



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 12:27 PM JST

PDB ID : 6KGX
EMDB ID : EMD-9976
Title : Structure of the phycobilisome from the red alga *Porphyridium purpureum*
Authors : Sui, S.F.; Ma, J.F.; You, X.; Sun, S.
Deposited on : 2019-07-12
Resolution : 2.80 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

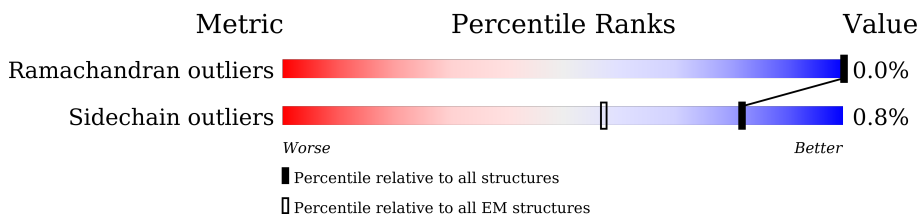
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A1	164	99% 99% .
1	A3	164	100% 99% .
1	A4	164	100% 99% .
1	AD	164	100% 99% .
1	AE	164	32% 100% .
1	AG	164	34% 99% .
1	B9	164	78% 99% .
1	BJ	164	79% 100% .
1	C1	164	100% 99% .

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Mol	Chain	Length	Quality of chain
1	C3	164	100% 99%
1	C4	164	99%
1	C8	164	24% 98%
1	CA	164	26% 100%
1	CD	164	100%
1	CE	164	41% 99%
1	CG	164	38% 98%
1	D9	164	29% 98%
1	DJ	164	27% 99%
1	E1	164	100% 99%
1	E3	164	100% 99%
1	E4	164	100% 99%
1	E8	164	67% 100%
1	EA	164	65% 100%
1	ED	164	100% 99%
1	EE	164	17% 99%
1	EG	164	18% 98%
1	F9	164	49% 99%
1	FJ	164	48% 99%
1	G1	164	96% 96%
1	G3	164	99% 99%
1	G4	164	96% 99%
1	G8	164	77% 99%
1	GA	164	76% 99%
1	GD	164	99% 99%

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Mol	Chain	Length	Quality of chain
1	GE	164	98%
1	GG	164	98%
1	H9	164	79% 100%
1	HJ	164	77% 99%
1	I1	164	95% 99%
1	I3	164	100% 98%
1	I4	164	95% 98%
1	I8	164	30% 99%
1	IA	164	31% 99%
1	ID	164	100% 98%
1	IE	164	98%
1	IG	164	98%
1	J5	164	99%
1	J9	164	97% 100%
1	JC	164	100% 98%
1	JJ	164	100% 100%
1	K1	164	98% 100%
1	K3	164	98% 98%
1	K4	164	99%
1	K8	164	9% 100%
1	KA	164	9% 100%
1	KD	164	100% 99%
1	KE	164	9% 99%
1	KG	164	7% 99%
1	L9	164	90% 99%

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Mol	Chain	Length	Quality of chain
1	LJ	164	90% 99%
1	M3	164	38% 100%
1	M8	164	100%
1	MA	164	100%
1	MD	164	39% 99%
1	ME	164	62% 99%
1	MG	164	65% 100%
1	N1	164	99%
1	N4	164	99%
1	N9	164	100% 99%
1	NJ	164	100% 98%
1	O2	164	100%
1	O3	164	99%
1	O6	164	99%
1	O7	164	97% 99%
1	O8	164	37% 99%
1	OA	164	40% 99%
1	OB	164	100%
1	OD	164	98%
1	OE	164	35% 100%
1	OF	164	96% 99%
1	OG	164	37% 100%
1	OI	164	100%
1	P1	164	24% 99%
1	P4	164	25% 99%

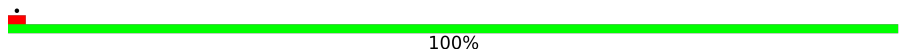
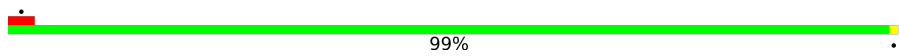
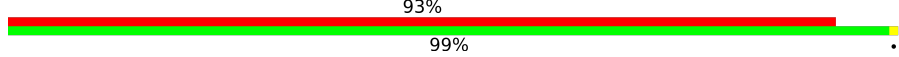
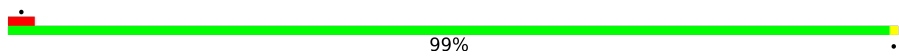
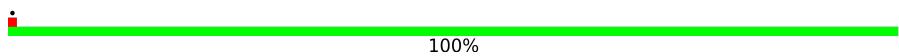
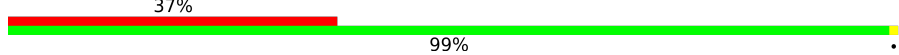

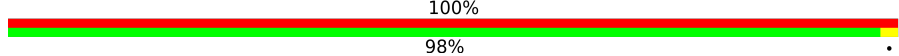


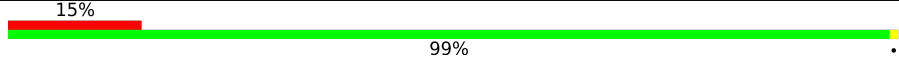

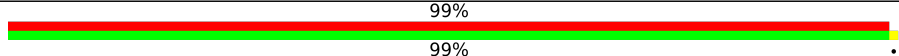
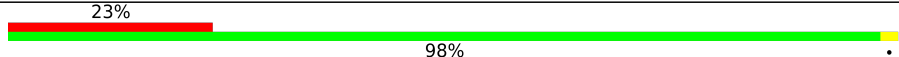
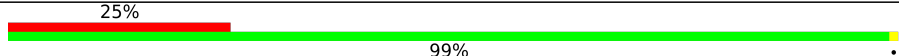
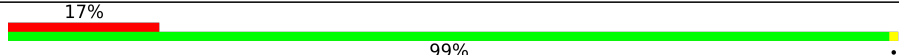
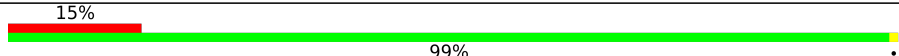
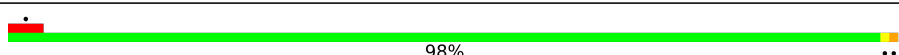
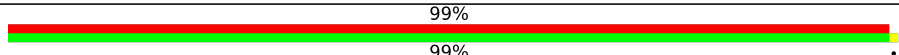
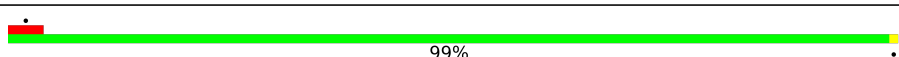
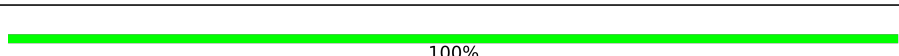
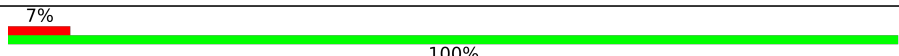
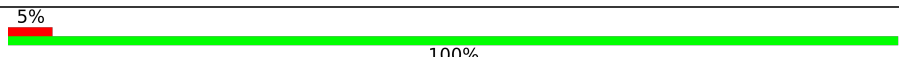
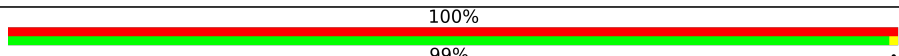
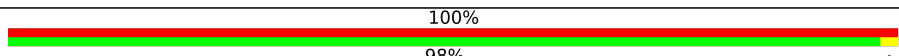
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Mol	Chain	Length	Quality of chain
1	P9	164	100%
1	PJ	164	100%
1	Q2	164	99%
1	Q3	164	99%
1	Q6	164	29%
1	Q7	164	90%
1	Q8	164	62%
1	QA	164	61%
1	QB	164	28%
1	QD	164	24%
1	QE	164	24%
1	QF	164	91%
1	QG	164	24%
1	QI	164	43%
1	R1	164	42%
1	R4	164	100%
1	R9	164	100%
1	RJ	164	100%
1	S2	164	100%
1	S3	164	30%
1	S6	164	95%
1	S7	164	66%
1	S8	164	65%
1	SA	164	30%
1	SB	164	30%

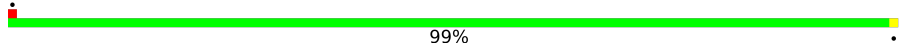
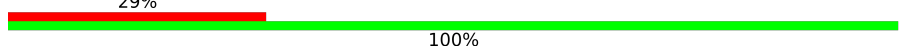
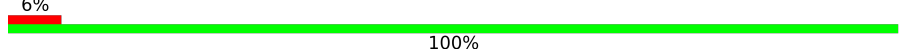


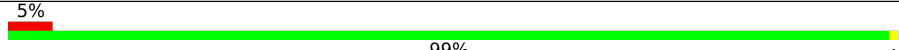
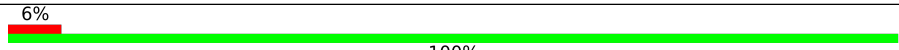
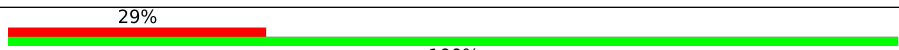
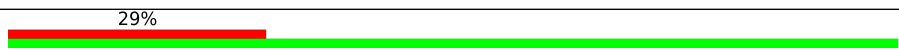
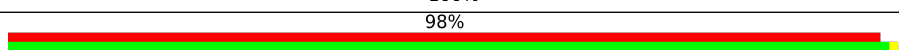
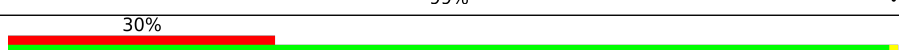
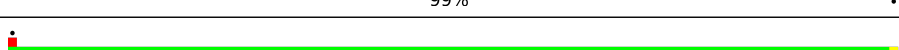
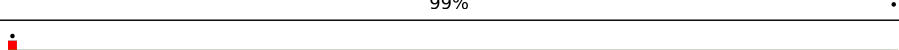
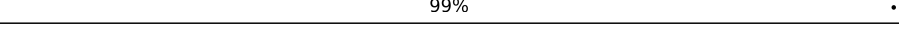
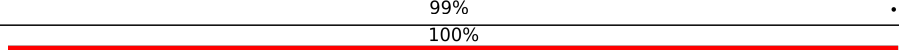
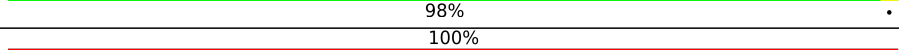
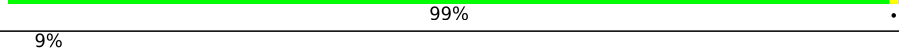
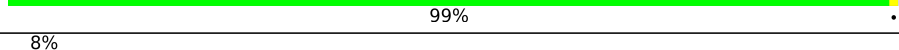
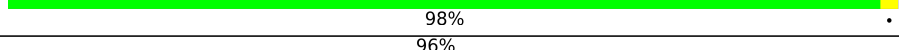
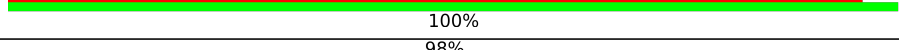
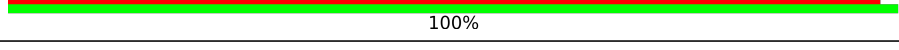
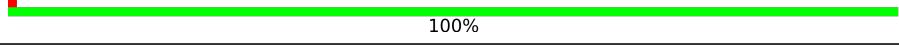
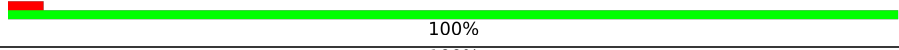
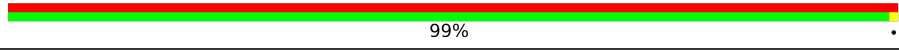
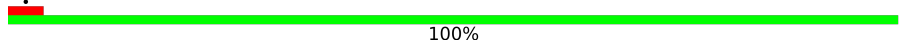
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Mol	Chain	Length	Quality of chain
1	SD	164	 100%
1	SE	164	 99%
1	SF	164	 93%
1	SG	164	 99%
1	SI	164	 100%
1	T1	164	 37%
1	T4	164	 37%
1	T9	164	 100%
1	TJ	164	 98%
1	U2	164	 100%
1	U3	164	 15%
1	U6	164	 18%
1	U7	164	 99%
1	U8	164	 23%
1	UA	164	 25%
1	UB	164	 17%
1	UD	164	 15%
1	UE	164	 98%
1	UF	164	 99%
1	UG	164	 99%
1	UI	164	 100%
1	V1	164	 7%
1	V4	164	 5%
1	V9	164	 100%
1	VJ	164	 99%

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Mol	Chain	Length	Quality of chain
1	W2	164	 99%
1	W3	164	 29% 100%
1	W6	164	 6% 100%
1	W7	164	 98% 100%
1	W8	164	 5% 100%
1	WA	164	 5% 99%
1	WB	164	 6% 100%
1	WD	164	 29% 100%
1	WE	164	 29% 100%
1	WF	164	 98% 99%
1	WG	164	 30% 99%
1	WI	164	 99%
1	X1	164	 99%
1	X4	164	 99%
1	X9	164	 100%
1	XJ	164	 98% 100%
1	Y8	164	 99%
1	YA	164	 8% 98%
1	YE	164	 96% 100%
1	YG	164	 98% 100%
1	Z2	164	 100%
1	Z6	164	 100%
1	Z7	164	 99%
1	ZB	164	 100%
1	ZF	164	 99%

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Mol	Chain	Length	Quality of chain
1	ZI	164	100%
1	a8	164	76%
1	aA	164	78%
1	aE	164	83%
1	aG	164	84%
1	b2	164	40%
1	b6	164	61%
1	b7	164	100%
1	bB	164	58%
1	bF	164	100%
1	bI	164	39%
1	c1	164	100%
1	c4	164	100%
1	cE	164	84%
1	cG	164	83%
1	d2	164	28%
1	d6	164	90%
1	d7	164	100%
1	d8	164	88%
1	dA	164	87%
1	dB	164	93%
1	dF	164	100%
1	dI	164	32%
1	e1	164	100%
1	e4	164	100%

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Mol	Chain	Length	Quality of chain
1	eE	164	79% 99%
1	eG	164	79% 98%
1	f2	164	45% 99%
1	f6	164	94% 99%
1	f7	164	100% 99%
1	f8	164	96% 99%
1	fA	164	95% 99%
1	fB	164	96% 99%
1	fF	164	100% 98%
1	fI	164	46% 100%
1	g1	164	100% 98%
1	g4	164	100% 99%
1	gE	164	76% 99%
1	gG	164	71% 100%
1	h2	164	20% 100%
1	h6	164	98% 99%
1	h7	164	100% 99%
1	h8	164	98% 98%
1	hA	164	98% 99%
1	hB	164	96% 99%
1	hF	164	100% 98%
1	hI	164	21% 100%
1	i1	164	100% 99%
1	i4	164	100% 99%
1	iE	164	82% 100%

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Mol	Chain	Length	Quality of chain
1	iG	164	83% 98%
1	j2	164	29% 100%
1	j6	164	82% 100%
1	j7	164	100% 99%
1	j8	164	93% 99%
1	jA	164	95% 100%
1	jB	164	83% 100%
1	jF	164	100% 98%
1	jI	164	32% 100%
1	k1	164	100% 99%
1	k4	164	100% 99%
1	kE	164	100% 97%
1	kG	164	100% 99%
1	l2	164	22% 100%
1	l6	164	78% 99%
1	l7	164	100% 100%
1	l8	164	51% 94% 6%
1	lA	164	52% 98%
1	lB	164	78% 100%
1	lF	164	100% 96%
1	lI	164	22% 100%
1	m1	164	100% 99%
1	m4	164	100% 99%
1	mE	164	99% 95%
1	mG	164	99% 98%

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Mol	Chain	Length	Quality of chain
1	oE	164	100%
1	oG	164	100%
1	p1	164	100%
1	p4	164	100%
1	qE	164	100%
1	qG	164	98%
1	r1	164	99%
1	r4	164	100%
1	sE	164	98%
1	sG	164	100%
1	t1	164	98%
1	t4	164	100%
1	uE	164	100%
1	uG	164	99%
1	v1	164	100%
1	v4	164	99%
1	x1	164	100%
1	x4	164	96%
1	z1	164	100%
1	z4	164	99%
2	11	177	100%
2	14	177	99%
2	A5	177	100%
2	AC	177	99%
2	B1	177	82%
2	B1	177	81%
2	B1	177	82%
2	B1	177	81%
2	B1	177	99%
2	B1	177	99%

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Mol	Chain	Length	Quality of chain
2	B3	177	100%
2	B4	177	99%
2	B5	177	82% 18%
2	BC	177	82% 76% 6% 18%
2	BD	177	100% 97%
2	BE	177	38% 99%
2	BG	177	36% 99%
2	C5	177	82% 82% 18%
2	C9	177	63% 99%
2	CC	177	82% 80% 18%
2	CJ	177	62% 99%
2	D1	177	99% 98%
2	D3	177	100% 97%
2	D4	177	100% 98%
2	D8	177	59% 98%
2	DA	177	60% 99%
2	DD	177	100% 99%
2	DE	177	28% 98%
2	DG	177	27% 99%
2	E9	177	44% 98%
2	EJ	177	42% 98%
2	F1	177	92% 99%
2	F3	177	100% 97%
2	F4	177	93% 99%
2	F5	177	36% 82% 18%

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Mol	Chain	Length	Quality of chain
2	F8	177	24% 99%
2	FA	177	21% 99%
2	FC	177	37% 82% 18%
2	FD	177	100% 98%
2	FE	177	98%
2	FG	177	99%
2	G5	177	81% 81% 18%
2	G9	177	90% 99%
2	GC	177	81% 82% 18%
2	GJ	177	88% 99%
2	H1	177	99% 98%
2	H3	177	99% 98%
2	H4	177	100% 99%
2	H5	177	10% 81% 18%
2	H8	177	50% 99%
2	HA	177	50% 99%
2	HC	177	10% 82% 18%
2	HD	177	99% 98%
2	HE	177	6% 99%
2	HG	177	5% 99%
2	I5	177	22% 97%
2	I9	177	21% 98%
2	IC	177	23% 99%
2	IJ	177	20% 99%
2	J1	177	98% 99%

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Mol	Chain	Length	Quality of chain
2	J3	177	100%
2	J4	177	98% 99%
2	J8	177	58% 99%
2	JA	177	58% 99%
2	JD	177	100% 99%
2	JE	177	98%
2	JG	177	98%
2	K5	177	10% 97%
2	K9	177	94% 99%
2	KC	177	10% 97%
2	KJ	177	93% 99%
2	L1	177	99% 98%
2	L3	177	99% 99%
2	L4	177	99% 99%
2	L5	177	11% 77% 6% 18%
2	L8	177	7% 99%
2	LA	177	7% 99%
2	LC	177	10% 79% 18%
2	LD	177	99% 99%
2	LE	177	99%
2	LG	177	98%
2	M9	177	84% 99%
2	MJ	177	84% 99%
2	N3	177	19% 99%
2	N8	177	5% 97%

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Mol	Chain	Length	Quality of chain
2	NA	177	5% 98%
2	ND	177	19% 99%
2	NE	177	56% 99%
2	NG	177	55% 99%
2	O1	177	5% 99%
2	O4	177	6% 98%
2	O9	177	100% 98%
2	OJ	177	100% 97%
2	P2	177	100%
2	P3	177	12% 98%
2	P6	177	7% 98%
2	P7	177	64% 99%
2	P8	177	69% 99%
2	PA	177	72% 98%
2	PB	177	6% 99%
2	PD	177	12% 98%
2	PE	177	38% 99%
2	PF	177	64% 98%
2	PG	177	38% 99%
2	PI	177	100%
2	Q1	177	7% 99%
2	Q4	177	6% 99%
2	Q9	177	100% 97%
2	QJ	177	99%
2	R2	177	99%

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Mol	Chain	Length	Quality of chain
2	R3	177	8% 99%
2	R6	177	19% 99%
2	R7	177	98% 99%
2	R8	177	33% 99%
2	RA	177	33% 98%
2	RB	177	18% 99%
2	RD	177	10% 99%
2	RE	177	14% 98%
2	RF	177	98% 99%
2	RG	177	14% 99%
2	RI	177	99%
2	S1	177	24% 98%
2	S4	177	27% 98%
2	S9	177	100% 99%
2	SJ	177	100% 98%
2	T2	177	5% 98%
2	T3	177	99%
2	T6	177	7% 99%
2	T7	177	95% 99%
2	T8	177	30% 99%
2	TA	177	30% 99%
2	TB	177	6% 99%
2	TD	177	99%
2	TE	177	8% 99%
2	TF	177	96% 99%

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Mol	Chain	Length	Quality of chain
2	TG	177	8% 99%
2	TI	177	5% 99%
2	U1	177	36% 98%
2	U4	177	36% 99%
2	U9	177	100% 98%
2	UJ	177	100% 99%
2	V2	177	98%
2	V3	177	45% 99%
2	V6	177	45% 98%
2	V7	177	99% 97%
2	V8	177	52% 99%
2	VA	177	55% 99%
2	VB	177	46% 98%
2	VD	177	44% 99%
2	VE	177	23% 97%
2	VF	177	98%
2	VG	177	23% 98%
2	VI	177	97%
2	W1	177	99%
2	W4	177	98%
2	W9	177	100% 96%
2	WJ	177	100% 99%
2	X3	177	11% 99%
2	X8	177	12% 98%
2	XA	177	12% 98%

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Mol	Chain	Length	Quality of chain
2	XD	177	12% 99%
2	XE	177	8% 98%
2	XG	177	7% 99%
2	Y1	177	7% 98%
2	Y2	177	99%
2	Y4	177	6% 97%
2	Y6	177	99%
2	Y7	177	98% 99%
2	Y9	177	100% 99%
2	YB	177	99%
2	YF	177	98% 99%
2	YI	177	99%
2	YJ	177	100% 99%
2	Z1	177	50% 82% 18%
2	Z4	177	49% 81% 18%
2	Z8	177	5% 99%
2	ZA	177	5% 99%
2	ZE	177	93% 98%
2	ZG	177	93% 97%
2	a1	177	79% 81% 18%
2	a2	177	97%
2	a4	177	79% 81% 18%
2	a6	177	18% 99%
2	a7	177	100% 99%
2	aB	177	19% 99%

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Mol	Chain	Length	Quality of chain
2	aF	177	100% 99%
2	aI	177	97%
2	bE	177	77% 98%
2	bG	177	76% 99%
2	c2	177	56% 99%
2	c6	177	74% 99%
2	c7	177	100% 99%
2	c8	177	96% 99%
2	cA	177	95% 99%
2	cB	177	73% 100%
2	cF	177	100% 98%
2	cI	177	57% 99%
2	d1	177	100% 99%
2	d4	177	100% 98%
2	dE	177	80% 99%
2	dG	177	79% 98%
2	e2	177	17% 99%
2	e6	177	85% 99%
2	e7	177	100% 99%
2	e8	177	44% 99%
2	eA	177	42% 99%
2	eB	177	85% 99%
2	eF	177	100% 98%
2	eI	177	18% 99%
2	f1	177	100% 98%

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Mol	Chain	Length	Quality of chain
2	f4	177	100% 98% ..
2	fE	177	69% 98% .
2	fG	177	68% 99% .
2	g2	177	51% 99% .
2	g6	177	77% 98% .
2	g7	177	100% 99% .
2	g8	177	98% 99% .
2	gA	177	98% 99% .
2	gB	177	77% 98% .
2	gF	177	100% 99% .
2	gI	177	47% 99% .
2	h1	177	100% 98% .
2	h4	177	100% 99% .
2	hE	177	92% 99% .
2	hG	177	91% 99% .
2	i2	177	11% 99% .
2	i6	177	98% 99% .
2	i7	177	100% 99% .
2	i8	177	90% 99% .
2	iA	177	89% 99% .
2	iB	177	98% 99% .
2	iF	177	100% 97% .
2	iI	177	14% 99% .
2	j1	177	100% 97% ..
2	j4	177	100% 99% .

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Mol	Chain	Length	Quality of chain
2	jE	177	54% 99%
2	jG	177	53% 99%
2	k2	177	44% 98%
2	k6	177	41% 99%
2	k7	177	100% 99%
2	k8	177	89% 99%
2	kA	177	88% 99%
2	kB	177	42% 99%
2	kF	177	100% 98%
2	kI	177	42% 98%
2	l1	177	100% 98%
2	l4	177	100% 98%
2	lE	177	100% 99%
2	lG	177	100% 97%
2	m2	177	14% 99%
2	m6	177	94% 99%
2	m7	177	100% 99%
2	m8	177	79% 98%
2	mA	177	80% 98%
2	mB	177	93% 98%
2	mF	177	100% 97%
2	mI	177	12% 99%
2	n1	177	98% 98%
2	n4	177	98% 99%
2	nE	177	100% 98%

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Mol	Chain	Length	Quality of chain
2	nG	177	100% 97% .
2	pE	177	100% 99% .
2	pG	177	100% 98% .
2	q1	177	100% 97% ..
2	q4	177	100% 97% .
2	rE	177	100% 98% .
2	rG	177	100% 97% .
2	s1	177	100% 97% .
2	s4	177	100% 98% .
2	tE	177	100% 98% .
2	tG	177	100% 99% .
2	u1	177	99% 98% .
2	u4	177	99% 98% ..
2	vE	177	99% 98% .
2	vG	177	98% 98% .
2	w1	177	100% 99% .
2	w4	177	100% 98% .
2	y1	177	100% 98% .
2	y4	177	100% 99% .
3	21	333	71% 68% 29% .
3	24	333	71% 68% 29% .
3	M1	333	69% 69% 29% .
3	M4	333	69% 69% 29% .
4	b1	405	16% 75% 20% .
4	b4	405	18% 76% 20% .

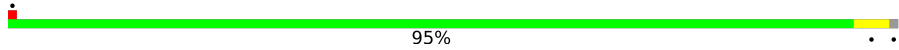
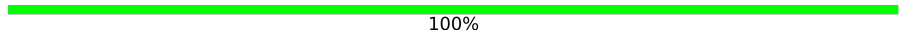






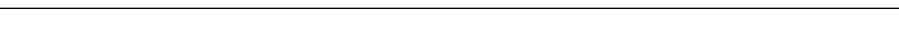
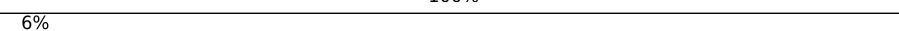
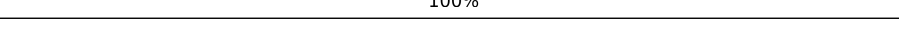
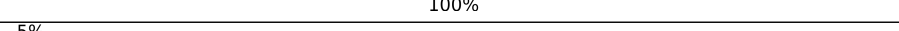
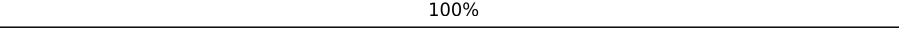
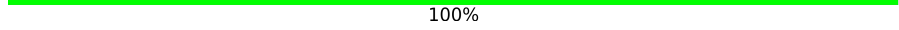
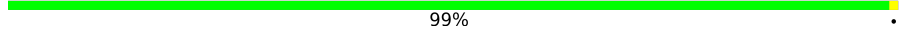


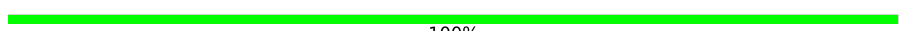




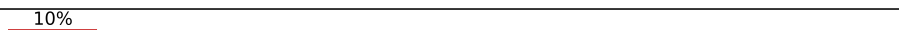
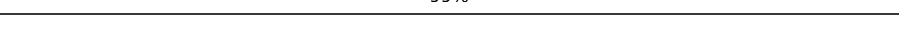
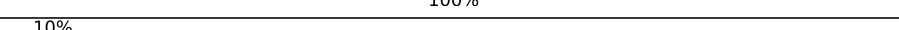
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Mol	Chain	Length	Quality of chain
4	o1	405	52% 51% 48%
4	o4	405	52% 50% 48%
5	31	288	95%
5	34	288	95%
6	X2	363	88% 11%
6	X6	363	88% 11%
6	X7	363	78% 88% 11%
6	XB	363	88% 11%
6	XF	363	77% 88% 11%
6	XI	363	88% 11%
7	A2	290	18% 88% 11%
7	A6	290	70% 88% 11%
7	A7	290	89% 88% 11%
7	A9	290	88% 87% 12%
7	AB	290	68% 88% 11%
7	AF	290	89% 88% 11%
7	AI	290	17% 89% 11%
7	AJ	290	88% 88% 12%
7	Y3	290	81% 80% 18%
7	YD	290	81% 81% 18%
8	B2	232	96%
8	B6	232	6% 97%
8	B7	232	27% 97%
8	BB	232	6% 95%
8	BF	232	27% 96%

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Mol	Chain	Length	Quality of chain
8	BI	232	 95%
9	C2	162	 100%
9	C6	162	 100%
9	C7	162	 91% 100%
9	CB	162	 100%
9	CF	162	 94% 99%
9	CI	162	 99%
9	E2	162	 100%
9	E6	162	 100%
9	E7	162	 6% 100%
9	EB	162	 100%
9	EF	162	 5% 100%
9	EI	162	 100%
9	G2	162	 99%
9	G6	162	 100%
9	G7	162	 72% 99%
9	GB	162	 100%
9	GF	162	 71% 99%
9	GI	162	 99%
9	I2	162	 100%
9	I6	162	 100%
9	I7	162	 10% 99%
9	IB	162	 100%
9	IF	162	 10% 100%
9	II	162	 100%

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Mol	Chain	Length	Quality of chain
9	K2	162	99%
9	K6	162	100%
9	K7	162	44% 99%
9	KB	162	100%
9	KF	162	43% 99%
9	KI	162	99%
9	M2	162	99%
9	M6	162	100%
9	M7	162	91% 99%
9	MB	162	100%
9	MF	162	90% 99%
9	MI	162	99%
10	D2	172	99%
10	D6	172	99%
10	D7	172	94% 99%
10	DB	172	99%
10	DF	172	94% 99%
10	DI	172	98%
10	F2	172	99%
10	F6	172	98%
10	F7	172	49% 98%
10	FB	172	99%
10	FF	172	49% 99%
10	FI	172	98%
10	H2	172	98%

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Mol	Chain	Length	Quality of chain
10	H6	172	99%
10	H7	172	33% 99%
10	HB	172	99%
10	HF	172	33% 98%
10	HI	172	98%
10	J2	172	98%
10	J6	172	97%
10	J7	172	36% 98%
10	JB	172	98%
10	JF	172	37% 98%
10	JI	172	99%
10	L2	172	98%
10	L6	172	98%
10	L7	172	5% 99%
10	LB	172	99%
10	LF	172	5% 99%
10	LI	172	98%
10	N2	172	98%
10	N6	172	99%
10	N7	172	72% 99%
10	NB	172	98%
10	NF	172	76% 99%
10	NI	172	98%
11	e3	303	9% 82% 18%
11	eD	303	8% 82% 18%

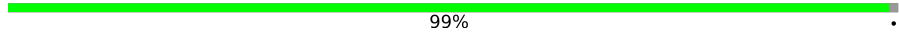
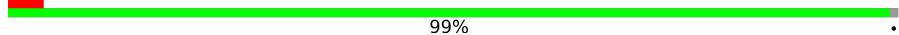
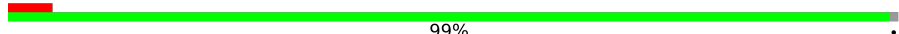
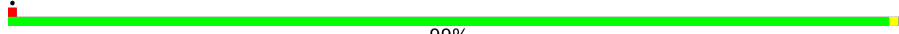


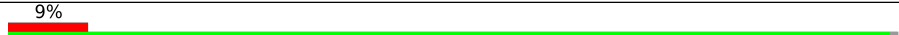
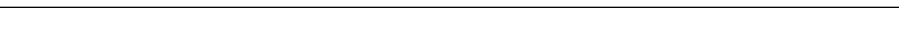
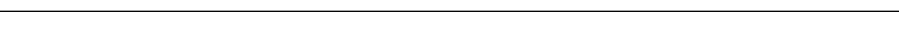
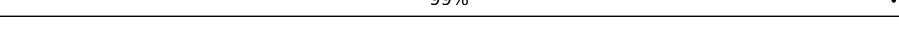
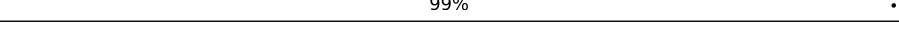
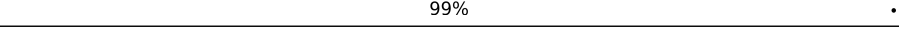
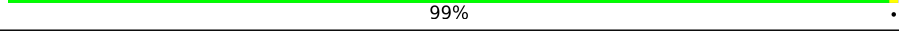
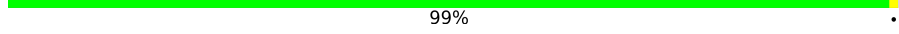
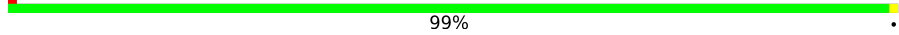
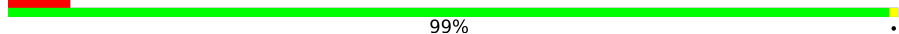
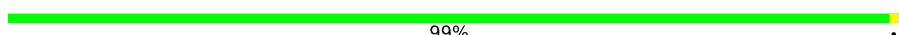
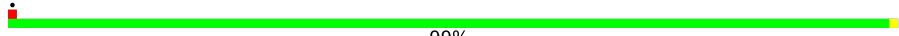





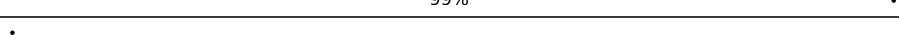
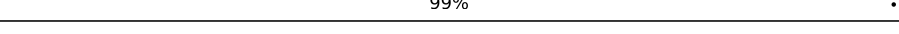
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Mol	Chain	Length	Quality of chain
12	b8	490	11% 74% 22%
12	bA	490	11% 75% 22%
13	A8	273	76% 86% 13%
13	AA	273	76% 87% 13%
13	wE	273	55% 85% 13%
13	wG	273	57% 87% 13%
13	xE	273	87% 86% 13%
13	xG	273	87% 87% 13%
14	B8	290	30% 86% 14%
14	BA	290	32% 86% 14%
14	yE	290	7% 86% 14%
14	yG	290	9% 86% 14%
15	d9	342	34% 79% 17%
15	dJ	342	34% 80% 17%
16	zE	498	6% 73% 26%
16	zG	498	6% 74% 26%
17	AH	161	5% 99%
17	CH	161	99%
17	EH	161	99%
17	GH	161	99%
17	JH	161	99%
17	KH	161	8% 99%
17	NH	161	99%
17	PH	161	99%
17	RH	161	99%

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Mol	Chain	Length	Quality of chain
17	TH	161	 99%
17	cH	161	 99%
17	eH	161	 99%
17	gH	161	 99%
17	iH	161	 99%
17	lH	161	 98%
17	mH	161	 99%
17	pH	161	 99%
17	rH	161	 99%
17	tH	161	 99%
17	vH	161	 99%
18	BH	161	 99%
18	DH	161	 99%
18	FH	161	 99%
18	HH	161	 99%
18	IH	161	 99%
18	LH	161	 99%
18	MH	161	 98%
18	OH	161	 99%
18	QH	161	 99%
18	SH	161	 99%
18	UH	161	 99%
18	dH	161	 99%
18	fH	161	 99%
18	hH	161	 99%

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Mol	Chain	Length	Quality of chain
18	jH	161	5% 99%
18	kH	161	99%
18	nH	161	99%
18	oH	161	96%
18	qH	161	10% 99%
18	sH	161	99%
18	uH	161	99%
18	wH	161	99%
19	VH	161	8% 99%
19	xH	161	17% 99%
20	WH	173	5% 100%
20	yH	173	5% 100%
21	XH	93	99%
21	zH	93	99%
22	1H	879	7% 95%
22	YH	879	7% 95%
23	2H	159	11% 83% 17%
23	ZH	159	11% 83% 17%
24	3H	288	5% 85% 12%
24	aH	288	5% 85% 12%
25	4H	253	5% 80% 19%
25	bH	253	5% 80% 19%

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 1014295 atoms, of which 1824 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	164	1250	779	219	245	7	0	0
1	C1	164	1250	779	219	245	7	0	0
1	E1	164	1250	779	219	245	7	0	0
1	G1	164	1250	779	219	245	7	0	0
1	I1	164	1250	779	219	245	7	0	0
1	K1	164	1250	779	219	245	7	0	0
1	N1	164	1250	779	219	245	7	0	0
1	P1	164	1250	779	219	245	7	0	0
1	R1	164	1250	779	219	245	7	0	0
1	T1	164	1250	779	219	245	7	0	0
1	V1	164	1250	779	219	245	7	0	0
1	X1	164	1250	779	219	245	7	0	0
1	c1	164	1250	779	219	245	7	0	0
1	e1	164	1250	779	219	245	7	0	0
1	g1	164	1250	779	219	245	7	0	0
1	i1	164	1250	779	219	245	7	0	0
1	k1	164	1250	779	219	245	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	p1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	r1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	t1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	v1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	x1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	z1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	h2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	E3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	M3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	N4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	P4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	X4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	c4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	e4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	g4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	i4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	k4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	m4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	p4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	r4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	t4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	v4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	x4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	z4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	J5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	d6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	h6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	h7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	K8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	M8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Y8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	a8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	h8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	B9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	D9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	F9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	H9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	J9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	L9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	N9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	P9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	X9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	jA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ED	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ID	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ME	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	eE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	kE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	qE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	sE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	uE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	eG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	kG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	qG	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	sG	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	uG	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	OI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	QI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	SI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	UI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	WI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ZI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	bI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	dI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	fI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	hI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	jI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	II	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	BJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	DJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	FJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	HJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	JJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	LJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 2 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	D1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H1	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	J1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	L1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	O1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Q1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	S1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	U1	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	W1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Z1	146	Total	C	N	O	S	0	0
			1065	654	187	213	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	a1	146	Total	C	N	O	S	0	0
			1065	654	187	213	11		
2	d1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	f1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	h1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	j1	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	l1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	n1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	q1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	s1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	u1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	w1	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	y1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	11	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	P2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	R2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	T2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	V2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	a2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	c2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	e2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	g2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i2	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	k2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	m2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	B3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	H3	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	N3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	R3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	T3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	V3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	X3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	B4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	H4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J4	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	O4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Q4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	S4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	U4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	W4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Y4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Z4	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	a4	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	d4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	f4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	h4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	j4	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	l4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	n4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	q4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	s4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	u4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	w4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	y4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	14	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	B5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	C5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	F5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	G5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	H5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	I5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	K5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	P6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	T6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	V6	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Y6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	a6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	c6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	e6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	g6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i6	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	k6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	m6	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	T7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	V7	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Y7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	a7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	c7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	e7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	g7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i7	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	k7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	m7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	F8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	H8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	J8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	L8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	N8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R8	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	T8	177	Total 1303	C 806	N 225	O 260	S 12	3	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	X8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Z8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	c8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	e8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	g8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	i8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	k8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	m8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	C9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	E9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	G9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	I9	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	K9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	M9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	O9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Q9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	S9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	U9	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	W9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Y9	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JA	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	LA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RA	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	TA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	VA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	XA	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	ZA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	cA	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	eA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	gA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	iA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	kA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	mA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TB	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	VB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	YB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	AC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	BC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	CC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	FC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	GC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	HC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	IC	176	Total 1286	C 795	N 224	O 256	S 11	0	0
2	KC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	BD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	DD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	FD	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	HD	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	JD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	ND	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	TD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	VD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	XD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	BE	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	DE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	LE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	TE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	VE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	XE	177	Total 1303	C 806	N 225	O 260	S 12	3	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	ZE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	bE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	dE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	fE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	hE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	jE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	lE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	nE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	pE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	rE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	tE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	vE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	YF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gF	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	iF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	BG	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	DG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	LG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	TG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	VG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	XG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	ZG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	bG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	dG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	fG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	hG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	jG	177	Total 1303	C 806	N 225	O 260	S 12	3	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	lG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	nG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	pG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	rG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	tG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	vG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	YI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iI	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	kI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	CJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	EJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	GJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	KJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	MJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	WJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

- Molecule 3 is a protein called LR7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M1	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		
3	21	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		
3	M4	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		
3	24	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		

- Molecule 4 is a protein called LR2_Hb.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b1	323	Total	C	N	O	S	0	0
			2485	1566	422	486	11		
4	o1	212	Total	C	N	O	S	0	0
			1645	1036	283	319	7		
4	b4	323	Total	C	N	O	S	0	0
			2485	1566	422	486	11		
4	o4	212	Total	C	N	O	S	0	0
			1645	1036	283	319	7		

- Molecule 5 is a protein called LR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	31	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		
5	34	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		

- Molecule 6 is a protein called LR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X2	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	X6	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	X7	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	XB	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	XF	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	XI	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		

- Molecule 7 is a protein called LR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A2	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	Y3	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
7	A6	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	A7	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	A9	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
7	AB	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	YD	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
7	AF	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	AI	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AJ	256	1979	1220	367	377	15	0	0

- Molecule 8 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B2	230	1889	1206	331	348	4	0	0
8	B6	231	1897	1212	332	349	4	0	0
8	B7	227	1874	1197	328	345	4	0	0
8	BB	231	1897	1212	332	349	4	0	0
8	BF	227	1874	1197	328	345	4	0	0
8	BI	230	1889	1206	331	348	4	0	0

- Molecule 9 is a protein called C-phycoyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C2	162	1228	773	209	240	6	0	0
9	E2	162	1228	773	209	240	6	0	0
9	G2	162	1228	773	209	240	6	0	0
9	I2	162	1228	773	209	240	6	0	0
9	K2	162	1228	773	209	240	6	0	0
9	M2	162	1228	773	209	240	6	0	0
9	C6	162	1228	773	209	240	6	0	0
9	E6	162	1228	773	209	240	6	0	0
9	G6	162	1228	773	209	240	6	0	0
9	I6	162	1228	773	209	240	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K6	162	1228	773	209	240	6	0	0
9	M6	162	1228	773	209	240	6	0	0
9	C7	162	1228	773	209	240	6	0	0
9	E7	162	1228	773	209	240	6	0	0
9	G7	162	1228	773	209	240	6	0	0
9	I7	162	1228	773	209	240	6	0	0
9	K7	162	1228	773	209	240	6	0	0
9	M7	162	1228	773	209	240	6	0	0
9	CB	162	1228	773	209	240	6	0	0
9	EB	162	1228	773	209	240	6	0	0
9	GB	162	1228	773	209	240	6	0	0
9	IB	162	1228	773	209	240	6	0	0
9	KB	162	1228	773	209	240	6	0	0
9	MB	162	1228	773	209	240	6	0	0
9	CF	162	1228	773	209	240	6	0	0
9	EF	162	1228	773	209	240	6	0	0
9	GF	162	1228	773	209	240	6	0	0
9	IF	162	1228	773	209	240	6	0	0
9	KF	162	1228	773	209	240	6	0	0
9	MF	162	1228	773	209	240	6	0	0
9	CI	162	1228	773	209	240	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	EI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	GI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	II	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

- Molecule 10 is a protein called C-phycoyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	H7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DB	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FB	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HB	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JB	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LB	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NB	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	NI	172	1272	786	224	253	9	0	0

- Molecule 11 is a protein called LR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e3	248	1932	1217	336	369	10	0	0
11	eD	248	1932	1217	336	369	10	0	0

- Molecule 12 is a protein called LRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	b8	380	2961	1867	514	565	15	0	0
12	bA	380	2961	1867	514	565	15	0	0

- Molecule 13 is a protein called LR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A8	238	1814	1122	335	342	15	0	0
13	AA	238	1814	1122	335	342	15	0	0
13	wE	238	1814	1122	335	342	15	0	0
13	xE	238	1814	1122	335	342	15	0	0
13	wG	238	1814	1122	335	342	15	0	0
13	xG	238	1814	1122	335	342	15	0	0

- Molecule 14 is a protein called LR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B8	250	1902	1184	346	358	14	0	0
14	BA	250	1902	1184	346	358	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	yE	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	yG	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		

- Molecule 15 is a protein called LR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	d9	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		
15	dJ	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		

- Molecule 16 is a protein called LRC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	zE	370	Total	C	N	O	S	0	0
			2901	1833	514	540	14		
16	zG	370	Total	C	N	O	S	0	0
			2901	1833	514	540	14		

- Molecule 17 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	CH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	EH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	GH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	JH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	KH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	NH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	PH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	RH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	TH	160	1225	768	211	239	7	0	0
17	cH	160	1225	768	211	239	7	0	0
17	eH	160	1225	768	211	239	7	0	0
17	gH	160	1225	768	211	239	7	0	0
17	iH	160	1225	768	211	239	7	0	0
17	lH	160	1225	768	211	239	7	0	0
17	mH	160	1225	768	211	239	7	0	0
17	pH	160	1225	768	211	239	7	0	0
17	rH	160	1225	768	211	239	7	0	0
17	tH	160	1225	768	211	239	7	0	0
17	vH	160	1225	768	211	239	7	0	0

- Molecule 18 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DH	161	1219	767	206	239	7	0	0
18	FH	161	1219	767	206	239	7	0	0
18	BH	161	1219	767	206	239	7	0	0
18	HH	161	1219	767	206	239	7	0	0
18	IH	161	1219	767	206	239	7	0	0
18	LH	161	1219	767	206	239	7	0	0
18	MH	161	1219	767	206	239	7	0	0
18	OH	161	1219	767	206	239	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	QH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	SH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	UH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	dH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	fH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	hH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	jH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	kH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	nH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	oH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	qH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	sH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	uH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	wH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 19 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	VH	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
19	xH	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 20 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	WH	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	yH	173	1376	881	230	261	4	0	0

- Molecule 21 is a protein called LC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	XH	92	720	453	127	135	5	0	0
21	zH	92	720	453	127	135	5	0	0

- Molecule 22 is a protein called Phycobilisome linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	YH	844	6756	4328	1169	1245	14	0	0
22	1H	844	6756	4328	1169	1245	14	0	0

- Molecule 23 is a protein called LRC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	ZH	132	1004	631	179	191	3	0	0
23	2H	132	1004	631	179	191	3	0	0

- Molecule 24 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	aH	253	1897	1190	325	375	7	0	0
24	3H	253	1897	1190	325	375	7	0	0

- Molecule 25 is a protein called LRC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	bH	206	1532	982	259	286	5	0	0
25	4H	206	1532	982	259	286	5	0	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	F1	1	Total 129	C 99	N 12	O 18	0
26	F1	1	Total 129	C 99	N 12	O 18	0
26	G1	1	Total 86	C 66	N 8	O 12	0
26	G1	1	Total 86	C 66	N 8	O 12	0
26	H1	1	Total 129	C 99	N 12	O 18	0
26	H1	1	Total 129	C 99	N 12	O 18	0
26	H1	1	Total 129	C 99	N 12	O 18	0
26	I1	1	Total 86	C 66	N 8	O 12	0
26	I1	1	Total 86	C 66	N 8	O 12	0
26	J1	1	Total 129	C 99	N 12	O 18	0
26	J1	1	Total 129	C 99	N 12	O 18	0
26	J1	1	Total 129	C 99	N 12	O 18	0
26	K1	1	Total 86	C 66	N 8	O 12	0
26	K1	1	Total 86	C 66	N 8	O 12	0
26	L1	1	Total 129	C 99	N 12	O 18	0
26	L1	1	Total 129	C 99	N 12	O 18	0
26	L1	1	Total 129	C 99	N 12	O 18	0
26	M1	1	Total 129	C 99	N 12	O 18	0
26	M1	1	Total 129	C 99	N 12	O 18	0
26	M1	1	Total 129	C 99	N 12	O 18	0
26	N1	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	N1	1	129	99	12	18	0
26	N1	1	129	99	12	18	0
26	O1	1	86	66	8	12	0
26	O1	1	86	66	8	12	0
26	P1	1	129	99	12	18	0
26	P1	1	129	99	12	18	0
26	P1	1	129	99	12	18	0
26	Q1	1	86	66	8	12	0
26	Q1	1	86	66	8	12	0
26	R1	1	129	99	12	18	0
26	R1	1	129	99	12	18	0
26	R1	1	129	99	12	18	0
26	S1	1	86	66	8	12	0
26	S1	1	86	66	8	12	0
26	T1	1	129	99	12	18	0
26	T1	1	129	99	12	18	0
26	T1	1	129	99	12	18	0
26	U1	1	86	66	8	12	0
26	U1	1	86	66	8	12	0
26	V1	1	129	99	12	18	0
26	V1	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	V1	1	Total 129	C 99	N 12	O 18	0
26	W1	1	Total 86	C 66	N 8	O 12	0
26	W1	1	Total 86	C 66	N 8	O 12	0
26	X1	1	Total 129	C 99	N 12	O 18	0
26	X1	1	Total 129	C 99	N 12	O 18	0
26	X1	1	Total 129	C 99	N 12	O 18	0
26	Y1	1	Total 86	C 66	N 8	O 12	0
26	Y1	1	Total 86	C 66	N 8	O 12	0
26	Z1	1	Total 86	C 66	N 8	O 12	0
26	Z1	1	Total 86	C 66	N 8	O 12	0
26	a1	1	Total 129	C 99	N 12	O 18	0
26	a1	1	Total 129	C 99	N 12	O 18	0
26	a1	1	Total 129	C 99	N 12	O 18	0
26	b1	1	Total 43	C 33	N 4	O 6	0
26	c1	1	Total 129	C 99	N 12	O 18	0
26	c1	1	Total 129	C 99	N 12	O 18	0
26	c1	1	Total 129	C 99	N 12	O 18	0
26	d1	1	Total 129	C 99	N 12	O 18	0
26	d1	1	Total 129	C 99	N 12	O 18	0
26	d1	1	Total 129	C 99	N 12	O 18	0
26	e1	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	e1	1	86	66	8	12	0
26	f1	1	86	66	8	12	0
26	f1	1	86	66	8	12	0
26	g1	1	129	99	12	18	0
26	g1	1	129	99	12	18	0
26	g1	1	129	99	12	18	0
26	h1	1	86	66	8	12	0
26	h1	1	86	66	8	12	0
26	i1	1	129	99	12	18	0
26	i1	1	129	99	12	18	0
26	i1	1	129	99	12	18	0
26	j1	1	86	66	8	12	0
26	j1	1	86	66	8	12	0
26	k1	1	129	99	12	18	0
26	k1	1	129	99	12	18	0
26	k1	1	129	99	12	18	0
26	l1	1	86	66	8	12	0
26	l1	1	86	66	8	12	0
26	m1	1	129	99	12	18	0
26	m1	1	129	99	12	18	0
26	m1	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	n1	1	43	33	4	6	0
26	o1	1	43	33	4	6	0
26	p1	1	86	66	8	12	0
26	p1	1	86	66	8	12	0
26	q1	1	129	99	12	18	0
26	q1	1	129	99	12	18	0
26	q1	1	129	99	12	18	0
26	r1	1	86	66	8	12	0
26	r1	1	86	66	8	12	0
26	s1	1	129	99	12	18	0
26	s1	1	129	99	12	18	0
26	s1	1	129	99	12	18	0
26	t1	1	86	66	8	12	0
26	t1	1	86	66	8	12	0
26	u1	1	129	99	12	18	0
26	u1	1	129	99	12	18	0
26	u1	1	129	99	12	18	0
26	v1	1	86	66	8	12	0
26	v1	1	86	66	8	12	0
26	w1	1	129	99	12	18	0
26	w1	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	w1	1	Total 129	C 99	N 12	O 18	0
26	x1	1	Total 86	C 66	N 8	O 12	0
26	x1	1	Total 86	C 66	N 8	O 12	0
26	y1	1	Total 129	C 99	N 12	O 18	0
26	y1	1	Total 129	C 99	N 12	O 18	0
26	y1	1	Total 129	C 99	N 12	O 18	0
26	z1	1	Total 86	C 66	N 8	O 12	0
26	z1	1	Total 86	C 66	N 8	O 12	0
26	11	1	Total 129	C 99	N 12	O 18	0
26	11	1	Total 129	C 99	N 12	O 18	0
26	11	1	Total 129	C 99	N 12	O 18	0
26	21	1	Total 129	C 99	N 12	O 18	0
26	21	1	Total 129	C 99	N 12	O 18	0
26	21	1	Total 129	C 99	N 12	O 18	0
26	A2	1	Total 129	C 99	N 12	O 18	0
26	A2	1	Total 129	C 99	N 12	O 18	0
26	A2	1	Total 129	C 99	N 12	O 18	0
26	D2	1	Total 43	C 33	N 4	O 6	0
26	F2	1	Total 43	C 33	N 4	O 6	0
26	H2	1	Total 43	C 33	N 4	O 6	0
26	J2	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	L2	1	43	33	4	6	0
26	N2	1	43	33	4	6	0
26	O2	1	86	66	8	12	0
26	O2	1	86	66	8	12	0
26	P2	1	129	99	12	18	0
26	P2	1	129	99	12	18	0
26	P2	1	129	99	12	18	0
26	Q2	1	86	66	8	12	0
26	Q2	1	86	66	8	12	0
26	R2	1	129	99	12	18	0
26	R2	1	129	99	12	18	0
26	R2	1	129	99	12	18	0
26	S2	1	86	66	8	12	0
26	S2	1	86	66	8	12	0
26	T2	1	129	99	12	18	0
26	T2	1	129	99	12	18	0
26	T2	1	129	99	12	18	0
26	U2	1	86	66	8	12	0
26	U2	1	86	66	8	12	0
26	V2	1	129	99	12	18	0
26	V2	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	V2	1	Total 129	C 99	N 12	O 18	0
26	W2	1	Total 43	C 33	N 4	O 6	0
26	Y2	1	Total 129	C 99	N 12	O 18	0
26	Y2	1	Total 129	C 99	N 12	O 18	0
26	Y2	1	Total 129	C 99	N 12	O 18	0
26	Z2	1	Total 86	C 66	N 8	O 12	0
26	Z2	1	Total 86	C 66	N 8	O 12	0
26	a2	1	Total 129	C 99	N 12	O 18	0
26	a2	1	Total 129	C 99	N 12	O 18	0
26	a2	1	Total 129	C 99	N 12	O 18	0
26	b2	1	Total 86	C 66	N 8	O 12	0
26	b2	1	Total 86	C 66	N 8	O 12	0
26	c2	1	Total 129	C 99	N 12	O 18	0
26	c2	1	Total 129	C 99	N 12	O 18	0
26	c2	1	Total 129	C 99	N 12	O 18	0
26	d2	1	Total 86	C 66	N 8	O 12	0
26	d2	1	Total 86	C 66	N 8	O 12	0
26	e2	1	Total 129	C 99	N 12	O 18	0
26	e2	1	Total 129	C 99	N 12	O 18	0
26	e2	1	Total 129	C 99	N 12	O 18	0
26	f2	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	f2	1	Total 86	C 66	N 8	O 12	0
26	g2	1	Total 129	C 99	N 12	O 18	0
26	g2	1	Total 129	C 99	N 12	O 18	0
26	g2	1	Total 129	C 99	N 12	O 18	0
26	h2	1	Total 86	C 66	N 8	O 12	0
26	h2	1	Total 86	C 66	N 8	O 12	0
26	i2	1	Total 129	C 99	N 12	O 18	0
26	i2	1	Total 129	C 99	N 12	O 18	0
26	i2	1	Total 129	C 99	N 12	O 18	0
26	j2	1	Total 86	C 66	N 8	O 12	0
26	j2	1	Total 86	C 66	N 8	O 12	0
26	k2	1	Total 129	C 99	N 12	O 18	0
26	k2	1	Total 129	C 99	N 12	O 18	0
26	k2	1	Total 129	C 99	N 12	O 18	0
26	l2	1	Total 86	C 66	N 8	O 12	0
26	l2	1	Total 86	C 66	N 8	O 12	0
26	m2	1	Total 129	C 99	N 12	O 18	0
26	m2	1	Total 129	C 99	N 12	O 18	0
26	m2	1	Total 129	C 99	N 12	O 18	0
26	e3	1	Total 43	C 33	N 4	O 6	0
26	A3	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A3	1	86	66	8	12	0
26	B3	1	129	99	12	18	0
26	B3	1	129	99	12	18	0
26	B3	1	129	99	12	18	0
26	C3	1	86	66	8	12	0
26	C3	1	86	66	8	12	0
26	D3	1	129	99	12	18	0
26	D3	1	129	99	12	18	0
26	D3	1	129	99	12	18	0
26	E3	1	86	66	8	12	0
26	E3	1	86	66	8	12	0
26	F3	1	129	99	12	18	0
26	F3	1	129	99	12	18	0
26	F3	1	129	99	12	18	0
26	G3	1	86	66	8	12	0
26	G3	1	86	66	8	12	0
26	H3	1	129	99	12	18	0
26	H3	1	129	99	12	18	0
26	H3	1	129	99	12	18	0
26	I3	1	86	66	8	12	0
26	I3	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	J3	1	Total 129	C 99	N 12	O 18	0
26	J3	1	Total 129	C 99	N 12	O 18	0
26	J3	1	Total 129	C 99	N 12	O 18	0
26	K3	1	Total 86	C 66	N 8	O 12	0
26	K3	1	Total 86	C 66	N 8	O 12	0
26	L3	1	Total 129	C 99	N 12	O 18	0
26	L3	1	Total 129	C 99	N 12	O 18	0
26	L3	1	Total 129	C 99	N 12	O 18	0
26	M3	1	Total 86	C 66	N 8	O 12	0
26	M3	1	Total 86	C 66	N 8	O 12	0
26	N3	1	Total 129	C 99	N 12	O 18	0
26	N3	1	Total 129	C 99	N 12	O 18	0
26	N3	1	Total 129	C 99	N 12	O 18	0
26	O3	1	Total 86	C 66	N 8	O 12	0
26	O3	1	Total 86	C 66	N 8	O 12	0
26	P3	1	Total 129	C 99	N 12	O 18	0
26	P3	1	Total 129	C 99	N 12	O 18	0
26	P3	1	Total 129	C 99	N 12	O 18	0
26	Q3	1	Total 86	C 66	N 8	O 12	0
26	Q3	1	Total 86	C 66	N 8	O 12	0
26	R3	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	R3	1	129	99	12	18	0
26	R3	1	129	99	12	18	0
26	S3	1	86	66	8	12	0
26	S3	1	86	66	8	12	0
26	T3	1	129	99	12	18	0
26	T3	1	129	99	12	18	0
26	T3	1	129	99	12	18	0
26	U3	1	86	66	8	12	0
26	U3	1	86	66	8	12	0
26	V3	1	129	99	12	18	0
26	V3	1	129	99	12	18	0
26	V3	1	129	99	12	18	0
26	W3	1	86	66	8	12	0
26	W3	1	86	66	8	12	0
26	X3	1	129	99	12	18	0
26	X3	1	129	99	12	18	0
26	X3	1	129	99	12	18	0
26	Y3	1	129	99	12	18	0
26	Y3	1	129	99	12	18	0
26	Y3	1	129	99	12	18	0
26	A4	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A4	1	86	66	8	12	0
26	B4	1	129	99	12	18	0
26	B4	1	129	99	12	18	0
26	B4	1	129	99	12	18	0
26	C4	1	86	66	8	12	0
26	C4	1	86	66	8	12	0
26	D4	1	129	99	12	18	0
26	D4	1	129	99	12	18	0
26	D4	1	129	99	12	18	0
26	E4	1	86	66	8	12	0
26	E4	1	86	66	8	12	0
26	F4	1	129	99	12	18	0
26	F4	1	129	99	12	18	0
26	F4	1	129	99	12	18	0
26	G4	1	86	66	8	12	0
26	G4	1	86	66	8	12	0
26	H4	1	129	99	12	18	0
26	H4	1	129	99	12	18	0
26	H4	1	129	99	12	18	0
26	I4	1	86	66	8	12	0
26	I4	1	86	66	8	12	0

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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	R4	1	Total 129	C 99	N 12	O 18	0
26	R4	1	Total 129	C 99	N 12	O 18	0
26	R4	1	Total 129	C 99	N 12	O 18	0
26	S4	1	Total 86	C 66	N 8	O 12	0
26	S4	1	Total 86	C 66	N 8	O 12	0
26	T4	1	Total 129	C 99	N 12	O 18	0
26	T4	1	Total 129	C 99	N 12	O 18	0
26	T4	1	Total 129	C 99	N 12	O 18	0
26	U4	1	Total 86	C 66	N 8	O 12	0
26	U4	1	Total 86	C 66	N 8	O 12	0
26	V4	1	Total 129	C 99	N 12	O 18	0
26	V4	1	Total 129	C 99	N 12	O 18	0
26	V4	1	Total 129	C 99	N 12	O 18	0
26	W4	1	Total 86	C 66	N 8	O 12	0
26	W4	1	Total 86	C 66	N 8	O 12	0
26	X4	1	Total 129	C 99	N 12	O 18	0
26	X4	1	Total 129	C 99	N 12	O 18	0
26	X4	1	Total 129	C 99	N 12	O 18	0
26	Y4	1	Total 86	C 66	N 8	O 12	0
26	Y4	1	Total 86	C 66	N 8	O 12	0
26	Z4	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	Z4	1	Total 86	C 66	N 8	O 12	0
26	a4	1	Total 129	C 99	N 12	O 18	0
26	a4	1	Total 129	C 99	N 12	O 18	0
26	a4	1	Total 129	C 99	N 12	O 18	0
26	b4	1	Total 43	C 33	N 4	O 6	0
26	c4	1	Total 129	C 99	N 12	O 18	0
26	c4	1	Total 129	C 99	N 12	O 18	0
26	c4	1	Total 129	C 99	N 12	O 18	0
26	d4	1	Total 129	C 99	N 12	O 18	0
26	d4	1	Total 129	C 99	N 12	O 18	0
26	d4	1	Total 129	C 99	N 12	O 18	0
26	e4	1	Total 86	C 66	N 8	O 12	0
26	e4	1	Total 86	C 66	N 8	O 12	0
26	f4	1	Total 86	C 66	N 8	O 12	0
26	f4	1	Total 86	C 66	N 8	O 12	0
26	g4	1	Total 129	C 99	N 12	O 18	0
26	g4	1	Total 129	C 99	N 12	O 18	0
26	g4	1	Total 129	C 99	N 12	O 18	0
26	h4	1	Total 129	C 99	N 12	O 18	0
26	h4	1	Total 129	C 99	N 12	O 18	0
26	h4	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	i4	1	Total 86	C 66	N 8	O 12	0
26	i4	1	Total 86	C 66	N 8	O 12	0
26	j4	1	Total 86	C 66	N 8	O 12	0
26	j4	1	Total 86	C 66	N 8	O 12	0
26	k4	1	Total 129	C 99	N 12	O 18	0
26	k4	1	Total 129	C 99	N 12	O 18	0
26	k4	1	Total 129	C 99	N 12	O 18	0
26	l4	1	Total 86	C 66	N 8	O 12	0
26	l4	1	Total 86	C 66	N 8	O 12	0
26	m4	1	Total 129	C 99	N 12	O 18	0
26	m4	1	Total 129	C 99	N 12	O 18	0
26	m4	1	Total 129	C 99	N 12	O 18	0
26	n4	1	Total 86	C 66	N 8	O 12	0
26	n4	1	Total 86	C 66	N 8	O 12	0
26	p4	1	Total 86	C 66	N 8	O 12	0
26	p4	1	Total 86	C 66	N 8	O 12	0
26	q4	1	Total 129	C 99	N 12	O 18	0
26	q4	1	Total 129	C 99	N 12	O 18	0
26	q4	1	Total 129	C 99	N 12	O 18	0
26	r4	1	Total 86	C 66	N 8	O 12	0
26	r4	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	s4	1	Total 129	C 99	N 12	O 18	0
26	s4	1	Total 129	C 99	N 12	O 18	0
26	s4	1	Total 129	C 99	N 12	O 18	0
26	t4	1	Total 86	C 66	N 8	O 12	0
26	t4	1	Total 86	C 66	N 8	O 12	0
26	u4	1	Total 129	C 99	N 12	O 18	0
26	u4	1	Total 129	C 99	N 12	O 18	0
26	u4	1	Total 129	C 99	N 12	O 18	0
26	v4	1	Total 86	C 66	N 8	O 12	0
26	v4	1	Total 86	C 66	N 8	O 12	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	x4	1	Total 86	C 66	N 8	O 12	0
26	x4	1	Total 86	C 66	N 8	O 12	0
26	y4	1	Total 129	C 99	N 12	O 18	0
26	y4	1	Total 129	C 99	N 12	O 18	0
26	y4	1	Total 129	C 99	N 12	O 18	0
26	z4	1	Total 86	C 66	N 8	O 12	0
26	z4	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	14	1	Total 129	C 99	N 12	O 18	0
26	14	1	Total 129	C 99	N 12	O 18	0
26	14	1	Total 129	C 99	N 12	O 18	0
26	24	1	Total 129	C 99	N 12	O 18	0
26	24	1	Total 129	C 99	N 12	O 18	0
26	24	1	Total 129	C 99	N 12	O 18	0
26	A5	1	Total 86	C 66	N 8	O 12	0
26	A5	1	Total 86	C 66	N 8	O 12	0
26	B5	1	Total 129	C 99	N 12	O 18	0
26	B5	1	Total 129	C 99	N 12	O 18	0
26	B5	1	Total 129	C 99	N 12	O 18	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	F5	1	Total 129	C 99	N 12	O 18	0
26	F5	1	Total 129	C 99	N 12	O 18	0
26	F5	1	Total 129	C 99	N 12	O 18	0
26	G5	1	Total 129	C 99	N 12	O 18	0
26	G5	1	Total 129	C 99	N 12	O 18	0
26	G5	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	H5	1	Total 129	C 99	N 12	O 18	0
26	H5	1	Total 129	C 99	N 12	O 18	0
26	H5	1	Total 129	C 99	N 12	O 18	0
26	I5	1	Total 129	C 99	N 12	O 18	0
26	I5	1	Total 129	C 99	N 12	O 18	0
26	I5	1	Total 129	C 99	N 12	O 18	0
26	J5	1	Total 86	C 66	N 8	O 12	0
26	J5	1	Total 86	C 66	N 8	O 12	0
26	K5	1	Total 129	C 99	N 12	O 18	0
26	K5	1	Total 129	C 99	N 12	O 18	0
26	K5	1	Total 129	C 99	N 12	O 18	0
26	L5	1	Total 129	C 99	N 12	O 18	0
26	L5	1	Total 129	C 99	N 12	O 18	0
26	L5	1	Total 129	C 99	N 12	O 18	0
26	A6	1	Total 86	C 66	N 8	O 12	0
26	A6	1	Total 86	C 66	N 8	O 12	0
26	D6	1	Total 43	C 33	N 4	O 6	0
26	G6	1	Total 43	C 33	N 4	O 6	0
26	H6	1	Total 43	C 33	N 4	O 6	0
26	K6	1	Total 43	C 33	N 4	O 6	0
26	L6	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	N6	1	43	33	4	6	0
26	O6	1	129	99	12	18	0
26	O6	1	129	99	12	18	0
26	O6	1	129	99	12	18	0
26	P6	1	86	66	8	12	0
26	P6	1	86	66	8	12	0
26	Q6	1	129	99	12	18	0
26	Q6	1	129	99	12	18	0
26	Q6	1	129	99	12	18	0
26	R6	1	86	66	8	12	0
26	R6	1	86	66	8	12	0
26	S6	1	129	99	12	18	0
26	S6	1	129	99	12	18	0
26	S6	1	129	99	12	18	0
26	T6	1	86	66	8	12	0
26	T6	1	86	66	8	12	0
26	U6	1	129	99	12	18	0
26	U6	1	129	99	12	18	0
26	U6	1	129	99	12	18	0
26	V6	1	86	66	8	12	0
26	V6	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	W6	1	Total 129	C 99	N 12	O 18	0
26	W6	1	Total 129	C 99	N 12	O 18	0
26	W6	1	Total 129	C 99	N 12	O 18	0
26	Y6	1	Total 86	C 66	N 8	O 12	0
26	Y6	1	Total 86	C 66	N 8	O 12	0
26	Z6	1	Total 129	C 99	N 12	O 18	0
26	Z6	1	Total 129	C 99	N 12	O 18	0
26	Z6	1	Total 129	C 99	N 12	O 18	0
26	a6	1	Total 86	C 66	N 8	O 12	0
26	a6	1	Total 86	C 66	N 8	O 12	0
26	b6	1	Total 86	C 66	N 8	O 12	0
26	b6	1	Total 86	C 66	N 8	O 12	0
26	c6	1	Total 86	C 66	N 8	O 12	0
26	c6	1	Total 86	C 66	N 8	O 12	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	e6	1	Total 129	C 99	N 12	O 18	0
26	e6	1	Total 129	C 99	N 12	O 18	0
26	e6	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	f6	1	Total 129	C 99	N 12	O 18	0
26	f6	1	Total 129	C 99	N 12	O 18	0
26	f6	1	Total 129	C 99	N 12	O 18	0
26	g6	1	Total 86	C 66	N 8	O 12	0
26	g6	1	Total 86	C 66	N 8	O 12	0
26	h6	1	Total 129	C 99	N 12	O 18	0
26	h6	1	Total 129	C 99	N 12	O 18	0
26	h6	1	Total 129	C 99	N 12	O 18	0
26	i6	1	Total 86	C 66	N 8	O 12	0
26	i6	1	Total 86	C 66	N 8	O 12	0
26	j6	1	Total 86	C 66	N 8	O 12	0
26	j6	1	Total 86	C 66	N 8	O 12	0
26	k6	1	Total 86	C 66	N 8	O 12	0
26	k6	1	Total 86	C 66	N 8	O 12	0
26	l6	1	Total 129	C 99	N 12	O 18	0
26	l6	1	Total 129	C 99	N 12	O 18	0
26	l6	1	Total 129	C 99	N 12	O 18	0
26	m6	1	Total 129	C 99	N 12	O 18	0
26	m6	1	Total 129	C 99	N 12	O 18	0
26	m6	1	Total 129	C 99	N 12	O 18	0
26	A7	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A7	1	Total 129	C 99	N 12	O 18	0
26	A7	1	Total 129	C 99	N 12	O 18	0
26	D7	1	Total 43	C 33	N 4	O 6	0
26	F7	1	Total 43	C 33	N 4	O 6	0
26	H7	1	Total 43	C 33	N 4	O 6	0
26	J7	1	Total 43	C 33	N 4	O 6	0
26	L7	1	Total 43	C 33	N 4	O 6	0
26	N7	1	Total 43	C 33	N 4	O 6	0
26	O7	1	Total 129	C 99	N 12	O 18	0
26	O7	1	Total 129	C 99	N 12	O 18	0
26	O7	1	Total 129	C 99	N 12	O 18	0
26	P7	1	Total 86	C 66	N 8	O 12	0
26	P7	1	Total 86	C 66	N 8	O 12	0
26	Q7	1	Total 129	C 99	N 12	O 18	0
26	Q7	1	Total 129	C 99	N 12	O 18	0
26	Q7	1	Total 129	C 99	N 12	O 18	0
26	R7	1	Total 86	C 66	N 8	O 12	0
26	R7	1	Total 86	C 66	N 8	O 12	0
26	S7	1	Total 129	C 99	N 12	O 18	0
26	S7	1	Total 129	C 99	N 12	O 18	0
26	S7	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	T7	1	86	66	8	12	0
26	T7	1	86	66	8	12	0
26	U7	1	129	99	12	18	0
26	U7	1	129	99	12	18	0
26	U7	1	129	99	12	18	0
26	V7	1	86	66	8	12	0
26	V7	1	86	66	8	12	0
26	W7	1	129	99	12	18	0
26	W7	1	129	99	12	18	0
26	W7	1	129	99	12	18	0
26	Y7	1	86	66	8	12	0
26	Y7	1	86	66	8	12	0
26	Z7	1	129	99	12	18	0
26	Z7	1	129	99	12	18	0
26	Z7	1	129	99	12	18	0
26	a7	1	86	66	8	12	0
26	a7	1	86	66	8	12	0
26	b7	1	129	99	12	18	0
26	b7	1	129	99	12	18	0
26	b7	1	129	99	12	18	0
26	c7	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	c7	1	Total 86	C 66	N 8	O 12	0
26	d7	1	Total 129	C 99	N 12	O 18	0
26	d7	1	Total 129	C 99	N 12	O 18	0
26	d7	1	Total 129	C 99	N 12	O 18	0
26	e7	1	Total 86	C 66	N 8	O 12	0
26	e7	1	Total 86	C 66	N 8	O 12	0
26	f7	1	Total 129	C 99	N 12	O 18	0
26	f7	1	Total 129	C 99	N 12	O 18	0
26	f7	1	Total 129	C 99	N 12	O 18	0
26	g7	1	Total 86	C 66	N 8	O 12	0
26	g7	1	Total 86	C 66	N 8	O 12	0
26	h7	1	Total 129	C 99	N 12	O 18	0
26	h7	1	Total 129	C 99	N 12	O 18	0
26	h7	1	Total 129	C 99	N 12	O 18	0
26	i7	1	Total 86	C 66	N 8	O 12	0
26	i7	1	Total 86	C 66	N 8	O 12	0
26	j7	1	Total 129	C 99	N 12	O 18	0
26	j7	1	Total 129	C 99	N 12	O 18	0
26	j7	1	Total 129	C 99	N 12	O 18	0
26	k7	1	Total 86	C 66	N 8	O 12	0
26	k7	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	l7	1	Total 129	C 99	N 12	O 18	0
26	l7	1	Total 129	C 99	N 12	O 18	0
26	l7	1	Total 129	C 99	N 12	O 18	0
26	m7	1	Total 86	C 66	N 8	O 12	0
26	m7	1	Total 86	C 66	N 8	O 12	0
26	A8	1	Total 86	C 66	N 8	O 12	0
26	A8	1	Total 86	C 66	N 8	O 12	0
26	B8	1	Total 43	C 33	N 4	O 6	0
26	C8	1	Total 129	C 99	N 12	O 18	0
26	C8	1	Total 129	C 99	N 12	O 18	0
26	C8	1	Total 129	C 99	N 12	O 18	0
26	D8	1	Total 86	C 66	N 8	O 12	0
26	D8	1	Total 86	C 66	N 8	O 12	0
26	E8	1	Total 129	C 99	N 12	O 18	0
26	E8	1	Total 129	C 99	N 12	O 18	0
26	E8	1	Total 129	C 99	N 12	O 18	0
26	F8	1	Total 86	C 66	N 8	O 12	0
26	F8	1	Total 86	C 66	N 8	O 12	0
26	G8	1	Total 129	C 99	N 12	O 18	0
26	G8	1	Total 129	C 99	N 12	O 18	0
26	G8	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	H8	1	86	66	8	12	0
26	H8	1	86	66	8	12	0
26	I8	1	129	99	12	18	0
26	I8	1	129	99	12	18	0
26	I8	1	129	99	12	18	0
26	J8	1	86	66	8	12	0
26	J8	1	86	66	8	12	0
26	K8	1	129	99	12	18	0
26	K8	1	129	99	12	18	0
26	K8	1	129	99	12	18	0
26	L8	1	86	66	8	12	0
26	L8	1	86	66	8	12	0
26	M8	1	129	99	12	18	0
26	M8	1	129	99	12	18	0
26	M8	1	129	99	12	18	0
26	N8	1	86	66	8	12	0
26	N8	1	86	66	8	12	0
26	O8	1	129	99	12	18	0
26	O8	1	129	99	12	18	0
26	O8	1	129	99	12	18	0
26	P8	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	P8	1	86	66	8	12	0
26	Q8	1	129	99	12	18	0
26	Q8	1	129	99	12	18	0
26	Q8	1	129	99	12	18	0
26	R8	1	86	66	8	12	0
26	R8	1	86	66	8	12	0
26	S8	1	129	99	12	18	0
26	S8	1	129	99	12	18	0
26	S8	1	129	99	12	18	0
26	T8	1	86	66	8	12	0
26	T8	1	86	66	8	12	0
26	U8	1	129	99	12	18	0
26	U8	1	129	99	12	18	0
26	U8	1	129	99	12	18	0
26	V8	1	86	66	8	12	0
26	V8	1	86	66	8	12	0
26	W8	1	129	99	12	18	0
26	W8	1	129	99	12	18	0
26	W8	1	129	99	12	18	0
26	X8	1	86	66	8	12	0
26	X8	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	Y8	1	Total 129	C 99	N 12	O 18	0
26	Y8	1	Total 129	C 99	N 12	O 18	0
26	Y8	1	Total 129	C 99	N 12	O 18	0
26	Z8	1	Total 86	C 66	N 8	O 12	0
26	Z8	1	Total 86	C 66	N 8	O 12	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	c8	1	Total 86	C 66	N 8	O 12	0
26	c8	1	Total 86	C 66	N 8	O 12	0
26	d8	1	Total 129	C 99	N 12	O 18	0
26	d8	1	Total 129	C 99	N 12	O 18	0
26	d8	1	Total 129	C 99	N 12	O 18	0
26	e8	1	Total 86	C 66	N 8	O 12	0
26	e8	1	Total 86	C 66	N 8	O 12	0
26	f8	1	Total 129	C 99	N 12	O 18	0
26	f8	1	Total 129	C 99	N 12	O 18	0
26	f8	1	Total 129	C 99	N 12	O 18	0
26	g8	1	Total 86	C 66	N 8	O 12	0
26	g8	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	h8	1	Total 129	C 99	N 12	O 18	0
26	h8	1	Total 129	C 99	N 12	O 18	0
26	h8	1	Total 129	C 99	N 12	O 18	0
26	i8	1	Total 86	C 66	N 8	O 12	0
26	i8	1	Total 86	C 66	N 8	O 12	0
26	j8	1	Total 129	C 99	N 12	O 18	0
26	j8	1	Total 129	C 99	N 12	O 18	0
26	j8	1	Total 129	C 99	N 12	O 18	0
26	k8	1	Total 86	C 66	N 8	O 12	0
26	k8	1	Total 86	C 66	N 8	O 12	0
26	l8	1	Total 129	C 99	N 12	O 18	0
26	l8	1	Total 129	C 99	N 12	O 18	0
26	l8	1	Total 129	C 99	N 12	O 18	0
26	m8	1	Total 86	C 66	N 8	O 12	0
26	m8	1	Total 86	C 66	N 8	O 12	0
26	A9	1	Total 129	C 99	N 12	O 18	0
26	A9	1	Total 129	C 99	N 12	O 18	0
26	A9	1	Total 129	C 99	N 12	O 18	0
26	B9	1	Total 129	C 99	N 12	O 18	0
26	B9	1	Total 129	C 99	N 12	O 18	0
26	B9	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	C9	1	86	66	8	12	0
26	C9	1	86	66	8	12	0
26	D9	1	129	99	12	18	0
26	D9	1	129	99	12	18	0
26	D9	1	129	99	12	18	0
26	E9	1	86	66	8	12	0
26	E9	1	86	66	8	12	0
26	F9	1	129	99	12	18	0
26	F9	1	129	99	12	18	0
26	F9	1	129	99	12	18	0
26	G9	1	86	66	8	12	0
26	G9	1	86	66	8	12	0
26	H9	1	129	99	12	18	0
26	H9	1	129	99	12	18	0
26	H9	1	129	99	12	18	0
26	I9	1	86	66	8	12	0
26	I9	1	86	66	8	12	0
26	J9	1	129	99	12	18	0
26	J9	1	129	99	12	18	0
26	J9	1	129	99	12	18	0
26	K9	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	K9	1	Total 86	C 66	N 8	O 12	0
26	L9	1	Total 129	C 99	N 12	O 18	0
26	L9	1	Total 129	C 99	N 12	O 18	0
26	L9	1	Total 129	C 99	N 12	O 18	0
26	M9	1	Total 86	C 66	N 8	O 12	0
26	M9	1	Total 86	C 66	N 8	O 12	0
26	N9	1	Total 129	C 99	N 12	O 18	0
26	N9	1	Total 129	C 99	N 12	O 18	0
26	N9	1	Total 129	C 99	N 12	O 18	0
26	O9	1	Total 86	C 66	N 8	O 12	0
26	O9	1	Total 86	C 66	N 8	O 12	0
26	P9	1	Total 129	C 99	N 12	O 18	0
26	P9	1	Total 129	C 99	N 12	O 18	0
26	P9	1	Total 129	C 99	N 12	O 18	0
26	Q9	1	Total 86	C 66	N 8	O 12	0
26	Q9	1	Total 86	C 66	N 8	O 12	0
26	R9	1	Total 129	C 99	N 12	O 18	0
26	R9	1	Total 129	C 99	N 12	O 18	0
26	R9	1	Total 129	C 99	N 12	O 18	0
26	S9	1	Total 86	C 66	N 8	O 12	0
26	S9	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	T9	1	Total 129	C 99	N 12	O 18	0
26	T9	1	Total 129	C 99	N 12	O 18	0
26	T9	1	Total 129	C 99	N 12	O 18	0
26	U9	1	Total 86	C 66	N 8	O 12	0
26	U9	1	Total 86	C 66	N 8	O 12	0
26	V9	1	Total 129	C 99	N 12	O 18	0
26	V9	1	Total 129	C 99	N 12	O 18	0
26	V9	1	Total 129	C 99	N 12	O 18	0
26	W9	1	Total 86	C 66	N 8	O 12	0
26	W9	1	Total 86	C 66	N 8	O 12	0
26	X9	1	Total 129	C 99	N 12	O 18	0
26	X9	1	Total 129	C 99	N 12	O 18	0
26	X9	1	Total 129	C 99	N 12	O 18	0
26	Y9	1	Total 86	C 66	N 8	O 12	0
26	Y9	1	Total 86	C 66	N 8	O 12	0
26	AA	1	Total 86	C 66	N 8	O 12	0
26	AA	1	Total 86	C 66	N 8	O 12	0
26	BA	1	Total 43	C 33	N 4	O 6	0
26	CA	1	Total 129	C 99	N 12	O 18	0
26	CA	1	Total 129	C 99	N 12	O 18	0
26	CA	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	DA	1	86	66	8	12	0
26	DA	1	86	66	8	12	0
26	EA	1	129	99	12	18	0
26	EA	1	129	99	12	18	0
26	EA	1	129	99	12	18	0
26	FA	1	86	66	8	12	0
26	FA	1	86	66	8	12	0
26	GA	1	129	99	12	18	0
26	GA	1	129	99	12	18	0
26	GA	1	129	99	12	18	0
26	HA	1	86	66	8	12	0
26	HA	1	86	66	8	12	0
26	IA	1	129	99	12	18	0
26	IA	1	129	99	12	18	0
26	IA	1	129	99	12	18	0
26	JA	1	86	66	8	12	0
26	JA	1	86	66	8	12	0
26	KA	1	129	99	12	18	0
26	KA	1	129	99	12	18	0
26	KA	1	129	99	12	18	0
26	LA	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	LA	1	Total 86	C 66	N 8	O 12	0
26	MA	1	Total 129	C 99	N 12	O 18	0
26	MA	1	Total 129	C 99	N 12	O 18	0
26	MA	1	Total 129	C 99	N 12	O 18	0
26	NA	1	Total 86	C 66	N 8	O 12	0
26	NA	1	Total 86	C 66	N 8	O 12	0
26	OA	1	Total 129	C 99	N 12	O 18	0
26	OA	1	Total 129	C 99	N 12	O 18	0
26	OA	1	Total 129	C 99	N 12	O 18	0
26	PA	1	Total 86	C 66	N 8	O 12	0
26	PA	1	Total 86	C 66	N 8	O 12	0
26	QA	1	Total 129	C 99	N 12	O 18	0
26	QA	1	Total 129	C 99	N 12	O 18	0
26	QA	1	Total 129	C 99	N 12	O 18	0
26	RA	1	Total 86	C 66	N 8	O 12	0
26	RA	1	Total 86	C 66	N 8	O 12	0
26	SA	1	Total 129	C 99	N 12	O 18	0
26	SA	1	Total 129	C 99	N 12	O 18	0
26	SA	1	Total 129	C 99	N 12	O 18	0
26	TA	1	Total 86	C 66	N 8	O 12	0
26	TA	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	UA	1	Total 129	C 99	N 12	O 18	0
26	UA	1	Total 129	C 99	N 12	O 18	0
26	UA	1	Total 129	C 99	N 12	O 18	0
26	VA	1	Total 86	C 66	N 8	O 12	0
26	VA	1	Total 86	C 66	N 8	O 12	0
26	WA	1	Total 129	C 99	N 12	O 18	0
26	WA	1	Total 129	C 99	N 12	O 18	0
26	WA	1	Total 129	C 99	N 12	O 18	0
26	XA	1	Total 86	C 66	N 8	O 12	0
26	XA	1	Total 86	C 66	N 8	O 12	0
26	YA	1	Total 129	C 99	N 12	O 18	0
26	YA	1	Total 129	C 99	N 12	O 18	0
26	YA	1	Total 129	C 99	N 12	O 18	0
26	ZA	1	Total 86	C 66	N 8	O 12	0
26	ZA	1	Total 86	C 66	N 8	O 12	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	cA	1	Total 129	C 99	N 12	O 18	0
26	cA	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	cA	1	Total 129	C 99	N 12	O 18	0
26	dA	1	Total 43	C 33	N 4	O 6	0
26	eA	1	Total 86	C 66	N 8	O 12	0
26	eA	1	Total 86	C 66	N 8	O 12	0
26	fA	1	Total 129	C 99	N 12	O 18	0
26	fA	1	Total 129	C 99	N 12	O 18	0
26	fA	1	Total 129	C 99	N 12	O 18	0
26	gA	1	Total 86	C 66	N 8	O 12	0
26	gA	1	Total 86	C 66	N 8	O 12	0
26	hA	1	Total 129	C 99	N 12	O 18	0
26	hA	1	Total 129	C 99	N 12	O 18	0
26	hA	1	Total 129	C 99	N 12	O 18	0
26	iA	1	Total 86	C 66	N 8	O 12	0
26	iA	1	Total 86	C 66	N 8	O 12	0
26	jA	1	Total 129	C 99	N 12	O 18	0
26	jA	1	Total 129	C 99	N 12	O 18	0
26	jA	1	Total 129	C 99	N 12	O 18	0
26	kA	1	Total 86	C 66	N 8	O 12	0
26	kA	1	Total 86	C 66	N 8	O 12	0
26	lA	1	Total 129	C 99	N 12	O 18	0
26	lA	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	lA	1	Total 129	C 99	N 12	O 18	0
26	mA	1	Total 86	C 66	N 8	O 12	0
26	mA	1	Total 86	C 66	N 8	O 12	0
26	AB	1	Total 86	C 66	N 8	O 12	0
26	AB	1	Total 86	C 66	N 8	O 12	0
26	DB	1	Total 43	C 33	N 4	O 6	0
26	GB	1	Total 43	C 33	N 4	O 6	0
26	HB	1	Total 43	C 33	N 4	O 6	0
26	KB	1	Total 43	C 33	N 4	O 6	0
26	LB	1	Total 43	C 33	N 4	O 6	0
26	NB	1	Total 43	C 33	N 4	O 6	0
26	OB	1	Total 129	C 99	N 12	O 18	0
26	OB	1	Total 129	C 99	N 12	O 18	0
26	OB	1	Total 129	C 99	N 12	O 18	0
26	PB	1	Total 86	C 66	N 8	O 12	0
26	PB	1	Total 86	C 66	N 8	O 12	0
26	QB	1	Total 129	C 99	N 12	O 18	0
26	QB	1	Total 129	C 99	N 12	O 18	0
26	QB	1	Total 129	C 99	N 12	O 18	0
26	RB	1	Total 86	C 66	N 8	O 12	0
26	RB	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	SB	1	Total 129	C 99	N 12	O 18	0
26	SB	1	Total 129	C 99	N 12	O 18	0
26	SB	1	Total 129	C 99	N 12	O 18	0
26	TB	1	Total 86	C 66	N 8	O 12	0
26	TB	1	Total 86	C 66	N 8	O 12	0
26	UB	1	Total 129	C 99	N 12	O 18	0
26	UB	1	Total 129	C 99	N 12	O 18	0
26	UB	1	Total 129	C 99	N 12	O 18	0
26	VB	1	Total 86	C 66	N 8	O 12	0
26	VB	1	Total 86	C 66	N 8	O 12	0
26	WB	1	Total 129	C 99	N 12	O 18	0
26	WB	1	Total 129	C 99	N 12	O 18	0
26	WB	1	Total 129	C 99	N 12	O 18	0
26	YB	1	Total 86	C 66	N 8	O 12	0
26	YB	1	Total 86	C 66	N 8	O 12	0
26	ZB	1	Total 129	C 99	N 12	O 18	0
26	ZB	1	Total 129	C 99	N 12	O 18	0
26	ZB	1	Total 129	C 99	N 12	O 18	0
26	aB	1	Total 86	C 66	N 8	O 12	0
26	aB	1	Total 86	C 66	N 8	O 12	0
26	bB	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	bB	1	86	66	8	12	0
26	cB	1	86	66	8	12	0
26	cB	1	86	66	8	12	0
26	dB	1	172	132	16	24	0
26	dB	1	172	132	16	24	0
26	dB	1	172	132	16	24	0
26	dB	1	172	132	16	24	0
26	eB	1	129	99	12	18	0
26	eB	1	129	99	12	18	0
26	eB	1	129	99	12	18	0
26	fB	1	129	99	12	18	0
26	fB	1	129	99	12	18	0
26	fB	1	129	99	12	18	0
26	gB	1	86	66	8	12	0
26	gB	1	86	66	8	12	0
26	hB	1	129	99	12	18	0
26	hB	1	129	99	12	18	0
26	hB	1	129	99	12	18	0
26	iB	1	86	66	8	12	0
26	iB	1	86	66	8	12	0
26	jB	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	jB	1	86	66	8	12	0
26	kB	1	86	66	8	12	0
26	kB	1	86	66	8	12	0
26	lB	1	129	99	12	18	0
26	lB	1	129	99	12	18	0
26	lB	1	129	99	12	18	0
26	mB	1	129	99	12	18	0
26	mB	1	129	99	12	18	0
26	mB	1	129	99	12	18	0
26	AC	1	129	99	12	18	0
26	AC	1	129	99	12	18	0
26	AC	1	129	99	12	18	0
26	BC	1	129	99	12	18	0
26	BC	1	129	99	12	18	0
26	BC	1	129	99	12	18	0
26	CC	1	129	99	12	18	0
26	CC	1	129	99	12	18	0
26	CC	1	129	99	12	18	0
26	FC	1	129	99	12	18	0
26	FC	1	129	99	12	18	0
26	FC	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	GC	1	Total 129	C 99	N 12	O 18	0
26	GC	1	Total 129	C 99	N 12	O 18	0
26	GC	1	Total 129	C 99	N 12	O 18	0
26	HC	1	Total 129	C 99	N 12	O 18	0
26	HC	1	Total 129	C 99	N 12	O 18	0
26	HC	1	Total 129	C 99	N 12	O 18	0
26	IC	1	Total 129	C 99	N 12	O 18	0
26	IC	1	Total 129	C 99	N 12	O 18	0
26	IC	1	Total 129	C 99	N 12	O 18	0
26	JC	1	Total 86	C 66	N 8	O 12	0
26	JC	1	Total 86	C 66	N 8	O 12	0
26	KC	1	Total 129	C 99	N 12	O 18	0
26	KC	1	Total 129	C 99	N 12	O 18	0
26	KC	1	Total 129	C 99	N 12	O 18	0
26	LC	1	Total 129	C 99	N 12	O 18	0
26	LC	1	Total 129	C 99	N 12	O 18	0
26	LC	1	Total 129	C 99	N 12	O 18	0
26	eD	1	Total 43	C 33	N 4	O 6	0
26	AD	1	Total 86	C 66	N 8	O 12	0
26	AD	1	Total 86	C 66	N 8	O 12	0
26	BD	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	BD	1	Total 129	C 99	N 12	O 18	0
26	BD	1	Total 129	C 99	N 12	O 18	0
26	CD	1	Total 86	C 66	N 8	O 12	0
26	CD	1	Total 86	C 66	N 8	O 12	0
26	DD	1	Total 129	C 99	N 12	O 18	0
26	DD	1	Total 129	C 99	N 12	O 18	0
26	DD	1	Total 129	C 99	N 12	O 18	0
26	ED	1	Total 86	C 66	N 8	O 12	0
26	ED	1	Total 86	C 66	N 8	O 12	0
26	FD	1	Total 129	C 99	N 12	O 18	0
26	FD	1	Total 129	C 99	N 12	O 18	0
26	FD	1	Total 129	C 99	N 12	O 18	0
26	GD	1	Total 86	C 66	N 8	O 12	0
26	GD	1	Total 86	C 66	N 8	O 12	0
26	HD	1	Total 129	C 99	N 12	O 18	0
26	HD	1	Total 129	C 99	N 12	O 18	0
26	HD	1	Total 129	C 99	N 12	O 18	0
26	ID	1	Total 86	C 66	N 8	O 12	0
26	ID	1	Total 86	C 66	N 8	O 12	0
26	JD	1	Total 129	C 99	N 12	O 18	0
26	JD	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	JD	1	Total 129	C 99	N 12	O 18	0
26	KD	1	Total 86	C 66	N 8	O 12	0
26	KD	1	Total 86	C 66	N 8	O 12	0
26	LD	1	Total 129	C 99	N 12	O 18	0
26	LD	1	Total 129	C 99	N 12	O 18	0
26	LD	1	Total 129	C 99	N 12	O 18	0
26	MD	1	Total 86	C 66	N 8	O 12	0
26	MD	1	Total 86	C 66	N 8	O 12	0
26	ND	1	Total 129	C 99	N 12	O 18	0
26	ND	1	Total 129	C 99	N 12	O 18	0
26	ND	1	Total 129	C 99	N 12	O 18	0
26	OD	1	Total 86	C 66	N 8	O 12	0
26	OD	1	Total 86	C 66	N 8	O 12	0
26	PD	1	Total 129	C 99	N 12	O 18	0
26	PD	1	Total 129	C 99	N 12	O 18	0
26	PD	1	Total 129	C 99	N 12	O 18	0
26	QD	1	Total 86	C 66	N 8	O 12	0
26	QD	1	Total 86	C 66	N 8	O 12	0
26	RD	1	Total 129	C 99	N 12	O 18	0
26	RD	1	Total 129	C 99	N 12	O 18	0
26	RD	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	SD	1	86	66	8	12	0
26	SD	1	86	66	8	12	0
26	TD	1	129	99	12	18	0
26	TD	1	129	99	12	18	0
26	TD	1	129	99	12	18	0
26	UD	1	86	66	8	12	0
26	UD	1	86	66	8	12	0
26	VD	1	129	99	12	18	0
26	VD	1	129	99	12	18	0
26	VD	1	129	99	12	18	0
26	WD	1	86	66	8	12	0
26	WD	1	86	66	8	12	0
26	XD	1	129	99	12	18	0
26	XD	1	129	99	12	18	0
26	XD	1	129	99	12	18	0
26	YD	1	129	99	12	18	0
26	YD	1	129	99	12	18	0
26	YD	1	129	99	12	18	0
26	AE	1	86	66	8	12	0
26	AE	1	86	66	8	12	0
26	BE	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	BE	1	Total 86	C 66	N 8	O 12	0
26	CE	1	Total 129	C 99	N 12	O 18	0
26	CE	1	Total 129	C 99	N 12	O 18	0
26	CE	1	Total 129	C 99	N 12	O 18	0
26	DE	1	Total 129	C 99	N 12	O 18	0
26	DE	1	Total 129	C 99	N 12	O 18	0
26	DE	1	Total 129	C 99	N 12	O 18	0
26	EE	1	Total 86	C 66	N 8	O 12	0
26	EE	1	Total 86	C 66	N 8	O 12	0
26	FE	1	Total 86	C 66	N 8	O 12	0
26	FE	1	Total 86	C 66	N 8	O 12	0
26	GE	1	Total 129	C 99	N 12	O 18	0
26	GE	1	Total 129	C 99	N 12	O 18	0
26	GE	1	Total 129	C 99	N 12	O 18	0
26	HE	1	Total 86	C 66	N 8	O 12	0
26	HE	1	Total 86	C 66	N 8	O 12	0
26	IE	1	Total 129	C 99	N 12	O 18	0
26	IE	1	Total 129	C 99	N 12	O 18	0
26	IE	1	Total 129	C 99	N 12	O 18	0
26	JE	1	Total 86	C 66	N 8	O 12	0
26	JE	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	KE	1	129	99	12	18	0
26	KE	1	129	99	12	18	0
26	KE	1	129	99	12	18	0
26	LE	1	86	66	8	12	0
26	LE	1	86	66	8	12	0
26	ME	1	129	99	12	18	0
26	ME	1	129	99	12	18	0
26	ME	1	129	99	12	18	0
26	NE	1	86	66	8	12	0
26	NE	1	86	66	8	12	0
26	OE	1	129	99	12	18	0
26	OE	1	129	99	12	18	0
26	OE	1	129	99	12	18	0
26	PE	1	86	66	8	12	0
26	PE	1	86	66	8	12	0
26	QE	1	129	99	12	18	0
26	QE	1	129	99	12	18	0
26	QE	1	129	99	12	18	0
26	RE	1	86	66	8	12	0
26	RE	1	86	66	8	12	0
26	SE	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	SE	1	Total 129	C 99	N 12	O 18	0
26	SE	1	Total 129	C 99	N 12	O 18	0
26	TE	1	Total 86	C 66	N 8	O 12	0
26	TE	1	Total 86	C 66	N 8	O 12	0
26	UE	1	Total 129	C 99	N 12	O 18	0
26	UE	1	Total 129	C 99	N 12	O 18	0
26	UE	1	Total 129	C 99	N 12	O 18	0
26	VE	1	Total 86	C 66	N 8	O 12	0
26	VE	1	Total 86	C 66	N 8	O 12	0
26	WE	1	Total 129	C 99	N 12	O 18	0
26	WE	1	Total 129	C 99	N 12	O 18	0
26	WE	1	Total 129	C 99	N 12	O 18	0
26	XE	1	Total 86	C 66	N 8	O 12	0
26	XE	1	Total 86	C 66	N 8	O 12	0
26	YE	1	Total 129	C 99	N 12	O 18	0
26	YE	1	Total 129	C 99	N 12	O 18	0
26	YE	1	Total 129	C 99	N 12	O 18	0
26	ZE	1	Total 86	C 66	N 8	O 12	0
26	ZE	1	Total 86	C 66	N 8	O 12	0
26	aE	1	Total 129	C 99	N 12	O 18	0
26	aE	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	aE	1	Total 129	C 99	N 12	O 18	0
26	bE	1	Total 86	C 66	N 8	O 12	0
26	bE	1	Total 86	C 66	N 8	O 12	0
26	cE	1	Total 129	C 99	N 12	O 18	0
26	cE	1	Total 129	C 99	N 12	O 18	0
26	cE	1	Total 129	C 99	N 12	O 18	0
26	dE	1	Total 86	C 66	N 8	O 12	0
26	dE	1	Total 86	C 66	N 8	O 12	0
26	eE	1	Total 129	C 99	N 12	O 18	0
26	eE	1	Total 129	C 99	N 12	O 18	0
26	eE	1	Total 129	C 99	N 12	O 18	0
26	fE	1	Total 86	C 66	N 8	O 12	0
26	fE	1	Total 86	C 66	N 8	O 12	0
26	gE	1	Total 129	C 99	N 12	O 18	0
26	gE	1	Total 129	C 99	N 12	O 18	0
26	gE	1	Total 129	C 99	N 12	O 18	0
26	hE	1	Total 86	C 66	N 8	O 12	0
26	hE	1	Total 86	C 66	N 8	O 12	0
26	iE	1	Total 129	C 99	N 12	O 18	0
26	iE	1	Total 129	C 99	N 12	O 18	0
26	iE	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	jE	1	86	66	8	12	0
26	jE	1	86	66	8	12	0
26	kE	1	129	99	12	18	0
26	kE	1	129	99	12	18	0
26	kE	1	129	99	12	18	0
26	lE	1	86	66	8	12	0
26	lE	1	86	66	8	12	0
26	mE	1	129	99	12	18	0
26	mE	1	129	99	12	18	0
26	mE	1	129	99	12	18	0
26	nE	1	86	66	8	12	0
26	nE	1	86	66	8	12	0
26	oE	1	129	99	12	18	0
26	oE	1	129	99	12	18	0
26	oE	1	129	99	12	18	0
26	pE	1	86	66	8	12	0
26	pE	1	86	66	8	12	0
26	qE	1	129	99	12	18	0
26	qE	1	129	99	12	18	0
26	qE	1	129	99	12	18	0
26	rE	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	rE	1	86	66	8	12	0
26	sE	1	129	99	12	18	0
26	sE	1	129	99	12	18	0
26	sE	1	129	99	12	18	0
26	tE	1	86	66	8	12	0
26	tE	1	86	66	8	12	0
26	uE	1	129	99	12	18	0
26	uE	1	129	99	12	18	0
26	uE	1	129	99	12	18	0
26	vE	1	86	66	8	12	0
26	vE	1	86	66	8	12	0
26	wE	1	129	99	12	18	0
26	wE	1	129	99	12	18	0
26	wE	1	129	99	12	18	0
26	xE	1	129	99	12	18	0
26	xE	1	129	99	12	18	0
26	xE	1	129	99	12	18	0
26	yE	1	43	33	4	6	0
26	zE	1	43	33	4	6	0
26	AF	1	129	99	12	18	0
26	AF	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	AF	1	Total 129	C 99	N 12	O 18	0
26	DF	1	Total 43	C 33	N 4	O 6	0
26	FF	1	Total 43	C 33	N 4	O 6	0
26	HF	1	Total 43	C 33	N 4	O 6	0
26	JF	1	Total 43	C 33	N 4	O 6	0
26	LF	1	Total 43	C 33	N 4	O 6	0
26	NF	1	Total 43	C 33	N 4	O 6	0
26	OF	1	Total 129	C 99	N 12	O 18	0
26	OF	1	Total 129	C 99	N 12	O 18	0
26	OF	1	Total 129	C 99	N 12	O 18	0
26	PF	1	Total 86	C 66	N 8	O 12	0
26	PF	1	Total 86	C 66	N 8	O 12	0
26	QF	1	Total 129	C 99	N 12	O 18	0
26	QF	1	Total 129	C 99	N 12	O 18	0
26	QF	1	Total 129	C 99	N 12	O 18	0
26	RF	1	Total 86	C 66	N 8	O 12	0
26	RF	1	Total 86	C 66	N 8	O 12	0
26	SF	1	Total 86	C 66	N 8	O 12	0
26	SF	1	Total 86	C 66	N 8	O 12	0
26	TF	1	Total 86	C 66	N 8	O 12	0
26	TF	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	UF	1	129	99	12	18	0
26	UF	1	129	99	12	18	0
26	UF	1	129	99	12	18	0
26	VF	1	129	99	12	18	0
26	VF	1	129	99	12	18	0
26	VF	1	129	99	12	18	0
26	WF	1	129	99	12	18	0
26	WF	1	129	99	12	18	0
26	WF	1	129	99	12	18	0
26	YF	1	86	66	8	12	0
26	YF	1	86	66	8	12	0
26	ZF	1	129	99	12	18	0
26	ZF	1	129	99	12	18	0
26	ZF	1	129	99	12	18	0
26	aF	1	86	66	8	12	0
26	aF	1	86	66	8	12	0
26	bF	1	129	99	12	18	0
26	bF	1	129	99	12	18	0
26	bF	1	129	99	12	18	0
26	cF	1	86	66	8	12	0
26	cF	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	dF	1	Total 129	C 99	N 12	O 18	0
26	dF	1	Total 129	C 99	N 12	O 18	0
26	dF	1	Total 129	C 99	N 12	O 18	0
26	eF	1	Total 86	C 66	N 8	O 12	0
26	eF	1	Total 86	C 66	N 8	O 12	0
26	fF	1	Total 129	C 99	N 12	O 18	0
26	fF	1	Total 129	C 99	N 12	O 18	0
26	fF	1	Total 129	C 99	N 12	O 18	0
26	gF	1	Total 86	C 66	N 8	O 12	0
26	gF	1	Total 86	C 66	N 8	O 12	0
26	hF	1	Total 129	C 99	N 12	O 18	0
26	hF	1	Total 129	C 99	N 12	O 18	0
26	hF	1	Total 129	C 99	N 12	O 18	0
26	iF	1	Total 86	C 66	N 8	O 12	0
26	iF	1	Total 86	C 66	N 8	O 12	0
26	jF	1	Total 129	C 99	N 12	O 18	0
26	jF	1	Total 129	C 99	N 12	O 18	0
26	jF	1	Total 129	C 99	N 12	O 18	0
26	kF	1	Total 86	C 66	N 8	O 12	0
26	kF	1	Total 86	C 66	N 8	O 12	0
26	lF	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	lF	1	Total 129	C 99	N 12	O 18	0
26	lF	1	Total 129	C 99	N 12	O 18	0
26	mF	1	Total 86	C 66	N 8	O 12	0
26	mF	1	Total 86	C 66	N 8	O 12	0
26	AG	1	Total 86	C 66	N 8	O 12	0
26	AG	1	Total 86	C 66	N 8	O 12	0
26	BG	1	Total 86	C 66	N 8	O 12	0
26	BG	1	Total 86	C 66	N 8	O 12	0
26	CG	1	Total 129	C 99	N 12	O 18	0
26	CG	1	Total 129	C 99	N 12	O 18	0
26	CG	1	Total 129	C 99	N 12	O 18	0
26	DG	1	Total 129	C 99	N 12	O 18	0
26	DG	1	Total 129	C 99	N 12	O 18	0
26	DG	1	Total 129	C 99	N 12	O 18	0
26	EG	1	Total 86	C 66	N 8	O 12	0
26	EG	1	Total 86	C 66	N 8	O 12	0
26	FG	1	Total 86	C 66	N 8	O 12	0
26	FG	1	Total 86	C 66	N 8	O 12	0
26	GG	1	Total 129	C 99	N 12	O 18	0
26	GG	1	Total 129	C 99	N 12	O 18	0
26	GG	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	HG	1	86	66	8	12	0
26	HG	1	86	66	8	12	0
26	IG	1	129	99	12	18	0
26	IG	1	129	99	12	18	0
26	IG	1	129	99	12	18	0
26	JG	1	86	66	8	12	0
26	JG	1	86	66	8	12	0
26	KG	1	129	99	12	18	0
26	KG	1	129	99	12	18	0
26	KG	1	129	99	12	18	0
26	LG	1	86	66	8	12	0
26	LG	1	86	66	8	12	0
26	MG	1	129	99	12	18	0
26	MG	1	129	99	12	18	0
26	MG	1	129	99	12	18	0
26	NG	1	86	66	8	12	0
26	NG	1	86	66	8	12	0
26	OG	1	129	99	12	18	0
26	OG	1	129	99	12	18	0
26	OG	1	129	99	12	18	0
26	PG	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	PG	1	86	66	8	12	0
26	QG	1	129	99	12	18	0
26	QG	1	129	99	12	18	0
26	QG	1	129	99	12	18	0
26	RG	1	86	66	8	12	0
26	RG	1	86	66	8	12	0
26	SG	1	129	99	12	18	0
26	SG	1	129	99	12	18	0
26	SG	1	129	99	12	18	0
26	TG	1	86	66	8	12	0
26	TG	1	86	66	8	12	0
26	UG	1	86	66	8	12	0
26	UG	1	86	66	8	12	0
26	VG	1	86	66	8	12	0
26	VG	1	86	66	8	12	0
26	WG	1	129	99	12	18	0
26	WG	1	129	99	12	18	0
26	WG	1	129	99	12	18	0
26	XG	1	129	99	12	18	0
26	XG	1	129	99	12	18	0
26	XG	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	YG	1	Total 129	C 99	N 12	O 18	0
26	YG	1	Total 129	C 99	N 12	O 18	0
26	YG	1	Total 129	C 99	N 12	O 18	0
26	ZG	1	Total 86	C 66	N 8	O 12	0
26	ZG	1	Total 86	C 66	N 8	O 12	0
26	aG	1	Total 129	C 99	N 12	O 18	0
26	aG	1	Total 129	C 99	N 12	O 18	0
26	aG	1	Total 129	C 99	N 12	O 18	0
26	bG	1	Total 86	C 66	N 8	O 12	0
26	bG	1	Total 86	C 66	N 8	O 12	0
26	cG	1	Total 129	C 99	N 12	O 18	0
26	cG	1	Total 129	C 99	N 12	O 18	0
26	cG	1	Total 129	C 99	N 12	O 18	0
26	dG	1	Total 86	C 66	N 8	O 12	0
26	dG	1	Total 86	C 66	N 8	O 12	0
26	eG	1	Total 129	C 99	N 12	O 18	0
26	eG	1	Total 129	C 99	N 12	O 18	0
26	eG	1	Total 129	C 99	N 12	O 18	0
26	fG	1	Total 86	C 66	N 8	O 12	0
26	fG	1	Total 86	C 66	N 8	O 12	0
26	gG	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	gG	1	Total 129	C 99	N 12	O 18	0
26	gG	1	Total 129	C 99	N 12	O 18	0
26	hG	1	Total 86	C 66	N 8	O 12	0
26	hG	1	Total 86	C 66	N 8	O 12	0
26	iG	1	Total 129	C 99	N 12	O 18	0
26	iG	1	Total 129	C 99	N 12	O 18	0
26	iG	1	Total 129	C 99	N 12	O 18	0
26	jG	1	Total 86	C 66	N 8	O 12	0
26	jG	1	Total 86	C 66	N 8	O 12	0
26	kG	1	Total 129	C 99	N 12	O 18	0
26	kG	1	Total 129	C 99	N 12	O 18	0
26	kG	1	Total 129	C 99	N 12	O 18	0
26	lG	1	Total 86	C 66	N 8	O 12	0
26	lG	1	Total 86	C 66	N 8	O 12	0
26	mG	1	Total 129	C 99	N 12	O 18	0
26	mG	1	Total 129	C 99	N 12	O 18	0
26	mG	1	Total 129	C 99	N 12	O 18	0
26	nG	1	Total 86	C 66	N 8	O 12	0
26	nG	1	Total 86	C 66	N 8	O 12	0
26	oG	1	Total 129	C 99	N 12	O 18	0
26	oG	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	oG	1	Total 129	C 99	N 12	O 18	0
26	pG	1	Total 86	C 66	N 8	O 12	0
26	pG	1	Total 86	C 66	N 8	O 12	0
26	qG	1	Total 129	C 99	N 12	O 18	0
26	qG	1	Total 129	C 99	N 12	O 18	0
26	qG	1	Total 129	C 99	N 12	O 18	0
26	rG	1	Total 86	C 66	N 8	O 12	0
26	rG	1	Total 86	C 66	N 8	O 12	0
26	sG	1	Total 129	C 99	N 12	O 18	0
26	sG	1	Total 129	C 99	N 12	O 18	0
26	sG	1	Total 129	C 99	N 12	O 18	0
26	tG	1	Total 86	C 66	N 8	O 12	0
26	tG	1	Total 86	C 66	N 8	O 12	0
26	uG	1	Total 129	C 99	N 12	O 18	0
26	uG	1	Total 129	C 99	N 12	O 18	0
26	uG	1	Total 129	C 99	N 12	O 18	0
26	vG	1	Total 86	C 66	N 8	O 12	0
26	vG	1	Total 86	C 66	N 8	O 12	0
26	wG	1	Total 129	C 99	N 12	O 18	0
26	wG	1	Total 129	C 99	N 12	O 18	0
26	wG	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	xG	1	Total 129	C 99	N 12	O 18	0
26	xG	1	Total 129	C 99	N 12	O 18	0
26	xG	1	Total 129	C 99	N 12	O 18	0
26	yG	1	Total 43	C 33	N 4	O 6	0
26	zG	1	Total 43	C 33	N 4	O 6	0
26	AI	1	Total 129	C 99	N 12	O 18	0
26	AI	1	Total 129	C 99	N 12	O 18	0
26	AI	1	Total 129	C 99	N 12	O 18	0
26	DI	1	Total 43	C 33	N 4	O 6	0
26	FI	1	Total 43	C 33	N 4	O 6	0
26	HI	1	Total 43	C 33	N 4	O 6	0
26	JI	1	Total 43	C 33	N 4	O 6	0
26	LI	1	Total 43	C 33	N 4	O 6	0
26	NI	1	Total 43	C 33	N 4	O 6	0
26	OI	1	Total 86	C 66	N 8	O 12	0
26	OI	1	Total 86	C 66	N 8	O 12	0
26	PI	1	Total 129	C 99	N 12	O 18	0
26	PI	1	Total 129	C 99	N 12	O 18	0
26	PI	1	Total 129	C 99	N 12	O 18	0
26	QI	1	Total 86	C 66	N 8	O 12	0
26	QI	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	RI	1	Total 129	C 99	N 12	O 18	0
26	RI	1	Total 129	C 99	N 12	O 18	0
26	RI	1	Total 129	C 99	N 12	O 18	0
26	SI	1	Total 86	C 66	N 8	O 12	0
26	SI	1	Total 86	C 66	N 8	O 12	0
26	TI	1	Total 129	C 99	N 12	O 18	0
26	TI	1	Total 129	C 99	N 12	O 18	0
26	TI	1	Total 129	C 99	N 12	O 18	0
26	UI	1	Total 86	C 66	N 8	O 12	0
26	UI	1	Total 86	C 66	N 8	O 12	0
26	VI	1	Total 129	C 99	N 12	O 18	0
26	VI	1	Total 129	C 99	N 12	O 18	0
26	VI	1	Total 129	C 99	N 12	O 18	0
26	WI	1	Total 43	C 33	N 4	O 6	0
26	YI	1	Total 129	C 99	N 12	O 18	0
26	YI	1	Total 129	C 99	N 12	O 18	0
26	YI	1	Total 129	C 99	N 12	O 18	0
26	ZI	1	Total 86	C 66	N 8	O 12	0
26	ZI	1	Total 86	C 66	N 8	O 12	0
26	aI	1	Total 129	C 99	N 12	O 18	0
26	aI	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	aI	1	Total 129	C 99	N 12	O 18	0
26	bI	1	Total 86	C 66	N 8	O 12	0
26	bI	1	Total 86	C 66	N 8	O 12	0
26	cI	1	Total 129	C 99	N 12	O 18	0
26	cI	1	Total 129	C 99	N 12	O 18	0
26	cI	1	Total 129	C 99	N 12	O 18	0
26	dI	1	Total 86	C 66	N 8	O 12	0
26	dI	1	Total 86	C 66	N 8	O 12	0
26	eI	1	Total 129	C 99	N 12	O 18	0
26	eI	1	Total 129	C 99	N 12	O 18	0
26	eI	1	Total 129	C 99	N 12	O 18	0
26	fI	1	Total 86	C 66	N 8	O 12	0
26	fI	1	Total 86	C 66	N 8	O 12	0
26	gI	1	Total 129	C 99	N 12	O 18	0
26	gI	1	Total 129	C 99	N 12	O 18	0
26	gI	1	Total 129	C 99	N 12	O 18	0
26	hI	1	Total 86	C 66	N 8	O 12	0
26	hI	1	Total 86	C 66	N 8	O 12	0
26	iI	1	Total 129	C 99	N 12	O 18	0
26	iI	1	Total 129	C 99	N 12	O 18	0
26	iI	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	jI	1	86	66	8	12	0
26	jI	1	86	66	8	12	0
26	kI	1	129	99	12	18	0
26	kI	1	129	99	12	18	0
26	kI	1	129	99	12	18	0
26	lI	1	86	66	8	12	0
26	lI	1	86	66	8	12	0
26	mI	1	129	99	12	18	0
26	mI	1	129	99	12	18	0
26	mI	1	129	99	12	18	0
26	AJ	1	172	132	16	24	0
26	AJ	1	172	132	16	24	0
26	AJ	1	172	132	16	24	0
26	AJ	1	172	132	16	24	0
26	BJ	1	129	99	12	18	0
26	BJ	1	129	99	12	18	0
26	BJ	1	129	99	12	18	0
26	CJ	1	86	66	8	12	0
26	CJ	1	86	66	8	12	0
26	DJ	1	129	99	12	18	0
26	DJ	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	DJ	1	Total 129	C 99	N 12	O 18	0
26	EJ	1	Total 86	C 66	N 8	O 12	0
26	EJ	1	Total 86	C 66	N 8	O 12	0
26	FJ	1	Total 86	C 66	N 8	O 12	0
26	FJ	1	Total 86	C 66	N 8	O 12	0
26	GJ	1	Total 86	C 66	N 8	O 12	0
26	GJ	1	Total 86	C 66	N 8	O 12	0
26	HJ	1	Total 129	C 99	N 12	O 18	0
26	HJ	1	Total 129	C 99	N 12	O 18	0
26	HJ	1	Total 129	C 99	N 12	O 18	0
26	IJ	1	Total 129	C 99	N 12	O 18	0
26	IJ	1	Total 129	C 99	N 12	O 18	0
26	IJ	1	Total 129	C 99	N 12	O 18	0
26	JJ	1	Total 129	C 99	N 12	O 18	0
26	JJ	1	Total 129	C 99	N 12	O 18	0
26	JJ	1	Total 129	C 99	N 12	O 18	0
26	KJ	1	Total 86	C 66	N 8	O 12	0
26	KJ	1	Total 86	C 66	N 8	O 12	0
26	LJ	1	Total 129	C 99	N 12	O 18	0
26	LJ	1	Total 129	C 99	N 12	O 18	0
26	LJ	1	Total 129	C 99	N 12	O 18	0

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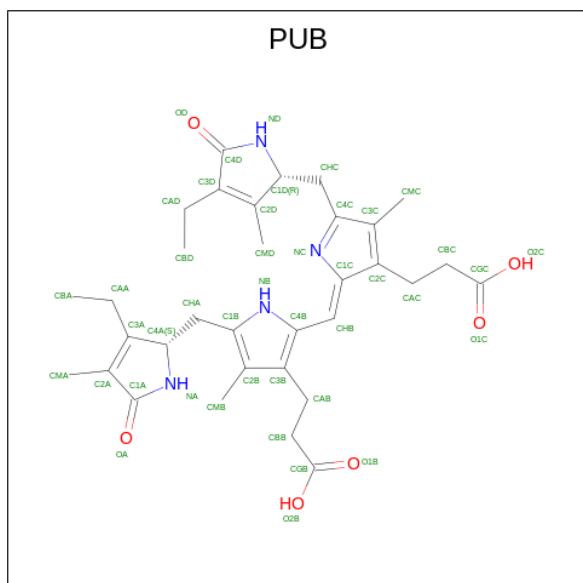
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	MJ	1	86	66	8	12	0
26	MJ	1	86	66	8	12	0
26	NJ	1	129	99	12	18	0
26	NJ	1	129	99	12	18	0
26	NJ	1	129	99	12	18	0
26	OJ	1	43	33	4	6	0
26	PJ	1	129	99	12	18	0
26	PJ	1	129	99	12	18	0
26	PJ	1	129	99	12	18	0
26	QJ	1	86	66	8	12	0
26	QJ	1	86	66	8	12	0
26	RJ	1	129	99	12	18	0
26	RJ	1	129	99	12	18	0
26	RJ	1	129	99	12	18	0
26	SJ	1	86	66	8	12	0
26	SJ	1	86	66	8	12	0
26	TJ	1	129	99	12	18	0
26	TJ	1	129	99	12	18	0
26	TJ	1	129	99	12	18	0
26	UJ	1	86	66	8	12	0
26	UJ	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	VJ	1	Total	C	N	O	0
			129	99	12	18	
26	VJ	1	Total	C	N	O	0
			129	99	12	18	
26	VJ	1	Total	C	N	O	0
			129	99	12	18	
26	WJ	1	Total	C	N	O	0
			86	66	8	12	
26	WJ	1	Total	C	N	O	0
			86	66	8	12	
26	XJ	1	Total	C	N	O	0
			129	99	12	18	
26	XJ	1	Total	C	N	O	0
			129	99	12	18	
26	XJ	1	Total	C	N	O	0
			129	99	12	18	
26	YJ	1	Total	C	N	O	0
			86	66	8	12	
26	YJ	1	Total	C	N	O	0
			86	66	8	12	

- Molecule 27 is PHYCOUROBILIN (three-letter code: PUB) (formula: $C_{33}H_{42}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	A1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	K1	1	Total 43	C 33	N 4	O 6	0
27	21	1	Total 86	C 66	N 8	O 12	0
27	21	1	Total 86	C 66	N 8	O 12	0
27	A2	1	Total 86	C 66	N 8	O 12	0
27	A2	1	Total 86	C 66	N 8	O 12	0
27	K3	1	Total 43	C 33	N 4	O 6	0
27	Y3	1	Total 43	C 33	N 4	O 6	0
27	A4	1	Total 43	C 33	N 4	O 6	0
27	K4	1	Total 43	C 33	N 4	O 6	0
27	24	1	Total 86	C 66	N 8	O 12	0
27	24	1	Total 86	C 66	N 8	O 12	0
27	A6	1	Total 86	C 66	N 8	O 12	0
27	A6	1	Total 86	C 66	N 8	O 12	0
27	A7	1	Total 86	C 66	N 8	O 12	0
27	A7	1	Total 86	C 66	N 8	O 12	0
27	A8	1	Total 86	C 66	N 8	O 12	0
27	A8	1	Total 86	C 66	N 8	O 12	0
27	B8	1	Total 43	C 33	N 4	O 6	0
27	Q8	1	Total 43	C 33	N 4	O 6	0
27	A9	1	Total 43	C 33	N 4	O 6	0
27	N9	1	Total 43	C 33	N 4	O 6	0

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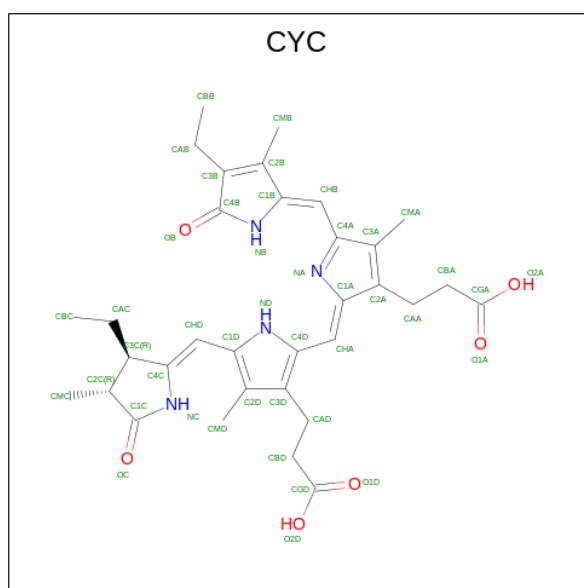
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	AA	1	Total 86	C 66	N 8	O 12	0
27	AA	1	Total 86	C 66	N 8	O 12	0
27	BA	1	Total 43	C 33	N 4	O 6	0
27	QA	1	Total 43	C 33	N 4	O 6	0
27	AB	1	Total 86	C 66	N 8	O 12	0
27	AB	1	Total 86	C 66	N 8	O 12	0
27	KD	1	Total 43	C 33	N 4	O 6	0
27	YD	1	Total 43	C 33	N 4	O 6	0
27	wE	1	Total 43	C 33	N 4	O 6	0
27	xE	1	Total 129	C 99	N 12	O 18	0
27	xE	1	Total 129	C 99	N 12	O 18	0
27	xE	1	Total 129	C 99	N 12	O 18	0
27	yE	1	Total 86	C 66	N 8	O 12	0
27	yE	1	Total 86	C 66	N 8	O 12	0
27	AF	1	Total 86	C 66	N 8	O 12	0
27	AF	1	Total 86	C 66	N 8	O 12	0
27	wG	1	Total 43	C 33	N 4	O 6	0
27	xG	1	Total 129	C 99	N 12	O 18	0
27	xG	1	Total 129	C 99	N 12	O 18	0
27	xG	1	Total 129	C 99	N 12	O 18	0
27	yG	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	yG	1	Total 86	C 66	N 8	O 12	0
27	AI	1	Total 86	C 66	N 8	O 12	0
27	AI	1	Total 86	C 66	N 8	O 12	0
27	AJ	1	Total 43	C 33	N 4	O 6	0
27	NJ	1	Total 43	C 33	N 4	O 6	0

- Molecule 28 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	C2	1	Total 43	C 33	N 4	O 6	0
28	D2	1	Total 43	C 33	N 4	O 6	0
28	E2	1	Total 43	C 33	N 4	O 6	0
28	F2	1	Total 43	C 33	N 4	O 6	0
28	G2	1	Total 43	C 33	N 4	O 6	0
28	H2	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
28	I2	1	Total 43	C 33	N 4	O 6	0
28	J2	1	Total 43	C 33	N 4	O 6	0
28	K2	1	Total 43	C 33	N 4	O 6	0
28	L2	1	Total 43	C 33	N 4	O 6	0
28	M2	1	Total 43	C 33	N 4	O 6	0
28	N2	1	Total 43	C 33	N 4	O 6	0
28	B6	1	Total 86	C 66	N 8	O 12	0
28	B6	1	Total 86	C 66	N 8	O 12	0
28	C6	1	Total 43	C 33	N 4	O 6	0
28	D6	1	Total 43	C 33	N 4	O 6	0
28	E6	1	Total 43	C 33	N 4	O 6	0
28	F6	1	Total 43	C 33	N 4	O 6	0
28	G6	1	Total 43	C 33	N 4	O 6	0
28	H6	1	Total 43	C 33	N 4	O 6	0
28	I6	1	Total 43	C 33	N 4	O 6	0
28	K6	1	Total 43	C 33	N 4	O 6	0
28	L6	1	Total 43	C 33	N 4	O 6	0
28	M6	1	Total 43	C 33	N 4	O 6	0
28	C7	1	Total 43	C 33	N 4	O 6	0
28	D7	1	Total 43	C 33	N 4	O 6	0
28	E7	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	F7	1	43	33	4	6	0
28	G7	1	43	33	4	6	0
28	H7	1	43	33	4	6	0
28	I7	1	43	33	4	6	0
28	J7	1	86	66	8	12	0
28	J7	1	86	66	8	12	0
28	K7	1	43	33	4	6	0
28	L7	1	43	33	4	6	0
28	N7	1	43	33	4	6	0
28	BB	1	43	33	4	6	0
28	CB	1	43	33	4	6	0
28	DB	1	43	33	4	6	0
28	EB	1	43	33	4	6	0
28	FB	1	43	33	4	6	0
28	GB	1	43	33	4	6	0
28	HB	1	43	33	4	6	0
28	IB	1	43	33	4	6	0
28	KB	1	43	33	4	6	0
28	LB	1	43	33	4	6	0
28	MB	1	43	33	4	6	0
28	NB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf	
28	CF	1	Total	C	N	O	0	
			43	33	4	6		
28	DF	1	Total	C	N	O	0	
			86	66	8	12		
28	DF	1	Total	C	N	O	0	
			86	66	8	12		
28	EF	1	Total	C	N	O	0	
			43	33	4	6		
28	FF	1	Total	C	N	O	0	
			43	33	4	6		
28	HF	1	Total	C	N	O	0	
			43	33	4	6		
28	IF	1	Total	C	N	O	0	
			43	33	4	6		
28	JF	1	Total	C	N	O	0	
			86	66	8	12		
28	JF	1	Total	C	N	O	0	
			86	66	8	12		
28	KF	1	Total	C	N	O	0	
			43	33	4	6		
28	LF	1	Total	C	N	O	0	
			43	33	4	6		
28	NF	1	Total	C	N	O	0	
			43	33	4	6		
28	AH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	CH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	FH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	EH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	GH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	IH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	JH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	KH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	LH	1	Total	C	H	N	O	0
			81	33	38	4	6	

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Mol	Chain	Residues	Atoms					AltConf
28	MH	1	Total 81	C 33	H 38	N 4	O 6	0
28	NH	1	Total 81	C 33	H 38	N 4	O 6	0
28	OH	1	Total 81	C 33	H 38	N 4	O 6	0
28	PH	1	Total 81	C 33	H 38	N 4	O 6	0
28	QH	1	Total 81	C 33	H 38	N 4	O 6	0
28	RH	1	Total 81	C 33	H 38	N 4	O 6	0
28	SH	1	Total 81	C 33	H 38	N 4	O 6	0
28	TH	1	Total 81	C 33	H 38	N 4	O 6	0
28	UH	1	Total 81	C 33	H 38	N 4	O 6	0
28	VH	1	Total 81	C 33	H 38	N 4	O 6	0
28	WH	1	Total 81	C 33	H 38	N 4	O 6	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	cH	1	Total 81	C 33	H 38	N 4	O 6	0
28	dH	1	Total 81	C 33	H 38	N 4	O 6	0
28	eH	1	Total 81	C 33	H 38	N 4	O 6	0
28	fH	1	Total 81	C 33	H 38	N 4	O 6	0
28	gH	1	Total 81	C 33	H 38	N 4	O 6	0
28	hH	1	Total 81	C 33	H 38	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
28	iH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	jH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	kH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	lH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	mH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	nH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	oH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	pH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	qH	1	Total	C	H	N	O	0
			162	66	76	8	12	
28	qH	1	Total	C	H	N	O	0
			162	66	76	8	12	
28	rH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	sH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	tH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	uH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	vH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	wH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	yH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	1H	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	CI	1	Total	C	N	O		0
			43	33	4	6		
28	DI	1	Total	C	N	O		0
			43	33	4	6		
28	EI	1	Total	C	N	O		0
			43	33	4	6		

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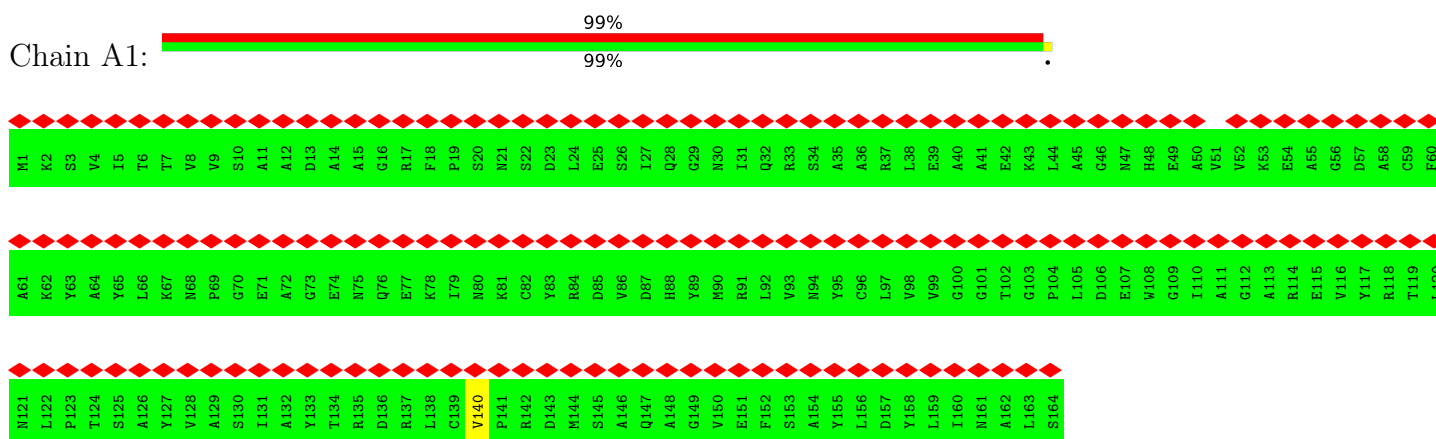
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
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28	GI	1	Total 43	C 33	N 4	O 6	0
28	HI	1	Total 43	C 33	N 4	O 6	0
28	II	1	Total 43	C 33	N 4	O 6	0
28	JI	1	Total 43	C 33	N 4	O 6	0
28	KI	1	Total 43	C 33	N 4	O 6	0
28	LI	1	Total 43	C 33	N 4	O 6	0
28	MI	1	Total 43	C 33	N 4	O 6	0
28	NI	1	Total 43	C 33	N 4	O 6	0

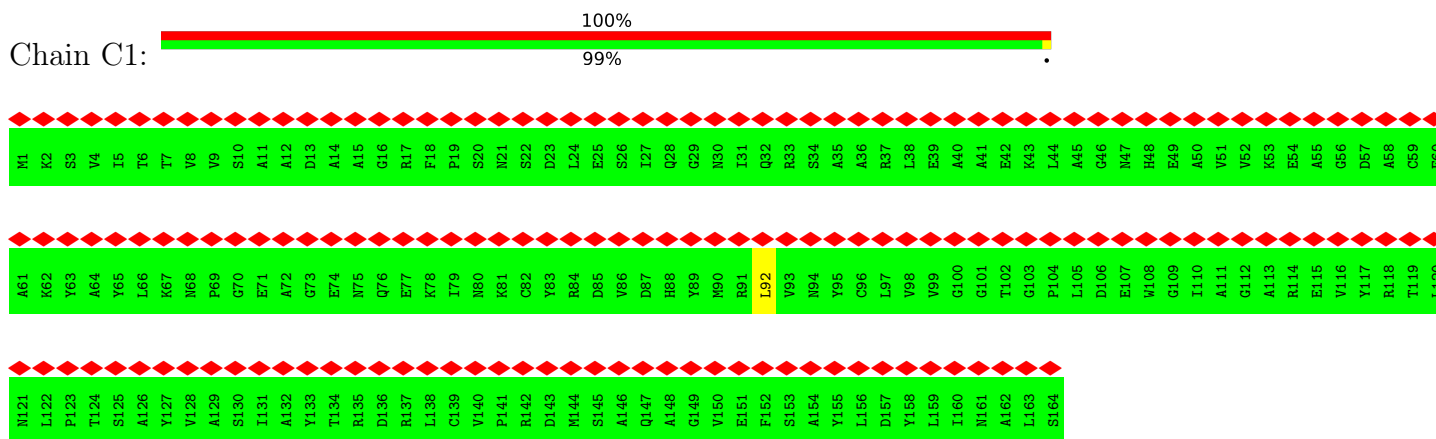
3 Residue-property plots

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

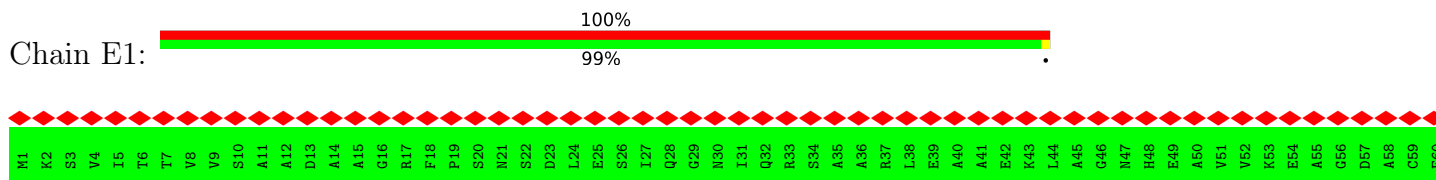
- Molecule 1: Phycoerythrin alpha subunit

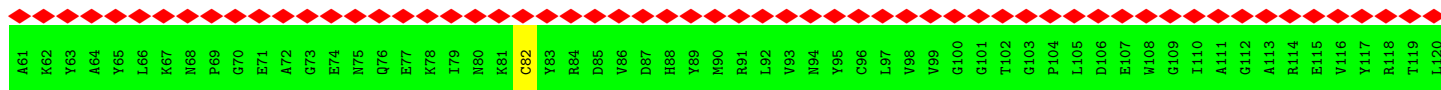


- Molecule 1: Phycoerythrin alpha subunit

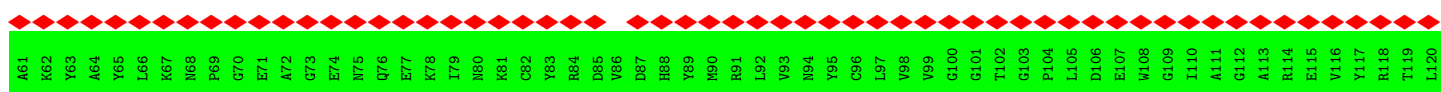
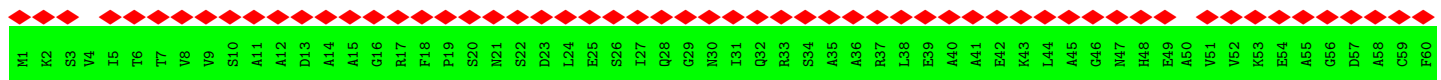


- Molecule 1: Phycoerythrin alpha subunit

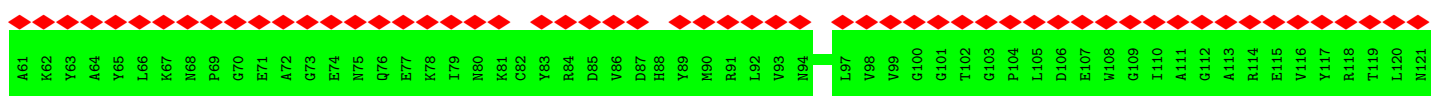
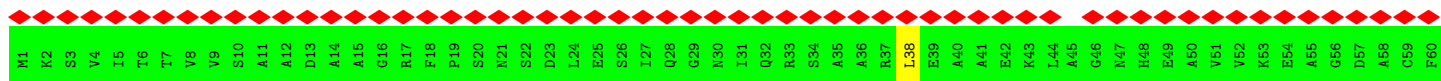




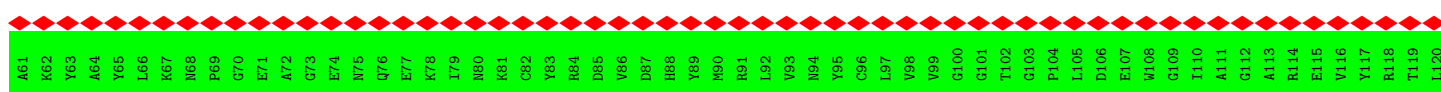
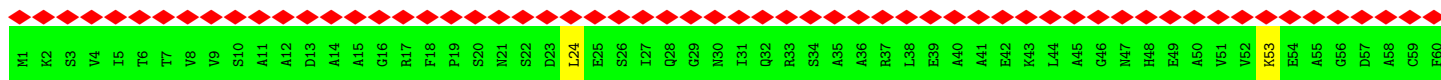
• Molecule 1: Phycoerythrin alpha subunit



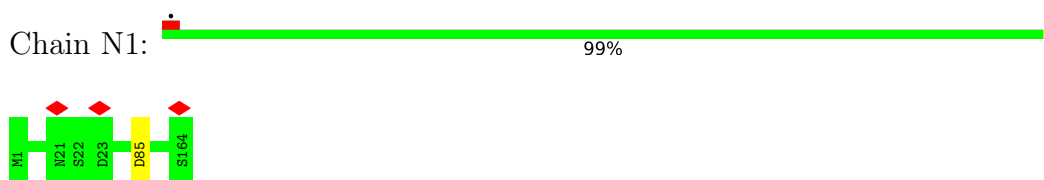
• Molecule 1: Phycoerythrin alpha subunit



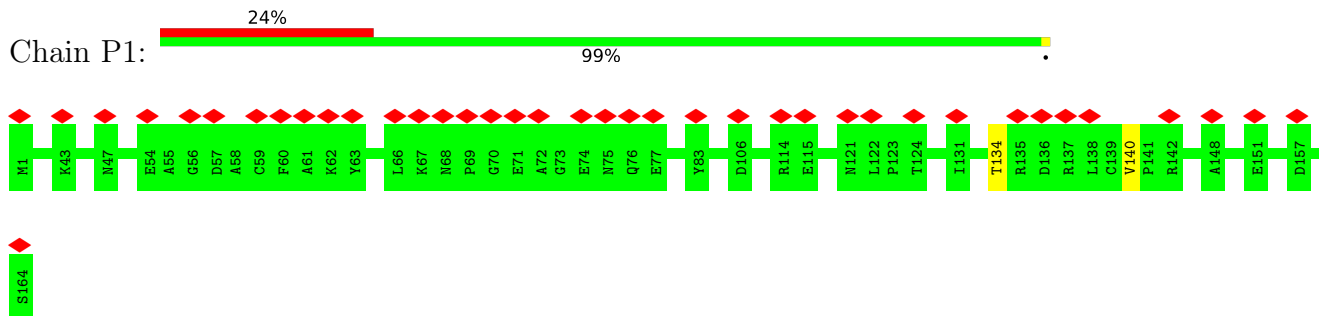
• Molecule 1: Phycoerythrin alpha subunit



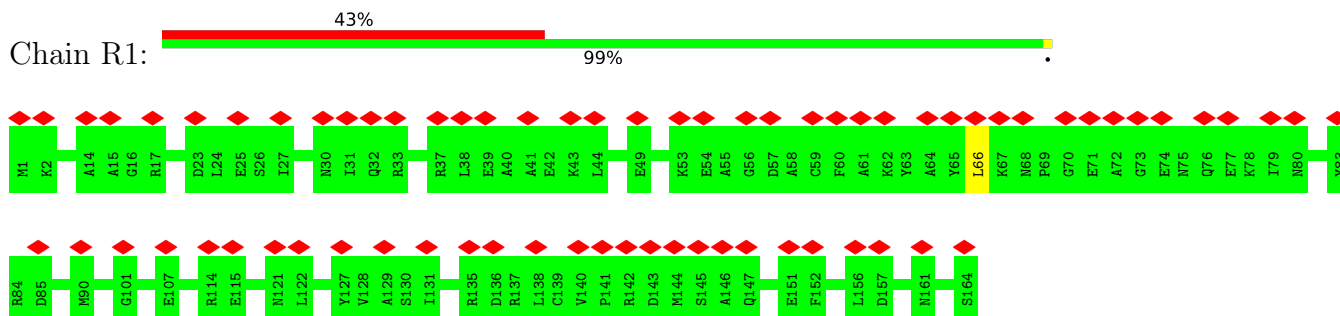
- Molecule 1: Phycoerythrin alpha subunit



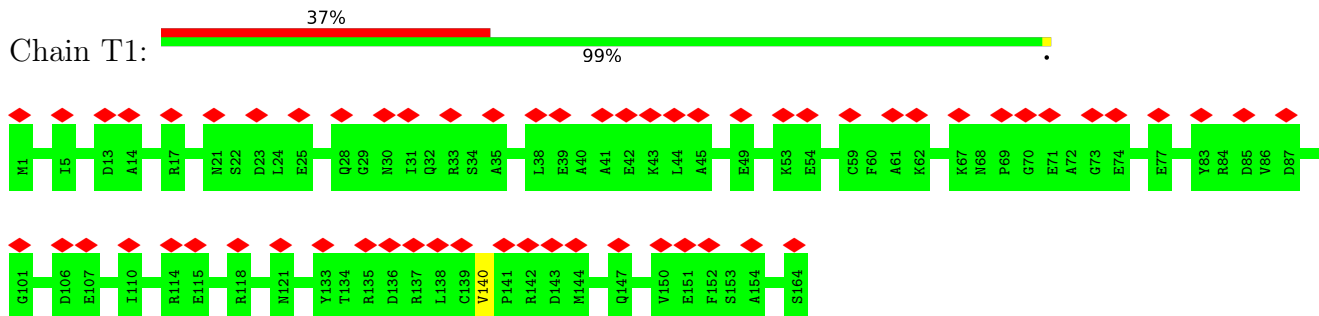
- Molecule 1: Phycoerythrin alpha subunit



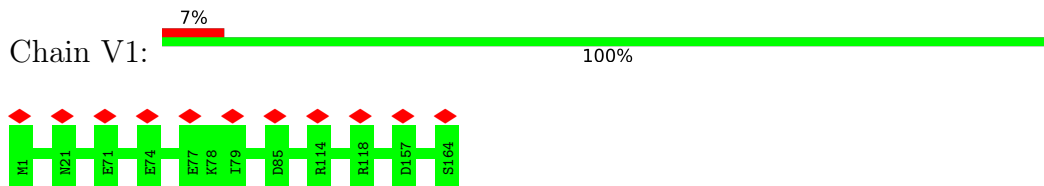
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit



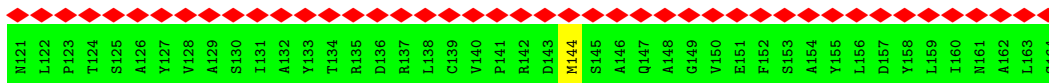
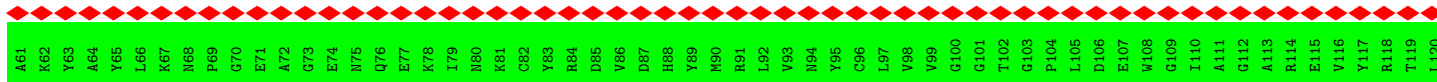
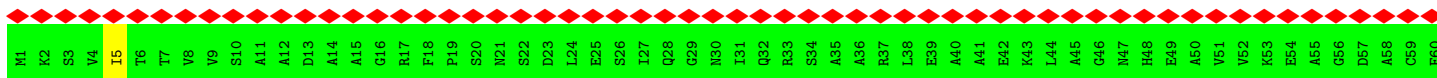
- Molecule 1: Phycoerythrin alpha subunit

Chain X1:  99%



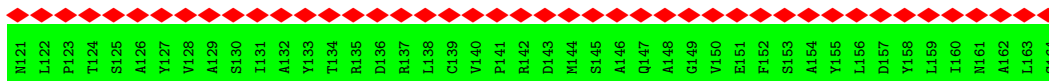
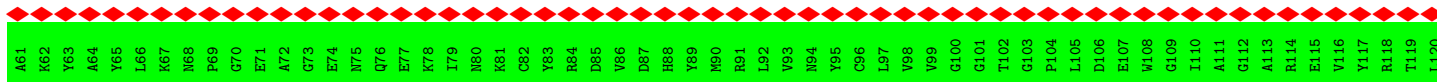
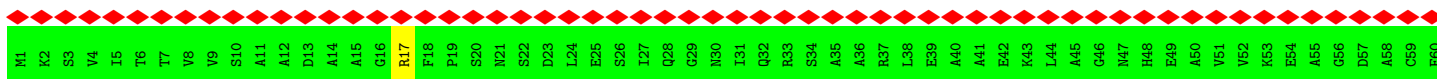
- Molecule 1: Phycoerythrin alpha subunit

Chain c1:  100%
99%



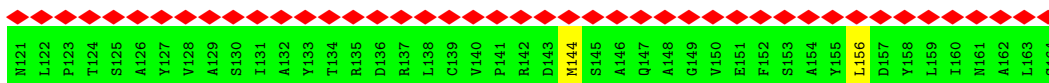
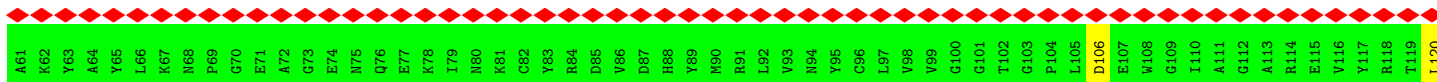
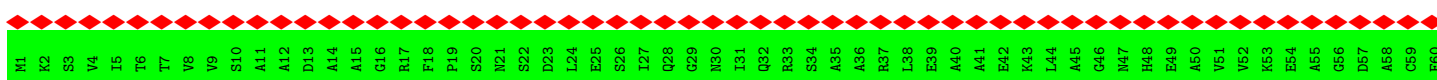
- Molecule 1: Phycoerythrin alpha subunit

Chain e1:  100%
99%

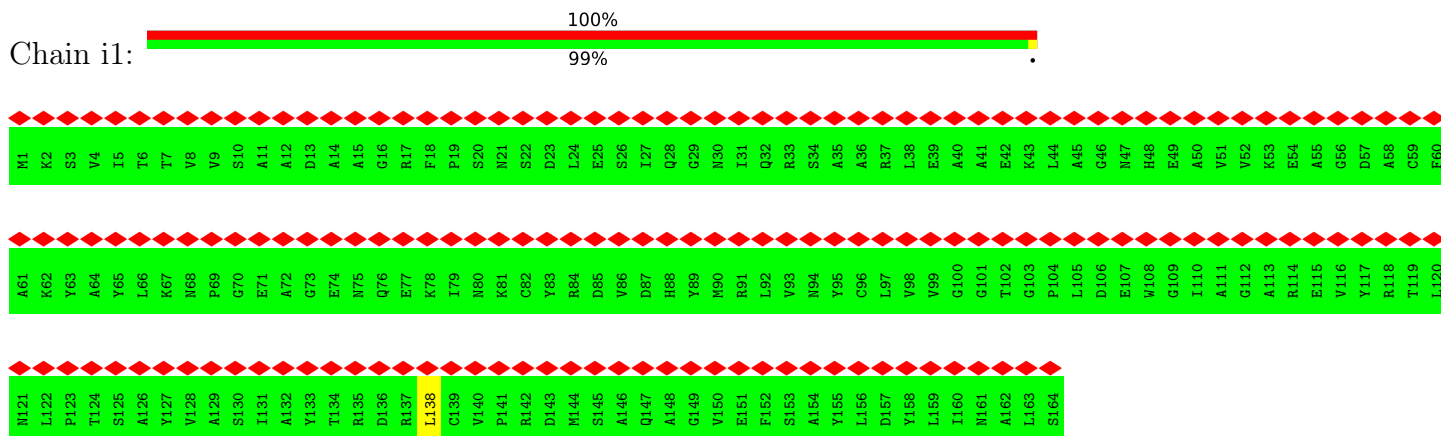


- Molecule 1: Phycoerythrin alpha subunit

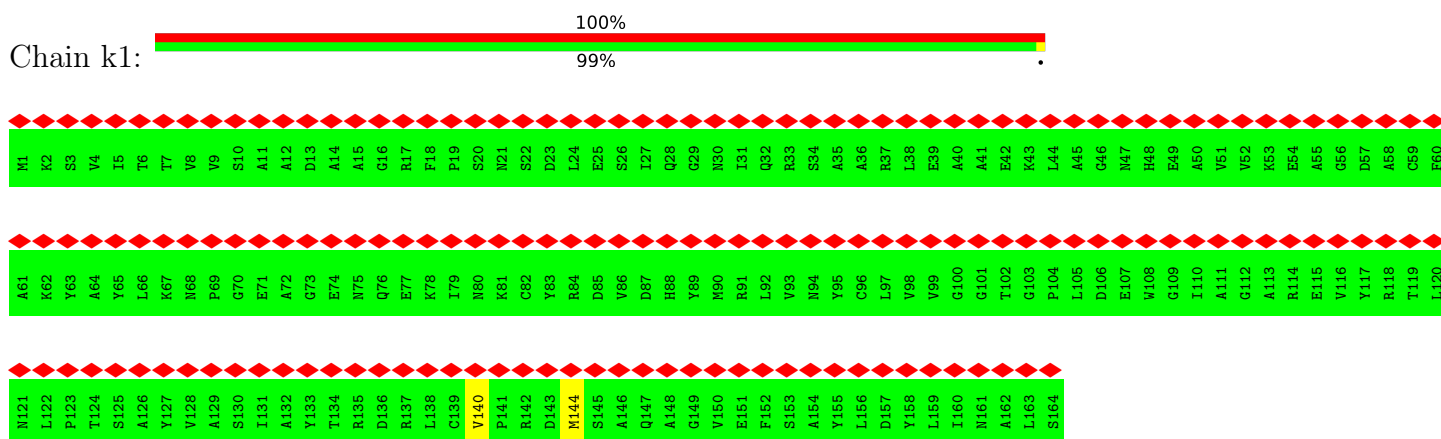
Chain g1:  100%
98%



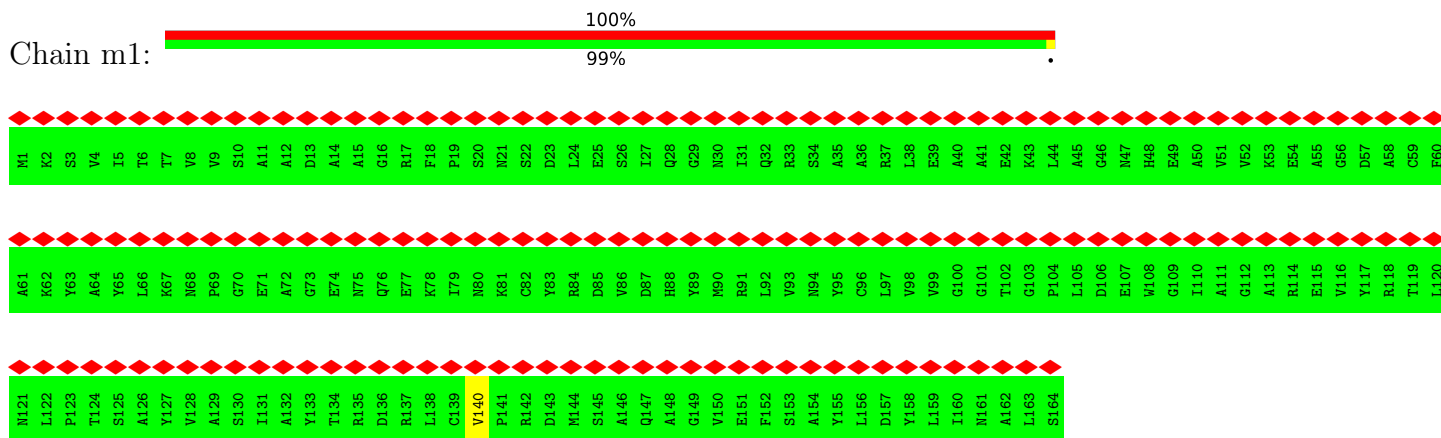
- Molecule 1: Phycoerythrin alpha subunit



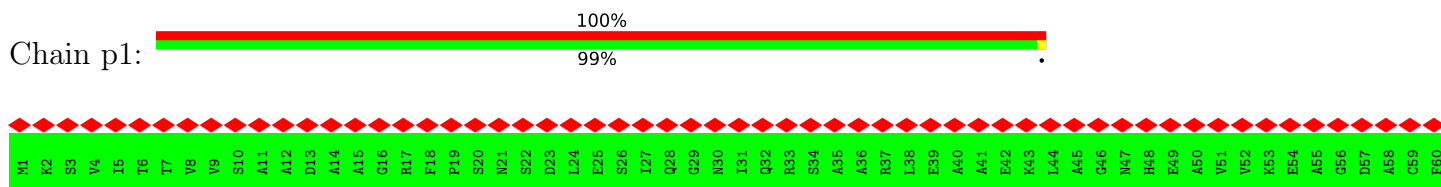
• Molecule 1: Phycoerythrin alpha subunit

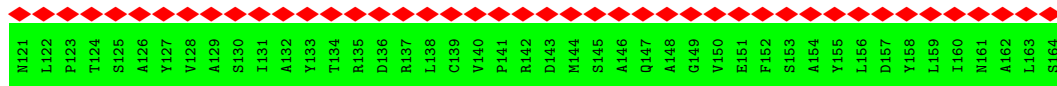
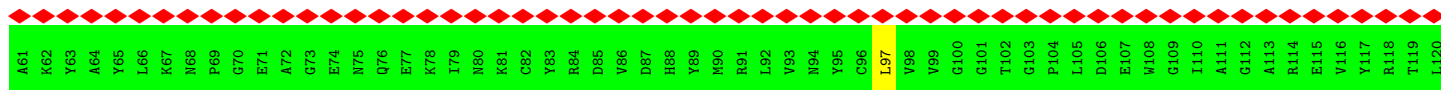


• Molecule 1: Phycoerythrin alpha subunit

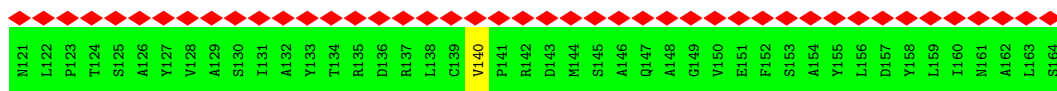
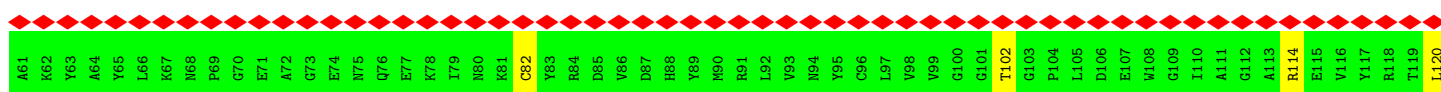
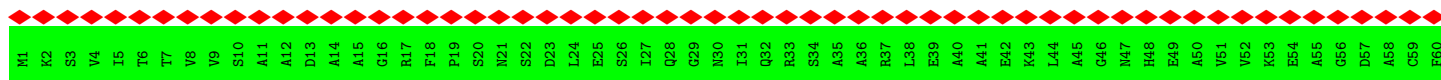


• Molecule 1: Phycoerythrin alpha subunit

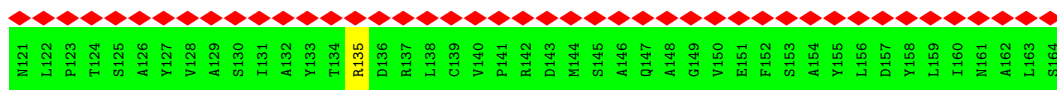
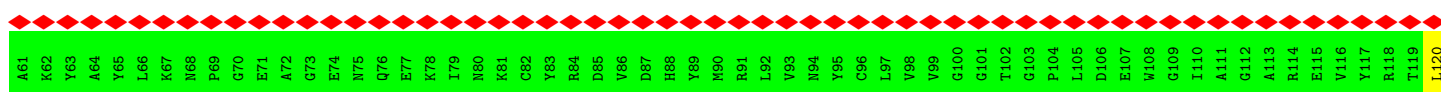
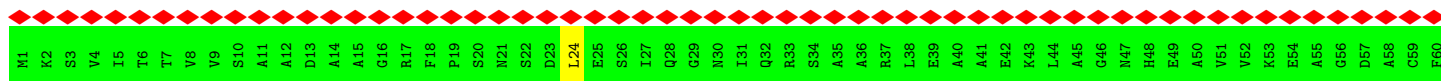




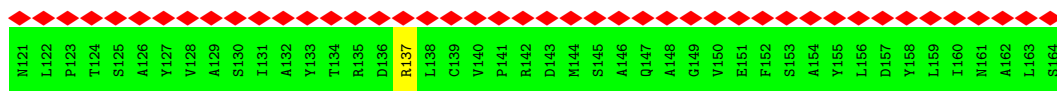
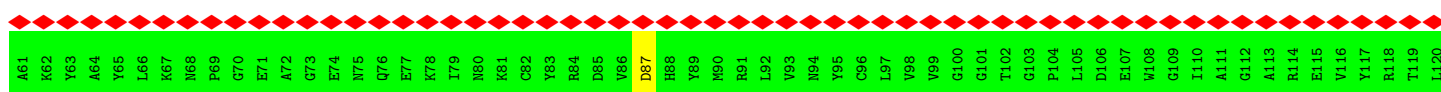
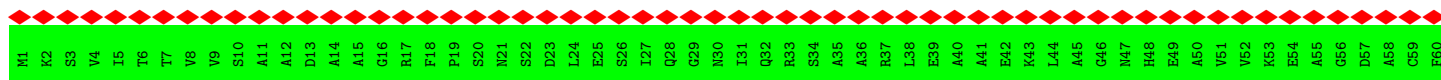
• Molecule 1: Phycoerythrin alpha subunit



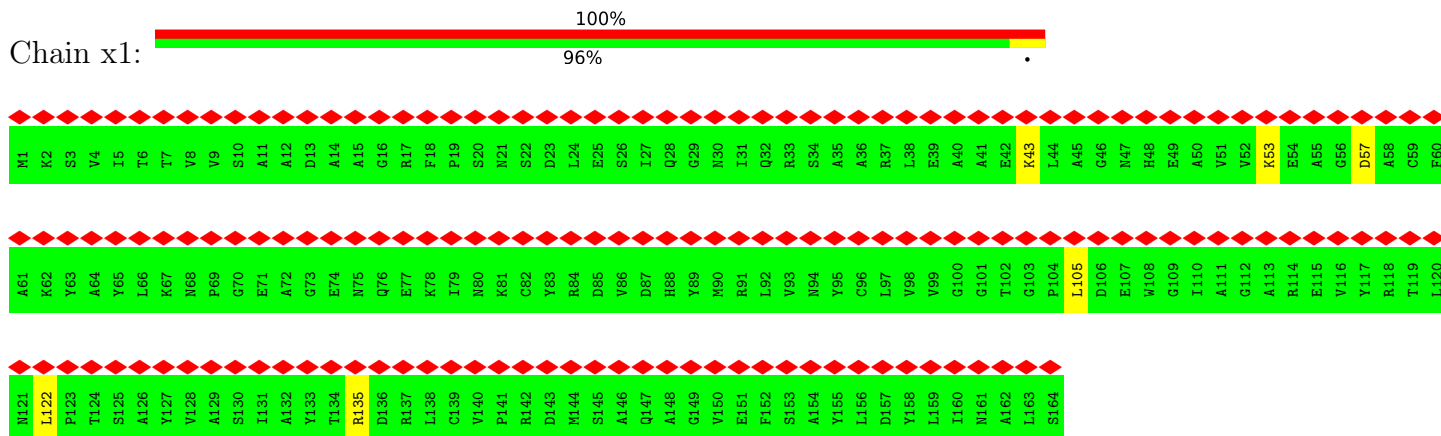
• Molecule 1: Phycoerythrin alpha subunit



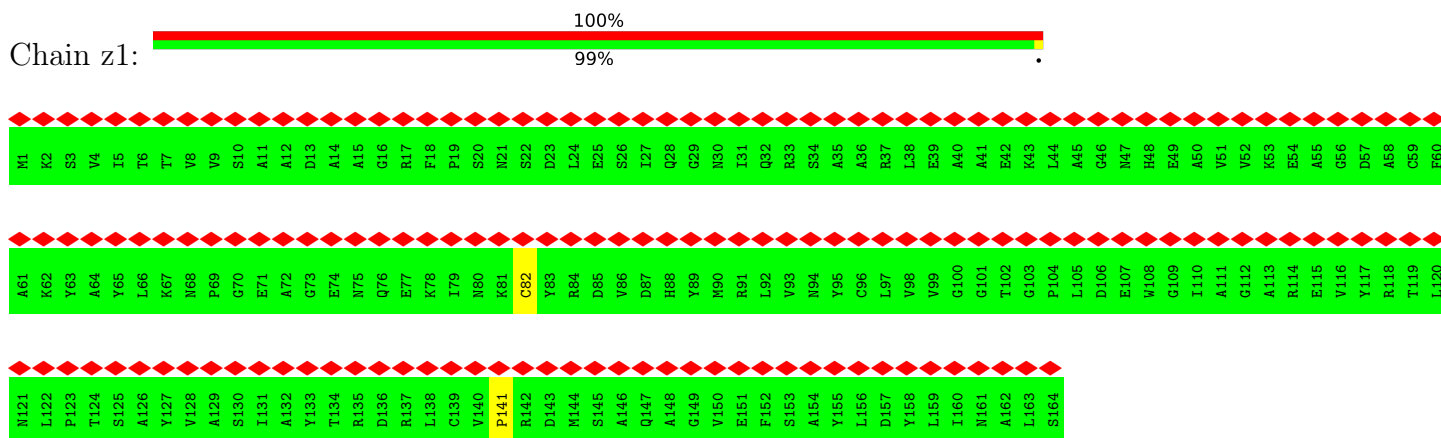
• Molecule 1: Phycoerythrin alpha subunit



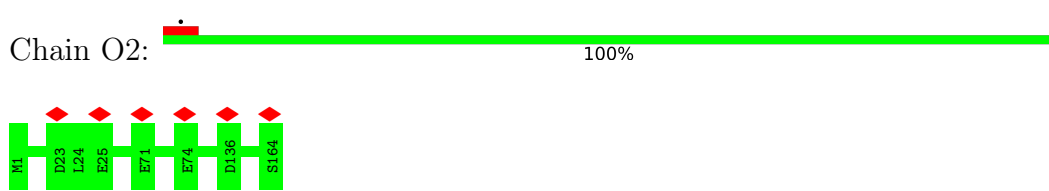
• Molecule 1: Phycoerythrin alpha subunit



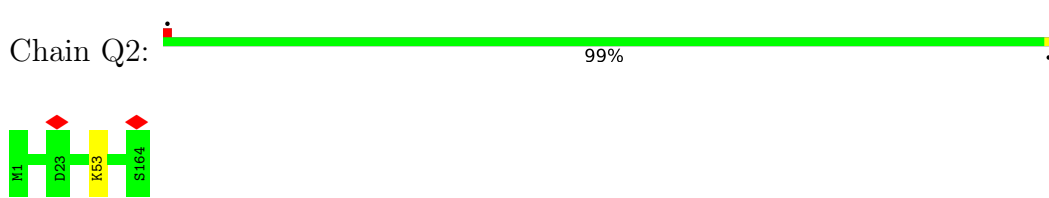
• Molecule 1: Phycoerythrin alpha subunit



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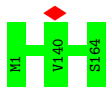


• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit





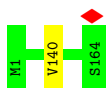
- Molecule 1: Phycoerythrin alpha subunit

Chain U2: 100%

There are no outlier residues recorded for this chain.

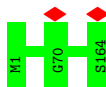
- Molecule 1: Phycoerythrin alpha subunit

Chain W2: 99%



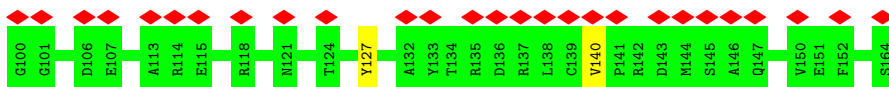
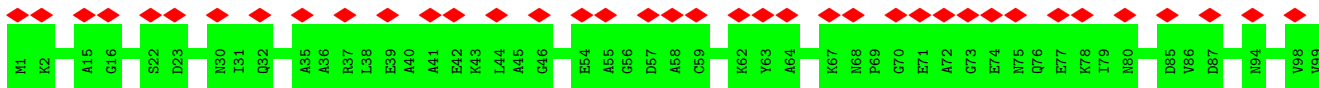
- Molecule 1: Phycoerythrin alpha subunit

Chain Z2: 100%



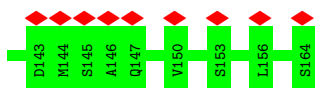
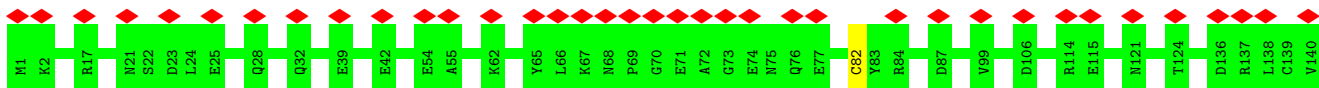
- Molecule 1: Phycoerythrin alpha subunit

Chain b2: 40% 99%



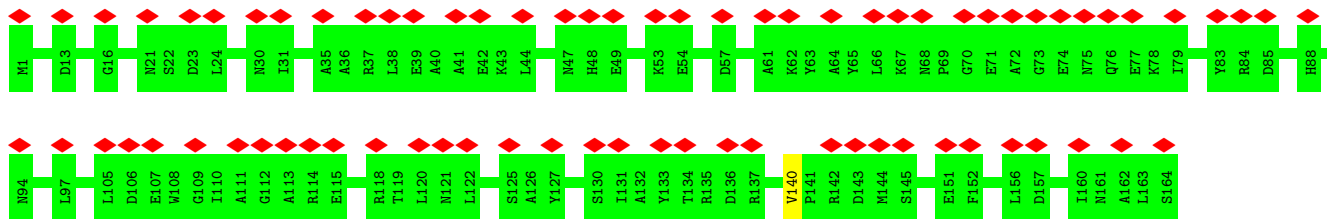
- Molecule 1: Phycoerythrin alpha subunit

Chain d2: 28% 99%

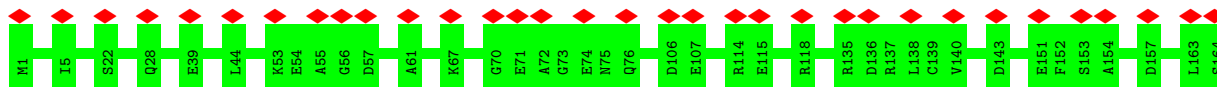


- Molecule 1: Phycoerythrin alpha subunit

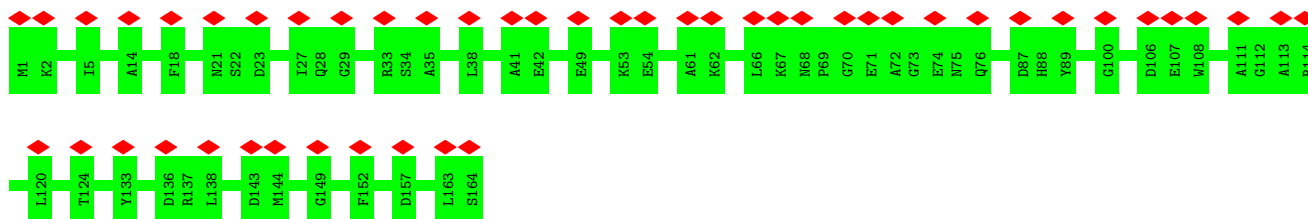
Chain f2: 45% 99%



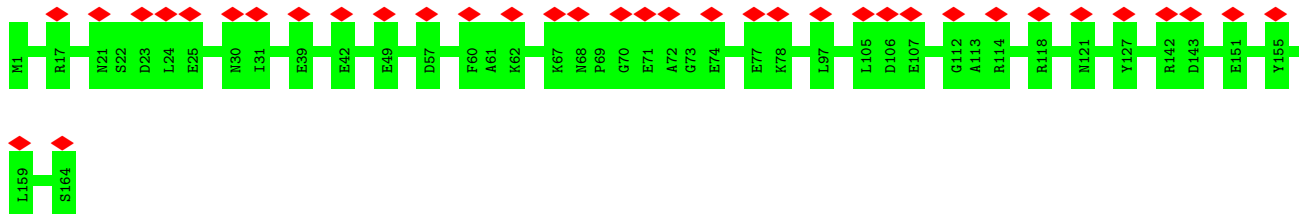
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

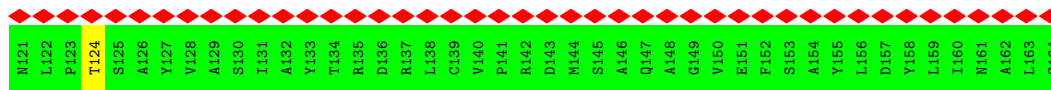


• Molecule 1: Phycoerythrin alpha subunit

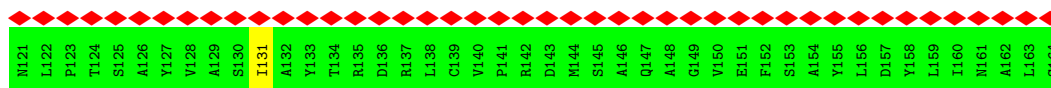
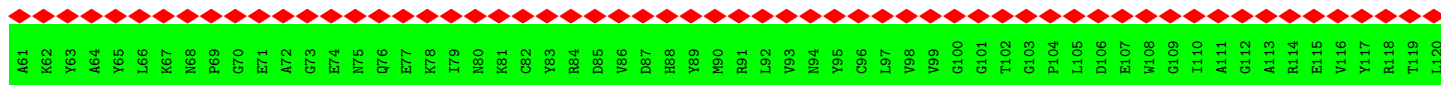
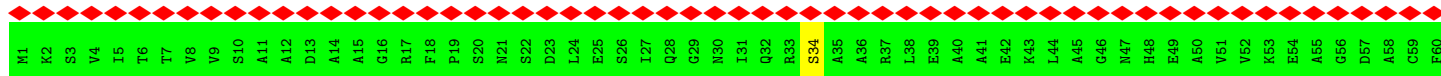


• Molecule 1: Phycoerythrin alpha subunit

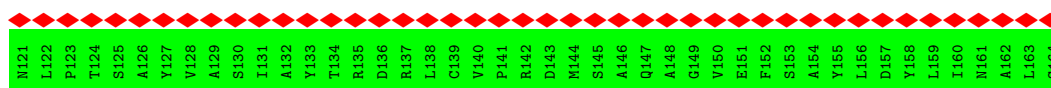
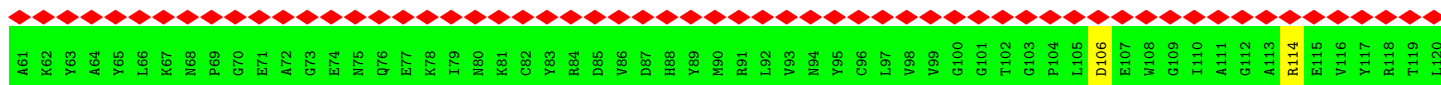
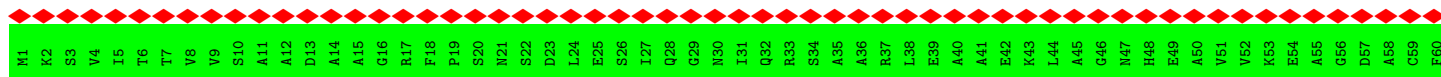




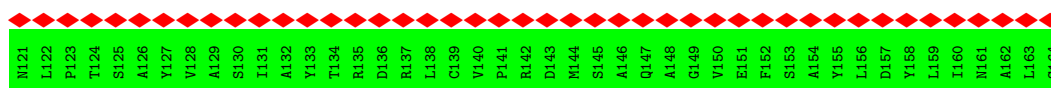
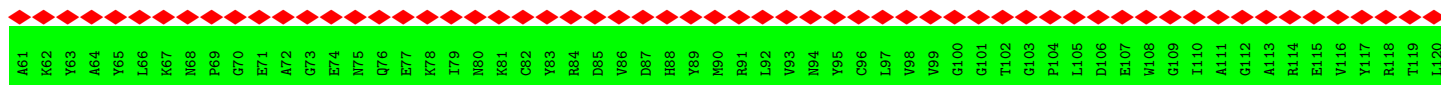
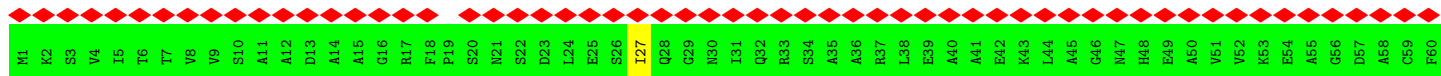
• Molecule 1: Phycoerythrin alpha subunit



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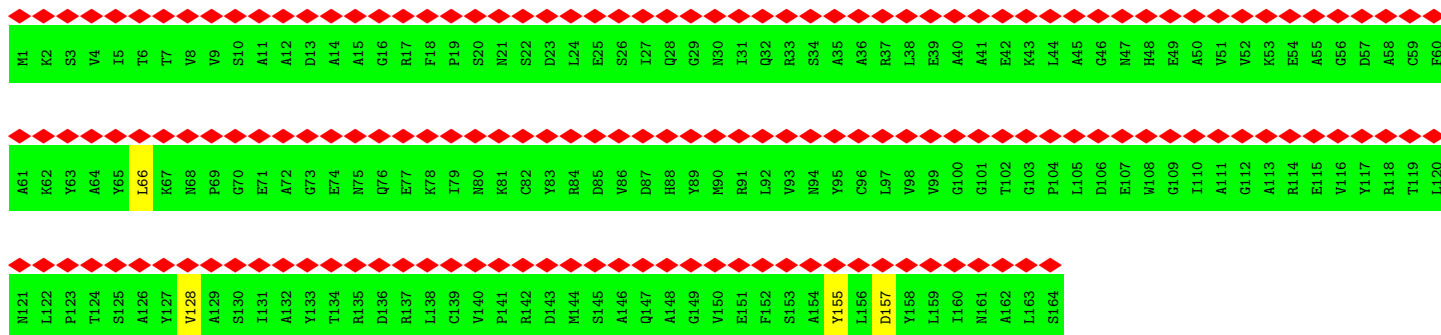


• Molecule 1: Phycoerythrin alpha subunit

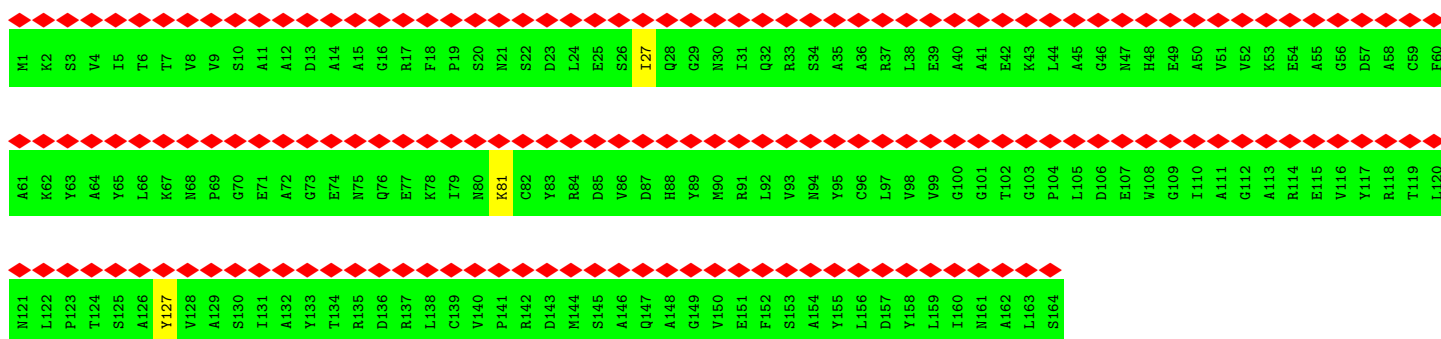


• Molecule 1: Phycoerythrin alpha subunit

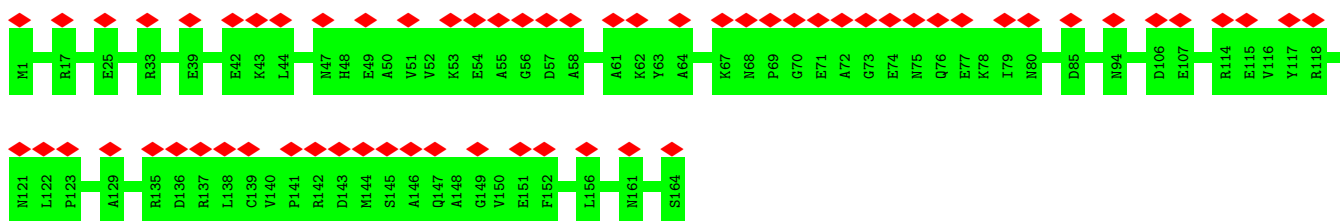
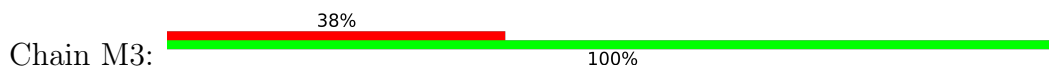




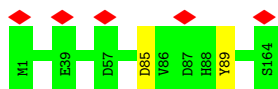
• Molecule 1: Phycoerythrin alpha subunit



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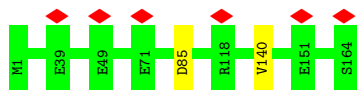


• Molecule 1: Phycoerythrin alpha subunit



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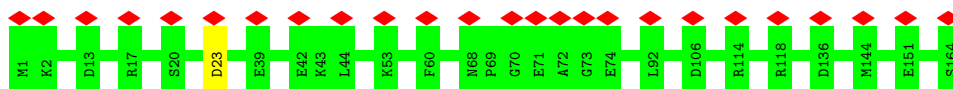




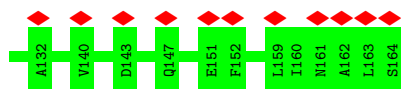
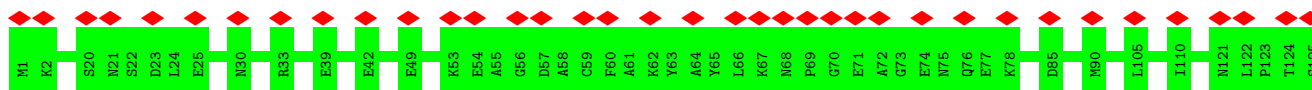
• Molecule 1: Phycoerythrin alpha subunit



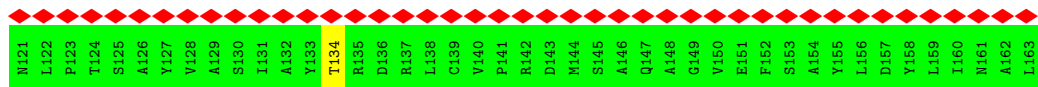
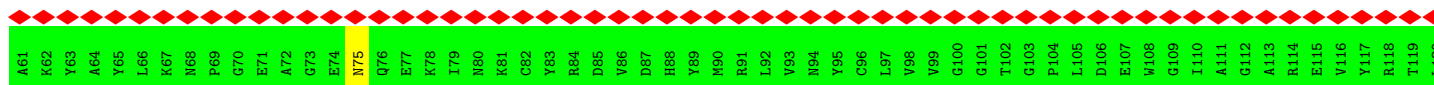
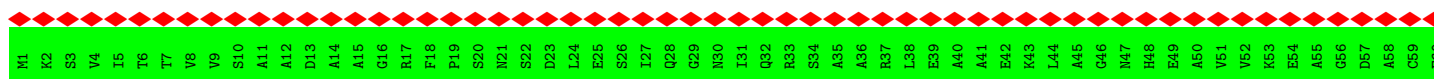
• Molecule 1: Phycoerythrin alpha subunit



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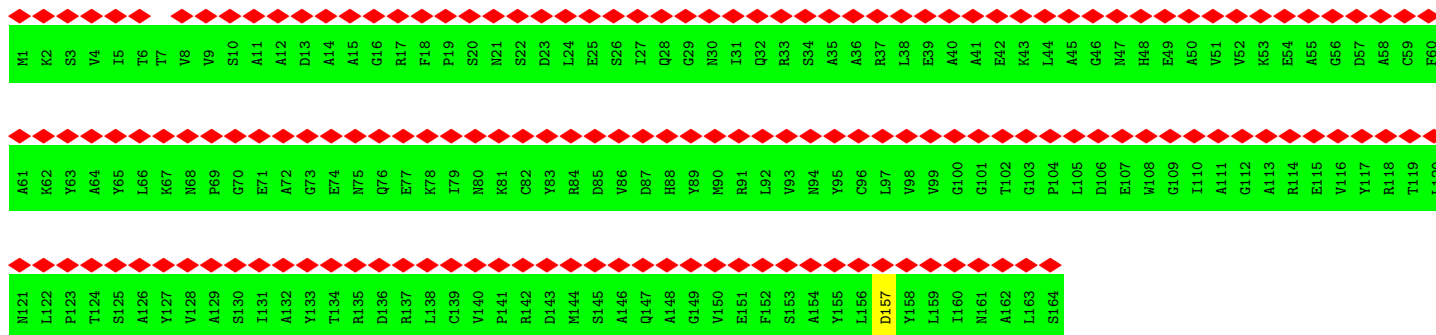


• Molecule 1: Phycoerythrin alpha subunit

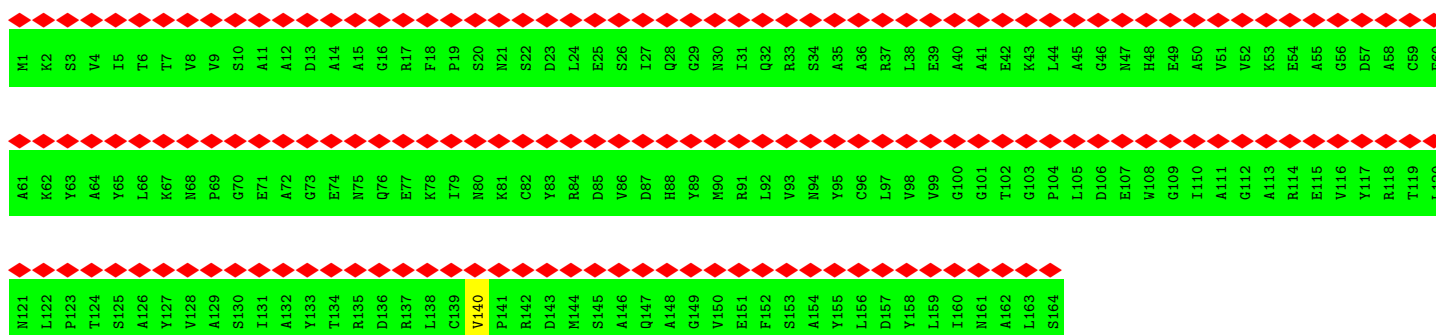


• Molecule 1: Phycoerythrin alpha subunit

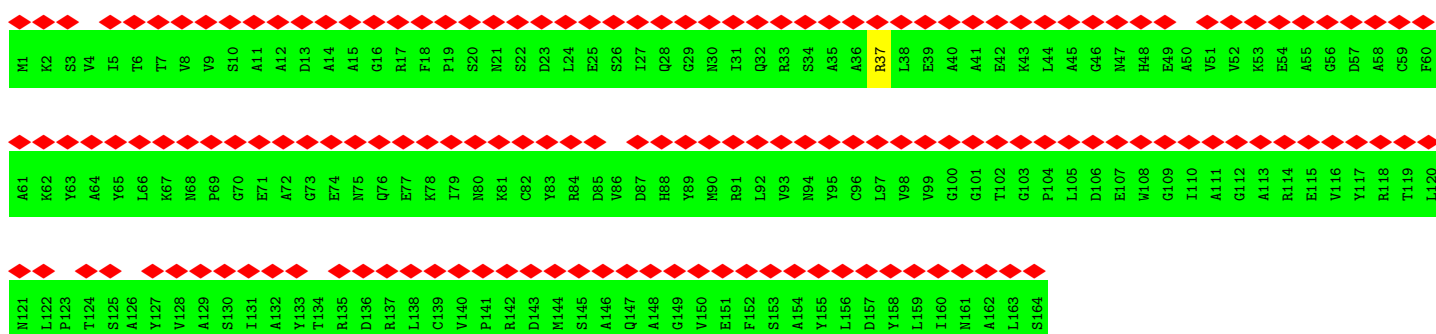




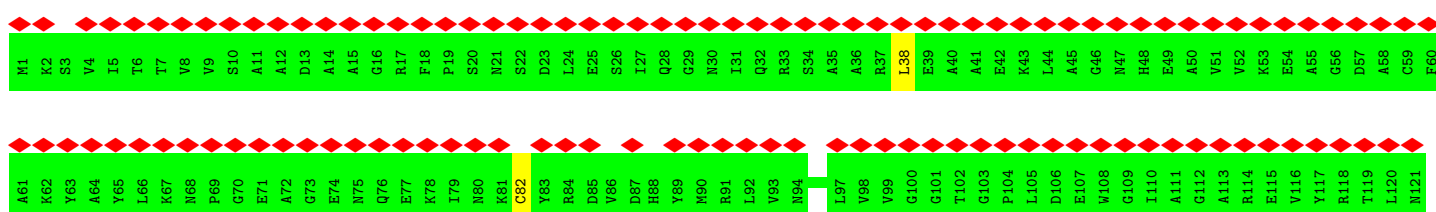
• Molecule 1: Phycoerythrin alpha subunit

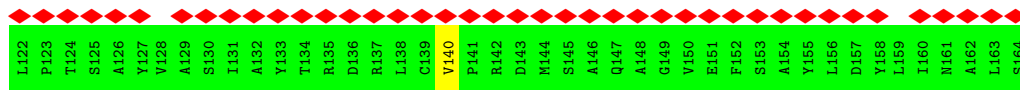


• Molecule 1: Phycoerythrin alpha subunit

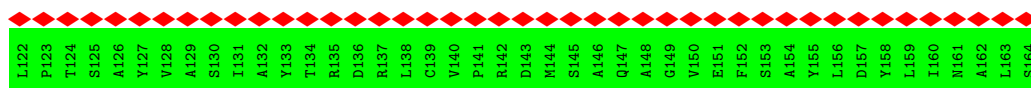
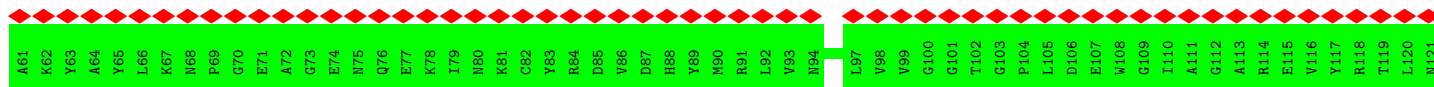
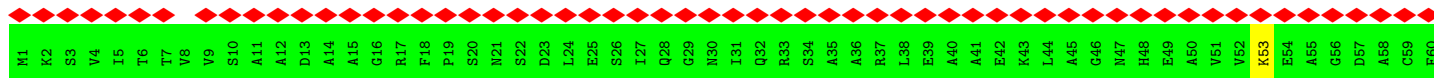


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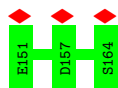
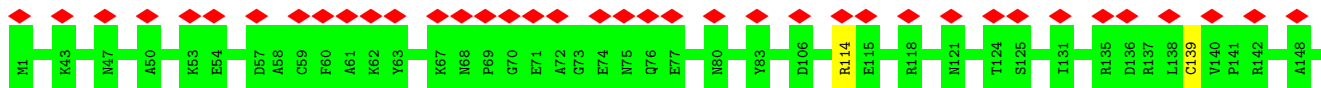
• Molecule 1: Phycoerythrin alpha subunit



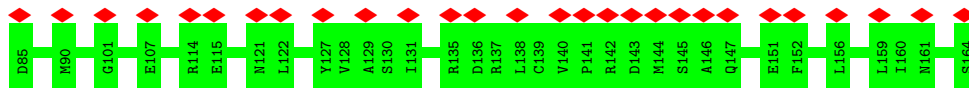
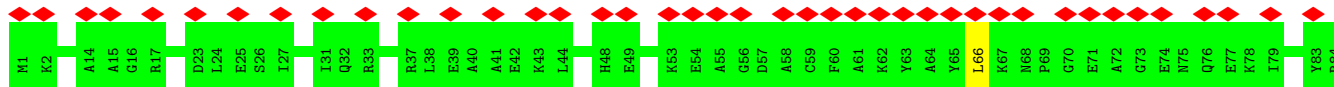
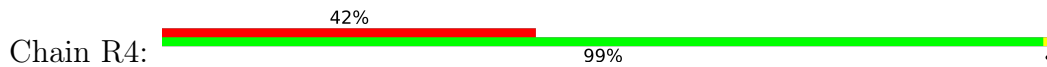
• Molecule 1: Phycoerythrin alpha subunit



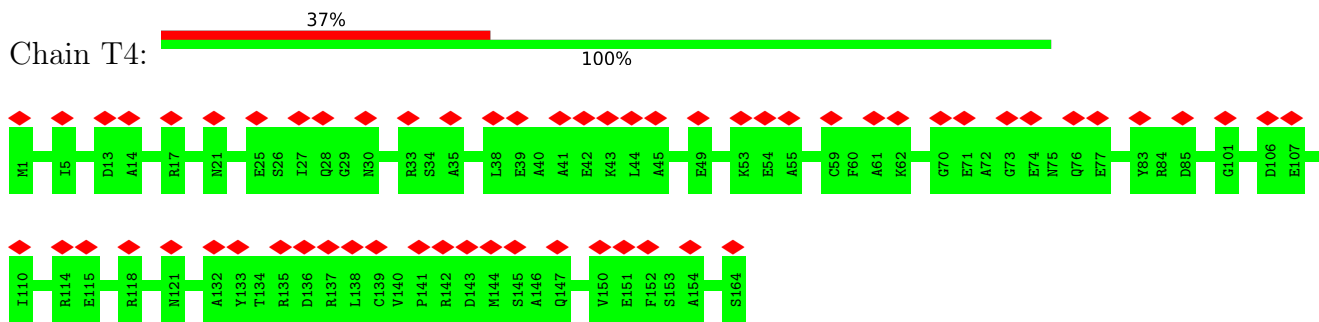
• Molecule 1: Phycoerythrin alpha subunit



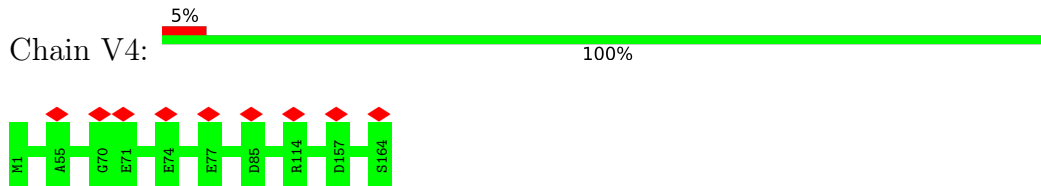
• Molecule 1: Phycoerythrin alpha subunit



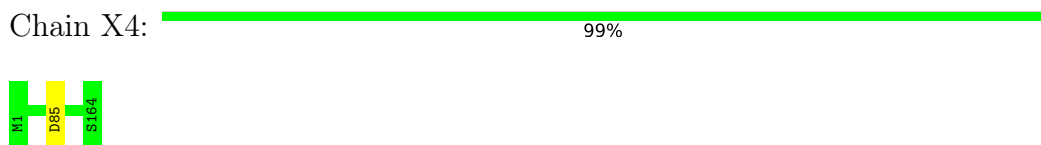
• Molecule 1: Phycoerythrin alpha subunit



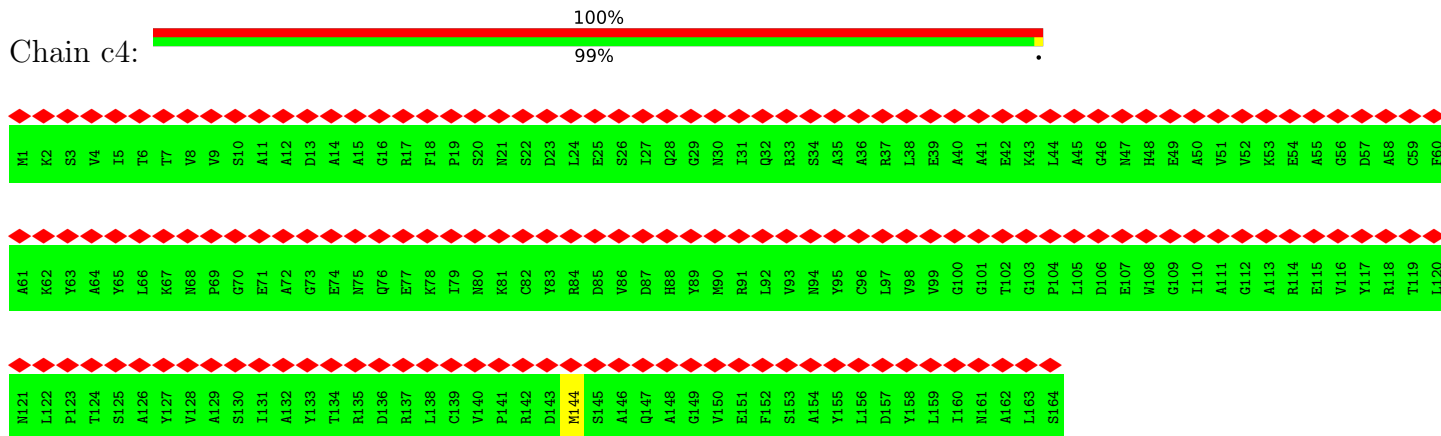
• Molecule 1: Phycoerythrin alpha subunit



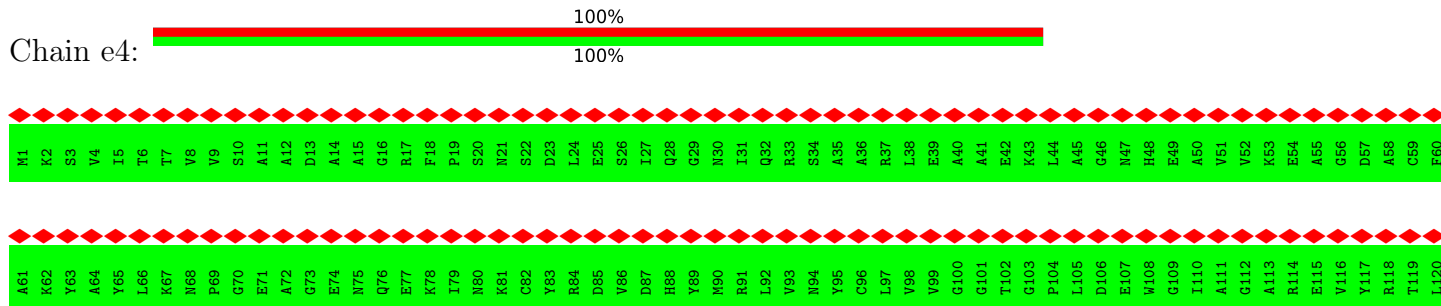
• Molecule 1: Phycoerythrin alpha subunit

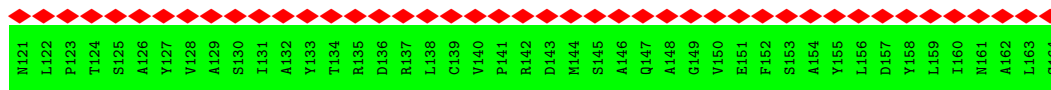


• Molecule 1: Phycoerythrin alpha subunit

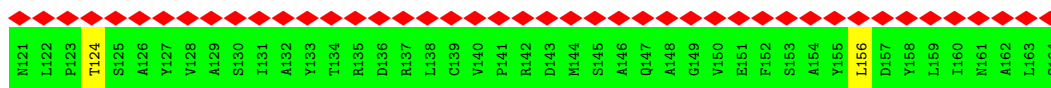
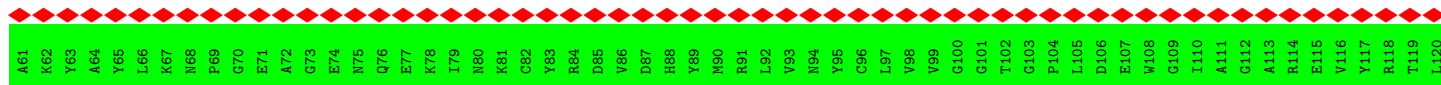


• Molecule 1: Phycoerythrin alpha subunit

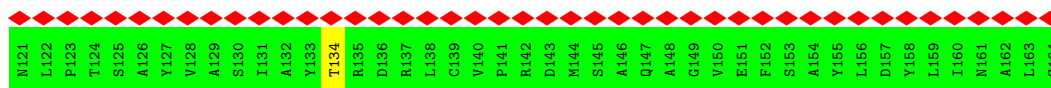
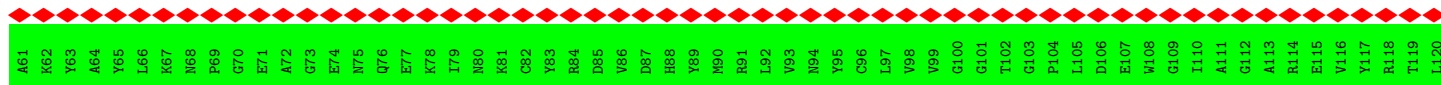
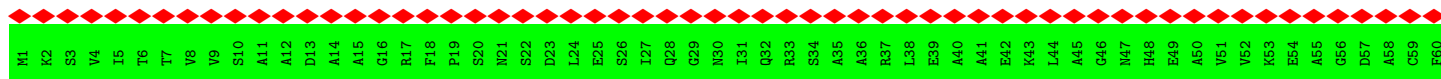




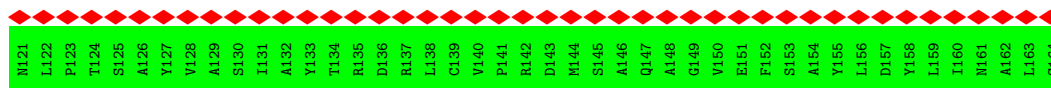
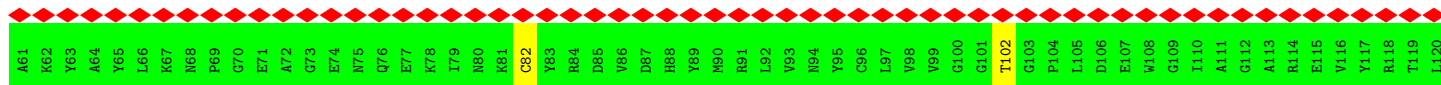
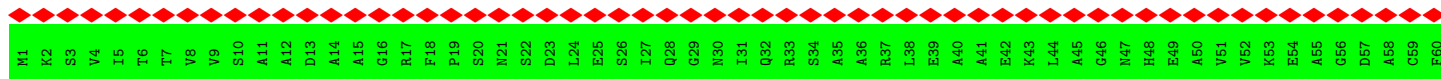
• Molecule 1: Phycoerythrin alpha subunit



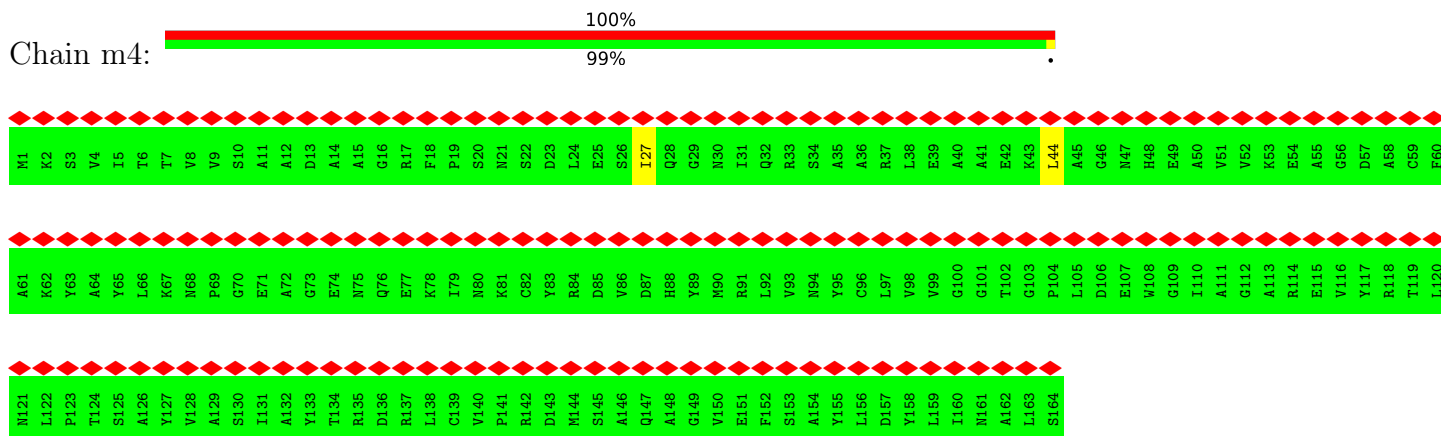
• Molecule 1: Phycoerythrin alpha subunit



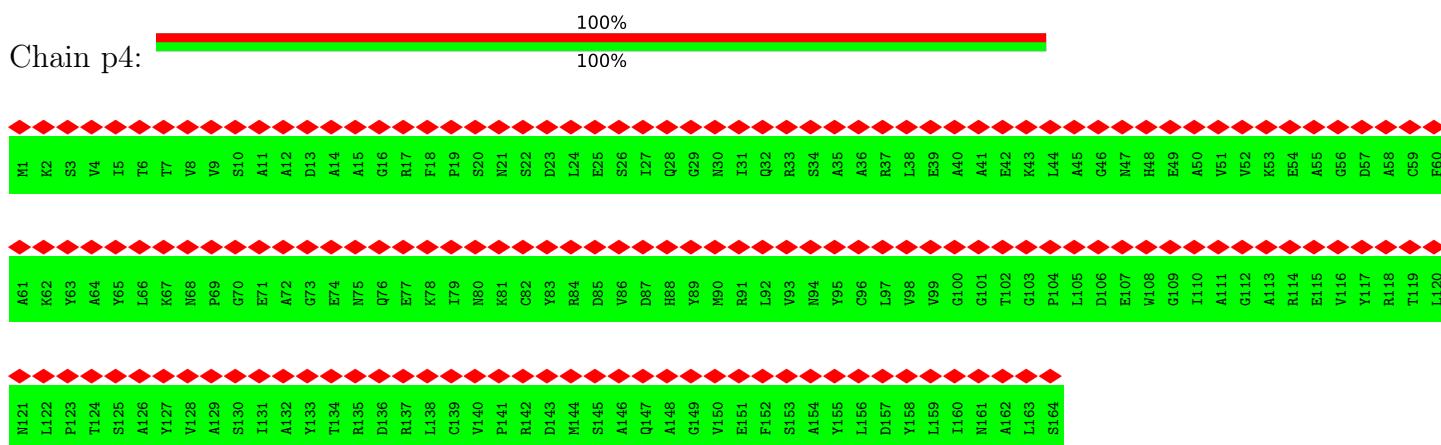
• Molecule 1: Phycoerythrin alpha subunit



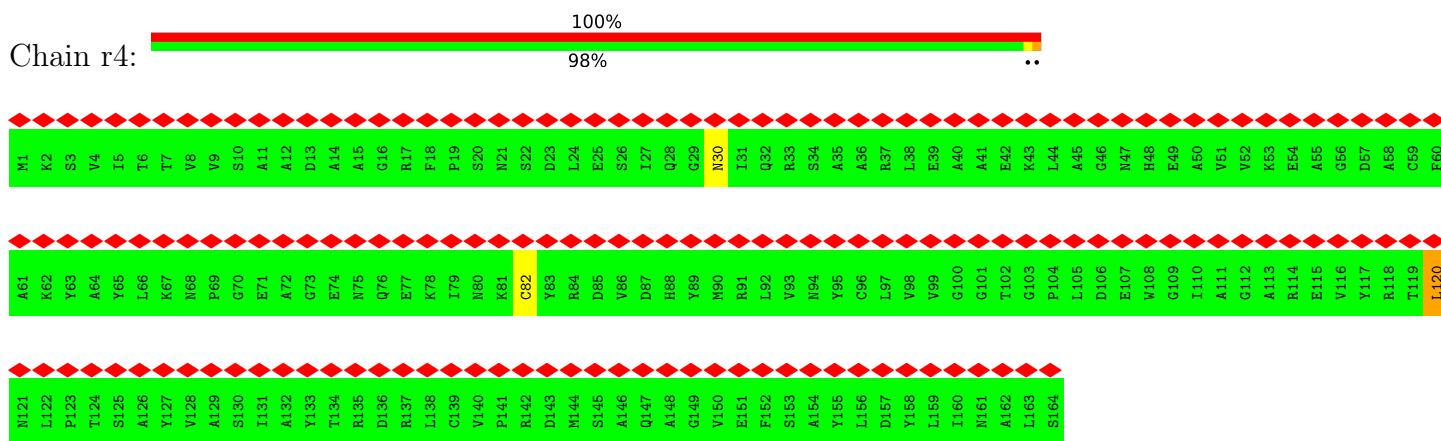
• Molecule 1: Phycoerythrin alpha subunit



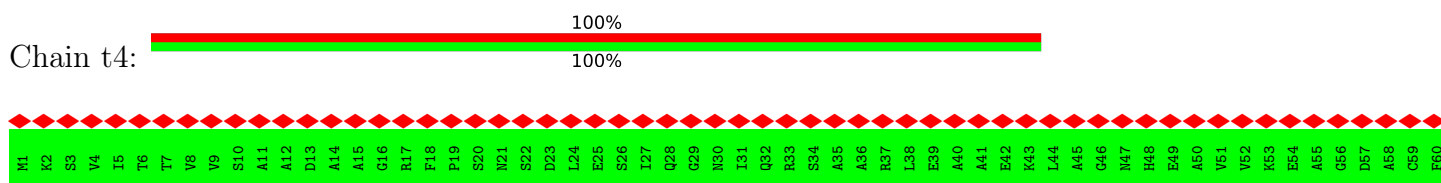
• Molecule 1: Phycoerythrin alpha subunit

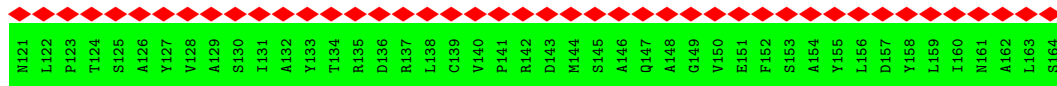
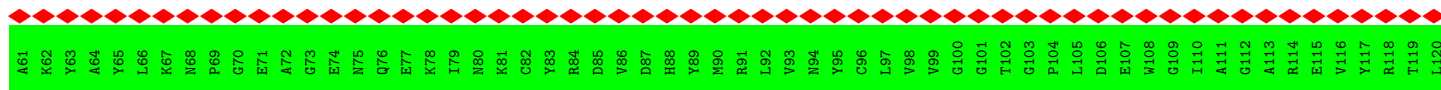


• Molecule 1: Phycoerythrin alpha subunit

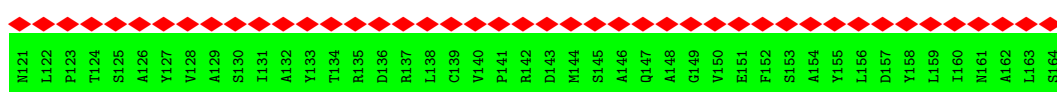
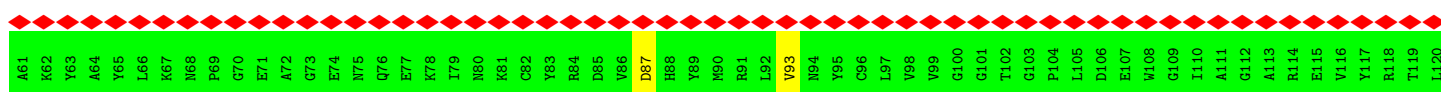
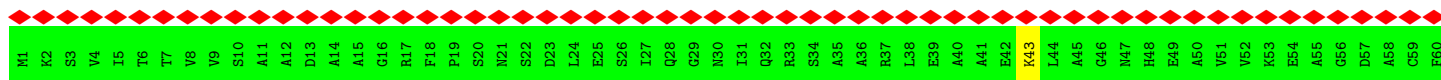


• Molecule 1: Phycoerythrin alpha subunit

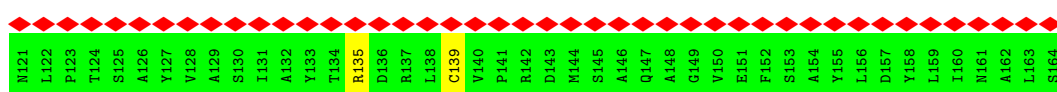
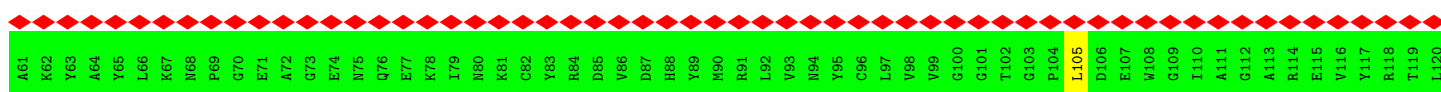
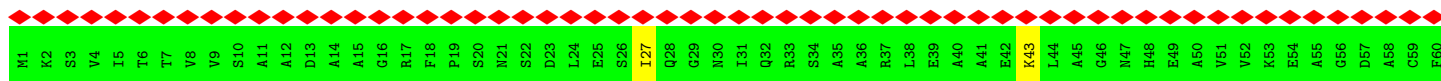




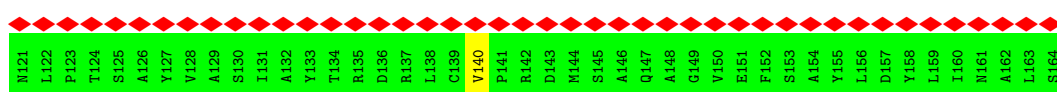
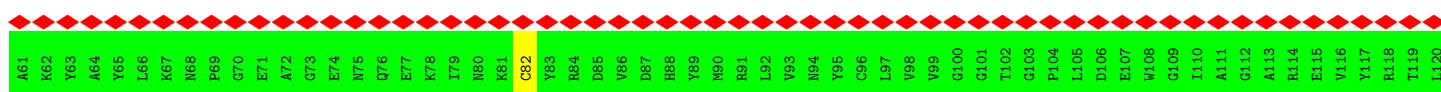
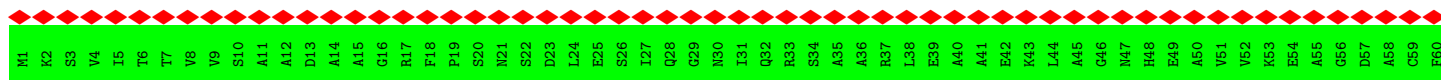
• Molecule 1: Phycoerythrin alpha subunit



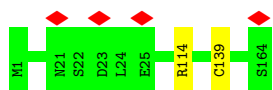
• Molecule 1: Phycoerythrin alpha subunit



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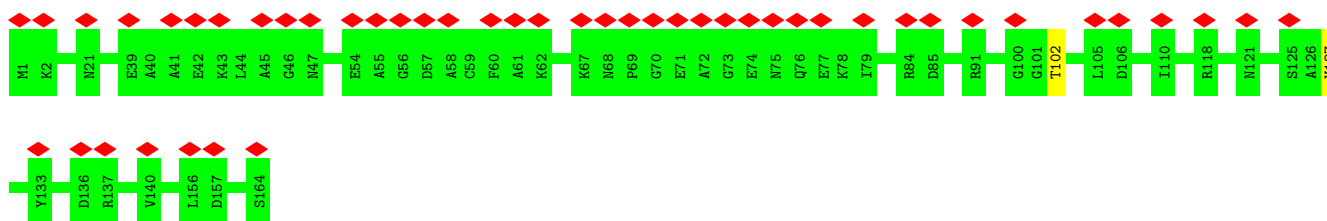
• Molecule 1: Phycoerythrin alpha subunit



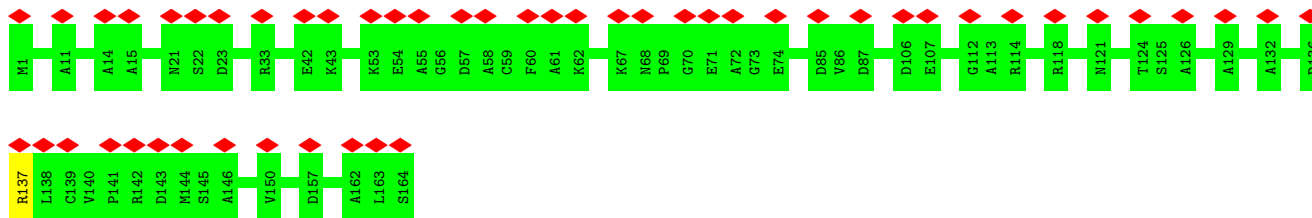
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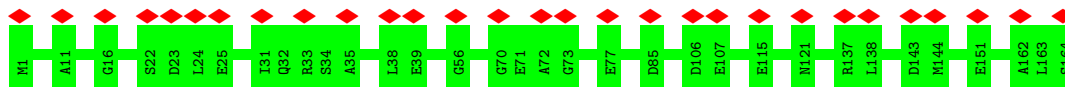
• Molecule 1: Phycoerythrin alpha subunit



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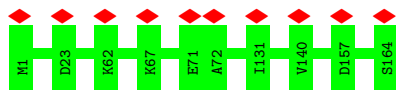


• Molecule 1: Phycoerythrin alpha subunit

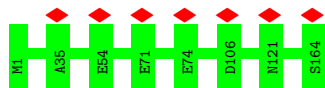


• Molecule 1: Phycoerythrin alpha subunit

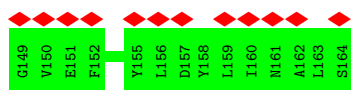
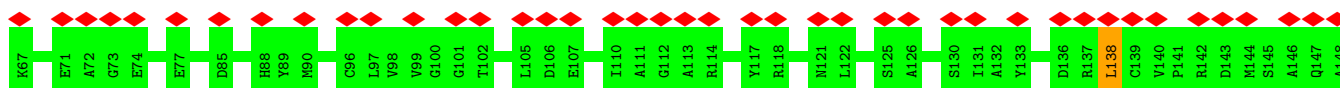
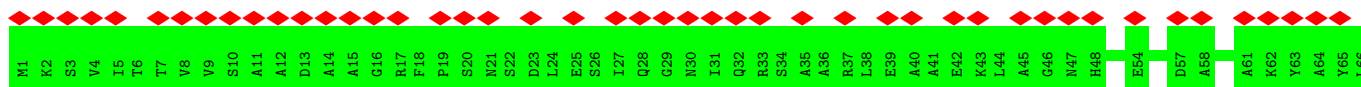




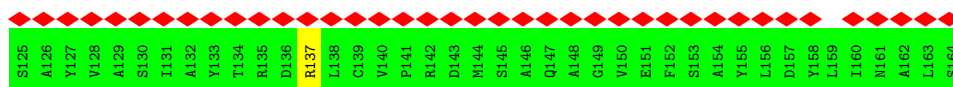
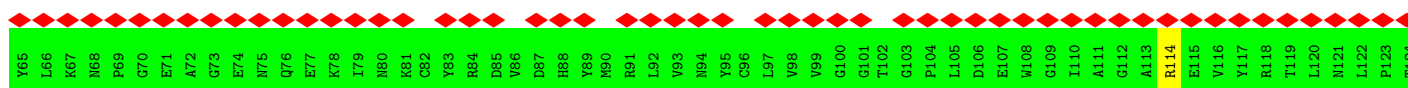
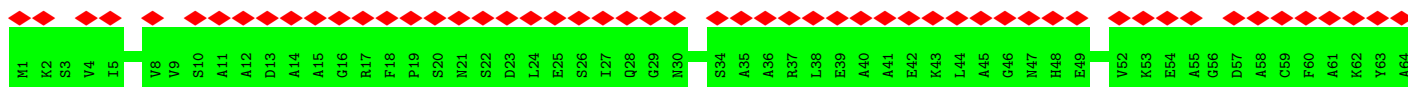
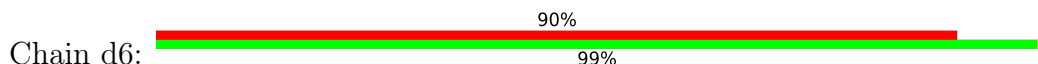
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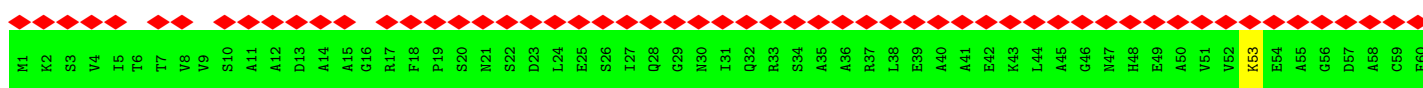
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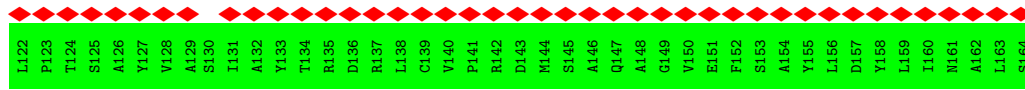
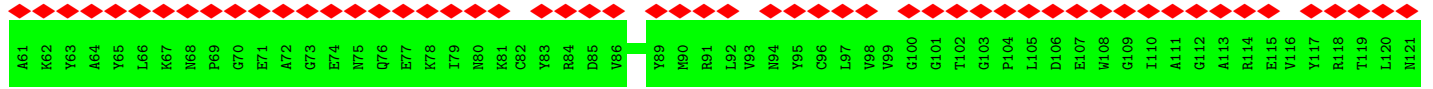


• Molecule 1: Phycoerythrin alpha subunit

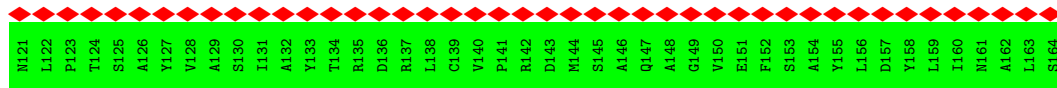
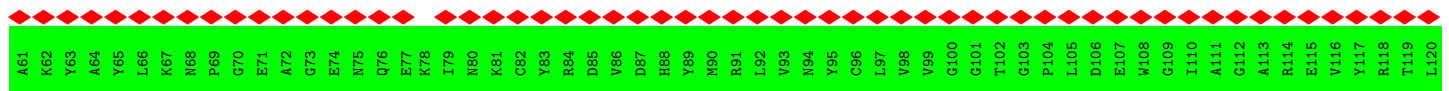
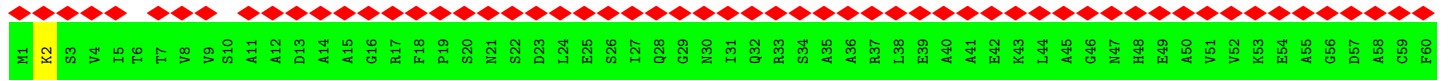


• Molecule 1: Phycoerythrin alpha subunit

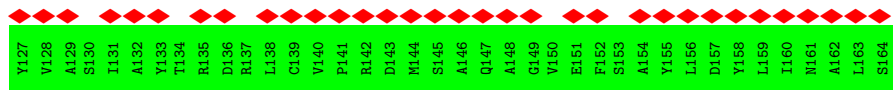
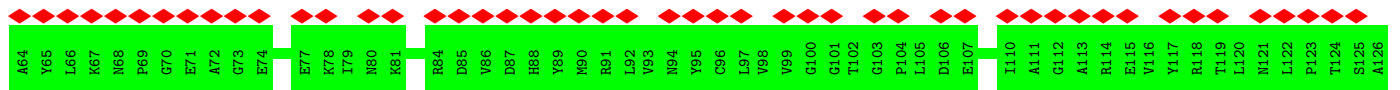
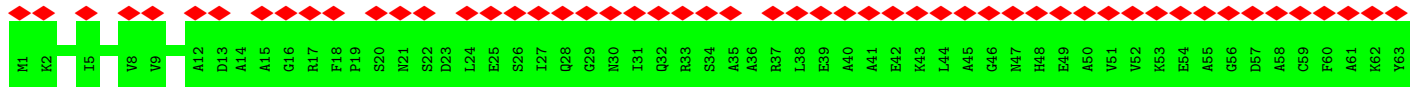
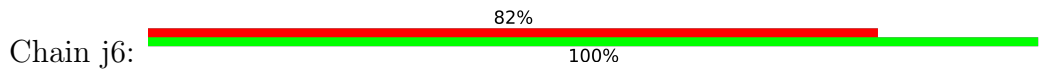




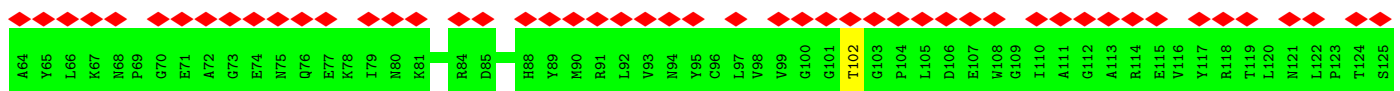
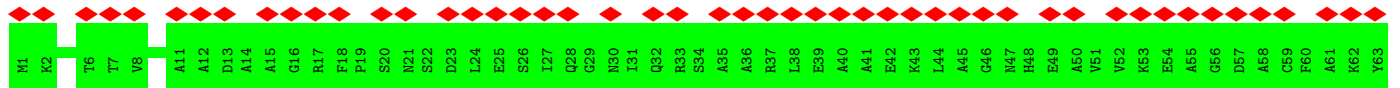
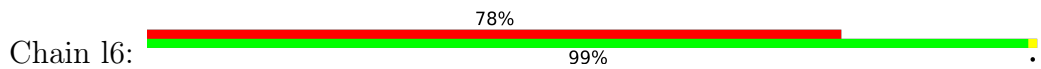
• Molecule 1: Phycoerythrin alpha subunit



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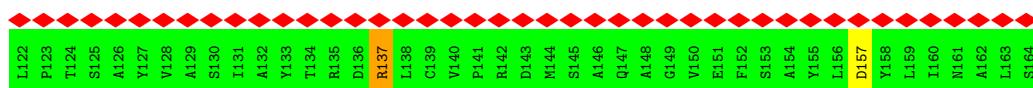
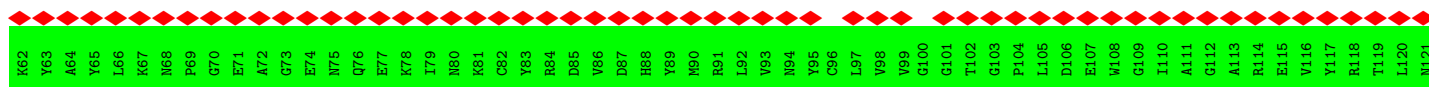
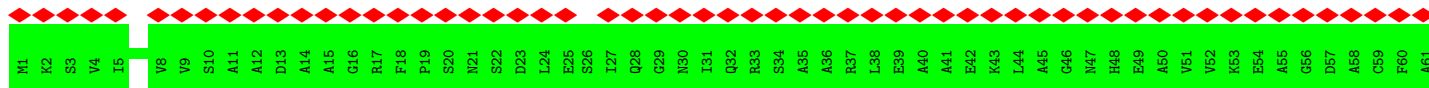


• Molecule 1: Phycoerythrin alpha subunit

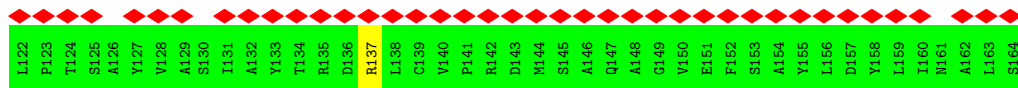
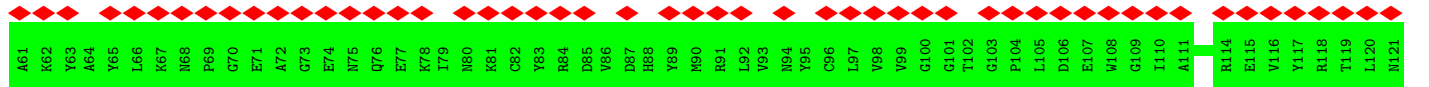
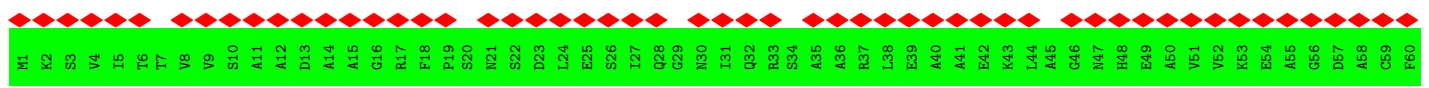




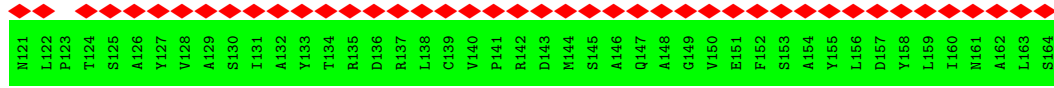
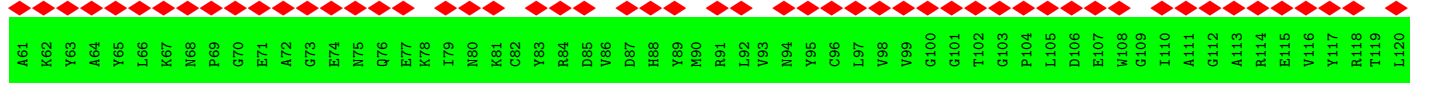
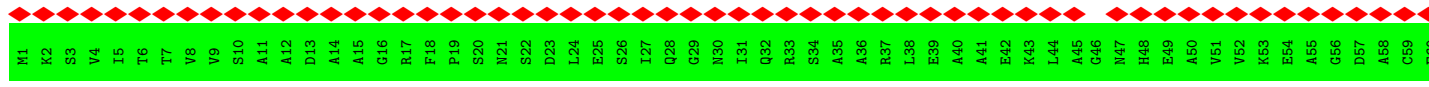
• Molecule 1: Phycoerythrin alpha subunit



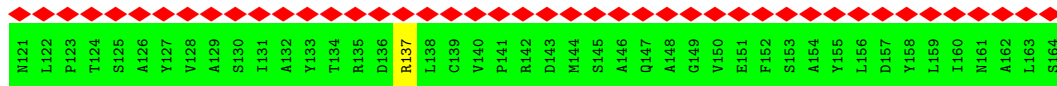
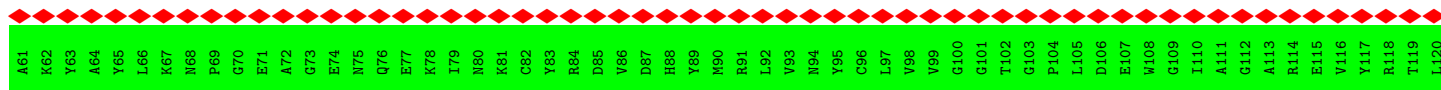
• Molecule 1: Phycoerythrin alpha subunit



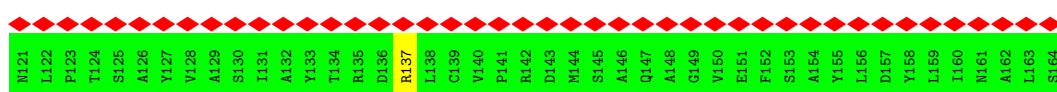
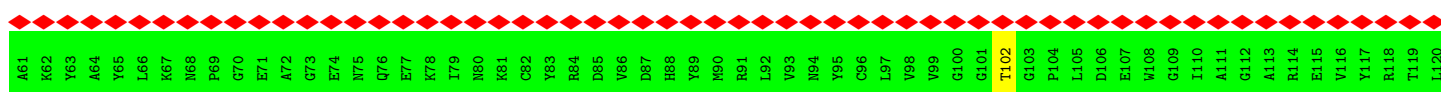
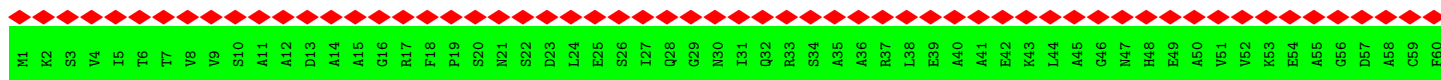
• Molecule 1: Phycoerythrin alpha subunit



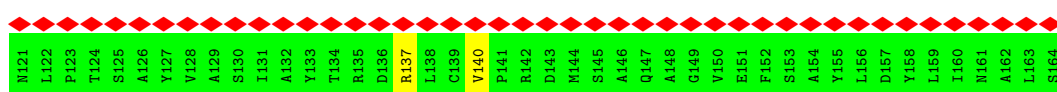
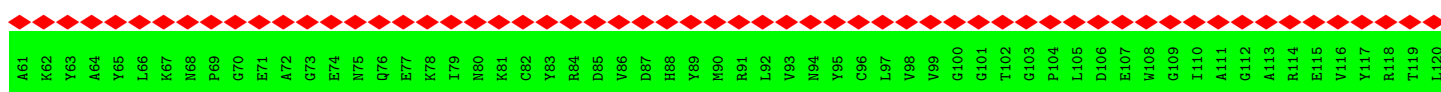
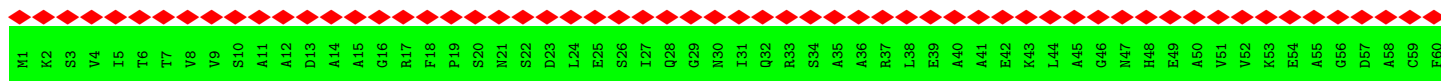
• Molecule 1: Phycoerythrin alpha subunit



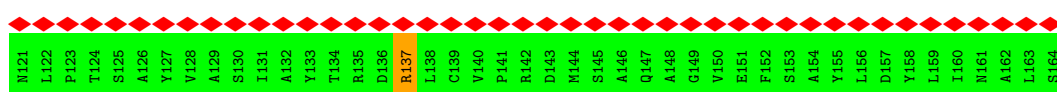
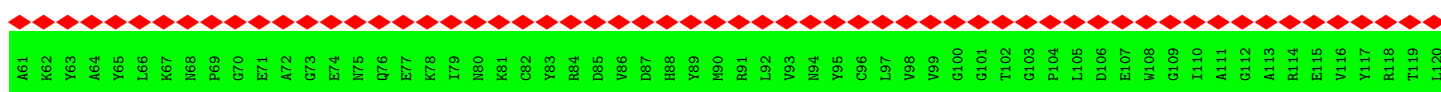
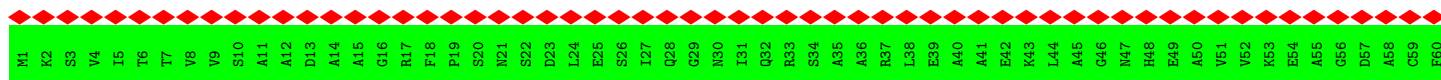
• Molecule 1: Phycoerythrin alpha subunit



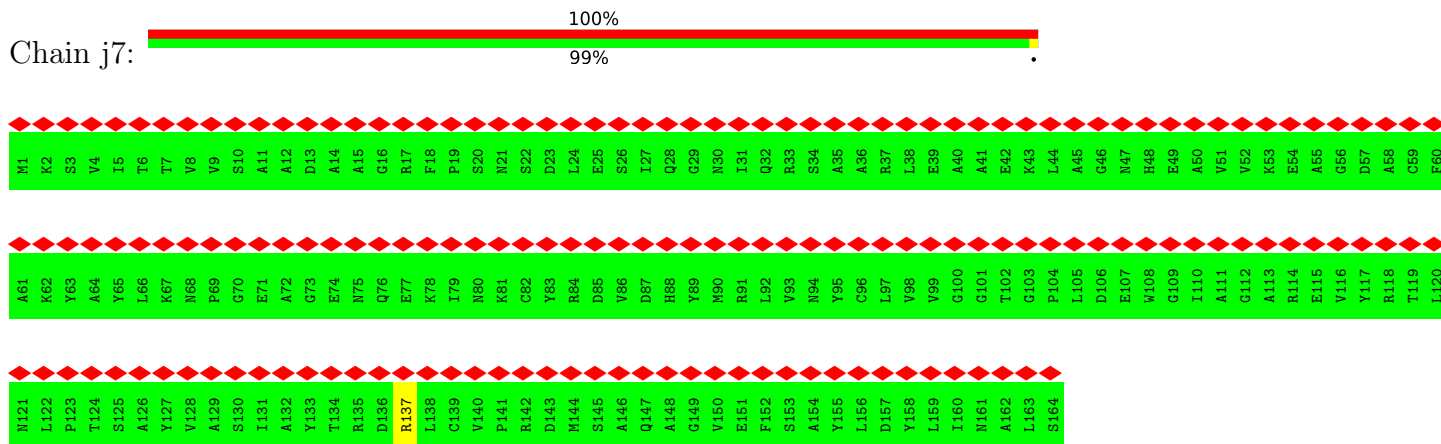
• Molecule 1: Phycoerythrin alpha subunit



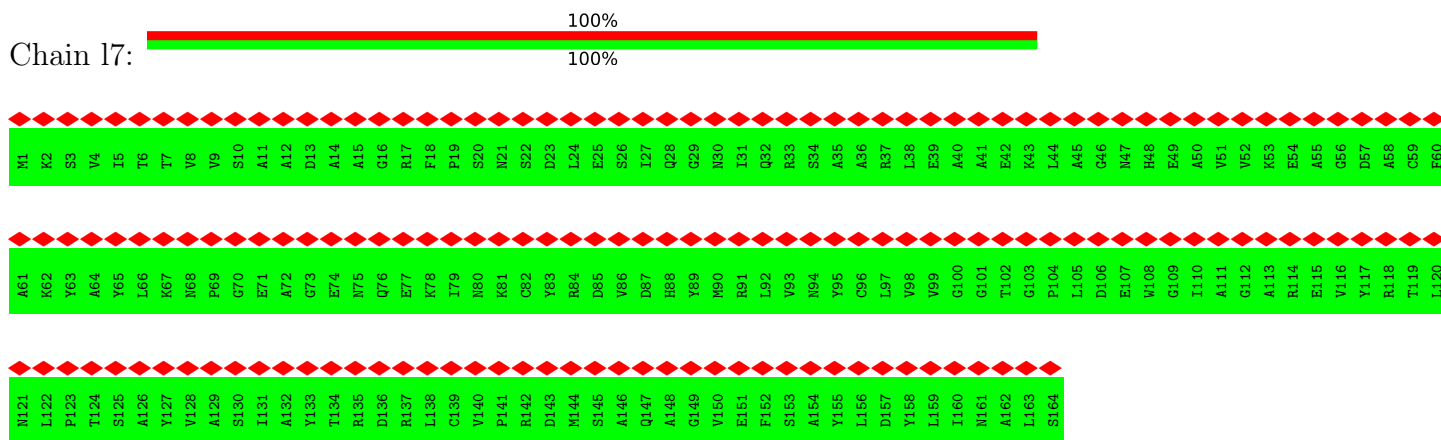
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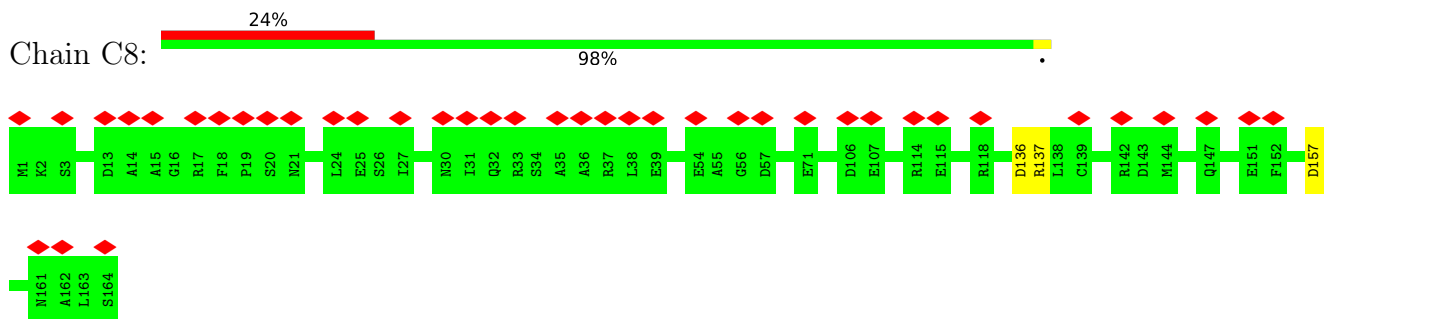
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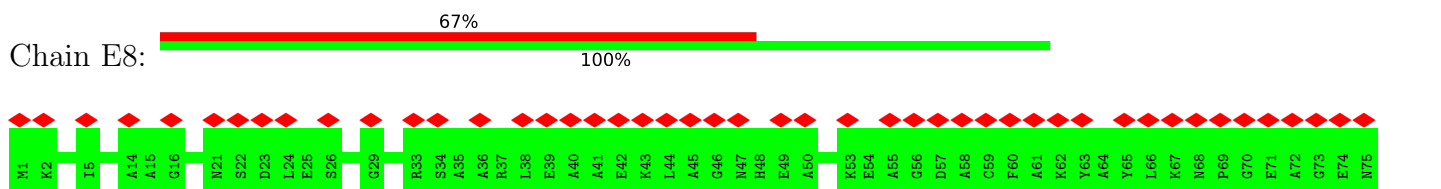
• Molecule 1: Phycoerythrin alpha subunit

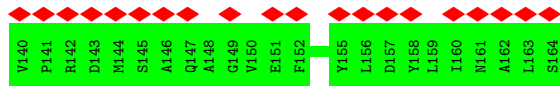
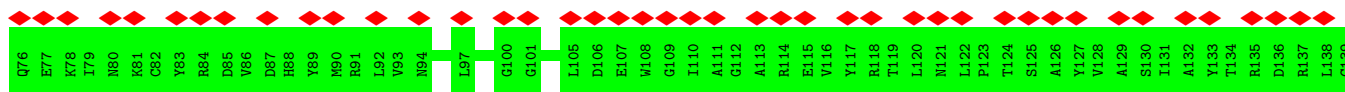


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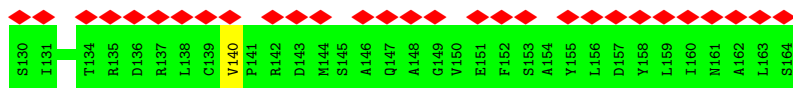
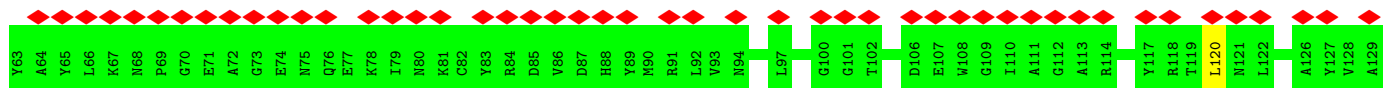
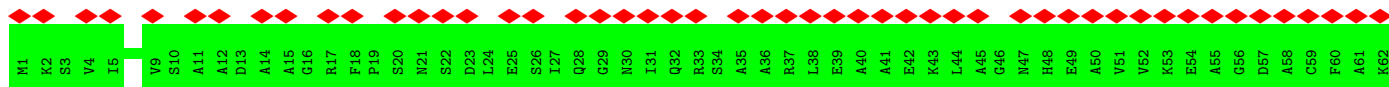
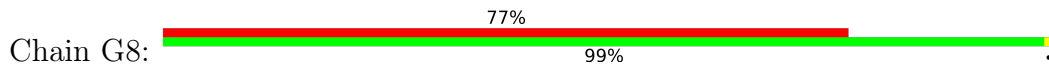


• Molecule 1: Phycoerythrin alpha subunit

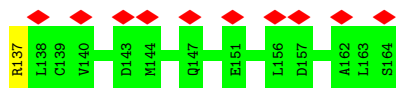
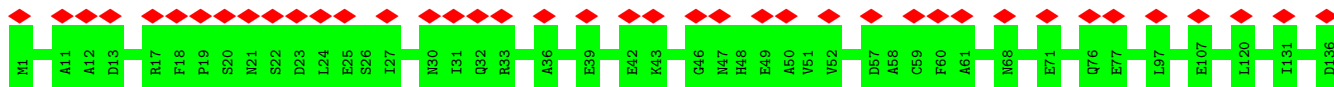




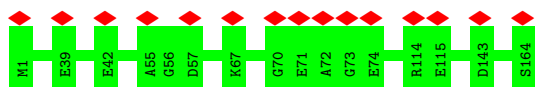
• Molecule 1: Phycoerythrin alpha subunit



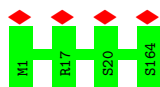
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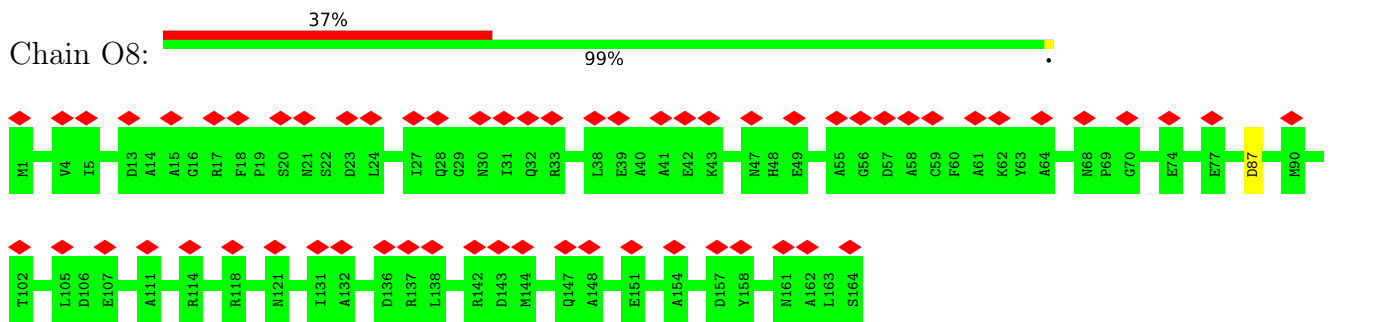
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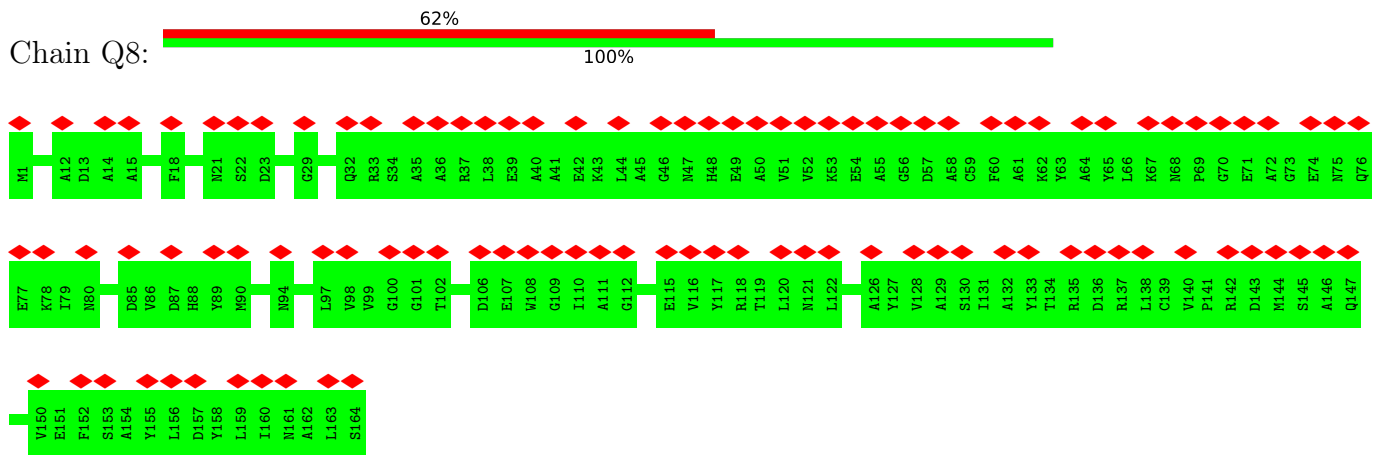
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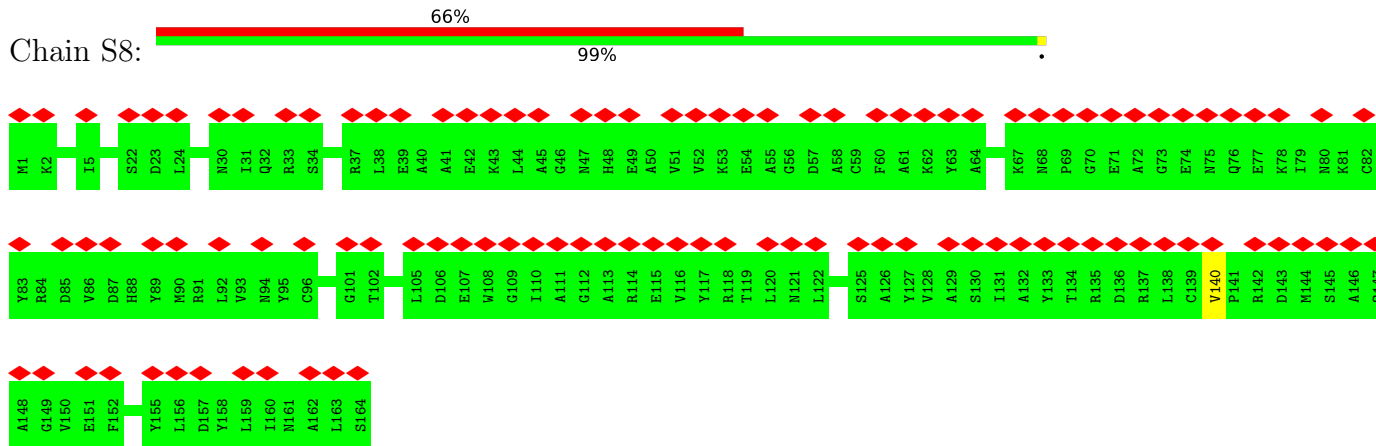
• Molecule 1: Phycoerythrin alpha subunit



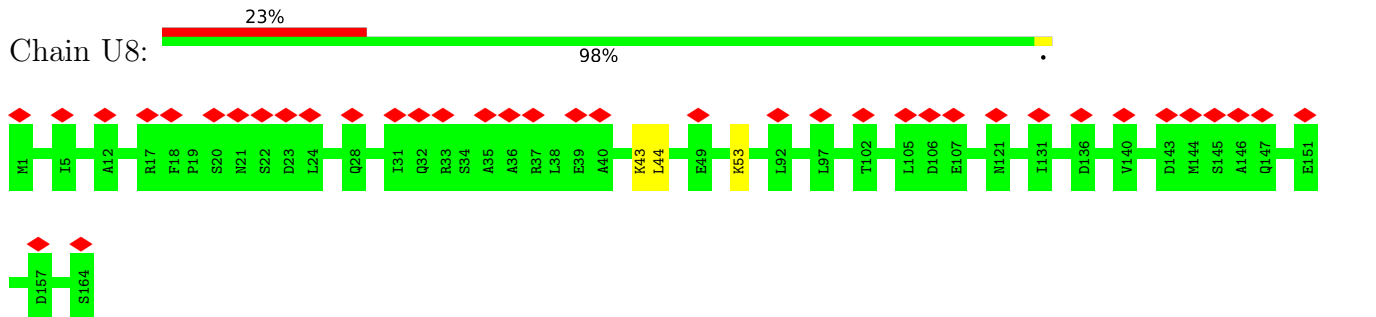
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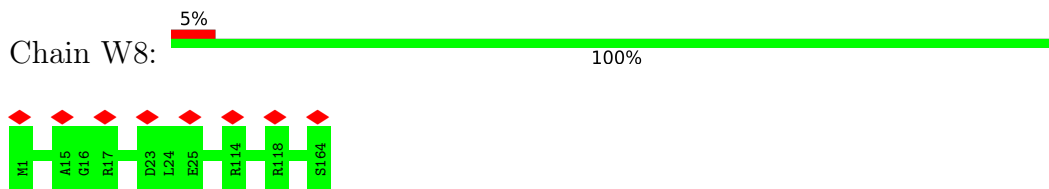
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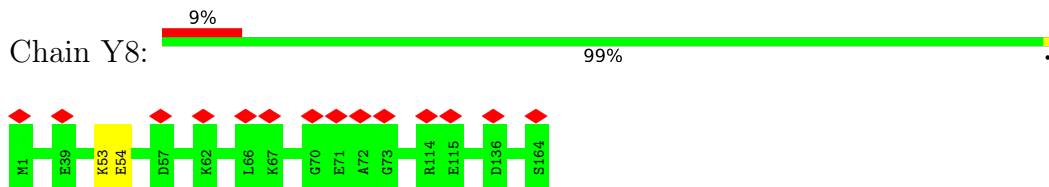
• Molecule 1: Phycoerythrin alpha subunit



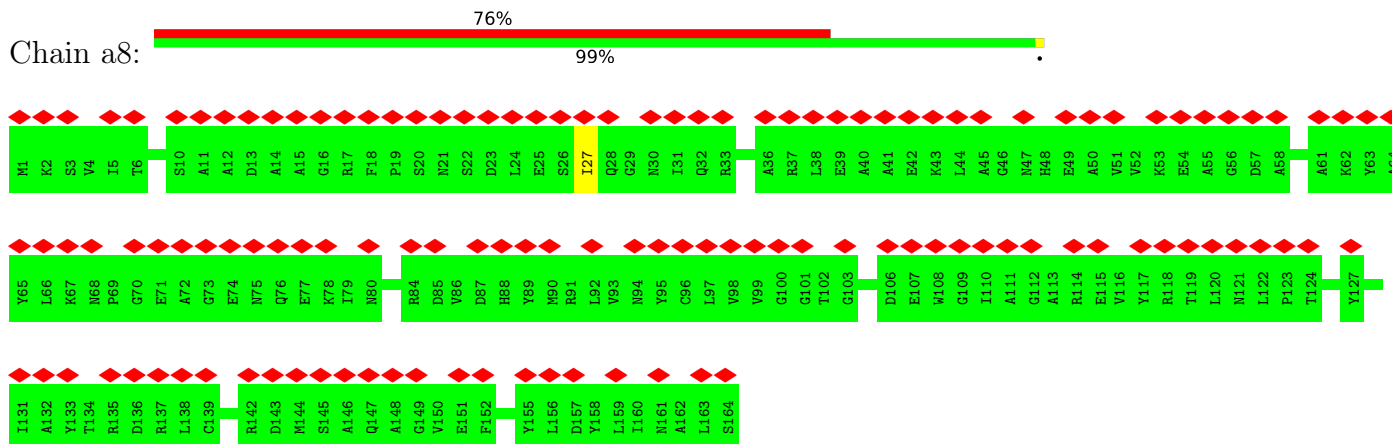
• Molecule 1: Phycoerythrin alpha subunit



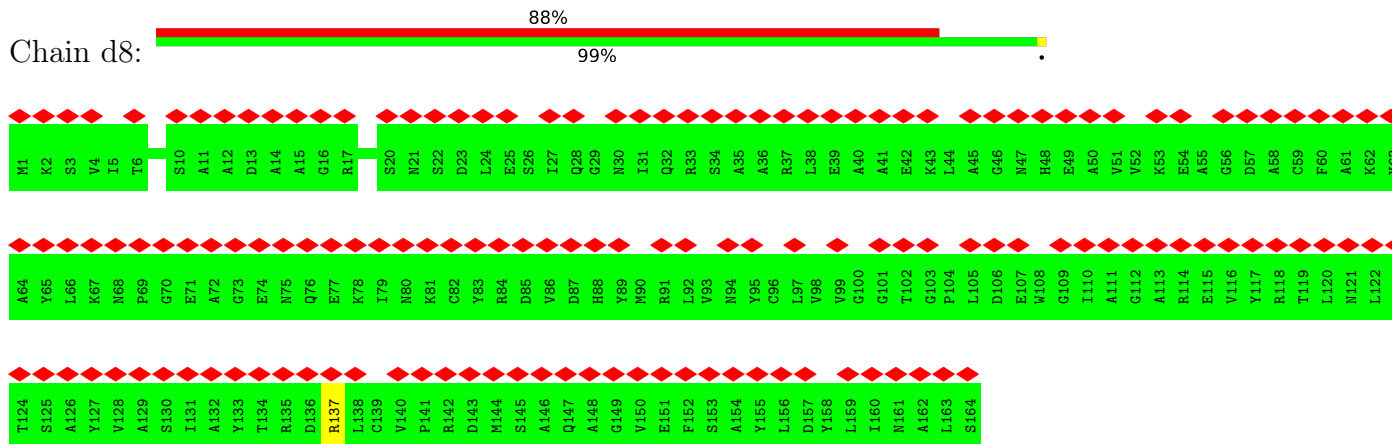
• Molecule 1: Phycoerythrin alpha subunit



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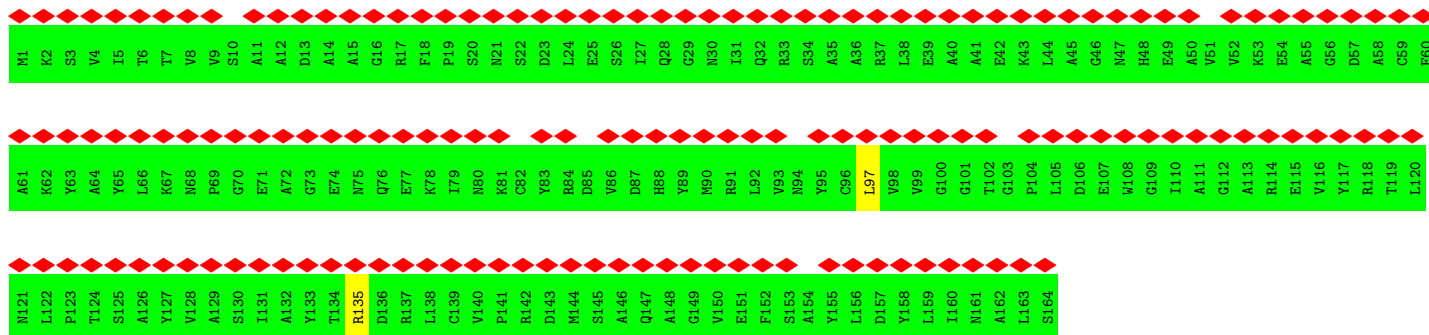


• Molecule 1: Phycoerythrin alpha subunit

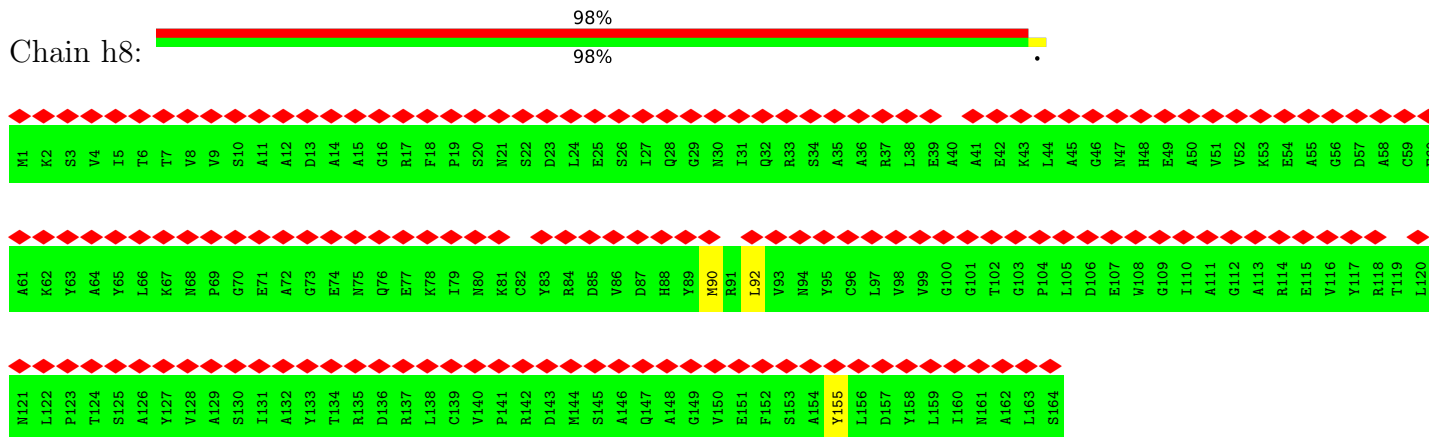


• Molecule 1: Phycoerythrin alpha subunit

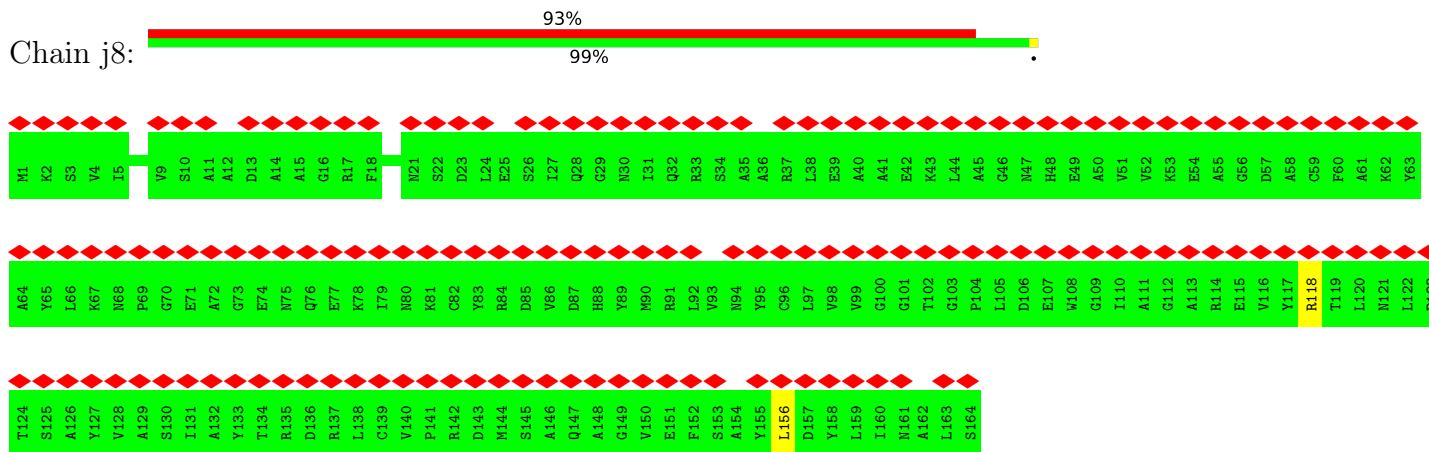




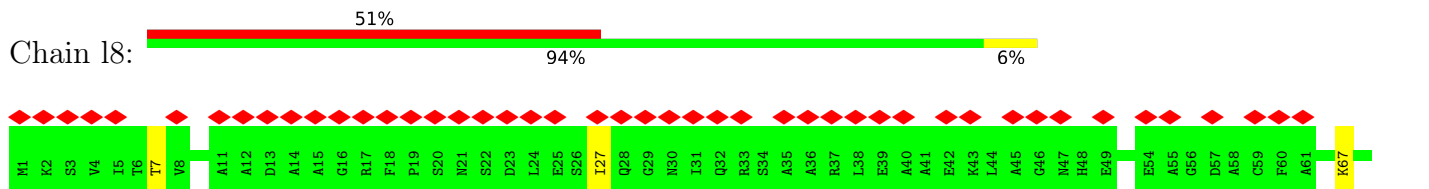
• Molecule 1: Phycoerythrin alpha subunit

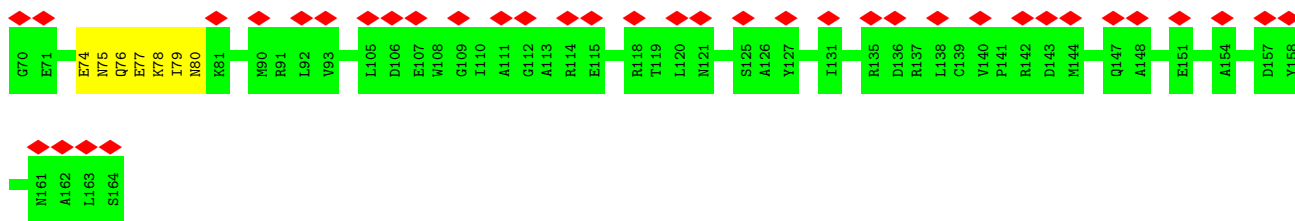


• Molecule 1: Phycoerythrin alpha subunit



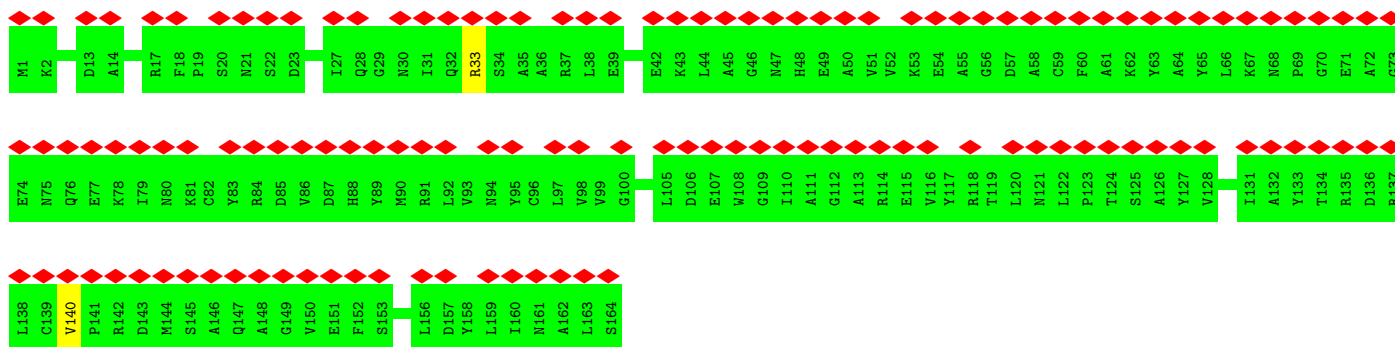
• Molecule 1: Phycoerythrin alpha subunit





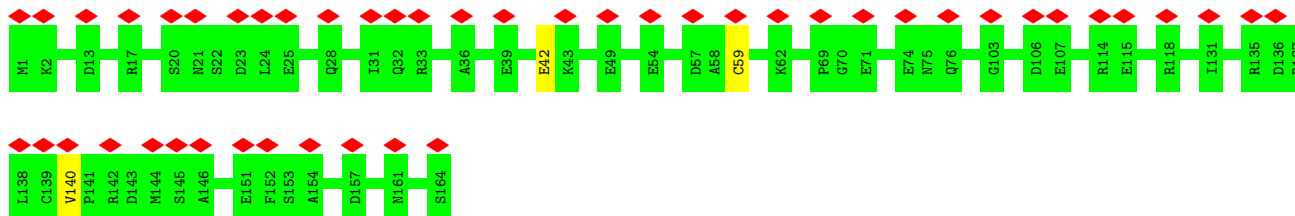
- Molecule 1: Phycoerythrin alpha subunit

Chain B9: 78%
99%



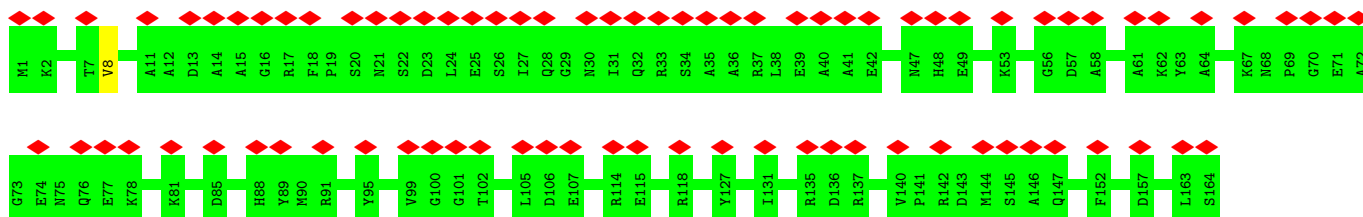
- Molecule 1: Phycoerythrin alpha subunit

Chain D9: 29%
98%



- Molecule 1: Phycoerythrin alpha subunit

Chain F9: 49%
99%

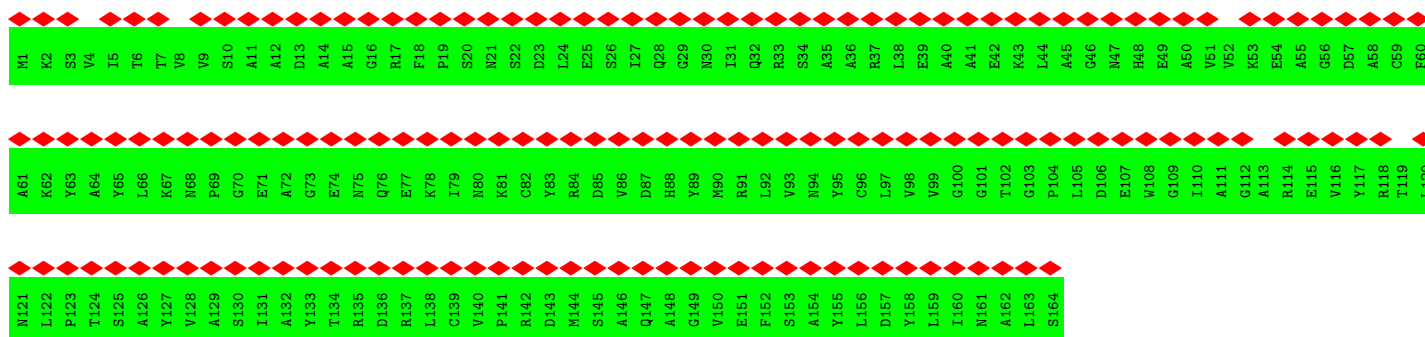


- Molecule 1: Phycoerythrin alpha subunit

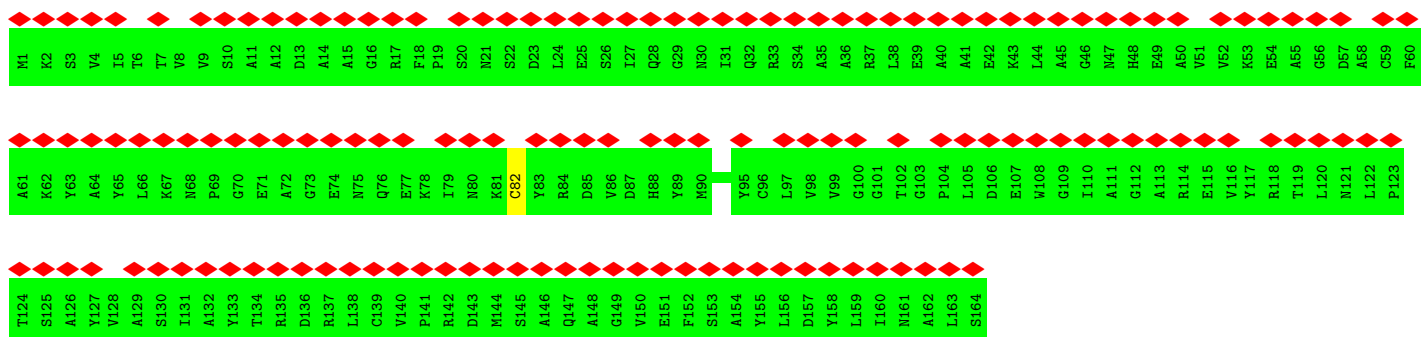
Chain H9: 79%
100%



- Molecule 1: Phycoerythrin alpha subunit

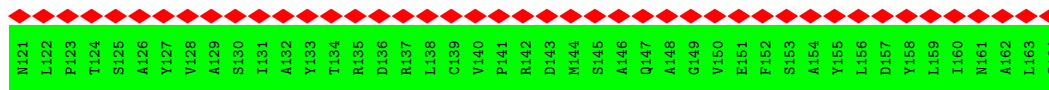


- Molecule 1: Phycoerythrin alpha subunit

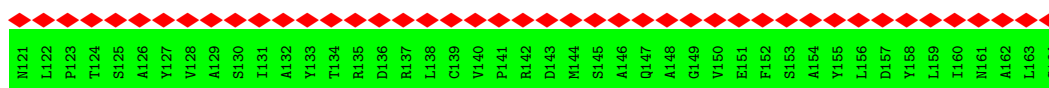
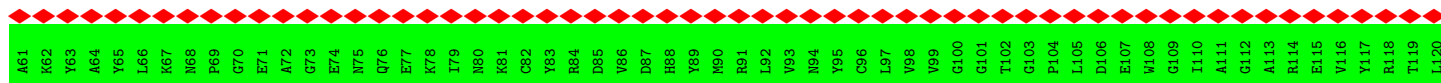
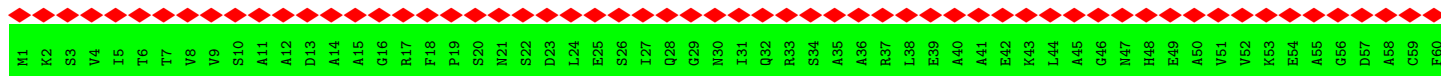


- Molecule 1: Phycoerythrin alpha subunit

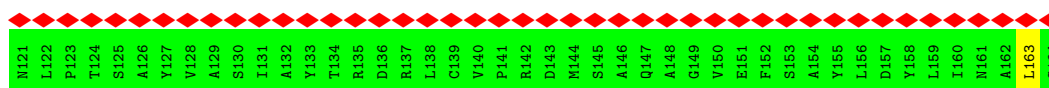
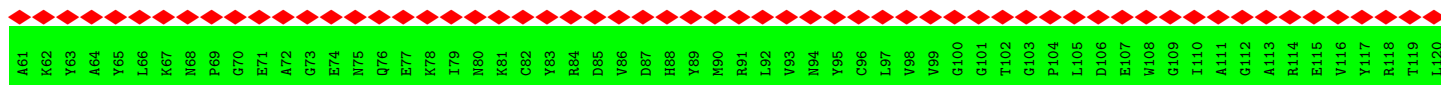
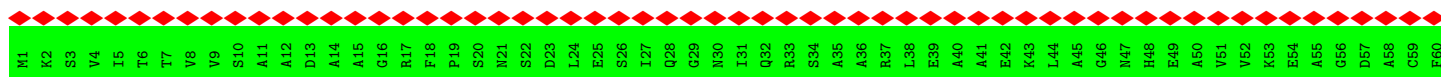




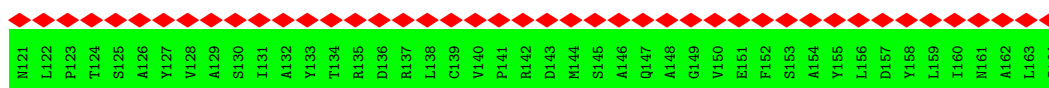
• Molecule 1: Phycoerythrin alpha subunit



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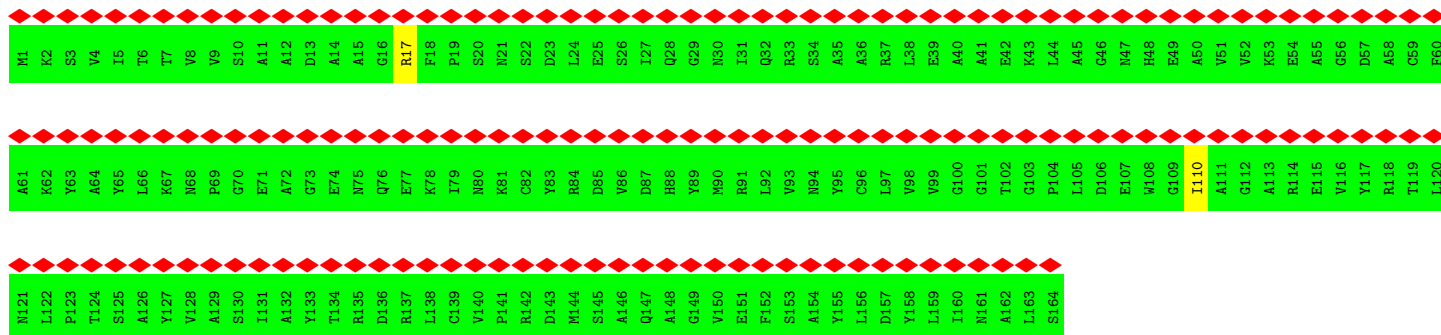


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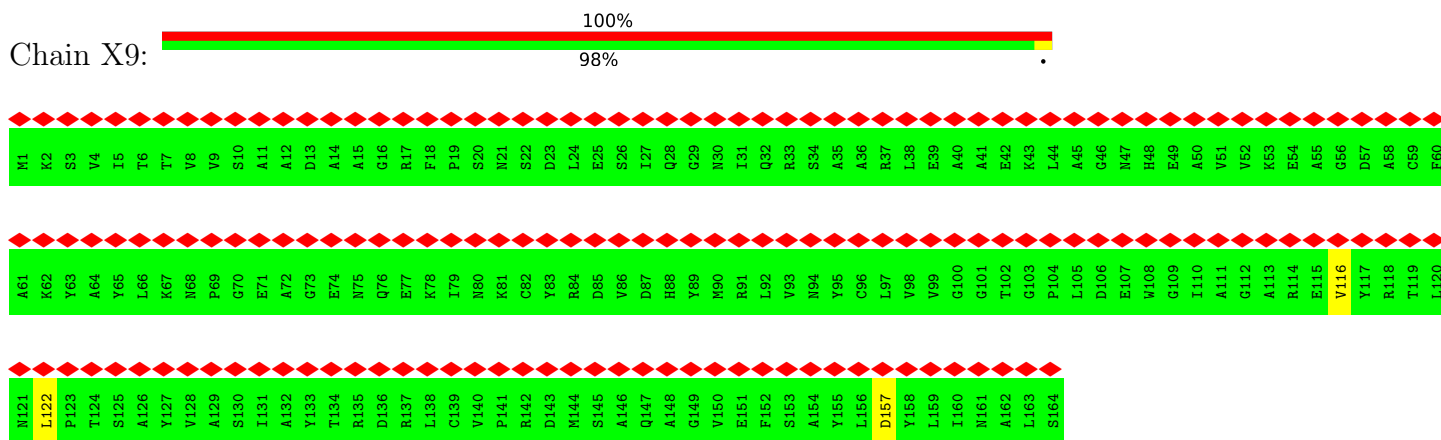


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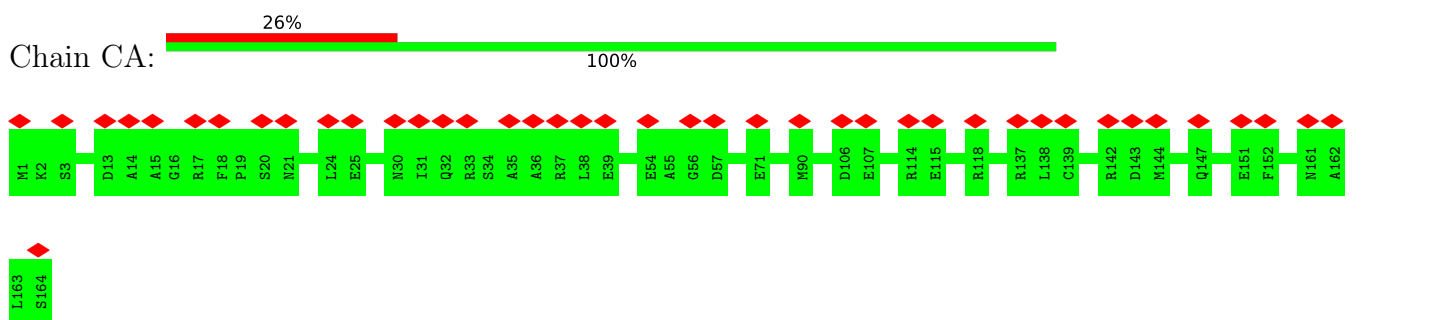




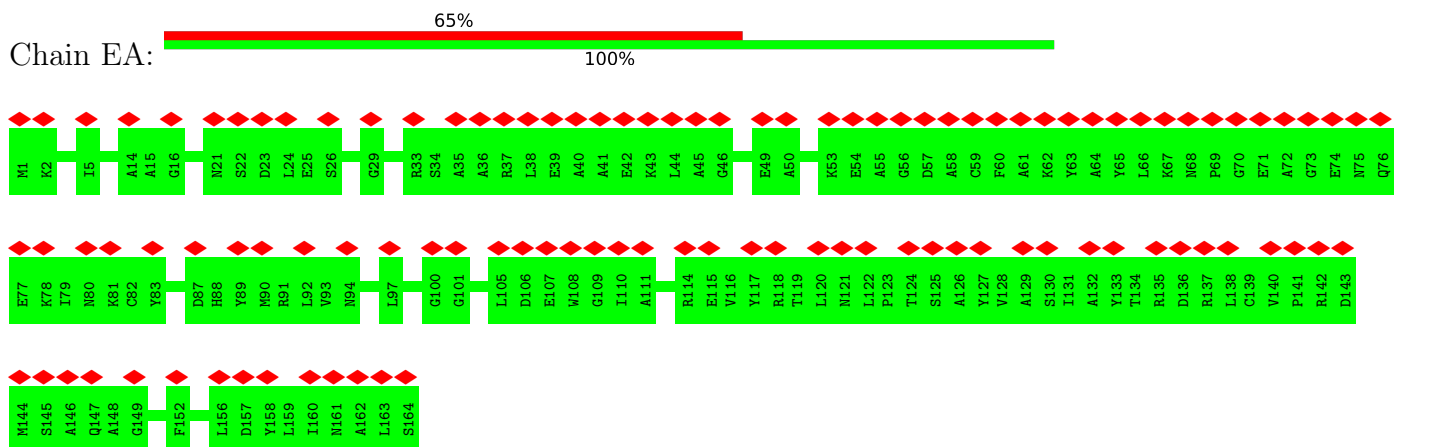
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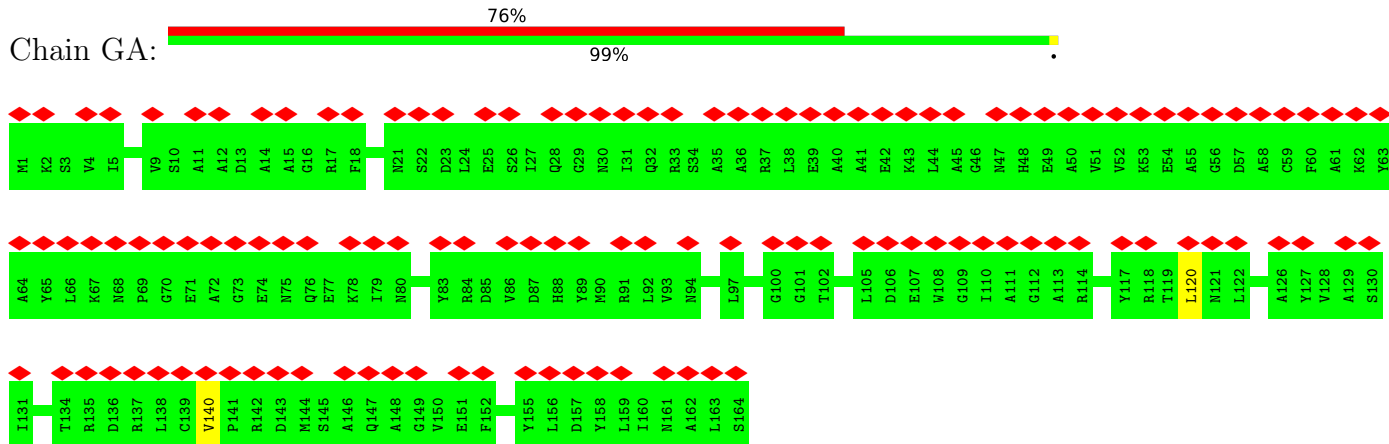
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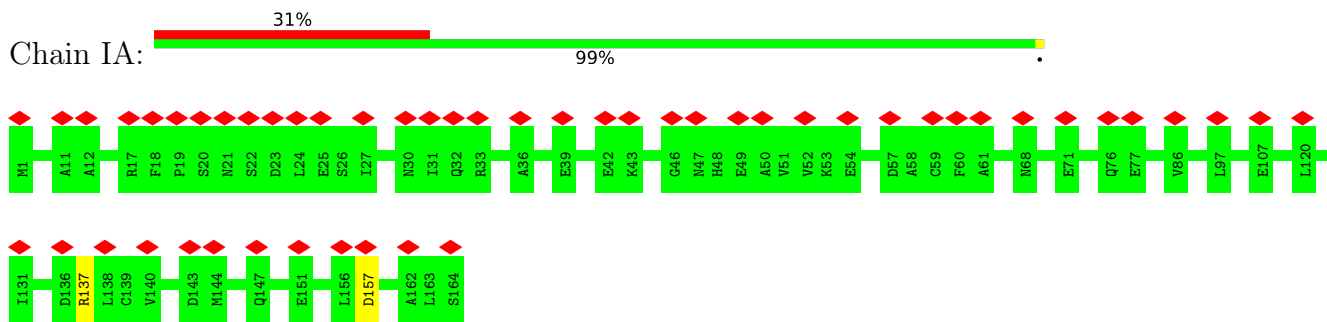
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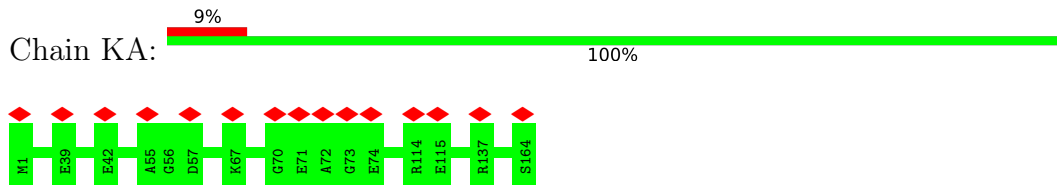
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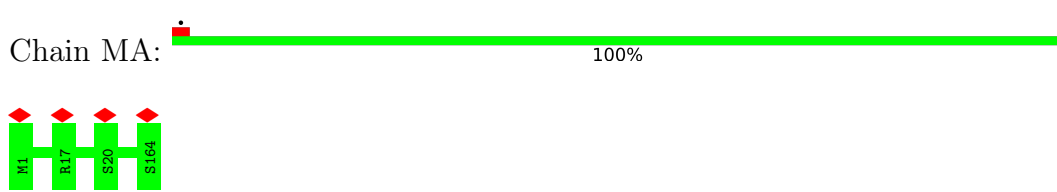
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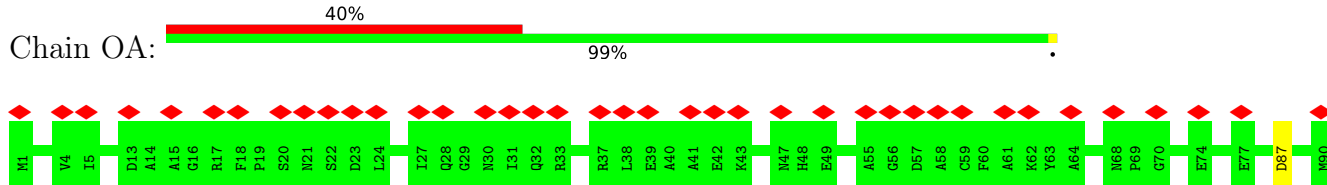
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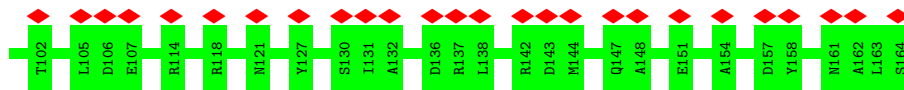


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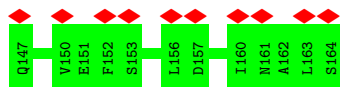
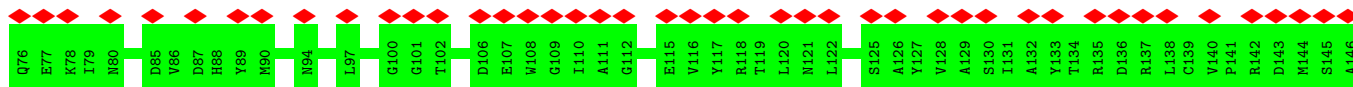
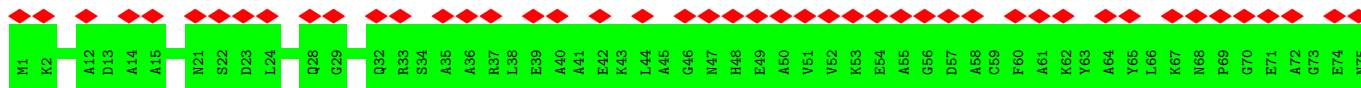


• Molecule 1: Phycoerythrin alpha subunit

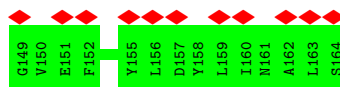
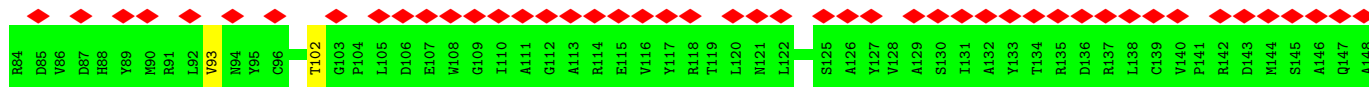
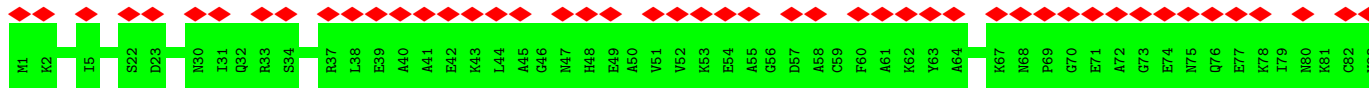




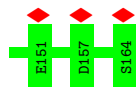
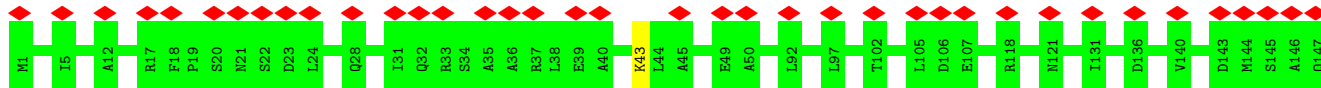
• Molecule 1: Phycoerythrin alpha subunit



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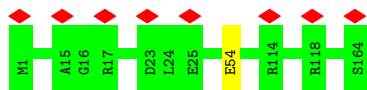


• Molecule 1: Phycoerythrin alpha subunit

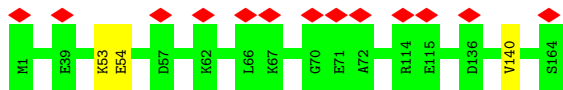


• Molecule 1: Phycoerythrin alpha subunit

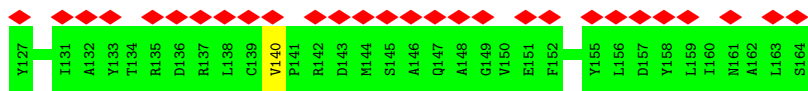
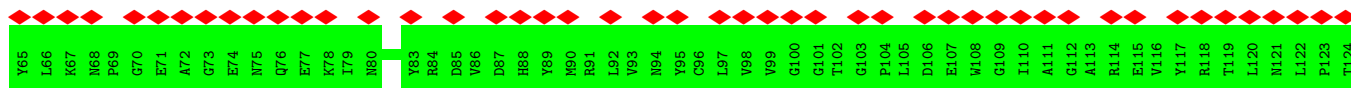
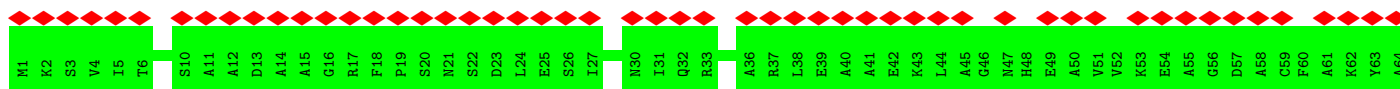
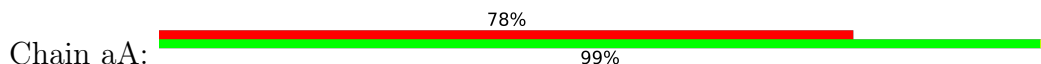




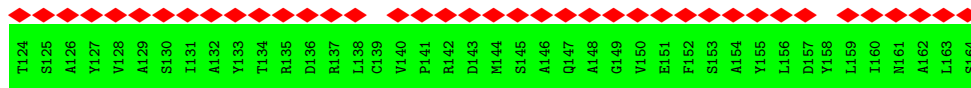
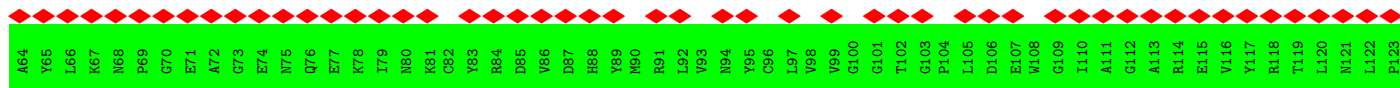
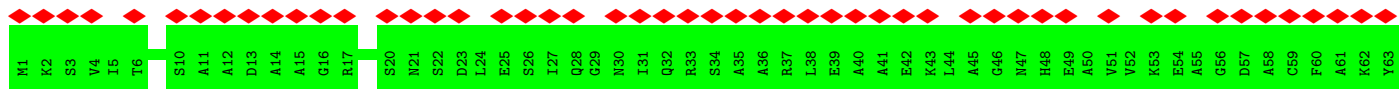
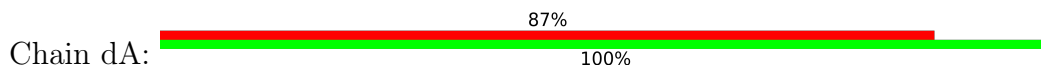
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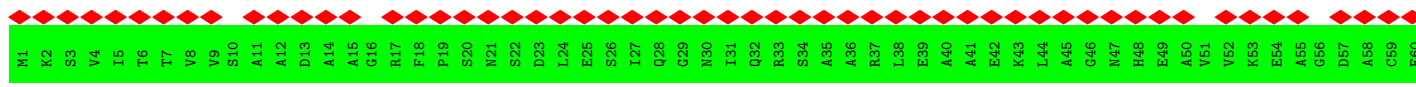
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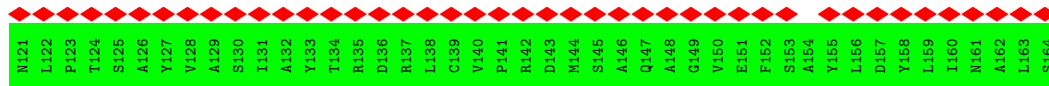
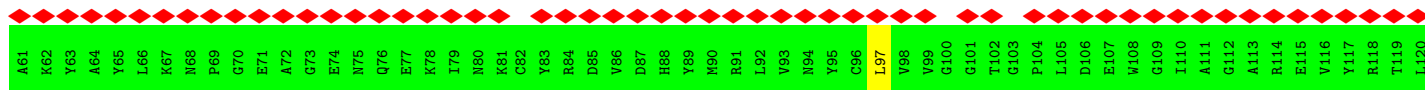


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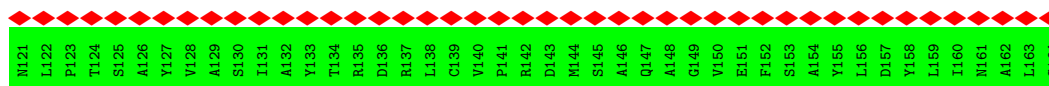
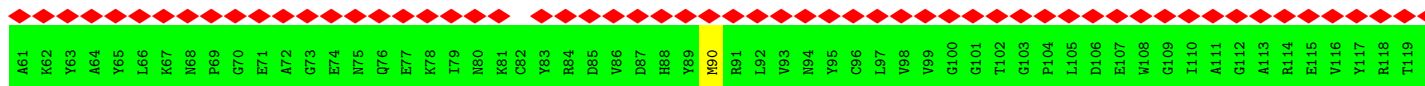


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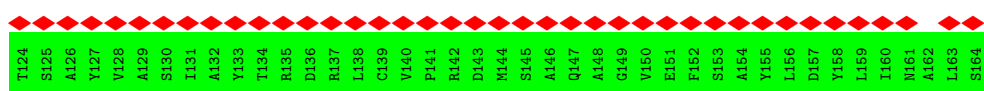
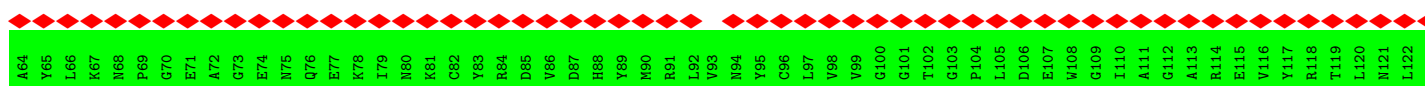




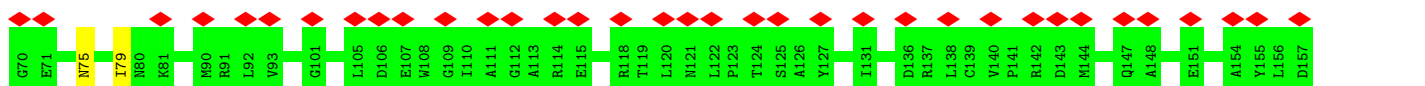
• Molecule 1: Phycoerythrin alpha subunit

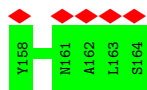


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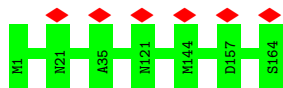


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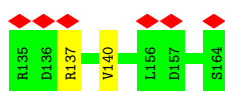
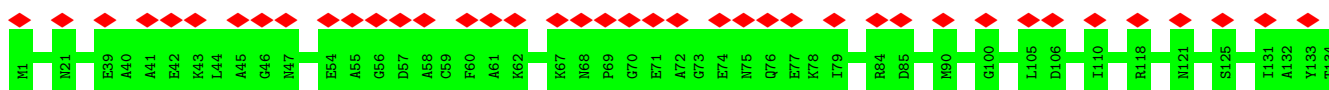




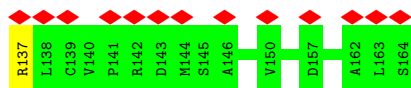
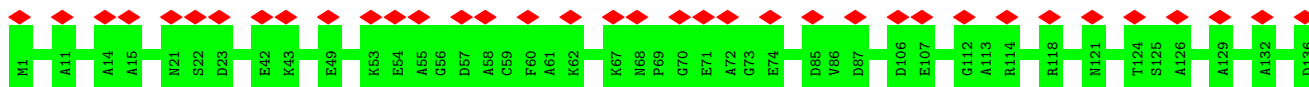
- Molecule 1: Phycoerythrin alpha subunit



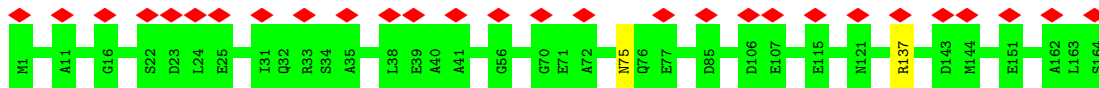
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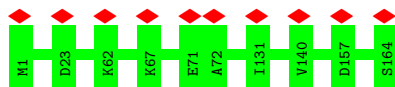
- Molecule 1: Phycoerythrin alpha subunit



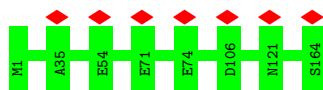
- Molecule 1: Phycoerythrin alpha subunit



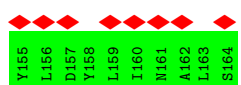
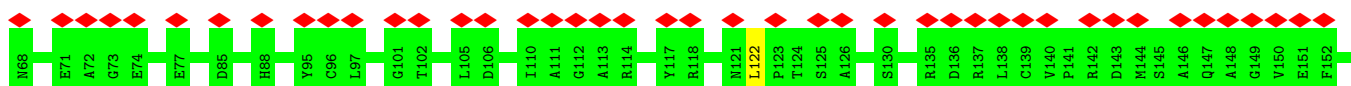
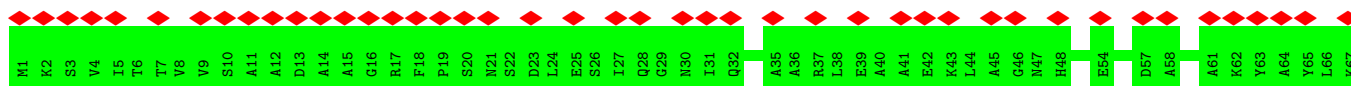
- Molecule 1: Phycoerythrin alpha subunit



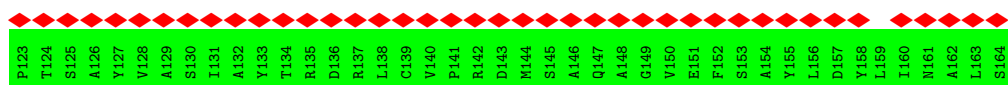
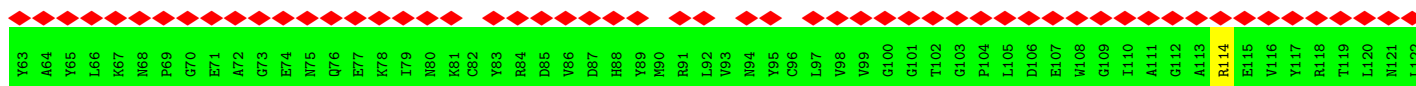
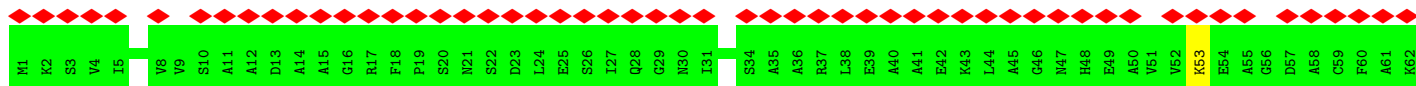
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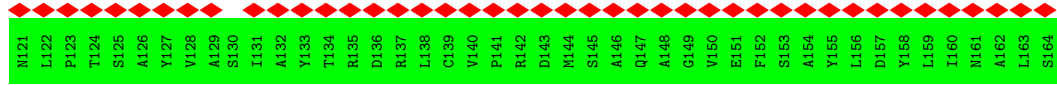
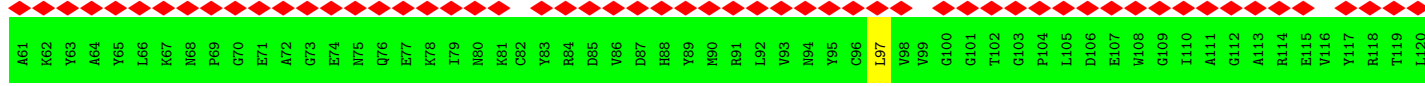
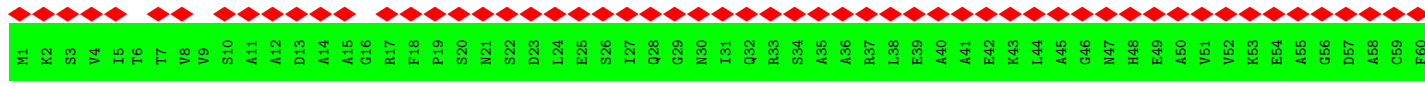
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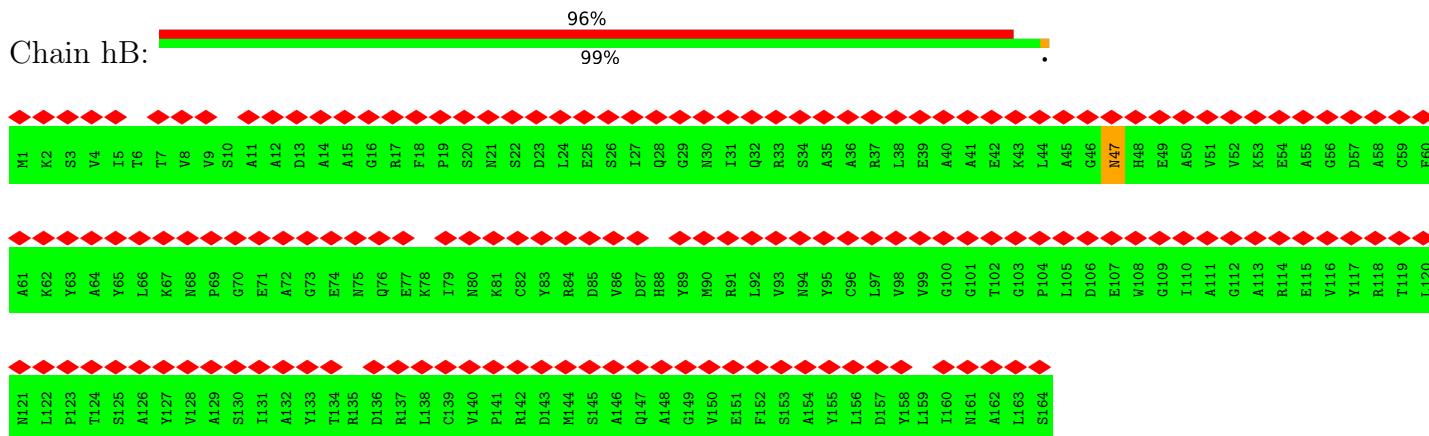
• Molecule 1: Phycoerythrin alpha subunit



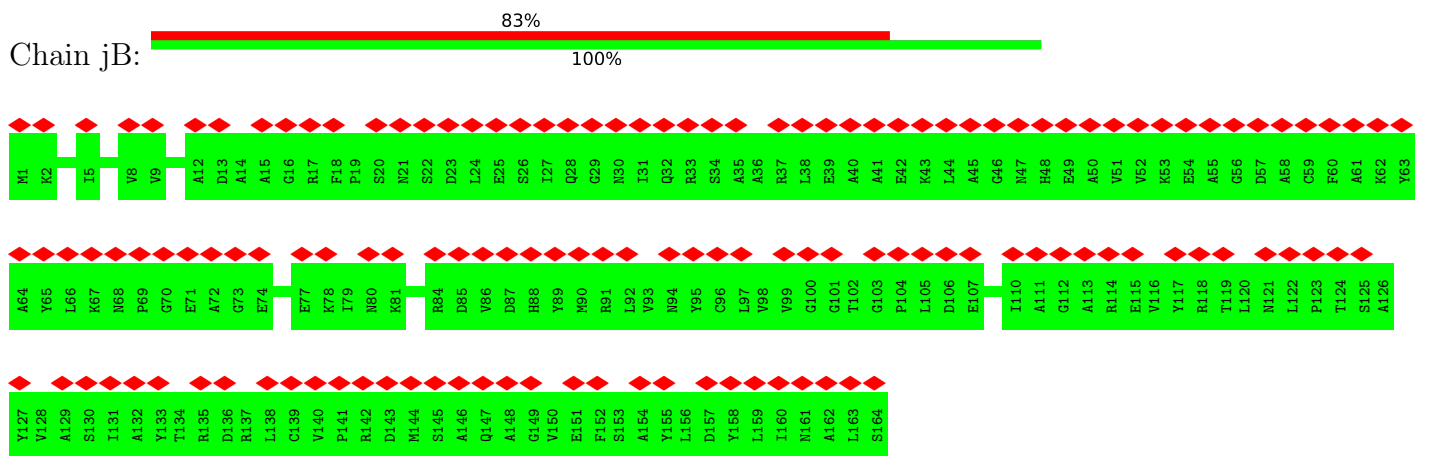
• Molecule 1: Phycoerythrin alpha subunit



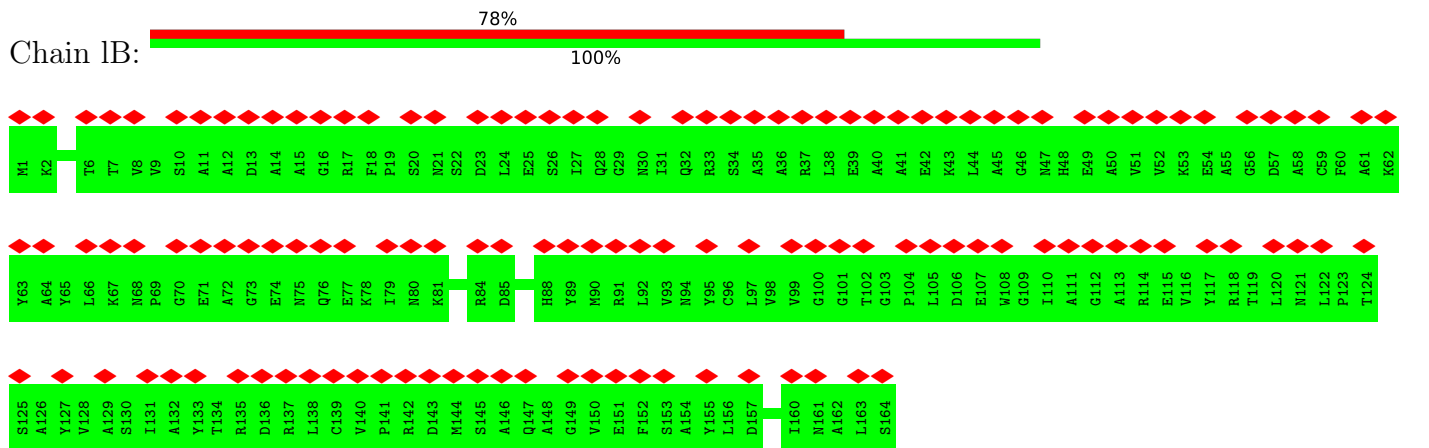
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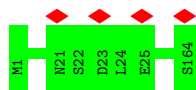


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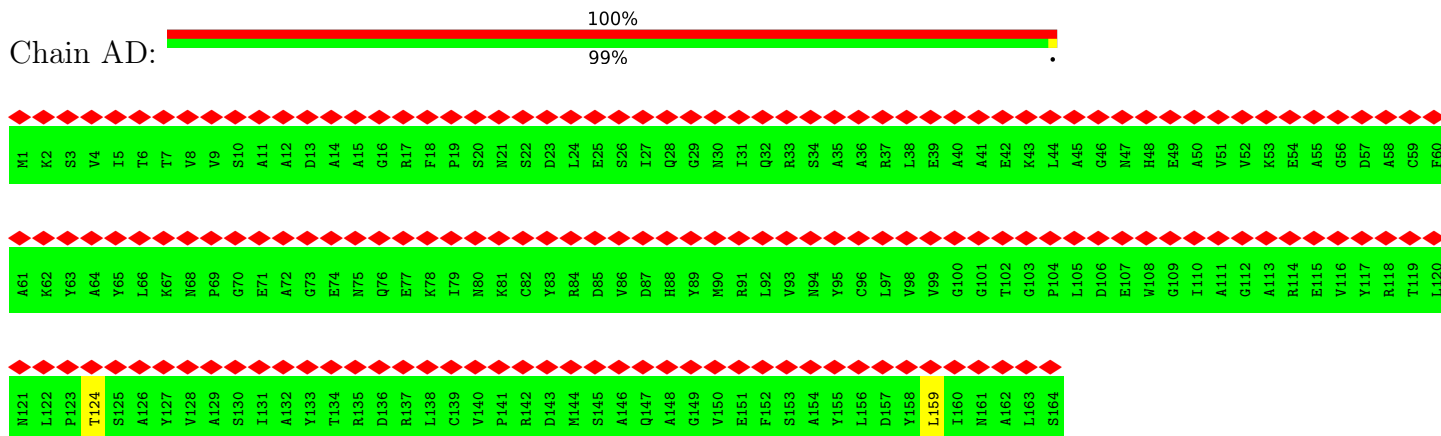


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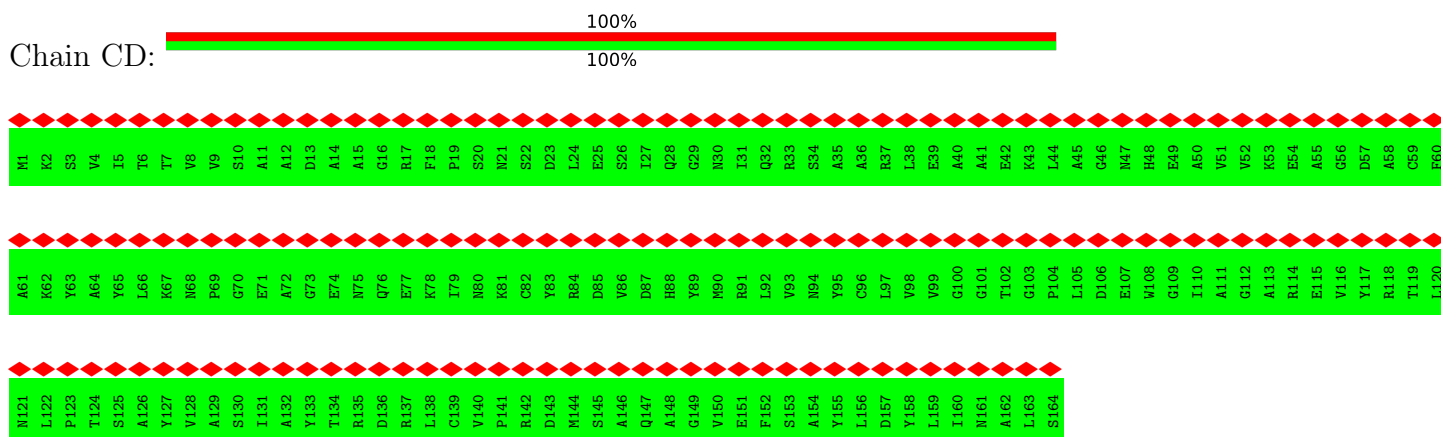




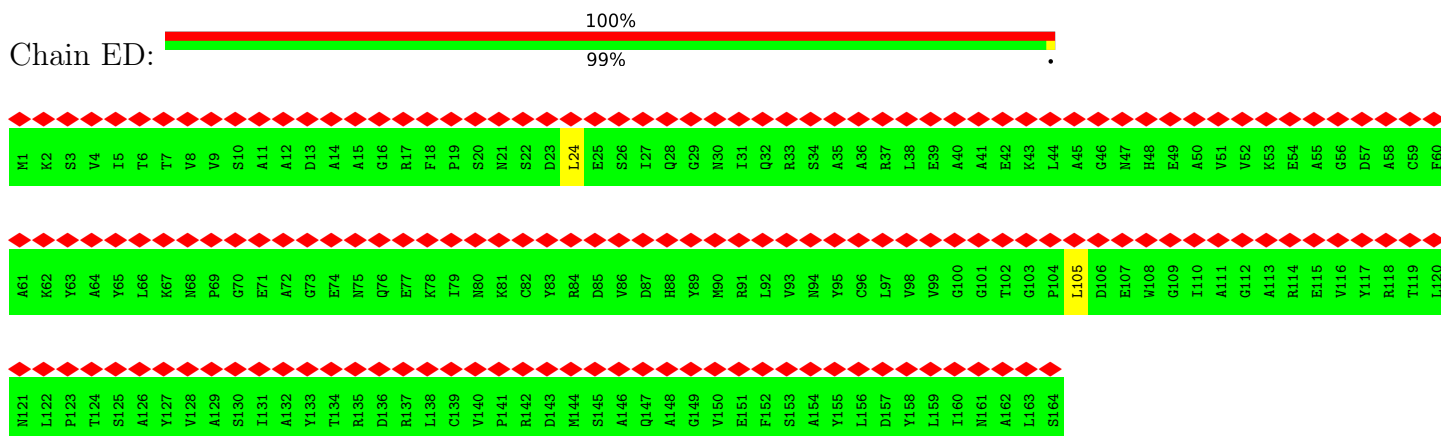
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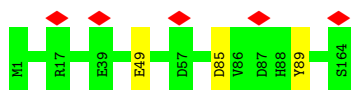
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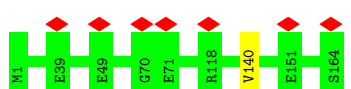
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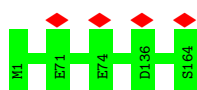
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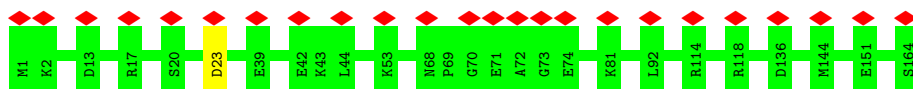
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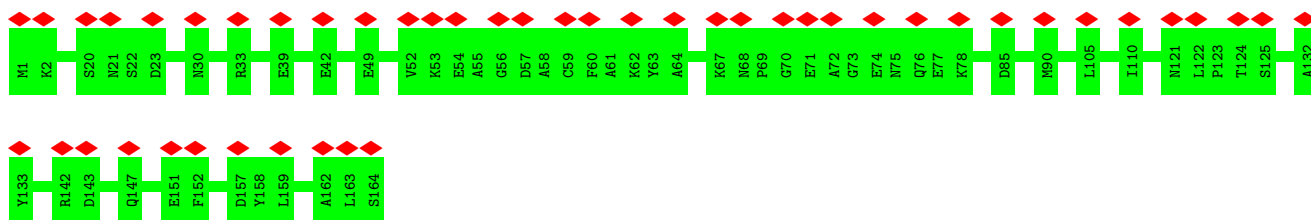
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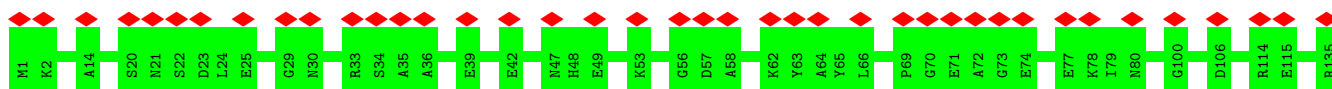
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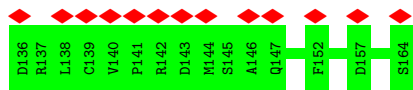


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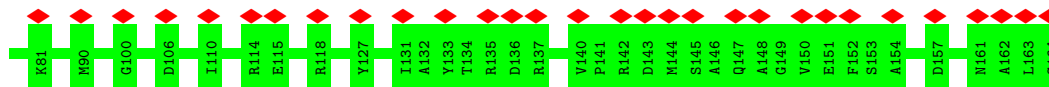
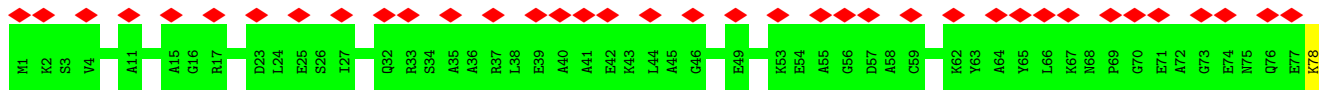
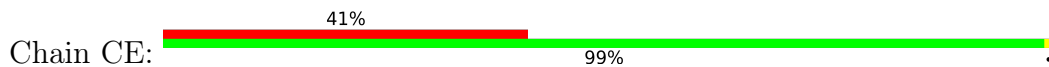


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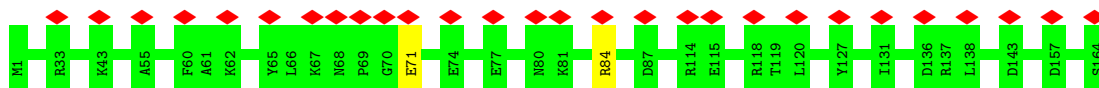




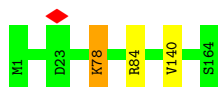
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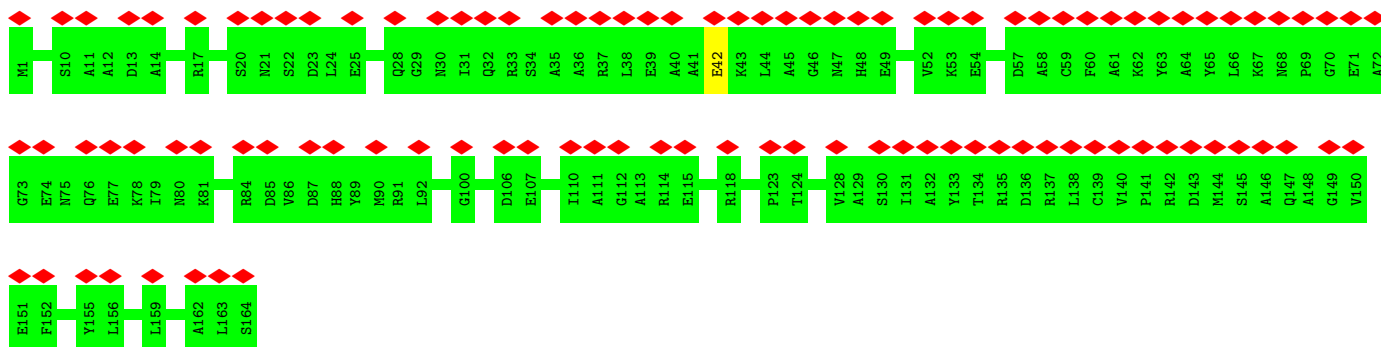


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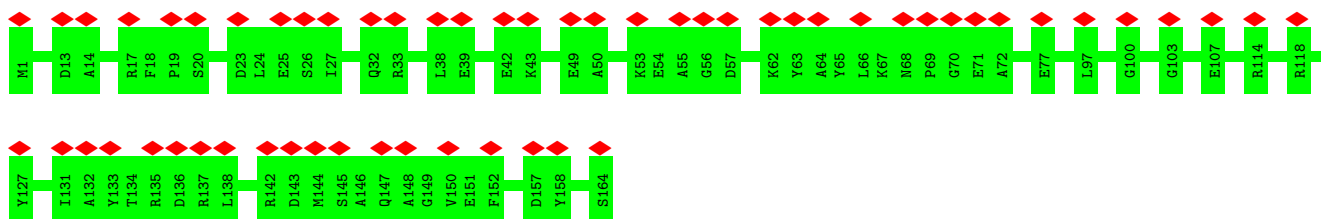


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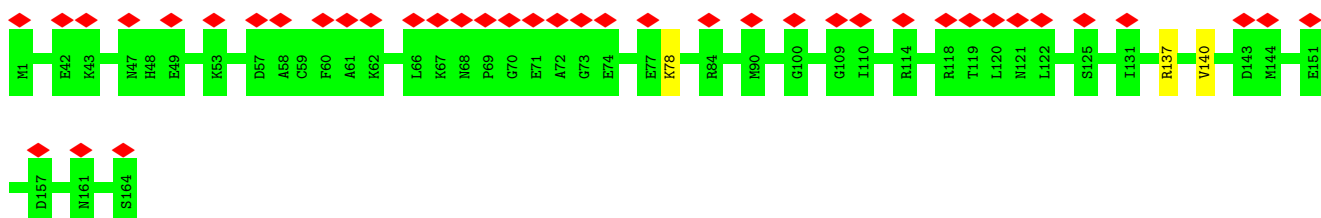




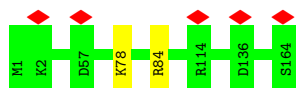
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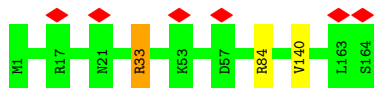
• Molecule 1: Phycoerythrin alpha subunit



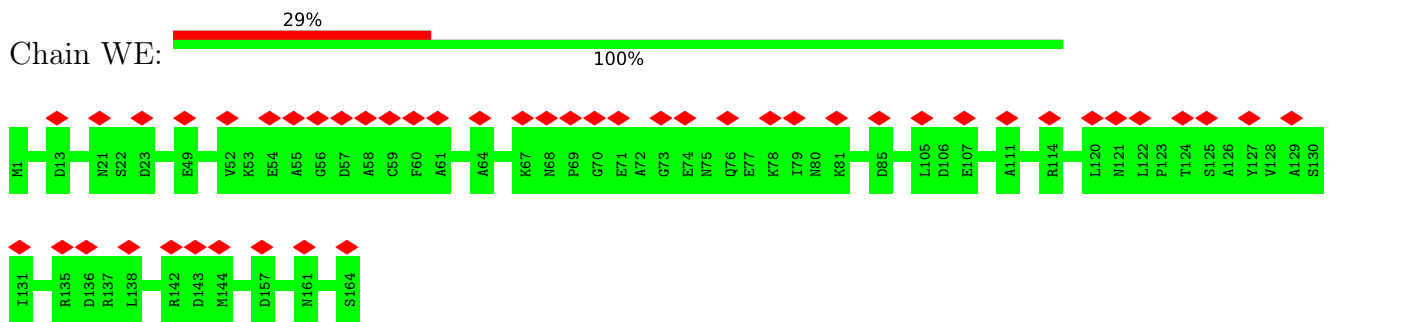
• Molecule 1: Phycoerythrin alpha subunit



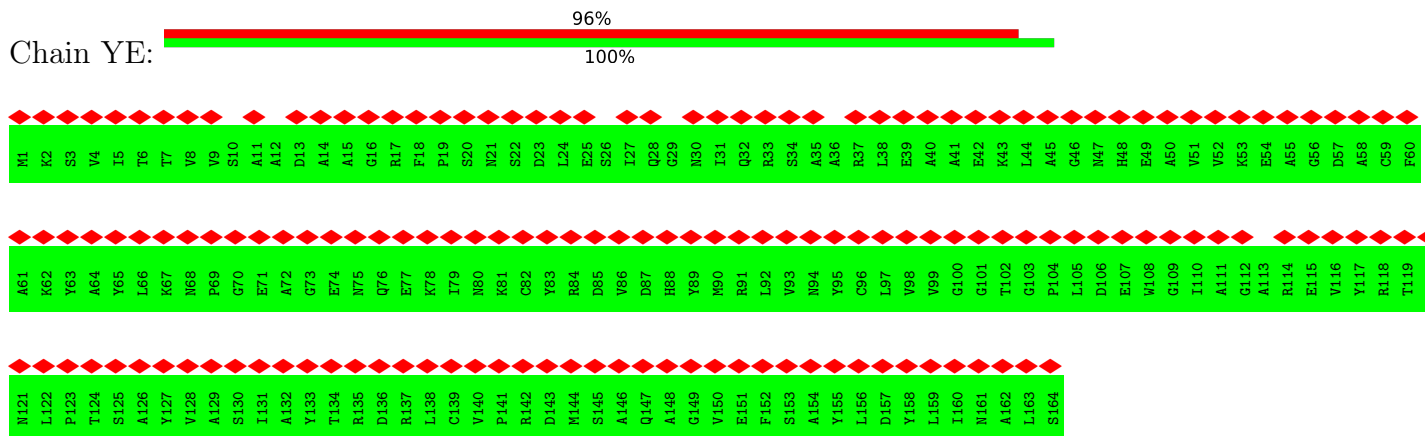
• Molecule 1: Phycoerythrin alpha subunit



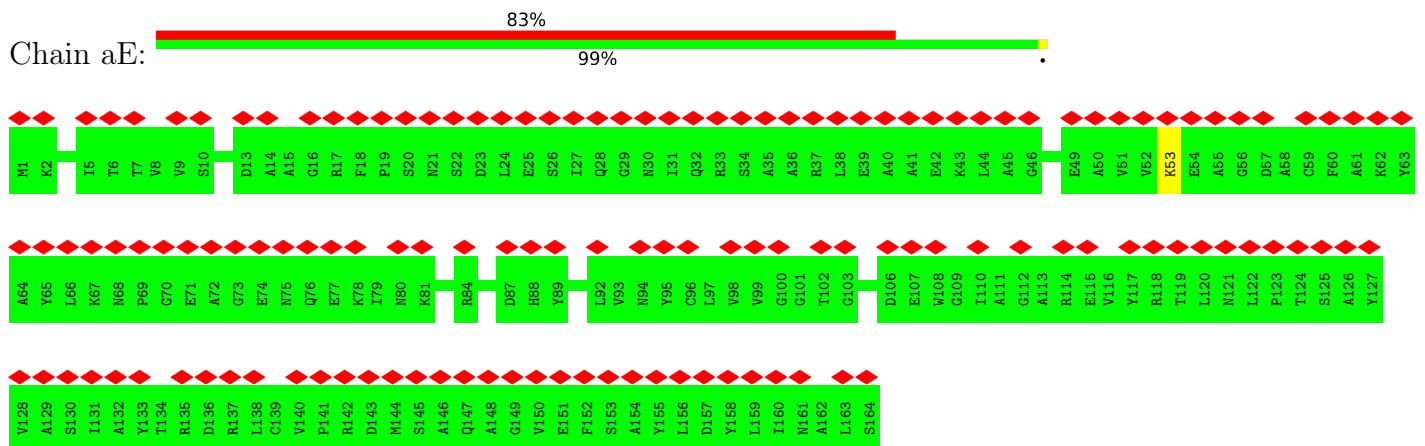
• Molecule 1: Phycoerythrin alpha subunit



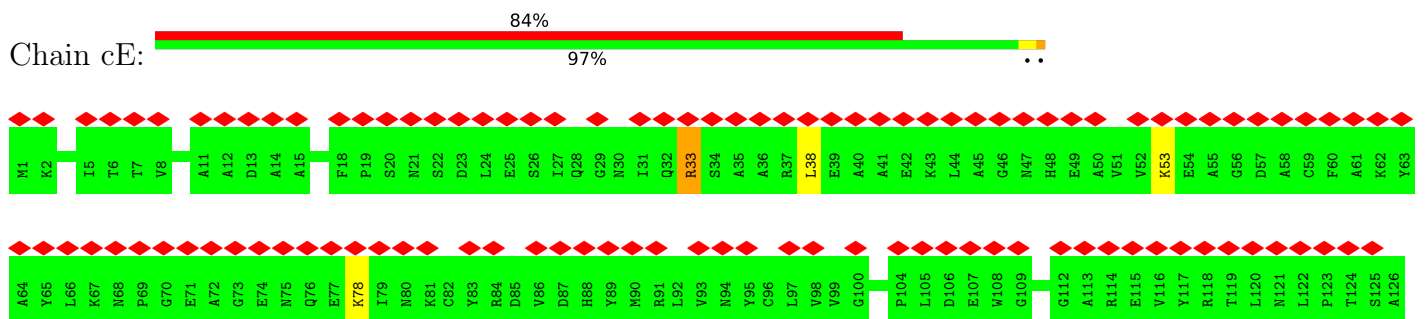
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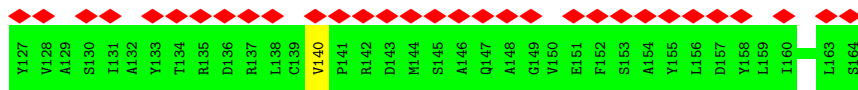


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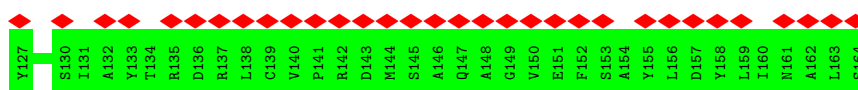
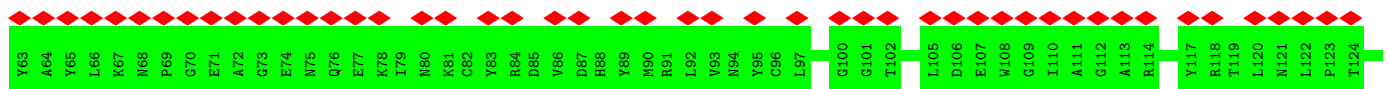
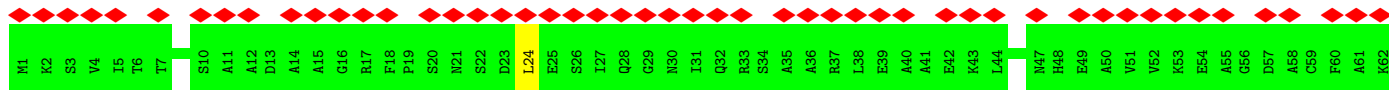
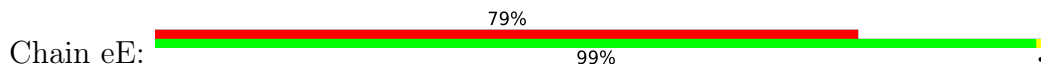


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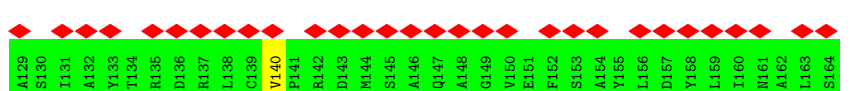
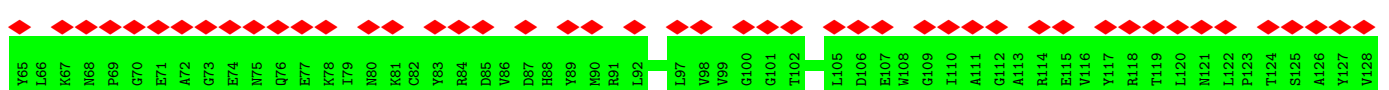
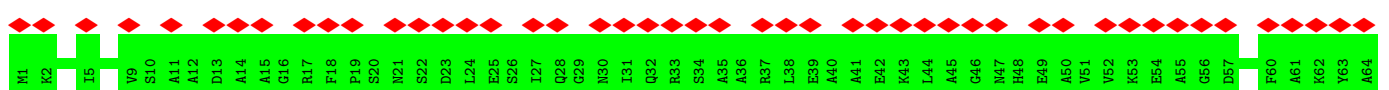
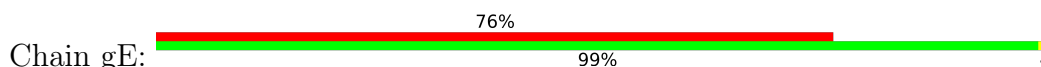




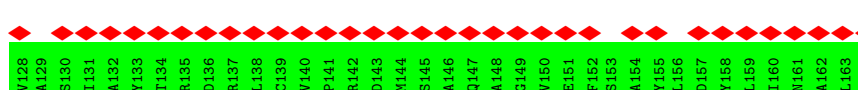
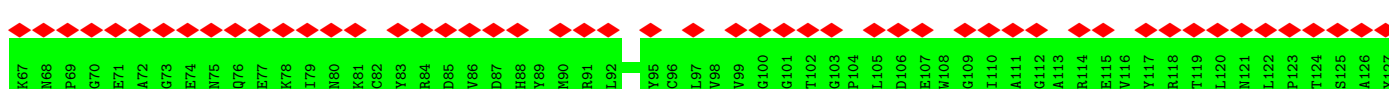
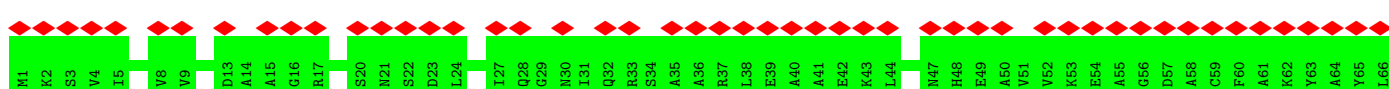
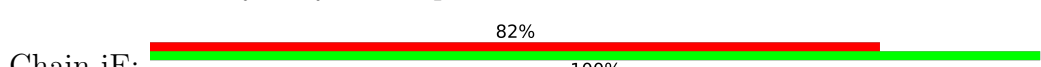
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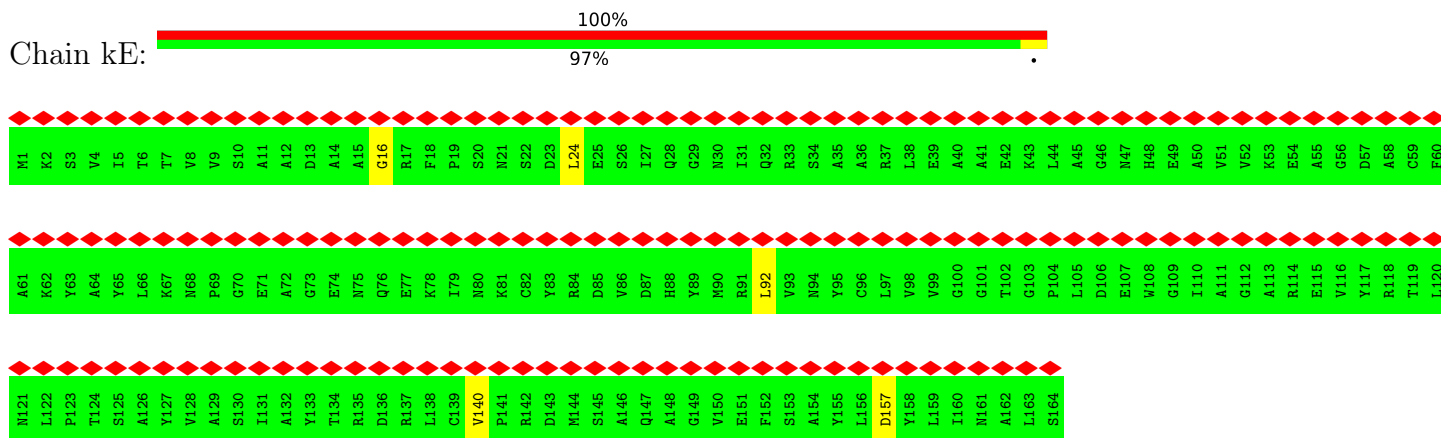
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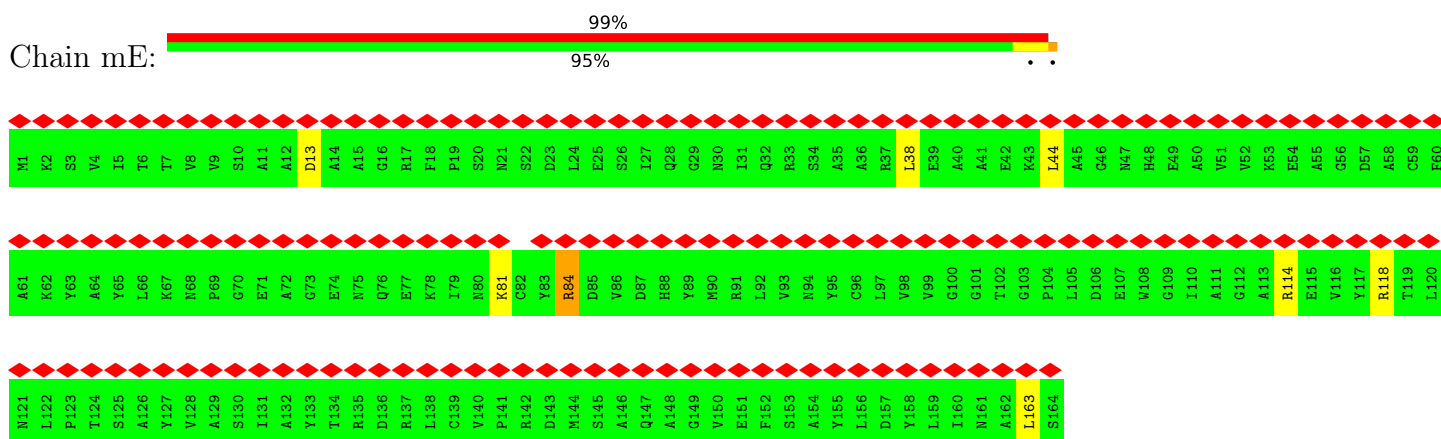
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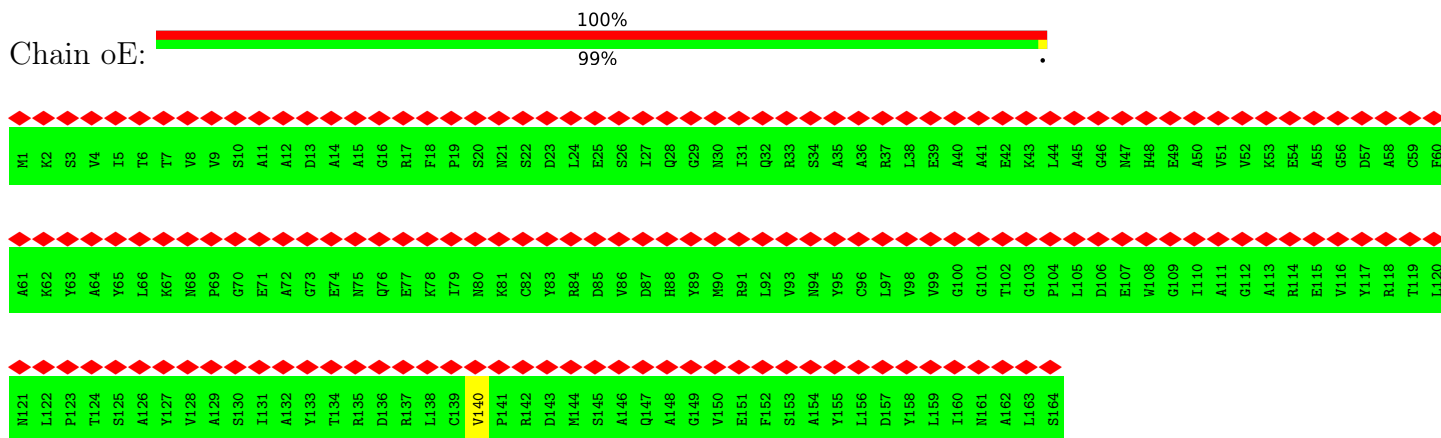
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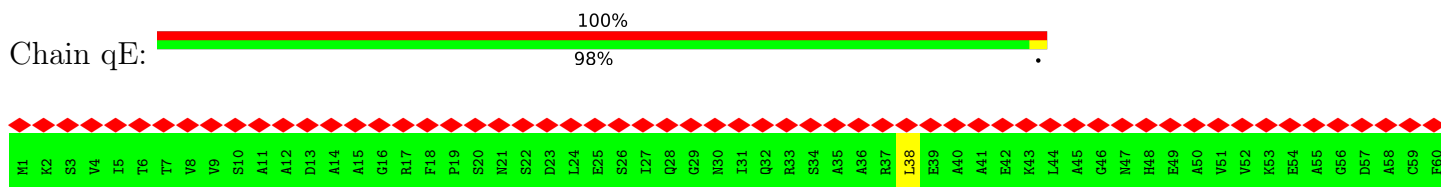
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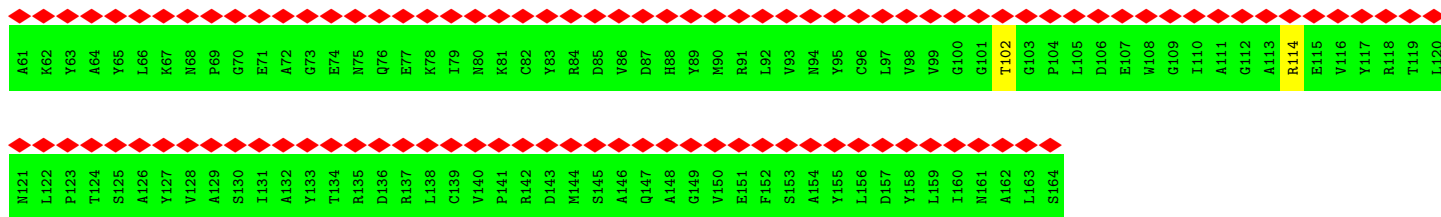


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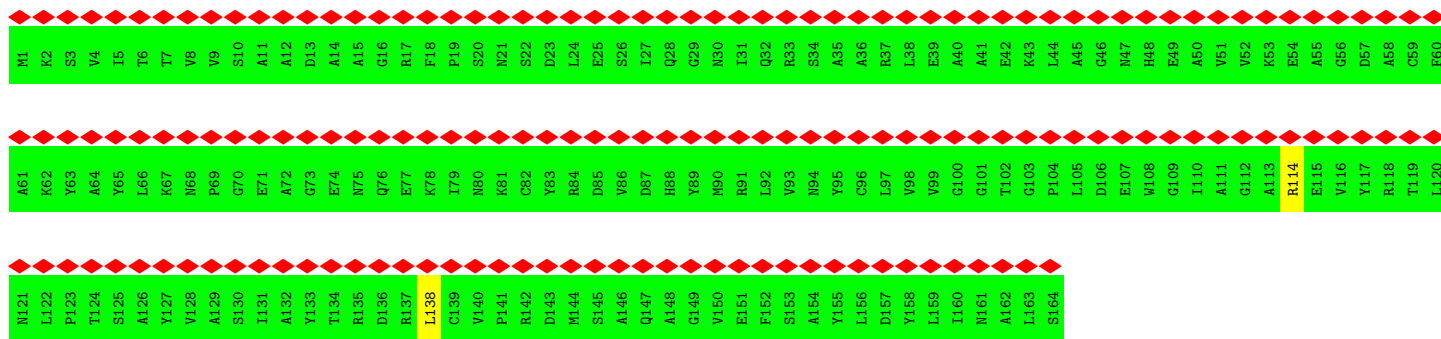


• Molecule 1: Phycoerythrin alpha subunit

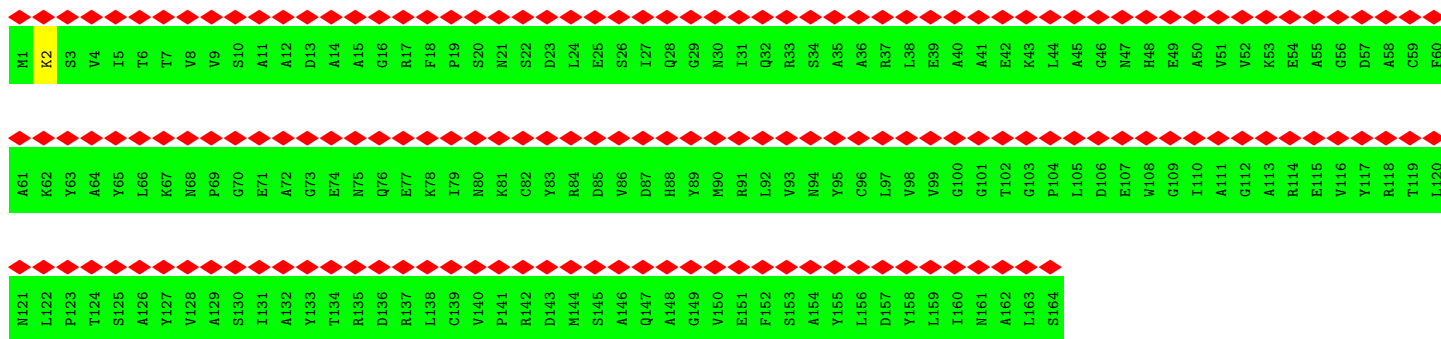




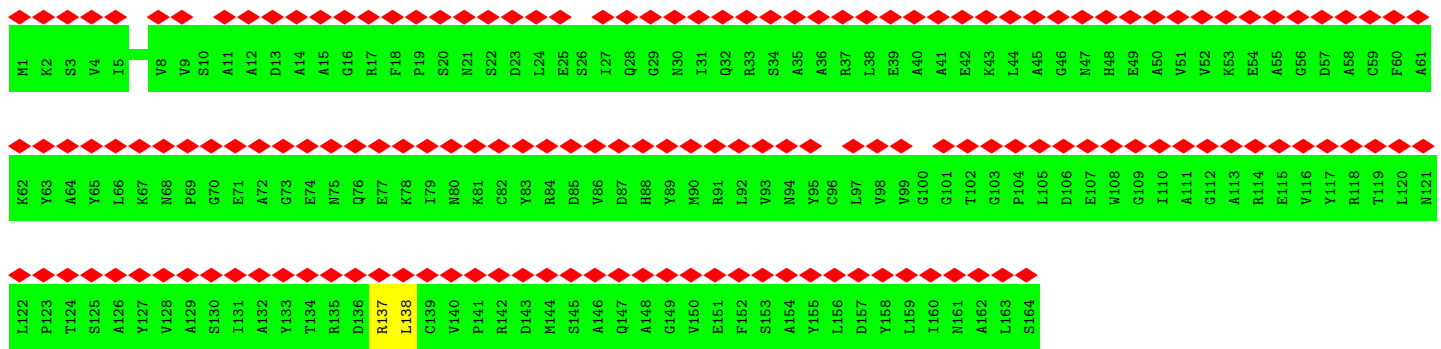
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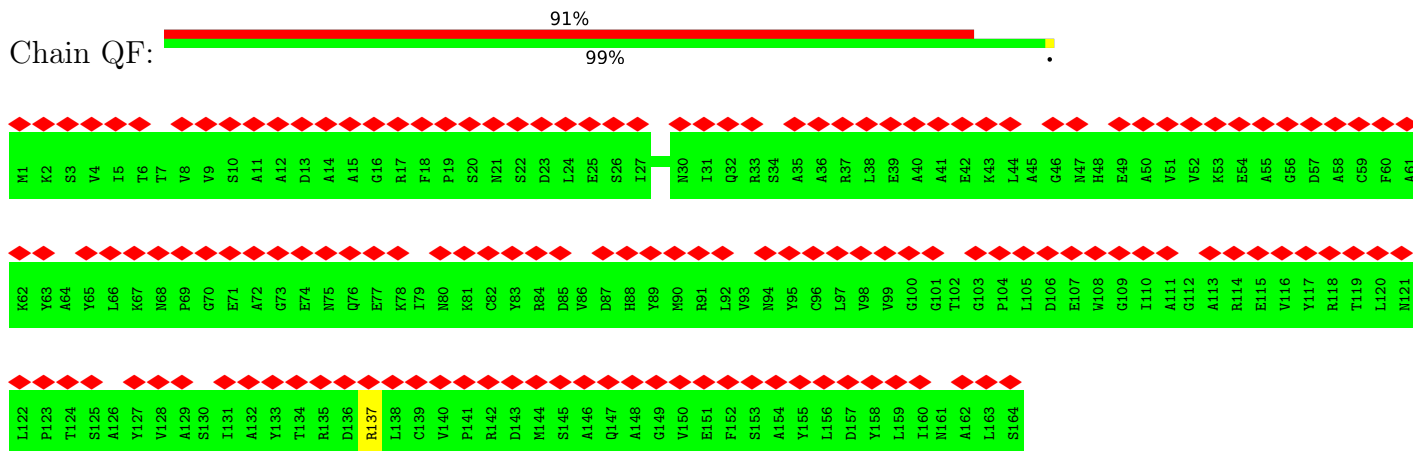
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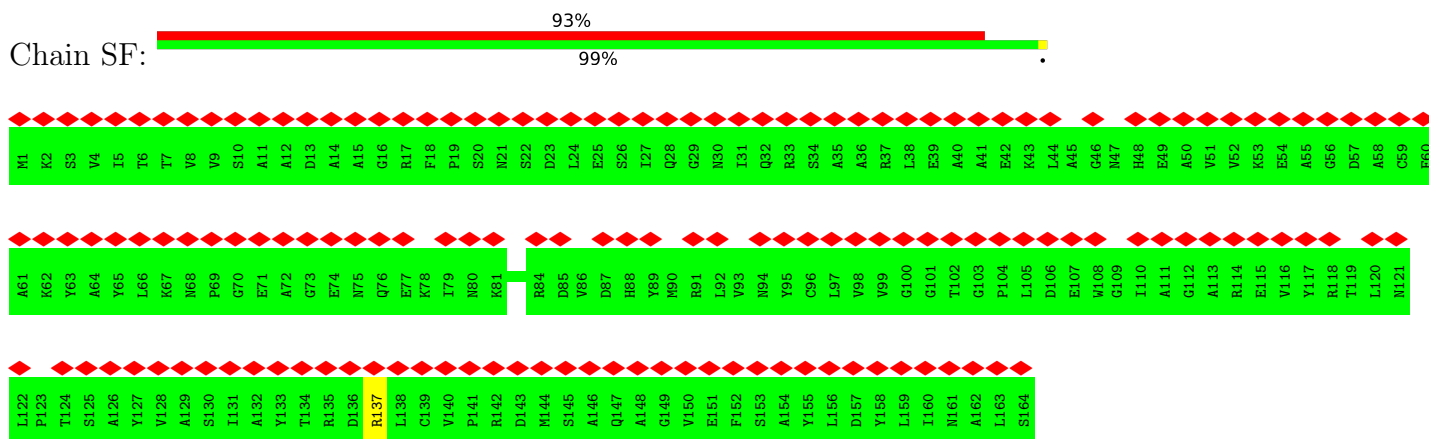
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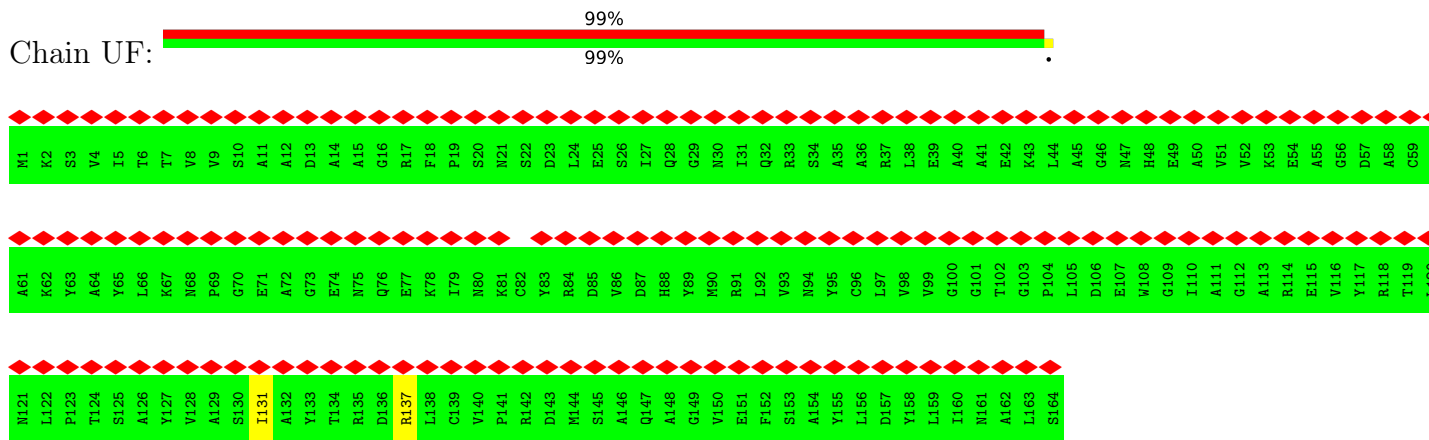
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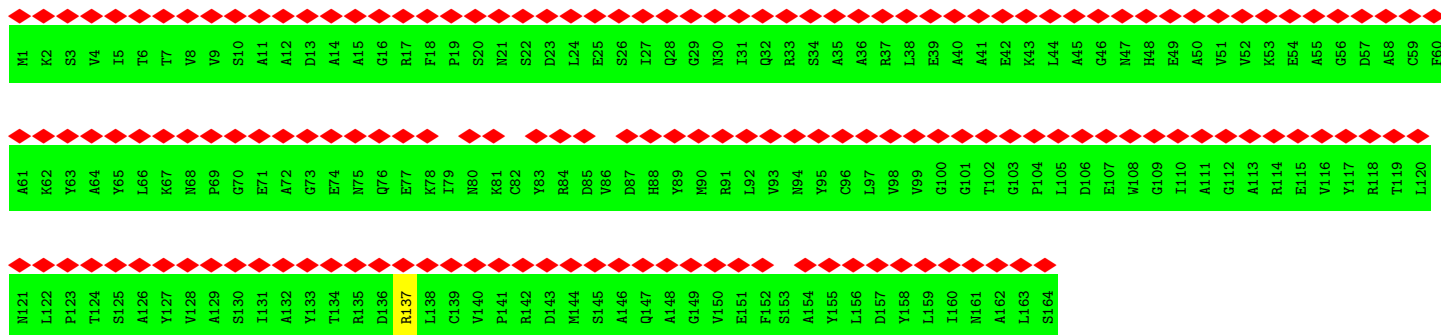


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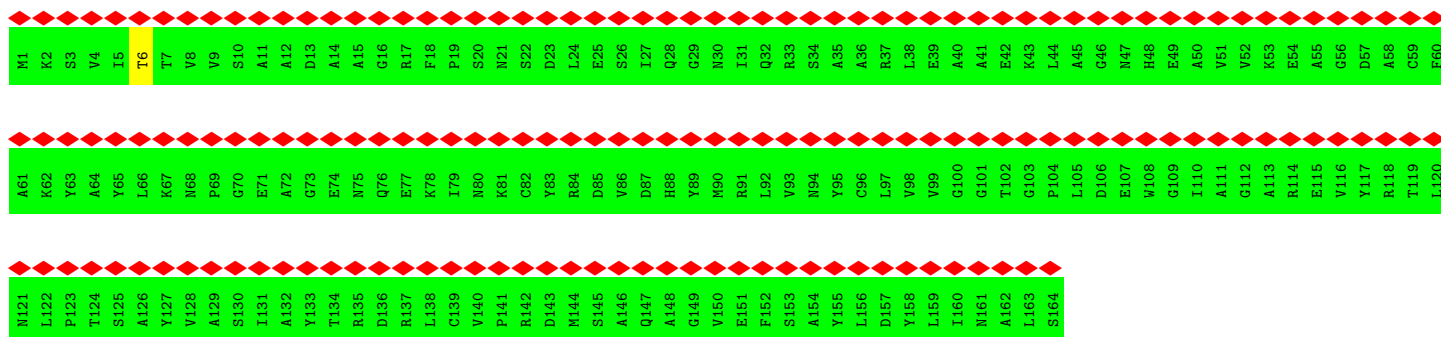


• Molecule 1: Phycoerythrin alpha subunit

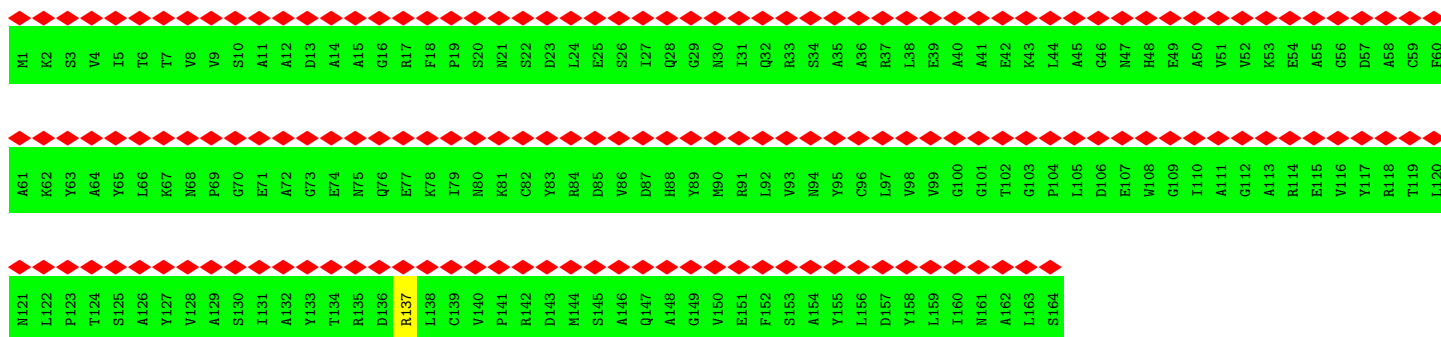




• Molecule 1: Phycoerythrin alpha subunit



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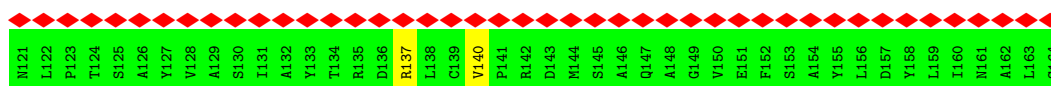
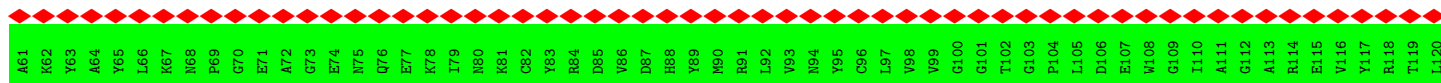
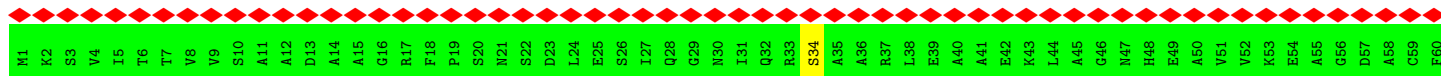


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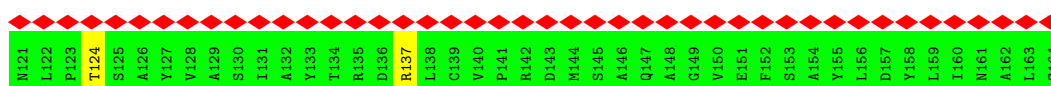
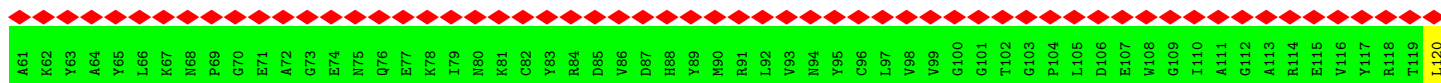
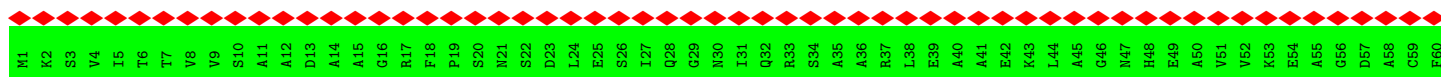




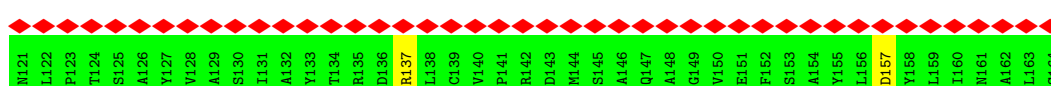
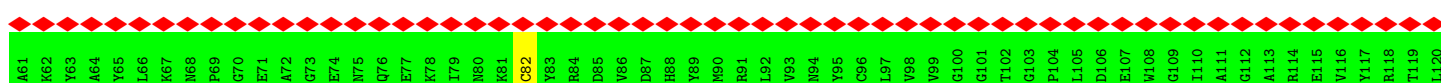
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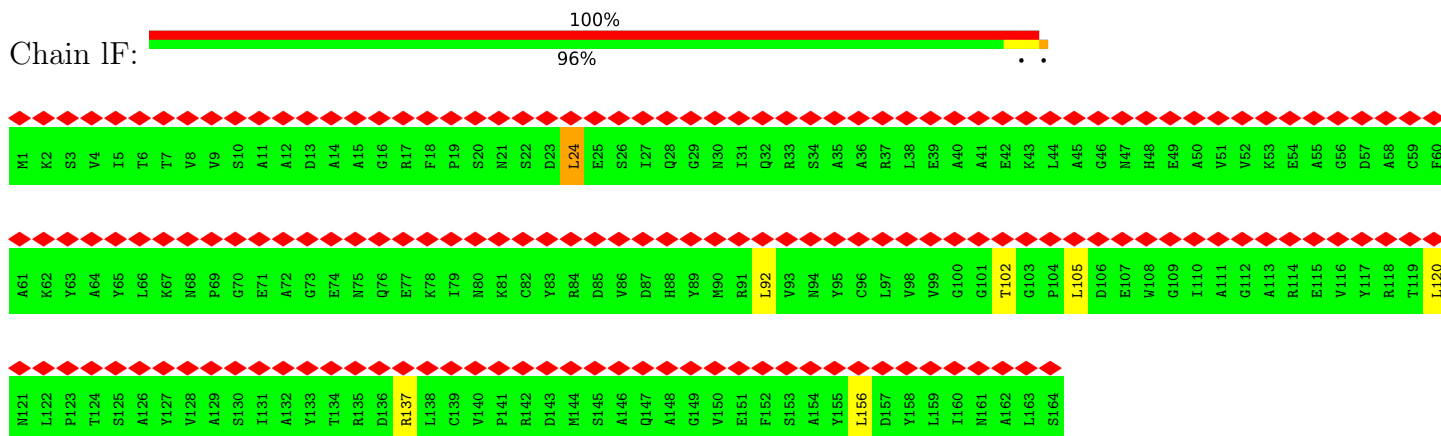
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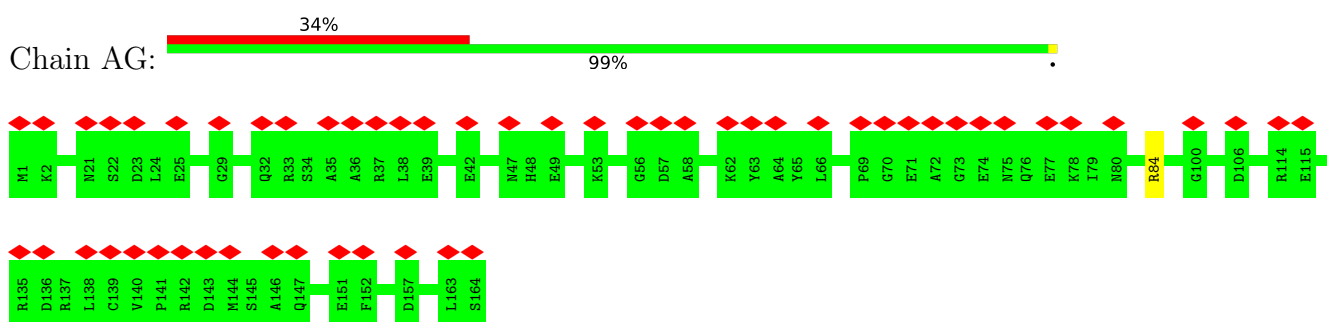
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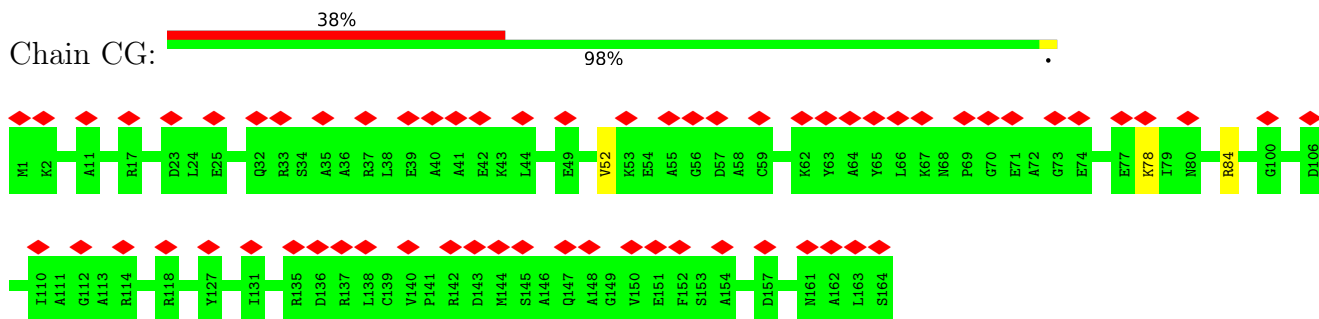
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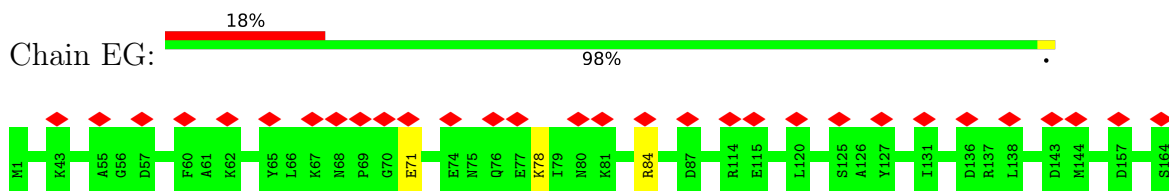
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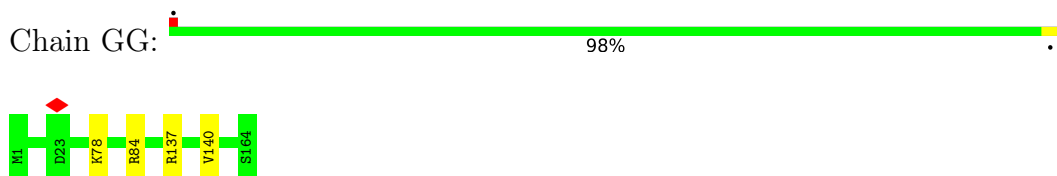
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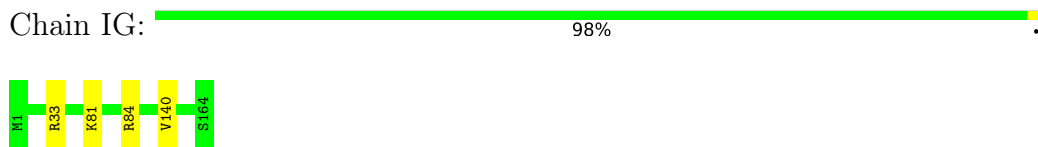
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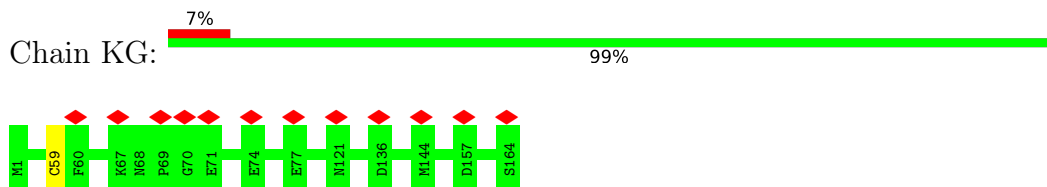
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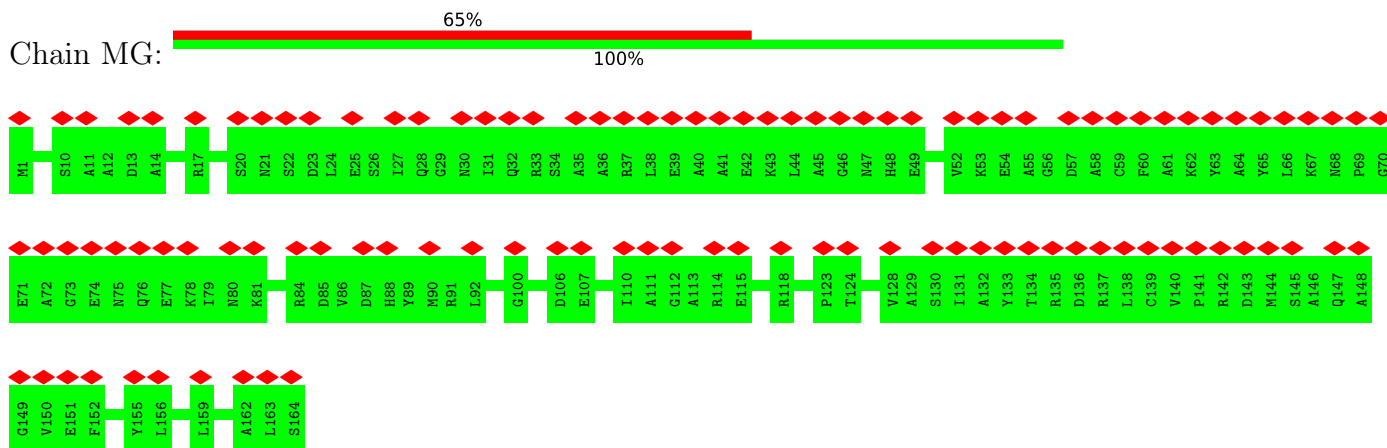
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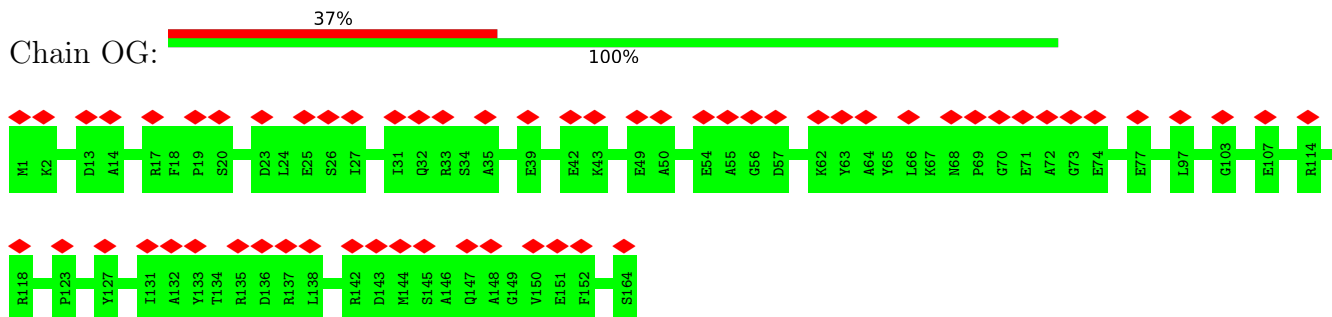
• Molecule 1: Phycoerythrin alpha subunit



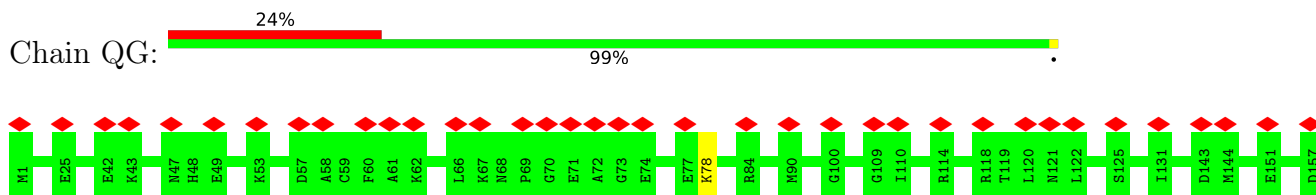
• Molecule 1: Phycoerythrin alpha subunit



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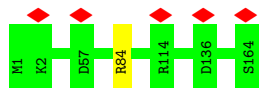


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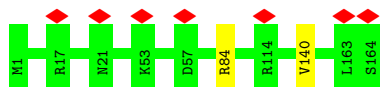




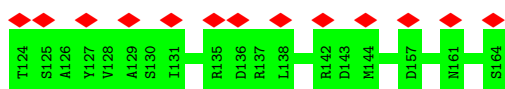
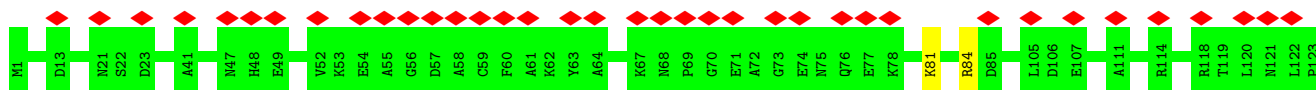
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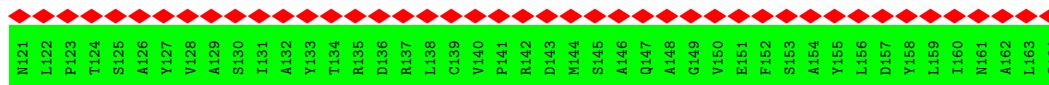
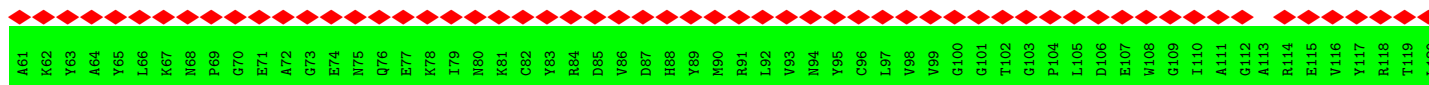
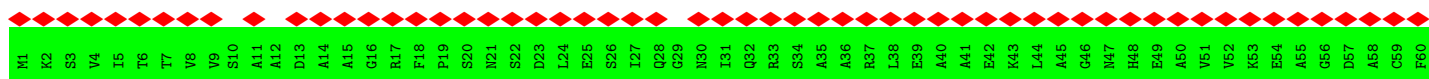
• Molecule 1: Phycoerythrin alpha subunit



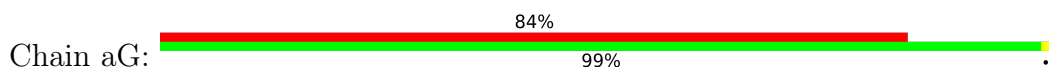
• Molecule 1: Phycoerythrin alpha subunit

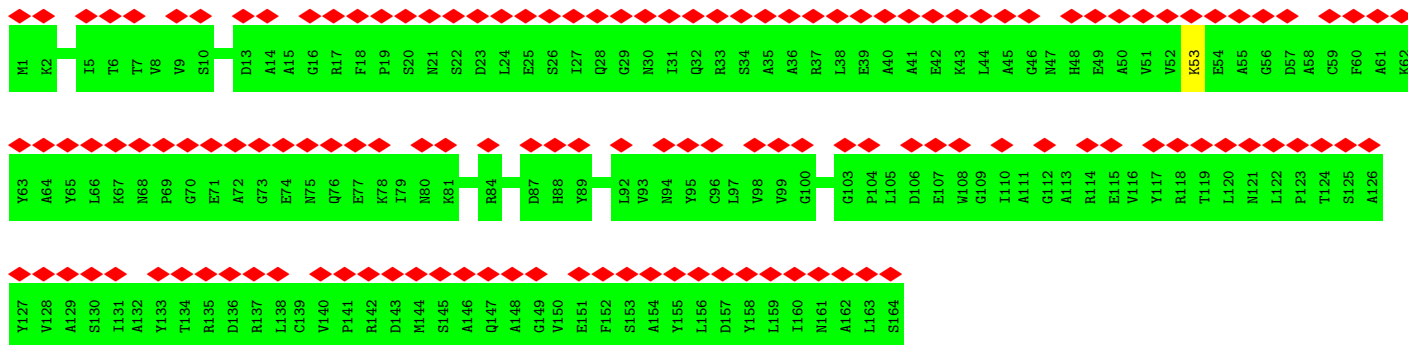


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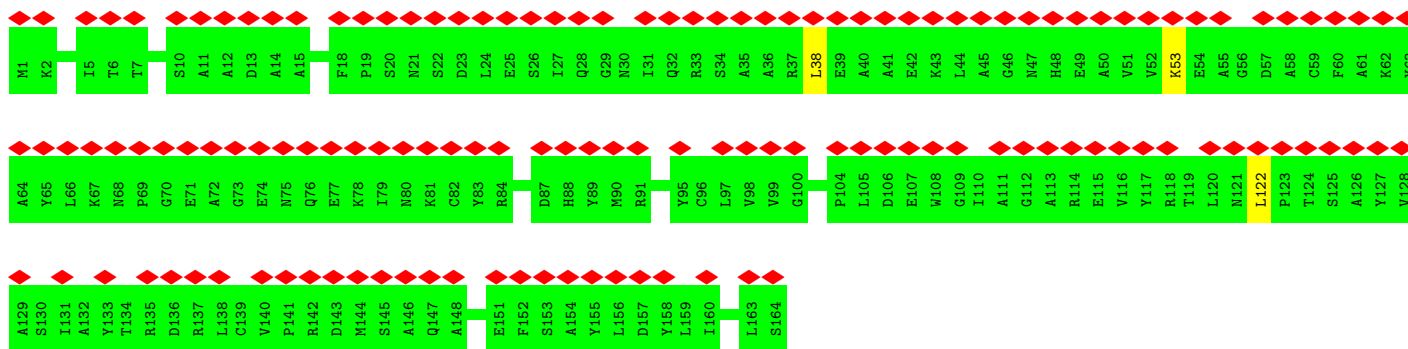
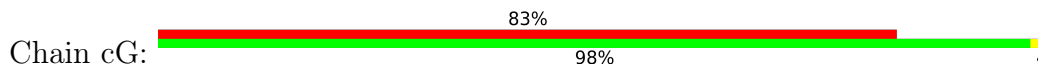


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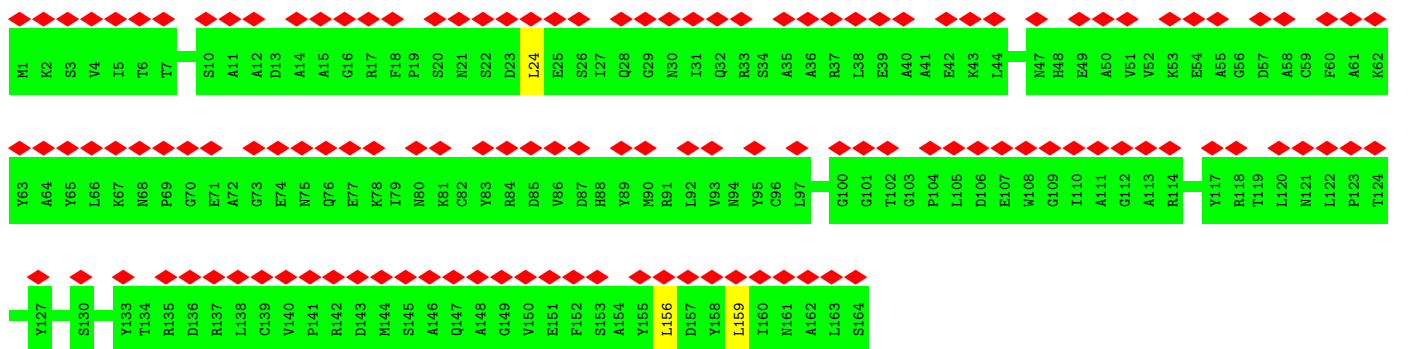
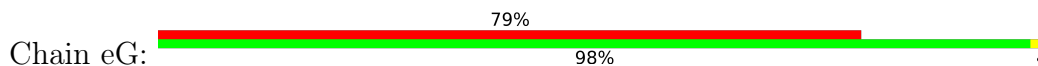




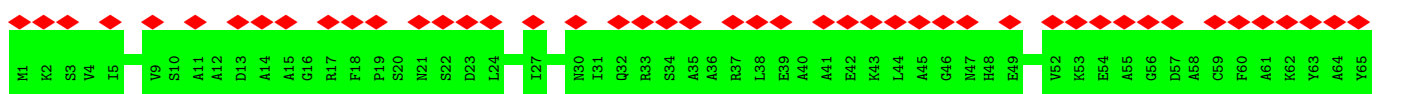
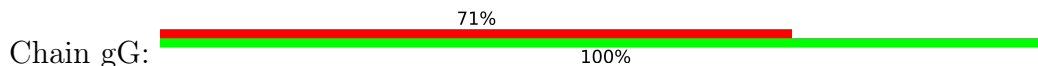
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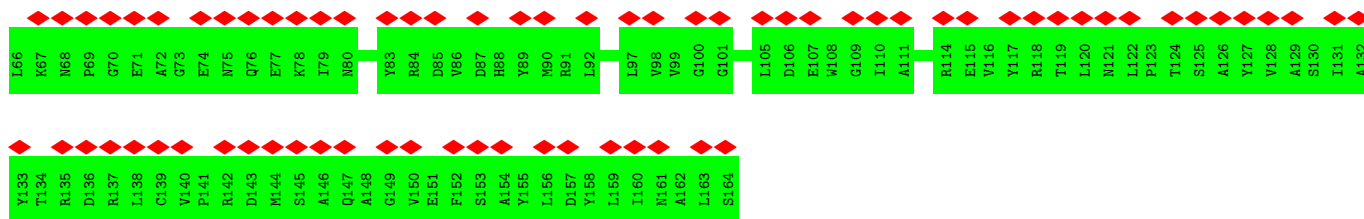


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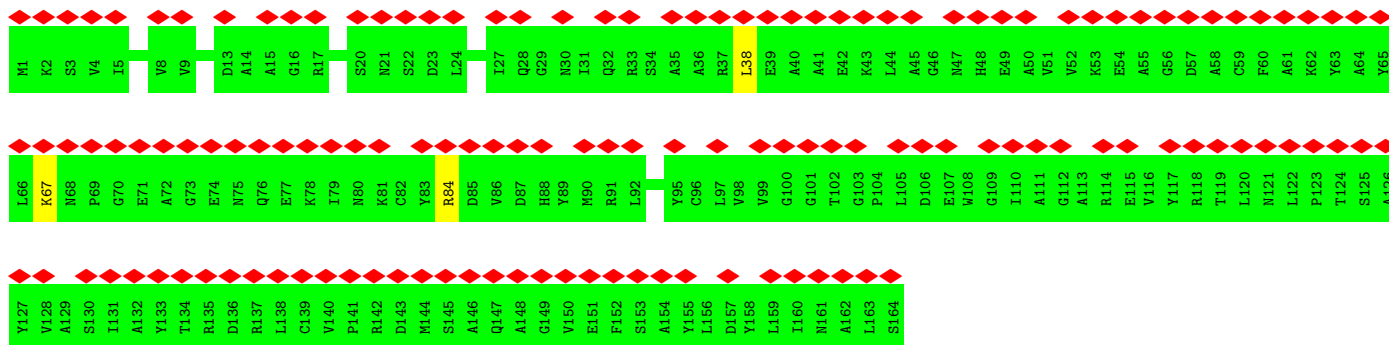
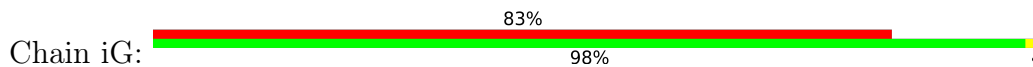


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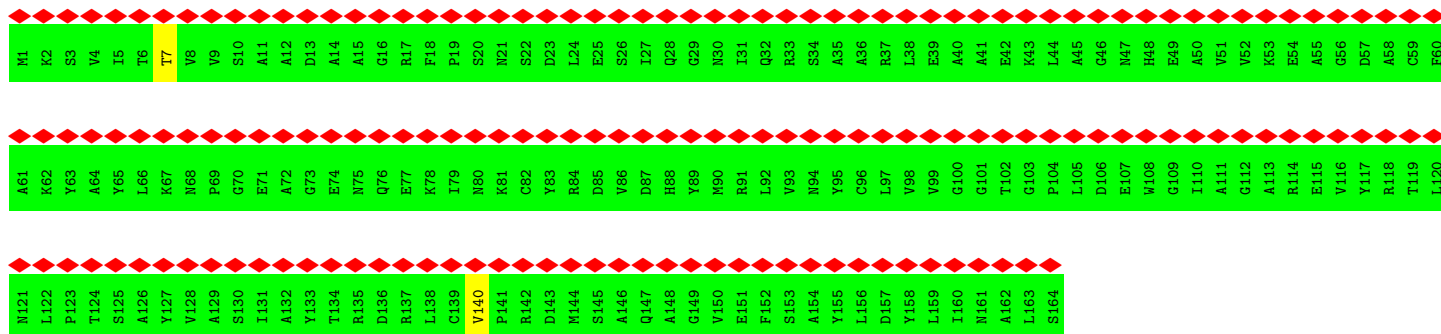




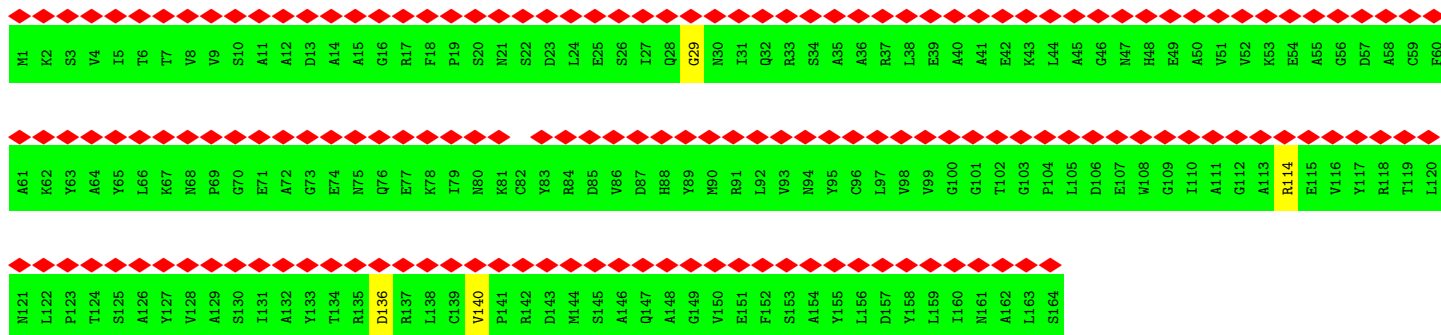
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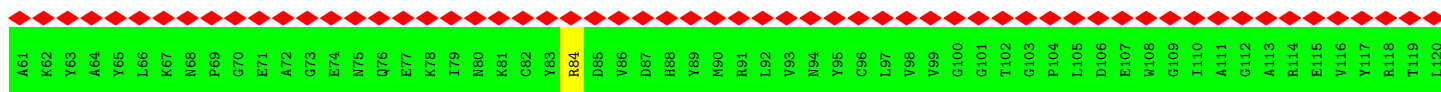


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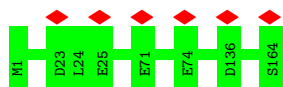


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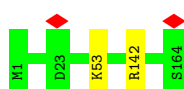




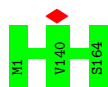
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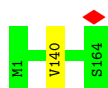


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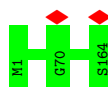


There are no outlier residues recorded for this chain.

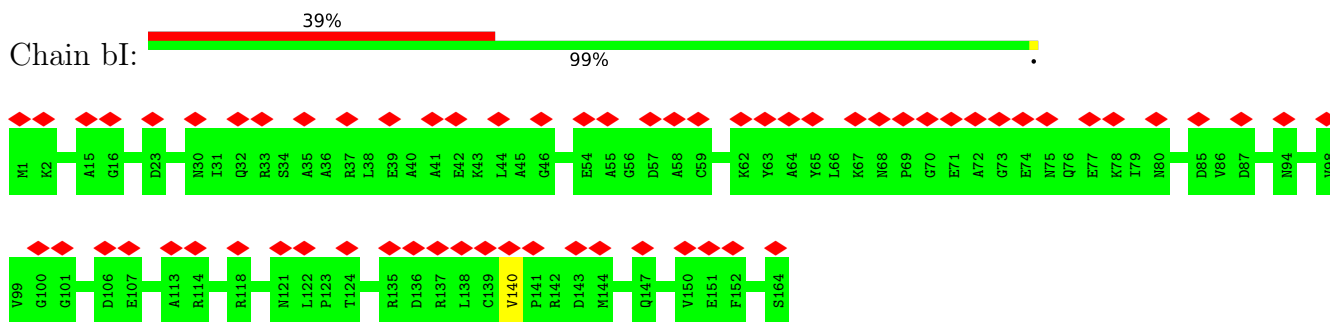
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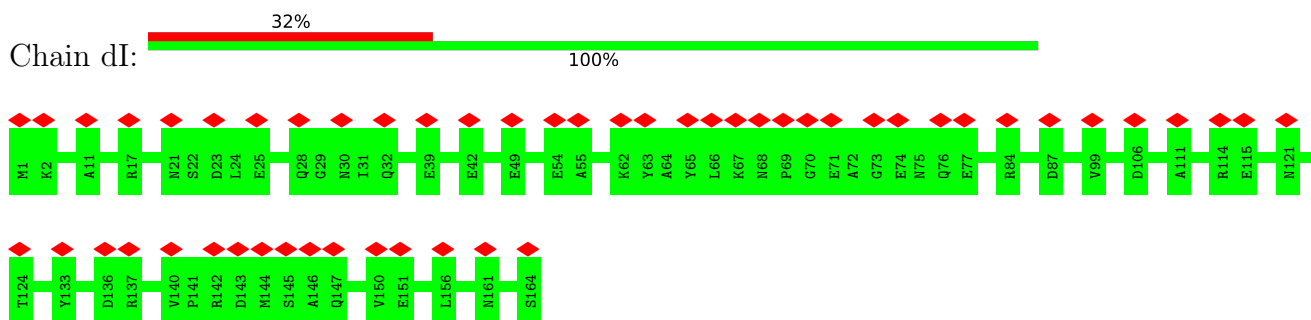
- Molecule 1: Phycoerythrin alpha subunit



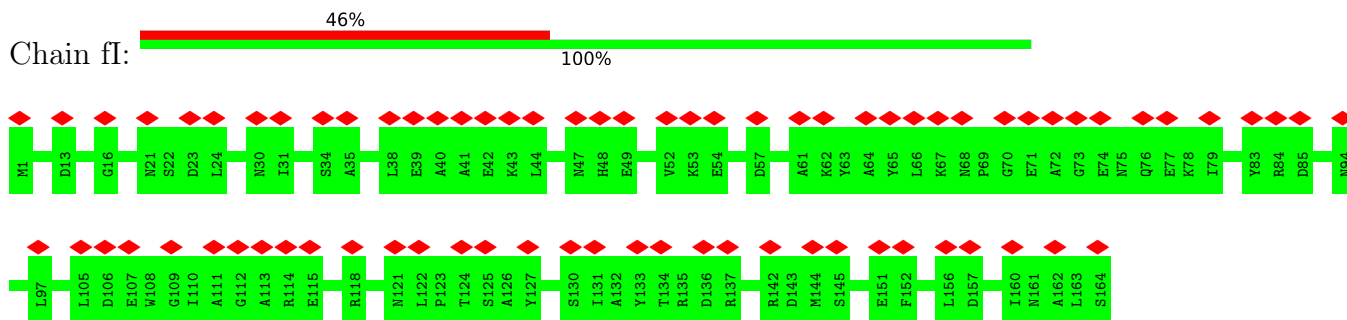
- Molecule 1: Phycoerythrin alpha subunit



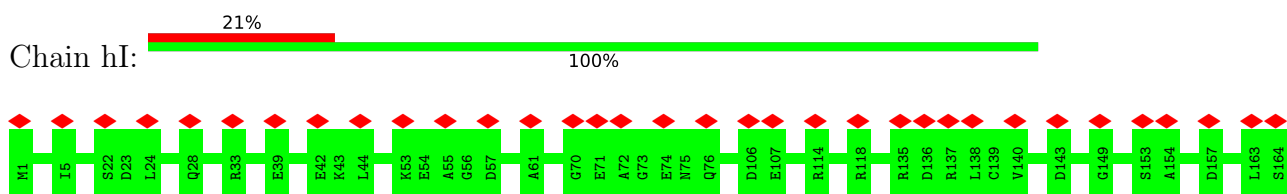
- Molecule 1: Phycoerythrin alpha subunit



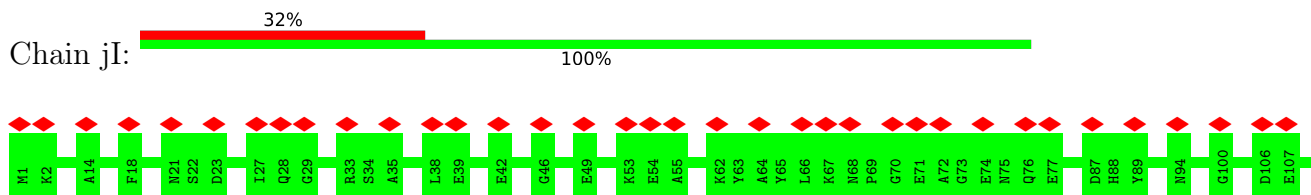
- Molecule 1: Phycoerythrin alpha subunit

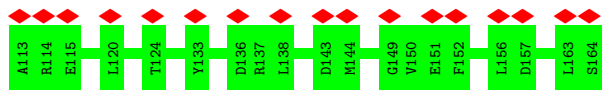


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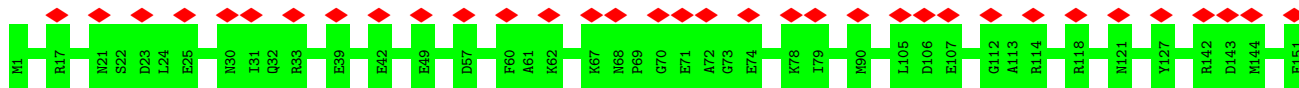


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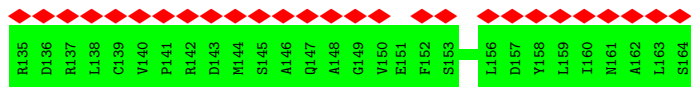
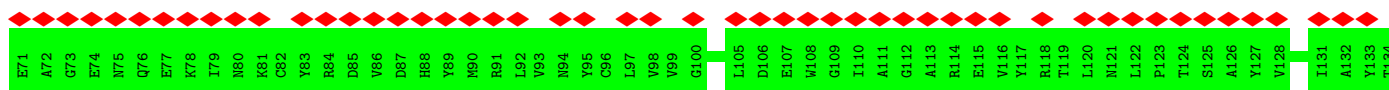
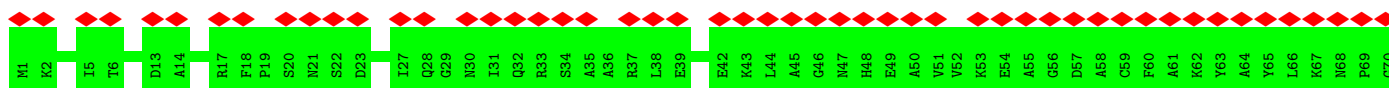
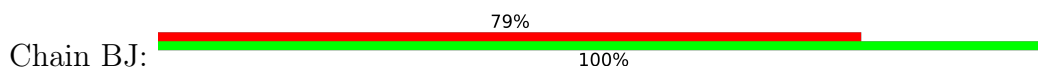




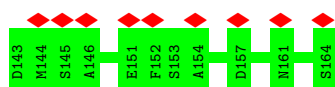
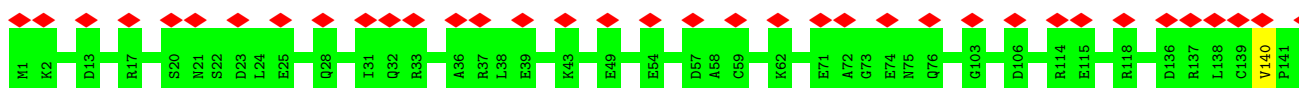
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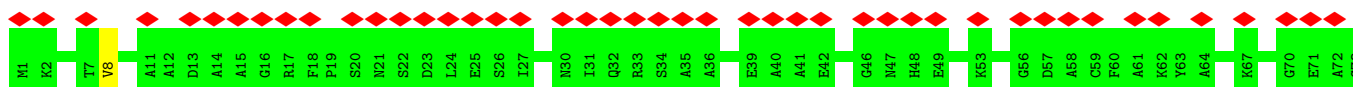
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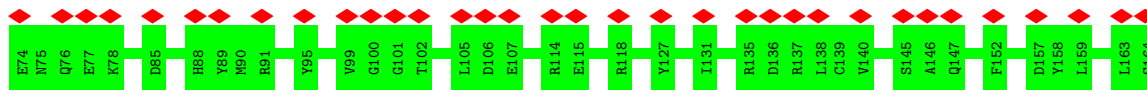


• Molecule 1: Phycoerythrin alpha subunit

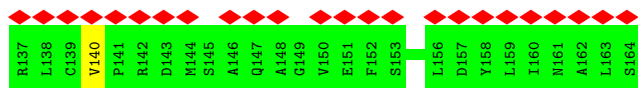
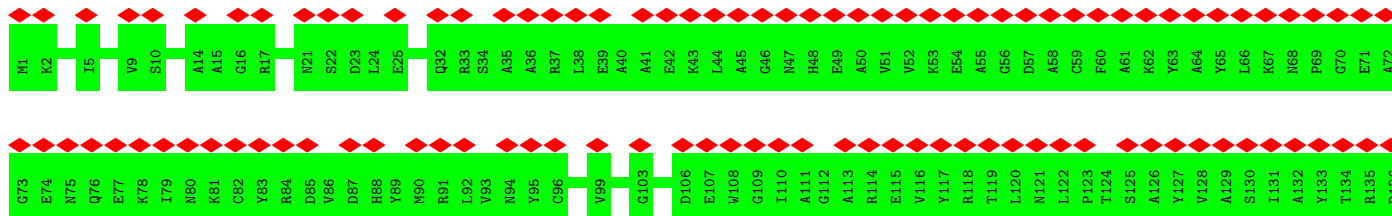
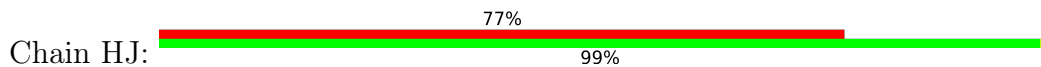


• Molecule 1: Phycoerythrin alpha subunit

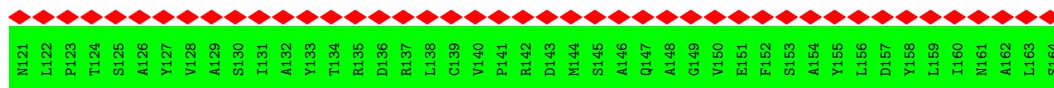
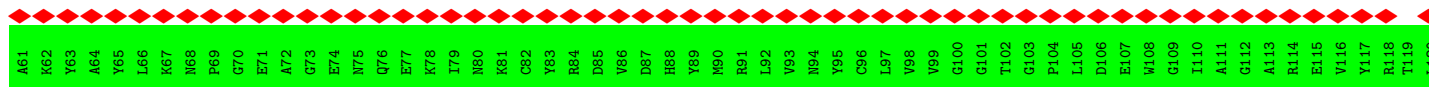
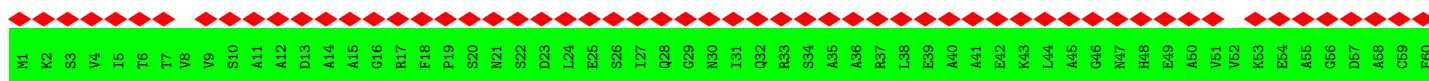




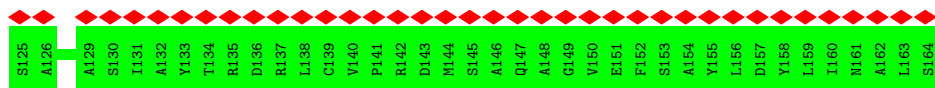
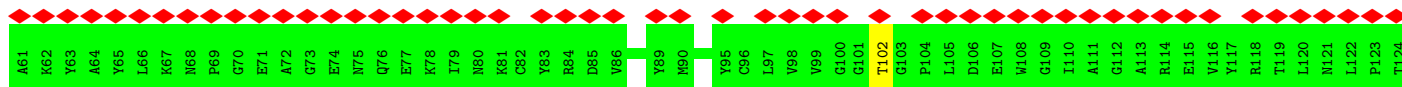
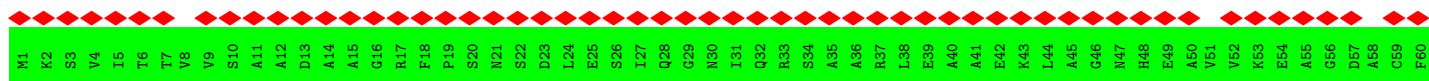
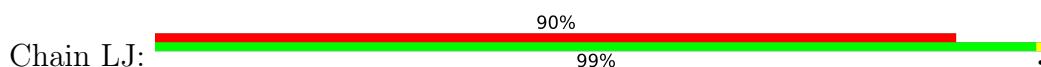
• Molecule 1: Phycoerythrin alpha subunit



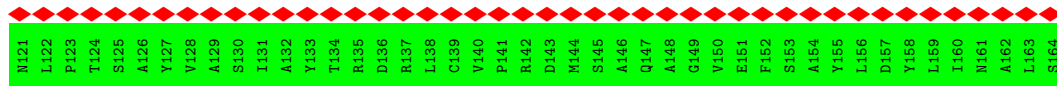
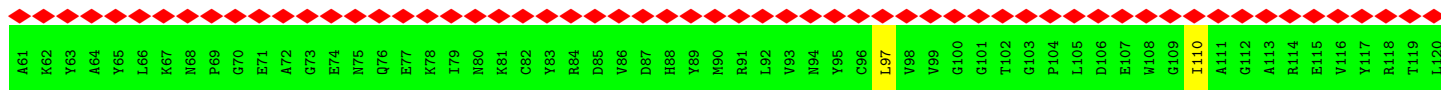
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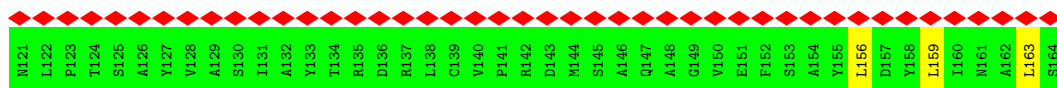
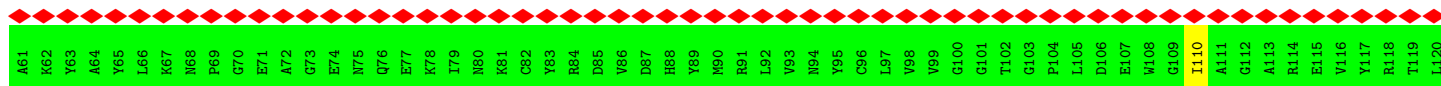
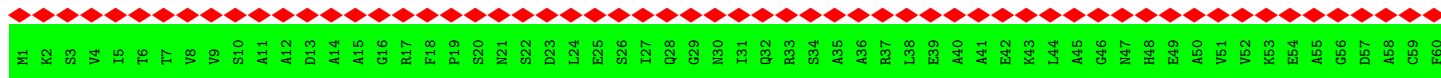
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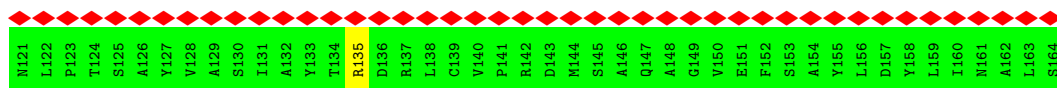
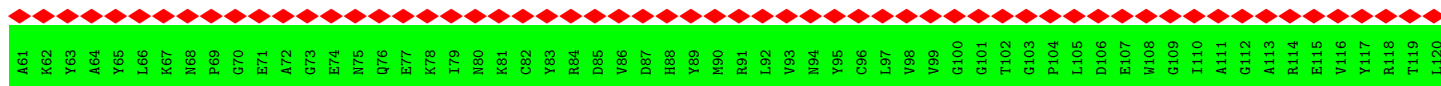
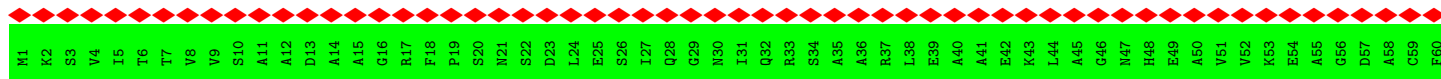
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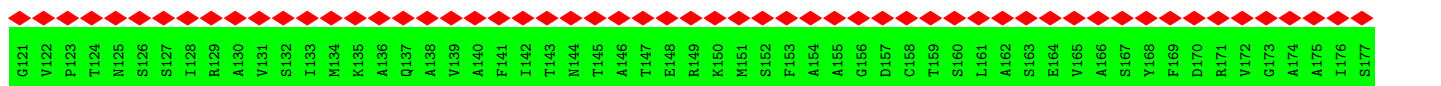
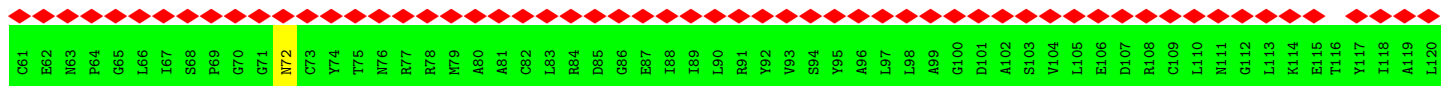
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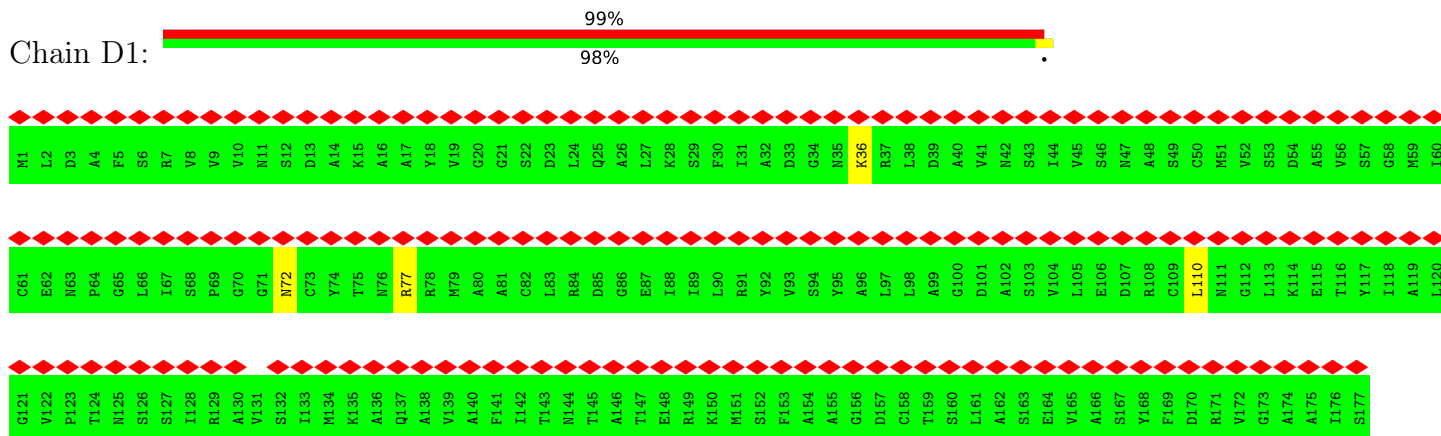
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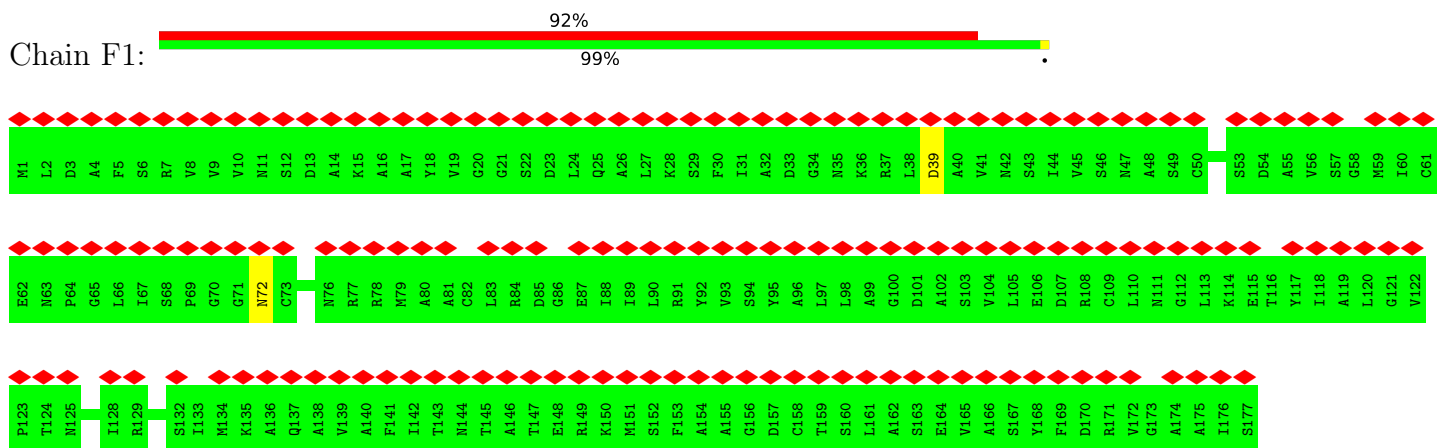
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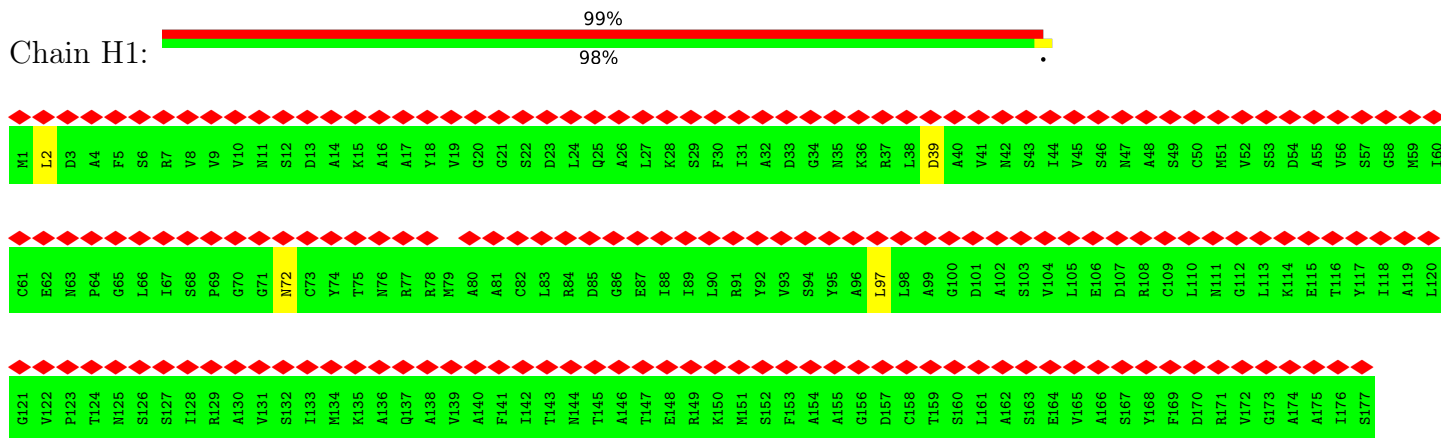
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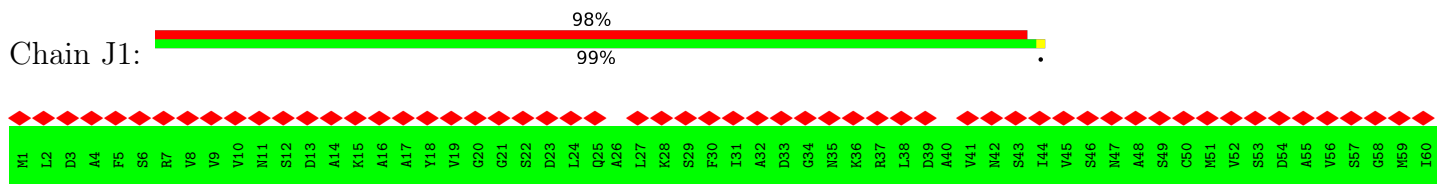
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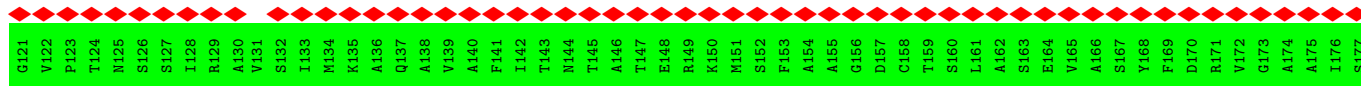
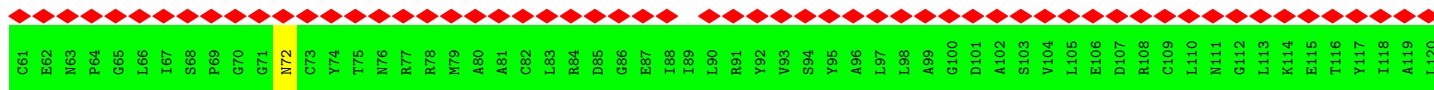


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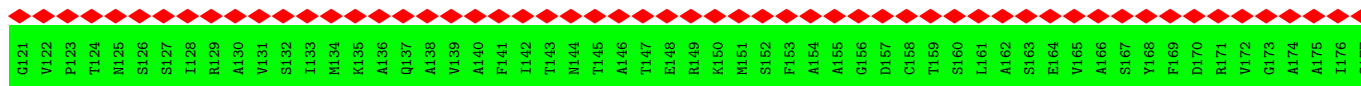
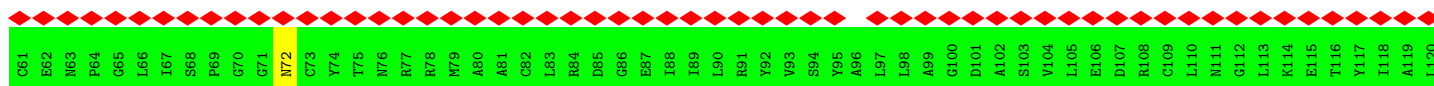
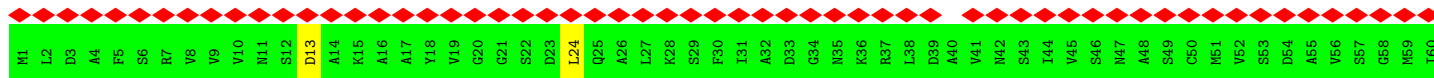


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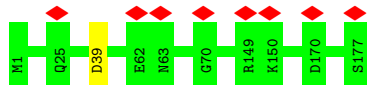




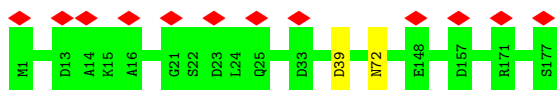
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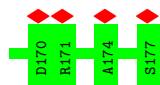
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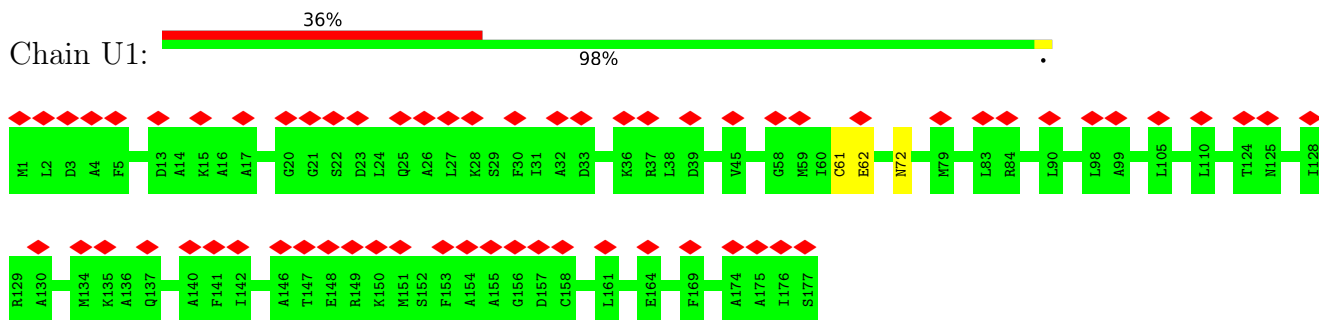
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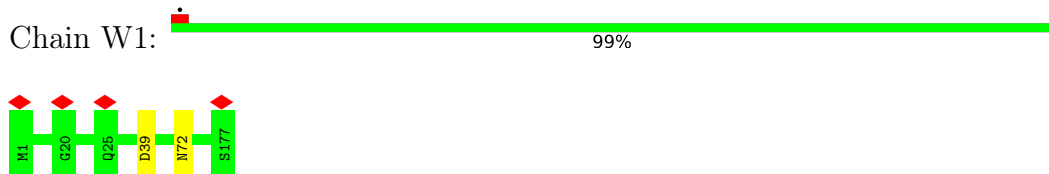
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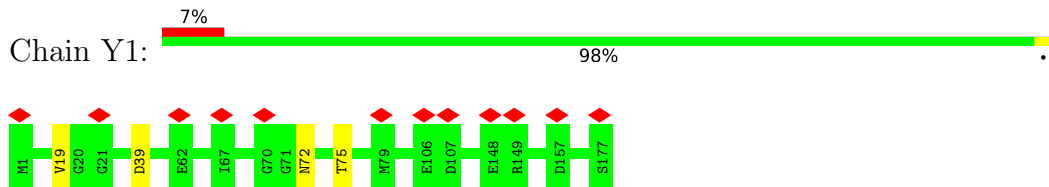
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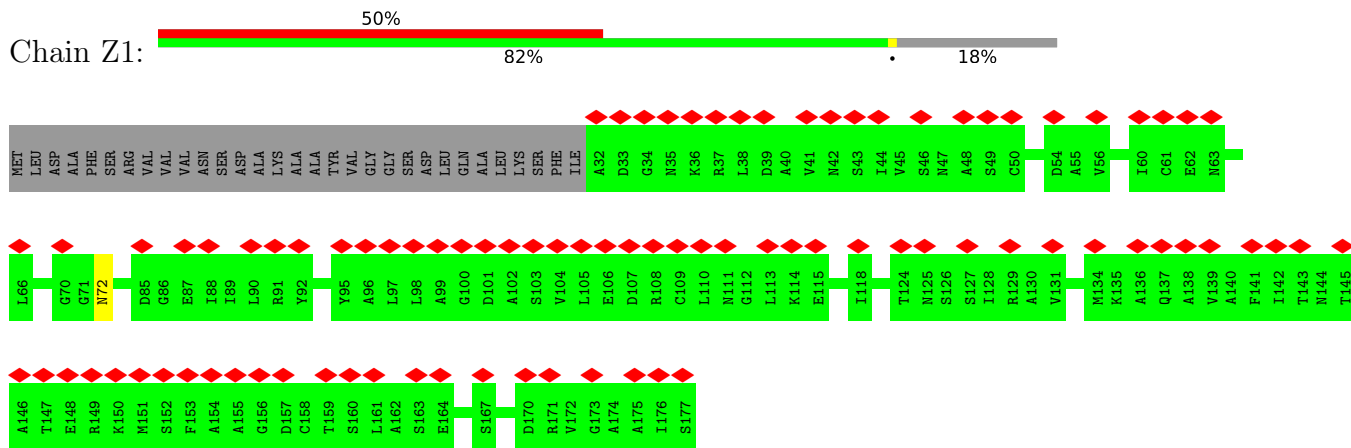
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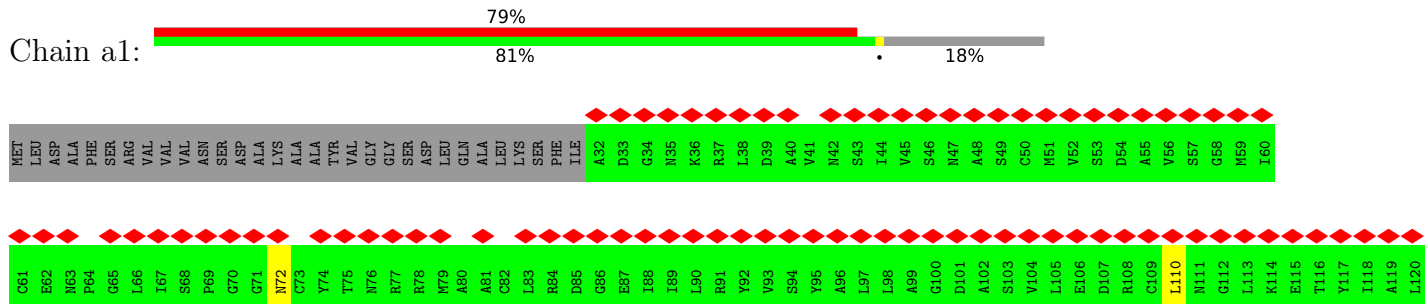
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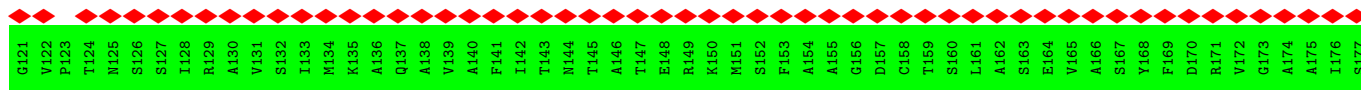


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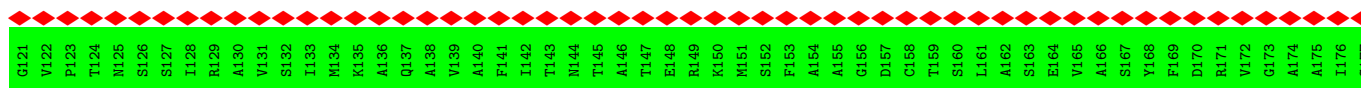
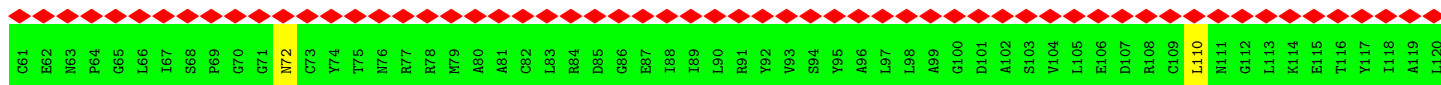
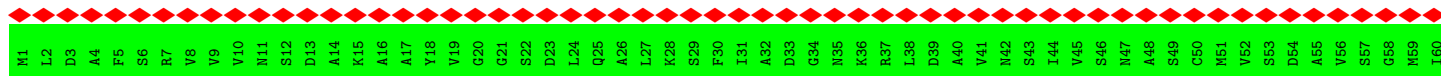


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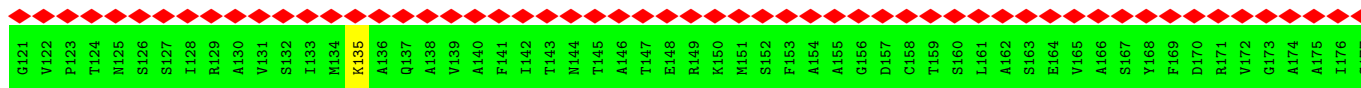
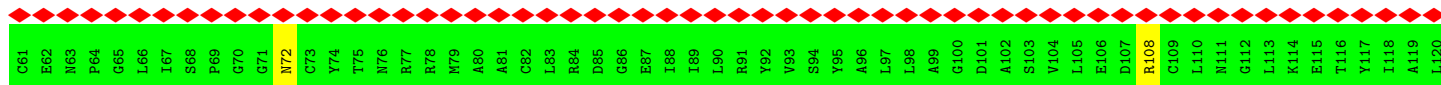
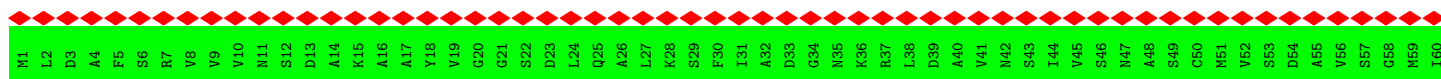




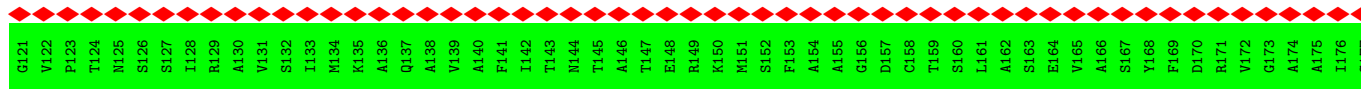
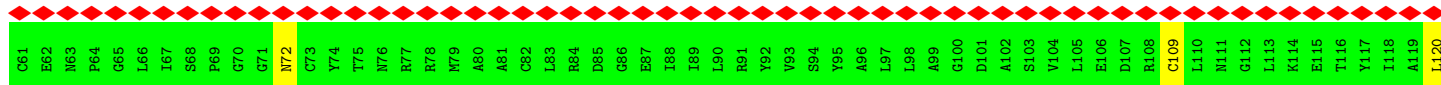
• Molecule 2: B-phycoerythrin beta chain



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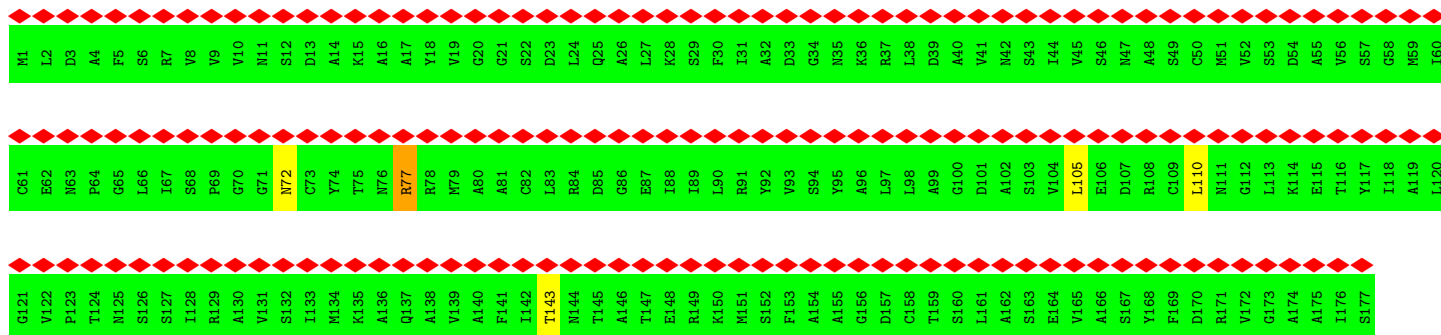


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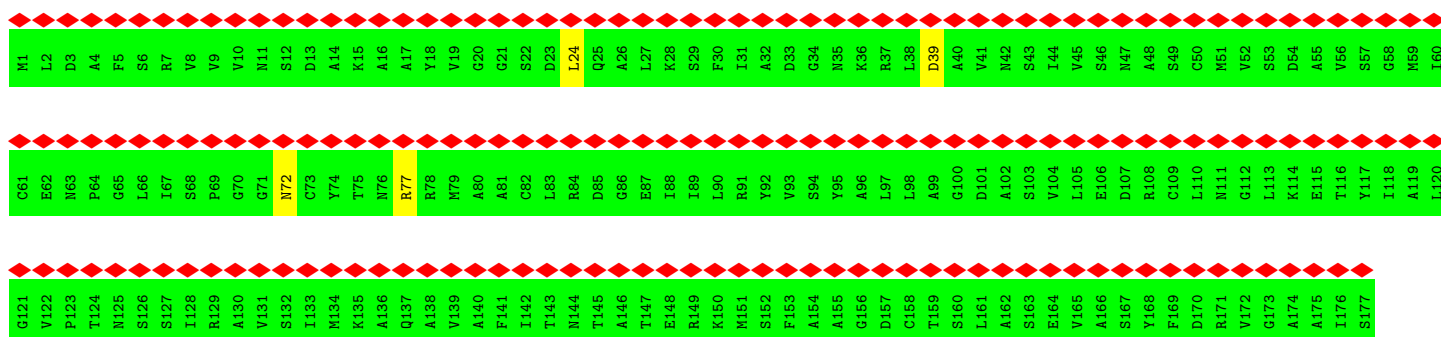


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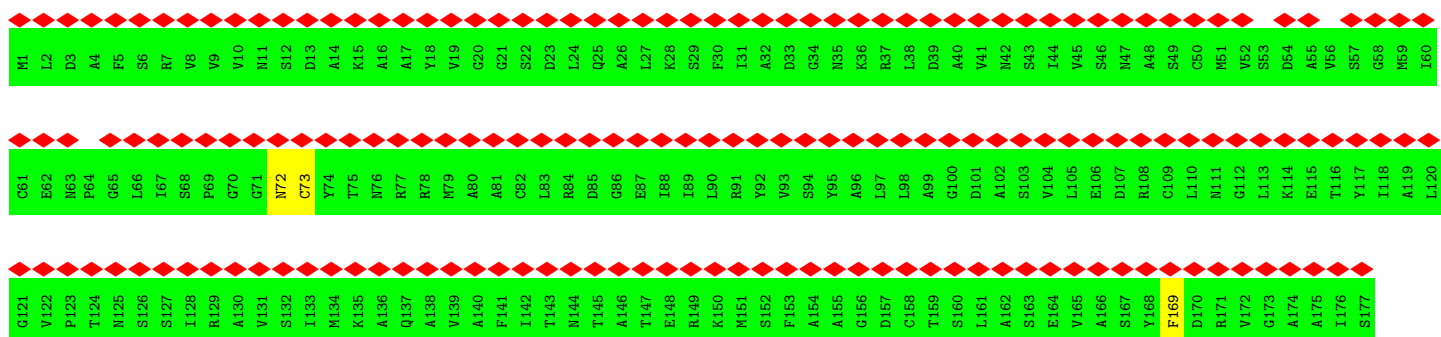




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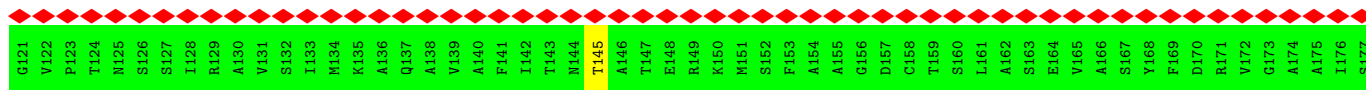


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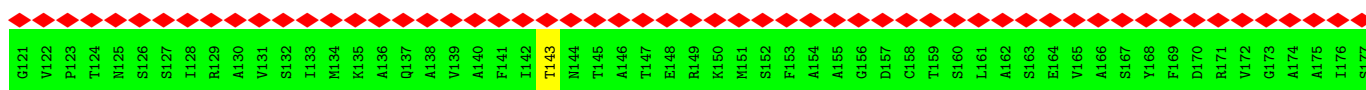
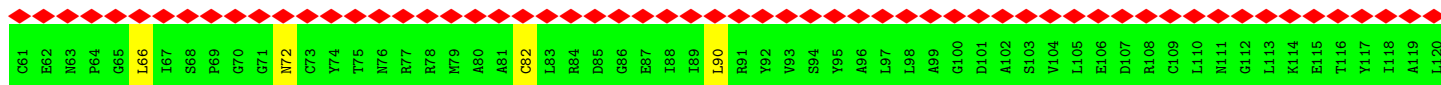


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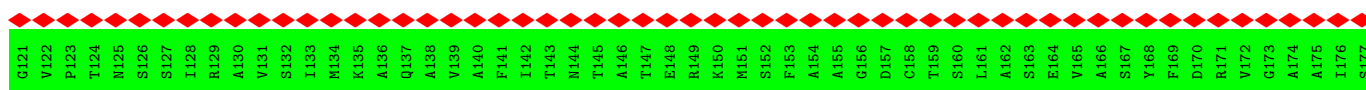
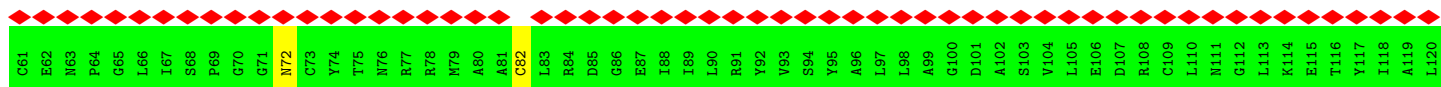




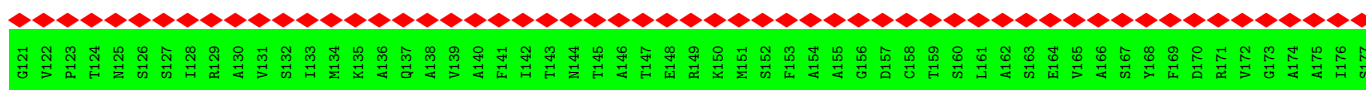
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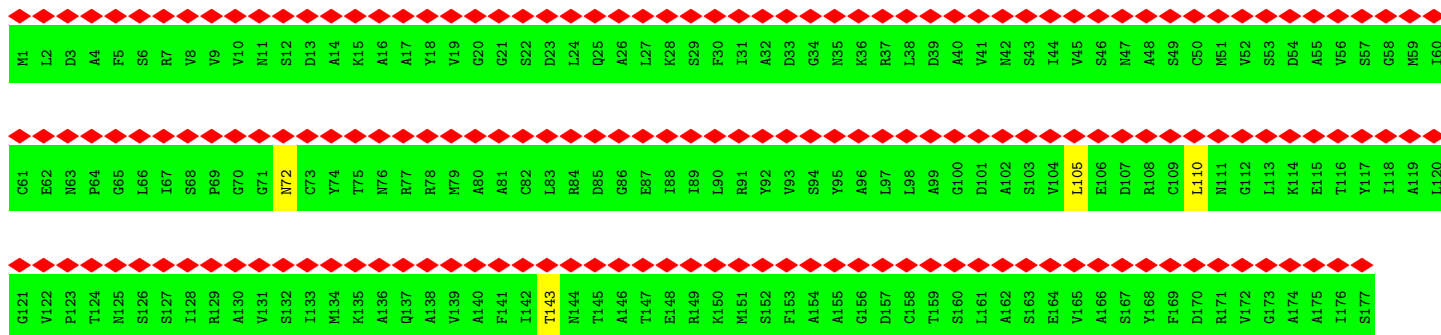


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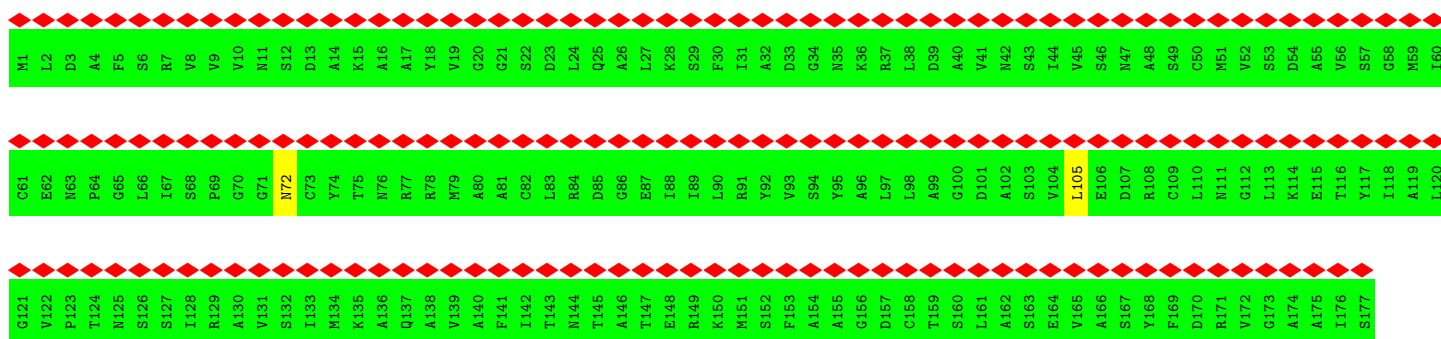


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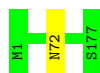
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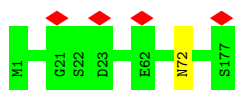
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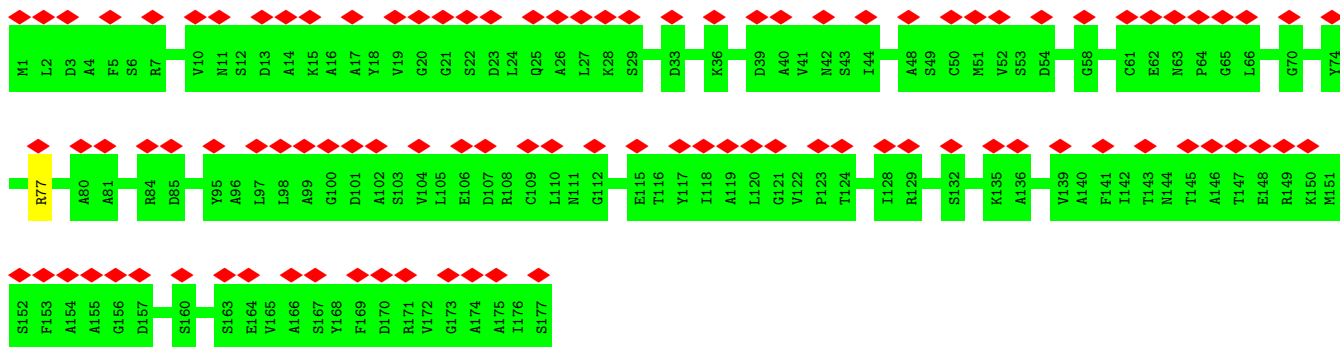
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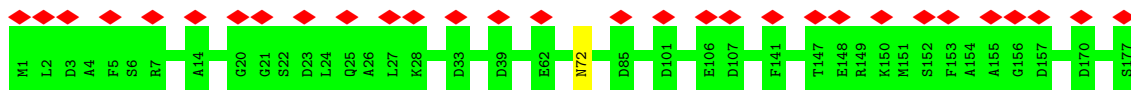
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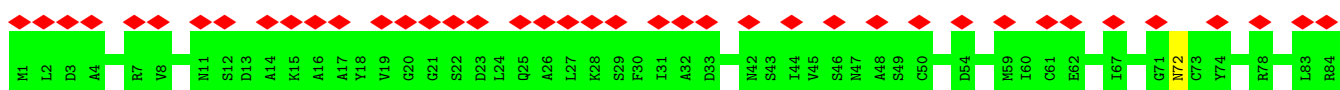
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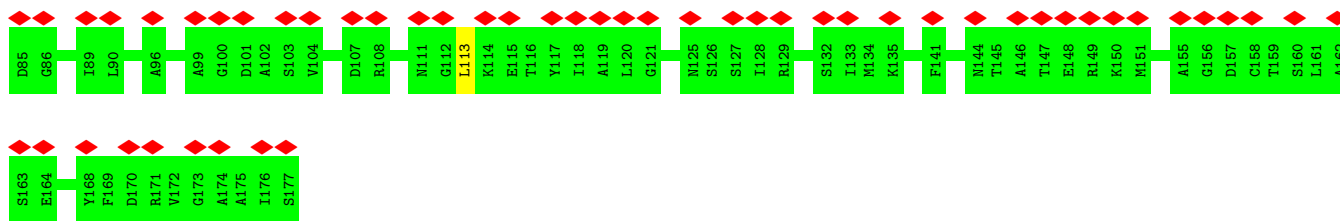


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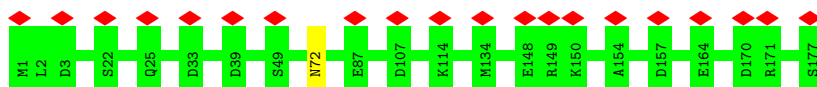


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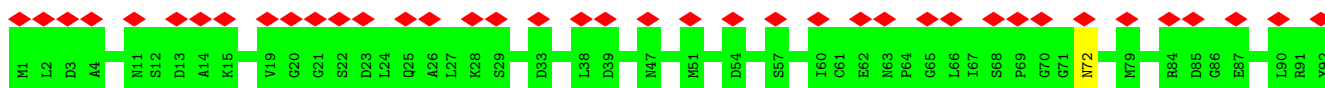
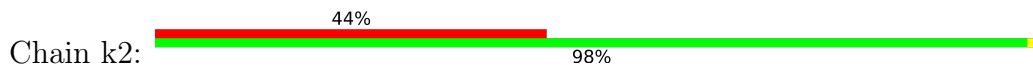




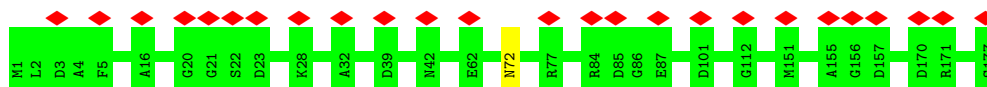
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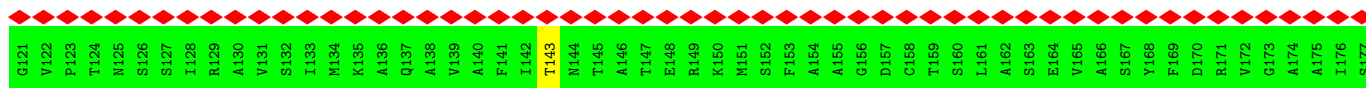
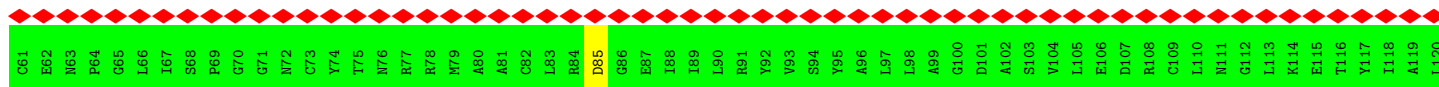
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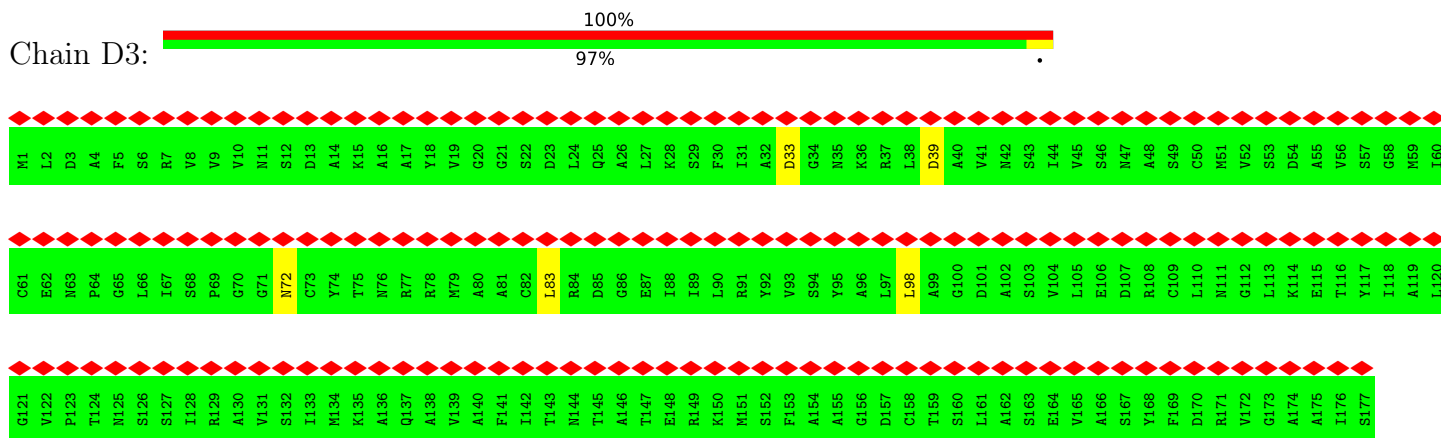
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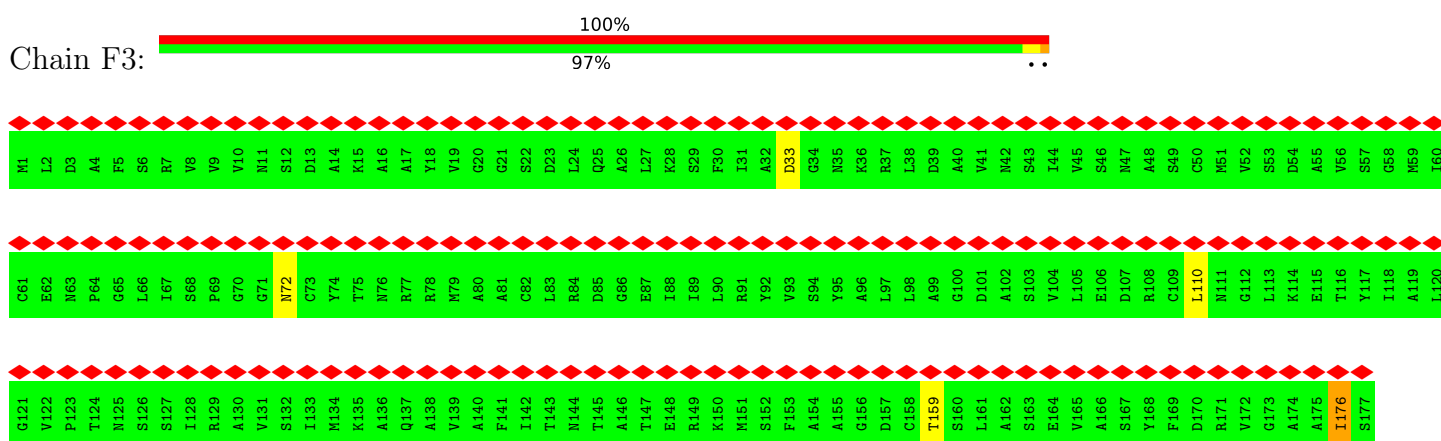
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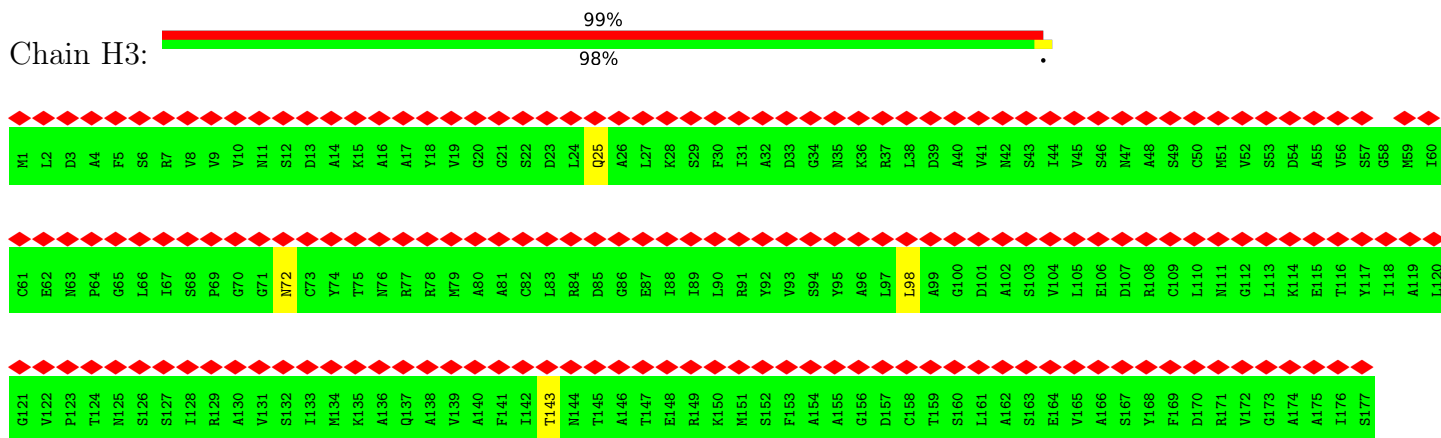
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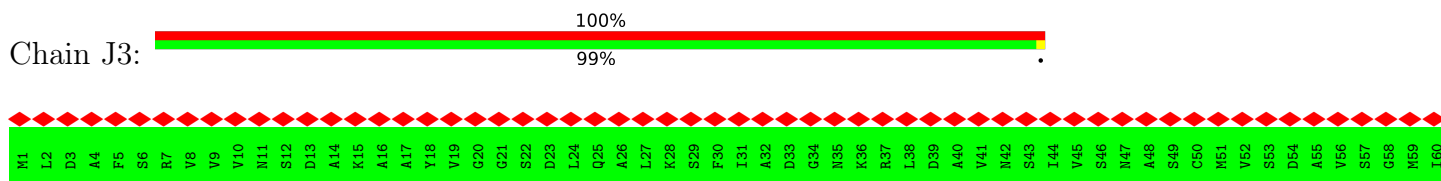
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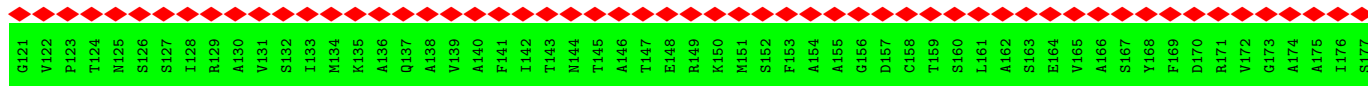
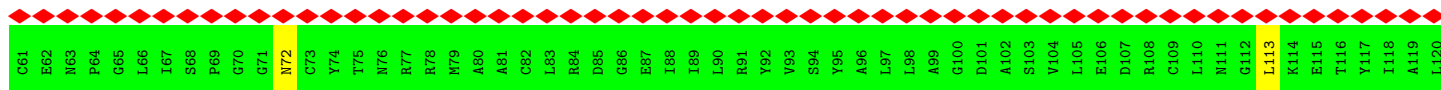


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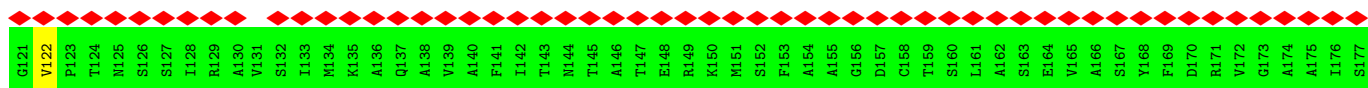
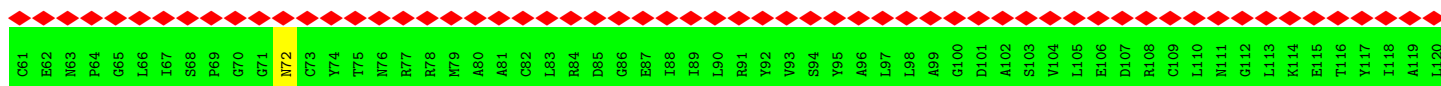


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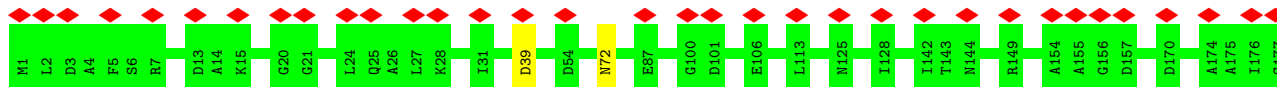




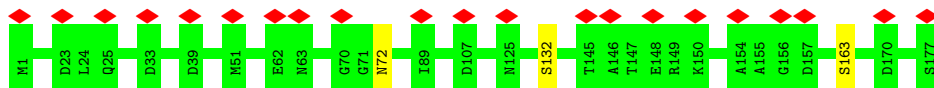
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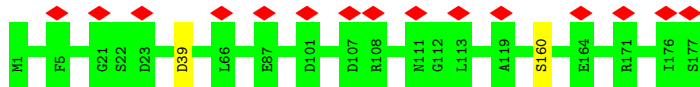
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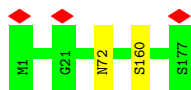


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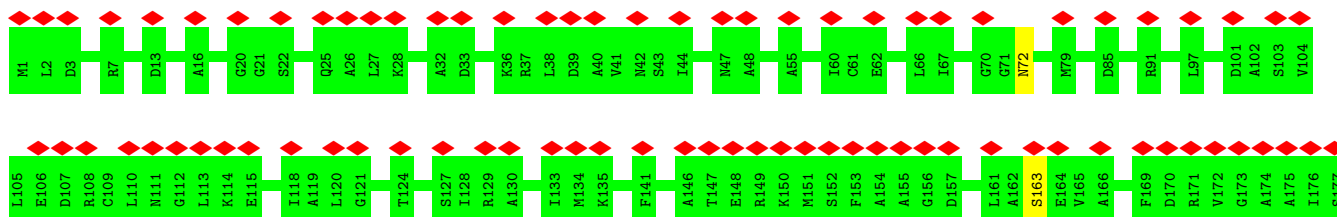


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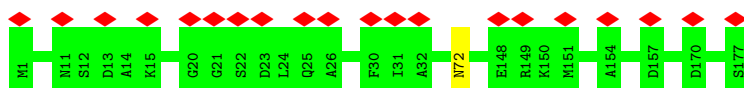




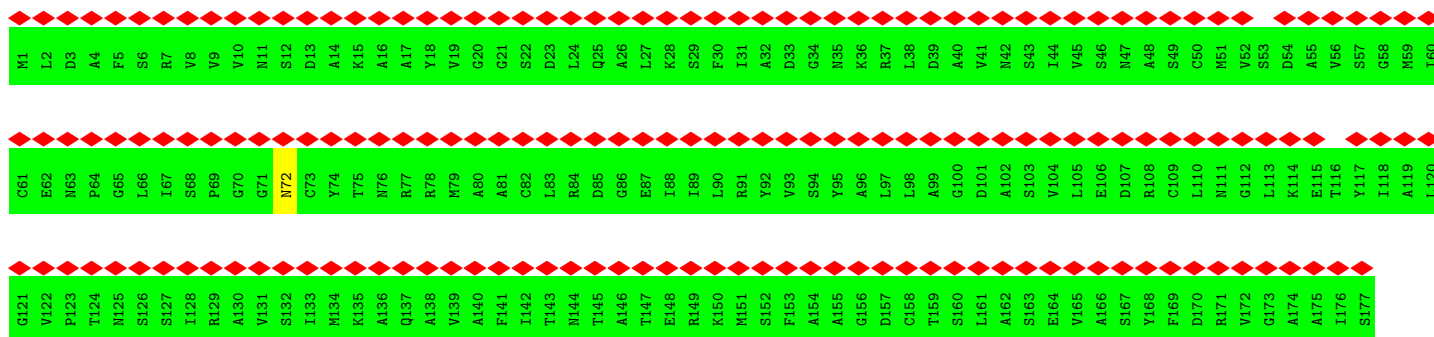
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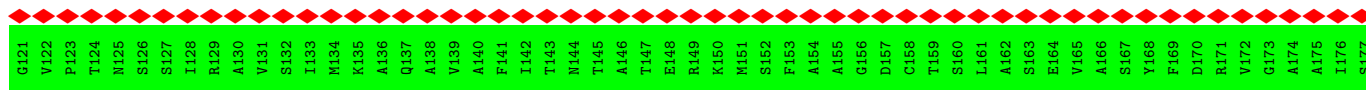


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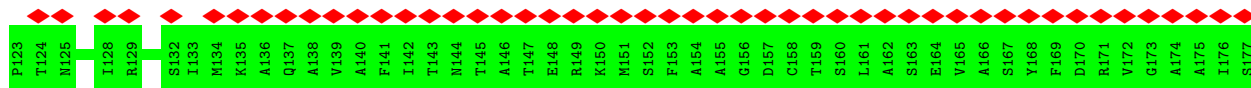
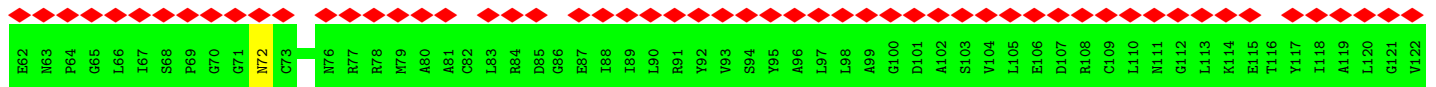
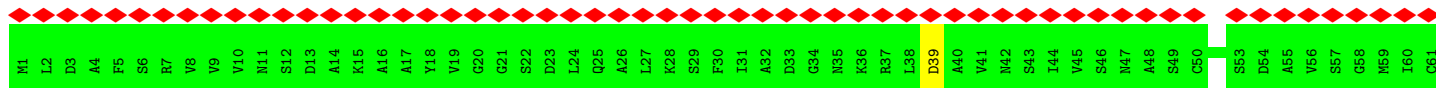


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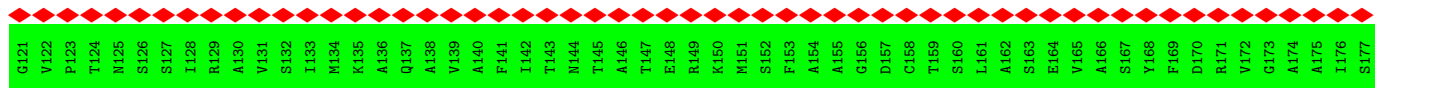
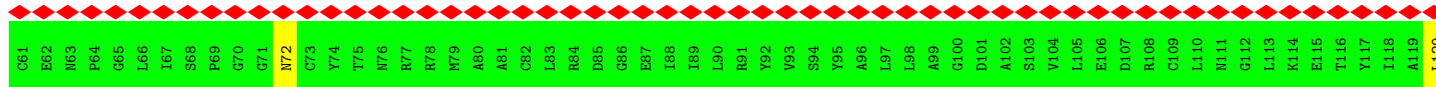




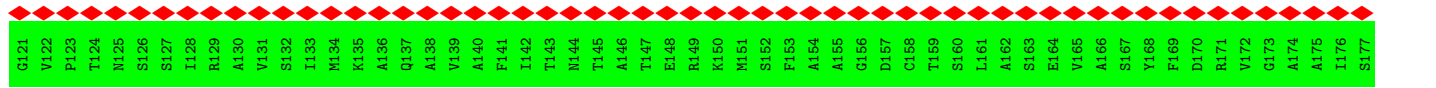
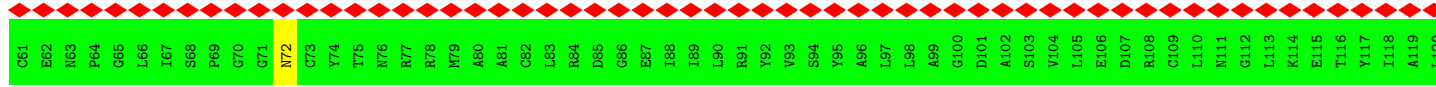
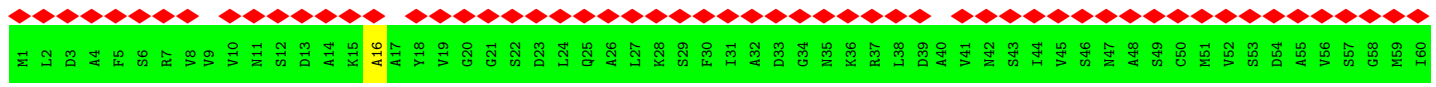
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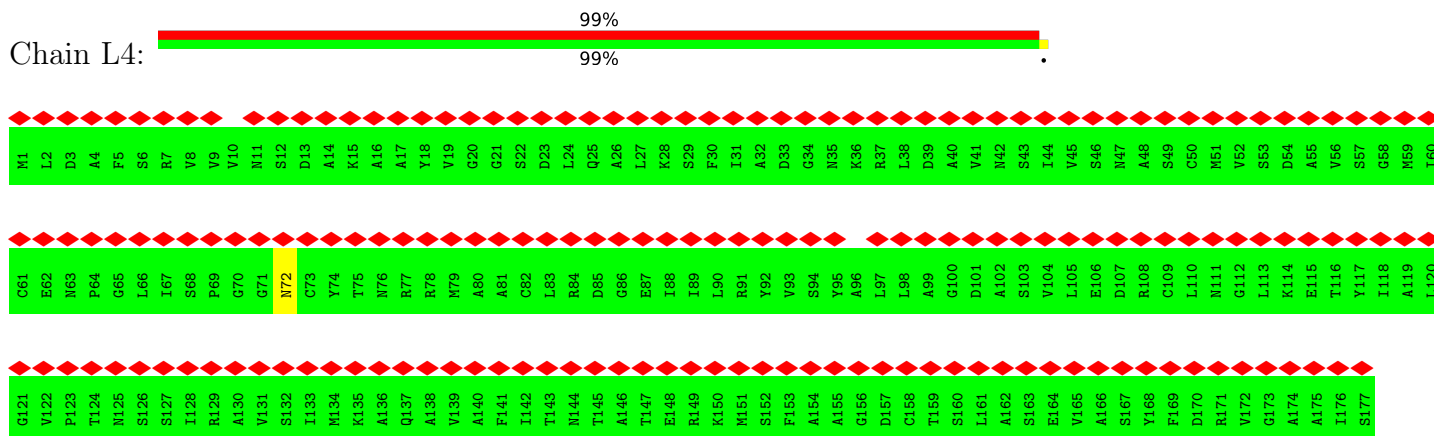
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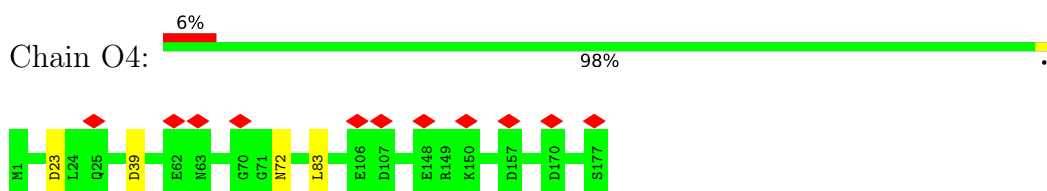
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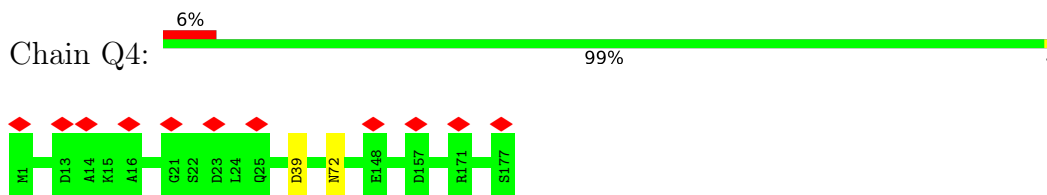
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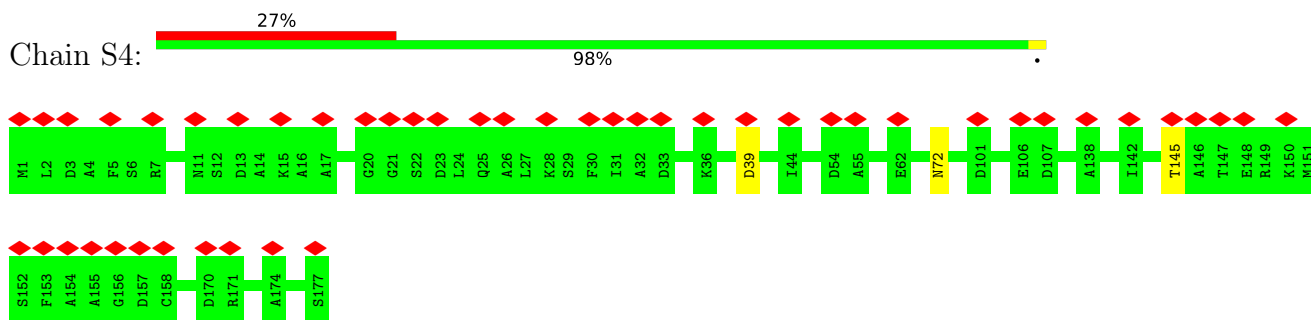
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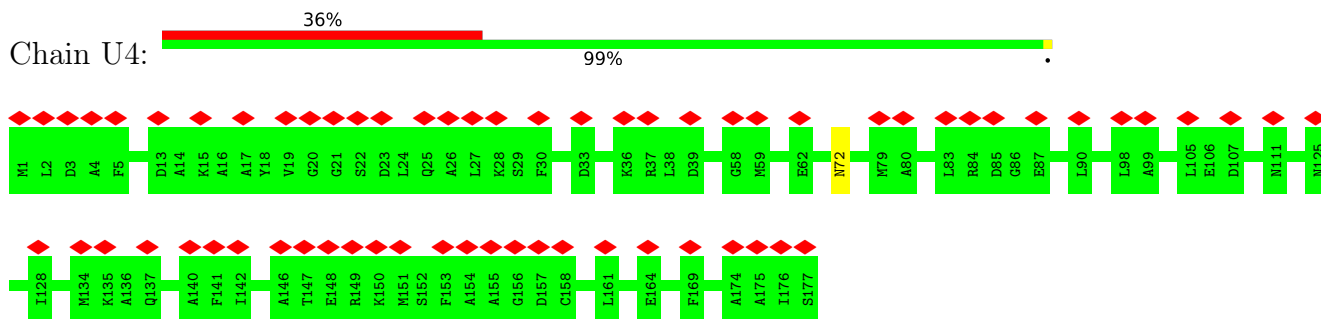
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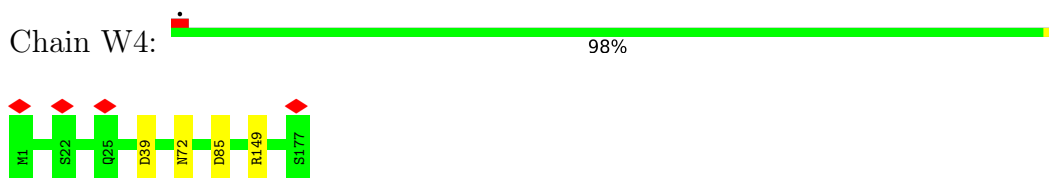
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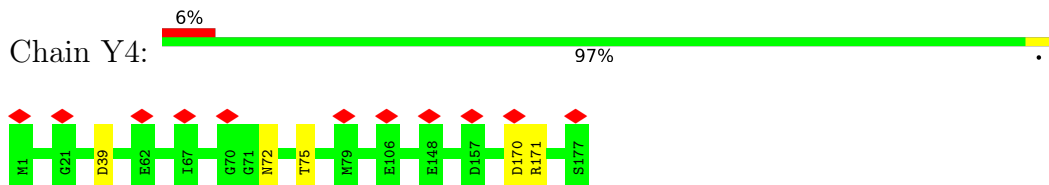
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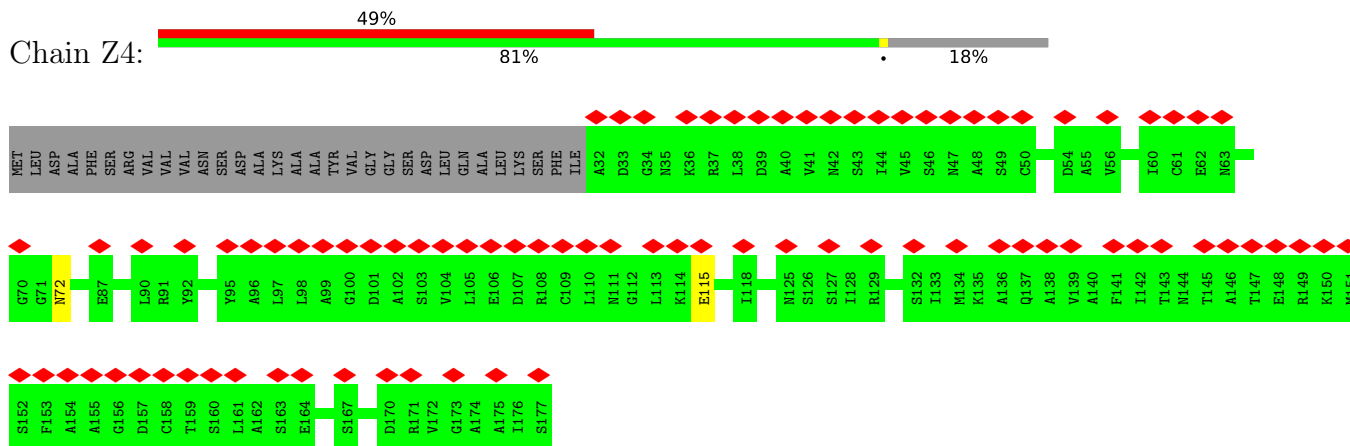
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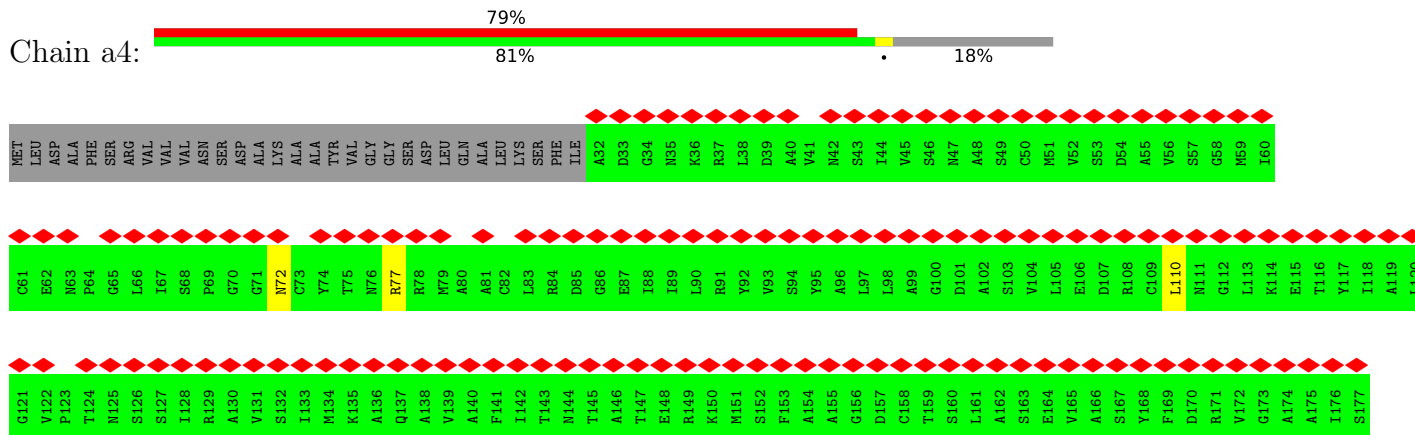
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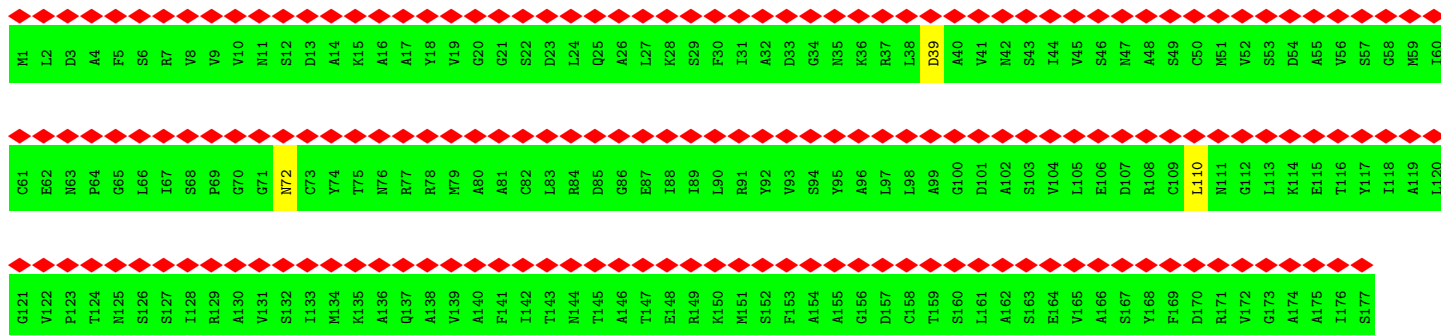


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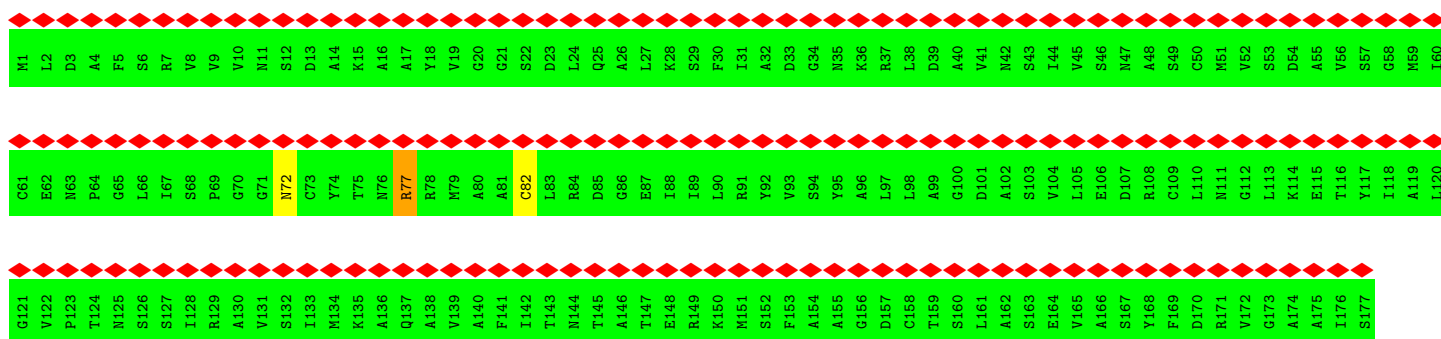


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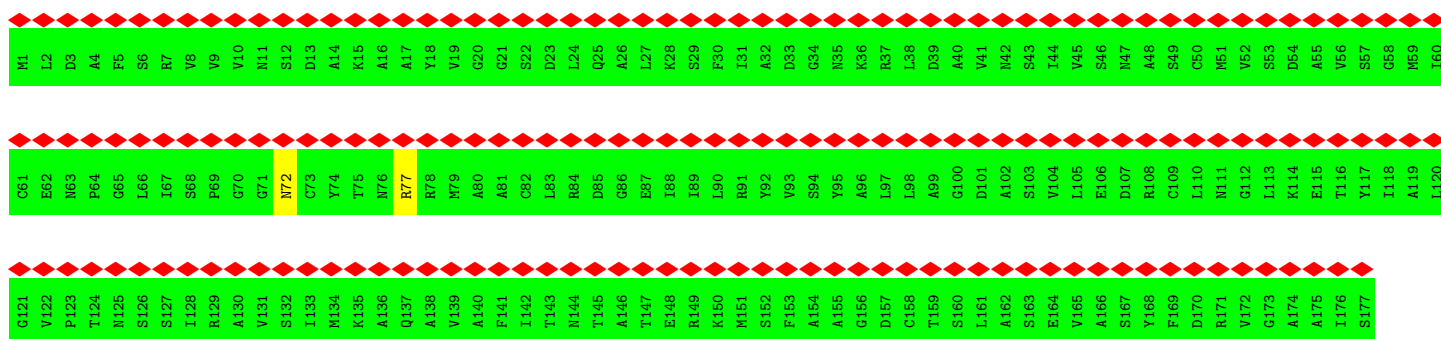




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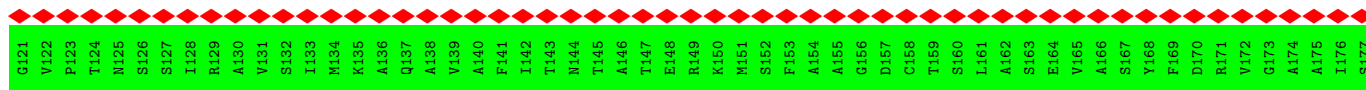


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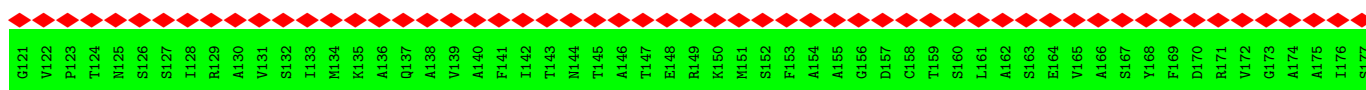
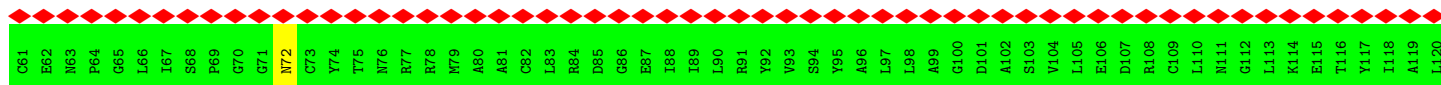


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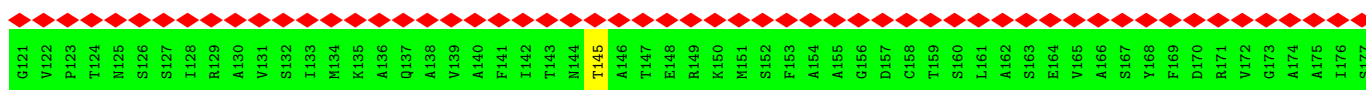
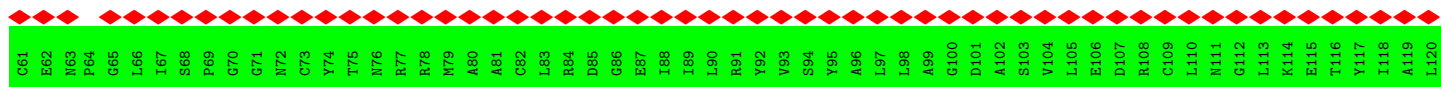
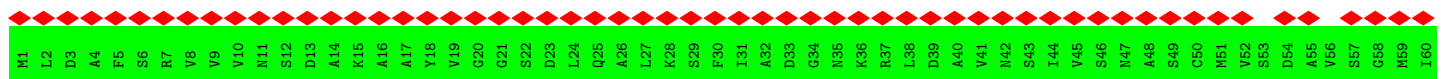




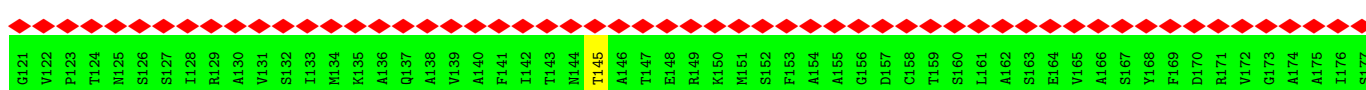
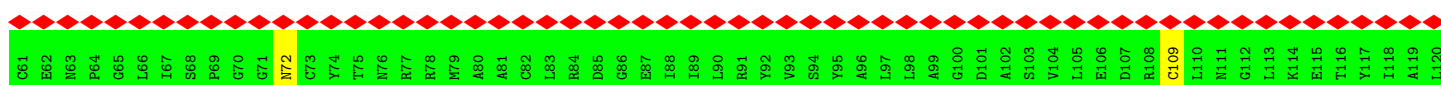
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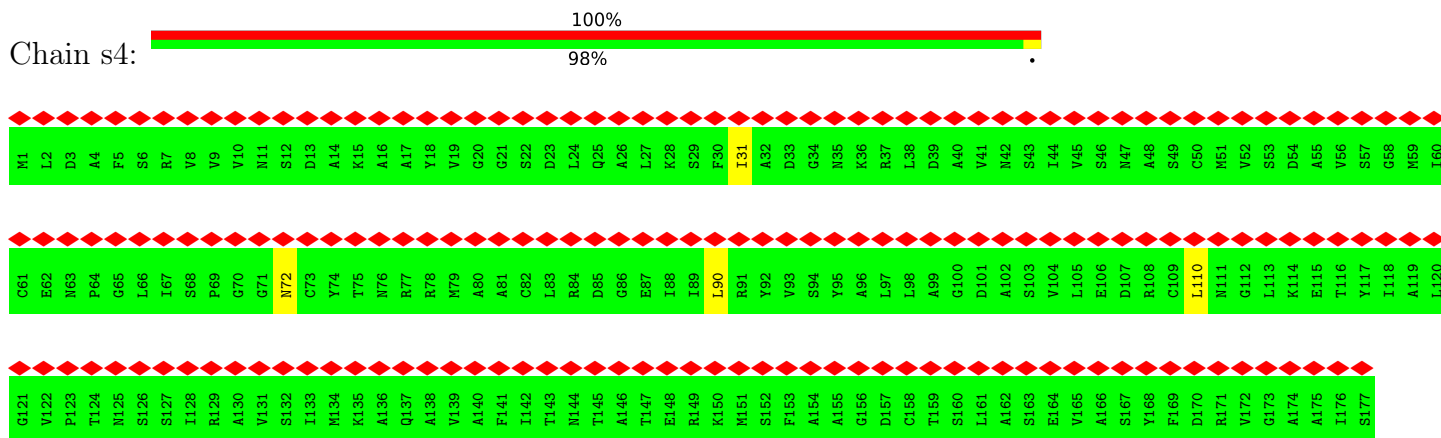
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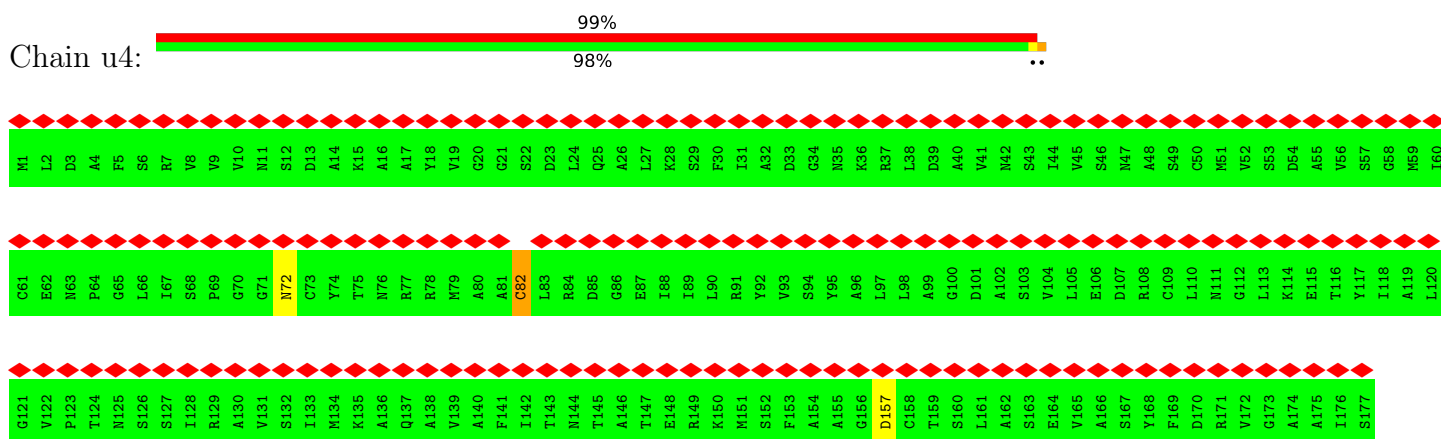
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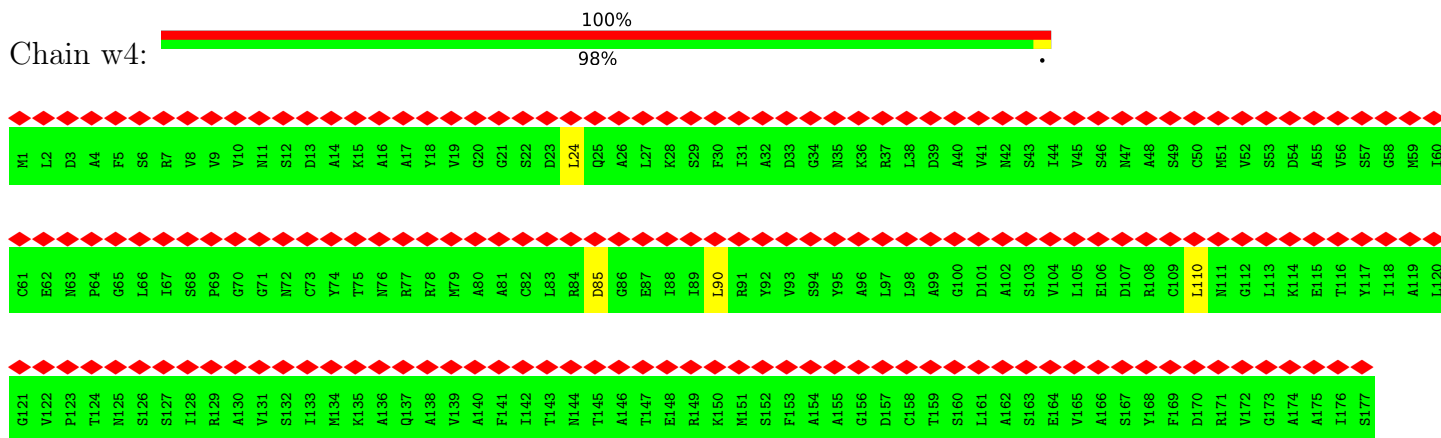
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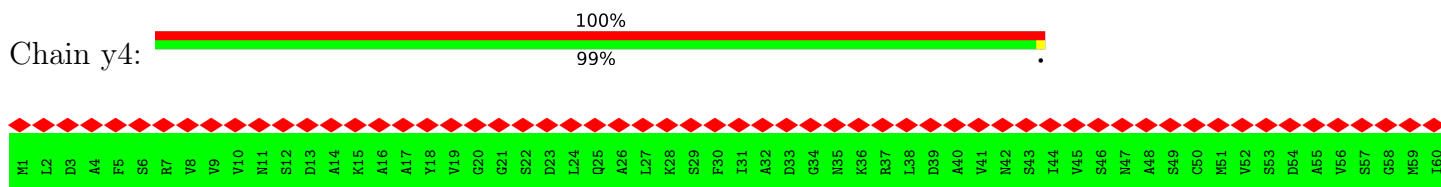
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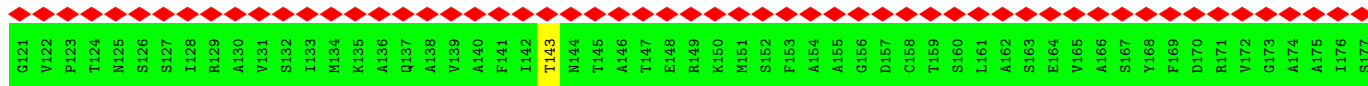
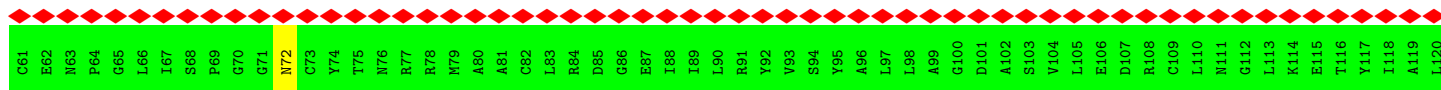


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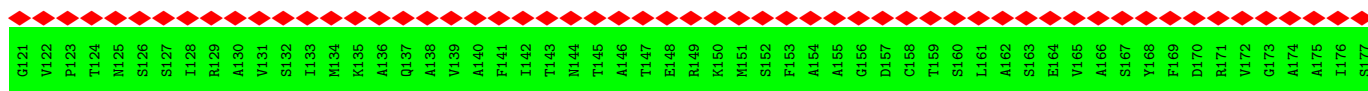
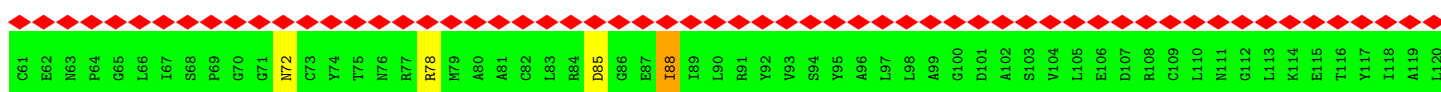


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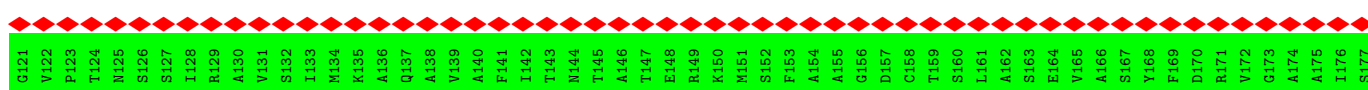
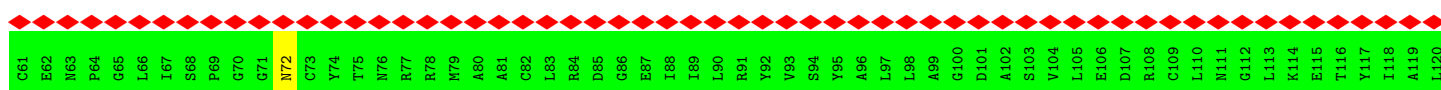
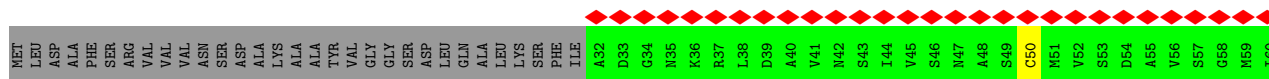
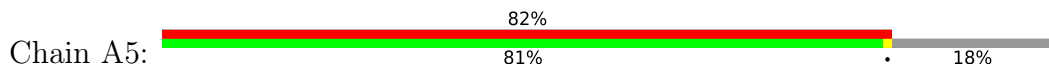




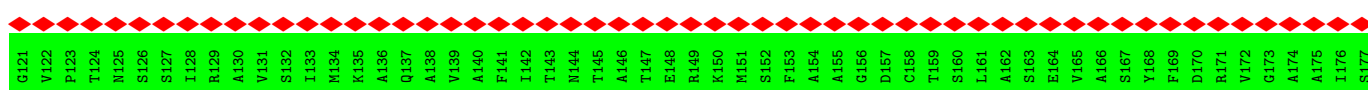
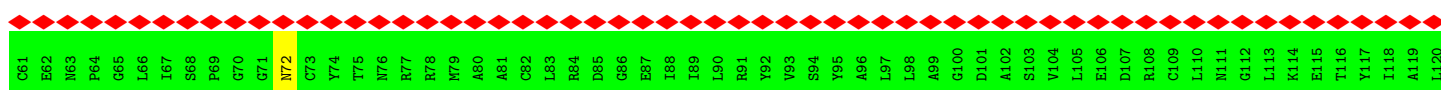
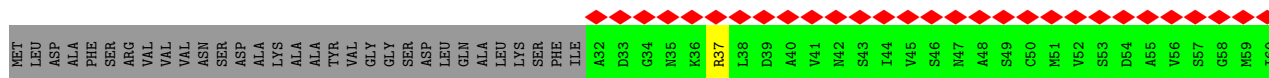
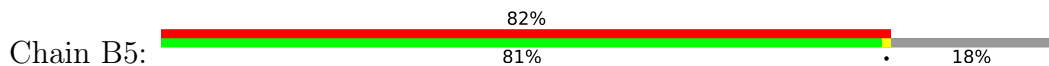
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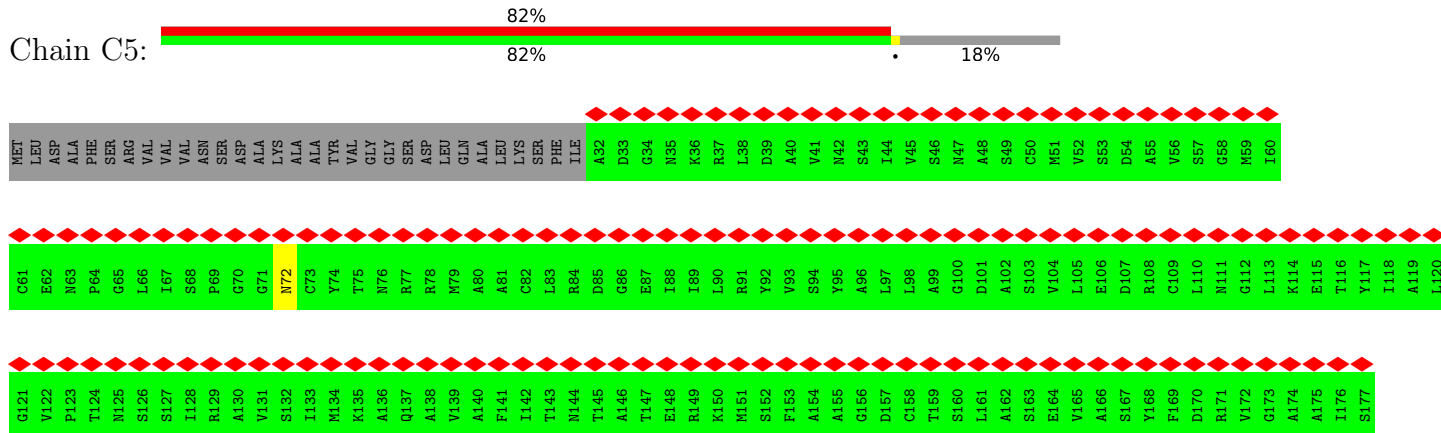
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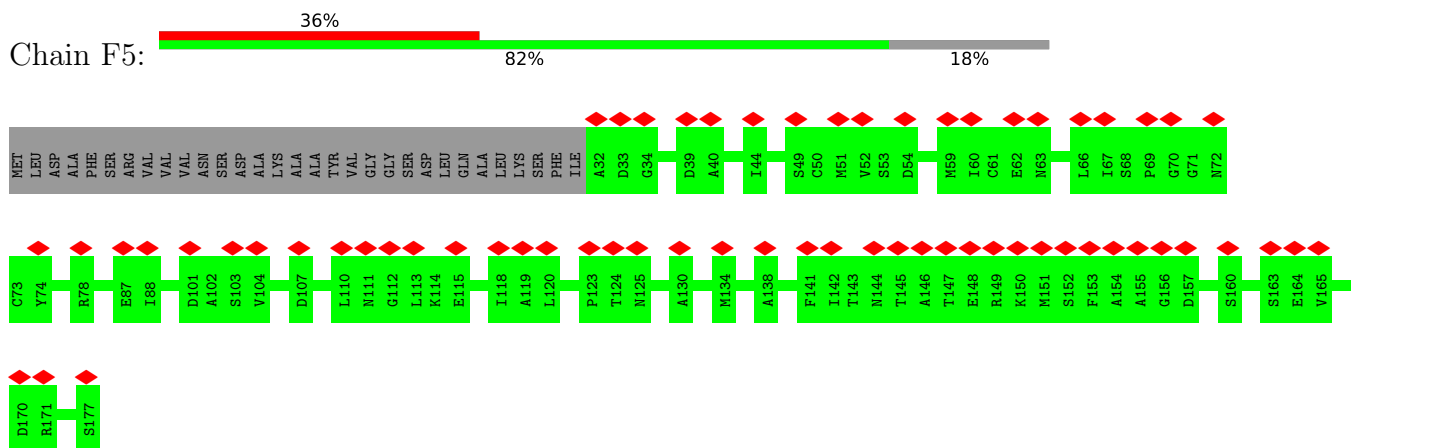
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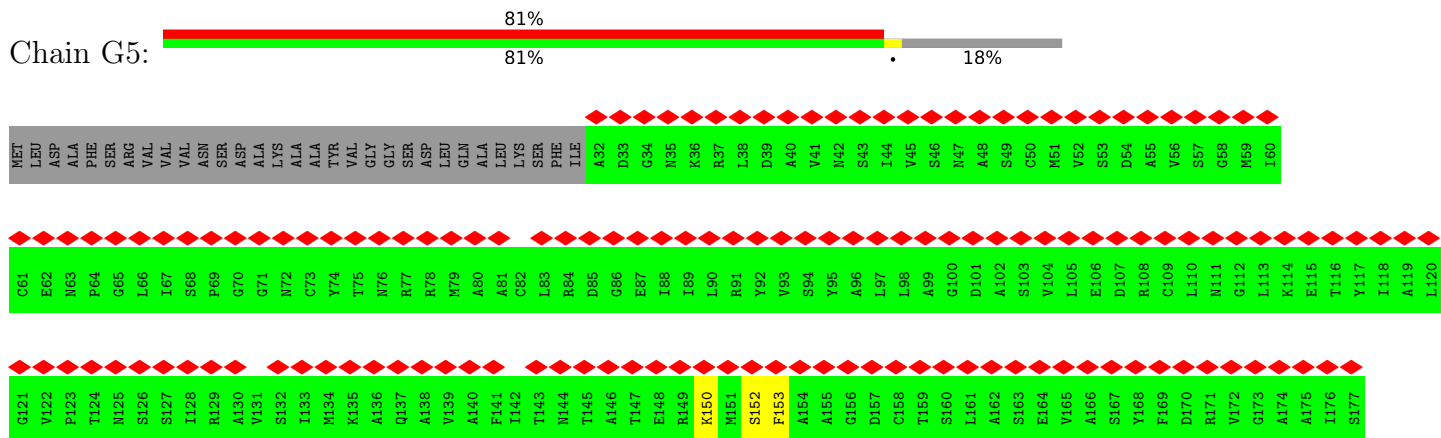
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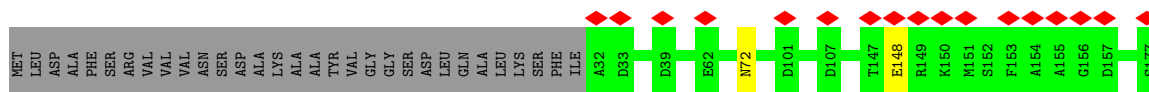


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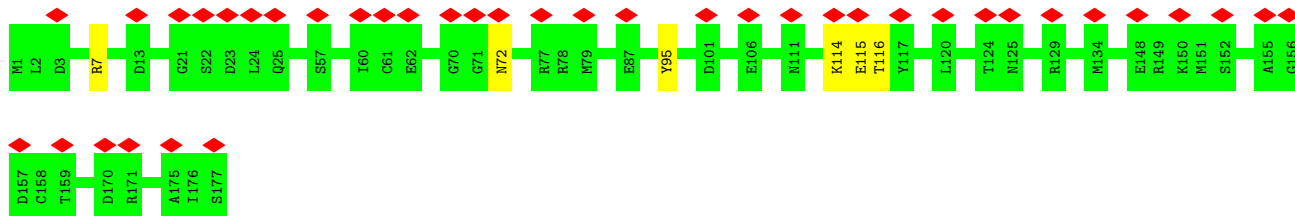


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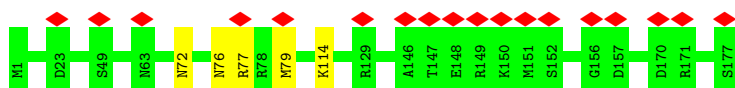




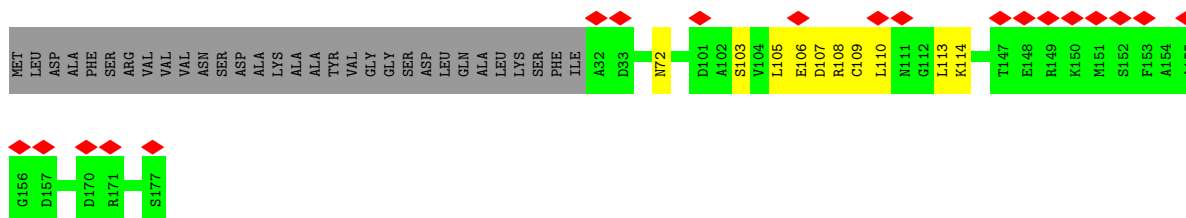
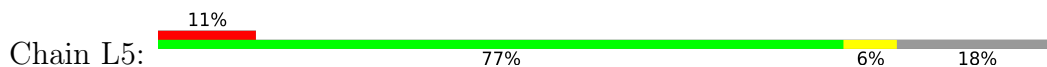
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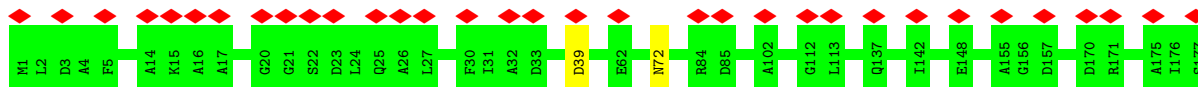
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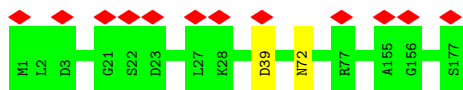
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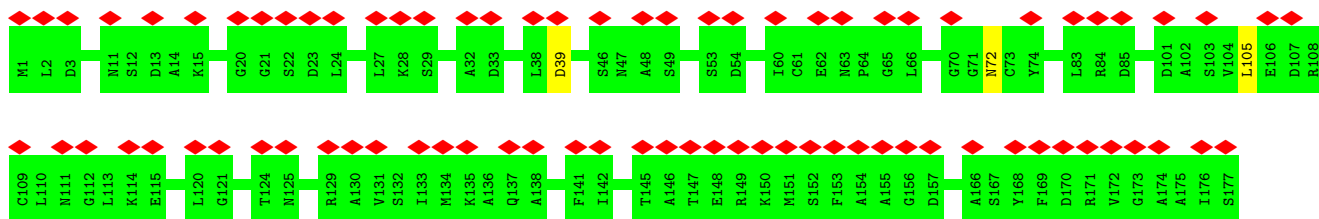
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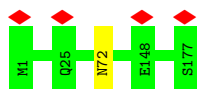
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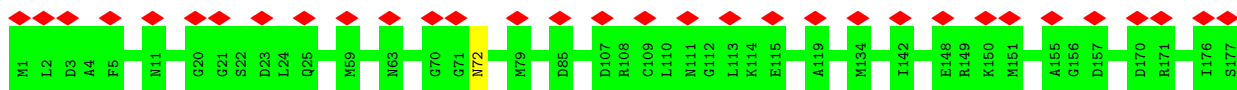
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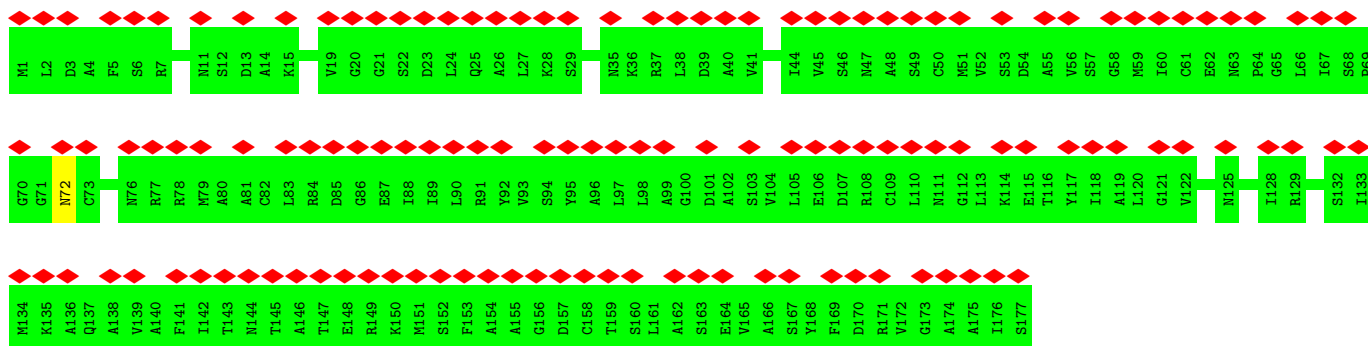
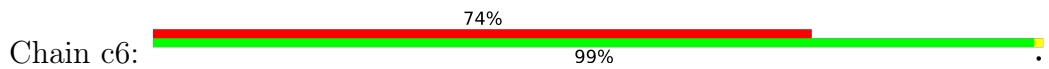
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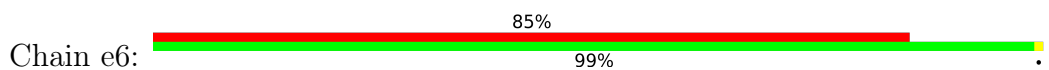
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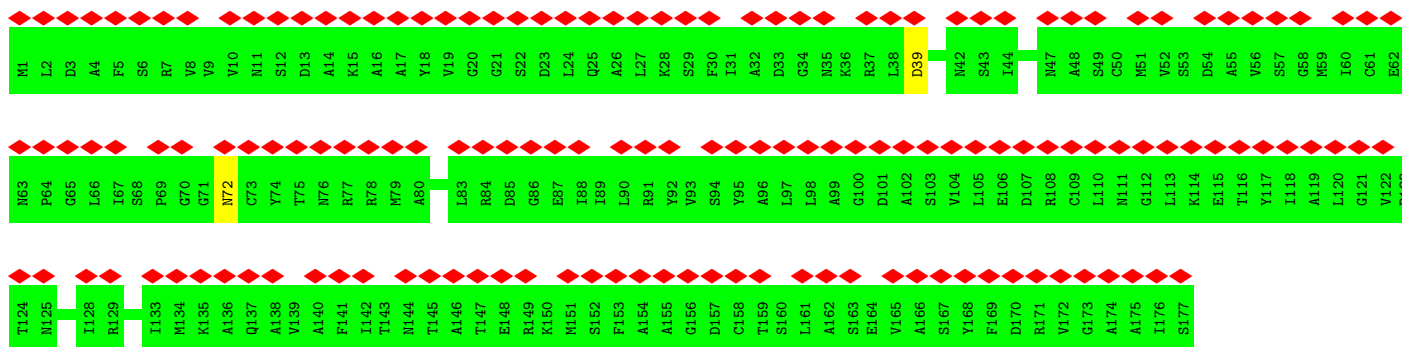


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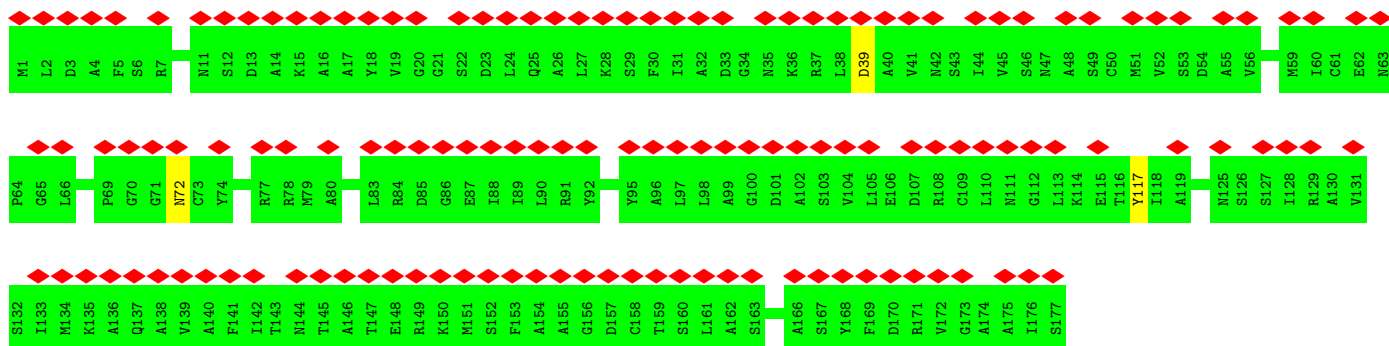
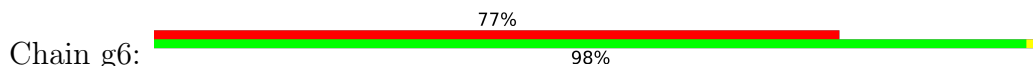


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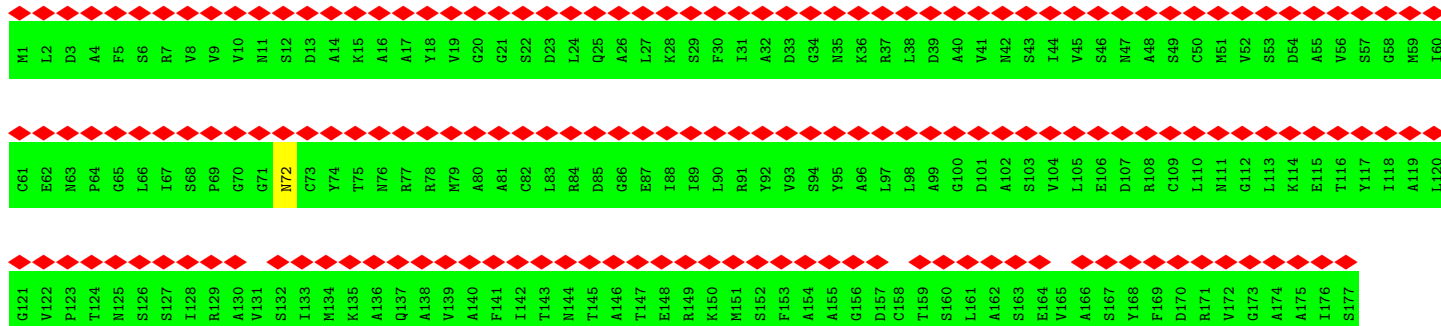




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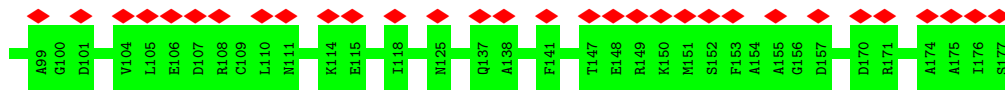


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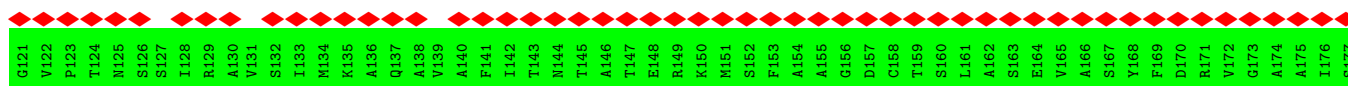
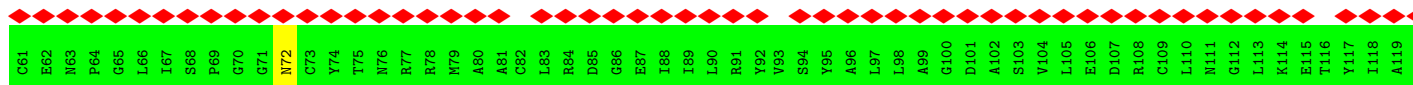
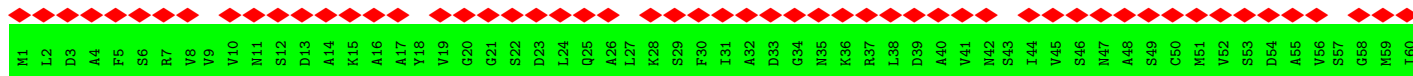


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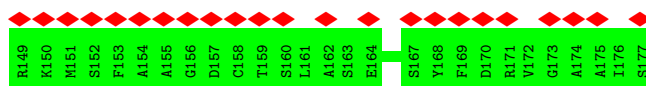
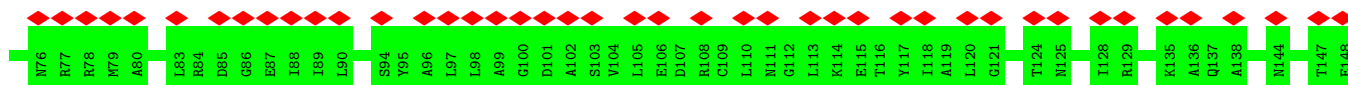
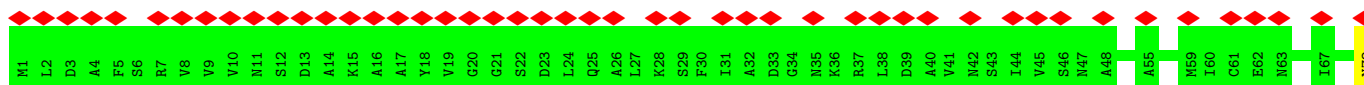




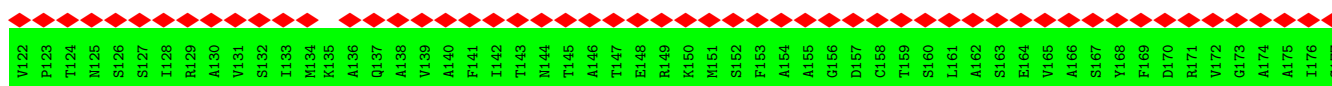
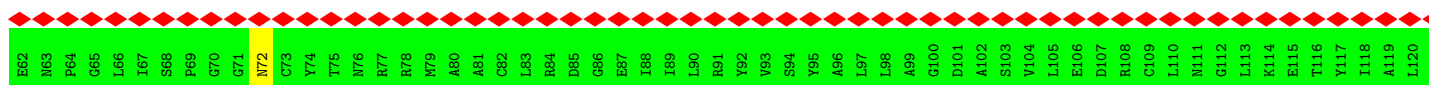
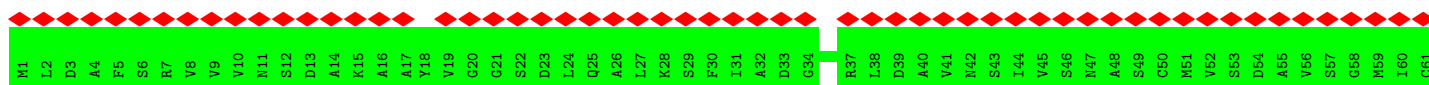
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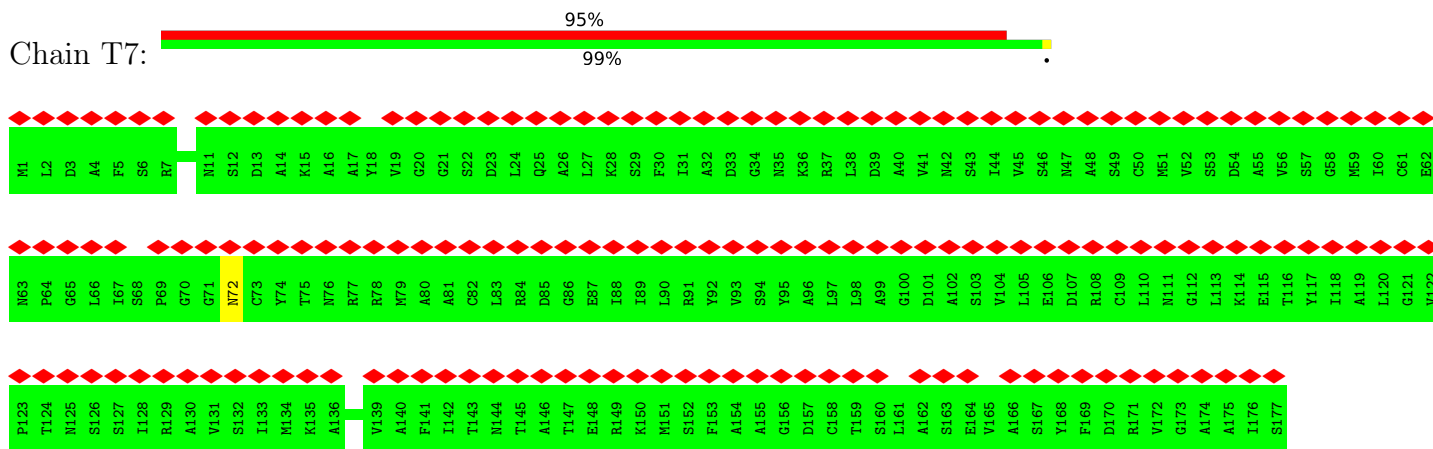
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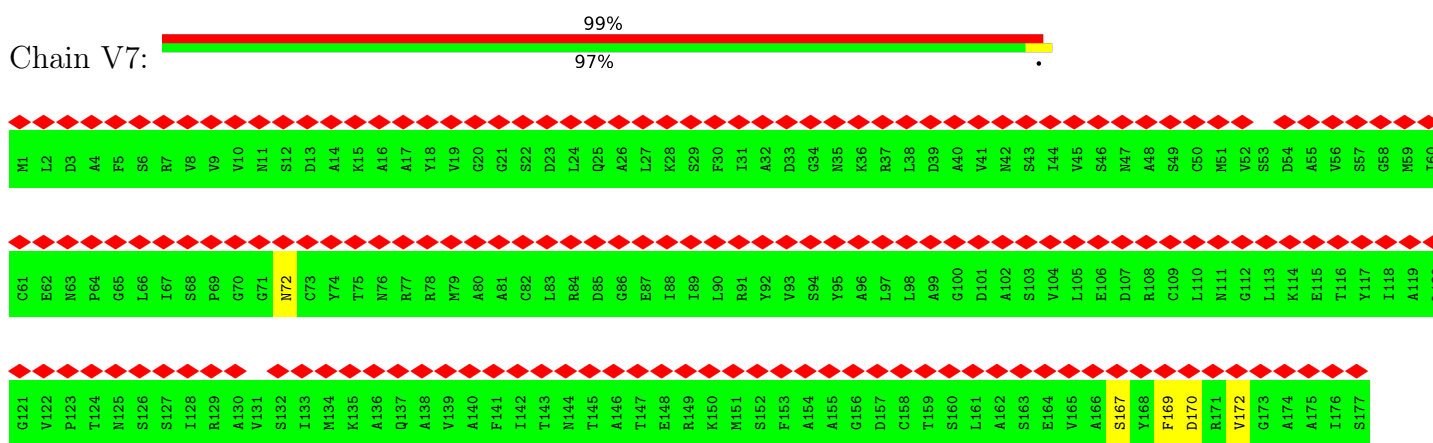
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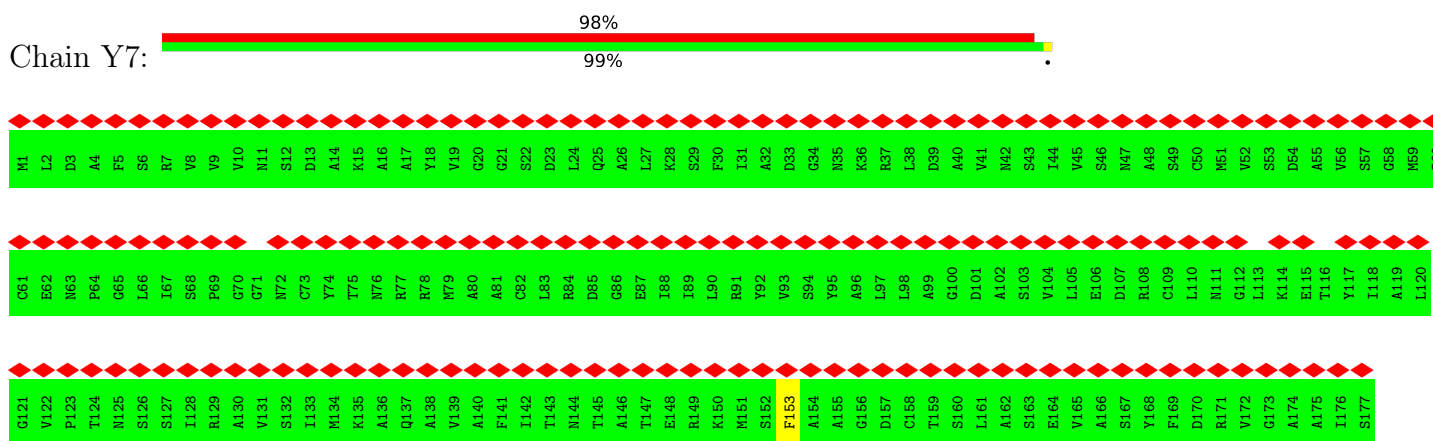
• Molecule 2: B-phycoerythrin beta chain



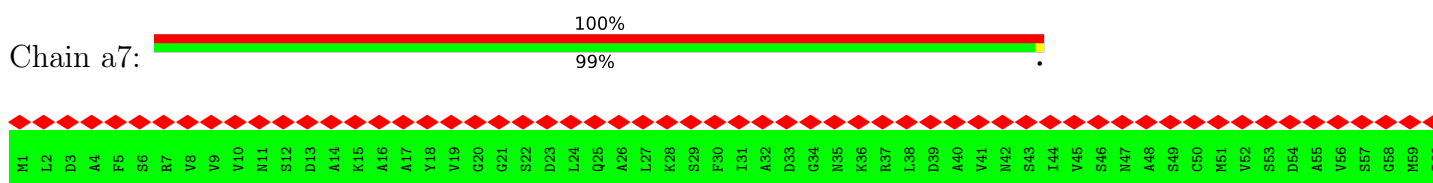
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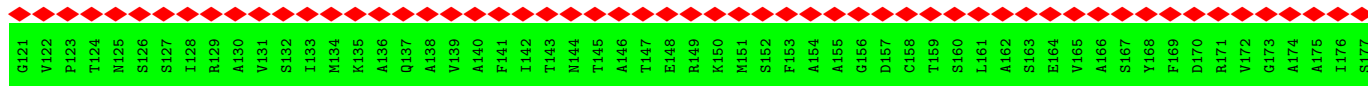
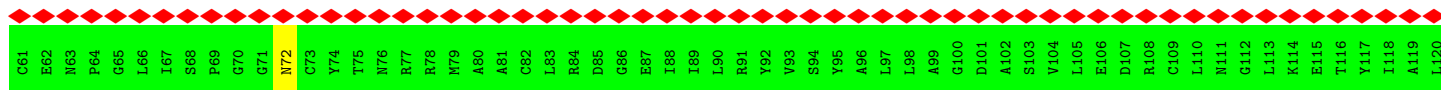


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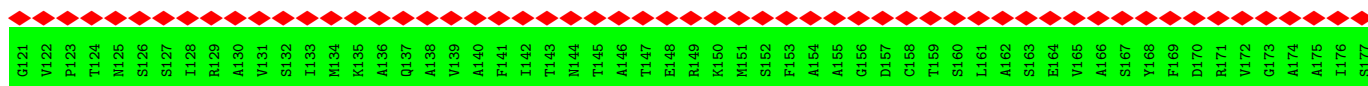
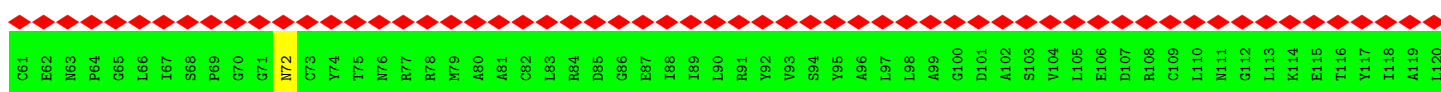
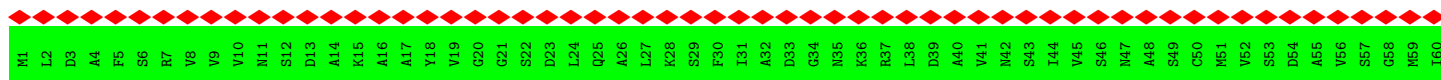


• Molecule 2: B-phycoerythrin beta chain

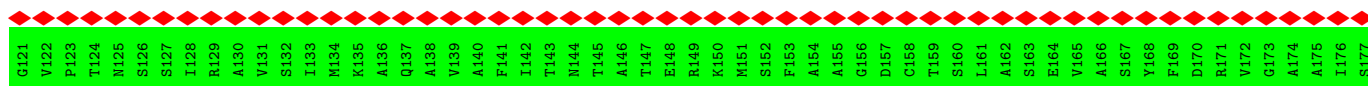
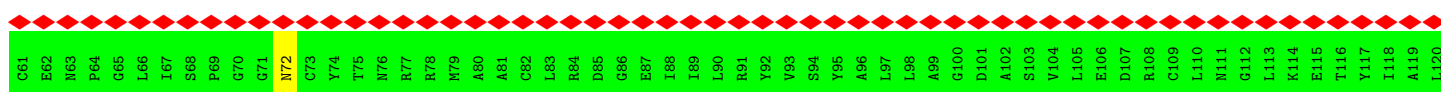
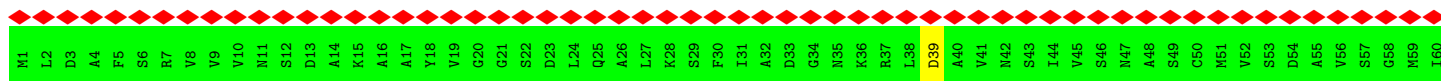




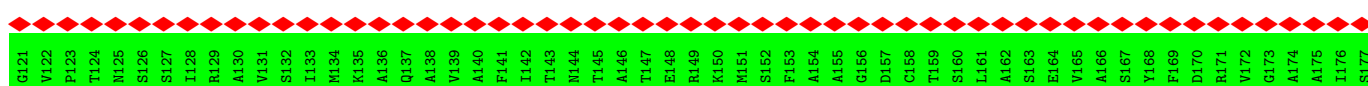
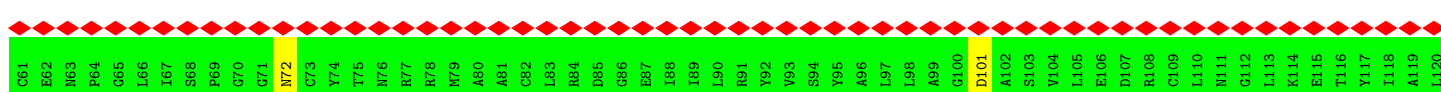
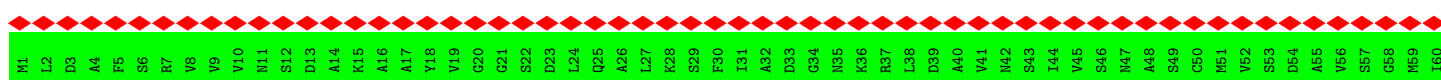
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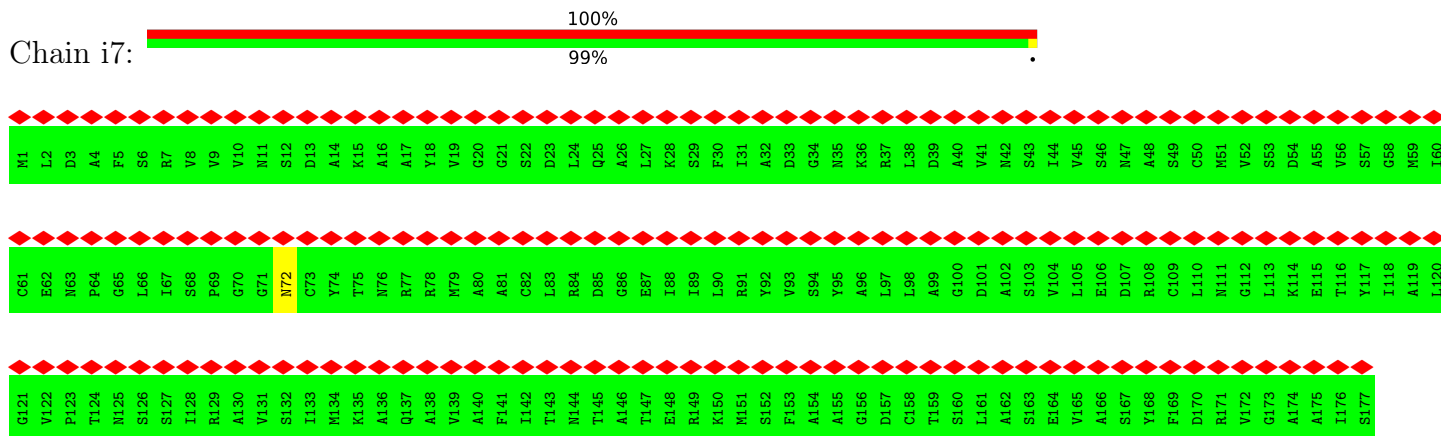
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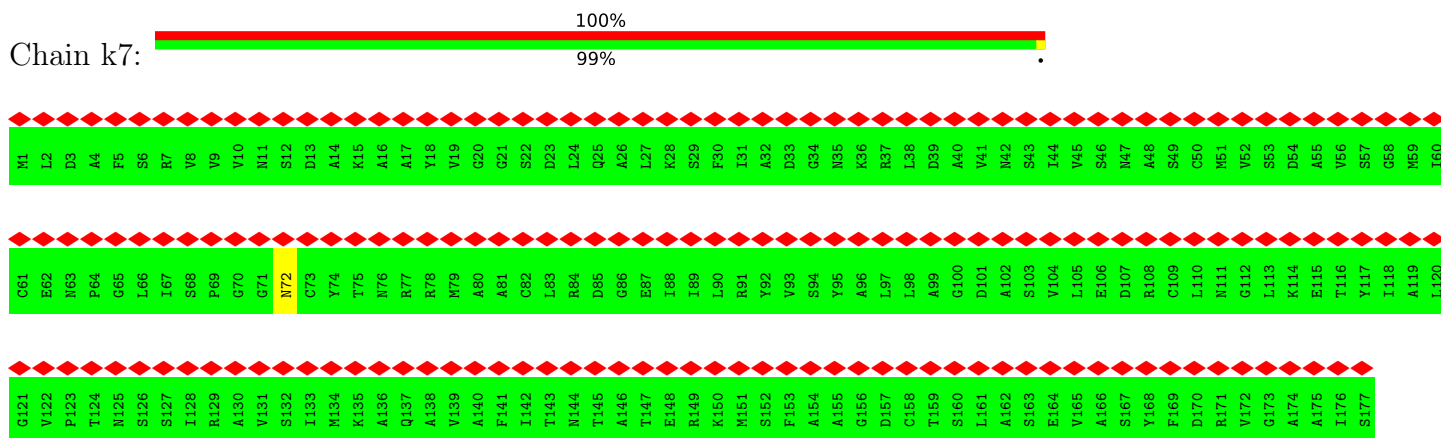
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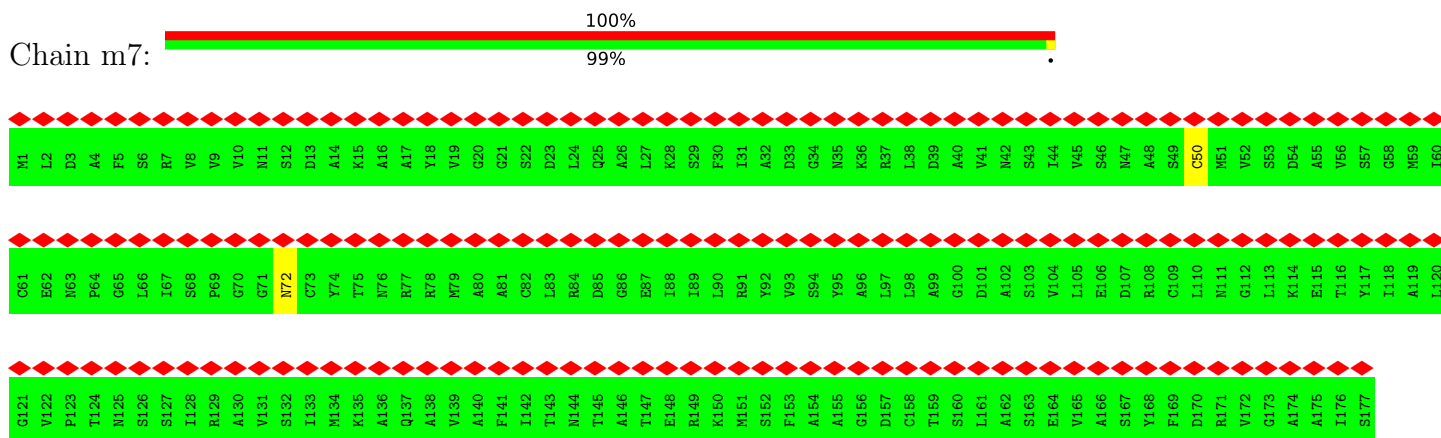
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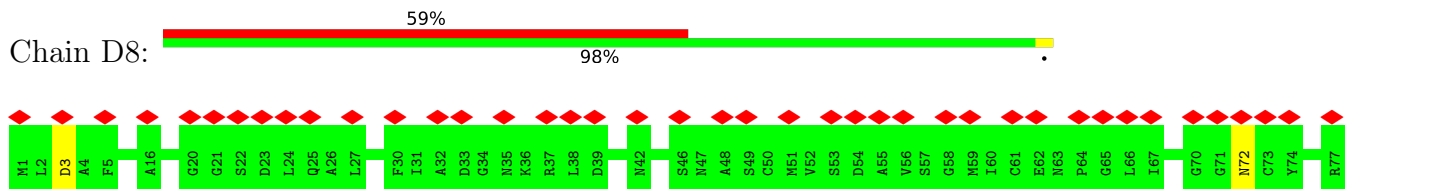
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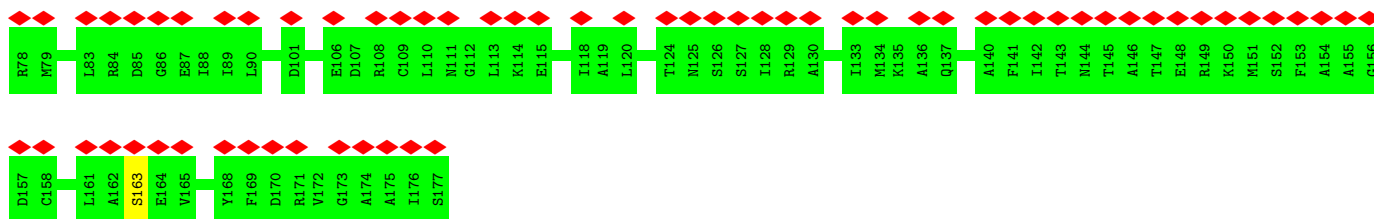


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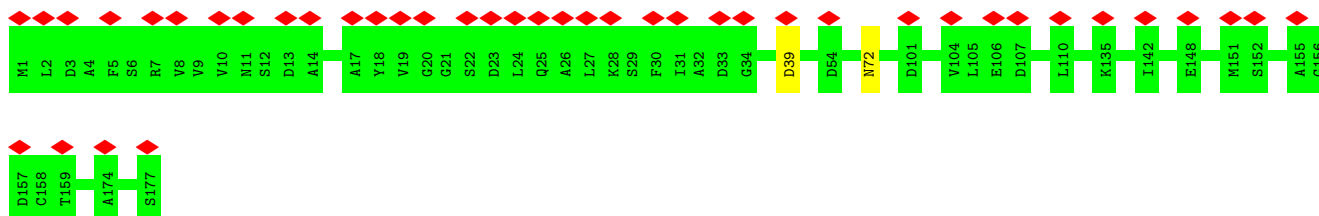


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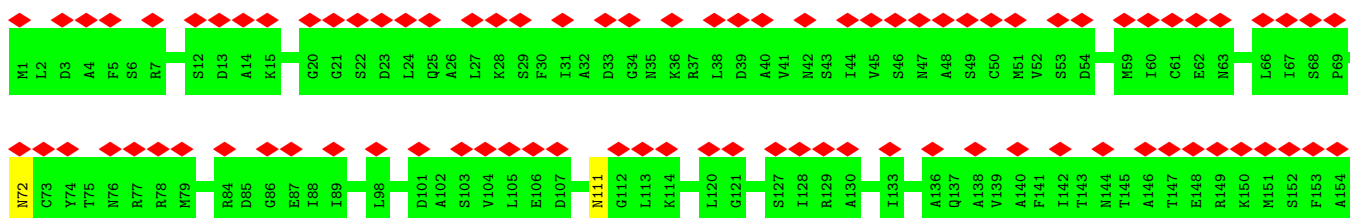
- Molecule 2: B-phycoerythrin beta chain



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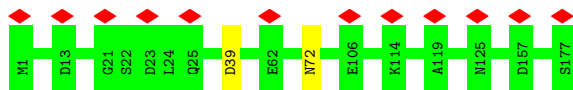


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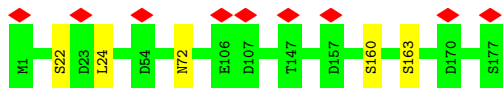


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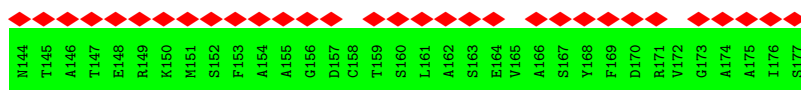
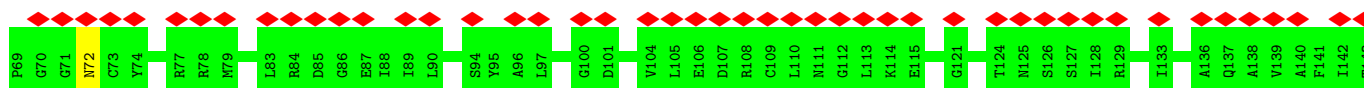
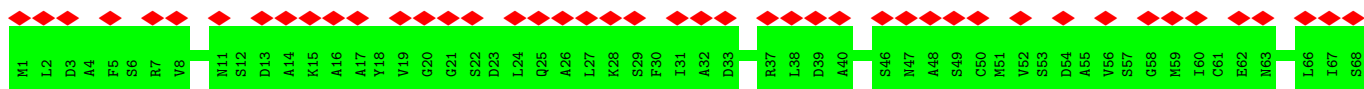




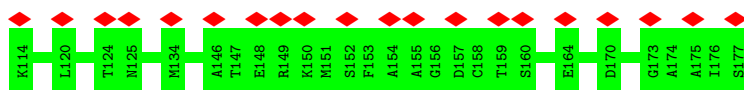
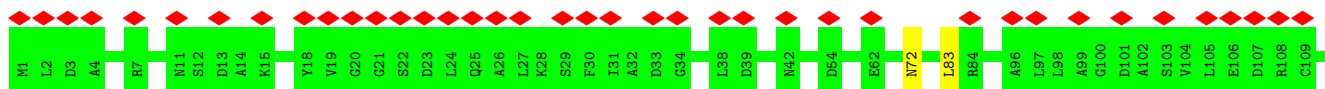
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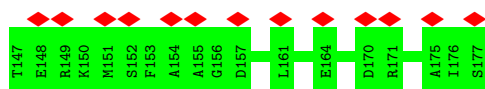
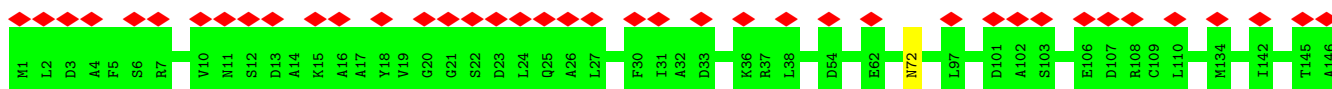
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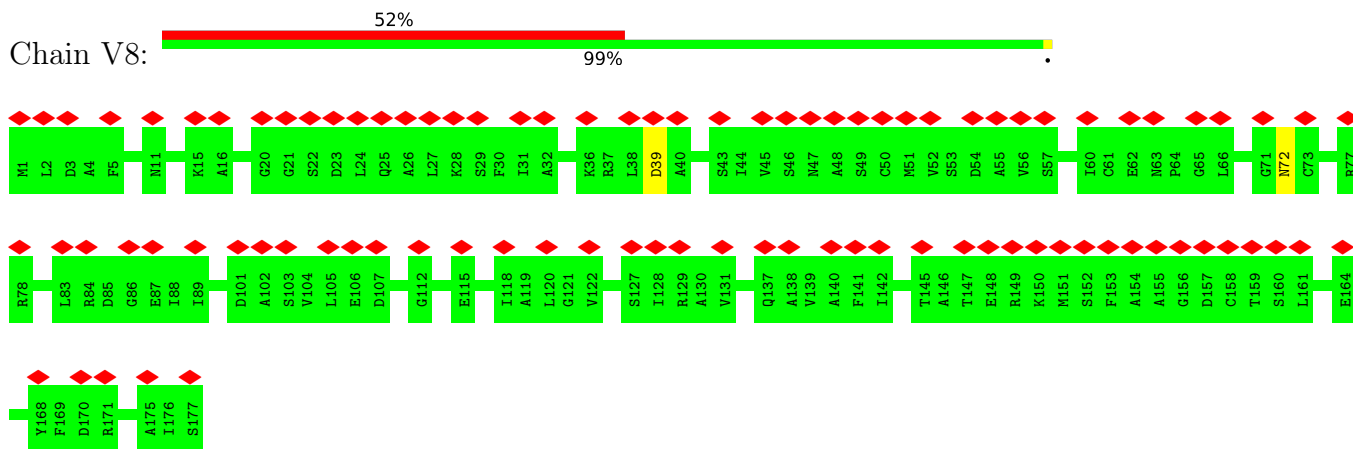
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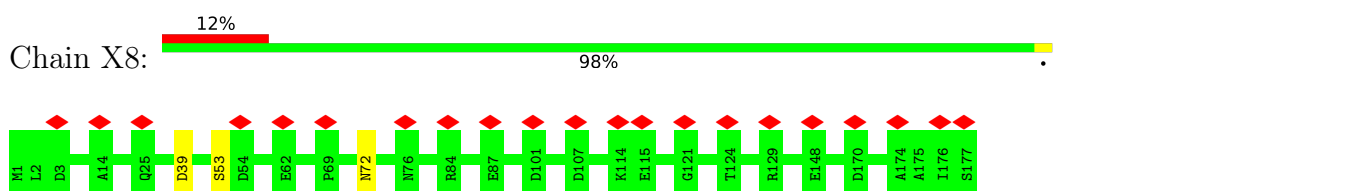
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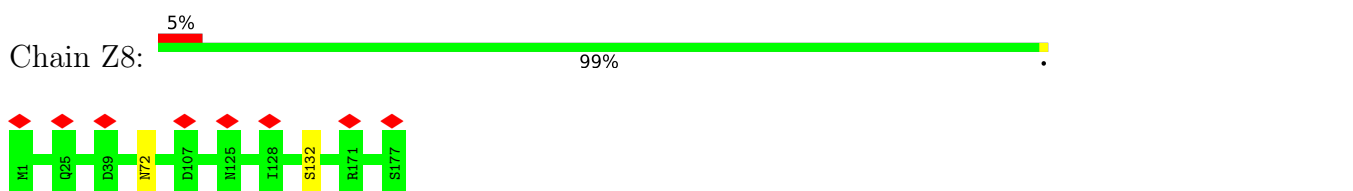
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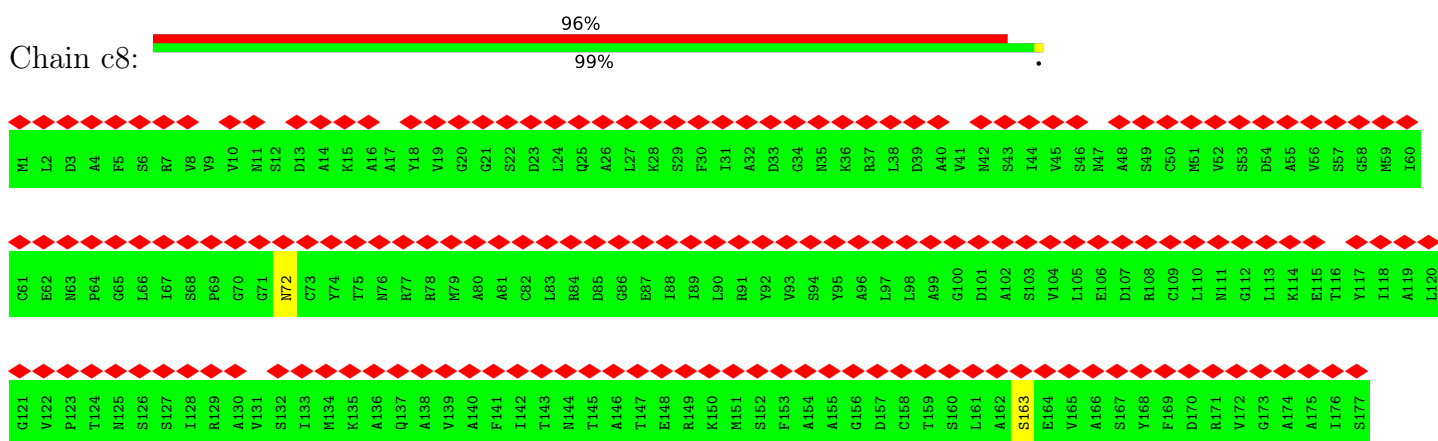
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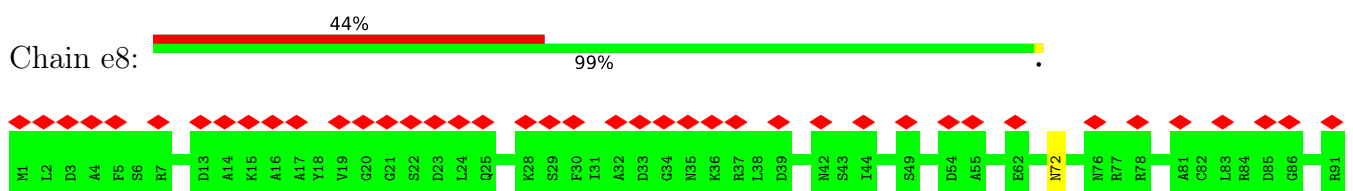
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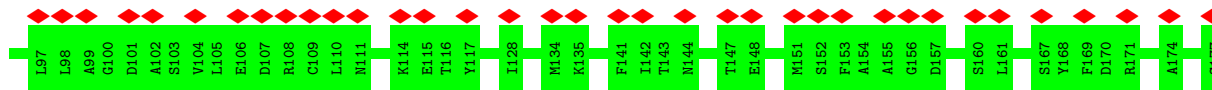


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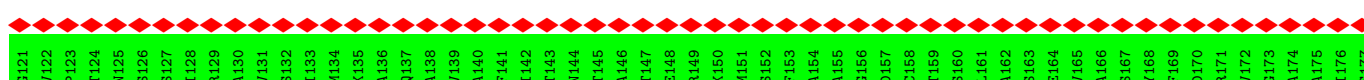
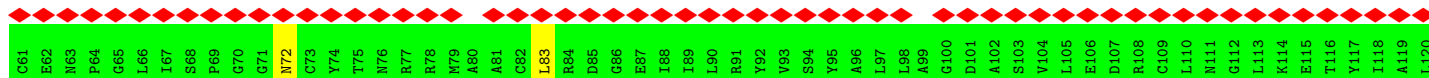
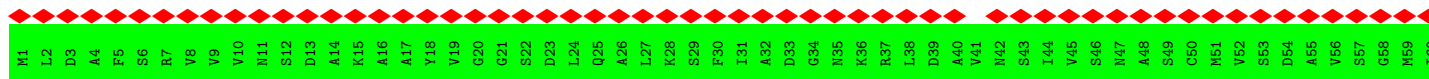


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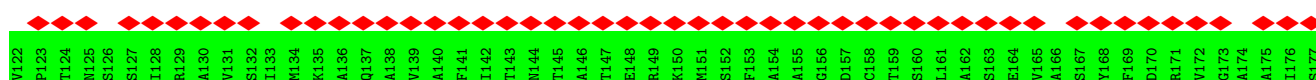
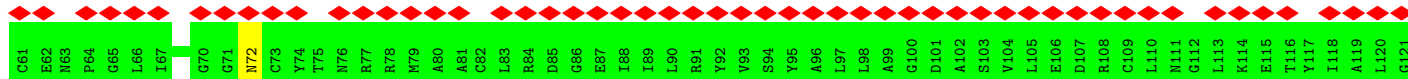




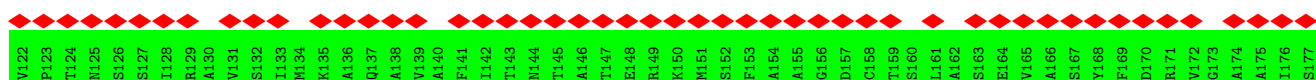
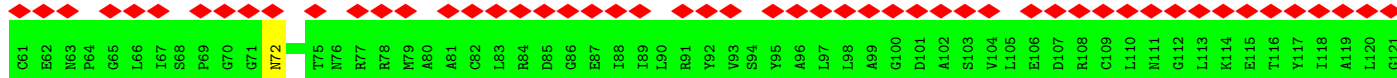
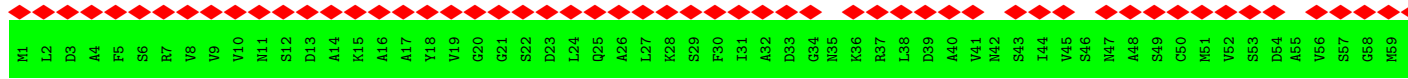
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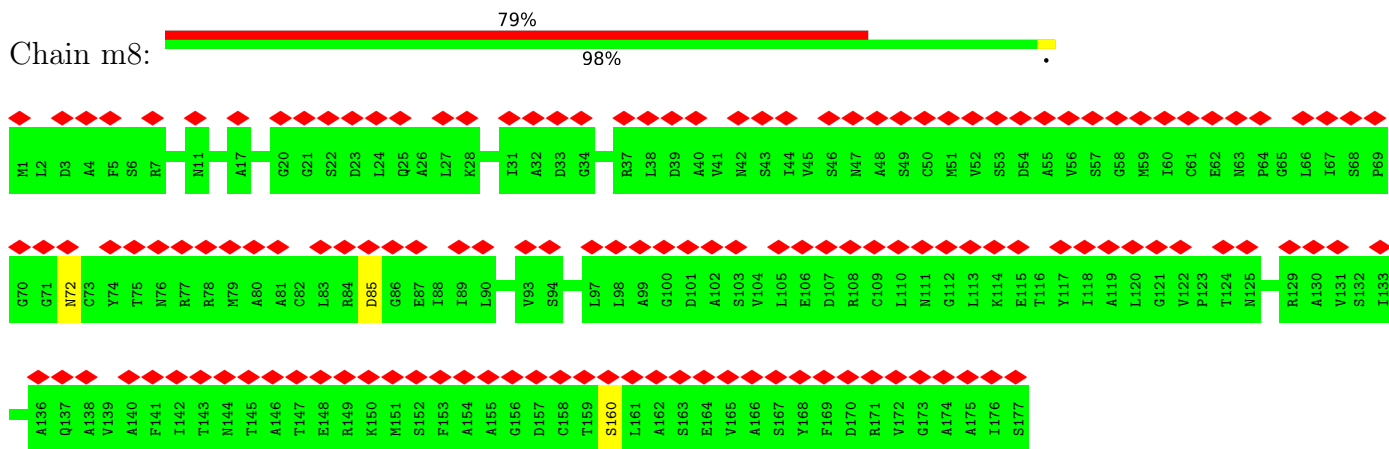
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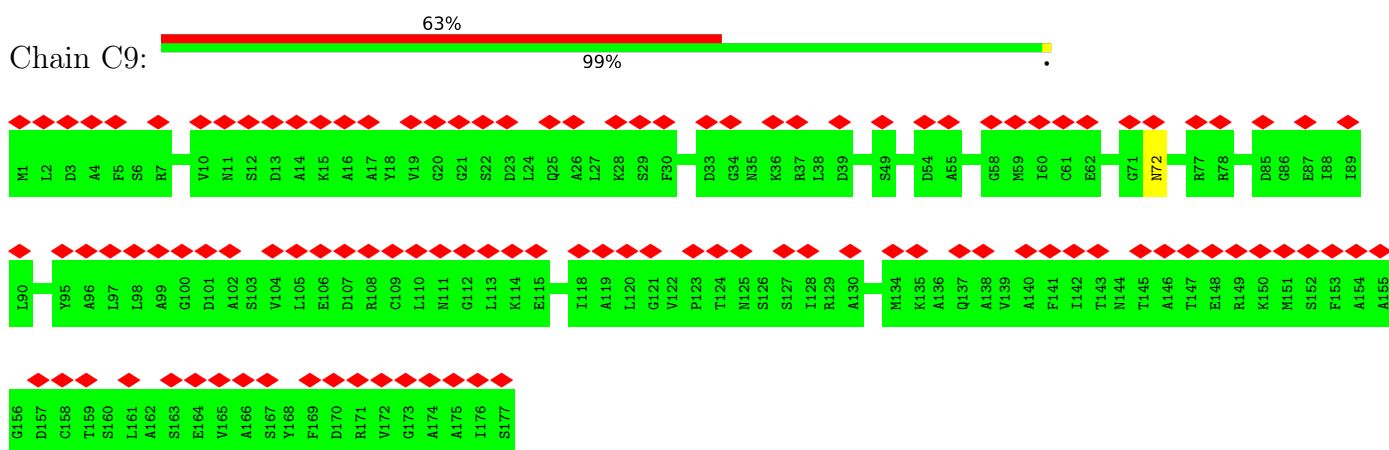
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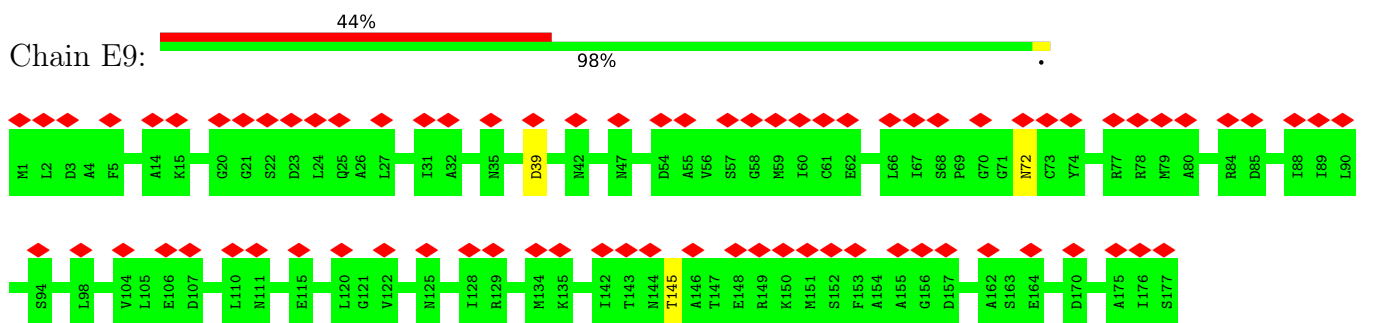
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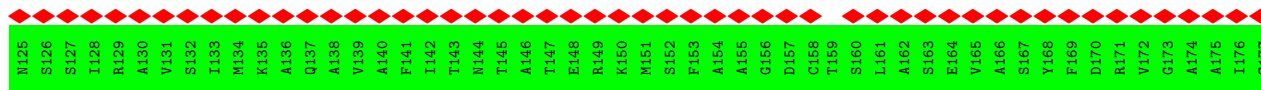


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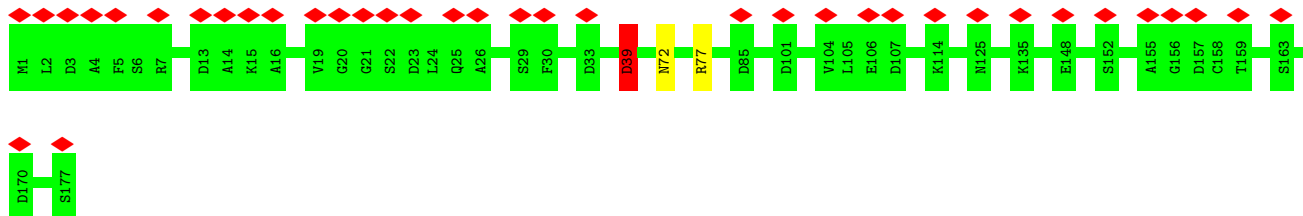


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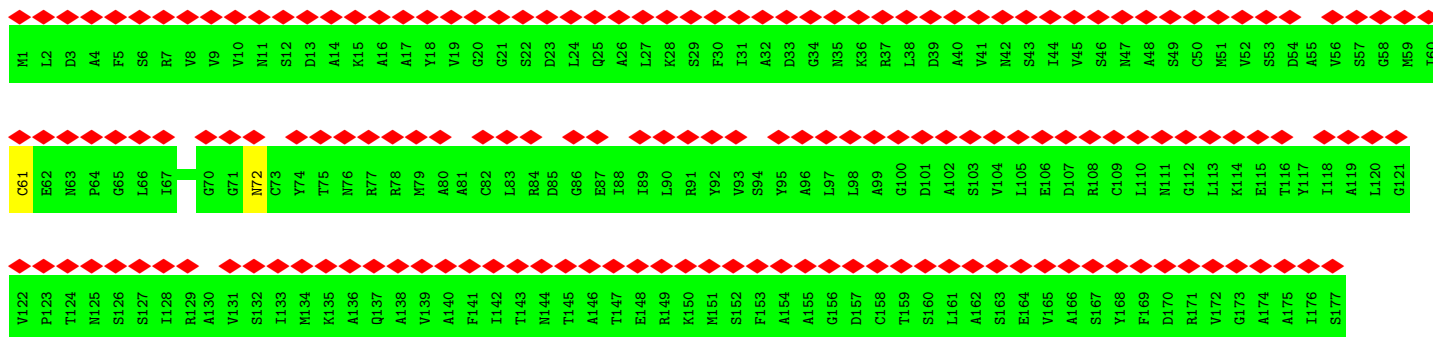




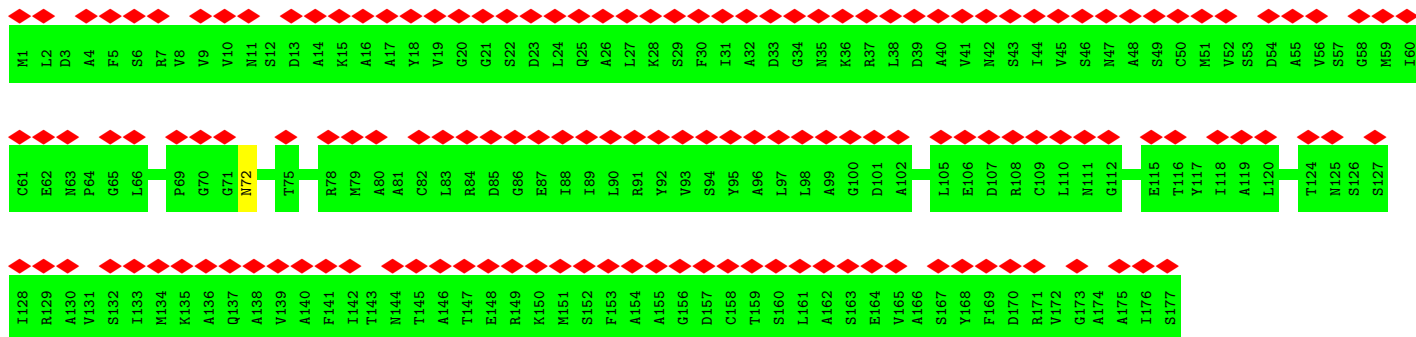
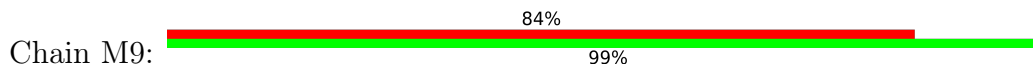
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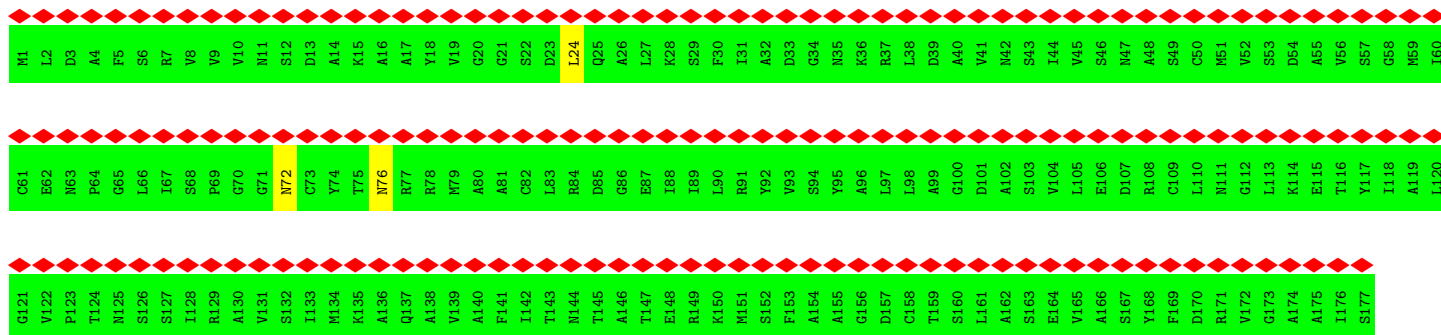


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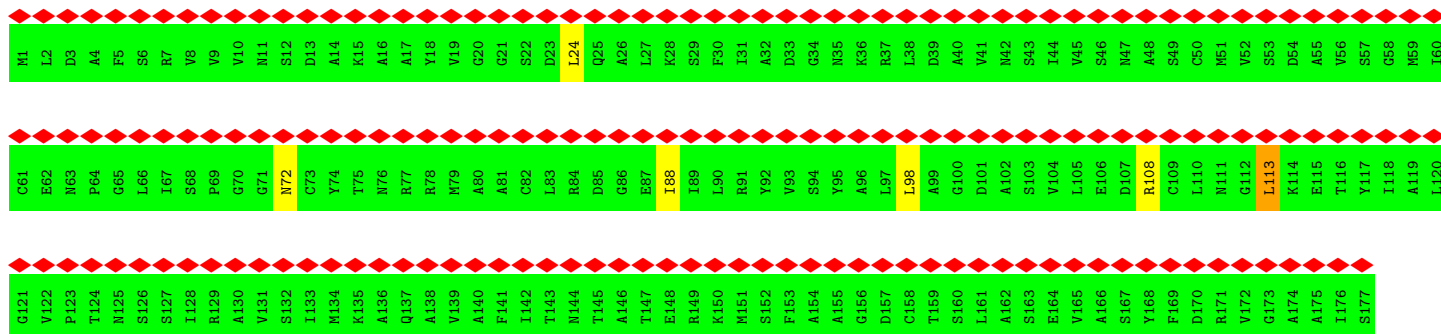


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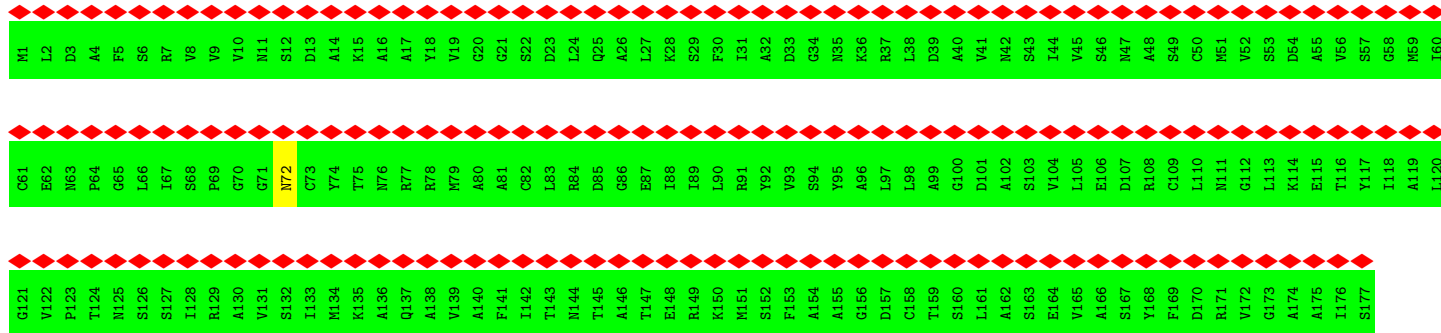




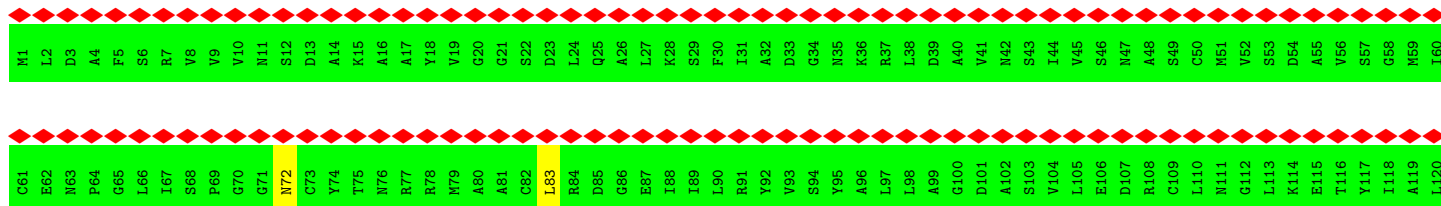
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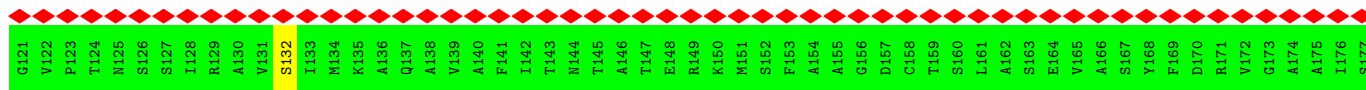


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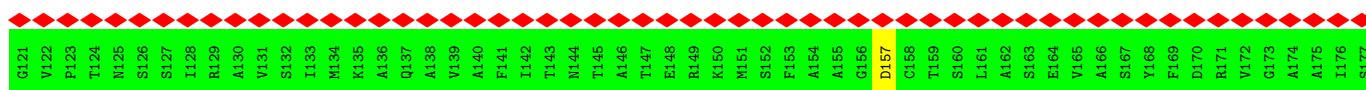
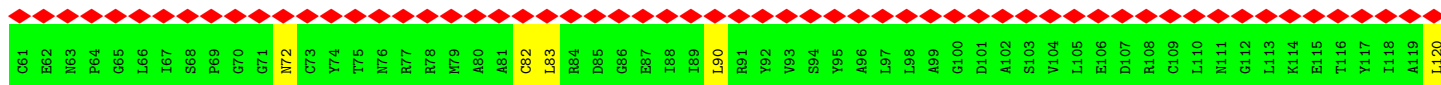


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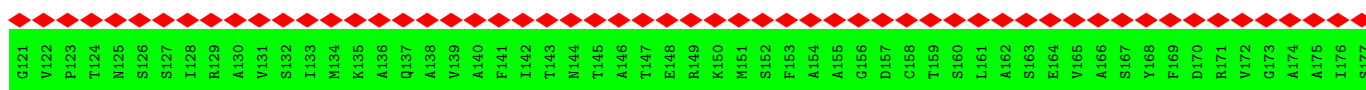
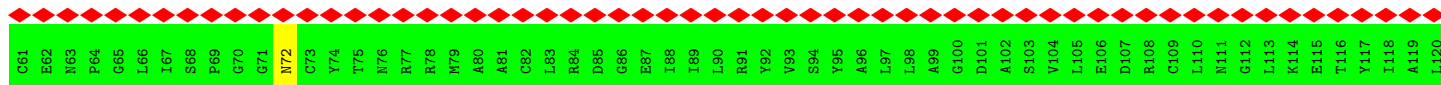




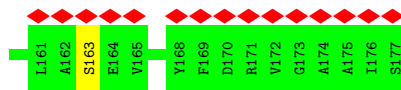
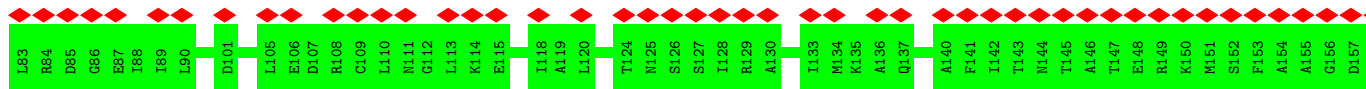
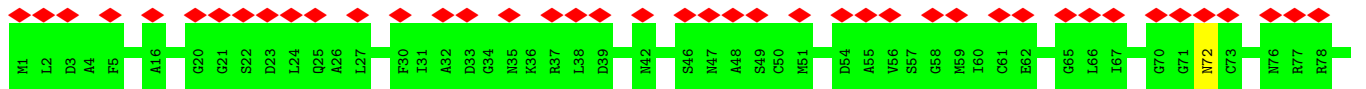
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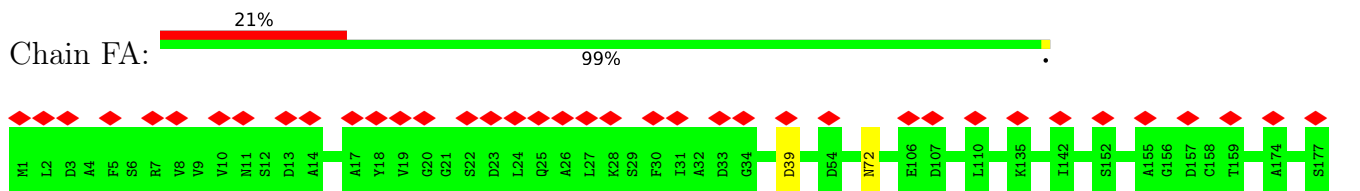
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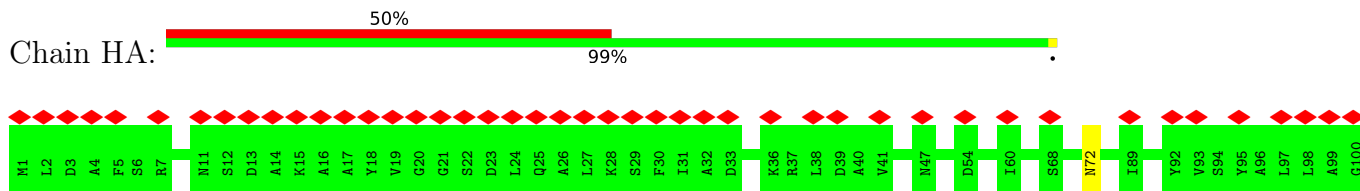
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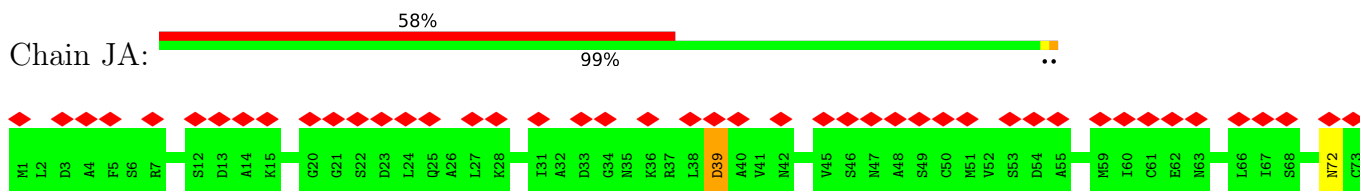
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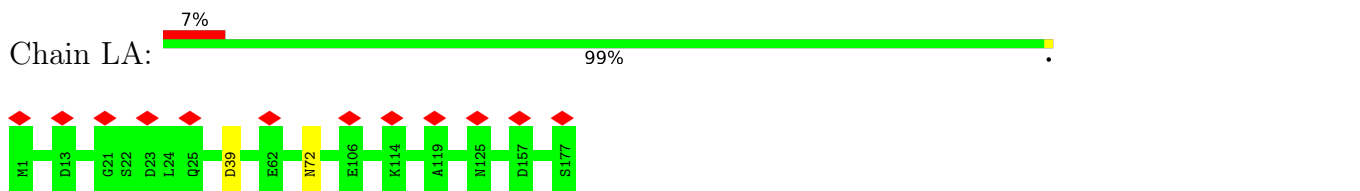
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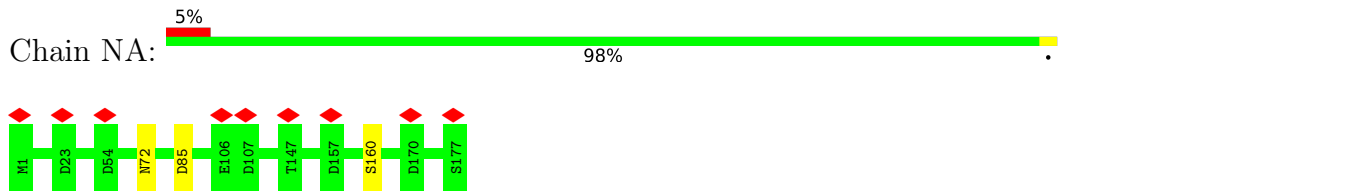
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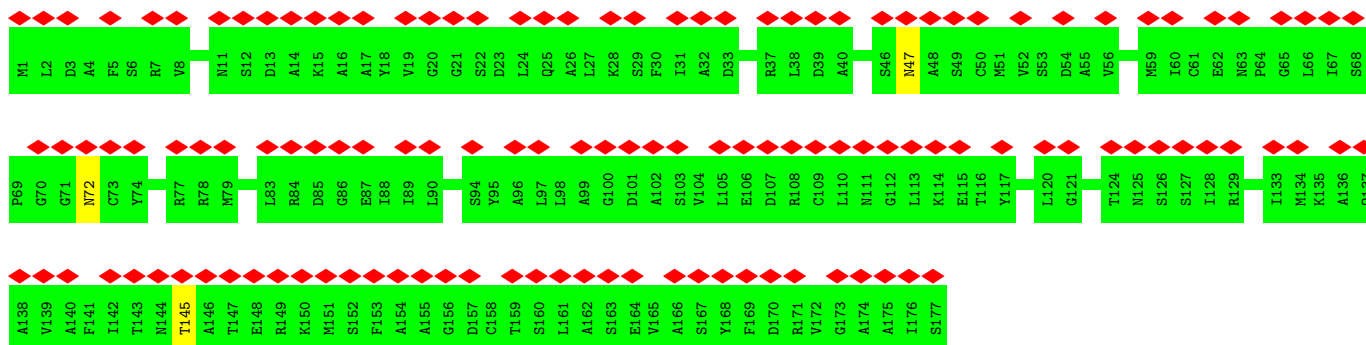


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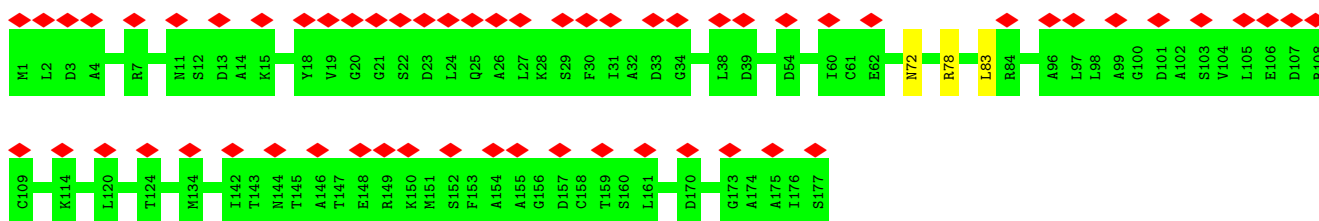
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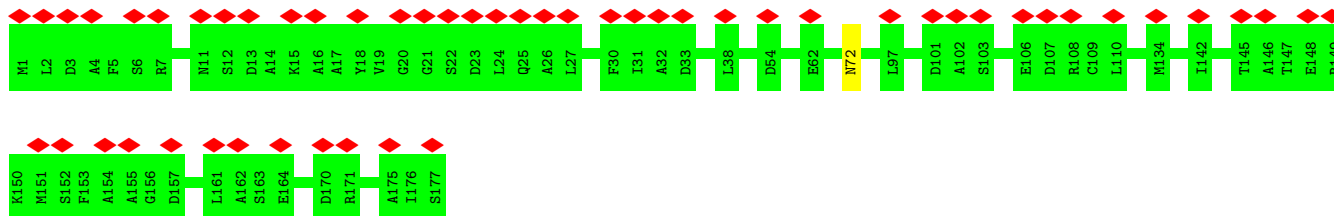
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Chain RA: 33% 98%



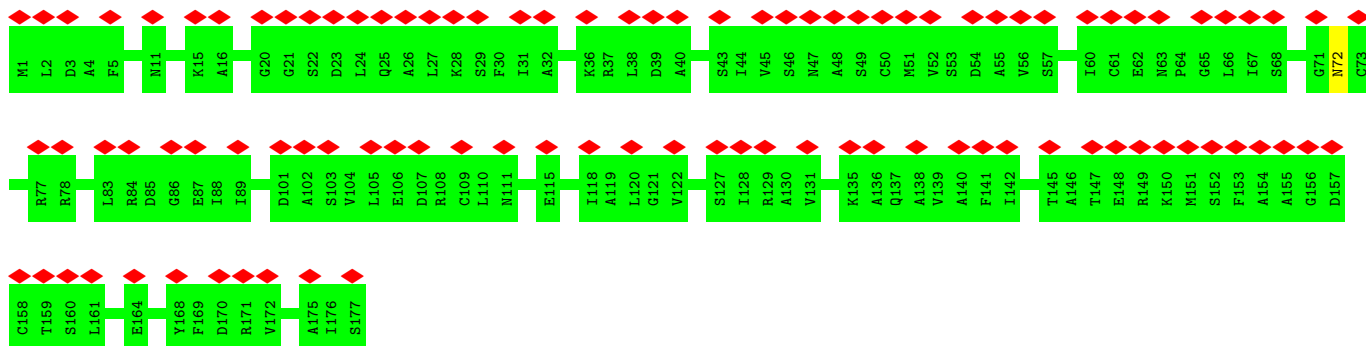
- Molecule 2: B-phycoerythrin beta chain

Chain TA: 30% 99%

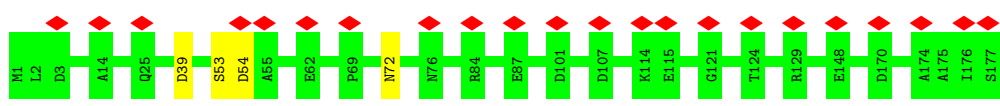


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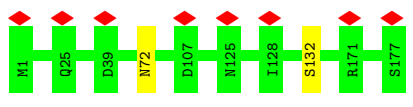
Chain VA: 55% 99%



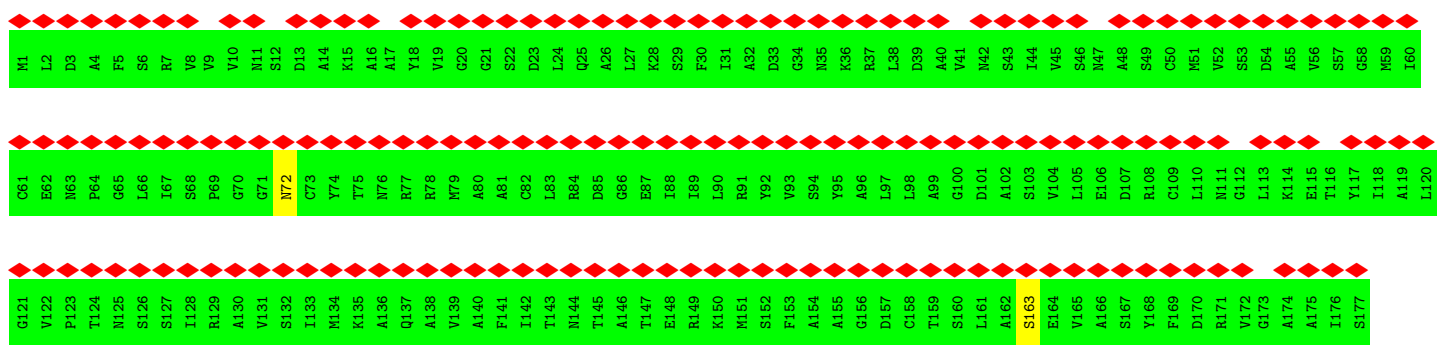
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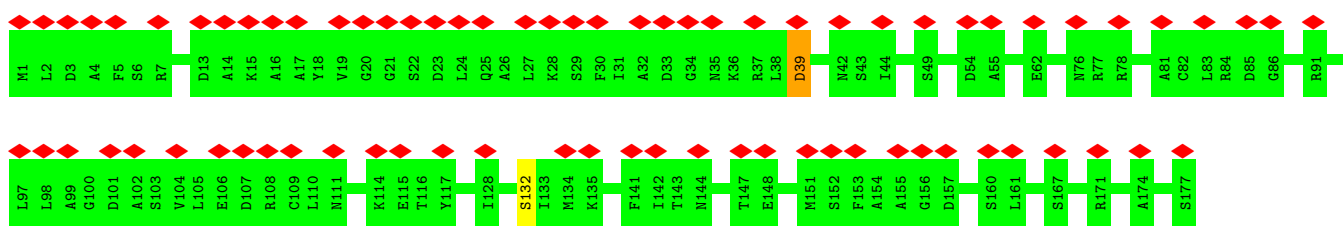
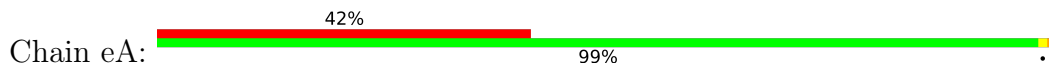
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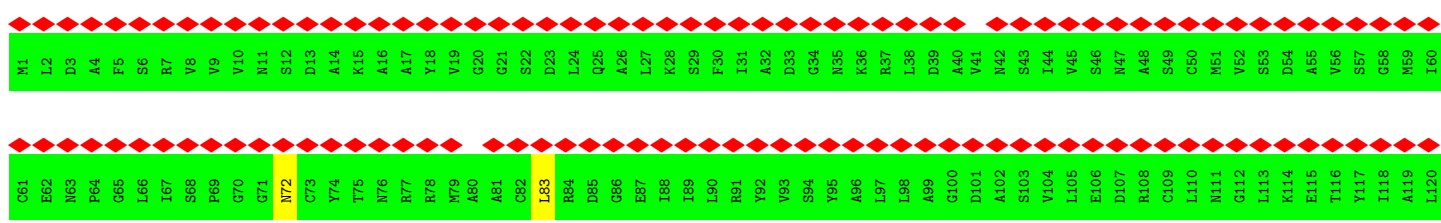
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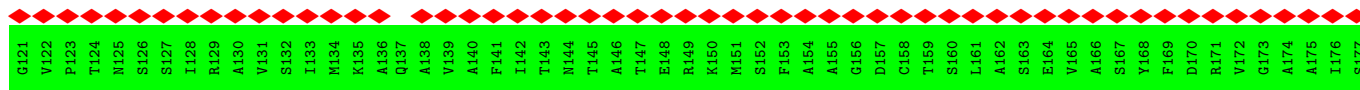


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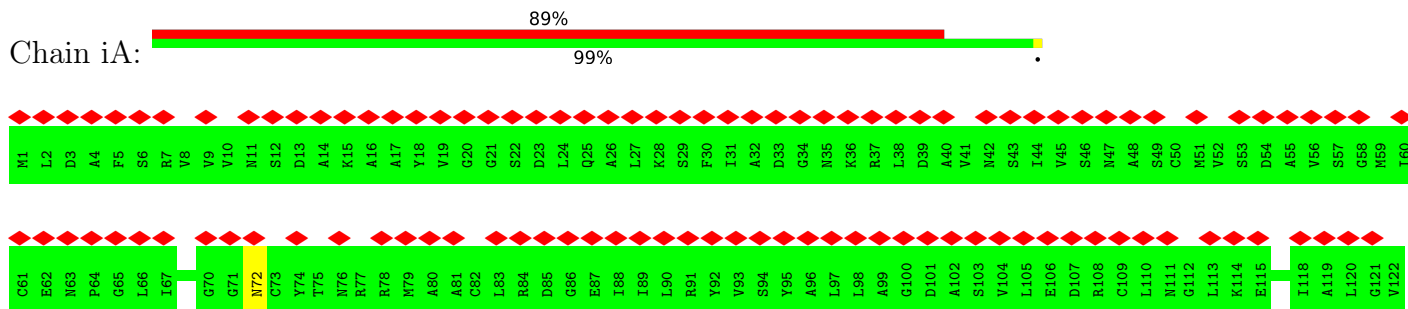


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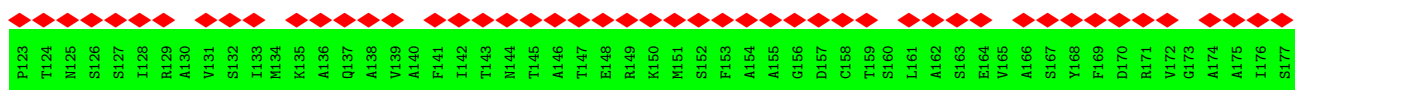
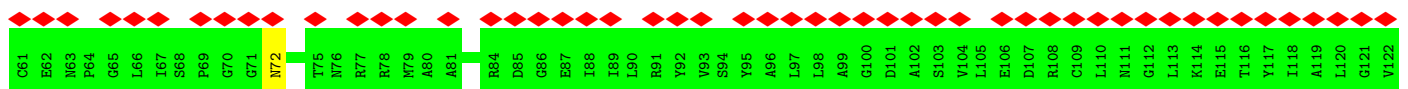
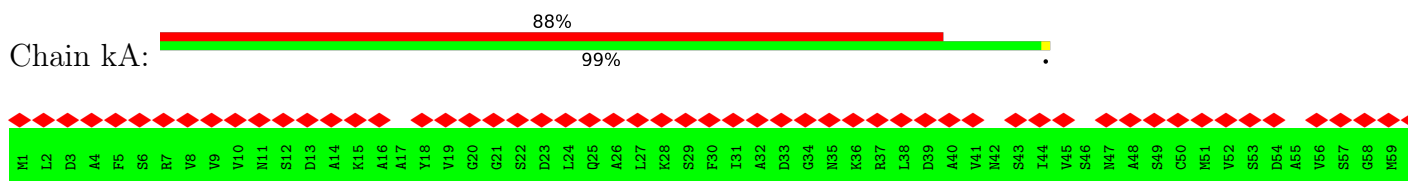




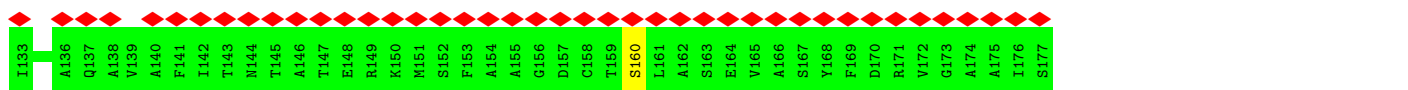
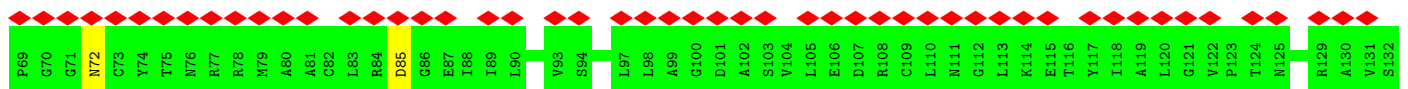
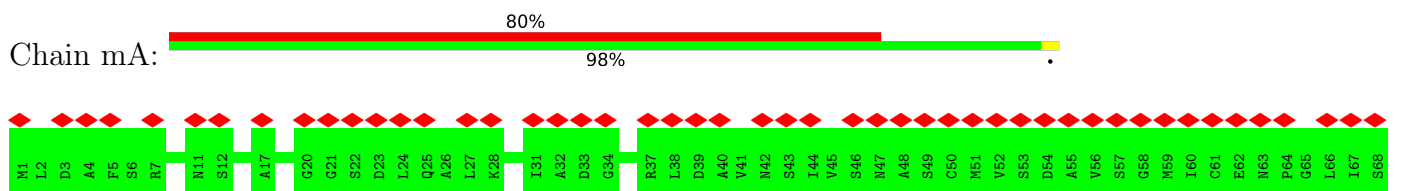
• Molecule 2: B-phycoerythrin beta chain



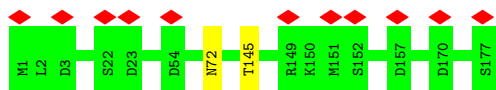
• Molecule 2: B-phycoerythrin beta chain



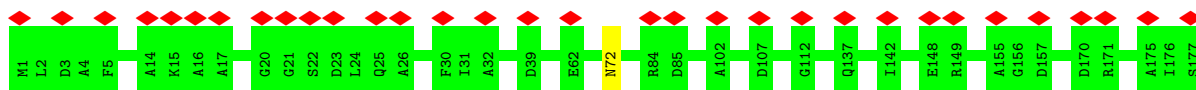
• Molecule 2: B-phycoerythrin beta chain



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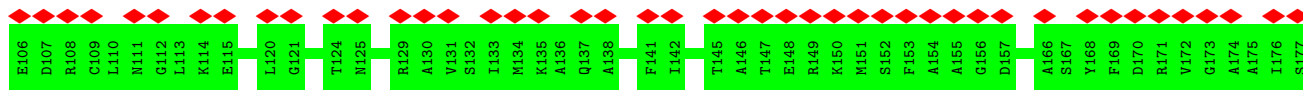
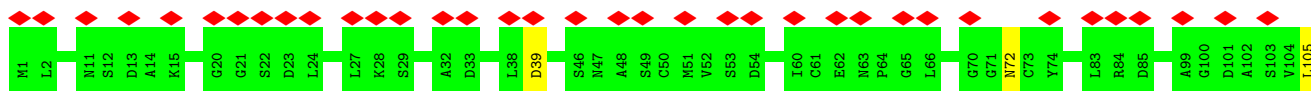
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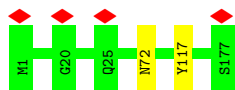
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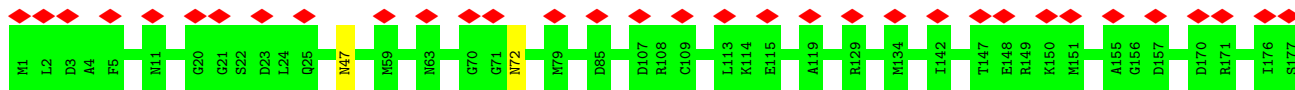
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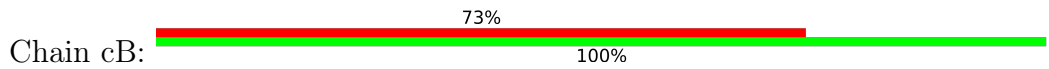
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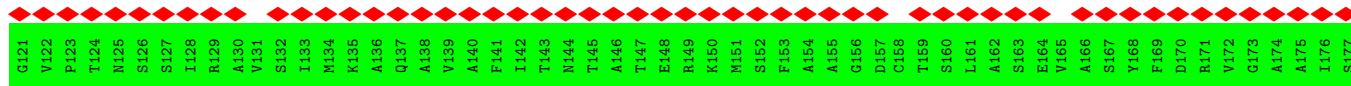
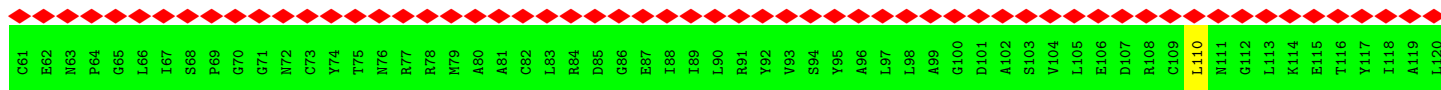


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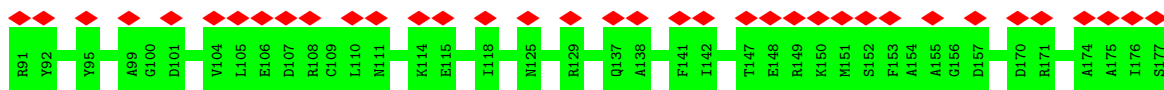
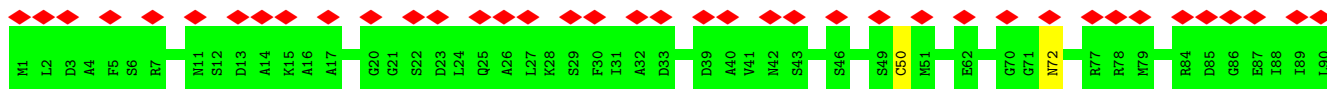
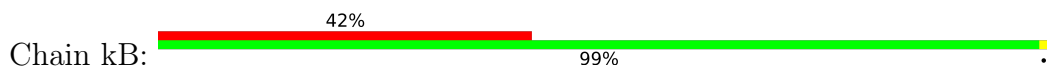


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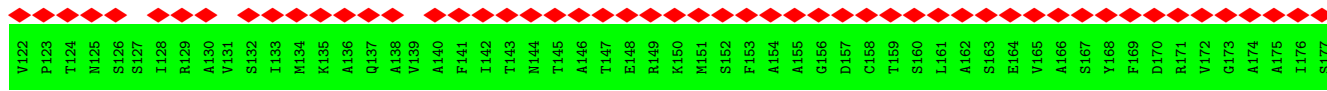
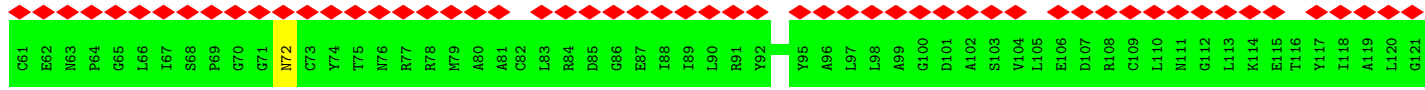
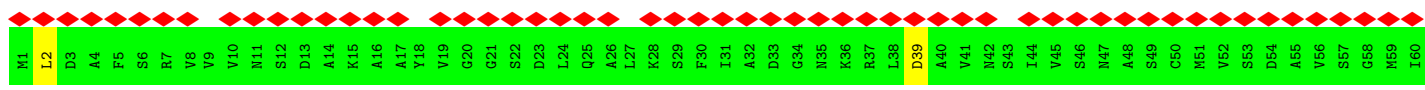




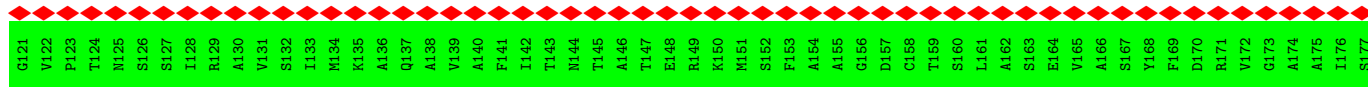
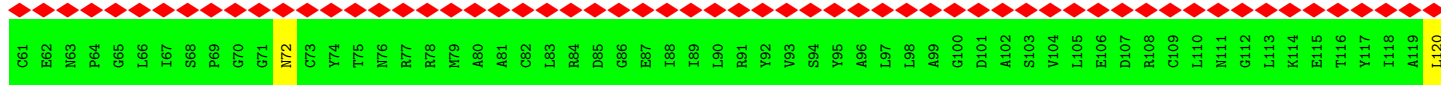
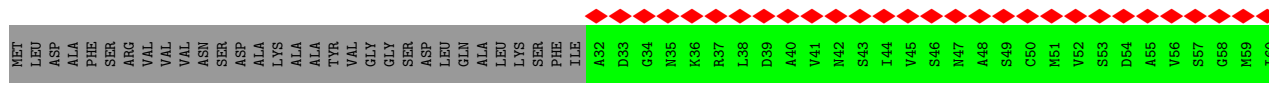
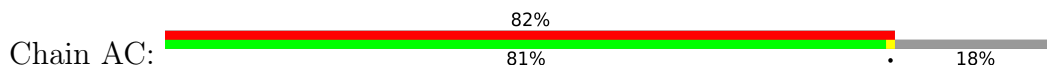
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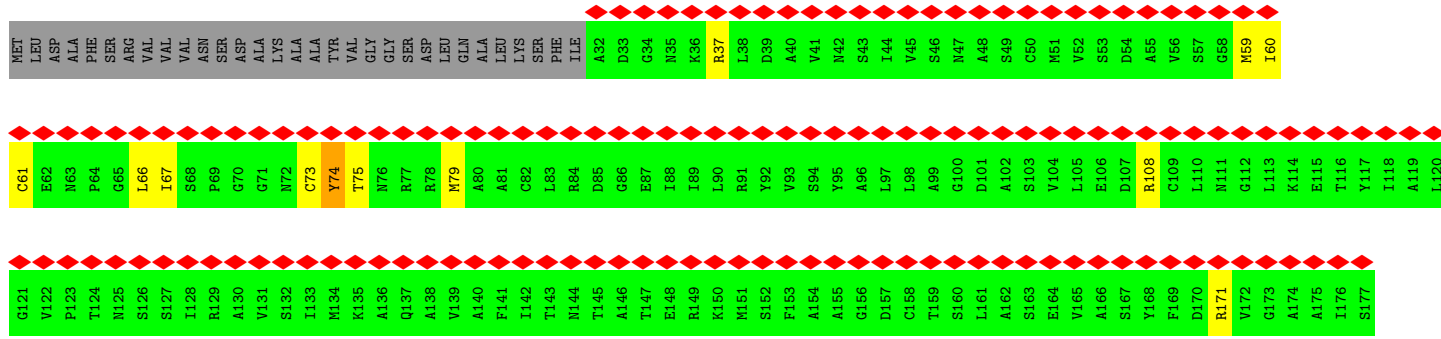
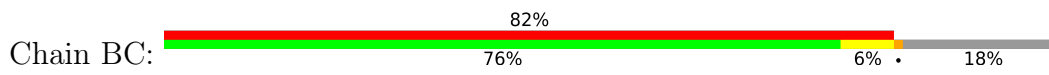
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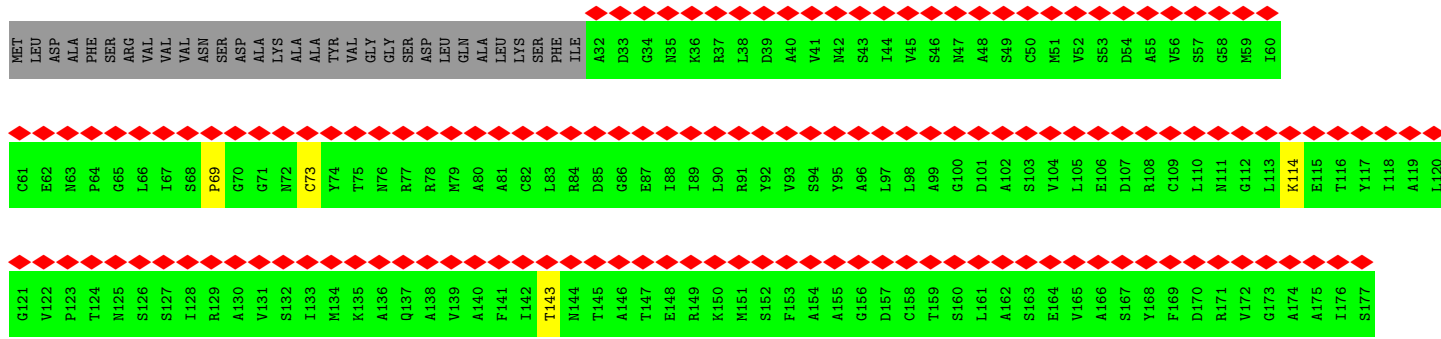
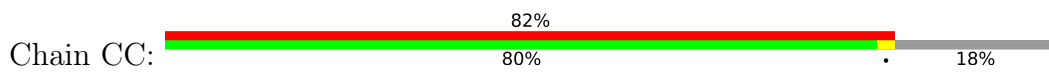
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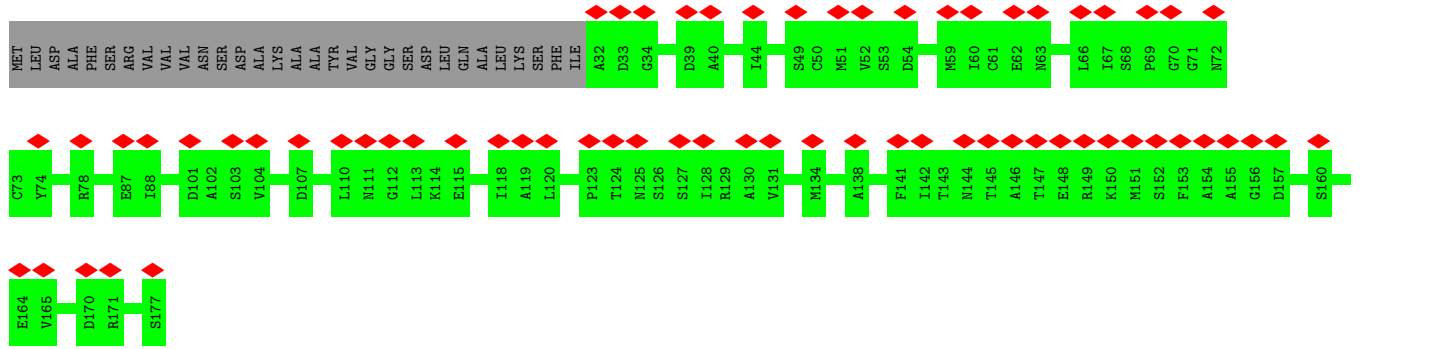
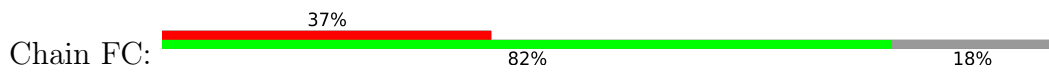
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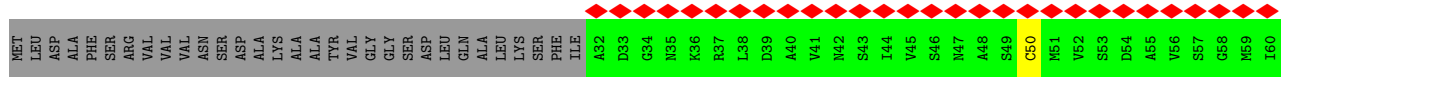
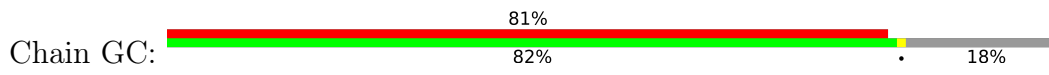
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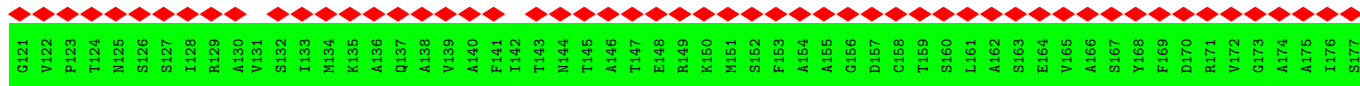
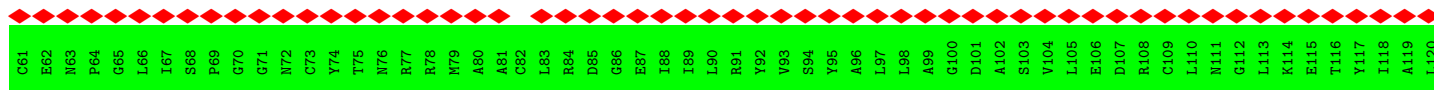


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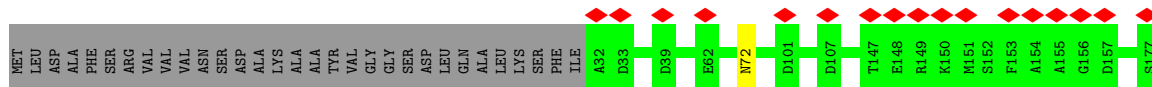
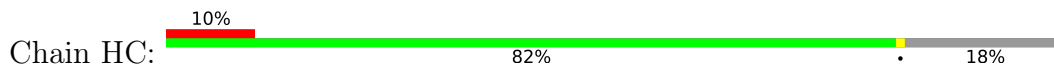


• Molecule 2: B-phycoerythrin beta chain

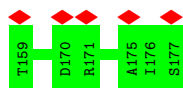
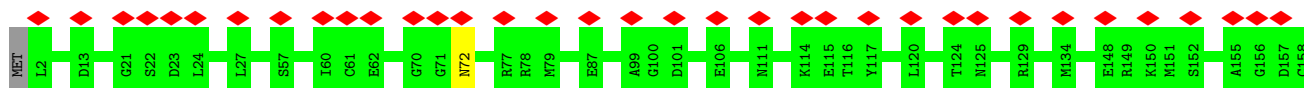




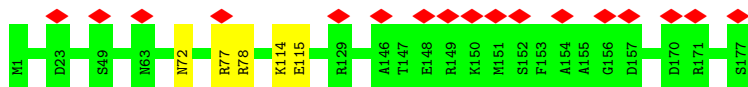
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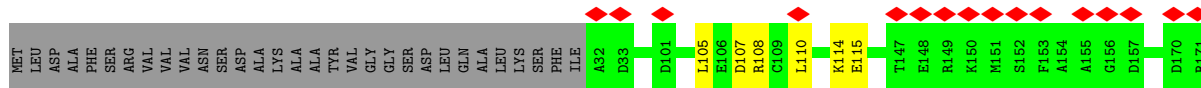
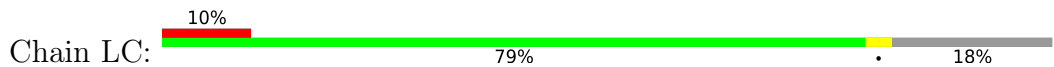
• Molecule 2: B-phycoerythrin beta chain



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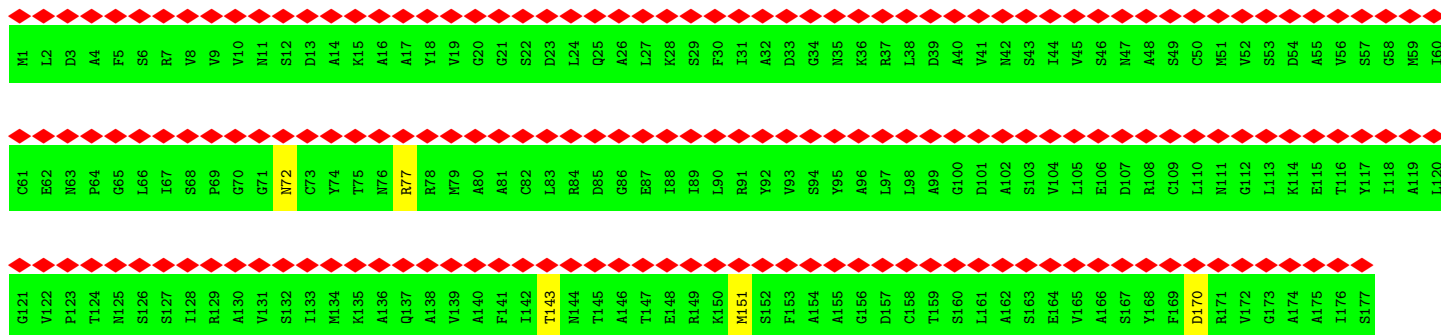


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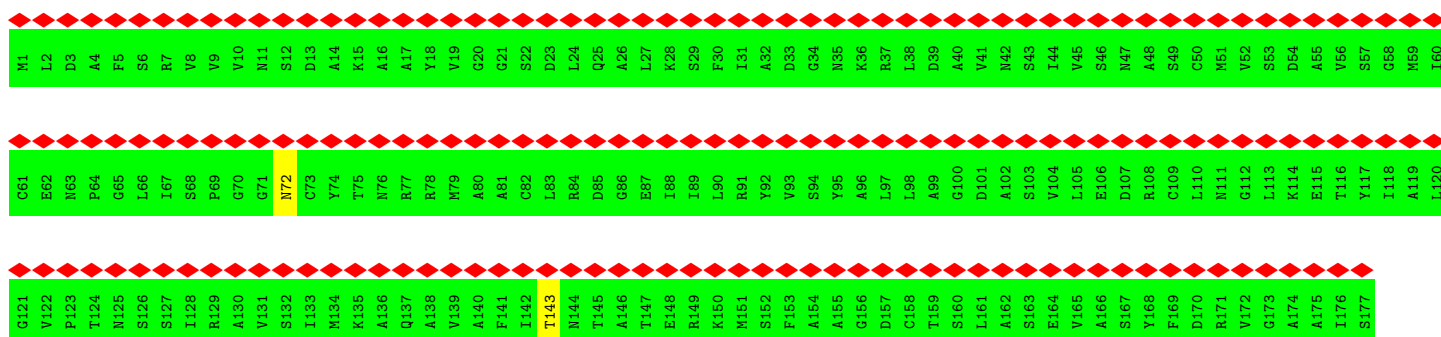


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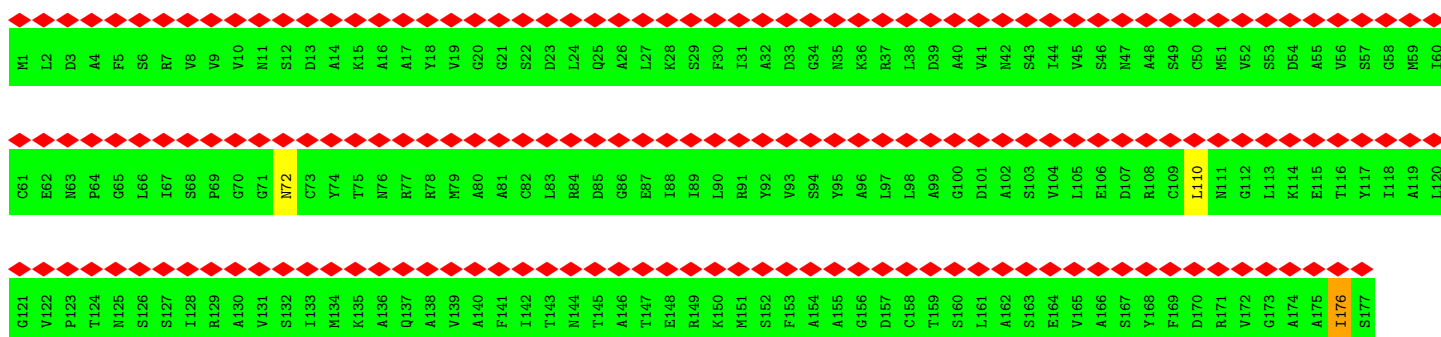




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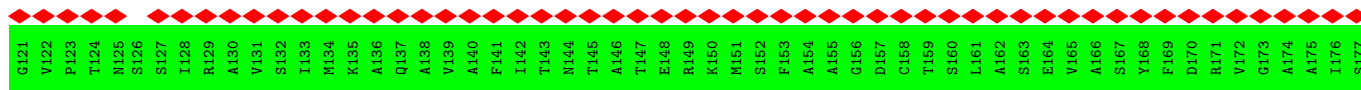


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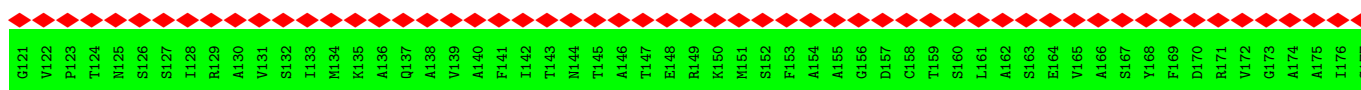
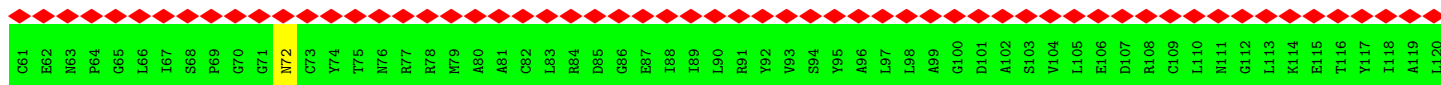
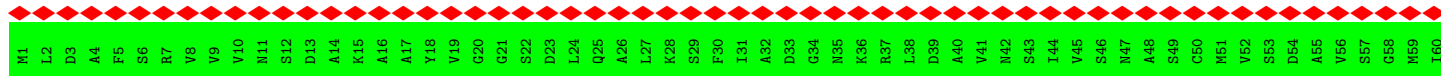


• Molecule 2: B-phycoerythrin beta chain

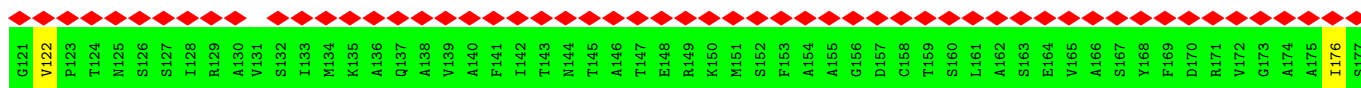
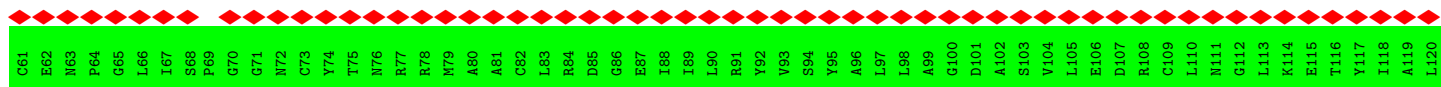
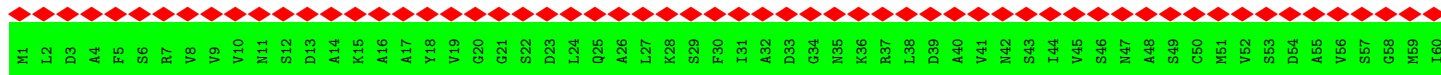




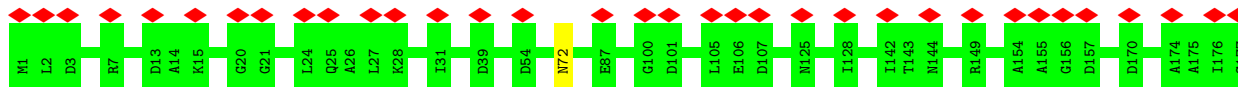
• Molecule 2: B-phycoerythrin beta chain



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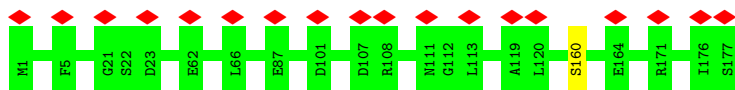


• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

Chain RD:  10% 99%



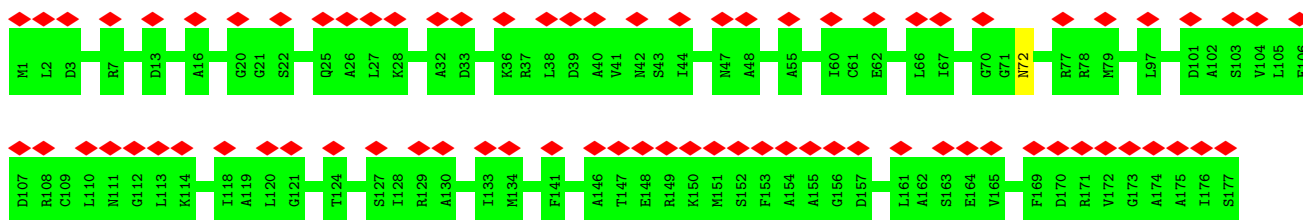
• Molecule 2: B-phycoerythrin beta chain

Chain TD:  99%



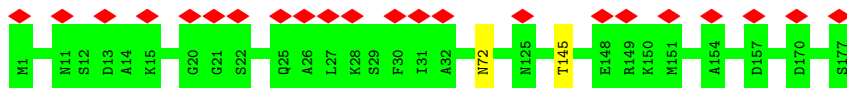
• Molecule 2: B-phycoerythrin beta chain

Chain VD:  44% 99%



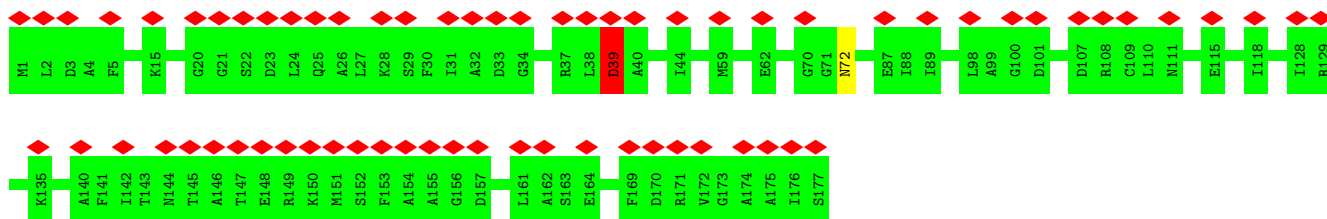
• Molecule 2: B-phycoerythrin beta chain

Chain XD:  12% 99%



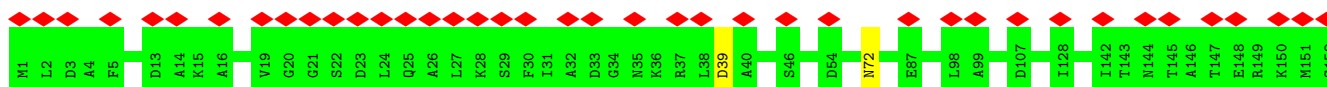
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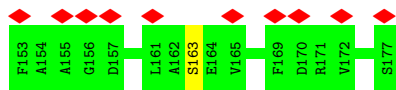
Chain BE:  38% 99%



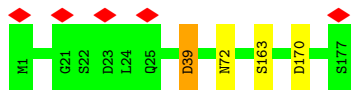
• Molecule 2: B-phycoerythrin beta chain

Chain DE:  28% 98%

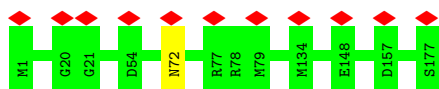




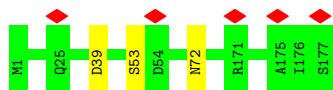
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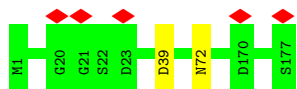
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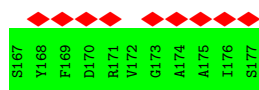
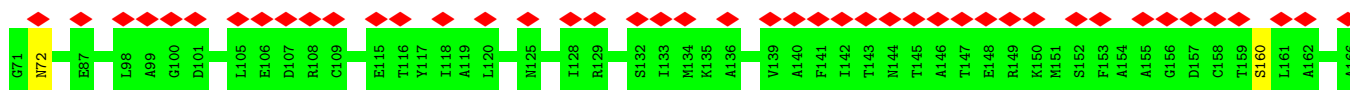
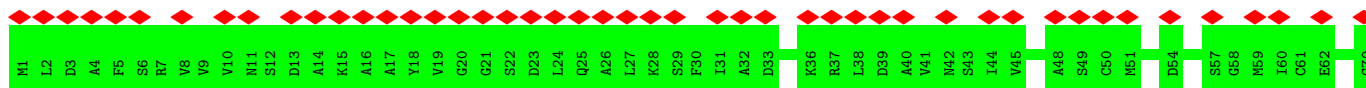
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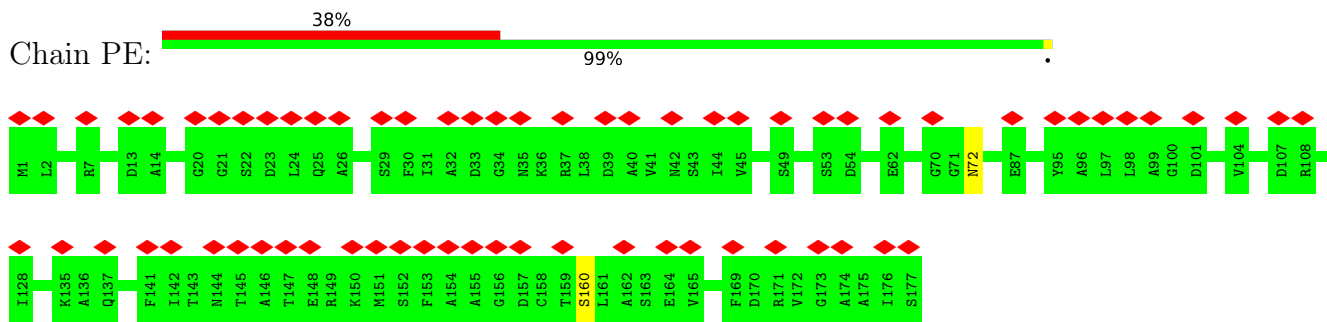
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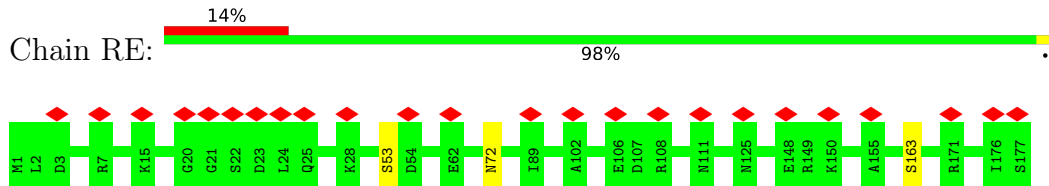
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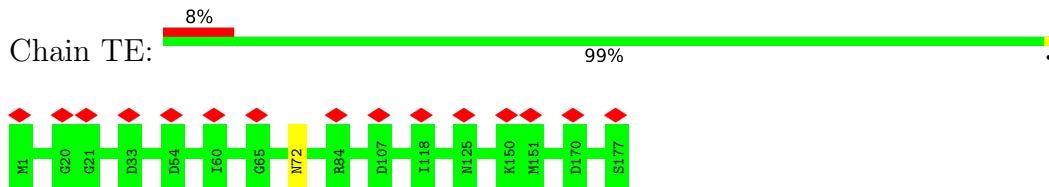
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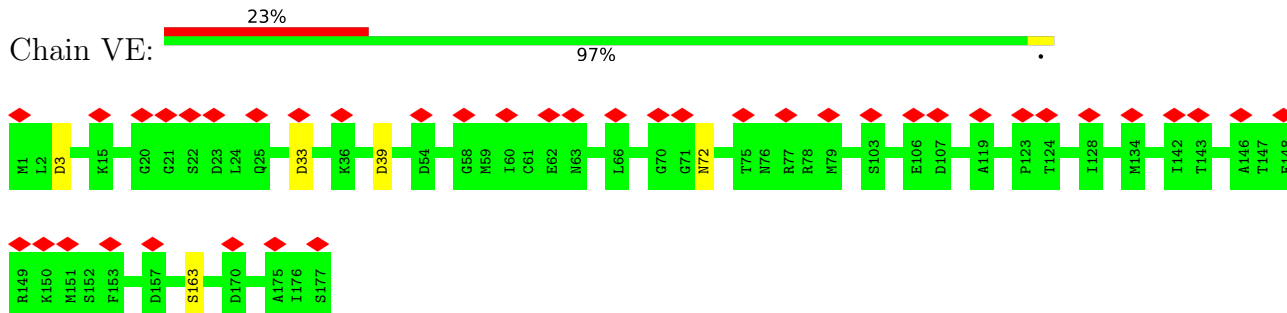
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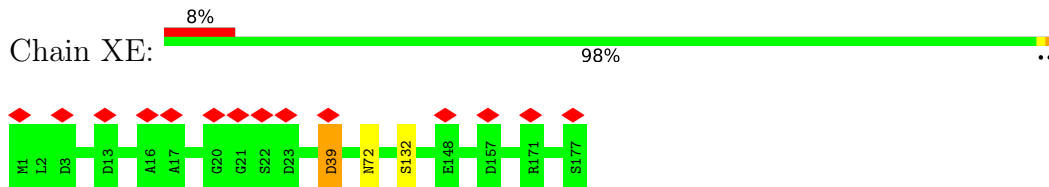
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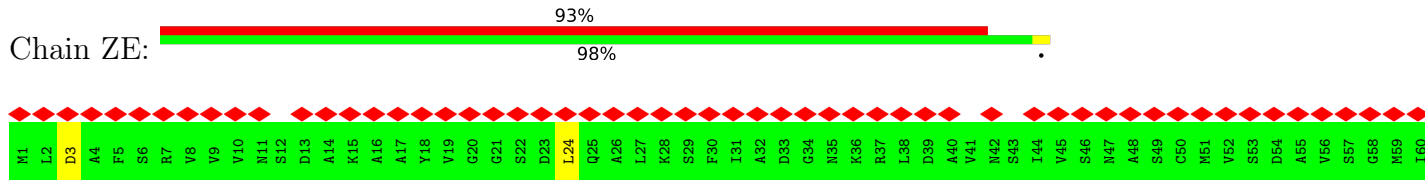
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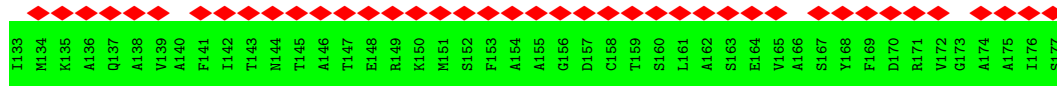
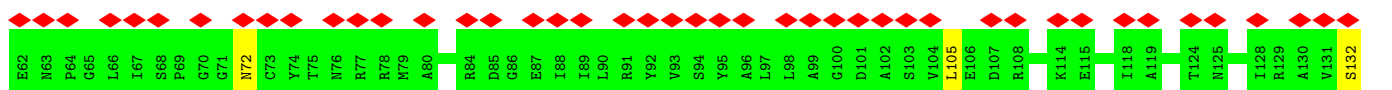


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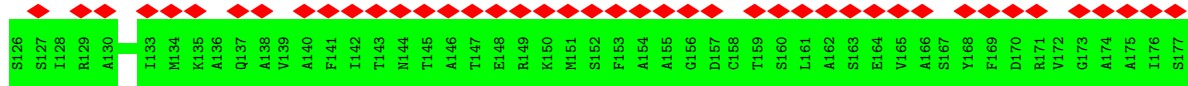
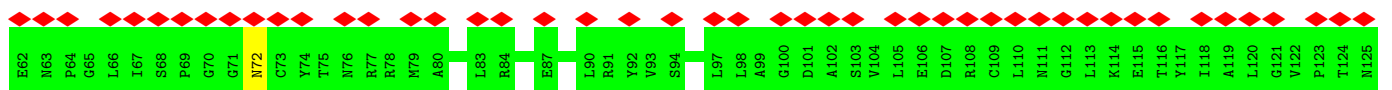
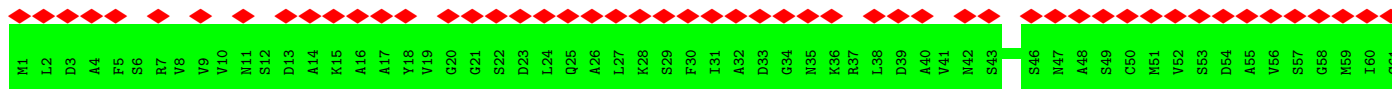




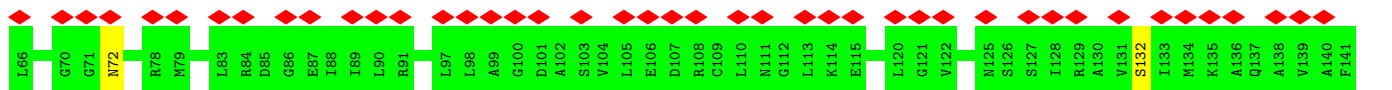
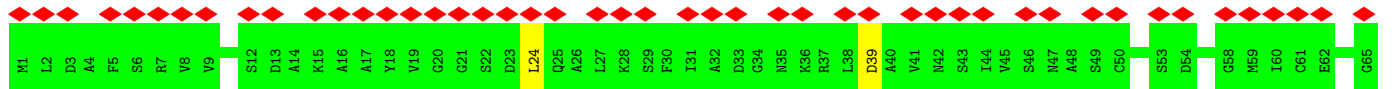
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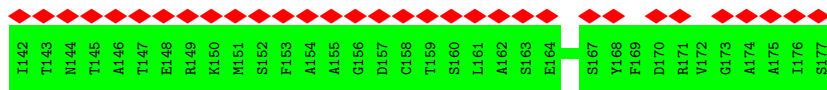


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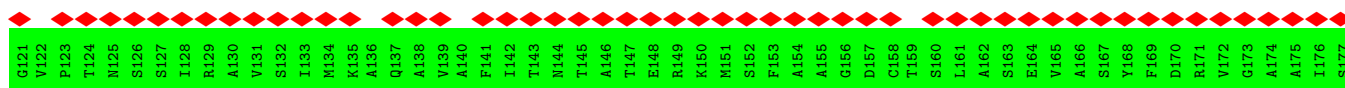
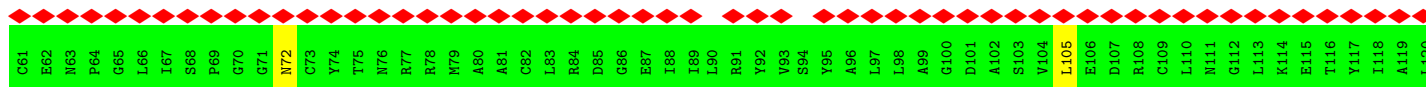
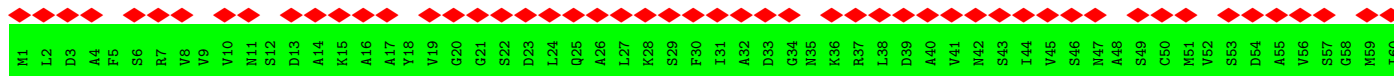


• Molecule 2: B-phycoerythrin beta chain

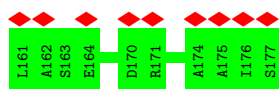
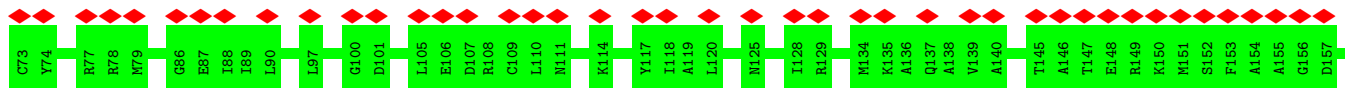




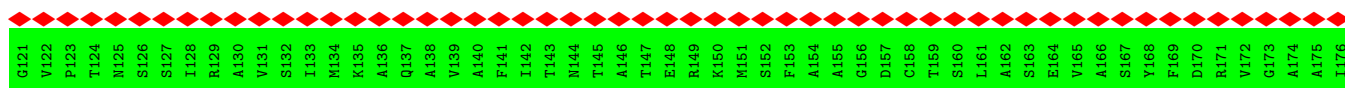
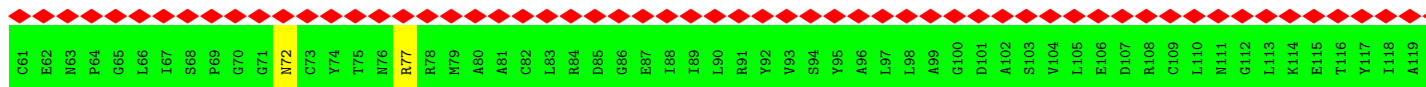
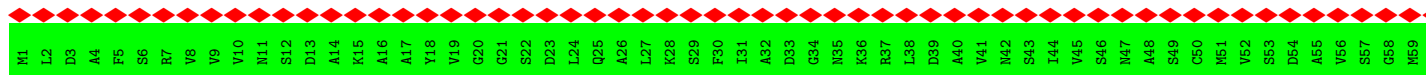
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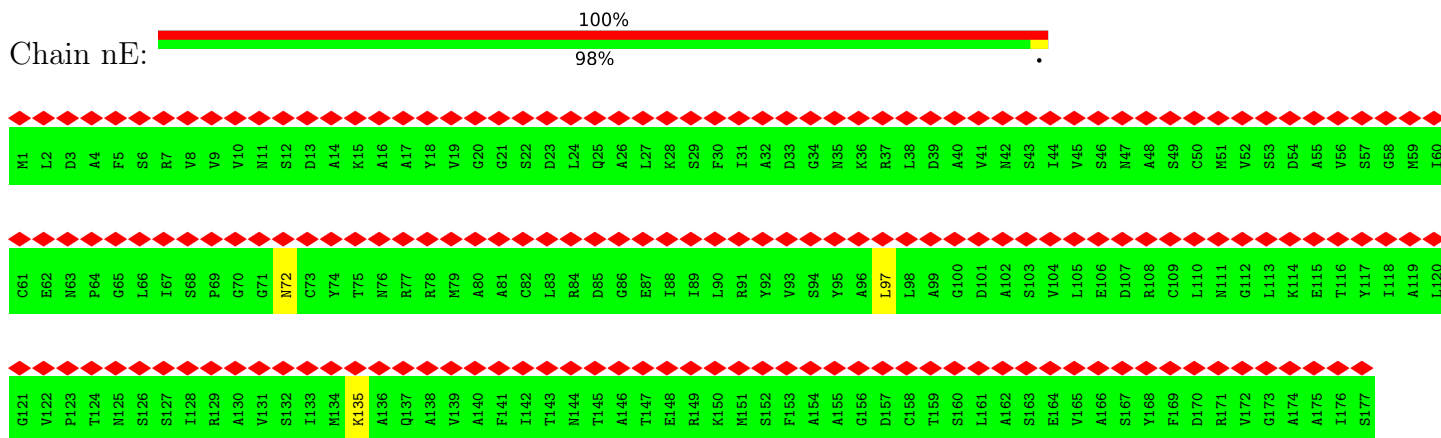
• Molecule 2: B-phycoerythrin beta chain



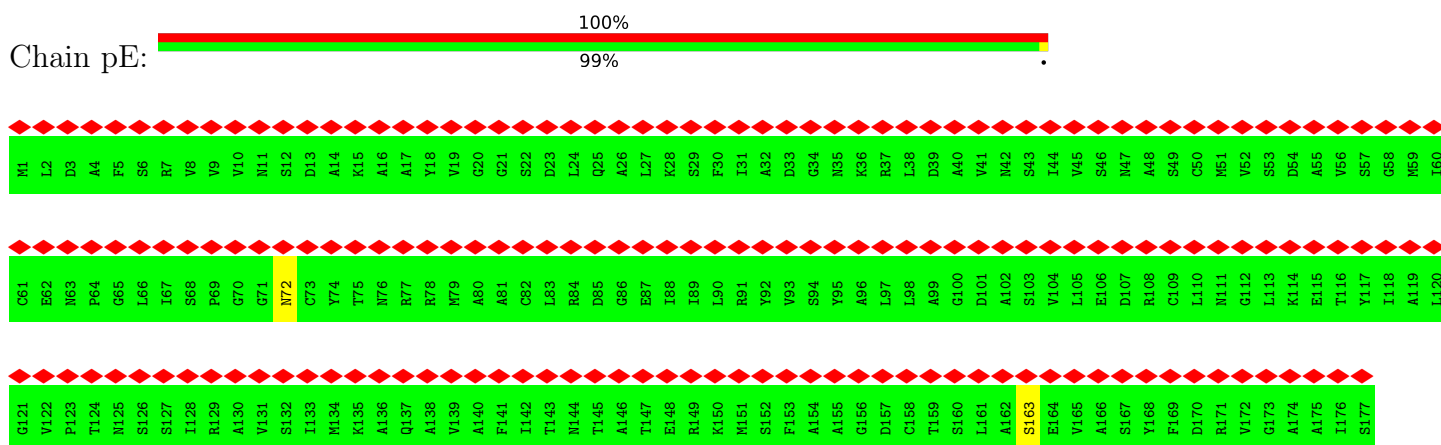
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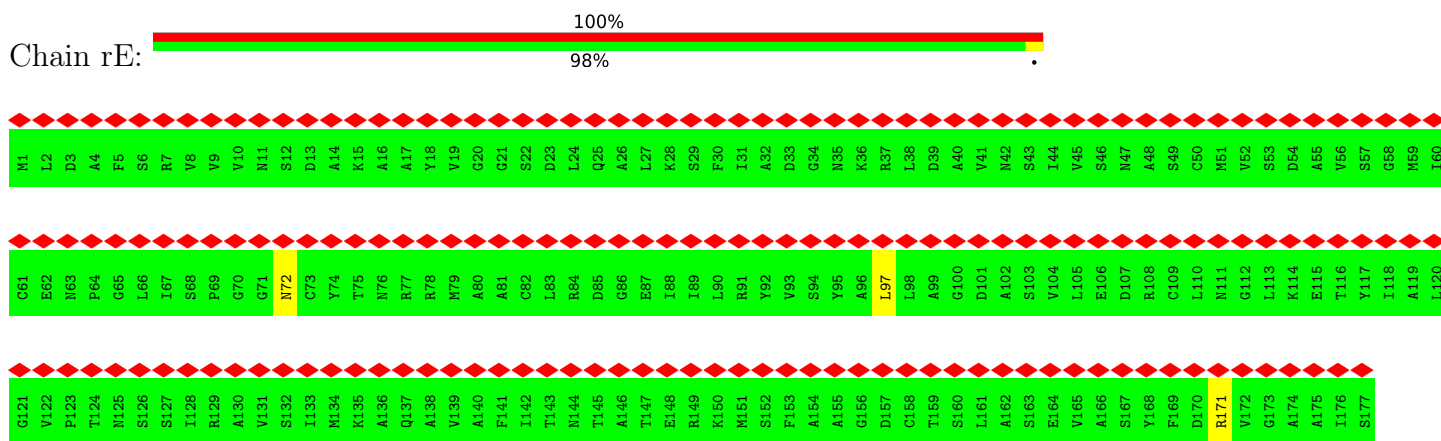
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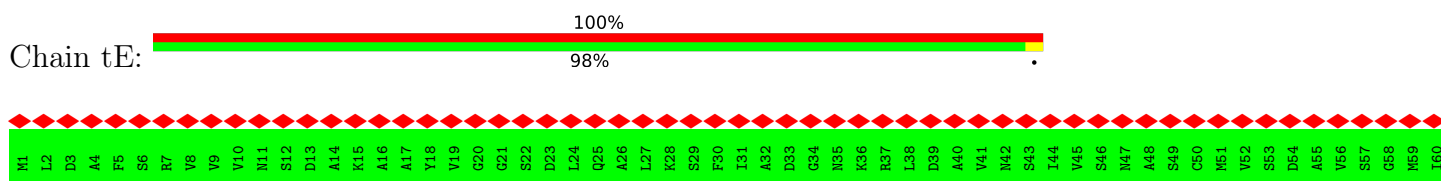
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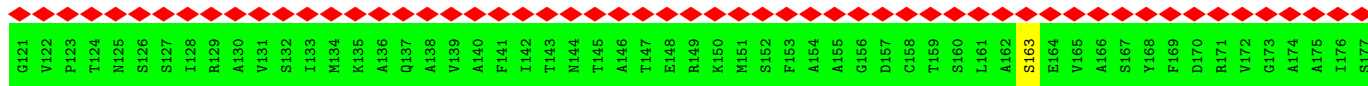
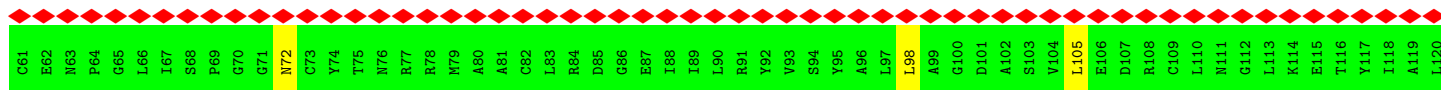


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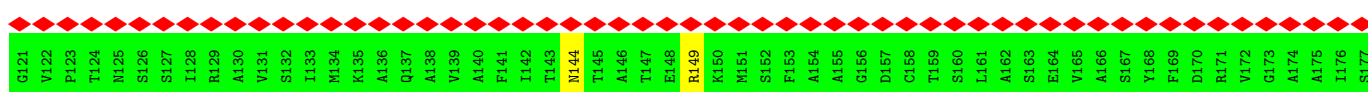
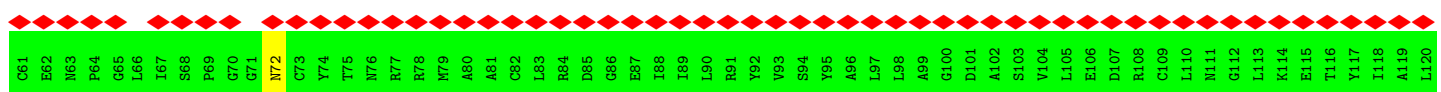
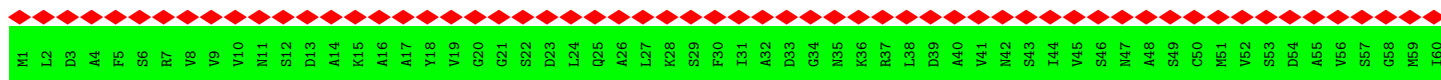


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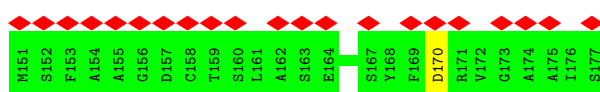
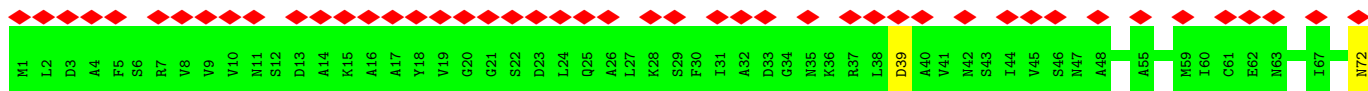




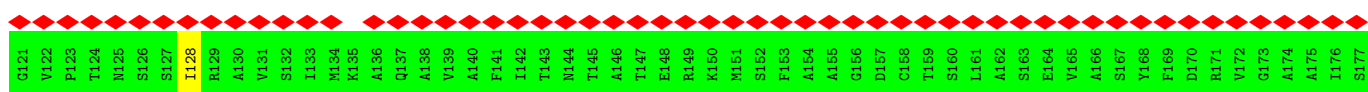
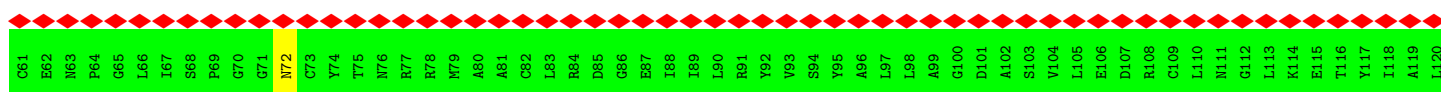
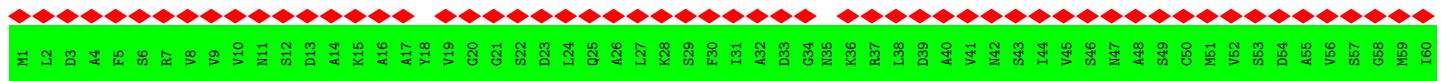
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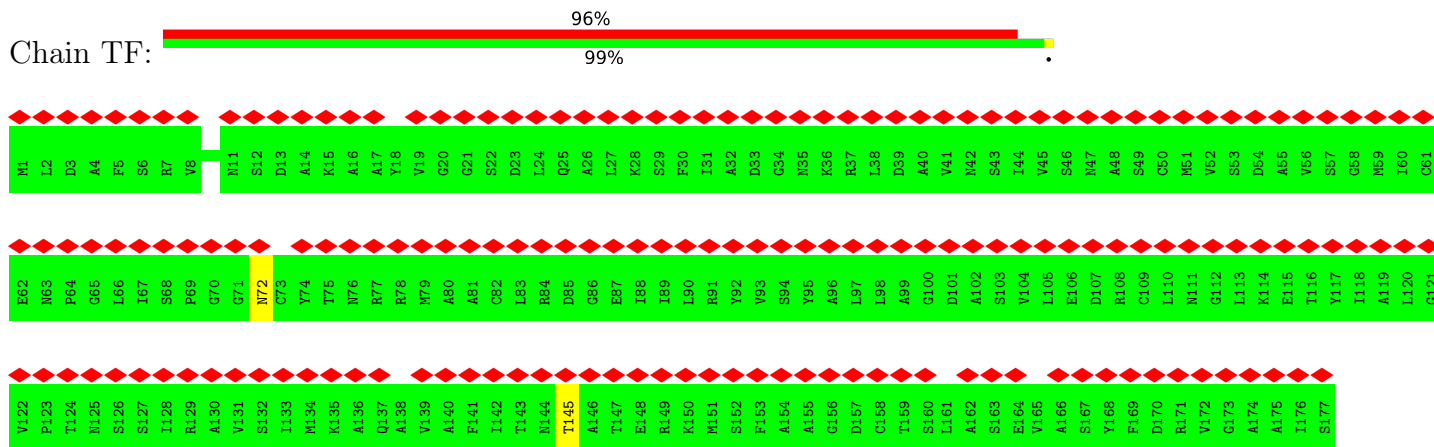
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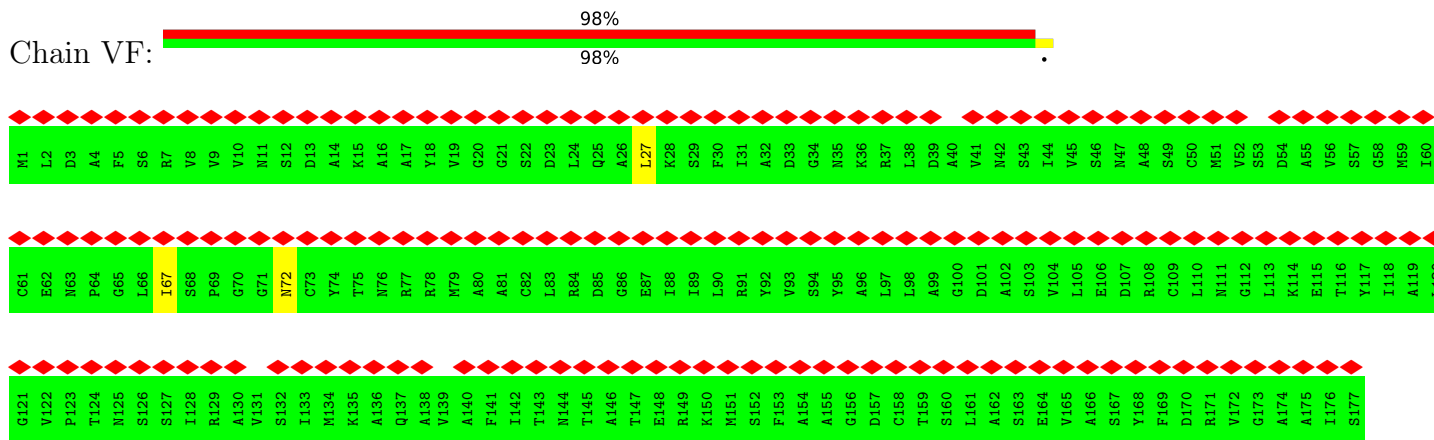
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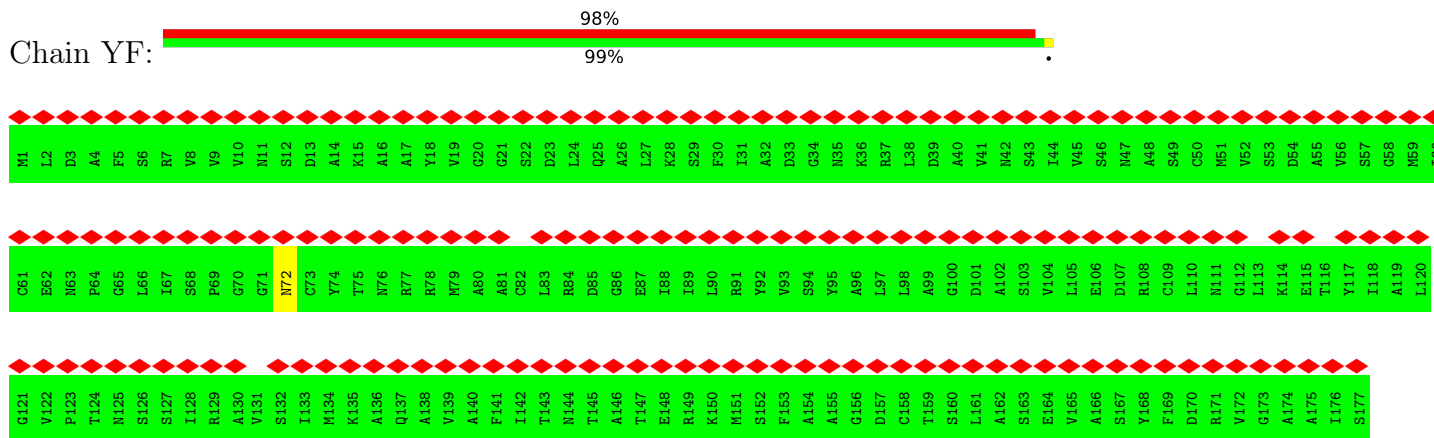
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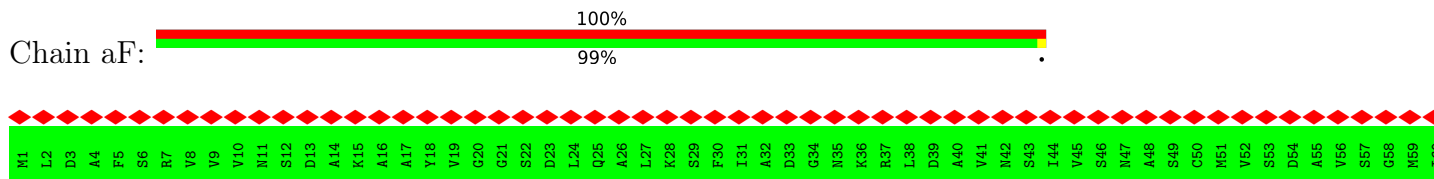
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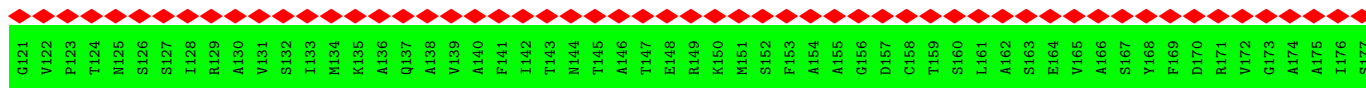
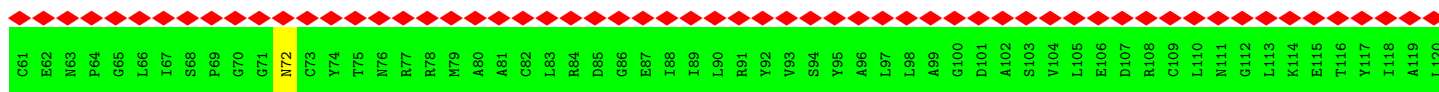


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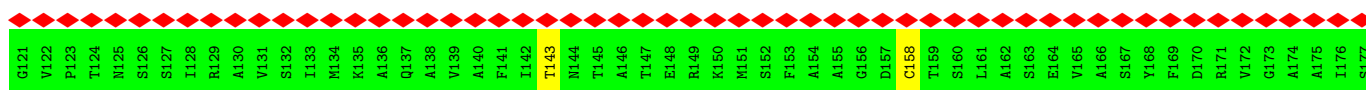
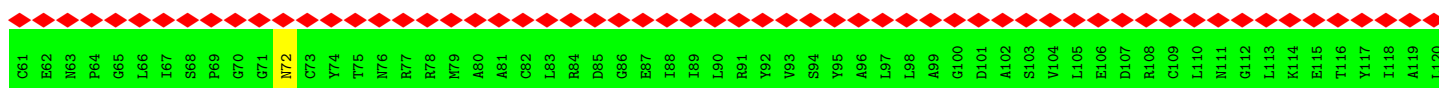
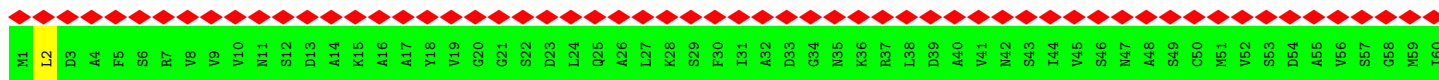


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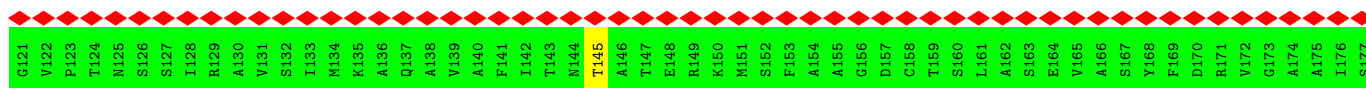
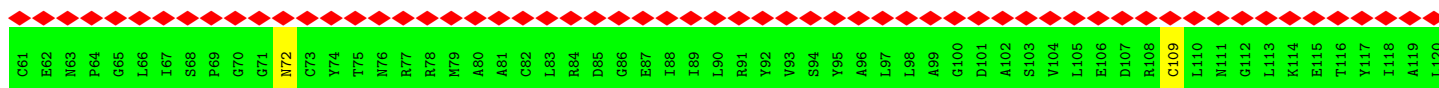
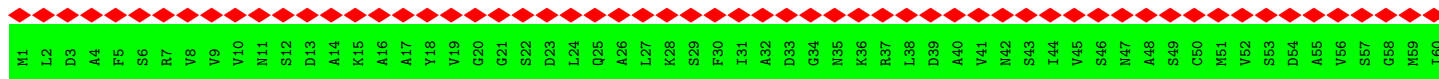




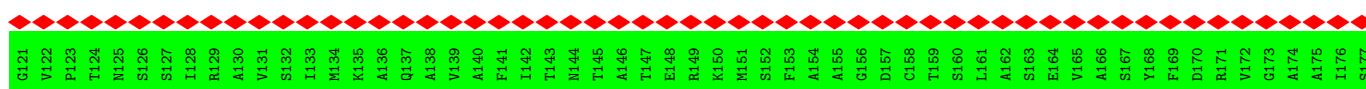
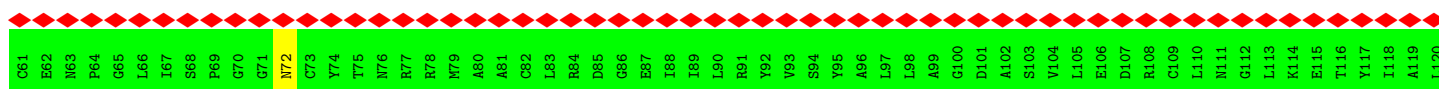
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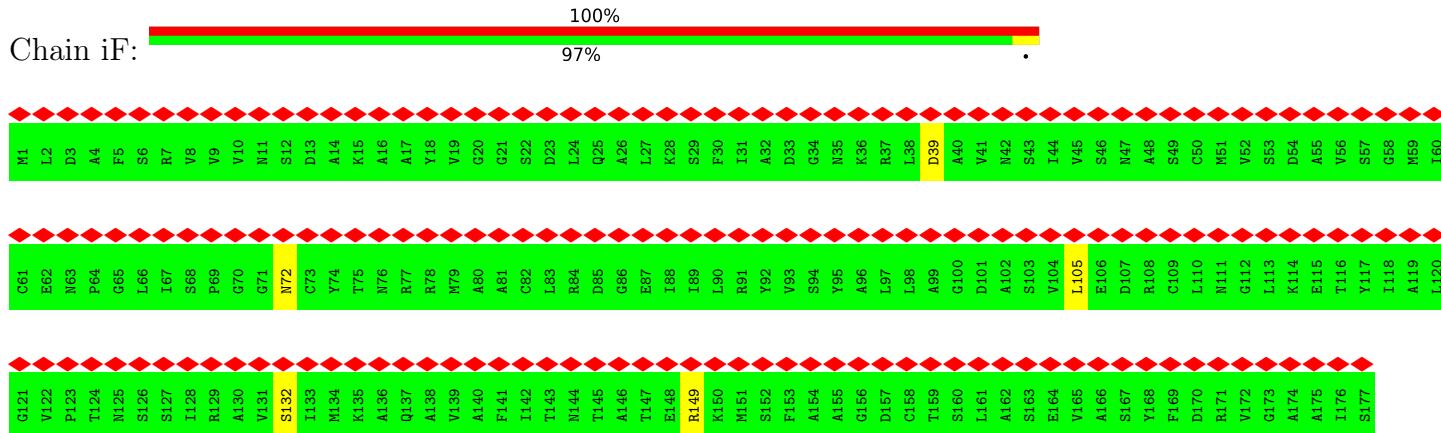
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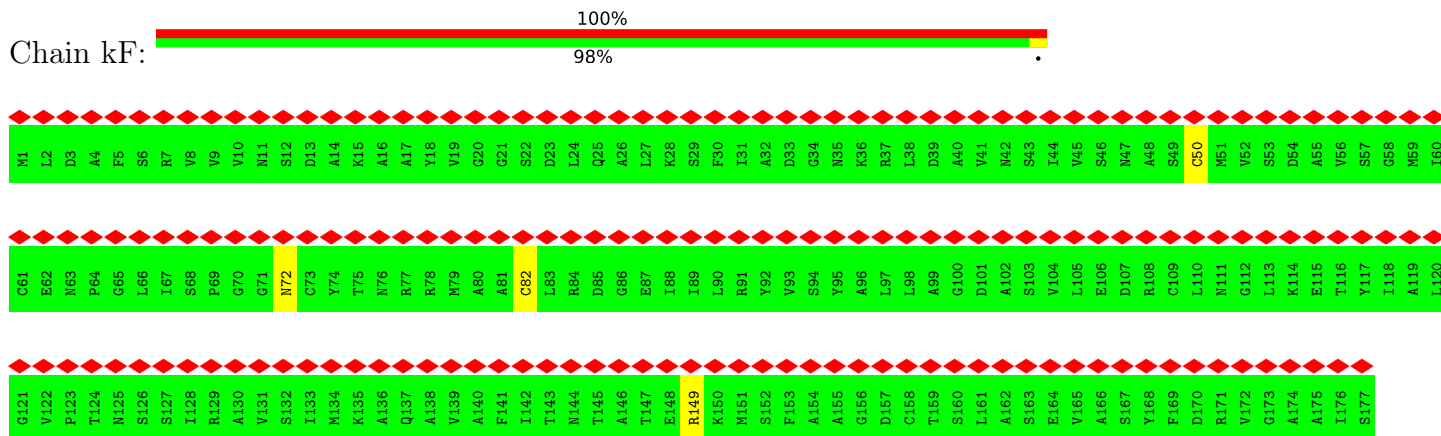
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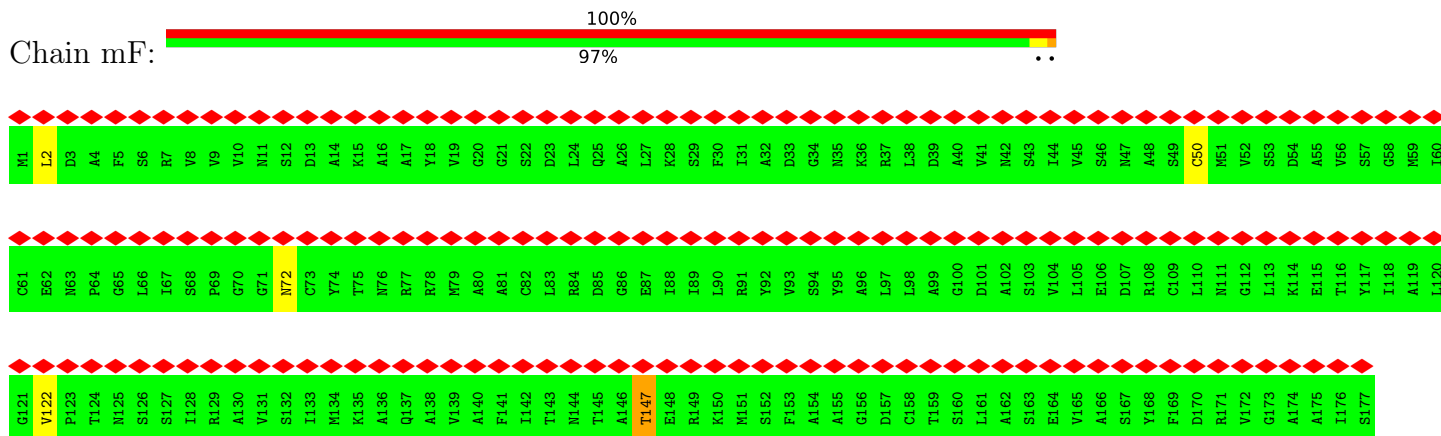
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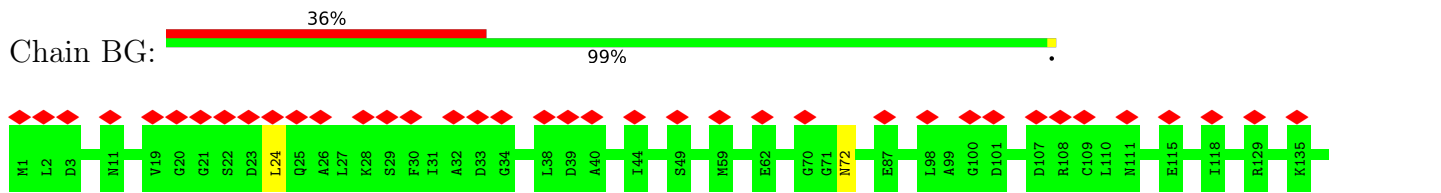
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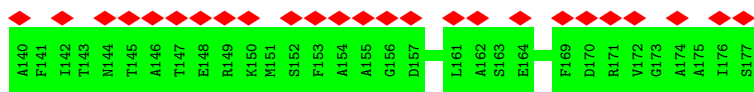


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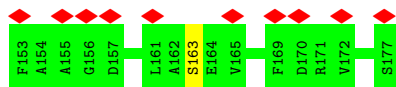
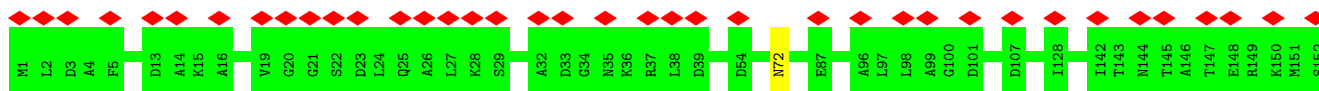


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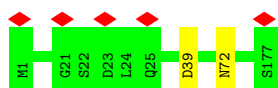




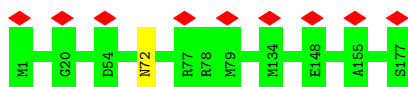
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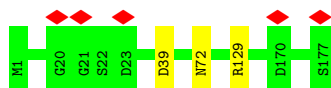
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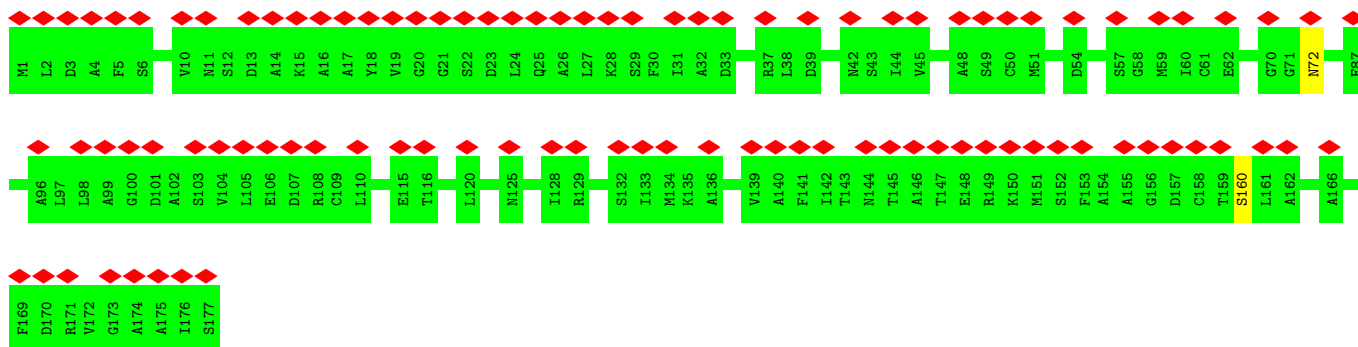


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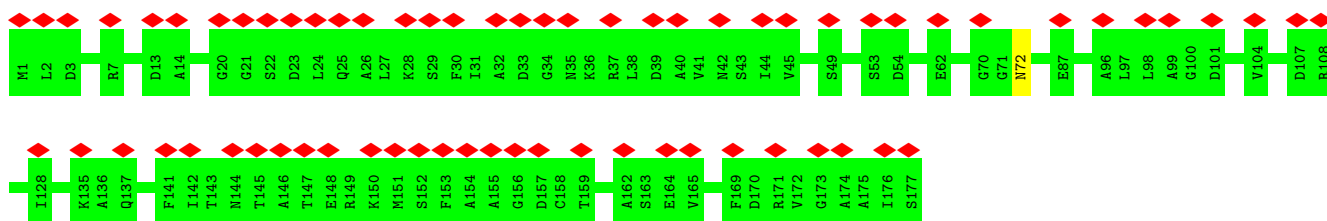
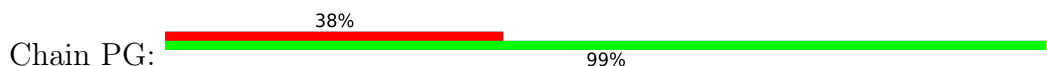


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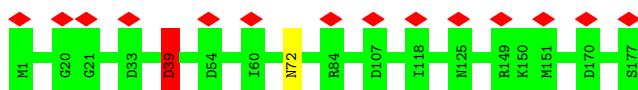
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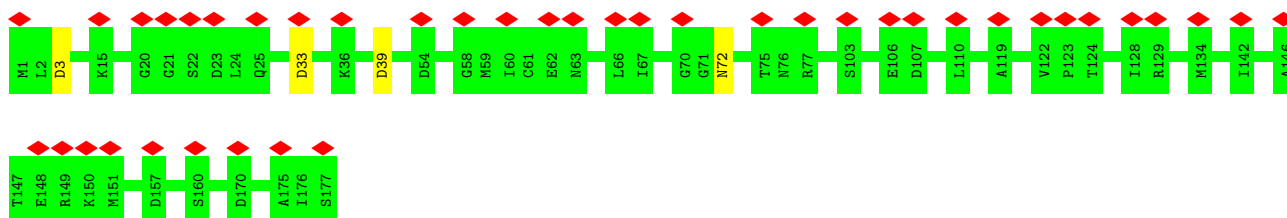
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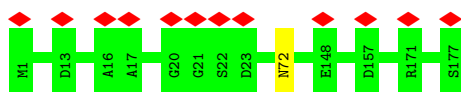
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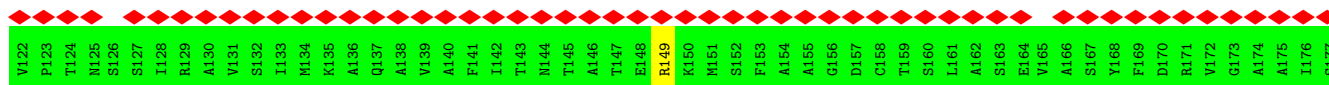
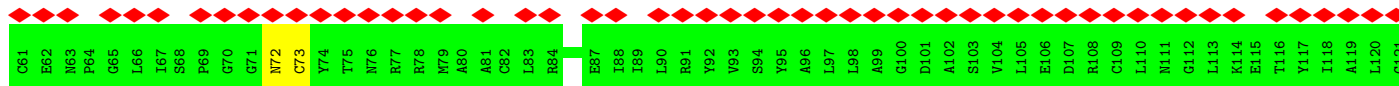
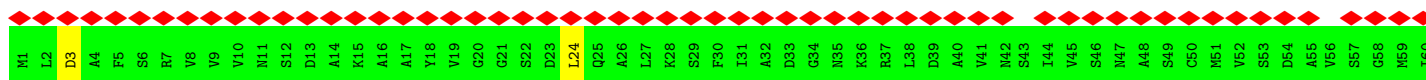
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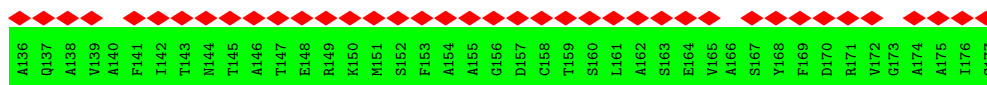
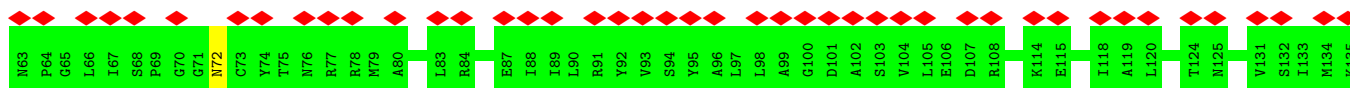
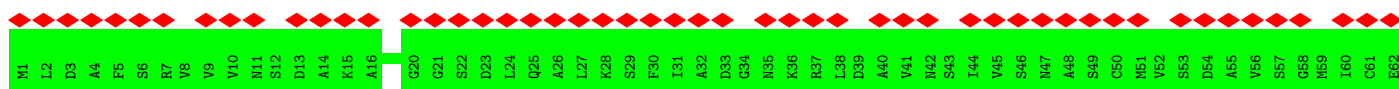
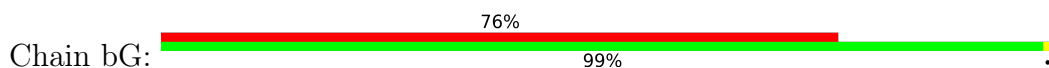
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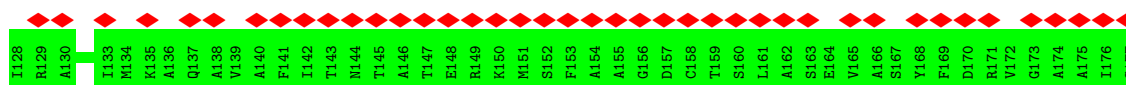
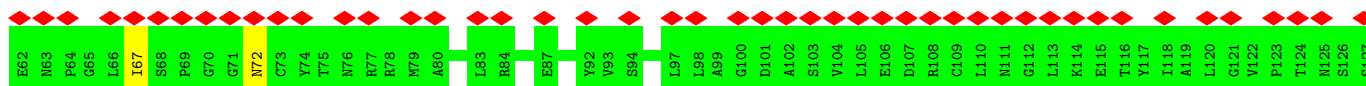
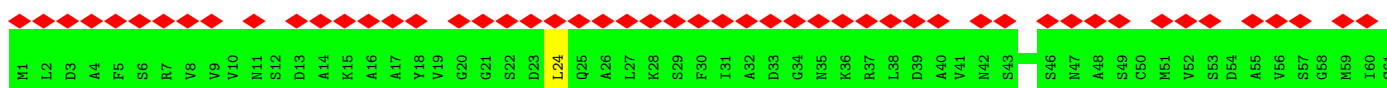
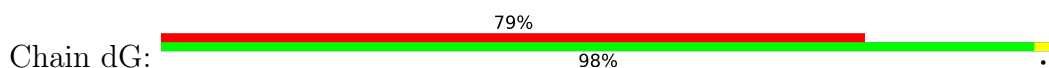
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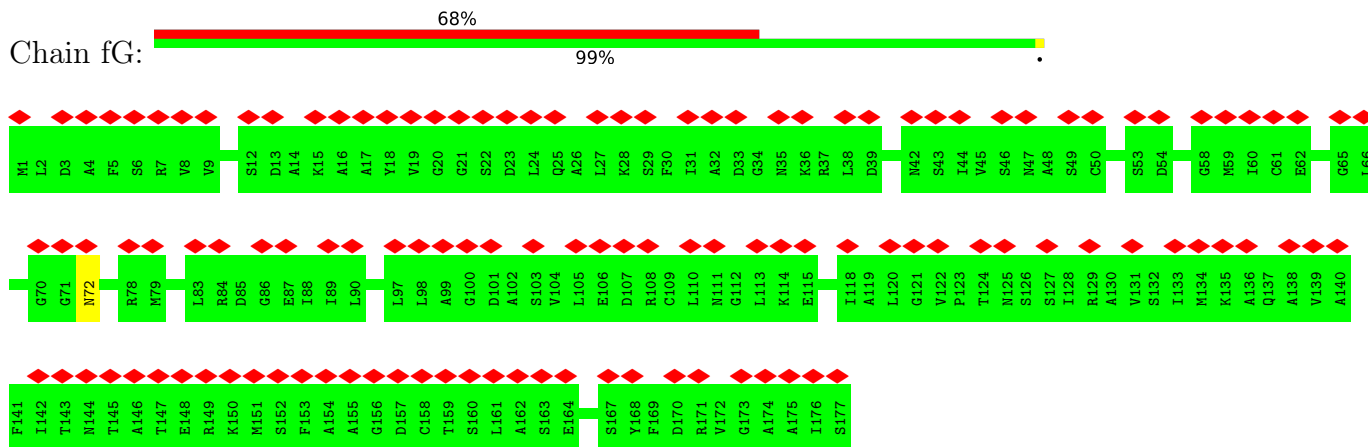
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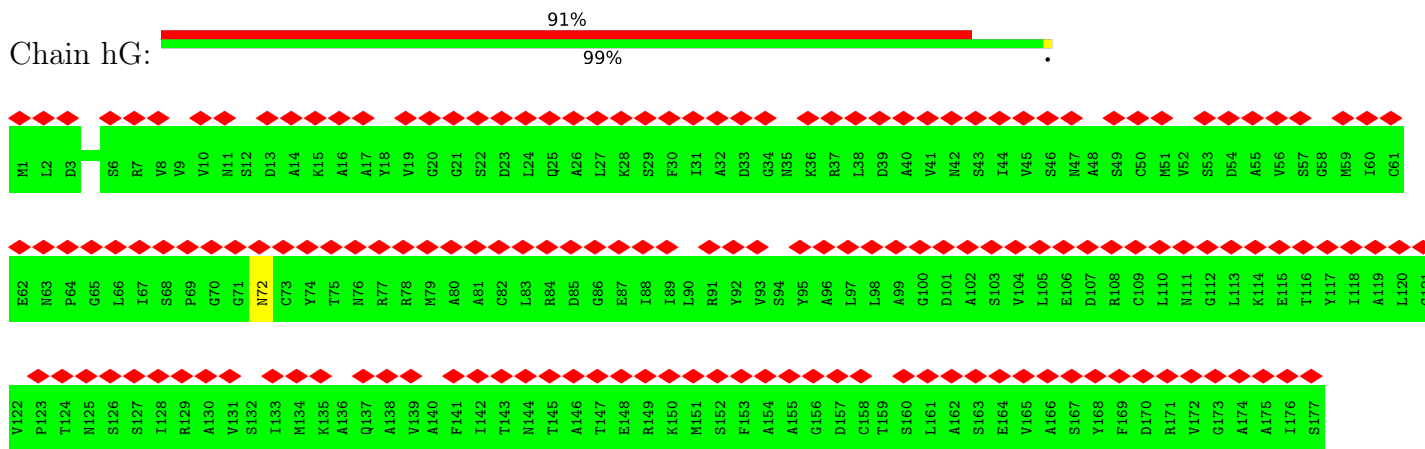
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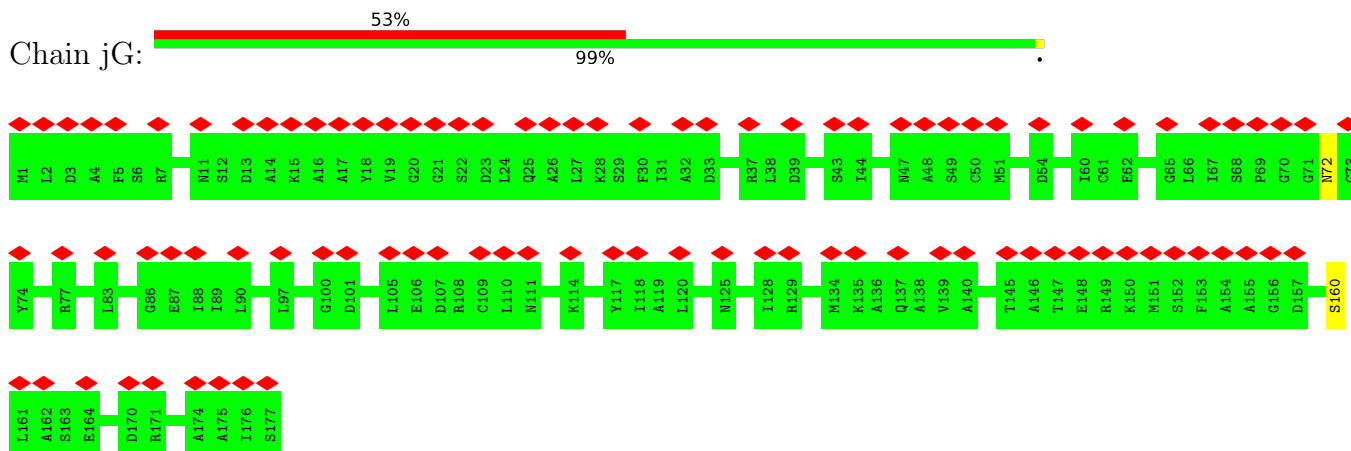
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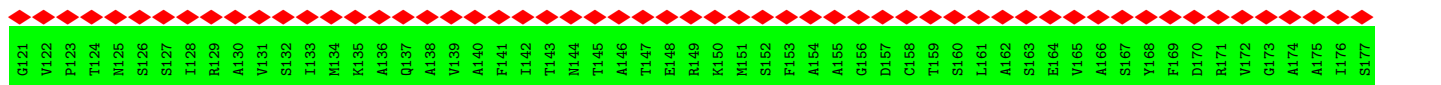
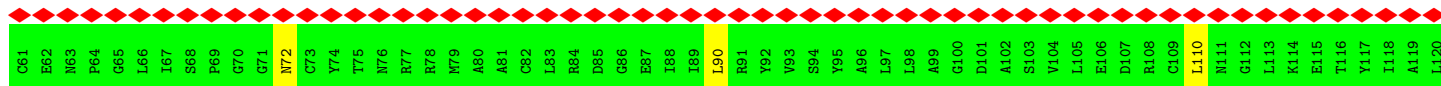
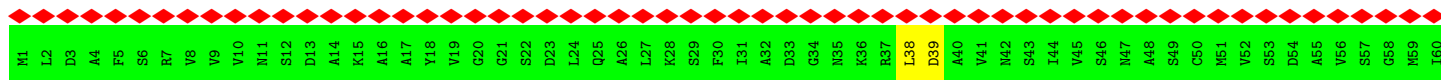


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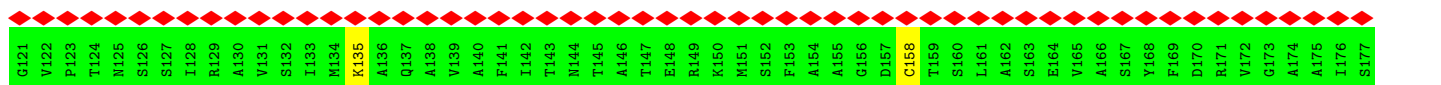
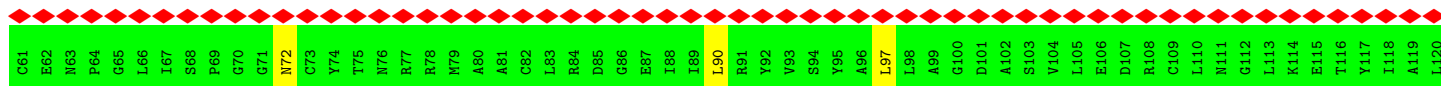
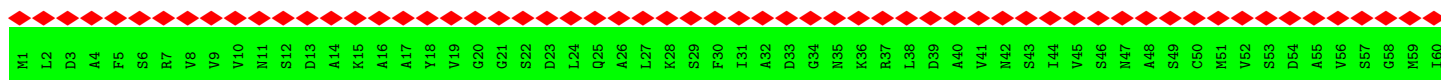


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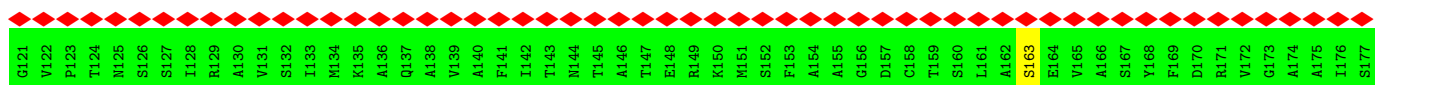
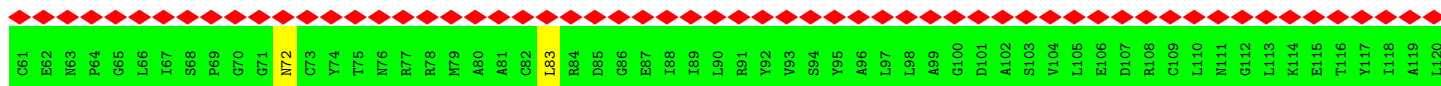
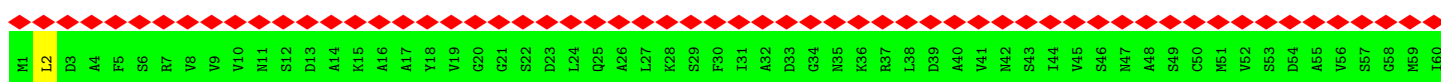




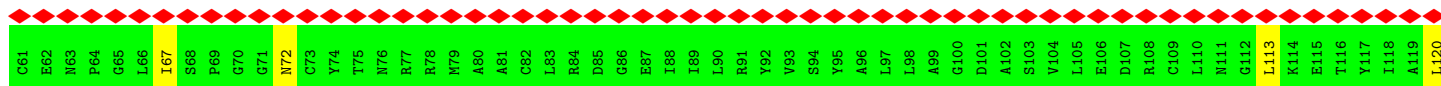
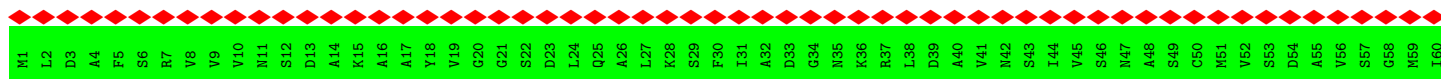
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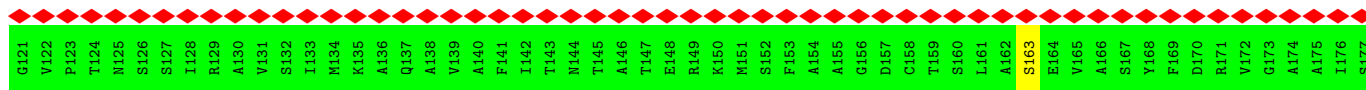


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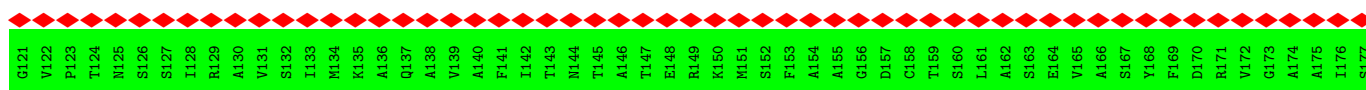
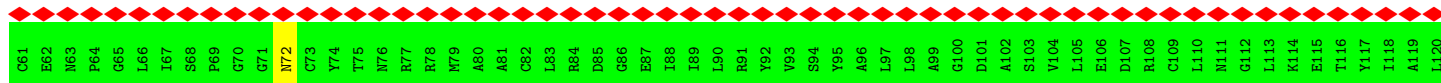
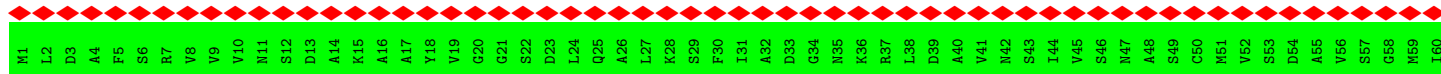


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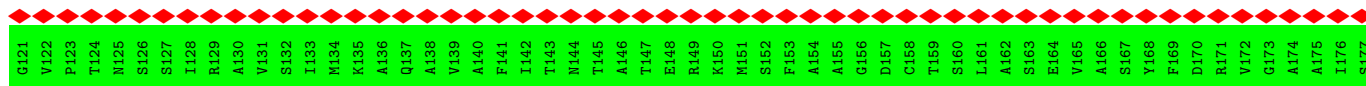
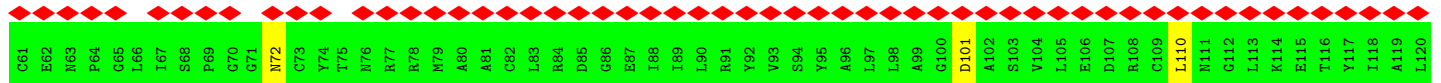
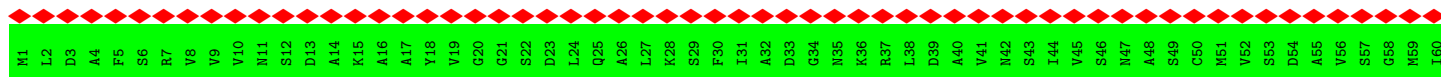




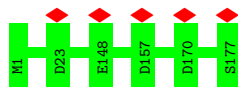
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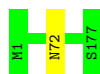
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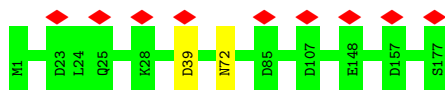
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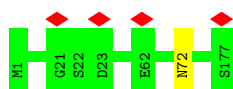
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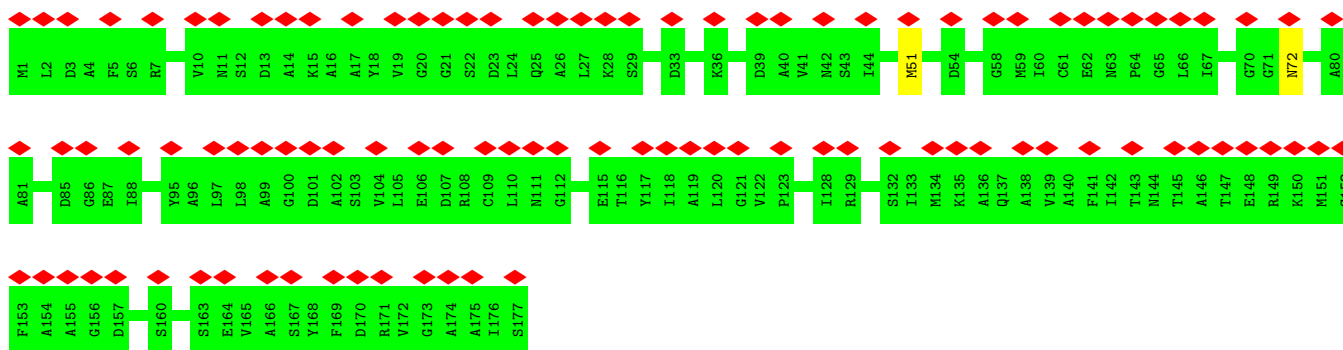
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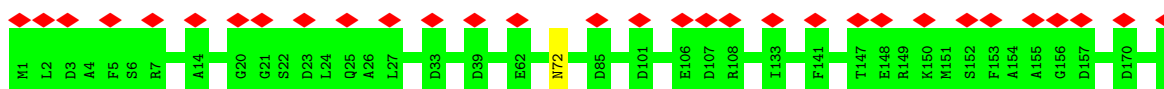
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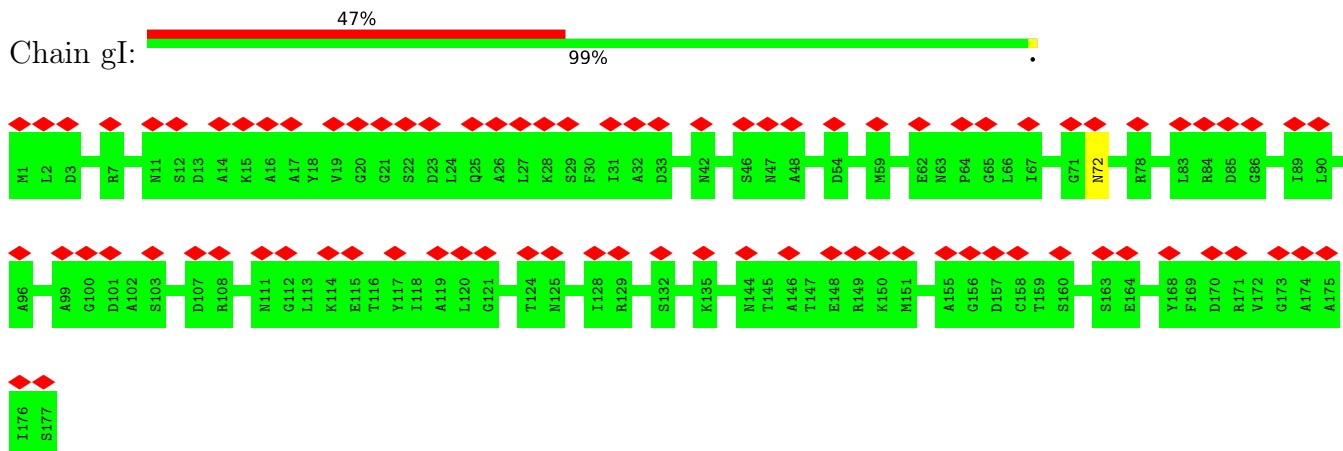
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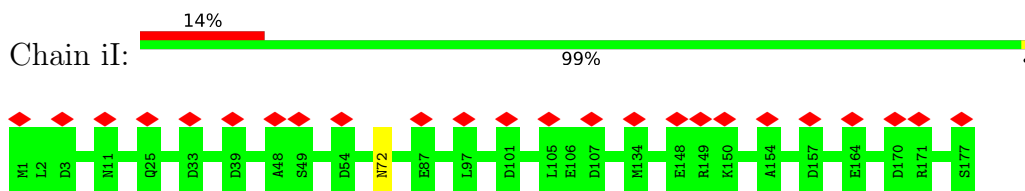
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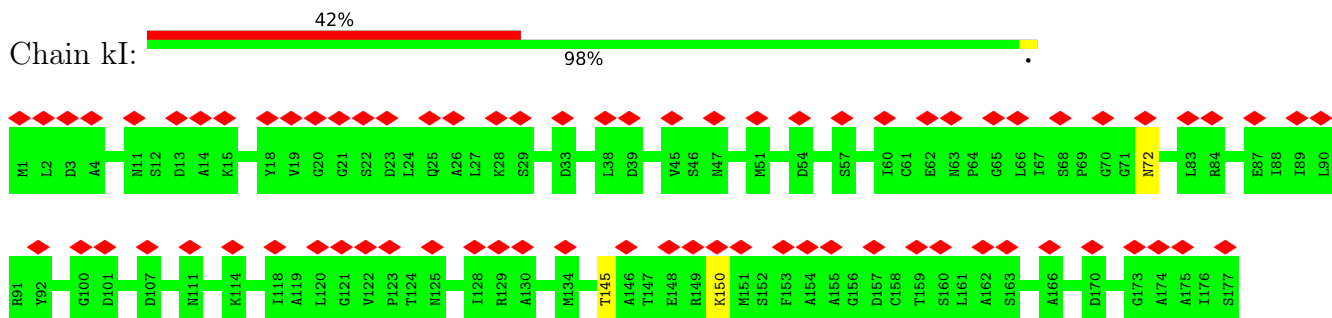
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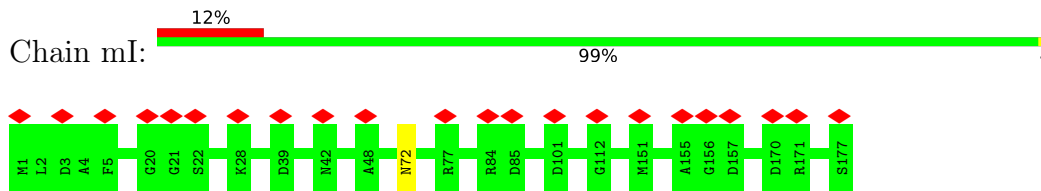
• Molecule 2: B-phycoerythrin beta chain



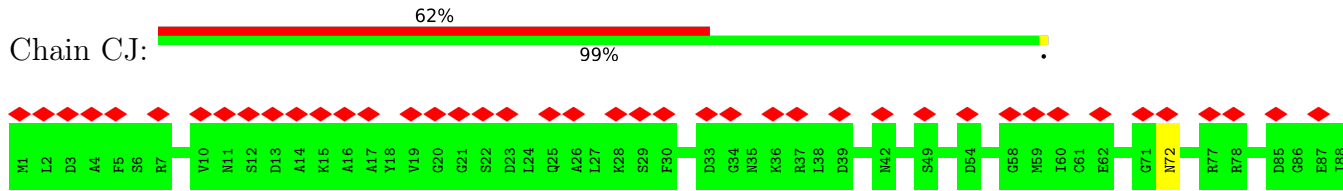
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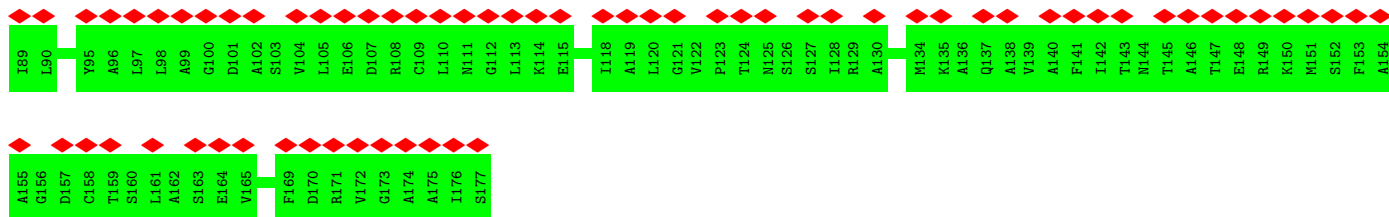


• Molecule 2: B-phycoerythrin beta chain

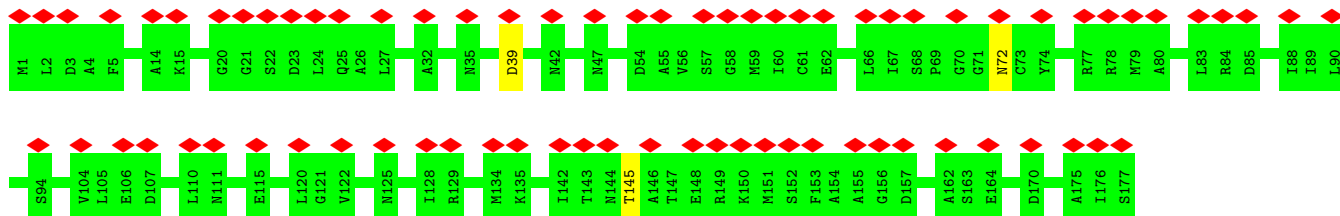
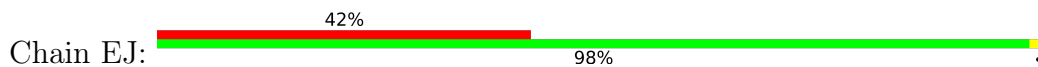


• Molecule 2: B-phycoerythrin beta chain

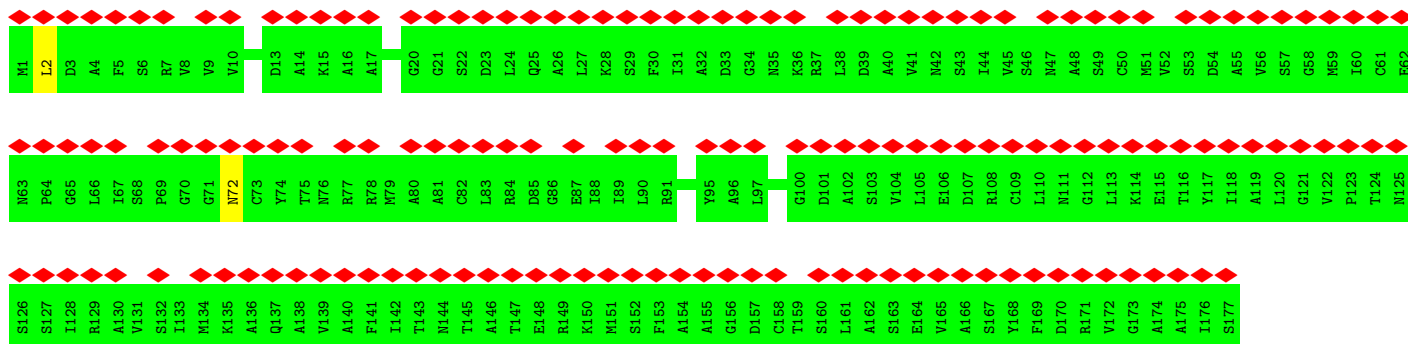
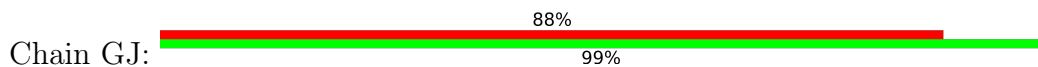




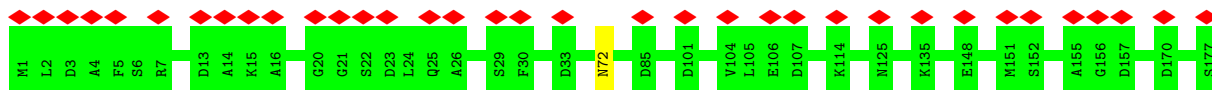
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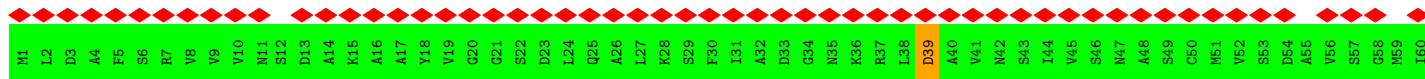
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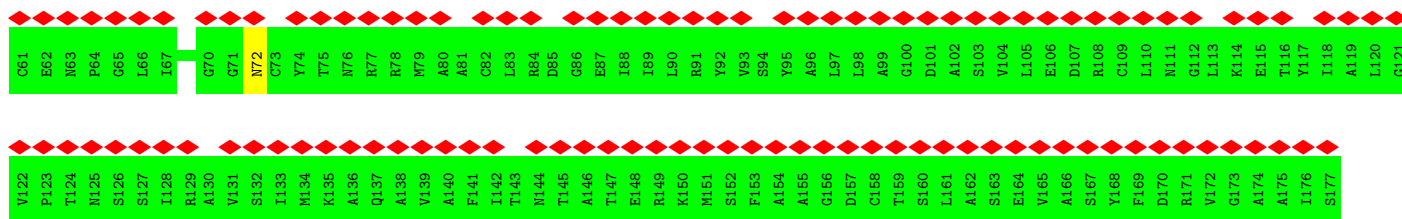


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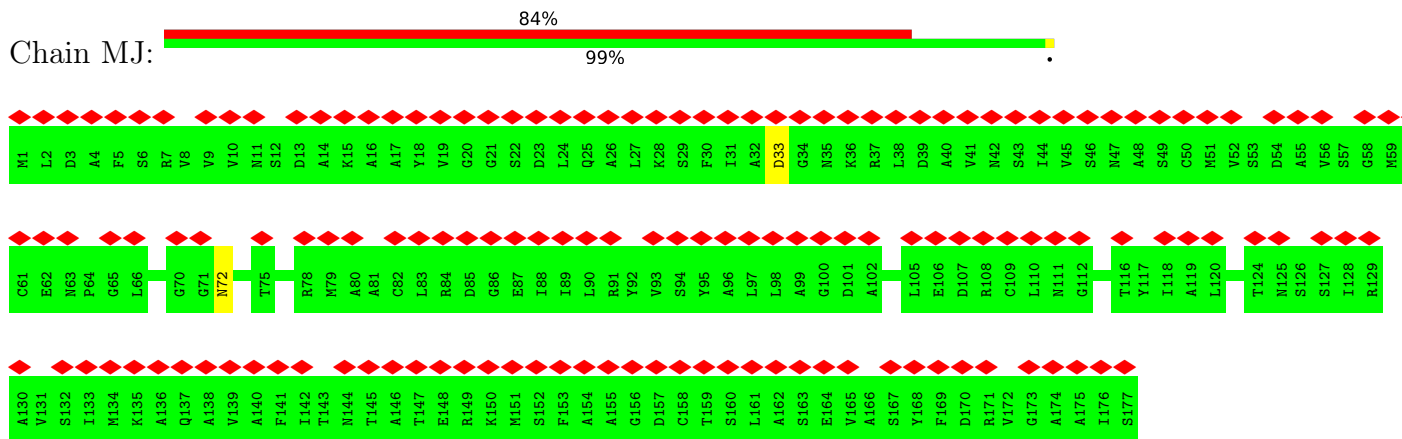


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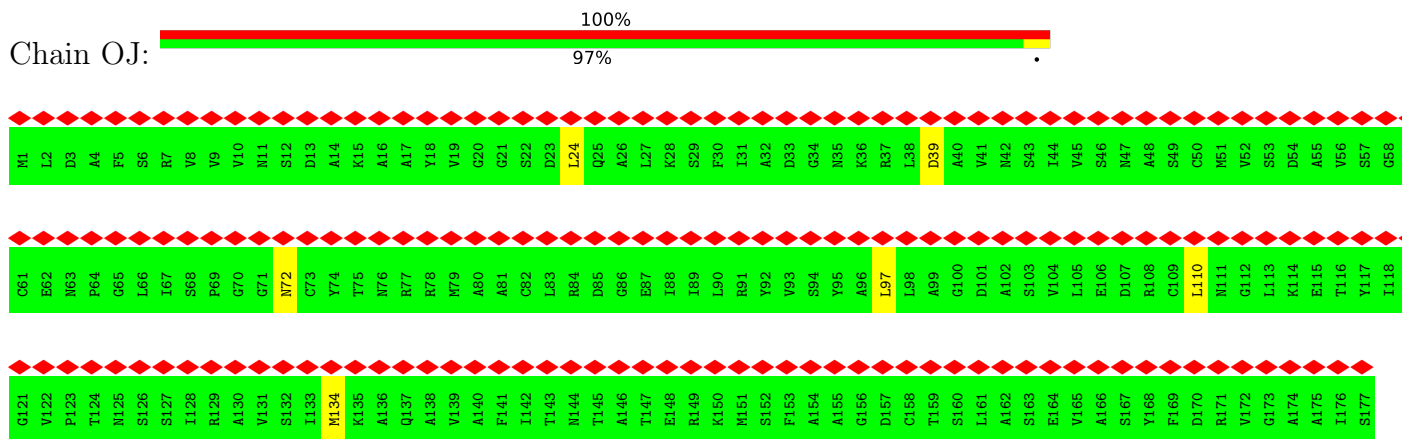




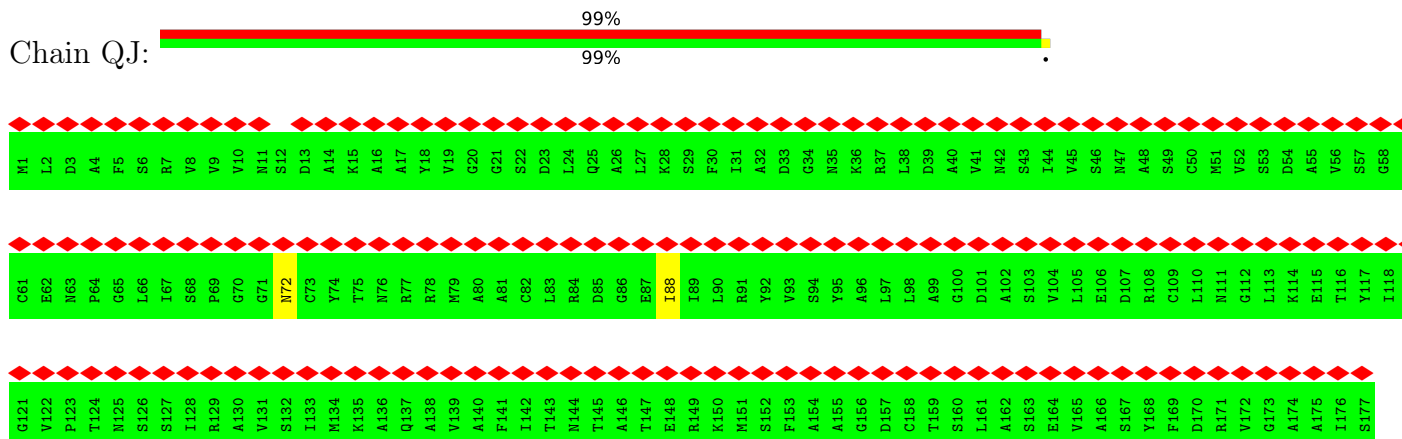
• Molecule 2: B-phycoerythrin beta chain



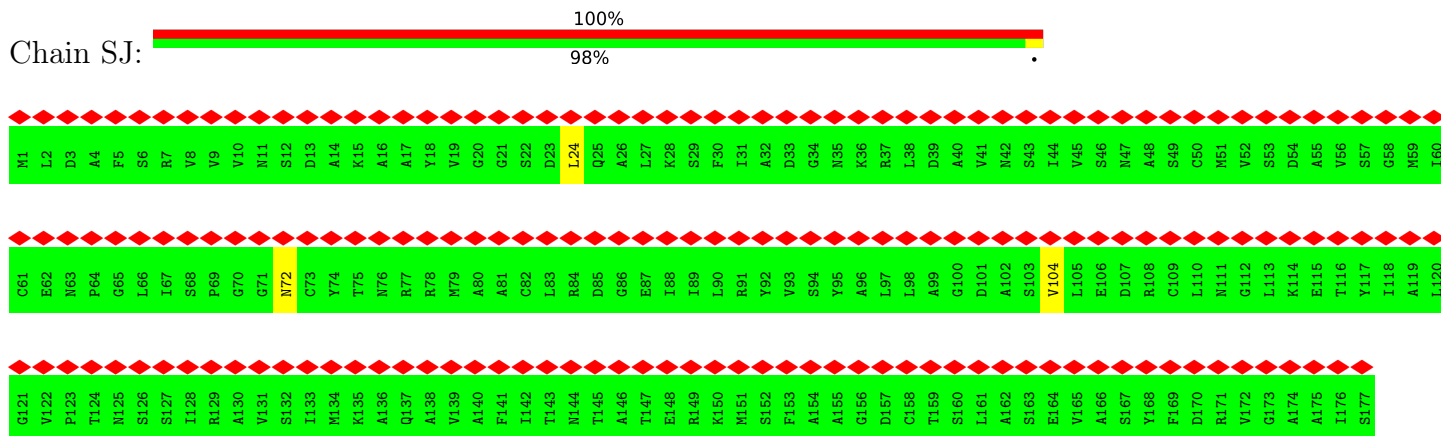
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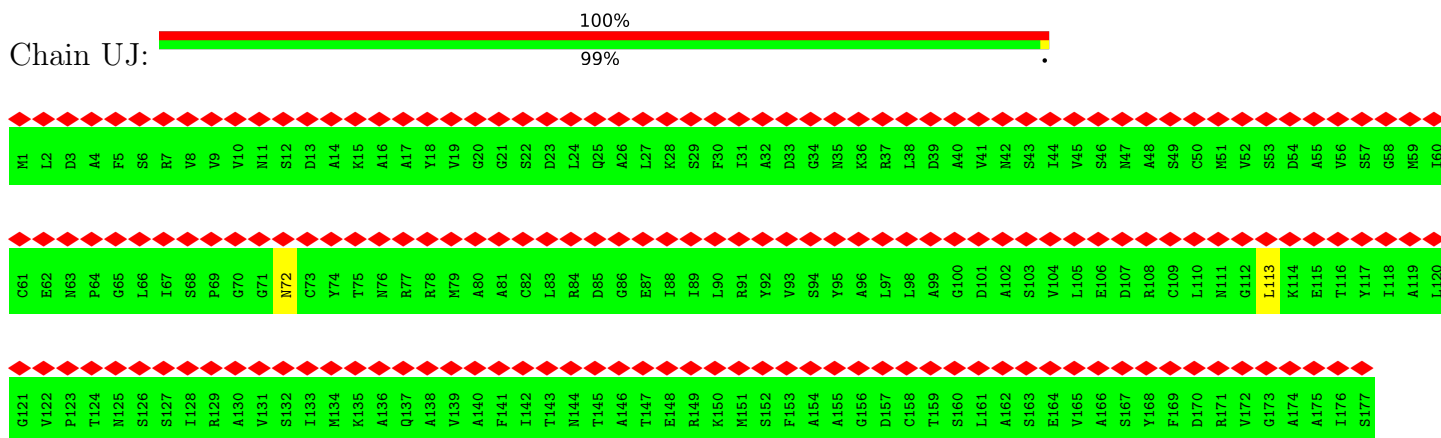
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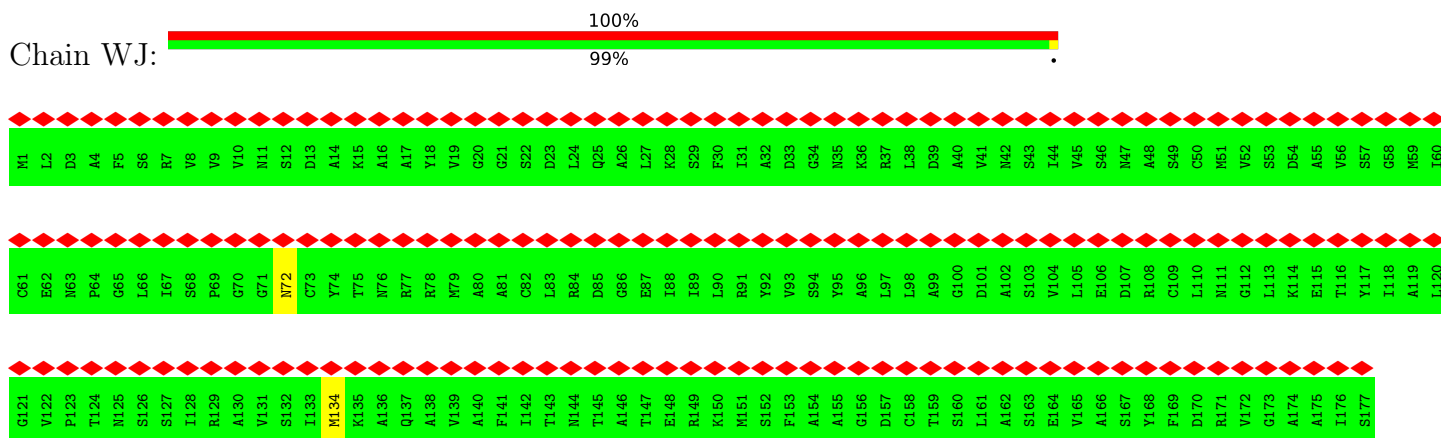
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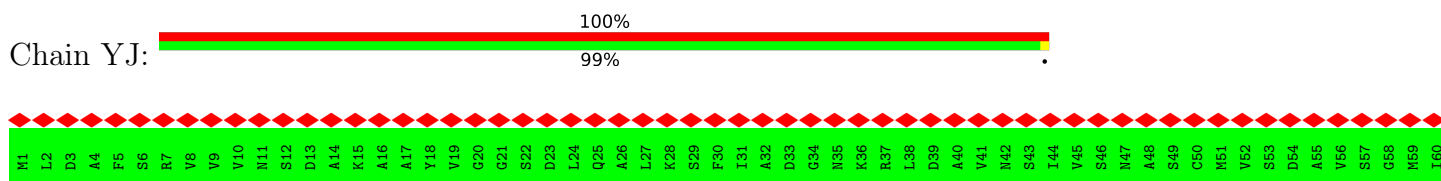
• Molecule 2: B-phycoerythrin beta chain

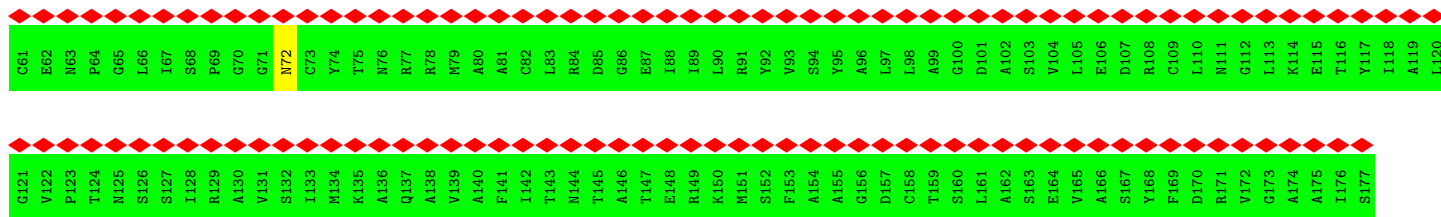


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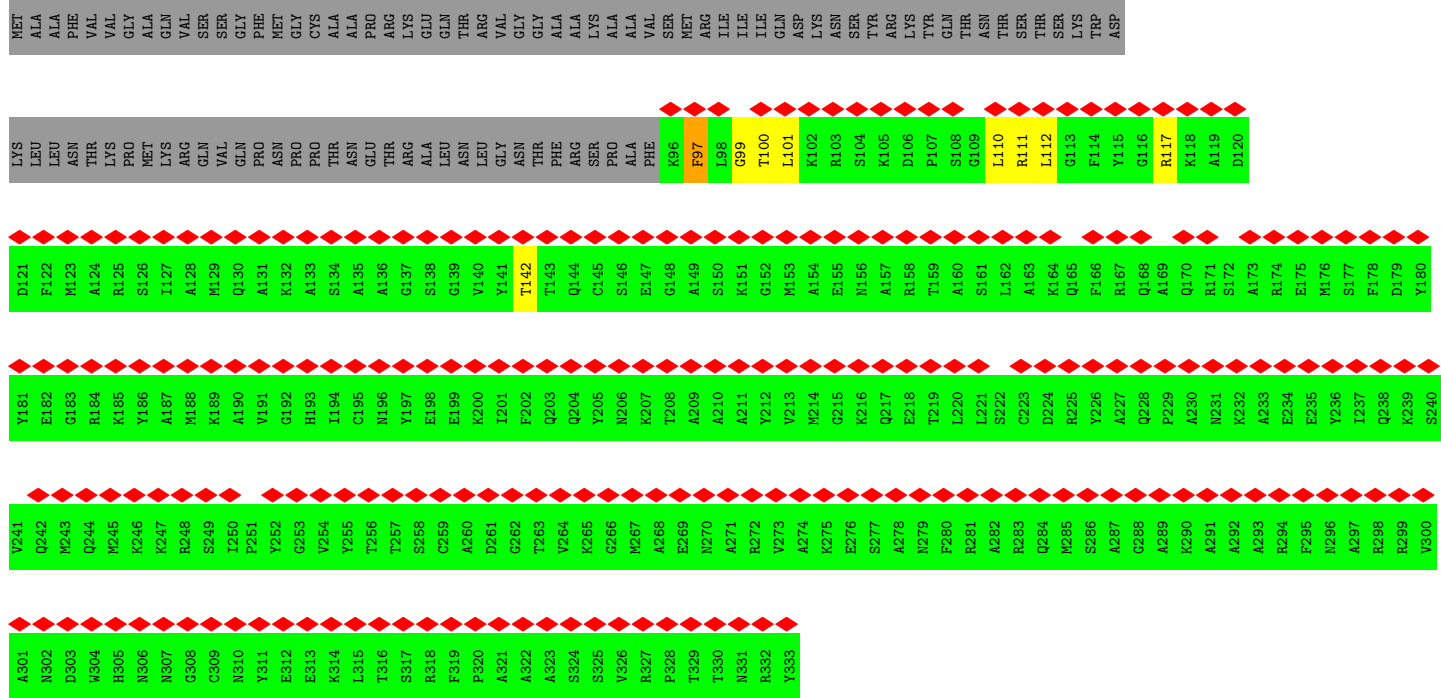


• Molecule 2: B-phycoerythrin beta chain

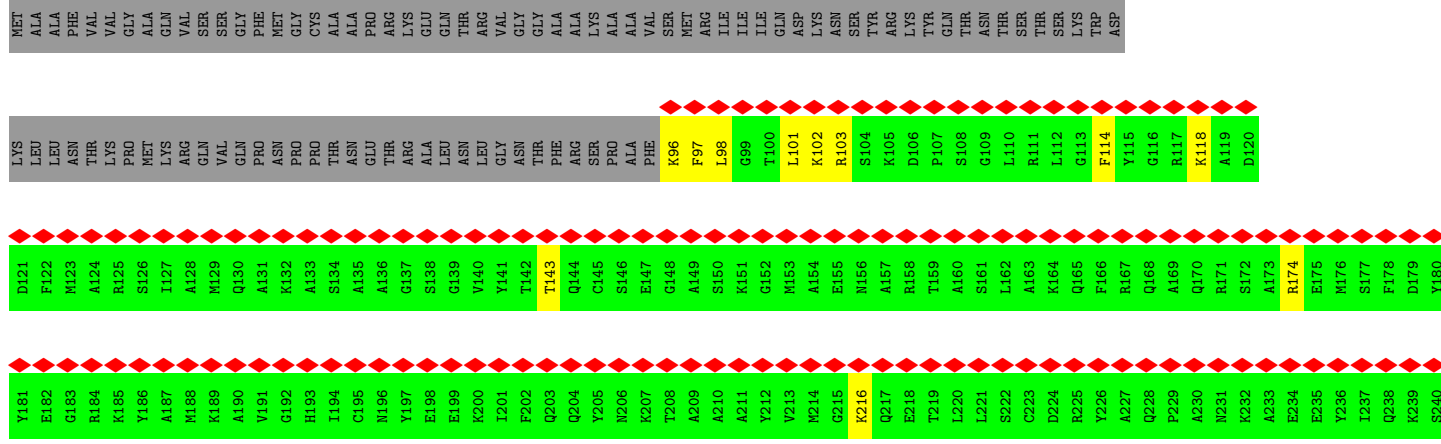


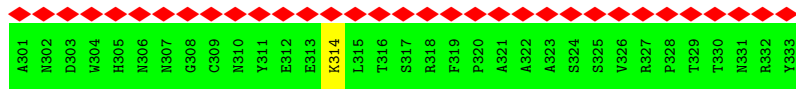
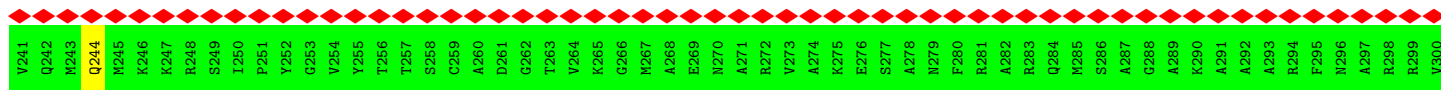


• Molecule 3: LR7



• Molecule 3: LR7

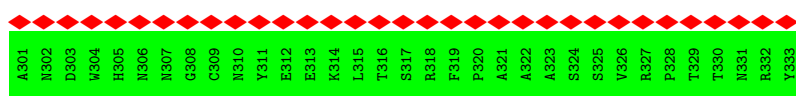
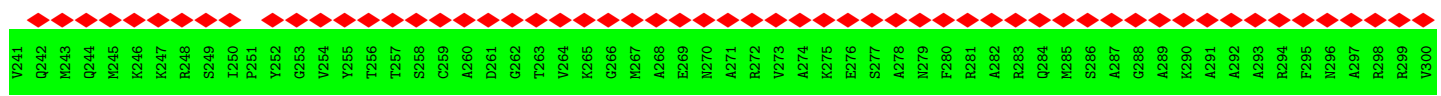
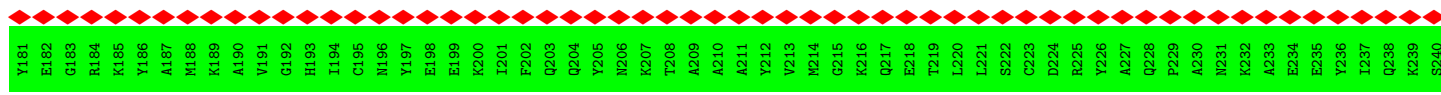
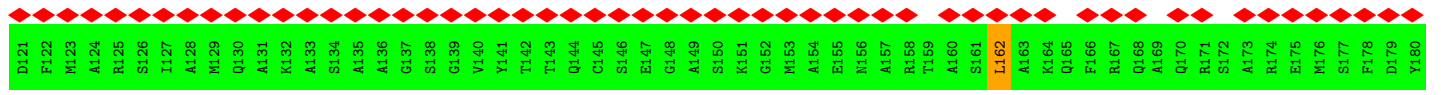
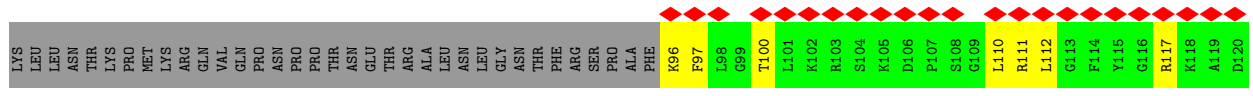




• Molecule 3: LR7



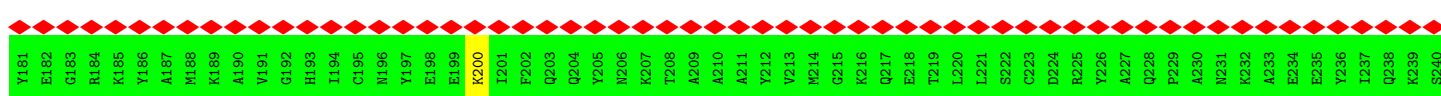
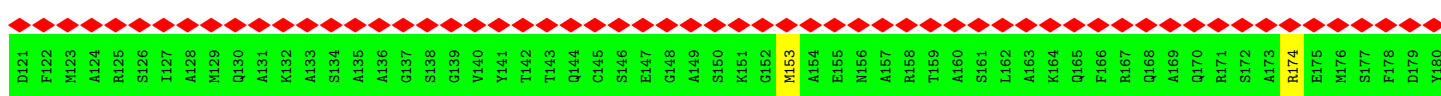
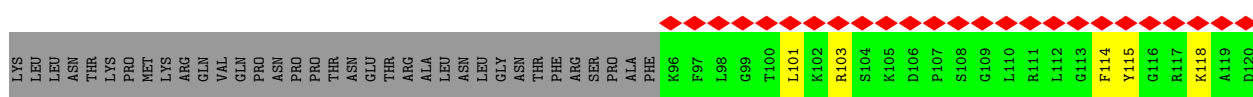
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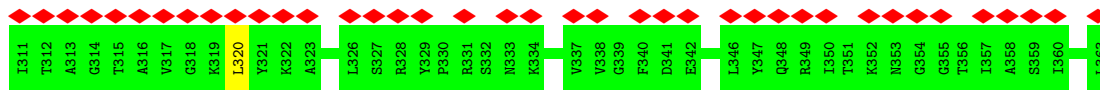


• Molecule 3: LR7

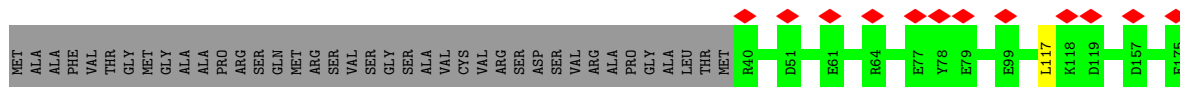
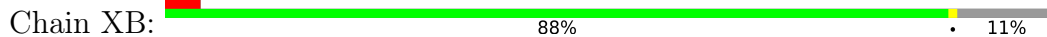


MET	ALA	VAL	VAL	GLY	ALA	GLN	VAL	SER	GLY	PHE	MET	GLY	CYS	ALA	ALA	PRO	ARG	THR	GLN	GLY	ALA	ALA	LYS	ASP
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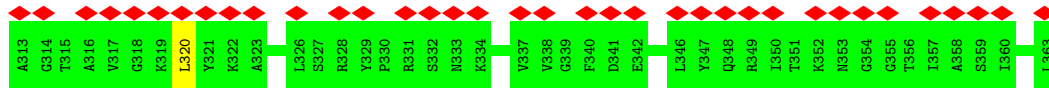
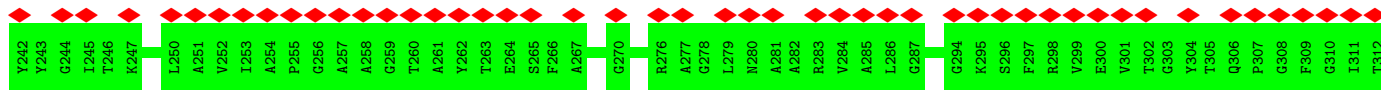
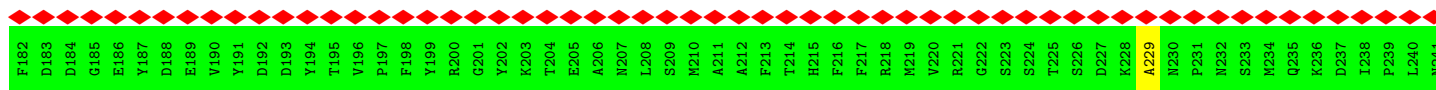
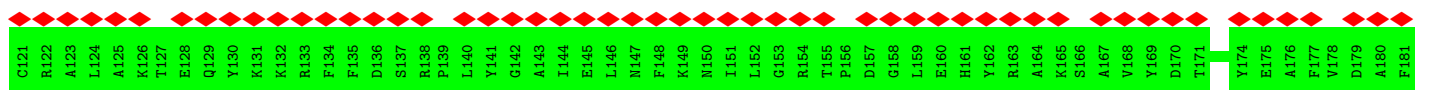
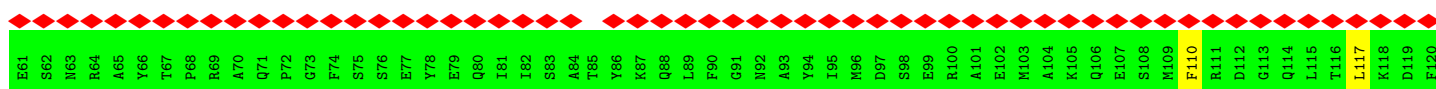
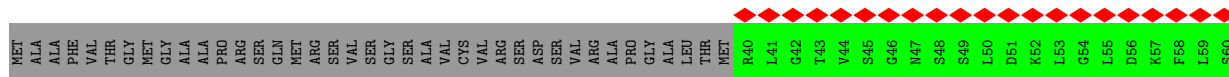
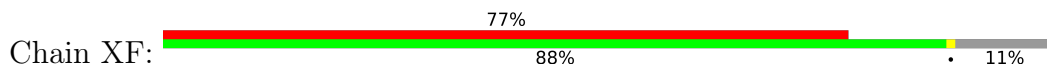




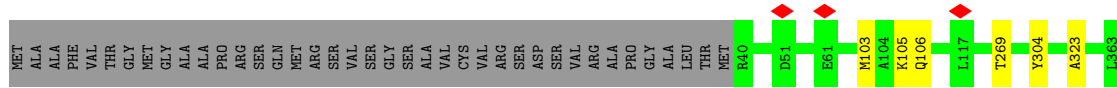
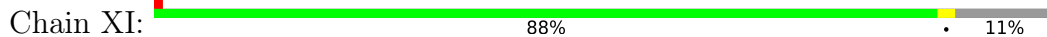
• Molecule 6: LR1



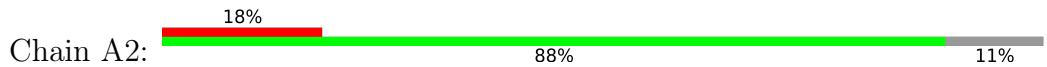
• Molecule 6: LR1

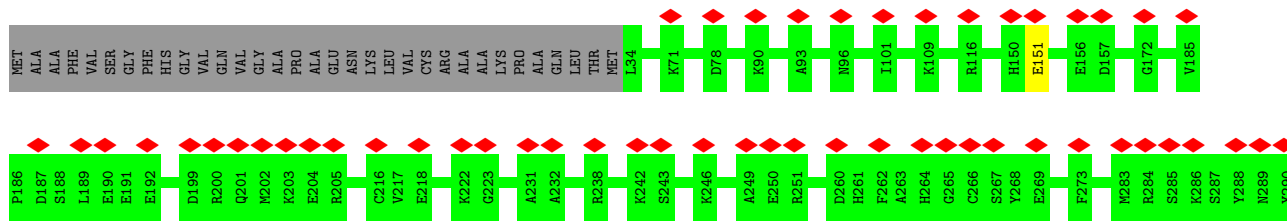


• Molecule 6: LR1

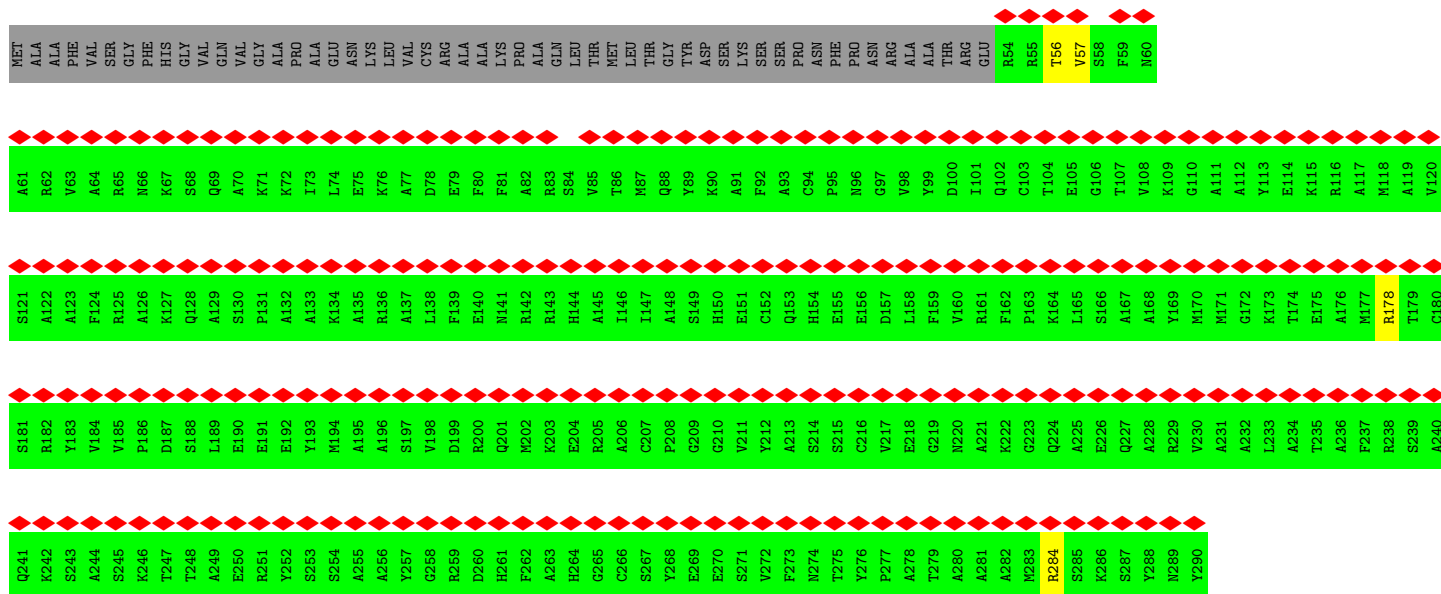
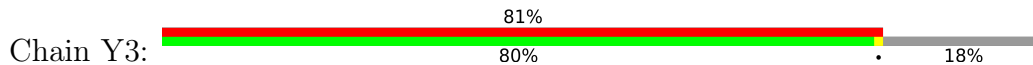


• Molecule 7: LR4

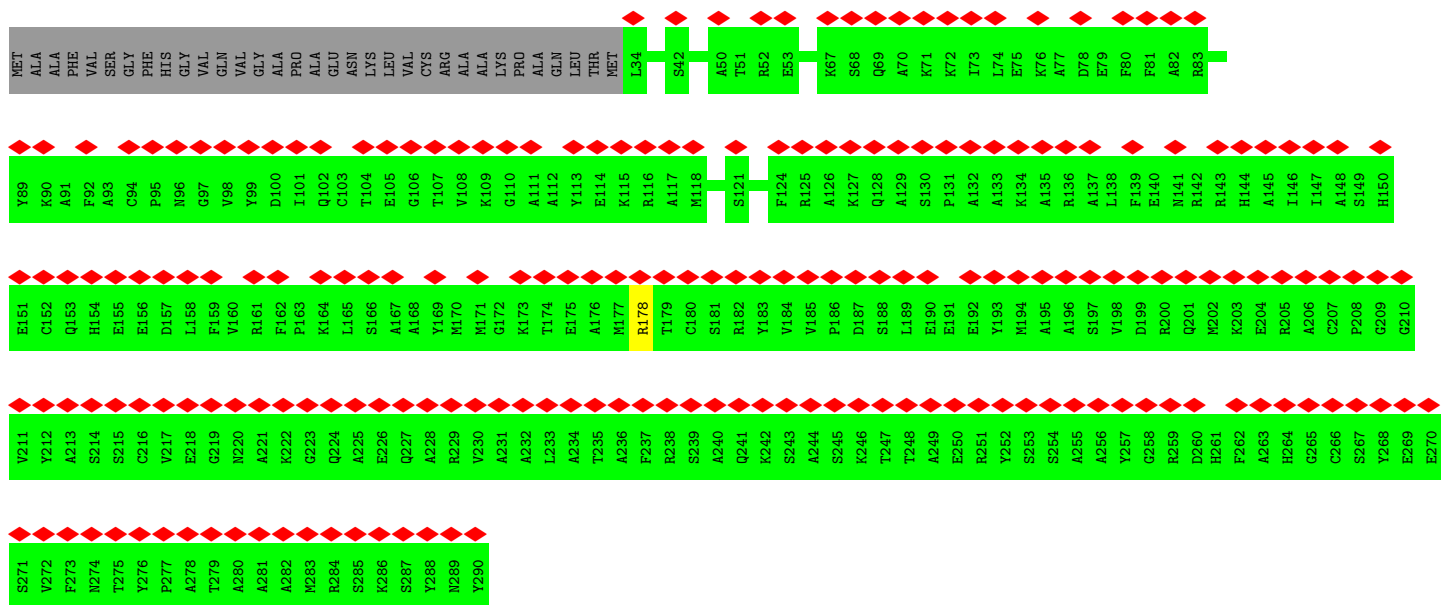
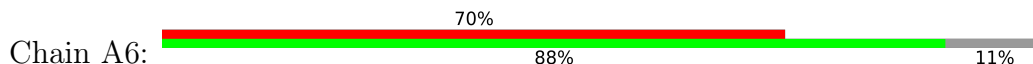




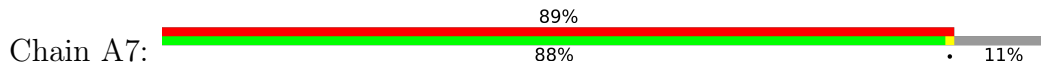
• Molecule 7: LR4



• Molecule 7: LR4

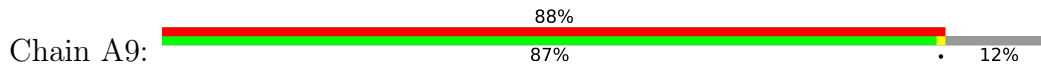


• Molecule 7: LR4



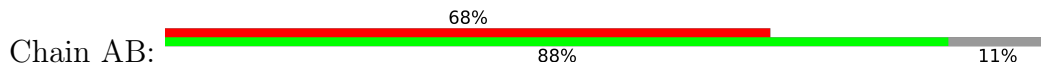
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A61	R62	W63	A64	R65	N66	K67	S68	Q69	A70	K71	K72	I73	L74	E75	K76	A77	D78	E79	F80	F81	A82	R83	S84	W85	T86	M87	Q88	R89	K90	A91	F92	A93	C94	P95	N96	G97	D98	V99	D100	I101	Q102	C103	T104	E105	G106	T107	V108	K109	G110	A111	A112	Y113	E114	K115	R116	A117	M118	A119	V120
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Q241	K242	S243	A244	S245	K246	T247	T248	A249	E250	R251	Y252	S253	S254	A255	A256	Y257	G258	R259	D260	H261	F262	A263	H264	G265	S266	S267	Y268	E269	E270	S271	V272	F273	N274	T275	Y276	P277	A278	T279	A280	A281	A282	M283	R284	S285	K286	S287	Y288	N289	Y290										

• Molecule 7: LR4

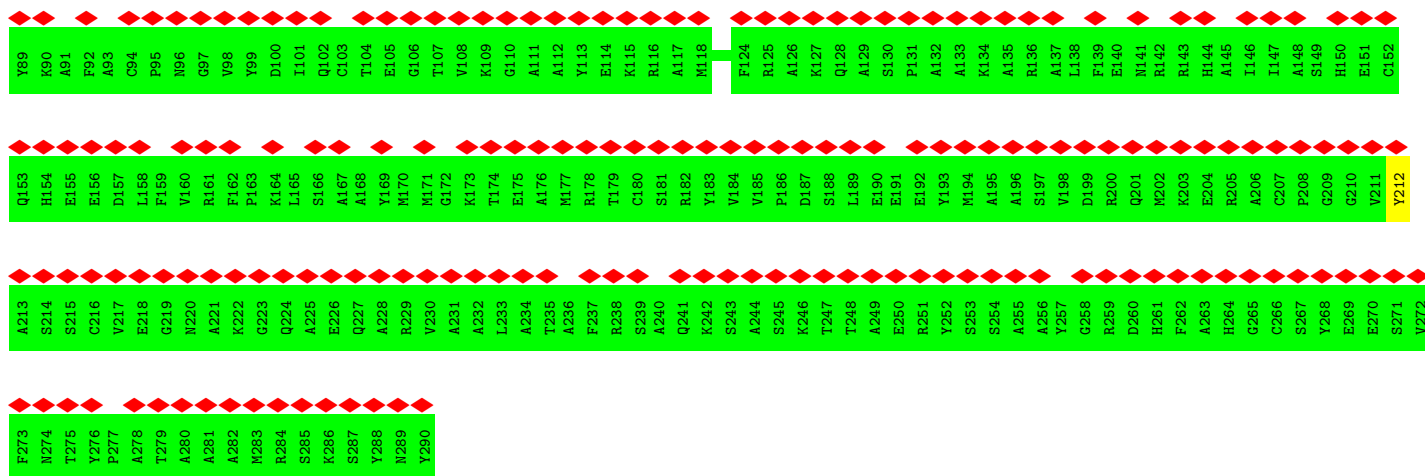


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A61	R62	W63	A64	R65	N66	K67	S68	Q69	A70	K71	K72	I73	L74	E75	K76	A77	D78	E79	F80	F81	A82	R83	S84	W85	T86	M87	Q88	R89	K90	A91	F92	A93	C94	P95	N96	G97	D98	V99	D100	I101	Q102	C103	T104	E105	G106	T107	V108	K109	G110	A111	A112	Y113	E114	K115	R116	A117	M118	A119	V120
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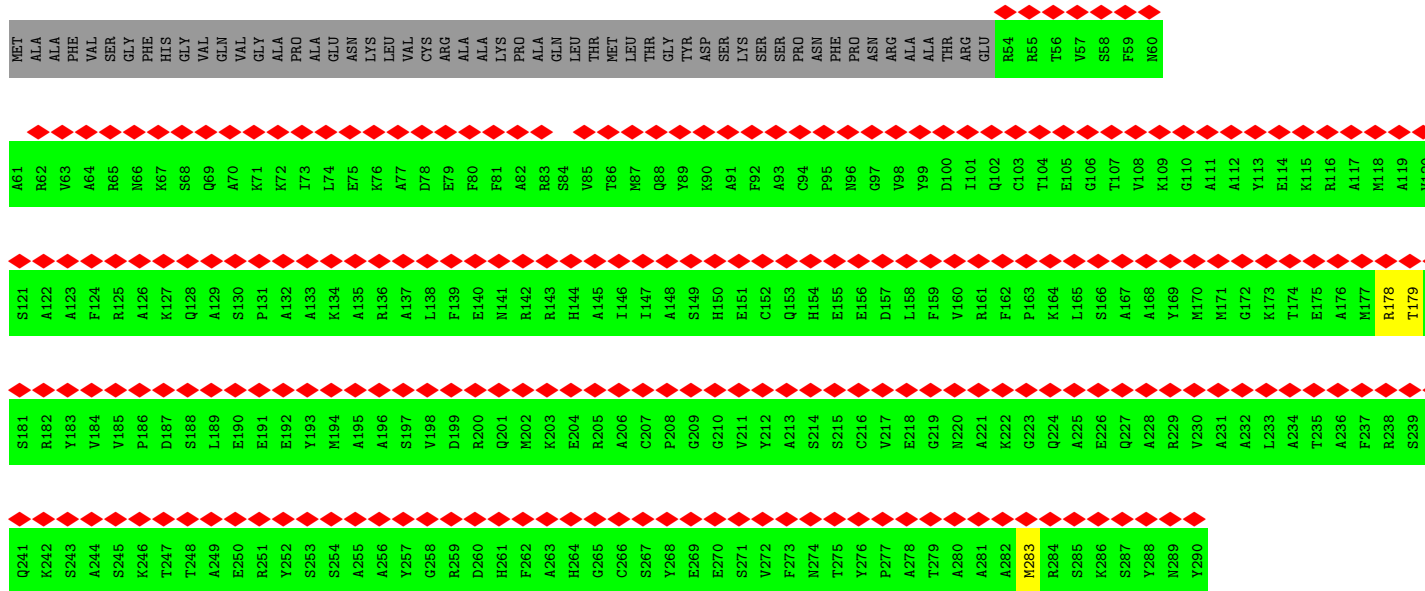
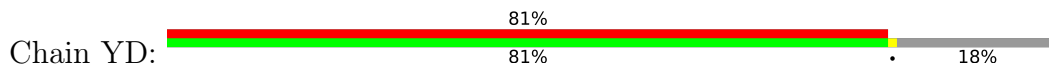
• Molecule 7: LR4



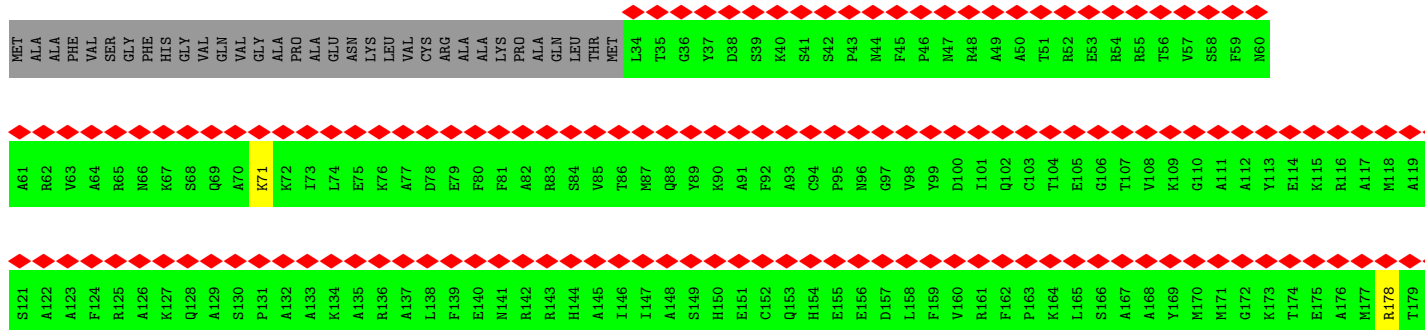
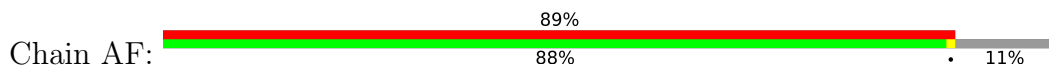
MET	ALA	ALA	PHE	VAL	SER	GLY	PHE	HIS	GLY	VAL	GLN	VAL	GLY	ALA	PRO	GLU	ASN	LYS	VAL	CYS	ARG	ALA	ALA	LYS	PRO	ALA	GLN	LEU	THR	MET	L34	D38	S42	R52	E53	K67	S68	Q69	A70	K71	K72	I73	L74	E75	K76	A77	D78	E79	F80	F81	A82	R83
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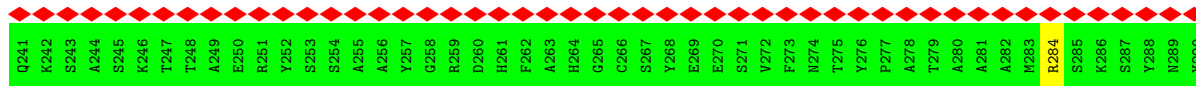
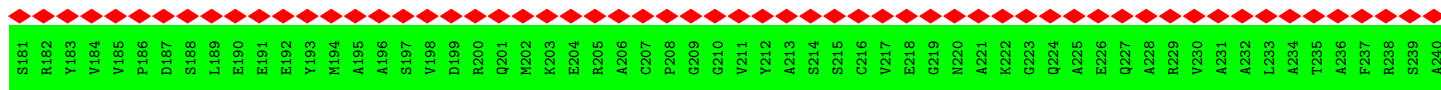


• Molecule 7: LR4

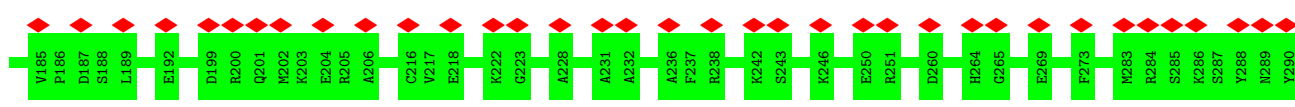
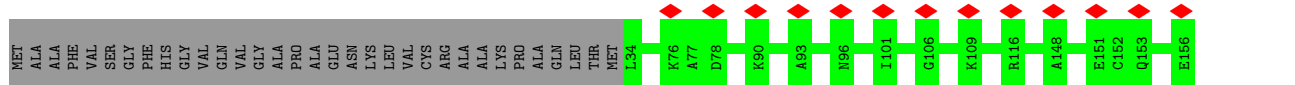
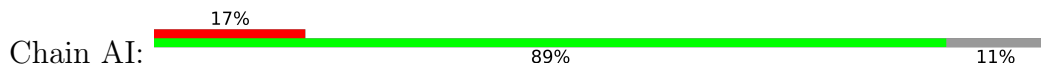


• Molecule 7: LR4

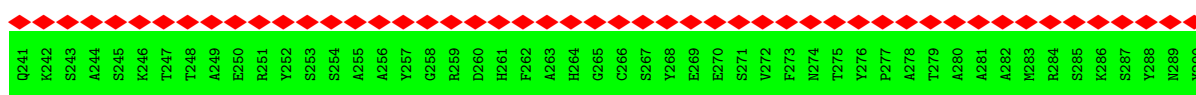
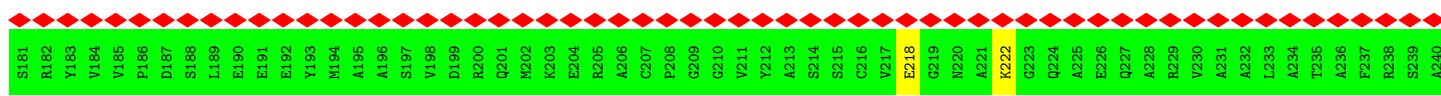
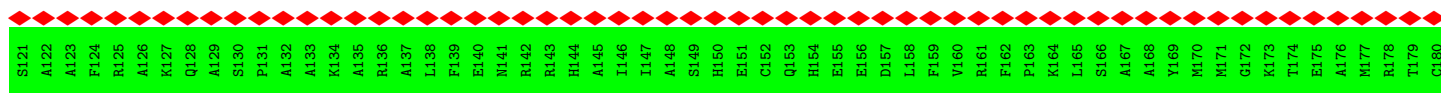
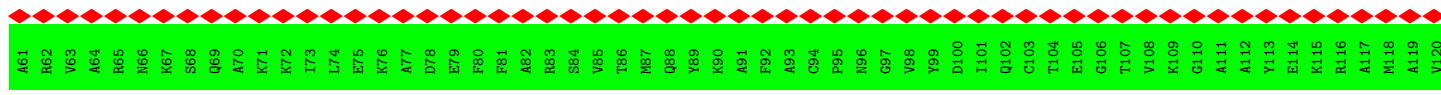
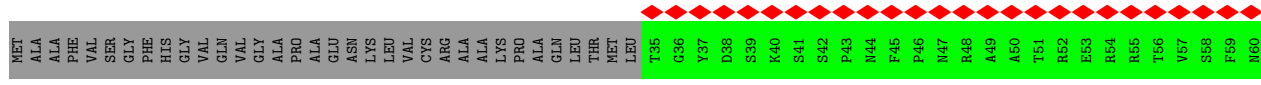
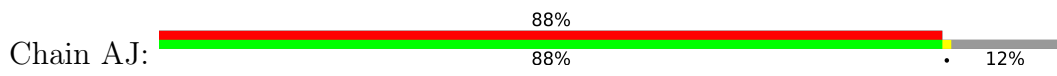




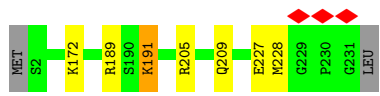
• Molecule 7: LR4



• Molecule 7: LR4

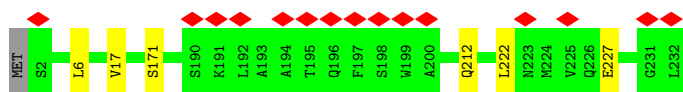


• Molecule 8: Phycobilisome rod-core linker polypeptide



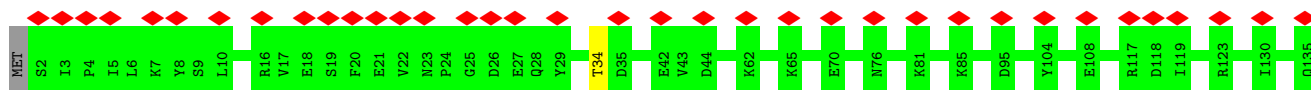
• Molecule 8: Phycobilisome rod-core linker polypeptide

Chain B6:  6% 97%



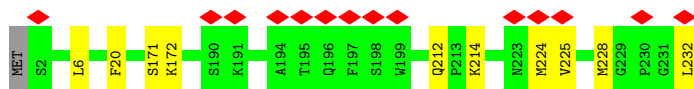
- Molecule 8: Phycobilisome rod-core linker polypeptide

Chain B7:  27% 97%



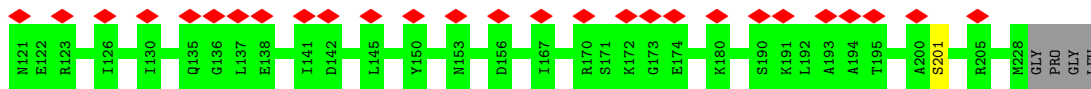
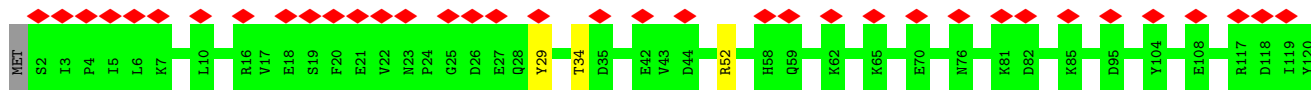
- Molecule 8: Phycobilisome rod-core linker polypeptide

Chain BB:  6% 95%



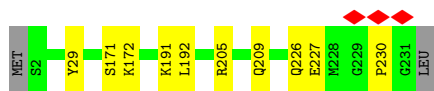
- Molecule 8: Phycobilisome rod-core linker polypeptide

Chain BF:  27% 96%



- Molecule 8: Phycobilisome rod-core linker polypeptide

Chain BI:  95%



- Molecule 9: C-phycoyanin alpha subunit

Chain C2:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoyanin alpha subunit

Chain E2:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain G2:  99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain I2:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain K2:  99%



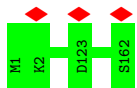
- Molecule 9: C-phyco cyanin alpha subunit

Chain M2:  99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain C6:  100%



- Molecule 9: C-phyco cyanin alpha subunit

Chain E6:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain G6:  100%

There are no outlier residues recorded for this chain.

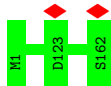
- Molecule 9: C-phyco cyanin alpha subunit

Chain I6:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain K6:  100%

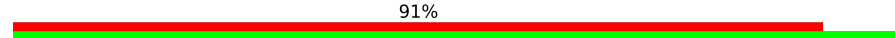


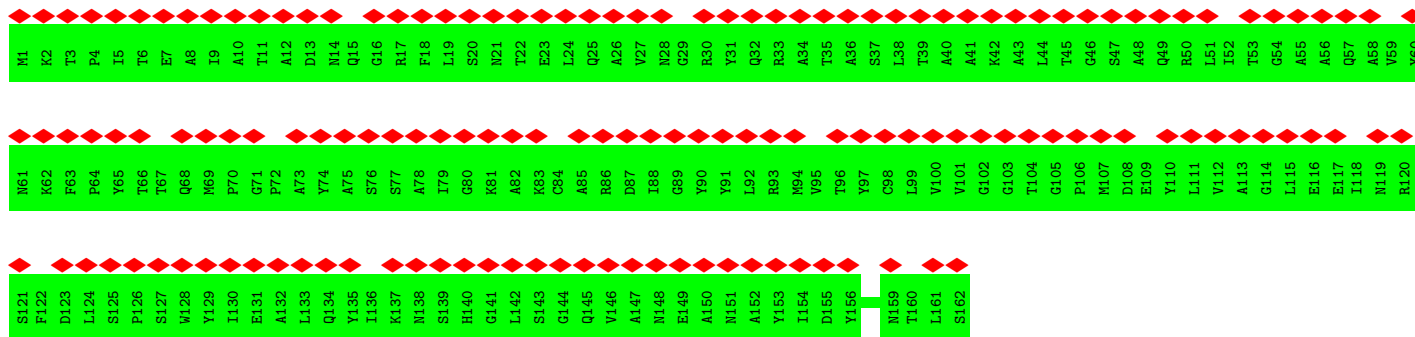
- Molecule 9: C-phycoerythrin alpha subunit

Chain M6:  100%

There are no outlier residues recorded for this chain.

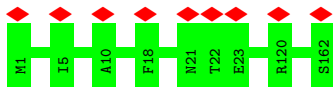
- Molecule 9: C-phycoerythrin alpha subunit

Chain C7:  91%
100%




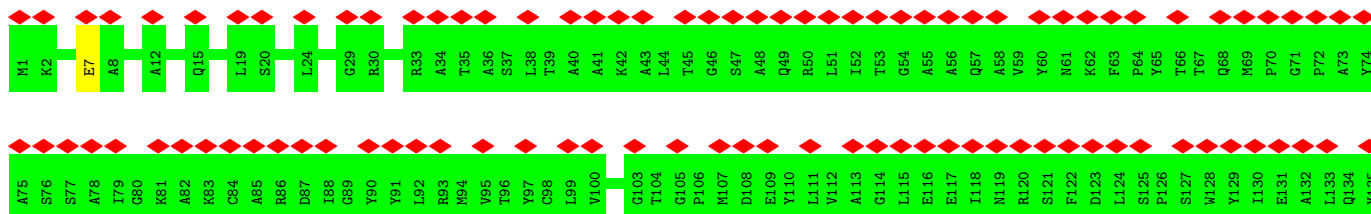
- Molecule 9: C-phycoerythrin alpha subunit

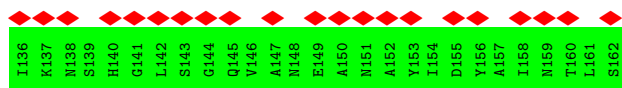
Chain E7:  6%
100%



- Molecule 9: C-phycoerythrin alpha subunit

Chain G7:  72%
99%

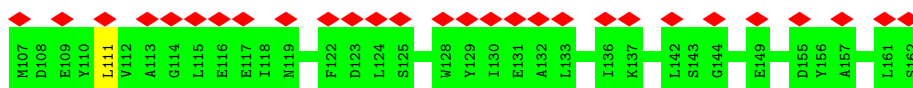
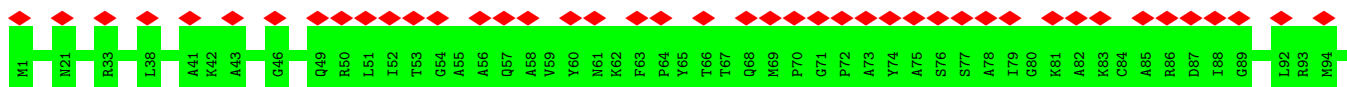




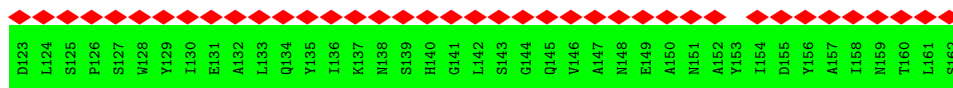
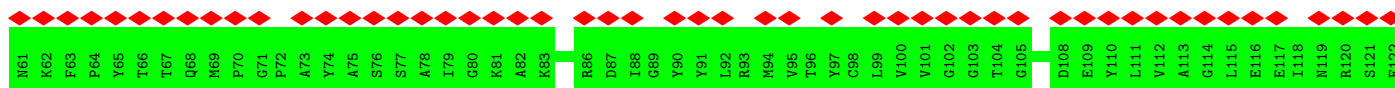
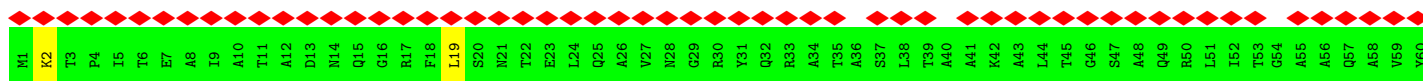
- Molecule 9: C-phycoerythrin alpha subunit



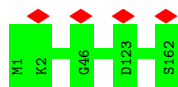
- Molecule 9: C-phycoerythrin alpha subunit



- Molecule 9: C-phycoerythrin alpha subunit



- Molecule 9: C-phycoerythrin alpha subunit



- Molecule 9: C-phycoerythrin alpha subunit



There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain GB:  100%

There are no outlier residues recorded for this chain.

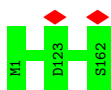
- Molecule 9: C-phycoerythrin alpha subunit

Chain IB:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain KB:  100%



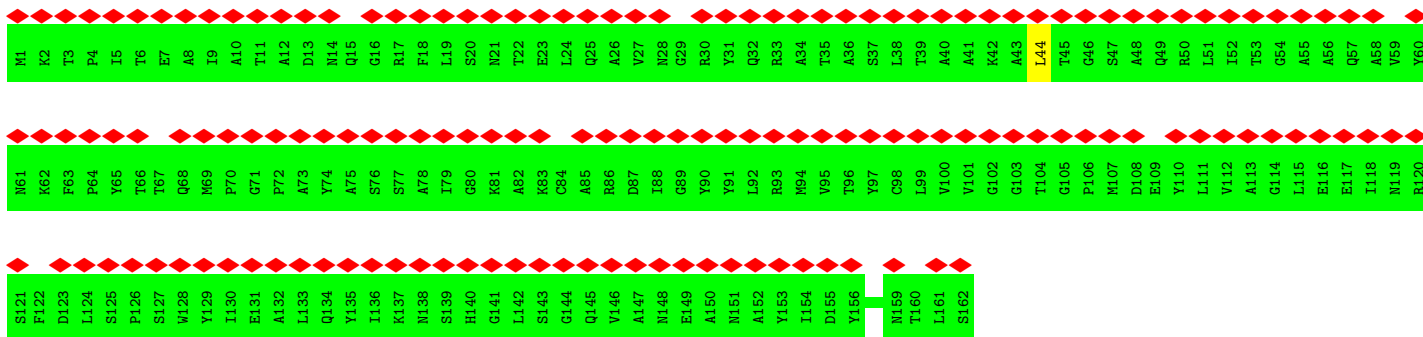
- Molecule 9: C-phycoerythrin alpha subunit

Chain MB:  100%

There are no outlier residues recorded for this chain.

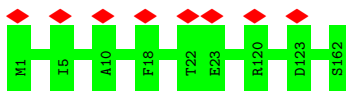
- Molecule 9: C-phycoerythrin alpha subunit

Chain CF:  94%
99%




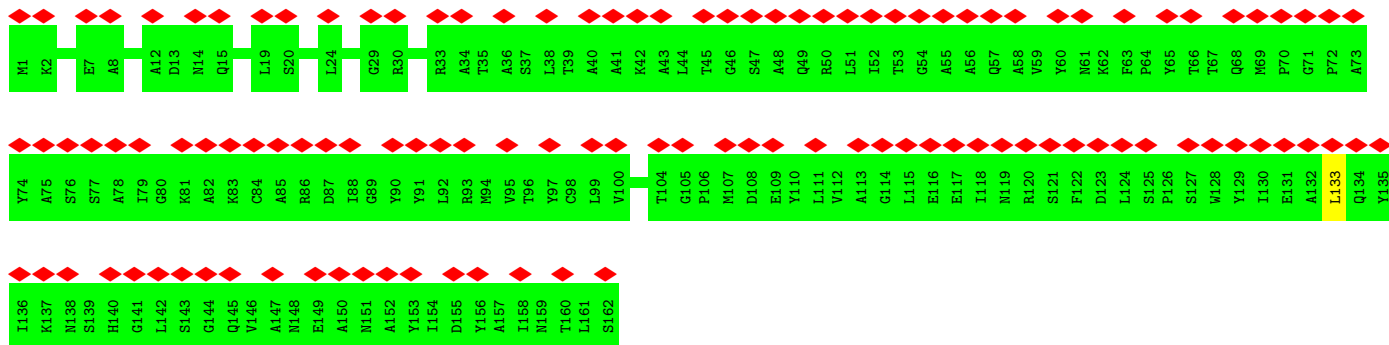
- Molecule 9: C-phycoerythrin alpha subunit

Chain EF:  5%
100%

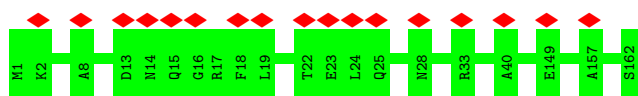


- Molecule 9: C-phycoerythrin alpha subunit

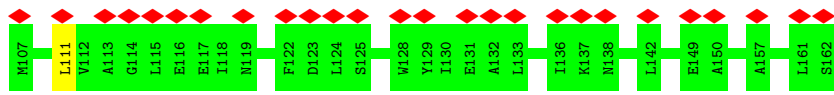
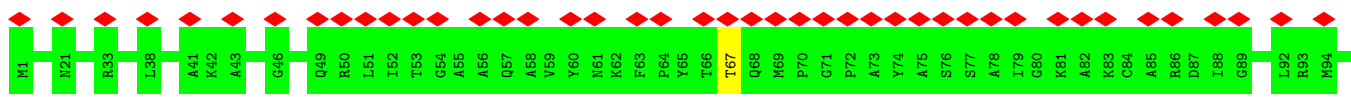
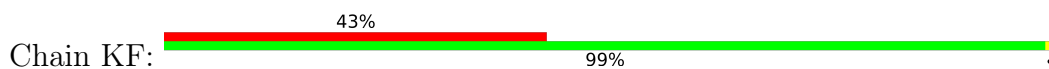
Chain GF:  71%
99%



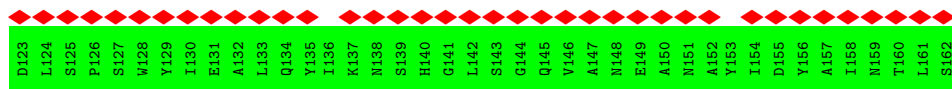
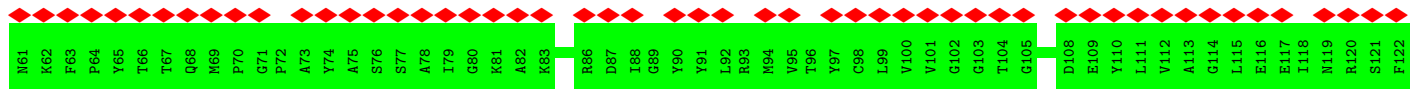
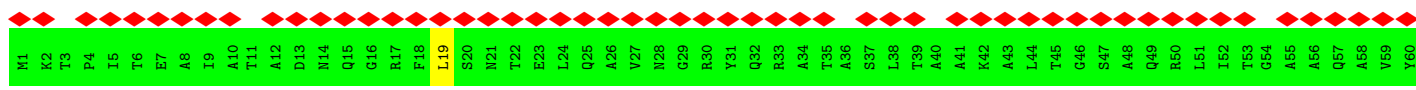
• Molecule 9: C-phycoyanin alpha subunit



• Molecule 9: C-phycoyanin alpha subunit



• Molecule 9: C-phycoyanin alpha subunit



• Molecule 9: C-phycoyanin alpha subunit





- Molecule 9: C-phyco cyanin alpha subunit

Chain EI:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain GI:  99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain II:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain KI:  99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain MI:  99%



- Molecule 10: C-phyco cyanin beta subunit

Chain D2:  99%



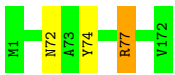
- Molecule 10: C-phyco cyanin beta subunit

Chain F2:  99%



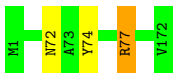
- Molecule 10: C-phyco cyanin beta subunit

Chain H2:  98% ..



● Molecule 10: C-phycocyanin beta subunit

Chain J2:  98% ..



● Molecule 10: C-phycocyanin beta subunit

Chain L2:  98% .



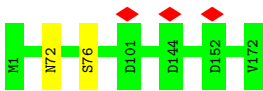
● Molecule 10: C-phycocyanin beta subunit

Chain N2:  98% .



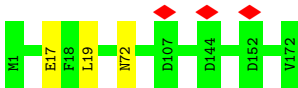
● Molecule 10: C-phycocyanin beta subunit

Chain D6:  99% .



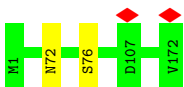
● Molecule 10: C-phycocyanin beta subunit

Chain F6:  98% .



● Molecule 10: C-phycocyanin beta subunit

Chain H6:  99% .



● Molecule 10: C-phycocyanin beta subunit

Chain J6:  97%



• Molecule 10: C-phyco cyanin beta subunit

Chain L6:  98%



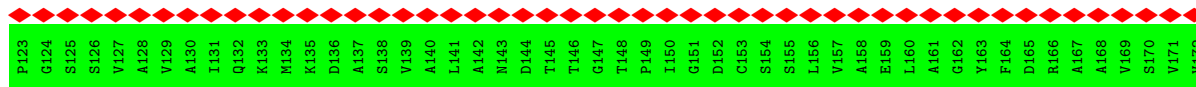
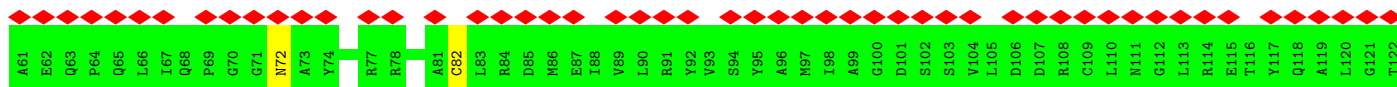
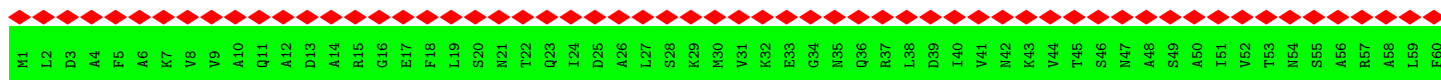
• Molecule 10: C-phyco cyanin beta subunit

Chain N6:  99%



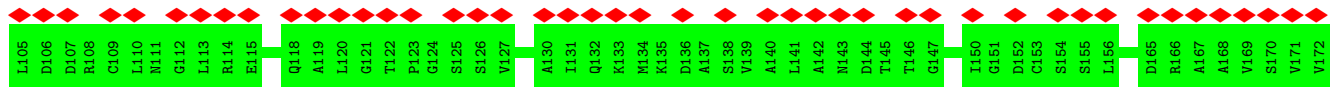
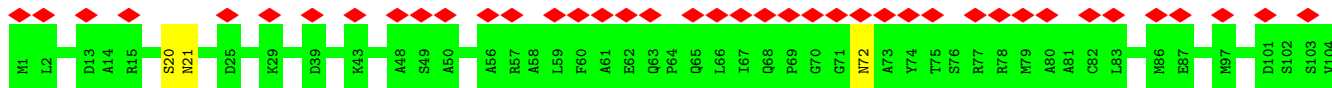
• Molecule 10: C-phyco cyanin beta subunit

Chain D7:  94%
99%



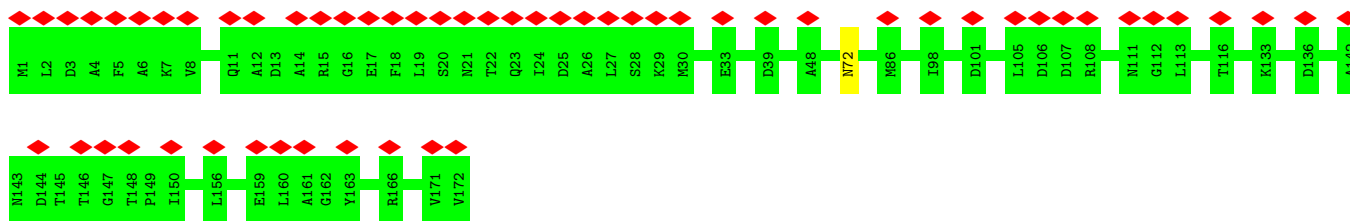
• Molecule 10: C-phyco cyanin beta subunit

Chain F7:  49%
98%

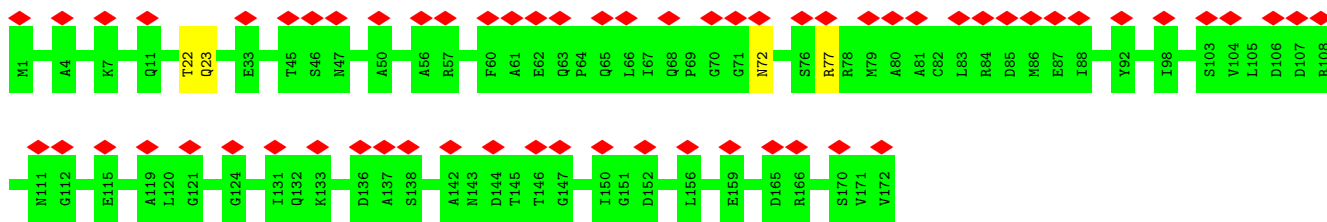


• Molecule 10: C-phyco cyanin beta subunit

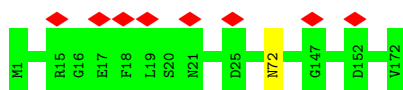
Chain H7:  33%
99%



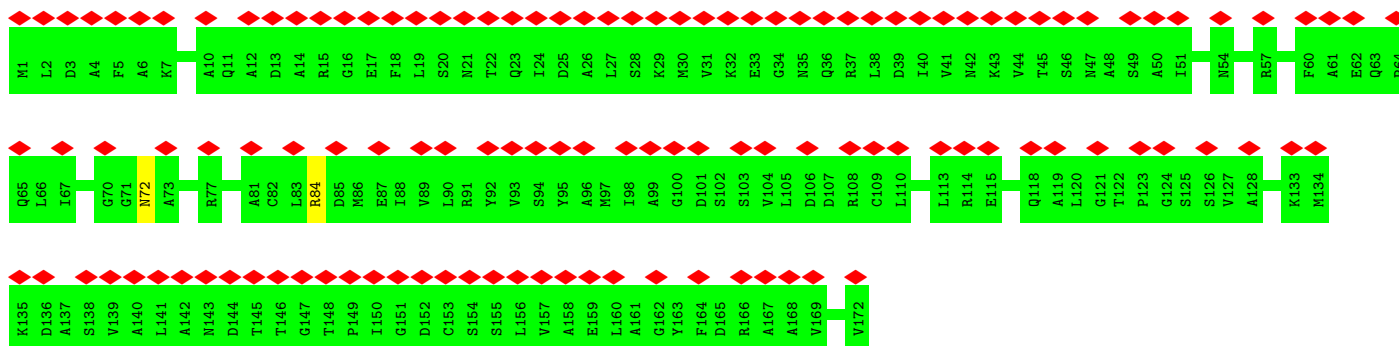
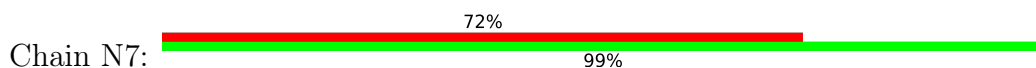
- Molecule 10: C-phycoerythrin beta subunit



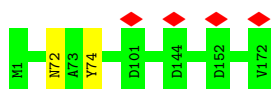
- Molecule 10: C-phycoerythrin beta subunit



- Molecule 10: C-phycoerythrin beta subunit



- Molecule 10: C-phycoerythrin beta subunit



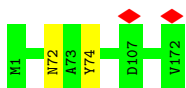
- Molecule 10: C-phycoerythrin beta subunit

Chain FB:  99%



- Molecule 10: C-phycoerythrin beta subunit

Chain HB:  99%



- Molecule 10: C-phycoerythrin beta subunit

Chain JB:  98%



- Molecule 10: C-phycoerythrin beta subunit

Chain LB:  99%



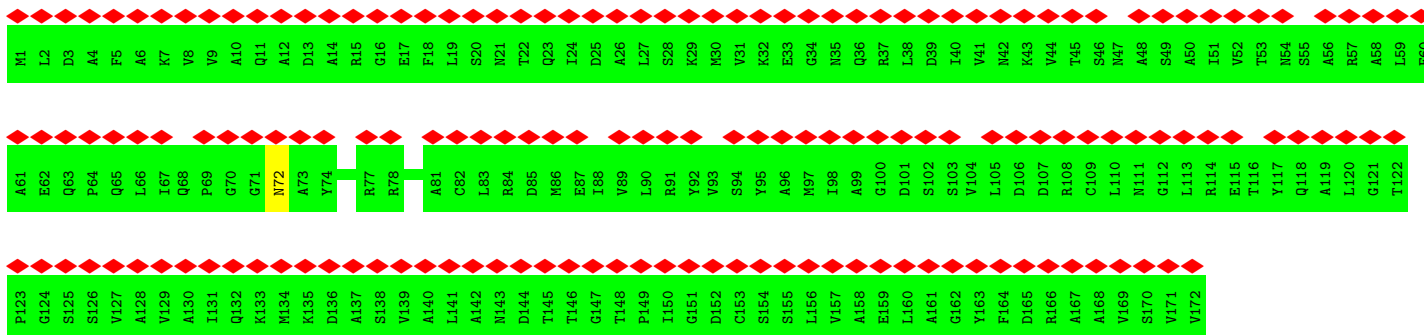
- Molecule 10: C-phycoerythrin beta subunit

Chain NB:  98%

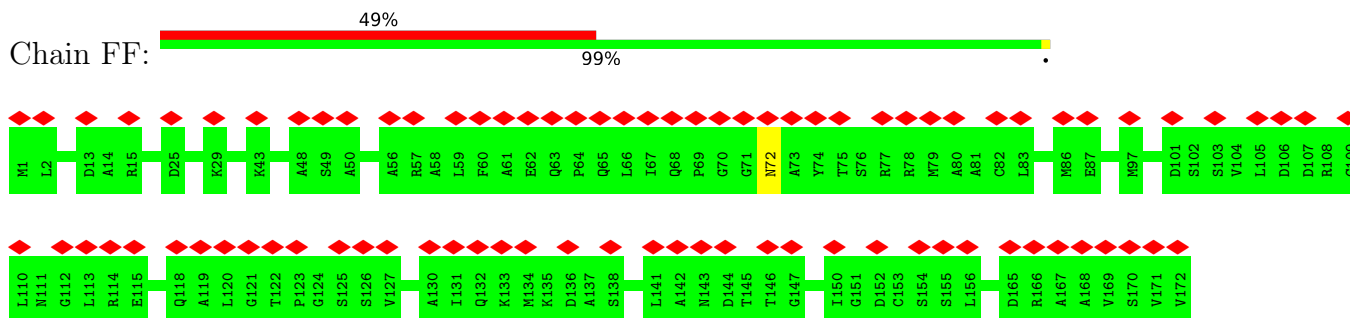


- Molecule 10: C-phycoerythrin beta subunit

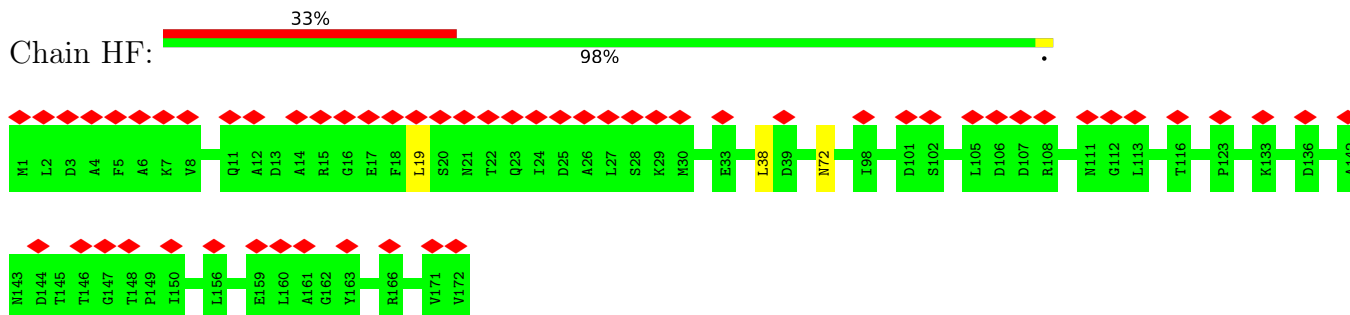
Chain DF:  94%



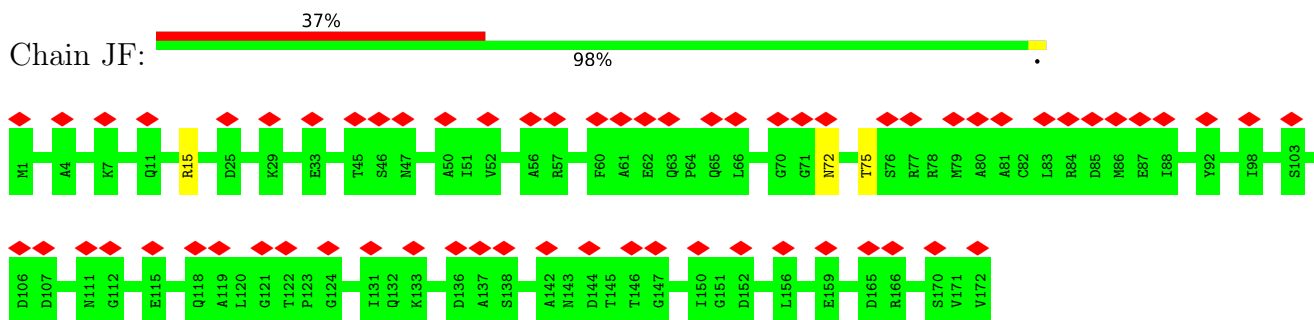
- Molecule 10: C-phycoerythrin beta subunit



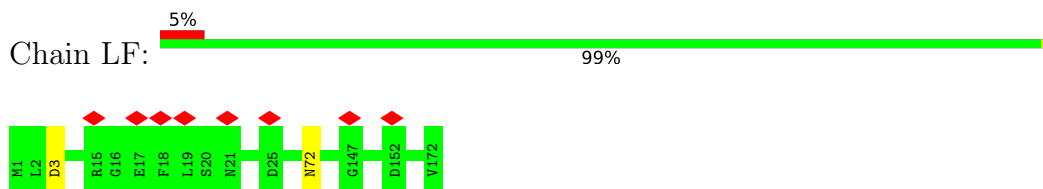
- Molecule 10: C-phycoerythrin beta subunit



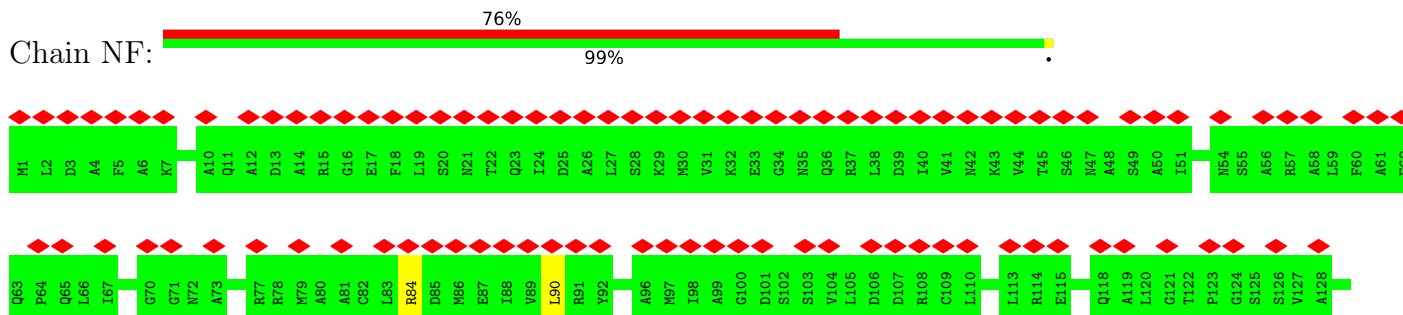
- Molecule 10: C-phycoerythrin beta subunit

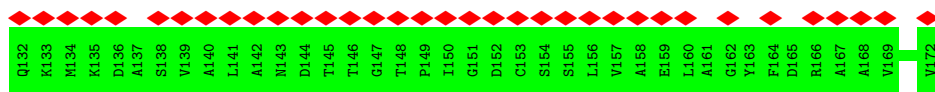


- Molecule 10: C-phycoerythrin beta subunit

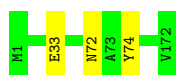


- Molecule 10: C-phycoerythrin beta subunit





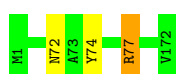
• Molecule 10: C-phyco cyanin beta subunit



• Molecule 10: C-phyco cyanin beta subunit



• Molecule 10: C-phyco cyanin beta subunit



• Molecule 10: C-phyco cyanin beta subunit



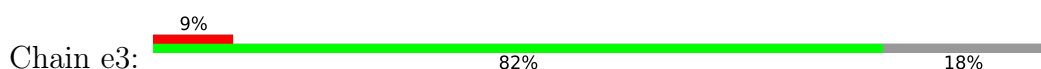
• Molecule 10: C-phyco cyanin beta subunit

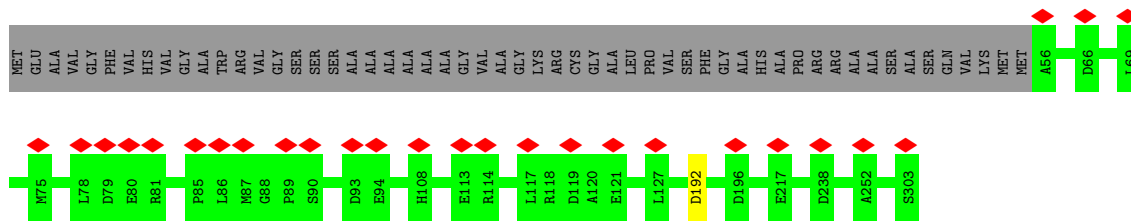


• Molecule 10: C-phyco cyanin beta subunit

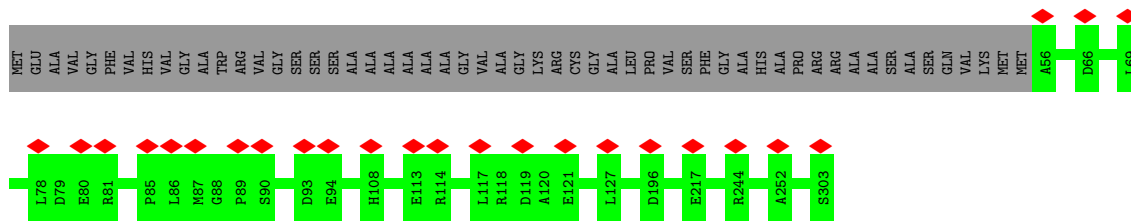
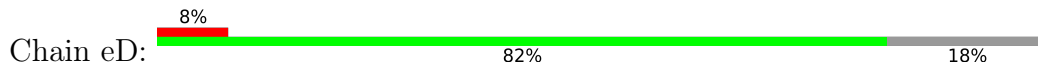


• Molecule 11: LR2

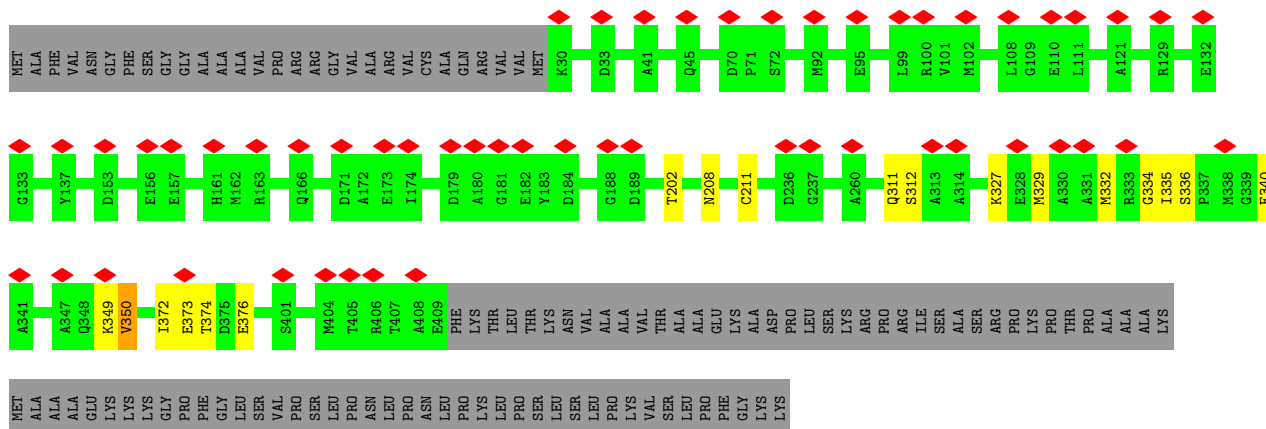
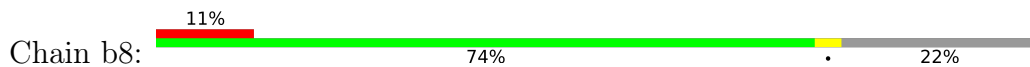




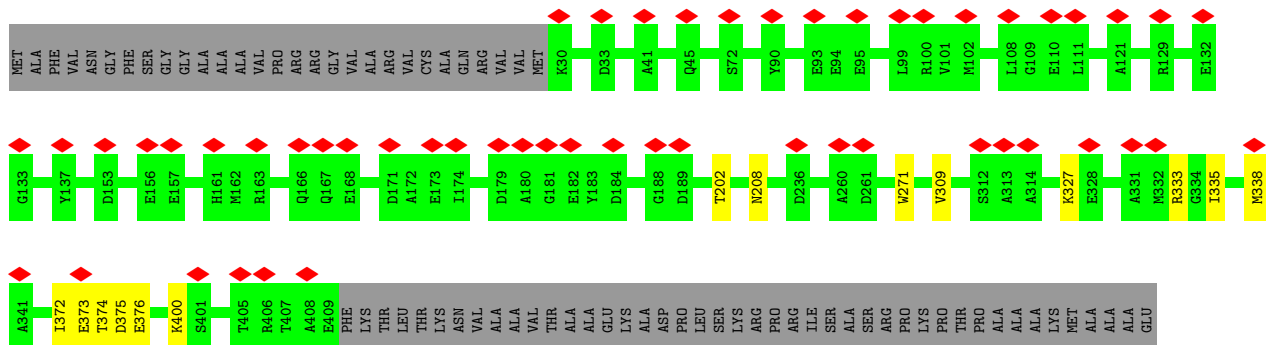
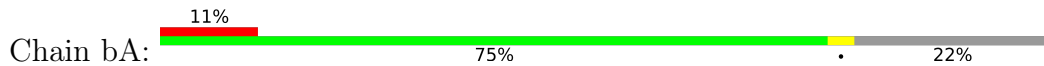
• Molecule 11: LR2

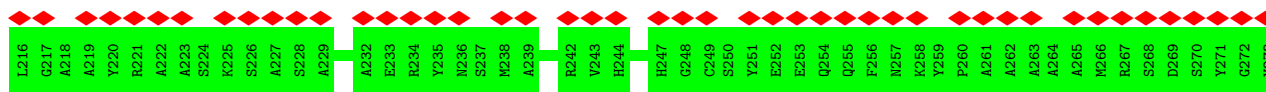


• Molecule 12: LRC2

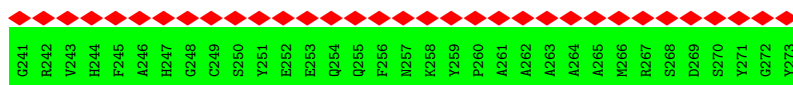
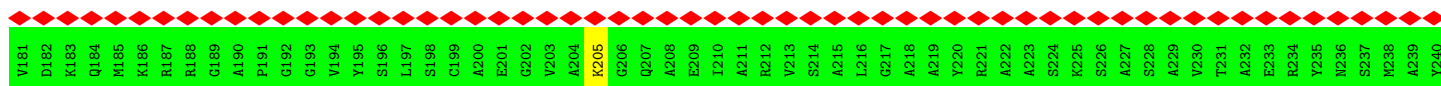
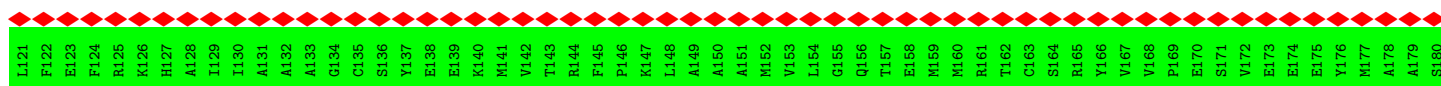
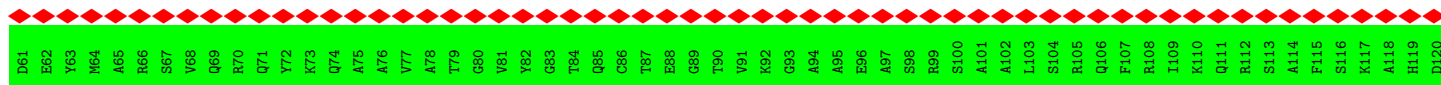
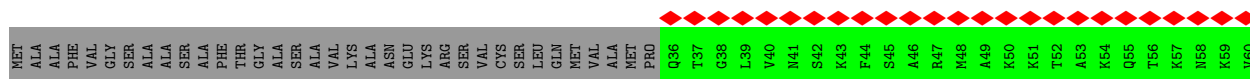
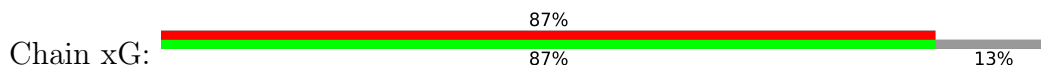


• Molecule 12: LRC2

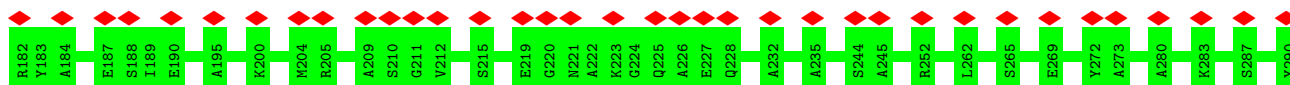
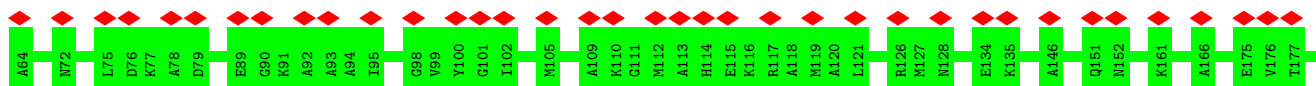
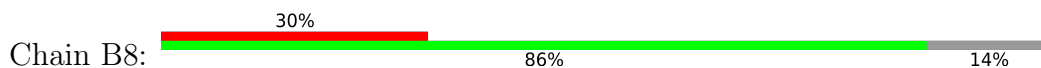




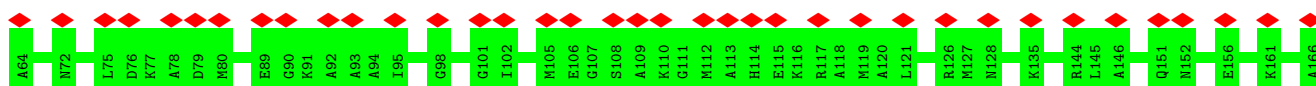
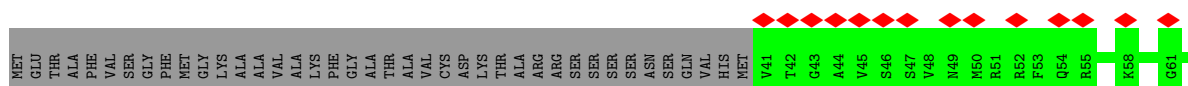
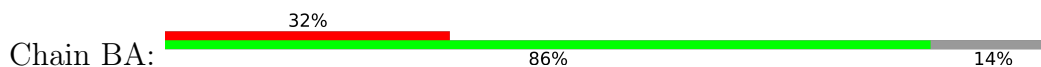
• Molecule 13: LR5

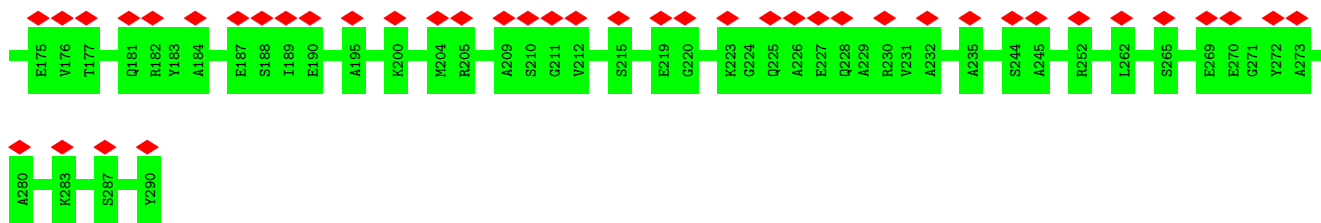


• Molecule 14: LR8

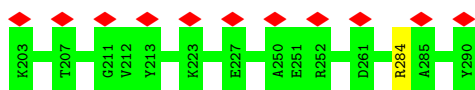
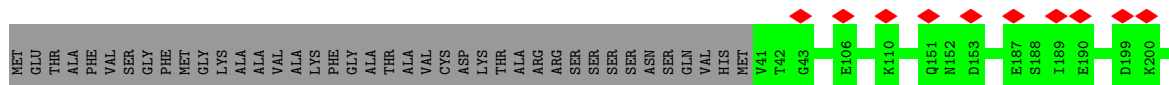
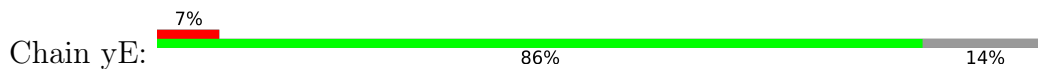


• Molecule 14: LR8

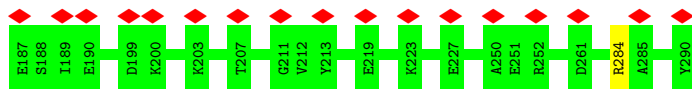
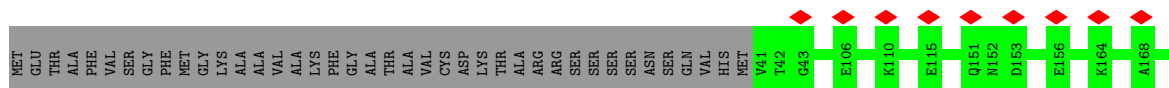
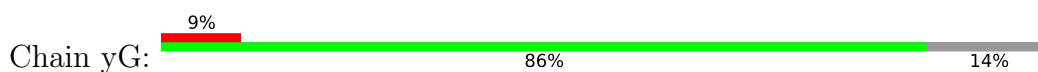




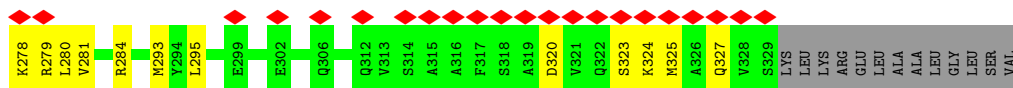
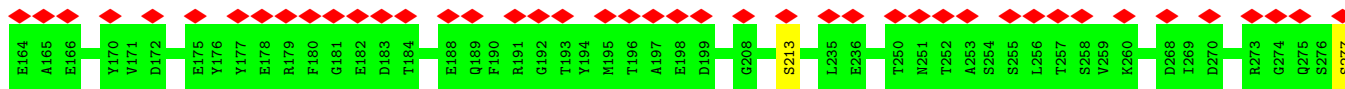
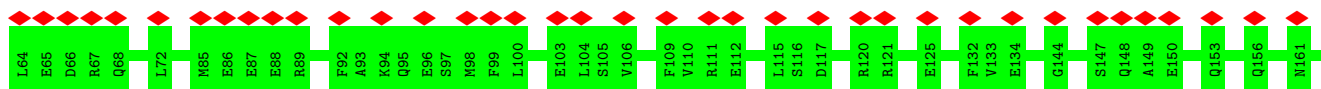
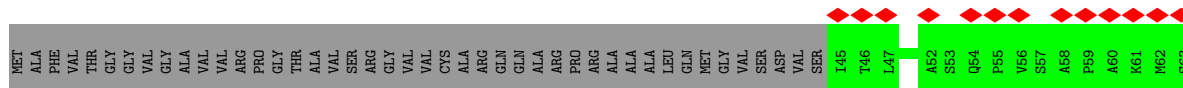
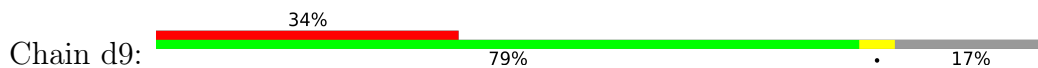
• Molecule 14: LR8



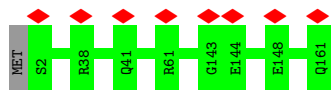
• Molecule 14: LR8



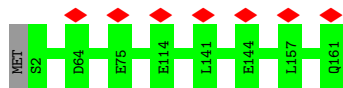
• Molecule 15: LR3



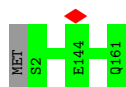
• Molecule 15: LR3



- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit



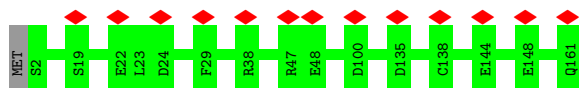
- Molecule 17: Allophycocyanin alpha subunit



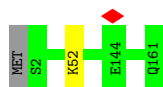
- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit

Chain PH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain RH:  99%



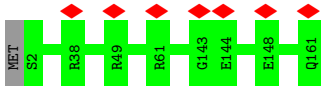
- Molecule 17: Allophycocyanin alpha subunit

Chain TH:  99%



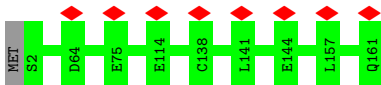
- Molecule 17: Allophycocyanin alpha subunit

Chain cH:  99%



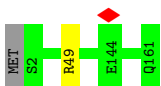
- Molecule 17: Allophycocyanin alpha subunit

Chain eH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain gH:  99%



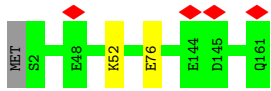
- Molecule 17: Allophycocyanin alpha subunit

Chain iH:  99%



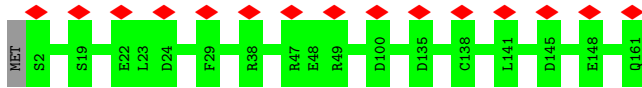
- Molecule 17: Allophycocyanin alpha subunit

Chain IH:  98%



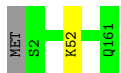
- Molecule 17: Allophycocyanin alpha subunit

Chain mH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain pH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain rH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain tH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain vH:  99%



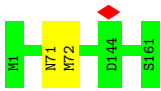
- Molecule 18: Allophycocyanin beta subunit

Chain DH:  99%



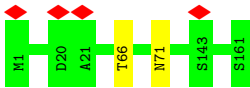
- Molecule 18: Allophycocyanin beta subunit

Chain FH:  99%



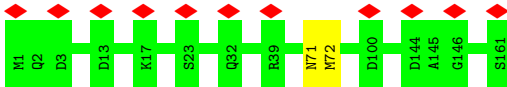
• Molecule 18: Allophycocyanin beta subunit

Chain BH:  99%



• Molecule 18: Allophycocyanin beta subunit

Chain HH:  99%



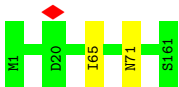
• Molecule 18: Allophycocyanin beta subunit

Chain IH:  99%



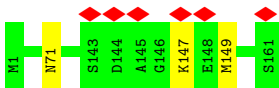
• Molecule 18: Allophycocyanin beta subunit

Chain LH:  99%



• Molecule 18: Allophycocyanin beta subunit

Chain MH:  98%



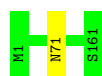
• Molecule 18: Allophycocyanin beta subunit

Chain OH:  99%



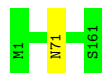
- Molecule 18: Allophycocyanin beta subunit

Chain QH:  99%



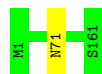
- Molecule 18: Allophycocyanin beta subunit

Chain SH:  99%



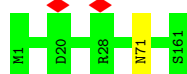
- Molecule 18: Allophycocyanin beta subunit

Chain UH:  99%



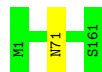
- Molecule 18: Allophycocyanin beta subunit

Chain dH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain fH:  99%



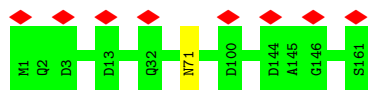
- Molecule 18: Allophycocyanin beta subunit

Chain hH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain jH:  99%



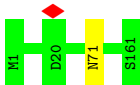
- Molecule 18: Allophycocyanin beta subunit

Chain kH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain nH:  99%



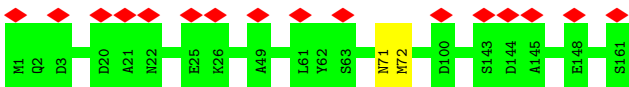
- Molecule 18: Allophycocyanin beta subunit

Chain oH:  96%



- Molecule 18: Allophycocyanin beta subunit

Chain qH:  10%  99%



- Molecule 18: Allophycocyanin beta subunit

Chain sH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain uH:  99%

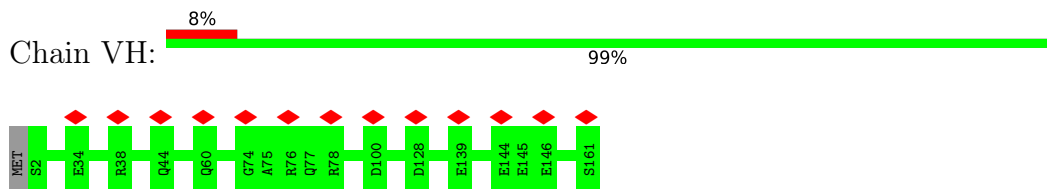


- Molecule 18: Allophycocyanin beta subunit

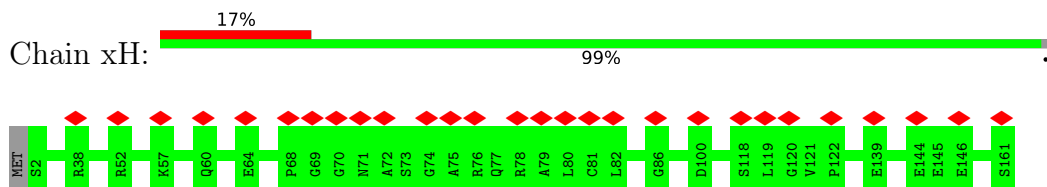
Chain wH:  99%



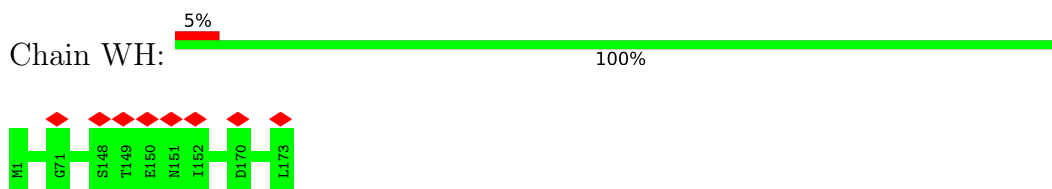
- Molecule 19: Allophycocyanin gamma subunit



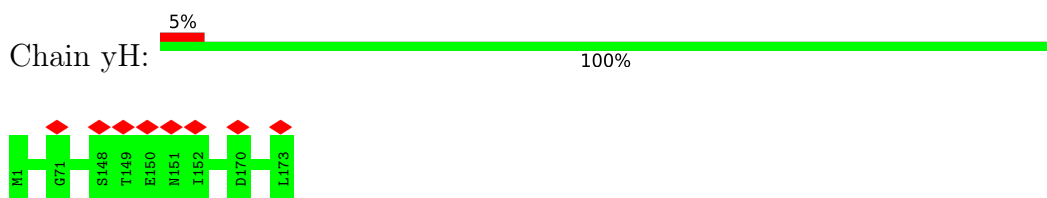
- Molecule 19: Allophycocyanin gamma subunit



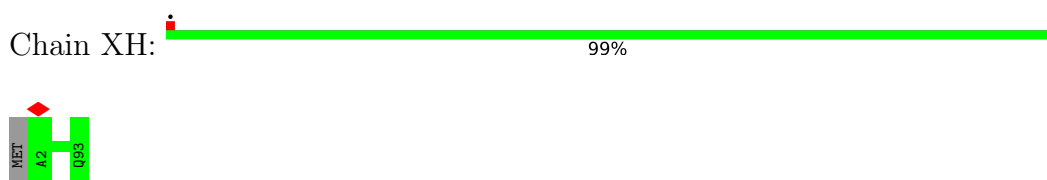
- Molecule 20: Allophycocyanin beta 18 subunit



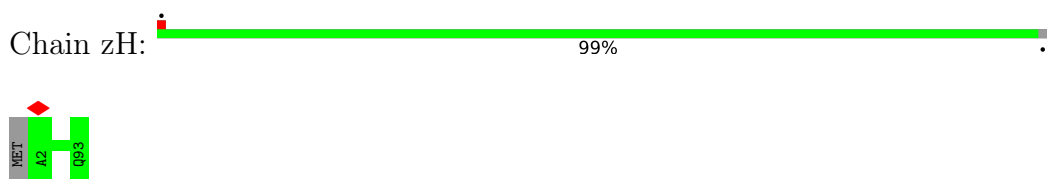
- Molecule 20: Allophycocyanin beta 18 subunit



- Molecule 21: LC

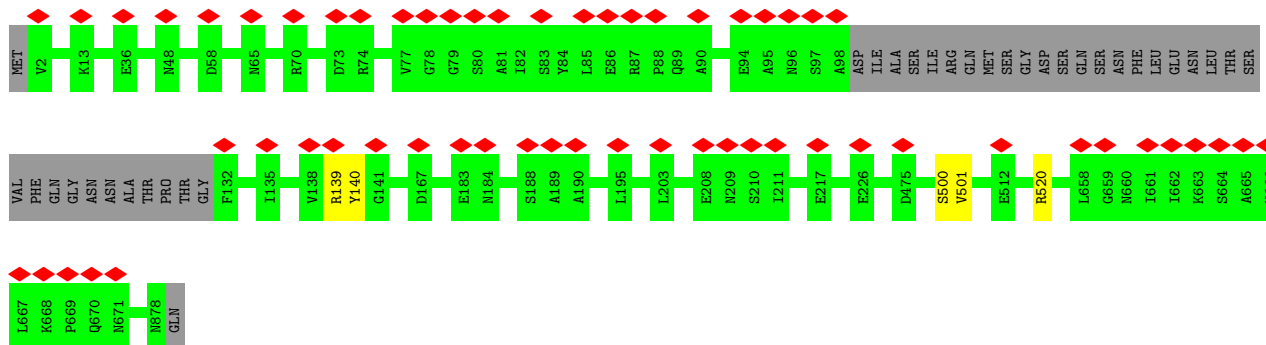


- Molecule 21: LC

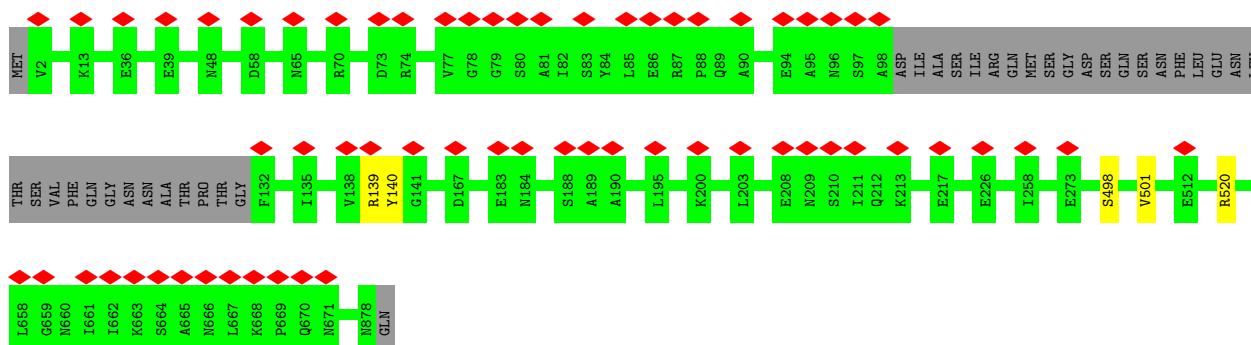


- Molecule 22: Phycobilisome linker polypeptide

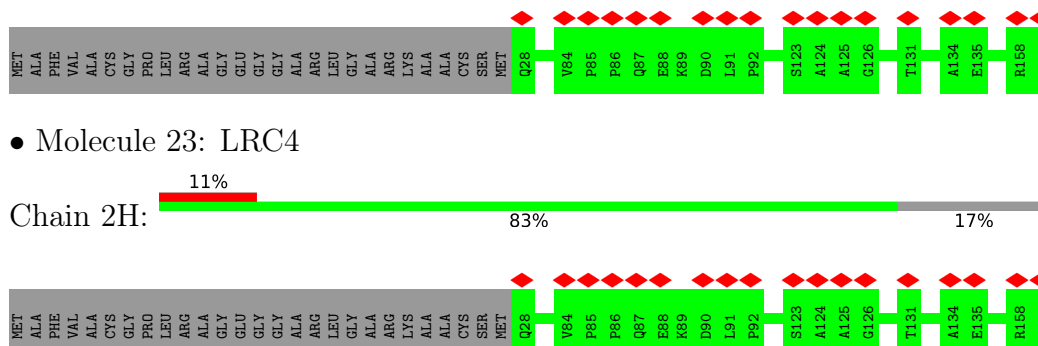
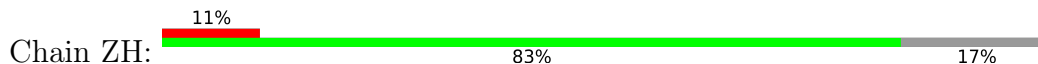




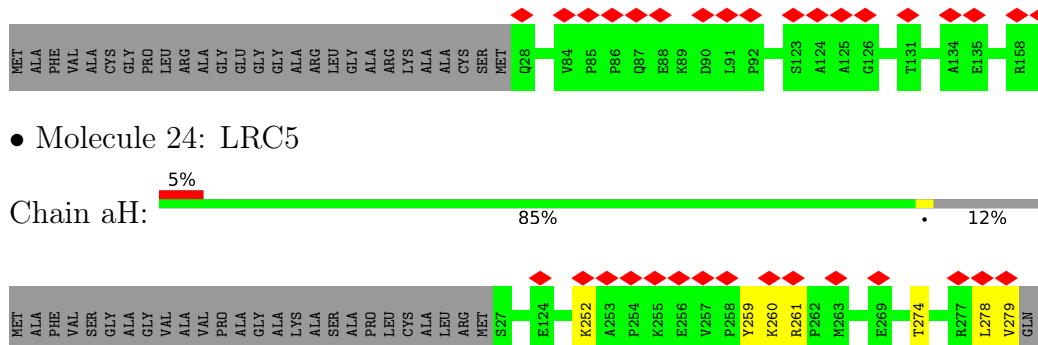
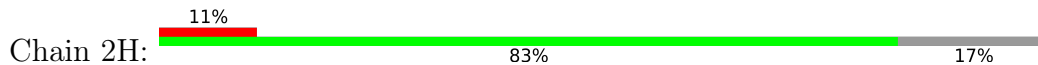
• Molecule 22: Phycobilisome linker polypeptide



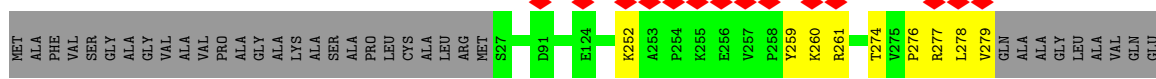
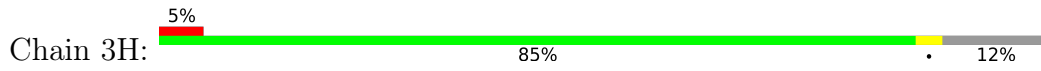
• Molecule 23: LRC4



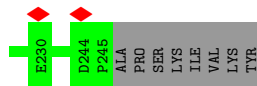
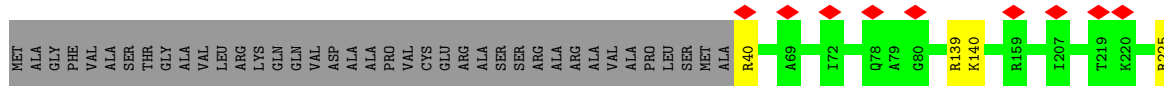
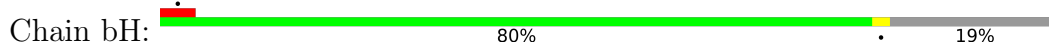
• Molecule 23: LRC4



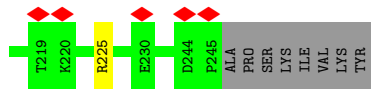
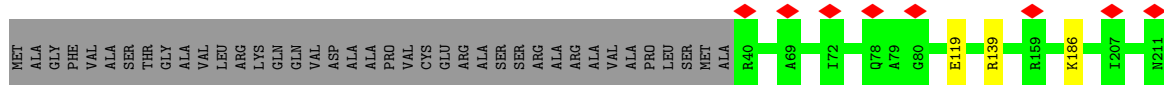
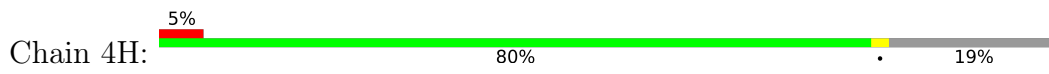
• Molecule 24: LRC5



• Molecule 25: LRC6



• Molecule 25: LRC6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	191825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	610.95996, 610.95996, 610.95996	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.33	0/1271	0.59	0/1721
1	A3	0.35	0/1271	0.63	0/1721
1	A4	0.32	0/1271	0.59	0/1721
1	AD	0.34	0/1271	0.64	0/1721
1	AE	0.33	0/1271	0.57	0/1721
1	AG	0.32	0/1271	0.59	1/1721 (0.1%)
1	B9	0.35	0/1271	0.60	0/1721
1	BJ	0.36	0/1271	0.61	0/1721
1	C1	0.32	0/1271	0.62	1/1721 (0.1%)
1	C3	0.36	0/1271	0.63	1/1721 (0.1%)
1	C4	0.32	0/1271	0.61	1/1721 (0.1%)
1	C8	0.42	0/1271	0.53	0/1721
1	CA	0.41	0/1271	0.54	0/1721
1	CD	0.33	0/1271	0.58	0/1721
1	CE	0.32	0/1271	0.63	0/1721
1	CG	0.33	0/1271	0.71	3/1721 (0.2%)
1	D9	0.38	0/1271	0.63	0/1721
1	DJ	0.43	0/1271	0.64	0/1721
1	E1	0.34	0/1271	0.62	0/1721
1	E3	0.34	0/1271	0.63	0/1721
1	E4	0.33	0/1271	0.61	0/1721
1	E8	0.38	0/1271	0.53	0/1721
1	EA	0.37	0/1271	0.55	0/1721
1	ED	0.33	0/1271	0.61	1/1721 (0.1%)
1	EE	0.36	0/1271	0.60	1/1721 (0.1%)
1	EG	0.38	0/1271	0.64	2/1721 (0.1%)
1	F9	0.38	0/1271	0.60	0/1721
1	FJ	0.39	0/1271	0.61	0/1721
1	G1	0.36	0/1271	0.62	0/1721
1	G3	0.36	0/1271	0.64	0/1721
1	G4	0.32	0/1271	0.61	0/1721
1	G8	0.35	0/1271	0.55	1/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GA	0.35	0/1271	0.54	1/1721 (0.1%)
1	GD	0.34	0/1271	0.61	1/1721 (0.1%)
1	GE	0.44	0/1271	0.69	3/1721 (0.2%)
1	GG	0.49	0/1271	0.83	5/1721 (0.3%)
1	H9	0.34	0/1271	0.60	0/1721
1	HJ	0.36	0/1271	0.63	0/1721
1	I1	0.34	0/1271	0.63	1/1721 (0.1%)
1	I3	0.35	0/1271	0.67	2/1721 (0.1%)
1	I4	0.31	0/1271	0.63	1/1721 (0.1%)
1	I8	0.41	0/1271	0.51	0/1721
1	IA	0.39	0/1271	0.51	1/1721 (0.1%)
1	ID	0.32	0/1271	0.62	1/1721 (0.1%)
1	IE	0.43	0/1271	0.70	3/1721 (0.2%)
1	IG	0.49	0/1271	0.78	4/1721 (0.2%)
1	J5	0.71	0/1271	0.59	0/1721
1	J9	0.33	0/1271	0.58	0/1721
1	JC	0.49	0/1271	0.53	0/1721
1	JJ	0.34	0/1271	0.59	0/1721
1	K1	0.34	0/1271	0.63	2/1721 (0.1%)
1	K3	0.37	0/1271	0.64	1/1721 (0.1%)
1	K4	0.33	0/1271	0.58	0/1721
1	K8	0.50	0/1271	0.56	0/1721
1	KA	0.48	0/1271	0.54	0/1721
1	KD	0.35	0/1271	0.64	1/1721 (0.1%)
1	KE	0.36	0/1271	0.61	1/1721 (0.1%)
1	KG	0.38	0/1271	0.60	0/1721
1	L9	0.35	0/1271	0.59	0/1721
1	LJ	0.35	0/1271	0.61	0/1721
1	M3	0.38	0/1271	0.59	0/1721
1	M8	0.60	0/1271	0.54	0/1721
1	MA	0.58	0/1271	0.54	0/1721
1	MD	0.35	0/1271	0.57	0/1721
1	ME	0.30	0/1271	0.60	0/1721
1	MG	0.31	0/1271	0.60	0/1721
1	N1	0.47	0/1271	0.65	1/1721 (0.1%)
1	N4	0.48	0/1271	0.63	1/1721 (0.1%)
1	N9	0.32	0/1271	0.60	1/1721 (0.1%)
1	NJ	0.33	0/1271	0.63	1/1721 (0.1%)
1	O2	0.34	0/1271	0.45	0/1721
1	O3	0.52	0/1271	0.66	1/1721 (0.1%)
1	O6	0.36	0/1271	0.48	0/1721
1	O7	0.28	0/1271	0.55	1/1721 (0.1%)
1	O8	0.39	0/1271	0.51	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	OA	0.37	0/1271	0.50	0/1721
1	OB	0.38	0/1271	0.49	0/1721
1	OD	0.47	0/1271	0.63	1/1721 (0.1%)
1	OE	0.33	0/1271	0.62	0/1721
1	OF	0.33	0/1271	0.59	0/1721
1	OG	0.34	0/1271	0.60	0/1721
1	OI	0.34	0/1271	0.47	0/1721
1	P1	0.35	0/1271	0.60	0/1721
1	P4	0.34	0/1271	0.60	0/1721
1	P9	0.34	0/1271	0.63	0/1721
1	PJ	0.34	0/1271	0.64	0/1721
1	Q2	0.39	0/1271	0.50	0/1721
1	Q3	0.50	0/1271	0.63	1/1721 (0.1%)
1	Q6	0.33	0/1271	0.50	0/1721
1	Q7	0.28	0/1271	0.51	1/1721 (0.1%)
1	Q8	0.36	0/1271	0.53	0/1721
1	QA	0.38	0/1271	0.51	0/1721
1	QB	0.33	0/1271	0.49	0/1721
1	QD	0.44	0/1271	0.60	0/1721
1	QE	0.33	0/1271	0.67	2/1721 (0.1%)
1	QF	0.34	0/1271	0.60	2/1721 (0.1%)
1	QG	0.35	0/1271	0.66	1/1721 (0.1%)
1	QI	0.39	0/1271	0.48	0/1721
1	R1	0.32	0/1271	0.57	1/1721 (0.1%)
1	R4	0.33	0/1271	0.57	1/1721 (0.1%)
1	R9	0.35	0/1271	0.63	1/1721 (0.1%)
1	RJ	0.37	0/1271	0.65	1/1721 (0.1%)
1	S2	0.36	0/1271	0.48	0/1721
1	S3	0.51	0/1271	0.66	1/1721 (0.1%)
1	S6	0.34	0/1271	0.49	0/1721
1	S7	0.29	0/1271	0.50	0/1721
1	S8	0.36	0/1271	0.52	0/1721
1	SA	0.35	0/1271	0.52	0/1721
1	SB	0.34	0/1271	0.49	0/1721
1	SD	0.45	0/1271	0.63	0/1721
1	SE	0.38	0/1271	0.76	3/1721 (0.2%)
1	SF	0.35	0/1271	0.65	2/1721 (0.1%)
1	SG	0.39	0/1271	0.67	2/1721 (0.1%)
1	SI	0.35	0/1271	0.49	0/1721
1	T1	0.33	0/1271	0.57	0/1721
1	T4	0.33	0/1271	0.57	0/1721
1	T9	0.35	0/1271	0.62	0/1721
1	TJ	0.36	0/1271	0.64	2/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	U2	0.40	0/1271	0.51	0/1721
1	U3	0.42	0/1271	0.61	0/1721
1	U6	0.32	0/1271	0.50	0/1721
1	U7	0.29	0/1271	0.60	2/1721 (0.1%)
1	U8	0.46	0/1271	0.55	0/1721
1	UA	0.43	0/1271	0.53	0/1721
1	UB	0.33	0/1271	0.52	0/1721
1	UD	0.38	0/1271	0.58	0/1721
1	UE	0.39	0/1271	0.72	5/1721 (0.3%)
1	UF	0.33	0/1271	0.69	3/1721 (0.2%)
1	UG	0.40	0/1271	0.67	2/1721 (0.1%)
1	UI	0.39	0/1271	0.48	0/1721
1	V1	0.38	0/1271	0.60	0/1721
1	V4	0.36	0/1271	0.57	0/1721
1	V9	0.34	0/1271	0.62	1/1721 (0.1%)
1	VJ	0.36	0/1271	0.66	3/1721 (0.2%)
1	W2	0.36	0/1271	0.48	0/1721
1	W3	0.42	0/1271	0.58	0/1721
1	W6	0.38	0/1271	0.50	0/1721
1	W7	0.29	0/1271	0.50	0/1721
1	W8	0.58	0/1271	0.55	0/1721
1	WA	0.57	0/1271	0.56	0/1721
1	WB	0.39	0/1271	0.51	0/1721
1	WD	0.38	0/1271	0.56	0/1721
1	WE	0.34	0/1271	0.56	0/1721
1	WF	0.33	0/1271	0.64	2/1721 (0.1%)
1	WG	0.34	0/1271	0.62	3/1721 (0.2%)
1	WI	0.36	0/1271	0.48	0/1721
1	X1	0.50	0/1271	0.66	0/1721
1	X4	0.50	0/1271	0.65	1/1721 (0.1%)
1	X9	0.34	0/1271	0.65	1/1721 (0.1%)
1	XJ	0.34	0/1271	0.62	0/1721
1	Y8	0.49	0/1271	0.53	0/1721
1	YA	0.47	0/1271	0.53	0/1721
1	YE	0.31	0/1271	0.58	0/1721
1	YG	0.33	0/1271	0.57	0/1721
1	Z2	0.38	0/1271	0.48	0/1721
1	Z6	0.36	0/1271	0.50	0/1721
1	Z7	0.28	0/1271	0.51	0/1721
1	ZB	0.37	0/1271	0.51	0/1721
1	ZF	0.32	0/1271	0.59	0/1721
1	ZI	0.39	0/1271	0.48	0/1721
1	a8	0.34	0/1271	0.51	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	aA	0.33	0/1271	0.52	0/1721
1	aE	0.34	0/1271	0.61	0/1721
1	aG	0.33	0/1271	0.62	0/1721
1	b2	0.30	0/1271	0.51	0/1721
1	b6	0.31	0/1271	0.53	1/1721 (0.1%)
1	b7	0.27	0/1271	0.53	1/1721 (0.1%)
1	bB	0.32	0/1271	0.53	0/1721
1	bF	0.32	0/1271	0.71	2/1721 (0.1%)
1	bI	0.29	0/1271	0.52	0/1721
1	c1	0.32	0/1271	0.63	1/1721 (0.1%)
1	c4	0.33	0/1271	0.58	0/1721
1	cE	0.33	0/1271	0.65	2/1721 (0.1%)
1	cG	0.33	0/1271	0.62	1/1721 (0.1%)
1	d2	0.31	0/1271	0.51	0/1721
1	d6	0.29	0/1271	0.50	0/1721
1	d7	0.28	0/1271	0.62	2/1721 (0.1%)
1	d8	0.35	0/1271	0.54	0/1721
1	dA	0.34	0/1271	0.54	0/1721
1	dB	0.29	0/1271	0.55	0/1721
1	dF	0.34	0/1271	0.70	2/1721 (0.1%)
1	dI	0.30	0/1271	0.51	0/1721
1	e1	0.34	0/1271	0.60	0/1721
1	e4	0.31	0/1271	0.60	0/1721
1	eE	0.32	0/1271	0.59	0/1721
1	eG	0.33	0/1271	0.65	1/1721 (0.1%)
1	f2	0.28	0/1271	0.52	0/1721
1	f6	0.28	0/1271	0.51	0/1721
1	f7	0.27	0/1271	0.51	1/1721 (0.1%)
1	f8	0.32	0/1271	0.56	1/1721 (0.1%)
1	fA	0.31	0/1271	0.57	1/1721 (0.1%)
1	fB	0.29	0/1271	0.50	0/1721
1	fF	0.34	0/1271	0.69	2/1721 (0.1%)
1	fI	0.29	0/1271	0.53	0/1721
1	g1	0.33	0/1271	0.69	3/1721 (0.2%)
1	g4	0.33	0/1271	0.64	1/1721 (0.1%)
1	gE	0.33	0/1271	0.59	0/1721
1	gG	0.31	0/1271	0.58	0/1721
1	h2	0.32	0/1271	0.50	0/1721
1	h6	0.30	0/1271	0.51	0/1721
1	h7	0.27	0/1271	0.55	1/1721 (0.1%)
1	h8	0.33	0/1271	0.59	1/1721 (0.1%)
1	hA	0.32	0/1271	0.55	0/1721
1	hB	0.31	0/1271	0.60	1/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	hF	0.32	0/1271	0.69	3/1721 (0.2%)
1	hI	0.31	0/1271	0.49	0/1721
1	i1	0.31	0/1271	0.59	0/1721
1	i4	0.32	0/1271	0.60	0/1721
1	iE	0.32	0/1271	0.61	0/1721
1	iG	0.35	0/1271	0.62	2/1721 (0.1%)
1	j2	0.31	0/1271	0.50	0/1721
1	j6	0.29	0/1271	0.47	0/1721
1	j7	0.28	0/1271	0.55	1/1721 (0.1%)
1	j8	0.33	0/1271	0.57	1/1721 (0.1%)
1	jA	0.31	0/1271	0.55	0/1721
1	jB	0.29	0/1271	0.47	0/1721
1	jF	0.35	0/1271	0.72	3/1721 (0.2%)
1	jI	0.30	0/1271	0.50	0/1721
1	k1	0.32	0/1271	0.62	0/1721
1	k4	0.31	0/1271	0.60	0/1721
1	kE	0.35	0/1271	0.64	3/1721 (0.2%)
1	kG	0.33	0/1271	0.63	0/1721
1	l2	0.31	0/1271	0.47	0/1721
1	l6	0.28	0/1271	0.50	0/1721
1	l7	0.29	0/1271	0.56	0/1721
1	l8	0.39	0/1271	0.58	1/1721 (0.1%)
1	lA	0.37	0/1271	0.57	0/1721
1	lB	0.29	0/1271	0.54	0/1721
1	lF	0.37	0/1271	0.76	7/1721 (0.4%)
1	lI	0.31	0/1271	0.48	0/1721
1	m1	0.34	0/1271	0.64	0/1721
1	m4	0.32	0/1271	0.62	2/1721 (0.1%)
1	mE	0.37	0/1271	0.86	9/1721 (0.5%)
1	mG	0.34	0/1271	0.65	0/1721
1	oE	0.32	0/1271	0.65	0/1721
1	oG	0.32	0/1271	0.64	0/1721
1	p1	0.34	0/1271	0.63	1/1721 (0.1%)
1	p4	0.33	0/1271	0.61	0/1721
1	qE	0.31	0/1271	0.63	1/1721 (0.1%)
1	qG	0.32	0/1271	0.65	1/1721 (0.1%)
1	r1	0.34	0/1271	0.64	1/1721 (0.1%)
1	r4	0.35	0/1271	0.63	1/1721 (0.1%)
1	sE	0.32	0/1271	0.58	1/1721 (0.1%)
1	sG	0.36	0/1271	0.60	2/1721 (0.1%)
1	t1	0.33	0/1271	0.64	2/1721 (0.1%)
1	t4	0.34	0/1271	0.61	0/1721
1	uE	0.32	0/1271	0.60	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	uG	0.33	0/1271	0.62	1/1721 (0.1%)
1	v1	0.34	0/1271	0.69	2/1721 (0.1%)
1	v4	0.34	0/1271	0.72	1/1721 (0.1%)
1	x1	0.36	0/1271	0.73	2/1721 (0.1%)
1	x4	0.33	0/1271	0.66	1/1721 (0.1%)
1	z1	0.33	0/1271	0.65	0/1721
1	z4	0.33	0/1271	0.64	0/1721
2	11	0.32	0/1297	0.63	1/1750 (0.1%)
2	14	0.32	0/1297	0.67	2/1750 (0.1%)
2	A5	0.29	0/1065	0.50	0/1437
2	AC	0.28	0/1065	0.49	0/1437
2	B1	0.32	0/1297	0.61	0/1750
2	B3	0.35	0/1297	0.67	1/1750 (0.1%)
2	B4	0.32	0/1297	0.59	0/1750
2	B5	0.28	0/1065	0.53	0/1437
2	BC	0.32	0/1065	0.52	0/1437
2	BD	0.32	0/1297	0.66	0/1750
2	BE	0.32	0/1303	0.63	1/1758 (0.1%)
2	BG	0.32	0/1303	0.56	1/1758 (0.1%)
2	C5	0.26	0/1065	0.49	0/1437
2	C9	0.37	0/1297	0.61	0/1750
2	CC	0.27	0/1065	0.46	0/1437
2	CJ	0.38	0/1297	0.63	0/1750
2	D1	0.32	0/1297	0.61	1/1750 (0.1%)
2	D3	0.34	0/1297	0.67	3/1750 (0.2%)
2	D4	0.32	0/1297	0.62	2/1750 (0.1%)
2	D8	0.36	0/1315	0.54	1/1774 (0.1%)
2	DA	0.36	0/1315	0.52	0/1774
2	DD	0.32	0/1297	0.62	0/1750
2	DE	0.33	0/1315	0.61	1/1774 (0.1%)
2	DG	0.34	0/1315	0.58	0/1774
2	E9	0.37	0/1297	0.63	1/1750 (0.1%)
2	EJ	0.39	0/1297	0.63	1/1750 (0.1%)
2	F1	0.31	0/1297	0.55	0/1750
2	F3	0.33	0/1297	0.63	1/1750 (0.1%)
2	F4	0.30	0/1297	0.55	0/1750
2	F5	0.41	0/1065	0.56	0/1437
2	F8	0.43	0/1315	0.58	1/1774 (0.1%)
2	FA	0.41	0/1315	0.57	1/1774 (0.1%)
2	FC	0.32	0/1065	0.51	0/1437
2	FD	0.33	0/1297	0.63	1/1750 (0.1%)
2	FE	0.40	0/1315	0.69	3/1774 (0.2%)
2	FG	0.43	0/1315	0.62	0/1774

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	G5	0.34	0/1065	0.51	0/1437
2	G9	0.32	0/1297	0.61	1/1750 (0.1%)
2	GC	0.27	0/1065	0.48	0/1437
2	GJ	0.34	0/1297	0.64	1/1750 (0.1%)
2	H1	0.32	0/1303	0.72	3/1758 (0.2%)
2	H3	0.34	0/1309	0.63	1/1766 (0.1%)
2	H4	0.32	0/1309	0.64	1/1766 (0.1%)
2	H5	0.54	0/1065	0.60	0/1437
2	H8	0.38	0/1315	0.59	1/1774 (0.1%)
2	HA	0.36	0/1315	0.55	0/1774
2	HC	0.39	0/1065	0.53	0/1437
2	HD	0.34	0/1309	0.64	0/1766
2	HE	0.34	0/1315	0.55	0/1774
2	HG	0.37	0/1315	0.56	0/1774
2	I5	0.44	0/1297	0.53	0/1750
2	I9	0.41	0/1309	0.71	3/1766 (0.2%)
2	IC	0.33	0/1289	0.49	0/1740
2	IJ	0.45	0/1309	0.66	0/1766
2	J1	0.32	0/1297	0.59	0/1750
2	J3	0.33	0/1297	0.64	1/1750 (0.1%)
2	J4	0.32	0/1297	0.55	0/1750
2	J8	0.37	0/1309	0.53	0/1766
2	JA	0.34	0/1309	0.56	1/1766 (0.1%)
2	JD	0.34	0/1297	0.65	0/1750
2	JE	0.35	0/1315	0.56	0/1774
2	JG	0.39	0/1315	0.60	2/1774 (0.1%)
2	K5	0.56	0/1297	0.56	0/1750
2	K9	0.33	0/1297	0.57	0/1750
2	KC	0.41	0/1297	0.50	0/1750
2	KJ	0.35	0/1297	0.60	1/1750 (0.1%)
2	L1	0.30	0/1297	0.61	1/1750 (0.1%)
2	L3	0.34	0/1297	0.65	0/1750
2	L4	0.30	0/1297	0.56	0/1750
2	L5	0.57	0/1065	0.58	0/1437
2	L8	0.49	0/1315	0.56	2/1774 (0.1%)
2	LA	0.47	0/1315	0.55	2/1774 (0.1%)
2	LC	0.43	0/1065	0.50	0/1437
2	LD	0.34	0/1297	0.65	0/1750
2	LE	0.43	0/1315	0.62	0/1774
2	LG	0.48	0/1315	0.67	2/1774 (0.1%)
2	M9	0.33	0/1297	0.61	0/1750
2	MJ	0.36	0/1297	0.63	1/1750 (0.1%)
2	N3	0.39	0/1315	0.60	1/1774 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	N8	0.53	0/1315	0.60	0/1774
2	NA	0.51	0/1315	0.61	1/1774 (0.1%)
2	ND	0.35	0/1315	0.56	0/1774
2	NE	0.31	0/1315	0.59	0/1774
2	NG	0.33	0/1315	0.62	0/1774
2	O1	0.36	0/1297	0.64	1/1750 (0.1%)
2	O4	0.37	0/1297	0.63	2/1750 (0.1%)
2	O9	0.33	0/1297	0.62	1/1750 (0.1%)
2	OJ	0.33	0/1297	0.68	2/1750 (0.1%)
2	P2	0.30	0/1297	0.47	0/1750
2	P3	0.44	0/1315	0.61	0/1774
2	P6	0.36	0/1297	0.47	0/1750
2	P7	0.30	0/1297	0.50	0/1750
2	P8	0.31	0/1297	0.50	0/1750
2	PA	0.31	0/1297	0.50	0/1750
2	PB	0.37	0/1297	0.48	0/1750
2	PD	0.41	0/1315	0.59	0/1774
2	PE	0.31	0/1315	0.59	0/1774
2	PF	0.34	0/1297	0.62	2/1750 (0.1%)
2	PG	0.33	0/1315	0.59	0/1774
2	PI	0.30	0/1297	0.47	0/1750
2	Q1	0.39	0/1297	0.64	1/1750 (0.1%)
2	Q4	0.39	0/1297	0.62	1/1750 (0.1%)
2	Q9	0.33	0/1297	0.67	4/1750 (0.2%)
2	QJ	0.34	0/1297	0.69	1/1750 (0.1%)
2	R2	0.35	0/1297	0.49	0/1750
2	R3	0.45	0/1315	0.60	0/1774
2	R6	0.32	0/1297	0.49	0/1750
2	R7	0.28	0/1297	0.50	0/1750
2	R8	0.39	0/1303	0.55	1/1758 (0.1%)
2	RA	0.37	0/1303	0.54	1/1758 (0.1%)
2	RB	0.34	0/1297	0.51	0/1750
2	RD	0.41	0/1315	0.58	0/1774
2	RE	0.33	0/1309	0.56	0/1766
2	RF	0.34	0/1297	0.62	1/1750 (0.1%)
2	RG	0.36	0/1309	0.58	0/1766
2	RI	0.35	0/1297	0.49	0/1750
2	S1	0.34	0/1297	0.65	2/1750 (0.1%)
2	S4	0.33	0/1297	0.65	2/1750 (0.1%)
2	S9	0.34	0/1297	0.60	0/1750
2	SJ	0.36	0/1297	0.67	1/1750 (0.1%)
2	T2	0.33	0/1297	0.47	0/1750
2	T3	0.62	0/1315	0.65	0/1774

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	T6	0.36	0/1297	0.49	0/1750
2	T7	0.29	0/1297	0.50	0/1750
2	T8	0.40	0/1315	0.54	0/1774
2	TA	0.39	0/1315	0.55	0/1774
2	TB	0.37	0/1297	0.50	0/1750
2	TD	0.54	0/1315	0.62	0/1774
2	TE	0.35	0/1309	0.57	0/1766
2	TF	0.33	0/1297	0.62	0/1750
2	TG	0.37	0/1309	0.61	1/1766 (0.1%)
2	TI	0.33	0/1297	0.47	0/1750
2	U1	0.35	0/1309	0.62	0/1766
2	U4	0.33	0/1309	0.60	0/1766
2	U9	0.35	0/1309	0.66	0/1766
2	UJ	0.34	0/1309	0.65	1/1766 (0.1%)
2	V2	0.37	0/1297	0.48	0/1750
2	V3	0.37	0/1315	0.61	0/1774
2	V6	0.31	0/1309	0.53	2/1766 (0.1%)
2	V7	0.31	0/1309	0.53	0/1766
2	V8	0.38	0/1315	0.57	1/1774 (0.1%)
2	VA	0.37	0/1315	0.55	0/1774
2	VB	0.31	0/1309	0.55	2/1766 (0.1%)
2	VD	0.34	0/1315	0.57	0/1774
2	VE	0.32	0/1309	0.62	2/1766 (0.1%)
2	VF	0.33	0/1309	0.64	1/1766 (0.1%)
2	VG	0.34	0/1309	0.60	2/1766 (0.1%)
2	VI	0.38	0/1297	0.49	0/1750
2	W1	0.45	0/1297	0.69	1/1750 (0.1%)
2	W4	0.44	0/1297	0.66	2/1750 (0.1%)
2	W9	0.32	0/1297	0.70	4/1750 (0.2%)
2	WJ	0.33	0/1297	0.64	0/1750
2	X3	0.46	0/1315	0.60	0/1774
2	X8	0.43	0/1309	0.56	1/1766 (0.1%)
2	XA	0.41	0/1309	0.57	1/1766 (0.1%)
2	XD	0.41	0/1315	0.59	0/1774
2	XE	0.35	0/1315	0.64	1/1774 (0.1%)
2	XG	0.37	0/1315	0.62	0/1774
2	Y1	0.37	0/1297	0.64	1/1750 (0.1%)
2	Y2	0.32	0/1297	0.47	0/1750
2	Y4	0.38	0/1297	0.64	1/1750 (0.1%)
2	Y6	0.40	0/1297	0.49	0/1750
2	Y7	0.29	0/1297	0.52	0/1750
2	Y9	0.33	0/1297	0.62	0/1750
2	YB	0.41	0/1297	0.49	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	YF	0.32	0/1297	0.61	0/1750
2	YI	0.31	0/1297	0.47	0/1750
2	YJ	0.36	0/1297	0.66	0/1750
2	Z1	0.33	0/1065	0.55	0/1437
2	Z4	0.34	0/1065	0.59	0/1437
2	Z8	0.51	0/1315	0.55	0/1774
2	ZA	0.49	0/1315	0.55	0/1774
2	ZE	0.34	0/1315	0.69	2/1774 (0.1%)
2	ZG	0.33	0/1315	0.69	2/1774 (0.1%)
2	a1	0.30	0/1065	0.60	1/1437 (0.1%)
2	a2	0.37	0/1297	0.51	0/1750
2	a4	0.30	0/1065	0.64	1/1437 (0.1%)
2	a6	0.32	0/1297	0.48	0/1750
2	a7	0.28	0/1297	0.52	0/1750
2	aB	0.33	0/1297	0.49	0/1750
2	aF	0.32	0/1297	0.63	0/1750
2	aI	0.37	0/1297	0.52	0/1750
2	bE	0.31	0/1315	0.56	1/1774 (0.1%)
2	bG	0.33	0/1315	0.58	0/1774
2	c2	0.28	0/1297	0.50	0/1750
2	c6	0.30	0/1297	0.53	0/1750
2	c7	0.27	0/1297	0.50	0/1750
2	c8	0.30	0/1309	0.57	0/1766
2	cA	0.30	0/1309	0.56	0/1766
2	cB	0.30	0/1297	0.51	0/1750
2	cF	0.33	0/1297	0.60	1/1750 (0.1%)
2	cI	0.26	0/1297	0.46	0/1750
2	d1	0.32	0/1297	0.64	1/1750 (0.1%)
2	d4	0.32	0/1297	0.65	2/1750 (0.1%)
2	dE	0.33	0/1309	0.60	0/1766
2	dG	0.33	0/1309	0.63	2/1766 (0.1%)
2	e2	0.29	0/1297	0.48	0/1750
2	e6	0.28	0/1297	0.52	0/1750
2	e7	0.30	0/1297	0.55	0/1750
2	e8	0.38	0/1315	0.56	0/1774
2	eA	0.37	0/1315	0.56	1/1774 (0.1%)
2	eB	0.29	0/1297	0.53	0/1750
2	eF	0.34	0/1297	0.63	0/1750
2	eI	0.28	0/1297	0.48	0/1750
2	f1	0.32	0/1297	0.61	0/1750
2	f4	0.33	0/1297	0.65	1/1750 (0.1%)
2	fE	0.32	0/1309	0.64	3/1766 (0.2%)
2	fG	0.33	0/1309	0.61	0/1766

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	g2	0.26	0/1297	0.54	1/1750 (0.1%)
2	g6	0.29	0/1297	0.50	0/1750
2	g7	0.29	0/1297	0.53	0/1750
2	g8	0.30	0/1315	0.58	1/1774 (0.1%)
2	gA	0.31	0/1315	0.58	1/1774 (0.1%)
2	gB	0.30	0/1297	0.51	0/1750
2	gF	0.34	0/1297	0.62	0/1750
2	gI	0.27	0/1297	0.50	0/1750
2	h1	0.32	0/1297	0.60	2/1750 (0.1%)
2	h4	0.32	0/1297	0.62	0/1750
2	hE	0.32	0/1315	0.59	1/1774 (0.1%)
2	hG	0.32	0/1315	0.61	0/1774
2	i2	0.28	0/1303	0.49	0/1758
2	i6	0.29	0/1309	0.57	0/1766
2	i7	0.28	0/1309	0.56	0/1766
2	i8	0.33	0/1315	0.58	0/1774
2	iA	0.34	0/1315	0.56	0/1774
2	iB	0.29	0/1309	0.59	1/1766 (0.1%)
2	iF	0.34	0/1309	0.68	1/1766 (0.1%)
2	iI	0.28	0/1303	0.51	0/1758
2	j1	0.33	0/1303	0.67	3/1758 (0.2%)
2	j4	0.32	0/1303	0.66	1/1758 (0.1%)
2	jE	0.30	0/1315	0.56	0/1774
2	jG	0.32	0/1315	0.58	0/1774
2	k2	0.30	0/1297	0.50	0/1750
2	k6	0.30	0/1297	0.50	0/1750
2	k7	0.27	0/1297	0.51	0/1750
2	k8	0.32	0/1315	0.56	0/1774
2	kA	0.31	0/1315	0.56	0/1774
2	kB	0.30	0/1297	0.51	0/1750
2	kF	0.32	0/1297	0.64	1/1750 (0.1%)
2	kI	0.29	0/1297	0.52	0/1750
2	l1	0.32	0/1297	0.63	2/1750 (0.1%)
2	l4	0.31	0/1297	0.61	2/1750 (0.1%)
2	lE	0.32	0/1315	0.65	1/1774 (0.1%)
2	lG	0.32	0/1315	0.64	2/1774 (0.1%)
2	m2	0.28	0/1297	0.46	0/1750
2	m6	0.28	0/1297	0.56	0/1750
2	m7	0.28	0/1297	0.49	0/1750
2	m8	0.34	0/1315	0.56	0/1774
2	mA	0.34	0/1315	0.56	0/1774
2	mB	0.28	0/1297	0.56	1/1750 (0.1%)
2	mF	0.35	0/1297	0.68	2/1750 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	mI	0.27	0/1297	0.46	0/1750
2	n1	0.31	0/1297	0.62	0/1750
2	n4	0.31	0/1297	0.63	0/1750
2	nE	0.34	0/1315	0.68	1/1774 (0.1%)
2	nG	0.34	0/1315	0.62	2/1774 (0.1%)
2	pE	0.32	0/1315	0.63	0/1774
2	pG	0.31	0/1315	0.66	2/1774 (0.1%)
2	q1	0.33	0/1297	0.69	2/1750 (0.1%)
2	q4	0.32	0/1297	0.60	0/1750
2	rE	0.32	0/1315	0.62	1/1774 (0.1%)
2	rG	0.32	0/1315	0.66	2/1774 (0.1%)
2	s1	0.33	0/1297	0.66	3/1750 (0.2%)
2	s4	0.31	0/1297	0.67	3/1750 (0.2%)
2	tE	0.34	0/1309	0.67	2/1766 (0.1%)
2	tG	0.33	0/1309	0.65	0/1766
2	u1	0.34	0/1297	0.62	1/1750 (0.1%)
2	u4	0.33	0/1297	0.60	1/1750 (0.1%)
2	vE	0.32	0/1315	0.61	0/1774
2	vG	0.33	0/1315	0.67	2/1774 (0.1%)
2	w1	0.31	0/1309	0.64	1/1766 (0.1%)
2	w4	0.33	0/1309	0.67	3/1766 (0.2%)
2	y1	0.33	0/1297	0.68	2/1750 (0.1%)
2	y4	0.33	0/1297	0.66	0/1750
3	21	0.37	0/1877	0.63	0/2511
3	24	0.38	0/1877	0.60	1/2511 (0.0%)
3	M1	0.37	0/1877	0.66	2/2511 (0.1%)
3	M4	0.36	0/1877	0.63	3/2511 (0.1%)
4	b1	0.44	0/2539	0.71	2/3449 (0.1%)
4	b4	0.44	0/2539	0.69	1/3449 (0.0%)
4	o1	0.38	0/1679	0.75	1/2276 (0.0%)
4	o4	0.38	0/1679	0.74	2/2276 (0.1%)
5	31	0.45	0/2233	0.65	1/3024 (0.0%)
5	34	0.45	0/2233	0.62	1/3024 (0.0%)
6	X2	0.43	0/2585	0.58	1/3492 (0.0%)
6	X6	0.44	0/2585	0.59	0/3492
6	X7	0.32	0/2585	0.56	2/3492 (0.1%)
6	XB	0.45	0/2585	0.58	1/3492 (0.0%)
6	XF	0.37	0/2585	0.67	3/3492 (0.1%)
6	XI	0.43	0/2585	0.58	1/3492 (0.0%)
7	A2	0.30	0/2025	0.50	0/2722
7	A6	0.30	0/2025	0.50	0/2722
7	A7	0.29	0/2025	0.50	0/2722
7	A9	0.36	0/2017	0.59	0/2711

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	AB	0.30	0/2025	0.49	0/2722
7	AF	0.35	0/2025	0.59	0/2722
7	AI	0.30	0/2025	0.48	0/2722
7	AJ	0.36	0/2017	0.62	0/2711
7	Y3	0.36	0/1866	0.64	0/2506
7	YD	0.35	0/1866	0.58	0/2506
8	B2	0.48	0/1933	0.59	0/2614
8	B6	0.53	0/1941	0.63	2/2625 (0.1%)
8	B7	0.35	0/1917	0.53	0/2592
8	BB	0.53	0/1941	0.63	1/2625 (0.0%)
8	BF	0.40	0/1917	0.64	0/2592
8	BI	0.48	0/1933	0.59	0/2614
9	C2	0.42	0/1251	0.50	0/1699
9	C6	0.37	0/1251	0.48	0/1699
9	C7	0.27	0/1251	0.49	0/1699
9	CB	0.38	0/1251	0.47	0/1699
9	CF	0.31	0/1251	0.59	0/1699
9	CI	0.43	0/1251	0.52	1/1699 (0.1%)
9	E2	0.41	0/1251	0.49	0/1699
9	E6	0.43	0/1251	0.50	0/1699
9	E7	0.38	0/1251	0.49	0/1699
9	EB	0.45	0/1251	0.51	0/1699
9	EF	0.41	0/1251	0.59	0/1699
9	EI	0.41	0/1251	0.49	0/1699
9	G2	0.40	0/1251	0.48	0/1699
9	G6	0.51	0/1251	0.52	0/1699
9	G7	0.28	0/1251	0.47	0/1699
9	GB	0.53	0/1251	0.54	0/1699
9	GF	0.32	0/1251	0.58	1/1699 (0.1%)
9	GI	0.40	0/1251	0.48	0/1699
9	I2	0.41	0/1251	0.48	0/1699
9	I6	0.50	0/1251	0.52	0/1699
9	I7	0.40	0/1251	0.51	0/1699
9	IB	0.51	0/1251	0.52	0/1699
9	IF	0.42	0/1251	0.59	0/1699
9	II	0.41	0/1251	0.48	0/1699
9	K2	0.45	0/1251	0.48	0/1699
9	K6	0.40	0/1251	0.46	0/1699
9	K7	0.31	0/1251	0.50	1/1699 (0.1%)
9	KB	0.42	0/1251	0.46	0/1699
9	KF	0.36	0/1251	0.56	1/1699 (0.1%)
9	KI	0.45	0/1251	0.49	0/1699
9	M2	0.42	0/1251	0.49	0/1699

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	M6	0.48	0/1251	0.50	0/1699
9	M7	0.28	0/1251	0.48	1/1699 (0.1%)
9	MB	0.50	0/1251	0.51	0/1699
9	MF	0.31	0/1251	0.55	1/1699 (0.1%)
9	MI	0.41	0/1251	0.49	0/1699
10	D2	0.38	0/1274	0.51	0/1723
10	D6	0.42	0/1274	0.50	0/1723
10	D7	0.28	0/1274	0.50	0/1723
10	DB	0.43	0/1274	0.52	0/1723
10	DF	0.31	0/1274	0.61	0/1723
10	DI	0.38	0/1274	0.52	0/1723
10	F2	0.41	0/1274	0.50	0/1723
10	F6	0.38	0/1274	0.48	0/1723
10	F7	0.31	0/1274	0.46	0/1723
10	FB	0.38	0/1274	0.50	0/1723
10	FF	0.32	0/1274	0.52	0/1723
10	FI	0.41	0/1274	0.50	0/1723
10	H2	0.39	0/1274	0.54	1/1723 (0.1%)
10	H6	0.44	0/1274	0.52	0/1723
10	H7	0.31	0/1274	0.54	0/1723
10	HB	0.46	0/1274	0.52	0/1723
10	HF	0.37	0/1274	0.60	1/1723 (0.1%)
10	HI	0.39	0/1274	0.55	1/1723 (0.1%)
10	J2	0.42	0/1274	0.62	2/1723 (0.1%)
10	J6	0.58	0/1274	0.61	2/1723 (0.1%)
10	J7	0.31	0/1274	0.47	0/1723
10	JB	0.60	0/1274	0.59	1/1723 (0.1%)
10	JF	0.34	0/1274	0.56	0/1723
10	JI	0.41	0/1274	0.54	0/1723
10	L2	0.44	0/1274	0.57	0/1723
10	L6	0.47	0/1274	0.53	0/1723
10	L7	0.40	0/1274	0.53	0/1723
10	LB	0.48	0/1274	0.52	0/1723
10	LF	0.46	0/1274	0.67	1/1723 (0.1%)
10	LI	0.44	0/1274	0.57	0/1723
10	N2	0.43	0/1274	0.53	0/1723
10	N6	0.43	0/1274	0.52	0/1723
10	N7	0.29	0/1274	0.53	1/1723 (0.1%)
10	NB	0.45	0/1274	0.54	0/1723
10	NF	0.32	0/1274	0.62	3/1723 (0.2%)
10	NI	0.43	0/1274	0.52	0/1723
11	e3	0.51	0/1973	0.68	1/2657 (0.0%)
11	eD	0.47	0/1973	0.65	0/2657

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	b8	0.52	0/3022	0.59	0/4084
12	bA	0.51	0/3022	0.58	0/4084
13	A8	0.34	0/1843	0.54	1/2469 (0.0%)
13	AA	0.34	0/1843	0.54	1/2469 (0.0%)
13	wE	0.33	0/1843	0.55	0/2469
13	wG	0.33	0/1843	0.55	0/2469
13	xE	0.32	0/1843	0.57	0/2469
13	xG	0.33	0/1843	0.57	0/2469
14	B8	0.40	0/1932	0.50	0/2590
14	BA	0.38	0/1932	0.51	0/2590
14	yE	0.34	0/1932	0.58	0/2590
14	yG	0.36	0/1932	0.56	0/2590
15	d9	0.42	0/2242	0.64	0/3026
15	dJ	0.45	0/2242	0.70	1/3026 (0.0%)
16	zE	0.39	0/2964	0.59	0/4003
16	zG	0.43	0/2964	0.59	0/4003
17	AH	0.25	0/1241	0.38	0/1676
17	CH	0.26	0/1241	0.39	0/1676
17	EH	0.27	0/1241	0.38	0/1676
17	GH	0.27	0/1241	0.38	0/1676
17	JH	0.28	0/1241	0.39	0/1676
17	KH	0.25	0/1241	0.38	0/1676
17	NH	0.28	0/1241	0.40	0/1676
17	PH	0.30	0/1241	0.39	0/1676
17	RH	0.29	0/1241	0.39	0/1676
17	TH	0.30	0/1241	0.39	0/1676
17	cH	0.27	0/1241	0.38	0/1676
17	eH	0.25	0/1241	0.37	0/1676
17	gH	0.27	0/1241	0.38	0/1676
17	iH	0.27	0/1241	0.39	0/1676
17	lH	0.29	0/1241	0.39	0/1676
17	mH	0.25	0/1241	0.38	0/1676
17	pH	0.28	0/1241	0.39	0/1676
17	rH	0.30	0/1241	0.39	0/1676
17	tH	0.30	0/1241	0.40	0/1676
17	vH	0.30	0/1241	0.39	0/1676
18	BH	0.25	0/1226	0.38	0/1655
18	DH	0.28	0/1226	0.39	0/1655
18	FH	0.26	0/1226	0.38	0/1655
18	HH	0.25	0/1226	0.37	0/1655
18	IH	0.28	0/1226	0.40	0/1655
18	LH	0.29	0/1226	0.39	0/1655
18	MH	0.28	0/1226	0.40	0/1655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	OH	0.25	0/1226	0.37	0/1655
18	QH	0.31	0/1226	0.42	0/1655
18	SH	0.31	0/1226	0.40	0/1655
18	UH	0.31	0/1226	0.40	0/1655
18	dH	0.27	0/1226	0.40	0/1655
18	fH	0.26	0/1226	0.39	0/1655
18	hH	0.25	0/1226	0.39	0/1655
18	jH	0.26	0/1226	0.38	0/1655
18	kH	0.28	0/1226	0.40	0/1655
18	nH	0.27	0/1226	0.39	0/1655
18	oH	0.29	0/1226	0.41	0/1655
18	qH	0.25	0/1226	0.37	0/1655
18	sH	0.31	0/1226	0.41	0/1655
18	uH	0.30	0/1226	0.41	0/1655
18	wH	0.30	0/1226	0.41	0/1655
19	VH	0.25	0/1281	0.38	0/1731
19	xH	0.25	0/1281	0.41	0/1731
20	WH	0.26	0/1396	0.37	0/1886
20	yH	0.26	0/1396	0.37	0/1886
21	XH	0.26	0/732	0.41	0/981
21	zH	0.26	0/732	0.42	0/981
22	1H	0.29	0/6891	0.42	0/9305
22	YH	0.28	0/6891	0.42	0/9305
23	2H	0.27	0/1027	0.45	0/1399
23	ZH	0.27	0/1027	0.46	0/1399
24	3H	0.32	0/1940	0.46	0/2637
24	aH	0.31	0/1940	0.45	0/2637
25	4H	0.31	0/1569	0.44	0/2147
25	bH	0.30	0/1569	0.44	0/2147
All	All	0.36	0/954792	0.57	378/1290312 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C3	0	1
1	C8	0	2
1	EE	0	1
1	EG	0	1
1	G1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	ID	0	1
1	J5	0	1
1	MD	0	1
1	ME	0	1
1	X9	0	1
1	a8	0	1
1	cE	0	1
1	cG	0	1
1	f7	0	1
1	fF	0	2
1	i1	0	1
1	k1	0	1
1	kE	0	1
1	mG	0	2
1	r4	0	1
1	x1	0	1
1	x4	0	1
1	z1	0	1
2	BE	0	2
2	FE	0	1
2	I9	0	1
2	JA	0	1
2	L1	0	1
2	O9	0	1
2	OJ	0	2
2	TG	0	1
2	U9	0	1
2	VF	0	1
2	XA	0	1
2	XE	0	1
2	eA	0	1
2	mF	0	1
2	nG	0	1
2	q4	0	1
2	w4	0	1
3	21	0	1
4	b1	0	1
4	o1	0	1
4	o4	0	2
5	31	0	1
5	34	0	1
7	A2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	AB	0	1
7	Y3	0	1
8	BB	0	1
8	BF	0	1
10	D2	0	1
10	DB	0	1
10	DI	0	2
10	F2	0	1
10	H2	0	1
10	HB	0	1
10	HF	0	1
10	HI	0	1
10	J2	0	1
10	JB	0	1
10	JI	0	1
10	L2	0	1
10	L6	0	1
10	LI	0	1
10	N2	0	2
10	N6	0	1
10	NB	0	1
10	NI	0	1
12	b8	0	1
12	bA	0	3
13	wE	0	1
15	dJ	0	2
16	zE	0	3
16	zG	0	1
All	All	0	88

There are no bond length outliers.

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GG	78	LYS	CD-CE-NZ	18.17	153.50	111.70
1	mE	84	ARG	NE-CZ-NH2	-12.59	114.00	120.30
1	SE	78	LYS	CD-CE-NZ	12.05	139.42	111.70
2	S1	39	ASP	CB-CG-OD1	10.70	127.93	118.30
1	ff	137	ARG	NE-CZ-NH2	-10.59	115.00	120.30
1	CG	78	LYS	CD-CE-NZ	10.39	135.60	111.70
2	S4	39	ASP	CB-CG-OD1	10.29	127.56	118.30
1	mE	84	ARG	NE-CZ-NH1	10.24	125.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bF	137	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	IG	84	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	jF	137	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	d7	137	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	QG	78	LYS	CD-CE-NZ	9.94	134.56	111.70
1	SE	84	ARG	NE-CZ-NH2	-9.87	115.37	120.30
2	JA	39	ASP	CB-CG-OD1	9.61	126.95	118.30
1	IG	84	ARG	NE-CZ-NH2	-9.59	115.50	120.30
2	FE	39	ASP	CB-CG-OD2	-9.48	109.77	118.30
2	W1	39	ASP	CB-CG-OD1	9.42	126.78	118.30
1	QE	78	LYS	CD-CE-NZ	9.40	133.31	111.70
1	SE	84	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	SG	84	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	SG	84	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	jF	137	ARG	NE-CZ-NH1	8.61	124.61	120.30
2	W4	39	ASP	CB-CG-OD1	8.51	125.96	118.30
4	b1	239	LEU	CA-CB-CG	8.51	134.87	115.30
1	U7	137	ARG	NE-CZ-NH2	-8.48	116.06	120.30
2	BE	39	ASP	CB-CA-C	8.38	127.15	110.40
1	hF	137	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	bF	137	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	Y4	39	ASP	CB-CG-OD1	8.27	125.74	118.30
1	GG	84	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	j4	110	LEU	CA-CB-CG	8.26	134.30	115.30
1	UF	137	ARG	NE-CZ-NH2	-8.23	116.19	120.30
2	Q1	39	ASP	CB-CG-OD1	8.17	125.65	118.30
2	Y1	39	ASP	CB-CG-OD1	8.11	125.60	118.30
2	O1	39	ASP	CB-CG-OD1	8.05	125.54	118.30
2	a4	110	LEU	CA-CB-CG	8.00	133.71	115.30
9	CI	2	LYS	C-N-CA	7.95	141.57	121.70
1	d7	137	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	KE	78	LYS	CD-CE-NZ	7.84	129.74	111.70
8	BB	6	LEU	CA-CB-CG	7.79	133.22	115.30
1	GE	84	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	fF	137	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	IE	84	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	XE	39	ASP	CB-CG-OD2	-7.49	111.56	118.30
10	J2	77	ARG	NE-CZ-NH1	-7.39	116.60	120.30
2	ZG	3	ASP	CB-CG-OD1	7.37	124.94	118.30
6	XF	229	ALA	C-N-CA	7.34	140.05	121.70
9	GF	133	LEU	CA-CB-CG	7.34	132.19	115.30
2	Q4	39	ASP	CB-CG-OD1	7.28	124.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J2	77	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	UE	33	ARG	NE-CZ-NH1	7.22	123.91	120.30
2	L8	39	ASP	CB-CG-OD2	7.21	124.79	118.30
1	lF	156	LEU	CA-CB-CG	7.19	131.84	115.30
2	rE	97	LEU	CA-CB-CG	7.18	131.81	115.30
2	ZE	3	ASP	CB-CG-OD1	7.18	124.76	118.30
1	x1	105	LEU	CA-CB-CG	7.18	131.81	115.30
2	OJ	110	LEU	CA-CB-CG	7.18	131.80	115.30
2	QJ	88	ILE	CG1-CB-CG2	-7.16	95.64	111.40
2	I9	39	ASP	CB-CG-OD1	7.16	124.74	118.30
2	LA	39	ASP	CB-CG-OD2	7.12	124.71	118.30
2	O4	39	ASP	CB-CG-OD1	7.12	124.70	118.30
2	a1	110	LEU	CA-CB-CG	7.11	131.65	115.30
8	B6	6	LEU	CA-CB-CG	7.04	131.49	115.30
3	M1	112	LEU	CA-CB-CG	7.04	131.49	115.30
6	XF	117	LEU	CA-CB-CG	7.00	131.40	115.30
1	U7	137	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	r4	120	LEU	CA-CB-CG	6.96	131.32	115.30
2	mF	50	CYS	CA-CB-SG	6.95	126.51	114.00
2	pG	83	LEU	CA-CB-CG	6.93	131.24	115.30
1	c1	5	ILE	CG1-CB-CG2	-6.85	96.33	111.40
2	y1	110	LEU	CA-CB-CG	6.81	130.97	115.30
1	UE	33	ARG	CD-NE-CZ	6.79	133.11	123.60
3	M4	112	LEU	CA-CB-CG	6.79	130.91	115.30
2	d1	110	LEU	CA-CB-CG	6.78	130.90	115.30
1	IE	78	LYS	CD-CE-NZ	6.78	127.29	111.70
1	dF	138	LEU	CA-CB-CG	6.73	130.78	115.30
1	UG	84	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	dG	67	ILE	CG1-CB-CG2	-6.71	96.65	111.40
2	W9	90	LEU	CA-CB-CG	6.70	130.72	115.30
2	dG	24	LEU	CA-CB-CG	6.70	130.70	115.30
2	H8	157	ASP	CB-CG-OD1	6.69	124.33	118.30
1	UE	33	ARG	CG-CD-NE	6.69	125.86	111.80
1	QF	137	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	hF	137	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	IG	33	ARG	NE-CZ-NH1	-6.67	116.96	120.30
3	M1	110	LEU	CA-CB-CG	6.62	130.52	115.30
1	sE	138	LEU	CA-CB-CG	6.61	130.51	115.30
1	mE	84	ARG	CG-CD-NE	6.61	125.68	111.80
2	y1	105	LEU	CA-CB-CG	6.58	130.44	115.30
2	14	78	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	qE	38	LEU	CA-CB-CG	6.58	130.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CG	84	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	VG	3	ASP	CB-CG-OD1	6.55	124.20	118.30
1	lF	137	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	lF	120	LEU	CA-CB-CG	6.55	130.35	115.30
2	rG	120	LEU	CA-CB-CG	6.55	130.36	115.30
1	UF	137	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	f4	77	ARG	NE-CZ-NH1	-6.51	117.04	120.30
6	X7	208	LEU	CA-CB-CG	6.51	130.28	115.30
10	LF	3	ASP	CB-CG-OD1	6.50	124.15	118.30
2	lE	77	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	cE	78	LYS	CD-CE-NZ	6.46	126.56	111.70
1	C1	92	LEU	CA-CB-CG	6.46	130.15	115.30
6	XF	320	LEU	CA-CB-CG	6.44	130.10	115.30
2	VG	33	ASP	CB-CG-OD1	6.43	124.09	118.30
2	w4	110	LEU	CA-CB-CG	6.43	130.09	115.30
1	mE	38	LEU	CA-CB-CG	6.43	130.08	115.30
9	MF	19	LEU	CA-CB-CG	6.42	130.07	115.30
1	dF	44	LEU	CA-CB-CG	6.42	130.06	115.30
2	vG	101	ASP	CB-CG-OD1	6.41	124.07	118.30
1	O7	137	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	ZG	24	LEU	CA-CB-CG	6.37	129.95	115.30
1	UE	84	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	R4	66	LEU	CA-CB-CG	6.35	129.91	115.30
2	VE	33	ASP	CB-CG-OD1	6.34	124.00	118.30
2	DE	39	ASP	CB-CG-OD2	6.33	124.00	118.30
2	TG	39	ASP	OD1-CG-OD2	-6.30	111.32	123.30
2	VE	3	ASP	CB-CG-OD1	6.30	123.97	118.30
2	N3	39	ASP	CB-CG-OD2	6.29	123.96	118.30
2	S1	39	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	b7	137	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	FD	176	ILE	CG1-CB-CG2	-6.27	97.60	111.40
2	Q9	88	ILE	CG1-CB-CG2	-6.27	97.61	111.40
1	QE	137	ARG	CA-CB-CG	6.25	127.15	113.40
1	K3	27	ILE	CG1-CB-CG2	-6.24	97.66	111.40
2	s4	110	LEU	CA-CB-CG	6.23	129.64	115.30
1	hB	47	ASN	CB-CA-C	6.21	122.83	110.40
1	C3	131	ILE	CG1-CB-CG2	-6.21	97.73	111.40
1	WG	81	LYS	CD-CE-NZ	6.21	125.98	111.70
1	O3	85	ASP	CB-CG-OD2	6.20	123.88	118.30
1	t1	120	LEU	CA-CB-CG	6.20	129.56	115.30
1	lE	84	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	GD	44	LEU	CA-CB-CG	6.17	129.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	w1	90	LEU	CA-CB-CG	6.15	129.46	115.30
1	x1	122	LEU	CA-CB-CG	6.15	129.45	115.30
1	kE	157	ASP	CB-CG-OD1	6.13	123.82	118.30
1	lF	105	LEU	CA-CB-CG	6.13	129.40	115.30
1	g4	156	LEU	CA-CB-CG	6.11	129.36	115.30
1	I3	157	ASP	CB-CG-OD1	6.11	123.80	118.30
10	NF	84	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	C4	157	ASP	CB-CG-OD1	6.10	123.79	118.30
2	ZE	24	LEU	CA-CB-CG	6.09	129.30	115.30
1	uG	84	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	mE	163	LEU	CA-CB-CG	6.07	129.27	115.30
1	WF	137	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	UG	84	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	VJ	163	LEU	CA-CB-CG	6.05	129.21	115.30
2	l1	39	ASP	CB-CG-OD2	6.04	123.74	118.30
1	l8	27	ILE	CG1-CB-CG2	-6.04	98.12	111.40
1	GG	84	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	H1	2	LEU	CA-CB-CG	6.00	129.10	115.30
1	CG	84	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	g1	156	LEU	CA-CB-CG	5.98	129.06	115.30
2	lG	90	LEU	CA-CB-CG	5.98	129.06	115.30
2	mF	2	LEU	CA-CB-CG	5.98	129.05	115.30
1	OD	85	ASP	CB-CG-OD2	5.97	123.67	118.30
2	q1	113	LEU	CA-CB-CG	5.96	129.01	115.30
1	K1	142	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	VJ	110	ILE	CG1-CB-CG2	-5.95	98.32	111.40
2	J3	113	LEU	CA-CB-CG	5.94	128.97	115.30
2	B3	85	ASP	CB-CG-OD1	5.94	123.65	118.30
1	X9	122	LEU	CA-CB-CG	5.93	128.94	115.30
2	H4	120	LEU	CA-CB-CG	5.92	128.93	115.30
1	f7	137	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	l4	24	LEU	CA-CB-CG	5.92	128.91	115.30
2	D3	98	LEU	CA-CB-CG	5.91	128.90	115.30
10	JB	141	LEU	CB-CG-CD2	-5.90	100.97	111.00
2	h1	120	LEU	CA-CB-CG	5.88	128.82	115.30
10	NF	90	LEU	CA-CB-CG	5.87	128.81	115.30
2	OJ	24	LEU	CA-CB-CG	5.87	128.80	115.30
4	o4	114	LEU	CA-CB-CG	5.87	128.79	115.30
1	kE	24	LEU	CA-CB-CG	5.87	128.79	115.30
1	r1	120	LEU	CA-CB-CG	5.86	128.78	115.30
1	UE	84	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	sG	138	LEU	CA-CB-CG	5.85	128.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R1	66	LEU	CA-CB-CG	5.85	128.75	115.30
2	Q9	24	LEU	CA-CB-CG	5.85	128.75	115.30
1	KD	27	ILE	CG1-CB-CG2	-5.83	98.58	111.40
10	NF	84	ARG	NE-CZ-NH2	5.82	123.21	120.30
2	GJ	2	LEU	CA-CB-CG	5.82	128.68	115.30
5	34	284	LEU	CA-CB-CG	5.82	128.68	115.30
1	SF	137	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	GE	84	ARG	NE-CZ-NH2	-5.81	117.40	120.30
10	J6	141	LEU	CB-CG-CD2	-5.79	101.16	111.00
2	s4	31	ILE	CG1-CB-CG2	-5.78	98.70	111.40
1	jF	157	ASP	CB-CG-OD1	5.77	123.49	118.30
1	j7	137	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	JG	39	ASP	CB-CG-OD2	5.75	123.47	118.30
9	M7	19	LEU	CA-CB-CG	5.75	128.52	115.30
2	tE	105	LEU	CA-CB-CG	5.74	128.50	115.30
2	LG	129	ARG	CA-CB-CG	5.74	126.02	113.40
2	RF	128	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	g1	106	ASP	CB-CG-OD1	5.72	123.45	118.30
9	K7	111	LEU	CA-CB-CG	5.71	128.44	115.30
6	X7	320	LEU	CA-CB-CG	5.71	128.44	115.30
10	J6	75	THR	CA-CB-CG2	5.71	120.39	112.40
2	s4	90	LEU	CA-CB-CG	5.71	128.42	115.30
10	HI	77	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	qG	138	LEU	CA-CB-CG	5.70	128.41	115.30
3	M4	110	LEU	CA-CB-CG	5.69	128.38	115.30
1	V9	110	ILE	CG1-CB-CG2	-5.69	98.89	111.40
2	O9	24	LEU	CA-CB-CG	5.68	128.37	115.30
1	mE	13	ASP	CB-CG-OD1	5.68	123.41	118.30
2	vG	110	LEU	CA-CB-CG	5.67	128.34	115.30
1	SF	137	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	FE	39	ASP	CB-CA-C	5.66	121.72	110.40
1	EE	84	ARG	NE-CZ-NH2	-5.65	117.47	120.30
2	iF	105	LEU	CA-CB-CG	5.64	128.28	115.30
2	fE	24	LEU	CA-CB-CG	5.64	128.27	115.30
1	v1	137	ARG	CA-CB-CG	5.64	125.80	113.40
10	H2	77	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	fA	97	LEU	CA-CB-CG	5.63	128.24	115.30
1	TJ	97	LEU	CA-CB-CG	5.62	128.23	115.30
1	ED	24	LEU	CA-CB-CG	5.62	128.22	115.30
1	lF	24	LEU	CA-CB-CG	5.62	128.22	115.30
2	E9	39	ASP	CB-CG-OD2	5.62	123.35	118.30
2	EJ	39	ASP	CB-CG-OD2	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	w4	90	LEU	CA-CB-CG	5.61	128.20	115.30
1	m4	27	ILE	CG1-CB-CG2	-5.61	99.06	111.40
2	g8	83	LEU	CA-CB-CG	5.60	128.19	115.30
5	31	284	LEU	CA-CB-CG	5.59	128.17	115.30
1	b6	138	LEU	CA-CB-CG	5.58	128.13	115.30
2	gA	83	LEU	CA-CB-CG	5.57	128.12	115.30
2	g2	113	LEU	CA-CB-CG	5.57	128.10	115.30
1	mE	44	LEU	CA-CB-CG	5.56	128.10	115.30
1	sG	137	ARG	CG-CD-NE	5.56	123.48	111.80
1	I3	66	LEU	CA-CB-CG	5.56	128.09	115.30
2	D3	33	ASP	CB-CG-OD1	5.55	123.30	118.30
2	u1	24	LEU	CA-CB-CG	5.55	128.07	115.30
1	EG	84	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	FA	39	ASP	CB-CG-OD2	5.53	123.28	118.30
2	KJ	39	ASP	CB-CG-OD2	5.52	123.27	118.30
2	D4	110	LEU	CA-CB-CG	5.51	127.98	115.30
2	j1	77	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	s1	90	LEU	CA-CB-CG	5.51	127.97	115.30
1	v4	87	ASP	CB-CG-OD1	5.50	123.25	118.30
2	VB	39	ASP	CB-CG-OD2	5.50	123.25	118.30
2	nG	90	LEU	CA-CB-CG	5.49	127.92	115.30
2	Q9	98	LEU	CA-CB-CG	5.49	127.92	115.30
1	hF	120	LEU	CA-CB-CG	5.46	127.86	115.30
2	F8	39	ASP	CB-CG-OD2	5.46	123.21	118.30
2	14	88	ILE	CG1-CB-CG2	-5.46	99.40	111.40
1	GG	137	ARG	CB-CG-CD	5.46	125.78	111.60
1	mE	81	LYS	CD-CE-NZ	5.45	124.23	111.70
2	fE	39	ASP	CB-CG-OD1	5.44	123.20	118.30
6	XB	117	LEU	CA-CB-CG	5.44	127.81	115.30
2	VB	105	LEU	CA-CB-CG	5.44	127.81	115.30
1	N9	27	ILE	CG1-CB-CG2	-5.43	99.45	111.40
1	lF	137	ARG	NE-CZ-NH1	5.43	123.01	120.30
2	mB	2	LEU	CA-CB-CG	5.42	127.78	115.30
1	NJ	27	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	x4	105	LEU	CA-CB-CG	5.42	127.77	115.30
2	hE	105	LEU	CA-CB-CG	5.42	127.77	115.30
11	e3	192	ASP	CB-CG-OD1	5.42	123.18	118.30
2	nE	97	LEU	CA-CB-CG	5.41	127.75	115.30
2	rG	67	ILE	CG1-CB-CG2	-5.41	99.49	111.40
2	V6	105	LEU	CA-CB-CG	5.41	127.75	115.30
2	S4	39	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	S3	85	ASP	CB-CG-OD2	5.41	123.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QF	137	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	RA	83	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	GE	78	LYS	CB-CG-CD	-5.40	97.57	111.60
2	G9	2	LEU	CA-CB-CG	5.38	127.67	115.30
4	b1	259	LEU	CA-CB-CG	5.38	127.66	115.30
1	I4	38	LEU	CA-CB-CG	5.37	127.65	115.30
1	cE	38	LEU	CA-CB-CG	5.36	127.62	115.30
1	Q3	85	ASP	CB-CG-OD2	5.35	123.12	118.30
2	W9	120	LEU	CA-CB-CG	5.35	127.61	115.30
2	l4	39	ASP	CB-CG-OD2	5.35	123.11	118.30
2	I9	77	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	ID	66	LEU	CA-CB-CG	5.34	127.58	115.30
1	VJ	159	LEU	CA-CB-CG	5.33	127.56	115.30
2	L8	39	ASP	CB-CG-OD1	-5.33	113.50	118.30
2	H1	97	LEU	CA-CB-CG	5.32	127.55	115.30
9	KF	111	LEU	CA-CB-CG	5.32	127.54	115.30
1	G8	120	LEU	CA-CB-CG	5.30	127.49	115.30
1	h8	92	LEU	CA-CB-CG	5.29	127.47	115.30
1	TJ	44	LEU	CA-CB-CG	5.29	127.47	115.30
1	R9	163	LEU	CA-CB-CG	5.29	127.46	115.30
2	l1	24	LEU	CA-CB-CG	5.28	127.45	115.30
2	PF	39	ASP	CB-CG-OD2	5.28	123.05	118.30
1	p1	97	LEU	CA-CB-CG	5.28	127.43	115.30
1	lF	92	LEU	CA-CB-CG	5.28	127.44	115.30
2	SJ	24	LEU	CA-CB-CG	5.28	127.44	115.30
2	LA	39	ASP	CB-CG-OD1	-5.27	113.55	118.30
1	f8	97	LEU	CA-CB-CG	5.27	127.42	115.30
2	UJ	113	LEU	CA-CB-CG	5.27	127.41	115.30
1	kE	92	LEU	CA-CB-CG	5.26	127.41	115.30
1	iG	38	LEU	CA-CB-CG	5.26	127.41	115.30
8	B6	222	LEU	CA-CB-CG	5.26	127.40	115.30
2	H3	98	LEU	CA-CB-CG	5.25	127.39	115.30
1	IG	81	LYS	CD-CE-NZ	5.25	123.78	111.70
2	X8	39	ASP	CB-CG-OD2	5.25	123.02	118.30
1	GA	120	LEU	CA-CB-CG	5.24	127.36	115.30
2	fE	39	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	RJ	38	LEU	CA-CB-CG	5.24	127.36	115.30
4	o4	106	PHE	C-N-CA	5.24	134.80	121.70
2	nG	97	LEU	CA-CB-CG	5.24	127.35	115.30
10	N7	84	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	K1	24	LEU	CA-CB-CG	5.23	127.34	115.30
2	FE	170	ASP	CB-CG-OD1	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	WG	84	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	j1	110	LEU	CA-CB-CG	5.23	127.33	115.30
2	JG	33	ASP	CB-CG-OD1	5.23	123.00	118.30
2	s1	31	ILE	CG1-CB-CG2	-5.22	99.91	111.40
3	24	153	MET	CA-CB-CG	5.22	122.17	113.30
2	bE	105	LEU	CA-CB-CG	5.21	127.29	115.30
2	LG	129	ARG	CB-CG-CD	5.21	125.15	111.60
2	pG	2	LEU	CA-CB-CG	5.21	127.28	115.30
1	j8	156	LEU	CA-CB-CG	5.21	127.28	115.30
1	mE	84	ARG	CD-NE-CZ	5.21	130.89	123.60
1	N1	85	ASP	CB-CG-OD2	5.20	122.98	118.30
2	XA	39	ASP	CB-CG-OD2	5.20	122.98	118.30
2	iB	110	LEU	CA-CB-CG	5.19	127.24	115.30
2	V6	39	ASP	CB-CG-OD2	5.19	122.97	118.30
1	Q7	137	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	s1	66	LEU	CA-CB-CG	5.19	127.23	115.30
1	eG	156	LEU	CA-CB-CG	5.19	127.23	115.30
2	O4	83	LEU	CA-CB-CG	5.18	127.22	115.30
4	b4	277	GLY	C-N-CA	5.18	134.65	121.70
2	11	105	LEU	CA-CB-CG	5.18	127.21	115.30
2	BG	24	LEU	CA-CB-CG	5.18	127.20	115.30
13	AA	48	MET	CA-CB-CG	5.17	122.08	113.30
2	L1	24	LEU	CA-CB-CG	5.16	127.17	115.30
2	h1	109	CYS	CA-CB-SG	5.16	123.30	114.00
2	d4	110	LEU	CA-CB-CG	5.16	127.16	115.30
2	lG	110	LEU	CA-CB-CG	5.16	127.16	115.30
1	g1	120	LEU	CA-CB-CG	5.15	127.15	115.30
2	H1	39	ASP	CB-CG-OD2	5.15	122.94	118.30
2	eA	39	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	X4	85	ASP	CB-CG-OD2	5.14	122.93	118.30
2	d4	39	ASP	CB-CG-OD2	5.14	122.93	118.30
10	HF	19	LEU	CA-CB-CG	5.14	127.12	115.30
1	AG	84	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	Q9	113	LEU	CA-CB-CG	5.13	127.10	115.30
1	UF	131	ILE	CG1-CB-CG2	-5.12	100.12	111.40
2	D1	110	LEU	CA-CB-CG	5.12	127.07	115.30
3	M4	162	LEU	CA-CB-CG	5.12	127.07	115.30
2	MJ	33	ASP	CB-CG-OD1	5.12	122.90	118.30
2	D8	3	ASP	CB-CG-OD1	5.11	122.90	118.30
13	A8	48	MET	CA-CB-CG	5.11	121.99	113.30
1	N4	85	ASP	CB-CG-OD2	5.11	122.90	118.30
2	W4	85	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IA	157	ASP	CB-CG-OD1	5.11	122.90	118.30
1	v1	87	ASP	CB-CG-OD1	5.10	122.89	118.30
2	I9	39	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	cG	38	LEU	CA-CB-CG	5.10	127.03	115.30
15	dJ	232	VAL	C-N-CA	5.10	134.45	121.70
1	h7	137	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	iG	67	LYS	C-N-CA	5.09	134.43	121.70
2	cF	2	LEU	CA-CB-CG	5.09	127.01	115.30
6	XI	323	ALA	C-N-CA	5.09	134.41	121.70
4	o1	72	ARG	CA-CB-CG	5.08	124.59	113.40
2	u4	82	CYS	CA-CB-SG	5.08	123.15	114.00
2	NA	85	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	t1	24	LEU	CA-CB-CG	5.08	126.97	115.30
2	q1	120	LEU	CA-CB-CG	5.07	126.97	115.30
6	X2	323	ALA	C-N-CA	5.07	134.37	121.70
1	m4	44	LEU	CA-CB-CG	5.06	126.94	115.30
2	j1	105	LEU	CA-CB-CG	5.05	126.91	115.30
2	VF	67	ILE	CG1-CB-CG2	-5.05	100.30	111.40
2	D3	83	LEU	CA-CB-CG	5.04	126.89	115.30
1	GG	137	ARG	CG-CD-NE	-5.03	101.23	111.80
2	R8	83	LEU	CB-CG-CD2	-5.03	102.45	111.00
2	W9	83	LEU	CA-CB-CG	5.03	126.86	115.30
2	w4	24	LEU	CA-CB-CG	5.03	126.86	115.30
2	F3	176	ILE	CG1-CB-CG2	-5.02	100.35	111.40
2	V8	39	ASP	CB-CG-OD2	5.02	122.82	118.30
2	W9	157	ASP	CB-CG-OD1	5.02	122.82	118.30
2	D4	24	LEU	CA-CB-CG	5.01	126.83	115.30
2	tE	98	LEU	CA-CB-CG	5.01	126.83	115.30
2	kF	50	CYS	CA-CB-SG	5.01	123.01	114.00
1	EG	78	LYS	CD-CE-NZ	5.01	123.22	111.70
1	WF	137	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	I1	38	LEU	CA-CB-CG	5.00	126.80	115.30
2	PF	170	ASP	CB-CG-OD1	5.00	122.80	118.30
1	WG	84	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	21	244	GLN	Peptide
5	31	210	GLY	Peptide
5	34	210	GLY	Peptide

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Mol	Chain	Res	Type	Group
7	A2	151	GLU	Peptide
7	AB	212	TYR	Peptide
8	BB	20	PHE	Peptide
2	BE	39	ASP	Sidechain,Peptide
8	BF	29	TYR	Peptide
1	C3	34	SER	Peptide
1	C8	136	ASP	Peptide
1	C8	157	ASP	Peptide
10	D2	74	TYR	Peptide
10	DB	74	TYR	Peptide
10	DI	33	GLU	Peptide
10	DI	74	TYR	Peptide
1	EE	71	GLU	Peptide
1	EG	71	GLU	Peptide
10	F2	74	TYR	Peptide
2	FE	39	ASP	Sidechain
1	G1	159	LEU	Peptide
10	H2	74	TYR	Peptide
10	HB	74	TYR	Peptide
10	HF	38	LEU	Peptide
10	HI	74	TYR	Peptide
2	I9	39	ASP	Sidechain
1	ID	94	ASN	Peptide
10	J2	74	TYR	Peptide
1	J5	139	CYS	Peptide
2	JA	39	ASP	Peptide
10	JB	74	TYR	Peptide
10	JI	74	TYR	Peptide
2	L1	13	ASP	Peptide
10	L2	74	TYR	Peptide
10	L6	74	TYR	Peptide
10	LI	74	TYR	Peptide
1	MD	140	VAL	Peptide
1	ME	42	GLU	Peptide
10	N2	33	GLU	Peptide
10	N2	74	TYR	Peptide
10	N6	74	TYR	Peptide
10	NB	74	TYR	Peptide
10	NI	74	TYR	Peptide
2	O9	76	ASN	Peptide
2	OJ	134	MET	Peptide
2	OJ	39	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	TG	39	ASP	Sidechain
2	U9	83	LEU	Peptide
2	VF	27	LEU	Peptide
1	X9	157	ASP	Peptide
2	XA	54	ASP	Sidechain
2	XE	39	ASP	Sidechain
7	Y3	56	THR	Peptide
1	a8	27	ILE	Peptide
4	b1	340	ALA	Peptide
12	b8	202	THR	Peptide
12	bA	202	THR	Peptide
12	bA	271	TRP	Peptide
12	bA	400	LYS	Peptide
1	cE	33	ARG	Peptide
1	cG	122	LEU	Peptide
15	dJ	232	VAL	Peptide
15	dJ	237	GLY	Peptide
2	eA	39	ASP	Sidechain
1	f7	140	VAL	Peptide
1	fF	140	VAL	Peptide
1	fF	34	SER	Peptide
1	i1	138	LEU	Peptide
1	k1	140	VAL	Peptide
1	kE	16	GLY	Peptide
2	mF	147	THR	Peptide
1	mG	136	ASP	Peptide
1	mG	29	GLY	Peptide
2	nG	158	CYS	Peptide
4	o1	118	GLU	Peptide
4	o4	115	THR	Peptide
4	o4	228	ASN	Peptide
2	q4	109	CYS	Peptide
1	r4	30	ASN	Peptide
2	w4	85	ASP	Peptide
13	wE	44	PHE	Peptide
1	x1	57	ASP	Peptide
1	x4	139	CYS	Peptide
1	z1	141	PRO	Peptide
16	zE	214	GLY	Peptide
16	zE	217	ALA	Peptide
16	zE	243	SER	Peptide
16	zG	217	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	A3	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	A4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	AD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	AE	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	AG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	B9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	BJ	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	C1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	C3	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	C4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	C8	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	CA	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	CD	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	CE	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	CG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	D9	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	DJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	E1	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	E3	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	E4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	EA	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	ED	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	EE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	EG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	F9	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	FJ	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	G1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	G3	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	G4	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	G8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	GA	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	GD	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	GE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	GG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	H9	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	HJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	I1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	I3	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	I4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	I8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	IA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	ID	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	IE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	IG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	J5	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	J9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	JC	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	JJ	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	K1	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	K3	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	K8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	KA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	KD	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	KE	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	KG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	L9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	LJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	M3	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	M8	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	MA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	MD	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	ME	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	MG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	N1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	N4	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	N9	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	NJ	162/164 (99%)	142 (88%)	20 (12%)	0	100	100
1	O2	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	O3	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	O6	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	O7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	O8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	OA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	OB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	OD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	OE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	OF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	OG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	OI	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	P1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	P9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	PJ	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	Q2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	Q3	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	Q6	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	Q7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	Q8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	QA	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	QB	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	QD	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	QE	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	QF	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	QG	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	QI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	R1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	R4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	R9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	RJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	S2	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	S3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	S6	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	S7	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	S8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	SA	162/164 (99%)	147 (91%)	15 (9%)	0	100	100
1	SB	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	SD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	SE	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	SF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	SG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	SI	162/164 (99%)	155 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	T4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	T9	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	TJ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	U2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	U3	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	U6	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	U7	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	U8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	UA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	UB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	UD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	UE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	UF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	UG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	UI	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	V1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	V4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	V9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	VJ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	W2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	W3	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	W6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	W7	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	W8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	WA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	WB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	WD	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	WE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	WF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	WG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WI	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	X1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	X4	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	X9	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	XJ	162/164 (99%)	145 (90%)	17 (10%)	0	100	100
1	Y8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	YA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	YE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	YG	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	Z2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	Z6	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	Z7	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	ZB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	ZF	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	ZI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	a8	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	aA	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	aE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	aG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	b2	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	b6	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	b7	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	bB	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	bF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	bI	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	c1	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	c4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	cE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	cG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	d2	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	d6	162/164 (99%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d7	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	d8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	dA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	dB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	dF	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	dI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	e1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	e4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	eE	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	eG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	f2	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	f6	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	f7	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	f8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	fA	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	fB	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	fF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	fI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	g1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	g4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	gE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	gG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	h2	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	h6	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	h7	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	h8	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	hA	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	hB	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	hF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	hI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	i1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	iE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	iG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	j2	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	j6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	j7	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	j8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	jA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	jB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	jF	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	jI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	k1	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	k4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	kE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	kG	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	l2	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	l6	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	l7	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	l8	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	lA	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	lB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	lF	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	lI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	m1	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	m4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	mE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	mG	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
1	oE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	oG	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
1	p1	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	p4	162/164 (99%)	147 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	qE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	qG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	r1	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	r4	162/164 (99%)	147 (91%)	15 (9%)	0	100	100
1	sE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	sG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	t1	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	t4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	uE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	uG	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	v1	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	v4	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	x1	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	x4	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	z1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	z4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
2	11	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	14	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	A5	143/177 (81%)	133 (93%)	10 (7%)	0	100	100
2	AC	143/177 (81%)	131 (92%)	12 (8%)	0	100	100
2	B1	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	B3	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	B4	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	B5	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	BC	143/177 (81%)	131 (92%)	11 (8%)	1 (1%)	22	53
2	BD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	BE	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	BG	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	C5	143/177 (81%)	139 (97%)	4 (3%)	0	100	100
2	C9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	CC	143/177 (81%)	132 (92%)	10 (7%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	D1	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	D3	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	D4	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	D8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	DA	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	DD	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	DE	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	DG	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	E9	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	EJ	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	F1	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	F3	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	F4	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	F5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	F8	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	FA	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	FC	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	FD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	FE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	FG	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	G5	143/177 (81%)	133 (93%)	10 (7%)	0	100	100
2	G9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	GC	143/177 (81%)	137 (96%)	6 (4%)	0	100	100
2	GJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	H1	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	H3	176/177 (99%)	169 (96%)	7 (4%)	0	100	100
2	H4	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	H5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	H8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	HA	177/177 (100%)	167 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	HC	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	HD	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	HE	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	HG	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	I5	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	I9	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	IC	173/177 (98%)	167 (96%)	6 (4%)	0	100	100
2	IJ	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	J1	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	J3	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	J4	174/177 (98%)	164 (94%)	9 (5%)	1 (1%)	25	56
2	J8	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	JA	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	JD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	JE	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	JG	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	K5	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	K9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	KC	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	KJ	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	L1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	L3	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	L4	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	L5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	L8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	LA	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	LC	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	LD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	LE	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	LG	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	M9	174/177 (98%)	168 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	MJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	N3	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	N8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	NA	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	ND	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	NE	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	NG	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	O1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	O4	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	O9	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	OJ	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	P2	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	P3	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	P6	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	P7	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	P8	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	PA	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	PB	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	PD	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	PE	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	PF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	PG	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	PI	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	Q1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	Q4	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	Q9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	QJ	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	R2	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	R3	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	R6	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	R7	174/177 (98%)	167 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R8	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
2	RA	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	RB	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	RD	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	RE	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	RF	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	RG	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	RI	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	S1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	S4	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	S9	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	SJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	T2	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	T3	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	T6	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	T7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	T8	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	TA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	TB	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	TD	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	TE	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	TF	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	TG	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	TI	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	U1	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	U4	176/177 (99%)	166 (94%)	10 (6%)	0	100	100
2	U9	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	UJ	176/177 (99%)	166 (94%)	10 (6%)	0	100	100
2	V2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	V3	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	V6	176/177 (99%)	170 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V7	176/177 (99%)	168 (96%)	8 (4%)	0	100	100
2	V8	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	VA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	VB	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	VD	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	VE	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	VF	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	VG	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	VI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	W1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	W4	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	W9	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	WJ	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	X3	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	X8	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	XA	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	XD	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	XE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	XG	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	Y1	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	Y2	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	Y4	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	Y6	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	Y7	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	Y9	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	YB	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	YF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	YI	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	YJ	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	Z1	143/177 (81%)	138 (96%)	5 (4%)	0	100	100
2	Z4	143/177 (81%)	137 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z8	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	ZA	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	ZE	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	ZG	177/177 (100%)	168 (95%)	8 (4%)	1 (1%)	25	56
2	a1	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	a2	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	a4	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	a6	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	a7	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	aB	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	aF	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	aI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	bE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	bG	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	c2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	c6	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	c7	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	c8	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	cA	176/177 (99%)	168 (96%)	8 (4%)	0	100	100
2	cB	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	cF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	cI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	d1	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
2	d4	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	dE	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	dG	176/177 (99%)	169 (96%)	7 (4%)	0	100	100
2	e2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	e6	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	e7	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	e8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	eA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	eB	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	eF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	eI	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	f1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	f4	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	fE	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	fG	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	g2	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	g6	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	g7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	g8	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	gA	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	gB	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	gF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	gI	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	h1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	h4	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	hE	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	hG	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	i2	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	i6	176/177 (99%)	161 (92%)	15 (8%)	0	100	100
2	i7	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	i8	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	iA	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	iB	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	iF	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
2	iI	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
2	j1	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	j4	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
2	jE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	jG	177/177 (100%)	173 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	k2	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	k6	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	k7	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	k8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	kA	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	kB	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	kF	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	kI	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	l1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	l4	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	lE	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	lG	177/177 (100%)	160 (90%)	17 (10%)	0	100	100
2	m2	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	m6	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	m7	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	m8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	mA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	mB	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	mF	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	mI	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	n1	174/177 (98%)	163 (94%)	10 (6%)	1 (1%)	25	56
2	n4	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
2	nE	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	nG	177/177 (100%)	164 (93%)	13 (7%)	0	100	100
2	pE	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	pG	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	q1	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	q4	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	rE	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	rG	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	s1	174/177 (98%)	158 (91%)	16 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	s4	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
2	tE	176/177 (99%)	168 (96%)	8 (4%)	0	100	100
2	tG	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	u1	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	u4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
2	vE	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	vG	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	w1	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	w4	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	y1	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	y4	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
3	21	236/333 (71%)	209 (89%)	27 (11%)	0	100	100
3	24	236/333 (71%)	216 (92%)	20 (8%)	0	100	100
3	M1	236/333 (71%)	209 (89%)	25 (11%)	2 (1%)	19	49
3	M4	236/333 (71%)	211 (89%)	25 (11%)	0	100	100
4	b1	321/405 (79%)	274 (85%)	44 (14%)	3 (1%)	17	46
4	b4	321/405 (79%)	276 (86%)	43 (13%)	2 (1%)	25	56
4	o1	210/405 (52%)	177 (84%)	32 (15%)	1 (0%)	29	61
4	o4	210/405 (52%)	179 (85%)	29 (14%)	2 (1%)	15	44
5	31	283/288 (98%)	264 (93%)	17 (6%)	2 (1%)	22	53
5	34	283/288 (98%)	260 (92%)	21 (7%)	2 (1%)	22	53
6	X2	322/363 (89%)	291 (90%)	31 (10%)	0	100	100
6	X6	322/363 (89%)	282 (88%)	40 (12%)	0	100	100
6	X7	322/363 (89%)	295 (92%)	26 (8%)	1 (0%)	41	72
6	XB	322/363 (89%)	280 (87%)	42 (13%)	0	100	100
6	XF	322/363 (89%)	295 (92%)	27 (8%)	0	100	100
6	XI	322/363 (89%)	290 (90%)	32 (10%)	0	100	100
7	A2	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
7	A6	255/290 (88%)	235 (92%)	20 (8%)	0	100	100
7	A7	255/290 (88%)	233 (91%)	22 (9%)	0	100	100
7	A9	254/290 (88%)	231 (91%)	23 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AB	255/290 (88%)	225 (88%)	30 (12%)	0	100	100
7	AF	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
7	AI	255/290 (88%)	238 (93%)	17 (7%)	0	100	100
7	AJ	254/290 (88%)	229 (90%)	25 (10%)	0	100	100
7	Y3	235/290 (81%)	216 (92%)	18 (8%)	1 (0%)	34	66
7	YD	235/290 (81%)	216 (92%)	19 (8%)	0	100	100
8	B2	228/232 (98%)	204 (90%)	23 (10%)	1 (0%)	34	66
8	B6	229/232 (99%)	209 (91%)	20 (9%)	0	100	100
8	B7	225/232 (97%)	199 (88%)	25 (11%)	1 (0%)	34	66
8	BB	229/232 (99%)	209 (91%)	20 (9%)	0	100	100
8	BF	225/232 (97%)	202 (90%)	22 (10%)	1 (0%)	34	66
8	BI	228/232 (98%)	207 (91%)	20 (9%)	1 (0%)	34	66
9	C2	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	C6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	C7	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
9	CB	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	CF	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
9	CI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	E2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	E6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	E7	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	EB	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	EF	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	EI	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	G2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	G6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	G7	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	GB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	GF	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	GI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
9	I2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I6	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	I7	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
9	IB	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	IF	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
9	II	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
9	K2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	K6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	K7	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
9	KB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	KF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	KI	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	M2	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	M6	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	M7	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	MB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	MF	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	MI	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
10	D2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	D6	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	56
10	D7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	DB	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
10	DF	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
10	DI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	F2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	F6	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
10	F7	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	FB	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	FF	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	FI	169/172 (98%)	158 (94%)	9 (5%)	2 (1%)	13	39
10	H2	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
10	H6	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H7	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	HB	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	HF	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	HI	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	J2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	J6	169/172 (98%)	164 (97%)	3 (2%)	2 (1%)	13	39
10	J7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	JB	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	JF	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	JI	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
10	L2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	L6	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	L7	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	LB	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
10	LF	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	LI	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	N2	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	N6	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	N7	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	NB	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	NF	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	NI	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
11	e3	246/303 (81%)	226 (92%)	20 (8%)	0	100	100
11	eD	246/303 (81%)	222 (90%)	24 (10%)	0	100	100
12	b8	378/490 (77%)	334 (88%)	39 (10%)	5 (1%)	12	36
12	bA	378/490 (77%)	334 (88%)	44 (12%)	0	100	100
13	A8	236/273 (86%)	217 (92%)	19 (8%)	0	100	100
13	AA	236/273 (86%)	218 (92%)	18 (8%)	0	100	100
13	wE	236/273 (86%)	223 (94%)	13 (6%)	0	100	100
13	wG	236/273 (86%)	223 (94%)	13 (6%)	0	100	100
13	xE	236/273 (86%)	221 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	xG	236/273 (86%)	221 (94%)	15 (6%)	0	100	100
14	B8	248/290 (86%)	234 (94%)	14 (6%)	0	100	100
14	BA	248/290 (86%)	235 (95%)	13 (5%)	0	100	100
14	yE	248/290 (86%)	239 (96%)	9 (4%)	0	100	100
14	yG	248/290 (86%)	237 (96%)	11 (4%)	0	100	100
15	d9	283/342 (83%)	250 (88%)	32 (11%)	1 (0%)	34	66
15	dJ	283/342 (83%)	241 (85%)	40 (14%)	2 (1%)	22	53
16	zE	368/498 (74%)	335 (91%)	33 (9%)	0	100	100
16	zG	368/498 (74%)	341 (93%)	27 (7%)	0	100	100
17	AH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	CH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	EH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	GH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	JH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	KH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	NH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	PH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	RH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	TH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
17	cH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	eH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	gH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	iH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	lH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	mH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	pH	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
17	rH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	tH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	vH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	BH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	DH	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	FH	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	25	56
18	HH	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	25	56
18	IH	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	56
18	LH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
18	MH	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
18	OH	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	25	56
18	QH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	SH	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
18	UH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	dH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	fH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	hH	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	25	56
18	jH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	kH	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
18	nH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
18	oH	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
18	qH	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	56
18	sH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	uH	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
18	wH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
19	VH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
19	xH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
20	WH	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
20	yH	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
21	XH	90/93 (97%)	86 (96%)	4 (4%)	0	100	100
21	zH	90/93 (97%)	86 (96%)	4 (4%)	0	100	100
22	1H	840/879 (96%)	785 (94%)	55 (6%)	0	100	100
22	YH	840/879 (96%)	787 (94%)	53 (6%)	0	100	100
23	2H	130/159 (82%)	122 (94%)	8 (6%)	0	100	100
23	ZH	130/159 (82%)	122 (94%)	8 (6%)	0	100	100
24	3H	251/288 (87%)	235 (94%)	15 (6%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	aH	251/288 (87%)	234 (93%)	17 (7%)	0	100	100
25	4H	204/253 (81%)	187 (92%)	17 (8%)	0	100	100
25	bH	204/253 (81%)	188 (92%)	16 (8%)	0	100	100
All	All	124066/129014 (96%)	117523 (95%)	6496 (5%)	47 (0%)	100	100

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	31	132	SER
7	Y3	57	VAL
2	J4	16	ALA
4	b4	302	CYS
2	BC	74	TYR
18	FH	72	MET
4	b1	337	MET
4	b1	341	ALA
4	o1	224	LYS
4	b4	343	MET
4	o4	249	GLY
10	D6	76	SER
10	H6	76	SER
10	J6	76	SER
2	ZG	73	CYS
18	IH	72	MET
10	FI	76	SER
3	M1	97	PHE
4	b1	344	LEU
12	b8	312	SER
15	d9	278	LYS
2	n1	73	CYS
5	31	108	GLY
8	B2	191	LYS
4	o4	246	VAL
5	34	164	GLY
12	b8	336	SER
12	b8	349	LYS
18	HH	72	MET
18	OH	72	MET
24	3H	276	PRO
15	dJ	278	LYS
10	J6	75	THR

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Mol	Chain	Res	Type
6	X7	117	LEU
12	b8	350	VAL
8	BF	201	SER
8	B7	201	SER
12	b8	334	GLY
18	DH	72	MET
18	hH	72	MET
18	qH	72	MET
10	FI	75	THR
5	34	5	PRO
15	dJ	281	VAL
2	CC	69	PRO
8	BI	230	PRO
3	M1	99	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A1	128/128 (100%)	127 (99%)	1 (1%)	81 94
1	A3	128/128 (100%)	127 (99%)	1 (1%)	81 94
1	A4	128/128 (100%)	126 (98%)	2 (2%)	62 88
1	AD	128/128 (100%)	126 (98%)	2 (2%)	62 88
1	AE	128/128 (100%)	128 (100%)	0	100 100
1	AG	128/128 (100%)	128 (100%)	0	100 100
1	B9	128/128 (100%)	126 (98%)	2 (2%)	62 88
1	BJ	128/128 (100%)	128 (100%)	0	100 100
1	C1	128/128 (100%)	128 (100%)	0	100 100
1	C3	128/128 (100%)	128 (100%)	0	100 100
1	C4	128/128 (100%)	128 (100%)	0	100 100
1	C8	128/128 (100%)	127 (99%)	1 (1%)	81 94
1	CA	128/128 (100%)	128 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	128/128 (100%)	128 (100%)	0	100	100
1	CE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	CG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	D9	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	DJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	E1	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	E3	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	E4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	E8	128/128 (100%)	128 (100%)	0	100	100
1	EA	128/128 (100%)	128 (100%)	0	100	100
1	ED	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	EE	128/128 (100%)	128 (100%)	0	100	100
1	EG	128/128 (100%)	128 (100%)	0	100	100
1	F9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	FJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	G1	128/128 (100%)	122 (95%)	6 (5%)	26	59
1	G3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	G4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	G8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	GA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	GD	128/128 (100%)	128 (100%)	0	100	100
1	GE	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	GG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	H9	128/128 (100%)	128 (100%)	0	100	100
1	HJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	I1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	I3	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	I4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	I8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	IA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	ID	128/128 (100%)	127 (99%)	1 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	IG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	J5	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	J9	128/128 (100%)	128 (100%)	0	100	100
1	JC	128/128 (100%)	128 (100%)	0	100	100
1	JJ	128/128 (100%)	128 (100%)	0	100	100
1	K1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	K3	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	K4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	K8	128/128 (100%)	128 (100%)	0	100	100
1	KA	128/128 (100%)	128 (100%)	0	100	100
1	KD	128/128 (100%)	128 (100%)	0	100	100
1	KE	128/128 (100%)	128 (100%)	0	100	100
1	KG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	L9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	LJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	M3	128/128 (100%)	128 (100%)	0	100	100
1	M8	128/128 (100%)	128 (100%)	0	100	100
1	MA	128/128 (100%)	128 (100%)	0	100	100
1	MD	128/128 (100%)	128 (100%)	0	100	100
1	ME	128/128 (100%)	128 (100%)	0	100	100
1	MG	128/128 (100%)	128 (100%)	0	100	100
1	N1	128/128 (100%)	128 (100%)	0	100	100
1	N4	128/128 (100%)	128 (100%)	0	100	100
1	N9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	NJ	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	O2	128/128 (100%)	128 (100%)	0	100	100
1	O3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	O6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	O7	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	O8	128/128 (100%)	127 (99%)	1 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	OA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	OB	128/128 (100%)	128 (100%)	0	100	100
1	OD	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	OE	128/128 (100%)	128 (100%)	0	100	100
1	OF	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	OG	128/128 (100%)	128 (100%)	0	100	100
1	OI	128/128 (100%)	128 (100%)	0	100	100
1	P1	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	P4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	P9	128/128 (100%)	128 (100%)	0	100	100
1	PJ	128/128 (100%)	128 (100%)	0	100	100
1	Q2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	Q3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	Q6	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	Q7	128/128 (100%)	128 (100%)	0	100	100
1	Q8	128/128 (100%)	128 (100%)	0	100	100
1	QA	128/128 (100%)	128 (100%)	0	100	100
1	QB	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	QD	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	QE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	QF	128/128 (100%)	128 (100%)	0	100	100
1	QG	128/128 (100%)	128 (100%)	0	100	100
1	QI	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	R1	128/128 (100%)	128 (100%)	0	100	100
1	R4	128/128 (100%)	128 (100%)	0	100	100
1	R9	128/128 (100%)	128 (100%)	0	100	100
1	RJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	S2	128/128 (100%)	128 (100%)	0	100	100
1	S3	128/128 (100%)	128 (100%)	0	100	100
1	S6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	S7	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	SA	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	SB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	SD	128/128 (100%)	128 (100%)	0	100	100
1	SE	128/128 (100%)	128 (100%)	0	100	100
1	SF	128/128 (100%)	128 (100%)	0	100	100
1	SG	128/128 (100%)	128 (100%)	0	100	100
1	SI	128/128 (100%)	128 (100%)	0	100	100
1	T1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	T4	128/128 (100%)	128 (100%)	0	100	100
1	T9	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	TJ	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	U2	128/128 (100%)	128 (100%)	0	100	100
1	U3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	U6	128/128 (100%)	128 (100%)	0	100	100
1	U7	128/128 (100%)	128 (100%)	0	100	100
1	U8	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	UA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	UB	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	UD	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	UE	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	UF	128/128 (100%)	128 (100%)	0	100	100
1	UG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	UI	128/128 (100%)	128 (100%)	0	100	100
1	V1	128/128 (100%)	128 (100%)	0	100	100
1	V4	128/128 (100%)	128 (100%)	0	100	100
1	V9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	VJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	W2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	W3	128/128 (100%)	128 (100%)	0	100	100
1	W6	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W7	128/128 (100%)	128 (100%)	0	100	100
1	W8	128/128 (100%)	128 (100%)	0	100	100
1	WA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	WB	128/128 (100%)	128 (100%)	0	100	100
1	WD	128/128 (100%)	128 (100%)	0	100	100
1	WE	128/128 (100%)	128 (100%)	0	100	100
1	WF	128/128 (100%)	128 (100%)	0	100	100
1	WG	128/128 (100%)	128 (100%)	0	100	100
1	WI	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	X1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	X4	128/128 (100%)	128 (100%)	0	100	100
1	X9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	XJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	Y8	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	YA	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	YE	128/128 (100%)	128 (100%)	0	100	100
1	YG	128/128 (100%)	128 (100%)	0	100	100
1	Z2	128/128 (100%)	128 (100%)	0	100	100
1	Z6	128/128 (100%)	128 (100%)	0	100	100
1	Z7	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	ZB	128/128 (100%)	128 (100%)	0	100	100
1	ZF	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	ZI	128/128 (100%)	128 (100%)	0	100	100
1	a8	128/128 (100%)	128 (100%)	0	100	100
1	aA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	aE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	aG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	b2	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	b6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	b7	128/128 (100%)	128 (100%)	0	100	100
1	bB	128/128 (100%)	127 (99%)	1 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bF	128/128 (100%)	128 (100%)	0	100	100
1	bI	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	c1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	c4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	cE	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	cG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	d2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	d6	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	d7	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	d8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	dA	128/128 (100%)	128 (100%)	0	100	100
1	dB	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	dF	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	dI	128/128 (100%)	128 (100%)	0	100	100
1	e1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	e4	128/128 (100%)	128 (100%)	0	100	100
1	eE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	eG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	f2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	f6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	f7	128/128 (100%)	128 (100%)	0	100	100
1	f8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	fA	128/128 (100%)	128 (100%)	0	100	100
1	fB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	fF	128/128 (100%)	128 (100%)	0	100	100
1	fI	128/128 (100%)	128 (100%)	0	100	100
1	g1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	g4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	gE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	gG	128/128 (100%)	128 (100%)	0	100	100
1	h2	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	h7	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	h8	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	hA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	hB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	hF	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	hI	128/128 (100%)	128 (100%)	0	100	100
1	i1	128/128 (100%)	128 (100%)	0	100	100
1	i4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	iE	128/128 (100%)	128 (100%)	0	100	100
1	iG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	j2	128/128 (100%)	128 (100%)	0	100	100
1	j6	128/128 (100%)	128 (100%)	0	100	100
1	j7	128/128 (100%)	128 (100%)	0	100	100
1	j8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	jA	128/128 (100%)	128 (100%)	0	100	100
1	jB	128/128 (100%)	128 (100%)	0	100	100
1	jF	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	jI	128/128 (100%)	128 (100%)	0	100	100
1	k1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	k4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	kE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	kG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	l2	128/128 (100%)	128 (100%)	0	100	100
1	l6	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	l7	128/128 (100%)	128 (100%)	0	100	100
1	l8	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	lA	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	lB	128/128 (100%)	128 (100%)	0	100	100
1	lF	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	lI	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	m4	128/128 (100%)	128 (100%)	0	100	100
1	mE	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	mG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	oE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	oG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	p1	128/128 (100%)	128 (100%)	0	100	100
1	p4	128/128 (100%)	128 (100%)	0	100	100
1	qE	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	qG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	r1	128/128 (100%)	124 (97%)	4 (3%)	40	74
1	r4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	sE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	sG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	t1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	t4	128/128 (100%)	128 (100%)	0	100	100
1	uE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	uG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	v1	128/128 (100%)	128 (100%)	0	100	100
1	v4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	x1	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	x4	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	z1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	z4	128/128 (100%)	126 (98%)	2 (2%)	62	88
2	11	137/137 (100%)	137 (100%)	0	100	100
2	14	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	A5	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	AC	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	B1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	B3	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	B4	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B5	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	BC	113/137 (82%)	101 (89%)	12 (11%)	6	20
2	BD	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	BE	138/137 (101%)	137 (99%)	1 (1%)	84	95
2	BG	138/137 (101%)	138 (100%)	0	100	100
2	C5	113/137 (82%)	113 (100%)	0	100	100
2	C9	137/137 (100%)	137 (100%)	0	100	100
2	CC	113/137 (82%)	110 (97%)	3 (3%)	44	78
2	CJ	137/137 (100%)	137 (100%)	0	100	100
2	D1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	D3	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	D4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	D8	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	DA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	DD	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	DE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	DG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	E9	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	EJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	F1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	F3	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	F4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	F5	113/137 (82%)	113 (100%)	0	100	100
2	F8	140/137 (102%)	140 (100%)	0	100	100
2	FA	140/137 (102%)	140 (100%)	0	100	100
2	FC	113/137 (82%)	113 (100%)	0	100	100
2	FD	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	FE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	FG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	G5	113/137 (82%)	110 (97%)	3 (3%)	44	78
2	G9	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	GC	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	GJ	137/137 (100%)	137 (100%)	0	100	100
2	H1	138/137 (101%)	138 (100%)	0	100	100
2	H3	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	H4	139/137 (102%)	139 (100%)	0	100	100
2	H5	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	H8	140/137 (102%)	140 (100%)	0	100	100
2	HA	140/137 (102%)	140 (100%)	0	100	100
2	HC	113/137 (82%)	113 (100%)	0	100	100
2	HD	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	HE	140/137 (102%)	140 (100%)	0	100	100
2	HG	140/137 (102%)	140 (100%)	0	100	100
2	I5	137/137 (100%)	132 (96%)	5 (4%)	35	69
2	I9	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	IC	136/137 (99%)	136 (100%)	0	100	100
2	IJ	139/137 (102%)	139 (100%)	0	100	100
2	J1	137/137 (100%)	137 (100%)	0	100	100
2	J3	137/137 (100%)	137 (100%)	0	100	100
2	J4	137/137 (100%)	137 (100%)	0	100	100
2	J8	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	JA	139/137 (102%)	139 (100%)	0	100	100
2	JD	137/137 (100%)	137 (100%)	0	100	100
2	JE	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	JG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	K5	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	K9	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	KC	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	KJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	L1	137/137 (100%)	137 (100%)	0	100	100
2	L3	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	L4	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L5	113/137 (82%)	104 (92%)	9 (8%)	12	34
2	L8	140/137 (102%)	140 (100%)	0	100	100
2	LA	140/137 (102%)	140 (100%)	0	100	100
2	LC	113/137 (82%)	107 (95%)	6 (5%)	22	54
2	LD	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	LE	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	LG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	M9	137/137 (100%)	137 (100%)	0	100	100
2	MJ	137/137 (100%)	137 (100%)	0	100	100
2	N3	140/137 (102%)	140 (100%)	0	100	100
2	N8	140/137 (102%)	134 (96%)	6 (4%)	29	62
2	NA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	ND	140/137 (102%)	140 (100%)	0	100	100
2	NE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	NG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	O1	137/137 (100%)	137 (100%)	0	100	100
2	O4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	O9	137/137 (100%)	137 (100%)	0	100	100
2	OJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	P2	137/137 (100%)	137 (100%)	0	100	100
2	P3	140/137 (102%)	136 (97%)	4 (3%)	42	76
2	P6	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	P7	137/137 (100%)	137 (100%)	0	100	100
2	P8	137/137 (100%)	137 (100%)	0	100	100
2	PA	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	PB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	PD	140/137 (102%)	135 (96%)	5 (4%)	35	69
2	PE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	PF	137/137 (100%)	137 (100%)	0	100	100
2	PG	140/137 (102%)	140 (100%)	0	100	100
2	PI	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q1	137/137 (100%)	137 (100%)	0	100	100
2	Q4	137/137 (100%)	137 (100%)	0	100	100
2	Q9	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	QJ	137/137 (100%)	137 (100%)	0	100	100
2	R2	137/137 (100%)	137 (100%)	0	100	100
2	R3	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	R6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	R7	137/137 (100%)	137 (100%)	0	100	100
2	R8	138/137 (101%)	138 (100%)	0	100	100
2	RA	138/137 (101%)	137 (99%)	1 (1%)	84	95
2	RB	137/137 (100%)	137 (100%)	0	100	100
2	RD	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	RE	139/137 (102%)	135 (97%)	4 (3%)	42	76
2	RF	137/137 (100%)	137 (100%)	0	100	100
2	RG	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	RI	137/137 (100%)	137 (100%)	0	100	100
2	S1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	S4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	S9	137/137 (100%)	137 (100%)	0	100	100
2	SJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	T2	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	T3	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	T6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	T7	137/137 (100%)	137 (100%)	0	100	100
2	T8	140/137 (102%)	140 (100%)	0	100	100
2	TA	140/137 (102%)	140 (100%)	0	100	100
2	TB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	TD	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	TE	139/137 (102%)	139 (100%)	0	100	100
2	TF	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	TG	139/137 (102%)	138 (99%)	1 (1%)	84	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	TI	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	U1	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	U4	139/137 (102%)	139 (100%)	0	100	100
2	U9	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	UJ	139/137 (102%)	139 (100%)	0	100	100
2	V2	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	V3	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	V6	139/137 (102%)	139 (100%)	0	100	100
2	V7	139/137 (102%)	135 (97%)	4 (3%)	42	76
2	V8	140/137 (102%)	140 (100%)	0	100	100
2	VA	140/137 (102%)	140 (100%)	0	100	100
2	VB	139/137 (102%)	139 (100%)	0	100	100
2	VD	140/137 (102%)	140 (100%)	0	100	100
2	VE	139/137 (102%)	136 (98%)	3 (2%)	52	83
2	VF	139/137 (102%)	139 (100%)	0	100	100
2	VG	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	VI	137/137 (100%)	132 (96%)	5 (4%)	35	69
2	W1	137/137 (100%)	137 (100%)	0	100	100
2	W4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	W9	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	WJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	X3	140/137 (102%)	140 (100%)	0	100	100
2	X8	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	XA	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	XD	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	XE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	XG	140/137 (102%)	140 (100%)	0	100	100
2	Y1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	Y2	137/137 (100%)	137 (100%)	0	100	100
2	Y4	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	Y6	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	Y9	137/137 (100%)	137 (100%)	0	100	100
2	YB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	YF	137/137 (100%)	137 (100%)	0	100	100
2	YI	137/137 (100%)	137 (100%)	0	100	100
2	YJ	137/137 (100%)	137 (100%)	0	100	100
2	Z1	113/137 (82%)	113 (100%)	0	100	100
2	Z4	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	Z8	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	ZA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	ZE	140/137 (102%)	140 (100%)	0	100	100
2	ZG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	a1	113/137 (82%)	113 (100%)	0	100	100
2	a2	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	a4	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	a6	137/137 (100%)	137 (100%)	0	100	100
2	a7	137/137 (100%)	137 (100%)	0	100	100
2	aB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	aF	137/137 (100%)	137 (100%)	0	100	100
2	aI	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	bE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	bG	140/137 (102%)	140 (100%)	0	100	100
2	c2	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	c6	137/137 (100%)	137 (100%)	0	100	100
2	c7	137/137 (100%)	137 (100%)	0	100	100
2	c8	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	cA	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	cB	137/137 (100%)	137 (100%)	0	100	100
2	cF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	cI	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	d1	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d4	137/137 (100%)	137 (100%)	0	100	100
2	dE	139/137 (102%)	139 (100%)	0	100	100
2	dG	139/137 (102%)	139 (100%)	0	100	100
2	e2	137/137 (100%)	137 (100%)	0	100	100
2	e6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	e7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	e8	140/137 (102%)	140 (100%)	0	100	100
2	eA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	eB	137/137 (100%)	137 (100%)	0	100	100
2	eF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	eI	137/137 (100%)	137 (100%)	0	100	100
2	f1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	f4	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	fE	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	fG	139/137 (102%)	139 (100%)	0	100	100
2	g2	137/137 (100%)	137 (100%)	0	100	100
2	g6	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	g7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	g8	140/137 (102%)	140 (100%)	0	100	100
2	gA	140/137 (102%)	140 (100%)	0	100	100
2	gB	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	gF	137/137 (100%)	137 (100%)	0	100	100
2	gI	137/137 (100%)	137 (100%)	0	100	100
2	h1	137/137 (100%)	137 (100%)	0	100	100
2	h4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	hE	140/137 (102%)	140 (100%)	0	100	100
2	hG	140/137 (102%)	140 (100%)	0	100	100
2	i2	138/137 (101%)	138 (100%)	0	100	100
2	i6	139/137 (102%)	139 (100%)	0	100	100
2	i7	139/137 (102%)	139 (100%)	0	100	100
2	i8	140/137 (102%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	iA	140/137 (102%)	140 (100%)	0	100	100
2	iB	139/137 (102%)	139 (100%)	0	100	100
2	iF	139/137 (102%)	135 (97%)	4 (3%)	42	76
2	iI	138/137 (101%)	138 (100%)	0	100	100
2	j1	138/137 (101%)	136 (99%)	2 (1%)	67	90
2	j4	138/137 (101%)	138 (100%)	0	100	100
2	jE	140/137 (102%)	140 (100%)	0	100	100
2	jG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	k2	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	k6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	k7	137/137 (100%)	137 (100%)	0	100	100
2	k8	140/137 (102%)	140 (100%)	0	100	100
2	kA	140/137 (102%)	140 (100%)	0	100	100
2	kB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	kF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	kI	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	l1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	l4	137/137 (100%)	137 (100%)	0	100	100
2	lE	140/137 (102%)	140 (100%)	0	100	100
2	lG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	m2	137/137 (100%)	137 (100%)	0	100	100
2	m6	137/137 (100%)	137 (100%)	0	100	100
2	m7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	m8	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	mA	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	mB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	mF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	mI	137/137 (100%)	137 (100%)	0	100	100
2	n1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	n4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	nE	140/137 (102%)	139 (99%)	1 (1%)	84	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	nG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	pE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	pG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	q1	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	q4	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	rE	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	rG	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	s1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	s4	137/137 (100%)	137 (100%)	0	100	100
2	tE	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	tG	139/137 (102%)	139 (100%)	0	100	100
2	u1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	u4	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	vE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	vG	140/137 (102%)	140 (100%)	0	100	100
2	w1	139/137 (102%)	139 (100%)	0	100	100
2	w4	139/137 (102%)	139 (100%)	0	100	100
2	y1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	y4	137/137 (100%)	136 (99%)	1 (1%)	84	95
3	21	183/262 (70%)	171 (93%)	12 (7%)	16	44
3	24	183/262 (70%)	174 (95%)	9 (5%)	25	57
3	M1	183/262 (70%)	177 (97%)	6 (3%)	38	72
3	M4	183/262 (70%)	177 (97%)	6 (3%)	38	72
4	b1	268/331 (81%)	254 (95%)	14 (5%)	23	55
4	b4	268/331 (81%)	254 (95%)	14 (5%)	23	55
4	o1	176/331 (53%)	172 (98%)	4 (2%)	50	82
4	o4	176/331 (53%)	169 (96%)	7 (4%)	31	65
5	31	227/229 (99%)	221 (97%)	6 (3%)	46	79
5	34	227/229 (99%)	221 (97%)	6 (3%)	46	79
6	X2	261/289 (90%)	259 (99%)	2 (1%)	81	94
6	X6	261/289 (90%)	255 (98%)	6 (2%)	50	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	X7	261/289 (90%)	260 (100%)	1 (0%)	91	97
6	XB	261/289 (90%)	258 (99%)	3 (1%)	73	92
6	XF	261/289 (90%)	260 (100%)	1 (0%)	91	97
6	XI	261/289 (90%)	256 (98%)	5 (2%)	57	85
7	A2	199/222 (90%)	199 (100%)	0	100	100
7	A6	199/222 (90%)	198 (100%)	1 (0%)	88	96
7	A7	199/222 (90%)	197 (99%)	2 (1%)	76	93
7	A9	198/222 (89%)	194 (98%)	4 (2%)	55	84
7	AB	199/222 (90%)	199 (100%)	0	100	100
7	AF	199/222 (90%)	196 (98%)	3 (2%)	65	89
7	AI	199/222 (90%)	199 (100%)	0	100	100
7	AJ	198/222 (89%)	196 (99%)	2 (1%)	76	93
7	Y3	182/222 (82%)	180 (99%)	2 (1%)	73	92
7	YD	182/222 (82%)	179 (98%)	3 (2%)	62	88
8	B2	209/211 (99%)	202 (97%)	7 (3%)	38	72
8	B6	210/211 (100%)	206 (98%)	4 (2%)	57	85
8	B7	208/211 (99%)	206 (99%)	2 (1%)	76	93
8	BB	210/211 (100%)	202 (96%)	8 (4%)	33	67
8	BF	208/211 (99%)	206 (99%)	2 (1%)	76	93
8	BI	209/211 (99%)	200 (96%)	9 (4%)	29	62
9	C2	125/125 (100%)	125 (100%)	0	100	100
9	C6	125/125 (100%)	125 (100%)	0	100	100
9	C7	125/125 (100%)	125 (100%)	0	100	100
9	CB	125/125 (100%)	125 (100%)	0	100	100
9	CF	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	CI	125/125 (100%)	125 (100%)	0	100	100
9	E2	125/125 (100%)	125 (100%)	0	100	100
9	E6	125/125 (100%)	125 (100%)	0	100	100
9	E7	125/125 (100%)	125 (100%)	0	100	100
9	EB	125/125 (100%)	125 (100%)	0	100	100
9	EF	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	EI	125/125 (100%)	125 (100%)	0	100	100
9	G2	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	G6	125/125 (100%)	125 (100%)	0	100	100
9	G7	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	GB	125/125 (100%)	125 (100%)	0	100	100
9	GF	125/125 (100%)	125 (100%)	0	100	100
9	GI	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	I2	125/125 (100%)	125 (100%)	0	100	100
9	I6	125/125 (100%)	125 (100%)	0	100	100
9	I7	125/125 (100%)	123 (98%)	2 (2%)	62	88
9	IB	125/125 (100%)	125 (100%)	0	100	100
9	IF	125/125 (100%)	125 (100%)	0	100	100
9	II	125/125 (100%)	125 (100%)	0	100	100
9	K2	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	K6	125/125 (100%)	125 (100%)	0	100	100
9	K7	125/125 (100%)	125 (100%)	0	100	100
9	KB	125/125 (100%)	125 (100%)	0	100	100
9	KF	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	KI	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	M2	125/125 (100%)	123 (98%)	2 (2%)	62	88
9	M6	125/125 (100%)	125 (100%)	0	100	100
9	M7	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	MB	125/125 (100%)	125 (100%)	0	100	100
9	MF	125/125 (100%)	125 (100%)	0	100	100
9	MI	125/125 (100%)	123 (98%)	2 (2%)	62	88
10	D2	134/134 (100%)	134 (100%)	0	100	100
10	D6	134/134 (100%)	134 (100%)	0	100	100
10	D7	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	DB	134/134 (100%)	134 (100%)	0	100	100
10	DF	134/134 (100%)	134 (100%)	0	100	100
10	DI	134/134 (100%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	F2	134/134 (100%)	134 (100%)	0	100	100
10	F6	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	F7	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	FB	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	FF	134/134 (100%)	134 (100%)	0	100	100
10	FI	134/134 (100%)	134 (100%)	0	100	100
10	H2	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	H6	134/134 (100%)	134 (100%)	0	100	100
10	H7	134/134 (100%)	134 (100%)	0	100	100
10	HB	134/134 (100%)	134 (100%)	0	100	100
10	HF	134/134 (100%)	134 (100%)	0	100	100
10	HI	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	J2	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	J6	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	J7	134/134 (100%)	131 (98%)	3 (2%)	52	83
10	JB	134/134 (100%)	134 (100%)	0	100	100
10	JF	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	JI	134/134 (100%)	134 (100%)	0	100	100
10	L2	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	L6	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	L7	134/134 (100%)	134 (100%)	0	100	100
10	LB	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	LF	134/134 (100%)	134 (100%)	0	100	100
10	LI	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	N2	134/134 (100%)	134 (100%)	0	100	100
10	N6	134/134 (100%)	134 (100%)	0	100	100
10	N7	134/134 (100%)	134 (100%)	0	100	100
10	NB	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	NF	134/134 (100%)	134 (100%)	0	100	100
10	NI	134/134 (100%)	133 (99%)	1 (1%)	84	95
11	e3	204/237 (86%)	204 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	eD	204/237 (86%)	204 (100%)	0	100	100
12	b8	304/389 (78%)	291 (96%)	13 (4%)	29	62
12	bA	304/389 (78%)	293 (96%)	11 (4%)	35	69
13	A8	179/203 (88%)	177 (99%)	2 (1%)	73	92
13	AA	179/203 (88%)	179 (100%)	0	100	100
13	wE	179/203 (88%)	175 (98%)	4 (2%)	52	83
13	wG	179/203 (88%)	178 (99%)	1 (1%)	86	96
13	xE	179/203 (88%)	177 (99%)	2 (1%)	73	92
13	xG	179/203 (88%)	178 (99%)	1 (1%)	86	96
14	B8	188/218 (86%)	188 (100%)	0	100	100
14	BA	188/218 (86%)	188 (100%)	0	100	100
14	yE	188/218 (86%)	187 (100%)	1 (0%)	88	96
14	yG	188/218 (86%)	187 (100%)	1 (0%)	88	96
15	d9	238/278 (86%)	225 (94%)	13 (6%)	21	52
15	dJ	238/278 (86%)	229 (96%)	9 (4%)	33	67
16	zE	303/406 (75%)	301 (99%)	2 (1%)	84	95
16	zG	303/406 (75%)	302 (100%)	1 (0%)	92	98
17	AH	130/131 (99%)	130 (100%)	0	100	100
17	CH	130/131 (99%)	130 (100%)	0	100	100
17	EH	130/131 (99%)	130 (100%)	0	100	100
17	GH	130/131 (99%)	130 (100%)	0	100	100
17	JH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	KH	130/131 (99%)	130 (100%)	0	100	100
17	NH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	PH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	RH	130/131 (99%)	130 (100%)	0	100	100
17	TH	130/131 (99%)	130 (100%)	0	100	100
17	cH	130/131 (99%)	130 (100%)	0	100	100
17	eH	130/131 (99%)	130 (100%)	0	100	100
17	gH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	iH	130/131 (99%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	lH	130/131 (99%)	128 (98%)	2 (2%)	65	89
17	mH	130/131 (99%)	130 (100%)	0	100	100
17	pH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	rH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	tH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	vH	130/131 (99%)	130 (100%)	0	100	100
18	BH	124/124 (100%)	123 (99%)	1 (1%)	81	94
18	DH	124/124 (100%)	124 (100%)	0	100	100
18	FH	124/124 (100%)	124 (100%)	0	100	100
18	HH	124/124 (100%)	124 (100%)	0	100	100
18	IH	124/124 (100%)	124 (100%)	0	100	100
18	LH	124/124 (100%)	123 (99%)	1 (1%)	81	94
18	MH	124/124 (100%)	122 (98%)	2 (2%)	62	88
18	OH	124/124 (100%)	124 (100%)	0	100	100
18	QH	124/124 (100%)	124 (100%)	0	100	100
18	SH	124/124 (100%)	124 (100%)	0	100	100
18	UH	124/124 (100%)	124 (100%)	0	100	100
18	dH	124/124 (100%)	124 (100%)	0	100	100
18	fH	124/124 (100%)	124 (100%)	0	100	100
18	hH	124/124 (100%)	124 (100%)	0	100	100
18	jH	124/124 (100%)	124 (100%)	0	100	100
18	kH	124/124 (100%)	123 (99%)	1 (1%)	81	94
18	nH	124/124 (100%)	124 (100%)	0	100	100
18	oH	124/124 (100%)	119 (96%)	5 (4%)	31	65
18	qH	124/124 (100%)	124 (100%)	0	100	100
18	sH	124/124 (100%)	124 (100%)	0	100	100
18	uH	124/124 (100%)	124 (100%)	0	100	100
18	wH	124/124 (100%)	124 (100%)	0	100	100
19	VH	133/136 (98%)	133 (100%)	0	100	100
19	xH	133/136 (98%)	133 (100%)	0	100	100
20	WH	147/153 (96%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	yH	147/153 (96%)	147 (100%)	0	100	100
21	XH	78/79 (99%)	78 (100%)	0	100	100
21	zH	78/79 (99%)	78 (100%)	0	100	100
22	1H	742/772 (96%)	737 (99%)	5 (1%)	84	95
22	YH	742/772 (96%)	737 (99%)	5 (1%)	84	95
23	2H	106/121 (88%)	106 (100%)	0	100	100
23	ZH	106/121 (88%)	106 (100%)	0	100	100
24	3H	194/214 (91%)	186 (96%)	8 (4%)	30	64
24	aH	194/214 (91%)	187 (96%)	7 (4%)	35	69
25	4H	165/199 (83%)	161 (98%)	4 (2%)	49	81
25	bH	165/199 (83%)	161 (98%)	4 (2%)	49	81
All	All	98470/100830 (98%)	97640 (99%)	830 (1%)	82	94

All (830) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	140	VAL
2	B1	45	VAL
2	D1	36	LYS
2	D1	77	ARG
1	E1	82	CYS
1	E1	140	VAL
2	F1	39	ASP
1	G1	137	ARG
1	G1	142	ARG
1	G1	143	ASP
1	G1	144	MET
1	G1	147	GLN
1	G1	151	GLU
1	I1	140	VAL
1	K1	53	LYS
3	M1	97	PHE
3	M1	100	THR
3	M1	101	LEU
3	M1	111	ARG
3	M1	117	ARG
3	M1	142	THR
1	P1	134	THR

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Mol	Chain	Res	Type
1	P1	140	VAL
2	S1	145	THR
1	T1	140	VAL
2	U1	61	CYS
2	U1	62	GLU
1	X1	137	ARG
2	Y1	19	VAL
2	Y1	75	THR
4	b1	72	ARG
4	b1	93	TYR
4	b1	116	VAL
4	b1	271	GLU
4	b1	300	SER
4	b1	301	LEU
4	b1	302	CYS
4	b1	303	SER
4	b1	305	ASP
4	b1	333	ILE
4	b1	336	ASP
4	b1	342	GLN
4	b1	343	MET
4	b1	344	LEU
1	c1	144	MET
1	e1	17	ARG
2	f1	108	ARG
2	f1	135	LYS
1	g1	144	MET
2	j1	77	ARG
2	j1	143	THR
1	k1	144	MET
2	l1	77	ARG
1	m1	140	VAL
2	n1	169	PHE
4	o1	72	ARG
4	o1	117	ARG
4	o1	244	ILE
4	o1	247	MET
2	q1	82	CYS
2	q1	120	LEU
2	q1	145	THR
1	r1	82	CYS
1	r1	102	THR

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Mol	Chain	Res	Type
1	r1	114	ARG
1	r1	140	VAL
2	s1	82	CYS
2	s1	143	THR
1	t1	135	ARG
2	u1	82	CYS
1	x1	43	LYS
1	x1	53	LYS
1	x1	135	ARG
2	y1	143	THR
1	z1	82	CYS
3	21	96	LYS
3	21	97	PHE
3	21	98	LEU
3	21	101	LEU
3	21	102	LYS
3	21	103	ARG
3	21	114	PHE
3	21	118	LYS
3	21	143	THR
3	21	174	ARG
3	21	216	LYS
3	21	314	LYS
5	31	4	LYS
5	31	7	GLU
5	31	130	GLU
5	31	161	ILE
5	31	177	THR
5	31	178	LYS
6	X2	106	GLN
6	X2	304	TYR
8	B2	172	LYS
8	B2	189	ARG
8	B2	191	LYS
8	B2	205	ARG
8	B2	209	GLN
8	B2	227	GLU
8	B2	228	MET
9	G2	30	ARG
10	H2	77	ARG
10	J2	77	ARG
9	K2	50	ARG

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Mol	Chain	Res	Type
10	L2	77	ARG
9	M2	30	ARG
9	M2	79	ILE
1	Q2	53	LYS
2	T2	39	ASP
2	T2	75	THR
2	V2	39	ASP
2	V2	150	LYS
2	V2	151	MET
1	W2	140	VAL
2	a2	39	ASP
2	a2	149	ARG
2	a2	150	LYS
2	a2	151	MET
1	b2	127	TYR
1	b2	140	VAL
2	c2	77	ARG
1	d2	82	CYS
1	f2	140	VAL
2	k2	149	ARG
2	k2	150	LYS
2	k2	151	MET
1	A3	124	THR
2	B3	143	THR
2	D3	39	ASP
1	E3	106	ASP
1	E3	114	ARG
2	F3	33	ASP
2	F3	110	LEU
2	F3	159	THR
2	F3	176	ILE
1	G3	27	ILE
2	H3	25	GLN
2	H3	143	THR
1	I3	128	VAL
1	I3	155	TYR
1	K3	81	LYS
1	K3	127	TYR
2	L3	122	VAL
1	O3	89	TYR
2	P3	132[A]	SER
2	P3	132[B]	SER

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Mol	Chain	Res	Type
2	P3	163[A]	SER
2	P3	163[B]	SER
1	Q3	140	VAL
2	R3	39	ASP
2	R3	160[A]	SER
2	R3	160[B]	SER
2	T3	160[A]	SER
2	T3	160[B]	SER
1	U3	23	ASP
2	V3	163[A]	SER
2	V3	163[B]	SER
7	Y3	178	ARG
7	Y3	284	ARG
1	A4	75	ASN
1	A4	134	THR
2	D4	77	ARG
1	E4	140	VAL
2	F4	39	ASP
1	G4	37	ARG
1	I4	82	CYS
1	I4	140	VAL
1	K4	53	LYS
3	M4	96	LYS
3	M4	97	PHE
3	M4	100	THR
3	M4	111	ARG
3	M4	117	ARG
3	M4	162	LEU
2	O4	23	ASP
1	P4	114	ARG
1	P4	139	CYS
2	S4	145	THR
2	W4	149	ARG
2	Y4	75	THR
2	Y4	170	ASP
2	Y4	171	ARG
2	Z4	115	GLU
2	a4	77	ARG
4	b4	72	ARG
4	b4	93	TYR
4	b4	224	LYS
4	b4	259	LEU

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Mol	Chain	Res	Type
4	b4	271	GLU
4	b4	272	LYS
4	b4	273	GLU
4	b4	301	LEU
4	b4	303	SER
4	b4	304	TYR
4	b4	305	ASP
4	b4	306	LYS
4	b4	343	MET
4	b4	344	LEU
1	c4	144	MET
2	f4	77	ARG
2	f4	82	CYS
1	g4	124	THR
2	h4	77	ARG
1	i4	134	THR
1	k4	82	CYS
1	k4	102	THR
2	n4	145	THR
4	o4	72	ARG
4	o4	189	PHE
4	o4	228	ASN
4	o4	244	ILE
4	o4	245	ASP
4	o4	246	VAL
4	o4	265	TYR
2	q4	2	LEU
2	q4	9	VAL
2	q4	145	THR
1	r4	82	CYS
1	r4	120	LEU
2	u4	82	CYS
2	u4	157	ASP
1	v4	43	LYS
1	v4	93	VAL
1	x4	27	ILE
1	x4	43	LYS
1	x4	135	ARG
2	y4	143	THR
1	z4	82	CYS
1	z4	140	VAL
2	14	85	ASP

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Mol	Chain	Res	Type
2	14	88	ILE
3	24	101	LEU
3	24	103	ARG
3	24	114	PHE
3	24	115	TYR
3	24	118	LYS
3	24	174	ARG
3	24	200	LYS
3	24	314	LYS
3	24	332	ARG
5	34	4	LYS
5	34	6	TYR
5	34	111	ILE
5	34	161	ILE
5	34	177	THR
5	34	178	LYS
2	A5	50	CYS
2	B5	37	ARG
2	G5	150	LYS
2	G5	152	SER
2	G5	153	PHE
2	H5	148	GLU
2	I5	7	ARG
2	I5	95	TYR
2	I5	114	LYS
2	I5	115	GLU
2	I5	116	THR
1	J5	114	ARG
2	K5	76	ASN
2	K5	77	ARG
2	K5	79	MET
2	K5	114	LYS
2	L5	103	SER
2	L5	105	LEU
2	L5	106	GLU
2	L5	107	ASP
2	L5	108	ARG
2	L5	109	CYS
2	L5	110	LEU
2	L5	113	LEU
2	L5	114	LYS
6	X6	103	MET

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Mol	Chain	Res	Type
6	X6	105	LYS
6	X6	106	GLN
6	X6	304	TYR
6	X6	312	THR
6	X6	344	THR
7	A6	178	ARG
8	B6	17	VAL
8	B6	171	SER
8	B6	212	GLN
8	B6	227	GLU
10	F6	17	GLU
10	F6	19	LEU
10	J6	8	VAL
10	J6	15	ARG
10	L6	39	ASP
1	O6	140	VAL
2	P6	145	THR
2	P6	150	LYS
1	Q6	102	THR
1	Q6	127	TYR
2	R6	39	ASP
1	S6	137	ARG
2	T6	39	ASP
1	b6	138	LEU
1	d6	114	ARG
1	d6	137	ARG
2	e6	39	ASP
1	f6	53	LYS
2	g6	39	ASP
2	g6	117	TYR
1	h6	2	LYS
2	k6	39	ASP
1	l6	102	THR
1	l6	140	VAL
6	X7	117	LEU
7	A7	71	LYS
7	A7	178	ARG
8	B7	34	THR
8	B7	214	LYS
10	D7	82	CYS
10	F7	20	SER
10	F7	21	ASN

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Mol	Chain	Res	Type
9	G7	7	GLU
9	I7	49	GLN
9	I7	50	ARG
10	J7	22	THR
10	J7	23	GLN
10	J7	77	ARG
9	M7	2	LYS
1	O7	137	ARG
1	O7	157	ASP
2	V7	167	SER
2	V7	169	PHE
2	V7	170	ASP
2	V7	172	VAL
2	Y7	153	PHE
1	Z7	137	ARG
1	d7	102	THR
2	e7	39	ASP
2	g7	101	ASP
1	h7	137	ARG
2	m7	50	CYS
12	b8	208	ASN
12	b8	211	CYS
12	b8	311	GLN
12	b8	327	LYS
12	b8	329	MET
12	b8	332	MET
12	b8	335	ILE
12	b8	340	GLU
12	b8	350	VAL
12	b8	372	ILE
12	b8	373	GLU
12	b8	374	THR
12	b8	376	GLU
13	A8	43	LYS
13	A8	47	ARG
1	C8	137	ARG
2	D8	163[A]	SER
2	D8	163[B]	SER
1	G8	140	VAL
1	I8	137	ARG
2	J8	111	ASN
2	N8	22	SER

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Mol	Chain	Res	Type
2	N8	24	LEU
2	N8	160[A]	SER
2	N8	160[B]	SER
2	N8	163[A]	SER
2	N8	163[B]	SER
1	O8	87	ASP
1	S8	140	VAL
1	U8	43	LYS
1	U8	44	LEU
1	U8	53	LYS
2	X8	53[A]	SER
2	X8	53[B]	SER
1	Y8	53	LYS
1	Y8	54	GLU
2	Z8	132[A]	SER
2	Z8	132[B]	SER
2	c8	163[A]	SER
2	c8	163[B]	SER
1	d8	137	ARG
1	f8	135	ARG
1	h8	90	MET
1	h8	155	TYR
1	j8	118	ARG
1	l8	7	THR
1	l8	67	LYS
1	l8	74	GLU
1	l8	75	ASN
1	l8	76	GLN
1	l8	77	GLU
1	l8	78	LYS
1	l8	79	ILE
1	l8	80	ASN
2	m8	85	ASP
2	m8	160[A]	SER
2	m8	160[B]	SER
15	d9	213	SER
15	d9	277	SER
15	d9	279	ARG
15	d9	280	LEU
15	d9	281	VAL
15	d9	284	ARG
15	d9	293	MET

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Mol	Chain	Res	Type
15	d9	295	LEU
15	d9	320	ASP
15	d9	323	SER
15	d9	324	LYS
15	d9	325	MET
15	d9	327	GLN
7	A9	52	ARG
7	A9	56	THR
7	A9	85	VAL
7	A9	266	CYS
1	B9	33	ARG
1	B9	140	VAL
1	D9	42	GLU
1	D9	59	CYS
1	D9	140	VAL
2	E9	145	THR
1	F9	8	VAL
2	I9	39	ASP
2	K9	61	CYS
1	L9	82	CYS
1	N9	114	ARG
2	Q9	108	ARG
2	Q9	113	LEU
1	T9	23	ASP
1	T9	88	HIS
1	T9	96	CYS
2	U9	132[A]	SER
2	U9	132[B]	SER
1	V9	17	ARG
2	W9	3	ASP
2	W9	82	CYS
1	X9	116	VAL
12	bA	208	ASN
12	bA	309	VAL
12	bA	327	LYS
12	bA	333	ARG
12	bA	335	ILE
12	bA	338	MET
12	bA	372	ILE
12	bA	373	GLU
12	bA	374	THR
12	bA	375	ASP

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Mol	Chain	Res	Type
12	bA	376	GLU
2	DA	163[A]	SER
2	DA	163[B]	SER
1	GA	140	VAL
1	IA	137	ARG
2	NA	160[A]	SER
2	NA	160[B]	SER
1	OA	87	ASP
2	PA	47	ASN
2	PA	145	THR
2	RA	78	ARG
1	SA	93	VAL
1	SA	102	THR
1	UA	43	LYS
1	WA	54	GLU
2	XA	53[A]	SER
2	XA	53[B]	SER
1	YA	53	LYS
1	YA	54	GLU
1	YA	140	VAL
2	ZA	132[A]	SER
2	ZA	132[B]	SER
1	aA	140	VAL
2	cA	163[A]	SER
2	cA	163[B]	SER
2	eA	132[A]	SER
2	eA	132[B]	SER
1	hA	90	MET
1	lA	67	LYS
1	lA	75	ASN
1	lA	79	ILE
2	mA	85	ASP
2	mA	160[A]	SER
2	mA	160[B]	SER
6	XB	304	TYR
6	XB	312	THR
6	XB	344	THR
8	BB	171	SER
8	BB	172	LYS
8	BB	212	GLN
8	BB	214	LYS
8	BB	224	MET

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Mol	Chain	Res	Type
8	BB	225	VAL
8	BB	228	MET
8	BB	232	LEU
10	FB	17	GLU
10	LB	39	ASP
10	NB	77	ARG
2	PB	145	THR
1	QB	137	ARG
1	QB	140	VAL
1	SB	137	ARG
2	TB	39	ASP
1	UB	75	ASN
1	UB	137	ARG
2	YB	117	TYR
2	aB	47	ASN
1	bB	122	LEU
1	dB	53	LYS
1	dB	114	ARG
1	fB	97	LEU
2	gB	28	LYS
2	gB	30	PHE
2	gB	117	TYR
1	hB	47	ASN
2	kB	50	CYS
2	mB	39	ASP
2	AC	120	LEU
2	BC	37	ARG
2	BC	59	MET
2	BC	60	ILE
2	BC	61	CYS
2	BC	66	LEU
2	BC	67	ILE
2	BC	73	CYS
2	BC	74	TYR
2	BC	75	THR
2	BC	79	MET
2	BC	108	ARG
2	BC	171	ARG
2	CC	73	CYS
2	CC	114	LYS
2	CC	143	THR
2	GC	50	CYS

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Mol	Chain	Res	Type
2	KC	77	ARG
2	KC	78	ARG
2	KC	114	LYS
2	KC	115	GLU
2	LC	105	LEU
2	LC	107	ASP
2	LC	108	ARG
2	LC	110	LEU
2	LC	114	LYS
2	LC	115	GLU
1	AD	124	THR
1	AD	159	LEU
2	BD	77	ARG
2	BD	143	THR
2	BD	151	MET
2	BD	170	ASP
2	DD	143	THR
1	ED	105	LEU
2	FD	110	LEU
2	FD	176	ILE
2	HD	24	LEU
2	HD	25	GLN
1	ID	140	VAL
2	LD	122	VAL
2	LD	176	ILE
1	OD	49	GLU
1	OD	89	TYR
2	PD	82	CYS
2	PD	132[A]	SER
2	PD	132[B]	SER
2	PD	163[A]	SER
2	PD	163[B]	SER
1	QD	140	VAL
2	RD	160[A]	SER
2	RD	160[B]	SER
2	TD	39	ASP
1	UD	23	ASP
2	XD	145	THR
7	YD	178	ARG
7	YD	179	THR
7	YD	283	MET
2	BE	39	ASP

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Mol	Chain	Res	Type
1	CE	78	LYS
2	DE	163[A]	SER
2	DE	163[B]	SER
2	FE	163[A]	SER
2	FE	163[B]	SER
1	GE	78	LYS
1	GE	140	VAL
1	IE	140	VAL
2	JE	39	ASP
2	JE	53[A]	SER
2	JE	53[B]	SER
2	LE	39	ASP
2	NE	160[A]	SER
2	NE	160[B]	SER
2	PE	160[A]	SER
2	PE	160[B]	SER
1	QE	140	VAL
2	RE	53[A]	SER
2	RE	53[B]	SER
2	RE	163[A]	SER
2	RE	163[B]	SER
1	UE	33	ARG
1	UE	140	VAL
2	VE	39	ASP
2	VE	163[A]	SER
2	VE	163[B]	SER
2	XE	132[A]	SER
2	XE	132[B]	SER
1	aE	53	LYS
2	bE	132[A]	SER
2	bE	132[B]	SER
1	cE	33	ARG
1	cE	53	LYS
1	cE	140	VAL
1	eE	24	LEU
2	fE	132[A]	SER
2	fE	132[B]	SER
1	gE	140	VAL
1	kE	140	VAL
1	mE	84	ARG
1	mE	114	ARG
1	mE	118	ARG

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Mol	Chain	Res	Type
2	nE	135	LYS
1	oE	140	VAL
2	pE	163[A]	SER
2	pE	163[B]	SER
1	qE	102	THR
1	qE	114	ARG
2	rE	171	ARG
1	sE	114	ARG
2	tE	163[A]	SER
2	tE	163[B]	SER
1	uE	2	LYS
2	vE	144	ASN
2	vE	149	ARG
13	wE	54	LYS
13	wE	88	GLU
13	wE	120	ASP
13	wE	234	ARG
13	xE	161	ARG
13	xE	267	ARG
14	yE	284	ARG
16	zE	213	ARG
16	zE	280	VAL
6	XF	110	PHE
7	AF	71	LYS
7	AF	178	ARG
7	AF	284	ARG
8	BF	34	THR
8	BF	52	ARG
9	CF	44	LEU
10	JF	15	ARG
10	JF	75	THR
9	KF	67	THR
1	OF	137	ARG
1	OF	138	LEU
2	TF	145	THR
1	ZF	6	THR
2	cF	143	THR
2	cF	158	CYS
1	dF	53	LYS
1	dF	102	THR
1	dF	114	ARG
2	eF	109	CYS

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Mol	Chain	Res	Type
2	eF	145	THR
1	hF	124	THR
2	iF	39	ASP
2	iF	132[A]	SER
2	iF	132[B]	SER
2	iF	149	ARG
1	jF	82	CYS
2	kF	82	CYS
2	kF	149	ARG
1	lF	24	LEU
1	lF	102	THR
2	mF	122	VAL
2	mF	147	THR
1	CG	52	VAL
2	DG	163[A]	SER
2	DG	163[B]	SER
2	FG	39	ASP
1	GG	140	VAL
1	IG	140	VAL
2	JG	53[A]	SER
2	JG	53[B]	SER
1	KG	59	CYS
2	LG	39	ASP
2	NG	160[A]	SER
2	NG	160[B]	SER
2	RG	53[A]	SER
2	RG	53[B]	SER
2	TG	39	ASP
1	UG	140	VAL
2	VG	39	ASP
2	ZG	149	ARG
1	aG	53	LYS
1	cG	53	LYS
1	eG	24	LEU
1	eG	159	LEU
1	iG	84	ARG
2	jG	160[A]	SER
2	jG	160[B]	SER
1	kG	7	THR
1	kG	140	VAL
2	lG	38	LEU
2	lG	39	ASP

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Mol	Chain	Res	Type
1	mG	114	ARG
1	mG	140	VAL
2	nG	135	LYS
1	oG	84	ARG
1	oG	140	VAL
2	pG	163[A]	SER
2	pG	163[B]	SER
1	qG	102	THR
1	qG	114	ARG
2	rG	113	LEU
2	rG	163[A]	SER
2	rG	163[B]	SER
1	sG	114	ARG
1	sG	137	ARG
1	uG	2	LYS
13	wG	54	LYS
13	xG	205	LYS
14	yG	284	ARG
16	zG	213	ARG
18	BH	66	THR
17	JH	52	LYS
18	LH	65	ILE
18	MH	147	LYS
18	MH	149	MET
17	NH	52	LYS
17	PH	52	LYS
22	YH	139	ARG
22	YH	140	TYR
22	YH	500	SER
22	YH	501	VAL
22	YH	520	ARG
24	aH	252	LYS
24	aH	259	TYR
24	aH	260	LYS
24	aH	261	ARG
24	aH	274	THR
24	aH	278	LEU
24	aH	279	VAL
25	bH	40	ARG
25	bH	139	ARG
25	bH	140	LYS
25	bH	225	ARG

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Mol	Chain	Res	Type
17	gH	49	ARG
18	kH	66	THR
17	lH	52	LYS
17	lH	76	GLU
18	oH	64	ASP
18	oH	81	CYS
18	oH	147	LYS
18	oH	148	GLU
18	oH	149	MET
17	pH	52	LYS
17	rH	52	LYS
17	tH	16	ARG
22	1H	139	ARG
22	1H	140	TYR
22	1H	498	SER
22	1H	501	VAL
22	1H	520	ARG
24	3H	252	LYS
24	3H	259	TYR
24	3H	260	LYS
24	3H	261	ARG
24	3H	274	THR
24	3H	277	ARG
24	3H	278	LEU
24	3H	279	VAL
25	4H	119	GLU
25	4H	139	ARG
25	4H	186	LYS
25	4H	225	ARG
6	XI	103	MET
6	XI	105	LYS
6	XI	106	GLN
6	XI	269	THR
6	XI	304	TYR
8	BI	29	TYR
8	BI	171	SER
8	BI	172	LYS
8	BI	191	LYS
8	BI	192	LEU
8	BI	205	ARG
8	BI	209	GLN
8	BI	226	GLN

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Mol	Chain	Res	Type
8	BI	227	GLU
9	GI	30	ARG
10	HI	77	ARG
9	KI	50	ARG
10	LI	77	ARG
9	MI	30	ARG
9	MI	79	ILE
10	NI	75	THR
1	QI	53	LYS
1	QI	142	ARG
2	TI	39	ASP
2	VI	61	CYS
2	VI	134	MET
2	VI	135	LYS
2	VI	149	ARG
2	VI	151	MET
1	WI	140	VAL
2	aI	39	ASP
2	aI	149	ARG
2	aI	150	LYS
2	aI	151	MET
1	bI	140	VAL
2	cI	51	MET
2	kI	145	THR
2	kI	150	LYS
15	dJ	196	THR
15	dJ	213	SER
15	dJ	222	ARG
15	dJ	244	THR
15	dJ	279	ARG
15	dJ	280	LEU
15	dJ	281	VAL
15	dJ	283	ARG
15	dJ	325	MET
7	AJ	218	GLU
7	AJ	222	LYS
1	DJ	140	VAL
2	EJ	145	THR
1	FJ	8	VAL
1	HJ	140	VAL
2	KJ	39	ASP
1	LJ	102	THR

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Mol	Chain	Res	Type
1	NJ	13	ASP
1	NJ	114	ARG
2	OJ	97	LEU
1	RJ	140	VAL
2	SJ	104	VAL
1	TJ	47	ASN
1	TJ	110	ILE
1	VJ	156	LEU
2	WJ	134	MET
1	XJ	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1083) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	32	GLN
2	B1	35	ASN
1	C1	47	ASN
1	C1	68	ASN
2	D1	25	GLN
2	D1	144	ASN
2	F1	11	ASN
1	G1	32	GLN
1	G1	47	ASN
1	G1	88	HIS
2	H1	144	ASN
1	I1	21	ASN
1	I1	28	GLN
1	I1	32	GLN
1	K1	68	ASN
1	K1	94	ASN
2	L1	111	ASN
2	L1	137	GLN
3	M1	170	GLN
3	M1	228	GLN
3	M1	279	ASN
1	N1	68	ASN
1	N1	88	HIS
2	O1	76	ASN
1	P1	88	HIS
1	R1	28	GLN
1	R1	68	ASN
2	S1	35	ASN

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Mol	Chain	Res	Type
1	T1	68	ASN
1	T1	88	HIS
1	V1	68	ASN
1	V1	94	ASN
1	X1	68	ASN
1	X1	88	HIS
2	Y1	11	ASN
2	Y1	76	ASN
2	a1	76	ASN
4	b1	312	GLN
1	c1	94	ASN
1	c1	161	ASN
2	d1	47	ASN
2	f1	137	GLN
1	m1	32	GLN
1	m1	76	GLN
1	m1	161	ASN
2	n1	47	ASN
2	n1	137	GLN
1	r1	161	ASN
2	s1	42	ASN
2	s1	137	GLN
1	t1	80	ASN
1	t1	94	ASN
2	u1	42	ASN
1	v1	76	GLN
1	v1	94	ASN
1	v1	161	ASN
1	x1	21	ASN
1	x1	28	GLN
2	y1	137	GLN
1	z1	28	GLN
1	z1	80	ASN
1	z1	161	ASN
2	11	35	ASN
2	11	42	ASN
3	21	193	HIS
3	21	204	GLN
3	21	244	GLN
3	21	296	ASN
3	21	310	ASN
5	31	43	ASN

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Mol	Chain	Res	Type
5	31	104	GLN
5	31	203	GLN
5	31	204	GLN
6	X2	80	GLN
6	X2	161	HIS
6	X2	273	GLN
6	X2	333	ASN
7	A2	60	ASN
7	A2	69	GLN
7	A2	224	GLN
7	A2	274	ASN
8	B2	53	GLN
8	B2	99	ASN
8	B2	121	ASN
8	B2	169	GLN
8	B2	178	ASN
9	E2	138	ASN
9	E2	148	ASN
10	F2	35	ASN
9	G2	138	ASN
9	G2	159	ASN
10	J2	35	ASN
9	K2	32	GLN
9	K2	57	GLN
9	K2	138	ASN
10	L2	35	ASN
10	L2	63	GLN
10	L2	65	GLN
9	M2	32	GLN
9	M2	148	ASN
10	N2	68	GLN
1	O2	21	ASN
2	P2	35	ASN
2	P2	76	ASN
1	Q2	76	GLN
1	Q2	161	ASN
2	R2	35	ASN
2	R2	47	ASN
2	R2	137	GLN
1	U2	80	ASN
2	V2	47	ASN
1	W2	76	GLN

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Mol	Chain	Res	Type
2	Y2	11	ASN
2	Y2	35	ASN
2	Y2	47	ASN
2	Y2	137	GLN
2	a2	35	ASN
2	a2	47	ASN
1	b2	28	GLN
1	b2	30	ASN
1	b2	88	HIS
2	c2	42	ASN
2	c2	111	ASN
1	d2	21	ASN
1	d2	76	GLN
1	d2	94	ASN
2	e2	76	ASN
2	e2	137	GLN
1	f2	28	GLN
1	f2	161	ASN
2	i2	35	ASN
1	j2	28	GLN
1	j2	32	GLN
1	j2	147	GLN
2	k2	11	ASN
2	k2	47	ASN
1	l2	28	GLN
11	e3	258	ASN
11	e3	284	ASN
1	A3	28	GLN
1	A3	68	ASN
1	A3	76	GLN
1	A3	88	HIS
1	A3	147	GLN
1	A3	161	ASN
1	C3	68	ASN
1	C3	76	GLN
1	C3	80	ASN
1	C3	94	ASN
2	D3	11	ASN
1	E3	68	ASN
2	F3	11	ASN
2	F3	111	ASN
2	H3	25	GLN

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Mol	Chain	Res	Type
2	J3	11	ASN
2	J3	47	ASN
2	L3	111	ASN
1	M3	88	HIS
1	M3	94	ASN
1	O3	21	ASN
1	Q3	76	GLN
1	W3	94	ASN
1	W3	147	GLN
7	Y3	60	ASN
7	Y3	220	ASN
7	Y3	241	GLN
1	A4	80	ASN
2	B4	25	GLN
2	B4	42	ASN
1	C4	28	GLN
1	C4	47	ASN
2	D4	42	ASN
1	G4	28	GLN
1	G4	76	GLN
1	G4	80	ASN
1	G4	88	HIS
2	H4	35	ASN
2	H4	63	ASN
1	I4	21	ASN
1	I4	47	ASN
2	J4	35	ASN
1	K4	94	ASN
2	L4	144	ASN
3	M4	170	GLN
1	N4	32	GLN
1	N4	68	ASN
1	N4	88	HIS
1	P4	88	HIS
1	R4	28	GLN
1	R4	68	ASN
2	S4	35	ASN
1	T4	68	ASN
1	T4	88	HIS
1	V4	68	ASN
1	V4	94	ASN
1	X4	68	ASN

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Mol	Chain	Res	Type
1	X4	88	HIS
4	b4	165	GLN
4	b4	312	GLN
1	c4	21	ASN
1	c4	32	GLN
2	d4	47	ASN
1	g4	30	ASN
1	g4	121	ASN
1	g4	147	GLN
2	h4	76	ASN
2	h4	137	GLN
1	i4	28	GLN
1	k4	147	GLN
2	l4	111	ASN
2	l4	137	GLN
2	n4	47	ASN
2	n4	137	GLN
4	o4	113	ASN
1	p4	32	GLN
2	q4	42	ASN
2	q4	144	ASN
1	r4	88	HIS
2	s4	137	GLN
1	v4	28	GLN
1	v4	76	GLN
1	x4	28	GLN
2	y4	25	GLN
2	y4	137	GLN
1	z4	28	GLN
1	z4	80	ASN
2	14	63	ASN
2	14	76	ASN
2	14	137	GLN
3	24	170	GLN
3	24	228	GLN
3	24	238	GLN
3	24	242	GLN
3	24	284	GLN
3	24	331	ASN
5	34	43	ASN
5	34	104	GLN
5	34	203	GLN

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Mol	Chain	Res	Type
5	34	204	GLN
5	34	275	GLN
2	B5	144	ASN
2	F5	35	ASN
2	G5	35	ASN
2	G5	144	ASN
2	I5	47	ASN
1	J5	28	GLN
1	J5	32	GLN
1	J5	68	ASN
1	J5	88	HIS
2	L5	47	ASN
6	X6	306	GLN
6	X6	333	ASN
7	A6	141	ASN
8	B6	226	GLN
9	C6	49	GLN
9	C6	61	ASN
9	C6	148	ASN
10	D6	35	ASN
10	D6	118	GLN
10	F6	35	ASN
10	F6	111	ASN
10	F6	118	GLN
9	G6	14	ASN
9	G6	145	GLN
10	H6	21	ASN
10	H6	35	ASN
10	H6	118	GLN
9	I6	15	GLN
9	I6	25	GLN
9	I6	32	GLN
9	I6	138	ASN
9	I6	145	GLN
10	J6	21	ASN
10	J6	35	ASN
10	J6	47	ASN
10	J6	118	GLN
10	J6	132	GLN
9	K6	25	GLN
9	K6	145	GLN
10	L6	23	GLN

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Mol	Chain	Res	Type
10	L6	35	ASN
10	L6	118	GLN
9	M6	49	GLN
9	M6	145	GLN
10	N6	21	ASN
10	N6	35	ASN
10	N6	118	GLN
1	O6	28	GLN
1	O6	88	HIS
1	O6	147	GLN
1	Q6	68	ASN
1	S6	94	ASN
1	S6	147	GLN
2	T6	125	ASN
2	T6	137	GLN
1	U6	28	GLN
1	U6	94	ASN
2	V6	25	GLN
2	V6	137	GLN
1	W6	88	HIS
1	W6	147	GLN
2	Y6	125	ASN
1	Z6	88	HIS
1	Z6	147	GLN
1	Z6	161	ASN
1	b6	21	ASN
1	b6	30	ASN
1	d6	28	GLN
1	d6	32	GLN
1	d6	94	ASN
1	f6	32	GLN
1	f6	147	GLN
2	g6	144	ASN
1	h6	121	ASN
2	i6	111	ASN
2	i6	137	GLN
2	i6	144	ASN
1	j6	28	GLN
1	j6	68	ASN
2	k6	11	ASN
2	m6	76	ASN
2	m6	125	ASN

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Mol	Chain	Res	Type
6	X7	333	ASN
7	A7	128	GLN
7	A7	141	ASN
7	A7	224	GLN
8	B7	23	ASN
8	B7	209	GLN
8	B7	211	GLN
9	C7	14	ASN
9	C7	61	ASN
9	C7	119	ASN
10	D7	21	ASN
10	D7	63	GLN
10	D7	111	ASN
9	E7	15	GLN
9	E7	145	GLN
10	F7	21	ASN
10	F7	143	ASN
9	G7	15	GLN
10	H7	23	GLN
10	H7	63	GLN
10	J7	23	GLN
10	J7	63	GLN
10	J7	111	ASN
10	J7	143	ASN
9	K7	14	ASN
9	K7	15	GLN
9	K7	61	ASN
10	L7	36	GLN
10	L7	68	GLN
10	L7	143	ASN
10	N7	21	ASN
1	O7	75	ASN
1	O7	94	ASN
1	O7	147	GLN
2	P7	111	ASN
1	Q7	32	GLN
1	Q7	80	ASN
1	Q7	94	ASN
2	R7	11	ASN
1	S7	76	GLN
1	S7	80	ASN
1	S7	88	HIS

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Mol	Chain	Res	Type
1	S7	94	ASN
1	U7	161	ASN
2	V7	63	ASN
1	W7	68	ASN
2	Y7	47	ASN
1	Z7	68	ASN
1	Z7	80	ASN
1	Z7	147	GLN
1	Z7	161	ASN
1	b7	94	ASN
2	e7	47	ASN
2	e7	144	ASN
1	f7	94	ASN
2	g7	76	ASN
1	h7	28	GLN
1	h7	32	GLN
1	h7	94	ASN
2	i7	47	ASN
1	j7	80	ASN
1	j7	94	ASN
2	k7	11	ASN
2	k7	144	ASN
1	l7	68	ASN
1	l7	80	ASN
1	l7	88	HIS
2	m7	111	ASN
12	b8	38	GLN
12	b8	155	HIS
12	b8	210	GLN
12	b8	276	ASN
12	b8	311	GLN
12	b8	348	GLN
13	A8	119	HIS
13	A8	236	ASN
14	B8	72	ASN
14	B8	128	ASN
14	B8	267	HIS
1	C8	32	GLN
1	E8	32	GLN
1	G8	32	GLN
2	H8	11	ASN
2	H8	137	GLN

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Mol	Chain	Res	Type
2	J8	111	ASN
2	N8	47	ASN
2	N8	125	ASN
2	P8	137	GLN
1	Q8	28	GLN
1	Q8	32	GLN
1	Q8	161	ASN
1	S8	32	GLN
1	S8	68	ASN
1	S8	94	ASN
1	U8	94	ASN
2	V8	125	ASN
1	W8	161	ASN
1	Y8	76	GLN
1	Y8	80	ASN
2	Z8	25	GLN
1	a8	21	ASN
1	a8	80	ASN
1	a8	94	ASN
2	c8	11	ASN
1	d8	94	ASN
1	d8	161	ASN
1	f8	68	ASN
1	f8	88	HIS
1	f8	94	ASN
1	f8	161	ASN
2	g8	11	ASN
2	g8	42	ASN
2	g8	137	GLN
1	h8	21	ASN
1	h8	28	GLN
1	h8	32	GLN
1	h8	94	ASN
1	h8	161	ASN
2	i8	25	GLN
2	k8	137	GLN
1	l8	75	ASN
1	l8	161	ASN
2	m8	63	ASN
15	d9	148	GLN
15	d9	161	ASN
15	d9	189	GLN

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Mol	Chain	Res	Type
15	d9	201	ASN
15	d9	322	GLN
7	A9	88	GLN
7	A9	102	GLN
7	A9	128	GLN
7	A9	141	ASN
7	A9	201	GLN
1	B9	68	ASN
2	C9	11	ASN
2	C9	63	ASN
1	D9	94	ASN
2	E9	11	ASN
1	F9	94	ASN
2	G9	11	ASN
1	H9	76	GLN
1	H9	80	ASN
1	H9	94	ASN
2	I9	11	ASN
2	I9	111	ASN
1	J9	21	ASN
1	J9	28	GLN
1	J9	147	GLN
1	L9	28	GLN
1	L9	147	GLN
2	M9	11	ASN
2	M9	25	GLN
2	O9	25	GLN
1	P9	68	ASN
1	P9	121	ASN
2	Q9	11	ASN
2	Q9	47	ASN
2	Q9	63	ASN
2	Q9	76	ASN
1	R9	94	ASN
1	R9	161	ASN
1	V9	21	ASN
1	V9	28	GLN
1	V9	88	HIS
2	W9	35	ASN
1	X9	94	ASN
2	Y9	11	ASN
2	Y9	137	GLN

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Mol	Chain	Res	Type
12	bA	38	GLN
12	bA	155	HIS
12	bA	208	ASN
12	bA	210	GLN
12	bA	311	GLN
13	AA	236	ASN
14	BA	72	ASN
14	BA	142	ASN
14	BA	267	HIS
14	BA	274	ASN
1	CA	28	GLN
2	DA	137	GLN
1	GA	32	GLN
2	HA	11	ASN
2	HA	137	GLN
2	JA	42	ASN
2	JA	111	ASN
2	PA	137	GLN
1	QA	28	GLN
1	QA	32	GLN
1	QA	94	ASN
1	QA	161	ASN
2	RA	137	GLN
1	SA	32	GLN
1	SA	68	ASN
1	SA	76	GLN
1	SA	80	ASN
1	SA	94	ASN
1	UA	94	ASN
2	VA	137	GLN
1	WA	161	ASN
1	YA	76	GLN
1	YA	80	ASN
1	aA	21	ASN
1	aA	28	GLN
2	cA	11	ASN
2	cA	111	ASN
1	dA	68	ASN
1	dA	94	ASN
1	fA	21	ASN
1	fA	94	ASN
2	gA	11	ASN

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Mol	Chain	Res	Type
2	gA	137	GLN
1	hA	21	ASN
1	hA	28	GLN
1	hA	32	GLN
1	hA	68	ASN
1	hA	94	ASN
1	hA	161	ASN
2	iA	11	ASN
2	iA	47	ASN
2	iA	76	ASN
2	kA	137	GLN
1	lA	21	ASN
2	mA	63	ASN
6	XB	147	ASN
6	XB	306	GLN
6	XB	333	ASN
8	BB	14	ASN
8	BB	212	GLN
9	CB	49	GLN
9	CB	61	ASN
10	DB	35	ASN
10	DB	118	GLN
9	EB	148	ASN
10	FB	35	ASN
10	FB	118	GLN
9	GB	15	GLN
9	GB	145	GLN
10	HB	21	ASN
10	HB	35	ASN
10	HB	118	GLN
9	IB	15	GLN
9	IB	25	GLN
9	IB	138	ASN
9	IB	145	GLN
10	JB	21	ASN
10	JB	35	ASN
10	JB	47	ASN
10	JB	68	GLN
10	JB	118	GLN
10	JB	132	GLN
9	KB	25	GLN
9	KB	145	GLN

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Mol	Chain	Res	Type
10	LB	23	GLN
10	LB	35	ASN
10	LB	118	GLN
9	MB	145	GLN
10	NB	21	ASN
10	NB	35	ASN
10	NB	118	GLN
1	OB	28	GLN
1	OB	88	HIS
1	OB	147	GLN
1	SB	32	GLN
1	SB	94	ASN
1	SB	147	GLN
2	TB	125	ASN
2	TB	137	GLN
1	UB	21	ASN
1	UB	94	ASN
2	VB	25	GLN
1	WB	88	HIS
2	YB	125	ASN
1	ZB	28	GLN
1	ZB	32	GLN
1	ZB	88	HIS
1	ZB	147	GLN
1	ZB	161	ASN
2	cB	76	ASN
1	dB	21	ASN
1	dB	28	GLN
1	dB	32	GLN
1	dB	88	HIS
1	dB	94	ASN
1	fB	30	ASN
1	fB	76	GLN
1	fB	147	GLN
2	iB	11	ASN
1	jB	68	ASN
2	kB	11	ASN
1	lB	68	ASN
2	mB	76	ASN
2	mB	125	ASN
2	AC	35	ASN
2	BC	144	ASN

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Mol	Chain	Res	Type
2	CC	144	ASN
2	FC	35	ASN
2	GC	35	ASN
2	IC	25	GLN
2	IC	47	ASN
1	JC	28	GLN
1	JC	32	GLN
1	JC	68	ASN
1	JC	88	HIS
2	KC	111	ASN
2	LC	76	ASN
11	eD	178	HIS
11	eD	258	ASN
11	eD	284	ASN
1	AD	68	ASN
1	CD	68	ASN
1	CD	76	GLN
1	CD	80	ASN
1	CD	94	ASN
2	DD	11	ASN
2	DD	35	ASN
2	DD	47	ASN
1	ED	28	GLN
1	ED	68	ASN
1	GD	28	GLN
1	GD	121	ASN
2	HD	25	GLN
2	JD	11	ASN
1	KD	80	ASN
1	KD	161	ASN
2	LD	111	ASN
1	OD	21	ASN
1	QD	76	GLN
1	QD	80	ASN
2	VD	47	ASN
1	WD	94	ASN
1	WD	147	GLN
7	YD	102	GLN
1	AE	30	ASN
1	AE	32	GLN
2	BE	47	ASN
1	CE	30	ASN

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Mol	Chain	Res	Type
1	CE	147	GLN
2	DE	35	ASN
2	DE	47	ASN
1	EE	68	ASN
1	EE	80	ASN
2	FE	47	ASN
1	GE	32	GLN
1	GE	94	ASN
1	IE	32	GLN
1	IE	94	ASN
1	IE	147	GLN
2	JE	47	ASN
1	KE	28	GLN
2	LE	11	ASN
2	LE	47	ASN
2	LE	125	ASN
1	ME	88	HIS
1	ME	147	GLN
2	NE	47	ASN
2	NE	111	ASN
2	PE	47	ASN
1	QE	76	GLN
1	QE	80	ASN
1	SE	147	GLN
2	TE	47	ASN
1	UE	76	GLN
1	UE	94	ASN
2	VE	35	ASN
1	WE	21	ASN
1	WE	68	ASN
1	WE	76	GLN
1	WE	80	ASN
1	WE	121	ASN
2	XE	35	ASN
2	XE	47	ASN
1	aE	75	ASN
1	cE	21	ASN
2	dE	47	ASN
1	eE	80	ASN
1	gE	94	ASN
2	hE	11	ASN
2	hE	76	ASN

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Mol	Chain	Res	Type
1	iE	80	ASN
2	lE	11	ASN
2	lE	47	ASN
2	lE	144	ASN
2	nE	11	ASN
2	nE	35	ASN
2	pE	76	ASN
2	tE	47	ASN
1	uE	32	GLN
1	uE	94	ASN
13	xE	111	GLN
14	yE	228	GLN
14	yE	267	HIS
16	zE	286	GLN
16	zE	300	GLN
6	XF	71	GLN
6	XF	333	ASN
7	AF	60	ASN
7	AF	224	GLN
8	BF	23	ASN
8	BF	209	GLN
8	BF	211	GLN
9	CF	14	ASN
9	CF	61	ASN
9	CF	119	ASN
10	DF	21	ASN
10	DF	23	GLN
10	DF	111	ASN
9	EF	145	GLN
10	FF	143	ASN
9	GF	61	ASN
10	HF	63	GLN
9	IF	21	ASN
10	JF	23	GLN
10	JF	143	ASN
9	KF	14	ASN
9	KF	61	ASN
10	LF	143	ASN
9	MF	15	GLN
10	NF	21	ASN
10	NF	118	GLN
10	NF	143	ASN

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Mol	Chain	Res	Type
1	OF	28	GLN
1	OF	75	ASN
1	OF	80	ASN
1	OF	94	ASN
1	OF	147	GLN
2	PF	76	ASN
2	PF	111	ASN
1	QF	80	ASN
1	QF	94	ASN
1	SF	88	HIS
1	UF	161	ASN
2	VF	63	ASN
1	WF	88	HIS
1	ZF	80	ASN
1	ZF	147	GLN
1	bF	161	ASN
2	cF	47	ASN
2	cF	63	ASN
1	dF	21	ASN
1	dF	28	GLN
2	eF	144	ASN
1	fF	94	ASN
2	gF	47	ASN
2	gF	76	ASN
1	hF	68	ASN
2	iF	47	ASN
2	iF	76	ASN
1	jF	32	GLN
2	kF	144	ASN
1	lF	68	ASN
1	lF	80	ASN
1	lF	147	GLN
2	mF	11	ASN
2	mF	76	ASN
2	mF	111	ASN
1	AG	30	ASN
1	AG	32	GLN
2	BG	47	ASN
2	BG	144	ASN
1	CG	30	ASN
2	DG	35	ASN
2	DG	47	ASN

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Mol	Chain	Res	Type
1	EG	80	ASN
2	FG	47	ASN
2	FG	125	ASN
1	GG	28	GLN
1	GG	94	ASN
2	HG	35	ASN
1	IG	32	GLN
1	IG	94	ASN
1	IG	147	GLN
2	JG	47	ASN
1	KG	32	GLN
2	LG	11	ASN
2	LG	35	ASN
2	LG	47	ASN
2	LG	125	ASN
1	MG	32	GLN
1	MG	88	HIS
1	MG	94	ASN
2	NG	47	ASN
1	OG	21	ASN
1	OG	80	ASN
2	PG	47	ASN
1	QG	76	GLN
1	QG	80	ASN
2	TG	47	ASN
1	UG	32	GLN
1	UG	76	GLN
1	UG	94	ASN
1	UG	147	GLN
2	VG	47	ASN
1	WG	21	ASN
1	WG	28	GLN
1	WG	32	GLN
1	WG	94	ASN
1	WG	121	ASN
2	XG	35	ASN
2	XG	47	ASN
1	YG	21	ASN
1	YG	76	GLN
2	ZG	47	ASN
1	aG	75	ASN
2	bG	47	ASN

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Mol	Chain	Res	Type
2	dG	47	ASN
2	dG	63	ASN
1	eG	80	ASN
1	gG	32	GLN
1	gG	94	ASN
2	hG	11	ASN
1	iG	161	ASN
1	kG	21	ASN
1	kG	32	GLN
2	lG	144	ASN
1	mG	147	GLN
1	mG	161	ASN
2	nG	42	ASN
2	nG	47	ASN
2	pG	76	ASN
1	uG	147	GLN
14	yG	155	GLN
14	yG	202	ASN
14	yG	267	HIS
16	zG	176	HIS
16	zG	286	GLN
16	zG	300	GLN
16	zG	351	GLN
17	AH	46	ASN
17	AH	53	GLN
17	AH	71	ASN
17	AH	161	GLN
18	DH	15	GLN
17	CH	46	ASN
18	FH	47	ASN
17	EH	34	GLN
17	EH	71	ASN
18	BH	15	GLN
17	GH	71	ASN
17	GH	161	GLN
18	HH	15	GLN
18	HH	22	ASN
18	HH	47	ASN
18	IH	47	ASN
17	JH	10	ASN
17	JH	53	GLN
17	JH	71	ASN

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Mol	Chain	Res	Type
17	KH	71	ASN
18	LH	47	ASN
18	MH	47	ASN
17	NH	53	GLN
17	NH	56	GLN
17	NH	71	ASN
18	OH	47	ASN
18	OH	110	ASN
18	OH	117	ASN
17	PH	53	GLN
17	PH	71	ASN
18	QH	15	GLN
18	QH	47	ASN
17	RH	46	ASN
17	RH	57	GLN
17	RH	71	ASN
18	SH	47	ASN
17	TH	34	GLN
17	TH	71	ASN
17	TH	161	GLN
19	VH	44	GLN
19	VH	60	GLN
19	VH	143	GLN
20	WH	137	GLN
21	XH	70	GLN
22	YH	27	GLN
22	YH	96	ASN
22	YH	169	ASN
22	YH	307	ASN
22	YH	331	GLN
22	YH	350	ASN
22	YH	415	GLN
22	YH	425	GLN
22	YH	660	ASN
22	YH	724	GLN
22	YH	755	GLN
22	YH	800	GLN
22	YH	808	GLN
22	YH	816	GLN
22	YH	849	ASN
23	ZH	28	GLN
23	ZH	42	ASN

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Mol	Chain	Res	Type
23	ZH	117	GLN
25	bH	135	ASN
25	bH	145	HIS
25	bH	177	ASN
25	bH	196	ASN
17	cH	71	ASN
17	eH	46	ASN
17	eH	71	ASN
17	gH	71	ASN
18	hH	15	GLN
17	iH	71	ASN
18	jH	47	ASN
18	kH	47	ASN
17	lH	71	ASN
17	mH	71	ASN
18	oH	47	ASN
17	pH	53	GLN
17	pH	71	ASN
18	qH	47	ASN
18	qH	117	ASN
17	rH	53	GLN
17	rH	71	ASN
18	sH	15	GLN
18	sH	47	ASN
18	sH	128	GLN
17	tH	56	GLN
17	tH	71	ASN
18	uH	47	ASN
17	vH	71	ASN
17	vH	161	GLN
19	xH	44	GLN
19	xH	60	GLN
19	xH	62	HIS
19	xH	143	GLN
20	yH	137	GLN
20	yH	172	ASN
21	zH	66	GLN
22	1H	27	GLN
22	1H	96	ASN
22	1H	169	ASN
22	1H	307	ASN
22	1H	331	GLN

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Mol	Chain	Res	Type
22	1H	350	ASN
22	1H	415	GLN
22	1H	425	GLN
22	1H	655	GLN
22	1H	724	GLN
22	1H	755	GLN
22	1H	800	GLN
22	1H	808	GLN
22	1H	816	GLN
23	2H	28	GLN
23	2H	42	ASN
23	2H	117	GLN
24	3H	194	ASN
25	4H	135	ASN
25	4H	145	HIS
6	XI	63	ASN
6	XI	161	HIS
6	XI	273	GLN
7	AI	60	ASN
7	AI	69	GLN
7	AI	144	HIS
7	AI	224	GLN
7	AI	227	GLN
7	AI	261	HIS
7	AI	274	ASN
8	BI	53	GLN
8	BI	99	ASN
8	BI	121	ASN
8	BI	178	ASN
10	DI	35	ASN
10	FI	35	ASN
9	GI	138	ASN
9	GI	159	ASN
10	JI	11	GLN
10	JI	35	ASN
9	KI	32	GLN
9	KI	138	ASN
10	LI	35	ASN
10	LI	63	GLN
10	LI	65	GLN
9	MI	25	GLN
9	MI	32	GLN

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Mol	Chain	Res	Type
9	MI	148	ASN
1	OI	21	ASN
2	PI	35	ASN
2	PI	76	ASN
1	QI	76	GLN
1	QI	161	ASN
2	RI	35	ASN
2	RI	47	ASN
2	RI	137	GLN
1	UI	80	ASN
2	VI	47	ASN
1	WI	76	GLN
2	YI	11	ASN
2	YI	35	ASN
2	YI	47	ASN
2	YI	137	GLN
2	aI	35	ASN
2	aI	47	ASN
1	bI	28	GLN
1	bI	76	GLN
1	bI	80	ASN
1	bI	161	ASN
2	cI	111	ASN
1	dI	21	ASN
1	dI	76	GLN
1	dI	94	ASN
2	eI	47	ASN
2	eI	76	ASN
1	fI	28	GLN
1	fI	94	ASN
1	fI	161	ASN
2	gI	35	ASN
1	hI	28	GLN
1	jI	32	GLN
2	kI	11	ASN
2	kI	35	ASN
2	kI	63	ASN
1	lI	32	GLN
2	mI	47	ASN
15	dJ	189	GLN
7	AJ	88	GLN
7	AJ	102	GLN

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Mol	Chain	Res	Type
7	AJ	201	GLN
1	BJ	68	ASN
2	CJ	11	ASN
2	CJ	63	ASN
1	DJ	32	GLN
1	DJ	94	ASN
2	EJ	11	ASN
1	FJ	28	GLN
1	FJ	94	ASN
2	GJ	11	ASN
2	GJ	47	ASN
1	HJ	76	GLN
1	HJ	80	ASN
2	IJ	11	ASN
2	IJ	25	GLN
1	JJ	68	ASN
2	KJ	11	ASN
1	LJ	76	GLN
1	LJ	80	ASN
1	LJ	147	GLN
2	MJ	11	ASN
2	MJ	25	GLN
2	MJ	47	ASN
1	NJ	28	GLN
1	NJ	32	GLN
2	OJ	11	ASN
2	OJ	111	ASN
1	PJ	68	ASN
1	PJ	121	ASN
1	PJ	147	GLN
1	PJ	161	ASN
2	QJ	11	ASN
2	QJ	47	ASN
2	QJ	63	ASN
2	QJ	76	ASN
1	RJ	28	GLN
1	RJ	94	ASN
1	RJ	161	ASN
1	TJ	161	ASN
2	UJ	63	ASN
1	VJ	21	ASN
1	VJ	28	GLN

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Mol	Chain	Res	Type
2	WJ	35	ASN
2	WJ	76	ASN
1	XJ	28	GLN
1	XJ	94	ASN
2	YJ	11	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

332 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MEN	FH	71	18	7,7,9	0.99	0	6,8,11	1.18	1 (16%)
2	MEN	s1	72	2	7,8,9	0.93	0	6,9,11	1.40	2 (33%)
2	MEN	XA	72	2	7,8,9	0.88	0	6,9,11	1.78	2 (33%)
2	MEN	RF	72	2	7,8,9	0.84	0	6,9,11	1.13	1 (16%)
2	MEN	LE	72	2,26	7,8,9	1.80	1 (14%)	6,9,11	3.66	3 (50%)
10	MEN	HI	72	10	7,8,9	0.86	0	6,9,11	1.67	2 (33%)
10	MEN	NB	72	10	7,8,9	0.84	0	6,9,11	1.64	2 (33%)
2	MEN	C9	72	2	7,8,9	0.85	0	6,9,11	1.48	2 (33%)
2	MEN	11	72	2	7,8,9	0.95	0	6,9,11	1.29	1 (16%)
18	MEN	qH	71	18	7,7,9	0.95	0	6,8,11	1.92	2 (33%)
2	MEN	XG	72	2,26	7,8,9	1.93	1 (14%)	6,9,11	3.18	2 (33%)
2	MEN	n4	72	2	7,8,9	0.88	0	6,9,11	1.05	0
2	MEN	gI	72	2	7,8,9	0.90	0	6,9,11	1.39	1 (16%)
2	MEN	y4	72	2	7,8,9	1.01	0	6,9,11	1.22	1 (16%)
2	MEN	H5	72	2	7,8,9	0.85	0	6,9,11	1.27	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	TA	72	2	7,8,9	0.84	0	6,9,11	1.74	2 (33%)
2	MEN	BD	72	2	7,8,9	0.97	0	6,9,11	1.13	1 (16%)
2	MEN	i2	72	2	7,8,9	0.88	0	6,9,11	1.53	1 (16%)
2	MEN	jE	72	2,26	7,8,9	1.29	1 (14%)	6,9,11	1.65	1 (16%)
18	MEN	uH	71	18	7,8,9	0.88	0	6,9,11	1.43	2 (33%)
2	MEN	kI	72	2	7,8,9	0.89	0	6,9,11	1.50	1 (16%)
18	MEN	hH	71	18	7,7,9	0.97	0	6,8,11	1.99	1 (16%)
2	MEN	YI	72	2	7,8,9	0.83	0	6,9,11	1.45	1 (16%)
2	MEN	a1	72	2	7,8,9	0.79	0	6,9,11	1.66	2 (33%)
18	MEN	oH	71	18	7,7,9	0.99	0	6,8,11	1.67	1 (16%)
2	MEN	m8	72	2	7,8,9	0.90	0	6,9,11	1.58	2 (33%)
2	MEN	k2	72	2	7,8,9	0.89	0	6,9,11	1.51	1 (16%)
2	MEN	C5	72	2	7,8,9	0.91	0	6,9,11	1.49	2 (33%)
2	MEN	H1	72	2	7,8,9	0.93	0	6,9,11	1.42	1 (16%)
2	MEN	gA	72	2	7,8,9	0.88	0	6,9,11	1.20	1 (16%)
2	MEN	u4	72	2	7,8,9	0.91	0	6,9,11	1.21	1 (16%)
2	MEN	ZE	72	2,26	7,8,9	1.65	1 (14%)	6,9,11	2.27	2 (33%)
18	MEN	wH	71	18	7,8,9	0.94	0	6,9,11	1.46	1 (16%)
2	MEN	vG	72	2,26	7,8,9	1.40	1 (14%)	6,9,11	1.16	1 (16%)
10	MEN	H6	72	10	7,8,9	0.90	0	6,9,11	1.41	2 (33%)
2	MEN	L1	72	2	7,8,9	0.89	0	6,9,11	1.60	1 (16%)
2	MEN	YB	72	2	7,8,9	0.94	0	6,9,11	1.37	1 (16%)
2	MEN	Z8	72	2	7,8,9	0.85	0	6,9,11	1.60	2 (33%)
2	MEN	g7	72	2	7,8,9	0.89	0	6,9,11	1.51	1 (16%)
2	MEN	VI	72	2	7,8,9	0.91	0	6,9,11	1.34	2 (33%)
2	MEN	DA	72	2	7,8,9	0.81	0	6,9,11	1.33	1 (16%)
10	MEN	J7	72	10	7,8,9	0.87	0	6,9,11	1.38	1 (16%)
2	MEN	T3	72	2	7,8,9	0.95	0	6,9,11	3.30	3 (50%)
2	MEN	L3	72	2	7,8,9	0.86	0	6,9,11	1.35	1 (16%)
2	MEN	WJ	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	d1	72	2	7,8,9	0.86	0	6,9,11	1.66	1 (16%)
18	MEN	UH	71	18	7,8,9	0.85	0	6,9,11	1.22	1 (16%)
2	MEN	G9	72	2	7,8,9	0.86	0	6,9,11	1.77	2 (33%)
2	MEN	FA	72	2	7,8,9	0.96	0	6,9,11	1.44	1 (16%)
2	MEN	TB	72	2	7,8,9	0.99	0	6,9,11	1.45	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	q1	72	2	7,8,9	0.94	0	6,9,11	1.50	2 (33%)
2	MEN	e7	72	2	7,8,9	0.89	0	6,9,11	1.40	2 (33%)
2	MEN	DG	72	2,26	7,8,9	1.58	1 (14%)	6,9,11	2.43	2 (33%)
2	MEN	L5	72	2	7,8,9	1.05	0	6,9,11	1.11	1 (16%)
2	MEN	iA	72	2	7,8,9	0.91	0	6,9,11	1.40	1 (16%)
2	MEN	M9	72	2	7,8,9	0.86	0	6,9,11	1.72	2 (33%)
2	MEN	LG	72	2,26	7,8,9	1.83	1 (14%)	6,9,11	3.79	3 (50%)
10	MEN	F2	72	10	7,8,9	0.90	0	6,9,11	1.63	1 (16%)
2	MEN	w1	72	2	7,8,9	0.94	0	6,9,11	1.24	1 (16%)
2	MEN	eA	72	2	7,8,9	0.87	0	6,9,11	1.33	0
2	MEN	jG	72	2,26	7,8,9	1.31	1 (14%)	6,9,11	1.80	2 (33%)
2	MEN	a7	72	2	7,8,9	0.89	0	6,9,11	1.25	1 (16%)
2	MEN	i7	72	2	7,8,9	0.86	0	6,9,11	1.62	2 (33%)
2	MEN	GJ	72	2	7,8,9	0.91	0	6,9,11	1.87	2 (33%)
2	MEN	F4	72	2	7,8,9	0.94	0	6,9,11	1.59	1 (16%)
2	MEN	P8	72	2	7,8,9	0.94	0	6,9,11	1.34	1 (16%)
10	MEN	DB	72	10,6	7,8,9	0.89	0	6,9,11	1.72	2 (33%)
2	MEN	U1	72	2	7,8,9	0.88	0	6,9,11	1.62	2 (33%)
2	MEN	e8	72	2	7,8,9	0.90	0	6,9,11	1.38	1 (16%)
2	MEN	RG	72	2,26	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	DE	72	2,26	7,8,9	1.50	1 (14%)	6,9,11	2.02	2 (33%)
2	MEN	tG	72	2,26	7,8,9	1.18	1 (14%)	6,9,11	1.44	1 (16%)
2	MEN	TE	72	2,26	7,8,9	1.40	1 (14%)	6,9,11	2.23	2 (33%)
2	MEN	hG	72	2,26	7,8,9	1.21	1 (14%)	6,9,11	0.86	0
2	MEN	aI	72	2	7,8,9	0.87	0	6,9,11	1.45	2 (33%)
2	MEN	eI	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	BG	72	2,26	7,8,9	1.62	1 (14%)	6,9,11	3.02	1 (16%)
2	MEN	MJ	72	2	7,8,9	0.84	0	6,9,11	1.82	2 (33%)
2	MEN	V2	72	2	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
10	MEN	LI	72	10	7,8,9	0.83	0	6,9,11	1.85	2 (33%)
2	MEN	j1	72	2	7,8,9	0.85	0	6,9,11	2.41	2 (33%)
10	MEN	DI	72	10	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
2	MEN	kB	72	2	7,8,9	0.89	0	6,9,11	1.51	1 (16%)
2	MEN	W4	72	2	7,8,9	0.87	0	6,9,11	1.61	1 (16%)
2	MEN	c6	72	2	7,8,9	0.89	0	6,9,11	1.10	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	RI	72	2	7,8,9	0.88	0	6,9,11	1.46	2 (33%)
2	MEN	PD	72	2	7,8,9	0.84	0	6,9,11	1.45	1 (16%)
2	MEN	l4	72	2	7,8,9	0.88	0	6,9,11	1.25	2 (33%)
2	MEN	q4	72	2	7,8,9	0.90	0	6,9,11	1.64	1 (16%)
2	MEN	F3	72	2	7,8,9	0.92	0	6,9,11	1.47	1 (16%)
2	MEN	JA	72	2	7,8,9	0.83	0	6,9,11	1.66	1 (16%)
2	MEN	ZG	72	2	7,8,9	0.90	0	6,9,11	1.38	1 (16%)
10	MEN	JI	72	10	7,8,9	0.84	0	6,9,11	1.86	2 (33%)
2	MEN	H3	72	2	7,8,9	0.91	0	6,9,11	1.68	1 (16%)
10	MEN	FF	72	10	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	mI	72	2	7,8,9	0.88	0	6,9,11	1.52	2 (33%)
18	MEN	SH	71	18	7,8,9	0.88	0	6,9,11	1.44	2 (33%)
2	MEN	S4	72	2	7,8,9	0.91	0	6,9,11	1.32	1 (16%)
2	MEN	HD	72	2	7,8,9	0.92	0	6,9,11	1.76	1 (16%)
18	MEN	dH	71	18	7,7,9	0.98	0	6,8,11	1.81	2 (33%)
2	MEN	FC	72	2	7,8,9	0.90	0	6,9,11	1.11	0
2	MEN	eB	72	2	7,8,9	0.86	0	6,9,11	1.50	1 (16%)
10	MEN	FB	72	10	7,8,9	0.87	0	6,9,11	1.60	1 (16%)
2	MEN	iB	72	2	7,8,9	0.93	0	6,9,11	0.94	0
2	MEN	i8	72	2	7,8,9	0.95	0	6,9,11	1.39	1 (16%)
2	MEN	l1	72	2	7,8,9	0.89	0	6,9,11	1.23	1 (16%)
2	MEN	mF	72	2	7,8,9	0.84	0	6,9,11	1.29	1 (16%)
2	MEN	K5	72	2	7,8,9	0.93	0	6,9,11	1.90	2 (33%)
18	MEN	jH	71	18	7,7,9	0.94	0	6,8,11	1.66	1 (16%)
18	MEN	OH	71	18	7,7,9	0.94	0	6,8,11	1.75	2 (33%)
2	MEN	HG	72	2,26	7,8,9	1.58	1 (14%)	6,9,11	2.44	2 (33%)
2	MEN	hE	72	2,26	7,8,9	1.24	1 (14%)	6,9,11	1.16	1 (16%)
2	MEN	P6	72	2	7,8,9	0.83	0	6,9,11	1.59	1 (16%)
18	MEN	BH	71	18	7,7,9	0.94	0	6,8,11	1.92	2 (33%)
2	MEN	V6	72	2	7,8,9	0.83	0	6,9,11	1.54	2 (33%)
18	MEN	IH	71	18	7,7,9	0.90	0	6,8,11	1.86	2 (33%)
2	MEN	k8	72	2	7,8,9	0.95	0	6,9,11	1.43	1 (16%)
2	MEN	Y9	72	2	7,8,9	0.90	0	6,9,11	1.64	1 (16%)
18	MEN	QH	71	18	7,8,9	0.88	0	6,9,11	1.84	2 (33%)
2	MEN	bG	72	2	7,8,9	0.92	0	6,9,11	1.30	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	FD	72	2	7,8,9	0.99	0	6,9,11	1.62	2 (33%)
2	MEN	Q4	72	2	7,8,9	0.89	0	6,9,11	1.65	2 (33%)
2	MEN	h1	72	2	7,8,9	0.92	0	6,9,11	1.76	2 (33%)
2	MEN	g2	72	2	7,8,9	0.89	0	6,9,11	1.41	1 (16%)
2	MEN	N3	72	2	7,8,9	0.93	0	6,9,11	1.47	1 (16%)
2	MEN	JD	72	2	7,8,9	0.86	0	6,9,11	1.43	1 (16%)
2	MEN	P3	72	2	7,8,9	0.86	0	6,9,11	2.01	2 (33%)
2	MEN	J4	72	2	7,8,9	0.87	0	6,9,11	1.53	2 (33%)
10	MEN	D2	72	10	7,8,9	0.87	0	6,9,11	1.40	2 (33%)
2	MEN	lG	72	2,26	7,8,9	1.03	0	6,9,11	1.69	2 (33%)
2	MEN	kA	72	2	7,8,9	0.93	0	6,9,11	1.49	2 (33%)
2	MEN	LC	72	2	7,8,9	0.97	0	6,9,11	0.78	0
2	MEN	NE	72	2,26	7,8,9	1.50	1 (14%)	6,9,11	2.66	2 (33%)
2	MEN	Y2	72	2	7,8,9	0.83	0	6,9,11	1.47	1 (16%)
2	MEN	B4	72	2	7,8,9	0.85	0	6,9,11	1.68	2 (33%)
10	MEN	LF	72	10	7,8,9	0.88	0	6,9,11	2.58	2 (33%)
2	MEN	e2	72	2	7,8,9	0.88	0	6,9,11	1.64	2 (33%)
2	MEN	Y6	72	2	7,8,9	0.93	0	6,9,11	1.33	1 (16%)
2	MEN	HC	72	2	7,8,9	0.81	0	6,9,11	1.18	1 (16%)
10	MEN	FI	72	10	7,8,9	0.90	0	6,9,11	1.55	1 (16%)
2	MEN	BE	72	2,26	7,8,9	1.54	1 (14%)	6,9,11	2.69	1 (16%)
2	MEN	CC	72	2	7,8,9	0.65	0	6,9,11	0.77	0
2	MEN	V8	72	2	7,8,9	0.81	0	6,9,11	1.57	2 (33%)
2	MEN	iF	72	2	7,8,9	0.84	0	6,9,11	1.40	1 (16%)
2	MEN	bE	72	2,26	7,8,9	1.48	1 (14%)	6,9,11	2.02	2 (33%)
2	MEN	D4	72	2	7,8,9	0.90	0	6,9,11	1.59	2 (33%)
2	MEN	YF	72	2	7,8,9	0.94	0	6,9,11	1.29	1 (16%)
2	MEN	c8	72	2	7,8,9	0.89	0	6,9,11	1.54	1 (16%)
2	MEN	D8	72	2	7,8,9	0.81	0	6,9,11	1.34	1 (16%)
10	MEN	NI	72	10	7,8,9	0.91	0	6,9,11	1.40	2 (33%)
10	MEN	L7	72	10	7,8,9	0.87	0	6,9,11	2.23	1 (16%)
2	MEN	X8	72	2	7,8,9	0.87	0	6,9,11	1.81	2 (33%)
2	MEN	n1	72	2	7,8,9	0.91	0	6,9,11	1.36	1 (16%)
2	MEN	IJ	72	2	7,8,9	0.84	0	6,9,11	1.72	1 (16%)
2	MEN	SJ	72	2	7,8,9	0.96	0	6,9,11	1.37	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	RA	72	2	7,8,9	0.86	0	6,9,11	1.47	1 (16%)
2	MEN	DD	72	2	7,8,9	0.90	0	6,9,11	1.10	1 (16%)
10	MEN	JB	72	10	7,8,9	0.91	0	6,9,11	1.59	1 (16%)
2	MEN	y1	72	2	7,8,9	0.94	0	6,9,11	1.21	1 (16%)
18	MEN	fH	71	18	7,7,9	0.95	0	6,8,11	1.78	2 (33%)
2	MEN	P2	72	2	7,8,9	0.90	0	6,9,11	1.28	0
2	MEN	X3	72	2	7,8,9	0.93	0	6,9,11	1.64	2 (33%)
2	MEN	XD	72	2	7,8,9	0.92	0	6,9,11	1.59	2 (33%)
2	MEN	YJ	72	2	7,8,9	0.85	0	6,9,11	1.94	2 (33%)
10	MEN	J6	72	10	7,8,9	0.88	0	6,9,11	1.56	1 (16%)
2	MEN	cA	72	2	7,8,9	0.87	0	6,9,11	1.63	1 (16%)
2	MEN	CJ	72	2	7,8,9	0.86	0	6,9,11	1.43	2 (33%)
10	MEN	L6	72	10	7,8,9	0.96	0	6,9,11	1.60	2 (33%)
2	MEN	L8	72	2	7,8,9	0.97	0	6,9,11	1.19	1 (16%)
2	MEN	lE	72	2,26	7,8,9	1.01	0	6,9,11	1.78	1 (16%)
2	MEN	cB	72	2	7,8,9	0.90	0	6,9,11	1.07	0
18	MEN	nH	71	18	7,7,9	0.95	0	6,8,11	1.86	2 (33%)
2	MEN	i6	72	2	7,8,9	0.92	0	6,9,11	1.19	1 (16%)
2	MEN	vE	72	2,26	7,8,9	1.39	1 (14%)	6,9,11	1.40	1 (16%)
2	MEN	LD	72	2	7,8,9	0.90	0	6,9,11	1.20	0
2	MEN	kF	72	2	7,8,9	0.91	0	6,9,11	1.11	1 (16%)
2	MEN	IC	72	2	7,8,9	0.90	0	6,9,11	1.69	1 (16%)
10	MEN	D6	72	10,6	7,8,9	0.88	0	6,9,11	1.60	2 (33%)
2	MEN	TG	72	2,26	7,8,9	1.41	1 (14%)	6,9,11	2.25	2 (33%)
2	MEN	a6	72	2	7,8,9	0.88	0	6,9,11	1.69	2 (33%)
2	MEN	LA	72	2	7,8,9	0.95	0	6,9,11	1.20	1 (16%)
2	MEN	m2	72	2	7,8,9	0.88	0	6,9,11	1.44	2 (33%)
2	MEN	g8	72	2	7,8,9	0.89	0	6,9,11	1.27	1 (16%)
2	MEN	u1	72	2	7,8,9	1.00	0	6,9,11	0.90	1 (16%)
2	MEN	rE	72	2,26	7,8,9	1.25	1 (14%)	6,9,11	1.09	1 (16%)
2	MEN	UJ	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
2	MEN	cI	72	2	7,8,9	0.89	0	6,9,11	1.27	1 (16%)
10	MEN	F6	72	10	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	TD	72	2,11	7,8,9	0.86	0	6,9,11	3.06	2 (33%)
2	MEN	O1	72	2	7,8,9	0.92	0	6,9,11	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	ND	72	2	7,8,9	0.93	0	6,9,11	1.45	1 (16%)
2	MEN	HA	72	2	7,8,9	0.87	0	6,9,11	1.62	1 (16%)
2	MEN	VB	72	2	7,8,9	0.82	0	6,9,11	1.58	1 (16%)
2	MEN	JG	72	2,26	7,8,9	1.47	1 (14%)	6,9,11	2.19	2 (33%)
2	MEN	pG	72	2,26	7,8,9	1.11	0	6,9,11	1.34	1 (16%)
2	MEN	O9	72	2	7,8,9	0.92	0	6,9,11	1.30	2 (33%)
2	MEN	PI	72	2	7,8,9	0.90	0	6,9,11	1.24	0
2	MEN	Y7	72	2	7,8,9	0.91	0	6,9,11	1.03	0
2	MEN	14	72	2	7,8,9	0.91	0	6,9,11	1.48	2 (33%)
2	MEN	PF	72	2	7,8,9	0.88	0	6,9,11	1.67	2 (33%)
2	MEN	S9	72	2	7,8,9	0.94	0	6,9,11	1.34	1 (16%)
2	MEN	Q1	72	2	7,8,9	0.89	0	6,9,11	1.69	2 (33%)
18	MEN	MH	71	18	7,7,9	0.93	0	6,8,11	1.89	2 (33%)
10	MEN	H2	72	10	7,8,9	0.87	0	6,9,11	1.53	2 (33%)
2	MEN	S1	72	2	7,8,9	0.91	0	6,9,11	1.31	1 (16%)
2	MEN	U4	72	2	7,8,9	0.85	0	6,9,11	1.62	1 (16%)
2	MEN	XE	72	2,26	7,8,9	1.87	1 (14%)	6,9,11	3.03	2 (33%)
2	MEN	g6	72	2	7,8,9	0.86	0	6,9,11	1.54	1 (16%)
2	MEN	TI	72	2	7,8,9	0.82	0	6,9,11	1.63	2 (33%)
2	MEN	RB	72	2	7,8,9	0.92	0	6,9,11	1.50	1 (16%)
2	MEN	dE	72	2,26	7,8,9	1.44	1 (14%)	6,9,11	1.79	1 (16%)
2	MEN	Z1	72	2	7,8,9	0.82	0	6,9,11	1.75	2 (33%)
2	MEN	aF	72	2	7,8,9	0.89	0	6,9,11	1.33	1 (16%)
2	MEN	c2	72	2	7,8,9	0.90	0	6,9,11	1.22	0
2	MEN	tE	72	2,26	7,8,9	1.20	1 (14%)	6,9,11	1.66	1 (16%)
2	MEN	W1	72	2	7,8,9	0.88	0	6,9,11	1.49	1 (16%)
2	MEN	f4	72	2	7,8,9	0.97	0	6,9,11	1.08	1 (16%)
2	MEN	R8	72	2	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	mA	72	2	7,8,9	0.91	0	6,9,11	1.52	2 (33%)
2	MEN	T6	72	2	7,8,9	0.96	0	6,9,11	1.44	1 (16%)
2	MEN	h4	72	2	7,8,9	0.91	0	6,9,11	1.91	2 (33%)
2	MEN	a4	72	2	7,8,9	0.81	0	6,9,11	1.71	2 (33%)
10	MEN	HF	72	10	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
2	MEN	rG	72	2,26	7,8,9	1.28	1 (14%)	6,9,11	0.99	1 (16%)
2	MEN	O4	72	2	7,8,9	0.94	0	6,9,11	1.29	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	N8	72	2	7,8,9	0.81	0	6,9,11	1.70	2 (33%)
2	MEN	eF	72	2	7,8,9	0.91	0	6,9,11	1.27	1 (16%)
2	MEN	EJ	72	2	7,8,9	0.80	0	6,9,11	1.57	2 (33%)
2	MEN	PB	72	2	7,8,9	0.85	0	6,9,11	1.61	2 (33%)
2	MEN	R7	72	2	7,8,9	0.86	0	6,9,11	1.22	1 (16%)
2	MEN	F1	72	2	7,8,9	1.04	0	6,9,11	2.71	2 (33%)
2	MEN	nG	72	2,26	7,8,9	1.39	1 (14%)	6,9,11	1.48	1 (16%)
2	MEN	dG	72	2,26	7,8,9	1.43	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	T8	72	2	7,8,9	0.83	0	6,9,11	1.72	1 (16%)
10	MEN	JF	72	10	7,8,9	0.82	0	6,9,11	1.66	1 (16%)
2	MEN	H4	72	2	7,8,9	0.94	0	6,9,11	1.42	1 (16%)
2	MEN	I5	72	2	7,8,9	0.89	0	6,9,11	1.79	1 (16%)
2	MEN	NA	72	2	7,8,9	0.80	0	6,9,11	1.73	2 (33%)
18	MEN	kH	71	18	7,7,9	0.93	0	6,8,11	2.09	2 (33%)
2	MEN	P7	72	2	7,8,9	0.86	0	6,9,11	1.54	1 (16%)
2	MEN	Z4	72	2	7,8,9	0.85	0	6,9,11	1.71	2 (33%)
2	MEN	AC	72	2	7,8,9	1.08	0	6,9,11	1.43	1 (16%)
18	MEN	HH	71	18	7,7,9	0.93	0	6,8,11	1.53	1 (16%)
2	MEN	G5	72	2	7,8,9	0.91	0	6,9,11	1.07	0
2	MEN	s4	72	2	7,8,9	0.86	0	6,9,11	1.39	2 (33%)
2	MEN	B5	72	2	7,8,9	0.90	0	6,9,11	1.26	2 (33%)
2	MEN	Q9	72	2	7,8,9	0.81	0	6,9,11	1.70	2 (33%)
2	MEN	d4	72	2	7,8,9	0.88	0	6,9,11	1.70	1 (16%)
2	MEN	V3	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	VA	72	2	7,8,9	0.80	0	6,9,11	1.70	2 (33%)
2	MEN	VG	72	2,26	7,8,9	1.36	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	GC	72	2	7,8,9	0.91	0	6,9,11	1.07	0
2	MEN	I9	72	2	7,8,9	0.85	0	6,9,11	1.65	1 (16%)
2	MEN	K9	72	2	7,8,9	0.90	0	6,9,11	1.43	1 (16%)
18	MEN	LH	71	18	7,7,9	0.96	0	6,8,11	1.68	2 (33%)
2	MEN	J3	72	2	7,8,9	0.89	0	6,9,11	1.21	1 (16%)
2	MEN	W9	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
18	MEN	sH	71	18	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	T2	72	2	7,8,9	0.83	0	6,9,11	1.61	2 (33%)
10	MEN	F7	72	10	7,8,9	0.89	0	6,9,11	1.38	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	RD	72	2	7,8,9	0.92	0	6,9,11	1.20	0
18	MEN	DH	71	18	7,7,9	0.95	0	6,8,11	1.74	2 (33%)
2	MEN	c7	72	2	7,8,9	0.84	0	6,9,11	1.64	1 (16%)
2	MEN	R3	72	2	7,8,9	0.93	0	6,9,11	1.23	0
10	MEN	LB	72	10	7,8,9	0.96	0	6,9,11	1.56	2 (33%)
2	MEN	H8	72	2	7,8,9	0.89	0	6,9,11	1.75	1 (16%)
10	MEN	J2	72	10	7,8,9	0.85	0	6,9,11	1.87	2 (33%)
2	MEN	VE	72	2,26	7,8,9	1.40	1 (14%)	6,9,11	1.50	1 (16%)
2	MEN	RE	72	2,26	7,8,9	1.72	1 (14%)	6,9,11	3.06	2 (33%)
2	MEN	KJ	72	2	7,8,9	0.87	0	6,9,11	1.63	2 (33%)
2	MEN	PE	72	2,26	7,8,9	1.60	1 (14%)	6,9,11	2.64	3 (50%)
2	MEN	D3	72	2	7,8,9	0.90	0	6,9,11	1.34	1 (16%)
2	MEN	mB	72	2	7,8,9	0.92	0	6,9,11	1.24	1 (16%)
2	MEN	VD	72	2	7,8,9	0.86	0	6,9,11	1.40	1 (16%)
10	MEN	HB	72	10	7,8,9	0.92	0	6,9,11	1.30	2 (33%)
2	MEN	k6	72	2	7,8,9	0.88	0	6,9,11	1.49	1 (16%)
2	MEN	V7	72	2	7,8,9	0.85	0	6,9,11	1.52	1 (16%)
2	MEN	k7	72	2	7,8,9	0.89	0	6,9,11	1.50	1 (16%)
10	MEN	H7	72	10	7,8,9	0.86	0	6,9,11	1.43	1 (16%)
2	MEN	T7	72	2	7,8,9	0.88	0	6,9,11	1.57	1 (16%)
2	MEN	cF	72	2	7,8,9	0.82	0	6,9,11	1.84	1 (16%)
2	MEN	D1	72	2	7,8,9	0.87	0	6,9,11	1.59	2 (33%)
2	MEN	Y4	72	2	7,8,9	0.88	0	6,9,11	1.36	1 (16%)
2	MEN	Y1	72	2	7,8,9	0.87	0	6,9,11	1.31	1 (16%)
2	MEN	FE	72	2,26	7,8,9	1.89	1 (14%)	6,9,11	3.65	3 (50%)
10	MEN	N7	72	10	7,8,9	0.94	0	6,9,11	1.26	1 (16%)
2	MEN	nE	72	2,26	7,8,9	1.34	1 (14%)	6,9,11	1.51	1 (16%)
2	MEN	gF	72	2	7,8,9	0.90	0	6,9,11	1.62	2 (33%)
2	MEN	j4	72	2	7,8,9	0.91	0	6,9,11	2.20	2 (33%)
2	MEN	ZA	72	2	7,8,9	0.86	0	6,9,11	1.65	2 (33%)
2	MEN	fE	72	2,26	7,8,9	1.29	1 (14%)	6,9,11	2.26	2 (33%)
2	MEN	m6	72	2	7,8,9	0.91	0	6,9,11	1.40	1 (16%)
2	MEN	PA	72	2	7,8,9	0.94	0	6,9,11	1.33	1 (16%)
2	MEN	R6	72	2	7,8,9	0.91	0	6,9,11	1.47	1 (16%)
2	MEN	F8	72	2	7,8,9	1.00	0	6,9,11	1.37	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MEN	N6	72	10	7,8,9	0.85	0	6,9,11	1.51	2 (33%)
2	MEN	e6	72	2	7,8,9	0.84	0	6,9,11	1.48	1 (16%)
2	MEN	U9	72	2	7,8,9	0.97	0	6,9,11	1.66	1 (16%)
2	MEN	R2	72	2	7,8,9	0.89	0	6,9,11	1.44	2 (33%)
2	MEN	F5	72	2	7,8,9	0.89	0	6,9,11	1.08	0
10	MEN	N2	72	10	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	gB	72	2	7,8,9	0.86	0	6,9,11	1.55	1 (16%)
2	MEN	VF	72	2	7,8,9	0.86	0	6,9,11	1.61	2 (33%)
2	MEN	pE	72	2,26	7,8,9	1.00	0	6,9,11	1.82	2 (33%)
2	MEN	FG	72	2,26	7,8,9	1.92	1 (14%)	6,9,11	3.70	3 (50%)
2	MEN	f1	72	2	7,8,9	0.96	0	6,9,11	1.09	1 (16%)
2	MEN	fG	72	2,26	7,8,9	1.30	1 (14%)	6,9,11	2.30	2 (33%)
2	MEN	QJ	72	2	7,8,9	0.82	0	6,9,11	1.77	2 (33%)
2	MEN	PG	72	2,26	7,8,9	1.56	1 (14%)	6,9,11	2.52	2 (33%)
2	MEN	m7	72	2	7,8,9	0.87	0	6,9,11	1.40	1 (16%)
2	MEN	JE	72	2,26	7,8,9	1.54	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	A5	72	2	7,8,9	1.16	0	6,9,11	1.89	2 (33%)
2	MEN	NG	72	2,26	7,8,9	1.51	1 (14%)	6,9,11	2.75	2 (33%)
2	MEN	B1	72	2	7,8,9	0.86	0	6,9,11	1.40	1 (16%)
2	MEN	J8	72	2	7,8,9	0.84	0	6,9,11	1.65	1 (16%)
2	MEN	a2	72	2	7,8,9	0.88	0	6,9,11	1.44	2 (33%)
2	MEN	iI	72	2	7,8,9	0.87	0	6,9,11	1.49	1 (16%)
2	MEN	HE	72	2,26	7,8,9	1.58	1 (14%)	6,9,11	2.51	2 (33%)
2	MEN	w4	72	2	7,8,9	0.93	0	6,9,11	0.94	0
2	MEN	E9	72	2	7,8,9	0.86	0	6,9,11	1.44	1 (16%)
2	MEN	TF	72	2	7,8,9	0.93	0	6,9,11	1.79	2 (33%)
2	MEN	B3	72	2	7,8,9	0.99	0	6,9,11	0.95	0
10	MEN	DF	72	10	7,8,9	0.85	0	6,9,11	1.59	2 (33%)
2	MEN	L4	72	2	7,8,9	0.90	0	6,9,11	1.52	1 (16%)
2	MEN	J1	72	2	7,8,9	0.93	0	6,9,11	1.55	1 (16%)
10	MEN	D7	72	10	7,8,9	0.89	0	6,9,11	1.59	2 (33%)
2	MEN	OJ	72	2	7,8,9	0.93	0	6,9,11	1.31	2 (33%)
2	MEN	KC	72	2	7,8,9	0.91	0	6,9,11	1.69	2 (33%)
10	MEN	L2	72	10	7,8,9	0.80	0	6,9,11	1.84	2 (33%)
2	MEN	BC	72	2	7,8,9	0.65	0	6,9,11	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	aB	72	2	7,8,9	0.86	0	6,9,11	1.71	2 (33%)
10	MEN	NF	72	10	7,8,9	0.96	0	6,9,11	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MEN	FH	71	18	-	4/6/6/10	-
2	MEN	s1	72	2	-	4/7/8/10	-
2	MEN	XA	72	2	-	4/7/8/10	-
2	MEN	RF	72	2	-	2/7/8/10	-
2	MEN	LE	72	2,26	-	3/7/8/10	-
10	MEN	HI	72	10	-	2/7/8/10	-
10	MEN	NB	72	10	-	4/7/8/10	-
2	MEN	C9	72	2	-	4/7/8/10	-
2	MEN	11	72	2	-	4/7/8/10	-
18	MEN	qH	71	18	-	2/6/6/10	-
2	MEN	XG	72	2,26	-	2/7/8/10	-
2	MEN	n4	72	2	-	2/7/8/10	-
2	MEN	gI	72	2	-	4/7/8/10	-
2	MEN	y4	72	2	-	3/7/8/10	-
2	MEN	H5	72	2	-	2/7/8/10	-
2	MEN	TA	72	2	-	2/7/8/10	-
2	MEN	BD	72	2	-	4/7/8/10	-
2	MEN	i2	72	2	-	4/7/8/10	-
2	MEN	jE	72	2,26	-	4/7/8/10	-
18	MEN	uH	71	18	-	4/7/8/10	-
2	MEN	kI	72	2	-	5/7/8/10	-
18	MEN	hH	71	18	-	2/6/6/10	-
2	MEN	YI	72	2	-	4/7/8/10	-
2	MEN	a1	72	2	-	4/7/8/10	-
18	MEN	oH	71	18	-	2/6/6/10	-
2	MEN	m8	72	2	-	4/7/8/10	-
2	MEN	k2	72	2	-	5/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	C5	72	2	-	4/7/8/10	-
2	MEN	H1	72	2	-	4/7/8/10	-
2	MEN	gA	72	2	-	3/7/8/10	-
2	MEN	u4	72	2	-	3/7/8/10	-
2	MEN	ZE	72	2,26	-	3/7/8/10	-
18	MEN	wH	71	18	-	4/7/8/10	-
2	MEN	vG	72	2,26	-	1/7/8/10	-
10	MEN	H6	72	10	-	4/7/8/10	-
2	MEN	L1	72	2	-	4/7/8/10	-
2	MEN	YB	72	2	-	5/7/8/10	-
2	MEN	Z8	72	2	-	4/7/8/10	-
2	MEN	g7	72	2	-	3/7/8/10	-
2	MEN	VI	72	2	-	2/7/8/10	-
2	MEN	DA	72	2	-	4/7/8/10	-
10	MEN	J7	72	10	-	3/7/8/10	-
2	MEN	T3	72	2	-	2/7/8/10	-
2	MEN	L3	72	2	-	5/7/8/10	-
2	MEN	WJ	72	2	-	5/7/8/10	-
2	MEN	d1	72	2	-	4/7/8/10	-
18	MEN	UH	71	18	-	2/7/8/10	-
2	MEN	G9	72	2	-	4/7/8/10	-
2	MEN	FA	72	2	-	4/7/8/10	-
2	MEN	TB	72	2	-	3/7/8/10	-
2	MEN	q1	72	2	-	2/7/8/10	-
2	MEN	e7	72	2	-	2/7/8/10	-
2	MEN	DG	72	2,26	-	2/7/8/10	-
2	MEN	L5	72	2	-	5/7/8/10	-
2	MEN	iA	72	2	-	4/7/8/10	-
2	MEN	M9	72	2	-	2/7/8/10	-
2	MEN	LG	72	2,26	-	3/7/8/10	-
10	MEN	F2	72	10	-	2/7/8/10	-
2	MEN	w1	72	2	-	2/7/8/10	-
2	MEN	eA	72	2	-	5/7/8/10	-
2	MEN	jG	72	2,26	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	a7	72	2	-	4/7/8/10	-
2	MEN	i7	72	2	-	3/7/8/10	-
2	MEN	GJ	72	2	-	4/7/8/10	-
2	MEN	F4	72	2	-	5/7/8/10	-
2	MEN	P8	72	2	-	4/7/8/10	-
10	MEN	DB	72	10,6	-	4/7/8/10	-
2	MEN	U1	72	2	-	4/7/8/10	-
2	MEN	e8	72	2	-	5/7/8/10	-
2	MEN	RG	72	2,26	-	2/7/8/10	-
2	MEN	DE	72	2,26	-	4/7/8/10	-
2	MEN	tG	72	2,26	-	4/7/8/10	-
2	MEN	TE	72	2,26	-	3/7/8/10	-
2	MEN	hG	72	2,26	-	2/7/8/10	-
2	MEN	aI	72	2	-	3/7/8/10	-
2	MEN	eI	72	2	-	5/7/8/10	-
2	MEN	BG	72	2,26	-	2/7/8/10	-
2	MEN	MJ	72	2	-	2/7/8/10	-
2	MEN	V2	72	2	-	2/7/8/10	-
10	MEN	LI	72	10	-	4/7/8/10	-
2	MEN	j1	72	2	-	4/7/8/10	-
10	MEN	DI	72	10	-	2/7/8/10	-
2	MEN	kB	72	2	-	4/7/8/10	-
2	MEN	W4	72	2	-	4/7/8/10	-
2	MEN	c6	72	2	-	3/7/8/10	-
2	MEN	RI	72	2	-	4/7/8/10	-
2	MEN	PD	72	2	-	4/7/8/10	-
2	MEN	l4	72	2	-	4/7/8/10	-
2	MEN	q4	72	2	-	3/7/8/10	-
2	MEN	F3	72	2	-	1/7/8/10	-
2	MEN	JA	72	2	-	4/7/8/10	-
2	MEN	ZG	72	2	-	5/7/8/10	-
10	MEN	JI	72	10	-	2/7/8/10	-
2	MEN	H3	72	2	-	4/7/8/10	-
10	MEN	FF	72	10	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	mI	72	2	-	4/7/8/10	-
18	MEN	SH	71	18	-	4/7/8/10	-
2	MEN	S4	72	2	-	4/7/8/10	-
2	MEN	HD	72	2	-	4/7/8/10	-
18	MEN	dH	71	18	-	2/6/6/10	-
2	MEN	FC	72	2	-	4/7/8/10	-
2	MEN	eB	72	2	-	4/7/8/10	-
10	MEN	FB	72	10	-	3/7/8/10	-
2	MEN	iB	72	2	-	2/7/8/10	-
2	MEN	i8	72	2	-	4/7/8/10	-
2	MEN	l1	72	2	-	5/7/8/10	-
2	MEN	mF	72	2	-	4/7/8/10	-
2	MEN	K5	72	2	-	2/7/8/10	-
18	MEN	jH	71	18	-	2/6/6/10	-
18	MEN	OH	71	18	-	0/6/6/10	-
2	MEN	HG	72	2,26	-	2/7/8/10	-
2	MEN	hE	72	2,26	-	1/7/8/10	-
2	MEN	P6	72	2	-	3/7/8/10	-
18	MEN	BH	71	18	-	2/6/6/10	-
2	MEN	V6	72	2	-	4/7/8/10	-
18	MEN	IH	71	18	-	3/6/6/10	-
2	MEN	k8	72	2	-	3/7/8/10	-
2	MEN	Y9	72	2	-	4/7/8/10	-
18	MEN	QH	71	18	-	2/7/8/10	-
2	MEN	bG	72	2	-	4/7/8/10	-
2	MEN	FD	72	2	-	4/7/8/10	-
2	MEN	Q4	72	2	-	4/7/8/10	-
2	MEN	h1	72	2	-	5/7/8/10	-
2	MEN	g2	72	2	-	4/7/8/10	-
2	MEN	N3	72	2	-	4/7/8/10	-
2	MEN	JD	72	2	-	1/7/8/10	-
2	MEN	P3	72	2	-	4/7/8/10	-
2	MEN	J4	72	2	-	5/7/8/10	-
10	MEN	D2	72	10	-	2/7/8/10	-
2	MEN	lG	72	2,26	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kA	72	2	-	4/7/8/10	-
2	MEN	LC	72	2	-	5/7/8/10	-
2	MEN	NE	72	2,26	-	2/7/8/10	-
2	MEN	Y2	72	2	-	4/7/8/10	-
2	MEN	B4	72	2	-	3/7/8/10	-
10	MEN	LF	72	10	-	2/7/8/10	-
2	MEN	e2	72	2	-	4/7/8/10	-
2	MEN	Y6	72	2	-	5/7/8/10	-
2	MEN	HC	72	2	-	2/7/8/10	-
10	MEN	FI	72	10	-	3/7/8/10	-
2	MEN	BE	72	2,26	-	2/7/8/10	-
2	MEN	CC	72	2	-	3/7/8/10	-
2	MEN	V8	72	2	-	4/7/8/10	-
2	MEN	iF	72	2	-	4/7/8/10	-
2	MEN	bE	72	2,26	-	4/7/8/10	-
2	MEN	D4	72	2	-	4/7/8/10	-
2	MEN	YF	72	2	-	4/7/8/10	-
2	MEN	c8	72	2	-	4/7/8/10	-
2	MEN	D8	72	2	-	4/7/8/10	-
10	MEN	NI	72	10	-	3/7/8/10	-
10	MEN	L7	72	10	-	2/7/8/10	-
2	MEN	X8	72	2	-	4/7/8/10	-
2	MEN	n1	72	2	-	4/7/8/10	-
2	MEN	IJ	72	2	-	4/7/8/10	-
2	MEN	SJ	72	2	-	4/7/8/10	-
2	MEN	RA	72	2	-	3/7/8/10	-
2	MEN	DD	72	2	-	3/7/8/10	-
10	MEN	JB	72	10	-	2/7/8/10	-
2	MEN	y1	72	2	-	2/7/8/10	-
18	MEN	fH	71	18	-	4/6/6/10	-
2	MEN	P2	72	2	-	4/7/8/10	-
2	MEN	X3	72	2	-	4/7/8/10	-
2	MEN	XD	72	2	-	4/7/8/10	-
2	MEN	YJ	72	2	-	0/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	J6	72	10	-	2/7/8/10	-
2	MEN	cA	72	2	-	4/7/8/10	-
2	MEN	CJ	72	2	-	4/7/8/10	-
10	MEN	L6	72	10	-	4/7/8/10	-
2	MEN	L8	72	2	-	4/7/8/10	-
2	MEN	lE	72	2,26	-	5/7/8/10	-
2	MEN	cB	72	2	-	3/7/8/10	-
18	MEN	nH	71	18	-	3/6/6/10	-
2	MEN	i6	72	2	-	3/7/8/10	-
2	MEN	vE	72	2,26	-	2/7/8/10	-
2	MEN	LD	72	2	-	5/7/8/10	-
2	MEN	kF	72	2	-	4/7/8/10	-
2	MEN	IC	72	2	-	2/7/8/10	-
10	MEN	D6	72	10,6	-	4/7/8/10	-
2	MEN	TG	72	2,26	-	2/7/8/10	-
2	MEN	a6	72	2	-	4/7/8/10	-
2	MEN	LA	72	2	-	4/7/8/10	-
2	MEN	m2	72	2	-	4/7/8/10	-
2	MEN	g8	72	2	-	2/7/8/10	-
2	MEN	u1	72	2	-	3/7/8/10	-
2	MEN	rE	72	2,26	-	4/7/8/10	-
2	MEN	UJ	72	2	-	4/7/8/10	-
2	MEN	cI	72	2	-	2/7/8/10	-
10	MEN	F6	72	10	-	3/7/8/10	-
2	MEN	TD	72	2,11	-	6/7/8/10	-
2	MEN	O1	72	2	-	4/7/8/10	-
2	MEN	ND	72	2	-	4/7/8/10	-
2	MEN	HA	72	2	-	4/7/8/10	-
2	MEN	VB	72	2	-	4/7/8/10	-
2	MEN	JG	72	2,26	-	2/7/8/10	-
2	MEN	pG	72	2,26	-	3/7/8/10	-
2	MEN	O9	72	2	-	2/7/8/10	-
2	MEN	PI	72	2	-	4/7/8/10	-
2	MEN	Y7	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	14	72	2	-	4/7/8/10	-
2	MEN	PF	72	2	-	4/7/8/10	-
2	MEN	S9	72	2	-	4/7/8/10	-
2	MEN	Q1	72	2	-	4/7/8/10	-
18	MEN	MH	71	18	-	2/6/6/10	-
10	MEN	H2	72	10	-	2/7/8/10	-
2	MEN	S1	72	2	-	4/7/8/10	-
2	MEN	U4	72	2	-	4/7/8/10	-
2	MEN	XE	72	2,26	-	2/7/8/10	-
2	MEN	g6	72	2	-	4/7/8/10	-
2	MEN	TI	72	2	-	3/7/8/10	-
2	MEN	RB	72	2	-	3/7/8/10	-
2	MEN	dE	72	2,26	-	2/7/8/10	-
2	MEN	Z1	72	2	-	4/7/8/10	-
2	MEN	aF	72	2	-	3/7/8/10	-
2	MEN	c2	72	2	-	2/7/8/10	-
2	MEN	tE	72	2,26	-	4/7/8/10	-
2	MEN	W1	72	2	-	4/7/8/10	-
2	MEN	f4	72	2	-	3/7/8/10	-
2	MEN	R8	72	2	-	3/7/8/10	-
2	MEN	mA	72	2	-	4/7/8/10	-
2	MEN	T6	72	2	-	3/7/8/10	-
2	MEN	h4	72	2	-	4/7/8/10	-
2	MEN	a4	72	2	-	4/7/8/10	-
10	MEN	HF	72	10	-	4/7/8/10	-
2	MEN	rG	72	2,26	-	3/7/8/10	-
2	MEN	O4	72	2	-	4/7/8/10	-
2	MEN	N8	72	2	-	2/7/8/10	-
2	MEN	eF	72	2	-	3/7/8/10	-
2	MEN	EJ	72	2	-	4/7/8/10	-
2	MEN	PB	72	2	-	3/7/8/10	-
2	MEN	R7	72	2	-	2/7/8/10	-
2	MEN	F1	72	2	-	6/7/8/10	-
2	MEN	nG	72	2,26	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	dG	72	2,26	-	3/7/8/10	-
2	MEN	T8	72	2	-	2/7/8/10	-
10	MEN	JF	72	10	-	1/7/8/10	-
2	MEN	H4	72	2	-	4/7/8/10	-
2	MEN	I5	72	2	-	2/7/8/10	-
2	MEN	NA	72	2	-	4/7/8/10	-
18	MEN	kH	71	18	-	1/6/6/10	-
2	MEN	P7	72	2	-	4/7/8/10	-
2	MEN	Z4	72	2	-	4/7/8/10	-
2	MEN	AC	72	2	-	2/7/8/10	-
18	MEN	HH	71	18	-	1/6/6/10	-
2	MEN	G5	72	2	-	4/7/8/10	-
2	MEN	s4	72	2	-	2/7/8/10	-
2	MEN	B5	72	2	-	4/7/8/10	-
2	MEN	Q9	72	2	-	4/7/8/10	-
2	MEN	d4	72	2	-	4/7/8/10	-
2	MEN	V3	72	2	-	4/7/8/10	-
2	MEN	VA	72	2	-	4/7/8/10	-
2	MEN	VG	72	2,26	-	4/7/8/10	-
2	MEN	GC	72	2	-	4/7/8/10	-
2	MEN	I9	72	2	-	4/7/8/10	-
2	MEN	K9	72	2	-	4/7/8/10	-
18	MEN	LH	71	18	-	4/6/6/10	-
2	MEN	J3	72	2	-	2/7/8/10	-
2	MEN	W9	72	2	-	4/7/8/10	-
18	MEN	sH	71	18	-	4/7/8/10	-
2	MEN	T2	72	2	-	3/7/8/10	-
10	MEN	F7	72	10	-	2/7/8/10	-
2	MEN	RD	72	2	-	4/7/8/10	-
18	MEN	DH	71	18	-	2/6/6/10	-
2	MEN	c7	72	2	-	4/7/8/10	-
2	MEN	R3	72	2	-	4/7/8/10	-
10	MEN	LB	72	10	-	4/7/8/10	-
2	MEN	H8	72	2	-	4/7/8/10	-
10	MEN	J2	72	10	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	VE	72	2,26	-	2/7/8/10	-
2	MEN	RE	72	2,26	-	2/7/8/10	-
2	MEN	KJ	72	2	-	5/7/8/10	-
2	MEN	PE	72	2,26	-	2/7/8/10	-
2	MEN	D3	72	2	-	2/7/8/10	-
2	MEN	mB	72	2	-	2/7/8/10	-
2	MEN	VD	72	2	-	4/7/8/10	-
10	MEN	HB	72	10	-	4/7/8/10	-
2	MEN	k6	72	2	-	4/7/8/10	-
2	MEN	V7	72	2	-	4/7/8/10	-
2	MEN	k7	72	2	-	3/7/8/10	-
10	MEN	H7	72	10	-	4/7/8/10	-
2	MEN	T7	72	2	-	4/7/8/10	-
2	MEN	cF	72	2	-	4/7/8/10	-
2	MEN	D1	72	2	-	4/7/8/10	-
2	MEN	Y4	72	2	-	4/7/8/10	-
2	MEN	Y1	72	2	-	4/7/8/10	-
2	MEN	FE	72	2,26	-	2/7/8/10	-
10	MEN	N7	72	10	-	2/7/8/10	-
2	MEN	nE	72	2,26	-	3/7/8/10	-
2	MEN	gF	72	2	-	3/7/8/10	-
2	MEN	j4	72	2	-	5/7/8/10	-
2	MEN	ZA	72	2	-	4/7/8/10	-
2	MEN	fE	72	2,26	-	2/7/8/10	-
2	MEN	m6	72	2	-	3/7/8/10	-
2	MEN	PA	72	2	-	4/7/8/10	-
2	MEN	R6	72	2	-	3/7/8/10	-
2	MEN	F8	72	2	-	4/7/8/10	-
10	MEN	N6	72	10	-	4/7/8/10	-
2	MEN	e6	72	2	-	2/7/8/10	-
2	MEN	U9	72	2	-	3/7/8/10	-
2	MEN	R2	72	2	-	4/7/8/10	-
2	MEN	F5	72	2	-	4/7/8/10	-
10	MEN	N2	72	10	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	gB	72	2	-	4/7/8/10	-
2	MEN	VF	72	2	-	4/7/8/10	-
2	MEN	pE	72	2,26	-	3/7/8/10	-
2	MEN	FG	72	2,26	-	2/7/8/10	-
2	MEN	f1	72	2	-	3/7/8/10	-
2	MEN	fG	72	2,26	-	2/7/8/10	-
2	MEN	QJ	72	2	-	4/7/8/10	-
2	MEN	PG	72	2,26	-	3/7/8/10	-
2	MEN	m7	72	2	-	4/7/8/10	-
2	MEN	JE	72	2,26	-	2/7/8/10	-
2	MEN	A5	72	2	-	2/7/8/10	-
2	MEN	NG	72	2,26	-	2/7/8/10	-
2	MEN	B1	72	2	-	2/7/8/10	-
2	MEN	J8	72	2	-	4/7/8/10	-
2	MEN	a2	72	2	-	3/7/8/10	-
2	MEN	iI	72	2	-	4/7/8/10	-
2	MEN	HE	72	2,26	-	2/7/8/10	-
2	MEN	w4	72	2	-	2/7/8/10	-
2	MEN	E9	72	2	-	3/7/8/10	-
2	MEN	TF	72	2	-	5/7/8/10	-
2	MEN	B3	72	2	-	4/7/8/10	-
10	MEN	DF	72	10	-	4/7/8/10	-
2	MEN	L4	72	2	-	4/7/8/10	-
2	MEN	J1	72	2	-	5/7/8/10	-
10	MEN	D7	72	10	-	2/7/8/10	-
2	MEN	OJ	72	2	-	4/7/8/10	-
2	MEN	KC	72	2	-	3/7/8/10	-
10	MEN	L2	72	10	-	4/7/8/10	-
2	MEN	BC	72	2	-	3/7/8/10	-
2	MEN	aB	72	2	-	4/7/8/10	-
10	MEN	NF	72	10	-	2/7/8/10	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	XG	72	MEN	OD1-CG	4.45	1.32	1.23
2	FG	72	MEN	OD1-CG	4.39	1.32	1.23
2	FE	72	MEN	OD1-CG	4.31	1.32	1.23
2	XE	72	MEN	OD1-CG	4.27	1.32	1.23
2	LG	72	MEN	OD1-CG	4.18	1.31	1.23
2	LE	72	MEN	OD1-CG	4.11	1.31	1.23
2	RG	72	MEN	OD1-CG	4.02	1.31	1.23
2	RE	72	MEN	OD1-CG	3.84	1.31	1.23
2	BG	72	MEN	OD1-CG	3.59	1.30	1.23
2	HG	72	MEN	OD1-CG	3.52	1.30	1.23
2	HE	72	MEN	OD1-CG	3.50	1.30	1.23
2	DG	72	MEN	OD1-CG	3.49	1.30	1.23
2	ZE	72	MEN	OD1-CG	3.46	1.30	1.23
2	PE	72	MEN	OD1-CG	3.44	1.30	1.23
2	BE	72	MEN	OD1-CG	3.38	1.30	1.23
2	JE	72	MEN	OD1-CG	3.37	1.30	1.23
2	PG	72	MEN	OD1-CG	3.37	1.30	1.23
2	NE	72	MEN	OD1-CG	3.22	1.29	1.23
2	DE	72	MEN	OD1-CG	3.21	1.29	1.23
2	NG	72	MEN	OD1-CG	3.19	1.29	1.23
2	bE	72	MEN	OD1-CG	3.16	1.29	1.23
2	JG	72	MEN	OD1-CG	3.15	1.29	1.23
2	TG	72	MEN	OD1-CG	2.95	1.29	1.23
2	TE	72	MEN	OD1-CG	2.94	1.29	1.23
2	VE	72	MEN	OD1-CG	2.93	1.29	1.23
2	nG	72	MEN	OD1-CG	2.87	1.29	1.23
2	vE	72	MEN	OD1-CG	2.80	1.29	1.23
2	VG	72	MEN	OD1-CG	2.77	1.28	1.23
2	dG	72	MEN	OD1-CG	2.74	1.28	1.23
2	vG	72	MEN	OD1-CG	2.72	1.28	1.23
2	dE	72	MEN	OD1-CG	2.69	1.28	1.23
2	jG	72	MEN	OD1-CG	2.67	1.28	1.23
2	nE	72	MEN	OD1-CG	2.67	1.28	1.23
2	jE	72	MEN	OD1-CG	2.58	1.28	1.23
2	fG	72	MEN	OD1-CG	2.55	1.28	1.23
2	fE	72	MEN	OD1-CG	2.52	1.28	1.23
2	hE	72	MEN	OD1-CG	2.41	1.28	1.23
2	tE	72	MEN	OD1-CG	2.38	1.28	1.23
2	hG	72	MEN	OD1-CG	2.33	1.28	1.23
2	tG	72	MEN	OD1-CG	2.33	1.28	1.23
2	rG	72	MEN	OD1-CG	2.30	1.27	1.23
2	rE	72	MEN	OD1-CG	2.16	1.27	1.23

All (459) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LG	72	MEN	CB-CG-ND2	-8.39	104.21	115.48
2	LE	72	MEN	CB-CG-ND2	-8.05	104.66	115.48
2	FG	72	MEN	CB-CG-ND2	-7.90	104.86	115.48
2	FE	72	MEN	CB-CG-ND2	-7.76	105.05	115.48
2	T3	72	MEN	CB-CG-ND2	6.91	124.78	115.48
2	XG	72	MEN	CB-CG-ND2	-6.86	106.26	115.48
2	RG	72	MEN	CB-CG-ND2	-6.76	106.39	115.48
2	TD	72	MEN	CB-CG-ND2	6.59	124.34	115.48
2	RE	72	MEN	CB-CG-ND2	-6.58	106.64	115.48
2	BG	72	MEN	CB-CG-ND2	-6.54	106.68	115.48
2	XE	72	MEN	CB-CG-ND2	-6.43	106.83	115.48
2	BE	72	MEN	CB-CG-ND2	-5.78	107.72	115.48
10	LF	72	MEN	CB-CG-ND2	5.59	123.00	115.48
2	PE	72	MEN	CB-CG-ND2	-5.47	108.13	115.48
2	NG	72	MEN	CB-CG-ND2	-5.36	108.28	115.48
2	PG	72	MEN	CB-CG-ND2	-5.28	108.38	115.48
2	NE	72	MEN	CB-CG-ND2	-5.16	108.55	115.48
2	j1	72	MEN	CB-CA-C	-5.11	101.90	111.47
2	JE	72	MEN	CB-CG-ND2	-5.04	108.70	115.48
2	HE	72	MEN	CB-CG-ND2	-5.00	108.77	115.48
2	HG	72	MEN	CB-CG-ND2	-4.77	109.07	115.48
2	F1	72	MEN	CB-CG-ND2	4.77	121.89	115.48
10	L7	72	MEN	CB-CG-ND2	4.75	121.88	115.48
18	hH	71	MEN	C-CA-CB	-4.51	106.73	111.94
2	TE	72	MEN	CB-CA-C	-4.44	103.15	111.47
2	j4	72	MEN	CB-CA-C	-4.41	103.20	111.47
2	TG	72	MEN	CB-CA-C	-4.39	103.25	111.47
2	JG	72	MEN	CB-CG-ND2	-4.35	109.63	115.48
2	ZE	72	MEN	CB-CG-ND2	-4.31	109.69	115.48
2	P3	72	MEN	CB-CA-C	-4.27	103.47	111.47
2	DG	72	MEN	CB-CG-ND2	-4.21	109.82	115.48
2	fG	72	MEN	CB-CG-ND2	-4.19	109.85	115.48
2	fE	72	MEN	CB-CG-ND2	-4.09	109.99	115.48
2	dG	72	MEN	CB-CG-ND2	-4.06	110.02	115.48
2	cF	72	MEN	CB-CA-C	-4.03	103.91	111.47
18	BH	71	MEN	C-CA-CB	-3.99	107.33	111.94
18	nH	71	MEN	C-CA-CB	-3.91	107.43	111.94
2	F1	72	MEN	CB-CA-C	-3.87	104.21	111.47
2	H8	72	MEN	CB-CA-C	-3.85	104.25	111.47
18	IH	71	MEN	C-CA-CB	-3.84	107.50	111.94
2	HD	72	MEN	CB-CA-C	-3.83	104.30	111.47
2	tE	72	MEN	CB-CA-C	-3.81	104.33	111.47
2	h4	72	MEN	CB-CA-C	-3.79	104.37	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DG	72	MEN	CB-CA-C	-3.78	104.38	111.47
18	dH	71	MEN	C-CA-CB	-3.76	107.60	111.94
2	lE	72	MEN	CB-CA-C	-3.73	104.48	111.47
2	pE	72	MEN	CB-CA-C	-3.72	104.49	111.47
2	IJ	72	MEN	CB-CG-ND2	3.72	120.48	115.48
18	fH	71	MEN	C-CA-CB	-3.69	107.68	111.94
18	DH	71	MEN	C-CA-CB	-3.63	107.75	111.94
2	MJ	72	MEN	CB-CG-ND2	3.62	120.36	115.48
10	JI	72	MEN	CB-CG-ND2	3.62	120.35	115.48
18	oH	71	MEN	C-CA-CB	-3.61	107.76	111.94
2	jG	72	MEN	CB-CG-ND2	-3.60	110.64	115.48
2	H3	72	MEN	CB-CA-C	-3.58	104.76	111.47
18	kH	71	MEN	C-CA-CB	-3.58	107.81	111.94
10	J2	72	MEN	CB-CG-ND2	3.56	120.27	115.48
18	qH	71	MEN	C-CA-CB	-3.55	107.84	111.94
2	QJ	72	MEN	CB-CA-C	-3.54	104.82	111.47
2	I5	72	MEN	CB-CA-C	-3.54	104.83	111.47
2	dE	72	MEN	CB-CG-ND2	-3.54	110.72	115.48
18	MH	71	MEN	C-CA-CB	-3.54	107.85	111.94
2	I9	72	MEN	CB-CG-ND2	3.53	120.23	115.48
18	jH	71	MEN	C-CA-CB	-3.53	107.87	111.94
2	HA	72	MEN	CB-CA-C	-3.49	104.92	111.47
2	Y9	72	MEN	CB-CA-C	-3.49	104.93	111.47
2	W4	72	MEN	CB-CG-ND2	3.49	120.17	115.48
2	A5	72	MEN	CA-CB-CG	3.48	122.60	112.70
2	bE	72	MEN	CB-CA-C	-3.48	104.95	111.47
2	TF	72	MEN	CB-CA-C	-3.46	104.98	111.47
2	c7	72	MEN	CB-CA-C	-3.43	105.03	111.47
2	lG	72	MEN	CB-CA-C	-3.43	105.05	111.47
2	YJ	72	MEN	CB-CG-ND2	3.42	120.08	115.48
2	DE	72	MEN	CB-CA-C	-3.42	105.06	111.47
18	LH	71	MEN	C-CA-CB	-3.40	108.02	111.94
2	M9	72	MEN	CB-CG-ND2	3.39	120.04	115.48
2	R8	72	MEN	CB-CA-C	-3.35	105.18	111.47
2	IC	72	MEN	CB-CA-C	-3.35	105.20	111.47
10	JF	72	MEN	CB-CA-C	-3.34	105.21	111.47
2	JA	72	MEN	CB-CA-C	-3.34	105.21	111.47
2	q4	72	MEN	CB-CA-C	-3.33	105.23	111.47
10	HI	72	MEN	CB-CG-ND2	3.32	119.95	115.48
2	X8	72	MEN	CA-CB-CG	-3.32	103.25	112.70
2	J8	72	MEN	CB-CA-C	-3.32	105.24	111.47
10	FB	72	MEN	CB-CG-ND2	3.32	119.94	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q9	72	MEN	CB-CA-C	-3.29	105.29	111.47
2	K5	72	MEN	CB-CA-C	-3.27	105.33	111.47
2	L1	72	MEN	CB-CA-C	-3.27	105.35	111.47
10	F2	72	MEN	CB-CG-ND2	3.26	119.87	115.48
2	d4	72	MEN	CB-CA-C	-3.25	105.38	111.47
2	XA	72	MEN	CA-CB-CG	-3.24	103.48	112.70
10	JB	72	MEN	CB-CG-ND2	3.24	119.84	115.48
18	kH	71	MEN	CB-CG-ND2	3.24	119.84	115.48
2	h1	72	MEN	CB-CA-C	-3.23	105.41	111.47
10	F6	72	MEN	CB-CG-ND2	3.22	119.81	115.48
2	VE	72	MEN	CB-CA-C	-3.22	105.44	111.47
2	bE	72	MEN	CB-CG-ND2	-3.21	111.16	115.48
2	a4	72	MEN	CB-CA-C	-3.21	105.46	111.47
2	jE	72	MEN	CB-CG-ND2	-3.19	111.19	115.48
2	GJ	72	MEN	CB-CA-C	-3.19	105.49	111.47
18	OH	71	MEN	C-CA-CB	-3.19	108.26	111.94
10	J6	72	MEN	CB-CG-ND2	3.18	119.76	115.48
2	W1	72	MEN	CB-CG-ND2	3.18	119.75	115.48
2	T3	72	MEN	OD1-CG-CB	-3.17	116.85	121.50
2	FE	72	MEN	CB-CA-C	-3.17	105.53	111.47
2	U9	72	MEN	CB-CA-C	-3.16	105.53	111.47
2	G9	72	MEN	CB-CA-C	-3.16	105.54	111.47
2	VG	72	MEN	CB-CA-C	-3.16	105.54	111.47
2	DE	72	MEN	CB-CG-ND2	-3.15	111.25	115.48
2	U4	72	MEN	CB-CA-C	-3.15	105.56	111.47
10	LI	72	MEN	CB-CG-ND2	3.15	119.72	115.48
2	RA	72	MEN	CB-CA-C	-3.15	105.57	111.47
2	FG	72	MEN	CB-CA-C	-3.14	105.58	111.47
10	FI	72	MEN	CB-CG-ND2	3.13	119.69	115.48
2	k7	72	MEN	CB-CA-C	-3.12	105.61	111.47
2	gF	72	MEN	CB-CA-C	-3.12	105.62	111.47
2	aB	72	MEN	CB-CA-C	-3.12	105.63	111.47
2	i7	72	MEN	CB-CA-C	-3.11	105.64	111.47
10	DB	72	MEN	CB-CA-C	-3.11	105.64	111.47
2	GJ	72	MEN	CA-CB-CG	-3.11	103.86	112.70
10	L2	72	MEN	CB-CA-C	-3.10	105.65	111.47
10	LI	72	MEN	CB-CA-C	-3.10	105.66	111.47
18	QH	71	MEN	CB-CA-C	-3.09	105.67	111.47
2	TA	72	MEN	CB-CA-C	-3.09	105.67	111.47
2	L4	72	MEN	CB-CA-C	-3.09	105.67	111.47
2	cA	72	MEN	CB-CA-C	-3.09	105.68	111.47
2	kB	72	MEN	CB-CA-C	-3.09	105.68	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J1	72	MEN	CB-CA-C	-3.08	105.69	111.47
2	g7	72	MEN	CB-CA-C	-3.08	105.69	111.47
2	kI	72	MEN	CB-CA-C	-3.08	105.69	111.47
2	V7	72	MEN	CB-CA-C	-3.08	105.70	111.47
2	T8	72	MEN	CB-CA-C	-3.08	105.70	111.47
10	L2	72	MEN	CB-CG-ND2	3.08	119.62	115.48
2	N3	72	MEN	CB-CA-C	-3.07	105.71	111.47
2	a6	72	MEN	CB-CA-C	-3.06	105.73	111.47
2	VF	72	MEN	CB-CA-C	-3.06	105.73	111.47
2	KJ	72	MEN	CB-CA-C	-3.06	105.73	111.47
2	k6	72	MEN	CB-CA-C	-3.06	105.74	111.47
18	HH	71	MEN	C-CA-CB	-3.05	108.41	111.94
18	sH	71	MEN	CB-CG-ND2	3.05	119.59	115.48
2	F4	72	MEN	CB-CA-C	-3.04	105.77	111.47
2	pG	72	MEN	CB-CA-C	-3.03	105.78	111.47
2	d1	72	MEN	CB-CA-C	-3.03	105.79	111.47
2	ND	72	MEN	CB-CA-C	-3.03	105.79	111.47
2	NG	72	MEN	CB-CA-C	-3.02	105.81	111.47
2	KC	72	MEN	CB-CA-C	-3.02	105.81	111.47
2	i2	72	MEN	CB-CA-C	-3.01	105.82	111.47
2	e2	72	MEN	CB-CA-C	-3.01	105.83	111.47
2	NE	72	MEN	CB-CA-C	-3.01	105.83	111.47
2	E9	72	MEN	CB-CA-C	-3.00	105.85	111.47
2	U1	72	MEN	CB-CA-C	-3.00	105.85	111.47
2	gB	72	MEN	CB-CA-C	-3.00	105.85	111.47
2	AC	72	MEN	CA-CB-CG	2.98	121.19	112.70
2	j4	72	MEN	CA-CB-CG	-2.98	104.22	112.70
2	c8	72	MEN	CB-CA-C	-2.98	105.89	111.47
2	D4	72	MEN	CB-CA-C	-2.97	105.89	111.47
2	eI	72	MEN	CB-CA-C	-2.97	105.90	111.47
2	N8	72	MEN	CB-CG-ND2	2.96	119.47	115.48
2	g6	72	MEN	CB-CA-C	-2.96	105.92	111.47
2	NA	72	MEN	CB-CG-ND2	2.96	119.46	115.48
10	D6	72	MEN	CB-CA-C	-2.95	105.95	111.47
2	P6	72	MEN	CB-CA-C	-2.93	105.97	111.47
2	tG	72	MEN	CB-CA-C	-2.93	105.98	111.47
2	iA	72	MEN	CB-CA-C	-2.92	105.99	111.47
2	PB	72	MEN	CB-CA-C	-2.92	105.99	111.47
2	k2	72	MEN	CB-CA-C	-2.92	106.00	111.47
2	Q1	72	MEN	CB-CA-C	-2.92	106.00	111.47
2	H1	72	MEN	CB-CA-C	-2.92	106.00	111.47
2	C5	72	MEN	CB-CA-C	-2.91	106.01	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T7	72	MEN	CB-CA-C	-2.91	106.01	111.47
2	ZA	72	MEN	CB-CG-ND2	2.91	119.39	115.48
10	NB	72	MEN	CB-CG-ND2	2.90	119.39	115.48
2	PD	72	MEN	CB-CA-C	-2.90	106.03	111.47
2	VB	72	MEN	CB-CA-C	-2.90	106.03	111.47
2	X8	72	MEN	CB-CA-C	-2.90	106.03	111.47
10	H2	72	MEN	CB-CG-ND2	2.89	119.38	115.48
2	iF	72	MEN	CB-CA-C	-2.89	106.05	111.47
2	Z1	72	MEN	CB-CA-C	-2.87	106.08	111.47
2	q1	72	MEN	CB-CA-C	-2.87	106.08	111.47
2	Q4	72	MEN	CB-CA-C	-2.87	106.08	111.47
2	Z4	72	MEN	CB-CA-C	-2.86	106.10	111.47
2	JE	72	MEN	CB-CA-C	-2.86	106.10	111.47
2	P7	72	MEN	CB-CA-C	-2.86	106.11	111.47
2	XA	72	MEN	CB-CA-C	-2.85	106.12	111.47
18	wH	71	MEN	CB-CG-ND2	2.85	119.32	115.48
2	VA	72	MEN	CB-CG-ND2	2.85	119.31	115.48
2	D1	72	MEN	CB-CA-C	-2.84	106.14	111.47
2	Z4	72	MEN	CB-CG-ND2	2.84	119.31	115.48
2	y4	72	MEN	CB-CA-C	-2.84	106.14	111.47
2	g2	72	MEN	CB-CA-C	-2.84	106.15	111.47
2	PF	72	MEN	CB-CA-C	-2.83	106.16	111.47
10	HF	72	MEN	CB-CA-C	-2.83	106.17	111.47
2	iI	72	MEN	CB-CA-C	-2.82	106.17	111.47
2	j1	72	MEN	CA-CB-CG	-2.82	104.67	112.70
2	J4	72	MEN	CB-CA-C	-2.81	106.20	111.47
2	G9	72	MEN	CA-CB-CG	-2.81	104.71	112.70
2	Z8	72	MEN	CB-CG-ND2	2.80	119.25	115.48
2	W9	72	MEN	CB-CA-C	-2.80	106.22	111.47
2	aF	72	MEN	CB-CG-ND2	2.80	119.24	115.48
2	T2	72	MEN	CB-CA-C	-2.79	106.24	111.47
2	TI	72	MEN	CB-CA-C	-2.78	106.26	111.47
18	QH	71	MEN	CB-CG-ND2	2.77	119.21	115.48
2	FD	72	MEN	CB-CA-C	-2.77	106.27	111.47
2	B4	72	MEN	CB-CA-C	-2.76	106.29	111.47
2	Z1	72	MEN	CB-CG-ND2	2.75	119.19	115.48
2	i8	72	MEN	CB-CA-C	-2.75	106.31	111.47
2	B1	72	MEN	CB-CA-C	-2.75	106.31	111.47
10	D7	72	MEN	CB-CA-C	-2.75	106.31	111.47
10	FF	72	MEN	CB-CA-C	-2.73	106.35	111.47
2	YB	72	MEN	CB-CG-ND2	2.71	119.13	115.48
2	nE	72	MEN	CB-CG-ND2	-2.71	111.84	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K9	72	MEN	CB-CA-C	-2.69	106.42	111.47
2	X3	72	MEN	CB-CA-C	-2.69	106.43	111.47
10	J7	72	MEN	CB-CA-C	-2.68	106.44	111.47
10	F7	72	MEN	CB-CA-C	-2.68	106.44	111.47
2	UJ	72	MEN	CB-CA-C	-2.68	106.45	111.47
2	a1	72	MEN	CB-CG-ND2	2.67	119.08	115.48
2	nG	72	MEN	CB-CG-ND2	-2.67	111.89	115.48
2	V8	72	MEN	CB-CG-ND2	2.67	119.07	115.48
2	EJ	72	MEN	CB-CG-ND2	2.67	119.07	115.48
2	k8	72	MEN	CB-CG-ND2	2.67	119.07	115.48
2	VA	72	MEN	CB-CA-C	-2.66	106.48	111.47
2	a1	72	MEN	CB-CA-C	-2.66	106.48	111.47
2	Y2	72	MEN	CB-CA-C	-2.66	106.48	111.47
2	TB	72	MEN	CB-CA-C	-2.66	106.49	111.47
10	J2	72	MEN	CB-CA-C	-2.64	106.52	111.47
18	qH	71	MEN	CB-CG-ND2	2.64	119.03	115.48
2	YI	72	MEN	CB-CA-C	-2.64	106.52	111.47
2	V6	72	MEN	CB-CA-C	-2.63	106.54	111.47
10	H6	72	MEN	CB-CG-ND2	2.61	119.00	115.48
2	F8	72	MEN	CB-CG-ND2	2.61	119.00	115.48
2	ZE	72	MEN	CB-CA-C	-2.61	106.57	111.47
10	H7	72	MEN	CB-CA-C	-2.61	106.57	111.47
2	gI	72	MEN	CB-CA-C	-2.61	106.57	111.47
2	JD	72	MEN	CB-CA-C	-2.61	106.58	111.47
2	XD	72	MEN	CB-CA-C	-2.61	106.58	111.47
2	LE	72	MEN	OD1-CG-CB	2.61	125.32	121.50
2	DA	72	MEN	CB-CA-C	-2.61	106.58	111.47
18	MH	71	MEN	CB-CG-ND2	2.60	118.99	115.48
2	D3	72	MEN	CB-CA-C	-2.60	106.59	111.47
2	FA	72	MEN	CB-CG-ND2	2.60	118.98	115.48
10	N2	72	MEN	CB-CA-C	-2.60	106.60	111.47
2	m6	72	MEN	CB-CA-C	-2.59	106.61	111.47
2	H4	72	MEN	CB-CA-C	-2.59	106.61	111.47
10	DB	72	MEN	CA-CB-CG	-2.59	105.34	112.70
2	T6	72	MEN	CB-CA-C	-2.58	106.62	111.47
2	s4	72	MEN	CB-CG-ND2	2.58	118.96	115.48
10	LB	72	MEN	CB-CA-C	-2.58	106.63	111.47
2	Y6	72	MEN	CB-CG-ND2	2.58	118.96	115.48
10	DF	72	MEN	CB-CA-C	-2.58	106.63	111.47
10	L6	72	MEN	CB-CA-C	-2.58	106.64	111.47
10	DF	72	MEN	CA-CB-CG	-2.57	105.37	112.70
2	n1	72	MEN	CB-CA-C	-2.57	106.65	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L6	72	MEN	CB-CG-ND2	2.57	118.94	115.48
2	kA	72	MEN	CB-CG-ND2	2.57	118.94	115.48
2	C9	72	MEN	CB-CA-C	-2.56	106.66	111.47
2	D8	72	MEN	CB-CA-C	-2.56	106.67	111.47
2	eB	72	MEN	CB-CA-C	-2.56	106.68	111.47
2	D1	72	MEN	CB-CG-ND2	2.55	118.91	115.48
2	14	72	MEN	CB-CA-C	-2.55	106.69	111.47
2	e6	72	MEN	CB-CA-C	-2.54	106.70	111.47
10	NB	72	MEN	CB-CA-C	-2.54	106.70	111.47
2	K5	72	MEN	CA-CB-CG	-2.54	105.48	112.70
10	D7	72	MEN	CA-CB-CG	-2.53	105.49	112.70
2	V3	72	MEN	CB-CA-C	-2.53	106.73	111.47
2	RB	72	MEN	CB-CA-C	-2.53	106.73	111.47
2	R6	72	MEN	CB-CA-C	-2.52	106.75	111.47
2	Y4	72	MEN	CB-CA-C	-2.50	106.78	111.47
2	TD	72	MEN	OD1-CG-CB	-2.50	117.83	121.50
18	OH	71	MEN	CB-CG-ND2	2.50	118.85	115.48
2	T3	72	MEN	CA-CB-CG	2.50	119.81	112.70
18	UH	71	MEN	CB-CG-ND2	2.50	118.84	115.48
2	FD	72	MEN	CB-CG-ND2	2.50	118.84	115.48
10	N6	72	MEN	CB-CG-ND2	2.49	118.84	115.48
2	a7	72	MEN	CB-CG-ND2	2.49	118.84	115.48
2	SJ	72	MEN	CB-CA-C	-2.49	106.80	111.47
10	N6	72	MEN	CB-CA-C	-2.49	106.80	111.47
2	WJ	72	MEN	CB-CA-C	-2.48	106.81	111.47
2	fE	72	MEN	CB-CA-C	-2.48	106.81	111.47
2	mI	72	MEN	CB-CG-ND2	2.48	118.82	115.48
2	m7	72	MEN	CB-CA-C	-2.48	106.82	111.47
2	m8	72	MEN	CB-CA-C	-2.48	106.83	111.47
2	X3	72	MEN	CB-CG-ND2	2.48	118.81	115.48
2	F3	72	MEN	CB-CG-ND2	2.47	118.81	115.48
18	SH	71	MEN	CB-CG-ND2	2.47	118.81	115.48
2	u4	72	MEN	CB-CA-C	-2.46	106.85	111.47
10	JI	72	MEN	CB-CA-C	-2.46	106.85	111.47
2	s1	72	MEN	CB-CG-ND2	2.46	118.80	115.48
2	TI	72	MEN	CB-CG-ND2	2.46	118.79	115.48
2	H5	72	MEN	CB-CA-C	-2.46	106.86	111.47
10	LB	72	MEN	CB-CG-ND2	2.45	118.78	115.48
2	y1	72	MEN	CB-CA-C	-2.45	106.88	111.47
2	TG	72	MEN	CB-CG-ND2	-2.45	112.19	115.48
2	XD	72	MEN	CB-CG-ND2	2.44	118.76	115.48
10	D2	72	MEN	CB-CG-ND2	2.43	118.75	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V8	72	MEN	CB-CA-C	-2.42	106.92	111.47
2	S9	72	MEN	CB-CA-C	-2.42	106.93	111.47
2	EJ	72	MEN	CB-CA-C	-2.41	106.95	111.47
2	LG	72	MEN	OD1-CG-CB	2.41	125.03	121.50
2	14	72	MEN	CB-CG-ND2	2.40	118.71	115.48
2	JG	72	MEN	CB-CA-C	-2.40	106.97	111.47
2	aI	72	MEN	CB-CG-ND2	2.39	118.70	115.48
2	T2	72	MEN	CB-CG-ND2	2.39	118.70	115.48
2	PA	72	MEN	CB-CA-C	-2.39	106.99	111.47
2	NA	72	MEN	CB-CA-C	-2.39	106.99	111.47
2	VD	72	MEN	CB-CA-C	-2.38	107.00	111.47
2	N8	72	MEN	CB-CA-C	-2.38	107.00	111.47
2	YJ	72	MEN	CA-CB-CG	-2.37	105.95	112.70
18	uH	71	MEN	CB-CG-ND2	2.37	118.67	115.48
2	P8	72	MEN	CB-CA-C	-2.36	107.04	111.47
2	h1	72	MEN	CB-CG-ND2	2.36	118.66	115.48
2	a2	72	MEN	CB-CG-ND2	2.36	118.66	115.48
2	R7	72	MEN	CB-CA-C	-2.35	107.06	111.47
10	DI	72	MEN	CB-CG-ND2	2.34	118.63	115.48
2	D4	72	MEN	CB-CG-ND2	2.34	118.63	115.48
2	R2	72	MEN	CB-CG-ND2	2.34	118.62	115.48
2	fG	72	MEN	CB-CA-C	-2.34	107.09	111.47
2	Y1	72	MEN	CB-CA-C	-2.33	107.09	111.47
2	CJ	72	MEN	CB-CA-C	-2.33	107.09	111.47
2	CJ	72	MEN	CB-CG-ND2	2.33	118.62	115.48
10	D6	72	MEN	CA-CB-CG	-2.33	106.08	112.70
2	XG	72	MEN	CA-CB-CG	2.33	119.33	112.70
2	HE	72	MEN	CB-CA-C	-2.32	107.12	111.47
2	FE	72	MEN	OD1-CG-CB	2.32	124.89	121.50
2	ZA	72	MEN	CB-CA-C	-2.31	107.13	111.47
2	PF	72	MEN	CB-CG-ND2	2.31	118.59	115.48
2	RI	72	MEN	CB-CG-ND2	2.31	118.59	115.48
2	TE	72	MEN	CB-CG-ND2	-2.31	112.38	115.48
2	kA	72	MEN	CB-CA-C	-2.30	107.17	111.47
2	m2	72	MEN	CB-CG-ND2	2.29	118.56	115.48
10	NI	72	MEN	CB-CA-C	-2.29	107.18	111.47
2	rE	72	MEN	CB-CA-C	-2.29	107.18	111.47
2	FG	72	MEN	OD1-CG-CB	2.28	124.84	121.50
18	BH	71	MEN	CB-CG-ND2	2.28	118.55	115.48
2	C9	72	MEN	CB-CG-ND2	2.28	118.55	115.48
2	RE	72	MEN	OD1-CG-CB	2.28	124.83	121.50
2	Q1	72	MEN	CB-CG-ND2	2.27	118.54	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B4	72	MEN	CB-CG-ND2	2.27	118.54	115.48
18	uH	71	MEN	CB-CA-C	-2.27	107.21	111.47
2	mA	72	MEN	CB-CA-C	-2.27	107.22	111.47
2	LG	72	MEN	CB-CA-C	-2.26	107.23	111.47
2	S1	72	MEN	CB-CA-C	-2.26	107.23	111.47
2	TF	72	MEN	CB-CG-ND2	2.26	118.52	115.48
18	IH	71	MEN	CB-CG-ND2	2.26	118.52	115.48
2	RG	72	MEN	OD1-CG-CB	2.26	124.80	121.50
2	S4	72	MEN	CB-CA-C	-2.25	107.24	111.47
18	sH	71	MEN	CB-CA-C	-2.25	107.25	111.47
2	11	72	MEN	CB-CA-C	-2.25	107.25	111.47
2	kF	72	MEN	CB-CA-C	-2.25	107.25	111.47
2	aB	72	MEN	CB-CG-ND2	2.25	118.51	115.48
2	ZG	72	MEN	CA-CB-CG	-2.25	106.30	112.70
2	P3	72	MEN	CB-CG-ND2	2.25	118.51	115.48
2	mI	72	MEN	CB-CA-C	-2.25	107.25	111.47
2	XE	72	MEN	CA-CB-CG	2.24	119.08	112.70
2	HC	72	MEN	CB-CA-C	-2.24	107.27	111.47
2	V2	72	MEN	CB-CG-ND2	2.24	118.49	115.48
2	L3	72	MEN	CB-CG-ND2	2.24	118.49	115.48
2	g8	72	MEN	CB-CA-C	-2.24	107.28	111.47
2	KC	72	MEN	CA-CB-CG	-2.23	106.35	112.70
2	vE	72	MEN	CB-CA-C	-2.23	107.29	111.47
2	l1	72	MEN	CB-CA-C	-2.23	107.29	111.47
2	Q4	72	MEN	CB-CG-ND2	2.23	118.48	115.48
2	HG	72	MEN	CB-CA-C	-2.23	107.29	111.47
2	f1	72	MEN	CB-CA-C	-2.23	107.30	111.47
2	mF	72	MEN	CB-CA-C	-2.22	107.30	111.47
2	a2	72	MEN	CB-CA-C	-2.22	107.30	111.47
2	VI	72	MEN	CB-CG-ND2	2.22	118.47	115.48
2	aI	72	MEN	CB-CA-C	-2.22	107.31	111.47
2	PE	72	MEN	CB-CA-C	-2.22	107.31	111.47
10	NI	72	MEN	CB-CG-ND2	2.21	118.46	115.48
18	dH	71	MEN	CB-CG-ND2	2.21	118.45	115.48
18	SH	71	MEN	CB-CA-C	-2.21	107.33	111.47
2	A5	72	MEN	CB-CA-C	-2.20	107.34	111.47
2	m2	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	YF	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	a6	72	MEN	CB-CG-ND2	2.19	118.43	115.48
18	LH	71	MEN	CB-CG-ND2	2.19	118.43	115.48
2	cI	72	MEN	CB-CA-C	-2.19	107.36	111.47
2	e7	72	MEN	CB-CA-C	-2.19	107.36	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	RI	72	MEN	CB-CA-C	-2.19	107.37	111.47
2	V2	72	MEN	CB-CA-C	-2.18	107.38	111.47
2	U1	72	MEN	CA-CB-CG	-2.18	106.50	112.70
2	bG	72	MEN	CB-CA-C	-2.18	107.39	111.47
18	nH	71	MEN	CB-CG-ND2	2.17	118.41	115.48
2	eI	72	MEN	CA-CB-CG	-2.17	106.52	112.70
2	e7	72	MEN	CB-CG-ND2	2.17	118.40	115.48
2	q1	72	MEN	CB-CG-ND2	2.17	118.40	115.48
2	f4	72	MEN	CB-CA-C	-2.16	107.42	111.47
2	s1	72	MEN	CB-CA-C	-2.16	107.42	111.47
18	fH	71	MEN	CB-CG-ND2	2.16	118.39	115.48
2	DD	72	MEN	CB-CG-ND2	2.16	118.38	115.48
2	L5	72	MEN	OD1-CG-CB	-2.15	118.34	121.50
2	J4	72	MEN	CB-CG-ND2	2.15	118.38	115.48
2	VI	72	MEN	CB-CA-C	-2.15	107.43	111.47
2	WJ	72	MEN	CB-CG-ND2	2.15	118.38	115.48
2	eF	72	MEN	CB-CA-C	-2.15	107.44	111.47
2	KJ	72	MEN	CB-CG-ND2	2.14	118.36	115.48
2	O4	72	MEN	CB-CA-C	-2.14	107.45	111.47
2	mB	72	MEN	CB-CA-C	-2.14	107.45	111.47
2	l4	72	MEN	CB-CA-C	-2.14	107.46	111.47
2	e2	72	MEN	CA-CB-CG	-2.14	106.62	112.70
2	VF	72	MEN	CB-CG-ND2	2.13	118.35	115.48
10	LF	72	MEN	CB-CA-C	-2.13	107.47	111.47
10	D2	72	MEN	CB-CA-C	-2.13	107.48	111.47
2	O9	72	MEN	CB-CG-ND2	2.12	118.33	115.48
18	FH	71	MEN	C-CA-CB	-2.12	109.49	111.94
2	V6	72	MEN	CB-CG-ND2	2.11	118.33	115.48
10	HB	72	MEN	CB-CG-ND2	2.11	118.32	115.48
2	M9	72	MEN	CB-CA-C	-2.11	107.52	111.47
2	LE	72	MEN	CB-CA-C	-2.11	107.52	111.47
2	Z8	72	MEN	CB-CA-C	-2.11	107.52	111.47
2	pE	72	MEN	CB-CG-ND2	2.10	118.31	115.48
2	BD	72	MEN	CB-CA-C	-2.10	107.52	111.47
2	rG	72	MEN	CB-CA-C	-2.10	107.52	111.47
2	MJ	72	MEN	CB-CA-C	-2.10	107.53	111.47
2	O4	72	MEN	CB-CG-ND2	2.09	118.30	115.48
2	B5	72	MEN	CB-CG-ND2	2.09	118.30	115.48
2	m8	72	MEN	CA-CB-CG	-2.09	106.75	112.70
10	H2	72	MEN	CB-CA-C	-2.09	107.55	111.47
2	PB	72	MEN	CB-CG-ND2	2.09	118.29	115.48
2	h4	72	MEN	CB-CG-ND2	2.09	118.29	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LA	72	MEN	CB-CA-C	-2.08	107.56	111.47
2	s4	72	MEN	CB-CA-C	-2.08	107.56	111.47
18	DH	71	MEN	CB-CG-ND2	2.08	118.28	115.48
2	OJ	72	MEN	CB-CA-C	-2.08	107.57	111.47
2	u1	72	MEN	CB-CA-C	-2.08	107.57	111.47
2	e8	72	MEN	CB-CA-C	-2.08	107.57	111.47
2	PE	72	MEN	OD1-CG-CB	2.07	124.53	121.50
2	J3	72	MEN	CB-CA-C	-2.07	107.58	111.47
2	RF	72	MEN	CB-CG-ND2	2.07	118.26	115.48
2	lG	72	MEN	CB-CG-ND2	2.07	118.26	115.48
2	B5	72	MEN	CB-CA-C	-2.06	107.60	111.47
10	HB	72	MEN	CB-CA-C	-2.06	107.60	111.47
2	i7	72	MEN	CA-CB-CG	-2.06	106.83	112.70
2	OJ	72	MEN	CB-CG-ND2	2.06	118.26	115.48
2	C5	72	MEN	CB-CG-ND2	2.06	118.25	115.48
2	R2	72	MEN	CB-CA-C	-2.05	107.62	111.47
2	gA	72	MEN	CB-CA-C	-2.05	107.63	111.47
2	O9	72	MEN	CB-CA-C	-2.05	107.63	111.47
10	DI	72	MEN	CB-CA-C	-2.04	107.64	111.47
2	Q9	72	MEN	CB-CG-ND2	2.04	118.22	115.48
2	gF	72	MEN	CB-CG-ND2	2.04	118.22	115.48
10	N7	72	MEN	CA-CB-CG	-2.04	106.91	112.70
2	L8	72	MEN	CB-CA-C	-2.04	107.65	111.47
2	c6	72	MEN	CB-CA-C	-2.03	107.67	111.47
2	mA	72	MEN	CA-CB-CG	-2.02	106.94	112.70
2	l4	72	MEN	CB-CG-ND2	2.02	118.21	115.48
10	HI	72	MEN	CB-CA-C	-2.02	107.68	111.47
10	H6	72	MEN	CB-CA-C	-2.02	107.69	111.47
2	hE	72	MEN	CB-CG-ND2	-2.02	112.77	115.48
2	V3	72	MEN	CB-CG-ND2	2.01	118.19	115.48
2	PG	72	MEN	OD1-CG-CB	2.01	124.44	121.50
2	i6	72	MEN	CB-CA-C	-2.01	107.70	111.47
2	QJ	72	MEN	CB-CG-ND2	2.01	118.18	115.48
2	jG	72	MEN	CB-CA-C	-2.01	107.71	111.47
2	w1	72	MEN	CB-CG-ND2	2.00	118.18	115.48
2	vG	72	MEN	CB-CA-C	-2.00	107.71	111.47
2	a4	72	MEN	CB-CG-ND2	2.00	118.18	115.48
2	TA	72	MEN	CB-CG-ND2	2.00	118.17	115.48

There are no chirality outliers.

All (1102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B1	72	MEN	C-CA-CB-CG
2	D1	72	MEN	C-CA-CB-CG
2	F1	72	MEN	CB-CG-ND2-CE2
2	F1	72	MEN	OD1-CG-ND2-CE2
2	H1	72	MEN	C-CA-CB-CG
2	J1	72	MEN	O-C-CA-CB
2	J1	72	MEN	N-CA-CB-CG
2	J1	72	MEN	C-CA-CB-CG
2	L1	72	MEN	C-CA-CB-CG
2	Q1	72	MEN	C-CA-CB-CG
2	S1	72	MEN	C-CA-CB-CG
2	U1	72	MEN	C-CA-CB-CG
2	Y1	72	MEN	C-CA-CB-CG
2	Z1	72	MEN	C-CA-CB-CG
2	a1	72	MEN	C-CA-CB-CG
2	f1	72	MEN	N-CA-CB-CG
2	f1	72	MEN	C-CA-CB-CG
2	h1	72	MEN	O-C-CA-CB
2	h1	72	MEN	CA-CB-CG-OD1
2	h1	72	MEN	CA-CB-CG-ND2
2	j1	72	MEN	C-CA-CB-CG
2	l1	72	MEN	O-C-CA-CB
2	l1	72	MEN	N-CA-CB-CG
2	s1	72	MEN	C-CA-CB-CG
2	11	72	MEN	N-CA-CB-CG
2	P2	72	MEN	C-CA-CB-CG
2	R2	72	MEN	C-CA-CB-CG
2	Y2	72	MEN	C-CA-CB-CG
2	g2	72	MEN	C-CA-CB-CG
2	i2	72	MEN	C-CA-CB-CG
2	k2	72	MEN	O-C-CA-CB
2	k2	72	MEN	C-CA-CB-CG
2	L3	72	MEN	O-C-CA-CB
2	L3	72	MEN	C-CA-CB-CG
2	N3	72	MEN	C-CA-CB-CG
2	R3	72	MEN	C-CA-CB-CG
2	T3	72	MEN	CB-CG-ND2-CE2
2	T3	72	MEN	OD1-CG-ND2-CE2
2	V3	72	MEN	C-CA-CB-CG
2	B4	72	MEN	O-C-CA-CB
2	B4	72	MEN	C-CA-CB-CG
2	D4	72	MEN	N-CA-CB-CG
2	D4	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	D4	72	MEN	CA-CB-CG-OD1
2	D4	72	MEN	CA-CB-CG-ND2
2	F4	72	MEN	O-C-CA-CB
2	F4	72	MEN	N-CA-CB-CG
2	F4	72	MEN	C-CA-CB-CG
2	J4	72	MEN	O-C-CA-CB
2	J4	72	MEN	C-CA-CB-CG
2	J4	72	MEN	CA-CB-CG-OD1
2	J4	72	MEN	CA-CB-CG-ND2
2	L4	72	MEN	C-CA-CB-CG
2	O4	72	MEN	C-CA-CB-CG
2	Q4	72	MEN	C-CA-CB-CG
2	S4	72	MEN	C-CA-CB-CG
2	U4	72	MEN	C-CA-CB-CG
2	Y4	72	MEN	C-CA-CB-CG
2	a4	72	MEN	C-CA-CB-CG
2	d4	72	MEN	O-C-CA-CB
2	d4	72	MEN	C-CA-CB-CG
2	h4	72	MEN	C-CA-CB-CG
2	j4	72	MEN	O-C-CA-CB
2	j4	72	MEN	C-CA-CB-CG
2	n4	72	MEN	C-CA-CB-CG
2	q4	72	MEN	N-CA-CB-CG
2	A5	72	MEN	CB-CG-ND2-CE2
2	A5	72	MEN	OD1-CG-ND2-CE2
2	B5	72	MEN	CB-CG-ND2-CE2
2	B5	72	MEN	OD1-CG-ND2-CE2
2	C5	72	MEN	N-CA-CB-CG
2	C5	72	MEN	C-CA-CB-CG
2	C5	72	MEN	CB-CG-ND2-CE2
2	C5	72	MEN	OD1-CG-ND2-CE2
2	F5	72	MEN	C-CA-CB-CG
2	F5	72	MEN	CB-CG-ND2-CE2
2	F5	72	MEN	OD1-CG-ND2-CE2
2	G5	72	MEN	C-CA-CB-CG
2	G5	72	MEN	CB-CG-ND2-CE2
2	G5	72	MEN	OD1-CG-ND2-CE2
2	H5	72	MEN	CB-CG-ND2-CE2
2	H5	72	MEN	OD1-CG-ND2-CE2
2	I5	72	MEN	C-CA-CB-CG
2	K5	72	MEN	C-CA-CB-CG
2	L5	72	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	L5	72	MEN	CB-CG-ND2-CE2
2	L5	72	MEN	OD1-CG-ND2-CE2
10	D6	72	MEN	C-CA-CB-CG
10	H6	72	MEN	C-CA-CB-CG
10	L6	72	MEN	C-CA-CB-CG
2	R6	72	MEN	C-CA-CB-CG
2	Y6	72	MEN	O-C-CA-CB
2	Y6	72	MEN	C-CA-CB-CG
2	a6	72	MEN	C-CA-CB-CG
2	c6	72	MEN	O-C-CA-CB
2	k6	72	MEN	C-CA-CB-CG
10	H7	72	MEN	C-CA-CB-CG
10	J7	72	MEN	O-C-CA-CB
2	P7	72	MEN	C-CA-CB-CG
2	R7	72	MEN	C-CA-CB-CG
2	T7	72	MEN	C-CA-CB-CG
2	V7	72	MEN	C-CA-CB-CG
2	Y7	72	MEN	C-CA-CB-CG
2	a7	72	MEN	O-C-CA-CB
2	c7	72	MEN	C-CA-CB-CG
2	D8	72	MEN	N-CA-CB-CG
2	F8	72	MEN	O-C-CA-CB
2	F8	72	MEN	C-CA-CB-CG
2	H8	72	MEN	C-CA-CB-CG
2	J8	72	MEN	C-CA-CB-CG
2	L8	72	MEN	C-CA-CB-CG
2	P8	72	MEN	C-CA-CB-CG
2	P8	72	MEN	CA-CB-CG-OD1
2	P8	72	MEN	CA-CB-CG-ND2
2	R8	72	MEN	C-CA-CB-CG
2	V8	72	MEN	C-CA-CB-CG
2	X8	72	MEN	C-CA-CB-CG
2	Z8	72	MEN	C-CA-CB-CG
2	c8	72	MEN	C-CA-CB-CG
2	e8	72	MEN	O-C-CA-CB
2	e8	72	MEN	C-CA-CB-CG
2	i8	72	MEN	C-CA-CB-CG
2	k8	72	MEN	O-C-CA-CB
2	k8	72	MEN	C-CA-CB-CG
2	m8	72	MEN	C-CA-CB-CG
2	C9	72	MEN	C-CA-CB-CG
2	G9	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	K9	72	MEN	C-CA-CB-CG
2	M9	72	MEN	C-CA-CB-CG
2	Q9	72	MEN	N-CA-CB-CG
2	Q9	72	MEN	C-CA-CB-CG
2	W9	72	MEN	C-CA-CB-CG
2	Y9	72	MEN	N-CA-CB-CG
2	FA	72	MEN	O-C-CA-CB
2	FA	72	MEN	C-CA-CB-CG
2	HA	72	MEN	C-CA-CB-CG
2	JA	72	MEN	C-CA-CB-CG
2	LA	72	MEN	C-CA-CB-CG
2	NA	72	MEN	O-C-CA-CB
2	PA	72	MEN	C-CA-CB-CG
2	RA	72	MEN	C-CA-CB-CG
2	VA	72	MEN	C-CA-CB-CG
2	XA	72	MEN	C-CA-CB-CG
2	ZA	72	MEN	C-CA-CB-CG
2	cA	72	MEN	C-CA-CB-CG
2	eA	72	MEN	O-C-CA-CB
2	eA	72	MEN	C-CA-CB-CG
2	gA	72	MEN	O-C-CA-CB
2	iA	72	MEN	C-CA-CB-CG
2	kA	72	MEN	O-C-CA-CB
2	kA	72	MEN	C-CA-CB-CG
2	mA	72	MEN	C-CA-CB-CG
2	mA	72	MEN	CA-CB-CG-OD1
2	mA	72	MEN	CA-CB-CG-ND2
10	DB	72	MEN	C-CA-CB-CG
10	LB	72	MEN	C-CA-CB-CG
10	NB	72	MEN	C-CA-CB-CG
2	RB	72	MEN	C-CA-CB-CG
2	VB	72	MEN	C-CA-CB-CG
2	YB	72	MEN	O-C-CA-CB
2	YB	72	MEN	C-CA-CB-CG
2	aB	72	MEN	C-CA-CB-CG
2	cB	72	MEN	O-C-CA-CB
2	gB	72	MEN	C-CA-CB-CG
2	kB	72	MEN	C-CA-CB-CG
2	AC	72	MEN	CB-CG-ND2-CE2
2	AC	72	MEN	OD1-CG-ND2-CE2
2	BC	72	MEN	CB-CG-ND2-CE2
2	BC	72	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
2	CC	72	MEN	O-C-CA-CB
2	CC	72	MEN	CB-CG-ND2-CE2
2	CC	72	MEN	OD1-CG-ND2-CE2
2	FC	72	MEN	C-CA-CB-CG
2	FC	72	MEN	CB-CG-ND2-CE2
2	FC	72	MEN	OD1-CG-ND2-CE2
2	GC	72	MEN	C-CA-CB-CG
2	GC	72	MEN	CB-CG-ND2-CE2
2	GC	72	MEN	OD1-CG-ND2-CE2
2	HC	72	MEN	CB-CG-ND2-CE2
2	HC	72	MEN	OD1-CG-ND2-CE2
2	IC	72	MEN	C-CA-CB-CG
2	KC	72	MEN	C-CA-CB-CG
2	LC	72	MEN	O-C-CA-CB
2	LC	72	MEN	CB-CG-ND2-CE2
2	LC	72	MEN	OD1-CG-ND2-CE2
2	BD	72	MEN	N-CA-CB-CG
2	DD	72	MEN	O-C-CA-CB
2	FD	72	MEN	C-CA-CB-CG
2	LD	72	MEN	O-C-CA-CB
2	LD	72	MEN	C-CA-CB-CG
2	ND	72	MEN	C-CA-CB-CG
2	PD	72	MEN	C-CA-CB-CG
2	RD	72	MEN	C-CA-CB-CG
2	TD	72	MEN	C-CA-CB-CG
2	TD	72	MEN	CB-CG-ND2-CE2
2	TD	72	MEN	OD1-CG-ND2-CE2
2	VD	72	MEN	C-CA-CB-CG
2	LE	72	MEN	O-C-CA-CB
2	bE	72	MEN	C-CA-CB-CG
2	lE	72	MEN	O-C-CA-CB
2	lE	72	MEN	N-CA-CB-CG
2	rE	72	MEN	C-CA-CB-CG
2	tE	72	MEN	C-CA-CB-CG
10	DF	72	MEN	C-CA-CB-CG
10	HF	72	MEN	N-CA-CB-CG
10	HF	72	MEN	C-CA-CB-CG
2	PF	72	MEN	C-CA-CB-CG
2	RF	72	MEN	C-CA-CB-CG
2	TF	72	MEN	O-C-CA-CB
2	TF	72	MEN	N-CA-CB-CG
2	TF	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	cF	72	MEN	C-CA-CB-CG
2	eF	72	MEN	O-C-CA-CB
2	gF	72	MEN	O-C-CA-CB
2	gF	72	MEN	CA-CB-CG-OD1
2	gF	72	MEN	CA-CB-CG-ND2
2	iF	72	MEN	C-CA-CB-CG
2	LG	72	MEN	O-C-CA-CB
2	PG	72	MEN	O-C-CA-CB
2	ZG	72	MEN	O-C-CA-CB
2	ZG	72	MEN	C-CA-CB-CG
2	bG	72	MEN	N-CA-CB-CG
2	bG	72	MEN	C-CA-CB-CG
2	dG	72	MEN	O-C-CA-CB
2	jG	72	MEN	C-CA-CB-CG
2	nG	72	MEN	C-CA-CB-CG
2	pG	72	MEN	O-C-CA-CB
2	rG	72	MEN	O-C-CA-CB
2	tG	72	MEN	C-CA-CB-CG
18	DH	71	MEN	N-CA-CB-CG
18	DH	71	MEN	C-CA-CB-CG
18	FH	71	MEN	N-CA-CB-CG
18	FH	71	MEN	C-CA-CB-CG
18	FH	71	MEN	CB-CG-ND2-CE2
18	FH	71	MEN	OD1-CG-ND2-CE2
18	BH	71	MEN	N-CA-CB-CG
18	LH	71	MEN	N-CA-CB-CG
18	MH	71	MEN	N-CA-CB-CG
18	QH	71	MEN	CB-CG-ND2-CE2
18	QH	71	MEN	OD1-CG-ND2-CE2
18	dH	71	MEN	N-CA-CB-CG
18	dH	71	MEN	C-CA-CB-CG
18	fH	71	MEN	N-CA-CB-CG
18	hH	71	MEN	CB-CG-ND2-CE2
18	hH	71	MEN	OD1-CG-ND2-CE2
18	jH	71	MEN	N-CA-CB-CG
18	jH	71	MEN	C-CA-CB-CG
18	kH	71	MEN	N-CA-CB-CG
18	nH	71	MEN	N-CA-CB-CG
18	nH	71	MEN	C-CA-CB-CG
18	oH	71	MEN	CB-CG-ND2-CE2
18	oH	71	MEN	OD1-CG-ND2-CE2
18	qH	71	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
18	sH	71	MEN	C-CA-CB-CG
18	wH	71	MEN	C-CA-CB-CG
10	NI	72	MEN	O-C-CA-CB
2	PI	72	MEN	C-CA-CB-CG
2	RI	72	MEN	C-CA-CB-CG
2	YI	72	MEN	C-CA-CB-CG
2	eI	72	MEN	O-C-CA-CB
2	gI	72	MEN	C-CA-CB-CG
2	iI	72	MEN	C-CA-CB-CG
2	kI	72	MEN	O-C-CA-CB
2	kI	72	MEN	C-CA-CB-CG
2	mI	72	MEN	C-CA-CB-CG
2	EJ	72	MEN	C-CA-CB-CG
2	GJ	72	MEN	C-CA-CB-CG
2	KJ	72	MEN	O-C-CA-CB
2	KJ	72	MEN	C-CA-CB-CG
2	MJ	72	MEN	C-CA-CB-CG
2	OJ	72	MEN	O-C-CA-CB
2	QJ	72	MEN	C-CA-CB-CG
2	UJ	72	MEN	O-C-CA-CB
2	WJ	72	MEN	O-C-CA-CB
2	WJ	72	MEN	C-CA-CB-CG
2	D1	72	MEN	CA-CB-CG-OD1
2	J1	72	MEN	CA-CB-CG-OD1
2	n1	72	MEN	CA-CB-CG-OD1
2	s1	72	MEN	CA-CB-CG-OD1
2	k2	72	MEN	CA-CB-CG-OD1
2	m2	72	MEN	CA-CB-CG-OD1
2	P3	72	MEN	CA-CB-CG-OD1
2	F4	72	MEN	CA-CB-CG-OD1
2	h4	72	MEN	CA-CB-CG-OD1
2	V6	72	MEN	CA-CB-CG-OD1
2	a6	72	MEN	CA-CB-CG-OD1
10	L7	72	MEN	CA-CB-CG-OD1
2	P7	72	MEN	CA-CB-CG-OD1
2	g7	72	MEN	CA-CB-CG-OD1
2	k7	72	MEN	CA-CB-CG-OD1
2	D8	72	MEN	CA-CB-CG-OD1
2	J8	72	MEN	CA-CB-CG-OD1
2	V8	72	MEN	CA-CB-CG-OD1
2	c8	72	MEN	CA-CB-CG-OD1
2	m8	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	O9	72	MEN	CA-CB-CG-OD1
2	S9	72	MEN	CA-CB-CG-OD1
2	Y9	72	MEN	CA-CB-CG-OD1
2	DA	72	MEN	CA-CB-CG-OD1
2	PA	72	MEN	CA-CB-CG-OD1
2	VA	72	MEN	CA-CB-CG-OD1
2	cA	72	MEN	CA-CB-CG-OD1
2	aB	72	MEN	CA-CB-CG-OD1
2	FD	72	MEN	CA-CB-CG-OD1
2	ZE	72	MEN	CA-CB-CG-OD1
2	VF	72	MEN	CA-CB-CG-OD1
2	kF	72	MEN	CA-CB-CG-OD1
2	mI	72	MEN	CA-CB-CG-OD1
2	OJ	72	MEN	CA-CB-CG-OD1
2	SJ	72	MEN	CA-CB-CG-OD1
2	D1	72	MEN	CA-CB-CG-ND2
2	J1	72	MEN	CA-CB-CG-ND2
2	n1	72	MEN	CA-CB-CG-ND2
2	s1	72	MEN	CA-CB-CG-ND2
2	T2	72	MEN	CA-CB-CG-ND2
2	g2	72	MEN	CA-CB-CG-ND2
2	k2	72	MEN	CA-CB-CG-ND2
2	m2	72	MEN	CA-CB-CG-ND2
2	P3	72	MEN	CA-CB-CG-ND2
2	F4	72	MEN	CA-CB-CG-ND2
2	h4	72	MEN	CA-CB-CG-ND2
2	V6	72	MEN	CA-CB-CG-ND2
2	a6	72	MEN	CA-CB-CG-ND2
10	L7	72	MEN	CA-CB-CG-ND2
2	P7	72	MEN	CA-CB-CG-ND2
2	T7	72	MEN	CA-CB-CG-ND2
2	g7	72	MEN	CA-CB-CG-ND2
2	k7	72	MEN	CA-CB-CG-ND2
2	D8	72	MEN	CA-CB-CG-ND2
2	J8	72	MEN	CA-CB-CG-ND2
2	V8	72	MEN	CA-CB-CG-ND2
2	c8	72	MEN	CA-CB-CG-ND2
2	m8	72	MEN	CA-CB-CG-ND2
2	O9	72	MEN	CA-CB-CG-ND2
2	S9	72	MEN	CA-CB-CG-ND2
2	Y9	72	MEN	CA-CB-CG-ND2
2	DA	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	PA	72	MEN	CA-CB-CG-ND2
2	VA	72	MEN	CA-CB-CG-ND2
2	cA	72	MEN	CA-CB-CG-ND2
2	aB	72	MEN	CA-CB-CG-ND2
2	FD	72	MEN	CA-CB-CG-ND2
2	ZE	72	MEN	CA-CB-CG-ND2
2	rE	72	MEN	CA-CB-CG-ND2
10	LF	72	MEN	CA-CB-CG-ND2
2	VF	72	MEN	CA-CB-CG-ND2
2	kF	72	MEN	CA-CB-CG-ND2
2	tG	72	MEN	CA-CB-CG-ND2
2	TI	72	MEN	CA-CB-CG-ND2
2	kI	72	MEN	CA-CB-CG-ND2
2	mI	72	MEN	CA-CB-CG-ND2
2	OJ	72	MEN	CA-CB-CG-ND2
2	SJ	72	MEN	CA-CB-CG-ND2
2	B1	72	MEN	N-CA-CB-CG
2	D1	72	MEN	N-CA-CB-CG
2	F1	72	MEN	N-CA-CB-CG
2	H1	72	MEN	N-CA-CB-CG
2	L1	72	MEN	N-CA-CB-CG
2	Q1	72	MEN	N-CA-CB-CG
2	U1	72	MEN	N-CA-CB-CG
2	Z1	72	MEN	N-CA-CB-CG
2	a1	72	MEN	N-CA-CB-CG
2	d1	72	MEN	N-CA-CB-CG
2	h1	72	MEN	N-CA-CB-CG
2	j1	72	MEN	N-CA-CB-CG
2	n1	72	MEN	N-CA-CB-CG
2	s1	72	MEN	N-CA-CB-CG
2	Y2	72	MEN	N-CA-CB-CG
2	i2	72	MEN	N-CA-CB-CG
2	k2	72	MEN	N-CA-CB-CG
2	B3	72	MEN	N-CA-CB-CG
2	R3	72	MEN	N-CA-CB-CG
2	V3	72	MEN	N-CA-CB-CG
2	B4	72	MEN	N-CA-CB-CG
2	H4	72	MEN	N-CA-CB-CG
2	J4	72	MEN	N-CA-CB-CG
2	L4	72	MEN	N-CA-CB-CG
2	O4	72	MEN	N-CA-CB-CG
2	Q4	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	U4	72	MEN	N-CA-CB-CG
2	a4	72	MEN	N-CA-CB-CG
2	d4	72	MEN	N-CA-CB-CG
2	f4	72	MEN	N-CA-CB-CG
2	h4	72	MEN	N-CA-CB-CG
2	j4	72	MEN	N-CA-CB-CG
2	l4	72	MEN	N-CA-CB-CG
2	l4	72	MEN	N-CA-CB-CG
2	F5	72	MEN	N-CA-CB-CG
2	G5	72	MEN	N-CA-CB-CG
2	I5	72	MEN	N-CA-CB-CG
2	K5	72	MEN	N-CA-CB-CG
10	D6	72	MEN	N-CA-CB-CG
2	R6	72	MEN	N-CA-CB-CG
2	a6	72	MEN	N-CA-CB-CG
2	k6	72	MEN	N-CA-CB-CG
10	H7	72	MEN	N-CA-CB-CG
2	P7	72	MEN	N-CA-CB-CG
2	R7	72	MEN	N-CA-CB-CG
2	T7	72	MEN	N-CA-CB-CG
2	V7	72	MEN	N-CA-CB-CG
2	Y7	72	MEN	N-CA-CB-CG
2	c7	72	MEN	N-CA-CB-CG
2	m7	72	MEN	N-CA-CB-CG
2	F8	72	MEN	N-CA-CB-CG
2	H8	72	MEN	N-CA-CB-CG
2	J8	72	MEN	N-CA-CB-CG
2	L8	72	MEN	N-CA-CB-CG
2	P8	72	MEN	N-CA-CB-CG
2	R8	72	MEN	N-CA-CB-CG
2	V8	72	MEN	N-CA-CB-CG
2	X8	72	MEN	N-CA-CB-CG
2	Z8	72	MEN	N-CA-CB-CG
2	c8	72	MEN	N-CA-CB-CG
2	e8	72	MEN	N-CA-CB-CG
2	i8	72	MEN	N-CA-CB-CG
2	m8	72	MEN	N-CA-CB-CG
2	C9	72	MEN	N-CA-CB-CG
2	G9	72	MEN	N-CA-CB-CG
2	K9	72	MEN	N-CA-CB-CG
2	M9	72	MEN	N-CA-CB-CG
2	S9	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	W9	72	MEN	N-CA-CB-CG
2	DA	72	MEN	N-CA-CB-CG
2	FA	72	MEN	N-CA-CB-CG
2	HA	72	MEN	N-CA-CB-CG
2	JA	72	MEN	N-CA-CB-CG
2	LA	72	MEN	N-CA-CB-CG
2	PA	72	MEN	N-CA-CB-CG
2	RA	72	MEN	N-CA-CB-CG
2	VA	72	MEN	N-CA-CB-CG
2	XA	72	MEN	N-CA-CB-CG
2	ZA	72	MEN	N-CA-CB-CG
2	cA	72	MEN	N-CA-CB-CG
2	eA	72	MEN	N-CA-CB-CG
2	iA	72	MEN	N-CA-CB-CG
2	mA	72	MEN	N-CA-CB-CG
10	DB	72	MEN	N-CA-CB-CG
2	RB	72	MEN	N-CA-CB-CG
2	VB	72	MEN	N-CA-CB-CG
2	aB	72	MEN	N-CA-CB-CG
2	kB	72	MEN	N-CA-CB-CG
2	FC	72	MEN	N-CA-CB-CG
2	GC	72	MEN	N-CA-CB-CG
2	IC	72	MEN	N-CA-CB-CG
2	KC	72	MEN	N-CA-CB-CG
2	LC	72	MEN	N-CA-CB-CG
2	FD	72	MEN	N-CA-CB-CG
2	PD	72	MEN	N-CA-CB-CG
2	RD	72	MEN	N-CA-CB-CG
2	TD	72	MEN	N-CA-CB-CG
2	VD	72	MEN	N-CA-CB-CG
2	bE	72	MEN	N-CA-CB-CG
2	rE	72	MEN	N-CA-CB-CG
2	tE	72	MEN	N-CA-CB-CG
10	DF	72	MEN	N-CA-CB-CG
2	PF	72	MEN	N-CA-CB-CG
2	RF	72	MEN	N-CA-CB-CG
2	VF	72	MEN	N-CA-CB-CG
2	cF	72	MEN	N-CA-CB-CG
2	iF	72	MEN	N-CA-CB-CG
2	ZG	72	MEN	N-CA-CB-CG
2	jG	72	MEN	N-CA-CB-CG
2	IG	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	tG	72	MEN	N-CA-CB-CG
18	sH	71	MEN	N-CA-CB-CG
2	YI	72	MEN	N-CA-CB-CG
2	gI	72	MEN	N-CA-CB-CG
2	iI	72	MEN	N-CA-CB-CG
2	kI	72	MEN	N-CA-CB-CG
2	GJ	72	MEN	N-CA-CB-CG
2	KJ	72	MEN	N-CA-CB-CG
2	MJ	72	MEN	N-CA-CB-CG
2	OJ	72	MEN	N-CA-CB-CG
2	QJ	72	MEN	N-CA-CB-CG
2	WJ	72	MEN	N-CA-CB-CG
2	T2	72	MEN	CA-CB-CG-OD1
10	LB	72	MEN	CA-CB-CG-OD1
2	jE	72	MEN	CA-CB-CG-OD1
2	rE	72	MEN	CA-CB-CG-OD1
10	LF	72	MEN	CA-CB-CG-OD1
2	tG	72	MEN	CA-CB-CG-OD1
2	TI	72	MEN	CA-CB-CG-OD1
2	kI	72	MEN	CA-CB-CG-OD1
2	V7	72	MEN	CA-CB-CG-ND2
2	Z8	72	MEN	CA-CB-CG-ND2
2	JA	72	MEN	CA-CB-CG-ND2
2	ZA	72	MEN	CA-CB-CG-ND2
2	PD	72	MEN	CA-CB-CG-ND2
2	PF	72	MEN	CA-CB-CG-ND2
2	rG	72	MEN	CA-CB-CG-ND2
18	wH	71	MEN	CA-CB-CG-ND2
2	L1	72	MEN	CA-CB-CG-OD1
2	O1	72	MEN	CA-CB-CG-OD1
2	a1	72	MEN	CA-CB-CG-OD1
2	j1	72	MEN	CA-CB-CG-OD1
2	q1	72	MEN	CA-CB-CG-OD1
10	D2	72	MEN	CA-CB-CG-OD1
10	H2	72	MEN	CA-CB-CG-OD1
2	R2	72	MEN	CA-CB-CG-OD1
2	g2	72	MEN	CA-CB-CG-OD1
2	H3	72	MEN	CA-CB-CG-OD1
2	R3	72	MEN	CA-CB-CG-OD1
2	O4	72	MEN	CA-CB-CG-OD1
2	S4	72	MEN	CA-CB-CG-OD1
2	a4	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	j4	72	MEN	CA-CB-CG-OD1
10	L6	72	MEN	CA-CB-CG-OD1
2	P6	72	MEN	CA-CB-CG-OD1
2	T6	72	MEN	CA-CB-CG-OD1
10	F7	72	MEN	CA-CB-CG-OD1
10	H7	72	MEN	CA-CB-CG-OD1
2	T7	72	MEN	CA-CB-CG-OD1
2	Y7	72	MEN	CA-CB-CG-OD1
2	a7	72	MEN	CA-CB-CG-OD1
2	L8	72	MEN	CA-CB-CG-OD1
2	N8	72	MEN	CA-CB-CG-OD1
2	X8	72	MEN	CA-CB-CG-OD1
2	Z8	72	MEN	CA-CB-CG-OD1
2	G9	72	MEN	CA-CB-CG-OD1
2	JA	72	MEN	CA-CB-CG-OD1
2	LA	72	MEN	CA-CB-CG-OD1
2	NA	72	MEN	CA-CB-CG-OD1
10	HB	72	MEN	CA-CB-CG-OD1
10	JB	72	MEN	CA-CB-CG-OD1
2	PB	72	MEN	CA-CB-CG-OD1
2	gB	72	MEN	CA-CB-CG-OD1
2	kB	72	MEN	CA-CB-CG-OD1
2	PD	72	MEN	CA-CB-CG-OD1
2	RD	72	MEN	CA-CB-CG-OD1
2	BE	72	MEN	CA-CB-CG-OD1
2	JE	72	MEN	CA-CB-CG-OD1
2	NE	72	MEN	CA-CB-CG-OD1
2	PE	72	MEN	CA-CB-CG-OD1
2	RE	72	MEN	CA-CB-CG-OD1
2	XE	72	MEN	CA-CB-CG-OD1
2	dE	72	MEN	CA-CB-CG-OD1
10	DF	72	MEN	CA-CB-CG-OD1
10	FF	72	MEN	CA-CB-CG-OD1
10	NF	72	MEN	CA-CB-CG-OD1
2	PF	72	MEN	CA-CB-CG-OD1
2	BG	72	MEN	CA-CB-CG-OD1
2	JG	72	MEN	CA-CB-CG-OD1
2	NG	72	MEN	CA-CB-CG-OD1
2	RG	72	MEN	CA-CB-CG-OD1
2	XG	72	MEN	CA-CB-CG-OD1
2	bG	72	MEN	CA-CB-CG-OD1
2	dG	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	rG	72	MEN	CA-CB-CG-OD1
18	LH	71	MEN	CA-CB-CG-OD1
18	wH	71	MEN	CA-CB-CG-OD1
10	DI	72	MEN	CA-CB-CG-OD1
10	HI	72	MEN	CA-CB-CG-OD1
2	RI	72	MEN	CA-CB-CG-OD1
2	EJ	72	MEN	CA-CB-CG-OD1
2	GJ	72	MEN	CA-CB-CG-OD1
2	H1	72	MEN	CA-CB-CG-ND2
2	Q1	72	MEN	CA-CB-CG-ND2
2	W1	72	MEN	CA-CB-CG-ND2
2	j1	72	MEN	CA-CB-CG-ND2
2	11	72	MEN	CA-CB-CG-ND2
10	D2	72	MEN	CA-CB-CG-ND2
10	J2	72	MEN	CA-CB-CG-ND2
2	R2	72	MEN	CA-CB-CG-ND2
2	i2	72	MEN	CA-CB-CG-ND2
2	B3	72	MEN	CA-CB-CG-ND2
2	L3	72	MEN	CA-CB-CG-ND2
2	R3	72	MEN	CA-CB-CG-ND2
2	V3	72	MEN	CA-CB-CG-ND2
2	X3	72	MEN	CA-CB-CG-ND2
2	H4	72	MEN	CA-CB-CG-ND2
2	Q4	72	MEN	CA-CB-CG-ND2
2	W4	72	MEN	CA-CB-CG-ND2
2	Z4	72	MEN	CA-CB-CG-ND2
2	a4	72	MEN	CA-CB-CG-ND2
2	l4	72	MEN	CA-CB-CG-ND2
10	D6	72	MEN	CA-CB-CG-ND2
10	N6	72	MEN	CA-CB-CG-ND2
2	g6	72	MEN	CA-CB-CG-ND2
2	m6	72	MEN	CA-CB-CG-ND2
10	D7	72	MEN	CA-CB-CG-ND2
10	F7	72	MEN	CA-CB-CG-ND2
10	N7	72	MEN	CA-CB-CG-ND2
2	Y7	72	MEN	CA-CB-CG-ND2
2	a7	72	MEN	CA-CB-CG-ND2
2	c7	72	MEN	CA-CB-CG-ND2
2	m7	72	MEN	CA-CB-CG-ND2
2	H8	72	MEN	CA-CB-CG-ND2
2	L8	72	MEN	CA-CB-CG-ND2
2	N8	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	X8	72	MEN	CA-CB-CG-ND2
2	e8	72	MEN	CA-CB-CG-ND2
2	g8	72	MEN	CA-CB-CG-ND2
2	E9	72	MEN	CA-CB-CG-ND2
2	G9	72	MEN	CA-CB-CG-ND2
2	K9	72	MEN	CA-CB-CG-ND2
2	U9	72	MEN	CA-CB-CG-ND2
2	W9	72	MEN	CA-CB-CG-ND2
2	HA	72	MEN	CA-CB-CG-ND2
2	LA	72	MEN	CA-CB-CG-ND2
2	NA	72	MEN	CA-CB-CG-ND2
2	XA	72	MEN	CA-CB-CG-ND2
2	eA	72	MEN	CA-CB-CG-ND2
2	gA	72	MEN	CA-CB-CG-ND2
10	DB	72	MEN	CA-CB-CG-ND2
10	HB	72	MEN	CA-CB-CG-ND2
10	NB	72	MEN	CA-CB-CG-ND2
2	VB	72	MEN	CA-CB-CG-ND2
2	gB	72	MEN	CA-CB-CG-ND2
2	kB	72	MEN	CA-CB-CG-ND2
2	BD	72	MEN	CA-CB-CG-ND2
2	HD	72	MEN	CA-CB-CG-ND2
2	RD	72	MEN	CA-CB-CG-ND2
2	VD	72	MEN	CA-CB-CG-ND2
2	XD	72	MEN	CA-CB-CG-ND2
2	BE	72	MEN	CA-CB-CG-ND2
2	DE	72	MEN	CA-CB-CG-ND2
2	FE	72	MEN	CA-CB-CG-ND2
2	HE	72	MEN	CA-CB-CG-ND2
2	JE	72	MEN	CA-CB-CG-ND2
2	NE	72	MEN	CA-CB-CG-ND2
2	dE	72	MEN	CA-CB-CG-ND2
2	fE	72	MEN	CA-CB-CG-ND2
2	lE	72	MEN	CA-CB-CG-ND2
10	DF	72	MEN	CA-CB-CG-ND2
10	FF	72	MEN	CA-CB-CG-ND2
10	NF	72	MEN	CA-CB-CG-ND2
2	TF	72	MEN	CA-CB-CG-ND2
2	cF	72	MEN	CA-CB-CG-ND2
2	mF	72	MEN	CA-CB-CG-ND2
2	FG	72	MEN	CA-CB-CG-ND2
2	JG	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	NG	72	MEN	CA-CB-CG-ND2
2	ZG	72	MEN	CA-CB-CG-ND2
2	dG	72	MEN	CA-CB-CG-ND2
2	fG	72	MEN	CA-CB-CG-ND2
2	lG	72	MEN	CA-CB-CG-ND2
18	LH	71	MEN	CA-CB-CG-ND2
10	DI	72	MEN	CA-CB-CG-ND2
2	RI	72	MEN	CA-CB-CG-ND2
2	cI	72	MEN	CA-CB-CG-ND2
2	iI	72	MEN	CA-CB-CG-ND2
2	EJ	72	MEN	CA-CB-CG-ND2
2	GJ	72	MEN	CA-CB-CG-ND2
2	KJ	72	MEN	CA-CB-CG-ND2
2	QJ	72	MEN	CA-CB-CG-ND2
2	S1	72	MEN	N-CA-CB-CG
10	N2	72	MEN	N-CA-CB-CG
2	g2	72	MEN	N-CA-CB-CG
2	S4	72	MEN	N-CA-CB-CG
2	Y4	72	MEN	N-CA-CB-CG
2	B5	72	MEN	N-CA-CB-CG
2	L5	72	MEN	N-CA-CB-CG
10	H6	72	MEN	N-CA-CB-CG
2	g7	72	MEN	N-CA-CB-CG
2	gB	72	MEN	N-CA-CB-CG
2	HD	72	MEN	N-CA-CB-CG
2	mF	72	MEN	N-CA-CB-CG
18	UH	71	MEN	N-CA-CB-CG
10	NI	72	MEN	N-CA-CB-CG
2	EJ	72	MEN	N-CA-CB-CG
2	SJ	72	MEN	N-CA-CB-CG
2	H1	72	MEN	CA-CB-CG-OD1
2	S1	72	MEN	CA-CB-CG-OD1
2	U1	72	MEN	CA-CB-CG-OD1
2	W1	72	MEN	CA-CB-CG-OD1
2	Z1	72	MEN	CA-CB-CG-OD1
2	11	72	MEN	CA-CB-CG-OD1
2	V2	72	MEN	CA-CB-CG-OD1
2	a2	72	MEN	CA-CB-CG-OD1
2	i2	72	MEN	CA-CB-CG-OD1
2	J3	72	MEN	CA-CB-CG-OD1
2	L3	72	MEN	CA-CB-CG-OD1
2	V3	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	H4	72	MEN	CA-CB-CG-OD1
2	U4	72	MEN	CA-CB-CG-OD1
2	W4	72	MEN	CA-CB-CG-OD1
2	Z4	72	MEN	CA-CB-CG-OD1
2	l4	72	MEN	CA-CB-CG-OD1
2	s4	72	MEN	CA-CB-CG-OD1
2	y4	72	MEN	CA-CB-CG-OD1
10	D6	72	MEN	CA-CB-CG-OD1
10	J6	72	MEN	CA-CB-CG-OD1
10	N6	72	MEN	CA-CB-CG-OD1
2	Y6	72	MEN	CA-CB-CG-OD1
2	c6	72	MEN	CA-CB-CG-OD1
2	g6	72	MEN	CA-CB-CG-OD1
2	k6	72	MEN	CA-CB-CG-OD1
2	m6	72	MEN	CA-CB-CG-OD1
10	D7	72	MEN	CA-CB-CG-OD1
2	V7	72	MEN	CA-CB-CG-OD1
2	c7	72	MEN	CA-CB-CG-OD1
2	m7	72	MEN	CA-CB-CG-OD1
2	H8	72	MEN	CA-CB-CG-OD1
2	e8	72	MEN	CA-CB-CG-OD1
2	g8	72	MEN	CA-CB-CG-OD1
2	E9	72	MEN	CA-CB-CG-OD1
2	K9	72	MEN	CA-CB-CG-OD1
2	U9	72	MEN	CA-CB-CG-OD1
2	XA	72	MEN	CA-CB-CG-OD1
2	ZA	72	MEN	CA-CB-CG-OD1
2	eA	72	MEN	CA-CB-CG-OD1
2	gA	72	MEN	CA-CB-CG-OD1
10	NB	72	MEN	CA-CB-CG-OD1
2	TB	72	MEN	CA-CB-CG-OD1
2	VB	72	MEN	CA-CB-CG-OD1
2	YB	72	MEN	CA-CB-CG-OD1
2	cB	72	MEN	CA-CB-CG-OD1
2	BD	72	MEN	CA-CB-CG-OD1
2	HD	72	MEN	CA-CB-CG-OD1
2	VD	72	MEN	CA-CB-CG-OD1
2	DE	72	MEN	CA-CB-CG-OD1
2	FE	72	MEN	CA-CB-CG-OD1
2	HE	72	MEN	CA-CB-CG-OD1
2	LE	72	MEN	CA-CB-CG-OD1
2	fE	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	pE	72	MEN	CA-CB-CG-OD1
2	tE	72	MEN	CA-CB-CG-OD1
2	TF	72	MEN	CA-CB-CG-OD1
2	YF	72	MEN	CA-CB-CG-OD1
2	aF	72	MEN	CA-CB-CG-OD1
2	cF	72	MEN	CA-CB-CG-OD1
2	mF	72	MEN	CA-CB-CG-OD1
2	FG	72	MEN	CA-CB-CG-OD1
2	HG	72	MEN	CA-CB-CG-OD1
2	LG	72	MEN	CA-CB-CG-OD1
2	PG	72	MEN	CA-CB-CG-OD1
2	ZG	72	MEN	CA-CB-CG-OD1
2	fG	72	MEN	CA-CB-CG-OD1
2	jG	72	MEN	CA-CB-CG-OD1
2	pG	72	MEN	CA-CB-CG-OD1
18	SH	71	MEN	CA-CB-CG-OD1
18	uH	71	MEN	CA-CB-CG-OD1
2	VI	72	MEN	CA-CB-CG-OD1
2	aI	72	MEN	CA-CB-CG-OD1
2	cI	72	MEN	CA-CB-CG-OD1
2	gI	72	MEN	CA-CB-CG-OD1
2	iI	72	MEN	CA-CB-CG-OD1
2	KJ	72	MEN	CA-CB-CG-OD1
2	UJ	72	MEN	CA-CB-CG-OD1
2	L1	72	MEN	CA-CB-CG-ND2
2	O1	72	MEN	CA-CB-CG-ND2
2	U1	72	MEN	CA-CB-CG-ND2
2	a1	72	MEN	CA-CB-CG-ND2
2	q1	72	MEN	CA-CB-CG-ND2
2	w1	72	MEN	CA-CB-CG-ND2
10	H2	72	MEN	CA-CB-CG-ND2
10	L2	72	MEN	CA-CB-CG-ND2
2	L4	72	MEN	CA-CB-CG-ND2
2	S4	72	MEN	CA-CB-CG-ND2
2	j4	72	MEN	CA-CB-CG-ND2
2	14	72	MEN	CA-CB-CG-ND2
10	L6	72	MEN	CA-CB-CG-ND2
2	P6	72	MEN	CA-CB-CG-ND2
2	T6	72	MEN	CA-CB-CG-ND2
2	Y6	72	MEN	CA-CB-CG-ND2
2	k6	72	MEN	CA-CB-CG-ND2
10	H7	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	iA	72	MEN	CA-CB-CG-ND2
2	PB	72	MEN	CA-CB-CG-ND2
2	TB	72	MEN	CA-CB-CG-ND2
2	YB	72	MEN	CA-CB-CG-ND2
2	mB	72	MEN	CA-CB-CG-ND2
2	LD	72	MEN	CA-CB-CG-ND2
2	PE	72	MEN	CA-CB-CG-ND2
2	XE	72	MEN	CA-CB-CG-ND2
2	jE	72	MEN	CA-CB-CG-ND2
2	pE	72	MEN	CA-CB-CG-ND2
2	tE	72	MEN	CA-CB-CG-ND2
10	HF	72	MEN	CA-CB-CG-ND2
2	YF	72	MEN	CA-CB-CG-ND2
2	aF	72	MEN	CA-CB-CG-ND2
2	BG	72	MEN	CA-CB-CG-ND2
2	LG	72	MEN	CA-CB-CG-ND2
2	RG	72	MEN	CA-CB-CG-ND2
2	VG	72	MEN	CA-CB-CG-ND2
2	bG	72	MEN	CA-CB-CG-ND2
2	hG	72	MEN	CA-CB-CG-ND2
2	pG	72	MEN	CA-CB-CG-ND2
18	SH	71	MEN	CA-CB-CG-ND2
18	fH	71	MEN	CA-CB-CG-ND2
18	uH	71	MEN	CA-CB-CG-ND2
10	HI	72	MEN	CA-CB-CG-ND2
10	JI	72	MEN	CA-CB-CG-ND2
2	O1	72	MEN	C-CA-CB-CG
2	W1	72	MEN	C-CA-CB-CG
2	d1	72	MEN	C-CA-CB-CG
2	h1	72	MEN	C-CA-CB-CG
2	l1	72	MEN	C-CA-CB-CG
2	n1	72	MEN	C-CA-CB-CG
2	11	72	MEN	C-CA-CB-CG
10	L2	72	MEN	C-CA-CB-CG
2	e2	72	MEN	C-CA-CB-CG
2	m2	72	MEN	C-CA-CB-CG
2	B3	72	MEN	C-CA-CB-CG
2	P3	72	MEN	C-CA-CB-CG
2	X3	72	MEN	C-CA-CB-CG
2	H4	72	MEN	C-CA-CB-CG
2	W4	72	MEN	C-CA-CB-CG
2	Z4	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	f4	72	MEN	C-CA-CB-CG
2	l4	72	MEN	C-CA-CB-CG
2	q4	72	MEN	C-CA-CB-CG
2	u4	72	MEN	C-CA-CB-CG
2	w4	72	MEN	C-CA-CB-CG
2	y4	72	MEN	C-CA-CB-CG
2	14	72	MEN	C-CA-CB-CG
2	B5	72	MEN	C-CA-CB-CG
2	L5	72	MEN	C-CA-CB-CG
10	N6	72	MEN	C-CA-CB-CG
2	V6	72	MEN	C-CA-CB-CG
2	g6	72	MEN	C-CA-CB-CG
2	i6	72	MEN	C-CA-CB-CG
2	a7	72	MEN	C-CA-CB-CG
2	m7	72	MEN	C-CA-CB-CG
2	D8	72	MEN	C-CA-CB-CG
2	I9	72	MEN	C-CA-CB-CG
2	S9	72	MEN	C-CA-CB-CG
2	Y9	72	MEN	C-CA-CB-CG
2	DA	72	MEN	C-CA-CB-CG
2	eB	72	MEN	C-CA-CB-CG
2	LC	72	MEN	C-CA-CB-CG
2	BD	72	MEN	C-CA-CB-CG
2	HD	72	MEN	C-CA-CB-CG
2	XD	72	MEN	C-CA-CB-CG
2	jE	72	MEN	C-CA-CB-CG
2	lE	72	MEN	C-CA-CB-CG
2	nE	72	MEN	C-CA-CB-CG
2	VF	72	MEN	C-CA-CB-CG
2	YF	72	MEN	C-CA-CB-CG
2	aF	72	MEN	C-CA-CB-CG
2	kF	72	MEN	C-CA-CB-CG
2	VG	72	MEN	C-CA-CB-CG
2	lG	72	MEN	C-CA-CB-CG
18	BH	71	MEN	C-CA-CB-CG
18	IH	71	MEN	N-CA-CB-CG
18	SH	71	MEN	C-CA-CB-CG
18	qH	71	MEN	C-CA-CB-CG
18	uH	71	MEN	C-CA-CB-CG
10	LI	72	MEN	C-CA-CB-CG
2	eI	72	MEN	C-CA-CB-CG
2	CJ	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	IJ	72	MEN	C-CA-CB-CG
2	SJ	72	MEN	C-CA-CB-CG
2	Q1	72	MEN	CA-CB-CG-OD1
10	J2	72	MEN	CA-CB-CG-OD1
10	L2	72	MEN	CA-CB-CG-OD1
2	e2	72	MEN	CA-CB-CG-OD1
2	B3	72	MEN	CA-CB-CG-OD1
2	X3	72	MEN	CA-CB-CG-OD1
2	Q4	72	MEN	CA-CB-CG-OD1
2	14	72	MEN	CA-CB-CG-OD1
10	N7	72	MEN	CA-CB-CG-OD1
2	Q9	72	MEN	CA-CB-CG-OD1
2	W9	72	MEN	CA-CB-CG-OD1
2	HA	72	MEN	CA-CB-CG-OD1
10	DB	72	MEN	CA-CB-CG-OD1
2	DD	72	MEN	CA-CB-CG-OD1
2	XD	72	MEN	CA-CB-CG-OD1
2	VE	72	MEN	CA-CB-CG-OD1
2	bE	72	MEN	CA-CB-CG-OD1
2	lE	72	MEN	CA-CB-CG-OD1
2	VG	72	MEN	CA-CB-CG-OD1
2	lG	72	MEN	CA-CB-CG-OD1
18	IH	71	MEN	CA-CB-CG-OD1
18	fH	71	MEN	CA-CB-CG-OD1
2	eI	72	MEN	CA-CB-CG-OD1
2	IJ	72	MEN	CA-CB-CG-OD1
2	QJ	72	MEN	CA-CB-CG-OD1
2	S1	72	MEN	CA-CB-CG-ND2
2	Z1	72	MEN	CA-CB-CG-ND2
2	u1	72	MEN	CA-CB-CG-ND2
2	P2	72	MEN	CA-CB-CG-ND2
2	V2	72	MEN	CA-CB-CG-ND2
2	Y2	72	MEN	CA-CB-CG-ND2
2	a2	72	MEN	CA-CB-CG-ND2
2	e2	72	MEN	CA-CB-CG-ND2
2	H3	72	MEN	CA-CB-CG-ND2
2	J3	72	MEN	CA-CB-CG-ND2
2	N3	72	MEN	CA-CB-CG-ND2
2	O4	72	MEN	CA-CB-CG-ND2
2	U4	72	MEN	CA-CB-CG-ND2
2	s4	72	MEN	CA-CB-CG-ND2
2	y4	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
10	H6	72	MEN	CA-CB-CG-ND2
10	J6	72	MEN	CA-CB-CG-ND2
2	c6	72	MEN	CA-CB-CG-ND2
2	i7	72	MEN	CA-CB-CG-ND2
2	C9	72	MEN	CA-CB-CG-ND2
2	I9	72	MEN	CA-CB-CG-ND2
2	Q9	72	MEN	CA-CB-CG-ND2
10	JB	72	MEN	CA-CB-CG-ND2
10	LB	72	MEN	CA-CB-CG-ND2
2	cB	72	MEN	CA-CB-CG-ND2
2	iB	72	MEN	CA-CB-CG-ND2
2	DD	72	MEN	CA-CB-CG-ND2
2	ND	72	MEN	CA-CB-CG-ND2
2	LE	72	MEN	CA-CB-CG-ND2
2	RE	72	MEN	CA-CB-CG-ND2
2	TE	72	MEN	CA-CB-CG-ND2
2	VE	72	MEN	CA-CB-CG-ND2
2	bE	72	MEN	CA-CB-CG-ND2
2	iF	72	MEN	CA-CB-CG-ND2
2	DG	72	MEN	CA-CB-CG-ND2
2	HG	72	MEN	CA-CB-CG-ND2
2	PG	72	MEN	CA-CB-CG-ND2
2	TG	72	MEN	CA-CB-CG-ND2
2	XG	72	MEN	CA-CB-CG-ND2
2	jG	72	MEN	CA-CB-CG-ND2
18	IH	71	MEN	CA-CB-CG-ND2
18	sH	71	MEN	CA-CB-CG-ND2
10	LI	72	MEN	CA-CB-CG-ND2
2	PI	72	MEN	CA-CB-CG-ND2
2	VI	72	MEN	CA-CB-CG-ND2
2	YI	72	MEN	CA-CB-CG-ND2
2	aI	72	MEN	CA-CB-CG-ND2
2	eI	72	MEN	CA-CB-CG-ND2
2	gI	72	MEN	CA-CB-CG-ND2
2	IJ	72	MEN	CA-CB-CG-ND2
2	UJ	72	MEN	CA-CB-CG-ND2
2	WJ	72	MEN	CA-CB-CG-ND2
2	O1	72	MEN	N-CA-CB-CG
2	W1	72	MEN	N-CA-CB-CG
2	Y1	72	MEN	N-CA-CB-CG
10	L2	72	MEN	N-CA-CB-CG
2	P2	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	R2	72	MEN	N-CA-CB-CG
2	e2	72	MEN	N-CA-CB-CG
2	m2	72	MEN	N-CA-CB-CG
2	H3	72	MEN	N-CA-CB-CG
2	L3	72	MEN	N-CA-CB-CG
2	N3	72	MEN	N-CA-CB-CG
2	P3	72	MEN	N-CA-CB-CG
2	Z4	72	MEN	N-CA-CB-CG
2	n4	72	MEN	N-CA-CB-CG
10	L6	72	MEN	N-CA-CB-CG
10	N6	72	MEN	N-CA-CB-CG
2	V6	72	MEN	N-CA-CB-CG
2	Y6	72	MEN	N-CA-CB-CG
2	g6	72	MEN	N-CA-CB-CG
2	k8	72	MEN	N-CA-CB-CG
2	kA	72	MEN	N-CA-CB-CG
10	LB	72	MEN	N-CA-CB-CG
10	NB	72	MEN	N-CA-CB-CG
2	YB	72	MEN	N-CA-CB-CG
2	LD	72	MEN	N-CA-CB-CG
2	ND	72	MEN	N-CA-CB-CG
2	jE	72	MEN	N-CA-CB-CG
18	wH	71	MEN	N-CA-CB-CG
10	LI	72	MEN	N-CA-CB-CG
2	PI	72	MEN	N-CA-CB-CG
2	RI	72	MEN	N-CA-CB-CG
2	eI	72	MEN	N-CA-CB-CG
2	mI	72	MEN	N-CA-CB-CG
2	CJ	72	MEN	N-CA-CB-CG
2	N3	72	MEN	CA-CB-CG-OD1
2	L4	72	MEN	CA-CB-CG-OD1
10	H6	72	MEN	CA-CB-CG-OD1
2	i7	72	MEN	CA-CB-CG-OD1
2	I9	72	MEN	CA-CB-CG-OD1
2	iB	72	MEN	CA-CB-CG-OD1
2	mB	72	MEN	CA-CB-CG-OD1
2	ND	72	MEN	CA-CB-CG-OD1
2	TE	72	MEN	CA-CB-CG-OD1
2	iF	72	MEN	CA-CB-CG-OD1
2	DG	72	MEN	CA-CB-CG-OD1
2	TG	72	MEN	CA-CB-CG-OD1
2	hG	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
18	sH	71	MEN	CA-CB-CG-OD1
10	JI	72	MEN	CA-CB-CG-OD1
10	LI	72	MEN	CA-CB-CG-OD1
2	YI	72	MEN	CA-CB-CG-OD1
2	WJ	72	MEN	CA-CB-CG-OD1
2	ll	72	MEN	CA-CB-CG-OD1
2	u1	72	MEN	CA-CB-CG-OD1
2	w1	72	MEN	CA-CB-CG-OD1
2	y1	72	MEN	CA-CB-CG-OD1
2	P2	72	MEN	CA-CB-CG-OD1
2	Y2	72	MEN	CA-CB-CG-OD1
2	c2	72	MEN	CA-CB-CG-OD1
2	u4	72	MEN	CA-CB-CG-OD1
2	i8	72	MEN	CA-CB-CG-OD1
2	C9	72	MEN	CA-CB-CG-OD1
2	iA	72	MEN	CA-CB-CG-OD1
2	LD	72	MEN	CA-CB-CG-OD1
2	hE	72	MEN	CA-CB-CG-OD1
2	vE	72	MEN	CA-CB-CG-OD1
10	HF	72	MEN	CA-CB-CG-OD1
2	PI	72	MEN	CA-CB-CG-OD1
2	u4	72	MEN	CA-CB-CG-ND2
2	T2	72	MEN	N-CA-CB-CG
2	X3	72	MEN	N-CA-CB-CG
2	W4	72	MEN	N-CA-CB-CG
10	F6	72	MEN	N-CA-CB-CG
2	T6	72	MEN	N-CA-CB-CG
2	i6	72	MEN	N-CA-CB-CG
2	i7	72	MEN	N-CA-CB-CG
2	k7	72	MEN	N-CA-CB-CG
2	T8	72	MEN	N-CA-CB-CG
2	E9	72	MEN	N-CA-CB-CG
2	I9	72	MEN	N-CA-CB-CG
2	U9	72	MEN	N-CA-CB-CG
2	NA	72	MEN	N-CA-CB-CG
2	TA	72	MEN	N-CA-CB-CG
10	HB	72	MEN	N-CA-CB-CG
2	PB	72	MEN	N-CA-CB-CG
2	TB	72	MEN	N-CA-CB-CG
2	XD	72	MEN	N-CA-CB-CG
2	DE	72	MEN	N-CA-CB-CG
2	TE	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	ZE	72	MEN	N-CA-CB-CG
2	nE	72	MEN	N-CA-CB-CG
2	pE	72	MEN	N-CA-CB-CG
2	YF	72	MEN	N-CA-CB-CG
2	kF	72	MEN	N-CA-CB-CG
2	VG	72	MEN	N-CA-CB-CG
2	nG	72	MEN	N-CA-CB-CG
18	SH	71	MEN	N-CA-CB-CG
18	uH	71	MEN	N-CA-CB-CG
10	FI	72	MEN	N-CA-CB-CG
2	TI	72	MEN	N-CA-CB-CG
2	aI	72	MEN	N-CA-CB-CG
2	IJ	72	MEN	N-CA-CB-CG
2	CJ	72	MEN	CA-CB-CG-OD1
2	Y4	72	MEN	CA-CB-CG-OD1
2	d4	72	MEN	CA-CB-CG-OD1
2	R8	72	MEN	CA-CB-CG-OD1
2	JD	72	MEN	CA-CB-CG-OD1
2	nE	72	MEN	CA-CB-CG-OD1
2	eF	72	MEN	CA-CB-CG-OD1
2	nG	72	MEN	CA-CB-CG-OD1
2	Y1	72	MEN	CA-CB-CG-ND2
2	y1	72	MEN	CA-CB-CG-ND2
10	F2	72	MEN	CA-CB-CG-ND2
2	D3	72	MEN	CA-CB-CG-ND2
2	e6	72	MEN	CA-CB-CG-ND2
10	J7	72	MEN	CA-CB-CG-ND2
10	FI	72	MEN	CA-CB-CG-ND2
2	a2	72	MEN	N-CA-CB-CG
2	P6	72	MEN	N-CA-CB-CG
10	FB	72	MEN	N-CA-CB-CG
2	eB	72	MEN	N-CA-CB-CG
2	UJ	72	MEN	N-CA-CB-CG
2	F1	72	MEN	C-CA-CB-CG
2	u1	72	MEN	C-CA-CB-CG
10	N2	72	MEN	C-CA-CB-CG
2	H3	72	MEN	C-CA-CB-CG
2	m6	72	MEN	C-CA-CB-CG
2	T8	72	MEN	C-CA-CB-CG
10	FB	72	MEN	C-CA-CB-CG
10	HB	72	MEN	C-CA-CB-CG
2	BC	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	DE	72	MEN	C-CA-CB-CG
2	mF	72	MEN	C-CA-CB-CG
18	LH	71	MEN	C-CA-CB-CG
18	MH	71	MEN	C-CA-CB-CG
18	UH	71	MEN	C-CA-CB-CG
18	fH	71	MEN	C-CA-CB-CG
10	NI	72	MEN	C-CA-CB-CG
2	F1	72	MEN	CA-CB-CG-OD1
2	Y1	72	MEN	CA-CB-CG-OD1
2	d1	72	MEN	CA-CB-CG-OD1
2	f1	72	MEN	CA-CB-CG-OD1
10	F2	72	MEN	CA-CB-CG-OD1
2	D3	72	MEN	CA-CB-CG-OD1
2	F3	72	MEN	CA-CB-CG-OD1
2	f4	72	MEN	CA-CB-CG-OD1
2	q4	72	MEN	CA-CB-CG-OD1
10	F6	72	MEN	CA-CB-CG-OD1
2	R6	72	MEN	CA-CB-CG-OD1
2	e6	72	MEN	CA-CB-CG-OD1
2	i6	72	MEN	CA-CB-CG-OD1
10	J7	72	MEN	CA-CB-CG-OD1
2	e7	72	MEN	CA-CB-CG-OD1
2	F8	72	MEN	CA-CB-CG-OD1
2	FA	72	MEN	CA-CB-CG-OD1
2	RA	72	MEN	CA-CB-CG-OD1
2	TA	72	MEN	CA-CB-CG-OD1
2	kA	72	MEN	CA-CB-CG-OD1
10	FB	72	MEN	CA-CB-CG-OD1
2	RB	72	MEN	CA-CB-CG-OD1
2	eB	72	MEN	CA-CB-CG-OD1
2	KC	72	MEN	CA-CB-CG-OD1
2	TD	72	MEN	CA-CB-CG-OD1
10	JF	72	MEN	CA-CB-CG-OD1
2	vG	72	MEN	CA-CB-CG-OD1
18	HH	71	MEN	CA-CB-CG-OD1
18	nH	71	MEN	CA-CB-CG-OD1
10	FI	72	MEN	CA-CB-CG-OD1
2	F1	72	MEN	CA-CB-CG-ND2
2	d1	72	MEN	CA-CB-CG-ND2
2	l1	72	MEN	CA-CB-CG-ND2
2	c2	72	MEN	CA-CB-CG-ND2
2	Y4	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	w4	72	MEN	CA-CB-CG-ND2
10	F6	72	MEN	CA-CB-CG-ND2
2	e7	72	MEN	CA-CB-CG-ND2
2	i8	72	MEN	CA-CB-CG-ND2
2	eB	72	MEN	CA-CB-CG-ND2
2	TD	72	MEN	CA-CB-CG-ND2
2	vE	72	MEN	CA-CB-CG-ND2
2	eF	72	MEN	CA-CB-CG-ND2
2	CJ	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1598 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	PEB	V2	203	2	43,46,46	3.42	12 (27%)	45,67,67	2.04	15 (33%)
26	PEB	LJ	202	1	43,46,46	3.34	10 (23%)	45,67,67	2.31	14 (31%)
26	PEB	WB	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.32	17 (37%)
26	PEB	L3	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.81	18 (40%)
26	PEB	K3	201	1	43,46,46	3.29	11 (25%)	45,67,67	2.26	16 (35%)
26	PEB	SE	202	1	43,46,46	2.83	11 (25%)	45,67,67	2.58	18 (40%)
26	PEB	I4	202	1	43,46,46	3.42	11 (25%)	45,67,67	1.96	12 (26%)
26	PEB	W7	201	1	43,46,46	3.37	10 (23%)	45,67,67	2.01	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	VE	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.79	16 (35%)
26	PEB	O3	201	1	43,46,46	3.06	10 (23%)	45,67,67	2.86	21 (46%)
26	PEB	e4	201	1	43,46,46	3.39	8 (18%)	45,67,67	1.90	13 (28%)
28	CYC	N2	1001	10	42,46,46	3.30	15 (35%)	50,67,67	2.78	21 (42%)
26	PEB	KG	203	1	43,46,46	3.33	9 (20%)	45,67,67	2.06	17 (37%)
26	PEB	g2	203	2	43,46,46	3.46	11 (25%)	45,67,67	2.18	15 (33%)
26	PEB	l6	202	1	43,46,46	3.34	11 (25%)	45,67,67	2.01	14 (31%)
26	PEB	NI	1002	10	43,46,46	3.31	10 (23%)	45,67,67	2.14	17 (37%)
26	PEB	d8	203	1	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
26	PEB	24	405	3	43,46,46	3.52	12 (27%)	45,67,67	2.52	15 (33%)
26	PEB	c4	203	2,1	43,46,46	3.35	12 (27%)	45,67,67	2.40	14 (31%)
26	PEB	b2	202	1	43,46,46	3.43	12 (27%)	45,67,67	1.97	13 (28%)
26	PEB	mB	201	2	43,46,46	3.46	12 (27%)	45,67,67	1.94	15 (33%)
26	PEB	OA	201	1	43,46,46	3.37	10 (23%)	45,67,67	1.99	15 (33%)
26	PEB	21	405	3	43,46,46	3.42	13 (30%)	45,67,67	2.61	16 (35%)
28	CYC	YH	1001	22	42,46,46	3.39	15 (35%)	50,67,67	3.17	19 (38%)
26	PEB	e6	201	2	43,46,46	3.39	11 (25%)	45,67,67	1.95	14 (31%)
28	CYC	dH	1001	-	42,46,46	3.39	15 (35%)	50,67,67	5.15	19 (38%)
26	PEB	iG	203	1	43,46,46	3.47	12 (27%)	45,67,67	2.04	14 (31%)
26	PEB	iA	201	2,13	43,46,46	3.46	11 (25%)	45,67,67	2.46	14 (31%)
26	PEB	sG	203	2,1	43,46,46	3.49	13 (30%)	45,67,67	2.76	16 (35%)
26	PEB	EE	201	1	43,46,46	3.10	8 (18%)	45,67,67	2.02	13 (28%)
26	PEB	DG	203	2	43,46,46	3.44	10 (23%)	45,67,67	2.02	14 (31%)
26	PEB	kG	202	1	43,46,46	3.59	11 (25%)	45,67,67	1.91	12 (26%)
26	PEB	WG	203	1	43,46,46	3.41	11 (25%)	45,67,67	2.15	12 (26%)
26	PEB	SB	203	2,1	43,46,46	3.23	10 (23%)	45,67,67	2.47	14 (31%)
26	PEB	w4	204	2,1	43,46,46	3.42	10 (23%)	45,67,67	1.93	11 (24%)
26	PEB	QJ	201	2,7	43,46,46	3.47	10 (23%)	45,67,67	2.33	19 (42%)
26	PEB	D1	202	2	43,46,46	3.34	12 (27%)	45,67,67	2.55	19 (42%)
26	PEB	J4	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.39	15 (33%)
26	PEB	Y4	202	2	43,46,46	3.40	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	Z6	201	2,1	43,46,46	3.14	10 (23%)	45,67,67	2.45	16 (35%)
26	PEB	TJ	203	1	43,46,46	3.35	8 (18%)	45,67,67	2.28	12 (26%)
26	PEB	m6	201	2	43,46,46	3.48	13 (30%)	45,67,67	1.94	13 (28%)
26	PEB	q4	201	2	43,46,46	3.53	12 (27%)	45,67,67	2.11	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	UA	201	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.41	15 (33%)
26	PEB	pG	201	2	43,46,46	3.33	9 (20%)	45,67,67	2.72	17 (37%)
26	PEB	j2	202	1	43,46,46	3.36	10 (23%)	45,67,67	1.93	12 (26%)
26	PEB	f6	202	1	43,46,46	3.43	11 (25%)	45,67,67	1.96	13 (28%)
26	PEB	IA	203	1	43,46,46	3.52	12 (27%)	45,67,67	2.16	15 (33%)
26	PEB	oE	202	1	43,46,46	3.49	11 (25%)	45,67,67	1.96	14 (31%)
26	PEB	II	201	1	43,46,46	3.32	11 (25%)	45,67,67	2.26	17 (37%)
27	PUB	24	402	3	42,46,46	3.54	8 (19%)	37,67,67	3.35	15 (40%)
27	PUB	yG	303	14	42,46,46	3.30	7 (16%)	37,67,67	3.12	13 (35%)
26	PEB	SE	201	2,1	43,46,46	3.25	11 (25%)	45,67,67	2.56	18 (40%)
26	PEB	U4	201	2,4	43,46,46	3.61	12 (27%)	45,67,67	2.17	17 (37%)
26	PEB	S6	203	2,1	43,46,46	3.22	9 (20%)	45,67,67	2.46	14 (31%)
26	PEB	pG	202	2	43,46,46	3.60	11 (25%)	45,67,67	2.73	18 (40%)
26	PEB	E8	203	1	43,46,46	3.45	10 (23%)	45,67,67	1.97	14 (31%)
26	PEB	OF	202	1	43,46,46	3.30	10 (23%)	45,67,67	2.47	15 (33%)
26	PEB	R6	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.18	17 (37%)
26	PEB	RI	201	2,6	43,46,46	3.32	10 (23%)	45,67,67	2.38	14 (31%)
26	PEB	Z7	202	1	43,46,46	3.20	9 (20%)	45,67,67	2.09	17 (37%)
26	PEB	SA	203	2,1	43,46,46	3.31	12 (27%)	45,67,67	2.41	14 (31%)
26	PEB	CE	203	1	43,46,46	3.39	11 (25%)	45,67,67	2.06	16 (35%)
26	PEB	g2	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.33	15 (33%)
26	PEB	RD	202	2	43,46,46	3.09	10 (23%)	45,67,67	2.93	15 (33%)
26	PEB	jE	202	2	43,46,46	3.49	10 (23%)	45,67,67	2.14	13 (28%)
26	PEB	U6	201	2,1	43,46,46	3.28	10 (23%)	45,67,67	2.38	16 (35%)
26	PEB	pE	201	2	43,46,46	3.43	9 (20%)	45,67,67	2.70	16 (35%)
26	PEB	U3	201	1	43,46,46	3.14	10 (23%)	45,67,67	2.69	15 (33%)
26	PEB	N1	202	1	43,46,46	3.31	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	D8	202	2	43,46,46	3.27	12 (27%)	45,67,67	2.67	17 (37%)
26	PEB	IG	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.57	15 (33%)
27	PUB	A7	304	7	42,46,46	3.53	8 (19%)	37,67,67	3.70	18 (48%)
26	PEB	u4	201	3,2	43,46,46	3.53	14 (32%)	45,67,67	2.26	18 (40%)
28	CYC	JH	1001	18,17	42,46,46	3.51	14 (33%)	50,67,67	2.91	22 (44%)
26	PEB	f8	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.03	14 (31%)
26	PEB	FC	201	2	43,46,46	3.35	10 (23%)	45,67,67	1.95	14 (31%)
26	PEB	CG	203	1	43,46,46	3.44	12 (27%)	45,67,67	1.99	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	NG	201	2	43,46,46	3.34	10 (23%)	45,67,67	3.07	17 (37%)
26	PEB	T3	202	2	43,46,46	2.67	9 (20%)	45,67,67	3.13	20 (44%)
26	PEB	hG	202	2	43,46,46	3.44	9 (20%)	45,67,67	1.99	15 (33%)
26	PEB	hB	202	1	43,46,46	3.44	11 (25%)	45,67,67	2.05	16 (35%)
26	PEB	M9	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	IE	203	2,1	43,46,46	3.01	10 (23%)	45,67,67	2.66	17 (37%)
26	PEB	M4	402	3,26	43,46,46	3.43	10 (23%)	45,67,67	2.18	14 (31%)
26	PEB	i6	201	2	43,46,46	3.45	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	JI	1002	10	43,46,46	3.31	11 (25%)	45,67,67	2.11	14 (31%)
26	PEB	L9	201	2,1	43,46,46	3.34	11 (25%)	45,67,67	2.42	16 (35%)
26	PEB	KB	201	9,10	43,46,46	3.32	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	P2	202	2	43,46,46	3.26	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	W8	202	1	43,46,46	3.30	10 (23%)	45,67,67	2.20	15 (33%)
26	PEB	LB	1002	9,10	43,46,46	3.32	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	JE	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.19	18 (40%)
26	PEB	c2	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.40	16 (35%)
26	PEB	aG	201	2,1	43,46,46	3.44	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	VF	201	2	43,46,46	3.40	12 (27%)	45,67,67	2.41	18 (40%)
26	PEB	EJ	201	2,15	43,46,46	3.27	11 (25%)	45,67,67	2.20	17 (37%)
26	PEB	tE	202	2	43,46,46	3.65	11 (25%)	45,67,67	2.46	15 (33%)
26	PEB	m4	201	2,1	43,46,46	3.22	12 (27%)	45,67,67	2.62	16 (35%)
26	PEB	d6	204	1	43,46,46	3.42	13 (30%)	45,67,67	2.12	13 (28%)
26	PEB	S4	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.14	15 (33%)
26	PEB	I5	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.29	16 (35%)
26	PEB	fG	201	2,13	43,46,46	3.41	10 (23%)	45,67,67	3.07	16 (35%)
28	CYC	qH	1002	-	42,46,46	3.48	14 (33%)	50,67,67	3.10	24 (48%)
26	PEB	A8	302	13	43,46,46	3.32	10 (23%)	45,67,67	2.77	18 (40%)
26	PEB	x4	202	1	43,46,46	3.41	10 (23%)	45,67,67	2.61	19 (42%)
28	CYC	D7	1001	10	42,46,46	3.34	13 (30%)	50,67,67	2.82	18 (36%)
26	PEB	IC	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.18	15 (33%)
26	PEB	c1	203	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.57	15 (33%)
28	CYC	J7	1003	9,10	42,46,46	3.24	12 (28%)	50,67,67	2.70	18 (36%)
26	PEB	BC	202	2	43,46,46	3.47	11 (25%)	45,67,67	1.93	13 (28%)
26	PEB	ZE	201	2	43,46,46	3.44	10 (23%)	45,67,67	3.41	16 (35%)
28	CYC	FH	1001	18	42,46,46	1.10	1 (2%)	50,67,67	0.95	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	X9	202	1	43,46,46	3.55	11 (25%)	45,67,67	1.92	14 (31%)
26	PEB	H9	202	1	43,46,46	3.40	12 (27%)	45,67,67	2.44	16 (35%)
26	PEB	Z4	201	2	43,46,46	3.47	11 (25%)	45,67,67	2.36	14 (31%)
26	PEB	KC	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.01	14 (31%)
26	PEB	VD	203	2	43,46,46	3.55	12 (27%)	45,67,67	1.97	16 (35%)
26	PEB	S6	202	1	43,46,46	1.08	2 (4%)	45,67,67	1.00	2 (4%)
26	PEB	y1	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.43	14 (31%)
26	PEB	ZG	202	2	43,46,46	3.58	12 (27%)	45,67,67	2.05	15 (33%)
27	PUB	xG	305	13	42,46,46	3.39	7 (16%)	37,67,67	3.26	15 (40%)
26	PEB	SA	202	1	43,46,46	3.28	11 (25%)	45,67,67	2.00	14 (31%)
26	PEB	S7	202	1	43,46,46	3.36	10 (23%)	45,67,67	2.62	13 (28%)
26	PEB	fA	203	2,1	43,46,46	3.36	12 (27%)	45,67,67	2.29	15 (33%)
26	PEB	Y7	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.14	15 (33%)
26	PEB	CG	202	1	43,46,46	3.08	9 (20%)	45,67,67	2.08	15 (33%)
26	PEB	N4	201	1	43,46,46	3.18	10 (23%)	45,67,67	2.74	21 (46%)
26	PEB	HC	201	2	43,46,46	3.47	11 (25%)	45,67,67	2.14	14 (31%)
26	PEB	n4	201	2,4	43,46,46	3.31	10 (23%)	45,67,67	2.35	19 (42%)
26	PEB	Y6	201	2	43,46,46	3.10	10 (23%)	45,67,67	2.60	19 (42%)
26	PEB	c8	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.59	16 (35%)
26	PEB	N9	203	1	43,46,46	3.36	8 (18%)	45,67,67	2.03	13 (28%)
26	PEB	X4	201	2,1	43,46,46	3.35	10 (23%)	45,67,67	2.00	13 (28%)
26	PEB	oG	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.26	15 (33%)
26	PEB	L1	201	3,2	43,46,46	3.51	12 (27%)	45,67,67	2.10	17 (37%)
26	PEB	C8	201	1	43,46,46	3.39	11 (25%)	45,67,67	2.24	19 (42%)
26	PEB	a2	203	2	43,46,46	3.43	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	PJ	203	1	43,46,46	3.38	10 (23%)	45,67,67	2.12	12 (26%)
26	PEB	v1	202	1	43,46,46	3.58	12 (27%)	45,67,67	2.87	20 (44%)
26	PEB	f2	201	1	43,46,46	3.30	11 (25%)	45,67,67	2.41	16 (35%)
26	PEB	kG	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.05	12 (26%)
26	PEB	aI	202	2	43,46,46	3.32	12 (27%)	45,67,67	2.57	15 (33%)
26	PEB	I8	201	2,1	43,46,46	3.33	11 (25%)	45,67,67	2.36	15 (33%)
26	PEB	l4	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	i4	201	1	43,46,46	3.52	12 (27%)	45,67,67	2.07	16 (35%)
26	PEB	YJ	201	2,26	43,46,46	3.48	10 (23%)	45,67,67	2.04	18 (40%)
26	PEB	TI	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.16	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	gG	201	1	43,46,46	3.11	11 (25%)	45,67,67	2.38	15 (33%)
26	PEB	k2	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.30	14 (31%)
28	CYC	J2	1001	10	42,46,46	3.03	16 (38%)	50,67,67	3.13	24 (48%)
26	PEB	Z2	201	1	43,46,46	3.33	12 (27%)	45,67,67	2.76	18 (40%)
26	PEB	vG	201	2	43,46,46	3.50	10 (23%)	45,67,67	2.87	18 (40%)
26	PEB	J1	203	2	43,46,46	3.53	10 (23%)	45,67,67	2.04	14 (31%)
26	PEB	OB	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	JD	201	2,7	43,46,46	3.30	9 (20%)	45,67,67	2.44	13 (28%)
26	PEB	K5	203	2	43,46,46	3.38	10 (23%)	45,67,67	1.96	14 (31%)
26	PEB	NJ	203	1	43,46,46	3.36	8 (18%)	45,67,67	2.12	13 (28%)
26	PEB	OI	202	1	43,46,46	3.37	11 (25%)	45,67,67	1.85	11 (24%)
26	PEB	LI	1002	10	43,46,46	3.35	10 (23%)	45,67,67	2.67	18 (40%)
26	PEB	M3	202	1	43,46,46	3.33	10 (23%)	45,67,67	1.96	14 (31%)
27	PUB	B8	302	14	42,46,46	3.25	8 (19%)	37,67,67	3.22	16 (43%)
26	PEB	V7	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.08	15 (33%)
28	CYC	NI	1001	10	42,46,46	3.36	15 (35%)	50,67,67	2.83	21 (42%)
26	PEB	gE	203	2,1	43,46,46	3.31	11 (25%)	45,67,67	2.61	16 (35%)
26	PEB	S8	201	1	43,46,46	3.26	10 (23%)	45,67,67	2.34	17 (37%)
26	PEB	rG	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	g4	201	1	43,46,46	3.37	9 (20%)	45,67,67	2.21	16 (35%)
26	PEB	UJ	202	2	43,46,46	3.53	10 (23%)	45,67,67	1.91	13 (28%)
26	PEB	HB	1002	9,10	43,46,46	3.29	12 (27%)	45,67,67	2.13	13 (28%)
26	PEB	TG	201	2	43,46,46	3.28	9 (20%)	45,67,67	2.94	15 (33%)
26	PEB	WI	201	1	43,46,46	3.29	11 (25%)	45,67,67	2.59	16 (35%)
26	PEB	FF	1002	10	43,46,46	3.32	10 (23%)	45,67,67	2.15	12 (26%)
26	PEB	mG	201	1	43,46,46	3.41	14 (32%)	45,67,67	2.54	16 (35%)
26	PEB	mB	202	2	43,46,46	3.41	11 (25%)	45,67,67	2.41	14 (31%)
26	PEB	a8	204	2,1	43,46,46	3.08	10 (23%)	45,67,67	2.35	17 (37%)
26	PEB	aA	204	2,1	43,46,46	3.07	11 (25%)	45,67,67	2.80	15 (33%)
28	CYC	CH	1001	18,17	42,46,46	3.49	15 (35%)	50,67,67	2.88	21 (42%)
26	PEB	WJ	201	2,7	43,46,46	3.62	9 (20%)	45,67,67	2.09	15 (33%)
26	PEB	UI	201	1	43,46,46	3.20	10 (23%)	45,67,67	2.80	19 (42%)
26	PEB	L5	202	2	43,46,46	3.20	10 (23%)	45,67,67	2.19	15 (33%)
26	PEB	eI	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.24	16 (35%)
26	PEB	mE	202	1	43,46,46	3.41	11 (25%)	45,67,67	2.01	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	J3	202	2	43,46,46	3.16	9 (20%)	45,67,67	3.13	18 (40%)
26	PEB	A2	305	7	43,46,46	3.35	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	FD	203	2	43,46,46	3.58	12 (27%)	45,67,67	1.98	17 (37%)
27	PUB	A2	302	7	42,46,46	3.48	8 (19%)	37,67,67	3.19	16 (43%)
26	PEB	CJ	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.01	15 (33%)
28	CYC	wH	1001	-	42,46,46	3.38	13 (30%)	50,67,67	2.90	22 (44%)
26	PEB	DJ	201	2,1	43,46,46	3.11	11 (25%)	45,67,67	2.83	14 (31%)
26	PEB	dF	202	1	43,46,46	3.41	12 (27%)	45,67,67	2.12	15 (33%)
26	PEB	mI	202	2	43,46,46	3.31	12 (27%)	45,67,67	2.38	15 (33%)
26	PEB	zG	501	2,16	43,46,46	3.39	10 (23%)	45,67,67	3.33	17 (37%)
26	PEB	MG	201	1	43,46,46	3.28	10 (23%)	45,67,67	1.88	13 (28%)
26	PEB	B5	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.02	13 (28%)
26	PEB	I1	201	1	43,46,46	3.43	9 (20%)	45,67,67	2.13	16 (35%)
28	CYC	I2	1001	9	42,46,46	3.18	13 (30%)	50,67,67	2.82	20 (40%)
26	PEB	aI	201	2	43,46,46	3.33	11 (25%)	45,67,67	2.30	17 (37%)
26	PEB	D1	201	3,2	43,46,46	3.37	10 (23%)	45,67,67	2.05	14 (31%)
28	CYC	kH	1001	-	42,46,46	3.41	13 (30%)	50,67,67	2.88	18 (36%)
26	PEB	lB	202	1	43,46,46	3.34	11 (25%)	45,67,67	2.02	13 (28%)
26	PEB	J7	1002	10	43,46,46	3.25	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	Z4	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.28	14 (31%)
26	PEB	C1	202	1	43,46,46	3.43	9 (20%)	45,67,67	1.86	12 (26%)
28	CYC	J7	1001	10	42,46,46	3.24	15 (35%)	50,67,67	2.89	23 (46%)
26	PEB	p1	202	1	43,46,46	3.75	11 (25%)	45,67,67	2.73	18 (40%)
26	PEB	U8	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.47	19 (42%)
26	PEB	VF	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	H6	1002	9,10	43,46,46	3.30	12 (27%)	45,67,67	2.12	12 (26%)
26	PEB	nG	202	2	43,46,46	3.60	13 (30%)	45,67,67	1.93	13 (28%)
26	PEB	N8	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.52	18 (40%)
26	PEB	aF	201	2	43,46,46	3.40	9 (20%)	45,67,67	2.13	13 (28%)
26	PEB	j2	201	1	43,46,46	3.36	11 (25%)	45,67,67	2.28	19 (42%)
26	PEB	VI	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.00	15 (33%)
26	PEB	K5	202	2	43,46,46	3.22	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	FJ	202	1	43,46,46	3.38	10 (23%)	45,67,67	2.01	14 (31%)
26	PEB	NJ	202	1	43,46,46	3.47	11 (25%)	45,67,67	1.94	14 (31%)
26	PEB	PG	202	2	43,46,46	3.58	11 (25%)	45,67,67	2.07	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	mF	201	2	43,46,46	3.48	11 (25%)	45,67,67	1.90	15 (33%)
28	CYC	hH	1001	22,18	42,46,46	3.47	14 (33%)	50,67,67	3.04	21 (42%)
26	PEB	C3	201	1	43,46,46	3.25	12 (27%)	45,67,67	2.58	17 (37%)
26	PEB	jB	201	1	43,46,46	3.43	13 (30%)	45,67,67	2.00	15 (33%)
26	PEB	P8	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.41	17 (37%)
26	PEB	Q8	203	1	43,46,46	3.26	10 (23%)	45,67,67	2.39	15 (33%)
26	PEB	J2	1002	10	43,46,46	3.35	11 (25%)	45,67,67	2.06	14 (31%)
27	PUB	yG	302	14	42,46,46	3.36	7 (16%)	37,67,67	3.16	19 (51%)
26	PEB	EG	201	1	43,46,46	3.08	9 (20%)	45,67,67	2.32	14 (31%)
26	PEB	JA	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.32	17 (37%)
28	CYC	JI	1001	10	42,46,46	3.13	16 (38%)	50,67,67	2.96	21 (42%)
26	PEB	c4	202	1	43,46,46	3.58	11 (25%)	45,67,67	2.26	16 (35%)
28	CYC	E7	1001	9,10	42,46,46	3.07	15 (35%)	50,67,67	3.04	18 (36%)
26	PEB	Y9	202	2	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
26	PEB	VE	202	2	43,46,46	3.43	11 (25%)	45,67,67	2.71	18 (40%)
26	PEB	S8	203	2,1	43,46,46	3.28	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	24	401	3	43,46,46	3.43	9 (20%)	45,67,67	2.19	14 (31%)
26	PEB	P8	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.53	18 (40%)
26	PEB	Y1	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.02	15 (33%)
26	PEB	Z1	202	2	43,46,46	3.24	10 (23%)	45,67,67	2.25	13 (28%)
26	PEB	rE	202	2	43,46,46	3.47	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	HA	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.25	17 (37%)
26	PEB	J5	202	1	43,46,46	3.16	10 (23%)	45,67,67	2.38	16 (35%)
26	PEB	K4	202	1	43,46,46	3.35	10 (23%)	45,67,67	1.93	13 (28%)
26	PEB	V4	202	1	43,46,46	3.30	12 (27%)	45,67,67	2.03	13 (28%)
26	PEB	OA	203	2,1	43,46,46	3.20	10 (23%)	45,67,67	2.68	17 (37%)
28	CYC	FI	1001	10	42,46,46	3.26	14 (33%)	50,67,67	2.99	20 (40%)
26	PEB	SB	201	1	43,46,46	3.29	10 (23%)	45,67,67	2.10	16 (35%)
26	PEB	A9	304	7,26	43,46,46	3.48	10 (23%)	45,67,67	2.65	15 (33%)
26	PEB	nE	201	2	43,46,46	3.47	9 (20%)	45,67,67	2.99	18 (40%)
26	PEB	H4	201	3,2	43,46,46	3.49	11 (25%)	45,67,67	2.02	15 (33%)
26	PEB	d2	201	1	43,46,46	3.26	10 (23%)	45,67,67	2.28	16 (35%)
26	PEB	gA	202	2	43,46,46	3.40	11 (25%)	45,67,67	2.39	16 (35%)
26	PEB	RG	202	2	43,46,46	3.38	11 (25%)	45,67,67	2.31	15 (33%)
27	PUB	24	403	3,1	42,46,46	3.37	8 (19%)	37,67,67	3.47	13 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	RJ	203	2,1	43,46,46	3.40	12 (27%)	45,67,67	2.35	15 (33%)
26	PEB	ME	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	A6	304	7	43,46,46	3.30	10 (23%)	45,67,67	2.15	16 (35%)
28	CYC	F2	1001	10	42,46,46	3.37	15 (35%)	50,67,67	3.37	23 (46%)
26	PEB	L1	203	2	43,46,46	3.41	10 (23%)	45,67,67	1.97	15 (33%)
26	PEB	CA	203	2,1	43,46,46	3.24	10 (23%)	45,67,67	2.48	16 (35%)
26	PEB	S9	202	2	43,46,46	3.36	9 (20%)	45,67,67	1.98	16 (35%)
26	PEB	ME	202	1	43,46,46	3.47	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	X9	201	2,1	43,46,46	3.34	11 (25%)	45,67,67	2.46	15 (33%)
26	PEB	i2	203	2	43,46,46	3.50	12 (27%)	45,67,67	1.89	12 (26%)
26	PEB	CC	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.12	16 (35%)
26	PEB	DD	201	2,7	43,46,46	3.40	13 (30%)	45,67,67	2.41	14 (31%)
26	PEB	eF	202	2	43,46,46	3.44	12 (27%)	45,67,67	1.96	14 (31%)
26	PEB	mG	202	1	43,46,46	3.38	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	OG	202	1	43,46,46	3.10	9 (20%)	45,67,67	2.20	15 (33%)
26	PEB	E8	201	2,1	43,46,46	3.28	11 (25%)	45,67,67	2.28	14 (31%)
26	PEB	u1	203	2	43,46,46	3.43	10 (23%)	45,67,67	2.07	14 (31%)
26	PEB	bE	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.88	16 (35%)
26	PEB	cG	202	1	43,46,46	3.36	10 (23%)	45,67,67	2.00	14 (31%)
26	PEB	B4	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.38	14 (31%)
26	PEB	NJ	204	2,1	43,46,46	3.47	10 (23%)	45,67,67	2.29	18 (40%)
26	PEB	uG	202	1	43,46,46	3.52	11 (25%)	45,67,67	2.03	14 (31%)
26	PEB	e1	201	1	43,46,46	3.50	12 (27%)	45,67,67	1.89	13 (28%)
26	PEB	SI	202	1	43,46,46	3.33	11 (25%)	45,67,67	1.96	13 (28%)
26	PEB	gB	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.99	16 (35%)
26	PEB	VJ	203	2,1	43,46,46	3.22	12 (27%)	45,67,67	2.28	14 (31%)
28	CYC	fH	1001	18	42,46,46	3.44	15 (35%)	50,67,67	2.94	21 (42%)
26	PEB	RD	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
26	PEB	M1	403	3	43,46,46	3.34	10 (23%)	45,67,67	2.29	17 (37%)
28	CYC	M2	1001	9	42,46,46	3.23	14 (33%)	50,67,67	2.89	20 (40%)
26	PEB	X8	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.66	19 (42%)
26	PEB	S3	202	1	43,46,46	3.23	10 (23%)	45,67,67	2.02	12 (26%)
26	PEB	K9	202	2	43,46,46	3.35	9 (20%)	45,67,67	2.15	15 (33%)
26	PEB	c8	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.34	16 (35%)
26	PEB	IG	202	1	43,46,46	3.19	10 (23%)	45,67,67	2.11	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	oG	202	1	43,46,46	3.51	9 (20%)	45,67,67	1.95	12 (26%)
26	PEB	CG	201	1	43,46,46	3.39	9 (20%)	45,67,67	2.28	14 (31%)
26	PEB	YF	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.03	12 (26%)
26	PEB	TF	201	2,6	43,46,46	3.35	12 (27%)	45,67,67	2.21	19 (42%)
26	PEB	BJ	203	2,1	43,46,46	2.91	9 (20%)	45,67,67	2.47	16 (35%)
26	PEB	sG	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.06	13 (28%)
26	PEB	OA	202	1	43,46,46	3.40	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	YG	203	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.69	17 (37%)
26	PEB	i4	202	1	43,46,46	3.38	9 (20%)	45,67,67	2.09	13 (28%)
26	PEB	e4	202	1	43,46,46	3.60	11 (25%)	45,67,67	2.17	15 (33%)
26	PEB	c2	201	2	43,46,46	3.36	11 (25%)	45,67,67	1.94	12 (26%)
26	PEB	VF	202	2,1	43,46,46	3.39	11 (25%)	45,67,67	2.53	16 (35%)
26	PEB	v4	202	1	43,46,46	3.53	11 (25%)	45,67,67	2.54	17 (37%)
26	PEB	qG	203	1	43,46,46	3.50	12 (27%)	45,67,67	2.31	16 (35%)
26	PEB	hI	202	1	43,46,46	3.41	10 (23%)	45,67,67	1.99	13 (28%)
26	PEB	lF	202	1	43,46,46	3.45	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	Q6	201	2,1	43,46,46	3.16	11 (25%)	45,67,67	2.64	17 (37%)
26	PEB	WG	201	2,1	43,46,46	3.23	11 (25%)	45,67,67	2.63	21 (46%)
26	PEB	e7	202	2	43,46,46	3.55	12 (27%)	45,67,67	1.96	14 (31%)
26	PEB	s1	202	2	43,46,46	3.43	11 (25%)	45,67,67	2.22	17 (37%)
26	PEB	T2	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.16	17 (37%)
26	PEB	XA	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.98	20 (44%)
26	PEB	aI	203	2	43,46,46	3.46	13 (30%)	45,67,67	2.00	14 (31%)
26	PEB	hF	201	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.45	16 (35%)
26	PEB	W2	201	1	43,46,46	3.33	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	R4	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.07	15 (33%)
26	PEB	GC	201	2	43,46,46	3.47	11 (25%)	45,67,67	2.04	16 (35%)
26	PEB	w1	202	2	43,46,46	3.55	12 (27%)	45,67,67	2.53	16 (35%)
26	PEB	u1	202	2	43,46,46	3.51	12 (27%)	45,67,67	2.42	14 (31%)
26	PEB	uG	201	2,1	43,46,46	3.49	12 (27%)	45,67,67	2.19	12 (26%)
26	PEB	P9	203	1	43,46,46	3.39	9 (20%)	45,67,67	2.11	12 (26%)
26	PEB	c1	202	1	43,46,46	3.57	10 (23%)	45,67,67	2.37	17 (37%)
26	PEB	k1	202	1	43,46,46	3.28	9 (20%)	45,67,67	2.07	15 (33%)
26	PEB	hA	202	1	43,46,46	3.30	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	q4	203	2	43,46,46	3.46	10 (23%)	45,67,67	2.09	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	O9	201	2,7,26	43,46,46	3.39	9 (20%)	45,67,67	1.99	15 (33%)
26	PEB	fI	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.23	16 (35%)
28	CYC	HF	1001	10	42,46,46	3.31	13 (30%)	50,67,67	2.89	22 (44%)
26	PEB	IE	202	2	43,46,46	3.53	11 (25%)	45,67,67	2.18	14 (31%)
26	PEB	AB	301	7	43,46,46	3.32	10 (23%)	45,67,67	2.45	17 (37%)
26	PEB	fE	202	2	43,46,46	3.58	13 (30%)	45,67,67	1.98	17 (37%)
27	PUB	A8	304	13	42,46,46	3.45	8 (19%)	37,67,67	3.08	13 (35%)
26	PEB	R9	202	1	43,46,46	3.37	12 (27%)	45,67,67	1.98	13 (28%)
26	PEB	VB	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.11	16 (35%)
26	PEB	C5	202	2	43,46,46	3.48	12 (27%)	45,67,67	2.07	13 (28%)
28	CYC	N7	1001	8,10	42,46,46	3.35	15 (35%)	50,67,67	2.77	19 (38%)
26	PEB	j6	201	1	43,46,46	3.43	12 (27%)	45,67,67	2.09	15 (33%)
26	PEB	TE	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.19	16 (35%)
26	PEB	DJ	202	1	43,46,46	3.13	11 (25%)	45,67,67	2.83	19 (42%)
26	PEB	z4	201	1	43,46,46	3.62	10 (23%)	45,67,67	2.30	19 (42%)
26	PEB	GA	202	1	43,46,46	3.39	11 (25%)	45,67,67	2.14	13 (28%)
26	PEB	II	202	1	43,46,46	3.47	12 (27%)	45,67,67	1.91	15 (33%)
28	CYC	EF	1001	9,10	42,46,46	3.04	14 (33%)	50,67,67	3.19	20 (40%)
26	PEB	U9	202	2	43,46,46	3.51	9 (20%)	45,67,67	1.89	15 (33%)
26	PEB	XE	202	2	43,46,46	3.48	11 (25%)	45,67,67	2.27	18 (40%)
26	PEB	fI	202	2	43,46,46	3.56	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	PJ	201	2,1	43,46,46	3.38	13 (30%)	45,67,67	2.44	13 (28%)
26	PEB	IF	201	2,1	43,46,46	3.36	10 (23%)	45,67,67	2.26	15 (33%)
26	PEB	KE	201	2,1	43,46,46	3.08	11 (25%)	45,67,67	2.82	20 (44%)
27	PUB	AB	302	7	42,46,46	3.50	8 (19%)	37,67,67	3.24	14 (37%)
28	CYC	SH	1001	18	42,46,46	3.33	13 (30%)	50,67,67	2.95	22 (44%)
26	PEB	II	202	2	43,46,46	3.71	12 (27%)	45,67,67	1.80	12 (26%)
26	PEB	g7	201	2	43,46,46	3.52	10 (23%)	45,67,67	1.88	15 (33%)
26	PEB	H3	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.55	17 (37%)
26	PEB	XA	201	2	43,46,46	3.29	11 (25%)	45,67,67	2.33	14 (31%)
26	PEB	XD	202	2	43,46,46	3.02	9 (20%)	45,67,67	2.62	19 (42%)
26	PEB	I5	201	2	43,46,46	3.23	10 (23%)	45,67,67	2.07	16 (35%)
26	PEB	F3	203	2	43,46,46	3.69	13 (30%)	45,67,67	2.12	15 (33%)
26	PEB	j8	203	2,1	43,46,46	3.22	11 (25%)	45,67,67	2.27	17 (37%)
26	PEB	P7	201	2,6	43,46,46	3.37	10 (23%)	45,67,67	2.11	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	D3	203	2	43,46,46	3.39	11 (25%)	45,67,67	1.88	16 (35%)
26	PEB	d6	203	1	43,46,46	3.49	12 (27%)	45,67,67	2.07	15 (33%)
26	PEB	J1	201	2	43,46,46	3.25	10 (23%)	45,67,67	1.97	15 (33%)
26	PEB	m1	203	1	43,46,46	3.50	12 (27%)	45,67,67	2.07	16 (35%)
26	PEB	I4	201	1	43,46,46	3.43	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	O7	202	1	43,46,46	3.42	12 (27%)	45,67,67	2.45	15 (33%)
26	PEB	gF	202	2	43,46,46	3.52	11 (25%)	45,67,67	2.21	14 (31%)
26	PEB	R9	201	1	43,46,46	3.51	12 (27%)	45,67,67	2.09	13 (28%)
26	PEB	eF	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.08	16 (35%)
26	PEB	YD	301	7	43,46,46	3.41	10 (23%)	45,67,67	2.73	18 (40%)
26	PEB	OG	201	2,1	43,46,46	3.30	12 (27%)	45,67,67	2.57	18 (40%)
26	PEB	X9	203	1	43,46,46	3.41	10 (23%)	45,67,67	1.97	13 (28%)
26	PEB	J1	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.51	15 (33%)
26	PEB	rG	201	2,13	43,46,46	3.46	11 (25%)	45,67,67	2.23	13 (28%)
26	PEB	B4	201	3,2,26	43,46,46	3.36	8 (18%)	45,67,67	1.94	12 (26%)
26	PEB	F5	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.00	16 (35%)
28	CYC	BB	1001	8,10	42,46,46	3.34	14 (33%)	50,67,67	2.82	22 (44%)
26	PEB	WB	203	2,1	43,46,46	3.11	10 (23%)	45,67,67	2.31	17 (37%)
28	CYC	MH	1001	18	42,46,46	3.42	15 (35%)	50,67,67	2.86	19 (38%)
27	PUB	A7	303	7	42,46,46	3.52	8 (19%)	37,67,67	3.12	15 (40%)
26	PEB	GA	201	1	43,46,46	3.27	11 (25%)	45,67,67	2.40	17 (37%)
26	PEB	iG	202	1	43,46,46	3.26	10 (23%)	45,67,67	2.31	18 (40%)
28	CYC	EI	1001	9	42,46,46	3.19	15 (35%)	50,67,67	2.95	19 (38%)
26	PEB	qE	203	1	43,46,46	3.46	12 (27%)	45,67,67	2.05	14 (31%)
26	PEB	XE	201	2	43,46,46	3.38	10 (23%)	45,67,67	3.69	17 (37%)
26	PEB	GJ	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.38	15 (33%)
26	PEB	K8	203	2,1	43,46,46	2.98	10 (23%)	45,67,67	2.46	16 (35%)
26	PEB	B3	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.99	18 (40%)
26	PEB	N7	1002	10	43,46,46	3.40	11 (25%)	45,67,67	2.20	14 (31%)
26	PEB	PB	201	2,6	43,46,46	3.34	10 (23%)	45,67,67	2.22	18 (40%)
28	CYC	eH	1001	18,17	42,46,46	3.45	15 (35%)	50,67,67	2.93	23 (46%)
26	PEB	ZI	201	1	43,46,46	3.33	12 (27%)	45,67,67	2.77	18 (40%)
26	PEB	D9	201	2,1	43,46,46	3.17	11 (25%)	45,67,67	2.39	14 (31%)
26	PEB	S2	202	1	43,46,46	3.37	11 (25%)	45,67,67	1.95	13 (28%)
27	PUB	A4	203	3,1	42,46,46	3.48	7 (16%)	37,67,67	3.21	16 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	YD	303	7,26	43,46,46	3.33	11 (25%)	45,67,67	3.20	18 (40%)
26	PEB	YE	202	1	43,46,46	3.43	12 (27%)	45,67,67	1.85	13 (28%)
26	PEB	UE	203	2,1	43,46,46	3.06	13 (30%)	45,67,67	3.16	17 (37%)
26	PEB	GD	201	1	43,46,46	3.11	10 (23%)	45,67,67	2.23	13 (28%)
26	PEB	RA	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.39	15 (33%)
26	PEB	Y6	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.28	17 (37%)
27	PUB	wG	304	13	42,46,46	3.41	8 (19%)	37,67,67	3.12	17 (45%)
26	PEB	V2	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.22	16 (35%)
26	PEB	J9	201	1	43,46,46	3.41	12 (27%)	45,67,67	2.19	15 (33%)
26	PEB	YD	304	7,26	43,46,46	3.30	11 (25%)	45,67,67	2.58	13 (28%)
26	PEB	iF	202	2	43,46,46	3.53	10 (23%)	45,67,67	1.85	12 (26%)
26	PEB	G3	202	1	43,46,46	3.33	11 (25%)	45,67,67	2.00	14 (31%)
26	PEB	S9	201	2,7	43,46,46	3.39	10 (23%)	45,67,67	2.09	13 (28%)
26	PEB	QE	202	1	43,46,46	3.52	11 (25%)	45,67,67	2.02	15 (33%)
26	PEB	P2	203	2	43,46,46	3.32	9 (20%)	45,67,67	1.90	12 (26%)
26	PEB	d4	203	2	43,46,46	3.49	10 (23%)	45,67,67	1.95	15 (33%)
28	CYC	YH	1004	22	42,46,46	3.44	13 (30%)	50,67,67	2.92	18 (36%)
26	PEB	F2	1002	10	43,46,46	3.27	10 (23%)	45,67,67	2.26	17 (37%)
26	PEB	k8	202	2	43,46,46	3.38	12 (27%)	45,67,67	2.54	17 (37%)
26	PEB	XJ	203	1	43,46,46	3.45	10 (23%)	45,67,67	2.04	13 (28%)
26	PEB	eB	203	2	43,46,46	3.56	11 (25%)	45,67,67	2.01	16 (35%)
26	PEB	VI	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.21	16 (35%)
26	PEB	GE	202	1	43,46,46	2.78	9 (20%)	45,67,67	2.92	21 (46%)
26	PEB	m1	202	1	43,46,46	3.53	12 (27%)	45,67,67	2.11	15 (33%)
26	PEB	UA	202	1	43,46,46	3.26	10 (23%)	45,67,67	2.46	18 (40%)
28	CYC	H2	1001	10	42,46,46	3.27	15 (35%)	50,67,67	3.07	23 (46%)
26	PEB	NA	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.50	18 (40%)
26	PEB	V3	201	2,11	43,46,46	3.31	10 (23%)	45,67,67	2.22	16 (35%)
26	PEB	DA	201	14,2	43,46,46	3.41	11 (25%)	45,67,67	2.45	13 (28%)
26	PEB	b7	201	1	43,46,46	3.37	11 (25%)	45,67,67	1.99	16 (35%)
26	PEB	Q1	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	T9	201	2,1	43,46,46	3.35	13 (30%)	45,67,67	2.30	13 (28%)
26	PEB	O8	203	2,1	43,46,46	3.23	10 (23%)	45,67,67	2.66	17 (37%)
26	PEB	n1	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.04	13 (28%)
26	PEB	U7	202	1	43,46,46	3.33	12 (27%)	45,67,67	2.07	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PUB	A8	303	13	42,46,46	3.41	9 (21%)	37,67,67	3.36	18 (48%)
26	PEB	cG	203	2,1	43,46,46	3.30	13 (30%)	45,67,67	2.77	17 (37%)
26	PEB	h4	203	2	43,46,46	3.44	9 (20%)	45,67,67	1.88	15 (33%)
26	PEB	Z8	202	2	43,46,46	3.07	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	O3	202	1	43,46,46	3.23	10 (23%)	45,67,67	2.05	16 (35%)
26	PEB	TI	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.24	14 (31%)
28	CYC	PH	1001	17	42,46,46	3.35	15 (35%)	50,67,67	3.00	22 (44%)
26	PEB	B9	203	2,1	43,46,46	2.94	9 (20%)	45,67,67	2.38	14 (31%)
26	PEB	ED	201	1	43,46,46	3.57	12 (27%)	45,67,67	2.31	14 (31%)
26	PEB	fB	203	2,1	43,46,46	3.48	10 (23%)	45,67,67	2.29	12 (26%)
26	PEB	mI	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	T3	201	2	43,46,46	3.58	11 (25%)	45,67,67	2.40	17 (37%)
26	PEB	AI	305	7	43,46,46	3.38	10 (23%)	45,67,67	2.00	13 (28%)
28	CYC	JF	1001	10	42,46,46	3.22	15 (35%)	50,67,67	2.85	23 (46%)
26	PEB	hE	201	2	43,46,46	3.49	12 (27%)	45,67,67	2.60	18 (40%)
26	PEB	A7	302	7	43,46,46	3.41	10 (23%)	45,67,67	1.95	13 (28%)
26	PEB	T6	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.29	19 (42%)
26	PEB	h1	202	2	43,46,46	3.47	9 (20%)	45,67,67	2.00	15 (33%)
26	PEB	H1	201	3,2	43,46,46	3.53	12 (27%)	45,67,67	1.92	12 (26%)
26	PEB	Q4	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	m2	202	2	43,46,46	3.31	12 (27%)	45,67,67	2.42	16 (35%)
26	PEB	P1	203	1	43,46,46	3.58	11 (25%)	45,67,67	1.80	12 (26%)
26	PEB	f8	203	2,1	43,46,46	3.32	12 (27%)	45,67,67	2.42	16 (35%)
26	PEB	FG	201	2	43,46,46	3.51	10 (23%)	45,67,67	3.86	16 (35%)
26	PEB	UE	202	1	43,46,46	3.27	9 (20%)	45,67,67	2.13	12 (26%)
26	PEB	KA	203	2,1	43,46,46	3.00	10 (23%)	45,67,67	2.45	16 (35%)
26	PEB	B1	201	3,2,26	43,46,46	3.37	9 (20%)	45,67,67	2.00	13 (28%)
26	PEB	RJ	201	1	43,46,46	3.53	12 (27%)	45,67,67	2.07	14 (31%)
26	PEB	xG	303	13	43,46,46	3.44	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	L4	203	2	43,46,46	3.43	10 (23%)	45,67,67	1.94	14 (31%)
26	PEB	hF	202	1	43,46,46	3.38	12 (27%)	45,67,67	2.16	14 (31%)
26	PEB	C9	201	2,7	43,46,46	3.13	11 (25%)	45,67,67	2.24	18 (40%)
26	PEB	WJ	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.86	15 (33%)
28	CYC	cH	1001	17	42,46,46	3.49	14 (33%)	50,67,67	4.76	20 (40%)
26	PEB	U1	201	2,4	43,46,46	3.61	12 (27%)	45,67,67	2.17	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	AC	201	2	43,46,46	3.49	9 (20%)	45,67,67	1.96	13 (28%)
26	PEB	AF	305	7	43,46,46	3.43	10 (23%)	45,67,67	2.42	15 (33%)
26	PEB	b1	501	2,4	43,46,46	3.48	9 (20%)	45,67,67	2.24	14 (31%)
26	PEB	yE	301	14	43,46,46	3.35	10 (23%)	45,67,67	2.11	16 (35%)
28	CYC	NB	1001	8,10	42,46,46	3.18	15 (35%)	50,67,67	2.93	27 (54%)
26	PEB	ZB	202	1	43,46,46	3.39	11 (25%)	45,67,67	2.16	16 (35%)
26	PEB	BE	202	2	43,46,46	3.49	10 (23%)	45,67,67	2.30	14 (31%)
26	PEB	ND	202	2	43,46,46	3.02	9 (20%)	45,67,67	3.13	17 (37%)
26	PEB	I8	203	1	43,46,46	3.52	12 (27%)	45,67,67	2.20	16 (35%)
26	PEB	xE	303	13	43,46,46	3.38	10 (23%)	45,67,67	2.32	15 (33%)
26	PEB	bI	201	1	43,46,46	3.39	10 (23%)	45,67,67	2.38	17 (37%)
26	PEB	fF	202	1	43,46,46	3.47	9 (20%)	45,67,67	2.59	15 (33%)
26	PEB	NB	1002	9,10	43,46,46	3.37	11 (25%)	45,67,67	2.21	15 (33%)
26	PEB	aB	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.17	19 (42%)
28	CYC	rH	1001	17	42,46,46	3.36	15 (35%)	50,67,67	3.04	21 (42%)
26	PEB	l7	201	2,1	43,46,46	3.34	9 (20%)	45,67,67	2.31	15 (33%)
26	PEB	e6	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.31	13 (28%)
26	PEB	WA	203	2,1	43,46,46	2.99	11 (25%)	45,67,67	2.52	16 (35%)
26	PEB	J8	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.42	17 (37%)
26	PEB	OI	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.50	18 (40%)
26	PEB	iI	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.00	15 (33%)
26	PEB	LF	1002	10	43,46,46	3.11	10 (23%)	45,67,67	2.37	15 (33%)
26	PEB	j6	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.95	14 (31%)
26	PEB	UD	202	1	43,46,46	3.34	10 (23%)	45,67,67	1.95	13 (28%)
26	PEB	dB	202	2,1	43,46,46	3.34	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	MD	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.00	13 (28%)
26	PEB	wG	303	13	43,46,46	3.47	11 (25%)	45,67,67	2.08	15 (33%)
26	PEB	xG	302	13	43,46,46	3.37	11 (25%)	45,67,67	2.91	13 (28%)
26	PEB	ZG	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.41	17 (37%)
26	PEB	EA	203	1	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
26	PEB	i8	201	2,13	43,46,46	3.43	12 (27%)	45,67,67	2.62	16 (35%)
26	PEB	cA	203	2	43,46,46	3.32	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	Z6	203	1	43,46,46	3.34	11 (25%)	45,67,67	2.15	16 (35%)
28	CYC	K2	1001	9	42,46,46	3.26	15 (35%)	50,67,67	2.88	19 (38%)
27	PUB	AB	303	7	42,46,46	3.42	7 (16%)	37,67,67	3.00	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	a2	202	2	43,46,46	3.28	13 (30%)	45,67,67	2.57	16 (35%)
26	PEB	BJ	201	1	43,46,46	3.18	11 (25%)	45,67,67	2.40	18 (40%)
26	PEB	NG	202	2	43,46,46	3.48	10 (23%)	45,67,67	1.92	13 (28%)
26	PEB	L5	203	2	43,46,46	3.16	11 (25%)	45,67,67	2.08	15 (33%)
26	PEB	J3	203	2	43,46,46	3.39	11 (25%)	45,67,67	2.32	14 (31%)
26	PEB	l6	203	1	43,46,46	3.46	11 (25%)	45,67,67	1.97	14 (31%)
26	PEB	mA	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.56	18 (40%)
26	PEB	G4	202	1	43,46,46	3.45	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	mF	202	2	43,46,46	3.71	10 (23%)	45,67,67	1.85	11 (24%)
26	PEB	GJ	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.22	17 (37%)
26	PEB	B5	203	2	43,46,46	3.55	12 (27%)	45,67,67	1.97	14 (31%)
26	PEB	RF	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.17	18 (40%)
26	PEB	E9	201	2,15	43,46,46	3.29	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	SB	202	1	43,46,46	3.43	10 (23%)	45,67,67	1.83	13 (28%)
26	PEB	m7	202	2	43,46,46	3.61	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	m8	201	2,13	43,46,46	3.42	11 (25%)	45,67,67	2.49	19 (42%)
27	PUB	AJ	302	1,7	42,46,46	3.54	8 (19%)	37,67,67	3.03	15 (40%)
26	PEB	e2	201	2	43,46,46	3.37	11 (25%)	45,67,67	2.14	15 (33%)
26	PEB	gE	202	1	43,46,46	3.37	10 (23%)	45,67,67	1.99	14 (31%)
28	CYC	C6	1001	9,10	42,46,46	3.25	15 (35%)	50,67,67	2.71	18 (36%)
26	PEB	B1	203	2	43,46,46	3.44	11 (25%)	45,67,67	1.96	14 (31%)
26	PEB	D4	201	3,2	43,46,46	3.32	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	X1	202	1	43,46,46	3.35	10 (23%)	45,67,67	2.58	16 (35%)
26	PEB	AJ	303	7,26	43,46,46	3.39	11 (25%)	45,67,67	2.54	15 (33%)
28	CYC	yH	1001	-	42,46,46	3.56	14 (33%)	50,67,67	2.88	19 (38%)
26	PEB	O7	203	2,1	43,46,46	3.23	9 (20%)	45,67,67	2.21	14 (31%)
26	PEB	AC	203	2	43,46,46	3.54	12 (27%)	45,67,67	1.84	13 (28%)
26	PEB	VD	201	2,11	43,46,46	3.34	10 (23%)	45,67,67	2.11	13 (28%)
26	PEB	V7	201	2	43,46,46	3.42	13 (30%)	45,67,67	2.17	18 (40%)
28	CYC	M6	1001	9,10	42,46,46	3.17	14 (33%)	50,67,67	2.89	19 (38%)
26	PEB	W3	201	1	43,46,46	3.18	10 (23%)	45,67,67	2.35	18 (40%)
26	PEB	FD	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.72	18 (40%)
26	PEB	Q2	201	1	43,46,46	3.32	11 (25%)	45,67,67	2.69	20 (44%)
26	PEB	cB	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	P9	202	1	43,46,46	3.48	11 (25%)	45,67,67	2.21	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	HD	203	2	43,46,46	3.56	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	f6	203	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.18	13 (28%)
26	PEB	LD	202	2	43,46,46	3.18	10 (23%)	45,67,67	2.76	17 (37%)
26	PEB	bE	202	2	43,46,46	3.64	10 (23%)	45,67,67	2.35	13 (28%)
26	PEB	RI	202	2	43,46,46	3.21	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	Q9	202	2	43,46,46	3.48	13 (30%)	45,67,67	1.83	13 (28%)
26	PEB	D4	202	2	43,46,46	3.47	13 (30%)	45,67,67	2.42	15 (33%)
28	CYC	C7	1001	9,10	42,46,46	3.32	13 (30%)	50,67,67	2.81	19 (38%)
26	PEB	tG	201	2	43,46,46	3.51	10 (23%)	45,67,67	2.85	16 (35%)
26	PEB	F4	202	2	43,46,46	3.49	12 (27%)	45,67,67	2.43	15 (33%)
26	PEB	R2	201	2,6	43,46,46	3.32	10 (23%)	45,67,67	2.38	15 (33%)
28	CYC	IB	1001	9,10	42,46,46	3.17	13 (30%)	50,67,67	2.81	18 (36%)
28	CYC	KB	202	9,10	42,46,46	3.19	14 (33%)	50,67,67	2.74	20 (40%)
26	PEB	SJ	202	2	43,46,46	3.36	9 (20%)	45,67,67	1.97	15 (33%)
26	PEB	H5	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.27	14 (31%)
26	PEB	d7	201	2,1	43,46,46	3.34	10 (23%)	45,67,67	2.23	14 (31%)
26	PEB	z4	202	1	43,46,46	3.53	9 (20%)	45,67,67	2.50	17 (37%)
26	PEB	kI	201	2	43,46,46	3.41	12 (27%)	45,67,67	1.96	12 (26%)
28	CYC	DI	1001	10	42,46,46	3.11	13 (30%)	50,67,67	2.80	20 (40%)
26	PEB	h8	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.17	16 (35%)
26	PEB	h7	203	2,1	43,46,46	3.48	13 (30%)	45,67,67	2.63	16 (35%)
26	PEB	a7	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.27	15 (33%)
26	PEB	IG	203	2,1	43,46,46	3.05	10 (23%)	45,67,67	2.73	18 (40%)
26	PEB	gB	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.59	13 (28%)
26	PEB	HI	1002	10	43,46,46	3.25	10 (23%)	45,67,67	2.08	16 (35%)
26	PEB	g7	202	2	43,46,46	3.49	11 (25%)	45,67,67	2.30	16 (35%)
26	PEB	f4	202	2	43,46,46	3.56	11 (25%)	45,67,67	2.18	14 (31%)
26	PEB	qG	201	2,1	43,46,46	3.41	12 (27%)	45,67,67	2.69	17 (37%)
26	PEB	hB	203	1	43,46,46	3.31	11 (25%)	45,67,67	2.09	16 (35%)
26	PEB	V4	203	2,1	43,46,46	3.39	11 (25%)	45,67,67	2.14	13 (28%)
28	CYC	iH	1001	18,17	42,46,46	3.44	15 (35%)	50,67,67	2.96	22 (44%)
26	PEB	OE	203	1	43,46,46	3.39	10 (23%)	45,67,67	2.09	17 (37%)
28	CYC	JF	1003	9,10	42,46,46	3.20	11 (26%)	50,67,67	2.65	19 (38%)
26	PEB	XD	201	2,11	43,46,46	3.64	11 (25%)	45,67,67	2.35	19 (42%)
26	PEB	MG	203	2,1	43,46,46	3.33	13 (30%)	45,67,67	2.57	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	T6	202	2	43,46,46	3.32	10 (23%)	45,67,67	2.31	19 (42%)
26	PEB	k6	201	2,7	43,46,46	3.45	12 (27%)	45,67,67	2.24	17 (37%)
26	PEB	eE	203	1	43,46,46	3.40	10 (23%)	45,67,67	2.32	15 (33%)
26	PEB	K1	201	1	43,46,46	3.41	10 (23%)	45,67,67	2.01	15 (33%)
26	PEB	e7	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.08	17 (37%)
26	PEB	lA	203	1	43,46,46	3.24	10 (23%)	45,67,67	2.06	13 (28%)
26	PEB	W8	203	2,1	43,46,46	3.00	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	QE	203	2,1	43,46,46	3.26	12 (27%)	45,67,67	2.72	17 (37%)
26	PEB	c2	203	2	43,46,46	3.47	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	O8	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.03	15 (33%)
28	CYC	pH	1001	17	42,46,46	3.46	14 (33%)	50,67,67	2.89	21 (42%)
26	PEB	j8	202	1	43,46,46	3.43	11 (25%)	45,67,67	2.61	17 (37%)
26	PEB	NF	1002	10	43,46,46	3.27	12 (27%)	45,67,67	2.09	12 (26%)
26	PEB	H2	1002	10	43,46,46	3.24	10 (23%)	45,67,67	2.09	16 (35%)
28	CYC	H7	1001	10	42,46,46	3.36	14 (33%)	50,67,67	2.92	20 (40%)
26	PEB	c7	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.20	14 (31%)
26	PEB	CE	202	1	43,46,46	3.03	9 (20%)	45,67,67	2.14	13 (28%)
26	PEB	Q8	202	2,1	43,46,46	3.29	11 (25%)	45,67,67	2.28	15 (33%)
26	PEB	wE	303	13	43,46,46	3.46	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	E3	202	1	43,46,46	3.40	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	bF	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.03	15 (33%)
26	PEB	11	203	2	43,46,46	3.43	9 (20%)	45,67,67	1.91	13 (28%)
26	PEB	iB	202	2	43,46,46	3.50	11 (25%)	45,67,67	2.00	13 (28%)
26	PEB	P9	201	2,1	43,46,46	3.47	12 (27%)	45,67,67	2.13	13 (28%)
26	PEB	T7	202	2	43,46,46	3.33	10 (23%)	45,67,67	1.78	12 (26%)
26	PEB	DE	203	2	43,46,46	3.46	10 (23%)	45,67,67	2.00	14 (31%)
26	PEB	i7	201	2	43,46,46	3.46	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	OB	202	1	43,46,46	3.39	10 (23%)	45,67,67	2.04	13 (28%)
26	PEB	N3	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.43	16 (35%)
26	PEB	Y9	201	2,26	43,46,46	3.51	11 (25%)	45,67,67	1.99	12 (26%)
26	PEB	LJ	201	2,1	43,46,46	3.30	10 (23%)	45,67,67	2.47	16 (35%)
26	PEB	O9	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.98	15 (33%)
26	PEB	AJ	305	2,7,26	43,46,46	3.45	11 (25%)	45,67,67	1.95	12 (26%)
26	PEB	f7	202	1	43,46,46	3.39	9 (20%)	45,67,67	2.66	14 (31%)
26	PEB	N1	201	1	43,46,46	3.23	10 (23%)	45,67,67	2.74	21 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	sE	201	1	43,46,46	3.32	9 (20%)	45,67,67	2.04	13 (28%)
26	PEB	TI	203	2	43,46,46	3.41	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	Y3	301	7	43,46,46	3.29	10 (23%)	45,67,67	2.62	16 (35%)
26	PEB	M9	202	2	43,46,46	3.31	9 (20%)	45,67,67	1.99	13 (28%)
26	PEB	wG	301	13	43,46,46	3.22	9 (20%)	45,67,67	2.29	15 (33%)
26	PEB	OJ	201	2	43,46,46	3.38	11 (25%)	45,67,67	2.53	16 (35%)
26	PEB	u4	203	2	43,46,46	3.59	11 (25%)	45,67,67	2.09	16 (35%)
26	PEB	fl	202	1	43,46,46	3.41	11 (25%)	45,67,67	1.97	14 (31%)
26	PEB	HE	201	2	43,46,46	3.13	13 (30%)	45,67,67	3.10	19 (42%)
26	PEB	YE	201	1	43,46,46	3.47	9 (20%)	45,67,67	1.88	15 (33%)
26	PEB	ZF	203	1	43,46,46	3.40	11 (25%)	45,67,67	2.50	16 (35%)
26	PEB	YA	201	2,1	43,46,46	3.08	10 (23%)	45,67,67	2.55	17 (37%)
26	PEB	JJ	202	1	43,46,46	3.17	9 (20%)	45,67,67	2.07	13 (28%)
26	PEB	cE	203	2,1	43,46,46	3.37	16 (37%)	45,67,67	3.00	17 (37%)
26	PEB	AG	201	1	43,46,46	3.25	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	G3	201	1	43,46,46	3.21	9 (20%)	45,67,67	2.15	13 (28%)
26	PEB	FI	1002	10	43,46,46	3.26	10 (23%)	45,67,67	2.23	17 (37%)
26	PEB	S4	201	2,4	43,46,46	3.47	12 (27%)	45,67,67	2.31	18 (40%)
26	PEB	eE	202	1	43,46,46	3.19	11 (25%)	45,67,67	2.33	19 (42%)
26	PEB	j8	201	1	43,46,46	3.31	11 (25%)	45,67,67	2.09	14 (31%)
26	PEB	lF	203	1	43,46,46	3.48	11 (25%)	45,67,67	2.75	15 (33%)
26	PEB	W9	201	2,7	43,46,46	3.43	11 (25%)	45,67,67	2.10	15 (33%)
26	PEB	UB	203	1	43,46,46	3.37	10 (23%)	45,67,67	2.02	15 (33%)
26	PEB	21	401	3	43,46,46	3.42	10 (23%)	45,67,67	2.28	17 (37%)
26	PEB	c7	201	2	43,46,46	3.36	10 (23%)	45,67,67	1.89	14 (31%)
26	PEB	E4	201	1	43,46,46	3.42	9 (20%)	45,67,67	1.91	12 (26%)
26	PEB	j1	201	2,4	43,46,46	3.54	11 (25%)	45,67,67	2.16	16 (35%)
26	PEB	M8	201	2,1	43,46,46	3.06	11 (25%)	45,67,67	2.68	15 (33%)
26	PEB	P3	201	2,11	43,46,46	3.43	10 (23%)	45,67,67	2.40	17 (37%)
26	PEB	VJ	202	1	43,46,46	3.46	11 (25%)	45,67,67	1.94	14 (31%)
26	PEB	J4	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.08	16 (35%)
26	PEB	A7	305	7	43,46,46	3.42	10 (23%)	45,67,67	2.38	14 (31%)
26	PEB	SF	202	1	43,46,46	3.31	10 (23%)	45,67,67	2.40	13 (28%)
26	PEB	W1	201	2	43,46,46	3.50	12 (27%)	45,67,67	2.40	23 (51%)
26	PEB	T4	201	2,1	43,46,46	3.47	12 (27%)	45,67,67	2.29	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	Y3	304	7,26	43,46,46	3.31	11 (25%)	45,67,67	2.42	13 (28%)
26	PEB	n4	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.05	14 (31%)
28	CYC	VH	1001	-	42,46,46	3.47	14 (33%)	50,67,67	3.12	19 (38%)
26	PEB	H8	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.27	15 (33%)
26	PEB	KC	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.10	14 (31%)
26	PEB	d1	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.01	14 (31%)
26	PEB	gI	203	2	43,46,46	3.46	11 (25%)	45,67,67	2.19	13 (28%)
26	PEB	oE	201	1	43,46,46	3.46	12 (27%)	45,67,67	2.53	17 (37%)
28	CYC	E2	1001	9	42,46,46	3.21	15 (35%)	50,67,67	2.92	20 (40%)
26	PEB	HG	201	2	43,46,46	3.14	12 (27%)	45,67,67	2.94	21 (46%)
26	PEB	N3	202	2	43,46,46	2.92	10 (23%)	45,67,67	3.31	18 (40%)
26	PEB	b7	203	2,1	43,46,46	3.45	11 (25%)	45,67,67	2.26	14 (31%)
26	PEB	i1	203	1	43,46,46	3.41	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	MA	201	2,1	43,46,46	3.05	11 (25%)	45,67,67	2.65	15 (33%)
26	PEB	k7	201	2	43,46,46	3.39	11 (25%)	45,67,67	1.92	13 (28%)
28	CYC	G7	1001	9,10	42,46,46	3.23	11 (26%)	50,67,67	2.88	19 (38%)
26	PEB	BJ	202	1	43,46,46	3.33	10 (23%)	45,67,67	1.97	15 (33%)
26	PEB	TA	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.34	14 (31%)
26	PEB	K8	201	1	43,46,46	3.35	10 (23%)	45,67,67	2.35	14 (31%)
26	PEB	C5	203	2	43,46,46	3.45	9 (20%)	45,67,67	2.22	14 (31%)
26	PEB	HF	1002	10	43,46,46	3.44	11 (25%)	45,67,67	2.30	14 (31%)
26	PEB	F1	201	3,2	43,46,46	3.56	12 (27%)	45,67,67	2.11	16 (35%)
26	PEB	vE	201	2	43,46,46	3.47	9 (20%)	45,67,67	3.06	17 (37%)
26	PEB	Q4	201	2	43,46,46	3.44	11 (25%)	45,67,67	2.32	20 (44%)
26	PEB	Q3	202	1	43,46,46	3.11	9 (20%)	45,67,67	1.98	14 (31%)
26	PEB	KA	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.30	15 (33%)
26	PEB	F1	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.39	16 (35%)
26	PEB	F8	202	2	43,46,46	3.31	11 (25%)	45,67,67	2.50	18 (40%)
26	PEB	aE	201	2,1	43,46,46	3.42	12 (27%)	45,67,67	2.60	16 (35%)
26	PEB	X8	201	2	43,46,46	3.28	11 (25%)	45,67,67	2.37	15 (33%)
26	PEB	JJ	201	1	43,46,46	3.38	13 (30%)	45,67,67	2.20	13 (28%)
27	PUB	xG	306	13	42,46,46	3.61	7 (16%)	37,67,67	2.91	15 (40%)
26	PEB	a4	203	2	43,46,46	3.29	9 (20%)	45,67,67	2.19	14 (31%)
26	PEB	V9	201	1	43,46,46	3.20	10 (23%)	45,67,67	2.30	12 (26%)
26	PEB	ZF	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.18	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	VA	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.56	18 (40%)
26	PEB	NE	201	2	43,46,46	3.35	10 (23%)	45,67,67	3.08	16 (35%)
26	PEB	H5	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
26	PEB	i2	202	2	43,46,46	3.29	11 (25%)	45,67,67	2.36	14 (31%)
26	PEB	L6	1002	9,10	43,46,46	3.33	10 (23%)	45,67,67	1.89	13 (28%)
26	PEB	g8	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.50	16 (35%)
26	PEB	l8	203	1	43,46,46	3.23	11 (25%)	45,67,67	2.06	13 (28%)
26	PEB	UB	202	1	43,46,46	3.46	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	T8	202	2	43,46,46	3.17	11 (25%)	45,67,67	2.36	16 (35%)
26	PEB	Q6	203	1	43,46,46	3.39	9 (20%)	45,67,67	2.00	15 (33%)
26	PEB	Y3	303	7,26	43,46,46	3.30	12 (27%)	45,67,67	2.79	14 (31%)
26	PEB	VJ	201	1	43,46,46	3.48	11 (25%)	45,67,67	1.86	13 (28%)
26	PEB	z1	201	1	43,46,46	3.56	11 (25%)	45,67,67	2.45	17 (37%)
26	PEB	i1	202	1	43,46,46	3.47	12 (27%)	45,67,67	2.12	18 (40%)
26	PEB	qE	201	2,1	43,46,46	3.39	11 (25%)	45,67,67	2.62	16 (35%)
26	PEB	F9	203	2,1	43,46,46	3.41	13 (30%)	45,67,67	3.08	13 (28%)
26	PEB	VD	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.57	18 (40%)
28	CYC	H6	1001	10	42,46,46	3.13	14 (33%)	50,67,67	3.07	21 (42%)
26	PEB	j7	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.45	17 (37%)
26	PEB	IC	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.05	15 (33%)
26	PEB	J8	202	2	43,46,46	3.35	12 (27%)	45,67,67	2.28	15 (33%)
26	PEB	Q7	202	1	43,46,46	3.38	12 (27%)	45,67,67	2.33	16 (35%)
26	PEB	b6	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	V3	202	2	43,46,46	3.18	9 (20%)	45,67,67	2.62	16 (35%)
26	PEB	R1	203	2,1	43,46,46	3.47	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	KJ	201	2	43,46,46	3.48	12 (27%)	45,67,67	2.02	15 (33%)
28	CYC	FF	1001	10	42,46,46	3.32	15 (35%)	50,67,67	2.89	18 (36%)
26	PEB	J3	201	2,7	43,46,46	3.20	10 (23%)	45,67,67	2.48	14 (31%)
26	PEB	D2	1002	10	43,46,46	3.30	10 (23%)	45,67,67	2.08	14 (31%)
26	PEB	F4	203	2	43,46,46	3.40	11 (25%)	45,67,67	1.91	15 (33%)
26	PEB	q1	202	2	43,46,46	3.37	12 (27%)	45,67,67	2.56	15 (33%)
28	CYC	HI	1001	10	42,46,46	3.24	14 (33%)	50,67,67	3.08	23 (46%)
27	PUB	A9	302	1,7	42,46,46	3.48	8 (19%)	37,67,67	3.18	15 (40%)
28	CYC	D2	1001	10	42,46,46	3.14	14 (33%)	50,67,67	2.83	21 (42%)
26	PEB	B3	203	2	43,46,46	3.48	13 (30%)	45,67,67	2.13	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	Y7	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.11	16 (35%)
28	CYC	jH	1001	22,18	42,46,46	3.50	15 (35%)	50,67,67	2.88	19 (38%)
26	PEB	dI	202	1	43,46,46	3.35	11 (25%)	45,67,67	1.89	12 (26%)
26	PEB	IJ	201	2,15	43,46,46	3.61	12 (27%)	45,67,67	2.28	15 (33%)
26	PEB	R6	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.24	17 (37%)
26	PEB	XG	203	2	43,46,46	3.48	11 (25%)	45,67,67	2.28	17 (37%)
26	PEB	iA	202	2	43,46,46	3.38	11 (25%)	45,67,67	2.21	16 (35%)
28	CYC	sH	1001	22,18	42,46,46	3.42	13 (30%)	50,67,67	2.85	17 (34%)
26	PEB	d6	202	2,1	43,46,46	3.36	10 (23%)	45,67,67	2.43	16 (35%)
26	PEB	BD	203	2	43,46,46	3.33	9 (20%)	45,67,67	1.99	14 (31%)
26	PEB	gF	201	2	43,46,46	3.57	10 (23%)	45,67,67	1.92	15 (33%)
26	PEB	lB	201	2,1	43,46,46	3.32	11 (25%)	45,67,67	2.37	14 (31%)
26	PEB	WF	201	1	43,46,46	3.21	11 (25%)	45,67,67	2.22	15 (33%)
26	PEB	w4	202	2	43,46,46	3.56	10 (23%)	45,67,67	2.61	14 (31%)
26	PEB	PD	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.19	16 (35%)
26	PEB	O2	201	1	43,46,46	3.38	11 (25%)	45,67,67	2.51	17 (37%)
26	PEB	O7	201	1	43,46,46	3.34	13 (30%)	45,67,67	2.27	18 (40%)
26	PEB	QD	201	1	43,46,46	3.23	11 (25%)	45,67,67	2.65	17 (37%)
26	PEB	j7	201	1	43,46,46	3.36	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	ID	202	1	43,46,46	3.43	11 (25%)	45,67,67	1.87	12 (26%)
26	PEB	kG	203	2,1	43,46,46	3.44	12 (27%)	45,67,67	2.31	11 (24%)
26	PEB	T9	203	1	43,46,46	3.39	8 (18%)	45,67,67	2.14	12 (26%)
26	PEB	FJ	201	1	43,46,46	3.23	11 (25%)	45,67,67	2.53	17 (37%)
26	PEB	z1	202	1	43,46,46	3.70	10 (23%)	45,67,67	2.58	19 (42%)
27	PUB	AA	304	13	42,46,46	3.47	9 (21%)	37,67,67	3.01	14 (37%)
26	PEB	C5	204	2	43,46,46	3.54	12 (27%)	45,67,67	1.88	15 (33%)
28	CYC	D6	1001	10	42,46,46	3.17	14 (33%)	50,67,67	3.01	21 (42%)
26	PEB	m2	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	ME	203	2,1	43,46,46	3.35	13 (30%)	45,67,67	2.46	15 (33%)
26	PEB	UA	203	3,1	43,46,46	3.33	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	QD	202	1	43,46,46	3.19	10 (23%)	45,67,67	1.99	13 (28%)
26	PEB	Q2	202	10,1	43,46,46	3.38	9 (20%)	45,67,67	1.87	12 (26%)
26	PEB	L2	1002	10	43,46,46	3.38	11 (25%)	45,67,67	2.75	16 (35%)
26	PEB	y4	202	2	43,46,46	3.37	9 (20%)	45,67,67	2.17	14 (31%)
26	PEB	A5	201	2	43,46,46	3.50	11 (25%)	45,67,67	2.17	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	OG	203	1	43,46,46	3.28	9 (20%)	45,67,67	2.00	16 (35%)
26	PEB	H9	203	1	43,46,46	3.42	11 (25%)	45,67,67	2.12	12 (26%)
26	PEB	J5	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.84	17 (37%)
26	PEB	M3	201	1	43,46,46	3.25	10 (23%)	45,67,67	2.48	16 (35%)
26	PEB	OB	203	2,1	43,46,46	3.19	11 (25%)	45,67,67	2.32	16 (35%)
26	PEB	SE	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.16	15 (33%)
26	PEB	iG	201	2,1	43,46,46	3.41	11 (25%)	45,67,67	2.38	14 (31%)
26	PEB	jI	202	1	43,46,46	3.34	11 (25%)	45,67,67	1.95	12 (26%)
26	PEB	wE	302	13	43,46,46	3.34	9 (20%)	45,67,67	2.19	15 (33%)
26	PEB	T4	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.06	16 (35%)
28	CYC	E6	1001	9,10	42,46,46	3.21	15 (35%)	50,67,67	2.76	21 (42%)
26	PEB	B4	203	2	43,46,46	3.42	10 (23%)	45,67,67	1.93	16 (35%)
26	PEB	SD	202	1	43,46,46	3.20	10 (23%)	45,67,67	1.96	12 (26%)
26	PEB	JG	201	2	43,46,46	3.41	10 (23%)	45,67,67	3.06	17 (37%)
26	PEB	p4	202	1	43,46,46	3.77	10 (23%)	45,67,67	2.77	17 (37%)
26	PEB	JG	202	2	43,46,46	3.47	11 (25%)	45,67,67	2.33	16 (35%)
26	PEB	P4	201	2,1	43,46,46	3.31	11 (25%)	45,67,67	2.23	14 (31%)
26	PEB	HC	203	2	43,46,46	3.27	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	R8	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	U6	203	1	43,46,46	3.41	11 (25%)	45,67,67	2.05	15 (33%)
26	PEB	WD	202	1	43,46,46	3.42	11 (25%)	45,67,67	2.05	13 (28%)
26	PEB	K4	201	1	43,46,46	3.44	11 (25%)	45,67,67	2.08	16 (35%)
26	PEB	IE	202	1	43,46,46	3.19	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	jF	203	2,1	43,46,46	3.48	13 (30%)	45,67,67	2.49	15 (33%)
26	PEB	Q3	201	1	43,46,46	3.26	11 (25%)	45,67,67	2.72	17 (37%)
26	PEB	hB	201	2,1	43,46,46	3.48	12 (27%)	45,67,67	2.23	14 (31%)
26	PEB	XJ	202	1	43,46,46	3.57	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	M4	401	3	43,46,46	3.43	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	eB	202	2	43,46,46	3.26	9 (20%)	45,67,67	2.27	14 (31%)
26	PEB	TJ	201	2,1	43,46,46	3.45	13 (30%)	45,67,67	2.35	13 (28%)
28	CYC	AH	1001	17	42,46,46	3.50	13 (30%)	50,67,67	4.72	20 (40%)
26	PEB	SG	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.13	14 (31%)
26	PEB	cI	203	2	43,46,46	3.46	12 (27%)	45,67,67	1.99	11 (24%)
26	PEB	h7	202	1	43,46,46	3.44	11 (25%)	45,67,67	2.03	15 (33%)
28	CYC	F7	1001	10	42,46,46	3.23	13 (30%)	50,67,67	2.97	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	x4	201	1	43,46,46	3.51	10 (23%)	45,67,67	1.86	14 (31%)
28	CYC	NF	1001	8,10	42,46,46	3.36	16 (38%)	50,67,67	2.86	23 (46%)
26	PEB	TB	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.33	19 (42%)
26	PEB	A2	301	7	43,46,46	3.39	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	x1	201	1	43,46,46	3.52	13 (30%)	45,67,67	1.87	15 (33%)
26	PEB	g1	203	2,1	43,46,46	3.36	12 (27%)	45,67,67	2.33	13 (28%)
26	PEB	dG	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.44	16 (35%)
26	PEB	V6	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.19	15 (33%)
28	CYC	GH	1001	17	42,46,46	3.44	15 (35%)	50,67,67	3.03	24 (48%)
28	CYC	CI	1001	9	42,46,46	3.25	14 (33%)	50,67,67	2.93	21 (42%)
26	PEB	B9	202	1	43,46,46	3.34	10 (23%)	45,67,67	2.01	15 (33%)
26	PEB	iB	201	2	43,46,46	3.43	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	ND	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.35	17 (37%)
27	PUB	KD	203	1,7	42,46,46	3.37	7 (16%)	37,67,67	3.59	17 (45%)
28	CYC	K7	1001	9,10	42,46,46	3.24	12 (28%)	50,67,67	2.86	19 (38%)
26	PEB	dB	201	1,7	43,46,46	3.36	8 (18%)	45,67,67	2.18	14 (31%)
26	PEB	e6	203	2	43,46,46	3.56	12 (27%)	45,67,67	2.70	18 (40%)
26	PEB	bB	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.21	14 (31%)
28	CYC	IF	1001	9,10	42,46,46	3.17	12 (28%)	50,67,67	2.96	22 (44%)
26	PEB	lG	202	2	43,46,46	3.44	9 (20%)	45,67,67	2.10	15 (33%)
26	PEB	DE	202	2,1	43,46,46	3.16	13 (30%)	45,67,67	3.17	16 (35%)
26	PEB	a4	201	2	43,46,46	3.44	11 (25%)	45,67,67	2.25	15 (33%)
26	PEB	f8	202	1	43,46,46	3.39	10 (23%)	45,67,67	2.05	15 (33%)
26	PEB	PI	202	2	43,46,46	3.29	11 (25%)	45,67,67	2.47	16 (35%)
26	PEB	AI	304	7	43,46,46	3.36	10 (23%)	45,67,67	2.06	13 (28%)
26	PEB	Y2	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.33	15 (33%)
26	PEB	I9	201	2,15	43,46,46	3.67	13 (30%)	45,67,67	2.35	18 (40%)
26	PEB	K9	201	2	43,46,46	3.35	11 (25%)	45,67,67	1.97	14 (31%)
26	PEB	O6	202	1	43,46,46	3.36	10 (23%)	45,67,67	2.06	14 (31%)
26	PEB	L7	1002	10	43,46,46	3.25	10 (23%)	45,67,67	2.23	14 (31%)
26	PEB	L4	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.34	15 (33%)
26	PEB	BG	201	2,16	43,46,46	3.38	12 (27%)	45,67,67	3.49	16 (35%)
26	PEB	c6	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	16 (35%)
26	PEB	R9	203	2,1	43,46,46	3.39	12 (27%)	45,67,67	2.33	16 (35%)
26	PEB	D6	1002	9,10	43,46,46	3.31	12 (27%)	45,67,67	2.25	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	k4	202	1	43,46,46	3.38	9 (20%)	45,67,67	1.95	14 (31%)
26	PEB	R3	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	N4	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.05	13 (28%)
26	PEB	WE	202	1	43,46,46	2.99	10 (23%)	45,67,67	2.23	15 (33%)
26	PEB	EJ	202	2	43,46,46	3.26	10 (23%)	45,67,67	2.10	14 (31%)
26	PEB	B8	301	14	43,46,46	3.42	10 (23%)	45,67,67	2.43	14 (31%)
26	PEB	QG	202	1	43,46,46	3.40	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	Y1	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.22	18 (40%)
26	PEB	SG	202	1	43,46,46	3.26	12 (27%)	45,67,67	2.40	16 (35%)
26	PEB	UB	201	2,1	43,46,46	3.30	10 (23%)	45,67,67	2.30	16 (35%)
26	PEB	V4	201	1	43,46,46	3.44	10 (23%)	45,67,67	2.04	17 (37%)
26	PEB	GG	201	2,1	43,46,46	3.18	12 (27%)	45,67,67	3.06	20 (44%)
26	PEB	WA	202	1	43,46,46	3.47	10 (23%)	45,67,67	2.26	13 (28%)
26	PEB	L3	201	2,26	43,46,46	3.39	10 (23%)	45,67,67	2.32	18 (40%)
26	PEB	g1	202	1	43,46,46	3.44	11 (25%)	45,67,67	2.12	14 (31%)
26	PEB	V6	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.05	16 (35%)
27	PUB	BA	302	14	42,46,46	3.29	7 (16%)	37,67,67	3.20	16 (43%)
26	PEB	QB	203	1	43,46,46	3.38	10 (23%)	45,67,67	2.01	15 (33%)
26	PEB	C8	203	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.45	16 (35%)
26	PEB	AB	304	7	43,46,46	3.29	9 (20%)	45,67,67	2.10	17 (37%)
26	PEB	B9	201	1	43,46,46	3.22	11 (25%)	45,67,67	2.32	16 (35%)
26	PEB	T7	201	2,6	43,46,46	3.40	12 (27%)	45,67,67	2.02	16 (35%)
26	PEB	L9	203	1	43,46,46	3.37	9 (20%)	45,67,67	2.04	14 (31%)
26	PEB	XD	203	2	43,46,46	3.49	11 (25%)	45,67,67	2.30	18 (40%)
26	PEB	LG	202	2	43,46,46	3.67	11 (25%)	45,67,67	2.71	15 (33%)
26	PEB	VI	202	2	43,46,46	3.13	10 (23%)	45,67,67	2.43	17 (37%)
26	PEB	aG	203	1	43,46,46	3.35	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	O8	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.98	13 (28%)
26	PEB	a8	201	1,13	43,46,46	3.10	10 (23%)	45,67,67	2.30	17 (37%)
26	PEB	cA	202	2,1	43,46,46	3.55	12 (27%)	45,67,67	2.28	13 (28%)
28	CYC	FB	1001	10	42,46,46	3.25	13 (30%)	50,67,67	2.90	18 (36%)
26	PEB	G9	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.09	17 (37%)
26	PEB	m4	203	1	43,46,46	3.54	11 (25%)	45,67,67	2.16	17 (37%)
26	PEB	U7	201	2,1	43,46,46	3.44	11 (25%)	45,67,67	2.24	14 (31%)
26	PEB	X1	203	1	43,46,46	3.22	11 (25%)	45,67,67	2.18	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	MD	201	1	43,46,46	3.28	11 (25%)	45,67,67	2.42	14 (31%)
26	PEB	m6	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.55	14 (31%)
26	PEB	DE	201	2	43,46,46	3.30	8 (18%)	45,67,67	2.95	17 (37%)
26	PEB	T1	202	1	43,46,46	3.31	10 (23%)	45,67,67	2.13	16 (35%)
26	PEB	K6	201	9,10	43,46,46	3.31	11 (25%)	45,67,67	2.10	15 (33%)
28	CYC	MI	1001	9	42,46,46	3.16	12 (28%)	50,67,67	2.89	17 (34%)
26	PEB	KC	203	2	43,46,46	3.40	10 (23%)	45,67,67	1.91	13 (28%)
26	PEB	gI	202	2	43,46,46	3.32	11 (25%)	45,67,67	2.31	14 (31%)
26	PEB	eI	201	2	43,46,46	3.35	11 (25%)	45,67,67	2.16	15 (33%)
26	PEB	Y2	201	2	43,46,46	3.37	11 (25%)	45,67,67	2.17	15 (33%)
26	PEB	k7	202	2	43,46,46	3.45	9 (20%)	45,67,67	2.09	16 (35%)
26	PEB	UJ	201	2,7	43,46,46	3.49	11 (25%)	45,67,67	2.10	17 (37%)
26	PEB	G5	203	2	43,46,46	3.43	9 (20%)	45,67,67	2.28	14 (31%)
26	PEB	r1	202	1	43,46,46	3.63	11 (25%)	45,67,67	2.49	14 (31%)
26	PEB	h1	201	2,4	43,46,46	3.64	11 (25%)	45,67,67	2.05	13 (28%)
26	PEB	O1	201	2,4	43,46,46	3.40	11 (25%)	45,67,67	2.36	20 (44%)
26	PEB	X3	202	2	43,46,46	2.97	9 (20%)	45,67,67	2.61	17 (37%)
26	PEB	g4	203	2,1	43,46,46	3.37	12 (27%)	45,67,67	2.44	13 (28%)
26	PEB	U4	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	e8	201	2,13	43,46,46	3.31	11 (25%)	45,67,67	2.39	16 (35%)
26	PEB	U3	202	1	43,46,46	3.36	9 (20%)	45,67,67	1.91	14 (31%)
28	CYC	EB	1001	9,10	42,46,46	3.24	16 (38%)	50,67,67	2.85	19 (38%)
26	PEB	M1	402	3,26	43,46,46	3.47	10 (23%)	45,67,67	2.08	14 (31%)
26	PEB	kA	201	2	43,46,46	3.36	10 (23%)	45,67,67	2.63	14 (31%)
26	PEB	t4	202	1	43,46,46	3.62	12 (27%)	45,67,67	2.47	16 (35%)
26	PEB	h8	203	1	43,46,46	3.47	11 (25%)	45,67,67	1.97	13 (28%)
26	PEB	H3	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	VA	202	2	43,46,46	3.46	14 (32%)	45,67,67	2.80	16 (35%)
26	PEB	U2	201	1	43,46,46	3.22	10 (23%)	45,67,67	2.77	19 (42%)
26	PEB	V8	202	2	43,46,46	3.45	13 (30%)	45,67,67	3.22	19 (42%)
26	PEB	g8	201	2	43,46,46	3.43	11 (25%)	45,67,67	2.54	16 (35%)
26	PEB	uE	201	2,1	43,46,46	3.37	13 (30%)	45,67,67	2.34	14 (31%)
26	PEB	AC	202	2	43,46,46	3.44	9 (20%)	45,67,67	2.19	14 (31%)
26	PEB	yG	301	14	43,46,46	3.36	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	HJ	202	1	43,46,46	3.39	12 (27%)	45,67,67	2.49	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	QF	201	2,1	43,46,46	3.32	11 (25%)	45,67,67	2.51	17 (37%)
26	PEB	F5	202	2	43,46,46	3.17	10 (23%)	45,67,67	1.94	12 (26%)
26	PEB	HD	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.58	17 (37%)
26	PEB	PF	201	2,6	43,46,46	3.38	10 (23%)	45,67,67	2.25	17 (37%)
26	PEB	C1	201	1	43,46,46	3.42	10 (23%)	45,67,67	1.98	12 (26%)
26	PEB	H7	1002	10	43,46,46	3.47	12 (27%)	45,67,67	2.24	15 (33%)
26	PEB	DD	203	2	43,46,46	3.39	10 (23%)	45,67,67	1.99	16 (35%)
26	PEB	KG	201	2,1	43,46,46	3.11	10 (23%)	45,67,67	2.52	14 (31%)
28	CYC	L2	1001	10	42,46,46	3.18	16 (38%)	50,67,67	2.97	22 (44%)
26	PEB	l4	202	2	43,46,46	3.63	11 (25%)	45,67,67	2.06	13 (28%)
27	PUB	A6	302	7	42,46,46	3.39	9 (21%)	37,67,67	3.30	16 (43%)
26	PEB	YA	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.31	16 (35%)
26	PEB	AD	201	1	43,46,46	3.47	12 (27%)	45,67,67	2.30	17 (37%)
26	PEB	gI	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	fG	202	2	43,46,46	3.60	12 (27%)	45,67,67	2.01	18 (40%)
27	PUB	21	402	3	42,46,46	3.49	8 (19%)	37,67,67	3.50	17 (45%)
26	PEB	LD	201	2,26	43,46,46	3.44	11 (25%)	45,67,67	2.25	15 (33%)
26	PEB	A3	202	1	43,46,46	3.49	11 (25%)	45,67,67	2.19	13 (28%)
26	PEB	KG	202	1	43,46,46	3.33	11 (25%)	45,67,67	2.36	16 (35%)
26	PEB	24	404	3	43,46,46	3.42	11 (25%)	45,67,67	2.73	16 (35%)
26	PEB	vG	202	2	43,46,46	3.49	10 (23%)	45,67,67	1.96	16 (35%)
26	PEB	d8	202	1	43,46,46	3.21	10 (23%)	45,67,67	2.22	15 (33%)
26	PEB	K3	202	1	43,46,46	3.43	9 (20%)	45,67,67	1.88	14 (31%)
26	PEB	AD	202	1	43,46,46	3.44	11 (25%)	45,67,67	1.98	12 (26%)
26	PEB	X3	201	2,11	43,46,46	3.64	11 (25%)	45,67,67	2.37	18 (40%)
26	PEB	C5	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.15	14 (31%)
26	PEB	21	404	3	43,46,46	3.40	11 (25%)	45,67,67	2.36	15 (33%)
26	PEB	U7	203	1	43,46,46	3.34	10 (23%)	45,67,67	2.25	15 (33%)
26	PEB	C4	202	1	43,46,46	3.46	10 (23%)	45,67,67	1.87	13 (28%)
28	CYC	LB	1001	10	42,46,46	3.22	15 (35%)	50,67,67	3.12	22 (44%)
26	PEB	TA	202	2	43,46,46	3.17	10 (23%)	45,67,67	2.36	16 (35%)
26	PEB	OE	202	1	43,46,46	3.07	10 (23%)	45,67,67	2.19	17 (37%)
26	PEB	LA	202	2	43,46,46	3.34	11 (25%)	45,67,67	2.64	18 (40%)
26	PEB	S2	201	1	43,46,46	3.42	11 (25%)	45,67,67	2.60	20 (44%)
26	PEB	HJ	201	2,1	43,46,46	3.14	10 (23%)	45,67,67	2.49	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	lA	202	1	43,46,46	3.27	10 (23%)	45,67,67	2.32	15 (33%)
26	PEB	UG	202	1	43,46,46	3.23	9 (20%)	45,67,67	2.16	13 (28%)
26	PEB	V8	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.52	18 (40%)
26	PEB	eA	201	2,13	43,46,46	3.32	10 (23%)	45,67,67	2.37	16 (35%)
26	PEB	x1	202	1	43,46,46	3.28	10 (23%)	45,67,67	2.88	17 (37%)
26	PEB	MJ	202	2	43,46,46	3.27	9 (20%)	45,67,67	2.03	14 (31%)
26	PEB	l1	202	2	43,46,46	3.51	11 (25%)	45,67,67	2.42	15 (33%)
27	PUB	A1	203	3,1	42,46,46	3.63	7 (16%)	37,67,67	3.36	17 (45%)
26	PEB	BC	201	2	43,46,46	3.50	10 (23%)	45,67,67	1.90	14 (31%)
26	PEB	jA	203	2,1	43,46,46	3.23	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	lB	203	1	43,46,46	3.44	10 (23%)	45,67,67	1.97	16 (35%)
26	PEB	GE	201	2,1	43,46,46	3.03	13 (30%)	45,67,67	3.31	19 (42%)
26	PEB	YB	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.38	17 (37%)
26	PEB	X4	203	1	43,46,46	3.20	11 (25%)	45,67,67	2.14	14 (31%)
26	PEB	hF	203	2,1	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
26	PEB	H4	203	2	43,46,46	3.54	11 (25%)	45,67,67	2.11	14 (31%)
26	PEB	s4	202	2	43,46,46	3.55	11 (25%)	45,67,67	2.38	15 (33%)
28	CYC	l7	1001	9,10	42,46,46	3.21	13 (30%)	50,67,67	2.85	18 (36%)
26	PEB	CE	201	2,1	43,46,46	3.16	13 (30%)	45,67,67	3.51	17 (37%)
27	PUB	A6	303	7	42,46,46	3.44	7 (16%)	37,67,67	3.00	14 (37%)
26	PEB	jG	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.16	13 (28%)
26	PEB	zE	501	2,16	43,46,46	3.37	10 (23%)	45,67,67	3.37	15 (33%)
26	PEB	bB	202	1	43,46,46	3.48	10 (23%)	45,67,67	2.36	15 (33%)
26	PEB	ED	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	Y4	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	Q1	201	2	43,46,46	3.40	12 (27%)	45,67,67	2.34	21 (46%)
26	PEB	VG	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.64	18 (40%)
26	PEB	T9	202	1	43,46,46	3.44	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	jE	201	2	43,46,46	3.29	9 (20%)	45,67,67	2.72	18 (40%)
26	PEB	QF	203	1	43,46,46	3.29	10 (23%)	45,67,67	2.07	14 (31%)
28	CYC	DF	1001	10	42,46,46	3.36	15 (35%)	50,67,67	2.85	18 (36%)
26	PEB	fF	203	2,1	43,46,46	3.46	11 (25%)	45,67,67	2.21	15 (33%)
26	PEB	D8	201	14,2	43,46,46	3.41	11 (25%)	45,67,67	2.47	13 (28%)
26	PEB	u4	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.44	13 (28%)
28	CYC	LI	1001	10	42,46,46	3.13	16 (38%)	50,67,67	2.97	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	dB	203	1	43,46,46	3.51	12 (27%)	45,67,67	2.04	15 (33%)
26	PEB	PA	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.51	16 (35%)
26	PEB	AI	301	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	14 (31%)
26	PEB	hI	201	1	43,46,46	3.41	11 (25%)	45,67,67	2.34	18 (40%)
27	PUB	AI	302	7	42,46,46	3.45	7 (16%)	37,67,67	3.14	16 (43%)
26	PEB	sE	203	2,1	43,46,46	3.40	13 (30%)	45,67,67	2.37	14 (31%)
26	PEB	R8	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.18	17 (37%)
26	PEB	W8	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.40	19 (42%)
26	PEB	UG	201	1	43,46,46	2.76	10 (23%)	45,67,67	2.99	16 (35%)
28	CYC	YH	1003	22	42,46,46	3.48	15 (35%)	50,67,67	2.89	20 (40%)
26	PEB	B3	201	2,26	43,46,46	3.37	9 (20%)	45,67,67	2.23	16 (35%)
26	PEB	DG	201	2	43,46,46	3.26	8 (18%)	45,67,67	3.08	17 (37%)
26	PEB	cI	201	2	43,46,46	3.38	10 (23%)	45,67,67	1.98	15 (33%)
26	PEB	JA	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.20	16 (35%)
28	CYC	GI	1001	9	42,46,46	3.31	14 (33%)	50,67,67	2.92	19 (38%)
26	PEB	MJ	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	P4	202	1	43,46,46	3.37	11 (25%)	45,67,67	2.08	17 (37%)
26	PEB	GG	203	1	43,46,46	3.40	11 (25%)	45,67,67	2.65	22 (48%)
28	CYC	G2	1001	9	42,46,46	3.26	14 (33%)	50,67,67	2.91	16 (32%)
26	PEB	HA	202	2	43,46,46	3.42	13 (30%)	45,67,67	2.45	15 (33%)
26	PEB	w4	203	2	43,46,46	3.51	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	cI	202	2	43,46,46	3.48	12 (27%)	45,67,67	2.37	14 (31%)
26	PEB	eG	203	1	43,46,46	3.36	10 (23%)	45,67,67	2.16	13 (28%)
26	PEB	CC	202	-	43,46,46	3.45	10 (23%)	45,67,67	2.21	14 (31%)
26	PEB	a6	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.16	20 (44%)
28	CYC	K6	202	9,10	42,46,46	3.19	14 (33%)	50,67,67	2.74	19 (38%)
26	PEB	u1	201	3,2	43,46,46	3.27	10 (23%)	45,67,67	2.49	21 (46%)
26	PEB	H5	203	2	43,46,46	3.14	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	ND	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	eB	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.01	16 (35%)
27	PUB	yE	303	14	42,46,46	3.37	7 (16%)	37,67,67	3.09	13 (35%)
26	PEB	H4	202	2	43,46,46	3.31	11 (25%)	45,67,67	2.42	17 (37%)
26	PEB	k8	201	2	43,46,46	3.40	9 (20%)	45,67,67	2.48	14 (31%)
26	PEB	R7	201	2	43,46,46	3.44	11 (25%)	45,67,67	2.04	16 (35%)
26	PEB	L8	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.73	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	KF	1001	9,10	42,46,46	3.17	11 (26%)	50,67,67	2.93	22 (44%)
26	PEB	RG	201	2	43,46,46	3.28	10 (23%)	45,67,67	3.69	21 (46%)
26	PEB	y1	201	2	43,46,46	3.54	11 (25%)	45,67,67	2.04	17 (37%)
26	PEB	JC	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.10	14 (31%)
26	PEB	fA	201	1	43,46,46	3.35	10 (23%)	45,67,67	2.11	17 (37%)
26	PEB	V1	203	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.16	13 (28%)
26	PEB	UD	201	1	43,46,46	3.22	10 (23%)	45,67,67	2.61	13 (28%)
26	PEB	fB	201	1	43,46,46	3.32	10 (23%)	45,67,67	2.11	17 (37%)
26	PEB	FA	202	2	43,46,46	3.32	12 (27%)	45,67,67	2.48	18 (40%)
26	PEB	R4	203	2,1	43,46,46	3.49	13 (30%)	45,67,67	1.96	13 (28%)
26	PEB	V2	202	2	43,46,46	3.15	10 (23%)	45,67,67	2.33	14 (31%)
26	PEB	GC	203	2	43,46,46	3.47	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	W4	201	2	43,46,46	3.52	12 (27%)	45,67,67	2.34	21 (46%)
28	CYC	L7	1001	10	42,46,46	3.36	14 (33%)	50,67,67	2.77	20 (40%)
26	PEB	iI	203	2	43,46,46	3.53	12 (27%)	45,67,67	1.90	14 (31%)
26	PEB	uG	203	1	43,46,46	3.45	11 (25%)	45,67,67	1.98	15 (33%)
26	PEB	Z7	203	1	43,46,46	3.43	11 (25%)	45,67,67	2.31	15 (33%)
26	PEB	fA	202	1	43,46,46	3.63	13 (30%)	45,67,67	1.99	13 (28%)
26	PEB	A6	301	7	43,46,46	3.34	11 (25%)	45,67,67	2.35	16 (35%)
26	PEB	fI	201	2	43,46,46	3.55	13 (30%)	45,67,67	2.13	17 (37%)
28	CYC	C2	1001	9	42,46,46	3.25	15 (35%)	50,67,67	2.93	21 (42%)
26	PEB	A5	202	2	43,46,46	3.56	12 (27%)	45,67,67	1.84	12 (26%)
26	PEB	IE	201	1	43,46,46	2.80	13 (30%)	45,67,67	2.85	18 (40%)
26	PEB	KD	202	1	43,46,46	3.44	10 (23%)	45,67,67	1.81	11 (24%)
26	PEB	c6	202	2	43,46,46	3.47	11 (25%)	45,67,67	1.99	13 (28%)
26	PEB	dE	201	2	43,46,46	3.48	10 (23%)	45,67,67	2.35	16 (35%)
26	PEB	WE	201	2,1	43,46,46	3.14	13 (30%)	45,67,67	2.85	20 (44%)
26	PEB	aE	202	1	43,46,46	3.10	9 (20%)	45,67,67	2.66	12 (26%)
26	PEB	G4	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.26	19 (42%)
26	PEB	l8	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.36	15 (33%)
26	PEB	U2	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.87	11 (24%)
27	PUB	AF	304	7	42,46,46	3.73	8 (19%)	37,67,67	3.97	17 (45%)
26	PEB	Q6	202	1	43,46,46	3.44	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	EG	202	1	43,46,46	3.37	11 (25%)	45,67,67	2.01	16 (35%)
26	PEB	R3	202	2	43,46,46	3.02	11 (25%)	45,67,67	3.00	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	QI	201	1	43,46,46	3.31	11 (25%)	45,67,67	2.70	20 (44%)
26	PEB	RB	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	cF	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	t1	202	1	43,46,46	3.68	10 (23%)	45,67,67	2.56	16 (35%)
26	PEB	F9	202	1	43,46,46	3.42	12 (27%)	45,67,67	2.00	15 (33%)
26	PEB	QA	204	1	43,46,46	3.21	10 (23%)	45,67,67	2.13	15 (33%)
28	CYC	MB	1001	9,10	42,46,46	3.16	14 (33%)	50,67,67	2.90	19 (38%)
26	PEB	QB	201	2,1	43,46,46	3.15	11 (25%)	45,67,67	2.73	17 (37%)
26	PEB	cE	201	1	43,46,46	2.91	10 (23%)	45,67,67	2.56	14 (31%)
26	PEB	E9	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.07	14 (31%)
26	PEB	PE	202	2	43,46,46	3.59	11 (25%)	45,67,67	2.06	15 (33%)
26	PEB	h7	201	2,1	43,46,46	3.30	10 (23%)	45,67,67	2.38	15 (33%)
26	PEB	TF	202	2	43,46,46	3.32	9 (20%)	45,67,67	1.81	13 (28%)
26	PEB	TD	202	2	43,46,46	2.76	9 (20%)	45,67,67	2.99	19 (42%)
26	PEB	Q7	201	2,1	43,46,46	3.24	11 (25%)	45,67,67	2.36	16 (35%)
26	PEB	kE	201	1	43,46,46	3.36	11 (25%)	45,67,67	2.31	16 (35%)
26	PEB	g1	201	1	43,46,46	3.36	10 (23%)	45,67,67	2.28	15 (33%)
26	PEB	P6	201	2,6	43,46,46	3.36	10 (23%)	45,67,67	2.23	18 (40%)
26	PEB	14	202	2	43,46,46	3.52	12 (27%)	45,67,67	2.32	14 (31%)
26	PEB	LE	201	2	43,46,46	3.34	8 (18%)	45,67,67	3.85	16 (35%)
28	CYC	nH	1001	-	42,46,46	3.48	14 (33%)	50,67,67	3.02	20 (40%)
26	PEB	BE	201	2,16	43,46,46	3.35	10 (23%)	45,67,67	3.49	16 (35%)
26	PEB	T2	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.38	15 (33%)
26	PEB	cA	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.59	15 (33%)
26	PEB	k2	201	2	43,46,46	3.33	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	eG	201	2,1	43,46,46	3.42	13 (30%)	45,67,67	2.23	17 (37%)
26	PEB	FD	201	2,7	43,46,46	3.43	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	b6	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.13	13 (28%)
26	PEB	d8	201	2,1	43,46,46	3.53	12 (27%)	45,67,67	2.37	13 (28%)
26	PEB	cB	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	19 (42%)
26	PEB	W7	202	1	43,46,46	3.43	10 (23%)	45,67,67	2.56	17 (37%)
26	PEB	OD	202	1	43,46,46	3.25	10 (23%)	45,67,67	1.98	15 (33%)
26	PEB	R4	202	1	43,46,46	3.32	8 (18%)	45,67,67	1.96	12 (26%)
26	PEB	iE	202	1	43,46,46	3.27	10 (23%)	45,67,67	2.32	14 (31%)
27	PUB	K3	203	1,7	42,46,46	3.41	7 (16%)	37,67,67	3.21	15 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	WH	1001	-	42,46,46	3.56	14 (33%)	50,67,67	2.88	19 (38%)
27	PUB	xE	305	13	42,46,46	3.40	8 (19%)	37,67,67	3.08	14 (37%)
26	PEB	S1	201	2,4	43,46,46	3.45	12 (27%)	45,67,67	2.27	18 (40%)
27	PUB	K4	203	3,1	42,46,46	3.49	7 (16%)	37,67,67	3.32	19 (51%)
26	PEB	XG	202	2	43,46,46	3.25	12 (27%)	45,67,67	2.63	16 (35%)
26	PEB	y4	203	2	43,46,46	3.51	11 (25%)	45,67,67	2.28	11 (24%)
26	PEB	SJ	201	2,7	43,46,46	3.39	9 (20%)	45,67,67	2.10	10 (22%)
26	PEB	h6	203	1	43,46,46	3.32	10 (23%)	45,67,67	2.00	13 (28%)
26	PEB	wG	302	13	43,46,46	3.30	9 (20%)	45,67,67	2.22	15 (33%)
26	PEB	BD	202	2	43,46,46	3.49	11 (25%)	45,67,67	3.06	18 (40%)
26	PEB	dF	201	2,1	43,46,46	3.26	9 (20%)	45,67,67	2.35	14 (31%)
26	PEB	RA	201	2	43,46,46	3.47	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	a8	203	1	43,46,46	3.13	10 (23%)	45,67,67	2.35	14 (31%)
26	PEB	PJ	202	1	43,46,46	3.50	10 (23%)	45,67,67	2.07	16 (35%)
26	PEB	M8	203	1	43,46,46	3.26	10 (23%)	45,67,67	2.27	15 (33%)
26	PEB	B5	201	2	43,46,46	3.48	11 (25%)	45,67,67	1.93	12 (26%)
26	PEB	O6	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.23	15 (33%)
26	PEB	R3	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.22	17 (37%)
28	CYC	DF	1003	9,10	42,46,46	3.14	12 (28%)	50,67,67	2.94	20 (40%)
26	PEB	GA	203	2,1	43,46,46	3.30	12 (27%)	45,67,67	2.55	14 (31%)
26	PEB	DI	1002	10	43,46,46	3.33	10 (23%)	45,67,67	2.19	17 (37%)
26	PEB	d1	203	2	43,46,46	3.45	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	CJ	201	2,7	43,46,46	3.09	11 (25%)	45,67,67	2.51	21 (46%)
26	PEB	ZB	203	1	43,46,46	3.33	10 (23%)	45,67,67	2.12	15 (33%)
28	CYC	oH	1001	18	42,46,46	3.43	15 (35%)	50,67,67	2.87	21 (42%)
26	PEB	D9	203	1	43,46,46	3.27	10 (23%)	45,67,67	2.25	15 (33%)
26	PEB	U8	201	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.44	15 (33%)
26	PEB	H3	203	2	43,46,46	3.55	12 (27%)	45,67,67	2.41	16 (35%)
27	PUB	Y3	302	7	42,46,46	3.56	8 (19%)	37,67,67	3.05	15 (40%)
26	PEB	PG	201	2	43,46,46	3.34	9 (20%)	45,67,67	3.22	18 (40%)
26	PEB	bG	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.08	15 (33%)
26	PEB	AF	302	7	43,46,46	3.39	10 (23%)	45,67,67	1.95	12 (26%)
27	PUB	21	403	3,1	42,46,46	3.47	7 (16%)	37,67,67	3.31	16 (43%)
26	PEB	IJ	203	2	43,46,46	3.39	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	OD	201	1	43,46,46	3.10	10 (23%)	45,67,67	2.81	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	RE	201	2	43,46,46	3.32	10 (23%)	45,67,67	3.60	19 (42%)
26	PEB	l7	203	1	43,46,46	3.35	12 (27%)	45,67,67	2.73	15 (33%)
26	PEB	DA	202	2	43,46,46	3.24	12 (27%)	45,67,67	2.74	19 (42%)
27	PUB	xE	301	13	42,46,46	3.39	7 (16%)	37,67,67	3.19	19 (51%)
28	CYC	LH	1001	-	42,46,46	3.45	14 (33%)	50,67,67	3.04	22 (44%)
26	PEB	X1	201	2,1	43,46,46	3.35	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	S3	201	1	43,46,46	3.11	10 (23%)	45,67,67	2.78	17 (37%)
26	PEB	W6	203	2,1	43,46,46	3.15	10 (23%)	45,67,67	2.28	16 (35%)
26	PEB	A9	303	7,26	43,46,46	3.45	11 (25%)	45,67,67	2.28	17 (37%)
26	PEB	HC	202	2	43,46,46	3.31	10 (23%)	45,67,67	1.99	13 (28%)
26	PEB	DF	1002	10	43,46,46	3.33	11 (25%)	45,67,67	2.14	15 (33%)
26	PEB	kF	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.10	16 (35%)
26	PEB	y1	203	2	43,46,46	3.45	11 (25%)	45,67,67	2.45	15 (33%)
26	PEB	c4	201	1	43,46,46	3.47	9 (20%)	45,67,67	2.22	15 (33%)
26	PEB	jF	202	1	43,46,46	3.41	12 (27%)	45,67,67	2.63	16 (35%)
26	PEB	rE	201	2,13	43,46,46	3.47	11 (25%)	45,67,67	2.31	16 (35%)
26	PEB	S8	202	1	43,46,46	3.27	11 (25%)	45,67,67	1.90	14 (31%)
26	PEB	PI	203	2	43,46,46	3.34	8 (18%)	45,67,67	1.85	13 (28%)
26	PEB	a8	202	1	43,46,46	3.21	10 (23%)	45,67,67	2.09	16 (35%)
26	PEB	AA	302	13	43,46,46	3.36	10 (23%)	45,67,67	2.82	18 (40%)
26	PEB	f2	202	1	43,46,46	3.49	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	h2	201	1	43,46,46	3.39	12 (27%)	45,67,67	2.31	20 (44%)
26	PEB	f7	201	1	43,46,46	3.50	13 (30%)	45,67,67	1.96	15 (33%)
26	PEB	l4	203	2	43,46,46	3.46	9 (20%)	45,67,67	1.83	12 (26%)
26	PEB	l1	202	1	43,46,46	3.40	10 (23%)	45,67,67	1.88	12 (26%)
26	PEB	h8	201	2,1	43,46,46	3.34	12 (27%)	45,67,67	2.56	15 (33%)
26	PEB	H1	203	2	43,46,46	3.51	10 (23%)	45,67,67	2.15	14 (31%)
26	PEB	YE	203	2,1	43,46,46	3.41	12 (27%)	45,67,67	2.15	14 (31%)
26	PEB	G1	202	1	43,46,46	3.44	11 (25%)	45,67,67	1.94	14 (31%)
26	PEB	m8	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.49	17 (37%)
26	PEB	V1	201	1	43,46,46	3.49	11 (25%)	45,67,67	1.96	15 (33%)
26	PEB	f4	201	2	43,46,46	3.50	13 (30%)	45,67,67	2.23	15 (33%)
26	PEB	P4	203	1	43,46,46	3.60	12 (27%)	45,67,67	1.71	10 (22%)
28	CYC	NH	1001	17	42,46,46	3.46	15 (35%)	50,67,67	2.93	23 (46%)
26	PEB	A4	201	1	43,46,46	3.37	10 (23%)	45,67,67	2.41	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PUB	A2	303	7	42,46,46	3.40	7 (16%)	37,67,67	2.99	14 (37%)
26	PEB	QJ	202	2	43,46,46	3.51	11 (25%)	45,67,67	2.11	17 (37%)
26	PEB	k1	201	1	43,46,46	3.48	10 (23%)	45,67,67	2.06	17 (37%)
26	PEB	IA	201	2,1	43,46,46	3.41	12 (27%)	45,67,67	2.31	14 (31%)
26	PEB	JD	203	2	43,46,46	3.39	10 (23%)	45,67,67	2.30	14 (31%)
26	PEB	hA	201	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.47	15 (33%)
26	PEB	iF	201	2	43,46,46	3.34	12 (27%)	45,67,67	2.05	16 (35%)
26	PEB	gA	201	2	43,46,46	3.46	11 (25%)	45,67,67	2.26	16 (35%)
26	PEB	GE	203	1	43,46,46	3.31	10 (23%)	45,67,67	2.16	17 (37%)
26	PEB	a1	203	2	43,46,46	3.34	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	jG	201	2	43,46,46	3.33	11 (25%)	45,67,67	2.84	18 (40%)
26	PEB	dB	204	1	43,46,46	3.42	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	h4	201	2,4	43,46,46	3.55	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	PF	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.00	17 (37%)
26	PEB	J9	203	2,1	43,46,46	3.21	12 (27%)	45,67,67	2.23	12 (26%)
26	PEB	m7	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	A1	202	1	43,46,46	3.51	12 (27%)	45,67,67	1.88	14 (31%)
28	CYC	I6	1001	9,10	42,46,46	3.18	13 (30%)	50,67,67	2.82	18 (36%)
26	PEB	gE	201	1	43,46,46	3.10	11 (25%)	45,67,67	2.73	19 (42%)
26	PEB	iE	201	2,1	43,46,46	3.37	11 (25%)	45,67,67	2.42	16 (35%)
26	PEB	QF	202	1	43,46,46	3.39	12 (27%)	45,67,67	2.50	17 (37%)
26	PEB	AJ	301	7	43,46,46	3.30	9 (20%)	45,67,67	2.05	17 (37%)
26	PEB	pE	202	2	43,46,46	3.66	12 (27%)	45,67,67	2.48	11 (24%)
26	PEB	U6	202	1	43,46,46	3.48	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	V3	203	2	43,46,46	3.57	12 (27%)	45,67,67	2.00	15 (33%)
28	CYC	G6	1001	9,10	42,46,46	3.18	13 (30%)	50,67,67	2.89	19 (38%)
26	PEB	FC	202	2	43,46,46	3.25	10 (23%)	45,67,67	1.95	12 (26%)
26	PEB	DG	202	2,1	43,46,46	3.15	10 (23%)	45,67,67	2.68	16 (35%)
26	PEB	v4	201	1	43,46,46	3.53	12 (27%)	45,67,67	2.11	14 (31%)
26	PEB	RJ	202	1	43,46,46	3.30	10 (23%)	45,67,67	1.99	14 (31%)
26	PEB	g6	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.02	16 (35%)
26	PEB	QB	202	1	43,46,46	3.40	10 (23%)	45,67,67	2.13	14 (31%)
26	PEB	L1	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.56	16 (35%)
26	PEB	i6	202	2	43,46,46	3.47	10 (23%)	45,67,67	2.02	15 (33%)
26	PEB	m2	203	2	43,46,46	3.46	13 (30%)	45,67,67	2.15	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	i7	202	2	43,46,46	3.43	10 (23%)	45,67,67	2.16	13 (28%)
26	PEB	a1	202	2	43,46,46	3.50	12 (27%)	45,67,67	1.99	12 (26%)
26	PEB	s1	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.15	15 (33%)
26	PEB	e3	401	1,11	43,46,46	3.38	10 (23%)	45,67,67	1.95	15 (33%)
26	PEB	L9	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.26	14 (31%)
26	PEB	dE	202	2	43,46,46	3.64	11 (25%)	45,67,67	2.00	14 (31%)
28	CYC	QH	1001	22,18	42,46,46	3.43	14 (33%)	50,67,67	2.90	18 (36%)
26	PEB	ZI	202	1	43,46,46	3.30	10 (23%)	45,67,67	1.94	12 (26%)
26	PEB	LG	201	2	43,46,46	3.36	11 (25%)	45,67,67	3.50	19 (42%)
26	PEB	aG	202	1	43,46,46	3.27	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	eA	202	2	43,46,46	3.26	11 (25%)	45,67,67	2.61	19 (42%)
26	PEB	xE	302	13	43,46,46	3.37	11 (25%)	45,67,67	2.95	15 (33%)
26	PEB	m4	202	1	43,46,46	3.46	12 (27%)	45,67,67	2.16	16 (35%)
26	PEB	YJ	202	2	43,46,46	3.47	9 (20%)	45,67,67	2.00	14 (31%)
27	PUB	N9	201	1,7	42,46,46	3.76	9 (21%)	37,67,67	3.15	12 (32%)
26	PEB	A8	301	13	43,46,46	3.20	11 (25%)	45,67,67	2.28	15 (33%)
26	PEB	JD	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.75	16 (35%)
26	PEB	c1	201	1	43,46,46	3.42	9 (20%)	45,67,67	2.10	14 (31%)
26	PEB	C9	202	2	43,46,46	3.45	10 (23%)	45,67,67	1.99	15 (33%)
26	PEB	R1	202	1	43,46,46	3.37	10 (23%)	45,67,67	1.86	13 (28%)
26	PEB	U1	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.09	16 (35%)
28	CYC	gH	1001	17	42,46,46	3.48	14 (33%)	50,67,67	2.95	21 (42%)
26	PEB	b4	501	2,4	43,46,46	3.47	10 (23%)	45,67,67	2.24	14 (31%)
26	PEB	UF	202	1	43,46,46	3.29	12 (27%)	45,67,67	2.13	16 (35%)
26	PEB	fE	201	2,13	43,46,46	3.43	10 (23%)	45,67,67	3.05	16 (35%)
26	PEB	DB	1002	9,10	43,46,46	3.34	12 (27%)	45,67,67	2.13	15 (33%)
26	PEB	G5	202	2	43,46,46	3.37	9 (20%)	45,67,67	1.94	13 (28%)
26	PEB	IA	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.36	17 (37%)
26	PEB	SF	201	1	43,46,46	3.31	12 (27%)	45,67,67	2.37	14 (31%)
28	CYC	qH	1001	-	42,46,46	3.47	15 (35%)	50,67,67	2.92	21 (42%)
26	PEB	TG	202	2	43,46,46	3.43	12 (27%)	45,67,67	2.22	17 (37%)
26	PEB	TE	201	2	43,46,46	3.32	8 (18%)	45,67,67	2.97	15 (33%)
26	PEB	QA	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.23	15 (33%)
26	PEB	w1	201	3,2	43,46,46	3.58	11 (25%)	45,67,67	2.25	14 (31%)
26	PEB	aB	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.39	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PUB	AF	303	7	42,46,46	3.60	8 (19%)	37,67,67	3.20	15 (40%)
26	PEB	U9	201	2,7	43,46,46	3.51	11 (25%)	45,67,67	2.13	17 (37%)
26	PEB	HG	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.37	16 (35%)
26	PEB	iI	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.31	14 (31%)
26	PEB	I3	202	1	43,46,46	3.45	11 (25%)	45,67,67	1.87	13 (28%)
26	PEB	A7	301	7	43,46,46	3.43	12 (27%)	45,67,67	2.80	14 (31%)
26	PEB	YG	202	1	43,46,46	3.41	10 (23%)	45,67,67	1.89	13 (28%)
26	PEB	wE	301	13	43,46,46	3.27	10 (23%)	45,67,67	2.21	15 (33%)
28	CYC	TH	1001	17	42,46,46	3.43	15 (35%)	50,67,67	2.90	19 (38%)
26	PEB	KD	201	1	43,46,46	3.26	11 (25%)	45,67,67	2.48	17 (37%)
27	PUB	xG	301	13	42,46,46	3.25	8 (19%)	37,67,67	3.35	19 (51%)
26	PEB	FE	201	2	43,46,46	3.48	10 (23%)	45,67,67	3.83	16 (35%)
26	PEB	T4	203	1	43,46,46	3.37	10 (23%)	45,67,67	2.04	14 (31%)
26	PEB	xE	304	13	43,46,46	3.44	11 (25%)	45,67,67	2.44	17 (37%)
26	PEB	D3	201	2,7	43,46,46	3.33	13 (30%)	45,67,67	2.12	13 (28%)
26	PEB	d6	201	1,7	43,46,46	3.35	8 (18%)	45,67,67	2.16	14 (31%)
26	PEB	kI	203	2	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
28	CYC	LF	1001	10	42,46,46	3.51	16 (38%)	50,67,67	3.08	24 (48%)
26	PEB	cE	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.07	14 (31%)
26	PEB	F3	202	2	43,46,46	3.28	10 (23%)	45,67,67	2.64	15 (33%)
26	PEB	C8	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.35	15 (33%)
26	PEB	w4	201	3,2	43,46,46	3.54	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	PA	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.32	17 (37%)
26	PEB	bG	202	2	43,46,46	3.62	9 (20%)	45,67,67	2.36	15 (33%)
26	PEB	RE	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.29	15 (33%)
26	PEB	aA	203	1	43,46,46	3.22	10 (23%)	45,67,67	2.19	14 (31%)
26	PEB	gG	202	1	43,46,46	3.34	10 (23%)	45,67,67	2.05	15 (33%)
26	PEB	D7	1002	10	43,46,46	3.37	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	UF	201	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.54	15 (33%)
26	PEB	j4	201	2,4	43,46,46	3.50	10 (23%)	45,67,67	1.88	14 (31%)
26	PEB	ZA	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.57	18 (40%)
26	PEB	P3	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.09	14 (31%)
26	PEB	Y8	203	1	43,46,46	3.21	10 (23%)	45,67,67	2.20	16 (35%)
26	PEB	D1	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.09	15 (33%)
26	PEB	s4	203	2	43,46,46	3.56	10 (23%)	45,67,67	1.96	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	RH	1001	17	42,46,46	3.35	14 (33%)	50,67,67	3.04	22 (44%)
26	PEB	P6	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.30	18 (40%)
26	PEB	C3	202	1	43,46,46	3.28	11 (25%)	45,67,67	2.02	12 (26%)
26	PEB	WB	202	1	43,46,46	3.29	9 (20%)	45,67,67	1.98	13 (28%)
26	PEB	jB	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.98	14 (31%)
26	PEB	e2	203	2	43,46,46	3.32	9 (20%)	45,67,67	1.95	12 (26%)
26	PEB	k2	203	2	43,46,46	3.49	10 (23%)	45,67,67	2.19	15 (33%)
26	PEB	bF	203	2,1	43,46,46	3.32	12 (27%)	45,67,67	2.58	16 (35%)
26	PEB	qE	202	1	43,46,46	3.50	12 (27%)	45,67,67	3.55	15 (33%)
26	PEB	LC	203	2	43,46,46	3.26	11 (25%)	45,67,67	2.11	15 (33%)
26	PEB	g4	202	1	43,46,46	3.47	11 (25%)	45,67,67	1.93	12 (26%)
26	PEB	LD	203	2	43,46,46	3.47	10 (23%)	45,67,67	1.81	13 (28%)
26	PEB	RI	203	2	43,46,46	3.44	10 (23%)	45,67,67	1.98	11 (24%)
26	PEB	IE	201	2	43,46,46	3.50	11 (25%)	45,67,67	2.65	17 (37%)
26	PEB	UE	201	1	43,46,46	2.80	10 (23%)	45,67,67	2.98	19 (42%)
26	PEB	D4	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.05	14 (31%)
26	PEB	W3	202	1	43,46,46	3.41	12 (27%)	45,67,67	2.08	15 (33%)
26	PEB	C4	201	1	43,46,46	3.44	10 (23%)	45,67,67	1.97	14 (31%)
28	CYC	UH	1001	-	42,46,46	3.37	15 (35%)	50,67,67	3.11	24 (48%)
26	PEB	LJ	203	1	43,46,46	3.37	9 (20%)	45,67,67	2.01	15 (33%)
26	PEB	N9	202	1	43,46,46	3.42	11 (25%)	45,67,67	1.83	12 (26%)
26	PEB	h6	202	1	43,46,46	3.37	11 (25%)	45,67,67	2.00	14 (31%)
26	PEB	d4	201	2	43,46,46	3.52	11 (25%)	45,67,67	1.94	15 (33%)
26	PEB	kB	201	2,7	43,46,46	3.40	12 (27%)	45,67,67	2.25	18 (40%)
26	PEB	WD	201	1	43,46,46	3.16	10 (23%)	45,67,67	2.30	15 (33%)
27	PUB	Q8	201	14,1	42,46,46	3.30	7 (16%)	37,67,67	3.36	18 (48%)
26	PEB	S1	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.07	16 (35%)
26	PEB	ZB	201	2,1	43,46,46	3.15	10 (23%)	45,67,67	2.45	17 (37%)
26	PEB	jA	202	1	43,46,46	3.52	10 (23%)	45,67,67	2.54	18 (40%)
26	PEB	JE	201	2	43,46,46	3.39	10 (23%)	45,67,67	3.30	17 (37%)
26	PEB	kI	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.37	14 (31%)
26	PEB	TJ	202	1	43,46,46	3.32	11 (25%)	45,67,67	2.07	15 (33%)
26	PEB	XG	201	2	43,46,46	3.38	10 (23%)	45,67,67	3.73	17 (37%)
26	PEB	dI	201	1	43,46,46	3.27	10 (23%)	45,67,67	2.20	16 (35%)
26	PEB	F3	201	2,7	43,46,46	3.46	11 (25%)	45,67,67	2.03	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	k4	203	2,1	43,46,46	3.27	10 (23%)	45,67,67	2.50	17 (37%)
26	PEB	YI	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.05	13 (28%)
26	PEB	d4	202	2,1	43,46,46	3.27	12 (27%)	45,67,67	2.41	13 (28%)
26	PEB	m1	201	2,1	43,46,46	3.18	11 (25%)	45,67,67	2.70	17 (37%)
26	PEB	O1	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.04	14 (31%)
26	PEB	fF	201	1	43,46,46	3.48	12 (27%)	45,67,67	1.99	14 (31%)
26	PEB	DD	202	2	43,46,46	3.22	11 (25%)	45,67,67	2.50	16 (35%)
28	CYC	vH	1001	17	42,46,46	3.45	15 (35%)	50,67,67	2.89	20 (40%)
26	PEB	YA	203	1	43,46,46	3.23	11 (25%)	45,67,67	2.16	14 (31%)
26	PEB	CC	203	2	43,46,46	3.50	11 (25%)	45,67,67	1.89	14 (31%)
26	PEB	aF	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.09	16 (35%)
26	PEB	ZE	202	2	43,46,46	3.59	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	H9	201	2,1	43,46,46	3.20	11 (25%)	45,67,67	2.43	16 (35%)
26	PEB	W1	202	2	43,46,46	3.49	12 (27%)	45,67,67	2.29	16 (35%)
26	PEB	N3	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.36	17 (37%)
26	PEB	e1	202	1	43,46,46	3.65	11 (25%)	45,67,67	2.21	15 (33%)
28	CYC	CB	1001	9,10	42,46,46	3.26	15 (35%)	50,67,67	2.74	17 (34%)
26	PEB	l2	202	1	43,46,46	3.38	12 (27%)	45,67,67	1.98	13 (28%)
26	PEB	J4	203	2	43,46,46	3.51	9 (20%)	45,67,67	1.95	13 (28%)
26	PEB	BC	203	2	43,46,46	3.51	12 (27%)	45,67,67	1.94	13 (28%)
26	PEB	sE	202	1	43,46,46	3.48	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	P1	201	2,1	43,46,46	3.31	12 (27%)	45,67,67	2.27	14 (31%)
26	PEB	E3	201	1	43,46,46	3.49	12 (27%)	45,67,67	2.29	15 (33%)
26	PEB	bF	202	1	43,46,46	3.53	11 (25%)	45,67,67	2.60	17 (37%)
26	PEB	mA	201	2,13	43,46,46	3.43	11 (25%)	45,67,67	2.50	19 (42%)
28	CYC	lH	1001	18,17	42,46,46	3.51	15 (35%)	50,67,67	2.98	23 (46%)
26	PEB	SA	201	1	43,46,46	3.26	10 (23%)	45,67,67	2.17	17 (37%)
26	PEB	jF	201	1	43,46,46	3.16	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	y4	201	2	43,46,46	3.46	11 (25%)	45,67,67	2.13	20 (44%)
26	PEB	oE	203	2,1	43,46,46	3.37	12 (27%)	45,67,67	2.57	16 (35%)
26	PEB	m6	203	2	43,46,46	3.48	11 (25%)	45,67,67	1.96	15 (33%)
26	PEB	h6	201	2,1	43,46,46	3.61	13 (30%)	45,67,67	2.56	10 (22%)
26	PEB	L4	201	3,2	43,46,46	3.49	12 (27%)	45,67,67	2.05	16 (35%)
26	PEB	PB	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.27	17 (37%)
27	PUB	QA	201	14,1	42,46,46	3.35	8 (19%)	37,67,67	3.56	16 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	Z8	201	2	43,46,46	3.19	10 (23%)	45,67,67	2.50	17 (37%)
26	PEB	HE	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.36	16 (35%)
26	PEB	GG	202	1	43,46,46	2.62	11 (25%)	45,67,67	3.01	20 (44%)
26	PEB	k4	201	1	43,46,46	3.48	11 (25%)	45,67,67	2.05	15 (33%)
26	PEB	G6	1002	9,10	43,46,46	3.23	10 (23%)	45,67,67	2.30	17 (37%)
26	PEB	RF	202	2	43,46,46	3.51	11 (25%)	45,67,67	1.72	10 (22%)
26	PEB	OF	203	2,1	43,46,46	3.25	10 (23%)	45,67,67	2.41	14 (31%)
26	PEB	eG	202	1	43,46,46	3.13	10 (23%)	45,67,67	2.25	20 (44%)
26	PEB	cF	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.32	16 (35%)
28	CYC	B6	1002	8,10	42,46,46	3.22	15 (35%)	50,67,67	2.91	23 (46%)
26	PEB	P7	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.06	15 (33%)
26	PEB	RD	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.24	19 (42%)
26	PEB	SG	201	2,1	43,46,46	3.22	11 (25%)	45,67,67	2.57	15 (33%)
26	PEB	aA	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.04	15 (33%)
27	PUB	YD	302	7	42,46,46	3.53	8 (19%)	37,67,67	3.04	16 (43%)
26	PEB	F1	203	2	43,46,46	3.36	10 (23%)	45,67,67	1.89	14 (31%)
26	PEB	mI	203	2	43,46,46	3.47	13 (30%)	45,67,67	2.18	14 (31%)
26	PEB	N1	203	2,1	43,46,46	3.45	11 (25%)	45,67,67	2.06	13 (28%)
26	PEB	WG	202	1	43,46,46	3.31	11 (25%)	45,67,67	2.28	18 (40%)
26	PEB	YI	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.34	15 (33%)
26	PEB	aE	203	1	43,46,46	3.40	11 (25%)	45,67,67	2.07	15 (33%)
26	PEB	G1	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.11	19 (42%)
27	PUB	AI	303	7	42,46,46	3.40	7 (16%)	37,67,67	3.00	14 (37%)
26	PEB	JJ	203	2,1	43,46,46	3.20	13 (30%)	45,67,67	2.26	13 (28%)
26	PEB	q1	201	2	43,46,46	3.50	11 (25%)	45,67,67	2.27	19 (42%)
26	PEB	X4	202	1	43,46,46	3.37	10 (23%)	45,67,67	2.59	16 (35%)
26	PEB	WA	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.40	18 (40%)
26	PEB	V1	202	1	43,46,46	3.25	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	V9	203	2,1	43,46,46	3.28	13 (30%)	45,67,67	2.38	13 (28%)
26	PEB	CA	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.22	18 (40%)
26	PEB	bI	202	1	43,46,46	3.43	11 (25%)	45,67,67	1.99	13 (28%)
26	PEB	d2	202	1	43,46,46	3.39	10 (23%)	45,67,67	1.88	12 (26%)
28	CYC	DB	1001	10	42,46,46	3.19	14 (33%)	50,67,67	3.00	21 (42%)
26	PEB	TD	203	2	43,46,46	3.31	10 (23%)	45,67,67	2.26	17 (37%)
26	PEB	GC	202	2	43,46,46	3.40	9 (20%)	45,67,67	1.93	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	i1	201	2,1	43,46,46	3.37	13 (30%)	45,67,67	2.28	14 (31%)
28	CYC	II	1001	9	42,46,46	3.20	13 (30%)	50,67,67	2.82	20 (40%)
26	PEB	A9	301	7	43,46,46	3.30	9 (20%)	45,67,67	1.99	16 (35%)
26	PEB	JC	201	1	43,46,46	3.39	11 (25%)	45,67,67	2.78	16 (35%)
26	PEB	G9	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	W9	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.97	16 (35%)
26	PEB	HJ	203	1	43,46,46	3.41	10 (23%)	45,67,67	2.25	14 (31%)
26	PEB	E8	202	1	43,46,46	3.41	11 (25%)	45,67,67	2.27	12 (26%)
26	PEB	AJ	304	7,26	43,46,46	3.51	11 (25%)	45,67,67	2.61	14 (31%)
26	PEB	E4	202	1	43,46,46	3.45	12 (27%)	45,67,67	1.77	12 (26%)
26	PEB	F5	203	2	43,46,46	3.37	11 (25%)	45,67,67	1.87	13 (28%)
26	PEB	eD	401	1,11	43,46,46	3.36	10 (23%)	45,67,67	1.96	13 (28%)
26	PEB	G8	201	1	43,46,46	3.30	11 (25%)	45,67,67	2.37	17 (37%)
26	PEB	VB	202	2	43,46,46	3.43	10 (23%)	45,67,67	2.19	15 (33%)
26	PEB	A1	201	1	43,46,46	3.42	14 (32%)	45,67,67	2.17	17 (37%)
26	PEB	W7	203	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.22	15 (33%)
26	PEB	H8	202	2	43,46,46	3.39	12 (27%)	45,67,67	2.59	17 (37%)
26	PEB	IC	203	2	43,46,46	3.37	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	Z6	202	1	43,46,46	3.35	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	PI	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.22	17 (37%)
26	PEB	K8	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.26	18 (40%)
26	PEB	Y8	201	2,1	43,46,46	3.07	10 (23%)	45,67,67	2.56	17 (37%)
26	PEB	YF	201	2	43,46,46	3.51	11 (25%)	45,67,67	2.31	18 (40%)
26	PEB	g6	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.50	13 (28%)
28	CYC	uH	1001	18	42,46,46	3.27	13 (30%)	50,67,67	3.25	26 (52%)
26	PEB	mE	203	1	43,46,46	3.48	12 (27%)	45,67,67	1.93	14 (31%)
26	PEB	14	201	2	43,46,46	3.63	11 (25%)	45,67,67	2.02	15 (33%)
26	PEB	a2	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.31	16 (35%)
26	PEB	t1	201	1	43,46,46	3.65	12 (27%)	45,67,67	1.83	12 (26%)
26	PEB	S7	203	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.39	15 (33%)
26	PEB	t4	201	1	43,46,46	3.68	11 (25%)	45,67,67	1.79	14 (31%)
26	PEB	h2	202	1	43,46,46	3.33	9 (20%)	45,67,67	2.01	16 (35%)
26	PEB	FE	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.48	17 (37%)
26	PEB	vE	202	2	43,46,46	3.52	10 (23%)	45,67,67	2.06	16 (35%)
26	PEB	PD	202	2	43,46,46	3.14	10 (23%)	45,67,67	2.64	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	I5	202	2	43,46,46	3.19	10 (23%)	45,67,67	2.34	18 (40%)
26	PEB	E1	201	1	43,46,46	3.43	11 (25%)	45,67,67	1.94	13 (28%)
26	PEB	V9	202	1	43,46,46	3.52	11 (25%)	45,67,67	2.07	12 (26%)
26	PEB	ID	201	1	43,46,46	3.35	12 (27%)	45,67,67	2.19	13 (28%)
26	PEB	A2	304	7	43,46,46	3.32	9 (20%)	45,67,67	2.12	14 (31%)
26	PEB	HD	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.13	14 (31%)
26	PEB	B1	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.33	15 (33%)
26	PEB	Z7	201	2,1	43,46,46	3.42	9 (20%)	45,67,67	3.11	14 (31%)
28	CYC	HB	1001	10	42,46,46	3.15	14 (33%)	50,67,67	3.09	21 (42%)
28	CYC	KI	1001	9	42,46,46	3.25	14 (33%)	50,67,67	2.87	19 (38%)
26	PEB	a6	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.35	15 (33%)
26	PEB	kE	203	2,1	43,46,46	3.42	11 (25%)	45,67,67	2.28	14 (31%)
26	PEB	WF	203	2,1	43,46,46	3.40	12 (27%)	45,67,67	2.33	16 (35%)
26	PEB	A4	202	1	43,46,46	3.49	10 (23%)	45,67,67	1.83	15 (33%)
26	PEB	EA	201	2,1	43,46,46	3.25	11 (25%)	45,67,67	2.29	14 (31%)
26	PEB	Z2	202	1	43,46,46	3.29	10 (23%)	45,67,67	1.93	12 (26%)
26	PEB	Q9	201	2,7	43,46,46	3.47	10 (23%)	45,67,67	2.26	18 (40%)
26	PEB	AG	202	1	43,46,46	3.51	12 (27%)	45,67,67	1.90	12 (26%)
26	PEB	AF	301	7	43,46,46	3.41	8 (18%)	45,67,67	2.12	14 (31%)
28	CYC	EH	1001	17	42,46,46	3.47	14 (33%)	50,67,67	3.00	20 (40%)
26	PEB	F4	201	3,2	43,46,46	3.51	12 (27%)	45,67,67	2.02	16 (35%)
26	PEB	j7	203	2,1	43,46,46	3.49	11 (25%)	45,67,67	2.27	16 (35%)
26	PEB	SD	201	1	43,46,46	3.17	10 (23%)	45,67,67	2.76	16 (35%)
26	PEB	Q7	203	1	43,46,46	3.33	10 (23%)	45,67,67	2.09	14 (31%)
26	PEB	j1	202	2	43,46,46	3.59	10 (23%)	45,67,67	2.68	16 (35%)
26	PEB	fB	202	1	43,46,46	3.44	11 (25%)	45,67,67	1.95	15 (33%)
26	PEB	R2	203	2	43,46,46	3.42	10 (23%)	45,67,67	1.98	12 (26%)
26	PEB	d1	202	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	W4	202	2	43,46,46	3.49	12 (27%)	45,67,67	2.25	16 (35%)
26	PEB	l6	201	2,1	43,46,46	3.36	12 (27%)	45,67,67	2.24	13 (28%)
26	PEB	d7	203	1	43,46,46	3.38	10 (23%)	45,67,67	2.79	15 (33%)
26	PEB	hG	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.44	17 (37%)
26	PEB	jI	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.31	17 (37%)
27	PUB	yE	302	14	42,46,46	3.33	7 (16%)	37,67,67	3.16	18 (48%)
26	PEB	D9	202	1	43,46,46	3.16	12 (27%)	45,67,67	2.77	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	p4	201	1	43,46,46	3.48	9 (20%)	45,67,67	1.94	14 (31%)
26	PEB	KJ	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.15	15 (33%)
26	PEB	qG	202	1	43,46,46	3.38	11 (25%)	45,67,67	3.43	18 (40%)
26	PEB	GD	202	1	43,46,46	3.37	10 (23%)	45,67,67	1.98	15 (33%)
26	PEB	q1	203	2	43,46,46	3.43	9 (20%)	45,67,67	2.11	15 (33%)
26	PEB	P2	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.23	17 (37%)
26	PEB	k6	202	2	43,46,46	3.34	9 (20%)	45,67,67	2.15	16 (35%)
26	PEB	mB	203	2	43,46,46	3.56	12 (27%)	45,67,67	1.99	15 (33%)
26	PEB	XJ	201	2,1	43,46,46	3.44	11 (25%)	45,67,67	2.24	14 (31%)
26	PEB	MG	202	1	43,46,46	3.46	12 (27%)	45,67,67	1.95	15 (33%)
26	PEB	EE	202	1	43,46,46	3.38	11 (25%)	45,67,67	2.00	16 (35%)
26	PEB	eI	203	2	43,46,46	3.31	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	f7	203	2,1	43,46,46	3.46	11 (25%)	45,67,67	2.36	14 (31%)
26	PEB	IJ	202	2	43,46,46	3.14	11 (25%)	45,67,67	2.53	15 (33%)
26	PEB	RB	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.22	17 (37%)
26	PEB	S6	201	1	43,46,46	3.29	10 (23%)	45,67,67	2.09	17 (37%)
26	PEB	O2	202	1	43,46,46	3.36	10 (23%)	45,67,67	1.86	12 (26%)
26	PEB	11	201	2	43,46,46	3.60	13 (30%)	45,67,67	1.78	12 (26%)
26	PEB	xG	304	13	43,46,46	3.48	11 (25%)	45,67,67	2.27	16 (35%)
26	PEB	17	202	1	43,46,46	3.39	13 (30%)	45,67,67	2.09	16 (35%)
27	PUB	AA	303	13	42,46,46	3.40	9 (21%)	37,67,67	3.35	17 (45%)
26	PEB	I8	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.37	17 (37%)
26	PEB	W6	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	CD	201	1	43,46,46	3.28	12 (27%)	45,67,67	2.55	17 (37%)
26	PEB	CD	202	1	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
26	PEB	ZA	202	2	43,46,46	3.07	11 (25%)	45,67,67	2.46	15 (33%)
26	PEB	kE	202	1	43,46,46	3.52	12 (27%)	45,67,67	2.27	13 (28%)
26	PEB	WF	202	1	43,46,46	3.36	9 (20%)	45,67,67	2.53	16 (35%)
28	CYC	L6	1001	10	42,46,46	3.24	15 (35%)	50,67,67	3.05	20 (40%)
26	PEB	cG	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.31	15 (33%)
26	PEB	f6	201	1	43,46,46	3.35	10 (23%)	45,67,67	2.12	17 (37%)
28	CYC	tH	1001	17	42,46,46	3.34	14 (33%)	50,67,67	3.03	20 (40%)
26	PEB	I3	201	1	43,46,46	3.45	13 (30%)	45,67,67	2.37	16 (35%)
26	PEB	LC	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.22	16 (35%)
28	CYC	B6	1001	8,10	42,46,46	3.34	14 (33%)	50,67,67	2.82	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	YG	201	1	43,46,46	3.26	9 (20%)	45,67,67	2.02	15 (33%)
26	PEB	U8	203	3,1	43,46,46	3.33	10 (23%)	45,67,67	2.07	13 (28%)
26	PEB	SI	201	1	43,46,46	3.42	11 (25%)	45,67,67	2.66	18 (40%)
26	PEB	tG	202	2	43,46,46	3.66	11 (25%)	45,67,67	2.63	16 (35%)
26	PEB	R2	202	2	43,46,46	3.19	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	A3	201	1	43,46,46	3.41	9 (20%)	45,67,67	2.02	15 (33%)
26	PEB	G8	203	2,1	43,46,46	3.35	12 (27%)	45,67,67	2.19	13 (28%)
26	PEB	BA	301	14	43,46,46	3.43	10 (23%)	45,67,67	2.42	14 (31%)
26	PEB	o1	501	2,4	43,46,46	3.24	10 (23%)	45,67,67	2.24	18 (40%)
26	PEB	d7	202	1	43,46,46	3.40	12 (27%)	45,67,67	2.02	15 (33%)
26	PEB	v1	201	1	43,46,46	3.54	12 (27%)	45,67,67	2.19	16 (35%)
28	CYC	F6	1001	10	42,46,46	3.26	13 (30%)	50,67,67	2.90	18 (36%)
26	PEB	LC	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
26	PEB	T3	203	2	43,46,46	3.20	10 (23%)	45,67,67	2.28	16 (35%)
26	PEB	g2	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	H1	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.49	16 (35%)
26	PEB	PD	203	2	43,46,46	3.39	10 (23%)	45,67,67	2.05	13 (28%)
26	PEB	IG	201	1	43,46,46	2.71	11 (25%)	45,67,67	2.79	15 (33%)
26	PEB	FG	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.52	17 (37%)
26	PEB	N2	1002	10	43,46,46	3.32	10 (23%)	45,67,67	2.14	17 (37%)
26	PEB	N9	204	2,1	43,46,46	3.49	9 (20%)	45,67,67	2.23	15 (33%)
26	PEB	dA	201	1	43,46,46	3.28	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	b2	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.57	18 (40%)
26	PEB	i2	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	FC	203	2	43,46,46	3.43	10 (23%)	45,67,67	1.88	12 (26%)
26	PEB	TB	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.34	21 (46%)
28	CYC	mH	1001	17	42,46,46	3.45	15 (35%)	50,67,67	3.02	22 (44%)
26	PEB	eE	201	2,1	43,46,46	3.46	14 (32%)	45,67,67	2.45	15 (33%)
26	PEB	LA	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.56	16 (35%)
26	PEB	lA	201	2,1	43,46,46	3.34	9 (20%)	45,67,67	2.62	18 (40%)
26	PEB	D3	202	2	43,46,46	3.24	11 (25%)	45,67,67	2.55	15 (33%)
26	PEB	QG	201	1	43,46,46	3.14	9 (20%)	45,67,67	2.27	14 (31%)
26	PEB	YI	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.15	16 (35%)
28	CYC	CF	1001	9,10	42,46,46	3.26	13 (30%)	50,67,67	2.72	20 (40%)
26	PEB	W6	201	1	43,46,46	3.33	10 (23%)	45,67,67	2.33	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	AE	201	1	43,46,46	3.06	9 (20%)	45,67,67	2.40	14 (31%)
26	PEB	dG	202	2	43,46,46	3.70	11 (25%)	45,67,67	1.85	15 (33%)
26	PEB	O4	201	2,4	43,46,46	3.42	10 (23%)	45,67,67	2.38	19 (42%)
26	PEB	J9	202	1	43,46,46	3.21	9 (20%)	45,67,67	2.07	13 (28%)
26	PEB	K1	202	1	43,46,46	3.30	12 (27%)	45,67,67	2.36	14 (31%)
26	PEB	nE	202	2	43,46,46	3.82	13 (30%)	45,67,67	2.28	15 (33%)
26	PEB	jA	201	1	43,46,46	3.35	10 (23%)	45,67,67	1.96	13 (28%)
28	CYC	YH	1002	22	42,46,46	3.46	14 (33%)	50,67,67	2.96	21 (42%)
26	PEB	T1	201	2,1	43,46,46	3.46	12 (27%)	45,67,67	2.23	17 (37%)
26	PEB	Q8	204	1	43,46,46	3.23	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	E1	202	1	43,46,46	3.43	10 (23%)	45,67,67	1.76	12 (26%)
26	PEB	L8	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.60	16 (35%)
26	PEB	s4	201	2	43,46,46	3.46	12 (27%)	45,67,67	2.34	15 (33%)
28	CYC	OH	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.90	20 (40%)
26	PEB	j4	202	2	43,46,46	3.47	9 (20%)	45,67,67	1.95	14 (31%)
26	PEB	G5	201	2	43,46,46	3.49	11 (25%)	45,67,67	2.05	17 (37%)
26	PEB	UF	203	1	43,46,46	3.32	10 (23%)	45,67,67	2.34	15 (33%)
26	PEB	FA	201	2,12	43,46,46	3.48	9 (20%)	45,67,67	2.43	16 (35%)
26	PEB	b7	202	1	43,46,46	3.46	10 (23%)	45,67,67	2.59	16 (35%)
26	PEB	MA	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.24	15 (33%)
26	PEB	kF	202	2	43,46,46	3.46	11 (25%)	45,67,67	2.05	14 (31%)
26	PEB	T2	203	2	43,46,46	3.40	10 (23%)	45,67,67	1.99	12 (26%)
26	PEB	mE	201	2,1	43,46,46	3.62	12 (27%)	45,67,67	2.51	14 (31%)
26	PEB	G8	202	1	43,46,46	3.35	12 (27%)	45,67,67	2.24	12 (26%)
26	PEB	mG	203	1	43,46,46	3.42	10 (23%)	45,67,67	2.19	14 (31%)
26	PEB	UI	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.90	12 (26%)
26	PEB	F8	201	2,12	43,46,46	3.48	9 (20%)	45,67,67	2.43	16 (35%)
26	PEB	r4	201	1	43,46,46	3.32	12 (27%)	45,67,67	2.12	16 (35%)
26	PEB	iE	203	1	43,46,46	3.54	12 (27%)	45,67,67	1.79	12 (26%)
26	PEB	JF	1002	10	43,46,46	3.19	10 (23%)	45,67,67	2.14	14 (31%)
26	PEB	ZF	201	2,1	43,46,46	3.26	9 (20%)	45,67,67	3.16	17 (37%)
26	PEB	Y2	203	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	12 (26%)
26	PEB	O6	203	2,1	43,46,46	3.23	11 (25%)	45,67,67	2.24	16 (35%)
26	PEB	a4	202	2	43,46,46	3.47	12 (27%)	45,67,67	1.98	12 (26%)
26	PEB	hE	202	2	43,46,46	3.53	9 (20%)	45,67,67	1.92	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	NA	201	2	43,46,46	3.24	10 (23%)	45,67,67	2.52	17 (37%)
26	PEB	l8	201	2,1	43,46,46	3.28	10 (23%)	45,67,67	2.53	19 (42%)
26	PEB	l9	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	r4	202	1	43,46,46	3.63	12 (27%)	45,67,67	2.49	15 (33%)
26	PEB	N4	203	2,1	43,46,46	3.41	11 (25%)	45,67,67	2.02	13 (28%)
26	PEB	a1	201	2	43,46,46	3.48	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	WE	203	1	43,46,46	3.47	12 (27%)	45,67,67	1.97	12 (26%)
26	PEB	BG	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.35	14 (31%)
26	PEB	M1	401	3	43,46,46	3.48	10 (23%)	45,67,67	2.12	15 (33%)
26	PEB	sG	202	1	43,46,46	3.45	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	l1	201	2	43,46,46	3.53	13 (30%)	45,67,67	2.08	13 (28%)
26	PEB	QG	203	2,1	43,46,46	3.44	13 (30%)	45,67,67	3.26	16 (35%)
26	PEB	PE	201	2	43,46,46	3.35	9 (20%)	45,67,67	3.44	18 (40%)
26	PEB	TD	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	OE	201	2,1	43,46,46	3.27	12 (27%)	45,67,67	2.85	19 (42%)
26	PEB	oG	203	1	43,46,46	3.37	12 (27%)	45,67,67	2.28	13 (28%)
28	CYC	1H	1000	22	42,46,46	3.43	13 (30%)	50,67,67	2.95	19 (38%)
26	PEB	CA	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.50	15 (33%)
26	PEB	p1	201	1	43,46,46	3.52	12 (27%)	45,67,67	1.84	12 (26%)
27	PUB	wE	304	13	42,46,46	3.56	9 (21%)	37,67,67	3.09	13 (35%)
26	PEB	N8	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.61	18 (40%)
26	PEB	LE	202	2	43,46,46	3.64	11 (25%)	45,67,67	2.68	18 (40%)
26	PEB	R1	201	1	43,46,46	3.38	11 (25%)	45,67,67	2.10	16 (35%)
26	PEB	QA	202	2,1	43,46,46	3.31	11 (25%)	45,67,67	2.25	15 (33%)
26	PEB	kB	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.11	16 (35%)
26	PEB	GB	1002	9,10	43,46,46	3.24	10 (23%)	45,67,67	2.24	16 (35%)
26	PEB	tE	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.48	14 (31%)
26	PEB	K5	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.14	17 (37%)
26	PEB	l2	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.24	17 (37%)
28	CYC	GB	1001	9,10	42,46,46	3.15	13 (30%)	50,67,67	2.93	18 (36%)
26	PEB	uE	203	1	43,46,46	3.55	12 (27%)	45,67,67	1.99	15 (33%)
26	PEB	T8	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.32	14 (31%)
26	PEB	KE	203	1	43,46,46	3.30	9 (20%)	45,67,67	1.99	16 (35%)
26	PEB	h4	202	2,1	43,46,46	3.29	11 (25%)	45,67,67	2.58	16 (35%)
26	PEB	gG	203	2,1	43,46,46	3.27	10 (23%)	45,67,67	2.57	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	s1	203	2	43,46,46	3.58	11 (25%)	45,67,67	1.96	14 (31%)
26	PEB	L3	203	2	43,46,46	3.49	9 (20%)	45,67,67	1.82	14 (31%)
26	PEB	M8	202	1	43,46,46	3.30	9 (20%)	45,67,67	2.33	19 (42%)
26	PEB	M4	403	3	43,46,46	3.35	10 (23%)	45,67,67	2.08	15 (33%)
26	PEB	T1	203	1	43,46,46	3.36	10 (23%)	45,67,67	1.98	13 (28%)
26	PEB	w1	203	2	43,46,46	3.49	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	P1	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.10	15 (33%)
26	PEB	BD	201	2,26	43,46,46	3.34	11 (25%)	45,67,67	2.17	17 (37%)
26	PEB	i8	202	2	43,46,46	3.32	10 (23%)	45,67,67	2.41	19 (42%)
26	PEB	k1	203	2,1	43,46,46	3.30	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	VG	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.57	15 (33%)
26	PEB	hA	203	1	43,46,46	3.42	9 (20%)	45,67,67	1.99	13 (28%)
26	PEB	L5	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.32	16 (35%)
26	PEB	R7	202	2	43,46,46	3.51	11 (25%)	45,67,67	2.17	14 (31%)
26	PEB	Z1	201	2	43,46,46	3.49	10 (23%)	45,67,67	2.38	15 (33%)
26	PEB	aA	201	1,13	43,46,46	3.09	10 (23%)	45,67,67	2.40	15 (33%)
26	PEB	KA	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.33	19 (42%)
26	PEB	S7	201	1	43,46,46	3.45	12 (27%)	45,67,67	2.20	15 (33%)
26	PEB	OF	201	1	43,46,46	3.35	13 (30%)	45,67,67	2.33	17 (37%)
27	PUB	NJ	201	1,7	42,46,46	3.65	7 (16%)	37,67,67	3.54	15 (40%)
26	PEB	dF	203	1	43,46,46	3.39	11 (25%)	45,67,67	2.81	15 (33%)
26	PEB	X3	203	2	43,46,46	3.50	11 (25%)	45,67,67	2.39	18 (40%)
26	PEB	O4	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	F7	1002	10	43,46,46	3.30	10 (23%)	45,67,67	2.04	13 (28%)
27	PUB	K1	203	3,1	42,46,46	3.39	7 (16%)	37,67,67	3.23	17 (45%)
26	PEB	a7	202	2	43,46,46	3.41	11 (25%)	45,67,67	2.05	15 (33%)
27	PUB	xE	306	13	42,46,46	3.69	8 (19%)	37,67,67	2.94	14 (37%)
26	PEB	r1	201	1	43,46,46	3.38	12 (27%)	45,67,67	2.22	17 (37%)
26	PEB	AA	301	13	43,46,46	3.18	11 (25%)	45,67,67	2.30	15 (33%)
28	CYC	KH	1001	17	42,46,46	3.58	16 (38%)	50,67,67	5.42	21 (42%)
26	PEB	QE	201	1	43,46,46	3.12	8 (18%)	45,67,67	2.31	14 (31%)
26	PEB	P3	202	2	43,46,46	3.05	10 (23%)	45,67,67	2.70	15 (33%)
26	PEB	DJ	203	1	43,46,46	3.22	10 (23%)	45,67,67	2.28	15 (33%)
26	PEB	KE	202	1	43,46,46	2.97	9 (20%)	45,67,67	2.13	15 (33%)
26	PEB	e8	202	2	43,46,46	3.28	10 (23%)	45,67,67	2.63	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	Y8	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.32	16 (35%)
26	PEB	F9	201	1	43,46,46	3.26	12 (27%)	45,67,67	2.63	17 (37%)
26	PEB	kA	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.42	16 (35%)
26	PEB	N6	201	9,10	43,46,46	3.37	11 (25%)	45,67,67	2.22	15 (33%)
28	CYC	IH	1001	-	42,46,46	3.40	14 (33%)	50,67,67	2.97	20 (40%)
26	PEB	e2	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.20	14 (31%)
26	PEB	YB	201	2	43,46,46	3.11	11 (25%)	45,67,67	2.67	20 (44%)
26	PEB	nG	201	2	43,46,46	3.47	10 (23%)	45,67,67	3.20	17 (37%)
26	PEB	MA	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	NE	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.00	14 (31%)
26	PEB	uE	202	1	43,46,46	3.54	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	EA	202	1	43,46,46	3.41	11 (25%)	45,67,67	2.31	14 (31%)
26	PEB	q4	202	2	43,46,46	3.38	12 (27%)	45,67,67	2.49	16 (35%)
26	PEB	QI	202	1	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
26	PEB	AE	202	1	43,46,46	3.42	11 (25%)	45,67,67	1.91	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	V2	203	2	-	11/24/74/74	0/4/4/4
26	PEB	LJ	202	1	-	9/24/74/74	0/4/4/4
26	PEB	WB	201	1	-	7/24/74/74	0/4/4/4
26	PEB	L3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	K3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	SE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	I4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	W7	201	1	-	6/24/74/74	0/4/4/4
26	PEB	VE	201	2	-	8/24/74/74	0/4/4/4
26	PEB	O3	201	1	-	9/24/74/74	0/4/4/4
26	PEB	e4	201	1	-	10/24/74/74	0/4/4/4
28	CYC	N2	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	KG	203	1	-	8/24/74/74	0/4/4/4
26	PEB	g2	203	2	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	l6	202	1	-	14/24/74/74	0/4/4/4
26	PEB	NI	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	d8	203	1	-	10/24/74/74	0/4/4/4
26	PEB	24	405	3	-	10/24/74/74	0/4/4/4
26	PEB	c4	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	b2	202	1	-	9/24/74/74	0/4/4/4
26	PEB	mB	201	2	-	10/24/74/74	0/4/4/4
26	PEB	OA	201	1	-	7/24/74/74	0/4/4/4
26	PEB	21	405	3	-	11/24/74/74	0/4/4/4
28	CYC	YH	1001	22	-	9/25/74/74	0/4/4/4
26	PEB	e6	201	2	-	9/24/74/74	0/4/4/4
28	CYC	dH	1001	-	-	11/25/74/74	0/4/4/4
26	PEB	iG	203	1	-	12/24/74/74	0/4/4/4
26	PEB	iA	201	2,13	-	8/24/74/74	0/4/4/4
26	PEB	sG	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	EE	201	1	-	7/24/74/74	0/4/4/4
26	PEB	DG	203	2	-	12/24/74/74	0/4/4/4
26	PEB	kG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	WG	203	1	-	13/24/74/74	0/4/4/4
26	PEB	SB	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	w4	204	2,1	-	8/24/74/74	0/4/4/4
26	PEB	QJ	201	2,7	-	3/24/74/74	0/4/4/4
26	PEB	D1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	J4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Y4	202	2	-	4/24/74/74	0/4/4/4
26	PEB	Z6	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	TJ	203	1	-	11/24/74/74	0/4/4/4
26	PEB	m6	201	2	-	6/24/74/74	0/4/4/4
26	PEB	q4	201	2	-	6/24/74/74	0/4/4/4
26	PEB	UA	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	pG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	j2	202	1	-	8/24/74/74	0/4/4/4
26	PEB	f6	202	1	-	8/24/74/74	0/4/4/4
26	PEB	IA	203	1	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	oE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	II	201	1	-	8/24/74/74	0/4/4/4
27	PUB	24	402	3	-	5/24/74/74	0/4/4/4
27	PUB	yG	303	14	-	5/24/74/74	0/4/4/4
26	PEB	SE	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	U4	201	2,4	-	7/24/74/74	0/4/4/4
26	PEB	S6	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	pG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	E8	203	1	-	10/24/74/74	0/4/4/4
26	PEB	OF	202	1	-	7/24/74/74	0/4/4/4
26	PEB	R6	202	2	-	11/24/74/74	0/4/4/4
26	PEB	RI	201	2,6	-	2/24/74/74	0/4/4/4
26	PEB	Z7	202	1	-	9/24/74/74	0/4/4/4
26	PEB	SA	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	CE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	g2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	RD	202	2	-	10/24/74/74	0/4/4/4
26	PEB	jE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	U6	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	pE	201	2	-	12/24/74/74	0/4/4/4
26	PEB	U3	201	1	-	6/24/74/74	0/4/4/4
26	PEB	N1	202	1	-	11/24/74/74	0/4/4/4
26	PEB	D8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	IG	201	2	-	11/24/74/74	0/4/4/4
27	PUB	A7	304	7	-	13/24/74/74	0/4/4/4
26	PEB	u4	201	3,2	-	12/24/74/74	0/4/4/4
28	CYC	JH	1001	18,17	-	6/25/74/74	0/4/4/4
26	PEB	f8	201	1	-	9/24/74/74	0/4/4/4
26	PEB	FC	201	2	-	6/24/74/74	0/4/4/4
26	PEB	CG	203	1	-	11/24/74/74	0/4/4/4
26	PEB	NG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	T3	202	2	-	9/24/74/74	0/4/4/4
26	PEB	hG	202	2	-	9/24/74/74	0/4/4/4
26	PEB	hB	202	1	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	M9	201	2	-	7/24/74/74	0/4/4/4
26	PEB	IE	203	2,1	-	5/24/74/74	0/4/4/4
26	PEB	M4	402	3,26	-	12/24/74/74	0/4/4/4
26	PEB	i6	201	2	-	10/24/74/74	0/4/4/4
26	PEB	JI	1002	10	-	12/24/74/74	0/4/4/4
26	PEB	L9	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	KB	201	9,10	-	6/24/74/74	0/4/4/4
26	PEB	P2	202	2	-	8/24/74/74	0/4/4/4
26	PEB	W8	202	1	-	13/24/74/74	0/4/4/4
26	PEB	LB	1002	9,10	-	11/24/74/74	0/4/4/4
26	PEB	JE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	c2	202	2	-	11/24/74/74	0/4/4/4
26	PEB	aG	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	VF	201	2	-	2/24/74/74	0/4/4/4
26	PEB	EJ	201	2,15	-	12/24/74/74	0/4/4/4
26	PEB	tE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	m4	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	d6	204	1	-	13/24/74/74	0/4/4/4
26	PEB	S4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	I5	203	2	-	11/24/74/74	0/4/4/4
26	PEB	fG	201	2,13	-	11/24/74/74	0/4/4/4
28	CYC	qH	1002	-	-	16/25/74/74	0/4/4/4
26	PEB	A8	302	13	-	10/24/74/74	0/4/4/4
26	PEB	x4	202	1	-	15/24/74/74	0/4/4/4
28	CYC	D7	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	IC	202	2	-	3/24/74/74	0/4/4/4
26	PEB	c1	203	2,1	-	9/24/74/74	0/4/4/4
28	CYC	J7	1003	9,10	-	6/25/74/74	0/4/4/4
26	PEB	BC	202	2	-	8/24/74/74	0/4/4/4
26	PEB	ZE	201	2	-	9/24/74/74	0/4/4/4
28	CYC	FH	1001	18	-	6/25/74/74	0/4/4/4
26	PEB	X9	202	1	-	11/24/74/74	0/4/4/4
26	PEB	H9	202	1	-	12/24/74/74	0/4/4/4
26	PEB	Z4	201	2	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	KC	202	2	-	6/24/74/74	0/4/4/4
26	PEB	VD	203	2	-	7/24/74/74	0/4/4/4
26	PEB	S6	202	1	-	10/24/74/74	0/4/4/4
26	PEB	y1	202	2	-	7/24/74/74	0/4/4/4
26	PEB	ZG	202	2	-	10/24/74/74	0/4/4/4
27	PUB	xG	305	13	-	8/24/74/74	0/4/4/4
26	PEB	SA	202	1	-	10/24/74/74	0/4/4/4
26	PEB	S7	202	1	-	8/24/74/74	0/4/4/4
26	PEB	fA	203	2,1	-	5/24/74/74	0/4/4/4
26	PEB	Y7	202	2	-	8/24/74/74	0/4/4/4
26	PEB	CG	202	1	-	6/24/74/74	0/4/4/4
26	PEB	N4	201	1	-	6/24/74/74	0/4/4/4
26	PEB	HC	201	2	-	8/24/74/74	0/4/4/4
26	PEB	n4	201	2,4	-	12/24/74/74	0/4/4/4
26	PEB	Y6	201	2	-	10/24/74/74	0/4/4/4
26	PEB	c8	201	2	-	10/24/74/74	0/4/4/4
26	PEB	N9	203	1	-	12/24/74/74	0/4/4/4
26	PEB	X4	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	oG	201	1	-	13/24/74/74	0/4/4/4
26	PEB	L1	201	3,2	-	12/24/74/74	0/4/4/4
26	PEB	C8	201	1	-	4/24/74/74	0/4/4/4
26	PEB	a2	203	2	-	10/24/74/74	0/4/4/4
26	PEB	PJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	v1	202	1	-	11/24/74/74	0/4/4/4
26	PEB	f2	201	1	-	9/24/74/74	0/4/4/4
26	PEB	kG	201	1	-	12/24/74/74	0/4/4/4
26	PEB	aI	202	2	-	7/24/74/74	0/4/4/4
26	PEB	I8	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	l4	201	2	-	9/24/74/74	0/4/4/4
26	PEB	i4	201	1	-	7/24/74/74	0/4/4/4
26	PEB	YJ	201	2,26	-	5/24/74/74	0/4/4/4
26	PEB	TI	201	2	-	5/24/74/74	0/4/4/4
26	PEB	gG	201	1	-	6/24/74/74	0/4/4/4
26	PEB	k2	202	2	-	16/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	J2	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	Z2	201	1	-	7/24/74/74	0/4/4/4
26	PEB	vG	201	2	-	9/24/74/74	0/4/4/4
26	PEB	J1	203	2	-	10/24/74/74	0/4/4/4
26	PEB	OB	201	1	-	9/24/74/74	0/4/4/4
26	PEB	JD	201	2,7	-	3/24/74/74	0/4/4/4
26	PEB	K5	203	2	-	9/24/74/74	0/4/4/4
26	PEB	NJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	OI	202	1	-	6/24/74/74	0/4/4/4
26	PEB	LI	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	M3	202	1	-	13/24/74/74	0/4/4/4
27	PUB	B8	302	14	-	4/24/74/74	0/4/4/4
26	PEB	V7	202	2	-	9/24/74/74	0/4/4/4
28	CYC	NI	1001	10	-	11/25/74/74	0/4/4/4
26	PEB	gE	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	S8	201	1	-	10/24/74/74	0/4/4/4
26	PEB	rG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	g4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	UJ	202	2	-	9/24/74/74	0/4/4/4
26	PEB	HB	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	TG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	WI	201	1	-	7/24/74/74	0/4/4/4
26	PEB	FF	1002	10	-	11/24/74/74	0/4/4/4
26	PEB	mG	201	1	-	10/24/74/74	0/4/4/4
26	PEB	mB	202	2	-	6/24/74/74	0/4/4/4
26	PEB	a8	204	2,1	-	7/24/74/74	0/4/4/4
26	PEB	aA	204	2,1	-	6/24/74/74	0/4/4/4
28	CYC	CH	1001	18,17	-	8/25/74/74	0/4/4/4
26	PEB	WJ	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	UI	201	1	-	9/24/74/74	0/4/4/4
26	PEB	L5	202	2	-	10/24/74/74	0/4/4/4
26	PEB	eI	202	2	-	10/24/74/74	0/4/4/4
26	PEB	mE	202	1	-	12/24/74/74	0/4/4/4
26	PEB	J3	202	2	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	A2	305	7	-	11/24/74/74	0/4/4/4
26	PEB	FD	203	2	-	11/24/74/74	0/4/4/4
27	PUB	A2	302	7	-	3/24/74/74	0/4/4/4
26	PEB	CJ	202	2	-	8/24/74/74	0/4/4/4
28	CYC	wH	1001	-	-	7/25/74/74	0/4/4/4
26	PEB	DJ	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	dF	202	1	-	10/24/74/74	0/4/4/4
26	PEB	mI	202	2	-	8/24/74/74	0/4/4/4
26	PEB	zG	501	2,16	-	6/24/74/74	0/4/4/4
26	PEB	MG	201	1	-	6/24/74/74	0/4/4/4
26	PEB	B5	202	2	-	9/24/74/74	0/4/4/4
26	PEB	I1	201	1	-	6/24/74/74	0/4/4/4
28	CYC	I2	1001	9	-	9/25/74/74	0/4/4/4
26	PEB	aI	201	2	-	2/24/74/74	0/4/4/4
26	PEB	D1	201	3,2	-	11/24/74/74	0/4/4/4
28	CYC	kH	1001	-	-	8/25/74/74	0/4/4/4
26	PEB	lB	202	1	-	14/24/74/74	0/4/4/4
26	PEB	J7	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	Z4	202	2	-	13/24/74/74	0/4/4/4
26	PEB	C1	202	1	-	15/24/74/74	0/4/4/4
28	CYC	J7	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	p1	202	1	-	17/24/74/74	0/4/4/4
26	PEB	U8	202	1	-	7/24/74/74	0/4/4/4
26	PEB	VF	203	2	-	9/24/74/74	0/4/4/4
26	PEB	H6	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	nG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	N8	202	2	-	8/24/74/74	0/4/4/4
26	PEB	aF	201	2	-	7/24/74/74	0/4/4/4
26	PEB	j2	201	1	-	10/24/74/74	0/4/4/4
26	PEB	VI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	K5	202	2	-	6/24/74/74	0/4/4/4
26	PEB	FJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	NJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	PG	202	2	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	mF	201	2	-	8/24/74/74	0/4/4/4
28	CYC	hH	1001	22,18	-	4/25/74/74	0/4/4/4
26	PEB	C3	201	1	-	11/24/74/74	0/4/4/4
26	PEB	jB	201	1	-	10/24/74/74	0/4/4/4
26	PEB	P8	201	2	-	10/24/74/74	0/4/4/4
26	PEB	Q8	203	1	-	4/24/74/74	0/4/4/4
26	PEB	J2	1002	10	-	11/24/74/74	0/4/4/4
27	PUB	yG	302	14	-	3/24/74/74	0/4/4/4
26	PEB	EG	201	1	-	9/24/74/74	0/4/4/4
26	PEB	JA	201	2	-	9/24/74/74	0/4/4/4
28	CYC	JI	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	c4	202	1	-	11/24/74/74	0/4/4/4
28	CYC	E7	1001	9,10	-	5/25/74/74	0/4/4/4
26	PEB	Y9	202	2	-	8/24/74/74	0/4/4/4
26	PEB	VE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	S8	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	24	401	3	-	15/24/74/74	0/4/4/4
26	PEB	P8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Y1	202	2	-	4/24/74/74	0/4/4/4
26	PEB	Z1	202	2	-	12/24/74/74	0/4/4/4
26	PEB	rE	202	2	-	10/24/74/74	0/4/4/4
26	PEB	HA	201	2	-	6/24/74/74	0/4/4/4
26	PEB	J5	202	1	-	7/24/74/74	0/4/4/4
26	PEB	K4	202	1	-	14/24/74/74	0/4/4/4
26	PEB	V4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	OA	203	2,1	-	6/24/74/74	0/4/4/4
28	CYC	FI	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	SB	201	1	-	10/24/74/74	0/4/4/4
26	PEB	A9	304	7,26	-	9/24/74/74	0/4/4/4
26	PEB	nE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	H4	201	3,2	-	9/24/74/74	0/4/4/4
26	PEB	d2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	gA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RG	202	2	-	13/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PUB	24	403	3,1	-	9/24/74/74	0/4/4/4
26	PEB	RJ	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	ME	201	1	-	6/24/74/74	0/4/4/4
26	PEB	A6	304	7	-	4/24/74/74	0/4/4/4
28	CYC	F2	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	L1	203	2	-	15/24/74/74	0/4/4/4
26	PEB	CA	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	S9	202	2	-	9/24/74/74	0/4/4/4
26	PEB	ME	202	1	-	10/24/74/74	0/4/4/4
26	PEB	X9	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	i2	203	2	-	14/24/74/74	0/4/4/4
26	PEB	CC	201	2	-	10/24/74/74	0/4/4/4
26	PEB	DD	201	2,7	-	11/24/74/74	0/4/4/4
26	PEB	eF	202	2	-	11/24/74/74	0/4/4/4
26	PEB	mG	202	1	-	6/24/74/74	0/4/4/4
26	PEB	OG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	E8	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	u1	203	2	-	5/24/74/74	0/4/4/4
26	PEB	bE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	cG	202	1	-	13/24/74/74	0/4/4/4
26	PEB	B4	202	2	-	7/24/74/74	0/4/4/4
26	PEB	NJ	204	2,1	-	12/24/74/74	0/4/4/4
26	PEB	uG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	e1	201	1	-	8/24/74/74	0/4/4/4
26	PEB	SI	202	1	-	10/24/74/74	0/4/4/4
26	PEB	gB	201	2	-	7/24/74/74	0/4/4/4
26	PEB	VJ	203	2,1	-	14/24/74/74	0/4/4/4
28	CYC	fH	1001	18	-	5/25/74/74	0/4/4/4
26	PEB	RD	201	2	-	5/24/74/74	0/4/4/4
26	PEB	M1	403	3	-	7/24/74/74	0/4/4/4
28	CYC	M2	1001	9	-	7/25/74/74	0/4/4/4
26	PEB	X8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	S3	202	1	-	8/24/74/74	0/4/4/4
26	PEB	K9	202	2	-	13/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	c8	202	2	-	10/24/74/74	0/4/4/4
26	PEB	IG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	oG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	CG	201	1	-	6/24/74/74	0/4/4/4
26	PEB	YF	202	2	-	8/24/74/74	0/4/4/4
26	PEB	TF	201	2,6	-	9/24/74/74	0/4/4/4
26	PEB	BJ	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	sG	201	1	-	12/24/74/74	0/4/4/4
26	PEB	OA	202	1	-	7/24/74/74	0/4/4/4
26	PEB	YG	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	i4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	e4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	c2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	VF	202	2,1	-	7/24/74/74	0/4/4/4
26	PEB	v4	202	1	-	13/24/74/74	0/4/4/4
26	PEB	qG	203	1	-	10/24/74/74	0/4/4/4
26	PEB	hI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	lF	202	1	-	10/24/74/74	0/4/4/4
26	PEB	Q6	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	WG	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	e7	202	2	-	10/24/74/74	0/4/4/4
26	PEB	s1	202	2	-	7/24/74/74	0/4/4/4
26	PEB	T2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	XA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	aI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	hF	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	W2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	R4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	GC	201	2	-	11/24/74/74	0/4/4/4
26	PEB	w1	202	2	-	13/24/74/74	0/4/4/4
26	PEB	u1	202	2	-	7/24/74/74	0/4/4/4
26	PEB	uG	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	P9	203	1	-	12/24/74/74	0/4/4/4
26	PEB	c1	202	1	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	k1	202	1	-	8/24/74/74	0/4/4/4
26	PEB	hA	202	1	-	6/24/74/74	0/4/4/4
26	PEB	q4	203	2	-	6/24/74/74	0/4/4/4
26	PEB	O9	201	2,7,26	-	8/24/74/74	0/4/4/4
26	PEB	fl	201	1	-	11/24/74/74	0/4/4/4
28	CYC	HF	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	lE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	AB	301	7	-	10/24/74/74	0/4/4/4
26	PEB	fE	202	2	-	11/24/74/74	0/4/4/4
27	PUB	A8	304	13	-	10/24/74/74	0/4/4/4
26	PEB	R9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	VB	201	2	-	9/24/74/74	0/4/4/4
26	PEB	C5	202	2	-	8/24/74/74	0/4/4/4
28	CYC	N7	1001	8,10	-	7/25/74/74	0/4/4/4
26	PEB	j6	201	1	-	9/24/74/74	0/4/4/4
26	PEB	TE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	DJ	202	1	-	13/24/74/74	0/4/4/4
26	PEB	z4	201	1	-	11/24/74/74	0/4/4/4
26	PEB	GA	202	1	-	5/24/74/74	0/4/4/4
26	PEB	lI	202	1	-	10/24/74/74	0/4/4/4
28	CYC	EF	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	U9	202	2	-	8/24/74/74	0/4/4/4
26	PEB	XE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	f1	202	2	-	5/24/74/74	0/4/4/4
26	PEB	PJ	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	lF	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	KE	201	2,1	-	6/24/74/74	0/4/4/4
27	PUB	AB	302	7	-	7/24/74/74	0/4/4/4
28	CYC	SH	1001	18	-	7/25/74/74	0/4/4/4
26	PEB	l1	202	2	-	11/24/74/74	0/4/4/4
26	PEB	g7	201	2	-	7/24/74/74	0/4/4/4
26	PEB	H3	202	2	-	8/24/74/74	0/4/4/4
26	PEB	XA	201	2	-	6/24/74/74	0/4/4/4
26	PEB	XD	202	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	I5	201	2	-	4/24/74/74	0/4/4/4
26	PEB	F3	203	2	-	11/24/74/74	0/4/4/4
26	PEB	j8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	P7	201	2,6	-	6/24/74/74	0/4/4/4
26	PEB	D3	203	2	-	11/24/74/74	0/4/4/4
26	PEB	d6	203	1	-	8/24/74/74	0/4/4/4
26	PEB	J1	201	2	-	12/24/74/74	0/4/4/4
26	PEB	m1	203	1	-	9/24/74/74	0/4/4/4
26	PEB	I4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	O7	202	1	-	7/24/74/74	0/4/4/4
26	PEB	gF	202	2	-	6/24/74/74	0/4/4/4
26	PEB	R9	201	1	-	12/24/74/74	0/4/4/4
26	PEB	eF	201	2	-	8/24/74/74	0/4/4/4
26	PEB	YD	301	7	-	16/24/74/74	0/4/4/4
26	PEB	OG	201	2,1	-	6/24/74/74	0/4/4/4
26	PEB	X9	203	1	-	10/24/74/74	0/4/4/4
26	PEB	J1	202	2	-	11/24/74/74	0/4/4/4
26	PEB	rG	201	2,13	-	11/24/74/74	0/4/4/4
26	PEB	B4	201	3,2,26	-	12/24/74/74	0/4/4/4
26	PEB	F5	201	2	-	6/24/74/74	0/4/4/4
28	CYC	BB	1001	8,10	-	12/25/74/74	0/4/4/4
26	PEB	WB	203	2,1	-	7/24/74/74	0/4/4/4
28	CYC	MH	1001	18	-	10/25/74/74	0/4/4/4
27	PUB	A7	303	7	-	5/24/74/74	0/4/4/4
26	PEB	GA	201	1	-	7/24/74/74	0/4/4/4
26	PEB	iG	202	1	-	13/24/74/74	0/4/4/4
28	CYC	EI	1001	9	-	8/25/74/74	0/4/4/4
26	PEB	qE	203	1	-	8/24/74/74	0/4/4/4
26	PEB	XE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	GJ	201	2	-	5/24/74/74	0/4/4/4
26	PEB	K8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	B3	202	2	-	8/24/74/74	0/4/4/4
26	PEB	N7	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	PB	201	2,6	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	eH	1001	18,17	-	8/25/74/74	0/4/4/4
26	PEB	ZI	201	1	-	7/24/74/74	0/4/4/4
26	PEB	D9	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	S2	202	1	-	10/24/74/74	0/4/4/4
27	PUB	A4	203	3,1	-	7/24/74/74	0/4/4/4
26	PEB	YD	303	7,26	-	13/24/74/74	0/4/4/4
26	PEB	YE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	UE	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	GD	201	1	-	6/24/74/74	0/4/4/4
26	PEB	RA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	Y6	202	2	-	12/24/74/74	0/4/4/4
27	PUB	wG	304	13	-	7/24/74/74	0/4/4/4
26	PEB	V2	201	2	-	4/24/74/74	0/4/4/4
26	PEB	J9	201	1	-	14/24/74/74	0/4/4/4
26	PEB	YD	304	7,26	-	13/24/74/74	0/4/4/4
26	PEB	iF	202	2	-	9/24/74/74	0/4/4/4
26	PEB	G3	202	1	-	13/24/74/74	0/4/4/4
26	PEB	S9	201	2,7	-	6/24/74/74	0/4/4/4
26	PEB	QE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	P2	203	2	-	7/24/74/74	0/4/4/4
26	PEB	d4	203	2	-	9/24/74/74	0/4/4/4
28	CYC	YH	1004	22	-	8/25/74/74	0/4/4/4
26	PEB	F2	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	k8	202	2	-	12/24/74/74	0/4/4/4
26	PEB	XJ	203	1	-	13/24/74/74	0/4/4/4
26	PEB	eB	203	2	-	13/24/74/74	0/4/4/4
26	PEB	VI	201	2	-	4/24/74/74	0/4/4/4
26	PEB	GE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	m1	202	1	-	9/24/74/74	0/4/4/4
26	PEB	UA	202	1	-	7/24/74/74	0/4/4/4
28	CYC	H2	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	NA	202	2	-	8/24/74/74	0/4/4/4
26	PEB	V3	201	2,11	-	11/24/74/74	0/4/4/4
26	PEB	DA	201	14,2	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	b7	201	1	-	12/24/74/74	0/4/4/4
26	PEB	Q1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	T9	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	O8	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	n1	201	2	-	9/24/74/74	0/4/4/4
26	PEB	U7	202	1	-	6/24/74/74	0/4/4/4
27	PUB	A8	303	13	-	7/24/74/74	0/4/4/4
26	PEB	cG	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	h4	203	2	-	7/24/74/74	0/4/4/4
26	PEB	Z8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	O3	202	1	-	10/24/74/74	0/4/4/4
26	PEB	TI	202	2	-	5/24/74/74	0/4/4/4
28	CYC	PH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	B9	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	ED	201	1	-	7/24/74/74	0/4/4/4
26	PEB	fB	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	mI	201	2	-	9/24/74/74	0/4/4/4
26	PEB	T3	201	2	-	5/24/74/74	0/4/4/4
26	PEB	AI	305	7	-	10/24/74/74	0/4/4/4
28	CYC	JF	1001	10	-	4/25/74/74	0/4/4/4
26	PEB	hE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	A7	302	7	-	10/24/74/74	0/4/4/4
26	PEB	T6	201	2	-	3/24/74/74	0/4/4/4
26	PEB	h1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	H1	201	3,2	-	9/24/74/74	0/4/4/4
26	PEB	Q4	202	2	-	10/24/74/74	0/4/4/4
26	PEB	m2	202	2	-	9/24/74/74	0/4/4/4
26	PEB	P1	203	1	-	10/24/74/74	0/4/4/4
26	PEB	f8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	FG	201	2	-	5/24/74/74	0/4/4/4
26	PEB	UE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	KA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	B1	201	3,2,26	-	10/24/74/74	0/4/4/4
26	PEB	RJ	201	1	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	xG	303	13	-	12/24/74/74	0/4/4/4
26	PEB	L4	203	2	-	13/24/74/74	0/4/4/4
26	PEB	hF	202	1	-	11/24/74/74	0/4/4/4
26	PEB	C9	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	WJ	202	2	-	7/24/74/74	0/4/4/4
28	CYC	cH	1001	17	-	10/25/74/74	0/4/4/4
26	PEB	U1	201	2,4	-	7/24/74/74	0/4/4/4
26	PEB	AC	201	2	-	9/24/74/74	0/4/4/4
26	PEB	AF	305	7	-	12/24/74/74	0/4/4/4
26	PEB	b1	501	2,4	-	7/24/74/74	0/4/4/4
26	PEB	yE	301	14	-	8/24/74/74	0/4/4/4
28	CYC	NB	1001	8,10	-	6/25/74/74	0/4/4/4
26	PEB	ZB	202	1	-	9/24/74/74	0/4/4/4
26	PEB	BE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	ND	202	2	-	8/24/74/74	0/4/4/4
26	PEB	I8	203	1	-	12/24/74/74	0/4/4/4
26	PEB	xE	303	13	-	11/24/74/74	0/4/4/4
26	PEB	bI	201	1	-	8/24/74/74	0/4/4/4
26	PEB	fF	202	1	-	9/24/74/74	0/4/4/4
26	PEB	NB	1002	9,10	-	10/24/74/74	0/4/4/4
26	PEB	aB	201	2	-	7/24/74/74	0/4/4/4
28	CYC	rH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	l7	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	e6	202	2	-	6/24/74/74	0/4/4/4
26	PEB	WA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	J8	201	2	-	9/24/74/74	0/4/4/4
26	PEB	OI	201	1	-	9/24/74/74	0/4/4/4
26	PEB	iI	201	2	-	6/24/74/74	0/4/4/4
26	PEB	LF	1002	10	-	7/24/74/74	0/4/4/4
26	PEB	j6	202	1	-	6/24/74/74	0/4/4/4
26	PEB	UD	202	1	-	11/24/74/74	0/4/4/4
26	PEB	dB	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	MD	202	1	-	13/24/74/74	0/4/4/4
26	PEB	wG	303	13	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	xG	302	13	-	12/24/74/74	0/4/4/4
26	PEB	ZG	201	2	-	9/24/74/74	0/4/4/4
26	PEB	EA	203	1	-	10/24/74/74	0/4/4/4
26	PEB	i8	201	2,13	-	5/24/74/74	0/4/4/4
26	PEB	cA	203	2	-	10/24/74/74	0/4/4/4
26	PEB	Z6	203	1	-	9/24/74/74	0/4/4/4
28	CYC	K2	1001	9	-	7/25/74/74	0/4/4/4
27	PUB	AB	303	7	-	9/24/74/74	0/4/4/4
26	PEB	a2	202	2	-	8/24/74/74	0/4/4/4
26	PEB	BJ	201	1	-	11/24/74/74	0/4/4/4
26	PEB	NG	202	2	-	10/24/74/74	0/4/4/4
26	PEB	L5	203	2	-	11/24/74/74	0/4/4/4
26	PEB	J3	203	2	-	14/24/74/74	0/4/4/4
26	PEB	l6	203	1	-	7/24/74/74	0/4/4/4
26	PEB	mA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	G4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	mF	202	2	-	10/24/74/74	0/4/4/4
26	PEB	GJ	202	2	-	12/24/74/74	0/4/4/4
26	PEB	B5	203	2	-	11/24/74/74	0/4/4/4
26	PEB	RF	201	2	-	7/24/74/74	0/4/4/4
26	PEB	E9	201	2,15	-	12/24/74/74	0/4/4/4
26	PEB	SB	202	1	-	9/24/74/74	0/4/4/4
26	PEB	m7	202	2	-	9/24/74/74	0/4/4/4
26	PEB	m8	201	2,13	-	9/24/74/74	0/4/4/4
27	PUB	AJ	302	1,7	-	7/24/74/74	0/4/4/4
26	PEB	e2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	gE	202	1	-	11/24/74/74	0/4/4/4
28	CYC	C6	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	B1	203	2	-	10/24/74/74	0/4/4/4
26	PEB	D4	201	3,2	-	10/24/74/74	0/4/4/4
26	PEB	X1	202	1	-	8/24/74/74	0/4/4/4
26	PEB	AJ	303	7,26	-	10/24/74/74	0/4/4/4
28	CYC	yH	1001	-	-	9/25/74/74	0/4/4/4
26	PEB	O7	203	2,1	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	AC	203	2	-	10/24/74/74	0/4/4/4
26	PEB	VD	201	2,11	-	11/24/74/74	0/4/4/4
26	PEB	V7	201	2	-	5/24/74/74	0/4/4/4
28	CYC	M6	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	W3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	FD	202	2	-	10/24/74/74	0/4/4/4
26	PEB	Q2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	cB	202	2	-	10/24/74/74	0/4/4/4
26	PEB	P9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	HD	203	2	-	12/24/74/74	0/4/4/4
26	PEB	f6	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	LD	202	2	-	9/24/74/74	0/4/4/4
26	PEB	bE	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RI	202	2	-	10/24/74/74	0/4/4/4
26	PEB	Q9	202	2	-	12/24/74/74	0/4/4/4
26	PEB	D4	202	2	-	8/24/74/74	0/4/4/4
28	CYC	C7	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	tG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	F4	202	2	-	10/24/74/74	0/4/4/4
26	PEB	R2	201	2,6	-	2/24/74/74	0/4/4/4
28	CYC	IB	1001	9,10	-	8/25/74/74	0/4/4/4
28	CYC	KB	202	9,10	-	9/25/74/74	0/4/4/4
26	PEB	SJ	202	2	-	8/24/74/74	0/4/4/4
26	PEB	H5	201	2	-	8/24/74/74	0/4/4/4
26	PEB	d7	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	z4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	kI	201	2	-	8/24/74/74	0/4/4/4
28	CYC	DI	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	h8	202	1	-	6/24/74/74	0/4/4/4
26	PEB	h7	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	a7	201	2	-	6/24/74/74	0/4/4/4
26	PEB	IG	203	2,1	-	4/24/74/74	0/4/4/4
26	PEB	gB	202	2	-	11/24/74/74	0/4/4/4
26	PEB	HI	1002	10	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	g7	202	2	-	4/24/74/74	0/4/4/4
26	PEB	f4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	qG	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	hB	203	1	-	9/24/74/74	0/4/4/4
26	PEB	V4	203	2,1	-	11/24/74/74	0/4/4/4
28	CYC	iH	1001	18,17	-	8/25/74/74	0/4/4/4
26	PEB	OE	203	1	-	12/24/74/74	0/4/4/4
28	CYC	JF	1003	9,10	-	9/25/74/74	0/4/4/4
26	PEB	XD	201	2,11	-	5/24/74/74	0/4/4/4
26	PEB	MG	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	T6	202	2	-	11/24/74/74	0/4/4/4
26	PEB	k6	201	2,7	-	8/24/74/74	0/4/4/4
26	PEB	eE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	K1	201	1	-	8/24/74/74	0/4/4/4
26	PEB	e7	201	2	-	6/24/74/74	0/4/4/4
26	PEB	lA	203	1	-	9/24/74/74	0/4/4/4
26	PEB	W8	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	QE	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	c2	203	2	-	13/24/74/74	0/4/4/4
26	PEB	O8	201	1	-	7/24/74/74	0/4/4/4
28	CYC	pH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	j8	202	1	-	11/24/74/74	0/4/4/4
26	PEB	NF	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	H2	1002	10	-	7/24/74/74	0/4/4/4
28	CYC	H7	1001	10	-	6/25/74/74	0/4/4/4
26	PEB	c7	202	2	-	9/24/74/74	0/4/4/4
26	PEB	CE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	Q8	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	wE	303	13	-	8/24/74/74	0/4/4/4
26	PEB	E3	202	1	-	13/24/74/74	0/4/4/4
26	PEB	bF	201	1	-	10/24/74/74	0/4/4/4
26	PEB	11	203	2	-	7/24/74/74	0/4/4/4
26	PEB	iB	202	2	-	10/24/74/74	0/4/4/4
26	PEB	P9	201	2,1	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	T7	202	2	-	12/24/74/74	0/4/4/4
26	PEB	DE	203	2	-	12/24/74/74	0/4/4/4
26	PEB	i7	201	2	-	4/24/74/74	0/4/4/4
26	PEB	OB	202	1	-	10/24/74/74	0/4/4/4
26	PEB	N3	203	2	-	8/24/74/74	0/4/4/4
26	PEB	Y9	201	2,26	-	7/24/74/74	0/4/4/4
26	PEB	LJ	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	O9	202	2	-	14/24/74/74	0/4/4/4
26	PEB	AJ	305	2,7,26	-	8/24/74/74	0/4/4/4
26	PEB	f7	202	1	-	10/24/74/74	0/4/4/4
26	PEB	N1	201	1	-	6/24/74/74	0/4/4/4
26	PEB	sE	201	1	-	14/24/74/74	0/4/4/4
26	PEB	TI	203	2	-	11/24/74/74	0/4/4/4
26	PEB	Y3	301	7	-	14/24/74/74	0/4/4/4
26	PEB	M9	202	2	-	10/24/74/74	0/4/4/4
26	PEB	wG	301	13	-	11/24/74/74	0/4/4/4
26	PEB	OJ	201	2	-	14/24/74/74	0/4/4/4
26	PEB	u4	203	2	-	2/24/74/74	0/4/4/4
26	PEB	fl	202	1	-	10/24/74/74	0/4/4/4
26	PEB	HE	201	2	-	11/24/74/74	0/4/4/4
26	PEB	YE	201	1	-	10/24/74/74	0/4/4/4
26	PEB	ZF	203	1	-	7/24/74/74	0/4/4/4
26	PEB	YA	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	JJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	cE	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	AG	201	1	-	9/24/74/74	0/4/4/4
26	PEB	G3	201	1	-	9/24/74/74	0/4/4/4
26	PEB	FI	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	S4	201	2,4	-	10/24/74/74	0/4/4/4
26	PEB	eE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	j8	201	1	-	7/24/74/74	0/4/4/4
26	PEB	lF	203	1	-	13/24/74/74	0/4/4/4
26	PEB	W9	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	UB	203	1	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	21	401	3	-	15/24/74/74	0/4/4/4
26	PEB	c7	201	2	-	7/24/74/74	0/4/4/4
26	PEB	E4	201	1	-	10/24/74/74	0/4/4/4
26	PEB	j1	201	2,4	-	12/24/74/74	0/4/4/4
26	PEB	M8	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	P3	201	2,11	-	9/24/74/74	0/4/4/4
26	PEB	VJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	J4	201	2	-	11/24/74/74	0/4/4/4
26	PEB	A7	305	7	-	12/24/74/74	0/4/4/4
26	PEB	SF	202	1	-	8/24/74/74	0/4/4/4
26	PEB	W1	201	2	-	8/24/74/74	0/4/4/4
26	PEB	T4	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	Y3	304	7,26	-	13/24/74/74	0/4/4/4
26	PEB	n4	202	2	-	7/24/74/74	0/4/4/4
28	CYC	VH	1001	-	-	11/25/74/74	0/4/4/4
26	PEB	H8	201	2	-	6/24/74/74	0/4/4/4
26	PEB	KC	201	2	-	5/24/74/74	0/4/4/4
26	PEB	d1	201	2	-	8/24/74/74	0/4/4/4
26	PEB	gI	203	2	-	10/24/74/74	0/4/4/4
26	PEB	oE	201	1	-	9/24/74/74	0/4/4/4
28	CYC	E2	1001	9	-	8/25/74/74	0/4/4/4
26	PEB	HG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	N3	202	2	-	8/24/74/74	0/4/4/4
26	PEB	b7	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	i1	203	1	-	10/24/74/74	0/4/4/4
26	PEB	MA	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	k7	201	2	-	10/24/74/74	0/4/4/4
28	CYC	G7	1001	9,10	-	10/25/74/74	0/4/4/4
26	PEB	BJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	TA	201	2	-	7/24/74/74	0/4/4/4
26	PEB	K8	201	1	-	6/24/74/74	0/4/4/4
26	PEB	C5	203	2	-	8/24/74/74	0/4/4/4
26	PEB	HF	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	F1	201	3,2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	vE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	Q4	201	2	-	4/24/74/74	0/4/4/4
26	PEB	Q3	202	1	-	9/24/74/74	0/4/4/4
26	PEB	KA	201	1	-	6/24/74/74	0/4/4/4
26	PEB	F1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	F8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	aE	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	X8	201	2	-	6/24/74/74	0/4/4/4
26	PEB	JJ	201	1	-	14/24/74/74	0/4/4/4
27	PUB	xG	306	13	-	6/24/74/74	0/4/4/4
26	PEB	a4	203	2	-	10/24/74/74	0/4/4/4
26	PEB	V9	201	1	-	12/24/74/74	0/4/4/4
26	PEB	ZF	202	1	-	9/24/74/74	0/4/4/4
26	PEB	VA	201	2	-	7/24/74/74	0/4/4/4
26	PEB	NE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	H5	202	2	-	8/24/74/74	0/4/4/4
26	PEB	i2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	L6	1002	9,10	-	10/24/74/74	0/4/4/4
26	PEB	g8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	l8	203	1	-	9/24/74/74	0/4/4/4
26	PEB	UB	202	1	-	9/24/74/74	0/4/4/4
26	PEB	T8	202	2	-	7/24/74/74	0/4/4/4
26	PEB	Q6	203	1	-	10/24/74/74	0/4/4/4
26	PEB	Y3	303	7,26	-	16/24/74/74	0/4/4/4
26	PEB	VJ	201	1	-	7/24/74/74	0/4/4/4
26	PEB	z1	201	1	-	11/24/74/74	0/4/4/4
26	PEB	i1	202	1	-	5/24/74/74	0/4/4/4
26	PEB	qE	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	F9	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	VD	202	2	-	10/24/74/74	0/4/4/4
28	CYC	H6	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	j7	202	1	-	7/24/74/74	0/4/4/4
26	PEB	IC	201	2	-	3/24/74/74	0/4/4/4
26	PEB	J8	202	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	Q7	202	1	-	8/24/74/74	0/4/4/4
26	PEB	b6	202	1	-	10/24/74/74	0/4/4/4
26	PEB	V3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	R1	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	KJ	201	2	-	9/24/74/74	0/4/4/4
28	CYC	FF	1001	10	-	6/25/74/74	0/4/4/4
26	PEB	J3	201	2,7	-	7/24/74/74	0/4/4/4
26	PEB	D2	1002	10	-	6/24/74/74	0/4/4/4
26	PEB	F4	203	2	-	9/24/74/74	0/4/4/4
26	PEB	q1	202	2	-	9/24/74/74	0/4/4/4
28	CYC	HI	1001	10	-	7/25/74/74	0/4/4/4
27	PUB	A9	302	1,7	-	8/24/74/74	0/4/4/4
28	CYC	D2	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	B3	203	2	-	10/24/74/74	0/4/4/4
26	PEB	Y7	201	2	-	10/24/74/74	0/4/4/4
28	CYC	jH	1001	22,18	-	8/25/74/74	0/4/4/4
26	PEB	dI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	IJ	201	2,15	-	9/24/74/74	0/4/4/4
26	PEB	R6	201	2	-	8/24/74/74	0/4/4/4
26	PEB	XG	203	2	-	11/24/74/74	0/4/4/4
26	PEB	iA	202	2	-	9/24/74/74	0/4/4/4
28	CYC	sH	1001	22,18	-	8/25/74/74	0/4/4/4
26	PEB	d6	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	BD	203	2	-	12/24/74/74	0/4/4/4
26	PEB	gF	201	2	-	10/24/74/74	0/4/4/4
26	PEB	lB	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	WF	201	1	-	8/24/74/74	0/4/4/4
26	PEB	w4	202	2	-	5/24/74/74	0/4/4/4
26	PEB	PD	201	2	-	4/24/74/74	0/4/4/4
26	PEB	O2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	O7	201	1	-	10/24/74/74	0/4/4/4
26	PEB	QD	201	1	-	6/24/74/74	0/4/4/4
26	PEB	j7	201	1	-	11/24/74/74	0/4/4/4
26	PEB	ID	202	1	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	kG	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	T9	203	1	-	13/24/74/74	0/4/4/4
26	PEB	FJ	201	1	-	12/24/74/74	0/4/4/4
26	PEB	z1	202	1	-	16/24/74/74	0/4/4/4
27	PUB	AA	304	13	-	10/24/74/74	0/4/4/4
26	PEB	C5	204	2	-	10/24/74/74	0/4/4/4
28	CYC	D6	1001	10	-	11/25/74/74	0/4/4/4
26	PEB	m2	201	2	-	9/24/74/74	0/4/4/4
26	PEB	ME	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	UA	203	3,1	-	8/24/74/74	0/4/4/4
26	PEB	QD	202	1	-	9/24/74/74	0/4/4/4
26	PEB	Q2	202	10,1	-	11/24/74/74	0/4/4/4
26	PEB	L2	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	y4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	A5	201	2	-	11/24/74/74	0/4/4/4
26	PEB	OG	203	1	-	10/24/74/74	0/4/4/4
26	PEB	H9	203	1	-	12/24/74/74	0/4/4/4
26	PEB	J5	201	1	-	9/24/74/74	0/4/4/4
26	PEB	M3	201	1	-	10/24/74/74	0/4/4/4
26	PEB	OB	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	SE	203	1	-	10/24/74/74	0/4/4/4
26	PEB	iG	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	jI	202	1	-	8/24/74/74	0/4/4/4
26	PEB	wE	302	13	-	11/24/74/74	0/4/4/4
26	PEB	T4	202	1	-	9/24/74/74	0/4/4/4
28	CYC	E6	1001	9,10	-	6/25/74/74	0/4/4/4
26	PEB	B4	203	2	-	12/24/74/74	0/4/4/4
26	PEB	SD	202	1	-	8/24/74/74	0/4/4/4
26	PEB	JG	201	2	-	8/24/74/74	0/4/4/4
26	PEB	p4	202	1	-	16/24/74/74	0/4/4/4
26	PEB	JG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	P4	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	HC	203	2	-	12/24/74/74	0/4/4/4
26	PEB	R8	201	2	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	U6	203	1	-	13/24/74/74	0/4/4/4
26	PEB	WD	202	1	-	12/24/74/74	0/4/4/4
26	PEB	K4	201	1	-	6/24/74/74	0/4/4/4
26	PEB	IE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	jF	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	Q3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	hB	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	XJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	M4	401	3	-	12/24/74/74	0/4/4/4
26	PEB	eB	202	2	-	6/24/74/74	0/4/4/4
26	PEB	TJ	201	2,1	-	14/24/74/74	0/4/4/4
28	CYC	AH	1001	17	-	7/25/74/74	0/4/4/4
26	PEB	SG	203	1	-	9/24/74/74	0/4/4/4
26	PEB	cI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	h7	202	1	-	14/24/74/74	0/4/4/4
28	CYC	F7	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	x4	201	1	-	11/24/74/74	0/4/4/4
28	CYC	NF	1001	8,10	-	8/25/74/74	0/4/4/4
26	PEB	TB	201	2	-	3/24/74/74	0/4/4/4
26	PEB	A2	301	7	-	8/24/74/74	0/4/4/4
26	PEB	x1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	g1	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	dG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	V6	202	2	-	10/24/74/74	0/4/4/4
28	CYC	GH	1001	17	-	9/25/74/74	0/4/4/4
28	CYC	CI	1001	9	-	9/25/74/74	0/4/4/4
26	PEB	B9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	iB	201	2	-	10/24/74/74	0/4/4/4
26	PEB	ND	203	2	-	8/24/74/74	0/4/4/4
27	PUB	KD	203	1,7	-	6/24/74/74	0/4/4/4
28	CYC	K7	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	dB	201	1,7	-	9/24/74/74	0/4/4/4
26	PEB	e6	203	2	-	13/24/74/74	0/4/4/4
26	PEB	bB	201	1	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	IF	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	IG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	DE	202	2,1	-	11/24/74/74	0/4/4/4
26	PEB	a4	201	2	-	4/24/74/74	0/4/4/4
26	PEB	f8	202	1	-	8/24/74/74	0/4/4/4
26	PEB	PI	202	2	-	6/24/74/74	0/4/4/4
26	PEB	AI	304	7	-	9/24/74/74	0/4/4/4
26	PEB	Y2	202	2	-	6/24/74/74	0/4/4/4
26	PEB	I9	201	2,15	-	7/24/74/74	0/4/4/4
26	PEB	K9	201	2	-	9/24/74/74	0/4/4/4
26	PEB	O6	202	1	-	10/24/74/74	0/4/4/4
26	PEB	L7	1002	10	-	10/24/74/74	0/4/4/4
26	PEB	L4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	BG	201	2,16	-	11/24/74/74	0/4/4/4
26	PEB	c6	201	2	-	5/24/74/74	0/4/4/4
26	PEB	R9	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	D6	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	k4	202	1	-	5/24/74/74	0/4/4/4
26	PEB	R3	203	2	-	12/24/74/74	0/4/4/4
26	PEB	N4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	WE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	EJ	202	2	-	7/24/74/74	0/4/4/4
26	PEB	B8	301	14	-	12/24/74/74	0/4/4/4
26	PEB	QG	202	1	-	7/24/74/74	0/4/4/4
26	PEB	Y1	201	2	-	7/24/74/74	0/4/4/4
26	PEB	SG	202	1	-	7/24/74/74	0/4/4/4
26	PEB	UB	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	V4	201	1	-	7/24/74/74	0/4/4/4
26	PEB	GG	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	WA	202	1	-	12/24/74/74	0/4/4/4
26	PEB	L3	201	2,26	-	5/24/74/74	0/4/4/4
26	PEB	g1	202	1	-	7/24/74/74	0/4/4/4
26	PEB	V6	201	2	-	8/24/74/74	0/4/4/4
27	PUB	BA	302	14	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	QB	203	1	-	10/24/74/74	0/4/4/4
26	PEB	C8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	AB	304	7	-	4/24/74/74	0/4/4/4
26	PEB	B9	201	1	-	11/24/74/74	0/4/4/4
26	PEB	T7	201	2,6	-	8/24/74/74	0/4/4/4
26	PEB	L9	203	1	-	11/24/74/74	0/4/4/4
26	PEB	XD	203	2	-	12/24/74/74	0/4/4/4
26	PEB	LG	202	2	-	14/24/74/74	0/4/4/4
26	PEB	VI	202	2	-	12/24/74/74	0/4/4/4
26	PEB	aG	203	1	-	11/24/74/74	0/4/4/4
26	PEB	O8	202	1	-	10/24/74/74	0/4/4/4
26	PEB	a8	201	1,13	-	10/24/74/74	0/4/4/4
26	PEB	cA	202	2,1	-	9/24/74/74	0/4/4/4
28	CYC	FB	1001	10	-	5/25/74/74	0/4/4/4
26	PEB	G9	202	2	-	13/24/74/74	0/4/4/4
26	PEB	m4	203	1	-	11/24/74/74	0/4/4/4
26	PEB	U7	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	X1	203	1	-	8/24/74/74	0/4/4/4
26	PEB	MD	201	1	-	10/24/74/74	0/4/4/4
26	PEB	m6	202	2	-	7/24/74/74	0/4/4/4
26	PEB	DE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	T1	202	1	-	8/24/74/74	0/4/4/4
26	PEB	K6	201	9,10	-	6/24/74/74	0/4/4/4
28	CYC	MI	1001	9	-	8/25/74/74	0/4/4/4
26	PEB	KC	203	2	-	8/24/74/74	0/4/4/4
26	PEB	gI	202	2	-	8/24/74/74	0/4/4/4
26	PEB	eI	201	2	-	5/24/74/74	0/4/4/4
26	PEB	Y2	201	2	-	3/24/74/74	0/4/4/4
26	PEB	k7	202	2	-	11/24/74/74	0/4/4/4
26	PEB	UJ	201	2,7	-	11/24/74/74	0/4/4/4
26	PEB	G5	203	2	-	12/24/74/74	0/4/4/4
26	PEB	r1	202	1	-	16/24/74/74	0/4/4/4
26	PEB	h1	201	2,4	-	9/24/74/74	0/4/4/4
26	PEB	O1	201	2,4	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	X3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	g4	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	U4	202	2	-	10/24/74/74	0/4/4/4
26	PEB	e8	201	2,13	-	6/24/74/74	0/4/4/4
26	PEB	U3	202	1	-	11/24/74/74	0/4/4/4
28	CYC	EB	1001	9,10	-	6/25/74/74	0/4/4/4
26	PEB	M1	402	3,26	-	13/24/74/74	0/4/4/4
26	PEB	kA	201	2	-	10/24/74/74	0/4/4/4
26	PEB	t4	202	1	-	18/24/74/74	0/4/4/4
26	PEB	h8	203	1	-	9/24/74/74	0/4/4/4
26	PEB	H3	201	2	-	4/24/74/74	0/4/4/4
26	PEB	VA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	U2	201	1	-	9/24/74/74	0/4/4/4
26	PEB	V8	202	2	-	10/24/74/74	0/4/4/4
26	PEB	g8	201	2	-	9/24/74/74	0/4/4/4
26	PEB	uE	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	AC	202	2	-	8/24/74/74	0/4/4/4
26	PEB	yG	301	14	-	8/24/74/74	0/4/4/4
26	PEB	HJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	QF	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	F5	202	2	-	11/24/74/74	0/4/4/4
26	PEB	HD	202	2	-	8/24/74/74	0/4/4/4
26	PEB	PF	201	2,6	-	5/24/74/74	0/4/4/4
26	PEB	C1	201	1	-	7/24/74/74	0/4/4/4
26	PEB	H7	1002	10	-	6/24/74/74	0/4/4/4
26	PEB	DD	203	2	-	11/24/74/74	0/4/4/4
26	PEB	KG	201	2,1	-	6/24/74/74	0/4/4/4
28	CYC	L2	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	l4	202	2	-	7/24/74/74	0/4/4/4
27	PUB	A6	302	7	-	9/24/74/74	0/4/4/4
26	PEB	YA	202	1	-	4/24/74/74	0/4/4/4
26	PEB	AD	201	1	-	11/24/74/74	0/4/4/4
26	PEB	gI	201	2	-	4/24/74/74	0/4/4/4
26	PEB	fG	202	2	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PUB	21	402	3	-	9/24/74/74	0/4/4/4
26	PEB	LD	201	2,26	-	6/24/74/74	0/4/4/4
26	PEB	A3	202	1	-	13/24/74/74	0/4/4/4
26	PEB	KG	202	1	-	4/24/74/74	0/4/4/4
26	PEB	24	404	3	-	12/24/74/74	0/4/4/4
26	PEB	vG	202	2	-	9/24/74/74	0/4/4/4
26	PEB	d8	202	1	-	5/24/74/74	0/4/4/4
26	PEB	K3	202	1	-	7/24/74/74	0/4/4/4
26	PEB	AD	202	1	-	12/24/74/74	0/4/4/4
26	PEB	X3	201	2,11	-	6/24/74/74	0/4/4/4
26	PEB	C5	201	2	-	8/24/74/74	0/4/4/4
26	PEB	21	404	3	-	7/24/74/74	0/4/4/4
26	PEB	U7	203	1	-	8/24/74/74	0/4/4/4
26	PEB	C4	202	1	-	13/24/74/74	0/4/4/4
28	CYC	LB	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	TA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	OE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	LA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	S2	201	1	-	7/24/74/74	0/4/4/4
26	PEB	HJ	201	2,1	-	14/24/74/74	0/4/4/4
26	PEB	lA	202	1	-	5/24/74/74	0/4/4/4
26	PEB	UG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	V8	201	2	-	7/24/74/74	0/4/4/4
26	PEB	eA	201	2,13	-	6/24/74/74	0/4/4/4
26	PEB	x1	202	1	-	13/24/74/74	0/4/4/4
26	PEB	MJ	202	2	-	10/24/74/74	0/4/4/4
26	PEB	11	202	2	-	10/24/74/74	0/4/4/4
27	PUB	A1	203	3,1	-	6/24/74/74	0/4/4/4
26	PEB	BC	201	2	-	8/24/74/74	0/4/4/4
26	PEB	jA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	lB	203	1	-	7/24/74/74	0/4/4/4
26	PEB	GE	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	YB	202	2	-	12/24/74/74	0/4/4/4
26	PEB	X4	203	1	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	hF	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	H4	203	2	-	10/24/74/74	0/4/4/4
26	PEB	s4	202	2	-	8/24/74/74	0/4/4/4
28	CYC	I7	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	CE	201	2,1	-	7/24/74/74	0/4/4/4
27	PUB	A6	303	7	-	8/24/74/74	0/4/4/4
26	PEB	jG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	zE	501	2,16	-	6/24/74/74	0/4/4/4
26	PEB	bB	202	1	-	7/24/74/74	0/4/4/4
26	PEB	ED	202	1	-	11/24/74/74	0/4/4/4
26	PEB	Y4	201	2	-	7/24/74/74	0/4/4/4
26	PEB	Q1	201	2	-	4/24/74/74	0/4/4/4
26	PEB	VG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	T9	202	1	-	9/24/74/74	0/4/4/4
26	PEB	jE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	QF	203	1	-	9/24/74/74	0/4/4/4
28	CYC	DF	1001	10	-	6/25/74/74	0/4/4/4
26	PEB	fF	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	D8	201	14,2	-	10/24/74/74	0/4/4/4
26	PEB	u4	202	2	-	7/24/74/74	0/4/4/4
28	CYC	LI	1001	10	-	5/25/74/74	0/4/4/4
26	PEB	dB	203	1	-	7/24/74/74	0/4/4/4
26	PEB	PA	201	2	-	10/24/74/74	0/4/4/4
26	PEB	AI	301	7	-	7/24/74/74	0/4/4/4
26	PEB	hI	201	1	-	10/24/74/74	0/4/4/4
27	PUB	AI	302	7	-	2/24/74/74	0/4/4/4
26	PEB	sE	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	R8	202	2	-	11/24/74/74	0/4/4/4
26	PEB	W8	201	1	-	7/24/74/74	0/4/4/4
26	PEB	UG	201	1	-	8/24/74/74	0/4/4/4
28	CYC	YH	1003	22	-	8/25/74/74	0/4/4/4
26	PEB	B3	201	2,26	-	6/24/74/74	0/4/4/4
26	PEB	DG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	cI	201	2	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	JA	202	2	-	9/24/74/74	0/4/4/4
28	CYC	GI	1001	9	-	6/25/74/74	0/4/4/4
26	PEB	MJ	201	2	-	7/24/74/74	0/4/4/4
26	PEB	P4	202	1	-	7/24/74/74	0/4/4/4
26	PEB	GG	203	1	-	9/24/74/74	0/4/4/4
28	CYC	G2	1001	9	-	6/25/74/74	0/4/4/4
26	PEB	HA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	w4	203	2	-	5/24/74/74	0/4/4/4
26	PEB	cI	202	2	-	11/24/74/74	0/4/4/4
26	PEB	eG	203	1	-	9/24/74/74	0/4/4/4
26	PEB	CC	202	-	-	7/24/74/74	0/4/4/4
26	PEB	a6	201	2	-	5/24/74/74	0/4/4/4
28	CYC	K6	202	9,10	-	9/25/74/74	0/4/4/4
26	PEB	u1	201	3,2	-	14/24/74/74	0/4/4/4
26	PEB	H5	203	2	-	12/24/74/74	0/4/4/4
26	PEB	ND	201	2	-	3/24/74/74	0/4/4/4
26	PEB	eB	201	2	-	9/24/74/74	0/4/4/4
27	PUB	yE	303	14	-	6/24/74/74	0/4/4/4
26	PEB	H4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	k8	201	2	-	11/24/74/74	0/4/4/4
26	PEB	R7	201	2	-	5/24/74/74	0/4/4/4
26	PEB	L8	202	2	-	9/24/74/74	0/4/4/4
28	CYC	KF	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	RG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	y1	201	2	-	11/24/74/74	0/4/4/4
26	PEB	JC	202	1	-	7/24/74/74	0/4/4/4
26	PEB	fA	201	1	-	9/24/74/74	0/4/4/4
26	PEB	V1	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	UD	201	1	-	5/24/74/74	0/4/4/4
26	PEB	fB	201	1	-	11/24/74/74	0/4/4/4
26	PEB	FA	202	2	-	8/24/74/74	0/4/4/4
26	PEB	R4	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	V2	202	2	-	12/24/74/74	0/4/4/4
26	PEB	GC	203	2	-	14/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	W4	201	2	-	8/24/74/74	0/4/4/4
28	CYC	L7	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	iI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	uG	203	1	-	9/24/74/74	0/4/4/4
26	PEB	Z7	203	1	-	7/24/74/74	0/4/4/4
26	PEB	fA	202	1	-	10/24/74/74	0/4/4/4
26	PEB	A6	301	7	-	10/24/74/74	0/4/4/4
26	PEB	f1	201	2	-	9/24/74/74	0/4/4/4
28	CYC	C2	1001	9	-	7/25/74/74	0/4/4/4
26	PEB	A5	202	2	-	10/24/74/74	0/4/4/4
26	PEB	IE	201	1	-	9/24/74/74	0/4/4/4
26	PEB	KD	202	1	-	10/24/74/74	0/4/4/4
26	PEB	c6	202	2	-	10/24/74/74	0/4/4/4
26	PEB	dE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	WE	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	aE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	G4	201	1	-	7/24/74/74	0/4/4/4
26	PEB	l8	202	1	-	5/24/74/74	0/4/4/4
26	PEB	U2	202	1	-	10/24/74/74	0/4/4/4
27	PUB	AF	304	7	-	15/24/74/74	0/4/4/4
26	PEB	Q6	202	1	-	9/24/74/74	0/4/4/4
26	PEB	EG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	R3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	QI	201	1	-	8/24/74/74	0/4/4/4
26	PEB	RB	201	2	-	9/24/74/74	0/4/4/4
26	PEB	cF	201	2	-	6/24/74/74	0/4/4/4
26	PEB	t1	202	1	-	17/24/74/74	0/4/4/4
26	PEB	F9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	QA	204	1	-	12/24/74/74	0/4/4/4
28	CYC	MB	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	QB	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	cE	201	1	-	12/24/74/74	0/4/4/4
26	PEB	E9	202	2	-	7/24/74/74	0/4/4/4
26	PEB	PE	202	2	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	h7	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	TF	202	2	-	15/24/74/74	0/4/4/4
26	PEB	TD	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Q7	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	kE	201	1	-	9/24/74/74	0/4/4/4
26	PEB	g1	201	1	-	6/24/74/74	0/4/4/4
26	PEB	P6	201	2,6	-	4/24/74/74	0/4/4/4
26	PEB	14	202	2	-	6/24/74/74	0/4/4/4
26	PEB	LE	201	2	-	7/24/74/74	0/4/4/4
28	CYC	nH	1001	-	-	4/25/74/74	0/4/4/4
26	PEB	BE	201	2,16	-	9/24/74/74	0/4/4/4
26	PEB	T2	202	2	-	5/24/74/74	0/4/4/4
26	PEB	cA	201	2	-	10/24/74/74	0/4/4/4
26	PEB	k2	201	2	-	7/24/74/74	0/4/4/4
26	PEB	eG	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	FD	201	2,7	-	3/24/74/74	0/4/4/4
26	PEB	b6	201	1	-	6/24/74/74	0/4/4/4
26	PEB	d8	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	cB	201	2	-	6/24/74/74	0/4/4/4
26	PEB	W7	202	1	-	11/24/74/74	0/4/4/4
26	PEB	OD	202	1	-	11/24/74/74	0/4/4/4
26	PEB	R4	202	1	-	9/24/74/74	0/4/4/4
26	PEB	iE	202	1	-	11/24/74/74	0/4/4/4
27	PUB	K3	203	1,7	-	9/24/74/74	0/4/4/4
28	CYC	WH	1001	-	-	9/25/74/74	0/4/4/4
27	PUB	xE	305	13	-	6/24/74/74	0/4/4/4
26	PEB	S1	201	2,4	-	9/24/74/74	0/4/4/4
27	PUB	K4	203	3,1	-	10/24/74/74	0/4/4/4
26	PEB	XG	202	2	-	5/24/74/74	0/4/4/4
26	PEB	y4	203	2	-	11/24/74/74	0/4/4/4
26	PEB	SJ	201	2,7	-	5/24/74/74	0/4/4/4
26	PEB	h6	203	1	-	7/24/74/74	0/4/4/4
26	PEB	wG	302	13	-	9/24/74/74	0/4/4/4
26	PEB	BD	202	2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	dF	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	RA	201	2	-	5/24/74/74	0/4/4/4
26	PEB	a8	203	1	-	11/24/74/74	0/4/4/4
26	PEB	PJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	M8	203	1	-	9/24/74/74	0/4/4/4
26	PEB	B5	201	2	-	8/24/74/74	0/4/4/4
26	PEB	O6	201	1	-	9/24/74/74	0/4/4/4
26	PEB	R3	201	2	-	5/24/74/74	0/4/4/4
28	CYC	DF	1003	9,10	-	10/25/74/74	0/4/4/4
26	PEB	GA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	DI	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	d1	203	2	-	8/24/74/74	0/4/4/4
26	PEB	CJ	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	ZB	203	1	-	9/24/74/74	0/4/4/4
28	CYC	oH	1001	18	-	9/25/74/74	0/4/4/4
26	PEB	D9	203	1	-	10/24/74/74	0/4/4/4
26	PEB	U8	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	H3	203	2	-	14/24/74/74	0/4/4/4
27	PUB	Y3	302	7	-	3/24/74/74	0/4/4/4
26	PEB	PG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	bG	201	2	-	4/24/74/74	0/4/4/4
26	PEB	AF	302	7	-	11/24/74/74	0/4/4/4
27	PUB	21	403	3,1	-	9/24/74/74	0/4/4/4
26	PEB	IJ	203	2	-	9/24/74/74	0/4/4/4
26	PEB	OD	201	1	-	9/24/74/74	0/4/4/4
26	PEB	RE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	l7	203	1	-	8/24/74/74	0/4/4/4
26	PEB	DA	202	2	-	8/24/74/74	0/4/4/4
27	PUB	xE	301	13	-	7/24/74/74	0/4/4/4
28	CYC	LH	1001	-	-	4/25/74/74	0/4/4/4
26	PEB	X1	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	S3	201	1	-	6/24/74/74	0/4/4/4
26	PEB	W6	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	A9	303	7,26	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	HC	202	2	-	8/24/74/74	0/4/4/4
26	PEB	DF	1002	10	-	11/24/74/74	0/4/4/4
26	PEB	kF	201	2	-	8/24/74/74	0/4/4/4
26	PEB	y1	203	2	-	8/24/74/74	0/4/4/4
26	PEB	c4	201	1	-	11/24/74/74	0/4/4/4
26	PEB	jF	202	1	-	8/24/74/74	0/4/4/4
26	PEB	rE	201	2,13	-	9/24/74/74	0/4/4/4
26	PEB	S8	202	1	-	10/24/74/74	0/4/4/4
26	PEB	PI	203	2	-	6/24/74/74	0/4/4/4
26	PEB	a8	202	1	-	6/24/74/74	0/4/4/4
26	PEB	AA	302	13	-	10/24/74/74	0/4/4/4
26	PEB	f2	202	1	-	10/24/74/74	0/4/4/4
26	PEB	h2	201	1	-	10/24/74/74	0/4/4/4
26	PEB	f7	201	1	-	10/24/74/74	0/4/4/4
26	PEB	14	203	2	-	8/24/74/74	0/4/4/4
26	PEB	I1	202	1	-	10/24/74/74	0/4/4/4
26	PEB	h8	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	H1	203	2	-	11/24/74/74	0/4/4/4
26	PEB	YE	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	G1	202	1	-	11/24/74/74	0/4/4/4
26	PEB	m8	202	2	-	10/24/74/74	0/4/4/4
26	PEB	V1	201	1	-	7/24/74/74	0/4/4/4
26	PEB	f4	201	2	-	9/24/74/74	0/4/4/4
26	PEB	P4	203	1	-	12/24/74/74	0/4/4/4
28	CYC	NH	1001	17	-	7/25/74/74	0/4/4/4
26	PEB	A4	201	1	-	12/24/74/74	0/4/4/4
27	PUB	A2	303	7	-	7/24/74/74	0/4/4/4
26	PEB	QJ	202	2	-	10/24/74/74	0/4/4/4
26	PEB	k1	201	1	-	8/24/74/74	0/4/4/4
26	PEB	IA	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	JD	203	2	-	16/24/74/74	0/4/4/4
26	PEB	hA	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	iF	201	2	-	8/24/74/74	0/4/4/4
26	PEB	gA	201	2	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	GE	203	1	-	10/24/74/74	0/4/4/4
26	PEB	a1	203	2	-	9/24/74/74	0/4/4/4
26	PEB	jG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	dB	204	1	-	11/24/74/74	0/4/4/4
26	PEB	h4	201	2,4	-	8/24/74/74	0/4/4/4
26	PEB	PF	202	2	-	8/24/74/74	0/4/4/4
26	PEB	J9	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	m7	201	2	-	9/24/74/74	0/4/4/4
26	PEB	A1	202	1	-	11/24/74/74	0/4/4/4
28	CYC	I6	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	gE	201	1	-	8/24/74/74	0/4/4/4
26	PEB	iE	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	QF	202	1	-	13/24/74/74	0/4/4/4
26	PEB	AJ	301	7	-	11/24/74/74	0/4/4/4
26	PEB	pE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	U6	202	1	-	9/24/74/74	0/4/4/4
26	PEB	V3	203	2	-	8/24/74/74	0/4/4/4
28	CYC	G6	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	FC	202	2	-	10/24/74/74	0/4/4/4
26	PEB	DG	202	2,1	-	12/24/74/74	0/4/4/4
26	PEB	v4	201	1	-	10/24/74/74	0/4/4/4
26	PEB	RJ	202	1	-	11/24/74/74	0/4/4/4
26	PEB	g6	201	2	-	6/24/74/74	0/4/4/4
26	PEB	QB	202	1	-	8/24/74/74	0/4/4/4
26	PEB	L1	202	2	-	10/24/74/74	0/4/4/4
26	PEB	i6	202	2	-	10/24/74/74	0/4/4/4
26	PEB	m2	203	2	-	9/24/74/74	0/4/4/4
26	PEB	i7	202	2	-	8/24/74/74	0/4/4/4
26	PEB	a1	202	2	-	6/24/74/74	0/4/4/4
26	PEB	s1	201	2	-	10/24/74/74	0/4/4/4
26	PEB	e3	401	1,11	-	9/24/74/74	0/4/4/4
26	PEB	L9	202	1	-	9/24/74/74	0/4/4/4
26	PEB	dE	202	2	-	12/24/74/74	0/4/4/4
28	CYC	QH	1001	22,18	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	ZI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	LG	201	2	-	9/24/74/74	0/4/4/4
26	PEB	aG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	eA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	xE	302	13	-	11/24/74/74	0/4/4/4
26	PEB	m4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	YJ	202	2	-	8/24/74/74	0/4/4/4
27	PUB	N9	201	1,7	-	3/24/74/74	0/4/4/4
26	PEB	A8	301	13	-	13/24/74/74	0/4/4/4
26	PEB	JD	202	2	-	10/24/74/74	0/4/4/4
26	PEB	c1	201	1	-	11/24/74/74	0/4/4/4
26	PEB	C9	202	2	-	7/24/74/74	0/4/4/4
26	PEB	R1	202	1	-	10/24/74/74	0/4/4/4
26	PEB	U1	202	2	-	8/24/74/74	0/4/4/4
28	CYC	gH	1001	17	-	9/25/74/74	0/4/4/4
26	PEB	b4	501	2,4	-	9/24/74/74	0/4/4/4
26	PEB	UF	202	1	-	6/24/74/74	0/4/4/4
26	PEB	fE	201	2,13	-	10/24/74/74	0/4/4/4
26	PEB	DB	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	G5	202	2	-	7/24/74/74	0/4/4/4
26	PEB	IA	202	1	-	4/24/74/74	0/4/4/4
26	PEB	SF	201	1	-	5/24/74/74	0/4/4/4
28	CYC	qH	1001	-	-	5/25/74/74	0/4/4/4
26	PEB	TG	202	2	-	15/24/74/74	0/4/4/4
26	PEB	TE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	QA	203	1	-	5/24/74/74	0/4/4/4
26	PEB	w1	201	3,2	-	13/24/74/74	0/4/4/4
26	PEB	aB	202	2	-	13/24/74/74	0/4/4/4
27	PUB	AF	303	7	-	5/24/74/74	0/4/4/4
26	PEB	U9	201	2,7	-	9/24/74/74	0/4/4/4
26	PEB	HG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	iI	202	2	-	8/24/74/74	0/4/4/4
26	PEB	I3	202	1	-	12/24/74/74	0/4/4/4
26	PEB	A7	301	7	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	YG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	wE	301	13	-	10/24/74/74	0/4/4/4
28	CYC	TH	1001	17	-	10/25/74/74	0/4/4/4
26	PEB	KD	201	1	-	7/24/74/74	0/4/4/4
27	PUB	xG	301	13	-	7/24/74/74	0/4/4/4
26	PEB	FE	201	2	-	5/24/74/74	0/4/4/4
26	PEB	T4	203	1	-	9/24/74/74	0/4/4/4
26	PEB	xE	304	13	-	9/24/74/74	0/4/4/4
26	PEB	D3	201	2,7	-	6/24/74/74	0/4/4/4
26	PEB	d6	201	1,7	-	11/24/74/74	0/4/4/4
26	PEB	kI	203	2	-	12/24/74/74	0/4/4/4
28	CYC	LF	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	cE	202	1	-	13/24/74/74	0/4/4/4
26	PEB	F3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	C8	202	1	-	9/24/74/74	0/4/4/4
26	PEB	w4	201	3,2	-	12/24/74/74	0/4/4/4
26	PEB	PA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	bG	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RE	202	2	-	15/24/74/74	0/4/4/4
26	PEB	aA	203	1	-	11/24/74/74	0/4/4/4
26	PEB	gG	202	1	-	11/24/74/74	0/4/4/4
26	PEB	D7	1002	10	-	11/24/74/74	0/4/4/4
26	PEB	UF	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	j4	201	2,4	-	10/24/74/74	0/4/4/4
26	PEB	ZA	201	2	-	4/24/74/74	0/4/4/4
26	PEB	P3	203	2	-	7/24/74/74	0/4/4/4
26	PEB	Y8	203	1	-	10/24/74/74	0/4/4/4
26	PEB	D1	203	2	-	11/24/74/74	0/4/4/4
26	PEB	s4	203	2	-	7/24/74/74	0/4/4/4
28	CYC	RH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	P6	202	2	-	14/24/74/74	0/4/4/4
26	PEB	C3	202	1	-	9/24/74/74	0/4/4/4
26	PEB	WB	202	1	-	8/24/74/74	0/4/4/4
26	PEB	jB	202	1	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	e2	203	2	-	8/24/74/74	0/4/4/4
26	PEB	k2	203	2	-	12/24/74/74	0/4/4/4
26	PEB	bF	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	qE	202	1	-	11/24/74/74	0/4/4/4
26	PEB	LC	203	2	-	11/24/74/74	0/4/4/4
26	PEB	g4	202	1	-	7/24/74/74	0/4/4/4
26	PEB	LD	203	2	-	9/24/74/74	0/4/4/4
26	PEB	RI	203	2	-	9/24/74/74	0/4/4/4
26	PEB	lE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	UE	201	1	-	8/24/74/74	0/4/4/4
26	PEB	D4	203	2	-	11/24/74/74	0/4/4/4
26	PEB	W3	202	1	-	12/24/74/74	0/4/4/4
26	PEB	C4	201	1	-	7/24/74/74	0/4/4/4
28	CYC	UH	1001	-	-	8/25/74/74	0/4/4/4
26	PEB	LJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	N9	202	1	-	11/24/74/74	0/4/4/4
26	PEB	h6	202	1	-	11/24/74/74	0/4/4/4
26	PEB	d4	201	2	-	10/24/74/74	0/4/4/4
26	PEB	kB	201	2,7	-	7/24/74/74	0/4/4/4
26	PEB	WD	201	1	-	7/24/74/74	0/4/4/4
27	PUB	Q8	201	14,1	-	7/24/74/74	0/4/4/4
26	PEB	S1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	ZB	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	jA	202	1	-	9/24/74/74	0/4/4/4
26	PEB	JE	201	2	-	8/24/74/74	0/4/4/4
26	PEB	kI	202	2	-	13/24/74/74	0/4/4/4
26	PEB	TJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	XG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	dI	201	1	-	8/24/74/74	0/4/4/4
26	PEB	F3	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	k4	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	YI	203	2	-	11/24/74/74	0/4/4/4
26	PEB	d4	202	2,1	-	8/24/74/74	0/4/4/4
26	PEB	m1	201	2,1	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	O1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	fF	201	1	-	9/24/74/74	0/4/4/4
26	PEB	DD	202	2	-	14/24/74/74	0/4/4/4
28	CYC	vH	1001	17	-	9/25/74/74	0/4/4/4
26	PEB	YA	203	1	-	11/24/74/74	0/4/4/4
26	PEB	CC	203	2	-	10/24/74/74	0/4/4/4
26	PEB	aF	202	2	-	10/24/74/74	0/4/4/4
26	PEB	ZE	202	2	-	10/24/74/74	0/4/4/4
26	PEB	H9	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	W1	202	2	-	5/24/74/74	0/4/4/4
26	PEB	N3	201	2	-	3/24/74/74	0/4/4/4
26	PEB	e1	202	1	-	12/24/74/74	0/4/4/4
28	CYC	CB	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	l2	202	1	-	8/24/74/74	0/4/4/4
26	PEB	J4	203	2	-	9/24/74/74	0/4/4/4
26	PEB	BC	203	2	-	11/24/74/74	0/4/4/4
26	PEB	sE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	P1	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	E3	201	1	-	9/24/74/74	0/4/4/4
26	PEB	bF	202	1	-	8/24/74/74	0/4/4/4
26	PEB	mA	201	2,13	-	9/24/74/74	0/4/4/4
28	CYC	lH	1001	18,17	-	7/25/74/74	0/4/4/4
26	PEB	SA	201	1	-	10/24/74/74	0/4/4/4
26	PEB	jF	201	1	-	9/24/74/74	0/4/4/4
26	PEB	y4	201	2	-	12/24/74/74	0/4/4/4
26	PEB	oE	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	m6	203	2	-	8/24/74/74	0/4/4/4
26	PEB	h6	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	L4	201	3,2	-	13/24/74/74	0/4/4/4
26	PEB	PB	202	2	-	12/24/74/74	0/4/4/4
27	PUB	QA	201	14,1	-	8/24/74/74	0/4/4/4
26	PEB	Z8	201	2	-	4/24/74/74	0/4/4/4
26	PEB	HE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	GG	202	1	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	k4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	G6	1002	9,10	-	9/24/74/74	0/4/4/4
26	PEB	RF	202	2	-	12/24/74/74	0/4/4/4
26	PEB	OF	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	eG	202	1	-	8/24/74/74	0/4/4/4
26	PEB	cF	202	2	-	11/24/74/74	0/4/4/4
28	CYC	B6	1002	8,10	-	5/25/74/74	0/4/4/4
26	PEB	P7	202	2	-	10/24/74/74	0/4/4/4
26	PEB	RD	203	2	-	11/24/74/74	0/4/4/4
26	PEB	SG	201	2,1	-	4/24/74/74	0/4/4/4
26	PEB	aA	202	1	-	6/24/74/74	0/4/4/4
27	PUB	YD	302	7	-	3/24/74/74	0/4/4/4
26	PEB	F1	203	2	-	9/24/74/74	0/4/4/4
26	PEB	mI	203	2	-	9/24/74/74	0/4/4/4
26	PEB	N1	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	WG	202	1	-	8/24/74/74	0/4/4/4
26	PEB	YI	202	2	-	6/24/74/74	0/4/4/4
26	PEB	aE	203	1	-	11/24/74/74	0/4/4/4
26	PEB	G1	201	1	-	9/24/74/74	0/4/4/4
27	PUB	AI	303	7	-	7/24/74/74	0/4/4/4
26	PEB	JJ	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	q1	201	2	-	12/24/74/74	0/4/4/4
26	PEB	X4	202	1	-	8/24/74/74	0/4/4/4
26	PEB	WA	201	1	-	7/24/74/74	0/4/4/4
26	PEB	V1	202	1	-	10/24/74/74	0/4/4/4
26	PEB	V9	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	CA	201	1	-	4/24/74/74	0/4/4/4
26	PEB	bI	202	1	-	8/24/74/74	0/4/4/4
26	PEB	d2	202	1	-	8/24/74/74	0/4/4/4
28	CYC	DB	1001	10	-	11/25/74/74	0/4/4/4
26	PEB	TD	203	2	-	7/24/74/74	0/4/4/4
26	PEB	GC	202	2	-	7/24/74/74	0/4/4/4
26	PEB	i1	201	2,1	-	12/24/74/74	0/4/4/4
28	CYC	II	1001	9	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	A9	301	7	-	10/24/74/74	0/4/4/4
26	PEB	JC	201	1	-	10/24/74/74	0/4/4/4
26	PEB	G9	201	2	-	4/24/74/74	0/4/4/4
26	PEB	W9	202	2	-	8/24/74/74	0/4/4/4
26	PEB	HJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	E8	202	1	-	9/24/74/74	0/4/4/4
26	PEB	AJ	304	7,26	-	9/24/74/74	0/4/4/4
26	PEB	E4	202	1	-	9/24/74/74	0/4/4/4
26	PEB	F5	203	2	-	10/24/74/74	0/4/4/4
26	PEB	eD	401	1,11	-	9/24/74/74	0/4/4/4
26	PEB	G8	201	1	-	7/24/74/74	0/4/4/4
26	PEB	VB	202	2	-	10/24/74/74	0/4/4/4
26	PEB	A1	201	1	-	5/24/74/74	0/4/4/4
26	PEB	W7	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	H8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	IC	203	2	-	10/24/74/74	0/4/4/4
26	PEB	Z6	202	1	-	9/24/74/74	0/4/4/4
26	PEB	PI	201	2	-	5/24/74/74	0/4/4/4
26	PEB	K8	202	1	-	8/24/74/74	0/4/4/4
26	PEB	Y8	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	YF	201	2	-	7/24/74/74	0/4/4/4
26	PEB	g6	202	2	-	11/24/74/74	0/4/4/4
28	CYC	uH	1001	18	-	8/25/74/74	0/4/4/4
26	PEB	mE	203	1	-	12/24/74/74	0/4/4/4
26	PEB	14	201	2	-	12/24/74/74	0/4/4/4
26	PEB	a2	201	2	-	2/24/74/74	0/4/4/4
26	PEB	t1	201	1	-	13/24/74/74	0/4/4/4
26	PEB	S7	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	t4	201	1	-	9/24/74/74	0/4/4/4
26	PEB	h2	202	1	-	11/24/74/74	0/4/4/4
26	PEB	FE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	vE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	PD	202	2	-	7/24/74/74	0/4/4/4
26	PEB	I5	202	2	-	3/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	E1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	V9	202	1	-	12/24/74/74	0/4/4/4
26	PEB	ID	201	1	-	13/24/74/74	0/4/4/4
26	PEB	A2	304	7	-	10/24/74/74	0/4/4/4
26	PEB	HD	201	2	-	4/24/74/74	0/4/4/4
26	PEB	B1	202	2	-	11/24/74/74	0/4/4/4
26	PEB	Z7	201	2,1	-	12/24/74/74	0/4/4/4
28	CYC	HB	1001	10	-	7/25/74/74	0/4/4/4
28	CYC	KI	1001	9	-	7/25/74/74	0/4/4/4
26	PEB	a6	202	2	-	13/24/74/74	0/4/4/4
26	PEB	kE	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	WF	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	A4	202	1	-	15/24/74/74	0/4/4/4
26	PEB	EA	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	Z2	202	1	-	9/24/74/74	0/4/4/4
26	PEB	Q9	201	2,7	-	2/24/74/74	0/4/4/4
26	PEB	AG	202	1	-	11/24/74/74	0/4/4/4
26	PEB	AF	301	7	-	7/24/74/74	0/4/4/4
28	CYC	EH	1001	17	-	9/25/74/74	0/4/4/4
26	PEB	F4	201	3,2	-	10/24/74/74	0/4/4/4
26	PEB	j7	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	SD	201	1	-	6/24/74/74	0/4/4/4
26	PEB	Q7	203	1	-	9/24/74/74	0/4/4/4
26	PEB	j1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	fB	202	1	-	8/24/74/74	0/4/4/4
26	PEB	R2	203	2	-	9/24/74/74	0/4/4/4
26	PEB	d1	202	2,1	-	4/24/74/74	0/4/4/4
26	PEB	W4	202	2	-	5/24/74/74	0/4/4/4
26	PEB	l6	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	d7	203	1	-	11/24/74/74	0/4/4/4
26	PEB	hG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	jI	201	1	-	11/24/74/74	0/4/4/4
27	PUB	yE	302	14	-	3/24/74/74	0/4/4/4
26	PEB	D9	202	1	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	p4	201	1	-	13/24/74/74	0/4/4/4
26	PEB	KJ	202	2	-	10/24/74/74	0/4/4/4
26	PEB	qG	202	1	-	15/24/74/74	0/4/4/4
26	PEB	GD	202	1	-	13/24/74/74	0/4/4/4
26	PEB	q1	203	2	-	9/24/74/74	0/4/4/4
26	PEB	P2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	k6	202	2	-	11/24/74/74	0/4/4/4
26	PEB	mB	203	2	-	9/24/74/74	0/4/4/4
26	PEB	XJ	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	MG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	EE	202	1	-	10/24/74/74	0/4/4/4
26	PEB	eI	203	2	-	8/24/74/74	0/4/4/4
26	PEB	f7	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	IJ	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RB	202	2	-	11/24/74/74	0/4/4/4
26	PEB	S6	201	1	-	10/24/74/74	0/4/4/4
26	PEB	O2	202	1	-	8/24/74/74	0/4/4/4
26	PEB	11	201	2	-	10/24/74/74	0/4/4/4
26	PEB	xG	304	13	-	9/24/74/74	0/4/4/4
26	PEB	17	202	1	-	11/24/74/74	0/4/4/4
27	PUB	AA	303	13	-	9/24/74/74	0/4/4/4
26	PEB	I8	202	1	-	4/24/74/74	0/4/4/4
26	PEB	W6	202	1	-	8/24/74/74	0/4/4/4
26	PEB	CD	201	1	-	9/24/74/74	0/4/4/4
26	PEB	CD	202	1	-	13/24/74/74	0/4/4/4
26	PEB	ZA	202	2	-	8/24/74/74	0/4/4/4
26	PEB	kE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	WF	202	1	-	9/24/74/74	0/4/4/4
28	CYC	L6	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	cG	201	1	-	11/24/74/74	0/4/4/4
26	PEB	f6	201	1	-	10/24/74/74	0/4/4/4
28	CYC	tH	1001	17	-	10/25/74/74	0/4/4/4
26	PEB	I3	201	1	-	14/24/74/74	0/4/4/4
26	PEB	LC	201	2	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	B6	1001	8,10	-	12/25/74/74	0/4/4/4
26	PEB	YG	201	1	-	7/24/74/74	0/4/4/4
26	PEB	U8	203	3,1	-	7/24/74/74	0/4/4/4
26	PEB	SI	201	1	-	10/24/74/74	0/4/4/4
26	PEB	tG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	R2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	A3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	G8	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	BA	301	14	-	13/24/74/74	0/4/4/4
26	PEB	o1	501	2,4	-	8/24/74/74	0/4/4/4
26	PEB	d7	202	1	-	10/24/74/74	0/4/4/4
26	PEB	v1	201	1	-	11/24/74/74	0/4/4/4
28	CYC	F6	1001	10	-	5/25/74/74	0/4/4/4
26	PEB	LC	202	2	-	10/24/74/74	0/4/4/4
26	PEB	T3	203	2	-	8/24/74/74	0/4/4/4
26	PEB	g2	201	2	-	4/24/74/74	0/4/4/4
26	PEB	H1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	PD	203	2	-	7/24/74/74	0/4/4/4
26	PEB	IG	201	1	-	9/24/74/74	0/4/4/4
26	PEB	FG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	N2	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	N9	204	2,1	-	12/24/74/74	0/4/4/4
26	PEB	dA	201	1	-	4/24/74/74	0/4/4/4
26	PEB	b2	201	1	-	9/24/74/74	0/4/4/4
26	PEB	i2	201	2	-	6/24/74/74	0/4/4/4
26	PEB	FC	203	2	-	11/24/74/74	0/4/4/4
26	PEB	TB	202	2	-	11/24/74/74	0/4/4/4
28	CYC	mH	1001	17	-	7/25/74/74	0/4/4/4
26	PEB	eE	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	LA	201	2	-	4/24/74/74	0/4/4/4
26	PEB	lA	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	D3	202	2	-	11/24/74/74	0/4/4/4
26	PEB	QG	201	1	-	8/24/74/74	0/4/4/4
26	PEB	YI	201	2	-	2/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	CF	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	W6	201	1	-	7/24/74/74	0/4/4/4
26	PEB	AE	201	1	-	9/24/74/74	0/4/4/4
26	PEB	dG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	O4	201	2,4	-	8/24/74/74	0/4/4/4
26	PEB	J9	202	1	-	12/24/74/74	0/4/4/4
26	PEB	K1	202	1	-	12/24/74/74	0/4/4/4
26	PEB	nE	202	2	-	9/24/74/74	0/4/4/4
26	PEB	jA	201	1	-	7/24/74/74	0/4/4/4
28	CYC	YH	1002	22	-	4/25/74/74	0/4/4/4
26	PEB	T1	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	Q8	204	1	-	10/24/74/74	0/4/4/4
26	PEB	E1	202	1	-	13/24/74/74	0/4/4/4
26	PEB	L8	201	2	-	4/24/74/74	0/4/4/4
26	PEB	s4	201	2	-	7/24/74/74	0/4/4/4
28	CYC	OH	1001	-	-	5/25/74/74	0/4/4/4
26	PEB	j4	202	2	-	7/24/74/74	0/4/4/4
26	PEB	G5	201	2	-	11/24/74/74	0/4/4/4
26	PEB	UF	203	1	-	9/24/74/74	0/4/4/4
26	PEB	FA	201	2,12	-	6/24/74/74	0/4/4/4
26	PEB	b7	202	1	-	7/24/74/74	0/4/4/4
26	PEB	MA	203	1	-	9/24/74/74	0/4/4/4
26	PEB	kF	202	2	-	9/24/74/74	0/4/4/4
26	PEB	T2	203	2	-	10/24/74/74	0/4/4/4
26	PEB	mE	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	G8	202	1	-	5/24/74/74	0/4/4/4
26	PEB	mG	203	1	-	11/24/74/74	0/4/4/4
26	PEB	UI	202	1	-	10/24/74/74	0/4/4/4
26	PEB	F8	201	2,12	-	6/24/74/74	0/4/4/4
26	PEB	r4	201	1	-	10/24/74/74	0/4/4/4
26	PEB	iE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	JF	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	ZF	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	Y2	203	2	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	O6	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	a4	202	2	-	6/24/74/74	0/4/4/4
26	PEB	hE	202	2	-	9/24/74/74	0/4/4/4
26	PEB	NA	201	2	-	6/24/74/74	0/4/4/4
26	PEB	l8	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	I9	202	2	-	7/24/74/74	0/4/4/4
26	PEB	r4	202	1	-	16/24/74/74	0/4/4/4
26	PEB	N4	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	a1	201	2	-	4/24/74/74	0/4/4/4
26	PEB	WE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	BG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	M1	401	3	-	13/24/74/74	0/4/4/4
26	PEB	sG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	l1	201	2	-	12/24/74/74	0/4/4/4
26	PEB	QG	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	PE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	TD	201	2	-	5/24/74/74	0/4/4/4
26	PEB	OE	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	oG	203	1	-	17/24/74/74	0/4/4/4
28	CYC	1H	1000	22	-	6/25/74/74	0/4/4/4
26	PEB	CA	202	1	-	10/24/74/74	0/4/4/4
26	PEB	p1	201	1	-	13/24/74/74	0/4/4/4
27	PUB	wE	304	13	-	9/24/74/74	0/4/4/4
26	PEB	N8	201	2	-	8/24/74/74	0/4/4/4
26	PEB	LE	202	2	-	14/24/74/74	0/4/4/4
26	PEB	R1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	QA	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	kB	202	2	-	11/24/74/74	0/4/4/4
26	PEB	GB	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	tE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	K5	201	2	-	3/24/74/74	0/4/4/4
26	PEB	l2	201	1	-	8/24/74/74	0/4/4/4
28	CYC	GB	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	uE	203	1	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	T8	201	2	-	7/24/74/74	0/4/4/4
26	PEB	KE	203	1	-	8/24/74/74	0/4/4/4
26	PEB	h4	202	2,1	-	13/24/74/74	0/4/4/4
26	PEB	gG	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	s1	203	2	-	7/24/74/74	0/4/4/4
26	PEB	L3	203	2	-	9/24/74/74	0/4/4/4
26	PEB	M8	202	1	-	4/24/74/74	0/4/4/4
26	PEB	M4	403	3	-	6/24/74/74	0/4/4/4
26	PEB	T1	203	1	-	10/24/74/74	0/4/4/4
26	PEB	w1	203	2	-	7/24/74/74	0/4/4/4
26	PEB	P1	202	1	-	5/24/74/74	0/4/4/4
26	PEB	BD	201	2,26	-	8/24/74/74	0/4/4/4
26	PEB	i8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	k1	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	VG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	hA	203	1	-	8/24/74/74	0/4/4/4
26	PEB	L5	201	2	-	7/24/74/74	0/4/4/4
26	PEB	R7	202	2	-	11/24/74/74	0/4/4/4
26	PEB	Z1	201	2	-	5/24/74/74	0/4/4/4
26	PEB	aA	201	1,13	-	8/24/74/74	0/4/4/4
26	PEB	KA	202	1	-	8/24/74/74	0/4/4/4
26	PEB	S7	201	1	-	8/24/74/74	0/4/4/4
26	PEB	OF	201	1	-	11/24/74/74	0/4/4/4
27	PUB	NJ	201	1,7	-	3/24/74/74	0/4/4/4
26	PEB	dF	203	1	-	10/24/74/74	0/4/4/4
26	PEB	X3	203	2	-	14/24/74/74	0/4/4/4
26	PEB	O4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	F7	1002	10	-	8/24/74/74	0/4/4/4
27	PUB	K1	203	3,1	-	9/24/74/74	0/4/4/4
26	PEB	a7	202	2	-	10/24/74/74	0/4/4/4
27	PUB	xE	306	13	-	4/24/74/74	0/4/4/4
26	PEB	r1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	AA	301	13	-	13/24/74/74	0/4/4/4
28	CYC	KH	1001	17	-	15/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	QE	201	1	-	8/24/74/74	0/4/4/4
26	PEB	P3	202	2	-	7/24/74/74	0/4/4/4
26	PEB	DJ	203	1	-	10/24/74/74	0/4/4/4
26	PEB	KE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	e8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Y8	202	1	-	4/24/74/74	0/4/4/4
26	PEB	F9	201	1	-	13/24/74/74	0/4/4/4
26	PEB	kA	202	2	-	11/24/74/74	0/4/4/4
26	PEB	N6	201	9,10	-	10/24/74/74	0/4/4/4
28	CYC	IH	1001	-	-	8/25/74/74	0/4/4/4
26	PEB	e2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	YB	201	2	-	10/24/74/74	0/4/4/4
26	PEB	nG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	MA	202	1	-	4/24/74/74	0/4/4/4
26	PEB	NE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	uE	202	1	-	10/24/74/74	0/4/4/4
26	PEB	EA	202	1	-	9/24/74/74	0/4/4/4
26	PEB	q4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	QI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	AE	202	1	-	11/24/74/74	0/4/4/4

All (17214) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p4	202	PEB	CHB-C4B	18.98	1.51	1.35
26	I9	201	PEB	CHB-C4B	18.86	1.50	1.35
26	LG	202	PEB	CHB-C4B	18.61	1.50	1.35
26	p1	202	PEB	CHB-C4B	18.61	1.50	1.35
27	N9	201	PUB	CHB-C1C	18.57	1.50	1.35
26	t4	201	PEB	CHB-C4B	18.56	1.50	1.35
26	nE	202	PEB	CHB-C4B	18.45	1.50	1.35
26	l1	202	PEB	CHB-C4B	18.43	1.50	1.35
26	IJ	201	PEB	CHB-C4B	18.40	1.50	1.35
26	z1	202	PEB	CHB-C4B	18.38	1.50	1.35
26	t1	202	PEB	CHB-C4B	18.31	1.50	1.35
26	LE	202	PEB	CHB-C4B	18.30	1.50	1.35
26	h6	201	PEB	CHB-C4B	18.26	1.50	1.35
26	P4	203	PEB	CHB-C4B	18.20	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h1	201	PEB	CHB-C4B	18.19	1.50	1.35
26	tG	202	PEB	CHB-C4B	18.15	1.50	1.35
26	mE	201	PEB	CHB-C4B	18.15	1.50	1.35
26	t1	201	PEB	CHB-C4B	18.13	1.50	1.35
27	xE	306	PUB	CHB-C1C	18.12	1.50	1.35
26	z4	201	PEB	CHB-C4B	18.11	1.50	1.35
26	fA	202	PEB	CHB-C4B	18.09	1.50	1.35
26	F3	203	PEB	CHB-C4B	18.05	1.50	1.35
26	XD	201	PEB	CHB-C4B	18.04	1.50	1.35
26	X3	201	PEB	CHB-C4B	18.04	1.50	1.35
26	j1	202	PEB	CHB-C4B	18.01	1.50	1.35
26	WJ	201	PEB	CHB-C4B	18.00	1.50	1.35
26	U1	201	PEB	CHB-C4B	17.98	1.50	1.35
26	U4	201	PEB	CHB-C4B	17.98	1.50	1.35
26	I8	203	PEB	CHB-C4B	17.96	1.50	1.35
26	mF	202	PEB	CHB-C4B	17.94	1.50	1.35
28	yH	1001	CYC	CHA-C1A	17.93	1.50	1.35
26	h4	201	PEB	CHB-C4B	17.93	1.50	1.35
26	e1	202	PEB	CHB-C4B	17.93	1.50	1.35
28	WH	1001	CYC	CHA-C1A	17.90	1.50	1.35
28	qH	1002	CYC	CHA-C1A	17.90	1.50	1.35
26	t4	202	PEB	CHB-C4B	17.89	1.50	1.35
26	P1	203	PEB	CHB-C4B	17.88	1.50	1.35
26	14	201	PEB	CHB-C4B	17.88	1.50	1.35
26	l4	202	PEB	CHB-C4B	17.87	1.50	1.35
26	dG	202	PEB	CHB-C4B	17.85	1.50	1.35
28	AH	1001	CYC	CHA-C1A	17.84	1.50	1.35
26	IA	203	PEB	CHB-C4B	17.82	1.50	1.35
26	f1	202	PEB	CHB-C4B	17.80	1.50	1.35
26	T3	201	PEB	CHB-C4B	17.77	1.50	1.35
26	WA	202	PEB	CHB-C4B	17.77	1.50	1.35
26	tE	202	PEB	CHB-C4B	17.77	1.50	1.35
27	NJ	201	PUB	CHB-C1C	17.76	1.50	1.35
26	11	201	PEB	CHB-C4B	17.75	1.49	1.35
26	kG	202	PEB	CHB-C4B	17.74	1.49	1.35
26	u4	203	PEB	CHB-C4B	17.73	1.49	1.35
26	w1	202	PEB	CHB-C4B	17.73	1.49	1.35
26	m7	202	PEB	CHB-C4B	17.73	1.49	1.35
26	FG	201	PEB	CHB-C4B	17.73	1.49	1.35
26	mB	203	PEB	CHB-C4B	17.69	1.49	1.35
26	H3	203	PEB	CHB-C4B	17.68	1.49	1.35
26	bE	202	PEB	CHB-C4B	17.67	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	cH	1001	CYC	CHA-C1A	17.66	1.49	1.35
26	w4	202	PEB	CHB-C4B	17.65	1.49	1.35
26	TD	201	PEB	CHB-C4B	17.65	1.49	1.35
26	V3	203	PEB	CHB-C4B	17.65	1.49	1.35
26	e4	202	PEB	CHB-C4B	17.65	1.49	1.35
26	r4	202	PEB	CHB-C4B	17.64	1.49	1.35
27	A1	203	PUB	CHB-C1C	17.62	1.49	1.35
28	KH	1001	CYC	CHA-C1A	17.61	1.49	1.35
26	w1	201	PEB	CHB-C4B	17.61	1.49	1.35
26	z1	201	PEB	CHB-C4B	17.61	1.49	1.35
26	XJ	202	PEB	CHB-C4B	17.60	1.49	1.35
26	r1	202	PEB	CHB-C4B	17.60	1.49	1.35
26	X9	202	PEB	CHB-C4B	17.59	1.49	1.35
26	m4	203	PEB	CHB-C4B	17.58	1.49	1.35
26	V1	201	PEB	CHB-C4B	17.55	1.49	1.35
26	FD	203	PEB	CHB-C4B	17.55	1.49	1.35
26	c4	202	PEB	CHB-C4B	17.55	1.49	1.35
26	v1	201	PEB	CHB-C4B	17.53	1.49	1.35
26	VD	203	PEB	CHB-C4B	17.53	1.49	1.35
26	gF	201	PEB	CHB-C4B	17.53	1.49	1.35
26	FE	201	PEB	CHB-C4B	17.52	1.49	1.35
26	s1	203	PEB	CHB-C4B	17.52	1.49	1.35
26	w4	201	PEB	CHB-C4B	17.52	1.49	1.35
26	nG	202	PEB	CHB-C4B	17.51	1.49	1.35
26	pG	202	PEB	CHB-C4B	17.51	1.49	1.35
26	pE	202	PEB	CHB-C4B	17.48	1.49	1.35
26	p1	201	PEB	CHB-C4B	17.48	1.49	1.35
26	ZE	202	PEB	CHB-C4B	17.48	1.49	1.35
26	X3	203	PEB	CHB-C4B	17.47	1.49	1.35
26	HD	203	PEB	CHB-C4B	17.47	1.49	1.35
26	cA	202	PEB	CHB-C4B	17.46	1.49	1.35
26	RJ	201	PEB	CHB-C4B	17.46	1.49	1.35
26	v1	202	PEB	CHB-C4B	17.44	1.49	1.35
26	v4	201	PEB	CHB-C4B	17.44	1.49	1.35
26	ED	201	PEB	CHB-C4B	17.44	1.49	1.35
27	xG	306	PUB	CHB-C1C	17.43	1.49	1.35
26	y1	201	PEB	CHB-C4B	17.43	1.49	1.35
26	x1	201	PEB	CHB-C4B	17.42	1.49	1.35
26	m1	203	PEB	CHB-C4B	17.41	1.49	1.35
26	x4	201	PEB	CHB-C4B	17.40	1.49	1.35
28	VH	1001	CYC	CHA-C1A	17.40	1.49	1.35
26	u4	201	PEB	CHB-C4B	17.39	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	i4	201	PEB	CHB-C4B	17.38	1.49	1.35
26	c1	202	PEB	CHB-C4B	17.38	1.49	1.35
26	f4	202	PEB	CHB-C4B	17.38	1.49	1.35
26	QE	202	PEB	CHB-C4B	17.37	1.49	1.35
26	s4	203	PEB	CHB-C4B	17.37	1.49	1.35
26	XD	203	PEB	CHB-C4B	17.37	1.49	1.35
28	JH	1001	CYC	CHA-C1A	17.37	1.49	1.35
26	iE	203	PEB	CHB-C4B	17.37	1.49	1.35
28	lH	1001	CYC	CHA-C1A	17.36	1.49	1.35
26	d8	201	PEB	CHB-C4B	17.36	1.49	1.35
26	vE	202	PEB	CHB-C4B	17.36	1.49	1.35
26	A5	201	PEB	CHB-C4B	17.36	1.49	1.35
26	g7	201	PEB	CHB-C4B	17.36	1.49	1.35
27	Y3	302	PUB	CHB-C1C	17.35	1.49	1.35
26	14	202	PEB	CHB-C4B	17.35	1.49	1.35
26	R9	201	PEB	CHB-C4B	17.35	1.49	1.35
26	PE	202	PEB	CHB-C4B	17.34	1.49	1.35
27	wE	304	PUB	CHB-C1C	17.34	1.49	1.35
26	u1	202	PEB	CHB-C4B	17.34	1.49	1.35
26	11	202	PEB	CHB-C4B	17.34	1.49	1.35
26	eB	203	PEB	CHB-C4B	17.33	1.49	1.35
26	bG	202	PEB	CHB-C4B	17.33	1.49	1.35
26	PG	202	PEB	CHB-C4B	17.32	1.49	1.35
28	1H	1000	CYC	CHA-C1A	17.31	1.49	1.35
26	HD	201	PEB	CHB-C4B	17.31	1.49	1.35
26	BD	202	PEB	CHB-C4B	17.31	1.49	1.35
26	v4	202	PEB	CHB-C4B	17.30	1.49	1.35
26	B3	202	PEB	CHB-C4B	17.29	1.49	1.35
26	G4	202	PEB	CHB-C4B	17.29	1.49	1.35
26	dB	203	PEB	CHB-C4B	17.29	1.49	1.35
26	ZG	202	PEB	CHB-C4B	17.29	1.49	1.35
28	LF	1001	CYC	CHA-C1A	17.29	1.49	1.35
28	YH	1004	CYC	CHA-C1A	17.29	1.49	1.35
26	U6	202	PEB	CHB-C4B	17.28	1.49	1.35
26	H1	201	PEB	CHB-C4B	17.27	1.49	1.35
26	g7	202	PEB	CHB-C4B	17.27	1.49	1.35
28	nH	1001	CYC	CHA-C1A	17.27	1.49	1.35
26	W4	201	PEB	CHB-C4B	17.26	1.49	1.35
26	hE	202	PEB	CHB-C4B	17.26	1.49	1.35
26	F1	201	PEB	CHB-C4B	17.26	1.49	1.35
26	kG	203	PEB	CHB-C4B	17.25	1.49	1.35
26	E8	203	PEB	CHB-C4B	17.25	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u4	202	PEB	CHB-C4B	17.25	1.49	1.35
28	LH	1001	CYC	CHA-C1A	17.22	1.49	1.35
28	gH	1001	CYC	CHA-C1A	17.22	1.49	1.35
28	EH	1001	CYC	CHA-C1A	17.22	1.49	1.35
26	tG	201	PEB	CHB-C4B	17.21	1.49	1.35
26	R7	202	PEB	CHB-C4B	17.20	1.49	1.35
26	z4	202	PEB	CHB-C4B	17.20	1.49	1.35
26	j4	201	PEB	CHB-C4B	17.20	1.49	1.35
26	lI	202	PEB	CHB-C4B	17.20	1.49	1.35
26	S4	201	PEB	CHB-C4B	17.19	1.49	1.35
26	bB	202	PEB	CHB-C4B	17.19	1.49	1.35
26	KJ	201	PEB	CHB-C4B	17.19	1.49	1.35
26	V4	201	PEB	CHB-C4B	17.19	1.49	1.35
26	J1	203	PEB	CHB-C4B	17.19	1.49	1.35
26	lE	202	PEB	CHB-C4B	17.19	1.49	1.35
26	a1	202	PEB	CHB-C4B	17.19	1.49	1.35
26	w4	203	PEB	CHB-C4B	17.19	1.49	1.35
26	f1	201	PEB	CHB-C4B	17.18	1.49	1.35
26	p4	201	PEB	CHB-C4B	17.17	1.49	1.35
26	RI	203	PEB	CHB-C4B	17.16	1.49	1.35
26	A1	202	PEB	CHB-C4B	17.16	1.49	1.35
26	l1	201	PEB	CHB-C4B	17.16	1.49	1.35
26	L3	203	PEB	CHB-C4B	17.16	1.49	1.35
26	f7	201	PEB	CHB-C4B	17.15	1.49	1.35
26	UB	202	PEB	CHB-C4B	17.15	1.49	1.35
28	CH	1001	CYC	CHA-C1A	17.15	1.49	1.35
26	gF	202	PEB	CHB-C4B	17.14	1.49	1.35
28	qH	1001	CYC	CHA-C1A	17.14	1.49	1.35
26	uG	201	PEB	CHB-C4B	17.14	1.49	1.35
26	vG	202	PEB	CHB-C4B	17.14	1.49	1.35
26	f7	203	PEB	CHB-C4B	17.13	1.49	1.35
26	A5	202	PEB	CHB-C4B	17.13	1.49	1.35
28	dH	1001	CYC	CHA-C1A	17.12	1.49	1.35
26	e7	202	PEB	CHB-C4B	17.12	1.49	1.35
26	dE	202	PEB	CHB-C4B	17.12	1.49	1.35
26	f2	202	PEB	CHB-C4B	17.11	1.49	1.35
26	oG	202	PEB	CHB-C4B	17.11	1.49	1.35
26	dG	201	PEB	CHB-C4B	17.11	1.49	1.35
28	jH	1001	CYC	CHA-C1A	17.11	1.49	1.35
26	AC	203	PEB	CHB-C4B	17.11	1.49	1.35
26	A4	202	PEB	CHB-C4B	17.10	1.49	1.35
26	jA	202	PEB	CHB-C4B	17.10	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B5	203	PEB	CHB-C4B	17.10	1.49	1.35
26	e1	201	PEB	CHB-C4B	17.10	1.49	1.35
26	e6	203	PEB	CHB-C4B	17.10	1.49	1.35
26	k4	201	PEB	CHB-C4B	17.09	1.49	1.35
26	q4	201	PEB	CHB-C4B	17.09	1.49	1.35
26	fF	201	PEB	CHB-C4B	17.09	1.49	1.35
26	d4	201	PEB	CHB-C4B	17.09	1.49	1.35
26	d6	203	PEB	CHB-C4B	17.09	1.49	1.35
26	j1	201	PEB	CHB-C4B	17.08	1.49	1.35
26	AC	201	PEB	CHB-C4B	17.08	1.49	1.35
26	AJ	304	PEB	CHB-C4B	17.08	1.49	1.35
26	R2	203	PEB	CHB-C4B	17.08	1.49	1.35
27	YD	302	PUB	CHB-C1C	17.07	1.49	1.35
28	DF	1001	CYC	CHA-C1A	17.06	1.49	1.35
28	vH	1001	CYC	CHA-C1A	17.06	1.49	1.35
26	G1	202	PEB	CHB-C4B	17.05	1.49	1.35
26	dE	201	PEB	CHB-C4B	17.05	1.49	1.35
26	AG	202	PEB	CHB-C4B	17.04	1.49	1.35
26	H4	203	PEB	CHB-C4B	17.04	1.49	1.35
26	hB	201	PEB	CHB-C4B	17.04	1.49	1.35
27	AF	303	PUB	CHB-C1C	17.04	1.49	1.35
26	i1	202	PEB	CHB-C4B	17.03	1.49	1.35
26	W1	201	PEB	CHB-C4B	17.03	1.49	1.35
26	m6	203	PEB	CHB-C4B	17.03	1.49	1.35
26	JG	201	PEB	CHB-C4B	17.02	1.49	1.35
26	R4	203	PEB	CHB-C4B	17.02	1.49	1.35
26	fB	203	PEB	CHB-C4B	17.01	1.49	1.35
26	D4	202	PEB	CHB-C4B	17.01	1.49	1.35
26	rG	201	PEB	CHB-C4B	17.01	1.49	1.35
26	W1	202	PEB	CHB-C4B	17.00	1.49	1.35
26	U9	201	PEB	CHB-C4B	17.00	1.49	1.35
26	k1	201	PEB	CHB-C4B	17.00	1.49	1.35
26	s4	202	PEB	CHB-C4B	17.00	1.49	1.35
28	OH	1001	CYC	CHA-C1A	17.00	1.49	1.35
26	H4	201	PEB	CHB-C4B	16.99	1.49	1.35
26	BC	201	PEB	CHB-C4B	16.99	1.49	1.35
26	vG	201	PEB	CHB-C4B	16.99	1.49	1.35
26	RF	202	PEB	CHB-C4B	16.99	1.49	1.35
26	rE	201	PEB	CHB-C4B	16.99	1.49	1.35
26	F3	201	PEB	CHB-C4B	16.98	1.49	1.35
26	C5	204	PEB	CHB-C4B	16.98	1.49	1.35
28	D7	1001	CYC	CHA-C1A	16.98	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	YH	1003	CYC	CHA-C1A	16.98	1.49	1.35
28	hH	1001	CYC	CHA-C1A	16.98	1.49	1.35
26	Y9	201	PEB	CHB-C4B	16.97	1.49	1.35
26	Y1	201	PEB	CHB-C4B	16.97	1.49	1.35
26	S1	201	PEB	CHB-C4B	16.97	1.49	1.35
26	iI	203	PEB	CHB-C4B	16.97	1.49	1.35
26	fG	202	PEB	CHB-C4B	16.97	1.49	1.35
26	bE	201	PEB	CHB-C4B	16.96	1.49	1.35
26	F4	202	PEB	CHB-C4B	16.96	1.49	1.35
26	y4	201	PEB	CHB-C4B	16.96	1.49	1.35
26	VI	203	PEB	CHB-C4B	16.96	1.49	1.35
26	j4	202	PEB	CHB-C4B	16.96	1.49	1.35
26	w1	203	PEB	CHB-C4B	16.95	1.49	1.35
26	A3	202	PEB	CHB-C4B	16.95	1.49	1.35
26	W4	202	PEB	CHB-C4B	16.95	1.49	1.35
26	UJ	202	PEB	CHB-C4B	16.95	1.49	1.35
26	Z4	201	PEB	CHB-C4B	16.95	1.49	1.35
28	C7	1001	CYC	CHA-C1A	16.94	1.49	1.35
28	pH	1001	CYC	CHA-C1A	16.94	1.49	1.35
26	E3	201	PEB	CHB-C4B	16.94	1.49	1.35
26	LD	203	PEB	CHB-C4B	16.94	1.49	1.35
28	eH	1001	CYC	CHA-C1A	16.94	1.49	1.35
26	uE	202	PEB	CHB-C4B	16.94	1.49	1.35
26	N9	204	PEB	CHB-C4B	16.94	1.49	1.35
26	fE	201	PEB	CHB-C4B	16.94	1.49	1.35
26	YF	201	PEB	CHB-C4B	16.94	1.49	1.35
26	J4	203	PEB	CHB-C4B	16.94	1.49	1.35
26	fG	201	PEB	CHB-C4B	16.94	1.49	1.35
26	ZE	201	PEB	CHB-C4B	16.93	1.49	1.35
26	iB	202	PEB	CHB-C4B	16.92	1.49	1.35
28	H7	1001	CYC	CHA-C1A	16.92	1.49	1.35
28	fH	1001	CYC	CHA-C1A	16.92	1.49	1.35
26	B5	201	PEB	CHB-C4B	16.92	1.49	1.35
27	AJ	302	PUB	CHB-C1C	16.92	1.49	1.35
26	m1	202	PEB	CHB-C4B	16.92	1.49	1.35
26	NJ	202	PEB	CHB-C4B	16.92	1.49	1.35
26	DE	203	PEB	CHB-C4B	16.92	1.49	1.35
26	AJ	305	PEB	CHB-C4B	16.92	1.49	1.35
28	TH	1001	CYC	CHA-C1A	16.91	1.49	1.35
28	L7	1001	CYC	CHA-C1A	16.91	1.49	1.35
26	GJ	202	PEB	CHB-C4B	16.91	1.49	1.35
26	Y4	201	PEB	CHB-C4B	16.90	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	XG	203	PEB	CHB-C4B	16.90	1.49	1.35
26	T9	202	PEB	CHB-C4B	16.90	1.49	1.35
26	q1	201	PEB	CHB-C4B	16.89	1.49	1.35
26	AD	201	PEB	CHB-C4B	16.89	1.49	1.35
26	g4	202	PEB	CHB-C4B	16.89	1.49	1.35
26	a4	202	PEB	CHB-C4B	16.89	1.49	1.35
26	l6	203	PEB	CHB-C4B	16.89	1.49	1.35
26	kE	202	PEB	CHB-C4B	16.89	1.49	1.35
26	VF	202	PEB	CHB-C4B	16.89	1.49	1.35
26	VG	201	PEB	CHB-C4B	16.88	1.49	1.35
27	AF	304	PUB	CHB-C1C	16.87	1.49	1.35
26	U9	202	PEB	CHB-C4B	16.86	1.49	1.35
26	YJ	202	PEB	CHB-C4B	16.86	1.49	1.35
26	I4	201	PEB	CHB-C4B	16.86	1.49	1.35
26	L4	201	PEB	CHB-C4B	16.86	1.49	1.35
26	k6	201	PEB	CHB-C4B	16.86	1.49	1.35
28	NH	1001	CYC	CHA-C1A	16.86	1.49	1.35
26	i7	201	PEB	CHB-C4B	16.86	1.49	1.35
26	F4	201	PEB	CHB-C4B	16.86	1.49	1.35
26	f4	201	PEB	CHB-C4B	16.86	1.49	1.35
26	j7	203	PEB	CHB-C4B	16.86	1.49	1.35
26	JE	201	PEB	CHB-C4B	16.86	1.49	1.35
26	c6	202	PEB	CHB-C4B	16.86	1.49	1.35
26	XE	202	PEB	CHB-C4B	16.86	1.49	1.35
26	GC	203	PEB	CHB-C4B	16.85	1.49	1.35
26	cI	202	PEB	CHB-C4B	16.85	1.49	1.35
28	YH	1002	CYC	CHA-C1A	16.85	1.49	1.35
26	i2	203	PEB	CHB-C4B	16.85	1.49	1.35
26	G5	201	PEB	CHB-C4B	16.85	1.49	1.35
26	BE	202	PEB	CHB-C4B	16.85	1.49	1.35
26	E8	202	PEB	CHB-C4B	16.85	1.49	1.35
26	bF	202	PEB	CHB-C4B	16.85	1.49	1.35
26	CJ	202	PEB	CHB-C4B	16.84	1.49	1.35
26	BC	203	PEB	CHB-C4B	16.84	1.49	1.35
26	lE	201	PEB	CHB-C4B	16.84	1.49	1.35
26	CC	203	PEB	CHB-C4B	16.84	1.49	1.35
26	R1	203	PEB	CHB-C4B	16.84	1.49	1.35
26	i6	202	PEB	CHB-C4B	16.84	1.49	1.35
26	h1	202	PEB	CHB-C4B	16.84	1.49	1.35
26	FE	202	PEB	CHB-C4B	16.84	1.49	1.35
26	TJ	201	PEB	CHB-C4B	16.83	1.49	1.35
26	iF	202	PEB	CHB-C4B	16.83	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V6	202	PEB	CHB-C4B	16.83	1.49	1.35
26	h8	203	PEB	CHB-C4B	16.83	1.49	1.35
28	mH	1001	CYC	CHA-C1A	16.82	1.49	1.35
26	a2	203	PEB	CHB-C4B	16.82	1.49	1.35
26	oE	202	PEB	CHB-C4B	16.82	1.49	1.35
26	uG	202	PEB	CHB-C4B	16.82	1.49	1.35
26	C5	202	PEB	CHB-C4B	16.82	1.49	1.35
26	A9	304	PEB	CHB-C4B	16.82	1.49	1.35
26	a7	201	PEB	CHB-C4B	16.82	1.49	1.35
26	P9	201	PEB	CHB-C4B	16.82	1.49	1.35
26	I9	202	PEB	CHB-C4B	16.81	1.49	1.35
26	24	405	PEB	CHB-C4B	16.81	1.49	1.35
26	Z1	201	PEB	CHB-C4B	16.81	1.49	1.35
26	GC	201	PEB	CHB-C4B	16.81	1.49	1.35
26	jF	203	PEB	CHB-C4B	16.81	1.49	1.35
26	HC	201	PEB	CHB-C4B	16.81	1.49	1.35
26	fF	203	PEB	CHB-C4B	16.81	1.49	1.35
26	lB	203	PEB	CHB-C4B	16.81	1.49	1.35
26	e3	401	PEB	CHB-C4B	16.80	1.49	1.35
26	jE	202	PEB	CHB-C4B	16.80	1.49	1.35
26	IJ	203	PEB	CHB-C4B	16.80	1.49	1.35
26	uE	203	PEB	CHB-C4B	16.80	1.49	1.35
26	UJ	201	PEB	CHB-C4B	16.80	1.49	1.35
26	k2	203	PEB	CHB-C4B	16.79	1.49	1.35
26	BC	202	PEB	CHB-C4B	16.79	1.49	1.35
26	hE	201	PEB	CHB-C4B	16.79	1.49	1.35
26	d4	203	PEB	CHB-C4B	16.79	1.49	1.35
28	GH	1001	CYC	CHA-C1A	16.79	1.49	1.35
28	MH	1001	CYC	CHA-C1A	16.79	1.49	1.35
26	CG	203	PEB	CHB-C4B	16.79	1.49	1.35
26	FG	202	PEB	CHB-C4B	16.79	1.49	1.35
26	XJ	201	PEB	CHB-C4B	16.79	1.49	1.35
26	kE	203	PEB	CHB-C4B	16.79	1.49	1.35
26	c4	201	PEB	CHB-C4B	16.78	1.49	1.35
26	H1	203	PEB	CHB-C4B	16.78	1.49	1.35
26	m6	202	PEB	CHB-C4B	16.78	1.49	1.35
26	V2	203	PEB	CHB-C4B	16.78	1.49	1.35
26	FD	201	PEB	CHB-C4B	16.78	1.49	1.35
26	vE	201	PEB	CHB-C4B	16.78	1.49	1.35
26	EA	202	PEB	CHB-C4B	16.78	1.49	1.35
28	oH	1001	CYC	CHA-C1A	16.78	1.49	1.35
26	L1	201	PEB	CHB-C4B	16.77	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ME	202	PEB	CHB-C4B	16.77	1.49	1.35
26	I1	201	PEB	CHB-C4B	16.77	1.49	1.35
26	HE	202	PEB	CHB-C4B	16.77	1.49	1.35
26	T2	203	PEB	CHB-C4B	16.76	1.49	1.35
26	fE	202	PEB	CHB-C4B	16.76	1.49	1.35
26	Q6	202	PEB	CHB-C4B	16.76	1.49	1.35
26	SB	202	PEB	CHB-C4B	16.76	1.49	1.35
26	VJ	201	PEB	CHB-C4B	16.75	1.49	1.35
26	E1	201	PEB	CHB-C4B	16.75	1.49	1.35
26	tE	201	PEB	CHB-C4B	16.74	1.49	1.35
26	c2	202	PEB	CHB-C4B	16.74	1.49	1.35
26	xG	304	PEB	CHB-C4B	16.74	1.49	1.35
26	B3	203	PEB	CHB-C4B	16.74	1.49	1.35
26	hG	202	PEB	CHB-C4B	16.74	1.49	1.35
26	C9	202	PEB	CHB-C4B	16.73	1.49	1.35
28	iH	1001	CYC	CHA-C1A	16.73	1.49	1.35
26	nG	201	PEB	CHB-C4B	16.72	1.49	1.35
26	WJ	202	PEB	CHB-C4B	16.72	1.49	1.35
26	TI	203	PEB	CHB-C4B	16.72	1.49	1.35
26	hB	202	PEB	CHB-C4B	16.71	1.49	1.35
26	q4	203	PEB	CHB-C4B	16.71	1.49	1.35
26	W9	201	PEB	CHB-C4B	16.70	1.49	1.35
26	S7	201	PEB	CHB-C4B	16.70	1.49	1.35
26	K8	202	PEB	CHB-C4B	16.70	1.49	1.35
26	OB	202	PEB	CHB-C4B	16.70	1.49	1.35
26	H5	201	PEB	CHB-C4B	16.70	1.49	1.35
26	i6	201	PEB	CHB-C4B	16.70	1.49	1.35
28	N7	1001	CYC	CHA-C1A	16.70	1.49	1.35
26	BG	202	PEB	CHB-C4B	16.69	1.49	1.35
28	F2	1001	CYC	CHA-C1A	16.69	1.49	1.35
26	mB	202	PEB	CHB-C4B	16.69	1.49	1.35
26	b2	202	PEB	CHB-C4B	16.69	1.49	1.35
26	M4	401	PEB	CHB-C4B	16.69	1.49	1.35
26	RF	201	PEB	CHB-C4B	16.69	1.49	1.35
26	DG	203	PEB	CHB-C4B	16.69	1.49	1.35
26	aI	203	PEB	CHB-C4B	16.68	1.49	1.35
26	xG	303	PEB	CHB-C4B	16.68	1.49	1.35
26	V9	202	PEB	CHB-C4B	16.68	1.49	1.35
26	iG	203	PEB	CHB-C4B	16.67	1.49	1.35
26	NJ	204	PEB	CHB-C4B	16.67	1.49	1.35
26	KA	202	PEB	CHB-C4B	16.67	1.49	1.35
26	m6	201	PEB	CHB-C4B	16.66	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R7	201	PEB	CHB-C4B	16.66	1.49	1.35
26	c7	202	PEB	CHB-C4B	16.66	1.49	1.35
26	OI	202	PEB	CHB-C4B	16.66	1.49	1.35
28	QH	1001	CYC	CHA-C1A	16.66	1.49	1.35
26	XG	201	PEB	CHB-C4B	16.65	1.49	1.35
26	K3	202	PEB	CHB-C4B	16.65	1.49	1.35
26	PJ	202	PEB	CHB-C4B	16.65	1.49	1.35
26	E4	202	PEB	CHB-C4B	16.64	1.49	1.35
26	y4	203	PEB	CHB-C4B	16.64	1.49	1.35
26	e6	202	PEB	CHB-C4B	16.64	1.49	1.35
26	CC	201	PEB	CHB-C4B	16.64	1.49	1.35
26	XE	201	PEB	CHB-C4B	16.64	1.49	1.35
26	J4	202	PEB	CHB-C4B	16.63	1.49	1.35
26	JA	201	PEB	CHB-C4B	16.63	1.49	1.35
26	q1	203	PEB	CHB-C4B	16.63	1.49	1.35
26	lF	202	PEB	CHB-C4B	16.63	1.49	1.35
26	d1	203	PEB	CHB-C4B	16.62	1.49	1.35
26	wG	303	PEB	CHB-C4B	16.62	1.49	1.35
26	c2	203	PEB	CHB-C4B	16.62	1.49	1.35
26	Q9	202	PEB	CHB-C4B	16.62	1.49	1.35
26	PD	201	PEB	CHB-C4B	16.62	1.49	1.35
26	V7	202	PEB	CHB-C4B	16.62	1.49	1.35
26	y1	202	PEB	CHB-C4B	16.62	1.49	1.35
26	L4	203	PEB	CHB-C4B	16.62	1.49	1.35
26	eD	401	PEB	CHB-C4B	16.61	1.49	1.35
26	mF	201	PEB	CHB-C4B	16.61	1.49	1.35
26	KD	202	PEB	CHB-C4B	16.61	1.49	1.35
26	VG	202	PEB	CHB-C4B	16.61	1.49	1.35
26	QJ	202	PEB	CHB-C4B	16.61	1.49	1.35
26	QG	202	PEB	CHB-C4B	16.61	1.49	1.35
26	qG	201	PEB	CHB-C4B	16.61	1.49	1.35
26	U7	201	PEB	CHB-C4B	16.61	1.49	1.35
26	fl	202	PEB	CHB-C4B	16.61	1.49	1.35
26	kI	201	PEB	CHB-C4B	16.61	1.49	1.35
26	VB	202	PEB	CHB-C4B	16.60	1.49	1.35
26	WE	203	PEB	CHB-C4B	16.60	1.49	1.35
26	nE	201	PEB	CHB-C4B	16.60	1.49	1.35
26	L4	202	PEB	CHB-C4B	16.60	1.49	1.35
26	iG	201	PEB	CHB-C4B	16.60	1.49	1.35
26	gB	201	PEB	CHB-C4B	16.60	1.49	1.35
26	YI	201	PEB	CHB-C4B	16.59	1.49	1.35
26	Q4	201	PEB	CHB-C4B	16.59	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cI	203	PEB	CHB-C4B	16.59	1.49	1.35
27	wG	304	PUB	CHB-C1C	16.59	1.49	1.35
26	Y9	202	PEB	CHB-C4B	16.59	1.49	1.35
26	P3	201	PEB	CHB-C4B	16.59	1.49	1.35
26	u1	203	PEB	CHB-C4B	16.59	1.49	1.35
26	h4	203	PEB	CHB-C4B	16.59	1.49	1.35
26	jB	201	PEB	CHB-C4B	16.58	1.49	1.35
26	bI	202	PEB	CHB-C4B	16.58	1.49	1.35
26	jG	202	PEB	CHB-C4B	16.58	1.49	1.35
26	s4	201	PEB	CHB-C4B	16.58	1.49	1.35
26	C5	201	PEB	CHB-C4B	16.58	1.49	1.35
28	FF	1001	CYC	CHA-C1A	16.58	1.49	1.35
26	j6	201	PEB	CHB-C4B	16.58	1.49	1.35
26	S7	203	PEB	CHB-C4B	16.58	1.49	1.35
26	Y7	201	PEB	CHB-C4B	16.57	1.49	1.35
26	D4	203	PEB	CHB-C4B	16.57	1.49	1.35
26	ME	203	PEB	CHB-C4B	16.57	1.49	1.35
26	mI	203	PEB	CHB-C4B	16.57	1.49	1.35
26	L1	202	PEB	CHB-C4B	16.57	1.49	1.35
27	A7	303	PUB	CHB-C1C	16.57	1.49	1.35
26	H3	201	PEB	CHB-C4B	16.57	1.49	1.35
26	J1	202	PEB	CHB-C4B	16.57	1.49	1.35
26	j8	202	PEB	CHB-C4B	16.56	1.49	1.35
26	AD	202	PEB	CHB-C4B	16.56	1.49	1.35
26	BG	201	PEB	CHB-C4B	16.56	1.49	1.35
26	mE	203	PEB	CHB-C4B	16.56	1.49	1.35
26	M9	201	PEB	CHB-C4B	16.56	1.49	1.35
26	OA	202	PEB	CHB-C4B	16.56	1.49	1.35
26	mB	201	PEB	CHB-C4B	16.56	1.49	1.35
26	PD	203	PEB	CHB-C4B	16.56	1.49	1.35
26	qG	203	PEB	CHB-C4B	16.56	1.49	1.35
26	O9	202	PEB	CHB-C4B	16.55	1.49	1.35
26	n4	202	PEB	CHB-C4B	16.55	1.48	1.35
26	kB	201	PEB	CHB-C4B	16.55	1.48	1.35
28	IH	1001	CYC	CHA-C1A	16.55	1.48	1.35
26	Y7	202	PEB	CHB-C4B	16.55	1.48	1.35
26	ED	202	PEB	CHB-C4B	16.55	1.48	1.35
26	V7	201	PEB	CHB-C4B	16.54	1.48	1.35
26	k7	202	PEB	CHB-C4B	16.54	1.48	1.35
26	VF	201	PEB	CHB-C4B	16.54	1.48	1.35
26	QF	202	PEB	CHB-C4B	16.54	1.48	1.35
26	Q2	202	PEB	CHB-C4B	16.54	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	iI	201	PEB	CHB-C4B	16.54	1.48	1.35
26	O2	202	PEB	CHB-C4B	16.54	1.48	1.35
26	W9	202	PEB	CHB-C4B	16.53	1.48	1.35
26	aF	201	PEB	CHB-C4B	16.53	1.48	1.35
27	A4	203	PUB	CHB-C1C	16.53	1.48	1.35
26	YJ	201	PEB	CHB-C4B	16.53	1.48	1.35
26	g1	202	PEB	CHB-C4B	16.53	1.48	1.35
26	EA	203	PEB	CHB-C4B	16.53	1.48	1.35
26	W8	202	PEB	CHB-C4B	16.53	1.48	1.35
26	E4	201	PEB	CHB-C4B	16.53	1.48	1.35
26	m2	203	PEB	CHB-C4B	16.52	1.48	1.35
26	PF	201	PEB	CHB-C4B	16.52	1.48	1.35
26	cF	202	PEB	CHB-C4B	16.52	1.48	1.35
26	iB	201	PEB	CHB-C4B	16.52	1.48	1.35
26	N9	202	PEB	CHB-C4B	16.52	1.48	1.35
26	hI	202	PEB	CHB-C4B	16.52	1.48	1.35
26	g2	203	PEB	CHB-C4B	16.52	1.48	1.35
26	CC	202	PEB	CHB-C4B	16.52	1.48	1.35
26	GA	202	PEB	CHB-C4B	16.52	1.48	1.35
26	PA	202	PEB	CHB-C4B	16.51	1.48	1.35
26	RA	201	PEB	CHB-C4B	16.51	1.48	1.35
26	T9	201	PEB	CHB-C4B	16.51	1.48	1.35
26	s1	201	PEB	CHB-C4B	16.51	1.48	1.35
26	E3	202	PEB	CHB-C4B	16.50	1.48	1.35
26	I3	201	PEB	CHB-C4B	16.50	1.48	1.35
26	l4	201	PEB	CHB-C4B	16.50	1.48	1.35
26	QB	202	PEB	CHB-C4B	16.50	1.48	1.35
26	pE	201	PEB	CHB-C4B	16.50	1.48	1.35
26	C5	203	PEB	CHB-C4B	16.50	1.48	1.35
26	fB	202	PEB	CHB-C4B	16.50	1.48	1.35
26	P3	203	PEB	CHB-C4B	16.50	1.48	1.35
28	UH	1001	CYC	CHA-C1A	16.50	1.48	1.35
26	G5	203	PEB	CHB-C4B	16.49	1.48	1.35
26	C4	201	PEB	CHB-C4B	16.49	1.48	1.35
28	kH	1001	CYC	CHA-C1A	16.49	1.48	1.35
26	C4	202	PEB	CHB-C4B	16.49	1.48	1.35
26	b7	203	PEB	CHB-C4B	16.49	1.48	1.35
26	h7	202	PEB	CHB-C4B	16.49	1.48	1.35
26	VE	201	PEB	CHB-C4B	16.48	1.48	1.35
27	A7	304	PUB	CHB-C1C	16.48	1.48	1.35
27	AB	302	PUB	CHB-C1C	16.48	1.48	1.35
26	K5	201	PEB	CHB-C4B	16.48	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V6	201	PEB	CHB-C4B	16.48	1.48	1.35
26	VB	201	PEB	CHB-C4B	16.48	1.48	1.35
26	YI	203	PEB	CHB-C4B	16.48	1.48	1.35
26	KC	201	PEB	CHB-C4B	16.47	1.48	1.35
28	NF	1001	CYC	CHA-C1A	16.47	1.48	1.35
26	14	203	PEB	CHB-C4B	16.47	1.48	1.35
26	S2	202	PEB	CHB-C4B	16.47	1.48	1.35
26	JG	202	PEB	CHB-C4B	16.47	1.48	1.35
26	IC	203	PEB	CHB-C4B	16.46	1.48	1.35
26	wE	303	PEB	CHB-C4B	16.46	1.48	1.35
26	eF	202	PEB	CHB-C4B	16.46	1.48	1.35
26	O6	201	PEB	CHB-C4B	16.46	1.48	1.35
26	L9	201	PEB	CHB-C4B	16.46	1.48	1.35
26	l2	202	PEB	CHB-C4B	16.46	1.48	1.35
26	AF	305	PEB	CHB-C4B	16.46	1.48	1.35
26	O4	201	PEB	CHB-C4B	16.46	1.48	1.35
26	kF	202	PEB	CHB-C4B	16.45	1.48	1.35
26	NG	202	PEB	CHB-C4B	16.45	1.48	1.35
26	Q9	201	PEB	CHB-C4B	16.45	1.48	1.35
26	D1	203	PEB	CHB-C4B	16.45	1.48	1.35
28	sH	1001	CYC	CHA-C1A	16.45	1.48	1.35
26	PF	202	PEB	CHB-C4B	16.45	1.48	1.35
28	YH	1001	CYC	CHA-C1A	16.45	1.48	1.35
26	T7	201	PEB	CHB-C4B	16.45	1.48	1.35
28	wH	1001	CYC	CHA-C1A	16.44	1.48	1.35
26	B1	203	PEB	CHB-C4B	16.44	1.48	1.35
26	P4	202	PEB	CHB-C4B	16.44	1.48	1.35
26	cB	201	PEB	CHB-C4B	16.44	1.48	1.35
26	E1	202	PEB	CHB-C4B	16.44	1.48	1.35
26	a1	201	PEB	CHB-C4B	16.44	1.48	1.35
26	rE	202	PEB	CHB-C4B	16.44	1.48	1.35
26	B8	301	PEB	CHB-C4B	16.43	1.48	1.35
26	lG	202	PEB	CHB-C4B	16.43	1.48	1.35
26	CG	201	PEB	CHB-C4B	16.43	1.48	1.35
26	Y2	203	PEB	CHB-C4B	16.43	1.48	1.35
26	k4	202	PEB	CHB-C4B	16.43	1.48	1.35
26	g6	201	PEB	CHB-C4B	16.43	1.48	1.35
26	G9	202	PEB	CHB-C4B	16.43	1.48	1.35
26	W7	203	PEB	CHB-C4B	16.43	1.48	1.35
26	b7	202	PEB	CHB-C4B	16.43	1.48	1.35
26	Y6	202	PEB	CHB-C4B	16.43	1.48	1.35
26	m4	202	PEB	CHB-C4B	16.43	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B5	202	PEB	CHB-C4B	16.43	1.48	1.35
26	HG	202	PEB	CHB-C4B	16.43	1.48	1.35
26	MG	202	PEB	CHB-C4B	16.43	1.48	1.35
26	L1	203	PEB	CHB-C4B	16.42	1.48	1.35
26	K4	202	PEB	CHB-C4B	16.42	1.48	1.35
26	sE	202	PEB	CHB-C4B	16.42	1.48	1.35
26	K4	201	PEB	CHB-C4B	16.42	1.48	1.35
26	iA	201	PEB	CHB-C4B	16.42	1.48	1.35
26	I1	202	PEB	CHB-C4B	16.42	1.48	1.35
26	BA	301	PEB	CHB-C4B	16.42	1.48	1.35
28	HF	1001	CYC	CHA-C1A	16.42	1.48	1.35
26	Y2	201	PEB	CHB-C4B	16.42	1.48	1.35
26	f6	202	PEB	CHB-C4B	16.42	1.48	1.35
26	QJ	201	PEB	CHB-C4B	16.42	1.48	1.35
28	F7	1001	CYC	CHA-C1A	16.42	1.48	1.35
26	AC	202	PEB	CHB-C4B	16.41	1.48	1.35
26	dB	204	PEB	CHB-C4B	16.41	1.48	1.35
26	YF	202	PEB	CHB-C4B	16.41	1.48	1.35
26	RJ	203	PEB	CHB-C4B	16.41	1.48	1.35
26	QG	203	PEB	CHB-C4B	16.41	1.48	1.35
26	d1	201	PEB	CHB-C4B	16.41	1.48	1.35
26	YE	201	PEB	CHB-C4B	16.40	1.48	1.35
26	hI	201	PEB	CHB-C4B	16.40	1.48	1.35
26	I4	202	PEB	CHB-C4B	16.40	1.48	1.35
26	11	203	PEB	CHB-C4B	16.40	1.48	1.35
26	O8	201	PEB	CHB-C4B	16.40	1.48	1.35
26	U6	203	PEB	CHB-C4B	16.40	1.48	1.35
26	HD	202	PEB	CHB-C4B	16.40	1.48	1.35
26	dF	202	PEB	CHB-C4B	16.40	1.48	1.35
27	AA	304	PUB	CHB-C1C	16.40	1.48	1.35
26	d6	202	PEB	CHB-C4B	16.39	1.48	1.35
26	NB	1002	PEB	CHB-C4B	16.39	1.48	1.35
26	OB	201	PEB	CHB-C4B	16.39	1.48	1.35
26	g2	201	PEB	CHB-C4B	16.39	1.48	1.35
26	g4	203	PEB	CHB-C4B	16.39	1.48	1.35
26	R6	202	PEB	CHB-C4B	16.39	1.48	1.35
26	k7	201	PEB	CHB-C4B	16.39	1.48	1.35
26	hF	201	PEB	CHB-C4B	16.39	1.48	1.35
26	kA	202	PEB	CHB-C4B	16.39	1.48	1.35
26	C1	202	PEB	CHB-C4B	16.39	1.48	1.35
26	I3	202	PEB	CHB-C4B	16.39	1.48	1.35
26	UF	201	PEB	CHB-C4B	16.39	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	RD	203	PEB	CHB-C4B	16.38	1.48	1.35
26	G1	201	PEB	CHB-C4B	16.38	1.48	1.35
26	O6	202	PEB	CHB-C4B	16.38	1.48	1.35
26	24	404	PEB	CHB-C4B	16.38	1.48	1.35
26	NE	202	PEB	CHB-C4B	16.38	1.48	1.35
26	G9	201	PEB	CHB-C4B	16.37	1.48	1.35
26	f8	202	PEB	CHB-C4B	16.37	1.48	1.35
26	xE	304	PEB	CHB-C4B	16.37	1.48	1.35
26	XJ	203	PEB	CHB-C4B	16.37	1.48	1.35
26	c1	201	PEB	CHB-C4B	16.37	1.48	1.35
26	lG	201	PEB	CHB-C4B	16.36	1.48	1.35
26	hA	203	PEB	CHB-C4B	16.36	1.48	1.35
26	PI	203	PEB	CHB-C4B	16.36	1.48	1.35
26	gA	201	PEB	CHB-C4B	16.36	1.48	1.35
26	YE	203	PEB	CHB-C4B	16.36	1.48	1.35
26	LG	201	PEB	CHB-C4B	16.36	1.48	1.35
26	PJ	201	PEB	CHB-C4B	16.36	1.48	1.35
26	K1	201	PEB	CHB-C4B	16.36	1.48	1.35
26	jI	201	PEB	CHB-C4B	16.36	1.48	1.35
26	KC	203	PEB	CHB-C4B	16.36	1.48	1.35
26	WF	203	PEB	CHB-C4B	16.35	1.48	1.35
26	gI	201	PEB	CHB-C4B	16.34	1.48	1.35
26	M1	401	PEB	CHB-C4B	16.34	1.48	1.35
26	f6	203	PEB	CHB-C4B	16.34	1.48	1.35
26	j6	202	PEB	CHB-C4B	16.34	1.48	1.35
26	N6	201	PEB	CHB-C4B	16.34	1.48	1.35
26	RB	202	PEB	CHB-C4B	16.34	1.48	1.35
26	VE	202	PEB	CHB-C4B	16.34	1.48	1.35
26	GG	203	PEB	CHB-C4B	16.34	1.48	1.35
26	R6	201	PEB	CHB-C4B	16.34	1.48	1.35
26	P2	203	PEB	CHB-C4B	16.34	1.48	1.35
26	U3	202	PEB	CHB-C4B	16.34	1.48	1.35
26	g4	201	PEB	CHB-C4B	16.33	1.48	1.35
26	s1	202	PEB	CHB-C4B	16.33	1.48	1.35
26	AI	301	PEB	CHB-C4B	16.33	1.48	1.35
26	eE	201	PEB	CHB-C4B	16.33	1.48	1.35
26	GC	202	PEB	CHB-C4B	16.33	1.48	1.35
26	lF	203	PEB	CHB-C4B	16.33	1.48	1.35
26	YE	202	PEB	CHB-C4B	16.33	1.48	1.35
26	TE	202	PEB	CHB-C4B	16.33	1.48	1.35
26	P7	201	PEB	CHB-C4B	16.32	1.48	1.35
26	d7	202	PEB	CHB-C4B	16.32	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A3	201	PEB	CHB-C4B	16.32	1.48	1.35
26	Y4	202	PEB	CHB-C4B	16.32	1.48	1.35
26	L3	202	PEB	CHB-C4B	16.32	1.48	1.35
26	c4	203	PEB	CHB-C4B	16.32	1.48	1.35
26	HJ	202	PEB	CHB-C4B	16.32	1.48	1.35
26	gI	203	PEB	CHB-C4B	16.32	1.48	1.35
26	i1	201	PEB	CHB-C4B	16.31	1.48	1.35
26	AI	305	PEB	CHB-C4B	16.31	1.48	1.35
26	i7	202	PEB	CHB-C4B	16.31	1.48	1.35
26	b1	501	PEB	CHB-C4B	16.31	1.48	1.35
26	S4	202	PEB	CHB-C4B	16.31	1.48	1.35
26	H7	1002	PEB	CHB-C4B	16.31	1.48	1.35
26	L2	1002	PEB	CHB-C4B	16.31	1.48	1.35
26	I5	203	PEB	CHB-C4B	16.31	1.48	1.35
26	A7	305	PEB	CHB-C4B	16.31	1.48	1.35
26	A9	303	PEB	CHB-C4B	16.31	1.48	1.35
26	QF	201	PEB	CHB-C4B	16.31	1.48	1.35
26	SI	202	PEB	CHB-C4B	16.30	1.48	1.35
26	H9	202	PEB	CHB-C4B	16.30	1.48	1.35
26	YG	202	PEB	CHB-C4B	16.30	1.48	1.35
27	24	402	PUB	CHB-C1C	16.30	1.48	1.35
26	sG	203	PEB	CHB-C4B	16.29	1.48	1.35
26	S1	202	PEB	CHB-C4B	16.29	1.48	1.35
26	W3	202	PEB	CHB-C4B	16.29	1.48	1.35
26	B4	203	PEB	CHB-C4B	16.29	1.48	1.35
26	W6	202	PEB	CHB-C4B	16.29	1.48	1.35
26	c6	201	PEB	CHB-C4B	16.29	1.48	1.35
26	i1	203	PEB	CHB-C4B	16.29	1.48	1.35
26	LD	201	PEB	CHB-C4B	16.29	1.48	1.35
26	jB	202	PEB	CHB-C4B	16.28	1.48	1.35
26	g8	202	PEB	CHB-C4B	16.28	1.48	1.35
28	GI	1001	CYC	CHA-C1A	16.28	1.48	1.35
26	d7	203	PEB	CHB-C4B	16.27	1.48	1.35
26	Q1	201	PEB	CHB-C4B	16.27	1.48	1.35
26	AE	202	PEB	CHB-C4B	16.27	1.48	1.35
26	Z7	201	PEB	CHB-C4B	16.27	1.48	1.35
26	l7	202	PEB	CHB-C4B	16.27	1.48	1.35
26	cB	202	PEB	CHB-C4B	16.27	1.48	1.35
26	kF	201	PEB	CHB-C4B	16.27	1.48	1.35
26	B4	201	PEB	CHB-C4B	16.27	1.48	1.35
26	b7	201	PEB	CHB-C4B	16.27	1.48	1.35
26	OA	201	PEB	CHB-C4B	16.27	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	RG	202	PEB	CHB-C4B	16.27	1.48	1.35
26	A2	301	PEB	CHB-C4B	16.26	1.48	1.35
26	Y1	202	PEB	CHB-C4B	16.26	1.48	1.35
26	lF	201	PEB	CHB-C4B	16.26	1.48	1.35
26	g1	201	PEB	CHB-C4B	16.26	1.48	1.35
26	qE	202	PEB	CHB-C4B	16.26	1.48	1.35
26	P2	201	PEB	CHB-C4B	16.26	1.48	1.35
26	mG	203	PEB	CHB-C4B	16.26	1.48	1.35
26	qE	203	PEB	CHB-C4B	16.25	1.48	1.35
26	TG	202	PEB	CHB-C4B	16.25	1.48	1.35
26	d2	202	PEB	CHB-C4B	16.25	1.48	1.35
26	A7	302	PEB	CHB-C4B	16.25	1.48	1.35
26	YB	202	PEB	CHB-C4B	16.25	1.48	1.35
26	MJ	201	PEB	CHB-C4B	16.25	1.48	1.35
26	h2	201	PEB	CHB-C4B	16.25	1.48	1.35
26	q4	202	PEB	CHB-C4B	16.25	1.48	1.35
26	d6	204	PEB	CHB-C4B	16.25	1.48	1.35
26	CE	203	PEB	CHB-C4B	16.25	1.48	1.35
26	N1	203	PEB	CHB-C4B	16.25	1.48	1.35
26	n1	201	PEB	CHB-C4B	16.25	1.48	1.35
26	UA	203	PEB	CHB-C4B	16.25	1.48	1.35
26	DD	201	PEB	CHB-C4B	16.25	1.48	1.35
26	zG	501	PEB	CHB-C4B	16.25	1.48	1.35
26	LI	1002	PEB	CHB-C4B	16.24	1.48	1.35
28	rH	1001	CYC	CHA-C1A	16.24	1.48	1.35
26	e4	201	PEB	CHB-C4B	16.24	1.48	1.35
26	hG	201	PEB	CHB-C4B	16.24	1.48	1.35
26	aE	201	PEB	CHB-C4B	16.24	1.48	1.35
26	g1	203	PEB	CHB-C4B	16.24	1.48	1.35
26	lB	202	PEB	CHB-C4B	16.24	1.48	1.35
28	PH	1001	CYC	CHA-C1A	16.24	1.48	1.35
26	b2	201	PEB	CHB-C4B	16.24	1.48	1.35
28	J7	1003	CYC	CHA-C1A	16.23	1.48	1.35
26	Q7	202	PEB	CHB-C4B	16.23	1.48	1.35
26	gA	202	PEB	CHB-C4B	16.23	1.48	1.35
26	T2	201	PEB	CHB-C4B	16.23	1.48	1.35
26	TF	201	PEB	CHB-C4B	16.23	1.48	1.35
26	eF	201	PEB	CHB-C4B	16.23	1.48	1.35
26	T2	202	PEB	CHB-C4B	16.23	1.48	1.35
26	RE	201	PEB	CHB-C4B	16.23	1.48	1.35
28	K7	1001	CYC	CHA-C1A	16.23	1.48	1.35
26	FD	202	PEB	CHB-C4B	16.23	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R8	201	PEB	CHB-C4B	16.23	1.48	1.35
26	VJ	202	PEB	CHB-C4B	16.23	1.48	1.35
26	B1	201	PEB	CHB-C4B	16.23	1.48	1.35
26	h2	202	PEB	CHB-C4B	16.23	1.48	1.35
27	A2	302	PUB	CHB-C1C	16.23	1.48	1.35
26	TE	201	PEB	CHB-C4B	16.22	1.48	1.35
26	O2	201	PEB	CHB-C4B	16.22	1.48	1.35
26	G8	203	PEB	CHB-C4B	16.22	1.48	1.35
26	P1	202	PEB	CHB-C4B	16.22	1.48	1.35
26	q1	202	PEB	CHB-C4B	16.22	1.48	1.35
26	OE	203	PEB	CHB-C4B	16.22	1.48	1.35
26	AF	301	PEB	CHB-C4B	16.22	1.48	1.35
26	F9	202	PEB	CHB-C4B	16.22	1.48	1.35
26	e2	201	PEB	CHB-C4B	16.21	1.48	1.35
26	DB	1002	PEB	CHB-C4B	16.21	1.48	1.35
26	l7	201	PEB	CHB-C4B	16.21	1.48	1.35
26	TI	202	PEB	CHB-C4B	16.21	1.48	1.35
26	a6	202	PEB	CHB-C4B	16.21	1.48	1.35
26	GJ	201	PEB	CHB-C4B	16.21	1.48	1.35
26	g8	201	PEB	CHB-C4B	16.21	1.48	1.35
26	VD	201	PEB	CHB-C4B	16.21	1.48	1.35
26	cE	203	PEB	CHB-C4B	16.21	1.48	1.35
28	B6	1001	CYC	CHA-C1A	16.21	1.48	1.35
26	24	401	PEB	CHB-C4B	16.20	1.48	1.35
26	W7	201	PEB	CHB-C4B	16.20	1.48	1.35
26	RE	202	PEB	CHB-C4B	16.20	1.48	1.35
26	d1	202	PEB	CHB-C4B	16.20	1.48	1.35
26	U8	203	PEB	CHB-C4B	16.20	1.48	1.35
26	kB	202	PEB	CHB-C4B	16.20	1.48	1.35
26	ND	203	PEB	CHB-C4B	16.20	1.48	1.35
26	aF	202	PEB	CHB-C4B	16.20	1.48	1.35
26	WG	203	PEB	CHB-C4B	16.20	1.48	1.35
26	cI	201	PEB	CHB-C4B	16.20	1.48	1.35
26	21	404	PEB	CHB-C4B	16.20	1.48	1.35
26	iA	202	PEB	CHB-C4B	16.20	1.48	1.35
26	ID	202	PEB	CHB-C4B	16.20	1.48	1.35
26	M4	403	PEB	CHB-C4B	16.19	1.48	1.35
26	qE	201	PEB	CHB-C4B	16.19	1.48	1.35
26	21	405	PEB	CHB-C4B	16.19	1.48	1.35
28	F6	1001	CYC	CHA-C1A	16.19	1.48	1.35
26	TI	201	PEB	CHB-C4B	16.19	1.48	1.35
26	dB	202	PEB	CHB-C4B	16.19	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	HJ	203	PEB	CHB-C4B	16.19	1.48	1.35
26	e7	201	PEB	CHB-C4B	16.18	1.48	1.35
26	b4	501	PEB	CHB-C4B	16.18	1.48	1.35
26	FC	201	PEB	CHB-C4B	16.18	1.48	1.35
26	J9	201	PEB	CHB-C4B	16.18	1.48	1.35
28	CF	1001	CYC	CHA-C1A	16.18	1.48	1.35
28	G7	1001	CYC	CHA-C1A	16.18	1.48	1.35
27	A9	302	PUB	CHB-C1C	16.18	1.48	1.35
26	a4	201	PEB	CHB-C4B	16.17	1.48	1.35
28	FI	1001	CYC	CHA-C1A	16.17	1.48	1.35
26	ZB	202	PEB	CHB-C4B	16.17	1.48	1.35
26	U1	202	PEB	CHB-C4B	16.17	1.48	1.35
26	X9	203	PEB	CHB-C4B	16.17	1.48	1.35
26	aG	201	PEB	CHB-C4B	16.17	1.48	1.35
26	SI	201	PEB	CHB-C4B	16.17	1.48	1.35
26	bI	201	PEB	CHB-C4B	16.17	1.48	1.35
26	NE	201	PEB	CHB-C4B	16.16	1.48	1.35
26	i2	201	PEB	CHB-C4B	16.16	1.48	1.35
26	T9	203	PEB	CHB-C4B	16.16	1.48	1.35
26	R1	202	PEB	CHB-C4B	16.16	1.48	1.35
26	k8	201	PEB	CHB-C4B	16.16	1.48	1.35
26	bG	201	PEB	CHB-C4B	16.16	1.48	1.35
26	NG	201	PEB	CHB-C4B	16.16	1.48	1.35
26	JJ	201	PEB	CHB-C4B	16.16	1.48	1.35
26	W7	202	PEB	CHB-C4B	16.16	1.48	1.35
26	P9	202	PEB	CHB-C4B	16.16	1.48	1.35
26	iE	201	PEB	CHB-C4B	16.16	1.48	1.35
28	BB	1001	CYC	CHA-C1A	16.16	1.48	1.35
26	EG	202	PEB	CHB-C4B	16.15	1.48	1.35
26	e2	203	PEB	CHB-C4B	16.15	1.48	1.35
26	T6	201	PEB	CHB-C4B	16.15	1.48	1.35
26	M3	202	PEB	CHB-C4B	16.15	1.48	1.35
26	qG	202	PEB	CHB-C4B	16.15	1.48	1.35
26	G4	201	PEB	CHB-C4B	16.15	1.48	1.35
28	RH	1001	CYC	CHA-C1A	16.15	1.48	1.35
26	R9	203	PEB	CHB-C4B	16.14	1.48	1.35
26	PI	201	PEB	CHB-C4B	16.14	1.48	1.35
26	H9	203	PEB	CHB-C4B	16.14	1.48	1.35
26	X9	201	PEB	CHB-C4B	16.14	1.48	1.35
26	oE	203	PEB	CHB-C4B	16.14	1.48	1.35
26	UI	202	PEB	CHB-C4B	16.14	1.48	1.35
26	hA	201	PEB	CHB-C4B	16.14	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a7	202	PEB	CHB-C4B	16.13	1.48	1.35
26	h7	203	PEB	CHB-C4B	16.13	1.48	1.35
26	IA	201	PEB	CHB-C4B	16.13	1.48	1.35
26	PE	201	PEB	CHB-C4B	16.13	1.48	1.35
26	H1	202	PEB	CHB-C4B	16.13	1.48	1.35
26	R1	201	PEB	CHB-C4B	16.13	1.48	1.35
26	TB	201	PEB	CHB-C4B	16.12	1.48	1.35
26	N3	203	PEB	CHB-C4B	16.12	1.48	1.35
26	UB	203	PEB	CHB-C4B	16.12	1.48	1.35
26	sG	202	PEB	CHB-C4B	16.12	1.48	1.35
26	m2	201	PEB	CHB-C4B	16.12	1.48	1.35
26	N4	203	PEB	CHB-C4B	16.12	1.48	1.35
26	K5	203	PEB	CHB-C4B	16.12	1.48	1.35
26	Q6	203	PEB	CHB-C4B	16.12	1.48	1.35
26	j2	202	PEB	CHB-C4B	16.12	1.48	1.35
26	oE	201	PEB	CHB-C4B	16.12	1.48	1.35
26	mI	201	PEB	CHB-C4B	16.12	1.48	1.35
26	l6	202	PEB	CHB-C4B	16.12	1.48	1.35
27	A8	304	PUB	CHB-C1C	16.12	1.48	1.35
26	LJ	201	PEB	CHB-C4B	16.11	1.48	1.35
26	N7	1002	PEB	CHB-C4B	16.11	1.48	1.35
26	S2	201	PEB	CHB-C4B	16.11	1.48	1.35
26	l6	201	PEB	CHB-C4B	16.11	1.48	1.35
26	AI	304	PEB	CHB-C4B	16.11	1.48	1.35
26	i8	201	PEB	CHB-C4B	16.10	1.48	1.35
28	FB	1001	CYC	CHA-C1A	16.10	1.48	1.35
26	l2	201	PEB	CHB-C4B	16.10	1.48	1.35
26	A6	301	PEB	CHB-C4B	16.10	1.48	1.35
26	eI	201	PEB	CHB-C4B	16.10	1.48	1.35
26	FJ	202	PEB	CHB-C4B	16.10	1.48	1.35
27	21	403	PUB	CHB-C1C	16.10	1.48	1.35
26	j2	201	PEB	CHB-C4B	16.10	1.48	1.35
26	B4	202	PEB	CHB-C4B	16.10	1.48	1.35
26	G5	202	PEB	CHB-C4B	16.10	1.48	1.35
26	OI	201	PEB	CHB-C4B	16.10	1.48	1.35
26	O1	201	PEB	CHB-C4B	16.09	1.48	1.35
26	A2	305	PEB	CHB-C4B	16.09	1.48	1.35
26	AA	302	PEB	CHB-C4B	16.09	1.48	1.35
26	VI	201	PEB	CHB-C4B	16.09	1.48	1.35
26	eI	203	PEB	CHB-C4B	16.09	1.48	1.35
26	B3	201	PEB	CHB-C4B	16.09	1.48	1.35
26	jI	202	PEB	CHB-C4B	16.09	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q4	202	PEB	CHB-C4B	16.08	1.48	1.35
26	WD	202	PEB	CHB-C4B	16.08	1.48	1.35
26	m7	201	PEB	CHB-C4B	16.08	1.48	1.35
26	C1	201	PEB	CHB-C4B	16.08	1.48	1.35
26	sE	203	PEB	CHB-C4B	16.08	1.48	1.35
26	TJ	202	PEB	CHB-C4B	16.08	1.48	1.35
26	AF	302	PEB	CHB-C4B	16.08	1.48	1.35
26	RB	201	PEB	CHB-C4B	16.08	1.48	1.35
26	bF	201	PEB	CHB-C4B	16.08	1.48	1.35
26	WB	201	PEB	CHB-C4B	16.08	1.48	1.35
26	G8	202	PEB	CHB-C4B	16.08	1.48	1.35
27	AI	302	PUB	CHB-C1C	16.08	1.48	1.35
26	h7	201	PEB	CHB-C4B	16.07	1.48	1.35
26	EE	202	PEB	CHB-C4B	16.07	1.48	1.35
26	B1	202	PEB	CHB-C4B	16.07	1.48	1.35
26	x4	202	PEB	CHB-C4B	16.07	1.48	1.35
26	gI	202	PEB	CHB-C4B	16.07	1.48	1.35
26	F4	203	PEB	CHB-C4B	16.07	1.48	1.35
26	O4	202	PEB	CHB-C4B	16.07	1.48	1.35
26	NA	202	PEB	CHB-C4B	16.07	1.48	1.35
26	cE	202	PEB	CHB-C4B	16.07	1.48	1.35
26	eI	202	PEB	CHB-C4B	16.07	1.48	1.35
26	rG	202	PEB	CHB-C4B	16.07	1.48	1.35
26	uE	201	PEB	CHB-C4B	16.06	1.48	1.35
26	V2	201	PEB	CHB-C4B	16.06	1.48	1.35
26	J8	201	PEB	CHB-C4B	16.06	1.48	1.35
26	f6	201	PEB	CHB-C4B	16.06	1.48	1.35
26	OG	201	PEB	CHB-C4B	16.06	1.48	1.35
26	K8	201	PEB	CHB-C4B	16.06	1.48	1.35
26	P6	201	PEB	CHB-C4B	16.06	1.48	1.35
26	Q1	202	PEB	CHB-C4B	16.05	1.48	1.35
26	h8	201	PEB	CHB-C4B	16.05	1.48	1.35
26	LE	201	PEB	CHB-C4B	16.05	1.48	1.35
26	fA	203	PEB	CHB-C4B	16.05	1.48	1.35
26	e6	201	PEB	CHB-C4B	16.05	1.48	1.35
26	L3	201	PEB	CHB-C4B	16.04	1.48	1.35
26	i4	202	PEB	CHB-C4B	16.04	1.48	1.35
26	N4	202	PEB	CHB-C4B	16.04	1.48	1.35
26	N8	202	PEB	CHB-C4B	16.04	1.48	1.35
26	S9	201	PEB	CHB-C4B	16.04	1.48	1.35
26	N1	202	PEB	CHB-C4B	16.04	1.48	1.35
28	uH	1001	CYC	CHA-C1A	16.04	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A7	301	PEB	CHB-C4B	16.04	1.48	1.35
26	D7	1002	PEB	CHB-C4B	16.04	1.48	1.35
26	QB	203	PEB	CHB-C4B	16.04	1.48	1.35
26	SJ	201	PEB	CHB-C4B	16.04	1.48	1.35
26	F1	202	PEB	CHB-C4B	16.03	1.48	1.35
26	F3	202	PEB	CHB-C4B	16.03	1.48	1.35
26	M8	203	PEB	CHB-C4B	16.03	1.48	1.35
28	J7	1001	CYC	CHA-C1A	16.03	1.48	1.35
26	P8	201	PEB	CHB-C4B	16.03	1.48	1.35
26	K9	201	PEB	CHB-C4B	16.03	1.48	1.35
26	m8	201	PEB	CHB-C4B	16.03	1.48	1.35
26	M1	402	PEB	CHB-C4B	16.03	1.48	1.35
26	R4	201	PEB	CHB-C4B	16.03	1.48	1.35
26	K9	202	PEB	CHB-C4B	16.03	1.48	1.35
26	N9	203	PEB	CHB-C4B	16.02	1.48	1.35
26	ID	201	PEB	CHB-C4B	16.02	1.48	1.35
26	JE	202	PEB	CHB-C4B	16.02	1.48	1.35
26	hF	202	PEB	CHB-C4B	16.02	1.48	1.35
26	r1	201	PEB	CHB-C4B	16.02	1.48	1.35
26	c2	201	PEB	CHB-C4B	16.02	1.48	1.35
26	GD	202	PEB	CHB-C4B	16.02	1.48	1.35
26	aB	202	PEB	CHB-C4B	16.02	1.48	1.35
26	WB	202	PEB	CHB-C4B	16.01	1.48	1.35
26	U2	202	PEB	CHB-C4B	16.01	1.48	1.35
26	gE	202	PEB	CHB-C4B	16.00	1.48	1.35
26	b6	201	PEB	CHB-C4B	16.00	1.48	1.35
26	CA	202	PEB	CHB-C4B	16.00	1.48	1.35
26	e2	202	PEB	CHB-C4B	16.00	1.48	1.35
26	HF	1002	PEB	CHB-C4B	16.00	1.48	1.35
26	a2	201	PEB	CHB-C4B	16.00	1.48	1.35
26	f8	203	PEB	CHB-C4B	16.00	1.48	1.35
26	T1	203	PEB	CHB-C4B	16.00	1.48	1.35
26	k2	202	PEB	CHB-C4B	16.00	1.48	1.35
26	bB	201	PEB	CHB-C4B	16.00	1.48	1.35
26	eG	201	PEB	CHB-C4B	16.00	1.48	1.35
26	cG	202	PEB	CHB-C4B	16.00	1.48	1.35
26	HC	202	PEB	CHB-C4B	15.99	1.48	1.35
26	FF	1002	PEB	CHB-C4B	15.99	1.48	1.35
26	MG	203	PEB	CHB-C4B	15.99	1.48	1.35
26	RG	201	PEB	CHB-C4B	15.99	1.48	1.35
26	k8	202	PEB	CHB-C4B	15.99	1.48	1.35
26	DF	1002	PEB	CHB-C4B	15.99	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c8	201	PEB	CHB-C4B	15.99	1.48	1.35
26	PG	201	PEB	CHB-C4B	15.99	1.48	1.35
26	J3	203	PEB	CHB-C4B	15.99	1.48	1.35
28	tH	1001	CYC	CHA-C1A	15.99	1.48	1.35
26	A1	201	PEB	CHB-C4B	15.99	1.48	1.35
26	L9	202	PEB	CHB-C4B	15.99	1.48	1.35
26	yG	301	PEB	CHB-C4B	15.99	1.48	1.35
28	JF	1003	CYC	CHA-C1A	15.99	1.48	1.35
26	DE	201	PEB	CHB-C4B	15.99	1.48	1.35
26	SA	203	PEB	CHB-C4B	15.98	1.48	1.35
26	MD	202	PEB	CHB-C4B	15.98	1.48	1.35
27	21	402	PUB	CHB-C1C	15.98	1.48	1.35
26	DA	201	PEB	CHB-C4B	15.98	1.48	1.35
26	LC	201	PEB	CHB-C4B	15.98	1.48	1.35
26	gE	203	PEB	CHB-C4B	15.98	1.48	1.35
26	TG	201	PEB	CHB-C4B	15.98	1.48	1.35
28	G2	1001	CYC	CHA-C1A	15.98	1.48	1.35
26	R3	203	PEB	CHB-C4B	15.98	1.48	1.35
26	O7	202	PEB	CHB-C4B	15.97	1.48	1.35
26	dB	201	PEB	CHB-C4B	15.97	1.48	1.35
26	DI	1002	PEB	CHB-C4B	15.97	1.48	1.35
26	AB	301	PEB	CHB-C4B	15.97	1.48	1.35
26	zE	501	PEB	CHB-C4B	15.97	1.48	1.35
26	uG	203	PEB	CHB-C4B	15.97	1.48	1.35
26	PB	202	PEB	CHB-C4B	15.97	1.48	1.35
26	LJ	202	PEB	CHB-C4B	15.97	1.48	1.35
26	w4	204	PEB	CHB-C4B	15.97	1.48	1.35
27	AI	303	PUB	CHB-C1C	15.97	1.48	1.35
26	Z6	202	PEB	CHB-C4B	15.96	1.48	1.35
28	NI	1001	CYC	CHA-C1A	15.96	1.48	1.35
27	A2	303	PUB	CHB-C1C	15.96	1.48	1.35
26	YG	203	PEB	CHB-C4B	15.96	1.48	1.35
26	PB	201	PEB	CHB-C4B	15.96	1.48	1.35
26	Z4	202	PEB	CHB-C4B	15.96	1.48	1.35
26	CA	201	PEB	CHB-C4B	15.96	1.48	1.35
26	d7	201	PEB	CHB-C4B	15.96	1.48	1.35
26	pG	201	PEB	CHB-C4B	15.96	1.48	1.35
26	D8	201	PEB	CHB-C4B	15.95	1.48	1.35
26	JD	203	PEB	CHB-C4B	15.95	1.48	1.35
28	SH	1001	CYC	CHA-C1A	15.95	1.48	1.35
26	M1	403	PEB	CHB-C4B	15.95	1.48	1.35
26	aI	201	PEB	CHB-C4B	15.95	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O1	202	PEB	CHB-C4B	15.95	1.48	1.35
26	O9	201	PEB	CHB-C4B	15.95	1.48	1.35
27	yG	302	PUB	CHB-C1C	15.95	1.48	1.35
26	W6	201	PEB	CHB-C4B	15.95	1.48	1.35
26	gB	202	PEB	CHB-C4B	15.95	1.48	1.35
26	L9	203	PEB	CHB-C4B	15.94	1.48	1.35
26	cA	201	PEB	CHB-C4B	15.94	1.48	1.35
26	kG	201	PEB	CHB-C4B	15.94	1.48	1.35
26	B9	202	PEB	CHB-C4B	15.94	1.48	1.35
28	K2	1001	CYC	CHA-C1A	15.93	1.48	1.35
26	aE	203	PEB	CHB-C4B	15.93	1.48	1.35
27	A6	303	PUB	CHB-C1C	15.93	1.48	1.35
26	xE	303	PEB	CHB-C4B	15.93	1.48	1.35
26	d6	201	PEB	CHB-C4B	15.93	1.48	1.35
26	mG	202	PEB	CHB-C4B	15.93	1.48	1.35
26	dI	202	PEB	CHB-C4B	15.93	1.48	1.35
26	g6	202	PEB	CHB-C4B	15.92	1.48	1.35
26	M9	202	PEB	CHB-C4B	15.92	1.48	1.35
26	mA	201	PEB	CHB-C4B	15.92	1.48	1.35
26	U4	202	PEB	CHB-C4B	15.92	1.48	1.35
26	h6	202	PEB	CHB-C4B	15.92	1.48	1.35
26	c7	201	PEB	CHB-C4B	15.92	1.48	1.35
26	J2	1002	PEB	CHB-C4B	15.91	1.48	1.35
26	V3	201	PEB	CHB-C4B	15.91	1.48	1.35
26	FC	203	PEB	CHB-C4B	15.91	1.48	1.35
26	i8	202	PEB	CHB-C4B	15.91	1.48	1.35
26	k2	201	PEB	CHB-C4B	15.91	1.48	1.35
26	D3	203	PEB	CHB-C4B	15.90	1.48	1.35
26	PA	201	PEB	CHB-C4B	15.90	1.48	1.35
26	KJ	202	PEB	CHB-C4B	15.90	1.48	1.35
26	Z6	203	PEB	CHB-C4B	15.89	1.48	1.35
26	BE	201	PEB	CHB-C4B	15.89	1.48	1.35
26	YD	303	PEB	CHB-C4B	15.89	1.48	1.35
26	ZG	201	PEB	CHB-C4B	15.89	1.48	1.35
26	WF	202	PEB	CHB-C4B	15.89	1.48	1.35
26	KC	202	PEB	CHB-C4B	15.89	1.48	1.35
26	KB	201	PEB	CHB-C4B	15.89	1.48	1.35
26	MA	203	PEB	CHB-C4B	15.88	1.48	1.35
26	O8	202	PEB	CHB-C4B	15.88	1.48	1.35
26	P9	203	PEB	CHB-C4B	15.87	1.48	1.35
26	II	201	PEB	CHB-C4B	15.87	1.48	1.35
26	eB	201	PEB	CHB-C4B	15.86	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PJ	203	PEB	CHB-C4B	15.86	1.48	1.35
26	X4	202	PEB	CHB-C4B	15.86	1.48	1.35
26	I8	202	PEB	CHB-C4B	15.86	1.48	1.35
26	Y8	202	PEB	CHB-C4B	15.86	1.48	1.35
26	H5	202	PEB	CHB-C4B	15.86	1.48	1.35
26	NJ	203	PEB	CHB-C4B	15.86	1.48	1.35
28	KI	1001	CYC	CHA-C1A	15.86	1.48	1.35
26	ME	201	PEB	CHB-C4B	15.86	1.48	1.35
26	VF	203	PEB	CHB-C4B	15.86	1.48	1.35
26	mG	201	PEB	CHB-C4B	15.86	1.48	1.35
26	y1	203	PEB	CHB-C4B	15.85	1.48	1.35
26	T4	202	PEB	CHB-C4B	15.85	1.48	1.35
26	ZI	202	PEB	CHB-C4B	15.85	1.48	1.35
26	V1	203	PEB	CHB-C4B	15.85	1.48	1.35
26	BJ	202	PEB	CHB-C4B	15.85	1.48	1.35
26	AJ	303	PEB	CHB-C4B	15.85	1.48	1.35
26	yE	301	PEB	CHB-C4B	15.85	1.48	1.35
26	ZB	203	PEB	CHB-C4B	15.85	1.48	1.35
26	mE	202	PEB	CHB-C4B	15.85	1.48	1.35
28	H2	1001	CYC	CHA-C1A	15.84	1.48	1.35
26	jG	201	PEB	CHB-C4B	15.84	1.48	1.35
26	T7	202	PEB	CHB-C4B	15.84	1.48	1.35
28	CB	1001	CYC	CHA-C1A	15.84	1.48	1.35
26	KA	201	PEB	CHB-C4B	15.84	1.48	1.35
26	C8	201	PEB	CHB-C4B	15.84	1.48	1.35
26	OF	201	PEB	CHB-C4B	15.84	1.48	1.35
26	D6	1002	PEB	CHB-C4B	15.84	1.48	1.35
26	DG	201	PEB	CHB-C4B	15.84	1.48	1.35
26	JJ	203	PEB	CHB-C4B	15.84	1.48	1.35
27	AB	303	PUB	CHB-C1C	15.84	1.48	1.35
26	21	401	PEB	CHB-C4B	15.83	1.48	1.35
26	Z7	203	PEB	CHB-C4B	15.83	1.48	1.35
26	IA	202	PEB	CHB-C4B	15.82	1.48	1.35
28	M2	1001	CYC	CHA-C1A	15.82	1.48	1.35
26	YA	203	PEB	CHB-C4B	15.82	1.48	1.35
26	y4	202	PEB	CHB-C4B	15.82	1.48	1.35
28	KF	1001	CYC	CHA-C1A	15.82	1.48	1.35
26	A2	304	PEB	CHB-C4B	15.82	1.48	1.35
26	T4	203	PEB	CHB-C4B	15.82	1.48	1.35
26	f8	201	PEB	CHB-C4B	15.82	1.48	1.35
26	A4	201	PEB	CHB-C4B	15.81	1.48	1.35
26	S6	201	PEB	CHB-C4B	15.81	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dF	203	PEB	CHB-C4B	15.81	1.48	1.35
26	K6	201	PEB	CHB-C4B	15.81	1.48	1.35
26	W2	201	PEB	CHB-C4B	15.81	1.48	1.35
26	YA	202	PEB	CHB-C4B	15.81	1.48	1.35
26	GE	203	PEB	CHB-C4B	15.81	1.48	1.35
26	g2	202	PEB	CHB-C4B	15.81	1.48	1.35
26	JA	202	PEB	CHB-C4B	15.81	1.48	1.35
26	V4	203	PEB	CHB-C4B	15.80	1.48	1.35
27	K4	203	PUB	CHB-C1C	15.80	1.48	1.35
26	UD	202	PEB	CHB-C4B	15.80	1.48	1.35
26	TF	202	PEB	CHB-C4B	15.80	1.48	1.35
26	D3	201	PEB	CHB-C4B	15.80	1.48	1.35
26	Z2	202	PEB	CHB-C4B	15.80	1.48	1.35
26	DD	203	PEB	CHB-C4B	15.80	1.48	1.35
28	C6	1001	CYC	CHA-C1A	15.80	1.48	1.35
26	a1	203	PEB	CHB-C4B	15.79	1.48	1.35
26	S9	202	PEB	CHB-C4B	15.79	1.48	1.35
26	R4	202	PEB	CHB-C4B	15.79	1.48	1.35
26	F7	1002	PEB	CHB-C4B	15.79	1.48	1.35
26	LJ	203	PEB	CHB-C4B	15.79	1.48	1.35
28	I7	1001	CYC	CHA-C1A	15.78	1.48	1.35
26	A8	302	PEB	CHB-C4B	15.78	1.48	1.35
26	kA	201	PEB	CHB-C4B	15.78	1.48	1.35
26	hA	202	PEB	CHB-C4B	15.78	1.48	1.35
26	gG	202	PEB	CHB-C4B	15.77	1.48	1.35
26	X1	201	PEB	CHB-C4B	15.77	1.48	1.35
26	TJ	203	PEB	CHB-C4B	15.77	1.48	1.35
26	j7	201	PEB	CHB-C4B	15.77	1.48	1.35
26	dI	201	PEB	CHB-C4B	15.77	1.48	1.35
26	P7	202	PEB	CHB-C4B	15.77	1.48	1.35
27	K3	203	PUB	CHB-C1C	15.77	1.48	1.35
27	yE	303	PUB	CHB-C1C	15.77	1.48	1.35
26	TA	201	PEB	CHB-C4B	15.77	1.48	1.35
26	lA	203	PEB	CHB-C4B	15.77	1.48	1.35
26	H6	1002	PEB	CHB-C4B	15.76	1.48	1.35
26	X4	201	PEB	CHB-C4B	15.76	1.48	1.35
26	N2	1002	PEB	CHB-C4B	15.76	1.48	1.35
26	P6	202	PEB	CHB-C4B	15.76	1.48	1.35
26	M8	202	PEB	CHB-C4B	15.76	1.48	1.35
26	fA	201	PEB	CHB-C4B	15.75	1.48	1.35
26	kI	202	PEB	CHB-C4B	15.75	1.48	1.35
26	GA	203	PEB	CHB-C4B	15.75	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	NI	1002	PEB	CHB-C4B	15.75	1.48	1.35
26	RA	202	PEB	CHB-C4B	15.75	1.48	1.35
26	D1	201	PEB	CHB-C4B	15.75	1.48	1.35
26	JD	202	PEB	CHB-C4B	15.75	1.48	1.35
26	jA	201	PEB	CHB-C4B	15.74	1.48	1.35
26	S8	202	PEB	CHB-C4B	15.74	1.48	1.35
26	aI	202	PEB	CHB-C4B	15.74	1.48	1.35
26	eE	203	PEB	CHB-C4B	15.74	1.48	1.35
26	k6	202	PEB	CHB-C4B	15.74	1.48	1.35
26	wE	302	PEB	CHB-C4B	15.74	1.48	1.35
26	T1	202	PEB	CHB-C4B	15.73	1.48	1.35
26	HA	202	PEB	CHB-C4B	15.73	1.48	1.35
26	O7	201	PEB	CHB-C4B	15.72	1.48	1.35
26	oG	203	PEB	CHB-C4B	15.72	1.48	1.35
26	H4	202	PEB	CHB-C4B	15.72	1.48	1.35
26	lB	201	PEB	CHB-C4B	15.72	1.48	1.35
26	G3	202	PEB	CHB-C4B	15.71	1.48	1.35
26	R9	202	PEB	CHB-C4B	15.71	1.48	1.35
26	fB	201	PEB	CHB-C4B	15.70	1.48	1.35
26	E8	201	PEB	CHB-C4B	15.70	1.48	1.35
26	KG	203	PEB	CHB-C4B	15.70	1.48	1.35
26	X1	202	PEB	CHB-C4B	15.70	1.48	1.35
26	ZI	201	PEB	CHB-C4B	15.70	1.48	1.35
26	MJ	202	PEB	CHB-C4B	15.69	1.48	1.35
26	MA	202	PEB	CHB-C4B	15.69	1.48	1.35
26	M4	402	PEB	CHB-C4B	15.69	1.48	1.35
26	C8	202	PEB	CHB-C4B	15.69	1.48	1.35
26	eA	201	PEB	CHB-C4B	15.69	1.48	1.35
26	IC	202	PEB	CHB-C4B	15.69	1.48	1.35
26	OE	201	PEB	CHB-C4B	15.69	1.48	1.35
26	n4	201	PEB	CHB-C4B	15.69	1.48	1.35
26	XG	202	PEB	CHB-C4B	15.68	1.48	1.35
26	sE	201	PEB	CHB-C4B	15.68	1.48	1.35
26	J9	203	PEB	CHB-C4B	15.68	1.48	1.35
26	fI	201	PEB	CHB-C4B	15.68	1.48	1.35
28	C2	1001	CYC	CHA-C1A	15.68	1.48	1.35
26	SB	201	PEB	CHB-C4B	15.68	1.48	1.35
26	RD	201	PEB	CHB-C4B	15.68	1.48	1.35
26	xE	302	PEB	CHB-C4B	15.68	1.48	1.35
26	S8	203	PEB	CHB-C4B	15.67	1.48	1.35
26	UB	201	PEB	CHB-C4B	15.67	1.48	1.35
26	VA	202	PEB	CHB-C4B	15.67	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J8	202	PEB	CHB-C4B	15.67	1.48	1.35
26	f2	201	PEB	CHB-C4B	15.67	1.48	1.35
26	eG	203	PEB	CHB-C4B	15.67	1.48	1.35
26	kE	201	PEB	CHB-C4B	15.67	1.48	1.35
26	TB	202	PEB	CHB-C4B	15.67	1.48	1.35
26	V4	202	PEB	CHB-C4B	15.66	1.48	1.35
26	JI	1002	PEB	CHB-C4B	15.66	1.48	1.35
26	AB	304	PEB	CHB-C4B	15.65	1.48	1.35
26	Y3	303	PEB	CHB-C4B	15.65	1.48	1.35
26	m2	202	PEB	CHB-C4B	15.65	1.48	1.35
26	h8	202	PEB	CHB-C4B	15.65	1.48	1.35
26	QA	202	PEB	CHB-C4B	15.65	1.48	1.35
26	Q2	201	PEB	CHB-C4B	15.65	1.48	1.35
26	bF	203	PEB	CHB-C4B	15.64	1.48	1.35
26	Z2	201	PEB	CHB-C4B	15.64	1.48	1.35
26	D1	202	PEB	CHB-C4B	15.64	1.48	1.35
26	A9	301	PEB	CHB-C4B	15.64	1.48	1.35
28	CI	1001	CYC	CHA-C1A	15.64	1.48	1.35
26	jF	202	PEB	CHB-C4B	15.63	1.48	1.35
26	SJ	202	PEB	CHB-C4B	15.63	1.48	1.35
26	OJ	201	PEB	CHB-C4B	15.63	1.48	1.35
26	F1	203	PEB	CHB-C4B	15.63	1.48	1.35
26	Q7	203	PEB	CHB-C4B	15.63	1.48	1.35
26	U7	202	PEB	CHB-C4B	15.63	1.48	1.35
28	JF	1001	CYC	CHA-C1A	15.63	1.48	1.35
26	HB	1002	PEB	CHB-C4B	15.63	1.48	1.35
26	wG	302	PEB	CHB-C4B	15.63	1.48	1.35
26	k1	203	PEB	CHB-C4B	15.62	1.48	1.35
26	T6	202	PEB	CHB-C4B	15.62	1.48	1.35
28	N2	1001	CYC	CHA-C1A	15.62	1.48	1.35
26	Y3	304	PEB	CHB-C4B	15.62	1.48	1.35
26	Y8	203	PEB	CHB-C4B	15.62	1.48	1.35
26	RI	201	PEB	CHB-C4B	15.62	1.48	1.35
26	c8	202	PEB	CHB-C4B	15.61	1.48	1.35
26	L6	1002	PEB	CHB-C4B	15.61	1.48	1.35
26	BD	203	PEB	CHB-C4B	15.61	1.48	1.35
26	BD	201	PEB	CHB-C4B	15.61	1.48	1.35
26	cF	201	PEB	CHB-C4B	15.61	1.48	1.35
26	l8	203	PEB	CHB-C4B	15.60	1.48	1.35
26	R8	202	PEB	CHB-C4B	15.60	1.48	1.35
26	T8	201	PEB	CHB-C4B	15.60	1.48	1.35
26	SA	202	PEB	CHB-C4B	15.60	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	i2	202	PEB	CHB-C4B	15.59	1.48	1.35
26	V8	202	PEB	CHB-C4B	15.59	1.48	1.35
26	k4	203	PEB	CHB-C4B	15.59	1.48	1.35
26	R2	201	PEB	CHB-C4B	15.59	1.48	1.35
26	OF	203	PEB	CHB-C4B	15.59	1.48	1.35
26	gG	203	PEB	CHB-C4B	15.59	1.48	1.35
26	H3	202	PEB	CHB-C4B	15.58	1.48	1.35
26	W3	201	PEB	CHB-C4B	15.58	1.48	1.35
26	L5	201	PEB	CHB-C4B	15.58	1.48	1.35
26	WI	201	PEB	CHB-C4B	15.58	1.48	1.35
26	h4	202	PEB	CHB-C4B	15.57	1.48	1.35
26	MD	201	PEB	CHB-C4B	15.57	1.48	1.35
26	d4	202	PEB	CHB-C4B	15.57	1.48	1.35
26	e8	201	PEB	CHB-C4B	15.57	1.48	1.35
27	xE	301	PUB	CHB-C1C	15.57	1.48	1.35
26	D2	1002	PEB	CHB-C4B	15.56	1.48	1.35
28	II	1001	CYC	CHA-C1A	15.56	1.48	1.35
26	cG	203	PEB	CHB-C4B	15.56	1.48	1.35
26	LA	201	PEB	CHB-C4B	15.56	1.48	1.35
26	h6	203	PEB	CHB-C4B	15.55	1.48	1.35
26	k1	202	PEB	CHB-C4B	15.55	1.48	1.35
26	E9	201	PEB	CHB-C4B	15.55	1.48	1.35
26	V8	201	PEB	CHB-C4B	15.55	1.48	1.35
26	P8	202	PEB	CHB-C4B	15.55	1.48	1.35
26	Q7	201	PEB	CHB-C4B	15.54	1.48	1.35
26	D4	201	PEB	CHB-C4B	15.53	1.48	1.35
26	cA	203	PEB	CHB-C4B	15.53	1.48	1.35
26	F5	201	PEB	CHB-C4B	15.53	1.48	1.35
26	A6	304	PEB	CHB-C4B	15.53	1.48	1.35
26	lA	202	PEB	CHB-C4B	15.52	1.48	1.35
27	A6	302	PUB	CHB-C1C	15.52	1.48	1.35
26	E9	202	PEB	CHB-C4B	15.52	1.48	1.35
26	aA	203	PEB	CHB-C4B	15.52	1.48	1.35
26	Q8	202	PEB	CHB-C4B	15.52	1.48	1.35
28	HI	1001	CYC	CHA-C1A	15.52	1.48	1.35
26	FA	201	PEB	CHB-C4B	15.52	1.48	1.35
26	LB	1002	PEB	CHB-C4B	15.52	1.48	1.35
26	VA	201	PEB	CHB-C4B	15.51	1.48	1.35
26	LC	202	PEB	CHB-C4B	15.51	1.48	1.35
26	PI	202	PEB	CHB-C4B	15.51	1.48	1.35
26	lA	201	PEB	CHB-C4B	15.50	1.48	1.35
26	YD	304	PEB	CHB-C4B	15.50	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	E2	1001	CYC	CHA-C1A	15.50	1.48	1.35
28	L6	1001	CYC	CHA-C1A	15.50	1.48	1.35
26	xG	302	PEB	CHB-C4B	15.50	1.48	1.35
26	U6	201	PEB	CHB-C4B	15.49	1.48	1.35
26	a4	203	PEB	CHB-C4B	15.49	1.48	1.35
26	a2	202	PEB	CHB-C4B	15.49	1.48	1.35
26	hB	203	PEB	CHB-C4B	15.49	1.48	1.35
26	d2	201	PEB	CHB-C4B	15.48	1.48	1.35
26	QI	201	PEB	CHB-C4B	15.48	1.48	1.35
26	QA	204	PEB	CHB-C4B	15.48	1.48	1.35
26	jE	201	PEB	CHB-C4B	15.48	1.48	1.35
26	F8	201	PEB	CHB-C4B	15.48	1.48	1.35
26	HI	1002	PEB	CHB-C4B	15.48	1.48	1.35
26	R3	201	PEB	CHB-C4B	15.47	1.48	1.35
26	iF	201	PEB	CHB-C4B	15.47	1.48	1.35
27	yE	302	PUB	CHB-C1C	15.47	1.48	1.35
26	a6	201	PEB	CHB-C4B	15.46	1.48	1.35
28	MI	1001	CYC	CHA-C1A	15.46	1.48	1.35
27	A8	303	PUB	CHB-C1C	15.46	1.48	1.35
26	L8	201	PEB	CHB-C4B	15.46	1.48	1.35
26	KE	203	PEB	CHB-C4B	15.46	1.48	1.35
26	SF	201	PEB	CHB-C4B	15.46	1.48	1.35
26	F9	203	PEB	CHB-C4B	15.44	1.48	1.35
26	OD	202	PEB	CHB-C4B	15.44	1.48	1.35
26	aG	203	PEB	CHB-C4B	15.44	1.48	1.35
26	j7	202	PEB	CHB-C4B	15.44	1.48	1.35
26	ND	201	PEB	CHB-C4B	15.44	1.48	1.35
27	AA	303	PUB	CHB-C1C	15.44	1.48	1.35
26	L7	1002	PEB	CHB-C4B	15.44	1.48	1.35
26	F9	201	PEB	CHB-C4B	15.44	1.48	1.35
26	S3	202	PEB	CHB-C4B	15.43	1.48	1.35
26	r4	201	PEB	CHB-C4B	15.43	1.48	1.35
26	FC	202	PEB	CHB-C4B	15.43	1.48	1.35
28	DF	1003	CYC	CHA-C1A	15.43	1.48	1.35
26	b6	202	PEB	CHB-C4B	15.43	1.48	1.35
26	QF	203	PEB	CHB-C4B	15.43	1.48	1.35
26	f7	202	PEB	CHB-C4B	15.43	1.48	1.35
26	D3	202	PEB	CHB-C4B	15.42	1.48	1.35
26	l7	203	PEB	CHB-C4B	15.42	1.48	1.35
26	I8	201	PEB	CHB-C4B	15.42	1.48	1.35
26	VD	202	PEB	CHB-C4B	15.42	1.48	1.35
26	Q8	204	PEB	CHB-C4B	15.41	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P2	202	PEB	CHB-C4B	15.41	1.48	1.35
26	O7	203	PEB	CHB-C4B	15.41	1.48	1.35
26	mI	202	PEB	CHB-C4B	15.41	1.48	1.35
26	LA	202	PEB	CHB-C4B	15.41	1.48	1.35
26	OG	203	PEB	CHB-C4B	15.40	1.48	1.35
26	H2	1002	PEB	CHB-C4B	15.40	1.48	1.35
26	IC	201	PEB	CHB-C4B	15.40	1.48	1.35
26	EA	201	PEB	CHB-C4B	15.39	1.48	1.35
26	aG	202	PEB	CHB-C4B	15.39	1.48	1.35
26	T1	201	PEB	CHB-C4B	15.38	1.48	1.35
26	EJ	201	PEB	CHB-C4B	15.38	1.48	1.35
26	ZF	203	PEB	CHB-C4B	15.38	1.48	1.35
26	MG	201	PEB	CHB-C4B	15.38	1.48	1.35
26	SA	201	PEB	CHB-C4B	15.38	1.48	1.35
26	aB	201	PEB	CHB-C4B	15.37	1.48	1.35
26	G3	201	PEB	CHB-C4B	15.37	1.48	1.35
26	eB	202	PEB	CHB-C4B	15.37	1.48	1.35
26	DD	202	PEB	CHB-C4B	15.36	1.48	1.35
28	I2	1001	CYC	CHA-C1A	15.36	1.47	1.35
26	X8	202	PEB	CHB-C4B	15.35	1.47	1.35
28	DB	1001	CYC	CHA-C1A	15.35	1.47	1.35
26	V1	202	PEB	CHB-C4B	15.35	1.47	1.35
26	K5	202	PEB	CHB-C4B	15.35	1.47	1.35
28	EI	1001	CYC	CHA-C1A	15.34	1.47	1.35
26	wE	301	PEB	CHB-C4B	15.34	1.47	1.35
26	AJ	301	PEB	CHB-C4B	15.34	1.47	1.35
26	G8	201	PEB	CHB-C4B	15.34	1.47	1.35
26	RJ	202	PEB	CHB-C4B	15.33	1.47	1.35
26	H8	202	PEB	CHB-C4B	15.33	1.47	1.35
26	JC	202	PEB	CHB-C4B	15.33	1.47	1.35
28	D6	1001	CYC	CHA-C1A	15.33	1.47	1.35
26	WD	201	PEB	CHB-C4B	15.32	1.47	1.35
26	F5	203	PEB	CHB-C4B	15.32	1.47	1.35
26	XA	202	PEB	CHB-C4B	15.32	1.47	1.35
26	iI	202	PEB	CHB-C4B	15.32	1.47	1.35
28	EB	1001	CYC	CHA-C1A	15.32	1.47	1.35
27	yG	303	PUB	CHB-C1C	15.31	1.47	1.35
26	T4	201	PEB	CHB-C4B	15.31	1.47	1.35
28	KB	202	CYC	CHA-C1A	15.30	1.47	1.35
26	P1	201	PEB	CHB-C4B	15.30	1.47	1.35
26	J7	1002	PEB	CHB-C4B	15.30	1.47	1.35
26	fF	202	PEB	CHB-C4B	15.29	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l8	202	PEB	CHB-C4B	15.29	1.47	1.35
26	F2	1002	PEB	CHB-C4B	15.29	1.47	1.35
26	UA	202	PEB	CHB-C4B	15.28	1.47	1.35
26	TD	203	PEB	CHB-C4B	15.28	1.47	1.35
26	K1	202	PEB	CHB-C4B	15.28	1.47	1.35
26	V3	202	PEB	CHB-C4B	15.27	1.47	1.35
26	HA	201	PEB	CHB-C4B	15.27	1.47	1.35
26	FJ	201	PEB	CHB-C4B	15.27	1.47	1.35
26	FI	1002	PEB	CHB-C4B	15.27	1.47	1.35
28	K6	202	CYC	CHA-C1A	15.27	1.47	1.35
26	OF	202	PEB	CHB-C4B	15.26	1.47	1.35
26	X1	203	PEB	CHB-C4B	15.26	1.47	1.35
26	S7	202	PEB	CHB-C4B	15.26	1.47	1.35
26	O3	202	PEB	CHB-C4B	15.26	1.47	1.35
26	P4	201	PEB	CHB-C4B	15.26	1.47	1.35
27	KD	203	PUB	CHB-C1C	15.25	1.47	1.35
26	K3	201	PEB	CHB-C4B	15.25	1.47	1.35
26	SE	201	PEB	CHB-C4B	15.25	1.47	1.35
26	YD	301	PEB	CHB-C4B	15.25	1.47	1.35
26	NF	1002	PEB	CHB-C4B	15.25	1.47	1.35
26	M3	201	PEB	CHB-C4B	15.24	1.47	1.35
26	ZF	202	PEB	CHB-C4B	15.24	1.47	1.35
26	EJ	202	PEB	CHB-C4B	15.23	1.47	1.35
28	D2	1001	CYC	CHA-C1A	15.23	1.47	1.35
26	j8	201	PEB	CHB-C4B	15.23	1.47	1.35
26	GB	1002	PEB	CHB-C4B	15.22	1.47	1.35
26	Q3	201	PEB	CHB-C4B	15.22	1.47	1.35
26	U2	201	PEB	CHB-C4B	15.21	1.47	1.35
26	L8	202	PEB	CHB-C4B	15.21	1.47	1.35
26	jA	203	PEB	CHB-C4B	15.21	1.47	1.35
26	B9	201	PEB	CHB-C4B	15.21	1.47	1.35
26	SF	202	PEB	CHB-C4B	15.21	1.47	1.35
26	SD	202	PEB	CHB-C4B	15.21	1.47	1.35
26	Q8	203	PEB	CHB-C4B	15.20	1.47	1.35
27	K1	203	PUB	CHB-C1C	15.20	1.47	1.35
26	GA	201	PEB	CHB-C4B	15.19	1.47	1.35
26	dF	201	PEB	CHB-C4B	15.18	1.47	1.35
27	24	403	PUB	CHB-C1C	15.18	1.47	1.35
26	X4	203	PEB	CHB-C4B	15.18	1.47	1.35
26	o1	501	PEB	CHB-C4B	15.18	1.47	1.35
26	G6	1002	PEB	CHB-C4B	15.17	1.47	1.35
28	HB	1001	CYC	CHA-C1A	15.17	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	LB	1001	CYC	CHA-C1A	15.17	1.47	1.35
26	l8	201	PEB	CHB-C4B	15.17	1.47	1.35
26	JC	201	PEB	CHB-C4B	15.17	1.47	1.35
26	KG	202	PEB	CHB-C4B	15.16	1.47	1.35
26	WG	201	PEB	CHB-C4B	15.16	1.47	1.35
26	N3	201	PEB	CHB-C4B	15.15	1.47	1.35
26	UE	202	PEB	CHB-C4B	15.15	1.47	1.35
28	E6	1001	CYC	CHA-C1A	15.15	1.47	1.35
26	u1	201	PEB	CHB-C4B	15.15	1.47	1.35
27	xE	305	PUB	CHB-C1C	15.15	1.47	1.35
26	mA	202	PEB	CHB-C4B	15.14	1.47	1.35
26	J4	201	PEB	CHB-C4B	15.14	1.47	1.35
26	U7	203	PEB	CHB-C4B	15.13	1.47	1.35
26	PD	202	PEB	CHB-C4B	15.13	1.47	1.35
26	JD	201	PEB	CHB-C4B	15.13	1.47	1.35
26	SG	201	PEB	CHB-C4B	15.12	1.47	1.35
26	I5	201	PEB	CHB-C4B	15.12	1.47	1.35
28	M6	1001	CYC	CHA-C1A	15.12	1.47	1.35
26	N1	201	PEB	CHB-C4B	15.11	1.47	1.35
26	J3	202	PEB	CHB-C4B	15.11	1.47	1.35
26	a8	202	PEB	CHB-C4B	15.11	1.47	1.35
26	U8	202	PEB	CHB-C4B	15.11	1.47	1.35
26	H8	201	PEB	CHB-C4B	15.10	1.47	1.35
26	O6	203	PEB	CHB-C4B	15.10	1.47	1.35
26	D9	201	PEB	CHB-C4B	15.10	1.47	1.35
26	FA	202	PEB	CHB-C4B	15.09	1.47	1.35
26	F5	202	PEB	CHB-C4B	15.09	1.47	1.35
26	dA	201	PEB	CHB-C4B	15.09	1.47	1.35
26	aA	202	PEB	CHB-C4B	15.09	1.47	1.35
28	H6	1001	CYC	CHA-C1A	15.09	1.47	1.35
26	QE	203	PEB	CHB-C4B	15.09	1.47	1.35
26	ZF	201	PEB	CHB-C4B	15.08	1.47	1.35
26	LD	202	PEB	CHB-C4B	15.08	1.47	1.35
26	S8	201	PEB	CHB-C4B	15.08	1.47	1.35
26	D8	202	PEB	CHB-C4B	15.08	1.47	1.35
27	BA	302	PUB	CHB-C1C	15.07	1.47	1.35
26	F8	202	PEB	CHB-C4B	15.07	1.47	1.35
26	V9	201	PEB	CHB-C4B	15.07	1.47	1.35
26	QD	201	PEB	CHB-C4B	15.07	1.47	1.35
28	DI	1001	CYC	CHA-C1A	15.07	1.47	1.35
26	CD	201	PEB	CHB-C4B	15.07	1.47	1.35
26	m4	201	PEB	CHB-C4B	15.06	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J5	201	PEB	CHB-C4B	15.06	1.47	1.35
26	c1	203	PEB	CHB-C4B	15.05	1.47	1.35
26	Z1	202	PEB	CHB-C4B	15.05	1.47	1.35
26	H9	201	PEB	CHB-C4B	15.04	1.47	1.35
26	wG	301	PEB	CHB-C4B	15.04	1.47	1.35
26	UI	201	PEB	CHB-C4B	15.04	1.47	1.35
26	CA	203	PEB	CHB-C4B	15.03	1.47	1.35
26	XA	201	PEB	CHB-C4B	15.03	1.47	1.35
26	WG	202	PEB	CHB-C4B	15.02	1.47	1.35
26	J1	201	PEB	CHB-C4B	15.01	1.47	1.35
26	eA	202	PEB	CHB-C4B	15.01	1.47	1.35
26	UF	202	PEB	CHB-C4B	15.01	1.47	1.35
26	IG	202	PEB	CHB-C4B	15.01	1.47	1.35
26	oG	201	PEB	CHB-C4B	15.01	1.47	1.35
26	AG	201	PEB	CHB-C4B	15.01	1.47	1.35
26	AA	301	PEB	CHB-C4B	15.01	1.47	1.35
28	IF	1001	CYC	CHA-C1A	15.01	1.47	1.35
26	HE	201	PEB	CHB-C4B	15.00	1.47	1.35
26	S6	203	PEB	CHB-C4B	15.00	1.47	1.35
26	UF	203	PEB	CHB-C4B	15.00	1.47	1.35
26	HC	203	PEB	CHB-C4B	15.00	1.47	1.35
26	QD	202	PEB	CHB-C4B	15.00	1.47	1.35
26	C3	201	PEB	CHB-C4B	14.98	1.47	1.35
26	Y2	202	PEB	CHB-C4B	14.98	1.47	1.35
26	A8	301	PEB	CHB-C4B	14.98	1.47	1.35
26	O8	203	PEB	CHB-C4B	14.98	1.47	1.35
28	MB	1001	CYC	CHA-C1A	14.98	1.47	1.35
26	j8	203	PEB	CHB-C4B	14.98	1.47	1.35
26	SG	202	PEB	CHB-C4B	14.97	1.47	1.35
26	WF	201	PEB	CHB-C4B	14.96	1.47	1.35
26	X8	201	PEB	CHB-C4B	14.96	1.47	1.35
27	xG	305	PUB	CHB-C1C	14.95	1.47	1.35
26	SE	203	PEB	CHB-C4B	14.95	1.47	1.35
26	YI	202	PEB	CHB-C4B	14.95	1.47	1.35
26	iG	202	PEB	CHB-C4B	14.95	1.47	1.35
26	DA	202	PEB	CHB-C4B	14.94	1.47	1.35
26	C3	202	PEB	CHB-C4B	14.94	1.47	1.35
26	m8	202	PEB	CHB-C4B	14.94	1.47	1.35
26	IE	202	PEB	CHB-C4B	14.94	1.47	1.35
26	OA	203	PEB	CHB-C4B	14.93	1.47	1.35
28	B6	1002	CYC	CHA-C1A	14.93	1.47	1.35
26	D9	203	PEB	CHB-C4B	14.92	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	QA	203	PEB	CHB-C4B	14.92	1.47	1.35
26	YG	201	PEB	CHB-C4B	14.91	1.47	1.35
26	d8	202	PEB	CHB-C4B	14.90	1.47	1.35
26	LC	203	PEB	CHB-C4B	14.90	1.47	1.35
26	SB	203	PEB	CHB-C4B	14.90	1.47	1.35
26	UG	202	PEB	CHB-C4B	14.89	1.47	1.35
26	I5	202	PEB	CHB-C4B	14.88	1.47	1.35
27	QA	201	PUB	CHB-C1C	14.87	1.47	1.35
26	JF	1002	PEB	CHB-C4B	14.87	1.47	1.35
26	C8	203	PEB	CHB-C4B	14.87	1.47	1.35
26	HJ	201	PEB	CHB-C4B	14.86	1.47	1.35
26	L5	202	PEB	CHB-C4B	14.86	1.47	1.35
26	sG	201	PEB	CHB-C4B	14.86	1.47	1.35
26	DG	202	PEB	CHB-C4B	14.86	1.47	1.35
28	I6	1001	CYC	CHA-C1A	14.86	1.47	1.35
26	SG	203	PEB	CHB-C4B	14.86	1.47	1.35
26	DE	202	PEB	CHB-C4B	14.85	1.47	1.35
26	BJ	201	PEB	CHB-C4B	14.85	1.47	1.35
28	G6	1001	CYC	CHA-C1A	14.85	1.47	1.35
26	CE	201	PEB	CHB-C4B	14.85	1.47	1.35
26	a8	203	PEB	CHB-C4B	14.84	1.47	1.35
28	L2	1001	CYC	CHA-C1A	14.84	1.47	1.35
26	x1	202	PEB	CHB-C4B	14.83	1.47	1.35
28	JI	1001	CYC	CHA-C1A	14.82	1.47	1.35
26	e8	202	PEB	CHB-C4B	14.82	1.47	1.35
28	IB	1001	CYC	CHA-C1A	14.81	1.47	1.35
26	WA	201	PEB	CHB-C4B	14.80	1.47	1.35
26	OB	203	PEB	CHB-C4B	14.79	1.47	1.35
26	J9	202	PEB	CHB-C4B	14.79	1.47	1.35
26	V9	203	PEB	CHB-C4B	14.78	1.47	1.35
26	UD	201	PEB	CHB-C4B	14.76	1.47	1.35
26	UA	201	PEB	CHB-C4B	14.75	1.47	1.35
26	N4	201	PEB	CHB-C4B	14.75	1.47	1.35
26	U8	201	PEB	CHB-C4B	14.75	1.47	1.35
26	W6	203	PEB	CHB-C4B	14.73	1.47	1.35
26	iE	202	PEB	CHB-C4B	14.72	1.47	1.35
26	m1	201	PEB	CHB-C4B	14.72	1.47	1.35
26	RI	202	PEB	CHB-C4B	14.71	1.47	1.35
26	WE	201	PEB	CHB-C4B	14.70	1.47	1.35
26	HG	201	PEB	CHB-C4B	14.67	1.47	1.35
26	W8	201	PEB	CHB-C4B	14.66	1.47	1.35
26	Z7	202	PEB	CHB-C4B	14.66	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aE	202	PEB	CHB-C4B	14.66	1.47	1.35
26	LF	1002	PEB	CHB-C4B	14.66	1.47	1.35
27	B8	302	PUB	CHB-C1C	14.65	1.47	1.35
28	NB	1001	CYC	CHA-C1A	14.65	1.47	1.35
26	R2	202	PEB	CHB-C4B	14.65	1.47	1.35
26	ZA	201	PEB	CHB-C4B	14.64	1.47	1.35
26	Y3	301	PEB	CHB-C4B	14.63	1.47	1.35
26	P3	202	PEB	CHB-C4B	14.62	1.47	1.35
27	Q8	201	PUB	CHB-C1C	14.62	1.47	1.35
26	QG	201	PEB	CHB-C4B	14.60	1.47	1.35
26	JJ	202	PEB	CHB-C4B	14.60	1.47	1.35
26	GG	201	PEB	CHB-C4B	14.58	1.47	1.35
26	DJ	201	PEB	CHB-C4B	14.56	1.47	1.35
26	cG	201	PEB	CHB-C4B	14.53	1.47	1.35
26	T3	203	PEB	CHB-C4B	14.51	1.47	1.35
28	LI	1001	CYC	CHA-C1A	14.51	1.47	1.35
26	J5	202	PEB	CHB-C4B	14.50	1.47	1.35
26	KG	201	PEB	CHB-C4B	14.49	1.47	1.35
28	E7	1001	CYC	CHA-C1A	14.49	1.47	1.35
28	GB	1001	CYC	CHA-C1A	14.48	1.47	1.35
26	KD	201	PEB	CHB-C4B	14.47	1.47	1.35
26	VJ	203	PEB	CHB-C4B	14.46	1.47	1.35
26	WB	203	PEB	CHB-C4B	14.45	1.47	1.35
26	Q3	202	PEB	CHB-C4B	14.44	1.47	1.35
26	V2	202	PEB	CHB-C4B	14.44	1.47	1.35
26	DJ	203	PEB	CHB-C4B	14.44	1.47	1.35
26	J3	201	PEB	CHB-C4B	14.42	1.47	1.35
26	eE	202	PEB	CHB-C4B	14.36	1.47	1.35
26	RD	202	PEB	CHB-C4B	14.35	1.47	1.35
26	ZB	201	PEB	CHB-C4B	14.32	1.47	1.35
27	xG	301	PUB	CHB-C1C	14.30	1.47	1.35
26	GD	201	PEB	CHB-C4B	14.30	1.47	1.35
26	EE	201	PEB	CHB-C4B	14.30	1.47	1.35
26	D9	202	PEB	CHB-C4B	14.27	1.47	1.35
26	Z6	201	PEB	CHB-C4B	14.26	1.47	1.35
26	QE	201	PEB	CHB-C4B	14.26	1.47	1.35
26	EG	201	PEB	CHB-C4B	14.25	1.47	1.35
26	Z8	201	PEB	CHB-C4B	14.23	1.47	1.35
26	Q6	201	PEB	CHB-C4B	14.22	1.47	1.35
26	OG	202	PEB	CHB-C4B	14.21	1.47	1.35
26	SD	201	PEB	CHB-C4B	14.21	1.47	1.35
26	ND	202	PEB	CHB-C4B	14.20	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	DJ	202	PEB	CHB-C4B	14.16	1.46	1.35
26	L5	203	PEB	CHB-C4B	14.15	1.46	1.35
26	N8	201	PEB	CHB-C4B	14.14	1.46	1.35
26	jF	201	PEB	CHB-C4B	14.11	1.46	1.35
28	J2	1001	CYC	CHA-C1A	14.07	1.46	1.35
26	U3	201	PEB	CHB-C4B	14.07	1.46	1.35
26	VI	202	PEB	CHB-C4B	14.06	1.46	1.35
26	QB	201	PEB	CHB-C4B	14.04	1.46	1.35
26	YA	201	PEB	CHB-C4B	14.03	1.46	1.35
26	IJ	202	PEB	CHB-C4B	14.02	1.46	1.35
26	NA	201	PEB	CHB-C4B	13.99	1.46	1.35
26	a8	201	PEB	CHB-C4B	13.98	1.46	1.35
26	Y8	201	PEB	CHB-C4B	13.97	1.46	1.35
26	CG	202	PEB	CHB-C4B	13.93	1.46	1.35
28	EF	1001	CYC	CHA-C1A	13.91	1.46	1.35
26	KE	201	PEB	CHB-C4B	13.91	1.46	1.35
26	XD	202	PEB	CHB-C4B	13.88	1.46	1.35
26	B9	203	PEB	CHB-C4B	13.88	1.46	1.35
26	TA	202	PEB	CHB-C4B	13.87	1.46	1.35
26	H5	203	PEB	CHB-C4B	13.87	1.46	1.35
26	aA	201	PEB	CHB-C4B	13.86	1.46	1.35
26	eG	202	PEB	CHB-C4B	13.85	1.46	1.35
26	R3	202	PEB	CHB-C4B	13.85	1.46	1.35
26	YB	201	PEB	CHB-C4B	13.84	1.46	1.35
26	Y6	201	PEB	CHB-C4B	13.82	1.46	1.35
26	BJ	203	PEB	CHB-C4B	13.81	1.46	1.35
26	T8	202	PEB	CHB-C4B	13.80	1.46	1.35
26	a8	204	PEB	CHB-C4B	13.78	1.46	1.35
26	aA	204	PEB	CHB-C4B	13.74	1.46	1.35
26	AE	201	PEB	CHB-C4B	13.74	1.46	1.35
26	UE	203	PEB	CHB-C4B	13.70	1.46	1.35
26	M8	201	PEB	CHB-C4B	13.70	1.46	1.35
26	IE	203	PEB	CHB-C4B	13.70	1.46	1.35
26	OE	202	PEB	CHB-C4B	13.68	1.46	1.35
26	S3	201	PEB	CHB-C4B	13.68	1.46	1.35
26	MA	201	PEB	CHB-C4B	13.60	1.46	1.35
26	X3	202	PEB	CHB-C4B	13.59	1.46	1.35
26	C9	201	PEB	CHB-C4B	13.59	1.46	1.35
26	N3	202	PEB	CHB-C4B	13.56	1.46	1.35
26	KA	203	PEB	CHB-C4B	13.52	1.46	1.35
27	AF	304	PUB	C3A-C2A	13.50	1.49	1.34
26	IG	203	PEB	CHB-C4B	13.48	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CE	202	PEB	CHB-C4B	13.48	1.46	1.35
26	K8	203	PEB	CHB-C4B	13.44	1.46	1.35
26	gG	201	PEB	CHB-C4B	13.41	1.46	1.35
26	OD	201	PEB	CHB-C4B	13.20	1.46	1.35
26	ZA	202	PEB	CHB-C4B	13.16	1.46	1.35
26	gE	201	PEB	CHB-C4B	13.13	1.46	1.35
26	O3	201	PEB	CHB-C4B	13.06	1.46	1.35
26	Z8	202	PEB	CHB-C4B	13.06	1.46	1.35
26	W8	203	PEB	CHB-C4B	13.02	1.46	1.35
26	WE	202	PEB	CHB-C4B	12.90	1.45	1.35
26	WA	203	PEB	CHB-C4B	12.87	1.45	1.35
26	GE	201	PEB	CHB-C4B	12.86	1.45	1.35
26	KE	202	PEB	CHB-C4B	12.70	1.45	1.35
26	CJ	201	PEB	CHB-C4B	12.30	1.45	1.35
26	SE	202	PEB	CHB-C4B	12.22	1.45	1.35
26	cE	201	PEB	CHB-C4B	12.17	1.45	1.35
27	K4	203	PUB	C3A-C2A	12.12	1.48	1.34
27	xG	305	PUB	C3A-C2A	12.06	1.48	1.34
26	TD	202	PEB	CHB-C4B	11.92	1.45	1.35
27	21	403	PUB	C3A-C2A	11.87	1.47	1.34
27	K1	203	PUB	C3A-C2A	11.85	1.47	1.34
27	24	402	PUB	C3A-C2A	11.78	1.47	1.34
27	xE	305	PUB	C3A-C2A	11.78	1.47	1.34
27	A9	302	PUB	C3A-C2A	11.70	1.47	1.34
27	NJ	201	PUB	C3A-C2A	11.69	1.47	1.34
27	xG	306	PUB	C3A-C2A	11.69	1.47	1.34
27	xG	301	PUB	C3A-C2A	11.65	1.47	1.34
27	24	403	PUB	C3A-C2A	11.65	1.47	1.34
27	xE	306	PUB	C3A-C2A	11.64	1.47	1.34
27	N9	201	PUB	C3A-C2A	11.63	1.47	1.34
27	xE	301	PUB	C3A-C2A	11.60	1.47	1.34
27	21	402	PUB	C3A-C2A	11.59	1.47	1.34
27	AF	303	PUB	C3A-C2A	11.58	1.47	1.34
27	A8	304	PUB	C3A-C2A	11.58	1.47	1.34
27	A7	304	PUB	C3A-C2A	11.55	1.47	1.34
27	AI	302	PUB	C3A-C2A	11.52	1.47	1.34
27	AB	302	PUB	C3A-C2A	11.50	1.47	1.34
27	A2	302	PUB	C3A-C2A	11.46	1.47	1.34
27	A6	302	PUB	C3A-C2A	11.46	1.47	1.34
27	A6	303	PUB	C3A-C2A	11.46	1.47	1.34
27	KD	203	PUB	C3A-C2A	11.45	1.47	1.34
27	A7	303	PUB	C3A-C2A	11.43	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	303	PUB	C3A-C2A	11.41	1.47	1.34
27	AJ	302	PUB	C3A-C2A	11.41	1.47	1.34
26	fF	202	PEB	C2D-C3D	11.38	1.49	1.34
27	QA	201	PUB	C3A-C2A	11.33	1.47	1.34
27	AA	304	PUB	C3A-C2A	11.33	1.47	1.34
27	K3	203	PUB	C3A-C2A	11.33	1.47	1.34
27	Q8	201	PUB	C3A-C2A	11.32	1.47	1.34
27	yE	303	PUB	C3A-C2A	11.29	1.47	1.34
27	A2	303	PUB	C3A-C2A	11.28	1.47	1.34
27	Y3	302	PUB	C3A-C2A	11.27	1.47	1.34
27	A8	303	PUB	C3A-C2A	11.27	1.47	1.34
27	AA	303	PUB	C3A-C2A	11.26	1.47	1.34
27	AI	303	PUB	C3A-C2A	11.23	1.47	1.34
27	B8	302	PUB	C3A-C2A	11.23	1.47	1.34
26	UE	201	PEB	CHB-C4B	11.20	1.44	1.35
27	A1	203	PUB	C3A-C2A	11.20	1.47	1.34
27	BA	302	PUB	C3A-C2A	11.19	1.47	1.34
27	yE	302	PUB	C3A-C2A	11.19	1.47	1.34
27	YD	302	PUB	C3A-C2A	11.16	1.47	1.34
27	yG	303	PUB	C3A-C2A	11.13	1.47	1.34
27	A4	203	PUB	C3A-C2A	11.07	1.46	1.34
27	yG	302	PUB	C3A-C2A	11.04	1.46	1.34
26	T3	202	PEB	CHB-C4B	11.02	1.44	1.35
26	M1	402	PEB	C2D-C3D	10.98	1.48	1.34
26	b4	501	PEB	C2D-C3D	10.96	1.48	1.34
26	b1	501	PEB	C2D-C3D	10.93	1.48	1.34
27	wE	304	PUB	C3A-C2A	10.87	1.46	1.34
26	FA	201	PEB	C2D-C3D	10.86	1.48	1.34
26	M4	402	PEB	C2D-C3D	10.86	1.48	1.34
26	IE	201	PEB	CHB-C4B	10.83	1.44	1.35
26	F8	201	PEB	C2D-C3D	10.81	1.48	1.34
26	M1	401	PEB	C2D-C3D	10.80	1.48	1.34
26	UG	201	PEB	CHB-C4B	10.60	1.44	1.35
26	f7	202	PEB	C2D-C3D	10.56	1.48	1.34
27	wG	304	PUB	C3A-C2A	10.49	1.46	1.34
26	UF	203	PEB	C2D-C3D	10.47	1.48	1.34
26	n1	201	PEB	C2D-C3D	10.47	1.48	1.34
26	h7	203	PEB	C2D-C3D	10.44	1.47	1.34
26	GE	202	PEB	CHB-C4B	10.42	1.43	1.35
26	YJ	201	PEB	C2D-C3D	10.38	1.47	1.34
26	S7	202	PEB	C2D-C3D	10.37	1.47	1.34
26	jF	202	PEB	C2D-C3D	10.34	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	WJ	201	PEB	C2D-C3D	10.33	1.47	1.34
26	N7	1002	PEB	C2D-C3D	10.32	1.47	1.34
26	CJ	201	PEB	C2D-C3D	10.32	1.47	1.34
26	uE	202	PEB	C2D-C3D	10.30	1.47	1.34
26	U7	203	PEB	C2D-C3D	10.28	1.47	1.34
26	21	401	PEB	C2D-C3D	10.27	1.47	1.34
26	z4	201	PEB	C2D-C3D	10.27	1.47	1.34
26	HF	1002	PEB	C2D-C3D	10.26	1.47	1.34
26	H7	1002	PEB	C2D-C3D	10.25	1.47	1.34
26	q1	201	PEB	C2D-C3D	10.22	1.47	1.34
26	bF	202	PEB	C2D-C3D	10.21	1.47	1.34
26	W9	201	PEB	C2D-C3D	10.20	1.47	1.34
26	UJ	202	PEB	C2D-C3D	10.20	1.47	1.34
26	A3	201	PEB	C2D-C3D	10.20	1.47	1.34
26	uE	203	PEB	C2D-C3D	10.17	1.47	1.34
26	J4	203	PEB	C2D-C3D	10.17	1.47	1.34
26	mF	201	PEB	C2D-C3D	10.16	1.47	1.34
26	L1	201	PEB	C2D-C3D	10.15	1.47	1.34
26	mE	202	PEB	C2D-C3D	10.15	1.47	1.34
26	C1	201	PEB	C2D-C3D	10.14	1.47	1.34
26	z1	201	PEB	C2D-C3D	10.14	1.47	1.34
26	b7	202	PEB	C2D-C3D	10.14	1.47	1.34
26	ZF	203	PEB	C2D-C3D	10.14	1.47	1.34
26	vE	201	PEB	C2D-C3D	10.13	1.47	1.34
26	U9	202	PEB	C2D-C3D	10.12	1.47	1.34
26	vG	201	PEB	C2D-C3D	10.12	1.47	1.34
26	XJ	203	PEB	C2D-C3D	10.11	1.47	1.34
26	gF	201	PEB	C2D-C3D	10.11	1.47	1.34
26	Y3	301	PEB	C2D-C3D	10.11	1.47	1.34
26	H1	203	PEB	C2D-C3D	10.09	1.47	1.34
26	iE	202	PEB	C2D-C3D	10.09	1.47	1.34
26	qE	202	PEB	C2D-C3D	10.09	1.47	1.34
26	iF	201	PEB	C2D-C3D	10.09	1.47	1.34
26	y1	203	PEB	C2D-C3D	10.07	1.47	1.34
26	14	203	PEB	C2D-C3D	10.07	1.47	1.34
26	tG	201	PEB	C2D-C3D	10.07	1.47	1.34
26	AJ	303	PEB	C2D-C3D	10.07	1.47	1.34
26	OF	202	PEB	C2D-C3D	10.07	1.47	1.34
26	A9	303	PEB	C2D-C3D	10.06	1.47	1.34
26	C9	201	PEB	C2D-C3D	10.06	1.47	1.34
26	w4	204	PEB	C2D-C3D	10.06	1.47	1.34
26	NJ	204	PEB	C2D-C3D	10.06	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l1	202	PEB	C2D-C3D	10.06	1.47	1.34
26	m7	201	PEB	C2D-C3D	10.06	1.47	1.34
26	f1	201	PEB	C2D-C3D	10.06	1.47	1.34
26	uG	203	PEB	C2D-C3D	10.05	1.47	1.34
26	VJ	202	PEB	C2D-C3D	10.05	1.47	1.34
26	s4	202	PEB	C2D-C3D	10.05	1.47	1.34
26	24	401	PEB	C2D-C3D	10.04	1.47	1.34
26	YJ	202	PEB	C2D-C3D	10.04	1.47	1.34
26	ED	201	PEB	C2D-C3D	10.03	1.47	1.34
26	nE	201	PEB	C2D-C3D	10.03	1.47	1.34
26	xG	302	PEB	C2D-C3D	10.03	1.47	1.34
26	L2	1002	PEB	C2D-C3D	10.02	1.47	1.34
26	l4	202	PEB	C2D-C3D	10.02	1.47	1.34
26	eB	203	PEB	C2D-C3D	10.02	1.47	1.34
26	sG	202	PEB	C2D-C3D	10.01	1.47	1.34
26	xG	304	PEB	C2D-C3D	10.01	1.47	1.34
26	D1	202	PEB	C2D-C3D	10.01	1.47	1.34
26	H4	203	PEB	C2D-C3D	10.01	1.47	1.34
26	uG	202	PEB	C2D-C3D	10.01	1.47	1.34
26	eE	203	PEB	C2D-C3D	10.00	1.47	1.34
26	y4	202	PEB	C2D-C3D	10.00	1.47	1.34
26	A5	202	PEB	C2D-C3D	10.00	1.47	1.34
26	lF	203	PEB	C2D-C3D	10.00	1.47	1.34
26	mF	202	PEB	C2D-C3D	10.00	1.47	1.34
26	O9	202	PEB	C2D-C3D	9.99	1.47	1.34
26	OJ	201	PEB	C2D-C3D	9.99	1.47	1.34
26	V9	202	PEB	C2D-C3D	9.99	1.47	1.34
26	nG	201	PEB	C2D-C3D	9.99	1.47	1.34
26	Z7	203	PEB	C2D-C3D	9.99	1.47	1.34
26	b7	203	PEB	C2D-C3D	9.99	1.47	1.34
26	P9	203	PEB	C2D-C3D	9.99	1.47	1.34
26	O9	201	PEB	C2D-C3D	9.98	1.47	1.34
26	W9	202	PEB	C2D-C3D	9.98	1.47	1.34
26	B1	203	PEB	C2D-C3D	9.98	1.47	1.34
26	oE	201	PEB	C2D-C3D	9.98	1.47	1.34
26	q4	201	PEB	C2D-C3D	9.98	1.47	1.34
26	sE	202	PEB	C2D-C3D	9.97	1.47	1.34
26	QJ	202	PEB	C2D-C3D	9.97	1.47	1.34
26	14	201	PEB	C2D-C3D	9.95	1.47	1.34
26	c1	201	PEB	C2D-C3D	9.95	1.47	1.34
26	C5	201	PEB	C2D-C3D	9.95	1.47	1.34
26	xE	304	PEB	C2D-C3D	9.95	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r1	202	PEB	C2D-C3D	9.95	1.47	1.34
26	MG	202	PEB	C2D-C3D	9.94	1.47	1.34
26	oG	201	PEB	C2D-C3D	9.94	1.47	1.34
26	J1	203	PEB	C2D-C3D	9.94	1.47	1.34
26	C5	204	PEB	C2D-C3D	9.94	1.47	1.34
26	YD	301	PEB	C2D-C3D	9.94	1.47	1.34
26	IA	201	PEB	C2D-C3D	9.94	1.47	1.34
26	oE	202	PEB	C2D-C3D	9.94	1.47	1.34
26	lG	201	PEB	C2D-C3D	9.94	1.47	1.34
26	O7	202	PEB	C2D-C3D	9.93	1.47	1.34
26	24	405	PEB	C2D-C3D	9.93	1.47	1.34
26	qG	203	PEB	C2D-C3D	9.93	1.47	1.34
26	s4	203	PEB	C2D-C3D	9.93	1.47	1.34
26	pE	201	PEB	C2D-C3D	9.93	1.47	1.34
26	C5	202	PEB	C2D-C3D	9.93	1.47	1.34
26	c1	202	PEB	C2D-C3D	9.92	1.47	1.34
26	iB	202	PEB	C2D-C3D	9.92	1.47	1.34
26	Y9	201	PEB	C2D-C3D	9.91	1.47	1.34
26	W7	202	PEB	C2D-C3D	9.91	1.47	1.34
26	JA	202	PEB	C2D-C3D	9.91	1.47	1.34
26	CC	202	PEB	C2D-C3D	9.91	1.47	1.34
26	SF	202	PEB	C2D-C3D	9.91	1.47	1.34
26	PJ	203	PEB	C2D-C3D	9.91	1.47	1.34
26	lE	201	PEB	C2D-C3D	9.91	1.47	1.34
26	qE	203	PEB	C2D-C3D	9.91	1.47	1.34
26	u1	201	PEB	C2D-C3D	9.91	1.47	1.34
26	mG	203	PEB	C2D-C3D	9.91	1.47	1.34
26	C5	203	PEB	C2D-C3D	9.90	1.47	1.34
26	J8	202	PEB	C2D-C3D	9.90	1.47	1.34
26	eE	201	PEB	C2D-C3D	9.90	1.47	1.34
26	V3	203	PEB	C2D-C3D	9.90	1.47	1.34
26	CC	201	PEB	C2D-C3D	9.90	1.47	1.34
26	xE	302	PEB	C2D-C3D	9.90	1.47	1.34
26	j7	202	PEB	C2D-C3D	9.90	1.47	1.34
26	nE	202	PEB	C2D-C3D	9.90	1.47	1.34
26	KD	201	PEB	C2D-C3D	9.90	1.47	1.34
26	j7	203	PEB	C2D-C3D	9.90	1.47	1.34
26	r4	202	PEB	C2D-C3D	9.90	1.47	1.34
26	e7	201	PEB	C2D-C3D	9.90	1.47	1.34
26	bE	201	PEB	C2D-C3D	9.90	1.47	1.34
26	YE	201	PEB	C2D-C3D	9.90	1.47	1.34
26	c4	201	PEB	C2D-C3D	9.89	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	w4	203	PEB	C2D-C3D	9.89	1.47	1.34
26	jF	203	PEB	C2D-C3D	9.89	1.47	1.34
26	aG	203	PEB	C2D-C3D	9.89	1.47	1.34
26	K4	201	PEB	C2D-C3D	9.89	1.47	1.34
26	Q9	201	PEB	C2D-C3D	9.89	1.47	1.34
26	ID	202	PEB	C2D-C3D	9.89	1.47	1.34
26	tE	201	PEB	C2D-C3D	9.89	1.47	1.34
26	bF	203	PEB	C2D-C3D	9.89	1.47	1.34
26	I3	202	PEB	C2D-C3D	9.88	1.47	1.34
26	dF	203	PEB	C2D-C3D	9.88	1.47	1.34
26	aF	202	PEB	C2D-C3D	9.88	1.47	1.34
26	AJ	301	PEB	C2D-C3D	9.88	1.47	1.34
26	11	203	PEB	C2D-C3D	9.88	1.47	1.34
26	d4	201	PEB	C2D-C3D	9.88	1.47	1.34
26	r4	201	PEB	C2D-C3D	9.88	1.47	1.34
26	cF	201	PEB	C2D-C3D	9.88	1.47	1.34
26	w4	202	PEB	C2D-C3D	9.88	1.47	1.34
26	DD	203	PEB	C2D-C3D	9.87	1.47	1.34
26	aE	203	PEB	C2D-C3D	9.87	1.47	1.34
26	c2	203	PEB	C2D-C3D	9.87	1.47	1.34
26	IG	201	PEB	CHB-C4B	9.87	1.43	1.35
26	s1	203	PEB	C2D-C3D	9.87	1.47	1.34
26	rE	201	PEB	C2D-C3D	9.87	1.47	1.34
26	G3	202	PEB	C2D-C3D	9.86	1.47	1.34
26	eG	201	PEB	C2D-C3D	9.86	1.47	1.34
26	q1	203	PEB	C2D-C3D	9.86	1.47	1.34
26	rG	201	PEB	C2D-C3D	9.86	1.47	1.34
26	BC	201	PEB	C2D-C3D	9.86	1.47	1.34
26	y1	202	PEB	C2D-C3D	9.85	1.47	1.34
26	ZF	201	PEB	C2D-C3D	9.85	1.47	1.34
26	j7	201	PEB	C2D-C3D	9.85	1.47	1.34
26	GD	202	PEB	C2D-C3D	9.85	1.47	1.34
26	w4	201	PEB	C2D-C3D	9.85	1.47	1.34
26	QJ	201	PEB	C2D-C3D	9.85	1.47	1.34
26	Q6	203	PEB	C2D-C3D	9.85	1.47	1.34
26	A7	302	PEB	C2D-C3D	9.85	1.47	1.34
26	N2	1002	PEB	C2D-C3D	9.85	1.47	1.34
26	gE	201	PEB	C2D-C3D	9.85	1.47	1.34
26	AC	202	PEB	C2D-C3D	9.84	1.47	1.34
26	f8	202	PEB	C2D-C3D	9.84	1.47	1.34
26	GJ	201	PEB	C2D-C3D	9.84	1.47	1.34
26	WD	202	PEB	C2D-C3D	9.84	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	HD	201	PEB	C2D-C3D	9.84	1.47	1.34
26	kG	202	PEB	C2D-C3D	9.84	1.47	1.34
26	S9	201	PEB	C2D-C3D	9.84	1.47	1.34
26	e7	202	PEB	C2D-C3D	9.84	1.47	1.34
26	jF	201	PEB	C2D-C3D	9.84	1.47	1.34
26	bI	201	PEB	C2D-C3D	9.84	1.47	1.34
26	l1	201	PEB	C2D-C3D	9.84	1.47	1.34
26	h1	201	PEB	C2D-C3D	9.83	1.47	1.34
26	m4	202	PEB	C2D-C3D	9.83	1.47	1.34
26	aG	201	PEB	C2D-C3D	9.83	1.47	1.34
26	c7	201	PEB	C2D-C3D	9.83	1.47	1.34
26	NF	1002	PEB	C2D-C3D	9.83	1.47	1.34
26	F2	1002	PEB	C2D-C3D	9.83	1.47	1.34
26	pG	201	PEB	C2D-C3D	9.83	1.47	1.34
26	fI	201	PEB	C2D-C3D	9.83	1.47	1.34
26	h6	202	PEB	C2D-C3D	9.82	1.47	1.34
26	ME	202	PEB	C2D-C3D	9.82	1.47	1.34
26	hE	201	PEB	C2D-C3D	9.82	1.47	1.34
26	iF	202	PEB	C2D-C3D	9.82	1.47	1.34
26	kF	202	PEB	C2D-C3D	9.82	1.47	1.34
26	qG	202	PEB	C2D-C3D	9.82	1.47	1.34
26	A1	202	PEB	C2D-C3D	9.82	1.47	1.34
26	LD	201	PEB	C2D-C3D	9.82	1.47	1.34
26	tE	202	PEB	C2D-C3D	9.82	1.47	1.34
26	k7	202	PEB	C2D-C3D	9.82	1.47	1.34
26	B4	203	PEB	C2D-C3D	9.82	1.47	1.34
26	c7	202	PEB	C2D-C3D	9.81	1.47	1.34
26	m7	202	PEB	C2D-C3D	9.81	1.47	1.34
26	ME	201	PEB	C2D-C3D	9.81	1.47	1.34
26	a7	202	PEB	C2D-C3D	9.81	1.47	1.34
26	YE	203	PEB	C2D-C3D	9.81	1.47	1.34
26	y4	203	PEB	C2D-C3D	9.81	1.47	1.34
26	b6	202	PEB	C2D-C3D	9.81	1.47	1.34
26	QB	203	PEB	C2D-C3D	9.81	1.47	1.34
26	w1	203	PEB	C2D-C3D	9.81	1.47	1.34
26	I8	201	PEB	C2D-C3D	9.81	1.47	1.34
26	X9	203	PEB	C2D-C3D	9.81	1.47	1.34
26	JD	203	PEB	C2D-C3D	9.81	1.47	1.34
26	NI	1002	PEB	C2D-C3D	9.81	1.47	1.34
26	j4	201	PEB	C2D-C3D	9.80	1.47	1.34
26	i4	202	PEB	C2D-C3D	9.80	1.47	1.34
26	q4	202	PEB	C2D-C3D	9.80	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j1	202	PEB	C2D-C3D	9.80	1.47	1.34
26	m1	202	PEB	C2D-C3D	9.80	1.47	1.34
26	l4	201	PEB	C2D-C3D	9.80	1.47	1.34
26	B5	203	PEB	C2D-C3D	9.80	1.47	1.34
26	VD	203	PEB	C2D-C3D	9.80	1.47	1.34
26	kE	202	PEB	C2D-C3D	9.80	1.47	1.34
26	C4	201	PEB	C2D-C3D	9.79	1.47	1.34
26	i7	202	PEB	C2D-C3D	9.79	1.47	1.34
26	W3	202	PEB	C2D-C3D	9.79	1.47	1.34
26	Y9	202	PEB	C2D-C3D	9.79	1.47	1.34
26	H8	202	PEB	C2D-C3D	9.79	1.47	1.34
26	J1	201	PEB	C2D-C3D	9.79	1.47	1.34
26	i1	203	PEB	C2D-C3D	9.79	1.47	1.34
26	D1	201	PEB	C2D-C3D	9.79	1.47	1.34
26	fA	201	PEB	C2D-C3D	9.79	1.47	1.34
26	LD	203	PEB	C2D-C3D	9.79	1.47	1.34
26	m6	201	PEB	C2D-C3D	9.78	1.47	1.34
26	G9	201	PEB	C2D-C3D	9.78	1.47	1.34
26	L3	203	PEB	C2D-C3D	9.78	1.47	1.34
26	t4	201	PEB	C2D-C3D	9.78	1.47	1.34
26	gF	202	PEB	C2D-C3D	9.77	1.47	1.34
26	VE	202	PEB	C2D-C3D	9.77	1.47	1.34
26	D4	203	PEB	C2D-C3D	9.77	1.47	1.34
26	FD	203	PEB	C2D-C3D	9.77	1.47	1.34
26	d2	202	PEB	C2D-C3D	9.77	1.47	1.34
26	F4	203	PEB	C2D-C3D	9.77	1.47	1.34
26	eG	203	PEB	C2D-C3D	9.77	1.47	1.34
26	WE	203	PEB	C2D-C3D	9.77	1.47	1.34
26	Y7	201	PEB	C2D-C3D	9.77	1.47	1.34
26	cF	202	PEB	C2D-C3D	9.77	1.47	1.34
26	D4	201	PEB	C2D-C3D	9.77	1.47	1.34
26	jA	202	PEB	C2D-C3D	9.77	1.47	1.34
26	WF	202	PEB	C2D-C3D	9.76	1.47	1.34
26	tG	202	PEB	C2D-C3D	9.76	1.47	1.34
26	CC	203	PEB	C2D-C3D	9.76	1.47	1.34
26	qE	201	PEB	C2D-C3D	9.76	1.47	1.34
26	mG	202	PEB	C2D-C3D	9.76	1.47	1.34
26	AF	302	PEB	C2D-C3D	9.76	1.47	1.34
26	iI	203	PEB	C2D-C3D	9.76	1.47	1.34
26	h7	202	PEB	C2D-C3D	9.76	1.47	1.34
26	cI	201	PEB	C2D-C3D	9.76	1.47	1.34
26	f4	202	PEB	C2D-C3D	9.75	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z7	201	PEB	C2D-C3D	9.75	1.47	1.34
26	r1	201	PEB	C2D-C3D	9.75	1.47	1.34
26	v1	202	PEB	C2D-C3D	9.75	1.47	1.34
26	y1	201	PEB	C2D-C3D	9.75	1.47	1.34
26	C3	202	PEB	C2D-C3D	9.75	1.47	1.34
26	j4	202	PEB	C2D-C3D	9.75	1.47	1.34
26	A7	305	PEB	C2D-C3D	9.75	1.47	1.34
26	E3	201	PEB	C2D-C3D	9.75	1.47	1.34
26	H9	203	PEB	C2D-C3D	9.75	1.47	1.34
26	e1	202	PEB	C2D-C3D	9.75	1.47	1.34
26	s1	201	PEB	C2D-C3D	9.75	1.47	1.34
26	t1	201	PEB	C2D-C3D	9.74	1.47	1.34
26	i2	201	PEB	C2D-C3D	9.74	1.47	1.34
26	d1	203	PEB	C2D-C3D	9.74	1.47	1.34
26	e1	201	PEB	C2D-C3D	9.74	1.47	1.34
26	pE	202	PEB	C2D-C3D	9.74	1.47	1.34
26	B5	201	PEB	C2D-C3D	9.74	1.47	1.34
26	PF	202	PEB	C2D-C3D	9.74	1.47	1.34
26	bG	201	PEB	C2D-C3D	9.74	1.47	1.34
26	D1	203	PEB	C2D-C3D	9.74	1.47	1.34
26	f4	201	PEB	C2D-C3D	9.74	1.47	1.34
26	cA	202	PEB	C2D-C3D	9.74	1.47	1.34
26	sG	203	PEB	C2D-C3D	9.74	1.47	1.34
26	G9	202	PEB	C2D-C3D	9.74	1.47	1.34
26	mA	202	PEB	C2D-C3D	9.74	1.47	1.34
26	mB	203	PEB	C2D-C3D	9.74	1.47	1.34
26	dE	202	PEB	C2D-C3D	9.74	1.47	1.34
26	eF	201	PEB	C2D-C3D	9.74	1.47	1.34
26	d1	201	PEB	C2D-C3D	9.74	1.47	1.34
26	l7	203	PEB	C2D-C3D	9.74	1.47	1.34
26	kF	201	PEB	C2D-C3D	9.73	1.47	1.34
26	c2	201	PEB	C2D-C3D	9.73	1.47	1.34
26	F1	203	PEB	C2D-C3D	9.73	1.47	1.34
26	N9	204	PEB	C2D-C3D	9.73	1.47	1.34
26	oG	202	PEB	C2D-C3D	9.73	1.47	1.34
26	YF	201	PEB	C2D-C3D	9.73	1.47	1.34
26	q4	203	PEB	C2D-C3D	9.73	1.47	1.34
26	g6	202	PEB	C2D-C3D	9.73	1.47	1.34
26	U7	201	PEB	C2D-C3D	9.73	1.47	1.34
26	iG	202	PEB	C2D-C3D	9.73	1.47	1.34
26	A9	304	PEB	C2D-C3D	9.73	1.47	1.34
26	iE	203	PEB	C2D-C3D	9.73	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j1	201	PEB	C2D-C3D	9.73	1.47	1.34
26	bI	202	PEB	C2D-C3D	9.73	1.47	1.34
26	AC	203	PEB	C2D-C3D	9.73	1.47	1.34
26	OE	203	PEB	C2D-C3D	9.73	1.47	1.34
26	cI	203	PEB	C2D-C3D	9.73	1.47	1.34
26	AJ	304	PEB	C2D-C3D	9.73	1.47	1.34
26	HD	202	PEB	C2D-C3D	9.73	1.47	1.34
26	xE	303	PEB	C2D-C3D	9.73	1.47	1.34
26	i1	202	PEB	C2D-C3D	9.72	1.47	1.34
26	Y7	202	PEB	C2D-C3D	9.72	1.47	1.34
26	jB	201	PEB	C2D-C3D	9.72	1.47	1.34
26	UF	202	PEB	C2D-C3D	9.72	1.47	1.34
26	mG	201	PEB	C2D-C3D	9.72	1.47	1.34
26	pG	202	PEB	C2D-C3D	9.72	1.47	1.34
26	c4	202	PEB	C2D-C3D	9.72	1.47	1.34
26	G4	201	PEB	C2D-C3D	9.72	1.47	1.34
26	v4	201	PEB	C2D-C3D	9.72	1.47	1.34
26	gB	202	PEB	C2D-C3D	9.72	1.47	1.34
26	KE	203	PEB	C2D-C3D	9.72	1.47	1.34
26	gI	203	PEB	C2D-C3D	9.72	1.47	1.34
26	J3	203	PEB	C2D-C3D	9.72	1.47	1.34
26	i6	202	PEB	C2D-C3D	9.72	1.47	1.34
26	i7	201	PEB	C2D-C3D	9.72	1.47	1.34
26	QE	201	PEB	C2D-C3D	9.72	1.47	1.34
26	gA	202	PEB	C2D-C3D	9.71	1.47	1.34
26	EE	202	PEB	C2D-C3D	9.71	1.47	1.34
26	SJ	201	PEB	C2D-C3D	9.71	1.47	1.34
26	b2	201	PEB	C2D-C3D	9.71	1.47	1.34
26	e4	201	PEB	C2D-C3D	9.71	1.47	1.34
26	LI	1002	PEB	C2D-C3D	9.71	1.47	1.34
26	I3	201	PEB	C2D-C3D	9.71	1.47	1.34
26	A4	202	PEB	C2D-C3D	9.71	1.47	1.34
26	VJ	201	PEB	C2D-C3D	9.71	1.47	1.34
26	l6	203	PEB	C2D-C3D	9.71	1.47	1.34
26	AF	301	PEB	C2D-C3D	9.71	1.47	1.34
26	y4	201	PEB	C2D-C3D	9.71	1.47	1.34
26	BD	202	PEB	C2D-C3D	9.71	1.47	1.34
26	Y2	203	PEB	C2D-C3D	9.71	1.47	1.34
26	VI	203	PEB	C2D-C3D	9.71	1.47	1.34
26	d6	203	PEB	C2D-C3D	9.70	1.47	1.34
26	e4	202	PEB	C2D-C3D	9.70	1.47	1.34
26	eF	202	PEB	C2D-C3D	9.70	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	zE	501	PEB	C2D-C3D	9.70	1.47	1.34
26	a1	201	PEB	C2D-C3D	9.70	1.47	1.34
26	dF	201	PEB	C2D-C3D	9.70	1.47	1.34
26	Z7	202	PEB	C2D-C3D	9.70	1.47	1.34
26	YF	202	PEB	C2D-C3D	9.70	1.47	1.34
26	i2	203	PEB	C2D-C3D	9.70	1.47	1.34
26	s1	202	PEB	C2D-C3D	9.70	1.47	1.34
26	HA	202	PEB	C2D-C3D	9.70	1.47	1.34
26	b2	202	PEB	C2D-C3D	9.70	1.47	1.34
26	m6	203	PEB	C2D-C3D	9.70	1.47	1.34
26	fB	201	PEB	C2D-C3D	9.70	1.47	1.34
26	u4	203	PEB	C2D-C3D	9.69	1.47	1.34
26	ZF	202	PEB	C2D-C3D	9.69	1.47	1.34
26	FI	1002	PEB	C2D-C3D	9.69	1.47	1.34
26	iI	201	PEB	C2D-C3D	9.69	1.47	1.34
26	VF	203	PEB	C2D-C3D	9.69	1.47	1.34
26	YI	203	PEB	C2D-C3D	9.69	1.47	1.34
26	J4	201	PEB	C2D-C3D	9.69	1.47	1.34
26	A7	301	PEB	C2D-C3D	9.69	1.47	1.34
26	d4	203	PEB	C2D-C3D	9.69	1.47	1.34
26	cI	202	PEB	C2D-C3D	9.69	1.47	1.34
26	NJ	203	PEB	C2D-C3D	9.69	1.47	1.34
26	N9	203	PEB	C2D-C3D	9.69	1.47	1.34
26	LJ	203	PEB	C2D-C3D	9.69	1.47	1.34
26	C1	202	PEB	C2D-C3D	9.68	1.47	1.34
26	u4	201	PEB	C2D-C3D	9.68	1.47	1.34
26	GC	201	PEB	C2D-C3D	9.68	1.47	1.34
26	VA	202	PEB	C2D-C3D	9.68	1.47	1.34
26	dB	204	PEB	C2D-C3D	9.68	1.47	1.34
26	MG	201	PEB	C2D-C3D	9.68	1.47	1.34
26	F3	203	PEB	C2D-C3D	9.68	1.47	1.34
26	P7	202	PEB	C2D-C3D	9.68	1.47	1.34
26	D3	203	PEB	C2D-C3D	9.67	1.47	1.34
26	C4	202	PEB	C2D-C3D	9.67	1.47	1.34
26	21	404	PEB	C2D-C3D	9.67	1.47	1.34
26	d8	201	PEB	C2D-C3D	9.67	1.47	1.34
26	e6	201	PEB	C2D-C3D	9.67	1.47	1.34
26	g2	202	PEB	C2D-C3D	9.67	1.47	1.34
26	fE	202	PEB	C2D-C3D	9.67	1.47	1.34
26	J7	1002	PEB	C2D-C3D	9.67	1.47	1.34
26	UB	203	PEB	C2D-C3D	9.67	1.47	1.34
26	cG	202	PEB	C2D-C3D	9.67	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	KG	203	PEB	C2D-C3D	9.67	1.47	1.34
26	ZG	202	PEB	C2D-C3D	9.67	1.47	1.34
26	V7	202	PEB	C2D-C3D	9.67	1.47	1.34
26	i4	201	PEB	C2D-C3D	9.66	1.47	1.34
26	a7	201	PEB	C2D-C3D	9.66	1.47	1.34
26	gE	202	PEB	C2D-C3D	9.66	1.47	1.34
26	AE	202	PEB	C2D-C3D	9.66	1.47	1.34
26	dE	201	PEB	C2D-C3D	9.66	1.47	1.34
26	j6	201	PEB	C2D-C3D	9.66	1.47	1.34
26	ZE	202	PEB	C2D-C3D	9.66	1.47	1.34
26	O1	201	PEB	C2D-C3D	9.66	1.47	1.34
26	dB	203	PEB	C2D-C3D	9.66	1.47	1.34
26	TJ	203	PEB	C2D-C3D	9.66	1.47	1.34
26	u1	203	PEB	C2D-C3D	9.66	1.46	1.34
26	L9	203	PEB	C2D-C3D	9.65	1.46	1.34
26	QE	202	PEB	C2D-C3D	9.65	1.46	1.34
26	R7	201	PEB	C2D-C3D	9.65	1.46	1.34
26	i8	201	PEB	C2D-C3D	9.65	1.46	1.34
26	gG	202	PEB	C2D-C3D	9.65	1.46	1.34
26	n4	201	PEB	C2D-C3D	9.65	1.46	1.34
26	21	405	PEB	C2D-C3D	9.65	1.46	1.34
26	BC	203	PEB	C2D-C3D	9.65	1.46	1.34
26	rE	202	PEB	C2D-C3D	9.65	1.46	1.34
26	wE	301	PEB	C2D-C3D	9.65	1.46	1.34
26	iG	203	PEB	C2D-C3D	9.65	1.46	1.34
26	H3	201	PEB	C2D-C3D	9.65	1.46	1.34
26	a4	201	PEB	C2D-C3D	9.65	1.46	1.34
26	gI	201	PEB	C2D-C3D	9.65	1.46	1.34
26	T9	203	PEB	C2D-C3D	9.64	1.46	1.34
26	mB	201	PEB	C2D-C3D	9.64	1.46	1.34
26	PA	202	PEB	C2D-C3D	9.64	1.46	1.34
26	M9	201	PEB	C2D-C3D	9.64	1.46	1.34
26	e2	202	PEB	C2D-C3D	9.64	1.46	1.34
26	SI	201	PEB	C2D-C3D	9.64	1.46	1.34
26	dB	201	PEB	C2D-C3D	9.64	1.46	1.34
26	SB	203	PEB	C2D-C3D	9.64	1.46	1.34
26	lA	201	PEB	C2D-C3D	9.64	1.46	1.34
26	s4	201	PEB	C2D-C3D	9.63	1.46	1.34
26	i6	201	PEB	C2D-C3D	9.63	1.46	1.34
26	L4	201	PEB	C2D-C3D	9.63	1.46	1.34
26	c6	202	PEB	C2D-C3D	9.63	1.46	1.34
26	I1	201	PEB	C2D-C3D	9.63	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V6	202	PEB	C2D-C3D	9.63	1.46	1.34
26	EG	202	PEB	C2D-C3D	9.63	1.46	1.34
26	BA	301	PEB	C2D-C3D	9.63	1.46	1.34
26	CE	203	PEB	C2D-C3D	9.63	1.46	1.34
26	G5	201	PEB	C2D-C3D	9.62	1.46	1.34
26	mA	201	PEB	C2D-C3D	9.62	1.46	1.34
26	eB	201	PEB	C2D-C3D	9.62	1.46	1.34
26	M4	401	PEB	C2D-C3D	9.62	1.46	1.34
26	V8	202	PEB	C2D-C3D	9.62	1.46	1.34
26	v4	202	PEB	C2D-C3D	9.62	1.46	1.34
26	fA	202	PEB	C2D-C3D	9.62	1.46	1.34
26	S2	201	PEB	C2D-C3D	9.62	1.46	1.34
26	p1	202	PEB	C2D-C3D	9.62	1.46	1.34
26	L3	201	PEB	C2D-C3D	9.62	1.46	1.34
26	A9	301	PEB	C2D-C3D	9.62	1.46	1.34
26	YG	203	PEB	C2D-C3D	9.62	1.46	1.34
26	U6	203	PEB	C2D-C3D	9.62	1.46	1.34
26	P9	201	PEB	C2D-C3D	9.62	1.46	1.34
26	d6	201	PEB	C2D-C3D	9.62	1.46	1.34
26	eB	202	PEB	C2D-C3D	9.62	1.46	1.34
26	U4	202	PEB	C2D-C3D	9.61	1.46	1.34
26	WJ	202	PEB	C2D-C3D	9.61	1.46	1.34
26	YG	202	PEB	C2D-C3D	9.61	1.46	1.34
26	Q7	203	PEB	C2D-C3D	9.61	1.46	1.34
26	P9	202	PEB	C2D-C3D	9.61	1.46	1.34
26	dA	201	PEB	C2D-C3D	9.61	1.46	1.34
26	R9	202	PEB	C2D-C3D	9.61	1.46	1.34
26	g8	202	PEB	C2D-C3D	9.61	1.46	1.34
26	AF	305	PEB	C2D-C3D	9.61	1.46	1.34
26	k2	203	PEB	C2D-C3D	9.60	1.46	1.34
26	b7	201	PEB	C2D-C3D	9.60	1.46	1.34
26	Q4	202	PEB	C2D-C3D	9.60	1.46	1.34
26	d7	201	PEB	C2D-C3D	9.60	1.46	1.34
26	mE	203	PEB	C2D-C3D	9.60	1.46	1.34
26	v1	201	PEB	C2D-C3D	9.60	1.46	1.34
26	U1	202	PEB	C2D-C3D	9.60	1.46	1.34
26	T4	203	PEB	C2D-C3D	9.60	1.46	1.34
26	xG	303	PEB	C2D-C3D	9.60	1.46	1.34
26	S1	202	PEB	C2D-C3D	9.60	1.46	1.34
26	Q9	202	PEB	C2D-C3D	9.60	1.46	1.34
26	iA	201	PEB	C2D-C3D	9.60	1.46	1.34
26	e6	203	PEB	C2D-C3D	9.60	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	RB	201	PEB	C2D-C3D	9.60	1.46	1.34
26	RF	201	PEB	C2D-C3D	9.60	1.46	1.34
26	mI	201	PEB	C2D-C3D	9.60	1.46	1.34
26	wE	302	PEB	C2D-C3D	9.59	1.46	1.34
26	fF	203	PEB	C2D-C3D	9.59	1.46	1.34
26	g2	201	PEB	C2D-C3D	9.59	1.46	1.34
26	U9	201	PEB	C2D-C3D	9.59	1.46	1.34
26	SJ	202	PEB	C2D-C3D	9.59	1.46	1.34
26	CA	203	PEB	C2D-C3D	9.59	1.46	1.34
26	WE	202	PEB	C2D-C3D	9.59	1.46	1.34
26	f8	201	PEB	C2D-C3D	9.59	1.46	1.34
26	w1	201	PEB	C2D-C3D	9.59	1.46	1.34
26	AG	202	PEB	C2D-C3D	9.59	1.46	1.34
26	YE	202	PEB	C2D-C3D	9.59	1.46	1.34
26	B8	301	PEB	C2D-C3D	9.59	1.46	1.34
26	cA	201	PEB	C2D-C3D	9.58	1.46	1.34
26	k1	203	PEB	C2D-C3D	9.58	1.46	1.34
26	ZE	201	PEB	C2D-C3D	9.58	1.46	1.34
26	O1	202	PEB	C2D-C3D	9.58	1.46	1.34
26	eI	202	PEB	C2D-C3D	9.58	1.46	1.34
26	A6	304	PEB	C2D-C3D	9.58	1.46	1.34
26	mI	202	PEB	C2D-C3D	9.58	1.46	1.34
26	gA	201	PEB	C2D-C3D	9.58	1.46	1.34
26	JD	201	PEB	C2D-C3D	9.58	1.46	1.34
26	HJ	203	PEB	C2D-C3D	9.58	1.46	1.34
26	UF	201	PEB	C2D-C3D	9.58	1.46	1.34
26	MJ	201	PEB	C2D-C3D	9.57	1.46	1.34
26	h6	203	PEB	C2D-C3D	9.57	1.46	1.34
26	cG	201	PEB	C2D-C3D	9.57	1.46	1.34
26	aI	203	PEB	C2D-C3D	9.57	1.46	1.34
26	HD	203	PEB	C2D-C3D	9.57	1.46	1.34
26	F1	202	PEB	C2D-C3D	9.57	1.46	1.34
26	n4	202	PEB	C2D-C3D	9.57	1.46	1.34
26	E4	201	PEB	C2D-C3D	9.57	1.46	1.34
26	YG	201	PEB	C2D-C3D	9.57	1.46	1.34
26	gG	201	PEB	C2D-C3D	9.57	1.46	1.34
26	XJ	202	PEB	C2D-C3D	9.57	1.46	1.34
26	D4	202	PEB	C2D-C3D	9.57	1.46	1.34
26	fA	203	PEB	C2D-C3D	9.57	1.46	1.34
26	FA	202	PEB	C2D-C3D	9.57	1.46	1.34
26	GC	202	PEB	C2D-C3D	9.57	1.46	1.34
26	dG	201	PEB	C2D-C3D	9.57	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dG	202	PEB	C2D-C3D	9.57	1.46	1.34
26	zG	501	PEB	C2D-C3D	9.57	1.46	1.34
26	PJ	202	PEB	C2D-C3D	9.57	1.46	1.34
26	RJ	201	PEB	C2D-C3D	9.57	1.46	1.34
26	fB	202	PEB	C2D-C3D	9.57	1.46	1.34
26	AJ	305	PEB	C2D-C3D	9.57	1.46	1.34
26	c8	202	PEB	C2D-C3D	9.56	1.46	1.34
26	G1	201	PEB	C2D-C3D	9.56	1.46	1.34
26	UE	202	PEB	C2D-C3D	9.56	1.46	1.34
26	H1	201	PEB	C2D-C3D	9.56	1.46	1.34
26	Q1	202	PEB	C2D-C3D	9.56	1.46	1.34
26	k2	201	PEB	C2D-C3D	9.56	1.46	1.34
26	iB	201	PEB	C2D-C3D	9.56	1.46	1.34
26	DA	202	PEB	C2D-C3D	9.56	1.46	1.34
26	A1	201	PEB	C2D-C3D	9.56	1.46	1.34
26	QG	202	PEB	C2D-C3D	9.56	1.46	1.34
26	I4	202	PEB	C2D-C3D	9.56	1.46	1.34
26	QA	203	PEB	C2D-C3D	9.56	1.46	1.34
26	aE	201	PEB	C2D-C3D	9.56	1.46	1.34
26	z1	202	PEB	C2D-C3D	9.56	1.46	1.34
26	g7	201	PEB	C2D-C3D	9.56	1.46	1.34
26	GJ	202	PEB	C2D-C3D	9.56	1.46	1.34
26	bF	201	PEB	C2D-C3D	9.55	1.46	1.34
26	p4	202	PEB	C2D-C3D	9.55	1.46	1.34
26	R9	201	PEB	C2D-C3D	9.55	1.46	1.34
26	wG	301	PEB	C2D-C3D	9.55	1.46	1.34
26	x4	201	PEB	C2D-C3D	9.55	1.46	1.34
26	I4	201	PEB	C2D-C3D	9.55	1.46	1.34
26	V9	203	PEB	C2D-C3D	9.55	1.46	1.34
26	E8	203	PEB	C2D-C3D	9.55	1.46	1.34
26	VB	202	PEB	C2D-C3D	9.55	1.46	1.34
26	D8	202	PEB	C2D-C3D	9.55	1.46	1.34
26	aF	201	PEB	C2D-C3D	9.55	1.46	1.34
26	M1	403	PEB	C2D-C3D	9.55	1.46	1.34
26	U7	202	PEB	C2D-C3D	9.55	1.46	1.34
26	h4	203	PEB	C2D-C3D	9.55	1.46	1.34
26	g7	202	PEB	C2D-C3D	9.55	1.46	1.34
26	K1	201	PEB	C2D-C3D	9.55	1.46	1.34
26	S9	202	PEB	C2D-C3D	9.55	1.46	1.34
26	cB	202	PEB	C2D-C3D	9.55	1.46	1.34
26	WG	203	PEB	C2D-C3D	9.55	1.46	1.34
26	F4	201	PEB	C2D-C3D	9.54	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bB	202	PEB	C2D-C3D	9.54	1.46	1.34
26	G5	203	PEB	C2D-C3D	9.54	1.46	1.34
26	m8	201	PEB	C2D-C3D	9.54	1.46	1.34
26	sE	203	PEB	C2D-C3D	9.54	1.46	1.34
26	H4	202	PEB	C2D-C3D	9.54	1.46	1.34
26	KC	201	PEB	C2D-C3D	9.54	1.46	1.34
26	BD	203	PEB	C2D-C3D	9.54	1.46	1.34
26	WF	203	PEB	C2D-C3D	9.54	1.46	1.34
26	R6	201	PEB	C2D-C3D	9.54	1.46	1.34
26	hB	201	PEB	C2D-C3D	9.54	1.46	1.34
26	jB	202	PEB	C2D-C3D	9.54	1.46	1.34
26	h1	202	PEB	C2D-C3D	9.54	1.46	1.34
26	q1	202	PEB	C2D-C3D	9.54	1.46	1.34
26	m2	201	PEB	C2D-C3D	9.54	1.46	1.34
26	11	201	PEB	C2D-C3D	9.54	1.46	1.34
26	lG	202	PEB	C2D-C3D	9.54	1.46	1.34
26	T1	202	PEB	C2D-C3D	9.53	1.46	1.34
26	JF	1002	PEB	C2D-C3D	9.53	1.46	1.34
26	cE	202	PEB	C2D-C3D	9.53	1.46	1.34
26	kE	201	PEB	C2D-C3D	9.53	1.46	1.34
26	Q6	201	PEB	C2D-C3D	9.53	1.46	1.34
26	C8	203	PEB	C2D-C3D	9.53	1.46	1.34
26	k6	202	PEB	C2D-C3D	9.53	1.46	1.34
26	kI	201	PEB	C2D-C3D	9.53	1.46	1.34
26	j6	202	PEB	C2D-C3D	9.53	1.46	1.34
26	D7	1002	PEB	C2D-C3D	9.53	1.46	1.34
26	X9	201	PEB	C2D-C3D	9.53	1.46	1.34
26	c2	202	PEB	C2D-C3D	9.53	1.46	1.34
26	QB	201	PEB	C2D-C3D	9.53	1.46	1.34
26	m2	203	PEB	C2D-C3D	9.53	1.46	1.34
26	k7	201	PEB	C2D-C3D	9.53	1.46	1.34
26	lF	202	PEB	C2D-C3D	9.52	1.46	1.34
26	Q8	203	PEB	C2D-C3D	9.52	1.46	1.34
26	R1	201	PEB	C2D-C3D	9.52	1.46	1.34
26	AE	201	PEB	C2D-C3D	9.52	1.46	1.34
26	AI	304	PEB	C2D-C3D	9.52	1.46	1.34
26	F8	202	PEB	C2D-C3D	9.52	1.46	1.34
26	U8	201	PEB	C2D-C3D	9.52	1.46	1.34
26	mI	203	PEB	C2D-C3D	9.52	1.46	1.34
26	h8	203	PEB	C2D-C3D	9.52	1.46	1.34
26	AC	201	PEB	C2D-C3D	9.52	1.46	1.34
26	HC	201	PEB	C2D-C3D	9.52	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g6	201	PEB	C2D-C3D	9.52	1.46	1.34
26	k4	201	PEB	C2D-C3D	9.52	1.46	1.34
26	NJ	202	PEB	C2D-C3D	9.52	1.46	1.34
26	a2	203	PEB	C2D-C3D	9.51	1.46	1.34
26	OG	203	PEB	C2D-C3D	9.51	1.46	1.34
26	x1	202	PEB	C2D-C3D	9.51	1.46	1.34
26	hA	203	PEB	C2D-C3D	9.51	1.46	1.34
26	jA	201	PEB	C2D-C3D	9.51	1.46	1.34
26	g2	203	PEB	C2D-C3D	9.51	1.46	1.34
26	UA	201	PEB	C2D-C3D	9.51	1.46	1.34
26	kB	202	PEB	C2D-C3D	9.51	1.46	1.34
26	GE	203	PEB	C2D-C3D	9.51	1.46	1.34
26	ED	202	PEB	C2D-C3D	9.51	1.46	1.34
26	m4	203	PEB	C2D-C3D	9.50	1.46	1.34
26	f6	203	PEB	C2D-C3D	9.50	1.46	1.34
26	BD	201	PEB	C2D-C3D	9.50	1.46	1.34
26	KE	202	PEB	C2D-C3D	9.50	1.46	1.34
26	lB	203	PEB	C2D-C3D	9.50	1.46	1.34
26	rG	202	PEB	C2D-C3D	9.50	1.46	1.34
26	M9	202	PEB	C2D-C3D	9.50	1.46	1.34
26	ZG	201	PEB	C2D-C3D	9.50	1.46	1.34
26	lE	202	PEB	C2D-C3D	9.50	1.46	1.34
26	AI	301	PEB	C2D-C3D	9.50	1.46	1.34
26	KD	202	PEB	C2D-C3D	9.50	1.46	1.34
26	l7	202	PEB	C2D-C3D	9.50	1.46	1.34
26	j8	202	PEB	C2D-C3D	9.49	1.46	1.34
26	cA	203	PEB	C2D-C3D	9.49	1.46	1.34
26	hI	201	PEB	C2D-C3D	9.49	1.46	1.34
26	CG	201	PEB	C2D-C3D	9.49	1.46	1.34
26	H3	202	PEB	C2D-C3D	9.49	1.46	1.34
26	O4	202	PEB	C2D-C3D	9.49	1.46	1.34
26	j8	201	PEB	C2D-C3D	9.49	1.46	1.34
26	eI	203	PEB	C2D-C3D	9.49	1.46	1.34
26	R7	202	PEB	C2D-C3D	9.49	1.46	1.34
26	k4	202	PEB	C2D-C3D	9.48	1.46	1.34
26	f1	202	PEB	C2D-C3D	9.48	1.46	1.34
26	V2	203	PEB	C2D-C3D	9.48	1.46	1.34
26	fB	203	PEB	C2D-C3D	9.48	1.46	1.34
26	K3	202	PEB	C2D-C3D	9.48	1.46	1.34
26	VB	201	PEB	C2D-C3D	9.48	1.46	1.34
26	c8	201	PEB	C2D-C3D	9.48	1.46	1.34
26	GC	203	PEB	C2D-C3D	9.48	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VG	202	PEB	C2D-C3D	9.48	1.46	1.34
26	k8	202	PEB	C2D-C3D	9.48	1.46	1.34
26	e2	203	PEB	C2D-C3D	9.48	1.46	1.34
26	TI	203	PEB	C2D-C3D	9.48	1.46	1.34
26	QF	203	PEB	C2D-C3D	9.48	1.46	1.34
26	E1	202	PEB	C2D-C3D	9.48	1.46	1.34
26	CG	203	PEB	C2D-C3D	9.48	1.46	1.34
26	T7	202	PEB	C2D-C3D	9.47	1.46	1.34
26	FD	201	PEB	C2D-C3D	9.47	1.46	1.34
26	uE	201	PEB	C2D-C3D	9.47	1.46	1.34
26	k1	201	PEB	C2D-C3D	9.47	1.46	1.34
26	Z1	201	PEB	C2D-C3D	9.47	1.46	1.34
26	AB	301	PEB	C2D-C3D	9.47	1.46	1.34
26	C9	202	PEB	C2D-C3D	9.47	1.46	1.34
26	RF	202	PEB	C2D-C3D	9.47	1.46	1.34
26	Q7	202	PEB	C2D-C3D	9.46	1.46	1.34
26	E1	201	PEB	C2D-C3D	9.46	1.46	1.34
26	d6	204	PEB	C2D-C3D	9.46	1.46	1.34
26	T4	202	PEB	C2D-C3D	9.46	1.46	1.34
26	W7	201	PEB	C2D-C3D	9.46	1.46	1.34
26	T2	203	PEB	C2D-C3D	9.46	1.46	1.34
26	f2	201	PEB	C2D-C3D	9.46	1.46	1.34
26	S4	202	PEB	C2D-C3D	9.46	1.46	1.34
26	VJ	203	PEB	C2D-C3D	9.46	1.46	1.34
26	H4	201	PEB	C2D-C3D	9.46	1.46	1.34
26	QG	201	PEB	C2D-C3D	9.46	1.46	1.34
26	UG	202	PEB	C2D-C3D	9.46	1.46	1.34
26	h4	201	PEB	C2D-C3D	9.46	1.46	1.34
26	kI	202	PEB	C2D-C3D	9.46	1.46	1.34
26	JJ	201	PEB	C2D-C3D	9.46	1.46	1.34
26	vE	202	PEB	C2D-C3D	9.45	1.46	1.34
26	hI	202	PEB	C2D-C3D	9.45	1.46	1.34
26	N9	202	PEB	C2D-C3D	9.45	1.46	1.34
26	Y4	201	PEB	C2D-C3D	9.45	1.46	1.34
26	p4	201	PEB	C2D-C3D	9.45	1.46	1.34
26	A4	201	PEB	C2D-C3D	9.45	1.46	1.34
26	R8	202	PEB	C2D-C3D	9.45	1.46	1.34
26	S6	203	PEB	C2D-C3D	9.45	1.46	1.34
26	SE	203	PEB	C2D-C3D	9.45	1.46	1.34
26	g8	201	PEB	C2D-C3D	9.45	1.46	1.34
26	X9	202	PEB	C2D-C3D	9.45	1.46	1.34
26	kA	202	PEB	C2D-C3D	9.45	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CD	201	PEB	C2D-C3D	9.45	1.46	1.34
26	PI	202	PEB	C2D-C3D	9.45	1.46	1.34
26	gB	201	PEB	C2D-C3D	9.45	1.46	1.34
26	I1	202	PEB	C2D-C3D	9.45	1.46	1.34
26	G5	202	PEB	C2D-C3D	9.45	1.46	1.34
26	E4	202	PEB	C2D-C3D	9.45	1.46	1.34
26	hB	202	PEB	C2D-C3D	9.45	1.46	1.34
26	nG	202	PEB	C2D-C3D	9.45	1.46	1.34
26	QI	201	PEB	C2D-C3D	9.45	1.46	1.34
26	g4	202	PEB	C2D-C3D	9.44	1.46	1.34
26	lB	201	PEB	C2D-C3D	9.44	1.46	1.34
26	f6	201	PEB	C2D-C3D	9.44	1.46	1.34
26	D9	203	PEB	C2D-C3D	9.44	1.46	1.34
26	f6	202	PEB	C2D-C3D	9.44	1.46	1.34
26	M4	403	PEB	C2D-C3D	9.44	1.46	1.34
26	g4	201	PEB	C2D-C3D	9.44	1.46	1.34
26	fG	202	PEB	C2D-C3D	9.44	1.46	1.34
26	F1	201	PEB	C2D-C3D	9.44	1.46	1.34
26	T8	202	PEB	C2D-C3D	9.44	1.46	1.34
26	IJ	202	PEB	C2D-C3D	9.44	1.46	1.34
26	a1	202	PEB	C2D-C3D	9.44	1.46	1.34
26	P6	201	PEB	C2D-C3D	9.44	1.46	1.34
26	RA	202	PEB	C2D-C3D	9.44	1.46	1.34
26	kG	201	PEB	C2D-C3D	9.44	1.46	1.34
26	g1	201	PEB	C2D-C3D	9.43	1.46	1.34
26	d7	202	PEB	C2D-C3D	9.43	1.46	1.34
26	R4	202	PEB	C2D-C3D	9.43	1.46	1.34
26	SA	202	PEB	C2D-C3D	9.43	1.46	1.34
26	fE	201	PEB	C2D-C3D	9.43	1.46	1.34
26	QA	202	PEB	C2D-C3D	9.43	1.46	1.34
26	e6	202	PEB	C2D-C3D	9.43	1.46	1.34
26	S7	201	PEB	C2D-C3D	9.43	1.46	1.34
26	M3	201	PEB	C2D-C3D	9.43	1.46	1.34
26	B3	201	PEB	C2D-C3D	9.43	1.46	1.34
26	D2	1002	PEB	C2D-C3D	9.43	1.46	1.34
26	WG	202	PEB	C2D-C3D	9.43	1.46	1.34
26	R1	202	PEB	C2D-C3D	9.43	1.46	1.34
26	iE	201	PEB	C2D-C3D	9.43	1.46	1.34
26	U1	201	PEB	C2D-C3D	9.42	1.46	1.34
26	IC	201	PEB	C2D-C3D	9.42	1.46	1.34
26	k1	202	PEB	C2D-C3D	9.42	1.46	1.34
26	U4	201	PEB	C2D-C3D	9.42	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	LC	202	PEB	C2D-C3D	9.42	1.46	1.34
26	PE	201	PEB	C2D-C3D	9.42	1.46	1.34
26	F4	202	PEB	C2D-C3D	9.42	1.46	1.34
26	jE	202	PEB	C2D-C3D	9.42	1.46	1.34
26	11	202	PEB	C2D-C3D	9.42	1.46	1.34
26	z4	202	PEB	C2D-C3D	9.42	1.46	1.34
26	24	404	PEB	C2D-C3D	9.42	1.46	1.34
26	mB	202	PEB	C2D-C3D	9.42	1.46	1.34
26	hG	201	PEB	C2D-C3D	9.42	1.46	1.34
26	h8	202	PEB	C2D-C3D	9.42	1.46	1.34
26	OA	201	PEB	C2D-C3D	9.42	1.46	1.34
26	SB	202	PEB	C2D-C3D	9.42	1.46	1.34
26	o1	501	PEB	C2D-C3D	9.41	1.46	1.34
26	HG	202	PEB	C2D-C3D	9.41	1.46	1.34
26	t4	202	PEB	C2D-C3D	9.41	1.46	1.34
26	hA	201	PEB	C2D-C3D	9.41	1.46	1.34
26	hA	202	PEB	C2D-C3D	9.41	1.46	1.34
26	W1	202	PEB	C2D-C3D	9.41	1.46	1.34
26	IE	202	PEB	C2D-C3D	9.41	1.46	1.34
26	dI	202	PEB	C2D-C3D	9.41	1.46	1.34
26	EA	203	PEB	C2D-C3D	9.41	1.46	1.34
26	K1	202	PEB	C2D-C3D	9.41	1.46	1.34
26	U8	203	PEB	C2D-C3D	9.41	1.46	1.34
26	DE	201	PEB	C2D-C3D	9.41	1.46	1.34
26	m8	202	PEB	C2D-C3D	9.41	1.46	1.34
26	BC	202	PEB	C2D-C3D	9.41	1.46	1.34
26	c6	201	PEB	C2D-C3D	9.40	1.46	1.34
26	GA	203	PEB	C2D-C3D	9.40	1.46	1.34
26	cB	201	PEB	C2D-C3D	9.40	1.46	1.34
26	dI	201	PEB	C2D-C3D	9.40	1.46	1.34
26	K3	201	PEB	C2D-C3D	9.40	1.46	1.34
26	LA	202	PEB	C2D-C3D	9.40	1.46	1.34
26	kA	201	PEB	C2D-C3D	9.40	1.46	1.34
26	R3	203	PEB	C2D-C3D	9.40	1.46	1.34
26	AD	201	PEB	C2D-C3D	9.40	1.46	1.34
26	h2	201	PEB	C2D-C3D	9.40	1.46	1.34
26	A6	301	PEB	C2D-C3D	9.40	1.46	1.34
26	C3	201	PEB	C2D-C3D	9.39	1.46	1.34
26	l8	201	PEB	C2D-C3D	9.39	1.46	1.34
26	qG	201	PEB	C2D-C3D	9.39	1.46	1.34
26	vG	202	PEB	C2D-C3D	9.39	1.46	1.34
26	AI	305	PEB	C2D-C3D	9.39	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q8	204	PEB	C2D-C3D	9.39	1.46	1.34
26	TA	202	PEB	C2D-C3D	9.39	1.46	1.34
26	UD	202	PEB	C2D-C3D	9.39	1.46	1.34
26	HE	202	PEB	C2D-C3D	9.39	1.46	1.34
26	Q8	202	PEB	C2D-C3D	9.39	1.46	1.34
26	S1	201	PEB	C2D-C3D	9.39	1.46	1.34
26	f2	202	PEB	C2D-C3D	9.39	1.46	1.34
26	b6	201	PEB	C2D-C3D	9.39	1.46	1.34
26	KJ	201	PEB	C2D-C3D	9.39	1.46	1.34
26	B5	202	PEB	C2D-C3D	9.38	1.46	1.34
26	m6	202	PEB	C2D-C3D	9.38	1.46	1.34
26	UA	203	PEB	C2D-C3D	9.38	1.46	1.34
26	F9	202	PEB	C2D-C3D	9.38	1.46	1.34
26	UJ	201	PEB	C2D-C3D	9.38	1.46	1.34
26	O7	201	PEB	C2D-C3D	9.38	1.46	1.34
26	hB	203	PEB	C2D-C3D	9.38	1.46	1.34
26	oE	203	PEB	C2D-C3D	9.38	1.46	1.34
26	P1	203	PEB	C2D-C3D	9.38	1.46	1.34
26	t1	202	PEB	C2D-C3D	9.38	1.46	1.34
26	F9	203	PEB	C2D-C3D	9.38	1.46	1.34
26	jI	201	PEB	C2D-C3D	9.38	1.46	1.34
26	SG	203	PEB	C2D-C3D	9.38	1.46	1.34
26	FC	202	PEB	C2D-C3D	9.38	1.46	1.34
26	T4	201	PEB	C2D-C3D	9.37	1.46	1.34
26	L8	202	PEB	C2D-C3D	9.37	1.46	1.34
26	j8	203	PEB	C2D-C3D	9.37	1.46	1.34
26	S7	203	PEB	C2D-C3D	9.37	1.46	1.34
26	jA	203	PEB	C2D-C3D	9.37	1.46	1.34
26	KC	203	PEB	C2D-C3D	9.37	1.46	1.34
26	g1	202	PEB	C2D-C3D	9.37	1.46	1.34
26	A2	305	PEB	C2D-C3D	9.37	1.46	1.34
26	OD	202	PEB	C2D-C3D	9.37	1.46	1.34
26	d2	201	PEB	C2D-C3D	9.37	1.46	1.34
26	H1	202	PEB	C2D-C3D	9.37	1.46	1.34
26	W4	202	PEB	C2D-C3D	9.37	1.46	1.34
26	14	202	PEB	C2D-C3D	9.37	1.46	1.34
26	B1	202	PEB	C2D-C3D	9.37	1.46	1.34
26	BE	202	PEB	C2D-C3D	9.36	1.46	1.34
26	AG	201	PEB	C2D-C3D	9.36	1.46	1.34
26	YI	202	PEB	C2D-C3D	9.36	1.46	1.34
26	L4	203	PEB	C2D-C3D	9.36	1.46	1.34
26	J3	201	PEB	C2D-C3D	9.36	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a4	202	PEB	C2D-C3D	9.36	1.46	1.34
26	B9	202	PEB	C2D-C3D	9.36	1.46	1.34
26	XD	202	PEB	C2D-C3D	9.36	1.46	1.34
26	OA	202	PEB	C2D-C3D	9.36	1.46	1.34
26	jE	201	PEB	C2D-C3D	9.36	1.46	1.34
26	x4	202	PEB	C2D-C3D	9.35	1.46	1.34
26	gG	203	PEB	C2D-C3D	9.35	1.46	1.34
26	RI	201	PEB	C2D-C3D	9.35	1.46	1.34
26	P2	201	PEB	C2D-C3D	9.35	1.46	1.34
26	jG	202	PEB	C2D-C3D	9.35	1.46	1.34
26	iA	202	PEB	C2D-C3D	9.35	1.46	1.34
26	FC	203	PEB	C2D-C3D	9.35	1.46	1.34
26	PB	201	PEB	C2D-C3D	9.35	1.46	1.34
26	T1	201	PEB	C2D-C3D	9.35	1.46	1.34
26	e8	202	PEB	C2D-C3D	9.35	1.46	1.34
26	XE	201	PEB	C2D-C3D	9.35	1.46	1.34
26	yE	301	PEB	C2D-C3D	9.35	1.46	1.34
26	eG	202	PEB	C2D-C3D	9.35	1.46	1.34
26	a6	201	PEB	C2D-C3D	9.35	1.46	1.34
26	PI	201	PEB	C2D-C3D	9.35	1.46	1.34
26	K5	201	PEB	C2D-C3D	9.34	1.46	1.34
26	RI	203	PEB	C2D-C3D	9.34	1.46	1.34
26	w1	202	PEB	C2D-C3D	9.34	1.46	1.34
26	x1	201	PEB	C2D-C3D	9.34	1.46	1.34
26	A2	301	PEB	C2D-C3D	9.34	1.46	1.34
26	O6	203	PEB	C2D-C3D	9.34	1.46	1.34
26	WF	201	PEB	C2D-C3D	9.34	1.46	1.34
26	A3	202	PEB	C2D-C3D	9.34	1.46	1.34
26	J9	201	PEB	C2D-C3D	9.34	1.46	1.34
26	DA	201	PEB	C2D-C3D	9.34	1.46	1.34
26	AB	304	PEB	C2D-C3D	9.34	1.46	1.34
26	XJ	201	PEB	C2D-C3D	9.34	1.46	1.34
26	G8	203	PEB	C2D-C3D	9.34	1.46	1.34
26	X3	202	PEB	C2D-C3D	9.33	1.46	1.34
26	GG	203	PEB	C2D-C3D	9.33	1.46	1.34
26	l2	202	PEB	C2D-C3D	9.33	1.46	1.34
26	V4	202	PEB	C2D-C3D	9.33	1.46	1.34
26	L4	202	PEB	C2D-C3D	9.33	1.46	1.34
26	TF	202	PEB	C2D-C3D	9.33	1.46	1.34
26	CG	202	PEB	C2D-C3D	9.33	1.46	1.34
26	PG	201	PEB	C2D-C3D	9.33	1.46	1.34
26	a4	203	PEB	C2D-C3D	9.33	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l7	201	PEB	C2D-C3D	9.32	1.46	1.34
26	O4	201	PEB	C2D-C3D	9.32	1.46	1.34
26	eA	202	PEB	C2D-C3D	9.32	1.46	1.34
26	RB	202	PEB	C2D-C3D	9.32	1.46	1.34
26	VD	202	PEB	C2D-C3D	9.32	1.46	1.34
26	O8	201	PEB	C2D-C3D	9.32	1.46	1.34
26	XD	203	PEB	C2D-C3D	9.32	1.46	1.34
26	C8	201	PEB	C2D-C3D	9.32	1.46	1.34
26	A2	304	PEB	C2D-C3D	9.32	1.46	1.34
26	CA	201	PEB	C2D-C3D	9.32	1.46	1.34
26	bG	202	PEB	C2D-C3D	9.32	1.46	1.34
26	R2	203	PEB	C2D-C3D	9.32	1.46	1.34
26	a8	204	PEB	C2D-C3D	9.32	1.46	1.34
26	ZB	202	PEB	C2D-C3D	9.32	1.46	1.34
26	bB	201	PEB	C2D-C3D	9.32	1.46	1.34
26	LD	202	PEB	C2D-C3D	9.32	1.46	1.34
26	hF	201	PEB	C2D-C3D	9.31	1.46	1.34
26	Y1	201	PEB	C2D-C3D	9.31	1.46	1.34
26	J8	201	PEB	C2D-C3D	9.31	1.46	1.34
26	JA	201	PEB	C2D-C3D	9.31	1.46	1.34
26	FC	201	PEB	C2D-C3D	9.31	1.46	1.34
26	c1	203	PEB	C2D-C3D	9.31	1.46	1.34
26	F3	201	PEB	C2D-C3D	9.31	1.46	1.34
26	V1	202	PEB	C2D-C3D	9.31	1.46	1.34
26	E9	202	PEB	C2D-C3D	9.31	1.46	1.34
26	m2	202	PEB	C2D-C3D	9.31	1.46	1.34
26	KC	202	PEB	C2D-C3D	9.30	1.46	1.34
26	SF	201	PEB	C2D-C3D	9.30	1.46	1.34
26	Y2	202	PEB	C2D-C3D	9.30	1.46	1.34
26	j2	202	PEB	C2D-C3D	9.30	1.46	1.34
26	JE	202	PEB	C2D-C3D	9.30	1.46	1.34
26	P6	202	PEB	C2D-C3D	9.30	1.46	1.34
26	R6	202	PEB	C2D-C3D	9.30	1.46	1.34
26	lI	201	PEB	C2D-C3D	9.30	1.46	1.34
26	P2	202	PEB	C2D-C3D	9.30	1.46	1.34
26	E3	202	PEB	C2D-C3D	9.30	1.46	1.34
26	G8	201	PEB	C2D-C3D	9.30	1.46	1.34
26	L1	202	PEB	C2D-C3D	9.30	1.46	1.34
26	U6	201	PEB	C2D-C3D	9.30	1.46	1.34
26	fI	202	PEB	C2D-C3D	9.30	1.46	1.34
26	VE	201	PEB	C2D-C3D	9.30	1.46	1.34
26	G8	202	PEB	C2D-C3D	9.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ZI	202	PEB	C2D-C3D	9.29	1.46	1.34
26	Y3	304	PEB	C2D-C3D	9.29	1.46	1.34
26	gI	202	PEB	C2D-C3D	9.29	1.46	1.34
26	KA	201	PEB	C2D-C3D	9.29	1.46	1.34
26	CJ	202	PEB	C2D-C3D	9.29	1.46	1.34
26	R2	201	PEB	C2D-C3D	9.29	1.46	1.34
26	DJ	203	PEB	C2D-C3D	9.29	1.46	1.34
26	Z6	202	PEB	C2D-C3D	9.29	1.46	1.34
26	e2	201	PEB	C2D-C3D	9.29	1.46	1.34
26	Z4	201	PEB	C2D-C3D	9.29	1.46	1.34
26	iI	202	PEB	C2D-C3D	9.29	1.46	1.34
26	j2	201	PEB	C2D-C3D	9.29	1.46	1.34
26	RE	201	PEB	C2D-C3D	9.28	1.46	1.34
26	VD	201	PEB	C2D-C3D	9.28	1.46	1.34
26	MD	202	PEB	C2D-C3D	9.28	1.46	1.34
26	CE	202	PEB	C2D-C3D	9.28	1.46	1.34
26	B3	203	PEB	C2D-C3D	9.28	1.46	1.34
26	f8	203	PEB	C2D-C3D	9.28	1.46	1.34
26	wE	303	PEB	C2D-C3D	9.28	1.46	1.34
26	Y4	202	PEB	C2D-C3D	9.28	1.46	1.34
26	f7	203	PEB	C2D-C3D	9.28	1.46	1.34
26	OF	201	PEB	C2D-C3D	9.28	1.46	1.34
26	MD	201	PEB	C2D-C3D	9.28	1.46	1.34
26	U6	202	PEB	C2D-C3D	9.28	1.46	1.34
26	l6	201	PEB	C2D-C3D	9.28	1.46	1.34
26	h2	202	PEB	C2D-C3D	9.28	1.46	1.34
26	F5	203	PEB	C2D-C3D	9.28	1.46	1.34
26	D8	201	PEB	C2D-C3D	9.28	1.46	1.34
26	QB	202	PEB	C2D-C3D	9.28	1.46	1.34
26	wG	302	PEB	C2D-C3D	9.28	1.46	1.34
26	OB	203	PEB	C2D-C3D	9.28	1.46	1.34
26	MJ	202	PEB	C2D-C3D	9.27	1.46	1.34
26	H9	202	PEB	C2D-C3D	9.27	1.46	1.34
26	U3	202	PEB	C2D-C3D	9.27	1.46	1.34
26	i1	201	PEB	C2D-C3D	9.27	1.46	1.34
26	aB	201	PEB	C2D-C3D	9.27	1.46	1.34
26	V6	201	PEB	C2D-C3D	9.27	1.46	1.34
26	K9	202	PEB	C2D-C3D	9.27	1.46	1.34
26	KG	202	PEB	C2D-C3D	9.27	1.46	1.34
26	Z2	202	PEB	C2D-C3D	9.26	1.46	1.34
26	S8	202	PEB	C2D-C3D	9.26	1.46	1.34
26	DI	1002	PEB	C2D-C3D	9.26	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	EE	201	PEB	C2D-C3D	9.26	1.46	1.34
26	UB	201	PEB	C2D-C3D	9.26	1.46	1.34
26	Q6	202	PEB	C2D-C3D	9.26	1.46	1.34
26	UB	202	PEB	C2D-C3D	9.26	1.46	1.34
26	Z6	201	PEB	C2D-C3D	9.26	1.46	1.34
26	W7	203	PEB	C2D-C3D	9.26	1.46	1.34
26	PB	202	PEB	C2D-C3D	9.26	1.46	1.34
26	D3	202	PEB	C2D-C3D	9.26	1.46	1.34
26	XG	201	PEB	C2D-C3D	9.26	1.46	1.34
26	B4	202	PEB	C2D-C3D	9.26	1.46	1.34
26	DG	203	PEB	C2D-C3D	9.25	1.46	1.34
26	O3	202	PEB	C2D-C3D	9.25	1.46	1.34
26	eI	201	PEB	C2D-C3D	9.25	1.46	1.34
26	K9	201	PEB	C2D-C3D	9.25	1.46	1.34
26	G1	202	PEB	C2D-C3D	9.25	1.46	1.34
26	X3	203	PEB	C2D-C3D	9.25	1.46	1.34
26	GA	201	PEB	C2D-C3D	9.24	1.46	1.34
26	R4	201	PEB	C2D-C3D	9.24	1.46	1.34
26	k8	201	PEB	C2D-C3D	9.24	1.46	1.34
26	bE	202	PEB	C2D-C3D	9.24	1.46	1.34
26	J9	202	PEB	C2D-C3D	9.24	1.46	1.34
26	G4	202	PEB	C2D-C3D	9.24	1.46	1.34
26	Q2	201	PEB	C2D-C3D	9.24	1.46	1.34
26	RD	203	PEB	C2D-C3D	9.24	1.46	1.34
26	SE	201	PEB	C2D-C3D	9.23	1.46	1.34
26	YD	304	PEB	C2D-C3D	9.23	1.46	1.34
26	W6	203	PEB	C2D-C3D	9.23	1.46	1.34
26	eE	202	PEB	C2D-C3D	9.23	1.46	1.34
26	IG	202	PEB	C2D-C3D	9.23	1.46	1.34
26	jG	201	PEB	C2D-C3D	9.23	1.46	1.34
26	O8	203	PEB	C2D-C3D	9.23	1.46	1.34
26	oG	203	PEB	C2D-C3D	9.23	1.46	1.34
26	BJ	202	PEB	C2D-C3D	9.23	1.46	1.34
26	a1	203	PEB	C2D-C3D	9.23	1.46	1.34
26	B3	202	PEB	C2D-C3D	9.23	1.46	1.34
26	DE	203	PEB	C2D-C3D	9.23	1.46	1.34
26	YI	201	PEB	C2D-C3D	9.23	1.46	1.34
26	AD	202	PEB	C2D-C3D	9.22	1.46	1.34
26	RG	201	PEB	C2D-C3D	9.22	1.46	1.34
26	sE	201	PEB	C2D-C3D	9.22	1.46	1.34
26	OD	201	PEB	C2D-C3D	9.22	1.46	1.34
26	GA	202	PEB	C2D-C3D	9.22	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	EJ	202	PEB	C2D-C3D	9.22	1.46	1.34
26	HC	202	PEB	C2D-C3D	9.22	1.46	1.34
26	iG	201	PEB	C2D-C3D	9.22	1.46	1.34
26	H3	203	PEB	C2D-C3D	9.22	1.46	1.34
26	FD	202	PEB	C2D-C3D	9.22	1.46	1.34
26	JG	202	PEB	C2D-C3D	9.21	1.46	1.34
26	l2	201	PEB	C2D-C3D	9.21	1.46	1.34
26	m1	203	PEB	C2D-C3D	9.21	1.46	1.34
26	YB	202	PEB	C2D-C3D	9.21	1.46	1.34
26	KJ	202	PEB	C2D-C3D	9.21	1.46	1.34
26	Q2	202	PEB	C2D-C3D	9.21	1.46	1.34
26	aA	202	PEB	C2D-C3D	9.21	1.46	1.34
26	a8	201	PEB	C2D-C3D	9.20	1.46	1.34
26	P7	201	PEB	C2D-C3D	9.20	1.46	1.34
26	f7	201	PEB	C2D-C3D	9.20	1.46	1.34
26	UE	201	PEB	C2D-C3D	9.20	1.46	1.34
26	K5	203	PEB	C2D-C3D	9.20	1.46	1.34
26	JE	201	PEB	C2D-C3D	9.20	1.46	1.34
26	CA	202	PEB	C2D-C3D	9.20	1.46	1.34
26	Z6	203	PEB	C2D-C3D	9.19	1.46	1.34
26	yG	301	PEB	C2D-C3D	9.19	1.46	1.34
26	R2	202	PEB	C2D-C3D	9.19	1.46	1.34
26	k6	201	PEB	C2D-C3D	9.19	1.46	1.34
26	YB	201	PEB	C2D-C3D	9.19	1.46	1.34
26	IC	202	PEB	C2D-C3D	9.19	1.46	1.34
26	B4	201	PEB	C2D-C3D	9.19	1.46	1.34
26	aI	202	PEB	C2D-C3D	9.19	1.46	1.34
26	L1	203	PEB	C2D-C3D	9.18	1.46	1.34
26	XA	201	PEB	C2D-C3D	9.18	1.46	1.34
26	V3	201	PEB	C2D-C3D	9.18	1.46	1.34
26	K6	201	PEB	C2D-C3D	9.18	1.46	1.34
26	P8	202	PEB	C2D-C3D	9.18	1.46	1.34
26	LE	201	PEB	C2D-C3D	9.18	1.46	1.34
26	RI	202	PEB	C2D-C3D	9.18	1.46	1.34
26	SB	201	PEB	C2D-C3D	9.18	1.46	1.34
26	ZB	203	PEB	C2D-C3D	9.18	1.46	1.34
26	hE	202	PEB	C2D-C3D	9.18	1.46	1.34
26	HJ	202	PEB	C2D-C3D	9.18	1.46	1.34
26	S8	201	PEB	C2D-C3D	9.18	1.46	1.34
26	aG	202	PEB	C2D-C3D	9.18	1.46	1.34
26	S2	202	PEB	C2D-C3D	9.18	1.46	1.34
26	Y6	202	PEB	C2D-C3D	9.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ID	201	PEB	C2D-C3D	9.17	1.46	1.34
26	S4	201	PEB	C2D-C3D	9.17	1.46	1.34
26	fG	201	PEB	C2D-C3D	9.17	1.46	1.34
26	RD	202	PEB	C2D-C3D	9.17	1.46	1.34
26	sG	201	PEB	C2D-C3D	9.17	1.46	1.34
26	i2	202	PEB	C2D-C3D	9.17	1.46	1.34
26	QE	203	PEB	C2D-C3D	9.17	1.46	1.34
26	K4	202	PEB	C2D-C3D	9.17	1.46	1.34
26	JD	202	PEB	C2D-C3D	9.17	1.46	1.34
26	O7	203	PEB	C2D-C3D	9.17	1.46	1.34
26	V7	201	PEB	C2D-C3D	9.17	1.46	1.34
26	BG	202	PEB	C2D-C3D	9.16	1.46	1.34
26	ZB	201	PEB	C2D-C3D	9.16	1.46	1.34
26	RJ	202	PEB	C2D-C3D	9.16	1.46	1.34
26	Q7	201	PEB	C2D-C3D	9.16	1.46	1.34
26	aA	204	PEB	C2D-C3D	9.16	1.46	1.34
26	cE	201	PEB	C2D-C3D	9.16	1.46	1.34
26	N6	201	PEB	C2D-C3D	9.16	1.46	1.34
26	WG	201	PEB	C2D-C3D	9.16	1.46	1.34
26	TI	201	PEB	C2D-C3D	9.16	1.46	1.34
26	X8	201	PEB	C2D-C3D	9.16	1.46	1.34
26	lF	201	PEB	C2D-C3D	9.16	1.46	1.34
26	TI	202	PEB	C2D-C3D	9.16	1.46	1.34
26	TD	203	PEB	C2D-C3D	9.15	1.46	1.34
26	l6	202	PEB	C2D-C3D	9.15	1.46	1.34
26	NE	201	PEB	C2D-C3D	9.15	1.46	1.34
26	i8	202	PEB	C2D-C3D	9.15	1.46	1.34
26	OA	203	PEB	C2D-C3D	9.15	1.46	1.34
26	H2	1002	PEB	C2D-C3D	9.15	1.46	1.34
26	mE	201	PEB	C2D-C3D	9.15	1.46	1.34
26	Y6	201	PEB	C2D-C3D	9.15	1.46	1.34
26	WB	203	PEB	C2D-C3D	9.15	1.46	1.34
26	O2	201	PEB	C2D-C3D	9.14	1.46	1.34
26	Y2	201	PEB	C2D-C3D	9.14	1.46	1.34
26	Y1	202	PEB	C2D-C3D	9.14	1.46	1.34
26	g1	203	PEB	C2D-C3D	9.14	1.46	1.34
26	d6	202	PEB	C2D-C3D	9.14	1.46	1.34
26	L5	202	PEB	C2D-C3D	9.14	1.46	1.34
26	JJ	202	PEB	C2D-C3D	9.14	1.46	1.34
26	A8	302	PEB	C2D-C3D	9.14	1.46	1.34
26	dF	202	PEB	C2D-C3D	9.14	1.46	1.34
26	P4	201	PEB	C2D-C3D	9.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I9	202	PEB	C2D-C3D	9.14	1.46	1.34
26	aE	202	PEB	C2D-C3D	9.14	1.46	1.34
26	g4	203	PEB	C2D-C3D	9.13	1.46	1.34
26	IA	203	PEB	C2D-C3D	9.13	1.46	1.34
26	V3	202	PEB	C2D-C3D	9.13	1.46	1.34
26	IE	201	PEB	C2D-C3D	9.13	1.46	1.34
26	KB	201	PEB	C2D-C3D	9.13	1.46	1.34
26	NB	1002	PEB	C2D-C3D	9.13	1.46	1.34
26	HI	1002	PEB	C2D-C3D	9.13	1.46	1.34
26	J1	202	PEB	C2D-C3D	9.12	1.46	1.34
26	DD	202	PEB	C2D-C3D	9.12	1.46	1.34
26	DG	201	PEB	C2D-C3D	9.12	1.46	1.34
26	B1	201	PEB	C2D-C3D	9.12	1.46	1.34
26	A5	201	PEB	C2D-C3D	9.12	1.46	1.34
26	hG	202	PEB	C2D-C3D	9.12	1.46	1.34
26	a6	202	PEB	C2D-C3D	9.12	1.46	1.34
26	QG	203	PEB	C2D-C3D	9.12	1.46	1.34
26	T2	201	PEB	C2D-C3D	9.11	1.46	1.34
26	VF	201	PEB	C2D-C3D	9.11	1.46	1.34
26	aA	201	PEB	C2D-C3D	9.11	1.46	1.34
26	DF	1002	PEB	C2D-C3D	9.11	1.46	1.34
26	PD	203	PEB	C2D-C3D	9.11	1.46	1.34
26	h8	201	PEB	C2D-C3D	9.11	1.46	1.34
26	p1	201	PEB	C2D-C3D	9.11	1.46	1.34
26	OI	201	PEB	C2D-C3D	9.11	1.46	1.34
26	K5	202	PEB	C2D-C3D	9.11	1.46	1.34
26	YD	303	PEB	C2D-C3D	9.11	1.46	1.34
26	FJ	202	PEB	C2D-C3D	9.11	1.46	1.34
26	H9	201	PEB	C2D-C3D	9.11	1.46	1.34
26	M3	202	PEB	C2D-C3D	9.10	1.46	1.34
26	h4	202	PEB	C2D-C3D	9.10	1.46	1.34
26	RA	201	PEB	C2D-C3D	9.10	1.46	1.34
26	VA	201	PEB	C2D-C3D	9.10	1.46	1.34
26	dB	202	PEB	C2D-C3D	9.10	1.46	1.34
26	T9	202	PEB	C2D-C3D	9.10	1.46	1.34
26	V9	201	PEB	C2D-C3D	9.10	1.46	1.34
26	lB	202	PEB	C2D-C3D	9.10	1.46	1.34
26	E9	201	PEB	C2D-C3D	9.10	1.46	1.34
26	F3	202	PEB	C2D-C3D	9.10	1.46	1.34
26	L3	202	PEB	C2D-C3D	9.10	1.46	1.34
26	SA	201	PEB	C2D-C3D	9.10	1.46	1.34
26	Q1	201	PEB	C2D-C3D	9.09	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	QA	204	PEB	C2D-C3D	9.09	1.46	1.34
26	O8	202	PEB	C2D-C3D	9.09	1.46	1.34
26	Q4	201	PEB	C2D-C3D	9.09	1.46	1.34
26	R8	201	PEB	C2D-C3D	9.08	1.46	1.34
26	GD	201	PEB	C2D-C3D	9.08	1.46	1.34
26	II	202	PEB	C2D-C3D	9.08	1.46	1.34
26	L9	201	PEB	C2D-C3D	9.08	1.46	1.34
26	F7	1002	PEB	C2D-C3D	9.08	1.46	1.34
26	J4	202	PEB	C2D-C3D	9.08	1.46	1.34
26	I8	203	PEB	C2D-C3D	9.08	1.46	1.34
26	d4	202	PEB	C2D-C3D	9.08	1.46	1.34
26	H6	1002	PEB	C2D-C3D	9.08	1.46	1.34
26	VI	201	PEB	C2D-C3D	9.08	1.46	1.34
26	U2	202	PEB	C2D-C3D	9.08	1.46	1.34
26	V8	201	PEB	C2D-C3D	9.08	1.46	1.34
26	TA	201	PEB	C2D-C3D	9.07	1.46	1.34
26	J2	1002	PEB	C2D-C3D	9.07	1.46	1.34
26	H5	201	PEB	C2D-C3D	9.07	1.46	1.34
26	VG	201	PEB	C2D-C3D	9.07	1.46	1.34
26	T1	203	PEB	C2D-C3D	9.07	1.46	1.34
26	I5	201	PEB	C2D-C3D	9.07	1.46	1.34
26	A8	301	PEB	C2D-C3D	9.07	1.46	1.34
26	gE	203	PEB	C2D-C3D	9.07	1.46	1.34
26	LG	201	PEB	C2D-C3D	9.07	1.46	1.34
26	XA	202	PEB	C2D-C3D	9.07	1.46	1.34
26	O6	202	PEB	C2D-C3D	9.06	1.46	1.34
26	wG	303	PEB	C2D-C3D	9.06	1.46	1.34
26	ND	201	PEB	C2D-C3D	9.06	1.46	1.34
26	UI	202	PEB	C2D-C3D	9.06	1.46	1.34
26	hF	202	PEB	C2D-C3D	9.06	1.46	1.34
26	SG	201	PEB	C2D-C3D	9.06	1.46	1.34
26	JG	201	PEB	C2D-C3D	9.05	1.46	1.34
26	O2	202	PEB	C2D-C3D	9.05	1.46	1.34
26	K8	201	PEB	C2D-C3D	9.05	1.46	1.34
26	X8	202	PEB	C2D-C3D	9.05	1.46	1.34
26	N1	203	PEB	C2D-C3D	9.05	1.46	1.34
26	kB	201	PEB	C2D-C3D	9.05	1.46	1.34
26	QF	202	PEB	C2D-C3D	9.05	1.46	1.34
26	S6	201	PEB	C2D-C3D	9.05	1.46	1.34
26	c4	203	PEB	C2D-C3D	9.05	1.46	1.34
26	AA	302	PEB	C2D-C3D	9.05	1.46	1.34
26	YA	202	PEB	C2D-C3D	9.05	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m1	201	PEB	C2D-C3D	9.04	1.46	1.34
26	ND	202	PEB	C2D-C3D	9.04	1.46	1.34
26	h6	201	PEB	C2D-C3D	9.04	1.46	1.34
26	aB	202	PEB	C2D-C3D	9.04	1.46	1.34
26	PI	203	PEB	C2D-C3D	9.04	1.46	1.34
26	P1	202	PEB	C2D-C3D	9.04	1.46	1.34
26	P3	201	PEB	C2D-C3D	9.04	1.46	1.34
26	P2	203	PEB	C2D-C3D	9.04	1.46	1.34
26	OF	203	PEB	C2D-C3D	9.03	1.46	1.34
26	PF	201	PEB	C2D-C3D	9.03	1.46	1.34
26	EJ	201	PEB	C2D-C3D	9.03	1.46	1.34
26	J3	202	PEB	C2D-C3D	9.03	1.46	1.34
26	kE	203	PEB	C2D-C3D	9.03	1.46	1.34
26	T8	201	PEB	C2D-C3D	9.03	1.46	1.34
26	MG	203	PEB	C2D-C3D	9.03	1.46	1.34
26	NG	202	PEB	C2D-C3D	9.03	1.46	1.34
26	W1	201	PEB	C2D-C3D	9.03	1.46	1.34
26	D3	201	PEB	C2D-C3D	9.03	1.46	1.34
26	EA	201	PEB	C2D-C3D	9.03	1.46	1.34
26	IC	203	PEB	C2D-C3D	9.03	1.46	1.34
26	OE	201	PEB	C2D-C3D	9.02	1.46	1.34
26	EG	201	PEB	C2D-C3D	9.02	1.46	1.34
26	PD	201	PEB	C2D-C3D	9.02	1.46	1.34
26	Y3	303	PEB	C2D-C3D	9.01	1.46	1.34
26	Y8	202	PEB	C2D-C3D	9.01	1.46	1.34
26	d8	202	PEB	C2D-C3D	9.01	1.46	1.34
26	PD	202	PEB	C2D-C3D	9.01	1.46	1.34
26	VI	202	PEB	C2D-C3D	9.01	1.46	1.34
26	QD	201	PEB	C2D-C3D	9.01	1.46	1.34
26	lA	202	PEB	C2D-C3D	9.01	1.46	1.34
26	LJ	201	PEB	C2D-C3D	9.01	1.46	1.34
26	k4	203	PEB	C2D-C3D	9.01	1.46	1.34
26	UG	201	PEB	C2D-C3D	9.01	1.46	1.34
26	u1	202	PEB	C2D-C3D	9.01	1.46	1.34
26	N3	201	PEB	C2D-C3D	9.01	1.46	1.34
26	SA	203	PEB	C2D-C3D	9.01	1.46	1.34
26	GE	202	PEB	C2D-C3D	9.01	1.46	1.34
26	E8	201	PEB	C2D-C3D	9.01	1.46	1.34
26	HB	1002	PEB	C2D-C3D	9.01	1.46	1.34
26	PE	202	PEB	C2D-C3D	9.01	1.46	1.34
26	NA	201	PEB	C2D-C3D	9.01	1.46	1.34
26	k2	202	PEB	C2D-C3D	9.01	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d1	202	PEB	C2D-C3D	9.01	1.46	1.34
26	W6	201	PEB	C2D-C3D	9.00	1.46	1.34
26	R3	202	PEB	C2D-C3D	9.00	1.46	1.34
26	eA	201	PEB	C2D-C3D	9.00	1.46	1.34
26	LC	201	PEB	C2D-C3D	9.00	1.46	1.34
26	KE	201	PEB	C2D-C3D	9.00	1.46	1.34
26	W4	201	PEB	C2D-C3D	9.00	1.46	1.34
26	TB	202	PEB	C2D-C3D	9.00	1.46	1.34
26	jI	202	PEB	C2D-C3D	8.99	1.46	1.34
26	V2	201	PEB	C2D-C3D	8.99	1.46	1.34
26	fF	201	PEB	C2D-C3D	8.99	1.46	1.34
26	kG	203	PEB	C2D-C3D	8.98	1.46	1.34
26	R9	203	PEB	C2D-C3D	8.98	1.46	1.34
26	XD	201	PEB	C2D-C3D	8.98	1.46	1.34
26	a2	201	PEB	C2D-C3D	8.98	1.46	1.34
26	TD	202	PEB	C2D-C3D	8.98	1.46	1.34
26	TJ	202	PEB	C2D-C3D	8.98	1.46	1.34
26	a8	202	PEB	C2D-C3D	8.98	1.46	1.34
26	O6	201	PEB	C2D-C3D	8.98	1.46	1.34
26	ZA	201	PEB	C2D-C3D	8.98	1.46	1.34
26	D9	202	PEB	C2D-C3D	8.98	1.46	1.34
26	N4	203	PEB	C2D-C3D	8.98	1.46	1.34
26	ZA	202	PEB	C2D-C3D	8.97	1.46	1.34
26	PJ	201	PEB	C2D-C3D	8.97	1.46	1.34
26	W6	202	PEB	C2D-C3D	8.97	1.46	1.34
26	X1	201	PEB	C2D-C3D	8.96	1.46	1.34
26	HC	203	PEB	C2D-C3D	8.96	1.46	1.34
26	W2	201	PEB	C2D-C3D	8.96	1.46	1.34
26	Q3	201	PEB	C2D-C3D	8.96	1.46	1.34
26	TE	201	PEB	C2D-C3D	8.96	1.46	1.34
26	P1	201	PEB	C2D-C3D	8.96	1.46	1.34
26	F5	201	PEB	C2D-C3D	8.96	1.46	1.34
26	d7	203	PEB	C2D-C3D	8.96	1.46	1.34
26	S8	203	PEB	C2D-C3D	8.96	1.46	1.34
26	X1	202	PEB	C2D-C3D	8.96	1.46	1.34
26	e8	201	PEB	C2D-C3D	8.96	1.46	1.34
26	R1	203	PEB	C2D-C3D	8.96	1.46	1.34
26	JI	1002	PEB	C2D-C3D	8.96	1.46	1.34
26	L7	1002	PEB	C2D-C3D	8.95	1.46	1.34
26	m4	201	PEB	C2D-C3D	8.95	1.46	1.34
26	YA	203	PEB	C2D-C3D	8.95	1.46	1.34
26	F5	202	PEB	C2D-C3D	8.94	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P3	203	PEB	C2D-C3D	8.94	1.46	1.34
26	Z2	201	PEB	C2D-C3D	8.94	1.46	1.34
26	N8	201	PEB	C2D-C3D	8.94	1.46	1.34
26	T6	202	PEB	C2D-C3D	8.94	1.46	1.34
26	SE	202	PEB	C2D-C3D	8.94	1.46	1.34
26	aI	201	PEB	C2D-C3D	8.94	1.46	1.34
26	SD	201	PEB	C2D-C3D	8.93	1.46	1.34
26	K8	202	PEB	C2D-C3D	8.93	1.46	1.34
26	WB	201	PEB	C2D-C3D	8.93	1.46	1.34
26	X4	202	PEB	C2D-C3D	8.93	1.46	1.34
26	RD	201	PEB	C2D-C3D	8.93	1.46	1.34
26	NE	202	PEB	C2D-C3D	8.93	1.46	1.34
26	T3	202	PEB	C2D-C3D	8.93	1.46	1.34
26	KG	201	PEB	C2D-C3D	8.93	1.46	1.34
26	TD	201	PEB	C2D-C3D	8.93	1.46	1.34
26	N4	202	PEB	C2D-C3D	8.93	1.46	1.34
26	P4	203	PEB	C2D-C3D	8.93	1.46	1.34
26	ND	203	PEB	C2D-C3D	8.92	1.46	1.34
26	QD	202	PEB	C2D-C3D	8.92	1.46	1.34
26	h7	201	PEB	C2D-C3D	8.92	1.46	1.34
26	ZI	201	PEB	C2D-C3D	8.91	1.46	1.34
26	cG	203	PEB	C2D-C3D	8.91	1.46	1.34
26	Z8	202	PEB	C2D-C3D	8.91	1.46	1.34
26	GG	202	PEB	CHB-C4B	8.91	1.42	1.35
26	DD	201	PEB	C2D-C3D	8.91	1.46	1.34
26	GE	201	PEB	C2D-C3D	8.91	1.46	1.34
26	WB	202	PEB	C2D-C3D	8.91	1.46	1.34
26	C8	202	PEB	C2D-C3D	8.90	1.46	1.34
26	TG	201	PEB	C2D-C3D	8.90	1.46	1.34
26	I5	202	PEB	C2D-C3D	8.90	1.46	1.34
26	N8	202	PEB	C2D-C3D	8.90	1.46	1.34
26	HA	201	PEB	C2D-C3D	8.90	1.46	1.34
26	NA	202	PEB	C2D-C3D	8.90	1.46	1.34
26	FF	1002	PEB	C2D-C3D	8.90	1.46	1.34
26	TJ	201	PEB	C2D-C3D	8.90	1.46	1.34
26	Y8	203	PEB	C2D-C3D	8.90	1.46	1.34
26	EA	202	PEB	C2D-C3D	8.90	1.46	1.34
26	H8	201	PEB	C2D-C3D	8.89	1.46	1.34
26	NG	201	PEB	C2D-C3D	8.89	1.46	1.34
26	P4	202	PEB	C2D-C3D	8.89	1.46	1.34
26	OB	202	PEB	C2D-C3D	8.89	1.46	1.34
26	T3	203	PEB	C2D-C3D	8.88	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	OB	201	PEB	C2D-C3D	8.88	1.46	1.34
26	AA	301	PEB	C2D-C3D	8.88	1.46	1.34
26	XE	202	PEB	C2D-C3D	8.88	1.46	1.34
26	eD	401	PEB	C2D-C3D	8.88	1.46	1.34
26	N3	202	PEB	C2D-C3D	8.88	1.46	1.34
26	DJ	202	PEB	C2D-C3D	8.88	1.46	1.34
26	IG	201	PEB	C2D-C3D	8.87	1.46	1.34
26	UI	201	PEB	C2D-C3D	8.87	1.46	1.34
26	U2	201	PEB	C2D-C3D	8.87	1.46	1.34
26	RJ	203	PEB	C2D-C3D	8.87	1.45	1.34
26	KA	202	PEB	C2D-C3D	8.87	1.45	1.34
26	OE	202	PEB	C2D-C3D	8.87	1.45	1.34
26	WA	203	PEB	C2D-C3D	8.87	1.45	1.34
26	R4	203	PEB	C2D-C3D	8.86	1.45	1.34
26	SD	202	PEB	C2D-C3D	8.86	1.45	1.34
26	X3	201	PEB	C2D-C3D	8.86	1.45	1.34
26	E8	202	PEB	C2D-C3D	8.86	1.45	1.34
26	V4	203	PEB	C2D-C3D	8.86	1.45	1.34
26	S3	202	PEB	C2D-C3D	8.85	1.45	1.34
26	S3	201	PEB	C2D-C3D	8.85	1.45	1.34
26	N3	203	PEB	C2D-C3D	8.85	1.45	1.34
26	IG	203	PEB	C2D-C3D	8.85	1.45	1.34
26	l8	202	PEB	C2D-C3D	8.85	1.45	1.34
26	V2	202	PEB	C2D-C3D	8.85	1.45	1.34
26	Z8	201	PEB	C2D-C3D	8.85	1.45	1.34
26	T2	202	PEB	C2D-C3D	8.85	1.45	1.34
26	N1	202	PEB	C2D-C3D	8.84	1.45	1.34
26	TE	202	PEB	C2D-C3D	8.84	1.45	1.34
26	D6	1002	PEB	C2D-C3D	8.84	1.45	1.34
26	GG	202	PEB	C2D-C3D	8.83	1.45	1.34
26	e3	401	PEB	C2D-C3D	8.83	1.45	1.34
26	HG	201	PEB	C2D-C3D	8.83	1.45	1.34
26	WI	201	PEB	C2D-C3D	8.82	1.45	1.34
26	uG	201	PEB	C2D-C3D	8.82	1.45	1.34
26	PG	202	PEB	C2D-C3D	8.82	1.45	1.34
26	a2	202	PEB	C2D-C3D	8.81	1.45	1.34
26	LB	1002	PEB	C2D-C3D	8.81	1.45	1.34
26	T7	201	PEB	C2D-C3D	8.81	1.45	1.34
26	a8	203	PEB	C2D-C3D	8.81	1.45	1.34
26	FE	201	PEB	C2D-C3D	8.81	1.45	1.34
26	I9	201	PEB	C2D-C3D	8.81	1.45	1.34
26	VF	202	PEB	C2D-C3D	8.81	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L9	202	PEB	C2D-C3D	8.80	1.45	1.34
26	R3	201	PEB	C2D-C3D	8.80	1.45	1.34
26	aA	203	PEB	C2D-C3D	8.80	1.45	1.34
26	XG	203	PEB	C2D-C3D	8.80	1.45	1.34
26	QF	201	PEB	C2D-C3D	8.80	1.45	1.34
26	P3	202	PEB	C2D-C3D	8.79	1.45	1.34
26	T6	201	PEB	C2D-C3D	8.79	1.45	1.34
26	FG	201	PEB	C2D-C3D	8.79	1.45	1.34
26	SG	202	PEB	C2D-C3D	8.78	1.45	1.34
26	RE	202	PEB	C2D-C3D	8.77	1.45	1.34
26	L6	1002	PEB	C2D-C3D	8.77	1.45	1.34
26	G6	1002	PEB	C2D-C3D	8.76	1.45	1.34
26	M8	202	PEB	C2D-C3D	8.76	1.45	1.34
26	DB	1002	PEB	C2D-C3D	8.75	1.45	1.34
26	W8	201	PEB	C2D-C3D	8.75	1.45	1.34
26	LA	201	PEB	C2D-C3D	8.75	1.45	1.34
26	G3	201	PEB	C2D-C3D	8.75	1.45	1.34
26	SI	202	PEB	C2D-C3D	8.75	1.45	1.34
26	Y8	201	PEB	C2D-C3D	8.74	1.45	1.34
26	GB	1002	PEB	C2D-C3D	8.74	1.45	1.34
26	YA	201	PEB	C2D-C3D	8.74	1.45	1.34
26	BJ	201	PEB	C2D-C3D	8.73	1.45	1.34
26	WE	201	PEB	C2D-C3D	8.72	1.45	1.34
26	MA	202	PEB	C2D-C3D	8.72	1.45	1.34
26	OI	202	PEB	C2D-C3D	8.72	1.45	1.34
26	UE	203	PEB	C2D-C3D	8.71	1.45	1.34
26	X4	201	PEB	C2D-C3D	8.71	1.45	1.34
26	W8	203	PEB	C2D-C3D	8.71	1.45	1.34
26	T3	201	PEB	C2D-C3D	8.71	1.45	1.34
26	JC	202	PEB	C2D-C3D	8.70	1.45	1.34
26	FE	202	PEB	C2D-C3D	8.69	1.45	1.34
26	B9	201	PEB	C2D-C3D	8.69	1.45	1.34
26	Z4	202	PEB	C2D-C3D	8.69	1.45	1.34
26	PA	201	PEB	C2D-C3D	8.69	1.45	1.34
26	L8	201	PEB	C2D-C3D	8.69	1.45	1.34
26	BG	201	PEB	C2D-C3D	8.68	1.45	1.34
26	U8	202	PEB	C2D-C3D	8.68	1.45	1.34
26	N1	201	PEB	C2D-C3D	8.68	1.45	1.34
26	OG	202	PEB	C2D-C3D	8.68	1.45	1.34
26	V1	201	PEB	C2D-C3D	8.68	1.45	1.34
26	l8	203	PEB	C2D-C3D	8.68	1.45	1.34
26	UA	202	PEB	C2D-C3D	8.67	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V1	203	PEB	C2D-C3D	8.67	1.45	1.34
26	LJ	202	PEB	C2D-C3D	8.67	1.45	1.34
26	IA	202	PEB	C2D-C3D	8.67	1.45	1.34
26	LC	203	PEB	C2D-C3D	8.67	1.45	1.34
26	TG	202	PEB	C2D-C3D	8.65	1.45	1.34
26	UD	201	PEB	C2D-C3D	8.65	1.45	1.34
26	N4	201	PEB	C2D-C3D	8.65	1.45	1.34
26	RG	202	PEB	C2D-C3D	8.65	1.45	1.34
26	lA	203	PEB	C2D-C3D	8.65	1.45	1.34
26	u4	202	PEB	C2D-C3D	8.64	1.45	1.34
26	V4	201	PEB	C2D-C3D	8.64	1.45	1.34
26	IJ	201	PEB	C2D-C3D	8.64	1.45	1.34
26	P8	201	PEB	C2D-C3D	8.63	1.45	1.34
26	MA	201	PEB	C2D-C3D	8.62	1.45	1.34
26	TB	201	PEB	C2D-C3D	8.62	1.45	1.34
26	DE	202	PEB	C2D-C3D	8.62	1.45	1.34
26	TF	201	PEB	C2D-C3D	8.61	1.45	1.34
26	Q3	202	PEB	C2D-C3D	8.61	1.45	1.34
26	OG	201	PEB	C2D-C3D	8.57	1.45	1.34
26	H5	202	PEB	C2D-C3D	8.57	1.45	1.34
26	X1	203	PEB	C2D-C3D	8.57	1.45	1.34
26	H5	203	PEB	C2D-C3D	8.57	1.45	1.34
26	FG	202	PEB	C2D-C3D	8.57	1.45	1.34
26	I5	203	PEB	C2D-C3D	8.56	1.45	1.34
26	WA	202	PEB	C2D-C3D	8.55	1.45	1.34
26	WA	201	PEB	C2D-C3D	8.55	1.45	1.34
26	M8	201	PEB	C2D-C3D	8.55	1.45	1.34
26	I8	202	PEB	C2D-C3D	8.55	1.45	1.34
26	O3	201	PEB	C2D-C3D	8.53	1.45	1.34
26	U3	201	PEB	C2D-C3D	8.53	1.45	1.34
26	L5	201	PEB	C2D-C3D	8.51	1.45	1.34
26	Z1	202	PEB	C2D-C3D	8.47	1.45	1.34
26	HJ	201	PEB	C2D-C3D	8.45	1.45	1.34
26	X4	203	PEB	C2D-C3D	8.44	1.45	1.34
26	IJ	203	PEB	C2D-C3D	8.44	1.45	1.34
26	XG	202	PEB	C2D-C3D	8.44	1.45	1.34
26	KA	203	PEB	C2D-C3D	8.43	1.45	1.34
26	DG	202	PEB	C2D-C3D	8.42	1.45	1.34
26	F9	201	PEB	C2D-C3D	8.40	1.45	1.34
26	LE	202	PEB	C2D-C3D	8.36	1.45	1.34
26	T4	201	PEB	C3C-C4C	8.31	1.55	1.42
26	FJ	201	PEB	C2D-C3D	8.28	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W3	201	PEB	C2D-C3D	8.27	1.45	1.34
26	L5	203	PEB	C2D-C3D	8.26	1.45	1.34
26	J9	203	PEB	C2D-C3D	8.26	1.45	1.34
26	LF	1002	PEB	C2D-C3D	8.25	1.45	1.34
26	GG	201	PEB	C2D-C3D	8.25	1.45	1.34
26	LG	202	PEB	C2D-C3D	8.24	1.45	1.34
26	W8	202	PEB	C2D-C3D	8.24	1.45	1.34
26	WD	201	PEB	C2D-C3D	8.24	1.45	1.34
26	M8	203	PEB	C2D-C3D	8.23	1.45	1.34
26	J5	202	PEB	C2D-C3D	8.23	1.45	1.34
26	MA	203	PEB	C2D-C3D	8.21	1.45	1.34
26	K8	203	PEB	C2D-C3D	8.21	1.45	1.34
26	IE	203	PEB	C2D-C3D	8.21	1.45	1.34
26	T9	201	PEB	C2D-C3D	8.19	1.45	1.34
26	JJ	203	PEB	C2D-C3D	8.16	1.45	1.34
26	DJ	201	PEB	C2D-C3D	8.15	1.45	1.34
26	D9	201	PEB	C2D-C3D	8.14	1.45	1.34
26	BE	201	PEB	C2D-C3D	8.14	1.45	1.34
26	cE	203	PEB	C2D-C3D	8.11	1.45	1.34
26	T1	201	PEB	C3C-C4C	8.05	1.54	1.42
26	HE	201	PEB	C2D-C3D	7.89	1.44	1.34
26	JC	201	PEB	C2D-C3D	7.86	1.44	1.34
26	ME	203	PEB	C2D-C3D	7.82	1.44	1.34
26	bG	202	PEB	C3C-C4C	7.69	1.54	1.42
26	nE	202	PEB	C3C-C4C	7.68	1.54	1.42
26	B9	203	PEB	C2D-C3D	7.55	1.44	1.34
26	CE	201	PEB	C2D-C3D	7.52	1.44	1.34
26	fG	202	PEB	C3C-C4C	7.51	1.53	1.42
26	YD	301	PEB	C3C-C4C	7.45	1.53	1.42
26	dE	202	PEB	C3C-C4C	7.43	1.53	1.42
26	PG	202	PEB	C3C-C4C	7.39	1.53	1.42
26	bE	202	PEB	C3C-C4C	7.37	1.53	1.42
26	BJ	203	PEB	C2D-C3D	7.34	1.44	1.34
26	fE	202	PEB	C3C-C4C	7.34	1.53	1.42
26	PE	202	PEB	C3C-C4C	7.33	1.53	1.42
28	KH	1001	CYC	C2A-C3A	7.27	1.52	1.36
26	NG	202	PEB	C3C-C4C	7.25	1.53	1.42
26	F5	203	PEB	C3C-C4C	7.23	1.53	1.42
26	NE	202	PEB	C3C-C4C	7.13	1.53	1.42
26	TE	202	PEB	C3C-C4C	7.03	1.53	1.42
26	FC	203	PEB	C3C-C4C	6.98	1.53	1.42
26	JE	202	PEB	C3C-C4C	6.92	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VA	202	PEB	C3B-C2B	6.89	1.51	1.36
26	TG	202	PEB	C3C-C4C	6.86	1.52	1.42
26	J5	201	PEB	C2D-C3D	6.83	1.43	1.34
26	dG	202	PEB	C3C-C4C	6.82	1.52	1.42
26	tE	202	PEB	C3C-C4C	6.80	1.52	1.42
26	rE	202	PEB	C3C-C4C	6.78	1.52	1.42
26	JG	202	PEB	C3C-C4C	6.75	1.52	1.42
26	J5	201	PEB	CHA-C1B	6.71	1.56	1.40
26	rG	202	PEB	C3C-C4C	6.68	1.52	1.42
26	HA	201	PEB	C3C-C4C	6.63	1.52	1.42
26	J5	201	PEB	C2A-C1A	-6.62	1.46	1.52
26	N1	203	PEB	C3C-C4C	6.59	1.52	1.42
26	H8	201	PEB	C3C-C4C	6.59	1.52	1.42
26	Z1	202	PEB	C3C-C4C	6.57	1.52	1.42
26	m8	202	PEB	C3B-C2B	6.54	1.50	1.36
26	ZG	202	PEB	C3C-C4C	6.54	1.52	1.42
28	F2	1001	CYC	C3B-C2B	6.53	1.50	1.36
26	JC	202	PEB	C3C-C4C	6.53	1.52	1.42
26	BE	202	PEB	C3C-C4C	6.53	1.52	1.42
26	mA	202	PEB	C3B-C2B	6.51	1.50	1.36
26	Y3	301	PEB	C3C-C4C	6.51	1.52	1.42
26	X4	201	PEB	C3C-C4C	6.50	1.52	1.42
26	V8	202	PEB	C3B-C2B	6.49	1.50	1.36
26	DJ	203	PEB	C3C-C4C	6.49	1.52	1.42
26	XE	202	PEB	C3C-C4C	6.48	1.52	1.42
26	V4	203	PEB	C3C-C4C	6.45	1.52	1.42
26	XG	203	PEB	C3C-C4C	6.42	1.52	1.42
26	D9	203	PEB	C3C-C4C	6.42	1.52	1.42
26	LC	203	PEB	C3C-C4C	6.42	1.52	1.42
26	A4	201	PEB	C3B-C2B	6.40	1.50	1.36
26	z1	202	PEB	C3B-C2B	6.38	1.50	1.36
26	sG	203	PEB	C3B-C2B	6.38	1.50	1.36
26	BG	202	PEB	C3C-C4C	6.36	1.52	1.42
26	JC	201	PEB	CHA-C1B	6.35	1.55	1.40
26	P1	201	PEB	C3C-C4C	6.34	1.52	1.42
26	lE	201	PEB	C3B-C2B	6.33	1.50	1.36
26	LE	202	PEB	C3C-C4C	6.32	1.51	1.42
26	qE	202	PEB	C3B-C2B	6.31	1.50	1.36
26	ZE	202	PEB	C3C-C4C	6.30	1.51	1.42
26	J5	202	PEB	C3C-C4C	6.29	1.51	1.42
26	V1	203	PEB	C3C-C4C	6.29	1.51	1.42
26	LB	1002	PEB	C3C-C4C	6.28	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	nG	202	PEB	C3C-C4C	6.28	1.51	1.42
26	gE	201	PEB	C3C-C4C	6.27	1.51	1.42
26	e1	202	PEB	C3B-C2B	6.27	1.50	1.36
26	L6	1002	PEB	C3C-C4C	6.26	1.51	1.42
26	r1	202	PEB	C3B-C2B	6.25	1.50	1.36
26	N4	203	PEB	C3C-C4C	6.25	1.51	1.42
26	ZG	201	PEB	C3B-C2B	6.24	1.50	1.36
26	mE	201	PEB	C3B-C2B	6.24	1.50	1.36
26	r4	202	PEB	C3B-C2B	6.23	1.50	1.36
26	Z4	202	PEB	C3C-C4C	6.22	1.51	1.42
26	N8	201	PEB	C3C-C4C	6.22	1.51	1.42
28	AH	1001	CYC	C2A-C3A	6.21	1.49	1.36
28	cH	1001	CYC	C2A-C3A	6.21	1.49	1.36
28	qH	1002	CYC	C3B-C2B	6.20	1.49	1.36
26	F9	203	PEB	C3B-C2B	6.20	1.49	1.36
26	x1	202	PEB	C3B-C2B	6.19	1.49	1.36
26	iG	201	PEB	C3B-C2B	6.18	1.49	1.36
26	HC	203	PEB	C3C-C4C	6.15	1.51	1.42
26	L5	203	PEB	C3C-C4C	6.15	1.51	1.42
26	p1	202	PEB	C3B-C2B	6.15	1.49	1.36
26	hE	202	PEB	C3C-C4C	6.15	1.51	1.42
26	F4	202	PEB	C3B-C2B	6.14	1.49	1.36
26	d7	203	PEB	C3B-C2B	6.14	1.49	1.36
26	BC	203	PEB	C3C-C4C	6.14	1.51	1.42
26	P4	201	PEB	C3C-C4C	6.14	1.51	1.42
26	K1	202	PEB	C3B-C2B	6.13	1.49	1.36
26	TA	201	PEB	C3C-C4C	6.13	1.51	1.42
26	cE	203	PEB	C3B-C2B	6.13	1.49	1.36
26	wG	303	PEB	C3B-C2B	6.12	1.49	1.36
26	j1	201	PEB	C3B-C2B	6.12	1.49	1.36
26	pE	202	PEB	C3C-C4C	6.11	1.51	1.42
26	ZF	201	PEB	C3C-C4C	6.11	1.51	1.42
26	kE	202	PEB	C3B-C2B	6.09	1.49	1.36
26	oG	203	PEB	C3B-C2B	6.09	1.49	1.36
26	gI	203	PEB	C3B-C2B	6.09	1.49	1.36
26	RE	202	PEB	C3C-C4C	6.09	1.51	1.42
26	H5	203	PEB	C3C-C4C	6.07	1.51	1.42
26	g2	203	PEB	C3B-C2B	6.06	1.49	1.36
26	d6	204	PEB	C3B-C2B	6.06	1.49	1.36
26	lF	203	PEB	C3B-C2B	6.06	1.49	1.36
26	PJ	201	PEB	C3B-C2B	6.06	1.49	1.36
26	dF	203	PEB	C3B-C2B	6.05	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	iE	202	PEB	C3C-C4C	6.05	1.51	1.42
26	CJ	201	PEB	C3C-C4C	6.04	1.51	1.42
26	A5	202	PEB	C3C-C4C	6.04	1.51	1.42
26	T8	201	PEB	C3C-C4C	6.04	1.51	1.42
26	ZA	201	PEB	C3C-C4C	6.04	1.51	1.42
26	x4	202	PEB	C3B-C2B	6.04	1.49	1.36
26	wE	303	PEB	C3B-C2B	6.04	1.49	1.36
26	RG	202	PEB	C3C-C4C	6.04	1.51	1.42
26	R1	203	PEB	C3C-C4C	6.03	1.51	1.42
26	mI	203	PEB	C3B-C2B	6.03	1.49	1.36
26	NA	201	PEB	C3C-C4C	6.02	1.51	1.42
26	wG	303	PEB	C3C-C4C	6.02	1.51	1.42
26	uG	203	PEB	C3B-C2B	6.02	1.49	1.36
26	B5	203	PEB	C3C-C4C	6.01	1.51	1.42
26	m2	203	PEB	C3B-C2B	6.01	1.49	1.36
26	R4	203	PEB	C3C-C4C	6.01	1.51	1.42
26	X1	201	PEB	C3C-C4C	6.00	1.51	1.42
26	wE	303	PEB	C3C-C4C	6.00	1.51	1.42
26	e4	202	PEB	C3B-C2B	5.99	1.49	1.36
26	VA	201	PEB	C3C-C4C	5.99	1.51	1.42
26	IG	201	PEB	C3C-C4C	5.99	1.51	1.42
26	iA	201	PEB	C3C-C4C	5.98	1.51	1.42
26	p4	202	PEB	C3B-C2B	5.97	1.49	1.36
26	uG	201	PEB	C3B-C2B	5.96	1.49	1.36
26	fF	202	PEB	C3B-C2B	5.96	1.49	1.36
26	Z7	201	PEB	C3C-C4C	5.96	1.51	1.42
26	A7	301	PEB	C3B-C2B	5.96	1.49	1.36
26	14	202	PEB	C3B-C2B	5.96	1.49	1.36
26	H1	203	PEB	C3B-C2B	5.95	1.49	1.36
26	a1	202	PEB	C3B-C2B	5.95	1.49	1.36
26	YD	304	PEB	C3B-C2B	5.95	1.49	1.36
26	oE	201	PEB	C3B-C2B	5.95	1.49	1.36
26	u1	202	PEB	C3B-C2B	5.95	1.49	1.36
26	aE	201	PEB	C3B-C2B	5.95	1.49	1.36
26	uE	203	PEB	C3B-C2B	5.94	1.49	1.36
26	gG	201	PEB	C3C-C4C	5.94	1.51	1.42
26	R7	202	PEB	C3B-C2B	5.94	1.49	1.36
26	qE	201	PEB	C3B-C2B	5.94	1.49	1.36
26	J3	203	PEB	C3B-C2B	5.93	1.49	1.36
26	F3	203	PEB	C3C-C4C	5.93	1.51	1.42
26	H9	203	PEB	C3C-C4C	5.93	1.51	1.42
26	xE	302	PEB	C3B-C2B	5.93	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cG	203	PEB	C3B-C2B	5.93	1.49	1.36
26	lG	202	PEB	C3C-C4C	5.92	1.51	1.42
26	aG	201	PEB	C3B-C2B	5.92	1.49	1.36
26	jE	202	PEB	C3C-C4C	5.92	1.51	1.42
26	t4	202	PEB	C3B-C2B	5.92	1.49	1.36
28	I6	1001	CYC	C3B-C2B	5.91	1.49	1.36
26	sE	203	PEB	C3B-C2B	5.91	1.49	1.36
26	z4	202	PEB	C3B-C2B	5.91	1.49	1.36
26	UE	201	PEB	C3C-C4C	5.91	1.51	1.42
26	t1	201	PEB	C3B-C2B	5.91	1.49	1.36
26	SJ	202	PEB	C3C-C4C	5.91	1.51	1.42
26	mG	201	PEB	C3B-C2B	5.91	1.49	1.36
26	L8	201	PEB	C3C-C4C	5.91	1.51	1.42
26	jF	202	PEB	C3B-C2B	5.90	1.49	1.36
26	C5	204	PEB	C3C-C4C	5.90	1.51	1.42
26	i8	201	PEB	C3C-C4C	5.90	1.51	1.42
26	lE	202	PEB	C3C-C4C	5.90	1.51	1.42
26	UG	201	PEB	C3C-C4C	5.90	1.51	1.42
26	RJ	203	PEB	C3B-C2B	5.90	1.49	1.36
26	DG	203	PEB	C3C-C4C	5.90	1.51	1.42
26	xE	304	PEB	C3B-C2B	5.90	1.49	1.36
26	e7	202	PEB	C3B-C2B	5.90	1.49	1.36
26	R9	203	PEB	C3B-C2B	5.90	1.49	1.36
26	QG	203	PEB	C3B-C2B	5.90	1.49	1.36
26	cE	201	PEB	C3C-C4C	5.89	1.51	1.42
26	aG	203	PEB	C3C-C4C	5.89	1.51	1.42
26	h7	203	PEB	C3B-C2B	5.89	1.49	1.36
26	iE	201	PEB	C3B-C2B	5.89	1.49	1.36
26	h8	203	PEB	C3C-C4C	5.89	1.51	1.42
26	tG	202	PEB	C3C-C4C	5.89	1.51	1.42
26	a4	202	PEB	C3B-C2B	5.88	1.49	1.36
26	d1	202	PEB	C3B-C2B	5.88	1.49	1.36
28	IB	1001	CYC	C3B-C2B	5.88	1.49	1.36
26	HJ	203	PEB	C3C-C4C	5.88	1.51	1.42
26	UJ	202	PEB	C3C-C4C	5.88	1.51	1.42
26	hE	201	PEB	C3B-C2B	5.88	1.49	1.36
26	hA	201	PEB	C3B-C2B	5.87	1.49	1.36
26	h8	201	PEB	C3B-C2B	5.87	1.49	1.36
26	ZE	201	PEB	C3B-C2B	5.87	1.49	1.36
26	E4	202	PEB	C3C-C4C	5.87	1.51	1.42
26	V9	203	PEB	C3C-C4C	5.87	1.51	1.42
26	OF	201	PEB	C3B-C2B	5.86	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c4	202	PEB	C3B-C2B	5.86	1.49	1.36
26	P9	201	PEB	C3B-C2B	5.86	1.49	1.36
26	AC	203	PEB	C3C-C4C	5.86	1.51	1.42
26	jG	202	PEB	C3C-C4C	5.86	1.51	1.42
26	SE	203	PEB	C3C-C4C	5.86	1.51	1.42
26	LA	201	PEB	C3C-C4C	5.86	1.51	1.42
26	Y3	304	PEB	C3B-C2B	5.86	1.49	1.36
26	AJ	304	PEB	C3B-C2B	5.86	1.49	1.36
26	xG	302	PEB	C3B-C2B	5.85	1.49	1.36
26	t1	202	PEB	C3B-C2B	5.85	1.49	1.36
26	V8	201	PEB	C3C-C4C	5.84	1.51	1.42
26	E1	202	PEB	C3C-C4C	5.84	1.51	1.42
26	cA	202	PEB	C3B-C2B	5.84	1.49	1.36
26	kE	203	PEB	C3B-C2B	5.84	1.49	1.36
26	VJ	202	PEB	C3C-C4C	5.84	1.51	1.42
26	UF	202	PEB	C3C-C4C	5.84	1.51	1.42
26	Z1	201	PEB	C3B-C2B	5.84	1.49	1.36
26	w4	204	PEB	C3C-C4C	5.83	1.51	1.42
28	FI	1001	CYC	C3B-C2B	5.83	1.49	1.36
26	LG	202	PEB	C3C-C4C	5.83	1.51	1.42
26	YF	202	PEB	C3C-C4C	5.83	1.51	1.42
26	K9	202	PEB	C3B-C2B	5.83	1.49	1.36
26	y1	203	PEB	C3C-C4C	5.83	1.51	1.42
26	TJ	201	PEB	C3B-C2B	5.83	1.49	1.36
26	S7	202	PEB	C3C-C4C	5.83	1.51	1.42
26	bF	202	PEB	C3B-C2B	5.83	1.49	1.36
26	s1	202	PEB	C3C-C4C	5.83	1.51	1.42
27	AF	304	PUB	C2C-C3C	5.83	1.49	1.36
26	FE	202	PEB	C3C-C4C	5.82	1.51	1.42
26	DE	203	PEB	C3C-C4C	5.82	1.51	1.42
26	iF	202	PEB	C3B-C2B	5.82	1.49	1.36
26	uE	201	PEB	C3B-C2B	5.82	1.49	1.36
26	BD	201	PEB	C3B-C2B	5.82	1.49	1.36
26	c8	201	PEB	C3B-C2B	5.82	1.49	1.36
28	oH	1001	CYC	C3B-C2B	5.82	1.49	1.36
26	V9	203	PEB	C3B-C2B	5.82	1.49	1.36
26	aF	202	PEB	C3C-C4C	5.81	1.51	1.42
26	nG	201	PEB	C3B-C2B	5.81	1.49	1.36
26	21	405	PEB	C3B-C2B	5.81	1.49	1.36
26	A9	304	PEB	C3B-C2B	5.81	1.49	1.36
26	h1	201	PEB	C3B-C2B	5.81	1.49	1.36
26	KJ	202	PEB	C3B-C2B	5.81	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D1	201	PEB	C3C-C4C	5.81	1.51	1.42
26	hB	203	PEB	C3C-C4C	5.81	1.51	1.42
26	24	405	PEB	C3B-C2B	5.81	1.49	1.36
26	IE	201	PEB	C3C-C4C	5.81	1.51	1.42
26	11	202	PEB	C3B-C2B	5.81	1.49	1.36
26	iI	203	PEB	C3B-C2B	5.81	1.49	1.36
26	WG	202	PEB	C3C-C4C	5.80	1.51	1.42
28	QH	1001	CYC	CHB-C1B	5.80	1.51	1.38
26	g1	202	PEB	C3B-C2B	5.80	1.49	1.36
26	11	203	PEB	C3C-C4C	5.80	1.51	1.42
26	YD	303	PEB	C3B-C2B	5.80	1.49	1.36
26	hG	202	PEB	C3C-C4C	5.80	1.51	1.42
26	oG	201	PEB	C3B-C2B	5.80	1.49	1.36
26	M4	401	PEB	C3B-C2B	5.80	1.49	1.36
26	AJ	303	PEB	C3B-C2B	5.79	1.49	1.36
26	Y7	202	PEB	C3C-C4C	5.79	1.51	1.42
26	nE	201	PEB	C3C-C4C	5.79	1.51	1.42
26	a1	203	PEB	C3C-C4C	5.79	1.51	1.42
26	Q9	202	PEB	C3C-C4C	5.79	1.51	1.42
26	iF	202	PEB	C3C-C4C	5.79	1.51	1.42
26	i2	203	PEB	C3B-C2B	5.79	1.49	1.36
26	l7	203	PEB	C3B-C2B	5.79	1.49	1.36
28	K7	1001	CYC	C3B-C2B	5.79	1.49	1.36
26	cA	201	PEB	C3B-C2B	5.78	1.49	1.36
26	AF	301	PEB	C3C-C4C	5.78	1.51	1.42
26	YE	201	PEB	C3B-C2B	5.78	1.49	1.36
28	K6	202	CYC	C3B-C2B	5.78	1.49	1.36
26	hF	202	PEB	C3B-C2B	5.78	1.49	1.36
26	JJ	201	PEB	C3B-C2B	5.78	1.49	1.36
26	F9	202	PEB	C3B-C2B	5.78	1.49	1.36
27	21	402	PUB	C2C-C3C	5.77	1.49	1.36
26	aB	202	PEB	C3B-C2B	5.77	1.49	1.36
26	GG	201	PEB	C3B-C2B	5.77	1.49	1.36
26	b1	501	PEB	C3B-C2B	5.77	1.49	1.36
28	N2	1001	CYC	C2A-C3A	5.77	1.49	1.36
26	N9	202	PEB	C3C-C4C	5.77	1.51	1.42
26	WG	203	PEB	C3B-C2B	5.77	1.49	1.36
26	kG	201	PEB	C3C-C4C	5.77	1.51	1.42
26	k2	202	PEB	C3B-C2B	5.77	1.49	1.36
28	MH	1001	CYC	C3B-C2B	5.77	1.49	1.36
26	k2	203	PEB	C3B-C2B	5.76	1.49	1.36
26	Y9	202	PEB	C3B-C2B	5.76	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	xG	304	PEB	C3B-C2B	5.76	1.49	1.36
26	L1	203	PEB	C3C-C4C	5.76	1.51	1.42
26	mF	202	PEB	C3B-C2B	5.76	1.49	1.36
26	U9	202	PEB	C3C-C4C	5.76	1.51	1.42
26	O7	202	PEB	C3B-C2B	5.76	1.49	1.36
26	v1	202	PEB	C3B-C2B	5.76	1.49	1.36
26	a6	202	PEB	C3B-C2B	5.76	1.49	1.36
26	h1	202	PEB	C3C-C4C	5.76	1.51	1.42
28	E2	1001	CYC	C3B-C2B	5.76	1.49	1.36
28	I2	1001	CYC	C3B-C2B	5.76	1.49	1.36
28	EI	1001	CYC	C3B-C2B	5.76	1.49	1.36
28	II	1001	CYC	C3B-C2B	5.76	1.49	1.36
26	J9	201	PEB	C3B-C2B	5.75	1.49	1.36
26	ED	201	PEB	C3B-C2B	5.75	1.49	1.36
26	hA	203	PEB	C3C-C4C	5.75	1.51	1.42
27	A7	304	PUB	C2C-C3C	5.75	1.49	1.36
26	JD	203	PEB	C3B-C2B	5.75	1.49	1.36
28	sH	1001	CYC	CHB-C1B	5.75	1.51	1.38
28	G2	1001	CYC	C3B-C2B	5.75	1.49	1.36
26	f7	202	PEB	C3B-C2B	5.75	1.48	1.36
28	NI	1001	CYC	C2A-C3A	5.75	1.48	1.36
26	F9	203	PEB	C3C-C4C	5.75	1.51	1.42
26	AG	202	PEB	C3B-C2B	5.75	1.48	1.36
26	Y3	303	PEB	C3B-C2B	5.75	1.48	1.36
26	YF	201	PEB	C3C-C4C	5.74	1.51	1.42
26	OJ	201	PEB	C3B-C2B	5.74	1.48	1.36
26	24	404	PEB	C3B-C2B	5.74	1.48	1.36
28	LF	1001	CYC	CHB-C1B	5.74	1.51	1.38
26	s4	202	PEB	C3B-C2B	5.74	1.48	1.36
26	BC	202	PEB	C3B-C2B	5.74	1.48	1.36
26	C4	202	PEB	C3C-C4C	5.74	1.51	1.42
28	C6	1001	CYC	C3B-C2B	5.74	1.48	1.36
26	d8	201	PEB	C3B-C2B	5.73	1.48	1.36
26	21	401	PEB	C3B-C2B	5.73	1.48	1.36
26	eF	202	PEB	C3B-C2B	5.73	1.48	1.36
28	yH	1001	CYC	CHB-C1B	5.73	1.51	1.38
26	pG	202	PEB	C3C-C4C	5.73	1.51	1.42
28	WH	1001	CYC	CHB-C1B	5.73	1.51	1.38
28	KI	1001	CYC	C3B-C2B	5.73	1.48	1.36
26	a7	202	PEB	C3C-C4C	5.73	1.51	1.42
26	VJ	203	PEB	C3C-C4C	5.73	1.51	1.42
26	lA	201	PEB	C3C-C4C	5.73	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z1	201	PEB	C3C-C4C	5.73	1.51	1.42
26	S9	202	PEB	C3C-C4C	5.73	1.51	1.42
26	c1	202	PEB	C3B-C2B	5.73	1.48	1.36
26	A9	303	PEB	C3B-C2B	5.72	1.48	1.36
26	CE	201	PEB	C3B-C2B	5.72	1.48	1.36
26	21	401	PEB	C3C-C4C	5.72	1.51	1.42
26	uG	203	PEB	C3C-C4C	5.72	1.51	1.42
26	C5	203	PEB	C3B-C2B	5.72	1.48	1.36
26	JD	201	PEB	C3C-C4C	5.72	1.51	1.42
26	YG	201	PEB	C3C-C4C	5.72	1.51	1.42
26	V9	202	PEB	C3B-C2B	5.72	1.48	1.36
26	lF	201	PEB	C3C-C4C	5.72	1.51	1.42
26	j7	202	PEB	C3B-C2B	5.72	1.48	1.36
26	FJ	202	PEB	C3B-C2B	5.72	1.48	1.36
26	TF	202	PEB	C3C-C4C	5.72	1.51	1.42
26	k8	201	PEB	C3B-C2B	5.72	1.48	1.36
26	g4	202	PEB	C3B-C2B	5.72	1.48	1.36
28	N2	1001	CYC	C3B-C2B	5.72	1.48	1.36
26	A7	305	PEB	C3B-C2B	5.71	1.48	1.36
28	GI	1001	CYC	C3B-C2B	5.71	1.48	1.36
26	DE	202	PEB	C3B-C2B	5.71	1.48	1.36
26	KE	202	PEB	C3C-C4C	5.71	1.51	1.42
26	VJ	201	PEB	C3C-C4C	5.71	1.51	1.42
26	b7	202	PEB	C3B-C2B	5.71	1.48	1.36
26	H4	203	PEB	C3B-C2B	5.71	1.48	1.36
26	kA	201	PEB	C3B-C2B	5.71	1.48	1.36
26	AF	301	PEB	C3B-C2B	5.71	1.48	1.36
28	J7	1003	CYC	C3B-C2B	5.71	1.48	1.36
28	KB	202	CYC	C3B-C2B	5.71	1.48	1.36
26	E9	202	PEB	C3C-C4C	5.71	1.51	1.42
26	n4	202	PEB	C3C-C4C	5.70	1.51	1.42
26	DA	201	PEB	C3B-C2B	5.70	1.48	1.36
26	jG	201	PEB	C3B-C2B	5.70	1.48	1.36
26	FG	202	PEB	C3C-C4C	5.70	1.51	1.42
26	g4	203	PEB	C3B-C2B	5.70	1.48	1.36
26	AD	202	PEB	C3B-C2B	5.70	1.48	1.36
26	gG	202	PEB	C3C-C4C	5.70	1.51	1.42
26	h7	202	PEB	C3B-C2B	5.70	1.48	1.36
28	CB	1001	CYC	C3B-C2B	5.70	1.48	1.36
28	NI	1001	CYC	C3B-C2B	5.70	1.48	1.36
26	LJ	203	PEB	C3C-C4C	5.70	1.50	1.42
26	fB	203	PEB	C3B-C2B	5.70	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	w1	201	PEB	C3B-C2B	5.70	1.48	1.36
26	A2	304	PEB	C3B-C2B	5.70	1.48	1.36
26	e6	203	PEB	C3B-C2B	5.70	1.48	1.36
26	sE	202	PEB	C3B-C2B	5.70	1.48	1.36
28	K2	1001	CYC	C3B-C2B	5.70	1.48	1.36
28	mH	1001	CYC	CHB-C1B	5.70	1.51	1.38
26	VE	202	PEB	C3C-C4C	5.69	1.50	1.42
26	q4	201	PEB	C3B-C2B	5.69	1.48	1.36
26	CC	203	PEB	C3C-C4C	5.69	1.50	1.42
28	D7	1001	CYC	C3B-C2B	5.69	1.48	1.36
26	g1	203	PEB	C3B-C2B	5.69	1.48	1.36
26	WE	203	PEB	C3B-C2B	5.69	1.48	1.36
26	b4	501	PEB	C3B-C2B	5.69	1.48	1.36
26	aE	203	PEB	C3B-C2B	5.69	1.48	1.36
26	xE	303	PEB	C3B-C2B	5.69	1.48	1.36
26	FA	201	PEB	C3C-C4C	5.69	1.50	1.42
26	l1	201	PEB	C3B-C2B	5.69	1.48	1.36
26	WD	202	PEB	C3B-C2B	5.69	1.48	1.36
26	LE	201	PEB	C3C-C4C	5.69	1.50	1.42
28	B6	1001	CYC	C3B-C2B	5.68	1.48	1.36
27	A2	302	PUB	C2C-C3C	5.68	1.48	1.36
26	mB	201	PEB	C3B-C2B	5.68	1.48	1.36
26	RF	202	PEB	C3B-C2B	5.68	1.48	1.36
26	ME	203	PEB	C3B-C2B	5.68	1.48	1.36
26	EJ	202	PEB	C3C-C4C	5.68	1.50	1.42
28	D6	1001	CYC	C3B-C2B	5.68	1.48	1.36
26	V9	202	PEB	C3C-C4C	5.68	1.50	1.42
26	uG	202	PEB	C3B-C2B	5.68	1.48	1.36
26	h6	201	PEB	C3B-C2B	5.68	1.48	1.36
28	JF	1003	CYC	C3B-C2B	5.68	1.48	1.36
26	O7	201	PEB	C3B-C2B	5.68	1.48	1.36
26	AC	202	PEB	C3B-C2B	5.68	1.48	1.36
26	eG	203	PEB	C3C-C4C	5.68	1.50	1.42
28	E6	1001	CYC	C3B-C2B	5.68	1.48	1.36
26	VF	203	PEB	C3C-C4C	5.67	1.50	1.42
28	DB	1001	CYC	C3B-C2B	5.67	1.48	1.36
26	X4	203	PEB	C3B-C2B	5.67	1.48	1.36
26	DD	201	PEB	C3B-C2B	5.67	1.48	1.36
28	CI	1001	CYC	C3B-C2B	5.67	1.48	1.36
26	g6	202	PEB	C3C-C4C	5.67	1.50	1.42
26	AF	305	PEB	C3B-C2B	5.67	1.48	1.36
26	GC	203	PEB	C3C-C4C	5.67	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	HJ	201	PEB	C3B-C2B	5.67	1.48	1.36
26	VE	201	PEB	C3B-C2B	5.67	1.48	1.36
28	dH	1001	CYC	C2A-C3A	5.67	1.48	1.36
28	JH	1001	CYC	C3B-C2B	5.67	1.48	1.36
26	V7	202	PEB	C3B-C2B	5.67	1.48	1.36
26	YE	201	PEB	C3C-C4C	5.67	1.50	1.42
26	eG	202	PEB	C3C-C4C	5.66	1.50	1.42
26	l1	202	PEB	C3B-C2B	5.66	1.48	1.36
26	G6	1002	PEB	C3B-C2B	5.66	1.48	1.36
26	YE	202	PEB	C3B-C2B	5.66	1.48	1.36
26	Z8	201	PEB	C3C-C4C	5.66	1.50	1.42
26	24	401	PEB	C3C-C4C	5.66	1.50	1.42
26	TJ	202	PEB	C3C-C4C	5.66	1.50	1.42
28	B6	1002	CYC	C3B-C2B	5.66	1.48	1.36
26	E3	201	PEB	C3B-C2B	5.66	1.48	1.36
26	B1	203	PEB	C3C-C4C	5.66	1.50	1.42
26	nE	201	PEB	C3B-C2B	5.66	1.48	1.36
26	N4	202	PEB	C3B-C2B	5.66	1.48	1.36
26	AF	302	PEB	C3B-C2B	5.66	1.48	1.36
26	dB	204	PEB	C3B-C2B	5.66	1.48	1.36
26	iG	202	PEB	C3C-C4C	5.66	1.50	1.42
26	u4	202	PEB	C3B-C2B	5.66	1.48	1.36
26	LJ	202	PEB	C3B-C2B	5.66	1.48	1.36
26	VJ	201	PEB	C3B-C2B	5.66	1.48	1.36
26	T7	202	PEB	C3C-C4C	5.66	1.50	1.42
26	mF	201	PEB	C3C-C4C	5.66	1.50	1.42
28	jH	1001	CYC	CHB-C1B	5.66	1.51	1.38
26	bI	201	PEB	C3C-C4C	5.66	1.50	1.42
26	m7	202	PEB	C3B-C2B	5.66	1.48	1.36
27	Q8	201	PUB	C2B-C1B	5.65	1.50	1.42
26	YD	301	PEB	C3B-C2B	5.65	1.48	1.36
26	UE	203	PEB	C3B-C2B	5.65	1.48	1.36
28	DF	1001	CYC	C3B-C2B	5.65	1.48	1.36
28	mH	1001	CYC	C3B-C2B	5.65	1.48	1.36
26	D7	1002	PEB	C3B-C2B	5.65	1.48	1.36
28	EB	1001	CYC	C3B-C2B	5.65	1.48	1.36
28	CH	1001	CYC	C3B-C2B	5.65	1.48	1.36
26	F9	202	PEB	C3C-C4C	5.65	1.50	1.42
26	RA	201	PEB	C3B-C2B	5.65	1.48	1.36
26	XJ	201	PEB	C3B-C2B	5.65	1.48	1.36
26	eE	203	PEB	C3C-C4C	5.64	1.50	1.42
26	CC	202	PEB	C3B-C2B	5.64	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A5	201	PEB	C3B-C2B	5.64	1.48	1.36
28	BB	1001	CYC	C3B-C2B	5.64	1.48	1.36
26	c1	201	PEB	C3C-C4C	5.64	1.50	1.42
26	i7	202	PEB	C3B-C2B	5.64	1.48	1.36
26	WG	203	PEB	C3C-C4C	5.64	1.50	1.42
26	j7	203	PEB	C3B-C2B	5.64	1.48	1.36
26	GB	1002	PEB	C3B-C2B	5.64	1.48	1.36
26	jF	203	PEB	C3B-C2B	5.64	1.48	1.36
28	C2	1001	CYC	C3B-C2B	5.64	1.48	1.36
28	G6	1001	CYC	C3B-C2B	5.64	1.48	1.36
26	UF	203	PEB	C3C-C4C	5.64	1.50	1.42
26	PA	201	PEB	C3B-C2B	5.64	1.48	1.36
26	HE	202	PEB	C3C-C4C	5.64	1.50	1.42
26	F1	202	PEB	C3B-C2B	5.64	1.48	1.36
28	M2	1001	CYC	C3B-C2B	5.63	1.48	1.36
28	DF	1003	CYC	C3B-C2B	5.63	1.48	1.36
26	C5	201	PEB	C3B-C2B	5.63	1.48	1.36
26	X1	203	PEB	C3B-C2B	5.63	1.48	1.36
27	AI	302	PUB	C2C-C3C	5.63	1.48	1.36
26	OF	202	PEB	C3B-C2B	5.63	1.48	1.36
26	DD	203	PEB	C3B-C2B	5.63	1.48	1.36
26	NJ	202	PEB	C3C-C4C	5.63	1.50	1.42
26	U7	203	PEB	C3B-C2B	5.63	1.48	1.36
26	XJ	202	PEB	C3B-C2B	5.63	1.48	1.36
26	VJ	203	PEB	C3B-C2B	5.63	1.48	1.36
26	i8	201	PEB	C3B-C2B	5.63	1.48	1.36
26	R9	202	PEB	C3C-C4C	5.63	1.50	1.42
28	KF	1001	CYC	C3B-C2B	5.63	1.48	1.36
26	H9	201	PEB	C3B-C2B	5.62	1.48	1.36
26	iB	201	PEB	C3B-C2B	5.62	1.48	1.36
26	YG	202	PEB	C3B-C2B	5.62	1.48	1.36
26	c4	201	PEB	C3C-C4C	5.62	1.50	1.42
26	GG	202	PEB	C3C-C4C	5.62	1.50	1.42
26	KE	203	PEB	C3C-C4C	5.62	1.50	1.42
26	sG	202	PEB	C3B-C2B	5.62	1.48	1.36
26	P4	203	PEB	C3B-C2B	5.62	1.48	1.36
28	NB	1001	CYC	C3B-C2B	5.62	1.48	1.36
28	WH	1001	CYC	C3B-C2B	5.62	1.48	1.36
26	JC	201	PEB	C2A-C1A	-5.62	1.47	1.52
26	AD	201	PEB	C3B-C2B	5.62	1.48	1.36
26	C1	202	PEB	C3C-C4C	5.62	1.50	1.42
26	m6	202	PEB	C3C-C4C	5.62	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	oH	1001	CYC	CHB-C1B	5.62	1.51	1.38
26	C3	202	PEB	C3B-C2B	5.62	1.48	1.36
28	JH	1001	CYC	CHB-C1B	5.62	1.51	1.38
28	yH	1001	CYC	C3B-C2B	5.61	1.48	1.36
26	J3	201	PEB	C3C-C4C	5.61	1.50	1.42
26	d4	203	PEB	C3C-C4C	5.61	1.50	1.42
28	1H	1000	CYC	C2A-C3A	5.61	1.48	1.36
26	mE	203	PEB	C3C-C4C	5.61	1.50	1.42
26	m4	202	PEB	C3B-C2B	5.61	1.48	1.36
26	MG	203	PEB	C3B-C2B	5.61	1.48	1.36
26	t4	201	PEB	C3B-C2B	5.61	1.48	1.36
26	m4	202	PEB	C3C-C4C	5.61	1.50	1.42
26	w1	202	PEB	C3B-C2B	5.61	1.48	1.36
28	YH	1003	CYC	CHB-C1B	5.61	1.51	1.38
26	AI	304	PEB	C3B-C2B	5.61	1.48	1.36
26	xG	303	PEB	C3B-C2B	5.61	1.48	1.36
26	fF	202	PEB	C3C-C4C	5.61	1.50	1.42
26	gF	202	PEB	C3B-C2B	5.61	1.48	1.36
26	uE	203	PEB	C3C-C4C	5.61	1.50	1.42
26	kE	201	PEB	C3C-C4C	5.61	1.50	1.42
26	RF	202	PEB	C3C-C4C	5.61	1.50	1.42
26	i6	201	PEB	C3B-C2B	5.61	1.48	1.36
26	YG	203	PEB	C3B-C2B	5.61	1.48	1.36
26	pE	201	PEB	C3B-C2B	5.60	1.48	1.36
26	P8	201	PEB	C3B-C2B	5.60	1.48	1.36
28	G7	1001	CYC	C3B-C2B	5.60	1.48	1.36
26	W7	202	PEB	C3B-C2B	5.60	1.48	1.36
26	S7	201	PEB	C3B-C2B	5.60	1.48	1.36
26	m1	201	PEB	C3B-C2B	5.60	1.48	1.36
26	D8	201	PEB	C3B-C2B	5.60	1.48	1.36
28	I7	1001	CYC	C3B-C2B	5.60	1.48	1.36
26	Z7	202	PEB	C3C-C4C	5.60	1.50	1.42
26	P9	203	PEB	C3C-C4C	5.60	1.50	1.42
26	KD	201	PEB	C3C-C4C	5.60	1.50	1.42
26	jA	202	PEB	C3B-C2B	5.60	1.48	1.36
26	A3	202	PEB	C3B-C2B	5.60	1.48	1.36
26	f4	201	PEB	C3B-C2B	5.60	1.48	1.36
26	HF	1002	PEB	C3B-C2B	5.60	1.48	1.36
26	SE	201	PEB	C3B-C2B	5.60	1.48	1.36
26	q1	203	PEB	C3B-C2B	5.60	1.48	1.36
28	CF	1001	CYC	C3B-C2B	5.60	1.48	1.36
26	d4	202	PEB	C3B-C2B	5.60	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	fH	1001	CYC	CHB-C1B	5.60	1.51	1.38
26	D3	203	PEB	C3B-C2B	5.60	1.48	1.36
26	Z4	201	PEB	C3B-C2B	5.60	1.48	1.36
28	LF	1001	CYC	C3B-C2B	5.60	1.48	1.36
27	24	402	PUB	C2C-C3C	5.60	1.48	1.36
28	M6	1001	CYC	C3B-C2B	5.60	1.48	1.36
26	oE	201	PEB	C3C-C4C	5.59	1.50	1.42
28	gH	1001	CYC	CHB-C1B	5.59	1.51	1.38
26	cG	201	PEB	C3C-C4C	5.59	1.50	1.42
28	jH	1001	CYC	C3B-C2B	5.59	1.48	1.36
26	jF	201	PEB	C3C-C4C	5.59	1.50	1.42
26	21	404	PEB	C3B-C2B	5.59	1.48	1.36
28	GB	1001	CYC	C3B-C2B	5.59	1.48	1.36
26	YE	203	PEB	C3B-C2B	5.59	1.48	1.36
27	KD	203	PUB	C2C-C3C	5.59	1.48	1.36
28	HI	1001	CYC	C3B-C2B	5.59	1.48	1.36
26	k7	202	PEB	C3C-C4C	5.59	1.50	1.42
26	cI	202	PEB	C3B-C2B	5.59	1.48	1.36
26	m6	201	PEB	C3B-C2B	5.59	1.48	1.36
26	H7	1002	PEB	C3B-C2B	5.59	1.48	1.36
26	HG	202	PEB	C3C-C4C	5.59	1.50	1.42
26	RJ	201	PEB	C3B-C2B	5.59	1.48	1.36
26	gB	202	PEB	C3C-C4C	5.59	1.50	1.42
28	YH	1003	CYC	C3B-C2B	5.59	1.48	1.36
26	M1	401	PEB	C3B-C2B	5.59	1.48	1.36
26	ZF	203	PEB	C3B-C2B	5.59	1.48	1.36
26	Y7	201	PEB	C3C-C4C	5.59	1.50	1.42
26	A7	302	PEB	C3B-C2B	5.59	1.48	1.36
26	FD	203	PEB	C3B-C2B	5.59	1.48	1.36
26	l6	201	PEB	C3B-C2B	5.58	1.48	1.36
26	gA	201	PEB	C3B-C2B	5.58	1.48	1.36
26	GJ	201	PEB	C3C-C4C	5.58	1.50	1.42
26	g6	202	PEB	C3B-C2B	5.58	1.48	1.36
26	XJ	203	PEB	C3B-C2B	5.58	1.48	1.36
26	F8	201	PEB	C3C-C4C	5.58	1.50	1.42
26	R9	201	PEB	C3B-C2B	5.58	1.48	1.36
26	F1	201	PEB	C3B-C2B	5.58	1.48	1.36
26	rE	201	PEB	C3B-C2B	5.58	1.48	1.36
26	U7	202	PEB	C3C-C4C	5.58	1.50	1.42
26	m4	201	PEB	C3B-C2B	5.58	1.48	1.36
26	J8	201	PEB	C3B-C2B	5.58	1.48	1.36
26	f4	202	PEB	C3C-C4C	5.57	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	oE	203	PEB	C3B-C2B	5.57	1.48	1.36
26	L4	201	PEB	C3B-C2B	5.57	1.48	1.36
26	fA	202	PEB	C3B-C2B	5.57	1.48	1.36
26	f2	201	PEB	C3C-C4C	5.57	1.50	1.42
28	YH	1004	CYC	C2A-C3A	5.57	1.48	1.36
26	l4	203	PEB	C3C-C4C	5.57	1.50	1.42
26	sE	201	PEB	C3B-C2B	5.57	1.48	1.36
26	gE	202	PEB	C3C-C4C	5.57	1.50	1.42
28	YH	1004	CYC	CHB-C1B	5.57	1.51	1.38
26	B5	202	PEB	C3B-C2B	5.57	1.48	1.36
28	lH	1001	CYC	C3B-C2B	5.57	1.48	1.36
26	A7	301	PEB	C3C-C4C	5.57	1.50	1.42
26	h7	201	PEB	C3B-C2B	5.57	1.48	1.36
28	MI	1001	CYC	C3B-C2B	5.57	1.48	1.36
26	eF	202	PEB	C3C-C4C	5.57	1.50	1.42
26	U6	201	PEB	C3C-C4C	5.57	1.50	1.42
26	C4	202	PEB	C3B-C2B	5.57	1.48	1.36
26	CA	202	PEB	C3B-C2B	5.57	1.48	1.36
28	H2	1001	CYC	C3B-C2B	5.57	1.48	1.36
26	F3	203	PEB	C3B-C2B	5.57	1.48	1.36
26	l8	201	PEB	C3C-C4C	5.57	1.50	1.42
26	uE	202	PEB	C3C-C4C	5.57	1.50	1.42
26	x4	202	PEB	C3C-C4C	5.57	1.50	1.42
26	i7	202	PEB	C3C-C4C	5.56	1.50	1.42
26	L9	203	PEB	C3C-C4C	5.56	1.50	1.42
26	TJ	203	PEB	C3B-C2B	5.56	1.48	1.36
26	y4	203	PEB	C3B-C2B	5.56	1.48	1.36
26	SG	203	PEB	C3C-C4C	5.56	1.50	1.42
26	iA	201	PEB	C3B-C2B	5.56	1.48	1.36
28	iH	1001	CYC	C3B-C2B	5.56	1.48	1.36
26	kE	201	PEB	C3B-C2B	5.56	1.48	1.36
28	C7	1001	CYC	C3B-C2B	5.56	1.48	1.36
26	l4	201	PEB	C3B-C2B	5.56	1.48	1.36
26	zG	501	PEB	C3B-C2B	5.56	1.48	1.36
26	lF	202	PEB	C3B-C2B	5.56	1.48	1.36
28	eH	1001	CYC	C3B-C2B	5.56	1.48	1.36
26	j8	202	PEB	C3B-C2B	5.56	1.48	1.36
28	QH	1001	CYC	C3B-C2B	5.56	1.48	1.36
28	VH	1001	CYC	C2A-C3A	5.56	1.48	1.36
26	Z7	203	PEB	C3B-C2B	5.56	1.48	1.36
26	oE	202	PEB	C3B-C2B	5.56	1.48	1.36
28	eH	1001	CYC	C2A-C3A	5.56	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BC	203	PEB	C3B-C2B	5.56	1.48	1.36
28	CH	1001	CYC	C2A-C3A	5.56	1.48	1.36
26	l1	202	PEB	C3C-C4C	5.56	1.50	1.42
28	mH	1001	CYC	C2A-C3A	5.56	1.48	1.36
28	sH	1001	CYC	C3B-C2B	5.56	1.48	1.36
26	XG	202	PEB	C3B-C2B	5.56	1.48	1.36
26	lG	201	PEB	C3B-C2B	5.56	1.48	1.36
26	J2	1002	PEB	C3C-C4C	5.56	1.50	1.42
26	q4	203	PEB	C3B-C2B	5.55	1.48	1.36
26	mB	202	PEB	C3C-C4C	5.55	1.50	1.42
26	s1	203	PEB	C3B-C2B	5.55	1.48	1.36
28	vH	1001	CYC	CHB-C1B	5.55	1.51	1.38
28	lH	1001	CYC	CHB-C1B	5.55	1.51	1.38
26	gE	203	PEB	C3B-C2B	5.55	1.48	1.36
26	pG	201	PEB	C3B-C2B	5.55	1.48	1.36
28	H2	1001	CYC	C2A-C3A	5.55	1.48	1.36
28	HI	1001	CYC	C2A-C3A	5.55	1.48	1.36
26	v4	202	PEB	C3B-C2B	5.55	1.48	1.36
28	kH	1001	CYC	C3B-C2B	5.55	1.48	1.36
26	HD	201	PEB	C3B-C2B	5.55	1.48	1.36
26	HA	202	PEB	C3B-C2B	5.55	1.48	1.36
26	wE	302	PEB	C3B-C2B	5.55	1.48	1.36
26	R4	203	PEB	C3B-C2B	5.55	1.48	1.36
26	SF	202	PEB	C3C-C4C	5.55	1.50	1.42
26	gB	202	PEB	C3B-C2B	5.55	1.48	1.36
26	SB	203	PEB	C3B-C2B	5.55	1.48	1.36
26	H4	201	PEB	C3B-C2B	5.55	1.48	1.36
28	MB	1001	CYC	C3B-C2B	5.54	1.48	1.36
26	RJ	202	PEB	C3C-C4C	5.54	1.50	1.42
26	DG	202	PEB	C3B-C2B	5.54	1.48	1.36
26	RJ	202	PEB	C3B-C2B	5.54	1.48	1.36
28	hH	1001	CYC	CHB-C1B	5.54	1.51	1.38
26	AC	203	PEB	C3B-C2B	5.54	1.48	1.36
28	L2	1001	CYC	C3B-C2B	5.54	1.48	1.36
26	N9	204	PEB	C3C-C4C	5.54	1.50	1.42
26	BD	203	PEB	C3C-C4C	5.54	1.50	1.42
26	R1	203	PEB	C3B-C2B	5.54	1.48	1.36
26	AE	202	PEB	C3B-C2B	5.54	1.48	1.36
26	y4	201	PEB	C3C-C4C	5.54	1.50	1.42
26	s4	203	PEB	C3B-C2B	5.54	1.48	1.36
26	tE	201	PEB	C3B-C2B	5.54	1.48	1.36
26	nG	201	PEB	C3C-C4C	5.54	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CG	201	PEB	C3B-C2B	5.54	1.48	1.36
26	u4	203	PEB	C3B-C2B	5.54	1.48	1.36
26	wG	302	PEB	C3B-C2B	5.54	1.48	1.36
26	B5	203	PEB	C3B-C2B	5.54	1.48	1.36
26	hF	201	PEB	C3B-C2B	5.54	1.48	1.36
28	VH	1001	CYC	CHB-C1B	5.54	1.51	1.38
26	A8	301	PEB	C3B-C2B	5.54	1.48	1.36
28	qH	1001	CYC	C3B-C2B	5.54	1.48	1.36
26	B4	203	PEB	C3C-C4C	5.53	1.50	1.42
26	mG	202	PEB	C3C-C4C	5.53	1.50	1.42
26	aF	202	PEB	C3B-C2B	5.53	1.48	1.36
26	G8	203	PEB	C3B-C2B	5.53	1.48	1.36
26	vE	201	PEB	C3B-C2B	5.53	1.48	1.36
26	T1	203	PEB	C3C-C4C	5.53	1.50	1.42
26	R9	202	PEB	C3B-C2B	5.53	1.48	1.36
26	mE	203	PEB	C3B-C2B	5.53	1.48	1.36
28	YH	1002	CYC	C2A-C3A	5.53	1.48	1.36
26	MG	202	PEB	C3C-C4C	5.53	1.50	1.42
28	FF	1001	CYC	C3B-C2B	5.53	1.48	1.36
26	DD	202	PEB	C3B-C2B	5.53	1.48	1.36
26	O9	201	PEB	C3B-C2B	5.53	1.48	1.36
26	aE	203	PEB	C3C-C4C	5.53	1.50	1.42
26	A1	201	PEB	C3B-C2B	5.53	1.48	1.36
26	e6	202	PEB	C3B-C2B	5.53	1.48	1.36
26	vE	202	PEB	C3C-C4C	5.53	1.50	1.42
28	YH	1001	CYC	C3B-C2B	5.53	1.48	1.36
26	H8	202	PEB	C3B-C2B	5.52	1.48	1.36
26	rG	201	PEB	C3B-C2B	5.52	1.48	1.36
26	F1	203	PEB	C3B-C2B	5.52	1.48	1.36
26	OE	202	PEB	C3C-C4C	5.52	1.50	1.42
26	jA	201	PEB	C3B-C2B	5.52	1.48	1.36
28	L7	1001	CYC	C3B-C2B	5.52	1.48	1.36
26	CD	201	PEB	C3C-C4C	5.52	1.50	1.42
26	kF	202	PEB	C3C-C4C	5.52	1.50	1.42
26	kG	202	PEB	C3B-C2B	5.52	1.48	1.36
26	mA	201	PEB	C3C-C4C	5.52	1.50	1.42
26	UB	201	PEB	C3C-C4C	5.52	1.50	1.42
26	JA	201	PEB	C3B-C2B	5.52	1.48	1.36
28	CH	1001	CYC	CHB-C1B	5.52	1.51	1.38
26	P6	201	PEB	C3C-C4C	5.52	1.50	1.42
26	f2	202	PEB	C3B-C2B	5.52	1.48	1.36
26	a8	201	PEB	C3B-C2B	5.52	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y9	201	PEB	C3B-C2B	5.52	1.48	1.36
28	hH	1001	CYC	C2A-C3A	5.52	1.48	1.36
26	zE	501	PEB	C3C-C4C	5.52	1.50	1.42
26	qG	203	PEB	C3C-C4C	5.52	1.50	1.42
26	fI	201	PEB	C3C-C4C	5.52	1.50	1.42
26	T7	201	PEB	C3B-C2B	5.52	1.48	1.36
26	R8	201	PEB	C3B-C2B	5.52	1.48	1.36
26	c1	203	PEB	C3B-C2B	5.52	1.48	1.36
26	F1	203	PEB	C3C-C4C	5.52	1.50	1.42
26	PA	201	PEB	C3C-C4C	5.52	1.50	1.42
26	m7	201	PEB	C3C-C4C	5.51	1.50	1.42
26	B3	202	PEB	C3B-C2B	5.51	1.48	1.36
26	D4	203	PEB	C3B-C2B	5.51	1.48	1.36
26	c4	203	PEB	C3B-C2B	5.51	1.48	1.36
26	c2	202	PEB	C3B-C2B	5.51	1.48	1.36
26	SG	201	PEB	C3B-C2B	5.51	1.48	1.36
26	m1	202	PEB	C3B-C2B	5.51	1.48	1.36
26	y1	201	PEB	C3C-C4C	5.51	1.50	1.42
26	D1	203	PEB	C3B-C2B	5.51	1.48	1.36
26	UF	203	PEB	C3B-C2B	5.51	1.48	1.36
28	JI	1001	CYC	C3B-C2B	5.51	1.48	1.36
26	a4	201	PEB	C3B-C2B	5.51	1.48	1.36
26	X8	201	PEB	C3B-C2B	5.51	1.48	1.36
26	L1	203	PEB	C3B-C2B	5.51	1.48	1.36
26	hG	201	PEB	C3B-C2B	5.51	1.48	1.36
26	B3	201	PEB	C3B-C2B	5.51	1.48	1.36
26	h4	203	PEB	C3C-C4C	5.51	1.50	1.42
26	X9	203	PEB	C3B-C2B	5.51	1.48	1.36
26	lB	201	PEB	C3B-C2B	5.51	1.48	1.36
26	P8	201	PEB	C3C-C4C	5.51	1.50	1.42
26	GA	202	PEB	C3B-C2B	5.51	1.48	1.36
26	X9	202	PEB	C3B-C2B	5.51	1.48	1.36
28	pH	1001	CYC	CHB-C1B	5.51	1.51	1.38
26	f6	203	PEB	C3B-C2B	5.51	1.48	1.36
28	tH	1001	CYC	C3B-C2B	5.51	1.48	1.36
26	C3	202	PEB	C3C-C4C	5.50	1.50	1.42
26	iB	202	PEB	C3B-C2B	5.50	1.48	1.36
26	WF	202	PEB	C3B-C2B	5.50	1.48	1.36
28	GI	1001	CYC	C2A-C3A	5.50	1.48	1.36
26	WF	201	PEB	C3B-C2B	5.50	1.48	1.36
26	L4	203	PEB	C3C-C4C	5.50	1.50	1.42
26	AA	301	PEB	C3B-C2B	5.50	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m1	202	PEB	C3C-C4C	5.50	1.50	1.42
28	TH	1001	CYC	CHB-C1B	5.50	1.51	1.38
26	i4	202	PEB	C3B-C2B	5.50	1.48	1.36
26	dE	201	PEB	C3B-C2B	5.50	1.48	1.36
28	F6	1001	CYC	C2A-C3A	5.50	1.48	1.36
26	WE	203	PEB	C3C-C4C	5.50	1.50	1.42
28	E7	1001	CYC	C3B-C2B	5.50	1.48	1.36
28	VH	1001	CYC	C3B-C2B	5.50	1.48	1.36
26	R9	203	PEB	C3C-C4C	5.50	1.50	1.42
26	PJ	203	PEB	C3C-C4C	5.50	1.50	1.42
26	NJ	203	PEB	C3B-C2B	5.50	1.48	1.36
28	YH	1002	CYC	CHB-C1B	5.50	1.51	1.38
26	T9	202	PEB	C3C-C4C	5.50	1.50	1.42
26	h6	203	PEB	C3B-C2B	5.50	1.48	1.36
26	W7	203	PEB	C3B-C2B	5.50	1.48	1.36
26	SE	202	PEB	C3C-C4C	5.50	1.50	1.42
26	fF	203	PEB	C3B-C2B	5.50	1.48	1.36
26	tG	201	PEB	C3B-C2B	5.50	1.48	1.36
26	NJ	203	PEB	C3C-C4C	5.50	1.50	1.42
26	EA	201	PEB	C3B-C2B	5.50	1.48	1.36
28	MH	1001	CYC	CHB-C1B	5.50	1.51	1.38
26	a1	201	PEB	C3B-C2B	5.50	1.48	1.36
26	jE	201	PEB	C3B-C2B	5.50	1.48	1.36
26	DF	1002	PEB	C3B-C2B	5.50	1.48	1.36
28	IH	1001	CYC	C3B-C2B	5.50	1.48	1.36
26	JD	203	PEB	C3C-C4C	5.50	1.50	1.42
26	W7	201	PEB	C3B-C2B	5.49	1.48	1.36
28	nH	1001	CYC	C2A-C3A	5.49	1.48	1.36
26	OG	202	PEB	C3C-C4C	5.49	1.50	1.42
26	y4	202	PEB	C3C-C4C	5.49	1.50	1.42
26	cG	202	PEB	C3C-C4C	5.49	1.50	1.42
26	K3	201	PEB	C3B-C2B	5.49	1.48	1.36
26	GE	201	PEB	C3B-C2B	5.49	1.48	1.36
26	L9	202	PEB	C3B-C2B	5.49	1.48	1.36
26	ME	202	PEB	C3C-C4C	5.49	1.50	1.42
26	EG	201	PEB	C3C-C4C	5.49	1.50	1.42
26	B3	203	PEB	C3B-C2B	5.49	1.48	1.36
26	N9	204	PEB	C3B-C2B	5.49	1.48	1.36
26	f7	203	PEB	C3B-C2B	5.49	1.48	1.36
27	K4	203	PUB	C2C-C3C	5.49	1.48	1.36
28	IF	1001	CYC	C3B-C2B	5.49	1.48	1.36
28	lH	1001	CYC	C2A-C3A	5.49	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J1	203	PEB	C3B-C2B	5.49	1.48	1.36
26	L1	201	PEB	C3B-C2B	5.49	1.48	1.36
27	AF	303	PUB	C2C-C3C	5.49	1.48	1.36
28	OH	1001	CYC	C3B-C2B	5.49	1.48	1.36
26	T9	201	PEB	C3B-C2B	5.49	1.48	1.36
26	zE	501	PEB	C3B-C2B	5.49	1.48	1.36
28	LI	1001	CYC	C3B-C2B	5.49	1.48	1.36
26	b2	201	PEB	C3C-C4C	5.49	1.50	1.42
26	HF	1002	PEB	C3C-C4C	5.49	1.50	1.42
26	iA	202	PEB	C3B-C2B	5.49	1.48	1.36
26	KJ	201	PEB	C3B-C2B	5.49	1.48	1.36
28	iH	1001	CYC	C2A-C3A	5.49	1.48	1.36
26	cA	201	PEB	C3C-C4C	5.49	1.50	1.42
27	K3	203	PUB	C2C-C3C	5.49	1.48	1.36
26	G8	202	PEB	C3B-C2B	5.48	1.48	1.36
26	N1	202	PEB	C3B-C2B	5.48	1.48	1.36
26	f7	201	PEB	C3B-C2B	5.48	1.48	1.36
26	V6	202	PEB	C3B-C2B	5.48	1.48	1.36
28	kH	1001	CYC	C2A-C3A	5.48	1.48	1.36
26	H1	201	PEB	C3B-C2B	5.48	1.48	1.36
26	qG	201	PEB	C3B-C2B	5.48	1.48	1.36
28	NH	1001	CYC	C2A-C3A	5.48	1.48	1.36
26	eE	202	PEB	C3C-C4C	5.48	1.50	1.42
26	KG	203	PEB	C3C-C4C	5.48	1.50	1.42
26	XA	201	PEB	C3B-C2B	5.48	1.48	1.36
26	eE	201	PEB	C3B-C2B	5.48	1.48	1.36
26	mE	202	PEB	C3C-C4C	5.48	1.50	1.42
26	PB	201	PEB	C3C-C4C	5.48	1.50	1.42
26	M1	403	PEB	C3B-C2B	5.48	1.48	1.36
26	B5	201	PEB	C3B-C2B	5.48	1.48	1.36
26	JI	1002	PEB	C3C-C4C	5.48	1.50	1.42
26	BC	201	PEB	C3B-C2B	5.48	1.48	1.36
26	VG	202	PEB	C3C-C4C	5.48	1.50	1.42
26	D1	201	PEB	C3B-C2B	5.48	1.48	1.36
27	wE	304	PUB	C2C-C3C	5.48	1.48	1.36
26	C8	202	PEB	C3B-C2B	5.48	1.48	1.36
26	g8	201	PEB	C3B-C2B	5.48	1.48	1.36
27	QA	201	PUB	C2C-C3C	5.48	1.48	1.36
26	V7	202	PEB	C3C-C4C	5.48	1.50	1.42
28	YH	1001	CYC	CHB-C1B	5.48	1.51	1.38
26	L4	203	PEB	C3B-C2B	5.48	1.48	1.36
26	DA	201	PEB	C3C-C4C	5.48	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X9	203	PEB	C3C-C4C	5.47	1.50	1.42
26	pG	202	PEB	C3B-C2B	5.47	1.48	1.36
28	YH	1002	CYC	C3B-C2B	5.47	1.48	1.36
26	AE	202	PEB	C3C-C4C	5.47	1.50	1.42
28	YH	1004	CYC	C3B-C2B	5.47	1.48	1.36
26	S7	202	PEB	C3B-C2B	5.47	1.48	1.36
26	HD	203	PEB	C3B-C2B	5.47	1.48	1.36
26	24	401	PEB	C3B-C2B	5.47	1.48	1.36
28	FB	1001	CYC	C2A-C3A	5.47	1.48	1.36
26	J8	202	PEB	C3B-C2B	5.47	1.48	1.36
26	lE	202	PEB	C3B-C2B	5.47	1.48	1.36
26	bI	202	PEB	C3B-C2B	5.47	1.48	1.36
26	H3	203	PEB	C3B-C2B	5.47	1.48	1.36
28	NF	1001	CYC	C2A-C3A	5.47	1.48	1.36
28	hH	1001	CYC	C3B-C2B	5.47	1.48	1.36
26	n1	201	PEB	C3C-C4C	5.47	1.50	1.42
26	vG	202	PEB	C3C-C4C	5.47	1.50	1.42
26	J3	203	PEB	C3C-C4C	5.47	1.50	1.42
26	i8	202	PEB	C3B-C2B	5.47	1.48	1.36
26	e1	201	PEB	C3B-C2B	5.47	1.48	1.36
26	T4	203	PEB	C3B-C2B	5.47	1.48	1.36
26	QF	202	PEB	C3B-C2B	5.47	1.48	1.36
26	V1	203	PEB	C3B-C2B	5.47	1.48	1.36
26	y1	203	PEB	C3B-C2B	5.47	1.48	1.36
26	kI	202	PEB	C3B-C2B	5.47	1.48	1.36
26	d1	201	PEB	C3C-C4C	5.47	1.50	1.42
26	a1	203	PEB	C3B-C2B	5.47	1.48	1.36
26	S6	203	PEB	C3B-C2B	5.47	1.48	1.36
26	Y6	202	PEB	C3B-C2B	5.47	1.48	1.36
26	iG	203	PEB	C3C-C4C	5.47	1.50	1.42
27	QA	201	PUB	C2B-C1B	5.47	1.50	1.42
26	l7	202	PEB	C3B-C2B	5.46	1.48	1.36
26	GE	202	PEB	C3C-C4C	5.46	1.50	1.42
26	oG	202	PEB	C3B-C2B	5.46	1.48	1.36
26	Q7	202	PEB	C3B-C2B	5.46	1.48	1.36
26	J1	203	PEB	C3C-C4C	5.46	1.50	1.42
26	Z7	203	PEB	C3C-C4C	5.46	1.50	1.42
26	n4	201	PEB	C3B-C2B	5.46	1.48	1.36
26	CE	202	PEB	C3C-C4C	5.46	1.50	1.42
26	cE	202	PEB	C3B-C2B	5.46	1.48	1.36
26	n4	202	PEB	C3B-C2B	5.46	1.48	1.36
26	i6	202	PEB	C3B-C2B	5.46	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T9	203	PEB	C3B-C2B	5.46	1.48	1.36
26	H9	203	PEB	C3B-C2B	5.46	1.48	1.36
26	jB	202	PEB	C3B-C2B	5.46	1.48	1.36
26	N9	203	PEB	C3C-C4C	5.46	1.50	1.42
26	fF	201	PEB	C3B-C2B	5.46	1.48	1.36
28	GH	1001	CYC	C2A-C3A	5.46	1.48	1.36
28	OH	1001	CYC	C2A-C3A	5.46	1.48	1.36
26	fE	201	PEB	C3B-C2B	5.46	1.48	1.36
26	iG	203	PEB	C3B-C2B	5.46	1.48	1.36
26	j6	202	PEB	C3B-C2B	5.46	1.48	1.36
26	JE	201	PEB	C3B-C2B	5.46	1.48	1.36
26	J9	202	PEB	C3B-C2B	5.46	1.48	1.36
26	XD	203	PEB	C3B-C2B	5.46	1.48	1.36
26	BD	202	PEB	C3B-C2B	5.46	1.48	1.36
26	AE	201	PEB	C3C-C4C	5.45	1.50	1.42
26	gE	202	PEB	C3B-C2B	5.45	1.48	1.36
26	j7	201	PEB	C3C-C4C	5.45	1.50	1.42
26	Q8	203	PEB	C3C-C4C	5.45	1.50	1.42
26	V9	201	PEB	C3B-C2B	5.45	1.48	1.36
26	vG	201	PEB	C3B-C2B	5.45	1.48	1.36
26	G9	201	PEB	C3C-C4C	5.45	1.50	1.42
26	M4	402	PEB	C3B-C2B	5.45	1.48	1.36
26	Q7	203	PEB	C3B-C2B	5.45	1.48	1.36
26	RA	201	PEB	C3C-C4C	5.45	1.50	1.42
26	aA	201	PEB	C3B-C2B	5.45	1.48	1.36
26	JD	201	PEB	C3B-C2B	5.45	1.48	1.36
26	kG	203	PEB	C3B-C2B	5.45	1.48	1.36
26	gF	201	PEB	C3C-C4C	5.45	1.50	1.42
28	qH	1001	CYC	C2A-C3A	5.45	1.48	1.36
26	g8	202	PEB	C3B-C2B	5.45	1.48	1.36
26	sG	201	PEB	C3C-C4C	5.45	1.50	1.42
26	N9	203	PEB	C3B-C2B	5.45	1.48	1.36
26	I4	202	PEB	C3C-C4C	5.45	1.50	1.42
26	i1	203	PEB	C3B-C2B	5.45	1.48	1.36
26	TI	202	PEB	C3B-C2B	5.45	1.48	1.36
28	gH	1001	CYC	C2A-C3A	5.45	1.48	1.36
26	q1	202	PEB	C3B-C2B	5.45	1.48	1.36
26	E8	201	PEB	C3B-C2B	5.45	1.48	1.36
26	A2	305	PEB	C3B-C2B	5.45	1.48	1.36
26	D3	202	PEB	C3B-C2B	5.45	1.48	1.36
26	iB	202	PEB	C3C-C4C	5.45	1.50	1.42
26	A4	202	PEB	C3C-C4C	5.45	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F4	201	PEB	C3C-C4C	5.45	1.50	1.42
26	AB	301	PEB	C3B-C2B	5.45	1.48	1.36
26	dA	201	PEB	C3B-C2B	5.45	1.48	1.36
26	OJ	201	PEB	C3C-C4C	5.45	1.50	1.42
26	f4	202	PEB	C3B-C2B	5.45	1.48	1.36
26	VJ	202	PEB	C3B-C2B	5.45	1.48	1.36
26	T4	203	PEB	C3C-C4C	5.44	1.50	1.42
26	oG	201	PEB	C3C-C4C	5.44	1.50	1.42
26	S8	201	PEB	C3B-C2B	5.44	1.48	1.36
28	EH	1001	CYC	CHB-C1B	5.44	1.51	1.38
28	1H	1000	CYC	CHB-C1B	5.44	1.51	1.38
26	JD	202	PEB	C3B-C2B	5.44	1.48	1.36
26	YJ	202	PEB	C3B-C2B	5.44	1.48	1.36
26	w4	201	PEB	C3B-C2B	5.44	1.48	1.36
28	F7	1001	CYC	C3B-C2B	5.44	1.48	1.36
26	h6	203	PEB	C3C-C4C	5.44	1.50	1.42
26	d7	201	PEB	C3B-C2B	5.44	1.48	1.36
26	CC	203	PEB	C3B-C2B	5.44	1.48	1.36
26	C5	202	PEB	C3B-C2B	5.44	1.48	1.36
26	AC	201	PEB	C3B-C2B	5.44	1.48	1.36
26	mI	202	PEB	C3B-C2B	5.44	1.48	1.36
26	aI	202	PEB	C3B-C2B	5.44	1.48	1.36
26	E1	201	PEB	C3B-C2B	5.44	1.48	1.36
26	14	201	PEB	C3B-C2B	5.44	1.48	1.36
26	L7	1002	PEB	C3B-C2B	5.44	1.48	1.36
28	tH	1001	CYC	CHB-C1B	5.44	1.51	1.38
26	J4	203	PEB	C3C-C4C	5.44	1.50	1.42
26	mG	202	PEB	C3B-C2B	5.43	1.48	1.36
28	qH	1001	CYC	CHB-C1B	5.43	1.51	1.38
26	d4	203	PEB	C3B-C2B	5.43	1.48	1.36
26	QF	201	PEB	C3B-C2B	5.43	1.48	1.36
26	c7	201	PEB	C3C-C4C	5.43	1.50	1.42
26	w4	204	PEB	C3B-C2B	5.43	1.48	1.36
26	R4	202	PEB	C3B-C2B	5.43	1.48	1.36
26	g7	202	PEB	C3B-C2B	5.43	1.48	1.36
26	Y1	202	PEB	C3B-C2B	5.43	1.48	1.36
26	O9	202	PEB	C3B-C2B	5.43	1.48	1.36
26	R8	201	PEB	C3C-C4C	5.43	1.50	1.42
26	uG	201	PEB	C3C-C4C	5.43	1.50	1.42
26	D8	201	PEB	C3C-C4C	5.43	1.50	1.42
26	VB	202	PEB	C3B-C2B	5.43	1.48	1.36
26	qE	203	PEB	C3B-C2B	5.43	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	EH	1001	CYC	C2A-C3A	5.43	1.48	1.36
26	U4	202	PEB	C3C-C4C	5.43	1.50	1.42
26	c2	203	PEB	C3B-C2B	5.43	1.48	1.36
26	gA	201	PEB	C3C-C4C	5.43	1.50	1.42
26	hF	202	PEB	C3C-C4C	5.43	1.50	1.42
26	lF	201	PEB	C3B-C2B	5.43	1.48	1.36
28	NH	1001	CYC	C3B-C2B	5.43	1.48	1.36
28	OH	1001	CYC	CHB-C1B	5.43	1.50	1.38
26	JJ	203	PEB	C3B-C2B	5.43	1.48	1.36
28	GH	1001	CYC	C3B-C2B	5.43	1.48	1.36
26	RD	202	PEB	C3C-C4C	5.43	1.50	1.42
26	f1	202	PEB	C3C-C4C	5.42	1.50	1.42
26	f6	203	PEB	C3C-C4C	5.42	1.50	1.42
26	AJ	301	PEB	C3C-C4C	5.42	1.50	1.42
26	w4	203	PEB	C3B-C2B	5.42	1.48	1.36
26	G5	201	PEB	C3B-C2B	5.42	1.48	1.36
26	I8	201	PEB	C3B-C2B	5.42	1.48	1.36
26	IC	203	PEB	C3B-C2B	5.42	1.48	1.36
26	eE	203	PEB	C3B-C2B	5.42	1.48	1.36
26	F1	201	PEB	C3C-C4C	5.42	1.50	1.42
26	lE	201	PEB	C3C-C4C	5.42	1.50	1.42
26	CG	202	PEB	C3C-C4C	5.42	1.50	1.42
27	A7	303	PUB	C2C-C3C	5.42	1.48	1.36
28	GH	1001	CYC	CHB-C1B	5.42	1.50	1.38
26	YB	202	PEB	C3B-C2B	5.42	1.48	1.36
28	jH	1001	CYC	C2A-C3A	5.42	1.48	1.36
26	s4	202	PEB	C3C-C4C	5.42	1.50	1.42
26	eI	202	PEB	C3B-C2B	5.42	1.48	1.36
28	JH	1001	CYC	C2A-C3A	5.42	1.48	1.36
26	d8	202	PEB	C3B-C2B	5.42	1.48	1.36
26	uG	202	PEB	C3C-C4C	5.42	1.50	1.42
27	xE	305	PUB	C2B-C1B	5.42	1.50	1.42
26	m2	202	PEB	C3B-C2B	5.42	1.48	1.36
26	FD	201	PEB	C3B-C2B	5.42	1.48	1.36
27	xG	305	PUB	C2C-C3C	5.42	1.48	1.36
28	RH	1001	CYC	C3B-C2B	5.42	1.48	1.36
26	AI	305	PEB	C3B-C2B	5.42	1.48	1.36
26	L1	202	PEB	C3B-C2B	5.42	1.48	1.36
26	LB	1002	PEB	C3B-C2B	5.42	1.48	1.36
26	j8	201	PEB	C3B-C2B	5.42	1.48	1.36
26	B4	201	PEB	C3C-C4C	5.42	1.50	1.42
26	zG	501	PEB	C3C-C4C	5.42	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bB	202	PEB	C3B-C2B	5.42	1.48	1.36
26	qE	203	PEB	C3C-C4C	5.42	1.50	1.42
26	OF	203	PEB	C3B-C2B	5.42	1.48	1.36
26	fG	201	PEB	C3B-C2B	5.42	1.48	1.36
26	dB	201	PEB	C3B-C2B	5.42	1.48	1.36
26	VG	201	PEB	C3B-C2B	5.42	1.48	1.36
26	JA	202	PEB	C3B-C2B	5.42	1.48	1.36
26	k8	201	PEB	C3C-C4C	5.42	1.50	1.42
27	A1	203	PUB	C2B-C1B	5.42	1.50	1.42
28	LB	1001	CYC	C3B-C2B	5.42	1.48	1.36
26	P6	202	PEB	C3B-C2B	5.42	1.48	1.36
26	hI	202	PEB	C3B-C2B	5.42	1.48	1.36
26	OG	203	PEB	C3C-C4C	5.42	1.50	1.42
26	A1	201	PEB	C3C-C4C	5.42	1.50	1.42
26	G5	203	PEB	C3C-C4C	5.42	1.50	1.42
26	C1	202	PEB	C3B-C2B	5.42	1.48	1.36
26	UA	201	PEB	C3C-C4C	5.41	1.50	1.42
26	H1	202	PEB	C3B-C2B	5.41	1.48	1.36
26	IG	202	PEB	C3B-C2B	5.41	1.48	1.36
26	X9	201	PEB	C3B-C2B	5.41	1.48	1.36
26	OA	202	PEB	C3B-C2B	5.41	1.48	1.36
26	gG	203	PEB	C3B-C2B	5.41	1.48	1.36
26	J4	203	PEB	C3B-C2B	5.41	1.48	1.36
28	kH	1001	CYC	CHB-C1B	5.41	1.50	1.38
26	F4	203	PEB	C3C-C4C	5.41	1.50	1.42
26	UD	202	PEB	C3C-C4C	5.41	1.50	1.42
26	WF	203	PEB	C3B-C2B	5.41	1.48	1.36
26	d6	201	PEB	C3B-C2B	5.41	1.48	1.36
26	A3	202	PEB	C3C-C4C	5.41	1.50	1.42
26	E4	201	PEB	C3B-C2B	5.41	1.48	1.36
26	A5	202	PEB	C3B-C2B	5.41	1.48	1.36
28	YH	1003	CYC	C2A-C3A	5.41	1.48	1.36
26	R1	202	PEB	C3B-C2B	5.41	1.48	1.36
26	S4	202	PEB	C3B-C2B	5.41	1.48	1.36
26	GA	203	PEB	C3B-C2B	5.41	1.48	1.36
26	AG	201	PEB	C3C-C4C	5.41	1.50	1.42
26	X3	203	PEB	C3B-C2B	5.41	1.48	1.36
26	jA	203	PEB	C3B-C2B	5.41	1.48	1.36
26	T6	202	PEB	C3B-C2B	5.41	1.48	1.36
26	II	202	PEB	C3B-C2B	5.41	1.48	1.36
26	m8	201	PEB	C3C-C4C	5.41	1.50	1.42
26	r4	201	PEB	C3B-C2B	5.41	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y4	203	PEB	C3C-C4C	5.41	1.50	1.42
26	b2	202	PEB	C3B-C2B	5.41	1.48	1.36
26	cI	203	PEB	C3B-C2B	5.41	1.48	1.36
26	U7	203	PEB	C3C-C4C	5.41	1.50	1.42
26	T9	203	PEB	C3C-C4C	5.41	1.50	1.42
26	VI	202	PEB	C3C-C4C	5.41	1.50	1.42
28	N7	1001	CYC	C3B-C2B	5.41	1.48	1.36
28	EF	1001	CYC	C3B-C2B	5.41	1.48	1.36
26	A9	301	PEB	C3B-C2B	5.41	1.48	1.36
26	H9	202	PEB	C3B-C2B	5.41	1.48	1.36
26	kA	202	PEB	C3B-C2B	5.41	1.48	1.36
26	WE	201	PEB	C3B-C2B	5.40	1.48	1.36
26	WE	202	PEB	C3C-C4C	5.40	1.50	1.42
26	L6	1002	PEB	C3B-C2B	5.40	1.48	1.36
28	vH	1001	CYC	C3B-C2B	5.40	1.48	1.36
26	UE	202	PEB	C3B-C2B	5.40	1.48	1.36
26	nE	202	PEB	C3B-C2B	5.40	1.48	1.36
26	TJ	203	PEB	C3C-C4C	5.40	1.50	1.42
26	VD	201	PEB	C3B-C2B	5.40	1.48	1.36
26	cG	202	PEB	C3B-C2B	5.40	1.48	1.36
28	G2	1001	CYC	C2A-C3A	5.40	1.48	1.36
26	ZF	203	PEB	C3C-C4C	5.40	1.50	1.42
26	J9	203	PEB	C3B-C2B	5.40	1.48	1.36
28	eH	1001	CYC	CHB-C1B	5.40	1.50	1.38
26	iI	201	PEB	C3B-C2B	5.40	1.48	1.36
26	24	405	PEB	C3C-C4C	5.40	1.50	1.42
26	FJ	202	PEB	C3C-C4C	5.40	1.50	1.42
26	14	203	PEB	C3B-C2B	5.40	1.48	1.36
26	JJ	202	PEB	C3B-C2B	5.40	1.48	1.36
26	f7	202	PEB	C3C-C4C	5.40	1.50	1.42
26	sG	202	PEB	C3C-C4C	5.40	1.50	1.42
28	LH	1001	CYC	C2A-C3A	5.40	1.48	1.36
26	V4	202	PEB	C3B-C2B	5.40	1.48	1.36
26	e4	201	PEB	C3B-C2B	5.40	1.48	1.36
26	V3	202	PEB	C3C-C4C	5.40	1.50	1.42
26	D3	201	PEB	C3B-C2B	5.40	1.48	1.36
26	gA	202	PEB	C3B-C2B	5.40	1.48	1.36
28	iH	1001	CYC	CHB-C1B	5.40	1.50	1.38
26	Z4	201	PEB	C3C-C4C	5.40	1.50	1.42
26	h8	203	PEB	C3B-C2B	5.40	1.48	1.36
26	j4	202	PEB	C3C-C4C	5.40	1.50	1.42
28	pH	1001	CYC	C2A-C3A	5.40	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	QJ	202	PEB	C3C-C4C	5.40	1.50	1.42
26	dG	201	PEB	C3B-C2B	5.40	1.48	1.36
28	fH	1001	CYC	C3B-C2B	5.40	1.48	1.36
26	I1	202	PEB	C3C-C4C	5.39	1.50	1.42
26	p1	201	PEB	C3B-C2B	5.39	1.48	1.36
26	QB	201	PEB	C3C-C4C	5.39	1.50	1.42
26	a7	202	PEB	C3B-C2B	5.39	1.48	1.36
26	f1	201	PEB	C3C-C4C	5.39	1.50	1.42
26	k1	202	PEB	C3C-C4C	5.39	1.50	1.42
26	c2	203	PEB	C3C-C4C	5.39	1.50	1.42
26	TD	203	PEB	C3B-C2B	5.39	1.48	1.36
28	IH	1001	CYC	C2A-C3A	5.39	1.48	1.36
26	T1	203	PEB	C3B-C2B	5.39	1.48	1.36
26	RD	203	PEB	C3B-C2B	5.39	1.48	1.36
26	H4	202	PEB	C3B-C2B	5.39	1.48	1.36
26	J4	202	PEB	C3B-C2B	5.39	1.48	1.36
26	V1	202	PEB	C3B-C2B	5.39	1.48	1.36
26	Y4	202	PEB	C3B-C2B	5.39	1.48	1.36
26	EE	201	PEB	C3C-C4C	5.39	1.50	1.42
26	D4	202	PEB	C3B-C2B	5.39	1.48	1.36
26	AJ	301	PEB	C3B-C2B	5.39	1.48	1.36
26	dF	202	PEB	C3B-C2B	5.39	1.48	1.36
26	I5	203	PEB	C3B-C2B	5.39	1.48	1.36
26	gG	202	PEB	C3B-C2B	5.39	1.48	1.36
28	pH	1001	CYC	C3B-C2B	5.39	1.48	1.36
26	QF	203	PEB	C3B-C2B	5.39	1.48	1.36
26	TB	202	PEB	C3B-C2B	5.39	1.48	1.36
28	1H	1000	CYC	C3B-C2B	5.39	1.48	1.36
26	t1	202	PEB	C3C-C4C	5.39	1.50	1.42
26	k4	202	PEB	C3B-C2B	5.38	1.48	1.36
26	B1	201	PEB	C3C-C4C	5.38	1.50	1.42
26	E8	202	PEB	C3B-C2B	5.38	1.48	1.36
26	WJ	202	PEB	C3B-C2B	5.38	1.48	1.36
26	CG	203	PEB	C3B-C2B	5.38	1.48	1.36
26	M1	402	PEB	C3B-C2B	5.38	1.48	1.36
26	A6	301	PEB	C3B-C2B	5.38	1.48	1.36
27	A6	302	PUB	C2C-C3C	5.38	1.48	1.36
26	bG	201	PEB	C3C-C4C	5.38	1.50	1.42
26	l8	201	PEB	C3B-C2B	5.38	1.48	1.36
26	CC	201	PEB	C3B-C2B	5.38	1.48	1.36
26	LC	202	PEB	C3B-C2B	5.38	1.48	1.36
26	GC	202	PEB	C3B-C2B	5.38	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D9	201	PEB	C3B-C2B	5.38	1.48	1.36
26	q4	202	PEB	C3B-C2B	5.38	1.48	1.36
26	W9	202	PEB	C3B-C2B	5.38	1.48	1.36
28	rH	1001	CYC	CHB-C1B	5.38	1.50	1.38
26	11	203	PEB	C3B-C2B	5.38	1.48	1.36
26	w4	202	PEB	C3B-C2B	5.38	1.48	1.36
26	P8	202	PEB	C3B-C2B	5.38	1.48	1.36
27	AB	302	PUB	C2C-C3C	5.38	1.48	1.36
26	p4	201	PEB	C3C-C4C	5.38	1.50	1.42
26	R7	202	PEB	C3C-C4C	5.38	1.50	1.42
26	kG	201	PEB	C3B-C2B	5.38	1.48	1.36
26	CJ	202	PEB	C3B-C2B	5.38	1.48	1.36
26	UJ	202	PEB	C3B-C2B	5.38	1.48	1.36
26	d7	202	PEB	C3B-C2B	5.38	1.48	1.36
26	IA	201	PEB	C3B-C2B	5.38	1.48	1.36
26	eG	203	PEB	C3B-C2B	5.37	1.48	1.36
26	B3	203	PEB	C3C-C4C	5.37	1.50	1.42
26	jI	201	PEB	C3C-C4C	5.37	1.50	1.42
26	IE	203	PEB	C3B-C2B	5.37	1.48	1.36
26	A1	202	PEB	C3C-C4C	5.37	1.50	1.42
26	l7	201	PEB	C3B-C2B	5.37	1.48	1.36
26	F4	203	PEB	C3B-C2B	5.37	1.48	1.36
26	a4	203	PEB	C3C-C4C	5.37	1.50	1.42
26	E4	202	PEB	C3B-C2B	5.37	1.48	1.36
26	C9	202	PEB	C3B-C2B	5.37	1.48	1.36
27	NJ	201	PUB	C2C-C3C	5.37	1.48	1.36
26	nG	202	PEB	C3B-C2B	5.37	1.48	1.36
26	X3	201	PEB	C2A-C1A	-5.37	1.47	1.52
28	nH	1001	CYC	C3B-C2B	5.37	1.48	1.36
26	yG	301	PEB	C3C-C4C	5.37	1.50	1.42
26	cI	203	PEB	C3C-C4C	5.37	1.50	1.42
26	k1	203	PEB	C3B-C2B	5.37	1.48	1.36
26	h1	202	PEB	C3B-C2B	5.37	1.48	1.36
26	tE	201	PEB	C3C-C4C	5.37	1.50	1.42
26	W3	202	PEB	C3B-C2B	5.37	1.48	1.36
26	l2	202	PEB	C3B-C2B	5.37	1.48	1.36
26	D4	201	PEB	C3B-C2B	5.37	1.48	1.36
26	hA	203	PEB	C3B-C2B	5.37	1.48	1.36
26	cB	202	PEB	C3B-C2B	5.37	1.48	1.36
26	G9	202	PEB	C3C-C4C	5.37	1.50	1.42
26	jG	201	PEB	C3C-C4C	5.37	1.50	1.42
26	L3	202	PEB	C3B-C2B	5.36	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C5	204	PEB	C3B-C2B	5.36	1.48	1.36
26	MD	202	PEB	C3B-C2B	5.36	1.48	1.36
26	wE	301	PEB	C3B-C2B	5.36	1.48	1.36
26	I3	202	PEB	C3B-C2B	5.36	1.48	1.36
28	gH	1001	CYC	C3B-C2B	5.36	1.48	1.36
26	KC	201	PEB	C3B-C2B	5.36	1.48	1.36
28	UH	1001	CYC	C3B-C2B	5.36	1.48	1.36
26	w1	203	PEB	C3B-C2B	5.36	1.48	1.36
26	i2	203	PEB	C3C-C4C	5.36	1.50	1.42
26	Y3	301	PEB	C3B-C2B	5.36	1.48	1.36
26	OG	201	PEB	C3B-C2B	5.36	1.48	1.36
26	bF	202	PEB	C3C-C4C	5.36	1.50	1.42
26	L4	202	PEB	C3B-C2B	5.36	1.48	1.36
26	c8	201	PEB	C3C-C4C	5.36	1.50	1.42
26	mF	202	PEB	C2A-C1A	-5.36	1.47	1.52
28	NH	1001	CYC	CHB-C1B	5.36	1.50	1.38
28	cH	1001	CYC	C3B-C2B	5.36	1.48	1.36
26	R3	202	PEB	C3C-C4C	5.36	1.50	1.42
26	j7	202	PEB	C3C-C4C	5.36	1.50	1.42
26	B8	301	PEB	C3B-C2B	5.36	1.48	1.36
26	l1	201	PEB	C3C-C4C	5.36	1.50	1.42
26	LF	1002	PEB	C3B-C2B	5.36	1.48	1.36
27	24	403	PUB	C2C-C3C	5.36	1.48	1.36
26	O9	202	PEB	C3C-C4C	5.36	1.50	1.42
28	TH	1001	CYC	C3B-C2B	5.36	1.48	1.36
26	k1	202	PEB	C3B-C2B	5.36	1.48	1.36
26	YF	202	PEB	C3B-C2B	5.36	1.48	1.36
26	KD	202	PEB	C3B-C2B	5.36	1.48	1.36
26	ZF	202	PEB	C3C-C4C	5.36	1.50	1.42
26	lF	202	PEB	C3C-C4C	5.36	1.50	1.42
28	wH	1001	CYC	CHB-C1B	5.36	1.50	1.38
26	Y7	201	PEB	C3B-C2B	5.35	1.48	1.36
26	f4	201	PEB	C3C-C4C	5.35	1.50	1.42
26	QE	203	PEB	C3B-C2B	5.35	1.48	1.36
26	QE	201	PEB	C3C-C4C	5.35	1.50	1.42
26	iE	203	PEB	C3B-C2B	5.35	1.48	1.36
26	C3	201	PEB	C3C-C4C	5.35	1.50	1.42
26	CE	203	PEB	C3C-C4C	5.35	1.50	1.42
26	N1	203	PEB	C3B-C2B	5.35	1.48	1.36
26	K3	202	PEB	C3B-C2B	5.35	1.48	1.36
26	kF	201	PEB	C3B-C2B	5.35	1.48	1.36
26	HJ	203	PEB	C3B-C2B	5.35	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V4	203	PEB	C3B-C2B	5.35	1.48	1.36
26	cF	201	PEB	C3C-C4C	5.35	1.50	1.42
26	TE	201	PEB	C3B-C2B	5.35	1.48	1.36
26	LG	201	PEB	C3B-C2B	5.35	1.48	1.36
26	qG	203	PEB	C3B-C2B	5.35	1.48	1.36
26	M4	403	PEB	C3B-C2B	5.35	1.48	1.36
26	UG	202	PEB	C3B-C2B	5.35	1.48	1.36
26	II	201	PEB	C3C-C4C	5.35	1.50	1.42
26	jB	202	PEB	C3C-C4C	5.35	1.50	1.42
26	bF	201	PEB	C3B-C2B	5.35	1.48	1.36
26	sG	201	PEB	C3B-C2B	5.35	1.48	1.36
26	C4	201	PEB	C3B-C2B	5.35	1.48	1.36
26	c6	202	PEB	C3B-C2B	5.35	1.48	1.36
26	E1	202	PEB	C3B-C2B	5.34	1.48	1.36
26	P7	201	PEB	C3B-C2B	5.34	1.48	1.36
26	JG	201	PEB	C3B-C2B	5.34	1.48	1.36
28	EH	1001	CYC	C3B-C2B	5.34	1.48	1.36
26	QE	202	PEB	C3B-C2B	5.34	1.48	1.36
26	JA	201	PEB	C3C-C4C	5.34	1.50	1.42
26	bE	202	PEB	C3B-C2B	5.34	1.48	1.36
26	k4	203	PEB	C3B-C2B	5.34	1.48	1.36
26	N7	1002	PEB	C3B-C2B	5.34	1.48	1.36
26	j8	203	PEB	C3B-C2B	5.34	1.48	1.36
26	M4	402	PEB	C3C-C4C	5.34	1.50	1.42
26	HD	202	PEB	C3B-C2B	5.34	1.48	1.36
28	PH	1001	CYC	CHB-C1B	5.34	1.50	1.38
26	TG	201	PEB	C3B-C2B	5.34	1.48	1.36
26	NE	201	PEB	C3B-C2B	5.34	1.48	1.36
26	TF	201	PEB	C3B-C2B	5.34	1.48	1.36
28	SH	1001	CYC	C3B-C2B	5.34	1.48	1.36
28	N7	1001	CYC	C2A-C3A	5.34	1.48	1.36
28	nH	1001	CYC	CHB-C1B	5.34	1.50	1.38
26	m1	203	PEB	C3B-C2B	5.34	1.48	1.36
26	G5	202	PEB	C3B-C2B	5.34	1.48	1.36
26	PB	202	PEB	C3B-C2B	5.34	1.48	1.36
26	NG	201	PEB	C3B-C2B	5.34	1.48	1.36
26	MD	201	PEB	C3B-C2B	5.34	1.48	1.36
26	fA	203	PEB	C3B-C2B	5.34	1.48	1.36
28	L6	1001	CYC	C3B-C2B	5.34	1.48	1.36
26	F3	201	PEB	C3B-C2B	5.33	1.48	1.36
26	k7	201	PEB	C3B-C2B	5.33	1.48	1.36
26	n1	201	PEB	C3B-C2B	5.33	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	OE	201	PEB	C3B-C2B	5.33	1.48	1.36
28	yH	1001	CYC	C2A-C3A	5.33	1.48	1.36
26	e7	201	PEB	C3C-C4C	5.33	1.50	1.42
28	G7	1001	CYC	C2A-C3A	5.33	1.48	1.36
26	R7	201	PEB	C3B-C2B	5.33	1.48	1.36
26	SA	201	PEB	C3B-C2B	5.33	1.48	1.36
26	A2	301	PEB	C3C-C4C	5.33	1.50	1.42
26	Q6	203	PEB	C3C-C4C	5.33	1.50	1.42
26	e7	201	PEB	C3B-C2B	5.33	1.48	1.36
26	J9	202	PEB	C3C-C4C	5.33	1.50	1.42
26	s4	201	PEB	C3B-C2B	5.33	1.48	1.36
26	PF	202	PEB	C3B-C2B	5.33	1.48	1.36
26	bG	202	PEB	C3B-C2B	5.33	1.48	1.36
26	J3	202	PEB	C3B-C2B	5.33	1.48	1.36
26	V2	202	PEB	C3C-C4C	5.33	1.50	1.42
26	dF	201	PEB	C3B-C2B	5.33	1.48	1.36
26	kA	201	PEB	C3C-C4C	5.33	1.50	1.42
26	BJ	202	PEB	C3C-C4C	5.33	1.50	1.42
26	B9	201	PEB	C3B-C2B	5.33	1.48	1.36
26	kI	201	PEB	C3B-C2B	5.33	1.48	1.36
26	mA	201	PEB	C3B-C2B	5.33	1.48	1.36
26	GC	201	PEB	C3B-C2B	5.33	1.48	1.36
28	LH	1001	CYC	C3B-C2B	5.33	1.48	1.36
26	d1	203	PEB	C3B-C2B	5.33	1.48	1.36
26	jE	201	PEB	C3C-C4C	5.33	1.50	1.42
26	BA	301	PEB	C3B-C2B	5.33	1.48	1.36
26	WA	202	PEB	C3B-C2B	5.33	1.48	1.36
28	wH	1001	CYC	C3B-C2B	5.33	1.48	1.36
26	l8	202	PEB	C3B-C2B	5.32	1.48	1.36
26	aG	203	PEB	C3B-C2B	5.32	1.48	1.36
26	I8	203	PEB	C3B-C2B	5.32	1.48	1.36
26	e6	201	PEB	C3B-C2B	5.32	1.48	1.36
26	g8	201	PEB	C3C-C4C	5.32	1.50	1.42
26	VD	202	PEB	C3C-C4C	5.32	1.50	1.42
26	W8	202	PEB	C3B-C2B	5.32	1.48	1.36
26	BD	203	PEB	C3B-C2B	5.32	1.48	1.36
28	F6	1001	CYC	C3B-C2B	5.32	1.48	1.36
26	J3	201	PEB	C3B-C2B	5.32	1.48	1.36
26	QJ	201	PEB	C3C-C4C	5.32	1.50	1.42
26	LD	201	PEB	C3B-C2B	5.32	1.48	1.36
26	DB	1002	PEB	C3B-C2B	5.32	1.48	1.36
26	l4	202	PEB	C3B-C2B	5.32	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K4	202	PEB	C3B-C2B	5.32	1.48	1.36
26	b7	203	PEB	C3B-C2B	5.32	1.48	1.36
26	OE	203	PEB	C3C-C4C	5.32	1.50	1.42
26	DG	201	PEB	C3C-C4C	5.32	1.50	1.42
26	VD	202	PEB	C3B-C2B	5.32	1.48	1.36
26	QA	203	PEB	C3C-C4C	5.32	1.50	1.42
26	KC	202	PEB	C3B-C2B	5.32	1.48	1.36
26	U7	202	PEB	C3B-C2B	5.32	1.48	1.36
28	fH	1001	CYC	C2A-C3A	5.32	1.48	1.36
26	D6	1002	PEB	C3B-C2B	5.32	1.48	1.36
26	L9	201	PEB	C3B-C2B	5.32	1.48	1.36
26	LE	201	PEB	C3B-C2B	5.32	1.48	1.36
26	k2	203	PEB	C3C-C4C	5.32	1.50	1.42
26	LJ	201	PEB	C3B-C2B	5.32	1.48	1.36
27	AA	303	PUB	C2C-C3C	5.32	1.48	1.36
26	U9	202	PEB	C3B-C2B	5.32	1.48	1.36
26	fF	203	PEB	C3C-C4C	5.32	1.50	1.42
26	e6	203	PEB	C3C-C4C	5.32	1.50	1.42
26	QG	201	PEB	C3C-C4C	5.32	1.50	1.42
26	fA	201	PEB	C3B-C2B	5.32	1.48	1.36
28	JF	1001	CYC	C3B-C2B	5.32	1.48	1.36
26	H7	1002	PEB	C3C-C4C	5.31	1.50	1.42
26	f1	202	PEB	C3B-C2B	5.31	1.48	1.36
28	JI	1001	CYC	C2A-C3A	5.31	1.48	1.36
26	DD	203	PEB	C3C-C4C	5.31	1.50	1.42
28	J2	1001	CYC	C3B-C2B	5.31	1.48	1.36
26	l2	201	PEB	C3C-C4C	5.31	1.50	1.42
26	b7	201	PEB	C3B-C2B	5.31	1.48	1.36
26	I3	201	PEB	C3B-C2B	5.31	1.48	1.36
26	IA	203	PEB	C3B-C2B	5.31	1.48	1.36
26	l6	203	PEB	C3B-C2B	5.31	1.48	1.36
26	TF	202	PEB	C3B-C2B	5.31	1.48	1.36
26	A4	201	PEB	C3C-C4C	5.31	1.50	1.42
26	ZI	202	PEB	C3B-C2B	5.31	1.48	1.36
26	Z2	202	PEB	C3B-C2B	5.31	1.48	1.36
26	MJ	202	PEB	C3C-C4C	5.31	1.50	1.42
27	AF	303	PUB	C2B-C1B	5.31	1.50	1.42
26	dI	202	PEB	C3B-C2B	5.31	1.48	1.36
26	a1	201	PEB	C3C-C4C	5.31	1.50	1.42
26	V7	201	PEB	C3B-C2B	5.31	1.48	1.36
26	A3	201	PEB	C3B-C2B	5.31	1.48	1.36
26	EA	202	PEB	C3B-C2B	5.31	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H7	1001	CYC	C3B-C2B	5.31	1.48	1.36
26	Q6	201	PEB	C3C-C4C	5.31	1.50	1.42
26	j6	202	PEB	C3C-C4C	5.31	1.50	1.42
26	e7	202	PEB	C3C-C4C	5.31	1.50	1.42
26	BA	301	PEB	C3C-C4C	5.31	1.50	1.42
26	PE	201	PEB	C3B-C2B	5.31	1.48	1.36
26	mG	203	PEB	C3B-C2B	5.31	1.48	1.36
26	bE	201	PEB	C3B-C2B	5.31	1.48	1.36
28	PH	1001	CYC	C3B-C2B	5.31	1.48	1.36
26	d8	202	PEB	C3C-C4C	5.31	1.50	1.42
26	YJ	201	PEB	C3C-C4C	5.31	1.50	1.42
26	k7	201	PEB	C3C-C4C	5.31	1.50	1.42
27	A8	303	PUB	C2C-C3C	5.31	1.48	1.36
26	M8	203	PEB	C3B-C2B	5.31	1.48	1.36
26	r1	201	PEB	C3B-C2B	5.30	1.48	1.36
26	O8	202	PEB	C3B-C2B	5.30	1.48	1.36
26	qG	202	PEB	C3B-C2B	5.30	1.48	1.36
28	BB	1001	CYC	C2A-C3A	5.30	1.48	1.36
26	g1	201	PEB	C3B-C2B	5.30	1.48	1.36
28	uH	1001	CYC	C3B-C2B	5.30	1.48	1.36
26	U1	202	PEB	C3B-C2B	5.30	1.48	1.36
26	lA	202	PEB	C3B-C2B	5.30	1.48	1.36
28	NF	1001	CYC	C3B-C2B	5.30	1.48	1.36
26	eA	201	PEB	C3C-C4C	5.30	1.50	1.42
26	d2	202	PEB	C3C-C4C	5.30	1.50	1.42
26	Q8	203	PEB	C3B-C2B	5.30	1.48	1.36
28	FB	1001	CYC	C3B-C2B	5.30	1.48	1.36
26	T2	202	PEB	C3B-C2B	5.30	1.48	1.36
26	f1	201	PEB	C3B-C2B	5.30	1.48	1.36
26	G3	202	PEB	C3B-C2B	5.30	1.48	1.36
26	DJ	203	PEB	C3B-C2B	5.30	1.48	1.36
28	AH	1001	CYC	C3B-C2B	5.30	1.48	1.36
26	P9	202	PEB	C3C-C4C	5.30	1.50	1.42
26	hG	202	PEB	C3B-C2B	5.30	1.48	1.36
28	J7	1001	CYC	C3B-C2B	5.30	1.48	1.36
26	f8	201	PEB	C3B-C2B	5.30	1.48	1.36
26	aI	203	PEB	C3B-C2B	5.30	1.48	1.36
27	A1	203	PUB	C2C-C3C	5.30	1.48	1.36
26	s4	201	PEB	C3C-C4C	5.30	1.50	1.42
26	f7	201	PEB	C3C-C4C	5.30	1.50	1.42
26	U8	201	PEB	C3C-C4C	5.30	1.50	1.42
26	GE	203	PEB	C3C-C4C	5.30	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UF	201	PEB	C3B-C2B	5.30	1.48	1.36
28	IH	1001	CYC	CHB-C1B	5.30	1.50	1.38
26	P9	203	PEB	C3B-C2B	5.30	1.48	1.36
26	QJ	202	PEB	C3B-C2B	5.30	1.48	1.36
26	D4	201	PEB	C3C-C4C	5.30	1.50	1.42
26	ME	202	PEB	C3B-C2B	5.30	1.48	1.36
26	mE	202	PEB	C3B-C2B	5.30	1.48	1.36
26	c2	201	PEB	C3B-C2B	5.30	1.48	1.36
26	HE	201	PEB	C3B-C2B	5.30	1.48	1.36
28	CI	1001	CYC	C2A-C3A	5.30	1.48	1.36
28	UH	1001	CYC	CHB-C1B	5.29	1.50	1.38
26	YG	201	PEB	C3B-C2B	5.29	1.48	1.36
26	ZI	201	PEB	C3C-C4C	5.29	1.50	1.42
26	H3	201	PEB	C3B-C2B	5.29	1.48	1.36
26	Y7	202	PEB	C3B-C2B	5.29	1.48	1.36
26	j7	201	PEB	C3B-C2B	5.29	1.48	1.36
26	lF	203	PEB	C3C-C4C	5.29	1.50	1.42
26	QA	202	PEB	C3B-C2B	5.29	1.48	1.36
26	sE	201	PEB	C3C-C4C	5.29	1.50	1.42
26	MG	202	PEB	C3B-C2B	5.29	1.48	1.36
26	NJ	204	PEB	C3C-C4C	5.29	1.50	1.42
27	xE	305	PUB	C2C-C3C	5.29	1.48	1.36
26	Z2	201	PEB	C3C-C4C	5.29	1.50	1.42
26	ID	202	PEB	C3B-C2B	5.29	1.48	1.36
26	NJ	204	PEB	C3B-C2B	5.29	1.48	1.36
26	BD	202	PEB	C3C-C4C	5.29	1.50	1.42
26	iI	203	PEB	C3C-C4C	5.29	1.50	1.42
26	a4	201	PEB	C3C-C4C	5.29	1.50	1.42
26	L5	202	PEB	C3B-C2B	5.29	1.48	1.36
26	BJ	201	PEB	C3B-C2B	5.29	1.48	1.36
26	lA	201	PEB	C3B-C2B	5.29	1.48	1.36
26	aE	202	PEB	C3C-C4C	5.29	1.50	1.42
26	y1	201	PEB	C3B-C2B	5.29	1.48	1.36
26	A2	301	PEB	C3B-C2B	5.29	1.48	1.36
26	GD	202	PEB	C3C-C4C	5.28	1.50	1.42
26	fI	202	PEB	C3B-C2B	5.28	1.48	1.36
28	rH	1001	CYC	C3B-C2B	5.28	1.48	1.36
26	vE	201	PEB	C3C-C4C	5.28	1.50	1.42
26	m8	201	PEB	C3B-C2B	5.28	1.48	1.36
28	MH	1001	CYC	C2A-C3A	5.28	1.48	1.36
26	kF	201	PEB	C3C-C4C	5.28	1.50	1.42
26	p1	202	PEB	C3C-C4C	5.28	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	WH	1001	CYC	C2A-C3A	5.28	1.48	1.36
26	SB	202	PEB	C3B-C2B	5.28	1.48	1.36
26	ED	202	PEB	C3B-C2B	5.28	1.48	1.36
26	e6	202	PEB	C3C-C4C	5.28	1.50	1.42
26	Q9	202	PEB	C3B-C2B	5.28	1.47	1.36
28	F7	1001	CYC	C2A-C3A	5.28	1.47	1.36
26	UB	201	PEB	C3B-C2B	5.28	1.47	1.36
28	RH	1001	CYC	C2A-C3A	5.28	1.47	1.36
26	J1	202	PEB	C3B-C2B	5.28	1.47	1.36
26	V3	201	PEB	C3B-C2B	5.28	1.47	1.36
26	bG	201	PEB	C3B-C2B	5.28	1.47	1.36
26	p4	202	PEB	C3C-C4C	5.28	1.50	1.42
26	dF	201	PEB	C3C-C4C	5.28	1.50	1.42
26	fF	201	PEB	C3C-C4C	5.28	1.50	1.42
26	f6	202	PEB	C3B-C2B	5.28	1.47	1.36
26	B8	301	PEB	C3C-C4C	5.28	1.50	1.42
26	N8	201	PEB	C3B-C2B	5.28	1.47	1.36
26	d4	201	PEB	C3B-C2B	5.27	1.47	1.36
26	Q6	202	PEB	C3B-C2B	5.27	1.47	1.36
26	rG	202	PEB	C3B-C2B	5.27	1.47	1.36
28	oH	1001	CYC	C2A-C3A	5.27	1.47	1.36
26	U4	201	PEB	C3B-C2B	5.27	1.47	1.36
26	f8	203	PEB	C3B-C2B	5.27	1.47	1.36
28	LH	1001	CYC	CHB-C1B	5.27	1.50	1.38
26	11	201	PEB	C3B-C2B	5.27	1.47	1.36
26	d6	202	PEB	C3B-C2B	5.27	1.47	1.36
27	AB	303	PUB	C2C-C3C	5.27	1.47	1.36
26	W9	202	PEB	C3C-C4C	5.27	1.50	1.42
26	kG	202	PEB	C3C-C4C	5.27	1.50	1.42
26	X1	202	PEB	C2A-C1A	-5.27	1.47	1.52
26	CE	203	PEB	C3B-C2B	5.27	1.47	1.36
26	jI	202	PEB	C3B-C2B	5.27	1.47	1.36
26	rE	201	PEB	C3C-C4C	5.27	1.50	1.42
26	Q8	202	PEB	C3B-C2B	5.27	1.47	1.36
26	11	201	PEB	C3C-C4C	5.27	1.50	1.42
26	D9	202	PEB	C3C-C4C	5.27	1.50	1.42
26	J8	201	PEB	C3C-C4C	5.27	1.50	1.42
26	A4	202	PEB	C3B-C2B	5.27	1.47	1.36
26	D9	203	PEB	C3B-C2B	5.27	1.47	1.36
26	VI	203	PEB	C3B-C2B	5.27	1.47	1.36
26	gI	202	PEB	C3B-C2B	5.27	1.47	1.36
26	a4	203	PEB	C3B-C2B	5.27	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S7	203	PEB	C3C-C4C	5.27	1.50	1.42
26	Q7	201	PEB	C3B-C2B	5.27	1.47	1.36
26	iG	202	PEB	C3B-C2B	5.27	1.47	1.36
27	Q8	201	PUB	C2C-C3C	5.27	1.47	1.36
26	U1	202	PEB	C3C-C4C	5.27	1.50	1.42
26	H8	201	PEB	C3B-C2B	5.27	1.47	1.36
26	a8	202	PEB	C3B-C2B	5.26	1.47	1.36
26	lB	203	PEB	C3B-C2B	5.26	1.47	1.36
26	y1	202	PEB	C3B-C2B	5.26	1.47	1.36
26	JC	202	PEB	C3B-C2B	5.26	1.47	1.36
26	hE	202	PEB	C3B-C2B	5.26	1.47	1.36
26	h7	203	PEB	C3C-C4C	5.26	1.50	1.42
28	C2	1001	CYC	C2A-C3A	5.26	1.47	1.36
26	s1	202	PEB	C3B-C2B	5.26	1.47	1.36
26	T2	202	PEB	C3C-C4C	5.26	1.50	1.42
26	yE	301	PEB	C3C-C4C	5.26	1.50	1.42
26	AI	301	PEB	C3B-C2B	5.26	1.47	1.36
28	UH	1001	CYC	C2A-C3A	5.26	1.47	1.36
28	YH	1001	CYC	C2A-C3A	5.26	1.47	1.36
26	cI	201	PEB	C3B-C2B	5.26	1.47	1.36
28	uH	1001	CYC	CHB-C1B	5.26	1.50	1.38
26	DE	201	PEB	C3C-C4C	5.26	1.50	1.42
28	tH	1001	CYC	C2A-C3A	5.26	1.47	1.36
26	J3	202	PEB	C3C-C4C	5.26	1.50	1.42
26	MA	203	PEB	C3B-C2B	5.26	1.47	1.36
26	j2	202	PEB	C3B-C2B	5.26	1.47	1.36
28	RH	1001	CYC	CHB-C1B	5.26	1.50	1.38
26	QB	203	PEB	C3C-C4C	5.26	1.50	1.42
27	A4	203	PUB	C2B-C1B	5.26	1.50	1.42
26	SF	202	PEB	C3B-C2B	5.26	1.47	1.36
26	O7	203	PEB	C3B-C2B	5.26	1.47	1.36
26	N1	201	PEB	C2A-C1A	-5.26	1.47	1.52
26	eF	201	PEB	C3C-C4C	5.26	1.50	1.42
26	QB	203	PEB	C3B-C2B	5.26	1.47	1.36
26	H3	202	PEB	C3B-C2B	5.26	1.47	1.36
26	RD	202	PEB	C3B-C2B	5.26	1.47	1.36
26	i6	202	PEB	C3C-C4C	5.26	1.50	1.42
26	AA	302	PEB	C3B-C2B	5.26	1.47	1.36
26	KD	201	PEB	C3B-C2B	5.26	1.47	1.36
26	D1	203	PEB	C3C-C4C	5.26	1.50	1.42
26	g7	201	PEB	C3C-C4C	5.26	1.50	1.42
26	VA	201	PEB	C3B-C2B	5.26	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J2	1001	CYC	C2A-C3A	5.26	1.47	1.36
26	ME	201	PEB	C3C-C4C	5.25	1.50	1.42
26	y4	202	PEB	C3B-C2B	5.25	1.47	1.36
26	C1	201	PEB	C3B-C2B	5.25	1.47	1.36
26	B9	202	PEB	C3C-C4C	5.25	1.50	1.42
26	pG	201	PEB	C3C-C4C	5.25	1.50	1.42
26	dB	202	PEB	C3B-C2B	5.25	1.47	1.36
26	h4	202	PEB	C3B-C2B	5.25	1.47	1.36
26	O2	201	PEB	C3C-C4C	5.25	1.50	1.42
28	wH	1001	CYC	C2A-C3A	5.25	1.47	1.36
26	21	404	PEB	C3C-C4C	5.25	1.50	1.42
26	L3	203	PEB	C3C-C4C	5.25	1.50	1.42
26	QF	203	PEB	C3C-C4C	5.25	1.50	1.42
26	NA	201	PEB	C3B-C2B	5.25	1.47	1.36
28	B6	1001	CYC	C2A-C3A	5.25	1.47	1.36
28	FF	1001	CYC	C2A-C3A	5.25	1.47	1.36
26	W7	202	PEB	C3C-C4C	5.25	1.50	1.42
26	FD	203	PEB	C3C-C4C	5.25	1.50	1.42
27	21	403	PUB	C2C-C3C	5.25	1.47	1.36
26	g2	202	PEB	C3B-C2B	5.25	1.47	1.36
26	m4	203	PEB	C3B-C2B	5.25	1.47	1.36
26	j4	201	PEB	C3B-C2B	5.25	1.47	1.36
26	aA	203	PEB	C3B-C2B	5.25	1.47	1.36
26	s1	201	PEB	C3C-C4C	5.25	1.50	1.42
26	PI	201	PEB	C3B-C2B	5.25	1.47	1.36
26	iF	201	PEB	C3C-C4C	5.25	1.50	1.42
26	a2	202	PEB	C3B-C2B	5.25	1.47	1.36
26	SF	201	PEB	C3B-C2B	5.25	1.47	1.36
26	T7	201	PEB	C3C-C4C	5.24	1.50	1.42
26	M3	202	PEB	C3B-C2B	5.24	1.47	1.36
26	i7	201	PEB	C3B-C2B	5.24	1.47	1.36
26	KC	203	PEB	C3B-C2B	5.24	1.47	1.36
26	E3	202	PEB	C3B-C2B	5.24	1.47	1.36
26	CA	203	PEB	C3B-C2B	5.24	1.47	1.36
28	SH	1001	CYC	CHB-C1B	5.24	1.50	1.38
26	DJ	201	PEB	C3B-C2B	5.24	1.47	1.36
26	OB	203	PEB	C3B-C2B	5.24	1.47	1.36
26	e2	202	PEB	C3C-C4C	5.24	1.50	1.42
26	BC	201	PEB	C3C-C4C	5.24	1.50	1.42
26	YE	202	PEB	C3C-C4C	5.24	1.50	1.42
26	k2	202	PEB	C3C-C4C	5.24	1.50	1.42
26	A9	301	PEB	C3C-C4C	5.24	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	GD	201	PEB	C3B-C2B	5.24	1.47	1.36
26	hB	203	PEB	C3B-C2B	5.24	1.47	1.36
26	U6	202	PEB	C3B-C2B	5.24	1.47	1.36
26	CA	201	PEB	C3B-C2B	5.24	1.47	1.36
26	GD	202	PEB	C3B-C2B	5.24	1.47	1.36
26	h2	202	PEB	C3B-C2B	5.24	1.47	1.36
26	X4	202	PEB	C2A-C1A	-5.24	1.47	1.52
26	AC	201	PEB	C3C-C4C	5.24	1.50	1.42
26	h4	201	PEB	C3B-C2B	5.23	1.47	1.36
26	S9	202	PEB	C3B-C2B	5.23	1.47	1.36
26	HA	201	PEB	C3B-C2B	5.23	1.47	1.36
28	rH	1001	CYC	C2A-C3A	5.23	1.47	1.36
26	X9	202	PEB	C3C-C4C	5.23	1.50	1.42
26	aA	201	PEB	C3C-C4C	5.23	1.50	1.42
26	d2	201	PEB	C3C-C4C	5.23	1.50	1.42
26	jI	202	PEB	C3C-C4C	5.23	1.50	1.42
26	jB	201	PEB	C3B-C2B	5.23	1.47	1.36
26	EE	202	PEB	C3B-C2B	5.23	1.47	1.36
28	JF	1001	CYC	C2A-C3A	5.23	1.47	1.36
26	O3	201	PEB	C1A-NA	-5.23	1.30	1.37
26	U7	201	PEB	C3B-C2B	5.23	1.47	1.36
26	aA	202	PEB	C3B-C2B	5.23	1.47	1.36
26	wG	301	PEB	C3B-C2B	5.23	1.47	1.36
28	CF	1001	CYC	C2A-C3A	5.23	1.47	1.36
26	q4	203	PEB	C3C-C4C	5.23	1.50	1.42
26	mF	202	PEB	C3C-C4C	5.23	1.50	1.42
26	S1	202	PEB	C3B-C2B	5.23	1.47	1.36
26	PJ	203	PEB	C3B-C2B	5.23	1.47	1.36
26	j2	201	PEB	C3C-C4C	5.23	1.50	1.42
26	UJ	201	PEB	C3C-C4C	5.23	1.50	1.42
26	K9	201	PEB	C3B-C2B	5.23	1.47	1.36
26	OA	201	PEB	C3B-C2B	5.23	1.47	1.36
26	q1	201	PEB	C3B-C2B	5.23	1.47	1.36
26	QJ	201	PEB	C3B-C2B	5.23	1.47	1.36
26	i4	201	PEB	C3B-C2B	5.23	1.47	1.36
26	ID	201	PEB	C3B-C2B	5.23	1.47	1.36
26	dB	201	PEB	C3C-C4C	5.23	1.50	1.42
26	YG	202	PEB	C3C-C4C	5.23	1.50	1.42
26	G9	202	PEB	C3B-C2B	5.23	1.47	1.36
27	A6	303	PUB	C2C-C3C	5.23	1.47	1.36
26	D8	202	PEB	C3B-C2B	5.23	1.47	1.36
26	gF	202	PEB	C3C-C4C	5.23	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JJ	202	PEB	C3C-C4C	5.23	1.50	1.42
26	K5	202	PEB	C3B-C2B	5.23	1.47	1.36
26	C8	201	PEB	C3B-C2B	5.23	1.47	1.36
26	G3	201	PEB	C3B-C2B	5.23	1.47	1.36
26	m6	203	PEB	C3B-C2B	5.23	1.47	1.36
26	OA	203	PEB	C3B-C2B	5.23	1.47	1.36
26	B4	202	PEB	C3B-C2B	5.23	1.47	1.36
26	x1	202	PEB	C3C-C4C	5.22	1.50	1.42
26	iI	201	PEB	C3B-C2B	5.22	1.47	1.36
26	b6	202	PEB	C3C-C4C	5.22	1.50	1.42
26	eB	201	PEB	C3B-C2B	5.22	1.47	1.36
26	Q6	203	PEB	C3B-C2B	5.22	1.47	1.36
26	P2	201	PEB	C3B-C2B	5.22	1.47	1.36
26	fE	202	PEB	C3B-C2B	5.22	1.47	1.36
26	kF	202	PEB	C3B-C2B	5.22	1.47	1.36
26	k8	202	PEB	C3C-C4C	5.22	1.50	1.42
26	AG	202	PEB	C3C-C4C	5.22	1.50	1.42
26	dI	202	PEB	C3C-C4C	5.22	1.50	1.42
26	GJ	202	PEB	C3B-C2B	5.22	1.47	1.36
26	EE	202	PEB	C3C-C4C	5.22	1.50	1.42
26	HJ	202	PEB	C3B-C2B	5.22	1.47	1.36
26	E9	202	PEB	C3B-C2B	5.22	1.47	1.36
26	lA	203	PEB	C3B-C2B	5.22	1.47	1.36
26	Q9	201	PEB	C3C-C4C	5.22	1.50	1.42
26	LD	202	PEB	C3B-C2B	5.22	1.47	1.36
26	fB	202	PEB	C3B-C2B	5.22	1.47	1.36
26	k4	201	PEB	C3B-C2B	5.22	1.47	1.36
26	l7	203	PEB	C3C-C4C	5.22	1.50	1.42
27	24	402	PUB	C2B-C1B	5.22	1.50	1.42
26	B4	203	PEB	C3B-C2B	5.22	1.47	1.36
26	SA	202	PEB	C3B-C2B	5.21	1.47	1.36
26	H4	203	PEB	C3C-C4C	5.21	1.50	1.42
26	e8	201	PEB	C3C-C4C	5.21	1.50	1.42
26	WF	203	PEB	C3C-C4C	5.21	1.50	1.42
26	FE	201	PEB	C3B-C2B	5.21	1.47	1.36
26	Q7	203	PEB	C3C-C4C	5.21	1.50	1.42
26	N6	201	PEB	C3B-C2B	5.21	1.47	1.36
26	aF	201	PEB	C3B-C2B	5.21	1.47	1.36
26	IC	202	PEB	C3B-C2B	5.21	1.47	1.36
26	IJ	202	PEB	C3B-C2B	5.21	1.47	1.36
28	J7	1001	CYC	C2A-C3A	5.21	1.47	1.36
26	h2	202	PEB	C3C-C4C	5.21	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K5	201	PEB	C3B-C2B	5.21	1.47	1.36
26	A7	302	PEB	C3C-C4C	5.21	1.50	1.42
26	LD	203	PEB	C3C-C4C	5.21	1.50	1.42
26	U1	201	PEB	C3B-C2B	5.21	1.47	1.36
26	S6	201	PEB	C3B-C2B	5.21	1.47	1.36
26	j2	202	PEB	C3C-C4C	5.21	1.50	1.42
26	h7	202	PEB	C3C-C4C	5.21	1.50	1.42
26	c6	201	PEB	C3B-C2B	5.21	1.47	1.36
26	DA	202	PEB	C3B-C2B	5.21	1.47	1.36
26	P7	202	PEB	C3B-C2B	5.21	1.47	1.36
26	U9	201	PEB	C3B-C2B	5.21	1.47	1.36
26	D3	203	PEB	C3C-C4C	5.21	1.50	1.42
26	fB	203	PEB	C3C-C4C	5.21	1.50	1.42
26	eI	202	PEB	C3C-C4C	5.21	1.50	1.42
26	k1	201	PEB	C3B-C2B	5.21	1.47	1.36
26	C8	203	PEB	C3B-C2B	5.21	1.47	1.36
26	RF	201	PEB	C3B-C2B	5.21	1.47	1.36
26	i2	202	PEB	C3B-C2B	5.21	1.47	1.36
26	U8	203	PEB	C3B-C2B	5.21	1.47	1.36
26	bE	201	PEB	C3C-C4C	5.21	1.50	1.42
28	PH	1001	CYC	C2A-C3A	5.21	1.47	1.36
26	UE	202	PEB	C3C-C4C	5.21	1.50	1.42
26	U6	201	PEB	C3B-C2B	5.21	1.47	1.36
26	tE	202	PEB	C3B-C2B	5.21	1.47	1.36
26	wE	302	PEB	C3C-C4C	5.21	1.50	1.42
26	e2	202	PEB	C3B-C2B	5.21	1.47	1.36
26	l4	201	PEB	C3C-C4C	5.21	1.50	1.42
26	sE	202	PEB	C3C-C4C	5.20	1.50	1.42
26	OI	201	PEB	C3C-C4C	5.20	1.50	1.42
26	eF	201	PEB	C3B-C2B	5.20	1.47	1.36
26	OB	202	PEB	C3B-C2B	5.20	1.47	1.36
26	O6	203	PEB	C3B-C2B	5.20	1.47	1.36
26	LD	203	PEB	C3B-C2B	5.20	1.47	1.36
26	tG	202	PEB	C3B-C2B	5.20	1.47	1.36
28	HF	1001	CYC	C3B-C2B	5.20	1.47	1.36
26	o1	501	PEB	C3C-C4C	5.20	1.50	1.42
26	kA	202	PEB	C3C-C4C	5.20	1.50	1.42
27	A2	303	PUB	C2C-C3C	5.20	1.47	1.36
26	U9	201	PEB	C3C-C4C	5.20	1.50	1.42
26	cF	202	PEB	C3C-C4C	5.20	1.50	1.42
26	z4	202	PEB	C3C-C4C	5.20	1.50	1.42
26	a7	201	PEB	C3C-C4C	5.20	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	vH	1001	CYC	C2A-C3A	5.20	1.47	1.36
26	H6	1002	PEB	C3B-C2B	5.20	1.47	1.36
26	j8	201	PEB	C3C-C4C	5.20	1.50	1.42
26	N4	203	PEB	C3B-C2B	5.20	1.47	1.36
26	TA	202	PEB	C3C-C4C	5.20	1.50	1.42
26	LA	201	PEB	C3B-C2B	5.20	1.47	1.36
26	jA	201	PEB	C3C-C4C	5.20	1.50	1.42
26	gI	203	PEB	C3C-C4C	5.20	1.50	1.42
28	FI	1001	CYC	C2A-C3A	5.20	1.47	1.36
26	kE	202	PEB	C3C-C4C	5.20	1.50	1.42
26	N4	201	PEB	C2A-C1A	-5.20	1.47	1.52
28	K2	1001	CYC	C2A-C3A	5.20	1.47	1.36
26	bF	203	PEB	C3B-C2B	5.20	1.47	1.36
26	P2	202	PEB	C3B-C2B	5.20	1.47	1.36
26	RI	202	PEB	C3C-C4C	5.20	1.50	1.42
26	P1	201	PEB	C3B-C2B	5.20	1.47	1.36
26	XD	201	PEB	C3B-C2B	5.20	1.47	1.36
26	RE	201	PEB	C3B-C2B	5.20	1.47	1.36
26	F3	202	PEB	C3B-C2B	5.19	1.47	1.36
26	O1	201	PEB	C3B-C2B	5.19	1.47	1.36
26	mG	203	PEB	C3C-C4C	5.19	1.50	1.42
26	V1	201	PEB	C3B-C2B	5.19	1.47	1.36
26	u1	201	PEB	C3C-C4C	5.19	1.50	1.42
26	V8	201	PEB	C3B-C2B	5.19	1.47	1.36
28	KI	1001	CYC	C2A-C3A	5.19	1.47	1.36
26	eB	203	PEB	C3B-C2B	5.19	1.47	1.36
26	SB	201	PEB	C3B-C2B	5.19	1.47	1.36
26	V3	202	PEB	C3B-C2B	5.19	1.47	1.36
26	eG	201	PEB	C3B-C2B	5.19	1.47	1.36
26	k2	201	PEB	C3B-C2B	5.19	1.47	1.36
27	AI	303	PUB	C2C-C3C	5.19	1.47	1.36
27	21	402	PUB	C2B-C1B	5.19	1.50	1.42
26	A1	202	PEB	C3B-C2B	5.19	1.47	1.36
26	UD	201	PEB	C3B-C2B	5.19	1.47	1.36
26	L1	201	PEB	C3C-C4C	5.19	1.50	1.42
26	SJ	201	PEB	C3C-C4C	5.19	1.50	1.42
28	NI	1001	CYC	CHB-C1B	5.19	1.50	1.38
26	L8	201	PEB	C2A-C1A	-5.19	1.47	1.52
26	S1	202	PEB	C3C-C4C	5.19	1.50	1.42
26	hB	202	PEB	C3B-C2B	5.19	1.47	1.36
26	PD	202	PEB	C3B-C2B	5.19	1.47	1.36
26	s4	203	PEB	C3C-C4C	5.19	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AF	305	PEB	C3C-C4C	5.19	1.50	1.42
26	PG	201	PEB	C3B-C2B	5.19	1.47	1.36
26	fG	202	PEB	C3B-C2B	5.19	1.47	1.36
27	xG	305	PUB	C2B-C1B	5.19	1.50	1.42
26	S2	202	PEB	C3B-C2B	5.19	1.47	1.36
26	hB	201	PEB	C3B-C2B	5.19	1.47	1.36
26	l6	202	PEB	C3C-C4C	5.19	1.50	1.42
26	R6	202	PEB	C3B-C2B	5.19	1.47	1.36
26	i4	202	PEB	C3C-C4C	5.19	1.50	1.42
26	AF	302	PEB	C3C-C4C	5.19	1.50	1.42
26	AB	304	PEB	C3B-C2B	5.19	1.47	1.36
26	R3	203	PEB	C3B-C2B	5.18	1.47	1.36
26	T3	203	PEB	C3B-C2B	5.18	1.47	1.36
26	A6	304	PEB	C3B-C2B	5.18	1.47	1.36
26	z1	202	PEB	C3C-C4C	5.18	1.50	1.42
26	O8	201	PEB	C3B-C2B	5.18	1.47	1.36
26	SJ	202	PEB	C3B-C2B	5.18	1.47	1.36
28	C7	1001	CYC	C2A-C3A	5.18	1.47	1.36
26	B4	202	PEB	C3C-C4C	5.18	1.50	1.42
26	K9	202	PEB	C3C-C4C	5.18	1.50	1.42
26	NE	201	PEB	C3C-C4C	5.18	1.50	1.42
26	eE	201	PEB	C3C-C4C	5.18	1.50	1.42
26	UA	203	PEB	C3B-C2B	5.18	1.47	1.36
26	PI	202	PEB	C3B-C2B	5.18	1.47	1.36
26	P4	201	PEB	C3B-C2B	5.18	1.47	1.36
26	GE	201	PEB	C3C-C4C	5.18	1.50	1.42
26	U6	203	PEB	C3B-C2B	5.18	1.47	1.36
26	gB	201	PEB	C3B-C2B	5.18	1.47	1.36
26	P1	203	PEB	C3B-C2B	5.18	1.47	1.36
28	qH	1002	CYC	CHB-C1B	5.18	1.50	1.38
26	G4	201	PEB	C3C-C4C	5.18	1.50	1.42
26	x1	201	PEB	C3B-C2B	5.18	1.47	1.36
28	DF	1001	CYC	C2A-C3A	5.18	1.47	1.36
26	ZE	201	PEB	C3C-C4C	5.18	1.50	1.42
26	HB	1002	PEB	C3B-C2B	5.18	1.47	1.36
26	U3	202	PEB	C3C-C4C	5.18	1.50	1.42
26	Y9	201	PEB	C3C-C4C	5.18	1.50	1.42
26	YI	201	PEB	C3C-C4C	5.18	1.50	1.42
26	b7	202	PEB	C3C-C4C	5.18	1.50	1.42
26	Q9	201	PEB	C3B-C2B	5.18	1.47	1.36
26	CC	202	PEB	C3C-C4C	5.18	1.50	1.42
26	P3	201	PEB	C3C-C4C	5.17	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M9	202	PEB	C3C-C4C	5.17	1.50	1.42
26	G4	202	PEB	C3B-C2B	5.17	1.47	1.36
26	O4	202	PEB	C3B-C2B	5.17	1.47	1.36
28	D7	1001	CYC	C2A-C3A	5.17	1.47	1.36
26	M1	401	PEB	C3C-C4C	5.17	1.50	1.42
26	TA	201	PEB	C3B-C2B	5.17	1.47	1.36
26	uE	202	PEB	C3B-C2B	5.17	1.47	1.36
26	ZB	201	PEB	C3C-C4C	5.17	1.50	1.42
26	vG	201	PEB	C3C-C4C	5.17	1.50	1.42
26	FI	1002	PEB	C3B-C2B	5.17	1.47	1.36
26	TJ	202	PEB	C3B-C2B	5.17	1.47	1.36
26	cF	202	PEB	C3B-C2B	5.17	1.47	1.36
26	RB	202	PEB	C3B-C2B	5.17	1.47	1.36
26	l4	202	PEB	C3C-C4C	5.17	1.50	1.42
26	e6	201	PEB	C3C-C4C	5.17	1.50	1.42
26	aF	201	PEB	C3C-C4C	5.17	1.50	1.42
28	SH	1001	CYC	C2A-C3A	5.17	1.47	1.36
26	UA	201	PEB	C3B-C2B	5.17	1.47	1.36
26	W2	201	PEB	C3C-C4C	5.17	1.50	1.42
26	V7	201	PEB	C3C-C4C	5.17	1.50	1.42
26	l8	203	PEB	C3B-C2B	5.17	1.47	1.36
28	TH	1001	CYC	C2A-C3A	5.17	1.47	1.36
26	AC	202	PEB	C3C-C4C	5.17	1.50	1.42
26	b6	202	PEB	C3B-C2B	5.17	1.47	1.36
26	d6	201	PEB	C3C-C4C	5.17	1.50	1.42
26	I8	201	PEB	C3C-C4C	5.17	1.50	1.42
26	wG	302	PEB	C3C-C4C	5.17	1.50	1.42
26	F2	1002	PEB	C3B-C2B	5.17	1.47	1.36
26	CC	201	PEB	C3C-C4C	5.17	1.50	1.42
26	VF	203	PEB	C3B-C2B	5.17	1.47	1.36
28	D2	1001	CYC	C3B-C2B	5.17	1.47	1.36
26	XA	201	PEB	C3C-C4C	5.16	1.50	1.42
26	WG	201	PEB	C3B-C2B	5.16	1.47	1.36
26	Z6	201	PEB	C3C-C4C	5.16	1.50	1.42
26	T7	202	PEB	C3B-C2B	5.16	1.47	1.36
26	U2	202	PEB	C3B-C2B	5.16	1.47	1.36
26	A8	302	PEB	C3B-C2B	5.16	1.47	1.36
26	C5	201	PEB	C3C-C4C	5.16	1.50	1.42
27	yG	303	PUB	C2B-C1B	5.16	1.50	1.42
26	TD	201	PEB	C3B-C2B	5.16	1.47	1.36
26	P7	202	PEB	C3C-C4C	5.16	1.50	1.42
26	PF	202	PEB	C3C-C4C	5.16	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UD	202	PEB	C3B-C2B	5.16	1.47	1.36
26	VF	202	PEB	C3B-C2B	5.16	1.47	1.36
27	xG	301	PUB	C2B-C1B	5.16	1.50	1.42
26	Q6	201	PEB	C3B-C2B	5.16	1.47	1.36
26	NB	1002	PEB	C3B-C2B	5.16	1.47	1.36
26	mG	201	PEB	C3C-C4C	5.16	1.50	1.42
26	eG	201	PEB	C3C-C4C	5.16	1.50	1.42
26	v1	201	PEB	C3B-C2B	5.16	1.47	1.36
26	a8	203	PEB	C3B-C2B	5.16	1.47	1.36
26	XJ	201	PEB	C3C-C4C	5.16	1.50	1.42
28	DI	1001	CYC	C3B-C2B	5.16	1.47	1.36
26	U8	201	PEB	C3B-C2B	5.16	1.47	1.36
28	uH	1001	CYC	C2A-C3A	5.16	1.47	1.36
26	k6	202	PEB	C3B-C2B	5.16	1.47	1.36
26	ND	203	PEB	C3B-C2B	5.16	1.47	1.36
26	VD	203	PEB	C3B-C2B	5.16	1.47	1.36
26	Y2	201	PEB	C3C-C4C	5.16	1.50	1.42
26	WI	201	PEB	C3C-C4C	5.16	1.50	1.42
26	S6	203	PEB	C3C-C4C	5.16	1.50	1.42
26	U3	201	PEB	C3B-C2B	5.15	1.47	1.36
26	P9	202	PEB	C3B-C2B	5.15	1.47	1.36
26	rE	202	PEB	C3B-C2B	5.15	1.47	1.36
26	C5	203	PEB	C3C-C4C	5.15	1.50	1.42
26	f6	202	PEB	C3C-C4C	5.15	1.50	1.42
26	S7	203	PEB	C3B-C2B	5.15	1.47	1.36
26	dI	201	PEB	C3C-C4C	5.15	1.50	1.42
26	PJ	202	PEB	C3C-C4C	5.15	1.50	1.42
26	HG	201	PEB	C3B-C2B	5.15	1.47	1.36
26	O8	203	PEB	C3B-C2B	5.15	1.47	1.36
26	QB	202	PEB	C3B-C2B	5.15	1.47	1.36
26	T3	201	PEB	C3B-C2B	5.15	1.47	1.36
26	pE	202	PEB	C3B-C2B	5.15	1.47	1.36
26	G1	201	PEB	C3C-C4C	5.15	1.50	1.42
26	f2	202	PEB	C3C-C4C	5.15	1.50	1.42
26	e4	201	PEB	C3C-C4C	5.15	1.50	1.42
26	QA	203	PEB	C3B-C2B	5.15	1.47	1.36
26	cA	203	PEB	C3B-C2B	5.15	1.47	1.36
26	M3	201	PEB	C3B-C2B	5.15	1.47	1.36
26	H1	203	PEB	C3C-C4C	5.15	1.50	1.42
26	G8	201	PEB	C3C-C4C	5.15	1.50	1.42
26	mB	203	PEB	C3B-C2B	5.15	1.47	1.36
26	g6	201	PEB	C3B-C2B	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	LI	1001	CYC	C2A-C3A	5.15	1.47	1.36
26	14	201	PEB	C3C-C4C	5.15	1.50	1.42
26	I1	202	PEB	C3B-C2B	5.15	1.47	1.36
26	W6	202	PEB	C3B-C2B	5.15	1.47	1.36
26	S4	202	PEB	C3C-C4C	5.15	1.50	1.42
26	L8	201	PEB	C3B-C2B	5.15	1.47	1.36
26	SI	202	PEB	C3B-C2B	5.15	1.47	1.36
26	R3	202	PEB	C3B-C2B	5.14	1.47	1.36
26	U3	201	PEB	C1A-NA	-5.14	1.30	1.37
26	I4	202	PEB	C3B-C2B	5.14	1.47	1.36
26	j4	202	PEB	C3B-C2B	5.14	1.47	1.36
26	UI	202	PEB	C3B-C2B	5.14	1.47	1.36
26	a6	201	PEB	C3C-C4C	5.14	1.50	1.42
26	hI	202	PEB	C3C-C4C	5.14	1.50	1.42
26	lB	202	PEB	C3B-C2B	5.14	1.47	1.36
26	pE	201	PEB	C3C-C4C	5.14	1.50	1.42
26	W4	202	PEB	C3B-C2B	5.14	1.47	1.36
26	XE	201	PEB	C3B-C2B	5.14	1.47	1.36
26	c7	202	PEB	C3B-C2B	5.14	1.47	1.36
26	FC	203	PEB	C3B-C2B	5.14	1.47	1.36
26	W1	202	PEB	C3B-C2B	5.14	1.47	1.36
26	O6	203	PEB	C3C-C4C	5.14	1.50	1.42
26	DJ	202	PEB	C3C-C4C	5.14	1.50	1.42
28	M2	1001	CYC	C2A-C3A	5.14	1.47	1.36
26	OI	202	PEB	C3B-C2B	5.14	1.47	1.36
26	A7	305	PEB	C3C-C4C	5.14	1.50	1.42
26	D3	201	PEB	C3C-C4C	5.14	1.50	1.42
27	xE	301	PUB	C2B-C1B	5.14	1.50	1.42
26	V2	203	PEB	C3B-C2B	5.14	1.47	1.36
26	R2	202	PEB	C3C-C4C	5.14	1.50	1.42
26	d4	201	PEB	C3C-C4C	5.14	1.50	1.42
26	HC	201	PEB	C3B-C2B	5.14	1.47	1.36
26	O4	202	PEB	C3C-C4C	5.13	1.50	1.42
26	k7	202	PEB	C3B-C2B	5.13	1.47	1.36
26	PI	202	PEB	C3C-C4C	5.13	1.50	1.42
26	cB	201	PEB	C3B-C2B	5.13	1.47	1.36
26	D3	202	PEB	C3C-C4C	5.13	1.50	1.42
26	H4	201	PEB	C3C-C4C	5.13	1.50	1.42
26	T2	203	PEB	C3B-C2B	5.13	1.47	1.36
26	O6	202	PEB	C3B-C2B	5.13	1.47	1.36
26	YI	202	PEB	C3B-C2B	5.13	1.47	1.36
26	F4	201	PEB	C3B-C2B	5.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c8	202	PEB	C3B-C2B	5.13	1.47	1.36
28	L2	1001	CYC	C2A-C3A	5.13	1.47	1.36
26	LC	201	PEB	C3B-C2B	5.13	1.47	1.36
26	c7	202	PEB	C3C-C4C	5.13	1.50	1.42
26	MD	202	PEB	C3C-C4C	5.13	1.50	1.42
28	EB	1001	CYC	C2A-C3A	5.13	1.47	1.36
26	k6	201	PEB	C3C-C4C	5.13	1.50	1.42
26	kB	201	PEB	C3C-C4C	5.13	1.50	1.42
28	dH	1001	CYC	C3B-C2B	5.13	1.47	1.36
26	g7	201	PEB	C3B-C2B	5.13	1.47	1.36
26	FC	202	PEB	C3B-C2B	5.13	1.47	1.36
26	cG	201	PEB	C3B-C2B	5.13	1.47	1.36
26	w1	203	PEB	C3C-C4C	5.13	1.50	1.42
26	Q8	202	PEB	C3C-C4C	5.13	1.50	1.42
26	SB	203	PEB	C3C-C4C	5.13	1.50	1.42
26	w1	201	PEB	C3C-C4C	5.13	1.50	1.42
28	E7	1001	CYC	C2A-C3A	5.13	1.47	1.36
26	IA	201	PEB	C3C-C4C	5.13	1.50	1.42
26	UG	202	PEB	C3C-C4C	5.13	1.50	1.42
26	aG	201	PEB	C3C-C4C	5.13	1.50	1.42
26	IG	203	PEB	C3B-C2B	5.13	1.47	1.36
26	u4	201	PEB	C3B-C2B	5.13	1.47	1.36
26	C5	202	PEB	C3C-C4C	5.13	1.50	1.42
26	D1	202	PEB	C3B-C2B	5.12	1.47	1.36
26	W7	203	PEB	C3C-C4C	5.12	1.50	1.42
26	l6	202	PEB	C3B-C2B	5.12	1.47	1.36
26	bI	202	PEB	C3C-C4C	5.12	1.50	1.42
26	j6	201	PEB	C3B-C2B	5.12	1.47	1.36
27	K1	203	PUB	C2C-C3C	5.12	1.47	1.36
26	dG	202	PEB	C3B-C2B	5.12	1.47	1.36
26	O1	202	PEB	C3C-C4C	5.12	1.50	1.42
26	T9	202	PEB	C3B-C2B	5.12	1.47	1.36
26	GA	201	PEB	C3B-C2B	5.12	1.47	1.36
26	mI	201	PEB	C3B-C2B	5.12	1.47	1.36
26	I3	202	PEB	C3C-C4C	5.12	1.50	1.42
26	aB	201	PEB	C3C-C4C	5.12	1.50	1.42
26	OF	202	PEB	C3C-C4C	5.12	1.50	1.42
26	WB	202	PEB	C3B-C2B	5.12	1.47	1.36
26	K1	201	PEB	C3C-C4C	5.12	1.50	1.42
26	p1	201	PEB	C3C-C4C	5.12	1.50	1.42
27	K1	203	PUB	C2B-C1B	5.12	1.50	1.42
26	q1	203	PEB	C3C-C4C	5.12	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	QG	202	PEB	C3B-C2B	5.12	1.47	1.36
26	xG	304	PEB	C3C-C4C	5.12	1.50	1.42
27	yE	303	PUB	C2C-C3C	5.12	1.47	1.36
26	UF	202	PEB	C3B-C2B	5.12	1.47	1.36
26	h2	201	PEB	C3C-C4C	5.12	1.50	1.42
26	PE	201	PEB	C3C-C4C	5.12	1.50	1.42
26	IC	201	PEB	C3B-C2B	5.12	1.47	1.36
26	UB	202	PEB	C3B-C2B	5.11	1.47	1.36
26	D4	203	PEB	C3C-C4C	5.11	1.50	1.42
26	D7	1002	PEB	C3C-C4C	5.11	1.50	1.42
26	l7	202	PEB	C3C-C4C	5.11	1.50	1.42
26	HD	203	PEB	C3C-C4C	5.11	1.50	1.42
28	DI	1001	CYC	C2A-C3A	5.11	1.47	1.36
26	S4	201	PEB	C3B-C2B	5.11	1.47	1.36
26	B9	202	PEB	C3B-C2B	5.11	1.47	1.36
26	G1	202	PEB	C3B-C2B	5.11	1.47	1.36
26	FG	201	PEB	C3B-C2B	5.11	1.47	1.36
26	WJ	201	PEB	C3C-C4C	5.11	1.50	1.42
27	A9	302	PUB	C2C-C3C	5.11	1.47	1.36
26	S2	201	PEB	C3C-C4C	5.11	1.50	1.42
26	K4	202	PEB	C3C-C4C	5.11	1.50	1.42
26	p4	201	PEB	C3B-C2B	5.11	1.47	1.36
26	AJ	305	PEB	C3B-C2B	5.11	1.47	1.36
26	LJ	203	PEB	C3B-C2B	5.11	1.47	1.36
27	AJ	302	PUB	C2C-C3C	5.11	1.47	1.36
26	XA	202	PEB	C3B-C2B	5.11	1.47	1.36
26	X3	201	PEB	C3B-C2B	5.11	1.47	1.36
26	eB	202	PEB	C3B-C2B	5.11	1.47	1.36
26	iF	201	PEB	C3B-C2B	5.11	1.47	1.36
28	I2	1001	CYC	C2A-C3A	5.11	1.47	1.36
26	eB	201	PEB	C3C-C4C	5.11	1.50	1.42
28	EF	1001	CYC	C2A-C3A	5.11	1.47	1.36
26	Q2	202	PEB	C3B-C2B	5.11	1.47	1.36
26	B5	201	PEB	C3C-C4C	5.11	1.50	1.42
26	WJ	202	PEB	C3C-C4C	5.11	1.50	1.42
26	h6	202	PEB	C3B-C2B	5.11	1.47	1.36
26	aG	202	PEB	C3C-C4C	5.11	1.50	1.42
28	MI	1001	CYC	C2A-C3A	5.11	1.47	1.36
26	QD	202	PEB	C3B-C2B	5.11	1.47	1.36
26	J5	202	PEB	C3B-C2B	5.11	1.47	1.36
26	k6	201	PEB	C3B-C2B	5.11	1.47	1.36
26	CJ	202	PEB	C3C-C4C	5.10	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	FC	201	PEB	C3B-C2B	5.10	1.47	1.36
26	SJ	201	PEB	C3B-C2B	5.10	1.47	1.36
26	GA	201	PEB	C3C-C4C	5.10	1.50	1.42
26	CG	203	PEB	C3C-C4C	5.10	1.50	1.42
26	ZE	202	PEB	C3B-C2B	5.10	1.47	1.36
26	XJ	202	PEB	C3C-C4C	5.10	1.50	1.42
26	K5	203	PEB	C3B-C2B	5.10	1.47	1.36
26	QA	202	PEB	C3C-C4C	5.10	1.50	1.42
26	O4	201	PEB	C3B-C2B	5.10	1.47	1.36
26	VI	202	PEB	C3B-C2B	5.10	1.47	1.36
26	S8	201	PEB	C3C-C4C	5.10	1.50	1.42
26	dB	203	PEB	C3C-C4C	5.10	1.50	1.42
26	f8	202	PEB	C3B-C2B	5.10	1.47	1.36
26	M3	202	PEB	C3C-C4C	5.10	1.50	1.42
26	QB	201	PEB	C3B-C2B	5.10	1.47	1.36
26	Y2	202	PEB	C3B-C2B	5.10	1.47	1.36
26	dB	202	PEB	C3C-C4C	5.10	1.50	1.42
26	g2	202	PEB	C3C-C4C	5.10	1.50	1.42
26	L3	203	PEB	C3B-C2B	5.10	1.47	1.36
26	S3	202	PEB	C3B-C2B	5.10	1.47	1.36
26	O7	202	PEB	C3C-C4C	5.10	1.50	1.42
26	P3	202	PEB	C3B-C2B	5.10	1.47	1.36
26	hB	202	PEB	C3C-C4C	5.10	1.50	1.42
26	S1	201	PEB	C3B-C2B	5.10	1.47	1.36
26	O2	202	PEB	C3B-C2B	5.10	1.47	1.36
26	Q2	201	PEB	C3C-C4C	5.10	1.50	1.42
26	BC	202	PEB	C3C-C4C	5.09	1.50	1.42
26	F7	1002	PEB	C3B-C2B	5.09	1.47	1.36
26	XG	201	PEB	C3B-C2B	5.09	1.47	1.36
26	gI	201	PEB	C3B-C2B	5.09	1.47	1.36
26	SD	202	PEB	C3B-C2B	5.09	1.47	1.36
26	V8	202	PEB	C2A-C1A	-5.09	1.47	1.52
26	V3	203	PEB	C3B-C2B	5.09	1.47	1.36
26	FG	201	PEB	C2A-C1A	-5.09	1.47	1.52
26	O1	202	PEB	C3B-C2B	5.09	1.47	1.36
26	K1	201	PEB	C3B-C2B	5.09	1.47	1.36
26	B1	203	PEB	C3B-C2B	5.09	1.47	1.36
26	vE	202	PEB	C3B-C2B	5.09	1.47	1.36
26	I5	202	PEB	C3B-C2B	5.09	1.47	1.36
26	KG	202	PEB	C3B-C2B	5.09	1.47	1.36
26	c6	202	PEB	C3C-C4C	5.09	1.50	1.42
26	a8	201	PEB	C3C-C4C	5.09	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	GB	1001	CYC	C2A-C3A	5.09	1.47	1.36
26	kB	201	PEB	C3B-C2B	5.09	1.47	1.36
26	ZG	201	PEB	C3C-C4C	5.09	1.50	1.42
26	SD	201	PEB	C1A-NA	-5.09	1.31	1.37
26	m2	201	PEB	C3B-C2B	5.09	1.47	1.36
26	BE	201	PEB	C3B-C2B	5.09	1.47	1.36
26	iI	202	PEB	C3B-C2B	5.09	1.47	1.36
27	AF	304	PUB	C2B-C1B	5.09	1.50	1.42
26	Q3	202	PEB	C3B-C2B	5.09	1.47	1.36
26	yE	301	PEB	C3B-C2B	5.09	1.47	1.36
26	Y2	203	PEB	C3B-C2B	5.09	1.47	1.36
26	I8	202	PEB	C3B-C2B	5.09	1.47	1.36
26	EG	202	PEB	C3B-C2B	5.08	1.47	1.36
26	i2	202	PEB	C3C-C4C	5.08	1.50	1.42
26	fI	202	PEB	C3C-C4C	5.08	1.50	1.42
26	G8	201	PEB	C3B-C2B	5.08	1.47	1.36
26	L8	202	PEB	C3B-C2B	5.08	1.47	1.36
26	OG	203	PEB	C3B-C2B	5.08	1.47	1.36
26	aI	203	PEB	C3C-C4C	5.08	1.50	1.42
26	L9	203	PEB	C3B-C2B	5.08	1.47	1.36
26	FD	202	PEB	C3B-C2B	5.08	1.47	1.36
26	eB	202	PEB	C3C-C4C	5.08	1.50	1.42
26	fB	202	PEB	C3C-C4C	5.08	1.50	1.42
28	D2	1001	CYC	C2A-C3A	5.08	1.47	1.36
28	II	1001	CYC	C2A-C3A	5.08	1.47	1.36
26	R1	202	PEB	C3C-C4C	5.08	1.50	1.42
26	iE	203	PEB	C3C-C4C	5.08	1.50	1.42
26	N9	202	PEB	C3B-C2B	5.08	1.47	1.36
28	KH	1001	CYC	C3B-C2B	5.08	1.47	1.36
26	cE	202	PEB	C3C-C4C	5.08	1.50	1.42
26	RJ	203	PEB	C3C-C4C	5.08	1.50	1.42
26	d6	203	PEB	C3C-C4C	5.08	1.50	1.42
26	MG	201	PEB	C3C-C4C	5.08	1.50	1.42
26	h6	202	PEB	C3C-C4C	5.08	1.50	1.42
27	N9	201	PUB	C2C-C3C	5.08	1.47	1.36
26	21	405	PEB	C3C-C4C	5.08	1.50	1.42
26	17	201	PEB	C3C-C4C	5.08	1.50	1.42
26	KD	202	PEB	C3C-C4C	5.08	1.50	1.42
26	dF	202	PEB	C3C-C4C	5.08	1.50	1.42
26	24	404	PEB	C3C-C4C	5.08	1.50	1.42
26	KE	203	PEB	C3B-C2B	5.08	1.47	1.36
26	TI	203	PEB	C3B-C2B	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YA	201	PEB	C3B-C2B	5.08	1.47	1.36
26	hA	202	PEB	C3B-C2B	5.08	1.47	1.36
26	t1	201	PEB	C3C-C4C	5.07	1.50	1.42
26	c4	202	PEB	C3C-C4C	5.07	1.50	1.42
26	DE	201	PEB	C3B-C2B	5.07	1.47	1.36
26	N8	201	PEB	C2A-C1A	-5.07	1.47	1.52
26	X8	201	PEB	C3C-C4C	5.07	1.50	1.42
26	oG	203	PEB	C3C-C4C	5.07	1.50	1.42
26	L3	201	PEB	C3B-C2B	5.07	1.47	1.36
26	g4	202	PEB	C3C-C4C	5.07	1.50	1.42
26	m7	202	PEB	C3C-C4C	5.07	1.50	1.42
26	AA	302	PEB	C3C-C4C	5.07	1.50	1.42
26	VB	201	PEB	C3C-C4C	5.07	1.50	1.42
26	Y8	201	PEB	C3B-C2B	5.07	1.47	1.36
26	g4	201	PEB	C3B-C2B	5.07	1.47	1.36
26	e8	202	PEB	C3B-C2B	5.07	1.47	1.36
26	T8	201	PEB	C3B-C2B	5.07	1.47	1.36
28	D6	1001	CYC	C2A-C3A	5.07	1.47	1.36
26	c2	202	PEB	C3C-C4C	5.07	1.50	1.42
26	gA	202	PEB	C3C-C4C	5.07	1.50	1.42
26	LC	202	PEB	C3C-C4C	5.07	1.50	1.42
26	M1	402	PEB	C3C-C4C	5.07	1.50	1.42
26	fA	201	PEB	C3C-C4C	5.07	1.50	1.42
26	iE	201	PEB	C3C-C4C	5.07	1.50	1.42
26	d1	203	PEB	C3C-C4C	5.07	1.50	1.42
26	V6	201	PEB	C3C-C4C	5.07	1.50	1.42
26	I4	201	PEB	C3B-C2B	5.07	1.47	1.36
26	dE	202	PEB	C3B-C2B	5.07	1.47	1.36
27	A4	203	PUB	C2C-C3C	5.07	1.47	1.36
26	J9	201	PEB	C3C-C4C	5.07	1.50	1.42
26	ZB	202	PEB	C3B-C2B	5.07	1.47	1.36
26	vG	202	PEB	C3B-C2B	5.07	1.47	1.36
26	q4	201	PEB	C3C-C4C	5.07	1.50	1.42
26	hI	201	PEB	C3C-C4C	5.07	1.50	1.42
27	xE	301	PUB	C2C-C3C	5.07	1.47	1.36
26	H1	201	PEB	C3C-C4C	5.06	1.50	1.42
26	lB	203	PEB	C3C-C4C	5.06	1.50	1.42
26	F5	202	PEB	C3B-C2B	5.06	1.47	1.36
26	s1	203	PEB	C3C-C4C	5.06	1.50	1.42
26	a2	202	PEB	C3C-C4C	5.06	1.50	1.42
26	PG	201	PEB	C3C-C4C	5.06	1.49	1.42
26	dB	203	PEB	C3B-C2B	5.06	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O7	203	PEB	C3C-C4C	5.06	1.49	1.42
26	SI	201	PEB	C3C-C4C	5.06	1.49	1.42
26	YJ	201	PEB	C3B-C2B	5.06	1.47	1.36
28	NF	1001	CYC	CHB-C1B	5.06	1.50	1.38
26	b6	201	PEB	C3C-C4C	5.06	1.49	1.42
26	IA	202	PEB	C3B-C2B	5.06	1.47	1.36
28	QH	1001	CYC	C2A-C3A	5.06	1.47	1.36
26	A9	304	PEB	C3C-C4C	5.06	1.49	1.42
26	ND	201	PEB	C3B-C2B	5.06	1.47	1.36
26	k4	201	PEB	C3C-C4C	5.06	1.49	1.42
26	u1	203	PEB	C3B-C2B	5.06	1.47	1.36
26	b6	201	PEB	C3B-C2B	5.06	1.47	1.36
27	AA	304	PUB	C2C-C3C	5.06	1.47	1.36
26	Z8	202	PEB	C3C-C4C	5.06	1.49	1.42
26	IE	202	PEB	C3C-C4C	5.06	1.49	1.42
28	G6	1001	CYC	C2A-C3A	5.06	1.47	1.36
26	cG	203	PEB	C3C-C4C	5.06	1.49	1.42
26	iI	202	PEB	C3C-C4C	5.06	1.49	1.42
26	aA	204	PEB	C3B-C2B	5.06	1.47	1.36
28	DB	1001	CYC	C2A-C3A	5.06	1.47	1.36
26	S9	201	PEB	C3B-C2B	5.06	1.47	1.36
26	UI	201	PEB	C3C-C4C	5.06	1.49	1.42
26	w4	201	PEB	C3C-C4C	5.06	1.49	1.42
26	RI	201	PEB	C3C-C4C	5.06	1.49	1.42
26	QB	202	PEB	C3C-C4C	5.06	1.49	1.42
26	RG	201	PEB	C3B-C2B	5.06	1.47	1.36
26	IC	201	PEB	C3C-C4C	5.06	1.49	1.42
26	CE	201	PEB	C3C-C4C	5.06	1.49	1.42
26	S3	201	PEB	C1A-NA	-5.06	1.31	1.37
26	F9	201	PEB	C3B-C2B	5.05	1.47	1.36
26	D2	1002	PEB	C3C-C4C	5.05	1.49	1.42
26	Q4	202	PEB	C3B-C2B	5.05	1.47	1.36
26	J2	1002	PEB	C3B-C2B	5.05	1.47	1.36
26	x4	201	PEB	C3B-C2B	5.05	1.47	1.36
27	A8	304	PUB	C2C-C3C	5.05	1.47	1.36
26	v1	201	PEB	C3C-C4C	5.05	1.49	1.42
26	K6	201	PEB	C3B-C2B	5.05	1.47	1.36
26	F7	1002	PEB	C3C-C4C	5.05	1.49	1.42
28	E6	1001	CYC	CHB-C1B	5.05	1.50	1.38
26	dB	204	PEB	C3C-C4C	5.05	1.49	1.42
26	XJ	203	PEB	C3C-C4C	5.05	1.49	1.42
26	JI	1002	PEB	C3B-C2B	5.05	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	HI	1002	PEB	C3B-C2B	5.05	1.47	1.36
26	a2	203	PEB	C3C-C4C	5.05	1.49	1.42
26	EG	202	PEB	C3C-C4C	5.05	1.49	1.42
26	Q1	202	PEB	C3B-C2B	5.05	1.47	1.36
26	A9	303	PEB	C3C-C4C	5.05	1.49	1.42
26	bB	201	PEB	C3C-C4C	5.05	1.49	1.42
26	mE	201	PEB	C3C-C4C	5.05	1.49	1.42
26	xE	303	PEB	C3C-C4C	5.05	1.49	1.42
26	j1	202	PEB	C3C-C4C	5.05	1.49	1.42
26	T8	202	PEB	C3C-C4C	5.05	1.49	1.42
26	GD	201	PEB	C3C-C4C	5.05	1.49	1.42
26	ZA	202	PEB	C3C-C4C	5.05	1.49	1.42
26	m6	202	PEB	C3B-C2B	5.05	1.47	1.36
26	tG	201	PEB	C3C-C4C	5.05	1.49	1.42
26	H2	1002	PEB	C3B-C2B	5.04	1.47	1.36
26	UJ	201	PEB	C3B-C2B	5.04	1.47	1.36
27	YD	302	PUB	C2C-C3C	5.04	1.47	1.36
28	FH	1001	CYC	CHA-C1A	5.04	1.39	1.35
26	VF	201	PEB	C3B-C2B	5.04	1.47	1.36
26	R2	201	PEB	C3C-C4C	5.04	1.49	1.42
26	PA	202	PEB	C3B-C2B	5.04	1.47	1.36
26	N3	203	PEB	C3B-C2B	5.04	1.47	1.36
26	AD	202	PEB	C3C-C4C	5.04	1.49	1.42
28	HB	1001	CYC	C3B-C2B	5.04	1.47	1.36
26	d7	202	PEB	C3C-C4C	5.04	1.49	1.42
26	d2	202	PEB	C3B-C2B	5.04	1.47	1.36
26	i2	201	PEB	C3B-C2B	5.04	1.47	1.36
26	CD	201	PEB	C3B-C2B	5.04	1.47	1.36
27	Y3	302	PUB	C2C-C3C	5.04	1.47	1.36
26	Z6	202	PEB	C3C-C4C	5.04	1.49	1.42
26	ZB	202	PEB	C3C-C4C	5.04	1.49	1.42
26	d1	201	PEB	C3B-C2B	5.04	1.47	1.36
26	g7	202	PEB	C3C-C4C	5.04	1.49	1.42
26	VD	203	PEB	C3C-C4C	5.04	1.49	1.42
27	xG	306	PUB	C2C-C3C	5.03	1.47	1.36
26	U4	202	PEB	C3B-C2B	5.03	1.47	1.36
26	OE	203	PEB	C3B-C2B	5.03	1.47	1.36
26	YF	201	PEB	C3B-C2B	5.03	1.47	1.36
26	B3	202	PEB	C3C-C4C	5.03	1.49	1.42
26	K3	201	PEB	C3C-C4C	5.03	1.49	1.42
26	R4	202	PEB	C3C-C4C	5.03	1.49	1.42
26	b7	201	PEB	C3C-C4C	5.03	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	SA	203	PEB	C3B-C2B	5.03	1.47	1.36
28	H6	1001	CYC	C3B-C2B	5.03	1.47	1.36
26	OB	203	PEB	C3C-C4C	5.03	1.49	1.42
26	hB	201	PEB	C3C-C4C	5.03	1.49	1.42
26	KA	201	PEB	C3B-C2B	5.03	1.47	1.36
26	HC	203	PEB	C3B-C2B	5.03	1.47	1.36
26	C9	202	PEB	C3C-C4C	5.03	1.49	1.42
26	e2	201	PEB	C3C-C4C	5.03	1.49	1.42
26	UD	201	PEB	C1A-NA	-5.03	1.31	1.37
26	E3	201	PEB	C3C-C4C	5.03	1.49	1.42
26	ID	202	PEB	C3C-C4C	5.03	1.49	1.42
27	yE	302	PUB	C2C-C3C	5.03	1.47	1.36
26	X4	202	PEB	C1A-NA	-5.03	1.31	1.37
26	UB	203	PEB	C3B-C2B	5.03	1.47	1.36
26	WG	202	PEB	C3B-C2B	5.03	1.47	1.36
26	v4	201	PEB	C3B-C2B	5.03	1.47	1.36
26	RI	202	PEB	C3B-C2B	5.03	1.47	1.36
26	b2	202	PEB	C3C-C4C	5.03	1.49	1.42
26	T3	202	PEB	C3C-C4C	5.03	1.49	1.42
26	cA	203	PEB	C3C-C4C	5.03	1.49	1.42
26	KB	201	PEB	C3B-C2B	5.03	1.47	1.36
26	aA	204	PEB	C3C-C4C	5.03	1.49	1.42
26	YI	202	PEB	C3C-C4C	5.03	1.49	1.42
26	F5	201	PEB	C3B-C2B	5.02	1.47	1.36
26	h6	201	PEB	C3C-C4C	5.02	1.49	1.42
26	lG	201	PEB	C3C-C4C	5.02	1.49	1.42
26	Y8	202	PEB	C3B-C2B	5.02	1.47	1.36
26	OD	201	PEB	C1A-NA	-5.02	1.31	1.37
26	Y3	304	PEB	C3C-C4C	5.02	1.49	1.42
26	aG	202	PEB	C3B-C2B	5.02	1.47	1.36
26	d6	202	PEB	C3C-C4C	5.02	1.49	1.42
26	K4	201	PEB	C3B-C2B	5.02	1.47	1.36
26	AD	201	PEB	C3C-C4C	5.02	1.49	1.42
26	L5	201	PEB	C3B-C2B	5.02	1.47	1.36
26	ZB	203	PEB	C3B-C2B	5.02	1.47	1.36
26	yG	301	PEB	C3B-C2B	5.02	1.47	1.36
26	GG	201	PEB	C3C-C4C	5.02	1.49	1.42
28	N7	1001	CYC	CHB-C1B	5.02	1.50	1.38
27	yE	302	PUB	C2B-C1B	5.02	1.49	1.42
28	DF	1003	CYC	C2A-C3A	5.02	1.47	1.36
26	r1	202	PEB	C3C-C4C	5.02	1.49	1.42
26	a4	202	PEB	C3C-C4C	5.02	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L5	202	PEB	C3C-C4C	5.02	1.49	1.42
26	K9	201	PEB	C3C-C4C	5.02	1.49	1.42
27	A7	303	PUB	C2B-C1B	5.02	1.49	1.42
26	J7	1002	PEB	C3B-C2B	5.02	1.47	1.36
26	V9	201	PEB	C3C-C4C	5.02	1.49	1.42
26	YI	203	PEB	C3B-C2B	5.02	1.47	1.36
26	U2	201	PEB	C3C-C4C	5.02	1.49	1.42
26	h8	202	PEB	C3B-C2B	5.02	1.47	1.36
26	i7	201	PEB	C3C-C4C	5.02	1.49	1.42
26	TD	202	PEB	C3C-C4C	5.01	1.49	1.42
26	BG	201	PEB	C3B-C2B	5.01	1.47	1.36
26	c7	201	PEB	C3B-C2B	5.01	1.47	1.36
26	YA	202	PEB	C3B-C2B	5.01	1.47	1.36
26	LA	202	PEB	C3B-C2B	5.01	1.47	1.36
26	B1	202	PEB	C3B-C2B	5.01	1.47	1.36
26	h4	203	PEB	C3B-C2B	5.01	1.47	1.36
26	v1	202	PEB	C3C-C4C	5.01	1.49	1.42
26	o1	501	PEB	C3B-C2B	5.01	1.47	1.36
26	FA	201	PEB	C3B-C2B	5.01	1.47	1.36
26	L4	201	PEB	C3C-C4C	5.01	1.49	1.42
26	J5	201	PEB	C1A-NA	-5.01	1.31	1.37
28	J7	1003	CYC	C2A-C3A	5.01	1.47	1.36
26	E4	201	PEB	C3C-C4C	5.01	1.49	1.42
26	v4	202	PEB	C3C-C4C	5.01	1.49	1.42
26	Z2	202	PEB	C3C-C4C	5.01	1.49	1.42
26	GC	202	PEB	C3C-C4C	5.01	1.49	1.42
26	IG	202	PEB	C3C-C4C	5.01	1.49	1.42
27	AA	304	PUB	C2B-C1B	5.01	1.49	1.42
26	eA	202	PEB	C3B-C2B	5.01	1.47	1.36
26	T3	201	PEB	C2A-C1A	-5.01	1.47	1.52
26	V6	201	PEB	C3B-C2B	5.01	1.47	1.36
26	Z6	203	PEB	C3B-C2B	5.01	1.47	1.36
26	g8	202	PEB	C3C-C4C	5.01	1.49	1.42
26	DJ	201	PEB	C3C-C4C	5.01	1.49	1.42
26	v4	201	PEB	C3C-C4C	5.01	1.49	1.42
26	NG	201	PEB	C3C-C4C	5.01	1.49	1.42
26	AI	305	PEB	C3C-C4C	5.01	1.49	1.42
28	N2	1001	CYC	CHB-C1B	5.01	1.49	1.38
26	U3	202	PEB	C3B-C2B	5.01	1.47	1.36
28	C6	1001	CYC	CHB-C1B	5.01	1.49	1.38
26	IC	202	PEB	C3C-C4C	5.01	1.49	1.42
26	TI	202	PEB	C3C-C4C	5.01	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K4	203	PUB	C2B-C1B	5.01	1.49	1.42
26	X1	202	PEB	C1A-NA	-5.00	1.31	1.37
26	S9	201	PEB	C3C-C4C	5.00	1.49	1.42
27	A7	304	PUB	C2B-C1B	5.00	1.49	1.42
26	w4	203	PEB	C3C-C4C	5.00	1.49	1.42
26	cB	201	PEB	C3C-C4C	5.00	1.49	1.42
26	u4	203	PEB	C3C-C4C	5.00	1.49	1.42
26	eD	401	PEB	C3B-C2B	5.00	1.47	1.36
26	cI	202	PEB	C3C-C4C	5.00	1.49	1.42
28	B6	1001	CYC	CHB-C1B	5.00	1.49	1.38
26	ZF	202	PEB	C3B-C2B	5.00	1.47	1.36
26	EJ	202	PEB	C3B-C2B	5.00	1.47	1.36
26	ZI	202	PEB	C3C-C4C	5.00	1.49	1.42
26	m2	201	PEB	C3C-C4C	5.00	1.49	1.42
26	dA	201	PEB	C3C-C4C	5.00	1.49	1.42
28	E6	1001	CYC	C2A-C3A	5.00	1.47	1.36
26	ED	201	PEB	C3C-C4C	5.00	1.49	1.42
26	YD	304	PEB	C3C-C4C	5.00	1.49	1.42
26	YI	201	PEB	C3B-C2B	5.00	1.47	1.36
26	HD	201	PEB	C3C-C4C	5.00	1.49	1.42
26	JD	202	PEB	C3C-C4C	5.00	1.49	1.42
26	X1	201	PEB	C3B-C2B	5.00	1.47	1.36
26	c1	201	PEB	C3B-C2B	5.00	1.47	1.36
26	RA	202	PEB	C3B-C2B	5.00	1.47	1.36
26	b1	501	PEB	C3C-C4C	5.00	1.49	1.42
26	AJ	304	PEB	C3C-C4C	5.00	1.49	1.42
26	O4	201	PEB	C3C-C4C	5.00	1.49	1.42
26	cB	202	PEB	C3C-C4C	5.00	1.49	1.42
26	OF	203	PEB	C3C-C4C	5.00	1.49	1.42
26	II	202	PEB	C3C-C4C	5.00	1.49	1.42
26	S6	202	PEB	CHB-C4B	4.99	1.39	1.35
26	UF	201	PEB	C3C-C4C	4.99	1.49	1.42
28	EB	1001	CYC	CHB-C1B	4.99	1.49	1.38
26	U2	202	PEB	C3C-C4C	4.99	1.49	1.42
26	F8	201	PEB	C3B-C2B	4.99	1.47	1.36
26	S8	202	PEB	C3B-C2B	4.99	1.47	1.36
26	VB	201	PEB	C3B-C2B	4.99	1.47	1.36
26	g2	203	PEB	C3C-C4C	4.99	1.49	1.42
26	G1	201	PEB	C3B-C2B	4.99	1.47	1.36
26	V2	202	PEB	C3B-C2B	4.99	1.47	1.36
26	f6	201	PEB	C3B-C2B	4.99	1.47	1.36
26	GJ	201	PEB	C3B-C2B	4.99	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y2	202	PEB	C3C-C4C	4.99	1.49	1.42
26	TF	201	PEB	C3C-C4C	4.99	1.49	1.42
26	LA	201	PEB	C2A-C1A	-4.99	1.47	1.52
26	XD	201	PEB	C2A-C1A	-4.99	1.47	1.52
26	G1	202	PEB	C3C-C4C	4.99	1.49	1.42
26	R4	201	PEB	C3C-C4C	4.99	1.49	1.42
26	TB	201	PEB	C3B-C2B	4.99	1.47	1.36
26	fB	201	PEB	C3C-C4C	4.99	1.49	1.42
26	LC	203	PEB	C3B-C2B	4.99	1.47	1.36
26	GC	203	PEB	C3B-C2B	4.99	1.47	1.36
26	JF	1002	PEB	C3C-C4C	4.99	1.49	1.42
26	T6	201	PEB	C3B-C2B	4.99	1.47	1.36
26	QI	202	PEB	CHB-C4B	4.99	1.39	1.35
26	c4	203	PEB	C3C-C4C	4.99	1.49	1.42
27	wG	304	PUB	C2C-C3C	4.99	1.47	1.36
26	d6	204	PEB	C3C-C4C	4.99	1.49	1.42
26	K6	201	PEB	C3C-C4C	4.99	1.49	1.42
26	d7	201	PEB	C3C-C4C	4.99	1.49	1.42
26	eI	201	PEB	C3C-C4C	4.99	1.49	1.42
26	V4	201	PEB	C3B-C2B	4.99	1.47	1.36
26	SG	203	PEB	C3B-C2B	4.99	1.47	1.36
26	R2	202	PEB	C3B-C2B	4.98	1.47	1.36
26	NI	1002	PEB	C3B-C2B	4.98	1.47	1.36
26	g1	202	PEB	C3C-C4C	4.98	1.49	1.42
28	L7	1001	CYC	CHB-C1B	4.98	1.49	1.38
26	iB	201	PEB	C3C-C4C	4.98	1.49	1.42
26	hG	201	PEB	C3C-C4C	4.98	1.49	1.42
26	d7	203	PEB	C3C-C4C	4.98	1.49	1.42
28	H7	1001	CYC	C2A-C3A	4.98	1.47	1.36
26	c4	201	PEB	C3B-C2B	4.98	1.47	1.36
26	DI	1002	PEB	C3B-C2B	4.98	1.47	1.36
28	MB	1001	CYC	C2A-C3A	4.98	1.47	1.36
26	A2	305	PEB	C3C-C4C	4.98	1.49	1.42
26	TB	201	PEB	C3C-C4C	4.98	1.49	1.42
27	KD	203	PUB	C2B-C1B	4.98	1.49	1.42
26	d6	203	PEB	C3B-C2B	4.98	1.47	1.36
28	JF	1003	CYC	CHB-C1B	4.98	1.49	1.38
26	Z6	201	PEB	C3B-C2B	4.98	1.47	1.36
26	f6	201	PEB	C3C-C4C	4.98	1.49	1.42
26	NF	1002	PEB	C3B-C2B	4.98	1.47	1.36
26	M9	202	PEB	C3B-C2B	4.98	1.47	1.36
26	BJ	203	PEB	C3B-C2B	4.98	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	HF	1001	CYC	CHB-C1B	4.98	1.49	1.38
26	CD	202	PEB	CHB-C4B	4.98	1.39	1.35
26	I1	201	PEB	C3B-C2B	4.98	1.47	1.36
26	P2	202	PEB	C3C-C4C	4.98	1.49	1.42
26	QI	201	PEB	C3C-C4C	4.98	1.49	1.42
26	N8	202	PEB	C3B-C2B	4.98	1.47	1.36
26	N2	1002	PEB	C3B-C2B	4.98	1.47	1.36
26	ZG	202	PEB	C3B-C2B	4.98	1.47	1.36
28	BB	1001	CYC	CHB-C1B	4.97	1.49	1.38
26	G3	202	PEB	C3C-C4C	4.97	1.49	1.42
26	PI	203	PEB	C3C-C4C	4.97	1.49	1.42
26	FF	1002	PEB	C3B-C2B	4.97	1.47	1.36
26	KG	202	PEB	C3C-C4C	4.97	1.49	1.42
26	mI	201	PEB	C3C-C4C	4.97	1.49	1.42
27	A6	302	PUB	C2B-C1B	4.97	1.49	1.42
26	e3	401	PEB	C3B-C2B	4.97	1.47	1.36
26	QE	203	PEB	C3C-C4C	4.97	1.49	1.42
26	X4	201	PEB	C3B-C2B	4.97	1.47	1.36
26	E1	201	PEB	C3C-C4C	4.97	1.49	1.42
26	c8	202	PEB	C3C-C4C	4.97	1.49	1.42
26	NA	202	PEB	C3B-C2B	4.97	1.47	1.36
26	NA	201	PEB	C2A-C1A	-4.97	1.47	1.52
26	RD	201	PEB	C3C-C4C	4.97	1.49	1.42
26	Y2	201	PEB	C3B-C2B	4.97	1.47	1.36
26	uE	201	PEB	C3C-C4C	4.97	1.49	1.42
26	e2	201	PEB	C3B-C2B	4.97	1.47	1.36
26	Z6	202	PEB	C3B-C2B	4.97	1.47	1.36
26	eI	201	PEB	C3B-C2B	4.97	1.47	1.36
26	j1	202	PEB	C3B-C2B	4.97	1.47	1.36
28	C6	1001	CYC	C2A-C3A	4.97	1.47	1.36
26	B3	201	PEB	C3C-C4C	4.97	1.49	1.42
26	FD	201	PEB	C3C-C4C	4.97	1.49	1.42
26	OG	201	PEB	C3C-C4C	4.97	1.49	1.42
26	A8	302	PEB	C3C-C4C	4.97	1.49	1.42
26	UB	203	PEB	C3C-C4C	4.97	1.49	1.42
26	gF	201	PEB	C3B-C2B	4.97	1.47	1.36
28	M6	1001	CYC	C2A-C3A	4.97	1.47	1.36
26	DG	201	PEB	C3B-C2B	4.97	1.47	1.36
28	sH	1001	CYC	C2A-C3A	4.97	1.47	1.36
26	q1	201	PEB	C3C-C4C	4.97	1.49	1.42
26	E9	201	PEB	C3C-C4C	4.97	1.49	1.42
26	Y8	203	PEB	C3B-C2B	4.97	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A8	304	PUB	C2B-C1B	4.97	1.49	1.42
26	i1	202	PEB	C3B-C2B	4.97	1.47	1.36
26	MJ	202	PEB	C3B-C2B	4.96	1.47	1.36
26	J1	201	PEB	C3C-C4C	4.96	1.49	1.42
26	s1	201	PEB	C3B-C2B	4.96	1.47	1.36
26	PJ	202	PEB	C3B-C2B	4.96	1.47	1.36
28	CB	1001	CYC	C2A-C3A	4.96	1.47	1.36
26	DF	1002	PEB	C3C-C4C	4.96	1.49	1.42
26	PF	201	PEB	C3B-C2B	4.96	1.47	1.36
28	I6	1001	CYC	CHB-C1B	4.96	1.49	1.38
26	W1	201	PEB	C3B-C2B	4.96	1.47	1.36
26	T6	201	PEB	C3C-C4C	4.96	1.49	1.42
26	RF	201	PEB	C3C-C4C	4.96	1.49	1.42
27	yG	303	PUB	C2C-C3C	4.96	1.47	1.36
26	HC	202	PEB	C3B-C2B	4.96	1.47	1.36
26	WD	202	PEB	C3C-C4C	4.96	1.49	1.42
28	JF	1003	CYC	C2A-C3A	4.96	1.47	1.36
26	KB	201	PEB	C3C-C4C	4.96	1.49	1.42
26	D9	202	PEB	C3B-C2B	4.96	1.47	1.36
26	I5	201	PEB	C3B-C2B	4.96	1.47	1.36
26	IE	202	PEB	C3B-C2B	4.96	1.47	1.36
28	CB	1001	CYC	CHB-C1B	4.96	1.49	1.38
26	N3	201	PEB	C3B-C2B	4.96	1.47	1.36
26	a2	201	PEB	C3C-C4C	4.96	1.49	1.42
26	WA	203	PEB	C3C-C4C	4.96	1.49	1.42
26	fA	203	PEB	C3C-C4C	4.96	1.49	1.42
26	kI	202	PEB	C3C-C4C	4.96	1.49	1.42
27	yG	302	PUB	C2C-C3C	4.95	1.47	1.36
26	Y1	202	PEB	C3C-C4C	4.95	1.49	1.42
26	n4	201	PEB	C3C-C4C	4.95	1.49	1.42
26	GG	203	PEB	C3C-C4C	4.95	1.49	1.42
26	mI	203	PEB	C3C-C4C	4.95	1.49	1.42
26	Q4	201	PEB	C3B-C2B	4.95	1.47	1.36
26	K8	201	PEB	C3B-C2B	4.95	1.47	1.36
26	F5	203	PEB	C3B-C2B	4.95	1.47	1.36
26	DD	202	PEB	C3C-C4C	4.95	1.49	1.42
26	x4	201	PEB	C3C-C4C	4.95	1.49	1.42
26	g2	201	PEB	C3B-C2B	4.95	1.47	1.36
26	cI	201	PEB	C3C-C4C	4.95	1.49	1.42
26	L5	203	PEB	C3B-C2B	4.95	1.47	1.36
26	O8	202	PEB	C3C-C4C	4.95	1.49	1.42
28	K7	1001	CYC	C2A-C3A	4.95	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q6	202	PEB	C3C-C4C	4.95	1.49	1.42
26	IJ	202	PEB	C3C-C4C	4.95	1.49	1.42
26	O6	202	PEB	C3C-C4C	4.95	1.49	1.42
26	S8	203	PEB	C3B-C2B	4.95	1.47	1.36
28	H7	1001	CYC	CHB-C1B	4.95	1.49	1.38
26	KA	202	PEB	C3B-C2B	4.95	1.47	1.36
26	ZB	201	PEB	C3B-C2B	4.95	1.47	1.36
26	xG	302	PEB	C3C-C4C	4.95	1.49	1.42
26	K8	202	PEB	C3B-C2B	4.95	1.47	1.36
26	V3	203	PEB	C3C-C4C	4.95	1.49	1.42
26	W4	201	PEB	C3B-C2B	4.95	1.47	1.36
26	R7	201	PEB	C3C-C4C	4.95	1.49	1.42
27	AA	303	PUB	C2B-C1B	4.95	1.49	1.42
26	m2	202	PEB	C3C-C4C	4.95	1.49	1.42
26	hE	201	PEB	C3C-C4C	4.95	1.49	1.42
26	IG	203	PEB	C3C-C4C	4.95	1.49	1.42
26	aI	202	PEB	C3C-C4C	4.95	1.49	1.42
26	R3	201	PEB	C3C-C4C	4.95	1.49	1.42
26	A5	201	PEB	C3C-C4C	4.95	1.49	1.42
26	W8	203	PEB	C3C-C4C	4.95	1.49	1.42
26	xG	303	PEB	C3C-C4C	4.95	1.49	1.42
26	Y4	202	PEB	C3C-C4C	4.94	1.49	1.42
26	J7	1002	PEB	C3C-C4C	4.94	1.49	1.42
26	aI	201	PEB	C3C-C4C	4.94	1.49	1.42
26	WD	201	PEB	C3B-C2B	4.94	1.47	1.36
28	IB	1001	CYC	CHB-C1B	4.94	1.49	1.38
26	e2	203	PEB	C3B-C2B	4.94	1.47	1.36
26	e1	201	PEB	C3C-C4C	4.94	1.49	1.42
26	kB	202	PEB	C3B-C2B	4.94	1.47	1.36
26	PD	203	PEB	C3C-C4C	4.94	1.49	1.42
26	B5	202	PEB	C3C-C4C	4.94	1.49	1.42
26	P6	202	PEB	C3C-C4C	4.94	1.49	1.42
26	W9	201	PEB	C3C-C4C	4.94	1.49	1.42
26	T1	201	PEB	C3B-C2B	4.94	1.47	1.36
26	F3	201	PEB	C3C-C4C	4.94	1.49	1.42
26	mI	202	PEB	C3C-C4C	4.94	1.49	1.42
26	QD	202	PEB	C3C-C4C	4.94	1.49	1.42
26	AI	301	PEB	C3C-C4C	4.94	1.49	1.42
26	c6	201	PEB	C3C-C4C	4.94	1.49	1.42
26	lB	201	PEB	C3C-C4C	4.94	1.49	1.42
26	NG	202	PEB	C3B-C2B	4.93	1.47	1.36
26	U6	203	PEB	C3C-C4C	4.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TD	203	PEB	C3C-C4C	4.93	1.49	1.42
28	GB	1001	CYC	C2C-C1C	-4.93	1.47	1.52
26	D2	1002	PEB	C3B-C2B	4.93	1.47	1.36
26	M4	401	PEB	C3C-C4C	4.93	1.49	1.42
26	a8	204	PEB	C3C-C4C	4.93	1.49	1.42
26	VI	201	PEB	C3C-C4C	4.93	1.49	1.42
26	Y9	202	PEB	C3C-C4C	4.93	1.49	1.42
26	lB	202	PEB	C3C-C4C	4.93	1.49	1.42
28	FF	1001	CYC	CHB-C1B	4.93	1.49	1.38
26	P2	203	PEB	C3C-C4C	4.93	1.49	1.42
26	ID	201	PEB	C3C-C4C	4.93	1.49	1.42
26	C3	201	PEB	C3B-C2B	4.93	1.47	1.36
26	G5	202	PEB	C3C-C4C	4.93	1.49	1.42
26	LI	1002	PEB	C3B-C2B	4.93	1.47	1.36
26	R2	203	PEB	C3B-C2B	4.93	1.47	1.36
26	B9	203	PEB	C3B-C2B	4.93	1.47	1.36
26	r4	202	PEB	C3C-C4C	4.93	1.49	1.42
26	F4	202	PEB	C3C-C4C	4.93	1.49	1.42
27	xG	301	PUB	C2C-C3C	4.93	1.47	1.36
26	XA	202	PEB	C3C-C4C	4.92	1.49	1.42
26	P3	203	PEB	C3C-C4C	4.92	1.49	1.42
26	RI	203	PEB	C3B-C2B	4.92	1.47	1.36
26	XD	201	PEB	C3C-C4C	4.92	1.49	1.42
26	FF	1002	PEB	C3C-C4C	4.92	1.49	1.42
26	X8	202	PEB	C3B-C2B	4.92	1.47	1.36
27	xE	306	PUB	C2C-C3C	4.92	1.47	1.36
26	u1	203	PEB	C3C-C4C	4.92	1.49	1.42
26	i6	201	PEB	C3C-C4C	4.92	1.49	1.42
27	A2	303	PUB	C2B-C1B	4.92	1.49	1.42
26	B1	201	PEB	C3B-C2B	4.92	1.47	1.36
26	i1	203	PEB	C3C-C4C	4.92	1.49	1.42
26	WB	203	PEB	C3B-C2B	4.92	1.47	1.36
28	F2	1001	CYC	C2A-C3A	4.92	1.47	1.36
26	K1	202	PEB	C3C-C4C	4.92	1.49	1.42
26	Q8	204	PEB	C3C-C4C	4.92	1.49	1.42
26	PF	201	PEB	C3C-C4C	4.92	1.49	1.42
26	PI	203	PEB	C3B-C2B	4.92	1.47	1.36
26	k1	201	PEB	C3C-C4C	4.91	1.49	1.42
26	P2	201	PEB	C3C-C4C	4.91	1.49	1.42
27	BA	302	PUB	C2C-C3C	4.91	1.47	1.36
26	Q1	201	PEB	C3B-C2B	4.91	1.47	1.36
26	t4	202	PEB	C3C-C4C	4.91	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	wE	301	PEB	C3C-C4C	4.91	1.49	1.42
26	J4	201	PEB	C3B-C2B	4.91	1.47	1.36
26	BJ	202	PEB	C3B-C2B	4.91	1.47	1.36
28	L6	1001	CYC	C2A-C3A	4.91	1.47	1.36
26	mB	202	PEB	C3B-C2B	4.91	1.47	1.36
26	R8	202	PEB	C3C-C4C	4.91	1.49	1.42
27	AI	303	PUB	C2B-C1B	4.91	1.49	1.42
26	m2	203	PEB	C3C-C4C	4.91	1.49	1.42
26	aA	202	PEB	C3C-C4C	4.91	1.49	1.42
26	EA	203	PEB	C3B-C2B	4.91	1.47	1.36
26	d8	203	PEB	CHB-C4B	4.91	1.39	1.35
28	K6	202	CYC	CHB-C1B	4.91	1.49	1.38
26	f8	201	PEB	C3C-C4C	4.91	1.49	1.42
26	aE	201	PEB	C3C-C4C	4.91	1.49	1.42
26	R1	201	PEB	C3B-C2B	4.91	1.47	1.36
26	BG	202	PEB	C3B-C2B	4.91	1.47	1.36
26	FJ	201	PEB	C3B-C2B	4.91	1.47	1.36
26	a6	202	PEB	C3C-C4C	4.91	1.49	1.42
26	a8	204	PEB	C3B-C2B	4.91	1.47	1.36
26	WB	203	PEB	C3C-C4C	4.91	1.49	1.42
26	aB	202	PEB	C3C-C4C	4.91	1.49	1.42
26	Q3	201	PEB	C1A-NA	-4.91	1.31	1.37
26	SG	201	PEB	C3C-C4C	4.90	1.49	1.42
28	CF	1001	CYC	CHB-C1B	4.90	1.49	1.38
28	JF	1001	CYC	CHB-C1B	4.90	1.49	1.38
26	z1	201	PEB	C3C-C4C	4.90	1.49	1.42
26	O2	202	PEB	C3C-C4C	4.90	1.49	1.42
26	kI	203	PEB	CHB-C4B	4.90	1.39	1.35
26	P7	201	PEB	C3C-C4C	4.90	1.49	1.42
26	K4	201	PEB	C3C-C4C	4.90	1.49	1.42
26	W6	203	PEB	C3B-C2B	4.90	1.47	1.36
26	E8	203	PEB	C3B-C2B	4.90	1.47	1.36
26	Q7	201	PEB	C3C-C4C	4.90	1.49	1.42
26	R1	201	PEB	C3C-C4C	4.90	1.49	1.42
26	H3	202	PEB	C3C-C4C	4.90	1.49	1.42
26	i8	202	PEB	C3C-C4C	4.90	1.49	1.42
26	T4	201	PEB	C3B-C2B	4.90	1.47	1.36
28	J7	1003	CYC	CHB-C1B	4.90	1.49	1.38
28	AH	1001	CYC	CHB-C1B	4.90	1.49	1.38
26	c1	202	PEB	C3C-C4C	4.90	1.49	1.42
26	W3	201	PEB	C3B-C2B	4.90	1.47	1.36
26	NE	202	PEB	C3B-C2B	4.90	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JE	202	PEB	C3B-C2B	4.90	1.47	1.36
26	J4	201	PEB	C3C-C4C	4.90	1.49	1.42
26	QD	201	PEB	C3B-C2B	4.90	1.47	1.36
26	xE	304	PEB	C3C-C4C	4.90	1.49	1.42
26	T6	202	PEB	C3C-C4C	4.90	1.49	1.42
26	DI	1002	PEB	C3C-C4C	4.90	1.49	1.42
28	J7	1001	CYC	CHB-C1B	4.89	1.49	1.38
26	T9	201	PEB	C3C-C4C	4.89	1.49	1.42
26	JF	1002	PEB	C3B-C2B	4.89	1.47	1.36
26	K8	203	PEB	C3B-C2B	4.89	1.47	1.36
26	b7	203	PEB	C3C-C4C	4.89	1.49	1.42
26	dE	201	PEB	C3C-C4C	4.89	1.49	1.42
27	A8	303	PUB	C2B-C1B	4.89	1.49	1.42
26	F8	202	PEB	C3B-C2B	4.89	1.47	1.36
26	IG	202	PEB	C3B-C2B	4.89	1.47	1.36
26	hF	203	PEB	CHB-C4B	4.89	1.39	1.35
26	P1	203	PEB	C3C-C4C	4.89	1.49	1.42
26	A3	201	PEB	C3C-C4C	4.89	1.49	1.42
26	DD	201	PEB	C3C-C4C	4.89	1.49	1.42
26	jF	202	PEB	C3C-C4C	4.89	1.49	1.42
26	QE	202	PEB	C3C-C4C	4.89	1.49	1.42
26	W7	201	PEB	C3C-C4C	4.89	1.49	1.42
28	G6	1001	CYC	CHB-C1B	4.89	1.49	1.38
26	mB	203	PEB	C3C-C4C	4.89	1.49	1.42
26	H5	203	PEB	C3B-C2B	4.89	1.47	1.36
26	O8	203	PEB	C3C-C4C	4.88	1.49	1.42
26	U7	201	PEB	C3C-C4C	4.88	1.49	1.42
26	G5	203	PEB	C3B-C2B	4.88	1.47	1.36
26	C4	201	PEB	C3C-C4C	4.88	1.49	1.42
26	z4	201	PEB	C3C-C4C	4.88	1.49	1.42
26	I5	202	PEB	C3C-C4C	4.88	1.49	1.42
26	m7	201	PEB	C3B-C2B	4.88	1.47	1.36
26	Q1	201	PEB	C3C-C4C	4.88	1.49	1.42
26	bB	201	PEB	C3B-C2B	4.88	1.47	1.36
26	ND	202	PEB	C3B-C2B	4.88	1.47	1.36
28	KB	202	CYC	CHB-C1B	4.88	1.49	1.38
26	B4	201	PEB	C3B-C2B	4.88	1.47	1.36
26	VF	201	PEB	C3C-C4C	4.88	1.49	1.42
28	HB	1001	CYC	C2A-C3A	4.88	1.47	1.36
26	G9	201	PEB	C3B-C2B	4.88	1.47	1.36
26	H1	202	PEB	C3C-C4C	4.88	1.49	1.42
26	RA	202	PEB	C3C-C4C	4.88	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ND	202	PEB	C3C-C4C	4.88	1.49	1.42
26	SD	202	PEB	C3C-C4C	4.88	1.49	1.42
26	h1	201	PEB	C3C-C4C	4.88	1.49	1.42
26	XE	201	PEB	C3C-C4C	4.88	1.49	1.42
26	KE	201	PEB	C3B-C2B	4.88	1.47	1.36
26	NJ	202	PEB	C3B-C2B	4.88	1.47	1.36
26	M9	201	PEB	C3C-C4C	4.87	1.49	1.42
26	SG	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	H5	202	PEB	C3B-C2B	4.87	1.47	1.36
26	P1	202	PEB	C3C-C4C	4.87	1.49	1.42
26	oG	202	PEB	C3C-C4C	4.87	1.49	1.42
26	TE	201	PEB	C3C-C4C	4.87	1.49	1.42
26	bF	201	PEB	C3C-C4C	4.87	1.49	1.42
26	KE	201	PEB	C3C-C4C	4.87	1.49	1.42
26	OE	201	PEB	C3C-C4C	4.87	1.49	1.42
26	PD	203	PEB	C3B-C2B	4.87	1.47	1.36
28	KF	1001	CYC	C2A-C3A	4.87	1.47	1.36
26	TB	202	PEB	C3C-C4C	4.87	1.49	1.42
26	PI	201	PEB	C3C-C4C	4.87	1.49	1.42
26	IJ	203	PEB	C3B-C2B	4.87	1.47	1.36
26	G3	201	PEB	C3C-C4C	4.87	1.49	1.42
26	EJ	201	PEB	C3C-C4C	4.87	1.49	1.42
26	O9	201	PEB	C3C-C4C	4.87	1.49	1.42
26	a7	201	PEB	C3B-C2B	4.87	1.47	1.36
26	m1	203	PEB	C3C-C4C	4.87	1.49	1.42
26	w4	202	PEB	C3C-C4C	4.87	1.49	1.42
26	U1	201	PEB	C3C-C4C	4.87	1.49	1.42
28	I7	1001	CYC	CHB-C1B	4.87	1.49	1.38
26	FA	202	PEB	C3B-C2B	4.87	1.47	1.36
26	BD	201	PEB	C3C-C4C	4.87	1.49	1.42
28	B6	1001	CYC	C2C-C1C	-4.86	1.47	1.52
26	Z1	202	PEB	C3B-C2B	4.86	1.47	1.36
26	Z7	202	PEB	C3B-C2B	4.86	1.47	1.36
26	PB	202	PEB	C3C-C4C	4.86	1.49	1.42
26	fB	201	PEB	C3B-C2B	4.86	1.47	1.36
28	L7	1001	CYC	C2A-C3A	4.86	1.47	1.36
26	l6	203	PEB	C3C-C4C	4.86	1.49	1.42
26	L7	1002	PEB	C3C-C4C	4.86	1.49	1.42
26	TI	201	PEB	C3B-C2B	4.86	1.47	1.36
26	j8	203	PEB	C3C-C4C	4.86	1.49	1.42
26	QG	203	PEB	C3C-C4C	4.86	1.49	1.42
26	e4	202	PEB	C3C-C4C	4.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TI	201	PEB	C3C-C4C	4.86	1.49	1.42
27	K3	203	PUB	C2B-C1B	4.86	1.49	1.42
26	Q3	202	PEB	C3C-C4C	4.86	1.49	1.42
26	j6	201	PEB	C3C-C4C	4.86	1.49	1.42
26	VF	202	PEB	C3C-C4C	4.86	1.49	1.42
26	SE	203	PEB	C3B-C2B	4.86	1.47	1.36
28	GB	1001	CYC	CHB-C1B	4.86	1.49	1.38
26	P2	203	PEB	C3B-C2B	4.86	1.47	1.36
28	LB	1001	CYC	C2C-C1C	-4.86	1.47	1.52
26	W6	203	PEB	C3C-C4C	4.86	1.49	1.42
26	gI	202	PEB	C3C-C4C	4.86	1.49	1.42
26	H5	201	PEB	C3B-C2B	4.85	1.47	1.36
26	AJ	305	PEB	C3C-C4C	4.85	1.49	1.42
26	P1	202	PEB	C3B-C2B	4.85	1.47	1.36
26	W8	201	PEB	C2A-C1A	-4.85	1.47	1.52
28	BB	1001	CYC	C2C-C1C	-4.85	1.47	1.52
26	C8	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	KG	203	PEB	C3B-C2B	4.85	1.47	1.36
28	HF	1001	CYC	C2A-C3A	4.85	1.47	1.36
26	XA	202	PEB	CHA-C1B	4.85	1.51	1.40
26	eB	203	PEB	C3C-C4C	4.85	1.49	1.42
26	E9	201	PEB	C3B-C2B	4.85	1.47	1.36
26	R8	202	PEB	C3B-C2B	4.85	1.47	1.36
26	C9	201	PEB	C3C-C4C	4.85	1.49	1.42
26	YI	203	PEB	C3C-C4C	4.85	1.49	1.42
26	R4	201	PEB	C3B-C2B	4.85	1.47	1.36
26	I9	202	PEB	C3B-C2B	4.85	1.47	1.36
26	GA	202	PEB	C3C-C4C	4.85	1.49	1.42
26	P4	202	PEB	C3B-C2B	4.85	1.47	1.36
26	V2	201	PEB	C3C-C4C	4.85	1.49	1.42
26	K3	202	PEB	C3C-C4C	4.85	1.49	1.42
26	k4	202	PEB	C3C-C4C	4.85	1.49	1.42
26	YJ	202	PEB	C3C-C4C	4.84	1.49	1.42
26	l6	201	PEB	C3C-C4C	4.84	1.49	1.42
26	L2	1002	PEB	C3B-C2B	4.84	1.47	1.36
26	x1	201	PEB	C3C-C4C	4.84	1.49	1.42
26	K8	203	PEB	C1A-NA	-4.84	1.31	1.37
26	VI	201	PEB	C3B-C2B	4.84	1.47	1.36
26	V2	201	PEB	C3B-C2B	4.84	1.47	1.36
26	m4	203	PEB	C3C-C4C	4.84	1.49	1.42
26	m6	201	PEB	C3C-C4C	4.84	1.49	1.42
27	A6	303	PUB	C2B-C1B	4.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H6	1001	CYC	C2A-C3A	4.84	1.47	1.36
26	eD	401	PEB	C3C-C4C	4.84	1.49	1.42
26	mF	201	PEB	C3B-C2B	4.84	1.47	1.36
26	eI	203	PEB	C3B-C2B	4.84	1.47	1.36
26	WA	201	PEB	C3C-C4C	4.84	1.49	1.42
26	jF	201	PEB	C3B-C2B	4.84	1.47	1.36
26	GJ	202	PEB	C3C-C4C	4.84	1.49	1.42
26	Y2	203	PEB	C3C-C4C	4.83	1.49	1.42
26	ZA	201	PEB	C3B-C2B	4.83	1.47	1.36
28	I7	1001	CYC	C2A-C3A	4.83	1.47	1.36
26	Q8	204	PEB	C3B-C2B	4.83	1.47	1.36
26	Q2	202	PEB	C3C-C4C	4.83	1.49	1.42
26	YA	203	PEB	C3C-C4C	4.83	1.49	1.42
26	P9	201	PEB	C3C-C4C	4.83	1.49	1.42
26	mB	201	PEB	C3C-C4C	4.83	1.49	1.42
26	hF	201	PEB	C3C-C4C	4.83	1.49	1.42
26	WB	201	PEB	C3C-C4C	4.83	1.49	1.42
26	wG	301	PEB	C3C-C4C	4.83	1.49	1.42
26	DJ	202	PEB	C3B-C2B	4.83	1.47	1.36
26	T2	201	PEB	C3C-C4C	4.83	1.49	1.42
26	e2	203	PEB	C3C-C4C	4.83	1.49	1.42
26	eI	203	PEB	C3C-C4C	4.83	1.49	1.42
27	AJ	302	PUB	C2B-C1B	4.83	1.49	1.42
26	R6	201	PEB	C3B-C2B	4.83	1.47	1.36
26	cF	201	PEB	C3B-C2B	4.83	1.47	1.36
26	G4	201	PEB	C3B-C2B	4.83	1.47	1.36
26	T2	201	PEB	C3B-C2B	4.83	1.47	1.36
26	k8	202	PEB	C3B-C2B	4.83	1.47	1.36
26	h7	201	PEB	C3C-C4C	4.83	1.49	1.42
28	H2	1001	CYC	CHB-C1B	4.82	1.49	1.38
28	KI	1001	CYC	CHB-C1B	4.82	1.49	1.38
27	N9	201	PUB	C2B-C1B	4.82	1.49	1.42
26	Q3	201	PEB	C3B-C2B	4.82	1.47	1.36
27	B8	302	PUB	C2C-C3C	4.82	1.47	1.36
26	J8	202	PEB	C3C-C4C	4.82	1.49	1.42
28	EI	1001	CYC	C2A-C3A	4.82	1.47	1.36
26	HC	202	PEB	C3C-C4C	4.82	1.49	1.42
26	SE	201	PEB	C3C-C4C	4.82	1.49	1.42
26	c2	201	PEB	C3C-C4C	4.82	1.49	1.42
26	a8	202	PEB	C3C-C4C	4.82	1.49	1.42
26	f8	202	PEB	C3C-C4C	4.82	1.49	1.42
26	XD	202	PEB	C3C-C4C	4.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C1	201	PEB	C3C-C4C	4.82	1.49	1.42
26	S3	202	PEB	C3C-C4C	4.82	1.49	1.42
26	l2	202	PEB	C3C-C4C	4.82	1.49	1.42
27	AB	303	PUB	C2B-C1B	4.81	1.49	1.42
26	A6	304	PEB	C3C-C4C	4.81	1.49	1.42
26	R6	201	PEB	C3C-C4C	4.81	1.49	1.42
26	W8	201	PEB	C3C-C4C	4.81	1.49	1.42
26	XG	201	PEB	C3C-C4C	4.81	1.49	1.42
26	Q4	201	PEB	C3C-C4C	4.81	1.49	1.42
26	YA	203	PEB	C3B-C2B	4.81	1.47	1.36
26	SB	202	PEB	C3C-C4C	4.81	1.49	1.42
26	V8	202	PEB	C3C-C4C	4.81	1.49	1.42
26	RJ	201	PEB	C3C-C4C	4.81	1.49	1.42
26	M4	403	PEB	C3C-C4C	4.81	1.49	1.42
26	VA	202	PEB	C3C-C4C	4.81	1.49	1.42
26	BE	202	PEB	C3B-C2B	4.81	1.46	1.36
26	c1	203	PEB	C3C-C4C	4.81	1.49	1.42
26	f7	203	PEB	C3C-C4C	4.81	1.49	1.42
26	M8	201	PEB	C3B-C2B	4.81	1.46	1.36
26	MA	201	PEB	C3B-C2B	4.81	1.46	1.36
26	G8	202	PEB	C3C-C4C	4.81	1.49	1.42
27	24	403	PUB	C2B-C1B	4.81	1.49	1.42
26	QA	204	PEB	C3B-C2B	4.81	1.46	1.36
26	P4	202	PEB	C3C-C4C	4.81	1.49	1.42
28	cH	1001	CYC	CHB-C1B	4.80	1.49	1.38
26	P3	203	PEB	C3B-C2B	4.80	1.46	1.36
28	E2	1001	CYC	C2A-C3A	4.80	1.46	1.36
28	B6	1002	CYC	C2A-C3A	4.80	1.46	1.36
26	k6	202	PEB	C3C-C4C	4.80	1.49	1.42
28	IB	1001	CYC	C2A-C3A	4.80	1.46	1.36
26	oE	202	PEB	C3C-C4C	4.80	1.49	1.42
26	D8	202	PEB	C3C-C4C	4.80	1.49	1.42
26	OD	202	PEB	C3B-C2B	4.80	1.46	1.36
26	e3	401	PEB	C3C-C4C	4.80	1.49	1.42
28	LB	1001	CYC	C2A-C3A	4.80	1.46	1.36
26	T3	203	PEB	C3C-C4C	4.80	1.49	1.42
26	I5	201	PEB	C3C-C4C	4.79	1.49	1.42
26	b4	501	PEB	C3C-C4C	4.79	1.49	1.42
26	m6	203	PEB	C3C-C4C	4.79	1.49	1.42
26	JJ	201	PEB	C3C-C4C	4.79	1.49	1.42
26	Z4	202	PEB	C3B-C2B	4.79	1.46	1.36
26	O3	202	PEB	C3B-C2B	4.79	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I3	201	PEB	C3C-C4C	4.79	1.49	1.42
26	JA	202	PEB	C3C-C4C	4.79	1.49	1.42
26	dF	203	PEB	C3C-C4C	4.79	1.49	1.42
26	MG	203	PEB	C3C-C4C	4.79	1.49	1.42
26	KA	203	PEB	C3B-C2B	4.79	1.46	1.36
26	X9	201	PEB	C3C-C4C	4.79	1.49	1.42
26	q1	202	PEB	C3C-C4C	4.79	1.49	1.42
26	N3	202	PEB	C3C-C4C	4.79	1.49	1.42
26	Y4	201	PEB	C3B-C2B	4.79	1.46	1.36
26	mA	202	PEB	C3C-C4C	4.79	1.49	1.42
26	M8	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	UI	202	PEB	C3C-C4C	4.79	1.49	1.42
26	m8	202	PEB	C3C-C4C	4.78	1.49	1.42
26	k2	201	PEB	C3C-C4C	4.78	1.49	1.42
26	RE	202	PEB	C3B-C2B	4.78	1.46	1.36
28	C7	1001	CYC	CHB-C1B	4.78	1.49	1.38
26	OI	202	PEB	C3C-C4C	4.78	1.49	1.42
26	HJ	202	PEB	C3C-C4C	4.78	1.49	1.42
26	a2	203	PEB	C3B-C2B	4.78	1.46	1.36
26	W6	201	PEB	C3C-C4C	4.78	1.49	1.42
26	QA	204	PEB	C3C-C4C	4.78	1.49	1.42
26	HC	201	PEB	C3C-C4C	4.78	1.49	1.42
26	UD	201	PEB	C3C-C4C	4.78	1.49	1.42
27	yG	302	PUB	C2B-C1B	4.78	1.49	1.42
26	FC	201	PEB	C3C-C4C	4.78	1.49	1.42
28	K2	1001	CYC	CHB-C1B	4.78	1.49	1.38
26	hA	201	PEB	C3C-C4C	4.78	1.49	1.42
26	C9	201	PEB	C3B-C2B	4.78	1.46	1.36
26	KG	201	PEB	C3C-C4C	4.78	1.49	1.42
28	IF	1001	CYC	C2A-C3A	4.77	1.46	1.36
26	e1	202	PEB	C3C-C4C	4.77	1.49	1.42
26	gI	201	PEB	C3C-C4C	4.77	1.49	1.42
26	PJ	201	PEB	C3C-C4C	4.77	1.49	1.42
26	F8	202	PEB	C2A-C1A	-4.77	1.47	1.52
26	Y1	201	PEB	C3B-C2B	4.77	1.46	1.36
26	t4	201	PEB	C3C-C4C	4.77	1.49	1.42
26	EJ	201	PEB	C3B-C2B	4.77	1.46	1.36
26	R9	201	PEB	C3C-C4C	4.77	1.49	1.42
26	jE	202	PEB	C3B-C2B	4.77	1.46	1.36
26	Q7	202	PEB	C3C-C4C	4.77	1.49	1.42
26	WA	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	h4	202	PEB	C3C-C4C	4.77	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u4	202	PEB	C3C-C4C	4.77	1.49	1.42
26	L9	202	PEB	C3C-C4C	4.77	1.49	1.42
26	g2	201	PEB	C3C-C4C	4.77	1.49	1.42
26	S8	203	PEB	C3C-C4C	4.77	1.49	1.42
28	I6	1001	CYC	C2A-C3A	4.77	1.46	1.36
26	WF	202	PEB	C3C-C4C	4.77	1.49	1.42
28	CI	1001	CYC	CHB-C1B	4.77	1.49	1.38
26	A6	301	PEB	C3C-C4C	4.77	1.49	1.42
26	h8	202	PEB	C3C-C4C	4.77	1.49	1.42
26	GC	201	PEB	C3C-C4C	4.77	1.49	1.42
26	RB	201	PEB	C3B-C2B	4.76	1.46	1.36
26	P4	203	PEB	C3C-C4C	4.76	1.49	1.42
26	I9	202	PEB	C3C-C4C	4.76	1.49	1.42
26	g1	201	PEB	C3C-C4C	4.76	1.49	1.42
26	W3	202	PEB	C3C-C4C	4.76	1.49	1.42
26	H9	202	PEB	C3C-C4C	4.76	1.49	1.42
26	S3	201	PEB	C3B-C2B	4.76	1.46	1.36
26	MJ	201	PEB	C3C-C4C	4.76	1.49	1.42
26	CA	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	TJ	201	PEB	C3C-C4C	4.76	1.49	1.42
28	M6	1001	CYC	CHB-C1B	4.76	1.49	1.38
26	M8	202	PEB	C3B-C2B	4.76	1.46	1.36
26	a6	201	PEB	C3B-C2B	4.76	1.46	1.36
26	MA	202	PEB	C3B-C2B	4.76	1.46	1.36
26	N3	202	PEB	C3B-C2B	4.76	1.46	1.36
26	ND	203	PEB	C3C-C4C	4.76	1.49	1.42
26	eA	201	PEB	C3B-C2B	4.76	1.46	1.36
26	j7	203	PEB	C3C-C4C	4.75	1.49	1.42
27	wE	304	PUB	C2B-C1B	4.75	1.49	1.42
26	QD	201	PEB	C3C-C4C	4.75	1.49	1.42
26	D1	202	PEB	C3C-C4C	4.75	1.49	1.42
26	U3	201	PEB	C3C-C4C	4.75	1.49	1.42
26	jA	202	PEB	C3C-C4C	4.75	1.49	1.42
26	u1	201	PEB	C3B-C2B	4.75	1.46	1.36
28	HI	1001	CYC	CHB-C1B	4.75	1.49	1.38
27	AB	302	PUB	C2B-C1B	4.75	1.49	1.42
26	B9	203	PEB	C3C-C4C	4.75	1.49	1.42
26	a1	202	PEB	C3C-C4C	4.74	1.49	1.42
26	GE	202	PEB	C1A-NA	-4.74	1.31	1.37
26	H3	201	PEB	C3C-C4C	4.74	1.49	1.42
26	Y8	203	PEB	C3C-C4C	4.74	1.49	1.42
26	RB	201	PEB	C3C-C4C	4.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	KC	203	PEB	C3C-C4C	4.74	1.49	1.42
28	IF	1001	CYC	CHB-C1B	4.74	1.49	1.38
26	DA	202	PEB	C3C-C4C	4.74	1.49	1.42
26	V4	202	PEB	C3C-C4C	4.74	1.49	1.42
26	iG	201	PEB	C3C-C4C	4.74	1.49	1.42
26	B1	202	PEB	C3C-C4C	4.74	1.49	1.42
26	YE	203	PEB	C3C-C4C	4.74	1.49	1.42
26	LG	201	PEB	C3C-C4C	4.74	1.49	1.42
26	L8	202	PEB	C2A-C1A	-4.74	1.47	1.52
26	H9	201	PEB	C3C-C4C	4.74	1.49	1.42
28	IF	1001	CYC	C2C-C1C	-4.74	1.47	1.52
26	fl	201	PEB	C3B-C2B	4.74	1.46	1.36
26	O7	201	PEB	C3C-C4C	4.74	1.49	1.42
26	IJ	203	PEB	C3C-C4C	4.74	1.49	1.42
28	C2	1001	CYC	CHB-C1B	4.73	1.49	1.38
26	R2	201	PEB	C3B-C2B	4.73	1.46	1.36
26	hA	202	PEB	C3C-C4C	4.73	1.49	1.42
26	A8	301	PEB	C3C-C4C	4.73	1.49	1.42
26	y1	202	PEB	C3C-C4C	4.73	1.49	1.42
26	OB	202	PEB	C3C-C4C	4.73	1.49	1.42
26	H8	202	PEB	C3C-C4C	4.73	1.49	1.42
26	SA	203	PEB	C3C-C4C	4.73	1.49	1.42
26	FA	202	PEB	C2A-C1A	-4.73	1.47	1.52
28	MB	1001	CYC	CHB-C1B	4.73	1.49	1.38
26	X3	202	PEB	C3C-C4C	4.73	1.49	1.42
26	jB	201	PEB	C3C-C4C	4.73	1.49	1.42
27	A2	302	PUB	C2B-C1B	4.73	1.49	1.42
26	OA	203	PEB	C3C-C4C	4.73	1.49	1.42
26	KA	203	PEB	C1A-NA	-4.73	1.31	1.37
26	HJ	201	PEB	C3C-C4C	4.73	1.49	1.42
26	kI	201	PEB	C3C-C4C	4.73	1.49	1.42
26	L5	201	PEB	C1A-NA	-4.73	1.31	1.37
26	PG	202	PEB	C3B-C2B	4.73	1.46	1.36
26	H3	203	PEB	C3C-C4C	4.73	1.49	1.42
26	N6	201	PEB	C3C-C4C	4.73	1.49	1.42
26	TG	201	PEB	C3C-C4C	4.73	1.49	1.42
26	U4	201	PEB	C3C-C4C	4.72	1.49	1.42
26	SG	202	PEB	C3B-C2B	4.72	1.46	1.36
26	kE	203	PEB	C3C-C4C	4.72	1.49	1.42
28	I2	1001	CYC	CHB-C1B	4.72	1.49	1.38
26	dG	201	PEB	C3C-C4C	4.72	1.49	1.42
26	GE	203	PEB	C3B-C2B	4.72	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UB	202	PEB	C3C-C4C	4.72	1.49	1.42
26	u4	201	PEB	C3C-C4C	4.72	1.49	1.42
26	xE	302	PEB	C3C-C4C	4.72	1.49	1.42
26	B9	201	PEB	C3C-C4C	4.72	1.49	1.42
26	HA	202	PEB	C3C-C4C	4.72	1.49	1.42
26	DG	202	PEB	C3C-C4C	4.72	1.49	1.42
26	OA	202	PEB	C3C-C4C	4.72	1.49	1.42
26	P3	201	PEB	C3B-C2B	4.72	1.46	1.36
28	NB	1001	CYC	C2A-C3A	4.72	1.46	1.36
26	D9	201	PEB	C3C-C4C	4.72	1.49	1.42
27	yE	303	PUB	C2B-C1B	4.72	1.49	1.42
27	xG	306	PUB	C2B-C1B	4.72	1.49	1.42
26	Z8	201	PEB	C3B-C2B	4.71	1.46	1.36
26	Q2	201	PEB	C2A-C1A	-4.71	1.47	1.52
26	FE	201	PEB	C2A-C1A	-4.71	1.47	1.52
26	iA	202	PEB	C3C-C4C	4.71	1.49	1.42
26	rG	201	PEB	C3C-C4C	4.71	1.49	1.42
26	W1	202	PEB	C3C-C4C	4.71	1.49	1.42
26	IE	203	PEB	C3C-C4C	4.71	1.49	1.42
26	UA	202	PEB	C1A-NA	-4.71	1.31	1.37
26	N3	203	PEB	C3C-C4C	4.71	1.49	1.42
26	D6	1002	PEB	C3C-C4C	4.71	1.49	1.42
28	II	1001	CYC	CHB-C1B	4.71	1.49	1.38
26	L8	202	PEB	C3C-C4C	4.71	1.49	1.42
28	KB	202	CYC	C2A-C3A	4.71	1.46	1.36
26	qG	201	PEB	C3C-C4C	4.71	1.49	1.42
28	dH	1001	CYC	CHB-C1B	4.71	1.49	1.38
26	W4	202	PEB	C3C-C4C	4.71	1.49	1.42
28	K6	202	CYC	C2A-C3A	4.71	1.46	1.36
26	NB	1002	PEB	C3C-C4C	4.70	1.49	1.42
26	ME	201	PEB	C3B-C2B	4.70	1.46	1.36
26	WJ	201	PEB	C3B-C2B	4.70	1.46	1.36
28	M2	1001	CYC	CHB-C1B	4.70	1.49	1.38
26	PE	202	PEB	C3B-C2B	4.70	1.46	1.36
26	aI	201	PEB	C3B-C2B	4.70	1.46	1.36
26	WD	201	PEB	C3C-C4C	4.70	1.49	1.42
26	X1	202	PEB	C3C-C4C	4.70	1.49	1.42
26	h4	201	PEB	C3C-C4C	4.70	1.49	1.42
28	E2	1001	CYC	CHB-C1B	4.70	1.49	1.38
26	SI	202	PEB	C3C-C4C	4.70	1.49	1.42
26	LJ	202	PEB	C3C-C4C	4.70	1.49	1.42
26	j1	201	PEB	C3C-C4C	4.70	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U8	202	PEB	C1A-NA	-4.70	1.31	1.37
26	N4	202	PEB	C3C-C4C	4.70	1.49	1.42
26	jA	203	PEB	C3C-C4C	4.69	1.49	1.42
26	VI	203	PEB	C3C-C4C	4.69	1.49	1.42
26	H2	1002	PEB	C3C-C4C	4.69	1.49	1.42
26	d1	202	PEB	C3C-C4C	4.69	1.49	1.42
26	C8	201	PEB	C3C-C4C	4.69	1.49	1.42
26	SF	201	PEB	C3C-C4C	4.69	1.49	1.42
26	e8	201	PEB	C3B-C2B	4.69	1.46	1.36
26	OD	201	PEB	C3B-C2B	4.69	1.46	1.36
28	NB	1001	CYC	CHB-C1B	4.69	1.49	1.38
26	hI	201	PEB	C3B-C2B	4.69	1.46	1.36
26	V6	202	PEB	C3C-C4C	4.69	1.49	1.42
26	T4	202	PEB	C3B-C2B	4.69	1.46	1.36
26	VB	202	PEB	C3C-C4C	4.69	1.49	1.42
26	TD	203	PEB	C1A-NA	-4.69	1.31	1.37
26	a2	201	PEB	C3B-C2B	4.69	1.46	1.36
26	h2	201	PEB	C3B-C2B	4.69	1.46	1.36
26	Y6	201	PEB	C3B-C2B	4.69	1.46	1.36
26	NF	1002	PEB	C3C-C4C	4.69	1.49	1.42
26	XD	202	PEB	C3B-C2B	4.69	1.46	1.36
28	EI	1001	CYC	CHB-C1B	4.69	1.49	1.38
27	BA	302	PUB	C2B-C1B	4.68	1.49	1.42
26	SD	201	PEB	C3B-C2B	4.68	1.46	1.36
26	q4	202	PEB	C3C-C4C	4.68	1.49	1.42
26	kB	202	PEB	C3C-C4C	4.68	1.49	1.42
26	Q4	202	PEB	C3C-C4C	4.68	1.49	1.42
26	Z6	203	PEB	C3C-C4C	4.68	1.49	1.42
28	GI	1001	CYC	CHB-C1B	4.68	1.49	1.38
26	N4	201	PEB	C3C-C4C	4.68	1.49	1.42
26	U8	202	PEB	C3C-C4C	4.68	1.49	1.42
26	eA	202	PEB	C3C-C4C	4.68	1.49	1.42
26	IC	203	PEB	C3C-C4C	4.68	1.49	1.42
26	QF	201	PEB	C3C-C4C	4.68	1.49	1.42
26	CG	201	PEB	C3C-C4C	4.68	1.49	1.42
26	RI	201	PEB	C3B-C2B	4.68	1.46	1.36
26	JG	202	PEB	C3B-C2B	4.68	1.46	1.36
26	aB	201	PEB	C3B-C2B	4.68	1.46	1.36
26	J1	201	PEB	C3B-C2B	4.68	1.46	1.36
26	i2	201	PEB	C3C-C4C	4.68	1.49	1.42
26	j4	201	PEB	C3C-C4C	4.68	1.49	1.42
26	LD	201	PEB	C3C-C4C	4.68	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P9	202	PEB	C1A-NA	-4.68	1.31	1.37
26	X3	201	PEB	C3C-C4C	4.68	1.49	1.42
26	TA	202	PEB	C3B-C2B	4.68	1.46	1.36
26	I4	201	PEB	C3C-C4C	4.68	1.49	1.42
26	ME	203	PEB	C3C-C4C	4.68	1.49	1.42
26	Q1	202	PEB	C3C-C4C	4.67	1.49	1.42
26	g4	201	PEB	C3C-C4C	4.67	1.49	1.42
26	RG	202	PEB	C3B-C2B	4.67	1.46	1.36
28	WH	1001	CYC	CHB-C4A	4.67	1.51	1.40
27	A9	302	PUB	C2B-C1B	4.67	1.49	1.42
26	MA	202	PEB	C2A-C1A	-4.67	1.47	1.52
26	V1	202	PEB	C3C-C4C	4.67	1.49	1.42
26	M1	403	PEB	C3C-C4C	4.67	1.49	1.42
26	S7	201	PEB	C3C-C4C	4.67	1.49	1.42
26	HD	202	PEB	C3C-C4C	4.67	1.49	1.42
26	S2	202	PEB	C3C-C4C	4.67	1.49	1.42
26	T8	202	PEB	C3B-C2B	4.67	1.46	1.36
26	TE	202	PEB	C3B-C2B	4.67	1.46	1.36
26	jG	202	PEB	C3B-C2B	4.67	1.46	1.36
26	i1	202	PEB	C3C-C4C	4.66	1.49	1.42
26	J9	203	PEB	C3C-C4C	4.66	1.49	1.42
26	SD	201	PEB	C3C-C4C	4.66	1.49	1.42
26	Z2	201	PEB	C1A-NA	-4.66	1.31	1.37
26	YA	202	PEB	C3C-C4C	4.66	1.49	1.42
28	IB	1001	CYC	C2C-C1C	-4.66	1.47	1.52
26	dI	201	PEB	C3B-C2B	4.66	1.46	1.36
26	SB	201	PEB	C3C-C4C	4.66	1.49	1.42
26	TI	203	PEB	C3C-C4C	4.66	1.49	1.42
26	U6	202	PEB	C3C-C4C	4.66	1.49	1.42
26	RD	203	PEB	C3C-C4C	4.66	1.49	1.42
26	k4	203	PEB	C3C-C4C	4.66	1.49	1.42
26	ZB	203	PEB	C3C-C4C	4.66	1.49	1.42
26	PD	201	PEB	C3C-C4C	4.66	1.49	1.42
26	u1	202	PEB	C3C-C4C	4.66	1.49	1.42
26	g6	201	PEB	C3C-C4C	4.66	1.49	1.42
28	G6	1001	CYC	C2C-C1C	-4.65	1.47	1.52
28	G2	1001	CYC	CHB-C1B	4.65	1.49	1.38
26	X4	202	PEB	C3C-C4C	4.65	1.49	1.42
26	X8	202	PEB	C3C-C4C	4.65	1.49	1.42
26	AB	304	PEB	C3C-C4C	4.65	1.49	1.42
27	B8	302	PUB	C2B-C1B	4.65	1.49	1.42
26	L3	202	PEB	C3C-C4C	4.65	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	E7	1001	CYC	CHB-C1B	4.64	1.49	1.38
28	DF	1001	CYC	CHB-C1B	4.64	1.49	1.38
28	EF	1001	CYC	CHB-C1B	4.64	1.49	1.38
26	iI	201	PEB	C3C-C4C	4.64	1.49	1.42
26	LJ	201	PEB	C3C-C4C	4.64	1.49	1.42
26	AB	301	PEB	C3C-C4C	4.64	1.49	1.42
26	RB	202	PEB	C3C-C4C	4.64	1.49	1.42
26	QI	201	PEB	C2A-C1A	-4.64	1.47	1.52
26	Z7	201	PEB	C3B-C2B	4.64	1.46	1.36
26	fA	202	PEB	C3C-C4C	4.64	1.49	1.42
26	KJ	201	PEB	C3C-C4C	4.64	1.49	1.42
26	S6	201	PEB	C3C-C4C	4.64	1.49	1.42
26	DB	1002	PEB	C3C-C4C	4.64	1.49	1.42
26	DE	203	PEB	C3B-C2B	4.64	1.46	1.36
26	X3	202	PEB	C3B-C2B	4.64	1.46	1.36
26	AA	301	PEB	C3C-C4C	4.64	1.49	1.42
26	oG	201	PEB	C1A-NA	-4.64	1.31	1.37
26	qE	202	PEB	C3C-C4C	4.64	1.49	1.42
28	L6	1001	CYC	C2C-C1C	-4.64	1.48	1.52
28	sH	1001	CYC	C2C-C1C	-4.64	1.48	1.52
26	XE	202	PEB	C3B-C2B	4.64	1.46	1.36
26	m1	201	PEB	C3C-C4C	4.64	1.49	1.42
28	RH	1001	CYC	C1C-NC	-4.64	1.31	1.37
26	FE	201	PEB	C3C-C4C	4.64	1.49	1.42
26	y4	201	PEB	C3B-C2B	4.63	1.46	1.36
26	CA	201	PEB	C3C-C4C	4.63	1.49	1.42
26	cA	202	PEB	C3C-C4C	4.63	1.49	1.42
26	T8	202	PEB	C1A-NA	-4.63	1.31	1.37
26	GG	203	PEB	C3B-C2B	4.63	1.46	1.36
26	Y1	201	PEB	C3C-C4C	4.63	1.49	1.42
26	w1	202	PEB	C3C-C4C	4.63	1.49	1.42
26	WF	201	PEB	C3C-C4C	4.63	1.49	1.42
26	T1	202	PEB	C3B-C2B	4.63	1.46	1.36
26	d2	201	PEB	C3B-C2B	4.63	1.46	1.36
26	QG	202	PEB	C3C-C4C	4.63	1.49	1.42
28	yH	1001	CYC	CHB-C4A	4.63	1.51	1.40
28	MI	1001	CYC	CHB-C1B	4.63	1.49	1.38
26	G5	201	PEB	C3C-C4C	4.63	1.49	1.42
26	Y6	201	PEB	C3C-C4C	4.62	1.49	1.42
26	J1	202	PEB	C3C-C4C	4.62	1.49	1.42
26	VE	201	PEB	C3C-C4C	4.62	1.49	1.42
26	M9	201	PEB	C3B-C2B	4.62	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VG	201	PEB	C3C-C4C	4.62	1.49	1.42
26	sG	202	PEB	CHA-C1B	4.62	1.51	1.40
26	OA	201	PEB	C3C-C4C	4.62	1.49	1.42
26	l4	202	PEB	CHA-C1B	4.62	1.51	1.40
26	WB	202	PEB	C3C-C4C	4.62	1.49	1.42
26	MD	201	PEB	C3C-C4C	4.62	1.49	1.42
26	ZI	201	PEB	C2A-C1A	-4.62	1.48	1.52
26	H6	1002	PEB	C3C-C4C	4.62	1.49	1.42
26	OB	201	PEB	C3C-C4C	4.62	1.49	1.42
26	U2	201	PEB	C1A-NA	-4.62	1.31	1.37
28	KF	1001	CYC	CHB-C1B	4.62	1.49	1.38
26	N1	202	PEB	C3C-C4C	4.62	1.49	1.42
28	D7	1001	CYC	CHB-C1B	4.62	1.49	1.38
26	OG	202	PEB	CHA-C1B	4.62	1.51	1.40
26	RA	202	PEB	CHA-C1B	4.62	1.51	1.40
26	HI	1002	PEB	C3C-C4C	4.62	1.49	1.42
26	PD	202	PEB	C3C-C4C	4.61	1.49	1.42
26	YD	303	PEB	C3C-C4C	4.61	1.49	1.42
26	R3	203	PEB	C3C-C4C	4.61	1.49	1.42
26	DE	202	PEB	C3C-C4C	4.61	1.49	1.42
26	T4	202	PEB	C3C-C4C	4.61	1.49	1.42
26	F9	201	PEB	C3C-C4C	4.61	1.49	1.42
26	T2	203	PEB	C3C-C4C	4.61	1.49	1.42
26	YB	201	PEB	C3B-C2B	4.61	1.46	1.36
28	mH	1001	CYC	CHB-C4A	4.61	1.51	1.40
26	OD	201	PEB	C3C-C4C	4.61	1.49	1.42
26	gB	201	PEB	C3C-C4C	4.61	1.49	1.42
26	O6	201	PEB	C3B-C2B	4.60	1.46	1.36
26	NG	201	PEB	C2A-C1A	-4.60	1.48	1.52
26	PA	202	PEB	C3C-C4C	4.60	1.49	1.42
26	ZF	201	PEB	C3B-C2B	4.60	1.46	1.36
26	O3	201	PEB	C3C-C4C	4.60	1.49	1.42
26	RI	203	PEB	C3C-C4C	4.60	1.49	1.42
28	DF	1003	CYC	CHB-C1B	4.60	1.49	1.38
26	A2	304	PEB	C3C-C4C	4.60	1.49	1.42
26	R6	202	PEB	C3C-C4C	4.60	1.49	1.42
26	FA	202	PEB	C3C-C4C	4.60	1.49	1.42
26	QD	201	PEB	C1A-NA	-4.60	1.31	1.37
28	JH	1001	CYC	CHB-C4A	4.60	1.51	1.40
26	T1	202	PEB	C3C-C4C	4.60	1.49	1.42
27	YD	302	PUB	C2B-C1B	4.60	1.49	1.42
26	FJ	201	PEB	C3C-C4C	4.60	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	KJ	202	PEB	C3C-C4C	4.60	1.49	1.42
26	HE	202	PEB	C3B-C2B	4.60	1.46	1.36
28	B6	1002	CYC	CHB-C1B	4.60	1.49	1.38
26	LA	202	PEB	C3C-C4C	4.59	1.49	1.42
26	FC	202	PEB	C3C-C4C	4.59	1.49	1.42
26	ND	201	PEB	C3C-C4C	4.59	1.49	1.42
26	BE	201	PEB	C4D-ND	4.59	1.41	1.35
26	BJ	201	PEB	C3C-C4C	4.59	1.49	1.42
26	UA	202	PEB	C3C-C4C	4.59	1.49	1.42
26	P4	203	PEB	CHA-C1B	4.59	1.51	1.40
26	L5	201	PEB	C2A-C1A	-4.59	1.48	1.52
26	QF	202	PEB	C3C-C4C	4.59	1.49	1.42
26	k1	203	PEB	C3C-C4C	4.59	1.49	1.42
26	YB	201	PEB	C3C-C4C	4.59	1.49	1.42
26	V2	203	PEB	C3C-C4C	4.59	1.49	1.42
26	PB	201	PEB	C3B-C2B	4.59	1.46	1.36
26	EA	201	PEB	C3C-C4C	4.59	1.49	1.42
26	H4	202	PEB	C3C-C4C	4.59	1.49	1.42
26	FI	1002	PEB	C3C-C4C	4.58	1.49	1.42
26	F8	202	PEB	C3C-C4C	4.58	1.49	1.42
26	Y8	201	PEB	C3C-C4C	4.58	1.49	1.42
26	KC	201	PEB	C3C-C4C	4.58	1.49	1.42
26	jF	203	PEB	C3C-C4C	4.58	1.49	1.42
26	RD	201	PEB	C3B-C2B	4.58	1.46	1.36
26	P8	202	PEB	C3C-C4C	4.58	1.49	1.42
26	N1	201	PEB	C3C-C4C	4.58	1.49	1.42
26	R2	203	PEB	C3C-C4C	4.58	1.49	1.42
26	TG	202	PEB	C3B-C2B	4.58	1.46	1.36
26	O8	201	PEB	C3C-C4C	4.58	1.49	1.42
26	eE	202	PEB	CHA-C1B	4.58	1.51	1.40
28	CH	1001	CYC	CHB-C4A	4.58	1.51	1.40
26	I1	201	PEB	C3C-C4C	4.58	1.49	1.42
26	Z8	202	PEB	C3B-C2B	4.58	1.46	1.36
26	E3	202	PEB	C3C-C4C	4.58	1.49	1.42
26	H5	202	PEB	C3C-C4C	4.58	1.49	1.42
26	e8	202	PEB	C3C-C4C	4.58	1.49	1.42
28	MB	1001	CYC	C2C-C1C	-4.58	1.48	1.52
26	JE	201	PEB	C3C-C4C	4.58	1.49	1.42
26	r4	201	PEB	C3C-C4C	4.58	1.49	1.42
26	O3	201	PEB	C3B-C2B	4.57	1.46	1.36
26	Q3	201	PEB	C3C-C4C	4.57	1.49	1.42
26	W4	201	PEB	C3C-C4C	4.57	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JC	201	PEB	C3B-C2B	4.57	1.46	1.36
26	X3	201	PEB	CHA-C1B	4.57	1.51	1.40
26	SG	202	PEB	C3C-C4C	4.57	1.49	1.42
27	wG	304	PUB	C2B-C1B	4.57	1.49	1.42
26	SI	201	PEB	C1A-NA	-4.57	1.31	1.37
26	V3	201	PEB	C3C-C4C	4.57	1.49	1.42
28	qH	1002	CYC	C2A-C3A	4.57	1.46	1.36
26	LD	202	PEB	C3C-C4C	4.57	1.49	1.42
28	rH	1001	CYC	C1C-NC	-4.57	1.31	1.37
26	L4	202	PEB	C3C-C4C	4.56	1.49	1.42
28	LF	1001	CYC	C2A-C3A	4.56	1.46	1.36
28	rH	1001	CYC	C2C-C1C	-4.56	1.48	1.52
26	iE	202	PEB	C3B-C2B	4.56	1.46	1.36
26	H8	202	PEB	C1A-NA	-4.56	1.31	1.37
26	L3	201	PEB	C3C-C4C	4.56	1.49	1.42
28	tH	1001	CYC	C1C-NC	-4.56	1.31	1.37
26	MA	202	PEB	C3C-C4C	4.56	1.49	1.42
26	j8	202	PEB	C3C-C4C	4.56	1.49	1.42
26	ZA	202	PEB	C3B-C2B	4.56	1.46	1.36
26	O6	201	PEB	C3C-C4C	4.56	1.49	1.42
26	E8	201	PEB	C3C-C4C	4.56	1.49	1.42
26	HB	1002	PEB	C3C-C4C	4.56	1.49	1.42
27	NJ	201	PUB	C2B-C1B	4.56	1.49	1.42
26	e8	202	PEB	C1A-NA	-4.56	1.31	1.37
26	F5	201	PEB	C3C-C4C	4.56	1.49	1.42
26	LF	1002	PEB	C3C-C4C	4.56	1.49	1.42
28	NI	1001	CYC	C2C-C1C	-4.56	1.48	1.52
26	Y8	202	PEB	C3C-C4C	4.56	1.49	1.42
26	OD	202	PEB	C3C-C4C	4.56	1.49	1.42
28	wH	1001	CYC	C1C-NC	-4.55	1.31	1.37
26	OF	201	PEB	C3C-C4C	4.55	1.49	1.42
26	AG	201	PEB	C3B-C2B	4.55	1.46	1.36
28	K7	1001	CYC	CHB-C1B	4.55	1.48	1.38
26	ZI	201	PEB	C1A-NA	-4.55	1.31	1.37
27	AI	302	PUB	C2B-C1B	4.55	1.49	1.42
26	XD	201	PEB	CHA-C1B	4.55	1.51	1.40
26	jI	201	PEB	C3B-C2B	4.55	1.46	1.36
26	D4	202	PEB	C3C-C4C	4.55	1.49	1.42
26	kG	203	PEB	C3C-C4C	4.55	1.49	1.42
26	P6	201	PEB	C3B-C2B	4.55	1.46	1.36
28	SH	1001	CYC	C2C-C1C	-4.55	1.48	1.52
26	I5	203	PEB	C3C-C4C	4.55	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YA	201	PEB	C3C-C4C	4.55	1.49	1.42
28	PH	1001	CYC	C1C-NC	-4.55	1.31	1.37
26	Z8	202	PEB	C2A-C1A	-4.55	1.48	1.52
26	AI	304	PEB	C3C-C4C	4.55	1.49	1.42
28	SH	1001	CYC	C1C-NC	-4.55	1.31	1.37
26	PD	201	PEB	C3B-C2B	4.54	1.46	1.36
26	bF	203	PEB	C3C-C4C	4.54	1.49	1.42
26	G4	202	PEB	C3C-C4C	4.54	1.49	1.42
26	W6	201	PEB	C3B-C2B	4.54	1.46	1.36
26	S3	201	PEB	C3C-C4C	4.54	1.49	1.42
26	TA	202	PEB	C1A-NA	-4.54	1.31	1.37
26	SG	202	PEB	C1A-NA	-4.54	1.31	1.37
26	KA	201	PEB	C3C-C4C	4.54	1.49	1.42
26	T3	203	PEB	C1A-NA	-4.54	1.31	1.37
26	j2	201	PEB	C3B-C2B	4.54	1.46	1.36
26	DG	203	PEB	C3B-C2B	4.54	1.46	1.36
28	D2	1001	CYC	CHB-C1B	4.54	1.48	1.38
26	GE	201	PEB	C1A-NA	-4.54	1.31	1.37
26	G6	1002	PEB	C3C-C4C	4.53	1.49	1.42
26	z4	201	PEB	C3B-C2B	4.53	1.46	1.36
28	L2	1001	CYC	CHB-C1B	4.53	1.48	1.38
26	K5	203	PEB	C3C-C4C	4.53	1.49	1.42
26	pE	202	PEB	CHA-C1B	4.53	1.51	1.40
26	JC	201	PEB	C1A-NA	-4.53	1.31	1.37
26	ED	202	PEB	C3C-C4C	4.53	1.49	1.42
26	P3	202	PEB	C3C-C4C	4.53	1.49	1.42
26	l8	203	PEB	C3C-C4C	4.53	1.49	1.42
27	Y3	302	PUB	C2B-C1B	4.53	1.49	1.42
26	y4	203	PEB	C1A-NA	-4.53	1.31	1.37
26	CJ	201	PEB	C3B-C2B	4.53	1.46	1.36
28	sH	1001	CYC	C1C-NC	-4.53	1.31	1.37
28	DI	1001	CYC	CHB-C1B	4.53	1.48	1.38
26	11	202	PEB	C3C-C4C	4.53	1.49	1.42
26	OB	201	PEB	C3B-C2B	4.52	1.46	1.36
26	KG	202	PEB	C1A-NA	-4.52	1.31	1.37
26	F2	1002	PEB	C3C-C4C	4.52	1.49	1.42
26	lA	203	PEB	C3C-C4C	4.52	1.49	1.42
26	mF	202	PEB	CHA-C1B	4.52	1.51	1.40
26	M8	202	PEB	C3C-C4C	4.52	1.49	1.42
26	H5	201	PEB	C1A-NA	-4.52	1.31	1.37
26	Z7	201	PEB	CHA-C1B	4.52	1.51	1.40
26	VG	202	PEB	C3B-C2B	4.52	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r1	201	PEB	C3C-C4C	4.52	1.49	1.42
26	l1	202	PEB	CHA-C1B	4.51	1.51	1.40
26	lA	202	PEB	C3C-C4C	4.51	1.49	1.42
28	wH	1001	CYC	C2C-C1C	-4.51	1.48	1.52
26	F8	201	PEB	C1A-NA	-4.51	1.31	1.37
26	XG	203	PEB	C3B-C2B	4.51	1.46	1.36
28	J2	1001	CYC	CHB-C1B	4.51	1.48	1.38
28	YH	1002	CYC	CHB-C4A	4.51	1.51	1.40
27	21	403	PUB	C2B-C1B	4.51	1.49	1.42
26	UA	202	PEB	C3B-C2B	4.51	1.46	1.36
26	h8	201	PEB	C3C-C4C	4.51	1.49	1.42
26	KA	203	PEB	C3C-C4C	4.51	1.49	1.42
26	HA	202	PEB	C1A-NA	-4.50	1.31	1.37
26	UI	201	PEB	C1A-NA	-4.50	1.31	1.37
26	i4	201	PEB	C3C-C4C	4.50	1.49	1.42
28	hH	1001	CYC	CHB-C4A	4.50	1.51	1.40
26	f8	203	PEB	C3C-C4C	4.50	1.49	1.42
26	JC	201	PEB	C3C-C4C	4.50	1.49	1.42
26	LC	201	PEB	C3C-C4C	4.50	1.49	1.42
26	W8	203	PEB	C2A-C1A	-4.50	1.48	1.52
26	TD	201	PEB	C2A-C1A	-4.50	1.48	1.52
28	YH	1003	CYC	CHB-C4A	4.50	1.51	1.40
26	RE	201	PEB	C3C-C4C	4.50	1.49	1.42
28	L6	1001	CYC	CHB-C1B	4.50	1.48	1.38
28	LI	1001	CYC	CHB-C1B	4.50	1.48	1.38
26	14	202	PEB	C3C-C4C	4.50	1.49	1.42
26	J5	201	PEB	C3B-C2B	4.50	1.46	1.36
26	cE	203	PEB	C3C-C4C	4.50	1.49	1.42
26	VD	201	PEB	C3C-C4C	4.50	1.49	1.42
26	sE	203	PEB	C3C-C4C	4.50	1.49	1.42
26	S8	202	PEB	C3C-C4C	4.49	1.49	1.42
26	m4	201	PEB	C3C-C4C	4.49	1.49	1.42
26	FE	202	PEB	C3B-C2B	4.49	1.46	1.36
26	W3	201	PEB	C3C-C4C	4.49	1.49	1.42
28	oH	1001	CYC	CHB-C4A	4.49	1.50	1.40
26	WE	201	PEB	C3C-C4C	4.49	1.49	1.42
26	y1	203	PEB	C1A-NA	-4.49	1.31	1.37
28	G7	1001	CYC	CHB-C1B	4.49	1.48	1.38
26	W2	201	PEB	C1A-NA	-4.49	1.31	1.37
26	OE	202	PEB	CHA-C1B	4.49	1.50	1.40
26	G8	203	PEB	C3C-C4C	4.48	1.49	1.42
28	jH	1001	CYC	CHB-C4A	4.48	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CA	203	PEB	C3C-C4C	4.48	1.49	1.42
28	kH	1001	CYC	C1C-NC	-4.48	1.31	1.37
26	VE	202	PEB	C3B-C2B	4.48	1.46	1.36
26	HG	202	PEB	C3B-C2B	4.48	1.46	1.36
26	OB	201	PEB	C2A-C1A	-4.48	1.48	1.52
26	O1	201	PEB	C1A-NA	-4.48	1.31	1.37
26	K8	201	PEB	C1A-NA	-4.48	1.31	1.37
26	YG	203	PEB	C3C-C4C	4.48	1.49	1.42
26	M3	201	PEB	C3C-C4C	4.48	1.49	1.42
26	Z2	201	PEB	C2A-C1A	-4.48	1.48	1.52
26	JG	201	PEB	C3C-C4C	4.48	1.49	1.42
28	I6	1001	CYC	C2C-C1C	-4.48	1.48	1.52
26	UE	203	PEB	C3C-C4C	4.48	1.49	1.42
26	C8	203	PEB	C3C-C4C	4.47	1.49	1.42
26	UJ	201	PEB	CHA-C1B	4.47	1.50	1.40
26	IJ	201	PEB	C3B-C2B	4.47	1.46	1.36
28	F2	1001	CYC	CHB-C1B	4.47	1.48	1.38
26	N3	201	PEB	C2A-C1A	-4.47	1.48	1.52
26	W1	201	PEB	C3C-C4C	4.47	1.49	1.42
26	FG	201	PEB	C3C-C4C	4.47	1.49	1.42
26	gG	201	PEB	CHA-C1B	4.47	1.50	1.40
26	FA	201	PEB	C1A-NA	-4.47	1.31	1.37
26	WB	201	PEB	C3B-C2B	4.47	1.46	1.36
26	BG	201	PEB	C2A-C1A	-4.46	1.48	1.52
26	W1	201	PEB	C1A-NA	-4.46	1.31	1.37
26	W9	201	PEB	C3B-C2B	4.46	1.46	1.36
26	YB	202	PEB	C3C-C4C	4.46	1.49	1.42
28	LB	1001	CYC	C1C-NC	-4.46	1.31	1.37
26	l8	202	PEB	C3C-C4C	4.46	1.49	1.42
28	LB	1001	CYC	CHB-C1B	4.46	1.48	1.38
26	ZF	203	PEB	CHA-C1B	4.46	1.50	1.40
28	YH	1004	CYC	CHB-C4A	4.46	1.50	1.40
26	R3	201	PEB	C1A-NA	-4.46	1.31	1.37
28	PH	1001	CYC	C2C-C1C	-4.46	1.48	1.52
26	W6	202	PEB	C3C-C4C	4.46	1.49	1.42
26	GB	1002	PEB	C3C-C4C	4.46	1.49	1.42
26	MG	201	PEB	C3B-C2B	4.45	1.46	1.36
26	T3	201	PEB	C1A-NA	-4.45	1.31	1.37
26	kF	202	PEB	CHA-C1B	4.45	1.50	1.40
26	N3	201	PEB	C3C-C4C	4.45	1.49	1.42
28	JI	1001	CYC	CHB-C1B	4.45	1.48	1.38
26	G4	201	PEB	CHA-C1B	4.45	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TD	202	PEB	C3B-C2B	4.45	1.46	1.36
26	PG	201	PEB	C2A-C1A	-4.45	1.48	1.52
26	F1	202	PEB	C3C-C4C	4.45	1.49	1.42
26	BG	201	PEB	C3C-C4C	4.45	1.49	1.42
26	N2	1002	PEB	C3C-C4C	4.45	1.49	1.42
28	VH	1001	CYC	CHB-C4A	4.44	1.50	1.40
26	R3	201	PEB	C3B-C2B	4.44	1.46	1.36
26	qE	201	PEB	C3C-C4C	4.44	1.49	1.42
26	f2	201	PEB	C3B-C2B	4.44	1.46	1.36
26	ZA	202	PEB	C2A-C1A	-4.44	1.48	1.52
26	sE	202	PEB	CHA-C1B	4.44	1.50	1.40
26	HG	201	PEB	C3C-C4C	4.44	1.49	1.42
26	FG	202	PEB	C3B-C2B	4.44	1.46	1.36
28	iH	1001	CYC	CHB-C4A	4.44	1.50	1.40
26	z1	201	PEB	C3B-C2B	4.44	1.46	1.36
26	Y6	202	PEB	C3C-C4C	4.43	1.49	1.42
26	R8	202	PEB	C1A-NA	-4.43	1.31	1.37
26	SA	201	PEB	C3C-C4C	4.43	1.49	1.42
26	i8	202	PEB	CHA-C1B	4.43	1.50	1.40
26	KG	201	PEB	C3B-C2B	4.43	1.46	1.36
26	cF	202	PEB	CHA-C1B	4.43	1.50	1.40
26	XA	202	PEB	C2A-C1A	-4.43	1.48	1.52
26	X4	203	PEB	C3C-C4C	4.43	1.49	1.42
28	gH	1001	CYC	CHB-C4A	4.43	1.50	1.40
28	IH	1001	CYC	CHB-C4A	4.43	1.50	1.40
26	BE	201	PEB	C1D-ND	4.43	1.52	1.45
26	MJ	201	PEB	C3B-C2B	4.43	1.46	1.36
26	WI	201	PEB	C1A-NA	-4.43	1.31	1.37
26	NA	202	PEB	C3C-C4C	4.43	1.49	1.42
28	FI	1001	CYC	CHB-C1B	4.43	1.48	1.38
28	MH	1001	CYC	CHB-C4A	4.42	1.50	1.40
26	I9	201	PEB	C3B-C2B	4.42	1.46	1.36
26	I8	202	PEB	C2A-C1A	-4.42	1.48	1.52
26	L9	202	PEB	C1A-NA	-4.42	1.31	1.37
28	KH	1001	CYC	C1C-NC	-4.42	1.31	1.37
26	AJ	303	PEB	C3C-C4C	4.41	1.48	1.42
26	S2	201	PEB	C1A-NA	-4.41	1.31	1.37
26	gE	203	PEB	C3C-C4C	4.41	1.48	1.42
26	sG	203	PEB	C3C-C4C	4.41	1.48	1.42
26	iA	202	PEB	CHA-C1B	4.41	1.50	1.40
26	S2	201	PEB	C2A-C1A	-4.41	1.48	1.52
26	GG	201	PEB	C1A-NA	-4.41	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	LF	1001	CYC	CHB-C4A	4.41	1.50	1.40
26	H5	201	PEB	C3C-C4C	4.41	1.48	1.42
28	DB	1001	CYC	C1C-NC	-4.41	1.31	1.37
28	TH	1001	CYC	C1C-NC	-4.41	1.31	1.37
28	GH	1001	CYC	CHB-C4A	4.41	1.50	1.40
26	N8	202	PEB	C3C-C4C	4.41	1.48	1.42
26	PJ	202	PEB	C1A-NA	-4.40	1.31	1.37
26	R8	202	PEB	CHA-C1B	4.40	1.50	1.40
26	L9	201	PEB	C3C-C4C	4.40	1.48	1.42
28	LF	1001	CYC	C1C-NC	-4.40	1.31	1.37
26	l2	201	PEB	C3B-C2B	4.40	1.46	1.36
26	MA	203	PEB	C3C-C4C	4.40	1.48	1.42
26	KA	201	PEB	C1A-NA	-4.39	1.31	1.37
28	EH	1001	CYC	C1C-NC	-4.39	1.31	1.37
26	IA	202	PEB	C2A-C1A	-4.39	1.48	1.52
26	N7	1002	PEB	C3C-C4C	4.39	1.48	1.42
26	RG	201	PEB	C3C-C4C	4.39	1.48	1.42
26	L8	202	PEB	CHA-C1B	4.39	1.50	1.40
26	W2	201	PEB	C2A-C1A	-4.39	1.48	1.52
26	H5	201	PEB	C2A-C1A	-4.39	1.48	1.52
26	gG	203	PEB	C3C-C4C	4.39	1.48	1.42
26	N1	201	PEB	C1A-NA	-4.39	1.31	1.37
28	vH	1001	CYC	C1C-NC	-4.39	1.31	1.37
26	CA	202	PEB	C3C-C4C	4.39	1.48	1.42
26	KC	202	PEB	C3C-C4C	4.38	1.48	1.42
26	K8	201	PEB	C3C-C4C	4.38	1.48	1.42
26	MA	201	PEB	C3C-C4C	4.38	1.48	1.42
26	U8	202	PEB	C3B-C2B	4.38	1.46	1.36
26	WA	201	PEB	C3B-C2B	4.38	1.46	1.36
28	F6	1001	CYC	CHB-C1B	4.38	1.48	1.38
26	HE	201	PEB	C3C-C4C	4.38	1.48	1.42
26	VA	202	PEB	CHA-C1B	4.38	1.50	1.40
26	kG	201	PEB	CHA-C1B	4.37	1.50	1.40
28	YH	1001	CYC	C1C-NC	-4.37	1.31	1.37
26	Q4	201	PEB	C1A-NA	-4.37	1.31	1.37
26	X1	203	PEB	C3C-C4C	4.37	1.48	1.42
26	W4	201	PEB	C1A-NA	-4.37	1.31	1.37
26	O3	201	PEB	C2A-C1A	-4.37	1.48	1.52
28	RH	1001	CYC	C2C-C1C	-4.37	1.48	1.52
26	LA	202	PEB	CHA-C1B	4.37	1.50	1.40
26	DJ	202	PEB	C1A-NA	-4.37	1.31	1.37
28	gH	1001	CYC	C1C-NC	-4.37	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1H	1000	CYC	CHB-C4A	4.36	1.50	1.40
28	HB	1001	CYC	C1C-NC	-4.36	1.31	1.37
26	LE	202	PEB	C3B-C2B	4.36	1.46	1.36
26	mE	203	PEB	CHA-C1B	4.36	1.50	1.40
28	qH	1001	CYC	CHB-C4A	4.36	1.50	1.40
26	GA	203	PEB	C3C-C4C	4.36	1.48	1.42
26	gE	201	PEB	CHA-C1B	4.36	1.50	1.40
26	M8	201	PEB	C1A-NA	-4.36	1.32	1.37
26	YF	202	PEB	CHA-C1B	4.36	1.50	1.40
26	bI	201	PEB	C3B-C2B	4.36	1.46	1.36
28	OH	1001	CYC	CHB-C4A	4.36	1.50	1.40
28	kH	1001	CYC	CHB-C4A	4.36	1.50	1.40
26	R3	203	PEB	C1A-NA	-4.36	1.32	1.37
28	NB	1001	CYC	C1C-NC	-4.36	1.32	1.37
28	FB	1001	CYC	CHB-C1B	4.36	1.48	1.38
28	HI	1001	CYC	C1C-NC	-4.36	1.32	1.37
26	O6	201	PEB	C2A-C1A	-4.36	1.48	1.52
26	NI	1002	PEB	C3C-C4C	4.36	1.48	1.42
26	iI	201	PEB	C3C-C4C	4.36	1.48	1.42
26	LA	202	PEB	C2A-C1A	-4.36	1.48	1.52
28	eH	1001	CYC	CHB-C4A	4.36	1.50	1.40
28	pH	1001	CYC	C1C-NC	-4.35	1.32	1.37
26	GJ	202	PEB	C2C-C3C	4.35	1.50	1.37
26	W8	201	PEB	C1A-NA	-4.35	1.32	1.37
28	IH	1001	CYC	CHB-C4A	4.35	1.50	1.40
26	Y4	201	PEB	C3C-C4C	4.35	1.48	1.42
26	II	201	PEB	C3B-C2B	4.35	1.46	1.36
28	L6	1001	CYC	C1C-NC	-4.35	1.32	1.37
26	O1	201	PEB	C3C-C4C	4.35	1.48	1.42
26	P9	202	PEB	CHA-C1B	4.35	1.50	1.40
26	WA	203	PEB	C2A-C1A	-4.34	1.48	1.52
26	ID	202	PEB	C1A-NA	-4.34	1.32	1.37
26	PE	201	PEB	C2A-C1A	-4.34	1.48	1.52
26	M8	203	PEB	C3C-C4C	4.34	1.48	1.42
26	ZB	201	PEB	C1A-NA	-4.34	1.32	1.37
28	fH	1001	CYC	CHB-C4A	4.34	1.50	1.40
28	F7	1001	CYC	CHB-C1B	4.34	1.48	1.38
26	P3	201	PEB	C2A-C1A	-4.34	1.48	1.52
28	H6	1001	CYC	CHB-C1B	4.34	1.48	1.38
28	NH	1001	CYC	C1C-NC	-4.34	1.32	1.37
26	PJ	202	PEB	CHA-C1B	4.34	1.50	1.40
28	CI	1001	CYC	C2C-C1C	-4.33	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P1	203	PEB	CHA-C1B	4.33	1.50	1.40
26	QG	201	PEB	CHA-C1B	4.33	1.50	1.40
26	eE	203	PEB	CHA-C1B	4.33	1.50	1.40
26	LE	201	PEB	C2A-C1A	-4.33	1.48	1.52
26	J4	202	PEB	C3C-C4C	4.33	1.48	1.42
26	fE	201	PEB	C3C-C4C	4.33	1.48	1.42
28	C2	1001	CYC	C2C-C1C	-4.32	1.48	1.52
26	Y3	303	PEB	C3C-C4C	4.32	1.48	1.42
28	HB	1001	CYC	C2C-C1C	-4.32	1.48	1.52
26	K5	203	PEB	C1A-NA	-4.32	1.32	1.37
28	NI	1001	CYC	C1C-NC	-4.32	1.32	1.37
26	U8	202	PEB	C2A-C1A	-4.32	1.48	1.52
26	T3	202	PEB	C3B-C2B	4.32	1.45	1.36
26	eG	202	PEB	C3B-C2B	4.32	1.45	1.36
26	Z7	203	PEB	CHA-C1B	4.32	1.50	1.40
28	DB	1001	CYC	C2C-C1C	-4.32	1.48	1.52
26	WG	201	PEB	C3C-C4C	4.32	1.48	1.42
28	EH	1001	CYC	CHB-C4A	4.32	1.50	1.40
26	QE	201	PEB	CHA-C1B	4.32	1.50	1.40
26	eE	202	PEB	C3B-C2B	4.31	1.45	1.36
28	HB	1001	CYC	CHB-C1B	4.31	1.48	1.38
26	b2	201	PEB	C3B-C2B	4.31	1.45	1.36
28	J2	1001	CYC	C1C-NC	-4.31	1.32	1.37
26	L1	202	PEB	C3C-C4C	4.31	1.48	1.42
26	BE	201	PEB	C3C-C4C	4.31	1.48	1.42
26	W4	201	PEB	C2A-C1A	-4.31	1.48	1.52
26	JJ	203	PEB	C3C-C4C	4.31	1.48	1.42
26	SA	202	PEB	C3C-C4C	4.31	1.48	1.42
26	eG	202	PEB	CHA-C1B	4.31	1.50	1.40
26	oE	203	PEB	CHA-C1B	4.31	1.50	1.40
28	IH	1001	CYC	C1C-NC	-4.31	1.32	1.37
26	N4	201	PEB	C1A-NA	-4.31	1.32	1.37
26	Y7	202	PEB	CHA-C1B	4.31	1.50	1.40
26	EJ	201	PEB	C1A-NA	-4.31	1.32	1.37
26	WG	202	PEB	CHA-C1B	4.31	1.50	1.40
28	QH	1001	CYC	CHB-C4A	4.30	1.50	1.40
26	c7	202	PEB	CHA-C1B	4.30	1.50	1.40
26	V1	201	PEB	C1A-NA	-4.30	1.32	1.37
26	VF	203	PEB	CHA-C1B	4.30	1.50	1.40
26	W6	201	PEB	C1A-NA	-4.30	1.32	1.37
28	L2	1001	CYC	C1C-NC	-4.30	1.32	1.37
26	EA	202	PEB	C3C-C4C	4.30	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T1	202	PEB	C1A-NA	-4.30	1.32	1.37
26	W8	203	PEB	C1A-NA	-4.30	1.32	1.37
26	LG	202	PEB	C2C-C3C	4.30	1.50	1.37
26	F5	202	PEB	C3C-C4C	4.30	1.48	1.42
26	H5	203	PEB	C1A-NA	-4.30	1.32	1.37
26	F3	202	PEB	C3C-C4C	4.30	1.48	1.42
28	QH	1001	CYC	C1C-NC	-4.30	1.32	1.37
27	xE	306	PUB	C2B-C1B	4.30	1.48	1.42
26	g1	203	PEB	C3C-C4C	4.29	1.48	1.42
26	QJ	202	PEB	CHA-C1B	4.29	1.50	1.40
26	gG	201	PEB	C3B-C2B	4.29	1.45	1.36
26	MJ	201	PEB	C1A-NA	-4.29	1.32	1.37
26	QJ	202	PEB	C1A-NA	-4.29	1.32	1.37
28	H6	1001	CYC	C1C-NC	-4.29	1.32	1.37
26	kB	202	PEB	C1A-NA	-4.29	1.32	1.37
26	BJ	203	PEB	C3C-C4C	4.29	1.48	1.42
26	F1	201	PEB	C2C-C3C	4.29	1.50	1.37
26	K8	203	PEB	C3C-C4C	4.29	1.48	1.42
26	Q1	201	PEB	C1A-NA	-4.29	1.32	1.37
26	RD	203	PEB	C1A-NA	-4.29	1.32	1.37
26	g4	203	PEB	C3C-C4C	4.29	1.48	1.42
26	EE	201	PEB	C3B-C2B	4.29	1.45	1.36
28	KH	1001	CYC	C3D-C2D	4.29	1.50	1.37
26	G5	203	PEB	CHA-C1B	4.29	1.50	1.40
28	pH	1001	CYC	C2C-C1C	-4.29	1.48	1.52
26	Z8	202	PEB	C1A-NA	-4.29	1.32	1.37
26	KG	202	PEB	C2A-C1A	-4.29	1.48	1.52
26	W8	203	PEB	C3B-C2B	4.28	1.45	1.36
28	tH	1001	CYC	C2C-C1C	-4.28	1.48	1.52
26	WJ	201	PEB	CHA-C1B	4.28	1.50	1.40
26	e6	203	PEB	C2C-C3C	4.28	1.50	1.37
26	H8	202	PEB	C2A-C1A	-4.28	1.48	1.52
28	D6	1001	CYC	C1C-NC	-4.28	1.32	1.37
26	IG	203	PEB	C1A-NA	-4.28	1.32	1.37
26	F8	201	PEB	C2A-C1A	-4.28	1.48	1.52
26	SI	201	PEB	C2A-C1A	-4.28	1.48	1.52
26	F4	201	PEB	C2C-C3C	4.28	1.50	1.37
26	W8	201	PEB	C3B-C2B	4.27	1.45	1.36
26	O2	201	PEB	C1A-NA	-4.27	1.32	1.37
28	sH	1001	CYC	CHB-C4A	4.27	1.50	1.40
26	X4	202	PEB	C3B-C2B	4.27	1.45	1.36
26	jA	202	PEB	C1A-NA	-4.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	WG	201	PEB	C1A-NA	-4.27	1.32	1.37
26	WB	201	PEB	C1A-NA	-4.27	1.32	1.37
26	B3	201	PEB	CHA-C1B	4.27	1.50	1.40
26	LC	201	PEB	C1A-NA	-4.27	1.32	1.37
28	EF	1001	CYC	C1C-NC	-4.27	1.32	1.37
28	CB	1001	CYC	CHB-C4A	4.27	1.50	1.40
28	H6	1001	CYC	C2C-C1C	-4.27	1.48	1.52
26	oE	202	PEB	CHA-C1B	4.27	1.50	1.40
28	GH	1001	CYC	C1C-NC	-4.26	1.32	1.37
26	HA	201	PEB	CHA-C1B	4.26	1.50	1.40
28	pH	1001	CYC	CHB-C4A	4.26	1.50	1.40
28	iH	1001	CYC	C1C-NC	-4.26	1.32	1.37
26	MG	201	PEB	C1A-NA	-4.26	1.32	1.37
28	YH	1002	CYC	C1C-NC	-4.26	1.32	1.37
26	ZA	202	PEB	C1A-NA	-4.26	1.32	1.37
26	d1	203	PEB	CHA-C1B	4.26	1.50	1.40
26	t1	202	PEB	C2C-C3C	4.26	1.50	1.37
26	O3	202	PEB	C3C-C4C	4.26	1.48	1.42
28	N2	1001	CYC	C2C-C1C	-4.26	1.48	1.52
26	LE	202	PEB	C2C-C3C	4.26	1.50	1.37
26	VI	202	PEB	C1A-NA	-4.26	1.32	1.37
26	K5	202	PEB	C3C-C4C	4.26	1.48	1.42
26	bB	202	PEB	C3C-C4C	4.26	1.48	1.42
26	V7	201	PEB	CHA-C1B	4.25	1.50	1.40
26	d4	202	PEB	C3C-C4C	4.25	1.48	1.42
26	D9	202	PEB	C1A-NA	-4.25	1.32	1.37
26	C8	202	PEB	C3C-C4C	4.25	1.48	1.42
28	B6	1002	CYC	C2C-C1C	-4.25	1.48	1.52
26	s4	201	PEB	CHA-C1B	4.25	1.50	1.40
28	NB	1001	CYC	C2C-C1C	-4.25	1.48	1.52
26	WA	203	PEB	C1A-NA	-4.25	1.32	1.37
26	tG	202	PEB	C2C-C3C	4.25	1.50	1.37
26	oE	203	PEB	C3C-C4C	4.25	1.48	1.42
26	m7	202	PEB	CHA-C1B	4.24	1.50	1.40
26	LG	202	PEB	C3B-C2B	4.24	1.45	1.36
26	XG	201	PEB	C2A-C1A	-4.24	1.48	1.52
26	VE	201	PEB	CHA-C1B	4.24	1.50	1.40
28	NH	1001	CYC	CHB-C4A	4.24	1.50	1.40
26	WA	203	PEB	C3B-C2B	4.24	1.45	1.36
26	M8	201	PEB	C3C-C4C	4.24	1.48	1.42
28	nH	1001	CYC	CHB-C4A	4.24	1.50	1.40
26	P3	203	PEB	C1A-NA	-4.24	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	uE	203	PEB	CHA-C1B	4.24	1.50	1.40
26	M9	201	PEB	C1A-NA	-4.24	1.32	1.37
26	aF	202	PEB	CHA-C1B	4.24	1.50	1.40
26	k6	202	PEB	C1A-NA	-4.24	1.32	1.37
26	d4	203	PEB	CHA-C1B	4.24	1.50	1.40
26	N8	201	PEB	CHA-C1B	4.23	1.50	1.40
26	F8	202	PEB	C1A-NA	-4.23	1.32	1.37
28	KH	1001	CYC	CHB-C1B	4.23	1.48	1.38
26	x4	202	PEB	C2C-C3C	4.23	1.50	1.37
26	G1	201	PEB	CHA-C1B	4.23	1.50	1.40
26	OE	202	PEB	C3B-C2B	4.23	1.45	1.36
26	LA	202	PEB	C1A-NA	-4.23	1.32	1.37
26	gE	201	PEB	C3B-C2B	4.23	1.45	1.36
26	TF	202	PEB	CHA-C1B	4.23	1.50	1.40
26	CG	202	PEB	CHA-C1B	4.23	1.50	1.40
26	PF	202	PEB	CHA-C1B	4.23	1.50	1.40
26	Z4	202	PEB	CHA-C1B	4.23	1.50	1.40
26	OI	201	PEB	C3B-C2B	4.23	1.45	1.36
26	PD	201	PEB	CHA-C1B	4.23	1.50	1.40
28	YH	1001	CYC	CHB-C4A	4.23	1.50	1.40
26	S9	201	PEB	CHA-C1B	4.22	1.50	1.40
26	CG	202	PEB	C3B-C2B	4.22	1.45	1.36
26	Q9	201	PEB	CHA-C1B	4.22	1.50	1.40
26	HA	202	PEB	C2A-C1A	-4.22	1.48	1.52
26	AG	201	PEB	CHA-C1B	4.22	1.50	1.40
26	b6	201	PEB	C1A-NA	-4.22	1.32	1.37
26	MA	201	PEB	C1A-NA	-4.22	1.32	1.37
26	uG	202	PEB	CHA-C1B	4.22	1.50	1.40
26	X1	202	PEB	C3B-C2B	4.22	1.45	1.36
26	z1	202	PEB	CHA-C1B	4.22	1.50	1.40
28	D2	1001	CYC	C1C-NC	-4.22	1.32	1.37
26	j1	202	PEB	CHA-C1B	4.22	1.50	1.40
26	YB	201	PEB	C2A-C1A	-4.22	1.48	1.52
26	H8	202	PEB	CHA-C1B	4.22	1.50	1.40
26	oG	202	PEB	CHA-C1B	4.22	1.50	1.40
26	gA	201	PEB	CHA-C1B	4.22	1.50	1.40
26	e7	202	PEB	CHA-C1B	4.22	1.50	1.40
26	eA	202	PEB	C1A-NA	-4.22	1.32	1.37
26	Q2	201	PEB	C1A-NA	-4.22	1.32	1.37
26	d8	201	PEB	C3C-C4C	4.21	1.48	1.42
28	NF	1001	CYC	CHB-C4A	4.21	1.50	1.40
28	B6	1002	CYC	C1C-NC	-4.21	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z8	201	PEB	C2A-C1A	-4.21	1.48	1.52
26	WA	201	PEB	C1A-NA	-4.21	1.32	1.37
26	J1	203	PEB	CHA-C1B	4.21	1.50	1.40
26	WI	201	PEB	C2A-C1A	-4.21	1.48	1.52
28	wH	1001	CYC	CHB-C4A	4.21	1.50	1.40
26	D1	203	PEB	CHA-C1B	4.21	1.50	1.40
26	FG	202	PEB	C1A-NA	-4.21	1.32	1.37
28	C6	1001	CYC	CHB-C4A	4.21	1.50	1.40
26	RD	203	PEB	CHA-C1B	4.21	1.50	1.40
26	IA	202	PEB	C3C-C4C	4.21	1.48	1.42
26	RD	201	PEB	C1A-NA	-4.21	1.32	1.37
26	TD	201	PEB	C3C-C4C	4.20	1.48	1.42
28	D6	1001	CYC	C2C-C1C	-4.20	1.48	1.52
26	fG	201	PEB	C3C-C4C	4.20	1.48	1.42
26	J5	201	PEB	C1B-C2B	4.20	1.54	1.45
28	jH	1001	CYC	C1C-NC	-4.20	1.32	1.37
26	ND	201	PEB	C2A-C1A	-4.20	1.48	1.52
28	kH	1001	CYC	C2C-C1C	-4.20	1.48	1.52
26	FD	202	PEB	C3C-C4C	4.20	1.48	1.42
26	bG	202	PEB	CHA-C1B	4.20	1.50	1.40
26	h2	201	PEB	C1A-NA	-4.20	1.32	1.37
26	X8	202	PEB	C2A-C1A	-4.20	1.48	1.52
28	NH	1001	CYC	C2C-C1C	-4.20	1.48	1.52
26	D3	203	PEB	CHA-C1B	4.20	1.50	1.40
26	Z8	201	PEB	C1A-NA	-4.20	1.32	1.37
26	CJ	201	PEB	C1A-NA	-4.20	1.32	1.37
26	N8	202	PEB	C1A-NA	-4.20	1.32	1.37
26	NE	201	PEB	C2A-C1A	-4.20	1.48	1.52
26	t4	201	PEB	CHA-C1B	4.19	1.50	1.40
26	Z6	201	PEB	C1A-NA	-4.19	1.32	1.37
26	N8	202	PEB	C2A-C1A	-4.19	1.48	1.52
26	FA	201	PEB	C2A-C1A	-4.19	1.48	1.52
28	jH	1001	CYC	C2C-C1C	-4.19	1.48	1.52
26	JC	201	PEB	C1B-C2B	4.19	1.54	1.45
28	NI	1001	CYC	CHB-C4A	4.19	1.50	1.40
28	B6	1002	CYC	CHB-C4A	4.19	1.50	1.40
28	UH	1001	CYC	C1C-NC	-4.19	1.32	1.37
28	vH	1001	CYC	CHB-C4A	4.19	1.50	1.40
26	bE	202	PEB	CHA-C1B	4.19	1.50	1.40
26	L8	201	PEB	CHA-C1B	4.19	1.50	1.40
26	VA	202	PEB	C2A-C1A	-4.19	1.48	1.52
28	UH	1001	CYC	C2C-C1C	-4.19	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YB	201	PEB	C1A-NA	-4.19	1.32	1.37
26	WE	202	PEB	C3B-C2B	4.18	1.45	1.36
26	qG	203	PEB	CHA-C1B	4.18	1.50	1.40
26	c1	202	PEB	C2C-C3C	4.18	1.50	1.37
26	B4	201	PEB	CHA-C1B	4.18	1.50	1.40
26	a7	202	PEB	CHA-C1B	4.18	1.50	1.40
28	LH	1001	CYC	CHB-C4A	4.18	1.50	1.40
26	H8	201	PEB	CHA-C1B	4.18	1.50	1.40
26	HA	201	PEB	C2A-C1A	-4.18	1.48	1.52
26	RB	201	PEB	C2A-C1A	-4.17	1.48	1.52
26	p1	202	PEB	CHA-C1B	4.17	1.50	1.40
26	qE	202	PEB	C1A-NA	-4.17	1.32	1.37
26	VG	202	PEB	CHA-C1B	4.17	1.50	1.40
28	qH	1001	CYC	C1C-NC	-4.17	1.32	1.37
26	iF	202	PEB	CHA-C1B	4.17	1.50	1.40
26	O2	201	PEB	C2A-C1A	-4.17	1.48	1.52
26	e1	202	PEB	C2C-C3C	4.17	1.50	1.37
28	tH	1001	CYC	CHB-C4A	4.17	1.50	1.40
26	QI	201	PEB	C1A-NA	-4.17	1.32	1.37
26	UA	202	PEB	C2A-C1A	-4.17	1.48	1.52
26	H9	202	PEB	CHA-C1B	4.17	1.50	1.40
26	FJ	202	PEB	CHA-C1B	4.17	1.50	1.40
26	VF	201	PEB	CHA-C1B	4.17	1.50	1.40
28	YH	1003	CYC	C1C-NC	-4.17	1.32	1.37
26	OG	202	PEB	C3B-C2B	4.17	1.45	1.36
26	V4	201	PEB	C3C-C4C	4.17	1.48	1.42
26	L3	201	PEB	CHA-C1B	4.17	1.50	1.40
26	E8	203	PEB	C3C-C4C	4.17	1.48	1.42
28	YH	1001	CYC	C2C-C1C	-4.17	1.48	1.52
26	TD	201	PEB	C1A-NA	-4.16	1.32	1.37
26	ZA	201	PEB	C2A-C1A	-4.16	1.48	1.52
28	M6	1001	CYC	C2C-C1C	-4.16	1.48	1.52
26	E9	201	PEB	C1A-NA	-4.16	1.32	1.37
26	NA	201	PEB	CHA-C1B	4.16	1.50	1.40
26	HA	202	PEB	CHA-C1B	4.16	1.50	1.40
26	L8	202	PEB	C1A-NA	-4.16	1.32	1.37
26	RA	202	PEB	C1A-NA	-4.16	1.32	1.37
26	K8	201	PEB	C2A-C1A	-4.16	1.48	1.52
26	iE	202	PEB	C1A-NA	-4.15	1.32	1.37
26	Y6	201	PEB	C1A-NA	-4.15	1.32	1.37
26	S2	201	PEB	C3B-C2B	4.15	1.45	1.36
26	OD	201	PEB	C2A-C1A	-4.15	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	jI	201	PEB	C1A-NA	-4.15	1.32	1.37
28	H2	1001	CYC	C1C-NC	-4.15	1.32	1.37
26	z1	201	PEB	CHA-C1B	4.15	1.50	1.40
26	XG	202	PEB	C3C-C4C	4.15	1.48	1.42
26	kA	202	PEB	C1A-NA	-4.15	1.32	1.37
28	RH	1001	CYC	CHB-C4A	4.15	1.50	1.40
26	HJ	202	PEB	CHA-C1B	4.15	1.50	1.40
28	vH	1001	CYC	C2C-C1C	-4.15	1.48	1.52
28	TH	1001	CYC	C2C-C1C	-4.14	1.48	1.52
26	qE	203	PEB	CHA-C1B	4.14	1.50	1.40
28	nH	1001	CYC	C1C-NC	-4.14	1.32	1.37
26	O2	201	PEB	C3B-C2B	4.14	1.45	1.36
26	LA	201	PEB	CHA-C1B	4.14	1.50	1.40
26	HC	201	PEB	CHA-C1B	4.14	1.50	1.40
26	Y8	202	PEB	C1A-NA	-4.14	1.32	1.37
26	OI	201	PEB	C1A-NA	-4.14	1.32	1.37
26	D4	203	PEB	CHA-C1B	4.14	1.50	1.40
26	HA	201	PEB	C1A-NA	-4.14	1.32	1.37
28	OH	1001	CYC	C1C-NC	-4.14	1.32	1.37
28	GH	1001	CYC	C2C-C1C	-4.13	1.48	1.52
28	PH	1001	CYC	CHB-C4A	4.13	1.50	1.40
26	pG	202	PEB	CHA-C1B	4.13	1.50	1.40
28	DI	1001	CYC	C1C-NC	-4.13	1.32	1.37
28	E6	1001	CYC	CHB-C4A	4.13	1.50	1.40
26	NA	202	PEB	CHA-C1B	4.13	1.50	1.40
26	T3	203	PEB	C2A-C1A	-4.13	1.48	1.52
26	B3	203	PEB	C1A-NA	-4.13	1.32	1.37
26	a4	201	PEB	CHA-C1B	4.13	1.50	1.40
26	SJ	201	PEB	CHA-C1B	4.13	1.50	1.40
26	I3	202	PEB	C1A-NA	-4.12	1.32	1.37
26	H5	201	PEB	CHA-C1B	4.12	1.50	1.40
28	N7	1001	CYC	CHB-C4A	4.12	1.50	1.40
26	WJ	202	PEB	CHA-C1B	4.12	1.50	1.40
26	dF	202	PEB	C1A-NA	-4.12	1.32	1.37
28	B6	1001	CYC	C1C-NC	-4.12	1.32	1.37
26	K5	201	PEB	C3C-C4C	4.12	1.48	1.42
28	rH	1001	CYC	CHB-C4A	4.12	1.50	1.40
26	N8	202	PEB	CHA-C1B	4.12	1.50	1.40
26	j2	201	PEB	C1A-NA	-4.12	1.32	1.37
26	T4	202	PEB	C1A-NA	-4.12	1.32	1.37
26	Y6	201	PEB	C2A-C1A	-4.12	1.48	1.52
26	V2	202	PEB	C1A-NA	-4.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	FA	202	PEB	C1A-NA	-4.12	1.32	1.37
26	GB	1002	PEB	C1A-NA	-4.12	1.32	1.37
26	e6	203	PEB	CHA-C1B	4.12	1.50	1.40
26	hF	202	PEB	C1A-NA	-4.12	1.32	1.37
26	IJ	201	PEB	C1A-NA	-4.12	1.32	1.37
26	W1	201	PEB	C2A-C1A	-4.12	1.48	1.52
26	NA	202	PEB	C1A-NA	-4.12	1.32	1.37
28	BB	1001	CYC	C1C-NC	-4.11	1.32	1.37
26	T8	202	PEB	C2A-C1A	-4.11	1.48	1.52
26	LG	201	PEB	C2A-C1A	-4.11	1.48	1.52
28	IH	1001	CYC	C2C-C1C	-4.11	1.48	1.52
28	YH	1003	CYC	C2C-C1C	-4.11	1.48	1.52
28	uH	1001	CYC	C2C-C1C	-4.11	1.48	1.52
26	HC	201	PEB	C1A-NA	-4.11	1.32	1.37
26	Q4	201	PEB	C2A-C1A	-4.11	1.48	1.52
28	HF	1001	CYC	C1C-NC	-4.11	1.32	1.37
28	NB	1001	CYC	CHB-C4A	4.11	1.50	1.40
26	Q4	202	PEB	C1A-NA	-4.11	1.32	1.37
26	e4	202	PEB	C2C-C3C	4.11	1.49	1.37
28	JF	1001	CYC	CHB-C4A	4.11	1.50	1.40
28	JI	1001	CYC	C1C-NC	-4.11	1.32	1.37
26	p4	202	PEB	CHA-C1B	4.11	1.50	1.40
28	UH	1001	CYC	CHB-C4A	4.11	1.50	1.40
26	dE	201	PEB	CHA-C1B	4.11	1.50	1.40
26	RG	201	PEB	C2A-C1A	-4.11	1.48	1.52
26	KC	203	PEB	C1A-NA	-4.11	1.32	1.37
26	OB	201	PEB	C1A-NA	-4.10	1.32	1.37
26	W4	202	PEB	C2A-C1A	-4.10	1.48	1.52
26	E8	202	PEB	C3C-C4C	4.10	1.48	1.42
28	TH	1001	CYC	CHB-C4A	4.10	1.50	1.40
26	PD	203	PEB	C1A-NA	-4.10	1.32	1.37
28	hH	1001	CYC	C1C-NC	-4.10	1.32	1.37
26	c4	202	PEB	C2C-C3C	4.10	1.49	1.37
28	QH	1001	CYC	C2C-C1C	-4.10	1.48	1.52
26	DD	203	PEB	CHA-C1B	4.10	1.50	1.40
28	LI	1001	CYC	C1C-NC	-4.10	1.32	1.37
26	O4	201	PEB	CHA-C1B	4.10	1.50	1.40
26	QJ	201	PEB	CHA-C1B	4.10	1.50	1.40
26	GC	203	PEB	CHA-C1B	4.10	1.50	1.40
26	F3	203	PEB	CHA-C1B	4.10	1.50	1.40
28	YH	1002	CYC	C2C-C1C	-4.10	1.48	1.52
26	L5	201	PEB	C3C-C4C	4.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YA	202	PEB	C1A-NA	-4.10	1.32	1.37
26	Z1	202	PEB	CHA-C1B	4.10	1.50	1.40
26	k7	202	PEB	CHA-C1B	4.10	1.50	1.40
28	DB	1001	CYC	CHB-C1B	4.10	1.47	1.38
26	tG	202	PEB	CHA-C1B	4.10	1.50	1.40
26	Q1	202	PEB	C1A-NA	-4.10	1.32	1.37
26	uG	203	PEB	CHA-C1B	4.10	1.50	1.40
28	EF	1001	CYC	C2C-C1C	-4.09	1.48	1.52
26	XD	203	PEB	C3C-C4C	4.09	1.48	1.42
26	UG	201	PEB	CHA-C1B	4.09	1.50	1.40
26	ZB	202	PEB	C1A-NA	-4.09	1.32	1.37
26	XG	202	PEB	C1A-NA	-4.09	1.32	1.37
26	EE	201	PEB	CHA-C1B	4.09	1.50	1.40
26	SI	201	PEB	C3B-C2B	4.09	1.45	1.36
26	P3	201	PEB	CHA-C1B	4.09	1.50	1.40
26	P3	201	PEB	C1A-NA	-4.09	1.32	1.37
26	C8	201	PEB	C1A-NA	-4.09	1.32	1.37
26	IJ	203	PEB	C1A-NA	-4.09	1.32	1.37
26	R6	201	PEB	C2A-C1A	-4.09	1.48	1.52
28	CF	1001	CYC	CHB-C4A	4.09	1.50	1.40
26	YE	201	PEB	CHA-C1B	4.09	1.50	1.40
26	ND	201	PEB	CHA-C1B	4.09	1.50	1.40
26	EA	202	PEB	CHA-C1B	4.08	1.50	1.40
26	P4	202	PEB	C1A-NA	-4.08	1.32	1.37
26	l2	201	PEB	C1A-NA	-4.08	1.32	1.37
28	fH	1001	CYC	C1C-NC	-4.08	1.32	1.37
28	EB	1001	CYC	CHB-C4A	4.08	1.50	1.40
28	JF	1001	CYC	C1C-NC	-4.08	1.32	1.37
28	EB	1001	CYC	C2C-C1C	-4.08	1.48	1.52
26	OI	201	PEB	C2A-C1A	-4.08	1.48	1.52
28	gH	1001	CYC	C2C-C1C	-4.08	1.48	1.52
26	FE	202	PEB	C1A-NA	-4.08	1.32	1.37
26	WG	202	PEB	C1A-NA	-4.08	1.32	1.37
26	m8	201	PEB	C1A-NA	-4.08	1.32	1.37
26	RI	202	PEB	C1A-NA	-4.08	1.32	1.37
26	VG	201	PEB	CHA-C1B	4.08	1.50	1.40
26	nE	202	PEB	CHA-C1B	4.08	1.50	1.40
26	x1	202	PEB	C2C-C3C	4.08	1.49	1.37
26	eB	203	PEB	CHA-C1B	4.07	1.50	1.40
26	HC	203	PEB	C1A-NA	-4.07	1.32	1.37
26	V8	202	PEB	CHA-C1B	4.07	1.50	1.40
26	EG	201	PEB	CHA-C1B	4.07	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f1	201	PEB	CHA-C1B	4.07	1.50	1.40
26	ME	201	PEB	CHA-C1B	4.07	1.49	1.40
26	CA	201	PEB	C1A-NA	-4.07	1.32	1.37
26	W1	202	PEB	C2A-C1A	-4.07	1.48	1.52
26	SJ	202	PEB	C1A-NA	-4.07	1.32	1.37
26	I8	202	PEB	C3C-C4C	4.07	1.48	1.42
26	EA	203	PEB	C3C-C4C	4.07	1.48	1.42
26	h4	203	PEB	CHA-C1B	4.07	1.49	1.40
26	K3	202	PEB	CHA-C1B	4.07	1.49	1.40
26	QJ	201	PEB	C2A-C1A	-4.07	1.48	1.52
28	qH	1002	CYC	C3D-C2D	4.07	1.49	1.37
28	dH	1001	CYC	C1C-NC	-4.07	1.32	1.37
26	t1	202	PEB	CHA-C1B	4.06	1.49	1.40
26	U4	201	PEB	C1A-NA	-4.06	1.32	1.37
26	eG	201	PEB	C1A-NA	-4.06	1.32	1.37
26	I5	201	PEB	C1A-NA	-4.06	1.32	1.37
26	J4	203	PEB	CHA-C1B	4.06	1.49	1.40
26	f2	201	PEB	C1A-NA	-4.06	1.32	1.37
26	TE	202	PEB	C1A-NA	-4.06	1.32	1.37
26	E8	202	PEB	CHA-C1B	4.06	1.49	1.40
26	VE	202	PEB	CHA-C1B	4.06	1.49	1.40
26	U1	201	PEB	CHA-C1B	4.06	1.49	1.40
26	hG	201	PEB	CHA-C1B	4.06	1.49	1.40
26	EG	201	PEB	C3B-C2B	4.06	1.45	1.36
26	U1	202	PEB	CHA-C1B	4.06	1.49	1.40
26	LD	201	PEB	CHA-C1B	4.06	1.49	1.40
26	W2	201	PEB	C3B-C2B	4.06	1.45	1.36
26	R1	201	PEB	C1A-NA	-4.06	1.32	1.37
26	a6	201	PEB	C1A-NA	-4.06	1.32	1.37
26	G6	1002	PEB	C1A-NA	-4.06	1.32	1.37
26	NA	202	PEB	C2A-C1A	-4.06	1.48	1.52
28	LH	1001	CYC	C2C-C1C	-4.06	1.48	1.52
27	K1	203	PUB	C3B-C2B	4.06	1.49	1.37
26	s1	203	PEB	CHA-C1B	4.06	1.49	1.40
28	G2	1001	CYC	C2C-C1C	-4.06	1.48	1.52
28	L2	1001	CYC	C2C-C1C	-4.05	1.48	1.52
26	oE	201	PEB	CHA-C1B	4.05	1.49	1.40
26	m6	203	PEB	CHA-C1B	4.05	1.49	1.40
26	T9	202	PEB	CHA-C1B	4.05	1.49	1.40
28	N2	1001	CYC	CHB-C4A	4.05	1.49	1.40
26	c6	202	PEB	CHA-C1B	4.05	1.49	1.40
26	DD	201	PEB	CHA-C1B	4.05	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VG	201	PEB	C2A-C1A	-4.05	1.48	1.52
28	N2	1001	CYC	C1C-NC	-4.05	1.32	1.37
26	dG	202	PEB	C2C-C3C	4.05	1.49	1.37
28	lH	1001	CYC	C1C-NC	-4.05	1.32	1.37
26	gF	202	PEB	CHA-C1B	4.05	1.49	1.40
26	XA	201	PEB	CHA-C1B	4.05	1.49	1.40
26	LJ	202	PEB	C1A-NA	-4.04	1.32	1.37
26	L3	203	PEB	CHA-C1B	4.04	1.49	1.40
26	cE	203	PEB	CHA-C1B	4.04	1.49	1.40
26	I9	202	PEB	CHA-C1B	4.04	1.49	1.40
26	H8	201	PEB	C1A-NA	-4.04	1.32	1.37
26	X8	201	PEB	CHA-C1B	4.04	1.49	1.40
26	r1	201	PEB	C2C-C3C	4.04	1.49	1.37
26	JG	201	PEB	CHA-C1B	4.04	1.49	1.40
26	O4	201	PEB	C1A-NA	-4.04	1.32	1.37
26	O6	201	PEB	C1A-NA	-4.04	1.32	1.37
26	Z1	201	PEB	CHA-C1B	4.04	1.49	1.40
26	V7	202	PEB	CHA-C1B	4.04	1.49	1.40
26	TG	202	PEB	C1A-NA	-4.04	1.32	1.37
28	D6	1001	CYC	CHB-C1B	4.04	1.47	1.38
26	Q1	201	PEB	C2A-C1A	-4.04	1.48	1.52
26	iI	203	PEB	CHA-C1B	4.04	1.49	1.40
26	dG	202	PEB	CHA-C1B	4.04	1.49	1.40
26	IJ	201	PEB	C3C-C4C	4.04	1.48	1.42
26	mA	202	PEB	CHA-C1B	4.03	1.49	1.40
28	uH	1001	CYC	CHB-C4A	4.03	1.49	1.40
26	TA	202	PEB	C2A-C1A	-4.03	1.48	1.52
26	R2	202	PEB	C1A-NA	-4.03	1.32	1.37
26	EJ	202	PEB	C1A-NA	-4.03	1.32	1.37
26	IJ	201	PEB	CHA-C1B	4.03	1.49	1.40
26	G5	201	PEB	C1A-NA	-4.03	1.32	1.37
26	T7	202	PEB	CHA-C1B	4.03	1.49	1.40
26	j8	201	PEB	C1A-NA	-4.03	1.32	1.37
26	XE	201	PEB	C2A-C1A	-4.03	1.48	1.52
26	FJ	201	PEB	C2A-C1A	-4.03	1.48	1.52
26	V1	201	PEB	C3C-C4C	4.03	1.48	1.42
26	m8	202	PEB	CHA-C1B	4.03	1.49	1.40
26	uE	202	PEB	CHA-C1B	4.03	1.49	1.40
26	h1	201	PEB	CHA-C1B	4.03	1.49	1.40
26	HE	202	PEB	CHA-C1B	4.02	1.49	1.40
26	PD	201	PEB	C2A-C1A	-4.02	1.48	1.52
26	K5	201	PEB	C1A-NA	-4.02	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B1	201	PEB	CHA-C1B	4.02	1.49	1.40
26	U4	201	PEB	CHA-C1B	4.02	1.49	1.40
26	fG	202	PEB	C1A-NA	-4.02	1.32	1.37
26	KD	202	PEB	CHA-C1B	4.02	1.49	1.40
28	LH	1001	CYC	C1C-NC	-4.02	1.32	1.37
26	F1	201	PEB	CHA-C1B	4.02	1.49	1.40
26	L9	202	PEB	CHA-C1B	4.02	1.49	1.40
26	HB	1002	PEB	C1A-NA	-4.02	1.32	1.37
28	iH	1001	CYC	C2C-C1C	-4.01	1.48	1.52
26	mF	201	PEB	C1A-NA	-4.01	1.32	1.37
26	qG	201	PEB	CHA-C1B	4.01	1.49	1.40
26	a8	204	PEB	C1A-NA	-4.01	1.32	1.37
26	I9	201	PEB	C3C-C4C	4.01	1.48	1.42
26	h4	203	PEB	C1A-NA	-4.01	1.32	1.37
26	K9	201	PEB	C1A-NA	-4.01	1.32	1.37
26	N3	201	PEB	CHA-C1B	4.01	1.49	1.40
26	I9	202	PEB	C1A-NA	-4.01	1.32	1.37
26	ZA	201	PEB	C1A-NA	-4.01	1.32	1.37
26	mA	201	PEB	C1A-NA	-4.01	1.32	1.37
26	IE	203	PEB	C1A-NA	-4.01	1.32	1.37
26	h1	202	PEB	CHA-C1B	4.01	1.49	1.40
26	hE	201	PEB	CHA-C1B	4.01	1.49	1.40
26	uE	203	PEB	C2C-C3C	4.01	1.49	1.37
26	LD	203	PEB	CHA-C1B	4.01	1.49	1.40
26	gG	201	PEB	C1A-NA	-4.01	1.32	1.37
28	HI	1001	CYC	C2C-C1C	-4.01	1.48	1.52
28	FB	1001	CYC	C1C-NC	-4.01	1.32	1.37
26	SF	201	PEB	C1A-NA	-4.01	1.32	1.37
26	g8	201	PEB	CHA-C1B	4.00	1.49	1.40
26	mB	203	PEB	CHA-C1B	4.00	1.49	1.40
26	fE	202	PEB	C1A-NA	-4.00	1.32	1.37
26	R3	203	PEB	CHA-C1B	4.00	1.49	1.40
26	j4	202	PEB	CHA-C1B	4.00	1.49	1.40
26	c4	201	PEB	CHA-C1B	4.00	1.49	1.40
26	PD	201	PEB	C1A-NA	-4.00	1.32	1.37
26	M8	201	PEB	C2A-C1A	-4.00	1.48	1.52
26	CJ	201	PEB	C2C-C3C	4.00	1.49	1.37
26	X3	201	PEB	C1A-NA	-4.00	1.32	1.37
26	L4	201	PEB	CHA-C1B	4.00	1.49	1.40
26	BE	201	PEB	OD-C4D	4.00	1.31	1.23
26	v1	202	PEB	C2C-C3C	4.00	1.49	1.37
28	H2	1001	CYC	C2C-C1C	-4.00	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	EI	1001	CYC	C2C-C1C	-4.00	1.48	1.52
26	S4	201	PEB	C3C-C4C	4.00	1.48	1.42
26	AB	304	PEB	C1A-NA	-4.00	1.32	1.37
26	HJ	202	PEB	C1A-NA	-4.00	1.32	1.37
26	s4	203	PEB	CHA-C1B	4.00	1.49	1.40
26	jG	202	PEB	CHA-C1B	4.00	1.49	1.40
28	JH	1001	CYC	C1C-NC	-4.00	1.32	1.37
26	I9	201	PEB	CHA-C1B	4.00	1.49	1.40
26	A1	201	PEB	CHA-C1B	3.99	1.49	1.40
26	HG	202	PEB	C1A-NA	-3.99	1.32	1.37
26	P1	202	PEB	C1A-NA	-3.99	1.32	1.37
26	aI	203	PEB	CHA-C1B	3.99	1.49	1.40
26	I9	201	PEB	C1A-NA	-3.99	1.32	1.37
26	kE	201	PEB	C2C-C3C	3.99	1.49	1.37
26	N3	201	PEB	C1A-NA	-3.99	1.32	1.37
26	KA	201	PEB	CHA-C1B	3.99	1.49	1.40
26	iE	203	PEB	CHA-C1B	3.99	1.49	1.40
26	e8	201	PEB	C1A-NA	-3.99	1.32	1.37
28	F2	1001	CYC	C1C-NC	-3.99	1.32	1.37
26	P8	202	PEB	CHA-C1B	3.99	1.49	1.40
26	TD	201	PEB	CHA-C1B	3.99	1.49	1.40
26	II	201	PEB	C1A-NA	-3.99	1.32	1.37
26	K1	201	PEB	CHA-C1B	3.99	1.49	1.40
26	ZB	202	PEB	CHA-C1B	3.99	1.49	1.40
28	SH	1001	CYC	CHB-C4A	3.99	1.49	1.40
28	EH	1001	CYC	C2C-C1C	-3.99	1.48	1.52
26	W4	201	PEB	C2C-C3C	3.99	1.49	1.37
26	11	201	PEB	CHA-C1B	3.99	1.49	1.40
26	a4	203	PEB	C1A-NA	-3.99	1.32	1.37
26	G8	201	PEB	C1A-NA	-3.99	1.32	1.37
26	jE	202	PEB	CHA-C1B	3.99	1.49	1.40
26	KD	201	PEB	C1A-NA	-3.98	1.32	1.37
26	U9	201	PEB	CHA-C1B	3.98	1.49	1.40
26	c8	202	PEB	C1A-NA	-3.98	1.32	1.37
26	QF	202	PEB	CHA-C1B	3.98	1.49	1.40
26	W1	201	PEB	C2C-C3C	3.98	1.49	1.37
27	A1	203	PUB	C3B-C2B	3.98	1.49	1.37
26	Q9	202	PEB	C1A-NA	-3.98	1.32	1.37
26	V4	201	PEB	C1A-NA	-3.98	1.32	1.37
28	M2	1001	CYC	C2C-C1C	-3.98	1.48	1.52
26	L5	203	PEB	C1A-NA	-3.98	1.32	1.37
28	nH	1001	CYC	C2C-C1C	-3.98	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aA	204	PEB	C1A-NA	-3.98	1.32	1.37
26	UG	201	PEB	C1A-NA	-3.98	1.32	1.37
26	aF	201	PEB	CHA-C1B	3.98	1.49	1.40
26	R3	201	PEB	C2A-C1A	-3.98	1.48	1.52
26	X4	202	PEB	CHA-C1B	3.98	1.49	1.40
26	G5	202	PEB	CHA-C1B	3.98	1.49	1.40
26	tE	202	PEB	C2C-C3C	3.98	1.49	1.37
26	Z6	202	PEB	C1A-NA	-3.98	1.32	1.37
28	F6	1001	CYC	C1C-NC	-3.98	1.32	1.37
28	mH	1001	CYC	C1C-NC	-3.98	1.32	1.37
26	N3	203	PEB	C1A-NA	-3.98	1.32	1.37
26	KE	201	PEB	C1A-NA	-3.98	1.32	1.37
26	lE	202	PEB	CHA-C1B	3.98	1.49	1.40
28	E2	1001	CYC	C2C-C1C	-3.98	1.48	1.52
26	zG	501	PEB	C2A-C1A	-3.97	1.48	1.52
26	K4	201	PEB	CHA-C1B	3.97	1.49	1.40
26	SG	202	PEB	CHA-C1B	3.97	1.49	1.40
26	r1	202	PEB	CHA-C1B	3.97	1.49	1.40
26	J1	201	PEB	CHA-C1B	3.97	1.49	1.40
26	CJ	202	PEB	CHA-C1B	3.97	1.49	1.40
26	PG	202	PEB	C2C-C3C	3.97	1.49	1.37
26	IG	201	PEB	C1A-NA	-3.97	1.32	1.37
28	FF	1001	CYC	CHB-C4A	3.97	1.49	1.40
26	F4	201	PEB	CHA-C1B	3.97	1.49	1.40
26	f4	202	PEB	CHA-C1B	3.97	1.49	1.40
26	r4	202	PEB	CHA-C1B	3.97	1.49	1.40
26	k8	202	PEB	C1A-NA	-3.97	1.32	1.37
26	S1	202	PEB	C1A-NA	-3.97	1.32	1.37
26	J5	202	PEB	C1A-NA	-3.97	1.32	1.37
26	m1	203	PEB	C2C-C3C	3.97	1.49	1.37
26	BJ	203	PEB	C1A-NA	-3.97	1.32	1.37
26	WJ	202	PEB	C1A-NA	-3.97	1.32	1.37
26	kA	202	PEB	CHA-C1B	3.97	1.49	1.40
26	11	201	PEB	C2C-C3C	3.97	1.49	1.37
26	H6	1002	PEB	C1A-NA	-3.97	1.32	1.37
28	B6	1001	CYC	CHB-C4A	3.97	1.49	1.40
26	T6	201	PEB	C1A-NA	-3.97	1.32	1.37
26	F9	201	PEB	C1A-NA	-3.97	1.32	1.37
26	FA	201	PEB	CHA-C1B	3.97	1.49	1.40
26	P7	202	PEB	CHA-C1B	3.96	1.49	1.40
26	E9	201	PEB	CHA-C1B	3.96	1.49	1.40
26	eI	201	PEB	CHA-C1B	3.96	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PE	202	PEB	C2C-C3C	3.96	1.49	1.37
26	u1	203	PEB	CHA-C1B	3.96	1.49	1.40
26	f6	202	PEB	CHA-C1B	3.96	1.49	1.40
26	W4	202	PEB	C1A-NA	-3.96	1.32	1.37
28	qH	1002	CYC	CHB-C4A	3.96	1.49	1.40
26	K8	201	PEB	CHA-C1B	3.96	1.49	1.40
26	F9	203	PEB	C4B-NB	-3.96	1.30	1.38
28	E6	1001	CYC	C1C-NC	-3.96	1.32	1.37
26	qG	202	PEB	C3C-C4C	3.96	1.48	1.42
26	m4	203	PEB	CHA-C1B	3.96	1.49	1.40
26	b6	202	PEB	C1A-NA	-3.96	1.32	1.37
26	bG	201	PEB	CHA-C1B	3.96	1.49	1.40
26	mG	202	PEB	CHA-C1B	3.96	1.49	1.40
26	Y1	202	PEB	C1A-NA	-3.96	1.32	1.37
26	X1	202	PEB	CHA-C1B	3.96	1.49	1.40
26	I5	201	PEB	CHA-C1B	3.96	1.49	1.40
26	jG	202	PEB	C1A-NA	-3.96	1.32	1.37
28	LI	1001	CYC	C2C-C1C	-3.96	1.48	1.52
26	e2	201	PEB	CHA-C1B	3.96	1.49	1.40
26	BA	301	PEB	C1A-NA	-3.95	1.32	1.37
26	a7	201	PEB	CHA-C1B	3.95	1.49	1.40
28	HF	1001	CYC	C2C-C1C	-3.95	1.48	1.52
26	j8	202	PEB	C1A-NA	-3.95	1.32	1.37
28	J7	1001	CYC	CHB-C4A	3.95	1.49	1.40
26	WI	201	PEB	C3B-C2B	3.95	1.45	1.36
26	P6	202	PEB	C2C-C3C	3.95	1.49	1.37
26	RE	201	PEB	C2A-C1A	-3.95	1.48	1.52
26	x1	201	PEB	CHA-C1B	3.95	1.49	1.40
26	eF	201	PEB	C1A-NA	-3.95	1.32	1.37
28	oH	1001	CYC	C1C-NC	-3.95	1.32	1.37
26	U7	201	PEB	CHA-C1B	3.95	1.49	1.40
26	SB	202	PEB	CHA-C1B	3.95	1.49	1.40
26	A8	301	PEB	CHA-C1B	3.95	1.49	1.40
26	O9	202	PEB	CHA-C1B	3.95	1.49	1.40
28	K2	1001	CYC	C2C-C1C	-3.95	1.48	1.52
26	G9	202	PEB	C2C-C3C	3.95	1.49	1.37
26	Z6	202	PEB	CHA-C1B	3.95	1.49	1.40
26	PB	202	PEB	C2C-C3C	3.95	1.49	1.37
27	Q8	201	PUB	C3B-C2B	3.95	1.49	1.37
26	F8	201	PEB	CHA-C1B	3.95	1.49	1.40
26	X4	201	PEB	C1A-NA	-3.95	1.32	1.37
26	GC	202	PEB	CHA-C1B	3.95	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	e8	202	PEB	C2A-C1A	-3.95	1.48	1.52
26	r4	202	PEB	C2C-C3C	3.95	1.49	1.37
26	c1	201	PEB	CHA-C1B	3.95	1.49	1.40
26	BD	201	PEB	CHA-C1B	3.95	1.49	1.40
26	KE	202	PEB	C1A-NA	-3.94	1.32	1.37
26	T3	201	PEB	CHA-C1B	3.94	1.49	1.40
26	CE	202	PEB	C3B-C2B	3.94	1.45	1.36
26	X3	203	PEB	C1A-NA	-3.94	1.32	1.37
28	IF	1001	CYC	C1C-NC	-3.94	1.32	1.37
26	KG	201	PEB	C1A-NA	-3.94	1.32	1.37
26	SG	201	PEB	C1A-NA	-3.94	1.32	1.37
28	C2	1001	CYC	CHB-C4A	3.94	1.49	1.40
28	L7	1001	CYC	C1C-NC	-3.94	1.32	1.37
26	f4	201	PEB	CHA-C1B	3.94	1.49	1.40
26	mI	201	PEB	CHA-C1B	3.94	1.49	1.40
26	aA	202	PEB	C1A-NA	-3.94	1.32	1.37
26	AF	301	PEB	C2C-C3C	3.94	1.49	1.37
26	S1	201	PEB	C3C-C4C	3.94	1.48	1.42
26	z4	202	PEB	C2C-C3C	3.94	1.49	1.37
26	JA	201	PEB	CHA-C1B	3.94	1.49	1.40
26	dG	201	PEB	CHA-C1B	3.94	1.49	1.40
26	g2	203	PEB	CHA-C1B	3.94	1.49	1.40
26	FD	201	PEB	CHA-C1B	3.94	1.49	1.40
26	I5	203	PEB	C2A-C1A	-3.94	1.48	1.52
28	CH	1001	CYC	C1C-NC	-3.94	1.32	1.37
26	TD	203	PEB	CHA-C1B	3.94	1.49	1.40
28	K6	202	CYC	CHB-C4A	3.94	1.49	1.40
26	TB	202	PEB	C2A-C1A	-3.94	1.48	1.52
28	MH	1001	CYC	C1C-NC	-3.93	1.32	1.37
26	BC	202	PEB	CHA-C1B	3.93	1.49	1.40
26	Q6	202	PEB	C1A-NA	-3.93	1.32	1.37
26	N3	203	PEB	CHA-C1B	3.93	1.49	1.40
26	U9	202	PEB	CHA-C1B	3.93	1.49	1.40
28	GB	1001	CYC	CHB-C4A	3.93	1.49	1.40
26	T7	201	PEB	CHA-C1B	3.93	1.49	1.40
26	H4	203	PEB	CHA-C1B	3.93	1.49	1.40
26	F5	201	PEB	C1A-NA	-3.93	1.32	1.37
26	x1	201	PEB	C2C-C3C	3.93	1.49	1.37
26	IC	201	PEB	CHA-C1B	3.93	1.49	1.40
26	MG	201	PEB	CHA-C1B	3.93	1.49	1.40
26	L3	201	PEB	C1A-NA	-3.93	1.32	1.37
26	BD	203	PEB	CHA-C1B	3.93	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y1	202	PEB	CHA-C1B	3.93	1.49	1.40
26	Y4	202	PEB	CHA-C1B	3.93	1.49	1.40
26	AC	201	PEB	CHA-C1B	3.93	1.49	1.40
26	J1	201	PEB	C1A-NA	-3.93	1.32	1.37
26	UB	203	PEB	C1A-NA	-3.93	1.32	1.37
26	24	401	PEB	CHA-C1B	3.93	1.49	1.40
26	eA	201	PEB	C1A-NA	-3.93	1.32	1.37
26	a2	201	PEB	C2A-C1A	-3.93	1.48	1.52
26	C1	201	PEB	CHA-C1B	3.93	1.49	1.40
26	RA	201	PEB	CHA-C1B	3.93	1.49	1.40
26	FG	201	PEB	CHA-C1B	3.93	1.49	1.40
26	aG	203	PEB	CHA-C1B	3.93	1.49	1.40
26	HG	202	PEB	CHA-C1B	3.93	1.49	1.40
26	k2	202	PEB	C1A-NA	-3.93	1.32	1.37
26	t1	201	PEB	CHA-C1B	3.93	1.49	1.40
26	WA	201	PEB	CHA-C1B	3.93	1.49	1.40
26	mF	201	PEB	CHA-C1B	3.93	1.49	1.40
26	AF	305	PEB	C2C-C3C	3.93	1.49	1.37
28	G6	1001	CYC	C1C-NC	-3.93	1.32	1.37
26	C9	202	PEB	CHA-C1B	3.93	1.49	1.40
28	KB	202	CYC	CHB-C4A	3.93	1.49	1.40
26	cG	203	PEB	CHA-C1B	3.92	1.49	1.40
26	nG	202	PEB	CHA-C1B	3.92	1.49	1.40
26	T3	201	PEB	C3C-C4C	3.92	1.48	1.42
26	nE	202	PEB	C2C-C3C	3.92	1.49	1.37
28	I6	1001	CYC	C1C-NC	-3.92	1.32	1.37
26	R2	201	PEB	C2A-C1A	-3.92	1.48	1.52
26	R2	201	PEB	C1A-NA	-3.92	1.32	1.37
26	QD	201	PEB	CHA-C1B	3.92	1.49	1.40
28	GI	1001	CYC	C2C-C1C	-3.92	1.48	1.52
26	SA	202	PEB	C1A-NA	-3.92	1.32	1.37
26	AE	201	PEB	C1A-NA	-3.92	1.32	1.37
26	aI	201	PEB	C2A-C1A	-3.92	1.48	1.52
26	i2	203	PEB	CHA-C1B	3.92	1.49	1.40
26	O6	201	PEB	CHA-C1B	3.92	1.49	1.40
26	BC	201	PEB	CHA-C1B	3.92	1.49	1.40
26	wG	303	PEB	CHA-C1B	3.92	1.49	1.40
26	R6	201	PEB	CHA-C1B	3.92	1.49	1.40
26	EJ	202	PEB	CHA-C1B	3.92	1.49	1.40
28	BB	1001	CYC	CHB-C4A	3.92	1.49	1.40
26	p4	202	PEB	C2C-C3C	3.92	1.49	1.37
26	OB	201	PEB	CHA-C1B	3.92	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	jE	201	PEB	CHA-C1B	3.92	1.49	1.40
28	hH	1001	CYC	C2C-C1C	-3.92	1.48	1.52
26	HG	201	PEB	C1A-NA	-3.92	1.32	1.37
26	ND	203	PEB	CHA-C1B	3.92	1.49	1.40
26	c8	202	PEB	CHA-C1B	3.92	1.49	1.40
26	F8	202	PEB	CHA-C1B	3.92	1.49	1.40
26	PG	202	PEB	CHA-C1B	3.92	1.49	1.40
26	tE	201	PEB	CHA-C1B	3.92	1.49	1.40
26	fA	202	PEB	CHA-C1B	3.92	1.49	1.40
26	IJ	203	PEB	CHA-C1B	3.92	1.49	1.40
26	P3	203	PEB	CHA-C1B	3.92	1.49	1.40
26	E9	202	PEB	CHA-C1B	3.92	1.49	1.40
26	n4	202	PEB	CHA-C1B	3.92	1.49	1.40
26	H5	202	PEB	C1A-NA	-3.91	1.32	1.37
26	k1	201	PEB	CHA-C1B	3.91	1.49	1.40
26	FA	202	PEB	CHA-C1B	3.91	1.49	1.40
26	KE	202	PEB	C3B-C2B	3.91	1.45	1.36
26	k8	202	PEB	CHA-C1B	3.91	1.49	1.40
26	LG	202	PEB	CHA-C1B	3.91	1.49	1.40
26	B8	301	PEB	C1A-NA	-3.91	1.32	1.37
26	H9	202	PEB	C1A-NA	-3.91	1.32	1.37
26	dE	202	PEB	C2C-C3C	3.91	1.49	1.37
26	fF	201	PEB	C1A-NA	-3.91	1.32	1.37
26	cA	203	PEB	C1A-NA	-3.91	1.32	1.37
26	CJ	202	PEB	C1A-NA	-3.91	1.32	1.37
26	e3	401	PEB	CHA-C1B	3.91	1.49	1.40
26	cA	203	PEB	CHA-C1B	3.91	1.49	1.40
26	hA	203	PEB	C1A-NA	-3.91	1.32	1.37
26	IJ	202	PEB	C1A-NA	-3.91	1.32	1.37
26	jE	202	PEB	C1A-NA	-3.91	1.32	1.37
26	j8	202	PEB	C2C-C3C	3.91	1.49	1.37
26	SE	201	PEB	C1A-NA	-3.91	1.32	1.37
26	Q9	202	PEB	CHA-C1B	3.91	1.49	1.40
26	k8	201	PEB	C1A-NA	-3.91	1.32	1.37
28	JF	1003	CYC	CHB-C4A	3.91	1.49	1.40
26	R4	201	PEB	C1A-NA	-3.91	1.32	1.37
26	I8	203	PEB	C3C-C4C	3.91	1.48	1.42
26	PD	203	PEB	CHA-C1B	3.91	1.49	1.40
26	W1	202	PEB	C1A-NA	-3.91	1.32	1.37
26	SB	201	PEB	C1A-NA	-3.91	1.32	1.37
26	HE	202	PEB	C1A-NA	-3.91	1.32	1.37
26	a2	203	PEB	CHA-C1B	3.91	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V4	203	PEB	C2A-C1A	-3.90	1.48	1.52
26	QE	203	PEB	C1A-NA	-3.90	1.32	1.37
26	hI	201	PEB	C1A-NA	-3.90	1.32	1.37
28	cH	1001	CYC	CHB-C4A	3.90	1.49	1.40
28	CI	1001	CYC	CHB-C4A	3.90	1.49	1.40
26	d1	202	PEB	C1A-NA	-3.90	1.32	1.37
26	aB	201	PEB	C1A-NA	-3.90	1.32	1.37
26	fF	202	PEB	C1A-NA	-3.90	1.32	1.37
26	Y6	202	PEB	CHA-C1B	3.90	1.49	1.40
26	e1	201	PEB	C2C-C3C	3.90	1.49	1.37
26	J4	201	PEB	C1A-NA	-3.90	1.32	1.37
26	GJ	201	PEB	C1A-NA	-3.90	1.32	1.37
26	BE	201	PEB	C2A-C1A	-3.90	1.48	1.52
26	VE	201	PEB	C2A-C1A	-3.90	1.48	1.52
26	fG	201	PEB	CHA-C1B	3.90	1.49	1.40
26	gI	203	PEB	CHA-C1B	3.90	1.49	1.40
26	F3	201	PEB	C1A-NA	-3.90	1.32	1.37
26	N8	201	PEB	C1A-NA	-3.90	1.32	1.37
26	C9	201	PEB	C1A-NA	-3.90	1.32	1.37
26	YD	303	PEB	C2C-C3C	3.90	1.49	1.37
28	AH	1001	CYC	CHB-C4A	3.90	1.49	1.40
26	G5	201	PEB	CHA-C1B	3.90	1.49	1.40
26	F3	201	PEB	CHA-C1B	3.90	1.49	1.40
26	Q4	202	PEB	CHA-C1B	3.90	1.49	1.40
26	w4	203	PEB	CHA-C1B	3.90	1.49	1.40
26	v1	201	PEB	CHA-C1B	3.90	1.49	1.40
26	PE	202	PEB	CHA-C1B	3.90	1.49	1.40
26	A1	201	PEB	C1A-NA	-3.90	1.32	1.37
26	a1	201	PEB	CHA-C1B	3.90	1.49	1.40
26	JA	202	PEB	CHA-C1B	3.90	1.49	1.40
26	X1	201	PEB	C1A-NA	-3.90	1.32	1.37
26	fl	201	PEB	C1A-NA	-3.90	1.32	1.37
26	SJ	202	PEB	CHA-C1B	3.90	1.49	1.40
26	SD	201	PEB	C2A-C1A	-3.90	1.48	1.52
26	R8	201	PEB	CHA-C1B	3.89	1.49	1.40
26	A6	304	PEB	C1A-NA	-3.89	1.32	1.37
26	ND	201	PEB	C1A-NA	-3.89	1.32	1.37
26	RI	201	PEB	C1A-NA	-3.89	1.32	1.37
26	K9	202	PEB	CHA-C1B	3.89	1.49	1.40
26	W9	202	PEB	CHA-C1B	3.89	1.49	1.40
26	NA	201	PEB	C1A-NA	-3.89	1.32	1.37
26	WE	201	PEB	C1A-NA	-3.89	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BJ	202	PEB	C1A-NA	-3.89	1.32	1.37
26	L1	201	PEB	CHA-C1B	3.89	1.49	1.40
28	LF	1001	CYC	C2C-C1C	-3.89	1.48	1.52
26	m4	203	PEB	C2C-C3C	3.89	1.49	1.37
26	jG	201	PEB	CHA-C1B	3.89	1.49	1.40
26	K4	201	PEB	C1A-NA	-3.89	1.32	1.37
26	W8	201	PEB	CHA-C1B	3.89	1.49	1.40
26	VB	202	PEB	CHA-C1B	3.89	1.49	1.40
26	wE	303	PEB	CHA-C1B	3.89	1.49	1.40
26	RF	202	PEB	CHA-C1B	3.89	1.49	1.40
26	TG	201	PEB	CHA-C1B	3.89	1.49	1.40
26	GG	202	PEB	C1A-NA	-3.89	1.32	1.37
28	WH	1001	CYC	C1C-NC	-3.89	1.32	1.37
26	Q1	202	PEB	CHA-C1B	3.89	1.49	1.40
26	LI	1002	PEB	C3C-C4C	3.89	1.48	1.42
26	mB	201	PEB	CHA-C1B	3.89	1.49	1.40
26	zE	501	PEB	C2A-C1A	-3.89	1.48	1.52
27	K4	203	PUB	C3B-C2B	3.89	1.49	1.37
26	dA	201	PEB	C1A-NA	-3.89	1.32	1.37
26	DG	203	PEB	C1A-NA	-3.89	1.32	1.37
26	S9	202	PEB	CHA-C1B	3.89	1.49	1.40
26	kB	201	PEB	CHA-C1B	3.89	1.49	1.40
26	X3	203	PEB	C3C-C4C	3.89	1.48	1.42
26	HF	1002	PEB	C1A-NA	-3.89	1.32	1.37
26	RG	202	PEB	C1A-NA	-3.89	1.32	1.37
28	NF	1001	CYC	C1C-NC	-3.89	1.32	1.37
26	Q2	201	PEB	C3B-C2B	3.89	1.45	1.36
26	YB	202	PEB	C2C-C3C	3.89	1.49	1.37
26	K3	201	PEB	C1A-NA	-3.89	1.32	1.37
26	S8	201	PEB	C1A-NA	-3.89	1.32	1.37
26	PF	202	PEB	C1A-NA	-3.89	1.32	1.37
26	RD	201	PEB	CHA-C1B	3.89	1.49	1.40
27	NJ	201	PUB	C3B-C2B	3.89	1.49	1.37
26	L5	203	PEB	C2A-C1A	-3.89	1.48	1.52
26	W1	201	PEB	CHA-C1B	3.88	1.49	1.40
26	M1	402	PEB	C1A-NA	-3.88	1.32	1.37
26	C8	203	PEB	C1A-NA	-3.88	1.32	1.37
26	LG	202	PEB	C2A-C1A	-3.88	1.48	1.52
26	cE	201	PEB	C3B-C2B	3.88	1.45	1.36
26	j7	202	PEB	CHA-C1B	3.88	1.49	1.40
26	KJ	202	PEB	CHA-C1B	3.88	1.49	1.40
26	A7	305	PEB	C2C-C3C	3.88	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	WE	202	PEB	CHA-C1B	3.88	1.49	1.40
27	A8	303	PUB	OD-C4D	3.88	1.31	1.23
26	x4	201	PEB	CHA-C1B	3.88	1.49	1.40
26	m1	203	PEB	CHA-C1B	3.88	1.49	1.40
28	K6	202	CYC	C1C-NC	-3.88	1.32	1.37
26	FE	201	PEB	CHA-C1B	3.88	1.49	1.40
26	KC	201	PEB	CHA-C1B	3.88	1.49	1.40
26	T9	203	PEB	C2C-C3C	3.88	1.49	1.37
26	Z6	202	PEB	C2A-C1A	-3.88	1.48	1.52
26	RB	201	PEB	CHA-C1B	3.88	1.49	1.40
26	Z1	202	PEB	C1A-NA	-3.88	1.32	1.37
28	GB	1001	CYC	C1C-NC	-3.88	1.32	1.37
26	UA	202	PEB	CHA-C1B	3.88	1.49	1.40
26	R3	203	PEB	C2A-C1A	-3.88	1.48	1.52
26	WB	201	PEB	C2A-C1A	-3.88	1.48	1.52
28	FI	1001	CYC	C1C-NC	-3.88	1.32	1.37
26	LC	201	PEB	CHA-C1B	3.88	1.49	1.40
26	B5	201	PEB	CHA-C1B	3.88	1.49	1.40
26	DA	201	PEB	CHA-C1B	3.88	1.49	1.40
26	FJ	201	PEB	C1A-NA	-3.88	1.32	1.37
28	JI	1001	CYC	CHB-C4A	3.88	1.49	1.40
26	W7	202	PEB	C2C-C3C	3.88	1.49	1.37
26	B3	203	PEB	CHA-C1B	3.88	1.49	1.40
26	X4	203	PEB	CHA-C1B	3.88	1.49	1.40
26	YF	201	PEB	CHA-C1B	3.88	1.49	1.40
28	M6	1001	CYC	CHB-C4A	3.88	1.49	1.40
26	L4	203	PEB	CHA-C1B	3.87	1.49	1.40
26	O8	203	PEB	C1A-NA	-3.87	1.32	1.37
26	Q1	201	PEB	CHA-C1B	3.87	1.49	1.40
26	E9	202	PEB	C1A-NA	-3.87	1.32	1.37
26	A9	304	PEB	C2C-C3C	3.87	1.49	1.37
26	S6	201	PEB	C1A-NA	-3.87	1.32	1.37
28	E7	1001	CYC	C1C-NC	-3.87	1.32	1.37
28	L2	1001	CYC	CHB-C4A	3.87	1.49	1.40
26	VJ	201	PEB	C2C-C3C	3.87	1.49	1.37
26	dE	202	PEB	C1A-NA	-3.87	1.32	1.37
26	LJ	201	PEB	C1A-NA	-3.87	1.32	1.37
26	a4	202	PEB	CHA-C1B	3.87	1.49	1.40
26	gA	202	PEB	CHA-C1B	3.87	1.49	1.40
26	RB	202	PEB	CHA-C1B	3.87	1.49	1.40
26	U6	203	PEB	C1A-NA	-3.87	1.32	1.37
26	HE	201	PEB	C1A-NA	-3.87	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	LJ	203	PEB	C1A-NA	-3.87	1.32	1.37
26	XE	202	PEB	C2C-C3C	3.87	1.49	1.37
26	OA	201	PEB	CHA-C1B	3.87	1.49	1.40
26	W4	202	PEB	CHA-C1B	3.87	1.49	1.40
26	VI	203	PEB	CHA-C1B	3.87	1.49	1.40
26	a2	201	PEB	C1A-NA	-3.87	1.32	1.37
26	EJ	201	PEB	CHA-C1B	3.87	1.49	1.40
26	D3	203	PEB	C1A-NA	-3.87	1.32	1.37
28	G6	1001	CYC	CHB-C4A	3.87	1.49	1.40
28	LI	1001	CYC	CHB-C4A	3.87	1.49	1.40
28	eH	1001	CYC	C1C-NC	-3.87	1.32	1.37
28	yH	1001	CYC	C1C-NC	-3.87	1.32	1.37
26	GA	201	PEB	C1A-NA	-3.87	1.32	1.37
26	aG	202	PEB	C1A-NA	-3.87	1.32	1.37
26	W4	201	PEB	CHA-C1B	3.87	1.49	1.40
26	rG	202	PEB	CHA-C1B	3.87	1.49	1.40
26	O8	201	PEB	CHA-C1B	3.87	1.49	1.40
26	r1	202	PEB	C2C-C3C	3.87	1.49	1.37
26	p1	201	PEB	CHA-C1B	3.87	1.49	1.40
26	D8	202	PEB	CHA-C1B	3.86	1.49	1.40
26	AE	201	PEB	C3B-C2B	3.86	1.44	1.36
26	QG	201	PEB	C3B-C2B	3.86	1.44	1.36
26	V1	201	PEB	C2A-C1A	-3.86	1.48	1.52
26	I1	201	PEB	C1A-NA	-3.86	1.32	1.37
28	NF	1001	CYC	C2C-C1C	-3.86	1.48	1.52
26	v1	202	PEB	C1A-NA	-3.86	1.32	1.37
26	D8	201	PEB	CHA-C1B	3.86	1.49	1.40
26	WF	202	PEB	CHA-C1B	3.86	1.49	1.40
26	14	201	PEB	C2C-C3C	3.86	1.49	1.37
27	N9	201	PUB	C3B-C2B	3.86	1.49	1.37
26	AJ	304	PEB	C2C-C3C	3.86	1.49	1.37
26	O1	201	PEB	C2C-C3C	3.86	1.49	1.37
26	DA	202	PEB	CHA-C1B	3.86	1.49	1.40
26	KC	203	PEB	CHA-C1B	3.86	1.49	1.40
26	pE	202	PEB	C1A-NA	-3.86	1.32	1.37
28	EB	1001	CYC	C1C-NC	-3.86	1.32	1.37
26	X1	203	PEB	CHA-C1B	3.86	1.49	1.40
28	J7	1003	CYC	CHB-C4A	3.86	1.49	1.40
26	XG	203	PEB	C2C-C3C	3.86	1.49	1.37
26	fB	202	PEB	CHA-C1B	3.86	1.49	1.40
26	UE	201	PEB	CHA-C1B	3.86	1.49	1.40
26	UA	203	PEB	C3C-C4C	3.86	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C4	201	PEB	CHA-C1B	3.86	1.49	1.40
26	t4	202	PEB	C2C-C3C	3.85	1.49	1.37
26	R2	201	PEB	CHA-C1B	3.85	1.49	1.40
26	C5	204	PEB	CHA-C1B	3.85	1.49	1.40
28	MB	1001	CYC	CHB-C4A	3.85	1.49	1.40
28	I6	1001	CYC	CHB-C4A	3.85	1.49	1.40
26	LG	201	PEB	CHA-C1B	3.85	1.49	1.40
26	A5	201	PEB	CHA-C1B	3.85	1.49	1.40
26	Y3	304	PEB	C2C-C3C	3.85	1.49	1.37
26	H8	201	PEB	C2A-C1A	-3.85	1.48	1.52
26	XD	203	PEB	C1A-NA	-3.85	1.32	1.37
26	Q4	201	PEB	CHA-C1B	3.85	1.49	1.40
28	K2	1001	CYC	CHB-C4A	3.85	1.49	1.40
28	KI	1001	CYC	CHB-C4A	3.85	1.49	1.40
26	nG	202	PEB	C2C-C3C	3.85	1.49	1.37
26	mI	202	PEB	C1A-NA	-3.85	1.32	1.37
26	KE	202	PEB	CHA-C1B	3.85	1.49	1.40
26	RJ	202	PEB	C1A-NA	-3.85	1.32	1.37
26	P1	202	PEB	CHA-C1B	3.85	1.49	1.40
26	r4	201	PEB	C2C-C3C	3.85	1.49	1.37
26	l8	202	PEB	CHA-C1B	3.85	1.49	1.40
26	TA	201	PEB	CHA-C1B	3.85	1.49	1.40
26	xG	302	PEB	C2C-C3C	3.85	1.49	1.37
26	lF	202	PEB	CHA-C1B	3.85	1.49	1.40
26	W8	202	PEB	C1A-NA	-3.85	1.32	1.37
26	XD	203	PEB	CHA-C1B	3.85	1.49	1.40
26	KA	201	PEB	C2A-C1A	-3.85	1.48	1.52
26	K5	201	PEB	C2A-C1A	-3.84	1.48	1.52
26	Q6	202	PEB	CHA-C1B	3.84	1.49	1.40
26	i7	202	PEB	CHA-C1B	3.84	1.49	1.40
28	MI	1001	CYC	C2C-C1C	-3.84	1.48	1.52
26	bB	202	PEB	C1A-NA	-3.84	1.32	1.37
26	QI	201	PEB	C3B-C2B	3.84	1.44	1.36
26	X3	203	PEB	CHA-C1B	3.84	1.49	1.40
26	aI	201	PEB	C1A-NA	-3.84	1.32	1.37
26	iE	202	PEB	CHA-C1B	3.84	1.49	1.40
26	V1	203	PEB	C2A-C1A	-3.84	1.48	1.52
26	A7	302	PEB	CHA-C1B	3.84	1.49	1.40
26	ZB	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	J3	201	PEB	C1A-NA	-3.84	1.32	1.37
26	fB	202	PEB	C1A-NA	-3.84	1.32	1.37
26	m2	201	PEB	CHA-C1B	3.84	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d6	203	PEB	CHA-C1B	3.84	1.49	1.40
26	TB	201	PEB	C1A-NA	-3.84	1.32	1.37
26	R6	202	PEB	CHA-C1B	3.84	1.49	1.40
26	XJ	202	PEB	CHA-C1B	3.84	1.49	1.40
26	S4	202	PEB	C1A-NA	-3.84	1.32	1.37
26	s4	202	PEB	CHA-C1B	3.84	1.49	1.40
26	K1	202	PEB	CHA-C1B	3.84	1.49	1.40
26	t1	201	PEB	C2C-C3C	3.84	1.49	1.37
26	L2	1002	PEB	C3C-C4C	3.84	1.48	1.42
26	eF	202	PEB	CHA-C1B	3.84	1.49	1.40
26	NG	202	PEB	CHA-C1B	3.84	1.49	1.40
26	fG	201	PEB	C2A-C1A	-3.84	1.48	1.52
28	H2	1001	CYC	CHB-C4A	3.84	1.49	1.40
26	D1	203	PEB	C1A-NA	-3.83	1.32	1.37
26	TB	201	PEB	CHA-C1B	3.83	1.49	1.40
26	aE	202	PEB	CHA-C1B	3.83	1.49	1.40
26	gE	201	PEB	C1A-NA	-3.83	1.32	1.37
26	fE	201	PEB	CHA-C1B	3.83	1.49	1.40
26	KG	202	PEB	CHA-C1B	3.83	1.49	1.40
26	pE	202	PEB	C2C-C3C	3.83	1.49	1.37
26	N1	201	PEB	C3B-C2B	3.83	1.44	1.36
26	U8	202	PEB	CHA-C1B	3.83	1.49	1.40
26	QE	202	PEB	CHA-C1B	3.83	1.49	1.40
28	HI	1001	CYC	CHB-C4A	3.83	1.49	1.40
26	W6	201	PEB	C2A-C1A	-3.83	1.48	1.52
26	MA	201	PEB	C2A-C1A	-3.83	1.48	1.52
26	KG	203	PEB	C1A-NA	-3.83	1.32	1.37
28	KI	1001	CYC	C2C-C1C	-3.83	1.48	1.52
28	E2	1001	CYC	C1C-NC	-3.83	1.32	1.37
26	Z4	201	PEB	CHA-C1B	3.83	1.49	1.40
26	W9	202	PEB	C1A-NA	-3.83	1.32	1.37
26	HD	203	PEB	C1A-NA	-3.83	1.32	1.37
26	I9	201	PEB	C2C-C3C	3.83	1.49	1.37
26	u1	201	PEB	C1A-NA	-3.83	1.32	1.37
26	IA	203	PEB	C3C-C4C	3.83	1.48	1.42
26	aE	203	PEB	CHA-C1B	3.83	1.49	1.40
26	RI	201	PEB	CHA-C1B	3.83	1.49	1.40
26	P2	201	PEB	CHA-C1B	3.83	1.49	1.40
26	TE	201	PEB	CHA-C1B	3.83	1.49	1.40
26	D7	1002	PEB	CHA-C1B	3.83	1.49	1.40
26	GG	203	PEB	C2A-C1A	-3.83	1.48	1.52
26	Y4	202	PEB	C1A-NA	-3.82	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W7	202	PEB	CHA-C1B	3.82	1.49	1.40
26	f6	202	PEB	C1A-NA	-3.82	1.32	1.37
26	K5	203	PEB	CHA-C1B	3.82	1.49	1.40
26	JA	202	PEB	C1A-NA	-3.82	1.32	1.37
28	I7	1001	CYC	CHB-C4A	3.82	1.49	1.40
26	AC	203	PEB	CHA-C1B	3.82	1.49	1.40
26	Q6	201	PEB	C1A-NA	-3.82	1.32	1.37
26	RB	202	PEB	C1A-NA	-3.82	1.32	1.37
26	m6	201	PEB	CHA-C1B	3.82	1.49	1.40
26	k6	201	PEB	CHA-C1B	3.82	1.49	1.40
26	eB	203	PEB	C1A-NA	-3.82	1.32	1.37
26	N4	201	PEB	C3B-C2B	3.82	1.44	1.36
26	W1	202	PEB	CHA-C1B	3.82	1.49	1.40
26	tE	202	PEB	CHA-C1B	3.82	1.49	1.40
28	L7	1001	CYC	CHB-C4A	3.82	1.49	1.40
26	Z6	203	PEB	CHA-C1B	3.82	1.49	1.40
26	eD	401	PEB	CHA-C1B	3.82	1.49	1.40
26	ZI	201	PEB	C3B-C2B	3.82	1.44	1.36
26	PA	201	PEB	CHA-C1B	3.82	1.49	1.40
28	EI	1001	CYC	CHB-C4A	3.82	1.49	1.40
26	j4	201	PEB	C2C-C3C	3.82	1.49	1.37
26	f1	202	PEB	CHA-C1B	3.82	1.49	1.40
26	A9	303	PEB	CHA-C1B	3.82	1.49	1.40
26	IA	202	PEB	CHA-C1B	3.82	1.49	1.40
26	jB	202	PEB	CHA-C1B	3.82	1.49	1.40
26	YB	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	D4	203	PEB	C1A-NA	-3.82	1.32	1.37
26	T6	201	PEB	CHA-C1B	3.82	1.49	1.40
26	GG	203	PEB	CHA-C1B	3.82	1.49	1.40
26	QE	201	PEB	C3B-C2B	3.81	1.44	1.36
26	DF	1002	PEB	CHA-C1B	3.81	1.49	1.40
26	11	201	PEB	C1A-NA	-3.81	1.32	1.37
26	K5	203	PEB	C2A-C1A	-3.81	1.48	1.52
26	JG	202	PEB	CHA-C1B	3.81	1.49	1.40
26	V2	201	PEB	C1A-NA	-3.81	1.32	1.37
28	IB	1001	CYC	C1C-NC	-3.81	1.32	1.37
26	I5	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	Y6	202	PEB	C2C-C3C	3.81	1.49	1.37
26	S8	203	PEB	C1A-NA	-3.81	1.32	1.37
26	a8	202	PEB	C1A-NA	-3.81	1.32	1.37
26	KJ	201	PEB	C1A-NA	-3.81	1.32	1.37
26	V6	202	PEB	CHA-C1B	3.81	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JD	201	PEB	CHA-C1B	3.81	1.49	1.40
26	ZE	202	PEB	CHA-C1B	3.81	1.49	1.40
26	eB	203	PEB	C2C-C3C	3.81	1.49	1.37
26	Z4	202	PEB	C1A-NA	-3.81	1.32	1.37
26	OA	203	PEB	C1A-NA	-3.81	1.32	1.37
26	GJ	201	PEB	CHA-C1B	3.81	1.49	1.40
26	V4	201	PEB	C2A-C1A	-3.81	1.48	1.52
26	QB	203	PEB	CHA-C1B	3.81	1.49	1.40
26	UJ	202	PEB	CHA-C1B	3.81	1.49	1.40
26	Y8	202	PEB	CHA-C1B	3.81	1.49	1.40
26	G3	201	PEB	CHA-C1B	3.81	1.49	1.40
26	NG	201	PEB	CHA-C1B	3.81	1.49	1.40
28	KB	202	CYC	C1C-NC	-3.81	1.32	1.37
26	WF	202	PEB	C2C-C3C	3.81	1.49	1.37
26	G8	201	PEB	CHA-C1B	3.81	1.49	1.40
26	LG	202	PEB	C1A-NA	-3.81	1.32	1.37
26	w1	203	PEB	CHA-C1B	3.81	1.49	1.40
26	U1	201	PEB	C1A-NA	-3.81	1.32	1.37
26	I3	201	PEB	C1A-NA	-3.81	1.32	1.37
26	ZF	202	PEB	C1A-NA	-3.81	1.32	1.37
26	L1	203	PEB	C2C-C3C	3.81	1.48	1.37
26	K5	201	PEB	CHA-C1B	3.81	1.49	1.40
26	z1	202	PEB	C2C-C3C	3.81	1.48	1.37
26	Y3	303	PEB	C2C-C3C	3.81	1.48	1.37
26	WA	202	PEB	C1A-NA	-3.81	1.32	1.37
26	x4	202	PEB	CHA-C1B	3.81	1.49	1.40
28	GI	1001	CYC	CHB-C4A	3.81	1.49	1.40
26	ZG	202	PEB	C2C-C3C	3.80	1.48	1.37
27	24	402	PUB	C3B-C2B	3.80	1.48	1.37
26	j6	202	PEB	CHA-C1B	3.80	1.49	1.40
27	QA	201	PUB	C3B-C2B	3.80	1.48	1.37
26	O8	202	PEB	C1A-NA	-3.80	1.32	1.37
26	G9	201	PEB	C1A-NA	-3.80	1.32	1.37
28	I2	1001	CYC	C2C-C1C	-3.80	1.48	1.52
26	G4	201	PEB	C1A-NA	-3.80	1.32	1.37
26	R3	201	PEB	CHA-C1B	3.80	1.49	1.40
26	O3	202	PEB	C1A-NA	-3.80	1.32	1.37
26	WF	203	PEB	C1A-NA	-3.80	1.32	1.37
26	u4	201	PEB	CHA-C1B	3.80	1.49	1.40
26	U9	202	PEB	C1A-NA	-3.80	1.32	1.37
26	IG	201	PEB	CHA-C1B	3.80	1.49	1.40
26	II	202	PEB	CHA-C1B	3.80	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	II	1001	CYC	CHB-C4A	3.80	1.49	1.40
26	SA	203	PEB	C1A-NA	-3.80	1.32	1.37
26	XD	201	PEB	C1A-NA	-3.80	1.32	1.37
26	WA	202	PEB	CHA-C1B	3.80	1.49	1.40
26	hB	202	PEB	CHA-C1B	3.80	1.49	1.40
28	fH	1001	CYC	C2C-C1C	-3.80	1.48	1.52
26	a2	202	PEB	C1A-NA	-3.80	1.32	1.37
28	CH	1001	CYC	C2C-C1C	-3.80	1.48	1.52
26	d4	201	PEB	CHA-C1B	3.80	1.49	1.40
26	YA	202	PEB	CHA-C1B	3.80	1.49	1.40
26	uG	203	PEB	C2C-C3C	3.80	1.48	1.37
26	ZB	203	PEB	C1A-NA	-3.80	1.32	1.37
26	u4	203	PEB	CHA-C1B	3.80	1.49	1.40
28	I2	1001	CYC	CHB-C4A	3.80	1.49	1.40
26	TJ	203	PEB	C2C-C3C	3.80	1.48	1.37
26	eA	201	PEB	CHA-C1B	3.80	1.49	1.40
26	d8	202	PEB	C1A-NA	-3.80	1.32	1.37
26	NG	202	PEB	C1A-NA	-3.80	1.32	1.37
26	YA	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	TG	201	PEB	C2A-C1A	-3.80	1.48	1.52
26	Q6	203	PEB	CHA-C1B	3.80	1.49	1.40
26	B9	201	PEB	C1A-NA	-3.80	1.32	1.37
26	DE	203	PEB	C1A-NA	-3.80	1.32	1.37
26	U8	203	PEB	C3C-C4C	3.80	1.48	1.42
26	L1	203	PEB	CHA-C1B	3.80	1.49	1.40
26	a1	202	PEB	CHA-C1B	3.80	1.49	1.40
26	PI	201	PEB	CHA-C1B	3.80	1.49	1.40
26	RI	203	PEB	CHA-C1B	3.80	1.49	1.40
26	KC	201	PEB	C1A-NA	-3.80	1.32	1.37
26	M9	201	PEB	CHA-C1B	3.80	1.49	1.40
26	A4	201	PEB	CHA-C1B	3.80	1.49	1.40
26	C1	201	PEB	C1A-NA	-3.80	1.32	1.37
28	CB	1001	CYC	C1C-NC	-3.80	1.32	1.37
26	hE	202	PEB	CHA-C1B	3.79	1.49	1.40
26	NE	202	PEB	CHA-C1B	3.79	1.49	1.40
26	PB	201	PEB	C1A-NA	-3.79	1.32	1.37
26	d4	201	PEB	C2C-C3C	3.79	1.48	1.37
26	vG	201	PEB	CHA-C1B	3.79	1.49	1.40
26	S8	202	PEB	C1A-NA	-3.79	1.32	1.37
26	B5	202	PEB	CHA-C1B	3.79	1.49	1.40
26	VA	201	PEB	CHA-C1B	3.79	1.49	1.40
26	TE	201	PEB	C2A-C1A	-3.79	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c6	202	PEB	C1A-NA	-3.79	1.32	1.37
26	BJ	201	PEB	C1A-NA	-3.79	1.32	1.37
26	VI	201	PEB	C1A-NA	-3.79	1.32	1.37
26	GG	202	PEB	C4A-NA	-3.79	1.29	1.37
26	GA	201	PEB	CHA-C1B	3.79	1.49	1.40
26	nG	201	PEB	CHA-C1B	3.79	1.49	1.40
28	IB	1001	CYC	CHB-C4A	3.79	1.49	1.40
26	H3	203	PEB	C1A-NA	-3.79	1.32	1.37
26	T6	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	RI	201	PEB	C2A-C1A	-3.79	1.48	1.52
28	E6	1001	CYC	C2C-C1C	-3.79	1.48	1.52
26	f7	202	PEB	C1A-NA	-3.79	1.32	1.37
26	dG	202	PEB	C1A-NA	-3.79	1.32	1.37
28	cH	1001	CYC	C1C-NC	-3.79	1.32	1.37
26	MJ	201	PEB	CHA-C1B	3.79	1.49	1.40
26	AA	301	PEB	CHA-C1B	3.79	1.49	1.40
26	QB	202	PEB	C1A-NA	-3.79	1.32	1.37
26	B9	202	PEB	C1A-NA	-3.79	1.32	1.37
26	PA	201	PEB	C1A-NA	-3.79	1.32	1.37
26	kB	202	PEB	CHA-C1B	3.79	1.49	1.40
26	x4	201	PEB	C2C-C3C	3.79	1.48	1.37
26	c2	202	PEB	CHA-C1B	3.79	1.49	1.40
28	C6	1001	CYC	C1C-NC	-3.79	1.32	1.37
26	TB	201	PEB	C2A-C1A	-3.79	1.48	1.52
26	V6	202	PEB	C2C-C3C	3.79	1.48	1.37
26	r1	201	PEB	CHA-C1B	3.79	1.49	1.40
26	J8	202	PEB	CHA-C1B	3.79	1.49	1.40
26	FD	203	PEB	C1A-NA	-3.79	1.32	1.37
26	H3	201	PEB	CHA-C1B	3.79	1.49	1.40
26	TI	202	PEB	C1A-NA	-3.78	1.32	1.37
26	cE	201	PEB	C2C-C3C	3.78	1.48	1.37
26	H1	202	PEB	C1A-NA	-3.78	1.32	1.37
26	IC	203	PEB	C1A-NA	-3.78	1.32	1.37
26	AF	302	PEB	CHA-C1B	3.78	1.49	1.40
28	H7	1001	CYC	CHB-C4A	3.78	1.49	1.40
28	CI	1001	CYC	C1C-NC	-3.78	1.32	1.37
26	CE	202	PEB	CHA-C1B	3.78	1.49	1.40
26	YD	304	PEB	C2C-C3C	3.78	1.48	1.37
26	XJ	203	PEB	CHA-C1B	3.78	1.49	1.40
26	j1	201	PEB	C2C-C3C	3.78	1.48	1.37
26	a1	201	PEB	C2A-C1A	-3.78	1.48	1.52
26	A2	304	PEB	CHA-C1B	3.78	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	e8	201	PEB	CHA-C1B	3.78	1.49	1.40
26	VI	201	PEB	CHA-C1B	3.78	1.49	1.40
26	sE	201	PEB	CHA-C1B	3.78	1.49	1.40
28	M2	1001	CYC	CHB-C4A	3.78	1.49	1.40
26	V4	201	PEB	CHA-C1B	3.78	1.49	1.40
26	h8	202	PEB	CHA-C1B	3.78	1.49	1.40
26	XG	203	PEB	CHA-C1B	3.78	1.49	1.40
26	D1	203	PEB	C2C-C3C	3.78	1.48	1.37
26	O4	201	PEB	C2C-C3C	3.78	1.48	1.37
26	ZB	203	PEB	CHA-C1B	3.78	1.49	1.40
26	UF	201	PEB	CHA-C1B	3.78	1.49	1.40
26	n1	201	PEB	CHA-C1B	3.78	1.49	1.40
26	d7	202	PEB	C1A-NA	-3.78	1.32	1.37
26	IC	201	PEB	C1A-NA	-3.78	1.32	1.37
27	AF	303	PUB	C3B-C2B	3.78	1.48	1.37
26	Q3	201	PEB	CHA-C1B	3.78	1.49	1.40
26	X9	203	PEB	CHA-C1B	3.78	1.49	1.40
26	e2	203	PEB	CHA-C1B	3.78	1.49	1.40
26	K3	202	PEB	C2C-C3C	3.78	1.48	1.37
26	W9	201	PEB	CHA-C1B	3.77	1.49	1.40
26	cI	203	PEB	CHA-C1B	3.77	1.49	1.40
26	PG	202	PEB	C1A-NA	-3.77	1.32	1.37
26	Z8	202	PEB	CHA-C1B	3.77	1.49	1.40
27	xE	306	PUB	C3B-C2B	3.77	1.48	1.37
26	R6	202	PEB	C1A-NA	-3.77	1.32	1.37
26	LB	1002	PEB	C1A-NA	-3.77	1.32	1.37
26	iA	201	PEB	CHA-C1B	3.77	1.49	1.40
26	T8	201	PEB	CHA-C1B	3.77	1.49	1.40
26	OD	202	PEB	C1A-NA	-3.77	1.32	1.37
26	FJ	202	PEB	C1A-NA	-3.77	1.32	1.37
28	EI	1001	CYC	C1C-NC	-3.77	1.32	1.37
26	mG	203	PEB	CHA-C1B	3.77	1.49	1.40
26	p1	201	PEB	C2C-C3C	3.77	1.48	1.37
26	g4	202	PEB	C2C-C3C	3.77	1.48	1.37
26	hG	202	PEB	CHA-C1B	3.77	1.49	1.40
26	S3	201	PEB	C2A-C1A	-3.77	1.48	1.52
28	D2	1001	CYC	C2C-C1C	-3.77	1.48	1.52
26	B5	203	PEB	CHA-C1B	3.77	1.49	1.40
26	v4	202	PEB	C2C-C3C	3.77	1.48	1.37
26	jA	202	PEB	C2C-C3C	3.77	1.48	1.37
26	m2	203	PEB	CHA-C1B	3.77	1.49	1.40
26	QB	201	PEB	C1A-NA	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V2	203	PEB	CHA-C1B	3.77	1.49	1.40
26	dB	203	PEB	CHA-C1B	3.77	1.49	1.40
26	BG	201	PEB	CHA-C1B	3.77	1.49	1.40
26	AJ	305	PEB	CHA-C1B	3.77	1.49	1.40
26	U8	203	PEB	C1A-NA	-3.77	1.32	1.37
26	GE	202	PEB	C4A-NA	-3.77	1.29	1.37
26	t4	202	PEB	CHA-C1B	3.77	1.49	1.40
26	F5	203	PEB	C1A-NA	-3.77	1.32	1.37
26	LD	201	PEB	C1A-NA	-3.77	1.32	1.37
26	iG	203	PEB	C1A-NA	-3.77	1.32	1.37
26	p1	202	PEB	C2C-C3C	3.77	1.48	1.37
26	l1	201	PEB	CHA-C1B	3.77	1.49	1.40
26	TA	202	PEB	CHA-C1B	3.77	1.49	1.40
26	A7	301	PEB	C2C-C3C	3.77	1.48	1.37
26	H7	1002	PEB	CHA-C1B	3.77	1.49	1.40
26	T4	203	PEB	C1A-NA	-3.77	1.32	1.37
26	Y4	201	PEB	C1A-NA	-3.77	1.32	1.37
26	A4	202	PEB	CHA-C1B	3.77	1.49	1.40
26	cI	202	PEB	CHA-C1B	3.77	1.49	1.40
28	cH	1001	CYC	C3D-C2D	3.77	1.48	1.37
26	eI	203	PEB	CHA-C1B	3.77	1.49	1.40
26	k8	202	PEB	C2C-C3C	3.77	1.48	1.37
26	vE	201	PEB	CHA-C1B	3.77	1.49	1.40
26	sG	203	PEB	C1A-NA	-3.77	1.32	1.37
26	Y3	303	PEB	CHA-C1B	3.76	1.49	1.40
26	UJ	201	PEB	C1A-NA	-3.76	1.32	1.37
26	c6	201	PEB	CHA-C1B	3.76	1.49	1.40
26	Z2	201	PEB	C3B-C2B	3.76	1.44	1.36
26	b7	202	PEB	C2C-C3C	3.76	1.48	1.37
26	HJ	203	PEB	C2C-C3C	3.76	1.48	1.37
26	w1	202	PEB	C1A-NA	-3.76	1.32	1.37
26	B9	203	PEB	C1A-NA	-3.76	1.32	1.37
26	iF	201	PEB	C1A-NA	-3.76	1.32	1.37
26	DJ	201	PEB	C1A-NA	-3.76	1.32	1.37
26	q4	203	PEB	CHA-C1B	3.76	1.49	1.40
26	R7	202	PEB	CHA-C1B	3.76	1.49	1.40
26	Y7	201	PEB	CHA-C1B	3.76	1.49	1.40
26	kA	201	PEB	CHA-C1B	3.76	1.49	1.40
28	IF	1001	CYC	CHB-C4A	3.76	1.49	1.40
26	NE	201	PEB	CHA-C1B	3.76	1.49	1.40
26	b2	201	PEB	C1A-NA	-3.76	1.32	1.37
26	IG	203	PEB	C2A-C1A	-3.76	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AJ	302	PUB	C3B-C2B	3.76	1.48	1.37
26	kG	203	PEB	CHA-C1B	3.76	1.49	1.40
26	mB	203	PEB	C2C-C3C	3.76	1.48	1.37
26	H1	203	PEB	CHA-C1B	3.76	1.49	1.40
26	G9	201	PEB	CHA-C1B	3.76	1.49	1.40
26	D1	202	PEB	C1A-NA	-3.76	1.32	1.37
26	fB	201	PEB	C1A-NA	-3.76	1.32	1.37
26	z4	202	PEB	CHA-C1B	3.76	1.49	1.40
26	YD	303	PEB	CHA-C1B	3.76	1.49	1.40
26	T2	202	PEB	C1A-NA	-3.76	1.32	1.37
26	R1	203	PEB	CHA-C1B	3.76	1.49	1.40
26	e6	201	PEB	C1A-NA	-3.76	1.32	1.37
26	i8	202	PEB	C1A-NA	-3.76	1.32	1.37
27	AA	303	PUB	OD-C4D	3.76	1.30	1.23
26	m2	202	PEB	C1A-NA	-3.76	1.32	1.37
26	SG	203	PEB	CHA-C1B	3.76	1.49	1.40
26	f7	201	PEB	C1A-NA	-3.76	1.32	1.37
26	Q7	202	PEB	CHA-C1B	3.76	1.49	1.40
26	dE	202	PEB	CHA-C1B	3.76	1.49	1.40
26	mI	203	PEB	CHA-C1B	3.76	1.49	1.40
28	HF	1001	CYC	CHB-C4A	3.76	1.49	1.40
26	qE	202	PEB	CHA-C1B	3.76	1.49	1.40
26	m7	201	PEB	C1A-NA	-3.76	1.32	1.37
26	R8	201	PEB	C1A-NA	-3.75	1.32	1.37
26	IJ	201	PEB	C2A-C1A	-3.75	1.48	1.52
26	24	405	PEB	C2C-C3C	3.75	1.48	1.37
26	ND	203	PEB	C1A-NA	-3.75	1.32	1.37
26	U4	202	PEB	CHA-C1B	3.75	1.49	1.40
26	fA	201	PEB	C1A-NA	-3.75	1.32	1.37
26	GC	201	PEB	CHA-C1B	3.75	1.49	1.40
26	L1	201	PEB	C1A-NA	-3.75	1.32	1.37
26	YE	202	PEB	CHA-C1B	3.75	1.49	1.40
26	P8	201	PEB	CHA-C1B	3.75	1.49	1.40
26	Q8	203	PEB	CHA-C1B	3.75	1.49	1.40
26	V2	201	PEB	CHA-C1B	3.75	1.49	1.40
26	FC	203	PEB	CHA-C1B	3.75	1.49	1.40
26	AF	301	PEB	CHA-C1B	3.75	1.49	1.40
28	VH	1001	CYC	C3D-C2D	3.75	1.48	1.37
26	GB	1002	PEB	C2A-C1A	-3.75	1.48	1.52
26	J8	202	PEB	C1A-NA	-3.75	1.32	1.37
26	R4	201	PEB	CHA-C1B	3.75	1.49	1.40
26	SE	203	PEB	CHA-C1B	3.75	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	DF	1001	CYC	CHB-C4A	3.75	1.49	1.40
28	OH	1001	CYC	C2C-C1C	-3.75	1.48	1.52
26	B1	202	PEB	CHA-C1B	3.75	1.49	1.40
26	M4	401	PEB	C2C-C3C	3.75	1.48	1.37
26	K1	201	PEB	C2C-C3C	3.74	1.48	1.37
26	RE	202	PEB	C1A-NA	-3.74	1.32	1.37
26	i1	201	PEB	CHA-C1B	3.74	1.49	1.40
26	pE	201	PEB	CHA-C1B	3.74	1.49	1.40
26	vG	202	PEB	CHA-C1B	3.74	1.49	1.40
26	Q3	202	PEB	C1A-NA	-3.74	1.32	1.37
26	e8	202	PEB	CHA-C1B	3.74	1.49	1.40
26	A2	301	PEB	C1A-NA	-3.74	1.32	1.37
26	C3	201	PEB	C1A-NA	-3.74	1.32	1.37
26	RB	201	PEB	C1A-NA	-3.74	1.32	1.37
26	V8	201	PEB	CHA-C1B	3.74	1.49	1.40
26	Y9	201	PEB	CHA-C1B	3.74	1.49	1.40
26	A3	202	PEB	C2C-C3C	3.74	1.48	1.37
28	II	1001	CYC	C2C-C1C	-3.74	1.48	1.52
26	FG	202	PEB	C2C-C3C	3.74	1.48	1.37
26	i6	202	PEB	CHA-C1B	3.74	1.49	1.40
26	14	201	PEB	C1A-NA	-3.74	1.32	1.37
26	y1	203	PEB	CHA-C1B	3.74	1.49	1.40
26	Y8	201	PEB	C1A-NA	-3.74	1.32	1.37
26	LE	202	PEB	C1A-NA	-3.74	1.32	1.37
26	D4	201	PEB	CHA-C1B	3.74	1.49	1.40
26	z4	201	PEB	CHA-C1B	3.74	1.49	1.40
26	HD	201	PEB	CHA-C1B	3.74	1.49	1.40
26	e7	201	PEB	C1A-NA	-3.74	1.32	1.37
26	t4	201	PEB	C2C-C3C	3.74	1.48	1.37
26	q4	201	PEB	CHA-C1B	3.74	1.49	1.40
26	I8	201	PEB	C1A-NA	-3.74	1.32	1.37
26	pE	201	PEB	C2C-C3C	3.74	1.48	1.37
26	lG	202	PEB	CHA-C1B	3.74	1.49	1.40
26	a1	201	PEB	C2C-C3C	3.74	1.48	1.37
26	q1	201	PEB	CHA-C1B	3.74	1.49	1.40
26	g7	201	PEB	CHA-C1B	3.74	1.49	1.40
26	TF	201	PEB	CHA-C1B	3.74	1.49	1.40
26	iG	202	PEB	C1A-NA	-3.74	1.32	1.37
26	D1	201	PEB	CHA-C1B	3.74	1.49	1.40
26	O1	202	PEB	CHA-C1B	3.74	1.49	1.40
26	B3	201	PEB	C2C-C3C	3.74	1.48	1.37
26	lA	201	PEB	C2A-C1A	-3.74	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E3	201	PEB	C1A-NA	-3.73	1.32	1.37
26	C9	202	PEB	C1A-NA	-3.73	1.32	1.37
26	XG	203	PEB	C1A-NA	-3.73	1.32	1.37
26	KC	202	PEB	CHA-C1B	3.73	1.49	1.40
26	T6	202	PEB	C1A-NA	-3.73	1.32	1.37
26	D8	201	PEB	C1A-NA	-3.73	1.32	1.37
26	c1	202	PEB	CHA-C1B	3.73	1.49	1.40
26	D6	1002	PEB	C1A-NA	-3.73	1.32	1.37
26	T8	202	PEB	CHA-C1B	3.73	1.49	1.40
26	DJ	201	PEB	C2A-C1A	-3.73	1.48	1.52
26	H4	203	PEB	C2C-C3C	3.73	1.48	1.37
26	xG	303	PEB	C2C-C3C	3.73	1.48	1.37
26	g7	202	PEB	CHA-C1B	3.73	1.49	1.40
26	iB	201	PEB	CHA-C1B	3.73	1.49	1.40
26	g8	201	PEB	C2C-C3C	3.73	1.48	1.37
26	MD	201	PEB	C1A-NA	-3.73	1.32	1.37
26	NJ	203	PEB	CHA-C1B	3.73	1.49	1.40
26	j2	202	PEB	C2C-C3C	3.73	1.48	1.37
26	A5	202	PEB	CHA-C1B	3.73	1.49	1.40
28	E7	1001	CYC	CHB-C4A	3.73	1.49	1.40
26	XE	202	PEB	CHA-C1B	3.73	1.49	1.40
28	E2	1001	CYC	CHB-C4A	3.73	1.49	1.40
26	P9	201	PEB	CHA-C1B	3.73	1.49	1.40
26	U6	201	PEB	C1A-NA	-3.73	1.32	1.37
26	RA	201	PEB	C1A-NA	-3.73	1.32	1.37
28	C2	1001	CYC	C1C-NC	-3.73	1.32	1.37
26	ZA	202	PEB	CHA-C1B	3.73	1.49	1.40
26	c2	203	PEB	CHA-C1B	3.73	1.49	1.40
26	X8	202	PEB	CHA-C1B	3.73	1.49	1.40
26	F4	201	PEB	C1A-NA	-3.73	1.32	1.37
26	UF	202	PEB	C1A-NA	-3.73	1.32	1.37
26	iB	202	PEB	CHA-C1B	3.73	1.49	1.40
26	fE	201	PEB	C2A-C1A	-3.73	1.48	1.52
26	oG	202	PEB	C2C-C3C	3.73	1.48	1.37
26	S1	201	PEB	CHA-C1B	3.73	1.49	1.40
26	E4	201	PEB	C1A-NA	-3.73	1.32	1.37
26	jA	201	PEB	C1A-NA	-3.73	1.32	1.37
26	bI	201	PEB	C1A-NA	-3.73	1.32	1.37
26	R2	203	PEB	CHA-C1B	3.73	1.49	1.40
26	ZA	201	PEB	CHA-C1B	3.73	1.49	1.40
26	zG	501	PEB	CHA-C1B	3.73	1.49	1.40
26	bF	202	PEB	C2C-C3C	3.73	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UA	203	PEB	C1A-NA	-3.73	1.32	1.37
26	V9	202	PEB	CHA-C1B	3.73	1.49	1.40
26	FE	202	PEB	C2C-C3C	3.73	1.48	1.37
26	D9	201	PEB	C1A-NA	-3.73	1.32	1.37
26	PE	202	PEB	C1A-NA	-3.73	1.32	1.37
26	d7	203	PEB	C2C-C3C	3.73	1.48	1.37
28	AH	1001	CYC	C3D-C2D	3.72	1.48	1.37
26	P6	201	PEB	C1A-NA	-3.72	1.32	1.37
26	I1	201	PEB	CHA-C1B	3.72	1.49	1.40
26	kG	202	PEB	CHA-C1B	3.72	1.49	1.40
26	J8	201	PEB	CHA-C1B	3.72	1.49	1.40
26	CA	203	PEB	C1A-NA	-3.72	1.32	1.37
26	UG	202	PEB	C1A-NA	-3.72	1.32	1.37
26	Y4	201	PEB	CHA-C1B	3.72	1.49	1.40
26	uG	201	PEB	CHA-C1B	3.72	1.49	1.40
26	TB	202	PEB	C2C-C3C	3.72	1.48	1.37
28	D7	1001	CYC	CHB-C4A	3.72	1.49	1.40
26	mF	202	PEB	C2C-C3C	3.72	1.48	1.37
26	h7	202	PEB	C1A-NA	-3.72	1.32	1.37
26	iG	201	PEB	CHA-C1B	3.72	1.49	1.40
26	tE	201	PEB	C2C-C3C	3.72	1.48	1.37
26	lB	203	PEB	CHA-C1B	3.72	1.49	1.40
26	FJ	201	PEB	CHA-C1B	3.72	1.49	1.40
26	O9	201	PEB	CHA-C1B	3.72	1.49	1.40
26	R4	203	PEB	C2C-C3C	3.72	1.48	1.37
26	LC	203	PEB	C1A-NA	-3.72	1.32	1.37
26	XD	201	PEB	C2C-C3C	3.72	1.48	1.37
26	AF	305	PEB	CHA-C1B	3.72	1.49	1.40
26	d1	201	PEB	C1A-NA	-3.72	1.32	1.37
26	R9	202	PEB	C1A-NA	-3.72	1.32	1.37
26	q1	203	PEB	CHA-C1B	3.72	1.49	1.40
26	z1	201	PEB	C2C-C3C	3.72	1.48	1.37
26	T6	202	PEB	C2C-C3C	3.72	1.48	1.37
26	y1	201	PEB	C2C-C3C	3.72	1.48	1.37
26	j8	202	PEB	CHA-C1B	3.72	1.49	1.40
28	I7	1001	CYC	C2C-C1C	-3.72	1.48	1.52
26	qG	202	PEB	CHA-C1B	3.72	1.49	1.40
26	Q8	203	PEB	C1A-NA	-3.72	1.32	1.37
26	y4	203	PEB	C2C-C3C	3.72	1.48	1.37
26	F9	201	PEB	C2A-C1A	-3.72	1.48	1.52
26	w1	201	PEB	CHA-C1B	3.71	1.49	1.40
26	VD	201	PEB	C1A-NA	-3.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u4	201	PEB	C2C-C3C	3.71	1.48	1.37
26	f2	202	PEB	CHA-C1B	3.71	1.49	1.40
26	A8	302	PEB	CHA-C1B	3.71	1.49	1.40
26	h7	203	PEB	C2C-C3C	3.71	1.48	1.37
26	Q2	202	PEB	C1A-NA	-3.71	1.32	1.37
26	CC	203	PEB	CHA-C1B	3.71	1.49	1.40
26	JE	201	PEB	CHA-C1B	3.71	1.49	1.40
26	T4	202	PEB	CHA-C1B	3.71	1.49	1.40
26	L4	201	PEB	C1A-NA	-3.71	1.32	1.37
26	z4	202	PEB	C1A-NA	-3.71	1.32	1.37
26	24	404	PEB	CHA-C1B	3.71	1.49	1.40
26	tG	201	PEB	CHA-C1B	3.71	1.49	1.40
26	X3	201	PEB	C2C-C3C	3.71	1.48	1.37
26	eB	201	PEB	C1A-NA	-3.71	1.32	1.37
26	A1	202	PEB	CHA-C1B	3.71	1.49	1.40
26	lA	202	PEB	CHA-C1B	3.71	1.49	1.40
26	iI	201	PEB	CHA-C1B	3.71	1.49	1.40
26	NF	1002	PEB	C1A-NA	-3.71	1.32	1.37
26	X4	201	PEB	CHA-C1B	3.71	1.49	1.40
26	h6	202	PEB	C1A-NA	-3.71	1.32	1.37
26	XA	201	PEB	C1A-NA	-3.71	1.32	1.37
26	ZE	202	PEB	C2C-C3C	3.71	1.48	1.37
28	NH	1001	CYC	C3D-C2D	3.71	1.48	1.37
26	YI	202	PEB	C1A-NA	-3.71	1.32	1.37
26	l7	203	PEB	C2C-C3C	3.71	1.48	1.37
26	F4	203	PEB	CHA-C1B	3.71	1.49	1.40
26	BC	203	PEB	CHA-C1B	3.71	1.49	1.40
26	k6	202	PEB	C2C-C3C	3.71	1.48	1.37
26	H7	1002	PEB	C1A-NA	-3.71	1.32	1.37
26	eE	202	PEB	C1A-NA	-3.71	1.32	1.37
26	i6	201	PEB	CHA-C1B	3.71	1.49	1.40
26	PG	201	PEB	CHA-C1B	3.71	1.49	1.40
26	Z6	203	PEB	C1A-NA	-3.71	1.32	1.37
26	OA	202	PEB	C1A-NA	-3.71	1.32	1.37
26	aG	203	PEB	C1A-NA	-3.71	1.32	1.37
26	I8	202	PEB	CHA-C1B	3.71	1.49	1.40
26	ff	202	PEB	C2C-C3C	3.71	1.48	1.37
26	BE	202	PEB	CHA-C1B	3.71	1.49	1.40
26	P4	202	PEB	CHA-C1B	3.71	1.49	1.40
26	i6	202	PEB	C2C-C3C	3.71	1.48	1.37
26	jI	202	PEB	C2C-C3C	3.71	1.48	1.37
26	L3	201	PEB	C2A-C1A	-3.71	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	e8	201	PEB	C2A-C1A	-3.71	1.48	1.52
26	I4	201	PEB	C1A-NA	-3.71	1.32	1.37
26	O4	202	PEB	CHA-C1B	3.71	1.49	1.40
26	G6	1002	PEB	C2A-C1A	-3.71	1.48	1.52
26	R8	201	PEB	C2A-C1A	-3.71	1.48	1.52
26	aF	202	PEB	C2C-C3C	3.71	1.48	1.37
26	NE	202	PEB	C2C-C3C	3.70	1.48	1.37
26	L9	203	PEB	CHA-C1B	3.70	1.49	1.40
26	R1	201	PEB	CHA-C1B	3.70	1.49	1.40
26	JC	202	PEB	C1A-NA	-3.70	1.32	1.37
26	YD	301	PEB	C2C-C3C	3.70	1.48	1.37
26	X8	201	PEB	C2A-C1A	-3.70	1.48	1.52
26	Y8	201	PEB	C2A-C1A	-3.70	1.48	1.52
26	jA	202	PEB	CHA-C1B	3.70	1.49	1.40
26	gA	201	PEB	C2C-C3C	3.70	1.48	1.37
26	aG	202	PEB	CHA-C1B	3.70	1.49	1.40
26	M3	201	PEB	C1A-NA	-3.70	1.32	1.37
26	f8	201	PEB	C1A-NA	-3.70	1.32	1.37
26	kA	201	PEB	C1A-NA	-3.70	1.32	1.37
28	qH	1001	CYC	C2C-C1C	-3.70	1.48	1.52
26	J7	1002	PEB	CHA-C1B	3.70	1.49	1.40
26	BE	201	PEB	CHA-C1B	3.70	1.49	1.40
26	gF	201	PEB	CHA-C1B	3.70	1.49	1.40
26	nE	201	PEB	CHA-C1B	3.70	1.49	1.40
26	R1	202	PEB	C1A-NA	-3.70	1.32	1.37
26	DB	1002	PEB	C1A-NA	-3.70	1.32	1.37
26	aI	201	PEB	CHA-C1B	3.70	1.49	1.40
26	b6	201	PEB	C2A-C1A	-3.70	1.48	1.52
26	AJ	303	PEB	CHA-C1B	3.70	1.49	1.40
26	KJ	201	PEB	CHA-C1B	3.70	1.49	1.40
26	EJ	201	PEB	C2A-C1A	-3.70	1.48	1.52
26	BC	202	PEB	C2C-C3C	3.70	1.48	1.37
27	xG	306	PUB	C3B-C2B	3.70	1.48	1.37
26	a1	203	PEB	C1A-NA	-3.70	1.32	1.37
26	TB	202	PEB	C1A-NA	-3.70	1.32	1.37
28	DF	1003	CYC	C1C-NC	-3.70	1.32	1.37
26	e4	201	PEB	C2C-C3C	3.70	1.48	1.37
26	l6	203	PEB	CHA-C1B	3.70	1.49	1.40
26	FC	203	PEB	C1A-NA	-3.70	1.32	1.37
26	PI	202	PEB	C1A-NA	-3.70	1.32	1.37
26	s1	202	PEB	C2C-C3C	3.70	1.48	1.37
26	T6	201	PEB	C2A-C1A	-3.70	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j4	201	PEB	CHA-C1B	3.70	1.49	1.40
26	AA	302	PEB	CHA-C1B	3.70	1.49	1.40
26	hA	202	PEB	CHA-C1B	3.70	1.49	1.40
26	m6	203	PEB	C2C-C3C	3.70	1.48	1.37
26	F1	203	PEB	CHA-C1B	3.70	1.49	1.40
26	kE	203	PEB	CHA-C1B	3.70	1.49	1.40
28	EF	1001	CYC	CHB-C4A	3.70	1.49	1.40
26	R7	202	PEB	C2C-C3C	3.70	1.48	1.37
26	UA	201	PEB	C1A-NA	-3.70	1.32	1.37
26	QA	203	PEB	C1A-NA	-3.70	1.32	1.37
26	a4	201	PEB	C2C-C3C	3.70	1.48	1.37
26	OJ	201	PEB	CHA-C1B	3.70	1.49	1.40
26	S4	201	PEB	CHA-C1B	3.70	1.49	1.40
26	V3	201	PEB	C1A-NA	-3.70	1.32	1.37
26	BD	203	PEB	C1A-NA	-3.70	1.32	1.37
26	g1	202	PEB	C2C-C3C	3.70	1.48	1.37
28	eH	1001	CYC	C3D-C2D	3.70	1.48	1.37
26	PI	203	PEB	CHA-C1B	3.69	1.49	1.40
26	GG	203	PEB	C1A-NA	-3.69	1.32	1.37
26	T6	202	PEB	CHA-C1B	3.69	1.49	1.40
26	hA	201	PEB	CHA-C1B	3.69	1.49	1.40
26	y4	201	PEB	C1A-NA	-3.69	1.32	1.37
26	eG	202	PEB	C1A-NA	-3.69	1.32	1.37
26	J4	201	PEB	CHA-C1B	3.69	1.49	1.40
26	Q8	202	PEB	C1A-NA	-3.69	1.32	1.37
26	FC	201	PEB	C1A-NA	-3.69	1.32	1.37
26	GD	201	PEB	C1A-NA	-3.69	1.32	1.37
26	PF	201	PEB	C1A-NA	-3.69	1.32	1.37
26	H4	201	PEB	C2C-C3C	3.69	1.48	1.37
26	L5	201	PEB	CHA-C1B	3.69	1.49	1.40
26	G5	202	PEB	C1A-NA	-3.69	1.32	1.37
26	W6	203	PEB	C1A-NA	-3.69	1.32	1.37
26	A2	305	PEB	CHA-C1B	3.69	1.49	1.40
26	G4	202	PEB	CHA-C1B	3.69	1.49	1.40
26	PJ	202	PEB	C2C-C3C	3.69	1.48	1.37
26	X8	201	PEB	C1A-NA	-3.69	1.32	1.37
26	N9	202	PEB	CHA-C1B	3.69	1.49	1.40
26	Y9	201	PEB	C2C-C3C	3.69	1.48	1.37
26	A8	302	PEB	C1A-NA	-3.69	1.32	1.37
26	DA	201	PEB	C1A-NA	-3.69	1.32	1.37
26	IA	201	PEB	C1A-NA	-3.69	1.32	1.37
26	C4	201	PEB	C2C-C3C	3.69	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	KD	202	PEB	C2C-C3C	3.69	1.48	1.37
26	S9	202	PEB	C1A-NA	-3.69	1.32	1.37
28	C7	1001	CYC	CHB-C4A	3.69	1.49	1.40
26	U2	201	PEB	C3B-C2B	3.69	1.44	1.36
26	m7	202	PEB	C2C-C3C	3.69	1.48	1.37
26	vE	201	PEB	C2C-C3C	3.69	1.48	1.37
26	YA	201	PEB	C2A-C1A	-3.69	1.48	1.52
26	S1	201	PEB	C1A-NA	-3.69	1.32	1.37
28	M6	1001	CYC	C1C-NC	-3.69	1.32	1.37
26	J5	201	PEB	C3C-C4C	3.69	1.47	1.42
26	mE	202	PEB	CHA-C1B	3.69	1.49	1.40
26	F1	203	PEB	C1A-NA	-3.68	1.32	1.37
26	k6	202	PEB	CHA-C1B	3.68	1.49	1.40
26	L9	201	PEB	C1A-NA	-3.68	1.32	1.37
26	f2	202	PEB	C2C-C3C	3.68	1.48	1.37
26	gA	202	PEB	C2C-C3C	3.68	1.48	1.37
28	L6	1001	CYC	CHB-C4A	3.68	1.49	1.40
26	bB	201	PEB	C1A-NA	-3.68	1.32	1.37
26	UI	201	PEB	C3B-C2B	3.68	1.44	1.36
26	T1	203	PEB	CHA-C1B	3.68	1.49	1.40
26	k8	201	PEB	CHA-C1B	3.68	1.49	1.40
26	ED	201	PEB	C1A-NA	-3.68	1.32	1.37
26	NJ	204	PEB	C1A-NA	-3.68	1.32	1.37
26	E1	202	PEB	C2C-C3C	3.68	1.48	1.37
26	a1	201	PEB	C1A-NA	-3.68	1.32	1.37
26	O7	201	PEB	C1A-NA	-3.68	1.32	1.37
26	a1	203	PEB	CHA-C1B	3.68	1.49	1.40
26	eA	202	PEB	CHA-C1B	3.68	1.49	1.40
26	eF	201	PEB	CHA-C1B	3.68	1.49	1.40
26	z4	201	PEB	C2C-C3C	3.68	1.48	1.37
26	V9	202	PEB	C2C-C3C	3.68	1.48	1.37
26	m8	202	PEB	C2C-C3C	3.68	1.48	1.37
28	hH	1001	CYC	C3D-C2D	3.68	1.48	1.37
26	SE	202	PEB	CHA-C1B	3.68	1.49	1.40
26	T2	201	PEB	C1A-NA	-3.68	1.32	1.37
26	T4	201	PEB	CHC-C4C	3.68	1.59	1.50
26	kA	202	PEB	C2C-C3C	3.68	1.48	1.37
26	II	202	PEB	C1A-NA	-3.68	1.32	1.37
26	YG	201	PEB	C2C-C3C	3.68	1.48	1.37
26	V6	201	PEB	C1A-NA	-3.68	1.32	1.37
26	M8	202	PEB	C1A-NA	-3.68	1.32	1.37
26	GC	201	PEB	C1A-NA	-3.68	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v4	201	PEB	CHA-C1B	3.68	1.49	1.40
26	H9	203	PEB	C2C-C3C	3.68	1.48	1.37
26	YB	202	PEB	C1A-NA	-3.68	1.32	1.37
26	mB	202	PEB	CHA-C1B	3.68	1.49	1.40
26	VB	202	PEB	C2C-C3C	3.68	1.48	1.37
26	C4	202	PEB	C1A-NA	-3.67	1.32	1.37
26	L5	202	PEB	C1A-NA	-3.67	1.32	1.37
26	P8	201	PEB	C1A-NA	-3.67	1.32	1.37
26	b6	201	PEB	CHA-C1B	3.67	1.49	1.40
26	K4	201	PEB	C2C-C3C	3.67	1.48	1.37
26	H1	203	PEB	C2C-C3C	3.67	1.48	1.37
26	F9	202	PEB	CHA-C1B	3.67	1.49	1.40
26	R4	203	PEB	CHA-C1B	3.67	1.49	1.40
26	N4	202	PEB	C1A-NA	-3.67	1.32	1.37
26	O6	203	PEB	C1A-NA	-3.67	1.32	1.37
26	q4	201	PEB	C2C-C3C	3.67	1.48	1.37
26	PB	202	PEB	CHA-C1B	3.67	1.49	1.40
26	QA	202	PEB	C1A-NA	-3.67	1.32	1.37
26	EE	202	PEB	C1A-NA	-3.67	1.32	1.37
26	n4	201	PEB	CHA-C1B	3.67	1.49	1.40
26	LC	203	PEB	CHA-C1B	3.67	1.49	1.40
26	n4	202	PEB	C2C-C3C	3.67	1.48	1.37
26	r4	201	PEB	CHA-C1B	3.67	1.49	1.40
26	L5	203	PEB	CHA-C1B	3.67	1.49	1.40
28	F2	1001	CYC	CHB-C4A	3.67	1.49	1.40
26	D4	202	PEB	C1A-NA	-3.67	1.32	1.37
26	YG	203	PEB	C2A-C1A	-3.67	1.48	1.52
26	d1	201	PEB	C2C-C3C	3.67	1.48	1.37
26	cF	201	PEB	C1A-NA	-3.67	1.32	1.37
28	I7	1001	CYC	C1C-NC	-3.67	1.32	1.37
26	P2	203	PEB	CHA-C1B	3.67	1.49	1.40
26	O9	202	PEB	C1A-NA	-3.67	1.32	1.37
26	B1	201	PEB	C2C-C3C	3.67	1.48	1.37
26	oG	203	PEB	CHA-C1B	3.67	1.49	1.40
26	f6	201	PEB	C1A-NA	-3.67	1.32	1.37
26	U8	201	PEB	C1A-NA	-3.67	1.32	1.37
26	h8	203	PEB	C1A-NA	-3.67	1.32	1.37
26	BG	202	PEB	CHA-C1B	3.67	1.49	1.40
26	AI	304	PEB	CHA-C1B	3.67	1.49	1.40
26	ZF	201	PEB	C2A-C1A	-3.67	1.48	1.52
26	v4	202	PEB	CHA-C1B	3.67	1.49	1.40
26	c8	201	PEB	CHA-C1B	3.67	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k4	201	PEB	CHA-C1B	3.67	1.49	1.40
26	QD	202	PEB	C1A-NA	-3.67	1.32	1.37
26	g7	202	PEB	C2C-C3C	3.67	1.48	1.37
26	YF	201	PEB	C2C-C3C	3.67	1.48	1.37
26	V4	203	PEB	CHA-C1B	3.67	1.49	1.40
26	LC	201	PEB	C2A-C1A	-3.67	1.48	1.52
26	K1	201	PEB	C1A-NA	-3.66	1.32	1.37
26	l7	202	PEB	C1A-NA	-3.66	1.32	1.37
26	dB	201	PEB	C2C-C3C	3.66	1.48	1.37
26	Y1	201	PEB	CHA-C1B	3.66	1.49	1.40
26	w4	201	PEB	CHA-C1B	3.66	1.49	1.40
26	C5	201	PEB	C2C-C3C	3.66	1.48	1.37
26	u1	201	PEB	C2C-C3C	3.66	1.48	1.37
26	R6	202	PEB	C2C-C3C	3.66	1.48	1.37
26	kB	202	PEB	C2C-C3C	3.66	1.48	1.37
26	O1	201	PEB	C2A-C1A	-3.66	1.48	1.52
26	X1	201	PEB	C2A-C1A	-3.66	1.48	1.52
26	P4	201	PEB	CHA-C1B	3.66	1.49	1.40
26	GG	202	PEB	CHA-C1B	3.66	1.49	1.40
26	M1	401	PEB	C2C-C3C	3.66	1.48	1.37
27	KD	203	PUB	C3B-C2B	3.66	1.48	1.37
26	OI	202	PEB	CHA-C1B	3.66	1.49	1.40
26	BD	201	PEB	C2C-C3C	3.66	1.48	1.37
26	BD	202	PEB	CHA-C1B	3.66	1.49	1.40
26	oE	203	PEB	C1A-NA	-3.66	1.32	1.37
26	V1	201	PEB	CHA-C1B	3.66	1.49	1.40
26	cA	201	PEB	CHA-C1B	3.66	1.49	1.40
26	NJ	202	PEB	CHA-C1B	3.66	1.49	1.40
26	Z4	201	PEB	C2C-C3C	3.66	1.48	1.37
26	AC	202	PEB	C2C-C3C	3.66	1.48	1.37
26	M1	402	PEB	CHA-C1B	3.66	1.49	1.40
26	VB	201	PEB	C1A-NA	-3.66	1.32	1.37
26	U3	201	PEB	C2A-C1A	-3.66	1.48	1.52
26	p4	201	PEB	C2C-C3C	3.66	1.48	1.37
26	B1	203	PEB	C1A-NA	-3.66	1.32	1.37
26	Z1	201	PEB	C2C-C3C	3.66	1.48	1.37
26	N9	203	PEB	C2C-C3C	3.66	1.48	1.37
26	AE	201	PEB	CHA-C1B	3.66	1.49	1.40
26	sG	201	PEB	CHA-C1B	3.66	1.49	1.40
26	D4	203	PEB	C2C-C3C	3.66	1.48	1.37
26	Y2	202	PEB	C1A-NA	-3.66	1.32	1.37
26	J9	201	PEB	C1A-NA	-3.66	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P9	203	PEB	CHA-C1B	3.66	1.49	1.40
26	jA	201	PEB	CHA-C1B	3.66	1.49	1.40
26	SJ	201	PEB	C2C-C3C	3.66	1.48	1.37
26	H1	201	PEB	C2C-C3C	3.66	1.48	1.37
26	iG	203	PEB	C2C-C3C	3.66	1.48	1.37
26	sE	203	PEB	C1A-NA	-3.66	1.32	1.37
26	ZG	201	PEB	C1A-NA	-3.66	1.32	1.37
26	C3	201	PEB	CHA-C1B	3.66	1.49	1.40
26	JE	202	PEB	CHA-C1B	3.66	1.49	1.40
26	v4	201	PEB	C2C-C3C	3.66	1.48	1.37
26	CD	201	PEB	CHA-C1B	3.66	1.49	1.40
26	gI	201	PEB	CHA-C1B	3.66	1.49	1.40
26	S4	201	PEB	C1A-NA	-3.66	1.32	1.37
26	WD	201	PEB	C1A-NA	-3.66	1.32	1.37
28	MB	1001	CYC	C1C-NC	-3.66	1.32	1.37
27	21	402	PUB	C3B-C2B	3.66	1.48	1.37
26	aA	203	PEB	C1A-NA	-3.66	1.32	1.37
26	s1	203	PEB	C2C-C3C	3.66	1.48	1.37
26	i2	201	PEB	CHA-C1B	3.66	1.49	1.40
26	g4	201	PEB	CHA-C1B	3.66	1.49	1.40
26	bB	201	PEB	CHA-C1B	3.65	1.49	1.40
26	SG	203	PEB	C1A-NA	-3.65	1.32	1.37
26	JG	201	PEB	C2A-C1A	-3.65	1.48	1.52
28	FB	1001	CYC	C2C-C1C	-3.65	1.48	1.52
26	B5	202	PEB	C2C-C3C	3.65	1.48	1.37
26	i2	202	PEB	C1A-NA	-3.65	1.32	1.37
26	g8	202	PEB	C2C-C3C	3.65	1.48	1.37
26	m4	202	PEB	CHA-C1B	3.65	1.49	1.40
26	O1	202	PEB	C1A-NA	-3.65	1.32	1.37
26	UE	201	PEB	C1A-NA	-3.65	1.32	1.37
26	aA	203	PEB	C2C-C3C	3.65	1.48	1.37
28	LB	1001	CYC	CHB-C4A	3.65	1.49	1.40
26	xE	302	PEB	C2C-C3C	3.65	1.48	1.37
26	a2	201	PEB	CHA-C1B	3.65	1.49	1.40
26	CC	202	PEB	C2C-C3C	3.65	1.48	1.37
26	oE	202	PEB	C2C-C3C	3.65	1.48	1.37
28	oH	1001	CYC	C3D-C2D	3.65	1.48	1.37
26	QA	203	PEB	CHA-C1B	3.65	1.49	1.40
28	H7	1001	CYC	C1C-NC	-3.65	1.32	1.37
26	11	202	PEB	C2C-C3C	3.65	1.48	1.37
26	X9	202	PEB	CHA-C1B	3.65	1.49	1.40
26	Q9	201	PEB	C2A-C1A	-3.65	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AD	202	PEB	C2C-C3C	3.65	1.48	1.37
26	i1	202	PEB	C1A-NA	-3.65	1.32	1.37
26	UJ	202	PEB	C1A-NA	-3.65	1.32	1.37
26	j7	202	PEB	C2C-C3C	3.65	1.48	1.37
26	CC	201	PEB	C2C-C3C	3.65	1.48	1.37
27	AF	304	PUB	C3B-C2B	3.65	1.48	1.37
26	kI	202	PEB	C1A-NA	-3.65	1.32	1.37
26	V1	203	PEB	CHA-C1B	3.65	1.49	1.40
26	LJ	203	PEB	CHA-C1B	3.65	1.49	1.40
28	D2	1001	CYC	CHB-C4A	3.65	1.49	1.40
26	j7	203	PEB	CHA-C1B	3.65	1.49	1.40
28	DI	1001	CYC	CHB-C4A	3.65	1.49	1.40
26	M9	202	PEB	C2C-C3C	3.65	1.48	1.37
26	B4	201	PEB	C2C-C3C	3.65	1.48	1.37
26	IG	201	PEB	C2C-C3C	3.65	1.48	1.37
26	xG	304	PEB	C2C-C3C	3.65	1.48	1.37
26	QF	202	PEB	C1A-NA	-3.65	1.32	1.37
26	VG	202	PEB	C2C-C3C	3.65	1.48	1.37
26	a6	202	PEB	CHA-C1B	3.65	1.49	1.40
26	T1	201	PEB	CHC-C4C	3.65	1.59	1.50
26	RA	201	PEB	C2A-C1A	-3.65	1.48	1.52
28	KB	202	CYC	C2C-C1C	-3.65	1.48	1.52
26	L6	1002	PEB	C1A-NA	-3.65	1.32	1.37
26	C5	203	PEB	C2C-C3C	3.65	1.48	1.37
26	d2	202	PEB	CHA-C1B	3.65	1.49	1.40
28	IH	1001	CYC	C3D-C2D	3.65	1.48	1.37
26	PJ	203	PEB	C2C-C3C	3.65	1.48	1.37
26	dF	203	PEB	CHA-C1B	3.65	1.49	1.40
26	I5	203	PEB	CHA-C1B	3.65	1.49	1.40
26	DE	203	PEB	C2C-C3C	3.65	1.48	1.37
26	iB	202	PEB	C2C-C3C	3.65	1.48	1.37
26	s1	201	PEB	CHA-C1B	3.65	1.49	1.40
28	F2	1001	CYC	C2C-C1C	-3.65	1.48	1.52
26	l4	201	PEB	C2C-C3C	3.65	1.48	1.37
26	kE	202	PEB	CHA-C1B	3.64	1.49	1.40
26	bE	201	PEB	CHA-C1B	3.64	1.49	1.40
26	LE	201	PEB	CHA-C1B	3.64	1.49	1.40
26	A9	303	PEB	C2C-C3C	3.64	1.48	1.37
26	jF	203	PEB	C1A-NA	-3.64	1.32	1.37
26	R1	203	PEB	C2C-C3C	3.64	1.48	1.37
26	p4	202	PEB	C4B-C3B	3.64	1.51	1.45
26	g2	201	PEB	CHA-C1B	3.64	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m1	201	PEB	C1A-NA	-3.64	1.32	1.37
26	z4	201	PEB	C1A-NA	-3.64	1.32	1.37
26	Y6	202	PEB	C1A-NA	-3.64	1.32	1.37
26	K4	202	PEB	CHA-C1B	3.64	1.48	1.40
26	k1	201	PEB	C2C-C3C	3.64	1.48	1.37
26	S1	202	PEB	CHA-C1B	3.64	1.48	1.40
26	d6	201	PEB	CHA-C1B	3.64	1.48	1.40
26	YA	201	PEB	C1A-NA	-3.64	1.32	1.37
26	dB	203	PEB	C1A-NA	-3.64	1.32	1.37
26	A7	305	PEB	CHA-C1B	3.64	1.48	1.40
26	Y8	202	PEB	C2A-C1A	-3.64	1.48	1.52
26	O2	202	PEB	CHA-C1B	3.64	1.48	1.40
26	IA	203	PEB	C1A-NA	-3.64	1.32	1.37
26	XE	202	PEB	C1A-NA	-3.64	1.32	1.37
26	d1	201	PEB	CHA-C1B	3.64	1.48	1.40
26	ZI	202	PEB	CHA-C1B	3.64	1.48	1.40
26	H1	201	PEB	CHA-C1B	3.64	1.48	1.40
28	DI	1001	CYC	C2C-C1C	-3.64	1.48	1.52
26	hB	202	PEB	C1A-NA	-3.64	1.32	1.37
26	kG	201	PEB	C1A-NA	-3.64	1.32	1.37
26	i4	201	PEB	C1A-NA	-3.64	1.32	1.37
26	vG	201	PEB	C2C-C3C	3.64	1.48	1.37
26	TB	202	PEB	CHA-C1B	3.64	1.48	1.40
26	d2	201	PEB	C1A-NA	-3.64	1.32	1.37
26	c4	202	PEB	CHA-C1B	3.64	1.48	1.40
26	rE	202	PEB	CHA-C1B	3.64	1.48	1.40
28	FI	1001	CYC	C2C-C1C	-3.64	1.48	1.52
26	P2	202	PEB	C1A-NA	-3.64	1.32	1.37
28	N7	1001	CYC	C1C-NC	-3.64	1.32	1.37
26	i4	202	PEB	C2C-C3C	3.64	1.48	1.37
26	mA	202	PEB	C2C-C3C	3.64	1.48	1.37
27	A7	304	PUB	C3B-C2B	3.64	1.48	1.37
26	Y2	203	PEB	CHA-C1B	3.64	1.48	1.40
26	24	405	PEB	CHA-C1B	3.64	1.48	1.40
26	UE	202	PEB	C1A-NA	-3.64	1.32	1.37
26	NG	202	PEB	C2C-C3C	3.63	1.48	1.37
26	Z7	201	PEB	C2A-C1A	-3.63	1.48	1.52
26	QB	203	PEB	C1A-NA	-3.63	1.32	1.37
26	HC	202	PEB	C1A-NA	-3.63	1.32	1.37
26	P6	202	PEB	CHA-C1B	3.63	1.48	1.40
26	E4	201	PEB	C2C-C3C	3.63	1.48	1.37
26	f8	201	PEB	C2C-C3C	3.63	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M1	403	PEB	CHA-C1B	3.63	1.48	1.40
26	g1	201	PEB	CHA-C1B	3.63	1.48	1.40
26	P9	202	PEB	C2A-C1A	-3.63	1.48	1.52
26	h4	201	PEB	C2C-C3C	3.63	1.48	1.37
26	F5	203	PEB	CHA-C1B	3.63	1.48	1.40
26	a1	202	PEB	C2C-C3C	3.63	1.48	1.37
26	oE	201	PEB	C2C-C3C	3.63	1.48	1.37
26	IC	203	PEB	CHA-C1B	3.63	1.48	1.40
26	fl	202	PEB	C2C-C3C	3.63	1.48	1.37
26	O4	201	PEB	C2A-C1A	-3.63	1.48	1.52
28	IH	1001	CYC	C2C-C1C	-3.63	1.48	1.52
26	DE	203	PEB	CHA-C1B	3.63	1.48	1.40
26	QG	202	PEB	CHA-C1B	3.63	1.48	1.40
26	AJ	303	PEB	C2C-C3C	3.63	1.48	1.37
26	HI	1002	PEB	C1A-NA	-3.63	1.32	1.37
26	HC	203	PEB	CHA-C1B	3.63	1.48	1.40
26	FG	202	PEB	CHA-C1B	3.63	1.48	1.40
26	RB	202	PEB	C2C-C3C	3.63	1.48	1.37
26	kE	202	PEB	C2C-C3C	3.63	1.48	1.37
26	aI	201	PEB	C2C-C3C	3.63	1.48	1.37
26	iI	202	PEB	C1A-NA	-3.63	1.32	1.37
26	JD	201	PEB	C2C-C3C	3.63	1.48	1.37
26	AI	305	PEB	CHA-C1B	3.63	1.48	1.40
26	F4	203	PEB	C1A-NA	-3.63	1.32	1.37
26	d4	201	PEB	C1A-NA	-3.63	1.32	1.37
26	Z7	202	PEB	C1A-NA	-3.63	1.32	1.37
26	aA	202	PEB	CHA-C1B	3.63	1.48	1.40
26	d6	201	PEB	C2C-C3C	3.63	1.48	1.37
26	jG	202	PEB	C2C-C3C	3.63	1.48	1.37
26	q4	203	PEB	C2C-C3C	3.63	1.48	1.37
26	R6	201	PEB	C1A-NA	-3.63	1.32	1.37
26	IC	202	PEB	CHA-C1B	3.63	1.48	1.40
26	y4	201	PEB	C2C-C3C	3.63	1.48	1.37
27	A7	303	PUB	C3B-C2B	3.63	1.48	1.37
26	pG	201	PEB	C2C-C3C	3.63	1.48	1.37
26	TE	202	PEB	CHA-C1B	3.63	1.48	1.40
28	pH	1001	CYC	C3D-C2D	3.63	1.48	1.37
26	X8	202	PEB	C1A-NA	-3.63	1.32	1.37
26	aI	202	PEB	C1A-NA	-3.63	1.32	1.37
26	C5	202	PEB	C2C-C3C	3.63	1.48	1.37
26	LE	202	PEB	CHA-C1B	3.63	1.48	1.40
26	GE	202	PEB	CHA-C1B	3.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k4	201	PEB	C2C-C3C	3.63	1.48	1.37
26	k8	201	PEB	C2C-C3C	3.63	1.48	1.37
26	TA	201	PEB	C2C-C3C	3.62	1.48	1.37
26	nE	202	PEB	C1A-NA	-3.62	1.32	1.37
26	m1	202	PEB	C2C-C3C	3.62	1.48	1.37
26	l1	201	PEB	C2C-C3C	3.62	1.48	1.37
26	HE	202	PEB	C2C-C3C	3.62	1.48	1.37
26	HG	202	PEB	C2C-C3C	3.62	1.48	1.37
26	AI	301	PEB	C1A-NA	-3.62	1.32	1.37
26	O1	201	PEB	CHA-C1B	3.62	1.48	1.40
26	vG	202	PEB	C1A-NA	-3.62	1.32	1.37
26	I4	201	PEB	CHA-C1B	3.62	1.48	1.40
26	K5	202	PEB	CHA-C1B	3.62	1.48	1.40
26	tG	201	PEB	C2C-C3C	3.62	1.48	1.37
26	e2	201	PEB	C1A-NA	-3.62	1.32	1.37
26	OB	203	PEB	C1A-NA	-3.62	1.32	1.37
28	L6	1001	CYC	C3D-C2D	3.62	1.48	1.37
26	A5	201	PEB	C2C-C3C	3.62	1.48	1.37
26	BG	202	PEB	C1A-NA	-3.62	1.32	1.37
26	YJ	201	PEB	CHA-C1B	3.62	1.48	1.40
26	JF	1002	PEB	CHA-C1B	3.62	1.48	1.40
28	KI	1001	CYC	C1C-NC	-3.62	1.32	1.37
26	O9	202	PEB	C2C-C3C	3.62	1.48	1.37
26	vE	202	PEB	C2C-C3C	3.62	1.48	1.37
26	e2	202	PEB	C1A-NA	-3.62	1.32	1.37
26	hE	202	PEB	C2C-C3C	3.62	1.48	1.37
26	21	404	PEB	C2C-C3C	3.62	1.48	1.37
26	N9	203	PEB	CHA-C1B	3.62	1.48	1.40
26	MA	202	PEB	C1A-NA	-3.62	1.32	1.37
26	PJ	201	PEB	C1A-NA	-3.62	1.32	1.37
26	PJ	203	PEB	C1A-NA	-3.62	1.32	1.37
26	eA	201	PEB	C2A-C1A	-3.62	1.48	1.52
26	B4	203	PEB	C1A-NA	-3.62	1.32	1.37
26	WB	203	PEB	C1A-NA	-3.62	1.32	1.37
26	DG	203	PEB	C2C-C3C	3.62	1.48	1.37
26	p4	201	PEB	CHA-C1B	3.62	1.48	1.40
26	DI	1002	PEB	CHA-C1B	3.62	1.48	1.40
26	e7	202	PEB	C2C-C3C	3.62	1.48	1.37
26	YE	201	PEB	C2C-C3C	3.62	1.48	1.37
26	T4	203	PEB	CHA-C1B	3.62	1.48	1.40
26	jE	202	PEB	C2C-C3C	3.62	1.48	1.37
26	X1	201	PEB	CHA-C1B	3.62	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N9	204	PEB	CHA-C1B	3.62	1.48	1.40
26	xG	302	PEB	C1A-NA	-3.62	1.32	1.37
26	VJ	202	PEB	C1A-NA	-3.62	1.32	1.37
28	G2	1001	CYC	CHB-C4A	3.62	1.48	1.40
26	SA	201	PEB	C1A-NA	-3.62	1.32	1.37
26	WF	202	PEB	C1A-NA	-3.62	1.32	1.37
26	QG	203	PEB	C1A-NA	-3.62	1.32	1.37
26	PF	201	PEB	C2C-C3C	3.62	1.48	1.37
28	JH	1001	CYC	C3D-C2D	3.62	1.48	1.37
26	F3	203	PEB	C2A-C1A	-3.62	1.48	1.52
26	K8	202	PEB	CHA-C1B	3.61	1.48	1.40
26	h1	202	PEB	C1A-NA	-3.61	1.32	1.37
26	K6	201	PEB	C1A-NA	-3.61	1.32	1.37
26	21	404	PEB	CHA-C1B	3.61	1.48	1.40
26	S4	202	PEB	CHA-C1B	3.61	1.48	1.40
26	24	401	PEB	C2C-C3C	3.61	1.48	1.37
26	R4	201	PEB	C2A-C1A	-3.61	1.48	1.52
26	aB	202	PEB	CHA-C1B	3.61	1.48	1.40
26	GA	202	PEB	C2C-C3C	3.61	1.48	1.37
26	fA	201	PEB	C2C-C3C	3.61	1.48	1.37
26	V8	201	PEB	C1A-NA	-3.61	1.32	1.37
28	K2	1001	CYC	C1C-NC	-3.61	1.32	1.37
26	dI	202	PEB	CHA-C1B	3.61	1.48	1.40
26	F9	201	PEB	CHA-C1B	3.61	1.48	1.40
26	WD	202	PEB	CHA-C1B	3.61	1.48	1.40
26	a2	201	PEB	C2C-C3C	3.61	1.48	1.37
26	aB	202	PEB	C2C-C3C	3.61	1.48	1.37
26	S2	202	PEB	CHA-C1B	3.61	1.48	1.40
26	V3	203	PEB	CHA-C1B	3.61	1.48	1.40
26	14	201	PEB	CHA-C1B	3.61	1.48	1.40
26	S6	201	PEB	CHA-C1B	3.61	1.48	1.40
26	BA	301	PEB	CHA-C1B	3.61	1.48	1.40
26	S9	201	PEB	C2C-C3C	3.61	1.48	1.37
26	Q4	202	PEB	C2A-C1A	-3.61	1.48	1.52
28	DF	1001	CYC	C2C-C1C	-3.61	1.48	1.52
26	O8	203	PEB	C2A-C1A	-3.61	1.48	1.52
26	HC	201	PEB	C2A-C1A	-3.61	1.48	1.52
26	B5	202	PEB	C1A-NA	-3.61	1.32	1.37
26	P1	201	PEB	CHA-C1B	3.61	1.48	1.40
26	14	203	PEB	CHA-C1B	3.61	1.48	1.40
26	w1	203	PEB	C2C-C3C	3.61	1.48	1.37
26	E1	202	PEB	CHA-C1B	3.61	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	OA	202	PEB	CHA-C1B	3.61	1.48	1.40
26	m1	202	PEB	C1A-NA	-3.61	1.32	1.37
26	y1	201	PEB	CHA-C1B	3.61	1.48	1.40
26	G8	202	PEB	C2C-C3C	3.61	1.48	1.37
28	nH	1001	CYC	C3D-C2D	3.61	1.48	1.37
26	FE	202	PEB	CHA-C1B	3.61	1.48	1.40
26	J3	201	PEB	C2C-C3C	3.61	1.48	1.37
26	H4	203	PEB	C1A-NA	-3.61	1.32	1.37
26	mG	203	PEB	C1A-NA	-3.61	1.32	1.37
26	G1	202	PEB	CHA-C1B	3.61	1.48	1.40
26	kA	201	PEB	C2C-C3C	3.61	1.48	1.37
26	i7	201	PEB	CHA-C1B	3.61	1.48	1.40
26	Z2	202	PEB	CHA-C1B	3.61	1.48	1.40
26	B8	301	PEB	CHA-C1B	3.61	1.48	1.40
26	CG	201	PEB	CHA-C1B	3.61	1.48	1.40
26	ZE	202	PEB	C1A-NA	-3.61	1.32	1.37
26	T8	201	PEB	C2C-C3C	3.61	1.48	1.37
26	FA	201	PEB	C2C-C3C	3.61	1.48	1.37
26	FC	202	PEB	CHA-C1B	3.61	1.48	1.40
26	HD	203	PEB	CHA-C1B	3.61	1.48	1.40
26	DE	201	PEB	CHA-C1B	3.61	1.48	1.40
28	CH	1001	CYC	C3D-C2D	3.61	1.48	1.37
26	aA	203	PEB	C3C-C4C	3.61	1.47	1.42
26	RD	201	PEB	C2A-C1A	-3.61	1.48	1.52
26	AD	202	PEB	C1A-NA	-3.61	1.32	1.37
26	f4	201	PEB	C2C-C3C	3.61	1.48	1.37
26	H3	203	PEB	CHA-C1B	3.61	1.48	1.40
26	AC	202	PEB	CHA-C1B	3.61	1.48	1.40
26	HF	1002	PEB	CHA-C1B	3.61	1.48	1.40
26	R2	201	PEB	C2C-C3C	3.61	1.48	1.37
26	j7	202	PEB	C1A-NA	-3.61	1.32	1.37
26	AA	302	PEB	C1A-NA	-3.61	1.32	1.37
26	YE	202	PEB	C1A-NA	-3.61	1.32	1.37
26	C1	202	PEB	C2C-C3C	3.61	1.48	1.37
26	W8	202	PEB	CHA-C1B	3.61	1.48	1.40
26	vE	202	PEB	CHA-C1B	3.60	1.48	1.40
26	NF	1002	PEB	CHA-C1B	3.60	1.48	1.40
26	AA	302	PEB	C2C-C3C	3.60	1.48	1.37
26	RI	201	PEB	C2C-C3C	3.60	1.48	1.37
26	C4	201	PEB	C1A-NA	-3.60	1.32	1.37
26	PA	202	PEB	C2C-C3C	3.60	1.48	1.37
26	YG	202	PEB	CHA-C1B	3.60	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AC	201	PEB	C2C-C3C	3.60	1.48	1.37
26	PI	201	PEB	C1A-NA	-3.60	1.32	1.37
26	h4	202	PEB	CHA-C1B	3.60	1.48	1.40
26	R1	202	PEB	CHA-C1B	3.60	1.48	1.40
26	fl	202	PEB	CHA-C1B	3.60	1.48	1.40
26	F8	201	PEB	C2C-C3C	3.60	1.48	1.37
26	qG	203	PEB	OD-C4D	3.60	1.30	1.23
26	KE	203	PEB	C1A-NA	-3.60	1.32	1.37
26	K8	202	PEB	C3C-C4C	3.60	1.47	1.42
26	R8	201	PEB	C2C-C3C	3.60	1.48	1.37
26	mG	203	PEB	C2C-C3C	3.60	1.48	1.37
26	P7	201	PEB	C1A-NA	-3.60	1.32	1.37
26	cB	202	PEB	CHA-C1B	3.60	1.48	1.40
27	A9	302	PUB	C3B-C2B	3.60	1.48	1.37
26	cB	201	PEB	CHA-C1B	3.60	1.48	1.40
26	CD	201	PEB	C1A-NA	-3.60	1.32	1.37
26	C1	201	PEB	C2C-C3C	3.60	1.48	1.37
26	xE	304	PEB	C2C-C3C	3.60	1.48	1.37
26	I5	202	PEB	C1A-NA	-3.60	1.32	1.37
26	Z8	201	PEB	CHA-C1B	3.60	1.48	1.40
26	R7	201	PEB	C2C-C3C	3.60	1.48	1.37
26	a7	202	PEB	C2C-C3C	3.60	1.48	1.37
26	kG	202	PEB	C2C-C3C	3.60	1.48	1.37
26	XA	201	PEB	C2C-C3C	3.60	1.48	1.37
26	DD	203	PEB	C1A-NA	-3.60	1.32	1.37
26	wG	301	PEB	C1A-NA	-3.60	1.32	1.37
26	RA	201	PEB	C2C-C3C	3.60	1.48	1.37
26	XA	201	PEB	C2A-C1A	-3.60	1.48	1.52
26	E4	202	PEB	CHA-C1B	3.60	1.48	1.40
26	DG	203	PEB	CHA-C1B	3.60	1.48	1.40
26	P9	203	PEB	C2C-C3C	3.60	1.48	1.37
26	FE	201	PEB	C2C-C3C	3.60	1.48	1.37
26	dI	202	PEB	C2C-C3C	3.60	1.48	1.37
26	N1	202	PEB	C1A-NA	-3.60	1.32	1.37
26	t4	202	PEB	C1A-NA	-3.60	1.32	1.37
26	mB	202	PEB	C1A-NA	-3.60	1.32	1.37
26	KA	202	PEB	C3C-C4C	3.60	1.47	1.42
26	P8	202	PEB	C2C-C3C	3.59	1.48	1.37
26	GJ	201	PEB	C2C-C3C	3.59	1.48	1.37
26	TI	201	PEB	CHA-C1B	3.59	1.48	1.40
26	LJ	202	PEB	CHA-C1B	3.59	1.48	1.40
26	h6	201	PEB	C1A-NA	-3.59	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X1	203	PEB	C1A-NA	-3.59	1.33	1.37
26	dB	202	PEB	C1A-NA	-3.59	1.33	1.37
26	D9	202	PEB	CHA-C1B	3.59	1.48	1.40
26	b2	202	PEB	CHA-C1B	3.59	1.48	1.40
26	e6	201	PEB	CHA-C1B	3.59	1.48	1.40
26	E1	201	PEB	C1A-NA	-3.59	1.33	1.37
26	i6	201	PEB	C1A-NA	-3.59	1.33	1.37
26	P7	202	PEB	C1A-NA	-3.59	1.33	1.37
26	b4	501	PEB	C2C-C3C	3.59	1.48	1.37
28	mH	1001	CYC	C3D-C2D	3.59	1.48	1.37
26	h4	201	PEB	CHA-C1B	3.59	1.48	1.40
26	K9	201	PEB	CHA-C1B	3.59	1.48	1.40
26	eI	201	PEB	C1A-NA	-3.59	1.33	1.37
26	b6	202	PEB	CHA-C1B	3.59	1.48	1.40
26	I1	202	PEB	CHA-C1B	3.59	1.48	1.40
26	g8	202	PEB	CHA-C1B	3.59	1.48	1.40
26	RJ	201	PEB	C2C-C3C	3.59	1.48	1.37
26	xE	303	PEB	C1A-NA	-3.59	1.33	1.37
28	J7	1001	CYC	C1C-NC	-3.59	1.33	1.37
26	g6	202	PEB	CHA-C1B	3.59	1.48	1.40
26	R9	202	PEB	CHA-C1B	3.59	1.48	1.40
26	JE	201	PEB	C2A-C1A	-3.59	1.48	1.52
26	N1	203	PEB	C1A-NA	-3.59	1.33	1.37
26	M4	403	PEB	C1A-NA	-3.59	1.33	1.37
26	VD	203	PEB	CHA-C1B	3.59	1.48	1.40
26	kE	201	PEB	CHA-C1B	3.59	1.48	1.40
26	RJ	202	PEB	CHA-C1B	3.59	1.48	1.40
26	eG	203	PEB	OD-C4D	3.59	1.30	1.23
26	U6	202	PEB	CHA-C1B	3.59	1.48	1.40
26	D3	201	PEB	C2C-C3C	3.59	1.48	1.37
26	V4	201	PEB	C2C-C3C	3.59	1.48	1.37
26	14	202	PEB	C2C-C3C	3.59	1.48	1.37
26	PJ	202	PEB	C2A-C1A	-3.59	1.48	1.52
26	P7	201	PEB	CHA-C1B	3.59	1.48	1.40
26	YI	202	PEB	CHA-C1B	3.59	1.48	1.40
26	gB	202	PEB	C2C-C3C	3.59	1.48	1.37
27	A2	302	PUB	C3B-C2B	3.59	1.48	1.37
26	dG	202	PEB	C2A-C1A	-3.59	1.48	1.52
26	eE	203	PEB	C1A-NA	-3.59	1.33	1.37
26	TG	202	PEB	CHA-C1B	3.59	1.48	1.40
26	k7	201	PEB	C2C-C3C	3.59	1.48	1.37
26	j1	201	PEB	CHA-C1B	3.59	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	xE	303	PEB	C2C-C3C	3.59	1.48	1.37
26	N1	203	PEB	CHA-C1B	3.58	1.48	1.40
26	N4	203	PEB	C2A-C1A	-3.58	1.48	1.52
26	s1	201	PEB	C2C-C3C	3.58	1.48	1.37
26	hG	202	PEB	C2C-C3C	3.58	1.48	1.37
26	w4	204	PEB	C1A-NA	-3.58	1.33	1.37
26	V9	202	PEB	C1A-NA	-3.58	1.33	1.37
26	a8	203	PEB	C3C-C4C	3.58	1.47	1.42
26	f7	202	PEB	C2C-C3C	3.58	1.48	1.37
26	hI	202	PEB	C2C-C3C	3.58	1.48	1.37
26	E1	201	PEB	CHA-C1B	3.58	1.48	1.40
26	P1	203	PEB	C1A-NA	-3.58	1.33	1.37
26	U6	202	PEB	C2C-C3C	3.58	1.48	1.37
26	21	401	PEB	C2C-C3C	3.58	1.48	1.37
26	I4	201	PEB	C2C-C3C	3.58	1.48	1.37
26	FF	1002	PEB	C1A-NA	-3.58	1.33	1.37
28	G7	1001	CYC	C1C-NC	-3.58	1.33	1.37
26	VF	202	PEB	CHA-C1B	3.58	1.48	1.40
26	YG	201	PEB	CHA-C1B	3.58	1.48	1.40
26	l8	202	PEB	C2A-C1A	-3.58	1.48	1.52
27	K3	203	PUB	C3B-C2B	3.58	1.48	1.37
26	L9	203	PEB	C1A-NA	-3.58	1.33	1.37
26	VA	201	PEB	C1A-NA	-3.58	1.33	1.37
26	cA	202	PEB	C1A-NA	-3.58	1.33	1.37
26	MG	202	PEB	C1A-NA	-3.58	1.33	1.37
26	yG	301	PEB	C1A-NA	-3.58	1.33	1.37
26	m8	201	PEB	CHA-C1B	3.58	1.48	1.40
26	b1	501	PEB	C2C-C3C	3.58	1.48	1.37
26	f1	202	PEB	C2C-C3C	3.58	1.48	1.37
26	T1	201	PEB	C1A-NA	-3.58	1.33	1.37
26	V1	202	PEB	C1A-NA	-3.58	1.33	1.37
26	hA	203	PEB	CHA-C1B	3.58	1.48	1.40
26	Q1	202	PEB	C2A-C1A	-3.58	1.48	1.52
28	F6	1001	CYC	C2C-C1C	-3.58	1.48	1.52
26	R4	202	PEB	C1A-NA	-3.58	1.33	1.37
28	K7	1001	CYC	C1C-NC	-3.58	1.33	1.37
26	C5	203	PEB	CHA-C1B	3.58	1.48	1.40
26	cI	203	PEB	C1A-NA	-3.58	1.33	1.37
26	lB	202	PEB	C2C-C3C	3.58	1.48	1.37
26	j8	201	PEB	C2C-C3C	3.58	1.48	1.37
26	UF	202	PEB	C2C-C3C	3.58	1.48	1.37
26	XJ	203	PEB	C2C-C3C	3.58	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T2	202	PEB	CHA-C1B	3.58	1.48	1.40
26	XG	202	PEB	CHA-C1B	3.58	1.48	1.40
26	V1	201	PEB	C2C-C3C	3.58	1.48	1.37
26	m2	201	PEB	C1A-NA	-3.58	1.33	1.37
26	O4	202	PEB	C1A-NA	-3.58	1.33	1.37
26	EA	201	PEB	C1A-NA	-3.58	1.33	1.37
26	J9	201	PEB	CHA-C1B	3.58	1.48	1.40
26	i1	203	PEB	C2C-C3C	3.58	1.48	1.37
26	I9	201	PEB	C2A-C1A	-3.58	1.48	1.52
26	d6	203	PEB	C1A-NA	-3.58	1.33	1.37
26	Y9	202	PEB	C1A-NA	-3.58	1.33	1.37
26	aG	201	PEB	C1A-NA	-3.58	1.33	1.37
26	cI	202	PEB	C1A-NA	-3.58	1.33	1.37
26	l6	202	PEB	C2C-C3C	3.58	1.48	1.37
26	TE	202	PEB	C2C-C3C	3.58	1.48	1.37
26	T1	202	PEB	CHA-C1B	3.58	1.48	1.40
26	EA	202	PEB	C2C-C3C	3.58	1.48	1.37
26	oG	201	PEB	C2C-C3C	3.58	1.48	1.37
26	P6	202	PEB	C1A-NA	-3.58	1.33	1.37
26	FD	203	PEB	CHA-C1B	3.58	1.48	1.40
26	PI	202	PEB	CHA-C1B	3.58	1.48	1.40
28	L7	1001	CYC	C2C-C1C	-3.57	1.48	1.52
26	E1	201	PEB	C2C-C3C	3.57	1.48	1.37
26	j2	202	PEB	CHA-C1B	3.57	1.48	1.40
26	rE	201	PEB	CHA-C1B	3.57	1.48	1.40
26	f1	201	PEB	C2C-C3C	3.57	1.48	1.37
26	c2	202	PEB	C1A-NA	-3.57	1.33	1.37
26	xE	302	PEB	C1A-NA	-3.57	1.33	1.37
26	qG	202	PEB	C1A-NA	-3.57	1.33	1.37
26	G9	201	PEB	C2C-C3C	3.57	1.48	1.37
26	SB	201	PEB	CHA-C1B	3.57	1.48	1.40
26	T4	203	PEB	C2C-C3C	3.57	1.48	1.37
26	AE	202	PEB	C1A-NA	-3.57	1.33	1.37
26	mE	203	PEB	C1A-NA	-3.57	1.33	1.37
26	a6	202	PEB	C2C-C3C	3.57	1.48	1.37
26	UB	202	PEB	C2C-C3C	3.57	1.48	1.37
26	J3	201	PEB	CHA-C1B	3.57	1.48	1.40
26	C5	201	PEB	CHA-C1B	3.57	1.48	1.40
26	bI	202	PEB	CHA-C1B	3.57	1.48	1.40
26	DD	201	PEB	C2C-C3C	3.57	1.48	1.37
26	T1	203	PEB	C1A-NA	-3.57	1.33	1.37
26	ED	202	PEB	C2C-C3C	3.57	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O8	202	PEB	CHA-C1B	3.57	1.48	1.40
26	OE	203	PEB	CHA-C1B	3.57	1.48	1.40
26	h1	201	PEB	C2C-C3C	3.57	1.48	1.37
26	CE	201	PEB	CHA-C1B	3.57	1.48	1.40
26	Y3	303	PEB	C1A-NA	-3.57	1.33	1.37
26	UD	202	PEB	C1A-NA	-3.57	1.33	1.37
26	xG	303	PEB	C1A-NA	-3.57	1.33	1.37
26	WG	202	PEB	C2C-C3C	3.57	1.48	1.37
28	JH	1001	CYC	C2C-C1C	-3.57	1.48	1.52
26	l6	203	PEB	C1A-NA	-3.57	1.33	1.37
26	NE	202	PEB	C1A-NA	-3.57	1.33	1.37
26	cB	202	PEB	C2C-C3C	3.57	1.48	1.37
26	h6	202	PEB	CHA-C1B	3.57	1.48	1.40
26	W7	201	PEB	C2C-C3C	3.57	1.48	1.37
26	H4	201	PEB	CHA-C1B	3.57	1.48	1.40
26	B4	201	PEB	C1A-NA	-3.57	1.33	1.37
26	wG	302	PEB	C2C-C3C	3.57	1.48	1.37
26	VD	203	PEB	C1A-NA	-3.57	1.33	1.37
28	1H	1000	CYC	C1C-NC	-3.57	1.33	1.37
26	R9	201	PEB	C2C-C3C	3.57	1.48	1.37
26	FG	201	PEB	C2C-C3C	3.57	1.48	1.37
26	o1	501	PEB	CHA-C1B	3.57	1.48	1.40
26	A8	302	PEB	C2C-C3C	3.57	1.48	1.37
26	W7	202	PEB	C1A-NA	-3.57	1.33	1.37
26	Y2	202	PEB	CHA-C1B	3.57	1.48	1.40
28	YH	1002	CYC	C3D-C2D	3.57	1.48	1.37
26	B4	202	PEB	C1A-NA	-3.57	1.33	1.37
26	YI	201	PEB	CHA-C1B	3.57	1.48	1.40
26	i7	201	PEB	C2C-C3C	3.57	1.48	1.37
26	AD	201	PEB	C1A-NA	-3.57	1.33	1.37
28	K6	202	CYC	C2C-C1C	-3.57	1.48	1.52
26	T2	201	PEB	CHA-C1B	3.57	1.48	1.40
26	a4	203	PEB	CHA-C1B	3.57	1.48	1.40
26	u4	201	PEB	C1A-NA	-3.57	1.33	1.37
26	P9	202	PEB	C2C-C3C	3.57	1.48	1.37
26	I1	201	PEB	C2C-C3C	3.56	1.48	1.37
28	LB	1001	CYC	C3D-C2D	3.56	1.48	1.37
26	jI	202	PEB	CHA-C1B	3.56	1.48	1.40
28	J2	1001	CYC	CHB-C4A	3.56	1.48	1.40
26	n4	201	PEB	C2C-C3C	3.56	1.48	1.37
26	ZF	203	PEB	C2C-C3C	3.56	1.48	1.37
26	I3	202	PEB	C2C-C3C	3.56	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UB	202	PEB	CHA-C1B	3.56	1.48	1.40
26	dB	201	PEB	CHA-C1B	3.56	1.48	1.40
26	LA	201	PEB	C1A-NA	-3.56	1.33	1.37
26	gG	203	PEB	C1A-NA	-3.56	1.33	1.37
26	VJ	203	PEB	C1A-NA	-3.56	1.33	1.37
26	wG	303	PEB	C2C-C3C	3.56	1.48	1.37
26	AB	304	PEB	CHA-C1B	3.56	1.48	1.40
26	P2	201	PEB	C1A-NA	-3.56	1.33	1.37
26	M4	402	PEB	C1A-NA	-3.56	1.33	1.37
26	g6	201	PEB	C1A-NA	-3.56	1.33	1.37
26	cE	201	PEB	C1A-NA	-3.56	1.33	1.37
26	MG	203	PEB	C1A-NA	-3.56	1.33	1.37
26	cI	201	PEB	C1A-NA	-3.56	1.33	1.37
26	U6	203	PEB	CHA-C1B	3.56	1.48	1.40
26	VJ	202	PEB	C2C-C3C	3.56	1.48	1.37
26	D2	1002	PEB	C1A-NA	-3.56	1.33	1.37
26	s4	203	PEB	C2C-C3C	3.56	1.48	1.37
26	Q9	202	PEB	C2C-C3C	3.56	1.48	1.37
26	e1	202	PEB	CHA-C1B	3.56	1.48	1.40
26	c6	202	PEB	C2C-C3C	3.56	1.48	1.37
26	c7	201	PEB	C1A-NA	-3.56	1.33	1.37
28	KF	1001	CYC	C1C-NC	-3.56	1.33	1.37
26	hB	201	PEB	CHA-C1B	3.56	1.48	1.40
26	fE	202	PEB	CHA-C1B	3.56	1.48	1.40
26	wE	302	PEB	C2C-C3C	3.56	1.48	1.37
26	i2	203	PEB	C2C-C3C	3.56	1.48	1.37
26	b1	501	PEB	CHA-C1B	3.56	1.48	1.40
26	PF	201	PEB	CHA-C1B	3.56	1.48	1.40
26	U7	201	PEB	C1A-NA	-3.56	1.33	1.37
26	L8	201	PEB	C1A-NA	-3.56	1.33	1.37
26	OB	202	PEB	C1A-NA	-3.56	1.33	1.37
26	CA	202	PEB	C2C-C3C	3.56	1.48	1.37
26	X4	201	PEB	C2A-C1A	-3.56	1.48	1.52
26	UD	201	PEB	C2A-C1A	-3.56	1.48	1.52
26	b4	501	PEB	CHA-C1B	3.56	1.48	1.40
26	HD	203	PEB	C4B-C3B	3.56	1.51	1.45
26	I4	202	PEB	CHA-C1B	3.56	1.48	1.40
26	hI	202	PEB	CHA-C1B	3.56	1.48	1.40
26	S7	201	PEB	C1A-NA	-3.56	1.33	1.37
26	N4	203	PEB	CHA-C1B	3.56	1.48	1.40
26	W6	202	PEB	CHA-C1B	3.56	1.48	1.40
26	WE	203	PEB	CHA-C1B	3.56	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	e7	201	PEB	C2C-C3C	3.56	1.48	1.37
26	Y9	202	PEB	C2C-C3C	3.56	1.48	1.37
26	OI	202	PEB	C2C-C3C	3.56	1.48	1.37
26	K5	202	PEB	C1A-NA	-3.56	1.33	1.37
26	P9	201	PEB	C1A-NA	-3.56	1.33	1.37
26	sG	201	PEB	C2C-C3C	3.56	1.48	1.37
26	TI	202	PEB	CHA-C1B	3.56	1.48	1.40
28	HB	1001	CYC	CHB-C4A	3.56	1.48	1.40
26	R7	201	PEB	CHA-C1B	3.56	1.48	1.40
26	b7	202	PEB	CHA-C1B	3.56	1.48	1.40
26	X9	202	PEB	C2C-C3C	3.56	1.48	1.37
26	mI	201	PEB	C2C-C3C	3.56	1.48	1.37
26	d4	202	PEB	C1A-NA	-3.56	1.33	1.37
26	OF	201	PEB	C1A-NA	-3.56	1.33	1.37
26	FG	202	PEB	C2A-C1A	-3.56	1.48	1.52
26	U9	201	PEB	C1A-NA	-3.56	1.33	1.37
26	SI	201	PEB	CHA-C1B	3.56	1.48	1.40
26	YI	203	PEB	CHA-C1B	3.56	1.48	1.40
26	TD	201	PEB	C2C-C3C	3.56	1.48	1.37
26	h7	203	PEB	CHA-C1B	3.56	1.48	1.40
26	SJ	201	PEB	C1A-NA	-3.56	1.33	1.37
28	F6	1001	CYC	CHB-C4A	3.56	1.48	1.40
26	iI	203	PEB	C2C-C3C	3.56	1.48	1.37
26	N6	201	PEB	C1A-NA	-3.56	1.33	1.37
26	VF	201	PEB	C1A-NA	-3.56	1.33	1.37
26	FC	201	PEB	CHA-C1B	3.56	1.48	1.40
27	QA	201	PUB	OD-C4D	3.55	1.30	1.23
26	m6	201	PEB	C1A-NA	-3.55	1.33	1.37
28	MH	1001	CYC	C3D-C2D	3.55	1.48	1.37
26	aE	203	PEB	C1A-NA	-3.55	1.33	1.37
26	ZF	203	PEB	C1A-NA	-3.55	1.33	1.37
26	cG	201	PEB	C1A-NA	-3.55	1.33	1.37
28	J7	1003	CYC	C1C-NC	-3.55	1.33	1.37
26	JE	202	PEB	C2C-C3C	3.55	1.48	1.37
26	wE	302	PEB	CHA-C1B	3.55	1.48	1.40
26	fB	202	PEB	C2C-C3C	3.55	1.48	1.37
26	H2	1002	PEB	C1A-NA	-3.55	1.33	1.37
26	E8	201	PEB	C1A-NA	-3.55	1.33	1.37
26	NB	1002	PEB	C1A-NA	-3.55	1.33	1.37
26	e4	201	PEB	CHA-C1B	3.55	1.48	1.40
26	H1	201	PEB	C1A-NA	-3.55	1.33	1.37
26	aB	202	PEB	C1A-NA	-3.55	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k2	203	PEB	C2C-C3C	3.55	1.48	1.37
26	24	404	PEB	C2C-C3C	3.55	1.48	1.37
26	ID	202	PEB	C2C-C3C	3.55	1.48	1.37
26	d6	202	PEB	C1A-NA	-3.55	1.33	1.37
26	BE	202	PEB	C1A-NA	-3.55	1.33	1.37
26	JD	203	PEB	CHA-C1B	3.55	1.48	1.40
26	P7	201	PEB	C2C-C3C	3.55	1.48	1.37
26	c2	201	PEB	CHA-C1B	3.55	1.48	1.40
26	YJ	201	PEB	C2C-C3C	3.55	1.48	1.37
26	O6	202	PEB	CHA-C1B	3.55	1.48	1.40
26	U7	202	PEB	C2C-C3C	3.55	1.48	1.37
26	b7	203	PEB	C1A-NA	-3.55	1.33	1.37
26	OE	203	PEB	C1A-NA	-3.55	1.33	1.37
26	D2	1002	PEB	CHA-C1B	3.55	1.48	1.40
26	KB	201	PEB	CHA-C1B	3.55	1.48	1.40
26	y1	203	PEB	C2C-C3C	3.55	1.48	1.37
26	Z7	203	PEB	C2C-C3C	3.55	1.48	1.37
26	u1	203	PEB	C1A-NA	-3.55	1.33	1.37
26	PB	201	PEB	CHA-C1B	3.55	1.48	1.40
26	GC	202	PEB	C2C-C3C	3.55	1.48	1.37
26	eF	202	PEB	C2C-C3C	3.55	1.48	1.37
28	EB	1001	CYC	C3D-C2D	3.55	1.48	1.37
26	e1	201	PEB	CHA-C1B	3.55	1.48	1.40
26	IE	201	PEB	CHA-C1B	3.55	1.48	1.40
26	W3	202	PEB	C1A-NA	-3.55	1.33	1.37
26	KB	201	PEB	C1A-NA	-3.55	1.33	1.37
26	J1	203	PEB	C2C-C3C	3.55	1.48	1.37
26	X8	201	PEB	C2C-C3C	3.55	1.48	1.37
26	C9	201	PEB	C2C-C3C	3.55	1.48	1.37
26	EA	203	PEB	CHA-C1B	3.55	1.48	1.40
26	T7	201	PEB	C1A-NA	-3.55	1.33	1.37
26	gB	201	PEB	C1A-NA	-3.55	1.33	1.37
26	EG	202	PEB	C1A-NA	-3.55	1.33	1.37
26	AJ	303	PEB	C1A-NA	-3.55	1.33	1.37
26	dF	203	PEB	C2C-C3C	3.55	1.48	1.37
26	CC	202	PEB	CHA-C1B	3.55	1.48	1.40
26	AB	304	PEB	C2C-C3C	3.55	1.48	1.37
26	H3	201	PEB	C1A-NA	-3.55	1.33	1.37
26	ED	202	PEB	C1A-NA	-3.55	1.33	1.37
26	W3	202	PEB	CHA-C1B	3.54	1.48	1.40
26	YJ	202	PEB	C2C-C3C	3.54	1.48	1.37
26	Q2	202	PEB	CHA-C1B	3.54	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	mB	201	PEB	C1A-NA	-3.54	1.33	1.37
26	AG	201	PEB	C1A-NA	-3.54	1.33	1.37
28	dH	1001	CYC	C3D-C2D	3.54	1.48	1.37
26	W6	201	PEB	CHA-C1B	3.54	1.48	1.40
26	M9	202	PEB	CHA-C1B	3.54	1.48	1.40
26	mA	201	PEB	CHA-C1B	3.54	1.48	1.40
26	VB	201	PEB	CHA-C1B	3.54	1.48	1.40
26	fF	202	PEB	CHA-C1B	3.54	1.48	1.40
26	GA	203	PEB	C1A-NA	-3.54	1.33	1.37
26	eD	401	PEB	C1A-NA	-3.54	1.33	1.37
26	PE	201	PEB	CHA-C1B	3.54	1.48	1.40
26	R1	201	PEB	C2A-C1A	-3.54	1.48	1.52
26	T4	201	PEB	C1A-NA	-3.54	1.33	1.37
26	Y2	201	PEB	CHA-C1B	3.54	1.48	1.40
26	GA	202	PEB	CHA-C1B	3.54	1.48	1.40
26	h8	203	PEB	CHA-C1B	3.54	1.48	1.40
26	d7	202	PEB	C2C-C3C	3.54	1.48	1.37
26	uG	202	PEB	C2C-C3C	3.54	1.48	1.37
26	g6	202	PEB	C1A-NA	-3.54	1.33	1.37
26	iA	202	PEB	C1A-NA	-3.54	1.33	1.37
26	DJ	202	PEB	CHA-C1B	3.54	1.48	1.40
26	K9	202	PEB	C2C-C3C	3.54	1.48	1.37
26	ZE	201	PEB	C2C-C3C	3.54	1.48	1.37
26	l4	201	PEB	CHA-C1B	3.54	1.48	1.40
26	21	401	PEB	CHA-C1B	3.54	1.48	1.40
26	E4	201	PEB	CHA-C1B	3.54	1.48	1.40
26	H5	203	PEB	CHA-C1B	3.54	1.48	1.40
26	uE	201	PEB	CHA-C1B	3.54	1.48	1.40
26	zE	501	PEB	CHA-C1B	3.54	1.48	1.40
26	qE	203	PEB	C1A-NA	-3.54	1.33	1.37
26	eI	202	PEB	C1A-NA	-3.54	1.33	1.37
26	TB	201	PEB	C2C-C3C	3.54	1.48	1.37
26	MJ	202	PEB	CHA-C1B	3.54	1.48	1.40
26	w4	202	PEB	C2C-C3C	3.54	1.48	1.37
26	PJ	203	PEB	CHA-C1B	3.54	1.48	1.40
28	FB	1001	CYC	CHB-C4A	3.54	1.48	1.40
26	c4	201	PEB	C1A-NA	-3.54	1.33	1.37
26	Q6	203	PEB	C1A-NA	-3.54	1.33	1.37
26	iI	201	PEB	C1A-NA	-3.54	1.33	1.37
26	bE	202	PEB	C2C-C3C	3.54	1.48	1.37
26	WB	201	PEB	CHA-C1B	3.54	1.48	1.40
26	P4	203	PEB	C2C-C3C	3.54	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	NJ	203	PEB	C2C-C3C	3.54	1.48	1.37
26	11	203	PEB	CHA-C1B	3.54	1.48	1.40
26	E8	203	PEB	CHA-C1B	3.54	1.48	1.40
26	kI	201	PEB	C2C-C3C	3.54	1.48	1.37
26	O6	202	PEB	C1A-NA	-3.54	1.33	1.37
26	21	405	PEB	C2C-C3C	3.54	1.48	1.37
26	P1	203	PEB	C2C-C3C	3.54	1.48	1.37
26	GJ	202	PEB	CHA-C1B	3.54	1.48	1.40
26	D3	201	PEB	C1A-NA	-3.54	1.33	1.37
26	c7	201	PEB	C2C-C3C	3.54	1.48	1.37
26	B1	203	PEB	CHA-C1B	3.54	1.48	1.40
26	UI	202	PEB	CHA-C1B	3.54	1.48	1.40
28	H6	1001	CYC	CHB-C4A	3.54	1.48	1.40
26	mE	203	PEB	C2C-C3C	3.54	1.48	1.37
26	SI	202	PEB	CHA-C1B	3.54	1.48	1.40
26	JI	1002	PEB	C1A-NA	-3.54	1.33	1.37
26	E8	202	PEB	C2C-C3C	3.54	1.48	1.37
26	h8	202	PEB	C2C-C3C	3.54	1.48	1.37
26	DB	1002	PEB	CHA-C1B	3.54	1.48	1.40
26	P9	203	PEB	C1A-NA	-3.54	1.33	1.37
26	a8	202	PEB	C2C-C3C	3.53	1.48	1.37
26	cA	201	PEB	C2C-C3C	3.53	1.48	1.37
27	A4	203	PUB	C3B-C2B	3.53	1.48	1.37
26	P6	201	PEB	CHA-C1B	3.53	1.48	1.40
26	cA	202	PEB	CHA-C1B	3.53	1.48	1.40
26	A3	202	PEB	C1A-NA	-3.53	1.33	1.37
26	V7	201	PEB	C1A-NA	-3.53	1.33	1.37
26	aE	202	PEB	C1A-NA	-3.53	1.33	1.37
26	k4	202	PEB	CHA-C1B	3.53	1.48	1.40
26	oG	203	PEB	C2C-C3C	3.53	1.48	1.37
26	OB	202	PEB	CHA-C1B	3.53	1.48	1.40
26	J2	1002	PEB	C1A-NA	-3.53	1.33	1.37
26	S2	202	PEB	C1A-NA	-3.53	1.33	1.37
26	DE	202	PEB	C1A-NA	-3.53	1.33	1.37
26	wE	301	PEB	C1A-NA	-3.53	1.33	1.37
26	lF	202	PEB	C1A-NA	-3.53	1.33	1.37
26	k4	203	PEB	CHA-C1B	3.53	1.48	1.40
26	a8	203	PEB	C2C-C3C	3.53	1.48	1.37
26	WG	203	PEB	C2C-C3C	3.53	1.48	1.37
26	S2	201	PEB	CHA-C1B	3.53	1.48	1.40
26	F7	1002	PEB	CHA-C1B	3.53	1.48	1.40
26	Y7	201	PEB	C2C-C3C	3.53	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U9	201	PEB	C2C-C3C	3.53	1.48	1.37
26	gF	202	PEB	C2C-C3C	3.53	1.48	1.37
26	c2	203	PEB	C1A-NA	-3.53	1.33	1.37
26	YB	202	PEB	CHA-C1B	3.53	1.48	1.40
26	TI	201	PEB	C1A-NA	-3.53	1.33	1.37
26	mE	202	PEB	C2C-C3C	3.53	1.48	1.37
28	jH	1001	CYC	C3D-C2D	3.53	1.48	1.37
28	MH	1001	CYC	C2C-C1C	-3.53	1.48	1.52
26	k2	201	PEB	C2C-C3C	3.53	1.48	1.37
26	m1	202	PEB	CHA-C1B	3.53	1.48	1.40
26	iB	201	PEB	C2C-C3C	3.53	1.48	1.37
26	m7	201	PEB	CHA-C1B	3.53	1.48	1.40
26	aA	202	PEB	C2C-C3C	3.53	1.48	1.37
26	dE	201	PEB	C2C-C3C	3.53	1.48	1.37
26	N4	203	PEB	C1A-NA	-3.53	1.33	1.37
26	JG	202	PEB	C1A-NA	-3.53	1.33	1.37
28	AH	1001	CYC	C1C-NC	-3.53	1.33	1.37
26	gB	202	PEB	CHA-C1B	3.53	1.48	1.40
26	AD	201	PEB	C2C-C3C	3.53	1.48	1.37
26	lE	201	PEB	C2C-C3C	3.53	1.48	1.37
26	BJ	202	PEB	CHA-C1B	3.53	1.48	1.40
26	g6	202	PEB	C2C-C3C	3.53	1.48	1.37
28	E6	1001	CYC	C3D-C2D	3.53	1.48	1.37
26	LD	201	PEB	C2A-C1A	-3.53	1.48	1.52
26	bF	202	PEB	CHA-C1B	3.53	1.48	1.40
26	L7	1002	PEB	C2C-C3C	3.53	1.48	1.37
26	gE	203	PEB	C1A-NA	-3.53	1.33	1.37
26	f7	201	PEB	C2C-C3C	3.53	1.48	1.37
26	bG	201	PEB	C2C-C3C	3.53	1.48	1.37
26	K6	201	PEB	CHA-C1B	3.53	1.48	1.40
26	YJ	202	PEB	CHA-C1B	3.53	1.48	1.40
28	H7	1001	CYC	C2C-C1C	-3.53	1.48	1.52
26	C8	202	PEB	C2C-C3C	3.53	1.48	1.37
26	ZG	202	PEB	C1A-NA	-3.53	1.33	1.37
26	C1	202	PEB	CHA-C1B	3.53	1.48	1.40
26	xE	303	PEB	CHA-C1B	3.53	1.48	1.40
26	q1	203	PEB	C2C-C3C	3.53	1.48	1.37
28	B6	1002	CYC	C1B-NB	-3.53	1.31	1.37
26	S4	201	PEB	C2A-C1A	-3.53	1.48	1.52
26	T3	201	PEB	C2C-C3C	3.53	1.48	1.37
26	eF	201	PEB	C2C-C3C	3.53	1.48	1.37
26	u1	202	PEB	C1A-NA	-3.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UB	202	PEB	C1A-NA	-3.52	1.33	1.37
26	fB	201	PEB	C2C-C3C	3.52	1.48	1.37
26	IJ	201	PEB	C2C-C3C	3.52	1.48	1.37
26	A1	202	PEB	C1A-NA	-3.52	1.33	1.37
26	jF	201	PEB	C1A-NA	-3.52	1.33	1.37
26	O2	202	PEB	C2C-C3C	3.52	1.48	1.37
26	CA	201	PEB	C2C-C3C	3.52	1.48	1.37
26	OE	203	PEB	C2C-C3C	3.52	1.48	1.37
26	B4	203	PEB	CHA-C1B	3.52	1.48	1.40
26	AJ	305	PEB	C1A-NA	-3.52	1.33	1.37
26	l2	202	PEB	CHA-C1B	3.52	1.48	1.40
26	VE	202	PEB	C2C-C3C	3.52	1.48	1.37
26	YG	202	PEB	C2C-C3C	3.52	1.48	1.37
26	AI	304	PEB	C2C-C3C	3.52	1.48	1.37
26	gB	202	PEB	C1A-NA	-3.52	1.33	1.37
26	T9	202	PEB	C2C-C3C	3.52	1.48	1.37
26	QB	202	PEB	CHA-C1B	3.52	1.48	1.40
26	lA	201	PEB	CHA-C1B	3.52	1.48	1.40
26	G9	202	PEB	CHA-C1B	3.52	1.48	1.40
26	PI	201	PEB	C2C-C3C	3.52	1.48	1.37
26	fA	202	PEB	C2C-C3C	3.52	1.48	1.37
26	m2	201	PEB	C2C-C3C	3.52	1.48	1.37
26	b7	203	PEB	CHA-C1B	3.52	1.48	1.40
26	CE	202	PEB	C2C-C3C	3.52	1.48	1.37
26	yE	301	PEB	C1A-NA	-3.52	1.33	1.37
26	SI	202	PEB	C1A-NA	-3.52	1.33	1.37
26	f7	201	PEB	CHA-C1B	3.52	1.48	1.40
26	I1	202	PEB	C2C-C3C	3.52	1.48	1.37
28	G7	1001	CYC	C3D-C2D	3.52	1.48	1.37
26	mI	202	PEB	CHA-C1B	3.52	1.48	1.40
26	V3	203	PEB	C1A-NA	-3.52	1.33	1.37
26	c8	201	PEB	C2C-C3C	3.52	1.48	1.37
26	FD	203	PEB	C2C-C3C	3.52	1.48	1.37
26	d7	203	PEB	CHA-C1B	3.52	1.48	1.40
26	A7	302	PEB	C2C-C3C	3.52	1.48	1.37
26	jA	201	PEB	C2C-C3C	3.52	1.48	1.37
26	aE	202	PEB	C3B-C2B	3.52	1.44	1.36
26	aE	201	PEB	C1A-NA	-3.52	1.33	1.37
26	P2	201	PEB	C2C-C3C	3.52	1.48	1.37
26	B5	201	PEB	C2C-C3C	3.52	1.48	1.37
26	WJ	201	PEB	C2C-C3C	3.52	1.48	1.37
26	e6	201	PEB	C2C-C3C	3.52	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	VH	1001	CYC	C1C-NC	-3.52	1.33	1.37
26	YE	202	PEB	C2C-C3C	3.52	1.48	1.37
28	DF	1003	CYC	C3D-C2D	3.52	1.48	1.37
26	q1	201	PEB	C1A-NA	-3.52	1.33	1.37
26	w4	203	PEB	C2C-C3C	3.52	1.48	1.37
26	M3	202	PEB	C2C-C3C	3.52	1.48	1.37
27	A8	303	PUB	C3B-C2B	3.52	1.48	1.37
28	TH	1001	CYC	C3D-C2D	3.52	1.48	1.37
26	gB	201	PEB	CHA-C1B	3.52	1.48	1.40
26	wG	302	PEB	CHA-C1B	3.52	1.48	1.40
26	Q9	201	PEB	C2C-C3C	3.52	1.48	1.37
26	g2	201	PEB	C1A-NA	-3.51	1.33	1.37
26	eE	201	PEB	C1A-NA	-3.51	1.33	1.37
26	OF	203	PEB	C1A-NA	-3.51	1.33	1.37
26	P2	202	PEB	CHA-C1B	3.51	1.48	1.40
26	C4	202	PEB	C2C-C3C	3.51	1.48	1.37
26	B3	202	PEB	CHA-C1B	3.51	1.48	1.40
26	V6	201	PEB	CHA-C1B	3.51	1.48	1.40
26	DG	201	PEB	CHA-C1B	3.51	1.48	1.40
26	hB	201	PEB	C1A-NA	-3.51	1.33	1.37
26	SF	202	PEB	C1A-NA	-3.51	1.33	1.37
26	wE	303	PEB	C2C-C3C	3.51	1.48	1.37
26	CG	202	PEB	C2C-C3C	3.51	1.48	1.37
26	fG	202	PEB	C2C-C3C	3.51	1.48	1.37
26	h8	201	PEB	CHA-C1B	3.51	1.48	1.40
26	RE	202	PEB	CHA-C1B	3.51	1.48	1.40
26	dF	202	PEB	CHA-C1B	3.51	1.48	1.40
26	p1	201	PEB	C1A-NA	-3.51	1.33	1.37
26	M8	203	PEB	C1A-NA	-3.51	1.33	1.37
26	w4	201	PEB	C2C-C3C	3.51	1.48	1.37
26	Q2	202	PEB	C2C-C3C	3.51	1.48	1.37
26	d8	201	PEB	C1A-NA	-3.51	1.33	1.37
26	EA	202	PEB	C1A-NA	-3.51	1.33	1.37
26	lB	203	PEB	C1A-NA	-3.51	1.33	1.37
26	gI	201	PEB	C1A-NA	-3.51	1.33	1.37
26	F2	1002	PEB	CHA-C1B	3.51	1.48	1.40
26	YD	304	PEB	CHA-C1B	3.51	1.48	1.40
26	FF	1002	PEB	CHA-C1B	3.51	1.48	1.40
26	U6	202	PEB	C1A-NA	-3.51	1.33	1.37
26	QE	202	PEB	C2C-C3C	3.51	1.48	1.37
26	IA	202	PEB	C1A-NA	-3.51	1.33	1.37
26	qE	201	PEB	CHA-C1B	3.51	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R4	202	PEB	CHA-C1B	3.51	1.48	1.40
26	Y2	201	PEB	C2C-C3C	3.51	1.48	1.37
26	A5	202	PEB	C2C-C3C	3.51	1.48	1.37
26	f8	201	PEB	CHA-C1B	3.51	1.48	1.40
26	11	203	PEB	C2C-C3C	3.51	1.48	1.37
28	LH	1001	CYC	C3D-C2D	3.51	1.48	1.37
28	qH	1001	CYC	C3D-C2D	3.51	1.48	1.37
26	J2	1002	PEB	CHA-C1B	3.51	1.48	1.40
26	LB	1002	PEB	CHA-C1B	3.51	1.48	1.40
26	mA	201	PEB	C2C-C3C	3.51	1.48	1.37
26	F7	1002	PEB	C1A-NA	-3.51	1.33	1.37
26	dI	202	PEB	C1A-NA	-3.51	1.33	1.37
26	G5	202	PEB	C2C-C3C	3.51	1.48	1.37
26	a8	202	PEB	CHA-C1B	3.51	1.48	1.40
26	UB	201	PEB	C1A-NA	-3.51	1.33	1.37
26	GC	202	PEB	C1A-NA	-3.51	1.33	1.37
28	GI	1001	CYC	C1C-NC	-3.51	1.33	1.37
26	X9	203	PEB	C2C-C3C	3.51	1.48	1.37
26	i2	201	PEB	C1A-NA	-3.51	1.33	1.37
26	UJ	201	PEB	C2C-C3C	3.51	1.48	1.37
26	O6	202	PEB	C2C-C3C	3.51	1.48	1.37
26	YI	201	PEB	C2C-C3C	3.51	1.48	1.37
26	A2	305	PEB	C2C-C3C	3.51	1.48	1.37
26	d4	203	PEB	C2C-C3C	3.51	1.48	1.37
26	d2	202	PEB	C1A-NA	-3.51	1.33	1.37
26	D4	201	PEB	C1A-NA	-3.51	1.33	1.37
26	O9	201	PEB	C1A-NA	-3.51	1.33	1.37
26	m2	202	PEB	CHA-C1B	3.51	1.48	1.40
26	jF	202	PEB	C2C-C3C	3.51	1.48	1.37
28	DF	1003	CYC	CHB-C4A	3.51	1.48	1.40
28	G2	1001	CYC	C3D-C2D	3.51	1.48	1.37
26	x1	201	PEB	C1A-NA	-3.51	1.33	1.37
26	F3	203	PEB	C1A-NA	-3.51	1.33	1.37
26	14	203	PEB	C2C-C3C	3.51	1.48	1.37
28	gH	1001	CYC	C3D-C2D	3.51	1.48	1.37
26	UB	203	PEB	CHA-C1B	3.51	1.48	1.40
26	O7	202	PEB	C2C-C3C	3.51	1.48	1.37
26	C4	202	PEB	CHA-C1B	3.51	1.48	1.40
28	G7	1001	CYC	CHB-C4A	3.51	1.48	1.40
26	cF	201	PEB	C2C-C3C	3.50	1.48	1.37
26	dG	201	PEB	C2C-C3C	3.50	1.48	1.37
26	AG	202	PEB	C1A-NA	-3.50	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PI	203	PEB	C1A-NA	-3.50	1.33	1.37
26	ME	202	PEB	C2C-C3C	3.50	1.48	1.37
28	MI	1001	CYC	CHB-C4A	3.50	1.48	1.40
26	O7	202	PEB	OD-C4D	3.50	1.30	1.23
26	BC	201	PEB	C2C-C3C	3.50	1.48	1.37
27	AI	302	PUB	C3B-C2B	3.50	1.48	1.37
26	RG	202	PEB	CHA-C1B	3.50	1.48	1.40
26	S9	201	PEB	C1A-NA	-3.50	1.33	1.37
26	A6	304	PEB	C2C-C3C	3.50	1.48	1.37
26	l6	203	PEB	C2C-C3C	3.50	1.48	1.37
28	yH	1001	CYC	C3D-C2D	3.50	1.48	1.37
26	cI	201	PEB	CHA-C1B	3.50	1.48	1.40
26	eB	201	PEB	C2C-C3C	3.50	1.48	1.37
27	AA	303	PUB	C3B-C2B	3.50	1.48	1.37
28	WH	1001	CYC	C3D-C2D	3.50	1.48	1.37
26	Y6	202	PEB	C2A-C1A	-3.50	1.49	1.52
26	lA	202	PEB	C2A-C1A	-3.50	1.49	1.52
26	N1	201	PEB	CHA-C1B	3.50	1.48	1.40
26	T4	201	PEB	CHA-C1B	3.50	1.48	1.40
26	l4	201	PEB	C1A-NA	-3.50	1.33	1.37
28	YH	1004	CYC	C1C-NC	-3.50	1.33	1.37
26	mB	201	PEB	C2C-C3C	3.50	1.48	1.37
28	YH	1003	CYC	C3D-C2D	3.50	1.48	1.37
26	Q7	203	PEB	CHA-C1B	3.50	1.48	1.40
26	I8	203	PEB	C2C-C3C	3.50	1.48	1.37
26	jB	202	PEB	C1A-NA	-3.50	1.33	1.37
26	B9	202	PEB	CHA-C1B	3.50	1.48	1.40
26	T6	201	PEB	C2C-C3C	3.50	1.48	1.37
26	gI	201	PEB	C2C-C3C	3.50	1.48	1.37
26	aA	203	PEB	CHA-C1B	3.50	1.48	1.40
26	N6	201	PEB	C2C-C3C	3.50	1.48	1.37
26	j7	203	PEB	C1A-NA	-3.50	1.33	1.37
26	cG	203	PEB	C1A-NA	-3.50	1.33	1.37
26	gI	202	PEB	C1A-NA	-3.50	1.33	1.37
26	FF	1002	PEB	C2C-C3C	3.50	1.48	1.37
26	iB	201	PEB	C1A-NA	-3.50	1.33	1.37
26	fl	202	PEB	C1A-NA	-3.50	1.33	1.37
26	lA	203	PEB	CHA-C1B	3.50	1.48	1.40
26	dB	203	PEB	C2C-C3C	3.50	1.48	1.37
28	OH	1001	CYC	C3D-C2D	3.50	1.48	1.37
26	f6	202	PEB	C2C-C3C	3.50	1.48	1.37
26	uE	202	PEB	C1A-NA	-3.50	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aB	201	PEB	CHA-C1B	3.50	1.48	1.40
26	TG	202	PEB	C2C-C3C	3.50	1.48	1.37
26	NB	1002	PEB	C2C-C3C	3.50	1.48	1.37
26	JG	202	PEB	C2C-C3C	3.50	1.48	1.37
26	d6	203	PEB	C2C-C3C	3.50	1.48	1.37
26	LA	201	PEB	C2C-C3C	3.50	1.48	1.37
26	a8	203	PEB	CHA-C1B	3.50	1.48	1.40
26	rG	201	PEB	CHA-C1B	3.50	1.48	1.40
26	Y1	201	PEB	C1A-NA	-3.50	1.33	1.37
26	AG	202	PEB	CHA-C1B	3.50	1.48	1.40
26	A1	202	PEB	C2C-C3C	3.50	1.48	1.37
28	C7	1001	CYC	C3D-C2D	3.50	1.48	1.37
26	i6	201	PEB	C2C-C3C	3.50	1.48	1.37
26	S7	203	PEB	CHA-C1B	3.50	1.48	1.40
26	kI	201	PEB	CHA-C1B	3.50	1.48	1.40
26	m6	202	PEB	C1A-NA	-3.50	1.33	1.37
26	fA	202	PEB	C1A-NA	-3.50	1.33	1.37
26	hB	203	PEB	C1A-NA	-3.50	1.33	1.37
26	IC	202	PEB	C1A-NA	-3.50	1.33	1.37
26	JJ	201	PEB	C1A-NA	-3.50	1.33	1.37
26	T1	201	PEB	CHA-C1B	3.50	1.48	1.40
26	t1	202	PEB	C1A-NA	-3.49	1.33	1.37
26	ID	201	PEB	C1A-NA	-3.49	1.33	1.37
26	RJ	203	PEB	C1A-NA	-3.49	1.33	1.37
26	i7	202	PEB	C2C-C3C	3.49	1.48	1.37
26	hA	202	PEB	C2C-C3C	3.49	1.48	1.37
28	I6	1001	CYC	C3D-C2D	3.49	1.48	1.37
26	GC	203	PEB	C2C-C3C	3.49	1.48	1.37
26	A7	301	PEB	C1A-NA	-3.49	1.33	1.37
26	eB	201	PEB	CHA-C1B	3.49	1.48	1.40
26	h1	202	PEB	C2C-C3C	3.49	1.48	1.37
26	n1	201	PEB	C2C-C3C	3.49	1.48	1.37
26	kF	201	PEB	CHA-C1B	3.49	1.48	1.40
26	MD	202	PEB	C2C-C3C	3.49	1.48	1.37
26	Y3	304	PEB	CHA-C1B	3.49	1.48	1.40
26	c2	201	PEB	C1A-NA	-3.49	1.33	1.37
26	gF	201	PEB	C2C-C3C	3.49	1.48	1.37
26	g7	201	PEB	C2C-C3C	3.49	1.48	1.37
26	S6	203	PEB	C1A-NA	-3.49	1.33	1.37
26	cA	203	PEB	C2C-C3C	3.49	1.48	1.37
26	U2	202	PEB	C2C-C3C	3.49	1.48	1.37
26	d6	204	PEB	C2C-C3C	3.49	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P2	201	PEB	C2A-C1A	-3.49	1.49	1.52
26	vG	201	PEB	C2A-C1A	-3.49	1.49	1.52
26	AI	305	PEB	C2C-C3C	3.49	1.48	1.37
26	e4	202	PEB	C1A-NA	-3.49	1.33	1.37
26	a6	202	PEB	C1A-NA	-3.49	1.33	1.37
26	v1	201	PEB	C2C-C3C	3.49	1.48	1.37
26	fE	202	PEB	C2C-C3C	3.49	1.48	1.37
28	vH	1001	CYC	C3D-C2D	3.49	1.48	1.37
26	QF	203	PEB	CHA-C1B	3.49	1.48	1.40
26	R4	202	PEB	C2C-C3C	3.49	1.48	1.37
26	R6	201	PEB	C2C-C3C	3.49	1.48	1.37
26	M4	402	PEB	CHA-C1B	3.49	1.48	1.40
26	gI	202	PEB	CHA-C1B	3.49	1.48	1.40
26	AF	302	PEB	C2C-C3C	3.49	1.48	1.37
26	C3	202	PEB	CHA-C1B	3.49	1.48	1.40
26	g4	202	PEB	CHA-C1B	3.49	1.48	1.40
28	KH	1001	CYC	C1A-C2A	3.49	1.51	1.45
26	F5	202	PEB	CHA-C1B	3.49	1.48	1.40
26	L6	1002	PEB	CHA-C1B	3.49	1.48	1.40
26	Y4	202	PEB	C2A-C1A	-3.49	1.49	1.52
26	ME	203	PEB	C1A-NA	-3.49	1.33	1.37
26	sE	202	PEB	C2C-C3C	3.49	1.48	1.37
26	xG	304	PEB	CHA-C1B	3.49	1.48	1.40
26	H7	1002	PEB	C2C-C3C	3.49	1.48	1.37
26	D8	201	PEB	C2C-C3C	3.49	1.48	1.37
26	y1	202	PEB	CHA-C1B	3.49	1.48	1.40
26	D8	202	PEB	C2C-C3C	3.49	1.48	1.37
26	I8	202	PEB	C1A-NA	-3.49	1.33	1.37
26	XJ	201	PEB	C1A-NA	-3.49	1.33	1.37
28	CF	1001	CYC	C1C-NC	-3.49	1.33	1.37
26	R2	202	PEB	CHA-C1B	3.49	1.48	1.40
26	l8	203	PEB	CHA-C1B	3.49	1.48	1.40
26	HC	202	PEB	CHA-C1B	3.49	1.48	1.40
26	F3	203	PEB	C2C-C3C	3.49	1.48	1.37
26	lF	203	PEB	C1A-NA	-3.48	1.33	1.37
26	FI	1002	PEB	CHA-C1B	3.48	1.48	1.40
26	OB	202	PEB	C2C-C3C	3.48	1.48	1.37
26	hG	201	PEB	C2C-C3C	3.48	1.48	1.37
26	A2	304	PEB	C2C-C3C	3.48	1.48	1.37
26	GE	203	PEB	C2C-C3C	3.48	1.48	1.37
26	mI	203	PEB	C2C-C3C	3.48	1.48	1.37
26	J3	203	PEB	CHA-C1B	3.48	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	WB	202	PEB	CHA-C1B	3.48	1.48	1.40
26	M1	403	PEB	C2C-C3C	3.48	1.48	1.37
26	o1	501	PEB	C2C-C3C	3.48	1.48	1.37
26	SJ	202	PEB	C2C-C3C	3.48	1.48	1.37
26	eB	202	PEB	CHA-C1B	3.48	1.48	1.40
26	j4	202	PEB	C1A-NA	-3.48	1.33	1.37
26	CC	203	PEB	C2C-C3C	3.48	1.48	1.37
26	S4	201	PEB	C2C-C3C	3.48	1.48	1.37
28	CF	1001	CYC	C3D-C2D	3.48	1.48	1.37
26	A9	304	PEB	CHA-C1B	3.48	1.48	1.40
26	lF	203	PEB	CHA-C1B	3.48	1.48	1.40
26	JI	1002	PEB	CHA-C1B	3.48	1.48	1.40
26	kF	201	PEB	C1A-NA	-3.48	1.33	1.37
26	DJ	203	PEB	C1A-NA	-3.48	1.33	1.37
26	j1	202	PEB	C2C-C3C	3.48	1.48	1.37
26	A4	202	PEB	C2C-C3C	3.48	1.48	1.37
26	VF	201	PEB	C2C-C3C	3.48	1.48	1.37
28	GH	1001	CYC	C3D-C2D	3.48	1.48	1.37
26	Z2	202	PEB	C1A-NA	-3.48	1.33	1.37
26	h4	202	PEB	C2C-C3C	3.48	1.48	1.37
26	c8	202	PEB	C2C-C3C	3.48	1.48	1.37
26	14	202	PEB	CHA-C1B	3.48	1.48	1.40
26	LC	202	PEB	CHA-C1B	3.48	1.48	1.40
26	YG	202	PEB	C1A-NA	-3.48	1.33	1.37
26	OF	202	PEB	C2C-C3C	3.48	1.48	1.37
26	A6	304	PEB	CHA-C1B	3.48	1.48	1.40
26	fG	202	PEB	CHA-C1B	3.48	1.48	1.40
28	II	1001	CYC	C1C-NC	-3.48	1.33	1.37
26	d2	202	PEB	C2C-C3C	3.48	1.48	1.37
26	j7	201	PEB	C2C-C3C	3.48	1.48	1.37
26	hA	203	PEB	C2C-C3C	3.48	1.48	1.37
26	lB	203	PEB	C2C-C3C	3.48	1.48	1.37
26	CC	201	PEB	CHA-C1B	3.48	1.48	1.40
26	WE	202	PEB	C1A-NA	-3.48	1.33	1.37
26	l6	201	PEB	CHA-C1B	3.48	1.48	1.40
26	e1	201	PEB	C1A-NA	-3.48	1.33	1.37
26	SB	203	PEB	C1A-NA	-3.48	1.33	1.37
26	dB	204	PEB	C2C-C3C	3.48	1.48	1.37
26	sG	202	PEB	C2C-C3C	3.48	1.48	1.37
28	rH	1001	CYC	C3D-C2D	3.48	1.48	1.37
26	D8	202	PEB	C1A-NA	-3.48	1.33	1.37
26	K1	202	PEB	C2C-C3C	3.48	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V7	201	PEB	C2C-C3C	3.48	1.48	1.37
26	G3	202	PEB	CHA-C1B	3.48	1.48	1.40
26	hB	203	PEB	OD-C4D	3.48	1.30	1.23
26	NI	1002	PEB	C1A-NA	-3.48	1.33	1.37
26	HF	1002	PEB	C2C-C3C	3.48	1.48	1.37
26	N4	202	PEB	CHA-C1B	3.48	1.48	1.40
26	TI	203	PEB	CHA-C1B	3.48	1.48	1.40
26	w4	204	PEB	C2C-C3C	3.48	1.48	1.37
26	O9	201	PEB	C2C-C3C	3.48	1.48	1.37
28	GI	1001	CYC	C3D-C2D	3.48	1.48	1.37
26	h6	203	PEB	C1A-NA	-3.48	1.33	1.37
26	AB	301	PEB	C2C-C3C	3.48	1.48	1.37
26	iG	202	PEB	CHA-C1B	3.48	1.48	1.40
26	RF	202	PEB	C2A-C1A	-3.47	1.49	1.52
26	m2	203	PEB	C2C-C3C	3.47	1.48	1.37
28	I2	1001	CYC	C1C-NC	-3.47	1.33	1.37
26	y4	203	PEB	CHA-C1B	3.47	1.48	1.40
26	I4	202	PEB	C2C-C3C	3.47	1.48	1.37
28	K7	1001	CYC	CHB-C4A	3.47	1.48	1.40
26	WA	202	PEB	C2A-C1A	-3.47	1.49	1.52
26	D7	1002	PEB	C2C-C3C	3.47	1.48	1.37
26	bB	201	PEB	C2C-C3C	3.47	1.48	1.37
26	IA	203	PEB	C2C-C3C	3.47	1.48	1.37
26	A2	301	PEB	C2C-C3C	3.47	1.48	1.37
28	sH	1001	CYC	C3D-C2D	3.47	1.48	1.37
26	TD	203	PEB	C2A-C1A	-3.47	1.49	1.52
28	WH	1001	CYC	C2C-C1C	-3.47	1.49	1.52
26	f8	203	PEB	C1A-NA	-3.47	1.33	1.37
26	YG	203	PEB	C1A-NA	-3.47	1.33	1.37
26	BE	202	PEB	C2C-C3C	3.47	1.48	1.37
28	PH	1001	CYC	C3D-C2D	3.47	1.48	1.37
26	IA	201	PEB	CHA-C1B	3.47	1.48	1.40
26	gI	203	PEB	C2C-C3C	3.47	1.48	1.37
26	aI	203	PEB	C1A-NA	-3.47	1.33	1.37
26	YJ	202	PEB	C1A-NA	-3.47	1.33	1.37
26	AD	202	PEB	OD-C4D	3.47	1.30	1.23
26	QJ	201	PEB	C2C-C3C	3.47	1.48	1.37
26	AI	301	PEB	CHA-C1B	3.47	1.48	1.40
28	F7	1001	CYC	CHB-C4A	3.47	1.48	1.40
26	f8	202	PEB	C2C-C3C	3.47	1.48	1.37
26	y4	202	PEB	C1A-NA	-3.47	1.33	1.37
26	E8	202	PEB	C1A-NA	-3.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	wG	303	PEB	C1A-NA	-3.47	1.33	1.37
26	aB	201	PEB	C2C-C3C	3.47	1.48	1.37
26	bB	201	PEB	C2A-C1A	-3.47	1.49	1.52
26	WF	203	PEB	CHA-C1B	3.47	1.48	1.40
26	R1	202	PEB	C2C-C3C	3.47	1.48	1.37
26	LC	202	PEB	C2C-C3C	3.47	1.48	1.37
26	m4	201	PEB	C1A-NA	-3.47	1.33	1.37
26	vG	202	PEB	C2C-C3C	3.47	1.48	1.37
26	CA	201	PEB	CHA-C1B	3.47	1.48	1.40
26	E3	202	PEB	C2C-C3C	3.47	1.48	1.37
26	OJ	201	PEB	C2C-C3C	3.47	1.48	1.37
26	G1	201	PEB	C1A-NA	-3.47	1.33	1.37
26	G4	202	PEB	C1A-NA	-3.47	1.33	1.37
26	N7	1002	PEB	C1A-NA	-3.47	1.33	1.37
26	J4	203	PEB	C2C-C3C	3.47	1.47	1.37
26	u1	201	PEB	CHA-C1B	3.47	1.48	1.40
26	j2	202	PEB	C1A-NA	-3.47	1.33	1.37
26	nG	202	PEB	C1A-NA	-3.47	1.33	1.37
26	m8	201	PEB	C2C-C3C	3.47	1.47	1.37
26	H9	203	PEB	CHA-C1B	3.47	1.48	1.40
28	dH	1001	CYC	CHB-C4A	3.47	1.48	1.40
26	B5	203	PEB	C2C-C3C	3.47	1.47	1.37
28	YH	1001	CYC	C3D-C2D	3.47	1.47	1.37
26	N2	1002	PEB	C1A-NA	-3.47	1.33	1.37
26	e3	401	PEB	C1A-NA	-3.47	1.33	1.37
26	TF	201	PEB	C1A-NA	-3.47	1.33	1.37
26	V8	202	PEB	C2C-C3C	3.47	1.47	1.37
26	N4	201	PEB	CHA-C1B	3.47	1.48	1.40
26	E9	201	PEB	C2A-C1A	-3.47	1.49	1.52
26	D1	201	PEB	C1A-NA	-3.47	1.33	1.37
26	21	405	PEB	C1A-NA	-3.47	1.33	1.37
26	AD	202	PEB	CHA-C1B	3.47	1.48	1.40
26	T3	203	PEB	CHA-C1B	3.47	1.48	1.40
26	G5	203	PEB	C2C-C3C	3.47	1.47	1.37
26	d6	202	PEB	CHA-C1B	3.47	1.48	1.40
28	eH	1001	CYC	C2C-C1C	-3.47	1.49	1.52
26	X8	202	PEB	C2C-C3C	3.47	1.47	1.37
26	e8	202	PEB	C2C-C3C	3.47	1.47	1.37
26	YG	201	PEB	C1A-NA	-3.46	1.33	1.37
26	C8	201	PEB	C2C-C3C	3.46	1.47	1.37
26	E3	202	PEB	C1A-NA	-3.46	1.33	1.37
26	i2	202	PEB	CHA-C1B	3.46	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	EA	201	PEB	CHA-C1B	3.46	1.48	1.40
26	CG	203	PEB	CHA-C1B	3.46	1.48	1.40
26	B4	203	PEB	C2C-C3C	3.46	1.47	1.37
26	R8	202	PEB	C2C-C3C	3.46	1.47	1.37
26	S9	202	PEB	C2C-C3C	3.46	1.47	1.37
28	UH	1001	CYC	C3D-C2D	3.46	1.47	1.37
26	mG	201	PEB	CHA-C1B	3.46	1.48	1.40
26	p1	202	PEB	C4B-C3B	3.46	1.51	1.45
26	O8	201	PEB	C2C-C3C	3.46	1.47	1.37
28	fH	1001	CYC	C3D-C2D	3.46	1.47	1.37
26	CE	203	PEB	CHA-C1B	3.46	1.48	1.40
26	h2	202	PEB	C2C-C3C	3.46	1.47	1.37
26	m6	202	PEB	CHA-C1B	3.46	1.48	1.40
26	PA	202	PEB	CHA-C1B	3.46	1.48	1.40
26	OG	202	PEB	C2C-C3C	3.46	1.47	1.37
26	a8	203	PEB	C1A-NA	-3.46	1.33	1.37
26	AJ	301	PEB	C1A-NA	-3.46	1.33	1.37
26	c6	201	PEB	C2C-C3C	3.46	1.47	1.37
26	b6	201	PEB	C2C-C3C	3.46	1.47	1.37
26	N9	204	PEB	C1A-NA	-3.46	1.33	1.37
26	ZI	202	PEB	C1A-NA	-3.46	1.33	1.37
26	M9	201	PEB	C2C-C3C	3.46	1.47	1.37
26	DD	203	PEB	C2C-C3C	3.46	1.47	1.37
26	xE	304	PEB	CHA-C1B	3.46	1.48	1.40
26	kI	202	PEB	CHA-C1B	3.46	1.48	1.40
26	k2	201	PEB	CHA-C1B	3.46	1.48	1.40
26	N6	201	PEB	CHA-C1B	3.46	1.48	1.40
26	ZG	202	PEB	CHA-C1B	3.46	1.48	1.40
26	O3	202	PEB	OD-C4D	3.46	1.30	1.23
26	P4	201	PEB	C1A-NA	-3.46	1.33	1.37
26	l6	202	PEB	C1A-NA	-3.46	1.33	1.37
28	FF	1001	CYC	C1C-NC	-3.46	1.33	1.37
26	w1	201	PEB	C2C-C3C	3.46	1.47	1.37
26	AC	203	PEB	C2C-C3C	3.46	1.47	1.37
26	MG	203	PEB	CHA-C1B	3.46	1.48	1.40
26	ZG	201	PEB	CHA-C1B	3.46	1.48	1.40
26	Y3	304	PEB	C1A-NA	-3.46	1.33	1.37
26	J9	203	PEB	C1A-NA	-3.46	1.33	1.37
26	UF	201	PEB	C1A-NA	-3.46	1.33	1.37
26	MG	202	PEB	CHA-C1B	3.46	1.48	1.40
26	k4	202	PEB	C2C-C3C	3.46	1.47	1.37
26	a6	201	PEB	CHA-C1B	3.46	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D3	203	PEB	C2C-C3C	3.46	1.47	1.37
26	eA	202	PEB	C2C-C3C	3.46	1.47	1.37
26	dB	202	PEB	CHA-C1B	3.46	1.48	1.40
26	DA	201	PEB	C2C-C3C	3.46	1.47	1.37
26	xG	303	PEB	CHA-C1B	3.46	1.48	1.40
26	14	202	PEB	C1A-NA	-3.46	1.33	1.37
26	N1	203	PEB	C2A-C1A	-3.46	1.49	1.52
26	A6	301	PEB	CHA-C1B	3.46	1.48	1.40
26	q1	201	PEB	C2C-C3C	3.46	1.47	1.37
26	kF	201	PEB	C2C-C3C	3.46	1.47	1.37
26	HD	201	PEB	C1A-NA	-3.46	1.33	1.37
26	qG	203	PEB	C1A-NA	-3.46	1.33	1.37
26	jA	203	PEB	CHA-C1B	3.46	1.48	1.40
26	lG	202	PEB	C2C-C3C	3.46	1.47	1.37
26	I8	203	PEB	C1A-NA	-3.46	1.33	1.37
26	u4	203	PEB	C2C-C3C	3.46	1.47	1.37
26	cB	201	PEB	C2C-C3C	3.46	1.47	1.37
26	rG	202	PEB	C2C-C3C	3.45	1.47	1.37
28	SH	1001	CYC	C3D-C2D	3.45	1.47	1.37
26	q4	202	PEB	CHA-C1B	3.45	1.48	1.40
26	RF	201	PEB	C2C-C3C	3.45	1.47	1.37
26	BJ	201	PEB	C2A-C1A	-3.45	1.49	1.52
26	v1	201	PEB	C1A-NA	-3.45	1.33	1.37
26	WG	203	PEB	C1A-NA	-3.45	1.33	1.37
26	V3	201	PEB	CHA-C1B	3.45	1.48	1.40
26	g2	201	PEB	C2C-C3C	3.45	1.47	1.37
26	gF	201	PEB	C1A-NA	-3.45	1.33	1.37
26	iF	202	PEB	C2C-C3C	3.45	1.47	1.37
26	OG	203	PEB	C2C-C3C	3.45	1.47	1.37
26	r4	201	PEB	C1A-NA	-3.45	1.33	1.37
26	C8	202	PEB	C1A-NA	-3.45	1.33	1.37
26	c2	203	PEB	C2C-C3C	3.45	1.47	1.37
26	d6	204	PEB	CHA-C1B	3.45	1.48	1.40
26	e7	201	PEB	CHA-C1B	3.45	1.48	1.40
26	a4	201	PEB	C2A-C1A	-3.45	1.49	1.52
27	AB	303	PUB	C3B-C2B	3.45	1.47	1.37
26	hB	202	PEB	C2C-C3C	3.45	1.47	1.37
26	dB	201	PEB	C1A-NA	-3.45	1.33	1.37
26	j8	203	PEB	CHA-C1B	3.45	1.48	1.40
26	s4	202	PEB	C2C-C3C	3.45	1.47	1.37
26	N3	203	PEB	C2A-C1A	-3.45	1.49	1.52
26	O2	202	PEB	C1A-NA	-3.45	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a6	201	PEB	C2C-C3C	3.45	1.47	1.37
26	m4	202	PEB	C2C-C3C	3.45	1.47	1.37
26	j6	201	PEB	CHA-C1B	3.45	1.48	1.40
26	C8	201	PEB	CHA-C1B	3.45	1.48	1.40
26	OE	202	PEB	C1A-NA	-3.45	1.33	1.37
26	PD	203	PEB	C2C-C3C	3.45	1.47	1.37
26	A2	301	PEB	CHA-C1B	3.45	1.48	1.40
26	L8	201	PEB	C2C-C3C	3.45	1.47	1.37
26	T9	203	PEB	CHA-C1B	3.45	1.48	1.40
26	z1	202	PEB	C1A-NA	-3.45	1.33	1.37
26	l8	203	PEB	C1A-NA	-3.45	1.33	1.37
26	Z7	203	PEB	C1A-NA	-3.45	1.33	1.37
26	P8	202	PEB	C1A-NA	-3.45	1.33	1.37
26	cE	202	PEB	C1A-NA	-3.45	1.33	1.37
27	A6	303	PUB	C3B-C2B	3.45	1.47	1.37
26	AE	202	PEB	CHA-C1B	3.45	1.48	1.40
26	XE	201	PEB	CHA-C1B	3.45	1.48	1.40
26	SF	202	PEB	CHA-C1B	3.45	1.48	1.40
27	Y3	302	PUB	C3B-C2B	3.45	1.47	1.37
26	g7	201	PEB	C1A-NA	-3.45	1.33	1.37
26	I5	202	PEB	CHA-C1B	3.45	1.48	1.40
26	DF	1002	PEB	C2C-C3C	3.45	1.47	1.37
26	BG	202	PEB	C2C-C3C	3.45	1.47	1.37
26	M4	403	PEB	CHA-C1B	3.45	1.48	1.40
26	J8	202	PEB	C2C-C3C	3.45	1.47	1.37
28	yH	1001	CYC	C2C-C1C	-3.45	1.49	1.52
26	YG	203	PEB	CHA-C1B	3.45	1.48	1.40
26	k6	201	PEB	C1A-NA	-3.45	1.33	1.37
27	AB	302	PUB	C3B-C2B	3.45	1.47	1.37
26	S7	201	PEB	CHA-C1B	3.45	1.48	1.40
26	g2	203	PEB	C2C-C3C	3.44	1.47	1.37
26	a8	201	PEB	C2C-C3C	3.44	1.47	1.37
26	QG	202	PEB	C1A-NA	-3.44	1.33	1.37
26	A6	301	PEB	C2C-C3C	3.44	1.47	1.37
26	iG	203	PEB	CHA-C1B	3.44	1.48	1.40
26	s4	201	PEB	C2C-C3C	3.44	1.47	1.37
26	XA	202	PEB	C1A-NA	-3.44	1.33	1.37
26	iI	203	PEB	C1A-NA	-3.44	1.33	1.37
26	P3	203	PEB	C2C-C3C	3.44	1.47	1.37
26	S7	202	PEB	C2C-C3C	3.44	1.47	1.37
26	l7	203	PEB	CHA-C1B	3.44	1.48	1.40
26	J9	201	PEB	C2C-C3C	3.44	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O7	202	PEB	C1A-NA	-3.44	1.33	1.37
26	AD	201	PEB	CHA-C1B	3.44	1.48	1.40
26	f7	203	PEB	C2C-C3C	3.44	1.47	1.37
26	V2	201	PEB	C2A-C1A	-3.44	1.49	1.52
26	eA	202	PEB	C2A-C1A	-3.44	1.49	1.52
26	VB	202	PEB	C1A-NA	-3.44	1.33	1.37
26	L9	203	PEB	C2C-C3C	3.44	1.47	1.37
26	f7	203	PEB	CHA-C1B	3.44	1.48	1.40
26	AB	301	PEB	C1A-NA	-3.44	1.33	1.37
26	OI	202	PEB	C1A-NA	-3.44	1.33	1.37
26	J5	202	PEB	C2C-C3C	3.44	1.47	1.37
26	V6	202	PEB	C1A-NA	-3.44	1.33	1.37
26	BD	201	PEB	C1A-NA	-3.44	1.33	1.37
26	LC	203	PEB	C2C-C3C	3.44	1.47	1.37
26	VI	201	PEB	C2A-C1A	-3.44	1.49	1.52
26	j6	202	PEB	C2C-C3C	3.44	1.47	1.37
26	OG	202	PEB	C1A-NA	-3.44	1.33	1.37
28	D7	1001	CYC	C1C-NC	-3.44	1.33	1.37
26	21	405	PEB	CHA-C1B	3.44	1.48	1.40
26	N7	1002	PEB	C2C-C3C	3.44	1.47	1.37
26	KD	201	PEB	C2C-C3C	3.44	1.47	1.37
28	IB	1001	CYC	C3D-C2D	3.44	1.47	1.37
26	V4	202	PEB	C1A-NA	-3.44	1.33	1.37
28	G2	1001	CYC	C1C-NC	-3.44	1.33	1.37
26	T1	203	PEB	C2C-C3C	3.44	1.47	1.37
26	AG	202	PEB	C2C-C3C	3.44	1.47	1.37
28	FI	1001	CYC	CHB-C4A	3.44	1.48	1.40
28	wH	1001	CYC	C3D-C2D	3.44	1.47	1.37
26	PB	201	PEB	C2A-C1A	-3.44	1.49	1.52
28	mH	1001	CYC	C2C-C1C	-3.44	1.49	1.52
26	RI	202	PEB	CHA-C1B	3.44	1.48	1.40
26	z1	201	PEB	C1A-NA	-3.44	1.33	1.37
26	mB	203	PEB	C1A-NA	-3.44	1.33	1.37
26	JC	202	PEB	C2C-C3C	3.44	1.47	1.37
26	W7	203	PEB	CHA-C1B	3.44	1.48	1.40
26	f1	201	PEB	C1A-NA	-3.44	1.33	1.37
26	V9	203	PEB	C1A-NA	-3.44	1.33	1.37
26	YF	202	PEB	C1A-NA	-3.44	1.33	1.37
26	UI	202	PEB	C1A-NA	-3.44	1.33	1.37
26	XA	202	PEB	C2C-C3C	3.44	1.47	1.37
26	C5	202	PEB	CHA-C1B	3.44	1.48	1.40
26	eA	201	PEB	C2C-C3C	3.44	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	pG	202	PEB	C2C-C3C	3.44	1.47	1.37
26	Z1	201	PEB	C1A-NA	-3.44	1.33	1.37
26	l2	202	PEB	C1A-NA	-3.44	1.33	1.37
26	cF	202	PEB	C1A-NA	-3.44	1.33	1.37
26	W6	202	PEB	C2C-C3C	3.44	1.47	1.37
26	rE	201	PEB	C2C-C3C	3.44	1.47	1.37
28	EH	1001	CYC	C3D-C2D	3.44	1.47	1.37
26	m7	201	PEB	C2C-C3C	3.44	1.47	1.37
26	d8	202	PEB	C2C-C3C	3.44	1.47	1.37
27	YD	302	PUB	C3B-C2B	3.44	1.47	1.37
26	fF	201	PEB	C2C-C3C	3.43	1.47	1.37
26	d6	204	PEB	C1A-NA	-3.43	1.33	1.37
26	sE	202	PEB	C1A-NA	-3.43	1.33	1.37
26	kG	201	PEB	C2C-C3C	3.43	1.47	1.37
27	wE	304	PUB	C3B-C2B	3.43	1.47	1.37
26	f4	202	PEB	C2C-C3C	3.43	1.47	1.37
26	gE	203	PEB	CHA-C1B	3.43	1.48	1.40
26	NE	201	PEB	C2C-C3C	3.43	1.47	1.37
26	eI	201	PEB	C2C-C3C	3.43	1.47	1.37
26	G1	202	PEB	C2C-C3C	3.43	1.47	1.37
26	JA	202	PEB	C2C-C3C	3.43	1.47	1.37
26	YA	203	PEB	CHA-C1B	3.43	1.48	1.40
26	k4	203	PEB	C2C-C3C	3.43	1.47	1.37
26	C5	204	PEB	C2C-C3C	3.43	1.47	1.37
26	V7	202	PEB	C2C-C3C	3.43	1.47	1.37
26	BC	203	PEB	C2C-C3C	3.43	1.47	1.37
26	h6	202	PEB	C2C-C3C	3.43	1.47	1.37
26	rG	201	PEB	C2C-C3C	3.43	1.47	1.37
26	e1	202	PEB	C1A-NA	-3.43	1.33	1.37
26	AI	301	PEB	C2C-C3C	3.43	1.47	1.37
26	c1	201	PEB	C1A-NA	-3.43	1.33	1.37
26	b7	201	PEB	C2C-C3C	3.43	1.47	1.37
26	A9	301	PEB	C2C-C3C	3.43	1.47	1.37
26	kE	203	PEB	C2C-C3C	3.43	1.47	1.37
26	EE	202	PEB	C2C-C3C	3.43	1.47	1.37
26	sE	201	PEB	C2C-C3C	3.43	1.47	1.37
26	dF	202	PEB	C2C-C3C	3.43	1.47	1.37
26	WB	202	PEB	C2C-C3C	3.43	1.47	1.37
26	UI	202	PEB	C2C-C3C	3.43	1.47	1.37
26	ME	203	PEB	CHA-C1B	3.43	1.48	1.40
26	WE	203	PEB	C2C-C3C	3.43	1.47	1.37
28	J7	1001	CYC	C3D-C2D	3.43	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L4	201	PEB	C2C-C3C	3.43	1.47	1.37
26	zE	501	PEB	C2C-C3C	3.43	1.47	1.37
26	UF	203	PEB	C1A-NA	-3.43	1.33	1.37
26	L4	203	PEB	C2C-C3C	3.43	1.47	1.37
26	cI	203	PEB	C2C-C3C	3.43	1.47	1.37
28	QH	1001	CYC	C3D-C2D	3.43	1.47	1.37
26	U7	202	PEB	C1A-NA	-3.43	1.33	1.37
26	LC	202	PEB	C1A-NA	-3.43	1.33	1.37
27	xE	305	PUB	C3B-C2B	3.43	1.47	1.37
26	u1	203	PEB	C2C-C3C	3.43	1.47	1.37
26	A4	201	PEB	C2C-C3C	3.43	1.47	1.37
26	UB	201	PEB	CHA-C1B	3.43	1.48	1.40
26	ED	202	PEB	CHA-C1B	3.43	1.48	1.40
27	AA	304	PUB	C3B-C2B	3.43	1.47	1.37
26	Z4	201	PEB	C1A-NA	-3.43	1.33	1.37
26	Q8	204	PEB	C1A-NA	-3.43	1.33	1.37
28	M2	1001	CYC	C1C-NC	-3.43	1.33	1.37
26	GC	201	PEB	C2C-C3C	3.43	1.47	1.37
26	TJ	203	PEB	CHA-C1B	3.43	1.48	1.40
26	d4	203	PEB	C1A-NA	-3.43	1.33	1.37
26	j7	201	PEB	C1A-NA	-3.43	1.33	1.37
26	JE	202	PEB	C1A-NA	-3.43	1.33	1.37
26	FC	203	PEB	C2C-C3C	3.43	1.47	1.37
26	s1	202	PEB	CHA-C1B	3.43	1.48	1.40
26	VA	202	PEB	C1A-NA	-3.42	1.33	1.37
26	U9	202	PEB	C2C-C3C	3.42	1.47	1.37
26	U8	201	PEB	CHA-C1B	3.42	1.48	1.40
26	11	203	PEB	C1A-NA	-3.42	1.33	1.37
26	h7	202	PEB	C2C-C3C	3.42	1.47	1.37
26	GG	203	PEB	C2C-C3C	3.42	1.47	1.37
26	RE	201	PEB	CHA-C1B	3.42	1.48	1.40
26	G5	201	PEB	C2C-C3C	3.42	1.47	1.37
26	bE	201	PEB	C2C-C3C	3.42	1.47	1.37
26	EG	202	PEB	C2C-C3C	3.42	1.47	1.37
26	AJ	301	PEB	C2C-C3C	3.42	1.47	1.37
26	O8	203	PEB	CHA-C1B	3.42	1.48	1.40
26	G3	202	PEB	C2C-C3C	3.42	1.47	1.37
26	Y1	202	PEB	C2A-C1A	-3.42	1.49	1.52
26	N7	1002	PEB	CHA-C1B	3.42	1.48	1.40
26	11	202	PEB	C2C-C3C	3.42	1.47	1.37
26	FC	202	PEB	C2C-C3C	3.42	1.47	1.37
26	QJ	202	PEB	C2C-C3C	3.42	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	KA	202	PEB	CHA-C1B	3.42	1.48	1.40
26	gA	201	PEB	C1A-NA	-3.42	1.33	1.37
26	I3	201	PEB	C2C-C3C	3.42	1.47	1.37
26	L6	1002	PEB	C2C-C3C	3.42	1.47	1.37
26	TJ	202	PEB	C2C-C3C	3.42	1.47	1.37
26	LE	202	PEB	C2A-C1A	-3.42	1.49	1.52
26	M1	402	PEB	C2C-C3C	3.42	1.47	1.37
26	V1	202	PEB	CHA-C1B	3.42	1.48	1.40
26	gG	203	PEB	CHA-C1B	3.42	1.48	1.40
28	F7	1001	CYC	C3D-C2D	3.42	1.47	1.37
26	w1	203	PEB	C1A-NA	-3.42	1.33	1.37
26	SB	202	PEB	C1A-NA	-3.42	1.33	1.37
26	e4	202	PEB	CHA-C1B	3.42	1.48	1.40
26	U3	202	PEB	C2C-C3C	3.42	1.47	1.37
26	U2	202	PEB	CHA-C1B	3.42	1.48	1.40
26	YE	203	PEB	CHA-C1B	3.42	1.48	1.40
26	V9	201	PEB	C1A-NA	-3.42	1.33	1.37
26	QF	203	PEB	C1A-NA	-3.42	1.33	1.37
26	jI	202	PEB	C1A-NA	-3.42	1.33	1.37
26	i4	201	PEB	CHA-C1B	3.42	1.48	1.40
26	HJ	203	PEB	CHA-C1B	3.42	1.48	1.40
26	e2	201	PEB	C2C-C3C	3.42	1.47	1.37
26	bI	202	PEB	C2C-C3C	3.42	1.47	1.37
26	pE	202	PEB	C2A-C1A	-3.42	1.49	1.52
26	F1	201	PEB	C1A-NA	-3.42	1.33	1.37
26	f2	202	PEB	C1A-NA	-3.42	1.33	1.37
26	L3	203	PEB	C1A-NA	-3.42	1.33	1.37
26	DA	202	PEB	C1A-NA	-3.42	1.33	1.37
26	KC	202	PEB	C1A-NA	-3.42	1.33	1.37
26	VF	203	PEB	C2C-C3C	3.42	1.47	1.37
26	NB	1002	PEB	CHA-C1B	3.42	1.48	1.40
26	GB	1002	PEB	CHA-C1B	3.42	1.48	1.40
26	X4	203	PEB	C1A-NA	-3.42	1.33	1.37
26	mI	201	PEB	C1A-NA	-3.42	1.33	1.37
26	u1	202	PEB	CHA-C1B	3.42	1.48	1.40
26	g2	202	PEB	C1A-NA	-3.42	1.33	1.37
26	F7	1002	PEB	C2C-C3C	3.42	1.47	1.37
26	DG	201	PEB	C2A-C1A	-3.42	1.49	1.52
26	QG	203	PEB	C4B-NB	-3.42	1.31	1.38
26	d7	202	PEB	CHA-C1B	3.42	1.48	1.40
26	L1	201	PEB	C2C-C3C	3.42	1.47	1.37
26	c1	201	PEB	C2C-C3C	3.42	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B1	202	PEB	C1A-NA	-3.42	1.33	1.37
26	i6	202	PEB	C1A-NA	-3.42	1.33	1.37
26	YF	201	PEB	C1A-NA	-3.42	1.33	1.37
26	NJ	204	PEB	CHA-C1B	3.42	1.48	1.40
26	ZF	202	PEB	C2C-C3C	3.42	1.47	1.37
26	cI	201	PEB	C2C-C3C	3.42	1.47	1.37
26	R8	202	PEB	C2A-C1A	-3.42	1.49	1.52
26	14	203	PEB	C1A-NA	-3.42	1.33	1.37
26	AB	301	PEB	CHA-C1B	3.41	1.48	1.40
26	CC	203	PEB	C1A-NA	-3.41	1.33	1.37
26	d1	203	PEB	C2C-C3C	3.41	1.47	1.37
26	RG	201	PEB	CHA-C1B	3.41	1.48	1.40
26	DE	201	PEB	C2A-C1A	-3.41	1.49	1.52
26	FI	1002	PEB	C2A-C1A	-3.41	1.49	1.52
27	21	403	PUB	C3B-C2B	3.41	1.47	1.37
26	L2	1002	PEB	CHA-C1B	3.41	1.48	1.40
26	f7	202	PEB	CHA-C1B	3.41	1.48	1.40
26	A4	202	PEB	C1A-NA	-3.41	1.33	1.37
26	WB	202	PEB	C1A-NA	-3.41	1.33	1.37
26	fF	203	PEB	C2C-C3C	3.41	1.47	1.37
26	iI	202	PEB	CHA-C1B	3.41	1.48	1.40
26	AI	304	PEB	C1A-NA	-3.41	1.33	1.37
26	F5	201	PEB	CHA-C1B	3.41	1.48	1.40
26	eG	203	PEB	CHA-C1B	3.41	1.48	1.40
28	I7	1001	CYC	C3D-C2D	3.41	1.47	1.37
26	V4	203	PEB	C1A-NA	-3.41	1.33	1.37
26	u4	203	PEB	C1A-NA	-3.41	1.33	1.37
26	j6	202	PEB	C1A-NA	-3.41	1.33	1.37
26	S7	202	PEB	C1A-NA	-3.41	1.33	1.37
26	R4	201	PEB	C2C-C3C	3.41	1.47	1.37
26	E8	203	PEB	C2C-C3C	3.41	1.47	1.37
26	c4	201	PEB	C2C-C3C	3.41	1.47	1.37
26	H5	202	PEB	CHA-C1B	3.41	1.48	1.40
26	dA	201	PEB	CHA-C1B	3.41	1.48	1.40
26	UD	201	PEB	CHA-C1B	3.41	1.48	1.40
26	JJ	201	PEB	CHA-C1B	3.41	1.48	1.40
26	PE	201	PEB	C2C-C3C	3.41	1.47	1.37
26	s4	203	PEB	C1A-NA	-3.41	1.33	1.37
26	HJ	201	PEB	C1A-NA	-3.41	1.33	1.37
26	Z6	203	PEB	C2C-C3C	3.41	1.47	1.37
26	OA	202	PEB	C2C-C3C	3.41	1.47	1.37
26	KG	202	PEB	C2C-C3C	3.41	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y7	201	PEB	C1A-NA	-3.41	1.33	1.37
26	IE	202	PEB	C1A-NA	-3.41	1.33	1.37
26	FI	1002	PEB	C1A-NA	-3.41	1.33	1.37
26	dI	201	PEB	CHA-C1B	3.41	1.48	1.40
26	k2	201	PEB	C1A-NA	-3.41	1.33	1.37
26	jB	202	PEB	C2C-C3C	3.41	1.47	1.37
26	iF	201	PEB	C2C-C3C	3.41	1.47	1.37
26	TJ	201	PEB	CHA-C1B	3.41	1.48	1.40
26	DA	202	PEB	C2C-C3C	3.41	1.47	1.37
26	RB	202	PEB	C2A-C1A	-3.41	1.49	1.52
26	OA	201	PEB	C2C-C3C	3.41	1.47	1.37
26	UD	202	PEB	C2C-C3C	3.41	1.47	1.37
26	S3	202	PEB	C2C-C3C	3.41	1.47	1.37
26	g1	202	PEB	C1A-NA	-3.41	1.33	1.37
28	E7	1001	CYC	C2C-C1C	-3.41	1.49	1.52
26	r1	201	PEB	C1A-NA	-3.41	1.33	1.37
26	RB	201	PEB	C2C-C3C	3.41	1.47	1.37
28	iH	1001	CYC	C3D-C2D	3.41	1.47	1.37
26	k7	201	PEB	C1A-NA	-3.41	1.33	1.37
26	b2	202	PEB	C2C-C3C	3.41	1.47	1.37
26	nE	201	PEB	C2C-C3C	3.41	1.47	1.37
26	xG	302	PEB	CHA-C1B	3.41	1.48	1.40
26	S2	202	PEB	C2C-C3C	3.41	1.47	1.37
26	RF	202	PEB	C2C-C3C	3.41	1.47	1.37
26	eI	203	PEB	C2C-C3C	3.41	1.47	1.37
26	S3	201	PEB	CHA-C1B	3.41	1.48	1.40
26	mF	201	PEB	C2C-C3C	3.41	1.47	1.37
26	N2	1002	PEB	CHA-C1B	3.40	1.48	1.40
26	i7	201	PEB	C1A-NA	-3.40	1.33	1.37
26	ED	201	PEB	CHA-C1B	3.40	1.48	1.40
26	VJ	201	PEB	CHA-C1B	3.40	1.48	1.40
26	U7	203	PEB	C1A-NA	-3.40	1.33	1.37
26	cB	201	PEB	C1A-NA	-3.40	1.33	1.37
26	XG	201	PEB	CHA-C1B	3.40	1.48	1.40
26	lF	202	PEB	C2C-C3C	3.40	1.47	1.37
27	AI	303	PUB	C3B-C2B	3.40	1.47	1.37
26	wE	303	PEB	C1A-NA	-3.40	1.33	1.37
26	fA	201	PEB	CHA-C1B	3.40	1.48	1.40
28	CB	1001	CYC	C3D-C2D	3.40	1.47	1.37
26	RG	202	PEB	C2C-C3C	3.40	1.47	1.37
26	bF	202	PEB	C1A-NA	-3.40	1.33	1.37
26	S1	201	PEB	C2C-C3C	3.40	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TE	201	PEB	C2C-C3C	3.40	1.47	1.37
26	IE	202	PEB	C2C-C3C	3.40	1.47	1.37
26	dB	204	PEB	CHA-C1B	3.40	1.48	1.40
26	TA	201	PEB	C1A-NA	-3.40	1.33	1.37
26	H6	1002	PEB	C2C-C3C	3.40	1.47	1.37
26	ZA	201	PEB	C2C-C3C	3.40	1.47	1.37
26	IE	203	PEB	CHA-C1B	3.40	1.48	1.40
26	V6	201	PEB	C2C-C3C	3.40	1.47	1.37
26	AG	201	PEB	C2C-C3C	3.40	1.47	1.37
26	d1	203	PEB	C1A-NA	-3.40	1.33	1.37
28	H7	1001	CYC	C3D-C2D	3.40	1.47	1.37
28	L7	1001	CYC	C3D-C2D	3.40	1.47	1.37
26	g1	203	PEB	CHA-C1B	3.40	1.48	1.40
26	h8	203	PEB	C2C-C3C	3.40	1.47	1.37
26	VJ	201	PEB	C1A-NA	-3.40	1.33	1.37
26	x1	202	PEB	CHA-C1B	3.40	1.48	1.40
26	LI	1002	PEB	C2A-C1A	-3.40	1.49	1.52
26	UA	201	PEB	CHA-C1B	3.40	1.48	1.40
26	IF	203	PEB	C2C-C3C	3.40	1.47	1.37
26	A6	301	PEB	C1A-NA	-3.40	1.33	1.37
26	FC	201	PEB	C2C-C3C	3.40	1.47	1.37
26	OE	202	PEB	C2C-C3C	3.40	1.47	1.37
26	jI	201	PEB	C2C-C3C	3.40	1.47	1.37
26	h7	203	PEB	OD-C4D	3.40	1.30	1.23
26	H1	202	PEB	C2C-C3C	3.40	1.47	1.37
26	SF	201	PEB	CHA-C1B	3.40	1.48	1.40
26	WG	203	PEB	CHA-C1B	3.40	1.48	1.40
26	j4	202	PEB	C2C-C3C	3.40	1.47	1.37
26	M4	403	PEB	C2C-C3C	3.40	1.47	1.37
26	T8	201	PEB	C1A-NA	-3.40	1.33	1.37
26	UE	203	PEB	C1A-NA	-3.40	1.33	1.37
26	S7	202	PEB	CHA-C1B	3.40	1.48	1.40
26	U1	201	PEB	C2C-C3C	3.40	1.47	1.37
26	RJ	203	PEB	C2C-C3C	3.40	1.47	1.37
26	P2	203	PEB	C1A-NA	-3.40	1.33	1.37
26	QE	202	PEB	C1A-NA	-3.40	1.33	1.37
26	a4	202	PEB	C2C-C3C	3.40	1.47	1.37
26	MJ	202	PEB	C2C-C3C	3.40	1.47	1.37
26	h4	203	PEB	C2C-C3C	3.40	1.47	1.37
26	g2	203	PEB	C1A-NA	-3.40	1.33	1.37
26	cE	203	PEB	C1A-NA	-3.40	1.33	1.37
26	G4	202	PEB	C2C-C3C	3.40	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U1	202	PEB	C2C-C3C	3.40	1.47	1.37
26	mA	202	PEB	C1A-NA	-3.40	1.33	1.37
26	mE	202	PEB	C1A-NA	-3.40	1.33	1.37
26	E8	201	PEB	CHA-C1B	3.40	1.48	1.40
26	WF	201	PEB	C1A-NA	-3.39	1.33	1.37
26	HD	201	PEB	C2C-C3C	3.39	1.47	1.37
26	jG	201	PEB	C2A-C1A	-3.39	1.49	1.52
26	d1	202	PEB	C2C-C3C	3.39	1.47	1.37
26	Q7	203	PEB	C2C-C3C	3.39	1.47	1.37
26	eE	201	PEB	C2C-C3C	3.39	1.47	1.37
26	AJ	305	PEB	C2C-C3C	3.39	1.47	1.37
26	N1	202	PEB	CHA-C1B	3.39	1.48	1.40
26	G1	202	PEB	C1A-NA	-3.39	1.33	1.37
26	F2	1002	PEB	C1A-NA	-3.39	1.33	1.37
26	R9	203	PEB	C1A-NA	-3.39	1.33	1.37
26	l4	202	PEB	C2C-C3C	3.39	1.47	1.37
26	L2	1002	PEB	C2C-C3C	3.39	1.47	1.37
26	GD	202	PEB	C2C-C3C	3.39	1.47	1.37
26	VE	201	PEB	C2C-C3C	3.39	1.47	1.37
26	SD	201	PEB	CHA-C1B	3.39	1.48	1.40
26	c6	201	PEB	C1A-NA	-3.39	1.33	1.37
26	H3	203	PEB	C2C-C3C	3.39	1.47	1.37
26	qE	203	PEB	C2C-C3C	3.39	1.47	1.37
26	CG	201	PEB	C2C-C3C	3.39	1.47	1.37
26	VB	201	PEB	C2C-C3C	3.39	1.47	1.37
26	TG	201	PEB	C2C-C3C	3.39	1.47	1.37
26	g1	201	PEB	C1A-NA	-3.39	1.33	1.37
26	BC	202	PEB	C1A-NA	-3.39	1.33	1.37
26	gE	202	PEB	CHA-C1B	3.39	1.48	1.40
26	MA	203	PEB	C1A-NA	-3.39	1.33	1.37
26	w4	204	PEB	CHA-C1B	3.39	1.48	1.40
26	HC	201	PEB	C2C-C3C	3.39	1.47	1.37
26	W3	201	PEB	CHA-C1B	3.39	1.48	1.40
26	J4	202	PEB	CHA-C1B	3.39	1.48	1.40
26	D6	1002	PEB	CHA-C1B	3.39	1.48	1.40
26	J2	1002	PEB	C2A-C1A	-3.39	1.49	1.52
26	TJ	202	PEB	C1A-NA	-3.39	1.33	1.37
28	JF	1003	CYC	C1C-NC	-3.39	1.33	1.37
26	f6	201	PEB	C2C-C3C	3.39	1.47	1.37
26	e8	201	PEB	C2C-C3C	3.39	1.47	1.37
26	gE	202	PEB	C2C-C3C	3.39	1.47	1.37
28	J7	1003	CYC	C3D-C2D	3.39	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	jF	202	PEB	CHA-C1B	3.39	1.48	1.40
26	H4	201	PEB	C1A-NA	-3.39	1.33	1.37
26	P1	201	PEB	C2C-C3C	3.39	1.47	1.37
26	eD	401	PEB	C2C-C3C	3.39	1.47	1.37
26	VA	202	PEB	C2C-C3C	3.39	1.47	1.37
28	M2	1001	CYC	C3D-C2D	3.39	1.47	1.37
26	R9	202	PEB	C2C-C3C	3.39	1.47	1.37
26	TI	201	PEB	C2A-C1A	-3.39	1.49	1.52
26	OF	201	PEB	C2C-C3C	3.39	1.47	1.37
26	jF	201	PEB	C2C-C3C	3.39	1.47	1.37
26	J1	202	PEB	C1A-NA	-3.39	1.33	1.37
26	EG	201	PEB	C1A-NA	-3.39	1.33	1.37
26	f8	202	PEB	CHA-C1B	3.39	1.48	1.40
26	U4	202	PEB	C2C-C3C	3.39	1.47	1.37
26	XJ	202	PEB	C2C-C3C	3.39	1.47	1.37
26	SI	202	PEB	C2C-C3C	3.39	1.47	1.37
26	IG	202	PEB	C1A-NA	-3.39	1.33	1.37
26	lA	202	PEB	C2C-C3C	3.39	1.47	1.37
26	hF	202	PEB	C2C-C3C	3.39	1.47	1.37
26	H3	203	PEB	C4B-C3B	3.39	1.51	1.45
26	eE	202	PEB	C2C-C3C	3.39	1.47	1.37
26	SE	203	PEB	C1A-NA	-3.39	1.33	1.37
26	T2	203	PEB	CHA-C1B	3.39	1.48	1.40
26	O3	202	PEB	CHA-C1B	3.39	1.48	1.40
26	hB	203	PEB	CHA-C1B	3.39	1.48	1.40
26	LI	1002	PEB	CHA-C1B	3.39	1.48	1.40
26	YJ	201	PEB	C1A-NA	-3.39	1.33	1.37
28	K7	1001	CYC	C3D-C2D	3.39	1.47	1.37
26	RF	201	PEB	CHA-C1B	3.39	1.48	1.40
26	II	202	PEB	C2C-C3C	3.39	1.47	1.37
26	ID	201	PEB	CHA-C1B	3.39	1.48	1.40
26	JJ	203	PEB	C1A-NA	-3.39	1.33	1.37
26	e3	401	PEB	C2C-C3C	3.39	1.47	1.37
26	J3	203	PEB	C2C-C3C	3.38	1.47	1.37
26	P8	201	PEB	C2C-C3C	3.38	1.47	1.37
26	a7	201	PEB	C2C-C3C	3.38	1.47	1.37
26	NG	201	PEB	C2C-C3C	3.38	1.47	1.37
26	L4	202	PEB	C2C-C3C	3.38	1.47	1.37
26	M4	402	PEB	C2C-C3C	3.38	1.47	1.37
26	L5	202	PEB	C2C-C3C	3.38	1.47	1.37
26	zG	501	PEB	C2C-C3C	3.38	1.47	1.37
26	F5	202	PEB	C1A-NA	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	iB	202	PEB	C1A-NA	-3.38	1.33	1.37
26	iF	201	PEB	CHA-C1B	3.38	1.48	1.40
26	R1	201	PEB	C2C-C3C	3.38	1.47	1.37
26	RA	202	PEB	C2C-C3C	3.38	1.47	1.37
26	B3	202	PEB	C2C-C3C	3.38	1.47	1.37
26	P4	201	PEB	C2C-C3C	3.38	1.47	1.37
26	FE	202	PEB	C2A-C1A	-3.38	1.49	1.52
26	a4	201	PEB	C1A-NA	-3.38	1.33	1.37
26	k4	202	PEB	C1A-NA	-3.38	1.33	1.37
26	FD	201	PEB	C2C-C3C	3.38	1.47	1.37
26	c7	201	PEB	CHA-C1B	3.38	1.48	1.40
26	P7	202	PEB	C2C-C3C	3.38	1.47	1.37
28	kH	1001	CYC	C3D-C2D	3.38	1.47	1.37
26	XJ	201	PEB	CHA-C1B	3.38	1.48	1.40
26	T1	201	PEB	C2C-C3C	3.38	1.47	1.37
26	N4	203	PEB	C2C-C3C	3.38	1.47	1.37
26	JF	1002	PEB	C2C-C3C	3.38	1.47	1.37
26	iI	201	PEB	C2C-C3C	3.38	1.47	1.37
28	IH	1001	CYC	C3D-C2D	3.38	1.47	1.37
26	P6	201	PEB	C2A-C1A	-3.38	1.49	1.52
26	P4	203	PEB	C1A-NA	-3.38	1.33	1.37
26	LF	1002	PEB	C1A-NA	-3.38	1.33	1.37
26	CG	201	PEB	C1A-NA	-3.38	1.33	1.37
26	U6	203	PEB	C2C-C3C	3.38	1.47	1.37
26	ID	201	PEB	C2C-C3C	3.38	1.47	1.37
26	h6	203	PEB	CHA-C1B	3.38	1.48	1.40
26	l2	201	PEB	C2C-C3C	3.38	1.47	1.37
26	s4	201	PEB	C1A-NA	-3.38	1.33	1.37
26	g2	202	PEB	CHA-C1B	3.38	1.48	1.40
26	k2	203	PEB	CHA-C1B	3.38	1.48	1.40
26	V4	202	PEB	CHA-C1B	3.38	1.48	1.40
26	SF	202	PEB	C2C-C3C	3.38	1.47	1.37
26	II	201	PEB	C2C-C3C	3.38	1.47	1.37
27	A2	303	PUB	C3B-C2B	3.38	1.47	1.37
26	iE	203	PEB	C1A-NA	-3.38	1.33	1.37
26	aA	201	PEB	C2C-C3C	3.38	1.47	1.37
26	T4	201	PEB	C2C-C3C	3.38	1.47	1.37
26	p4	202	PEB	C1A-NA	-3.38	1.33	1.37
26	e6	203	PEB	C1A-NA	-3.38	1.33	1.37
26	O8	201	PEB	C1A-NA	-3.38	1.33	1.37
26	JD	201	PEB	C1A-NA	-3.38	1.33	1.37
26	UJ	202	PEB	C2C-C3C	3.38	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U2	201	PEB	C2A-C1A	-3.38	1.49	1.52
26	G6	1002	PEB	CHA-C1B	3.38	1.48	1.40
26	QB	203	PEB	C2C-C3C	3.38	1.47	1.37
26	J7	1002	PEB	C2C-C3C	3.38	1.47	1.37
26	w4	202	PEB	CHA-C1B	3.38	1.48	1.40
26	PF	201	PEB	C2A-C1A	-3.38	1.49	1.52
26	JI	1002	PEB	C2A-C1A	-3.38	1.49	1.52
26	a2	203	PEB	C2C-C3C	3.38	1.47	1.37
26	s1	203	PEB	C1A-NA	-3.38	1.33	1.37
26	cE	202	PEB	CHA-C1B	3.38	1.48	1.40
26	MA	202	PEB	C2C-C3C	3.38	1.47	1.37
28	KF	1001	CYC	CHB-C4A	3.38	1.48	1.40
26	SD	202	PEB	C2C-C3C	3.38	1.47	1.37
26	y1	202	PEB	C1A-NA	-3.38	1.33	1.37
26	Y9	201	PEB	C1A-NA	-3.38	1.33	1.37
26	N1	203	PEB	C2C-C3C	3.38	1.47	1.37
26	WD	201	PEB	CHA-C1B	3.38	1.48	1.40
26	O8	202	PEB	C2C-C3C	3.37	1.47	1.37
26	CE	203	PEB	C2C-C3C	3.37	1.47	1.37
26	hE	202	PEB	C1A-NA	-3.37	1.33	1.37
26	bG	202	PEB	C2C-C3C	3.37	1.47	1.37
28	oH	1001	CYC	C2C-C1C	-3.37	1.49	1.52
27	A8	304	PUB	C3B-C2B	3.37	1.47	1.37
26	l6	201	PEB	C2C-C3C	3.37	1.47	1.37
26	aF	201	PEB	C2C-C3C	3.37	1.47	1.37
26	A3	202	PEB	CHA-C1B	3.37	1.48	1.40
26	w1	201	PEB	C1A-NA	-3.37	1.33	1.37
26	b7	202	PEB	C1A-NA	-3.37	1.33	1.37
26	GE	202	PEB	C3B-C2B	3.37	1.43	1.36
26	IG	201	PEB	CMB-C2B	-3.37	1.43	1.50
26	H6	1002	PEB	CHA-C1B	3.37	1.48	1.40
26	NI	1002	PEB	CHA-C1B	3.37	1.48	1.40
26	d6	201	PEB	C1A-NA	-3.37	1.33	1.37
26	pG	202	PEB	C1A-NA	-3.37	1.33	1.37
26	QA	204	PEB	C1A-NA	-3.37	1.33	1.37
26	TI	203	PEB	C1A-NA	-3.37	1.33	1.37
26	O7	201	PEB	C2C-C3C	3.37	1.47	1.37
26	iE	203	PEB	C2C-C3C	3.37	1.47	1.37
26	LI	1002	PEB	C2C-C3C	3.37	1.47	1.37
28	MI	1001	CYC	C3D-C2D	3.37	1.47	1.37
26	jF	202	PEB	OD-C4D	3.37	1.30	1.23
26	gG	202	PEB	C2C-C3C	3.37	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JI	1002	PEB	C2C-C3C	3.37	1.47	1.37
26	F9	203	PEB	C1A-NA	-3.37	1.33	1.37
26	K3	201	PEB	C2C-C3C	3.37	1.47	1.37
26	HC	202	PEB	C2C-C3C	3.37	1.47	1.37
26	IC	201	PEB	C2C-C3C	3.37	1.47	1.37
26	B3	203	PEB	C2C-C3C	3.37	1.47	1.37
26	E3	202	PEB	CHA-C1B	3.37	1.48	1.40
26	bB	202	PEB	CHA-C1B	3.37	1.48	1.40
26	U2	202	PEB	C1A-NA	-3.37	1.33	1.37
26	bF	203	PEB	C1A-NA	-3.37	1.33	1.37
28	C6	1001	CYC	C3D-C2D	3.37	1.47	1.37
26	e2	203	PEB	C2C-C3C	3.37	1.47	1.37
26	LJ	203	PEB	C2C-C3C	3.37	1.47	1.37
26	oG	201	PEB	CHA-C1B	3.37	1.48	1.40
26	EE	201	PEB	C2C-C3C	3.37	1.47	1.37
26	B1	201	PEB	C1A-NA	-3.37	1.33	1.37
26	n4	202	PEB	C1A-NA	-3.37	1.33	1.37
26	k6	201	PEB	C2C-C3C	3.37	1.47	1.37
26	Y8	203	PEB	C2C-C3C	3.37	1.47	1.37
26	C9	202	PEB	C2C-C3C	3.37	1.47	1.37
26	jF	203	PEB	CHA-C1B	3.37	1.48	1.40
26	gI	203	PEB	C1A-NA	-3.37	1.33	1.37
26	pG	201	PEB	CHA-C1B	3.37	1.48	1.40
26	HB	1002	PEB	C2C-C3C	3.37	1.47	1.37
26	eG	202	PEB	C2C-C3C	3.37	1.47	1.37
26	T1	202	PEB	C2A-C1A	-3.37	1.49	1.52
26	V2	201	PEB	C2C-C3C	3.37	1.47	1.37
26	F4	203	PEB	C2C-C3C	3.37	1.47	1.37
26	W6	201	PEB	C2C-C3C	3.37	1.47	1.37
26	hF	201	PEB	CHA-C1B	3.37	1.48	1.40
26	iE	203	PEB	OD-C4D	3.37	1.30	1.23
26	b7	203	PEB	C2C-C3C	3.37	1.47	1.37
26	qG	203	PEB	C2C-C3C	3.37	1.47	1.37
26	l7	201	PEB	CHA-C1B	3.37	1.48	1.40
26	VE	202	PEB	C1A-NA	-3.37	1.33	1.37
26	k1	201	PEB	C1A-NA	-3.36	1.33	1.37
26	p1	202	PEB	C1A-NA	-3.36	1.33	1.37
26	H9	201	PEB	C1A-NA	-3.36	1.33	1.37
26	L3	202	PEB	CHA-C1B	3.36	1.48	1.40
26	OI	201	PEB	CHA-C1B	3.36	1.48	1.40
26	G8	202	PEB	CHA-C1B	3.36	1.48	1.40
26	Q6	202	PEB	C2C-C3C	3.36	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P1	201	PEB	C1A-NA	-3.36	1.33	1.37
26	l8	202	PEB	C2C-C3C	3.36	1.47	1.37
26	RE	202	PEB	C2C-C3C	3.36	1.47	1.37
26	MJ	201	PEB	C2C-C3C	3.36	1.47	1.37
26	fB	203	PEB	CHA-C1B	3.36	1.48	1.40
26	D1	201	PEB	C2C-C3C	3.36	1.47	1.37
26	PG	201	PEB	C2C-C3C	3.36	1.47	1.37
26	hI	201	PEB	C2C-C3C	3.36	1.47	1.37
26	U4	202	PEB	C1A-NA	-3.36	1.33	1.37
26	m8	202	PEB	C1A-NA	-3.36	1.33	1.37
26	f6	201	PEB	CHA-C1B	3.36	1.48	1.40
26	ZB	203	PEB	C2C-C3C	3.36	1.47	1.37
26	cG	201	PEB	C2C-C3C	3.36	1.47	1.37
26	TJ	201	PEB	C2C-C3C	3.36	1.47	1.37
28	RH	1001	CYC	C3D-C2D	3.36	1.47	1.37
26	K4	202	PEB	C2C-C3C	3.36	1.47	1.37
26	nG	201	PEB	C2C-C3C	3.36	1.47	1.37
26	v1	202	PEB	CHA-C1B	3.36	1.48	1.40
26	F1	203	PEB	C2C-C3C	3.36	1.47	1.37
28	tH	1001	CYC	C3D-C2D	3.36	1.47	1.37
26	aI	202	PEB	CHA-C1B	3.36	1.48	1.40
26	VG	201	PEB	C2C-C3C	3.36	1.47	1.37
26	I3	202	PEB	CHA-C1B	3.36	1.48	1.40
26	UF	203	PEB	C2C-C3C	3.36	1.47	1.37
28	MI	1001	CYC	C1C-NC	-3.36	1.33	1.37
26	l2	202	PEB	C2C-C3C	3.36	1.47	1.37
26	oG	202	PEB	OD-C4D	3.36	1.30	1.23
26	c7	202	PEB	C2C-C3C	3.36	1.47	1.37
26	T9	201	PEB	C2C-C3C	3.36	1.47	1.37
26	G8	203	PEB	C1A-NA	-3.36	1.33	1.37
26	e6	202	PEB	CHA-C1B	3.36	1.48	1.40
26	g4	201	PEB	C2C-C3C	3.36	1.47	1.37
26	QB	202	PEB	C2C-C3C	3.36	1.47	1.37
26	lB	201	PEB	CHA-C1B	3.36	1.48	1.40
26	k2	202	PEB	CHA-C1B	3.36	1.48	1.40
26	V2	202	PEB	CHA-C1B	3.36	1.48	1.40
26	F4	202	PEB	CHA-C1B	3.36	1.48	1.40
26	g6	201	PEB	CHA-C1B	3.36	1.48	1.40
26	k7	202	PEB	C2C-C3C	3.36	1.47	1.37
26	U1	202	PEB	C1A-NA	-3.36	1.33	1.37
26	Q9	201	PEB	C1A-NA	-3.36	1.33	1.37
26	W1	202	PEB	C2C-C3C	3.36	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C1	202	PEB	C1A-NA	-3.36	1.33	1.37
26	f8	202	PEB	C1A-NA	-3.36	1.33	1.37
26	PB	202	PEB	C1A-NA	-3.36	1.33	1.37
26	LF	1002	PEB	C2C-C3C	3.36	1.47	1.37
26	ED	201	PEB	C2C-C3C	3.36	1.47	1.37
26	E4	202	PEB	C1A-NA	-3.36	1.33	1.37
26	v4	202	PEB	C1A-NA	-3.36	1.33	1.37
28	E2	1001	CYC	C3D-C2D	3.36	1.47	1.37
26	A9	301	PEB	CHA-C1B	3.36	1.48	1.40
26	fF	201	PEB	CHA-C1B	3.36	1.48	1.40
26	V1	203	PEB	C1A-NA	-3.36	1.33	1.37
26	Y2	201	PEB	C1A-NA	-3.36	1.33	1.37
26	YE	203	PEB	C1A-NA	-3.36	1.33	1.37
26	PD	201	PEB	C2C-C3C	3.36	1.47	1.37
26	V8	201	PEB	C2A-C1A	-3.35	1.49	1.52
26	hF	201	PEB	C2C-C3C	3.35	1.47	1.37
26	XJ	201	PEB	C2C-C3C	3.35	1.47	1.37
26	K9	201	PEB	C2C-C3C	3.35	1.47	1.37
26	BD	203	PEB	C2C-C3C	3.35	1.47	1.37
26	uE	202	PEB	C2C-C3C	3.35	1.47	1.37
26	CE	201	PEB	C1A-NA	-3.35	1.33	1.37
26	cG	202	PEB	C1A-NA	-3.35	1.33	1.37
26	q1	202	PEB	CHA-C1B	3.35	1.48	1.40
26	MA	203	PEB	C2C-C3C	3.35	1.47	1.37
26	dF	201	PEB	C1A-NA	-3.35	1.33	1.37
26	B9	201	PEB	C2A-C1A	-3.35	1.49	1.52
26	W9	202	PEB	C2C-C3C	3.35	1.47	1.37
26	BD	202	PEB	C2C-C3C	3.35	1.47	1.37
26	O7	203	PEB	C1A-NA	-3.35	1.33	1.37
26	E8	203	PEB	C1A-NA	-3.35	1.33	1.37
26	l7	202	PEB	C2C-C3C	3.35	1.47	1.37
26	YA	203	PEB	C2C-C3C	3.35	1.47	1.37
26	ME	201	PEB	C2C-C3C	3.35	1.47	1.37
26	HI	1002	PEB	CHA-C1B	3.35	1.48	1.40
26	cE	202	PEB	C2C-C3C	3.35	1.47	1.37
26	fG	201	PEB	C2C-C3C	3.35	1.47	1.37
26	L4	203	PEB	C1A-NA	-3.35	1.33	1.37
26	fA	203	PEB	C1A-NA	-3.35	1.33	1.37
26	u4	202	PEB	CHA-C1B	3.35	1.48	1.40
26	ZF	201	PEB	CHA-C1B	3.35	1.48	1.40
26	H3	201	PEB	C2C-C3C	3.35	1.47	1.37
26	dA	201	PEB	C2C-C3C	3.35	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	kB	201	PEB	C2C-C3C	3.35	1.47	1.37
26	W3	201	PEB	C1A-NA	-3.35	1.33	1.37
26	U7	203	PEB	C2C-C3C	3.35	1.47	1.37
26	M8	203	PEB	C2C-C3C	3.35	1.47	1.37
26	m6	201	PEB	C2C-C3C	3.35	1.47	1.37
26	Y8	203	PEB	CHA-C1B	3.35	1.48	1.40
26	d8	201	PEB	CHA-C1B	3.35	1.48	1.40
26	LD	203	PEB	C2C-C3C	3.35	1.47	1.37
28	uH	1001	CYC	C3D-C2D	3.35	1.47	1.37
26	O7	202	PEB	CHA-C1B	3.35	1.48	1.40
26	KJ	202	PEB	C2C-C3C	3.35	1.47	1.37
26	RG	202	PEB	C2A-C1A	-3.35	1.49	1.52
26	wG	301	PEB	C2C-C3C	3.35	1.47	1.37
26	U4	201	PEB	C2C-C3C	3.35	1.47	1.37
28	DF	1001	CYC	C3D-C2D	3.35	1.47	1.37
26	j4	201	PEB	C1A-NA	-3.35	1.33	1.37
26	W6	202	PEB	C1A-NA	-3.35	1.33	1.37
26	fB	201	PEB	CHA-C1B	3.35	1.48	1.40
26	y4	202	PEB	CHA-C1B	3.35	1.48	1.40
26	JC	201	PEB	C2C-C3C	3.35	1.47	1.37
26	lB	202	PEB	C1A-NA	-3.35	1.33	1.37
26	D9	201	PEB	CHA-C1B	3.35	1.48	1.40
26	lA	203	PEB	C2C-C3C	3.35	1.47	1.37
26	AE	201	PEB	C2C-C3C	3.35	1.47	1.37
26	uG	201	PEB	C2C-C3C	3.35	1.47	1.37
26	i1	202	PEB	CHA-C1B	3.35	1.48	1.40
26	W7	203	PEB	C1A-NA	-3.35	1.33	1.37
26	G8	202	PEB	C1A-NA	-3.35	1.33	1.37
26	D2	1002	PEB	C2C-C3C	3.35	1.47	1.37
26	MA	202	PEB	CHA-C1B	3.35	1.48	1.40
26	HB	1002	PEB	CHA-C1B	3.35	1.48	1.40
26	K6	201	PEB	C2C-C3C	3.35	1.47	1.37
26	hB	201	PEB	C2C-C3C	3.35	1.47	1.37
26	KE	202	PEB	C2C-C3C	3.35	1.47	1.37
26	C5	204	PEB	C1A-NA	-3.35	1.33	1.37
28	EI	1001	CYC	C3D-C2D	3.34	1.47	1.37
26	R9	203	PEB	C2C-C3C	3.34	1.47	1.37
26	VI	201	PEB	C2C-C3C	3.34	1.47	1.37
26	A9	304	PEB	C1A-NA	-3.34	1.33	1.37
26	aE	202	PEB	C2C-C3C	3.34	1.47	1.37
26	d7	201	PEB	CHA-C1B	3.34	1.48	1.40
26	J2	1002	PEB	C2C-C3C	3.34	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F2	1002	PEB	C2A-C1A	-3.34	1.49	1.52
26	lA	203	PEB	C1A-NA	-3.34	1.33	1.37
26	WB	201	PEB	C2C-C3C	3.34	1.47	1.37
26	K3	201	PEB	CHA-C1B	3.34	1.48	1.40
26	Y6	201	PEB	CHA-C1B	3.34	1.48	1.40
26	G8	201	PEB	C2C-C3C	3.34	1.47	1.37
26	J9	202	PEB	C2C-C3C	3.34	1.47	1.37
26	a2	202	PEB	CHA-C1B	3.34	1.48	1.40
26	cF	201	PEB	CHA-C1B	3.34	1.48	1.40
26	i1	201	PEB	C2C-C3C	3.34	1.47	1.37
26	JD	203	PEB	C2C-C3C	3.34	1.47	1.37
26	CG	203	PEB	C1A-NA	-3.34	1.33	1.37
26	GD	201	PEB	CHA-C1B	3.34	1.48	1.40
26	I1	202	PEB	C1A-NA	-3.34	1.33	1.37
26	AC	203	PEB	C1A-NA	-3.34	1.33	1.37
26	Y2	203	PEB	C2C-C3C	3.34	1.47	1.37
26	P6	201	PEB	C2C-C3C	3.34	1.47	1.37
26	E1	202	PEB	C1A-NA	-3.34	1.33	1.37
26	CE	202	PEB	C1A-NA	-3.34	1.33	1.37
26	ME	202	PEB	C1A-NA	-3.34	1.33	1.37
26	W4	202	PEB	C2C-C3C	3.34	1.47	1.37
26	C3	202	PEB	C2C-C3C	3.34	1.47	1.37
26	F3	201	PEB	C2C-C3C	3.34	1.47	1.37
26	T9	201	PEB	CHA-C1B	3.34	1.48	1.40
26	U8	202	PEB	C2C-C3C	3.34	1.47	1.37
26	JJ	202	PEB	C2C-C3C	3.34	1.47	1.37
26	CE	203	PEB	C1A-NA	-3.34	1.33	1.37
26	oE	202	PEB	C1A-NA	-3.34	1.33	1.37
26	Q8	202	PEB	C2A-C1A	-3.34	1.49	1.52
26	l8	201	PEB	CHA-C1B	3.34	1.48	1.40
26	bF	201	PEB	C2C-C3C	3.34	1.47	1.37
26	e2	202	PEB	CHA-C1B	3.34	1.48	1.40
26	rE	202	PEB	C2C-C3C	3.34	1.47	1.37
26	UA	203	PEB	CHA-C1B	3.34	1.48	1.40
26	FF	1002	PEB	C2A-C1A	-3.34	1.49	1.52
26	bG	201	PEB	C1A-NA	-3.34	1.33	1.37
26	bI	201	PEB	CHA-C1B	3.34	1.48	1.40
26	yG	301	PEB	C2C-C3C	3.34	1.47	1.37
26	Q7	203	PEB	C1A-NA	-3.34	1.33	1.37
26	YD	304	PEB	C1A-NA	-3.34	1.33	1.37
26	DG	202	PEB	C1A-NA	-3.34	1.33	1.37
26	S3	202	PEB	OD-C4D	3.34	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V4	202	PEB	C2C-C3C	3.34	1.47	1.37
26	OB	201	PEB	C2C-C3C	3.34	1.47	1.37
26	CG	203	PEB	C2C-C3C	3.34	1.47	1.37
26	A2	304	PEB	C1A-NA	-3.34	1.33	1.37
26	ZB	202	PEB	C2C-C3C	3.33	1.47	1.37
26	DG	202	PEB	C2A-C1A	-3.33	1.49	1.52
26	D6	1002	PEB	C2C-C3C	3.33	1.47	1.37
26	PI	203	PEB	C2C-C3C	3.33	1.47	1.37
28	D7	1001	CYC	C3D-C2D	3.33	1.47	1.37
26	mE	201	PEB	C2C-C3C	3.33	1.47	1.37
26	QD	202	PEB	CHA-C1B	3.33	1.48	1.40
26	SB	201	PEB	C2C-C3C	3.33	1.47	1.37
26	MG	202	PEB	C2C-C3C	3.33	1.47	1.37
26	f6	203	PEB	C2C-C3C	3.33	1.47	1.37
26	H2	1002	PEB	CHA-C1B	3.33	1.48	1.40
26	P2	203	PEB	C2C-C3C	3.33	1.47	1.37
26	YE	203	PEB	C2C-C3C	3.33	1.47	1.37
26	fE	201	PEB	C2C-C3C	3.33	1.47	1.37
27	wG	304	PUB	C3B-C2B	3.33	1.47	1.37
26	J4	203	PEB	C1A-NA	-3.33	1.33	1.37
26	e4	201	PEB	C1A-NA	-3.33	1.33	1.37
26	cE	203	PEB	OD-C4D	3.33	1.29	1.23
26	F5	201	PEB	C2C-C3C	3.33	1.47	1.37
26	G1	201	PEB	C2C-C3C	3.33	1.47	1.37
26	Z6	202	PEB	C2C-C3C	3.33	1.47	1.37
26	KD	201	PEB	CHA-C1B	3.33	1.48	1.40
26	h4	202	PEB	OD-C4D	3.33	1.29	1.23
26	i8	201	PEB	CHA-C1B	3.33	1.48	1.40
26	KB	201	PEB	C2C-C3C	3.33	1.47	1.37
26	O6	201	PEB	C2C-C3C	3.33	1.47	1.37
26	G8	203	PEB	CHA-C1B	3.33	1.48	1.40
26	rG	202	PEB	C1A-NA	-3.33	1.33	1.37
26	LD	201	PEB	C2C-C3C	3.33	1.47	1.37
26	YI	203	PEB	C2C-C3C	3.33	1.47	1.37
26	W7	201	PEB	CHA-C1B	3.33	1.48	1.40
26	UA	202	PEB	C2C-C3C	3.33	1.47	1.37
26	RD	203	PEB	C2C-C3C	3.33	1.47	1.37
26	AE	202	PEB	C2C-C3C	3.33	1.47	1.37
26	DI	1002	PEB	C1A-NA	-3.33	1.33	1.37
26	NJ	202	PEB	C1A-NA	-3.33	1.33	1.37
26	WF	201	PEB	C2C-C3C	3.33	1.47	1.37
26	CJ	202	PEB	C2C-C3C	3.33	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y1	202	PEB	C2C-C3C	3.33	1.47	1.37
26	l6	202	PEB	CHA-C1B	3.33	1.48	1.40
26	OA	203	PEB	C2A-C1A	-3.33	1.49	1.52
28	B6	1002	CYC	C4B-NB	-3.33	1.30	1.38
26	OG	203	PEB	C1A-NA	-3.33	1.33	1.37
26	cG	202	PEB	C2C-C3C	3.33	1.47	1.37
26	Y9	202	PEB	CHA-C1B	3.33	1.48	1.40
26	f4	202	PEB	C1A-NA	-3.33	1.33	1.37
26	h6	201	PEB	CHA-C1B	3.33	1.48	1.40
26	EE	202	PEB	CHA-C1B	3.33	1.48	1.40
26	eG	203	PEB	C1A-NA	-3.33	1.33	1.37
26	AJ	304	PEB	C1A-NA	-3.33	1.33	1.37
26	M8	202	PEB	C2C-C3C	3.33	1.47	1.37
26	HC	203	PEB	C2C-C3C	3.33	1.47	1.37
26	Y6	201	PEB	C2C-C3C	3.33	1.47	1.37
26	QG	202	PEB	C2C-C3C	3.33	1.47	1.37
26	lA	202	PEB	C1A-NA	-3.33	1.33	1.37
26	VD	201	PEB	CHA-C1B	3.32	1.48	1.40
26	H5	202	PEB	C2C-C3C	3.32	1.47	1.37
26	g6	201	PEB	C2C-C3C	3.32	1.47	1.37
26	KC	202	PEB	C2C-C3C	3.32	1.47	1.37
28	K6	202	CYC	C3D-C2D	3.32	1.47	1.37
26	E8	202	PEB	C2A-C1A	-3.32	1.49	1.52
26	OD	202	PEB	CHA-C1B	3.32	1.48	1.40
26	o1	501	PEB	C1A-NA	-3.32	1.33	1.37
26	hG	202	PEB	C1A-NA	-3.32	1.33	1.37
26	KC	201	PEB	C2A-C1A	-3.32	1.49	1.52
28	dH	1001	CYC	C2C-C1C	-3.32	1.49	1.52
28	KB	202	CYC	C3D-C2D	3.32	1.47	1.37
26	A3	201	PEB	CHA-C1B	3.32	1.48	1.40
26	L9	202	PEB	C2C-C3C	3.32	1.47	1.37
26	u4	202	PEB	C1A-NA	-3.32	1.33	1.37
26	dB	204	PEB	C1A-NA	-3.32	1.33	1.37
26	DB	1002	PEB	C2C-C3C	3.32	1.47	1.37
26	A9	301	PEB	C1A-NA	-3.32	1.33	1.37
26	LI	1002	PEB	C1A-NA	-3.32	1.33	1.37
26	S6	201	PEB	C2C-C3C	3.32	1.47	1.37
26	WJ	202	PEB	C2C-C3C	3.32	1.47	1.37
26	Z2	202	PEB	C2C-C3C	3.32	1.47	1.37
26	O8	201	PEB	C2A-C1A	-3.32	1.49	1.52
26	fA	203	PEB	CHA-C1B	3.32	1.48	1.40
26	i2	201	PEB	C2C-C3C	3.32	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h7	202	PEB	CHA-C1B	3.32	1.48	1.40
26	eI	202	PEB	CHA-C1B	3.32	1.48	1.40
26	B1	203	PEB	C2C-C3C	3.32	1.47	1.37
26	i4	201	PEB	C2C-C3C	3.32	1.47	1.37
26	Z8	201	PEB	C2C-C3C	3.32	1.47	1.37
26	jB	201	PEB	C2C-C3C	3.32	1.47	1.37
26	QF	203	PEB	C2C-C3C	3.32	1.47	1.37
26	E4	202	PEB	C2C-C3C	3.32	1.47	1.37
26	j7	203	PEB	C2C-C3C	3.32	1.47	1.37
26	GA	201	PEB	C2C-C3C	3.32	1.47	1.37
26	PB	201	PEB	C2C-C3C	3.32	1.47	1.37
26	l8	203	PEB	C2C-C3C	3.32	1.47	1.37
26	Z1	202	PEB	C2C-C3C	3.32	1.47	1.37
26	g8	201	PEB	C1A-NA	-3.32	1.33	1.37
26	qG	201	PEB	C1A-NA	-3.32	1.33	1.37
26	M8	202	PEB	CHA-C1B	3.32	1.48	1.40
26	EG	202	PEB	CHA-C1B	3.32	1.48	1.40
26	JC	202	PEB	CHA-C1B	3.32	1.48	1.40
26	yE	301	PEB	CHA-C1B	3.32	1.48	1.40
26	OD	202	PEB	OD-C4D	3.32	1.29	1.23
26	K4	202	PEB	C1A-NA	-3.32	1.33	1.37
26	m7	202	PEB	C1A-NA	-3.32	1.33	1.37
26	KC	203	PEB	C2C-C3C	3.32	1.47	1.37
26	F4	202	PEB	C1A-NA	-3.32	1.33	1.37
26	LD	203	PEB	C1A-NA	-3.32	1.33	1.37
26	kB	201	PEB	C1A-NA	-3.31	1.33	1.37
26	VI	202	PEB	CHA-C1B	3.31	1.48	1.40
26	EA	203	PEB	C2C-C3C	3.31	1.47	1.37
26	QF	201	PEB	C2C-C3C	3.31	1.47	1.37
26	h7	201	PEB	CHA-C1B	3.31	1.48	1.40
26	i2	203	PEB	C1A-NA	-3.31	1.33	1.37
26	I4	202	PEB	C1A-NA	-3.31	1.33	1.37
26	JA	201	PEB	C2C-C3C	3.31	1.47	1.37
26	PA	201	PEB	C2C-C3C	3.31	1.47	1.37
26	FJ	202	PEB	C2C-C3C	3.31	1.47	1.37
26	V1	202	PEB	C2C-C3C	3.31	1.47	1.37
26	hE	201	PEB	C2C-C3C	3.31	1.47	1.37
26	wE	301	PEB	C2C-C3C	3.31	1.47	1.37
26	LB	1002	PEB	C2C-C3C	3.31	1.47	1.37
26	lB	202	PEB	CHA-C1B	3.31	1.48	1.40
26	IC	203	PEB	C2C-C3C	3.31	1.47	1.37
26	ZI	202	PEB	C2C-C3C	3.31	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	i7	202	PEB	C1A-NA	-3.31	1.33	1.37
26	ZI	201	PEB	CHA-C1B	3.31	1.48	1.40
26	I3	202	PEB	OD-C4D	3.31	1.29	1.23
26	YD	303	PEB	C1A-NA	-3.31	1.33	1.37
26	lF	203	PEB	OD-C4D	3.31	1.29	1.23
26	AJ	304	PEB	CHA-C1B	3.31	1.48	1.40
26	RI	202	PEB	C2A-C1A	-3.31	1.49	1.52
26	Q6	203	PEB	C2C-C3C	3.31	1.47	1.37
26	aI	203	PEB	C2C-C3C	3.31	1.47	1.37
26	R2	202	PEB	C2A-C1A	-3.31	1.49	1.52
26	g4	201	PEB	C1A-NA	-3.31	1.33	1.37
26	GD	202	PEB	CHA-C1B	3.31	1.48	1.40
26	T2	203	PEB	C2C-C3C	3.31	1.47	1.37
26	SI	201	PEB	C2C-C3C	3.31	1.47	1.37
26	Y4	202	PEB	C2C-C3C	3.31	1.47	1.37
26	B9	202	PEB	C2C-C3C	3.31	1.47	1.37
26	L3	201	PEB	C2C-C3C	3.31	1.47	1.37
26	eE	203	PEB	C2C-C3C	3.31	1.47	1.37
26	HD	203	PEB	C2C-C3C	3.31	1.47	1.37
26	gG	201	PEB	C2C-C3C	3.31	1.47	1.37
28	KF	1001	CYC	C3D-C2D	3.31	1.47	1.37
26	k1	202	PEB	C2C-C3C	3.31	1.47	1.37
26	F5	203	PEB	C2C-C3C	3.31	1.47	1.37
26	Z2	201	PEB	CHA-C1B	3.31	1.48	1.40
26	JD	203	PEB	C1A-NA	-3.31	1.33	1.37
26	j2	201	PEB	C2C-C3C	3.31	1.47	1.37
26	N9	202	PEB	C2C-C3C	3.31	1.47	1.37
26	h6	203	PEB	C2C-C3C	3.31	1.47	1.37
26	GE	203	PEB	C1A-NA	-3.30	1.33	1.37
26	g1	203	PEB	C2C-C3C	3.30	1.47	1.37
26	kF	202	PEB	C2C-C3C	3.30	1.47	1.37
26	bB	202	PEB	C2C-C3C	3.30	1.47	1.37
26	A9	303	PEB	C1A-NA	-3.30	1.33	1.37
26	PA	202	PEB	C1A-NA	-3.30	1.33	1.37
26	AC	202	PEB	C1A-NA	-3.30	1.33	1.37
26	Q8	203	PEB	C2C-C3C	3.30	1.47	1.37
26	S8	201	PEB	C2C-C3C	3.30	1.47	1.37
26	FA	202	PEB	C2C-C3C	3.30	1.47	1.37
26	f8	203	PEB	CHA-C1B	3.30	1.48	1.40
26	L7	1002	PEB	C1A-NA	-3.30	1.33	1.37
26	yE	301	PEB	C2C-C3C	3.30	1.47	1.37
27	xG	305	PUB	C3B-C2B	3.30	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D4	202	PEB	CHA-C1B	3.30	1.48	1.40
26	MD	202	PEB	CHA-C1B	3.30	1.48	1.40
26	a4	203	PEB	C2C-C3C	3.30	1.47	1.37
26	U1	201	PEB	C2A-C1A	-3.30	1.49	1.52
26	jE	201	PEB	C2A-C1A	-3.30	1.49	1.52
26	U7	203	PEB	OD-C4D	3.30	1.29	1.23
26	k7	201	PEB	CHA-C1B	3.30	1.48	1.40
26	F9	203	PEB	CHA-C1B	3.30	1.48	1.40
26	A8	301	PEB	C2C-C3C	3.30	1.47	1.37
26	V2	203	PEB	C2C-C3C	3.30	1.47	1.37
26	S2	201	PEB	C2C-C3C	3.30	1.47	1.37
26	Y3	301	PEB	C2C-C3C	3.30	1.47	1.37
26	VG	202	PEB	C1A-NA	-3.30	1.33	1.37
26	AA	301	PEB	C2C-C3C	3.30	1.47	1.37
26	NJ	204	PEB	C2C-C3C	3.30	1.47	1.37
26	TI	203	PEB	C2C-C3C	3.30	1.47	1.37
26	V9	201	PEB	C2C-C3C	3.30	1.47	1.37
26	OA	203	PEB	CHA-C1B	3.30	1.48	1.40
26	A3	201	PEB	C2C-C3C	3.30	1.47	1.37
26	J5	202	PEB	C2A-C1A	-3.30	1.49	1.52
26	bF	201	PEB	CHA-C1B	3.30	1.48	1.40
26	DJ	203	PEB	C2C-C3C	3.30	1.47	1.37
26	ID	202	PEB	OD-C4D	3.30	1.29	1.23
26	OG	203	PEB	CHA-C1B	3.30	1.48	1.40
26	GG	201	PEB	C2A-C1A	-3.30	1.49	1.52
26	LJ	202	PEB	C2C-C3C	3.30	1.47	1.37
26	RD	201	PEB	C2C-C3C	3.30	1.47	1.37
26	MG	201	PEB	C2C-C3C	3.30	1.47	1.37
26	D8	201	PEB	C2A-C1A	-3.30	1.49	1.52
26	OF	202	PEB	C1A-NA	-3.30	1.33	1.37
26	jB	201	PEB	CHA-C1B	3.30	1.48	1.40
26	NF	1002	PEB	C2C-C3C	3.30	1.47	1.37
26	UG	201	PEB	C2C-C3C	3.30	1.47	1.37
26	ZI	201	PEB	C2C-C3C	3.30	1.47	1.37
26	OA	201	PEB	C1A-NA	-3.30	1.33	1.37
26	F9	202	PEB	OD-C4D	3.30	1.29	1.23
26	aG	202	PEB	C2C-C3C	3.30	1.47	1.37
26	S1	202	PEB	C2A-C1A	-3.30	1.49	1.52
26	k1	201	PEB	C2A-C1A	-3.30	1.49	1.52
26	l7	202	PEB	CHA-C1B	3.30	1.48	1.40
26	Q7	202	PEB	C1A-NA	-3.29	1.33	1.37
26	AC	201	PEB	C1A-NA	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ZE	201	PEB	CHA-C1B	3.29	1.48	1.40
28	MB	1001	CYC	C3D-C2D	3.29	1.47	1.37
26	U8	203	PEB	C2C-C3C	3.29	1.47	1.37
28	N7	1001	CYC	C3D-C2D	3.29	1.47	1.37
26	x1	202	PEB	C1A-NA	-3.29	1.33	1.37
26	ME	202	PEB	CHA-C1B	3.29	1.48	1.40
26	R2	203	PEB	C2C-C3C	3.29	1.47	1.37
26	UB	203	PEB	C2C-C3C	3.29	1.47	1.37
26	dI	201	PEB	C2C-C3C	3.29	1.47	1.37
26	aB	201	PEB	C2A-C1A	-3.29	1.49	1.52
26	L4	202	PEB	C1A-NA	-3.29	1.33	1.37
26	AI	305	PEB	C1A-NA	-3.29	1.33	1.37
26	RI	203	PEB	C2C-C3C	3.29	1.47	1.37
26	YD	301	PEB	CHA-C1B	3.29	1.48	1.40
26	t4	202	PEB	C4B-C3B	3.29	1.50	1.45
28	M6	1001	CYC	C3D-C2D	3.29	1.47	1.37
26	LA	202	PEB	C2C-C3C	3.29	1.47	1.37
26	T4	202	PEB	C2A-C1A	-3.29	1.49	1.52
26	cG	202	PEB	CHA-C1B	3.29	1.48	1.40
26	cF	202	PEB	C2C-C3C	3.29	1.47	1.37
26	L2	1002	PEB	C1A-NA	-3.29	1.33	1.37
26	SD	202	PEB	OD-C4D	3.29	1.29	1.23
28	CB	1001	CYC	C2C-C1C	-3.29	1.49	1.52
26	fB	203	PEB	C2C-C3C	3.29	1.47	1.37
26	h7	201	PEB	C2C-C3C	3.29	1.47	1.37
26	NA	202	PEB	C2C-C3C	3.29	1.47	1.37
26	RJ	202	PEB	C2C-C3C	3.29	1.47	1.37
28	IF	1001	CYC	C3D-C2D	3.29	1.47	1.37
26	AJ	301	PEB	CHA-C1B	3.29	1.48	1.40
26	ND	203	PEB	C2A-C1A	-3.29	1.49	1.52
26	c2	201	PEB	C2C-C3C	3.29	1.47	1.37
26	S7	201	PEB	C2C-C3C	3.29	1.47	1.37
26	M1	403	PEB	C1A-NA	-3.29	1.33	1.37
26	R1	203	PEB	C1A-NA	-3.29	1.33	1.37
26	bF	201	PEB	C1A-NA	-3.29	1.33	1.37
26	g1	202	PEB	CHA-C1B	3.29	1.48	1.40
26	YB	201	PEB	CHA-C1B	3.29	1.48	1.40
26	j6	201	PEB	C2C-C3C	3.29	1.47	1.37
28	II	1001	CYC	C3D-C2D	3.29	1.47	1.37
26	a8	204	PEB	CHA-C1B	3.29	1.48	1.40
26	b2	201	PEB	C2C-C3C	3.29	1.47	1.37
26	n1	201	PEB	C1A-NA	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PF	202	PEB	C2C-C3C	3.29	1.47	1.37
26	VI	203	PEB	C2C-C3C	3.29	1.47	1.37
26	F5	202	PEB	C2C-C3C	3.28	1.47	1.37
26	M3	202	PEB	CHA-C1B	3.28	1.48	1.40
26	PI	201	PEB	C2A-C1A	-3.28	1.49	1.52
26	l4	202	PEB	C1A-NA	-3.28	1.33	1.37
26	d2	201	PEB	C2C-C3C	3.28	1.47	1.37
26	h2	202	PEB	CHA-C1B	3.28	1.48	1.40
26	L2	1002	PEB	C2A-C1A	-3.28	1.49	1.52
26	W8	202	PEB	C2C-C3C	3.28	1.47	1.37
26	KE	203	PEB	C2C-C3C	3.28	1.47	1.37
26	U3	202	PEB	C1A-NA	-3.28	1.33	1.37
26	v4	201	PEB	C1A-NA	-3.28	1.33	1.37
28	KH	1001	CYC	CHB-C4A	3.28	1.48	1.40
26	mA	202	PEB	C2A-C1A	-3.28	1.49	1.52
26	UI	201	PEB	C2A-C1A	-3.28	1.49	1.52
26	hI	201	PEB	C2A-C1A	-3.28	1.49	1.52
26	CJ	201	PEB	C2A-C1A	-3.28	1.49	1.52
26	dI	201	PEB	C1A-NA	-3.28	1.33	1.37
26	N9	204	PEB	C2C-C3C	3.28	1.47	1.37
26	ZG	201	PEB	C2C-C3C	3.28	1.47	1.37
26	D9	201	PEB	C2A-C1A	-3.28	1.49	1.52
26	T4	202	PEB	C2C-C3C	3.28	1.47	1.37
26	i8	202	PEB	C2C-C3C	3.28	1.47	1.37
26	gB	201	PEB	C2C-C3C	3.28	1.47	1.37
26	U7	203	PEB	CHA-C1B	3.28	1.48	1.40
28	mH	1001	CYC	C1B-C2B	3.28	1.51	1.45
26	P1	202	PEB	C2C-C3C	3.28	1.47	1.37
26	q1	202	PEB	C2C-C3C	3.28	1.47	1.37
26	ff	203	PEB	CHA-C1B	3.28	1.48	1.40
26	bE	202	PEB	C1A-NA	-3.28	1.33	1.37
28	NB	1001	CYC	C1B-NB	-3.28	1.32	1.37
26	UE	201	PEB	C2C-C3C	3.28	1.47	1.37
26	aE	203	PEB	C2C-C3C	3.28	1.47	1.37
26	C8	202	PEB	CHA-C1B	3.28	1.48	1.40
26	m2	203	PEB	C1A-NA	-3.28	1.33	1.37
26	f6	203	PEB	CHA-C1B	3.28	1.48	1.40
26	BG	201	PEB	OD-C4D	3.28	1.29	1.23
26	UG	201	PEB	C3B-C2B	3.28	1.43	1.36
26	C5	203	PEB	C1A-NA	-3.28	1.33	1.37
26	hA	202	PEB	C1A-NA	-3.28	1.33	1.37
26	iA	201	PEB	C2C-C3C	3.28	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L1	202	PEB	C2C-C3C	3.28	1.47	1.37
26	K8	202	PEB	C1A-NA	-3.28	1.33	1.37
26	gG	202	PEB	CHA-C1B	3.28	1.48	1.40
26	yG	301	PEB	CHA-C1B	3.28	1.48	1.40
26	V4	203	PEB	C2C-C3C	3.28	1.47	1.37
26	lG	201	PEB	CHA-C1B	3.28	1.48	1.40
26	R4	203	PEB	C1A-NA	-3.28	1.33	1.37
26	m6	203	PEB	C1A-NA	-3.28	1.33	1.37
26	T2	203	PEB	C1A-NA	-3.28	1.33	1.37
26	G3	201	PEB	C1A-NA	-3.28	1.33	1.37
26	jB	201	PEB	C1A-NA	-3.28	1.33	1.37
26	E3	202	PEB	OD-C4D	3.28	1.29	1.23
26	B9	201	PEB	CHA-C1B	3.28	1.48	1.40
26	jE	201	PEB	C2C-C3C	3.27	1.47	1.37
26	mG	202	PEB	C2C-C3C	3.27	1.47	1.37
26	Q8	202	PEB	CHA-C1B	3.27	1.48	1.40
26	m1	203	PEB	C1A-NA	-3.27	1.33	1.37
26	TG	202	PEB	C2A-C1A	-3.27	1.49	1.52
26	f2	201	PEB	C2C-C3C	3.27	1.47	1.37
26	P4	202	PEB	C2C-C3C	3.27	1.47	1.37
26	y4	201	PEB	CHA-C1B	3.27	1.48	1.40
26	A2	305	PEB	C1A-NA	-3.27	1.33	1.37
26	K3	202	PEB	C1A-NA	-3.27	1.33	1.37
26	c4	203	PEB	C1A-NA	-3.27	1.33	1.37
27	B8	302	PUB	OD-C4D	3.27	1.29	1.23
26	C5	201	PEB	C1A-NA	-3.27	1.33	1.37
26	QE	201	PEB	C2C-C3C	3.27	1.47	1.37
26	gE	201	PEB	C2C-C3C	3.27	1.47	1.37
26	DI	1002	PEB	C2C-C3C	3.27	1.47	1.37
28	JI	1001	CYC	C2C-C1C	-3.27	1.49	1.52
26	P3	201	PEB	C2C-C3C	3.27	1.47	1.37
26	g4	203	PEB	CHA-C1B	3.27	1.48	1.40
26	WD	202	PEB	OD-C4D	3.27	1.29	1.23
26	R3	203	PEB	C2C-C3C	3.27	1.47	1.37
26	x1	202	PEB	OD-C4D	3.27	1.29	1.23
26	SE	203	PEB	C2C-C3C	3.27	1.47	1.37
26	D2	1002	PEB	C2A-C1A	-3.27	1.49	1.52
26	V1	203	PEB	C2C-C3C	3.27	1.47	1.37
26	YB	201	PEB	C2C-C3C	3.27	1.47	1.37
28	YH	1004	CYC	C3D-C2D	3.27	1.47	1.37
26	F9	202	PEB	C1A-NA	-3.27	1.33	1.37
26	vE	202	PEB	C1A-NA	-3.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D9	203	PEB	C2C-C3C	3.27	1.47	1.37
28	1H	1000	CYC	C3D-C2D	3.27	1.47	1.37
26	L5	203	PEB	C2C-C3C	3.27	1.47	1.37
26	EG	201	PEB	C2C-C3C	3.27	1.47	1.37
26	IE	203	PEB	C2A-C1A	-3.27	1.49	1.52
26	S6	203	PEB	CHA-C1B	3.27	1.48	1.40
28	I2	1001	CYC	C3D-C2D	3.27	1.47	1.37
26	i1	203	PEB	CHA-C1B	3.27	1.48	1.40
26	IE	202	PEB	CHA-C1B	3.27	1.48	1.40
28	NB	1001	CYC	C3D-C2D	3.27	1.47	1.37
26	j7	201	PEB	CHA-C1B	3.27	1.48	1.40
26	F1	202	PEB	C1A-NA	-3.27	1.33	1.37
26	l7	203	PEB	OD-C4D	3.27	1.29	1.23
26	T7	201	PEB	C2C-C3C	3.27	1.47	1.37
26	QA	203	PEB	C2C-C3C	3.27	1.47	1.37
26	U8	203	PEB	CHA-C1B	3.27	1.48	1.40
26	b2	202	PEB	C1A-NA	-3.27	1.33	1.37
26	g4	202	PEB	C1A-NA	-3.27	1.33	1.37
26	W8	202	PEB	C2A-C1A	-3.27	1.49	1.52
26	D9	202	PEB	C2A-C1A	-3.27	1.49	1.52
26	H4	202	PEB	C2C-C3C	3.27	1.47	1.37
26	SA	202	PEB	C2C-C3C	3.27	1.47	1.37
26	W7	201	PEB	C1A-NA	-3.26	1.33	1.37
26	O2	201	PEB	C2C-C3C	3.26	1.47	1.37
26	L9	201	PEB	C2C-C3C	3.26	1.47	1.37
28	E7	1001	CYC	C3D-C2D	3.26	1.47	1.37
26	l8	201	PEB	C2A-C1A	-3.26	1.49	1.52
26	SA	201	PEB	C2A-C1A	-3.26	1.49	1.52
26	UA	203	PEB	C2C-C3C	3.26	1.47	1.37
26	U6	201	PEB	CHA-C1B	3.26	1.48	1.40
26	TI	201	PEB	C2C-C3C	3.26	1.47	1.37
26	BJ	202	PEB	C2C-C3C	3.26	1.47	1.37
26	C9	201	PEB	CHA-C1B	3.26	1.48	1.40
26	F8	202	PEB	C2C-C3C	3.26	1.47	1.37
26	YI	201	PEB	C1A-NA	-3.26	1.33	1.37
26	NI	1002	PEB	C2C-C3C	3.26	1.47	1.37
28	K2	1001	CYC	C3D-C2D	3.26	1.47	1.37
28	KI	1001	CYC	C3D-C2D	3.26	1.47	1.37
26	E3	201	PEB	C2C-C3C	3.26	1.47	1.37
26	QA	202	PEB	CHA-C1B	3.26	1.48	1.40
26	DJ	201	PEB	CHA-C1B	3.26	1.48	1.40
26	J8	201	PEB	C2C-C3C	3.26	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T2	201	PEB	C2A-C1A	-3.26	1.49	1.52
26	GE	201	PEB	C2A-C1A	-3.26	1.49	1.52
26	g4	203	PEB	C2C-C3C	3.26	1.47	1.37
26	b7	201	PEB	C1A-NA	-3.26	1.33	1.37
26	QG	201	PEB	C1A-NA	-3.26	1.33	1.37
28	JF	1003	CYC	C3D-C2D	3.26	1.47	1.37
26	H5	201	PEB	C2C-C3C	3.26	1.47	1.37
26	HD	202	PEB	C2C-C3C	3.26	1.47	1.37
26	QG	202	PEB	OD-C4D	3.26	1.29	1.23
26	h2	201	PEB	C2C-C3C	3.26	1.47	1.37
26	G5	203	PEB	C1A-NA	-3.26	1.33	1.37
26	X9	203	PEB	C1A-NA	-3.26	1.33	1.37
26	FD	201	PEB	C1A-NA	-3.26	1.33	1.37
26	kI	201	PEB	C1A-NA	-3.26	1.33	1.37
26	UE	201	PEB	C3B-C2B	3.26	1.43	1.36
26	cA	202	PEB	C2C-C3C	3.26	1.47	1.37
26	H2	1002	PEB	C2C-C3C	3.26	1.47	1.37
26	T7	202	PEB	C2C-C3C	3.26	1.47	1.37
26	ME	203	PEB	C2C-C3C	3.26	1.47	1.37
26	NJ	202	PEB	C2C-C3C	3.26	1.47	1.37
26	k1	203	PEB	C2C-C3C	3.25	1.47	1.37
26	J4	202	PEB	C1A-NA	-3.25	1.33	1.37
26	W8	202	PEB	C3C-C4C	3.25	1.47	1.42
26	KD	202	PEB	OD-C4D	3.25	1.29	1.23
26	Q3	202	PEB	OD-C4D	3.25	1.29	1.23
26	O2	201	PEB	CHA-C1B	3.25	1.48	1.40
26	A5	202	PEB	C1A-NA	-3.25	1.33	1.37
26	l8	202	PEB	C1A-NA	-3.25	1.33	1.37
26	bI	202	PEB	C1A-NA	-3.25	1.33	1.37
26	SA	201	PEB	CHA-C1B	3.25	1.48	1.40
26	H5	203	PEB	C2C-C3C	3.25	1.47	1.37
26	HA	201	PEB	C2C-C3C	3.25	1.47	1.37
28	F7	1001	CYC	C1C-NC	-3.25	1.33	1.37
26	W3	202	PEB	OD-C4D	3.25	1.29	1.23
26	S4	202	PEB	C2C-C3C	3.25	1.47	1.37
26	WD	202	PEB	C2C-C3C	3.25	1.47	1.37
26	aG	203	PEB	C2C-C3C	3.25	1.47	1.37
26	x4	201	PEB	C1A-NA	-3.25	1.33	1.37
26	h8	202	PEB	C1A-NA	-3.25	1.33	1.37
26	Y3	301	PEB	CHA-C1B	3.25	1.48	1.40
26	BC	201	PEB	C1A-NA	-3.25	1.33	1.37
26	Q8	204	PEB	C2C-C3C	3.25	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	LC	203	PEB	C2A-C1A	-3.25	1.49	1.52
26	SB	202	PEB	C2C-C3C	3.25	1.47	1.37
26	KG	203	PEB	C2C-C3C	3.25	1.47	1.37
26	m4	203	PEB	C1A-NA	-3.25	1.33	1.37
26	24	405	PEB	C1A-NA	-3.25	1.33	1.37
26	L3	202	PEB	C2A-C1A	-3.25	1.49	1.52
26	L5	202	PEB	CHA-C1B	3.25	1.48	1.40
26	HI	1002	PEB	C2C-C3C	3.25	1.47	1.37
26	N4	202	PEB	C2C-C3C	3.25	1.47	1.37
26	DF	1002	PEB	C1A-NA	-3.25	1.33	1.37
26	SG	203	PEB	C2C-C3C	3.25	1.47	1.37
26	a2	202	PEB	C2A-C1A	-3.25	1.49	1.52
26	IE	201	PEB	C2C-C3C	3.25	1.47	1.37
26	gE	203	PEB	C2C-C3C	3.25	1.47	1.37
26	jF	202	PEB	C1A-NA	-3.25	1.33	1.37
26	OG	201	PEB	C1A-NA	-3.25	1.33	1.37
26	UE	202	PEB	C2C-C3C	3.25	1.47	1.37
26	M1	401	PEB	CHA-C1B	3.25	1.48	1.40
26	N8	202	PEB	C2C-C3C	3.25	1.47	1.37
26	VA	201	PEB	C2C-C3C	3.25	1.47	1.37
26	R6	202	PEB	C2A-C1A	-3.25	1.49	1.52
26	tG	201	PEB	C2A-C1A	-3.25	1.49	1.52
26	a8	201	PEB	CHA-C1B	3.25	1.48	1.40
26	Z2	201	PEB	C2C-C3C	3.25	1.47	1.37
26	SA	203	PEB	CHA-C1B	3.25	1.48	1.40
26	U3	201	PEB	CHA-C1B	3.25	1.48	1.40
26	PF	202	PEB	C2A-C1A	-3.24	1.49	1.52
26	F3	202	PEB	C1A-NA	-3.24	1.33	1.37
26	X9	201	PEB	C1A-NA	-3.24	1.33	1.37
26	H4	202	PEB	CHA-C1B	3.24	1.48	1.40
26	N2	1002	PEB	C2C-C3C	3.24	1.47	1.37
26	11	202	PEB	CHA-C1B	3.24	1.48	1.40
26	RF	202	PEB	C1A-NA	-3.24	1.33	1.37
26	Q3	202	PEB	CHA-C1B	3.24	1.48	1.40
26	w1	202	PEB	CHA-C1B	3.24	1.48	1.40
26	T1	202	PEB	C2C-C3C	3.24	1.47	1.37
26	G4	201	PEB	C2C-C3C	3.24	1.47	1.37
26	WE	202	PEB	C2C-C3C	3.24	1.47	1.37
26	kG	203	PEB	C2C-C3C	3.24	1.47	1.37
26	xE	302	PEB	CHA-C1B	3.24	1.48	1.40
26	j1	201	PEB	C1A-NA	-3.24	1.33	1.37
26	Z4	202	PEB	C2C-C3C	3.24	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	lF	201	PEB	CHA-C1B	3.24	1.48	1.40
26	BJ	201	PEB	CHA-C1B	3.24	1.48	1.40
26	A7	305	PEB	C1A-NA	-3.24	1.33	1.37
26	E3	201	PEB	CHA-C1B	3.24	1.48	1.40
26	M9	202	PEB	C1A-NA	-3.24	1.33	1.37
26	QA	202	PEB	C2A-C1A	-3.24	1.49	1.52
26	mI	203	PEB	C1A-NA	-3.24	1.33	1.37
26	m1	201	PEB	CHA-C1B	3.24	1.48	1.40
26	H8	201	PEB	C2C-C3C	3.24	1.47	1.37
26	L3	203	PEB	C2C-C3C	3.24	1.47	1.37
26	LJ	201	PEB	C2C-C3C	3.24	1.47	1.37
26	uE	203	PEB	C1A-NA	-3.24	1.33	1.37
28	NF	1001	CYC	C3D-C2D	3.24	1.47	1.37
26	IE	201	PEB	C3B-C2B	3.24	1.43	1.36
26	S8	201	PEB	C2A-C1A	-3.24	1.49	1.52
26	DE	201	PEB	C2C-C3C	3.24	1.47	1.37
26	A3	201	PEB	C1A-NA	-3.24	1.33	1.37
26	S1	202	PEB	C2C-C3C	3.24	1.47	1.37
26	GA	202	PEB	C1A-NA	-3.23	1.33	1.37
26	a1	203	PEB	C2C-C3C	3.23	1.47	1.37
26	UG	202	PEB	C2C-C3C	3.23	1.47	1.37
26	IE	202	PEB	C2C-C3C	3.23	1.47	1.37
26	f4	201	PEB	C1A-NA	-3.23	1.33	1.37
26	D9	203	PEB	C1A-NA	-3.23	1.33	1.37
26	i1	202	PEB	C2C-C3C	3.23	1.47	1.37
26	iE	201	PEB	CHA-C1B	3.23	1.48	1.40
26	K5	202	PEB	C2C-C3C	3.23	1.47	1.37
28	YH	1002	CYC	C1B-C2B	3.23	1.50	1.45
26	eF	202	PEB	C1A-NA	-3.23	1.33	1.37
26	UG	202	PEB	OD-C4D	3.23	1.29	1.23
26	iA	202	PEB	C2C-C3C	3.23	1.47	1.37
26	h6	201	PEB	C2C-C3C	3.23	1.47	1.37
26	LF	1002	PEB	C2A-C1A	-3.23	1.49	1.52
26	l7	203	PEB	C1A-NA	-3.23	1.33	1.37
28	hH	1001	CYC	C1B-C2B	3.23	1.50	1.45
26	cB	202	PEB	C1A-NA	-3.23	1.33	1.37
26	IG	202	PEB	C2C-C3C	3.23	1.47	1.37
26	T9	203	PEB	C1A-NA	-3.23	1.33	1.37
26	DD	201	PEB	C1A-NA	-3.23	1.33	1.37
26	iF	202	PEB	C1A-NA	-3.23	1.33	1.37
26	MJ	202	PEB	C1A-NA	-3.23	1.33	1.37
26	I5	201	PEB	C2C-C3C	3.23	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m4	202	PEB	C1A-NA	-3.23	1.33	1.37
26	D4	202	PEB	C2C-C3C	3.23	1.47	1.37
26	24	404	PEB	C1A-NA	-3.23	1.33	1.37
26	DI	1002	PEB	C2A-C1A	-3.23	1.49	1.52
26	eE	203	PEB	OD-C4D	3.23	1.29	1.23
26	oG	202	PEB	C1A-NA	-3.23	1.33	1.37
26	fA	203	PEB	C2C-C3C	3.23	1.47	1.37
26	eB	202	PEB	C1A-NA	-3.23	1.33	1.37
26	U4	201	PEB	C2A-C1A	-3.23	1.49	1.52
26	H5	203	PEB	C2A-C1A	-3.23	1.49	1.52
26	RE	202	PEB	C2A-C1A	-3.23	1.49	1.52
26	Q7	202	PEB	C2C-C3C	3.23	1.47	1.37
26	MG	203	PEB	C2C-C3C	3.23	1.47	1.37
26	bI	201	PEB	C2C-C3C	3.23	1.47	1.37
26	C3	202	PEB	C1A-NA	-3.23	1.33	1.37
26	i4	202	PEB	C1A-NA	-3.23	1.33	1.37
26	R7	201	PEB	C1A-NA	-3.23	1.33	1.37
26	J1	201	PEB	C2C-C3C	3.23	1.47	1.37
26	d4	202	PEB	CHA-C1B	3.23	1.48	1.40
26	S8	202	PEB	C2C-C3C	3.22	1.47	1.37
26	WD	202	PEB	C1A-NA	-3.22	1.33	1.37
26	W6	203	PEB	CHA-C1B	3.22	1.48	1.40
28	LF	1001	CYC	C3D-C2D	3.22	1.47	1.37
26	YE	201	PEB	C1A-NA	-3.22	1.33	1.37
26	S8	203	PEB	CHA-C1B	3.22	1.48	1.40
26	S1	201	PEB	C2A-C1A	-3.22	1.49	1.52
26	yG	301	PEB	C2A-C1A	-3.22	1.49	1.52
26	Y4	201	PEB	C2C-C3C	3.22	1.47	1.37
26	c7	202	PEB	C1A-NA	-3.22	1.33	1.37
26	dF	203	PEB	C1A-NA	-3.22	1.33	1.37
28	C7	1001	CYC	C1C-NC	-3.22	1.33	1.37
26	DG	201	PEB	C2C-C3C	3.22	1.47	1.37
26	SB	203	PEB	CHA-C1B	3.22	1.48	1.40
26	H1	203	PEB	C1A-NA	-3.22	1.33	1.37
26	H4	202	PEB	C1A-NA	-3.22	1.33	1.37
26	YA	202	PEB	C2C-C3C	3.22	1.47	1.37
26	lB	201	PEB	C2C-C3C	3.22	1.47	1.37
28	N7	1001	CYC	C2C-C1C	-3.22	1.49	1.52
26	R3	201	PEB	C2C-C3C	3.22	1.47	1.37
26	TF	202	PEB	C2C-C3C	3.22	1.47	1.37
26	XD	203	PEB	C2C-C3C	3.22	1.47	1.37
26	uG	203	PEB	C1A-NA	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	DF	1001	CYC	C1C-NC	-3.22	1.33	1.37
26	Y8	201	PEB	CHA-C1B	3.22	1.48	1.40
26	bE	201	PEB	C2A-C1A	-3.22	1.49	1.52
26	G3	202	PEB	C1A-NA	-3.22	1.33	1.37
26	wE	301	PEB	CHA-C1B	3.22	1.48	1.40
26	T2	201	PEB	C2C-C3C	3.22	1.47	1.37
28	FF	1001	CYC	C3D-C2D	3.22	1.47	1.37
26	L7	1002	PEB	CHA-C1B	3.22	1.48	1.40
26	VA	201	PEB	C2A-C1A	-3.22	1.49	1.52
26	R9	201	PEB	C1A-NA	-3.22	1.33	1.37
26	FC	202	PEB	C1A-NA	-3.22	1.33	1.37
26	TF	201	PEB	C2C-C3C	3.22	1.47	1.37
28	FF	1001	CYC	C2C-C1C	-3.22	1.49	1.52
26	JJ	201	PEB	C2C-C3C	3.22	1.47	1.37
26	G9	202	PEB	C1A-NA	-3.22	1.33	1.37
27	A6	302	PUB	C3B-C2B	3.22	1.47	1.37
26	sG	203	PEB	C2C-C3C	3.22	1.47	1.37
26	T9	202	PEB	C1A-NA	-3.22	1.33	1.37
26	XJ	202	PEB	C1A-NA	-3.22	1.33	1.37
26	X9	201	PEB	CHA-C1B	3.22	1.48	1.40
26	Y8	202	PEB	C2C-C3C	3.22	1.47	1.37
26	hB	203	PEB	C2C-C3C	3.22	1.47	1.37
26	OD	201	PEB	CHA-C1B	3.22	1.48	1.40
26	mG	202	PEB	C1A-NA	-3.22	1.33	1.37
26	Q1	201	PEB	C2C-C3C	3.22	1.47	1.37
26	KC	201	PEB	C2C-C3C	3.22	1.47	1.37
26	h7	203	PEB	C1A-NA	-3.22	1.33	1.37
26	lA	201	PEB	C1A-NA	-3.21	1.33	1.37
26	kF	202	PEB	C2A-C1A	-3.21	1.49	1.52
26	QG	201	PEB	C2C-C3C	3.21	1.47	1.37
27	24	403	PUB	C3B-C2B	3.21	1.47	1.37
26	oG	203	PEB	C1A-NA	-3.21	1.33	1.37
26	I8	202	PEB	C2C-C3C	3.21	1.47	1.37
26	J7	1002	PEB	C1A-NA	-3.21	1.33	1.37
26	S7	203	PEB	C1A-NA	-3.21	1.33	1.37
26	QI	201	PEB	C2C-C3C	3.21	1.47	1.37
26	H9	202	PEB	C2C-C3C	3.21	1.47	1.37
26	SA	201	PEB	C2C-C3C	3.21	1.47	1.37
26	d2	201	PEB	CHA-C1B	3.21	1.47	1.40
26	x4	202	PEB	C1A-NA	-3.21	1.33	1.37
26	V4	202	PEB	OD-C4D	3.21	1.29	1.23
26	oE	202	PEB	OD-C4D	3.21	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VD	203	PEB	C2C-C3C	3.21	1.47	1.37
26	K5	203	PEB	C2C-C3C	3.21	1.47	1.37
26	F9	202	PEB	C2C-C3C	3.21	1.47	1.37
26	k2	203	PEB	C1A-NA	-3.21	1.33	1.37
26	dF	201	PEB	CHA-C1B	3.21	1.47	1.40
26	WA	202	PEB	C3C-C4C	3.21	1.47	1.42
26	B5	201	PEB	C1A-NA	-3.21	1.33	1.37
26	bG	202	PEB	C1A-NA	-3.21	1.33	1.37
26	UE	202	PEB	OD-C4D	3.21	1.29	1.23
26	GD	202	PEB	C1A-NA	-3.21	1.33	1.37
26	aG	201	PEB	C2C-C3C	3.21	1.47	1.37
26	L8	202	PEB	C2C-C3C	3.21	1.47	1.37
26	CC	202	PEB	C1A-NA	-3.21	1.33	1.37
26	iE	202	PEB	C2C-C3C	3.21	1.47	1.37
26	VF	203	PEB	C2A-C1A	-3.21	1.49	1.52
26	V8	202	PEB	C1A-NA	-3.21	1.33	1.37
26	jG	201	PEB	C2C-C3C	3.21	1.47	1.37
26	D1	202	PEB	CHA-C1B	3.21	1.47	1.40
26	XE	201	PEB	C2C-C3C	3.20	1.47	1.37
26	w1	201	PEB	C4B-C3B	3.20	1.50	1.45
26	OI	201	PEB	C2C-C3C	3.20	1.47	1.37
26	hI	202	PEB	C1A-NA	-3.20	1.33	1.37
26	RE	201	PEB	C2C-C3C	3.20	1.47	1.37
26	qE	203	PEB	OD-C4D	3.20	1.29	1.23
26	SF	201	PEB	C2C-C3C	3.20	1.47	1.37
26	s4	202	PEB	C1A-NA	-3.20	1.33	1.37
26	M3	201	PEB	CHA-C1B	3.20	1.47	1.40
26	Q4	201	PEB	C2C-C3C	3.20	1.47	1.37
26	YA	201	PEB	CHA-C1B	3.20	1.47	1.40
26	CA	202	PEB	C1A-NA	-3.20	1.33	1.37
26	rE	202	PEB	C1A-NA	-3.20	1.33	1.37
26	AF	302	PEB	C1A-NA	-3.20	1.33	1.37
26	W7	203	PEB	C2C-C3C	3.20	1.47	1.37
26	cI	202	PEB	C2C-C3C	3.20	1.47	1.37
26	iG	202	PEB	C2C-C3C	3.20	1.47	1.37
28	HF	1001	CYC	C3D-C2D	3.20	1.47	1.37
26	fI	201	PEB	C2C-C3C	3.20	1.47	1.37
26	D3	201	PEB	CHA-C1B	3.20	1.47	1.40
26	W3	201	PEB	C2A-C1A	-3.20	1.49	1.52
26	K8	203	PEB	C2A-C1A	-3.20	1.49	1.52
26	DJ	202	PEB	C2A-C1A	-3.20	1.49	1.52
26	f6	203	PEB	C1A-NA	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cE	201	PEB	CHA-C1B	3.20	1.47	1.40
26	UF	203	PEB	CHA-C1B	3.20	1.47	1.40
26	N9	202	PEB	C1A-NA	-3.20	1.33	1.37
26	W9	201	PEB	C1A-NA	-3.20	1.33	1.37
26	i8	201	PEB	C2C-C3C	3.20	1.47	1.37
26	d6	202	PEB	C2C-C3C	3.20	1.47	1.37
26	w1	202	PEB	C2C-C3C	3.20	1.47	1.37
26	V2	203	PEB	C1A-NA	-3.20	1.33	1.37
26	j6	201	PEB	C1A-NA	-3.20	1.33	1.37
26	D9	203	PEB	OD-C4D	3.20	1.29	1.23
26	Y1	201	PEB	C2A-C1A	-3.20	1.49	1.52
26	hE	201	PEB	C2A-C1A	-3.20	1.49	1.52
26	s4	202	PEB	C2A-C1A	-3.20	1.49	1.52
26	E8	201	PEB	C2A-C1A	-3.20	1.49	1.52
26	F2	1002	PEB	C2C-C3C	3.20	1.47	1.37
28	LF	1001	CYC	C1B-C2B	3.20	1.50	1.45
26	N2	1002	PEB	C2A-C1A	-3.20	1.49	1.52
26	dE	201	PEB	C2A-C1A	-3.20	1.49	1.52
28	C6	1001	CYC	C2C-C1C	-3.20	1.49	1.52
26	wG	301	PEB	CHA-C1B	3.20	1.47	1.40
26	L1	203	PEB	C1A-NA	-3.20	1.33	1.37
26	t4	201	PEB	C1A-NA	-3.20	1.33	1.37
26	N1	202	PEB	C2C-C3C	3.20	1.47	1.37
26	ED	202	PEB	OD-C4D	3.19	1.29	1.23
26	H3	202	PEB	C2C-C3C	3.19	1.47	1.37
26	IG	202	PEB	CHA-C1B	3.19	1.47	1.40
26	aE	201	PEB	C2C-C3C	3.19	1.47	1.37
26	KA	201	PEB	C2C-C3C	3.19	1.47	1.37
26	e6	202	PEB	C1A-NA	-3.19	1.33	1.37
26	Q4	202	PEB	C2C-C3C	3.19	1.47	1.37
26	hA	201	PEB	C2C-C3C	3.19	1.47	1.37
26	M4	401	PEB	CHA-C1B	3.19	1.47	1.40
26	L1	202	PEB	C1A-NA	-3.19	1.33	1.37
26	A7	302	PEB	C1A-NA	-3.19	1.33	1.37
26	FI	1002	PEB	C2C-C3C	3.19	1.47	1.37
26	P1	202	PEB	C2A-C1A	-3.19	1.49	1.52
26	m8	202	PEB	C2A-C1A	-3.19	1.49	1.52
26	j8	203	PEB	C1A-NA	-3.19	1.33	1.37
28	YH	1004	CYC	C1B-C2B	3.19	1.50	1.45
26	K8	201	PEB	C2C-C3C	3.19	1.47	1.37
26	GG	203	PEB	OD-C4D	3.19	1.29	1.23
26	UD	202	PEB	CHA-C1B	3.19	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W8	201	PEB	C2C-C3C	3.19	1.47	1.37
26	kB	201	PEB	C2A-C1A	-3.19	1.49	1.52
26	QA	204	PEB	C2C-C3C	3.19	1.47	1.37
26	eG	203	PEB	C2C-C3C	3.19	1.47	1.37
26	mB	202	PEB	C2C-C3C	3.19	1.47	1.37
26	J5	201	PEB	C2C-C3C	3.19	1.47	1.37
26	k4	201	PEB	C1A-NA	-3.19	1.33	1.37
26	V8	201	PEB	C2C-C3C	3.19	1.47	1.37
26	JE	201	PEB	C2C-C3C	3.19	1.47	1.37
26	c4	203	PEB	C2C-C3C	3.19	1.47	1.37
26	mE	201	PEB	CHA-C1B	3.19	1.47	1.40
26	X9	201	PEB	C2C-C3C	3.19	1.47	1.37
26	IC	202	PEB	C2C-C3C	3.19	1.47	1.37
28	NI	1001	CYC	C3D-C2D	3.19	1.47	1.37
26	Q1	202	PEB	C2C-C3C	3.19	1.47	1.37
26	k1	203	PEB	OD-C4D	3.19	1.29	1.23
26	j1	202	PEB	C1A-NA	-3.19	1.33	1.37
26	Q7	201	PEB	C1A-NA	-3.19	1.33	1.37
26	g1	203	PEB	OD-C4D	3.19	1.29	1.23
26	M3	201	PEB	C2A-C1A	-3.18	1.49	1.52
26	X3	203	PEB	C2C-C3C	3.18	1.47	1.37
26	N4	201	PEB	C2C-C3C	3.18	1.47	1.37
26	c2	202	PEB	C2C-C3C	3.18	1.47	1.37
26	Y4	201	PEB	C2A-C1A	-3.18	1.49	1.52
26	GA	201	PEB	C2A-C1A	-3.18	1.49	1.52
26	l8	201	PEB	C1A-NA	-3.18	1.33	1.37
26	A3	202	PEB	OD-C4D	3.18	1.29	1.23
28	G6	1001	CYC	C3D-C2D	3.18	1.47	1.37
26	g1	202	PEB	OD-C4D	3.18	1.29	1.23
26	H8	202	PEB	C2C-C3C	3.18	1.47	1.37
26	N1	201	PEB	C2C-C3C	3.18	1.47	1.37
26	NJ	203	PEB	C1A-NA	-3.18	1.33	1.37
26	S8	203	PEB	C2A-C1A	-3.18	1.49	1.52
26	X4	202	PEB	C2C-C3C	3.18	1.47	1.37
26	GC	203	PEB	C1A-NA	-3.18	1.33	1.37
26	uG	202	PEB	C1A-NA	-3.18	1.33	1.37
26	GJ	202	PEB	C1A-NA	-3.18	1.33	1.37
26	YG	203	PEB	OD-C4D	3.18	1.29	1.23
26	GE	203	PEB	CHA-C1B	3.18	1.47	1.40
26	V3	203	PEB	C2C-C3C	3.18	1.47	1.37
26	tG	202	PEB	C1A-NA	-3.18	1.33	1.37
26	VI	203	PEB	C1A-NA	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UE	202	PEB	CHA-C1B	3.18	1.47	1.40
26	g1	201	PEB	C2C-C3C	3.18	1.47	1.37
26	b6	202	PEB	C2C-C3C	3.18	1.47	1.37
26	dB	202	PEB	C2C-C3C	3.18	1.47	1.37
26	UF	201	PEB	C2C-C3C	3.18	1.47	1.37
26	U6	203	PEB	OD-C4D	3.18	1.29	1.23
26	IA	202	PEB	C2C-C3C	3.18	1.47	1.37
26	T7	202	PEB	C1A-NA	-3.18	1.33	1.37
26	a6	201	PEB	C2A-C1A	-3.18	1.49	1.52
26	V7	202	PEB	C2A-C1A	-3.18	1.49	1.52
26	J1	202	PEB	CHA-C1B	3.18	1.47	1.40
26	r1	202	PEB	C1A-NA	-3.18	1.33	1.37
26	AF	305	PEB	C1A-NA	-3.18	1.33	1.37
26	u4	202	PEB	C2C-C3C	3.18	1.47	1.37
26	MD	201	PEB	CHA-C1B	3.18	1.47	1.40
26	WA	201	PEB	C2C-C3C	3.18	1.47	1.37
26	HA	202	PEB	C2C-C3C	3.17	1.47	1.37
26	DD	202	PEB	CHA-C1B	3.17	1.47	1.40
26	sG	202	PEB	OD-C4D	3.17	1.29	1.23
26	g4	203	PEB	C1A-NA	-3.17	1.33	1.37
26	J9	202	PEB	C1A-NA	-3.17	1.33	1.37
26	mG	201	PEB	C2C-C3C	3.17	1.47	1.37
26	P9	201	PEB	C2C-C3C	3.17	1.47	1.37
26	IG	201	PEB	C2C-C3C	3.17	1.47	1.37
28	GB	1001	CYC	C3D-C2D	3.17	1.47	1.37
28	J2	1001	CYC	C2C-C1C	-3.17	1.49	1.52
26	D4	201	PEB	C2C-C3C	3.17	1.47	1.37
26	U7	201	PEB	C2C-C3C	3.17	1.47	1.37
26	ZA	202	PEB	C2C-C3C	3.17	1.47	1.37
26	GE	203	PEB	OD-C4D	3.17	1.29	1.23
26	KB	201	PEB	C2A-C1A	-3.17	1.49	1.52
26	RD	203	PEB	C2A-C1A	-3.17	1.49	1.52
26	Z7	202	PEB	C2C-C3C	3.17	1.47	1.37
26	LE	201	PEB	C2C-C3C	3.17	1.47	1.37
26	SA	202	PEB	CHA-C1B	3.17	1.47	1.40
26	Y1	201	PEB	C2C-C3C	3.17	1.47	1.37
26	P4	202	PEB	C2A-C1A	-3.17	1.49	1.52
26	WE	203	PEB	C1A-NA	-3.17	1.33	1.37
26	V9	202	PEB	OD-C4D	3.17	1.29	1.23
26	QD	202	PEB	OD-C4D	3.17	1.29	1.23
26	mG	201	PEB	OD-C4D	3.17	1.29	1.23
26	t1	202	PEB	C4B-C3B	3.17	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CD	201	PEB	C2A-C1A	-3.17	1.49	1.52
26	W9	201	PEB	C2C-C3C	3.17	1.47	1.37
26	H1	202	PEB	CHA-C1B	3.17	1.47	1.40
26	wE	302	PEB	C1A-NA	-3.17	1.33	1.37
26	m4	201	PEB	CHA-C1B	3.17	1.47	1.40
26	P4	201	PEB	C2A-C1A	-3.17	1.49	1.52
26	X1	202	PEB	C2C-C3C	3.16	1.47	1.37
26	W3	202	PEB	C2C-C3C	3.16	1.47	1.37
26	Q8	204	PEB	CHA-C1B	3.16	1.47	1.40
26	hF	201	PEB	OD-C4D	3.16	1.29	1.23
26	S3	202	PEB	C1A-NA	-3.16	1.33	1.37
26	BG	201	PEB	C2C-C3C	3.16	1.47	1.37
26	bF	203	PEB	CHA-C1B	3.16	1.47	1.40
26	O4	202	PEB	C2C-C3C	3.16	1.47	1.37
26	JG	201	PEB	C2C-C3C	3.16	1.47	1.37
26	lG	202	PEB	C1A-NA	-3.16	1.33	1.37
28	CI	1001	CYC	C3D-C2D	3.16	1.47	1.37
26	Z8	202	PEB	C2C-C3C	3.16	1.47	1.37
26	d8	201	PEB	C2C-C3C	3.16	1.47	1.37
26	J1	202	PEB	C2C-C3C	3.16	1.47	1.37
26	W2	201	PEB	C2C-C3C	3.16	1.47	1.37
26	DA	201	PEB	C2A-C1A	-3.16	1.49	1.52
26	j8	201	PEB	CHA-C1B	3.16	1.47	1.40
26	VJ	202	PEB	CHA-C1B	3.16	1.47	1.40
26	11	202	PEB	C1A-NA	-3.16	1.33	1.37
26	a7	201	PEB	C1A-NA	-3.16	1.33	1.37
26	YG	203	PEB	C2C-C3C	3.16	1.47	1.37
28	BB	1001	CYC	C3D-C2D	3.16	1.47	1.37
26	H5	202	PEB	C2A-C1A	-3.16	1.49	1.52
26	f8	203	PEB	C2C-C3C	3.16	1.47	1.37
26	I5	203	PEB	C2C-C3C	3.16	1.47	1.37
26	Y7	202	PEB	C2C-C3C	3.16	1.47	1.37
26	RJ	201	PEB	C1A-NA	-3.16	1.33	1.37
26	Q2	201	PEB	C2C-C3C	3.15	1.47	1.37
26	sE	203	PEB	C2C-C3C	3.15	1.47	1.37
26	VF	203	PEB	C1A-NA	-3.15	1.33	1.37
26	F9	203	PEB	C2A-C1A	-3.15	1.49	1.52
27	A4	203	PUB	OD-C4D	3.15	1.29	1.23
26	OE	201	PEB	C1A-NA	-3.15	1.33	1.37
26	b7	201	PEB	CHA-C1B	3.15	1.47	1.40
26	UE	203	PEB	OD-C4D	3.15	1.29	1.23
26	J4	202	PEB	C2C-C3C	3.15	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M1	401	PEB	C1A-NA	-3.15	1.33	1.37
26	f1	202	PEB	C1A-NA	-3.15	1.33	1.37
26	SB	202	PEB	OD-C4D	3.15	1.29	1.23
26	Q2	201	PEB	CHA-C1B	3.15	1.47	1.40
26	G3	201	PEB	C2C-C3C	3.15	1.47	1.37
26	CD	201	PEB	C2C-C3C	3.15	1.47	1.37
27	A6	303	PUB	OD-C4D	3.15	1.29	1.23
26	k1	202	PEB	CHA-C1B	3.15	1.47	1.40
26	c1	202	PEB	C1A-NA	-3.15	1.33	1.37
26	D7	1002	PEB	C1A-NA	-3.15	1.33	1.37
26	lE	202	PEB	C1A-NA	-3.15	1.33	1.37
26	h4	202	PEB	C1A-NA	-3.15	1.33	1.37
26	JF	1002	PEB	C1A-NA	-3.15	1.33	1.37
26	B4	202	PEB	CHA-C1B	3.15	1.47	1.40
28	C2	1001	CYC	C3D-C2D	3.15	1.47	1.37
26	dE	202	PEB	C2A-C1A	-3.15	1.49	1.52
26	OJ	201	PEB	C1A-NA	-3.15	1.33	1.37
26	A1	201	PEB	C2C-C3C	3.15	1.47	1.37
26	DJ	203	PEB	OD-C4D	3.15	1.29	1.23
26	F4	202	PEB	C2C-C3C	3.15	1.47	1.37
28	EF	1001	CYC	C3D-C2D	3.15	1.47	1.37
26	KE	203	PEB	CHA-C1B	3.15	1.47	1.40
26	QI	201	PEB	CHA-C1B	3.15	1.47	1.40
26	IJ	202	PEB	C2A-C1A	-3.15	1.49	1.52
26	O1	202	PEB	C2C-C3C	3.15	1.47	1.37
26	XG	201	PEB	C2C-C3C	3.15	1.47	1.37
27	xE	301	PUB	C3B-C2B	3.15	1.47	1.37
26	SF	202	PEB	OD-C4D	3.15	1.29	1.23
28	F6	1001	CYC	C3D-C2D	3.15	1.47	1.37
28	KH	1001	CYC	C2C-C1C	-3.15	1.49	1.52
26	UB	203	PEB	OD-C4D	3.15	1.29	1.23
26	c1	203	PEB	C1A-NA	-3.15	1.33	1.37
26	d7	201	PEB	C2C-C3C	3.15	1.47	1.37
26	WA	202	PEB	C2C-C3C	3.15	1.47	1.37
26	y1	202	PEB	C2C-C3C	3.15	1.47	1.37
26	TJ	203	PEB	C1A-NA	-3.15	1.33	1.37
26	m6	202	PEB	C2C-C3C	3.15	1.47	1.37
26	gG	202	PEB	C1A-NA	-3.15	1.33	1.37
26	OA	201	PEB	C2A-C1A	-3.14	1.49	1.52
26	b4	501	PEB	C1A-NA	-3.14	1.33	1.37
26	T4	201	PEB	OD-C4D	3.14	1.29	1.23
26	N6	201	PEB	C2A-C1A	-3.14	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	WH	1001	CYC	C1B-C2B	3.14	1.50	1.45
26	f7	203	PEB	C1A-NA	-3.14	1.33	1.37
26	u1	202	PEB	C2C-C3C	3.14	1.47	1.37
26	U3	202	PEB	CHA-C1B	3.14	1.47	1.40
26	YF	202	PEB	C2A-C1A	-3.14	1.49	1.52
28	B6	1001	CYC	C3D-C2D	3.14	1.47	1.37
26	k1	202	PEB	C1A-NA	-3.14	1.33	1.37
28	FB	1001	CYC	C3D-C2D	3.14	1.47	1.37
26	GD	201	PEB	C2C-C3C	3.14	1.47	1.37
26	QD	202	PEB	C2C-C3C	3.14	1.47	1.37
26	SG	202	PEB	C2C-C3C	3.14	1.47	1.37
26	WI	201	PEB	C2C-C3C	3.14	1.47	1.37
26	K6	201	PEB	C2A-C1A	-3.14	1.49	1.52
26	G8	201	PEB	C2A-C1A	-3.14	1.49	1.52
28	JH	1001	CYC	C1B-C2B	3.14	1.50	1.45
26	RF	201	PEB	C1A-NA	-3.14	1.33	1.37
26	l2	201	PEB	CHA-C1B	3.14	1.47	1.40
26	V9	201	PEB	CHA-C1B	3.14	1.47	1.40
26	OF	202	PEB	CHA-C1B	3.14	1.47	1.40
26	j2	201	PEB	CHA-C1B	3.14	1.47	1.40
26	jF	203	PEB	C2C-C3C	3.14	1.47	1.37
26	PD	202	PEB	CHA-C1B	3.14	1.47	1.40
26	J5	201	PEB	C4A-NA	-3.14	1.30	1.37
26	r4	202	PEB	C4B-C3B	3.14	1.50	1.45
26	k4	203	PEB	OD-C4D	3.14	1.29	1.23
26	LJ	202	PEB	C2A-C1A	-3.14	1.49	1.52
26	XJ	203	PEB	C1A-NA	-3.14	1.33	1.37
26	E9	202	PEB	C2C-C3C	3.14	1.47	1.37
26	SE	202	PEB	C2C-C3C	3.14	1.47	1.37
26	F1	202	PEB	CHA-C1B	3.14	1.47	1.40
26	X1	203	PEB	C2C-C3C	3.14	1.47	1.37
26	YF	202	PEB	C2C-C3C	3.13	1.47	1.37
26	t1	201	PEB	C1A-NA	-3.13	1.33	1.37
26	p4	201	PEB	C1A-NA	-3.13	1.33	1.37
26	i1	203	PEB	C1A-NA	-3.13	1.33	1.37
26	QF	202	PEB	C2C-C3C	3.13	1.47	1.37
26	HJ	202	PEB	C2C-C3C	3.13	1.47	1.37
26	QE	203	PEB	C2A-C1A	-3.13	1.49	1.52
26	XG	203	PEB	C2A-C1A	-3.13	1.49	1.52
26	T4	203	PEB	OD-C4D	3.13	1.29	1.23
26	K5	201	PEB	C2C-C3C	3.13	1.47	1.37
26	MJ	201	PEB	C2A-C1A	-3.13	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JA	201	PEB	C1A-NA	-3.13	1.33	1.37
26	H9	203	PEB	C1A-NA	-3.13	1.33	1.37
26	mA	201	PEB	C2A-C1A	-3.13	1.49	1.52
26	TA	202	PEB	C2C-C3C	3.13	1.46	1.37
26	c1	203	PEB	C2C-C3C	3.13	1.46	1.37
26	LG	201	PEB	C2C-C3C	3.13	1.46	1.37
26	O7	201	PEB	CHA-C1B	3.13	1.47	1.40
26	R9	203	PEB	CHA-C1B	3.13	1.47	1.40
26	M3	202	PEB	C1A-NA	-3.13	1.33	1.37
26	i8	201	PEB	C1A-NA	-3.13	1.33	1.37
26	qG	201	PEB	C2C-C3C	3.13	1.46	1.37
26	tE	202	PEB	C1A-NA	-3.13	1.33	1.37
26	wG	302	PEB	C1A-NA	-3.13	1.33	1.37
26	HJ	203	PEB	C1A-NA	-3.13	1.33	1.37
26	sG	203	PEB	C2A-C1A	-3.13	1.49	1.52
26	d7	201	PEB	C1A-NA	-3.13	1.33	1.37
26	ND	203	PEB	C2C-C3C	3.13	1.46	1.37
26	i4	202	PEB	CHA-C1B	3.13	1.47	1.40
26	T9	201	PEB	OD-C4D	3.13	1.29	1.23
26	KJ	201	PEB	C2C-C3C	3.12	1.46	1.37
26	cG	202	PEB	OD-C4D	3.12	1.29	1.23
28	B6	1002	CYC	C3D-C2D	3.12	1.46	1.37
26	LC	201	PEB	C2C-C3C	3.12	1.46	1.37
26	Y7	202	PEB	C1A-NA	-3.12	1.33	1.37
26	uE	201	PEB	C2C-C3C	3.12	1.46	1.37
26	VF	202	PEB	C2C-C3C	3.12	1.46	1.37
26	C8	203	PEB	CHA-C1B	3.12	1.47	1.40
26	J4	201	PEB	C2C-C3C	3.12	1.46	1.37
26	V1	202	PEB	OD-C4D	3.12	1.29	1.23
26	HD	201	PEB	C2A-C1A	-3.12	1.49	1.52
26	Z7	202	PEB	CHA-C1B	3.12	1.47	1.40
28	DB	1001	CYC	CHB-C4A	3.12	1.47	1.40
26	DE	202	PEB	C2A-C1A	-3.12	1.49	1.52
26	YF	201	PEB	C2A-C1A	-3.12	1.49	1.52
26	Q6	203	PEB	OD-C4D	3.12	1.29	1.23
26	J3	203	PEB	C1A-NA	-3.12	1.33	1.37
26	IJ	203	PEB	C2C-C3C	3.12	1.46	1.37
26	w4	202	PEB	C1A-NA	-3.12	1.33	1.37
26	QG	203	PEB	C2A-C1A	-3.12	1.49	1.52
26	jA	203	PEB	C2C-C3C	3.12	1.46	1.37
27	AB	303	PUB	OD-C4D	3.12	1.29	1.23
26	Z1	201	PEB	C2A-C1A	-3.12	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N4	202	PEB	OD-C4D	3.11	1.29	1.23
26	gE	202	PEB	C1A-NA	-3.11	1.33	1.37
26	SD	202	PEB	C1A-NA	-3.11	1.33	1.37
26	kG	202	PEB	C1A-NA	-3.11	1.33	1.37
28	lH	1001	CYC	C1B-C2B	3.11	1.50	1.45
26	U9	201	PEB	OD-C4D	3.11	1.29	1.23
26	fB	203	PEB	C1A-NA	-3.11	1.33	1.37
26	P1	201	PEB	C2A-C1A	-3.11	1.49	1.52
26	S8	202	PEB	CHA-C1B	3.11	1.47	1.40
26	m4	201	PEB	C2C-C3C	3.11	1.46	1.37
26	fF	203	PEB	C1A-NA	-3.11	1.33	1.37
26	WJ	201	PEB	C1A-NA	-3.11	1.33	1.37
26	WI	201	PEB	CHA-C1B	3.11	1.47	1.40
26	u1	202	PEB	C4B-C3B	3.11	1.50	1.45
27	BA	302	PUB	C3B-C2B	3.11	1.46	1.37
26	l1	202	PEB	C1A-NA	-3.11	1.33	1.37
26	iA	201	PEB	C1A-NA	-3.11	1.33	1.37
26	N3	203	PEB	C2C-C3C	3.11	1.46	1.37
26	bI	201	PEB	C2A-C1A	-3.11	1.49	1.52
26	SF	201	PEB	C2A-C1A	-3.11	1.49	1.52
26	DG	202	PEB	CHA-C1B	3.11	1.47	1.40
26	dF	201	PEB	C2C-C3C	3.11	1.46	1.37
26	M4	401	PEB	C1A-NA	-3.11	1.33	1.37
26	g8	201	PEB	C2A-C1A	-3.11	1.49	1.52
26	I9	202	PEB	C2C-C3C	3.10	1.46	1.37
26	X4	203	PEB	C2C-C3C	3.10	1.46	1.37
28	CH	1001	CYC	C1B-C2B	3.10	1.50	1.45
26	eE	202	PEB	C2A-C1A	-3.10	1.49	1.52
26	dG	201	PEB	C2A-C1A	-3.10	1.49	1.52
26	DD	202	PEB	C2C-C3C	3.10	1.46	1.37
26	S7	203	PEB	C2C-C3C	3.10	1.46	1.37
26	KA	202	PEB	C2C-C3C	3.10	1.46	1.37
26	KD	202	PEB	C1A-NA	-3.10	1.33	1.37
26	iE	201	PEB	C1A-NA	-3.10	1.33	1.37
26	L9	202	PEB	C2A-C1A	-3.10	1.49	1.52
26	PA	201	PEB	C2A-C1A	-3.10	1.49	1.52
26	I8	201	PEB	CHA-C1B	3.10	1.47	1.40
26	m2	202	PEB	C2C-C3C	3.10	1.46	1.37
26	n4	201	PEB	C1A-NA	-3.10	1.33	1.37
26	k2	202	PEB	C2C-C3C	3.10	1.46	1.37
26	T1	203	PEB	OD-C4D	3.10	1.29	1.23
26	F1	202	PEB	C2C-C3C	3.10	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	VH	1001	CYC	C2C-C1C	-3.10	1.49	1.52
26	q4	202	PEB	C2C-C3C	3.10	1.46	1.37
26	K8	202	PEB	C2C-C3C	3.10	1.46	1.37
28	oH	1001	CYC	C1B-C2B	3.10	1.50	1.45
26	KG	203	PEB	CHA-C1B	3.10	1.47	1.40
26	WG	203	PEB	OD-C4D	3.10	1.29	1.23
26	B1	202	PEB	C2C-C3C	3.10	1.46	1.37
26	gG	203	PEB	C2C-C3C	3.10	1.46	1.37
26	KA	203	PEB	C2A-C1A	-3.10	1.49	1.52
26	IC	202	PEB	C2A-C1A	-3.10	1.49	1.52
26	K1	202	PEB	C1A-NA	-3.09	1.33	1.37
26	w4	201	PEB	C1A-NA	-3.09	1.33	1.37
26	Z6	203	PEB	C2A-C1A	-3.09	1.49	1.52
26	ND	201	PEB	C2C-C3C	3.09	1.46	1.37
26	eG	201	PEB	C2C-C3C	3.09	1.46	1.37
26	L1	202	PEB	CHA-C1B	3.09	1.47	1.40
26	QF	201	PEB	CHA-C1B	3.09	1.47	1.40
28	YH	1003	CYC	C1B-C2B	3.09	1.50	1.45
26	H3	201	PEB	C2A-C1A	-3.09	1.49	1.52
26	g4	201	PEB	C2A-C1A	-3.09	1.49	1.52
26	vE	201	PEB	C2A-C1A	-3.09	1.49	1.52
26	AG	201	PEB	C2A-C1A	-3.09	1.49	1.52
26	J9	202	PEB	CHA-C1B	3.09	1.47	1.40
26	q4	201	PEB	C1A-NA	-3.09	1.33	1.37
26	O6	203	PEB	CHA-C1B	3.09	1.47	1.40
26	X9	202	PEB	C1A-NA	-3.09	1.33	1.37
26	lB	201	PEB	C1A-NA	-3.09	1.33	1.37
28	jH	1001	CYC	C1B-C2B	3.09	1.50	1.45
26	I4	202	PEB	C2A-C1A	-3.09	1.49	1.52
26	UJ	201	PEB	C2A-C1A	-3.09	1.49	1.52
26	L3	202	PEB	C2C-C3C	3.09	1.46	1.37
26	JD	202	PEB	C2C-C3C	3.09	1.46	1.37
26	LF	1002	PEB	CHA-C1B	3.09	1.47	1.40
26	h2	202	PEB	C1A-NA	-3.09	1.33	1.37
26	eF	201	PEB	C2A-C1A	-3.09	1.49	1.52
26	CJ	202	PEB	C2A-C1A	-3.09	1.49	1.52
28	yH	1001	CYC	C1B-C2B	3.09	1.50	1.45
28	F2	1001	CYC	C3D-C2D	3.09	1.46	1.37
26	l7	201	PEB	C2C-C3C	3.09	1.46	1.37
28	FI	1001	CYC	C3D-C2D	3.09	1.46	1.37
26	O9	202	PEB	C2A-C1A	-3.09	1.49	1.52
26	SG	201	PEB	CHA-C1B	3.09	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	SA	203	PEB	C2C-C3C	3.09	1.46	1.37
26	IA	203	PEB	CHA-C1B	3.09	1.47	1.40
26	Q3	202	PEB	C2C-C3C	3.09	1.46	1.37
27	yE	302	PUB	C3B-C2B	3.09	1.46	1.37
26	D1	202	PEB	C2C-C3C	3.09	1.46	1.37
26	I8	203	PEB	CHA-C1B	3.09	1.47	1.40
26	W2	201	PEB	CHA-C1B	3.09	1.47	1.40
26	SA	203	PEB	C2A-C1A	-3.09	1.49	1.52
28	KF	1001	CYC	C2C-C1C	-3.09	1.49	1.52
26	n4	202	PEB	C2A-C1A	-3.08	1.49	1.52
26	NI	1002	PEB	C2A-C1A	-3.08	1.49	1.52
26	U3	202	PEB	OD-C4D	3.08	1.29	1.23
26	EJ	202	PEB	C2C-C3C	3.08	1.46	1.37
26	P1	203	PEB	OD-C4D	3.08	1.29	1.23
26	T1	201	PEB	OD-C4D	3.08	1.29	1.23
26	KG	203	PEB	OD-C4D	3.08	1.29	1.23
27	B8	302	PUB	C3B-C2B	3.08	1.46	1.37
26	j1	201	PEB	OD-C4D	3.08	1.29	1.23
27	yG	302	PUB	C3B-C2B	3.08	1.46	1.37
26	K5	202	PEB	C2A-C1A	-3.08	1.49	1.52
26	EA	202	PEB	C2A-C1A	-3.08	1.49	1.52
26	PJ	201	PEB	CHA-C1B	3.08	1.47	1.40
26	VF	202	PEB	C1A-NA	-3.08	1.33	1.37
26	k6	201	PEB	C2A-C1A	-3.08	1.49	1.52
26	X4	201	PEB	C2C-C3C	3.08	1.46	1.37
26	gA	202	PEB	C1A-NA	-3.08	1.33	1.37
26	j4	201	PEB	OD-C4D	3.08	1.29	1.23
26	j6	201	PEB	C2A-C1A	-3.08	1.49	1.52
26	E9	201	PEB	C2C-C3C	3.08	1.46	1.37
26	QJ	201	PEB	C1A-NA	-3.08	1.33	1.37
28	VH	1001	CYC	C1B-C2B	3.08	1.50	1.45
26	S4	202	PEB	C2A-C1A	-3.08	1.49	1.52
26	P6	202	PEB	C2A-C1A	-3.08	1.49	1.52
26	a2	203	PEB	C1A-NA	-3.08	1.33	1.37
26	sE	201	PEB	C1A-NA	-3.08	1.33	1.37
26	A3	201	PEB	OD-C4D	3.08	1.29	1.23
26	AG	202	PEB	OD-C4D	3.08	1.29	1.23
27	yE	303	PUB	C3B-C2B	3.08	1.46	1.37
26	c4	203	PEB	CHA-C1B	3.08	1.47	1.40
26	HD	202	PEB	CHA-C1B	3.08	1.47	1.40
26	T8	202	PEB	C2C-C3C	3.08	1.46	1.37
26	N9	203	PEB	OD-C4D	3.08	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O9	201	PEB	OD-C4D	3.08	1.29	1.23
26	EA	201	PEB	C2A-C1A	-3.08	1.49	1.52
26	CA	203	PEB	CHA-C1B	3.08	1.47	1.40
26	MA	203	PEB	CHA-C1B	3.08	1.47	1.40
26	RJ	203	PEB	CHA-C1B	3.08	1.47	1.40
28	N2	1001	CYC	C3D-C2D	3.08	1.46	1.37
26	TJ	203	PEB	OD-C4D	3.08	1.29	1.23
26	RG	201	PEB	C2C-C3C	3.07	1.46	1.37
26	A8	302	PEB	C2A-C1A	-3.07	1.49	1.52
26	eE	201	PEB	CHA-C1B	3.07	1.47	1.40
26	sG	201	PEB	C1A-NA	-3.07	1.33	1.37
26	nE	201	PEB	C2A-C1A	-3.07	1.49	1.52
26	B5	203	PEB	C1A-NA	-3.07	1.33	1.37
28	GH	1001	CYC	C1B-C2B	3.07	1.50	1.45
26	AE	202	PEB	OD-C4D	3.07	1.29	1.23
26	L4	202	PEB	CHA-C1B	3.07	1.47	1.40
26	e2	202	PEB	C2C-C3C	3.07	1.46	1.37
26	k1	203	PEB	CHA-C1B	3.07	1.47	1.40
26	Q7	201	PEB	C2C-C3C	3.07	1.46	1.37
26	IE	201	PEB	C1A-NA	-3.07	1.33	1.37
26	B3	201	PEB	C1A-NA	-3.07	1.33	1.37
26	uE	201	PEB	C1A-NA	-3.07	1.33	1.37
26	C3	201	PEB	C2C-C3C	3.07	1.46	1.37
26	u4	201	PEB	OD-C4D	3.07	1.29	1.23
26	uG	203	PEB	OD-C4D	3.07	1.29	1.23
26	aA	201	PEB	CHA-C1B	3.07	1.47	1.40
26	CA	202	PEB	CHA-C1B	3.07	1.47	1.40
26	r1	202	PEB	C4B-C3B	3.07	1.50	1.45
26	jF	201	PEB	CHA-C1B	3.07	1.47	1.40
26	A9	303	PEB	OD-C4D	3.07	1.29	1.23
26	oG	203	PEB	OD-C4D	3.07	1.29	1.23
26	V3	201	PEB	C2C-C3C	3.07	1.46	1.37
26	fF	202	PEB	OD-C4D	3.07	1.29	1.23
26	aI	202	PEB	C2A-C1A	-3.06	1.49	1.52
26	e1	202	PEB	OD-C4D	3.06	1.29	1.23
26	l1	201	PEB	C1A-NA	-3.06	1.33	1.37
26	UJ	201	PEB	OD-C4D	3.06	1.29	1.23
26	C3	202	PEB	OD-C4D	3.06	1.29	1.23
26	R9	202	PEB	OD-C4D	3.06	1.29	1.23
26	kG	202	PEB	OD-C4D	3.06	1.29	1.23
26	pG	202	PEB	C4B-C3B	3.06	1.50	1.45
26	II	201	PEB	CHA-C1B	3.06	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D6	1001	CYC	CHB-C4A	3.06	1.47	1.40
26	UD	202	PEB	OD-C4D	3.06	1.29	1.23
26	iE	201	PEB	C2C-C3C	3.06	1.46	1.37
26	e4	202	PEB	OD-C4D	3.06	1.29	1.23
26	NA	201	PEB	C2C-C3C	3.06	1.46	1.37
26	D3	202	PEB	C2C-C3C	3.06	1.46	1.37
26	qE	201	PEB	C2C-C3C	3.06	1.46	1.37
26	j8	203	PEB	C2C-C3C	3.06	1.46	1.37
26	l6	201	PEB	C1A-NA	-3.06	1.33	1.37
26	sG	203	PEB	CHA-C1B	3.06	1.47	1.40
26	hF	202	PEB	CHA-C1B	3.06	1.47	1.40
26	mI	201	PEB	C2A-C1A	-3.06	1.49	1.52
26	jA	203	PEB	C1A-NA	-3.06	1.33	1.37
26	O3	201	PEB	C4A-NA	-3.06	1.30	1.37
26	V9	203	PEB	C2C-C3C	3.06	1.46	1.37
26	MD	202	PEB	C1A-NA	-3.06	1.33	1.37
26	RJ	202	PEB	OD-C4D	3.06	1.29	1.23
26	lF	201	PEB	C2C-C3C	3.06	1.46	1.37
26	IG	201	PEB	C4A-NA	-3.05	1.30	1.37
26	O3	201	PEB	CHA-C1B	3.05	1.47	1.40
26	TF	202	PEB	C1A-NA	-3.05	1.33	1.37
26	TE	202	PEB	C2A-C1A	-3.05	1.49	1.52
26	OF	203	PEB	C2C-C3C	3.05	1.46	1.37
26	FJ	201	PEB	C2C-C3C	3.05	1.46	1.37
26	UG	202	PEB	CHA-C1B	3.05	1.47	1.40
26	O7	203	PEB	C2C-C3C	3.05	1.46	1.37
26	m2	201	PEB	C2A-C1A	-3.05	1.49	1.52
26	QF	201	PEB	C1A-NA	-3.05	1.33	1.37
26	JJ	202	PEB	C1A-NA	-3.05	1.33	1.37
26	fB	202	PEB	OD-C4D	3.05	1.29	1.23
26	IE	202	PEB	OD-C4D	3.05	1.29	1.23
26	a4	202	PEB	C1A-NA	-3.05	1.33	1.37
26	h4	201	PEB	C1A-NA	-3.05	1.33	1.37
26	E8	201	PEB	C2C-C3C	3.05	1.46	1.37
26	IG	202	PEB	OD-C4D	3.05	1.29	1.23
26	kG	203	PEB	C1A-NA	-3.05	1.33	1.37
26	i2	202	PEB	C2C-C3C	3.05	1.46	1.37
28	NH	1001	CYC	C1B-C2B	3.05	1.50	1.45
26	MD	201	PEB	C2C-C3C	3.05	1.46	1.37
26	v4	202	PEB	OD-C4D	3.05	1.29	1.23
26	X1	201	PEB	C2C-C3C	3.05	1.46	1.37
26	bF	203	PEB	C2C-C3C	3.05	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	EE	201	PEB	C1A-NA	-3.05	1.33	1.37
26	KE	203	PEB	OD-C4D	3.05	1.29	1.23
26	OG	203	PEB	OD-C4D	3.05	1.29	1.23
26	f2	201	PEB	CHA-C1B	3.05	1.47	1.40
26	F3	202	PEB	CHA-C1B	3.05	1.47	1.40
26	CC	201	PEB	C1A-NA	-3.05	1.33	1.37
26	d7	203	PEB	C1A-NA	-3.04	1.33	1.37
26	QE	201	PEB	C1A-NA	-3.04	1.33	1.37
26	r4	202	PEB	C1A-NA	-3.04	1.33	1.37
26	M8	203	PEB	CHA-C1B	3.04	1.47	1.40
26	h2	201	PEB	C2A-C1A	-3.04	1.49	1.52
26	g4	202	PEB	OD-C4D	3.04	1.29	1.23
26	H9	203	PEB	OD-C4D	3.04	1.29	1.23
26	s4	203	PEB	OD-C4D	3.04	1.29	1.23
26	VJ	202	PEB	OD-C4D	3.04	1.29	1.23
26	s1	201	PEB	C1A-NA	-3.04	1.33	1.37
26	q4	202	PEB	C1A-NA	-3.04	1.33	1.37
26	sG	202	PEB	C1A-NA	-3.04	1.33	1.37
26	oE	203	PEB	C2C-C3C	3.04	1.46	1.37
26	JJ	202	PEB	CHA-C1B	3.04	1.47	1.40
26	iI	202	PEB	C2C-C3C	3.04	1.46	1.37
26	h6	203	PEB	OD-C4D	3.04	1.29	1.23
26	ID	202	PEB	CHA-C1B	3.04	1.47	1.40
26	k1	203	PEB	C1A-NA	-3.04	1.33	1.37
28	uH	1001	CYC	C1C-NC	-3.04	1.33	1.37
26	ZB	203	PEB	OD-C4D	3.04	1.29	1.23
26	WE	203	PEB	OD-C4D	3.04	1.29	1.23
26	NB	1002	PEB	C2A-C1A	-3.04	1.49	1.52
26	iG	201	PEB	C2C-C3C	3.04	1.46	1.37
26	S8	203	PEB	C2C-C3C	3.04	1.46	1.37
26	y1	201	PEB	C1A-NA	-3.04	1.33	1.37
26	jG	202	PEB	C2A-C1A	-3.04	1.49	1.52
26	X4	203	PEB	OD-C4D	3.04	1.29	1.23
26	j1	201	PEB	C4B-C3B	3.04	1.50	1.45
26	e7	202	PEB	C1A-NA	-3.04	1.33	1.37
26	gF	202	PEB	OD-C4D	3.04	1.29	1.23
28	fH	1001	CYC	C1B-C2B	3.03	1.50	1.45
26	Z7	201	PEB	C2C-C3C	3.03	1.46	1.37
26	Q7	201	PEB	CHA-C1B	3.03	1.47	1.40
26	M3	201	PEB	C2C-C3C	3.03	1.46	1.37
28	DB	1001	CYC	C3D-C2D	3.03	1.46	1.37
26	J1	203	PEB	C1A-NA	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d4	202	PEB	C2C-C3C	3.03	1.46	1.37
26	WB	203	PEB	CHA-C1B	3.03	1.47	1.40
26	hA	201	PEB	C1A-NA	-3.03	1.33	1.37
26	L9	201	PEB	CHA-C1B	3.03	1.47	1.40
26	nG	201	PEB	C2A-C1A	-3.03	1.49	1.52
26	b6	202	PEB	OD-C4D	3.03	1.29	1.23
26	SE	202	PEB	C3B-C2B	3.03	1.43	1.36
26	VD	201	PEB	C2C-C3C	3.03	1.46	1.37
26	ZB	203	PEB	C2A-C1A	-3.03	1.49	1.52
26	f7	202	PEB	OD-C4D	3.03	1.29	1.23
26	I5	201	PEB	C2A-C1A	-3.03	1.49	1.52
26	Z6	203	PEB	OD-C4D	3.03	1.29	1.23
26	TJ	201	PEB	OD-C4D	3.03	1.29	1.23
26	B4	202	PEB	C2C-C3C	3.03	1.46	1.37
26	g4	203	PEB	OD-C4D	3.03	1.29	1.23
26	jB	202	PEB	OD-C4D	3.03	1.29	1.23
28	qH	1002	CYC	C1B-C2B	3.03	1.50	1.45
26	KA	202	PEB	C1A-NA	-3.03	1.33	1.37
26	W6	202	PEB	C2A-C1A	-3.02	1.49	1.52
26	QB	201	PEB	C2A-C1A	-3.02	1.49	1.52
26	g2	202	PEB	C2C-C3C	3.02	1.46	1.37
26	QB	203	PEB	OD-C4D	3.02	1.29	1.23
26	dF	203	PEB	OD-C4D	3.02	1.29	1.23
26	SG	203	PEB	OD-C4D	3.02	1.29	1.23
26	a1	202	PEB	C1A-NA	-3.02	1.33	1.37
26	l7	201	PEB	C1A-NA	-3.02	1.33	1.37
27	xG	301	PUB	C3B-C2B	3.02	1.46	1.37
26	P4	203	PEB	OD-C4D	3.02	1.29	1.23
26	m1	201	PEB	C2C-C3C	3.02	1.46	1.37
26	WD	201	PEB	C2C-C3C	3.02	1.46	1.37
26	EA	201	PEB	C2C-C3C	3.02	1.46	1.37
26	N1	202	PEB	OD-C4D	3.02	1.29	1.23
26	WF	203	PEB	C2C-C3C	3.02	1.46	1.37
26	kE	201	PEB	C1A-NA	-3.02	1.33	1.37
26	QA	204	PEB	CHA-C1B	3.02	1.47	1.40
28	MH	1001	CYC	C1B-C2B	3.02	1.50	1.45
26	EA	203	PEB	C1A-NA	-3.02	1.33	1.37
26	k7	202	PEB	C2A-C1A	-3.02	1.49	1.52
26	H2	1002	PEB	C2A-C1A	-3.02	1.49	1.52
26	ZB	201	PEB	C2A-C1A	-3.02	1.49	1.52
26	a8	204	PEB	C2C-C3C	3.02	1.46	1.37
26	O7	203	PEB	CHA-C1B	3.02	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d4	202	PEB	OD-C4D	3.02	1.29	1.23
26	d8	201	PEB	OD-C4D	3.02	1.29	1.23
26	eE	202	PEB	OD-C4D	3.02	1.29	1.23
26	T3	203	PEB	C2C-C3C	3.01	1.46	1.37
26	NJ	203	PEB	OD-C4D	3.01	1.29	1.23
26	Z4	201	PEB	C2A-C1A	-3.01	1.49	1.52
26	JG	202	PEB	C2A-C1A	-3.01	1.49	1.52
26	GE	202	PEB	C2C-C3C	3.01	1.46	1.37
26	YE	203	PEB	OD-C4D	3.01	1.29	1.23
26	OB	203	PEB	CHA-C1B	3.01	1.47	1.40
26	i1	201	PEB	OD-C4D	3.01	1.29	1.23
26	f6	202	PEB	OD-C4D	3.01	1.29	1.23
26	FD	202	PEB	C2C-C3C	3.01	1.46	1.37
26	SE	203	PEB	OD-C4D	3.01	1.29	1.23
26	BA	301	PEB	C2C-C3C	3.01	1.46	1.37
26	BC	203	PEB	C1A-NA	-3.01	1.33	1.37
26	sE	203	PEB	CHA-C1B	3.01	1.47	1.40
26	ME	203	PEB	OD-C4D	3.01	1.29	1.23
26	T9	203	PEB	OD-C4D	3.01	1.29	1.23
26	sE	202	PEB	OD-C4D	3.01	1.29	1.23
28	kH	1001	CYC	C1B-C2B	3.01	1.50	1.45
26	U2	201	PEB	CHA-C1B	3.01	1.47	1.40
26	DD	201	PEB	C2A-C1A	-3.01	1.49	1.52
26	qE	202	PEB	C4B-C3B	3.01	1.50	1.45
26	U2	201	PEB	C2C-C3C	3.01	1.46	1.37
26	WF	202	PEB	OD-C4D	3.01	1.29	1.23
26	UI	201	PEB	CHA-C1B	3.01	1.47	1.40
26	iF	202	PEB	C2A-C1A	-3.01	1.49	1.52
26	QE	202	PEB	OD-C4D	3.01	1.29	1.23
26	eI	202	PEB	C2C-C3C	3.00	1.46	1.37
26	T2	202	PEB	C2C-C3C	3.00	1.46	1.37
28	LI	1001	CYC	C3D-C2D	3.00	1.46	1.37
26	m8	201	PEB	C2A-C1A	-3.00	1.49	1.52
26	OF	201	PEB	CHA-C1B	3.00	1.47	1.40
26	CG	202	PEB	C1A-NA	-3.00	1.33	1.37
26	WG	201	PEB	C2C-C3C	3.00	1.46	1.37
28	QH	1001	CYC	C1B-C2B	3.00	1.50	1.45
26	SB	201	PEB	C2A-C1A	-3.00	1.49	1.52
26	R9	201	PEB	CHA-C1B	3.00	1.47	1.40
26	SE	201	PEB	CHA-C1B	3.00	1.47	1.40
26	oG	203	PEB	C2A-C1A	-3.00	1.49	1.52
26	Q7	203	PEB	OD-C4D	3.00	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	mE	201	PEB	C1A-NA	-3.00	1.33	1.37
26	UI	201	PEB	C2C-C3C	3.00	1.46	1.37
28	pH	1001	CYC	C1B-C2B	3.00	1.50	1.45
26	RI	203	PEB	C1A-NA	-3.00	1.33	1.37
26	14	203	PEB	OD-C4D	3.00	1.29	1.23
26	YI	203	PEB	C1A-NA	-3.00	1.33	1.37
26	jB	201	PEB	C2A-C1A	-3.00	1.49	1.52
26	w4	202	PEB	C4B-C3B	3.00	1.50	1.45
26	TD	203	PEB	C2C-C3C	3.00	1.46	1.37
28	L2	1001	CYC	C3D-C2D	3.00	1.46	1.37
26	w4	203	PEB	C1A-NA	-3.00	1.33	1.37
26	lE	201	PEB	CHA-C1B	3.00	1.47	1.40
26	YE	202	PEB	OD-C4D	3.00	1.29	1.23
26	T4	201	PEB	C2A-C1A	-3.00	1.49	1.52
26	cE	203	PEB	C2C-C3C	3.00	1.46	1.37
26	fl	201	PEB	CHA-C1B	3.00	1.47	1.40
26	hF	201	PEB	C1A-NA	-3.00	1.33	1.37
26	l8	201	PEB	C2C-C3C	3.00	1.46	1.37
26	A5	202	PEB	OD-C4D	3.00	1.29	1.23
26	GG	201	PEB	C4B-NB	-3.00	1.32	1.38
28	JF	1001	CYC	C3D-C2D	3.00	1.46	1.37
26	H3	202	PEB	CHA-C1B	3.00	1.47	1.40
26	LB	1002	PEB	C2A-C1A	-3.00	1.49	1.52
26	Z6	201	PEB	CHA-C1B	3.00	1.47	1.40
26	MA	201	PEB	CHA-C1B	3.00	1.47	1.40
26	lE	201	PEB	OD-C4D	2.99	1.29	1.23
26	fG	202	PEB	OD-C4D	2.99	1.29	1.23
26	D3	202	PEB	CHA-C1B	2.99	1.47	1.40
26	W6	202	PEB	OD-C4D	2.99	1.29	1.23
26	q4	203	PEB	C1A-NA	-2.99	1.33	1.37
26	G6	1002	PEB	C2C-C3C	2.99	1.46	1.37
26	V9	203	PEB	CHA-C1B	2.99	1.47	1.40
26	F5	201	PEB	C2A-C1A	-2.99	1.49	1.52
26	QF	203	PEB	OD-C4D	2.99	1.29	1.23
26	IA	201	PEB	C2C-C3C	2.99	1.46	1.37
26	Y7	202	PEB	C2A-C1A	-2.99	1.49	1.52
26	a8	202	PEB	C2A-C1A	-2.99	1.49	1.52
26	eI	201	PEB	C2A-C1A	-2.99	1.49	1.52
28	D6	1001	CYC	C3D-C2D	2.99	1.46	1.37
26	N8	201	PEB	C2C-C3C	2.99	1.46	1.37
26	e6	202	PEB	C2C-C3C	2.99	1.46	1.37
26	TJ	201	PEB	C1A-NA	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c4	201	PEB	OD-C4D	2.99	1.29	1.23
26	C5	204	PEB	OD-C4D	2.99	1.29	1.23
26	cA	201	PEB	C1A-NA	-2.99	1.33	1.37
26	B5	203	PEB	OD-C4D	2.99	1.29	1.23
26	J9	202	PEB	OD-C4D	2.99	1.29	1.23
26	C3	201	PEB	C2A-C1A	-2.99	1.49	1.52
26	PB	202	PEB	C2A-C1A	-2.99	1.49	1.52
26	AA	301	PEB	C1A-NA	-2.99	1.33	1.37
26	KC	203	PEB	C2A-C1A	-2.99	1.49	1.52
26	yE	301	PEB	C2A-C1A	-2.99	1.49	1.52
26	i1	203	PEB	OD-C4D	2.99	1.29	1.23
26	d8	202	PEB	CHA-C1B	2.98	1.47	1.40
26	mI	202	PEB	C2C-C3C	2.98	1.46	1.37
26	p4	201	PEB	C2A-C1A	-2.98	1.49	1.52
26	r4	201	PEB	OD-C4D	2.98	1.29	1.23
26	LJ	203	PEB	OD-C4D	2.98	1.29	1.23
26	aG	201	PEB	CHA-C1B	2.98	1.47	1.40
26	a7	202	PEB	C1A-NA	-2.98	1.33	1.37
26	F9	201	PEB	C2C-C3C	2.98	1.46	1.37
26	F1	202	PEB	C2A-C1A	-2.98	1.49	1.52
26	S7	202	PEB	OD-C4D	2.98	1.29	1.23
26	j6	202	PEB	OD-C4D	2.98	1.29	1.23
26	JE	202	PEB	C2A-C1A	-2.98	1.49	1.52
26	UD	201	PEB	C2C-C3C	2.98	1.46	1.37
26	b1	501	PEB	C1A-NA	-2.98	1.33	1.37
26	N3	201	PEB	C2C-C3C	2.98	1.46	1.37
26	OG	201	PEB	C2C-C3C	2.98	1.46	1.37
28	HB	1001	CYC	C3D-C2D	2.98	1.46	1.37
28	NB	1001	CYC	C4B-NB	-2.98	1.31	1.38
26	r1	201	PEB	OD-C4D	2.98	1.29	1.23
26	J8	201	PEB	C1A-NA	-2.98	1.33	1.37
26	11	202	PEB	C4B-C3B	2.98	1.50	1.45
26	G5	201	PEB	C2A-C1A	-2.98	1.49	1.52
26	g8	202	PEB	C2A-C1A	-2.98	1.49	1.52
26	OE	201	PEB	C2A-C1A	-2.98	1.49	1.52
26	GA	203	PEB	CHA-C1B	2.98	1.47	1.40
26	kI	202	PEB	C2C-C3C	2.98	1.46	1.37
26	ZF	203	PEB	OD-C4D	2.98	1.29	1.23
26	B8	301	PEB	C2A-C1A	-2.98	1.49	1.52
26	Z7	203	PEB	OD-C4D	2.98	1.29	1.23
26	c4	202	PEB	C1A-NA	-2.98	1.33	1.37
26	h7	201	PEB	C1A-NA	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B9	201	PEB	C2C-C3C	2.98	1.46	1.37
26	iG	203	PEB	OD-C4D	2.98	1.29	1.23
26	HI	1002	PEB	C2A-C1A	-2.98	1.49	1.52
26	iG	201	PEB	C1A-NA	-2.98	1.33	1.37
26	QA	202	PEB	C2C-C3C	2.97	1.46	1.37
26	KG	201	PEB	CHA-C1B	2.97	1.47	1.40
26	jI	201	PEB	CHA-C1B	2.97	1.47	1.40
28	gH	1001	CYC	C1B-C2B	2.97	1.50	1.45
26	fE	202	PEB	OD-C4D	2.97	1.29	1.23
26	SJ	201	PEB	C2A-C1A	-2.97	1.49	1.52
26	SD	202	PEB	CHA-C1B	2.97	1.47	1.40
26	s4	201	PEB	OD-C4D	2.97	1.29	1.23
26	d7	203	PEB	OD-C4D	2.97	1.29	1.23
26	v1	202	PEB	OD-C4D	2.97	1.29	1.23
26	aF	202	PEB	C1A-NA	-2.97	1.33	1.37
26	gI	202	PEB	C2C-C3C	2.97	1.46	1.37
26	JJ	203	PEB	C2C-C3C	2.97	1.46	1.37
26	c4	202	PEB	OD-C4D	2.97	1.29	1.23
26	D6	1002	PEB	C2A-C1A	-2.97	1.49	1.52
26	kE	202	PEB	C1A-NA	-2.97	1.33	1.37
26	B5	201	PEB	OD-C4D	2.97	1.29	1.23
26	ZB	201	PEB	CHA-C1B	2.97	1.47	1.40
26	aI	203	PEB	C2A-C1A	-2.97	1.49	1.52
26	F3	202	PEB	C2C-C3C	2.97	1.46	1.37
26	M8	201	PEB	CHA-C1B	2.96	1.47	1.40
28	tH	1001	CYC	C1B-C2B	2.96	1.50	1.45
26	m4	201	PEB	OD-C4D	2.96	1.29	1.23
26	c8	201	PEB	C1A-NA	-2.96	1.33	1.37
26	qG	202	PEB	C2C-C3C	2.96	1.46	1.37
26	YG	202	PEB	OD-C4D	2.96	1.29	1.23
26	S9	201	PEB	C2A-C1A	-2.96	1.49	1.52
26	L5	201	PEB	C2C-C3C	2.96	1.46	1.37
26	GB	1002	PEB	C2C-C3C	2.96	1.46	1.37
26	R2	203	PEB	C1A-NA	-2.96	1.33	1.37
27	A1	203	PUB	OD-C4D	2.96	1.29	1.23
28	EH	1001	CYC	C1B-C2B	2.96	1.50	1.45
28	nH	1001	CYC	C1B-C2B	2.96	1.50	1.45
26	YI	201	PEB	C2A-C1A	-2.96	1.49	1.52
26	AD	201	PEB	C4B-C3B	2.96	1.50	1.45
26	j2	201	PEB	C2A-C1A	-2.96	1.49	1.52
26	S6	201	PEB	C2A-C1A	-2.96	1.49	1.52
26	rE	202	PEB	OD-C4D	2.96	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C9	201	PEB	C2A-C1A	-2.96	1.49	1.52
26	J9	203	PEB	C2C-C3C	2.96	1.46	1.37
26	FD	202	PEB	CHA-C1B	2.96	1.47	1.40
26	W3	201	PEB	C2C-C3C	2.96	1.46	1.37
26	B8	301	PEB	C2C-C3C	2.96	1.46	1.37
26	sE	203	PEB	OD-C4D	2.96	1.29	1.23
26	C5	202	PEB	C1A-NA	-2.96	1.33	1.37
26	WD	201	PEB	C2A-C1A	-2.96	1.49	1.52
26	S8	201	PEB	CHA-C1B	2.96	1.47	1.40
26	GE	201	PEB	C4B-NB	-2.96	1.32	1.38
26	G8	203	PEB	C2C-C3C	2.95	1.46	1.37
26	L6	1002	PEB	C2A-C1A	-2.95	1.49	1.52
26	pG	202	PEB	C2A-C1A	-2.95	1.49	1.52
28	iH	1001	CYC	C1B-C2B	2.95	1.50	1.45
26	OE	201	PEB	C2C-C3C	2.95	1.46	1.37
26	jE	202	PEB	C2A-C1A	-2.95	1.49	1.52
26	V7	202	PEB	C1A-NA	-2.95	1.33	1.37
26	I5	202	PEB	C2C-C3C	2.95	1.46	1.37
26	i6	201	PEB	OD-C4D	2.95	1.29	1.23
26	U3	201	PEB	C2C-C3C	2.95	1.46	1.37
28	1H	1000	CYC	C1B-C2B	2.95	1.50	1.45
26	aA	202	PEB	C2A-C1A	-2.95	1.49	1.52
26	ZF	202	PEB	CHA-C1B	2.95	1.47	1.40
26	I5	203	PEB	C1A-NA	-2.95	1.33	1.37
26	h8	201	PEB	C1A-NA	-2.95	1.33	1.37
26	n4	202	PEB	OD-C4D	2.95	1.29	1.23
26	W7	202	PEB	OD-C4D	2.95	1.29	1.23
26	X1	203	PEB	OD-C4D	2.95	1.29	1.23
26	s4	202	PEB	OD-C4D	2.95	1.29	1.23
26	V3	202	PEB	C2C-C3C	2.95	1.46	1.37
26	I8	201	PEB	C2C-C3C	2.95	1.46	1.37
26	X9	201	PEB	OD-C4D	2.95	1.29	1.23
26	OE	203	PEB	OD-C4D	2.95	1.29	1.23
26	gF	201	PEB	OD-C4D	2.95	1.29	1.23
26	s1	203	PEB	OD-C4D	2.95	1.29	1.23
26	cE	201	PEB	OD-C4D	2.95	1.29	1.23
26	F4	201	PEB	C2A-C1A	-2.95	1.49	1.52
26	Y9	201	PEB	OD-C4D	2.95	1.29	1.23
26	kE	202	PEB	OD-C4D	2.95	1.29	1.23
26	MG	202	PEB	OD-C4D	2.95	1.29	1.23
26	e2	203	PEB	C1A-NA	-2.95	1.33	1.37
26	A5	201	PEB	C1A-NA	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F1	203	PEB	OD-C4D	2.95	1.29	1.23
26	KG	201	PEB	C2A-C1A	-2.95	1.49	1.52
26	kE	203	PEB	C1A-NA	-2.94	1.33	1.37
26	eF	201	PEB	OD-C4D	2.94	1.29	1.23
26	J8	201	PEB	C2A-C1A	-2.94	1.49	1.52
28	qH	1002	CYC	C1A-C2A	2.94	1.50	1.45
26	EJ	201	PEB	C2C-C3C	2.94	1.46	1.37
26	14	202	PEB	C4B-C3B	2.94	1.50	1.45
26	i1	201	PEB	C1A-NA	-2.94	1.33	1.37
26	G5	203	PEB	C2A-C1A	-2.94	1.49	1.52
26	rE	201	PEB	OD-C4D	2.94	1.29	1.23
26	lG	201	PEB	OD-C4D	2.94	1.29	1.23
26	O8	203	PEB	C2C-C3C	2.94	1.46	1.37
26	UA	201	PEB	C2C-C3C	2.94	1.46	1.37
26	LD	202	PEB	CHA-C1B	2.94	1.47	1.40
26	eG	201	PEB	OD-C4D	2.94	1.29	1.23
26	U4	201	PEB	C4B-C3B	2.94	1.50	1.45
26	hG	201	PEB	C2A-C1A	-2.94	1.49	1.52
28	eH	1001	CYC	C1B-C2B	2.94	1.50	1.45
26	P9	201	PEB	OD-C4D	2.94	1.29	1.23
26	Y3	301	PEB	C1A-NA	-2.94	1.33	1.37
26	AD	201	PEB	OD-C4D	2.94	1.29	1.23
26	GD	202	PEB	OD-C4D	2.94	1.29	1.23
28	KH	1001	CYC	C1D-CHD	2.94	1.52	1.41
26	P7	202	PEB	C2A-C1A	-2.94	1.49	1.52
26	iB	201	PEB	OD-C4D	2.94	1.29	1.23
28	D2	1001	CYC	C3D-C2D	2.94	1.46	1.37
26	R9	203	PEB	OD-C4D	2.94	1.29	1.23
26	QB	201	PEB	C2C-C3C	2.93	1.46	1.37
26	JD	202	PEB	CHA-C1B	2.93	1.47	1.40
26	lF	201	PEB	OD-C4D	2.93	1.29	1.23
26	JC	201	PEB	C4A-NA	-2.93	1.31	1.37
26	DJ	202	PEB	C2C-C3C	2.93	1.46	1.37
26	uE	203	PEB	OD-C4D	2.93	1.29	1.23
26	WF	201	PEB	CHA-C1B	2.93	1.47	1.40
26	hI	201	PEB	CHA-C1B	2.93	1.47	1.40
26	V3	203	PEB	OD-C4D	2.93	1.29	1.23
27	24	402	PUB	OD-C4D	2.93	1.29	1.23
28	YH	1001	CYC	C1B-C2B	2.93	1.50	1.45
26	A8	301	PEB	C1A-NA	-2.93	1.33	1.37
26	w1	202	PEB	C4B-C3B	2.93	1.50	1.45
26	T9	201	PEB	C1A-NA	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eB	202	PEB	C2C-C3C	2.93	1.46	1.37
26	c7	201	PEB	OD-C4D	2.93	1.29	1.23
28	D7	1001	CYC	C2C-C1C	-2.93	1.49	1.52
26	eI	203	PEB	C1A-NA	-2.93	1.33	1.37
26	A5	201	PEB	C2A-C1A	-2.93	1.49	1.52
26	hE	202	PEB	OD-C4D	2.93	1.29	1.23
26	RA	202	PEB	C2A-C1A	-2.92	1.49	1.52
26	QE	203	PEB	OD-C4D	2.92	1.29	1.23
26	J3	202	PEB	CHA-C1B	2.92	1.47	1.40
26	ZF	201	PEB	OD-C4D	2.92	1.29	1.23
26	WG	201	PEB	CHA-C1B	2.92	1.47	1.40
26	s1	202	PEB	OD-C4D	2.92	1.29	1.23
26	Q8	202	PEB	C2C-C3C	2.92	1.46	1.37
28	sH	1001	CYC	C1B-C2B	2.92	1.50	1.45
26	IJ	202	PEB	CHA-C1B	2.92	1.47	1.40
26	aF	201	PEB	OD-C4D	2.92	1.29	1.23
27	KD	203	PUB	OA-C1A	2.92	1.29	1.23
26	RD	202	PEB	C2C-C3C	2.92	1.46	1.37
28	IH	1001	CYC	C1B-C2B	2.92	1.50	1.45
26	VJ	203	PEB	C2C-C3C	2.92	1.46	1.37
26	Q6	201	PEB	CHA-C1B	2.92	1.47	1.40
26	G9	202	PEB	OD-C4D	2.92	1.29	1.23
26	PE	202	PEB	OD-C4D	2.92	1.29	1.23
26	wE	302	PEB	OD-C4D	2.92	1.29	1.23
26	kF	202	PEB	OD-C4D	2.92	1.29	1.23
26	D9	202	PEB	C2C-C3C	2.92	1.46	1.37
26	G3	201	PEB	C2A-C1A	-2.92	1.49	1.52
26	cF	201	PEB	OD-C4D	2.92	1.29	1.23
28	qH	1001	CYC	C1B-C2B	2.92	1.50	1.45
27	K3	203	PUB	OA-C1A	2.92	1.29	1.23
26	XJ	202	PEB	C2A-C1A	-2.92	1.49	1.52
26	l4	202	PEB	OD-C4D	2.92	1.29	1.23
26	a7	201	PEB	OD-C4D	2.92	1.29	1.23
26	m1	202	PEB	C2A-C1A	-2.92	1.49	1.52
26	C9	202	PEB	C2A-C1A	-2.92	1.49	1.52
26	SB	203	PEB	C2C-C3C	2.92	1.46	1.37
26	k2	203	PEB	C4B-C3B	2.92	1.50	1.45
26	VJ	203	PEB	CHA-C1B	2.92	1.47	1.40
28	DI	1001	CYC	C3D-C2D	2.92	1.46	1.37
26	h2	201	PEB	CHA-C1B	2.91	1.47	1.40
26	lB	203	PEB	OD-C4D	2.91	1.29	1.23
26	ME	201	PEB	C2A-C1A	-2.91	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I3	201	PEB	CHA-C1B	2.91	1.47	1.40
26	h8	201	PEB	C2C-C3C	2.91	1.46	1.37
26	OD	202	PEB	C2C-C3C	2.91	1.46	1.37
26	e7	202	PEB	OD-C4D	2.91	1.29	1.23
26	g1	203	PEB	C1A-NA	-2.91	1.33	1.37
26	CC	203	PEB	OD-C4D	2.91	1.29	1.23
27	21	402	PUB	OD-C4D	2.91	1.29	1.23
26	F4	202	PEB	C2A-C1A	-2.91	1.49	1.52
28	H2	1001	CYC	C3D-C2D	2.91	1.46	1.37
26	E8	203	PEB	OD-C4D	2.91	1.29	1.23
26	kF	202	PEB	C1A-NA	-2.91	1.33	1.37
26	OD	201	PEB	C4A-NA	-2.91	1.31	1.37
26	V2	202	PEB	C2A-C1A	-2.91	1.49	1.52
26	Q6	202	PEB	C2A-C1A	-2.91	1.49	1.52
26	KJ	201	PEB	C2A-C1A	-2.91	1.49	1.52
26	hG	201	PEB	C1A-NA	-2.91	1.33	1.37
26	CJ	201	PEB	CHA-C1B	2.91	1.47	1.40
26	l6	201	PEB	C2A-C1A	-2.91	1.49	1.52
26	i8	201	PEB	C2A-C1A	-2.91	1.49	1.52
26	Y2	202	PEB	C2C-C3C	2.91	1.46	1.37
26	K3	202	PEB	OD-C4D	2.91	1.29	1.23
26	k4	201	PEB	OD-C4D	2.91	1.29	1.23
26	OA	203	PEB	C2C-C3C	2.91	1.46	1.37
26	F4	203	PEB	OD-C4D	2.91	1.29	1.23
26	bF	203	PEB	OD-C4D	2.91	1.29	1.23
26	D6	1002	PEB	C4B-C3B	2.91	1.50	1.45
26	U8	201	PEB	C2C-C3C	2.91	1.46	1.37
26	rG	202	PEB	OD-C4D	2.91	1.29	1.23
26	HJ	203	PEB	OD-C4D	2.91	1.29	1.23
26	aG	201	PEB	C4B-C3B	2.91	1.50	1.45
26	Y2	203	PEB	C1A-NA	-2.91	1.33	1.37
26	RI	202	PEB	C2C-C3C	2.91	1.46	1.37
26	S7	201	PEB	C2A-C1A	-2.91	1.49	1.52
26	21	401	PEB	C1A-NA	-2.91	1.33	1.37
26	gE	202	PEB	OD-C4D	2.91	1.29	1.23
26	GG	202	PEB	C2C-C3C	2.91	1.46	1.37
26	U1	201	PEB	C4B-C3B	2.90	1.50	1.45
26	aA	204	PEB	CHA-C1B	2.90	1.47	1.40
26	RJ	201	PEB	CHA-C1B	2.90	1.47	1.40
26	BJ	202	PEB	OD-C4D	2.90	1.29	1.23
26	LD	202	PEB	C2C-C3C	2.90	1.46	1.37
26	b7	203	PEB	OD-C4D	2.90	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	EG	202	PEB	OD-C4D	2.90	1.29	1.23
26	TI	202	PEB	C2C-C3C	2.90	1.46	1.37
26	aA	201	PEB	C1A-NA	-2.90	1.33	1.37
26	A7	301	PEB	CHA-C1B	2.90	1.47	1.40
26	f7	201	PEB	OD-C4D	2.90	1.29	1.23
26	J9	203	PEB	CHA-C1B	2.90	1.47	1.40
26	J3	202	PEB	C1A-NA	-2.90	1.33	1.37
26	GG	202	PEB	C3B-C2B	2.90	1.42	1.36
27	A9	302	PUB	OA-C1A	2.90	1.29	1.23
26	R2	202	PEB	C2C-C3C	2.90	1.46	1.37
26	XE	202	PEB	C2A-C1A	-2.90	1.49	1.52
28	AH	1001	CYC	C1B-C2B	2.90	1.50	1.45
26	Y7	202	PEB	OD-C4D	2.90	1.29	1.23
26	NJ	202	PEB	OD-C4D	2.90	1.29	1.23
26	r1	202	PEB	OD-C4D	2.90	1.29	1.23
26	lA	201	PEB	C2C-C3C	2.90	1.46	1.37
26	K9	202	PEB	C1A-NA	-2.90	1.33	1.37
26	t4	201	PEB	OD-C4D	2.90	1.29	1.23
26	eG	201	PEB	CHA-C1B	2.90	1.47	1.40
26	k7	202	PEB	OD-C4D	2.90	1.29	1.23
26	AC	201	PEB	OD-C4D	2.90	1.29	1.23
26	BJ	201	PEB	C2C-C3C	2.90	1.46	1.37
26	S6	203	PEB	C2C-C3C	2.90	1.46	1.37
26	k1	201	PEB	OD-C4D	2.90	1.29	1.23
26	OB	202	PEB	OD-C4D	2.90	1.29	1.23
26	WB	202	PEB	OD-C4D	2.90	1.29	1.23
28	OH	1001	CYC	C1B-C2B	2.89	1.50	1.45
26	H9	202	PEB	C2A-C1A	-2.89	1.49	1.52
26	gA	201	PEB	OD-C4D	2.89	1.29	1.23
26	YI	202	PEB	C2C-C3C	2.89	1.46	1.37
26	FJ	202	PEB	OD-C4D	2.89	1.29	1.23
26	P3	202	PEB	CHA-C1B	2.89	1.47	1.40
26	y1	201	PEB	OD-C4D	2.89	1.29	1.23
26	dB	201	PEB	OD-C4D	2.89	1.29	1.23
27	A8	304	PUB	OD-C4D	2.89	1.29	1.23
26	BC	203	PEB	OD-C4D	2.89	1.29	1.23
26	aE	203	PEB	OD-C4D	2.89	1.29	1.23
26	SG	203	PEB	C2A-C1A	-2.89	1.49	1.52
26	UE	203	PEB	CHA-C1B	2.89	1.47	1.40
26	E4	202	PEB	OD-C4D	2.89	1.29	1.23
26	AC	202	PEB	OD-C4D	2.89	1.29	1.23
26	F7	1002	PEB	C2A-C1A	-2.89	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ZE	201	PEB	C2A-C1A	-2.89	1.49	1.52
26	U7	202	PEB	CHA-C1B	2.89	1.47	1.40
26	aG	203	PEB	OD-C4D	2.89	1.29	1.23
26	cG	201	PEB	OD-C4D	2.89	1.29	1.23
26	ID	201	PEB	C2A-C1A	-2.89	1.49	1.52
26	u1	203	PEB	OD-C4D	2.89	1.29	1.23
26	mI	202	PEB	C2A-C1A	-2.89	1.49	1.52
26	q4	202	PEB	OD-C4D	2.89	1.29	1.23
26	e7	201	PEB	OD-C4D	2.89	1.29	1.23
26	X9	203	PEB	OD-C4D	2.89	1.29	1.23
26	j7	202	PEB	OD-C4D	2.89	1.29	1.23
26	j7	203	PEB	OD-C4D	2.89	1.29	1.23
27	21	403	PUB	OA-C1A	2.89	1.29	1.23
26	W6	203	PEB	C2C-C3C	2.89	1.46	1.37
26	CC	201	PEB	OD-C4D	2.89	1.29	1.23
26	y4	202	PEB	C2C-C3C	2.89	1.46	1.37
28	L2	1001	CYC	C1B-NB	-2.89	1.33	1.37
26	VD	203	PEB	OD-C4D	2.89	1.29	1.23
26	ME	202	PEB	OD-C4D	2.88	1.29	1.23
26	WB	202	PEB	C2A-C1A	-2.88	1.49	1.52
26	C1	202	PEB	OD-C4D	2.88	1.29	1.23
26	BD	203	PEB	OD-C4D	2.88	1.29	1.23
26	C5	202	PEB	OD-C4D	2.88	1.29	1.23
26	uG	201	PEB	OD-C4D	2.88	1.29	1.23
26	jF	203	PEB	OD-C4D	2.88	1.29	1.23
26	kE	201	PEB	OD-C4D	2.88	1.29	1.23
26	vE	201	PEB	OD-C4D	2.88	1.29	1.23
26	f6	201	PEB	C2A-C1A	-2.88	1.49	1.52
26	A4	201	PEB	C1A-NA	-2.88	1.33	1.37
26	Y8	203	PEB	C1A-NA	-2.88	1.33	1.37
26	KJ	202	PEB	C1A-NA	-2.88	1.33	1.37
26	O7	201	PEB	OD-C4D	2.88	1.29	1.23
26	l2	201	PEB	C2A-C1A	-2.88	1.49	1.52
26	QE	203	PEB	CHA-C1B	2.88	1.47	1.40
26	T3	202	PEB	C1A-NA	-2.88	1.33	1.37
26	H3	201	PEB	OD-C4D	2.88	1.29	1.23
26	AA	302	PEB	C2A-C1A	-2.88	1.49	1.52
26	DE	202	PEB	CHA-C1B	2.88	1.47	1.40
26	xG	302	PEB	OD-C4D	2.88	1.29	1.23
26	U8	201	PEB	C2A-C1A	-2.88	1.49	1.52
26	g7	202	PEB	OD-C4D	2.88	1.29	1.23
26	AF	302	PEB	OD-C4D	2.88	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JJ	202	PEB	OD-C4D	2.88	1.29	1.23
28	H6	1001	CYC	C3D-C2D	2.88	1.46	1.37
26	EE	202	PEB	OD-C4D	2.88	1.29	1.23
26	b2	201	PEB	CHA-C1B	2.88	1.47	1.40
26	HE	201	PEB	C2C-C3C	2.88	1.46	1.37
26	d6	201	PEB	OD-C4D	2.88	1.29	1.23
26	nE	202	PEB	OD-C4D	2.88	1.29	1.23
26	hG	202	PEB	OD-C4D	2.88	1.29	1.23
26	WF	201	PEB	OD-C4D	2.88	1.29	1.23
26	GA	203	PEB	C2C-C3C	2.87	1.46	1.37
26	aG	201	PEB	OD-C4D	2.87	1.29	1.23
26	M8	203	PEB	C2A-C1A	-2.87	1.49	1.52
26	Z7	201	PEB	OD-C4D	2.87	1.29	1.23
26	cG	201	PEB	CHA-C1B	2.87	1.47	1.40
26	qE	202	PEB	C2C-C3C	2.87	1.46	1.37
26	B4	203	PEB	OD-C4D	2.87	1.29	1.23
26	W7	201	PEB	OD-C4D	2.87	1.29	1.23
26	F5	203	PEB	OD-C4D	2.87	1.29	1.23
26	eB	203	PEB	C2A-C1A	-2.87	1.49	1.52
26	sG	203	PEB	OD-C4D	2.87	1.29	1.23
26	WE	201	PEB	C2C-C3C	2.87	1.46	1.37
26	gF	202	PEB	C2A-C1A	-2.87	1.49	1.52
26	xE	304	PEB	C1A-NA	-2.87	1.33	1.37
26	B3	203	PEB	OD-C4D	2.87	1.29	1.23
26	G3	202	PEB	OD-C4D	2.87	1.29	1.23
26	m4	203	PEB	OD-C4D	2.87	1.29	1.23
26	RJ	203	PEB	OD-C4D	2.87	1.29	1.23
26	Z6	201	PEB	C2A-C1A	-2.87	1.49	1.52
26	rG	201	PEB	C2A-C1A	-2.87	1.49	1.52
26	YA	203	PEB	C1A-NA	-2.87	1.33	1.37
26	j2	202	PEB	OD-C4D	2.87	1.29	1.23
26	z4	201	PEB	OD-C4D	2.87	1.29	1.23
26	M9	201	PEB	C2A-C1A	-2.87	1.49	1.52
26	c1	201	PEB	OD-C4D	2.87	1.29	1.23
26	CC	202	PEB	OD-C4D	2.87	1.29	1.23
26	ZF	201	PEB	C2C-C3C	2.87	1.46	1.37
26	PG	202	PEB	OD-C4D	2.87	1.29	1.23
26	O6	203	PEB	C2C-C3C	2.87	1.46	1.37
26	xG	303	PEB	OD-C4D	2.87	1.29	1.23
26	TJ	202	PEB	CHA-C1B	2.87	1.47	1.40
26	gG	202	PEB	OD-C4D	2.87	1.29	1.23
27	xG	305	PUB	OA-C1A	2.87	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	MD	202	PEB	OD-C4D	2.87	1.29	1.23
26	QB	201	PEB	CHA-C1B	2.87	1.47	1.40
26	a1	203	PEB	OD-C4D	2.87	1.29	1.23
26	P9	203	PEB	OD-C4D	2.87	1.29	1.23
26	WJ	202	PEB	OD-C4D	2.87	1.29	1.23
26	e6	203	PEB	C2A-C1A	-2.87	1.49	1.52
26	P7	201	PEB	C2A-C1A	-2.87	1.49	1.52
26	A4	201	PEB	OD-C4D	2.87	1.29	1.23
26	fA	202	PEB	OD-C4D	2.87	1.29	1.23
26	aF	201	PEB	C1A-NA	-2.86	1.33	1.37
26	j6	201	PEB	OD-C4D	2.86	1.29	1.23
26	AJ	305	PEB	OD-C4D	2.86	1.29	1.23
26	p4	202	PEB	C2A-C1A	-2.86	1.49	1.52
26	I8	203	PEB	C4B-C3B	2.86	1.50	1.45
26	L9	203	PEB	OD-C4D	2.86	1.29	1.23
26	jB	201	PEB	OD-C4D	2.86	1.29	1.23
27	xG	306	PUB	OA-C1A	2.86	1.29	1.23
28	NF	1001	CYC	OB-C4B	2.86	1.29	1.23
26	e2	201	PEB	C2A-C1A	-2.86	1.49	1.52
26	WG	201	PEB	OD-C4D	2.86	1.29	1.23
26	PJ	201	PEB	OD-C4D	2.86	1.29	1.23
26	I3	201	PEB	OD-C4D	2.86	1.29	1.23
26	g8	201	PEB	OD-C4D	2.86	1.29	1.23
26	NE	202	PEB	OD-C4D	2.86	1.29	1.23
26	C5	201	PEB	OD-C4D	2.86	1.29	1.23
26	mB	202	PEB	OD-C4D	2.86	1.29	1.23
26	HD	202	PEB	OD-C4D	2.86	1.29	1.23
27	AA	304	PUB	OD-C4D	2.86	1.29	1.23
26	AF	301	PEB	C1A-NA	-2.86	1.33	1.37
26	T7	201	PEB	OD-C4D	2.86	1.29	1.23
26	OF	201	PEB	OD-C4D	2.86	1.29	1.23
26	YJ	201	PEB	OD-C4D	2.86	1.29	1.23
28	eH	1001	CYC	C1D-CHD	2.86	1.52	1.41
26	f4	202	PEB	C2A-C1A	-2.86	1.49	1.52
26	xE	304	PEB	OD-C4D	2.86	1.29	1.23
26	aE	201	PEB	C4B-C3B	2.86	1.50	1.45
26	R3	202	PEB	C2C-C3C	2.86	1.46	1.37
26	R4	202	PEB	OD-C4D	2.86	1.29	1.23
26	YF	202	PEB	OD-C4D	2.86	1.29	1.23
26	f8	202	PEB	OD-C4D	2.86	1.29	1.23
26	g8	202	PEB	C1A-NA	-2.86	1.33	1.37
26	q1	202	PEB	C1A-NA	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	FJ	201	PEB	OD-C4D	2.86	1.29	1.23
26	A1	201	PEB	C2A-C1A	-2.86	1.49	1.52
26	OF	203	PEB	CHA-C1B	2.86	1.47	1.40
26	K4	201	PEB	OD-C4D	2.86	1.29	1.23
26	EA	203	PEB	OD-C4D	2.86	1.29	1.23
26	BA	301	PEB	C2A-C1A	-2.86	1.49	1.52
26	HJ	202	PEB	C2A-C1A	-2.86	1.49	1.52
26	YD	301	PEB	C1A-NA	-2.86	1.33	1.37
26	N7	1002	PEB	OD-C4D	2.86	1.29	1.23
28	LB	1001	CYC	C1B-NB	-2.86	1.33	1.37
26	24	404	PEB	OD-C4D	2.86	1.29	1.23
27	A6	302	PUB	OD-C4D	2.86	1.29	1.23
26	R3	201	PEB	C4A-NA	-2.86	1.31	1.37
26	GG	201	PEB	C4A-NA	-2.86	1.31	1.37
28	L2	1001	CYC	C4B-NB	-2.86	1.31	1.38
26	E3	202	PEB	C1D-ND	2.86	1.50	1.45
26	z1	201	PEB	OD-C4D	2.86	1.29	1.23
26	G1	201	PEB	OD-C4D	2.85	1.29	1.23
26	A9	304	PEB	OD-C4D	2.85	1.29	1.23
26	FC	203	PEB	OD-C4D	2.85	1.29	1.23
26	Q6	201	PEB	C2C-C3C	2.85	1.46	1.37
26	VG	202	PEB	C2A-C1A	-2.85	1.49	1.52
26	uG	201	PEB	C1A-NA	-2.85	1.33	1.37
26	n1	201	PEB	OD-C4D	2.85	1.29	1.23
26	QE	203	PEB	C2C-C3C	2.85	1.46	1.37
26	KG	201	PEB	C2C-C3C	2.85	1.46	1.37
26	Q3	201	PEB	C4A-NA	-2.85	1.31	1.37
26	f1	202	PEB	OD-C4D	2.85	1.29	1.23
26	W9	201	PEB	OD-C4D	2.85	1.29	1.23
26	TF	201	PEB	OD-C4D	2.85	1.29	1.23
26	pE	201	PEB	C2A-C1A	-2.85	1.49	1.52
26	y1	203	PEB	OD-C4D	2.85	1.29	1.23
26	g7	201	PEB	OD-C4D	2.85	1.29	1.23
26	CE	203	PEB	OD-C4D	2.85	1.29	1.23
26	24	401	PEB	C1A-NA	-2.85	1.33	1.37
26	IJ	203	PEB	C4B-C3B	2.85	1.50	1.45
26	F3	201	PEB	OD-C4D	2.85	1.29	1.23
26	BC	201	PEB	OD-C4D	2.85	1.29	1.23
26	JE	202	PEB	OD-C4D	2.85	1.29	1.23
26	a2	202	PEB	C2C-C3C	2.85	1.46	1.37
26	v1	202	PEB	C4B-C3B	2.85	1.50	1.45
26	H1	203	PEB	OD-C4D	2.85	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q1	203	PEB	OD-C4D	2.85	1.29	1.23
26	H4	203	PEB	OD-C4D	2.85	1.29	1.23
28	JF	1001	CYC	C2C-C1C	-2.85	1.49	1.52
26	HG	201	PEB	C2C-C3C	2.85	1.46	1.37
26	f4	202	PEB	OD-C4D	2.85	1.29	1.23
26	dE	201	PEB	OD-C4D	2.85	1.29	1.23
27	Q8	201	PUB	OA-C1A	2.85	1.29	1.23
28	LI	1001	CYC	C4B-NB	-2.85	1.31	1.38
26	D8	202	PEB	C2A-C1A	-2.85	1.49	1.52
26	WB	203	PEB	C2C-C3C	2.85	1.46	1.37
26	m1	203	PEB	OD-C4D	2.85	1.29	1.23
26	R7	201	PEB	OD-C4D	2.85	1.29	1.23
26	tG	201	PEB	OD-C4D	2.85	1.29	1.23
26	R3	203	PEB	OD-C4D	2.85	1.29	1.23
26	JC	202	PEB	C2A-C1A	-2.85	1.49	1.52
26	e4	201	PEB	OD-C4D	2.85	1.29	1.23
26	T7	202	PEB	OD-C4D	2.85	1.29	1.23
26	AJ	304	PEB	OD-C4D	2.85	1.29	1.23
26	DB	1002	PEB	C2A-C1A	-2.85	1.49	1.52
26	u4	203	PEB	OD-C4D	2.85	1.29	1.23
26	OI	202	PEB	OD-C4D	2.85	1.29	1.23
26	R4	203	PEB	OD-C4D	2.84	1.29	1.23
26	m6	202	PEB	OD-C4D	2.84	1.29	1.23
26	lE	202	PEB	OD-C4D	2.84	1.29	1.23
26	ME	201	PEB	C1A-NA	-2.84	1.33	1.37
26	F1	201	PEB	OD-C4D	2.84	1.29	1.23
26	r4	202	PEB	OD-C4D	2.84	1.29	1.23
26	uE	202	PEB	OD-C4D	2.84	1.29	1.23
26	HD	201	PEB	OD-C4D	2.84	1.29	1.23
26	PJ	202	PEB	OD-C4D	2.84	1.29	1.23
26	gA	201	PEB	C2A-C1A	-2.84	1.49	1.52
26	J9	203	PEB	OD-C4D	2.84	1.29	1.23
26	hB	201	PEB	OD-C4D	2.84	1.29	1.23
26	jF	201	PEB	OD-C4D	2.84	1.29	1.23
26	V7	201	PEB	C2A-C1A	-2.84	1.49	1.52
26	G4	201	PEB	OD-C4D	2.84	1.29	1.23
26	aF	202	PEB	OD-C4D	2.84	1.29	1.23
26	XJ	203	PEB	OD-C4D	2.84	1.29	1.23
26	uE	201	PEB	OD-C4D	2.84	1.29	1.23
26	mG	202	PEB	OD-C4D	2.84	1.29	1.23
26	qE	201	PEB	OD-C4D	2.84	1.29	1.23
26	xE	303	PEB	OD-C4D	2.84	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ZF	202	PEB	OD-C4D	2.84	1.29	1.23
26	21	404	PEB	OD-C4D	2.84	1.29	1.23
26	j8	201	PEB	OD-C4D	2.84	1.29	1.23
27	yG	303	PUB	C3B-C2B	2.84	1.46	1.37
26	JD	202	PEB	C1A-NA	-2.84	1.33	1.37
26	q1	201	PEB	OD-C4D	2.84	1.29	1.23
26	C5	203	PEB	OD-C4D	2.84	1.29	1.23
26	cF	202	PEB	OD-C4D	2.84	1.29	1.23
27	BA	302	PUB	OD-C4D	2.84	1.29	1.23
26	IA	203	PEB	C4B-C3B	2.84	1.50	1.45
26	p1	201	PEB	OD-C4D	2.84	1.29	1.23
26	H3	202	PEB	OD-C4D	2.84	1.29	1.23
26	q4	203	PEB	OD-C4D	2.84	1.29	1.23
26	OF	202	PEB	OD-C4D	2.84	1.29	1.23
28	FF	1001	CYC	C1B-C2B	2.84	1.50	1.45
26	U7	201	PEB	OD-C4D	2.84	1.29	1.23
26	F9	201	PEB	OD-C4D	2.84	1.29	1.23
27	AB	302	PUB	OD-C4D	2.84	1.29	1.23
28	DF	1001	CYC	OB-C4B	2.84	1.29	1.23
26	iA	202	PEB	OD-C4D	2.84	1.29	1.23
26	e1	201	PEB	OD-C4D	2.83	1.29	1.23
26	b7	203	PEB	C2A-C1A	-2.83	1.49	1.52
26	UA	201	PEB	C2A-C1A	-2.83	1.49	1.52
26	d7	201	PEB	OD-C4D	2.83	1.29	1.23
26	wG	302	PEB	OD-C4D	2.83	1.29	1.23
26	lF	201	PEB	C1A-NA	-2.83	1.33	1.37
26	BD	201	PEB	OD-C4D	2.83	1.29	1.23
26	cG	203	PEB	C2C-C3C	2.83	1.46	1.37
26	w4	202	PEB	OD-C4D	2.83	1.29	1.23
26	AJ	303	PEB	OD-C4D	2.83	1.29	1.23
26	t4	202	PEB	OD-C4D	2.83	1.29	1.23
26	XA	202	PEB	C1B-C2B	2.83	1.51	1.45
26	VD	202	PEB	C2C-C3C	2.83	1.46	1.37
26	M9	202	PEB	OD-C4D	2.83	1.29	1.23
26	24	405	PEB	OD-C4D	2.83	1.29	1.23
26	c7	202	PEB	OD-C4D	2.83	1.29	1.23
26	HC	203	PEB	C2A-C1A	-2.83	1.49	1.52
26	VI	202	PEB	C2A-C1A	-2.83	1.49	1.52
26	bE	201	PEB	OD-C4D	2.83	1.29	1.23
26	NG	202	PEB	OD-C4D	2.83	1.29	1.23
26	jA	201	PEB	OD-C4D	2.83	1.29	1.23
26	bG	201	PEB	OD-C4D	2.83	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K5	201	PEB	C4A-NA	-2.83	1.31	1.37
26	cE	203	PEB	C1D-ND	2.83	1.50	1.45
26	y4	201	PEB	OD-C4D	2.83	1.29	1.23
26	m2	202	PEB	OD-C4D	2.83	1.29	1.23
26	O6	202	PEB	OD-C4D	2.83	1.29	1.23
26	DD	203	PEB	OD-C4D	2.83	1.29	1.23
26	YE	201	PEB	OD-C4D	2.83	1.29	1.23
27	A2	302	PUB	OA-C1A	2.83	1.29	1.23
26	l1	201	PEB	C2A-C1A	-2.83	1.49	1.52
26	fB	201	PEB	C2A-C1A	-2.83	1.49	1.52
26	w1	202	PEB	OD-C4D	2.83	1.29	1.23
26	u1	201	PEB	OD-C4D	2.83	1.29	1.23
26	AF	305	PEB	OD-C4D	2.83	1.29	1.23
26	QG	203	PEB	OD-C4D	2.83	1.29	1.23
26	SD	201	PEB	C2C-C3C	2.83	1.46	1.37
26	eG	201	PEB	C2A-C1A	-2.83	1.49	1.52
26	CA	203	PEB	C2C-C3C	2.83	1.46	1.37
26	B9	202	PEB	OD-C4D	2.83	1.29	1.23
26	K1	201	PEB	OD-C4D	2.83	1.29	1.23
26	fB	203	PEB	OD-C4D	2.83	1.29	1.23
26	m6	203	PEB	OD-C4D	2.82	1.29	1.23
26	f8	203	PEB	OD-C4D	2.82	1.29	1.23
26	fF	201	PEB	OD-C4D	2.82	1.29	1.23
26	p1	202	PEB	C2A-C1A	-2.82	1.49	1.52
26	c6	201	PEB	C2A-C1A	-2.82	1.49	1.52
26	ZE	202	PEB	OD-C4D	2.82	1.29	1.23
26	dE	202	PEB	OD-C4D	2.82	1.29	1.23
27	AJ	302	PUB	OA-C1A	2.82	1.29	1.23
26	P3	203	PEB	C2A-C1A	-2.82	1.49	1.52
26	A7	305	PEB	OD-C4D	2.82	1.29	1.23
26	QG	203	PEB	C4A-NA	-2.82	1.31	1.37
26	kE	203	PEB	OD-C4D	2.82	1.29	1.23
26	X4	202	PEB	C4A-NA	-2.82	1.31	1.37
26	F4	201	PEB	OD-C4D	2.82	1.28	1.23
26	H4	201	PEB	OD-C4D	2.82	1.28	1.23
26	L4	203	PEB	OD-C4D	2.82	1.28	1.23
26	d6	204	PEB	OD-C4D	2.82	1.28	1.23
26	aI	202	PEB	C2C-C3C	2.82	1.46	1.37
26	mB	203	PEB	OD-C4D	2.82	1.28	1.23
26	gA	202	PEB	OD-C4D	2.82	1.28	1.23
27	wE	304	PUB	OD-C4D	2.82	1.28	1.23
26	Z2	201	PEB	C4A-NA	-2.82	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	IE	201	PEB	OA-C1A	2.82	1.29	1.23
28	cH	1001	CYC	C1B-C2B	2.82	1.50	1.45
26	e6	203	PEB	OD-C4D	2.82	1.28	1.23
26	jG	202	PEB	OD-C4D	2.82	1.28	1.23
26	PJ	201	PEB	C2C-C3C	2.82	1.46	1.37
26	FD	203	PEB	OD-C4D	2.82	1.28	1.23
26	TJ	201	PEB	C1D-ND	2.82	1.50	1.45
26	i4	202	PEB	OD-C4D	2.82	1.28	1.23
26	GC	203	PEB	OD-C4D	2.82	1.28	1.23
26	e1	202	PEB	C4B-C3B	2.82	1.50	1.45
26	H9	201	PEB	C2C-C3C	2.82	1.46	1.37
26	dG	202	PEB	OD-C4D	2.82	1.28	1.23
26	V3	203	PEB	C2A-C1A	-2.82	1.49	1.52
26	iA	201	PEB	C2A-C1A	-2.82	1.49	1.52
26	DE	203	PEB	OD-C4D	2.82	1.28	1.23
26	dG	201	PEB	OD-C4D	2.82	1.28	1.23
26	PJ	203	PEB	OD-C4D	2.82	1.28	1.23
26	WJ	201	PEB	OD-C4D	2.82	1.28	1.23
26	b2	201	PEB	C2A-C1A	-2.81	1.49	1.52
26	qG	202	PEB	OD-C4D	2.81	1.28	1.23
26	xG	304	PEB	OD-C4D	2.81	1.28	1.23
26	hI	202	PEB	OD-C4D	2.81	1.28	1.23
28	lH	1001	CYC	C1D-CHD	2.81	1.52	1.41
26	c2	201	PEB	OD-C4D	2.81	1.28	1.23
26	cI	201	PEB	OD-C4D	2.81	1.28	1.23
26	J3	202	PEB	C2C-C3C	2.81	1.46	1.37
26	AC	203	PEB	OD-C4D	2.81	1.28	1.23
26	C4	201	PEB	OD-C4D	2.81	1.28	1.23
26	vG	201	PEB	OD-C4D	2.81	1.28	1.23
26	cI	203	PEB	OD-C4D	2.81	1.28	1.23
26	XD	202	PEB	C2C-C3C	2.81	1.46	1.37
26	GE	201	PEB	C4A-NA	-2.81	1.31	1.37
26	B1	203	PEB	OD-C4D	2.81	1.28	1.23
26	G5	203	PEB	OD-C4D	2.81	1.28	1.23
26	k7	202	PEB	C1A-NA	-2.81	1.34	1.37
26	wE	301	PEB	OD-C4D	2.81	1.28	1.23
28	N7	1001	CYC	OB-C4B	2.81	1.28	1.23
26	d1	203	PEB	OD-C4D	2.81	1.28	1.23
26	p4	201	PEB	OD-C4D	2.81	1.28	1.23
26	ZG	202	PEB	OD-C4D	2.81	1.28	1.23
26	f6	203	PEB	OD-C4D	2.81	1.28	1.23
26	P8	202	PEB	OD-C4D	2.81	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UF	203	PEB	OD-C4D	2.81	1.28	1.23
26	V3	202	PEB	OD-C4D	2.81	1.28	1.23
26	gI	203	PEB	OD-C4D	2.81	1.28	1.23
28	AH	1001	CYC	C2C-C1C	-2.81	1.49	1.52
26	N9	203	PEB	C1A-NA	-2.81	1.34	1.37
26	mG	201	PEB	C1A-NA	-2.81	1.34	1.37
26	k2	201	PEB	OD-C4D	2.81	1.28	1.23
26	m6	201	PEB	OD-C4D	2.81	1.28	1.23
26	yG	301	PEB	OD-C4D	2.81	1.28	1.23
26	GG	202	PEB	CMB-C2B	-2.81	1.44	1.50
26	H1	201	PEB	OD-C4D	2.81	1.28	1.23
26	IA	201	PEB	OD-C4D	2.81	1.28	1.23
28	NH	1001	CYC	C1D-CHD	2.81	1.52	1.41
26	U6	202	PEB	C2A-C1A	-2.81	1.49	1.52
26	D3	203	PEB	OD-C4D	2.81	1.28	1.23
28	JF	1001	CYC	OB-C4B	2.81	1.28	1.23
26	C8	203	PEB	C2C-C3C	2.81	1.46	1.37
26	PA	202	PEB	OD-C4D	2.81	1.28	1.23
26	CE	201	PEB	OD-C4D	2.81	1.28	1.23
26	A6	304	PEB	OD-C4D	2.81	1.28	1.23
26	Z7	202	PEB	OD-C4D	2.81	1.28	1.23
27	xG	305	PUB	OD-C4D	2.81	1.28	1.23
26	L7	1002	PEB	C2A-C1A	-2.81	1.49	1.52
26	WG	202	PEB	C2A-C1A	-2.81	1.49	1.52
26	E1	202	PEB	OD-C4D	2.81	1.28	1.23
26	mB	201	PEB	OD-C4D	2.81	1.28	1.23
26	jI	202	PEB	OD-C4D	2.81	1.28	1.23
26	R1	202	PEB	OD-C4D	2.81	1.28	1.23
26	g2	202	PEB	OD-C4D	2.81	1.28	1.23
26	pG	202	PEB	OD-C4D	2.81	1.28	1.23
26	m2	202	PEB	C2A-C1A	-2.80	1.49	1.52
26	k8	202	PEB	C2A-C1A	-2.80	1.49	1.52
26	rG	201	PEB	OD-C4D	2.80	1.28	1.23
28	LH	1001	CYC	C1B-C2B	2.80	1.50	1.45
26	O3	202	PEB	C2C-C3C	2.80	1.46	1.37
26	XG	202	PEB	C2C-C3C	2.80	1.46	1.37
28	rH	1001	CYC	C1B-C2B	2.80	1.50	1.45
26	U7	202	PEB	OD-C4D	2.80	1.28	1.23
26	nE	201	PEB	OD-C4D	2.80	1.28	1.23
26	fI	202	PEB	OD-C4D	2.80	1.28	1.23
26	FD	201	PEB	OD-C4D	2.80	1.28	1.23
26	CG	203	PEB	OD-C4D	2.80	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l4	202	PEB	C2A-C1A	-2.80	1.49	1.52
26	A2	305	PEB	OD-C4D	2.80	1.28	1.23
26	d4	201	PEB	OD-C4D	2.80	1.28	1.23
26	F7	1002	PEB	OD-C4D	2.80	1.28	1.23
28	LI	1001	CYC	C1B-NB	-2.80	1.33	1.37
26	yE	301	PEB	OD-C4D	2.80	1.28	1.23
26	AI	301	PEB	OD-C4D	2.80	1.28	1.23
26	T3	202	PEB	C4B-NB	-2.80	1.32	1.38
26	i4	201	PEB	OD-C4D	2.80	1.28	1.23
26	g6	201	PEB	OD-C4D	2.80	1.28	1.23
27	K1	203	PUB	OD-C4D	2.80	1.28	1.23
26	TD	202	PEB	C1A-NA	-2.80	1.34	1.37
26	oE	201	PEB	C1A-NA	-2.80	1.34	1.37
26	k6	201	PEB	OD-C4D	2.80	1.28	1.23
26	W7	203	PEB	OD-C4D	2.80	1.28	1.23
26	RJ	201	PEB	OD-C4D	2.80	1.28	1.23
26	d1	202	PEB	CHA-C1B	2.80	1.47	1.40
26	ZI	201	PEB	C4A-NA	-2.80	1.31	1.37
26	PF	202	PEB	OD-C4D	2.80	1.28	1.23
26	MJ	202	PEB	OD-C4D	2.80	1.28	1.23
26	HB	1002	PEB	C4B-C3B	2.80	1.50	1.45
26	N9	202	PEB	OD-C4D	2.80	1.28	1.23
26	c1	203	PEB	CHA-C1B	2.80	1.47	1.40
26	P9	202	PEB	OD-C4D	2.80	1.28	1.23
26	gB	201	PEB	OD-C4D	2.80	1.28	1.23
26	FC	201	PEB	OD-C4D	2.80	1.28	1.23
26	U6	201	PEB	C2C-C3C	2.80	1.46	1.37
26	y4	203	PEB	OD-C4D	2.80	1.28	1.23
26	U9	202	PEB	OD-C4D	2.80	1.28	1.23
27	21	403	PUB	OD-C4D	2.80	1.28	1.23
26	u1	203	PEB	C2A-C1A	-2.80	1.49	1.52
26	a7	201	PEB	C2A-C1A	-2.80	1.49	1.52
26	A5	201	PEB	OD-C4D	2.80	1.28	1.23
28	LB	1001	CYC	C4B-NB	-2.80	1.32	1.38
26	JJ	203	PEB	CHA-C1B	2.80	1.47	1.40
26	f2	202	PEB	OD-C4D	2.80	1.28	1.23
26	RA	202	PEB	OD-C4D	2.80	1.28	1.23
27	xE	306	PUB	OD-C4D	2.80	1.28	1.23
26	O2	202	PEB	OD-C4D	2.80	1.28	1.23
26	h6	201	PEB	OD-C4D	2.80	1.28	1.23
26	mE	201	PEB	C4B-C3B	2.80	1.50	1.45
26	B9	203	PEB	C2C-C3C	2.80	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	IC	201	PEB	C2A-C1A	-2.79	1.49	1.52
26	D1	203	PEB	OD-C4D	2.79	1.28	1.23
27	K4	203	PUB	OD-C4D	2.79	1.28	1.23
26	L1	203	PEB	OD-C4D	2.79	1.28	1.23
26	c2	203	PEB	OD-C4D	2.79	1.28	1.23
26	iI	203	PEB	OD-C4D	2.79	1.28	1.23
26	M3	202	PEB	OD-C4D	2.79	1.28	1.23
26	JG	202	PEB	OD-C4D	2.79	1.28	1.23
27	A7	304	PUB	OD-C4D	2.79	1.28	1.23
26	J3	203	PEB	C4B-C3B	2.79	1.50	1.45
26	h7	201	PEB	OD-C4D	2.79	1.28	1.23
27	AF	304	PUB	OD-C4D	2.79	1.28	1.23
26	V2	202	PEB	C2C-C3C	2.79	1.45	1.37
26	d6	203	PEB	OD-C4D	2.79	1.28	1.23
26	c1	202	PEB	OD-C4D	2.79	1.28	1.23
26	ID	201	PEB	OD-C4D	2.79	1.28	1.23
26	jE	202	PEB	OD-C4D	2.79	1.28	1.23
26	qE	202	PEB	OD-C4D	2.79	1.28	1.23
26	lB	201	PEB	C2A-C1A	-2.79	1.49	1.52
28	LF	1001	CYC	C4B-NB	-2.79	1.32	1.38
26	l6	201	PEB	OD-C4D	2.79	1.28	1.23
26	eB	203	PEB	OD-C4D	2.79	1.28	1.23
26	IC	203	PEB	OD-C4D	2.79	1.28	1.23
26	r4	202	PEB	C2A-C1A	-2.79	1.49	1.52
26	KA	202	PEB	C2A-C1A	-2.79	1.49	1.52
26	dE	201	PEB	C1A-NA	-2.79	1.34	1.37
26	Q6	201	PEB	C2A-C1A	-2.79	1.49	1.52
26	B9	203	PEB	CHA-C1B	2.79	1.47	1.40
26	p1	202	PEB	OD-C4D	2.79	1.28	1.23
26	E4	201	PEB	OD-C4D	2.79	1.28	1.23
26	TF	202	PEB	OD-C4D	2.79	1.28	1.23
27	NJ	201	PUB	OA-C1A	2.79	1.28	1.23
26	D3	201	PEB	C2A-C1A	-2.79	1.49	1.52
26	m7	202	PEB	C2A-C1A	-2.79	1.49	1.52
26	VF	202	PEB	C2A-C1A	-2.79	1.49	1.52
26	I4	202	PEB	OD-C4D	2.79	1.28	1.23
26	m7	202	PEB	OD-C4D	2.79	1.28	1.23
26	lB	201	PEB	OD-C4D	2.79	1.28	1.23
26	pE	202	PEB	OD-C4D	2.79	1.28	1.23
28	HI	1001	CYC	C3D-C2D	2.79	1.45	1.37
26	Q2	202	PEB	OD-C4D	2.79	1.28	1.23
26	F3	203	PEB	OD-C4D	2.79	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C4	202	PEB	OD-C4D	2.79	1.28	1.23
26	i8	202	PEB	OD-C4D	2.79	1.28	1.23
26	aA	203	PEB	OD-C4D	2.79	1.28	1.23
26	vG	202	PEB	OD-C4D	2.79	1.28	1.23
26	AI	305	PEB	OD-C4D	2.79	1.28	1.23
26	DG	202	PEB	C2C-C3C	2.79	1.45	1.37
26	h2	202	PEB	OD-C4D	2.79	1.28	1.23
26	k2	203	PEB	OD-C4D	2.79	1.28	1.23
26	sE	201	PEB	OD-C4D	2.79	1.28	1.23
26	dI	202	PEB	OD-C4D	2.79	1.28	1.23
27	A9	302	PUB	OD-C4D	2.79	1.28	1.23
26	W9	202	PEB	OD-C4D	2.78	1.28	1.23
26	LD	203	PEB	OD-C4D	2.78	1.28	1.23
26	y1	202	PEB	OD-C4D	2.78	1.28	1.23
27	Q8	201	PUB	OD-C4D	2.78	1.28	1.23
26	y4	202	PEB	OD-C4D	2.78	1.28	1.23
26	YG	201	PEB	OD-C4D	2.78	1.28	1.23
26	11	203	PEB	OD-C4D	2.78	1.28	1.23
27	xE	301	PUB	OD-C4D	2.78	1.28	1.23
26	IG	203	PEB	CHA-C1B	2.78	1.46	1.40
26	b2	202	PEB	OD-C4D	2.78	1.28	1.23
26	x4	201	PEB	OD-C4D	2.78	1.28	1.23
26	eF	202	PEB	OD-C4D	2.78	1.28	1.23
26	x4	202	PEB	OD-C4D	2.78	1.28	1.23
26	dB	203	PEB	OD-C4D	2.78	1.28	1.23
26	mE	203	PEB	OD-C4D	2.78	1.28	1.23
26	H6	1002	PEB	C4B-C3B	2.78	1.50	1.45
26	S3	202	PEB	CHA-C1B	2.78	1.46	1.40
26	s1	202	PEB	C2A-C1A	-2.78	1.49	1.52
26	Y2	201	PEB	C2A-C1A	-2.78	1.49	1.52
26	oE	203	PEB	OD-C4D	2.78	1.28	1.23
27	AI	302	PUB	OA-C1A	2.78	1.28	1.23
26	R7	202	PEB	C1A-NA	-2.78	1.34	1.37
26	a1	202	PEB	OD-C4D	2.78	1.28	1.23
26	k1	202	PEB	OD-C4D	2.78	1.28	1.23
26	fA	203	PEB	OD-C4D	2.78	1.28	1.23
26	eE	202	PEB	OD-C4D	2.78	1.28	1.23
26	v1	201	PEB	OD-C4D	2.78	1.28	1.23
26	h4	201	PEB	OD-C4D	2.78	1.28	1.23
26	14	201	PEB	OD-C4D	2.78	1.28	1.23
26	D8	202	PEB	OD-C4D	2.78	1.28	1.23
26	bE	202	PEB	OD-C4D	2.78	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	i1	201	PEB	C2A-C1A	-2.78	1.49	1.52
26	A1	202	PEB	OD-C4D	2.78	1.28	1.23
26	kI	201	PEB	OD-C4D	2.78	1.28	1.23
26	g2	203	PEB	OD-C4D	2.78	1.28	1.23
27	24	402	PUB	OA-C1A	2.78	1.28	1.23
27	24	403	PUB	OA-C1A	2.78	1.28	1.23
26	cF	202	PEB	C2A-C1A	-2.78	1.49	1.52
26	OG	201	PEB	C2A-C1A	-2.78	1.49	1.52
26	bI	202	PEB	OD-C4D	2.78	1.28	1.23
26	D9	201	PEB	C2C-C3C	2.78	1.45	1.37
26	ME	201	PEB	OD-C4D	2.78	1.28	1.23
26	xE	302	PEB	OD-C4D	2.78	1.28	1.23
27	xE	305	PUB	OD-C4D	2.78	1.28	1.23
26	KE	201	PEB	C2C-C3C	2.78	1.45	1.37
26	q1	203	PEB	C1A-NA	-2.78	1.34	1.37
26	d2	202	PEB	OD-C4D	2.78	1.28	1.23
26	A1	201	PEB	OD-C4D	2.78	1.28	1.23
26	L3	203	PEB	OD-C4D	2.78	1.28	1.23
26	d4	203	PEB	OD-C4D	2.78	1.28	1.23
26	t1	201	PEB	OD-C4D	2.78	1.28	1.23
27	xE	306	PUB	OA-C1A	2.78	1.28	1.23
26	aE	201	PEB	CHA-C1B	2.78	1.46	1.40
26	n4	201	PEB	OD-C4D	2.77	1.28	1.23
26	o1	501	PEB	OD-C4D	2.77	1.28	1.23
26	B3	201	PEB	OD-C4D	2.77	1.28	1.23
26	fE	201	PEB	OD-C4D	2.77	1.28	1.23
26	nG	202	PEB	OD-C4D	2.77	1.28	1.23
28	JI	1001	CYC	C3D-C2D	2.77	1.45	1.37
28	JI	1001	CYC	C1B-NB	-2.77	1.33	1.37
26	a7	202	PEB	OD-C4D	2.77	1.28	1.23
26	fG	201	PEB	OD-C4D	2.77	1.28	1.23
26	hA	201	PEB	C2A-C1A	-2.77	1.49	1.52
26	DE	202	PEB	C2C-C3C	2.77	1.45	1.37
28	SH	1001	CYC	C1D-CHD	2.77	1.51	1.41
26	OG	201	PEB	CHA-C1B	2.77	1.46	1.40
26	I5	203	PEB	OD-C4D	2.77	1.28	1.23
26	RG	202	PEB	OD-C4D	2.77	1.28	1.23
28	J7	1003	CYC	OB-C4B	2.77	1.28	1.23
26	I1	202	PEB	OD-C4D	2.77	1.28	1.23
26	Y3	301	PEB	OD-C4D	2.77	1.28	1.23
26	AB	304	PEB	OD-C4D	2.77	1.28	1.23
26	j1	202	PEB	OD-C4D	2.77	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TG	202	PEB	OD-C4D	2.77	1.28	1.23
26	i2	202	PEB	C2A-C1A	-2.77	1.49	1.52
26	eG	202	PEB	C2A-C1A	-2.77	1.49	1.52
26	14	201	PEB	C4B-C3B	2.77	1.50	1.45
26	j7	201	PEB	OD-C4D	2.77	1.28	1.23
28	D7	1001	CYC	OB-C4B	2.77	1.28	1.23
26	21	404	PEB	C1A-NA	-2.77	1.34	1.37
26	k4	203	PEB	C1A-NA	-2.77	1.34	1.37
26	q1	202	PEB	OD-C4D	2.77	1.28	1.23
26	11	201	PEB	OD-C4D	2.77	1.28	1.23
26	FF	1002	PEB	OD-C4D	2.77	1.28	1.23
26	D3	201	PEB	OD-C4D	2.77	1.28	1.23
26	P8	202	PEB	C2A-C1A	-2.77	1.49	1.52
26	QB	202	PEB	C2A-C1A	-2.77	1.49	1.52
28	J7	1001	CYC	C2C-C1C	-2.77	1.49	1.52
26	A7	302	PEB	OD-C4D	2.77	1.28	1.23
26	UF	202	PEB	OD-C4D	2.77	1.28	1.23
26	a8	201	PEB	C1A-NA	-2.77	1.34	1.37
26	a4	202	PEB	OD-C4D	2.77	1.28	1.23
26	eG	202	PEB	OD-C4D	2.77	1.28	1.23
26	OE	201	PEB	CHA-C1B	2.77	1.46	1.40
26	a4	202	PEB	C2A-C1A	-2.77	1.49	1.52
26	A8	301	PEB	OD-C4D	2.77	1.28	1.23
26	g8	202	PEB	OD-C4D	2.77	1.28	1.23
26	RA	201	PEB	OD-C4D	2.77	1.28	1.23
27	xE	305	PUB	OA-C1A	2.77	1.28	1.23
26	X1	202	PEB	C4A-NA	-2.77	1.31	1.37
26	e6	201	PEB	OD-C4D	2.77	1.28	1.23
26	I8	201	PEB	OD-C4D	2.77	1.28	1.23
26	b7	201	PEB	OD-C4D	2.77	1.28	1.23
26	z4	202	PEB	OD-C4D	2.77	1.28	1.23
26	D1	202	PEB	C2A-C1A	-2.77	1.49	1.52
26	B3	201	PEB	C2A-C1A	-2.77	1.49	1.52
26	HB	1002	PEB	C2A-C1A	-2.77	1.49	1.52
26	BJ	202	PEB	C2A-C1A	-2.77	1.49	1.52
26	BJ	203	PEB	C2C-C3C	2.77	1.45	1.37
26	A6	301	PEB	OD-C4D	2.76	1.28	1.23
26	l7	202	PEB	OD-C4D	2.76	1.28	1.23
26	HD	203	PEB	OD-C4D	2.76	1.28	1.23
27	A7	303	PUB	OD-C4D	2.76	1.28	1.23
26	dF	202	PEB	C2A-C1A	-2.76	1.49	1.52
26	cA	202	PEB	OD-C4D	2.76	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X3	203	PEB	C4A-NA	-2.76	1.31	1.37
26	b7	202	PEB	OD-C4D	2.76	1.28	1.23
26	kB	202	PEB	C2A-C1A	-2.76	1.49	1.52
26	II	201	PEB	C2A-C1A	-2.76	1.49	1.52
26	UB	201	PEB	C2C-C3C	2.76	1.45	1.37
26	x1	201	PEB	OD-C4D	2.76	1.28	1.23
26	j4	202	PEB	OD-C4D	2.76	1.28	1.23
26	P7	202	PEB	OD-C4D	2.76	1.28	1.23
26	UG	201	PEB	C4A-NA	-2.76	1.31	1.37
28	JH	1001	CYC	C1D-CHD	2.76	1.51	1.41
26	QD	201	PEB	C2C-C3C	2.76	1.45	1.37
26	H3	203	PEB	OD-C4D	2.76	1.28	1.23
26	R6	202	PEB	OD-C4D	2.76	1.28	1.23
26	l8	201	PEB	OD-C4D	2.76	1.28	1.23
26	Y9	202	PEB	OD-C4D	2.76	1.28	1.23
26	TE	202	PEB	OD-C4D	2.76	1.28	1.23
27	K1	203	PUB	OA-C1A	2.76	1.28	1.23
26	K9	201	PEB	C2A-C1A	-2.76	1.49	1.52
26	JA	201	PEB	C2A-C1A	-2.76	1.49	1.52
26	K3	201	PEB	OD-C4D	2.76	1.28	1.23
26	KD	201	PEB	OD-C4D	2.76	1.28	1.23
26	L4	201	PEB	OD-C4D	2.76	1.28	1.23
26	i1	202	PEB	C2A-C1A	-2.76	1.49	1.52
26	dA	201	PEB	OD-C4D	2.76	1.28	1.23
26	RF	201	PEB	OD-C4D	2.76	1.28	1.23
28	hH	1001	CYC	C1D-CHD	2.76	1.51	1.41
26	I4	201	PEB	OD-C4D	2.76	1.28	1.23
26	dB	204	PEB	OD-C4D	2.76	1.28	1.23
26	hE	201	PEB	OD-C4D	2.76	1.28	1.23
26	i2	203	PEB	OD-C4D	2.76	1.28	1.23
26	BE	201	PEB	C2C-C3C	2.76	1.45	1.37
26	d1	202	PEB	C4B-C3B	2.76	1.50	1.45
26	lE	201	PEB	C4B-C3B	2.76	1.50	1.45
26	S1	202	PEB	OD-C4D	2.76	1.28	1.23
26	iE	202	PEB	OD-C4D	2.76	1.28	1.23
26	kE	202	PEB	C4B-C3B	2.76	1.50	1.45
28	cH	1001	CYC	C1D-CHD	2.76	1.51	1.41
26	R1	203	PEB	OD-C4D	2.76	1.28	1.23
26	k6	202	PEB	OD-C4D	2.76	1.28	1.23
26	RB	201	PEB	OD-C4D	2.76	1.28	1.23
27	21	402	PUB	OA-C1A	2.76	1.28	1.23
26	U3	201	PEB	C4A-NA	-2.76	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	qH	1001	CYC	C1D-CHD	2.76	1.51	1.41
26	C9	202	PEB	OD-C4D	2.76	1.28	1.23
26	s1	202	PEB	C1A-NA	-2.76	1.34	1.37
26	R8	201	PEB	OD-C4D	2.76	1.28	1.23
26	TE	201	PEB	OD-C4D	2.76	1.28	1.23
26	bF	202	PEB	OD-C4D	2.76	1.28	1.23
26	z4	202	PEB	C4B-C3B	2.76	1.50	1.45
26	L4	202	PEB	OD-C4D	2.76	1.28	1.23
26	VF	201	PEB	C2A-C1A	-2.76	1.49	1.52
26	YI	202	PEB	C2A-C1A	-2.76	1.49	1.52
26	g1	201	PEB	OD-C4D	2.76	1.28	1.23
26	RB	202	PEB	OD-C4D	2.76	1.28	1.23
26	bG	202	PEB	OD-C4D	2.76	1.28	1.23
26	aA	204	PEB	C2C-C3C	2.76	1.45	1.37
26	OB	203	PEB	C2C-C3C	2.76	1.45	1.37
26	JD	203	PEB	OD-C4D	2.76	1.28	1.23
26	iF	201	PEB	OD-C4D	2.76	1.28	1.23
26	U6	201	PEB	C2A-C1A	-2.76	1.49	1.52
26	mE	203	PEB	C2A-C1A	-2.76	1.49	1.52
26	YF	201	PEB	OD-C4D	2.76	1.28	1.23
26	nG	201	PEB	OD-C4D	2.76	1.28	1.23
27	AI	302	PUB	OD-C4D	2.76	1.28	1.23
26	KA	203	PEB	CHA-C1B	2.76	1.46	1.40
26	sG	203	PEB	C4B-C3B	2.75	1.50	1.45
26	lG	202	PEB	OD-C4D	2.75	1.28	1.23
26	gI	201	PEB	OD-C4D	2.75	1.28	1.23
27	wG	304	PUB	OD-C4D	2.75	1.28	1.23
28	jH	1001	CYC	OB-C4B	2.75	1.28	1.23
28	qH	1001	CYC	OB-C4B	2.75	1.28	1.23
26	GC	202	PEB	OD-C4D	2.75	1.28	1.23
26	DB	1002	PEB	C4B-C3B	2.75	1.50	1.45
26	m1	201	PEB	C2A-C1A	-2.75	1.49	1.52
26	R7	202	PEB	OD-C4D	2.75	1.28	1.23
26	uG	202	PEB	OD-C4D	2.75	1.28	1.23
26	I9	201	PEB	OD-C4D	2.75	1.28	1.23
26	S9	202	PEB	OD-C4D	2.75	1.28	1.23
26	DA	202	PEB	OD-C4D	2.75	1.28	1.23
26	FD	202	PEB	C1A-NA	-2.75	1.34	1.37
26	T1	201	PEB	C2A-C1A	-2.75	1.49	1.52
26	J1	201	PEB	OD-C4D	2.75	1.28	1.23
26	e2	203	PEB	OD-C4D	2.75	1.28	1.23
26	J7	1002	PEB	OD-C4D	2.75	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C9	201	PEB	OD-C4D	2.75	1.28	1.23
26	kA	202	PEB	OD-C4D	2.75	1.28	1.23
26	BC	202	PEB	OD-C4D	2.75	1.28	1.23
27	K4	203	PUB	OA-C1A	2.75	1.28	1.23
27	xG	301	PUB	OD-C4D	2.75	1.28	1.23
26	e4	202	PEB	C4B-C3B	2.75	1.50	1.45
26	21	401	PEB	OD-C4D	2.75	1.28	1.23
26	21	405	PEB	OD-C4D	2.75	1.28	1.23
26	e8	202	PEB	OD-C4D	2.75	1.28	1.23
26	AA	301	PEB	OD-C4D	2.75	1.28	1.23
28	YH	1003	CYC	C1D-CHD	2.75	1.51	1.41
26	D4	203	PEB	OD-C4D	2.75	1.28	1.23
26	UF	202	PEB	CHA-C1B	2.75	1.46	1.40
26	AI	304	PEB	OD-C4D	2.75	1.28	1.23
26	B1	201	PEB	OD-C4D	2.75	1.28	1.23
26	J3	203	PEB	OD-C4D	2.75	1.28	1.23
26	RE	202	PEB	OD-C4D	2.75	1.28	1.23
26	J4	201	PEB	OD-C4D	2.75	1.28	1.23
26	Y7	201	PEB	OD-C4D	2.75	1.28	1.23
26	E9	202	PEB	OD-C4D	2.75	1.28	1.23
28	jH	1001	CYC	C1D-CHD	2.75	1.51	1.41
26	LD	202	PEB	OD-C4D	2.75	1.28	1.23
26	BE	202	PEB	OD-C4D	2.75	1.28	1.23
27	xG	306	PUB	OD-C4D	2.75	1.28	1.23
26	Y2	202	PEB	C2A-C1A	-2.75	1.49	1.52
26	LD	202	PEB	C2A-C1A	-2.75	1.49	1.52
26	oE	203	PEB	C2A-C1A	-2.75	1.49	1.52
26	u1	202	PEB	OD-C4D	2.75	1.28	1.23
26	w4	201	PEB	OD-C4D	2.75	1.28	1.23
26	h1	201	PEB	OD-C4D	2.75	1.28	1.23
26	vE	202	PEB	OD-C4D	2.75	1.28	1.23
26	dF	201	PEB	OD-C4D	2.75	1.28	1.23
28	J2	1001	CYC	C1B-NB	-2.75	1.33	1.37
26	KE	201	PEB	C2A-C1A	-2.75	1.49	1.52
26	g4	201	PEB	OD-C4D	2.75	1.28	1.23
27	A7	304	PUB	OA-C1A	2.75	1.28	1.23
26	h1	202	PEB	OD-C4D	2.74	1.28	1.23
26	U4	202	PEB	OD-C4D	2.74	1.28	1.23
26	FC	202	PEB	OD-C4D	2.74	1.28	1.23
26	OE	202	PEB	OD-C4D	2.74	1.28	1.23
28	uH	1001	CYC	C1D-CHD	2.74	1.51	1.41
26	U1	202	PEB	C2A-C1A	-2.74	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m6	201	PEB	C2A-C1A	-2.74	1.49	1.52
26	w1	201	PEB	OD-C4D	2.74	1.28	1.23
26	R9	201	PEB	OD-C4D	2.74	1.28	1.23
27	AB	302	PUB	OA-C1A	2.74	1.28	1.23
26	ZE	201	PEB	OD-C4D	2.74	1.28	1.23
26	bF	201	PEB	OD-C4D	2.74	1.28	1.23
26	X3	203	PEB	C2A-C1A	-2.74	1.49	1.52
26	a4	203	PEB	OD-C4D	2.74	1.28	1.23
26	a6	202	PEB	OD-C4D	2.74	1.28	1.23
26	S8	202	PEB	OD-C4D	2.74	1.28	1.23
27	A2	302	PUB	OD-C4D	2.74	1.28	1.23
26	lF	203	PEB	C4B-C3B	2.74	1.50	1.45
26	J1	202	PEB	OD-C4D	2.74	1.28	1.23
26	A2	304	PEB	OD-C4D	2.74	1.28	1.23
26	F5	201	PEB	OD-C4D	2.74	1.28	1.23
26	sG	201	PEB	OD-C4D	2.74	1.28	1.23
26	d6	202	PEB	OD-C4D	2.74	1.28	1.23
26	a8	201	PEB	OD-C4D	2.74	1.28	1.23
28	L6	1001	CYC	C1B-NB	-2.74	1.33	1.37
26	tE	201	PEB	OD-C4D	2.74	1.28	1.23
26	mI	203	PEB	OD-C4D	2.74	1.28	1.23
26	R6	201	PEB	OD-C4D	2.74	1.28	1.23
26	MA	203	PEB	C2A-C1A	-2.74	1.49	1.52
28	RH	1001	CYC	C1B-C2B	2.74	1.50	1.45
26	e2	201	PEB	OD-C4D	2.74	1.28	1.23
26	VE	201	PEB	OD-C4D	2.74	1.28	1.23
26	eI	201	PEB	OD-C4D	2.74	1.28	1.23
26	gI	202	PEB	OD-C4D	2.74	1.28	1.23
26	d7	202	PEB	OD-C4D	2.74	1.28	1.23
26	kB	202	PEB	OD-C4D	2.74	1.28	1.23
28	mH	1001	CYC	C1D-CHD	2.74	1.51	1.41
26	hA	201	PEB	OD-C4D	2.74	1.28	1.23
26	UD	201	PEB	C4A-NA	-2.74	1.31	1.37
26	i7	201	PEB	OD-C4D	2.74	1.28	1.23
26	XJ	201	PEB	OD-C4D	2.74	1.28	1.23
28	MH	1001	CYC	OB-C4B	2.74	1.28	1.23
26	T8	201	PEB	C2A-C1A	-2.74	1.49	1.52
26	UB	202	PEB	C2A-C1A	-2.74	1.49	1.52
26	L2	1002	PEB	OD-C4D	2.74	1.28	1.23
28	YH	1004	CYC	OB-C4B	2.74	1.28	1.23
26	t1	202	PEB	OD-C4D	2.74	1.28	1.23
26	w4	203	PEB	OD-C4D	2.74	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W9	202	PEB	C2A-C1A	-2.74	1.49	1.52
26	eE	201	PEB	C2A-C1A	-2.74	1.49	1.52
26	i6	202	PEB	OD-C4D	2.74	1.28	1.23
26	ZG	201	PEB	OD-C4D	2.74	1.28	1.23
26	kG	203	PEB	OD-C4D	2.74	1.28	1.23
28	CH	1001	CYC	C1D-CHD	2.74	1.51	1.41
26	XE	202	PEB	OD-C4D	2.74	1.28	1.23
26	MD	201	PEB	C2A-C1A	-2.74	1.49	1.52
26	T9	201	PEB	C1D-ND	2.74	1.49	1.45
26	F1	202	PEB	OD-C4D	2.73	1.28	1.23
26	v4	201	PEB	OD-C4D	2.73	1.28	1.23
26	D7	1002	PEB	OD-C4D	2.73	1.28	1.23
26	L9	202	PEB	OD-C4D	2.73	1.28	1.23
26	oE	201	PEB	OD-C4D	2.73	1.28	1.23
26	pE	201	PEB	OD-C4D	2.73	1.28	1.23
26	h8	201	PEB	OD-C4D	2.73	1.28	1.23
26	PB	202	PEB	OD-C4D	2.73	1.28	1.23
28	EF	1001	CYC	C4C-NC	-2.73	1.31	1.37
26	e6	202	PEB	OD-C4D	2.73	1.28	1.23
26	aB	202	PEB	OD-C4D	2.73	1.28	1.23
26	KC	203	PEB	OD-C4D	2.73	1.28	1.23
26	VD	201	PEB	OD-C4D	2.73	1.28	1.23
26	AE	201	PEB	OD-C4D	2.73	1.28	1.23
26	DE	201	PEB	OD-C4D	2.73	1.28	1.23
26	Y7	201	PEB	C2A-C1A	-2.73	1.49	1.52
26	HC	202	PEB	C2A-C1A	-2.73	1.49	1.52
26	k4	202	PEB	OD-C4D	2.73	1.28	1.23
26	P6	202	PEB	OD-C4D	2.73	1.28	1.23
27	AB	303	PUB	OA-C1A	2.73	1.28	1.23
26	C1	201	PEB	OD-C4D	2.73	1.28	1.23
26	h7	202	PEB	OD-C4D	2.73	1.28	1.23
26	fl	201	PEB	OD-C4D	2.73	1.28	1.23
26	c2	202	PEB	OD-C4D	2.73	1.28	1.23
26	KC	201	PEB	OD-C4D	2.73	1.28	1.23
26	XG	203	PEB	OD-C4D	2.73	1.28	1.23
26	s1	201	PEB	OD-C4D	2.73	1.28	1.23
26	h4	203	PEB	OD-C4D	2.73	1.28	1.23
26	NE	201	PEB	OD-C4D	2.73	1.28	1.23
26	WF	203	PEB	OD-C4D	2.73	1.28	1.23
27	QA	201	PUB	OA-C1A	2.73	1.28	1.23
26	eB	202	PEB	OD-C4D	2.73	1.28	1.23
26	cA	203	PEB	OD-C4D	2.73	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VB	202	PEB	OD-C4D	2.73	1.28	1.23
27	A6	303	PUB	OA-C1A	2.73	1.28	1.23
26	GC	201	PEB	OD-C4D	2.73	1.28	1.23
26	JF	1002	PEB	OD-C4D	2.73	1.28	1.23
26	OG	202	PEB	OD-C4D	2.73	1.28	1.23
26	q4	202	PEB	C2A-C1A	-2.73	1.49	1.52
26	O7	203	PEB	OD-C4D	2.73	1.28	1.23
26	QE	201	PEB	OD-C4D	2.73	1.28	1.23
26	iF	202	PEB	OD-C4D	2.73	1.28	1.23
26	O1	201	PEB	OD-C4D	2.73	1.28	1.23
26	a8	203	PEB	OD-C4D	2.73	1.28	1.23
26	cA	201	PEB	OD-C4D	2.73	1.28	1.23
26	eB	201	PEB	OD-C4D	2.73	1.28	1.23
26	VD	202	PEB	OD-C4D	2.73	1.28	1.23
26	HE	202	PEB	OD-C4D	2.73	1.28	1.23
26	x4	202	PEB	C4B-C3B	2.73	1.50	1.45
26	t4	202	PEB	C2A-C1A	-2.73	1.49	1.52
26	gA	202	PEB	C2A-C1A	-2.73	1.49	1.52
26	l2	201	PEB	OD-C4D	2.73	1.28	1.23
26	f4	201	PEB	OD-C4D	2.73	1.28	1.23
26	E1	201	PEB	OD-C4D	2.73	1.28	1.23
26	WE	202	PEB	OD-C4D	2.73	1.28	1.23
26	f2	201	PEB	OD-C4D	2.73	1.28	1.23
26	L9	201	PEB	OD-C4D	2.73	1.28	1.23
26	cI	202	PEB	OD-C4D	2.73	1.28	1.23
26	Y3	301	PEB	C2A-C1A	-2.73	1.49	1.52
26	I8	201	PEB	C2A-C1A	-2.73	1.49	1.52
26	cB	201	PEB	C2A-C1A	-2.73	1.49	1.52
26	PI	202	PEB	C2C-C3C	2.73	1.45	1.37
26	A4	202	PEB	OD-C4D	2.72	1.28	1.23
26	U1	202	PEB	OD-C4D	2.72	1.28	1.23
26	mI	202	PEB	OD-C4D	2.72	1.28	1.23
28	OH	1001	CYC	OB-C4B	2.72	1.28	1.23
26	kI	202	PEB	C2A-C1A	-2.72	1.49	1.52
26	MG	201	PEB	OD-C4D	2.72	1.28	1.23
26	CJ	202	PEB	OD-C4D	2.72	1.28	1.23
26	xG	304	PEB	C1A-NA	-2.72	1.34	1.37
26	RF	202	PEB	OD-C4D	2.72	1.28	1.23
26	kG	201	PEB	OD-C4D	2.72	1.28	1.23
26	LI	1002	PEB	OD-C4D	2.72	1.28	1.23
26	QJ	202	PEB	OD-C4D	2.72	1.28	1.23
27	BA	302	PUB	OA-C1A	2.72	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m4	201	PEB	C1D-ND	2.72	1.49	1.45
26	SE	201	PEB	C2C-C3C	2.72	1.45	1.37
26	f8	201	PEB	OD-C4D	2.72	1.28	1.23
26	TF	201	PEB	C2A-C1A	-2.72	1.49	1.52
26	d1	201	PEB	OD-C4D	2.72	1.28	1.23
26	QG	201	PEB	OD-C4D	2.72	1.28	1.23
26	hG	201	PEB	OD-C4D	2.72	1.28	1.23
26	c1	203	PEB	OD-C4D	2.72	1.28	1.23
26	YB	202	PEB	OD-C4D	2.72	1.28	1.23
26	iB	202	PEB	OD-C4D	2.72	1.28	1.23
26	IJ	201	PEB	OD-C4D	2.72	1.28	1.23
26	q4	201	PEB	OD-C4D	2.72	1.28	1.23
26	iI	201	PEB	OD-C4D	2.72	1.28	1.23
28	L6	1001	CYC	C4B-NB	-2.72	1.32	1.38
26	s4	201	PEB	C2A-C1A	-2.72	1.49	1.52
26	J1	203	PEB	OD-C4D	2.72	1.28	1.23
26	g2	201	PEB	OD-C4D	2.72	1.28	1.23
26	aE	201	PEB	OD-C4D	2.72	1.28	1.23
28	TH	1001	CYC	C1B-C2B	2.72	1.50	1.45
26	qE	202	PEB	C4A-NA	-2.72	1.31	1.37
26	J9	201	PEB	C2A-C1A	-2.72	1.49	1.52
26	i2	202	PEB	OD-C4D	2.72	1.28	1.23
26	V6	202	PEB	OD-C4D	2.72	1.28	1.23
28	J2	1001	CYC	C3D-C2D	2.72	1.45	1.37
26	fA	201	PEB	OD-C4D	2.72	1.28	1.23
26	VB	201	PEB	OD-C4D	2.72	1.28	1.23
26	qG	202	PEB	C4B-C3B	2.72	1.50	1.45
26	c8	201	PEB	OD-C4D	2.72	1.28	1.23
28	1H	1000	CYC	OB-C4B	2.72	1.28	1.23
28	qH	1002	CYC	OB-C4B	2.72	1.28	1.23
26	g1	203	PEB	C1D-ND	2.72	1.49	1.45
26	m2	203	PEB	OD-C4D	2.71	1.28	1.23
26	DG	203	PEB	OD-C4D	2.71	1.28	1.23
26	f4	201	PEB	C4B-C3B	2.71	1.50	1.45
26	A7	301	PEB	OD-C4D	2.71	1.28	1.23
26	iI	202	PEB	OD-C4D	2.71	1.28	1.23
26	XJ	202	PEB	OD-C4D	2.71	1.28	1.23
26	DA	202	PEB	C2A-C1A	-2.71	1.49	1.52
28	vH	1001	CYC	C1B-C2B	2.71	1.50	1.45
28	YH	1002	CYC	C1D-CHD	2.71	1.51	1.41
26	K5	203	PEB	OD-C4D	2.71	1.28	1.23
26	K9	201	PEB	OD-C4D	2.71	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eA	202	PEB	OD-C4D	2.71	1.28	1.23
26	TF	201	PEB	C4B-C3B	2.71	1.50	1.45
26	k7	201	PEB	OD-C4D	2.71	1.28	1.23
26	AB	301	PEB	OD-C4D	2.71	1.28	1.23
28	CF	1001	CYC	OB-C4B	2.71	1.28	1.23
28	DF	1003	CYC	C2C-C1C	-2.71	1.49	1.52
26	G5	201	PEB	OD-C4D	2.71	1.28	1.23
26	GA	203	PEB	OD-C4D	2.71	1.28	1.23
28	G7	1001	CYC	OB-C4B	2.71	1.28	1.23
26	W8	201	PEB	C4A-NA	-2.71	1.31	1.37
26	B4	201	PEB	OD-C4D	2.71	1.28	1.23
26	RD	203	PEB	OD-C4D	2.71	1.28	1.23
27	B8	302	PUB	OA-C1A	2.71	1.28	1.23
26	P8	201	PEB	C2A-C1A	-2.71	1.49	1.52
26	A2	301	PEB	OD-C4D	2.71	1.28	1.23
26	TJ	201	PEB	C4B-C3B	2.71	1.50	1.45
26	kB	201	PEB	OD-C4D	2.71	1.28	1.23
28	B6	1002	CYC	OB-C4B	2.71	1.28	1.23
26	w4	201	PEB	C4B-C3B	2.71	1.50	1.45
26	S9	201	PEB	OD-C4D	2.71	1.28	1.23
28	OH	1001	CYC	C1D-CHD	2.71	1.51	1.41
26	Q7	202	PEB	OD-C4D	2.71	1.28	1.23
28	J7	1001	CYC	OB-C4B	2.71	1.28	1.23
26	PD	203	PEB	OD-C4D	2.71	1.28	1.23
26	mG	203	PEB	OD-C4D	2.71	1.28	1.23
26	K4	201	PEB	C2A-C1A	-2.71	1.49	1.52
26	IJ	203	PEB	C2A-C1A	-2.71	1.49	1.52
28	1H	1000	CYC	C2C-C1C	-2.71	1.49	1.52
26	HJ	201	PEB	C2C-C3C	2.71	1.45	1.37
26	DF	1002	PEB	OD-C4D	2.71	1.28	1.23
26	JD	203	PEB	C4B-C3B	2.71	1.50	1.45
26	jI	201	PEB	OD-C4D	2.71	1.28	1.23
26	UJ	202	PEB	C2A-C1A	-2.71	1.49	1.52
26	b2	201	PEB	OD-C4D	2.71	1.28	1.23
26	R8	202	PEB	OD-C4D	2.71	1.28	1.23
26	l1	202	PEB	OD-C4D	2.71	1.28	1.23
26	M4	403	PEB	OD-C4D	2.71	1.28	1.23
26	D8	201	PEB	OD-C4D	2.71	1.28	1.23
26	X9	202	PEB	OD-C4D	2.71	1.28	1.23
26	KE	201	PEB	CHA-C1B	2.71	1.46	1.40
28	F7	1001	CYC	C2C-C1C	-2.71	1.49	1.52
26	Z1	202	PEB	OD-C4D	2.71	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VA	202	PEB	OD-C4D	2.71	1.28	1.23
26	eE	201	PEB	OD-C4D	2.71	1.28	1.23
26	dG	201	PEB	C1A-NA	-2.71	1.34	1.37
26	w4	204	PEB	OD-C4D	2.70	1.28	1.23
26	AG	201	PEB	OD-C4D	2.70	1.28	1.23
26	Q6	202	PEB	OD-C4D	2.70	1.28	1.23
27	AF	303	PUB	OD-C4D	2.70	1.28	1.23
26	hE	201	PEB	C1A-NA	-2.70	1.34	1.37
26	Y6	202	PEB	OD-C4D	2.70	1.28	1.23
26	SJ	202	PEB	OD-C4D	2.70	1.28	1.23
26	Q9	201	PEB	OD-C4D	2.70	1.28	1.23
26	O3	201	PEB	C2C-C3C	2.70	1.45	1.37
26	jE	201	PEB	OD-C4D	2.70	1.28	1.23
26	wE	303	PEB	OD-C4D	2.70	1.28	1.23
27	yE	303	PUB	OD-C4D	2.70	1.28	1.23
28	CH	1001	CYC	OB-C4B	2.70	1.28	1.23
26	X3	202	PEB	C2C-C3C	2.70	1.45	1.37
26	h1	201	PEB	C2A-C1A	-2.70	1.49	1.52
26	cA	203	PEB	C2A-C1A	-2.70	1.49	1.52
26	hF	202	PEB	OD-C4D	2.70	1.28	1.23
28	YH	1001	CYC	OB-C4B	2.70	1.28	1.23
28	YH	1002	CYC	OB-C4B	2.70	1.28	1.23
26	S3	201	PEB	C4A-NA	-2.70	1.31	1.37
28	J7	1001	CYC	C1B-C2B	2.70	1.50	1.45
26	TG	201	PEB	OD-C4D	2.70	1.28	1.23
28	oH	1001	CYC	OB-C4B	2.70	1.28	1.23
26	v1	202	PEB	C2A-C1A	-2.70	1.49	1.52
26	V9	203	PEB	C2A-C1A	-2.70	1.49	1.52
26	hB	201	PEB	C2A-C1A	-2.70	1.49	1.52
26	jA	202	PEB	OD-C4D	2.70	1.28	1.23
26	bB	202	PEB	OD-C4D	2.70	1.28	1.23
26	VJ	201	PEB	OD-C4D	2.70	1.28	1.23
26	h4	202	PEB	C1D-ND	2.70	1.49	1.45
26	A9	301	PEB	OD-C4D	2.70	1.28	1.23
26	TA	201	PEB	OD-C4D	2.70	1.28	1.23
26	J1	203	PEB	C2A-C1A	-2.70	1.49	1.52
26	K5	203	PEB	C4A-NA	-2.70	1.31	1.37
26	j2	201	PEB	OD-C4D	2.70	1.28	1.23
26	eI	203	PEB	OD-C4D	2.70	1.28	1.23
26	ND	202	PEB	C2C-C3C	2.70	1.45	1.37
26	Q3	201	PEB	C2C-C3C	2.70	1.45	1.37
26	i2	201	PEB	OD-C4D	2.70	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	LJ	201	PEB	CHA-C1B	2.70	1.46	1.40
26	DA	201	PEB	OD-C4D	2.70	1.28	1.23
26	gG	201	PEB	OD-C4D	2.70	1.28	1.23
26	II	201	PEB	OD-C4D	2.70	1.28	1.23
26	KE	202	PEB	C4A-NA	-2.70	1.31	1.37
28	SH	1001	CYC	C1B-C2B	2.70	1.50	1.45
26	B3	203	PEB	C4B-C3B	2.70	1.50	1.45
26	L1	201	PEB	OD-C4D	2.70	1.28	1.23
26	jG	201	PEB	OD-C4D	2.70	1.28	1.23
26	Z6	201	PEB	C2C-C3C	2.70	1.45	1.37
26	P2	203	PEB	OD-C4D	2.70	1.28	1.23
26	UI	202	PEB	OD-C4D	2.70	1.28	1.23
28	K7	1001	CYC	OB-C4B	2.70	1.28	1.23
26	QG	203	PEB	C1C-CHB	2.69	1.51	1.41
26	QD	201	PEB	C4A-NA	-2.69	1.31	1.37
26	e2	202	PEB	OD-C4D	2.69	1.28	1.23
26	P3	203	PEB	OD-C4D	2.69	1.28	1.23
26	cB	202	PEB	OD-C4D	2.69	1.28	1.23
26	VF	202	PEB	OD-C4D	2.69	1.28	1.23
26	R9	201	PEB	C4B-C3B	2.69	1.50	1.45
26	V8	202	PEB	OD-C4D	2.69	1.28	1.23
26	kI	202	PEB	OD-C4D	2.69	1.28	1.23
26	OD	201	PEB	C2C-C3C	2.69	1.45	1.37
26	H9	201	PEB	CHA-C1B	2.69	1.46	1.40
26	C1	201	PEB	C2A-C1A	-2.69	1.49	1.52
26	T9	202	PEB	C2A-C1A	-2.69	1.49	1.52
26	VE	202	PEB	OD-C4D	2.69	1.28	1.23
26	H7	1002	PEB	OD-C4D	2.69	1.28	1.23
26	m7	201	PEB	OD-C4D	2.69	1.28	1.23
26	WG	202	PEB	OD-C4D	2.69	1.28	1.23
26	V3	201	PEB	OD-C4D	2.69	1.28	1.23
26	V6	201	PEB	OD-C4D	2.69	1.28	1.23
26	G8	203	PEB	OD-C4D	2.69	1.28	1.23
26	JA	202	PEB	OD-C4D	2.69	1.28	1.23
26	VG	201	PEB	OD-C4D	2.69	1.28	1.23
26	K8	203	PEB	CHA-C1B	2.69	1.46	1.40
26	c6	202	PEB	OD-C4D	2.69	1.28	1.23
26	dF	202	PEB	OD-C4D	2.69	1.28	1.23
26	JJ	203	PEB	OD-C4D	2.69	1.28	1.23
26	G1	202	PEB	OD-C4D	2.69	1.28	1.23
26	11	202	PEB	OD-C4D	2.69	1.28	1.23
26	H4	202	PEB	C2A-C1A	-2.69	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	XD	202	PEB	C2A-C1A	-2.69	1.49	1.52
26	SI	202	PEB	OD-C4D	2.69	1.28	1.23
26	GJ	202	PEB	OD-C4D	2.69	1.28	1.23
26	mG	203	PEB	C2A-C1A	-2.69	1.49	1.52
26	J5	202	PEB	C4A-NA	-2.69	1.31	1.37
26	k8	201	PEB	OD-C4D	2.69	1.28	1.23
26	VA	201	PEB	OD-C4D	2.69	1.28	1.23
27	K3	203	PUB	OD-C4D	2.69	1.28	1.23
28	YH	1003	CYC	OB-C4B	2.69	1.28	1.23
26	u4	203	PEB	C2A-C1A	-2.69	1.49	1.52
26	XD	202	PEB	CHA-C1B	2.69	1.46	1.40
26	dB	202	PEB	OD-C4D	2.69	1.28	1.23
26	u4	202	PEB	C4B-C3B	2.69	1.50	1.45
26	I1	201	PEB	OD-C4D	2.69	1.28	1.23
26	J4	202	PEB	OD-C4D	2.69	1.28	1.23
26	c6	201	PEB	OD-C4D	2.69	1.28	1.23
26	DD	201	PEB	OD-C4D	2.69	1.28	1.23
26	q1	202	PEB	C2A-C1A	-2.69	1.49	1.52
26	qE	201	PEB	C1A-NA	-2.69	1.34	1.37
26	D1	202	PEB	OD-C4D	2.69	1.28	1.23
26	FC	201	PEB	C2A-C1A	-2.69	1.49	1.52
26	m1	201	PEB	OD-C4D	2.69	1.28	1.23
26	EJ	202	PEB	OD-C4D	2.69	1.28	1.23
28	pH	1001	CYC	C1D-CHD	2.69	1.51	1.41
26	P3	202	PEB	C1A-NA	-2.69	1.34	1.37
26	G5	202	PEB	OD-C4D	2.69	1.28	1.23
26	oG	201	PEB	OD-C4D	2.69	1.28	1.23
26	M1	403	PEB	OD-C4D	2.69	1.28	1.23
26	H9	201	PEB	OD-C4D	2.69	1.28	1.23
26	PE	201	PEB	OD-C4D	2.69	1.28	1.23
28	dH	1001	CYC	OB-C4B	2.69	1.28	1.23
26	mE	202	PEB	OD-C4D	2.69	1.28	1.23
26	TI	203	PEB	OD-C4D	2.69	1.28	1.23
26	V2	203	PEB	OD-C4D	2.68	1.28	1.23
26	gE	201	PEB	OD-C4D	2.68	1.28	1.23
26	J5	202	PEB	CHA-C1B	2.68	1.46	1.40
26	RJ	201	PEB	C4B-C3B	2.68	1.50	1.45
28	LI	1001	CYC	OB-C4B	2.68	1.28	1.23
26	K1	202	PEB	OD-C4D	2.68	1.28	1.23
27	A2	303	PUB	OA-C1A	2.68	1.28	1.23
27	N9	201	PUB	OA-C1A	2.68	1.28	1.23
26	F5	202	PEB	C2A-C1A	-2.68	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PD	203	PEB	C2A-C1A	-2.68	1.49	1.52
26	wG	301	PEB	OD-C4D	2.68	1.28	1.23
28	EF	1001	CYC	C1B-NB	-2.68	1.33	1.37
26	l6	203	PEB	OD-C4D	2.68	1.28	1.23
26	DG	201	PEB	OD-C4D	2.68	1.28	1.23
27	YD	302	PUB	OA-C1A	2.68	1.28	1.23
26	WJ	202	PEB	C2A-C1A	-2.68	1.49	1.52
26	k8	202	PEB	OD-C4D	2.68	1.28	1.23
26	J9	201	PEB	OD-C4D	2.68	1.28	1.23
26	HJ	201	PEB	CHA-C1B	2.68	1.46	1.40
26	B1	201	PEB	C2A-C1A	-2.68	1.49	1.52
26	ZF	203	PEB	C1B-C2B	2.68	1.51	1.45
26	c8	202	PEB	OD-C4D	2.68	1.28	1.23
27	AF	303	PUB	OA-C1A	2.68	1.28	1.23
26	l1	201	PEB	OD-C4D	2.68	1.28	1.23
26	Z4	202	PEB	OD-C4D	2.68	1.28	1.23
26	mE	201	PEB	OD-C4D	2.68	1.28	1.23
26	L3	201	PEB	OD-C4D	2.68	1.28	1.23
26	AJ	303	PEB	C2A-C1A	-2.68	1.49	1.52
26	Y1	202	PEB	OD-C4D	2.68	1.28	1.23
26	w1	203	PEB	OD-C4D	2.68	1.28	1.23
26	cB	201	PEB	OD-C4D	2.68	1.28	1.23
26	LC	203	PEB	OD-C4D	2.68	1.28	1.23
26	C8	203	PEB	C4A-NA	-2.68	1.31	1.37
26	W8	203	PEB	C4A-NA	-2.68	1.31	1.37
26	H4	202	PEB	OD-C4D	2.68	1.28	1.23
26	UF	201	PEB	OD-C4D	2.68	1.28	1.23
26	YJ	202	PEB	OD-C4D	2.68	1.28	1.23
26	aA	201	PEB	OD-C4D	2.68	1.28	1.23
28	hH	1001	CYC	OB-C4B	2.68	1.28	1.23
26	PI	203	PEB	OD-C4D	2.68	1.28	1.23
26	b4	501	PEB	OD-C4D	2.68	1.28	1.23
26	BG	202	PEB	OD-C4D	2.68	1.28	1.23
26	mI	201	PEB	OD-C4D	2.68	1.28	1.23
28	L2	1001	CYC	OB-C4B	2.68	1.28	1.23
26	XD	203	PEB	C4A-NA	-2.68	1.31	1.37
26	T2	203	PEB	OD-C4D	2.68	1.28	1.23
27	AI	303	PUB	OA-C1A	2.68	1.28	1.23
26	F5	202	PEB	OD-C4D	2.67	1.28	1.23
26	i7	202	PEB	OD-C4D	2.67	1.28	1.23
26	V8	201	PEB	OD-C4D	2.67	1.28	1.23
26	P6	201	PEB	OD-C4D	2.67	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	YI	203	PEB	OD-C4D	2.67	1.28	1.23
26	PD	202	PEB	C2C-C3C	2.67	1.45	1.37
26	J4	203	PEB	OD-C4D	2.67	1.28	1.23
26	O8	201	PEB	OD-C4D	2.67	1.28	1.23
26	SF	201	PEB	OD-C4D	2.67	1.28	1.23
26	H6	1002	PEB	C2A-C1A	-2.67	1.49	1.52
28	K7	1001	CYC	C2C-C1C	-2.67	1.49	1.52
26	LJ	202	PEB	OD-C4D	2.67	1.28	1.23
26	S3	201	PEB	C2C-C3C	2.67	1.45	1.37
26	m2	201	PEB	OD-C4D	2.67	1.28	1.23
26	KG	201	PEB	OD-C4D	2.67	1.28	1.23
27	A6	302	PUB	OA-C1A	2.67	1.28	1.23
27	xE	301	PUB	OA-C1A	2.67	1.28	1.23
28	VH	1001	CYC	C1D-CHD	2.67	1.51	1.41
26	DD	202	PEB	OD-C4D	2.67	1.28	1.23
26	HJ	201	PEB	C2A-C1A	-2.67	1.49	1.52
26	T6	201	PEB	OD-C4D	2.67	1.28	1.23
26	IG	201	PEB	C3B-C2B	2.67	1.42	1.36
26	d2	201	PEB	C2A-C1A	-2.67	1.49	1.52
26	i2	201	PEB	C2A-C1A	-2.67	1.49	1.52
26	TB	202	PEB	OD-C4D	2.67	1.28	1.23
26	CG	202	PEB	OD-C4D	2.67	1.28	1.23
27	A2	303	PUB	OD-C4D	2.67	1.28	1.23
28	fH	1001	CYC	OB-C4B	2.67	1.28	1.23
28	YH	1004	CYC	C2C-C1C	-2.67	1.49	1.52
26	V7	201	PEB	OD-C4D	2.67	1.28	1.23
26	Y4	202	PEB	OD-C4D	2.67	1.28	1.23
26	QB	202	PEB	OD-C4D	2.67	1.28	1.23
26	HG	202	PEB	OD-C4D	2.67	1.28	1.23
26	iG	202	PEB	OD-C4D	2.67	1.28	1.23
26	UE	203	PEB	C4B-NB	-2.67	1.32	1.38
26	T8	201	PEB	OD-C4D	2.67	1.28	1.23
26	j8	202	PEB	OD-C4D	2.67	1.28	1.23
26	V3	202	PEB	CHA-C1B	2.67	1.46	1.40
26	MA	201	PEB	C2C-C3C	2.67	1.45	1.37
27	Y3	302	PUB	OA-C1A	2.67	1.28	1.23
26	G4	201	PEB	C1B-C2B	2.67	1.51	1.45
26	l2	202	PEB	OD-C4D	2.67	1.28	1.23
26	l6	202	PEB	OD-C4D	2.67	1.28	1.23
26	PI	201	PEB	OD-C4D	2.67	1.28	1.23
28	F7	1001	CYC	OB-C4B	2.67	1.28	1.23
26	ZB	201	PEB	C2C-C3C	2.67	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S7	201	PEB	OD-C4D	2.67	1.28	1.23
26	TB	201	PEB	OD-C4D	2.67	1.28	1.23
28	QH	1001	CYC	C1D-CHD	2.66	1.51	1.41
26	g1	202	PEB	C4B-C3B	2.66	1.50	1.45
26	V7	202	PEB	OD-C4D	2.66	1.28	1.23
26	a8	204	PEB	OD-C4D	2.66	1.28	1.23
26	QB	201	PEB	OD-C4D	2.66	1.28	1.23
26	oE	201	PEB	C1B-C2B	2.66	1.51	1.45
26	NJ	202	PEB	C2A-C1A	-2.66	1.49	1.52
26	VJ	203	PEB	C2A-C1A	-2.66	1.49	1.52
28	uH	1001	CYC	C1B-C2B	2.66	1.49	1.45
26	aI	203	PEB	OD-C4D	2.66	1.28	1.23
26	P2	202	PEB	C2C-C3C	2.66	1.45	1.37
26	VI	203	PEB	OD-C4D	2.66	1.28	1.23
26	RI	203	PEB	C4B-C3B	2.66	1.50	1.45
26	U1	201	PEB	OD-C4D	2.66	1.28	1.23
26	QG	203	PEB	CHA-C1B	2.66	1.46	1.40
26	WG	201	PEB	C4A-NA	-2.66	1.31	1.37
26	S4	202	PEB	OD-C4D	2.66	1.28	1.23
28	M6	1001	CYC	C4C-NC	-2.66	1.31	1.37
26	VD	202	PEB	CHA-C1B	2.66	1.46	1.40
26	d1	202	PEB	OD-C4D	2.66	1.28	1.23
26	e3	401	PEB	OD-C4D	2.66	1.28	1.23
28	IF	1001	CYC	C1B-NB	-2.66	1.33	1.37
26	SD	201	PEB	C4A-NA	-2.66	1.31	1.37
26	Y2	203	PEB	OD-C4D	2.66	1.28	1.23
26	D4	202	PEB	OD-C4D	2.66	1.28	1.23
26	h6	201	PEB	C1C-CHB	2.66	1.51	1.41
27	AI	303	PUB	OD-C4D	2.66	1.28	1.23
26	L1	202	PEB	OD-C4D	2.66	1.28	1.23
26	V1	203	PEB	OD-C4D	2.66	1.28	1.23
26	V4	203	PEB	OD-C4D	2.66	1.28	1.23
26	RI	202	PEB	OD-C4D	2.66	1.28	1.23
28	WH	1001	CYC	OB-C4B	2.66	1.28	1.23
26	pE	202	PEB	C4B-C3B	2.66	1.49	1.45
26	UA	202	PEB	C4A-NA	-2.66	1.31	1.37
27	NJ	201	PUB	OD-C4D	2.66	1.28	1.23
26	l6	202	PEB	C2A-C1A	-2.66	1.49	1.52
26	N1	203	PEB	OD-C4D	2.66	1.28	1.23
26	fF	203	PEB	OD-C4D	2.66	1.28	1.23
26	wG	303	PEB	OD-C4D	2.66	1.28	1.23
28	eH	1001	CYC	OB-C4B	2.66	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	OA	201	PEB	OD-C4D	2.66	1.28	1.23
26	mA	201	PEB	OD-C4D	2.66	1.28	1.23
28	LH	1001	CYC	OB-C4B	2.66	1.28	1.23
26	CE	201	PEB	C1D-ND	2.66	1.49	1.45
26	IC	201	PEB	OD-C4D	2.66	1.28	1.23
26	UJ	202	PEB	OD-C4D	2.66	1.28	1.23
26	U8	202	PEB	C4A-NA	-2.66	1.31	1.37
26	I1	202	PEB	C2A-C1A	-2.66	1.49	1.52
26	EA	201	PEB	OD-C4D	2.66	1.28	1.23
28	EH	1001	CYC	C1D-CHD	2.66	1.51	1.41
26	IJ	202	PEB	C4A-NA	-2.66	1.31	1.37
26	gG	201	PEB	C2A-C1A	-2.66	1.49	1.52
26	a4	201	PEB	OD-C4D	2.66	1.28	1.23
26	CE	202	PEB	OD-C4D	2.66	1.28	1.23
26	qG	201	PEB	OD-C4D	2.66	1.28	1.23
26	L3	202	PEB	OD-C4D	2.65	1.28	1.23
26	I3	201	PEB	C2A-C1A	-2.65	1.49	1.52
26	c4	203	PEB	OD-C4D	2.65	1.28	1.23
26	h8	203	PEB	OD-C4D	2.65	1.28	1.23
27	A4	203	PUB	OA-C1A	2.65	1.28	1.23
26	VF	203	PEB	OD-C4D	2.65	1.28	1.23
26	mF	202	PEB	OD-C4D	2.65	1.28	1.23
26	T6	202	PEB	OD-C4D	2.65	1.28	1.23
26	p1	201	PEB	C2A-C1A	-2.65	1.49	1.52
28	JF	1003	CYC	OB-C4B	2.65	1.28	1.23
28	kH	1001	CYC	OB-C4B	2.65	1.28	1.23
28	TH	1001	CYC	C1D-CHD	2.65	1.51	1.41
26	S7	203	PEB	OD-C4D	2.65	1.28	1.23
27	yG	303	PUB	OD-C4D	2.65	1.28	1.23
26	f1	201	PEB	OD-C4D	2.65	1.28	1.23
26	R3	201	PEB	OD-C4D	2.65	1.28	1.23
26	hA	203	PEB	OD-C4D	2.65	1.28	1.23
26	JD	201	PEB	OD-C4D	2.65	1.28	1.23
28	yH	1001	CYC	OB-C4B	2.65	1.28	1.23
26	gE	201	PEB	C2A-C1A	-2.65	1.49	1.52
28	nH	1001	CYC	C1D-CHD	2.65	1.51	1.41
26	CA	203	PEB	OD-C4D	2.65	1.28	1.23
26	Y4	201	PEB	OD-C4D	2.65	1.28	1.23
26	hB	202	PEB	OD-C4D	2.65	1.28	1.23
28	PH	1001	CYC	C1B-C2B	2.65	1.49	1.45
26	NG	202	PEB	C2A-C1A	-2.65	1.49	1.52
28	JI	1001	CYC	C4B-NB	-2.65	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AG	202	PEB	C4B-C3B	2.65	1.49	1.45
26	SA	202	PEB	OD-C4D	2.65	1.28	1.23
26	RD	201	PEB	OD-C4D	2.65	1.28	1.23
26	iA	201	PEB	OD-C4D	2.65	1.28	1.23
26	B1	202	PEB	OD-C4D	2.65	1.28	1.23
28	LB	1001	CYC	C4C-NC	-2.65	1.31	1.37
26	T2	202	PEB	OD-C4D	2.65	1.28	1.23
26	K5	201	PEB	OD-C4D	2.65	1.28	1.23
26	l8	202	PEB	OD-C4D	2.65	1.28	1.23
28	nH	1001	CYC	OB-C4B	2.65	1.28	1.23
26	D1	201	PEB	OD-C4D	2.65	1.28	1.23
26	C8	203	PEB	OD-C4D	2.65	1.28	1.23
26	ND	202	PEB	OD-C4D	2.65	1.28	1.23
26	YI	201	PEB	OD-C4D	2.65	1.28	1.23
27	KD	203	PUB	OD-C4D	2.65	1.28	1.23
26	H4	203	PEB	C2A-C1A	-2.65	1.49	1.52
27	AA	304	PUB	OA-C1A	2.65	1.28	1.23
28	NB	1001	CYC	C4C-NC	-2.64	1.31	1.37
26	h1	201	PEB	C1A-NA	-2.64	1.34	1.37
26	S2	202	PEB	OD-C4D	2.64	1.28	1.23
26	lA	202	PEB	OD-C4D	2.64	1.28	1.23
26	MG	202	PEB	C2A-C1A	-2.64	1.49	1.52
26	F9	203	PEB	C1C-CHB	2.64	1.51	1.41
28	HF	1001	CYC	OB-C4B	2.64	1.28	1.23
26	DG	203	PEB	C2A-C1A	-2.64	1.49	1.52
26	KE	201	PEB	OD-C4D	2.64	1.28	1.23
26	24	401	PEB	OD-C4D	2.64	1.28	1.23
26	O9	202	PEB	OD-C4D	2.64	1.28	1.23
26	m4	202	PEB	OD-C4D	2.64	1.28	1.23
28	C7	1001	CYC	OB-C4B	2.64	1.28	1.23
26	UB	201	PEB	C2A-C1A	-2.64	1.49	1.52
26	a2	203	PEB	OD-C4D	2.64	1.28	1.23
26	O8	203	PEB	OD-C4D	2.64	1.28	1.23
26	HA	202	PEB	OD-C4D	2.64	1.28	1.23
27	YD	302	PUB	OD-C4D	2.64	1.28	1.23
26	hE	202	PEB	C4B-C3B	2.64	1.49	1.45
26	P1	202	PEB	C4A-NA	-2.64	1.31	1.37
26	J1	201	PEB	C2A-C1A	-2.64	1.49	1.52
26	L5	201	PEB	C4A-NA	-2.64	1.31	1.37
26	WA	201	PEB	C4A-NA	-2.64	1.31	1.37
26	R4	201	PEB	OD-C4D	2.64	1.28	1.23
26	e7	202	PEB	C2A-C1A	-2.64	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R2	202	PEB	OD-C4D	2.64	1.28	1.23
26	T3	203	PEB	C4A-NA	-2.64	1.31	1.37
28	LH	1001	CYC	C1D-CHD	2.64	1.51	1.41
26	f6	201	PEB	OD-C4D	2.64	1.28	1.23
26	W8	202	PEB	C4A-NA	-2.64	1.31	1.37
26	HG	202	PEB	C2A-C1A	-2.64	1.49	1.52
26	ED	202	PEB	C1D-ND	2.64	1.49	1.45
26	NF	1002	PEB	OD-C4D	2.64	1.28	1.23
26	bI	201	PEB	OD-C4D	2.64	1.28	1.23
28	N2	1001	CYC	C1B-NB	-2.64	1.33	1.37
27	AA	303	PUB	OA-C1A	2.64	1.28	1.23
26	I9	202	PEB	C2A-C1A	-2.64	1.49	1.52
26	N3	202	PEB	C1A-NA	-2.64	1.34	1.37
26	J8	202	PEB	OD-C4D	2.64	1.28	1.23
26	sE	203	PEB	C4B-C3B	2.64	1.49	1.45
26	kA	201	PEB	OD-C4D	2.64	1.28	1.23
26	LC	202	PEB	OD-C4D	2.64	1.28	1.23
26	eD	401	PEB	OD-C4D	2.64	1.28	1.23
26	lF	202	PEB	OD-C4D	2.64	1.28	1.23
26	YD	301	PEB	C2A-C1A	-2.64	1.49	1.52
26	jA	203	PEB	OD-C4D	2.64	1.28	1.23
26	NJ	204	PEB	OD-C4D	2.64	1.28	1.23
26	ND	202	PEB	CHA-C1B	2.63	1.46	1.40
26	D2	1002	PEB	OD-C4D	2.63	1.28	1.23
26	N3	203	PEB	OD-C4D	2.63	1.28	1.23
26	h6	202	PEB	OD-C4D	2.63	1.28	1.23
26	a8	204	PEB	C2A-C1A	-2.63	1.49	1.52
26	iI	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	VF	201	PEB	OD-C4D	2.63	1.28	1.23
26	W6	203	PEB	OD-C4D	2.63	1.28	1.23
26	HE	201	PEB	C4B-NB	-2.63	1.32	1.38
28	iH	1001	CYC	C1D-CHD	2.63	1.51	1.41
26	oE	203	PEB	C1B-C2B	2.63	1.51	1.45
26	l8	203	PEB	OD-C4D	2.63	1.28	1.23
26	NG	201	PEB	OD-C4D	2.63	1.28	1.23
26	h8	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	DJ	201	PEB	C2C-C3C	2.63	1.45	1.37
26	m8	201	PEB	C4A-NA	-2.63	1.31	1.37
26	g6	202	PEB	OD-C4D	2.63	1.28	1.23
26	GC	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	VD	203	PEB	C4B-C3B	2.63	1.49	1.45
26	AJ	301	PEB	OD-C4D	2.63	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BG	202	PEB	C2A-C1A	-2.63	1.49	1.52
26	BJ	203	PEB	CHA-C1B	2.63	1.46	1.40
26	M8	201	PEB	C2C-C3C	2.63	1.45	1.37
26	U2	201	PEB	CHA-C4A	-2.63	1.31	1.36
26	E8	201	PEB	OD-C4D	2.63	1.28	1.23
26	i8	201	PEB	OD-C4D	2.63	1.28	1.23
26	lB	202	PEB	OD-C4D	2.63	1.28	1.23
26	ND	201	PEB	OD-C4D	2.63	1.28	1.23
27	Y3	302	PUB	OD-C4D	2.63	1.28	1.23
28	MB	1001	CYC	C4C-NC	-2.63	1.31	1.37
26	jI	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	QF	202	PEB	OD-C4D	2.63	1.28	1.23
26	z1	202	PEB	C4B-C3B	2.63	1.49	1.45
26	u4	202	PEB	OD-C4D	2.63	1.28	1.23
26	H8	202	PEB	OD-C4D	2.63	1.28	1.23
26	FD	202	PEB	OD-C4D	2.63	1.28	1.23
26	CJ	201	PEB	OD-C4D	2.63	1.28	1.23
28	qH	1002	CYC	C1C-NC	-2.63	1.34	1.37
26	n1	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	U9	201	PEB	C2A-C1A	-2.63	1.49	1.52
28	FF	1001	CYC	OB-C4B	2.63	1.28	1.23
26	jI	201	PEB	CHA-C4A	-2.63	1.31	1.36
26	TA	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	VD	203	PEB	C2A-C1A	-2.63	1.49	1.52
26	ZA	202	PEB	OD-C4D	2.63	1.28	1.23
26	O4	202	PEB	OD-C4D	2.63	1.28	1.23
26	14	202	PEB	OD-C4D	2.63	1.28	1.23
27	yG	303	PUB	OA-C1A	2.63	1.28	1.23
26	rE	201	PEB	C2A-C1A	-2.63	1.49	1.52
26	f4	202	PEB	C4B-C3B	2.62	1.49	1.45
26	W8	203	PEB	CHA-C1B	2.62	1.46	1.40
26	SE	202	PEB	C1A-NA	-2.62	1.34	1.37
26	OF	203	PEB	OD-C4D	2.62	1.28	1.23
27	A8	304	PUB	OA-C1A	2.62	1.28	1.23
26	TD	203	PEB	C4A-NA	-2.62	1.31	1.37
28	GH	1001	CYC	C1D-CHD	2.62	1.51	1.41
26	WA	203	PEB	C4A-NA	-2.62	1.31	1.37
26	h8	202	PEB	OD-C4D	2.62	1.28	1.23
28	gH	1001	CYC	C1D-CHD	2.62	1.51	1.41
26	Q7	201	PEB	OD-C4D	2.62	1.28	1.23
26	G8	201	PEB	OD-C4D	2.62	1.28	1.23
26	mF	201	PEB	OD-C4D	2.62	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	KF	1001	CYC	OB-C4B	2.62	1.28	1.23
26	m1	202	PEB	OD-C4D	2.62	1.28	1.23
27	AF	304	PUB	OA-C1A	2.62	1.28	1.23
28	wH	1001	CYC	C1B-C2B	2.62	1.49	1.45
26	Y6	201	PEB	OD-C4D	2.62	1.28	1.23
26	I9	202	PEB	C4B-C3B	2.62	1.49	1.45
26	KJ	202	PEB	OD-C4D	2.62	1.28	1.23
26	ZE	202	PEB	C4B-C3B	2.62	1.49	1.45
28	BB	1001	CYC	C4B-NB	-2.62	1.32	1.38
26	KC	202	PEB	OD-C4D	2.62	1.28	1.23
26	IE	203	PEB	C4A-NA	-2.62	1.31	1.37
26	R2	203	PEB	C4B-C3B	2.62	1.49	1.45
26	S4	201	PEB	C4B-C3B	2.62	1.49	1.45
26	UF	201	PEB	C2A-C1A	-2.62	1.49	1.52
26	a1	201	PEB	OD-C4D	2.62	1.28	1.23
26	Y2	201	PEB	OD-C4D	2.62	1.28	1.23
26	jE	201	PEB	C1A-NA	-2.62	1.34	1.37
26	G8	202	PEB	OD-C4D	2.62	1.28	1.23
26	lA	203	PEB	OD-C4D	2.62	1.28	1.23
26	JE	201	PEB	OD-C4D	2.62	1.28	1.23
26	SG	201	PEB	C2C-C3C	2.62	1.45	1.37
26	M4	402	PEB	OD-C4D	2.62	1.28	1.23
26	l4	202	PEB	C2A-C1A	-2.62	1.49	1.52
26	VB	202	PEB	C2A-C1A	-2.62	1.49	1.52
26	HG	201	PEB	C4A-NA	-2.62	1.31	1.37
28	B6	1002	CYC	C4A-C3A	2.62	1.51	1.45
27	yE	303	PUB	OA-C1A	2.62	1.28	1.23
26	w4	203	PEB	C2A-C1A	-2.62	1.49	1.52
28	G7	1001	CYC	C2C-C1C	-2.62	1.49	1.52
26	BG	201	PEB	C4D-ND	2.61	1.38	1.35
26	Y1	201	PEB	OD-C4D	2.61	1.28	1.23
26	OJ	201	PEB	OD-C4D	2.61	1.28	1.23
26	Q4	202	PEB	OD-C4D	2.61	1.28	1.23
26	l4	201	PEB	OD-C4D	2.61	1.28	1.23
26	PA	201	PEB	OD-C4D	2.61	1.28	1.23
26	ZB	202	PEB	OD-C4D	2.61	1.28	1.23
26	DI	1002	PEB	OD-C4D	2.61	1.28	1.23
26	WE	201	PEB	C4A-NA	-2.61	1.31	1.37
26	Z4	202	PEB	C2A-C1A	-2.61	1.49	1.52
26	k4	201	PEB	C2A-C1A	-2.61	1.49	1.52
28	CF	1001	CYC	C2C-C1C	-2.61	1.49	1.52
28	N2	1001	CYC	C4B-NB	-2.61	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	sH	1001	CYC	C1D-CHD	2.61	1.51	1.41
26	AC	201	PEB	C2A-C1A	-2.61	1.49	1.52
26	b1	501	PEB	OD-C4D	2.61	1.28	1.23
26	Q6	201	PEB	OD-C4D	2.61	1.28	1.23
26	kG	202	PEB	C4B-C3B	2.61	1.49	1.45
26	OB	203	PEB	OD-C4D	2.61	1.28	1.23
26	LJ	201	PEB	OD-C4D	2.61	1.28	1.23
26	KC	202	PEB	C2A-C1A	-2.61	1.49	1.52
26	L5	203	PEB	OD-C4D	2.61	1.28	1.23
26	P2	201	PEB	OD-C4D	2.61	1.28	1.23
26	K9	202	PEB	OD-C4D	2.61	1.28	1.23
26	tE	201	PEB	C2A-C1A	-2.61	1.49	1.52
26	PI	202	PEB	C2A-C1A	-2.61	1.49	1.52
26	GA	201	PEB	OD-C4D	2.61	1.28	1.23
26	PG	201	PEB	OD-C4D	2.61	1.28	1.23
26	xG	304	PEB	C4B-C3B	2.61	1.49	1.45
26	H5	201	PEB	C4A-NA	-2.61	1.31	1.37
26	U2	202	PEB	OD-C4D	2.61	1.28	1.23
26	BJ	201	PEB	OD-C4D	2.61	1.28	1.23
26	DE	203	PEB	C2A-C1A	-2.61	1.49	1.52
26	QJ	201	PEB	OD-C4D	2.61	1.28	1.23
27	A8	303	PUB	OA-C1A	2.61	1.28	1.23
26	rG	201	PEB	C1A-NA	-2.61	1.34	1.37
28	WH	1001	CYC	C1D-CHD	2.61	1.51	1.41
26	YI	202	PEB	OD-C4D	2.61	1.28	1.23
28	IH	1001	CYC	C1D-CHD	2.61	1.51	1.41
26	MG	202	PEB	C4B-C3B	2.61	1.49	1.45
26	M1	402	PEB	OD-C4D	2.61	1.28	1.23
26	XA	202	PEB	OD-C4D	2.61	1.28	1.23
28	DF	1003	CYC	OB-C4B	2.61	1.28	1.23
28	NB	1001	CYC	OB-C4B	2.61	1.28	1.23
26	c4	202	PEB	C4B-C3B	2.61	1.49	1.45
28	YH	1001	CYC	C1D-CHD	2.61	1.51	1.41
26	y4	203	PEB	C4B-C3B	2.61	1.49	1.45
26	i4	201	PEB	C2A-C1A	-2.61	1.49	1.52
26	aG	202	PEB	C2A-C1A	-2.61	1.49	1.52
26	rG	202	PEB	C2A-C1A	-2.61	1.49	1.52
26	h2	201	PEB	CHA-C4A	-2.60	1.31	1.36
26	U6	201	PEB	OD-C4D	2.60	1.28	1.23
26	RE	201	PEB	OD-C4D	2.60	1.28	1.23
26	D4	202	PEB	C4B-C3B	2.60	1.49	1.45
26	B3	202	PEB	OD-C4D	2.60	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	IH	1001	CYC	OB-C4B	2.60	1.28	1.23
26	XG	202	PEB	C4A-NA	-2.60	1.31	1.37
28	cH	1001	CYC	C2C-C1C	-2.60	1.49	1.52
28	IF	1001	CYC	C4B-NB	-2.60	1.32	1.38
26	TJ	202	PEB	OD-C4D	2.60	1.28	1.23
26	QF	201	PEB	OD-C4D	2.60	1.28	1.23
26	F9	203	PEB	C4A-NA	-2.60	1.31	1.37
26	VE	202	PEB	C2A-C1A	-2.60	1.49	1.52
26	SE	202	PEB	OA-C1A	2.60	1.28	1.23
26	F4	202	PEB	OD-C4D	2.60	1.28	1.23
26	UA	201	PEB	OD-C4D	2.60	1.28	1.23
26	KE	201	PEB	C4A-NA	-2.60	1.31	1.37
26	Z8	202	PEB	OD-C4D	2.60	1.28	1.23
26	HA	201	PEB	OD-C4D	2.60	1.28	1.23
26	CA	203	PEB	C4A-NA	-2.60	1.31	1.37
28	yH	1001	CYC	C1D-CHD	2.60	1.51	1.41
26	j8	203	PEB	OD-C4D	2.60	1.28	1.23
26	GA	202	PEB	OD-C4D	2.60	1.28	1.23
26	NE	202	PEB	C2A-C1A	-2.60	1.49	1.52
26	AF	301	PEB	OD-C4D	2.60	1.28	1.23
26	EJ	201	PEB	OD-C4D	2.60	1.28	1.23
27	xG	301	PUB	OA-C1A	2.60	1.28	1.23
28	F2	1001	CYC	C1A-C2A	2.60	1.49	1.45
28	IB	1001	CYC	C4C-NC	-2.60	1.31	1.37
26	N4	203	PEB	OD-C4D	2.60	1.28	1.23
26	hA	202	PEB	OD-C4D	2.60	1.28	1.23
26	aB	201	PEB	OD-C4D	2.60	1.28	1.23
26	F5	203	PEB	C2A-C1A	-2.60	1.49	1.52
26	B9	201	PEB	OD-C4D	2.60	1.28	1.23
26	pG	201	PEB	OD-C4D	2.60	1.28	1.23
26	h1	201	PEB	C4B-C3B	2.60	1.49	1.45
26	V3	203	PEB	C4B-C3B	2.60	1.49	1.45
26	N3	202	PEB	OD-C4D	2.60	1.28	1.23
26	YB	201	PEB	OD-C4D	2.60	1.28	1.23
26	FG	201	PEB	C4B-C3B	2.60	1.49	1.45
26	T3	201	PEB	C4A-NA	-2.60	1.31	1.37
26	mI	203	PEB	C4B-C3B	2.60	1.49	1.45
26	aI	202	PEB	OD-C4D	2.60	1.28	1.23
26	lA	201	PEB	OD-C4D	2.60	1.28	1.23
28	M2	1001	CYC	OB-C4B	2.60	1.28	1.23
26	X3	202	PEB	C1A-NA	-2.60	1.34	1.37
26	U4	202	PEB	C2A-C1A	-2.60	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V9	203	PEB	OD-C4D	2.60	1.28	1.23
26	H3	202	PEB	C1A-NA	-2.60	1.34	1.37
26	Z7	203	PEB	C1B-C2B	2.60	1.51	1.45
26	e8	201	PEB	OD-C4D	2.59	1.28	1.23
26	L4	201	PEB	C2A-C1A	-2.59	1.49	1.52
26	CE	201	PEB	C2C-C3C	2.59	1.45	1.37
26	GE	201	PEB	OD-C4D	2.59	1.28	1.23
28	QH	1001	CYC	OB-C4B	2.59	1.28	1.23
28	fH	1001	CYC	C1D-CHD	2.59	1.51	1.41
26	mA	202	PEB	OD-C4D	2.59	1.28	1.23
26	XD	202	PEB	C1A-NA	-2.59	1.34	1.37
28	KH	1001	CYC	C1B-C2B	2.59	1.49	1.45
26	M1	401	PEB	OD-C4D	2.59	1.28	1.23
26	aA	204	PEB	OD-C4D	2.59	1.28	1.23
26	QA	204	PEB	OD-C4D	2.59	1.28	1.23
26	HE	201	PEB	C4A-NA	-2.59	1.31	1.37
26	CA	202	PEB	OD-C4D	2.59	1.28	1.23
26	MG	203	PEB	OD-C4D	2.59	1.28	1.23
28	sH	1001	CYC	OB-C4B	2.59	1.28	1.23
26	V2	201	PEB	OD-C4D	2.59	1.28	1.23
26	LD	201	PEB	OD-C4D	2.59	1.28	1.23
26	QF	201	PEB	C4B-C3B	2.59	1.49	1.45
28	JF	1003	CYC	C2C-C1C	-2.59	1.49	1.52
26	FE	201	PEB	C4B-C3B	2.59	1.49	1.45
26	V9	201	PEB	OD-C4D	2.59	1.28	1.23
26	QA	202	PEB	OD-C4D	2.59	1.28	1.23
26	gG	203	PEB	OD-C4D	2.59	1.28	1.23
26	Z6	203	PEB	C4A-NA	-2.59	1.31	1.37
26	X9	202	PEB	C4B-C3B	2.59	1.49	1.45
26	E3	201	PEB	C2A-C1A	-2.59	1.49	1.52
26	FI	1002	PEB	OD-C4D	2.59	1.28	1.23
26	F3	202	PEB	OD-C4D	2.59	1.28	1.23
26	SJ	201	PEB	OD-C4D	2.59	1.28	1.23
27	yE	302	PUB	OA-C1A	2.59	1.28	1.23
26	IJ	201	PEB	C4A-NA	-2.59	1.31	1.37
28	UH	1001	CYC	C1D-CHD	2.59	1.51	1.41
26	B9	202	PEB	C2A-C1A	-2.59	1.49	1.52
26	JD	201	PEB	C2A-C1A	-2.59	1.49	1.52
26	M4	401	PEB	OD-C4D	2.59	1.28	1.23
26	d8	202	PEB	OD-C4D	2.59	1.28	1.23
26	MA	201	PEB	OD-C4D	2.59	1.28	1.23
28	H7	1001	CYC	OB-C4B	2.59	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cF	202	PEB	C1B-C2B	2.59	1.51	1.45
26	FD	202	PEB	C4B-C3B	2.59	1.49	1.45
26	kA	202	PEB	C2A-C1A	-2.59	1.49	1.52
26	O1	202	PEB	OD-C4D	2.59	1.28	1.23
26	Q9	202	PEB	OD-C4D	2.59	1.28	1.23
26	UB	201	PEB	OD-C4D	2.59	1.28	1.23
26	X3	202	PEB	CHA-C1B	2.59	1.46	1.40
26	a6	201	PEB	OD-C4D	2.59	1.28	1.23
26	JJ	201	PEB	OD-C4D	2.59	1.28	1.23
26	mE	201	PEB	C1C-CHB	2.59	1.51	1.41
26	WA	202	PEB	C4A-NA	-2.59	1.31	1.37
26	H1	202	PEB	OD-C4D	2.58	1.28	1.23
26	PI	202	PEB	OD-C4D	2.58	1.28	1.23
26	a2	202	PEB	OD-C4D	2.58	1.28	1.23
26	EE	201	PEB	OD-C4D	2.58	1.28	1.23
27	wE	304	PUB	OA-C1A	2.58	1.28	1.23
28	F2	1001	CYC	C4B-NB	-2.58	1.32	1.38
26	RD	201	PEB	C4A-NA	-2.58	1.31	1.37
26	AA	302	PEB	OD-C4D	2.58	1.28	1.23
26	TI	201	PEB	OD-C4D	2.58	1.28	1.23
28	K6	202	CYC	OB-C4B	2.58	1.28	1.23
26	YA	201	PEB	C2C-C3C	2.58	1.45	1.37
26	X4	202	PEB	C1B-C2B	2.58	1.51	1.45
26	T2	201	PEB	OD-C4D	2.58	1.28	1.23
28	KI	1001	CYC	OB-C4B	2.58	1.28	1.23
26	Y9	201	PEB	C2A-C1A	-2.58	1.49	1.52
26	bG	202	PEB	C2A-C1A	-2.58	1.49	1.52
28	CH	1001	CYC	C4A-C3A	2.58	1.51	1.45
26	lG	201	PEB	C4B-C3B	2.58	1.49	1.45
26	W4	202	PEB	OD-C4D	2.58	1.28	1.23
26	CG	201	PEB	OD-C4D	2.58	1.28	1.23
26	d4	202	PEB	C1D-ND	2.58	1.49	1.45
26	l7	201	PEB	OD-C4D	2.58	1.28	1.23
26	X8	202	PEB	OD-C4D	2.58	1.28	1.23
26	KJ	201	PEB	OD-C4D	2.58	1.28	1.23
26	i1	202	PEB	OD-C4D	2.58	1.28	1.23
26	HC	203	PEB	OD-C4D	2.58	1.28	1.23
26	SE	202	PEB	CMB-C2B	-2.58	1.45	1.50
28	oH	1001	CYC	C1D-CHD	2.58	1.51	1.41
26	HG	201	PEB	CHA-C1B	2.58	1.46	1.40
26	EA	202	PEB	OD-C4D	2.58	1.28	1.23
26	UI	201	PEB	C4A-NA	-2.58	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eA	201	PEB	OD-C4D	2.58	1.28	1.23
26	O6	203	PEB	OD-C4D	2.58	1.28	1.23
26	aA	204	PEB	C2A-C1A	-2.58	1.49	1.52
26	K4	202	PEB	OD-C4D	2.58	1.28	1.23
26	UE	203	PEB	C4A-NA	-2.58	1.31	1.37
26	D6	1002	PEB	OD-C4D	2.58	1.28	1.23
26	LE	202	PEB	OD-C4D	2.58	1.28	1.23
26	aF	202	PEB	C2A-C1A	-2.58	1.49	1.52
26	VI	203	PEB	C2A-C1A	-2.58	1.49	1.52
26	WE	201	PEB	C4B-NB	-2.58	1.33	1.38
26	RI	203	PEB	OD-C4D	2.58	1.28	1.23
26	Y2	202	PEB	OD-C4D	2.58	1.28	1.23
26	D3	202	PEB	OD-C4D	2.58	1.28	1.23
26	DB	1002	PEB	OD-C4D	2.58	1.28	1.23
27	AJ	302	PUB	OD-C4D	2.58	1.28	1.23
26	F1	201	PEB	C2A-C1A	-2.57	1.49	1.52
26	g2	203	PEB	C2A-C1A	-2.57	1.49	1.52
26	S7	203	PEB	C2A-C1A	-2.57	1.49	1.52
26	WA	203	PEB	CHA-C1B	2.57	1.46	1.40
26	PD	202	PEB	C1A-NA	-2.57	1.34	1.37
26	fB	201	PEB	OD-C4D	2.57	1.28	1.23
26	G4	202	PEB	OD-C4D	2.57	1.28	1.23
28	F7	1001	CYC	C1B-C2B	2.57	1.49	1.45
26	G8	203	PEB	C2A-C1A	-2.57	1.49	1.52
26	U8	203	PEB	OD-C4D	2.57	1.28	1.23
26	e8	202	PEB	C4A-NA	-2.57	1.31	1.37
28	PH	1001	CYC	C1D-CHD	2.57	1.51	1.41
26	l1	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	V3	201	PEB	C4A-NA	-2.57	1.31	1.37
26	X3	202	PEB	OD-C4D	2.57	1.28	1.23
26	gE	203	PEB	OD-C4D	2.57	1.28	1.23
26	XG	202	PEB	OD-C4D	2.57	1.28	1.23
26	XJ	202	PEB	C4B-C3B	2.57	1.49	1.45
26	ND	203	PEB	OD-C4D	2.57	1.28	1.23
26	BD	201	PEB	C2A-C1A	-2.57	1.49	1.52
26	OE	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	YD	301	PEB	OD-C4D	2.57	1.28	1.23
26	QE	203	PEB	C4A-NA	-2.57	1.31	1.37
26	BD	202	PEB	OD-C4D	2.57	1.28	1.23
26	HE	201	PEB	CHA-C1B	2.57	1.46	1.40
26	cA	201	PEB	C2A-C1A	-2.57	1.49	1.52
28	pH	1001	CYC	OB-C4B	2.57	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U4	201	PEB	OD-C4D	2.57	1.28	1.23
26	U8	201	PEB	OD-C4D	2.57	1.28	1.23
26	eI	202	PEB	OD-C4D	2.57	1.28	1.23
27	yE	302	PUB	OD-C4D	2.57	1.28	1.23
26	VI	202	PEB	C2C-C3C	2.57	1.45	1.37
26	K6	201	PEB	OD-C4D	2.57	1.28	1.23
26	HC	202	PEB	OD-C4D	2.57	1.28	1.23
28	K2	1001	CYC	OB-C4B	2.57	1.28	1.23
26	L1	201	PEB	C2A-C1A	-2.57	1.49	1.52
26	FD	203	PEB	C2A-C1A	-2.57	1.49	1.52
26	WB	203	PEB	OD-C4D	2.57	1.28	1.23
26	D9	201	PEB	OD-C4D	2.57	1.28	1.23
26	PD	202	PEB	OD-C4D	2.57	1.28	1.23
26	CG	201	PEB	C2A-C1A	-2.57	1.49	1.52
28	KB	202	CYC	C4C-NC	-2.57	1.32	1.37
26	aE	202	PEB	OD-C4D	2.56	1.28	1.23
26	MJ	201	PEB	OD-C4D	2.56	1.28	1.23
27	A1	203	PUB	OA-C1A	2.56	1.28	1.23
26	HF	1002	PEB	OD-C4D	2.56	1.28	1.23
26	J1	202	PEB	C4B-C3B	2.56	1.49	1.45
26	XG	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	U2	201	PEB	C4A-NA	-2.56	1.32	1.37
26	c8	202	PEB	C2A-C1A	-2.56	1.49	1.52
27	AA	303	PUB	C3C-C4C	2.56	1.52	1.43
26	iI	201	PEB	C1D-ND	2.56	1.49	1.45
26	P7	201	PEB	OD-C4D	2.56	1.28	1.23
26	mA	201	PEB	C4A-NA	-2.56	1.32	1.37
26	iF	201	PEB	C2A-C1A	-2.56	1.49	1.52
26	W1	202	PEB	OD-C4D	2.56	1.28	1.23
26	m8	201	PEB	OD-C4D	2.56	1.28	1.23
26	XE	201	PEB	OD-C4D	2.56	1.28	1.23
26	P4	202	PEB	C4A-NA	-2.56	1.32	1.37
26	GG	201	PEB	CHA-C1B	2.56	1.46	1.40
26	E9	201	PEB	OD-C4D	2.56	1.28	1.23
26	HE	202	PEB	C2A-C1A	-2.56	1.49	1.52
28	sH	1001	CYC	C4B-NB	-2.56	1.32	1.38
26	IJ	201	PEB	CAC-C2C	2.56	1.55	1.52
26	XD	202	PEB	OD-C4D	2.56	1.28	1.23
28	B6	1001	CYC	C4B-NB	-2.56	1.32	1.38
26	G9	201	PEB	OD-C4D	2.56	1.28	1.23
26	aI	201	PEB	OD-C4D	2.56	1.28	1.23
27	wG	304	PUB	OA-C1A	2.56	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W4	201	PEB	C4B-C3B	2.56	1.49	1.45
28	L6	1001	CYC	C4C-NC	-2.56	1.32	1.37
26	R2	201	PEB	OD-C4D	2.56	1.28	1.23
26	E9	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	L5	202	PEB	C4A-NA	-2.56	1.32	1.37
26	B5	202	PEB	OD-C4D	2.56	1.28	1.23
26	TI	202	PEB	OD-C4D	2.56	1.28	1.23
26	NI	1002	PEB	OD-C4D	2.56	1.28	1.23
26	RD	202	PEB	OD-C4D	2.55	1.28	1.23
26	cG	203	PEB	OD-C4D	2.55	1.28	1.23
26	hI	201	PEB	OD-C4D	2.55	1.28	1.23
26	v4	202	PEB	C4B-C3B	2.55	1.49	1.45
26	IG	203	PEB	C4A-NA	-2.55	1.32	1.37
28	N7	1001	CYC	C1B-C2B	2.55	1.49	1.45
26	BG	201	PEB	C1D-ND	2.55	1.49	1.45
28	UH	1001	CYC	C1B-C2B	2.55	1.49	1.45
26	SI	201	PEB	OD-C4D	2.55	1.28	1.23
26	M8	201	PEB	C4A-NA	-2.55	1.32	1.37
26	X1	202	PEB	C1B-C2B	2.55	1.51	1.45
26	fF	201	PEB	C4B-C3B	2.55	1.49	1.45
26	N3	201	PEB	OD-C4D	2.55	1.28	1.23
26	QG	203	PEB	C2C-C3C	2.55	1.45	1.37
26	KC	201	PEB	C4A-NA	-2.55	1.32	1.37
26	V6	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	H8	201	PEB	OD-C4D	2.55	1.28	1.23
26	SA	201	PEB	OD-C4D	2.55	1.28	1.23
26	YD	304	PEB	OD-C4D	2.55	1.28	1.23
28	EB	1001	CYC	OB-C4B	2.55	1.28	1.23
28	KH	1001	CYC	C4A-NA	-2.55	1.30	1.36
26	R2	203	PEB	OD-C4D	2.55	1.28	1.23
26	gB	202	PEB	OD-C4D	2.55	1.28	1.23
26	SB	203	PEB	OD-C4D	2.55	1.28	1.23
26	Y3	303	PEB	OD-C4D	2.55	1.28	1.23
26	YD	303	PEB	OD-C4D	2.55	1.28	1.23
26	UA	203	PEB	OD-C4D	2.55	1.28	1.23
26	KB	201	PEB	OD-C4D	2.55	1.28	1.23
26	KA	201	PEB	C4A-NA	-2.55	1.32	1.37
26	IA	203	PEB	OD-C4D	2.55	1.28	1.23
26	RI	201	PEB	OD-C4D	2.55	1.28	1.23
26	M1	402	PEB	C2A-C1A	-2.55	1.49	1.52
26	FA	202	PEB	OD-C4D	2.55	1.28	1.23
26	z1	202	PEB	OD-C4D	2.55	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	kG	201	PEB	C1B-C2B	2.55	1.51	1.45
26	M9	201	PEB	OD-C4D	2.55	1.28	1.23
28	EB	1001	CYC	C4C-NC	-2.55	1.32	1.37
26	X3	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	d7	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	ND	202	PEB	C1A-NA	-2.55	1.34	1.37
27	24	403	PUB	OD-C4D	2.54	1.28	1.23
28	SH	1001	CYC	OB-C4B	2.54	1.28	1.23
26	BJ	203	PEB	C4A-NA	-2.54	1.32	1.37
26	WE	201	PEB	CHA-C1B	2.54	1.46	1.40
26	EJ	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	B4	202	PEB	OD-C4D	2.54	1.28	1.23
26	N6	201	PEB	OD-C4D	2.54	1.28	1.23
26	Z6	201	PEB	OD-C4D	2.54	1.28	1.23
28	rH	1001	CYC	C1D-CHD	2.54	1.51	1.41
26	h2	201	PEB	OD-C4D	2.54	1.28	1.23
26	eE	203	PEB	C1B-C2B	2.54	1.51	1.45
28	K6	202	CYC	C4C-NC	-2.54	1.32	1.37
26	VJ	203	PEB	OD-C4D	2.54	1.28	1.23
28	AH	1001	CYC	C1D-CHD	2.54	1.51	1.41
26	S6	203	PEB	OD-C4D	2.54	1.28	1.23
26	A8	302	PEB	OD-C4D	2.54	1.28	1.23
28	KB	202	CYC	OB-C4B	2.54	1.28	1.23
28	wH	1001	CYC	C1D-CHD	2.54	1.51	1.41
26	m4	201	PEB	C2A-C1A	-2.54	1.49	1.52
26	w1	201	PEB	C1C-CHB	2.54	1.51	1.41
26	UI	201	PEB	CHA-C4A	-2.54	1.31	1.36
26	VI	201	PEB	OD-C4D	2.54	1.28	1.23
26	CA	203	PEB	C2A-C1A	-2.54	1.49	1.52
26	lB	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	MG	201	PEB	C2A-C1A	-2.54	1.49	1.52
26	aA	202	PEB	OD-C4D	2.54	1.28	1.23
26	D1	203	PEB	C2A-C1A	-2.54	1.49	1.52
26	P2	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	F3	202	PEB	C2A-C1A	-2.54	1.49	1.52
28	uH	1001	CYC	OB-C4B	2.54	1.28	1.23
28	HF	1001	CYC	C4C-NC	-2.54	1.32	1.37
26	H1	201	PEB	C4B-C3B	2.54	1.49	1.45
26	VB	201	PEB	C2A-C1A	-2.54	1.49	1.52
26	IE	201	PEB	CMB-C2B	-2.54	1.45	1.50
26	NA	202	PEB	OD-C4D	2.54	1.28	1.23
26	RG	201	PEB	OD-C4D	2.54	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I3	201	PEB	C4B-C3B	2.54	1.49	1.45
28	mH	1001	CYC	C4A-C3A	2.54	1.51	1.45
26	VG	202	PEB	OD-C4D	2.54	1.28	1.23
26	t1	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	m1	202	PEB	C4B-C3B	2.54	1.49	1.45
26	N9	204	PEB	OD-C4D	2.54	1.28	1.23
26	G8	201	PEB	C4A-NA	-2.54	1.32	1.37
26	uG	201	PEB	C1D-ND	2.54	1.49	1.45
26	T4	202	PEB	OD-C4D	2.54	1.28	1.23
26	L5	202	PEB	OD-C4D	2.54	1.28	1.23
28	BB	1001	CYC	C1B-NB	-2.54	1.33	1.37
26	HE	201	PEB	C2A-C1A	-2.54	1.49	1.52
26	mG	201	PEB	C2A-C1A	-2.54	1.49	1.52
26	P8	201	PEB	OD-C4D	2.54	1.28	1.23
26	k6	202	PEB	C4A-NA	-2.53	1.32	1.37
26	HG	201	PEB	C2A-C1A	-2.53	1.49	1.52
26	EG	201	PEB	OD-C4D	2.53	1.28	1.23
26	KE	202	PEB	OD-C4D	2.53	1.28	1.23
26	MA	201	PEB	C4A-NA	-2.53	1.32	1.37
28	C2	1001	CYC	C4C-NC	-2.53	1.32	1.37
26	Q2	201	PEB	C4A-NA	-2.53	1.32	1.37
28	YH	1002	CYC	C4A-C3A	2.53	1.51	1.45
26	u1	202	PEB	C1C-CHB	2.53	1.50	1.41
26	H9	202	PEB	C1B-C2B	2.53	1.51	1.45
28	IF	1001	CYC	C4C-NC	-2.53	1.32	1.37
26	fA	202	PEB	C4B-C3B	2.53	1.49	1.45
26	JI	1002	PEB	OD-C4D	2.53	1.28	1.23
26	TI	203	PEB	C4B-C3B	2.53	1.49	1.45
28	vH	1001	CYC	C1D-CHD	2.53	1.50	1.41
26	K8	203	PEB	C4A-NA	-2.53	1.32	1.37
26	R3	202	PEB	OD-C4D	2.53	1.28	1.23
26	I5	201	PEB	OD-C4D	2.53	1.28	1.23
27	N9	201	PUB	OD-C4D	2.53	1.28	1.23
26	24	405	PEB	C2A-C1A	-2.53	1.49	1.52
26	T7	201	PEB	C2A-C1A	-2.53	1.49	1.52
26	iI	202	PEB	C2A-C1A	-2.53	1.49	1.52
28	G7	1001	CYC	C1B-C2B	2.53	1.49	1.45
26	Q8	202	PEB	OD-C4D	2.53	1.28	1.23
26	II	202	PEB	OD-C4D	2.53	1.28	1.23
26	11	201	PEB	C4B-C3B	2.53	1.49	1.45
26	d1	201	PEB	C2A-C1A	-2.53	1.49	1.52
26	I8	203	PEB	OD-C4D	2.53	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H7	1001	CYC	C1B-C2B	2.53	1.49	1.45
26	L8	202	PEB	OD-C4D	2.53	1.28	1.23
26	ZB	201	PEB	OD-C4D	2.53	1.28	1.23
28	JH	1001	CYC	OB-C4B	2.53	1.28	1.23
26	c8	201	PEB	C4B-C3B	2.53	1.49	1.45
28	RH	1001	CYC	C1D-CHD	2.53	1.50	1.41
26	LG	202	PEB	OD-C4D	2.53	1.28	1.23
26	OB	203	PEB	C2A-C1A	-2.53	1.49	1.52
26	S4	201	PEB	OD-C4D	2.52	1.28	1.23
26	C8	202	PEB	OD-C4D	2.52	1.28	1.23
26	SF	201	PEB	C4A-NA	-2.52	1.32	1.37
26	M8	201	PEB	OD-C4D	2.52	1.28	1.23
26	G4	201	PEB	C4A-NA	-2.52	1.32	1.37
26	fA	201	PEB	C2A-C1A	-2.52	1.49	1.52
26	Z2	202	PEB	OD-C4D	2.52	1.28	1.23
26	LA	201	PEB	OD-C4D	2.52	1.28	1.23
28	VH	1001	CYC	OB-C4B	2.52	1.28	1.23
26	DG	202	PEB	OD-C4D	2.52	1.28	1.23
26	u1	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	aB	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	JA	201	PEB	OD-C4D	2.52	1.28	1.23
26	GC	203	PEB	C2A-C1A	-2.52	1.49	1.52
26	D4	201	PEB	OD-C4D	2.52	1.28	1.23
26	f7	203	PEB	OD-C4D	2.52	1.28	1.23
26	Z8	201	PEB	C4A-NA	-2.52	1.32	1.37
26	EG	202	PEB	C2A-C1A	-2.52	1.49	1.52
28	CI	1001	CYC	C4C-NC	-2.52	1.32	1.37
26	J8	201	PEB	OD-C4D	2.52	1.28	1.23
28	H2	1001	CYC	C1B-C2B	2.52	1.49	1.45
26	ZA	201	PEB	C4A-NA	-2.52	1.32	1.37
28	E6	1001	CYC	OB-C4B	2.52	1.28	1.23
26	N8	202	PEB	OD-C4D	2.52	1.28	1.23
28	C6	1001	CYC	OB-C4B	2.52	1.28	1.23
28	QH	1001	CYC	C4B-NB	-2.52	1.32	1.38
26	P3	202	PEB	OD-C4D	2.52	1.28	1.23
28	B6	1002	CYC	C4C-NC	-2.52	1.32	1.37
28	HB	1001	CYC	C4C-NC	-2.52	1.32	1.37
26	k4	203	PEB	C1D-ND	2.52	1.49	1.45
26	m8	202	PEB	OD-C4D	2.52	1.28	1.23
28	kH	1001	CYC	C4A-C3A	2.52	1.51	1.45
28	LF	1001	CYC	OB-C4B	2.51	1.28	1.23
28	DB	1001	CYC	C1B-NB	-2.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ZG	202	PEB	C4B-C3B	2.51	1.49	1.45
26	A2	301	PEB	C2A-C1A	-2.51	1.49	1.52
26	U6	202	PEB	OD-C4D	2.51	1.28	1.23
26	vE	202	PEB	C4B-C3B	2.51	1.49	1.45
28	E6	1001	CYC	C4C-NC	-2.51	1.32	1.37
26	DD	201	PEB	C4B-C3B	2.51	1.49	1.45
26	X1	203	PEB	C4A-NA	-2.51	1.32	1.37
26	N2	1002	PEB	OD-C4D	2.51	1.28	1.23
26	Q4	201	PEB	C4A-NA	-2.51	1.32	1.37
26	C3	201	PEB	OD-C4D	2.51	1.28	1.23
26	AC	203	PEB	C4B-C3B	2.51	1.49	1.45
26	AJ	304	PEB	C4B-C3B	2.51	1.49	1.45
28	dH	1001	CYC	C1D-CHD	2.51	1.50	1.41
26	F8	202	PEB	OD-C4D	2.51	1.28	1.23
26	NB	1002	PEB	OD-C4D	2.51	1.28	1.23
28	L7	1001	CYC	OB-C4B	2.51	1.28	1.23
28	iH	1001	CYC	C4A-C3A	2.51	1.51	1.45
26	S2	201	PEB	OD-C4D	2.51	1.28	1.23
26	a2	201	PEB	OD-C4D	2.51	1.28	1.23
26	K5	202	PEB	OD-C4D	2.51	1.28	1.23
26	JG	201	PEB	OD-C4D	2.51	1.28	1.23
27	yG	302	PUB	OA-C1A	2.51	1.28	1.23
28	KH	1001	CYC	C4D-CHA	2.51	1.50	1.41
26	R3	203	PEB	C4A-NA	-2.51	1.32	1.37
28	D6	1001	CYC	C1B-NB	-2.51	1.33	1.37
26	A5	201	PEB	C4B-C3B	2.51	1.49	1.45
26	R1	203	PEB	C2A-C1A	-2.51	1.49	1.52
26	V3	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	U8	202	PEB	OD-C4D	2.51	1.28	1.23
26	UA	202	PEB	OD-C4D	2.50	1.28	1.23
28	KH	1001	CYC	C1A-NA	-2.50	1.33	1.38
26	T2	203	PEB	C4B-C3B	2.50	1.49	1.45
26	gI	203	PEB	C4B-C3B	2.50	1.49	1.45
26	dI	201	PEB	OD-C4D	2.50	1.28	1.23
26	g4	202	PEB	C4B-C3B	2.50	1.49	1.45
26	xE	304	PEB	C4B-C3B	2.50	1.49	1.45
26	V6	201	PEB	C2A-C1A	-2.50	1.49	1.52
26	UB	202	PEB	OD-C4D	2.50	1.28	1.23
26	KA	203	PEB	C4A-NA	-2.50	1.32	1.37
28	JF	1001	CYC	C4A-C3A	2.50	1.51	1.45
26	P2	202	PEB	OD-C4D	2.50	1.28	1.23
26	FE	202	PEB	OD-C4D	2.50	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	IJ	203	PEB	OD-C4D	2.50	1.28	1.23
26	W2	201	PEB	C4A-NA	-2.50	1.32	1.37
26	d2	201	PEB	OD-C4D	2.50	1.28	1.23
26	Z7	203	PEB	C2A-C1A	-2.50	1.49	1.52
26	B4	202	PEB	C4B-C3B	2.50	1.49	1.45
26	iA	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	tE	202	PEB	C4B-C3B	2.50	1.49	1.45
28	G2	1001	CYC	OB-C4B	2.50	1.28	1.23
28	N2	1001	CYC	OB-C4B	2.50	1.28	1.23
26	I9	201	PEB	C4A-NA	-2.50	1.32	1.37
26	QI	201	PEB	C4A-NA	-2.50	1.32	1.37
28	NI	1001	CYC	C4B-NB	-2.50	1.32	1.38
28	AH	1001	CYC	C4D-CHA	2.50	1.50	1.41
26	L8	201	PEB	OD-C4D	2.50	1.28	1.23
26	PF	201	PEB	OD-C4D	2.50	1.28	1.23
26	S1	201	PEB	C4B-C3B	2.50	1.49	1.45
26	P3	201	PEB	C4A-NA	-2.50	1.32	1.37
28	oH	1001	CYC	C4A-C3A	2.50	1.51	1.45
26	R1	201	PEB	OD-C4D	2.50	1.28	1.23
26	J2	1002	PEB	OD-C4D	2.50	1.28	1.23
28	HB	1001	CYC	C1B-NB	-2.50	1.33	1.37
26	T2	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	O3	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	cF	201	PEB	C2A-C1A	-2.50	1.49	1.52
26	SB	201	PEB	OD-C4D	2.50	1.28	1.23
26	y4	201	PEB	C4B-C3B	2.50	1.49	1.45
28	NH	1001	CYC	OB-C4B	2.50	1.28	1.23
28	NF	1001	CYC	C1B-C2B	2.50	1.49	1.45
26	IJ	202	PEB	C2C-C3C	2.49	1.45	1.37
26	O4	201	PEB	OD-C4D	2.49	1.28	1.23
26	K8	201	PEB	C4A-NA	-2.49	1.32	1.37
26	HJ	202	PEB	C1B-C2B	2.49	1.51	1.45
26	a8	203	PEB	C2A-C1A	-2.49	1.49	1.52
28	F2	1001	CYC	C1B-NB	-2.49	1.33	1.37
26	l4	201	PEB	C2A-C1A	-2.49	1.49	1.52
26	tE	202	PEB	OD-C4D	2.49	1.28	1.23
26	TD	202	PEB	C4B-NB	-2.49	1.33	1.38
26	ZI	202	PEB	OD-C4D	2.49	1.28	1.23
27	A8	303	PUB	C3C-C4C	2.49	1.51	1.43
28	E7	1001	CYC	C1B-NB	-2.49	1.33	1.37
26	iF	202	PEB	C1B-C2B	2.49	1.51	1.45
26	Q3	201	PEB	C2A-C1A	-2.49	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O3	202	PEB	C4A-NA	-2.49	1.32	1.37
26	kF	201	PEB	OD-C4D	2.49	1.28	1.23
26	MJ	201	PEB	C4A-NA	-2.49	1.32	1.37
26	N3	202	PEB	C2C-C3C	2.49	1.45	1.37
26	Q1	202	PEB	OD-C4D	2.49	1.28	1.23
26	x1	202	PEB	C4B-C3B	2.49	1.49	1.45
26	AE	202	PEB	C4B-C3B	2.49	1.49	1.45
26	IJ	203	PEB	C4A-NA	-2.49	1.32	1.37
26	QJ	202	PEB	C2A-C1A	-2.49	1.49	1.52
28	C6	1001	CYC	C1B-C2B	2.49	1.49	1.45
26	E8	202	PEB	OD-C4D	2.49	1.28	1.23
26	LA	202	PEB	OD-C4D	2.49	1.28	1.23
28	H6	1001	CYC	C4C-NC	-2.49	1.32	1.37
26	B5	203	PEB	C2A-C1A	-2.49	1.49	1.52
26	W1	201	PEB	C4B-C3B	2.49	1.49	1.45
28	E7	1001	CYC	C4C-NC	-2.49	1.32	1.37
28	JH	1001	CYC	C4A-C3A	2.49	1.51	1.45
28	YH	1004	CYC	C4A-C3A	2.49	1.51	1.45
26	g4	203	PEB	C1D-ND	2.49	1.49	1.45
26	IA	201	PEB	C2A-C1A	-2.49	1.49	1.52
26	DJ	203	PEB	C2A-C1A	-2.49	1.49	1.52
28	GI	1001	CYC	OB-C4B	2.49	1.28	1.23
26	N4	201	PEB	C4A-NA	-2.49	1.32	1.37
26	OF	201	PEB	C4B-C3B	2.49	1.49	1.45
26	s4	201	PEB	C1B-C2B	2.49	1.51	1.45
26	Z6	201	PEB	C4A-NA	-2.49	1.32	1.37
26	WB	201	PEB	C4A-NA	-2.48	1.32	1.37
26	VD	201	PEB	C4A-NA	-2.48	1.32	1.37
26	y1	201	PEB	C4B-C3B	2.48	1.49	1.45
26	Q4	201	PEB	OD-C4D	2.48	1.28	1.23
26	F2	1002	PEB	OD-C4D	2.48	1.28	1.23
26	c7	202	PEB	C2A-C1A	-2.48	1.49	1.52
28	HI	1001	CYC	OB-C4B	2.48	1.28	1.23
28	MI	1001	CYC	OB-C4B	2.48	1.28	1.23
26	X4	203	PEB	C4A-NA	-2.48	1.32	1.37
26	zE	501	PEB	OD-C4D	2.48	1.28	1.23
28	CB	1001	CYC	C1B-C2B	2.48	1.49	1.45
26	f8	201	PEB	C2A-C1A	-2.48	1.49	1.52
26	bG	201	PEB	C2A-C1A	-2.48	1.49	1.52
26	c1	202	PEB	C4B-C3B	2.48	1.49	1.45
26	S6	201	PEB	OD-C4D	2.48	1.28	1.23
26	TD	202	PEB	C2C-C3C	2.48	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H1	201	PEB	C2A-C1A	-2.48	1.49	1.52
26	R4	203	PEB	C2A-C1A	-2.48	1.49	1.52
26	OA	202	PEB	OD-C4D	2.48	1.28	1.23
26	pE	202	PEB	C1B-C2B	2.48	1.51	1.45
26	L1	202	PEB	C2A-C1A	-2.48	1.49	1.52
26	TD	201	PEB	C4A-NA	-2.48	1.32	1.37
26	F8	201	PEB	C4A-NA	-2.48	1.32	1.37
26	FA	201	PEB	C4A-NA	-2.48	1.32	1.37
28	I6	1001	CYC	C4C-NC	-2.48	1.32	1.37
26	OA	203	PEB	OD-C4D	2.48	1.28	1.23
26	VI	203	PEB	C4B-C3B	2.48	1.49	1.45
26	Q1	201	PEB	OD-C4D	2.48	1.28	1.23
26	HI	1002	PEB	OD-C4D	2.48	1.28	1.23
26	g7	202	PEB	C1A-NA	-2.48	1.34	1.37
26	X9	202	PEB	C2A-C1A	-2.48	1.49	1.52
28	IH	1001	CYC	C4A-C3A	2.48	1.51	1.45
28	HI	1001	CYC	C1B-C2B	2.48	1.49	1.45
26	q4	203	PEB	C4B-C3B	2.48	1.49	1.45
26	JD	202	PEB	OD-C4D	2.47	1.28	1.23
26	S2	201	PEB	C4A-NA	-2.47	1.32	1.37
26	BD	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	gE	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	CD	201	PEB	OD-C4D	2.47	1.28	1.23
28	NI	1001	CYC	OB-C4B	2.47	1.28	1.23
26	W8	203	PEB	C2C-C3C	2.47	1.45	1.37
28	cH	1001	CYC	C4D-CHA	2.47	1.50	1.41
26	p4	202	PEB	OD-C4D	2.47	1.28	1.23
26	eD	401	PEB	C2A-C1A	-2.47	1.49	1.52
26	c2	203	PEB	C4B-C3B	2.47	1.49	1.45
28	jH	1001	CYC	C1A-C2A	2.47	1.49	1.45
26	aG	202	PEB	OD-C4D	2.47	1.28	1.23
28	CB	1001	CYC	OB-C4B	2.47	1.28	1.23
26	r1	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	N1	201	PEB	C4A-NA	-2.47	1.32	1.37
26	Q8	204	PEB	OD-C4D	2.47	1.28	1.23
28	kH	1001	CYC	C1D-CHD	2.47	1.50	1.41
26	H2	1002	PEB	OD-C4D	2.47	1.28	1.23
26	h6	201	PEB	C4B-C3B	2.47	1.49	1.45
26	ZB	201	PEB	C4A-NA	-2.47	1.32	1.37
26	DJ	202	PEB	C4A-NA	-2.47	1.32	1.37
28	NI	1001	CYC	C1B-C2B	2.47	1.49	1.45
26	Q1	201	PEB	C4A-NA	-2.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W6	201	PEB	C4A-NA	-2.47	1.32	1.37
26	J4	203	PEB	C2A-C1A	-2.47	1.49	1.52
28	YH	1003	CYC	C1A-C2A	2.47	1.49	1.45
28	H2	1001	CYC	OB-C4B	2.47	1.28	1.23
27	A7	303	PUB	OA-C1A	2.47	1.28	1.23
28	J2	1001	CYC	C4A-C3A	2.47	1.51	1.45
26	h4	201	PEB	C2A-C1A	-2.47	1.49	1.52
26	FE	201	PEB	OD-C4D	2.47	1.28	1.23
26	XG	201	PEB	OD-C4D	2.47	1.28	1.23
26	U7	203	PEB	C1D-ND	2.47	1.49	1.45
26	C4	201	PEB	C2A-C1A	-2.47	1.49	1.52
26	L5	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	IG	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	HG	201	PEB	C4B-NB	-2.47	1.33	1.38
26	TG	202	PEB	C4A-NA	-2.47	1.32	1.37
26	H4	202	PEB	C4B-C3B	2.47	1.49	1.45
26	Y8	201	PEB	C4A-NA	-2.47	1.32	1.37
26	D9	203	PEB	CHA-C1B	2.47	1.46	1.40
26	T9	202	PEB	OD-C4D	2.47	1.28	1.23
26	HA	202	PEB	C4A-NA	-2.47	1.32	1.37
26	TI	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	Z6	202	PEB	OD-C4D	2.47	1.28	1.23
28	mH	1001	CYC	OB-C4B	2.47	1.28	1.23
28	NI	1001	CYC	C1B-NB	-2.47	1.33	1.37
26	A7	301	PEB	C4B-C3B	2.46	1.49	1.45
28	MH	1001	CYC	C1D-CHD	2.46	1.50	1.41
26	LG	201	PEB	C4B-C3B	2.46	1.49	1.45
26	XA	201	PEB	OD-C4D	2.46	1.28	1.23
28	F6	1001	CYC	OB-C4B	2.46	1.28	1.23
28	GB	1001	CYC	C1B-NB	-2.46	1.33	1.37
26	ZB	203	PEB	C4A-NA	-2.46	1.32	1.37
28	BB	1001	CYC	C4C-NC	-2.46	1.32	1.37
26	c8	201	PEB	C2A-C1A	-2.46	1.49	1.52
26	b6	201	PEB	OD-C4D	2.46	1.28	1.23
28	tH	1001	CYC	C4B-NB	-2.46	1.32	1.38
28	FB	1001	CYC	C1D-CHD	2.46	1.50	1.41
26	A3	202	PEB	C1D-ND	2.46	1.49	1.45
26	FC	202	PEB	C2A-C1A	-2.46	1.49	1.52
28	EI	1001	CYC	OB-C4B	2.46	1.28	1.23
28	H6	1001	CYC	C1B-NB	-2.46	1.33	1.37
26	GG	202	PEB	OA-C1A	2.46	1.28	1.23
28	NH	1001	CYC	C4A-C3A	2.46	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hF	202	PEB	C4A-NA	-2.46	1.32	1.37
28	DF	1003	CYC	C1B-C2B	2.46	1.49	1.45
26	d4	201	PEB	C4B-C3B	2.46	1.49	1.45
26	GG	203	PEB	C4B-C3B	2.46	1.49	1.45
26	RA	202	PEB	C1B-C2B	2.46	1.51	1.45
28	hH	1001	CYC	C4A-C3A	2.46	1.51	1.45
26	P1	201	PEB	OD-C4D	2.46	1.28	1.23
26	LG	201	PEB	OD-C4D	2.46	1.28	1.23
26	IJ	202	PEB	OD-C4D	2.46	1.28	1.23
28	EB	1001	CYC	C1B-NB	-2.46	1.33	1.37
26	X8	201	PEB	OD-C4D	2.46	1.28	1.23
26	J3	202	PEB	OD-C4D	2.46	1.28	1.23
26	XD	203	PEB	C2A-C1A	-2.46	1.49	1.52
26	Y3	304	PEB	OD-C4D	2.46	1.28	1.23
28	tH	1001	CYC	C1D-CHD	2.46	1.50	1.41
26	F9	203	PEB	OD-C4D	2.46	1.28	1.23
28	CB	1001	CYC	C4C-NC	-2.46	1.32	1.37
26	GA	201	PEB	C4A-NA	-2.45	1.32	1.37
26	ME	202	PEB	C4B-C3B	2.45	1.49	1.45
28	vH	1001	CYC	C4B-NB	-2.45	1.32	1.38
26	bB	201	PEB	OD-C4D	2.45	1.28	1.23
26	GJ	201	PEB	C4B-C3B	2.45	1.49	1.45
26	SI	201	PEB	C4A-NA	-2.45	1.32	1.37
28	GI	1001	CYC	C1D-CHD	2.45	1.50	1.41
26	fG	202	PEB	C4B-C3B	2.45	1.49	1.45
26	L7	1002	PEB	OD-C4D	2.45	1.28	1.23
26	SI	202	PEB	C1D-ND	2.45	1.49	1.45
26	N3	202	PEB	CHA-C1B	2.45	1.46	1.40
26	P1	203	PEB	C2A-C1A	-2.45	1.49	1.52
26	qE	203	PEB	C2A-C1A	-2.45	1.49	1.52
26	B9	203	PEB	OD-C4D	2.45	1.28	1.23
26	jF	203	PEB	C4B-C3B	2.45	1.49	1.45
26	jF	202	PEB	C2A-C1A	-2.45	1.49	1.52
26	mF	201	PEB	C2A-C1A	-2.45	1.49	1.52
26	IC	202	PEB	OD-C4D	2.45	1.28	1.23
28	JI	1001	CYC	OB-C4B	2.45	1.28	1.23
26	OG	201	PEB	C4B-C3B	2.45	1.49	1.45
28	B6	1001	CYC	C1B-NB	-2.45	1.33	1.37
26	GJ	201	PEB	OD-C4D	2.45	1.28	1.23
26	jF	202	PEB	C4B-C3B	2.45	1.49	1.45
26	b6	201	PEB	C4A-NA	-2.45	1.32	1.37
26	hB	202	PEB	C2A-C1A	-2.45	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TD	203	PEB	OD-C4D	2.45	1.28	1.23
28	DB	1001	CYC	C4C-NC	-2.45	1.32	1.37
26	C8	203	PEB	C2A-C1A	-2.45	1.49	1.52
26	kI	202	PEB	C4B-C3B	2.45	1.49	1.45
26	VJ	202	PEB	C4B-C3B	2.45	1.49	1.45
26	X1	203	PEB	C2A-C1A	-2.45	1.49	1.52
26	FC	203	PEB	C2A-C1A	-2.45	1.49	1.52
26	DD	203	PEB	C2A-C1A	-2.45	1.49	1.52
26	WE	203	PEB	C4B-C3B	2.45	1.49	1.45
26	u4	202	PEB	C1C-CHB	2.45	1.50	1.41
28	D6	1001	CYC	C4C-NC	-2.45	1.32	1.37
26	XD	203	PEB	OD-C4D	2.45	1.28	1.23
26	jF	203	PEB	C1C-CHB	2.45	1.50	1.41
26	PB	201	PEB	C4A-NA	-2.45	1.32	1.37
26	sG	203	PEB	C4B-NB	-2.45	1.33	1.38
26	Y8	201	PEB	C2C-C3C	2.45	1.44	1.37
28	N2	1001	CYC	C1B-C2B	2.45	1.49	1.45
26	YA	201	PEB	OD-C4D	2.45	1.28	1.23
26	P3	202	PEB	C2C-C3C	2.45	1.44	1.37
26	a8	202	PEB	OD-C4D	2.45	1.28	1.23
26	m2	203	PEB	C4B-C3B	2.44	1.49	1.45
26	O6	203	PEB	C2A-C1A	-2.44	1.49	1.52
26	R7	201	PEB	C2A-C1A	-2.44	1.49	1.52
26	j8	203	PEB	C2A-C1A	-2.44	1.49	1.52
26	QD	201	PEB	C2A-C1A	-2.44	1.49	1.52
26	T9	201	PEB	C4B-C3B	2.44	1.49	1.45
26	I5	201	PEB	C4A-NA	-2.44	1.32	1.37
28	rH	1001	CYC	C4B-NB	-2.44	1.32	1.38
26	KC	203	PEB	C4A-NA	-2.44	1.32	1.37
26	NA	201	PEB	OD-C4D	2.44	1.28	1.23
28	UH	1001	CYC	OB-C4B	2.44	1.28	1.23
26	aB	201	PEB	C4A-NA	-2.44	1.32	1.37
28	EI	1001	CYC	C4C-NC	-2.44	1.32	1.37
26	d8	201	PEB	C2A-C1A	-2.44	1.49	1.52
26	GA	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	iB	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	nE	202	PEB	C2A-C1A	-2.44	1.49	1.52
28	LI	1001	CYC	C4C-NC	-2.44	1.32	1.37
26	IE	203	PEB	C2C-C3C	2.44	1.44	1.37
28	I2	1001	CYC	OB-C4B	2.44	1.28	1.23
26	e4	202	PEB	C1D-ND	2.44	1.49	1.45
26	H4	201	PEB	C4B-C3B	2.44	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	kF	201	PEB	C4B-C3B	2.44	1.49	1.45
26	OG	202	PEB	C4A-NA	-2.44	1.32	1.37
28	F6	1001	CYC	C1D-CHD	2.44	1.50	1.41
26	I9	202	PEB	OD-C4D	2.44	1.28	1.23
28	OH	1001	CYC	C4A-C3A	2.44	1.51	1.45
26	N8	201	PEB	OD-C4D	2.44	1.28	1.23
26	ED	201	PEB	OD-C4D	2.44	1.28	1.23
26	F3	201	PEB	C2A-C1A	-2.44	1.49	1.52
26	i7	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	KD	201	PEB	C2A-C1A	-2.44	1.49	1.52
28	G6	1001	CYC	C1B-NB	-2.44	1.33	1.37
26	OJ	201	PEB	C2A-C1A	-2.44	1.49	1.52
26	LB	1002	PEB	OD-C4D	2.44	1.28	1.23
26	JC	202	PEB	OD-C4D	2.44	1.28	1.23
28	J2	1001	CYC	C4B-NB	-2.44	1.32	1.38
28	H6	1001	CYC	C4B-NB	-2.44	1.32	1.38
26	FG	202	PEB	OD-C4D	2.44	1.28	1.23
26	t1	201	PEB	C4B-C3B	2.44	1.49	1.45
26	QG	203	PEB	C4B-C3B	2.44	1.49	1.45
26	R2	201	PEB	C4A-NA	-2.44	1.32	1.37
26	N3	203	PEB	C4A-NA	-2.44	1.32	1.37
26	ZB	202	PEB	C4A-NA	-2.44	1.32	1.37
28	C6	1001	CYC	C4C-NC	-2.44	1.32	1.37
26	kG	203	PEB	C4A-NA	-2.43	1.32	1.37
26	WD	202	PEB	C2A-C1A	-2.43	1.49	1.52
26	JJ	201	PEB	C2A-C1A	-2.43	1.49	1.52
26	d8	201	PEB	C4B-C3B	2.43	1.49	1.45
28	eH	1001	CYC	C4A-C3A	2.43	1.51	1.45
28	qH	1001	CYC	C4A-C3A	2.43	1.51	1.45
26	kA	202	PEB	C4B-C3B	2.43	1.49	1.45
26	21	405	PEB	C2A-C1A	-2.43	1.49	1.52
26	U9	202	PEB	C2A-C1A	-2.43	1.49	1.52
26	LJ	202	PEB	C4A-NA	-2.43	1.32	1.37
28	YH	1001	CYC	C4A-C3A	2.43	1.51	1.45
26	HD	203	PEB	C2A-C1A	-2.43	1.49	1.52
28	HB	1001	CYC	C4B-NB	-2.43	1.32	1.38
26	KA	202	PEB	OD-C4D	2.43	1.28	1.23
28	E2	1001	CYC	OB-C4B	2.43	1.28	1.23
26	Y9	202	PEB	C4B-C3B	2.43	1.49	1.45
26	HB	1002	PEB	OD-C4D	2.43	1.28	1.23
28	II	1001	CYC	OB-C4B	2.43	1.28	1.23
26	e7	201	PEB	C2A-C1A	-2.43	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TJ	202	PEB	C4B-C3B	2.43	1.49	1.45
26	CE	202	PEB	C4A-NA	-2.43	1.32	1.37
26	GG	201	PEB	C4B-C3B	2.43	1.49	1.45
26	T8	202	PEB	C4A-NA	-2.43	1.32	1.37
28	iH	1001	CYC	C4B-NB	-2.43	1.32	1.38
28	J7	1003	CYC	C1B-C2B	2.43	1.49	1.45
26	D9	203	PEB	C2A-C1A	-2.43	1.49	1.52
28	GB	1001	CYC	C4C-NC	-2.43	1.32	1.37
28	EF	1001	CYC	C4B-NB	-2.43	1.32	1.38
26	hI	201	PEB	CHA-C4A	-2.43	1.32	1.36
26	UE	201	PEB	OD-C4D	2.43	1.28	1.23
28	KF	1001	CYC	C1D-CHD	2.43	1.50	1.41
26	T7	201	PEB	C4B-C3B	2.43	1.49	1.45
26	mB	201	PEB	C4B-C3B	2.43	1.49	1.45
26	m4	203	PEB	C2A-C1A	-2.43	1.49	1.52
26	h6	201	PEB	C2A-C1A	-2.43	1.49	1.52
26	KD	201	PEB	C4A-NA	-2.43	1.32	1.37
28	G2	1001	CYC	C1D-CHD	2.43	1.50	1.41
26	P4	201	PEB	OD-C4D	2.43	1.28	1.23
26	PB	201	PEB	OD-C4D	2.43	1.28	1.23
26	O3	201	PEB	C4B-NB	-2.43	1.33	1.38
26	A9	303	PEB	C2A-C1A	-2.43	1.49	1.52
28	J7	1003	CYC	C2C-C1C	-2.43	1.49	1.52
26	V2	203	PEB	C4B-C3B	2.43	1.49	1.45
26	iI	203	PEB	C4B-C3B	2.43	1.49	1.45
26	H5	202	PEB	OD-C4D	2.43	1.28	1.23
26	IA	203	PEB	C4A-NA	-2.43	1.32	1.37
26	cE	203	PEB	C1B-C2B	2.43	1.51	1.45
26	C8	201	PEB	OD-C4D	2.43	1.28	1.23
26	CA	201	PEB	OD-C4D	2.43	1.28	1.23
26	kB	202	PEB	C4A-NA	-2.43	1.32	1.37
26	F4	202	PEB	C1C-CHB	2.43	1.50	1.41
26	h2	201	PEB	C4A-NA	-2.43	1.32	1.37
26	HJ	202	PEB	C4A-NA	-2.43	1.32	1.37
26	RD	202	PEB	CHA-C1B	2.42	1.46	1.40
28	L7	1001	CYC	C1B-C2B	2.42	1.49	1.45
26	D4	203	PEB	C2A-C1A	-2.42	1.49	1.52
26	O4	202	PEB	C2A-C1A	-2.42	1.49	1.52
26	H5	202	PEB	C4A-NA	-2.42	1.32	1.37
26	kE	201	PEB	C4A-NA	-2.42	1.32	1.37
26	g2	203	PEB	C4B-C3B	2.42	1.49	1.45
26	TJ	201	PEB	C1C-CHB	2.42	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F9	203	PEB	C2C-C3C	2.42	1.44	1.37
26	H8	202	PEB	C4A-NA	-2.42	1.32	1.37
28	E2	1001	CYC	C4C-NC	-2.42	1.32	1.37
26	aG	203	PEB	C1B-C2B	2.42	1.51	1.45
26	R1	201	PEB	C4A-NA	-2.42	1.32	1.37
26	qG	202	PEB	C4A-NA	-2.42	1.32	1.37
28	J2	1001	CYC	OB-C4B	2.42	1.28	1.23
26	ZF	203	PEB	C4A-NA	-2.42	1.32	1.37
28	JF	1001	CYC	C1B-C2B	2.42	1.49	1.45
26	hG	202	PEB	C4B-C3B	2.42	1.49	1.45
26	YA	201	PEB	C4A-NA	-2.42	1.32	1.37
26	AE	201	PEB	C4A-NA	-2.42	1.32	1.37
26	tG	202	PEB	OD-C4D	2.42	1.28	1.23
28	wH	1001	CYC	OB-C4B	2.42	1.28	1.23
26	S1	201	PEB	OD-C4D	2.42	1.28	1.23
26	SE	201	PEB	OD-C4D	2.42	1.28	1.23
26	A5	202	PEB	C4B-C3B	2.42	1.49	1.45
26	g1	201	PEB	C2A-C1A	-2.42	1.49	1.52
26	g7	201	PEB	C2A-C1A	-2.42	1.49	1.52
26	mE	202	PEB	C2A-C1A	-2.42	1.49	1.52
28	CI	1001	CYC	OB-C4B	2.42	1.28	1.23
26	f1	202	PEB	C4B-C3B	2.42	1.49	1.45
26	f7	201	PEB	C4B-C3B	2.42	1.49	1.45
26	O7	202	PEB	C1D-ND	2.42	1.49	1.45
26	W1	201	PEB	C4A-NA	-2.42	1.32	1.37
26	P8	202	PEB	C4A-NA	-2.42	1.32	1.37
26	hE	201	PEB	C4B-C3B	2.42	1.49	1.45
26	fB	202	PEB	C2A-C1A	-2.42	1.49	1.52
28	G6	1001	CYC	OB-C4B	2.42	1.28	1.23
28	I6	1001	CYC	C4B-NB	-2.42	1.32	1.38
26	B9	203	PEB	C4A-NA	-2.42	1.32	1.37
26	fE	202	PEB	C4B-C3B	2.42	1.49	1.45
28	TH	1001	CYC	OB-C4B	2.42	1.28	1.23
26	eG	201	PEB	C4B-C3B	2.42	1.49	1.45
28	B6	1001	CYC	C4C-NC	-2.42	1.32	1.37
26	I8	202	PEB	OD-C4D	2.42	1.28	1.23
26	cA	202	PEB	C4B-C3B	2.41	1.49	1.45
26	YF	202	PEB	C1B-C2B	2.41	1.51	1.45
26	ZA	201	PEB	OD-C4D	2.41	1.28	1.23
26	iG	202	PEB	C2A-C1A	-2.41	1.49	1.52
26	RF	202	PEB	C4B-C3B	2.41	1.49	1.45
26	M9	201	PEB	C4A-NA	-2.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R3	202	PEB	C2A-C1A	-2.41	1.49	1.52
26	Y3	303	PEB	C2A-C1A	-2.41	1.49	1.52
26	CE	203	PEB	C2A-C1A	-2.41	1.49	1.52
28	IF	1001	CYC	C1D-CHD	2.41	1.50	1.41
26	VI	202	PEB	OD-C4D	2.41	1.28	1.23
28	I6	1001	CYC	OB-C4B	2.41	1.28	1.23
26	U6	202	PEB	C4A-NA	-2.41	1.32	1.37
26	P6	201	PEB	C4A-NA	-2.41	1.32	1.37
26	k2	202	PEB	C2A-C1A	-2.41	1.49	1.52
26	gG	202	PEB	C2A-C1A	-2.41	1.49	1.52
26	IA	202	PEB	OD-C4D	2.41	1.28	1.23
28	GB	1001	CYC	OB-C4B	2.41	1.28	1.23
26	bB	202	PEB	C4A-NA	-2.41	1.32	1.37
26	F9	203	PEB	C4B-C3B	2.41	1.49	1.45
26	O8	202	PEB	OD-C4D	2.41	1.28	1.23
28	NB	1001	CYC	C4A-C3A	2.41	1.51	1.45
26	fF	203	PEB	C4B-C3B	2.41	1.49	1.45
28	FB	1001	CYC	OB-C4B	2.41	1.28	1.23
26	Z7	201	PEB	C1A-NA	-2.41	1.34	1.37
26	SE	203	PEB	C2A-C1A	-2.41	1.49	1.52
26	S8	201	PEB	OD-C4D	2.41	1.28	1.23
28	MH	1001	CYC	C4A-C3A	2.41	1.51	1.45
26	U3	202	PEB	C4A-NA	-2.41	1.32	1.37
26	X3	203	PEB	OD-C4D	2.41	1.28	1.23
26	QA	203	PEB	C2A-C1A	-2.41	1.49	1.52
26	cG	203	PEB	C1B-C2B	2.41	1.51	1.45
28	VH	1001	CYC	C4A-C3A	2.41	1.51	1.45
26	YB	201	PEB	C4A-NA	-2.41	1.32	1.37
26	C4	202	PEB	C4B-C3B	2.41	1.49	1.45
26	lG	202	PEB	C4B-C3B	2.41	1.49	1.45
28	EB	1001	CYC	C1D-CHD	2.41	1.50	1.41
26	F5	201	PEB	C4A-NA	-2.41	1.32	1.37
26	11	202	PEB	C1C-CHB	2.41	1.50	1.41
26	c2	201	PEB	C2A-C1A	-2.41	1.49	1.52
26	f6	202	PEB	C2A-C1A	-2.41	1.49	1.52
26	BE	202	PEB	C2A-C1A	-2.41	1.49	1.52
26	SG	201	PEB	C2A-C1A	-2.41	1.49	1.52
26	G5	201	PEB	C4A-NA	-2.41	1.32	1.37
26	k2	202	PEB	C4B-C3B	2.41	1.49	1.45
26	R8	202	PEB	C1B-C2B	2.41	1.51	1.45
26	UB	202	PEB	C4A-NA	-2.41	1.32	1.37
26	WI	201	PEB	C4A-NA	-2.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	fH	1001	CYC	C4A-C3A	2.41	1.51	1.45
26	d4	202	PEB	C4B-C3B	2.41	1.49	1.45
26	oE	201	PEB	C2A-C1A	-2.41	1.49	1.52
26	zG	501	PEB	OD-C4D	2.41	1.28	1.23
28	IB	1001	CYC	C4B-NB	-2.41	1.32	1.38
26	IE	201	PEB	C4A-NA	-2.41	1.32	1.37
26	FG	202	PEB	C4A-NA	-2.41	1.32	1.37
26	sG	203	PEB	C1C-CHB	2.41	1.50	1.41
26	ME	203	PEB	C1D-ND	2.41	1.49	1.45
26	w4	203	PEB	C4B-C3B	2.41	1.49	1.45
26	D9	202	PEB	C4A-NA	-2.40	1.32	1.37
26	C5	202	PEB	C4B-C3B	2.40	1.49	1.45
26	PD	201	PEB	OD-C4D	2.40	1.28	1.23
26	uG	202	PEB	C1D-ND	2.40	1.49	1.45
26	LF	1002	PEB	OD-C4D	2.40	1.28	1.23
26	UG	201	PEB	CMB-C2B	-2.40	1.45	1.50
28	YH	1003	CYC	C4A-C3A	2.40	1.51	1.45
26	CJ	201	PEB	C4A-NA	-2.40	1.32	1.37
26	S8	201	PEB	C4A-NA	-2.40	1.32	1.37
26	RG	202	PEB	C4A-NA	-2.40	1.32	1.37
26	P9	202	PEB	C1B-C2B	2.40	1.51	1.45
26	lF	203	PEB	C2A-C1A	-2.40	1.49	1.52
26	M8	203	PEB	C4A-NA	-2.40	1.32	1.37
26	jI	201	PEB	C4A-NA	-2.40	1.32	1.37
26	VD	201	PEB	C2A-C1A	-2.40	1.49	1.52
26	c7	202	PEB	C1B-C2B	2.40	1.51	1.45
26	jG	201	PEB	C1A-NA	-2.40	1.34	1.37
26	a6	201	PEB	C4A-NA	-2.40	1.32	1.37
26	Y8	201	PEB	OD-C4D	2.40	1.28	1.23
26	XD	201	PEB	OD-C4D	2.40	1.28	1.23
26	GA	203	PEB	C2A-C1A	-2.40	1.49	1.52
26	HG	201	PEB	OD-C4D	2.40	1.28	1.23
28	lH	1001	CYC	C4A-C3A	2.40	1.51	1.45
28	L2	1001	CYC	C4C-NC	-2.40	1.32	1.37
26	RF	201	PEB	C4B-C3B	2.40	1.49	1.45
26	PJ	202	PEB	C4A-NA	-2.40	1.32	1.37
28	I2	1001	CYC	C4C-NC	-2.40	1.32	1.37
26	KB	201	PEB	C4A-NA	-2.40	1.32	1.37
28	N2	1001	CYC	C4C-NC	-2.40	1.32	1.37
28	dH	1001	CYC	C4D-CHA	2.40	1.50	1.41
26	TA	202	PEB	OD-C4D	2.40	1.28	1.23
26	k8	202	PEB	C4B-C3B	2.40	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cG	201	PEB	C4B-C3B	2.40	1.49	1.45
26	H5	203	PEB	C4A-NA	-2.40	1.32	1.37
26	SE	202	PEB	OD-C4D	2.40	1.28	1.23
26	U7	201	PEB	C2A-C1A	-2.40	1.49	1.52
26	f1	201	PEB	C2A-C1A	-2.40	1.50	1.52
26	VB	201	PEB	C4B-C3B	2.40	1.49	1.45
26	O1	201	PEB	C4A-NA	-2.40	1.32	1.37
26	T8	202	PEB	OD-C4D	2.40	1.28	1.23
26	LD	202	PEB	C1A-NA	-2.39	1.34	1.37
26	PJ	201	PEB	C1D-ND	2.39	1.49	1.45
26	H9	202	PEB	C4A-NA	-2.39	1.32	1.37
26	V8	202	PEB	C4B-C3B	2.39	1.49	1.45
26	YI	203	PEB	C4B-C3B	2.39	1.49	1.45
26	GG	201	PEB	C2C-C3C	2.39	1.44	1.37
26	kB	201	PEB	C4B-C3B	2.39	1.49	1.45
26	U8	201	PEB	C4A-NA	-2.39	1.32	1.37
26	RD	202	PEB	C2A-C1A	-2.39	1.50	1.52
26	L5	203	PEB	C4A-NA	-2.39	1.32	1.37
26	cA	201	PEB	C4B-C3B	2.39	1.49	1.45
26	C3	201	PEB	C4A-NA	-2.39	1.32	1.37
26	MA	203	PEB	C4A-NA	-2.39	1.32	1.37
26	JD	202	PEB	C4B-C3B	2.39	1.49	1.45
26	X4	201	PEB	OD-C4D	2.39	1.28	1.23
26	Z1	202	PEB	C2A-C1A	-2.39	1.50	1.52
26	e3	401	PEB	C2A-C1A	-2.39	1.50	1.52
26	dA	201	PEB	C2A-C1A	-2.39	1.50	1.52
26	14	202	PEB	C1C-CHB	2.39	1.50	1.41
26	X3	201	PEB	OD-C4D	2.39	1.28	1.23
26	H6	1002	PEB	OD-C4D	2.39	1.28	1.23
26	K8	202	PEB	C2A-C1A	-2.39	1.50	1.52
26	U8	203	PEB	C4A-NA	-2.39	1.32	1.37
26	S8	203	PEB	OD-C4D	2.39	1.28	1.23
26	CC	203	PEB	C4B-C3B	2.39	1.49	1.45
26	D3	202	PEB	C1A-NA	-2.39	1.34	1.37
28	I7	1001	CYC	C1B-NB	-2.39	1.33	1.37
26	21	404	PEB	C2A-C1A	-2.39	1.50	1.52
26	IE	201	PEB	C2A-C1A	2.39	1.54	1.52
28	DI	1001	CYC	C4B-NB	-2.39	1.32	1.38
26	mG	201	PEB	C4B-NB	-2.39	1.33	1.38
26	VG	201	PEB	C1A-NA	-2.39	1.34	1.37
26	LC	201	PEB	C4A-NA	-2.39	1.32	1.37
26	cE	201	PEB	C4A-NA	-2.39	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V3	201	PEB	C2A-C1A	-2.39	1.50	1.52
26	aE	201	PEB	C1C-CHB	2.39	1.50	1.41
26	V1	203	PEB	CHC-C4C	2.39	1.56	1.50
26	c8	202	PEB	C4B-C3B	2.39	1.49	1.45
26	T3	203	PEB	OD-C4D	2.39	1.28	1.23
26	Y2	203	PEB	C4B-C3B	2.39	1.49	1.45
26	k6	201	PEB	C4B-C3B	2.39	1.49	1.45
26	cI	203	PEB	C4B-C3B	2.39	1.49	1.45
26	KG	202	PEB	C4A-NA	-2.39	1.32	1.37
26	m6	203	PEB	C4B-C3B	2.39	1.49	1.45
26	RI	201	PEB	C4A-NA	-2.39	1.32	1.37
26	c4	203	PEB	C4B-C3B	2.38	1.49	1.45
26	O6	202	PEB	C2A-C1A	-2.38	1.50	1.52
28	K6	202	CYC	C1B-NB	-2.38	1.33	1.37
26	V9	203	PEB	C4B-NB	-2.38	1.33	1.38
28	G6	1001	CYC	C4C-NC	-2.38	1.32	1.37
26	Y1	202	PEB	C4A-NA	-2.38	1.32	1.37
26	mE	203	PEB	C1B-C2B	2.38	1.50	1.45
26	RB	201	PEB	C4A-NA	-2.38	1.32	1.37
26	JD	203	PEB	C2A-C1A	-2.38	1.50	1.52
26	qG	203	PEB	C2A-C1A	-2.38	1.50	1.52
26	I9	201	PEB	CAC-C2C	2.38	1.55	1.52
28	1H	1000	CYC	C4A-C3A	2.38	1.50	1.45
26	I5	202	PEB	C4A-NA	-2.38	1.32	1.37
26	GC	201	PEB	C4A-NA	-2.38	1.32	1.37
26	Z8	201	PEB	OD-C4D	2.38	1.28	1.23
26	SA	203	PEB	OD-C4D	2.38	1.28	1.23
28	iH	1001	CYC	OB-C4B	2.38	1.28	1.23
26	QI	202	PEB	C3C-C4C	-2.38	1.38	1.42
26	QJ	202	PEB	C4A-NA	-2.38	1.32	1.37
26	m4	202	PEB	C4B-C3B	2.38	1.49	1.45
27	YD	302	PUB	C4C-NC	2.38	1.39	1.35
26	PJ	201	PEB	C1C-CHB	2.38	1.50	1.41
27	N9	201	PUB	C4C-NC	2.38	1.39	1.35
26	K1	202	PEB	C4A-NA	-2.38	1.32	1.37
26	II	202	PEB	C1D-ND	2.38	1.49	1.45
26	R6	201	PEB	C4A-NA	-2.38	1.32	1.37
26	D8	201	PEB	C4A-NA	-2.38	1.32	1.37
26	V6	201	PEB	C4B-C3B	2.38	1.49	1.45
26	k7	201	PEB	C4B-C3B	2.38	1.49	1.45
28	HI	1001	CYC	C1D-CHD	2.38	1.50	1.41
26	fF	203	PEB	C1C-CHB	2.38	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	E2	1001	CYC	C1B-NB	-2.38	1.33	1.37
26	f4	201	PEB	C2A-C1A	-2.38	1.50	1.52
26	Q8	203	PEB	C2A-C1A	-2.38	1.50	1.52
26	S3	201	PEB	C4B-NB	-2.38	1.33	1.38
26	JE	201	PEB	C4B-C3B	2.38	1.49	1.45
26	HD	202	PEB	C1A-NA	-2.38	1.34	1.37
26	H9	202	PEB	OD-C4D	2.38	1.28	1.23
28	vH	1001	CYC	OB-C4B	2.38	1.28	1.23
26	mI	203	PEB	C2A-C1A	-2.38	1.50	1.52
28	EI	1001	CYC	C1B-NB	-2.38	1.33	1.37
26	PJ	203	PEB	C4A-NA	-2.38	1.32	1.37
28	AH	1001	CYC	OB-C4B	2.38	1.28	1.23
26	i6	202	PEB	C2A-C1A	-2.38	1.50	1.52
26	f7	203	PEB	C2A-C1A	-2.38	1.50	1.52
26	T6	202	PEB	C4A-NA	-2.37	1.32	1.37
28	C2	1001	CYC	OB-C4B	2.37	1.28	1.23
26	ED	201	PEB	C1C-CHB	2.37	1.50	1.41
26	SA	202	PEB	C2A-C1A	-2.37	1.50	1.52
26	cA	202	PEB	C2A-C1A	-2.37	1.50	1.52
26	fI	202	PEB	C2A-C1A	-2.37	1.50	1.52
26	VI	202	PEB	C4A-NA	-2.37	1.32	1.37
28	IB	1001	CYC	C1B-NB	-2.37	1.33	1.37
26	VE	201	PEB	C4B-C3B	2.37	1.49	1.45
26	h6	202	PEB	C2A-C1A	-2.37	1.50	1.52
26	fF	203	PEB	C2A-C1A	-2.37	1.50	1.52
26	BJ	203	PEB	OD-C4D	2.37	1.28	1.23
26	W4	201	PEB	C4A-NA	-2.37	1.32	1.37
26	hI	201	PEB	C4A-NA	-2.37	1.32	1.37
26	OD	201	PEB	C4B-NB	-2.37	1.33	1.38
26	EJ	202	PEB	C4A-NA	-2.37	1.32	1.37
26	C8	201	PEB	C4A-NA	-2.37	1.32	1.37
26	S6	202	PEB	C3C-C4C	-2.37	1.38	1.42
26	HC	201	PEB	OD-C4D	2.37	1.28	1.23
26	KG	202	PEB	OD-C4D	2.37	1.28	1.23
26	UE	201	PEB	C4A-NA	-2.37	1.32	1.37
26	B5	202	PEB	C2A-C1A	-2.37	1.50	1.52
26	H5	203	PEB	OD-C4D	2.37	1.28	1.23
26	G5	202	PEB	C4A-NA	-2.37	1.32	1.37
26	uG	202	PEB	C1B-C2B	2.37	1.50	1.45
26	TF	201	PEB	C4A-NA	-2.37	1.32	1.37
26	SG	201	PEB	C4A-NA	-2.37	1.32	1.37
28	C7	1001	CYC	C1B-C2B	2.37	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d4	201	PEB	C2A-C1A	-2.37	1.50	1.52
26	Q4	202	PEB	C4A-NA	-2.37	1.32	1.37
26	SE	201	PEB	C4A-NA	-2.37	1.32	1.37
26	fB	203	PEB	C1C-CHB	2.37	1.50	1.41
28	D7	1001	CYC	C1B-C2B	2.37	1.49	1.45
26	gE	201	PEB	C1B-C2B	2.37	1.50	1.45
26	a6	202	PEB	C2A-C1A	-2.37	1.50	1.52
26	JC	202	PEB	C4A-NA	-2.37	1.32	1.37
26	WG	203	PEB	C4B-C3B	2.37	1.49	1.45
26	K8	202	PEB	OD-C4D	2.37	1.28	1.23
26	Y6	201	PEB	C4A-NA	-2.37	1.32	1.37
26	QF	203	PEB	C2A-C1A	-2.37	1.50	1.52
26	G1	202	PEB	C4B-C3B	2.37	1.49	1.45
26	i1	203	PEB	C4B-C3B	2.37	1.49	1.45
26	cE	203	PEB	C1C-CHB	2.37	1.50	1.41
26	f7	203	PEB	C1C-CHB	2.37	1.50	1.41
26	gG	203	PEB	C4A-NA	-2.37	1.32	1.37
26	xE	302	PEB	C4B-C3B	2.37	1.49	1.45
26	bE	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	K3	201	PEB	C4A-NA	-2.36	1.32	1.37
28	KB	202	CYC	C1B-NB	-2.36	1.33	1.37
26	dA	201	PEB	C4A-NA	-2.36	1.32	1.37
26	RD	203	PEB	C4A-NA	-2.36	1.32	1.37
28	IB	1001	CYC	OB-C4B	2.36	1.28	1.23
26	CE	201	PEB	C4A-NA	-2.36	1.32	1.37
26	g7	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	LE	201	PEB	C4B-C3B	2.36	1.49	1.45
26	bB	202	PEB	C1C-CHB	2.36	1.50	1.41
26	I9	202	PEB	C4A-NA	-2.36	1.32	1.37
26	KD	202	PEB	C1D-ND	2.36	1.49	1.45
26	w1	202	PEB	C1C-CHB	2.36	1.50	1.41
28	TH	1001	CYC	C4B-NB	-2.36	1.33	1.38
26	aA	204	PEB	C4A-NA	-2.36	1.32	1.37
26	dB	204	PEB	C4A-NA	-2.36	1.32	1.37
26	l2	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	v4	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	s1	203	PEB	C4B-C3B	2.36	1.49	1.45
26	v4	201	PEB	C4B-C3B	2.36	1.49	1.45
26	fA	203	PEB	C4B-C3B	2.36	1.49	1.45
28	HF	1001	CYC	C4B-NB	-2.36	1.33	1.38
26	BA	301	PEB	C4A-NA	-2.36	1.32	1.37
28	C6	1001	CYC	C1B-NB	-2.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	OD	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	eE	201	PEB	C4B-C3B	2.36	1.49	1.45
28	FI	1001	CYC	C1D-CHD	2.36	1.50	1.41
26	XA	201	PEB	C4A-NA	-2.36	1.32	1.37
26	i2	203	PEB	C4B-C3B	2.36	1.49	1.45
26	B8	301	PEB	C4A-NA	-2.36	1.32	1.37
28	I7	1001	CYC	C4C-NC	-2.36	1.32	1.37
26	gI	203	PEB	C2A-C1A	-2.36	1.50	1.52
28	cH	1001	CYC	OB-C4B	2.36	1.28	1.23
26	X8	201	PEB	C4A-NA	-2.36	1.32	1.37
28	I6	1001	CYC	C1B-NB	-2.36	1.33	1.37
26	Q1	202	PEB	C4A-NA	-2.36	1.32	1.37
26	UF	202	PEB	C4A-NA	-2.36	1.32	1.37
26	11	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	R9	201	PEB	C2A-C1A	-2.36	1.50	1.52
26	eE	203	PEB	C2A-C1A	-2.36	1.50	1.52
26	UA	201	PEB	C4A-NA	-2.36	1.32	1.37
26	OD	202	PEB	C4A-NA	-2.36	1.32	1.37
26	L4	202	PEB	C4B-C3B	2.36	1.49	1.45
28	D2	1001	CYC	C4B-NB	-2.36	1.33	1.38
26	e8	201	PEB	C4A-NA	-2.36	1.32	1.37
26	T2	202	PEB	C1C-CHB	2.36	1.50	1.41
26	11	201	PEB	C2A-C1A	-2.36	1.50	1.52
26	FJ	201	PEB	C4A-NA	-2.36	1.32	1.37
28	E6	1001	CYC	C1B-NB	-2.36	1.33	1.37
26	tE	201	PEB	C4B-C3B	2.36	1.49	1.45
28	gH	1001	CYC	OB-C4B	2.36	1.28	1.23
26	j8	201	PEB	C4A-NA	-2.36	1.32	1.37
26	C9	201	PEB	C4A-NA	-2.36	1.32	1.37
26	OE	202	PEB	C4A-NA	-2.36	1.32	1.37
26	OB	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	AI	305	PEB	C2A-C1A	-2.36	1.50	1.52
26	VA	201	PEB	C4A-NA	-2.36	1.32	1.37
28	J2	1001	CYC	C1A-NA	-2.36	1.33	1.38
26	R7	202	PEB	C4B-C3B	2.36	1.49	1.45
26	HC	201	PEB	C4A-NA	-2.36	1.32	1.37
28	lH	1001	CYC	OB-C4B	2.36	1.28	1.23
26	m4	202	PEB	C2A-C1A	-2.36	1.50	1.52
26	dI	201	PEB	C2A-C1A	-2.36	1.50	1.52
26	hF	203	PEB	C3C-C4C	-2.36	1.38	1.42
28	vH	1001	CYC	C4A-C3A	2.36	1.50	1.45
26	kI	203	PEB	C3C-C4C	-2.36	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H2	1001	CYC	C1D-CHD	2.36	1.50	1.41
26	TE	202	PEB	C4A-NA	-2.35	1.32	1.37
26	NB	1002	PEB	C4A-NA	-2.35	1.32	1.37
26	24	404	PEB	C2A-C1A	-2.35	1.50	1.52
26	KA	203	PEB	C2C-C3C	2.35	1.44	1.37
26	KG	203	PEB	C4A-NA	-2.35	1.32	1.37
26	K8	203	PEB	C2C-C3C	2.35	1.44	1.37
26	K1	201	PEB	C2A-C1A	-2.35	1.50	1.52
26	H1	202	PEB	C4B-C3B	2.35	1.49	1.45
26	nE	202	PEB	C4B-C3B	2.35	1.49	1.45
26	eA	201	PEB	C4A-NA	-2.35	1.32	1.37
26	qG	203	PEB	C1D-ND	2.35	1.49	1.45
26	TA	202	PEB	C4A-NA	-2.35	1.32	1.37
26	OF	201	PEB	C2A-C1A	-2.35	1.50	1.52
26	bF	203	PEB	C2A-C1A	-2.35	1.50	1.52
27	wE	304	PUB	CHC-C4C	2.35	1.53	1.50
26	O7	201	PEB	C4B-C3B	2.35	1.49	1.45
26	O1	202	PEB	C2A-C1A	-2.35	1.50	1.52
26	v1	201	PEB	C2A-C1A	-2.35	1.50	1.52
26	d6	203	PEB	C2A-C1A	-2.35	1.50	1.52
26	OA	203	PEB	C4A-NA	-2.35	1.32	1.37
26	VB	202	PEB	C4A-NA	-2.35	1.32	1.37
26	GE	203	PEB	C4A-NA	-2.35	1.32	1.37
26	i7	202	PEB	C1B-C2B	2.35	1.50	1.45
26	mG	201	PEB	C4B-C3B	2.35	1.49	1.45
26	N9	202	PEB	C2A-C1A	-2.35	1.50	1.52
26	FD	202	PEB	C2A-C1A	-2.35	1.50	1.52
26	fG	202	PEB	C2A-C1A	-2.35	1.50	1.52
26	TJ	201	PEB	C2A-C1A	-2.35	1.50	1.52
26	G6	1002	PEB	C4A-NA	-2.35	1.32	1.37
26	N6	201	PEB	C4A-NA	-2.35	1.32	1.37
26	21	405	PEB	C4B-C3B	2.35	1.49	1.45
26	eG	202	PEB	C4A-NA	-2.35	1.32	1.37
28	K2	1001	CYC	C4C-NC	-2.35	1.32	1.37
28	KI	1001	CYC	C4C-NC	-2.35	1.32	1.37
28	KI	1001	CYC	C1B-NB	-2.35	1.33	1.37
26	A7	301	PEB	C2A-C1A	-2.35	1.50	1.52
26	OI	202	PEB	C2A-C1A	-2.35	1.50	1.52
26	E3	201	PEB	OD-C4D	2.35	1.28	1.23
27	AF	303	PUB	C4B-CHB	2.35	1.50	1.41
28	1H	1000	CYC	C1D-CHD	2.35	1.50	1.41
26	YA	202	PEB	C4A-NA	-2.35	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J4	202	PEB	C4B-C3B	2.35	1.49	1.45
26	sE	202	PEB	C1B-C2B	2.35	1.50	1.45
28	JF	1003	CYC	C1B-C2B	2.35	1.49	1.45
26	T2	202	PEB	C4A-NA	-2.35	1.32	1.37
26	Y4	202	PEB	C4A-NA	-2.35	1.32	1.37
26	PA	202	PEB	C4A-NA	-2.35	1.32	1.37
26	OB	201	PEB	C4A-NA	-2.35	1.32	1.37
28	CB	1001	CYC	C1B-NB	-2.35	1.33	1.37
27	yG	302	PUB	OD-C4D	2.35	1.28	1.23
26	V3	202	PEB	C1A-NA	-2.35	1.34	1.37
26	KE	201	PEB	C4B-NB	-2.35	1.33	1.38
26	iI	203	PEB	C2A-C1A	-2.35	1.50	1.52
26	V4	203	PEB	CHC-C4C	2.35	1.56	1.50
26	l2	201	PEB	C4A-NA	-2.35	1.32	1.37
26	RI	202	PEB	C4A-NA	-2.35	1.32	1.37
26	P8	201	PEB	C4A-NA	-2.34	1.32	1.37
28	H2	1001	CYC	C4C-NC	-2.34	1.32	1.37
26	mB	201	PEB	C2A-C1A	-2.34	1.50	1.52
26	L6	1002	PEB	OD-C4D	2.34	1.28	1.23
28	HI	1001	CYC	C1B-NB	-2.34	1.33	1.37
26	gE	203	PEB	C4A-NA	-2.34	1.32	1.37
28	CF	1001	CYC	C1D-CHD	2.34	1.50	1.41
26	W3	202	PEB	C1D-ND	2.34	1.49	1.45
26	J3	201	PEB	C2A-C1A	-2.34	1.50	1.52
26	SD	202	PEB	C2A-C1A	-2.34	1.50	1.52
26	DA	201	PEB	C4A-NA	-2.34	1.32	1.37
26	v1	201	PEB	C4B-C3B	2.34	1.49	1.45
26	d2	201	PEB	C4A-NA	-2.34	1.32	1.37
28	K7	1001	CYC	C1D-CHD	2.34	1.50	1.41
28	MB	1001	CYC	C4B-NB	-2.34	1.33	1.38
26	G4	202	PEB	C4B-C3B	2.34	1.49	1.45
26	q4	201	PEB	C4B-C3B	2.34	1.49	1.45
28	CH	1001	CYC	C4B-NB	-2.34	1.33	1.38
26	K3	201	PEB	C2A-C1A	-2.34	1.50	1.52
26	PG	202	PEB	C2A-C1A	-2.34	1.50	1.52
26	V8	201	PEB	C4A-NA	-2.34	1.32	1.37
26	P4	202	PEB	OD-C4D	2.34	1.28	1.23
26	S1	202	PEB	C4A-NA	-2.34	1.32	1.37
26	GB	1002	PEB	C4A-NA	-2.34	1.32	1.37
28	JF	1001	CYC	C4C-NC	-2.34	1.32	1.37
26	OE	201	PEB	C4B-C3B	2.34	1.49	1.45
28	HI	1001	CYC	C4C-NC	-2.34	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	GH	1001	CYC	C4B-NB	-2.34	1.33	1.38
28	NF	1001	CYC	C4C-NC	-2.34	1.32	1.37
26	eF	202	PEB	C2A-C1A	-2.34	1.50	1.52
26	R3	202	PEB	CHA-C1B	2.34	1.45	1.40
28	DI	1001	CYC	C1D-CHD	2.34	1.50	1.41
28	PH	1001	CYC	C4B-NB	-2.34	1.33	1.38
26	X1	201	PEB	C4A-NA	-2.34	1.32	1.37
26	W4	202	PEB	C4A-NA	-2.34	1.32	1.37
28	CI	1001	CYC	C1B-NB	-2.34	1.33	1.37
26	S7	201	PEB	C4A-NA	-2.34	1.32	1.37
28	DB	1001	CYC	C4B-NB	-2.34	1.33	1.38
26	F8	202	PEB	C4A-NA	-2.34	1.32	1.37
26	jA	203	PEB	C2A-C1A	-2.34	1.50	1.52
26	h7	203	PEB	C4B-C3B	2.34	1.49	1.45
26	dG	202	PEB	C4A-NA	-2.34	1.32	1.37
26	O7	202	PEB	C4B-C3B	2.33	1.49	1.45
26	e1	202	PEB	C1C-CHB	2.33	1.50	1.41
26	W6	203	PEB	C4A-NA	-2.33	1.32	1.37
26	ZF	202	PEB	C4A-NA	-2.33	1.32	1.37
28	pH	1001	CYC	C4A-C3A	2.33	1.50	1.45
26	L4	202	PEB	C2A-C1A	-2.33	1.50	1.52
26	AG	202	PEB	C2A-C1A	-2.33	1.50	1.52
26	V6	202	PEB	C4A-NA	-2.33	1.32	1.37
26	d1	202	PEB	C2A-C1A	-2.33	1.50	1.52
26	WF	203	PEB	C2A-C1A	-2.33	1.50	1.52
28	II	1001	CYC	C4C-NC	-2.33	1.32	1.37
26	qE	203	PEB	C1D-ND	2.33	1.49	1.45
26	vG	202	PEB	C4B-C3B	2.33	1.49	1.45
28	D2	1001	CYC	C4C-NC	-2.33	1.32	1.37
28	jH	1001	CYC	C4A-C3A	2.33	1.50	1.45
26	WF	203	PEB	C4A-NA	-2.33	1.32	1.37
26	q1	201	PEB	C2A-C1A	-2.33	1.50	1.52
26	H4	201	PEB	C2A-C1A	-2.33	1.50	1.52
26	IG	203	PEB	C2C-C3C	2.33	1.44	1.37
26	SG	202	PEB	C4A-NA	-2.33	1.32	1.37
26	L8	202	PEB	C1B-C2B	2.33	1.50	1.45
28	HF	1001	CYC	C1B-C2B	2.33	1.49	1.45
26	B5	202	PEB	C4A-NA	-2.33	1.32	1.37
26	EJ	201	PEB	C4A-NA	-2.33	1.32	1.37
26	CD	202	PEB	C3C-C4C	-2.33	1.38	1.42
28	NF	1001	CYC	C1D-CHD	2.33	1.50	1.41
26	V2	202	PEB	C4A-NA	-2.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S3	202	PEB	C4A-NA	-2.33	1.32	1.37
26	TB	202	PEB	C4A-NA	-2.33	1.32	1.37
26	fG	202	PEB	C4A-NA	-2.33	1.32	1.37
26	sE	202	PEB	C2A-C1A	-2.33	1.50	1.52
26	S4	201	PEB	C4A-NA	-2.33	1.32	1.37
26	U4	201	PEB	C4A-NA	-2.33	1.32	1.37
26	X4	201	PEB	C4A-NA	-2.33	1.32	1.37
28	WH	1001	CYC	C4A-C3A	2.33	1.50	1.45
28	LF	1001	CYC	CBA-CGA	2.33	1.56	1.50
28	KH	1001	CYC	OB-C4B	2.33	1.28	1.23
26	mB	203	PEB	C4B-C3B	2.33	1.49	1.45
26	oG	201	PEB	C4B-C3B	2.33	1.49	1.45
26	R3	202	PEB	C1A-NA	-2.33	1.34	1.37
26	gA	201	PEB	C1B-C2B	2.33	1.50	1.45
26	d8	203	PEB	C3C-C4C	-2.33	1.38	1.42
26	dB	204	PEB	C2A-C1A	-2.33	1.50	1.52
26	hB	203	PEB	C2A-C1A	-2.33	1.50	1.52
26	ND	202	PEB	C2A-C1A	-2.33	1.50	1.52
26	MG	203	PEB	C2A-C1A	-2.33	1.50	1.52
26	fl	201	PEB	C2A-C1A	-2.33	1.50	1.52
28	FI	1001	CYC	C4B-NB	-2.33	1.33	1.38
26	OF	201	PEB	C1C-CHB	2.33	1.50	1.41
26	k2	202	PEB	OD-C4D	2.33	1.28	1.23
26	UG	201	PEB	OD-C4D	2.33	1.28	1.23
26	mG	201	PEB	C1C-CHB	2.33	1.50	1.41
26	FD	203	PEB	C4B-C3B	2.33	1.49	1.45
28	F2	1001	CYC	C1D-CHD	2.33	1.50	1.41
28	YH	1004	CYC	C1D-CHD	2.33	1.50	1.41
26	iE	201	PEB	C1C-CHB	2.33	1.50	1.41
26	a1	202	PEB	C4B-C3B	2.33	1.49	1.45
26	eG	201	PEB	CHA-C4A	-2.33	1.32	1.36
28	J2	1001	CYC	C4C-NC	-2.33	1.32	1.37
26	D4	202	PEB	C2A-C1A	-2.33	1.50	1.52
28	E7	1001	CYC	C1B-C2B	2.33	1.49	1.45
26	N1	201	PEB	C1B-C2B	2.32	1.50	1.45
26	iE	201	PEB	OD-C4D	2.32	1.28	1.23
26	LC	202	PEB	C4A-NA	-2.32	1.32	1.37
28	yH	1001	CYC	C4A-C3A	2.32	1.50	1.45
26	J9	203	PEB	C1D-ND	2.32	1.49	1.45
28	D6	1001	CYC	OB-C4B	2.32	1.28	1.23
26	f8	203	PEB	C4B-C3B	2.32	1.49	1.45
26	lF	202	PEB	C2A-C1A	-2.32	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	SG	202	PEB	OD-C4D	2.32	1.28	1.23
26	bF	201	PEB	C1D-ND	2.32	1.49	1.45
27	AA	303	PUB	CHC-C4C	2.32	1.53	1.50
26	AC	202	PEB	C4B-C3B	2.32	1.49	1.45
26	II	202	PEB	C2A-C1A	-2.32	1.50	1.52
26	dF	202	PEB	C1C-CHB	2.32	1.50	1.41
26	w4	202	PEB	C1C-CHB	2.32	1.50	1.41
26	a2	202	PEB	C4A-NA	-2.32	1.32	1.37
26	PD	201	PEB	C4A-NA	-2.32	1.32	1.37
28	E2	1001	CYC	C4B-NB	-2.32	1.33	1.38
26	s1	203	PEB	C2A-C1A	-2.32	1.50	1.52
26	L9	203	PEB	C2A-C1A	-2.32	1.50	1.52
26	CG	203	PEB	C2A-C1A	-2.32	1.50	1.52
26	W1	202	PEB	C4A-NA	-2.32	1.32	1.37
26	I8	203	PEB	C4A-NA	-2.32	1.32	1.37
26	HJ	201	PEB	C4A-NA	-2.32	1.32	1.37
26	cE	202	PEB	C4B-C3B	2.32	1.49	1.45
26	ZG	201	PEB	C4B-C3B	2.32	1.49	1.45
26	j2	201	PEB	C4A-NA	-2.32	1.32	1.37
26	cG	203	PEB	C2A-C1A	-2.32	1.50	1.52
26	mF	202	PEB	C4B-C3B	2.32	1.49	1.45
26	y1	203	PEB	C4A-NA	-2.32	1.32	1.37
26	XG	201	PEB	C4B-C3B	2.32	1.49	1.45
26	B3	202	PEB	C1C-CHB	2.32	1.50	1.41
26	N3	202	PEB	C2A-C1A	-2.32	1.50	1.52
26	v4	201	PEB	C2A-C1A	-2.32	1.50	1.52
26	O6	201	PEB	C4A-NA	-2.32	1.32	1.37
26	AB	304	PEB	C4A-NA	-2.32	1.32	1.37
26	hB	201	PEB	C1D-ND	2.32	1.49	1.45
26	MD	201	PEB	C4A-NA	-2.32	1.32	1.37
26	LC	202	PEB	C2A-C1A	-2.32	1.50	1.52
26	jF	201	PEB	C4A-NA	-2.32	1.32	1.37
28	K6	202	CYC	C1B-C2B	2.32	1.49	1.45
28	CF	1001	CYC	C1B-C2B	2.32	1.49	1.45
26	mG	201	PEB	C1D-ND	2.32	1.49	1.45
26	V2	202	PEB	OD-C4D	2.32	1.28	1.23
26	Q6	202	PEB	C4A-NA	-2.32	1.32	1.37
28	NI	1001	CYC	C4C-NC	-2.32	1.32	1.37
26	R9	202	PEB	C2A-C1A	-2.32	1.50	1.52
26	WJ	201	PEB	C2A-C1A	-2.32	1.50	1.52
26	oE	201	PEB	C4B-C3B	2.32	1.49	1.45
26	J2	1002	PEB	C4A-NA	-2.32	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a8	204	PEB	C4A-NA	-2.32	1.32	1.37
26	aI	201	PEB	C4A-NA	-2.32	1.32	1.37
28	EH	1001	CYC	OB-C4B	2.32	1.28	1.23
26	sE	203	PEB	C2A-C1A	-2.32	1.50	1.52
26	WG	201	PEB	C2A-C1A	-2.32	1.50	1.52
26	WA	203	PEB	C2C-C3C	2.32	1.44	1.37
26	u4	203	PEB	C4B-C3B	2.32	1.49	1.45
26	G9	201	PEB	C4B-C3B	2.32	1.49	1.45
26	eB	201	PEB	C4A-NA	-2.31	1.32	1.37
26	j7	203	PEB	C4B-C3B	2.31	1.49	1.45
26	iG	203	PEB	C2A-C1A	-2.31	1.50	1.52
26	FE	202	PEB	C4A-NA	-2.31	1.32	1.37
26	RE	202	PEB	C4A-NA	-2.31	1.32	1.37
26	T9	201	PEB	C1C-CHB	2.31	1.50	1.41
26	O2	201	PEB	C4A-NA	-2.31	1.32	1.37
26	WB	203	PEB	C4A-NA	-2.31	1.32	1.37
28	DF	1001	CYC	C1D-CHD	2.31	1.50	1.41
26	HJ	203	PEB	C2A-C1A	-2.31	1.50	1.52
26	e6	201	PEB	C4A-NA	-2.31	1.32	1.37
26	F9	201	PEB	C4A-NA	-2.31	1.32	1.37
26	CA	201	PEB	C4A-NA	-2.31	1.32	1.37
26	y4	201	PEB	C4A-NA	-2.31	1.32	1.37
26	I8	201	PEB	C4A-NA	-2.31	1.32	1.37
26	P9	202	PEB	C4A-NA	-2.31	1.32	1.37
26	U3	201	PEB	C4B-NB	-2.31	1.33	1.38
26	CC	202	PEB	C4B-C3B	2.31	1.49	1.45
26	Y8	202	PEB	C4A-NA	-2.31	1.32	1.37
26	KG	201	PEB	C4A-NA	-2.31	1.32	1.37
26	e7	202	PEB	C1D-ND	2.31	1.49	1.45
26	RD	202	PEB	C4B-C3B	2.31	1.49	1.45
26	VD	202	PEB	C1A-NA	-2.31	1.34	1.37
26	P9	203	PEB	C4A-NA	-2.31	1.32	1.37
26	FA	202	PEB	C4A-NA	-2.31	1.32	1.37
26	H1	202	PEB	C2A-C1A	-2.31	1.50	1.52
26	u4	202	PEB	C2A-C1A	-2.31	1.50	1.52
26	OG	201	PEB	OD-C4D	2.31	1.28	1.23
26	II	201	PEB	C4A-NA	-2.31	1.32	1.37
28	RH	1001	CYC	C4A-C3A	2.31	1.50	1.45
26	a2	201	PEB	C4A-NA	-2.31	1.32	1.37
26	NA	201	PEB	C4A-NA	-2.31	1.32	1.37
26	H3	203	PEB	C2A-C1A	-2.31	1.50	1.52
26	fE	202	PEB	C4A-NA	-2.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cE	202	PEB	C1D-ND	2.31	1.49	1.45
26	S1	201	PEB	C4A-NA	-2.31	1.32	1.37
26	W3	201	PEB	C4A-NA	-2.31	1.32	1.37
26	Z4	202	PEB	C4A-NA	-2.31	1.32	1.37
26	IA	201	PEB	C4A-NA	-2.31	1.32	1.37
28	gH	1001	CYC	C4A-C3A	2.31	1.50	1.45
26	uG	201	PEB	C4B-C3B	2.31	1.49	1.45
26	mB	203	PEB	C2A-C1A	-2.31	1.50	1.52
26	SE	201	PEB	C2A-C1A	-2.31	1.50	1.52
26	E8	203	PEB	C4A-NA	-2.31	1.32	1.37
26	W9	202	PEB	C4A-NA	-2.31	1.32	1.37
28	RH	1001	CYC	C4B-NB	-2.31	1.33	1.38
26	WD	202	PEB	C1D-ND	2.31	1.49	1.45
26	K3	201	PEB	C4B-C3B	2.31	1.49	1.45
26	h4	203	PEB	C4A-NA	-2.31	1.32	1.37
26	w4	204	PEB	C4A-NA	-2.31	1.32	1.37
26	E4	202	PEB	C2A-C1A	-2.31	1.50	1.52
28	C7	1001	CYC	C2C-C1C	-2.31	1.50	1.52
28	LH	1001	CYC	C4A-C3A	2.31	1.50	1.45
26	R2	202	PEB	C4A-NA	-2.31	1.32	1.37
26	T8	201	PEB	C4A-NA	-2.31	1.32	1.37
26	ND	203	PEB	C4A-NA	-2.31	1.32	1.37
26	OI	201	PEB	C4A-NA	-2.31	1.32	1.37
26	jI	202	PEB	C1D-ND	2.31	1.49	1.45
28	K7	1001	CYC	C1B-C2B	2.31	1.49	1.45
26	k4	203	PEB	C2A-C1A	-2.31	1.50	1.52
26	iE	203	PEB	C2A-C1A	-2.31	1.50	1.52
26	SJ	202	PEB	C2A-C1A	-2.31	1.50	1.52
26	c6	202	PEB	C4A-NA	-2.31	1.32	1.37
26	DJ	201	PEB	C4A-NA	-2.31	1.32	1.37
26	LJ	201	PEB	C4B-C3B	2.31	1.49	1.45
28	BB	1001	CYC	OB-C4B	2.31	1.28	1.23
26	L8	201	PEB	C4A-NA	-2.30	1.32	1.37
26	cG	203	PEB	C4A-NA	-2.30	1.32	1.37
26	jF	202	PEB	C1D-ND	2.30	1.49	1.45
26	q4	201	PEB	C2A-C1A	-2.30	1.50	1.52
26	YA	202	PEB	OD-C4D	2.30	1.28	1.23
26	A9	304	PEB	C4B-C3B	2.30	1.49	1.45
26	SA	202	PEB	C4A-NA	-2.30	1.32	1.37
26	CD	201	PEB	C4A-NA	-2.30	1.32	1.37
26	OI	202	PEB	C1D-ND	2.30	1.49	1.45
26	T3	202	PEB	C2C-C3C	2.30	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j2	202	PEB	C2A-C1A	-2.30	1.50	1.52
26	oE	202	PEB	C1B-C2B	2.30	1.50	1.45
28	H7	1001	CYC	C4C-NC	-2.30	1.32	1.37
28	DI	1001	CYC	C4C-NC	-2.30	1.32	1.37
26	C5	203	PEB	C4B-C3B	2.30	1.49	1.45
26	JI	1002	PEB	C4A-NA	-2.30	1.32	1.37
26	Y2	203	PEB	C2A-C1A	-2.30	1.50	1.52
26	GA	201	PEB	C1B-C2B	2.30	1.50	1.45
26	J4	201	PEB	C4A-NA	-2.30	1.32	1.37
26	O4	201	PEB	C4A-NA	-2.30	1.32	1.37
26	L9	201	PEB	C1C-CHB	2.30	1.50	1.41
26	W4	201	PEB	OD-C4D	2.30	1.28	1.23
26	e1	202	PEB	C1D-ND	2.30	1.49	1.45
26	F4	202	PEB	C4B-C3B	2.30	1.49	1.45
26	l7	202	PEB	C4B-C3B	2.30	1.49	1.45
26	RF	201	PEB	C4A-NA	-2.30	1.32	1.37
26	ME	203	PEB	C1C-CHB	2.30	1.50	1.41
26	W1	201	PEB	OD-C4D	2.30	1.28	1.23
26	XE	201	PEB	C4B-C3B	2.30	1.49	1.45
26	X1	201	PEB	OD-C4D	2.30	1.28	1.23
26	G8	202	PEB	C2A-C1A	-2.30	1.50	1.52
26	Q9	202	PEB	C2A-C1A	-2.30	1.50	1.52
26	WD	201	PEB	C4A-NA	-2.30	1.32	1.37
26	wG	302	PEB	C4A-NA	-2.30	1.32	1.37
26	M4	401	PEB	C4B-C3B	2.30	1.49	1.45
26	QF	202	PEB	C1B-C2B	2.30	1.50	1.45
26	YA	203	PEB	OD-C4D	2.30	1.28	1.23
26	IC	201	PEB	C4A-NA	-2.30	1.32	1.37
26	C5	201	PEB	C4B-C3B	2.30	1.49	1.45
26	fB	203	PEB	C4B-C3B	2.30	1.49	1.45
26	VF	202	PEB	C4B-C3B	2.30	1.49	1.45
26	N7	1002	PEB	C2A-C1A	-2.30	1.50	1.52
26	uE	203	PEB	C1B-C2B	2.30	1.50	1.45
26	CC	201	PEB	C4B-C3B	2.30	1.49	1.45
26	IC	203	PEB	C4A-NA	-2.30	1.32	1.37
26	G1	201	PEB	C2A-C1A	-2.30	1.50	1.52
26	LC	201	PEB	OD-C4D	2.30	1.28	1.23
28	GH	1001	CYC	C4A-C3A	2.30	1.50	1.45
26	w1	203	PEB	C2A-C1A	-2.30	1.50	1.52
26	b6	202	PEB	C2A-C1A	-2.30	1.50	1.52
26	IE	202	PEB	C2A-C1A	-2.30	1.50	1.52
26	L3	202	PEB	C1A-NA	-2.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	DG	203	PEB	C4A-NA	-2.29	1.32	1.37
26	O8	202	PEB	C4A-NA	-2.29	1.32	1.37
26	O7	201	PEB	C2A-C1A	-2.29	1.50	1.52
26	ED	201	PEB	C2A-C1A	-2.29	1.50	1.52
26	sE	203	PEB	C1C-CHB	2.29	1.50	1.41
26	iE	201	PEB	C4A-NA	-2.29	1.32	1.37
26	gG	201	PEB	C4A-NA	-2.29	1.32	1.37
26	J9	201	PEB	C1D-ND	2.29	1.49	1.45
26	RJ	201	PEB	C1C-CHB	2.29	1.50	1.41
26	SG	201	PEB	OD-C4D	2.29	1.27	1.23
26	O6	202	PEB	C4A-NA	-2.29	1.32	1.37
26	aG	201	PEB	C1C-CHB	2.29	1.50	1.41
26	Y8	202	PEB	OD-C4D	2.29	1.27	1.23
26	M4	402	PEB	C2A-C1A	-2.29	1.50	1.52
26	g4	203	PEB	C2A-C1A	-2.29	1.50	1.52
26	24	401	PEB	C2A-C1A	-2.29	1.50	1.52
26	B3	203	PEB	C4A-NA	-2.29	1.32	1.37
26	FG	201	PEB	OD-C4D	2.29	1.27	1.23
26	fA	201	PEB	C4B-C3B	2.29	1.49	1.45
26	M3	202	PEB	C2A-C1A	-2.29	1.50	1.52
28	qH	1002	CYC	C2C-C1C	-2.29	1.50	1.52
26	oG	203	PEB	C1D-ND	2.29	1.49	1.45
28	KB	202	CYC	C1B-C2B	2.29	1.49	1.45
26	OF	203	PEB	C4A-NA	-2.29	1.32	1.37
26	SD	201	PEB	C4B-NB	-2.29	1.33	1.38
28	KB	202	CYC	C4B-NB	-2.29	1.33	1.38
26	y4	203	PEB	C4A-NA	-2.29	1.32	1.37
26	R9	201	PEB	C1C-CHB	2.29	1.50	1.41
26	IA	203	PEB	C2A-C1A	-2.29	1.50	1.52
26	BC	203	PEB	C2A-C1A	-2.29	1.50	1.52
26	PE	202	PEB	C2A-C1A	-2.29	1.50	1.52
26	sG	203	PEB	C4A-NA	-2.29	1.32	1.37
26	WJ	202	PEB	C1D-ND	2.29	1.49	1.45
26	BD	202	PEB	C1C-CHB	2.29	1.50	1.41
26	WF	203	PEB	C1C-CHB	2.29	1.50	1.41
26	G8	201	PEB	C1B-C2B	2.29	1.50	1.45
26	x1	201	PEB	C2A-C1A	-2.29	1.50	1.52
26	ID	202	PEB	C2A-C1A	-2.29	1.50	1.52
26	gI	201	PEB	C2A-C1A	-2.29	1.50	1.52
26	RJ	202	PEB	C2A-C1A	-2.29	1.50	1.52
26	B5	203	PEB	C4B-C3B	2.29	1.49	1.45
26	UE	203	PEB	C2C-C3C	2.29	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	JH	1001	CYC	C4B-NB	-2.29	1.33	1.38
28	EI	1001	CYC	C4B-NB	-2.29	1.33	1.38
26	mA	201	PEB	C1D-ND	2.29	1.49	1.45
26	AD	202	PEB	C1D-ND	2.29	1.49	1.45
26	D1	203	PEB	C1B-C2B	2.29	1.50	1.45
26	A6	304	PEB	C4A-NA	-2.29	1.32	1.37
26	K6	201	PEB	C4A-NA	-2.29	1.32	1.37
26	H9	201	PEB	C2A-C1A	-2.29	1.50	1.52
26	AJ	304	PEB	C2A-C1A	-2.29	1.50	1.52
26	kI	201	PEB	C4B-C3B	2.29	1.49	1.45
26	X3	201	PEB	C4A-NA	-2.29	1.32	1.37
26	EA	202	PEB	C4A-NA	-2.29	1.32	1.37
26	LF	1002	PEB	C4A-NA	-2.29	1.32	1.37
26	OB	201	PEB	OD-C4D	2.29	1.27	1.23
26	t4	201	PEB	C2A-C1A	-2.29	1.50	1.52
26	W6	203	PEB	C2A-C1A	-2.29	1.50	1.52
26	OA	202	PEB	C4A-NA	-2.29	1.32	1.37
26	UA	203	PEB	C4A-NA	-2.29	1.32	1.37
26	P1	202	PEB	OD-C4D	2.29	1.27	1.23
26	g7	201	PEB	C4B-C3B	2.29	1.49	1.45
26	R7	201	PEB	C4B-C3B	2.29	1.49	1.45
26	gF	202	PEB	C4B-C3B	2.29	1.49	1.45
28	MB	1001	CYC	C1B-NB	-2.29	1.34	1.37
26	X8	202	PEB	C1B-C2B	2.29	1.50	1.45
26	Z6	202	PEB	C4A-NA	-2.29	1.32	1.37
26	AD	201	PEB	C4A-NA	-2.29	1.32	1.37
26	EE	202	PEB	C2A-C1A	-2.29	1.50	1.52
26	mF	201	PEB	C1B-C2B	2.29	1.50	1.45
26	tG	202	PEB	C4B-C3B	2.29	1.49	1.45
26	QE	203	PEB	C4B-NB	-2.29	1.33	1.38
26	B1	202	PEB	C2A-C1A	-2.29	1.50	1.52
26	e6	202	PEB	C2A-C1A	-2.29	1.50	1.52
28	D7	1001	CYC	C1D-CHD	2.28	1.50	1.41
26	jB	201	PEB	C4B-C3B	2.28	1.49	1.45
26	N8	201	PEB	C4A-NA	-2.28	1.32	1.37
26	E9	202	PEB	C4A-NA	-2.28	1.32	1.37
28	H2	1001	CYC	C1B-NB	-2.28	1.34	1.37
26	e4	202	PEB	C1C-CHB	2.28	1.50	1.41
26	K8	203	PEB	OD-C4D	2.28	1.27	1.23
28	D2	1001	CYC	OB-C4B	2.28	1.27	1.23
28	C2	1001	CYC	C1B-NB	-2.28	1.34	1.37
28	K2	1001	CYC	C1B-NB	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	xG	302	PEB	C4B-C3B	2.28	1.49	1.45
26	fl	201	PEB	C4A-NA	-2.28	1.32	1.37
26	m1	203	PEB	C2A-C1A	-2.28	1.50	1.52
26	bF	202	PEB	C4B-C3B	2.28	1.49	1.45
28	sH	1001	CYC	C1A-C2A	2.28	1.49	1.45
26	fA	202	PEB	C1C-CHB	2.28	1.50	1.41
26	SB	201	PEB	C4A-NA	-2.28	1.32	1.37
26	T1	202	PEB	OD-C4D	2.28	1.27	1.23
28	K7	1001	CYC	C4C-NC	-2.28	1.32	1.37
26	D9	201	PEB	C4B-C3B	2.28	1.49	1.45
26	uG	201	PEB	C1C-CHB	2.28	1.50	1.41
26	XJ	201	PEB	C1C-CHB	2.28	1.50	1.41
28	J7	1001	CYC	C4A-C3A	2.28	1.50	1.45
26	KA	203	PEB	OD-C4D	2.28	1.27	1.23
26	a2	203	PEB	C2A-C1A	-2.28	1.50	1.52
26	W3	202	PEB	C4A-NA	-2.28	1.32	1.37
26	PI	202	PEB	C4A-NA	-2.28	1.32	1.37
26	QF	201	PEB	C1C-CHB	2.28	1.50	1.41
26	BC	203	PEB	C4B-C3B	2.28	1.49	1.45
26	P3	201	PEB	OD-C4D	2.28	1.27	1.23
26	OB	202	PEB	C4A-NA	-2.28	1.32	1.37
26	eB	203	PEB	C4A-NA	-2.28	1.32	1.37
26	RJ	203	PEB	C4B-C3B	2.28	1.49	1.45
26	S7	201	PEB	C1C-CHB	2.28	1.50	1.41
26	jG	202	PEB	C4A-NA	-2.28	1.32	1.37
26	hB	203	PEB	C4B-C3B	2.28	1.49	1.45
26	d8	202	PEB	C4A-NA	-2.28	1.32	1.37
28	LI	1001	CYC	C1D-CHD	2.28	1.49	1.41
28	M6	1001	CYC	C4B-NB	-2.28	1.33	1.38
26	D2	1002	PEB	C4A-NA	-2.28	1.32	1.37
26	S8	203	PEB	C4A-NA	-2.28	1.32	1.37
26	HD	202	PEB	C1C-CHB	2.28	1.49	1.41
28	MI	1001	CYC	C4C-NC	-2.28	1.32	1.37
26	kI	201	PEB	C2A-C1A	-2.28	1.50	1.52
26	RJ	201	PEB	C2A-C1A	-2.28	1.50	1.52
26	y4	202	PEB	C4B-C3B	2.28	1.49	1.45
28	FB	1001	CYC	C4C-NC	-2.28	1.32	1.37
26	R4	201	PEB	C4A-NA	-2.28	1.32	1.37
26	VB	201	PEB	C4A-NA	-2.28	1.32	1.37
26	FC	201	PEB	C4A-NA	-2.28	1.32	1.37
28	JF	1001	CYC	C1B-NB	-2.28	1.34	1.37
28	L2	1001	CYC	C1D-CHD	2.28	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	LG	202	PEB	C4A-NA	-2.28	1.32	1.37
28	M2	1001	CYC	C4C-NC	-2.28	1.32	1.37
26	L9	202	PEB	C1B-C2B	2.28	1.50	1.45
26	FJ	202	PEB	C1B-C2B	2.28	1.50	1.45
28	JI	1001	CYC	C4A-C3A	2.28	1.50	1.45
26	WA	203	PEB	OD-C4D	2.28	1.27	1.23
26	QI	201	PEB	OD-C4D	2.28	1.27	1.23
28	N2	1001	CYC	C1D-CHD	2.28	1.49	1.41
26	kG	202	PEB	C1C-CHB	2.27	1.49	1.41
26	T6	201	PEB	C4A-NA	-2.27	1.32	1.37
26	IC	202	PEB	C4A-NA	-2.27	1.32	1.37
26	L9	201	PEB	C4B-C3B	2.27	1.49	1.45
26	UG	202	PEB	C4A-NA	-2.27	1.32	1.37
26	Z1	202	PEB	C4A-NA	-2.27	1.32	1.37
26	H3	202	PEB	C2A-C1A	-2.27	1.50	1.52
26	DJ	203	PEB	CHA-C1B	2.27	1.45	1.40
26	iE	201	PEB	C4B-C3B	2.27	1.49	1.45
26	m2	203	PEB	C4A-NA	-2.27	1.32	1.37
28	B6	1001	CYC	OB-C4B	2.27	1.27	1.23
26	s4	202	PEB	C1C-CHB	2.27	1.49	1.41
26	L9	202	PEB	C4A-NA	-2.27	1.32	1.37
26	jE	202	PEB	C4A-NA	-2.27	1.32	1.37
26	AJ	303	PEB	C4A-NA	-2.27	1.32	1.37
26	RD	202	PEB	C1A-NA	-2.27	1.34	1.37
26	w1	202	PEB	C2A-C1A	-2.27	1.50	1.52
26	F4	203	PEB	C2A-C1A	-2.27	1.50	1.52
26	P2	201	PEB	C4A-NA	-2.27	1.32	1.37
26	M8	202	PEB	C4A-NA	-2.27	1.32	1.37
28	NF	1001	CYC	C1B-NB	-2.27	1.34	1.37
26	NF	1002	PEB	C4B-C3B	2.27	1.49	1.45
26	SA	201	PEB	C4A-NA	-2.27	1.32	1.37
26	f6	203	PEB	C4B-C3B	2.27	1.49	1.45
26	T1	201	PEB	C4A-NA	-2.27	1.32	1.37
26	KG	202	PEB	C1B-C2B	2.27	1.50	1.45
26	J4	201	PEB	C2A-C1A	-2.27	1.50	1.52
26	g6	201	PEB	C2A-C1A	-2.27	1.50	1.52
26	PG	202	PEB	C4A-NA	-2.27	1.32	1.37
28	nH	1001	CYC	C4A-C3A	2.27	1.50	1.45
26	f7	203	PEB	C4B-C3B	2.27	1.49	1.45
26	ED	201	PEB	C4B-C3B	2.27	1.49	1.45
26	Z2	201	PEB	OD-C4D	2.27	1.27	1.23
26	MA	203	PEB	OD-C4D	2.27	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U1	201	PEB	C4A-NA	-2.27	1.32	1.37
26	g2	201	PEB	C4A-NA	-2.27	1.32	1.37
26	L4	202	PEB	C1C-CHB	2.27	1.49	1.41
28	K6	202	CYC	C1D-CHD	2.27	1.49	1.41
26	SD	202	PEB	C4A-NA	-2.27	1.32	1.37
26	UD	202	PEB	C4A-NA	-2.27	1.32	1.37
26	P3	203	PEB	C4A-NA	-2.27	1.32	1.37
28	eH	1001	CYC	C4D-CHA	2.27	1.49	1.41
26	C1	202	PEB	C4B-C3B	2.27	1.49	1.45
26	N2	1002	PEB	C4A-NA	-2.27	1.32	1.37
26	LA	201	PEB	C4A-NA	-2.27	1.32	1.37
26	yG	301	PEB	C4A-NA	-2.27	1.32	1.37
26	L1	202	PEB	C1C-CHB	2.27	1.49	1.41
26	GD	202	PEB	C4B-C3B	2.27	1.49	1.45
26	M4	402	PEB	C4A-NA	-2.27	1.32	1.37
26	jI	202	PEB	C2A-C1A	-2.27	1.50	1.52
28	E6	1001	CYC	C1D-CHD	2.27	1.49	1.41
26	j7	203	PEB	C1C-CHB	2.27	1.49	1.41
26	aE	201	PEB	C4B-NB	-2.27	1.33	1.38
26	eI	202	PEB	C4A-NA	-2.27	1.32	1.37
26	N9	204	PEB	C1C-CHB	2.27	1.49	1.41
26	D3	202	PEB	C4B-NB	-2.27	1.33	1.38
26	N4	203	PEB	C4A-NA	-2.27	1.32	1.37
28	F6	1001	CYC	C4C-NC	-2.27	1.32	1.37
26	N7	1002	PEB	C4B-C3B	2.27	1.49	1.45
26	K1	202	PEB	C4B-C3B	2.27	1.49	1.45
28	LF	1001	CYC	C4C-NC	-2.27	1.32	1.37
26	Q7	203	PEB	C2A-C1A	-2.27	1.50	1.52
26	A9	304	PEB	C2A-C1A	-2.27	1.50	1.52
26	AD	201	PEB	C2A-C1A	-2.27	1.50	1.52
26	J3	201	PEB	OD-C4D	2.26	1.27	1.23
26	G8	203	PEB	C4A-NA	-2.26	1.32	1.37
26	RJ	203	PEB	C1C-CHB	2.26	1.49	1.41
26	iG	201	PEB	OD-C4D	2.26	1.27	1.23
26	HC	203	PEB	C4A-NA	-2.26	1.32	1.37
26	P4	203	PEB	C2A-C1A	-2.26	1.50	1.52
26	T3	201	PEB	C1C-CHB	2.26	1.49	1.41
28	FF	1001	CYC	C1D-CHD	2.26	1.49	1.41
26	IG	203	PEB	OD-C4D	2.26	1.27	1.23
26	TB	201	PEB	C4A-NA	-2.26	1.32	1.37
28	N7	1001	CYC	C4C-NC	-2.26	1.32	1.37
26	DD	202	PEB	C1A-NA	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E1	201	PEB	C4B-C3B	2.26	1.49	1.45
28	K6	202	CYC	C4B-NB	-2.26	1.33	1.38
26	rE	202	PEB	C2A-C1A	-2.26	1.50	1.52
26	ZG	202	PEB	C2A-C1A	-2.26	1.50	1.52
26	J1	201	PEB	C4A-NA	-2.26	1.32	1.37
26	FF	1002	PEB	C4A-NA	-2.26	1.32	1.37
26	gF	202	PEB	C1C-CHB	2.26	1.49	1.41
26	kE	203	PEB	C4B-C3B	2.26	1.49	1.45
26	TJ	202	PEB	C1C-CHB	2.26	1.49	1.41
26	ME	203	PEB	C4A-NA	-2.26	1.32	1.37
26	d1	202	PEB	C1C-CHB	2.26	1.49	1.41
26	e2	201	PEB	C4A-NA	-2.26	1.32	1.37
26	LJ	203	PEB	C2A-C1A	-2.26	1.50	1.52
26	xE	303	PEB	C4B-C3B	2.26	1.49	1.45
28	EB	1001	CYC	C4B-NB	-2.26	1.33	1.38
26	O8	203	PEB	C4A-NA	-2.26	1.32	1.37
26	g4	203	PEB	C4B-C3B	2.26	1.49	1.45
28	YH	1001	CYC	C4B-NB	-2.26	1.33	1.38
28	IH	1001	CYC	C4B-NB	-2.26	1.33	1.38
26	UJ	201	PEB	C1B-C2B	2.26	1.50	1.45
26	hF	201	PEB	C1C-CHB	2.26	1.49	1.41
26	q1	202	PEB	C1C-CHB	2.26	1.49	1.41
26	sE	201	PEB	C1D-ND	2.26	1.49	1.45
28	LF	1001	CYC	C1B-NB	-2.26	1.34	1.37
26	l6	201	PEB	C4B-C3B	2.26	1.49	1.45
26	gB	202	PEB	C2A-C1A	-2.26	1.50	1.52
26	NI	1002	PEB	C4A-NA	-2.26	1.32	1.37
26	TI	202	PEB	C4A-NA	-2.26	1.32	1.37
26	WG	202	PEB	C1B-C2B	2.26	1.50	1.45
28	C2	1001	CYC	C4B-NB	-2.26	1.33	1.38
26	V1	201	PEB	C4A-NA	-2.26	1.32	1.37
26	TA	201	PEB	C4A-NA	-2.26	1.32	1.37
26	XE	202	PEB	C4B-C3B	2.26	1.49	1.45
26	JJ	201	PEB	C1D-ND	2.26	1.49	1.45
26	A8	301	PEB	C2A-C1A	-2.26	1.50	1.52
28	E6	1001	CYC	C4B-NB	-2.26	1.33	1.38
28	I7	1001	CYC	C1D-CHD	2.26	1.49	1.41
26	U2	202	PEB	C4A-NA	-2.26	1.32	1.37
26	E9	201	PEB	C4A-NA	-2.26	1.32	1.37
27	QA	201	PUB	C3C-C4C	2.26	1.51	1.43
26	gG	201	PEB	C1B-C2B	2.26	1.50	1.45
26	m6	203	PEB	C2A-C1A	-2.26	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	jF	203	PEB	C2A-C1A	-2.26	1.50	1.52
26	PA	201	PEB	C4A-NA	-2.26	1.32	1.37
26	gE	201	PEB	C4A-NA	-2.26	1.32	1.37
26	nG	201	PEB	C4B-C3B	2.26	1.49	1.45
26	a2	202	PEB	C1C-CHB	2.26	1.49	1.41
26	TD	201	PEB	C1C-CHB	2.26	1.49	1.41
26	FG	201	PEB	C1C-CHB	2.26	1.49	1.41
26	Q7	201	PEB	C4B-C3B	2.26	1.49	1.45
27	AF	304	PUB	C1C-C2C	2.26	1.49	1.45
26	r4	201	PEB	C2A-C1A	-2.26	1.50	1.52
28	eH	1001	CYC	C1A-C2A	2.26	1.49	1.45
28	D6	1001	CYC	C4B-NB	-2.26	1.33	1.38
26	rG	201	PEB	C4B-C3B	2.26	1.49	1.45
28	G6	1001	CYC	C1D-CHD	2.25	1.49	1.41
28	KB	202	CYC	C1D-CHD	2.25	1.49	1.41
26	n4	201	PEB	C2A-C1A	-2.25	1.50	1.52
26	hA	202	PEB	C2A-C1A	-2.25	1.50	1.52
28	GH	1001	CYC	OB-C4B	2.25	1.27	1.23
26	LJ	201	PEB	C1C-CHB	2.25	1.49	1.41
28	DF	1001	CYC	C1B-C2B	2.25	1.49	1.45
26	F3	203	PEB	C4B-C3B	2.25	1.49	1.45
26	R9	203	PEB	C4B-C3B	2.25	1.49	1.45
28	oH	1001	CYC	C4B-NB	-2.25	1.33	1.38
28	pH	1001	CYC	C4B-NB	-2.25	1.33	1.38
28	CI	1001	CYC	C4B-NB	-2.25	1.33	1.38
26	I5	202	PEB	OD-C4D	2.25	1.27	1.23
26	D8	202	PEB	C4A-NA	-2.25	1.32	1.37
28	KF	1001	CYC	C4C-NC	-2.25	1.32	1.37
26	eE	201	PEB	C1C-CHB	2.25	1.49	1.41
26	aF	202	PEB	C1B-C2B	2.25	1.50	1.45
28	UH	1001	CYC	C1A-C2A	2.25	1.49	1.45
26	N1	203	PEB	C4A-NA	-2.25	1.32	1.37
26	aG	202	PEB	C1B-C2B	2.25	1.50	1.45
28	LF	1001	CYC	C4A-C3A	2.25	1.50	1.45
26	QB	202	PEB	C4A-NA	-2.25	1.32	1.37
26	MG	203	PEB	C4A-NA	-2.25	1.32	1.37
26	tE	202	PEB	C1C-CHB	2.25	1.49	1.41
26	Y6	202	PEB	C4A-NA	-2.25	1.32	1.37
26	XJ	203	PEB	C2A-C1A	-2.25	1.50	1.52
28	L2	1001	CYC	C4A-C3A	2.25	1.50	1.45
26	c2	202	PEB	C4B-C3B	2.25	1.49	1.45
26	i4	201	PEB	C4B-C3B	2.25	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E1	202	PEB	C4A-NA	-2.25	1.32	1.37
26	H8	201	PEB	C4A-NA	-2.25	1.32	1.37
26	N8	202	PEB	C4A-NA	-2.25	1.32	1.37
26	NA	202	PEB	C4A-NA	-2.25	1.32	1.37
26	J5	201	PEB	CHA-C4A	2.25	1.41	1.36
26	N4	201	PEB	C1B-C2B	2.25	1.50	1.45
26	O2	201	PEB	OD-C4D	2.25	1.27	1.23
26	b4	501	PEB	C2A-C1A	-2.25	1.50	1.52
26	y1	203	PEB	C4B-C3B	2.25	1.49	1.45
26	S4	202	PEB	C4A-NA	-2.25	1.32	1.37
26	WI	201	PEB	OD-C4D	2.25	1.27	1.23
26	WA	203	PEB	C4B-NB	-2.25	1.33	1.38
26	UD	201	PEB	C4B-NB	-2.25	1.33	1.38
26	RI	203	PEB	C1C-CHB	2.25	1.49	1.41
26	P2	202	PEB	C4A-NA	-2.25	1.32	1.37
28	DB	1001	CYC	OB-C4B	2.25	1.27	1.23
26	gI	201	PEB	C4A-NA	-2.25	1.32	1.37
26	TI	201	PEB	C4A-NA	-2.25	1.32	1.37
26	f2	201	PEB	C2A-C1A	-2.25	1.50	1.52
26	F1	203	PEB	C4A-NA	-2.25	1.32	1.37
26	eI	201	PEB	C4A-NA	-2.25	1.32	1.37
26	C5	204	PEB	C4B-C3B	2.25	1.49	1.45
26	Q3	202	PEB	C4A-NA	-2.25	1.32	1.37
26	EA	201	PEB	C4A-NA	-2.25	1.32	1.37
26	j7	202	PEB	C2A-C1A	-2.25	1.50	1.52
26	j8	201	PEB	C2A-C1A	-2.25	1.50	1.52
26	jA	202	PEB	C2A-C1A	-2.25	1.50	1.52
26	G3	201	PEB	C4A-NA	-2.25	1.32	1.37
28	JI	1001	CYC	C1D-CHD	2.25	1.49	1.41
26	iG	201	PEB	C4A-NA	-2.25	1.32	1.37
26	P1	201	PEB	CHC-C4C	2.25	1.55	1.50
26	FE	201	PEB	C1C-CHB	2.25	1.49	1.41
26	HG	202	PEB	C4A-NA	-2.25	1.32	1.37
28	L7	1001	CYC	C4C-NC	-2.25	1.32	1.37
26	sG	202	PEB	C1B-C2B	2.25	1.50	1.45
26	gF	201	PEB	C4B-C3B	2.25	1.49	1.45
26	SA	203	PEB	C4A-NA	-2.25	1.32	1.37
26	zE	501	PEB	C4B-C3B	2.25	1.49	1.45
28	cH	1001	CYC	C4A-C3A	2.25	1.50	1.45
28	BB	1001	CYC	C1D-CHD	2.25	1.49	1.41
26	iA	201	PEB	C1D-ND	2.25	1.49	1.45
26	CJ	201	PEB	C1B-C2B	2.25	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	nG	202	PEB	C4A-NA	-2.25	1.32	1.37
26	E3	201	PEB	C1C-CHB	2.25	1.49	1.41
28	D2	1001	CYC	C1B-NB	-2.25	1.34	1.37
26	GA	203	PEB	C4A-NA	-2.25	1.32	1.37
26	NG	202	PEB	C4A-NA	-2.25	1.32	1.37
26	xG	303	PEB	C4B-C3B	2.24	1.49	1.45
26	I3	201	PEB	C4A-NA	-2.24	1.32	1.37
26	M3	201	PEB	C4A-NA	-2.24	1.32	1.37
28	NH	1001	CYC	C4B-NB	-2.24	1.33	1.38
26	m1	202	PEB	C1C-CHB	2.24	1.49	1.41
26	f2	201	PEB	C4A-NA	-2.24	1.32	1.37
28	L7	1001	CYC	C1D-CHD	2.24	1.49	1.41
26	E4	201	PEB	C4B-C3B	2.24	1.49	1.45
26	fA	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	SF	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	T1	203	PEB	C4A-NA	-2.24	1.32	1.37
26	BD	203	PEB	C4A-NA	-2.24	1.32	1.37
26	QB	201	PEB	C4A-NA	-2.24	1.32	1.37
28	FF	1001	CYC	C4C-NC	-2.24	1.32	1.37
26	C8	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	AA	301	PEB	C2A-C1A	-2.24	1.50	1.52
26	KD	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	e1	201	PEB	C4B-C3B	2.24	1.49	1.45
28	L7	1001	CYC	C4B-NB	-2.24	1.33	1.38
26	fF	201	PEB	C4A-NA	-2.24	1.32	1.37
26	XJ	202	PEB	C4A-NA	-2.24	1.32	1.37
26	c2	202	PEB	C1C-CHB	2.24	1.49	1.41
26	cI	202	PEB	C1C-CHB	2.24	1.49	1.41
28	dH	1001	CYC	C4A-C3A	2.24	1.50	1.45
26	P2	202	PEB	C4B-C3B	2.24	1.49	1.45
26	i2	202	PEB	C4B-C3B	2.24	1.49	1.45
28	C7	1001	CYC	C1D-CHD	2.24	1.49	1.41
26	lG	201	PEB	C2A-C1A	-2.24	1.50	1.52
26	wG	303	PEB	C1B-C2B	2.24	1.50	1.45
26	E8	202	PEB	C4A-NA	-2.24	1.32	1.37
26	wE	302	PEB	C4A-NA	-2.24	1.32	1.37
26	cG	201	PEB	C4A-NA	-2.24	1.32	1.37
28	F2	1001	CYC	C4C-NC	-2.24	1.32	1.37
26	WA	202	PEB	OD-C4D	2.24	1.27	1.23
26	o1	501	PEB	C4A-NA	-2.24	1.32	1.37
26	W2	201	PEB	CHA-C4A	-2.24	1.32	1.36
26	vG	201	PEB	C4B-C3B	2.24	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I7	1001	CYC	C4B-NB	-2.24	1.33	1.38
26	a7	202	PEB	C1B-C2B	2.24	1.50	1.45
26	E8	201	PEB	C4A-NA	-2.24	1.32	1.37
26	B4	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	B4	203	PEB	C2A-C1A	-2.24	1.50	1.52
26	C5	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	AE	202	PEB	C2A-C1A	-2.24	1.50	1.52
28	wH	1001	CYC	C4B-NB	-2.24	1.33	1.38
26	Y8	203	PEB	OD-C4D	2.24	1.27	1.23
26	QA	204	PEB	C4B-C3B	2.24	1.49	1.45
26	H2	1002	PEB	C4A-NA	-2.24	1.32	1.37
26	mA	202	PEB	C4A-NA	-2.24	1.32	1.37
26	m4	201	PEB	C4B-C3B	2.24	1.49	1.45
26	a1	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	f1	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	aA	203	PEB	C2A-C1A	-2.24	1.50	1.52
26	AI	301	PEB	C2A-C1A	-2.24	1.50	1.52
26	H8	202	PEB	C1B-C2B	2.24	1.50	1.45
26	oE	203	PEB	C4A-NA	-2.24	1.32	1.37
26	kE	203	PEB	C1C-CHB	2.24	1.49	1.41
26	aI	202	PEB	C1C-CHB	2.24	1.49	1.41
26	S8	202	PEB	C4A-NA	-2.24	1.32	1.37
26	i1	202	PEB	C4B-C3B	2.24	1.49	1.45
26	W7	203	PEB	C4B-C3B	2.24	1.49	1.45
26	e2	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	M3	201	PEB	OD-C4D	2.24	1.27	1.23
26	HJ	201	PEB	OD-C4D	2.24	1.27	1.23
26	dI	202	PEB	C1D-ND	2.24	1.49	1.45
26	g6	201	PEB	C4A-NA	-2.24	1.32	1.37
28	DI	1001	CYC	OB-C4B	2.24	1.27	1.23
26	Q2	202	PEB	C4A-NA	-2.24	1.32	1.37
26	h8	202	PEB	C2A-C1A	-2.24	1.50	1.52
26	TG	202	PEB	C4B-C3B	2.24	1.49	1.45
28	EF	1001	CYC	C1B-C2B	2.24	1.49	1.45
28	N7	1001	CYC	C1D-CHD	2.24	1.49	1.41
26	g8	202	PEB	C4B-C3B	2.24	1.49	1.45
26	aA	201	PEB	C4A-NA	-2.24	1.32	1.37
26	dI	202	PEB	C2A-C1A	-2.24	1.50	1.52
28	GB	1001	CYC	C4B-NB	-2.24	1.33	1.38
26	R2	203	PEB	C1C-CHB	2.24	1.49	1.41
26	GC	202	PEB	C4A-NA	-2.24	1.32	1.37
26	U7	202	PEB	C4B-C3B	2.24	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	uH	1001	CYC	C4B-NB	-2.24	1.33	1.38
28	L6	1001	CYC	C1D-CHD	2.24	1.49	1.41
28	nH	1001	CYC	C4D-CHA	2.24	1.49	1.41
28	qH	1002	CYC	C4D-CHA	2.24	1.49	1.41
26	T4	201	PEB	C4A-NA	-2.24	1.32	1.37
26	Z8	202	PEB	C4A-NA	-2.24	1.32	1.37
28	M6	1001	CYC	C1B-NB	-2.24	1.34	1.37
26	i7	201	PEB	C4B-C3B	2.23	1.49	1.45
26	oG	203	PEB	C4B-C3B	2.23	1.49	1.45
26	UF	202	PEB	CHA-C4A	-2.23	1.32	1.36
26	lB	201	PEB	C4B-C3B	2.23	1.49	1.45
28	B6	1001	CYC	C1D-CHD	2.23	1.49	1.41
26	H1	203	PEB	C4B-C3B	2.23	1.49	1.45
26	c2	201	PEB	C4A-NA	-2.23	1.32	1.37
26	T4	203	PEB	C4A-NA	-2.23	1.32	1.37
26	D3	203	PEB	C2A-C1A	-2.23	1.50	1.52
26	gF	202	PEB	C1A-NA	-2.23	1.34	1.37
26	W8	203	PEB	OD-C4D	2.23	1.27	1.23
26	DD	202	PEB	C4B-C3B	2.23	1.49	1.45
28	jH	1001	CYC	C4B-NB	-2.23	1.33	1.38
26	UF	201	PEB	C1C-CHB	2.23	1.49	1.41
26	m1	202	PEB	C4A-NA	-2.23	1.32	1.37
26	AA	302	PEB	C4A-NA	-2.23	1.32	1.37
26	eA	202	PEB	C4A-NA	-2.23	1.32	1.37
26	a4	201	PEB	C1B-C2B	2.23	1.50	1.45
28	LI	1001	CYC	C4A-C3A	2.23	1.50	1.45
26	O9	201	PEB	C1D-ND	2.23	1.49	1.45
26	fA	202	PEB	C1D-ND	2.23	1.49	1.45
26	QD	202	PEB	C4A-NA	-2.23	1.32	1.37
26	D4	202	PEB	C1C-CHB	2.23	1.49	1.41
26	W2	201	PEB	OD-C4D	2.23	1.27	1.23
28	EI	1001	CYC	C1D-CHD	2.23	1.49	1.41
26	l1	203	PEB	C2A-C1A	-2.23	1.50	1.52
26	nG	202	PEB	C2A-C1A	-2.23	1.50	1.52
26	S6	201	PEB	C4A-NA	-2.23	1.32	1.37
26	h7	202	PEB	C4A-NA	-2.23	1.32	1.37
26	TF	201	PEB	C1D-ND	2.23	1.49	1.45
26	qG	203	PEB	C4B-C3B	2.23	1.49	1.45
28	MH	1001	CYC	C4B-NB	-2.23	1.33	1.38
26	kE	202	PEB	C1C-CHB	2.23	1.49	1.41
26	PI	201	PEB	C4A-NA	-2.23	1.32	1.37
26	e7	202	PEB	C4B-C3B	2.23	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t1	201	PEB	C2A-C1A	-2.23	1.50	1.52
26	P9	201	PEB	C2A-C1A	-2.23	1.50	1.52
26	cE	203	PEB	C2A-C1A	-2.23	1.50	1.52
26	i4	202	PEB	C4B-C3B	2.23	1.49	1.45
26	yE	301	PEB	C4A-NA	-2.23	1.32	1.37
28	EH	1001	CYC	C4A-C3A	2.23	1.50	1.45
26	D1	201	PEB	C2A-C1A	-2.23	1.50	1.52
26	e6	203	PEB	C4A-NA	-2.23	1.32	1.37
26	JA	202	PEB	C4A-NA	-2.23	1.32	1.37
26	NG	201	PEB	C1A-NA	-2.23	1.34	1.37
26	b7	202	PEB	C4B-C3B	2.23	1.49	1.45
26	A2	304	PEB	C4A-NA	-2.23	1.32	1.37
26	k2	202	PEB	C4A-NA	-2.23	1.32	1.37
28	SH	1001	CYC	C4B-NB	-2.23	1.33	1.38
26	j4	201	PEB	C4B-C3B	2.23	1.49	1.45
26	IG	201	PEB	O1C-CGC	2.23	1.29	1.22
26	U7	201	PEB	C4A-NA	-2.23	1.32	1.37
26	QA	203	PEB	C4A-NA	-2.23	1.32	1.37
26	cA	202	PEB	C4A-NA	-2.23	1.32	1.37
26	dB	202	PEB	C2A-C1A	-2.23	1.50	1.52
26	NJ	204	PEB	C1C-CHB	2.23	1.49	1.41
26	XJ	202	PEB	C1C-CHB	2.23	1.49	1.41
26	A8	302	PEB	C4A-NA	-2.23	1.32	1.37
26	dE	202	PEB	C4A-NA	-2.23	1.32	1.37
26	hA	201	PEB	C1C-CHB	2.23	1.49	1.41
26	Z7	203	PEB	C4A-NA	-2.23	1.32	1.37
26	F1	203	PEB	C2A-C1A	-2.23	1.50	1.52
28	G6	1001	CYC	C4B-NB	-2.23	1.33	1.38
28	qH	1002	CYC	C4B-NB	-2.23	1.33	1.38
26	W4	202	PEB	C4B-C3B	2.23	1.49	1.45
26	qE	203	PEB	C1B-C2B	2.23	1.50	1.45
26	OI	201	PEB	OD-C4D	2.23	1.27	1.23
26	U2	202	PEB	C2A-C1A	-2.23	1.50	1.52
26	S3	202	PEB	C2A-C1A	-2.23	1.50	1.52
26	GD	201	PEB	C4A-NA	-2.23	1.32	1.37
26	h7	201	PEB	C1C-CHB	2.23	1.49	1.41
27	21	402	PUB	C3C-C4C	2.23	1.51	1.43
26	w1	203	PEB	C4B-C3B	2.22	1.49	1.45
26	ME	203	PEB	C4B-C3B	2.22	1.49	1.45
26	T9	201	PEB	C2A-C1A	-2.22	1.50	1.52
28	JI	1001	CYC	C4C-NC	-2.22	1.32	1.37
28	NF	1001	CYC	C4A-C3A	2.22	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cA	202	PEB	C1C-CHB	2.22	1.49	1.41
26	O6	201	PEB	OD-C4D	2.22	1.27	1.23
26	c7	201	PEB	C2A-C1A	-2.22	1.50	1.52
26	G9	201	PEB	C2A-C1A	-2.22	1.50	1.52
28	M2	1001	CYC	C1D-CHD	2.22	1.49	1.41
26	a1	201	PEB	C1B-C2B	2.22	1.50	1.45
26	V2	201	PEB	C4A-NA	-2.22	1.32	1.37
26	V6	201	PEB	C4A-NA	-2.22	1.32	1.37
26	A9	303	PEB	C4A-NA	-2.22	1.32	1.37
26	DB	1002	PEB	C1C-CHB	2.22	1.49	1.41
28	jH	1001	CYC	C4D-CHA	2.22	1.49	1.41
28	GI	1001	CYC	C4D-CHA	2.22	1.49	1.41
26	T1	201	PEB	C1D-ND	2.22	1.49	1.45
26	s4	203	PEB	C4B-C3B	2.22	1.49	1.45
26	nE	202	PEB	C1C-CHB	2.22	1.49	1.41
26	RJ	203	PEB	C4B-NB	-2.22	1.33	1.38
26	U6	203	PEB	C4A-NA	-2.22	1.32	1.37
28	M6	1001	CYC	OB-C4B	2.22	1.27	1.23
26	t1	201	PEB	C1C-CHB	2.22	1.49	1.41
26	PE	202	PEB	C4B-C3B	2.22	1.49	1.45
26	eB	201	PEB	C2A-C1A	-2.22	1.50	1.52
26	RF	201	PEB	C2A-C1A	-2.22	1.50	1.52
26	tG	202	PEB	C1C-CHB	2.22	1.49	1.41
26	l1	202	PEB	C1C-CHB	2.22	1.49	1.41
26	UF	201	PEB	C4A-NA	-2.22	1.32	1.37
26	f6	203	PEB	C1C-CHB	2.22	1.49	1.41
26	T2	201	PEB	C4A-NA	-2.22	1.32	1.37
26	E4	202	PEB	C4A-NA	-2.22	1.32	1.37
26	xE	302	PEB	C1D-ND	2.22	1.49	1.45
26	l7	203	PEB	C4B-C3B	2.22	1.49	1.45
26	H3	203	PEB	C4A-NA	-2.22	1.32	1.37
26	D9	201	PEB	C4A-NA	-2.22	1.32	1.37
26	HC	202	PEB	C4A-NA	-2.22	1.32	1.37
26	HF	1002	PEB	C4B-C3B	2.22	1.49	1.45
26	D6	1002	PEB	C4A-NA	-2.22	1.32	1.37
26	lB	201	PEB	C4A-NA	-2.22	1.32	1.37
26	KE	203	PEB	C4A-NA	-2.22	1.32	1.37
26	aI	202	PEB	C4B-NB	-2.22	1.33	1.38
26	DE	202	PEB	OD-C4D	2.22	1.27	1.23
26	d8	201	PEB	C1C-CHB	2.22	1.49	1.41
26	nG	201	PEB	C1C-CHB	2.22	1.49	1.41
26	R8	202	PEB	C4A-NA	-2.22	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M1	401	PEB	C4B-C3B	2.22	1.49	1.45
26	h7	201	PEB	C4B-C3B	2.22	1.49	1.45
26	gE	203	PEB	C1C-CHB	2.22	1.49	1.41
26	vE	202	PEB	C2A-C1A	-2.22	1.50	1.52
26	QA	203	PEB	OD-C4D	2.22	1.27	1.23
26	21	404	PEB	C4B-C3B	2.22	1.49	1.45
26	b2	201	PEB	C4A-NA	-2.22	1.32	1.37
26	DE	202	PEB	C4A-NA	-2.22	1.32	1.37
28	G2	1001	CYC	C4C-NC	-2.22	1.32	1.37
28	FB	1001	CYC	C1B-NB	-2.22	1.34	1.37
26	GJ	201	PEB	C2A-C1A	-2.22	1.50	1.52
26	QE	202	PEB	C1C-CHB	2.22	1.49	1.41
28	CB	1001	CYC	C4B-NB	-2.22	1.33	1.38
26	C3	201	PEB	C1B-C2B	2.22	1.50	1.45
26	CE	201	PEB	C1B-C2B	2.22	1.50	1.45
26	jA	201	PEB	C4A-NA	-2.22	1.32	1.37
26	S7	203	PEB	C4B-C3B	2.22	1.49	1.45
26	WF	203	PEB	C4B-C3B	2.22	1.49	1.45
26	W7	203	PEB	C1C-CHB	2.22	1.49	1.41
28	LH	1001	CYC	C4D-CHA	2.22	1.49	1.41
26	LA	202	PEB	C1B-C2B	2.22	1.50	1.45
26	oG	202	PEB	C1B-C2B	2.22	1.50	1.45
26	k1	203	PEB	C1D-ND	2.22	1.49	1.45
28	K2	1001	CYC	C4B-NB	-2.22	1.33	1.38
28	GB	1001	CYC	C1D-CHD	2.22	1.49	1.41
26	V4	203	PEB	C4A-NA	-2.22	1.32	1.37
26	MA	202	PEB	C4A-NA	-2.22	1.32	1.37
26	YB	202	PEB	C4A-NA	-2.22	1.32	1.37
26	YE	203	PEB	C4B-C3B	2.22	1.49	1.45
26	uE	201	PEB	C4B-C3B	2.22	1.49	1.45
26	g8	201	PEB	C1B-C2B	2.22	1.50	1.45
28	FI	1001	CYC	OB-C4B	2.22	1.27	1.23
26	hF	202	PEB	C1C-CHB	2.22	1.49	1.41
26	iB	201	PEB	C4A-NA	-2.22	1.32	1.37
26	RJ	203	PEB	C4A-NA	-2.22	1.32	1.37
26	TJ	201	PEB	C4A-NA	-2.22	1.32	1.37
26	W3	202	PEB	C2A-C1A	-2.22	1.50	1.52
26	V4	202	PEB	C2A-C1A	-2.22	1.50	1.52
26	R3	202	PEB	C4B-C3B	2.22	1.49	1.45
28	YH	1003	CYC	C4D-CHA	2.22	1.49	1.41
26	D3	203	PEB	C4A-NA	-2.22	1.32	1.37
26	GG	201	PEB	C1C-CHB	2.22	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	E7	1001	CYC	C4B-NB	-2.21	1.33	1.38
26	HJ	202	PEB	C1C-CHB	2.21	1.49	1.41
26	K4	201	PEB	C4A-NA	-2.21	1.32	1.37
26	U4	201	PEB	C1C-CHB	2.21	1.49	1.41
26	hB	201	PEB	C1C-CHB	2.21	1.49	1.41
26	HJ	203	PEB	C4A-NA	-2.21	1.32	1.37
26	e2	202	PEB	C4A-NA	-2.21	1.32	1.37
28	hH	1001	CYC	C4D-CHA	2.21	1.49	1.41
28	lH	1001	CYC	C4D-CHA	2.21	1.49	1.41
26	W1	202	PEB	C4B-C3B	2.21	1.49	1.45
26	q1	203	PEB	C4B-C3B	2.21	1.49	1.45
26	TE	202	PEB	C4B-C3B	2.21	1.49	1.45
26	R9	203	PEB	C1C-CHB	2.21	1.49	1.41
28	CF	1001	CYC	C4A-C3A	2.21	1.50	1.45
26	xG	302	PEB	C1D-ND	2.21	1.49	1.45
26	rE	201	PEB	C4B-C3B	2.21	1.49	1.45
26	AG	201	PEB	C4A-NA	-2.21	1.32	1.37
26	H1	203	PEB	C2A-C1A	-2.21	1.50	1.52
28	E2	1001	CYC	C1D-CHD	2.21	1.49	1.41
26	iG	203	PEB	C4B-C3B	2.21	1.49	1.45
26	J5	202	PEB	OD-C4D	2.21	1.27	1.23
26	iE	202	PEB	C2A-C1A	-2.21	1.50	1.52
26	YJ	202	PEB	C4B-C3B	2.21	1.49	1.45
26	a1	202	PEB	C1C-CHB	2.21	1.49	1.41
26	HD	203	PEB	C4A-NA	-2.21	1.32	1.37
26	UJ	201	PEB	C4A-NA	-2.21	1.32	1.37
26	MD	201	PEB	OD-C4D	2.21	1.27	1.23
26	XD	201	PEB	C4A-NA	-2.21	1.32	1.37
26	TJ	202	PEB	C4A-NA	-2.21	1.32	1.37
26	V9	203	PEB	C1C-CHB	2.21	1.49	1.41
26	Y7	202	PEB	C1B-C2B	2.21	1.50	1.45
26	W8	203	PEB	C4B-NB	-2.21	1.33	1.38
26	V1	201	PEB	OD-C4D	2.21	1.27	1.23
26	SB	202	PEB	C4A-NA	-2.21	1.32	1.37
26	q1	201	PEB	C4B-C3B	2.21	1.49	1.45
26	S2	202	PEB	C4A-NA	-2.21	1.32	1.37
26	OG	201	PEB	C1C-CHB	2.21	1.49	1.41
28	FI	1001	CYC	C4C-NC	-2.21	1.32	1.37
26	VA	202	PEB	C4B-NB	-2.21	1.33	1.38
26	m7	202	PEB	C4B-C3B	2.21	1.49	1.45
26	O7	201	PEB	C1C-CHB	2.21	1.49	1.41
26	Y4	201	PEB	C4A-NA	-2.21	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I8	202	PEB	C4A-NA	-2.21	1.32	1.37
26	hB	202	PEB	C4A-NA	-2.21	1.32	1.37
26	d6	204	PEB	C2A-C1A	-2.21	1.50	1.52
26	WB	203	PEB	C2A-C1A	-2.21	1.50	1.52
26	T1	202	PEB	C4A-NA	-2.21	1.32	1.37
28	E2	1001	CYC	C1B-C2B	2.21	1.49	1.45
26	j2	201	PEB	CHA-C4A	-2.21	1.32	1.36
26	QI	201	PEB	CHA-C4A	-2.21	1.32	1.36
26	a2	202	PEB	C4B-NB	-2.21	1.33	1.38
26	Z1	201	PEB	OD-C4D	2.21	1.27	1.23
28	PH	1001	CYC	OB-C4B	2.21	1.27	1.23
26	gA	202	PEB	C4B-C3B	2.21	1.49	1.45
26	i6	201	PEB	C2A-C1A	-2.21	1.50	1.52
26	mI	203	PEB	C4A-NA	-2.21	1.32	1.37
26	rG	202	PEB	C1B-C2B	2.21	1.50	1.45
26	k2	203	PEB	C1C-CHB	2.21	1.49	1.41
26	PD	203	PEB	C4A-NA	-2.21	1.32	1.37
26	SI	202	PEB	C4A-NA	-2.21	1.32	1.37
26	N1	203	PEB	CHC-C4C	2.21	1.55	1.50
26	Q6	201	PEB	C4A-NA	-2.21	1.32	1.37
26	f2	202	PEB	C2A-C1A	-2.21	1.50	1.52
26	JF	1002	PEB	C2A-C1A	-2.21	1.50	1.52
26	cE	203	PEB	C4B-C3B	2.21	1.49	1.45
26	Q2	201	PEB	CHA-C4A	-2.21	1.32	1.36
26	WI	201	PEB	CHA-C4A	-2.21	1.32	1.36
26	F4	203	PEB	C4A-NA	-2.21	1.32	1.37
26	HF	1002	PEB	C4A-NA	-2.21	1.32	1.37
28	H7	1001	CYC	C1D-CHD	2.21	1.49	1.41
26	D1	202	PEB	C4B-C3B	2.20	1.49	1.45
26	D4	203	PEB	C4A-NA	-2.20	1.32	1.37
26	R7	201	PEB	C4A-NA	-2.20	1.32	1.37
26	R8	201	PEB	C4A-NA	-2.20	1.32	1.37
28	DI	1001	CYC	C1B-NB	-2.20	1.34	1.37
26	u4	201	PEB	C1D-ND	2.20	1.49	1.45
26	L4	203	PEB	C2A-C1A	-2.20	1.50	1.52
26	Q2	201	PEB	OD-C4D	2.20	1.27	1.23
26	HJ	202	PEB	OD-C4D	2.20	1.27	1.23
26	b6	202	PEB	C4A-NA	-2.20	1.32	1.37
26	f8	201	PEB	C4B-C3B	2.20	1.49	1.45
28	UH	1001	CYC	C4B-NB	-2.20	1.33	1.38
26	k2	202	PEB	C1C-CHB	2.20	1.49	1.41
28	YH	1003	CYC	C4B-NB	-2.20	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aI	203	PEB	C4B-C3B	2.20	1.49	1.45
28	CB	1001	CYC	C4A-C3A	2.20	1.50	1.45
26	W9	201	PEB	C2A-C1A	-2.20	1.50	1.52
26	X9	203	PEB	C2A-C1A	-2.20	1.50	1.52
26	eI	202	PEB	C2A-C1A	-2.20	1.50	1.52
26	D1	203	PEB	C4A-NA	-2.20	1.32	1.37
26	J8	201	PEB	C4A-NA	-2.20	1.32	1.37
27	A7	303	PUB	C4B-CHB	2.20	1.49	1.41
26	OJ	201	PEB	C1D-ND	2.20	1.49	1.45
28	mH	1001	CYC	C4D-CHA	2.20	1.49	1.41
26	D9	202	PEB	C1B-C2B	2.20	1.50	1.45
26	xE	302	PEB	C4A-NA	-2.20	1.32	1.37
26	aG	202	PEB	C4A-NA	-2.20	1.32	1.37
26	e7	201	PEB	C4B-C3B	2.20	1.49	1.45
26	k1	203	PEB	C2A-C1A	-2.20	1.50	1.52
26	c4	203	PEB	C1C-CHB	2.20	1.49	1.41
26	VF	201	PEB	C1B-C2B	2.20	1.50	1.45
26	F4	201	PEB	C4A-NA	-2.20	1.32	1.37
26	m6	201	PEB	C4A-NA	-2.20	1.32	1.37
28	yH	1001	CYC	C4B-NB	-2.20	1.33	1.38
26	D3	201	PEB	C4B-C3B	2.20	1.49	1.45
26	B3	202	PEB	C4B-C3B	2.20	1.49	1.45
26	V3	203	PEB	C4A-NA	-2.20	1.32	1.37
26	lF	203	PEB	C1C-CHB	2.20	1.49	1.41
28	TH	1001	CYC	C4A-C3A	2.20	1.50	1.45
26	N3	201	PEB	C4A-NA	-2.20	1.32	1.37
26	MG	201	PEB	C4A-NA	-2.20	1.32	1.37
26	R7	202	PEB	C2A-C1A	-2.20	1.50	1.52
26	h6	203	PEB	C4B-C3B	2.20	1.49	1.45
26	P7	201	PEB	C4A-NA	-2.20	1.32	1.37
26	C8	202	PEB	C4A-NA	-2.20	1.32	1.37
26	DI	1002	PEB	C4A-NA	-2.20	1.32	1.37
26	YG	203	PEB	C1C-CHB	2.20	1.49	1.41
26	iG	201	PEB	C1C-CHB	2.20	1.49	1.41
26	DB	1002	PEB	C4A-NA	-2.20	1.32	1.37
26	rG	202	PEB	C4A-NA	-2.20	1.32	1.37
27	AB	302	PUB	C4B-CHB	2.20	1.49	1.41
26	V2	203	PEB	C2A-C1A	-2.20	1.50	1.52
26	wG	301	PEB	C2A-C1A	-2.20	1.50	1.52
28	GH	1001	CYC	C4D-CHA	2.20	1.49	1.41
26	F2	1002	PEB	C4A-NA	-2.20	1.32	1.37
26	g8	201	PEB	C4A-NA	-2.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VI	201	PEB	C4A-NA	-2.20	1.32	1.37
26	u4	201	PEB	C4B-C3B	2.20	1.49	1.45
26	h8	201	PEB	C1C-CHB	2.20	1.49	1.41
26	F3	203	PEB	C1C-CHB	2.20	1.49	1.41
26	lG	201	PEB	C1C-CHB	2.20	1.49	1.41
26	HE	202	PEB	C4A-NA	-2.20	1.32	1.37
28	C6	1001	CYC	C4B-NB	-2.20	1.33	1.38
26	P1	202	PEB	C1B-C2B	2.20	1.50	1.45
26	A1	201	PEB	C4A-NA	-2.20	1.32	1.37
26	S2	202	PEB	C1D-ND	2.20	1.49	1.45
26	OF	202	PEB	C4B-C3B	2.20	1.49	1.45
26	c1	202	PEB	C2A-C1A	-2.20	1.50	1.52
26	P3	202	PEB	C2A-C1A	-2.20	1.50	1.52
26	MD	202	PEB	C2A-C1A	-2.20	1.50	1.52
26	FA	202	PEB	C1B-C2B	2.20	1.50	1.45
26	qG	201	PEB	C1B-C2B	2.20	1.50	1.45
28	C6	1001	CYC	C4A-C3A	2.20	1.50	1.45
26	GB	1002	PEB	OD-C4D	2.20	1.27	1.23
26	h8	202	PEB	C4A-NA	-2.20	1.32	1.37
26	W9	202	PEB	C4B-C3B	2.20	1.49	1.45
28	I2	1001	CYC	C4B-NB	-2.20	1.33	1.38
26	PE	202	PEB	C4A-NA	-2.20	1.32	1.37
28	GI	1001	CYC	C4C-NC	-2.20	1.32	1.37
26	U1	202	PEB	C4A-NA	-2.20	1.32	1.37
26	P7	202	PEB	C1B-C2B	2.19	1.50	1.45
26	TD	202	PEB	OD-C4D	2.19	1.27	1.23
26	cI	202	PEB	C4A-NA	-2.19	1.32	1.37
26	g1	203	PEB	C4B-C3B	2.19	1.49	1.45
26	iB	201	PEB	C2A-C1A	-2.19	1.50	1.52
26	fE	202	PEB	C2A-C1A	-2.19	1.50	1.52
26	V1	203	PEB	C4A-NA	-2.19	1.32	1.37
26	O6	203	PEB	C4A-NA	-2.19	1.32	1.37
26	L7	1002	PEB	C4A-NA	-2.19	1.32	1.37
26	OB	203	PEB	C4A-NA	-2.19	1.32	1.37
26	c6	201	PEB	C4B-C3B	2.19	1.49	1.45
26	nG	202	PEB	C4B-C3B	2.19	1.49	1.45
28	EF	1001	CYC	C1D-CHD	2.19	1.49	1.41
26	P6	202	PEB	C4A-NA	-2.19	1.32	1.37
26	Q8	203	PEB	C4A-NA	-2.19	1.32	1.37
26	aI	202	PEB	C4A-NA	-2.19	1.32	1.37
26	A1	201	PEB	C1B-C2B	2.19	1.50	1.45
26	l6	201	PEB	C4A-NA	-2.19	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	UB	203	PEB	C4A-NA	-2.19	1.32	1.37
26	d6	204	PEB	C1D-ND	2.19	1.49	1.45
26	sG	201	PEB	C1D-ND	2.19	1.49	1.45
26	g4	203	PEB	C1C-CHB	2.19	1.49	1.41
26	v1	201	PEB	C4A-NA	-2.19	1.32	1.37
26	aA	202	PEB	C4A-NA	-2.19	1.32	1.37
26	JG	202	PEB	C4A-NA	-2.19	1.32	1.37
26	a2	203	PEB	C4B-C3B	2.19	1.49	1.45
26	d7	203	PEB	C4B-C3B	2.19	1.49	1.45
26	M8	203	PEB	OD-C4D	2.19	1.27	1.23
28	rH	1001	CYC	OB-C4B	2.19	1.27	1.23
26	bI	201	PEB	C4A-NA	-2.19	1.32	1.37
28	rH	1001	CYC	C4A-C3A	2.19	1.50	1.45
26	VD	203	PEB	C4A-NA	-2.19	1.32	1.37
26	DE	203	PEB	C4A-NA	-2.19	1.32	1.37
26	F8	202	PEB	C1B-C2B	2.19	1.50	1.45
28	LF	1001	CYC	C1D-CHD	2.19	1.49	1.41
26	KJ	201	PEB	C4B-C3B	2.19	1.49	1.45
26	hA	202	PEB	C4A-NA	-2.19	1.32	1.37
26	Q8	204	PEB	C4B-C3B	2.19	1.49	1.45
26	xG	302	PEB	C4A-NA	-2.19	1.32	1.37
26	x1	202	PEB	C1D-ND	2.19	1.49	1.45
26	GA	202	PEB	C4A-NA	-2.19	1.32	1.37
26	mE	201	PEB	C4A-NA	-2.19	1.32	1.37
26	YF	201	PEB	C4A-NA	-2.19	1.32	1.37
28	NH	1001	CYC	C4D-CHA	2.19	1.49	1.41
26	GA	203	PEB	C4B-C3B	2.19	1.49	1.45
26	m2	202	PEB	C4A-NA	-2.19	1.32	1.37
26	B3	203	PEB	C2A-C1A	-2.19	1.50	1.52
26	Q6	201	PEB	C4B-C3B	2.19	1.49	1.45
26	TI	203	PEB	C1C-CHB	2.19	1.49	1.41
28	WH	1001	CYC	C4D-CHA	2.19	1.49	1.41
26	a8	202	PEB	C4A-NA	-2.19	1.32	1.37
26	l8	202	PEB	C4A-NA	-2.19	1.32	1.37
26	R9	203	PEB	C4A-NA	-2.19	1.32	1.37
26	JA	201	PEB	C4A-NA	-2.19	1.32	1.37
26	21	401	PEB	C4B-C3B	2.19	1.49	1.45
28	LH	1001	CYC	C1A-C2A	2.19	1.49	1.45
26	r1	201	PEB	C1B-C2B	2.19	1.50	1.45
26	j7	203	PEB	C2A-C1A	-2.19	1.50	1.52
26	hI	202	PEB	C2A-C1A	-2.19	1.50	1.52
28	D2	1001	CYC	C1D-CHD	2.19	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fA	202	PEB	C4A-NA	-2.19	1.32	1.37
26	A1	202	PEB	C4B-C3B	2.19	1.49	1.45
26	c8	201	PEB	C1D-ND	2.19	1.49	1.45
26	AJ	305	PEB	C1D-ND	2.19	1.49	1.45
28	CH	1001	CYC	C1A-C2A	2.19	1.49	1.45
26	QB	203	PEB	C4A-NA	-2.19	1.32	1.37
26	N4	202	PEB	C2A-C1A	-2.19	1.50	1.52
28	FI	1001	CYC	C1B-NB	-2.19	1.34	1.37
26	J1	203	PEB	C4B-C3B	2.19	1.49	1.45
26	h4	201	PEB	C4B-C3B	2.19	1.49	1.45
26	V9	201	PEB	C4A-NA	-2.19	1.32	1.37
26	ZA	202	PEB	C4A-NA	-2.19	1.32	1.37
26	XG	203	PEB	C4A-NA	-2.19	1.32	1.37
26	B5	203	PEB	C1C-CHB	2.19	1.49	1.41
26	f8	202	PEB	C4B-C3B	2.19	1.49	1.45
26	JG	201	PEB	C4B-C3B	2.19	1.49	1.45
28	JF	1001	CYC	C4B-NB	-2.19	1.33	1.38
26	m7	201	PEB	C2A-C1A	-2.19	1.50	1.52
26	cI	201	PEB	C4A-NA	-2.19	1.32	1.37
26	iI	201	PEB	C4A-NA	-2.19	1.32	1.37
26	CD	201	PEB	C1B-C2B	2.19	1.50	1.45
28	J2	1001	CYC	C1D-CHD	2.19	1.49	1.41
28	TH	1001	CYC	C1A-C2A	2.19	1.49	1.45
26	H9	201	PEB	C4A-NA	-2.19	1.32	1.37
26	C9	201	PEB	C1B-C2B	2.19	1.50	1.45
26	RA	201	PEB	C4A-NA	-2.19	1.32	1.37
26	KJ	202	PEB	C1D-ND	2.19	1.49	1.45
26	bF	202	PEB	C1C-CHB	2.19	1.49	1.41
26	VJ	203	PEB	C4B-NB	-2.18	1.33	1.38
28	VH	1001	CYC	C4D-CHA	2.18	1.49	1.41
26	Z2	201	PEB	CHA-C4A	-2.18	1.32	1.36
28	eH	1001	CYC	C4B-NB	-2.18	1.33	1.38
28	II	1001	CYC	C4B-NB	-2.18	1.33	1.38
26	eE	201	PEB	C1D-ND	2.18	1.49	1.45
26	tG	202	PEB	C1D-ND	2.18	1.49	1.45
26	c4	203	PEB	C2A-C1A	-2.18	1.50	1.52
26	d4	203	PEB	C2A-C1A	-2.18	1.50	1.52
26	rE	201	PEB	C1A-NA	-2.18	1.34	1.37
26	M1	402	PEB	C4A-NA	-2.18	1.32	1.37
26	U6	201	PEB	C4A-NA	-2.18	1.32	1.37
26	mB	201	PEB	C4A-NA	-2.18	1.32	1.37
26	SF	201	PEB	C1C-CHB	2.18	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	MI	1001	CYC	C1D-CHD	2.18	1.49	1.41
26	L1	202	PEB	C4B-C3B	2.18	1.49	1.45
26	mI	202	PEB	C4B-C3B	2.18	1.49	1.45
26	iE	203	PEB	C1D-ND	2.18	1.49	1.45
26	T4	202	PEB	C4A-NA	-2.18	1.32	1.37
26	JE	202	PEB	C4A-NA	-2.18	1.32	1.37
28	NI	1001	CYC	C1D-CHD	2.18	1.49	1.41
26	g1	202	PEB	C1C-CHB	2.18	1.49	1.41
28	WH	1001	CYC	C4B-NB	-2.18	1.33	1.38
26	e2	203	PEB	C4B-C3B	2.18	1.49	1.45
26	V9	202	PEB	C4B-C3B	2.18	1.49	1.45
26	qE	201	PEB	C4B-C3B	2.18	1.49	1.45
28	E7	1001	CYC	C1D-CHD	2.18	1.49	1.41
26	11	201	PEB	C4A-NA	-2.18	1.32	1.37
26	EG	202	PEB	C4A-NA	-2.18	1.32	1.37
26	R4	203	PEB	C4B-C3B	2.18	1.49	1.45
28	DB	1001	CYC	C1A-C2A	2.18	1.49	1.45
26	L3	201	PEB	C4A-NA	-2.18	1.32	1.37
26	Y3	301	PEB	C4A-NA	-2.18	1.32	1.37
28	II	1001	CYC	C1B-NB	-2.18	1.34	1.37
26	d4	203	PEB	C1B-C2B	2.18	1.50	1.45
26	g4	202	PEB	C1C-CHB	2.18	1.49	1.41
26	X9	202	PEB	C1C-CHB	2.18	1.49	1.41
26	YE	202	PEB	C4B-C3B	2.18	1.49	1.45
26	y1	203	PEB	C2A-C1A	-2.18	1.50	1.52
26	ZG	201	PEB	C2A-C1A	-2.18	1.50	1.52
26	k6	201	PEB	C4A-NA	-2.18	1.32	1.37
26	UE	201	PEB	CMB-C2B	-2.18	1.46	1.50
26	WJ	202	PEB	C1B-C2B	2.18	1.50	1.45
26	s1	201	PEB	C2A-C1A	-2.18	1.50	1.52
26	gB	201	PEB	C2A-C1A	-2.18	1.50	1.52
26	T2	203	PEB	C1C-CHB	2.18	1.49	1.41
26	D3	201	PEB	C4A-NA	-2.18	1.32	1.37
26	SI	201	PEB	C1B-C2B	2.18	1.50	1.45
26	eE	202	PEB	C4A-NA	-2.18	1.32	1.37
26	J9	203	PEB	C1C-CHB	2.18	1.49	1.41
26	O9	202	PEB	C1D-ND	2.18	1.49	1.45
26	cA	201	PEB	C1D-ND	2.18	1.49	1.45
26	l1	201	PEB	C4B-C3B	2.18	1.49	1.45
26	H4	203	PEB	C4B-C3B	2.18	1.49	1.45
26	j1	201	PEB	C4A-NA	-2.18	1.32	1.37
26	F5	203	PEB	C4A-NA	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T3	202	PEB	CHA-C4A	-2.18	1.32	1.36
26	h6	202	PEB	C4A-NA	-2.18	1.32	1.37
26	T7	201	PEB	C4A-NA	-2.18	1.32	1.37
26	hE	201	PEB	C1C-CHB	2.18	1.49	1.41
26	V4	201	PEB	OD-C4D	2.18	1.27	1.23
26	g1	203	PEB	C1C-CHB	2.18	1.49	1.41
28	yH	1001	CYC	C4D-CHA	2.18	1.49	1.41
28	JI	1001	CYC	C1B-C2B	2.18	1.49	1.45
26	k4	201	PEB	C4B-C3B	2.18	1.49	1.45
26	I9	201	PEB	C4B-C3B	2.18	1.49	1.45
28	MB	1001	CYC	OB-C4B	2.18	1.27	1.23
26	O8	201	PEB	C4A-NA	-2.18	1.32	1.37
26	ID	201	PEB	C4A-NA	-2.18	1.32	1.37
28	I6	1001	CYC	C1D-CHD	2.18	1.49	1.41
26	R4	203	PEB	C1D-ND	2.18	1.49	1.45
26	BC	202	PEB	C4A-NA	-2.18	1.32	1.37
26	Q3	201	PEB	C4B-NB	-2.18	1.33	1.38
28	H7	1001	CYC	C4B-NB	-2.18	1.33	1.38
28	tH	1001	CYC	C4A-C3A	2.18	1.50	1.45
28	NI	1001	CYC	C4A-C3A	2.17	1.50	1.45
26	K5	202	PEB	C4A-NA	-2.17	1.32	1.37
26	f6	202	PEB	C4A-NA	-2.17	1.32	1.37
26	m8	202	PEB	C4A-NA	-2.17	1.32	1.37
26	IA	202	PEB	C4A-NA	-2.17	1.32	1.37
26	WD	202	PEB	C4A-NA	-2.17	1.32	1.37
26	eG	201	PEB	C4A-NA	-2.17	1.32	1.37
26	qE	201	PEB	C1C-CHB	2.17	1.49	1.41
26	r1	201	PEB	C2A-C1A	-2.17	1.50	1.52
26	uE	201	PEB	C2A-C1A	-2.17	1.50	1.52
26	lF	201	PEB	C1C-CHB	2.17	1.49	1.41
26	q4	202	PEB	C4B-C3B	2.17	1.49	1.45
26	WG	202	PEB	C4A-NA	-2.17	1.32	1.37
28	F6	1001	CYC	C1B-NB	-2.17	1.34	1.37
26	N4	202	PEB	C4A-NA	-2.17	1.32	1.37
26	mF	201	PEB	C4A-NA	-2.17	1.32	1.37
28	DF	1003	CYC	C4C-NC	-2.17	1.32	1.37
26	DA	202	PEB	C4B-C3B	2.17	1.49	1.45
26	K3	202	PEB	C2A-C1A	-2.17	1.50	1.52
26	X8	202	PEB	C4A-NA	-2.17	1.32	1.37
26	F1	202	PEB	C1C-CHB	2.17	1.49	1.41
26	b7	201	PEB	C1D-ND	2.17	1.49	1.45
26	PF	201	PEB	C4A-NA	-2.17	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JC	201	PEB	OD-C4D	2.17	1.27	1.23
26	b7	201	PEB	C4B-C3B	2.17	1.49	1.45
26	CJ	202	PEB	C4A-NA	-2.17	1.32	1.37
26	M4	403	PEB	C4A-NA	-2.17	1.32	1.37
26	J9	203	PEB	C4B-C3B	2.17	1.49	1.45
26	wE	301	PEB	C4B-C3B	2.17	1.49	1.45
26	ZI	201	PEB	OD-C4D	2.17	1.27	1.23
26	Y1	201	PEB	C4A-NA	-2.17	1.32	1.37
26	DF	1002	PEB	C4A-NA	-2.17	1.32	1.37
26	WJ	202	PEB	C4A-NA	-2.17	1.32	1.37
26	u4	203	PEB	C1C-CHB	2.17	1.49	1.41
26	GE	202	PEB	CMB-C2B	-2.17	1.46	1.50
26	ID	201	PEB	C4B-C3B	2.17	1.49	1.45
26	S2	202	PEB	C2A-C1A	-2.17	1.50	1.52
26	OA	202	PEB	C2A-C1A	-2.17	1.50	1.52
26	YE	203	PEB	C1C-CHB	2.17	1.49	1.41
26	G3	202	PEB	C4A-NA	-2.17	1.32	1.37
26	d8	201	PEB	C4A-NA	-2.17	1.32	1.37
28	G2	1001	CYC	C4D-CHA	2.17	1.49	1.41
26	m4	203	PEB	C4B-C3B	2.17	1.49	1.45
26	h8	201	PEB	C4B-C3B	2.17	1.49	1.45
26	YD	303	PEB	C4B-C3B	2.17	1.49	1.45
26	WE	201	PEB	OD-C4D	2.17	1.27	1.23
26	m2	202	PEB	C4B-C3B	2.17	1.49	1.45
26	14	201	PEB	C1C-CHB	2.17	1.49	1.41
26	J9	202	PEB	C1D-ND	2.17	1.49	1.45
26	c1	203	PEB	C4B-C3B	2.17	1.49	1.45
26	g2	202	PEB	C2A-C1A	-2.17	1.50	1.52
26	24	405	PEB	C4B-C3B	2.17	1.49	1.45
26	HD	201	PEB	C1C-CHB	2.17	1.49	1.41
26	HA	201	PEB	C4A-NA	-2.17	1.32	1.37
26	G3	202	PEB	C4B-C3B	2.17	1.49	1.45
26	eG	201	PEB	C1C-CHB	2.17	1.49	1.41
26	x4	202	PEB	C2A-C1A	-2.17	1.50	1.52
26	gA	201	PEB	C4A-NA	-2.17	1.32	1.37
26	qE	202	PEB	C1B-C2B	2.17	1.50	1.45
28	KI	1001	CYC	C4B-NB	-2.17	1.33	1.38
26	iF	201	PEB	C1B-C2B	2.17	1.50	1.45
26	tE	202	PEB	C1D-ND	2.17	1.49	1.45
26	14	203	PEB	C2A-C1A	-2.17	1.50	1.52
26	mI	201	PEB	C4A-NA	-2.17	1.32	1.37
28	MB	1001	CYC	C1D-CHD	2.17	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	JJ	203	PEB	C4B-C3B	2.17	1.49	1.45
26	q4	201	PEB	C4A-NA	-2.17	1.32	1.37
26	14	201	PEB	C4A-NA	-2.17	1.32	1.37
26	YD	301	PEB	C4A-NA	-2.17	1.32	1.37
26	w4	201	PEB	C1C-CHB	2.17	1.49	1.41
26	AC	203	PEB	C1C-CHB	2.17	1.49	1.41
26	W9	201	PEB	C1B-C2B	2.17	1.50	1.45
26	eA	202	PEB	C4B-C3B	2.17	1.49	1.45
26	aG	201	PEB	C4A-NA	-2.16	1.32	1.37
26	ZF	201	PEB	C1A-NA	-2.16	1.34	1.37
26	x1	201	PEB	C4B-C3B	2.16	1.49	1.45
26	zG	501	PEB	C4B-C3B	2.16	1.49	1.45
26	l1	202	PEB	C1D-ND	2.16	1.49	1.45
26	UE	202	PEB	C4A-NA	-2.16	1.32	1.37
26	A5	202	PEB	C1C-CHB	2.16	1.49	1.41
26	m6	202	PEB	C1C-CHB	2.16	1.49	1.41
26	UA	203	PEB	C2A-C1A	-2.16	1.50	1.52
26	XJ	203	PEB	C4B-C3B	2.16	1.49	1.45
28	hH	1001	CYC	C1A-C2A	2.16	1.49	1.45
26	U9	201	PEB	C4A-NA	-2.16	1.32	1.37
26	U1	201	PEB	C1C-CHB	2.16	1.49	1.41
26	e6	202	PEB	C1C-CHB	2.16	1.49	1.41
28	mH	1001	CYC	C4B-NB	-2.16	1.33	1.38
28	M6	1001	CYC	C1D-CHD	2.16	1.49	1.41
28	EI	1001	CYC	C1B-C2B	2.16	1.49	1.45
26	J3	201	PEB	C4A-NA	-2.16	1.32	1.37
26	F5	202	PEB	C4A-NA	-2.16	1.32	1.37
26	jI	202	PEB	C4A-NA	-2.16	1.32	1.37
28	L2	1001	CYC	C1A-NA	-2.16	1.33	1.38
26	i4	201	PEB	C4A-NA	-2.16	1.32	1.37
26	H7	1002	PEB	C4A-NA	-2.16	1.32	1.37
28	KI	1001	CYC	C1B-C2B	2.16	1.49	1.45
26	UB	203	PEB	C2A-C1A	-2.16	1.50	1.52
26	YG	202	PEB	C4B-C3B	2.16	1.49	1.45
26	q4	202	PEB	C1C-CHB	2.16	1.49	1.41
26	G8	203	PEB	C1C-CHB	2.16	1.49	1.41
26	J4	202	PEB	C1C-CHB	2.16	1.49	1.41
26	l4	202	PEB	C1C-CHB	2.16	1.49	1.41
26	m2	201	PEB	C4A-NA	-2.16	1.32	1.37
26	fB	202	PEB	C4A-NA	-2.16	1.32	1.37
26	EA	203	PEB	C2A-C1A	-2.16	1.50	1.52
26	HD	202	PEB	C2A-C1A	-2.16	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PD	202	PEB	C2A-C1A	-2.16	1.50	1.52
26	D6	1002	PEB	C1C-CHB	2.16	1.49	1.41
26	f2	202	PEB	C4B-C3B	2.16	1.49	1.45
26	ZE	201	PEB	C4B-C3B	2.16	1.49	1.45
26	jB	201	PEB	C1C-CHB	2.16	1.49	1.41
26	Y3	304	PEB	C1D-ND	2.16	1.49	1.45
26	QG	202	PEB	C1D-ND	2.16	1.49	1.45
26	G1	201	PEB	C4A-NA	-2.16	1.32	1.37
26	X9	201	PEB	C1C-CHB	2.16	1.49	1.41
26	lE	202	PEB	C2A-C1A	-2.16	1.50	1.52
26	KA	202	PEB	C4A-NA	-2.16	1.32	1.37
26	HI	1002	PEB	C4A-NA	-2.16	1.32	1.37
26	cB	201	PEB	C4A-NA	-2.16	1.32	1.37
26	AI	304	PEB	C4A-NA	-2.16	1.32	1.37
28	LI	1001	CYC	C1A-NA	-2.16	1.33	1.38
26	gB	201	PEB	C4A-NA	-2.16	1.32	1.37
26	xE	303	PEB	C4A-NA	-2.16	1.32	1.37
26	E3	201	PEB	C4B-C3B	2.16	1.49	1.45
26	BD	202	PEB	C4B-C3B	2.16	1.49	1.45
26	e6	201	PEB	C2A-C1A	-2.16	1.50	1.52
26	ED	202	PEB	C2A-C1A	-2.16	1.50	1.52
26	JE	201	PEB	C1C-CHB	2.16	1.49	1.41
28	IB	1001	CYC	C1D-CHD	2.16	1.49	1.41
28	I2	1001	CYC	C1B-NB	-2.16	1.34	1.37
26	YD	304	PEB	C4A-NA	-2.16	1.32	1.37
26	ID	201	PEB	C1D-ND	2.16	1.49	1.45
26	mE	203	PEB	C1D-ND	2.16	1.49	1.45
28	K2	1001	CYC	C1D-CHD	2.16	1.49	1.41
28	JH	1001	CYC	C4D-CHA	2.16	1.49	1.41
26	U6	203	PEB	C2A-C1A	-2.16	1.50	1.52
26	a7	202	PEB	C2A-C1A	-2.16	1.50	1.52
26	AD	202	PEB	C2A-C1A	-2.16	1.50	1.52
26	LE	202	PEB	C4B-C3B	2.16	1.49	1.45
26	A3	201	PEB	C1C-CHB	2.16	1.49	1.41
26	z4	201	PEB	C4A-NA	-2.16	1.32	1.37
26	XJ	201	PEB	C4A-NA	-2.16	1.32	1.37
26	f1	202	PEB	C1C-CHB	2.16	1.49	1.41
26	JJ	202	PEB	C1D-ND	2.16	1.49	1.45
26	XE	202	PEB	C4A-NA	-2.16	1.32	1.37
26	nE	202	PEB	C4A-NA	-2.16	1.32	1.37
26	N9	202	PEB	C4B-C3B	2.16	1.49	1.45
26	jF	202	PEB	C1C-CHB	2.16	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A9	302	PUB	C4B-CHB	2.16	1.49	1.41
26	F9	201	PEB	C1B-C2B	2.16	1.50	1.45
26	C9	202	PEB	C4A-NA	-2.16	1.32	1.37
28	B6	1002	CYC	C1D-CHD	2.16	1.49	1.41
26	O6	203	PEB	C4B-C3B	2.16	1.49	1.45
26	cA	203	PEB	C4B-C3B	2.16	1.49	1.45
26	QE	202	PEB	C4B-C3B	2.16	1.49	1.45
26	hF	201	PEB	C4B-C3B	2.16	1.49	1.45
26	h1	201	PEB	C1C-CHB	2.16	1.49	1.41
26	HE	201	PEB	C1C-CHB	2.16	1.49	1.41
26	mI	202	PEB	C4A-NA	-2.16	1.32	1.37
26	FJ	201	PEB	C1B-C2B	2.16	1.50	1.45
26	f7	201	PEB	C1D-ND	2.16	1.49	1.45
26	W8	202	PEB	OD-C4D	2.16	1.27	1.23
26	J3	202	PEB	C4B-C3B	2.16	1.49	1.45
26	B5	202	PEB	C4B-C3B	2.16	1.49	1.45
26	YI	202	PEB	C4A-NA	-2.16	1.32	1.37
26	BC	203	PEB	C1C-CHB	2.16	1.49	1.41
26	J8	202	PEB	C4A-NA	-2.16	1.32	1.37
26	LE	202	PEB	C4A-NA	-2.16	1.32	1.37
26	j8	201	PEB	C1D-ND	2.16	1.49	1.45
26	PD	202	PEB	C4B-C3B	2.16	1.49	1.45
28	MI	1001	CYC	C1B-NB	-2.16	1.34	1.37
26	u1	202	PEB	C4A-NA	-2.16	1.32	1.37
26	Z2	202	PEB	C2A-C1A	-2.16	1.50	1.52
26	l6	203	PEB	C2A-C1A	-2.16	1.50	1.52
28	G2	1001	CYC	C1B-NB	-2.15	1.34	1.37
26	v4	201	PEB	C4A-NA	-2.15	1.32	1.37
26	t4	201	PEB	C1C-CHB	2.15	1.49	1.41
26	G8	203	PEB	C4B-C3B	2.15	1.49	1.45
28	KI	1001	CYC	C1D-CHD	2.15	1.49	1.41
26	S8	202	PEB	C2A-C1A	-2.15	1.50	1.52
26	DF	1002	PEB	C2A-C1A	-2.15	1.50	1.52
28	mH	1001	CYC	C1A-C2A	2.15	1.49	1.45
26	VF	202	PEB	C1C-CHB	2.15	1.49	1.41
26	D8	201	PEB	C1D-ND	2.15	1.49	1.45
26	i2	203	PEB	C4A-NA	-2.15	1.32	1.37
26	A1	201	PEB	C4B-C3B	2.15	1.49	1.45
26	Y3	303	PEB	C4A-NA	-2.15	1.32	1.37
26	z1	202	PEB	C2A-C1A	-2.15	1.50	1.52
26	PI	202	PEB	C4B-C3B	2.15	1.49	1.45
26	E8	202	PEB	C1C-CHB	2.15	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bB	201	PEB	C4A-NA	-2.15	1.32	1.37
26	24	405	PEB	C1D-ND	2.15	1.49	1.45
26	VA	202	PEB	C1C-CHB	2.15	1.49	1.41
26	NJ	202	PEB	C1C-CHB	2.15	1.49	1.41
26	G6	1002	PEB	OD-C4D	2.15	1.27	1.23
26	kB	201	PEB	C4A-NA	-2.15	1.32	1.37
26	D4	201	PEB	C4B-C3B	2.15	1.49	1.45
28	K2	1001	CYC	C1B-C2B	2.15	1.49	1.45
26	F1	201	PEB	C1C-CHB	2.15	1.49	1.41
26	DJ	201	PEB	OD-C4D	2.15	1.27	1.23
26	f6	201	PEB	C4A-NA	-2.15	1.32	1.37
26	H9	203	PEB	C4A-NA	-2.15	1.32	1.37
26	LC	203	PEB	C4A-NA	-2.15	1.32	1.37
28	CH	1001	CYC	C4D-CHA	2.15	1.49	1.41
28	EH	1001	CYC	C4D-CHA	2.15	1.49	1.41
26	X3	203	PEB	C4B-C3B	2.15	1.49	1.45
26	DA	202	PEB	C4A-NA	-2.15	1.32	1.37
26	D8	202	PEB	C4B-C3B	2.15	1.49	1.45
26	H9	202	PEB	C1C-CHB	2.15	1.49	1.41
26	XD	201	PEB	C1C-CHB	2.15	1.49	1.41
26	V9	203	PEB	C4A-NA	-2.15	1.32	1.37
26	B5	201	PEB	C4B-C3B	2.15	1.49	1.45
26	M4	403	PEB	C2A-C1A	-2.15	1.50	1.52
26	TI	202	PEB	C1C-CHB	2.15	1.49	1.41
26	H3	201	PEB	C4A-NA	-2.15	1.32	1.37
26	a2	203	PEB	C1C-CHB	2.15	1.49	1.41
28	TH	1001	CYC	C4D-CHA	2.15	1.49	1.41
28	YH	1002	CYC	C4D-CHA	2.15	1.49	1.41
26	d1	203	PEB	C1B-C2B	2.15	1.50	1.45
26	a4	202	PEB	C4B-C3B	2.15	1.49	1.45
28	QH	1001	CYC	C1A-C2A	2.15	1.49	1.45
26	dF	202	PEB	C4A-NA	-2.15	1.32	1.37
26	Z8	202	PEB	C1B-C2B	2.15	1.50	1.45
26	j4	201	PEB	C4A-NA	-2.15	1.32	1.37
26	f8	203	PEB	C4A-NA	-2.15	1.32	1.37
26	lA	202	PEB	C4A-NA	-2.15	1.32	1.37
26	iB	202	PEB	C4B-C3B	2.15	1.49	1.45
28	L6	1001	CYC	OB-C4B	2.15	1.27	1.23
27	24	402	PUB	C3C-C4C	2.15	1.50	1.43
26	IG	202	PEB	C4A-NA	-2.15	1.32	1.37
26	XG	203	PEB	C4B-C3B	2.15	1.49	1.45
26	O7	203	PEB	C4A-NA	-2.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b7	203	PEB	C1C-CHB	2.15	1.49	1.41
26	d1	201	PEB	C4B-C3B	2.15	1.49	1.45
26	DD	201	PEB	C4A-NA	-2.15	1.32	1.37
26	eE	201	PEB	C4A-NA	-2.15	1.32	1.37
26	ZI	202	PEB	C4A-NA	-2.15	1.32	1.37
26	d6	204	PEB	C4B-C3B	2.15	1.49	1.45
26	TD	201	PEB	C4B-C3B	2.15	1.49	1.45
26	DG	202	PEB	C4A-NA	-2.15	1.32	1.37
26	EJ	201	PEB	C1B-C2B	2.15	1.50	1.45
26	IE	201	PEB	C1C-CHB	2.15	1.49	1.41
26	QF	202	PEB	C1C-CHB	2.15	1.49	1.41
26	YD	304	PEB	C1D-ND	2.15	1.49	1.45
26	X9	203	PEB	C4B-C3B	2.15	1.49	1.45
26	uE	203	PEB	C2A-C1A	-2.14	1.50	1.52
26	OA	201	PEB	C4A-NA	-2.14	1.32	1.37
26	GJ	201	PEB	C4A-NA	-2.14	1.32	1.37
26	t4	201	PEB	C4B-C3B	2.14	1.49	1.45
26	BC	202	PEB	C4B-C3B	2.14	1.49	1.45
26	ZI	201	PEB	CHA-C4A	-2.14	1.32	1.36
26	u4	201	PEB	C4A-NA	-2.14	1.32	1.37
28	kH	1001	CYC	C4B-NB	-2.14	1.33	1.38
26	LD	201	PEB	C4A-NA	-2.14	1.32	1.37
26	ZG	202	PEB	C4A-NA	-2.14	1.32	1.37
26	z1	201	PEB	C2A-C1A	-2.14	1.50	1.52
27	AA	304	PUB	C3C-C4C	2.14	1.50	1.43
28	IH	1001	CYC	C4B-NB	-2.14	1.33	1.38
28	J7	1001	CYC	C4C-NC	-2.14	1.32	1.37
26	A1	201	PEB	C1D-ND	2.14	1.49	1.45
26	W9	202	PEB	C1D-ND	2.14	1.49	1.45
26	HD	201	PEB	C4A-NA	-2.14	1.32	1.37
26	eB	202	PEB	C2A-C1A	-2.14	1.50	1.52
26	vG	202	PEB	C2A-C1A	-2.14	1.50	1.52
26	i1	201	PEB	C4B-C3B	2.14	1.49	1.45
26	d7	201	PEB	C4B-C3B	2.14	1.49	1.45
26	i2	201	PEB	C4A-NA	-2.14	1.32	1.37
26	LB	1002	PEB	C4A-NA	-2.14	1.32	1.37
26	IE	202	PEB	C4A-NA	-2.14	1.32	1.37
26	s4	203	PEB	C1C-CHB	2.14	1.49	1.41
26	FC	203	PEB	C4A-NA	-2.14	1.32	1.37
26	E4	202	PEB	C4B-C3B	2.14	1.49	1.45
26	f7	201	PEB	C4A-NA	-2.14	1.32	1.37
28	H6	1001	CYC	C1D-CHD	2.14	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B1	203	PEB	C4B-C3B	2.14	1.49	1.45
26	x4	201	PEB	C4B-C3B	2.14	1.49	1.45
26	j7	202	PEB	C4B-C3B	2.14	1.49	1.45
26	YF	201	PEB	C4B-C3B	2.14	1.49	1.45
26	l7	202	PEB	C4A-NA	-2.14	1.32	1.37
28	CF	1001	CYC	C4C-NC	-2.14	1.32	1.37
26	JD	202	PEB	C1C-CHB	2.14	1.49	1.41
26	VE	201	PEB	C1C-CHB	2.14	1.49	1.41
26	aI	203	PEB	O1B-CGB	2.14	1.29	1.22
26	qG	201	PEB	C4B-C3B	2.14	1.49	1.45
27	A6	302	PUB	C4B-CHB	2.14	1.49	1.41
26	ID	202	PEB	C1D-ND	2.14	1.49	1.45
26	WE	201	PEB	C1C-CHB	2.14	1.49	1.41
26	fF	201	PEB	C1C-CHB	2.14	1.49	1.41
26	O7	201	PEB	C4A-NA	-2.14	1.32	1.37
26	FD	203	PEB	C4A-NA	-2.14	1.32	1.37
26	dI	202	PEB	C4A-NA	-2.14	1.32	1.37
26	XD	203	PEB	C4B-C3B	2.14	1.49	1.45
26	W9	202	PEB	C1B-C2B	2.14	1.50	1.45
26	aE	203	PEB	C1B-C2B	2.14	1.50	1.45
26	Y3	303	PEB	C1D-ND	2.14	1.49	1.45
26	GA	203	PEB	C1C-CHB	2.14	1.49	1.41
26	i6	202	PEB	C4B-C3B	2.14	1.49	1.45
26	a1	203	PEB	C2A-C1A	-2.14	1.50	1.52
28	dH	1001	CYC	C4C-NC	-2.14	1.32	1.37
26	ZA	202	PEB	C1B-C2B	2.14	1.50	1.45
26	hG	201	PEB	C1B-C2B	2.14	1.50	1.45
26	dF	201	PEB	C4B-C3B	2.14	1.49	1.45
26	JJ	201	PEB	C4B-C3B	2.14	1.49	1.45
26	a4	202	PEB	C1C-CHB	2.14	1.49	1.41
26	V1	202	PEB	C4A-NA	-2.14	1.32	1.37
26	a6	202	PEB	C4A-NA	-2.14	1.32	1.37
26	F7	1002	PEB	C4A-NA	-2.14	1.32	1.37
26	kA	202	PEB	C4A-NA	-2.14	1.32	1.37
26	q1	201	PEB	C4A-NA	-2.14	1.32	1.37
26	R6	202	PEB	C4A-NA	-2.14	1.32	1.37
26	AA	301	PEB	C4A-NA	-2.14	1.32	1.37
26	ND	201	PEB	C4A-NA	-2.14	1.32	1.37
26	BG	202	PEB	C4A-NA	-2.14	1.32	1.37
26	21	401	PEB	C2A-C1A	-2.14	1.50	1.52
28	I7	1001	CYC	OB-C4B	2.14	1.27	1.23
26	QD	201	PEB	C1B-C2B	2.14	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eI	201	PEB	C1B-C2B	2.14	1.50	1.45
26	f4	201	PEB	C4A-NA	-2.14	1.32	1.37
26	h7	202	PEB	C1C-CHB	2.14	1.49	1.41
26	D3	202	PEB	C4B-C3B	2.14	1.49	1.45
26	G8	202	PEB	C4B-C3B	2.14	1.49	1.45
26	OB	203	PEB	C4B-C3B	2.14	1.49	1.45
26	V3	203	PEB	C1C-CHB	2.14	1.49	1.41
28	C2	1001	CYC	C1B-C2B	2.14	1.49	1.45
26	bF	203	PEB	C4A-NA	-2.14	1.32	1.37
26	bG	201	PEB	C4A-NA	-2.14	1.32	1.37
26	k2	201	PEB	C2A-C1A	-2.14	1.50	1.52
26	H7	1002	PEB	C2A-C1A	-2.14	1.50	1.52
26	l7	201	PEB	C1C-CHB	2.14	1.49	1.41
26	HF	1002	PEB	C1C-CHB	2.14	1.49	1.41
26	U9	201	PEB	C4B-C3B	2.14	1.49	1.45
26	lE	202	PEB	C4B-C3B	2.14	1.49	1.45
26	LG	202	PEB	C4B-C3B	2.14	1.49	1.45
26	A4	201	PEB	C4A-NA	-2.14	1.32	1.37
26	BD	201	PEB	C4A-NA	-2.14	1.32	1.37
26	A5	202	PEB	C1D-ND	2.14	1.49	1.45
26	B5	201	PEB	C1D-ND	2.14	1.49	1.45
26	NE	202	PEB	C4A-NA	-2.14	1.32	1.37
26	b1	501	PEB	C2A-C1A	-2.14	1.50	1.52
26	uE	202	PEB	C1C-CHB	2.14	1.49	1.41
26	VI	203	PEB	C1C-CHB	2.14	1.49	1.41
26	i6	201	PEB	C4A-NA	-2.14	1.32	1.37
26	A8	301	PEB	C4A-NA	-2.14	1.32	1.37
26	D9	202	PEB	C4B-NB	-2.14	1.34	1.38
26	S4	201	PEB	C1C-CHB	2.14	1.49	1.41
26	k4	201	PEB	C1C-CHB	2.14	1.49	1.41
26	YD	303	PEB	C4A-NA	-2.14	1.32	1.37
26	V7	202	PEB	C1B-C2B	2.14	1.50	1.45
28	L2	1001	CYC	C1B-C2B	2.14	1.48	1.45
26	a8	201	PEB	C4A-NA	-2.13	1.32	1.37
26	O8	202	PEB	C2A-C1A	-2.13	1.50	1.52
26	WE	203	PEB	C2A-C1A	-2.13	1.50	1.52
26	SI	202	PEB	C2A-C1A	-2.13	1.50	1.52
26	f4	201	PEB	C1B-C2B	2.13	1.50	1.45
26	mF	202	PEB	C1C-CHB	2.13	1.49	1.41
28	fH	1001	CYC	C1A-C2A	2.13	1.49	1.45
26	pE	202	PEB	C4A-NA	-2.13	1.32	1.37
26	J1	202	PEB	C2A-C1A	-2.13	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	pG	201	PEB	C2A-C1A	-2.13	1.50	1.52
26	EA	202	PEB	C1C-CHB	2.13	1.49	1.41
26	fA	203	PEB	C1C-CHB	2.13	1.49	1.41
26	O1	201	PEB	C1B-C2B	2.13	1.50	1.45
26	XA	201	PEB	C1B-C2B	2.13	1.50	1.45
26	G8	202	PEB	C4A-NA	-2.13	1.32	1.37
26	qG	201	PEB	C1C-CHB	2.13	1.49	1.41
28	HB	1001	CYC	C1D-CHD	2.13	1.49	1.41
26	L1	203	PEB	C2A-C1A	-2.13	1.50	1.52
26	MG	203	PEB	C1C-CHB	2.13	1.49	1.41
26	w4	204	PEB	C4B-C3B	2.13	1.49	1.45
28	nH	1001	CYC	C1A-C2A	2.13	1.49	1.45
28	FF	1001	CYC	C4B-NB	-2.13	1.33	1.38
26	K8	201	PEB	C1B-C2B	2.13	1.50	1.45
26	E9	201	PEB	C1B-C2B	2.13	1.50	1.45
28	LB	1001	CYC	OB-C4B	2.13	1.27	1.23
26	s4	201	PEB	C4A-NA	-2.13	1.32	1.37
26	AD	201	PEB	C1C-CHB	2.13	1.49	1.41
26	A2	305	PEB	C2A-C1A	-2.13	1.50	1.52
26	A4	202	PEB	C4B-C3B	2.13	1.49	1.45
26	Y3	304	PEB	C4A-NA	-2.13	1.32	1.37
26	AG	202	PEB	C4A-NA	-2.13	1.32	1.37
26	C5	204	PEB	C1D-ND	2.13	1.48	1.45
26	KJ	201	PEB	C1C-CHB	2.13	1.49	1.41
26	V7	201	PEB	C1B-C2B	2.13	1.50	1.45
26	A1	202	PEB	C4A-NA	-2.13	1.32	1.37
26	AF	305	PEB	C4B-C3B	2.13	1.49	1.45
26	RI	202	PEB	C4B-C3B	2.13	1.49	1.45
26	vG	201	PEB	C1C-CHB	2.13	1.49	1.41
26	f2	201	PEB	C1D-ND	2.13	1.48	1.45
26	DD	202	PEB	C1D-ND	2.13	1.48	1.45
26	E1	202	PEB	C2A-C1A	-2.13	1.50	1.52
26	J7	1002	PEB	C2A-C1A	-2.13	1.50	1.52
26	I8	203	PEB	C2A-C1A	-2.13	1.50	1.52
26	T9	202	PEB	C1C-CHB	2.13	1.49	1.41
26	f4	202	PEB	C1C-CHB	2.13	1.49	1.41
26	a2	202	PEB	C4B-C3B	2.13	1.49	1.45
26	jA	202	PEB	C4B-C3B	2.13	1.49	1.45
26	JJ	203	PEB	C1C-CHB	2.13	1.49	1.41
26	ZG	201	PEB	C4A-NA	-2.13	1.32	1.37
26	H7	1002	PEB	C4B-C3B	2.13	1.49	1.45
26	V9	203	PEB	C4B-C3B	2.13	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	uG	203	PEB	C2A-C1A	-2.13	1.50	1.52
26	21	405	PEB	C4A-NA	-2.13	1.32	1.37
26	P9	201	PEB	C1D-ND	2.13	1.48	1.45
26	VJ	201	PEB	C1C-CHB	2.13	1.49	1.41
26	s1	203	PEB	C1C-CHB	2.13	1.49	1.41
26	B3	203	PEB	C1C-CHB	2.13	1.49	1.41
26	d6	204	PEB	C4A-NA	-2.13	1.32	1.37
28	GI	1001	CYC	C4B-NB	-2.13	1.33	1.38
26	l7	202	PEB	C1D-ND	2.13	1.48	1.45
26	P4	201	PEB	C4A-NA	-2.13	1.32	1.37
26	WE	203	PEB	C1C-CHB	2.13	1.49	1.41
26	m1	203	PEB	C4B-C3B	2.13	1.49	1.45
26	B1	203	PEB	C2A-C1A	-2.13	1.50	1.52
28	CI	1001	CYC	C1B-C2B	2.13	1.48	1.45
26	f7	201	PEB	C1C-CHB	2.13	1.49	1.41
26	i8	201	PEB	C4B-C3B	2.13	1.49	1.45
28	D6	1001	CYC	C1D-CHD	2.13	1.49	1.41
26	rE	201	PEB	C1C-CHB	2.13	1.49	1.41
26	M1	403	PEB	C2A-C1A	-2.13	1.50	1.52
26	c2	203	PEB	C2A-C1A	-2.13	1.50	1.52
26	JA	202	PEB	C2A-C1A	-2.13	1.50	1.52
26	WA	201	PEB	C4B-NB	-2.13	1.34	1.38
26	q1	202	PEB	C4B-C3B	2.13	1.49	1.45
27	A7	304	PUB	C1C-C2C	2.13	1.49	1.45
26	L2	1002	PEB	C4A-NA	-2.13	1.32	1.37
26	eD	401	PEB	C4A-NA	-2.13	1.32	1.37
26	VJ	201	PEB	C4A-NA	-2.13	1.32	1.37
26	Q7	202	PEB	C1B-C2B	2.13	1.50	1.45
26	HA	202	PEB	C1B-C2B	2.13	1.50	1.45
26	xG	304	PEB	C1C-CHB	2.13	1.49	1.41
26	CC	201	PEB	C4A-NA	-2.13	1.32	1.37
26	KA	201	PEB	C1B-C2B	2.13	1.50	1.45
28	B6	1001	CYC	C1B-C2B	2.13	1.48	1.45
26	CC	203	PEB	C1C-CHB	2.13	1.49	1.41
26	OE	201	PEB	C1C-CHB	2.13	1.49	1.41
26	UI	202	PEB	C2A-C1A	-2.13	1.50	1.52
26	jG	201	PEB	C4B-C3B	2.13	1.49	1.45
26	LI	1002	PEB	C4A-NA	-2.13	1.32	1.37
26	VD	203	PEB	C1C-CHB	2.13	1.49	1.41
28	dH	1001	CYC	C1B-C2B	2.13	1.48	1.45
26	fA	203	PEB	C4A-NA	-2.12	1.32	1.37
26	wG	303	PEB	C4A-NA	-2.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ME	203	PEB	C2A-C1A	-2.12	1.50	1.52
26	GD	202	PEB	C4A-NA	-2.12	1.32	1.37
26	F1	201	PEB	C4B-C3B	2.12	1.49	1.45
26	QB	201	PEB	C4B-C3B	2.12	1.49	1.45
26	PG	202	PEB	C4B-C3B	2.12	1.49	1.45
26	Y3	303	PEB	C1B-C2B	2.12	1.50	1.45
26	F3	202	PEB	C4B-C3B	2.12	1.49	1.45
26	O2	202	PEB	C2A-C1A	-2.12	1.50	1.52
26	h7	203	PEB	C2A-C1A	-2.12	1.50	1.52
26	EE	202	PEB	C4A-NA	-2.12	1.32	1.37
26	C5	204	PEB	C1C-CHB	2.12	1.49	1.41
26	K8	202	PEB	C4A-NA	-2.12	1.32	1.37
28	JI	1001	CYC	C1A-NA	-2.12	1.34	1.38
26	iA	202	PEB	C4A-NA	-2.12	1.32	1.37
28	LI	1001	CYC	C1B-C2B	2.12	1.48	1.45
26	G1	201	PEB	C1B-C2B	2.12	1.50	1.45
26	X1	203	PEB	C1B-C2B	2.12	1.50	1.45
26	G9	201	PEB	C4A-NA	-2.12	1.32	1.37
26	f6	202	PEB	C4B-C3B	2.12	1.49	1.45
26	i1	203	PEB	C1D-ND	2.12	1.48	1.45
26	mB	201	PEB	C1D-ND	2.12	1.48	1.45
26	eF	202	PEB	C1D-ND	2.12	1.48	1.45
26	AJ	303	PEB	C1D-ND	2.12	1.48	1.45
26	wE	303	PEB	C1B-C2B	2.12	1.50	1.45
26	w1	201	PEB	C4A-NA	-2.12	1.32	1.37
26	Y7	201	PEB	C4A-NA	-2.12	1.32	1.37
26	IC	203	PEB	C2A-C1A	-2.12	1.50	1.52
26	X3	201	PEB	C1C-CHB	2.12	1.49	1.41
26	lF	201	PEB	C4B-C3B	2.12	1.49	1.45
26	kG	202	PEB	C1D-ND	2.12	1.48	1.45
26	SE	202	PEB	O1C-CGC	2.12	1.29	1.22
26	RE	201	PEB	C1C-CHB	2.12	1.49	1.41
26	zG	501	PEB	C1C-CHB	2.12	1.49	1.41
26	S7	202	PEB	C2A-C1A	-2.12	1.50	1.52
26	cI	201	PEB	C2A-C1A	-2.12	1.50	1.52
26	u1	201	PEB	C4A-NA	-2.12	1.32	1.37
26	YA	203	PEB	C4A-NA	-2.12	1.32	1.37
26	VE	202	PEB	C4A-NA	-2.12	1.32	1.37
26	BJ	201	PEB	C4A-NA	-2.12	1.32	1.37
26	S7	203	PEB	C1C-CHB	2.12	1.49	1.41
26	w1	202	PEB	C4A-NA	-2.12	1.32	1.37
26	Y8	203	PEB	C4A-NA	-2.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	EG	201	PEB	C4A-NA	-2.12	1.32	1.37
28	gH	1001	CYC	C4D-CHA	2.12	1.49	1.41
28	PH	1001	CYC	C4A-C3A	2.12	1.50	1.45
26	kG	203	PEB	C4B-C3B	2.12	1.49	1.45
26	y1	202	PEB	C1C-CHB	2.12	1.49	1.41
26	YD	304	PEB	C2A-C1A	-2.12	1.50	1.52
26	kE	201	PEB	C2A-C1A	-2.12	1.50	1.52
26	WD	201	PEB	OD-C4D	2.12	1.27	1.23
26	m7	202	PEB	C1C-CHB	2.12	1.49	1.41
28	qH	1001	CYC	C4D-CHA	2.12	1.49	1.41
26	11	201	PEB	C1C-CHB	2.12	1.49	1.41
28	DF	1001	CYC	C1B-NB	-2.12	1.34	1.37
26	e2	201	PEB	C1B-C2B	2.12	1.50	1.45
26	i8	201	PEB	C1D-ND	2.12	1.48	1.45
26	Y9	201	PEB	C4B-C3B	2.12	1.49	1.45
26	PJ	201	PEB	C2A-C1A	-2.12	1.50	1.52
26	jF	201	PEB	C1B-C2B	2.12	1.50	1.45
26	lI	202	PEB	C4A-NA	-2.12	1.32	1.37
26	aA	201	PEB	C1D-ND	2.12	1.48	1.45
26	L5	203	PEB	O1B-CGB	2.12	1.29	1.22
26	FD	203	PEB	C1C-CHB	2.12	1.49	1.41
27	xE	306	PUB	C4C-NC	2.12	1.38	1.35
26	aI	203	PEB	C1C-CHB	2.12	1.49	1.41
26	m6	201	PEB	C4B-C3B	2.12	1.49	1.45
26	UE	203	PEB	C4B-C3B	2.12	1.49	1.45
26	A2	305	PEB	C4A-NA	-2.12	1.32	1.37
26	j8	203	PEB	C4A-NA	-2.12	1.32	1.37
26	EA	203	PEB	C4A-NA	-2.12	1.32	1.37
28	MH	1001	CYC	C4D-CHA	2.12	1.49	1.41
28	fH	1001	CYC	C4B-NB	-2.12	1.33	1.38
28	wH	1001	CYC	C4A-C3A	2.12	1.50	1.45
26	g2	201	PEB	C2A-C1A	-2.12	1.50	1.52
26	Y2	202	PEB	C4A-NA	-2.12	1.32	1.37
28	BB	1001	CYC	C1B-C2B	2.12	1.48	1.45
26	XJ	201	PEB	C4B-C3B	2.12	1.49	1.45
26	P4	203	PEB	C1C-CHB	2.12	1.49	1.41
26	d7	202	PEB	C1C-CHB	2.12	1.49	1.41
26	nG	202	PEB	C1D-ND	2.12	1.48	1.45
26	A7	305	PEB	C4B-C3B	2.12	1.49	1.45
26	EA	201	PEB	C1C-CHB	2.12	1.49	1.41
26	r4	201	PEB	C1D-ND	2.12	1.48	1.45
26	fE	201	PEB	C1C-CHB	2.12	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	SH	1001	CYC	C4A-C3A	2.12	1.50	1.45
26	iE	203	PEB	C4B-C3B	2.12	1.49	1.45
26	V4	202	PEB	C4A-NA	-2.12	1.32	1.37
26	cB	202	PEB	C4A-NA	-2.12	1.32	1.37
26	H3	202	PEB	C1C-CHB	2.12	1.49	1.41
26	P1	201	PEB	C4A-NA	-2.11	1.32	1.37
26	t4	202	PEB	C1C-CHB	2.11	1.49	1.41
26	c2	202	PEB	C2A-C1A	-2.11	1.50	1.52
26	U4	202	PEB	C4A-NA	-2.11	1.32	1.37
26	OG	201	PEB	C4A-NA	-2.11	1.32	1.37
26	WG	203	PEB	C4A-NA	-2.11	1.32	1.37
26	eB	201	PEB	C4B-C3B	2.11	1.49	1.45
26	E8	201	PEB	C1C-CHB	2.11	1.49	1.41
28	OH	1001	CYC	C4D-CHA	2.11	1.49	1.41
26	Q9	202	PEB	C4A-NA	-2.11	1.32	1.37
26	hA	203	PEB	C4A-NA	-2.11	1.32	1.37
26	lA	203	PEB	C4A-NA	-2.11	1.32	1.37
28	F7	1001	CYC	C4C-NC	-2.11	1.32	1.37
26	T3	201	PEB	C4B-C3B	2.11	1.49	1.45
26	J9	201	PEB	C4B-C3B	2.11	1.49	1.45
26	B4	202	PEB	C1C-CHB	2.11	1.49	1.41
26	H6	1002	PEB	C1C-CHB	2.11	1.49	1.41
26	PB	202	PEB	C4A-NA	-2.11	1.32	1.37
26	SB	203	PEB	C4A-NA	-2.11	1.32	1.37
26	i2	203	PEB	C2A-C1A	-2.11	1.50	1.52
26	AI	304	PEB	C2A-C1A	-2.11	1.50	1.52
26	NF	1002	PEB	C4A-NA	-2.11	1.32	1.37
26	f1	201	PEB	C4B-C3B	2.11	1.49	1.45
26	y1	202	PEB	C4B-C3B	2.11	1.49	1.45
26	B4	203	PEB	C4B-C3B	2.11	1.49	1.45
26	JG	201	PEB	C1C-CHB	2.11	1.49	1.41
26	b4	501	PEB	C4A-NA	-2.11	1.32	1.37
26	lB	202	PEB	C4A-NA	-2.11	1.32	1.37
26	jA	201	PEB	C1D-ND	2.11	1.48	1.45
26	l7	202	PEB	C2A-C1A	-2.11	1.50	1.52
26	tG	201	PEB	C1C-CHB	2.11	1.49	1.41
26	W1	201	PEB	C1B-C2B	2.11	1.50	1.45
28	F2	1001	CYC	C1B-C2B	2.11	1.48	1.45
26	fB	202	PEB	C4B-C3B	2.11	1.49	1.45
28	DB	1001	CYC	C1D-CHD	2.11	1.49	1.41
26	f6	203	PEB	C2A-C1A	-2.11	1.50	1.52
26	eG	203	PEB	C2A-C1A	-2.11	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cF	201	PEB	C4A-NA	-2.11	1.32	1.37
26	IA	201	PEB	C4B-C3B	2.11	1.49	1.45
26	f8	203	PEB	C1C-CHB	2.11	1.49	1.41
28	UH	1001	CYC	C4D-CHA	2.11	1.49	1.41
26	M8	201	PEB	C4B-NB	-2.11	1.34	1.38
26	c2	202	PEB	C4A-NA	-2.11	1.32	1.37
26	iG	202	PEB	C4A-NA	-2.11	1.32	1.37
28	J7	1003	CYC	C1D-CHD	2.11	1.49	1.41
26	S2	201	PEB	C1B-C2B	2.11	1.50	1.45
26	rG	201	PEB	C1C-CHB	2.11	1.49	1.41
26	l6	202	PEB	C4A-NA	-2.11	1.32	1.37
26	gF	201	PEB	C4A-NA	-2.11	1.32	1.37
26	gG	202	PEB	C4A-NA	-2.11	1.32	1.37
26	C3	202	PEB	C1B-C2B	2.11	1.50	1.45
28	NB	1001	CYC	C1D-CHD	2.11	1.49	1.41
28	iH	1001	CYC	C4D-CHA	2.11	1.49	1.41
26	YJ	201	PEB	C4A-NA	-2.11	1.32	1.37
26	Q3	201	PEB	C1B-C2B	2.11	1.50	1.45
26	cG	203	PEB	C1C-CHB	2.11	1.49	1.41
26	Z2	202	PEB	C4A-NA	-2.11	1.32	1.37
26	d2	202	PEB	C4A-NA	-2.11	1.32	1.37
26	S9	201	PEB	C4A-NA	-2.11	1.32	1.37
26	fF	202	PEB	C4A-NA	-2.11	1.32	1.37
26	K1	202	PEB	C1C-CHB	2.11	1.49	1.41
26	qG	203	PEB	C1B-C2B	2.11	1.50	1.45
26	UB	201	PEB	C4A-NA	-2.11	1.32	1.37
26	D4	203	PEB	C1B-C2B	2.11	1.50	1.45
26	j6	201	PEB	C1C-CHB	2.11	1.49	1.41
26	mB	202	PEB	C1C-CHB	2.11	1.49	1.41
26	W3	201	PEB	OD-C4D	2.11	1.27	1.23
26	Q9	202	PEB	C4B-C3B	2.11	1.49	1.45
26	h8	203	PEB	C4A-NA	-2.11	1.32	1.37
28	DF	1003	CYC	C1D-CHD	2.11	1.49	1.41
26	K9	201	PEB	C4A-NA	-2.11	1.32	1.37
26	lE	201	PEB	C2A-C1A	-2.11	1.50	1.52
26	QF	202	PEB	C2A-C1A	-2.11	1.50	1.52
26	gI	202	PEB	C2A-C1A	-2.11	1.50	1.52
26	CE	201	PEB	C1C-CHB	2.11	1.49	1.41
26	j6	202	PEB	C4A-NA	-2.11	1.32	1.37
26	aA	203	PEB	C4A-NA	-2.11	1.32	1.37
26	ZE	202	PEB	C4A-NA	-2.11	1.32	1.37
26	rE	202	PEB	C4A-NA	-2.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j6	201	PEB	C4B-C3B	2.11	1.49	1.45
26	dB	203	PEB	C4A-NA	-2.11	1.32	1.37
26	hF	202	PEB	C1D-ND	2.11	1.48	1.45
26	e7	202	PEB	C1C-CHB	2.11	1.49	1.41
26	oE	201	PEB	C1C-CHB	2.11	1.49	1.41
26	VJ	203	PEB	C1C-CHB	2.11	1.49	1.41
26	aE	203	PEB	C2A-C1A	-2.11	1.50	1.52
26	S7	201	PEB	C4B-C3B	2.11	1.49	1.45
26	j2	202	PEB	C4A-NA	-2.11	1.32	1.37
26	Q7	202	PEB	C4A-NA	-2.10	1.32	1.37
26	aI	203	PEB	C4A-NA	-2.10	1.32	1.37
26	D9	202	PEB	OD-C4D	2.10	1.27	1.23
26	FE	202	PEB	C4B-C3B	2.10	1.49	1.45
28	F7	1001	CYC	C1D-CHD	2.10	1.49	1.41
26	AJ	305	PEB	C2A-C1A	-2.10	1.50	1.52
26	W7	201	PEB	C1C-CHB	2.10	1.49	1.41
26	VA	202	PEB	C1D-ND	2.10	1.48	1.45
26	Q4	201	PEB	C4B-C3B	2.10	1.49	1.45
26	HA	202	PEB	C4B-C3B	2.10	1.49	1.45
26	Q7	202	PEB	C1C-CHB	2.10	1.49	1.41
26	wE	303	PEB	C4A-NA	-2.10	1.32	1.37
26	v4	202	PEB	C1D-ND	2.10	1.48	1.45
26	HB	1002	PEB	C1C-CHB	2.10	1.49	1.41
26	cB	201	PEB	C4B-C3B	2.10	1.49	1.45
26	C3	202	PEB	C4A-NA	-2.10	1.32	1.37
26	kA	201	PEB	C2A-C1A	-2.10	1.50	1.52
26	ZI	202	PEB	C2A-C1A	-2.10	1.50	1.52
26	S8	203	PEB	C4B-C3B	2.10	1.49	1.45
26	PA	201	PEB	C4B-C3B	2.10	1.49	1.45
26	D8	202	PEB	C1C-CHB	2.10	1.49	1.41
26	mI	203	PEB	C1C-CHB	2.10	1.49	1.41
26	I5	203	PEB	C4A-NA	-2.10	1.32	1.37
26	A7	301	PEB	C4A-NA	-2.10	1.32	1.37
26	F4	202	PEB	C4B-NB	-2.10	1.34	1.38
28	E6	1001	CYC	C1B-C2B	2.10	1.48	1.45
26	A3	202	PEB	C4B-C3B	2.10	1.49	1.45
26	dF	203	PEB	C4B-C3B	2.10	1.49	1.45
26	UE	203	PEB	C2A-C1A	-2.10	1.50	1.52
26	YJ	201	PEB	C2A-C1A	-2.10	1.50	1.52
26	M1	403	PEB	C4A-NA	-2.10	1.32	1.37
26	WF	201	PEB	C4A-NA	-2.10	1.32	1.37
26	iG	203	PEB	C4A-NA	-2.10	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	DE	202	PEB	C4B-NB	-2.10	1.34	1.38
26	DA	201	PEB	C1D-ND	2.10	1.48	1.45
26	h1	202	PEB	C4A-NA	-2.10	1.32	1.37
26	uG	201	PEB	C2A-C1A	-2.10	1.50	1.52
26	C3	201	PEB	C4B-NB	-2.10	1.34	1.38
26	kG	203	PEB	C1C-CHB	2.10	1.49	1.41
28	EH	1001	CYC	C4B-NB	-2.10	1.33	1.38
28	qH	1001	CYC	C4B-NB	-2.10	1.33	1.38
26	V2	203	PEB	C1C-CHB	2.10	1.49	1.41
26	D7	1002	PEB	C4A-NA	-2.10	1.32	1.37
26	fB	201	PEB	C4A-NA	-2.10	1.32	1.37
26	GG	203	PEB	C4A-NA	-2.10	1.32	1.37
26	gI	203	PEB	C4A-NA	-2.10	1.32	1.37
26	eE	201	PEB	CHA-C4A	-2.10	1.32	1.36
28	NF	1001	CYC	C4D-CHA	2.10	1.49	1.41
26	U1	202	PEB	C1B-C2B	2.10	1.50	1.45
26	d6	204	PEB	C1C-CHB	2.10	1.49	1.41
26	bF	203	PEB	C1C-CHB	2.10	1.49	1.41
26	a4	203	PEB	C4A-NA	-2.10	1.32	1.37
26	S6	203	PEB	C4A-NA	-2.10	1.32	1.37
26	FJ	202	PEB	C4A-NA	-2.10	1.32	1.37
26	MD	202	PEB	C4A-NA	-2.10	1.32	1.37
28	HB	1001	CYC	OB-C4B	2.10	1.27	1.23
26	nE	201	PEB	C1C-CHB	2.10	1.49	1.41
28	HF	1001	CYC	C1B-NB	-2.10	1.34	1.37
26	e6	203	PEB	C1C-CHB	2.10	1.49	1.41
26	g7	202	PEB	C1C-CHB	2.10	1.49	1.41
26	dF	202	PEB	C1B-C2B	2.10	1.50	1.45
26	DJ	202	PEB	C4B-NB	-2.10	1.34	1.38
26	l2	201	PEB	CHA-C4A	-2.10	1.32	1.36
26	r1	201	PEB	C4B-C3B	2.10	1.49	1.45
26	bF	201	PEB	C1C-CHB	2.10	1.49	1.41
26	TG	202	PEB	C1D-ND	2.10	1.48	1.45
26	d6	202	PEB	C4A-NA	-2.10	1.32	1.37
26	g6	202	PEB	C4A-NA	-2.10	1.32	1.37
26	Q7	201	PEB	C1C-CHB	2.10	1.49	1.41
26	QJ	202	PEB	C1B-C2B	2.10	1.50	1.45
26	CG	203	PEB	C4A-NA	-2.10	1.32	1.37
26	FI	1002	PEB	C4A-NA	-2.10	1.32	1.37
26	c1	201	PEB	C2A-C1A	-2.10	1.50	1.52
26	m8	201	PEB	C1D-ND	2.10	1.48	1.45
26	VA	202	PEB	C1B-C2B	2.10	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fG	201	PEB	C1C-CHB	2.10	1.49	1.41
26	W6	201	PEB	C1B-C2B	2.10	1.50	1.45
26	V8	201	PEB	C1D-ND	2.10	1.48	1.45
26	Q6	203	PEB	C4A-NA	-2.10	1.32	1.37
26	CD	201	PEB	C4B-NB	-2.10	1.34	1.38
28	dH	1001	CYC	C4B-NB	-2.10	1.33	1.38
26	VJ	202	PEB	C1C-CHB	2.10	1.49	1.41
26	f8	203	PEB	C2A-C1A	-2.10	1.50	1.52
28	E7	1001	CYC	OB-C4B	2.10	1.27	1.23
26	CA	202	PEB	C4A-NA	-2.10	1.32	1.37
26	H7	1002	PEB	C1C-CHB	2.10	1.49	1.41
26	24	404	PEB	C1B-C2B	2.10	1.50	1.45
26	aB	202	PEB	C4A-NA	-2.10	1.32	1.37
26	BE	202	PEB	C4A-NA	-2.10	1.32	1.37
28	uH	1001	CYC	C4A-C3A	2.10	1.50	1.45
26	g6	202	PEB	C2A-C1A	-2.10	1.50	1.52
26	E8	203	PEB	C2A-C1A	-2.10	1.50	1.52
26	U7	201	PEB	C1C-CHB	2.10	1.49	1.41
26	V9	202	PEB	C1C-CHB	2.10	1.49	1.41
26	pG	202	PEB	C1B-C2B	2.10	1.50	1.45
26	QA	202	PEB	C1C-CHB	2.10	1.49	1.41
26	r1	201	PEB	C1D-ND	2.10	1.48	1.45
28	D7	1001	CYC	C4D-CHA	2.09	1.49	1.41
26	qG	202	PEB	C1B-C2B	2.09	1.50	1.45
26	i1	201	PEB	C4A-NA	-2.09	1.32	1.37
28	J7	1003	CYC	C4C-NC	-2.09	1.32	1.37
26	dB	203	PEB	C2A-C1A	-2.09	1.50	1.52
26	21	405	PEB	C1D-ND	2.09	1.48	1.45
26	Z4	201	PEB	C1C-CHB	2.09	1.49	1.41
26	C3	202	PEB	C1D-ND	2.09	1.48	1.45
26	nE	202	PEB	C1D-ND	2.09	1.48	1.45
26	RB	202	PEB	C4A-NA	-2.09	1.32	1.37
26	OI	202	PEB	C4A-NA	-2.09	1.32	1.37
26	AB	301	PEB	C4B-C3B	2.09	1.49	1.45
26	j1	202	PEB	C2A-C1A	-2.09	1.50	1.52
26	o1	501	PEB	C2A-C1A	-2.09	1.50	1.52
26	G4	201	PEB	C2A-C1A	-2.09	1.50	1.52
26	A5	202	PEB	C2A-C1A	-2.09	1.50	1.52
26	YE	201	PEB	C1C-CHB	2.09	1.49	1.41
26	SG	202	PEB	O1C-CGC	2.09	1.29	1.22
26	s4	202	PEB	C4B-C3B	2.09	1.49	1.45
28	NB	1001	CYC	C1B-C2B	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r4	201	PEB	C1B-C2B	2.09	1.50	1.45
26	f2	202	PEB	C1D-ND	2.09	1.48	1.45
26	A1	202	PEB	C2A-C1A	-2.09	1.50	1.52
26	L6	1002	PEB	C4A-NA	-2.09	1.33	1.37
26	QF	202	PEB	C4A-NA	-2.09	1.33	1.37
27	xE	305	PUB	C4B-CHB	2.09	1.49	1.41
26	H5	203	PEB	O1B-CGB	2.09	1.29	1.22
26	LA	202	PEB	C4A-NA	-2.09	1.33	1.37
26	F5	203	PEB	O1B-CGB	2.09	1.29	1.22
26	u1	201	PEB	C2A-C1A	-2.09	1.50	1.52
26	VA	201	PEB	C1D-ND	2.09	1.48	1.45
26	lE	201	PEB	C1D-ND	2.09	1.48	1.45
26	bF	201	PEB	C4B-C3B	2.09	1.49	1.45
27	Y3	302	PUB	C4C-NC	2.09	1.38	1.35
26	RG	201	PEB	C1C-CHB	2.09	1.49	1.41
26	m1	203	PEB	C1D-ND	2.09	1.48	1.45
26	HB	1002	PEB	C4A-NA	-2.09	1.33	1.37
26	CE	203	PEB	C4A-NA	-2.09	1.33	1.37
26	cG	202	PEB	C4A-NA	-2.09	1.33	1.37
26	J1	202	PEB	C1C-CHB	2.09	1.49	1.41
26	uE	202	PEB	C2A-C1A	-2.09	1.50	1.52
26	sG	202	PEB	C2A-C1A	-2.09	1.50	1.52
26	m1	201	PEB	C4A-NA	-2.09	1.33	1.37
26	gB	202	PEB	C4A-NA	-2.09	1.33	1.37
26	AF	305	PEB	C4A-NA	-2.09	1.33	1.37
26	h7	203	PEB	C1C-CHB	2.09	1.49	1.41
28	RH	1001	CYC	C4D-CHA	2.09	1.49	1.41
26	u4	202	PEB	C4A-NA	-2.09	1.33	1.37
26	l8	203	PEB	C4A-NA	-2.09	1.33	1.37
28	E2	1001	CYC	C4A-C3A	2.09	1.50	1.45
26	VA	202	PEB	C4B-C3B	2.09	1.49	1.45
26	S1	201	PEB	C1C-CHB	2.09	1.49	1.41
26	I3	201	PEB	C1C-CHB	2.09	1.49	1.41
26	P4	201	PEB	CHC-C4C	2.09	1.55	1.50
26	R9	203	PEB	C4B-NB	-2.09	1.34	1.38
26	ID	202	PEB	C4A-NA	-2.09	1.33	1.37
26	ME	202	PEB	C4A-NA	-2.09	1.33	1.37
26	X4	203	PEB	C2A-C1A	-2.09	1.50	1.52
26	k6	201	PEB	C1C-CHB	2.09	1.49	1.41
26	FD	202	PEB	C1C-CHB	2.09	1.49	1.41
28	DF	1001	CYC	C4D-CHA	2.09	1.49	1.41
26	LD	202	PEB	C4B-C3B	2.09	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	WJ	202	PEB	C4B-C3B	2.09	1.49	1.45
28	J2	1001	CYC	C1B-C2B	2.09	1.48	1.45
26	bF	203	PEB	C1D-ND	2.09	1.48	1.45
28	N7	1001	CYC	C4A-C3A	2.09	1.50	1.45
26	PF	202	PEB	C4B-C3B	2.09	1.49	1.45
26	ZB	202	PEB	C1B-C2B	2.09	1.50	1.45
26	l6	203	PEB	C4A-NA	-2.09	1.33	1.37
28	AH	1001	CYC	C4A-C3A	2.09	1.50	1.45
27	A8	303	PUB	CHC-C4C	2.09	1.52	1.50
26	uE	202	PEB	C1D-ND	2.09	1.48	1.45
26	D1	201	PEB	C4A-NA	-2.09	1.33	1.37
26	m1	201	PEB	C4B-C3B	2.09	1.49	1.45
26	I8	201	PEB	C4B-C3B	2.09	1.49	1.45
26	SA	203	PEB	C4B-C3B	2.09	1.49	1.45
26	DJ	201	PEB	C4B-C3B	2.09	1.49	1.45
26	AE	202	PEB	C4A-NA	-2.09	1.33	1.37
26	B5	201	PEB	C1C-CHB	2.09	1.49	1.41
28	gH	1001	CYC	C4B-NB	-2.09	1.33	1.38
26	D3	201	PEB	C1D-ND	2.09	1.48	1.45
26	h7	203	PEB	C1D-ND	2.09	1.48	1.45
26	L1	201	PEB	C4A-NA	-2.09	1.33	1.37
28	F2	1001	CYC	OB-C4B	2.09	1.27	1.23
28	RH	1001	CYC	OB-C4B	2.09	1.27	1.23
26	A6	301	PEB	C2A-C1A	-2.09	1.50	1.52
26	dB	203	PEB	C4B-C3B	2.09	1.49	1.45
26	LG	201	PEB	C1A-NA	-2.09	1.34	1.37
26	V7	201	PEB	C4A-NA	-2.09	1.33	1.37
26	mG	202	PEB	C4A-NA	-2.09	1.33	1.37
26	JJ	201	PEB	C4A-NA	-2.09	1.33	1.37
26	JJ	203	PEB	C4A-NA	-2.09	1.33	1.37
26	bE	202	PEB	C1C-CHB	2.08	1.49	1.41
26	T2	202	PEB	C4B-C3B	2.08	1.49	1.45
26	dF	203	PEB	C1C-CHB	2.08	1.49	1.41
26	L4	203	PEB	C4A-NA	-2.08	1.33	1.37
28	N2	1001	CYC	C4A-C3A	2.08	1.50	1.45
26	xE	304	PEB	C1C-CHB	2.08	1.49	1.41
26	Q8	203	PEB	OD-C4D	2.08	1.27	1.23
26	g1	202	PEB	C1D-ND	2.08	1.48	1.45
26	h6	202	PEB	C1D-ND	2.08	1.48	1.45
26	S9	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	d7	202	PEB	C4B-C3B	2.08	1.49	1.45
26	F3	201	PEB	C1C-CHB	2.08	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cE	203	PEB	C4B-NB	-2.08	1.34	1.38
26	IA	203	PEB	C1C-CHB	2.08	1.49	1.41
26	N1	202	PEB	C4A-NA	-2.08	1.33	1.37
26	m4	201	PEB	C4A-NA	-2.08	1.33	1.37
26	Y2	203	PEB	C1C-CHB	2.08	1.49	1.41
26	lB	203	PEB	C2A-C1A	-2.08	1.50	1.52
26	mA	202	PEB	C1B-C2B	2.08	1.50	1.45
26	c4	203	PEB	C4A-NA	-2.08	1.33	1.37
26	OA	202	PEB	C4B-C3B	2.08	1.49	1.45
26	BC	201	PEB	C4B-C3B	2.08	1.49	1.45
26	eF	201	PEB	C4B-C3B	2.08	1.49	1.45
26	h4	202	PEB	C4A-NA	-2.08	1.33	1.37
26	j4	202	PEB	C1C-CHB	2.08	1.49	1.41
26	kI	202	PEB	C4A-NA	-2.08	1.33	1.37
26	VG	201	PEB	C1C-CHB	2.08	1.49	1.41
26	sE	203	PEB	C4A-NA	-2.08	1.33	1.37
28	GI	1001	CYC	C1B-NB	-2.08	1.34	1.37
26	DD	201	PEB	C1C-CHB	2.08	1.49	1.41
26	k8	202	PEB	C4A-NA	-2.08	1.33	1.37
26	C4	201	PEB	C1D-ND	2.08	1.48	1.45
26	lG	201	PEB	C1D-ND	2.08	1.48	1.45
26	K9	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	jB	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	i1	201	PEB	C1C-CHB	2.08	1.49	1.41
26	O2	202	PEB	C4A-NA	-2.08	1.33	1.37
26	d6	203	PEB	C4A-NA	-2.08	1.33	1.37
28	FB	1001	CYC	C1B-C2B	2.08	1.48	1.45
26	YI	203	PEB	C1C-CHB	2.08	1.49	1.41
26	IG	201	PEB	CBC-CGC	2.08	1.55	1.50
26	AC	203	PEB	C1D-ND	2.08	1.48	1.45
26	d8	202	PEB	C4B-C3B	2.08	1.49	1.45
26	HE	201	PEB	C4B-C3B	2.08	1.49	1.45
26	UD	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	f1	201	PEB	C4A-NA	-2.08	1.33	1.37
26	P2	203	PEB	C4B-C3B	2.08	1.49	1.45
26	R3	202	PEB	C4B-NB	-2.08	1.34	1.38
26	l7	203	PEB	C1C-CHB	2.08	1.49	1.41
26	QG	202	PEB	C1C-CHB	2.08	1.49	1.41
26	a7	201	PEB	C1C-CHB	2.08	1.49	1.41
26	bE	201	PEB	C4B-C3B	2.08	1.49	1.45
28	J7	1001	CYC	C1B-NB	-2.08	1.34	1.37
26	X8	201	PEB	C1B-C2B	2.08	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z7	202	PEB	C4A-NA	-2.08	1.33	1.37
26	XE	201	PEB	C1C-CHB	2.08	1.49	1.41
27	B8	302	PUB	C3C-C4C	2.08	1.50	1.43
26	cI	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	KJ	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	fI	201	PEB	C1B-C2B	2.08	1.50	1.45
26	DJ	202	PEB	C1B-C2B	2.08	1.50	1.45
26	V4	201	PEB	C4A-NA	-2.08	1.33	1.37
26	LD	203	PEB	C4A-NA	-2.08	1.33	1.37
26	BC	203	PEB	C1D-ND	2.08	1.48	1.45
26	W8	201	PEB	C4B-NB	-2.08	1.34	1.38
26	L3	202	PEB	C1C-CHB	2.08	1.49	1.41
26	j7	201	PEB	C4B-C3B	2.08	1.49	1.45
26	wE	303	PEB	C1C-CHB	2.08	1.49	1.41
26	h8	203	PEB	C2A-C1A	-2.08	1.50	1.52
26	p1	202	PEB	C1B-C2B	2.08	1.50	1.45
26	e1	201	PEB	C1C-CHB	2.08	1.49	1.41
26	QG	201	PEB	C4A-NA	-2.08	1.33	1.37
28	EB	1001	CYC	C1B-C2B	2.08	1.48	1.45
26	I3	202	PEB	C1C-CHB	2.08	1.49	1.41
26	mE	202	PEB	O1C-CGC	2.08	1.29	1.22
26	NB	1002	PEB	C4B-C3B	2.08	1.49	1.45
26	kF	202	PEB	C4B-C3B	2.08	1.49	1.45
26	RG	202	PEB	C4B-C3B	2.08	1.49	1.45
26	QD	201	PEB	C4B-NB	-2.08	1.34	1.38
26	j1	202	PEB	C1C-CHB	2.08	1.49	1.41
26	L3	202	PEB	C4B-C3B	2.08	1.49	1.45
28	1H	1000	CYC	C4D-CHA	2.08	1.49	1.41
26	K1	201	PEB	C4A-NA	-2.08	1.33	1.37
26	T1	203	PEB	C2A-C1A	-2.08	1.50	1.52
26	U8	203	PEB	C2A-C1A	-2.08	1.50	1.52
27	A6	302	PUB	C1C-NC	-2.08	1.34	1.38
26	O7	202	PEB	C1C-CHB	2.08	1.49	1.41
26	ZF	202	PEB	C4B-C3B	2.08	1.49	1.45
26	F4	201	PEB	C1B-C2B	2.08	1.50	1.45
26	YE	202	PEB	C1D-ND	2.08	1.48	1.45
26	fI	202	PEB	C1D-ND	2.08	1.48	1.45
26	X1	201	PEB	CHC-C4C	2.08	1.55	1.50
26	x4	201	PEB	C1C-CHB	2.08	1.49	1.41
28	C2	1001	CYC	C1D-CHD	2.08	1.49	1.41
26	U7	202	PEB	C2A-C1A	-2.08	1.50	1.52
26	j8	202	PEB	C2A-C1A	-2.08	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	tG	201	PEB	C4B-C3B	2.08	1.49	1.45
26	A8	301	PEB	C1B-C2B	2.08	1.50	1.45
26	P9	201	PEB	C1C-CHB	2.08	1.49	1.41
26	MG	202	PEB	C1C-CHB	2.08	1.49	1.41
26	Y2	201	PEB	C4A-NA	-2.08	1.33	1.37
26	h2	202	PEB	C4A-NA	-2.08	1.33	1.37
26	M3	202	PEB	C4A-NA	-2.08	1.33	1.37
26	AD	202	PEB	C4A-NA	-2.08	1.33	1.37
26	AJ	305	PEB	C4A-NA	-2.08	1.33	1.37
26	NJ	202	PEB	C1D-ND	2.08	1.48	1.45
26	V8	202	PEB	C1C-CHB	2.07	1.49	1.41
26	cE	203	PEB	C4D-ND	2.07	1.37	1.35
26	g2	202	PEB	C4B-C3B	2.07	1.49	1.45
26	TG	201	PEB	C1A-NA	-2.07	1.34	1.37
26	aE	202	PEB	C4A-NA	-2.07	1.33	1.37
26	l7	202	PEB	C1C-CHB	2.07	1.49	1.41
26	u4	201	PEB	C1B-C2B	2.07	1.50	1.45
26	a1	201	PEB	C1C-CHB	2.07	1.49	1.41
26	w4	203	PEB	C1C-CHB	2.07	1.49	1.41
26	KC	202	PEB	C4A-NA	-2.07	1.33	1.37
26	fG	201	PEB	C1A-NA	-2.07	1.34	1.37
26	m2	203	PEB	C1C-CHB	2.07	1.49	1.41
26	24	405	PEB	C1C-CHB	2.07	1.49	1.41
26	X4	203	PEB	C1B-C2B	2.07	1.50	1.45
26	SE	203	PEB	C1B-C2B	2.07	1.50	1.45
26	Q9	201	PEB	C1C-CHB	2.07	1.49	1.41
26	GJ	202	PEB	C2A-C1A	-2.07	1.50	1.52
26	T7	202	PEB	C1D-ND	2.07	1.48	1.45
26	uE	201	PEB	C1D-ND	2.07	1.48	1.45
26	MA	201	PEB	C4B-NB	-2.07	1.34	1.38
26	I8	203	PEB	C1C-CHB	2.07	1.49	1.41
26	YG	201	PEB	C4A-NA	-2.07	1.33	1.37
26	H1	201	PEB	C1C-CHB	2.07	1.49	1.41
26	s1	201	PEB	C4A-NA	-2.07	1.33	1.37
26	c6	201	PEB	C4A-NA	-2.07	1.33	1.37
26	OG	203	PEB	C4A-NA	-2.07	1.33	1.37
26	h7	202	PEB	C4B-C3B	2.07	1.49	1.45
26	j8	203	PEB	C4B-C3B	2.07	1.49	1.45
28	F6	1001	CYC	C1B-C2B	2.07	1.48	1.45
26	e1	201	PEB	C4A-NA	-2.07	1.33	1.37
28	E7	1001	CYC	C4A-C3A	2.07	1.50	1.45
26	A5	201	PEB	C1C-CHB	2.07	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D1	202	PEB	C4A-NA	-2.07	1.33	1.37
26	U7	203	PEB	C4A-NA	-2.07	1.33	1.37
26	cE	202	PEB	C4A-NA	-2.07	1.33	1.37
26	uE	202	PEB	C4A-NA	-2.07	1.33	1.37
26	kG	201	PEB	C4A-NA	-2.07	1.33	1.37
26	s1	202	PEB	C4B-C3B	2.07	1.49	1.45
26	dE	202	PEB	C4B-C3B	2.07	1.49	1.45
26	O2	201	PEB	CHA-C4A	-2.07	1.32	1.36
26	N3	202	PEB	C4B-NB	-2.07	1.34	1.38
26	WB	201	PEB	C1B-C2B	2.07	1.50	1.45
26	m4	203	PEB	C1C-CHB	2.07	1.49	1.41
28	J7	1001	CYC	C1D-CHD	2.07	1.49	1.41
26	x1	201	PEB	C4A-NA	-2.07	1.33	1.37
26	m4	202	PEB	C4A-NA	-2.07	1.33	1.37
26	JE	202	PEB	C4B-C3B	2.07	1.49	1.45
26	L1	203	PEB	C4A-NA	-2.07	1.33	1.37
26	UF	203	PEB	C4A-NA	-2.07	1.33	1.37
26	PJ	201	PEB	C4A-NA	-2.07	1.33	1.37
26	D3	202	PEB	C1C-CHB	2.07	1.49	1.41
26	IA	201	PEB	C1C-CHB	2.07	1.49	1.41
26	BC	201	PEB	C1C-CHB	2.07	1.49	1.41
28	IH	1001	CYC	C4D-CHA	2.07	1.49	1.41
26	Y3	304	PEB	C2A-C1A	-2.07	1.50	1.52
26	A4	201	PEB	C2A-C1A	-2.07	1.50	1.52
26	ZF	203	PEB	C2A-C1A	-2.07	1.50	1.52
26	Z4	201	PEB	C4B-C3B	2.07	1.49	1.45
26	eI	203	PEB	C4B-C3B	2.07	1.49	1.45
28	D6	1001	CYC	C1A-C2A	2.07	1.49	1.45
26	A9	301	PEB	C4A-NA	-2.07	1.33	1.37
26	aG	203	PEB	C4A-NA	-2.07	1.33	1.37
26	IE	201	PEB	OD-C4D	2.07	1.27	1.23
26	YG	202	PEB	C1C-CHB	2.07	1.49	1.41
26	RE	201	PEB	C4B-C3B	2.07	1.49	1.45
26	XG	202	PEB	C4B-C3B	2.07	1.49	1.45
26	H1	201	PEB	C4A-NA	-2.07	1.33	1.37
26	JF	1002	PEB	C4A-NA	-2.07	1.33	1.37
26	GE	201	PEB	C2C-C3C	2.07	1.43	1.37
26	u4	201	PEB	C1C-CHB	2.07	1.49	1.41
26	uG	203	PEB	C4B-C3B	2.07	1.49	1.45
27	xG	301	PUB	C1C-NC	-2.07	1.34	1.38
26	BD	201	PEB	C1B-C2B	2.07	1.50	1.45
26	VD	202	PEB	C4B-C3B	2.07	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	OE	203	PEB	C4B-C3B	2.07	1.49	1.45
26	LD	201	PEB	C1C-CHB	2.07	1.49	1.41
26	H6	1002	PEB	C4A-NA	-2.07	1.33	1.37
26	VG	202	PEB	C4A-NA	-2.07	1.33	1.37
26	Q1	201	PEB	C1B-C2B	2.07	1.50	1.45
28	L6	1001	CYC	C4A-C3A	2.07	1.50	1.45
26	oE	202	PEB	C1C-CHB	2.07	1.49	1.41
26	e6	201	PEB	C4B-C3B	2.07	1.49	1.45
26	G5	201	PEB	C1C-CHB	2.07	1.49	1.41
28	HI	1001	CYC	C4B-NB	-2.07	1.33	1.38
26	V8	202	PEB	C4B-NB	-2.07	1.34	1.38
26	R2	202	PEB	C4B-C3B	2.07	1.49	1.45
26	AI	305	PEB	C4A-NA	-2.07	1.33	1.37
28	H2	1001	CYC	C4B-NB	-2.07	1.33	1.38
26	lE	202	PEB	C1D-ND	2.07	1.48	1.45
28	II	1001	CYC	C1B-C2B	2.07	1.48	1.45
26	b7	201	PEB	C1C-CHB	2.07	1.49	1.41
26	QJ	201	PEB	C1C-CHB	2.07	1.49	1.41
28	pH	1001	CYC	C4D-CHA	2.07	1.49	1.41
26	M4	401	PEB	C4A-NA	-2.07	1.33	1.37
28	tH	1001	CYC	OB-C4B	2.07	1.27	1.23
26	l6	201	PEB	C1C-CHB	2.07	1.49	1.41
28	EI	1001	CYC	C4A-C3A	2.07	1.50	1.45
26	DA	202	PEB	C1C-CHB	2.07	1.49	1.41
26	lB	202	PEB	C1D-ND	2.07	1.48	1.45
26	kE	203	PEB	C4A-NA	-2.07	1.33	1.37
26	T3	202	PEB	OD-C4D	2.07	1.27	1.23
28	N7	1001	CYC	C4D-CHA	2.07	1.49	1.41
26	I1	202	PEB	C4A-NA	-2.07	1.33	1.37
26	R1	201	PEB	C1B-C2B	2.07	1.50	1.45
26	B3	203	PEB	C1B-C2B	2.07	1.50	1.45
26	R1	203	PEB	C1D-ND	2.06	1.48	1.45
26	V4	202	PEB	C1D-ND	2.06	1.48	1.45
28	YH	1004	CYC	C4D-CHA	2.06	1.49	1.41
26	OE	201	PEB	OD-C4D	2.06	1.27	1.23
28	LB	1001	CYC	C1D-CHD	2.06	1.49	1.41
26	V4	202	PEB	C4B-C3B	2.06	1.49	1.45
26	cB	202	PEB	C4B-C3B	2.06	1.49	1.45
26	iF	201	PEB	C4B-C3B	2.06	1.49	1.45
26	g2	203	PEB	C4A-NA	-2.06	1.33	1.37
26	iA	201	PEB	C4A-NA	-2.06	1.33	1.37
26	i8	202	PEB	C2A-C1A	-2.06	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	wE	301	PEB	C2A-C1A	-2.06	1.50	1.52
28	J7	1001	CYC	C4B-NB	-2.06	1.33	1.38
26	F1	202	PEB	C4B-C3B	2.06	1.49	1.45
26	hA	201	PEB	C4B-C3B	2.06	1.49	1.45
26	kE	201	PEB	C4B-C3B	2.06	1.49	1.45
26	ZE	201	PEB	C1C-CHB	2.06	1.49	1.41
28	H6	1001	CYC	OB-C4B	2.06	1.27	1.23
26	t4	202	PEB	C1D-ND	2.06	1.48	1.45
26	x1	201	PEB	C1C-CHB	2.06	1.49	1.41
28	YH	1002	CYC	C1A-C2A	2.06	1.49	1.45
26	QA	202	PEB	C4A-NA	-2.06	1.33	1.37
26	GE	201	PEB	CHA-C1B	2.06	1.45	1.40
26	ME	202	PEB	C2A-C1A	-2.06	1.50	1.52
26	NF	1002	PEB	C2A-C1A	-2.06	1.50	1.52
28	oH	1001	CYC	C1A-C2A	2.06	1.49	1.45
26	M9	202	PEB	C4A-NA	-2.06	1.33	1.37
26	dB	202	PEB	C4A-NA	-2.06	1.33	1.37
26	d7	201	PEB	C1C-CHB	2.06	1.49	1.41
28	oH	1001	CYC	C4D-CHA	2.06	1.49	1.41
26	iI	203	PEB	C4A-NA	-2.06	1.33	1.37
26	cI	202	PEB	C4B-C3B	2.06	1.49	1.45
28	MH	1001	CYC	C1A-C2A	2.06	1.49	1.45
26	oE	202	PEB	C1D-ND	2.06	1.48	1.45
26	X9	201	PEB	C4B-C3B	2.06	1.49	1.45
26	BG	201	PEB	C4B-C3B	2.06	1.49	1.45
26	CG	203	PEB	C4B-C3B	2.06	1.49	1.45
26	JI	1002	PEB	C4B-C3B	2.06	1.49	1.45
26	j6	202	PEB	C1C-CHB	2.06	1.49	1.41
26	fE	202	PEB	C1D-ND	2.06	1.48	1.45
26	WF	202	PEB	C1B-C2B	2.06	1.50	1.45
26	iA	202	PEB	C4B-C3B	2.06	1.49	1.45
26	A2	301	PEB	C4A-NA	-2.06	1.33	1.37
26	eG	203	PEB	C4A-NA	-2.06	1.33	1.37
26	QB	203	PEB	C2A-C1A	-2.06	1.50	1.52
28	I2	1001	CYC	C1B-C2B	2.06	1.48	1.45
26	uG	203	PEB	C1B-C2B	2.06	1.50	1.45
26	A9	303	PEB	C1D-ND	2.06	1.48	1.45
26	D9	203	PEB	C4B-C3B	2.06	1.49	1.45
26	HE	201	PEB	OD-C4D	2.06	1.27	1.23
28	M2	1001	CYC	C1B-C2B	2.06	1.48	1.45
26	jB	202	PEB	C4A-NA	-2.06	1.33	1.37
26	m4	202	PEB	C1C-CHB	2.06	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V8	202	PEB	C1D-ND	2.06	1.48	1.45
26	A6	301	PEB	C4B-C3B	2.06	1.49	1.45
26	m6	203	PEB	C4A-NA	-2.06	1.33	1.37
26	lF	202	PEB	C4A-NA	-2.06	1.33	1.37
26	f4	201	PEB	C1C-CHB	2.06	1.49	1.41
26	hB	201	PEB	C4B-C3B	2.06	1.49	1.45
26	cG	202	PEB	C4B-C3B	2.06	1.49	1.45
28	VH	1001	CYC	C1A-C2A	2.06	1.49	1.45
26	q1	202	PEB	C4A-NA	-2.06	1.33	1.37
26	l4	201	PEB	C4A-NA	-2.06	1.33	1.37
26	i7	201	PEB	C2A-C1A	-2.06	1.50	1.52
26	K1	202	PEB	C4B-NB	-2.06	1.34	1.38
26	W6	202	PEB	C4A-NA	-2.06	1.33	1.37
26	T4	201	PEB	C1D-ND	2.06	1.48	1.45
26	XG	201	PEB	C1C-CHB	2.06	1.49	1.41
26	gI	202	PEB	C1C-CHB	2.06	1.49	1.41
27	AA	304	PUB	C4B-CHB	2.06	1.49	1.41
26	i1	202	PEB	C4A-NA	-2.06	1.33	1.37
26	O9	202	PEB	C4A-NA	-2.06	1.33	1.37
26	bI	202	PEB	C4A-NA	-2.06	1.33	1.37
26	j8	202	PEB	C4B-C3B	2.06	1.49	1.45
26	m7	202	PEB	C1B-C2B	2.06	1.50	1.45
26	VF	203	PEB	C1B-C2B	2.06	1.50	1.45
28	M2	1001	CYC	C1B-NB	-2.06	1.34	1.37
26	P9	201	PEB	C4A-NA	-2.06	1.33	1.37
26	F9	202	PEB	C2A-C1A	-2.06	1.50	1.52
26	WE	201	PEB	C2A-C1A	-2.06	1.50	1.52
26	N9	202	PEB	C1C-CHB	2.06	1.49	1.41
26	l6	203	PEB	C4B-C3B	2.06	1.49	1.45
26	uE	203	PEB	C4B-C3B	2.06	1.49	1.45
26	BG	201	PEB	C1C-CHB	2.06	1.49	1.41
26	O1	202	PEB	C4A-NA	-2.06	1.33	1.37
26	MJ	202	PEB	C4A-NA	-2.06	1.33	1.37
26	O7	201	PEB	C1D-ND	2.06	1.48	1.45
26	oG	201	PEB	C1B-C2B	2.06	1.50	1.45
26	z1	201	PEB	C4A-NA	-2.06	1.33	1.37
26	h8	201	PEB	C4A-NA	-2.06	1.33	1.37
26	Y9	201	PEB	C4A-NA	-2.06	1.33	1.37
26	OF	203	PEB	C1C-CHB	2.06	1.49	1.41
28	NF	1001	CYC	C4B-NB	-2.06	1.33	1.38
26	C1	201	PEB	C1D-ND	2.06	1.48	1.45
26	B5	203	PEB	C1D-ND	2.06	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W1	202	PEB	C1C-CHB	2.06	1.49	1.41
26	NE	201	PEB	C1C-CHB	2.06	1.49	1.41
26	H4	203	PEB	C4A-NA	-2.06	1.33	1.37
26	OF	201	PEB	C4A-NA	-2.06	1.33	1.37
26	HD	202	PEB	C4B-C3B	2.06	1.49	1.45
26	fF	201	PEB	C1D-ND	2.06	1.48	1.45
26	L4	201	PEB	C4A-NA	-2.06	1.33	1.37
26	BJ	202	PEB	C4A-NA	-2.06	1.33	1.37
26	i1	202	PEB	C1C-CHB	2.06	1.49	1.41
26	RG	201	PEB	C4B-C3B	2.06	1.49	1.45
26	fA	203	PEB	C2A-C1A	-2.06	1.50	1.52
26	GJ	202	PEB	C4A-NA	-2.06	1.33	1.37
26	OF	201	PEB	C1D-ND	2.05	1.48	1.45
28	fH	1001	CYC	C4D-CHA	2.05	1.49	1.41
26	F4	203	PEB	C4B-C3B	2.05	1.49	1.45
26	QE	203	PEB	C1C-CHB	2.05	1.49	1.41
26	l7	203	PEB	C1D-ND	2.05	1.48	1.45
26	AG	202	PEB	C1C-CHB	2.05	1.49	1.41
26	H4	202	PEB	C4A-NA	-2.05	1.33	1.37
26	a7	202	PEB	C4A-NA	-2.05	1.33	1.37
26	a8	203	PEB	C4A-NA	-2.05	1.33	1.37
26	mG	201	PEB	C4A-NA	-2.05	1.33	1.37
26	m2	203	PEB	C2A-C1A	-2.05	1.50	1.52
26	mG	202	PEB	C2A-C1A	-2.05	1.50	1.52
26	GJ	202	PEB	C4B-C3B	2.05	1.49	1.45
28	NH	1001	CYC	C1A-C2A	2.05	1.49	1.45
26	F9	201	PEB	C4B-NB	-2.05	1.34	1.38
26	H4	201	PEB	C1C-CHB	2.05	1.49	1.41
26	RF	202	PEB	C1C-CHB	2.05	1.49	1.41
26	e1	201	PEB	C1D-ND	2.05	1.48	1.45
26	S8	202	PEB	C1D-ND	2.05	1.48	1.45
28	M6	1001	CYC	C1B-C2B	2.05	1.48	1.45
26	sE	203	PEB	C4B-NB	-2.05	1.34	1.38
26	F9	202	PEB	C4B-C3B	2.05	1.49	1.45
26	QG	202	PEB	C4B-C3B	2.05	1.49	1.45
26	VJ	201	PEB	C4B-C3B	2.05	1.49	1.45
26	AB	301	PEB	C4A-NA	-2.05	1.33	1.37
26	OE	203	PEB	C4A-NA	-2.05	1.33	1.37
26	n4	202	PEB	C1C-CHB	2.05	1.49	1.41
26	qE	201	PEB	C2A-C1A	-2.05	1.50	1.52
26	aE	201	PEB	C4A-NA	-2.05	1.33	1.37
26	uG	202	PEB	C4A-NA	-2.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	PJ	201	PEB	C4B-C3B	2.05	1.49	1.45
26	jA	203	PEB	C4A-NA	-2.05	1.33	1.37
26	R7	202	PEB	C1C-CHB	2.05	1.49	1.41
26	WG	201	PEB	C1C-CHB	2.05	1.49	1.41
26	B9	201	PEB	C4B-C3B	2.05	1.49	1.45
26	IE	203	PEB	C4B-NB	-2.05	1.34	1.38
28	C6	1001	CYC	C1D-CHD	2.05	1.49	1.41
26	v1	202	PEB	C4A-NA	-2.05	1.33	1.37
26	L3	203	PEB	C4A-NA	-2.05	1.33	1.37
26	d7	202	PEB	C4A-NA	-2.05	1.33	1.37
26	B3	202	PEB	C2A-C1A	-2.05	1.50	1.52
26	c4	202	PEB	C2A-C1A	-2.05	1.50	1.52
26	SG	203	PEB	C1B-C2B	2.05	1.50	1.45
26	lB	203	PEB	C4B-C3B	2.05	1.49	1.45
26	l2	202	PEB	C4A-NA	-2.05	1.33	1.37
26	Z4	201	PEB	C4A-NA	-2.05	1.33	1.37
26	J9	203	PEB	C4A-NA	-2.05	1.33	1.37
26	lI	202	PEB	C1C-CHB	2.05	1.49	1.41
26	I3	202	PEB	C4A-NA	-2.05	1.33	1.37
26	h4	202	PEB	C2A-C1A	-2.05	1.50	1.52
26	i4	201	PEB	C1C-CHB	2.05	1.49	1.41
26	Q8	202	PEB	C1C-CHB	2.05	1.49	1.41
27	A2	302	PUB	C4B-CHB	2.05	1.49	1.41
26	hB	202	PEB	C1C-CHB	2.05	1.49	1.41
26	B1	203	PEB	C4A-NA	-2.05	1.33	1.37
26	D4	202	PEB	C4A-NA	-2.05	1.33	1.37
26	j6	201	PEB	C1D-ND	2.05	1.48	1.45
26	JJ	203	PEB	C1D-ND	2.05	1.48	1.45
26	h2	201	PEB	C4B-C3B	2.05	1.49	1.45
26	lA	203	PEB	C1C-CHB	2.05	1.49	1.41
26	xE	304	PEB	C4A-NA	-2.05	1.33	1.37
26	mG	203	PEB	C4A-NA	-2.05	1.33	1.37
26	VF	201	PEB	C1C-CHB	2.05	1.49	1.41
28	CI	1001	CYC	C1D-CHD	2.05	1.49	1.41
26	I3	201	PEB	C1D-ND	2.05	1.48	1.45
28	G2	1001	CYC	C4B-NB	-2.05	1.33	1.38
28	H6	1001	CYC	C1B-C2B	2.05	1.48	1.45
26	x1	201	PEB	C1D-ND	2.05	1.48	1.45
26	V9	201	PEB	C1D-ND	2.05	1.48	1.45
26	NG	201	PEB	C1C-CHB	2.05	1.49	1.41
26	q4	201	PEB	C1C-CHB	2.05	1.49	1.41
26	Y8	203	PEB	C1C-CHB	2.05	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	WG	203	PEB	C1C-CHB	2.05	1.49	1.41
26	M1	401	PEB	C4A-NA	-2.05	1.33	1.37
26	mB	203	PEB	C4A-NA	-2.05	1.33	1.37
26	J8	202	PEB	C2A-C1A	-2.05	1.50	1.52
26	mB	202	PEB	C2A-C1A	-2.05	1.50	1.52
26	cI	203	PEB	C2A-C1A	-2.05	1.50	1.52
26	C5	202	PEB	C1C-CHB	2.05	1.49	1.41
26	O9	202	PEB	C4B-C3B	2.05	1.49	1.45
26	EE	202	PEB	C4B-C3B	2.05	1.49	1.45
28	L7	1001	CYC	C4D-CHA	2.05	1.49	1.41
28	LB	1001	CYC	C4A-C3A	2.05	1.50	1.45
26	mB	203	PEB	C1C-CHB	2.05	1.49	1.41
26	D3	201	PEB	C1C-CHB	2.05	1.49	1.41
26	e3	401	PEB	C4A-NA	-2.05	1.33	1.37
26	W7	202	PEB	C1B-C2B	2.05	1.50	1.45
26	L4	201	PEB	C1C-CHB	2.05	1.49	1.41
26	uE	201	PEB	C1C-CHB	2.05	1.49	1.41
28	C7	1001	CYC	C4D-CHA	2.05	1.49	1.41
26	c2	203	PEB	C4A-NA	-2.05	1.33	1.37
26	X9	201	PEB	C4A-NA	-2.05	1.33	1.37
28	PH	1001	CYC	C4C-NC	-2.05	1.33	1.37
26	p1	201	PEB	C4B-C3B	2.05	1.49	1.45
26	m6	201	PEB	C1B-C2B	2.05	1.50	1.45
26	DF	1002	PEB	C1B-C2B	2.05	1.50	1.45
26	iG	201	PEB	C4B-C3B	2.05	1.49	1.45
28	F7	1001	CYC	C1A-C2A	2.05	1.49	1.45
26	k8	201	PEB	C4A-NA	-2.05	1.33	1.37
26	FC	202	PEB	C4A-NA	-2.05	1.33	1.37
26	H3	203	PEB	C1C-CHB	2.05	1.49	1.41
26	qE	202	PEB	C4B-NB	-2.05	1.34	1.38
26	a1	203	PEB	C1C-CHB	2.05	1.49	1.41
26	I4	202	PEB	C4A-NA	-2.05	1.33	1.37
26	m6	202	PEB	C4A-NA	-2.05	1.33	1.37
26	21	405	PEB	C1C-CHB	2.05	1.49	1.41
28	QH	1001	CYC	C4D-CHA	2.05	1.49	1.41
26	CG	203	PEB	C1C-CHB	2.05	1.49	1.41
26	bI	202	PEB	C4B-C3B	2.05	1.49	1.45
26	a1	203	PEB	C4A-NA	-2.05	1.33	1.37
26	C5	202	PEB	C4A-NA	-2.05	1.33	1.37
26	dI	201	PEB	C4A-NA	-2.05	1.33	1.37
26	T4	203	PEB	C2A-C1A	-2.05	1.50	1.52
26	q4	203	PEB	C2A-C1A	-2.05	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ME	202	PEB	C1C-CHB	2.04	1.49	1.41
28	JF	1001	CYC	C1D-CHD	2.04	1.49	1.41
26	H5	201	PEB	OD-C4D	2.04	1.27	1.23
26	L1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	b7	202	PEB	C1C-CHB	2.04	1.49	1.41
26	YE	203	PEB	C4A-NA	-2.04	1.33	1.37
26	YI	201	PEB	C4A-NA	-2.04	1.33	1.37
26	I4	202	PEB	C4B-C3B	2.04	1.49	1.45
26	dB	203	PEB	C1C-CHB	2.04	1.49	1.41
26	jG	201	PEB	C1C-CHB	2.04	1.49	1.41
26	mI	202	PEB	C1C-CHB	2.04	1.49	1.41
26	B8	301	PEB	OD-C4D	2.04	1.27	1.23
26	l8	203	PEB	C1C-CHB	2.04	1.49	1.41
26	wG	303	PEB	C1C-CHB	2.04	1.49	1.41
26	d6	202	PEB	C2A-C1A	-2.04	1.50	1.52
26	Q7	202	PEB	C2A-C1A	-2.04	1.50	1.52
26	GC	201	PEB	C1C-CHB	2.04	1.49	1.41
26	NF	1002	PEB	C1D-ND	2.04	1.48	1.45
26	TF	202	PEB	C1D-ND	2.04	1.48	1.45
26	CE	201	PEB	C4B-NB	-2.04	1.34	1.38
26	cG	203	PEB	C4B-NB	-2.04	1.34	1.38
26	R4	203	PEB	C1C-CHB	2.04	1.49	1.41
26	kA	202	PEB	C1C-CHB	2.04	1.49	1.41
26	lF	202	PEB	C1C-CHB	2.04	1.49	1.41
28	FF	1001	CYC	C4D-CHA	2.04	1.49	1.41
26	C5	204	PEB	C2A-C1A	-2.04	1.50	1.52
26	f7	201	PEB	C2A-C1A	-2.04	1.50	1.52
26	A4	202	PEB	C1C-CHB	2.04	1.49	1.41
26	k7	201	PEB	C1C-CHB	2.04	1.49	1.41
26	g7	202	PEB	C4B-C3B	2.04	1.49	1.45
26	gE	203	PEB	C4B-C3B	2.04	1.49	1.45
26	v1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	f2	202	PEB	C1C-CHB	2.04	1.49	1.41
26	Z2	201	PEB	C1B-C2B	2.04	1.50	1.45
26	P1	203	PEB	C1C-CHB	2.04	1.49	1.41
26	N8	202	PEB	C1C-CHB	2.04	1.49	1.41
26	R9	202	PEB	C1C-CHB	2.04	1.49	1.41
26	k2	201	PEB	C4B-C3B	2.04	1.49	1.45
26	k1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	i6	201	PEB	C1C-CHB	2.04	1.49	1.41
26	zE	501	PEB	C1C-CHB	2.04	1.49	1.41
26	SG	202	PEB	C1B-C2B	2.04	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C7	1001	CYC	C4C-NC	-2.04	1.33	1.37
28	HB	1001	CYC	C1B-C2B	2.04	1.48	1.45
26	J8	202	PEB	C1C-CHB	2.04	1.49	1.41
26	f1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	iI	202	PEB	C4A-NA	-2.04	1.33	1.37
26	KJ	201	PEB	C4A-NA	-2.04	1.33	1.37
27	wG	304	PUB	C4C-NC	2.04	1.38	1.35
26	HC	201	PEB	C1C-CHB	2.04	1.49	1.41
26	l6	202	PEB	C1D-ND	2.04	1.48	1.45
26	kE	202	PEB	C1D-ND	2.04	1.48	1.45
26	h7	203	PEB	C4A-NA	-2.04	1.33	1.37
26	WE	202	PEB	C4A-NA	-2.04	1.33	1.37
26	eB	203	PEB	C4B-C3B	2.04	1.49	1.45
26	GE	201	PEB	C4B-C3B	2.04	1.49	1.45
26	G4	202	PEB	C1C-CHB	2.04	1.49	1.41
26	aF	201	PEB	C1C-CHB	2.04	1.49	1.41
26	FD	201	PEB	C2A-C1A	-2.04	1.50	1.52
26	k4	202	PEB	C4A-NA	-2.04	1.33	1.37
26	ME	201	PEB	C4A-NA	-2.04	1.33	1.37
28	OH	1001	CYC	C4B-NB	-2.04	1.33	1.38
26	WF	201	PEB	C1D-ND	2.04	1.48	1.45
26	fG	202	PEB	C1C-CHB	2.04	1.49	1.41
26	W9	201	PEB	C4A-NA	-2.04	1.33	1.37
26	YA	203	PEB	C1C-CHB	2.04	1.49	1.41
26	iI	203	PEB	C1C-CHB	2.04	1.49	1.41
26	T8	202	PEB	C4B-NB	-2.04	1.34	1.38
26	jB	201	PEB	C1D-ND	2.04	1.48	1.45
26	A1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	iI	203	PEB	C4A-NA	-2.04	1.33	1.37
26	H9	203	PEB	C2A-C1A	-2.04	1.50	1.52
26	ED	201	PEB	C4A-NA	-2.04	1.33	1.37
26	JG	202	PEB	C4B-C3B	2.04	1.49	1.45
26	jB	202	PEB	C1C-CHB	2.04	1.49	1.41
26	WF	201	PEB	C1C-CHB	2.04	1.49	1.41
26	HA	201	PEB	C1B-C2B	2.04	1.50	1.45
26	kE	202	PEB	C4A-NA	-2.04	1.33	1.37
26	m1	203	PEB	C1C-CHB	2.04	1.49	1.41
26	JA	202	PEB	C1C-CHB	2.04	1.49	1.41
26	hF	202	PEB	C4B-C3B	2.04	1.49	1.45
26	BJ	201	PEB	C4B-C3B	2.04	1.49	1.45
28	YH	1001	CYC	C1A-C2A	2.04	1.49	1.45
28	E6	1001	CYC	C4A-C3A	2.04	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b2	202	PEB	C4A-NA	-2.04	1.33	1.37
26	C4	202	PEB	C4A-NA	-2.04	1.33	1.37
26	A7	305	PEB	C4A-NA	-2.04	1.33	1.37
26	T9	201	PEB	C4A-NA	-2.04	1.33	1.37
26	LG	201	PEB	C1C-CHB	2.04	1.49	1.41
26	jB	201	PEB	C4A-NA	-2.04	1.33	1.37
26	kF	201	PEB	C4A-NA	-2.04	1.33	1.37
26	BD	202	PEB	C1A-NA	-2.04	1.35	1.37
26	f7	202	PEB	C2A-C1A	-2.04	1.50	1.52
26	F3	203	PEB	C4A-NA	-2.04	1.33	1.37
28	K2	1001	CYC	C4D-CHA	2.04	1.49	1.41
26	D7	1002	PEB	C1C-CHB	2.04	1.49	1.41
26	r4	201	PEB	C4A-NA	-2.04	1.33	1.37
26	mB	202	PEB	C4A-NA	-2.04	1.33	1.37
26	GD	201	PEB	OD-C4D	2.04	1.27	1.23
26	gA	202	PEB	C1C-CHB	2.04	1.49	1.41
26	DD	202	PEB	C1C-CHB	2.04	1.49	1.41
26	p1	201	PEB	C1D-ND	2.04	1.48	1.45
26	YE	203	PEB	C1D-ND	2.04	1.48	1.45
26	f8	202	PEB	C1C-CHB	2.04	1.49	1.41
26	TD	202	PEB	CHA-C4A	-2.04	1.32	1.36
26	kI	201	PEB	C4A-NA	-2.04	1.33	1.37
26	c1	203	PEB	C1C-CHB	2.04	1.49	1.41
26	l1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	W4	202	PEB	C1C-CHB	2.04	1.49	1.41
26	U7	202	PEB	C1C-CHB	2.04	1.49	1.41
28	YH	1001	CYC	C4D-CHA	2.04	1.49	1.41
26	ZI	201	PEB	C1B-C2B	2.04	1.50	1.45
26	W7	202	PEB	C4B-C3B	2.04	1.49	1.45
26	H8	202	PEB	C4B-C3B	2.04	1.49	1.45
26	Y9	202	PEB	C4A-NA	-2.04	1.33	1.37
26	iF	201	PEB	C4A-NA	-2.04	1.33	1.37
26	V1	201	PEB	C1C-CHB	2.04	1.49	1.41
26	uE	201	PEB	C4A-NA	-2.04	1.33	1.37
26	MD	201	PEB	C1C-CHB	2.03	1.49	1.41
26	j7	202	PEB	C1D-ND	2.03	1.48	1.45
26	QD	202	PEB	C2A-C1A	-2.03	1.50	1.52
26	VD	202	PEB	C2A-C1A	-2.03	1.50	1.52
26	MG	203	PEB	C1B-C2B	2.03	1.50	1.45
28	G7	1001	CYC	C1D-CHD	2.03	1.49	1.41
26	A7	302	PEB	C4A-NA	-2.03	1.33	1.37
26	B9	201	PEB	C4A-NA	-2.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	DD	203	PEB	C4A-NA	-2.03	1.33	1.37
26	OE	201	PEB	C4A-NA	-2.03	1.33	1.37
26	d4	202	PEB	C1C-CHB	2.03	1.49	1.41
26	c6	202	PEB	C4B-C3B	2.03	1.48	1.45
26	U6	203	PEB	C1D-ND	2.03	1.48	1.45
26	O4	202	PEB	C4A-NA	-2.03	1.33	1.37
26	UI	202	PEB	C4A-NA	-2.03	1.33	1.37
26	VJ	203	PEB	C4A-NA	-2.03	1.33	1.37
26	y4	203	PEB	C1C-CHB	2.03	1.49	1.41
26	24	404	PEB	C4B-C3B	2.03	1.48	1.45
26	I1	201	PEB	C2A-C1A	-2.03	1.50	1.52
26	y1	201	PEB	C2A-C1A	-2.03	1.50	1.52
26	YE	202	PEB	C2A-C1A	-2.03	1.50	1.52
26	cA	203	PEB	C4A-NA	-2.03	1.33	1.37
27	AJ	302	PUB	C4B-CHB	2.03	1.49	1.41
26	cE	201	PEB	C1D-ND	2.03	1.48	1.45
26	r4	202	PEB	C1C-CHB	2.03	1.49	1.41
26	c6	202	PEB	C1C-CHB	2.03	1.49	1.41
26	k2	201	PEB	C4A-NA	-2.03	1.33	1.37
26	bE	201	PEB	C1C-CHB	2.03	1.49	1.41
26	eI	202	PEB	C1C-CHB	2.03	1.49	1.41
26	N6	201	PEB	C4B-C3B	2.03	1.48	1.45
26	ED	202	PEB	C4B-C3B	2.03	1.48	1.45
26	DE	202	PEB	C4B-C3B	2.03	1.48	1.45
26	MG	203	PEB	C4B-C3B	2.03	1.48	1.45
26	a4	201	PEB	C1C-CHB	2.03	1.49	1.41
26	MG	202	PEB	C4A-NA	-2.03	1.33	1.37
28	DF	1001	CYC	C4C-NC	-2.03	1.33	1.37
26	H9	201	PEB	C4B-C3B	2.03	1.48	1.45
26	D4	201	PEB	C4A-NA	-2.03	1.33	1.37
26	j8	202	PEB	C4A-NA	-2.03	1.33	1.37
26	F9	202	PEB	C4A-NA	-2.03	1.33	1.37
26	QF	203	PEB	C4A-NA	-2.03	1.33	1.37
26	CC	203	PEB	C1D-ND	2.03	1.48	1.45
26	mE	202	PEB	C1D-ND	2.03	1.48	1.45
26	PE	201	PEB	C1C-CHB	2.03	1.49	1.41
26	eF	202	PEB	C1C-CHB	2.03	1.49	1.41
26	pE	201	PEB	C4B-C3B	2.03	1.48	1.45
26	YG	203	PEB	C4B-C3B	2.03	1.48	1.45
26	P4	203	PEB	C4A-NA	-2.03	1.33	1.37
26	SA	203	PEB	C1C-CHB	2.03	1.49	1.41
26	gG	203	PEB	C1C-CHB	2.03	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	kF	202	PEB	C1B-C2B	2.03	1.50	1.45
26	bF	202	PEB	C4A-NA	-2.03	1.33	1.37
26	j6	202	PEB	C4B-C3B	2.03	1.48	1.45
26	WE	201	PEB	C4B-C3B	2.03	1.48	1.45
26	cE	203	PEB	C4A-NA	-2.03	1.33	1.37
26	sG	201	PEB	C4A-NA	-2.03	1.33	1.37
26	P3	202	PEB	C4B-C3B	2.03	1.48	1.45
26	b2	202	PEB	C2A-C1A	-2.03	1.50	1.52
26	G3	202	PEB	C2A-C1A	-2.03	1.50	1.52
26	14	202	PEB	C4A-NA	-2.03	1.33	1.37
26	V7	201	PEB	C1C-CHB	2.03	1.49	1.41
26	UF	202	PEB	C1C-CHB	2.03	1.49	1.41
26	w4	201	PEB	C1D-ND	2.03	1.48	1.45
26	z1	201	PEB	C1B-C2B	2.03	1.50	1.45
26	b2	202	PEB	C4B-C3B	2.03	1.48	1.45
26	DJ	203	PEB	C4B-C3B	2.03	1.48	1.45
26	QA	204	PEB	C4A-NA	-2.03	1.33	1.37
26	ED	202	PEB	C4A-NA	-2.03	1.33	1.37
26	OF	202	PEB	C4A-NA	-2.03	1.33	1.37
26	J3	203	PEB	C1D-ND	2.03	1.48	1.45
26	TE	202	PEB	C1D-ND	2.03	1.48	1.45
26	s1	202	PEB	C1C-CHB	2.03	1.49	1.41
28	D2	1001	CYC	C1B-C2B	2.03	1.48	1.45
26	hI	202	PEB	C4A-NA	-2.03	1.33	1.37
26	NA	202	PEB	C1C-CHB	2.03	1.49	1.41
26	BA	301	PEB	OD-C4D	2.03	1.27	1.23
26	R9	202	PEB	C4A-NA	-2.03	1.33	1.37
26	SG	201	PEB	C4B-NB	-2.03	1.34	1.38
26	dG	201	PEB	C1C-CHB	2.03	1.49	1.41
26	R1	203	PEB	C4B-C3B	2.03	1.48	1.45
26	P4	203	PEB	C4B-C3B	2.03	1.48	1.45
26	mI	203	PEB	O1B-CGB	2.03	1.28	1.22
26	UE	203	PEB	C1C-CHB	2.03	1.49	1.41
26	d4	202	PEB	C4A-NA	-2.03	1.33	1.37
26	jF	203	PEB	C4B-NB	-2.03	1.34	1.38
28	EB	1001	CYC	C4D-CHA	2.03	1.49	1.41
26	CA	202	PEB	C2A-C1A	-2.03	1.50	1.52
26	fE	202	PEB	C1C-CHB	2.03	1.49	1.41
26	hF	201	PEB	C4A-NA	-2.03	1.33	1.37
26	R4	201	PEB	C1B-C2B	2.03	1.50	1.45
26	g4	202	PEB	C1D-ND	2.03	1.48	1.45
26	p1	201	PEB	C1C-CHB	2.03	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g8	202	PEB	C1C-CHB	2.03	1.49	1.41
26	FD	201	PEB	C1C-CHB	2.03	1.49	1.41
26	Q7	201	PEB	C4A-NA	-2.03	1.33	1.37
26	i8	201	PEB	C4A-NA	-2.03	1.33	1.37
26	c2	201	PEB	C4B-C3B	2.03	1.48	1.45
26	YE	202	PEB	C1C-CHB	2.03	1.49	1.41
26	BC	202	PEB	C2A-C1A	-2.03	1.50	1.52
28	PH	1001	CYC	C4D-CHA	2.03	1.49	1.41
26	MA	202	PEB	OD-C4D	2.03	1.27	1.23
26	E4	202	PEB	C1C-CHB	2.03	1.49	1.41
26	XG	202	PEB	C1C-CHB	2.03	1.49	1.41
26	NJ	204	PEB	C4A-NA	-2.03	1.33	1.37
26	hE	201	PEB	C1B-C2B	2.03	1.50	1.45
28	EF	1001	CYC	C4A-C3A	2.03	1.50	1.45
28	UH	1001	CYC	C4A-C3A	2.03	1.50	1.45
26	IJ	201	PEB	C1C-CHB	2.03	1.49	1.41
26	t1	201	PEB	C4A-NA	-2.03	1.33	1.37
26	L8	202	PEB	C4A-NA	-2.03	1.33	1.37
26	AJ	301	PEB	C4A-NA	-2.03	1.33	1.37
28	cH	1001	CYC	C4C-NC	-2.03	1.33	1.37
26	L2	1002	PEB	C4B-C3B	2.03	1.48	1.45
26	R9	201	PEB	C1D-ND	2.03	1.48	1.45
26	cI	203	PEB	C4A-NA	-2.03	1.33	1.37
28	EB	1001	CYC	C4A-C3A	2.03	1.50	1.45
26	GA	202	PEB	C4B-C3B	2.03	1.48	1.45
26	dB	204	PEB	C1D-ND	2.02	1.48	1.45
26	j6	202	PEB	C2A-C1A	-2.02	1.50	1.52
26	d7	203	PEB	C1C-CHB	2.02	1.49	1.41
26	GC	203	PEB	C1C-CHB	2.02	1.49	1.41
26	P1	203	PEB	C4A-NA	-2.02	1.33	1.37
26	n4	201	PEB	C4A-NA	-2.02	1.33	1.37
26	c8	202	PEB	C4A-NA	-2.02	1.33	1.37
26	VF	201	PEB	C4A-NA	-2.02	1.33	1.37
27	A8	304	PUB	C3C-C4C	2.02	1.50	1.43
26	kB	201	PEB	C1C-CHB	2.02	1.49	1.41
26	11	201	PEB	C1D-ND	2.02	1.48	1.45
26	IJ	202	PEB	C4B-NB	-2.02	1.34	1.38
26	dE	201	PEB	C1C-CHB	2.02	1.49	1.41
26	qE	203	PEB	C1C-CHB	2.02	1.49	1.41
28	tH	1001	CYC	C4D-CHA	2.02	1.49	1.41
26	dG	202	PEB	C1B-C2B	2.02	1.50	1.45
26	C5	201	PEB	C1C-CHB	2.02	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	jB	202	PEB	C4B-C3B	2.02	1.48	1.45
26	g1	201	PEB	C4A-NA	-2.02	1.33	1.37
26	S7	202	PEB	C4A-NA	-2.02	1.33	1.37
26	RJ	202	PEB	C4A-NA	-2.02	1.33	1.37
26	JJ	201	PEB	C1C-CHB	2.02	1.49	1.41
26	d1	203	PEB	C2A-C1A	-2.02	1.50	1.52
26	PJ	203	PEB	C2A-C1A	-2.02	1.50	1.52
26	Q9	202	PEB	C1D-ND	2.02	1.48	1.45
26	PG	201	PEB	C1A-NA	-2.02	1.35	1.37
28	vH	1001	CYC	C4D-CHA	2.02	1.49	1.41
28	GH	1001	CYC	C1A-C2A	2.02	1.48	1.45
26	HG	201	PEB	C1C-CHB	2.02	1.49	1.41
28	MB	1001	CYC	C1B-C2B	2.02	1.48	1.45
26	y1	201	PEB	C4A-NA	-2.02	1.33	1.37
26	I4	201	PEB	C4A-NA	-2.02	1.33	1.37
26	JJ	203	PEB	C2A-C1A	-2.02	1.50	1.52
26	OJ	201	PEB	C4B-C3B	2.02	1.48	1.45
28	C2	1001	CYC	C4D-CHA	2.02	1.48	1.41
26	a8	201	PEB	C1D-ND	2.02	1.48	1.45
26	aA	204	PEB	C4B-NB	-2.02	1.34	1.38
26	R4	203	PEB	C4A-NA	-2.02	1.33	1.37
26	A6	301	PEB	C4A-NA	-2.02	1.33	1.37
26	W7	203	PEB	C4A-NA	-2.02	1.33	1.37
26	LD	203	PEB	C1C-CHB	2.02	1.48	1.41
27	N9	201	PUB	C4B-CHB	2.02	1.48	1.41
26	D4	202	PEB	C1D-ND	2.02	1.48	1.45
26	aG	203	PEB	C2A-C1A	-2.02	1.50	1.52
26	k7	201	PEB	C4A-NA	-2.02	1.33	1.37
26	kI	201	PEB	C1C-CHB	2.02	1.48	1.41
26	Z6	203	PEB	C1B-C2B	2.02	1.50	1.45
26	AA	301	PEB	C1B-C2B	2.02	1.50	1.45
26	F4	201	PEB	C1C-CHB	2.02	1.48	1.41
28	M2	1001	CYC	C4B-NB	-2.02	1.33	1.38
26	Z1	201	PEB	C1C-CHB	2.02	1.48	1.41
26	l7	203	PEB	C4A-NA	-2.02	1.33	1.37
26	A6	304	PEB	C2A-C1A	-2.02	1.50	1.52
26	mE	201	PEB	C1D-ND	2.02	1.48	1.45
26	kG	203	PEB	C1D-ND	2.02	1.48	1.45
26	M4	401	PEB	C1C-CHB	2.02	1.48	1.41
26	tE	201	PEB	C1C-CHB	2.02	1.48	1.41
26	z4	201	PEB	C1C-CHB	2.02	1.48	1.41
26	LC	203	PEB	O1B-CGB	2.02	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G1	202	PEB	C1C-CHB	2.02	1.48	1.41
26	K6	201	PEB	C1C-CHB	2.02	1.48	1.41
26	CE	203	PEB	C4B-C3B	2.02	1.48	1.45
26	J3	203	PEB	C2A-C1A	-2.02	1.50	1.52
26	T7	202	PEB	C2A-C1A	-2.02	1.50	1.52
26	YB	201	PEB	C1B-C2B	2.02	1.50	1.45
26	jF	203	PEB	C4A-NA	-2.02	1.33	1.37
26	L4	201	PEB	C1D-ND	2.02	1.48	1.45
26	r4	202	PEB	C1D-ND	2.02	1.48	1.45
26	Q9	202	PEB	C1B-C2B	2.02	1.50	1.45
26	aI	201	PEB	C1B-C2B	2.02	1.50	1.45
26	v4	201	PEB	C1C-CHB	2.02	1.48	1.41
26	G8	202	PEB	C1C-CHB	2.02	1.48	1.41
26	QE	202	PEB	C2A-C1A	-2.02	1.50	1.52
26	k1	203	PEB	C4A-NA	-2.02	1.33	1.37
26	fE	201	PEB	C1A-NA	-2.02	1.35	1.37
26	F9	202	PEB	C1C-CHB	2.02	1.48	1.41
28	CB	1001	CYC	C1D-CHD	2.02	1.48	1.41
26	V7	201	PEB	C4B-C3B	2.02	1.48	1.45
27	24	403	PUB	C1C-C2C	2.02	1.48	1.45
26	n1	201	PEB	C1C-CHB	2.02	1.48	1.41
26	l4	202	PEB	C1B-C2B	2.02	1.50	1.45
26	eE	202	PEB	C1B-C2B	2.02	1.50	1.45
26	l8	201	PEB	C4A-NA	-2.02	1.33	1.37
26	B1	202	PEB	C1C-CHB	2.02	1.48	1.41
26	C8	201	PEB	C1C-CHB	2.02	1.48	1.41
26	l2	202	PEB	C1D-ND	2.02	1.48	1.45
28	FF	1001	CYC	C1B-NB	-2.02	1.34	1.37
26	SB	203	PEB	C4B-C3B	2.02	1.48	1.45
26	CC	202	PEB	C1C-CHB	2.02	1.48	1.41
26	OI	201	PEB	CHA-C4A	-2.02	1.32	1.36
26	w1	203	PEB	C4A-NA	-2.02	1.33	1.37
26	DE	202	PEB	C1C-CHB	2.02	1.48	1.41
26	l1	201	PEB	C1D-ND	2.02	1.48	1.45
26	FA	202	PEB	C4B-C3B	2.02	1.48	1.45
26	B4	202	PEB	C4A-NA	-2.02	1.33	1.37
26	K4	202	PEB	C4A-NA	-2.02	1.33	1.37
26	U7	202	PEB	C4A-NA	-2.02	1.33	1.37
26	g2	202	PEB	C1C-CHB	2.02	1.48	1.41
26	m2	203	PEB	O1B-CGB	2.02	1.28	1.22
26	WE	202	PEB	C2A-C1A	-2.02	1.50	1.52
26	mA	202	PEB	C4B-NB	-2.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	uE	203	PEB	C1C-CHB	2.02	1.48	1.41
26	21	404	PEB	C4A-NA	-2.02	1.33	1.37
26	a4	202	PEB	C4A-NA	-2.02	1.33	1.37
26	T7	201	PEB	C1D-ND	2.02	1.48	1.45
26	d6	203	PEB	C4B-C3B	2.02	1.48	1.45
26	q4	202	PEB	C4A-NA	-2.02	1.33	1.37
26	J7	1002	PEB	C4A-NA	-2.02	1.33	1.37
26	gE	202	PEB	C4A-NA	-2.02	1.33	1.37
28	JF	1003	CYC	C4D-CHA	2.02	1.48	1.41
26	J2	1002	PEB	C4B-C3B	2.01	1.48	1.45
26	I3	202	PEB	C1D-ND	2.01	1.48	1.45
26	A7	301	PEB	C1C-CHB	2.01	1.48	1.41
26	k1	202	PEB	C4A-NA	-2.01	1.33	1.37
26	G9	202	PEB	C2A-C1A	-2.01	1.50	1.52
26	H9	203	PEB	C4B-C3B	2.01	1.48	1.45
26	V9	202	PEB	C1D-ND	2.01	1.48	1.45
26	O7	202	PEB	C4A-NA	-2.01	1.33	1.37
26	HA	202	PEB	C1C-CHB	2.01	1.48	1.41
26	A1	202	PEB	C1C-CHB	2.01	1.48	1.41
26	I9	201	PEB	C1C-CHB	2.01	1.48	1.41
26	G1	202	PEB	C4A-NA	-2.01	1.33	1.37
26	e6	202	PEB	C4A-NA	-2.01	1.33	1.37
26	J9	201	PEB	C4A-NA	-2.01	1.33	1.37
26	UF	203	PEB	C4B-C3B	2.01	1.48	1.45
28	iH	1001	CYC	C1A-C2A	2.01	1.48	1.45
28	vH	1001	CYC	C1A-C2A	2.01	1.48	1.45
26	N4	203	PEB	CHC-C4C	2.01	1.55	1.50
26	l8	203	PEB	C1D-ND	2.01	1.48	1.45
26	V1	202	PEB	C2A-C1A	-2.01	1.50	1.52
26	bI	202	PEB	C2A-C1A	-2.01	1.50	1.52
26	l1	201	PEB	C4A-NA	-2.01	1.33	1.37
26	hB	203	PEB	C4A-NA	-2.01	1.33	1.37
26	E1	201	PEB	C1C-CHB	2.01	1.48	1.41
28	lH	1001	CYC	C1A-C2A	2.01	1.48	1.45
26	SF	201	PEB	C4B-NB	-2.01	1.34	1.38
26	P1	201	PEB	C1D-ND	2.01	1.48	1.45
26	v1	202	PEB	C1D-ND	2.01	1.48	1.45
26	VJ	202	PEB	C1D-ND	2.01	1.48	1.45
26	j7	201	PEB	C4A-NA	-2.01	1.33	1.37
26	UJ	202	PEB	C4A-NA	-2.01	1.33	1.37
26	pG	201	PEB	C1A-NA	-2.01	1.35	1.37
26	GG	202	PEB	O1C-CGC	2.01	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h6	203	PEB	C2A-C1A	-2.01	1.50	1.52
26	CA	201	PEB	C1C-CHB	2.01	1.48	1.41
26	QF	201	PEB	C4A-NA	-2.01	1.33	1.37
26	j1	201	PEB	C1D-ND	2.01	1.48	1.45
26	y4	201	PEB	C1C-CHB	2.01	1.48	1.41
26	A3	202	PEB	C1B-C2B	2.01	1.50	1.45
26	m2	202	PEB	C1C-CHB	2.01	1.48	1.41
26	AJ	304	PEB	C1C-CHB	2.01	1.48	1.41
26	R1	203	PEB	C4A-NA	-2.01	1.33	1.37
26	NE	201	PEB	C1A-NA	-2.01	1.35	1.37
26	D1	202	PEB	C1C-CHB	2.01	1.48	1.41
26	c2	203	PEB	C1C-CHB	2.01	1.48	1.41
26	F3	203	PEB	C1D-ND	2.01	1.48	1.45
26	W3	202	PEB	C1C-CHB	2.01	1.48	1.41
26	i2	202	PEB	C4A-NA	-2.01	1.33	1.37
26	aF	202	PEB	C4A-NA	-2.01	1.33	1.37
26	SB	202	PEB	C2A-C1A	-2.01	1.50	1.52
26	CG	202	PEB	C2A-C1A	-2.01	1.50	1.52
26	qG	201	PEB	C2A-C1A	-2.01	1.50	1.52
26	KD	201	PEB	C4B-C3B	2.01	1.48	1.45
28	H7	1001	CYC	C4D-CHA	2.01	1.48	1.41
26	nG	202	PEB	C1C-CHB	2.01	1.48	1.41
28	L6	1001	CYC	C1A-NA	-2.01	1.34	1.38
26	FG	202	PEB	C4B-C3B	2.01	1.48	1.45
26	Q8	202	PEB	C4A-NA	-2.01	1.33	1.37
26	G9	202	PEB	C4A-NA	-2.01	1.33	1.37
26	SF	202	PEB	C4A-NA	-2.01	1.33	1.37
26	h6	201	PEB	C1D-ND	2.01	1.48	1.45
26	P4	202	PEB	C1B-C2B	2.01	1.50	1.45
26	W4	201	PEB	C1B-C2B	2.01	1.50	1.45
26	II	201	PEB	CHA-C4A	-2.01	1.32	1.36
26	E3	201	PEB	C4A-NA	-2.01	1.33	1.37
26	xG	304	PEB	C4A-NA	-2.01	1.33	1.37
26	l2	202	PEB	C1C-CHB	2.01	1.48	1.41
26	iG	203	PEB	C1C-CHB	2.01	1.48	1.41
26	K4	202	PEB	C4B-C3B	2.01	1.48	1.45
26	m7	201	PEB	C4B-C3B	2.01	1.48	1.45
26	J8	202	PEB	C4B-C3B	2.01	1.48	1.45
26	oE	203	PEB	C1C-CHB	2.01	1.48	1.41
26	s4	201	PEB	C1D-ND	2.01	1.48	1.45
26	cI	203	PEB	C1C-CHB	2.01	1.48	1.41
26	e6	203	PEB	C4B-C3B	2.01	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	VE	202	PEB	C4B-C3B	2.01	1.48	1.45
28	qH	1001	CYC	C1A-C2A	2.01	1.48	1.45
26	c4	202	PEB	C1C-CHB	2.01	1.48	1.41
26	Z6	202	PEB	C1B-C2B	2.01	1.50	1.45
26	vE	201	PEB	C1C-CHB	2.01	1.48	1.41
26	F1	201	PEB	C4A-NA	-2.01	1.33	1.37
26	d2	202	PEB	C2A-C1A	-2.01	1.50	1.52
28	LB	1001	CYC	C1A-NA	-2.01	1.34	1.38
26	U6	202	PEB	C1C-CHB	2.01	1.48	1.41
26	iE	203	PEB	C1C-CHB	2.01	1.48	1.41
26	d4	201	PEB	C4A-NA	-2.01	1.33	1.37
26	h4	201	PEB	C4A-NA	-2.01	1.33	1.37
26	i8	202	PEB	C4A-NA	-2.01	1.33	1.37
26	L9	201	PEB	C4A-NA	-2.01	1.33	1.37
26	jA	203	PEB	C1C-CHB	2.01	1.48	1.41
26	fl	202	PEB	C4B-C3B	2.01	1.48	1.45
26	GE	201	PEB	CHA-C4A	-2.01	1.32	1.36
26	u4	201	PEB	C2A-C1A	-2.01	1.50	1.52
26	l1	202	PEB	C4B-C3B	2.01	1.48	1.45
26	eF	202	PEB	C4B-C3B	2.01	1.48	1.45
26	EG	202	PEB	C4B-C3B	2.01	1.48	1.45
28	DF	1001	CYC	C4B-NB	-2.01	1.33	1.38
26	b2	202	PEB	C1C-CHB	2.01	1.48	1.41
26	sG	202	PEB	C1C-CHB	2.01	1.48	1.41
26	J4	202	PEB	C4A-NA	-2.01	1.33	1.37
26	h8	203	PEB	C4B-C3B	2.01	1.48	1.45
26	O9	202	PEB	C1B-C2B	2.01	1.50	1.45
26	L5	201	PEB	OD-C4D	2.01	1.27	1.23
26	i2	203	PEB	C1C-CHB	2.01	1.48	1.41
28	qH	1002	CYC	C1D-CHD	2.01	1.48	1.41
26	A7	302	PEB	C2A-C1A	-2.01	1.50	1.52
26	GD	201	PEB	C2A-C1A	-2.01	1.50	1.52
26	e7	201	PEB	C4A-NA	-2.01	1.33	1.37
27	wE	304	PUB	C3C-C4C	2.01	1.50	1.43
26	Q1	201	PEB	C4B-C3B	2.01	1.48	1.45
26	sE	202	PEB	C1C-CHB	2.01	1.48	1.41
26	iB	202	PEB	C4A-NA	-2.01	1.33	1.37
28	FI	1001	CYC	C4D-CHA	2.01	1.48	1.41
26	R1	202	PEB	C1D-ND	2.00	1.48	1.45
26	RJ	201	PEB	C1D-ND	2.00	1.48	1.45
26	gI	202	PEB	C4B-C3B	2.00	1.48	1.45
26	iE	202	PEB	C4A-NA	-2.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AF	302	PEB	C4A-NA	-2.00	1.33	1.37
28	D7	1001	CYC	C4C-NC	-2.00	1.33	1.37
26	R1	202	PEB	C2A-C1A	-2.00	1.50	1.52
26	I4	201	PEB	C2A-C1A	-2.00	1.50	1.52
26	AC	203	PEB	C2A-C1A	-2.00	1.50	1.52
26	QG	202	PEB	C2A-C1A	-2.00	1.50	1.52
28	N7	1001	CYC	C1B-NB	-2.00	1.34	1.37
26	Q8	204	PEB	C4A-NA	-2.00	1.33	1.37
26	K9	201	PEB	C4B-C3B	2.00	1.48	1.45
26	r1	202	PEB	C1C-CHB	2.00	1.48	1.41
26	D3	203	PEB	C1D-ND	2.00	1.48	1.45
26	b7	203	PEB	C4A-NA	-2.00	1.33	1.37
26	kA	201	PEB	C4A-NA	-2.00	1.33	1.37
28	H2	1001	CYC	C4A-C3A	2.00	1.50	1.45
26	oG	203	PEB	C1C-CHB	2.00	1.48	1.41
28	KH	1001	CYC	C1B-NB	-2.00	1.34	1.37
26	dB	202	PEB	C4B-C3B	2.00	1.48	1.45
26	GE	203	PEB	C4B-C3B	2.00	1.48	1.45
26	SA	202	PEB	C1D-ND	2.00	1.48	1.45
28	rH	1001	CYC	C4D-CHA	2.00	1.48	1.41
26	AF	302	PEB	C2A-C1A	-2.00	1.50	1.52
26	y1	202	PEB	C4A-NA	-2.00	1.33	1.37
26	Q7	203	PEB	C4A-NA	-2.00	1.33	1.37
26	WE	203	PEB	C4A-NA	-2.00	1.33	1.37
26	R9	202	PEB	C4B-C3B	2.00	1.48	1.45
26	PA	202	PEB	C4B-C3B	2.00	1.48	1.45
26	W7	201	PEB	C1D-ND	2.00	1.48	1.45
26	a1	202	PEB	C4A-NA	-2.00	1.33	1.37
26	B9	202	PEB	C4A-NA	-2.00	1.33	1.37
26	a2	201	PEB	C1B-C2B	2.00	1.50	1.45
26	dF	203	PEB	C1B-C2B	2.00	1.50	1.45
26	F3	201	PEB	C4A-NA	-2.00	1.33	1.37
26	N7	1002	PEB	C4A-NA	-2.00	1.33	1.37
26	m6	202	PEB	C2A-C1A	-2.00	1.50	1.52
26	rE	202	PEB	C1D-ND	2.00	1.48	1.45
26	aE	203	PEB	C1C-CHB	2.00	1.48	1.41
26	kG	201	PEB	C1C-CHB	2.00	1.48	1.41
26	u1	203	PEB	C4A-NA	-2.00	1.33	1.37
26	h6	201	PEB	C4A-NA	-2.00	1.33	1.37
26	d6	203	PEB	C1C-CHB	2.00	1.48	1.41
26	mE	203	PEB	C1C-CHB	2.00	1.48	1.41
26	kI	202	PEB	C1C-CHB	2.00	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L1	201	PEB	C1B-C2B	2.00	1.50	1.45
28	rH	1001	CYC	C4C-NC	-2.00	1.33	1.37
26	V2	203	PEB	O1B-CGB	2.00	1.28	1.22
26	YA	203	PEB	C2A-C1A	-2.00	1.50	1.52
26	Y2	201	PEB	C4B-C3B	2.00	1.48	1.45
26	UF	202	PEB	C4B-C3B	2.00	1.48	1.45
26	IE	201	PEB	O1C-CGC	2.00	1.28	1.22
26	K4	201	PEB	C1B-C2B	2.00	1.50	1.45
26	ZG	202	PEB	C1C-CHB	2.00	1.48	1.41
28	B6	1002	CYC	C1B-C2B	2.00	1.48	1.45
26	m6	201	PEB	C1D-ND	2.00	1.48	1.45
26	e8	201	PEB	C1D-ND	2.00	1.48	1.45
26	c8	202	PEB	C1C-CHB	2.00	1.48	1.41
26	k8	202	PEB	C1C-CHB	2.00	1.48	1.41
26	YD	303	PEB	C1C-CHB	2.00	1.48	1.41
26	SE	201	PEB	C1C-CHB	2.00	1.48	1.41
26	DD	201	PEB	C1B-C2B	2.00	1.50	1.45
26	E1	201	PEB	C4A-NA	-2.00	1.33	1.37
26	g1	203	PEB	C4A-NA	-2.00	1.33	1.37
26	c4	201	PEB	C4A-NA	-2.00	1.33	1.37
26	c7	201	PEB	C4A-NA	-2.00	1.33	1.37
26	i7	201	PEB	C4A-NA	-2.00	1.33	1.37

All (24889) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	dH	1001	CYC	C4D-CHA-C1A	26.78	160.79	128.81
28	cH	1001	CYC	C4D-CHA-C1A	23.60	157.00	128.81
28	AH	1001	CYC	C4D-CHA-C1A	23.35	156.70	128.81
28	KH	1001	CYC	CHA-C1A-NA	-22.36	97.82	128.83
26	FG	201	PEB	OA-C1A-C2A	-17.62	112.17	126.17
26	FE	201	PEB	OA-C1A-C2A	-17.55	112.22	126.17
26	XG	201	PEB	OA-C1A-C2A	-16.31	113.20	126.17
26	XE	201	PEB	OA-C1A-C2A	-16.25	113.26	126.17
26	RG	201	PEB	OA-C1A-C2A	-16.11	113.36	126.17
26	qE	202	PEB	CHB-C4B-NB	-15.73	107.01	128.83
26	RE	201	PEB	OA-C1A-C2A	-15.63	113.74	126.17
26	LE	201	PEB	OA-C1A-C2A	-15.19	114.09	126.17
28	KH	1001	CYC	C4D-CHA-C1A	15.18	146.94	128.81
26	BG	201	PEB	OA-C1A-C2A	-15.09	114.17	126.17
26	PE	201	PEB	OA-C1A-C2A	-15.05	114.21	126.17
26	qG	202	PEB	CHB-C4B-NB	-14.36	108.91	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	zE	501	PEB	OA-C1A-C2A	-14.36	114.76	126.17
26	ZE	201	PEB	OA-C1A-C2A	-14.31	114.79	126.17
26	zG	501	PEB	OA-C1A-C2A	-14.18	114.90	126.17
26	Z7	201	PEB	C1C-CHB-C4B	13.88	145.38	128.81
26	LG	201	PEB	OA-C1A-C2A	-13.86	115.16	126.17
26	BE	201	PEB	OA-C1A-C2A	-13.79	115.21	126.17
26	JE	201	PEB	OA-C1A-C2A	-13.65	115.32	126.17
26	PG	201	PEB	OA-C1A-C2A	-13.32	115.58	126.17
28	dH	1001	CYC	C1B-CHB-C4A	13.08	160.04	128.08
28	F2	1001	CYC	C3B-C4B-NB	12.99	117.27	106.78
26	ZF	201	PEB	C1C-CHB-C4B	12.87	144.18	128.81
28	EF	1001	CYC	C3B-C4B-NB	12.59	116.95	106.78
26	NE	201	PEB	OA-C1A-C2A	-12.54	116.20	126.17
26	J3	202	PEB	C1C-CHB-C4B	12.53	143.78	128.81
26	nG	201	PEB	OA-C1A-C2A	-12.53	116.21	126.17
26	DG	201	PEB	OA-C1A-C2A	-12.49	116.24	126.17
26	NG	201	PEB	OA-C1A-C2A	-12.47	116.26	126.17
26	vE	201	PEB	OA-C1A-C2A	-12.41	116.31	126.17
26	fG	201	PEB	OA-C1A-C2A	-12.32	116.38	126.17
28	E7	1001	CYC	C3B-C4B-NB	12.20	116.63	106.78
26	DE	202	PEB	CHC-C1D-ND	-12.13	99.87	113.95
26	fE	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
26	JG	201	PEB	OA-C1A-C2A	-12.06	116.58	126.17
28	tH	1001	CYC	C3B-C4B-NB	11.92	116.41	106.78
26	TE	201	PEB	OA-C1A-C2A	-11.88	116.73	126.17
26	DE	201	PEB	OA-C1A-C2A	-11.78	116.81	126.17
27	AF	304	PUB	C2A-C1A-NA	11.75	117.64	107.21
26	j1	202	PEB	C1C-CHB-C4B	11.73	142.82	128.81
28	FI	1001	CYC	C3B-C4B-NB	11.72	116.25	106.78
26	TG	201	PEB	OA-C1A-C2A	-11.71	116.86	126.17
26	pG	202	PEB	C1C-CHB-C4B	11.68	142.77	128.81
28	HI	1001	CYC	C3B-C4B-NB	11.68	116.22	106.78
28	KH	1001	CYC	C3B-C4B-NB	11.67	116.20	106.78
28	H2	1001	CYC	C3B-C4B-NB	11.66	116.20	106.78
28	RH	1001	CYC	C3B-C4B-NB	11.64	116.19	106.78
26	v1	202	PEB	CHB-C4B-NB	-11.64	112.68	128.83
26	bE	201	PEB	OA-C1A-C2A	-11.60	116.95	126.17
28	IF	1001	CYC	C3B-C4B-NB	11.59	116.14	106.78
28	rH	1001	CYC	C3B-C4B-NB	11.59	116.14	106.78
28	I7	1001	CYC	C3B-C4B-NB	11.57	116.12	106.78
28	EH	1001	CYC	C3B-C4B-NB	11.54	116.10	106.78
26	m6	202	PEB	C1C-CHB-C4B	11.53	142.58	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	xG	302	PEB	C1C-CHB-C4B	-11.50	115.07	128.81
28	PH	1001	CYC	C3B-C4B-NB	11.48	116.06	106.78
28	GH	1001	CYC	C3B-C4B-NB	11.48	116.05	106.78
28	AH	1001	CYC	C3B-C4B-NB	11.47	116.05	106.78
28	cH	1001	CYC	C3B-C4B-NB	11.47	116.05	106.78
28	lH	1001	CYC	C3B-C4B-NB	11.45	116.03	106.78
26	h6	201	PEB	C1C-CHB-C4B	11.45	142.48	128.81
28	D6	1001	CYC	C3B-C4B-NB	11.44	116.02	106.78
26	xE	302	PEB	C1C-CHB-C4B	-11.43	115.16	128.81
27	24	403	PUB	C2A-C1A-NA	11.40	117.32	107.21
28	FB	1001	CYC	C3B-C4B-NB	11.40	115.99	106.78
28	F6	1001	CYC	C3B-C4B-NB	11.39	115.98	106.78
28	gH	1001	CYC	C3B-C4B-NB	11.37	115.96	106.78
26	tG	201	PEB	OA-C1A-C2A	-11.36	117.14	126.17
28	HB	1001	CYC	C3B-C4B-NB	11.32	115.92	106.78
28	EI	1001	CYC	C3B-C4B-NB	11.32	115.92	106.78
27	Q8	201	PUB	C2A-C1A-NA	11.27	117.21	107.21
28	MB	1001	CYC	C3B-C4B-NB	11.26	115.88	106.78
28	M6	1001	CYC	C3B-C4B-NB	11.26	115.88	106.78
28	C2	1001	CYC	C3B-C4B-NB	11.26	115.88	106.78
28	iH	1001	CYC	C3B-C4B-NB	11.25	115.87	106.78
28	H6	1001	CYC	C3B-C4B-NB	11.25	115.86	106.78
27	yE	303	PUB	C2A-C1A-NA	11.23	117.17	107.21
26	x1	202	PEB	CHB-C4B-NB	-11.22	113.27	128.83
28	VH	1001	CYC	C3B-C4B-NB	11.21	115.84	106.78
28	KH	1001	CYC	CHA-C1A-C2A	11.21	151.22	125.32
28	E2	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
28	G2	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
28	CI	1001	CYC	C3B-C4B-NB	11.20	115.83	106.78
28	DB	1001	CYC	C3B-C4B-NB	11.19	115.82	106.78
26	YD	303	PEB	C1C-CHB-C4B	-11.18	115.45	128.81
28	GI	1001	CYC	C3B-C4B-NB	11.17	115.81	106.78
28	mH	1001	CYC	C3B-C4B-NB	11.15	115.79	106.78
27	QA	201	PUB	C2A-C1A-NA	11.15	117.10	107.21
28	JH	1001	CYC	C3B-C4B-NB	11.14	115.78	106.78
27	yG	303	PUB	C2A-C1A-NA	11.14	117.09	107.21
27	A8	304	PUB	C2A-C1A-NA	11.13	117.09	107.21
27	BA	302	PUB	C2A-C1A-NA	11.10	117.05	107.21
28	DF	1003	CYC	C3B-C4B-NB	11.09	115.74	106.78
28	I2	1001	CYC	C3B-C4B-NB	11.09	115.74	106.78
28	G7	1001	CYC	C3B-C4B-NB	11.09	115.74	106.78
27	A4	203	PUB	C2A-C1A-NA	11.08	117.04	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	nE	201	PEB	OA-C1A-C2A	-11.07	117.38	126.17
27	A6	303	PUB	C2A-C1A-NA	11.06	117.02	107.21
27	A8	303	PUB	C2A-C1A-NA	11.06	117.02	107.21
26	vG	201	PEB	OA-C1A-C2A	-11.06	117.38	126.17
27	AA	303	PUB	C2A-C1A-NA	11.05	117.01	107.21
27	AB	303	PUB	C2A-C1A-NA	11.05	117.01	107.21
28	II	1001	CYC	C3B-C4B-NB	11.04	115.70	106.78
28	M2	1001	CYC	C3B-C4B-NB	11.04	115.70	106.78
28	yH	1001	CYC	C3B-C4B-NB	11.03	115.69	106.78
27	N9	201	PUB	C2A-C1A-NA	11.03	116.99	107.21
27	AA	304	PUB	C2A-C1A-NA	11.03	116.99	107.21
27	B8	302	PUB	C2A-C1A-NA	11.01	116.98	107.21
27	AI	303	PUB	C2A-C1A-NA	11.01	116.97	107.21
28	dH	1001	CYC	C3B-C4B-NB	10.99	115.66	106.78
28	WH	1001	CYC	C3B-C4B-NB	10.98	115.65	106.78
28	GB	1001	CYC	C3B-C4B-NB	10.98	115.65	106.78
28	KI	1001	CYC	C3B-C4B-NB	10.96	115.63	106.78
28	K2	1001	CYC	C3B-C4B-NB	10.95	115.62	106.78
27	A2	303	PUB	C2A-C1A-NA	10.94	116.91	107.21
27	AF	303	PUB	C2A-C1A-NA	10.94	116.91	107.21
28	G6	1001	CYC	C3B-C4B-NB	10.90	115.59	106.78
28	F7	1001	CYC	C3B-C4B-NB	10.90	115.59	106.78
28	MI	1001	CYC	C3B-C4B-NB	10.90	115.59	106.78
28	J7	1003	CYC	C3B-C4B-NB	10.89	115.58	106.78
28	KB	202	CYC	C3B-C4B-NB	10.88	115.57	106.78
27	Y3	302	PUB	C2A-C1A-NA	10.88	116.86	107.21
28	K6	202	CYC	C3B-C4B-NB	10.88	115.57	106.78
28	YH	1004	CYC	C3B-C4B-NB	10.88	115.56	106.78
27	K4	203	PUB	C2A-C1A-NA	10.87	116.85	107.21
28	EB	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78
26	CE	201	PEB	CHC-C4C-C3C	-10.86	111.82	130.34
28	CB	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
27	A7	304	PUB	C2A-C1A-NA	10.85	116.83	107.21
27	24	402	PUB	C2A-C1A-NA	10.85	116.83	107.21
26	tG	202	PEB	C1C-CHB-C4B	10.84	141.76	128.81
28	kH	1001	CYC	C3B-C4B-NB	10.84	115.53	106.78
27	A2	302	PUB	C2A-C1A-NA	10.83	116.82	107.21
28	vH	1001	CYC	C3B-C4B-NB	10.83	115.53	106.78
26	DJ	201	PEB	CHC-C1D-ND	-10.83	101.37	113.95
28	KF	1001	CYC	C3B-C4B-NB	10.83	115.53	106.78
28	TH	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78
28	pH	1001	CYC	C3B-C4B-NB	10.82	115.52	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	qH	1001	CYC	C3B-C4B-NB	10.81	115.51	106.78
27	A7	303	PUB	C2A-C1A-NA	10.81	116.80	107.21
28	I6	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
28	UH	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
28	C6	1001	CYC	C3B-C4B-NB	10.79	115.50	106.78
26	aE	202	PEB	C1C-CHB-C4B	10.79	141.70	128.81
27	AI	302	PUB	C2A-C1A-NA	10.79	116.78	107.21
28	NH	1001	CYC	C3B-C4B-NB	10.78	115.49	106.78
28	E6	1001	CYC	C3B-C4B-NB	10.78	115.48	106.78
28	hH	1001	CYC	C3B-C4B-NB	10.78	115.48	106.78
28	C7	1001	CYC	C3B-C4B-NB	10.76	115.47	106.78
28	wH	1001	CYC	C3B-C4B-NB	10.75	115.46	106.78
28	OH	1001	CYC	C3B-C4B-NB	10.74	115.46	106.78
28	nH	1001	CYC	C3B-C4B-NB	10.74	115.46	106.78
28	SH	1001	CYC	C3B-C4B-NB	10.72	115.44	106.78
28	1H	1000	CYC	C3B-C4B-NB	10.72	115.44	106.78
27	AB	302	PUB	C2A-C1A-NA	10.72	116.72	107.21
28	IH	1001	CYC	C3B-C4B-NB	10.72	115.44	106.78
28	LH	1001	CYC	C3B-C4B-NB	10.71	115.43	106.78
28	eH	1001	CYC	C3B-C4B-NB	10.71	115.43	106.78
28	jH	1001	CYC	C3B-C4B-NB	10.71	115.43	106.78
28	IB	1001	CYC	C3B-C4B-NB	10.70	115.42	106.78
28	MH	1001	CYC	C3B-C4B-NB	10.70	115.42	106.78
27	21	403	PUB	C2A-C1A-NA	10.70	116.70	107.21
28	KH	1001	CYC	CHB-C4A-NA	-10.68	102.60	124.93
28	D7	1001	CYC	C3B-C4B-NB	10.67	115.40	106.78
27	wE	304	PUB	C2A-C1A-NA	10.66	116.66	107.21
28	oH	1001	CYC	C3B-C4B-NB	10.64	115.38	106.78
27	YD	302	PUB	C2A-C1A-NA	10.64	116.65	107.21
28	DI	1001	CYC	C3B-C4B-NB	10.63	115.37	106.78
28	qH	1002	CYC	C3B-C4B-NB	10.63	115.37	106.78
28	sH	1001	CYC	C3B-C4B-NB	10.63	115.37	106.78
26	JC	201	PEB	CMB-C2B-C1B	10.63	141.43	125.06
28	JF	1003	CYC	C3B-C4B-NB	10.63	115.36	106.78
27	xG	301	PUB	C2A-C1A-NA	10.62	116.63	107.21
28	fH	1001	CYC	C3B-C4B-NB	10.62	115.36	106.78
27	xE	305	PUB	C2A-C1A-NA	10.61	116.62	107.21
26	J5	201	PEB	CMB-C2B-C1B	10.61	141.40	125.06
27	NJ	201	PUB	C2A-C1A-NA	10.61	116.62	107.21
28	D2	1001	CYC	C3B-C4B-NB	10.60	115.34	106.78
28	YH	1002	CYC	C3B-C4B-NB	10.60	115.34	106.78
28	K7	1001	CYC	C3B-C4B-NB	10.59	115.34	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K1	203	PUB	C2A-C1A-NA	10.59	116.61	107.21
27	K3	203	PUB	C2A-C1A-NA	10.59	116.60	107.21
28	L7	1001	CYC	C3B-C4B-NB	10.59	115.33	106.78
27	A1	203	PUB	C2A-C1A-NA	10.58	116.60	107.21
28	YH	1003	CYC	C3B-C4B-NB	10.58	115.33	106.78
27	A6	302	PUB	C2A-C1A-NA	10.58	116.60	107.21
27	KD	203	PUB	C2A-C1A-NA	10.58	116.59	107.21
28	J7	1001	CYC	C3B-C4B-NB	10.57	115.31	106.78
27	xG	305	PUB	C2A-C1A-NA	10.56	116.58	107.21
27	A9	302	PUB	C2A-C1A-NA	10.56	116.57	107.21
27	xE	306	PUB	C2A-C1A-NA	10.55	116.56	107.21
27	yG	302	PUB	C2A-C1A-NA	10.54	116.56	107.21
26	V8	202	PEB	CHB-C4B-NB	-10.51	114.25	128.83
27	xE	301	PUB	C2A-C1A-NA	10.51	116.53	107.21
28	QH	1001	CYC	C3B-C4B-NB	10.50	115.27	106.78
27	21	402	PUB	C2A-C1A-NA	10.50	116.53	107.21
27	wG	304	PUB	C2A-C1A-NA	10.50	116.52	107.21
28	uH	1001	CYC	C3B-C4B-NB	10.49	115.25	106.78
27	xG	306	PUB	C2A-C1A-NA	10.48	116.51	107.21
27	yE	302	PUB	C2A-C1A-NA	10.48	116.51	107.21
26	CE	201	PEB	C1C-CHB-C4B	10.46	141.31	128.81
28	FF	1001	CYC	C3B-C4B-NB	10.45	115.22	106.78
28	DF	1001	CYC	C3B-C4B-NB	10.45	115.22	106.78
27	AJ	302	PUB	C2A-C1A-NA	10.45	116.48	107.21
28	YH	1001	CYC	C3B-C4B-NB	10.45	115.22	106.78
26	pE	202	PEB	C1C-CHB-C4B	10.43	141.27	128.81
28	CH	1001	CYC	C3B-C4B-NB	10.39	115.17	106.78
26	mB	202	PEB	C1C-CHB-C4B	10.39	141.22	128.81
28	CF	1001	CYC	C3B-C4B-NB	10.37	115.15	106.78
28	H7	1001	CYC	C3B-C4B-NB	10.36	115.15	106.78
26	x4	202	PEB	CHB-C4B-NB	-10.34	114.49	128.83
26	VE	201	PEB	OA-C1A-C2A	-10.27	118.00	126.17
28	BB	1001	CYC	C3B-C4B-NB	10.26	115.07	106.78
26	r4	202	PEB	CHB-C4B-NB	-10.26	114.59	128.83
27	AF	304	PUB	C4B-CHB-C1C	-10.26	116.55	128.81
28	B6	1001	CYC	C3B-C4B-NB	10.26	115.07	106.78
26	N3	202	PEB	C1C-CHB-C4B	10.26	141.06	128.81
28	N2	1001	CYC	C3B-C4B-NB	10.25	115.06	106.78
28	JF	1001	CYC	C3B-C4B-NB	10.25	115.06	106.78
26	p1	202	PEB	CHB-C4B-NB	-10.23	114.64	128.83
26	VE	202	PEB	C1C-CHB-C4B	10.23	141.02	128.81
28	LB	1001	CYC	C3B-C4B-NB	10.20	115.02	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J2	1001	CYC	C3B-C4B-NB	10.17	115.00	106.78
28	NI	1001	CYC	C3B-C4B-NB	10.17	115.00	106.78
26	r1	202	PEB	CHB-C4B-NB	-10.16	114.73	128.83
26	lA	201	PEB	C1C-CHB-C4B	10.15	140.93	128.81
26	z4	202	PEB	CHB-C4B-NB	-10.14	114.76	128.83
26	LG	202	PEB	C1C-CHB-C4B	10.14	140.92	128.81
26	GE	202	PEB	OA-C1A-C2A	10.13	134.22	126.17
28	L6	1001	CYC	C3B-C4B-NB	10.12	114.95	106.78
26	jF	202	PEB	CHB-C4B-NB	-10.09	114.83	128.83
26	L2	1002	PEB	CHC-C1D-ND	-10.09	102.23	113.95
28	HF	1001	CYC	C3B-C4B-NB	10.09	114.93	106.78
28	N7	1001	CYC	C3B-C4B-NB	10.03	114.88	106.78
26	Y3	303	PEB	C1C-CHB-C4B	-10.03	116.83	128.81
26	p4	202	PEB	CHB-C4B-NB	-10.02	114.93	128.83
26	tE	202	PEB	C1C-CHB-C4B	9.97	140.72	128.81
26	QG	203	PEB	C1C-CHB-C4B	9.97	140.71	128.81
28	YH	1001	CYC	CAA-CBA-CGA	9.96	135.03	113.60
26	UE	203	PEB	CHC-C4C-C3C	-9.92	113.42	130.34
26	GE	201	PEB	CHC-C4C-C3C	-9.86	113.52	130.34
28	JI	1001	CYC	C3B-C4B-NB	9.85	114.73	106.78
26	A7	301	PEB	C1C-CHB-C4B	-9.83	117.07	128.81
26	jG	201	PEB	OA-C1A-C2A	-9.81	118.37	126.17
26	z1	202	PEB	CHB-C4B-NB	-9.76	115.28	128.83
26	t1	202	PEB	CHB-C4B-NB	-9.72	115.35	128.83
26	j8	202	PEB	C1C-CHB-C4B	-9.72	117.20	128.81
26	v4	202	PEB	CHB-C4B-NB	-9.71	115.36	128.83
26	gB	202	PEB	C1C-CHB-C4B	-9.70	117.22	128.81
27	A7	304	PUB	C4B-CHB-C1C	-9.70	117.22	128.81
26	JD	202	PEB	C1C-CHB-C4B	9.60	140.28	128.81
26	CE	201	PEB	CHC-C1D-ND	9.59	125.08	113.95
28	LF	1001	CYC	C3B-C4B-NB	9.59	114.52	106.78
26	ND	202	PEB	C1C-CHB-C4B	9.58	140.25	128.81
28	NF	1001	CYC	C3B-C4B-NB	9.56	114.50	106.78
26	xE	302	PEB	CHB-C4B-NB	-9.56	115.57	128.83
26	GA	203	PEB	CHC-C4C-C3C	-9.54	114.07	130.34
26	YD	303	PEB	CHB-C4B-NB	-9.53	115.61	128.83
28	NB	1001	CYC	C3B-C4B-NB	9.53	114.48	106.78
26	F9	203	PEB	CHB-C4B-NB	-9.49	115.67	128.83
26	VG	202	PEB	C1C-CHB-C4B	9.42	140.07	128.81
26	LE	202	PEB	C1C-CHB-C4B	9.37	140.00	128.81
26	kA	201	PEB	C1C-CHB-C4B	-9.35	117.64	128.81
26	dF	203	PEB	CHB-C4B-NB	-9.34	115.87	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lF	203	PEB	CHB-C4B-NB	-9.34	115.87	128.83
26	xG	302	PEB	CHB-C4B-NB	-9.33	115.88	128.83
26	A9	304	PEB	C1C-CHB-C4B	-9.33	117.67	128.81
26	GG	202	PEB	OA-C1A-C2A	9.32	133.59	126.17
26	cE	203	PEB	CHC-C4C-C3C	-9.31	114.46	130.34
26	LI	1002	PEB	CHC-C1D-ND	-9.31	103.14	113.95
26	l7	203	PEB	C1C-CHB-C4B	-9.28	117.72	128.81
26	FE	202	PEB	C1C-CHB-C4B	9.27	139.89	128.81
26	ZE	201	PEB	CHA-C4A-NA	9.27	136.23	125.20
26	VA	202	PEB	CHB-C4B-NB	-9.26	115.98	128.83
26	FG	202	PEB	C1C-CHB-C4B	9.26	139.87	128.81
26	BD	202	PEB	C1C-CHB-C4B	9.25	139.86	128.81
26	VG	201	PEB	OA-C1A-C2A	-9.25	118.82	126.17
26	bE	202	PEB	C1C-CHB-C4B	9.23	139.84	128.81
26	pE	201	PEB	OA-C1A-C2A	-9.19	118.86	126.17
26	g6	202	PEB	C1C-CHB-C4B	-9.15	117.88	128.81
26	jA	202	PEB	C1C-CHB-C4B	-9.14	117.89	128.81
26	DA	202	PEB	CHB-C4B-NB	-9.13	116.17	128.83
26	l7	203	PEB	CHB-C4B-NB	-9.11	116.19	128.83
26	LE	201	PEB	CHC-C1D-ND	-9.08	103.41	113.95
26	A7	301	PEB	CHB-C4B-NB	-9.05	116.27	128.83
26	FG	201	PEB	C2A-C1A-NA	9.05	116.07	108.27
26	d7	203	PEB	C1C-CHB-C4B	-9.05	118.00	128.81
26	Y3	301	PEB	CHC-C1D-ND	-9.03	103.46	113.95
26	aA	204	PEB	C1C-CHB-C4B	9.02	139.59	128.81
26	YD	303	PEB	CHC-C1D-ND	-9.02	103.47	113.95
26	FD	202	PEB	CHC-C4C-C3C	-9.01	114.97	130.34
28	L2	1001	CYC	C3B-C4B-NB	9.01	114.06	106.78
26	L3	202	PEB	C1C-CHB-C4B	8.98	139.54	128.81
26	XA	202	PEB	C1C-CHB-C4B	-8.97	118.09	128.81
27	AF	304	PUB	CHB-C1C-NC	-8.97	116.38	128.83
28	LI	1001	CYC	C3B-C4B-NB	8.96	114.01	106.78
26	BD	202	PEB	OA-C1A-C2A	-8.94	119.06	126.17
26	f7	202	PEB	C1C-CHB-C4B	-8.94	118.13	128.81
26	YD	301	PEB	C1C-CHB-C4B	-8.92	118.15	128.81
26	BG	202	PEB	C1C-CHB-C4B	8.91	139.45	128.81
26	F9	203	PEB	C1C-CHB-C4B	8.89	139.43	128.81
26	t4	202	PEB	CHB-C4B-NB	-8.89	116.50	128.83
26	GG	201	PEB	CHB-C4B-NB	-8.88	116.50	128.83
26	D8	202	PEB	CHB-C4B-NB	-8.87	116.53	128.83
26	V8	202	PEB	OA-C1A-C2A	-8.87	119.12	126.17
26	b2	201	PEB	C1C-CHB-C4B	8.82	139.34	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d7	203	PEB	CHB-C4B-NB	-8.81	116.61	128.83
26	LE	201	PEB	CHA-C4A-NA	8.80	135.67	125.20
27	A7	304	PUB	CHB-C1C-NC	-8.79	116.63	128.83
26	w4	202	PEB	C1C-CHB-C4B	8.79	139.31	128.81
26	UF	201	PEB	C1C-CHB-C4B	8.78	139.30	128.81
26	e8	202	PEB	CHB-C4B-NB	-8.78	116.65	128.83
26	21	405	PEB	CHB-C4B-NB	-8.74	116.70	128.83
27	KD	203	PUB	C4B-CHB-C1C	-8.73	118.38	128.81
26	jE	201	PEB	OA-C1A-C2A	-8.73	119.23	126.17
26	qG	203	PEB	C1C-CHB-C4B	8.71	139.22	128.81
26	FE	201	PEB	C2A-C1A-NA	8.71	115.78	108.27
26	B3	202	PEB	OA-C1A-C2A	-8.70	119.26	126.17
26	AF	305	PEB	C1C-CHB-C4B	-8.70	118.42	128.81
26	Y3	303	PEB	CHB-C4B-NB	-8.69	116.78	128.83
26	cE	203	PEB	C1C-CHB-C4B	8.68	139.18	128.81
26	F3	202	PEB	CHC-C4C-C3C	-8.67	115.56	130.34
26	XG	201	PEB	C2A-C1A-NA	8.66	115.74	108.27
26	CA	202	PEB	C1C-CHB-C4B	-8.66	118.47	128.81
28	B6	1002	CYC	C3B-C4B-NB	8.65	113.77	106.78
26	BE	202	PEB	C1C-CHB-C4B	8.64	139.13	128.81
26	iE	202	PEB	C1C-CHB-C4B	8.63	139.11	128.81
26	cE	201	PEB	C1C-CHB-C4B	8.62	139.10	128.81
26	fF	202	PEB	C1C-CHB-C4B	-8.62	118.52	128.81
26	eA	202	PEB	CHB-C4B-NB	-8.58	116.92	128.83
28	cH	1001	CYC	CHB-C4A-NA	-8.57	107.00	124.93
26	VF	202	PEB	C1C-CHB-C4B	8.56	139.03	128.81
26	HE	201	PEB	CHC-C4C-C3C	-8.54	115.78	130.34
26	x1	202	PEB	C1C-CHB-C4B	8.53	139.00	128.81
26	O7	202	PEB	CHB-C4B-NB	-8.50	117.04	128.83
26	cA	201	PEB	C1C-CHB-C4B	-8.49	118.67	128.81
26	y1	203	PEB	C1C-CHB-C4B	-8.47	118.69	128.81
26	XE	201	PEB	C2A-C1A-NA	8.46	115.57	108.27
26	b7	202	PEB	C1C-CHB-C4B	-8.45	118.71	128.81
26	L8	201	PEB	OA-C1A-C2A	-8.45	119.46	126.17
26	l8	201	PEB	C1C-CHB-C4B	8.44	138.89	128.81
26	OE	201	PEB	CHC-C1D-ND	-8.42	104.16	113.95
26	aA	204	PEB	CHC-C4C-C3C	-8.41	115.99	130.34
26	tE	201	PEB	OA-C1A-C2A	-8.41	119.49	126.17
26	HG	202	PEB	C1C-CHB-C4B	8.40	138.85	128.81
26	HE	202	PEB	C1C-CHB-C4B	8.40	138.84	128.81
26	GE	201	PEB	CHB-C4B-NB	-8.39	117.18	128.83
26	H8	202	PEB	CHB-C4B-NB	-8.39	117.19	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	qE	202	PEB	C1C-CHB-C4B	8.38	138.82	128.81
26	W7	202	PEB	C1C-CHB-C4B	-8.37	118.81	128.81
26	lG	201	PEB	OA-C1A-C2A	-8.36	119.52	126.17
26	c8	201	PEB	CHB-C4B-NB	-8.35	117.25	128.83
27	NJ	201	PUB	C4B-CHB-C1C	-8.35	118.84	128.81
26	oE	203	PEB	CHC-C4C-C3C	-8.34	116.11	130.34
26	LD	202	PEB	C1C-CHB-C4B	8.34	138.78	128.81
26	AJ	304	PEB	C1C-CHB-C4B	-8.34	118.85	128.81
26	IE	201	PEB	OA-C1A-C2A	8.33	132.80	126.17
26	L3	202	PEB	OA-C1A-C2A	-8.32	119.56	126.17
26	RG	201	PEB	C2A-C1A-NA	8.31	115.44	108.27
26	PJ	201	PEB	C1C-CHB-C4B	8.31	138.74	128.81
26	FG	201	PEB	CHA-C4A-NA	8.31	135.09	125.20
26	XE	201	PEB	CHA-C4A-NA	8.31	135.08	125.20
26	FE	201	PEB	CHA-C4A-NA	8.29	135.06	125.20
26	ND	202	PEB	OA-C1A-C2A	-8.29	119.58	126.17
26	K1	202	PEB	CHB-C4B-NB	-8.29	117.33	128.83
26	S7	202	PEB	C1C-CHB-C4B	-8.28	118.91	128.81
26	HJ	203	PEB	CHC-C1D-ND	-8.28	104.33	113.95
26	kG	203	PEB	C1C-CHB-C4B	8.28	138.70	128.81
26	BJ	203	PEB	CHC-C4C-C3C	-8.27	116.23	130.34
26	24	404	PEB	CHB-C4B-NB	-8.26	117.36	128.83
26	N3	202	PEB	OA-C1A-C2A	-8.25	119.61	126.17
26	h7	203	PEB	CHB-C4B-NB	-8.25	117.39	128.83
26	AJ	303	PEB	C1C-CHB-C4B	-8.24	118.96	128.81
26	KD	201	PEB	C1C-CHB-C4B	8.24	138.66	128.81
26	XG	201	PEB	CHA-C4A-NA	8.24	135.00	125.20
26	B3	202	PEB	C1C-CHB-C4B	8.24	138.65	128.81
26	QG	203	PEB	CHC-C4C-C3C	-8.22	116.32	130.34
26	g8	201	PEB	C1C-CHB-C4B	-8.22	119.00	128.81
26	XA	202	PEB	CHB-C4B-NB	-8.21	117.44	128.83
26	V8	202	PEB	C1C-CHB-C4B	-8.19	119.02	128.81
26	LG	201	PEB	CHA-C4A-NA	8.18	134.94	125.20
26	LA	201	PEB	OA-C1A-C2A	-8.18	119.67	126.17
28	LF	1001	CYC	C4D-CHA-C1A	8.18	138.58	128.81
28	AH	1001	CYC	CHB-C4A-NA	-8.16	107.87	124.93
26	AJ	304	PEB	CHB-C4B-NB	-8.16	117.51	128.83
26	J3	203	PEB	CHB-C4B-NB	-8.15	117.52	128.83
26	kA	202	PEB	CHB-C4B-NB	-8.15	117.53	128.83
26	cA	201	PEB	CHB-C4B-NB	-8.14	117.53	128.83
26	z1	201	PEB	C1C-CHB-C4B	8.13	138.52	128.81
26	24	404	PEB	C1C-CHB-C4B	-8.11	119.13	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d4	202	PEB	CHC-C4C-C3C	-8.09	116.54	130.34
26	X8	202	PEB	CHB-C4B-NB	-8.08	117.62	128.83
26	lE	202	PEB	C1C-CHB-C4B	8.07	138.45	128.81
26	A9	304	PEB	CHB-C4B-NB	-8.07	117.64	128.83
26	ZF	201	PEB	OA-C1A-C2A	-8.07	119.76	126.17
26	c8	201	PEB	C1C-CHB-C4B	-8.06	119.17	128.81
26	UG	201	PEB	CMB-C2B-C1B	8.06	137.47	125.06
26	S7	203	PEB	C1C-CHB-C4B	8.04	138.42	128.81
26	f7	203	PEB	C1C-CHB-C4B	8.04	138.42	128.81
26	21	405	PEB	C1C-CHB-C4B	-8.03	119.22	128.81
26	hE	201	PEB	OA-C1A-C2A	-8.02	119.80	126.17
28	KH	1001	CYC	CHB-C4A-C3A	8.01	145.50	124.90
26	XG	202	PEB	CHC-C4C-C3C	-8.00	116.70	130.34
26	RE	201	PEB	CHA-C4A-NA	7.99	134.70	125.20
26	lE	201	PEB	OA-C1A-C2A	-7.98	119.83	126.17
26	YD	304	PEB	C1C-CHB-C4B	-7.98	119.27	128.81
26	24	405	PEB	CHB-C4B-NB	-7.98	117.76	128.83
26	y1	202	PEB	C1C-CHB-C4B	7.98	138.34	128.81
26	B8	301	PEB	CHC-C1D-ND	-7.97	104.69	113.95
26	NE	201	PEB	CHA-C4A-NA	7.97	134.68	125.20
26	gF	202	PEB	OA-C1A-C2A	-7.97	119.83	126.17
26	RG	201	PEB	CHA-C4A-NA	7.97	134.68	125.20
26	DE	202	PEB	CHC-C4C-C3C	-7.97	116.74	130.34
26	HG	201	PEB	CHC-C4C-C3C	-7.97	116.75	130.34
26	bF	202	PEB	CHB-C4B-NB	-7.96	117.78	128.83
26	qG	201	PEB	C1C-CHB-C4B	7.96	138.32	128.81
26	QF	201	PEB	CHC-C4C-C3C	-7.95	116.77	130.34
26	AE	201	PEB	C1C-CHB-C4B	7.95	138.31	128.81
26	y4	203	PEB	CHB-C4B-NB	-7.95	117.80	128.83
26	RE	201	PEB	C2A-C1A-NA	7.95	115.12	108.27
26	f2	201	PEB	C1C-CHB-C4B	7.93	138.28	128.81
26	OJ	201	PEB	C1C-CHB-C4B	-7.93	119.34	128.81
26	OA	203	PEB	C1C-CHB-C4B	7.92	138.27	128.81
26	OF	202	PEB	CHB-C4B-NB	-7.92	117.84	128.83
26	k8	202	PEB	CHB-C4B-NB	-7.92	117.84	128.83
26	G5	203	PEB	C1C-CHB-C4B	7.91	138.26	128.81
26	QG	203	PEB	CHB-C4B-NB	-7.90	117.86	128.83
27	21	402	PUB	CHB-C1C-NC	-7.89	117.88	128.83
26	jF	203	PEB	CHC-C4C-C3C	-7.89	116.88	130.34
26	zE	501	PEB	CHA-C4A-NA	7.88	134.57	125.20
28	cH	1001	CYC	CHA-C1A-NA	-7.87	117.91	128.83
26	AA	302	PEB	C1C-CHB-C4B	-7.87	119.41	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j7	202	PEB	CHB-C4B-NB	-7.87	117.92	128.83
26	BA	301	PEB	CHC-C1D-ND	-7.86	104.82	113.95
26	N1	201	PEB	CMB-C2B-C1B	7.86	137.16	125.06
26	QE	203	PEB	CHC-C4C-C3C	-7.85	116.94	130.34
26	c1	203	PEB	CHC-C4C-C3C	-7.84	116.97	130.34
26	f7	202	PEB	CHB-C4B-NB	-7.84	117.95	128.83
26	A7	305	PEB	C1C-CHB-C4B	-7.84	119.44	128.81
26	nE	202	PEB	CHC-C1D-ND	7.84	123.05	113.95
26	fF	202	PEB	CHB-C4B-NB	-7.84	117.96	128.83
26	a4	203	PEB	CHC-C1D-ND	-7.83	104.86	113.95
26	X4	202	PEB	CMB-C2B-C1B	7.83	137.12	125.06
26	JD	201	PEB	C1C-CHB-C4B	-7.81	119.48	128.81
26	JE	201	PEB	CHA-C4A-NA	7.81	134.49	125.20
26	LG	201	PEB	C2A-C1A-NA	7.80	115.00	108.27
28	AH	1001	CYC	CHA-C1A-NA	-7.80	118.01	128.83
26	m4	201	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
26	e6	202	PEB	C1C-CHB-C4B	7.80	138.12	128.81
26	WE	201	PEB	CHC-C4C-C3C	-7.79	117.05	130.34
26	LD	202	PEB	OA-C1A-C2A	-7.79	119.98	126.17
28	NF	1001	CYC	C4D-CHA-C1A	7.79	138.12	128.81
27	24	402	PUB	C4B-CHB-C1C	-7.79	119.51	128.81
26	WE	201	PEB	CHB-C4B-NB	-7.79	118.03	128.83
26	g4	203	PEB	CHC-C4C-C3C	-7.78	117.06	130.34
26	R3	202	PEB	OA-C1A-C2A	-7.78	119.99	126.17
26	BG	201	PEB	C2A-C1A-NA	7.77	114.97	108.27
26	NG	201	PEB	CHA-C4A-NA	7.77	134.45	125.20
26	dG	201	PEB	OA-C1A-C2A	-7.77	119.99	126.17
26	LE	201	PEB	C2A-C1A-NA	7.77	114.97	108.27
26	L8	202	PEB	C1C-CHB-C4B	-7.77	119.53	128.81
28	LF	1001	CYC	CMA-C3A-C4A	7.77	137.03	125.06
26	O8	203	PEB	C1C-CHB-C4B	7.76	138.08	128.81
26	d8	201	PEB	CHC-C4C-C3C	-7.75	117.11	130.34
26	s4	202	PEB	C1C-CHB-C4B	7.75	138.07	128.81
26	kE	202	PEB	CHB-C4B-NB	-7.75	118.08	128.83
26	RE	202	PEB	C1C-CHB-C4B	7.75	138.06	128.81
26	RD	202	PEB	OA-C1A-C2A	-7.75	120.01	126.17
26	i8	201	PEB	CHB-C4B-NB	-7.75	118.08	128.83
26	qE	201	PEB	CHC-C4C-C3C	-7.74	117.14	130.34
26	X1	202	PEB	CMB-C2B-C1B	7.74	136.98	125.06
26	YD	304	PEB	CHB-C4B-NB	-7.73	118.10	128.83
26	c2	202	PEB	C1C-CHB-C4B	7.73	138.04	128.81
26	nG	201	PEB	CHA-C4A-NA	7.72	134.39	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H4	202	PEB	CHC-C4C-C3C	-7.71	117.19	130.34
26	k8	201	PEB	CHB-C4B-NB	-7.71	118.13	128.83
26	bF	202	PEB	C1C-CHB-C4B	-7.71	119.60	128.81
28	B6	1002	CYC	CMA-C3A-C4A	7.71	136.93	125.06
26	N4	201	PEB	CMB-C2B-C1B	7.70	136.93	125.06
26	y1	203	PEB	CHB-C4B-NB	-7.70	118.14	128.83
26	gE	201	PEB	CMB-C2B-C1B	7.69	136.91	125.06
26	U7	201	PEB	C1C-CHB-C4B	7.69	138.00	128.81
26	XD	202	PEB	OA-C1A-C2A	-7.69	120.06	126.17
26	vE	201	PEB	CHA-C4A-NA	7.68	134.34	125.20
26	e6	203	PEB	C1C-CHB-C4B	-7.68	119.64	128.81
26	k1	203	PEB	C1C-CHB-C4B	7.68	137.98	128.81
26	ZE	201	PEB	C2A-C1A-NA	7.67	114.89	108.27
26	UE	201	PEB	C1C-CHB-C4B	7.67	137.97	128.81
26	xE	304	PEB	CHB-C4B-NB	-7.67	118.19	128.83
26	HE	201	PEB	CHB-C4B-NB	-7.67	118.19	128.83
26	X9	201	PEB	C1C-CHB-C4B	7.66	137.96	128.81
26	bG	202	PEB	C1C-CHB-C4B	7.66	137.96	128.81
26	HA	202	PEB	CHB-C4B-NB	-7.66	118.21	128.83
26	GE	201	PEB	CHA-C1B-NB	-7.65	108.92	124.93
26	J8	202	PEB	CHB-C4B-NB	-7.65	118.21	128.83
26	24	405	PEB	C1C-CHB-C4B	-7.65	119.67	128.81
26	L8	202	PEB	CHB-C4B-NB	-7.65	118.22	128.83
26	kA	201	PEB	CHB-C4B-NB	-7.65	118.22	128.83
26	pG	201	PEB	OA-C1A-C2A	-7.65	120.09	126.17
26	UE	203	PEB	CHB-C4B-NB	-7.64	118.23	128.83
26	sG	203	PEB	CHC-C4C-C3C	-7.64	117.31	130.34
26	P9	201	PEB	C1C-CHB-C4B	7.63	137.93	128.81
26	XJ	201	PEB	C1C-CHB-C4B	7.63	137.92	128.81
26	MA	201	PEB	CHC-C4C-C3C	-7.62	117.34	130.34
26	GJ	201	PEB	C1C-CHB-C4B	7.62	137.91	128.81
26	cA	202	PEB	C1C-CHB-C4B	7.60	137.89	128.81
26	OJ	201	PEB	CHB-C4B-NB	-7.59	118.29	128.83
26	IA	201	PEB	C1C-CHB-C4B	7.59	137.88	128.81
26	cI	202	PEB	C1C-CHB-C4B	7.59	137.88	128.81
26	P3	202	PEB	CHC-C4C-C3C	-7.58	117.40	130.34
26	rE	201	PEB	OA-C1A-C2A	-7.58	120.14	126.17
26	u1	201	PEB	C1C-CHB-C4B	7.58	137.87	128.81
26	b7	202	PEB	CHB-C4B-NB	-7.56	118.34	128.83
26	AA	302	PEB	CHB-C4B-NB	-7.56	118.34	128.83
26	WF	202	PEB	C1C-CHB-C4B	-7.56	119.78	128.81
26	S7	202	PEB	CHB-C4B-NB	-7.56	118.34	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D6	1002	PEB	CHB-C4B-NB	-7.56	118.35	128.83
26	BE	201	PEB	CHA-C4A-NA	7.55	134.19	125.20
26	MG	203	PEB	CHC-C4C-C3C	-7.55	117.46	130.34
26	k2	203	PEB	CHB-C4B-NB	-7.55	118.36	128.83
26	sE	203	PEB	CHC-C4C-C3C	-7.55	117.47	130.34
26	M8	201	PEB	CHC-C4C-C3C	-7.55	117.47	130.34
26	bF	203	PEB	C1C-CHB-C4B	7.54	137.82	128.81
26	BG	201	PEB	CHA-C4A-NA	7.54	134.17	125.20
26	sG	203	PEB	CHB-C4B-NB	-7.54	118.36	128.83
26	i1	201	PEB	CHC-C4C-C3C	-7.53	117.50	130.34
26	zG	501	PEB	C2A-C1A-NA	7.53	114.76	108.27
26	JD	203	PEB	CHB-C4B-NB	-7.52	118.39	128.83
26	e6	203	PEB	CHB-C4B-NB	-7.52	118.39	128.83
26	Q3	201	PEB	CHC-C4C-C3C	-7.52	117.51	130.34
26	zG	501	PEB	CHA-C4A-NA	7.52	134.15	125.20
26	G4	202	PEB	CHC-C1D-ND	-7.50	105.23	113.95
26	PE	201	PEB	CHA-C4A-NA	7.50	134.12	125.20
26	bI	201	PEB	C1C-CHB-C4B	7.50	137.77	128.81
26	LD	202	PEB	CHC-C4C-C3C	-7.50	117.55	130.34
26	D4	202	PEB	C1C-CHB-C4B	7.49	137.76	128.81
26	N8	202	PEB	CHB-C4B-NB	-7.49	118.44	128.83
26	NA	202	PEB	CHB-C4B-NB	-7.49	118.44	128.83
26	T2	202	PEB	C1C-CHB-C4B	7.48	137.75	128.81
26	QG	203	PEB	CHA-C1B-NB	-7.48	109.28	124.93
26	A8	302	PEB	C1C-CHB-C4B	-7.47	119.88	128.81
26	AA	302	PEB	CHC-C1D-ND	-7.47	105.28	113.95
26	UE	201	PEB	CMB-C2B-C1B	7.47	136.56	125.06
26	11	202	PEB	CHC-C4C-C3C	-7.45	117.63	130.34
26	U3	201	PEB	CHA-C1B-NB	-7.44	109.38	124.93
26	k8	201	PEB	C1C-CHB-C4B	-7.43	119.93	128.81
26	a2	202	PEB	C1C-CHB-C4B	7.43	137.68	128.81
26	w4	202	PEB	CHC-C4C-C3C	-7.43	117.67	130.34
26	RG	202	PEB	C1C-CHB-C4B	7.42	137.68	128.81
26	W7	202	PEB	CHB-C4B-NB	-7.42	118.53	128.83
26	g1	203	PEB	CHC-C4C-C3C	-7.42	117.69	130.34
26	X3	202	PEB	OA-C1A-C2A	-7.42	120.28	126.17
26	UE	203	PEB	CHA-C1B-NB	-7.42	109.42	124.93
26	uE	201	PEB	CHC-C4C-C3C	-7.40	117.71	130.34
26	h7	203	PEB	C1C-CHB-C4B	-7.40	119.97	128.81
26	aE	201	PEB	CHB-C4B-NB	-7.40	118.56	128.83
26	Z7	201	PEB	OA-C1A-C2A	-7.40	120.29	126.17
26	DG	202	PEB	CHC-C1D-ND	-7.40	105.35	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	pG	201	PEB	C1C-CHB-C4B	-7.40	119.97	128.81
26	m1	201	PEB	CHC-C4C-C3C	-7.39	117.73	130.34
26	YG	203	PEB	CHC-C4C-C3C	-7.39	117.73	130.34
26	WG	201	PEB	CHC-C4C-C3C	-7.39	117.73	130.34
26	u1	202	PEB	CHC-C4C-C3C	-7.38	117.75	130.34
26	k4	203	PEB	C1C-CHB-C4B	7.37	137.62	128.81
26	IG	203	PEB	CHC-C1D-ND	-7.37	105.39	113.95
26	aE	201	PEB	CHC-C4C-C3C	-7.37	117.77	130.34
26	H1	202	PEB	CHC-C4C-C3C	-7.37	117.77	130.34
26	H1	202	PEB	C1C-CHB-C4B	7.36	137.60	128.81
26	N4	201	PEB	CHC-C1D-ND	-7.36	105.40	113.95
26	aI	202	PEB	C1C-CHB-C4B	7.36	137.60	128.81
28	RH	1001	CYC	OB-C4B-C3B	-7.36	120.06	128.04
26	L1	202	PEB	CHC-C4C-C3C	-7.35	117.80	130.34
26	u1	202	PEB	C1C-CHB-C4B	7.35	137.59	128.81
26	a7	201	PEB	C1C-CHB-C4B	7.34	137.58	128.81
28	NB	1001	CYC	CMA-C3A-C4A	7.34	136.37	125.06
26	gE	203	PEB	CHC-C4C-C3C	-7.34	117.83	130.34
26	JJ	203	PEB	CHC-C4C-C3C	-7.33	117.83	130.34
26	QD	201	PEB	CHC-C4C-C3C	-7.33	117.83	130.34
26	P8	202	PEB	CHB-C4B-NB	-7.33	118.66	128.83
26	zE	501	PEB	C2A-C1A-NA	7.32	114.58	108.27
26	tG	201	PEB	CHA-C4A-NA	7.31	133.90	125.20
28	F2	1001	CYC	OB-C4B-C3B	-7.31	120.11	128.04
26	A8	302	PEB	CHB-C4B-NB	-7.31	118.69	128.83
26	c8	202	PEB	CHB-C4B-NB	-7.31	118.69	128.83
26	oG	201	PEB	CHB-C4B-NB	-7.30	118.70	128.83
26	PA	201	PEB	CHB-C4B-NB	-7.29	118.71	128.83
26	PE	201	PEB	C2A-C1A-NA	7.29	114.56	108.27
26	SF	202	PEB	C1C-CHB-C4B	-7.28	120.11	128.81
27	A8	304	PUB	CAD-C3D-C4D	7.28	132.88	121.38
26	L9	201	PEB	CHC-C4C-C3C	-7.27	117.93	130.34
26	qE	202	PEB	CHA-C1B-NB	-7.27	109.72	124.93
26	ZG	201	PEB	CHB-C4B-NB	-7.27	118.75	128.83
26	bF	203	PEB	CHC-C4C-C3C	-7.26	117.95	130.34
26	iG	201	PEB	CHC-C4C-C3C	-7.26	117.95	130.34
26	B9	203	PEB	CHC-C4C-C3C	-7.26	117.96	130.34
26	ME	203	PEB	CHC-C4C-C3C	-7.25	117.97	130.34
26	IE	203	PEB	CHC-C4C-C3C	-7.25	117.97	130.34
26	XE	202	PEB	C1C-CHB-C4B	7.25	137.47	128.81
26	h4	202	PEB	C1C-CHB-C4B	-7.25	120.15	128.81
26	I3	201	PEB	CHB-C4B-NB	-7.25	118.78	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LA	202	PEB	CHB-C4B-NB	-7.25	118.78	128.83
26	gB	202	PEB	CHB-C4B-NB	-7.25	118.78	128.83
26	F9	201	PEB	CHC-C4C-C3C	-7.24	117.98	130.34
26	C8	203	PEB	CHC-C4C-C3C	-7.23	118.00	130.34
26	kE	201	PEB	CHB-C4B-NB	-7.23	118.80	128.83
26	S3	201	PEB	CHA-C1B-NB	-7.23	109.81	124.93
26	CA	203	PEB	CHC-C4C-C3C	-7.22	118.02	130.34
26	xE	303	PEB	CHB-C4B-NB	-7.22	118.81	128.83
27	xG	305	PUB	CHB-C1C-NC	-7.22	118.81	128.83
26	q4	202	PEB	CHC-C4C-C3C	-7.22	118.03	130.34
26	G9	201	PEB	C1C-CHB-C4B	7.21	137.43	128.81
26	UD	201	PEB	CHA-C1B-NB	-7.21	109.85	124.93
26	gG	201	PEB	CMB-C2B-C1B	7.21	136.17	125.06
27	B8	302	PUB	CAD-C3D-C4D	7.21	132.77	121.38
27	24	402	PUB	CHB-C1C-NC	-7.21	118.83	128.83
26	VD	202	PEB	CHC-C4C-C3C	-7.21	118.05	130.34
26	KE	201	PEB	CHC-C4C-C3C	-7.21	118.05	130.34
28	uH	1001	CYC	CHD-C4C-NC	7.20	133.76	125.20
26	T3	202	PEB	CHB-C4B-NB	-7.20	118.85	128.83
26	WF	203	PEB	C1C-CHB-C4B	7.19	137.40	128.81
26	q4	202	PEB	C1C-CHB-C4B	7.19	137.40	128.81
26	JA	202	PEB	CHB-C4B-NB	-7.19	118.86	128.83
26	hB	201	PEB	C1C-CHB-C4B	7.18	137.39	128.81
26	D8	201	PEB	C1C-CHB-C4B	-7.18	120.23	128.81
27	KD	203	PUB	CAD-C3D-C4D	7.18	132.72	121.38
26	Z4	201	PEB	CHC-C1D-ND	-7.18	105.61	113.95
26	bE	201	PEB	CHA-C4A-NA	7.18	133.74	125.20
26	vG	201	PEB	CHA-C4A-NA	7.18	133.74	125.20
26	V3	202	PEB	OA-C1A-C2A	-7.17	120.47	126.17
26	PD	202	PEB	CHC-C4C-C3C	-7.17	118.11	130.34
26	SD	201	PEB	CHA-C1B-NB	-7.16	109.95	124.93
26	ZF	203	PEB	CHB-C4B-NB	-7.16	118.90	128.83
26	J3	201	PEB	C1C-CHB-C4B	-7.16	120.26	128.81
26	O3	201	PEB	CHA-C1B-NB	-7.15	109.98	124.93
26	V9	201	PEB	CHB-C4B-NB	-7.14	118.92	128.83
26	Z4	202	PEB	C1C-CHB-C4B	7.14	137.34	128.81
26	LA	202	PEB	C1C-CHB-C4B	-7.14	120.28	128.81
27	21	402	PUB	C4B-CHB-C1C	-7.14	120.28	128.81
26	j8	202	PEB	CHB-C4B-NB	-7.14	118.93	128.83
26	GG	203	PEB	C1C-CHB-C4B	7.13	137.33	128.81
26	i8	201	PEB	C1C-CHB-C4B	-7.13	120.29	128.81
26	XG	202	PEB	C1C-CHB-C4B	7.13	137.32	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	302	PUB	CAD-C3D-C4D	7.12	132.63	121.38
26	UG	201	PEB	CHC-C1D-ND	-7.12	105.68	113.95
26	U7	203	PEB	CHB-C4B-NB	-7.12	118.95	128.83
26	TJ	203	PEB	CHC-C1D-ND	-7.11	105.69	113.95
26	sG	203	PEB	CHA-C1B-NB	-7.11	110.05	124.93
28	J2	1001	CYC	CHB-C4A-NA	-7.11	110.06	124.93
26	U6	201	PEB	C1C-CHB-C4B	7.11	137.30	128.81
26	cA	203	PEB	CHB-C4B-NB	-7.11	118.97	128.83
26	S8	203	PEB	C1C-CHB-C4B	7.10	137.30	128.81
26	dF	203	PEB	C1C-CHB-C4B	-7.10	120.32	128.81
26	iG	202	PEB	C1C-CHB-C4B	7.10	137.29	128.81
26	JG	201	PEB	CHA-C4A-NA	7.10	133.65	125.20
27	24	403	PUB	CHC-C1D-ND	-7.10	104.75	113.72
26	DA	201	PEB	C1C-CHB-C4B	-7.09	120.34	128.81
26	SA	203	PEB	C1C-CHB-C4B	7.09	137.28	128.81
26	IG	203	PEB	CHC-C4C-C3C	-7.09	118.25	130.34
26	g8	202	PEB	CHB-C4B-NB	-7.08	119.00	128.83
26	SF	202	PEB	CHB-C4B-NB	-7.08	119.00	128.83
26	v1	201	PEB	C1C-CHB-C4B	7.08	137.27	128.81
26	cG	203	PEB	CHA-C1B-NB	-7.08	110.12	124.93
26	dE	201	PEB	OA-C1A-C2A	-7.08	120.54	126.17
26	lB	201	PEB	C1C-CHB-C4B	7.08	137.27	128.81
27	AA	303	PUB	C4B-CHB-C1C	-7.08	120.35	128.81
26	PG	201	PEB	CHA-C4A-NA	7.08	133.62	125.20
26	J4	202	PEB	CHC-C4C-C3C	-7.08	118.27	130.34
26	OD	201	PEB	CHA-C1B-NB	-7.07	110.14	124.93
26	J1	202	PEB	C1C-CHB-C4B	7.07	137.25	128.81
26	JE	201	PEB	C2A-C1A-NA	7.07	114.36	108.27
26	D4	202	PEB	CHC-C4C-C3C	-7.06	118.29	130.34
26	OA	203	PEB	CHC-C4C-C3C	-7.06	118.30	130.34
26	JG	202	PEB	C1C-CHB-C4B	7.06	137.24	128.81
26	gA	202	PEB	CHB-C4B-NB	-7.05	119.04	128.83
26	WG	203	PEB	CHB-C4B-NB	-7.05	119.05	128.83
26	LJ	201	PEB	CHC-C4C-C3C	-7.05	118.31	130.34
26	PJ	201	PEB	CHC-C4C-C3C	-7.05	118.32	130.34
26	KG	201	PEB	CHC-C4C-C3C	-7.05	118.32	130.34
26	HD	202	PEB	C1C-CHB-C4B	7.04	137.22	128.81
26	P3	202	PEB	OA-C1A-C2A	-7.04	120.58	126.17
26	y4	203	PEB	C1C-CHB-C4B	-7.03	120.41	128.81
26	DG	201	PEB	C2A-C1A-NA	7.03	114.33	108.27
27	K3	203	PUB	CAD-C3D-C4D	7.03	132.48	121.38
26	F3	202	PEB	C1C-CHB-C4B	7.03	137.20	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D3	202	PEB	OA-C1A-C2A	-7.02	120.59	126.17
26	kG	203	PEB	CHC-C4C-C3C	-7.02	118.36	130.34
26	Y3	304	PEB	CHB-C4B-NB	-7.02	119.09	128.83
26	WF	202	PEB	CHB-C4B-NB	-7.02	119.09	128.83
26	u4	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
26	nE	201	PEB	CHA-C4A-NA	7.02	133.55	125.20
26	Z1	201	PEB	CHC-C1D-ND	-7.01	105.81	113.95
26	A8	302	PEB	CHC-C1D-ND	-7.01	105.81	113.95
26	BE	201	PEB	C2A-C1A-NA	7.01	114.31	108.27
26	w1	202	PEB	CHC-C4C-C3C	-7.00	118.39	130.34
26	GG	202	PEB	C4B-C3B-C2B	-7.00	99.03	106.78
26	XG	203	PEB	C1C-CHB-C4B	7.00	137.17	128.81
27	KD	203	PUB	CHB-C1C-NC	-7.00	119.12	128.83
26	HD	202	PEB	OA-C1A-C2A	-7.00	120.61	126.17
26	B3	202	PEB	CHC-C4C-C3C	-7.00	118.40	130.34
26	Y3	304	PEB	C1C-CHB-C4B	-7.00	120.45	128.81
26	P8	201	PEB	CHB-C4B-NB	-7.00	119.12	128.83
26	N1	201	PEB	CHC-C1D-ND	-6.99	105.83	113.95
26	AJ	303	PEB	CHB-C4B-NB	-6.99	119.13	128.83
26	DD	202	PEB	OA-C1A-C2A	-6.99	120.62	126.17
26	V3	202	PEB	CHC-C4C-C3C	-6.98	118.43	130.34
26	iE	201	PEB	CHB-C4B-NB	-6.98	119.14	128.83
28	tH	1001	CYC	OB-C4B-C3B	-6.98	120.46	128.04
26	j7	202	PEB	C1C-CHB-C4B	-6.98	120.47	128.81
26	T3	202	PEB	CHC-C4C-C3C	-6.98	118.43	130.34
26	F1	202	PEB	CHC-C4C-C3C	-6.98	118.44	130.34
26	fE	201	PEB	CHA-C4A-NA	6.97	133.50	125.20
26	Y8	201	PEB	CHC-C4C-C3C	-6.97	118.45	130.34
28	KF	1001	CYC	C4D-CHA-C1A	6.97	137.13	128.81
26	g6	202	PEB	CHB-C4B-NB	-6.97	119.16	128.83
26	DJ	202	PEB	CHC-C1D-ND	-6.97	105.86	113.95
26	M3	201	PEB	CHC-C4C-C3C	-6.96	118.46	130.34
26	YA	201	PEB	CHC-C4C-C3C	-6.96	118.46	130.34
26	R3	202	PEB	CHC-C1D-ND	-6.96	105.86	113.95
26	K8	203	PEB	CHC-C4C-C3C	-6.96	118.47	130.34
26	aA	201	PEB	CHB-C4B-NB	-6.96	119.17	128.83
26	14	202	PEB	CHC-C4C-C3C	-6.96	118.47	130.34
28	JI	1001	CYC	CHB-C4A-NA	-6.96	110.38	124.93
26	AF	305	PEB	CHB-C4B-NB	-6.95	119.19	128.83
26	N3	202	PEB	CHC-C1D-ND	-6.95	105.88	113.95
26	A7	305	PEB	CHB-C4B-NB	-6.94	119.19	128.83
26	D9	201	PEB	CHC-C4C-C3C	-6.94	118.50	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mA	202	PEB	CHB-C4B-NB	-6.94	119.20	128.83
26	h8	201	PEB	CHC-C4C-C3C	-6.94	118.50	130.34
28	rH	1001	CYC	OB-C4B-C3B	-6.92	120.53	128.04
28	kH	1001	CYC	CHB-C4A-NA	-6.92	110.46	124.93
26	qG	202	PEB	C1C-CHB-C4B	6.91	137.06	128.81
26	qG	201	PEB	CHC-C4C-C3C	-6.91	118.55	130.34
28	I6	1001	CYC	OC-C1C-C2C	-6.91	120.68	126.17
26	PJ	203	PEB	CHC-C1D-ND	-6.90	105.93	113.95
26	L4	202	PEB	CHC-C4C-C3C	-6.90	118.57	130.34
26	V9	203	PEB	CHB-C4B-NB	-6.90	119.26	128.83
26	B3	203	PEB	CHB-C4B-NB	-6.90	119.26	128.83
27	AA	304	PUB	CAD-C3D-C4D	6.90	132.27	121.38
26	TA	202	PEB	CHB-C4B-NB	-6.90	119.26	128.83
26	TE	201	PEB	CHA-C4A-NA	6.89	133.40	125.20
26	I8	201	PEB	C1C-CHB-C4B	6.89	137.04	128.81
26	KA	203	PEB	CHC-C4C-C3C	-6.89	118.58	130.34
26	PD	202	PEB	OA-C1A-C2A	-6.89	120.69	126.17
26	YD	301	PEB	CHB-C4B-NB	-6.89	119.27	128.83
26	aB	202	PEB	CHB-C4B-NB	-6.89	119.28	128.83
26	WA	203	PEB	CHC-C4C-C3C	-6.88	118.60	130.34
26	e4	202	PEB	CHB-C4B-NB	-6.88	119.28	128.83
26	i2	202	PEB	C1C-CHB-C4B	6.88	137.02	128.81
26	k8	202	PEB	C1C-CHB-C4B	-6.88	120.59	128.81
26	z4	201	PEB	C1C-CHB-C4B	6.87	137.02	128.81
26	J3	202	PEB	OA-C1A-C2A	-6.87	120.71	126.17
26	N3	202	PEB	CHC-C4C-C3C	-6.87	118.63	130.34
26	fG	201	PEB	CHA-C4A-NA	6.87	133.37	125.20
27	A2	302	PUB	CHB-C1C-NC	-6.86	119.31	128.83
26	a6	202	PEB	CHB-C4B-NB	-6.86	119.31	128.83
26	aF	201	PEB	C1C-CHB-C4B	6.86	137.00	128.81
26	L3	202	PEB	CHC-C4C-C3C	-6.86	118.65	130.34
26	cG	203	PEB	CHC-C4C-C3C	-6.86	118.65	130.34
26	UB	201	PEB	C1C-CHB-C4B	6.85	136.99	128.81
26	lF	203	PEB	C1C-CHB-C4B	-6.85	120.63	128.81
26	UI	201	PEB	CMB-C2B-C1B	6.85	135.61	125.06
28	DF	1001	CYC	C4D-CHA-C1A	6.85	136.99	128.81
26	UF	203	PEB	CHB-C4B-NB	-6.84	119.34	128.83
26	H3	202	PEB	OA-C1A-C2A	-6.84	120.74	126.17
26	c4	201	PEB	C1C-CHB-C4B	6.84	136.97	128.81
26	O7	202	PEB	C1C-CHB-C4B	-6.83	120.64	128.81
26	T8	202	PEB	CHB-C4B-NB	-6.82	119.36	128.83
26	F9	203	PEB	CHC-C4C-C3C	-6.82	118.70	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HG	201	PEB	CHB-C4B-NB	-6.82	119.37	128.83
26	cG	201	PEB	CHB-C4B-NB	-6.82	119.37	128.83
26	AB	301	PEB	CHB-C4B-NB	-6.82	119.37	128.83
26	X9	201	PEB	CHC-C4C-C3C	-6.82	118.71	130.34
26	U2	201	PEB	CMB-C2B-C1B	6.82	135.56	125.06
28	1H	1000	CYC	CHB-C4A-NA	-6.82	110.67	124.93
26	D1	202	PEB	C1C-CHB-C4B	6.81	136.95	128.81
26	eE	201	PEB	CHC-C4C-C3C	-6.81	118.72	130.34
26	pG	201	PEB	CHB-C4B-NB	-6.81	119.38	128.83
26	J9	203	PEB	CHC-C4C-C3C	-6.81	118.72	130.34
26	H3	202	PEB	C1C-CHB-C4B	6.81	136.94	128.81
27	QA	201	PUB	CHB-C1C-NC	-6.81	119.39	128.83
26	21	404	PEB	CHB-C4B-NB	-6.80	119.39	128.83
26	T9	201	PEB	CHC-C4C-C3C	-6.80	118.74	130.34
26	AB	301	PEB	C1C-CHB-C4B	-6.80	120.69	128.81
26	OG	202	PEB	CMB-C2B-C1B	6.80	135.53	125.06
26	xG	304	PEB	CHB-C4B-NB	-6.80	119.40	128.83
27	AJ	302	PUB	OD-C4D-C3D	-6.80	120.66	128.04
26	P9	203	PEB	CHC-C1D-ND	-6.80	106.05	113.95
26	f8	203	PEB	C1C-CHB-C4B	6.80	136.93	128.81
26	SD	201	PEB	CHB-C4B-NB	-6.79	119.41	128.83
27	AA	303	PUB	CAD-C3D-C4D	6.79	132.10	121.38
26	H9	203	PEB	CHC-C1D-ND	-6.79	106.06	113.95
26	J3	201	PEB	CHB-C4B-NB	-6.79	119.41	128.83
26	kl	202	PEB	CHC-C4C-C3C	-6.79	118.76	130.34
26	fl	201	PEB	C1C-CHB-C4B	6.79	136.92	128.81
26	Z8	202	PEB	CHB-C4B-NB	-6.79	119.42	128.83
26	TI	202	PEB	C1C-CHB-C4B	6.78	136.91	128.81
26	D9	202	PEB	CHA-C1B-NB	-6.78	110.74	124.93
27	Y3	302	PUB	CAD-C3D-C4D	6.78	132.09	121.38
26	j4	202	PEB	C1C-CHB-C4B	6.78	136.91	128.81
26	m8	202	PEB	CHB-C4B-NB	-6.78	119.42	128.83
28	IH	1001	CYC	CHB-C4A-NA	-6.78	110.75	124.93
26	d8	201	PEB	C1C-CHB-C4B	6.78	136.91	128.81
26	S3	201	PEB	CHC-C4C-C3C	-6.78	118.78	130.34
26	FA	202	PEB	CHB-C4B-NB	-6.78	119.42	128.83
26	f8	203	PEB	CHC-C4C-C3C	-6.78	118.78	130.34
26	q1	201	PEB	C1C-CHB-C4B	6.78	136.91	128.81
26	SG	201	PEB	CHC-C1D-ND	-6.78	106.08	113.95
26	DG	202	PEB	CHC-C4C-C3C	-6.77	118.80	130.34
28	nH	1001	CYC	CHB-C4A-NA	-6.76	110.79	124.93
26	TD	202	PEB	CHC-C4C-C3C	-6.76	118.81	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	NJ	204	PEB	C1C-CHB-C4B	6.76	136.88	128.81
26	ZA	202	PEB	CHB-C4B-NB	-6.76	119.45	128.83
26	gG	203	PEB	CHC-C4C-C3C	-6.76	118.81	130.34
26	VA	201	PEB	C1C-CHB-C4B	-6.76	120.74	128.81
28	VH	1001	CYC	CHB-C4A-NA	-6.75	110.81	124.93
26	aG	201	PEB	CHB-C4B-NB	-6.75	119.46	128.83
26	JD	202	PEB	OA-C1A-C2A	-6.75	120.81	126.17
28	EH	1001	CYC	OB-C4B-C3B	-6.75	120.71	128.04
26	F8	202	PEB	CHB-C4B-NB	-6.74	119.47	128.83
26	TJ	201	PEB	CHC-C4C-C3C	-6.74	118.84	130.34
26	T8	201	PEB	C1C-CHB-C4B	-6.74	120.76	128.81
26	qG	202	PEB	CHA-C1B-NB	-6.74	110.83	124.93
28	LI	1001	CYC	CHB-C4A-NA	-6.74	110.83	124.93
26	H9	201	PEB	CHC-C4C-C3C	-6.74	118.84	130.34
26	S8	201	PEB	CHB-C4B-NB	-6.74	119.48	128.83
28	AH	1001	CYC	OB-C4B-C3B	-6.73	120.74	128.04
26	JD	201	PEB	CHB-C4B-NB	-6.73	119.50	128.83
26	G8	202	PEB	CHB-C4B-NB	-6.72	119.50	128.83
26	SB	203	PEB	CHC-C4C-C3C	-6.72	118.88	130.34
26	e8	202	PEB	C1C-CHB-C4B	-6.72	120.78	128.81
26	GG	201	PEB	CHA-C1B-NB	-6.72	110.88	124.93
26	G4	201	PEB	CMB-C2B-C1B	6.72	135.41	125.06
26	TG	201	PEB	CHA-C4A-NA	6.71	133.19	125.20
26	OF	202	PEB	C1C-CHB-C4B	-6.71	120.79	128.81
27	QA	201	PUB	CHC-C1D-ND	-6.71	105.23	113.72
26	SI	201	PEB	CMB-C2B-C1B	6.71	135.40	125.06
26	u4	202	PEB	C1C-CHB-C4B	6.71	136.83	128.81
26	DD	201	PEB	CHB-C4B-NB	-6.71	119.52	128.83
28	YH	1002	CYC	CHB-C4A-NA	-6.71	110.90	124.93
26	J1	202	PEB	CHC-C4C-C3C	-6.70	118.91	130.34
26	sE	203	PEB	CHB-C4B-NB	-6.70	119.53	128.83
26	S3	201	PEB	CHB-C4B-NB	-6.70	119.54	128.83
26	HF	1002	PEB	CHC-C1D-ND	-6.69	106.17	113.95
28	KH	1001	CYC	OB-C4B-C3B	-6.69	120.78	128.04
26	U8	201	PEB	C1C-CHB-C4B	6.69	136.80	128.81
28	L2	1001	CYC	CHB-C4A-NA	-6.69	110.93	124.93
26	AD	201	PEB	CHB-C4B-NB	-6.69	119.55	128.83
26	jG	201	PEB	CHA-C4A-NA	6.69	133.16	125.20
28	IB	1001	CYC	OC-C1C-C2C	-6.69	120.86	126.17
27	A8	303	PUB	CAD-C3D-C4D	6.68	131.94	121.38
26	C5	203	PEB	CHB-C4B-NB	-6.68	119.56	128.83
26	oE	201	PEB	CHA-C1B-NB	-6.68	110.95	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e1	202	PEB	CHB-C4B-NB	-6.68	119.56	128.83
27	YD	302	PUB	CAD-C3D-C4D	6.68	131.94	121.38
26	DA	201	PEB	CHB-C4B-NB	-6.68	119.56	128.83
26	OF	203	PEB	CHC-C4C-C3C	-6.68	118.94	130.34
28	EF	1001	CYC	C4D-CHA-C1A	6.68	136.79	128.81
26	m4	201	PEB	C1C-CHB-C4B	6.68	136.78	128.81
26	G8	203	PEB	CHC-C4C-C3C	-6.67	118.95	130.34
26	IG	201	PEB	CMB-C2B-C1B	6.67	135.34	125.06
26	J9	201	PEB	CHB-C4B-NB	-6.67	119.58	128.83
28	cH	1001	CYC	OB-C4B-C3B	-6.66	120.81	128.04
26	JJ	203	PEB	C1C-CHB-C4B	6.66	136.77	128.81
26	Q3	201	PEB	CMB-C2B-C1B	6.66	135.32	125.06
26	OE	201	PEB	CHC-C4C-C3C	-6.66	118.98	130.34
28	YH	1004	CYC	CHB-C4A-NA	-6.66	111.00	124.93
28	hH	1001	CYC	CHB-C4A-NA	-6.66	111.01	124.93
26	DG	201	PEB	CHA-C4A-NA	6.66	133.12	125.20
26	L1	202	PEB	C1C-CHB-C4B	6.66	136.76	128.81
28	RH	1001	CYC	CHB-C4A-NA	-6.65	111.01	124.93
26	SD	201	PEB	CMB-C2B-C1B	6.65	135.31	125.06
26	R3	202	PEB	CHC-C4C-C3C	-6.65	119.00	130.34
27	A4	203	PUB	CAD-C3D-C4D	6.65	131.88	121.38
26	iE	201	PEB	CHC-C4C-C3C	-6.65	119.00	130.34
26	JJ	201	PEB	CHB-C4B-NB	-6.65	119.61	128.83
26	jA	202	PEB	CHB-C4B-NB	-6.65	119.61	128.83
26	B1	202	PEB	CHC-C4C-C3C	-6.64	119.01	130.34
26	SE	201	PEB	CHC-C4C-C3C	-6.64	119.01	130.34
26	F4	202	PEB	CHC-C4C-C3C	-6.64	119.02	130.34
26	h4	202	PEB	CHB-C4B-NB	-6.64	119.62	128.83
26	CC	202	PEB	CHB-C4B-NB	-6.64	119.62	128.83
26	S6	203	PEB	CHC-C4C-C3C	-6.64	119.02	130.34
26	g7	202	PEB	OA-C1A-C2A	-6.64	120.90	126.17
26	D8	201	PEB	CHB-C4B-NB	-6.63	119.63	128.83
26	OF	203	PEB	C1C-CHB-C4B	6.63	136.72	128.81
26	T3	202	PEB	OA-C1A-C2A	-6.63	120.91	126.17
26	J9	203	PEB	C1C-CHB-C4B	6.62	136.72	128.81
28	rH	1001	CYC	CHB-C4A-NA	-6.62	111.07	124.93
26	SA	203	PEB	CHC-C4C-C3C	-6.62	119.04	130.34
26	SI	201	PEB	C1C-CHB-C4B	6.62	136.72	128.81
26	m1	201	PEB	C1C-CHB-C4B	6.62	136.71	128.81
26	cE	203	PEB	CHA-C1B-NB	-6.61	111.09	124.93
28	NH	1001	CYC	CHB-C4A-NA	-6.61	111.09	124.93
28	PH	1001	CYC	OB-C4B-C3B	-6.61	120.86	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	gI	202	PEB	CHC-C4C-C3C	-6.61	119.06	130.34
27	A1	203	PUB	CAD-C3D-C4D	6.60	131.81	121.38
26	TD	202	PEB	OA-C1A-C2A	-6.60	120.92	126.17
28	F2	1001	CYC	CAB-C3B-C2B	6.60	138.82	127.53
26	24	401	PEB	CHC-C1D-ND	-6.60	106.29	113.95
26	UA	201	PEB	C1C-CHB-C4B	6.59	136.69	128.81
26	Q7	201	PEB	CHC-C4C-C3C	-6.59	119.10	130.34
26	EA	201	PEB	CHC-C4C-C3C	-6.59	119.10	130.34
27	21	403	PUB	CHA-C1B-C2B	-6.59	119.11	130.34
26	iA	201	PEB	CHB-C4B-NB	-6.58	119.69	128.83
28	GH	1001	CYC	OB-C4B-C3B	-6.58	120.90	128.04
27	N9	201	PUB	CAD-C3D-C4D	6.58	131.77	121.38
26	jG	202	PEB	C1C-CHB-C4B	6.58	136.67	128.81
26	wG	301	PEB	CHB-C4B-NB	-6.58	119.70	128.83
26	DE	201	PEB	C2A-C1A-NA	6.57	113.94	108.27
26	I5	203	PEB	OA-C1A-C2A	-6.57	120.95	126.17
26	RA	201	PEB	CHB-C4B-NB	-6.57	119.71	128.83
28	LH	1001	CYC	CHB-C4A-NA	-6.57	111.19	124.93
26	RD	202	PEB	C1C-CHB-C4B	6.57	136.66	128.81
26	i7	202	PEB	CHB-C4B-NB	-6.57	119.72	128.83
26	L9	201	PEB	C1C-CHB-C4B	6.57	136.65	128.81
26	E8	201	PEB	CHC-C4C-C3C	-6.57	119.14	130.34
26	SD	201	PEB	CHC-C4C-C3C	-6.56	119.15	130.34
26	a8	204	PEB	C1C-CHB-C4B	6.56	136.65	128.81
26	AC	202	PEB	CHB-C4B-NB	-6.56	119.73	128.83
26	TA	201	PEB	C1C-CHB-C4B	-6.55	120.98	128.81
26	P3	201	PEB	CHC-C1D-ND	-6.55	106.34	113.95
26	EG	201	PEB	C1C-CHB-C4B	6.55	136.63	128.81
26	B4	202	PEB	CHC-C4C-C3C	-6.55	119.17	130.34
28	OH	1001	CYC	CHB-C4A-NA	-6.54	111.24	124.93
26	FD	202	PEB	OA-C1A-C2A	-6.54	120.97	126.17
26	IJ	202	PEB	CHC-C4C-C3C	-6.54	119.18	130.34
26	OF	201	PEB	CHB-C4B-NB	-6.54	119.75	128.83
26	SG	202	PEB	CMB-C2B-C1B	6.54	135.14	125.06
26	q1	202	PEB	C1C-CHB-C4B	6.54	136.62	128.81
26	VA	201	PEB	CHB-C4B-NB	-6.54	119.76	128.83
26	MD	201	PEB	CHB-C4B-NB	-6.54	119.76	128.83
26	S7	202	PEB	CHC-C1D-ND	-6.54	106.36	113.95
26	fF	203	PEB	C1C-CHB-C4B	6.53	136.61	128.81
26	V8	201	PEB	C1C-CHB-C4B	-6.53	121.00	128.81
26	HJ	201	PEB	CHC-C4C-C3C	-6.53	119.19	130.34
26	S8	203	PEB	CHC-C4C-C3C	-6.53	119.20	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	24	403	PUB	CAD-C3D-C4D	6.53	131.70	121.38
26	SJ	201	PEB	CHC-C1D-ND	-6.53	106.36	113.95
27	QA	201	PUB	CAD-C3D-C4D	6.53	131.69	121.38
26	h7	201	PEB	CHC-C4C-C3C	-6.53	119.20	130.34
26	j7	203	PEB	CHC-C4C-C3C	-6.53	119.20	130.34
27	xE	306	PUB	CAD-C3D-C4D	6.53	131.69	121.38
26	d1	202	PEB	CHB-C4B-NB	-6.53	119.78	128.83
26	H6	1002	PEB	CHB-C4B-NB	-6.52	119.78	128.83
26	DB	1002	PEB	CHB-C4B-NB	-6.52	119.79	128.83
27	A6	302	PUB	CHB-C1C-NC	-6.52	119.79	128.83
26	iA	201	PEB	C1C-CHB-C4B	-6.52	121.03	128.81
28	FF	1001	CYC	C4D-CHA-C1A	6.51	136.59	128.81
26	DA	202	PEB	C1C-CHB-C4B	-6.51	121.03	128.81
26	R3	202	PEB	C1C-CHB-C4B	6.51	136.59	128.81
26	F9	201	PEB	CHA-C1B-NB	-6.51	111.31	124.93
26	lA	202	PEB	OA-C1A-C2A	-6.51	121.00	126.17
28	qH	1001	CYC	CHB-C4A-NA	-6.50	111.33	124.93
28	uH	1001	CYC	CHB-C4A-NA	-6.50	111.33	124.93
26	GA	203	PEB	C1C-CHB-C4B	6.50	136.58	128.81
26	hG	201	PEB	OA-C1A-C2A	-6.50	121.00	126.17
28	GB	1001	CYC	OC-C1C-C2C	-6.50	121.00	126.17
26	lE	201	PEB	CHB-C4B-NB	-6.50	119.81	128.83
27	QA	201	PUB	C4B-CHB-C1C	-6.50	121.04	128.81
26	HB	1002	PEB	CHB-C4B-NB	-6.50	119.81	128.83
28	QH	1001	CYC	CHD-C4C-NC	6.50	132.93	125.20
28	eH	1001	CYC	CHB-C4A-NA	-6.50	111.34	124.93
27	A9	302	PUB	CAD-C3D-C4D	6.50	131.64	121.38
26	KG	201	PEB	C1C-CHB-C4B	6.50	136.57	128.81
26	l8	202	PEB	OA-C1A-C2A	-6.50	121.01	126.17
26	g1	202	PEB	CHB-C4B-NB	-6.49	119.82	128.83
26	O8	203	PEB	CHC-C4C-C3C	-6.49	119.27	130.34
26	mI	202	PEB	CHC-C4C-C3C	-6.49	119.27	130.34
26	gE	201	PEB	C1C-CHB-C4B	6.49	136.56	128.81
26	X3	202	PEB	CHC-C4C-C3C	-6.49	119.28	130.34
26	14	202	PEB	C1C-CHB-C4B	6.48	136.56	128.81
26	g8	201	PEB	CHB-C4B-NB	-6.48	119.83	128.83
28	mH	1001	CYC	CHB-C4A-NA	-6.48	111.37	124.93
28	G6	1001	CYC	OC-C1C-C2C	-6.48	121.02	126.17
26	kE	203	PEB	CHC-C4C-C3C	-6.48	119.29	130.34
26	X3	203	PEB	C1C-CHB-C4B	6.48	136.55	128.81
26	Q3	201	PEB	CHA-C1B-NB	-6.48	111.38	124.93
26	s4	201	PEB	C1C-CHB-C4B	6.48	136.54	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	WE	201	PEB	CHA-C1B-NB	-6.47	111.40	124.93
26	RD	202	PEB	CHC-C4C-C3C	-6.47	119.30	130.34
26	mG	201	PEB	CHC-C4C-C3C	-6.47	119.30	130.34
26	TD	202	PEB	CHB-C4B-NB	-6.47	119.85	128.83
26	TD	203	PEB	CHC-C1D-ND	-6.46	106.44	113.95
26	VD	202	PEB	OA-C1A-C2A	-6.46	121.03	126.17
26	UG	201	PEB	C1C-CHB-C4B	6.46	136.53	128.81
26	RD	202	PEB	CHC-C1D-ND	-6.46	106.44	113.95
26	PG	201	PEB	C2A-C1A-NA	6.46	113.84	108.27
26	cE	201	PEB	CMB-C2B-C1B	6.46	135.01	125.06
26	T9	203	PEB	CHC-C1D-ND	-6.46	106.44	113.95
26	cF	202	PEB	CMB-C2B-C1B	6.46	135.01	125.06
26	EG	201	PEB	CMB-C2B-C1B	6.46	135.01	125.06
26	lG	201	PEB	CHB-C4B-NB	-6.46	119.87	128.83
26	ZI	201	PEB	CHB-C4B-C3B	-6.46	110.40	125.32
28	HF	1001	CYC	CAB-C3B-C4B	6.46	131.58	121.38
28	F2	1001	CYC	C4D-CHA-C1A	6.46	136.52	128.81
26	UA	202	PEB	CMB-C2B-C1B	6.46	135.00	125.06
27	AI	302	PUB	CAD-C3D-C4D	6.46	131.57	121.38
26	BD	202	PEB	CHC-C4C-C3C	-6.46	119.33	130.34
26	eI	202	PEB	CHC-C4C-C3C	-6.45	119.33	130.34
28	oH	1001	CYC	CHD-C4C-NC	6.45	132.87	125.20
26	iI	202	PEB	C1C-CHB-C4B	6.45	136.51	128.81
26	aB	202	PEB	C1C-CHB-C4B	-6.44	121.11	128.81
26	C3	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
28	fH	1001	CYC	CHB-C4A-NA	-6.44	111.46	124.93
26	q1	202	PEB	CHC-C4C-C3C	-6.44	119.35	130.34
26	e2	202	PEB	CHC-C4C-C3C	-6.44	119.36	130.34
26	mI	203	PEB	CHB-C4B-NB	-6.44	119.90	128.83
28	dH	1001	CYC	CHA-C1A-NA	-6.44	119.90	128.83
27	24	403	PUB	CHB-C1C-NC	-6.44	119.90	128.83
26	rG	201	PEB	OA-C1A-C2A	-6.44	121.06	126.17
26	hF	201	PEB	C1C-CHB-C4B	6.44	136.50	128.81
26	d1	202	PEB	CHC-C4C-C3C	-6.43	119.36	130.34
28	tH	1001	CYC	CHB-C4A-NA	-6.43	111.47	124.93
27	A8	303	PUB	C4B-CHB-C1C	-6.43	121.12	128.81
28	SH	1001	CYC	CHB-C4A-NA	-6.43	111.47	124.93
28	B6	1001	CYC	OC-C1C-C2C	-6.43	121.06	126.17
26	mG	203	PEB	CHA-C4A-NA	-6.43	117.56	125.20
27	xE	305	PUB	CAD-C3D-C4D	6.43	131.53	121.38
26	QB	201	PEB	CHC-C1D-ND	-6.43	106.48	113.95
26	oG	203	PEB	CHB-C4B-NB	-6.43	119.91	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K3	201	PEB	CBC-CAC-C2C	6.42	123.58	112.62
26	YA	201	PEB	C1C-CHB-C4B	6.42	136.48	128.81
26	MD	201	PEB	CHC-C4C-C3C	-6.42	119.39	130.34
26	ZI	201	PEB	CMB-C2B-C1B	6.42	134.95	125.06
26	U8	202	PEB	CMB-C2B-C1B	6.42	134.95	125.06
26	QD	201	PEB	CHA-C1B-NB	-6.42	111.50	124.93
26	g2	202	PEB	CHC-C4C-C3C	-6.42	119.40	130.34
26	KD	201	PEB	CBC-CAC-C2C	6.41	123.56	112.62
27	A2	302	PUB	CAD-C3D-C4D	6.41	131.50	121.38
26	GG	203	PEB	CHA-C4A-NA	-6.41	117.58	125.20
28	VH	1001	CYC	OB-C4B-C3B	-6.41	121.08	128.04
26	mG	201	PEB	CHB-C4B-NB	-6.41	119.94	128.83
26	jE	202	PEB	C1C-CHB-C4B	6.41	136.47	128.81
26	y1	202	PEB	CHC-C4C-C3C	-6.41	119.41	130.34
26	RJ	203	PEB	CHB-C4B-NB	-6.40	119.95	128.83
26	CE	201	PEB	CHA-C1B-NB	-6.40	111.54	124.93
28	EB	1001	CYC	C4D-CHA-C1A	6.40	136.45	128.81
28	gH	1001	CYC	OB-C4B-C3B	-6.40	121.10	128.04
26	KE	201	PEB	CHB-C4B-NB	-6.39	119.96	128.83
26	CA	202	PEB	CHB-C4B-NB	-6.39	119.96	128.83
26	Z2	201	PEB	CHB-C4B-C3B	-6.39	110.55	125.32
28	HB	1001	CYC	C4D-CHA-C1A	6.39	136.44	128.81
26	V8	201	PEB	CHB-C4B-NB	-6.39	119.96	128.83
26	mE	201	PEB	C1C-CHB-C4B	6.39	136.44	128.81
26	m2	203	PEB	CHB-C4B-NB	-6.39	119.97	128.83
26	i8	202	PEB	CHB-C4B-NB	-6.39	119.97	128.83
26	tG	202	PEB	CBC-CAC-C2C	6.39	123.52	112.62
26	gE	201	PEB	CHC-C1D-ND	-6.39	106.53	113.95
26	R2	201	PEB	CHC-C1D-ND	-6.38	106.54	113.95
26	D3	202	PEB	CHB-C4B-NB	-6.38	119.98	128.83
27	21	403	PUB	CAD-C3D-C4D	6.38	131.45	121.38
26	PI	202	PEB	C1C-CHB-C4B	6.38	136.43	128.81
28	UH	1001	CYC	CHB-C4A-NA	-6.37	111.61	124.93
26	kA	202	PEB	C1C-CHB-C4B	-6.37	121.20	128.81
26	RI	201	PEB	CHC-C1D-ND	-6.37	106.55	113.95
26	HE	201	PEB	CHA-C1B-NB	-6.37	111.62	124.93
26	Y8	201	PEB	C1C-CHB-C4B	6.36	136.41	128.81
28	GI	1001	CYC	OC-C1C-C2C	-6.36	121.11	126.17
26	XD	202	PEB	CHC-C4C-C3C	-6.36	119.48	130.34
26	OE	202	PEB	CMB-C2B-C1B	6.36	134.86	125.06
26	J8	201	PEB	CHB-C4B-NB	-6.36	120.00	128.83
27	AA	303	PUB	CHB-C1C-NC	-6.36	120.00	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	DE	201	PEB	CHA-C4A-NA	6.36	132.77	125.20
28	lH	1001	CYC	OB-C4B-C3B	-6.36	121.14	128.04
26	ND	202	PEB	CHC-C4C-C3C	-6.36	119.49	130.34
28	iH	1001	CYC	CHB-C4A-NA	-6.36	111.63	124.93
26	a8	203	PEB	CHC-C4C-C3C	-6.36	119.49	130.34
26	gA	202	PEB	C1C-CHB-C4B	-6.36	121.21	128.81
27	Q8	201	PUB	CAD-C3D-C4D	6.36	131.42	121.38
26	aG	203	PEB	C1C-CHB-C4B	6.35	136.40	128.81
26	M1	401	PEB	CHB-C4B-NB	-6.35	120.01	128.83
27	xE	301	PUB	CAD-C3D-C4D	6.34	131.40	121.38
27	AF	303	PUB	OD-C4D-C3D	-6.34	121.16	128.04
26	XA	202	PEB	CMB-C2B-C1B	6.34	134.83	125.06
26	eE	202	PEB	CMB-C2B-C1B	6.34	134.83	125.06
28	PH	1001	CYC	CHB-C4A-NA	-6.34	111.67	124.93
28	NI	1001	CYC	OC-C1C-C2C	-6.34	121.13	126.17
26	jE	201	PEB	CHA-C4A-NA	6.34	132.74	125.20
27	xG	301	PUB	CHB-C1C-NC	-6.34	120.04	128.83
28	lH	1001	CYC	CHB-C4A-NA	-6.33	111.68	124.93
26	aI	202	PEB	CHB-C4B-NB	-6.33	120.04	128.83
26	eE	201	PEB	C1C-CHB-C4B	6.33	136.37	128.81
26	Z2	201	PEB	CMB-C2B-C1B	6.33	134.81	125.06
26	d6	204	PEB	CHB-C4B-NB	-6.33	120.05	128.83
26	P3	202	PEB	C1C-CHB-C4B	6.33	136.37	128.81
26	QF	202	PEB	C1C-CHB-C4B	6.33	136.37	128.81
26	OG	201	PEB	CHC-C4C-C3C	-6.32	119.55	130.34
26	C8	202	PEB	C1C-CHB-C4B	-6.32	121.26	128.81
26	R2	202	PEB	C1C-CHB-C4B	6.32	136.36	128.81
28	WH	1001	CYC	CHD-C4C-NC	6.32	132.71	125.20
26	N9	204	PEB	C1C-CHB-C4B	6.31	136.35	128.81
26	HF	1002	PEB	CHB-C4B-NB	-6.31	120.07	128.83
28	yH	1001	CYC	CHD-C4C-NC	6.31	132.71	125.20
26	O7	201	PEB	CHB-C4B-NB	-6.31	120.08	128.83
26	OA	203	PEB	CHC-C1D-ND	-6.31	106.62	113.95
26	X8	201	PEB	CHB-C4B-NB	-6.31	120.08	128.83
27	xG	301	PUB	CAD-C3D-C4D	6.31	131.34	121.38
26	j8	201	PEB	CHB-C4B-NB	-6.31	120.08	128.83
26	s1	202	PEB	OA-C1A-C2A	-6.30	121.16	126.17
26	mA	201	PEB	CHB-C4B-NB	-6.30	120.08	128.83
26	a8	201	PEB	CHB-C4B-NB	-6.30	120.08	128.83
28	G2	1001	CYC	OC-C1C-C2C	-6.30	121.16	126.17
26	W3	201	PEB	CHC-C4C-C3C	-6.30	119.59	130.34
26	HD	203	PEB	C1C-CHB-C4B	6.30	136.34	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A6	301	PEB	CHB-C4B-NB	-6.30	120.09	128.83
26	XD	201	PEB	OA-C1A-C2A	-6.30	121.16	126.17
26	C5	201	PEB	CHB-C4B-NB	-6.30	120.09	128.83
26	D8	202	PEB	C1C-CHB-C4B	-6.30	121.28	128.81
26	D9	202	PEB	CMB-C2B-C1B	6.30	134.76	125.06
26	g8	202	PEB	C1C-CHB-C4B	-6.30	121.29	128.81
27	wE	304	PUB	CAD-C3D-C4D	6.30	131.32	121.38
26	X3	201	PEB	OA-C1A-C2A	-6.30	121.17	126.17
26	QD	201	PEB	CMB-C2B-C1B	6.29	134.76	125.06
26	aE	202	PEB	CMB-C2B-C1B	6.29	134.76	125.06
26	J4	202	PEB	C1C-CHB-C4B	6.29	136.33	128.81
26	LJ	201	PEB	C1C-CHB-C4B	6.29	136.32	128.81
28	L6	1001	CYC	CHB-C4A-NA	-6.29	111.78	124.93
28	oH	1001	CYC	CMA-C3A-C4A	6.29	134.75	125.06
26	Q6	201	PEB	CHC-C1D-ND	-6.29	106.64	113.95
28	cH	1001	CYC	CHB-C4A-C3A	6.29	141.07	124.90
28	wH	1001	CYC	CHB-C4A-NA	-6.29	111.78	124.93
28	EI	1001	CYC	C4D-CHA-C1A	6.29	136.32	128.81
26	wE	301	PEB	CHB-C4B-NB	-6.29	120.11	128.83
26	DJ	201	PEB	CHC-C4C-C3C	-6.28	119.62	130.34
28	E2	1001	CYC	C4D-CHA-C1A	6.28	136.31	128.81
26	dB	202	PEB	CHC-C1D-ND	-6.28	106.66	113.95
28	CH	1001	CYC	CHB-C4A-NA	-6.27	111.81	124.93
26	P8	202	PEB	C1C-CHB-C4B	-6.27	121.32	128.81
26	hF	201	PEB	CHC-C4C-C3C	-6.26	119.66	130.34
26	HD	202	PEB	CHC-C4C-C3C	-6.26	119.66	130.34
28	GH	1001	CYC	CHB-C4A-NA	-6.26	111.83	124.93
26	fA	203	PEB	C1C-CHB-C4B	6.26	136.29	128.81
26	VJ	203	PEB	CHB-C4B-NB	-6.26	120.15	128.83
26	a2	202	PEB	CHB-C4B-NB	-6.26	120.15	128.83
26	H7	1002	PEB	CHB-C4B-NB	-6.26	120.15	128.83
26	m8	201	PEB	CHB-C4B-NB	-6.26	120.15	128.83
28	LB	1001	CYC	CHB-C4A-NA	-6.26	111.85	124.93
28	qH	1002	CYC	CHB-C1B-NB	-6.26	112.63	126.06
26	dB	202	PEB	C1C-CHB-C4B	6.25	136.28	128.81
26	RI	202	PEB	C1C-CHB-C4B	6.25	136.28	128.81
26	DD	202	PEB	CHC-C4C-C3C	-6.25	119.67	130.34
26	GG	202	PEB	C2A-C1A-NA	-6.25	102.88	108.27
26	HJ	202	PEB	CMB-C2B-C1B	6.25	134.69	125.06
28	LI	1001	CYC	CMA-C3A-C4A	6.25	134.69	125.06
26	d6	202	PEB	C1C-CHB-C4B	6.25	136.28	128.81
26	RA	202	PEB	CHB-C4B-NB	-6.25	120.16	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IJ	203	PEB	C1C-CHB-C4B	6.25	136.28	128.81
26	mE	201	PEB	CHC-C4C-C3C	-6.25	119.68	130.34
26	BE	201	PEB	OD-C4D-C3D	-6.25	115.30	129.46
26	F9	203	PEB	CHA-C1B-NB	-6.25	111.87	124.93
26	FJ	201	PEB	CHA-C1B-NB	-6.24	111.87	124.93
26	UG	202	PEB	CHB-C4B-NB	-6.24	120.17	128.83
26	cE	202	PEB	CHB-C4B-NB	-6.24	120.18	128.83
28	mH	1001	CYC	CHD-C4C-NC	6.23	132.62	125.20
26	h6	201	PEB	CHC-C4C-C3C	-6.23	119.71	130.34
26	FJ	201	PEB	CHC-C4C-C3C	-6.23	119.71	130.34
26	VF	201	PEB	C1C-CHB-C4B	6.23	136.25	128.81
26	TD	202	PEB	C1C-CHB-C4B	6.23	136.25	128.81
28	pH	1001	CYC	CHB-C4A-NA	-6.23	111.91	124.93
26	oE	201	PEB	CHB-C4B-NB	-6.22	120.19	128.83
26	WF	203	PEB	CHC-C4C-C3C	-6.22	119.73	130.34
26	DJ	202	PEB	CHA-C1B-NB	-6.22	111.92	124.93
28	BB	1001	CYC	OC-C1C-C2C	-6.22	121.23	126.17
26	m2	202	PEB	CHC-C4C-C3C	-6.22	119.73	130.34
26	QB	201	PEB	CHB-C4B-NB	-6.22	120.20	128.83
27	A2	303	PUB	CAD-C3D-C4D	6.22	131.20	121.38
26	YB	201	PEB	CHC-C1D-ND	-6.22	106.73	113.95
27	AI	303	PUB	CAD-C3D-C4D	6.21	131.19	121.38
26	T3	202	PEB	C1C-CHB-C4B	6.21	136.23	128.81
26	P2	202	PEB	C1C-CHB-C4B	6.21	136.23	128.81
26	M3	201	PEB	CHB-C4B-NB	-6.21	120.21	128.83
26	SG	201	PEB	C1C-CHB-C4B	6.21	136.22	128.81
26	UI	201	PEB	CHB-C4B-C3B	-6.21	110.98	125.32
28	H2	1001	CYC	C4D-CHA-C1A	6.21	136.22	128.81
26	i8	202	PEB	C1C-CHB-C4B	-6.20	121.40	128.81
26	R9	203	PEB	CHB-C4B-NB	-6.20	120.23	128.83
26	UE	201	PEB	CHC-C1D-ND	-6.20	106.75	113.95
26	jF	203	PEB	CHB-C4B-NB	-6.20	120.23	128.83
28	H6	1001	CYC	C4D-CHA-C1A	6.20	136.21	128.81
26	A3	202	PEB	CHB-C4B-NB	-6.19	120.24	128.83
26	SG	201	PEB	CHC-C4C-C3C	-6.19	119.78	130.34
26	K8	201	PEB	CMB-C2B-C1B	6.19	134.60	125.06
28	B6	1002	CYC	CHB-C4A-NA	-6.19	111.99	124.93
26	VF	202	PEB	CHC-C4C-C3C	-6.18	119.79	130.34
26	H7	1002	PEB	CHC-C1D-ND	-6.18	106.77	113.95
26	VD	202	PEB	C1C-CHB-C4B	6.18	136.19	128.81
26	RD	203	PEB	CHC-C1D-ND	-6.18	106.78	113.95
28	L2	1001	CYC	CMA-C3A-C4A	6.18	134.57	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R7	202	PEB	CHB-C4B-NB	-6.17	120.26	128.83
26	B9	203	PEB	C1C-CHB-C4B	6.17	136.18	128.81
27	yE	302	PUB	OD-C4D-C3D	-6.17	121.34	128.04
26	U2	201	PEB	CHB-C4B-C3B	-6.17	111.07	125.32
26	TG	202	PEB	C1C-CHB-C4B	6.17	136.18	128.81
26	S2	201	PEB	C1C-CHB-C4B	6.17	136.18	128.81
26	eA	202	PEB	C1C-CHB-C4B	-6.17	121.44	128.81
26	GC	203	PEB	C1C-CHB-C4B	6.17	136.17	128.81
26	a6	202	PEB	C1C-CHB-C4B	-6.16	121.44	128.81
26	CD	201	PEB	CHA-C1B-NB	-6.16	112.04	124.93
26	R8	201	PEB	CHB-C4B-NB	-6.16	120.28	128.83
26	KG	202	PEB	CMB-C2B-C1B	6.16	134.55	125.06
26	ZB	201	PEB	CHC-C4C-C3C	-6.16	119.83	130.34
26	C3	201	PEB	CHA-C1B-NB	-6.16	112.05	124.93
26	WI	201	PEB	CMB-C2B-C1B	6.16	134.54	125.06
28	YH	1001	CYC	CHB-C4A-NA	-6.16	112.06	124.93
27	xG	306	PUB	CAD-C3D-C4D	6.16	131.10	121.38
27	N9	201	PUB	CHA-C4A-NA	-6.16	106.80	113.95
26	GE	201	PEB	C1C-CHB-C4B	6.16	136.16	128.81
26	Z6	201	PEB	CHC-C4C-C3C	-6.15	119.85	130.34
26	eB	202	PEB	CHC-C4C-C3C	-6.15	119.85	130.34
26	WB	201	PEB	CMB-C2B-C1B	6.15	134.53	125.06
27	A8	303	PUB	CHB-C1C-NC	-6.15	120.30	128.83
26	UD	201	PEB	CHB-C4B-NB	-6.15	120.30	128.83
26	y4	202	PEB	CHC-C4C-C3C	-6.15	119.86	130.34
26	QE	203	PEB	CHB-C4B-NB	-6.15	120.30	128.83
27	xG	305	PUB	CAD-C3D-C4D	6.14	131.08	121.38
26	UE	201	PEB	CHB-C4B-C3B	-6.14	111.13	125.32
26	g4	201	PEB	OA-C1A-C2A	-6.14	121.29	126.17
26	S2	201	PEB	CMB-C2B-C1B	6.14	134.52	125.06
26	HJ	202	PEB	CHA-C1B-NB	-6.14	112.09	124.93
26	k1	203	PEB	CHC-C4C-C3C	-6.14	119.86	130.34
26	dA	201	PEB	CHB-C4B-NB	-6.14	120.31	128.83
26	lF	201	PEB	C1C-CHB-C4B	6.14	136.14	128.81
26	BJ	201	PEB	CHC-C4C-C3C	-6.14	119.87	130.34
26	H9	202	PEB	CHA-C1B-NB	-6.13	112.10	124.93
27	xE	306	PUB	OD-C4D-C3D	-6.13	121.39	128.04
26	jA	203	PEB	CHC-C4C-C3C	-6.13	119.88	130.34
26	DJ	202	PEB	CMB-C2B-C1B	6.13	134.50	125.06
28	E6	1001	CYC	CAB-C3B-C4B	6.13	131.06	121.38
26	gI	203	PEB	CHB-C4B-NB	-6.13	120.33	128.83
26	OE	201	PEB	OA-C1A-C2A	-6.13	121.30	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	WF	201	PEB	CHB-C4B-NB	-6.13	120.33	128.83
26	TJ	201	PEB	C1C-CHB-C4B	6.12	136.12	128.81
28	N7	1001	CYC	C4D-CHA-C1A	6.12	136.12	128.81
26	N3	203	PEB	CHC-C1D-ND	-6.12	106.84	113.95
26	S3	201	PEB	CMB-C2B-C1B	6.12	134.49	125.06
26	ZI	201	PEB	C1C-CHB-C4B	6.12	136.12	128.81
26	g8	202	PEB	OA-C1A-C2A	-6.12	121.31	126.17
26	YG	203	PEB	CHA-C1B-NB	-6.12	112.13	124.93
26	RF	201	PEB	CHC-C1D-ND	-6.11	106.85	113.95
26	GA	201	PEB	CHA-C1B-NB	-6.11	112.14	124.93
28	JI	1001	CYC	CMA-C3A-C4A	6.11	134.48	125.06
26	O3	201	PEB	CHC-C4C-C3C	-6.11	119.91	130.34
26	gE	203	PEB	CHA-C1B-NB	-6.11	112.15	124.93
28	MH	1001	CYC	CHD-C4C-NC	6.11	132.47	125.20
26	Q6	201	PEB	CHB-C4B-NB	-6.11	120.35	128.83
28	MH	1001	CYC	CMA-C3A-C4A	6.11	134.47	125.06
26	J3	202	PEB	CHC-C4C-C3C	-6.11	119.92	130.34
26	XA	201	PEB	CHB-C4B-NB	-6.10	120.36	128.83
28	NB	1001	CYC	CHB-C4A-NA	-6.10	112.16	124.93
26	CD	201	PEB	CMB-C2B-C1B	6.10	134.47	125.06
27	K4	203	PUB	CAD-C3D-C4D	6.10	131.02	121.38
26	i7	202	PEB	C1C-CHB-C4B	-6.10	121.52	128.81
28	EB	1001	CYC	CAB-C3B-C4B	6.10	131.02	121.38
26	B1	202	PEB	CHC-C1D-ND	-6.10	106.86	113.95
26	aI	202	PEB	CHC-C4C-C3C	-6.10	119.93	130.34
26	X4	202	PEB	CHA-C1B-NB	-6.10	112.17	124.93
26	IG	201	PEB	C4B-C3B-C2B	-6.10	100.03	106.78
26	GG	201	PEB	CHC-C4C-C3C	-6.10	119.94	130.34
28	YH	1001	CYC	CMA-C3A-C4A	6.10	134.45	125.06
28	JH	1001	CYC	CHB-C4A-NA	-6.10	112.18	124.93
26	IE	201	PEB	CHA-C4A-NA	6.10	132.45	125.20
26	UE	203	PEB	C1C-CHB-C4B	6.09	136.09	128.81
26	G8	201	PEB	CMB-C2B-C1B	6.09	134.45	125.06
26	OD	201	PEB	CMB-C2B-C1B	6.09	134.45	125.06
26	vE	201	PEB	C2A-C1A-NA	6.09	113.52	108.27
26	W6	201	PEB	CMB-C2B-C1B	6.09	134.44	125.06
26	KG	202	PEB	CHA-C1B-NB	-6.09	112.20	124.93
26	wG	302	PEB	CHB-C4B-NB	-6.09	120.38	128.83
26	Q2	201	PEB	C1C-CHB-C4B	6.09	136.08	128.81
26	T2	203	PEB	CHB-C4B-NB	-6.08	120.39	128.83
26	pE	201	PEB	CHA-C4A-NA	6.08	132.44	125.20
26	QJ	201	PEB	C1C-CHB-C4B	6.08	136.07	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	wE	302	PEB	CHB-C4B-NB	-6.08	120.39	128.83
26	nG	201	PEB	C2A-C1A-NA	6.08	113.51	108.27
26	FJ	201	PEB	CMB-C2B-C1B	6.08	134.43	125.06
26	B9	201	PEB	CHC-C4C-C3C	-6.08	119.97	130.34
27	K1	203	PUB	OD-C4D-C3D	-6.07	121.45	128.04
27	NJ	201	PUB	CAD-C3D-C4D	6.07	130.97	121.38
26	JF	1002	PEB	CHC-C1D-ND	-6.07	106.89	113.95
26	w1	201	PEB	C1C-CHB-C4B	6.07	136.06	128.81
26	O3	201	PEB	CMB-C2B-C1B	6.07	134.41	125.06
26	w1	202	PEB	C1C-CHB-C4B	6.07	136.06	128.81
26	qE	202	PEB	CHB-C4B-C3B	6.06	139.33	125.32
26	BE	201	PEB	CHC-C4C-C3C	-6.06	120.00	130.34
27	AI	302	PUB	CHB-C1C-NC	-6.06	120.42	128.83
26	O8	203	PEB	CHC-C1D-ND	-6.06	106.91	113.95
26	GE	202	PEB	C4B-C3B-C2B	-6.06	100.08	106.78
26	bB	202	PEB	CHC-C4C-C3C	-6.06	120.01	130.34
26	M1	403	PEB	CHB-C4B-NB	-6.05	120.43	128.83
26	R9	201	PEB	CHB-C4B-NB	-6.05	120.44	128.83
28	FI	1001	CYC	OB-C4B-C3B	-6.05	121.47	128.04
26	T3	202	PEB	C2A-C1A-NA	6.05	113.49	108.27
26	zG	501	PEB	CHB-C4B-NB	-6.05	120.44	128.83
26	QF	202	PEB	CHC-C4C-C3C	-6.05	120.02	130.34
26	C8	202	PEB	CHB-C4B-NB	-6.05	120.44	128.83
28	vH	1001	CYC	CMA-C3A-C4A	6.05	134.38	125.06
26	F3	203	PEB	OA-C1A-C2A	-6.05	121.37	126.17
28	QH	1001	CYC	CMA-C3A-C4A	6.04	134.37	125.06
26	HG	201	PEB	CHA-C1B-NB	-6.04	112.29	124.93
26	jE	201	PEB	CHB-C4B-NB	-6.04	120.45	128.83
28	IF	1001	CYC	C4D-CHA-C1A	6.04	136.03	128.81
28	EH	1001	CYC	CHB-C4A-NA	-6.04	112.30	124.93
28	HI	1001	CYC	C4D-CHA-C1A	6.04	136.02	128.81
26	iI	202	PEB	CHC-C4C-C3C	-6.04	120.04	130.34
26	W7	203	PEB	CHC-C4C-C3C	-6.04	120.04	130.34
26	YE	203	PEB	CHC-C4C-C3C	-6.04	120.04	130.34
26	cA	202	PEB	CHC-C4C-C3C	-6.03	120.05	130.34
27	24	402	PUB	CAD-C3D-C4D	6.03	130.90	121.38
28	C7	1001	CYC	C4D-CHA-C1A	6.03	136.01	128.81
26	GG	202	PEB	C3B-C4B-NB	6.03	118.82	110.05
28	GB	1001	CYC	C4D-CHA-C1A	6.03	136.01	128.81
26	PD	202	PEB	C1C-CHB-C4B	6.02	136.01	128.81
28	iH	1001	CYC	OB-C4B-C3B	-6.02	121.50	128.04
26	aG	201	PEB	CHC-C4C-C3C	-6.02	120.06	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AG	201	PEB	CMB-C2B-C1B	6.02	134.34	125.06
26	OD	201	PEB	CHC-C4C-C3C	-6.02	120.08	130.34
26	GA	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
26	Z2	201	PEB	C1C-CHB-C4B	6.01	135.99	128.81
26	SF	201	PEB	CHB-C4B-NB	-6.01	120.48	128.83
28	AH	1001	CYC	CHD-C4C-NC	6.01	132.35	125.20
27	A6	302	PUB	CAD-C3D-C4D	6.01	130.88	121.38
26	AA	301	PEB	CHB-C4B-NB	-6.01	120.49	128.83
28	D6	1001	CYC	OB-C4B-C3B	-6.01	121.52	128.04
26	IE	201	PEB	C2A-C1A-NA	-6.01	103.09	108.27
26	ND	203	PEB	CHC-C1D-ND	-6.01	106.97	113.95
26	T3	203	PEB	CHC-C1D-ND	-6.01	106.97	113.95
26	QB	201	PEB	C1C-CHB-C4B	6.01	135.99	128.81
26	UD	201	PEB	CHC-C4C-C3C	-6.01	120.09	130.34
26	a2	202	PEB	CHC-C4C-C3C	-6.01	120.09	130.34
26	c4	201	PEB	CHC-C1D-ND	-6.01	106.97	113.95
26	X1	202	PEB	CHA-C1B-NB	-6.00	112.37	124.93
26	P2	202	PEB	CHC-C4C-C3C	-6.00	120.10	130.34
26	V7	202	PEB	OA-C1A-C2A	-6.00	121.40	126.17
28	hH	1001	CYC	CHD-C4C-NC	6.00	132.34	125.20
26	IG	201	PEB	OA-C1A-C2A	6.00	130.94	126.17
26	c4	203	PEB	CHC-C4C-C3C	-6.00	120.11	130.34
27	AB	303	PUB	CAD-C3D-C4D	6.00	130.85	121.38
26	fB	203	PEB	C1C-CHB-C4B	6.00	135.97	128.81
27	A6	303	PUB	CAD-C3D-C4D	6.00	130.85	121.38
27	yG	302	PUB	OD-C4D-C3D	-6.00	121.53	128.04
26	N6	201	PEB	CHB-C4B-NB	-5.99	120.51	128.83
26	l7	201	PEB	CHC-C4C-C3C	-5.99	120.12	130.34
26	Q3	201	PEB	CHB-C4B-NB	-5.99	120.52	128.83
26	SF	201	PEB	CHA-C1B-NB	-5.99	112.40	124.93
26	F9	201	PEB	CMB-C2B-C1B	5.99	134.29	125.06
26	G8	201	PEB	CHA-C1B-NB	-5.99	112.40	124.93
26	WE	202	PEB	C1C-CHB-C4B	5.99	135.96	128.81
26	P9	202	PEB	CMB-C2B-C1B	5.99	134.29	125.06
26	HD	203	PEB	CAB-C3B-C4B	5.99	135.61	125.01
26	WD	201	PEB	CHC-C4C-C3C	-5.99	120.12	130.34
26	d8	202	PEB	CHB-C4B-NB	-5.99	120.52	128.83
28	qH	1002	CYC	C4D-CHA-C1A	5.99	135.96	128.81
27	A7	304	PUB	CAD-C3D-C4D	5.99	130.83	121.38
28	mH	1001	CYC	OB-C4B-C3B	-5.98	121.55	128.04
26	QI	201	PEB	CHB-C4B-C3B	-5.98	111.50	125.32
26	UF	202	PEB	CHB-C4B-NB	-5.98	120.53	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D1	202	PEB	CHC-C4C-C3C	-5.98	120.14	130.34
27	K4	203	PUB	OD-C4D-C3D	-5.98	121.55	128.04
26	U7	202	PEB	CHB-C4B-NB	-5.98	120.53	128.83
26	N3	203	PEB	C1C-CHB-C4B	5.98	135.95	128.81
27	AB	302	PUB	CAD-C3D-C4D	5.98	130.82	121.38
26	N3	201	PEB	OA-C1A-C2A	-5.98	121.42	126.17
26	eB	202	PEB	C1C-CHB-C4B	5.98	135.95	128.81
26	Q9	201	PEB	C1C-CHB-C4B	5.97	135.95	128.81
26	J8	201	PEB	C1C-CHB-C4B	-5.97	121.67	128.81
28	UH	1001	CYC	CHD-C4C-NC	5.97	132.30	125.20
26	i2	202	PEB	CHC-C4C-C3C	-5.97	120.16	130.34
28	DB	1001	CYC	OB-C4B-C3B	-5.97	121.56	128.04
26	H3	202	PEB	CHC-C4C-C3C	-5.96	120.16	130.34
27	AB	302	PUB	CHC-C1D-ND	-5.96	106.18	113.72
26	UG	201	PEB	CHB-C4B-C3B	-5.96	111.54	125.32
26	c4	202	PEB	CHB-C4B-NB	-5.96	120.55	128.83
28	hH	1001	CYC	OB-C4B-C3B	-5.96	121.57	128.04
28	gH	1001	CYC	CHB-C4A-NA	-5.96	112.46	124.93
26	RJ	201	PEB	CHB-C4B-NB	-5.96	120.56	128.83
26	lB	201	PEB	CHC-C4C-C3C	-5.96	120.17	130.34
26	GE	202	PEB	C3B-C4B-NB	5.96	118.72	110.05
26	DD	202	PEB	CHB-C4B-NB	-5.96	120.56	128.83
26	KE	201	PEB	CHA-C1B-NB	-5.96	112.47	124.93
27	Q8	201	PUB	OD-C4D-C3D	-5.96	121.57	128.04
26	Q8	203	PEB	CHB-C4B-NB	-5.96	120.56	128.83
27	yE	303	PUB	CAD-C3D-C4D	5.96	130.79	121.38
26	R3	201	PEB	CHC-C1D-ND	-5.96	107.03	113.95
26	XD	203	PEB	C1C-CHB-C4B	5.95	135.92	128.81
26	h8	201	PEB	CHB-C4B-NB	-5.95	120.57	128.83
26	K9	202	PEB	CHB-C4B-NB	-5.95	120.57	128.83
26	gI	202	PEB	C1C-CHB-C4B	5.95	135.92	128.81
26	fE	201	PEB	C2A-C1A-NA	5.95	113.40	108.27
26	xE	303	PEB	C1C-CHB-C4B	-5.95	121.70	128.81
26	v4	201	PEB	C1C-CHB-C4B	5.95	135.91	128.81
26	Q2	201	PEB	CHB-C4B-C3B	-5.95	111.58	125.32
26	cB	202	PEB	CHB-C4B-NB	-5.94	120.58	128.83
28	LB	1001	CYC	CMA-C3A-C4A	5.94	134.22	125.06
26	S9	201	PEB	CHC-C1D-ND	-5.94	107.05	113.95
28	AH	1001	CYC	CHB-C4A-C3A	5.94	140.18	124.90
26	iA	202	PEB	CHB-C4B-NB	-5.94	120.59	128.83
27	yG	303	PUB	OD-C4D-C3D	-5.94	121.59	128.04
26	SB	203	PEB	C1C-CHB-C4B	5.94	135.90	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SE	202	PEB	OA-C1A-C2A	5.94	130.89	126.17
26	fG	201	PEB	C2A-C1A-NA	5.94	113.39	108.27
26	k4	203	PEB	OA-C1A-C2A	-5.94	121.45	126.17
28	L6	1001	CYC	CMA-C3A-C4A	5.93	134.20	125.06
26	UE	202	PEB	CHB-C4B-NB	-5.93	120.60	128.83
26	BJ	201	PEB	CHB-C4B-NB	-5.93	120.60	128.83
26	SE	201	PEB	C1C-CHB-C4B	5.93	135.89	128.81
27	AF	304	PUB	OD-C4D-C3D	-5.93	121.60	128.04
26	jG	201	PEB	CHB-C4B-NB	-5.93	120.60	128.83
26	QJ	202	PEB	CHB-C4B-NB	-5.93	120.60	128.83
26	uG	203	PEB	CHB-C4B-NB	-5.93	120.61	128.83
26	A9	303	PEB	CHB-C4B-NB	-5.92	120.61	128.83
26	Z7	203	PEB	CHB-C4B-NB	-5.92	120.61	128.83
27	A6	302	PUB	CHC-C1D-ND	-5.92	106.23	113.72
26	24	404	PEB	CHA-C1B-NB	-5.92	112.55	124.93
28	MI	1001	CYC	OC-C1C-C2C	-5.92	121.47	126.17
27	xG	306	PUB	OD-C4D-C3D	-5.92	121.62	128.04
27	xE	305	PUB	OD-C4D-C3D	-5.92	121.62	128.04
26	KA	201	PEB	CMB-C2B-C1B	5.92	134.18	125.06
28	VH	1001	CYC	CHD-C4C-NC	5.92	132.24	125.20
26	S6	203	PEB	C1C-CHB-C4B	5.92	135.88	128.81
27	AB	303	PUB	OD-C4D-C3D	-5.91	121.62	128.04
26	NA	201	PEB	CHB-C4B-NB	-5.91	120.62	128.83
26	RA	202	PEB	C1C-CHB-C4B	-5.91	121.75	128.81
26	Z6	201	PEB	C1C-CHB-C4B	5.91	135.87	128.81
27	yG	303	PUB	CAD-C3D-C4D	5.91	130.72	121.38
26	ZA	201	PEB	OA-C1A-C2A	-5.91	121.47	126.17
26	KA	202	PEB	CHC-C4C-C3C	-5.91	120.26	130.34
27	NJ	201	PUB	C1D-CHC-C4C	-5.91	100.51	113.37
27	yE	303	PUB	OD-C4D-C3D	-5.91	121.63	128.04
27	AI	303	PUB	OD-C4D-C3D	-5.91	121.63	128.04
28	GI	1001	CYC	C4D-CHA-C1A	5.91	135.87	128.81
26	D9	202	PEB	CHB-C4B-NB	-5.91	120.63	128.83
28	qH	1001	CYC	CMA-C3A-C4A	5.91	134.16	125.06
26	h7	201	PEB	C1C-CHB-C4B	5.91	135.86	128.81
26	D9	201	PEB	C1C-CHB-C4B	5.91	135.86	128.81
26	ZB	201	PEB	C1C-CHB-C4B	5.90	135.86	128.81
28	TH	1001	CYC	CMA-C3A-C4A	5.90	134.15	125.06
26	dB	201	PEB	CHB-C4B-NB	-5.90	120.64	128.83
26	V9	202	PEB	CHC-C1D-ND	-5.90	107.09	113.95
26	F4	202	PEB	CHB-C4B-NB	-5.90	120.64	128.83
27	NJ	201	PUB	CHC-C1D-ND	-5.89	106.27	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AI	302	PUB	OD-C4D-C3D	-5.89	121.65	128.04
28	OH	1001	CYC	CMA-C3A-C4A	5.89	134.13	125.06
27	K1	203	PUB	CBB-CAB-C3B	5.89	122.67	112.62
26	fA	201	PEB	CHB-C4B-NB	-5.89	120.66	128.83
27	wG	304	PUB	CAD-C3D-C4D	5.88	130.67	121.38
26	Y8	202	PEB	CMB-C2B-C1B	5.88	134.13	125.06
26	H1	203	PEB	CHB-C4B-NB	-5.88	120.67	128.83
26	hA	201	PEB	CHC-C4C-C3C	-5.88	120.30	130.34
26	R8	202	PEB	CHB-C4B-NB	-5.88	120.67	128.83
26	I3	201	PEB	CHC-C4C-C3C	-5.88	120.31	130.34
26	U3	201	PEB	CHC-C4C-C3C	-5.88	120.31	130.34
26	V3	202	PEB	C1C-CHB-C4B	5.88	135.83	128.81
26	WG	202	PEB	CMB-C2B-C1B	5.88	134.12	125.06
26	11	202	PEB	C1C-CHB-C4B	5.88	135.83	128.81
26	WA	202	PEB	CHC-C4C-C3C	-5.87	120.32	130.34
26	TI	203	PEB	CHB-C4B-NB	-5.87	120.68	128.83
26	QG	201	PEB	C1C-CHB-C4B	5.87	135.82	128.81
28	nH	1001	CYC	CHD-C4C-NC	5.87	132.19	125.20
26	YA	202	PEB	CMB-C2B-C1B	5.87	134.10	125.06
26	c1	203	PEB	CHB-C4B-NB	-5.87	120.68	128.83
26	K8	201	PEB	CHA-C1B-NB	-5.87	112.65	124.93
26	oE	203	PEB	CMB-C2B-C1B	5.87	134.10	125.06
26	JD	202	PEB	CHC-C4C-C3C	-5.87	120.33	130.34
26	I8	202	PEB	OA-C1A-C2A	-5.86	121.51	126.17
26	GA	202	PEB	CHB-C4B-NB	-5.86	120.70	128.83
28	MH	1001	CYC	CHB-C4A-NA	-5.86	112.67	124.93
27	A2	303	PUB	OD-C4D-C3D	-5.86	121.69	128.04
26	VE	201	PEB	CHA-C4A-NA	5.85	132.17	125.20
26	M8	201	PEB	CHC-C1D-ND	-5.85	107.15	113.95
28	YH	1003	CYC	CHB-C4A-NA	-5.85	112.69	124.93
28	uH	1001	CYC	CMC-C2C-C1C	5.85	125.02	112.40
26	D3	201	PEB	CHB-C4B-NB	-5.85	120.71	128.83
26	d6	202	PEB	CHC-C1D-ND	-5.85	107.16	113.95
26	lF	203	PEB	CHA-C1B-NB	-5.85	112.70	124.93
26	eG	201	PEB	C1C-CHB-C4B	5.84	135.79	128.81
26	QI	201	PEB	C1C-CHB-C4B	5.84	135.79	128.81
26	oG	203	PEB	OA-C1A-C2A	-5.84	121.53	126.17
26	N7	1002	PEB	CHB-C4B-NB	-5.84	120.72	128.83
26	K8	202	PEB	CHC-C4C-C3C	-5.84	120.38	130.34
26	c1	202	PEB	CHB-C4B-NB	-5.84	120.73	128.83
26	TE	202	PEB	C1C-CHB-C4B	5.84	135.78	128.81
28	EF	1001	CYC	OB-C4B-C3B	-5.84	121.71	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	xG	303	PEB	CHB-C4B-NB	-5.84	120.73	128.83
26	IA	202	PEB	OA-C1A-C2A	-5.83	121.53	126.17
26	CG	201	PEB	CHB-C4B-NB	-5.83	120.73	128.83
26	KA	201	PEB	CHA-C1B-NB	-5.83	112.73	124.93
26	JG	201	PEB	C2A-C1A-NA	5.83	113.30	108.27
26	q4	203	PEB	CHB-C4B-NB	-5.83	120.74	128.83
26	DE	202	PEB	CHB-C4B-NB	-5.83	120.74	128.83
26	FE	201	PEB	OA-C1A-NA	5.83	132.00	124.94
26	R3	202	PEB	CHB-C4B-NB	-5.83	120.74	128.83
27	A9	302	PUB	OD-C4D-C3D	-5.82	121.72	128.04
26	SG	202	PEB	CHA-C1B-NB	-5.82	112.75	124.93
26	VI	202	PEB	CHB-C4B-NB	-5.82	120.75	128.83
26	Q7	201	PEB	C1C-CHB-C4B	5.82	135.76	128.81
28	M2	1001	CYC	OC-C1C-C2C	-5.82	121.55	126.17
26	TD	202	PEB	C2A-C1A-NA	5.82	113.29	108.27
26	M4	401	PEB	CHB-C4B-NB	-5.82	120.76	128.83
27	K1	203	PUB	CAD-C3D-C4D	5.82	130.57	121.38
26	gE	203	PEB	CHB-C4B-NB	-5.82	120.76	128.83
28	J2	1001	CYC	CMA-C3A-C4A	5.82	134.02	125.06
28	TH	1001	CYC	CHB-C4A-NA	-5.81	112.77	124.93
26	TE	201	PEB	C2A-C1A-NA	5.81	113.28	108.27
26	kF	202	PEB	C1C-CHB-C4B	5.81	135.75	128.81
26	U3	201	PEB	CHB-C4B-NB	-5.81	120.76	128.83
28	JH	1001	CYC	OB-C4B-C3B	-5.81	121.73	128.04
26	Z1	202	PEB	CHC-C1D-ND	-5.81	107.20	113.95
26	UF	201	PEB	CHC-C4C-C3C	-5.81	120.43	130.34
26	FA	201	PEB	C1C-CHB-C4B	-5.81	121.87	128.81
26	CJ	201	PEB	CHC-C1D-ND	-5.81	107.20	113.95
26	hE	202	PEB	C1C-CHB-C4B	5.81	135.75	128.81
26	A6	301	PEB	C1C-CHB-C4B	-5.81	121.87	128.81
27	AF	303	PUB	CAD-C3D-C4D	5.80	130.54	121.38
27	xG	305	PUB	OD-C4D-C3D	-5.80	121.75	128.04
26	A8	301	PEB	CHB-C4B-NB	-5.80	120.79	128.83
27	A7	303	PUB	OD-C4D-C3D	-5.80	121.75	128.04
26	PI	202	PEB	CHC-C4C-C3C	-5.80	120.45	130.34
28	MB	1001	CYC	C4D-CHA-C1A	5.80	135.73	128.81
26	a1	201	PEB	CHA-C1B-NB	-5.79	112.81	124.93
26	OE	201	PEB	CHB-C4B-NB	-5.79	120.79	128.83
26	QB	201	PEB	CHC-C4C-C3C	-5.79	120.46	130.34
26	W1	202	PEB	OA-C1A-C2A	-5.79	121.57	126.17
28	G6	1001	CYC	C4D-CHA-C1A	5.79	135.72	128.81
26	gG	203	PEB	CHA-C1B-NB	-5.79	112.82	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V9	201	PEB	C1C-CHB-C4B	-5.79	121.89	128.81
26	A1	201	PEB	CHB-C4B-NB	-5.79	120.80	128.83
26	H8	202	PEB	C1C-CHB-C4B	-5.79	121.90	128.81
26	JI	1002	PEB	CHB-C4B-NB	-5.79	120.80	128.83
26	OB	203	PEB	CHC-C4C-C3C	-5.79	120.47	130.34
26	QF	201	PEB	C1C-CHB-C4B	5.79	135.72	128.81
27	21	403	PUB	CHC-C1D-ND	-5.78	106.41	113.72
26	NB	1002	PEB	CHB-C4B-NB	-5.78	120.80	128.83
27	A7	304	PUB	OD-C4D-C3D	-5.78	121.76	128.04
26	d4	202	PEB	C1C-CHB-C4B	5.78	135.72	128.81
26	P1	201	PEB	CBC-CAC-C2C	5.78	122.48	112.62
26	ND	201	PEB	OA-C1A-C2A	-5.78	121.58	126.17
27	24	403	PUB	OD-C4D-C3D	-5.78	121.77	128.04
28	jH	1001	CYC	CHB-C4A-NA	-5.78	112.85	124.93
26	F8	201	PEB	C1C-CHB-C4B	-5.78	121.91	128.81
26	h8	201	PEB	CHA-C1B-NB	-5.77	112.85	124.93
27	AF	304	PUB	CAD-C3D-C4D	5.77	130.50	121.38
26	H9	202	PEB	CMB-C2B-C1B	5.77	133.95	125.06
26	jI	201	PEB	C1C-CHB-C4B	5.77	135.70	128.81
26	dF	203	PEB	CHA-C1B-NB	-5.77	112.86	124.93
26	C3	202	PEB	CHB-C4B-NB	-5.77	120.82	128.83
28	B6	1001	CYC	CAB-C3B-C4B	5.77	130.49	121.38
26	dF	201	PEB	C1C-CHB-C4B	5.77	135.70	128.81
26	HD	203	PEB	CHB-C4B-NB	-5.77	120.82	128.83
26	hI	201	PEB	C1C-CHB-C4B	5.77	135.70	128.81
26	Y8	202	PEB	CHA-C1B-NB	-5.77	112.87	124.93
26	EJ	202	PEB	CHC-C1D-ND	-5.77	107.25	113.95
26	kG	202	PEB	CHB-C4B-NB	-5.77	120.83	128.83
28	oH	1001	CYC	CHB-C4A-NA	-5.77	112.87	124.93
26	m1	201	PEB	CHC-C1D-ND	-5.77	107.25	113.95
28	GI	1001	CYC	CAB-C3B-C4B	5.77	130.49	121.38
28	BB	1001	CYC	CAB-C3B-C4B	5.76	130.48	121.38
26	H4	202	PEB	CHB-C4B-NB	-5.76	120.83	128.83
26	N8	201	PEB	CHB-C4B-NB	-5.76	120.83	128.83
26	QE	203	PEB	CHA-C1B-NB	-5.76	112.88	124.93
26	I8	203	PEB	CHB-C4B-NB	-5.76	120.84	128.83
26	DJ	202	PEB	CHB-C4B-NB	-5.76	120.84	128.83
26	j8	203	PEB	CHC-C4C-C3C	-5.76	120.52	130.34
26	HE	201	PEB	CHC-C1D-ND	-5.76	107.26	113.95
26	BJ	203	PEB	C1C-CHB-C4B	5.76	135.69	128.81
26	M4	402	PEB	CHB-C4B-NB	-5.76	120.84	128.83
28	CH	1001	CYC	CMA-C3A-C4A	5.76	133.93	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R3	203	PEB	CHC-C1D-ND	-5.75	107.27	113.95
26	OF	201	PEB	CHC-C4C-C3C	-5.75	120.53	130.34
26	w1	201	PEB	CHC-C4C-C3C	-5.75	120.53	130.34
26	NJ	203	PEB	CHC-C1D-ND	-5.75	107.28	113.95
28	M6	1001	CYC	C4D-CHA-C1A	5.75	135.67	128.81
26	H3	203	PEB	CAB-C3B-C4B	5.75	135.18	125.01
26	YI	202	PEB	CHC-C4C-C3C	-5.74	120.54	130.34
28	K2	1001	CYC	OC-C1C-C2C	-5.74	121.61	126.17
28	DF	1001	CYC	OC-C1C-C2C	-5.74	121.61	126.17
28	fH	1001	CYC	CMA-C3A-C4A	5.74	133.91	125.06
26	w1	201	PEB	CHB-C4B-NB	-5.74	120.86	128.83
26	LF	1002	PEB	CHB-C4B-NB	-5.74	120.86	128.83
27	Q8	201	PUB	CHB-C1C-NC	-5.74	120.86	128.83
27	xG	301	PUB	C1D-CHC-C4C	-5.74	100.88	113.37
26	Y2	202	PEB	CHC-C4C-C3C	-5.74	120.55	130.34
27	A2	302	PUB	OD-C4D-C3D	-5.74	121.81	128.04
26	d6	201	PEB	CHB-C4B-NB	-5.74	120.87	128.83
26	hA	201	PEB	OA-C1A-C2A	-5.74	121.61	126.17
26	QE	202	PEB	C1C-CHB-C4B	5.74	135.66	128.81
26	FA	201	PEB	CHB-C4B-NB	-5.73	120.87	128.83
26	fB	203	PEB	CHC-C4C-C3C	-5.73	120.56	130.34
26	mG	201	PEB	CHA-C1B-NB	-5.73	112.94	124.93
26	B8	301	PEB	CHB-C4B-NB	-5.73	120.88	128.83
26	l1	201	PEB	OA-C1A-C2A	-5.73	121.62	126.17
26	b1	501	PEB	CHB-C4B-NB	-5.73	120.88	128.83
27	21	402	PUB	CAD-C3D-C4D	5.73	130.43	121.38
28	IH	1001	CYC	CHD-C4C-NC	5.73	132.01	125.20
26	s4	201	PEB	CMB-C2B-C1B	5.73	133.88	125.06
26	g2	203	PEB	CHB-C4B-NB	-5.73	120.88	128.83
28	D7	1001	CYC	C4D-CHA-C1A	5.73	135.65	128.81
26	aE	201	PEB	CHA-C1B-NB	-5.73	112.96	124.93
27	AF	303	PUB	CBB-CAB-C3B	5.73	122.39	112.62
26	FF	1002	PEB	OA-C1A-C2A	-5.72	121.62	126.17
26	W8	201	PEB	CMB-C2B-C1B	5.72	133.88	125.06
26	nE	201	PEB	C2A-C1A-NA	5.72	113.21	108.27
28	IH	1001	CYC	CMA-C3A-C4A	5.72	133.88	125.06
28	JF	1001	CYC	CMA-C3A-C4A	5.72	133.88	125.06
28	LH	1001	CYC	CMA-C3A-C4A	5.72	133.88	125.06
27	A7	303	PUB	CAD-C3D-C4D	5.72	130.42	121.38
26	QD	201	PEB	CHB-C4B-NB	-5.72	120.89	128.83
26	RI	202	PEB	CHC-C4C-C3C	-5.72	120.58	130.34
26	L9	202	PEB	CHA-C1B-NB	-5.72	112.97	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	YA	202	PEB	CHA-C1B-NB	-5.72	112.98	124.93
28	vH	1001	CYC	CHB-C4A-NA	-5.71	112.98	124.93
26	mE	201	PEB	CHA-C1B-NB	-5.71	112.98	124.93
26	k6	202	PEB	CHB-C4B-NB	-5.71	120.90	128.83
28	LB	1001	CYC	CBD-CAD-C3D	5.71	122.37	112.62
26	O2	201	PEB	C1C-CHB-C4B	5.71	135.63	128.81
26	NE	201	PEB	C2A-C1A-NA	5.71	113.20	108.27
26	aF	202	PEB	CHB-C4B-NB	-5.71	120.91	128.83
26	NF	1002	PEB	CHB-C4B-NB	-5.71	120.91	128.83
26	JJ	202	PEB	CHB-C4B-NB	-5.71	120.91	128.83
26	TG	201	PEB	C2A-C1A-NA	5.71	113.19	108.27
26	w1	202	PEB	CHB-C4B-NB	-5.71	120.91	128.83
26	c7	202	PEB	CMB-C2B-C1B	5.71	133.85	125.06
28	G2	1001	CYC	C4D-CHA-C1A	5.70	135.62	128.81
28	HI	1001	CYC	OB-C4B-C3B	-5.70	121.85	128.04
26	21	401	PEB	CHC-C1D-ND	-5.70	107.32	113.95
26	VJ	202	PEB	CHB-C4B-NB	-5.70	120.92	128.83
26	QE	201	PEB	C1C-CHB-C4B	5.70	135.62	128.81
26	MA	201	PEB	CHC-C1D-ND	-5.70	107.33	113.95
26	V9	202	PEB	CHB-C4B-NB	-5.70	120.92	128.83
26	O7	203	PEB	CHC-C4C-C3C	-5.70	120.61	130.34
26	lG	202	PEB	C1C-CHB-C4B	5.70	135.62	128.81
26	J9	202	PEB	CHB-C4B-NB	-5.70	120.92	128.83
27	N9	201	PUB	C1D-CHC-C4C	-5.70	100.97	113.37
28	KI	1001	CYC	OC-C1C-C2C	-5.70	121.64	126.17
28	NF	1001	CYC	OC-C1C-C2C	-5.69	121.64	126.17
27	xE	305	PUB	CHB-C1C-NC	-5.69	120.93	128.83
26	hA	201	PEB	CHB-C4B-NB	-5.69	120.93	128.83
28	KH	1001	CYC	CAB-C3B-C4B	5.69	130.37	121.38
26	ND	202	PEB	CHC-C1D-ND	-5.69	107.34	113.95
26	A6	304	PEB	CHB-C4B-NB	-5.69	120.93	128.83
26	f8	202	PEB	CHB-C4B-NB	-5.69	120.94	128.83
28	VH	1001	CYC	CMA-C3A-C4A	5.69	133.82	125.06
26	F8	201	PEB	CHB-C4B-NB	-5.69	120.94	128.83
26	mI	202	PEB	C1C-CHB-C4B	5.69	135.60	128.81
26	H4	203	PEB	CHB-C4B-NB	-5.69	120.94	128.83
26	v1	202	PEB	CHA-C4A-NA	-5.69	118.44	125.20
26	B9	201	PEB	CHB-C4B-NB	-5.69	120.94	128.83
26	dI	201	PEB	C1C-CHB-C4B	5.69	135.60	128.81
26	QG	201	PEB	CMB-C2B-C1B	5.69	133.82	125.06
26	D8	201	PEB	OA-C1A-C2A	-5.68	121.65	126.17
26	LE	201	PEB	CHB-C4B-NB	-5.68	120.94	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	nH	1001	CYC	OB-C4B-C3B	-5.68	121.87	128.04
26	eE	203	PEB	C1C-CHB-C4B	5.68	135.60	128.81
26	Q6	201	PEB	CHC-C4C-C3C	-5.68	120.65	130.34
28	C6	1001	CYC	CAB-C3B-C4B	5.68	130.35	121.38
26	oE	203	PEB	CHA-C1B-NB	-5.68	113.05	124.93
26	W3	201	PEB	OA-C1A-C2A	-5.68	121.66	126.17
26	wG	301	PEB	C1C-CHB-C4B	-5.68	122.03	128.81
26	CJ	201	PEB	C3B-C4B-NB	5.68	118.31	110.05
26	O3	201	PEB	CHB-C4B-NB	-5.68	120.95	128.83
26	TA	201	PEB	CHB-C4B-NB	-5.68	120.95	128.83
26	ND	202	PEB	C2A-C1A-NA	5.68	113.17	108.27
26	ZF	203	PEB	CHC-C1D-ND	-5.68	107.36	113.95
26	H8	201	PEB	CHB-C4B-NB	-5.68	120.95	128.83
26	TJ	203	PEB	CHB-C4B-NB	-5.67	120.96	128.83
26	BA	301	PEB	CHB-C4B-NB	-5.67	120.96	128.83
26	RD	202	PEB	CHB-C4B-NB	-5.67	120.96	128.83
28	kH	1001	CYC	CMA-C3A-C4A	5.67	133.80	125.06
28	H2	1001	CYC	OB-C4B-C3B	-5.67	121.89	128.04
26	b7	203	PEB	C1C-CHB-C4B	5.67	135.58	128.81
27	A6	303	PUB	OD-C4D-C3D	-5.67	121.89	128.04
26	OB	203	PEB	CHB-C4B-NB	-5.67	120.97	128.83
26	W7	203	PEB	C1C-CHB-C4B	5.66	135.58	128.81
26	SE	202	PEB	C4B-C3B-C2B	-5.66	100.51	106.78
26	T4	201	PEB	CMC-C3C-C2C	-5.66	114.26	124.94
26	f4	201	PEB	OA-C1A-C2A	-5.66	121.67	126.17
28	C2	1001	CYC	C4D-CHA-C1A	5.66	135.57	128.81
26	S6	203	PEB	CHC-C1D-ND	-5.66	107.37	113.95
26	qE	201	PEB	C1C-CHB-C4B	5.66	135.57	128.81
28	CB	1001	CYC	CAB-C3B-C4B	5.66	130.32	121.38
26	R2	202	PEB	CHC-C4C-C3C	-5.66	120.69	130.34
26	U8	201	PEB	CHC-C4C-C3C	-5.66	120.69	130.34
26	c2	202	PEB	CHC-C4C-C3C	-5.66	120.69	130.34
26	qG	202	PEB	CMB-C2B-C1B	5.66	133.77	125.06
26	hA	201	PEB	CHA-C1B-NB	-5.66	113.10	124.93
26	L7	1002	PEB	CHB-C4B-NB	-5.66	120.98	128.83
28	LF	1001	CYC	CMB-C2B-C1B	5.65	131.22	124.17
26	eE	203	PEB	CMB-C2B-C1B	5.65	133.77	125.06
26	TJ	201	PEB	CHB-C4B-NB	-5.65	120.99	128.83
26	P4	201	PEB	CBC-CAC-C2C	5.65	122.26	112.62
26	b4	501	PEB	CHB-C4B-NB	-5.65	120.99	128.83
26	MD	202	PEB	CHB-C4B-NB	-5.65	120.99	128.83
26	W6	203	PEB	C1C-CHB-C4B	5.65	135.56	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J1	203	PEB	OA-C1A-C2A	-5.65	121.68	126.17
26	FD	202	PEB	C1C-CHB-C4B	5.64	135.55	128.81
28	DF	1003	CYC	OB-C4B-C3B	-5.64	121.92	128.04
28	sH	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
28	HB	1001	CYC	OB-C4B-C3B	-5.64	121.92	128.04
28	nH	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
26	EA	202	PEB	CHA-C1B-NB	-5.64	113.14	124.93
28	JF	1001	CYC	CHB-C4A-NA	-5.64	113.14	124.93
27	AJ	302	PUB	CAD-C3D-C4D	5.64	130.28	121.38
26	OD	201	PEB	CHB-C4B-NB	-5.63	121.01	128.83
26	IJ	201	PEB	CMB-C2B-C1B	5.63	133.74	125.06
26	A5	201	PEB	OA-C1A-C2A	-5.63	121.70	126.17
26	FG	201	PEB	OA-C1A-NA	5.63	131.76	124.94
26	zE	501	PEB	CHB-C4B-NB	-5.63	121.02	128.83
26	QF	202	PEB	CHA-C1B-NB	-5.63	113.16	124.93
26	PD	201	PEB	CMB-C2B-C1B	5.63	133.73	125.06
26	QE	201	PEB	CMB-C2B-C1B	5.63	133.73	125.06
26	H3	203	PEB	CHB-C4B-NB	-5.63	121.02	128.83
26	b7	203	PEB	CHC-C4C-C3C	-5.63	120.74	130.34
28	BB	1001	CYC	C4D-CHA-C1A	5.63	135.53	128.81
28	DF	1003	CYC	C4D-CHA-C1A	5.63	135.53	128.81
26	d6	202	PEB	CHC-C4C-C3C	-5.63	120.74	130.34
26	VF	202	PEB	OA-C1A-C2A	-5.63	121.70	126.17
26	OG	201	PEB	OA-C1A-C2A	-5.63	121.70	126.17
26	D7	1002	PEB	CHB-C4B-NB	-5.62	121.03	128.83
26	mA	202	PEB	OA-C1A-C2A	-5.62	121.71	126.17
26	fF	201	PEB	CHB-C4B-NB	-5.62	121.03	128.83
28	EI	1001	CYC	CAB-C3B-C4B	5.62	130.25	121.38
26	D9	202	PEB	CHC-C1D-ND	-5.62	107.43	113.95
26	IG	203	PEB	CHB-C4B-NB	-5.61	121.04	128.83
26	DE	203	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	LJ	202	PEB	CHA-C1B-NB	-5.61	113.19	124.93
26	PF	201	PEB	CHC-C1D-ND	-5.61	107.43	113.95
26	DA	201	PEB	OA-C1A-C2A	-5.61	121.71	126.17
26	QJ	201	PEB	OA-C1A-C2A	-5.61	121.71	126.17
26	JA	201	PEB	C1C-CHB-C4B	-5.61	122.11	128.81
26	g4	202	PEB	CHB-C4B-NB	-5.60	121.05	128.83
26	JA	201	PEB	CHB-C4B-NB	-5.60	121.06	128.83
26	JE	201	PEB	CHB-C4B-NB	-5.60	121.06	128.83
28	TH	1001	CYC	OB-C4B-C3B	-5.60	121.96	128.04
26	ID	201	PEB	CHB-C4B-NB	-5.60	121.06	128.83
26	M8	201	PEB	C1C-CHB-C4B	5.60	135.50	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	i8	202	PEB	CHC-C1D-ND	-5.60	107.45	113.95
26	WG	201	PEB	CHB-C4B-NB	-5.60	121.06	128.83
28	tH	1001	CYC	CMA-C3A-C4A	5.60	133.68	125.06
26	jF	201	PEB	C1C-CHB-C4B	5.60	135.49	128.81
27	xE	301	PUB	CHB-C1C-NC	-5.60	121.06	128.83
26	J5	201	PEB	CHA-C1B-C2B	5.60	139.29	124.90
26	lG	201	PEB	CHA-C4A-NA	5.60	131.86	125.20
26	Y3	301	PEB	C1C-CHB-C4B	-5.59	122.13	128.81
26	Q8	203	PEB	C1C-CHB-C4B	-5.59	122.13	128.81
26	W8	203	PEB	CHC-C4C-C3C	-5.59	120.80	130.34
26	IA	203	PEB	CHB-C4B-NB	-5.59	121.07	128.83
26	eG	202	PEB	CMB-C2B-C1B	5.59	133.67	125.06
26	Y6	201	PEB	CHC-C1D-ND	-5.59	107.46	113.95
26	WJ	201	PEB	CHC-C1D-ND	-5.59	107.46	113.95
28	E2	1001	CYC	CAB-C3B-C4B	5.59	130.20	121.38
26	DG	202	PEB	OA-C1A-C2A	-5.59	121.73	126.17
26	aG	203	PEB	CMB-C2B-C1B	5.58	133.66	125.06
26	YB	202	PEB	CHB-C4B-NB	-5.58	121.08	128.83
27	yG	303	PUB	CHA-C4A-NA	-5.58	107.46	113.95
26	pG	202	PEB	OA-C1A-C2A	-5.58	121.73	126.17
26	h1	201	PEB	OA-C1A-C2A	-5.58	121.74	126.17
26	UD	201	PEB	CMB-C2B-C1B	5.58	133.65	125.06
26	N8	201	PEB	OA-C1A-C2A	-5.58	121.74	126.17
28	E7	1001	CYC	OB-C4B-C3B	-5.58	121.99	128.04
26	N3	202	PEB	C2A-C1A-NA	5.58	113.08	108.27
28	FF	1001	CYC	CMB-C2B-C1B	5.58	131.13	124.17
26	I8	201	PEB	CHC-C4C-C3C	-5.58	120.83	130.34
28	pH	1001	CYC	OB-C4B-C3B	-5.57	121.99	128.04
28	YH	1003	CYC	CMA-C3A-C4A	5.57	133.65	125.06
26	aG	202	PEB	CMB-C2B-C1B	5.57	133.65	125.06
26	V2	202	PEB	CHB-C4B-NB	-5.57	121.10	128.83
27	N9	201	PUB	OD-C4D-C3D	-5.57	121.99	128.04
26	h8	203	PEB	CHC-C1D-ND	-5.57	107.48	113.95
26	f7	201	PEB	CHB-C4B-NB	-5.57	121.10	128.83
26	T8	201	PEB	CHB-C4B-NB	-5.57	121.10	128.83
26	LG	201	PEB	CBC-CAC-C2C	-5.57	103.12	112.62
28	G7	1001	CYC	OB-C4B-C3B	-5.57	122.00	128.04
26	B4	202	PEB	CHC-C1D-ND	-5.56	107.49	113.95
26	m4	202	PEB	CHB-C4B-NB	-5.56	121.11	128.83
26	UA	201	PEB	CHC-C1D-ND	-5.56	107.49	113.95
26	W2	201	PEB	CMB-C2B-C1B	5.56	133.63	125.06
28	H6	1001	CYC	OB-C4B-C3B	-5.56	122.01	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IA	201	PEB	CHC-C4C-C3C	-5.56	120.86	130.34
26	G5	203	PEB	OA-C1A-C2A	-5.56	121.75	126.17
26	YG	203	PEB	CHB-C4B-NB	-5.56	121.12	128.83
26	CC	201	PEB	CHB-C4B-NB	-5.56	121.12	128.83
26	LC	202	PEB	CHB-C4B-NB	-5.55	121.12	128.83
26	G3	201	PEB	CHC-C4C-C3C	-5.55	120.87	130.34
26	h4	202	PEB	CHC-C1D-ND	5.55	120.39	113.95
26	uG	201	PEB	CHC-C4C-C3C	-5.55	120.87	130.34
26	l7	202	PEB	CHB-C4B-NB	-5.55	121.13	128.83
26	QA	203	PEB	CHB-C4B-NB	-5.55	121.13	128.83
28	UH	1001	CYC	OB-C4B-C3B	-5.55	122.02	128.04
26	TB	202	PEB	CHB-C4B-NB	-5.55	121.13	128.83
26	IG	201	PEB	CHC-C1D-ND	-5.55	107.51	113.95
26	O2	201	PEB	CMB-C2B-C1B	5.54	133.60	125.06
26	21	401	PEB	CHB-C4B-NB	-5.54	121.14	128.83
26	dB	202	PEB	CHC-C4C-C3C	-5.54	120.88	130.34
28	F6	1001	CYC	CAB-C3B-C4B	5.54	130.13	121.38
26	OB	201	PEB	CMB-C2B-C1B	5.54	133.60	125.06
26	KJ	202	PEB	CHB-C4B-NB	-5.54	121.14	128.83
26	RD	201	PEB	CHC-C1D-ND	-5.54	107.51	113.95
26	WI	201	PEB	CHB-C4B-C3B	-5.54	112.52	125.32
26	m1	202	PEB	CHB-C4B-NB	-5.54	121.14	128.83
26	NB	1002	PEB	OA-C1A-C2A	-5.54	121.77	126.17
26	OI	201	PEB	C1C-CHB-C4B	5.54	135.43	128.81
26	X1	202	PEB	CHC-C1D-ND	-5.54	107.52	113.95
26	BG	201	PEB	CHC-C4C-C3C	-5.54	120.90	130.34
26	wG	303	PEB	CHA-C1B-NB	-5.53	113.36	124.93
28	iH	1001	CYC	CMA-C3A-C4A	5.53	133.58	125.06
26	ND	203	PEB	C1C-CHB-C4B	5.53	135.42	128.81
26	N1	203	PEB	OA-C1A-C2A	-5.53	121.78	126.17
26	ME	203	PEB	C1C-CHB-C4B	5.53	135.41	128.81
28	C2	1001	CYC	OC-C1C-C2C	-5.53	121.78	126.17
26	d2	201	PEB	C1C-CHB-C4B	5.53	135.41	128.81
28	YH	1002	CYC	CMA-C3A-C4A	5.53	133.58	125.06
26	DJ	203	PEB	CHB-C4B-NB	-5.52	121.17	128.83
26	eF	202	PEB	CHB-C4B-NB	-5.52	121.17	128.83
26	l6	201	PEB	C1C-CHB-C4B	5.52	135.41	128.81
26	L5	202	PEB	CHB-C4B-NB	-5.52	121.17	128.83
26	DJ	202	PEB	CHC-C4C-C3C	-5.52	120.93	130.34
26	J2	1002	PEB	CHB-C4B-NB	-5.52	121.17	128.83
28	CI	1001	CYC	OC-C1C-C2C	-5.52	121.79	126.17
27	wG	304	PUB	C1D-CHC-C4C	-5.52	101.37	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	bF	201	PEB	CHC-C4C-C3C	-5.52	120.93	130.34
26	ZB	202	PEB	CMB-C2B-C1B	5.52	133.56	125.06
27	YD	302	PUB	OD-C4D-C3D	-5.51	122.06	128.04
26	a1	202	PEB	CHB-C4B-NB	-5.51	121.18	128.83
26	l6	201	PEB	CHC-C4C-C3C	-5.51	120.93	130.34
26	bB	202	PEB	CHC-C1D-ND	-5.51	107.55	113.95
26	WA	201	PEB	CMB-C2B-C1B	5.51	133.55	125.06
26	D9	203	PEB	CHB-C4B-NB	-5.51	121.18	128.83
26	X4	202	PEB	CHC-C1D-ND	-5.51	107.55	113.95
26	mA	201	PEB	CBC-CAC-C2C	-5.51	103.22	112.62
27	BA	302	PUB	OD-C4D-C3D	-5.51	122.06	128.04
26	SJ	202	PEB	C1C-CHB-C4B	5.51	135.39	128.81
26	bE	201	PEB	C2A-C1A-NA	5.51	113.02	108.27
26	HJ	201	PEB	C1C-CHB-C4B	5.51	135.39	128.81
27	24	403	PUB	CHA-C1B-C2B	-5.51	120.94	130.34
26	T3	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
26	BD	202	PEB	CHA-C4A-NA	5.50	131.75	125.20
26	L2	1002	PEB	OA-C1A-C2A	-5.50	121.80	126.17
26	VF	203	PEB	OA-C1A-C2A	-5.50	121.80	126.17
26	V8	202	PEB	C4B-C3B-C2B	-5.50	100.70	106.78
26	Y2	202	PEB	C1C-CHB-C4B	5.50	135.38	128.81
28	dH	1001	CYC	CHD-C4C-NC	5.50	131.74	125.20
26	pE	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
26	UA	202	PEB	CHA-C1B-NB	-5.50	113.43	124.93
28	LB	1001	CYC	OC-C1C-C2C	-5.50	121.80	126.17
28	WH	1001	CYC	CHB-C4A-NA	-5.50	113.43	124.93
27	21	403	PUB	OD-C4D-C3D	-5.49	122.08	128.04
28	C7	1001	CYC	OB-C4B-C3B	-5.49	122.08	128.04
26	N9	203	PEB	CHC-C1D-ND	-5.49	107.57	113.95
26	H9	201	PEB	C1C-CHB-C4B	5.49	135.37	128.81
26	S7	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
26	A2	304	PEB	CHB-C4B-NB	-5.49	121.21	128.83
26	MA	201	PEB	C1C-CHB-C4B	5.49	135.37	128.81
26	VA	202	PEB	C4B-C3B-C2B	-5.49	100.71	106.78
26	l8	201	PEB	CHC-C4C-C3C	-5.49	120.97	130.34
26	iA	201	PEB	OA-C1A-C2A	-5.49	121.81	126.17
26	JC	201	PEB	CHA-C1B-NB	-5.49	113.45	124.93
28	yH	1001	CYC	CHB-C4A-NA	-5.49	113.45	124.93
26	S4	202	PEB	CHB-C4B-NB	-5.49	121.22	128.83
26	g1	201	PEB	CHC-C1D-ND	-5.48	107.58	113.95
28	HF	1001	CYC	OC-C1C-C2C	-5.48	121.81	126.17
26	UA	201	PEB	CHC-C4C-C3C	-5.48	120.98	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q6	201	PEB	C1C-CHB-C4B	5.48	135.36	128.81
26	J5	201	PEB	CHA-C1B-NB	-5.48	113.46	124.93
27	A4	203	PUB	OD-C4D-C3D	-5.48	122.09	128.04
26	CA	203	PEB	C1C-CHB-C4B	5.48	135.36	128.81
28	NI	1001	CYC	C4D-CHA-C1A	5.48	135.36	128.81
26	U8	203	PEB	CHB-C4B-NB	-5.48	121.22	128.83
26	cG	203	PEB	CHB-C4B-NB	-5.48	121.22	128.83
27	NJ	201	PUB	CHB-C1C-NC	-5.48	121.23	128.83
26	LJ	202	PEB	CHC-C4C-C3C	-5.48	120.99	130.34
26	IE	203	PEB	CHB-C4B-NB	-5.48	121.23	128.83
26	T1	201	PEB	CMC-C3C-C2C	-5.48	114.61	124.94
26	QI	201	PEB	CMB-C2B-C1B	5.48	133.50	125.06
26	k4	203	PEB	CHC-C4C-C3C	-5.48	121.00	130.34
26	hA	203	PEB	CHC-C1D-ND	-5.48	107.59	113.95
26	e2	202	PEB	C1C-CHB-C4B	5.48	135.35	128.81
26	k2	202	PEB	CHB-C4B-NB	-5.47	121.24	128.83
28	CI	1001	CYC	C4D-CHA-C1A	5.47	135.34	128.81
28	uH	1001	CYC	CMA-C3A-C4A	5.47	133.49	125.06
26	f4	202	PEB	OA-C1A-C2A	-5.47	121.83	126.17
26	Q8	203	PEB	CHC-C1D-ND	-5.47	107.60	113.95
28	FB	1001	CYC	OB-C4B-C3B	-5.47	122.11	128.04
26	jF	203	PEB	C1C-CHB-C4B	5.46	135.34	128.81
27	A1	203	PUB	C4B-CHB-C1C	-5.46	122.28	128.81
26	IE	201	PEB	CMB-C2B-C1B	5.46	133.47	125.06
28	RH	1001	CYC	CMA-C3A-C4A	5.46	133.47	125.06
28	sH	1001	CYC	CHD-C4C-NC	5.46	131.70	125.20
28	cH	1001	CYC	CHD-C4C-NC	5.46	131.70	125.20
26	C5	202	PEB	CHB-C4B-NB	-5.46	121.25	128.83
26	MJ	202	PEB	CHC-C1D-ND	-5.46	107.61	113.95
26	e6	202	PEB	CHC-C4C-C3C	-5.46	121.03	130.34
26	cI	202	PEB	CHC-C4C-C3C	-5.45	121.03	130.34
26	AE	201	PEB	CMB-C2B-C1B	5.45	133.46	125.06
26	c2	203	PEB	CHB-C4B-NB	-5.45	121.26	128.83
28	jH	1001	CYC	CMA-C3A-C4A	5.45	133.46	125.06
26	C3	201	PEB	CHC-C4C-C3C	-5.45	121.04	130.34
26	YD	304	PEB	CHA-C1B-NB	-5.45	113.53	124.93
26	IG	201	PEB	CHB-C4B-C3B	-5.45	112.73	125.32
26	YI	202	PEB	C1C-CHB-C4B	5.45	135.32	128.81
26	ED	201	PEB	CHC-C4C-C3C	-5.45	121.04	130.34
26	XD	202	PEB	C1C-CHB-C4B	5.45	135.32	128.81
28	E6	1001	CYC	C4D-CHA-C1A	5.45	135.32	128.81
26	bB	202	PEB	C1C-CHB-C4B	5.45	135.32	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T6	202	PEB	CHB-C4B-NB	-5.45	121.27	128.83
28	hH	1001	CYC	CMA-C3A-C4A	5.45	133.45	125.06
28	dH	1001	CYC	OB-C4B-C3B	-5.44	122.13	128.04
26	fA	203	PEB	CHC-C4C-C3C	-5.44	121.05	130.34
26	WB	203	PEB	CHC-C4C-C3C	-5.44	121.05	130.34
26	E3	201	PEB	CHC-C4C-C3C	-5.44	121.05	130.34
26	R6	202	PEB	CHB-C4B-NB	-5.44	121.28	128.83
26	aE	201	PEB	C1C-CHB-C4B	5.44	135.31	128.81
27	B8	302	PUB	CHB-C1C-NC	-5.44	121.28	128.83
26	DG	203	PEB	C1C-CHB-C4B	5.44	135.31	128.81
26	O7	201	PEB	CHC-C4C-C3C	-5.44	121.07	130.34
26	W4	202	PEB	OA-C1A-C2A	-5.44	121.85	126.17
28	EF	1001	CYC	CHB-C4A-NA	-5.44	113.56	124.93
27	AB	302	PUB	CHB-C1C-NC	-5.44	121.29	128.83
26	h2	201	PEB	C1C-CHB-C4B	5.43	135.30	128.81
26	HE	201	PEB	OD-C4D-ND	-5.43	117.88	125.93
26	dF	201	PEB	CHC-C4C-C3C	-5.43	121.07	130.34
26	LG	202	PEB	CBC-CAC-C2C	5.43	121.89	112.62
28	fH	1001	CYC	CHD-C4C-NC	5.43	131.66	125.20
28	G2	1001	CYC	CAB-C3B-C4B	5.43	129.96	121.38
26	I9	202	PEB	C1C-CHB-C4B	5.43	135.29	128.81
26	GD	201	PEB	CHC-C4C-C3C	-5.43	121.08	130.34
26	qG	202	PEB	CHB-C4B-C3B	5.43	137.86	125.32
28	VH	1001	CYC	CMC-C2C-C1C	5.43	124.10	112.40
26	RI	201	PEB	OA-C1A-C2A	-5.43	121.86	126.17
26	W6	203	PEB	CHC-C4C-C3C	-5.42	121.08	130.34
26	YD	301	PEB	OA-C1A-C2A	-5.42	121.86	126.17
26	gG	203	PEB	CHB-C4B-NB	-5.42	121.30	128.83
26	Q2	201	PEB	CMB-C2B-C1B	5.42	133.41	125.06
26	aA	201	PEB	C1C-CHB-C4B	-5.42	122.33	128.81
26	hE	201	PEB	CHA-C4A-NA	5.42	131.65	125.20
28	SH	1001	CYC	CMA-C3A-C4A	5.42	133.41	125.06
26	VB	202	PEB	CHB-C4B-NB	-5.42	121.31	128.83
28	B6	1001	CYC	C4D-CHA-C1A	5.42	135.28	128.81
26	Z7	203	PEB	CMB-C2B-C1B	5.42	133.41	125.06
28	YH	1004	CYC	CMA-C3A-C4A	5.42	133.41	125.06
26	N1	201	PEB	CHA-C1B-NB	-5.42	113.60	124.93
28	vH	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
26	U3	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06
26	R3	202	PEB	C2A-C1A-NA	5.41	112.94	108.27
26	D3	202	PEB	CHC-C4C-C3C	-5.41	121.11	130.34
27	NJ	201	PUB	OD-C4D-C3D	-5.41	122.17	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z7	203	PEB	CHA-C1B-NB	-5.41	113.61	124.93
26	L4	202	PEB	C1C-CHB-C4B	5.41	135.27	128.81
26	AF	301	PEB	CHB-C4B-NB	-5.41	121.33	128.83
26	ZF	202	PEB	CHB-C4B-NB	-5.41	121.33	128.83
26	VA	202	PEB	OA-C1A-C2A	-5.41	121.87	126.17
26	c1	201	PEB	CHC-C1D-ND	-5.41	107.67	113.95
26	D9	202	PEB	CHC-C4C-C3C	-5.40	121.12	130.34
26	N6	201	PEB	OA-C1A-C2A	-5.40	121.88	126.17
26	LJ	202	PEB	CHB-C4B-NB	-5.40	121.33	128.83
26	ZA	201	PEB	CHC-C1D-ND	5.40	120.22	113.95
26	O6	203	PEB	CHB-C4B-NB	-5.40	121.33	128.83
26	d7	203	PEB	CHA-C1B-NB	-5.40	113.63	124.93
26	J1	202	PEB	CHC-C1D-ND	-5.40	107.67	113.95
26	Y3	301	PEB	CHB-C4B-NB	-5.40	121.33	128.83
26	R4	203	PEB	CHB-C4B-NB	-5.40	121.33	128.83
28	qH	1002	CYC	OB-C4B-C3B	-5.40	122.18	128.04
26	U8	202	PEB	CHC-C1D-ND	-5.40	107.68	113.95
26	QA	202	PEB	CHC-C4C-C3C	-5.40	121.13	130.34
26	VI	202	PEB	CHC-C4C-C3C	-5.40	121.13	130.34
28	I7	1001	CYC	OB-C4B-C3B	-5.40	122.18	128.04
26	bF	203	PEB	OA-C1A-C2A	-5.40	121.88	126.17
28	M6	1001	CYC	OC-C1C-C2C	-5.40	121.88	126.17
26	kI	202	PEB	CHB-C4B-NB	-5.40	121.34	128.83
26	c1	202	PEB	C1C-CHB-C4B	-5.40	122.36	128.81
26	R1	203	PEB	CHB-C4B-NB	-5.39	121.34	128.83
28	wH	1001	CYC	OB-C4B-C3B	-5.39	122.19	128.04
26	PA	202	PEB	CHC-C1D-ND	-5.39	107.69	113.95
28	FB	1001	CYC	CAB-C3B-C4B	5.39	129.89	121.38
26	u4	202	PEB	CHC-C1D-ND	-5.39	107.69	113.95
26	C8	203	PEB	C1C-CHB-C4B	5.39	135.25	128.81
26	NG	201	PEB	C2A-C1A-NA	5.39	112.92	108.27
26	L3	201	PEB	CMB-C2B-C1B	5.39	133.36	125.06
26	f7	203	PEB	CHC-C4C-C3C	-5.39	121.15	130.34
26	cG	203	PEB	C1C-CHB-C4B	5.39	135.24	128.81
26	Z8	201	PEB	CHB-C4B-NB	-5.39	121.36	128.83
26	B3	202	PEB	CHA-C4A-NA	5.39	131.61	125.20
28	MI	1001	CYC	CAB-C3B-C4B	5.39	129.88	121.38
26	GG	201	PEB	C1C-CHB-C4B	5.39	135.24	128.81
26	eI	202	PEB	C1C-CHB-C4B	5.38	135.24	128.81
26	W6	201	PEB	CHA-C1B-NB	-5.38	113.67	124.93
26	TJ	202	PEB	CHB-C4B-NB	-5.38	121.36	128.83
26	Z6	202	PEB	CMB-C2B-C1B	5.38	133.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	GH	1001	CYC	CMA-C3A-C4A	5.38	133.35	125.06
28	MI	1001	CYC	C4D-CHA-C1A	5.38	135.24	128.81
26	I9	201	PEB	CMB-C2B-C1B	5.38	133.35	125.06
28	EB	1001	CYC	OC-C1C-C2C	-5.38	121.89	126.17
26	a2	201	PEB	CHC-C1D-ND	-5.38	107.70	113.95
26	cE	201	PEB	CBC-CAC-C2C	5.38	121.80	112.62
28	1H	1000	CYC	CHD-C4C-NC	5.38	131.60	125.20
26	NA	201	PEB	OA-C1A-C2A	-5.38	121.90	126.17
26	d7	201	PEB	CHC-C4C-C3C	-5.38	121.17	130.34
26	LI	1002	PEB	OA-C1A-C2A	-5.38	121.90	126.17
26	B4	202	PEB	CHB-C4B-NB	-5.38	121.37	128.83
26	jA	201	PEB	CHB-C4B-NB	-5.38	121.37	128.83
26	B5	202	PEB	CHB-C4B-NB	-5.38	121.37	128.83
26	P3	201	PEB	CMB-C2B-C1B	5.37	133.34	125.06
28	EF	1001	CYC	CMA-C3A-C4A	5.37	133.34	125.06
26	Z1	202	PEB	C1C-CHB-C4B	5.37	135.23	128.81
26	RB	202	PEB	CHB-C4B-NB	-5.37	121.38	128.83
26	bG	202	PEB	OA-C1A-C2A	-5.37	121.90	126.17
28	I2	1001	CYC	OC-C1C-C2C	-5.37	121.90	126.17
26	YF	201	PEB	C1C-CHB-C4B	5.37	135.22	128.81
28	LH	1001	CYC	CHD-C4C-NC	5.37	131.59	125.20
28	L7	1001	CYC	OC-C1C-C2C	-5.37	121.90	126.17
26	s4	202	PEB	CHC-C4C-C3C	-5.37	121.18	130.34
28	HF	1001	CYC	C4D-CHA-C1A	5.37	135.22	128.81
26	U7	203	PEB	C1C-CHB-C4B	-5.37	122.40	128.81
26	h4	201	PEB	OA-C1A-C2A	-5.37	121.91	126.17
28	KB	202	CYC	CAB-C3B-C4B	5.37	129.86	121.38
26	qG	201	PEB	CHC-C1D-ND	-5.37	107.72	113.95
28	YH	1002	CYC	OB-C4B-C3B	-5.37	122.22	128.04
26	q1	203	PEB	CHB-C4B-NB	-5.36	121.39	128.83
26	R2	201	PEB	OA-C1A-C2A	-5.36	121.91	126.17
26	IG	201	PEB	C3B-C4B-NB	5.36	117.85	110.05
26	R7	202	PEB	OA-C1A-C2A	-5.36	121.91	126.17
26	U8	202	PEB	CHA-C1B-NB	-5.36	113.72	124.93
26	ZA	201	PEB	CHB-C4B-NB	-5.36	121.39	128.83
26	LE	201	PEB	OD-C4D-ND	-5.36	117.99	125.93
28	1H	1000	CYC	CMA-C3A-C4A	5.36	133.32	125.06
26	J5	202	PEB	CHB-C4B-NB	-5.36	121.39	128.83
26	Q7	203	PEB	CHB-C4B-NB	-5.36	121.39	128.83
26	cG	202	PEB	CHB-C4B-NB	-5.36	121.39	128.83
26	o1	501	PEB	CHC-C1D-ND	-5.36	107.73	113.95
26	LF	1002	PEB	OA-C1A-C2A	-5.36	121.91	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V6	202	PEB	CHB-C4B-NB	-5.36	121.40	128.83
26	eG	201	PEB	CHC-C4C-C3C	-5.36	121.20	130.34
26	O8	203	PEB	OA-C1A-C2A	-5.36	121.92	126.17
26	h8	201	PEB	OA-C1A-C2A	-5.36	121.92	126.17
28	rH	1001	CYC	CMA-C3A-C4A	5.35	133.31	125.06
26	H3	203	PEB	C1C-CHB-C4B	5.35	135.21	128.81
26	P1	201	PEB	OA-C1A-C2A	-5.35	121.92	126.17
26	OG	201	PEB	CHB-C4B-NB	-5.35	121.40	128.83
26	T9	201	PEB	C1C-CHB-C4B	5.35	135.20	128.81
26	uG	201	PEB	C1C-CHB-C4B	5.35	135.20	128.81
26	V9	203	PEB	CHC-C4C-C3C	-5.35	121.21	130.34
26	W8	203	PEB	OA-C1A-C2A	-5.35	121.92	126.17
27	A6	302	PUB	OD-C4D-C3D	-5.35	122.23	128.04
26	aI	201	PEB	CHC-C1D-ND	-5.35	107.73	113.95
26	Y2	201	PEB	OA-C1A-C2A	-5.35	121.92	126.17
26	P4	201	PEB	OA-C1A-C2A	-5.35	121.92	126.17
26	k7	202	PEB	OA-C1A-C2A	-5.35	121.92	126.17
27	AF	303	PUB	CHB-C1C-NC	-5.35	121.41	128.83
28	WH	1001	CYC	OB-C4B-C3B	-5.35	122.24	128.04
28	kH	1001	CYC	OB-C4B-C3B	-5.35	122.24	128.04
26	A4	201	PEB	CAB-C3B-C2B	5.34	137.83	127.88
28	NH	1001	CYC	OB-C4B-C3B	-5.34	122.24	128.04
26	CJ	201	PEB	CMB-C2B-C1B	5.34	133.29	125.06
26	qG	202	PEB	CAB-C3B-C4B	5.34	134.46	125.01
28	K6	202	CYC	CAB-C3B-C4B	5.34	129.82	121.38
26	P2	201	PEB	OA-C1A-C2A	-5.34	121.93	126.17
26	PA	201	PEB	OA-C1A-C2A	-5.34	121.93	126.17
26	SI	201	PEB	CHB-C4B-C3B	-5.34	112.98	125.32
26	g1	201	PEB	OA-C1A-C2A	-5.34	121.93	126.17
26	U2	201	PEB	C3B-C4B-NB	5.34	117.81	110.05
26	T2	202	PEB	CHC-C4C-C3C	-5.34	121.23	130.34
28	JH	1001	CYC	CMA-C3A-C4A	5.34	133.28	125.06
26	N4	201	PEB	CHA-C1B-NB	-5.34	113.77	124.93
26	AJ	301	PEB	CHB-C4B-NB	-5.34	121.42	128.83
26	WB	201	PEB	CHA-C1B-NB	-5.33	113.77	124.93
26	nG	202	PEB	C1C-CHB-C4B	5.33	135.18	128.81
26	Q8	202	PEB	CHC-C4C-C3C	-5.33	121.24	130.34
26	LE	202	PEB	CBC-CAC-C2C	5.33	121.72	112.62
26	L8	201	PEB	C2A-C1A-NA	5.33	112.87	108.27
26	j7	203	PEB	CHB-C4B-NB	-5.33	121.43	128.83
26	WA	201	PEB	CHA-C1B-NB	-5.33	113.78	124.93
26	VA	202	PEB	C1C-CHB-C4B	-5.33	122.44	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FA	201	PEB	C3D-C4D-ND	5.33	117.71	107.26
26	TD	201	PEB	CHB-C4B-NB	-5.33	121.44	128.83
26	ME	203	PEB	CHA-C1B-NB	-5.33	113.79	124.93
26	T3	202	PEB	C3B-C4B-NB	5.33	117.80	110.05
28	M2	1001	CYC	C4D-CHA-C1A	5.32	135.17	128.81
28	PH	1001	CYC	CMA-C3A-C4A	5.32	133.26	125.06
26	h4	202	PEB	CHC-C4C-C3C	-5.32	121.26	130.34
26	UI	201	PEB	C3B-C4B-NB	5.32	117.79	110.05
26	Z8	202	PEB	CMB-C2B-C1B	5.32	133.26	125.06
26	LC	203	PEB	OA-C1A-C2A	-5.32	121.94	126.17
28	IH	1001	CYC	CMA-C3A-C4A	5.32	133.26	125.06
28	L6	1001	CYC	CBD-CAD-C3D	5.32	121.70	112.62
26	iG	203	PEB	CHB-C4B-NB	-5.32	121.45	128.83
27	AB	302	PUB	OD-C4D-C3D	-5.32	122.27	128.04
26	j2	201	PEB	C1C-CHB-C4B	5.32	135.16	128.81
26	nG	201	PEB	C1C-CHB-C4B	5.32	135.16	128.81
26	l4	202	PEB	C1C-CHB-C4B	5.32	135.16	128.81
28	YH	1004	CYC	OB-C4B-C3B	-5.32	122.27	128.04
26	ZI	201	PEB	C3B-C4B-NB	5.32	117.78	110.05
26	PI	201	PEB	OA-C1A-C2A	-5.32	121.95	126.17
26	W8	201	PEB	CHA-C1B-NB	-5.32	113.81	124.93
26	LE	202	PEB	CMB-C2B-C1B	5.32	133.25	125.06
28	F6	1001	CYC	OB-C4B-C3B	-5.31	122.27	128.04
26	e8	201	PEB	CHB-C4B-NB	-5.31	121.46	128.83
26	OI	201	PEB	CMB-C2B-C1B	5.31	133.25	125.06
28	M2	1001	CYC	CAB-C3B-C4B	5.31	129.77	121.38
26	S7	203	PEB	OA-C1A-C2A	-5.31	121.95	126.17
26	V4	202	PEB	CHB-C4B-NB	-5.31	121.46	128.83
26	Y1	201	PEB	OA-C1A-C2A	-5.31	121.95	126.17
26	QG	203	PEB	OA-C1A-C2A	-5.31	121.95	126.17
26	Q7	202	PEB	CHC-C4C-C3C	-5.31	121.28	130.34
26	Z2	201	PEB	C3B-C4B-NB	5.31	117.77	110.05
26	e2	203	PEB	CHB-C4B-NB	-5.31	121.46	128.83
26	YI	201	PEB	OA-C1A-C2A	-5.31	121.95	126.17
26	q1	202	PEB	OA-C1A-C2A	-5.31	121.95	126.17
28	N2	1001	CYC	OC-C1C-C2C	-5.31	121.95	126.17
26	hF	202	PEB	CHB-C4B-NB	-5.31	121.47	128.83
26	LJ	201	PEB	CHB-C4B-NB	-5.31	121.47	128.83
26	SA	202	PEB	CHC-C4C-C3C	-5.31	121.29	130.34
26	F8	201	PEB	C3D-C4D-ND	5.31	117.67	107.26
28	yH	1001	CYC	OB-C4B-C3B	-5.30	122.28	128.04
26	n4	201	PEB	OA-C1A-C2A	-5.30	121.96	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X3	203	PEB	CHC-C1D-ND	-5.30	107.79	113.95
27	KD	203	PUB	OD-C4D-C3D	-5.30	122.28	128.04
28	II	1001	CYC	OC-C1C-C2C	-5.30	121.96	126.17
26	kG	201	PEB	CMB-C2B-C1B	5.30	133.23	125.06
27	A7	303	PUB	CHB-C1C-NC	-5.30	121.47	128.83
28	DF	1001	CYC	CAB-C3B-C4B	5.30	129.75	121.38
26	gA	201	PEB	C1C-CHB-C4B	-5.30	122.48	128.81
26	DF	1002	PEB	CHB-C4B-NB	-5.30	121.48	128.83
27	Y3	302	PUB	OD-C4D-C3D	-5.30	122.29	128.04
26	UF	201	PEB	CHC-C1D-ND	-5.30	107.80	113.95
28	qH	1001	CYC	OB-C4B-C3B	-5.30	122.29	128.04
26	AB	304	PEB	CHB-C4B-NB	-5.30	121.48	128.83
28	IH	1001	CYC	OB-C4B-C3B	-5.29	122.29	128.04
28	E7	1001	CYC	CMA-C3A-C4A	5.29	133.22	125.06
26	N8	201	PEB	CBC-CAC-C2C	-5.29	103.59	112.62
28	hH	1001	CYC	CMB-C2B-C1B	5.29	130.78	124.17
26	WA	203	PEB	OA-C1A-C2A	-5.29	121.97	126.17
28	LH	1001	CYC	OB-C4B-C3B	-5.29	122.30	128.04
26	JC	201	PEB	CHA-C1B-C2B	5.29	138.50	124.90
28	YH	1002	CYC	CMB-C2B-C1B	5.29	130.77	124.17
28	MB	1001	CYC	OC-C1C-C2C	-5.29	121.97	126.17
26	LG	201	PEB	CHB-C4B-NB	-5.29	121.49	128.83
26	e8	201	PEB	OA-C1A-C2A	-5.29	121.97	126.17
26	R3	203	PEB	CAB-CBB-CGB	-5.29	102.22	113.60
26	GA	201	PEB	CHB-C4B-NB	-5.29	121.49	128.83
27	K3	203	PUB	OD-C4D-C3D	-5.29	122.30	128.04
28	YH	1004	CYC	CHD-C4C-NC	5.29	131.49	125.20
26	M4	403	PEB	CHB-C4B-NB	-5.29	121.50	128.83
28	mH	1001	CYC	CMA-C3A-C4A	5.29	133.20	125.06
26	gA	201	PEB	CHB-C4B-NB	-5.28	121.50	128.83
26	g4	203	PEB	C1C-CHB-C4B	5.28	135.12	128.81
26	I5	203	PEB	CHB-C4B-NB	-5.28	121.50	128.83
28	J7	1003	CYC	OB-C4B-C3B	-5.28	122.31	128.04
28	fH	1001	CYC	OB-C4B-C3B	-5.28	122.31	128.04
27	A9	302	PUB	CHA-C1B-C2B	-5.28	121.33	130.34
27	BA	302	PUB	CHB-C1C-NC	-5.28	121.50	128.83
27	A4	203	PUB	CHC-C1D-ND	-5.28	107.04	113.72
28	SH	1001	CYC	CHD-C4C-NC	5.28	131.48	125.20
26	R2	203	PEB	CHB-C4B-NB	-5.28	121.51	128.83
26	Z6	203	PEB	CMB-C2B-C1B	5.28	133.19	125.06
27	21	402	PUB	C1D-CHC-C4C	-5.27	101.89	113.37
26	rG	202	PEB	C1C-CHB-C4B	5.27	135.11	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	eA	201	PEB	CHB-C4B-NB	-5.27	121.51	128.83
26	ED	201	PEB	CHA-C1B-NB	-5.27	113.90	124.93
28	eH	1001	CYC	CHD-C4C-NC	5.27	131.47	125.20
26	k2	202	PEB	CHC-C4C-C3C	-5.27	121.34	130.34
26	HA	201	PEB	CHB-C4B-NB	-5.27	121.52	128.83
26	lA	201	PEB	OA-C1A-C2A	-5.27	121.98	126.17
28	gH	1001	CYC	CMA-C3A-C4A	5.27	133.18	125.06
26	a8	204	PEB	CHC-C4C-C3C	-5.27	121.35	130.34
26	JJ	201	PEB	CHC-C4C-C3C	-5.27	121.35	130.34
26	QI	201	PEB	C3B-C4B-NB	5.27	117.71	110.05
26	XJ	203	PEB	CHB-C4B-NB	-5.27	121.52	128.83
28	EI	1001	CYC	OC-C1C-C2C	-5.27	121.98	126.17
28	H7	1001	CYC	C4D-CHA-C1A	5.27	135.10	128.81
26	P1	202	PEB	CMB-C2B-C1B	5.27	133.18	125.06
26	O6	201	PEB	CMB-C2B-C1B	5.27	133.18	125.06
26	W2	201	PEB	CHB-C4B-C3B	-5.27	113.15	125.32
26	IE	202	PEB	C1C-CHB-C4B	5.27	135.10	128.81
26	NJ	204	PEB	CHC-C4C-C3C	-5.27	121.36	130.34
26	UF	203	PEB	C1C-CHB-C4B	-5.26	122.52	128.81
26	lA	201	PEB	CHC-C4C-C3C	-5.26	121.36	130.34
28	pH	1001	CYC	CMA-C3A-C4A	5.26	133.17	125.06
26	F8	202	PEB	CMB-C2B-C1B	5.26	133.17	125.06
28	OH	1001	CYC	OB-C4B-C3B	-5.26	122.33	128.04
26	i4	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
26	jB	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
26	CD	201	PEB	CHB-C4B-NB	-5.26	121.53	128.83
26	PB	202	PEB	OA-C1A-C2A	-5.26	121.99	126.17
26	c1	201	PEB	C1C-CHB-C4B	5.26	135.09	128.81
26	TI	202	PEB	CHC-C4C-C3C	-5.26	121.37	130.34
26	N9	204	PEB	CHC-C4C-C3C	-5.26	121.37	130.34
26	Y9	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
26	Z8	201	PEB	OA-C1A-C2A	-5.26	121.99	126.17
26	ZF	201	PEB	CHC-C1D-ND	-5.25	107.84	113.95
26	M8	201	PEB	OA-C1A-C2A	-5.25	122.00	126.17
26	aI	201	PEB	OA-C1A-C2A	-5.25	122.00	126.17
28	MB	1001	CYC	OB-C4B-C3B	-5.25	122.34	128.04
26	S2	201	PEB	CHB-C4B-C3B	-5.25	113.18	125.32
26	MG	203	PEB	C1C-CHB-C4B	5.25	135.08	128.81
26	sG	202	PEB	C1C-CHB-C4B	5.25	135.08	128.81
26	iG	201	PEB	C1C-CHB-C4B	5.25	135.08	128.81
28	J7	1001	CYC	OB-C4B-C3B	-5.25	122.34	128.04
26	SB	203	PEB	CHB-C4B-NB	-5.25	121.55	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	IF	1001	CYC	OB-C4B-C3B	-5.25	122.34	128.04
26	T4	203	PEB	CHB-C4B-NB	-5.25	121.55	128.83
28	eH	1001	CYC	CMA-C3A-C4A	5.25	133.14	125.06
26	L4	202	PEB	CHB-C4B-NB	-5.25	121.55	128.83
28	D6	1001	CYC	C2B-C1B-NB	5.24	114.66	106.99
26	Y7	202	PEB	OA-C1A-C2A	-5.24	122.00	126.17
26	V1	203	PEB	CHB-C4B-NB	-5.24	121.56	128.83
26	L8	202	PEB	CMB-C2B-C1B	5.24	133.13	125.06
26	a1	201	PEB	CMB-C2B-C1B	5.24	133.13	125.06
26	PJ	202	PEB	CMB-C2B-C1B	5.24	133.13	125.06
26	a1	203	PEB	CHC-C1D-ND	-5.24	107.87	113.95
26	AE	202	PEB	CHB-C4B-NB	-5.24	121.56	128.83
26	AA	301	PEB	C1C-CHB-C4B	-5.24	122.56	128.81
26	SE	201	PEB	CHC-C1D-ND	-5.24	107.87	113.95
26	VG	201	PEB	CHA-C4A-NA	5.23	131.43	125.20
26	nE	202	PEB	C1C-CHB-C4B	5.23	135.06	128.81
26	GG	202	PEB	CMB-C2B-C1B	5.23	133.12	125.06
26	BE	201	PEB	CHB-C4B-NB	-5.23	121.57	128.83
26	E8	202	PEB	CHA-C1B-NB	-5.23	113.99	124.93
28	1H	1000	CYC	CAB-C3B-C4B	5.23	129.64	121.38
26	Y2	201	PEB	CHC-C1D-ND	-5.23	107.87	113.95
26	SB	203	PEB	CHC-C1D-ND	-5.23	107.87	113.95
26	tG	201	PEB	C2A-C1A-NA	5.23	112.78	108.27
26	TI	201	PEB	OA-C1A-C2A	-5.23	122.02	126.17
26	KE	202	PEB	CMB-C2B-C1B	5.23	133.12	125.06
28	E2	1001	CYC	OC-C1C-C2C	-5.23	122.02	126.17
26	O2	201	PEB	CHB-C4B-C3B	-5.23	113.25	125.32
26	HD	201	PEB	OA-C1A-C2A	-5.23	122.02	126.17
26	F9	202	PEB	CHB-C4B-NB	-5.23	121.58	128.83
26	a2	201	PEB	OA-C1A-C2A	-5.22	122.02	126.17
26	N4	203	PEB	OA-C1A-C2A	-5.22	122.02	126.17
26	OB	201	PEB	CHC-C1D-ND	-5.22	107.88	113.95
26	VG	202	PEB	CHB-C4B-C3B	-5.22	113.26	125.32
26	hF	202	PEB	CHC-C4C-C3C	-5.22	121.43	130.34
26	X8	202	PEB	C1C-CHB-C4B	-5.22	122.57	128.81
27	AA	304	PUB	OD-C4D-C3D	-5.22	122.38	128.04
26	GE	203	PEB	C1C-CHB-C4B	5.22	135.04	128.81
26	JC	202	PEB	CHB-C4B-NB	-5.22	121.59	128.83
27	wE	304	PUB	CBA-CAA-C3A	-5.22	105.06	112.98
26	U8	203	PEB	CHC-C4C-C3C	-5.22	121.44	130.34
26	RD	202	PEB	C2A-C1A-NA	5.22	112.77	108.27
26	h7	203	PEB	CHA-C1B-NB	-5.22	114.02	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T2	201	PEB	OA-C1A-C2A	-5.22	122.03	126.17
27	A1	203	PUB	CHC-C1D-ND	-5.21	107.13	113.72
28	jH	1001	CYC	CHD-C4C-NC	5.21	131.41	125.20
26	X3	202	PEB	C1C-CHB-C4B	5.21	135.04	128.81
26	LG	202	PEB	CMB-C2B-C1B	5.21	133.09	125.06
26	f8	201	PEB	CHB-C4B-NB	-5.21	121.60	128.83
26	c6	202	PEB	CHB-C4B-NB	-5.21	121.60	128.83
26	G1	201	PEB	CMB-C2B-C1B	5.21	133.09	125.06
26	c4	203	PEB	CHB-C4B-NB	-5.21	121.60	128.83
28	H7	1001	CYC	CAB-C3B-C4B	5.21	129.61	121.38
26	O7	203	PEB	C1C-CHB-C4B	5.21	135.03	128.81
26	OI	201	PEB	CHB-C4B-C3B	-5.21	113.28	125.32
28	KF	1001	CYC	CAB-C3B-C4B	5.21	129.61	121.38
26	a4	201	PEB	CHA-C1B-NB	-5.20	114.05	124.93
28	J7	1001	CYC	CMA-C3A-C4A	5.20	133.08	125.06
26	G8	203	PEB	C1C-CHB-C4B	5.20	135.02	128.81
26	QF	201	PEB	CHB-C4B-NB	-5.20	121.61	128.83
26	c8	202	PEB	C1C-CHB-C4B	-5.20	122.60	128.81
26	U8	201	PEB	CHC-C1D-ND	-5.20	107.91	113.95
26	IE	201	PEB	C4B-C3B-C2B	-5.20	101.03	106.78
26	PE	201	PEB	OA-C1A-NA	5.19	131.23	124.94
28	EF	1001	CYC	OC-C1C-C2C	-5.19	122.04	126.17
26	ID	201	PEB	CHC-C4C-C3C	-5.19	121.48	130.34
26	gA	201	PEB	CHA-C1B-NB	-5.19	114.07	124.93
26	S7	201	PEB	CHC-C4C-C3C	-5.19	121.48	130.34
26	FA	202	PEB	CMB-C2B-C1B	5.19	133.06	125.06
26	VF	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
28	CF	1001	CYC	OB-C4B-C3B	-5.19	122.41	128.04
26	A3	202	PEB	C1C-CHB-C4B	-5.19	122.61	128.81
26	YB	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
26	Q2	201	PEB	C3B-C4B-NB	5.19	117.60	110.05
26	wE	303	PEB	CHB-C4B-NB	-5.19	121.63	128.83
28	EH	1001	CYC	CMA-C3A-C4A	5.19	133.05	125.06
26	U7	201	PEB	CHC-C4C-C3C	-5.19	121.49	130.34
26	RI	203	PEB	CHB-C4B-NB	-5.19	121.63	128.83
26	IJ	202	PEB	C1C-CHB-C4B	5.19	135.00	128.81
26	dE	201	PEB	CHA-C4A-NA	5.19	131.37	125.20
26	L8	201	PEB	C1C-CHB-C4B	-5.19	122.61	128.81
26	LA	201	PEB	C1C-CHB-C4B	-5.19	122.61	128.81
26	m8	202	PEB	OA-C1A-C2A	-5.18	122.05	126.17
26	N7	1002	PEB	CHC-C4C-C3C	-5.18	121.50	130.34
28	yH	1001	CYC	CMA-C3A-C4A	5.18	133.04	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	i8	201	PEB	OA-C1A-C2A	-5.18	122.06	126.17
26	AG	202	PEB	CHB-C4B-NB	-5.18	121.64	128.83
26	ZA	202	PEB	CMB-C2B-C1B	5.18	133.04	125.06
26	CE	202	PEB	C4B-C3B-C2B	-5.18	101.05	106.78
26	kE	201	PEB	C1C-CHB-C4B	-5.18	122.62	128.81
26	uE	202	PEB	C1C-CHB-C4B	5.18	134.99	128.81
26	L2	1002	PEB	CHC-C4C-C3C	-5.18	121.51	130.34
26	gG	203	PEB	CHC-C1D-ND	-5.18	107.94	113.95
28	QH	1001	CYC	OB-C4B-C3B	-5.18	122.42	128.04
26	WB	203	PEB	C1C-CHB-C4B	5.17	134.99	128.81
28	K2	1001	CYC	C4D-CHA-C1A	5.17	134.99	128.81
26	N4	202	PEB	CHB-C4B-NB	-5.17	121.65	128.83
26	f4	202	PEB	CHB-C4B-NB	-5.17	121.65	128.83
26	P9	201	PEB	CHC-C4C-C3C	-5.17	121.52	130.34
28	1H	1000	CYC	OB-C4B-C3B	-5.17	122.43	128.04
26	e7	202	PEB	CHA-C1B-NB	-5.17	114.11	124.93
26	eI	203	PEB	CHB-C4B-NB	-5.17	121.66	128.83
26	RJ	203	PEB	C1C-CHB-C4B	5.17	134.99	128.81
26	I9	202	PEB	CHC-C1D-ND	-5.17	107.94	113.95
28	wH	1001	CYC	CMA-C3A-C4A	5.17	133.03	125.06
26	SF	201	PEB	CHC-C4C-C3C	-5.17	121.52	130.34
26	KG	201	PEB	CHC-C1D-ND	-5.17	107.95	113.95
28	NH	1001	CYC	CMA-C3A-C4A	5.17	133.02	125.06
27	A6	302	PUB	CHA-C1B-C2B	-5.17	121.53	130.34
26	LA	202	PEB	CMB-C2B-C1B	5.17	133.02	125.06
27	24	403	PUB	C1C-C2C-C3C	-5.17	101.06	106.78
26	VG	201	PEB	C1C-CHB-C4B	5.17	134.98	128.81
26	I1	201	PEB	CHC-C1D-ND	-5.16	107.95	113.95
26	GE	201	PEB	CMA-C2A-C1A	-5.16	101.27	112.40
28	YH	1001	CYC	CAB-C3B-C4B	5.16	129.53	121.38
26	e6	203	PEB	CHA-C1B-NB	-5.16	114.13	124.93
26	OG	201	PEB	C1C-CHB-C4B	5.16	134.98	128.81
26	oE	201	PEB	OA-C1A-C2A	-5.16	122.07	126.17
26	ZF	203	PEB	C1C-CHB-C4B	-5.16	122.64	128.81
26	GC	203	PEB	OA-C1A-C2A	-5.16	122.07	126.17
26	T9	201	PEB	CHB-C4B-NB	-5.16	121.67	128.83
26	WE	203	PEB	CHB-C4B-NB	-5.16	121.67	128.83
26	jF	202	PEB	CHC-C4C-C3C	-5.16	121.54	130.34
26	X3	203	PEB	CAB-CBB-CGB	-5.16	102.50	113.60
26	n4	201	PEB	CHC-C1D-ND	-5.16	107.96	113.95
26	DJ	203	PEB	CHC-C1D-ND	-5.16	107.96	113.95
26	wG	302	PEB	C1C-CHB-C4B	-5.16	122.65	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	hB	203	PEB	CHB-C4B-NB	-5.16	121.68	128.83
26	f2	201	PEB	CHC-C4C-C3C	-5.15	121.55	130.34
28	F7	1001	CYC	C1B-CHB-C4A	-5.15	115.49	128.08
26	b7	203	PEB	OA-C1A-C2A	-5.15	122.08	126.17
27	K3	203	PUB	CHB-C1C-NC	-5.15	121.68	128.83
26	RG	201	PEB	OA-C1A-NA	5.15	131.18	124.94
26	IJ	202	PEB	CHB-C4B-NB	-5.15	121.68	128.83
26	T4	201	PEB	CMD-C2D-C3D	-5.15	122.80	130.06
26	II	201	PEB	C1C-CHB-C4B	5.15	134.96	128.81
26	EA	202	PEB	CHB-C4B-NB	-5.15	121.68	128.83
26	LA	201	PEB	C2A-C1A-NA	5.15	112.71	108.27
26	xG	304	PEB	OA-C1A-C2A	-5.15	122.08	126.17
26	cI	203	PEB	CHB-C4B-NB	-5.15	121.69	128.83
26	ZF	203	PEB	CMB-C2B-C1B	5.15	132.99	125.06
26	ED	201	PEB	CHB-C4B-NB	-5.15	121.69	128.83
26	Y6	202	PEB	OA-C1A-C2A	-5.15	122.08	126.17
26	R9	202	PEB	CHB-C4B-NB	-5.15	121.69	128.83
28	UH	1001	CYC	CMA-C3A-C4A	5.15	132.99	125.06
26	cA	203	PEB	C1C-CHB-C4B	-5.15	122.66	128.81
28	JF	1001	CYC	C4D-CHA-C1A	5.15	134.96	128.81
26	n4	202	PEB	OA-C1A-C2A	-5.15	122.08	126.17
28	M6	1001	CYC	OB-C4B-C3B	-5.15	122.45	128.04
26	h1	202	PEB	CHB-C4B-NB	-5.15	121.69	128.83
26	ME	201	PEB	CMB-C2B-C1B	5.15	132.99	125.06
26	g2	202	PEB	C1C-CHB-C4B	5.14	134.95	128.81
26	MA	201	PEB	OA-C1A-C2A	-5.14	122.08	126.17
26	u4	201	PEB	C1C-CHB-C4B	5.14	134.95	128.81
26	V4	203	PEB	CHB-C4B-NB	-5.14	121.69	128.83
27	A1	203	PUB	CHA-C4A-NA	-5.14	107.98	113.95
26	BC	202	PEB	CHB-C4B-NB	-5.14	121.70	128.83
26	z1	201	PEB	CHB-C4B-C3B	-5.14	113.45	125.32
26	UA	203	PEB	CHC-C4C-C3C	-5.14	121.57	130.34
26	E8	202	PEB	CHB-C4B-NB	-5.14	121.70	128.83
26	UG	201	PEB	C3B-C4B-NB	5.14	117.52	110.05
26	a7	202	PEB	CHB-C4B-NB	-5.14	121.70	128.83
26	j7	203	PEB	C1C-CHB-C4B	5.14	134.94	128.81
26	eA	201	PEB	OA-C1A-C2A	-5.14	122.09	126.17
26	G3	202	PEB	CHB-C4B-NB	-5.13	121.70	128.83
28	SH	1001	CYC	OB-C4B-C3B	-5.13	122.47	128.04
26	F7	1002	PEB	OA-C1A-C2A	-5.13	122.09	126.17
26	UE	201	PEB	C3B-C4B-NB	5.13	117.52	110.05
26	WF	202	PEB	CHC-C1D-ND	-5.13	107.99	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SE	203	PEB	CHC-C1D-ND	-5.13	107.99	113.95
28	GB	1001	CYC	CAB-C3B-C4B	5.13	129.48	121.38
26	A2	301	PEB	CHB-C4B-NB	-5.13	121.71	128.83
26	Y2	203	PEB	CHB-C4B-NB	-5.13	121.71	128.83
26	XE	201	PEB	OA-C1A-NA	5.13	131.16	124.94
27	A1	203	PUB	CHB-C1C-NC	-5.13	121.71	128.83
26	ZB	203	PEB	CMB-C2B-C1B	5.13	132.97	125.06
28	nH	1001	CYC	CMB-C2B-C1B	5.13	130.57	124.17
28	qH	1002	CYC	CAA-C2A-C1A	5.13	134.08	125.01
26	b7	202	PEB	CHC-C1D-ND	-5.13	107.99	113.95
26	UG	201	PEB	C4B-C3B-C2B	-5.13	101.11	106.78
28	H7	1001	CYC	OC-C1C-C2C	-5.13	122.10	126.17
26	RB	202	PEB	OA-C1A-C2A	-5.13	122.10	126.17
26	H5	201	PEB	CMB-C2B-C1B	5.12	132.95	125.06
26	RJ	203	PEB	CHC-C4C-C3C	-5.12	121.61	130.34
28	jH	1001	CYC	OB-C4B-C3B	-5.12	122.49	128.04
26	hE	201	PEB	CHB-C4B-NB	-5.12	121.73	128.83
26	N3	202	PEB	CHA-C1B-NB	-5.11	114.23	124.93
28	LI	1001	CYC	CHA-C1A-NA	-5.11	121.73	128.83
26	Q9	201	PEB	OA-C1A-C2A	-5.11	122.11	126.17
26	H9	202	PEB	CHC-C4C-C3C	-5.11	121.62	130.34
26	c1	203	PEB	CHC-C1D-ND	-5.11	108.01	113.95
26	k1	203	PEB	OA-C1A-C2A	-5.11	122.11	126.17
26	GD	201	PEB	CHB-C4B-NB	-5.11	121.74	128.83
26	Y3	301	PEB	OA-C1A-C2A	-5.11	122.11	126.17
26	SG	201	PEB	CHB-C4B-NB	-5.11	121.74	128.83
26	S6	203	PEB	CHB-C4B-NB	-5.11	121.74	128.83
28	WH	1001	CYC	CMA-C3A-C4A	5.11	132.93	125.06
26	WI	201	PEB	C1C-CHB-C4B	5.11	134.91	128.81
26	S4	201	PEB	OA-C1A-C2A	-5.11	122.11	126.17
26	IE	201	PEB	C1C-CHB-C4B	5.11	134.91	128.81
26	SA	201	PEB	CHB-C4B-NB	-5.11	121.74	128.83
26	lF	203	PEB	CHC-C4C-C3C	-5.11	121.63	130.34
26	X8	201	PEB	CHA-C1B-NB	-5.11	114.25	124.93
28	J2	1001	CYC	CAB-C3B-C4B	5.11	129.44	121.38
26	O8	201	PEB	OA-C1A-C2A	-5.10	122.11	126.17
28	gH	1001	CYC	CHD-C4C-NC	5.10	131.27	125.20
28	YH	1003	CYC	OB-C4B-C3B	-5.10	122.50	128.04
26	aG	203	PEB	CHA-C1B-NB	-5.10	114.26	124.93
26	AI	304	PEB	CHB-C4B-NB	-5.10	121.75	128.83
28	YH	1003	CYC	CHD-C4C-NC	5.10	131.27	125.20
28	N7	1001	CYC	OC-C1C-C2C	-5.10	122.12	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FD	203	PEB	CHB-C4B-NB	-5.10	121.75	128.83
28	KI	1001	CYC	C4D-CHA-C1A	5.10	134.90	128.81
26	d6	203	PEB	CMB-C2B-C1B	5.10	132.92	125.06
26	Y6	201	PEB	OA-C1A-C2A	-5.10	122.12	126.17
26	DG	202	PEB	CHB-C4B-NB	-5.10	121.76	128.83
26	iG	201	PEB	CHA-C1B-NB	-5.10	114.27	124.93
26	Z1	201	PEB	OA-C1A-C2A	-5.10	122.12	126.17
28	NH	1001	CYC	CMB-C2B-C1B	5.10	130.53	124.17
26	CD	201	PEB	CHC-C4C-C3C	-5.09	121.65	130.34
26	NF	1002	PEB	CHC-C4C-C3C	-5.09	121.65	130.34
26	hB	203	PEB	CHC-C1D-ND	-5.09	108.03	113.95
26	RE	201	PEB	OA-C1A-NA	5.09	131.11	124.94
28	G6	1001	CYC	CAB-C3B-C4B	5.09	129.42	121.38
28	LB	1001	CYC	C4D-CHA-C1A	5.09	134.89	128.81
27	wE	304	PUB	OD-C4D-C3D	-5.09	122.52	128.04
28	UH	1001	CYC	C4D-CHA-C1A	5.09	134.89	128.81
26	E3	201	PEB	CHB-C4B-NB	-5.09	121.77	128.83
26	hG	201	PEB	CHA-C4A-NA	5.09	131.26	125.20
26	W3	202	PEB	CHC-C4C-C3C	-5.09	121.66	130.34
26	P4	202	PEB	CMB-C2B-C1B	5.09	132.90	125.06
26	YB	202	PEB	OA-C1A-C2A	-5.09	122.13	126.17
28	K7	1001	CYC	OB-C4B-C3B	-5.09	122.52	128.04
26	eG	203	PEB	CHC-C1D-ND	-5.09	108.04	113.95
28	CH	1001	CYC	CHD-C4C-NC	5.09	131.25	125.20
26	m2	202	PEB	C1C-CHB-C4B	5.09	134.88	128.81
26	eE	203	PEB	CHC-C1D-ND	-5.08	108.04	113.95
26	h7	202	PEB	CHB-C4B-NB	-5.08	121.78	128.83
27	xE	301	PUB	OD-C4D-C3D	-5.08	122.53	128.04
26	W4	202	PEB	CHB-C4B-NB	-5.08	121.78	128.83
26	B3	201	PEB	OA-C1A-C2A	-5.08	122.13	126.17
28	L7	1001	CYC	CAB-C3B-C4B	5.08	129.40	121.38
26	RJ	202	PEB	CHB-C4B-NB	-5.08	121.78	128.83
28	F7	1001	CYC	C2B-C1B-NB	5.08	114.42	106.99
26	LI	1002	PEB	CHC-C4C-C3C	-5.08	121.68	130.34
28	DB	1001	CYC	C2B-C1B-NB	5.08	114.42	106.99
26	I5	202	PEB	OA-C1A-C2A	-5.07	122.14	126.17
28	F6	1001	CYC	C4D-CHA-C1A	5.07	134.87	128.81
26	F4	202	PEB	C1C-CHB-C4B	5.07	134.87	128.81
26	A9	303	PEB	C1C-CHB-C4B	-5.07	122.75	128.81
26	j1	201	PEB	C4B-C3B-C2B	-5.07	101.17	106.78
26	iI	203	PEB	CHB-C4B-NB	-5.07	121.80	128.83
26	dG	201	PEB	CHA-C4A-NA	5.07	131.23	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	uH	1001	CYC	OB-C4B-C3B	-5.07	122.54	128.04
26	W1	202	PEB	CHB-C4B-NB	-5.07	121.80	128.83
27	AF	304	PUB	CHA-C4A-NA	-5.07	108.06	113.95
28	LB	1001	CYC	CAB-C3B-C4B	5.07	129.38	121.38
28	L6	1001	CYC	OC-C1C-C2C	-5.06	122.15	126.17
26	O6	201	PEB	CHC-C1D-ND	-5.06	108.07	113.95
26	R9	203	PEB	C1C-CHB-C4B	5.06	134.86	128.81
26	T3	202	PEB	C4B-C3B-C2B	-5.06	101.18	106.78
26	P9	202	PEB	CHA-C1B-NB	-5.06	114.34	124.93
26	hG	202	PEB	C1C-CHB-C4B	5.06	134.85	128.81
26	XA	201	PEB	CHA-C1B-NB	-5.06	114.35	124.93
26	aE	203	PEB	CHB-C4B-NB	-5.06	121.81	128.83
26	l7	201	PEB	C1C-CHB-C4B	5.06	134.85	128.81
26	E8	202	PEB	CHC-C4C-C3C	-5.06	121.71	130.34
28	IF	1001	CYC	OC-C1C-C2C	-5.06	122.15	126.17
28	E7	1001	CYC	CHB-C4A-NA	-5.06	114.36	124.93
26	D1	201	PEB	CHC-C1D-ND	-5.06	108.08	113.95
26	mI	201	PEB	OA-C1A-C2A	-5.05	122.15	126.17
28	QH	1001	CYC	C4D-CHA-C1A	5.05	134.85	128.81
26	VE	201	PEB	CHB-C4B-NB	-5.05	121.82	128.83
26	s1	202	PEB	CHB-C4B-NB	-5.05	121.82	128.83
26	aA	203	PEB	CHC-C4C-C3C	-5.05	121.72	130.34
26	m2	201	PEB	OA-C1A-C2A	-5.05	122.16	126.17
26	21	404	PEB	OA-C1A-C2A	-5.05	122.16	126.17
26	GJ	201	PEB	CHC-C1D-ND	-5.05	108.08	113.95
26	J8	202	PEB	C1C-CHB-C4B	-5.05	122.78	128.81
26	Z7	201	PEB	CHC-C1D-ND	-5.05	108.08	113.95
26	WE	202	PEB	CMB-C2B-C1B	5.05	132.84	125.06
28	EI	1001	CYC	CMA-C3A-C4A	5.05	132.84	125.06
26	AC	201	PEB	OA-C1A-C2A	-5.05	122.16	126.17
26	FC	203	PEB	CHB-C4B-NB	-5.05	121.83	128.83
26	BC	203	PEB	CHB-C4B-NB	-5.05	121.83	128.83
28	L2	1001	CYC	CHA-C1A-NA	-5.04	121.83	128.83
26	Y4	201	PEB	OA-C1A-C2A	-5.04	122.16	126.17
26	Y8	201	PEB	OA-C1A-C2A	-5.04	122.16	126.17
28	YH	1002	CYC	CHD-C4C-NC	5.04	131.20	125.20
26	Q1	202	PEB	CHC-C1D-ND	-5.04	108.09	113.95
26	uG	202	PEB	CHA-C1B-NB	-5.04	114.39	124.93
26	IC	203	PEB	CHB-C4B-NB	-5.04	121.83	128.83
28	KF	1001	CYC	OB-C4B-C3B	-5.04	122.57	128.04
28	KH	1001	CYC	C2B-C1B-NB	5.04	114.37	106.99
26	G5	201	PEB	CHC-C4C-C3C	-5.04	121.74	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	VE	202	PEB	CHB-C4B-C3B	-5.04	113.68	125.32
28	KI	1001	CYC	CAB-C3B-C4B	5.04	129.34	121.38
26	XG	201	PEB	OA-C1A-NA	5.04	131.04	124.94
26	kB	201	PEB	OA-C1A-C2A	-5.04	122.17	126.17
28	EH	1001	CYC	CHD-C4C-NC	5.04	131.19	125.20
26	R9	203	PEB	CHA-C1B-NB	-5.04	114.39	124.93
26	FG	202	PEB	CMB-C2B-C1B	5.04	132.82	125.06
26	s4	202	PEB	OA-C1A-C2A	-5.03	122.17	126.17
26	C5	203	PEB	C1C-CHB-C4B	-5.03	122.80	128.81
26	R2	201	PEB	CMB-C2B-C1B	5.03	132.82	125.06
26	mI	202	PEB	CHB-C4B-NB	-5.03	121.84	128.83
28	NF	1001	CYC	CAB-C3B-C4B	5.03	129.33	121.38
26	YB	201	PEB	OA-C1A-C2A	-5.03	122.17	126.17
26	M9	202	PEB	CHC-C1D-ND	-5.03	108.11	113.95
26	M3	202	PEB	CHB-C4B-NB	-5.03	121.85	128.83
26	WD	202	PEB	CHB-C4B-NB	-5.03	121.85	128.83
26	D1	203	PEB	CHB-C4B-NB	-5.03	121.85	128.83
26	e6	203	PEB	OA-C1A-C2A	-5.03	122.18	126.17
26	A8	301	PEB	C1C-CHB-C4B	-5.03	122.80	128.81
26	P6	202	PEB	CHB-C4B-NB	-5.03	121.86	128.83
27	A1	203	PUB	CBA-CAA-C3A	-5.03	105.36	112.98
26	DA	202	PEB	OA-C1A-C2A	-5.03	122.18	126.17
28	H7	1001	CYC	CMB-C2B-C1B	5.02	130.44	124.17
28	DB	1001	CYC	C1B-C2B-C3B	-5.02	102.63	107.87
26	Y3	304	PEB	CHA-C1B-NB	-5.02	114.42	124.93
26	T2	202	PEB	CHB-C4B-NB	-5.02	121.86	128.83
28	rH	1001	CYC	CMB-C2B-C1B	5.02	130.44	124.17
26	VJ	203	PEB	CHC-C4C-C3C	-5.02	121.77	130.34
26	E9	202	PEB	CHC-C1D-ND	-5.02	108.11	113.95
26	L5	203	PEB	CHB-C4B-NB	-5.02	121.86	128.83
26	e7	202	PEB	CHB-C4B-NB	-5.02	121.86	128.83
26	k6	201	PEB	OA-C1A-C2A	-5.02	122.18	126.17
26	EA	202	PEB	CMB-C2B-C1B	5.02	132.79	125.06
26	IG	202	PEB	C1C-CHB-C4B	5.02	134.81	128.81
28	KH	1001	CYC	C1B-NB-C4B	-5.02	104.28	110.67
26	NA	202	PEB	C1C-CHB-C4B	-5.02	122.82	128.81
28	DI	1001	CYC	OB-C4B-C3B	-5.02	122.60	128.04
26	IE	203	PEB	CHA-C1B-NB	-5.01	114.44	124.93
26	eE	203	PEB	CHA-C1B-NB	-5.01	114.44	124.93
26	L9	202	PEB	CHC-C4C-C3C	-5.01	121.79	130.34
26	m2	202	PEB	CHC-C1D-ND	-5.01	108.13	113.95
26	m4	203	PEB	CHC-C4C-C3C	-5.01	121.79	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V9	201	PEB	CHC-C4C-C3C	-5.01	121.79	130.34
26	XG	202	PEB	CHA-C1B-NB	-5.01	114.45	124.93
26	KA	202	PEB	OA-C1A-C2A	-5.01	122.19	126.17
26	c4	203	PEB	CHC-C1D-ND	-5.01	108.13	113.95
27	AF	304	PUB	CBA-CAA-C3A	5.01	120.57	112.98
26	CG	203	PEB	C1C-CHB-C4B	5.01	134.79	128.81
28	pH	1001	CYC	CMB-C2B-C1B	5.01	130.42	124.17
26	hB	201	PEB	CHC-C4C-C3C	-5.01	121.80	130.34
26	VI	201	PEB	CHC-C1D-ND	-5.01	108.13	113.95
28	F2	1001	CYC	C2B-C1B-NB	5.01	114.32	106.99
26	YI	201	PEB	CHC-C1D-ND	-5.01	108.14	113.95
26	CE	203	PEB	C1C-CHB-C4B	5.01	134.79	128.81
26	Y8	203	PEB	CHB-C4B-NB	-5.00	121.89	128.83
26	t1	202	PEB	CHA-C4A-NA	-5.00	119.26	125.20
26	H3	202	PEB	C2A-C1A-NA	5.00	112.58	108.27
26	i1	203	PEB	CHB-C4B-NB	-5.00	121.89	128.83
26	SE	201	PEB	CHB-C4B-NB	-5.00	121.89	128.83
28	LH	1001	CYC	CAB-C3B-C4B	5.00	129.27	121.38
26	u1	202	PEB	CHB-C4B-NB	-5.00	121.90	128.83
26	UA	202	PEB	CHC-C1D-ND	-4.99	108.15	113.95
26	X9	202	PEB	CHB-C4B-NB	-4.99	121.90	128.83
26	cG	201	PEB	CHA-C1B-NB	-4.99	114.48	124.93
26	a4	202	PEB	CHB-C4B-NB	-4.99	121.90	128.83
26	P8	201	PEB	C1C-CHB-C4B	-4.99	122.84	128.81
26	j8	202	PEB	CHC-C1D-ND	-4.99	108.15	113.95
26	XJ	201	PEB	CHC-C4C-C3C	-4.99	121.83	130.34
26	C3	201	PEB	CHB-C4B-NB	-4.99	121.91	128.83
26	H5	201	PEB	OA-C1A-C2A	-4.99	122.21	126.17
26	FI	1002	PEB	OA-C1A-C2A	-4.99	122.21	126.17
26	DD	201	PEB	CHA-C1B-NB	-4.99	114.50	124.93
26	V2	202	PEB	CHC-C4C-C3C	-4.99	121.83	130.34
26	RI	201	PEB	CMB-C2B-C1B	4.98	132.74	125.06
26	m2	202	PEB	CHB-C4B-NB	-4.98	121.91	128.83
28	K2	1001	CYC	CAB-C3B-C4B	4.98	129.25	121.38
26	R1	201	PEB	CMB-C2B-C1B	4.98	132.74	125.06
26	L9	202	PEB	CMB-C2B-C1B	4.98	132.74	125.06
28	C2	1001	CYC	CAB-C3B-C4B	4.98	129.25	121.38
26	TB	201	PEB	CHC-C1D-ND	-4.98	108.16	113.95
26	QJ	202	PEB	C1C-CHB-C4B	-4.98	122.86	128.81
28	HF	1001	CYC	CMB-C2B-C1B	4.98	130.39	124.17
26	RJ	203	PEB	CHA-C1B-NB	-4.98	114.51	124.93
26	c7	202	PEB	OA-C1A-C2A	-4.98	122.21	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V2	201	PEB	CHC-C1D-ND	-4.98	108.16	113.95
28	NI	1001	CYC	CAB-C3B-C4B	4.98	129.24	121.38
26	S1	201	PEB	OA-C1A-C2A	-4.98	122.21	126.17
26	U6	203	PEB	CHB-C4B-NB	-4.98	121.92	128.83
26	CA	201	PEB	CHB-C4B-NB	-4.98	121.92	128.83
28	B6	1002	CYC	OC-C1C-C2C	-4.98	122.22	126.17
26	CC	202	PEB	C1C-CHB-C4B	-4.98	122.86	128.81
26	B8	301	PEB	OD-C4D-ND	-4.98	118.56	125.93
27	KD	203	PUB	CHC-C1D-ND	-4.97	107.43	113.72
26	k8	202	PEB	CAB-C3B-C4B	4.97	133.81	125.01
26	aE	202	PEB	CHB-C4B-C3B	-4.97	113.84	125.32
26	j6	202	PEB	CHB-C4B-NB	-4.97	121.93	128.83
26	DD	201	PEB	OA-C1A-C2A	-4.97	122.22	126.17
27	yE	302	PUB	CHB-C1C-NC	-4.97	121.93	128.83
28	D2	1001	CYC	OB-C4B-C3B	-4.97	122.65	128.04
28	sH	1001	CYC	OB-C4B-C3B	-4.97	122.65	128.04
26	K8	203	PEB	C1C-CHB-C4B	4.97	134.75	128.81
26	F4	202	PEB	CHA-C1B-NB	-4.97	114.54	124.93
26	G4	202	PEB	CHC-C4C-C3C	-4.97	121.86	130.34
26	tE	201	PEB	C2A-C1A-NA	4.97	112.56	108.27
28	FI	1001	CYC	C2B-C1B-NB	4.97	114.26	106.99
26	B5	203	PEB	OA-C1A-C2A	-4.97	122.22	126.17
26	D8	202	PEB	OA-C1A-C2A	-4.97	122.22	126.17
26	AA	302	PEB	CHA-C1B-NB	-4.97	114.55	124.93
28	AH	1001	CYC	CMB-C2B-C1B	4.96	130.37	124.17
26	UF	203	PEB	CHC-C1D-ND	-4.96	108.18	113.95
26	h6	203	PEB	CHB-C4B-NB	-4.96	121.94	128.83
26	f6	203	PEB	CHC-C4C-C3C	-4.96	121.87	130.34
26	GC	201	PEB	CHC-C4C-C3C	-4.96	121.87	130.34
26	WA	202	PEB	OA-C1A-C2A	-4.96	122.23	126.17
26	X1	203	PEB	CHA-C1B-NB	-4.96	114.55	124.93
26	MG	203	PEB	CHA-C1B-NB	-4.96	114.55	124.93
26	RG	201	PEB	CHC-C4C-C3C	-4.96	121.88	130.34
26	vE	202	PEB	C1C-CHB-C4B	4.96	134.73	128.81
26	GG	203	PEB	CAB-C3B-C4B	4.96	133.78	125.01
26	Q7	202	PEB	CHA-C1B-NB	-4.95	114.57	124.93
26	mG	201	PEB	C1C-CHB-C4B	4.95	134.73	128.81
26	W9	201	PEB	CMB-C2B-C1B	4.95	132.69	125.06
26	XD	203	PEB	CHC-C1D-ND	-4.95	108.19	113.95
26	C8	201	PEB	CHB-C4B-NB	-4.95	121.96	128.83
26	RI	202	PEB	CHB-C4B-NB	-4.95	121.96	128.83
27	xG	301	PUB	OD-C4D-C3D	-4.95	122.67	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E3	201	PEB	CHA-C1B-NB	-4.95	114.57	124.93
28	sH	1001	CYC	CHB-C4A-NA	-4.95	114.58	124.93
26	A3	201	PEB	CHC-C4C-C3C	-4.95	121.89	130.34
26	m4	202	PEB	OA-C1A-C2A	-4.95	122.24	126.17
26	L7	1002	PEB	OA-C1A-C2A	-4.95	122.24	126.17
26	L1	202	PEB	CHC-C1D-ND	-4.95	108.20	113.95
26	qE	201	PEB	OA-C1A-C2A	-4.95	122.24	126.17
26	P7	202	PEB	CHB-C4B-NB	-4.95	121.97	128.83
26	VE	201	PEB	C4B-C3B-C2B	-4.95	101.31	106.78
26	D9	203	PEB	CHC-C1D-ND	-4.95	108.20	113.95
28	KB	202	CYC	CMA-C3A-C4A	4.94	132.68	125.06
28	F7	1001	CYC	OB-C4B-C3B	-4.94	122.67	128.04
26	WA	203	PEB	CHB-C4B-NB	-4.94	121.97	128.83
26	N8	202	PEB	C1C-CHB-C4B	-4.94	122.90	128.81
28	NI	1001	CYC	C2C-C1C-NC	4.94	112.53	108.27
26	w4	202	PEB	CHB-C4B-NB	-4.94	121.97	128.83
26	DI	1002	PEB	OA-C1A-C2A	-4.94	122.24	126.17
26	ZE	202	PEB	C1C-CHB-C4B	4.94	134.71	128.81
28	FB	1001	CYC	C4D-CHA-C1A	4.94	134.71	128.81
26	WG	201	PEB	CHA-C1B-NB	-4.94	114.59	124.93
26	qG	201	PEB	CMB-C2B-C1B	4.94	132.67	125.06
26	W3	202	PEB	C1C-CHB-C4B	4.94	134.71	128.81
26	F3	203	PEB	CHB-C4B-NB	-4.94	121.98	128.83
26	gE	201	PEB	CHA-C1B-NB	-4.94	114.60	124.93
28	KH	1001	CYC	CHD-C4C-NC	-4.94	119.33	125.20
26	BD	202	PEB	CHC-C1D-ND	-4.94	108.21	113.95
26	F2	1002	PEB	OA-C1A-C2A	-4.94	122.25	126.17
26	r1	201	PEB	CAA-C3A-C2A	-4.94	101.93	114.26
26	f6	203	PEB	C1C-CHB-C4B	4.94	134.71	128.81
26	DE	202	PEB	OA-C1A-C2A	-4.94	122.25	126.17
26	WG	202	PEB	CHA-C1B-NB	-4.93	114.61	124.93
26	HD	202	PEB	C2A-C1A-NA	4.93	112.53	108.27
26	T8	202	PEB	CMB-C2B-C1B	4.93	132.66	125.06
28	II	1001	CYC	CAB-C3B-C4B	4.93	129.17	121.38
26	D3	201	PEB	OA-C1A-C2A	-4.93	122.25	126.17
26	S1	202	PEB	CHB-C4B-NB	-4.93	121.98	128.83
26	mE	201	PEB	CHB-C4B-NB	-4.93	121.98	128.83
28	F2	1001	CYC	C1B-C2B-C3B	-4.93	102.72	107.87
27	AF	304	PUB	C1C-C2C-C3C	-4.93	101.32	106.78
26	bB	202	PEB	CHB-C4B-NB	-4.93	121.99	128.83
26	BJ	201	PEB	CHA-C1B-NB	-4.93	114.62	124.93
28	YH	1001	CYC	CHD-C4C-NC	4.93	131.07	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	GH	1001	CYC	CHD-C4C-NC	4.93	131.06	125.20
28	wH	1001	CYC	CHD-C4C-NC	4.93	131.06	125.20
26	EJ	201	PEB	CHC-C1D-ND	-4.93	108.23	113.95
26	BA	301	PEB	OD-C4D-ND	-4.93	118.63	125.93
26	QD	202	PEB	CHB-C4B-NB	-4.93	122.00	128.83
26	J3	201	PEB	CHC-C1D-ND	-4.92	108.23	113.95
28	KH	1001	CYC	CMB-C2B-C1B	4.92	130.32	124.17
26	KA	203	PEB	C1C-CHB-C4B	4.92	134.69	128.81
26	wG	303	PEB	CHB-C4B-NB	-4.92	122.00	128.83
26	FD	201	PEB	OA-C1A-C2A	-4.92	122.26	126.17
26	E3	202	PEB	CHB-C4B-NB	-4.92	122.00	128.83
28	N7	1001	CYC	CAB-C3B-C4B	4.92	129.15	121.38
26	UD	202	PEB	CHB-C4B-NB	-4.92	122.00	128.83
26	tE	201	PEB	CHB-C4B-NB	-4.92	122.00	128.83
26	H5	201	PEB	CHC-C1D-ND	-4.92	108.23	113.95
26	T6	201	PEB	CHC-C1D-ND	-4.92	108.23	113.95
28	CI	1001	CYC	CAB-C3B-C4B	4.92	129.15	121.38
28	F7	1001	CYC	C1B-C2B-C3B	-4.92	102.74	107.87
26	l4	201	PEB	CHB-C4B-NB	-4.92	122.00	128.83
26	IJ	201	PEB	CAB-CBB-CGB	-4.92	103.02	113.60
26	YJ	202	PEB	CHB-C4B-NB	-4.92	122.00	128.83
26	t4	202	PEB	CHA-C4A-NA	-4.92	119.36	125.20
27	xG	301	PUB	CHC-C1D-ND	-4.92	107.50	113.72
26	M9	201	PEB	CHC-C1D-ND	-4.92	108.24	113.95
26	YI	203	PEB	CHB-C4B-NB	-4.92	122.00	128.83
26	UE	201	PEB	C4B-C3B-C2B	-4.92	101.34	106.78
26	RD	203	PEB	CAB-CBB-CGB	-4.92	103.02	113.60
26	HF	1002	PEB	CHA-C1B-NB	-4.92	114.65	124.93
26	a8	203	PEB	CHC-C1D-ND	-4.92	108.24	113.95
26	aG	201	PEB	C1C-CHB-C4B	4.92	134.68	128.81
28	CB	1001	CYC	CMA-C3A-C4A	4.92	132.63	125.06
26	tE	201	PEB	CHA-C4A-NA	4.92	131.05	125.20
26	VI	202	PEB	C1C-CHB-C4B	4.92	134.68	128.81
26	P3	201	PEB	OA-C1A-C2A	-4.92	122.27	126.17
26	R4	202	PEB	CHB-C4B-NB	-4.91	122.01	128.83
26	NE	201	PEB	CHB-C4B-NB	-4.91	122.01	128.83
26	QG	203	PEB	C2A-C1A-NA	4.91	112.51	108.27
28	F7	1001	CYC	CMB-C2B-C1B	4.91	130.30	124.17
26	WI	201	PEB	C3B-C4B-NB	4.91	117.19	110.05
26	G8	201	PEB	CHB-C4B-NB	-4.91	122.01	128.83
26	OF	203	PEB	CHC-C1D-ND	-4.91	108.25	113.95
26	21	405	PEB	CHA-C1B-NB	-4.91	114.66	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q8	202	PEB	OA-C1A-C2A	-4.91	122.27	126.17
26	d4	202	PEB	CHB-C4B-NB	-4.91	122.02	128.83
26	ZG	201	PEB	CHA-C1B-NB	-4.91	114.66	124.93
26	a1	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
26	NA	201	PEB	CHA-C1B-NB	-4.91	114.67	124.93
28	L7	1001	CYC	C4D-CHA-C1A	4.91	134.67	128.81
26	JG	202	PEB	CMB-C2B-C1B	4.91	132.62	125.06
26	O6	203	PEB	CHC-C4C-C3C	-4.91	121.97	130.34
26	21	404	PEB	C1C-CHB-C4B	-4.91	122.95	128.81
27	wG	304	PUB	OD-C4D-C3D	-4.91	122.72	128.04
28	FF	1001	CYC	CHB-C1B-NB	-4.90	115.53	126.06
28	I7	1001	CYC	CAB-C3B-C4B	4.90	129.12	121.38
28	E2	1001	CYC	CMA-C3A-C4A	4.90	132.62	125.06
26	J5	202	PEB	CHA-C1B-NB	-4.90	114.68	124.93
26	X4	203	PEB	CHB-C4B-NB	-4.90	122.03	128.83
26	lF	202	PEB	CHB-C4B-NB	-4.90	122.03	128.83
28	dH	1001	CYC	CMA-C3A-C4A	4.90	132.61	125.06
26	24	405	PEB	CHA-C1B-NB	-4.90	114.68	124.93
28	L6	1001	CYC	CAB-C3B-C4B	4.90	129.12	121.38
26	XG	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
26	gE	202	PEB	OA-C1A-C2A	-4.90	122.28	126.17
26	V4	203	PEB	OA-C1A-C2A	-4.90	122.28	126.17
26	P6	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
28	D7	1001	CYC	CAB-C3B-C4B	4.90	129.11	121.38
28	C2	1001	CYC	OB-C4B-C3B	-4.90	122.73	128.04
27	A8	303	PUB	CBA-CAA-C3A	-4.90	105.55	112.98
26	a7	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
26	X8	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
28	VH	1001	CYC	CHB-C4A-C3A	4.90	137.49	124.90
26	m4	201	PEB	OA-C1A-C2A	-4.89	122.28	126.17
26	Y6	201	PEB	CMB-C2B-C1B	4.89	132.60	125.06
26	S9	202	PEB	C1C-CHB-C4B	4.89	134.66	128.81
28	F2	1001	CYC	CAA-C2A-C1A	4.89	133.67	125.01
26	Y6	202	PEB	CHB-C4B-NB	-4.89	122.04	128.83
28	CF	1001	CYC	CAB-C3B-C4B	4.89	129.10	121.38
26	YA	201	PEB	CHC-C1D-ND	-4.89	108.27	113.95
28	G7	1001	CYC	C4D-CHA-C1A	4.89	134.65	128.81
28	K6	202	CYC	CMA-C3A-C4A	4.89	132.59	125.06
26	YA	201	PEB	OA-C1A-C2A	-4.89	122.28	126.17
28	MH	1001	CYC	OB-C4B-C3B	-4.89	122.73	128.04
26	LD	201	PEB	CHB-C4B-NB	-4.89	122.05	128.83
28	kH	1001	CYC	CHB-C4A-C3A	4.89	137.47	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fF	203	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
27	AB	302	PUB	CHA-C1B-C2B	-4.89	122.00	130.34
28	FI	1001	CYC	C4D-CHA-C1A	4.89	134.65	128.81
26	WF	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
28	NF	1001	CYC	CMB-C2B-C1B	4.89	130.27	124.17
28	D6	1001	CYC	C1B-C2B-C3B	-4.89	102.77	107.87
26	M1	402	PEB	CHB-C4B-NB	-4.89	122.05	128.83
26	s1	201	PEB	C1C-CHB-C4B	4.89	134.65	128.81
26	b2	201	PEB	CHB-C4B-C3B	-4.89	114.03	125.32
27	B8	302	PUB	OD-C4D-C3D	-4.88	122.74	128.04
26	BD	203	PEB	CHC-C1D-ND	-4.88	108.28	113.95
26	iF	202	PEB	CHB-C4B-NB	-4.88	122.05	128.83
26	XA	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
26	Q4	202	PEB	CHC-C1D-ND	-4.88	108.28	113.95
26	PB	201	PEB	CMB-C2B-C1B	4.88	132.58	125.06
26	A4	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
28	F7	1001	CYC	CAB-C3B-C4B	4.88	129.09	121.38
26	a8	202	PEB	CHB-C4B-NB	-4.88	122.06	128.83
26	Y6	202	PEB	CHC-C4C-C3C	-4.88	122.01	130.34
26	EA	203	PEB	CHC-C4C-C3C	-4.88	122.01	130.34
26	21	401	PEB	OA-C1A-C2A	-4.88	122.29	126.17
26	UB	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
26	QE	203	PEB	C1C-CHB-C4B	4.88	134.64	128.81
26	BG	201	PEB	OA-C1A-NA	4.88	130.85	124.94
26	vG	201	PEB	C2A-C1A-NA	4.88	112.48	108.27
26	YB	201	PEB	C3B-C4B-NB	4.88	117.14	110.05
26	d7	201	PEB	OA-C1A-C2A	-4.88	122.30	126.17
26	L8	201	PEB	CHB-C4B-NB	-4.88	122.06	128.83
26	X8	202	PEB	CMB-C2B-C1B	4.88	132.57	125.06
26	cE	203	PEB	CHB-C4B-NB	-4.88	122.06	128.83
26	DJ	201	PEB	C1C-CHB-C4B	4.88	134.63	128.81
26	TB	201	PEB	OA-C1A-C2A	-4.88	122.30	126.17
26	24	401	PEB	CHB-C4B-NB	-4.88	122.06	128.83
26	E4	201	PEB	CHB-C4B-NB	-4.87	122.06	128.83
26	bE	202	PEB	OA-C1A-C2A	-4.87	122.30	126.17
28	M2	1001	CYC	OB-C4B-C3B	-4.87	122.75	128.04
28	F7	1001	CYC	CHB-C1B-NB	-4.87	115.59	126.06
26	QB	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
26	WD	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
26	QF	202	PEB	CMB-C2B-C1B	4.87	132.57	125.06
28	E7	1001	CYC	C4D-CHA-C1A	4.87	134.63	128.81
26	h8	203	PEB	CHB-C4B-NB	-4.87	122.07	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V3	201	PEB	CHB-C4B-NB	-4.87	122.07	128.83
27	K4	203	PUB	CHB-C1C-NC	-4.87	122.07	128.83
26	V1	203	PEB	OA-C1A-C2A	-4.87	122.30	126.17
26	DJ	201	PEB	CHB-C4B-NB	-4.87	122.07	128.83
28	LI	1001	CYC	C1B-C2B-C3B	-4.87	102.79	107.87
26	UA	203	PEB	CHB-C4B-NB	-4.87	122.07	128.83
26	cF	202	PEB	CHA-C1B-NB	-4.87	114.75	124.93
26	IA	202	PEB	CHB-C4B-NB	-4.87	122.07	128.83
26	ZG	202	PEB	C1C-CHB-C4B	4.87	134.62	128.81
26	YB	202	PEB	CHC-C4C-C3C	-4.87	122.03	130.34
26	n1	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
28	K7	1001	CYC	C2B-C1B-NB	4.86	114.11	106.99
26	gI	203	PEB	C4B-C3B-C2B	-4.86	101.40	106.78
26	dF	202	PEB	CHC-C4C-C3C	-4.86	122.04	130.34
26	TJ	202	PEB	CHC-C4C-C3C	-4.86	122.04	130.34
26	LE	201	PEB	OA-C1A-NA	4.86	130.83	124.94
26	LA	201	PEB	CHB-C4B-NB	-4.86	122.08	128.83
26	a4	201	PEB	CMB-C2B-C1B	4.86	132.55	125.06
26	qG	201	PEB	CHA-C1B-NB	-4.86	114.76	124.93
28	vH	1001	CYC	CHD-C4C-NC	4.86	130.99	125.20
26	Z4	201	PEB	CHB-C4B-NB	-4.86	122.08	128.83
26	wE	303	PEB	CHA-C1B-NB	-4.86	114.76	124.93
28	1H	1000	CYC	CHB-C4A-C3A	4.86	137.39	124.90
26	bB	201	PEB	OA-C1A-C2A	-4.86	122.31	126.17
26	KG	203	PEB	CHC-C1D-ND	-4.86	108.31	113.95
28	TH	1001	CYC	C4D-CHA-C1A	4.86	134.61	128.81
26	RE	201	PEB	CHC-C4C-C3C	-4.86	122.06	130.34
26	B5	203	PEB	CHB-C4B-NB	-4.86	122.09	128.83
28	CI	1001	CYC	OB-C4B-C3B	-4.86	122.77	128.04
27	yG	302	PUB	C1D-CHC-C4C	-4.86	102.81	113.37
28	cH	1001	CYC	CMA-C3A-C4A	4.85	132.54	125.06
28	uH	1001	CYC	CAC-C3C-C4C	4.85	125.14	112.67
26	PD	201	PEB	OA-C1A-C2A	-4.85	122.31	126.17
26	P6	201	PEB	CMB-C2B-C1B	4.85	132.54	125.06
28	I2	1001	CYC	CAB-C3B-C4B	4.85	129.04	121.38
28	I2	1001	CYC	C4D-CHA-C1A	4.85	134.61	128.81
26	CA	203	PEB	CHC-C1D-ND	-4.85	108.31	113.95
26	T3	201	PEB	OA-C1A-C2A	-4.85	122.31	126.17
28	K6	202	CYC	OC-C1C-C2C	-4.85	122.31	126.17
26	IJ	201	PEB	CHC-C1D-ND	-4.85	108.31	113.95
26	i2	203	PEB	CHB-C4B-NB	-4.85	122.10	128.83
26	OA	202	PEB	CHB-C4B-NB	-4.85	122.10	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FE	202	PEB	CMB-C2B-C1B	4.85	132.53	125.06
28	D2	1001	CYC	C4D-CHA-C1A	4.85	134.60	128.81
26	XD	203	PEB	CAB-CBB-CGB	-4.85	103.17	113.60
28	CF	1001	CYC	CMA-C3A-C4A	4.85	132.53	125.06
26	BD	202	PEB	C2A-C1A-NA	4.85	112.45	108.27
26	n1	201	PEB	CHC-C1D-ND	-4.85	108.32	113.95
26	jA	203	PEB	CHB-C4B-NB	-4.85	122.10	128.83
26	YF	201	PEB	OA-C1A-C2A	-4.85	122.32	126.17
26	gG	202	PEB	OA-C1A-C2A	-4.85	122.32	126.17
26	uE	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
28	oH	1001	CYC	OB-C4B-C3B	-4.85	122.78	128.04
26	Y6	201	PEB	C3B-C4B-NB	4.85	117.10	110.05
26	C9	201	PEB	C3B-C4B-NB	4.85	117.10	110.05
26	HJ	202	PEB	CHC-C4C-C3C	-4.84	122.08	130.34
26	PD	202	PEB	CHC-C1D-ND	-4.84	108.32	113.95
28	eH	1001	CYC	OB-C4B-C3B	-4.84	122.78	128.04
28	KB	202	CYC	OC-C1C-C2C	-4.84	122.32	126.17
26	fA	202	PEB	CHB-C4B-NB	-4.84	122.11	128.83
26	l7	201	PEB	CHC-C1D-ND	-4.84	108.33	113.95
26	h2	201	PEB	CHC-C4C-C3C	-4.84	122.08	130.34
26	D4	203	PEB	CHB-C4B-NB	-4.84	122.11	128.83
26	e8	201	PEB	C1C-CHB-C4B	-4.84	123.03	128.81
26	C1	201	PEB	CHB-C4B-NB	-4.84	122.12	128.83
26	a4	201	PEB	OA-C1A-C2A	-4.84	122.33	126.17
26	v4	201	PEB	OA-C1A-C2A	-4.84	122.33	126.17
26	S3	201	PEB	C3D-C4D-ND	4.84	116.75	107.26
26	A8	302	PEB	CHA-C1B-NB	-4.84	114.82	124.93
26	rE	202	PEB	C1C-CHB-C4B	4.84	134.59	128.81
28	II	1001	CYC	C4D-CHA-C1A	4.84	134.59	128.81
26	Z8	201	PEB	C1C-CHB-C4B	-4.84	123.03	128.81
28	YH	1004	CYC	CHB-C4A-C3A	4.84	137.33	124.90
26	kE	203	PEB	CHB-C4B-NB	-4.84	122.12	128.83
28	H6	1001	CYC	CMA-C3A-C4A	4.83	132.51	125.06
26	cG	203	PEB	CHA-C1B-C2B	4.83	137.33	124.90
26	TA	201	PEB	CHC-C1D-ND	4.83	119.56	113.95
28	L6	1001	CYC	C4D-CHA-C1A	4.83	134.58	128.81
26	v1	202	PEB	CHA-C1B-NB	-4.83	114.82	124.93
28	D6	1001	CYC	CHA-C1A-NA	-4.83	122.12	128.83
27	K4	203	PUB	CBB-CAB-C3B	4.83	120.86	112.62
26	IE	203	PEB	C3D-C4D-ND	4.83	116.74	107.26
27	24	402	PUB	OD-C4D-C3D	-4.83	122.80	128.04
26	W7	201	PEB	CHB-C4B-NB	-4.83	122.13	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L2	1001	CYC	C1B-C2B-C3B	-4.83	102.83	107.87
26	hE	201	PEB	CHC-C4C-C3C	-4.82	122.11	130.34
26	hA	203	PEB	CHB-C4B-NB	-4.82	122.14	128.83
26	GB	1002	PEB	C4B-C3B-C2B	-4.82	101.44	106.78
27	xE	306	PUB	CHA-C4A-NA	-4.82	108.35	113.95
26	l6	201	PEB	OA-C1A-C2A	-4.82	122.34	126.17
26	xE	304	PEB	OA-C1A-C2A	-4.82	122.34	126.17
26	R4	201	PEB	CMB-C2B-C1B	4.82	132.49	125.06
26	g1	203	PEB	CHB-C4B-NB	-4.82	122.14	128.83
26	IE	203	PEB	CHC-C1D-ND	-4.82	108.35	113.95
28	C6	1001	CYC	CMA-C3A-C4A	4.82	132.49	125.06
26	l8	203	PEB	CHC-C4C-C3C	-4.82	122.11	130.34
28	I6	1001	CYC	CAB-C3B-C4B	4.82	128.99	121.38
28	DI	1001	CYC	C4D-CHA-C1A	4.82	134.57	128.81
28	TH	1001	CYC	CHD-C4C-NC	4.82	130.94	125.20
26	a8	203	PEB	OA-C1A-C2A	-4.82	122.34	126.17
26	UI	201	PEB	CHA-C4A-NA	4.82	130.93	125.20
26	ME	203	PEB	CHB-C4B-NB	-4.82	122.14	128.83
26	O4	201	PEB	OA-C1A-C2A	-4.82	122.34	126.17
26	PB	202	PEB	CHB-C4B-NB	-4.82	122.15	128.83
26	HC	201	PEB	CMB-C2B-C1B	4.82	132.48	125.06
26	g4	203	PEB	OA-C1A-C2A	-4.82	122.34	126.17
27	A1	203	PUB	OD-C4D-C3D	-4.82	122.81	128.04
26	qE	201	PEB	CHA-C1B-NB	-4.82	114.86	124.93
26	l1	202	PEB	CHB-C4B-NB	-4.82	122.15	128.83
26	qE	202	PEB	CHA-C1B-C2B	4.81	137.28	124.90
26	DE	202	PEB	C1C-CHB-C4B	4.81	134.56	128.81
26	LG	202	PEB	OA-C1A-C2A	-4.81	122.35	126.17
26	g8	201	PEB	CHA-C1B-NB	-4.81	114.87	124.93
26	Y8	201	PEB	CHC-C1D-ND	-4.81	108.36	113.95
26	d4	201	PEB	CHB-C4B-NB	-4.81	122.15	128.83
26	W8	202	PEB	CHC-C1D-ND	-4.81	108.36	113.95
26	U3	201	PEB	C3D-C4D-ND	4.81	116.70	107.26
26	DJ	202	PEB	OD-C4D-ND	-4.81	118.80	125.93
26	Z2	201	PEB	CMA-C2A-C1A	-4.81	102.04	112.40
26	I8	202	PEB	CHA-C1B-NB	-4.81	114.87	124.93
26	NA	201	PEB	CHC-C1D-ND	4.81	119.53	113.95
26	QA	203	PEB	CHC-C1D-ND	-4.81	108.36	113.95
28	YH	1002	CYC	CHB-C4A-C3A	4.81	137.26	124.90
26	MG	203	PEB	CHC-C1D-ND	-4.81	108.36	113.95
26	I8	202	PEB	CHB-C4B-NB	-4.81	122.16	128.83
26	ZB	202	PEB	CHA-C1B-NB	-4.81	114.88	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SE	202	PEB	C2A-C1A-NA	-4.81	104.13	108.27
26	WA	202	PEB	C1C-CHB-C4B	-4.81	123.07	128.81
26	YG	203	PEB	OA-C1A-C2A	-4.81	122.35	126.17
26	P2	202	PEB	CHB-C4B-NB	-4.80	122.16	128.83
26	AD	202	PEB	CHB-C4B-NB	-4.80	122.16	128.83
26	TF	202	PEB	CHB-C4B-NB	-4.80	122.16	128.83
26	z1	201	PEB	CMB-C2B-C1B	4.80	132.46	125.06
26	L5	201	PEB	OA-C1A-C2A	-4.80	122.35	126.17
26	ED	202	PEB	CHB-C4B-NB	-4.80	122.16	128.83
26	g1	201	PEB	C1C-CHB-C4B	4.80	134.55	128.81
26	iE	201	PEB	CHA-C1B-NB	-4.80	114.89	124.93
26	aI	202	PEB	OA-C1A-C2A	-4.80	122.35	126.17
26	eE	201	PEB	CHB-C4B-NB	-4.80	122.17	128.83
26	14	202	PEB	CHB-C4B-NB	-4.80	122.17	128.83
28	HB	1001	CYC	CMA-C3A-C4A	4.80	132.46	125.06
26	l8	201	PEB	OA-C1A-C2A	-4.80	122.36	126.17
26	QA	202	PEB	OA-C1A-C2A	-4.80	122.36	126.17
26	hF	201	PEB	OA-C1A-C2A	-4.80	122.36	126.17
26	i1	201	PEB	OA-C1A-C2A	-4.80	122.36	126.17
26	WA	201	PEB	OA-C1A-C2A	-4.80	122.36	126.17
26	F9	201	PEB	CHB-C4B-NB	-4.80	122.17	128.83
26	ZB	201	PEB	CHB-C4B-NB	-4.80	122.17	128.83
26	J5	201	PEB	CMB-C2B-C3B	-4.80	113.09	126.12
28	JI	1001	CYC	C4D-CHA-C1A	4.80	134.54	128.81
26	NG	201	PEB	OA-C1A-NA	4.80	130.75	124.94
28	JF	1003	CYC	CAB-C3B-C4B	4.80	128.96	121.38
26	F1	201	PEB	C1C-CHB-C4B	4.80	134.54	128.81
26	cF	201	PEB	CHC-C1D-ND	-4.80	108.38	113.95
26	FJ	201	PEB	CHB-C4B-NB	-4.79	122.18	128.83
26	kG	201	PEB	CHA-C1B-NB	-4.79	114.91	124.93
26	GA	203	PEB	CHB-C4B-NB	-4.79	122.18	128.83
26	XJ	202	PEB	CHB-C4B-NB	-4.79	122.18	128.83
26	nE	201	PEB	C1C-CHB-C4B	4.79	134.53	128.81
26	LG	201	PEB	CHC-C1D-ND	-4.79	108.39	113.95
28	II	1001	CYC	OB-C4B-C3B	-4.79	122.84	128.04
26	x1	202	PEB	C4B-C3B-C2B	-4.79	101.48	106.78
26	O9	202	PEB	CHB-C4B-NB	-4.79	122.18	128.83
26	qE	201	PEB	CHB-C4B-NB	-4.79	122.19	128.83
28	I2	1001	CYC	OB-C4B-C3B	-4.79	122.84	128.04
26	R2	202	PEB	CHB-C4B-NB	-4.79	122.19	128.83
26	J9	201	PEB	CHA-C1B-NB	-4.79	114.92	124.93
26	U9	201	PEB	OA-C1A-C2A	-4.79	122.37	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	YA	203	PEB	OA-C1A-C2A	-4.79	122.37	126.17
26	Z8	202	PEB	C4B-C3B-C2B	-4.79	101.49	106.78
28	J2	1001	CYC	C4D-CHA-C1A	4.78	134.53	128.81
26	FE	201	PEB	CHB-C4B-NB	-4.78	122.19	128.83
26	I5	201	PEB	CMB-C2B-C1B	4.78	132.43	125.06
26	TD	202	PEB	C3B-C4B-NB	4.78	117.01	110.05
26	s4	201	PEB	CHA-C1B-NB	-4.78	114.93	124.93
26	nE	201	PEB	CHA-C1B-NB	-4.78	114.93	124.93
26	Z4	202	PEB	CHC-C1D-ND	-4.78	108.39	113.95
26	R6	202	PEB	OA-C1A-C2A	-4.78	122.37	126.17
26	W9	202	PEB	CHB-C4B-NB	-4.78	122.19	128.83
26	mG	202	PEB	CHB-C4B-NB	-4.78	122.19	128.83
26	R6	201	PEB	OA-C1A-C2A	-4.78	122.37	126.17
26	kF	201	PEB	CHB-C4B-NB	-4.78	122.19	128.83
26	Z6	201	PEB	CHB-C4B-NB	-4.78	122.20	128.83
26	P2	203	PEB	CHB-C4B-NB	-4.78	122.20	128.83
26	g4	203	PEB	CHB-C4B-NB	-4.78	122.20	128.83
26	R9	203	PEB	CHC-C4C-C3C	-4.78	122.19	130.34
26	kE	203	PEB	C1C-CHB-C4B	4.78	134.52	128.81
28	N2	1001	CYC	C4D-CHA-C1A	4.78	134.52	128.81
28	G7	1001	CYC	C2B-C1B-NB	4.78	113.98	106.99
26	f4	201	PEB	C2A-C1A-NA	4.78	112.39	108.27
26	L3	201	PEB	CHA-C1B-NB	-4.78	114.94	124.93
26	lF	201	PEB	CHC-C4C-C3C	-4.78	122.19	130.34
26	HG	201	PEB	C2A-C1A-NA	4.78	112.39	108.27
28	iH	1001	CYC	CHD-C4C-NC	4.78	130.88	125.20
26	DA	202	PEB	C4B-C3B-C2B	-4.78	101.50	106.78
26	y4	202	PEB	C1C-CHB-C4B	4.77	134.51	128.81
26	N9	203	PEB	CHB-C4B-NB	-4.77	122.20	128.83
26	cA	201	PEB	OA-C1A-C2A	-4.77	122.38	126.17
26	wE	302	PEB	C1C-CHB-C4B	-4.77	123.11	128.81
26	z1	202	PEB	CHA-C4A-NA	-4.77	119.53	125.20
26	SE	202	PEB	CHC-C1D-ND	-4.77	108.40	113.95
26	Q3	202	PEB	CHB-C4B-NB	-4.77	122.21	128.83
26	aA	203	PEB	CHB-C4B-NB	-4.77	122.21	128.83
26	q1	203	PEB	OA-C1A-C2A	-4.77	122.38	126.17
28	N7	1001	CYC	OB-C4B-C3B	-4.77	122.86	128.04
26	E8	202	PEB	OA-C1A-C2A	-4.77	122.38	126.17
26	gA	201	PEB	CMB-C2B-C1B	4.77	132.41	125.06
26	X1	203	PEB	CHB-C4B-NB	-4.77	122.21	128.83
26	TB	201	PEB	CMB-C2B-C1B	4.77	132.41	125.06
26	T9	203	PEB	CHB-C4B-NB	-4.77	122.21	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L2	1002	PEB	CMD-C2D-C3D	4.77	136.79	130.06
26	AC	203	PEB	CHB-C4B-NB	-4.77	122.21	128.83
26	IC	202	PEB	CHB-C4B-NB	-4.77	122.22	128.83
26	PB	201	PEB	OA-C1A-C2A	-4.77	122.38	126.17
26	XJ	202	PEB	C1C-CHB-C4B	4.77	134.50	128.81
26	c4	203	PEB	OA-C1A-C2A	-4.77	122.38	126.17
26	bF	201	PEB	CHB-C4B-NB	-4.77	122.22	128.83
26	dB	203	PEB	CMB-C2B-C1B	4.77	132.40	125.06
26	e1	201	PEB	CHB-C4B-NB	-4.76	122.22	128.83
26	z1	202	PEB	CHA-C1B-NB	-4.76	114.97	124.93
26	SE	202	PEB	C3B-C4B-NB	4.76	116.98	110.05
26	s4	203	PEB	C1C-CHB-C4B	4.76	134.50	128.81
26	f7	202	PEB	CHC-C1D-ND	-4.76	108.42	113.95
28	JF	1003	CYC	C4D-CHA-C1A	4.76	134.50	128.81
28	IH	1001	CYC	CHB-C4A-C3A	4.76	137.14	124.90
28	PH	1001	CYC	CHD-C4C-NC	4.76	130.87	125.20
26	QB	201	PEB	C4B-C3B-C2B	-4.76	101.51	106.78
26	HG	201	PEB	OA-C1A-C2A	-4.76	122.39	126.17
27	21	403	PUB	CHB-C1C-NC	-4.76	122.23	128.83
26	dE	202	PEB	C1C-CHB-C4B	4.76	134.49	128.81
26	LG	202	PEB	CHB-C4B-C3B	-4.76	114.33	125.32
28	E7	1001	CYC	CAB-C3B-C4B	4.76	128.89	121.38
26	H9	202	PEB	C1C-CHB-C4B	4.76	134.49	128.81
26	gE	203	PEB	CHC-C1D-ND	-4.76	108.42	113.95
28	hH	1001	CYC	CHB-C4A-C3A	4.76	137.13	124.90
28	CF	1001	CYC	C4D-CHA-C1A	4.76	134.49	128.81
26	C1	201	PEB	CHC-C4C-C3C	-4.76	122.23	130.34
28	pH	1001	CYC	CHD-C4C-NC	4.76	130.86	125.20
26	K3	201	PEB	CHB-C4B-NB	-4.76	122.23	128.83
26	GC	202	PEB	CHB-C4B-NB	-4.76	122.23	128.83
26	W4	202	PEB	CHC-C1D-ND	-4.75	108.43	113.95
26	M8	203	PEB	CHC-C4C-C3C	-4.75	122.23	130.34
26	fB	203	PEB	CHB-C4B-NB	-4.75	122.23	128.83
28	HB	1001	CYC	CAB-C3B-C4B	4.75	128.89	121.38
28	fH	1001	CYC	CMB-C2B-C1B	4.75	130.10	124.17
26	OJ	201	PEB	OA-C1A-C2A	-4.75	122.39	126.17
26	NG	201	PEB	CHB-C4B-NB	-4.75	122.24	128.83
26	YF	201	PEB	CHC-C1D-ND	-4.75	108.43	113.95
26	ED	202	PEB	CHC-C4C-C3C	-4.75	122.23	130.34
26	U3	201	PEB	CHA-C1B-C2B	4.75	137.12	124.90
26	SA	201	PEB	OA-C1A-C2A	-4.75	122.40	126.17
26	T6	201	PEB	CMB-C2B-C1B	4.75	132.38	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lA	203	PEB	CHC-C4C-C3C	-4.75	122.24	130.34
28	L2	1001	CYC	OC-C1C-C2C	-4.75	122.40	126.17
26	TA	202	PEB	CMB-C2B-C1B	4.75	132.38	125.06
26	g8	202	PEB	CHC-C1D-ND	-4.75	108.43	113.95
26	f2	202	PEB	CHB-C4B-NB	-4.75	122.24	128.83
26	kI	202	PEB	C1C-CHB-C4B	4.75	134.48	128.81
28	mH	1001	CYC	CMB-C2B-C1B	4.75	130.09	124.17
28	qH	1001	CYC	CHD-C4C-NC	4.75	130.85	125.20
26	l4	202	PEB	OA-C1A-C2A	-4.74	122.40	126.17
26	YF	202	PEB	CMB-C2B-C1B	4.74	132.37	125.06
26	SD	201	PEB	C3D-C4D-ND	4.74	116.56	107.26
26	LC	203	PEB	CHB-C4B-NB	-4.74	122.25	128.83
26	UI	201	PEB	C1C-CHB-C4B	4.74	134.47	128.81
26	M8	202	PEB	CHB-C4B-NB	-4.74	122.25	128.83
26	FD	202	PEB	CHB-C4B-NB	-4.74	122.25	128.83
26	J8	201	PEB	OA-C1A-C2A	-4.74	122.41	126.17
27	A7	304	PUB	C1C-C2C-C3C	-4.74	101.54	106.78
26	P3	202	PEB	C2A-C1A-NA	4.74	112.36	108.27
26	E3	202	PEB	CHC-C4C-C3C	-4.74	122.26	130.34
26	G5	202	PEB	CHB-C4B-NB	-4.74	122.25	128.83
26	T6	202	PEB	OA-C1A-C2A	-4.74	122.41	126.17
26	C8	203	PEB	CHC-C1D-ND	-4.74	108.45	113.95
26	YF	201	PEB	CMB-C2B-C1B	4.74	132.36	125.06
26	AC	202	PEB	C1C-CHB-C4B	-4.74	123.15	128.81
26	FG	201	PEB	CHC-C1D-ND	-4.74	108.45	113.95
26	FG	201	PEB	CHB-C4B-NB	-4.73	122.26	128.83
26	J3	202	PEB	CHC-C1D-ND	-4.73	108.45	113.95
26	M8	202	PEB	OA-C1A-C2A	-4.73	122.41	126.17
28	LI	1001	CYC	CBB-CAB-C3B	-4.73	99.38	112.43
26	lB	201	PEB	OA-C1A-C2A	-4.73	122.41	126.17
26	QG	203	PEB	CHA-C1B-C2B	4.73	137.07	124.90
26	WD	202	PEB	CHC-C4C-C3C	-4.73	122.27	130.34
28	FF	1001	CYC	CAB-C3B-C4B	4.73	128.85	121.38
28	GB	1001	CYC	OB-C4B-C3B	-4.73	122.91	128.04
26	UJ	201	PEB	CMB-C2B-C1B	4.73	132.35	125.06
26	EA	201	PEB	C1C-CHB-C4B	4.73	134.46	128.81
26	V8	201	PEB	CHA-C1B-NB	-4.73	115.04	124.93
26	iE	203	PEB	CHC-C4C-C3C	-4.73	122.27	130.34
28	J7	1003	CYC	CAB-C3B-C4B	4.73	128.85	121.38
26	O3	201	PEB	C3D-C4D-ND	4.73	116.54	107.26
26	m6	202	PEB	OA-C1A-C2A	-4.73	122.41	126.17
26	uE	201	PEB	OA-C1A-C2A	-4.73	122.41	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I5	202	PEB	CMB-C2B-C1B	4.73	132.34	125.06
26	T3	201	PEB	CHC-C4C-C3C	-4.73	122.28	130.34
26	A5	201	PEB	C2A-C1A-NA	4.73	112.35	108.27
26	A9	301	PEB	CHB-C4B-NB	-4.73	122.27	128.83
26	gA	202	PEB	OA-C1A-C2A	-4.73	122.42	126.17
26	d7	201	PEB	C1C-CHB-C4B	4.72	134.45	128.81
26	U2	201	PEB	CHA-C1B-NB	-4.72	115.05	124.93
26	w1	202	PEB	CHC-C1D-ND	-4.72	108.46	113.95
28	IB	1001	CYC	CAB-C3B-C4B	4.72	128.84	121.38
26	e8	201	PEB	CMB-C2B-C1B	4.72	132.34	125.06
26	W2	201	PEB	C1C-CHB-C4B	4.72	134.45	128.81
26	h7	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
26	UD	201	PEB	C3D-C4D-ND	4.72	116.52	107.26
27	21	402	PUB	OD-C4D-C3D	-4.72	122.92	128.04
28	GH	1001	CYC	CMB-C2B-C1B	4.72	130.06	124.17
26	RF	202	PEB	CHB-C4B-NB	-4.72	122.28	128.83
28	I6	1001	CYC	CMA-C3A-C4A	4.72	132.33	125.06
26	HE	201	PEB	C2A-C1A-NA	4.72	112.34	108.27
26	QF	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
28	FF	1001	CYC	OB-C4B-C3B	-4.72	122.92	128.04
26	FA	201	PEB	CMB-C2B-C1B	4.72	132.33	125.06
26	hE	201	PEB	CHA-C1B-NB	-4.72	115.06	124.93
26	U6	202	PEB	OA-C1A-C2A	-4.72	122.42	126.17
26	TB	202	PEB	OA-C1A-C2A	-4.72	122.42	126.17
28	K7	1001	CYC	C1B-C2B-C3B	-4.72	102.95	107.87
26	V2	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
26	B1	203	PEB	C1C-CHB-C4B	4.72	134.44	128.81
26	lE	201	PEB	C2A-C1A-NA	4.72	112.34	108.27
26	IA	203	PEB	CHC-C4C-C3C	-4.72	122.30	130.34
26	a2	201	PEB	CMB-C2B-C1B	4.72	132.32	125.06
28	DB	1001	CYC	CHA-C1A-NA	-4.71	122.29	128.83
26	UI	201	PEB	CHA-C1B-NB	-4.71	115.07	124.93
26	ZI	201	PEB	CMA-C2A-C1A	-4.71	102.24	112.40
26	O3	202	PEB	CHC-C4C-C3C	-4.71	122.30	130.34
26	f1	202	PEB	OA-C1A-C2A	-4.71	122.43	126.17
26	K1	202	PEB	CHC-C1D-ND	-4.71	108.47	113.95
26	w4	204	PEB	CHC-C1D-ND	-4.71	108.47	113.95
26	Y3	303	PEB	CHA-C1B-NB	-4.71	115.08	124.93
26	eI	201	PEB	CMB-C2B-C1B	4.71	132.32	125.06
28	H6	1001	CYC	CAB-C3B-C4B	4.71	128.82	121.38
26	MG	201	PEB	CMB-C2B-C1B	4.71	132.32	125.06
26	TD	202	PEB	CHC-C1D-ND	-4.71	108.48	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P6	202	PEB	OA-C1A-C2A	-4.71	122.43	126.17
26	YB	201	PEB	CHA-C1B-NB	-4.71	115.08	124.93
27	yE	302	PUB	CMD-C2D-C3D	4.71	134.84	127.77
26	ZA	202	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
26	N8	201	PEB	CHA-C1B-NB	-4.71	115.08	124.93
26	TI	202	PEB	CHB-C4B-NB	-4.71	122.30	128.83
26	zE	501	PEB	OA-C1A-NA	4.71	130.64	124.94
28	N7	1001	CYC	CMB-C2B-C1B	4.71	130.05	124.17
26	k1	201	PEB	OA-C1A-C2A	-4.71	122.43	126.17
26	YE	203	PEB	C1C-CHB-C4B	4.71	134.43	128.81
28	FI	1001	CYC	C1B-C2B-C3B	-4.71	102.96	107.87
26	ZA	201	PEB	C1C-CHB-C4B	-4.71	123.19	128.81
26	D1	202	PEB	CHC-C1D-ND	-4.70	108.48	113.95
26	JG	201	PEB	CHB-C4B-NB	-4.70	122.30	128.83
26	jG	202	PEB	CMB-C2B-C1B	4.70	132.31	125.06
26	eA	201	PEB	C1C-CHB-C4B	-4.70	123.19	128.81
26	SE	202	PEB	CMB-C2B-C1B	4.70	132.30	125.06
26	W2	201	PEB	C3B-C4B-NB	4.70	116.89	110.05
26	fG	201	PEB	CHC-C4C-C3C	-4.70	122.32	130.34
26	Q6	201	PEB	OA-C1A-C2A	-4.70	122.44	126.17
26	i2	201	PEB	OA-C1A-C2A	-4.70	122.44	126.17
26	aI	201	PEB	CMB-C2B-C1B	4.70	132.30	125.06
26	AB	301	PEB	CHC-C1D-ND	-4.70	108.49	113.95
26	ZB	202	PEB	CHC-C1D-ND	-4.70	108.49	113.95
26	fE	201	PEB	CHC-C4C-C3C	-4.70	122.33	130.34
26	B5	201	PEB	CHB-C4B-NB	-4.70	122.31	128.83
28	VH	1001	CYC	CMB-C2B-C1B	4.70	130.03	124.17
26	ZF	203	PEB	CHA-C1B-NB	-4.70	115.11	124.93
26	mG	201	PEB	OA-C1A-C2A	-4.70	122.44	126.17
26	W6	202	PEB	CHC-C4C-C3C	-4.70	122.33	130.34
26	B3	202	PEB	C2A-C1A-NA	4.70	112.32	108.27
26	c8	201	PEB	OA-C1A-C2A	-4.69	122.44	126.17
26	SG	201	PEB	CHA-C1B-NB	-4.69	115.11	124.93
26	L1	201	PEB	C1C-CHB-C4B	4.69	134.42	128.81
27	A6	303	PUB	CHA-C1B-C2B	-4.69	122.33	130.34
26	TA	202	PEB	CHC-C1D-ND	-4.69	108.50	113.95
28	IB	1001	CYC	CMA-C3A-C4A	4.69	132.29	125.06
26	SG	203	PEB	CHC-C1D-ND	-4.69	108.50	113.95
26	IF	202	PEB	OA-C1A-C2A	-4.69	122.44	126.17
26	G6	1002	PEB	OA-C1A-C2A	-4.69	122.44	126.17
26	L3	203	PEB	CHC-C1D-ND	-4.69	108.50	113.95
28	G6	1001	CYC	OB-C4B-C3B	-4.69	122.95	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J7	1002	PEB	CHC-C1D-ND	-4.68	108.51	113.95
26	PD	202	PEB	C2A-C1A-NA	4.68	112.31	108.27
26	H4	201	PEB	OA-C1A-C2A	-4.68	122.45	126.17
26	h6	202	PEB	CHB-C4B-NB	-4.68	122.33	128.83
26	IA	202	PEB	CHA-C1B-NB	-4.68	115.14	124.93
26	F8	201	PEB	CMB-C2B-C1B	4.68	132.28	125.06
26	l8	202	PEB	C2A-C1A-NA	4.68	112.31	108.27
26	G4	201	PEB	C1C-CHB-C4B	4.68	134.40	128.81
26	HB	1002	PEB	C4B-C3B-C2B	-4.68	101.60	106.78
26	EA	202	PEB	CHC-C4C-C3C	-4.68	122.36	130.34
26	l1	201	PEB	CHB-C4B-NB	-4.68	122.34	128.83
26	q1	201	PEB	CHC-C4C-C3C	-4.68	122.36	130.34
26	L9	201	PEB	CHB-C4B-NB	-4.68	122.34	128.83
26	JC	201	PEB	CMB-C2B-C3B	-4.68	113.42	126.12
26	LE	202	PEB	CHB-C4B-C3B	-4.68	114.52	125.32
26	VE	202	PEB	CMB-C2B-C1B	4.68	132.26	125.06
26	VG	202	PEB	CMB-C2B-C1B	4.67	132.26	125.06
28	dH	1001	CYC	CAB-C3B-C4B	4.67	128.76	121.38
26	y4	202	PEB	CHB-C4B-NB	-4.67	122.34	128.83
26	dB	201	PEB	C1C-CHB-C4B	-4.67	123.23	128.81
26	m8	201	PEB	CBC-CAC-C2C	-4.67	104.64	112.62
26	ND	202	PEB	CHA-C1B-NB	-4.67	115.16	124.93
26	S8	202	PEB	CHC-C4C-C3C	-4.67	122.37	130.34
26	E9	201	PEB	CMB-C2B-C1B	4.67	132.26	125.06
26	UD	201	PEB	CHA-C1B-C2B	4.67	136.91	124.90
28	NB	1001	CYC	OC-C1C-C2C	-4.67	122.46	126.17
28	J7	1001	CYC	CHB-C4A-NA	-4.67	115.16	124.93
26	W8	202	PEB	CHC-C4C-C3C	-4.67	122.37	130.34
26	l8	203	PEB	CBC-CAC-C2C	-4.67	104.65	112.62
26	gA	202	PEB	CHC-C1D-ND	-4.67	108.52	113.95
26	XE	201	PEB	CHB-C4B-NB	-4.67	122.35	128.83
26	Q7	201	PEB	CHB-C4B-NB	-4.67	122.35	128.83
26	A8	302	PEB	CMB-C2B-C1B	4.67	132.25	125.06
26	u4	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
26	qE	201	PEB	CHC-C1D-ND	-4.67	108.53	113.95
26	HE	201	PEB	OA-C1A-C2A	-4.67	122.46	126.17
26	Z6	202	PEB	CHA-C1B-NB	-4.67	115.17	124.93
26	q4	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
26	w4	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
28	mH	1001	CYC	CHB-C4A-C3A	4.67	136.90	124.90
26	OA	201	PEB	OA-C1A-C2A	-4.66	122.46	126.17
26	A2	305	PEB	CHB-C4B-NB	-4.66	122.36	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	oE	202	PEB	CHB-C4B-NB	-4.66	122.36	128.83
28	rH	1001	CYC	CHD-C4C-NC	4.66	130.75	125.20
27	A8	304	PUB	OD-C4D-C3D	-4.66	122.98	128.04
26	f4	201	PEB	CHB-C4B-NB	-4.66	122.36	128.83
26	rE	201	PEB	CHB-C4B-NB	-4.66	122.36	128.83
26	O6	203	PEB	C1C-CHB-C4B	4.66	134.38	128.81
26	j1	202	PEB	CHC-C1D-ND	-4.66	108.53	113.95
26	CG	202	PEB	C4B-C3B-C2B	-4.66	101.62	106.78
26	q4	201	PEB	OA-C1A-C2A	-4.66	122.47	126.17
26	a8	201	PEB	C1C-CHB-C4B	-4.66	123.24	128.81
26	B9	201	PEB	CHA-C1B-NB	-4.66	115.19	124.93
28	nH	1001	CYC	CHB-C4A-C3A	4.66	136.88	124.90
26	T1	203	PEB	CHB-C4B-NB	-4.66	122.37	128.83
26	NA	201	PEB	C4B-C3B-C2B	-4.66	101.63	106.78
26	VA	202	PEB	CAB-C3B-C2B	4.66	136.55	127.88
26	W1	202	PEB	CHC-C1D-ND	-4.66	108.54	113.95
26	iG	203	PEB	CHC-C1D-ND	-4.66	108.54	113.95
26	j8	203	PEB	CHB-C4B-NB	-4.66	122.37	128.83
26	YG	202	PEB	CHB-C4B-NB	-4.66	122.37	128.83
26	rG	201	PEB	CHB-C4B-NB	-4.66	122.37	128.83
28	E6	1001	CYC	OC-C1C-C2C	-4.66	122.47	126.17
28	EF	1001	CYC	CAB-C3B-C4B	4.66	128.73	121.38
26	S3	201	PEB	CHA-C1B-C2B	4.66	136.87	124.90
26	z4	202	PEB	CHA-C4A-NA	-4.66	119.67	125.20
26	H3	201	PEB	OA-C1A-C2A	-4.65	122.47	126.17
26	hI	201	PEB	CHC-C4C-C3C	-4.65	122.40	130.34
26	Z6	202	PEB	CHC-C1D-ND	-4.65	108.54	113.95
26	BD	201	PEB	CHB-C4B-NB	-4.65	122.37	128.83
26	RA	201	PEB	CHA-C1B-NB	-4.65	115.20	124.93
26	G1	202	PEB	CHC-C1D-ND	-4.65	108.55	113.95
26	uG	201	PEB	OA-C1A-C2A	-4.65	122.47	126.17
26	eA	201	PEB	CMB-C2B-C1B	4.65	132.22	125.06
26	kB	202	PEB	CHC-C4C-C3C	-4.65	122.41	130.34
28	LF	1001	CYC	OC-C1C-C2C	-4.65	122.48	126.17
28	KF	1001	CYC	C2B-C1B-NB	4.65	113.79	106.99
26	b1	501	PEB	OA-C1A-C2A	-4.65	122.48	126.17
26	s1	201	PEB	OA-C1A-C2A	-4.65	122.48	126.17
26	D2	1002	PEB	OA-C1A-C2A	-4.65	122.48	126.17
26	cF	202	PEB	OA-C1A-C2A	-4.65	122.48	126.17
26	n4	202	PEB	CHC-C1D-ND	-4.65	108.55	113.95
26	kE	201	PEB	CHA-C1B-NB	-4.65	115.21	124.93
27	A9	302	PUB	CHA-C4A-NA	-4.65	108.55	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e2	201	PEB	CMB-C2B-C1B	4.64	132.22	125.06
28	FB	1001	CYC	C2B-C1B-NB	4.64	113.79	106.99
26	I3	202	PEB	CHB-C4B-NB	-4.64	122.39	128.83
28	H6	1001	CYC	OC-C1C-C2C	-4.64	122.48	126.17
26	l6	202	PEB	CHB-C4B-NB	-4.64	122.39	128.83
28	QH	1001	CYC	CHB-C4A-NA	-4.64	115.22	124.93
26	W8	203	PEB	C1C-CHB-C4B	4.64	134.35	128.81
26	QG	202	PEB	CHC-C4C-C3C	-4.64	122.42	130.34
26	S2	201	PEB	C3B-C4B-NB	4.64	116.80	110.05
26	WB	202	PEB	CHC-C4C-C3C	-4.64	122.42	130.34
26	mI	203	PEB	C4B-C3B-C2B	-4.64	101.65	106.78
26	t1	202	PEB	CHC-C1D-ND	-4.64	108.56	113.95
26	M8	203	PEB	CHB-C4B-NB	-4.64	122.39	128.83
26	cB	201	PEB	OA-C1A-C2A	-4.64	122.48	126.17
26	m2	203	PEB	C4B-C3B-C2B	-4.64	101.65	106.78
26	N8	201	PEB	C4B-C3B-C2B	-4.64	101.65	106.78
26	R2	202	PEB	CHC-C1D-ND	-4.64	108.56	113.95
26	G9	201	PEB	CHC-C1D-ND	-4.64	108.56	113.95
26	DD	202	PEB	C2A-C1A-NA	4.64	112.27	108.27
26	k4	201	PEB	OA-C1A-C2A	-4.64	122.49	126.17
26	K8	201	PEB	C3D-C4D-ND	4.64	116.35	107.26
26	WB	203	PEB	CHC-C1D-ND	-4.63	108.57	113.95
28	F6	1001	CYC	C2B-C1B-NB	4.63	113.77	106.99
26	t4	202	PEB	CHA-C1B-NB	-4.63	115.24	124.93
26	R9	201	PEB	OA-C1A-C2A	-4.63	122.49	126.17
26	fB	203	PEB	CHC-C1D-ND	-4.63	108.57	113.95
26	LJ	203	PEB	CHC-C1D-ND	-4.63	108.57	113.95
26	U6	201	PEB	CHC-C4C-C3C	-4.63	122.44	130.34
26	LE	201	PEB	CBC-CAC-C2C	-4.63	104.72	112.62
26	b6	201	PEB	CMB-C2B-C1B	4.63	132.19	125.06
26	H6	1002	PEB	C4B-C3B-C2B	-4.63	101.66	106.78
26	p1	202	PEB	CHA-C1B-NB	-4.63	115.25	124.93
26	jF	202	PEB	C1C-CHB-C4B	-4.63	123.28	128.81
28	BB	1001	CYC	C2C-C1C-NC	4.63	112.26	108.27
26	k8	201	PEB	CHA-C1B-NB	-4.63	115.25	124.93
28	sH	1001	CYC	C4D-CHA-C1A	4.63	134.34	128.81
28	J2	1001	CYC	CHB-C4A-C3A	4.63	136.79	124.90
26	sG	203	PEB	C1C-CHB-C4B	4.63	134.33	128.81
26	jG	201	PEB	CHA-C1B-NB	-4.62	115.26	124.93
26	p1	202	PEB	OA-C1A-C2A	-4.62	122.50	126.17
26	fF	202	PEB	CHC-C1D-ND	-4.62	108.58	113.95
26	AA	302	PEB	CMB-C2B-C1B	4.62	132.18	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m1	203	PEB	CHC-C4C-C3C	-4.62	122.45	130.34
26	UG	202	PEB	CHA-C1B-NB	-4.62	115.26	124.93
26	aE	202	PEB	CHC-C1D-ND	-4.62	108.58	113.95
26	z4	201	PEB	CHB-C4B-C3B	-4.62	114.64	125.32
26	R3	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
26	LD	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
26	T6	201	PEB	OA-C1A-C2A	-4.62	122.50	126.17
26	Y9	201	PEB	CHC-C1D-ND	-4.62	108.58	113.95
26	yE	301	PEB	CHB-C4B-NB	-4.62	122.42	128.83
26	PG	201	PEB	OA-C1A-NA	4.62	130.53	124.94
26	F4	203	PEB	CHB-C4B-NB	-4.62	122.42	128.83
26	P8	202	PEB	CHC-C4C-C3C	-4.62	122.46	130.34
26	fA	202	PEB	CHC-C4C-C3C	-4.62	122.46	130.34
26	VI	201	PEB	OA-C1A-C2A	-4.62	122.50	126.17
26	W9	201	PEB	CHC-C1D-ND	-4.62	108.59	113.95
26	TF	201	PEB	C1C-CHB-C4B	4.62	134.32	128.81
26	XD	201	PEB	CHC-C1D-ND	-4.62	108.59	113.95
28	EH	1001	CYC	CMB-C2B-C1B	4.62	129.93	124.17
28	qH	1002	CYC	CMB-C2B-C1B	4.62	129.93	124.17
28	M6	1001	CYC	CAB-C3B-C4B	4.62	128.67	121.38
27	xE	301	PUB	C1D-CHC-C4C	-4.61	103.33	113.37
26	NE	201	PEB	OA-C1A-NA	4.61	130.53	124.94
26	CC	203	PEB	CHB-C4B-NB	-4.61	122.43	128.83
28	MI	1001	CYC	OB-C4B-C3B	-4.61	123.03	128.04
26	i1	201	PEB	C1C-CHB-C4B	4.61	134.32	128.81
26	RI	202	PEB	CHC-C1D-ND	-4.61	108.59	113.95
28	B6	1001	CYC	C2C-C1C-NC	4.61	112.25	108.27
28	OH	1001	CYC	CHB-C4A-C3A	4.61	136.76	124.90
28	D2	1001	CYC	CAB-C3B-C4B	4.61	128.66	121.38
28	LI	1001	CYC	OC-C1C-C2C	-4.61	122.51	126.17
26	VA	201	PEB	CHA-C1B-NB	-4.61	115.29	124.93
26	kA	201	PEB	CHA-C1B-NB	-4.61	115.29	124.93
26	D2	1002	PEB	CHB-C4B-NB	-4.61	122.43	128.83
28	B6	1002	CYC	C1B-C2B-C3B	-4.61	103.06	107.87
26	f6	203	PEB	CHB-C4B-NB	-4.61	122.43	128.83
28	CH	1001	CYC	CMB-C2B-C1B	4.61	129.92	124.17
28	CH	1001	CYC	CHB-C4A-C3A	4.61	136.75	124.90
26	N3	201	PEB	CHC-C1D-ND	-4.61	108.60	113.95
26	kF	202	PEB	OA-C1A-C2A	-4.61	122.51	126.17
27	xG	305	PUB	C1C-C2C-C3C	-4.61	101.68	106.78
26	X3	202	PEB	C2A-C1A-NA	4.61	112.25	108.27
26	lA	203	PEB	CBC-CAC-C2C	-4.61	104.76	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	NI	1002	PEB	OA-C1A-C2A	-4.61	122.51	126.17
26	SE	201	PEB	CHA-C1B-NB	-4.61	115.30	124.93
26	W6	202	PEB	OA-C1A-C2A	-4.61	122.51	126.17
28	IH	1001	CYC	CHD-C4C-NC	4.61	130.68	125.20
27	Q8	201	PUB	CHC-C1D-ND	-4.61	107.90	113.72
27	yG	302	PUB	CHC-C1D-ND	-4.61	107.90	113.72
26	X3	201	PEB	CHC-C1D-ND	-4.61	108.60	113.95
26	I4	201	PEB	CHC-C1D-ND	-4.61	108.60	113.95
26	U4	202	PEB	CHB-C4B-NB	-4.60	122.44	128.83
26	fF	203	PEB	CHB-C4B-NB	-4.60	122.44	128.83
27	Q8	201	PUB	C1C-C2C-C3C	-4.60	101.69	106.78
28	nH	1001	CYC	CAB-C3B-C4B	4.60	128.65	121.38
26	OE	203	PEB	C1C-CHB-C4B	4.60	134.31	128.81
26	sE	202	PEB	C1C-CHB-C4B	4.60	134.31	128.81
26	MA	202	PEB	CHB-C4B-NB	-4.60	122.44	128.83
26	X4	202	PEB	C3D-C4D-ND	4.60	116.29	107.26
28	BB	1001	CYC	CHB-C4A-NA	-4.60	115.31	124.93
26	X8	202	PEB	OA-C1A-C2A	-4.60	122.51	126.17
26	k7	201	PEB	CHB-C4B-NB	-4.60	122.44	128.83
26	V9	203	PEB	CHC-C1D-ND	-4.60	108.60	113.95
26	YG	203	PEB	C1C-CHB-C4B	4.60	134.31	128.81
26	JE	202	PEB	OA-C1A-C2A	-4.60	122.52	126.17
26	EJ	201	PEB	CMB-C2B-C1B	4.60	132.15	125.06
26	G6	1002	PEB	C4B-C3B-C2B	-4.60	101.69	106.78
26	WE	202	PEB	C4B-C3B-C2B	-4.60	101.69	106.78
26	X4	203	PEB	CHA-C1B-NB	-4.60	115.31	124.93
26	aG	201	PEB	CHA-C1B-NB	-4.60	115.31	124.93
26	oE	201	PEB	CMB-C2B-C1B	4.60	132.14	125.06
26	T7	202	PEB	CHB-C4B-NB	-4.60	122.45	128.83
26	MJ	201	PEB	CMB-C2B-C1B	4.60	132.14	125.06
26	N1	202	PEB	CHC-C4C-C3C	-4.60	122.50	130.34
26	F9	203	PEB	C2A-C1A-NA	4.59	112.23	108.27
26	V2	203	PEB	CHB-C4B-NB	-4.59	122.45	128.83
26	J4	202	PEB	CHB-C4B-NB	-4.59	122.45	128.83
28	DI	1001	CYC	CAB-C3B-C4B	4.59	128.63	121.38
26	K9	202	PEB	C1C-CHB-C4B	-4.59	123.32	128.81
26	jA	203	PEB	OA-C1A-C2A	-4.59	122.52	126.17
26	Q1	201	PEB	CHC-C1D-ND	-4.59	108.62	113.95
26	I1	201	PEB	CMB-C2B-C1B	4.59	132.13	125.06
26	A7	301	PEB	OA-C1A-C2A	-4.59	122.52	126.17
28	K7	1001	CYC	CAB-C3B-C4B	4.59	128.63	121.38
26	U2	201	PEB	C1C-CHB-C4B	4.59	134.29	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A1	201	PEB	CHA-C1B-NB	-4.59	115.33	124.93
26	X9	201	PEB	CHC-C1D-ND	-4.59	108.62	113.95
28	JH	1001	CYC	CHD-C4C-NC	4.59	130.66	125.20
26	E1	201	PEB	CHB-C4B-NB	-4.59	122.47	128.83
26	S8	203	PEB	OA-C1A-C2A	-4.59	122.53	126.17
26	QE	203	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	GG	203	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	L9	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
26	F1	202	PEB	C1C-CHB-C4B	4.58	134.28	128.81
26	EA	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	UB	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
28	MB	1001	CYC	CAB-C3B-C4B	4.58	128.62	121.38
26	MA	202	PEB	C3D-C4D-ND	4.58	116.25	107.26
28	JF	1001	CYC	CAB-C3B-C4B	4.58	128.62	121.38
26	O8	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
26	S1	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	ID	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
26	YE	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
26	bB	201	PEB	CMB-C2B-C1B	4.58	132.12	125.06
28	L2	1001	CYC	CBB-CAB-C3B	-4.58	99.80	112.43
26	bG	202	PEB	CHC-C1D-ND	4.58	119.27	113.95
26	l1	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	S7	201	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	MA	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	VB	201	PEB	CHC-C1D-ND	-4.58	108.63	113.95
26	d7	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
26	x1	202	PEB	C3B-C4B-NB	4.58	116.71	110.05
26	C9	201	PEB	CMB-C2B-C1B	4.58	132.12	125.06
28	HB	1001	CYC	OC-C1C-C2C	-4.58	122.53	126.17
26	G3	201	PEB	C3D-C4D-ND	4.58	116.24	107.26
27	K3	203	PUB	C4B-CHB-C1C	-4.58	123.34	128.81
26	W7	202	PEB	CHC-C1D-ND	-4.58	108.63	113.95
26	oE	203	PEB	CHC-C1D-ND	-4.58	108.63	113.95
26	GD	202	PEB	CHB-C4B-NB	-4.58	122.48	128.83
26	U4	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	Z4	201	PEB	OA-C1A-C2A	-4.58	122.53	126.17
28	eH	1001	CYC	CHB-C4A-C3A	4.58	136.67	124.90
26	I4	202	PEB	OA-C1A-C2A	-4.58	122.53	126.17
26	eG	202	PEB	C4B-C3B-C2B	-4.58	101.72	106.78
26	R8	201	PEB	C1C-CHB-C4B	-4.57	123.34	128.81
26	O3	201	PEB	CHA-C1B-C2B	4.57	136.66	124.90
26	TD	202	PEB	C4B-C3B-C2B	-4.57	101.72	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E7	1001	CYC	OC-C1C-C2C	-4.57	122.54	126.17
27	K4	203	PUB	CHA-C4A-NA	-4.57	108.64	113.95
26	YI	202	PEB	CHB-C4B-NB	-4.57	122.48	128.83
26	GJ	202	PEB	CHB-C4B-NB	-4.57	122.48	128.83
26	A1	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
28	D6	1001	CYC	C1B-NB-C4B	-4.57	104.85	110.67
26	b7	201	PEB	CHB-C4B-NB	-4.57	122.48	128.83
27	A8	304	PUB	CHA-C1B-C2B	-4.57	122.54	130.34
26	uG	202	PEB	CMB-C2B-C1B	4.57	132.10	125.06
28	D7	1001	CYC	OB-C4B-C3B	-4.57	123.08	128.04
26	Z1	201	PEB	CHB-C4B-NB	-4.57	122.49	128.83
26	tE	202	PEB	CBC-CAC-C2C	4.57	120.42	112.62
26	hF	201	PEB	CHC-C1D-ND	-4.57	108.64	113.95
26	SI	201	PEB	C3B-C4B-NB	4.57	116.70	110.05
26	l2	201	PEB	C1C-CHB-C4B	4.57	134.27	128.81
26	H1	203	PEB	OA-C1A-C2A	-4.57	122.54	126.17
26	W1	201	PEB	CHC-C1D-ND	-4.57	108.64	113.95
26	Z8	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
26	OD	201	PEB	C3D-C4D-ND	4.57	116.22	107.26
26	GG	201	PEB	C3D-C4D-ND	4.57	116.22	107.26
26	D7	1002	PEB	CHA-C1B-NB	-4.57	115.38	124.93
26	g8	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
26	HA	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
26	ZA	201	PEB	CMB-C2B-C1B	4.57	132.10	125.06
26	Q8	202	PEB	CHB-C4B-NB	-4.57	122.49	128.83
26	SD	201	PEB	CHA-C1B-C2B	4.57	136.65	124.90
28	cH	1001	CYC	CMB-C2B-C1B	4.57	129.87	124.17
26	MD	201	PEB	OA-C1A-C2A	-4.57	122.54	126.17
26	gG	201	PEB	CHA-C1B-NB	-4.57	115.38	124.93
26	g2	203	PEB	C4B-C3B-C2B	-4.57	101.73	106.78
28	H6	1001	CYC	C2B-C1B-NB	4.57	113.67	106.99
26	y1	201	PEB	OA-C1A-C2A	-4.56	122.54	126.17
26	L1	203	PEB	CHB-C4B-NB	-4.56	122.50	128.83
26	N1	202	PEB	CHB-C4B-NB	-4.56	122.50	128.83
26	S7	203	PEB	CHC-C4C-C3C	-4.56	122.55	130.34
26	IE	201	PEB	C3B-C4B-NB	4.56	116.69	110.05
28	NH	1001	CYC	CHB-C4A-C3A	4.56	136.64	124.90
27	A8	304	PUB	CHC-C1D-ND	-4.56	107.95	113.72
26	jA	202	PEB	CHC-C1D-ND	-4.56	108.65	113.95
26	OI	201	PEB	C3B-C4B-NB	4.56	116.69	110.05
26	g1	203	PEB	C1C-CHB-C4B	4.56	134.26	128.81
26	Q2	201	PEB	CMA-C2A-C1A	-4.56	102.57	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S4	202	PEB	OA-C1A-C2A	-4.56	122.55	126.17
26	lA	202	PEB	C2A-C1A-NA	4.56	112.21	108.27
26	d1	203	PEB	CMB-C2B-C1B	4.56	132.09	125.06
26	E8	203	PEB	CHC-C4C-C3C	-4.56	122.56	130.34
26	m8	202	PEB	C1C-CHB-C4B	-4.56	123.36	128.81
26	gG	203	PEB	CMB-C2B-C1B	4.56	132.09	125.06
26	MA	203	PEB	CHC-C4C-C3C	-4.56	122.56	130.34
26	L5	201	PEB	CHA-C1B-NB	-4.56	115.39	124.93
26	I8	203	PEB	CHC-C4C-C3C	-4.56	122.56	130.34
28	HB	1001	CYC	C2B-C1B-NB	4.56	113.66	106.99
28	qH	1002	CYC	CMA-C3A-C4A	4.56	132.09	125.06
26	m6	202	PEB	CHC-C4C-C3C	-4.56	122.56	130.34
26	E8	201	PEB	C1C-CHB-C4B	4.56	134.25	128.81
26	P8	202	PEB	CMB-C2B-C1B	4.56	132.08	125.06
26	BE	201	PEB	OA-C1A-NA	4.56	130.46	124.94
28	DF	1003	CYC	C2B-C1B-NB	4.56	113.66	106.99
26	W8	202	PEB	OA-C1A-C2A	-4.56	122.55	126.17
26	Y8	203	PEB	OA-C1A-C2A	-4.56	122.55	126.17
26	w4	203	PEB	CHB-C4B-NB	-4.55	122.51	128.83
26	EA	203	PEB	OA-C1A-C2A	-4.55	122.55	126.17
26	RG	201	PEB	CHB-C4B-NB	-4.55	122.51	128.83
26	aE	203	PEB	CHA-C1B-NB	-4.55	115.41	124.93
26	X1	202	PEB	C3D-C4D-ND	4.55	116.19	107.26
26	f7	203	PEB	OA-C1A-C2A	-4.55	122.55	126.17
26	TD	201	PEB	OA-C1A-C2A	-4.55	122.55	126.17
26	WD	202	PEB	OA-C1A-C2A	-4.55	122.55	126.17
26	UI	201	PEB	C3D-C4D-ND	4.55	116.19	107.26
26	TD	201	PEB	CHC-C4C-C3C	-4.55	122.57	130.34
26	VB	202	PEB	OA-C1A-C2A	-4.55	122.55	126.17
26	N4	203	PEB	CHB-C4B-NB	-4.55	122.52	128.83
26	14	201	PEB	CHB-C4B-NB	-4.55	122.52	128.83
26	dF	201	PEB	OA-C1A-C2A	-4.55	122.56	126.17
28	YH	1004	CYC	CAB-C3B-C4B	4.55	128.56	121.38
26	PI	202	PEB	CHB-C4B-NB	-4.55	122.52	128.83
28	DB	1001	CYC	C4D-CHA-C1A	4.55	134.24	128.81
26	c1	202	PEB	OA-C1A-C2A	-4.55	122.56	126.17
26	M3	201	PEB	OA-C1A-C2A	-4.55	122.56	126.17
26	cE	203	PEB	OA-C1A-C2A	-4.55	122.56	126.17
26	F9	203	PEB	OA-C1A-C2A	-4.55	122.56	126.17
26	E9	201	PEB	CHC-C1D-ND	-4.55	108.67	113.95
28	qH	1001	CYC	CHB-C4A-C3A	4.55	136.59	124.90
26	C3	201	PEB	C1C-CHB-C4B	4.55	134.24	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	hI	202	PEB	CHB-C4B-NB	-4.55	122.52	128.83
26	a2	202	PEB	OA-C1A-C2A	-4.54	122.56	126.17
26	UE	203	PEB	OA-C1A-C2A	-4.54	122.56	126.17
26	jE	202	PEB	CMB-C2B-C1B	4.54	132.06	125.06
26	HA	202	PEB	C1C-CHB-C4B	-4.54	123.38	128.81
26	mA	202	PEB	CHA-C1B-NB	-4.54	115.43	124.93
26	T1	201	PEB	CMD-C2D-C3D	-4.54	123.66	130.06
28	F2	1001	CYC	C1B-NB-C4B	-4.54	104.89	110.67
26	qE	203	PEB	C1C-CHB-C4B	4.54	134.23	128.81
26	D6	1002	PEB	C4B-C3B-C2B	-4.54	101.76	106.78
26	b6	202	PEB	CHB-C4B-NB	-4.54	122.53	128.83
26	N3	203	PEB	OA-C1A-C2A	-4.54	122.56	126.17
27	A4	203	PUB	CHA-C4A-NA	-4.54	108.67	113.95
26	U2	201	PEB	C3D-C4D-ND	4.54	116.17	107.26
26	A4	201	PEB	C4B-C3B-C2B	-4.54	101.76	106.78
26	c4	203	PEB	C1C-CHB-C4B	4.54	134.23	128.81
26	VG	201	PEB	CHC-C4C-C3C	-4.54	122.60	130.34
26	fE	201	PEB	CHB-C4B-NB	-4.54	122.53	128.83
26	OD	201	PEB	CHA-C1B-C2B	4.54	136.56	124.90
26	UE	202	PEB	CHA-C1B-NB	-4.54	115.45	124.93
28	gH	1001	CYC	CMB-C2B-C1B	4.53	129.83	124.17
26	J4	201	PEB	C1C-CHB-C4B	4.53	134.23	128.81
26	V2	201	PEB	CMB-C2B-C1B	4.53	132.05	125.06
26	LE	201	PEB	C3D-C4D-ND	4.53	116.15	107.26
26	LC	201	PEB	CHB-C4B-NB	-4.53	122.54	128.83
26	R4	202	PEB	CHC-C4C-C3C	-4.53	122.61	130.34
26	KC	202	PEB	CHC-C4C-C3C	-4.53	122.61	130.34
26	E9	202	PEB	OA-C1A-C2A	-4.53	122.57	126.17
28	CB	1001	CYC	C4D-CHA-C1A	4.53	134.22	128.81
26	lG	201	PEB	C2A-C1A-NA	4.53	112.18	108.27
28	Jl	1001	CYC	CAB-C3B-C4B	4.53	128.53	121.38
26	LD	203	PEB	CHC-C1D-ND	-4.53	108.69	113.95
26	a4	201	PEB	CHB-C4B-NB	-4.53	122.55	128.83
26	F1	202	PEB	CHA-C1B-NB	-4.53	115.46	124.93
26	l4	201	PEB	OA-C1A-C2A	-4.53	122.57	126.17
26	k6	202	PEB	CHC-C4C-C3C	-4.53	122.62	130.34
28	PH	1001	CYC	CMB-C2B-C1B	4.53	129.82	124.17
26	Y2	202	PEB	CHB-C4B-NB	-4.53	122.55	128.83
26	Q1	202	PEB	OA-C1A-C2A	-4.52	122.58	126.17
26	MA	202	PEB	CHC-C4C-C3C	-4.52	122.62	130.34
26	h1	202	PEB	C1C-CHB-C4B	-4.52	123.41	128.81
26	D3	202	PEB	C2A-C1A-NA	4.52	112.17	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HJ	202	PEB	C1C-CHB-C4B	4.52	134.21	128.81
26	Q4	202	PEB	OA-C1A-C2A	-4.52	122.58	126.17
26	WB	202	PEB	OA-C1A-C2A	-4.52	122.58	126.17
26	k2	202	PEB	CHC-C1D-ND	-4.52	108.70	113.95
28	HI	1001	CYC	CHB-C4A-NA	-4.52	115.48	124.93
26	dG	201	PEB	CHC-C4C-C3C	-4.52	122.63	130.34
26	QA	202	PEB	CHB-C4B-NB	-4.52	122.56	128.83
26	JD	201	PEB	CHC-C1D-ND	-4.52	108.70	113.95
26	yG	301	PEB	CHB-C4B-NB	-4.52	122.56	128.83
26	RA	202	PEB	CMB-C2B-C1B	4.52	132.02	125.06
26	eF	201	PEB	OA-C1A-C2A	-4.52	122.58	126.17
26	RA	201	PEB	C1C-CHB-C4B	-4.52	123.41	128.81
26	SF	202	PEB	CHC-C1D-ND	-4.52	108.70	113.95
26	LD	201	PEB	CHA-C1B-NB	-4.52	115.48	124.93
28	OH	1001	CYC	CHD-C4C-NC	4.52	130.58	125.20
26	PE	202	PEB	C1C-CHB-C4B	4.52	134.21	128.81
26	m1	203	PEB	OA-C1A-C2A	-4.52	122.58	126.17
27	AB	303	PUB	CHA-C1B-C2B	-4.52	122.63	130.34
26	JD	202	PEB	C2A-C1A-NA	4.52	112.17	108.27
26	XD	202	PEB	C2A-C1A-NA	4.52	112.17	108.27
28	IF	1001	CYC	CMA-C3A-C4A	4.52	132.02	125.06
26	l7	203	PEB	CHA-C1B-NB	-4.52	115.48	124.93
28	CB	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
26	UB	203	PEB	CHB-C4B-NB	-4.52	122.56	128.83
26	uE	203	PEB	CHB-C4B-NB	-4.52	122.56	128.83
26	SE	202	PEB	CHB-C4B-C3B	-4.52	114.89	125.32
28	B6	1001	CYC	CHB-C4A-NA	-4.52	115.49	124.93
26	Y7	202	PEB	C1C-CHB-C4B	4.52	134.20	128.81
26	WE	203	PEB	OA-C1A-C2A	-4.52	122.58	126.17
26	LF	1002	PEB	CHA-C1B-NB	-4.51	115.49	124.93
28	MI	1001	CYC	C2B-C1B-NB	4.51	113.60	106.99
26	F1	202	PEB	CHB-C4B-NB	-4.51	122.56	128.83
27	21	402	PUB	C1C-C2C-C3C	-4.51	101.79	106.78
27	yG	302	PUB	CMD-C2D-C3D	4.51	134.54	127.77
26	I5	202	PEB	CHB-C4B-NB	-4.51	122.57	128.83
27	A8	303	PUB	CMA-C2A-C1A	4.51	132.01	121.39
28	YH	1002	CYC	CAB-C3B-C4B	4.51	128.51	121.38
26	U6	203	PEB	C1C-CHB-C4B	-4.51	123.42	128.81
26	A4	201	PEB	C3B-C4B-NB	4.51	116.61	110.05
27	AA	303	PUB	CMA-C2A-C1A	4.51	132.00	121.39
26	qG	202	PEB	CHA-C1B-C2B	4.51	136.50	124.90
26	q1	202	PEB	CHB-C4B-NB	-4.51	122.57	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	XJ	203	PEB	OA-C1A-C2A	-4.51	122.59	126.17
26	FE	201	PEB	CHC-C1D-ND	-4.51	108.71	113.95
26	eE	202	PEB	CAA-C3A-C2A	-4.51	102.99	114.26
27	yE	302	PUB	C1D-CHC-C4C	-4.51	103.56	113.37
26	g1	202	PEB	CHC-C4C-C3C	-4.51	122.65	130.34
28	tH	1001	CYC	CHD-C4C-NC	4.51	130.57	125.20
26	M8	202	PEB	CHC-C4C-C3C	-4.51	122.65	130.34
26	N2	1002	PEB	OA-C1A-C2A	-4.51	122.59	126.17
26	VE	202	PEB	OA-C1A-C2A	-4.51	122.59	126.17
26	H5	201	PEB	CHA-C1B-NB	-4.51	115.50	124.93
26	WG	201	PEB	C1C-CHB-C4B	4.51	134.19	128.81
26	KB	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
26	ME	202	PEB	C1C-CHB-C4B	4.51	134.19	128.81
26	g7	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
26	RE	201	PEB	CHB-C4B-NB	-4.51	122.58	128.83
26	i1	202	PEB	C1C-CHB-C4B	4.51	134.19	128.81
26	k4	201	PEB	CHC-C1D-ND	-4.50	108.72	113.95
26	RB	201	PEB	CHC-C1D-ND	-4.50	108.72	113.95
26	VI	201	PEB	CMB-C2B-C1B	4.50	132.00	125.06
28	fH	1001	CYC	CHB-C4A-C3A	4.50	136.48	124.90
26	Y7	202	PEB	CMB-C2B-C1B	4.50	132.00	125.06
26	DE	202	PEB	C3D-C4D-ND	4.50	116.09	107.26
26	IJ	202	PEB	CHA-C1B-NB	-4.50	115.51	124.93
26	YE	203	PEB	CHB-C4B-NB	-4.50	122.58	128.83
26	FA	201	PEB	CHA-C1B-NB	-4.50	115.52	124.93
26	f4	202	PEB	CHC-C1D-ND	-4.50	108.72	113.95
26	SG	203	PEB	CMB-C2B-C1B	4.50	132.00	125.06
26	GD	201	PEB	C3D-C4D-ND	4.50	116.09	107.26
26	Y7	201	PEB	OA-C1A-C2A	-4.50	122.59	126.17
26	RB	201	PEB	OA-C1A-C2A	-4.50	122.59	126.17
26	VI	203	PEB	CHB-C4B-NB	-4.50	122.59	128.83
26	rG	201	PEB	CHC-C4C-C3C	-4.50	122.66	130.34
26	Y3	303	PEB	CMB-C2B-C1B	4.50	131.99	125.06
27	A7	303	PUB	CMA-C2A-C1A	4.50	131.97	121.39
28	fH	1001	CYC	CAB-C3B-C4B	4.50	128.48	121.38
26	AF	302	PEB	CHB-C4B-NB	-4.50	122.59	128.83
26	MA	203	PEB	CHB-C4B-NB	-4.50	122.59	128.83
26	rE	201	PEB	CHA-C4A-NA	4.50	130.55	125.20
26	WE	201	PEB	C3D-C4D-ND	4.49	116.08	107.26
28	GB	1001	CYC	CMA-C3A-C4A	4.49	131.99	125.06
26	L5	201	PEB	CHC-C1D-ND	-4.49	108.73	113.95
28	F7	1001	CYC	C1B-NB-C4B	-4.49	104.95	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U3	201	PEB	OD-C4D-ND	-4.49	119.27	125.93
26	fA	203	PEB	CHB-C4B-NB	-4.49	122.59	128.83
26	HJ	202	PEB	CHB-C4B-NB	-4.49	122.59	128.83
26	k7	202	PEB	C1C-CHB-C4B	4.49	134.18	128.81
26	O1	201	PEB	C3B-C4B-NB	4.49	116.58	110.05
27	wE	304	PUB	CHA-C1B-C2B	-4.49	122.67	130.34
28	JI	1001	CYC	CHB-C4A-C3A	4.49	136.45	124.90
26	N1	203	PEB	CHB-C4B-NB	-4.49	122.60	128.83
26	J9	203	PEB	CHB-C4B-NB	-4.49	122.60	128.83
28	wH	1001	CYC	CAB-C3B-C4B	4.49	128.47	121.38
26	F5	203	PEB	CHB-C4B-NB	-4.49	122.60	128.83
26	J4	203	PEB	OA-C1A-C2A	-4.49	122.60	126.17
26	bF	202	PEB	CHA-C1B-NB	-4.49	115.54	124.93
26	IJ	202	PEB	OA-C1A-C2A	-4.49	122.60	126.17
26	MG	203	PEB	CHB-C4B-NB	-4.49	122.60	128.83
26	D3	202	PEB	CHA-C1B-NB	-4.49	115.54	124.93
26	L1	202	PEB	OA-C1A-C2A	-4.49	122.60	126.17
26	p4	202	PEB	OA-C1A-C2A	-4.49	122.60	126.17
26	J3	202	PEB	C2A-C1A-NA	4.49	112.14	108.27
26	KE	202	PEB	C4B-C3B-C2B	-4.49	101.81	106.78
26	i4	201	PEB	C1C-CHB-C4B	4.49	134.17	128.81
26	C9	201	PEB	CHC-C1D-ND	-4.49	108.74	113.95
26	V3	201	PEB	CMB-C2B-C1B	4.49	131.97	125.06
28	uH	1001	CYC	CAB-C3B-C4B	4.49	128.46	121.38
26	GG	201	PEB	CMA-C2A-C1A	-4.49	102.73	112.40
26	jF	201	PEB	CMB-C2B-C1B	4.48	131.97	125.06
26	X9	203	PEB	CHC-C1D-ND	-4.48	108.74	113.95
26	Z8	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
26	F3	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
26	NB	1002	PEB	C2A-C1A-NA	4.48	112.14	108.27
26	NF	1002	PEB	C4B-C3B-C2B	-4.48	101.82	106.78
28	TH	1001	CYC	CMB-C2B-C1B	4.48	129.76	124.17
26	KC	201	PEB	CHB-C4B-NB	-4.48	122.61	128.83
26	A6	301	PEB	CHC-C1D-ND	-4.48	108.74	113.95
26	Z8	202	PEB	CHC-C1D-ND	-4.48	108.74	113.95
26	M8	203	PEB	C3D-C4D-ND	4.48	116.05	107.26
26	G8	202	PEB	CHC-C4C-C3C	-4.48	122.69	130.34
26	mE	203	PEB	CMB-C2B-C1B	4.48	131.97	125.06
26	M1	403	PEB	CHA-C1B-NB	-4.48	115.56	124.93
26	j1	201	PEB	C3B-C4B-NB	4.48	116.57	110.05
26	TI	203	PEB	CHC-C4C-C3C	-4.48	122.69	130.34
26	M8	202	PEB	C3D-C4D-ND	4.48	116.05	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q7	202	PEB	CHB-C4B-NB	-4.48	122.61	128.83
26	X9	203	PEB	CHB-C4B-NB	-4.48	122.61	128.83
26	m4	203	PEB	OA-C1A-C2A	-4.48	122.61	126.17
27	yE	303	PUB	CHA-C4A-NA	-4.48	108.75	113.95
26	g1	201	PEB	CHC-C4C-C3C	-4.48	122.70	130.34
28	SH	1001	CYC	CAB-C3B-C4B	4.48	128.45	121.38
26	X1	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
26	NJ	202	PEB	OA-C1A-C2A	-4.48	122.61	126.17
26	WD	201	PEB	C3D-C4D-ND	4.48	116.04	107.26
26	d1	203	PEB	CHB-C4B-NB	-4.48	122.62	128.83
26	W8	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
27	BA	302	PUB	CHA-C4A-NA	-4.48	108.75	113.95
26	AD	201	PEB	CHC-C4C-C3C	-4.47	122.70	130.34
26	QF	201	PEB	CHC-C1D-ND	-4.47	108.75	113.95
26	V8	201	PEB	CBC-CAC-C2C	-4.47	104.98	112.62
26	N3	201	PEB	CHB-C4B-NB	-4.47	122.62	128.83
26	eG	201	PEB	CHB-C4B-NB	-4.47	122.62	128.83
26	B3	202	PEB	CHC-C1D-ND	-4.47	108.75	113.95
26	D9	201	PEB	CHB-C4B-NB	-4.47	122.62	128.83
28	iH	1001	CYC	CHB-C4A-C3A	4.47	136.40	124.90
26	W3	201	PEB	C3D-C4D-ND	4.47	116.03	107.26
26	QD	201	PEB	C3D-C4D-ND	4.47	116.03	107.26
26	GJ	202	PEB	CBC-CAC-C2C	4.47	120.25	112.62
26	mF	201	PEB	CMB-C2B-C1B	4.47	131.95	125.06
26	cE	201	PEB	C3B-C4B-NB	4.47	116.56	110.05
26	F8	201	PEB	CHA-C1B-NB	-4.47	115.58	124.93
26	j1	201	PEB	CHB-C4B-NB	-4.47	122.62	128.83
26	OA	203	PEB	OA-C1A-C2A	-4.47	122.62	126.17
26	A3	201	PEB	C1C-CHB-C4B	4.47	134.15	128.81
28	C6	1001	CYC	C4D-CHA-C1A	4.47	134.15	128.81
26	JD	203	PEB	C4B-C3B-C2B	-4.47	101.83	106.78
26	P8	202	PEB	CHA-C1B-NB	-4.47	115.58	124.93
26	pE	202	PEB	CMB-C2B-C1B	4.47	131.95	125.06
28	G7	1001	CYC	C1B-C2B-C3B	-4.47	103.21	107.87
26	c6	201	PEB	OA-C1A-C2A	-4.47	122.62	126.17
28	OH	1001	CYC	CAB-C3B-C4B	4.47	128.44	121.38
26	SA	203	PEB	OA-C1A-C2A	-4.47	122.62	126.17
26	RB	201	PEB	CMB-C2B-C1B	4.47	131.94	125.06
27	A7	303	PUB	CBB-CAB-C3B	4.47	120.24	112.62
28	vH	1001	CYC	CMB-C2B-C1B	4.47	129.74	124.17
26	k1	202	PEB	CHC-C1D-ND	-4.47	108.76	113.95
28	IH	1001	CYC	CAB-C3B-C4B	4.47	128.43	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C4	201	PEB	CHC-C4C-C3C	-4.46	122.72	130.34
26	M9	201	PEB	CMB-C2B-C1B	4.46	131.94	125.06
26	IJ	203	PEB	CAB-C3B-C4B	4.46	132.91	125.01
26	j6	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
26	J7	1002	PEB	CHB-C4B-NB	-4.46	122.64	128.83
26	e2	201	PEB	CHC-C1D-ND	-4.46	108.77	113.95
26	N1	201	PEB	C3D-C4D-ND	4.46	116.01	107.26
26	N3	203	PEB	CAB-CBB-CGB	-4.46	104.00	113.60
26	X1	203	PEB	CHC-C4C-C3C	-4.46	122.73	130.34
26	HJ	201	PEB	CHA-C1B-NB	-4.46	115.60	124.93
26	Q1	201	PEB	CMB-C2B-C1B	4.46	131.94	125.06
26	P7	202	PEB	CMB-C2B-C1B	4.46	131.94	125.06
26	oE	202	PEB	CHC-C4C-C3C	-4.46	122.73	130.34
26	D9	203	PEB	OA-C1A-C2A	-4.46	122.63	126.17
26	D8	201	PEB	C2A-C1A-NA	4.46	112.12	108.27
26	II	201	PEB	CMB-C2B-C1B	4.46	131.93	125.06
28	FI	1001	CYC	C1B-NB-C4B	-4.46	104.99	110.67
26	f8	203	PEB	CHC-C1D-ND	-4.46	108.77	113.95
26	QE	203	PEB	C2A-C1A-NA	4.46	112.12	108.27
27	AA	303	PUB	C1D-CHC-C4C	4.46	123.06	113.37
26	dF	202	PEB	CHB-C4B-NB	-4.46	122.64	128.83
26	oG	201	PEB	CHA-C1B-NB	-4.46	115.61	124.93
26	L4	201	PEB	C1C-CHB-C4B	4.46	134.13	128.81
26	I5	202	PEB	CHC-C1D-ND	-4.46	108.77	113.95
28	IH	1001	CYC	CHB-C4A-C3A	4.46	136.36	124.90
26	f1	202	PEB	CHC-C1D-ND	-4.46	108.77	113.95
26	ME	201	PEB	OA-C1A-C2A	-4.46	122.63	126.17
26	p4	202	PEB	CHA-C4A-NA	-4.46	119.91	125.20
26	DF	1002	PEB	CHA-C1B-NB	-4.46	115.61	124.93
26	Z7	201	PEB	CMB-C2B-C1B	4.46	131.93	125.06
27	K1	203	PUB	CHA-C4A-NA	-4.46	108.77	113.95
26	AG	201	PEB	CHA-C1B-NB	-4.46	115.61	124.93
26	WB	201	PEB	C3D-C4D-ND	4.46	116.00	107.26
26	P3	203	PEB	C1C-CHB-C4B	4.45	134.13	128.81
26	SE	203	PEB	C1C-CHB-C4B	4.45	134.13	128.81
27	N9	201	PUB	CMA-C2A-C1A	4.45	131.87	121.39
26	b4	501	PEB	C1C-CHB-C4B	-4.45	123.49	128.81
28	LH	1001	CYC	CMB-C2B-C1B	4.45	129.73	124.17
28	tH	1001	CYC	CMB-C2B-C1B	4.45	129.73	124.17
26	ZE	201	PEB	CHB-C4B-NB	-4.45	122.65	128.83
26	zG	501	PEB	OA-C1A-NA	4.45	130.33	124.94
26	RA	201	PEB	OA-C1A-C2A	-4.45	122.63	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	LI	1001	CYC	CHB-C4A-C3A	4.45	136.35	124.90
26	OE	201	PEB	C3D-C4D-ND	4.45	115.99	107.26
28	I7	1001	CYC	CMA-C3A-C4A	4.45	131.92	125.06
26	d6	201	PEB	C1C-CHB-C4B	-4.45	123.49	128.81
26	CG	201	PEB	OA-C1A-C2A	-4.45	122.63	126.17
26	FJ	202	PEB	CHA-C1B-NB	-4.45	115.62	124.93
26	PE	201	PEB	CHB-C4B-NB	-4.45	122.65	128.83
28	LH	1001	CYC	CHB-C4A-C3A	4.45	136.34	124.90
26	VF	202	PEB	CHC-C1D-ND	-4.45	108.78	113.95
26	V3	203	PEB	OA-C1A-C2A	-4.45	122.64	126.17
26	AF	301	PEB	OA-C1A-C2A	-4.45	122.64	126.17
26	J3	201	PEB	C4B-C3B-C2B	-4.45	101.86	106.78
26	Z8	201	PEB	CHA-C1B-NB	-4.45	115.63	124.93
27	QA	201	PUB	C1C-C2C-C3C	-4.45	101.86	106.78
26	cE	203	PEB	CHA-C1B-C2B	4.45	136.34	124.90
26	W6	201	PEB	C3D-C4D-ND	4.45	115.98	107.26
28	rH	1001	CYC	CHB-C4A-C3A	4.45	136.34	124.90
26	L5	201	PEB	CHB-C4B-NB	-4.45	122.66	128.83
26	N1	201	PEB	C3B-C4B-NB	4.45	116.52	110.05
26	Q3	201	PEB	C3D-C4D-ND	4.45	115.98	107.26
26	P2	201	PEB	CHC-C1D-ND	-4.45	108.78	113.95
28	kH	1001	CYC	CHD-C4C-NC	4.44	130.49	125.20
28	IB	1001	CYC	C2C-C1C-NC	4.44	112.10	108.27
26	b2	201	PEB	OA-C1A-C2A	-4.44	122.64	126.17
26	i2	203	PEB	C4B-C3B-C2B	-4.44	101.86	106.78
26	VF	201	PEB	CHA-C1B-NB	-4.44	115.64	124.93
26	BC	203	PEB	OA-C1A-C2A	-4.44	122.64	126.17
28	J7	1001	CYC	CMB-C2B-C1B	4.44	129.71	124.17
26	QI	201	PEB	C3D-C4D-ND	4.44	115.97	107.26
26	a7	201	PEB	CMB-C2B-C1B	4.44	131.90	125.06
26	Y6	201	PEB	CHA-C1B-NB	-4.44	115.64	124.93
26	R7	202	PEB	C1C-CHB-C4B	-4.44	123.50	128.81
26	mA	202	PEB	C1C-CHB-C4B	-4.44	123.50	128.81
26	EJ	202	PEB	OA-C1A-C2A	-4.44	122.64	126.17
26	AD	201	PEB	CAB-C3B-C4B	4.44	132.87	125.01
26	JE	201	PEB	OA-C1A-NA	4.44	130.32	124.94
26	O2	201	PEB	C3B-C4B-NB	4.44	116.51	110.05
26	dF	203	PEB	CHC-C1D-ND	-4.44	108.79	113.95
26	HI	1002	PEB	OA-C1A-C2A	-4.44	122.64	126.17
26	l2	201	PEB	CMB-C2B-C1B	4.44	131.90	125.06
27	xG	305	PUB	C4B-CHB-C1C	-4.44	123.51	128.81
26	E8	202	PEB	CMB-C2B-C1B	4.44	131.90	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	RH	1001	CYC	CHB-C4A-C3A	4.44	136.31	124.90
26	U2	201	PEB	CHA-C4A-NA	4.44	130.48	125.20
26	w1	203	PEB	CHB-C4B-NB	-4.44	122.67	128.83
28	tH	1001	CYC	CHB-C4A-C3A	4.44	136.31	124.90
26	N6	201	PEB	C2A-C1A-NA	4.44	112.10	108.27
26	Z4	201	PEB	OD-C4D-ND	-4.44	119.36	125.93
26	MA	203	PEB	OA-C1A-C2A	-4.43	122.65	126.17
26	P8	201	PEB	OA-C1A-C2A	-4.43	122.65	126.17
26	V2	203	PEB	CHC-C4C-C3C	-4.43	122.78	130.34
26	ZE	201	PEB	OA-C1A-NA	4.43	130.31	124.94
26	kB	202	PEB	CHB-C4B-NB	-4.43	122.68	128.83
26	gE	203	PEB	CMB-C2B-C1B	4.43	131.89	125.06
26	EE	201	PEB	CMB-C2B-C1B	4.43	131.89	125.06
28	CH	1001	CYC	CAB-C3B-C4B	4.43	128.38	121.38
26	H9	203	PEB	CHB-C4B-NB	-4.43	122.68	128.83
26	HJ	201	PEB	CHB-C4B-NB	-4.43	122.68	128.83
28	qH	1001	CYC	CAB-C3B-C4B	4.43	128.37	121.38
26	BA	301	PEB	C3D-C4D-ND	4.43	115.95	107.26
26	LA	202	PEB	C4B-C3B-C2B	-4.43	101.88	106.78
26	N4	201	PEB	C3B-C4B-NB	4.43	116.49	110.05
26	w4	204	PEB	CHB-C4B-NB	-4.43	122.69	128.83
26	jG	201	PEB	C2A-C1A-NA	4.43	112.09	108.27
26	N4	201	PEB	C3D-C4D-ND	4.43	115.95	107.26
26	C8	201	PEB	CHC-C4C-C3C	-4.43	122.79	130.34
26	P7	202	PEB	OA-C1A-C2A	-4.43	122.65	126.17
26	gG	203	PEB	C1C-CHB-C4B	4.43	134.10	128.81
26	ND	203	PEB	OA-C1A-C2A	-4.43	122.65	126.17
26	VG	202	PEB	OA-C1A-C2A	-4.43	122.65	126.17
26	H2	1002	PEB	CHB-C4B-NB	-4.43	122.69	128.83
28	RH	1001	CYC	CHD-C4C-NC	4.43	130.47	125.20
26	11	203	PEB	CHB-C4B-NB	-4.42	122.69	128.83
26	e7	201	PEB	CHC-C1D-ND	-4.42	108.81	113.95
26	J1	202	PEB	OA-C1A-C2A	-4.42	122.66	126.17
26	O4	202	PEB	CHB-C4B-NB	-4.42	122.69	128.83
26	lA	203	PEB	CHB-C4B-NB	-4.42	122.69	128.83
26	dF	201	PEB	CHB-C4B-NB	-4.42	122.69	128.83
28	NF	1001	CYC	CMA-C3A-C4A	4.42	131.88	125.06
26	J3	203	PEB	C4B-C3B-C2B	-4.42	101.89	106.78
28	D2	1001	CYC	CMA-C3A-C4A	4.42	131.88	125.06
26	H8	201	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
26	R6	201	PEB	CMB-C2B-C1B	4.42	131.88	125.06
26	mA	201	PEB	CHA-C1B-NB	-4.42	115.68	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IG	202	PEB	OA-C1A-C2A	-4.42	122.66	126.17
28	G2	1001	CYC	C2B-C1B-NB	4.42	113.46	106.99
26	ID	202	PEB	CHC-C4C-C3C	-4.42	122.80	130.34
26	M8	203	PEB	OA-C1A-C2A	-4.42	122.66	126.17
26	DA	201	PEB	C2A-C1A-NA	4.42	112.08	108.27
26	X1	202	PEB	CMA-C2A-C1A	-4.42	102.87	112.40
28	H2	1001	CYC	OC-C1C-C2C	-4.42	122.66	126.17
28	C6	1001	CYC	OC-C1C-C2C	-4.42	122.66	126.17
26	lB	203	PEB	CHB-C4B-NB	-4.42	122.70	128.83
26	i4	202	PEB	OA-C1A-C2A	-4.42	122.66	126.17
28	LH	1001	CYC	CMC-C2C-C1C	4.42	121.93	112.40
26	lB	202	PEB	CHB-C4B-NB	-4.42	122.70	128.83
26	P2	202	PEB	CHC-C1D-ND	-4.42	108.82	113.95
26	MA	203	PEB	C3D-C4D-ND	4.42	115.92	107.26
28	I6	1001	CYC	C2C-C1C-NC	4.42	112.08	108.27
26	H4	203	PEB	OA-C1A-C2A	-4.42	122.66	126.17
26	K6	201	PEB	OA-C1A-C2A	-4.42	122.66	126.17
26	QF	203	PEB	CMB-C2B-C1B	4.42	131.86	125.06
27	wG	304	PUB	CMA-C2A-C1A	4.42	131.78	121.39
26	GG	202	PEB	CHC-C1D-ND	-4.42	108.82	113.95
26	L8	202	PEB	C4B-C3B-C2B	-4.41	101.90	106.78
26	T9	202	PEB	OA-C1A-C2A	-4.41	122.66	126.17
26	M3	201	PEB	CHA-C1B-NB	-4.41	115.70	124.93
27	A7	303	PUB	C1D-CHC-C4C	-4.41	103.77	113.37
26	JA	201	PEB	CHA-C1B-NB	-4.41	115.70	124.93
26	c4	202	PEB	OA-C1A-C2A	-4.41	122.67	126.17
26	KG	201	PEB	OA-C1A-C2A	-4.41	122.67	126.17
26	SF	201	PEB	CMB-C2B-C1B	4.41	131.86	125.06
26	WA	203	PEB	C1C-CHB-C4B	4.41	134.08	128.81
28	I7	1001	CYC	C4D-CHA-C1A	4.41	134.08	128.81
26	IC	201	PEB	CMB-C2B-C1B	4.41	131.86	125.06
26	O4	202	PEB	CHC-C1D-ND	-4.41	108.83	113.95
26	r4	201	PEB	CHB-C4B-NB	-4.41	122.71	128.83
26	J3	201	PEB	C3D-C4D-ND	4.41	115.91	107.26
26	R3	202	PEB	C4B-C3B-C2B	-4.41	101.90	106.78
26	ND	201	PEB	CMB-C2B-C1B	4.41	131.85	125.06
26	FF	1002	PEB	C2A-C1A-NA	4.41	112.07	108.27
26	F5	202	PEB	CHC-C4C-C3C	-4.41	122.82	130.34
28	J2	1001	CYC	C2B-C1B-NB	4.41	113.44	106.99
26	jF	202	PEB	CHA-C1B-NB	-4.41	115.71	124.93
26	CA	201	PEB	CHC-C4C-C3C	-4.41	122.82	130.34
26	A7	301	PEB	CHA-C1B-NB	-4.41	115.71	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y4	202	PEB	OA-C1A-C2A	-4.41	122.67	126.17
26	W8	202	PEB	C3D-C4D-ND	4.41	115.90	107.26
26	W8	203	PEB	CHB-C4B-NB	-4.41	122.72	128.83
26	f1	201	PEB	CMB-C2B-C1B	4.41	131.85	125.06
26	I9	202	PEB	CAB-C3B-C4B	4.40	132.80	125.01
26	IJ	202	PEB	C4B-C3B-C2B	-4.40	101.91	106.78
26	RD	201	PEB	CMB-C2B-C1B	4.40	131.85	125.06
26	F8	201	PEB	OA-C1A-C2A	-4.40	122.67	126.17
26	D9	201	PEB	OA-C1A-C2A	-4.40	122.67	126.17
26	KC	202	PEB	OA-C1A-C2A	-4.40	122.67	126.17
26	yG	301	PEB	OA-C1A-C2A	-4.40	122.67	126.17
28	I7	1001	CYC	OC-C1C-C2C	-4.40	122.67	126.17
26	d8	202	PEB	CHC-C1D-ND	-4.40	108.83	113.95
26	WE	202	PEB	C3B-C4B-NB	4.40	116.45	110.05
28	FI	1001	CYC	OC-C1C-C2C	-4.40	122.67	126.17
26	D8	202	PEB	C4B-C3B-C2B	-4.40	101.91	106.78
26	J5	202	PEB	C3D-C4D-ND	4.40	115.89	107.26
26	nG	201	PEB	OA-C1A-NA	4.40	130.27	124.94
28	LB	1001	CYC	C2C-C1C-NC	4.40	112.07	108.27
26	C4	201	PEB	CHB-C4B-NB	-4.40	122.72	128.83
26	l6	201	PEB	CHB-C4B-NB	-4.40	122.72	128.83
28	AH	1001	CYC	CMA-C3A-C4A	4.40	131.84	125.06
26	lA	202	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
26	21	404	PEB	CHA-C1B-NB	-4.40	115.73	124.93
26	l8	202	PEB	CHC-C4C-C3C	-4.40	122.84	130.34
28	L2	1001	CYC	CHB-C4A-C3A	4.40	136.21	124.90
26	N4	202	PEB	CHC-C4C-C3C	-4.40	122.84	130.34
28	N7	1001	CYC	CMA-C3A-C4A	4.40	131.83	125.06
28	J2	1001	CYC	C1B-C2B-C3B	-4.40	103.28	107.87
26	QA	202	PEB	C1C-CHB-C4B	4.39	134.06	128.81
26	I5	202	PEB	CHA-C1B-NB	-4.39	115.74	124.93
26	hF	202	PEB	CHA-C1B-NB	-4.39	115.74	124.93
26	ME	201	PEB	C1C-CHB-C4B	4.39	134.06	128.81
26	ZA	202	PEB	CHC-C1D-ND	-4.39	108.84	113.95
28	dH	1001	CYC	C1B-NB-C4B	-4.39	105.08	110.67
28	JF	1003	CYC	OB-C4B-C3B	-4.39	123.27	128.04
26	T2	203	PEB	CHC-C4C-C3C	-4.39	122.84	130.34
26	i2	202	PEB	CHB-C4B-NB	-4.39	122.73	128.83
26	M3	201	PEB	C3D-C4D-ND	4.39	115.88	107.26
26	T3	202	PEB	CHC-C1D-ND	-4.39	108.85	113.95
26	LC	201	PEB	CHA-C1B-NB	-4.39	115.75	124.93
26	C8	203	PEB	CHB-C4B-NB	-4.39	122.74	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D7	1001	CYC	C2B-C1B-NB	4.39	113.42	106.99
26	DE	202	PEB	CHA-C1B-NB	-4.39	115.75	124.93
26	iA	201	PEB	C4B-C3B-C2B	-4.39	101.92	106.78
26	G8	203	PEB	CHB-C4B-NB	-4.39	122.74	128.83
26	X9	203	PEB	OA-C1A-C2A	-4.39	122.68	126.17
26	P9	203	PEB	CHB-C4B-NB	-4.39	122.74	128.83
28	JF	1001	CYC	OB-C4B-C3B	-4.39	123.28	128.04
26	UF	201	PEB	CMB-C2B-C1B	4.39	131.82	125.06
26	UJ	202	PEB	CHC-C1D-ND	-4.39	108.85	113.95
26	h8	202	PEB	OA-C1A-C2A	-4.39	122.69	126.17
26	M8	201	PEB	CHB-C4B-NB	-4.39	122.74	128.83
26	UE	203	PEB	C2A-C1A-NA	4.39	112.05	108.27
28	LF	1001	CYC	CAB-C3B-C4B	4.39	128.31	121.38
26	eE	202	PEB	C4B-C3B-C2B	-4.39	101.93	106.78
26	V9	203	PEB	CHA-C1B-NB	-4.39	115.76	124.93
26	Q6	202	PEB	CMB-C2B-C1B	4.38	131.82	125.06
28	DB	1001	CYC	OC-C1C-C2C	-4.38	122.69	126.17
26	C1	202	PEB	CHB-C4B-NB	-4.38	122.75	128.83
26	B3	201	PEB	CHB-C4B-NB	-4.38	122.75	128.83
26	H5	202	PEB	OA-C1A-C2A	-4.38	122.69	126.17
28	H2	1001	CYC	CHB-C4A-NA	-4.38	115.77	124.93
26	XA	202	PEB	C4B-C3B-C2B	-4.38	101.93	106.78
28	G7	1001	CYC	C1B-NB-C4B	-4.38	105.09	110.67
26	U6	201	PEB	OA-C1A-C2A	-4.38	122.69	126.17
26	iB	202	PEB	CHB-C4B-NB	-4.38	122.75	128.83
26	X1	203	PEB	CMB-C2B-C1B	4.38	131.81	125.06
26	HC	201	PEB	CHA-C1B-NB	-4.38	115.77	124.93
26	N3	201	PEB	CMB-C2B-C1B	4.38	131.81	125.06
28	J7	1001	CYC	CAB-C3B-C4B	4.38	128.29	121.38
26	F2	1002	PEB	CHC-C1D-ND	-4.38	108.86	113.95
26	HG	201	PEB	CHC-C1D-ND	-4.38	108.86	113.95
26	l8	203	PEB	CHB-C4B-NB	-4.38	122.75	128.83
26	F4	202	PEB	OA-C1A-C2A	-4.38	122.69	126.17
26	FG	202	PEB	CHB-C4B-C3B	-4.38	115.21	125.32
28	NH	1001	CYC	CAB-C3B-C4B	4.38	128.29	121.38
26	Z8	202	PEB	C3B-C4B-NB	4.38	116.42	110.05
26	W1	201	PEB	C4B-C3B-C2B	-4.38	101.94	106.78
26	H2	1002	PEB	OA-C1A-C2A	-4.38	122.69	126.17
26	h1	201	PEB	CHB-C4B-NB	-4.38	122.76	128.83
26	F3	201	PEB	CHC-C4C-C3C	-4.38	122.87	130.34
26	Q6	201	PEB	C4B-C3B-C2B	-4.38	101.94	106.78
28	E7	1001	CYC	C2B-C1B-NB	4.38	113.39	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C7	1001	CYC	CAB-C3B-C4B	4.38	128.29	121.38
28	DF	1003	CYC	OC-C1C-C2C	-4.38	122.69	126.17
28	JI	1001	CYC	C1B-C2B-C3B	-4.38	103.31	107.87
26	LG	202	PEB	C3D-C4D-ND	4.38	115.84	107.26
26	sE	201	PEB	CHB-C4B-NB	-4.37	122.76	128.83
26	p1	202	PEB	CBA-CAA-C3A	-4.37	103.73	113.47
26	H7	1002	PEB	CHA-C1B-NB	-4.37	115.78	124.93
26	B8	301	PEB	C3D-C4D-ND	4.37	115.84	107.26
26	GA	202	PEB	OA-C1A-C2A	-4.37	122.70	126.17
26	HA	201	PEB	OA-C1A-C2A	-4.37	122.70	126.17
28	H6	1001	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
26	FA	202	PEB	C1C-CHB-C4B	-4.37	123.59	128.81
27	AA	304	PUB	CHA-C1B-C2B	-4.37	122.88	130.34
26	g2	202	PEB	CHC-C1D-ND	-4.37	108.87	113.95
26	KE	203	PEB	CHC-C1D-ND	-4.37	108.87	113.95
26	K5	203	PEB	OA-C1A-C2A	-4.37	122.70	126.17
26	Q4	201	PEB	CMB-C2B-C1B	4.37	131.79	125.06
27	yE	303	PUB	CHB-C1C-NC	-4.37	122.77	128.83
27	AI	303	PUB	CHB-C1C-NC	-4.37	122.77	128.83
26	SI	202	PEB	C3D-C4D-ND	4.37	115.83	107.26
26	CE	202	PEB	C1C-CHB-C4B	4.37	134.03	128.81
26	HG	202	PEB	CHB-C4B-C3B	-4.37	115.23	125.32
27	21	403	PUB	C1C-C2C-C3C	-4.37	101.95	106.78
27	A9	302	PUB	CMA-C2A-C1A	4.37	131.66	121.39
26	lF	201	PEB	CHB-C4B-NB	-4.37	122.77	128.83
28	HB	1001	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
28	hH	1001	CYC	CAB-C3B-C4B	4.37	128.28	121.38
26	f6	201	PEB	CHC-C4C-C3C	-4.37	122.89	130.34
26	g2	202	PEB	CHB-C4B-NB	-4.37	122.77	128.83
26	j7	201	PEB	CHB-C4B-NB	-4.37	122.77	128.83
26	XG	202	PEB	CHB-C4B-NB	-4.37	122.77	128.83
26	xE	304	PEB	C1C-CHB-C4B	-4.37	123.59	128.81
26	ZA	201	PEB	CHA-C1B-NB	-4.37	115.80	124.93
26	eI	201	PEB	OA-C1A-C2A	-4.37	122.70	126.17
26	AI	301	PEB	CHB-C4B-NB	-4.37	122.77	128.83
26	VJ	203	PEB	CHA-C1B-NB	-4.37	115.80	124.93
26	G9	202	PEB	CHB-C4B-NB	-4.37	122.77	128.83
26	IC	202	PEB	OA-C1A-C2A	-4.37	122.70	126.17
26	cG	203	PEB	C3D-C4D-ND	4.36	115.82	107.26
27	A1	203	PUB	CMA-C2A-C1A	4.36	131.66	121.39
26	TB	201	PEB	CHA-C1B-NB	-4.36	115.80	124.93
26	IG	203	PEB	C4B-C3B-C2B	-4.36	101.95	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	xG	306	PUB	CHA-C4A-NA	-4.36	108.88	113.95
28	CF	1001	CYC	CHB-C4A-NA	-4.36	115.81	124.93
26	SE	203	PEB	CMB-C2B-C1B	4.36	131.78	125.06
26	KA	202	PEB	CHB-C4B-NB	-4.36	122.78	128.83
26	eB	203	PEB	CHB-C4B-NB	-4.36	122.78	128.83
26	ZF	201	PEB	C2A-C1A-NA	4.36	112.03	108.27
26	Z7	201	PEB	CHB-C4B-C3B	-4.36	115.24	125.32
26	T3	201	PEB	CHA-C1B-NB	-4.36	115.81	124.93
26	f6	203	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	iA	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	ZG	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	w4	201	PEB	CHC-C4C-C3C	-4.36	122.90	130.34
26	WF	202	PEB	CHA-C1B-NB	-4.36	115.81	124.93
28	dH	1001	CYC	CHB-C4A-NA	-4.36	115.81	124.93
26	K5	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	IE	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	JG	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
28	YH	1001	CYC	CMB-C2B-C1B	4.36	129.61	124.17
26	Z4	201	PEB	C3D-C4D-ND	4.36	115.81	107.26
26	LE	202	PEB	C3D-C4D-ND	4.36	115.81	107.26
26	bF	202	PEB	CHC-C1D-ND	-4.36	108.89	113.95
28	FB	1001	CYC	C1B-NB-C4B	-4.36	105.12	110.67
28	NF	1001	CYC	OB-C4B-C3B	-4.36	123.31	128.04
26	T3	203	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	r4	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	u4	202	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	JA	201	PEB	OA-C1A-C2A	-4.36	122.71	126.17
26	uE	202	PEB	CMB-C2B-C1B	4.36	131.77	125.06
26	Q2	201	PEB	CHC-C4C-C3C	-4.36	122.91	130.34
26	V3	201	PEB	CHA-C1B-NB	-4.35	115.82	124.93
28	DI	1001	CYC	CMA-C3A-C4A	4.35	131.77	125.06
26	MG	202	PEB	CHB-C4B-NB	-4.35	122.79	128.83
26	V6	202	PEB	C1C-CHB-C4B	-4.35	123.61	128.81
26	IG	203	PEB	C3D-C4D-ND	4.35	115.80	107.26
26	d1	201	PEB	CHC-C1D-ND	-4.35	108.89	113.95
26	14	201	PEB	CHC-C1D-ND	-4.35	108.89	113.95
26	h1	202	PEB	CHC-C1D-ND	-4.35	108.89	113.95
26	DJ	201	PEB	C4B-C3B-C2B	-4.35	101.97	106.78
26	V1	203	PEB	CMD-C2D-C3D	-4.35	123.93	130.06
26	CE	202	PEB	C3B-C4B-NB	4.35	116.38	110.05
26	cI	202	PEB	CHB-C4B-NB	-4.35	122.79	128.83
28	G7	1001	CYC	CAB-C3B-C4B	4.35	128.25	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W7	203	PEB	CHB-C4B-NB	-4.35	122.79	128.83
26	PA	201	PEB	CHA-C1B-NB	-4.35	115.83	124.93
26	eF	202	PEB	CHA-C1B-NB	-4.35	115.83	124.93
26	iB	202	PEB	OA-C1A-C2A	-4.35	122.72	126.17
28	JF	1003	CYC	OC-C1C-C2C	-4.35	122.72	126.17
26	B4	202	PEB	C1C-CHB-C4B	4.35	134.00	128.81
26	L3	201	PEB	CHB-C4B-NB	-4.35	122.80	128.83
26	N8	202	PEB	CMB-C2B-C1B	4.35	131.76	125.06
26	II	201	PEB	CHB-C4B-C3B	-4.35	115.28	125.32
26	IG	201	PEB	C4B-C3B-C2B	-4.35	101.97	106.78
27	A9	302	PUB	CHB-C1C-NC	-4.35	122.80	128.83
28	F6	1001	CYC	C1B-NB-C4B	-4.35	105.13	110.67
26	CG	201	PEB	CHC-C1D-ND	-4.35	108.90	113.95
27	A2	302	PUB	C1C-C2C-C3C	-4.35	101.97	106.78
28	wH	1001	CYC	CHB-C4A-C3A	4.35	136.08	124.90
26	AJ	303	PEB	CHA-C1B-NB	-4.35	115.84	124.93
26	LF	1002	PEB	C2A-C1A-NA	4.35	112.02	108.27
26	P3	203	PEB	CHC-C1D-ND	-4.35	108.90	113.95
28	G6	1001	CYC	CMA-C3A-C4A	4.35	131.76	125.06
26	m1	201	PEB	CHB-C4B-NB	-4.35	122.80	128.83
26	V4	203	PEB	CMD-C2D-C3D	-4.35	123.94	130.06
26	LE	201	PEB	C4B-C3B-C2B	-4.35	101.97	106.78
26	W2	201	PEB	CMA-C2A-C1A	-4.35	103.04	112.40
26	v4	202	PEB	CHA-C4A-NA	-4.34	120.04	125.20
28	eH	1001	CYC	CAB-C3B-C4B	4.34	128.24	121.38
26	p4	202	PEB	CBA-CAA-C3A	-4.34	103.79	113.47
26	N9	204	PEB	CHB-C4B-NB	-4.34	122.80	128.83
26	D1	202	PEB	OA-C1A-C2A	-4.34	122.72	126.17
26	S9	201	PEB	C4B-C3B-C2B	-4.34	101.97	106.78
26	JI	1002	PEB	OA-C1A-C2A	-4.34	122.72	126.17
26	L9	203	PEB	C1C-CHB-C4B	4.34	134.00	128.81
26	LF	1002	PEB	CHC-C4C-C3C	-4.34	122.93	130.34
26	gF	201	PEB	C1C-CHB-C4B	4.34	134.00	128.81
26	jI	201	PEB	C3B-C4B-NB	4.34	116.36	110.05
28	JH	1001	CYC	CHB-C4A-C3A	4.34	136.06	124.90
26	Q2	201	PEB	C3D-C4D-ND	4.34	115.78	107.26
26	JE	202	PEB	C1C-CHB-C4B	4.34	133.99	128.81
28	D6	1001	CYC	C4D-CHA-C1A	4.34	133.99	128.81
26	W4	201	PEB	CHC-C1D-ND	-4.34	108.91	113.95
26	K9	201	PEB	CHC-C1D-ND	-4.34	108.91	113.95
26	DJ	202	PEB	C3D-C4D-ND	4.34	115.77	107.26
28	F2	1001	CYC	CHA-C1A-NA	-4.34	122.81	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	q1	202	PEB	CHC-C1D-ND	-4.34	108.91	113.95
28	MB	1001	CYC	CMA-C3A-C4A	4.34	131.75	125.06
26	QI	201	PEB	CHC-C4C-C3C	-4.34	122.94	130.34
26	BE	201	PEB	CHC-C1D-ND	4.34	118.98	113.95
26	J5	202	PEB	C2A-C1A-NA	4.34	112.01	108.27
28	YH	1004	CYC	CMB-C2B-C1B	4.34	129.58	124.17
28	1H	1000	CYC	CMB-C2B-C1B	4.34	129.58	124.17
26	g7	202	PEB	CHB-C4B-NB	-4.34	122.81	128.83
26	HD	201	PEB	CHC-C4C-C3C	-4.34	122.94	130.34
26	HE	202	PEB	CHB-C4B-C3B	-4.34	115.30	125.32
26	hG	201	PEB	CHB-C4B-NB	-4.34	122.81	128.83
26	tE	202	PEB	C3D-C4D-ND	4.34	115.77	107.26
26	jE	201	PEB	CHA-C1B-NB	-4.34	115.86	124.93
26	CJ	201	PEB	C4B-C3B-C2B	-4.34	101.98	106.78
26	rG	202	PEB	CMB-C2B-C1B	4.34	131.74	125.06
26	fE	201	PEB	CHA-C1B-NB	-4.34	115.86	124.93
26	J1	203	PEB	CHB-C4B-NB	-4.33	122.81	128.83
28	KH	1001	CYC	C1B-C2B-C3B	-4.33	103.35	107.87
26	L8	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
26	JD	203	PEB	OA-C1A-C2A	-4.33	122.73	126.17
28	F6	1001	CYC	OC-C1C-C2C	-4.33	122.73	126.17
26	OD	202	PEB	CHC-C4C-C3C	-4.33	122.95	130.34
26	GE	201	PEB	C1B-C2B-C3B	-4.33	101.53	106.51
26	y1	203	PEB	CHC-C1D-ND	-4.33	108.92	113.95
28	M2	1001	CYC	C2B-C1B-NB	4.33	113.33	106.99
26	P9	202	PEB	C1C-CHB-C4B	4.33	133.98	128.81
26	PA	201	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
26	b4	501	PEB	C3D-C4D-ND	4.33	115.76	107.26
26	J2	1002	PEB	OA-C1A-C2A	-4.33	122.73	126.17
26	VA	201	PEB	OA-C1A-C2A	-4.33	122.73	126.17
26	PI	203	PEB	CHB-C4B-NB	-4.33	122.82	128.83
26	J8	201	PEB	CHA-C1B-NB	-4.33	115.88	124.93
26	Y1	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
27	AI	302	PUB	C1C-C2C-C3C	-4.33	101.99	106.78
26	dI	201	PEB	CHC-C4C-C3C	-4.33	122.95	130.34
26	K4	201	PEB	CMB-C2B-C1B	4.33	131.73	125.06
26	V9	201	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
26	MD	201	PEB	C3D-C4D-ND	4.33	115.75	107.26
26	fG	201	PEB	OA-C1A-NA	4.33	130.18	124.94
26	CG	202	PEB	CMB-C2B-C1B	4.33	131.73	125.06
28	DB	1001	CYC	C1B-NB-C4B	-4.33	105.16	110.67
28	IB	1001	CYC	C4D-CHA-C1A	4.33	133.98	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IA	202	PEB	CHC-C4C-C3C	-4.33	122.96	130.34
26	kG	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
26	eI	201	PEB	CHC-C1D-ND	-4.32	108.92	113.95
28	DF	1003	CYC	C1B-C2B-C3B	-4.32	103.36	107.87
26	g1	203	PEB	CHA-C1B-NB	-4.32	115.89	124.93
26	V3	201	PEB	OA-C1A-C2A	-4.32	122.74	126.17
26	JF	1002	PEB	CHB-C4B-NB	-4.32	122.83	128.83
26	ZI	201	PEB	C3D-C4D-ND	4.32	115.74	107.26
26	iG	201	PEB	CHB-C4B-NB	-4.32	122.83	128.83
26	C5	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
26	n4	202	PEB	CHB-C4B-NB	-4.32	122.83	128.83
26	K5	201	PEB	CMB-C2B-C1B	4.32	131.72	125.06
28	N2	1001	CYC	CAB-C3B-C4B	4.32	128.20	121.38
26	N3	202	PEB	C3B-C4B-NB	4.32	116.33	110.05
26	kE	202	PEB	C2A-C1A-NA	4.32	112.00	108.27
28	AH	1001	CYC	CAB-C3B-C4B	4.32	128.20	121.38
26	KA	201	PEB	C3D-C4D-ND	4.32	115.73	107.26
26	H8	201	PEB	CMB-C2B-C1B	4.32	131.72	125.06
27	B8	302	PUB	CHA-C4A-NA	-4.32	108.93	113.95
26	Y4	202	PEB	CHC-C1D-ND	-4.32	108.93	113.95
26	MJ	201	PEB	CHC-C1D-ND	-4.32	108.93	113.95
26	XG	201	PEB	CHC-C4C-C3C	-4.32	122.97	130.34
26	V6	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
26	aI	203	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
26	BC	201	PEB	CHB-C4B-NB	-4.32	122.84	128.83
26	H3	201	PEB	CHC-C4C-C3C	-4.32	122.97	130.34
26	S4	202	PEB	CHC-C1D-ND	-4.32	108.94	113.95
26	KJ	201	PEB	CHC-C1D-ND	-4.32	108.94	113.95
26	I3	202	PEB	CHC-C4C-C3C	-4.31	122.98	130.34
26	i6	202	PEB	CHC-C1D-ND	-4.31	108.94	113.95
26	bF	203	PEB	C2A-C1A-NA	4.31	111.99	108.27
26	IJ	203	PEB	CHC-C1D-ND	-4.31	108.94	113.95
26	MA	201	PEB	CHB-C4B-NB	-4.31	122.84	128.83
26	DI	1002	PEB	CHB-C4B-NB	-4.31	122.84	128.83
26	24	404	PEB	CMB-C2B-C1B	4.31	131.71	125.06
28	E6	1001	CYC	CMA-C3A-C4A	4.31	131.71	125.06
26	VE	201	PEB	CHC-C4C-C3C	-4.31	122.98	130.34
26	t1	201	PEB	OA-C1A-C2A	-4.31	122.75	126.17
26	FC	202	PEB	OA-C1A-C2A	-4.31	122.75	126.17
26	YI	203	PEB	CHC-C4C-C3C	-4.31	122.98	130.34
28	GH	1001	CYC	CHB-C4A-C3A	4.31	135.99	124.90
26	e8	202	PEB	CHC-C4C-C3C	-4.31	122.98	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z2	201	PEB	C3D-C4D-ND	4.31	115.72	107.26
26	iG	201	PEB	C3D-C4D-ND	4.31	115.72	107.26
28	I6	1001	CYC	C4D-CHA-C1A	4.31	133.96	128.81
26	jI	202	PEB	CHB-C4B-NB	-4.31	122.85	128.83
26	b7	201	PEB	CHC-C4C-C3C	-4.31	122.99	130.34
26	O6	202	PEB	CHB-C4B-NB	-4.31	122.85	128.83
26	ND	201	PEB	CHB-C4B-NB	-4.31	122.85	128.83
26	PI	201	PEB	CHC-C1D-ND	-4.31	108.94	113.95
26	V1	201	PEB	C3D-C4D-ND	4.31	115.71	107.26
26	gE	203	PEB	C3D-C4D-ND	4.31	115.71	107.26
26	V4	201	PEB	C3D-C4D-ND	4.31	115.71	107.26
26	K5	202	PEB	CHC-C4C-C3C	-4.31	122.99	130.34
26	s1	203	PEB	OA-C1A-C2A	-4.31	122.75	126.17
28	UH	1001	CYC	CHB-C4A-C3A	4.31	135.97	124.90
26	rE	202	PEB	OA-C1A-C2A	-4.31	122.75	126.17
26	Y2	203	PEB	CHC-C4C-C3C	-4.31	122.99	130.34
26	x1	201	PEB	CMB-C2B-C1B	4.31	131.69	125.06
26	DD	202	PEB	CHA-C1B-NB	-4.31	115.93	124.93
28	GI	1001	CYC	C2B-C1B-NB	4.30	113.29	106.99
28	uH	1001	CYC	CHB-C4A-C3A	4.30	135.97	124.90
26	bG	201	PEB	CMB-C2B-C1B	4.30	131.69	125.06
28	sH	1001	CYC	CMB-C2B-C1B	4.30	129.54	124.17
26	II	201	PEB	C3B-C4B-NB	4.30	116.31	110.05
26	fG	201	PEB	CHB-C4B-NB	-4.30	122.86	128.83
26	W4	201	PEB	OA-C1A-C2A	-4.30	122.75	126.17
26	Q8	204	PEB	OA-C1A-C2A	-4.30	122.75	126.17
26	kE	202	PEB	OA-C1A-C2A	-4.30	122.75	126.17
26	Y1	202	PEB	CHC-C1D-ND	-4.30	108.95	113.95
26	C4	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
26	B5	202	PEB	CHC-C4C-C3C	-4.30	123.00	130.34
26	S8	201	PEB	OA-C1A-C2A	-4.30	122.75	126.17
26	bI	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
26	WA	202	PEB	C3D-C4D-ND	4.30	115.70	107.26
28	IF	1001	CYC	CHB-C4A-NA	-4.30	115.94	124.93
26	KG	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
26	NA	202	PEB	CMB-C2B-C1B	4.30	131.69	125.06
26	L5	202	PEB	OA-C1A-C2A	-4.30	122.75	126.17
26	i6	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
26	X8	201	PEB	C1C-CHB-C4B	-4.30	123.67	128.81
28	LF	1001	CYC	CHB-C1B-NB	-4.30	116.83	126.06
26	XG	203	PEB	CMB-C2B-C1B	4.30	131.68	125.06
26	vE	201	PEB	OA-C1A-NA	4.30	130.15	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	EE	201	PEB	C1C-CHB-C4B	4.30	133.94	128.81
26	aG	202	PEB	C1C-CHB-C4B	4.30	133.94	128.81
26	mB	201	PEB	CHB-C4B-NB	-4.30	122.86	128.83
26	TG	201	PEB	C1C-CHB-C4B	4.30	133.94	128.81
26	I8	203	PEB	C1C-CHB-C4B	-4.30	123.67	128.81
28	NI	1001	CYC	CHB-C4A-NA	-4.30	115.94	124.93
26	V7	201	PEB	CMB-C2B-C1B	4.30	131.68	125.06
26	IE	201	PEB	CHC-C1D-ND	-4.30	108.96	113.95
28	qH	1002	CYC	C1B-C2B-C3B	-4.30	103.39	107.87
26	GB	1002	PEB	C3D-C4D-ND	4.30	115.69	107.26
26	WG	203	PEB	CHA-C1B-NB	-4.30	115.95	124.93
26	w1	202	PEB	CHA-C1B-NB	-4.30	115.95	124.93
26	TG	202	PEB	CMB-C2B-C1B	4.29	131.68	125.06
26	VA	201	PEB	CBC-CAC-C2C	-4.29	105.29	112.62
26	F9	203	PEB	CHA-C1B-C2B	4.29	135.94	124.90
26	x4	202	PEB	CHC-C1D-ND	-4.29	108.96	113.95
26	R2	202	PEB	OA-C1A-C2A	-4.29	122.76	126.17
28	UH	1001	CYC	CBD-CAD-C3D	4.29	119.95	112.62
26	RI	203	PEB	CAB-C3B-C4B	4.29	132.60	125.01
26	OB	203	PEB	C1C-CHB-C4B	4.29	133.94	128.81
26	D3	201	PEB	C2A-C1A-NA	4.29	111.97	108.27
26	PD	203	PEB	C1C-CHB-C4B	4.29	133.94	128.81
26	UA	202	PEB	CHC-C4C-C3C	-4.29	123.02	130.34
26	b1	501	PEB	C3D-C4D-ND	4.29	115.68	107.26
28	cH	1001	CYC	CAB-C3B-C4B	4.29	128.16	121.38
26	PF	202	PEB	CHB-C4B-NB	-4.29	122.88	128.83
26	hA	202	PEB	OA-C1A-C2A	-4.29	122.76	126.17
26	T8	202	PEB	CHC-C1D-ND	-4.29	108.97	113.95
26	XA	201	PEB	CMB-C2B-C1B	4.29	131.67	125.06
26	KE	201	PEB	C1C-CHB-C4B	4.29	133.93	128.81
26	bG	202	PEB	C3D-C4D-ND	4.29	115.67	107.26
27	AJ	302	PUB	CMA-C2A-C1A	4.29	131.47	121.39
26	E8	201	PEB	OA-C1A-C2A	-4.29	122.76	126.17
26	GB	1002	PEB	OA-C1A-C2A	-4.29	122.76	126.17
26	RF	202	PEB	OA-C1A-C2A	-4.29	122.76	126.17
26	HG	202	PEB	CMB-C2B-C1B	4.29	131.67	125.06
26	HD	203	PEB	C4B-C3B-C2B	-4.29	102.04	106.78
26	T8	201	PEB	OA-C1A-C2A	-4.29	122.77	126.17
28	M6	1001	CYC	CMA-C3A-C4A	4.29	131.66	125.06
26	cE	201	PEB	C4B-C3B-C2B	-4.29	102.04	106.78
26	BG	201	PEB	OD-C4D-C3D	-4.29	119.75	129.46
26	HD	201	PEB	C1C-CHB-C4B	4.29	133.93	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FJ	202	PEB	CHB-C4B-NB	-4.29	122.88	128.83
26	W1	201	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	24	401	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	D9	202	PEB	OD-C4D-ND	-4.28	119.58	125.93
26	ME	201	PEB	CHC-C4C-C3C	-4.28	123.03	130.34
26	fG	201	PEB	CHA-C1B-NB	-4.28	115.97	124.93
26	H9	201	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	A9	304	PEB	CHC-C1D-ND	-4.28	108.97	113.95
26	WD	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
28	RH	1001	CYC	CMB-C2B-C1B	4.28	129.51	124.17
26	L5	203	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	YD	303	PEB	CHA-C1B-NB	-4.28	115.97	124.93
26	SJ	201	PEB	C4B-C3B-C2B	-4.28	102.04	106.78
26	UB	203	PEB	C1C-CHB-C4B	-4.28	123.69	128.81
26	GE	203	PEB	CHC-C1D-ND	-4.28	108.97	113.95
26	Z6	203	PEB	CHB-C4B-NB	-4.28	122.89	128.83
26	ZF	201	PEB	CHC-C4C-C3C	-4.28	123.03	130.34
26	cG	201	PEB	CHC-C4C-C3C	-4.28	123.03	130.34
26	LI	1002	PEB	C1C-CHB-C4B	4.28	133.92	128.81
26	L4	203	PEB	CHB-C4B-NB	-4.28	122.89	128.83
26	QD	201	PEB	CHA-C1B-C2B	4.28	135.91	124.90
26	DB	1002	PEB	C4B-C3B-C2B	-4.28	102.05	106.78
26	A8	301	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	dG	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
28	D6	1001	CYC	OC-C1C-C2C	-4.28	122.77	126.17
28	pH	1001	CYC	CHB-C4A-C3A	4.28	135.91	124.90
26	JA	202	PEB	C1C-CHB-C4B	-4.28	123.70	128.81
26	I9	201	PEB	CHC-C1D-ND	-4.28	108.98	113.95
26	D4	201	PEB	C3B-C4B-NB	4.28	116.27	110.05
27	yG	302	PUB	CHB-C1C-NC	-4.28	122.89	128.83
26	JA	201	PEB	C3D-C4D-ND	4.28	115.65	107.26
26	a1	201	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	LC	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
26	HI	1002	PEB	CHB-C4B-NB	-4.28	122.89	128.83
27	QA	201	PUB	OD-C4D-ND	-4.28	119.59	125.93
26	H9	201	PEB	CHB-C4B-NB	-4.27	122.90	128.83
26	GG	202	PEB	CHB-C4B-C3B	-4.27	115.45	125.32
26	ZA	202	PEB	C3B-C4B-NB	4.27	116.27	110.05
26	FA	201	PEB	OA-C1A-C2A	-4.27	122.78	126.17
26	TA	201	PEB	OA-C1A-C2A	-4.27	122.78	126.17
26	LC	201	PEB	CMB-C2B-C1B	4.27	131.65	125.06
28	UH	1001	CYC	CAB-C3B-C4B	4.27	128.13	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OG	202	PEB	C1C-CHB-C4B	4.27	133.91	128.81
26	aE	201	PEB	C1B-C2B-C3B	-4.27	101.60	106.51
26	KE	201	PEB	C2A-C1A-NA	4.27	111.95	108.27
26	u1	203	PEB	OA-C1A-C2A	-4.27	122.78	126.17
26	A3	202	PEB	CHA-C1B-NB	-4.27	116.00	124.93
26	L5	203	PEB	C3D-C4D-ND	4.27	115.63	107.26
26	HC	201	PEB	OA-C1A-C2A	-4.27	122.78	126.17
26	GE	201	PEB	C4B-C3B-C2B	-4.27	102.06	106.78
26	R2	203	PEB	CAB-C3B-C4B	4.27	132.56	125.01
26	I8	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
26	PG	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
26	jA	203	PEB	C1C-CHB-C4B	4.27	133.91	128.81
26	uG	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
28	E7	1001	CYC	C1B-NB-C4B	-4.27	105.24	110.67
26	VD	202	PEB	CHB-C4B-NB	-4.27	122.91	128.83
26	FF	1002	PEB	CHC-C1D-ND	-4.27	108.99	113.95
26	M1	402	PEB	C3D-C4D-ND	4.27	115.63	107.26
26	G6	1002	PEB	C3D-C4D-ND	4.27	115.63	107.26
26	jI	201	PEB	CHC-C4C-C3C	-4.27	123.06	130.34
26	H1	201	PEB	OA-C1A-C2A	-4.26	122.78	126.17
26	mB	202	PEB	OA-C1A-C2A	-4.26	122.78	126.17
26	OE	202	PEB	C4B-C3B-C2B	-4.26	102.06	106.78
28	HI	1001	CYC	C2B-C1B-NB	4.26	113.23	106.99
26	I8	202	PEB	CHC-C4C-C3C	-4.26	123.06	130.34
26	LJ	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
26	l2	201	PEB	C3B-C4B-NB	4.26	116.25	110.05
26	Y7	201	PEB	C1C-CHB-C4B	4.26	133.90	128.81
26	l6	203	PEB	CHB-C4B-NB	-4.26	122.92	128.83
26	RI	203	PEB	CHC-C4C-C3C	-4.26	123.07	130.34
28	L7	1001	CYC	C2C-C1C-NC	4.26	111.95	108.27
26	vG	201	PEB	OA-C1A-NA	4.26	130.10	124.94
26	JJ	203	PEB	CHB-C4B-NB	-4.26	122.92	128.83
28	H7	1001	CYC	OB-C4B-C3B	-4.26	123.42	128.04
28	DB	1001	CYC	CMA-C3A-C4A	4.26	131.62	125.06
28	N2	1001	CYC	CHB-C4A-NA	-4.26	116.02	124.93
28	QH	1001	CYC	CMB-C2B-C1B	4.26	129.49	124.17
26	O6	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
26	b4	501	PEB	OA-C1A-C2A	-4.26	122.79	126.17
26	eI	203	PEB	CHC-C4C-C3C	-4.26	123.07	130.34
26	SB	203	PEB	CHA-C1B-NB	-4.26	116.03	124.93
26	aI	203	PEB	CHB-C4B-NB	-4.26	122.92	128.83
26	V2	202	PEB	C1C-CHB-C4B	4.26	133.90	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X4	203	PEB	CHC-C4C-C3C	-4.26	123.08	130.34
26	F3	202	PEB	CHB-C4B-NB	-4.26	122.92	128.83
26	UE	203	PEB	CHA-C1B-C2B	4.26	135.85	124.90
26	K8	202	PEB	CHB-C4B-NB	-4.26	122.92	128.83
27	A2	303	PUB	CHB-C1C-NC	-4.26	122.92	128.83
26	G3	201	PEB	OA-C1A-C2A	-4.26	122.79	126.17
26	LE	202	PEB	OA-C1A-C2A	-4.26	122.79	126.17
26	TE	202	PEB	CMB-C2B-C1B	4.26	131.62	125.06
26	D9	202	PEB	C3D-C4D-ND	4.26	115.61	107.26
27	A6	302	PUB	C1C-C2C-C3C	-4.26	102.07	106.78
26	Q4	201	PEB	CHC-C1D-ND	-4.26	109.01	113.95
26	m8	201	PEB	CHA-C1B-NB	-4.25	116.03	124.93
26	IG	203	PEB	OA-C1A-C2A	-4.25	122.79	126.17
28	sH	1001	CYC	CAB-C3B-C4B	4.25	128.10	121.38
26	j8	203	PEB	OA-C1A-C2A	-4.25	122.79	126.17
26	d7	201	PEB	CHB-C4B-NB	-4.25	122.93	128.83
26	IC	202	PEB	CMB-C2B-C1B	4.25	131.61	125.06
26	VE	201	PEB	OA-C1A-NA	4.25	130.09	124.94
26	c2	202	PEB	CHB-C4B-NB	-4.25	122.93	128.83
27	wE	304	PUB	CMA-C2A-C1A	4.25	131.39	121.39
28	IF	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
28	FF	1001	CYC	C1B-CHB-C4A	-4.25	117.69	128.08
26	K1	202	PEB	C4B-C3B-C2B	-4.25	102.08	106.78
26	m1	202	PEB	CMB-C2B-C1B	4.25	131.61	125.06
26	pG	201	PEB	CHA-C4A-NA	4.25	130.26	125.20
28	qH	1002	CYC	CHD-C4C-NC	4.25	130.26	125.20
26	V1	202	PEB	CHB-C4B-NB	-4.25	122.93	128.83
26	Z7	202	PEB	CHB-C4B-NB	-4.25	122.93	128.83
26	K4	201	PEB	C2A-C1A-NA	4.25	111.94	108.27
26	a7	202	PEB	CMB-C2B-C1B	4.25	131.61	125.06
26	HE	202	PEB	CMB-C2B-C1B	4.25	131.61	125.06
26	LB	1002	PEB	OA-C1A-C2A	-4.25	122.79	126.17
26	V3	201	PEB	CHC-C4C-C3C	-4.25	123.09	130.34
26	CE	201	PEB	CMD-C2D-C3D	-4.25	124.07	130.06
27	xE	305	PUB	C1C-C2C-C3C	-4.25	102.08	106.78
27	K3	203	PUB	CHA-C4A-NA	-4.25	109.01	113.95
26	pE	201	PEB	C2A-C1A-NA	4.25	111.94	108.27
26	JE	202	PEB	CMB-C2B-C1B	4.25	131.61	125.06
26	e8	201	PEB	C3D-C4D-ND	4.25	115.59	107.26
26	eA	202	PEB	CHC-C4C-C3C	-4.25	123.09	130.34
26	D4	202	PEB	OA-C1A-C2A	-4.25	122.80	126.17
26	AJ	303	PEB	OA-C1A-C2A	-4.25	122.80	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	u1	203	PEB	C1C-CHB-C4B	4.25	133.88	128.81
26	TD	201	PEB	CHA-C1B-NB	-4.25	116.05	124.93
26	JC	202	PEB	C3D-C4D-ND	4.25	115.59	107.26
26	h7	201	PEB	CHB-C4B-NB	-4.25	122.94	128.83
28	EB	1001	CYC	CMA-C3A-C4A	4.25	131.60	125.06
28	DF	1001	CYC	C2B-C1B-NB	4.25	113.21	106.99
26	j8	203	PEB	C1C-CHB-C4B	4.25	133.88	128.81
28	SH	1001	CYC	CHB-C4A-C3A	4.25	135.82	124.90
26	N2	1002	PEB	CHC-C4C-C3C	-4.24	123.10	130.34
26	R2	203	PEB	CHC-C4C-C3C	-4.24	123.10	130.34
26	oE	201	PEB	CHA-C1B-C2B	4.24	135.82	124.90
26	Q6	202	PEB	CHC-C1D-ND	-4.24	109.02	113.95
26	e2	201	PEB	OA-C1A-C2A	-4.24	122.80	126.17
26	KJ	201	PEB	CHB-C4B-NB	-4.24	122.94	128.83
26	FE	202	PEB	CHB-C4B-C3B	-4.24	115.51	125.32
26	GE	202	PEB	CHB-C4B-C3B	-4.24	115.52	125.32
26	CA	203	PEB	CHB-C4B-NB	-4.24	122.94	128.83
26	k2	201	PEB	OA-C1A-C2A	-4.24	122.80	126.17
28	F2	1001	CYC	OC-C1C-C2C	-4.24	122.80	126.17
26	D9	202	PEB	CHA-C1B-C2B	4.24	135.81	124.90
26	WE	201	PEB	CHC-C1D-ND	-4.24	109.02	113.95
26	GG	201	PEB	C2A-C1A-NA	4.24	111.93	108.27
26	CE	201	PEB	C3D-C4D-ND	4.24	115.58	107.26
26	FG	202	PEB	C3D-C4D-ND	4.24	115.58	107.26
26	L5	201	PEB	C2A-C1A-NA	4.24	111.93	108.27
26	CJ	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
26	wE	301	PEB	C1C-CHB-C4B	-4.24	123.74	128.81
27	AF	303	PUB	CMA-C2A-C1A	4.24	131.36	121.39
26	PJ	202	PEB	CHA-C1B-NB	-4.24	116.06	124.93
26	E8	201	PEB	CHB-C4B-NB	-4.24	122.95	128.83
26	mG	202	PEB	CBC-CAC-C2C	-4.24	105.39	112.62
26	W8	202	PEB	C2A-C1A-NA	4.24	111.93	108.27
26	AE	201	PEB	C4B-C3B-C2B	-4.24	102.09	106.78
26	ZF	201	PEB	CHB-C4B-C3B	-4.24	115.53	125.32
26	LC	201	PEB	OA-C1A-C2A	-4.24	122.80	126.17
26	tG	201	PEB	OA-C1A-NA	4.24	130.07	124.94
26	k6	201	PEB	C1C-CHB-C4B	4.24	133.87	128.81
26	H9	201	PEB	C3D-C4D-ND	4.24	115.57	107.26
26	R7	201	PEB	CHC-C1D-ND	-4.24	109.03	113.95
26	p4	202	PEB	CHA-C1B-NB	-4.24	116.07	124.93
26	AA	301	PEB	OA-C1A-C2A	-4.24	122.80	126.17
26	HJ	201	PEB	C3D-C4D-ND	4.24	115.57	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U8	202	PEB	CHC-C4C-C3C	-4.24	123.11	130.34
26	WA	201	PEB	CHB-C4B-NB	-4.24	122.95	128.83
28	EF	1001	CYC	C1B-NB-C4B	-4.24	105.28	110.67
27	24	402	PUB	CMA-C2A-C1A	4.24	131.35	121.39
26	qE	203	PEB	CHC-C4C-C3C	-4.24	123.11	130.34
26	Q7	202	PEB	C1C-CHB-C4B	4.23	133.87	128.81
26	KJ	202	PEB	CHA-C1B-NB	-4.23	116.08	124.93
26	m8	201	PEB	CHC-C1D-ND	4.23	118.86	113.95
26	W8	201	PEB	C3D-C4D-ND	4.23	115.56	107.26
26	KE	201	PEB	OA-C1A-C2A	-4.23	122.81	126.17
26	iI	201	PEB	OA-C1A-C2A	-4.23	122.81	126.17
26	L3	201	PEB	CHC-C4C-C3C	-4.23	123.12	130.34
26	EA	201	PEB	CHB-C4B-NB	-4.23	122.96	128.83
26	m8	202	PEB	CAB-C3B-C2B	4.23	135.76	127.88
28	DF	1003	CYC	CAB-C3B-C4B	4.23	128.06	121.38
26	kF	201	PEB	C3D-C4D-ND	4.23	115.56	107.26
26	RD	202	PEB	C4B-C3B-C2B	-4.23	102.10	106.78
26	X1	201	PEB	CHB-C4B-NB	-4.23	122.96	128.83
26	Y8	203	PEB	C3D-C4D-ND	4.23	115.56	107.26
27	A7	304	PUB	CMA-C2A-C1A	4.23	131.34	121.39
26	W4	201	PEB	C4B-C3B-C2B	-4.23	102.10	106.78
26	H8	201	PEB	CHA-C1B-NB	-4.23	116.08	124.93
26	dI	202	PEB	CHB-C4B-NB	-4.23	122.96	128.83
27	B8	302	PUB	CHC-C1D-ND	-4.23	108.37	113.72
26	V2	202	PEB	C3D-C4D-ND	4.23	115.56	107.26
26	QB	202	PEB	CHC-C1D-ND	-4.23	109.04	113.95
26	m1	201	PEB	CHA-C1B-NB	-4.23	116.09	124.93
26	XE	202	PEB	CMB-C2B-C1B	4.23	131.57	125.06
26	J8	201	PEB	C3D-C4D-ND	4.23	115.55	107.26
26	eA	201	PEB	C3D-C4D-ND	4.23	115.55	107.26
26	m8	201	PEB	CMB-C2B-C1B	4.23	131.57	125.06
26	HA	201	PEB	CHA-C1B-NB	-4.22	116.10	124.93
26	d1	202	PEB	C1C-CHB-C4B	4.22	133.85	128.81
28	kH	1001	CYC	CAB-C3B-C4B	4.22	128.05	121.38
26	YA	203	PEB	C3D-C4D-ND	4.22	115.54	107.26
26	a1	202	PEB	CHC-C4C-C3C	-4.22	123.14	130.34
26	YJ	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
26	A7	302	PEB	CHB-C4B-NB	-4.22	122.97	128.83
26	Q7	202	PEB	CMB-C2B-C1B	4.22	131.56	125.06
26	o1	501	PEB	OA-C1A-C2A	-4.22	122.82	126.17
26	D6	1002	PEB	OA-C1A-C2A	-4.22	122.82	126.17
26	gG	201	PEB	C4B-C3B-C2B	-4.22	102.11	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A4	203	PUB	CMA-C2A-C1A	4.22	131.32	121.39
26	m8	201	PEB	C3D-C4D-ND	4.22	115.54	107.26
26	hF	201	PEB	CHB-C4B-NB	-4.22	122.97	128.83
26	F8	202	PEB	C1C-CHB-C4B	-4.22	123.77	128.81
26	M4	402	PEB	C3D-C4D-ND	4.22	115.54	107.26
26	dB	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
26	V4	202	PEB	CHC-C4C-C3C	-4.22	123.14	130.34
26	MG	201	PEB	CHC-C4C-C3C	-4.22	123.14	130.34
26	I9	201	PEB	CAB-C3B-C4B	4.22	132.47	125.01
26	mE	201	PEB	OA-C1A-C2A	-4.22	122.82	126.17
26	Q8	202	PEB	C1C-CHB-C4B	4.22	133.85	128.81
26	I8	202	PEB	C3D-C4D-ND	4.22	115.53	107.26
28	DI	1001	CYC	C2B-C1B-NB	4.22	113.16	106.99
26	W8	201	PEB	CHB-C4B-NB	-4.22	122.98	128.83
26	F2	1002	PEB	CHC-C4C-C3C	-4.22	123.14	130.34
26	RB	202	PEB	CHC-C4C-C3C	-4.22	123.14	130.34
26	r4	201	PEB	CAA-C3A-C2A	-4.22	103.72	114.26
26	tG	202	PEB	C3D-C4D-ND	4.22	115.53	107.26
26	C8	202	PEB	CHC-C1D-ND	-4.22	109.05	113.95
26	NA	201	PEB	CMB-C2B-C1B	4.22	131.56	125.06
26	W1	201	PEB	C3B-C4B-NB	4.22	116.18	110.05
26	gF	202	PEB	CHB-C4B-NB	-4.22	122.98	128.83
26	VF	203	PEB	CMB-C2B-C1B	4.22	131.56	125.06
28	HB	1001	CYC	C1B-NB-C4B	-4.22	105.30	110.67
28	PH	1001	CYC	CHB-C4A-C3A	4.22	135.74	124.90
28	C7	1001	CYC	C2B-C1B-NB	4.22	113.16	106.99
26	GD	201	PEB	CHA-C1B-NB	-4.22	116.11	124.93
27	24	403	PUB	CMA-C2A-C1A	4.22	131.31	121.39
26	N8	202	PEB	C4B-C3B-C2B	-4.22	102.12	106.78
26	m4	201	PEB	CHB-C4B-NB	-4.21	122.98	128.83
26	aA	202	PEB	CHB-C4B-NB	-4.21	122.98	128.83
26	F4	201	PEB	CMB-C2B-C1B	4.21	131.55	125.06
26	IG	201	PEB	C3D-C4D-ND	4.21	115.53	107.26
26	VA	202	PEB	CHC-C4C-C3C	-4.21	123.15	130.34
27	AI	303	PUB	C1C-C2C-C3C	-4.21	102.12	106.78
26	y1	202	PEB	OA-C1A-C2A	-4.21	122.82	126.17
26	24	405	PEB	OA-C1A-C2A	-4.21	122.82	126.17
26	Y8	201	PEB	C4B-C3B-C2B	-4.21	102.12	106.78
26	DJ	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
26	TB	202	PEB	CHA-C1B-NB	-4.21	116.12	124.93
28	G6	1001	CYC	C2C-C1C-NC	4.21	111.90	108.27
27	xG	301	PUB	C1C-C2C-C3C	-4.21	102.12	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c1	203	PEB	CHA-C1B-NB	-4.21	116.13	124.93
26	FJ	202	PEB	CMB-C2B-C1B	4.21	131.55	125.06
26	T8	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
26	RJ	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
26	vG	201	PEB	CHC-C1D-ND	-4.21	109.06	113.95
26	J1	202	PEB	CHB-C4B-NB	-4.21	122.99	128.83
26	Q6	202	PEB	CHA-C1B-NB	-4.21	116.13	124.93
28	WH	1001	CYC	CMB-C2B-C1B	4.21	129.42	124.17
26	PI	202	PEB	OA-C1A-C2A	-4.21	122.83	126.17
26	TE	201	PEB	C1C-CHB-C4B	4.21	133.84	128.81
26	XE	201	PEB	CHC-C4C-C3C	-4.21	123.16	130.34
26	NA	202	PEB	C4B-C3B-C2B	-4.21	102.12	106.78
26	IE	203	PEB	C4B-C3B-C2B	-4.21	102.13	106.78
26	qE	202	PEB	C4B-C3B-C2B	-4.21	102.13	106.78
26	tE	201	PEB	C4B-C3B-C2B	-4.21	102.13	106.78
26	X4	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
26	K8	202	PEB	C3D-C4D-ND	4.21	115.51	107.26
26	TG	201	PEB	CHC-C4C-C3C	-4.21	123.16	130.34
26	HG	201	PEB	C1C-CHB-C4B	4.21	133.83	128.81
28	J7	1003	CYC	C2B-C1B-NB	4.21	113.15	106.99
26	gG	201	PEB	CHC-C1D-ND	-4.21	109.06	113.95
26	aA	204	PEB	CHB-C4B-NB	-4.21	122.99	128.83
26	Q3	201	PEB	CHA-C1B-C2B	4.21	135.71	124.90
26	i4	201	PEB	CHC-C4C-C3C	-4.21	123.17	130.34
26	BJ	203	PEB	CHB-C4B-NB	-4.20	123.00	128.83
26	CJ	201	PEB	C1C-CHB-C4B	4.20	133.83	128.81
26	OI	201	PEB	C3D-C4D-ND	4.20	115.51	107.26
26	VI	203	PEB	CHC-C4C-C3C	-4.20	123.17	130.34
26	d1	201	PEB	CHB-C4B-NB	-4.20	123.00	128.83
26	yE	301	PEB	OA-C1A-C2A	-4.20	122.83	126.17
26	aA	201	PEB	CHA-C1B-NB	-4.20	116.14	124.93
26	H5	203	PEB	C3D-C4D-ND	4.20	115.50	107.26
26	l8	202	PEB	CHB-C4B-NB	-4.20	123.00	128.83
26	FI	1002	PEB	CHC-C4C-C3C	-4.20	123.17	130.34
26	WA	203	PEB	C3B-C4B-NB	4.20	116.16	110.05
26	jB	201	PEB	CHB-C4B-NB	-4.20	123.00	128.83
26	VD	203	PEB	OA-C1A-C2A	-4.20	122.83	126.17
26	b1	501	PEB	C1C-CHB-C4B	-4.20	123.79	128.81
26	JD	201	PEB	C4B-C3B-C2B	-4.20	102.13	106.78
26	T3	203	PEB	C2A-C1A-NA	4.20	111.89	108.27
26	HC	203	PEB	CHB-C4B-NB	-4.20	123.00	128.83
28	K7	1001	CYC	C1B-CHB-C4A	-4.20	117.82	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W8	203	PEB	C3B-C4B-NB	4.20	116.16	110.05
27	K3	203	PUB	CMA-C2A-C1A	4.20	131.27	121.39
26	IA	202	PEB	C3D-C4D-ND	4.20	115.50	107.26
26	T6	201	PEB	CHA-C1B-NB	-4.20	116.15	124.93
26	P1	203	PEB	CMB-C2B-C1B	4.20	131.53	125.06
26	UF	201	PEB	CHA-C1B-NB	-4.20	116.15	124.93
26	hG	201	PEB	CHA-C1B-NB	-4.20	116.15	124.93
28	EF	1001	CYC	C2B-C1B-NB	4.20	113.13	106.99
26	m7	202	PEB	OA-C1A-C2A	-4.20	122.83	126.17
26	LD	202	PEB	C2A-C1A-NA	4.20	111.89	108.27
26	jE	201	PEB	C4B-C3B-C2B	-4.20	102.14	106.78
26	X8	201	PEB	CMB-C2B-C1B	4.20	131.53	125.06
26	qE	203	PEB	CMB-C2B-C1B	4.20	131.53	125.06
26	TE	201	PEB	CHC-C4C-C3C	-4.20	123.18	130.34
28	H6	1001	CYC	C1B-NB-C4B	-4.20	105.33	110.67
28	KH	1001	CYC	C1A-C2A-C3A	-4.20	102.14	106.78
26	F5	202	PEB	OA-C1A-C2A	-4.20	122.84	126.17
26	O9	202	PEB	OA-C1A-C2A	-4.20	122.84	126.17
28	GB	1001	CYC	C2C-C1C-NC	4.20	111.89	108.27
26	f6	202	PEB	CHB-C4B-NB	-4.20	123.01	128.83
26	NJ	204	PEB	CHB-C4B-NB	-4.20	123.01	128.83
26	P1	202	PEB	C3D-C4D-ND	4.20	115.49	107.26
26	QE	201	PEB	C4B-C3B-C2B	-4.20	102.14	106.78
26	KA	203	PEB	CHB-C4B-NB	-4.20	123.01	128.83
26	K4	201	PEB	OA-C1A-C2A	-4.20	122.84	126.17
26	OF	201	PEB	CHA-C1B-NB	-4.20	116.16	124.93
26	GE	202	PEB	CMB-C2B-C1B	4.19	131.52	125.06
26	B3	203	PEB	CHC-C1D-ND	-4.19	109.08	113.95
26	NE	202	PEB	C1C-CHB-C4B	4.19	133.82	128.81
28	pH	1001	CYC	CAB-C3B-C4B	4.19	128.00	121.38
27	Y3	302	PUB	CMA-C2A-C1A	4.19	131.26	121.39
26	R6	202	PEB	CHC-C4C-C3C	-4.19	123.18	130.34
26	O1	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
26	c8	201	PEB	C4B-C3B-C2B	-4.19	102.14	106.78
26	kA	202	PEB	CAB-CBB-CGB	4.19	122.63	113.60
26	RB	201	PEB	CAB-C3B-C4B	4.19	132.43	125.01
26	H5	201	PEB	C3D-C4D-ND	4.19	115.49	107.26
26	C8	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
26	U6	201	PEB	CHC-C1D-ND	-4.19	109.08	113.95
26	JG	201	PEB	OA-C1A-NA	4.19	130.02	124.94
28	II	1001	CYC	C2B-C1B-NB	4.19	113.12	106.99
28	DF	1003	CYC	C1B-NB-C4B	-4.19	105.33	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	PA	202	PEB	CHC-C4C-C3C	-4.19	123.19	130.34
26	W2	201	PEB	C3D-C4D-ND	4.19	115.48	107.26
27	BA	302	PUB	CMA-C2A-C1A	4.19	131.25	121.39
26	q1	202	PEB	C2A-C1A-NA	4.19	111.89	108.27
26	m8	202	PEB	C4B-C3B-C2B	-4.19	102.14	106.78
28	yH	1001	CYC	CAB-C3B-C4B	4.19	128.00	121.38
26	jI	202	PEB	C3D-C4D-ND	4.19	115.48	107.26
26	C5	204	PEB	OA-C1A-C2A	-4.19	122.84	126.17
26	IJ	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
26	iI	203	PEB	C4B-C3B-C2B	-4.19	102.15	106.78
27	KD	203	PUB	CMA-C2A-C1A	4.19	131.24	121.39
26	cF	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
26	d2	201	PEB	CHC-C4C-C3C	-4.19	123.19	130.34
26	AC	201	PEB	C2A-C1A-NA	4.19	111.88	108.27
28	NB	1001	CYC	CHB-C4A-C3A	4.19	135.67	124.90
26	XA	201	PEB	C1C-CHB-C4B	-4.19	123.81	128.81
28	KF	1001	CYC	C1B-NB-C4B	-4.19	105.34	110.67
27	KD	203	PUB	C1C-C2C-C3C	-4.19	102.15	106.78
26	bE	202	PEB	C3D-C4D-ND	4.19	115.47	107.26
27	AF	304	PUB	CAC-C2C-C1C	4.19	132.42	125.01
26	pE	201	PEB	C1C-CHB-C4B	-4.19	123.81	128.81
26	G3	202	PEB	CHC-C4C-C3C	-4.19	123.20	130.34
26	nG	201	PEB	CHA-C1B-NB	-4.19	116.18	124.93
26	O2	201	PEB	C3D-C4D-ND	4.19	115.47	107.26
26	X4	202	PEB	CMA-C2A-C1A	-4.19	103.38	112.40
27	YD	302	PUB	CMA-C2A-C1A	4.19	131.24	121.39
26	d1	203	PEB	CHA-C1B-NB	-4.19	116.18	124.93
26	c1	203	PEB	C1C-CHB-C4B	4.19	133.81	128.81
26	jF	203	PEB	OA-C1A-C2A	-4.19	122.84	126.17
26	p4	201	PEB	CHC-C1D-ND	-4.19	109.09	113.95
28	IH	1001	CYC	CMB-C2B-C1B	4.19	129.39	124.17
26	IJ	203	PEB	CHB-C4B-NB	-4.18	123.02	128.83
26	OG	201	PEB	CHC-C1D-ND	-4.18	109.09	113.95
26	N8	201	PEB	CMB-C2B-C1B	4.18	131.51	125.06
26	e6	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
26	N7	1002	PEB	OA-C1A-C2A	-4.18	122.85	126.17
26	mA	201	PEB	CHC-C1D-ND	4.18	118.81	113.95
26	J3	203	PEB	OA-C1A-C2A	-4.18	122.85	126.17
26	TA	201	PEB	C3D-C4D-ND	4.18	115.47	107.26
26	OB	201	PEB	C3D-C4D-ND	4.18	115.47	107.26
26	f8	202	PEB	CHC-C4C-C3C	-4.18	123.20	130.34
26	xG	303	PEB	CHC-C4C-C3C	-4.18	123.20	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V8	201	PEB	CMB-C2B-C1B	4.18	131.50	125.06
26	YG	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
26	q4	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
26	kE	203	PEB	OA-C1A-C2A	-4.18	122.85	126.17
26	K4	202	PEB	C3D-C4D-ND	4.18	115.46	107.26
28	jH	1001	CYC	CMB-C2B-C1B	4.18	129.39	124.17
26	h4	203	PEB	CHB-C4B-NB	-4.18	123.03	128.83
26	h8	202	PEB	CMB-C2B-C1B	4.18	131.50	125.06
28	D2	1001	CYC	C2B-C1B-NB	4.18	113.11	106.99
27	24	402	PUB	C1C-C2C-C3C	-4.18	102.16	106.78
26	M4	401	PEB	C3D-C4D-ND	4.18	115.46	107.26
26	G9	202	PEB	CBC-CAC-C2C	4.18	119.75	112.62
26	EJ	201	PEB	C3B-C4B-NB	4.18	116.13	110.05
26	P8	201	PEB	CHA-C1B-NB	-4.18	116.19	124.93
26	p1	202	PEB	CHA-C4A-NA	-4.18	120.24	125.20
26	KC	201	PEB	CMB-C2B-C1B	4.18	131.50	125.06
26	P4	202	PEB	C3D-C4D-ND	4.18	115.45	107.26
26	WE	201	PEB	C1B-C2B-C3B	-4.18	101.71	106.51
26	FI	1002	PEB	CHC-C1D-ND	-4.18	109.10	113.95
26	MD	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
26	OG	201	PEB	C2A-C1A-NA	4.17	111.87	108.27
26	LB	1002	PEB	CHB-C4B-NB	-4.17	123.04	128.83
26	SD	202	PEB	CHB-C4B-NB	-4.17	123.04	128.83
26	l2	202	PEB	CHC-C4C-C3C	-4.17	123.22	130.34
26	iA	202	PEB	C4B-C3B-C2B	-4.17	102.16	106.78
26	qG	203	PEB	CHC-C4C-C3C	-4.17	123.22	130.34
26	fE	201	PEB	OA-C1A-NA	4.17	130.00	124.94
26	Z1	201	PEB	CHA-C1B-NB	-4.17	116.20	124.93
26	c8	202	PEB	C4B-C3B-C2B	-4.17	102.16	106.78
26	R6	201	PEB	CHC-C1D-ND	-4.17	109.10	113.95
26	iF	201	PEB	C3B-C4B-NB	4.17	116.12	110.05
26	L3	202	PEB	C2A-C1A-NA	4.17	111.87	108.27
26	IE	201	PEB	CHB-C4B-C3B	-4.17	115.68	125.32
26	D9	201	PEB	C4B-C3B-C2B	-4.17	102.17	106.78
28	EH	1001	CYC	C4D-CHA-C1A	4.17	133.79	128.81
26	aI	202	PEB	CHA-C1B-NB	-4.17	116.21	124.93
28	kH	1001	CYC	CMB-C2B-C1B	4.17	129.38	124.17
26	h7	201	PEB	CHC-C1D-ND	-4.17	109.10	113.95
26	FA	202	PEB	CAB-C3B-C4B	4.17	132.39	125.01
26	OA	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
26	bB	201	PEB	C3D-C4D-ND	4.17	115.44	107.26
28	I2	1001	CYC	C2B-C1B-NB	4.17	113.09	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	302	PUB	CMA-C2A-C1A	4.17	131.20	121.39
26	fF	203	PEB	OA-C1A-C2A	-4.17	122.86	126.17
26	TD	201	PEB	CMB-C2B-C1B	4.17	131.48	125.06
26	d7	202	PEB	CHC-C4C-C3C	-4.17	123.23	130.34
26	dE	201	PEB	CHC-C4C-C3C	-4.17	123.23	130.34
26	j2	201	PEB	C3B-C4B-NB	4.17	116.11	110.05
28	FB	1001	CYC	OC-C1C-C2C	-4.17	122.86	126.17
26	oG	202	PEB	CMB-C2B-C1B	4.17	131.48	125.06
27	B8	302	PUB	CMA-C2A-C1A	4.17	131.19	121.39
28	K2	1001	CYC	C2B-C1B-NB	4.17	113.09	106.99
27	AI	302	PUB	CHA-C1B-C2B	-4.17	123.23	130.34
26	D1	203	PEB	OA-C1A-C2A	-4.17	122.86	126.17
26	F3	202	PEB	OA-C1A-C2A	-4.17	122.86	126.17
26	F8	202	PEB	OA-C1A-C2A	-4.17	122.86	126.17
26	XA	202	PEB	CAA-C3A-C2A	-4.17	103.85	114.26
26	BE	202	PEB	C3D-C4D-ND	4.17	115.43	107.26
26	kG	201	PEB	CHB-C4B-NB	-4.17	123.05	128.83
26	T3	202	PEB	CHA-C1B-NB	-4.17	116.22	124.93
26	DD	203	PEB	CHC-C1D-ND	-4.17	109.11	113.95
26	N3	201	PEB	C2A-C1A-NA	4.17	111.86	108.27
26	VF	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17
28	KF	1001	CYC	OC-C1C-C2C	-4.17	122.86	126.17
26	H8	202	PEB	C4B-C3B-C2B	-4.17	102.17	106.78
28	YH	1003	CYC	CMB-C2B-C1B	4.17	129.37	124.17
26	F9	201	PEB	CHA-C1B-C2B	4.16	135.61	124.90
26	c1	203	PEB	OA-C1A-C2A	-4.16	122.86	126.17
26	GJ	202	PEB	OA-C1A-C2A	-4.16	122.86	126.17
28	J7	1003	CYC	OC-C1C-C2C	-4.16	122.86	126.17
26	Z6	203	PEB	CHA-C1B-NB	-4.16	116.22	124.93
26	I9	201	PEB	CAB-CBB-CGB	-4.16	104.64	113.60
26	WA	201	PEB	C3D-C4D-ND	4.16	115.43	107.26
27	AA	304	PUB	CMA-C2A-C1A	4.16	131.18	121.39
26	WA	202	PEB	C2A-C1A-NA	4.16	111.86	108.27
26	HA	201	PEB	C1C-CHB-C4B	-4.16	123.84	128.81
26	CA	201	PEB	OA-C1A-C2A	-4.16	122.86	126.17
26	FC	202	PEB	CHC-C4C-C3C	-4.16	123.24	130.34
28	FB	1001	CYC	CHA-C1A-NA	-4.16	123.05	128.83
26	PG	202	PEB	CMB-C2B-C1B	4.16	131.47	125.06
26	FE	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
26	RA	202	PEB	CAA-C3A-C2A	-4.16	103.86	114.26
27	yE	302	PUB	CHC-C1D-ND	-4.16	108.46	113.72
28	dH	1001	CYC	C2B-C1B-NB	4.16	113.08	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M8	202	PEB	CHA-C1B-NB	-4.16	116.23	124.93
26	B5	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
26	L8	201	PEB	CHA-C1B-NB	-4.16	116.23	124.93
26	BG	202	PEB	OA-C1A-C2A	-4.16	122.86	126.17
26	DJ	201	PEB	OA-C1A-C2A	-4.16	122.86	126.17
26	F1	203	PEB	CHB-C4B-NB	-4.16	123.06	128.83
27	A2	302	PUB	CMA-C2A-C1A	4.16	131.18	121.39
26	G6	1002	PEB	CAB-C3B-C2B	4.16	135.62	127.88
26	Z2	201	PEB	C4B-NB-C1B	-4.16	98.67	106.51
26	b6	202	PEB	CHC-C1D-ND	-4.16	109.12	113.95
26	XG	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
26	AJ	304	PEB	CHC-C1D-ND	-4.16	109.12	113.95
28	TH	1001	CYC	CAB-C3B-C4B	4.16	127.95	121.38
26	KA	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
26	u1	201	PEB	C3B-C4B-NB	4.16	116.10	110.05
26	T1	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
26	eD	401	PEB	C3D-C4D-ND	4.16	115.42	107.26
26	l1	201	PEB	C2A-C1A-NA	4.16	111.86	108.27
26	V8	202	PEB	OA-C1A-NA	4.16	129.98	124.94
26	l7	202	PEB	CHC-C4C-C3C	-4.16	123.25	130.34
26	cI	203	PEB	C4B-C3B-C2B	-4.16	102.18	106.78
26	a2	201	PEB	C3D-C4D-ND	4.16	115.41	107.26
26	JD	202	PEB	C3D-C4D-ND	4.16	115.41	107.26
26	ZG	202	PEB	C3D-C4D-ND	4.16	115.41	107.26
26	VE	201	PEB	C2A-C1A-NA	4.16	111.86	108.27
26	F8	202	PEB	CAB-C3B-C4B	4.15	132.36	125.01
26	F5	202	PEB	CHB-C4B-NB	-4.15	123.06	128.83
26	LF	1002	PEB	C3D-C4D-ND	4.15	115.41	107.26
26	GG	201	PEB	C1B-C2B-C3B	-4.15	101.74	106.51
26	ZI	201	PEB	C4B-NB-C1B	-4.15	98.69	106.51
26	BG	202	PEB	C3D-C4D-ND	4.15	115.41	107.26
26	K4	202	PEB	CHC-C1D-ND	-4.15	109.12	113.95
28	KI	1001	CYC	C2B-C1B-NB	4.15	113.07	106.99
26	cE	203	PEB	CMB-C2B-C1B	4.15	131.46	125.06
26	g7	202	PEB	CHC-C4C-C3C	-4.15	123.26	130.34
26	UA	202	PEB	CHB-C4B-NB	-4.15	123.07	128.83
26	mG	201	PEB	C2A-C1A-NA	4.15	111.85	108.27
28	YH	1001	CYC	CHB-C4A-C3A	4.15	135.58	124.90
26	M1	403	PEB	CMB-C2B-C1B	4.15	131.46	125.06
28	K2	1001	CYC	CMA-C3A-C4A	4.15	131.46	125.06
26	l6	201	PEB	C2A-C1A-NA	4.15	111.85	108.27
26	B1	202	PEB	C1C-CHB-C4B	4.15	133.77	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S6	203	PEB	CHA-C1B-NB	-4.15	116.25	124.93
26	IG	203	PEB	C3B-C4B-NB	4.15	116.09	110.05
26	dG	202	PEB	CMB-C2B-C1B	4.15	131.46	125.06
26	K8	201	PEB	CHC-C1D-ND	-4.15	109.13	113.95
27	Q8	201	PUB	CHA-C4A-NA	-4.15	109.13	113.95
26	i4	202	PEB	C1B-C2B-C3B	-4.15	101.74	106.51
26	Q8	203	PEB	C3D-C4D-ND	4.15	115.40	107.26
26	VI	202	PEB	C3D-C4D-ND	4.15	115.40	107.26
26	PA	201	PEB	C2A-C1A-NA	4.15	111.85	108.27
26	LG	201	PEB	C4B-C3B-C2B	-4.15	102.19	106.78
26	ID	201	PEB	OA-C1A-C2A	-4.15	122.87	126.17
26	MA	202	PEB	CHA-C1B-NB	-4.15	116.25	124.93
26	gG	203	PEB	C3D-C4D-ND	4.15	115.40	107.26
26	LD	201	PEB	CHC-C4C-C3C	-4.15	123.26	130.34
26	c7	202	PEB	CHA-C1B-NB	-4.15	116.26	124.93
26	H5	202	PEB	C3D-C4D-ND	4.15	115.40	107.26
26	UB	202	PEB	C3D-C4D-ND	4.15	115.40	107.26
27	K4	203	PUB	CBA-CAA-C3A	-4.15	106.69	112.98
26	ND	203	PEB	CAB-CBB-CGB	-4.15	104.68	113.60
27	A2	303	PUB	C1C-C2C-C3C	-4.15	102.19	106.78
26	GE	202	PEB	C2A-C1A-NA	-4.15	104.70	108.27
26	R8	201	PEB	CHA-C1B-NB	-4.15	116.26	124.93
28	gH	1001	CYC	CAB-C3B-C4B	4.15	127.93	121.38
27	A7	304	PUB	CHA-C4A-NA	-4.15	109.13	113.95
26	QI	201	PEB	CMA-C2A-C1A	-4.15	103.47	112.40
26	N8	201	PEB	CHC-C1D-ND	4.15	118.76	113.95
26	oE	202	PEB	CMB-C2B-C1B	4.15	131.45	125.06
26	i6	202	PEB	OA-C1A-C2A	-4.15	122.88	126.17
26	V1	201	PEB	CHC-C4C-C3C	-4.15	123.27	130.34
26	GG	201	PEB	CHC-C1D-ND	-4.14	109.13	113.95
26	e1	202	PEB	CBC-CAC-C2C	4.14	119.69	112.62
26	gG	201	PEB	C1C-CHB-C4B	4.14	133.76	128.81
26	gE	201	PEB	CHB-C4B-C3B	-4.14	115.75	125.32
26	DG	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
26	f2	201	PEB	CHB-C4B-C3B	-4.14	115.75	125.32
28	HB	1001	CYC	CMB-C2B-C1B	4.14	129.34	124.17
26	d1	202	PEB	CHC-C1D-ND	-4.14	109.14	113.95
26	f6	203	PEB	CHC-C1D-ND	-4.14	109.14	113.95
28	F6	1001	CYC	CHA-C1A-NA	-4.14	123.08	128.83
26	qG	203	PEB	CMB-C2B-C1B	4.14	131.44	125.06
26	H3	203	PEB	C4B-C3B-C2B	-4.14	102.20	106.78
26	h6	201	PEB	OA-C1A-C2A	-4.14	122.88	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	PF	202	PEB	OA-C1A-C2A	-4.14	122.88	126.17
26	cA	201	PEB	C4B-C3B-C2B	-4.14	102.20	106.78
26	O4	201	PEB	CMB-C2B-C1B	4.14	131.44	125.06
26	QB	202	PEB	CBB-CAB-C3B	-4.14	101.12	112.63
26	g1	203	PEB	OA-C1A-C2A	-4.14	122.88	126.17
26	H5	202	PEB	CHC-C4C-C3C	-4.14	123.28	130.34
26	NI	1002	PEB	CHC-C4C-C3C	-4.14	123.28	130.34
26	mA	201	PEB	CMB-C2B-C1B	4.14	131.44	125.06
26	O8	202	PEB	C3D-C4D-ND	4.14	115.38	107.26
26	h2	201	PEB	C3B-C4B-NB	4.14	116.07	110.05
26	ZF	202	PEB	CHC-C4C-C3C	-4.14	123.28	130.34
28	D2	1001	CYC	C1B-C2B-C3B	-4.14	103.55	107.87
26	DJ	203	PEB	C1B-C2B-C3B	-4.14	101.76	106.51
26	aF	201	PEB	CHC-C4C-C3C	-4.14	123.28	130.34
26	WI	201	PEB	C3D-C4D-ND	4.14	115.38	107.26
26	EE	201	PEB	C4B-C3B-C2B	-4.14	102.20	106.78
26	xE	302	PEB	CHA-C1B-NB	-4.14	116.28	124.93
26	OG	201	PEB	C3D-C4D-ND	4.14	115.38	107.26
26	j2	202	PEB	CHB-C4B-NB	-4.14	123.09	128.83
26	fl	202	PEB	CHB-C4B-NB	-4.14	123.09	128.83
28	KI	1001	CYC	CMA-C3A-C4A	4.14	131.43	125.06
26	M3	201	PEB	CMB-C2B-C1B	4.14	131.43	125.06
26	k2	202	PEB	C3D-C4D-ND	4.14	115.37	107.26
26	ND	201	PEB	CHC-C1D-ND	-4.13	109.15	113.95
26	CE	201	PEB	CHB-C4B-NB	-4.13	123.09	128.83
26	V4	201	PEB	CHC-C4C-C3C	-4.13	123.29	130.34
26	t4	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
26	YA	201	PEB	C4B-C3B-C2B	-4.13	102.21	106.78
26	H1	202	PEB	C3D-C4D-ND	4.13	115.37	107.26
26	W7	201	PEB	CHC-C4C-C3C	-4.13	123.29	130.34
28	B6	1002	CYC	CHB-C4A-C3A	4.13	135.53	124.90
26	sG	203	PEB	C1B-C2B-C3B	-4.13	101.76	106.51
26	C5	201	PEB	OA-C1A-C2A	-4.13	122.89	126.17
26	dF	203	PEB	OA-C1A-C2A	-4.13	122.89	126.17
26	lF	201	PEB	OA-C1A-C2A	-4.13	122.89	126.17
26	SA	202	PEB	CHB-C4B-NB	-4.13	123.10	128.83
28	MB	1001	CYC	C2B-C1B-NB	4.13	113.04	106.99
26	mB	202	PEB	CHC-C4C-C3C	-4.13	123.29	130.34
28	FF	1001	CYC	C1B-C2B-C3B	-4.13	103.56	107.87
26	k4	203	PEB	C2A-C1A-NA	4.13	111.83	108.27
26	iF	202	PEB	C1C-CHB-C4B	-4.13	123.88	128.81
26	r1	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aB	201	PEB	OA-C1A-C2A	-4.13	122.89	126.17
28	F7	1001	CYC	OC-C1C-C2C	-4.13	122.89	126.17
28	FF	1001	CYC	OC-C1C-C2C	-4.13	122.89	126.17
26	U9	202	PEB	CHC-C1D-ND	-4.13	109.15	113.95
26	T3	201	PEB	C3D-C4D-ND	4.13	115.36	107.26
26	ZI	202	PEB	C3D-C4D-ND	4.13	115.36	107.26
26	UE	203	PEB	CMB-C2B-C1B	4.13	131.42	125.06
28	J7	1001	CYC	C1B-C2B-C3B	-4.13	103.56	107.87
26	G3	201	PEB	CHB-C4B-NB	-4.13	123.10	128.83
26	J5	201	PEB	C3D-C4D-ND	4.13	115.36	107.26
27	21	402	PUB	CMA-C2A-C1A	4.13	131.10	121.39
26	Z1	201	PEB	OD-C4D-ND	-4.13	119.81	125.93
27	A6	302	PUB	CMA-C2A-C1A	4.13	131.10	121.39
26	Q2	202	PEB	CHC-C4C-C3C	-4.13	123.30	130.34
26	H3	203	PEB	CHC-C4C-C3C	-4.13	123.30	130.34
26	bE	201	PEB	OA-C1A-NA	4.13	129.94	124.94
26	cG	203	PEB	CMB-C2B-C1B	4.13	131.42	125.06
26	l8	202	PEB	CHA-C1B-NB	-4.13	116.30	124.93
28	NB	1001	CYC	C1B-C2B-C3B	-4.13	103.56	107.87
28	DI	1001	CYC	C1B-C2B-C3B	-4.13	103.56	107.87
26	A4	201	PEB	C2A-C1A-NA	4.13	111.83	108.27
26	K1	201	PEB	CMB-C2B-C1B	4.13	131.42	125.06
26	S1	202	PEB	CHC-C1D-ND	-4.13	109.16	113.95
26	p4	202	PEB	CHC-C1D-ND	-4.13	109.16	113.95
26	KE	202	PEB	C3B-C4B-NB	4.12	116.05	110.05
26	jF	201	PEB	C3B-C4B-NB	4.12	116.05	110.05
26	LA	201	PEB	CHA-C1B-NB	-4.12	116.31	124.93
26	e3	401	PEB	C3D-C4D-ND	4.12	115.35	107.26
26	UI	201	PEB	CHC-C4C-C3C	-4.12	123.30	130.34
26	i8	201	PEB	C3D-C4D-ND	4.12	115.35	107.26
28	vH	1001	CYC	CAB-C3B-C4B	4.12	127.89	121.38
26	LI	1002	PEB	CMD-C2D-C3D	4.12	135.88	130.06
26	f7	203	PEB	CHC-C1D-ND	-4.12	109.16	113.95
26	R2	201	PEB	C2A-C1A-NA	4.12	111.83	108.27
26	D1	202	PEB	CHB-C4B-NB	-4.12	123.11	128.83
26	w4	203	PEB	CHC-C4C-C3C	-4.12	123.31	130.34
26	J5	202	PEB	CMB-C2B-C1B	4.12	131.41	125.06
26	AI	305	PEB	CHB-C4B-NB	-4.12	123.11	128.83
26	s1	203	PEB	C1C-CHB-C4B	4.12	133.73	128.81
26	O1	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
26	c2	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
26	b6	201	PEB	C3D-C4D-ND	4.12	115.34	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J5	202	PEB	C1B-C2B-C3B	-4.12	101.78	106.51
26	B1	202	PEB	OA-C1A-C2A	-4.12	122.90	126.17
26	T6	202	PEB	CHA-C1B-NB	-4.12	116.31	124.93
26	f8	203	PEB	CHB-C4B-NB	-4.12	123.11	128.83
26	L5	201	PEB	CMB-C2B-C1B	4.12	131.41	125.06
26	g4	201	PEB	CHC-C4C-C3C	-4.12	123.31	130.34
28	YH	1003	CYC	CHB-C4A-C3A	4.12	135.49	124.90
26	K8	203	PEB	CHB-C4B-NB	-4.12	123.11	128.83
26	sG	201	PEB	CHB-C4B-NB	-4.12	123.11	128.83
26	r1	201	PEB	C3B-C4B-NB	4.12	116.04	110.05
26	X3	202	PEB	C3B-C4B-NB	4.12	116.04	110.05
26	U6	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
26	H1	202	PEB	CHC-C1D-ND	-4.12	109.17	113.95
26	k8	201	PEB	C3D-C4D-ND	4.12	115.34	107.26
26	d2	201	PEB	C3B-C4B-NB	4.12	116.04	110.05
27	Q8	201	PUB	C4B-CHB-C1C	-4.12	123.89	128.81
27	QA	201	PUB	CHA-C4A-NA	-4.12	109.17	113.95
26	d2	201	PEB	OA-C1A-C2A	-4.12	122.90	126.17
26	L8	201	PEB	CMB-C2B-C1B	4.12	131.40	125.06
26	hG	201	PEB	C3D-C4D-ND	4.12	115.33	107.26
26	PA	202	PEB	CHA-C1B-NB	-4.12	116.32	124.93
26	mA	202	PEB	C4B-C3B-C2B	-4.12	102.23	106.78
27	B8	302	PUB	C1C-C2C-C3C	-4.12	102.23	106.78
26	R3	202	PEB	C3B-C4B-NB	4.12	116.04	110.05
26	OF	203	PEB	CHB-C4B-NB	-4.12	123.12	128.83
28	H6	1001	CYC	CMB-C2B-C1B	4.12	129.31	124.17
26	SE	201	PEB	C3D-C4D-ND	4.12	115.33	107.26
26	G6	1002	PEB	CHB-C4B-NB	-4.11	123.12	128.83
26	L6	1002	PEB	CHB-C4B-NB	-4.11	123.12	128.83
26	HC	202	PEB	OA-C1A-C2A	-4.11	122.90	126.17
26	d4	203	PEB	CMB-C2B-C1B	4.11	131.40	125.06
26	a2	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
26	P3	201	PEB	C3D-C4D-ND	4.11	115.33	107.26
26	u4	201	PEB	CHC-C4C-C3C	-4.11	123.32	130.34
26	p4	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
27	xG	305	PUB	CMA-C2A-C1A	4.11	131.06	121.39
26	EG	201	PEB	CHC-C4C-C3C	-4.11	123.32	130.34
26	p4	201	PEB	OA-C1A-C2A	-4.11	122.90	126.17
28	L6	1001	CYC	CHB-C4A-C3A	4.11	135.47	124.90
26	lB	201	PEB	C2A-C1A-NA	4.11	111.82	108.27
26	BJ	203	PEB	C4B-C3B-C2B	-4.11	102.23	106.78
26	XG	203	PEB	C3D-C4D-ND	4.11	115.33	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a2	202	PEB	CHA-C1B-NB	-4.11	116.33	124.93
26	W9	201	PEB	CHB-C4B-C3B	-4.11	115.82	125.32
28	K7	1001	CYC	C1B-NB-C4B	-4.11	105.44	110.67
26	i8	202	PEB	C4B-C3B-C2B	-4.11	102.23	106.78
26	bG	201	PEB	OA-C1A-C2A	-4.11	122.91	126.17
26	UJ	202	PEB	OA-C1A-C2A	-4.11	122.91	126.17
27	BA	302	PUB	CHA-C1B-C2B	-4.11	123.33	130.34
26	nE	202	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	AF	301	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	dI	202	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	DE	202	PEB	C1B-C2B-C3B	-4.11	101.79	106.51
26	aI	201	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	eA	202	PEB	CAB-C3B-C4B	4.11	132.28	125.01
26	S2	202	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	a8	202	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	m6	203	PEB	OA-C1A-C2A	-4.11	122.91	126.17
26	pG	201	PEB	C2A-C1A-NA	4.11	111.81	108.27
26	C8	202	PEB	C3D-C4D-ND	4.11	115.32	107.26
26	T2	201	PEB	CMB-C2B-C1B	4.11	131.39	125.06
27	AJ	302	PUB	CHA-C1B-C2B	-4.11	123.33	130.34
26	sG	203	PEB	CHA-C1B-C2B	4.11	135.46	124.90
26	L7	1002	PEB	CHC-C4C-C3C	-4.11	123.33	130.34
26	f4	201	PEB	C4B-C3B-C2B	-4.11	102.24	106.78
28	D7	1001	CYC	OC-C1C-C2C	-4.11	122.91	126.17
26	P4	201	PEB	CHB-C4B-NB	-4.11	123.13	128.83
26	e7	201	PEB	CHB-C4B-NB	-4.11	123.13	128.83
26	G8	202	PEB	C3D-C4D-ND	4.11	115.31	107.26
26	vG	202	PEB	C1C-CHB-C4B	4.11	133.71	128.81
26	P2	202	PEB	OA-C1A-C2A	-4.11	122.91	126.17
26	VB	201	PEB	OA-C1A-C2A	-4.11	122.91	126.17
26	hB	201	PEB	OA-C1A-C2A	-4.11	122.91	126.17
26	I4	201	PEB	CMB-C2B-C1B	4.10	131.38	125.06
26	E3	201	PEB	C3D-C4D-ND	4.10	115.31	107.26
26	OG	201	PEB	CHA-C1B-NB	-4.10	116.35	124.93
26	m8	202	PEB	C2A-C1A-NA	4.10	111.81	108.27
26	GE	201	PEB	C2A-C1A-NA	4.10	111.81	108.27
26	iE	201	PEB	C3D-C4D-ND	4.10	115.31	107.26
26	E8	203	PEB	OA-C1A-C2A	-4.10	122.91	126.17
28	uH	1001	CYC	CMB-C2B-C1B	4.10	129.29	124.17
26	b6	201	PEB	CHA-C1B-NB	-4.10	116.35	124.93
26	u4	202	PEB	CHB-C4B-NB	-4.10	123.14	128.83
26	O4	201	PEB	CHC-C1D-ND	-4.10	109.18	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	VI	202	PEB	C4B-C3B-C2B	-4.10	102.24	106.78
26	J3	202	PEB	C1B-C2B-C3B	-4.10	101.80	106.51
26	IA	202	PEB	CMB-C2B-C1B	4.10	131.38	125.06
28	EH	1001	CYC	CHB-C4A-C3A	4.10	135.44	124.90
26	G8	202	PEB	C1C-CHB-C4B	-4.10	123.91	128.81
26	P3	202	PEB	CHC-C1D-ND	-4.10	109.19	113.95
26	HJ	203	PEB	CHB-C4B-NB	-4.10	123.14	128.83
26	d1	203	PEB	CHC-C4C-C3C	-4.10	123.34	130.34
28	gH	1001	CYC	CHB-C4A-C3A	4.10	135.44	124.90
26	m4	201	PEB	C3D-C4D-ND	4.10	115.30	107.26
26	RI	202	PEB	OA-C1A-C2A	-4.10	122.91	126.17
26	kI	201	PEB	OA-C1A-C2A	-4.10	122.91	126.17
26	VD	201	PEB	CHA-C1B-NB	-4.10	116.36	124.93
26	VB	202	PEB	C1C-CHB-C4B	-4.10	123.91	128.81
26	TJ	202	PEB	C4B-C3B-C2B	-4.10	102.25	106.78
26	TJ	201	PEB	OA-C1A-C2A	-4.10	122.92	126.17
26	sG	201	PEB	CMB-C2B-C1B	4.10	131.37	125.06
26	W1	202	PEB	C2A-C1A-NA	4.10	111.81	108.27
26	V3	201	PEB	C2A-C1A-NA	4.10	111.81	108.27
26	VJ	201	PEB	CHB-C4B-NB	-4.10	123.14	128.83
26	KE	201	PEB	CHC-C1D-ND	-4.10	109.19	113.95
28	HI	1001	CYC	OC-C1C-C2C	-4.10	122.92	126.17
28	CB	1001	CYC	OB-C4B-C3B	-4.10	123.59	128.04
26	GA	202	PEB	C3D-C4D-ND	4.10	115.30	107.26
26	xE	304	PEB	CHA-C1B-NB	-4.10	116.36	124.93
26	sE	202	PEB	CHC-C4C-C3C	-4.10	123.35	130.34
26	eI	202	PEB	C3D-C4D-ND	4.10	115.29	107.26
26	k2	202	PEB	C1C-CHB-C4B	4.10	133.70	128.81
26	f6	201	PEB	OA-C1A-C2A	-4.10	122.92	126.17
26	HA	202	PEB	OA-C1A-C2A	-4.10	122.92	126.17
26	RG	202	PEB	OA-C1A-C2A	-4.10	122.92	126.17
26	YJ	201	PEB	CMB-C2B-C1B	4.09	131.37	125.06
26	eB	201	PEB	CHB-C4B-NB	-4.09	123.15	128.83
27	xE	305	PUB	CMA-C2A-C1A	4.09	131.02	121.39
26	F8	202	PEB	CHC-C4C-C3C	-4.09	123.35	130.34
26	FA	202	PEB	CHC-C4C-C3C	-4.09	123.35	130.34
26	IG	201	PEB	CHC-C4C-C3C	-4.09	123.35	130.34
26	DF	1002	PEB	CMB-C2B-C1B	4.09	131.37	125.06
26	H4	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	X9	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	eB	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	pG	202	PEB	C3D-C4D-ND	4.09	115.29	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	WH	1001	CYC	CAB-C3B-C4B	4.09	127.84	121.38
26	IG	203	PEB	C1C-CHB-C4B	4.09	133.70	128.81
26	eG	203	PEB	C1C-CHB-C4B	4.09	133.70	128.81
26	i2	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	lE	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	W7	202	PEB	CHA-C1B-NB	-4.09	116.37	124.93
27	QA	201	PUB	C1D-CHC-C4C	-4.09	104.46	113.37
28	GI	1001	CYC	OB-C4B-C3B	-4.09	123.60	128.04
28	H2	1001	CYC	C2B-C1B-NB	4.09	112.98	106.99
28	wH	1001	CYC	CMB-C2B-C1B	4.09	129.28	124.17
26	Y2	202	PEB	CHC-C1D-ND	-4.09	109.20	113.95
26	U2	201	PEB	C4B-NB-C1B	-4.09	98.80	106.51
26	h2	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	fB	203	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	F2	1002	PEB	C3D-C4D-ND	4.09	115.29	107.26
26	K3	202	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
26	AI	305	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
26	LC	201	PEB	CHC-C1D-ND	-4.09	109.20	113.95
26	L1	202	PEB	CHB-C4B-NB	-4.09	123.15	128.83
28	M6	1001	CYC	C2B-C1B-NB	4.09	112.98	106.99
26	B3	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	RI	201	PEB	C2A-C1A-NA	4.09	111.80	108.27
26	V8	201	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	aG	201	PEB	C1B-C2B-C3B	-4.09	101.81	106.51
26	QA	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	ZA	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
27	yG	302	PUB	CMA-C2A-C1A	4.09	131.01	121.39
26	MG	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	H4	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	jF	203	PEB	CHA-C1B-NB	-4.09	116.38	124.93
26	L7	1002	PEB	C2A-C1A-NA	4.09	111.80	108.27
26	K6	201	PEB	CHB-C4B-NB	-4.09	123.16	128.83
26	g2	203	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	Y9	201	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	EA	201	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	lE	202	PEB	CHC-C4C-C3C	-4.09	123.37	130.34
26	v1	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	T9	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	F1	202	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	U1	201	PEB	OA-C1A-C2A	-4.09	122.92	126.17
26	F8	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	BG	201	PEB	C3D-C4D-ND	4.09	115.28	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O3	202	PEB	C1C-CHB-C4B	4.09	133.69	128.81
28	qH	1001	CYC	CMB-C2B-C1B	4.09	129.27	124.17
28	H7	1001	CYC	C1B-CHB-C4A	-4.09	118.10	128.08
26	B4	201	PEB	CAA-C3A-C2A	-4.09	104.05	114.26
26	hE	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	dI	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
26	PD	201	PEB	CHC-C4C-C3C	-4.09	123.37	130.34
26	H9	202	PEB	CHB-C4B-NB	-4.09	123.16	128.83
26	C5	201	PEB	C1C-CHB-C4B	-4.09	123.93	128.81
26	mB	203	PEB	OA-C1A-C2A	-4.08	122.92	126.17
26	a2	203	PEB	CAB-C3B-C4B	4.08	132.24	125.01
26	c1	202	PEB	CHC-C1D-ND	-4.08	109.20	113.95
26	O4	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
26	FA	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
26	T3	201	PEB	CMB-C2B-C1B	4.08	131.35	125.06
26	HC	202	PEB	CHC-C4C-C3C	-4.08	123.37	130.34
28	yH	1001	CYC	CMB-C2B-C1B	4.08	129.27	124.17
28	CI	1001	CYC	C2B-C1B-NB	4.08	112.97	106.99
27	wG	304	PUB	CHC-C1D-ND	-4.08	108.56	113.72
26	gE	201	PEB	C3B-C4B-NB	4.08	115.99	110.05
26	V4	203	PEB	C2A-C1A-NA	4.08	111.79	108.27
26	S2	201	PEB	CMA-C2A-C1A	-4.08	103.60	112.40
26	Y2	203	PEB	OA-C1A-C2A	-4.08	122.93	126.17
26	CC	201	PEB	OA-C1A-C2A	-4.08	122.93	126.17
26	VE	202	PEB	C3B-C4B-NB	4.08	115.99	110.05
26	II	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
26	q4	201	PEB	CHB-C4B-NB	-4.08	123.17	128.83
26	Z7	202	PEB	C4B-C3B-C2B	-4.08	102.27	106.78
26	PG	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
26	OB	202	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
26	d4	203	PEB	CHB-C4B-NB	-4.08	123.17	128.83
26	14	203	PEB	CHB-C4B-NB	-4.08	123.17	128.83
26	kI	201	PEB	CHB-C4B-NB	-4.08	123.17	128.83
26	e2	203	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
26	s1	201	PEB	CBA-CAA-C3A	4.08	122.55	113.47
26	m1	201	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	HJ	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	F3	202	PEB	C1B-C2B-C3B	-4.08	101.82	106.51
26	R9	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
26	CA	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	ZA	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	Q7	201	PEB	OA-C1A-C2A	-4.08	122.93	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P1	202	PEB	CHA-C1B-NB	-4.08	116.40	124.93
26	L7	1002	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	C8	201	PEB	CHA-C1B-NB	-4.08	116.40	124.93
26	ND	201	PEB	CHA-C1B-NB	-4.08	116.40	124.93
26	pE	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	lE	201	PEB	C4B-C3B-C2B	-4.08	102.27	106.78
26	P6	202	PEB	CHA-C1B-NB	-4.08	116.40	124.93
26	H8	201	PEB	OA-C1A-C2A	-4.08	122.93	126.17
26	VG	202	PEB	C3B-C4B-NB	4.08	115.98	110.05
26	Z1	201	PEB	CAB-CBB-CGB	-4.08	104.83	113.60
26	GG	201	PEB	OD-C4D-ND	-4.08	119.89	125.93
26	TI	201	PEB	CMB-C2B-C1B	4.08	131.34	125.06
26	Q8	204	PEB	CHB-C4B-NB	-4.08	123.17	128.83
26	O8	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
26	LC	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
26	a4	202	PEB	C2A-C1A-NA	4.08	111.79	108.27
26	U2	201	PEB	CHC-C4C-C3C	-4.08	123.39	130.34
26	PJ	201	PEB	CHB-C4B-NB	-4.08	123.17	128.83
26	QB	203	PEB	CHC-C1D-ND	-4.08	109.22	113.95
27	A4	203	PUB	C1C-C2C-C3C	-4.08	102.27	106.78
26	TE	201	PEB	OA-C1A-NA	4.07	129.88	124.94
26	I1	202	PEB	OA-C1A-C2A	-4.07	122.93	126.17
26	i1	203	PEB	OA-C1A-C2A	-4.07	122.93	126.17
26	QG	201	PEB	C4B-C3B-C2B	-4.07	102.27	106.78
26	e6	201	PEB	CHB-C4B-NB	-4.07	123.18	128.83
26	L9	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
26	N8	202	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
26	J4	202	PEB	CHC-C1D-ND	-4.07	109.22	113.95
26	XE	201	PEB	CHC-C1D-ND	-4.07	109.22	113.95
26	m1	201	PEB	OA-C1A-C2A	-4.07	122.94	126.17
26	GE	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
26	H9	202	PEB	CHA-C1B-C2B	4.07	135.37	124.90
26	Z8	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
26	eI	202	PEB	CHB-C4B-NB	-4.07	123.18	128.83
26	P3	202	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
26	B9	203	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
26	OE	201	PEB	CHA-C1B-NB	-4.07	116.42	124.93
26	gE	202	PEB	CHB-C4B-NB	-4.07	123.18	128.83
26	HC	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
26	VG	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
26	m6	203	PEB	CHB-C4B-NB	-4.07	123.18	128.83
28	J7	1001	CYC	C2B-C1B-NB	4.07	112.95	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X1	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
26	O1	202	PEB	CHB-C4B-NB	-4.07	123.18	128.83
26	jG	202	PEB	CHB-C4B-C3B	-4.07	115.92	125.32
28	H7	1001	CYC	CHB-C1B-NB	-4.07	117.32	126.06
26	aG	201	PEB	CHC-C1D-ND	-4.07	109.22	113.95
28	CI	1001	CYC	CMA-C3A-C4A	4.07	131.33	125.06
26	HC	201	PEB	CHB-C4B-NB	-4.07	123.18	128.83
26	xE	302	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
26	U6	202	PEB	C2A-C1A-NA	4.07	111.78	108.27
26	JE	201	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
28	C2	1001	CYC	CMA-C3A-C4A	4.07	131.33	125.06
28	jH	1001	CYC	CHB-C4A-C3A	4.07	135.36	124.90
26	lG	202	PEB	OA-C1A-C2A	-4.07	122.94	126.17
28	G2	1001	CYC	OB-C4B-C3B	-4.07	123.63	128.04
26	z1	202	PEB	CHC-C1D-ND	-4.07	109.22	113.95
26	HC	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
26	V1	202	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
26	QA	204	PEB	OA-C1A-C2A	-4.07	122.94	126.17
28	EI	1001	CYC	C2B-C1B-NB	4.07	112.94	106.99
27	yE	302	PUB	CMA-C2A-C1A	4.07	130.95	121.39
26	XE	202	PEB	C3D-C4D-ND	4.06	115.23	107.26
26	V1	203	PEB	C2A-C1A-NA	4.06	111.78	108.27
26	y1	203	PEB	C4B-C3B-C2B	-4.06	102.28	106.78
28	EI	1001	CYC	OB-C4B-C3B	-4.06	123.63	128.04
26	dE	202	PEB	CMB-C2B-C1B	4.06	131.32	125.06
26	IJ	202	PEB	C2A-C1A-NA	4.06	111.78	108.27
26	hA	202	PEB	CMB-C2B-C1B	4.06	131.32	125.06
26	bI	201	PEB	CHB-C4B-C3B	-4.06	115.93	125.32
26	Z1	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
26	kG	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
26	QD	202	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
26	DG	202	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	LA	201	PEB	CMB-C2B-C1B	4.06	131.32	125.06
26	GJ	202	PEB	CMC-C3C-C2C	4.06	132.60	124.94
26	VD	201	PEB	OA-C1A-C2A	-4.06	122.94	126.17
26	mG	203	PEB	OA-C1A-C2A	-4.06	122.94	126.17
26	YI	202	PEB	CHC-C1D-ND	-4.06	109.23	113.95
26	AB	301	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
27	yG	303	PUB	CHB-C1C-NC	-4.06	123.19	128.83
26	V9	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
26	N9	204	PEB	OA-C1A-C2A	-4.06	122.94	126.17
26	aA	204	PEB	CHA-C1B-NB	-4.06	116.44	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	jI	201	PEB	CHB-C4B-C3B	-4.06	115.94	125.32
26	L8	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
26	UI	201	PEB	C4B-NB-C1B	-4.06	98.86	106.51
26	a1	202	PEB	C2A-C1A-NA	4.06	111.77	108.27
26	HJ	201	PEB	C2A-C1A-NA	4.06	111.77	108.27
26	Y2	202	PEB	OA-C1A-C2A	-4.06	122.94	126.17
26	N8	202	PEB	OA-C1A-C2A	-4.06	122.94	126.17
26	eD	401	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
26	F3	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
28	L6	1001	CYC	C1B-C2B-C3B	-4.06	103.64	107.87
26	DB	1002	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
27	AI	302	PUB	CMA-C2A-C1A	4.06	130.94	121.39
26	H5	203	PEB	C4B-C3B-C2B	-4.06	102.29	106.78
28	EH	1001	CYC	CAB-C3B-C4B	4.06	127.79	121.38
26	lF	202	PEB	CHC-C4C-C3C	-4.06	123.42	130.34
26	O1	202	PEB	CHC-C1D-ND	-4.06	109.23	113.95
26	M8	201	PEB	C2A-C1A-NA	4.06	111.77	108.27
26	I9	201	PEB	OA-C1A-C2A	-4.06	122.95	126.17
26	D3	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
26	C8	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
26	DG	202	PEB	CHA-C1B-NB	-4.06	116.45	124.93
26	u1	203	PEB	CHC-C4C-C3C	-4.06	123.42	130.34
26	YA	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
26	y4	201	PEB	CHA-C1B-C2B	-4.06	114.47	124.90
26	Y8	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
26	JC	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
27	A6	303	PUB	CMA-C2A-C1A	4.05	130.93	121.39
26	XA	202	PEB	OA-C1A-C2A	-4.05	122.95	126.17
26	CA	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
26	X3	203	PEB	CBC-CAC-C2C	4.05	119.54	112.62
26	S1	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
26	JG	201	PEB	CHC-C4C-C3C	-4.05	123.42	130.34
26	Z2	202	PEB	C3D-C4D-ND	4.05	115.21	107.26
26	wG	303	PEB	C3D-C4D-ND	4.05	115.21	107.26
26	ZF	202	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
26	E9	202	PEB	CHB-C4B-NB	-4.05	123.20	128.83
28	C6	1001	CYC	OB-C4B-C3B	-4.05	123.64	128.04
26	v1	201	PEB	OA-C1A-C2A	-4.05	122.95	126.17
26	d7	203	PEB	OA-C1A-C2A	-4.05	122.95	126.17
26	H5	203	PEB	CHB-C4B-NB	-4.05	123.21	128.83
26	U9	201	PEB	CBC-CAC-C2C	-4.05	105.70	112.62
26	o1	501	PEB	C3B-C4B-NB	4.05	115.94	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HJ	202	PEB	CHA-C1B-C2B	4.05	135.32	124.90
28	dH	1001	CYC	C1B-C2B-C3B	-4.05	103.64	107.87
26	mE	202	PEB	CHC-C4C-C3C	-4.05	123.43	130.34
26	TJ	203	PEB	OD-C4D-ND	-4.05	119.93	125.93
26	f4	201	PEB	CAA-C3A-C2A	-4.05	104.14	114.26
26	U1	202	PEB	CMB-C2B-C1B	4.05	131.30	125.06
26	Y6	202	PEB	C2A-C1A-NA	4.05	111.77	108.27
26	b6	201	PEB	CHC-C1D-ND	-4.05	109.24	113.95
26	kB	202	PEB	CHC-C1D-ND	-4.05	109.24	113.95
26	S4	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	FG	202	PEB	C3B-C4B-NB	4.05	115.94	110.05
26	QG	203	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
26	PD	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	NB	1002	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	RB	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	RF	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	KE	201	PEB	CMB-C2B-C1B	4.05	131.30	125.06
26	O9	201	PEB	C3B-C4B-NB	4.05	115.94	110.05
26	GE	201	PEB	C3B-C4B-NB	4.05	115.94	110.05
26	TD	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
28	KI	1001	CYC	OB-C4B-C3B	-4.05	123.65	128.04
26	IG	202	PEB	CHC-C4C-C3C	-4.05	123.44	130.34
26	T2	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	JD	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	PA	202	PEB	CHA-C4A-NA	4.05	130.02	125.20
26	hA	202	PEB	CHC-C4C-C3C	-4.05	123.44	130.34
28	C2	1001	CYC	C2B-C1B-NB	4.05	112.91	106.99
26	J3	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	LA	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	HG	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
26	WJ	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	C9	202	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	WJ	201	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	lA	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	OF	203	PEB	C2A-C1A-NA	4.04	111.76	108.27
26	T3	203	PEB	CHB-C4B-NB	-4.04	123.22	128.83
26	k4	201	PEB	CHB-C4B-NB	-4.04	123.22	128.83
26	gB	202	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	RD	201	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	K8	203	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	R8	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	X8	202	PEB	C3D-C4D-ND	4.04	115.19	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	vH	1001	CYC	C4D-CHA-C1A	4.04	133.64	128.81
26	p4	202	PEB	CAB-C3B-C4B	4.04	132.16	125.01
26	G4	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	OI	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	kB	201	PEB	CMB-C2B-C1B	4.04	131.29	125.06
26	AE	201	PEB	C3B-C4B-NB	4.04	115.93	110.05
26	a8	203	PEB	CHB-C4B-NB	-4.04	123.22	128.83
26	U4	201	PEB	CAC-CBC-CGC	-4.04	102.43	113.76
26	d2	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	cA	203	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	HE	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	P8	201	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
26	Z8	201	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
26	L1	201	PEB	CHC-C1D-ND	-4.04	109.25	113.95
28	LB	1001	CYC	CHB-C4A-C3A	4.04	135.29	124.90
28	lH	1001	CYC	CMB-C2B-C1B	4.04	129.21	124.17
26	b2	201	PEB	C1B-C2B-C3B	-4.04	101.87	106.51
26	Q1	201	PEB	C3B-C4B-NB	4.04	115.93	110.05
26	YE	201	PEB	CHB-C4B-NB	-4.04	123.22	128.83
28	I7	1001	CYC	C2B-C1B-NB	4.04	112.90	106.99
26	RE	202	PEB	C3B-C4B-NB	4.04	115.93	110.05
26	R1	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
26	tE	202	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	DJ	203	PEB	OA-C1A-C2A	-4.04	122.96	126.17
28	uH	1001	CYC	C4D-CHA-C1A	4.04	133.63	128.81
26	aF	202	PEB	CMB-C2B-C1B	4.04	131.28	125.06
26	SI	201	PEB	CHA-C1B-NB	-4.04	116.48	124.93
26	RE	202	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	N3	201	PEB	CHA-C1B-NB	-4.04	116.49	124.93
27	AI	303	PUB	CMA-C2A-C1A	4.04	130.89	121.39
26	n1	201	PEB	CHB-C4B-NB	-4.04	123.23	128.83
26	P4	203	PEB	CHC-C4C-C3C	-4.04	123.45	130.34
28	qH	1002	CYC	CHB-C1B-C2B	4.04	134.95	126.95
26	f8	201	PEB	C3D-C4D-ND	4.04	115.18	107.26
28	L7	1001	CYC	C2B-C1B-NB	4.04	112.90	106.99
26	VD	203	PEB	CHB-C4B-NB	-4.04	123.23	128.83
26	bI	201	PEB	CHC-C4C-C3C	-4.04	123.45	130.34
27	21	403	PUB	CMA-C2A-C1A	4.04	130.88	121.39
26	u4	201	PEB	OA-C1A-C2A	-4.04	122.96	126.17
26	k8	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
26	ZB	203	PEB	CHB-C4B-NB	-4.04	123.23	128.83
28	MH	1001	CYC	CHB-C4A-C3A	4.04	135.28	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H7	1001	CYC	C1B-C2B-C3B	-4.04	103.66	107.87
26	TG	201	PEB	OA-C1A-NA	4.04	129.83	124.94
27	yG	303	PUB	CMA-C2A-C1A	4.03	130.88	121.39
26	a4	202	PEB	OA-C1A-C2A	-4.03	122.97	126.17
28	OH	1001	CYC	CMB-C2B-C1B	4.03	129.21	124.17
26	Y3	304	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	G5	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	HC	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	GB	1002	PEB	CHB-C4B-NB	-4.03	123.23	128.83
26	A5	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	mA	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	c1	203	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
26	Z7	202	PEB	CHC-C4C-C3C	-4.03	123.46	130.34
28	KH	1001	CYC	CAA-C2A-C1A	4.03	132.15	125.01
26	a1	203	PEB	OA-C1A-C2A	-4.03	122.97	126.17
26	d6	204	PEB	CHC-C4C-C3C	-4.03	123.46	130.34
26	CG	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	R4	203	PEB	OA-C1A-C2A	-4.03	122.97	126.17
26	V4	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
26	HA	202	PEB	C4B-C3B-C2B	-4.03	102.32	106.78
28	WH	1001	CYC	C4D-CHA-C1A	4.03	133.62	128.81
26	Q1	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	A8	302	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	O8	203	PEB	C2A-C1A-NA	4.03	111.75	108.27
26	SB	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	m8	201	PEB	CAB-CBB-CGB	-4.03	104.93	113.60
26	GG	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
26	c2	203	PEB	C4B-C3B-C2B	-4.03	102.32	106.78
26	K5	201	PEB	CHC-C4C-C3C	-4.03	123.46	130.34
26	R3	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
28	CH	1001	CYC	OC-C1C-C2C	-4.03	122.97	126.17
28	SH	1001	CYC	CMB-C2B-C1B	4.03	129.20	124.17
28	F2	1001	CYC	CMA-C3A-C4A	4.03	131.27	125.06
26	N6	201	PEB	C3D-C4D-ND	4.03	115.16	107.26
27	BA	302	PUB	C1C-C2C-C3C	-4.03	102.32	106.78
26	T2	202	PEB	CHA-C1B-NB	-4.03	116.51	124.93
26	ND	201	PEB	C2A-C1A-NA	4.03	111.75	108.27
26	ZE	202	PEB	C3D-C4D-ND	4.03	115.16	107.26
26	QJ	202	PEB	C3D-C4D-ND	4.03	115.16	107.26
26	T8	201	PEB	CHC-C1D-ND	4.03	118.62	113.95
26	X9	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
26	l4	202	PEB	CHC-C4C-C3C	-4.03	123.47	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K3	201	PEB	C3D-C4D-ND	4.03	115.16	107.26
26	PE	202	PEB	CMB-C2B-C1B	4.03	131.26	125.06
26	HG	201	PEB	CMB-C2B-C1B	4.03	131.26	125.06
26	IG	201	PEB	C2A-C1A-NA	-4.03	104.80	108.27
26	h1	201	PEB	C3D-C4D-ND	4.02	115.16	107.26
26	A9	303	PEB	OA-C1A-C2A	-4.02	122.97	126.17
26	D4	201	PEB	C4B-C3B-C2B	-4.02	102.33	106.78
26	bI	201	PEB	C3B-C4B-NB	4.02	115.90	110.05
26	F3	202	PEB	CHA-C1B-NB	-4.02	116.52	124.93
26	SI	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
26	JJ	201	PEB	CHA-C1B-NB	-4.02	116.52	124.93
26	DA	201	PEB	C4B-C3B-C2B	-4.02	102.33	106.78
26	u1	203	PEB	CHC-C1D-ND	-4.02	109.28	113.95
26	S7	203	PEB	CHC-C1D-ND	-4.02	109.28	113.95
26	Z8	202	PEB	CAB-C3B-C4B	4.02	132.13	125.01
26	E9	201	PEB	C3B-C4B-NB	4.02	115.90	110.05
26	e8	202	PEB	C4B-C3B-C2B	-4.02	102.33	106.78
26	QA	203	PEB	C1C-CHB-C4B	-4.02	124.00	128.81
26	E8	203	PEB	C2A-C1A-NA	4.02	111.74	108.27
28	K7	1001	CYC	C4D-CHA-C1A	4.02	133.61	128.81
26	L5	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
28	cH	1001	CYC	C1B-NB-C4B	-4.02	105.55	110.67
27	AB	303	PUB	CMA-C2A-C1A	4.02	130.85	121.39
26	i6	201	PEB	CHB-C4B-NB	-4.02	123.25	128.83
26	YA	203	PEB	CHB-C4B-NB	-4.02	123.25	128.83
26	XA	202	PEB	C3D-C4D-ND	4.02	115.15	107.26
26	i1	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
26	SA	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
26	O2	201	PEB	CMA-C2A-C1A	-4.02	103.74	112.40
26	f2	201	PEB	CMB-C2B-C1B	4.02	131.25	125.06
28	VH	1001	CYC	CAB-C3B-C4B	4.02	127.73	121.38
26	dE	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
26	PD	203	PEB	CHC-C1D-ND	-4.02	109.28	113.95
26	m8	202	PEB	CHA-C1B-NB	-4.02	116.53	124.93
26	eA	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
26	Q3	202	PEB	CHC-C4C-C3C	-4.02	123.48	130.34
26	c8	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
26	HE	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
26	aA	203	PEB	OA-C1A-C2A	-4.02	122.98	126.17
26	hI	201	PEB	C3B-C4B-NB	4.02	115.89	110.05
26	NA	202	PEB	CHC-C4C-C3C	-4.02	123.48	130.34
26	PA	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	202	PEB	C3D-C4D-ND	4.02	115.14	107.26
26	T4	201	PEB	CMB-C2B-C1B	4.02	131.25	125.06
26	NJ	203	PEB	CHB-C4B-NB	-4.02	123.26	128.83
26	f2	201	PEB	C3B-C4B-NB	4.02	115.89	110.05
28	H7	1001	CYC	C2B-C1B-NB	4.02	112.87	106.99
26	V6	201	PEB	OA-C1A-C2A	-4.02	122.98	126.17
26	PB	202	PEB	CHC-C4C-C3C	-4.02	123.49	130.34
26	XD	202	PEB	C3B-C4B-NB	4.02	115.89	110.05
26	g7	202	PEB	CHA-C4A-NA	4.02	129.98	125.20
26	VA	201	PEB	C4B-C3B-C2B	-4.01	102.34	106.78
26	A4	201	PEB	CHA-C1B-NB	-4.01	116.53	124.93
26	OB	202	PEB	OA-C1A-C2A	-4.01	122.98	126.17
26	AD	202	PEB	CHC-C4C-C3C	-4.01	123.49	130.34
26	S6	201	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	e8	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	iA	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	kA	201	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	WF	202	PEB	CMB-C2B-C1B	4.01	131.25	125.06
26	h8	201	PEB	C2A-C1A-NA	4.01	111.73	108.27
26	F5	201	PEB	CHC-C4C-C3C	-4.01	123.49	130.34
26	EG	201	PEB	C3D-C4D-ND	4.01	115.13	107.26
28	DB	1001	CYC	CBD-CAD-C3D	-4.01	105.77	112.62
26	Z6	201	PEB	C4B-C3B-C2B	-4.01	102.34	106.78
26	qE	203	PEB	CHB-C4B-NB	-4.01	123.26	128.83
26	o1	501	PEB	C2A-C1A-NA	4.01	111.73	108.27
26	CA	201	PEB	CHA-C1B-NB	-4.01	116.54	124.93
26	QB	201	PEB	C3B-C4B-NB	4.01	115.89	110.05
26	B1	202	PEB	CHB-C4B-NB	-4.01	123.26	128.83
26	U1	202	PEB	CHB-C4B-NB	-4.01	123.26	128.83
26	fB	202	PEB	CHB-C4B-NB	-4.01	123.26	128.83
26	j7	201	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
26	SI	202	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
28	JI	1001	CYC	C2B-C1B-NB	4.01	112.86	106.99
26	R1	203	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	KG	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	AI	304	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
26	f1	201	PEB	CHA-C1B-NB	-4.01	116.55	124.93
26	J8	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	BE	201	PEB	C3D-C4D-ND	4.01	115.13	107.26
26	j2	201	PEB	CHB-C4B-C3B	-4.01	116.06	125.32
26	K1	202	PEB	CHA-C4A-NA	-4.01	120.44	125.20
26	ED	201	PEB	C3D-C4D-ND	4.01	115.12	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c4	203	PEB	C2A-C1A-NA	4.01	111.73	108.27
26	M8	203	PEB	C2A-C1A-NA	4.01	111.73	108.27
26	cE	202	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
26	c8	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
26	cA	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
26	G5	202	PEB	CMB-C2B-C1B	4.01	131.24	125.06
26	CJ	201	PEB	CHB-C4B-C3B	-4.01	116.06	125.32
26	c7	201	PEB	OA-C1A-C2A	-4.01	122.99	126.17
26	dB	204	PEB	OA-C1A-C2A	-4.01	122.99	126.17
26	YF	202	PEB	OA-C1A-C2A	-4.01	122.99	126.17
26	oG	202	PEB	CHB-C4B-NB	-4.01	123.27	128.83
26	OF	201	PEB	C1B-C2B-C3B	-4.01	101.91	106.51
26	l8	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
26	O3	201	PEB	OD-C4D-ND	-4.01	119.99	125.93
26	PD	201	PEB	OD-C4D-ND	-4.01	119.99	125.93
28	D7	1001	CYC	C1B-C2B-C3B	-4.01	103.69	107.87
26	gG	201	PEB	C3B-C4B-NB	4.01	115.88	110.05
28	HI	1001	CYC	C1B-NB-C4B	-4.01	105.57	110.67
26	C4	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
26	iA	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
27	24	402	PUB	C1D-CHC-C4C	-4.01	104.65	113.37
26	F7	1002	PEB	C2A-C1A-NA	4.01	111.73	108.27
26	VI	203	PEB	CHC-C1D-ND	-4.01	109.30	113.95
26	J4	203	PEB	CHB-C4B-NB	-4.01	123.27	128.83
26	14	201	PEB	C3D-C4D-ND	4.00	115.12	107.26
26	TG	202	PEB	C3B-C4B-NB	4.00	115.87	110.05
26	GA	202	PEB	CHC-C4C-C3C	-4.00	123.51	130.34
26	nG	202	PEB	OA-C1A-C2A	-4.00	122.99	126.17
26	hI	202	PEB	OA-C1A-C2A	-4.00	122.99	126.17
28	yH	1001	CYC	C4D-CHA-C1A	4.00	133.59	128.81
28	IB	1001	CYC	OB-C4B-C3B	-4.00	123.70	128.04
26	Q2	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
27	A8	304	PUB	CMA-C2A-C1A	4.00	130.81	121.39
26	c1	202	PEB	CBC-CAC-C2C	4.00	119.45	112.62
26	V7	201	PEB	CHA-C1B-NB	-4.00	116.56	124.93
26	IA	203	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	P7	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
26	pE	202	PEB	OA-C1A-C2A	-4.00	122.99	126.17
26	QI	201	PEB	C4B-NB-C1B	-4.00	98.97	106.51
26	j1	201	PEB	CBB-CAB-C3B	4.00	123.75	112.63
26	WA	203	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	BD	202	PEB	C3D-C4D-ND	4.00	115.11	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	wE	303	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	YD	301	PEB	CHC-C1D-ND	-4.00	109.30	113.95
26	eA	202	PEB	C4B-C3B-C2B	-4.00	102.35	106.78
26	BE	201	PEB	C4B-C3B-C2B	-4.00	102.35	106.78
26	S2	201	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	Q4	201	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	C9	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	O7	203	PEB	CHB-C4B-NB	-4.00	123.28	128.83
26	RD	202	PEB	C3B-C4B-NB	4.00	115.87	110.05
26	J2	1002	PEB	C2A-C1A-NA	4.00	111.72	108.27
28	K2	1001	CYC	OB-C4B-C3B	-4.00	123.70	128.04
28	CH	1001	CYC	OB-C4B-C3B	-4.00	123.70	128.04
26	YA	203	PEB	CHC-C1D-ND	-4.00	109.30	113.95
26	UE	203	PEB	C4B-C3B-C2B	-4.00	102.36	106.78
26	R3	202	PEB	OD-C4D-ND	-4.00	120.00	125.93
26	P7	201	PEB	C3D-C4D-ND	4.00	115.11	107.26
27	B8	302	PUB	CHA-C1B-C2B	-4.00	123.52	130.34
26	q4	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
26	FI	1002	PEB	C2A-C1A-NA	4.00	111.72	108.27
26	j2	202	PEB	OA-C1A-C2A	-4.00	122.99	126.17
26	G9	202	PEB	OA-C1A-C2A	-4.00	122.99	126.17
26	lA	202	PEB	CHB-C4B-NB	-4.00	123.28	128.83
26	e3	401	PEB	CHC-C4C-C3C	-4.00	123.52	130.34
27	yG	303	PUB	C1C-C2C-C3C	-4.00	102.36	106.78
26	h2	201	PEB	C3D-C4D-ND	4.00	115.10	107.26
28	KB	202	CYC	C4D-CHA-C1A	4.00	133.58	128.81
26	BE	202	PEB	OA-C1A-C2A	-4.00	123.00	126.17
26	S8	201	PEB	C3D-C4D-ND	4.00	115.10	107.26
26	T3	202	PEB	OD-C4D-ND	-4.00	120.01	125.93
26	S8	203	PEB	C3D-C4D-ND	4.00	115.10	107.26
28	MI	1001	CYC	C1B-NB-C4B	-4.00	105.58	110.67
26	M1	401	PEB	C3D-C4D-ND	4.00	115.10	107.26
26	i1	202	PEB	C3D-C4D-ND	4.00	115.10	107.26
26	r4	201	PEB	CHC-C4C-C3C	-4.00	123.52	130.34
26	H6	1002	PEB	CHC-C4C-C3C	-4.00	123.52	130.34
26	PJ	202	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	Z1	202	PEB	CMB-C2B-C1B	4.00	131.22	125.06
26	b2	201	PEB	C3B-C4B-NB	4.00	115.86	110.05
26	cB	201	PEB	C3D-C4D-ND	3.99	115.10	107.26
26	d2	201	PEB	CHB-C4B-C3B	-3.99	116.09	125.32
26	l2	201	PEB	CHB-C4B-C3B	-3.99	116.09	125.32
26	P6	201	PEB	C3D-C4D-ND	3.99	115.10	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	YD	302	PUB	CBA-CAA-C3A	-3.99	106.92	112.98
26	IJ	202	PEB	C3B-C4B-NB	3.99	115.86	110.05
26	SG	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	qG	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	RI	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	jG	201	PEB	C4B-C3B-C2B	-3.99	102.36	106.78
26	S3	202	PEB	CHB-C4B-NB	-3.99	123.29	128.83
28	cH	1001	CYC	C2B-C1B-NB	3.99	112.83	106.99
26	RA	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	R8	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	B9	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
28	C2	1001	CYC	CHB-C4A-NA	-3.99	116.58	124.93
26	K8	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
26	EA	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	mA	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
28	D6	1001	CYC	CMA-C3A-C4A	3.99	131.21	125.06
26	gA	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	PE	202	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	D1	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
26	I8	202	PEB	CMB-C2B-C1B	3.99	131.21	125.06
26	O1	201	PEB	CHA-C1B-NB	-3.99	116.58	124.93
26	RG	201	PEB	CHA-C1B-NB	-3.99	116.58	124.93
26	PG	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	W4	201	PEB	C3B-C4B-NB	3.99	115.86	110.05
28	C7	1001	CYC	C1B-C2B-C3B	-3.99	103.71	107.87
26	X4	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	RG	202	PEB	C3B-C4B-NB	3.99	115.85	110.05
26	S2	202	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
26	OB	201	PEB	OD-C4D-ND	-3.99	120.02	125.93
26	m7	202	PEB	CHC-C1D-ND	-3.99	109.31	113.95
26	fB	201	PEB	CHC-C1D-ND	-3.99	109.31	113.95
26	W7	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	l7	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	jG	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
28	qH	1002	CYC	OC-C1C-C2C	-3.99	123.00	126.17
26	g2	201	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
26	FE	201	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
26	FF	1002	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
26	M9	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
26	KD	201	PEB	C3B-C4B-NB	3.99	115.85	110.05
26	UB	202	PEB	C2A-C1A-NA	3.99	111.71	108.27
26	L9	203	PEB	CHC-C1D-ND	-3.99	109.31	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G5	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	L6	1002	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	W1	201	PEB	CMB-C2B-C1B	3.99	131.21	125.06
26	NJ	204	PEB	CHA-C1B-NB	-3.99	116.59	124.93
26	Z6	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	iG	202	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
26	t1	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	O4	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	24	404	PEB	OA-C1A-C2A	-3.99	123.00	126.17
28	MI	1001	CYC	C2C-C1C-NC	3.99	111.71	108.27
26	FD	203	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	X4	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
26	L5	203	PEB	C4B-C3B-C2B	-3.99	102.37	106.78
28	JH	1001	CYC	CMB-C2B-C1B	3.99	129.15	124.17
26	J4	203	PEB	CHC-C1D-ND	-3.99	109.32	113.95
26	N8	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
27	A2	303	PUB	CMA-C2A-C1A	3.99	130.77	121.39
28	FI	1001	CYC	CBD-CAD-C3D	-3.99	105.82	112.62
26	G4	201	PEB	CHA-C1B-NB	-3.99	116.59	124.93
26	ZE	201	PEB	CHC-C4C-C3C	-3.99	123.54	130.34
26	c6	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	IE	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	MJ	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
27	A4	203	PUB	CHB-C1C-NC	-3.99	123.30	128.83
26	X3	201	PEB	OD-C4D-ND	-3.99	120.03	125.93
26	UD	201	PEB	OD-C4D-ND	-3.99	120.03	125.93
26	m1	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	ZB	201	PEB	C4B-C3B-C2B	-3.99	102.37	106.78
26	a6	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	OG	203	PEB	OA-C1A-C2A	-3.99	123.00	126.17
26	d4	203	PEB	CHA-C1B-NB	-3.99	116.60	124.93
26	E1	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	hI	201	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	YJ	202	PEB	C3D-C4D-ND	3.99	115.08	107.26
26	i7	202	PEB	CMB-C2B-C1B	3.99	131.20	125.06
28	QH	1001	CYC	CAA-C2A-C1A	3.98	132.06	125.01
26	h4	202	PEB	OD-C4D-C3D	-3.98	120.43	129.46
26	m4	201	PEB	CHA-C1B-NB	-3.98	116.60	124.93
26	V7	201	PEB	OA-C1A-C2A	-3.98	123.00	126.17
26	PF	201	PEB	OA-C1A-C2A	-3.98	123.00	126.17
26	c6	201	PEB	C3D-C4D-ND	3.98	115.08	107.26
26	ZF	201	PEB	CHA-C4A-NA	3.98	129.94	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	GH	1001	CYC	CAB-C3B-C4B	3.98	127.67	121.38
26	bB	201	PEB	CHC-C1D-ND	-3.98	109.32	113.95
28	GB	1001	CYC	C2B-C1B-NB	3.98	112.82	106.99
26	Z8	201	PEB	C3D-C4D-ND	3.98	115.08	107.26
26	R3	201	PEB	C2A-C1A-NA	3.98	111.71	108.27
28	L6	1001	CYC	C2C-C1C-NC	3.98	111.71	108.27
26	JG	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
26	ZA	201	PEB	C4B-C3B-C2B	-3.98	102.37	106.78
26	V6	201	PEB	CHC-C1D-ND	-3.98	109.32	113.95
26	P6	202	PEB	CHC-C4C-C3C	-3.98	123.54	130.34
26	VG	201	PEB	OA-C1A-NA	3.98	129.76	124.94
26	U8	202	PEB	CHB-C4B-NB	-3.98	123.30	128.83
26	cG	203	PEB	OD-C4D-ND	-3.98	120.03	125.93
26	Q2	201	PEB	C4B-NB-C1B	-3.98	99.01	106.51
26	MD	201	PEB	CHA-C1B-NB	-3.98	116.61	124.93
26	DB	1002	PEB	OA-C1A-C2A	-3.98	123.01	126.17
26	KC	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
28	D2	1001	CYC	OC-C1C-C2C	-3.98	123.01	126.17
26	Y1	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
26	j6	201	PEB	CHB-C4B-NB	-3.98	123.31	128.83
26	R7	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
26	k7	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
26	EE	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
26	V2	203	PEB	CHC-C1D-ND	-3.98	109.33	113.95
26	DA	202	PEB	CAB-C3B-C4B	3.98	132.05	125.01
26	A5	201	PEB	CHB-C4B-NB	-3.98	123.31	128.83
26	u4	203	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
26	FA	202	PEB	OA-C1A-C2A	-3.98	123.01	126.17
26	VA	201	PEB	CMB-C2B-C1B	3.98	131.19	125.06
26	II	201	PEB	C1B-C2B-C3B	-3.98	101.94	106.51
26	S6	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
26	P8	201	PEB	C2A-C1A-NA	3.98	111.70	108.27
26	K3	201	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
26	VE	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	xE	303	PEB	C3D-C4D-ND	3.98	115.06	107.26
28	E2	1001	CYC	C2B-C1B-NB	3.98	112.81	106.99
26	DI	1002	PEB	C2A-C1A-NA	3.98	111.70	108.27
26	OA	202	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
26	J1	201	PEB	C3B-C4B-NB	3.98	115.83	110.05
26	KA	203	PEB	C3B-C4B-NB	3.98	115.83	110.05
26	QE	201	PEB	C3B-C4B-NB	3.98	115.83	110.05
26	11	202	PEB	C3D-C4D-ND	3.98	115.06	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	dB	201	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	sE	202	PEB	CMB-C2B-C1B	3.98	131.19	125.06
26	R6	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	I8	203	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	B9	202	PEB	CHB-C4B-NB	-3.98	123.31	128.83
27	xE	301	PUB	CMA-C2A-C1A	3.98	130.74	121.39
26	QF	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
28	iH	1001	CYC	CMB-C2B-C1B	3.98	129.13	124.17
26	BE	202	PEB	CHB-C4B-C3B	-3.98	116.14	125.32
26	VA	201	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	FD	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	TE	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
26	XD	201	PEB	CMB-C2B-C1B	3.97	131.19	125.06
26	QA	204	PEB	CHC-C4C-C3C	-3.97	123.56	130.34
26	B5	201	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	vG	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	B1	201	PEB	OA-C1A-C2A	-3.97	123.01	126.17
26	hA	201	PEB	C2A-C1A-NA	3.97	111.70	108.27
26	YJ	202	PEB	C2A-C1A-NA	3.97	111.70	108.27
26	VI	202	PEB	C3B-C4B-NB	3.97	115.83	110.05
26	tG	201	PEB	CHC-C4C-C3C	-3.97	123.56	130.34
26	g8	201	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	SB	203	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	vE	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	DD	201	PEB	C4B-C3B-C2B	-3.97	102.38	106.78
26	K1	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	P4	201	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	H9	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	TB	202	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	UB	201	PEB	C3D-C4D-ND	3.97	115.06	107.26
26	xG	304	PEB	C2A-C1A-NA	3.97	111.70	108.27
26	Q8	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
26	V7	202	PEB	CHB-C4B-NB	-3.97	123.32	128.83
26	kA	201	PEB	C4B-C3B-C2B	-3.97	102.39	106.78
26	h8	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	K5	201	PEB	CHB-C4B-NB	-3.97	123.32	128.83
26	HD	201	PEB	C2A-C1A-NA	3.97	111.70	108.27
26	lB	202	PEB	OA-C1A-C2A	-3.97	123.02	126.17
26	h8	202	PEB	CHC-C4C-C3C	-3.97	123.56	130.34
28	oH	1001	CYC	CHB-C4A-C3A	3.97	135.11	124.90
26	JG	201	PEB	C3D-C4D-ND	3.97	115.05	107.26
26	R8	202	PEB	C1C-CHB-C4B	-3.97	124.07	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N1	201	PEB	CHB-C4B-C3B	-3.97	116.15	125.32
28	G6	1001	CYC	C2B-C1B-NB	3.97	112.80	106.99
28	QH	1001	CYC	CAB-C3B-C4B	3.97	127.65	121.38
26	G1	202	PEB	C3D-C4D-ND	3.97	115.05	107.26
26	k4	202	PEB	CHC-C4C-C3C	-3.97	123.57	130.34
26	J3	201	PEB	C3B-C4B-NB	3.97	115.82	110.05
26	GC	201	PEB	OA-C1A-C2A	-3.97	123.02	126.17
26	u1	201	PEB	CBA-CAA-C3A	3.97	122.30	113.47
26	m4	203	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	VD	201	PEB	C1B-C2B-C3B	-3.97	101.95	106.51
26	JD	201	PEB	OA-C1A-C2A	-3.97	123.02	126.17
26	KD	202	PEB	OA-C1A-C2A	-3.97	123.02	126.17
26	JA	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	KB	201	PEB	CHB-C4B-NB	-3.97	123.32	128.83
28	PH	1001	CYC	CAB-C3B-C4B	3.97	127.64	121.38
26	nG	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	CD	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
27	A8	303	PUB	C1D-CHC-C4C	3.97	122.00	113.37
26	i7	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	E8	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	T8	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	fE	202	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	W6	203	PEB	OA-C1A-C2A	-3.97	123.02	126.17
26	fI	201	PEB	C3B-C4B-NB	3.97	115.82	110.05
26	bE	201	PEB	CHC-C4C-C3C	-3.97	123.57	130.34
26	JE	201	PEB	C3D-C4D-ND	3.97	115.04	107.26
26	21	401	PEB	CHA-C1B-NB	-3.97	116.64	124.93
26	i8	201	PEB	C2A-C1A-NA	3.97	111.69	108.27
26	HE	202	PEB	C2A-C1A-NA	3.97	111.69	108.27
26	i1	203	PEB	CHC-C4C-C3C	-3.97	123.57	130.34
27	wG	304	PUB	CHA-C1B-C2B	-3.97	123.57	130.34
26	j2	201	PEB	CMB-C2B-C1B	3.97	131.17	125.06
28	NH	1001	CYC	CHD-C4C-NC	3.97	129.92	125.20
26	u4	203	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	21	401	PEB	C2A-C1A-NA	3.96	111.69	108.27
26	FD	202	PEB	C2A-C1A-NA	3.96	111.69	108.27
26	MD	201	PEB	C2A-C1A-NA	3.96	111.69	108.27
28	N2	1001	CYC	C2C-C1C-NC	3.96	111.69	108.27
26	i8	201	PEB	CBC-CAC-C2C	-3.96	105.85	112.62
26	N4	201	PEB	CHB-C4B-C3B	-3.96	116.16	125.32
26	A7	301	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	W8	203	PEB	C3D-C4D-ND	3.96	115.04	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W9	201	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	JE	202	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	qE	201	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	TI	202	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	CJ	202	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	M1	403	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	j1	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	Q7	203	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	YI	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	sG	203	PEB	CBA-CAA-C3A	-3.96	104.64	113.47
26	i8	201	PEB	C4B-C3B-C2B	-3.96	102.39	106.78
26	w4	203	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	YB	201	PEB	C3D-C4D-ND	3.96	115.04	107.26
26	fG	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	SG	202	PEB	CHC-C1D-ND	-3.96	109.34	113.95
26	TE	202	PEB	C3B-C4B-NB	3.96	115.81	110.05
26	cB	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	NE	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	AI	305	PEB	OA-C1A-C2A	-3.96	123.02	126.17
26	P3	201	PEB	CHA-C1B-NB	-3.96	116.64	124.93
26	K9	202	PEB	CHA-C1B-NB	-3.96	116.64	124.93
26	ZB	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	d1	202	PEB	CHA-C1B-NB	-3.96	116.64	124.93
26	WG	201	PEB	C1B-C2B-C3B	-3.96	101.96	106.51
26	l1	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	NA	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	XA	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	fB	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	GC	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	JI	1002	PEB	C2A-C1A-NA	3.96	111.69	108.27
26	SI	201	PEB	CMA-C2A-C1A	-3.96	103.86	112.40
26	CE	201	PEB	C4B-C3B-C2B	-3.96	102.40	106.78
26	YF	202	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	SF	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	ND	202	PEB	C3B-C4B-NB	3.96	115.81	110.05
26	m8	201	PEB	C2A-C1A-NA	3.96	111.69	108.27
26	U2	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	Y9	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	PA	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	QE	201	PEB	CHB-C4B-C3B	-3.96	116.17	125.32
28	G2	1001	CYC	C1B-NB-C4B	-3.96	105.63	110.67
26	lF	203	PEB	CHC-C1D-ND	-3.96	109.35	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aI	202	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	aF	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
26	SG	203	PEB	OA-C1A-C2A	-3.96	123.03	126.17
26	I3	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	JJ	202	PEB	C1B-C2B-C3B	-3.96	101.96	106.51
26	VD	201	PEB	CHC-C4C-C3C	-3.96	123.58	130.34
26	w1	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	GC	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	ZA	202	PEB	CAB-C3B-C4B	3.96	132.01	125.01
26	aA	201	PEB	C3B-C4B-NB	3.96	115.81	110.05
26	QF	203	PEB	C1B-C2B-C3B	-3.96	101.96	106.51
26	yG	301	PEB	C3D-C4D-ND	3.96	115.03	107.26
26	L6	1002	PEB	OA-C1A-C2A	-3.96	123.03	126.17
28	sH	1001	CYC	OC-C1C-C2C	-3.96	123.03	126.17
26	B1	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	X9	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	pG	201	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	J8	202	PEB	CHC-C4C-C3C	-3.96	123.59	130.34
26	IE	203	PEB	C1C-CHB-C4B	3.96	133.54	128.81
27	A2	302	PUB	CHA-C1B-C2B	-3.96	123.59	130.34
26	u4	203	PEB	CHB-C4B-NB	-3.96	123.34	128.83
26	MA	203	PEB	C2A-C1A-NA	3.96	111.68	108.27
26	CE	203	PEB	OA-C1A-C2A	-3.96	123.03	126.17
26	QF	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	RE	201	PEB	CHA-C1B-NB	-3.96	116.66	124.93
26	M1	403	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	UA	203	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	mG	203	PEB	CHB-C4B-NB	-3.96	123.34	128.83
26	K5	202	PEB	C3D-C4D-ND	3.96	115.02	107.26
26	RJ	201	PEB	CHC-C4C-C3C	-3.95	123.59	130.34
26	AA	302	PEB	C3D-C4D-ND	3.95	115.02	107.26
26	H5	203	PEB	C3B-C4B-NB	3.95	115.80	110.05
26	II	202	PEB	CHC-C4C-C3C	-3.95	123.59	130.34
26	S4	201	PEB	CHB-C4B-NB	-3.95	123.34	128.83
26	f7	202	PEB	OD-C4D-ND	-3.95	120.07	125.93
26	OA	203	PEB	C3D-C4D-ND	3.95	115.02	107.26
26	kA	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
26	U8	202	PEB	CAB-CBB-CGB	-3.95	105.09	113.60
26	XD	201	PEB	C3D-C4D-ND	3.95	115.02	107.26
26	nG	201	PEB	CHC-C4C-C3C	-3.95	123.59	130.34
26	PA	201	PEB	C3D-C4D-ND	3.95	115.02	107.26
26	NG	202	PEB	C3D-C4D-ND	3.95	115.02	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	bI	201	PEB	C3D-C4D-ND	3.95	115.02	107.26
26	T4	202	PEB	CHC-C1D-ND	-3.95	109.36	113.95
26	X3	201	PEB	CMB-C2B-C1B	3.95	131.15	125.06
26	b2	202	PEB	C3D-C4D-ND	3.95	115.01	107.26
26	PE	201	PEB	CHC-C4C-C3C	-3.95	123.60	130.34
26	UJ	202	PEB	C3D-C4D-ND	3.95	115.01	107.26
28	K6	202	CYC	C4D-CHA-C1A	3.95	133.53	128.81
26	AG	202	PEB	CHC-C1D-ND	-3.95	109.36	113.95
28	jH	1001	CYC	CAB-C3B-C4B	3.95	127.62	121.38
26	u1	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	C5	203	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	H2	1002	PEB	C3D-C4D-ND	3.95	115.01	107.26
26	Y4	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
26	Y6	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
26	v1	202	PEB	CHB-C4B-C3B	3.95	134.45	125.32
26	gB	202	PEB	C3D-C4D-ND	3.95	115.01	107.26
26	SB	202	PEB	CHC-C4C-C3C	-3.95	123.60	130.34
26	a1	203	PEB	C2A-C1A-NA	3.95	111.68	108.27
26	Y8	201	PEB	C2A-C1A-NA	3.95	111.68	108.27
26	CA	203	PEB	C2A-C1A-NA	3.95	111.68	108.27
28	I6	1001	CYC	OB-C4B-C3B	-3.95	123.75	128.04
28	B6	1001	CYC	CMA-C3A-C4A	3.95	131.15	125.06
26	HC	201	PEB	CHC-C1D-ND	-3.95	109.36	113.95
26	aF	202	PEB	CHC-C1D-ND	-3.95	109.36	113.95
26	w4	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	HJ	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	SA	201	PEB	CHC-C4C-C3C	-3.95	123.60	130.34
26	kI	201	PEB	CHC-C4C-C3C	-3.95	123.60	130.34
26	N4	201	PEB	CMA-C2A-C1A	-3.95	103.89	112.40
28	CI	1001	CYC	CHB-C4A-NA	-3.95	116.67	124.93
27	yE	303	PUB	CMA-C2A-C1A	3.95	130.68	121.39
26	HB	1002	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	T9	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	NA	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	c4	203	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	TA	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	UA	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	SE	202	PEB	CAB-C3B-C4B	3.95	131.99	125.01
26	x4	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	G8	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	UA	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
26	PG	201	PEB	CHC-C4C-C3C	-3.95	123.61	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U8	203	PEB	C3D-C4D-ND	3.95	115.00	107.26
28	F7	1001	CYC	C4D-CHA-C1A	3.95	133.52	128.81
26	S7	201	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	ZB	203	PEB	CHA-C1B-NB	-3.95	116.68	124.93
26	l6	203	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	d7	202	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	FI	1002	PEB	C3D-C4D-ND	3.95	115.00	107.26
26	IG	202	PEB	C2A-C1A-NA	3.95	111.67	108.27
26	DG	203	PEB	C3D-C4D-ND	3.94	115.00	107.26
26	BE	202	PEB	CMB-C2B-C1B	3.94	131.14	125.06
26	rG	202	PEB	C3D-C4D-ND	3.94	115.00	107.26
28	HI	1001	CYC	CHB-C1B-NB	-3.94	117.59	126.06
27	A4	203	PUB	CBA-CAA-C3A	-3.94	107.00	112.98
26	YG	201	PEB	CHB-C4B-NB	-3.94	123.36	128.83
26	kF	201	PEB	CBA-CAA-C3A	3.94	122.25	113.47
26	dF	201	PEB	CHC-C1D-ND	-3.94	109.37	113.95
26	kF	202	PEB	CHC-C1D-ND	-3.94	109.37	113.95
26	T3	203	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
26	G8	203	PEB	C3D-C4D-ND	3.94	115.00	107.26
26	11	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	W4	202	PEB	C2A-C1A-NA	3.94	111.67	108.27
26	WE	201	PEB	C2A-C1A-NA	3.94	111.67	108.27
26	OI	201	PEB	CMA-C2A-C1A	-3.94	103.90	112.40
26	F3	203	PEB	C3D-C4D-ND	3.94	114.99	107.26
26	IC	202	PEB	CHA-C1B-NB	-3.94	116.69	124.93
26	C3	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
26	d6	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
26	V3	203	PEB	CHB-C4B-NB	-3.94	123.36	128.83
26	S9	201	PEB	C3B-C4B-NB	3.94	115.78	110.05
26	f1	201	PEB	CHC-C1D-ND	-3.94	109.37	113.95
26	R2	203	PEB	C3D-C4D-ND	3.94	114.99	107.26
26	SA	203	PEB	C3D-C4D-ND	3.94	114.99	107.26
26	sE	201	PEB	CHC-C4C-C3C	-3.94	123.61	130.34
26	CG	203	PEB	CHC-C4C-C3C	-3.94	123.61	130.34
26	f2	202	PEB	C3D-C4D-ND	3.94	114.99	107.26
26	LG	201	PEB	OA-C1A-NA	3.94	129.71	124.94
26	kE	202	PEB	CHA-C1B-NB	-3.94	116.69	124.93
26	jE	202	PEB	CHB-C4B-C3B	-3.94	116.22	125.32
26	WF	203	PEB	CHB-C4B-NB	-3.94	123.36	128.83
26	NJ	203	PEB	CHA-C1B-NB	-3.94	116.69	124.93
26	BG	201	PEB	CHB-C4B-NB	-3.94	123.36	128.83
26	fB	201	PEB	CMB-C2B-C1B	3.94	131.13	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N3	202	PEB	C1B-C2B-C3B	-3.94	101.99	106.51
26	Q4	201	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	GA	203	PEB	C3D-C4D-ND	3.94	114.98	107.26
28	E2	1001	CYC	OB-C4B-C3B	-3.94	123.77	128.04
26	BC	202	PEB	C3D-C4D-ND	3.94	114.98	107.26
26	bI	202	PEB	C3D-C4D-ND	3.94	114.98	107.26
28	CI	1001	CYC	CBD-CAD-C3D	-3.94	105.90	112.62
26	YB	201	PEB	CBC-CAC-C2C	3.94	119.34	112.62
26	s1	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
26	X8	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
26	RG	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
26	TD	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	nE	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	N4	201	PEB	OD-C4D-ND	-3.94	120.10	125.93
26	O6	201	PEB	OD-C4D-ND	-3.94	120.10	125.93
26	HG	201	PEB	C1B-C2B-C3B	-3.94	101.99	106.51
26	y4	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
26	PJ	203	PEB	CHB-C4B-NB	-3.94	123.37	128.83
26	j1	202	PEB	CHB-C4B-C3B	-3.94	116.23	125.32
26	U8	201	PEB	C2A-C1A-NA	3.94	111.67	108.27
26	VB	202	PEB	C2A-C1A-NA	3.94	111.67	108.27
26	dF	203	PEB	C2A-C1A-NA	3.94	111.67	108.27
26	O4	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
27	wE	304	PUB	C1D-CHC-C4C	-3.94	104.81	113.37
26	D9	203	PEB	C1B-C2B-C3B	-3.94	101.99	106.51
26	iB	202	PEB	CHC-C1D-ND	-3.94	109.38	113.95
26	R1	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	g6	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	d8	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	cG	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
26	UE	201	PEB	OA-C1A-C2A	3.94	129.30	126.17
26	UF	202	PEB	OD-C4D-ND	-3.94	120.10	125.93
26	F5	201	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	H6	1002	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	IA	201	PEB	C2A-C1A-NA	3.93	111.67	108.27
26	l7	201	PEB	CHB-C4B-NB	-3.93	123.37	128.83
28	YH	1001	CYC	C4D-CHA-C1A	3.93	133.51	128.81
26	V1	203	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	A4	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	L8	201	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	TG	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	OE	202	PEB	CHA-C1B-NB	-3.93	116.70	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A1	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	T3	203	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	IG	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	SJ	201	PEB	C3B-C4B-NB	3.93	115.77	110.05
26	YA	201	PEB	C2A-C1A-NA	3.93	111.66	108.27
28	AH	1001	CYC	C1B-NB-C4B	-3.93	105.66	110.67
26	C1	202	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	f6	201	PEB	C3D-C4D-ND	3.93	114.98	107.26
26	QF	203	PEB	OA-C1A-C2A	-3.93	123.05	126.17
26	aF	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
28	JI	1001	CYC	OC-C1C-C2C	-3.93	123.05	126.17
26	AJ	301	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	N1	201	PEB	CMA-C2A-C1A	-3.93	103.93	112.40
26	SG	202	PEB	CHA-C1B-C2B	3.93	135.01	124.90
26	v1	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	AD	202	PEB	CHA-C1B-NB	-3.93	116.71	124.93
28	LB	1001	CYC	C1B-C2B-C3B	-3.93	103.77	107.87
26	T6	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	Q7	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	aA	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	TD	203	PEB	C2A-C1A-NA	3.93	111.66	108.27
28	EB	1001	CYC	C2C-C1C-NC	3.93	111.66	108.27
26	e1	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	BC	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	XD	201	PEB	CHB-C4B-NB	-3.93	123.37	128.83
26	EJ	202	PEB	CHB-C4B-NB	-3.93	123.37	128.83
26	N8	202	PEB	CAB-C3B-C4B	3.93	131.96	125.01
26	ZB	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
26	kA	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	dB	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	MJ	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	S2	201	PEB	CHC-C4C-C3C	-3.93	123.63	130.34
26	jA	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	XD	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	HB	1002	PEB	CHC-C4C-C3C	-3.93	123.64	130.34
26	oG	202	PEB	CHC-C4C-C3C	-3.93	123.64	130.34
26	y4	203	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	JI	1002	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	P1	201	PEB	CMD-C2D-C3D	-3.93	124.52	130.06
26	jE	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
26	X3	202	PEB	C3D-C4D-ND	3.93	114.97	107.26
26	LA	201	PEB	C3D-C4D-ND	3.93	114.97	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AC	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
26	QB	202	PEB	CMB-C2B-C1B	3.93	131.11	125.06
26	Z6	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
26	k8	201	PEB	C4B-C3B-C2B	-3.93	102.44	106.78
26	d8	202	PEB	C2A-C1A-NA	3.93	111.66	108.27
26	TI	201	PEB	C2A-C1A-NA	3.93	111.66	108.27
26	YG	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
26	k7	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
26	VF	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
26	E9	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
26	K5	201	PEB	C2A-C1A-NA	3.93	111.66	108.27
26	d2	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
28	LI	1001	CYC	C2B-C1B-NB	3.93	112.73	106.99
26	F5	203	PEB	C3D-C4D-ND	3.93	114.96	107.26
26	b2	202	PEB	CHC-C4C-C3C	-3.92	123.64	130.34
26	l2	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	jE	201	PEB	C2A-C1A-NA	3.92	111.66	108.27
26	u1	201	PEB	CHC-C4C-C3C	-3.92	123.64	130.34
26	A2	305	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	j8	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	bF	202	PEB	OA-C1A-C2A	-3.92	123.05	126.17
26	k2	203	PEB	C1C-CHB-C4B	-3.92	124.12	128.81
26	m8	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	AI	305	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	i4	202	PEB	C2A-C1A-NA	3.92	111.66	108.27
26	fB	202	PEB	CHC-C4C-C3C	-3.92	123.65	130.34
28	L6	1001	CYC	C2B-C1B-NB	3.92	112.73	106.99
26	X3	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	h7	202	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	yE	301	PEB	C3D-C4D-ND	3.92	114.96	107.26
26	BG	202	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
26	g8	201	PEB	OA-C1A-C2A	-3.92	123.05	126.17
26	BJ	201	PEB	OA-C1A-C2A	-3.92	123.05	126.17
26	A2	304	PEB	CHA-C1B-NB	-3.92	116.73	124.93
26	e8	202	PEB	CMB-C2B-C1B	3.92	131.10	125.06
26	s1	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	D2	1002	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	h4	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	xG	304	PEB	C3D-C4D-ND	3.92	114.95	107.26
28	KB	202	CYC	CHB-C4A-NA	-3.92	116.73	124.93
26	S3	202	PEB	OD-C4D-ND	-3.92	120.12	125.93
26	T1	201	PEB	CMB-C2B-C1B	3.92	131.10	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GC	203	PEB	CMB-C2B-C1B	3.92	131.10	125.06
26	l6	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	W7	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	ZB	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	lB	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	DE	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	kE	203	PEB	CHA-C1B-NB	-3.92	116.73	124.93
26	D1	201	PEB	C3B-C4B-NB	3.92	115.75	110.05
26	eE	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
26	IJ	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	Y2	201	PEB	C2A-C1A-NA	3.92	111.65	108.27
26	F3	201	PEB	CHB-C4B-NB	-3.92	123.39	128.83
26	l2	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
26	L9	201	PEB	CHC-C1D-ND	-3.92	109.39	113.95
26	dF	203	PEB	CHC-C4C-C3C	-3.92	123.65	130.34
26	Z7	202	PEB	C3B-C4B-NB	3.92	115.75	110.05
26	PD	202	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
26	y4	201	PEB	C2A-C1A-NA	3.92	111.65	108.27
26	mF	202	PEB	CHC-C1D-ND	-3.92	109.40	113.95
26	E3	201	PEB	OA-C1A-C2A	-3.92	123.06	126.17
26	HG	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	Y4	201	PEB	CMB-C2B-C1B	3.92	131.10	125.06
26	r1	202	PEB	CHA-C4A-NA	-3.92	120.55	125.20
26	TD	202	PEB	CHA-C1B-NB	-3.92	116.74	124.93
26	OA	203	PEB	C2A-C1A-NA	3.92	111.65	108.27
26	J4	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	xE	304	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	gG	202	PEB	CHC-C1D-ND	-3.92	109.40	113.95
26	V8	202	PEB	CHC-C4C-C3C	-3.92	123.65	130.34
26	mA	202	PEB	CAB-C3B-C2B	3.92	135.18	127.88
26	E8	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	PJ	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
26	K8	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
26	YD	304	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	F2	1002	PEB	C2A-C1A-NA	3.92	111.65	108.27
26	f6	202	PEB	CHC-C4C-C3C	-3.92	123.66	130.34
26	QA	202	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	K1	201	PEB	CHC-C1D-ND	-3.92	109.40	113.95
26	I3	201	PEB	OA-C1A-C2A	-3.92	123.06	126.17
26	h7	203	PEB	OA-C1A-C2A	-3.92	123.06	126.17
26	bI	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
26	K8	203	PEB	CHA-C1B-NB	-3.92	116.74	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TF	201	PEB	CHC-C4C-C3C	-3.92	123.66	130.34
26	P1	201	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	ND	203	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	UF	202	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	LJ	202	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	V8	202	PEB	C3B-C4B-NB	3.92	115.75	110.05
26	i7	201	PEB	CHC-C4C-C3C	-3.92	123.66	130.34
26	VI	203	PEB	C3D-C4D-ND	3.92	114.94	107.26
26	wE	301	PEB	C3D-C4D-ND	3.91	114.94	107.26
26	mG	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
26	V2	201	PEB	C3D-C4D-ND	3.91	114.94	107.26
26	k4	203	PEB	C3D-C4D-ND	3.91	114.94	107.26
26	kI	202	PEB	C3D-C4D-ND	3.91	114.94	107.26
28	L2	1001	CYC	C2B-C1B-NB	3.91	112.72	106.99
26	g1	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
26	L9	203	PEB	OA-C1A-C2A	-3.91	123.06	126.17
26	K8	202	PEB	CHC-C1D-ND	-3.91	109.40	113.95
26	UI	202	PEB	CHB-C4B-NB	-3.91	123.40	128.83
26	TI	201	PEB	C3D-C4D-ND	3.91	114.94	107.26
26	GG	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
26	M1	403	PEB	CHC-C4C-C3C	-3.91	123.66	130.34
26	bI	201	PEB	CMB-C2B-C1B	3.91	131.09	125.06
26	PI	202	PEB	CHC-C1D-ND	-3.91	109.40	113.95
26	X3	203	PEB	C3D-C4D-ND	3.91	114.94	107.26
26	TG	201	PEB	C3D-C4D-ND	3.91	114.94	107.26
26	K8	203	PEB	C3B-C4B-NB	3.91	115.74	110.05
26	C9	202	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
26	fA	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	Y6	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
26	fF	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
26	P3	201	PEB	CHB-C4B-NB	-3.91	123.40	128.83
26	FE	202	PEB	C3B-C4B-NB	3.91	115.74	110.05
28	MB	1001	CYC	C2C-C1C-NC	3.91	111.64	108.27
26	H8	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
26	D6	1002	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
26	iF	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	wG	301	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	hF	202	PEB	C1B-C2B-C3B	-3.91	102.02	106.51
26	F9	203	PEB	OD-C4D-ND	-3.91	120.14	125.93
26	P1	201	PEB	CHB-C4B-NB	-3.91	123.40	128.83
26	PG	201	PEB	CHA-C1B-NB	-3.91	116.75	124.93
26	e4	201	PEB	C3D-C4D-ND	3.91	114.93	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g4	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	k4	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	J4	201	PEB	CMB-C2B-C1B	3.91	131.09	125.06
26	YD	301	PEB	C2A-C1A-NA	3.91	111.64	108.27
26	CD	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	D7	1002	PEB	OA-C1A-C2A	-3.91	123.06	126.17
26	m8	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
26	O8	202	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
26	UA	202	PEB	CAB-CBB-CGB	-3.91	105.19	113.60
26	G5	203	PEB	CMB-C2B-C1B	3.91	131.09	125.06
26	c1	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	Q8	203	PEB	OD-C4D-ND	-3.91	120.14	125.93
26	EA	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	hF	201	PEB	C2A-C1A-NA	3.91	111.64	108.27
26	F3	202	PEB	CMB-C2B-C1B	3.91	131.08	125.06
27	AF	303	PUB	C1D-CHC-C4C	-3.91	104.86	113.37
26	QA	203	PEB	CMB-C2B-C1B	3.91	131.08	125.06
26	VD	201	PEB	CMB-C2B-C1B	3.91	131.08	125.06
26	KA	203	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	hE	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	EJ	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
26	N8	201	PEB	C2A-C1A-NA	3.91	111.64	108.27
26	mE	201	PEB	C2A-C1A-NA	3.91	111.64	108.27
26	WA	203	PEB	C4B-C3B-C2B	-3.91	102.46	106.78
26	UG	201	PEB	OD-C4D-ND	-3.91	120.14	125.93
26	RJ	201	PEB	C3D-C4D-ND	3.91	114.92	107.26
26	m4	203	PEB	CHC-C1D-ND	-3.91	109.41	113.95
26	AC	201	PEB	C3D-C4D-ND	3.91	114.92	107.26
26	NF	1002	PEB	C3D-C4D-ND	3.91	114.92	107.26
26	DI	1002	PEB	C3D-C4D-ND	3.91	114.92	107.26
26	NA	202	PEB	CAB-C3B-C4B	3.91	131.92	125.01
26	SB	201	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
26	UD	202	PEB	OA-C1A-C2A	-3.91	123.07	126.17
26	GD	202	PEB	CHC-C1D-ND	-3.91	109.41	113.95
26	HI	1002	PEB	C3D-C4D-ND	3.91	114.92	107.26
28	DF	1001	CYC	OB-C4B-C3B	-3.91	123.80	128.04
26	BJ	202	PEB	C1C-CHB-C4B	3.91	133.47	128.81
26	I1	202	PEB	C3D-C4D-ND	3.91	114.92	107.26
26	TD	203	PEB	C3D-C4D-ND	3.91	114.92	107.26
26	ME	203	PEB	OD-C4D-C3D	-3.91	120.61	129.46
26	A2	305	PEB	CHC-C4C-C3C	-3.90	123.68	130.34
26	z1	202	PEB	C3D-C4D-ND	3.90	114.92	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j2	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	L3	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	I9	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	I5	201	PEB	CHC-C1D-ND	-3.90	109.41	113.95
26	iA	201	PEB	C2A-C1A-NA	3.90	111.64	108.27
28	M2	1001	CYC	C2C-C1C-NC	3.90	111.64	108.27
26	VB	202	PEB	CHC-C4C-C3C	-3.90	123.68	130.34
26	fl	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
28	MB	1001	CYC	CHB-C4A-NA	-3.90	116.77	124.93
26	U3	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
26	M4	402	PEB	OA-C1A-C2A	-3.90	123.07	126.17
28	gH	1001	CYC	C4D-CHA-C1A	3.90	133.47	128.81
26	H1	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	TE	201	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	N4	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	mI	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
28	LB	1001	CYC	C2B-C1B-NB	3.90	112.70	106.99
26	XD	202	PEB	CHB-C4B-NB	-3.90	123.41	128.83
26	k1	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	L9	202	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	R9	201	PEB	C3D-C4D-ND	3.90	114.92	107.26
26	l7	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	T9	202	PEB	CMB-C2B-C1B	3.90	131.07	125.06
26	K1	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
26	U8	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
26	O9	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
26	OI	201	PEB	CHC-C4C-C3C	-3.90	123.68	130.34
26	YD	304	PEB	C2A-C1A-NA	3.90	111.64	108.27
26	Y2	203	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
26	P3	203	PEB	CAB-CBB-CGB	-3.90	105.21	113.60
26	d1	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
28	K6	202	CYC	C2B-C1B-NB	3.90	112.70	106.99
26	b2	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
26	w4	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	U6	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	NE	202	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	Y1	201	PEB	C2A-C1A-NA	3.90	111.64	108.27
26	Y3	304	PEB	C2A-C1A-NA	3.90	111.64	108.27
26	BD	202	PEB	CHA-C1B-NB	-3.90	116.78	124.93
27	Q8	201	PUB	CMA-C2A-C1A	3.90	130.56	121.39
28	L7	1001	CYC	C1B-C2B-C3B	-3.90	103.80	107.87
28	IF	1001	CYC	C2B-C1B-NB	3.90	112.70	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L1	203	PEB	OA-C1A-C2A	-3.90	123.07	126.17
26	FG	201	PEB	OD-C4D-ND	-3.90	120.15	125.93
26	WJ	201	PEB	OD-C4D-ND	-3.90	120.15	125.93
26	vE	201	PEB	CHB-C4B-NB	-3.90	123.42	128.83
26	O2	201	PEB	CHC-C4C-C3C	-3.90	123.69	130.34
26	JA	202	PEB	CHC-C4C-C3C	-3.90	123.69	130.34
26	eB	203	PEB	CMB-C2B-C1B	3.90	131.07	125.06
26	H8	201	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
26	g6	202	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	h6	202	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	I9	202	PEB	CHB-C4B-NB	-3.90	123.42	128.83
26	ZB	201	PEB	CHC-C1D-ND	-3.90	109.42	113.95
26	RD	202	PEB	OD-C4D-ND	-3.90	120.16	125.93
28	H2	1001	CYC	C1B-NB-C4B	-3.90	105.71	110.67
26	M9	202	PEB	C3D-C4D-ND	3.90	114.91	107.26
26	fG	202	PEB	CHB-C4B-NB	-3.90	123.42	128.83
26	QB	201	PEB	C2A-C1A-NA	3.90	111.63	108.27
26	D1	201	PEB	OA-C1A-C2A	-3.90	123.08	126.17
26	D4	203	PEB	OA-C1A-C2A	-3.90	123.08	126.17
26	hB	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
26	k2	203	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
26	F8	202	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
26	eG	201	PEB	C1B-C2B-C3B	-3.90	102.03	106.51
26	UI	202	PEB	C3D-C4D-ND	3.90	114.90	107.26
26	ZA	201	PEB	C2A-C1A-NA	3.90	111.63	108.27
26	IE	203	PEB	C3B-C4B-NB	3.90	115.72	110.05
27	AF	304	PUB	CBB-CAB-C3B	-3.90	105.97	112.62
26	a4	203	PEB	CHB-C4B-NB	-3.89	123.42	128.83
26	f4	201	PEB	C3D-C4D-ND	3.89	114.90	107.26
26	NE	202	PEB	CMB-C2B-C1B	3.89	131.06	125.06
26	S7	201	PEB	CHA-C1B-NB	-3.89	116.79	124.93
26	rE	202	PEB	C3D-C4D-ND	3.89	114.90	107.26
26	FF	1002	PEB	C3D-C4D-ND	3.89	114.90	107.26
28	N2	1001	CYC	C1B-C2B-C3B	-3.89	103.81	107.87
26	DG	201	PEB	CHB-C4B-NB	-3.89	123.42	128.83
26	j1	202	PEB	C2A-C1A-NA	3.89	111.63	108.27
28	D6	1001	CYC	CBD-CAD-C3D	-3.89	105.97	112.62
26	UG	201	PEB	OA-C1A-C2A	3.89	129.27	126.17
26	eG	203	PEB	OA-C1A-C2A	-3.89	123.08	126.17
26	hG	202	PEB	C3D-C4D-ND	3.89	114.90	107.26
26	h6	203	PEB	CHC-C1D-ND	-3.89	109.43	113.95
26	mI	203	PEB	CHC-C1D-ND	-3.89	109.43	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B1	201	PEB	C3B-C4B-NB	3.89	115.71	110.05
26	M8	201	PEB	C3B-C4B-NB	3.89	115.71	110.05
26	S4	201	PEB	C2A-C1A-NA	3.89	111.63	108.27
26	k2	203	PEB	C3D-C4D-ND	3.89	114.90	107.26
26	k6	202	PEB	C3D-C4D-ND	3.89	114.90	107.26
26	U2	202	PEB	CHB-C4B-NB	-3.89	123.43	128.83
26	KC	203	PEB	CHB-C4B-NB	-3.89	123.43	128.83
26	L7	1002	PEB	CHA-C1B-NB	-3.89	116.79	124.93
26	mE	201	PEB	C1B-C2B-C3B	-3.89	102.04	106.51
26	T2	201	PEB	C2A-C1A-NA	3.89	111.63	108.27
26	MA	201	PEB	C2A-C1A-NA	3.89	111.63	108.27
28	C7	1001	CYC	CMA-C3A-C4A	3.89	131.06	125.06
28	YH	1001	CYC	OB-C4B-C3B	-3.89	123.82	128.04
26	hB	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	XJ	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	dB	203	PEB	CHB-C4B-NB	-3.89	123.43	128.83
26	OA	201	PEB	CHC-C4C-C3C	-3.89	123.70	130.34
26	WB	203	PEB	OA-C1A-C2A	-3.89	123.08	126.17
28	HI	1001	CYC	CAB-C3B-C4B	3.89	127.52	121.38
26	T2	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	LB	1002	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	JI	1002	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
28	KF	1001	CYC	C1B-C2B-C3B	-3.89	103.81	107.87
26	x4	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	a6	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	Z6	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
26	M4	403	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	pE	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	KA	203	PEB	CMB-C2B-C1B	3.89	131.05	125.06
26	W1	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	N3	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	BD	203	PEB	CHB-C4B-NB	-3.89	123.43	128.83
26	FJ	201	PEB	CHA-C1B-C2B	3.89	134.90	124.90
26	VB	201	PEB	CMB-C2B-C1B	3.89	131.05	125.06
26	g4	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	aG	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	OE	203	PEB	OA-C1A-C2A	-3.89	123.08	126.17
28	UH	1001	CYC	OC-C1C-C2C	-3.89	123.08	126.17
28	M2	1001	CYC	C1B-NB-C4B	-3.89	105.72	110.67
26	DA	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	PF	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	iI	201	PEB	C3D-C4D-ND	3.89	114.89	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aA	204	PEB	C3B-C4B-NB	3.89	115.70	110.05
26	FA	202	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
26	U8	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	N9	202	PEB	CHB-C4B-NB	-3.89	123.43	128.83
28	DF	1003	CYC	C1B-CHB-C4A	-3.89	118.58	128.08
26	A9	301	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	zG	501	PEB	C3D-C4D-ND	3.89	114.89	107.26
26	CG	202	PEB	C3B-C4B-NB	3.89	115.70	110.05
26	AD	201	PEB	CAB-CBB-CGB	-3.89	105.24	113.60
28	YH	1003	CYC	CAB-C3B-C4B	3.89	127.52	121.38
26	F9	203	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
26	J2	1002	PEB	C3D-C4D-ND	3.89	114.88	107.26
26	SE	202	PEB	C3D-C4D-ND	3.89	114.88	107.26
26	iI	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
26	T3	203	PEB	C3B-C4B-NB	3.89	115.70	110.05
26	S1	201	PEB	CHC-C4C-C3C	-3.89	123.71	130.34
26	H8	202	PEB	CHC-C4C-C3C	-3.89	123.71	130.34
26	hB	202	PEB	C3D-C4D-ND	3.89	114.88	107.26
26	B1	201	PEB	CHC-C1D-ND	-3.89	109.44	113.95
26	C9	201	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
26	I4	202	PEB	C3D-C4D-ND	3.89	114.88	107.26
26	lE	202	PEB	C3D-C4D-ND	3.89	114.88	107.26
26	I4	201	PEB	C2A-C1A-NA	3.88	111.62	108.27
26	A8	301	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	QA	204	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	dF	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	Y8	201	PEB	C3B-C4B-NB	3.88	115.70	110.05
26	s4	202	PEB	CHA-C1B-NB	-3.88	116.81	124.93
26	m2	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	U8	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	fI	201	PEB	CHB-C4B-NB	-3.88	123.44	128.83
26	n4	201	PEB	C3B-C4B-NB	3.88	115.70	110.05
26	KC	201	PEB	CHA-C1B-NB	-3.88	116.81	124.93
28	HB	1001	CYC	CHB-C4A-NA	-3.88	116.81	124.93
26	j8	203	PEB	CHC-C1D-ND	-3.88	109.44	113.95
26	CE	202	PEB	CHB-C4B-C3B	-3.88	116.35	125.32
26	mE	202	PEB	CHB-C4B-NB	-3.88	123.44	128.83
26	d8	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	aB	202	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	fI	201	PEB	CHC-C4C-C3C	-3.88	123.71	130.34
26	a8	203	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	OJ	201	PEB	C3D-C4D-ND	3.88	114.88	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FC	202	PEB	CHB-C4B-NB	-3.88	123.44	128.83
26	AF	302	PEB	CHC-C4C-C3C	-3.88	123.72	130.34
27	A2	303	PUB	CHA-C1B-C2B	-3.88	123.72	130.34
26	hG	201	PEB	CMB-C2B-C1B	3.88	131.04	125.06
26	S3	202	PEB	C2A-C1A-NA	3.88	111.62	108.27
26	I8	202	PEB	C2A-C1A-NA	3.88	111.62	108.27
26	m2	202	PEB	CHA-C1B-NB	-3.88	116.81	124.93
26	V2	202	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
26	Y9	202	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
26	aA	203	PEB	C3D-C4D-ND	3.88	114.88	107.26
26	K5	201	PEB	CHA-C1B-NB	-3.88	116.81	124.93
26	P9	202	PEB	CHC-C4C-C3C	-3.88	123.72	130.34
28	JF	1001	CYC	C2B-C1B-NB	3.88	112.67	106.99
26	U7	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	FC	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	FC	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	eI	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
28	J7	1003	CYC	C1B-C2B-C3B	-3.88	103.82	107.87
26	JG	202	PEB	CHB-C4B-C3B	-3.88	116.35	125.32
27	K3	203	PUB	C1C-C2C-C3C	-3.88	102.49	106.78
26	c2	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	V4	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	m4	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	PI	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	h7	202	PEB	CHC-C4C-C3C	-3.88	123.72	130.34
26	UD	202	PEB	C2A-C1A-NA	3.88	111.62	108.27
26	HG	202	PEB	C2A-C1A-NA	3.88	111.62	108.27
28	K2	1001	CYC	C2C-C1C-NC	3.88	111.62	108.27
26	d2	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	NI	1002	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	AE	201	PEB	CHB-C4B-C3B	-3.88	116.36	125.32
26	QB	203	PEB	C1C-CHB-C4B	3.88	133.44	128.81
26	W3	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
26	J7	1002	PEB	OA-C1A-C2A	-3.88	123.09	126.17
26	XG	203	PEB	OA-C1A-C2A	-3.88	123.09	126.17
26	W2	201	PEB	C1B-C2B-C3B	-3.88	102.05	106.51
26	H3	202	PEB	C1B-C2B-C3B	-3.88	102.05	106.51
26	a2	203	PEB	CHB-C4B-NB	-3.88	123.44	128.83
26	F4	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	d4	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	xG	303	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	VI	201	PEB	C3D-C4D-ND	3.88	114.87	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OA	201	PEB	CHB-C4B-NB	-3.88	123.45	128.83
26	B5	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
26	WJ	201	PEB	CMB-C2B-C1B	3.88	131.04	125.06
26	kG	203	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	c4	202	PEB	CHC-C1D-ND	-3.88	109.44	113.95
27	K1	203	PUB	CHC-C1D-ND	-3.88	108.82	113.72
26	U9	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	y4	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
26	KB	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	uG	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
26	M4	403	PEB	CHC-C4C-C3C	-3.88	123.72	130.34
26	FG	201	PEB	C3D-C4D-ND	3.88	114.86	107.26
26	J1	201	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
27	QA	201	PUB	CMA-C2A-C1A	3.88	130.51	121.39
26	N9	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
26	A5	202	PEB	C3D-C4D-ND	3.88	114.86	107.26
27	xG	306	PUB	CMA-C2A-C1A	3.88	130.51	121.39
26	LC	201	PEB	C3D-C4D-ND	3.88	114.86	107.26
26	AI	304	PEB	C3D-C4D-ND	3.88	114.86	107.26
26	G6	1002	PEB	C3B-C4B-NB	3.88	115.69	110.05
26	H5	202	PEB	C1C-CHB-C4B	3.88	133.44	128.81
26	g2	203	PEB	CHC-C4C-C3C	-3.87	123.73	130.34
26	AB	304	PEB	CHC-C4C-C3C	-3.87	123.73	130.34
26	m1	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
28	C7	1001	CYC	OC-C1C-C2C	-3.87	123.09	126.17
26	P8	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	XG	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	aB	202	PEB	CHC-C4C-C3C	-3.87	123.73	130.34
26	A2	301	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	F7	1002	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	Z4	202	PEB	C2A-C1A-NA	3.87	111.61	108.27
26	IJ	203	PEB	C2A-C1A-NA	3.87	111.61	108.27
26	B1	203	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	N2	1002	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	TI	203	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	G1	202	PEB	CHC-C4C-C3C	-3.87	123.73	130.34
26	X8	201	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
26	V7	201	PEB	C1C-CHB-C4B	3.87	133.43	128.81
26	O8	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
26	mA	201	PEB	OA-C1A-C2A	-3.87	123.09	126.17
26	E1	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	K9	201	PEB	C3D-C4D-ND	3.87	114.85	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	RE	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	YI	203	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	KJ	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	CJ	202	PEB	C2A-C1A-NA	3.87	111.61	108.27
26	H2	1002	PEB	CHC-C4C-C3C	-3.87	123.73	130.34
26	uE	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	HF	1002	PEB	OD-C4D-ND	-3.87	120.20	125.93
26	u1	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	L4	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
26	Y4	201	PEB	C2A-C1A-NA	3.87	111.61	108.27
28	EF	1001	CYC	C2C-C1C-NC	3.87	111.61	108.27
26	A7	302	PEB	CHC-C4C-C3C	-3.87	123.74	130.34
26	GJ	202	PEB	CHC-C4C-C3C	-3.87	123.74	130.34
26	DJ	201	PEB	C3B-C4B-NB	3.87	115.68	110.05
26	NJ	203	PEB	CMB-C2B-C1B	3.87	131.02	125.06
26	A2	304	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	oG	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	TF	201	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
26	S3	202	PEB	CHC-C4C-C3C	-3.87	123.74	130.34
26	j7	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	kI	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	Z4	201	PEB	CHA-C1B-NB	-3.87	116.84	124.93
26	KA	202	PEB	C2A-C1A-NA	3.87	111.61	108.27
26	i2	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	f7	203	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	SA	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	KJ	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	i2	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	P3	203	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	h8	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	J9	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	hA	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	HE	201	PEB	C1B-C2B-C3B	-3.87	102.07	106.51
26	D8	201	PEB	CHC-C1D-ND	3.87	118.44	113.95
26	tE	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	QF	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	RG	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
26	O1	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
26	GB	1002	PEB	C3B-C4B-NB	3.87	115.67	110.05
26	KC	202	PEB	CHB-C4B-NB	-3.87	123.46	128.83
26	rE	201	PEB	CHC-C4C-C3C	-3.87	123.74	130.34
26	VI	203	PEB	C4B-C3B-C2B	-3.87	102.50	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l4	202	PEB	CMB-C2B-C1B	3.87	131.02	125.06
26	RE	202	PEB	CMB-C2B-C1B	3.87	131.02	125.06
26	GE	201	PEB	CHA-C1B-C2B	3.87	134.84	124.90
26	i1	203	PEB	C1B-C2B-C3B	-3.87	102.07	106.51
26	t1	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
26	mE	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
26	g4	201	PEB	CHC-C1D-ND	-3.87	109.46	113.95
26	VJ	203	PEB	C1C-CHB-C4B	3.87	133.43	128.81
28	NB	1001	CYC	C4D-CHA-C1A	3.87	133.43	128.81
26	eB	203	PEB	C3D-C4D-ND	3.87	114.84	107.26
26	tG	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
26	u1	203	PEB	CMB-C2B-C1B	3.87	131.02	125.06
26	I3	201	PEB	CHA-C1B-NB	-3.86	116.85	124.93
26	H9	201	PEB	CHA-C1B-NB	-3.86	116.85	124.93
26	H8	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	HA	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
27	yE	302	PUB	CBA-CAA-C3A	-3.86	107.12	112.98
26	B9	203	PEB	CHB-C4B-NB	-3.86	123.47	128.83
26	RI	202	PEB	C4B-C3B-C2B	-3.86	102.50	106.78
26	N4	202	PEB	CHA-C1B-NB	-3.86	116.85	124.93
26	gB	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	DD	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	NG	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	gE	201	PEB	C4B-C3B-C2B	-3.86	102.51	106.78
27	yE	302	PUB	C1C-C2C-C3C	-3.86	102.51	106.78
26	V8	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	I3	201	PEB	C1B-C2B-C3B	-3.86	102.07	106.51
26	hI	201	PEB	C1B-C2B-C3B	-3.86	102.07	106.51
26	d1	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	AB	304	PEB	C3D-C4D-ND	3.86	114.84	107.26
28	HF	1001	CYC	CHB-C1B-NB	-3.86	117.77	126.06
26	21	404	PEB	C2A-C1A-NA	3.86	111.60	108.27
26	SE	203	PEB	OA-C1A-C2A	-3.86	123.10	126.17
26	jI	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
26	l2	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	W9	201	PEB	OD-C4D-ND	-3.86	120.21	125.93
26	sG	202	PEB	CHC-C4C-C3C	-3.86	123.75	130.34
28	H2	1001	CYC	CHB-C1B-NB	-3.86	117.77	126.06
28	cH	1001	CYC	C1B-C2B-C3B	-3.86	103.84	107.87
26	D4	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	Q7	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
26	k6	201	PEB	CMB-C2B-C1B	3.86	131.01	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UE	201	PEB	C2A-C1A-NA	-3.86	104.94	108.27
28	H6	1001	CYC	CHB-C4A-NA	-3.86	116.86	124.93
28	KB	202	CYC	C2B-C1B-NB	3.86	112.64	106.99
26	JJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	OE	201	PEB	OD-C4D-ND	-3.86	120.21	125.93
26	YB	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	JD	202	PEB	C1B-C2B-C3B	-3.86	102.08	106.51
26	lG	202	PEB	C2A-C1A-NA	3.86	111.60	108.27
26	R2	202	PEB	CMB-C2B-C1B	3.86	131.01	125.06
26	I4	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	F4	202	PEB	C1B-C2B-C3B	-3.86	102.08	106.51
26	sG	202	PEB	CMB-C2B-C1B	3.86	131.01	125.06
26	i4	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	e6	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	QB	202	PEB	CHA-C1B-NB	-3.86	116.86	124.93
26	rG	201	PEB	CHA-C4A-NA	3.86	129.79	125.20
26	d7	203	PEB	C2A-C1A-NA	3.86	111.60	108.27
26	y1	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	D8	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	mE	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	KJ	201	PEB	CHC-C4C-C3C	-3.86	123.75	130.34
26	C1	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	Q1	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	h8	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	KA	203	PEB	CHA-C1B-NB	-3.86	116.86	124.93
26	a7	202	PEB	OA-C1A-C2A	-3.86	123.11	126.17
26	j7	203	PEB	OA-C1A-C2A	-3.86	123.11	126.17
26	O6	203	PEB	C4B-C3B-C2B	-3.86	102.51	106.78
26	R3	203	PEB	C1C-CHB-C4B	3.86	133.42	128.81
26	CG	201	PEB	C1C-CHB-C4B	-3.86	124.20	128.81
26	F2	1002	PEB	OD-C4D-ND	-3.86	120.21	125.93
26	LD	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	UG	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	mI	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	bG	201	PEB	CHB-C4B-NB	-3.86	123.47	128.83
26	XJ	203	PEB	CHC-C1D-ND	-3.86	109.47	113.95
26	e6	203	PEB	CMB-C2B-C1B	3.86	131.00	125.06
26	r1	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	GE	201	PEB	OD-C4D-ND	-3.86	120.22	125.93
26	X3	201	PEB	CHB-C4B-NB	-3.86	123.48	128.83
26	fE	202	PEB	CHB-C4B-NB	-3.86	123.48	128.83
26	AJ	304	PEB	CHA-C1B-NB	-3.86	116.86	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J1	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	J4	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	K5	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	cF	202	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	a7	201	PEB	CHC-C4C-C3C	-3.86	123.76	130.34
26	dF	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	O4	201	PEB	C1C-CHB-C4B	3.86	133.42	128.81
26	BJ	201	PEB	C4B-C3B-C2B	-3.86	102.51	106.78
26	WI	201	PEB	CMA-C2A-C1A	-3.86	104.09	112.40
26	K8	201	PEB	CHA-C1B-C2B	3.86	134.82	124.90
26	KE	201	PEB	C1B-C2B-C3B	-3.86	102.08	106.51
26	EA	201	PEB	CHA-C1B-NB	-3.86	116.87	124.93
26	PB	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
26	KG	202	PEB	CHC-C4C-C3C	-3.86	123.76	130.34
28	JF	1001	CYC	CMB-C2B-C1B	3.86	128.98	124.17
26	F5	202	PEB	C3D-C4D-ND	3.86	114.82	107.26
26	PD	203	PEB	C3D-C4D-ND	3.86	114.82	107.26
26	KJ	202	PEB	CHC-C4C-C3C	-3.86	123.76	130.34
26	YD	301	PEB	C3D-C4D-ND	3.86	114.82	107.26
26	jI	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
26	Y6	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
26	Q8	204	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	FC	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	K8	202	PEB	CMB-C2B-C1B	3.85	131.00	125.06
28	J2	1001	CYC	CMB-C2B-C1B	3.85	128.98	124.17
26	gF	202	PEB	CHC-C4C-C3C	-3.85	123.76	130.34
26	m2	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	XD	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	Q8	203	PEB	CMB-C2B-C1B	3.85	131.00	125.06
26	O4	201	PEB	CHA-C1B-NB	-3.85	116.87	124.93
26	T3	202	PEB	C1B-C2B-C3B	-3.85	102.08	106.51
26	T4	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	FD	201	PEB	C2A-C1A-NA	3.85	111.59	108.27
28	FF	1001	CYC	C2B-C1B-NB	3.85	112.63	106.99
26	q1	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	F9	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	O9	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	jE	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	Z6	201	PEB	CHC-C1D-ND	-3.85	109.47	113.95
26	BD	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	iI	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	e4	202	PEB	C1C-CHB-C4B	-3.85	124.21	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e3	401	PEB	OA-C1A-C2A	-3.85	123.11	126.17
26	WB	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	aI	203	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	FG	201	PEB	CHC-C4C-C3C	-3.85	123.77	130.34
26	H8	202	PEB	CHC-C1D-ND	-3.85	109.47	113.95
26	y1	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
26	oE	203	PEB	CHA-C1B-C2B	3.85	134.81	124.90
26	OA	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	dB	204	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	KE	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
26	L4	202	PEB	CHC-C1D-ND	-3.85	109.47	113.95
26	v4	201	PEB	C2A-C1A-NA	3.85	111.59	108.27
26	Y6	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	oE	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	iI	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	CC	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
26	DD	201	PEB	CMB-C2B-C1B	3.85	130.99	125.06
26	j8	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	O8	201	PEB	CHB-C4B-NB	-3.85	123.49	128.83
26	aA	201	PEB	C1B-C2B-C3B	-3.85	102.09	106.51
26	a7	202	PEB	CHA-C1B-NB	-3.85	116.88	124.93
26	Q4	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	eI	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	mI	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	c4	202	PEB	C1C-CHB-C4B	-3.85	124.21	128.81
26	HA	202	PEB	CHC-C4C-C3C	-3.85	123.77	130.34
26	Y2	203	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	d6	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	uE	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	vG	202	PEB	CHC-C1D-ND	-3.85	109.48	113.95
26	R8	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
27	A8	304	PUB	C1C-C2C-C3C	-3.85	102.52	106.78
26	aG	202	PEB	CHA-C1B-NB	-3.85	116.88	124.93
26	GJ	201	PEB	CAB-C3B-C4B	3.85	131.82	125.01
26	RE	202	PEB	CHB-C4B-C3B	-3.85	116.43	125.32
26	x4	201	PEB	CMB-C2B-C1B	3.85	130.99	125.06
26	sE	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	GJ	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	m2	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
28	FB	1001	CYC	C1B-C2B-C3B	-3.85	103.86	107.87
26	N3	203	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
28	WH	1001	CYC	CHB-C4A-C3A	3.85	134.79	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	HB	1001	CYC	C2C-C1C-NC	3.85	111.59	108.27
26	S3	202	PEB	C1B-C2B-C3B	-3.85	102.09	106.51
26	C5	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	j7	203	PEB	C3D-C4D-ND	3.85	114.81	107.26
28	HI	1001	CYC	C1A-C2A-C3A	-3.85	102.52	106.78
26	aE	203	PEB	CMB-C2B-C1B	3.85	130.99	125.06
26	AA	301	PEB	CHC-C4C-C3C	-3.85	123.78	130.34
26	HI	1002	PEB	CHC-C4C-C3C	-3.85	123.78	130.34
26	eD	401	PEB	OA-C1A-C2A	-3.85	123.11	126.17
26	P2	203	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	e2	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	K6	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	F7	1002	PEB	CHC-C4C-C3C	-3.85	123.78	130.34
26	N1	203	PEB	C2A-C1A-NA	3.85	111.59	108.27
26	J8	201	PEB	C2A-C1A-NA	3.85	111.59	108.27
26	P3	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	W4	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	A6	304	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	W6	203	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	YE	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	mF	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	QJ	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	W9	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	VA	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	II	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
26	U2	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
26	Y3	303	PEB	OA-C1A-C2A	-3.85	123.11	126.17
26	O2	202	PEB	C3D-C4D-ND	3.85	114.80	107.26
26	D6	1002	PEB	C3D-C4D-ND	3.85	114.80	107.26
28	KI	1001	CYC	C2C-C1C-NC	3.85	111.59	108.27
26	IA	202	PEB	CHA-C1B-NB	-3.85	116.89	124.93
26	ZI	202	PEB	CHB-C4B-NB	-3.85	123.49	128.83
26	UF	201	PEB	C3D-C4D-ND	3.85	114.80	107.26
26	mF	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
26	gI	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
26	DD	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
26	zE	501	PEB	CHA-C1B-NB	-3.84	116.89	124.93
26	a2	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
26	i1	202	PEB	CHC-C4C-C3C	-3.84	123.78	130.34
26	wE	302	PEB	CHC-C1D-ND	-3.84	109.48	113.95
26	YI	201	PEB	C2A-C1A-NA	3.84	111.59	108.27
27	A9	302	PUB	C1C-C2C-C3C	-3.84	102.53	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b7	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
28	BB	1001	CYC	CMA-C3A-C4A	3.84	130.98	125.06
27	NJ	201	PUB	CMA-C2A-C1A	3.84	130.43	121.39
26	q4	201	PEB	OD-C4D-ND	-3.84	120.24	125.93
26	D4	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
26	YG	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95
26	K8	203	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
26	J9	202	PEB	C1B-C2B-C3B	-3.84	102.10	106.51
28	K6	202	CYC	CHB-C4A-NA	-3.84	116.90	124.93
26	IC	203	PEB	C3D-C4D-ND	3.84	114.80	107.26
26	cI	202	PEB	CHA-C1B-NB	-3.84	116.90	124.93
26	BG	202	PEB	CMB-C2B-C1B	3.84	130.98	125.06
26	ME	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
26	lE	201	PEB	CHC-C4C-C3C	-3.84	123.79	130.34
26	jG	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
28	JF	1001	CYC	C1B-C2B-C3B	-3.84	103.86	107.87
26	C9	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
26	i2	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	g7	202	PEB	CMB-C2B-C1B	3.84	130.98	125.06
26	wG	302	PEB	CMB-C2B-C1B	3.84	130.98	125.06
26	WE	203	PEB	C2A-C1A-NA	3.84	111.58	108.27
26	D4	202	PEB	CHB-C4B-NB	-3.84	123.50	128.83
26	H4	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	q4	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	P9	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	XG	203	PEB	C3B-C4B-NB	3.84	115.63	110.05
26	AJ	305	PEB	CHC-C4C-C3C	-3.84	123.79	130.34
26	R4	201	PEB	CHC-C1D-ND	-3.84	109.49	113.95
26	bG	201	PEB	CHC-C1D-ND	-3.84	109.49	113.95
26	B4	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	j8	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	BC	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	X8	202	PEB	CAB-C3B-C4B	3.84	131.80	125.01
26	GA	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	jA	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	aB	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
28	GI	1001	CYC	C1B-NB-C4B	-3.84	105.78	110.67
26	gI	201	PEB	CHC-C4C-C3C	-3.84	123.79	130.34
26	jA	203	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	oE	201	PEB	CHA-C4A-NA	3.84	129.77	125.20
26	S1	201	PEB	CMB-C2B-C1B	3.84	130.97	125.06
26	GB	1002	PEB	CHC-C4C-C3C	-3.84	123.79	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g6	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	Q4	201	PEB	C3B-C4B-NB	3.84	115.63	110.05
26	W8	202	PEB	CHB-C4B-NB	-3.84	123.50	128.83
26	G3	201	PEB	CMB-C2B-C1B	3.84	130.97	125.06
26	W1	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	J9	203	PEB	C4B-C3B-C2B	-3.84	102.54	106.78
26	hA	201	PEB	C1C-CHB-C4B	3.84	133.39	128.81
26	VE	201	PEB	C1C-CHB-C4B	3.84	133.39	128.81
26	p1	202	PEB	C3D-C4D-ND	3.84	114.79	107.26
26	K1	201	PEB	C2A-C1A-NA	3.84	111.58	108.27
26	V6	202	PEB	C2A-C1A-NA	3.84	111.58	108.27
26	w1	203	PEB	C3D-C4D-ND	3.84	114.78	107.26
26	a6	201	PEB	C3D-C4D-ND	3.84	114.78	107.26
26	kB	202	PEB	C3D-C4D-ND	3.84	114.78	107.26
26	jF	201	PEB	CHC-C4C-C3C	-3.84	123.80	130.34
26	c8	202	PEB	CAB-C3B-C4B	3.84	131.79	125.01
26	JC	202	PEB	C2A-C1A-NA	3.83	111.58	108.27
26	SG	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	F1	201	PEB	OA-C1A-C2A	-3.83	123.12	126.17
26	CE	201	PEB	CHA-C1B-C2B	3.83	134.76	124.90
26	N3	202	PEB	CMB-C2B-C1B	3.83	130.97	125.06
26	d4	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
28	DF	1001	CYC	C1B-C2B-C3B	-3.83	103.87	107.87
26	D8	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
26	cB	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	H3	201	PEB	C2A-C1A-NA	3.83	111.58	108.27
26	bB	201	PEB	CHA-C1B-NB	-3.83	116.91	124.93
26	C5	203	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	D8	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	CC	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	JG	201	PEB	CHC-C1D-ND	-3.83	109.50	113.95
26	h4	202	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
26	YI	202	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
28	C7	1001	CYC	C1B-NB-C4B	-3.83	105.79	110.67
26	VD	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	g4	201	PEB	C2A-C1A-NA	3.83	111.58	108.27
26	iG	202	PEB	C3B-C4B-NB	3.83	115.62	110.05
28	YH	1003	CYC	C4D-CHA-C1A	3.83	133.39	128.81
26	PI	203	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	IC	201	PEB	CHB-C4B-NB	-3.83	123.51	128.83
26	OB	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	K9	202	PEB	C3D-C4D-ND	3.83	114.78	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GJ	201	PEB	OD-C4D-ND	-3.83	120.25	125.93
26	U4	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	i8	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	eE	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	MG	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
26	d4	202	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
26	IE	202	PEB	C2A-C1A-NA	3.83	111.58	108.27
26	OE	203	PEB	C2A-C1A-NA	3.83	111.58	108.27
26	L2	1002	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	B5	201	PEB	CHC-C4C-C3C	-3.83	123.81	130.34
26	P6	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	P8	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	VE	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	DF	1002	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	UF	201	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	sG	201	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	ND	202	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
26	J9	201	PEB	CHC-C4C-C3C	-3.83	123.81	130.34
26	QB	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
28	UH	1001	CYC	CAD-CBD-CGD	-3.83	103.03	113.76
26	h4	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	24	404	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	PJ	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	k2	201	PEB	C4B-C3B-C2B	-3.83	102.55	106.78
26	B4	202	PEB	C4B-C3B-C2B	-3.83	102.55	106.78
26	BC	201	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	eG	202	PEB	C3B-C4B-NB	3.83	115.62	110.05
26	L3	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	Y3	303	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	K5	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	c7	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	eE	201	PEB	CHA-C1B-NB	-3.83	116.92	124.93
26	CC	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
28	yH	1001	CYC	CHB-C4A-C3A	3.83	134.74	124.90
26	UA	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	ID	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	cI	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	YD	303	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	B1	201	PEB	CAA-C3A-C2A	-3.83	104.70	114.26
26	R4	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	bB	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	bF	201	PEB	C3D-C4D-ND	3.83	114.77	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N2	1001	CYC	CHB-C1B-NB	-3.83	117.84	126.06
28	eH	1001	CYC	CMB-C2B-C1B	3.83	128.94	124.17
26	a4	203	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	f8	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
26	k2	201	PEB	CHB-C4B-NB	-3.83	123.52	128.83
26	lF	201	PEB	C2A-C1A-NA	3.83	111.57	108.27
26	k1	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	RE	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	YI	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	YI	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
26	q4	203	PEB	C3D-C4D-ND	3.83	114.76	107.26
26	i2	201	PEB	CHC-C4C-C3C	-3.83	123.81	130.34
26	x4	202	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
27	NJ	201	PUB	C1C-C2C-C3C	-3.82	102.55	106.78
27	A9	302	PUB	CHC-C1D-ND	-3.82	108.89	113.72
26	PA	201	PEB	C1C-CHB-C4B	-3.82	124.24	128.81
26	WJ	202	PEB	CMB-C2B-C1B	3.82	130.95	125.06
26	BD	201	PEB	OA-C1A-C2A	-3.82	123.13	126.17
26	gI	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	RJ	202	PEB	CHC-C1D-ND	-3.82	109.51	113.95
26	aG	202	PEB	CHC-C4C-C3C	-3.82	123.81	130.34
28	H6	1001	CYC	C2C-C1C-NC	3.82	111.57	108.27
28	EI	1001	CYC	C2C-C1C-NC	3.82	111.57	108.27
28	G2	1001	CYC	CHA-C1A-NA	-3.82	123.52	128.83
26	l2	201	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
26	KC	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	D7	1002	PEB	CMB-C2B-C1B	3.82	130.95	125.06
26	U7	203	PEB	CHC-C4C-C3C	-3.82	123.81	130.34
28	oH	1001	CYC	CAB-C3B-C4B	3.82	127.42	121.38
26	lB	201	PEB	CHB-C4B-NB	-3.82	123.52	128.83
26	Q9	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	MA	201	PEB	C3B-C4B-NB	3.82	115.61	110.05
26	dB	204	PEB	CHC-C4C-C3C	-3.82	123.82	130.34
26	E4	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	M8	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	o1	501	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	dA	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	KE	202	PEB	C1C-CHB-C4B	3.82	133.38	128.81
26	N8	201	PEB	C3B-C4B-NB	3.82	115.61	110.05
26	NA	201	PEB	C3B-C4B-NB	3.82	115.61	110.05
26	l4	201	PEB	C2A-C1A-NA	3.82	111.57	108.27
26	b7	203	PEB	C2A-C1A-NA	3.82	111.57	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L5	201	PEB	CHC-C4C-C3C	-3.82	123.82	130.34
26	w4	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	C5	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	eF	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	RI	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
28	J2	1001	CYC	O2A-CGA-CBA	3.82	126.31	114.03
26	q1	203	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	V8	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
26	jI	201	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
26	dI	201	PEB	CHB-C4B-C3B	-3.82	116.49	125.32
26	e6	203	PEB	C3D-C4D-ND	3.82	114.76	107.26
28	AH	1001	CYC	OC-C1C-C2C	-3.82	123.14	126.17
26	Z4	202	PEB	CMB-C2B-C1B	3.82	130.95	125.06
26	NG	202	PEB	CMB-C2B-C1B	3.82	130.95	125.06
26	T2	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	a1	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	aE	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	gI	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	J1	203	PEB	C2A-C1A-NA	3.82	111.57	108.27
26	D2	1002	PEB	C2A-C1A-NA	3.82	111.57	108.27
26	l6	203	PEB	CHC-C4C-C3C	-3.82	123.82	130.34
26	S3	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
26	d6	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
26	V7	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	a8	204	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	LG	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	dB	202	PEB	CHB-C4B-NB	-3.82	123.53	128.83
28	HI	1001	CYC	C1B-C2B-C3B	-3.82	103.89	107.87
26	S1	201	PEB	C2A-C1A-NA	3.82	111.56	108.27
26	eF	201	PEB	CHB-C4B-NB	-3.82	123.53	128.83
26	NJ	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	v4	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	TJ	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	nG	201	PEB	CHB-C4B-NB	-3.82	123.53	128.83
26	l7	201	PEB	C2A-C1A-NA	3.82	111.56	108.27
26	N1	203	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	CE	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	O7	201	PEB	CHA-C1B-NB	-3.82	116.95	124.93
26	J5	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
26	A9	304	PEB	OA-C1A-C2A	-3.82	123.14	126.17
26	u4	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	V1	203	PEB	C4B-C3B-C2B	-3.82	102.56	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S2	201	PEB	CHA-C1B-NB	-3.82	116.95	124.93
26	Y1	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	i7	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	aA	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
26	Q8	203	PEB	CHA-C1B-NB	-3.82	116.95	124.93
26	P6	201	PEB	C3B-C4B-NB	3.82	115.60	110.05
26	mI	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
26	d8	202	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
26	mB	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
26	tG	201	PEB	CHB-C4B-NB	-3.81	123.53	128.83
26	P2	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	lB	203	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	XG	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	a8	201	PEB	C3B-C4B-NB	3.81	115.60	110.05
26	l6	203	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	K3	202	PEB	CHB-C4B-NB	-3.81	123.54	128.83
26	T3	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	KG	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	AA	301	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	fE	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	DJ	203	PEB	C3B-C4B-NB	3.81	115.60	110.05
26	e7	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	iI	201	PEB	CHC-C4C-C3C	-3.81	123.83	130.34
26	Z8	201	PEB	C3B-C4B-NB	3.81	115.59	110.05
26	s1	202	PEB	CHA-C4A-NA	3.81	129.74	125.20
26	WI	201	PEB	C4B-NB-C1B	-3.81	99.33	106.51
26	XG	202	PEB	CMB-C2B-C1B	3.81	130.94	125.06
26	r1	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
26	w4	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	a6	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	AJ	304	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	lF	203	PEB	C1B-C2B-C3B	-3.81	102.13	106.51
26	Q6	201	PEB	C3B-C4B-NB	3.81	115.59	110.05
26	CC	203	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	O7	203	PEB	C2A-C1A-NA	3.81	111.56	108.27
26	Y2	202	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
27	AB	302	PUB	C1C-C2C-C3C	-3.81	102.56	106.78
26	R4	203	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	KC	203	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	iB	201	PEB	CHB-C4B-NB	-3.81	123.54	128.83
26	YA	201	PEB	C3B-C4B-NB	3.81	115.59	110.05
26	R2	202	PEB	C3D-C4D-ND	3.81	114.74	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	bE	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
26	mG	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	bE	202	PEB	CHC-C1D-ND	3.81	118.37	113.95
26	dG	201	PEB	CHB-C4B-NB	-3.81	123.54	128.83
26	H9	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
26	PJ	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
26	aF	201	PEB	CMB-C2B-C1B	3.81	130.93	125.06
26	H3	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	TD	202	PEB	C1B-C2B-C3B	-3.81	102.13	106.51
26	IC	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	ZG	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	v4	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	A5	202	PEB	OA-C1A-C2A	-3.81	123.14	126.17
26	WD	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
26	Q6	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
28	J7	1003	CYC	C1B-NB-C4B	-3.81	105.82	110.67
26	HG	202	PEB	C3B-C4B-NB	3.81	115.59	110.05
26	BD	201	PEB	C1C-CHB-C4B	-3.81	124.26	128.81
26	g2	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	H3	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	S4	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	Y8	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	kB	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	W8	203	PEB	CMB-C2B-C1B	3.81	130.93	125.06
26	Y8	202	PEB	CHC-C4C-C3C	-3.81	123.84	130.34
26	A7	302	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	eF	201	PEB	C3B-C4B-NB	3.81	115.59	110.05
26	dI	201	PEB	C3B-C4B-NB	3.81	115.59	110.05
26	vG	202	PEB	OD-C4D-ND	-3.81	120.29	125.93
26	A2	304	PEB	CHC-C4C-C3C	-3.81	123.84	130.34
26	XA	202	PEB	CHC-C1D-ND	-3.81	109.53	113.95
26	RB	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	AC	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	zE	501	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	eA	202	PEB	OA-C1A-C2A	-3.81	123.15	126.17
26	t1	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	l6	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	UJ	201	PEB	CBC-CAC-C2C	-3.81	106.12	112.62
26	lA	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	PB	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	PG	201	PEB	C4B-C3B-C2B	-3.81	102.57	106.78
27	K4	203	PUB	C1C-C2C-C3C	-3.81	102.57	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K6	202	CYC	OB-C4B-C3B	-3.81	123.91	128.04
26	Y2	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	B4	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	iB	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
26	T9	203	PEB	OA-C1A-C2A	-3.81	123.15	126.17
26	CA	203	PEB	OA-C1A-C2A	-3.81	123.15	126.17
26	XD	201	PEB	OD-C4D-ND	-3.81	120.29	125.93
26	V3	201	PEB	C3D-C4D-ND	3.81	114.72	107.26
26	U4	202	PEB	C3D-C4D-ND	3.81	114.72	107.26
26	i4	202	PEB	CHA-C1B-NB	-3.81	116.97	124.93
26	G6	1002	PEB	CHC-C4C-C3C	-3.81	123.85	130.34
26	c1	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	F9	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	f2	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
26	SF	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
26	XE	202	PEB	C3B-C4B-NB	3.80	115.58	110.05
26	h4	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	UE	203	PEB	C1B-C2B-C3B	-3.80	102.14	106.51
26	V3	201	PEB	CAC-CBC-CGC	-3.80	103.09	113.76
26	j6	201	PEB	CHC-C4C-C3C	-3.80	123.85	130.34
26	W4	202	PEB	CAB-C3B-C4B	3.80	131.74	125.01
26	W8	203	PEB	C4B-C3B-C2B	-3.80	102.57	106.78
26	C4	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	H4	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	GC	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	R1	202	PEB	CHC-C4C-C3C	-3.80	123.85	130.34
26	k2	201	PEB	CHC-C4C-C3C	-3.80	123.85	130.34
26	CA	202	PEB	CHC-C4C-C3C	-3.80	123.85	130.34
26	B5	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	G8	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	KA	201	PEB	CHA-C1B-C2B	3.80	134.68	124.90
26	iE	202	PEB	C4B-C3B-C2B	-3.80	102.57	106.78
26	AF	301	PEB	CHA-C1B-NB	-3.80	116.98	124.93
26	c2	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	L3	201	PEB	CHC-C1D-ND	-3.80	109.53	113.95
26	kE	203	PEB	CHC-C1D-ND	-3.80	109.53	113.95
26	cF	202	PEB	CHC-C1D-ND	-3.80	109.53	113.95
26	W1	202	PEB	CAB-C3B-C4B	3.80	131.74	125.01
26	JF	1002	PEB	OA-C1A-C2A	-3.80	123.15	126.17
26	k1	202	PEB	CHB-C4B-NB	-3.80	123.55	128.83
26	V7	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	sG	201	PEB	C3D-C4D-ND	3.80	114.72	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AI	301	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	Z7	201	PEB	CHC-C4C-C3C	-3.80	123.85	130.34
26	N1	201	PEB	OD-C4D-ND	-3.80	120.30	125.93
26	MG	203	PEB	C1B-C2B-C3B	-3.80	102.14	106.51
28	M6	1001	CYC	C2C-C1C-NC	3.80	111.55	108.27
26	X3	202	PEB	CHB-C4B-NB	-3.80	123.55	128.83
26	i6	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	a8	201	PEB	CHA-C1B-NB	-3.80	116.98	124.93
26	u1	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	O6	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	a8	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	P2	203	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
26	YA	202	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
26	GD	202	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
26	e2	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	KC	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
26	PE	201	PEB	CHA-C1B-NB	-3.80	116.98	124.93
26	UD	202	PEB	C1B-C2B-C3B	-3.80	102.14	106.51
26	g1	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	VG	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	I8	201	PEB	C1B-C2B-C3B	-3.80	102.15	106.51
26	Z6	201	PEB	C3B-C4B-NB	3.80	115.58	110.05
26	e2	203	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	DB	1002	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	fG	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	AJ	305	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	c4	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
26	a6	202	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
26	SG	202	PEB	CMA-C2A-C1A	-3.80	104.22	112.40
26	xE	304	PEB	C2A-C1A-NA	3.80	111.55	108.27
26	wG	302	PEB	CHC-C1D-ND	-3.80	109.54	113.95
26	d6	204	PEB	CHA-C1B-NB	-3.80	116.99	124.93
26	A3	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	PI	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
26	O9	201	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
26	r1	201	PEB	OA-C1A-C2A	-3.80	123.15	126.17
26	a2	202	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
26	VD	201	PEB	C2A-C1A-NA	3.80	111.55	108.27
26	VE	202	PEB	C2A-C1A-NA	3.80	111.55	108.27
26	Y4	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	R6	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	mB	201	PEB	C3D-C4D-ND	3.80	114.71	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	RI	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	mA	202	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
26	dF	202	PEB	C1B-C2B-C3B	-3.80	102.15	106.51
26	A9	303	PEB	CHA-C1B-NB	-3.80	116.99	124.93
28	M6	1001	CYC	CHB-C4A-NA	-3.80	116.99	124.93
26	I5	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	ZE	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	J4	201	PEB	C3B-C4B-NB	3.80	115.57	110.05
26	M8	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
28	F6	1001	CYC	C1B-C2B-C3B	-3.80	103.91	107.87
26	S9	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	hA	201	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	WF	203	PEB	C3D-C4D-ND	3.80	114.71	107.26
26	ZB	201	PEB	C3B-C4B-NB	3.80	115.57	110.05
26	DG	203	PEB	CHB-C4B-C3B	-3.80	116.55	125.32
26	V2	203	PEB	C3D-C4D-ND	3.80	114.70	107.26
26	m6	201	PEB	C3D-C4D-ND	3.80	114.70	107.26
26	iB	202	PEB	C3D-C4D-ND	3.80	114.70	107.26
26	HD	201	PEB	C3D-C4D-ND	3.80	114.70	107.26
26	PD	202	PEB	CHB-C4B-NB	-3.79	123.56	128.83
26	Q6	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	e6	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	C8	203	PEB	C2A-C1A-NA	3.79	111.54	108.27
26	R6	201	PEB	CAB-C3B-C4B	3.79	131.72	125.01
28	B6	1002	CYC	CBB-CAB-C3B	-3.79	101.97	112.43
26	DF	1002	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	PB	201	PEB	C3B-C4B-NB	3.79	115.57	110.05
26	U1	201	PEB	CAC-CBC-CGC	-3.79	103.12	113.76
26	Y7	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	WG	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	A9	301	PEB	CHC-C1D-ND	-3.79	109.54	113.95
26	UE	201	PEB	OD-C4D-ND	-3.79	120.31	125.93
26	n4	201	PEB	C4B-C3B-C2B	-3.79	102.58	106.78
26	lB	203	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	KE	201	PEB	CAA-C3A-C2A	3.79	123.74	114.26
26	W4	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	d7	203	PEB	CHC-C1D-ND	-3.79	109.54	113.95
28	F2	1001	CYC	CHB-C1B-NB	-3.79	117.92	126.06
26	lA	203	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	FJ	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	B3	202	PEB	CHA-C1B-NB	-3.79	117.00	124.93
26	O1	201	PEB	CMB-C2B-C1B	3.79	130.90	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h4	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	B8	301	PEB	CHA-C1B-NB	-3.79	117.00	124.93
26	IC	202	PEB	CHC-C1D-ND	-3.79	109.54	113.95
26	CG	201	PEB	CHC-C4C-C3C	-3.79	123.87	130.34
26	YF	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	dG	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
26	aA	204	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	rG	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	KJ	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
28	J2	1001	CYC	OB-C4B-C3B	-3.79	123.93	128.04
26	W6	203	PEB	CHC-C1D-ND	-3.79	109.55	113.95
26	B4	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	n4	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	k1	202	PEB	CHA-C1B-NB	-3.79	117.00	124.93
26	uG	201	PEB	CHA-C1B-NB	-3.79	117.00	124.93
26	I9	202	PEB	C2A-C1A-NA	3.79	111.54	108.27
26	RA	202	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
26	KD	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
28	DI	1001	CYC	CMB-C2B-C1B	3.79	128.90	124.17
26	NA	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	AC	203	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	VF	203	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	TI	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
26	AG	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	WI	201	PEB	C1B-C2B-C3B	-3.79	102.16	106.51
26	XA	202	PEB	CAB-C3B-C4B	3.79	131.71	125.01
27	yE	303	PUB	C1C-C2C-C3C	-3.79	102.59	106.78
26	SD	202	PEB	CHC-C4C-C3C	-3.79	123.88	130.34
26	OE	201	PEB	C2A-C1A-NA	3.79	111.54	108.27
26	f2	201	PEB	C1B-C2B-C3B	-3.79	102.16	106.51
26	Z2	202	PEB	CHB-C4B-NB	-3.79	123.57	128.83
26	xE	303	PEB	CHC-C4C-C3C	-3.79	123.88	130.34
26	b7	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	AF	305	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	eE	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
26	y4	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
26	TD	203	PEB	C3B-C4B-NB	3.79	115.56	110.05
28	H2	1001	CYC	CAB-C3B-C4B	3.79	127.36	121.38
26	IC	203	PEB	CHC-C4C-C3C	-3.79	123.88	130.34
26	iE	202	PEB	CHC-C1D-ND	-3.79	109.55	113.95
26	D1	203	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	Y2	202	PEB	C3D-C4D-ND	3.79	114.69	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aA	204	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	AF	302	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	X4	203	PEB	OD-C4D-ND	-3.79	120.32	125.93
26	GA	201	PEB	CHA-C1B-C2B	3.79	134.64	124.90
26	J1	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	u4	201	PEB	C2A-C1A-NA	3.79	111.54	108.27
26	GA	202	PEB	C2A-C1A-NA	3.79	111.54	108.27
26	GE	203	PEB	CHB-C4B-NB	-3.79	123.58	128.83
26	hB	203	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
26	eG	203	PEB	CHA-C1B-NB	-3.79	117.01	124.93
28	GB	1001	CYC	CHB-C4A-NA	-3.79	117.01	124.93
26	R2	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	cA	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	jF	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
26	CJ	202	PEB	C1C-CHB-C4B	3.79	133.33	128.81
26	NE	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
26	c6	201	PEB	CHC-C4C-C3C	-3.79	123.88	130.34
26	g7	202	PEB	CHA-C1B-NB	-3.79	117.02	124.93
26	SE	201	PEB	C1B-C2B-C3B	-3.78	102.16	106.51
26	y1	202	PEB	CHC-C1D-ND	-3.78	109.55	113.95
26	eA	201	PEB	CHC-C1D-ND	3.78	118.34	113.95
26	Z4	202	PEB	C3D-C4D-ND	3.78	114.69	107.26
26	I5	203	PEB	C3D-C4D-ND	3.78	114.69	107.26
26	T6	201	PEB	C3D-C4D-ND	3.78	114.69	107.26
26	O1	201	PEB	CHC-C4C-C3C	-3.78	123.88	130.34
26	FC	201	PEB	CHC-C4C-C3C	-3.78	123.88	130.34
26	s4	201	PEB	OA-C1A-C2A	-3.78	123.16	126.17
26	XE	202	PEB	OA-C1A-C2A	-3.78	123.16	126.17
26	cI	203	PEB	C3D-C4D-ND	3.78	114.68	107.26
26	SI	201	PEB	CHC-C4C-C3C	-3.78	123.88	130.34
26	PG	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
26	eE	201	PEB	C1B-C2B-C3B	-3.78	102.16	106.51
26	KG	202	PEB	CHA-C1B-C2B	3.78	134.63	124.90
26	ME	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
26	H5	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	PG	202	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	P4	202	PEB	CHA-C1B-NB	-3.78	117.02	124.93
26	VA	202	PEB	CHA-C1B-NB	-3.78	117.02	124.93
26	m2	201	PEB	CMB-C2B-C1B	3.78	130.89	125.06
26	U8	201	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	JG	202	PEB	C3B-C4B-NB	3.78	115.55	110.05
26	WF	201	PEB	C3D-C4D-ND	3.78	114.68	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KC	201	PEB	CHC-C4C-C3C	-3.78	123.89	130.34
28	G7	1001	CYC	CHB-C1B-NB	-3.78	117.94	126.06
28	I7	1001	CYC	C1B-NB-C4B	-3.78	105.85	110.67
26	XD	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	TA	202	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	OG	202	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	UE	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
26	e8	202	PEB	CAB-C3B-C4B	3.78	131.70	125.01
26	OB	202	PEB	CHB-C4B-NB	-3.78	123.58	128.83
26	IG	202	PEB	C3B-C4B-NB	3.78	115.55	110.05
26	jF	203	PEB	C3D-C4D-ND	3.78	114.68	107.26
26	AG	201	PEB	C3D-C4D-ND	3.78	114.68	107.26
26	t4	201	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	A7	305	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	k7	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
28	II	1001	CYC	C1B-C2B-C3B	-3.78	103.93	107.87
26	gI	201	PEB	CHB-C4B-NB	-3.78	123.58	128.83
26	mI	201	PEB	CMB-C2B-C1B	3.78	130.88	125.06
26	LC	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	YG	201	PEB	C1C-CHB-C4B	3.78	133.32	128.81
26	U8	201	PEB	C3B-C4B-NB	3.78	115.55	110.05
26	jB	201	PEB	CHC-C4C-C3C	-3.78	123.89	130.34
26	U1	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	UF	203	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	PE	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	RG	202	PEB	CMB-C2B-C1B	3.78	130.88	125.06
26	mF	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
28	HF	1001	CYC	C2B-C1B-NB	3.78	112.52	106.99
26	lE	202	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	c6	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	QG	201	PEB	CHB-C4B-C3B	-3.78	116.59	125.32
26	mI	202	PEB	CMB-C2B-C1B	3.78	130.88	125.06
26	V4	203	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	xG	302	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	k4	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	DD	201	PEB	CHC-C4C-C3C	-3.78	123.89	130.34
26	JA	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	M3	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	Z4	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	mI	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	J1	203	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	l4	201	PEB	C3D-C4D-ND	3.78	114.67	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	VB	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	w4	201	PEB	C1C-CHB-C4B	3.78	133.32	128.81
26	r4	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	jF	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	cA	203	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
26	X3	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	h7	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
26	a4	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	PD	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
26	gE	203	PEB	CHA-C1B-C2B	3.78	134.61	124.90
27	Y3	302	PUB	C4B-CHB-C1C	3.78	133.32	128.81
26	Q7	203	PEB	CMB-C2B-C1B	3.78	130.88	125.06
26	HD	202	PEB	C1B-C2B-C3B	-3.78	102.17	106.51
26	g2	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	S8	202	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	TJ	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
26	RB	201	PEB	CAB-CBB-CGB	-3.78	105.48	113.60
26	PE	202	PEB	C2A-C1A-NA	3.77	111.53	108.27
26	k2	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
28	JF	1003	CYC	C2B-C1B-NB	3.77	112.51	106.99
26	C8	202	PEB	CHC-C4C-C3C	-3.77	123.90	130.34
26	aA	203	PEB	C1C-CHB-C4B	-3.77	124.30	128.81
26	JD	203	PEB	C1C-CHB-C4B	-3.77	124.30	128.81
28	M2	1001	CYC	C1B-C2B-C3B	-3.77	103.93	107.87
26	e3	401	PEB	CMB-C2B-C1B	3.77	130.88	125.06
26	RI	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	UG	201	PEB	CMB-C2B-C3B	-3.77	115.87	126.12
26	p4	202	PEB	OD-C4D-ND	-3.77	120.34	125.93
26	r4	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
26	Q7	203	PEB	C1B-C2B-C3B	-3.77	102.18	106.51
28	D6	1001	CYC	C4A-C3A-C2A	-3.77	102.18	106.51
26	L1	203	PEB	C3D-C4D-ND	3.77	114.66	107.26
26	z4	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
28	G7	1001	CYC	C1B-CHB-C4A	-3.77	118.86	128.08
26	H3	203	PEB	C2A-C1A-NA	3.77	111.53	108.27
26	SE	203	PEB	CHA-C4A-NA	3.77	129.69	125.20
26	i1	203	PEB	C3D-C4D-ND	3.77	114.66	107.26
26	i7	201	PEB	C1C-CHB-C4B	3.77	133.31	128.81
26	F9	202	PEB	OA-C1A-C2A	-3.77	123.17	126.17
26	CC	203	PEB	OA-C1A-C2A	-3.77	123.17	126.17
26	q1	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
26	m7	202	PEB	C3D-C4D-ND	3.77	114.66	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X9	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
26	R8	202	PEB	CMB-C2B-C1B	3.77	130.87	125.06
26	L9	202	PEB	CHA-C1B-C2B	3.77	134.60	124.90
26	VF	203	PEB	CHC-C1D-ND	-3.77	109.57	113.95
26	XE	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
26	SJ	201	PEB	C3D-C4D-ND	3.77	114.66	107.26
28	MB	1001	CYC	C1B-C2B-C3B	-3.77	103.94	107.87
26	DG	201	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	CJ	202	PEB	CHC-C4C-C3C	-3.77	123.91	130.34
28	D2	1001	CYC	CMB-C2B-C1B	3.77	128.88	124.17
26	h4	203	PEB	CHC-C1D-ND	-3.77	109.57	113.95
26	ME	203	PEB	CMB-C2B-C1B	3.77	130.87	125.06
26	EA	202	PEB	CHA-C1B-C2B	3.77	134.59	124.90
26	Q6	201	PEB	C2A-C1A-NA	3.77	111.52	108.27
28	L2	1001	CYC	C2C-C1C-NC	3.77	111.52	108.27
26	Y3	301	PEB	C3D-C4D-ND	3.77	114.66	107.26
26	g7	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
27	21	402	PUB	CHC-C1D-ND	-3.77	108.95	113.72
26	uE	203	PEB	CHC-C1D-ND	-3.77	109.57	113.95
26	w1	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
26	ZA	201	PEB	OD-C4D-ND	-3.77	120.35	125.93
26	R2	202	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	a2	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	V8	201	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	IJ	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	d6	203	PEB	CHB-C4B-NB	-3.77	123.60	128.83
26	QA	204	PEB	C1B-C2B-C3B	-3.77	102.18	106.51
26	c4	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
28	DI	1001	CYC	OC-C1C-C2C	-3.77	123.18	126.17
26	Y6	201	PEB	C2A-C1A-NA	3.77	111.52	108.27
26	cI	201	PEB	CHC-C4C-C3C	-3.77	123.91	130.34
26	eB	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	jE	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	qG	201	PEB	CHB-C4B-NB	-3.77	123.60	128.83
26	JJ	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	fF	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	W7	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	FD	201	PEB	CHC-C4C-C3C	-3.77	123.91	130.34
27	AI	303	PUB	CHA-C1B-C2B	-3.77	123.91	130.34
27	AJ	302	PUB	C1C-C2C-C3C	-3.77	102.61	106.78
26	J5	201	PEB	CBB-CAB-C3B	-3.77	102.16	112.63
28	E7	1001	CYC	C1B-C2B-C3B	-3.77	103.94	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k1	202	PEB	C1B-C2B-C3B	-3.77	102.18	106.51
28	dH	1001	CYC	CMB-C2B-C1B	3.77	128.87	124.17
26	C8	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
26	D1	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	y1	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	Q9	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	VJ	201	PEB	C3D-C4D-ND	3.77	114.65	107.26
26	uE	201	PEB	C1C-CHB-C4B	3.77	133.31	128.81
26	S8	201	PEB	C2A-C1A-NA	3.77	111.52	108.27
26	XA	201	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
26	rG	201	PEB	OD-C4D-ND	-3.77	120.35	125.93
26	D4	202	PEB	C3D-C4D-ND	3.76	114.65	107.26
26	TD	202	PEB	C3D-C4D-ND	3.76	114.65	107.26
26	BC	202	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
26	YB	201	PEB	CHB-C4B-C3B	-3.76	116.62	125.32
26	M1	401	PEB	C1C-CHB-C4B	-3.76	124.31	128.81
26	d6	204	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	P7	202	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	R2	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
26	Q1	201	PEB	OA-C1A-C2A	-3.76	123.18	126.17
26	T4	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
26	KC	203	PEB	OA-C1A-C2A	-3.76	123.18	126.17
26	S1	202	PEB	C2A-C1A-NA	3.76	111.52	108.27
26	X8	201	PEB	C2A-C1A-NA	3.76	111.52	108.27
26	LD	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	dE	201	PEB	CHB-C4B-NB	-3.76	123.61	128.83
26	SF	201	PEB	C1C-CHB-C4B	3.76	133.31	128.81
26	D1	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	d7	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	h7	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	dB	203	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	q1	201	PEB	CMB-C2B-C1B	3.76	130.86	125.06
28	HF	1001	CYC	CMA-C3A-C4A	3.76	130.86	125.06
26	21	405	PEB	OA-C1A-C2A	-3.76	123.18	126.17
26	A6	301	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
26	q4	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
26	RI	202	PEB	CMB-C2B-C1B	3.76	130.86	125.06
26	TB	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	FD	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	MA	202	PEB	CMB-C2B-C1B	3.76	130.86	125.06
28	jH	1001	CYC	OC-C1C-C2C	-3.76	123.18	126.17
26	k8	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OB	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
28	oH	1001	CYC	CMB-C2B-C1B	3.76	128.86	124.17
26	DA	202	PEB	C3D-C4D-ND	3.76	114.64	107.26
28	jH	1001	CYC	C4D-CHA-C1A	3.76	133.30	128.81
26	PJ	203	PEB	C3D-C4D-ND	3.76	114.64	107.26
28	E2	1001	CYC	C2C-C1C-NC	3.76	111.52	108.27
26	Z2	201	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
26	X9	201	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
26	tG	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
28	AH	1001	CYC	C2B-C1B-NB	3.76	112.49	106.99
26	eG	203	PEB	CMB-C2B-C1B	3.76	130.85	125.06
26	hG	201	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
26	h1	202	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	a7	202	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	BJ	201	PEB	C3D-C4D-ND	3.76	114.64	107.26
26	T9	203	PEB	OD-C4D-ND	-3.76	120.36	125.93
26	RJ	203	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
26	g4	202	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
28	iH	1001	CYC	OC-C1C-C2C	-3.76	123.18	126.17
26	HA	201	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
26	oG	203	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
27	AA	304	PUB	C1C-C2C-C3C	-3.76	102.62	106.78
26	V6	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	DG	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
26	NA	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
26	R3	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	XD	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
26	A2	304	PEB	OA-C1A-C2A	-3.76	123.19	126.17
26	V4	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
26	W9	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
26	TD	202	PEB	OD-C4D-ND	-3.76	120.36	125.93
26	PD	202	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	R3	203	PEB	CHB-C4B-C3B	-3.76	116.64	125.32
26	HA	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	S3	201	PEB	CBB-CAB-C3B	-3.76	102.19	112.63
26	P7	201	PEB	CHC-C1D-ND	-3.76	109.58	113.95
26	S1	202	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	m7	201	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	g1	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
26	q1	203	PEB	C2A-C1A-NA	3.76	111.51	108.27
26	Z1	202	PEB	C4B-C3B-C2B	-3.76	102.63	106.78
26	H9	201	PEB	C1B-C2B-C3B	-3.76	102.20	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m6	203	PEB	C3D-C4D-ND	3.76	114.63	107.26
26	P3	202	PEB	CHB-C4B-NB	-3.76	123.62	128.83
28	D7	1001	CYC	C1B-NB-C4B	-3.76	105.89	110.67
26	l8	203	PEB	C3D-C4D-ND	3.75	114.63	107.26
26	kE	203	PEB	C3D-C4D-ND	3.75	114.63	107.26
26	wG	301	PEB	CHC-C1D-ND	-3.75	109.59	113.95
26	U3	202	PEB	CHB-C4B-NB	-3.75	123.62	128.83
26	g2	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	MA	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	X4	202	PEB	CHB-C4B-C3B	-3.75	116.65	125.32
26	cI	203	PEB	OA-C1A-C2A	-3.75	123.19	126.17
28	DB	1001	CYC	CHB-C4A-NA	-3.75	117.08	124.93
26	b7	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	VB	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	AJ	303	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	B9	203	PEB	C3B-C4B-NB	3.75	115.51	110.05
26	H1	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
27	yE	303	PUB	CHA-C1B-C2B	-3.75	123.94	130.34
26	e2	202	PEB	CHB-C4B-NB	-3.75	123.62	128.83
26	a8	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	h2	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	WG	201	PEB	CMB-C2B-C1B	3.75	130.84	125.06
26	M3	201	PEB	OD-C4D-C3D	-3.75	120.96	129.46
26	c6	202	PEB	CHC-C4C-C3C	-3.75	123.94	130.34
26	F1	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	mB	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	P2	202	PEB	CHA-C1B-NB	-3.75	117.08	124.93
26	UA	201	PEB	C3B-C4B-NB	3.75	115.51	110.05
26	ZG	201	PEB	CHC-C4C-C3C	-3.75	123.94	130.34
26	j7	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
26	B4	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	LA	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	G9	201	PEB	OD-C4D-ND	-3.75	120.37	125.93
26	DJ	202	PEB	CHA-C1B-C2B	3.75	134.55	124.90
26	a8	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
26	iA	202	PEB	C2A-C1A-NA	3.75	111.51	108.27
26	mA	201	PEB	C2A-C1A-NA	3.75	111.51	108.27
26	D9	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	P9	203	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	QA	204	PEB	CHB-C4B-NB	-3.75	123.62	128.83
26	dG	201	PEB	C3D-C4D-ND	3.75	114.62	107.26
26	A6	304	PEB	CHC-C4C-C3C	-3.75	123.94	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J9	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	Q4	202	PEB	C2A-C1A-NA	3.75	111.51	108.27
27	K3	203	PUB	CHA-C1B-C2B	-3.75	123.94	130.34
26	cG	203	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
27	A7	303	PUB	C1C-C2C-C3C	-3.75	102.63	106.78
26	WI	201	PEB	CHA-C1B-NB	-3.75	117.09	124.93
26	S9	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	D4	202	PEB	C2A-C1A-NA	3.75	111.50	108.27
26	I5	203	PEB	C2A-C1A-NA	3.75	111.50	108.27
26	ZG	202	PEB	C2A-C1A-NA	3.75	111.50	108.27
26	mI	201	PEB	C2A-C1A-NA	3.75	111.50	108.27
26	pE	202	PEB	OD-C4D-ND	-3.75	120.38	125.93
26	P8	202	PEB	CHC-C1D-ND	-3.75	109.59	113.95
26	L1	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	YI	203	PEB	CAB-C3B-C4B	3.75	131.64	125.01
26	N7	1002	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	l8	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	eG	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	Q1	201	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
27	xE	301	PUB	C1C-C2C-C3C	-3.75	102.63	106.78
26	C3	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	I4	201	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	TI	203	PEB	CAB-C3B-C4B	3.75	131.64	125.01
28	KB	202	CYC	OB-C4B-C3B	-3.75	123.97	128.04
26	h2	201	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
26	a8	201	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
26	a1	203	PEB	C4B-C3B-C2B	-3.75	102.64	106.78
26	mG	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	sG	203	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	KA	203	PEB	C1B-C2B-C3B	-3.75	102.21	106.51
26	t4	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	Z7	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	q4	202	PEB	C2A-C1A-NA	3.75	111.50	108.27
28	HF	1001	CYC	C2C-C1C-NC	3.75	111.50	108.27
26	SJ	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
26	pG	201	PEB	C4B-C3B-C2B	-3.75	102.64	106.78
26	aB	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
26	VD	201	PEB	CHB-C4B-NB	-3.75	123.63	128.83
26	a1	201	PEB	C3D-C4D-ND	3.74	114.61	107.26
26	V2	203	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
26	W8	202	PEB	OD-C4D-C3D	-3.74	120.97	129.46
26	uE	201	PEB	C2A-C1A-NA	3.74	111.50	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P7	201	PEB	CHB-C4B-NB	-3.74	123.63	128.83
28	L7	1001	CYC	OB-C4B-C3B	-3.74	123.98	128.04
26	GE	201	PEB	OA-C1A-C2A	-3.74	123.20	126.17
26	C5	204	PEB	C3D-C4D-ND	3.74	114.61	107.26
26	YA	201	PEB	C3D-C4D-ND	3.74	114.61	107.26
26	fl	201	PEB	CHB-C4B-C3B	-3.74	116.67	125.32
26	U1	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
26	h6	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	BA	301	PEB	CHA-C1B-NB	-3.74	117.10	124.93
26	iG	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	lB	202	PEB	CHC-C4C-C3C	-3.74	123.95	130.34
26	KC	203	PEB	CHC-C4C-C3C	-3.74	123.95	130.34
26	sG	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
26	wG	301	PEB	OD-C4D-ND	-3.74	120.39	125.93
26	hB	202	PEB	CHB-C4B-NB	-3.74	123.64	128.83
26	YB	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
26	HA	202	PEB	CHC-C1D-ND	-3.74	109.60	113.95
26	XJ	201	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
26	jI	201	PEB	CMB-C2B-C1B	3.74	130.83	125.06
28	J2	1001	CYC	CAA-CBA-CGA	3.74	121.66	113.60
26	KB	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
28	GI	1001	CYC	C2C-C1C-NC	3.74	111.50	108.27
26	U1	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	RD	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	A8	301	PEB	CHC-C4C-C3C	-3.74	123.95	130.34
26	l1	203	PEB	OA-C1A-C2A	-3.74	123.20	126.17
26	Y3	304	PEB	OA-C1A-C2A	-3.74	123.20	126.17
26	fA	203	PEB	OA-C1A-C2A	-3.74	123.20	126.17
26	A7	305	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	R7	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	lE	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	RF	201	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	i1	201	PEB	CHB-C4B-NB	-3.74	123.64	128.83
26	VD	202	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
26	K5	203	PEB	CHC-C4C-C3C	-3.74	123.96	130.34
26	LG	201	PEB	CHA-C1B-NB	-3.74	117.11	124.93
28	l2	1001	CYC	C1B-C2B-C3B	-3.74	103.97	107.87
26	OD	202	PEB	CHB-C4B-NB	-3.74	123.64	128.83
26	HF	1002	PEB	C3D-C4D-ND	3.74	114.60	107.26
26	CE	201	PEB	CMB-C2B-C1B	3.74	130.82	125.06
26	RB	201	PEB	CHB-C4B-NB	-3.74	123.64	128.83
26	MG	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O7	201	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
26	C9	202	PEB	C2A-C1A-NA	3.74	111.50	108.27
26	cI	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
26	k6	202	PEB	CHC-C1D-ND	-3.74	109.61	113.95
26	DE	201	PEB	CHC-C1D-ND	-3.74	109.61	113.95
26	I8	201	PEB	C2A-C1A-NA	3.74	111.50	108.27
26	L5	202	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	H8	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	DA	202	PEB	CHC-C4C-C3C	-3.74	123.96	130.34
26	e7	201	PEB	C3B-C4B-NB	3.74	115.48	110.05
26	IE	202	PEB	C3B-C4B-NB	3.74	115.48	110.05
26	d1	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	J4	203	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	J9	201	PEB	OA-C1A-C2A	-3.74	123.20	126.17
26	G5	202	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	N9	202	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	aE	202	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	B3	201	PEB	C4B-C3B-C2B	-3.74	102.65	106.78
28	DB	1001	CYC	C4A-C3A-C2A	-3.74	102.22	106.51
26	t4	201	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	m1	202	PEB	CHA-C1B-NB	-3.74	117.12	124.93
26	AF	305	PEB	C3D-C4D-ND	3.74	114.59	107.26
26	ZG	201	PEB	C1C-CHB-C4B	-3.74	124.35	128.81
26	m6	203	PEB	C2A-C1A-NA	3.74	111.49	108.27
28	M2	1001	CYC	CMA-C3A-C4A	3.74	130.82	125.06
26	I1	201	PEB	C3D-C4D-ND	3.73	114.59	107.26
26	CG	202	PEB	C3D-C4D-ND	3.73	114.59	107.26
28	IB	1001	CYC	C2B-C1B-NB	3.73	112.45	106.99
26	OE	201	PEB	C1C-CHB-C4B	3.73	133.27	128.81
26	SD	202	PEB	OD-C4D-ND	-3.73	120.40	125.93
26	O7	203	PEB	OA-C1A-C2A	-3.73	123.20	126.17
26	JJ	202	PEB	CHA-C1B-NB	-3.73	117.12	124.93
26	M3	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	d4	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	g7	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	cA	203	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
26	XJ	202	PEB	CHA-C1B-NB	-3.73	117.12	124.93
26	k4	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	K5	201	PEB	OA-C1A-C2A	-3.73	123.20	126.17
26	bI	201	PEB	OA-C1A-C2A	-3.73	123.20	126.17
26	O9	201	PEB	C4B-C3B-C2B	-3.73	102.65	106.78
26	H1	203	PEB	CHC-C4C-C3C	-3.73	123.97	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CG	202	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
26	z4	202	PEB	CHC-C1D-ND	-3.73	109.61	113.95
26	ZG	201	PEB	C4B-C3B-C2B	-3.73	102.65	106.78
26	FD	201	PEB	C1C-CHB-C4B	3.73	133.27	128.81
26	gB	201	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
26	rG	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	PI	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	d8	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	U4	201	PEB	OA-C1A-C2A	-3.73	123.21	126.17
26	EE	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
26	RF	201	PEB	C3B-C4B-NB	3.73	115.48	110.05
26	11	203	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	P2	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
28	SH	1001	CYC	C4D-CHA-C1A	3.73	133.27	128.81
26	LC	203	PEB	C4B-C3B-C2B	-3.73	102.65	106.78
26	ME	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	AI	301	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
26	gI	202	PEB	CHC-C1D-ND	-3.73	109.61	113.95
27	K1	203	PUB	CHB-C1C-NC	-3.73	123.65	128.83
26	14	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	C3	201	PEB	CHA-C1B-C2B	3.73	134.49	124.90
26	eB	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	P7	201	PEB	CHA-C1B-NB	-3.73	117.13	124.93
26	UA	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	LC	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	i6	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	oG	201	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
26	U7	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
26	L1	203	PEB	CHC-C1D-ND	-3.73	109.62	113.95
27	NJ	201	PUB	CHA-C4A-NA	-3.73	109.62	113.95
26	cG	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	cI	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
26	gI	203	PEB	C3B-C4B-NB	3.73	115.47	110.05
26	K9	201	PEB	CHB-C4B-NB	-3.73	123.66	128.83
26	OF	202	PEB	CHA-C1B-NB	-3.73	117.13	124.93
28	LF	1001	CYC	C2C-C1C-NC	3.73	111.49	108.27
26	JE	202	PEB	C3B-C4B-NB	3.73	115.47	110.05
26	p1	201	PEB	CMB-C2B-C1B	3.73	130.81	125.06
26	z4	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
26	a6	202	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
26	GG	203	PEB	OD-C4D-ND	-3.73	120.41	125.93
28	DF	1003	CYC	CHB-C1B-NB	-3.73	118.06	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b2	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
26	Y9	202	PEB	CHC-C4C-C3C	-3.73	123.98	130.34
26	X9	203	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	PB	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
26	BD	201	PEB	CHC-C4C-C3C	-3.73	123.98	130.34
26	CA	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
26	MA	201	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
26	zG	501	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
26	E4	202	PEB	C3D-C4D-ND	3.73	114.57	107.26
26	aF	202	PEB	C3D-C4D-ND	3.73	114.57	107.26
26	gG	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
26	xG	302	PEB	CHC-C4C-C3C	-3.73	123.98	130.34
28	MB	1001	CYC	C1B-NB-C4B	-3.73	105.92	110.67
26	O4	201	PEB	C2A-C1A-NA	3.73	111.48	108.27
26	DD	203	PEB	C3D-C4D-ND	3.73	114.57	107.26
26	a8	204	PEB	CHC-C1D-ND	-3.73	109.62	113.95
26	D8	202	PEB	CHC-C4C-C3C	-3.73	123.98	130.34
26	AC	201	PEB	CHC-C4C-C3C	-3.73	123.98	130.34
26	JJ	201	PEB	OA-C1A-C2A	-3.73	123.21	126.17
26	i6	201	PEB	CHA-C1B-NB	-3.72	117.14	124.93
26	A4	201	PEB	CHB-C4B-NB	-3.72	123.66	128.83
27	yG	302	PUB	C1C-C2C-C3C	-3.72	102.66	106.78
27	xG	301	PUB	CMA-C2A-C1A	3.72	130.15	121.39
26	f1	201	PEB	OA-C1A-C2A	-3.72	123.21	126.17
26	d6	204	PEB	OA-C1A-C2A	-3.72	123.21	126.17
26	N9	203	PEB	OA-C1A-C2A	-3.72	123.21	126.17
26	HD	201	PEB	OD-C4D-ND	-3.72	120.41	125.93
26	O8	203	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	W3	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	F8	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	PF	201	PEB	CMB-C2B-C1B	3.72	130.80	125.06
26	g8	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	gA	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	w1	203	PEB	CHC-C1D-ND	-3.72	109.62	113.95
26	B9	201	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
26	W2	201	PEB	C4B-NB-C1B	-3.72	99.50	106.51
26	P3	202	PEB	C3B-C4B-NB	3.72	115.46	110.05
26	oG	201	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
26	VJ	203	PEB	OD-C4D-C3D	-3.72	121.03	129.46
26	K4	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	AB	301	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	vE	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KJ	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
26	W1	202	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
26	KD	202	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
28	DI	1001	CYC	C1B-NB-C4B	-3.72	105.93	110.67
26	a2	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	Z8	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	B4	203	PEB	CHB-C4B-NB	-3.72	123.67	128.83
26	h8	202	PEB	CHB-C4B-NB	-3.72	123.67	128.83
28	L6	1001	CYC	CHA-C1A-NA	-3.72	123.67	128.83
26	x4	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	I5	201	PEB	CHA-C1B-NB	-3.72	117.15	124.93
27	A1	203	PUB	C1C-C2C-C3C	-3.72	102.66	106.78
26	sE	201	PEB	C1C-CHB-C4B	3.72	133.25	128.81
28	KI	1001	CYC	C1B-C2B-C3B	-3.72	103.99	107.87
26	x1	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	AJ	304	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	eG	203	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
26	LD	201	PEB	CHC-C1D-ND	-3.72	109.63	113.95
26	RD	203	PEB	C1C-CHB-C4B	3.72	133.25	128.81
26	V6	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
28	mH	1001	CYC	CAB-C3B-C4B	3.72	127.25	121.38
26	s4	203	PEB	C3D-C4D-ND	3.72	114.56	107.26
28	EB	1001	CYC	C2B-C1B-NB	3.72	112.43	106.99
26	HD	203	PEB	CHC-C1D-ND	-3.72	109.63	113.95
26	UA	201	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
26	21	404	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	T4	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	G8	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	ED	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	qE	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	AG	201	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
26	eA	202	PEB	CMB-C2B-C1B	3.72	130.79	125.06
26	RA	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	fF	203	PEB	C3D-C4D-ND	3.72	114.56	107.26
26	O1	201	PEB	CHC-C1D-ND	-3.72	109.63	113.95
27	K1	203	PUB	C1C-C2C-C3C	-3.72	102.67	106.78
26	vG	201	PEB	CHB-C4B-NB	-3.72	123.67	128.83
26	X4	201	PEB	CMC-C3C-C2C	-3.72	117.93	124.94
26	B3	202	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	dE	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	K6	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	kG	202	PEB	C2A-C1A-NA	3.72	111.48	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mB	203	PEB	CHC-C1D-ND	-3.72	109.63	113.95
26	z1	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	IA	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	qG	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	gE	203	PEB	C1C-CHB-C4B	3.72	133.25	128.81
26	WB	202	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	WI	201	PEB	CHC-C4C-C3C	-3.72	124.00	130.34
26	T7	202	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	ME	203	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
26	gG	202	PEB	CHB-C4B-NB	-3.72	123.67	128.83
26	X9	201	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	k6	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	XJ	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	ND	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	w1	201	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
26	T7	201	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
26	H3	202	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	mB	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
26	kI	202	PEB	OA-C1A-C2A	-3.72	123.22	126.17
26	j1	201	PEB	CHC-C1D-ND	-3.72	109.63	113.95
26	N9	203	PEB	C3D-C4D-ND	3.72	114.55	107.26
26	K1	202	PEB	CHC-C4C-C3C	-3.71	124.00	130.34
26	S6	201	PEB	CHC-C4C-C3C	-3.71	124.00	130.34
26	XG	201	PEB	C4B-C3B-C2B	-3.71	102.67	106.78
26	D7	1002	PEB	C3D-C4D-ND	3.71	114.55	107.26
26	I5	203	PEB	CHA-C1B-NB	-3.71	117.16	124.93
26	PI	201	PEB	CHA-C1B-NB	-3.71	117.16	124.93
26	h7	203	PEB	C2A-C1A-NA	3.71	111.47	108.27
28	G2	1001	CYC	C2C-C1C-NC	3.71	111.47	108.27
28	IF	1001	CYC	C2C-C1C-NC	3.71	111.47	108.27
26	T9	203	PEB	C3D-C4D-ND	3.71	114.55	107.26
26	kE	202	PEB	C3D-C4D-ND	3.71	114.55	107.26
26	xE	302	PEB	C3D-C4D-ND	3.71	114.55	107.26
26	T1	201	PEB	OA-C1A-C2A	-3.71	123.22	126.17
26	R3	201	PEB	CAB-CBB-CGB	-3.71	105.61	113.60
26	TF	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
26	Q8	204	PEB	C1B-C2B-C3B	-3.71	102.24	106.51
26	m6	202	PEB	C3D-C4D-ND	3.71	114.55	107.26
26	QG	202	PEB	C1C-CHB-C4B	3.71	133.25	128.81
26	XG	202	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	LJ	202	PEB	OD-C4D-ND	-3.71	120.43	125.93
26	L4	201	PEB	C3D-C4D-ND	3.71	114.54	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H7	1002	PEB	C3D-C4D-ND	3.71	114.54	107.26
26	Y8	203	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	XG	203	PEB	CHB-C4B-C3B	-3.71	116.74	125.32
26	NG	202	PEB	C3B-C4B-NB	3.71	115.45	110.05
26	GG	201	PEB	C4B-C3B-C2B	-3.71	102.67	106.78
26	eA	201	PEB	C2A-C1A-NA	3.71	111.47	108.27
26	KE	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
26	pG	202	PEB	OD-C4D-ND	-3.71	120.43	125.93
26	P2	201	PEB	CMB-C2B-C1B	3.71	130.78	125.06
26	PB	201	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	ZF	202	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	VA	202	PEB	C3B-C4B-NB	3.71	115.45	110.05
26	G3	201	PEB	CHA-C1B-NB	-3.71	117.17	124.93
26	bE	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
28	CF	1001	CYC	C2B-C1B-NB	3.71	112.42	106.99
26	W4	201	PEB	CMB-C2B-C1B	3.71	130.78	125.06
28	K2	1001	CYC	C1B-C2B-C3B	-3.71	104.00	107.87
26	I9	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
26	P3	203	PEB	OA-C1A-C2A	-3.71	123.22	126.17
26	F4	203	PEB	OA-C1A-C2A	-3.71	123.22	126.17
26	N7	1002	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	M4	402	PEB	CMD-C2D-C3D	3.71	135.30	130.06
26	b7	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
26	GC	201	PEB	CHB-C4B-NB	-3.71	123.68	128.83
26	m2	201	PEB	C2A-C1A-NA	3.71	111.47	108.27
28	L7	1001	CYC	CMB-C2B-C1B	3.71	128.80	124.17
26	sE	201	PEB	CHA-C1B-NB	-3.71	117.17	124.93
26	ZF	202	PEB	C3D-C4D-ND	3.71	114.54	107.26
26	LI	1002	PEB	C3D-C4D-ND	3.71	114.54	107.26
26	GC	202	PEB	CMB-C2B-C1B	3.71	130.78	125.06
26	dF	201	PEB	C2A-C1A-NA	3.71	111.47	108.27
26	D8	202	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	CA	202	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	OE	203	PEB	CHC-C1D-ND	-3.71	109.64	113.95
26	QE	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
26	Z7	203	PEB	C1C-CHB-C4B	-3.71	124.38	128.81
26	T1	202	PEB	C3B-C4B-NB	3.71	115.44	110.05
26	bF	202	PEB	C3D-C4D-ND	3.71	114.53	107.26
26	WG	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
26	d7	201	PEB	C2A-C1A-NA	3.71	111.47	108.27
28	C2	1001	CYC	CBD-CAD-C3D	-3.71	106.29	112.62
26	mA	201	PEB	CAB-CBB-CGB	-3.71	105.63	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	wG	304	PUB	C4B-CHB-C1C	3.71	133.24	128.81
27	Y3	302	PUB	CHA-C1B-C2B	-3.71	124.02	130.34
26	TD	203	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
26	O1	202	PEB	CMB-C2B-C1B	3.71	130.77	125.06
26	Y9	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
26	EJ	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
26	i6	201	PEB	CHC-C4C-C3C	-3.71	124.02	130.34
26	oG	203	PEB	CHC-C4C-C3C	-3.71	124.02	130.34
26	p1	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
26	D3	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
28	MH	1001	CYC	CAB-C3B-C4B	3.71	127.23	121.38
28	EB	1001	CYC	OB-C4B-C3B	-3.71	124.02	128.04
26	J7	1002	PEB	C3D-C4D-ND	3.71	114.53	107.26
26	n1	201	PEB	C2A-C1A-NA	3.71	111.47	108.27
27	xE	306	PUB	CMA-C2A-C1A	3.70	130.10	121.39
28	H2	1001	CYC	C1B-C2B-C3B	-3.70	104.00	107.87
28	M6	1001	CYC	C1B-C2B-C3B	-3.70	104.00	107.87
28	I6	1001	CYC	C2B-C1B-NB	3.70	112.41	106.99
26	MD	201	PEB	OD-C4D-C3D	-3.70	121.07	129.46
26	Z1	202	PEB	C3D-C4D-ND	3.70	114.53	107.26
27	YD	302	PUB	C4B-CHB-C1C	3.70	133.23	128.81
28	GH	1001	CYC	C4D-CHA-C1A	3.70	133.23	128.81
28	M6	1001	CYC	C1B-NB-C4B	-3.70	105.95	110.67
26	Z2	201	PEB	C1B-C2B-C3B	-3.70	102.25	106.51
26	X8	202	PEB	CHC-C1D-ND	-3.70	109.65	113.95
26	r1	202	PEB	C3D-C4D-ND	3.70	114.53	107.26
26	N3	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
26	Z6	203	PEB	CHC-C4C-C3C	-3.70	124.02	130.34
26	Y3	303	PEB	OD-C4D-C3D	-3.70	121.07	129.46
26	V2	201	PEB	C2A-C1A-NA	3.70	111.47	108.27
26	XA	201	PEB	C2A-C1A-NA	3.70	111.47	108.27
26	Z7	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	OI	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	XJ	202	PEB	CHC-C4C-C3C	-3.70	124.02	130.34
26	W9	201	PEB	C3B-C4B-NB	3.70	115.43	110.05
26	jG	202	PEB	C3B-C4B-NB	3.70	115.43	110.05
26	S2	202	PEB	CHB-C4B-NB	-3.70	123.69	128.83
26	iA	202	PEB	CAA-C3A-C4A	3.70	122.18	112.67
26	m6	202	PEB	C2A-C1A-NA	3.70	111.46	108.27
26	K9	201	PEB	C2A-C1A-NA	3.70	111.46	108.27
26	QF	203	PEB	CHC-C4C-C3C	-3.70	124.02	130.34
26	ZI	201	PEB	CHC-C4C-C3C	-3.70	124.02	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T7	201	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	IJ	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
28	H2	1001	CYC	C1A-C2A-C3A	-3.70	102.69	106.78
26	Y6	201	PEB	CBC-CAC-C2C	3.70	118.94	112.62
26	R1	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	f8	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	D9	202	PEB	CHA-C4A-NA	3.70	129.60	125.20
26	c7	201	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	UI	202	PEB	CHC-C4C-C3C	-3.70	124.03	130.34
26	F9	202	PEB	CHA-C1B-NB	-3.70	117.19	124.93
26	e6	203	PEB	C2A-C1A-NA	3.70	111.46	108.27
26	QB	201	PEB	C3D-C4D-ND	3.70	114.52	107.26
28	K2	1001	CYC	CHB-C4A-NA	-3.70	117.19	124.93
26	14	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	A6	301	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	AG	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	e7	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	sE	203	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	N3	202	PEB	OD-C4D-ND	-3.70	120.45	125.93
26	DG	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
26	QG	202	PEB	CHB-C4B-NB	-3.70	123.70	128.83
26	k1	203	PEB	C2A-C1A-NA	3.70	111.46	108.27
26	AJ	301	PEB	CHC-C1D-ND	-3.70	109.65	113.95
26	W2	201	PEB	CHC-C4C-C3C	-3.70	124.03	130.34
26	JF	1002	PEB	C3D-C4D-ND	3.70	114.51	107.26
26	h6	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	AI	304	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	II	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	C5	204	PEB	CHB-C4B-NB	-3.70	123.70	128.83
26	Y8	202	PEB	CHB-C4B-NB	-3.70	123.70	128.83
26	PD	203	PEB	CHC-C4C-C3C	-3.70	124.03	130.34
26	d6	203	PEB	C3D-C4D-ND	3.70	114.51	107.26
26	OJ	201	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
28	K7	1001	CYC	CHB-C1B-NB	-3.70	118.12	126.06
26	k1	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	L4	203	PEB	C3D-C4D-ND	3.70	114.51	107.26
26	gA	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
26	a2	202	PEB	C2A-C1A-NA	3.70	111.46	108.27
26	fA	203	PEB	C3D-C4D-ND	3.70	114.51	107.26
26	jG	201	PEB	C3D-C4D-ND	3.70	114.51	107.26
26	PI	202	PEB	CMB-C2B-C1B	3.70	130.75	125.06
26	U1	202	PEB	CHC-C1D-ND	-3.70	109.66	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OF	202	PEB	C3D-C4D-ND	3.70	114.51	107.26
26	gI	202	PEB	C3D-C4D-ND	3.70	114.51	107.26
28	AH	1001	CYC	C1B-C2B-C3B	-3.70	104.02	107.87
26	TJ	201	PEB	OD-C4D-C3D	-3.70	121.09	129.46
26	L4	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
26	N3	203	PEB	C3B-C4B-NB	3.70	115.42	110.05
26	LE	202	PEB	C3B-C4B-NB	3.70	115.42	110.05
26	O7	202	PEB	CHC-C4C-C3C	-3.69	124.03	130.34
26	Q7	203	PEB	CHC-C4C-C3C	-3.69	124.03	130.34
26	I4	201	PEB	CHA-C1B-NB	-3.69	117.20	124.93
26	NE	201	PEB	CHA-C1B-NB	-3.69	117.20	124.93
26	PA	201	PEB	CBC-CAC-C2C	-3.69	106.31	112.62
26	hA	203	PEB	C3D-C4D-ND	3.69	114.51	107.26
26	q4	201	PEB	CHC-C4C-C3C	-3.69	124.04	130.34
26	jE	202	PEB	C3B-C4B-NB	3.69	115.42	110.05
26	GE	201	PEB	C3D-C4D-ND	3.69	114.51	107.26
26	O2	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
28	GH	1001	CYC	OC-C1C-C2C	-3.69	123.24	126.17
26	lB	201	PEB	C3D-C4D-ND	3.69	114.51	107.26
26	uG	201	PEB	C2A-C1A-NA	3.69	111.46	108.27
26	O2	201	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
26	UG	202	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
26	g1	203	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	S4	201	PEB	CHC-C4C-C3C	-3.69	124.04	130.34
26	H5	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
28	K7	1001	CYC	OC-C1C-C2C	-3.69	123.24	126.17
26	EJ	201	PEB	CHB-C4B-C3B	-3.69	116.79	125.32
26	X3	202	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
26	y1	203	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	A6	301	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	S3	201	PEB	OD-C4D-C3D	-3.69	121.09	129.46
26	D6	1002	PEB	CAB-C3B-C4B	3.69	131.54	125.01
26	P2	201	PEB	CHA-C1B-NB	-3.69	117.21	124.93
26	L4	203	PEB	CHC-C1D-ND	-3.69	109.66	113.95
26	D9	201	PEB	C3B-C4B-NB	3.69	115.42	110.05
26	AE	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	vE	201	PEB	CHA-C1B-NB	-3.69	117.21	124.93
26	OF	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
26	C3	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	F1	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	wE	302	PEB	CMB-C2B-C1B	3.69	130.75	125.06
26	P2	203	PEB	CAB-C3B-C4B	3.69	131.54	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V6	202	PEB	CHC-C4C-C3C	-3.69	124.04	130.34
26	X4	201	PEB	CHB-C4B-NB	-3.69	123.71	128.83
26	iE	201	PEB	CHC-C1D-ND	-3.69	109.66	113.95
26	I1	201	PEB	CHA-C1B-NB	-3.69	117.21	124.93
26	HD	203	PEB	C2A-C1A-NA	3.69	111.45	108.27
26	O3	201	PEB	CBA-CAA-C3A	-3.69	105.25	113.47
26	JD	203	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	gE	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	LB	1002	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
26	KE	203	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
26	N8	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	lF	202	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	Y4	201	PEB	C3B-C4B-NB	3.69	115.42	110.05
26	IE	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
26	gF	201	PEB	C2A-C1A-NA	3.69	111.45	108.27
26	X8	202	PEB	CHA-C1B-NB	-3.69	117.22	124.93
26	F1	202	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
26	YA	202	PEB	CHB-C4B-NB	-3.69	123.71	128.83
26	SI	202	PEB	CHB-C4B-NB	-3.69	123.71	128.83
28	eH	1001	CYC	CHA-C1A-NA	-3.69	123.71	128.83
26	B9	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
26	G1	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
26	JJ	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
26	L2	1002	PEB	C1C-CHB-C4B	3.69	133.21	128.81
26	f6	201	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
26	a1	203	PEB	C3D-C4D-ND	3.69	114.49	107.26
26	A7	301	PEB	CAA-C3A-C4A	-3.69	103.21	112.67
26	B4	201	PEB	C3B-C4B-NB	3.69	115.41	110.05
26	KE	203	PEB	C3B-C4B-NB	3.69	115.41	110.05
26	QG	201	PEB	C3B-C4B-NB	3.69	115.41	110.05
26	K3	201	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
26	e8	201	PEB	CHC-C1D-ND	3.69	118.23	113.95
26	TJ	203	PEB	C1C-CHB-C4B	-3.69	124.41	128.81
26	pG	202	PEB	CAB-C3B-C4B	3.69	131.53	125.01
26	CG	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
26	iE	202	PEB	C3B-C4B-NB	3.69	115.41	110.05
26	WE	202	PEB	C3D-C4D-ND	3.69	114.49	107.26
26	iE	202	PEB	CMB-C2B-C1B	3.69	130.74	125.06
26	ZI	201	PEB	C1B-C2B-C3B	-3.69	102.28	106.51
26	VD	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
26	gE	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
27	A7	304	PUB	CAC-C2C-C1C	3.69	131.53	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HE	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
26	X1	201	PEB	C4B-C3B-C2B	-3.68	102.70	106.78
26	F9	202	PEB	C4B-C3B-C2B	-3.68	102.70	106.78
26	SD	202	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
26	LC	203	PEB	CMB-C2B-C1B	3.68	130.74	125.06
26	s4	201	PEB	C3D-C4D-ND	3.68	114.49	107.26
26	d8	201	PEB	C3D-C4D-ND	3.68	114.49	107.26
26	bG	201	PEB	C3D-C4D-ND	3.68	114.49	107.26
26	mG	202	PEB	C3D-C4D-ND	3.68	114.49	107.26
26	U7	201	PEB	CMB-C2B-C1B	3.68	130.74	125.06
26	G5	201	PEB	CHB-C4B-NB	-3.68	123.72	128.83
26	N2	1002	PEB	C2A-C1A-NA	3.68	111.45	108.27
26	O1	201	PEB	CHB-C4B-C3B	-3.68	116.81	125.32
26	C3	202	PEB	C3B-C4B-NB	3.68	115.41	110.05
26	G9	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	YE	201	PEB	C1C-CHB-C4B	3.68	133.21	128.81
26	WB	203	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
26	K3	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
26	TB	201	PEB	C2A-C1A-NA	3.68	111.45	108.27
26	S4	201	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
26	dE	202	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	HC	203	PEB	CMB-C2B-C1B	3.68	130.73	125.06
26	cB	202	PEB	CHC-C4C-C3C	-3.68	124.06	130.34
26	T4	203	PEB	CHC-C1D-ND	-3.68	109.67	113.95
26	Q1	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
26	bG	202	PEB	CMC-C3C-C2C	-3.68	118.00	124.94
26	p4	201	PEB	C3D-C4D-ND	3.68	114.48	107.26
26	fB	203	PEB	C3D-C4D-ND	3.68	114.48	107.26
26	c2	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	dB	203	PEB	CHA-C1B-NB	-3.68	117.23	124.93
26	OB	202	PEB	CMB-C2B-C1B	3.68	130.73	125.06
26	C5	202	PEB	CHC-C4C-C3C	-3.68	124.06	130.34
26	R1	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
26	K4	201	PEB	CHC-C1D-ND	-3.68	109.67	113.95
26	HD	202	PEB	CHC-C1D-ND	-3.68	109.67	113.95
26	eI	203	PEB	CAB-C3B-C4B	3.68	131.52	125.01
28	D7	1001	CYC	CHB-C1B-NB	-3.68	118.16	126.06
26	QF	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
26	D4	203	PEB	CMB-C2B-C1B	3.68	130.73	125.06
26	j8	201	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
26	e8	201	PEB	C2A-C1A-NA	3.68	111.44	108.27
26	uG	201	PEB	C3D-C4D-ND	3.68	114.48	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V9	203	PEB	C1C-CHB-C4B	3.68	133.20	128.81
28	rH	1001	CYC	CAB-C3B-C4B	3.68	127.19	121.38
26	fI	201	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
26	f2	201	PEB	C3D-C4D-ND	3.68	114.47	107.26
26	a7	201	PEB	C3D-C4D-ND	3.68	114.47	107.26
26	a1	202	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
26	AC	203	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	YD	304	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	LJ	203	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	kE	201	PEB	CMB-C2B-C1B	3.68	130.73	125.06
26	mF	201	PEB	CHC-C1D-ND	-3.68	109.68	113.95
26	KE	201	PEB	CMA-C2A-C1A	-3.68	104.48	112.40
26	kI	202	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
26	E8	203	PEB	C3D-C4D-ND	3.68	114.47	107.26
26	b2	201	PEB	CMB-C2B-C1B	3.68	130.73	125.06
26	W7	202	PEB	CMB-C2B-C1B	3.68	130.73	125.06
26	sE	202	PEB	CHA-C1B-NB	-3.68	117.24	124.93
26	L1	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
26	Y7	201	PEB	C3D-C4D-ND	3.68	114.47	107.26
26	jB	201	PEB	OA-C1A-C2A	-3.68	123.25	126.17
26	SD	201	PEB	OD-C4D-C3D	-3.68	121.13	129.46
26	d6	203	PEB	CHA-C1B-NB	-3.68	117.24	124.93
26	GJ	202	PEB	CHC-C1D-ND	-3.68	109.68	113.95
26	HE	201	PEB	CMB-C2B-C1B	3.68	130.72	125.06
26	GE	203	PEB	OD-C4D-ND	-3.68	120.48	125.93
26	NG	201	PEB	CHA-C1B-NB	-3.68	117.25	124.93
26	AG	201	PEB	C4B-C3B-C2B	-3.68	102.72	106.78
26	WG	203	PEB	C4B-C3B-C2B	-3.68	102.72	106.78
26	Z6	203	PEB	OA-C1A-C2A	-3.67	123.25	126.17
26	WF	201	PEB	OA-C1A-C2A	-3.67	123.25	126.17
26	PI	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	X1	201	PEB	CMC-C3C-C2C	-3.67	118.01	124.94
26	w4	202	PEB	CAB-C3B-C4B	3.67	131.51	125.01
26	d1	202	PEB	C1B-C2B-C3B	-3.67	102.29	106.51
28	F2	1001	CYC	CBD-CAD-C3D	-3.67	106.35	112.62
26	K6	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
26	nE	202	PEB	OD-C4D-ND	-3.67	120.49	125.93
28	NB	1001	CYC	CAB-C3B-C4B	3.67	127.18	121.38
26	fI	201	PEB	C3D-C4D-ND	3.67	114.47	107.26
26	P2	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	ZF	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
26	qE	201	PEB	C1B-C2B-C3B	-3.67	102.29	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mE	202	PEB	CMB-C2B-C1B	3.67	130.72	125.06
26	z1	201	PEB	C3D-C4D-ND	3.67	114.47	107.26
26	jF	202	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
28	MH	1001	CYC	CMB-C2B-C1B	3.67	128.75	124.17
26	N9	204	PEB	C3D-C4D-ND	3.67	114.47	107.26
26	m4	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	VI	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	II	202	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	iE	201	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
26	eF	201	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
26	j1	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	IC	201	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	HD	203	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	H1	201	PEB	CHB-C4B-NB	-3.67	123.73	128.83
28	D2	1001	CYC	C1B-NB-C4B	-3.67	105.99	110.67
26	VD	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	eG	202	PEB	CHB-C4B-NB	-3.67	123.73	128.83
26	f7	201	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	aE	203	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	bF	203	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	HJ	201	PEB	C1B-C2B-C3B	-3.67	102.29	106.51
26	eE	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	aA	204	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
26	A1	201	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	PF	201	PEB	CHA-C1B-NB	-3.67	117.26	124.93
26	l1	201	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	L5	202	PEB	C4B-C3B-C2B	-3.67	102.72	106.78
26	WA	202	PEB	CHB-C4B-NB	-3.67	123.74	128.83
26	KC	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	gG	202	PEB	C2A-C1A-NA	3.67	111.44	108.27
26	GD	202	PEB	OA-C1A-C2A	-3.67	123.26	126.17
26	fA	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
26	V2	202	PEB	OD-C4D-C3D	-3.67	121.15	129.46
26	gB	201	PEB	CMB-C2B-C1B	3.67	130.71	125.06
26	dF	202	PEB	CMB-C2B-C1B	3.67	130.71	125.06
26	J3	202	PEB	C3B-C4B-NB	3.67	115.39	110.05
26	xG	302	PEB	CHA-C1B-NB	-3.67	117.26	124.93
26	hA	202	PEB	CHB-C4B-NB	-3.67	123.74	128.83
26	K5	202	PEB	CHC-C1D-ND	-3.67	109.69	113.95
28	IB	1001	CYC	CHB-C4A-NA	-3.67	117.26	124.93
26	H1	202	PEB	OA-C1A-C2A	-3.67	123.26	126.17
26	nE	201	PEB	OA-C1A-NA	3.67	129.38	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	MD	202	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	nG	201	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	S7	202	PEB	OA-C1A-C2A	-3.67	123.26	126.17
26	C8	203	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	GD	201	PEB	CMB-C2B-C1B	3.67	130.71	125.06
26	FD	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
26	F3	201	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	q4	202	PEB	CHC-C1D-ND	-3.67	109.69	113.95
26	mE	203	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	sE	202	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	XJ	201	PEB	C3D-C4D-ND	3.67	114.45	107.26
26	m4	201	PEB	C4B-C3B-C2B	-3.67	102.73	106.78
26	mI	202	PEB	C4B-C3B-C2B	-3.67	102.73	106.78
26	u1	201	PEB	CMB-C2B-C1B	3.67	130.71	125.06
26	YJ	201	PEB	OA-C1A-C2A	-3.66	123.26	126.17
26	H9	203	PEB	OD-C4D-ND	-3.66	120.50	125.93
26	B1	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	G9	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	FE	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	kG	202	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	y1	202	PEB	C2A-C1A-NA	3.66	111.43	108.27
26	N4	203	PEB	C2A-C1A-NA	3.66	111.43	108.27
26	TA	202	PEB	CAB-C3B-C4B	3.66	131.49	125.01
26	UJ	202	PEB	OD-C4D-ND	-3.66	120.50	125.93
26	fF	202	PEB	CMD-C2D-C3D	3.66	135.23	130.06
26	bI	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
26	Q4	202	PEB	CMB-C2B-C1B	3.66	130.71	125.06
26	B4	201	PEB	OA-C1A-C2A	-3.66	123.26	126.17
26	CE	201	PEB	OA-C1A-C2A	-3.66	123.26	126.17
26	a4	201	PEB	CHC-C1D-ND	-3.66	109.69	113.95
26	L2	1002	PEB	C2A-C1A-NA	3.66	111.43	108.27
26	P2	202	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
26	C3	202	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
26	J9	202	PEB	CHA-C1B-NB	-3.66	117.27	124.93
26	KB	201	PEB	CMB-C2B-C1B	3.66	130.71	125.06
26	K1	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	11	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	O7	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
26	k1	203	PEB	C1B-C2B-C3B	-3.66	102.30	106.51
26	ID	201	PEB	CHA-C1B-NB	-3.66	117.27	124.93
26	ZA	201	PEB	C3B-C4B-NB	3.66	115.38	110.05
26	DG	203	PEB	C3B-C4B-NB	3.66	115.38	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GB	1002	PEB	CAB-C3B-C2B	3.66	134.70	127.88
26	T9	202	PEB	C1C-CHB-C4B	3.66	133.18	128.81
26	cI	202	PEB	OA-C1A-C2A	-3.66	123.26	126.17
26	iI	201	PEB	C2A-C1A-NA	3.66	111.43	108.27
26	QG	201	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
26	RJ	202	PEB	CHA-C1B-NB	-3.66	117.27	124.93
26	lF	201	PEB	CHC-C1D-ND	-3.66	109.69	113.95
26	YE	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
26	ND	203	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
26	M8	203	PEB	C1B-C2B-C3B	-3.66	102.30	106.51
28	1H	1000	CYC	OC-C1C-C2C	-3.66	123.26	126.17
26	j6	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
26	e1	201	PEB	C2A-C1A-NA	3.66	111.43	108.27
28	HI	1001	CYC	CHA-C1A-NA	-3.66	123.75	128.83
26	HE	202	PEB	C3B-C4B-NB	3.66	115.37	110.05
26	aA	204	PEB	C1B-C2B-C3B	-3.66	102.31	106.51
26	GA	201	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
26	KG	203	PEB	OD-C4D-ND	-3.66	120.51	125.93
26	cB	201	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
26	Q4	201	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
26	I8	201	PEB	C3B-C4B-NB	3.66	115.37	110.05
26	f4	201	PEB	CHC-C1D-ND	-3.66	109.70	113.95
26	f6	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
26	g4	203	PEB	CHA-C1B-NB	-3.66	117.28	124.93
28	KI	1001	CYC	CHB-C4A-NA	-3.66	117.28	124.93
27	wE	304	PUB	CHC-C1D-ND	-3.66	109.09	113.72
28	CI	1001	CYC	C1B-C2B-C3B	-3.66	104.05	107.87
26	A2	305	PEB	OA-C1A-C2A	-3.66	123.26	126.17
26	QJ	202	PEB	OD-C4D-ND	-3.66	120.51	125.93
26	A3	201	PEB	CHB-C4B-NB	-3.66	123.75	128.83
26	aF	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
28	HF	1001	CYC	C1B-CHB-C4A	-3.66	119.14	128.08
28	UH	1001	CYC	CMB-C2B-C1B	3.66	128.74	124.17
26	y4	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
26	hB	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
26	eD	401	PEB	CMB-C2B-C1B	3.66	130.70	125.06
28	I2	1001	CYC	C1B-NB-C4B	-3.66	106.01	110.67
26	B9	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
26	CD	201	PEB	CHA-C1B-C2B	3.66	134.31	124.90
26	DE	203	PEB	CHB-C4B-C3B	-3.66	116.87	125.32
26	SF	202	PEB	CMB-C2B-C1B	3.66	130.70	125.06
26	BG	201	PEB	C4B-C3B-C2B	-3.66	102.73	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a8	202	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
26	OB	203	PEB	CHC-C1D-ND	-3.66	109.70	113.95
26	T4	202	PEB	C3B-C4B-NB	3.66	115.37	110.05
26	OG	201	PEB	C1B-C2B-C3B	-3.66	102.31	106.51
28	eH	1001	CYC	CBD-CAD-C3D	-3.66	106.38	112.62
26	TF	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
28	MI	1001	CYC	C1B-C2B-C3B	-3.66	104.06	107.87
26	S8	201	PEB	C1C-CHB-C4B	-3.66	124.44	128.81
28	fH	1001	CYC	C4D-CHA-C1A	3.66	133.18	128.81
26	c8	202	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
26	LC	202	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
26	h2	202	PEB	CHB-C4B-NB	-3.66	123.76	128.83
26	G3	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
26	P4	203	PEB	C3D-C4D-ND	3.66	114.43	107.26
26	l7	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
26	OB	203	PEB	C3D-C4D-ND	3.66	114.43	107.26
26	FA	201	PEB	C2A-C1A-NA	3.66	111.42	108.27
27	AF	304	PUB	OA-C1A-NA	-3.66	120.52	125.93
26	X4	201	PEB	C4B-C3B-C2B	-3.66	102.74	106.78
26	e7	201	PEB	C4B-C3B-C2B	-3.66	102.74	106.78
26	m6	201	PEB	CHB-C4B-NB	-3.65	123.76	128.83
26	g4	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
26	m6	201	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	cG	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	W9	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
26	iF	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
26	W6	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
26	nG	201	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
26	A3	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
26	JA	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
26	D3	203	PEB	C3D-C4D-ND	3.65	114.43	107.26
26	u4	203	PEB	C3D-C4D-ND	3.65	114.43	107.26
26	U1	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	EG	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	eG	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	N3	202	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
26	gB	202	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
26	s4	203	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
26	IC	201	PEB	CHA-C1B-NB	-3.65	117.29	124.93
26	CA	203	PEB	C3D-C4D-ND	3.65	114.43	107.26
26	jB	201	PEB	C3D-C4D-ND	3.65	114.43	107.26
26	TJ	203	PEB	C3D-C4D-ND	3.65	114.43	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h2	202	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	d6	202	PEB	CHB-C4B-NB	-3.65	123.76	128.83
26	B3	201	PEB	CHA-C4A-NA	3.65	129.55	125.20
26	H8	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
26	u4	203	PEB	CHA-C1B-NB	-3.65	117.29	124.93
28	II	1001	CYC	C1B-NB-C4B	-3.65	106.02	110.67
26	HD	202	PEB	CHA-C4A-NA	3.65	129.55	125.20
26	lG	201	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	TJ	202	PEB	C3B-C4B-NB	3.65	115.36	110.05
26	g7	202	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	KJ	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
27	AB	303	PUB	C1C-C2C-C3C	-3.65	102.74	106.78
26	R3	203	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	CG	203	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	QA	203	PEB	OD-C4D-ND	-3.65	120.52	125.93
26	a1	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	f7	201	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	fB	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	PI	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
26	YJ	201	PEB	C1C-CHB-C4B	3.65	133.17	128.81
26	L5	202	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	D4	203	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
26	RD	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	iE	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	X1	203	PEB	OD-C4D-ND	-3.65	120.52	125.93
26	O6	202	PEB	CMB-C2B-C1B	3.65	130.68	125.06
26	V6	201	PEB	CMB-C2B-C1B	3.65	130.68	125.06
26	D1	202	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	T9	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	qG	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	H5	201	PEB	CHB-C4B-NB	-3.65	123.77	128.83
26	QB	202	PEB	CHB-C4B-NB	-3.65	123.77	128.83
26	iG	201	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
26	P2	202	PEB	CMB-C2B-C1B	3.65	130.68	125.06
26	e4	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	I9	202	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
26	ZB	203	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
26	IC	202	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
26	SD	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	EA	203	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	c4	202	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
26	S4	201	PEB	CMB-C2B-C1B	3.65	130.68	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	WJ	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
26	Z1	202	PEB	C3B-C4B-NB	3.65	115.36	110.05
26	M4	401	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
28	SH	1001	CYC	OC-C1C-C2C	-3.65	123.27	126.17
26	NI	1002	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	aI	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
26	bE	201	PEB	CHB-C4B-NB	-3.65	123.77	128.83
26	LJ	203	PEB	CHB-C4B-NB	-3.65	123.77	128.83
26	x1	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
26	gF	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
26	S1	201	PEB	CHB-C4B-NB	-3.65	123.77	128.83
26	P8	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	ZB	203	PEB	OA-C1A-C2A	-3.65	123.27	126.17
26	QB	203	PEB	C3D-C4D-ND	3.65	114.41	107.26
26	VJ	203	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
26	nE	201	PEB	CAB-CBB-CGB	-3.65	105.76	113.60
26	SB	203	PEB	C4B-C3B-C2B	-3.65	102.75	106.78
26	lB	203	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
26	V2	202	PEB	C3B-C4B-NB	3.64	115.35	110.05
26	j7	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
26	E3	201	PEB	C1B-C2B-C3B	-3.64	102.32	106.51
26	Q9	202	PEB	C2A-C1A-NA	3.64	111.42	108.27
26	gE	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	M8	202	PEB	CMB-C2B-C1B	3.64	130.68	125.06
26	R4	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	m4	203	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	j6	201	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	k2	201	PEB	C3B-C4B-NB	3.64	115.35	110.05
26	F9	201	PEB	C1C-CHB-C4B	3.64	133.16	128.81
26	rG	202	PEB	C1B-C2B-C3B	-3.64	102.32	106.51
26	L4	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	j4	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	JJ	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	RB	202	PEB	CMB-C2B-C1B	3.64	130.68	125.06
26	bG	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
26	G3	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
26	zE	501	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
26	cF	201	PEB	C3B-C4B-NB	3.64	115.35	110.05
26	Q7	203	PEB	C3D-C4D-ND	3.64	114.41	107.26
26	RA	201	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
26	JF	1002	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
26	S7	202	PEB	CHA-C1B-NB	-3.64	117.31	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CD	201	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
28	G2	1001	CYC	CBD-CAD-C3D	-3.64	106.41	112.62
26	14	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	BD	201	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
26	n1	201	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	ED	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
26	Q6	203	PEB	CHC-C1D-ND	-3.64	109.72	113.95
26	IF	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	U3	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
26	LF	1002	PEB	C3B-C4B-NB	3.64	115.34	110.05
26	f7	202	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
26	g2	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
26	R3	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	b6	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	m2	203	PEB	CHC-C1D-ND	-3.64	109.72	113.95
26	T4	201	PEB	CHC-C1D-ND	-3.64	109.72	113.95
26	g6	201	PEB	C3B-C4B-NB	3.64	115.34	110.05
26	OG	203	PEB	C3B-C4B-NB	3.64	115.34	110.05
26	DI	1002	PEB	CHC-C4C-C3C	-3.64	124.13	130.34
26	qE	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	ND	202	PEB	OD-C4D-ND	-3.64	120.54	125.93
26	cA	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
26	PI	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
26	H4	202	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
26	m2	203	PEB	C3B-C4B-NB	3.64	115.34	110.05
26	n4	201	PEB	CAB-CBB-CGB	-3.64	105.77	113.60
26	FC	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
28	JI	1001	CYC	CHA-C1A-NA	-3.64	123.78	128.83
26	RJ	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	J2	1002	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
26	h2	202	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
26	cI	202	PEB	CMB-C2B-C1B	3.64	130.67	125.06
28	GI	1001	CYC	CHA-C1A-NA	-3.64	123.78	128.83
26	F4	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	O9	201	PEB	C3D-C4D-ND	3.64	114.40	107.26
26	O3	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
26	fF	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
26	JD	203	PEB	CAB-C3B-C4B	3.64	131.44	125.01
26	WA	203	PEB	CMB-C2B-C1B	3.64	130.66	125.06
26	L6	1002	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
26	FE	201	PEB	OD-C4D-ND	-3.64	120.54	125.93
26	v1	201	PEB	C2A-C1A-NA	3.64	111.41	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c1	201	PEB	C3D-C4D-ND	3.64	114.39	107.26
26	I5	201	PEB	C3D-C4D-ND	3.64	114.39	107.26
26	YD	303	PEB	C3D-C4D-ND	3.64	114.39	107.26
26	j2	201	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
26	T3	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
26	Q6	202	PEB	CHB-C4B-NB	-3.64	123.78	128.83
26	m2	202	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
26	sE	203	PEB	C4B-C3B-C2B	-3.64	102.76	106.78
26	XE	202	PEB	CHB-C4B-C3B	-3.64	116.92	125.32
26	T4	202	PEB	CHC-C4C-C3C	-3.64	124.14	130.34
26	BJ	203	PEB	C3D-C4D-ND	3.64	114.39	107.26
26	jG	201	PEB	OA-C1A-NA	3.63	129.34	124.94
26	l6	202	PEB	OA-C1A-C2A	-3.63	123.28	126.17
26	a4	201	PEB	C3D-C4D-ND	3.63	114.39	107.26
26	a8	204	PEB	C2A-C1A-NA	3.63	111.41	108.27
26	P9	201	PEB	C2A-C1A-NA	3.63	111.41	108.27
26	mF	202	PEB	CAA-C3A-C4A	3.63	122.00	112.67
26	SB	201	PEB	CHC-C1D-ND	-3.63	109.73	113.95
26	NJ	202	PEB	C3D-C4D-ND	3.63	114.39	107.26
26	e1	202	PEB	CHA-C1B-NB	-3.63	117.33	124.93
26	S6	203	PEB	C4B-C3B-C2B	-3.63	102.76	106.78
26	R9	203	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
26	H5	202	PEB	C2A-C1A-NA	3.63	111.41	108.27
26	A9	304	PEB	C3D-C4D-ND	3.63	114.39	107.26
26	VJ	202	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
26	L8	202	PEB	CHC-C1D-ND	-3.63	109.73	113.95
26	O6	202	PEB	C3D-C4D-ND	3.63	114.39	107.26
26	G8	201	PEB	CHA-C1B-C2B	3.63	134.24	124.90
26	W3	202	PEB	C2A-C1A-NA	3.63	111.40	108.27
26	f1	202	PEB	C3D-C4D-ND	3.63	114.39	107.26
26	KA	201	PEB	CHB-C4B-NB	-3.63	123.79	128.83
26	D4	201	PEB	CHC-C1D-ND	-3.63	109.73	113.95
26	a4	202	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
26	OB	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
28	GI	1001	CYC	CBD-CAD-C3D	-3.63	106.42	112.62
28	MI	1001	CYC	CMA-C3A-C4A	3.63	130.66	125.06
26	eG	203	PEB	CHB-C4B-NB	-3.63	123.79	128.83
26	PF	201	PEB	C3B-C4B-NB	3.63	115.33	110.05
26	X3	201	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
26	K9	201	PEB	OA-C1A-C2A	-3.63	123.29	126.17
26	ZI	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
26	oE	203	PEB	C3D-C4D-ND	3.63	114.38	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	iF	201	PEB	CHC-C1D-ND	-3.63	109.73	113.95
26	IJ	203	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
26	l4	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
28	C2	1001	CYC	C1B-NB-C4B	-3.63	106.05	110.67
26	SG	201	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
26	e1	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
26	s1	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
26	aB	202	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	PE	201	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	QA	204	PEB	C3B-C4B-NB	3.63	115.33	110.05
28	YH	1004	CYC	OC-C1C-C2C	-3.63	123.29	126.17
26	N1	203	PEB	CMC-C3C-C2C	-3.63	118.10	124.94
26	GE	201	PEB	CAA-C3A-C2A	3.63	123.33	114.26
26	BG	202	PEB	C3B-C4B-NB	3.63	115.33	110.05
26	Q4	201	PEB	CBC-CAC-C2C	-3.63	106.43	112.62
26	aI	202	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	c2	201	PEB	CHB-C4B-NB	-3.63	123.79	128.83
28	E6	1001	CYC	C2B-C1B-NB	3.63	112.30	106.99
26	eB	201	PEB	CMB-C2B-C1B	3.63	130.65	125.06
28	TH	1001	CYC	CHB-C4A-C3A	3.63	134.23	124.90
28	J7	1001	CYC	OC-C1C-C2C	-3.63	123.29	126.17
26	hI	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
26	D3	202	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
26	dB	201	PEB	CHC-C1D-ND	-3.63	109.73	113.95
26	G4	202	PEB	OD-C4D-ND	-3.63	120.56	125.93
26	e1	202	PEB	CHC-C4C-C3C	-3.63	124.15	130.34
26	T8	202	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	CA	203	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	W6	203	PEB	CMB-C2B-C1B	3.63	130.65	125.06
26	t1	202	PEB	CAB-C3B-C4B	3.63	131.43	125.01
26	Q2	202	PEB	CHB-C4B-NB	-3.63	123.80	128.83
26	J9	203	PEB	C3D-C4D-ND	3.63	114.38	107.26
26	PF	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
26	WG	202	PEB	C1C-CHB-C4B	3.63	133.14	128.81
26	iG	203	PEB	OA-C1A-C2A	-3.63	123.29	126.17
26	N7	1002	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	R6	201	PEB	CAB-CBB-CGB	-3.63	105.80	113.60
26	QG	201	PEB	C3D-C4D-ND	3.63	114.38	107.26
26	A3	201	PEB	OD-C4D-ND	-3.63	120.56	125.93
26	wE	301	PEB	OD-C4D-ND	-3.63	120.56	125.93
26	R3	203	PEB	OA-C1A-C2A	-3.63	123.29	126.17
26	Z6	203	PEB	C3D-C4D-ND	3.63	114.37	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	gG	202	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
26	oG	201	PEB	C4B-C3B-C2B	-3.63	102.77	106.78
26	WD	201	PEB	CHA-C1B-NB	-3.62	117.35	124.93
26	qE	201	PEB	C2A-C1A-NA	3.62	111.40	108.27
26	u1	203	PEB	C3D-C4D-ND	3.62	114.37	107.26
26	P6	201	PEB	CHC-C1D-ND	-3.62	109.74	113.95
27	21	403	PUB	CHA-C4A-NA	-3.62	109.74	113.95
26	C4	201	PEB	OA-C1A-C2A	-3.62	123.29	126.17
28	vH	1001	CYC	CHB-C4A-C3A	3.62	134.22	124.90
26	ND	202	PEB	CMB-C2B-C1B	3.62	130.65	125.06
26	YD	304	PEB	C4B-C3B-C2B	-3.62	102.77	106.78
26	xE	302	PEB	C4B-C3B-C2B	-3.62	102.77	106.78
26	f1	201	PEB	C3D-C4D-ND	3.62	114.37	107.26
26	XD	203	PEB	CBC-CAC-C2C	3.62	118.80	112.62
26	W3	201	PEB	CHB-C4B-NB	-3.62	123.80	128.83
26	J4	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
26	f7	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	D9	203	PEB	C3B-C4B-NB	3.62	115.32	110.05
26	qE	202	PEB	OD-C4D-ND	-3.62	120.56	125.93
26	J1	203	PEB	CHC-C1D-ND	-3.62	109.74	113.95
26	T1	202	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
26	c2	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
26	GD	201	PEB	OA-C1A-C2A	-3.62	123.29	126.17
26	pE	201	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
26	TG	201	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
26	c2	202	PEB	CHA-C1B-NB	-3.62	117.36	124.93
26	ZB	203	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	eF	201	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	LJ	201	PEB	CHA-C1B-NB	-3.62	117.36	124.93
26	SJ	201	PEB	CHB-C4B-C3B	-3.62	116.96	125.32
26	j2	201	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	j7	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	AG	201	PEB	CHB-C4B-NB	-3.62	123.81	128.83
26	H5	203	PEB	C2A-C1A-NA	3.62	111.39	108.27
26	YB	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
26	JA	202	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
26	fA	201	PEB	C4B-C3B-C2B	-3.62	102.78	106.78
26	C3	202	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
26	MA	203	PEB	C1B-C2B-C3B	-3.62	102.35	106.51
28	JI	1001	CYC	CMB-C2B-C1B	3.62	128.69	124.17
26	s4	203	PEB	OA-C1A-C2A	-3.62	123.30	126.17
26	JC	202	PEB	OA-C1A-C2A	-3.62	123.30	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	sE	203	PEB	C1C-CHB-C4B	3.62	133.13	128.81
26	e6	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
26	U2	201	PEB	C1B-C2B-C3B	-3.62	102.35	106.51
26	ZE	201	PEB	C1B-C2B-C3B	-3.62	102.35	106.51
26	ND	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	L3	202	PEB	CHA-C4A-NA	3.62	129.51	125.20
26	F8	201	PEB	OD-C4D-C3D	-3.62	121.26	129.46
26	iI	202	PEB	CMB-C2B-C1B	3.62	130.63	125.06
26	U2	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
26	w4	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
26	EA	203	PEB	C2A-C1A-NA	3.62	111.39	108.27
26	A7	301	PEB	C1B-C2B-C3B	-3.62	102.36	106.51
26	YE	203	PEB	C3D-C4D-ND	3.62	114.36	107.26
26	b7	202	PEB	CHA-C1B-NB	-3.62	117.37	124.93
26	m8	202	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
26	Y1	201	PEB	CMB-C2B-C1B	3.62	130.63	125.06
27	AA	303	PUB	CBA-CAA-C3A	-3.62	107.49	112.98
26	GJ	201	PEB	C3D-C4D-ND	3.62	114.35	107.26
26	S6	201	PEB	CHC-C1D-ND	-3.62	109.75	113.95
26	gB	202	PEB	CHC-C1D-ND	-3.62	109.75	113.95
26	cG	202	PEB	C1B-C2B-C3B	-3.62	102.36	106.51
26	R1	201	PEB	OD-C4D-ND	-3.62	120.57	125.93
26	aA	202	PEB	OA-C1A-C2A	-3.62	123.30	126.17
26	h6	202	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
26	PD	203	PEB	CAB-CBB-CGB	-3.62	105.82	113.60
26	24	404	PEB	CHA-C1B-C2B	3.62	134.20	124.90
26	A6	304	PEB	CMB-C2B-C1B	3.62	130.63	125.06
26	T1	202	PEB	CHC-C1D-ND	-3.62	109.75	113.95
26	c2	201	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
26	UE	202	PEB	C1B-C2B-C3B	-3.62	102.36	106.51
26	W7	202	PEB	C3D-C4D-ND	3.62	114.35	107.26
26	dF	203	PEB	C3D-C4D-ND	3.61	114.35	107.26
26	R7	201	PEB	OA-C1A-C2A	-3.61	123.30	126.17
26	H1	203	PEB	C2A-C1A-NA	3.61	111.39	108.27
26	g4	203	PEB	C2A-C1A-NA	3.61	111.39	108.27
26	QF	203	PEB	C2A-C1A-NA	3.61	111.39	108.27
26	GJ	201	PEB	CHB-C4B-NB	-3.61	123.81	128.83
26	YI	203	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
26	O7	202	PEB	CHA-C1B-NB	-3.61	117.37	124.93
26	SB	202	PEB	C3D-C4D-ND	3.61	114.35	107.26
28	FI	1001	CYC	CHA-C1A-NA	-3.61	123.81	128.83
26	f6	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IJ	201	PEB	C3D-C4D-ND	3.61	114.35	107.26
26	kE	202	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
26	m4	202	PEB	CHA-C1B-NB	-3.61	117.37	124.93
26	OE	201	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
26	N3	202	PEB	C3D-C4D-ND	3.61	114.35	107.26
28	C2	1001	CYC	C1B-C2B-C3B	-3.61	104.10	107.87
26	C8	203	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
26	FA	201	PEB	OD-C4D-C3D	-3.61	121.27	129.46
26	i4	201	PEB	C3D-C4D-ND	3.61	114.35	107.26
26	L9	201	PEB	CHA-C1B-NB	-3.61	117.38	124.93
28	I6	1001	CYC	CHB-C4A-NA	-3.61	117.38	124.93
26	i7	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
26	l7	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
26	LD	201	PEB	OA-C1A-C2A	-3.61	123.30	126.17
26	I9	202	PEB	C4B-C3B-C2B	-3.61	102.78	106.78
26	PJ	203	PEB	CMB-C2B-C1B	3.61	130.63	125.06
26	r1	202	PEB	CHA-C1B-NB	-3.61	117.38	124.93
26	bG	201	PEB	CHA-C1B-NB	-3.61	117.38	124.93
26	TF	201	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	O4	202	PEB	CMB-C2B-C1B	3.61	130.62	125.06
26	b2	201	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	FI	1002	PEB	OD-C4D-ND	-3.61	120.58	125.93
26	gG	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	L5	202	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	fF	201	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	a8	204	PEB	CMB-C2B-C1B	3.61	130.62	125.06
26	d6	201	PEB	CHC-C1D-ND	-3.61	109.75	113.95
26	YG	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	oG	203	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	k4	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
26	m4	202	PEB	C2A-C1A-NA	3.61	111.39	108.27
26	aI	202	PEB	C2A-C1A-NA	3.61	111.39	108.27
26	e4	202	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	NJ	202	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	cE	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	XJ	203	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	U7	202	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	r1	202	PEB	OD-C4D-ND	-3.61	120.58	125.93
26	Y1	202	PEB	CMB-C2B-C1B	3.61	130.62	125.06
26	PA	202	PEB	CMB-C2B-C1B	3.61	130.62	125.06
26	cG	201	PEB	C1B-C2B-C3B	-3.61	102.36	106.51
26	LI	1002	PEB	C2A-C1A-NA	3.61	111.38	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LC	201	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	H3	201	PEB	OD-C4D-ND	-3.61	120.58	125.93
26	YF	201	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	V2	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
26	U7	203	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
26	E3	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	cG	201	PEB	CMB-C2B-C1B	3.61	130.62	125.06
26	H1	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
26	aE	203	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
26	k7	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	zG	501	PEB	CHA-C1B-NB	-3.61	117.39	124.93
26	OF	202	PEB	C1B-C2B-C3B	-3.61	102.37	106.51
26	OF	201	PEB	OA-C1A-C2A	-3.61	123.31	126.17
26	I5	202	PEB	CHC-C4C-C3C	-3.61	124.19	130.34
26	MG	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
26	cE	201	PEB	CHB-C4B-C3B	-3.61	116.99	125.32
26	Z8	201	PEB	OD-C4D-ND	-3.61	120.59	125.93
26	kE	201	PEB	C3D-C4D-ND	3.61	114.33	107.26
26	SB	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
26	CG	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
26	dF	203	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
26	DJ	203	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
28	HF	1001	CYC	C1B-C2B-C3B	-3.61	104.11	107.87
26	DE	203	PEB	OA-C1A-C2A	-3.61	123.31	126.17
26	RF	201	PEB	OA-C1A-C2A	-3.61	123.31	126.17
26	Z1	202	PEB	CAA-C3A-C4A	3.61	121.93	112.67
28	CI	1001	CYC	C1B-NB-C4B	-3.61	106.08	110.67
26	U7	201	PEB	C3D-C4D-ND	3.60	114.33	107.26
26	U9	201	PEB	C3D-C4D-ND	3.60	114.33	107.26
26	P3	203	PEB	C4B-C3B-C2B	-3.60	102.79	106.78
26	IE	201	PEB	C2A-C3A-C4A	-3.60	95.94	101.34
26	h6	203	PEB	C3D-C4D-ND	3.60	114.33	107.26
26	RA	202	PEB	CAB-C3B-C4B	3.60	131.39	125.01
26	DG	201	PEB	OA-C1A-NA	3.60	129.31	124.94
26	f4	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	C8	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	hB	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	g6	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
26	bF	203	PEB	C1B-C2B-C3B	-3.60	102.37	106.51
26	OF	201	PEB	C3D-C4D-ND	3.60	114.33	107.26
26	Y2	203	PEB	CAB-C3B-C4B	3.60	131.38	125.01
26	A9	303	PEB	CBC-CAC-C2C	-3.60	106.47	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IJ	202	PEB	OD-C4D-ND	-3.60	120.59	125.93
28	GI	1001	CYC	C1B-C2B-C3B	-3.60	104.11	107.87
26	L3	203	PEB	C3D-C4D-ND	3.60	114.33	107.26
26	ZF	203	PEB	C3D-C4D-ND	3.60	114.33	107.26
26	W4	202	PEB	CHC-C4C-C3C	-3.60	124.19	130.34
26	LF	1002	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	pG	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	H3	202	PEB	CHC-C1D-ND	-3.60	109.76	113.95
26	uE	201	PEB	CHA-C1B-NB	-3.60	117.40	124.93
26	b6	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	IC	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	CD	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	T3	201	PEB	CHC-C1D-ND	-3.60	109.77	113.95
26	W6	201	PEB	CHC-C1D-ND	-3.60	109.77	113.95
26	WF	201	PEB	C1B-C2B-C3B	-3.60	102.37	106.51
26	v4	202	PEB	OD-C4D-ND	-3.60	120.59	125.93
26	GC	202	PEB	CHC-C4C-C3C	-3.60	124.19	130.34
26	A4	201	PEB	C3D-C4D-ND	3.60	114.32	107.26
26	K3	202	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	QG	202	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	gI	203	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	i6	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	SD	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	eG	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	TD	201	PEB	CHC-C1D-ND	-3.60	109.77	113.95
26	l2	201	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
26	jG	201	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
26	UA	202	PEB	CHA-C1B-C2B	3.60	134.16	124.90
26	dG	201	PEB	CHA-C1B-NB	-3.60	117.40	124.93
26	EG	201	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	WA	202	PEB	OD-C4D-C3D	-3.60	121.30	129.46
26	dA	201	PEB	CHA-C1B-NB	-3.60	117.40	124.93
26	S6	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
28	G7	1001	CYC	OC-C1C-C2C	-3.60	123.31	126.17
26	k1	201	PEB	CAB-CBB-CGB	-3.60	105.86	113.60
26	R7	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
26	f8	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
28	LI	1001	CYC	C2C-C1C-NC	3.60	111.38	108.27
26	u1	201	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	K8	203	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	KA	203	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	RI	201	PEB	OD-C4D-ND	-3.60	120.60	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C8	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
26	Q8	204	PEB	C2A-C1A-NA	3.60	111.38	108.27
28	H2	1001	CYC	C2C-C1C-NC	3.60	111.38	108.27
26	i2	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	LG	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
28	EF	1001	CYC	C2A-C1A-NA	3.60	115.28	110.05
27	xE	301	PUB	CHC-C1D-ND	-3.60	109.17	113.72
26	oE	201	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
26	NE	202	PEB	CHB-C4B-C3B	-3.60	117.01	125.32
26	b6	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
26	J3	203	PEB	C3D-C4D-ND	3.60	114.32	107.26
26	k1	202	PEB	C2A-C1A-NA	3.60	111.37	108.27
26	DD	203	PEB	OA-C1A-C2A	-3.60	123.31	126.17
26	d2	201	PEB	C1B-C2B-C3B	-3.60	102.38	106.51
26	C8	203	PEB	CHA-C1B-NB	-3.60	117.41	124.93
26	dB	204	PEB	CHB-C4B-NB	-3.60	123.84	128.83
26	aI	201	PEB	C3B-C4B-NB	3.60	115.28	110.05
26	d7	202	PEB	C1B-C2B-C3B	-3.60	102.38	106.51
26	y4	203	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
26	Q6	203	PEB	C3D-C4D-ND	3.60	114.31	107.26
26	A5	202	PEB	CHB-C4B-NB	-3.60	123.84	128.83
27	K3	203	PUB	CHC-C1D-ND	-3.59	109.18	113.72
26	VF	201	PEB	CHA-C4A-NA	3.59	129.48	125.20
26	l7	203	PEB	OA-C1A-C2A	-3.59	123.31	126.17
26	a8	204	PEB	OA-C1A-C2A	-3.59	123.31	126.17
26	OG	202	PEB	CHA-C1B-NB	-3.59	117.41	124.93
26	m1	201	PEB	C1B-C2B-C3B	-3.59	102.38	106.51
26	QE	203	PEB	C1B-C2B-C3B	-3.59	102.38	106.51
28	IF	1001	CYC	C1B-NB-C4B	-3.59	106.09	110.67
26	mI	203	PEB	C3B-C4B-NB	3.59	115.28	110.05
26	n1	201	PEB	OD-C4D-ND	-3.59	120.61	125.93
26	lG	202	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	G9	202	PEB	C2A-C1A-NA	3.59	111.37	108.27
28	E6	1001	CYC	C2C-C1C-NC	3.59	111.37	108.27
26	q1	202	PEB	C1B-C2B-C3B	-3.59	102.38	106.51
28	KF	1001	CYC	C2A-C1A-NA	3.59	115.28	110.05
26	wG	302	PEB	OA-C1A-C2A	-3.59	123.32	126.17
26	E3	201	PEB	OD-C4D-ND	-3.59	120.61	125.93
26	UB	201	PEB	CHC-C1D-ND	-3.59	109.78	113.95
26	VJ	203	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	sG	201	PEB	CHA-C1B-NB	-3.59	117.42	124.93
26	rE	202	PEB	C1B-C2B-C3B	-3.59	102.38	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F5	201	PEB	CHB-C4B-NB	-3.59	123.84	128.83
26	N3	203	PEB	CAC-CBC-CGC	-3.59	103.69	113.76
26	UJ	201	PEB	CHA-C1B-NB	-3.59	117.42	124.93
26	J4	201	PEB	CHC-C4C-C3C	-3.59	124.21	130.34
27	wG	304	PUB	OD-C4D-ND	-3.59	120.61	125.93
28	I7	1001	CYC	CHB-C4A-NA	-3.59	117.42	124.93
26	E9	202	PEB	C2A-C1A-NA	3.59	111.37	108.27
26	a6	201	PEB	C3B-C4B-NB	3.59	115.27	110.05
26	Q4	202	PEB	OD-C4D-ND	-3.59	120.61	125.93
26	SE	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	TJ	203	PEB	OA-C1A-C2A	-3.59	123.32	126.17
26	t4	201	PEB	CAB-CBB-CGB	-3.59	105.88	113.60
26	RD	203	PEB	C3D-C4D-ND	3.59	114.30	107.26
26	H1	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	V9	203	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
27	wE	304	PUB	C1C-C2C-C3C	-3.59	102.81	106.78
26	r1	201	PEB	CBA-CAA-C3A	3.59	121.46	113.47
26	WF	201	PEB	CHA-C1B-NB	-3.59	117.42	124.93
26	E1	202	PEB	OA-C1A-C2A	-3.59	123.32	126.17
26	K9	202	PEB	OA-C1A-C2A	-3.59	123.32	126.17
26	P3	203	PEB	CHC-C4C-C3C	-3.59	124.22	130.34
26	g6	202	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	kF	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	U4	201	PEB	CMB-C2B-C1B	3.59	130.59	125.06
26	s4	201	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
26	l8	201	PEB	C1B-C2B-C3B	-3.59	102.39	106.51
26	Q1	202	PEB	OD-C4D-ND	-3.59	120.61	125.93
26	YA	202	PEB	CHA-C1B-C2B	3.59	134.13	124.90
26	C9	201	PEB	CHB-C4B-C3B	-3.59	117.03	125.32
26	SG	203	PEB	CHB-C4B-NB	-3.59	123.85	128.83
27	wE	304	PUB	CHB-C1C-NC	-3.59	123.85	128.83
26	Y8	202	PEB	CHA-C1B-C2B	3.59	134.13	124.90
26	AE	202	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	eI	203	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
26	WA	203	PEB	C2A-C1A-NA	3.59	111.37	108.27
26	e4	201	PEB	CHB-C4B-NB	-3.59	123.85	128.83
26	B3	201	PEB	CHC-C4C-C3C	-3.59	124.22	130.34
26	jB	202	PEB	C3D-C4D-ND	3.59	114.30	107.26
26	mB	202	PEB	C3D-C4D-ND	3.59	114.30	107.26
26	UE	203	PEB	C3D-C4D-ND	3.59	114.30	107.26
26	u1	201	PEB	CHB-C4B-C3B	-3.59	117.03	125.32
26	JJ	203	PEB	C3D-C4D-ND	3.59	114.30	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KD	201	PEB	CHC-C4C-C3C	-3.59	124.22	130.34
26	NE	202	PEB	C3B-C4B-NB	3.59	115.27	110.05
26	y4	201	PEB	CAB-C3B-C4B	3.59	131.35	125.01
26	uG	201	PEB	OD-C4D-C3D	-3.59	121.33	129.46
26	aB	201	PEB	CHC-C1D-ND	-3.59	109.78	113.95
28	G6	1001	CYC	CHB-C4A-NA	-3.59	117.43	124.93
26	G4	201	PEB	C3D-C4D-ND	3.59	114.29	107.26
26	U9	201	PEB	C2A-C1A-NA	3.59	111.36	108.27
28	dH	1001	CYC	C4A-C3A-C2A	-3.59	102.39	106.51
26	YG	203	PEB	CHA-C1B-C2B	3.58	134.12	124.90
27	A8	304	PUB	OD-C4D-ND	-3.58	120.62	125.93
26	a1	201	PEB	CHA-C1B-C2B	3.58	134.12	124.90
26	X1	203	PEB	C3D-C4D-ND	3.58	114.29	107.26
26	dI	202	PEB	OA-C1A-C2A	-3.58	123.32	126.17
26	eE	202	PEB	C3B-C4B-NB	3.58	115.26	110.05
26	P9	202	PEB	CHB-C4B-NB	-3.58	123.86	128.83
26	S9	201	PEB	CHB-C4B-C3B	-3.58	117.04	125.32
26	Y1	201	PEB	CHC-C4C-C3C	-3.58	124.22	130.34
26	Q1	202	PEB	CMB-C2B-C1B	3.58	130.58	125.06
28	J7	1001	CYC	C1B-NB-C4B	-3.58	106.11	110.67
27	N9	201	PUB	OA-C1A-NA	-3.58	120.62	125.93
26	R8	201	PEB	C3D-C4D-ND	3.58	114.29	107.26
26	DE	201	PEB	C3D-C4D-ND	3.58	114.29	107.26
26	TB	202	PEB	CHC-C4C-C3C	-3.58	124.22	130.34
26	c1	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
26	e4	201	PEB	OA-C1A-C2A	-3.58	123.32	126.17
26	QE	202	PEB	OA-C1A-C2A	-3.58	123.32	126.17
26	X1	202	PEB	C3B-C4B-NB	3.58	115.26	110.05
26	U3	202	PEB	C1B-C2B-C3B	-3.58	102.39	106.51
26	SG	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
28	B6	1002	CYC	C4D-CHA-C1A	3.58	133.09	128.81
26	g2	201	PEB	CHB-C4B-NB	-3.58	123.86	128.83
26	d8	202	PEB	C3B-C4B-NB	3.58	115.26	110.05
26	ZF	202	PEB	C3B-C4B-NB	3.58	115.26	110.05
26	sE	203	PEB	CHA-C1B-NB	-3.58	117.44	124.93
26	M4	401	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	gE	201	PEB	CHA-C1B-C2B	3.58	134.11	124.90
26	D9	202	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
26	tG	202	PEB	CHB-C4B-C3B	-3.58	117.05	125.32
26	e2	201	PEB	CHA-C1B-NB	-3.58	117.44	124.93
26	Q8	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
26	R2	201	PEB	C3B-C4B-NB	3.58	115.26	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V2	203	PEB	CAB-CBB-CGB	3.58	121.31	113.60
26	h6	202	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	A7	302	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	K5	203	PEB	CHB-C4B-NB	-3.58	123.86	128.83
27	AB	303	PUB	CHB-C1C-NC	-3.58	123.86	128.83
26	RD	201	PEB	CAB-CBB-CGB	-3.58	105.90	113.60
26	j7	202	PEB	CHA-C4A-NA	-3.58	120.95	125.20
26	l7	203	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
26	YG	203	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
26	TA	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
26	xE	304	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
26	F4	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
26	KD	201	PEB	CMB-C2B-C1B	3.58	130.58	125.06
26	t1	201	PEB	CHB-C4B-NB	-3.58	123.86	128.83
26	f6	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
26	m2	203	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
26	i6	201	PEB	CMB-C2B-C1B	3.58	130.58	125.06
28	FI	1001	CYC	CMA-C3A-C4A	3.58	130.58	125.06
27	AA	303	PUB	C1C-C2C-C3C	-3.58	102.82	106.78
26	V9	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
26	R9	202	PEB	CHA-C1B-NB	-3.58	117.45	124.93
26	OA	202	PEB	C2A-C1A-NA	3.58	111.36	108.27
26	HJ	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
26	H4	203	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
26	hF	203	PEB	CHC-C1D-ND	-3.58	109.79	113.95
26	b7	202	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	gI	201	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	oE	203	PEB	C1C-CHB-C4B	3.58	133.08	128.81
26	OB	202	PEB	CHA-C1B-NB	-3.58	117.45	124.93
26	C5	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
26	vE	202	PEB	OD-C4D-ND	-3.58	120.63	125.93
26	d7	203	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
26	YD	303	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
26	B9	202	PEB	C3D-C4D-ND	3.58	114.28	107.26
26	pG	202	PEB	CMB-C2B-C1B	3.58	130.57	125.06
26	EE	201	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
26	Z8	202	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	dI	201	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	D8	202	PEB	CAB-C3B-C4B	3.58	131.34	125.01
27	xG	305	PUB	CHC-C1D-ND	-3.58	109.20	113.72
26	YF	202	PEB	CHC-C1D-ND	-3.58	109.79	113.95
26	hI	202	PEB	CHC-C1D-ND	-3.58	109.79	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m1	203	PEB	C3D-C4D-ND	3.58	114.28	107.26
26	YA	203	PEB	C2A-C1A-NA	3.58	111.36	108.27
26	GE	202	PEB	C2A-C3A-C4A	-3.58	95.98	101.34
26	WB	203	PEB	C3B-C4B-NB	3.58	115.25	110.05
26	eG	201	PEB	C3D-C4D-ND	3.58	114.28	107.26
26	PB	202	PEB	CBC-CAC-C2C	3.58	118.72	112.62
26	S9	201	PEB	OA-C1A-C2A	-3.58	123.33	126.17
26	xE	304	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
26	W6	203	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
26	QB	202	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
26	T2	203	PEB	CAB-C3B-C4B	3.58	131.33	125.01
26	WJ	202	PEB	CHB-C4B-NB	-3.57	123.87	128.83
26	a4	202	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
26	ED	201	PEB	C1C-CHB-C4B	3.57	133.08	128.81
26	eE	201	PEB	OA-C1A-C2A	-3.57	123.33	126.17
26	LD	202	PEB	C1B-C2B-C3B	-3.57	102.40	106.51
26	h1	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	O1	201	PEB	C3D-C4D-ND	3.57	114.27	107.26
28	HI	1001	CYC	CMB-C2B-C1B	3.57	128.63	124.17
26	PI	203	PEB	CHC-C4C-C3C	-3.57	124.24	130.34
26	P9	203	PEB	OA-C1A-C2A	-3.57	123.33	126.17
26	UB	201	PEB	OA-C1A-C2A	-3.57	123.33	126.17
26	i1	202	PEB	OD-C4D-ND	-3.57	120.64	125.93
26	oG	201	PEB	C3B-C4B-NB	3.57	115.25	110.05
26	JG	201	PEB	CAA-C3A-C2A	-3.57	105.33	114.26
26	Y7	202	PEB	CBC-CAC-C2C	-3.57	106.52	112.62
26	H1	202	PEB	OD-C4D-ND	-3.57	120.64	125.93
26	LJ	202	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
28	J2	1001	CYC	C2A-C1A-NA	3.57	115.25	110.05
26	d4	201	PEB	OA-C1A-C2A	-3.57	123.33	126.17
26	O6	202	PEB	OA-C1A-C2A	-3.57	123.33	126.17
26	cE	201	PEB	C3D-C4D-ND	3.57	114.27	107.26
26	WG	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	IC	201	PEB	CHC-C1D-ND	-3.57	109.80	113.95
26	l8	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
26	m7	202	PEB	CMB-C2B-C1B	3.57	130.56	125.06
26	v4	202	PEB	C3D-C4D-ND	3.57	114.27	107.26
26	C3	201	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
27	yG	302	PUB	CHA-C1B-C2B	-3.57	124.25	130.34
28	YH	1003	CYC	OC-C1C-C2C	-3.57	123.33	126.17
26	PF	202	PEB	CHC-C1D-ND	-3.57	109.80	113.95
26	CE	203	PEB	C2A-C1A-NA	3.57	111.35	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h8	203	PEB	C3D-C4D-ND	3.57	114.26	107.26
26	e6	201	PEB	CMB-C2B-C1B	3.57	130.56	125.06
26	m6	203	PEB	CHC-C4C-C3C	-3.57	124.25	130.34
27	AB	302	PUB	C1D-CHC-C4C	-3.57	105.60	113.37
27	xE	305	PUB	CHC-C1D-ND	-3.57	109.21	113.72
26	i8	201	PEB	CHA-C1B-NB	-3.57	117.47	124.93
26	Y1	202	PEB	CHC-C4C-C3C	-3.57	124.25	130.34
26	QF	203	PEB	C3D-C4D-ND	3.57	114.26	107.26
26	KG	203	PEB	C1C-CHB-C4B	3.57	133.07	128.81
26	H1	203	PEB	C1C-CHB-C4B	-3.57	124.55	128.81
26	a2	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
26	q1	203	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
26	LA	202	PEB	CAB-C3B-C4B	3.57	131.32	125.01
26	l2	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	T6	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	M1	402	PEB	CMD-C2D-C3D	3.57	135.10	130.06
26	aF	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
26	l4	202	PEB	OD-C4D-ND	-3.57	120.64	125.93
26	21	405	PEB	C3D-C4D-ND	3.57	114.26	107.26
26	RD	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	j6	202	PEB	OA-C1A-C2A	-3.57	123.34	126.17
26	OD	201	PEB	CBA-CAA-C3A	-3.57	105.53	113.47
26	k4	203	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
27	A6	302	PUB	C1D-CHC-C4C	-3.57	105.61	113.37
26	i8	202	PEB	CAA-C3A-C4A	3.57	121.83	112.67
26	w4	204	PEB	C3D-C4D-ND	3.57	114.26	107.26
26	eI	203	PEB	CHC-C1D-ND	-3.57	109.81	113.95
26	Z1	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	j1	201	PEB	C2A-C1A-NA	3.57	111.35	108.27
26	V9	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
26	aA	201	PEB	C4B-C3B-C2B	-3.57	102.84	106.78
26	uG	203	PEB	OA-C1A-C2A	-3.57	123.34	126.17
26	nE	201	PEB	C3D-C4D-ND	3.57	114.25	107.26
26	BJ	203	PEB	C3B-C4B-NB	3.57	115.23	110.05
26	NG	202	PEB	CHB-C4B-C3B	-3.57	117.08	125.32
26	P2	203	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
26	PI	202	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
26	T9	202	PEB	CHC-C4C-C3C	-3.56	124.26	130.34
26	AC	202	PEB	CHC-C4C-C3C	-3.56	124.26	130.34
26	m2	202	PEB	C3D-C4D-ND	3.56	114.25	107.26
26	aA	204	PEB	CHC-C1D-ND	-3.56	109.81	113.95
26	T1	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O8	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
26	OG	202	PEB	C3D-C4D-ND	3.56	114.25	107.26
26	rE	201	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
26	lF	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
26	M1	402	PEB	CMB-C2B-C1B	3.56	130.55	125.06
26	BD	203	PEB	C3D-C4D-ND	3.56	114.25	107.26
26	CJ	201	PEB	C3D-C4D-ND	3.56	114.25	107.26
26	kB	201	PEB	C1C-CHB-C4B	3.56	133.07	128.81
26	M4	401	PEB	C2A-C1A-NA	3.56	111.34	108.27
26	p1	201	PEB	CHA-C1B-NB	-3.56	117.48	124.93
26	G9	202	PEB	C3D-C4D-ND	3.56	114.25	107.26
26	O6	203	PEB	C3B-C4B-NB	3.56	115.23	110.05
26	e7	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
26	cI	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
28	D6	1001	CYC	CHB-C4A-NA	-3.56	117.48	124.93
26	J3	203	PEB	C1C-CHB-C4B	-3.56	124.55	128.81
26	l1	201	PEB	CHC-C1D-ND	-3.56	109.81	113.95
26	Y2	203	PEB	CHC-C1D-ND	-3.56	109.81	113.95
26	ZG	202	PEB	OD-C4D-ND	-3.56	120.65	125.93
26	V3	202	PEB	C3D-C4D-ND	3.56	114.25	107.26
26	kA	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
26	NG	201	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
26	ED	201	PEB	OD-C4D-ND	-3.56	120.65	125.93
26	HJ	201	PEB	OD-C4D-ND	-3.56	120.65	125.93
26	vE	202	PEB	CHC-C1D-ND	-3.56	109.81	113.95
28	CF	1001	CYC	OC-C1C-C2C	-3.56	123.34	126.17
26	G9	201	PEB	CMB-C2B-C1B	3.56	130.55	125.06
28	N2	1001	CYC	C2B-C1B-NB	3.56	112.20	106.99
26	sG	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
26	mG	203	PEB	CHC-C4C-C3C	-3.56	124.26	130.34
26	a4	203	PEB	C3B-C4B-NB	3.56	115.23	110.05
26	TB	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
26	T8	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
26	ZE	201	PEB	CHA-C1B-NB	-3.56	117.48	124.93
28	K2	1001	CYC	C1B-NB-C4B	-3.56	106.14	110.67
28	B6	1002	CYC	CHB-C1B-NB	-3.56	118.42	126.06
26	F1	203	PEB	C3D-C4D-ND	3.56	114.24	107.26
26	K6	201	PEB	CHC-C4C-C3C	-3.56	124.27	130.34
26	AF	302	PEB	CHA-C1B-NB	-3.56	117.49	124.93
26	i6	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
26	OA	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
26	m7	201	PEB	CMB-C2B-C1B	3.56	130.54	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	DE	201	PEB	CHB-C4B-NB	-3.56	123.89	128.83
26	VG	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
26	J7	1002	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
26	mI	203	PEB	CHC-C4C-C3C	-3.56	124.27	130.34
26	YE	203	PEB	OA-C1A-C2A	-3.56	123.34	126.17
28	IH	1001	CYC	OC-C1C-C2C	-3.56	123.34	126.17
26	LD	203	PEB	C3D-C4D-ND	3.56	114.24	107.26
26	KJ	202	PEB	CMB-C2B-C1B	3.56	130.54	125.06
28	EI	1001	CYC	C1B-NB-C4B	-3.56	106.14	110.67
26	FJ	201	PEB	CMA-C2A-C1A	-3.56	104.74	112.40
26	sE	203	PEB	OA-C1A-C2A	-3.56	123.34	126.17
26	F3	201	PEB	C4B-C3B-C2B	-3.56	102.85	106.78
26	bB	202	PEB	OD-C4D-ND	-3.56	120.66	125.93
26	UE	202	PEB	CMB-C2B-C1B	3.56	130.54	125.06
26	cF	201	PEB	C3D-C4D-ND	3.56	114.24	107.26
26	OF	201	PEB	C1C-CHB-C4B	3.56	133.06	128.81
26	DF	1002	PEB	CHC-C4C-C3C	-3.56	124.27	130.34
26	DD	202	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
26	v4	202	PEB	CHA-C1B-NB	-3.56	117.50	124.93
26	eB	203	PEB	OA-C1A-C2A	-3.56	123.35	126.17
26	rE	201	PEB	C3D-C4D-ND	3.56	114.23	107.26
26	UJ	201	PEB	C3D-C4D-ND	3.56	114.23	107.26
26	c6	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
26	h7	201	PEB	C1B-C2B-C3B	-3.56	102.43	106.51
26	aG	202	PEB	C1B-C2B-C3B	-3.56	102.43	106.51
26	T9	201	PEB	OD-C4D-C3D	-3.55	121.41	129.46
26	L8	202	PEB	CAB-C3B-C4B	3.55	131.30	125.01
26	U4	202	PEB	CMB-C2B-C1B	3.55	130.54	125.06
26	A5	201	PEB	C1C-CHB-C4B	3.55	133.06	128.81
26	GJ	202	PEB	C2A-C1A-NA	3.55	111.34	108.27
26	sE	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
26	K4	202	PEB	CHC-C4C-C3C	-3.55	124.28	130.34
26	HJ	202	PEB	CHC-C1D-ND	-3.55	109.82	113.95
26	LD	202	PEB	C3B-C4B-NB	3.55	115.22	110.05
26	EJ	201	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
26	R2	201	PEB	OD-C4D-ND	-3.55	120.67	125.93
26	G5	203	PEB	CHB-C4B-C3B	-3.55	117.11	125.32
26	l2	202	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
26	E8	201	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
27	KD	203	PUB	CHA-C4A-NA	-3.55	109.82	113.95
26	IG	203	PEB	OD-C4D-ND	-3.55	120.67	125.93
26	SA	201	PEB	C2A-C1A-NA	3.55	111.34	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OG	203	PEB	C2A-C1A-NA	3.55	111.34	108.27
26	DD	201	PEB	CAB-C3B-C4B	3.55	131.29	125.01
26	NJ	204	PEB	OA-C1A-C2A	-3.55	123.35	126.17
26	ID	202	PEB	C3D-C4D-ND	3.55	114.23	107.26
26	BE	202	PEB	C3B-C4B-NB	3.55	115.22	110.05
26	rE	202	PEB	CMB-C2B-C1B	3.55	130.53	125.06
26	k1	201	PEB	CHC-C4C-C3C	-3.55	124.28	130.34
26	21	401	PEB	C3D-C4D-ND	3.55	114.23	107.26
26	QE	203	PEB	C3D-C4D-ND	3.55	114.23	107.26
26	UF	202	PEB	CHC-C1D-ND	-3.55	109.82	113.95
26	ZF	201	PEB	CMB-C2B-C1B	3.55	130.53	125.06
26	T8	202	PEB	CAB-C3B-C4B	3.55	131.29	125.01
26	L4	201	PEB	OD-C4D-C3D	-3.55	121.41	129.46
26	aG	201	PEB	C3D-C4D-ND	3.55	114.23	107.26
28	uH	1001	CYC	CMC-C2C-C3C	3.55	128.15	113.83
26	g4	201	PEB	C1C-CHB-C4B	3.55	133.05	128.81
26	vE	201	PEB	C3D-C4D-ND	3.55	114.23	107.26
26	WG	203	PEB	CHC-C1D-ND	-3.55	109.82	113.95
26	F1	201	PEB	OD-C4D-ND	-3.55	120.67	125.93
26	PA	201	PEB	OD-C4D-ND	-3.55	120.67	125.93
26	G5	202	PEB	CHC-C4C-C3C	-3.55	124.28	130.34
28	H7	1001	CYC	CMA-C3A-C4A	3.55	130.53	125.06
26	UB	203	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	k1	203	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	D4	201	PEB	OA-C1A-C2A	-3.55	123.35	126.17
26	I9	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
27	yG	303	PUB	CHC-C1D-ND	-3.55	109.23	113.72
26	g1	202	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
26	L9	203	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	RI	201	PEB	C3B-C4B-NB	3.55	115.21	110.05
26	wE	303	PEB	C4B-C3B-C2B	-3.55	102.86	106.78
26	QA	202	PEB	CHA-C1B-NB	-3.55	117.51	124.93
26	J5	201	PEB	OD-C4D-ND	-3.55	120.67	125.93
26	CA	201	PEB	CMB-C2B-C1B	3.55	130.53	125.06
26	d8	203	PEB	CHC-C1D-ND	-3.55	109.83	113.95
26	aG	203	PEB	CHC-C1D-ND	-3.55	109.83	113.95
26	QJ	201	PEB	CHC-C1D-ND	-3.55	109.83	113.95
26	ID	202	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
26	WD	201	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
26	A3	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
26	f4	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	U9	202	PEB	OD-C4D-ND	-3.55	120.67	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OF	202	PEB	OD-C4D-ND	-3.55	120.67	125.93
26	X4	203	PEB	C4B-C3B-C2B	-3.55	102.86	106.78
28	KI	1001	CYC	CBD-CAD-C3D	-3.55	106.57	112.62
26	U6	201	PEB	CHB-C4B-NB	-3.55	123.91	128.83
26	f7	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
26	DE	202	PEB	C2A-C1A-NA	3.55	111.33	108.27
26	O6	203	PEB	CHC-C1D-ND	-3.55	109.83	113.95
26	CJ	202	PEB	CHC-C1D-ND	-3.55	109.83	113.95
26	OB	202	PEB	C1B-C2B-C3B	-3.55	102.44	106.51
26	m7	202	PEB	CHC-C4C-C3C	-3.55	124.29	130.34
26	IG	201	PEB	CAC-CBC-CGC	3.55	123.70	113.76
26	ME	202	PEB	CHB-C4B-NB	-3.55	123.91	128.83
26	PJ	202	PEB	CHC-C4C-C3C	-3.55	124.29	130.34
26	Q2	201	PEB	OD-C4D-ND	-3.55	120.68	125.93
26	E9	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	Z4	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
26	kI	201	PEB	C2A-C1A-NA	3.55	111.33	108.27
26	a8	204	PEB	C3B-C4B-NB	3.55	115.21	110.05
26	w1	201	PEB	OD-C4D-ND	-3.55	120.68	125.93
26	g1	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	J9	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	OE	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
26	K8	201	PEB	CHC-C4C-C3C	-3.55	124.29	130.34
26	jF	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
27	A1	203	PUB	OD-C4D-ND	-3.55	120.68	125.93
26	VF	203	PEB	C2A-C1A-NA	3.54	111.33	108.27
26	WB	203	PEB	CMB-C2B-C1B	3.54	130.52	125.06
26	UE	202	PEB	CHC-C4C-C3C	-3.54	124.29	130.34
26	S6	202	PEB	CHC-C1D-ND	-3.54	109.83	113.95
26	OB	203	PEB	C3B-C4B-NB	3.54	115.20	110.05
26	CG	202	PEB	C1C-CHB-C4B	3.54	133.04	128.81
26	S7	203	PEB	C3D-C4D-ND	3.54	114.21	107.26
26	CE	203	PEB	C3D-C4D-ND	3.54	114.21	107.26
26	T7	201	PEB	CHC-C4C-C3C	-3.54	124.29	130.34
26	I8	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
26	T8	201	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
26	QA	204	PEB	C2A-C1A-NA	3.54	111.33	108.27
26	V9	203	PEB	OD-C4D-C3D	-3.54	121.43	129.46
26	T6	202	PEB	CHC-C4C-C3C	-3.54	124.29	130.34
26	u4	201	PEB	CHB-C4B-C3B	-3.54	117.13	125.32
26	B3	203	PEB	C3D-C4D-ND	3.54	114.21	107.26
26	24	405	PEB	C3D-C4D-ND	3.54	114.21	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U9	201	PEB	CHB-C4B-NB	-3.54	123.91	128.83
26	NJ	203	PEB	OD-C4D-ND	-3.54	120.68	125.93
26	fF	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
28	KI	1001	CYC	C1B-NB-C4B	-3.54	106.16	110.67
26	f7	202	PEB	CMD-C2D-C3D	3.54	135.06	130.06
26	m7	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
26	FC	201	PEB	CHB-C4B-NB	-3.54	123.91	128.83
26	F5	201	PEB	CMB-C2B-C1B	3.54	130.52	125.06
26	FJ	202	PEB	C3D-C4D-ND	3.54	114.21	107.26
26	YJ	201	PEB	C3D-C4D-ND	3.54	114.21	107.26
26	H6	1002	PEB	CAB-C3B-C4B	3.54	131.28	125.01
26	Z2	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
28	vH	1001	CYC	OC-C1C-C2C	-3.54	123.36	126.17
26	fF	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
26	oG	203	PEB	C2A-C1A-NA	3.54	111.33	108.27
26	eI	201	PEB	CHA-C1B-NB	-3.54	117.53	124.93
26	o1	501	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
26	e2	203	PEB	CHC-C1D-ND	-3.54	109.83	113.95
26	V9	203	PEB	C1B-C2B-C3B	-3.54	102.44	106.51
26	UF	203	PEB	C3B-C4B-NB	3.54	115.20	110.05
26	KD	202	PEB	CHB-C4B-NB	-3.54	123.92	128.83
26	l7	203	PEB	C3D-C4D-ND	3.54	114.21	107.26
26	q1	203	PEB	OD-C4D-ND	-3.54	120.69	125.93
26	FC	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
26	HC	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
26	QJ	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
26	T4	201	PEB	C1C-CHB-C4B	3.54	133.04	128.81
26	G8	201	PEB	CHC-C4C-C3C	-3.54	124.30	130.34
26	H5	203	PEB	CMB-C2B-C1B	3.54	130.51	125.06
26	mF	202	PEB	CHB-C4B-NB	-3.54	123.92	128.83
26	W8	203	PEB	CHA-C1B-NB	-3.54	117.53	124.93
26	U1	201	PEB	CAB-C3B-C4B	3.54	131.27	125.01
26	KG	201	PEB	C2A-C1A-NA	3.54	111.32	108.27
28	DF	1001	CYC	C2C-C1C-NC	3.54	111.32	108.27
26	xG	302	PEB	OA-C1A-C2A	-3.54	123.36	126.17
26	GD	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
28	D7	1001	CYC	C4A-C3A-C2A	-3.54	102.44	106.51
26	WD	201	PEB	CMB-C2B-C1B	3.54	130.51	125.06
26	U6	202	PEB	CHC-C4C-C3C	-3.54	124.30	130.34
26	DG	201	PEB	C3D-C4D-ND	3.54	114.20	107.26
28	K6	202	CYC	C1B-C2B-C3B	-3.54	104.18	107.87
26	AE	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T2	201	PEB	CHC-C1D-ND	-3.54	109.84	113.95
26	jA	203	PEB	CHC-C1D-ND	-3.54	109.84	113.95
26	A8	301	PEB	CMB-C2B-C1B	3.54	130.51	125.06
26	iF	201	PEB	OD-C4D-ND	-3.54	120.69	125.93
26	PB	201	PEB	CAB-CBB-CGB	-3.54	105.99	113.60
26	V1	202	PEB	C3D-C4D-ND	3.54	114.20	107.26
26	L1	202	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
26	QA	202	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
26	gI	203	PEB	CHC-C4C-C3C	-3.54	124.30	130.34
26	R7	201	PEB	C3B-C4B-NB	3.54	115.19	110.05
26	mB	202	PEB	C2A-C1A-NA	3.54	111.32	108.27
26	oG	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
27	K4	203	PUB	CHC-C1D-ND	-3.54	109.25	113.72
26	W6	203	PEB	C3B-C4B-NB	3.54	115.19	110.05
26	QG	203	PEB	C3D-C4D-ND	3.54	114.20	107.26
26	d1	202	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
26	21	405	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
26	EJ	202	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
26	A3	202	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
26	P1	201	PEB	CMC-C3C-C2C	-3.54	118.28	124.94
26	wE	302	PEB	CHA-C1B-NB	-3.54	117.54	124.93
26	Y8	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
26	g4	203	PEB	CHC-C1D-ND	-3.54	109.84	113.95
26	g2	203	PEB	C3B-C4B-NB	3.53	115.19	110.05
27	A2	302	PUB	CHC-C1D-ND	-3.53	109.25	113.72
26	YB	202	PEB	C2A-C1A-NA	3.53	111.32	108.27
28	H7	1001	CYC	C2C-C1C-NC	3.53	111.32	108.27
26	HA	202	PEB	OD-C4D-ND	-3.53	120.69	125.93
26	UF	203	PEB	OD-C4D-ND	-3.53	120.69	125.93
26	YB	202	PEB	CHA-C1B-NB	-3.53	117.54	124.93
26	RG	202	PEB	CHB-C4B-C3B	-3.53	117.16	125.32
26	gE	201	PEB	OD-C4D-ND	-3.53	120.69	125.93
26	OF	203	PEB	C3D-C4D-ND	3.53	114.19	107.26
26	r1	202	PEB	C2A-C1A-NA	3.53	111.32	108.27
26	H4	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
26	EG	202	PEB	C2A-C1A-NA	3.53	111.32	108.27
27	wG	304	PUB	CBA-CAA-C3A	-3.53	107.62	112.98
26	iF	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
26	NG	202	PEB	CHC-C4C-C3C	3.53	136.36	130.34
26	f8	203	PEB	C3D-C4D-ND	3.53	114.19	107.26
26	cA	203	PEB	OA-C1A-C2A	-3.53	123.36	126.17
26	X4	202	PEB	C3B-C4B-NB	3.53	115.19	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OD	201	PEB	OD-C4D-ND	-3.53	120.70	125.93
27	AF	303	PUB	C1C-C2C-C3C	-3.53	102.87	106.78
26	G5	202	PEB	CHA-C1B-NB	-3.53	117.54	124.93
26	14	201	PEB	CHC-C4C-C3C	-3.53	124.31	130.34
26	X8	202	PEB	OD-C4D-ND	-3.53	120.70	125.93
26	OF	203	PEB	OA-C1A-C2A	-3.53	123.36	126.17
26	AI	301	PEB	OA-C1A-C2A	-3.53	123.36	126.17
26	OA	202	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
26	FE	201	PEB	C4B-C3B-C2B	-3.53	102.87	106.78
26	XE	201	PEB	C4B-C3B-C2B	-3.53	102.87	106.78
26	RG	202	PEB	C4B-C3B-C2B	-3.53	102.87	106.78
26	v1	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
26	YI	203	PEB	CHC-C1D-ND	-3.53	109.85	113.95
26	L5	202	PEB	CHA-C1B-NB	-3.53	117.55	124.93
26	bF	203	PEB	CHA-C1B-NB	-3.53	117.55	124.93
26	OE	202	PEB	C3B-C4B-NB	3.53	115.19	110.05
26	g2	201	PEB	OA-C1A-C2A	-3.53	123.37	126.17
26	V9	203	PEB	OA-C1A-C2A	-3.53	123.37	126.17
26	U8	202	PEB	CHA-C1B-C2B	3.53	133.98	124.90
26	UB	202	PEB	CHC-C4C-C3C	-3.53	124.32	130.34
26	GD	202	PEB	C3D-C4D-ND	3.53	114.19	107.26
26	sG	202	PEB	C3D-C4D-ND	3.53	114.19	107.26
26	a2	201	PEB	CHA-C1B-NB	-3.53	117.55	124.93
26	A7	301	PEB	C2A-C1A-NA	3.53	111.32	108.27
26	UG	201	PEB	C2A-C1A-NA	-3.53	105.23	108.27
26	Q3	202	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
26	RJ	202	PEB	CHC-C4C-C3C	-3.53	124.32	130.34
26	N4	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	ID	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
26	A8	302	PEB	OA-C1A-C2A	-3.53	123.37	126.17
26	EJ	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	ZF	202	PEB	C2A-C1A-NA	3.53	111.31	108.27
26	X1	203	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	H2	1002	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	xG	304	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	kA	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
26	V2	201	PEB	CHA-C1B-NB	-3.53	117.55	124.93
26	h7	203	PEB	CHC-C1D-ND	-3.53	109.85	113.95
27	21	402	PUB	OD-C4D-ND	-3.53	120.70	125.93
26	C8	201	PEB	C1B-C2B-C3B	-3.53	102.46	106.51
26	J1	201	PEB	CMB-C2B-C1B	3.53	130.50	125.06
26	Y4	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X1	203	PEB	C3B-C4B-NB	3.53	115.18	110.05
26	N1	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	S1	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	fA	203	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	a2	201	PEB	OD-C4D-ND	-3.53	120.70	125.93
26	dG	201	PEB	C2A-C1A-NA	3.53	111.31	108.27
27	K4	203	PUB	CMA-C2A-C1A	3.53	129.69	121.39
26	aG	203	PEB	C3D-C4D-ND	3.53	114.18	107.26
28	H2	1001	CYC	CMB-C2B-C1B	3.53	128.57	124.17
26	mG	201	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	XA	202	PEB	OD-C4D-ND	-3.53	120.70	125.93
26	P1	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	U4	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
28	E6	1001	CYC	OB-C4B-C3B	-3.53	124.21	128.04
26	m2	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
26	HB	1002	PEB	CAB-C3B-C4B	3.53	131.25	125.01
26	U6	203	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	r4	202	PEB	OD-C4D-ND	-3.53	120.71	125.93
26	u4	201	PEB	CBA-CAA-C3A	3.53	121.32	113.47
26	X1	202	PEB	CHB-C4B-C3B	-3.53	117.17	125.32
26	O7	203	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
26	RG	201	PEB	C1C-CHB-C4B	3.53	133.02	128.81
26	ED	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	D9	203	PEB	OD-C4D-ND	-3.53	120.71	125.93
28	N2	1001	CYC	CMB-C2B-C1B	3.53	128.57	124.17
26	WF	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
26	aB	201	PEB	CMB-C2B-C1B	3.53	130.49	125.06
26	IA	203	PEB	OA-C1A-C2A	-3.53	123.37	126.17
26	LC	203	PEB	C2A-C1A-NA	3.53	111.31	108.27
28	FB	1001	CYC	CHB-C4A-NA	-3.53	117.56	124.93
26	P1	203	PEB	C3D-C4D-ND	3.52	114.17	107.26
26	wG	302	PEB	CHA-C1B-NB	-3.52	117.56	124.93
26	I8	201	PEB	C3D-C4D-ND	3.52	114.17	107.26
28	DF	1001	CYC	C1B-NB-C4B	-3.52	106.18	110.67
26	k2	201	PEB	C2A-C1A-NA	3.52	111.31	108.27
28	I7	1001	CYC	C2C-C1C-NC	3.52	111.31	108.27
26	kI	203	PEB	CHC-C1D-ND	-3.52	109.86	113.95
26	T4	202	PEB	CHB-C4B-C3B	-3.52	117.18	125.32
26	TI	201	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	SG	202	PEB	CHB-C4B-NB	-3.52	123.94	128.83
26	w1	203	PEB	OD-C4D-ND	-3.52	120.71	125.93
26	dF	202	PEB	OD-C4D-ND	-3.52	120.71	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	WG	202	PEB	OD-C4D-ND	-3.52	120.71	125.93
26	BD	203	PEB	C4B-C3B-C2B	-3.52	102.88	106.78
26	M4	402	PEB	CHA-C1B-NB	-3.52	117.56	124.93
26	j8	201	PEB	CHC-C4C-C3C	-3.52	124.33	130.34
26	CD	202	PEB	CHC-C1D-ND	-3.52	109.86	113.95
26	n4	201	PEB	C2A-C1A-NA	3.52	111.31	108.27
26	LJ	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
28	G2	1001	CYC	C1B-C2B-C3B	-3.52	104.19	107.87
26	LB	1002	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	uE	202	PEB	CHC-C4C-C3C	-3.52	124.33	130.34
26	BD	203	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	I9	201	PEB	OD-C4D-ND	-3.52	120.71	125.93
26	uG	203	PEB	C3D-C4D-ND	3.52	114.17	107.26
26	r4	201	PEB	CBA-CAA-C3A	3.52	121.31	113.47
26	EG	201	PEB	CAB-C3B-C4B	3.52	131.24	125.01
26	W8	203	PEB	C2A-C1A-NA	3.52	111.31	108.27
26	IF	202	PEB	C2A-C1A-NA	3.52	111.31	108.27
26	PJ	201	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
26	M9	202	PEB	OA-C1A-C2A	-3.52	123.37	126.17
26	RD	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
26	UG	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
26	VF	202	PEB	C3D-C4D-ND	3.52	114.17	107.26
26	C8	203	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	vE	202	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	JF	1002	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	I3	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
26	Q8	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
26	F2	1002	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	f1	202	PEB	CHC-C4C-C3C	-3.52	124.33	130.34
26	N3	201	PEB	CHC-C4C-C3C	-3.52	124.33	130.34
26	WF	203	PEB	CMB-C2B-C1B	3.52	130.48	125.06
26	a6	201	PEB	CHC-C1D-ND	-3.52	109.86	113.95
26	OE	203	PEB	C3D-C4D-ND	3.52	114.16	107.26
26	f1	202	PEB	CHB-C4B-NB	-3.52	123.95	128.83
26	k2	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
28	E7	1001	CYC	C2C-C1C-NC	3.52	111.31	108.27
26	KA	202	PEB	CMB-C2B-C1B	3.52	130.48	125.06
26	P1	202	PEB	CHC-C1D-ND	-3.52	109.86	113.95
26	XJ	201	PEB	CHC-C1D-ND	-3.52	109.86	113.95
26	VI	201	PEB	CHA-C1B-NB	-3.52	117.57	124.93
26	c1	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
26	U9	202	PEB	OA-C1A-C2A	-3.52	123.38	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	jB	202	PEB	OA-C1A-C2A	-3.52	123.38	126.17
26	a1	203	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	ED	201	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
26	kE	202	PEB	C1C-CHB-C4B	-3.52	124.61	128.81
26	i1	203	PEB	C2A-C1A-NA	3.52	111.31	108.27
26	F3	201	PEB	C2A-C1A-NA	3.52	111.31	108.27
26	bF	202	PEB	C2A-C1A-NA	3.52	111.31	108.27
26	Y1	201	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	O4	201	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	aB	201	PEB	C3B-C4B-NB	3.52	115.17	110.05
26	c4	203	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
26	g6	201	PEB	CHC-C4C-C3C	-3.52	124.34	130.34
26	l8	201	PEB	CHA-C1B-NB	-3.52	117.58	124.93
26	SB	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
26	J9	202	PEB	C3B-C4B-NB	3.52	115.16	110.05
26	H8	202	PEB	OD-C4D-ND	-3.52	120.72	125.93
27	24	402	PUB	OD-C4D-ND	-3.52	120.72	125.93
26	iG	203	PEB	C3D-C4D-ND	3.52	114.16	107.26
26	F2	1002	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
28	LI	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
26	pE	201	PEB	OA-C1A-NA	3.52	129.20	124.94
26	VB	201	PEB	C3B-C4B-NB	3.51	115.16	110.05
26	jE	201	PEB	CHC-C4C-C3C	-3.51	124.34	130.34
27	yG	302	PUB	CBA-CAA-C3A	-3.51	107.65	112.98
26	fF	202	PEB	C3D-C4D-ND	3.51	114.16	107.26
26	24	401	PEB	CMB-C2B-C1B	3.51	130.48	125.06
26	FD	203	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
26	H5	203	PEB	OD-C4D-ND	-3.51	120.72	125.93
28	qH	1002	CYC	C2B-C1B-NB	3.51	112.13	106.99
26	QE	202	PEB	C3D-C4D-ND	3.51	114.15	107.26
26	WB	201	PEB	CHC-C1D-ND	-3.51	109.87	113.95
28	F6	1001	CYC	CHB-C4A-NA	-3.51	117.58	124.93
26	KE	201	PEB	C3B-C4B-NB	3.51	115.16	110.05
26	QE	201	PEB	OD-C4D-ND	-3.51	120.72	125.93
26	eG	203	PEB	OD-C4D-ND	-3.51	120.72	125.93
28	JF	1003	CYC	C1B-C2B-C3B	-3.51	104.20	107.87
26	FG	202	PEB	OD-C4D-ND	-3.51	120.73	125.93
26	D7	1002	PEB	CHC-C4C-C3C	-3.51	124.35	130.34
26	jA	201	PEB	CHC-C4C-C3C	-3.51	124.35	130.34
26	i1	201	PEB	C2A-C1A-NA	3.51	111.30	108.27
26	j4	201	PEB	C2A-C1A-NA	3.51	111.30	108.27
26	LC	202	PEB	C2A-C1A-NA	3.51	111.30	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K2	1001	CYC	CBD-CAD-C3D	-3.51	106.63	112.62
26	NJ	203	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
28	H2	1001	CYC	CHA-C1A-NA	-3.51	123.95	128.83
26	UG	202	PEB	CHC-C1D-ND	-3.51	109.87	113.95
26	gE	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
26	UE	203	PEB	C3B-C4B-NB	3.51	115.16	110.05
26	UJ	201	PEB	CHB-C4B-NB	-3.51	123.96	128.83
26	HI	1002	PEB	C2A-C1A-NA	3.51	111.30	108.27
26	aI	201	PEB	CHA-C1B-NB	-3.51	117.59	124.93
26	P6	201	PEB	CAB-CBB-CGB	-3.51	106.05	113.60
26	AJ	301	PEB	C3B-C4B-NB	3.51	115.16	110.05
26	l4	201	PEB	OD-C4D-ND	-3.51	120.73	125.93
26	IE	203	PEB	OD-C4D-ND	-3.51	120.73	125.93
26	N9	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	U3	201	PEB	CBB-CAB-C3B	-3.51	102.87	112.63
26	kA	201	PEB	OA-C1A-C2A	-3.51	123.38	126.17
26	gF	201	PEB	OA-C1A-C2A	-3.51	123.38	126.17
26	iB	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
26	HD	202	PEB	C3D-C4D-ND	3.51	114.15	107.26
26	D3	201	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	WF	201	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	EE	202	PEB	C3D-C4D-ND	3.51	114.14	107.26
26	EG	202	PEB	C3D-C4D-ND	3.51	114.14	107.26
26	EE	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
26	E9	201	PEB	OA-C1A-C2A	-3.51	123.38	126.17
26	YF	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
26	F3	201	PEB	OD-C4D-ND	-3.51	120.73	125.93
26	VD	201	PEB	CAC-CBC-CGC	-3.51	103.92	113.76
26	N1	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	S4	201	PEB	CHA-C1B-NB	-3.51	117.59	124.93
26	HJ	203	PEB	CMB-C2B-C1B	3.51	130.47	125.06
26	E9	201	PEB	CHB-C4B-C3B	-3.51	117.22	125.32
26	EE	201	PEB	C3B-C4B-NB	3.51	115.15	110.05
26	UG	202	PEB	CHC-C4C-C3C	-3.51	124.36	130.34
26	ND	202	PEB	CHA-C4A-NA	3.51	129.38	125.20
28	FB	1001	CYC	CMB-C2B-C1B	3.51	128.55	124.17
26	O3	202	PEB	CHB-C4B-NB	-3.51	123.96	128.83
26	R6	201	PEB	CHB-C4B-NB	-3.51	123.96	128.83
26	Y3	301	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	OB	201	PEB	CHA-C1B-NB	-3.51	117.60	124.93
26	h2	202	PEB	CHC-C1D-ND	-3.51	109.88	113.95
26	YA	202	PEB	OA-C1A-C2A	-3.51	123.39	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	VI	202	PEB	OA-C1A-C2A	-3.51	123.39	126.17
26	BJ	203	PEB	OA-C1A-C2A	-3.51	123.39	126.17
26	UB	201	PEB	CHB-C4B-NB	-3.51	123.96	128.83
28	EF	1001	CYC	C1B-C2B-C3B	-3.51	104.21	107.87
26	d1	201	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	e2	203	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	z4	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
26	G9	201	PEB	CAB-C3B-C4B	3.51	131.21	125.01
26	NF	1002	PEB	C3B-C4B-NB	3.51	115.15	110.05
26	D3	202	PEB	C1C-CHB-C4B	3.51	133.00	128.81
26	PJ	201	PEB	CHA-C1B-NB	-3.51	117.60	124.93
26	G3	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
26	KE	203	PEB	OD-C4D-ND	-3.51	120.74	125.93
26	yG	301	PEB	OD-C4D-ND	-3.51	120.74	125.93
26	X4	203	PEB	C3B-C4B-NB	3.51	115.15	110.05
26	BC	202	PEB	OA-C1A-C2A	-3.51	123.39	126.17
26	VD	203	PEB	C3D-C4D-ND	3.51	114.14	107.26
26	JJ	202	PEB	C3B-C4B-NB	3.50	115.15	110.05
26	X4	203	PEB	C3D-C4D-ND	3.50	114.14	107.26
26	Z7	203	PEB	CHA-C1B-C2B	3.50	133.91	124.90
26	e2	203	PEB	CAB-C3B-C4B	3.50	131.21	125.01
26	M4	402	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	tE	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	U6	201	PEB	C4B-C3B-C2B	-3.50	102.90	106.78
26	cG	201	PEB	C4B-C3B-C2B	-3.50	102.90	106.78
27	AJ	302	PUB	CHC-C1D-ND	-3.50	109.29	113.72
26	CE	201	PEB	C3B-C4B-NB	3.50	115.15	110.05
26	cA	203	PEB	CAB-C3B-C4B	3.50	131.21	125.01
26	A1	201	PEB	CHC-C4C-C3C	-3.50	124.36	130.34
26	U3	201	PEB	C1B-C2B-C3B	-3.50	102.48	106.51
26	PG	201	PEB	CHC-C1D-ND	-3.50	109.88	113.95
26	cE	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	uE	203	PEB	C3D-C4D-ND	3.50	114.13	107.26
26	X3	202	PEB	OD-C4D-C3D	-3.50	121.52	129.46
26	DG	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	BG	201	PEB	C1C-CHB-C4B	3.50	132.99	128.81
28	wH	1001	CYC	C4D-CHA-C1A	3.50	132.99	128.81
26	m1	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	J8	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	tE	202	PEB	CHC-C1D-ND	3.50	118.01	113.95
26	vG	201	PEB	C3D-C4D-ND	3.50	114.13	107.26
26	UB	202	PEB	OD-C4D-ND	-3.50	120.74	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t1	202	PEB	CHA-C1B-NB	-3.50	117.61	124.93
26	a6	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	ME	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	DA	201	PEB	CHC-C1D-ND	3.50	118.01	113.95
26	O1	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	eB	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	IJ	201	PEB	OD-C4D-ND	-3.50	120.74	125.93
26	XG	201	PEB	C1C-CHB-C4B	3.50	132.99	128.81
26	AG	202	PEB	C3D-C4D-ND	3.50	114.13	107.26
26	G5	203	PEB	OD-C4D-ND	-3.50	120.75	125.93
26	A9	304	PEB	OD-C4D-ND	-3.50	120.75	125.93
28	F6	1001	CYC	CMB-C2B-C1B	3.50	128.54	124.17
26	DA	202	PEB	CAA-C3A-C4A	3.50	121.66	112.67
26	r1	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	DG	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
28	CB	1001	CYC	C2C-C1C-NC	3.50	111.29	108.27
26	a2	203	PEB	CHC-C4C-C3C	-3.50	124.37	130.34
26	CC	202	PEB	CHC-C4C-C3C	-3.50	124.37	130.34
26	Z7	203	PEB	C3D-C4D-ND	3.50	114.12	107.26
26	V3	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
26	XD	201	PEB	CHA-C1B-NB	-3.50	117.61	124.93
26	zG	501	PEB	OD-C4D-ND	-3.50	120.75	125.93
26	JD	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
26	SE	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
28	DF	1003	CYC	CMB-C2B-C1B	3.50	128.54	124.17
26	uG	202	PEB	OA-C1A-C2A	-3.50	123.39	126.17
28	J2	1001	CYC	OC-C1C-C2C	-3.50	123.39	126.17
26	a4	203	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	DE	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	lF	201	PEB	CHA-C1B-NB	-3.50	117.61	124.93
28	CI	1001	CYC	C2C-C1C-NC	3.50	111.29	108.27
26	b2	202	PEB	CHB-C4B-NB	-3.50	123.97	128.83
26	T2	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
28	NB	1001	CYC	C2B-C1B-NB	3.50	112.11	106.99
26	O4	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	G5	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
26	AD	201	PEB	C1C-CHB-C4B	3.50	132.99	128.81
26	cF	201	PEB	CMB-C2B-C1B	3.50	130.45	125.06
26	RB	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
27	A6	303	PUB	C1C-C2C-C3C	-3.50	102.91	106.78
26	RB	201	PEB	CHA-C1B-NB	-3.50	117.62	124.93
26	r1	201	PEB	C1C-CHB-C4B	3.50	132.99	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J5	202	PEB	C1C-CHB-C4B	-3.50	124.63	128.81
26	qE	203	PEB	C3D-C4D-ND	3.50	114.12	107.26
26	DA	202	PEB	C3B-C4B-NB	3.50	115.14	110.05
26	q4	202	PEB	CHB-C4B-NB	-3.50	123.98	128.83
26	X9	203	PEB	C3D-C4D-ND	3.50	114.12	107.26
26	L7	1002	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
26	SF	201	PEB	CHA-C1B-C2B	3.50	133.89	124.90
26	KA	201	PEB	CHC-C1D-ND	-3.50	109.89	113.95
26	hB	202	PEB	CMB-C2B-C1B	3.50	130.45	125.06
26	dF	201	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
26	F9	201	PEB	CMA-C2A-C1A	-3.50	104.87	112.40
26	O7	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
28	JH	1001	CYC	OC-C1C-C2C	-3.50	123.39	126.17
26	fA	203	PEB	C2A-C1A-NA	3.50	111.29	108.27
26	CA	203	PEB	CHA-C1B-NB	-3.49	117.62	124.93
26	wE	302	PEB	C3D-C4D-ND	3.49	114.12	107.26
26	gF	201	PEB	C3D-C4D-ND	3.49	114.12	107.26
27	yE	302	PUB	OD-C4D-ND	-3.49	120.75	125.93
26	qG	202	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	S2	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	UI	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	A8	301	PEB	CHA-C1B-NB	-3.49	117.62	124.93
26	r4	201	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	hF	201	PEB	C3D-C4D-ND	3.49	114.11	107.26
26	F4	201	PEB	CHC-C1D-ND	-3.49	109.89	113.95
26	HA	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
26	PG	202	PEB	OA-C1A-C2A	-3.49	123.40	126.17
26	h8	201	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	U6	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
26	SD	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	J5	202	PEB	CBB-CAB-C3B	-3.49	102.92	112.63
26	C5	203	PEB	CHC-C4C-C3C	-3.49	124.38	130.34
26	j6	202	PEB	CHC-C4C-C3C	-3.49	124.38	130.34
26	Z6	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
26	h6	203	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	dF	202	PEB	CHA-C1B-NB	-3.49	117.63	124.93
26	O4	202	PEB	C2A-C1A-NA	3.49	111.28	108.27
26	A5	202	PEB	C2A-C1A-NA	3.49	111.28	108.27
26	CE	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
28	K7	1001	CYC	C4A-C3A-C2A	-3.49	102.50	106.51
26	WJ	202	PEB	CHC-C4C-C3C	-3.49	124.38	130.34
26	Q7	202	PEB	OA-C1A-C2A	-3.49	123.40	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A8	303	PUB	CBB-CAB-C3B	3.49	118.58	112.62
26	xG	302	PEB	C3D-C4D-ND	3.49	114.11	107.26
26	R2	202	PEB	CHA-C1B-NB	-3.49	117.63	124.93
26	dA	201	PEB	CHC-C4C-C3C	-3.49	124.38	130.34
26	QD	202	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	CG	203	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	b4	501	PEB	CHC-C4C-C3C	-3.49	124.38	130.34
26	GG	203	PEB	CHC-C4C-C3C	-3.49	124.38	130.34
28	G6	1001	CYC	C1B-C2B-C3B	-3.49	104.23	107.87
26	h7	202	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	I8	203	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	IG	201	PEB	CMB-C2B-C3B	-3.49	116.64	126.12
28	C6	1001	CYC	C2B-C1B-NB	3.49	112.10	106.99
26	H2	1002	PEB	C2A-C1A-NA	3.49	111.28	108.27
26	kF	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
28	F2	1001	CYC	C2C-C1C-NC	3.49	111.28	108.27
28	I2	1001	CYC	C2C-C1C-NC	3.49	111.28	108.27
28	C7	1001	CYC	C4A-C3A-C2A	-3.49	102.50	106.51
28	LB	1001	CYC	CAD-C3D-C2D	3.49	137.27	127.25
26	WA	203	PEB	CHA-C1B-NB	-3.49	117.64	124.93
26	O7	203	PEB	C3D-C4D-ND	3.49	114.10	107.26
28	GB	1001	CYC	C1B-C2B-C3B	-3.49	104.23	107.87
26	V9	201	PEB	C3B-C4B-NB	3.49	115.12	110.05
26	LF	1002	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	QB	202	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
26	r4	202	PEB	CHA-C1B-NB	-3.49	117.64	124.93
26	q4	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
26	eB	202	PEB	CHB-C4B-NB	-3.49	123.99	128.83
26	OG	203	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	R3	202	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
26	D4	203	PEB	OD-C4D-ND	-3.49	120.76	125.93
26	Y3	304	PEB	CMB-C2B-C1B	3.49	130.43	125.06
26	QE	202	PEB	CHC-C1D-ND	-3.49	109.90	113.95
26	CE	203	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
26	VI	202	PEB	OD-C4D-C3D	-3.49	121.56	129.46
26	T1	203	PEB	OA-C1A-C2A	-3.49	123.40	126.17
26	T1	201	PEB	C3B-C4B-NB	3.49	115.12	110.05
26	ME	203	PEB	C2A-C1A-NA	3.49	111.28	108.27
26	XJ	203	PEB	C2A-C1A-NA	3.49	111.28	108.27
26	J3	203	PEB	CAB-C3B-C4B	3.49	131.18	125.01
26	CA	203	PEB	C3B-C4B-NB	3.49	115.12	110.05
26	AB	301	PEB	C4B-C3B-C2B	-3.49	102.92	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TB	201	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	HC	203	PEB	C4B-C3B-C2B	-3.49	102.92	106.78
26	T1	203	PEB	C3D-C4D-ND	3.49	114.10	107.26
26	KD	201	PEB	C3D-C4D-ND	3.49	114.10	107.26
26	KB	201	PEB	CHC-C4C-C3C	-3.48	124.39	130.34
26	O8	203	PEB	C3B-C4B-NB	3.48	115.12	110.05
26	O8	202	PEB	C2A-C1A-NA	3.48	111.28	108.27
26	T9	203	PEB	C2A-C1A-NA	3.48	111.28	108.27
28	FI	1001	CYC	C2C-C1C-NC	3.48	111.28	108.27
26	A2	305	PEB	CHA-C1B-NB	-3.48	117.64	124.93
26	SB	202	PEB	CHB-C4B-NB	-3.48	123.99	128.83
26	kF	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
26	VD	203	PEB	CHC-C4C-C3C	-3.48	124.39	130.34
26	kF	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
26	NJ	204	PEB	C3D-C4D-ND	3.48	114.09	107.26
26	V2	202	PEB	CHC-C1D-ND	-3.48	109.90	113.95
26	s1	202	PEB	C2A-C1A-NA	3.48	111.28	108.27
26	A6	301	PEB	C2A-C1A-NA	3.48	111.28	108.27
26	L8	201	PEB	CMA-C2A-C1A	-3.48	104.89	112.40
26	C8	202	PEB	OD-C4D-ND	-3.48	120.77	125.93
27	yG	302	PUB	OD-C4D-ND	-3.48	120.77	125.93
26	Q6	202	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
26	NG	201	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
26	PD	202	PEB	C3B-C4B-NB	3.48	115.11	110.05
27	AA	304	PUB	CHB-C1C-NC	-3.48	124.00	128.83
28	EB	1001	CYC	CHB-C4A-NA	-3.48	117.65	124.93
26	P6	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
26	CE	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
26	MG	203	PEB	CMB-C2B-C1B	3.48	130.43	125.06
26	XA	202	PEB	C3B-C4B-NB	3.48	115.11	110.05
26	a8	204	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
26	IA	203	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
26	D1	201	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	F1	203	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	DI	1002	PEB	C1C-CHB-C4B	3.48	132.97	128.81
26	hB	202	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
26	xE	303	PEB	CHA-C1B-NB	-3.48	117.65	124.93
26	ZF	203	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	m7	202	PEB	CHB-C4B-NB	-3.48	124.00	128.83
26	V7	202	PEB	CHA-C4A-NA	3.48	129.34	125.20
26	G1	201	PEB	C3D-C4D-ND	3.48	114.09	107.26
26	OD	202	PEB	OA-C1A-C2A	-3.48	123.41	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UJ	201	PEB	OA-C1A-C2A	-3.48	123.41	126.17
26	WG	203	PEB	C2A-C1A-NA	3.48	111.27	108.27
26	aI	203	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
26	u4	202	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
26	GE	202	PEB	CHC-C1D-ND	-3.48	109.91	113.95
26	DE	203	PEB	C3B-C4B-NB	3.48	115.11	110.05
26	OE	203	PEB	C3B-C4B-NB	3.48	115.11	110.05
26	O8	203	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	dA	201	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	RD	203	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
26	BJ	202	PEB	CHB-C4B-NB	-3.48	124.00	128.83
26	B1	202	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	P4	201	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	AG	202	PEB	C4B-C3B-C2B	-3.48	102.93	106.78
26	GG	201	PEB	CHA-C1B-C2B	3.48	133.84	124.90
26	s1	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
26	Y4	201	PEB	OD-C4D-ND	-3.48	120.78	125.93
26	iB	201	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
26	kI	202	PEB	CHA-C1B-NB	-3.48	117.66	124.93
28	H7	1001	CYC	C1B-NB-C4B	-3.48	106.24	110.67
26	KA	201	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
26	P3	201	PEB	CBC-CAC-C2C	-3.48	106.69	112.62
26	g4	202	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
26	T8	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
26	GC	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
26	oG	203	PEB	C3B-C4B-NB	3.48	115.11	110.05
28	CB	1001	CYC	C2B-C1B-NB	3.48	112.08	106.99
26	A2	305	PEB	CMB-C2B-C1B	3.48	130.42	125.06
26	AD	201	PEB	CHA-C1B-NB	-3.48	117.66	124.93
26	d6	204	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
26	EE	202	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
26	V3	203	PEB	C3D-C4D-ND	3.48	114.08	107.26
26	DE	201	PEB	OA-C1A-NA	3.48	129.15	124.94
26	uE	201	PEB	C4B-C3B-C2B	-3.48	102.94	106.78
26	H9	203	PEB	C2A-C1A-NA	3.48	111.27	108.27
26	cB	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
28	C6	1001	CYC	C2C-C1C-NC	3.48	111.27	108.27
26	R1	201	PEB	C3B-C4B-NB	3.48	115.10	110.05
26	AB	301	PEB	OA-C1A-C2A	-3.47	123.41	126.17
26	X4	202	PEB	OD-C4D-ND	-3.47	120.78	125.93
26	u4	201	PEB	C3D-C4D-ND	3.47	114.08	107.26
26	N9	204	PEB	CHA-C1B-NB	-3.47	117.67	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S7	201	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	VG	202	PEB	OD-C4D-ND	-3.47	120.78	125.93
26	R9	203	PEB	C3D-C4D-ND	3.47	114.07	107.26
28	K7	1001	CYC	CHA-C1A-NA	-3.47	124.01	128.83
26	EA	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
26	yG	301	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	QF	203	PEB	CHA-C1B-NB	-3.47	117.67	124.93
26	c4	203	PEB	OD-C4D-ND	-3.47	120.78	125.93
26	UD	202	PEB	OD-C4D-ND	-3.47	120.78	125.93
26	sG	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
26	mG	201	PEB	CHA-C1B-C2B	3.47	133.83	124.90
27	K1	203	PUB	CMA-C2A-C1A	3.47	129.56	121.39
26	a6	201	PEB	CHB-C4B-NB	-3.47	124.01	128.83
26	f6	201	PEB	CHB-C4B-NB	-3.47	124.01	128.83
26	mE	203	PEB	CHB-C4B-NB	-3.47	124.01	128.83
28	L2	1001	CYC	C4D-CHA-C1A	3.47	132.96	128.81
26	q1	201	PEB	C3D-C4D-ND	3.47	114.07	107.26
26	J1	202	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	j7	201	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	sG	202	PEB	C2A-C1A-NA	3.47	111.27	108.27
27	AJ	302	PUB	CHB-C1C-NC	-3.47	124.01	128.83
26	p1	202	PEB	CAB-C3B-C4B	3.47	131.15	125.01
26	VI	201	PEB	C3B-C4B-NB	3.47	115.10	110.05
26	CG	202	PEB	CHB-C4B-C3B	-3.47	117.30	125.32
26	TI	202	PEB	CMB-C2B-C1B	3.47	130.41	125.06
26	B3	201	PEB	CHC-C1D-ND	-3.47	109.92	113.95
26	ME	202	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
26	G1	201	PEB	CHA-C1B-NB	-3.47	117.67	124.93
26	OD	201	PEB	CHA-C4A-NA	3.47	129.33	125.20
26	A8	302	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
26	D9	203	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
26	ZF	201	PEB	C3D-C4D-ND	3.47	114.07	107.26
26	a6	201	PEB	CMB-C2B-C1B	3.47	130.41	125.06
26	FC	203	PEB	CMB-C2B-C1B	3.47	130.41	125.06
26	M1	401	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	h7	202	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	YG	201	PEB	C2A-C1A-NA	3.47	111.27	108.27
26	EG	202	PEB	C1C-CHB-C4B	3.47	132.96	128.81
26	W7	203	PEB	CHA-C1B-NB	-3.47	117.67	124.93
28	sH	1001	CYC	CAA-C2A-C1A	3.47	131.15	125.01
26	WF	202	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
26	YJ	202	PEB	CHC-C4C-C3C	-3.47	124.42	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fB	201	PEB	CHB-C4B-NB	-3.47	124.01	128.83
26	ND	203	PEB	C3B-C4B-NB	3.47	115.10	110.05
26	GD	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
26	C8	203	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
26	ZG	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
26	P6	202	PEB	CBC-CAC-C2C	3.47	118.54	112.62
26	N9	204	PEB	C2A-C1A-NA	3.47	111.26	108.27
26	VJ	203	PEB	C3D-C4D-ND	3.47	114.07	107.26
28	GB	1001	CYC	C1B-NB-C4B	-3.47	106.25	110.67
26	O4	201	PEB	OD-C4D-ND	-3.47	120.79	125.93
26	KG	202	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
26	k4	202	PEB	OA-C1A-C2A	-3.47	123.42	126.17
26	BE	201	PEB	CHA-C1B-NB	-3.47	117.68	124.93
26	T4	203	PEB	C3D-C4D-ND	3.47	114.06	107.26
26	c4	203	PEB	CHA-C1B-NB	-3.47	117.68	124.93
26	T1	201	PEB	C1C-CHB-C4B	3.47	132.95	128.81
28	E2	1001	CYC	C1B-C2B-C3B	-3.47	104.25	107.87
26	GA	203	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
26	lA	201	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
26	DJ	202	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
28	CB	1001	CYC	CMB-C2B-C1B	3.47	128.50	124.17
26	Y9	201	PEB	C3D-C4D-ND	3.47	114.06	107.26
26	QE	203	PEB	CMB-C2B-C1B	3.47	130.40	125.06
26	kF	201	PEB	OA-C1A-C2A	-3.47	123.42	126.17
26	l1	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
26	T3	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
26	OG	203	PEB	CHC-C1D-ND	-3.47	109.92	113.95
26	R7	201	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
26	mB	203	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
26	BC	201	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
26	JE	202	PEB	CHA-C1B-NB	-3.47	117.68	124.93
28	L7	1001	CYC	C1B-NB-C4B	-3.47	106.25	110.67
26	l1	201	PEB	CHB-C4B-NB	-3.47	124.02	128.83
26	U8	203	PEB	C4B-C3B-C2B	-3.47	102.95	106.78
26	I3	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
26	F1	201	PEB	CHC-C1D-ND	-3.47	109.92	113.95
26	aE	201	PEB	OA-C1A-C2A	-3.47	123.42	126.17
26	LG	201	PEB	CHC-C4C-C3C	-3.47	124.43	130.34
26	IA	201	PEB	C3D-C4D-ND	3.47	114.06	107.26
26	WD	202	PEB	C2A-C1A-NA	3.46	111.26	108.27
26	c7	201	PEB	C3B-C4B-NB	3.46	115.09	110.05
26	KG	201	PEB	C3B-C4B-NB	3.46	115.09	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	rG	202	PEB	CHB-C4B-C3B	-3.46	117.32	125.32
26	a8	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
26	HD	203	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	Q8	204	PEB	CMB-C2B-C1B	3.46	130.40	125.06
26	B4	203	PEB	OD-C4D-ND	-3.46	120.80	125.93
26	yE	301	PEB	OD-C4D-ND	-3.46	120.80	125.93
28	II	1001	CYC	C2C-C1C-NC	3.46	111.26	108.27
26	R6	202	PEB	CMB-C2B-C1B	3.46	130.40	125.06
26	E9	202	PEB	CMB-C2B-C1B	3.46	130.40	125.06
28	N2	1001	CYC	OB-C4B-C3B	-3.46	124.28	128.04
26	14	201	PEB	OD-C4D-ND	-3.46	120.80	125.93
26	I8	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
26	V3	203	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	EG	202	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	Z7	201	PEB	C3D-C4D-ND	3.46	114.05	107.26
26	H4	201	PEB	CHB-C4B-NB	-3.46	124.02	128.83
26	GG	203	PEB	CHB-C4B-NB	-3.46	124.02	128.83
26	C4	202	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
26	WE	201	PEB	CMB-C2B-C1B	3.46	130.40	125.06
26	yE	301	PEB	CMB-C2B-C1B	3.46	130.40	125.06
26	SG	202	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	H4	202	PEB	C1C-CHB-C4B	3.46	132.94	128.81
26	t4	202	PEB	CAB-C3B-C4B	3.46	131.13	125.01
26	G8	203	PEB	C2A-C1A-NA	3.46	111.26	108.27
26	hI	202	PEB	C2A-C1A-NA	3.46	111.26	108.27
26	hB	203	PEB	OA-C1A-C2A	-3.46	123.42	126.17
26	sE	201	PEB	OA-C1A-C2A	-3.46	123.42	126.17
28	FI	1001	CYC	CHB-C4A-NA	-3.46	117.69	124.93
26	a1	201	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
26	Q1	202	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	m6	201	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	iB	201	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
26	c2	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
26	H4	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
26	V3	202	PEB	CHB-C4B-NB	-3.46	124.03	128.83
26	T1	202	PEB	CHB-C4B-C3B	-3.46	117.33	125.32
28	G7	1001	CYC	CMB-C2B-C1B	3.46	128.49	124.17
26	oE	202	PEB	C3D-C4D-ND	3.46	114.05	107.26
26	M9	201	PEB	C1C-CHB-C4B	3.46	132.94	128.81
26	mG	202	PEB	CHC-C4C-C3C	-3.46	124.44	130.34
26	V4	202	PEB	C2A-C1A-NA	3.46	111.26	108.27
26	dB	204	PEB	C1B-C2B-C3B	-3.46	102.53	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	QF	201	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
26	U4	201	PEB	OD-C4D-ND	-3.46	120.80	125.93
26	YD	301	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
26	Q8	204	PEB	C3B-C4B-NB	3.46	115.08	110.05
26	e1	201	PEB	OA-C1A-C2A	-3.46	123.42	126.17
26	d6	203	PEB	OA-C1A-C2A	-3.46	123.42	126.17
28	NI	1001	CYC	CMB-C2B-C1B	3.46	128.49	124.17
26	T2	202	PEB	CMB-C2B-C1B	3.46	130.39	125.06
26	k2	202	PEB	OD-C4D-C3D	-3.46	121.62	129.46
26	CC	201	PEB	CHC-C4C-C3C	-3.46	124.44	130.34
26	XJ	201	PEB	C2A-C1A-NA	3.46	111.25	108.27
26	G1	201	PEB	CBC-CAC-C2C	-3.46	106.72	112.62
28	LF	1001	CYC	CBD-CAD-C3D	3.46	118.52	112.62
26	E3	202	PEB	OA-C1A-C2A	-3.46	123.42	126.17
26	ZA	202	PEB	OA-C1A-C2A	-3.46	123.42	126.17
26	uE	203	PEB	OA-C1A-C2A	-3.46	123.42	126.17
28	B6	1002	CYC	C2B-C1B-NB	3.46	112.05	106.99
26	hB	203	PEB	C3B-C4B-NB	3.46	115.08	110.05
28	II	1001	CYC	CMA-C3A-C4A	3.46	130.39	125.06
26	O3	201	PEB	CHA-C4A-NA	3.46	129.32	125.20
26	LG	201	PEB	OD-C4D-ND	-3.46	120.81	125.93
28	L7	1001	CYC	CMA-C3A-C4A	3.46	130.39	125.06
26	HD	203	PEB	CBB-CAB-C3B	3.46	122.23	112.63
26	24	401	PEB	C3D-C4D-ND	3.46	114.04	107.26
26	AE	202	PEB	C3D-C4D-ND	3.46	114.04	107.26
26	M8	202	PEB	CMA-C2A-C1A	-3.46	104.95	112.40
28	dH	1001	CYC	OC-C1C-C2C	-3.46	123.42	126.17
26	e7	202	PEB	CMB-C2B-C1B	3.46	130.39	125.06
26	d1	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
26	wE	301	PEB	CHC-C1D-ND	-3.46	109.93	113.95
26	TI	201	PEB	CHC-C1D-ND	-3.46	109.93	113.95
26	TA	201	PEB	C2A-C1A-NA	3.46	111.25	108.27
26	SG	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
26	bG	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
26	RJ	201	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
28	FI	1001	CYC	C4A-C3A-C2A	-3.46	102.54	106.51
26	KG	201	PEB	CHB-C4B-NB	-3.46	124.03	128.83
26	n4	202	PEB	C3D-C4D-ND	3.46	114.04	107.26
26	ND	203	PEB	CAC-CBC-CGC	-3.46	104.07	113.76
26	Q1	201	PEB	CHA-C1B-NB	-3.46	117.70	124.93
26	V6	201	PEB	C3B-C4B-NB	3.46	115.08	110.05
28	HI	1001	CYC	C2A-C1A-NA	3.46	115.08	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I5	203	PEB	CHC-C4C-C3C	-3.46	124.44	130.34
28	NI	1001	CYC	C1B-C2B-C3B	-3.46	104.27	107.87
26	J4	203	PEB	CMB-C2B-C1B	3.46	130.38	125.06
26	k6	202	PEB	CMB-C2B-C1B	3.46	130.38	125.06
26	VF	203	PEB	CHA-C4A-NA	3.46	129.31	125.20
26	wG	302	PEB	C3D-C4D-ND	3.46	114.04	107.26
26	HJ	203	PEB	C3D-C4D-ND	3.46	114.04	107.26
26	g4	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
26	k2	202	PEB	CHA-C1B-NB	-3.45	117.71	124.93
26	J5	202	PEB	OD-C4D-ND	-3.45	120.81	125.93
26	JE	201	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
26	bG	202	PEB	CMB-C2B-C1B	3.45	130.38	125.06
26	SJ	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
28	DF	1001	CYC	CHB-C1B-NB	-3.45	118.64	126.06
26	fA	203	PEB	CHC-C1D-ND	-3.45	109.94	113.95
26	WG	201	PEB	CHC-C1D-ND	-3.45	109.94	113.95
26	hF	201	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
26	c6	201	PEB	CMB-C2B-C1B	3.45	130.38	125.06
26	Y3	301	PEB	C3B-C4B-NB	3.45	115.07	110.05
26	LJ	203	PEB	C3B-C4B-NB	3.45	115.07	110.05
26	bF	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
26	TF	201	PEB	CAB-C3B-C4B	3.45	131.12	125.01
27	xE	306	PUB	CHB-C1C-C2C	-3.45	117.34	125.32
26	oG	201	PEB	CHA-C4A-NA	-3.45	121.10	125.20
26	ZI	202	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
26	I9	202	PEB	CBC-CAC-C2C	-3.45	106.73	112.62
26	r4	202	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
26	FG	201	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
28	KB	202	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
26	l4	201	PEB	C1C-CHB-C4B	-3.45	124.69	128.81
26	iG	203	PEB	OD-C4D-ND	-3.45	120.82	125.93
28	C6	1001	CYC	CMB-C2B-C1B	3.45	128.48	124.17
26	UG	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
26	R9	202	PEB	CHC-C1D-ND	-3.45	109.94	113.95
28	CB	1001	CYC	CHB-C4A-NA	-3.45	117.71	124.93
26	X1	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	z1	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
26	YG	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
28	wH	1001	CYC	OC-C1C-C2C	-3.45	123.43	126.17
26	11	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
26	Y4	202	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
28	LB	1001	CYC	CHA-C1A-NA	-3.45	124.04	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I7	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
26	V7	202	PEB	CMB-C2B-C1B	3.45	130.38	125.06
26	c6	201	PEB	C3B-C4B-NB	3.45	115.07	110.05
26	CE	201	PEB	OD-C4D-C3D	-3.45	121.64	129.46
26	V8	202	PEB	CHA-C1B-NB	-3.45	117.72	124.93
26	MJ	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
28	EI	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
26	d6	201	PEB	CMB-C2B-C1B	3.45	130.38	125.06
26	VJ	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
26	f8	201	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
26	FE	202	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	SE	202	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	aF	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	j1	201	PEB	C3D-C4D-ND	3.45	114.03	107.26
26	pE	202	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
26	RD	203	PEB	CHB-C4B-C3B	-3.45	117.35	125.32
26	CE	202	PEB	CHC-C4C-C3C	-3.45	124.46	130.34
26	bG	201	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	B3	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
26	V2	201	PEB	C3B-C4B-NB	3.45	115.06	110.05
26	e4	201	PEB	C2A-C1A-NA	3.45	111.25	108.27
26	cG	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
26	I4	201	PEB	CHC-C4C-C3C	-3.45	124.46	130.34
26	BJ	202	PEB	C3D-C4D-ND	3.45	114.02	107.26
26	NE	201	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
26	M1	401	PEB	OA-C1A-C2A	-3.45	123.43	126.17
26	E4	202	PEB	OA-C1A-C2A	-3.45	123.43	126.17
26	hB	203	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	dE	201	PEB	CHA-C1B-NB	-3.45	117.72	124.93
26	S8	203	PEB	OD-C4D-C3D	-3.45	121.65	129.46
26	Y8	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
26	V9	202	PEB	C3D-C4D-ND	3.45	114.02	107.26
26	X8	202	PEB	CHC-C4C-C3C	-3.45	124.46	130.34
26	AB	304	PEB	CMB-C2B-C1B	3.45	130.37	125.06
26	ZB	202	PEB	OD-C4D-ND	-3.45	120.82	125.93
26	q4	201	PEB	C1C-CHB-C4B	3.45	132.93	128.81
26	TD	201	PEB	C2A-C1A-NA	3.45	111.24	108.27
26	Q3	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
26	UD	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
26	HJ	203	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
26	i2	203	PEB	C3B-C4B-NB	3.45	115.06	110.05
26	J5	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HJ	203	PEB	OA-C1A-C2A	-3.45	123.43	126.17
26	X1	202	PEB	OD-C4D-ND	-3.45	120.83	125.93
26	G8	201	PEB	OD-C4D-ND	-3.45	120.83	125.93
26	k8	201	PEB	CMB-C2B-C1B	3.45	130.37	125.06
26	OA	203	PEB	C3B-C4B-NB	3.45	115.06	110.05
26	N3	203	PEB	CHB-C4B-C3B	-3.45	117.36	125.32
26	sE	201	PEB	CMB-C2B-C1B	3.44	130.37	125.06
26	i1	202	PEB	OA-C1A-C2A	-3.44	123.43	126.17
26	K4	202	PEB	OA-C1A-C2A	-3.44	123.43	126.17
26	MG	203	PEB	OA-C1A-C2A	-3.44	123.43	126.17
28	YH	1002	CYC	OC-C1C-C2C	-3.44	123.43	126.17
26	WF	203	PEB	CHA-C1B-NB	-3.44	117.73	124.93
26	QI	202	PEB	CHC-C1D-ND	-3.44	109.95	113.95
26	HI	1002	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
26	P9	203	PEB	OD-C4D-ND	-3.44	120.83	125.93
26	VB	201	PEB	CHB-C4B-NB	-3.44	124.05	128.83
26	u4	201	PEB	CMB-C2B-C1B	3.44	130.37	125.06
26	cG	201	PEB	C3B-C4B-NB	3.44	115.06	110.05
26	p1	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
26	Y7	201	PEB	CHC-C1D-ND	-3.44	109.95	113.95
26	ND	202	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
26	bF	201	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
26	RG	201	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
26	T7	201	PEB	CHB-C4B-NB	-3.44	124.05	128.83
26	OA	203	PEB	C1B-C2B-C3B	-3.44	102.55	106.51
26	SB	203	PEB	C1B-C2B-C3B	-3.44	102.55	106.51
26	fG	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17
26	T6	201	PEB	C3B-C4B-NB	3.44	115.06	110.05
26	m8	202	PEB	C3B-C4B-NB	3.44	115.06	110.05
26	lA	201	PEB	C3B-C4B-NB	3.44	115.06	110.05
26	Q8	204	PEB	CHC-C4C-C3C	-3.44	124.46	130.34
26	VJ	202	PEB	OD-C4D-ND	-3.44	120.83	125.93
26	WB	203	PEB	CHB-C4B-NB	-3.44	124.05	128.83
26	iG	202	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
28	F6	1001	CYC	C2C-C1C-NC	3.44	111.24	108.27
26	TF	202	PEB	C1C-CHB-C4B	-3.44	124.70	128.81
26	11	202	PEB	CHC-C1D-ND	-3.44	109.95	113.95
26	LJ	202	PEB	CHA-C1B-C2B	3.44	133.75	124.90
26	m1	201	PEB	C3B-C4B-NB	3.44	115.06	110.05
26	PI	201	PEB	C3B-C4B-NB	3.44	115.06	110.05
26	N4	202	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
26	f8	203	PEB	C4B-C3B-C2B	-3.44	102.97	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aA	202	PEB	CHC-C4C-C3C	-3.44	124.47	130.34
26	X3	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
26	U7	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
26	OF	203	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
28	FB	1001	CYC	C4A-C3A-C2A	-3.44	102.56	106.51
26	SG	201	PEB	C3B-C4B-NB	3.44	115.05	110.05
26	S7	203	PEB	C2A-C1A-NA	3.44	111.24	108.27
26	KA	203	PEB	C2A-C1A-NA	3.44	111.24	108.27
26	S8	201	PEB	OD-C4D-ND	-3.44	120.83	125.93
26	c4	201	PEB	CMB-C2B-C1B	3.44	130.36	125.06
28	JH	1001	CYC	CAB-C3B-C4B	3.44	126.81	121.38
26	h1	201	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
26	PD	203	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
28	F6	1001	CYC	C4A-C3A-C2A	-3.44	102.56	106.51
26	HD	201	PEB	CHA-C1B-NB	-3.44	117.74	124.93
26	j6	201	PEB	CMB-C2B-C1B	3.44	130.36	125.06
26	q4	201	PEB	C2A-C1A-NA	3.44	111.24	108.27
26	QG	202	PEB	C3D-C4D-ND	3.44	114.01	107.26
28	E2	1001	CYC	C1B-NB-C4B	-3.44	106.29	110.67
26	UF	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
28	JF	1001	CYC	CHB-C4A-C3A	3.44	133.74	124.90
26	l8	203	PEB	OA-C1A-C2A	-3.44	123.44	126.17
26	A4	201	PEB	CBB-CAB-C3B	3.44	122.18	112.63
26	VF	201	PEB	C2A-C1A-NA	3.44	111.24	108.27
28	N7	1001	CYC	C2C-C1C-NC	3.44	111.24	108.27
26	c4	202	PEB	CBC-CAC-C2C	3.44	118.49	112.62
26	k7	202	PEB	CHC-C1D-ND	-3.44	109.95	113.95
26	R1	201	PEB	CHA-C1B-NB	-3.44	117.74	124.93
26	YG	202	PEB	CHC-C4C-C3C	-3.44	124.47	130.34
26	B1	201	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
26	aE	202	PEB	C3B-C4B-NB	3.44	115.05	110.05
26	U4	201	PEB	CAB-C3B-C4B	3.44	131.09	125.01
26	V4	202	PEB	C3D-C4D-ND	3.44	114.00	107.26
26	IG	203	PEB	CMA-C2A-C1A	-3.44	105.00	112.40
26	AA	301	PEB	CHA-C1B-NB	-3.44	117.74	124.93
28	K7	1001	CYC	CMB-C2B-C1B	3.44	128.46	124.17
26	TA	202	PEB	C3B-C4B-NB	3.44	115.05	110.05
26	eB	201	PEB	C3B-C4B-NB	3.44	115.05	110.05
28	D7	1001	CYC	CMA-C3A-C4A	3.44	130.36	125.06
26	ND	201	PEB	CHC-C4C-C3C	-3.44	124.48	130.34
26	ME	201	PEB	CBC-CAC-C2C	-3.44	106.76	112.62
26	H3	203	PEB	CBB-CAB-C3B	3.44	122.17	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S2	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17
26	14	203	PEB	OA-C1A-C2A	-3.44	123.44	126.17
26	V3	203	PEB	C2A-C1A-NA	3.44	111.23	108.27
26	OF	202	PEB	CHC-C4C-C3C	-3.44	124.48	130.34
26	K8	201	PEB	OD-C4D-C3D	-3.44	121.67	129.46
28	D7	1001	CYC	C1B-CHB-C4A	-3.44	119.69	128.08
26	aI	201	PEB	OD-C4D-ND	-3.44	120.84	125.93
26	WA	203	PEB	C1B-C2B-C3B	-3.43	102.56	106.51
26	AJ	301	PEB	C1B-C2B-C3B	-3.43	102.56	106.51
26	RF	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	A9	301	PEB	OA-C1A-C2A	-3.43	123.44	126.17
26	X4	202	PEB	CHA-C1B-C2B	3.43	133.73	124.90
26	CE	203	PEB	C1B-C2B-C3B	-3.43	102.56	106.51
26	SF	202	PEB	C3B-C4B-NB	3.43	115.04	110.05
26	RI	202	PEB	C3B-C4B-NB	3.43	115.04	110.05
26	R4	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	L9	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	H9	203	PEB	OA-C1A-C2A	-3.43	123.44	126.17
26	iI	203	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
26	JC	202	PEB	CMB-C2B-C1B	3.43	130.35	125.06
26	F9	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
26	gB	201	PEB	C3B-C4B-NB	3.43	115.04	110.05
26	MA	201	PEB	CHA-C1B-NB	-3.43	117.75	124.93
26	E1	201	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
26	VI	203	PEB	CAB-CBB-CGB	3.43	120.99	113.60
26	V3	203	PEB	CAB-C3B-C4B	3.43	131.08	125.01
26	C5	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	AC	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	WB	201	PEB	C3B-C4B-NB	3.43	115.04	110.05
26	V9	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
26	ID	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
26	SI	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
26	O7	202	PEB	OA-C1A-C2A	-3.43	123.44	126.17
26	j8	203	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
28	FI	1001	CYC	CHB-C1B-NB	-3.43	118.69	126.06
26	S1	201	PEB	CHA-C1B-NB	-3.43	117.75	124.93
26	B4	201	PEB	CHC-C1D-ND	-3.43	109.96	113.95
26	XD	201	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
26	YE	202	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
26	II	201	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
26	gI	202	PEB	CHB-C4B-NB	-3.43	124.07	128.83
26	aB	201	PEB	C2A-C1A-NA	3.43	111.23	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D3	201	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
26	eG	201	PEB	OA-C1A-C2A	-3.43	123.44	126.17
26	V3	203	PEB	CHC-C1D-ND	-3.43	109.96	113.95
26	d1	202	PEB	OD-C4D-ND	-3.43	120.85	125.93
26	L6	1002	PEB	C3B-C4B-NB	3.43	115.04	110.05
26	D2	1002	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
26	RA	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	VD	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	ME	203	PEB	C3D-C4D-ND	3.43	113.99	107.26
26	E8	201	PEB	CHA-C1B-NB	-3.43	117.76	124.93
26	GA	201	PEB	OD-C4D-ND	-3.43	120.85	125.93
28	NF	1001	CYC	CHB-C1B-NB	-3.43	118.69	126.06
28	HF	1001	CYC	C4A-C3A-C2A	-3.43	102.57	106.51
26	I1	201	PEB	CHC-C4C-C3C	-3.43	124.49	130.34
26	MD	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	AI	305	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	DJ	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
28	iH	1001	CYC	CAB-C3B-C4B	3.43	126.79	121.38
26	O6	202	PEB	CBA-CAA-C3A	-3.43	105.83	113.47
26	hB	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
26	L8	202	PEB	C3B-C4B-NB	3.43	115.04	110.05
26	U3	202	PEB	CHC-C4C-C3C	-3.43	124.49	130.34
26	NI	1002	PEB	CHB-C4B-NB	-3.43	124.07	128.83
26	RI	202	PEB	CAB-C3B-C4B	3.43	131.07	125.01
26	WE	201	PEB	OA-C1A-C2A	-3.43	123.45	126.17
26	dB	204	PEB	C3B-C4B-NB	3.43	115.03	110.05
26	S1	202	PEB	CMB-C2B-C1B	3.43	130.34	125.06
26	K8	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	TJ	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
26	ZI	201	PEB	OD-C4D-ND	-3.43	120.85	125.93
26	HE	201	PEB	CHA-C1B-C2B	3.43	133.71	124.90
26	f1	201	PEB	OD-C4D-ND	-3.43	120.86	125.93
26	S7	202	PEB	OD-C4D-ND	-3.43	120.86	125.93
26	DD	203	PEB	C3B-C4B-NB	3.43	115.03	110.05
26	MJ	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
26	KG	201	PEB	CMB-C2B-C1B	3.43	130.34	125.06
26	E9	201	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
26	ZF	201	PEB	C4B-C3B-C2B	-3.42	102.99	106.78
26	YG	203	PEB	CHA-C4A-NA	3.42	129.28	125.20
26	u4	201	PEB	CAA-C3A-C2A	-3.42	105.70	114.26
26	qE	201	PEB	OD-C4D-ND	-3.42	120.86	125.93
26	Z6	201	PEB	C2A-C1A-NA	3.42	111.22	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AE	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	yG	301	PEB	CMB-C2B-C1B	3.42	130.34	125.06
26	AJ	303	PEB	CHC-C4C-C3C	-3.42	124.50	130.34
26	P2	201	PEB	C3B-C4B-NB	3.42	115.03	110.05
26	x4	202	PEB	C3B-C4B-NB	3.42	115.03	110.05
26	O2	202	PEB	CHB-C4B-NB	-3.42	124.08	128.83
26	OF	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
26	f1	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	C5	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	l6	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	k2	203	PEB	CHC-C4C-C3C	-3.42	124.50	130.34
26	LA	202	PEB	C3B-C4B-NB	3.42	115.03	110.05
26	W2	201	PEB	CHA-C1B-NB	-3.42	117.77	124.93
26	cE	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
26	jA	203	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
26	J4	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
28	C2	1001	CYC	C2C-C1C-NC	3.42	111.22	108.27
26	f4	201	PEB	C3B-C4B-NB	3.42	115.03	110.05
26	wG	301	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
26	U8	202	PEB	OD-C4D-ND	-3.42	120.86	125.93
26	SF	202	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
28	DF	1001	CYC	C4A-C3A-C2A	-3.42	102.58	106.51
26	GA	203	PEB	OA-C1A-C2A	-3.42	123.45	126.17
28	I7	1001	CYC	CBD-CAD-C3D	-3.42	106.78	112.62
26	d4	201	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
26	TE	201	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
26	jB	202	PEB	CHC-C4C-C3C	-3.42	124.50	130.34
26	VF	203	PEB	CHB-C4B-NB	-3.42	124.08	128.83
26	P2	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	hF	202	PEB	CAB-CBB-CGB	-3.42	106.24	113.60
26	N3	201	PEB	OD-C4D-ND	-3.42	120.86	125.93
26	I9	201	PEB	CHC-C4C-C3C	-3.42	124.50	130.34
26	jF	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
26	QG	203	PEB	CMA-C2A-C1A	-3.42	105.03	112.40
26	BG	201	PEB	CHA-C1B-NB	-3.42	117.78	124.93
26	m8	201	PEB	C1C-CHB-C4B	-3.42	124.72	128.81
26	F4	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	C5	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
26	LJ	203	PEB	C3D-C4D-ND	3.42	113.97	107.26
26	L8	202	PEB	OD-C4D-ND	-3.42	120.87	125.93
26	Q9	201	PEB	CMB-C2B-C1B	3.42	130.33	125.06
26	W6	201	PEB	C3B-C4B-NB	3.42	115.02	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H1	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
26	21	401	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
28	I2	1001	CYC	CMA-C3A-C4A	3.42	130.33	125.06
26	S1	202	PEB	OD-C4D-ND	-3.42	120.87	125.93
26	w1	202	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
26	A9	301	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
26	R9	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	dF	201	PEB	C3B-C4B-NB	3.42	115.02	110.05
26	QJ	201	PEB	C3B-C4B-NB	3.42	115.02	110.05
26	XG	202	PEB	OA-C1A-C2A	-3.42	123.46	126.17
26	X3	201	PEB	CHA-C1B-NB	-3.42	117.78	124.93
26	D1	203	PEB	CHC-C4C-C3C	-3.42	124.51	130.34
26	K1	202	PEB	OD-C4D-ND	-3.42	120.87	125.93
26	fB	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
26	OI	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
26	P2	203	PEB	CHC-C1D-ND	-3.42	109.98	113.95
26	TF	201	PEB	OD-C4D-C3D	-3.42	121.72	129.46
26	E8	202	PEB	CHA-C1B-C2B	3.42	133.69	124.90
26	a8	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	LG	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	SG	203	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	KA	203	PEB	OA-C1A-C2A	-3.42	123.46	126.17
26	M1	402	PEB	CHC-C4C-C3C	-3.42	124.51	130.34
26	PJ	203	PEB	C1B-C2B-C3B	-3.42	102.59	106.51
26	a2	202	PEB	CMB-C2B-C1B	3.42	130.32	125.06
26	iE	203	PEB	CHB-C4B-NB	-3.42	124.09	128.83
26	O7	203	PEB	CHC-C1D-ND	-3.42	109.98	113.95
26	w1	202	PEB	C3D-C4D-ND	3.42	113.96	107.26
26	PA	202	PEB	C3B-C4B-NB	3.42	115.02	110.05
26	mF	201	PEB	C3B-C4B-NB	3.42	115.02	110.05
28	D7	1001	CYC	CMB-C2B-C1B	3.42	128.43	124.17
26	hF	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
26	GD	201	PEB	OD-C4D-C3D	-3.41	121.72	129.46
26	E4	201	PEB	OD-C4D-ND	-3.41	120.87	125.93
27	A8	304	PUB	OA-C1A-NA	-3.41	120.87	125.93
26	j1	202	PEB	CHC-C4C-C3C	-3.41	124.51	130.34
26	C9	201	PEB	C3D-C4D-ND	3.41	113.96	107.26
26	l2	202	PEB	CHB-C4B-NB	-3.41	124.09	128.83
26	L4	203	PEB	C2A-C1A-NA	3.41	111.22	108.27
26	DG	202	PEB	C3B-C4B-NB	3.41	115.02	110.05
26	p4	202	PEB	C1C-CHB-C4B	-3.41	124.73	128.81
26	R6	201	PEB	CHA-C1B-NB	-3.41	117.79	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LA	202	PEB	OD-C4D-ND	-3.41	120.87	125.93
26	ND	201	PEB	OD-C4D-ND	-3.41	120.87	125.93
26	UI	202	PEB	OA-C1A-C2A	-3.41	123.46	126.17
28	G6	1001	CYC	C1B-NB-C4B	-3.41	106.32	110.67
26	A5	201	PEB	C4B-C3B-C2B	-3.41	103.00	106.78
26	Q7	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	CA	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	H3	202	PEB	CHA-C4A-NA	3.41	129.26	125.20
26	a8	202	PEB	OD-C4D-ND	-3.41	120.87	125.93
28	KF	1001	CYC	C1B-CHB-C4A	-3.41	119.74	128.08
26	s1	201	PEB	CMB-C2B-C1B	3.41	130.32	125.06
26	T2	203	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
26	dE	201	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
26	AJ	305	PEB	OA-C1A-C2A	-3.41	123.46	126.17
26	XG	201	PEB	CHA-C1B-NB	-3.41	117.80	124.93
26	QE	201	PEB	CHC-C4C-C3C	-3.41	124.52	130.34
26	m1	203	PEB	C2A-C1A-NA	3.41	111.21	108.27
26	WA	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
26	W8	203	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	u4	201	PEB	CAB-CBB-CGB	-3.41	106.26	113.60
26	TI	203	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
28	sH	1001	CYC	C1A-C2A-C3A	-3.41	103.01	106.78
26	x4	202	PEB	C1C-CHB-C4B	3.41	132.88	128.81
26	kB	201	PEB	CHB-C4B-NB	-3.41	124.09	128.83
26	zG	501	PEB	CHC-C4C-C3C	-3.41	124.52	130.34
28	IF	1001	CYC	C1B-C2B-C3B	-3.41	104.31	107.87
26	X4	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	bB	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
28	K6	202	CYC	C2C-C1C-NC	3.41	111.21	108.27
26	E9	202	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
26	DE	202	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
26	iG	202	PEB	OD-C4D-ND	-3.41	120.88	125.93
26	YA	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
28	KF	1001	CYC	C4A-C3A-C2A	-3.41	102.59	106.51
26	T1	203	PEB	CHC-C4C-C3C	-3.41	124.52	130.34
27	21	402	PUB	CBA-CAA-C3A	-3.41	107.81	112.98
26	S6	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
26	U7	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
26	X1	202	PEB	CHA-C1B-C2B	3.41	133.67	124.90
26	r4	201	PEB	C3B-C4B-NB	3.41	115.01	110.05
26	O9	201	PEB	CHB-C4B-NB	-3.41	124.10	128.83
26	RE	201	PEB	C1C-CHB-C4B	3.41	132.88	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S8	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	IA	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	aA	203	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
26	F5	203	PEB	CMB-C2B-C1B	3.41	130.31	125.06
26	gG	203	PEB	CHA-C1B-C2B	3.41	133.66	124.90
26	iE	201	PEB	OA-C1A-C2A	-3.41	123.46	126.17
26	c4	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
26	gI	201	PEB	CMB-C2B-C1B	3.41	130.31	125.06
26	K8	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
28	J2	1001	CYC	C1B-NB-C4B	-3.41	106.33	110.67
26	iF	201	PEB	C3D-C4D-ND	3.41	113.94	107.26
26	y4	202	PEB	OD-C4D-ND	-3.41	120.88	125.93
26	HC	203	PEB	C3B-C4B-NB	3.41	115.00	110.05
26	X1	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
26	i1	202	PEB	CMB-C2B-C1B	3.41	130.31	125.06
26	J3	202	PEB	CMB-C2B-C1B	3.41	130.31	125.06
26	FI	1002	PEB	C3B-C4B-NB	3.41	115.00	110.05
26	mA	201	PEB	C1C-CHB-C4B	-3.41	124.74	128.81
26	NI	1002	PEB	OD-C4D-ND	-3.41	120.88	125.93
26	Z2	201	PEB	CHC-C1D-ND	-3.41	109.99	113.95
26	cE	203	PEB	C4B-C3B-C2B	-3.41	103.01	106.78
26	u4	201	PEB	CBC-CAC-C2C	-3.41	106.81	112.62
26	eB	202	PEB	C2A-C1A-NA	3.41	111.21	108.27
28	D2	1001	CYC	C2C-C1C-NC	3.41	111.21	108.27
26	h2	201	PEB	OD-C4D-ND	-3.41	120.89	125.93
26	IA	202	PEB	OD-C4D-ND	-3.41	120.89	125.93
26	S2	202	PEB	CMB-C2B-C1B	3.41	130.31	125.06
26	O8	202	PEB	C1B-C2B-C3B	-3.41	102.60	106.51
26	S8	202	PEB	C1B-C2B-C3B	-3.41	102.60	106.51
27	AB	302	PUB	CHA-C4A-NA	-3.41	109.99	113.95
26	OF	203	PEB	C4B-C3B-C2B	-3.40	103.01	106.78
26	LJ	201	PEB	C4B-C3B-C2B	-3.40	103.01	106.78
26	KE	202	PEB	CHB-C4B-C3B	-3.40	117.45	125.32
26	TG	202	PEB	OD-C4D-C3D	-3.40	121.75	129.46
26	PG	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	w1	203	PEB	CHC-C4C-C3C	-3.40	124.53	130.34
26	m1	201	PEB	CHA-C4A-NA	-3.40	121.16	125.20
26	Q9	202	PEB	CHC-C1D-ND	-3.40	109.99	113.95
28	NI	1001	CYC	OB-C4B-C3B	-3.40	124.35	128.04
26	d6	201	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	B8	301	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	s4	202	PEB	C3D-C4D-ND	3.40	113.94	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k6	201	PEB	C2A-C1A-NA	3.40	111.21	108.27
28	YH	1003	CYC	CHA-C1A-NA	-3.40	124.11	128.83
26	f1	201	PEB	CHA-C4A-NA	3.40	129.25	125.20
26	eI	201	PEB	C3B-C4B-NB	3.40	115.00	110.05
28	N2	1001	CYC	C2A-C1A-NA	3.40	115.00	110.05
26	GE	202	PEB	OA-C1A-NA	-3.40	120.82	124.94
26	i4	201	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
26	W8	201	PEB	CHA-C1B-C2B	3.40	133.65	124.90
26	h4	201	PEB	C2A-C1A-NA	3.40	111.21	108.27
26	WD	202	PEB	CHA-C1B-NB	-3.40	117.82	124.93
26	K9	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	wE	301	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	iF	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	jF	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	QB	201	PEB	CAB-C3B-C4B	3.40	131.03	125.01
26	M9	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	JD	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	IJ	203	PEB	OA-C1A-C2A	-3.40	123.47	126.17
26	hF	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
26	vG	202	PEB	C3B-C4B-NB	3.40	115.00	110.05
26	h8	201	PEB	CHA-C1B-C2B	3.40	133.65	124.90
26	HJ	203	PEB	C2A-C1A-NA	3.40	111.20	108.27
26	g1	201	PEB	C3B-C4B-NB	3.40	115.00	110.05
26	SG	203	PEB	OD-C4D-ND	-3.40	120.89	125.93
27	K1	203	PUB	CBA-CAA-C3A	-3.40	107.82	112.98
26	V3	202	PEB	CBC-CAC-C2C	3.40	118.42	112.62
26	l7	202	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	KE	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	UF	202	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	AJ	305	PEB	CMB-C2B-C1B	3.40	130.30	125.06
26	H5	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	CA	203	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
26	e8	201	PEB	CHA-C1B-NB	-3.40	117.82	124.93
26	G1	202	PEB	CHB-C4B-NB	-3.40	124.11	128.83
26	D1	203	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	y1	203	PEB	C3B-C4B-NB	3.40	114.99	110.05
26	AF	301	PEB	C1C-CHB-C4B	-3.40	124.75	128.81
26	I8	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	eI	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
26	vG	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	C1	202	PEB	OA-C1A-C2A	-3.40	123.47	126.17
26	KE	202	PEB	CHC-C1D-ND	-3.40	110.00	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OF	202	PEB	CHC-C1D-ND	-3.40	110.00	113.95
26	O3	201	PEB	C2A-C1A-NA	3.40	111.20	108.27
26	l8	203	PEB	C2A-C1A-NA	3.40	111.20	108.27
26	K8	201	PEB	CHB-C4B-NB	-3.40	124.11	128.83
26	m4	201	PEB	C3B-C4B-NB	3.40	114.99	110.05
26	P7	201	PEB	C3B-C4B-NB	3.40	114.99	110.05
26	U6	203	PEB	CHC-C4C-C3C	-3.40	124.54	130.34
26	IE	202	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	N1	202	PEB	C3B-C4B-NB	3.40	114.99	110.05
26	F5	201	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
26	S8	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
26	l7	202	PEB	CBC-CAC-C2C	-3.40	106.82	112.62
26	H7	1002	PEB	OD-C4D-ND	-3.40	120.90	125.93
26	H4	201	PEB	C3B-C4B-NB	3.40	114.99	110.05
26	e6	201	PEB	C3B-C4B-NB	3.40	114.99	110.05
26	LC	202	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
26	FI	1002	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
28	L2	1001	CYC	C1A-C2A-C3A	-3.40	103.02	106.78
26	SI	202	PEB	OA-C1A-C2A	-3.40	123.47	126.17
26	T9	203	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
26	JC	202	PEB	CHA-C1B-NB	-3.40	117.83	124.93
26	U1	201	PEB	CMB-C2B-C1B	3.40	130.29	125.06
26	i2	201	PEB	C2A-C1A-NA	3.40	111.20	108.27
28	NF	1001	CYC	C2C-C1C-NC	3.40	111.20	108.27
26	W6	201	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
26	RI	201	PEB	CHA-C1B-NB	-3.39	117.83	124.93
26	T7	201	PEB	C3B-C4B-NB	3.39	114.99	110.05
28	jH	1001	CYC	CHA-C1A-NA	-3.39	124.12	128.83
26	pE	202	PEB	CHB-C4B-C3B	-3.39	117.48	125.32
26	hF	202	PEB	C1C-CHB-C4B	3.39	132.86	128.81
26	iG	201	PEB	OA-C1A-C2A	-3.39	123.47	126.17
28	pH	1001	CYC	OC-C1C-C2C	-3.39	123.47	126.17
26	AD	202	PEB	C3D-C4D-ND	3.39	113.92	107.26
28	LI	1001	CYC	CMB-C2B-C1B	3.39	128.41	124.17
26	B3	201	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	J4	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	MG	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	WE	203	PEB	CHC-C4C-C3C	-3.39	124.55	130.34
26	BD	202	PEB	OD-C4D-ND	-3.39	120.90	125.93
26	AE	201	PEB	OD-C4D-ND	-3.39	120.90	125.93
26	jF	203	PEB	OD-C4D-ND	-3.39	120.90	125.93
26	L1	201	PEB	C3B-C4B-NB	3.39	114.99	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AJ	304	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
26	F7	1002	PEB	CHB-C4B-NB	-3.39	124.12	128.83
26	S2	201	PEB	C4B-NB-C1B	-3.39	100.12	106.51
26	PA	201	PEB	CMB-C2B-C1B	3.39	130.29	125.06
26	I5	201	PEB	OA-C1A-C2A	-3.39	123.47	126.17
26	GE	203	PEB	C3B-C4B-NB	3.39	114.98	110.05
26	S7	202	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
26	cF	201	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
26	g1	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	s4	203	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	W3	201	PEB	CHA-C4A-NA	3.39	129.24	125.20
26	JA	201	PEB	OD-C4D-ND	-3.39	120.90	125.93
28	N2	1001	CYC	C1A-C2A-C3A	-3.39	103.03	106.78
26	G9	201	PEB	CAB-CBB-CGB	-3.39	106.30	113.60
26	hI	201	PEB	CMA-C2A-C1A	-3.39	105.09	112.40
26	GJ	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
26	VE	202	PEB	OD-C4D-ND	-3.39	120.91	125.93
26	PJ	203	PEB	C3B-C4B-NB	3.39	114.98	110.05
26	f8	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
28	KB	202	CYC	C2C-C1C-NC	3.39	111.20	108.27
28	DI	1001	CYC	CHB-C4A-NA	-3.39	117.84	124.93
26	eA	201	PEB	CHA-C1B-NB	-3.39	117.84	124.93
26	R1	203	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	JE	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	WJ	201	PEB	C2A-C1A-NA	3.39	111.20	108.27
26	WE	202	PEB	CHB-C4B-C3B	-3.39	117.49	125.32
26	S4	202	PEB	OD-C4D-ND	-3.39	120.91	125.93
26	rG	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
26	aI	203	PEB	CHC-C1D-ND	-3.39	110.01	113.95
26	KG	203	PEB	C3B-C4B-NB	3.39	114.98	110.05
26	k8	202	PEB	CAB-CBB-CGB	3.39	120.90	113.60
26	N2	1002	PEB	CHB-C4B-NB	-3.39	124.12	128.83
26	KJ	202	PEB	CBC-CAC-C2C	-3.39	106.83	112.62
26	EG	202	PEB	C3B-C4B-NB	3.39	114.98	110.05
26	c1	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
26	UF	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
26	a8	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
26	qG	203	PEB	C3D-C4D-ND	3.39	113.91	107.26
26	x1	201	PEB	CHA-C1B-NB	-3.39	117.84	124.93
26	F1	201	PEB	CHB-C4B-NB	-3.39	124.13	128.83
26	WE	203	PEB	C3D-C4D-ND	3.39	113.91	107.26
26	OG	203	PEB	C3D-C4D-ND	3.39	113.91	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	QI	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
26	GE	201	PEB	CMB-C2B-C1B	3.39	130.28	125.06
26	G1	201	PEB	C2A-C1A-NA	3.39	111.19	108.27
26	h4	201	PEB	CHB-C4B-NB	-3.39	124.13	128.83
28	nH	1001	CYC	CHA-C1A-NA	-3.39	124.13	128.83
26	Q4	201	PEB	CHA-C1B-NB	-3.39	117.85	124.93
26	h6	201	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
26	W7	201	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
26	L2	1002	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
26	QB	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
26	j4	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
26	JE	201	PEB	CHC-C1D-ND	-3.39	110.01	113.95
26	X8	201	PEB	CHC-C1D-ND	3.39	117.88	113.95
26	c4	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
26	EE	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
26	RE	202	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
28	VH	1001	CYC	CHA-C1A-NA	-3.39	124.13	128.83
26	DJ	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
26	TE	202	PEB	OD-C4D-C3D	-3.39	121.79	129.46
26	D9	203	PEB	C2A-C1A-NA	3.39	111.19	108.27
26	WF	201	PEB	C2A-C1A-NA	3.39	111.19	108.27
26	M8	201	PEB	CHA-C1B-NB	-3.39	117.85	124.93
26	S6	201	PEB	OD-C4D-ND	-3.39	120.92	125.93
26	d2	201	PEB	CMB-C2B-C1B	3.39	130.28	125.06
26	dB	201	PEB	CMB-C2B-C1B	3.39	130.28	125.06
26	W4	202	PEB	C4B-C3B-C2B	-3.39	103.04	106.78
26	U7	203	PEB	CHA-C1B-NB	-3.39	117.85	124.93
26	Y8	203	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	gF	202	PEB	OA-C1A-NA	3.38	129.04	124.94
26	L5	202	PEB	OD-C4D-ND	-3.38	120.92	125.93
26	V6	201	PEB	CHB-C4B-NB	-3.38	124.13	128.83
27	AJ	302	PUB	CHA-C4A-NA	-3.38	110.02	113.95
26	fl	202	PEB	OA-C1A-C2A	-3.38	123.48	126.17
26	hA	201	PEB	CHA-C1B-C2B	3.38	133.60	124.90
26	O7	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
26	kB	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
27	xG	306	PUB	C1C-C2C-C3C	-3.38	103.04	106.78
26	n4	202	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	q4	203	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	aA	203	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	O2	201	PEB	C4B-NB-C1B	-3.38	100.14	106.51
28	iH	1001	CYC	C4D-CHA-C1A	3.38	132.85	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KA	202	PEB	OD-C4D-C3D	-3.38	121.79	129.46
26	M8	203	PEB	CHA-C1B-NB	-3.38	117.86	124.93
26	WA	201	PEB	CHA-C1B-C2B	3.38	133.60	124.90
26	c7	202	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
28	N7	1001	CYC	C2B-C1B-NB	3.38	111.94	106.99
26	zE	501	PEB	OD-C4D-ND	-3.38	120.92	125.93
26	YB	201	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
26	EG	201	PEB	C3B-C4B-NB	3.38	114.97	110.05
26	sE	203	PEB	C1B-C2B-C3B	-3.38	102.62	106.51
26	z1	201	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
26	U2	202	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
26	YJ	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
28	L6	1001	CYC	CAD-C3D-C2D	3.38	136.97	127.25
26	EA	203	PEB	C3B-C4B-NB	3.38	114.97	110.05
26	UE	202	PEB	C3B-C4B-NB	3.38	114.97	110.05
26	UD	202	PEB	C3D-C4D-ND	3.38	113.89	107.26
26	g6	201	PEB	OA-C1A-C2A	-3.38	123.48	126.17
26	VG	202	PEB	CBC-CAC-C2C	3.38	118.39	112.62
26	xE	303	PEB	C1B-C2B-C3B	-3.38	102.62	106.51
26	WA	201	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
26	QD	202	PEB	C3D-C4D-ND	3.38	113.89	107.26
28	IH	1001	CYC	C4D-CHA-C1A	3.38	132.85	128.81
26	BD	201	PEB	C3B-C4B-NB	3.38	114.97	110.05
26	S8	201	PEB	CHA-C1B-NB	-3.38	117.86	124.93
28	NH	1001	CYC	OC-C1C-C2C	-3.38	123.48	126.17
26	U4	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
28	DF	1003	CYC	C1A-C2A-C3A	-3.38	103.04	106.78
26	DJ	203	PEB	OD-C4D-ND	-3.38	120.92	125.93
28	MI	1001	CYC	CHB-C4A-NA	-3.38	117.86	124.93
26	CC	202	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	hE	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	s4	201	PEB	CAB-CBB-CGB	-3.38	106.33	113.60
26	V7	201	PEB	CHC-C1D-ND	-3.38	110.02	113.95
26	j4	201	PEB	C3D-C4D-ND	3.38	113.89	107.26
26	FC	201	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
26	AF	302	PEB	CMB-C2B-C1B	3.38	130.27	125.06
26	ZF	203	PEB	OD-C4D-ND	-3.38	120.92	125.93
26	gG	201	PEB	OD-C4D-ND	-3.38	120.92	125.93
26	QE	203	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
26	L3	203	PEB	CHB-C4B-NB	-3.38	124.14	128.83
26	d6	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
26	W7	203	PEB	OA-C1A-C2A	-3.38	123.49	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HD	203	PEB	OA-C1A-C2A	-3.38	123.49	126.17
26	F9	202	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	ZB	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	GG	202	PEB	CAB-C3B-C4B	3.38	130.99	125.01
26	cF	202	PEB	CHA-C1B-C2B	3.38	133.59	124.90
26	U1	202	PEB	CAA-C3A-C2A	-3.38	105.82	114.26
26	xE	304	PEB	OD-C4D-ND	-3.38	120.92	125.93
26	UF	203	PEB	CHA-C1B-NB	-3.38	117.87	124.93
26	Q6	203	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
26	NE	201	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
27	Y3	302	PUB	CBA-CAA-C3A	-3.38	107.86	112.98
26	mB	201	PEB	C3B-C4B-NB	3.38	114.96	110.05
26	c2	202	PEB	CMB-C2B-C1B	3.38	130.27	125.06
26	E8	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
26	bE	201	PEB	OD-C4D-ND	-3.38	120.93	125.93
26	R9	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
26	D2	1002	PEB	CMB-C2B-C1B	3.38	130.26	125.06
26	R2	202	PEB	CAB-C3B-C4B	3.38	130.98	125.01
26	SI	202	PEB	OD-C4D-C3D	-3.38	121.81	129.46
26	WE	203	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	kE	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	O6	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
26	SJ	201	PEB	OA-C1A-C2A	-3.38	123.49	126.17
26	mA	202	PEB	C2A-C1A-NA	3.38	111.18	108.27
26	AB	301	PEB	C2A-C1A-NA	3.38	111.18	108.27
26	Y4	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	d6	204	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	O9	202	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	aA	202	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	Q3	202	PEB	C3B-C4B-NB	3.38	114.96	110.05
26	U7	203	PEB	C3B-C4B-NB	3.38	114.96	110.05
26	EE	202	PEB	C3B-C4B-NB	3.38	114.96	110.05
26	x4	202	PEB	CHA-C4A-NA	-3.38	121.19	125.20
26	F3	203	PEB	CAC-CBC-CGC	-3.38	104.30	113.76
26	O1	202	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
26	W8	201	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
26	iG	202	PEB	CHC-C1D-ND	-3.38	110.03	113.95
26	CG	201	PEB	OD-C4D-ND	-3.38	120.93	125.93
26	xG	303	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
26	mG	202	PEB	C2A-C1A-NA	3.38	111.18	108.27
26	iB	201	PEB	CHA-C1B-NB	-3.38	117.87	124.93
26	X3	203	PEB	CMB-C2B-C1B	3.38	130.26	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SB	203	PEB	C3B-C4B-NB	3.38	114.96	110.05
28	J7	1001	CYC	CBD-CAD-C3D	3.38	118.38	112.62
26	GJ	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
26	RG	201	PEB	OD-C4D-ND	-3.38	120.93	125.93
26	H8	202	PEB	CAB-C3B-C4B	3.38	130.98	125.01
26	gG	201	PEB	CHA-C1B-C2B	3.38	133.58	124.90
26	gG	201	PEB	CHB-C4B-C3B	-3.37	117.52	125.32
26	VI	202	PEB	CHA-C1B-NB	-3.37	117.87	124.93
26	IA	203	PEB	C1C-CHB-C4B	-3.37	124.78	128.81
26	K5	202	PEB	CHB-C4B-NB	-3.37	124.15	128.83
26	B9	202	PEB	OA-C1A-C2A	-3.37	123.49	126.17
26	W9	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
28	LF	1001	CYC	C1B-C2B-C3B	-3.37	104.35	107.87
26	P4	202	PEB	C1B-C2B-C3B	-3.37	102.63	106.51
26	YG	201	PEB	C1B-C2B-C3B	-3.37	102.63	106.51
26	q1	202	PEB	OD-C4D-ND	-3.37	120.93	125.93
26	bB	201	PEB	OD-C4D-ND	-3.37	120.93	125.93
26	CC	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
26	H2	1002	PEB	C3B-C4B-NB	3.37	114.96	110.05
26	l7	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
26	ZI	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
26	eI	202	PEB	OA-C1A-C2A	-3.37	123.49	126.17
26	fF	203	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
26	d6	202	PEB	CMB-C2B-C1B	3.37	130.26	125.06
26	YD	301	PEB	CHA-C1B-NB	-3.37	117.88	124.93
26	T4	201	PEB	C3B-C4B-NB	3.37	114.95	110.05
26	UF	203	PEB	C3D-C4D-ND	3.37	113.88	107.26
28	II	1001	CYC	C1A-C2A-C3A	-3.37	103.05	106.78
26	R1	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
26	F9	201	PEB	OD-C4D-ND	-3.37	120.93	125.93
26	l6	202	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
26	O1	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
26	O7	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
26	lG	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
26	AD	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
26	JG	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
26	PI	203	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
26	g6	201	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
26	cB	201	PEB	C3B-C4B-NB	3.37	114.95	110.05
26	V3	203	PEB	OD-C4D-ND	-3.37	120.94	125.93
26	VD	203	PEB	OD-C4D-ND	-3.37	120.94	125.93
26	kB	201	PEB	C2A-C1A-NA	3.37	111.18	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	DJ	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
26	LC	202	PEB	CHA-C1B-NB	-3.37	117.88	124.93
26	R9	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
26	iB	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
26	dF	201	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
26	nG	202	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
26	v1	202	PEB	CHC-C1D-ND	-3.37	110.03	113.95
26	g6	201	PEB	CHA-C1B-NB	-3.37	117.88	124.93
26	SB	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
26	dB	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
26	W7	203	PEB	CMB-C2B-C1B	3.37	130.25	125.06
26	i7	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
26	rG	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
26	p1	202	PEB	CHC-C1D-ND	-3.37	110.03	113.95
26	b4	501	PEB	CMD-C2D-C3D	3.37	134.81	130.06
26	RE	201	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
26	lG	202	PEB	CHB-C4B-NB	-3.37	124.15	128.83
26	aA	203	PEB	CMC-C3C-C2C	3.37	131.29	124.94
26	YG	201	PEB	C3B-C4B-NB	3.37	114.95	110.05
26	RA	201	PEB	CMB-C2B-C1B	3.37	130.25	125.06
26	m2	201	PEB	CHC-C1D-ND	-3.37	110.04	113.95
26	S4	201	PEB	CHC-C1D-ND	-3.37	110.04	113.95
26	Q7	203	PEB	CHA-C1B-NB	-3.37	117.89	124.93
26	FJ	201	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
28	J7	1001	CYC	C4A-C3A-C2A	-3.37	102.64	106.51
26	Q6	201	PEB	CAB-C3B-C4B	3.37	130.97	125.01
26	c6	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
26	IA	201	PEB	CHB-C4B-NB	-3.37	124.16	128.83
26	NF	1002	PEB	CAB-C3B-C4B	3.37	130.97	125.01
26	a1	203	PEB	C1C-CHB-C4B	3.37	132.83	128.81
26	NJ	203	PEB	OA-C1A-C2A	-3.37	123.50	126.17
26	YI	202	PEB	C2A-C1A-NA	3.37	111.17	108.27
26	I9	201	PEB	C1C-CHB-C4B	3.37	132.83	128.81
26	oG	203	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
26	cI	201	PEB	CMB-C2B-C1B	3.37	130.25	125.06
26	FD	202	PEB	CHC-C1D-ND	-3.37	110.04	113.95
26	bG	201	PEB	CHC-C4C-C3C	-3.37	124.60	130.34
26	wG	301	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
28	JI	1001	CYC	C4A-C3A-C2A	-3.37	102.64	106.51
26	ZB	203	PEB	C2A-C1A-NA	3.37	111.17	108.27
26	S6	203	PEB	C3B-C4B-NB	3.37	114.94	110.05
26	pE	202	PEB	C3B-C4B-NB	3.37	114.94	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	wG	301	PEB	C3B-C4B-NB	3.37	114.94	110.05
26	H1	202	PEB	CHB-C4B-NB	-3.37	124.16	128.83
28	NI	1001	CYC	CMA-C3A-C4A	3.37	130.25	125.06
26	T1	202	PEB	OD-C4D-ND	-3.36	120.94	125.93
26	R9	203	PEB	CHC-C1D-ND	-3.36	110.04	113.95
26	P9	201	PEB	C3D-C4D-ND	3.36	113.86	107.26
26	MJ	202	PEB	OA-C1A-C2A	-3.36	123.50	126.17
26	W1	202	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
26	TD	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
26	WB	201	PEB	C1B-C2B-C3B	-3.36	102.64	106.51
26	P8	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
26	i2	203	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
26	J7	1002	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	N7	1002	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	dB	202	PEB	CMB-C2B-C1B	3.36	130.24	125.06
26	qG	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
26	D1	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
26	v1	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	a8	203	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	fE	202	PEB	CHC-C1D-ND	3.36	117.85	113.95
26	zE	501	PEB	CHC-C1D-ND	-3.36	110.04	113.95
26	q4	203	PEB	OD-C4D-ND	-3.36	120.95	125.93
28	FB	1001	CYC	C2C-C1C-NC	3.36	111.17	108.27
26	II	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	GG	203	PEB	CMB-C2B-C1B	3.36	130.24	125.06
26	c4	201	PEB	C3D-C4D-ND	3.36	113.86	107.26
26	m1	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
26	L9	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
26	cE	201	PEB	CHA-C1B-NB	-3.36	117.90	124.93
26	f1	201	PEB	CAB-CBB-CGB	-3.36	106.37	113.60
26	I4	202	PEB	C1C-CHB-C4B	3.36	132.82	128.81
26	O6	203	PEB	OA-C1A-C2A	-3.36	123.50	126.17
26	m1	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	f1	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	V6	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	A7	305	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	AF	301	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	a6	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
28	I2	1001	CYC	C1A-C2A-C3A	-3.36	103.06	106.78
28	E6	1001	CYC	C1A-C2A-C3A	-3.36	103.06	106.78
26	e8	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
26	e6	202	PEB	CHB-C4B-NB	-3.36	124.17	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	301	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
26	aB	202	PEB	CHA-C1B-NB	-3.36	117.90	124.93
28	L2	1001	CYC	CMB-C2B-C1B	3.36	128.36	124.17
26	RJ	203	PEB	OA-C1A-C2A	-3.36	123.50	126.17
26	c7	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
28	J7	1003	CYC	C2C-C1C-NC	3.36	111.17	108.27
26	i2	201	PEB	CHC-C1D-ND	-3.36	110.05	113.95
26	oE	202	PEB	CHA-C1B-NB	-3.36	117.90	124.93
26	Z2	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
26	LA	201	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
26	j2	201	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
26	fl	202	PEB	CHC-C1D-ND	-3.36	110.05	113.95
26	G4	202	PEB	OA-C1A-C2A	-3.36	123.50	126.17
26	RI	202	PEB	CHA-C1B-NB	-3.36	117.91	124.93
26	YG	203	PEB	C3D-C4D-ND	3.36	113.85	107.26
26	tE	201	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
26	A9	304	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
26	XG	203	PEB	OD-C4D-ND	-3.36	120.95	125.93
26	U1	201	PEB	C3B-C4B-NB	3.36	114.94	110.05
26	k1	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
26	B1	203	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
26	B4	203	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
26	G4	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
26	O7	203	PEB	C3B-C4B-NB	3.36	114.93	110.05
26	i4	201	PEB	OA-C1A-C2A	-3.36	123.50	126.17
26	FJ	202	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
26	j7	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
26	C9	201	PEB	CBC-CAC-C2C	3.36	118.35	112.62
28	E7	1001	CYC	C2A-C1A-NA	3.36	114.93	110.05
26	wG	303	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	AI	301	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	GC	202	PEB	CHA-C1B-NB	-3.36	117.91	124.93
26	p4	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	DB	1002	PEB	CAB-C3B-C4B	3.36	130.95	125.01
26	A9	304	PEB	CHA-C1B-NB	-3.36	117.91	124.93
26	R2	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
26	aI	202	PEB	CMB-C2B-C1B	3.36	130.23	125.06
26	B9	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	bI	201	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
26	AJ	301	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
26	pE	201	PEB	OD-C4D-ND	-3.36	120.96	125.93
26	H3	201	PEB	C1C-CHB-C4B	3.36	132.82	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	v4	202	PEB	C1C-CHB-C4B	3.36	132.82	128.81
28	EI	1001	CYC	CHB-C4A-NA	-3.36	117.91	124.93
26	A3	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
26	u1	202	PEB	C1B-C2B-C3B	-3.36	102.66	106.51
26	P3	202	PEB	OD-C4D-ND	-3.36	120.96	125.93
26	S9	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
26	K8	202	PEB	OD-C4D-C3D	-3.36	121.86	129.46
26	V4	201	PEB	CMB-C2B-C1B	3.36	130.23	125.06
26	l8	202	PEB	CMB-C2B-C1B	3.36	130.23	125.06
26	PI	203	PEB	CAB-C3B-C4B	3.36	130.94	125.01
28	E6	1001	CYC	C2A-C1A-NA	3.35	114.93	110.05
26	C5	202	PEB	C2A-C1A-NA	3.35	111.17	108.27
26	H9	203	PEB	C3D-C4D-ND	3.35	113.84	107.26
26	FD	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
26	jA	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
26	HC	202	PEB	OD-C4D-ND	-3.35	120.96	125.93
26	QG	201	PEB	OD-C4D-ND	-3.35	120.96	125.93
27	xG	301	PUB	OD-C4D-ND	-3.35	120.96	125.93
26	DJ	202	PEB	CHA-C4A-NA	3.35	129.19	125.20
26	h2	201	PEB	CMA-C2A-C1A	-3.35	105.17	112.40
26	D3	203	PEB	C3B-C4B-NB	3.35	114.93	110.05
28	C6	1001	CYC	CHB-C4A-NA	-3.35	117.92	124.93
26	EJ	202	PEB	CMB-C2B-C1B	3.35	130.23	125.06
26	F9	202	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
26	eD	401	PEB	C2A-C1A-NA	3.35	111.16	108.27
26	R2	201	PEB	CHA-C1B-NB	-3.35	117.92	124.93
26	OA	203	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
26	wG	303	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
26	UE	202	PEB	OD-C4D-ND	-3.35	120.96	125.93
26	a2	203	PEB	CHC-C1D-ND	-3.35	110.05	113.95
26	H3	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
28	DF	1001	CYC	CMA-C3A-C4A	3.35	130.23	125.06
26	gG	203	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
26	DE	201	PEB	OD-C4D-ND	-3.35	120.96	125.93
27	QA	201	PUB	OD-C4D-C3D	-3.35	124.40	128.04
28	E6	1001	CYC	CHB-C4A-NA	-3.35	117.92	124.93
26	JC	202	PEB	OD-C4D-ND	-3.35	120.96	125.93
26	S3	201	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
26	QF	202	PEB	CHA-C1B-C2B	3.35	133.52	124.90
27	xE	306	PUB	C1C-C2C-C3C	-3.35	103.07	106.78
28	EB	1001	CYC	C1A-C2A-C3A	-3.35	103.07	106.78
26	BD	201	PEB	CHA-C1B-NB	-3.35	117.92	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	NJ	201	PUB	OD-C4D-ND	-3.35	120.97	125.93
26	OI	202	PEB	CHB-C4B-NB	-3.35	124.18	128.83
26	VJ	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
28	CF	1001	CYC	CHD-C4C-NC	3.35	129.19	125.20
26	b6	201	PEB	C3B-C4B-NB	3.35	114.92	110.05
28	CF	1001	CYC	C1B-NB-C4B	-3.35	106.40	110.67
26	C3	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
26	B4	203	PEB	OA-C1A-C2A	-3.35	123.51	126.17
28	QH	1001	CYC	OC-C1C-C2C	-3.35	123.51	126.17
26	T8	202	PEB	CHA-C1B-NB	-3.35	117.92	124.93
28	CF	1001	CYC	C1B-C2B-C3B	-3.35	104.38	107.87
26	LC	203	PEB	C3B-C4B-NB	3.35	114.92	110.05
26	f7	203	PEB	CHB-C4B-NB	-3.35	124.18	128.83
26	d8	201	PEB	CHB-C4B-NB	-3.35	124.18	128.83
28	CH	1001	CYC	CHA-C1A-NA	-3.35	124.18	128.83
26	b1	501	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
26	DE	201	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
26	wE	301	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
26	A2	305	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
27	K3	203	PUB	OA-C1A-NA	-3.35	120.97	125.93
28	H2	1001	CYC	C2A-C1A-NA	3.35	114.92	110.05
26	q4	202	PEB	CHA-C1B-NB	-3.35	117.93	124.93
26	YD	301	PEB	CMD-C2D-C3D	3.35	134.79	130.06
26	y4	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
26	S4	202	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
26	V4	203	PEB	CMC-C3C-C2C	-3.35	118.63	124.94
26	sG	202	PEB	CHA-C1B-NB	-3.35	117.93	124.93
28	N7	1001	CYC	C1B-C2B-C3B	-3.35	104.38	107.87
26	eE	203	PEB	CHA-C1B-C2B	3.35	133.51	124.90
26	N2	1002	PEB	OD-C4D-ND	-3.35	120.97	125.93
26	kI	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
26	KD	202	PEB	C3D-C4D-ND	3.35	113.83	107.26
26	fB	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
26	Q6	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
26	y1	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
26	gG	203	PEB	OD-C4D-ND	-3.35	120.97	125.93
26	c2	201	PEB	C3B-C4B-NB	3.35	114.92	110.05
26	J5	202	PEB	C3B-C4B-NB	3.35	114.92	110.05
26	iI	202	PEB	CHB-C4B-NB	-3.35	124.18	128.83
26	h7	203	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
26	IC	203	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
26	U7	202	PEB	OD-C4D-ND	-3.35	120.97	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W7	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
26	LE	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
26	l2	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
26	ZF	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
26	LJ	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
28	sH	1001	CYC	CHB-C4A-C3A	3.35	133.51	124.90
26	g1	203	PEB	C2A-C1A-NA	3.35	111.16	108.27
26	NJ	204	PEB	C2A-C1A-NA	3.35	111.16	108.27
26	e4	202	PEB	CHA-C1B-NB	-3.35	117.93	124.93
26	b4	501	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
26	A9	303	PEB	C3D-C4D-ND	3.35	113.82	107.26
26	mI	201	PEB	CHC-C1D-ND	-3.35	110.06	113.95
26	OI	201	PEB	C4B-NB-C1B	-3.35	100.21	106.51
26	B5	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
26	dB	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
26	RE	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
26	T6	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
28	lH	1001	CYC	CAB-C3B-C4B	3.35	126.66	121.38
26	S7	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
26	KA	201	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
26	z4	201	PEB	CMB-C2B-C1B	3.34	130.22	125.06
26	V3	202	PEB	CHC-C1D-ND	-3.34	110.06	113.95
26	SE	203	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
26	GG	203	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
26	HI	1002	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	LA	201	PEB	CMA-C2A-C1A	-3.34	105.19	112.40
26	H4	203	PEB	C1C-CHB-C4B	-3.34	124.81	128.81
26	AA	302	PEB	OA-C1A-C2A	-3.34	123.51	126.17
26	m2	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
26	A9	304	PEB	CHC-C4C-C3C	-3.34	124.63	130.34
26	u1	202	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
26	U7	202	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
26	AD	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	xE	302	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	EG	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	c4	202	PEB	C2A-C1A-NA	3.34	111.16	108.27
26	g6	202	PEB	C2A-C1A-NA	3.34	111.16	108.27
26	m2	201	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	HB	1002	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	dI	201	PEB	CMB-C2B-C1B	3.34	130.21	125.06
26	SA	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	eB	203	PEB	CHC-C4C-C3C	-3.34	124.64	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	LI	1001	CYC	C2A-C1A-NA	3.34	114.91	110.05
26	LD	202	PEB	CHA-C4A-NA	3.34	129.18	125.20
26	PJ	203	PEB	OD-C4D-ND	-3.34	120.98	125.93
27	21	403	PUB	OA-C1A-NA	-3.34	120.98	125.93
26	V7	202	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	W7	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	m1	202	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
26	J1	203	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
26	J4	201	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
26	PE	202	PEB	OA-C1A-C2A	-3.34	123.52	126.17
26	h6	203	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	mG	201	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	TJ	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	SA	203	PEB	OD-C4D-C3D	-3.34	121.89	129.46
26	H9	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	jF	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
26	b1	501	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	s1	202	PEB	CHA-C1B-NB	-3.34	117.94	124.93
26	PE	201	PEB	CHC-C1D-ND	-3.34	110.07	113.95
26	E3	201	PEB	CMB-C2B-C1B	3.34	130.21	125.06
26	T6	202	PEB	CMB-C2B-C1B	3.34	130.21	125.06
26	YI	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	L1	202	PEB	CHA-C1B-NB	-3.34	117.95	124.93
26	Y2	202	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	Y3	301	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	b4	501	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	V1	202	PEB	OA-C1A-C2A	-3.34	123.52	126.17
26	M4	403	PEB	OA-C1A-C2A	-3.34	123.52	126.17
26	I1	202	PEB	CHB-C4B-NB	-3.34	124.19	128.83
26	P9	203	PEB	CMB-C2B-C1B	3.34	130.21	125.06
27	A8	303	PUB	C1C-C2C-C3C	-3.34	103.09	106.78
26	q4	203	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
26	iA	202	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
26	UG	201	PEB	CAC-CBC-CGC	3.34	123.12	113.76
26	EG	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
26	hG	201	PEB	CAB-CBB-CGB	-3.34	106.42	113.60
26	Z2	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
26	ZE	202	PEB	OD-C4D-ND	-3.34	120.98	125.93
26	d2	202	PEB	CMB-C2B-C1B	3.34	130.21	125.06
26	mA	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	mI	201	PEB	C3B-C4B-NB	3.34	114.91	110.05
26	D1	202	PEB	CHA-C1B-NB	-3.34	117.95	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AF	305	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
26	F4	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
26	g2	201	PEB	CMB-C2B-C1B	3.34	130.20	125.06
26	yE	301	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	BD	202	PEB	C1B-C2B-C3B	-3.34	102.68	106.51
26	P9	202	PEB	CHA-C1B-C2B	3.34	133.48	124.90
26	A8	301	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
26	KG	201	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
28	IF	1001	CYC	C1A-C2A-C3A	-3.34	103.09	106.78
26	QE	203	PEB	CMA-C2A-C1A	-3.34	105.21	112.40
26	G3	201	PEB	OD-C4D-C3D	-3.34	121.90	129.46
26	QA	204	PEB	OD-C4D-C3D	-3.34	121.90	129.46
26	Y2	201	PEB	C3B-C4B-NB	3.34	114.90	110.05
26	DG	203	PEB	OA-C1A-C2A	-3.34	123.52	126.17
26	OB	203	PEB	C1B-C2B-C3B	-3.34	102.68	106.51
26	k7	202	PEB	CMB-C2B-C1B	3.34	130.20	125.06
26	f8	201	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
26	aE	202	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
26	F1	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
26	s1	203	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	w4	204	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	g6	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	cE	203	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	RI	202	PEB	C2A-C1A-NA	3.34	111.15	108.27
26	kI	202	PEB	CAB-C3B-C4B	3.34	130.91	125.01
26	F4	202	PEB	OD-C4D-ND	-3.34	120.99	125.93
26	R4	202	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
26	T9	201	PEB	C3D-C4D-ND	3.34	113.80	107.26
26	SG	203	PEB	C3D-C4D-ND	3.34	113.80	107.26
26	SE	203	PEB	OD-C4D-ND	-3.34	120.99	125.93
26	aA	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
26	gA	201	PEB	CHA-C1B-C2B	3.33	133.48	124.90
26	R3	203	PEB	C3B-C4B-NB	3.33	114.90	110.05
26	hA	201	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	gE	203	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	f6	202	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
26	dA	201	PEB	CMB-C2B-C1B	3.33	130.20	125.06
26	GJ	201	PEB	CMB-C2B-C1B	3.33	130.20	125.06
26	WE	202	PEB	CHC-C4C-C3C	-3.33	124.65	130.34
26	GE	203	PEB	C3D-C4D-ND	3.33	113.80	107.26
26	D4	201	PEB	CHB-C4B-NB	-3.33	124.20	128.83
26	IG	203	PEB	CHA-C1B-NB	-3.33	117.96	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L1	203	PEB	C2A-C1A-NA	3.33	111.15	108.27
26	M3	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
26	nE	201	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	e1	201	PEB	CHC-C4C-C3C	-3.33	124.65	130.34
26	GA	202	PEB	C1C-CHB-C4B	-3.33	124.83	128.81
26	AA	301	PEB	CMB-C2B-C1B	3.33	130.20	125.06
26	R1	201	PEB	CHC-C4C-C3C	-3.33	124.65	130.34
26	T4	201	PEB	CHC-C4C-C3C	3.33	136.02	130.34
26	D7	1002	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	gB	201	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	PB	201	PEB	CHA-C1B-NB	-3.33	117.96	124.93
26	TA	202	PEB	OA-C1A-C2A	-3.33	123.52	126.17
26	AA	301	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
26	kE	203	PEB	C2A-C1A-NA	3.33	111.15	108.27
26	RG	202	PEB	CAB-C3B-C4B	3.33	130.91	125.01
26	a1	201	PEB	OD-C4D-ND	-3.33	120.99	125.93
26	YF	201	PEB	CHA-C1B-NB	-3.33	117.96	124.93
28	JI	1001	CYC	OB-C4B-C3B	-3.33	124.42	128.04
26	d7	203	PEB	C3D-C4D-ND	3.33	113.80	107.26
26	SE	203	PEB	C3D-C4D-ND	3.33	113.80	107.26
26	QF	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	JD	202	PEB	CHA-C1B-NB	-3.33	117.96	124.93
26	M9	201	PEB	CAB-CBB-CGB	-3.33	106.43	113.60
26	k6	201	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
26	i2	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	S4	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	f6	203	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	bF	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
28	JF	1001	CYC	C4A-C3A-C2A	-3.33	102.68	106.51
26	s4	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
26	L5	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
26	R9	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	aB	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	MJ	201	PEB	CAB-CBB-CGB	-3.33	106.44	113.60
26	c8	201	PEB	CAB-C3B-C4B	3.33	130.90	125.01
26	ED	202	PEB	OA-C1A-C2A	-3.33	123.53	126.17
26	lA	203	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	V4	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	wE	301	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
26	XD	202	PEB	OD-C4D-C3D	-3.33	121.91	129.46
26	O4	202	PEB	CHC-C4C-C3C	-3.33	124.66	130.34
28	D2	1001	CYC	CHB-C4A-NA	-3.33	117.97	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aG	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	VA	201	PEB	C3B-C4B-NB	3.33	114.89	110.05
26	KE	203	PEB	C3D-C4D-ND	3.33	113.79	107.26
26	s1	203	PEB	CHC-C4C-C3C	-3.33	124.66	130.34
26	gF	202	PEB	CAA-C3A-C2A	-3.33	105.94	114.26
26	LJ	202	PEB	OA-C1A-C2A	-3.33	123.53	126.17
26	eB	201	PEB	CHA-C1B-NB	-3.33	117.97	124.93
26	QI	201	PEB	CHA-C1B-NB	-3.33	117.97	124.93
26	SI	202	PEB	CMB-C2B-C1B	3.33	130.19	125.06
28	DF	1003	CYC	C2A-C1A-NA	3.33	114.89	110.05
26	c1	202	PEB	OD-C4D-ND	-3.33	121.00	125.93
26	JD	202	PEB	CHB-C4B-NB	-3.33	124.21	128.83
26	B4	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
27	wG	304	PUB	C1C-C2C-C3C	-3.33	103.10	106.78
27	K3	203	PUB	OD-C4D-ND	-3.33	121.00	125.93
26	S6	203	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
26	fG	202	PEB	CMC-C3C-C2C	-3.33	118.67	124.94
26	YA	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	mE	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	UE	203	PEB	OD-C4D-ND	-3.33	121.00	125.93
26	IA	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	LD	203	PEB	CHB-C4B-NB	-3.33	124.21	128.83
26	U4	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
26	FG	202	PEB	OA-C1A-C2A	-3.33	123.53	126.17
26	dF	203	PEB	CHA-C1B-C2B	3.33	133.45	124.90
26	kG	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
28	NI	1001	CYC	C1A-C2A-C3A	-3.33	103.10	106.78
26	WG	202	PEB	CHB-C4B-NB	-3.33	124.21	128.83
26	j4	202	PEB	CHC-C4C-C3C	-3.33	124.66	130.34
26	O7	202	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
26	f7	203	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
26	PA	201	PEB	CAB-C3B-C4B	3.33	130.89	125.01
26	e3	401	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	SE	203	PEB	C2A-C1A-NA	3.33	111.14	108.27
26	j4	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	Y6	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	L8	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
26	UA	203	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
28	JF	1003	CYC	C1B-NB-C4B	-3.32	106.44	110.67
26	DE	203	PEB	OD-C4D-ND	-3.32	121.00	125.93
26	dB	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
26	HE	201	PEB	CMA-C2A-C1A	-3.32	105.24	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e2	201	PEB	C3B-C4B-NB	3.32	114.88	110.05
26	fB	201	PEB	C3B-C4B-NB	3.32	114.88	110.05
26	C1	202	PEB	C4B-C3B-C2B	-3.32	103.10	106.78
26	k2	202	PEB	C4B-C3B-C2B	-3.32	103.10	106.78
26	C4	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
26	YD	304	PEB	CMB-C2B-C1B	3.32	130.18	125.06
26	Q2	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
26	W3	201	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
26	j2	201	PEB	CHC-C1D-ND	-3.32	110.09	113.95
26	aB	201	PEB	CHB-C4B-NB	-3.32	124.22	128.83
26	DG	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	j7	203	PEB	CHA-C1B-NB	-3.32	117.98	124.93
26	F5	201	PEB	OA-C1A-C2A	-3.32	123.53	126.17
28	L7	1001	CYC	CHB-C1B-NB	-3.32	118.92	126.06
26	P4	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	FA	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	f2	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
26	fI	202	PEB	CMB-C2B-C1B	3.32	130.18	125.06
26	UA	202	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	c8	202	PEB	C3B-C4B-NB	3.32	114.88	110.05
26	nE	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
26	RJ	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
26	w1	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
27	xE	305	PUB	CHA-C1B-C2B	-3.32	124.67	130.34
26	SB	203	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	eI	201	PEB	C2A-C1A-NA	3.32	111.14	108.27
26	F7	1002	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	cI	203	PEB	CHC-C4C-C3C	-3.32	124.67	130.34
26	V7	202	PEB	CHC-C1D-ND	-3.32	110.09	113.95
26	K8	202	PEB	CMD-C2D-C3D	3.32	134.75	130.06
27	yE	303	PUB	CHC-C1D-ND	-3.32	109.52	113.72
26	P6	201	PEB	CHA-C1B-NB	-3.32	117.99	124.93
26	VD	202	PEB	CHA-C1B-NB	-3.32	117.99	124.93
26	QB	203	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	ME	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	tG	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	24	404	PEB	CHC-C4C-C3C	-3.32	124.67	130.34
26	m6	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	T2	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
26	V8	202	PEB	CAB-C3B-C2B	3.32	134.06	127.88
28	C7	1001	CYC	CMB-C2B-C1B	3.32	128.31	124.17
26	QD	202	PEB	OD-C4D-ND	-3.32	121.01	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GD	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
26	L5	203	PEB	CBB-CAB-C3B	-3.32	103.41	112.63
26	jA	203	PEB	C2A-C1A-NA	3.32	111.13	108.27
26	YE	203	PEB	C2A-C1A-NA	3.32	111.13	108.27
26	L1	201	PEB	CHA-C1B-NB	-3.32	117.99	124.93
26	aG	202	PEB	OD-C4D-ND	-3.32	121.01	125.93
26	DD	203	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	IG	202	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	MG	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
26	mF	202	PEB	CHC-C4C-C3C	-3.32	124.68	130.34
26	lA	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
26	JC	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
26	E1	202	PEB	C3B-C4B-NB	3.32	114.88	110.05
26	T8	202	PEB	C3B-C4B-NB	3.32	114.88	110.05
28	MI	1001	CYC	C2A-C1A-NA	3.32	114.88	110.05
26	h8	201	PEB	CMB-C2B-C1B	3.32	130.17	125.06
26	oG	202	PEB	C3D-C4D-ND	3.32	113.77	107.26
26	cE	202	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	U7	203	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
26	XJ	201	PEB	CHA-C1B-NB	-3.32	117.99	124.93
26	E1	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
28	IB	1001	CYC	C1B-C2B-C3B	-3.32	104.41	107.87
26	HG	202	PEB	OA-C1A-C2A	-3.32	123.54	126.17
26	h7	203	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	UG	202	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	L4	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
26	e4	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
26	HD	201	PEB	CHB-C4B-NB	-3.32	124.23	128.83
26	E3	201	PEB	C1C-CHB-C4B	3.32	132.77	128.81
26	mE	203	PEB	C1C-CHB-C4B	3.32	132.77	128.81
28	I6	1001	CYC	C1B-C2B-C3B	-3.32	104.41	107.87
26	UB	203	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
26	cA	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
26	YD	301	PEB	CHC-C4C-C3C	3.32	135.99	130.34
26	G6	1002	PEB	C2A-C1A-NA	3.32	111.13	108.27
28	tH	1001	CYC	OC-C1C-C2C	-3.32	123.54	126.17
26	LA	202	PEB	CHC-C1D-ND	-3.31	110.10	113.95
26	LJ	203	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
26	G4	202	PEB	CHB-C4B-NB	-3.31	124.23	128.83
26	F4	203	PEB	CHC-C4C-C3C	-3.31	124.68	130.34
26	RJ	203	PEB	C2A-C1A-NA	3.31	111.13	108.27
26	B1	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SF	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	SA	203	PEB	CHB-C4B-NB	-3.31	124.23	128.83
26	iE	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
26	S4	201	PEB	C3B-C4B-NB	3.31	114.87	110.05
26	LJ	201	PEB	CHC-C1D-ND	-3.31	110.10	113.95
26	N1	202	PEB	OD-C4D-ND	-3.31	121.02	125.93
26	G5	201	PEB	C2A-C1A-NA	3.31	111.13	108.27
26	tG	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
26	lB	202	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
26	VD	203	PEB	CAB-C3B-C4B	3.31	130.87	125.01
26	AD	201	PEB	C3D-C4D-ND	3.31	113.76	107.26
26	Q7	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
26	K3	201	PEB	C3B-C4B-NB	3.31	114.87	110.05
26	m6	201	PEB	C3B-C4B-NB	3.31	114.87	110.05
26	OG	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
26	C8	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	HC	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	KD	201	PEB	CHB-C4B-NB	-3.31	124.23	128.83
26	c1	203	PEB	OD-C4D-ND	-3.31	121.02	125.93
26	Y8	203	PEB	OD-C4D-C3D	-3.31	121.95	129.46
26	KA	203	PEB	CHC-C1D-ND	-3.31	110.10	113.95
26	wG	302	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
28	H7	1001	CYC	C4A-C3A-C2A	-3.31	102.70	106.51
26	D2	1002	PEB	CHC-C4C-C3C	-3.31	124.69	130.34
26	FJ	202	PEB	CHC-C4C-C3C	-3.31	124.69	130.34
26	V2	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
26	d8	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	eB	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	H6	1002	PEB	C3B-C4B-NB	3.31	114.87	110.05
26	l4	202	PEB	CHC-C1D-ND	-3.31	110.10	113.95
26	l7	201	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
26	f6	202	PEB	CMB-C2B-C1B	3.31	130.16	125.06
26	J9	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
26	lF	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
28	LH	1001	CYC	CMC-C2C-C3C	3.31	127.18	113.83
26	YJ	201	PEB	CHC-C4C-C3C	-3.31	124.69	130.34
26	V8	202	PEB	CBB-CAB-C3B	3.31	121.83	112.63
26	UI	201	PEB	OD-C4D-C3D	-3.31	121.96	129.46
26	AI	305	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
28	GB	1001	CYC	C1A-C2A-C3A	-3.31	103.12	106.78
26	KJ	202	PEB	C1C-CHB-C4B	-3.31	124.86	128.81
26	a6	202	PEB	CHA-C1B-NB	-3.31	118.01	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P1	201	PEB	C2A-C1A-NA	3.31	111.13	108.27
26	d8	201	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
26	IG	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
26	D6	1002	PEB	C3B-C4B-NB	3.31	114.86	110.05
28	M2	1001	CYC	CHB-C4A-NA	-3.31	118.01	124.93
26	JC	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	J8	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
26	BD	203	PEB	OD-C4D-ND	-3.31	121.03	125.93
26	mE	201	PEB	CHA-C4A-NA	3.31	129.14	125.20
26	H1	201	PEB	C3B-C4B-NB	3.31	114.86	110.05
26	xG	302	PEB	C2A-C1A-NA	3.31	111.12	108.27
26	HC	201	PEB	CHC-C4C-C3C	-3.31	124.69	130.34
26	z4	201	PEB	CHC-C1D-ND	-3.31	110.11	113.95
26	lB	201	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
26	YB	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
26	RI	202	PEB	OD-C4D-ND	-3.31	121.03	125.93
26	A6	301	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
26	MD	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
26	Y8	201	PEB	CHB-C4B-NB	-3.31	124.24	128.83
26	mI	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
26	IA	203	PEB	C2A-C1A-NA	3.31	111.12	108.27
26	LB	1002	PEB	C2A-C1A-NA	3.31	111.12	108.27
26	fF	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
26	S1	201	PEB	CHC-C1D-ND	-3.31	110.11	113.95
26	s1	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
26	sG	201	PEB	CHC-C4C-C3C	-3.31	124.70	130.34
26	L9	203	PEB	C3B-C4B-NB	3.31	114.86	110.05
26	ZG	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
26	kB	202	PEB	CMB-C2B-C1B	3.31	130.16	125.06
26	q4	201	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
28	J2	1001	CYC	C1A-C2A-C3A	-3.31	103.12	106.78
26	c2	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	YG	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
26	N9	203	PEB	OD-C4D-ND	-3.31	121.03	125.93
26	wG	301	PEB	CHC-C4C-C3C	-3.31	124.70	130.34
26	c2	201	PEB	C2A-C1A-NA	3.31	111.12	108.27
26	f7	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
26	TB	202	PEB	CMB-C2B-C1B	3.31	130.16	125.06
26	X8	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
26	Q4	202	PEB	CHC-C4C-C3C	-3.31	124.70	130.34
26	LF	1002	PEB	OD-C4D-C3D	-3.31	121.97	129.46
26	u1	203	PEB	OD-C4D-ND	-3.31	121.03	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	wE	303	PEB	OD-C4D-ND	-3.31	121.03	125.93
26	hA	201	PEB	CMB-C2B-C1B	3.31	130.15	125.06
26	IE	203	PEB	CMB-C2B-C1B	3.31	130.15	125.06
26	TI	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
26	W8	202	PEB	CBC-CAC-C2C	-3.30	106.98	112.62
26	W4	202	PEB	OD-C4D-ND	-3.30	121.03	125.93
26	y4	201	PEB	OD-C4D-ND	-3.30	121.03	125.93
26	hI	201	PEB	OD-C4D-ND	-3.30	121.03	125.93
26	K5	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	oG	202	PEB	CHA-C1B-NB	-3.30	118.02	124.93
26	FF	1002	PEB	C4B-C3B-C2B	-3.30	103.12	106.78
26	QJ	201	PEB	CMB-C2B-C1B	3.30	130.15	125.06
26	y4	201	PEB	C3B-C4B-NB	3.30	114.86	110.05
26	eB	202	PEB	C3B-C4B-NB	3.30	114.86	110.05
26	XD	202	PEB	C1B-C2B-C3B	-3.30	102.71	106.51
26	U3	202	PEB	C1C-CHB-C4B	3.30	132.76	128.81
26	AJ	301	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	cI	203	PEB	C3B-C4B-NB	3.30	114.86	110.05
26	WG	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	SG	202	PEB	CBC-CAC-C2C	-3.30	106.98	112.62
26	aA	204	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	cB	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	JF	1002	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	gF	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	qG	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
26	iG	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
26	W6	201	PEB	CHC-C4C-C3C	-3.30	124.70	130.34
26	AA	302	PEB	CHC-C4C-C3C	-3.30	124.70	130.34
26	ND	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
26	UB	203	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	WE	201	PEB	CHA-C1B-C2B	3.30	133.39	124.90
28	J7	1003	CYC	CMB-C2B-C1B	3.30	128.29	124.17
26	QJ	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	iE	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
28	rH	1001	CYC	OC-C1C-C2C	-3.30	123.55	126.17
26	lI	202	PEB	CMB-C2B-C1B	3.30	130.15	125.06
26	YB	202	PEB	CBC-CAC-C2C	3.30	118.26	112.62
27	YD	302	PUB	CHA-C1B-C2B	-3.30	124.70	130.34
26	h8	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	h8	202	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	RB	201	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	mF	201	PEB	OD-C4D-ND	-3.30	121.04	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U9	201	PEB	CMB-C2B-C1B	3.30	130.15	125.06
26	C5	203	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	d6	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	m6	203	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
28	LH	1001	CYC	C4D-CHA-C1A	3.30	132.75	128.81
26	E3	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
26	k4	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
26	VJ	201	PEB	CHC-C4C-C3C	-3.30	124.71	130.34
26	T2	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	P4	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	kE	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	O6	201	PEB	CHA-C1B-NB	-3.30	118.03	124.93
26	D8	202	PEB	CMB-C2B-C1B	3.30	130.15	125.06
26	y1	201	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	A9	301	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	DD	201	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	Q9	201	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	SD	202	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	e6	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	eG	202	PEB	CHC-C1D-ND	-3.30	110.11	113.95
26	SE	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
26	XE	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
26	KG	202	PEB	CMA-C2A-C1A	-3.30	105.29	112.40
26	Q7	201	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	O8	201	PEB	C2A-C1A-NA	3.30	111.12	108.27
28	G7	1001	CYC	CHA-C1A-NA	-3.30	124.25	128.83
26	NJ	202	PEB	C1C-CHB-C4B	3.30	132.75	128.81
26	A2	301	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
26	TG	202	PEB	CHB-C4B-C3B	-3.30	117.70	125.32
26	j8	201	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	A9	301	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	C3	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
26	fB	202	PEB	CMB-C2B-C1B	3.30	130.15	125.06
28	JF	1003	CYC	CMA-C3A-C4A	3.30	130.15	125.06
26	L9	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	yG	301	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	OJ	201	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	O1	201	PEB	C2A-C1A-NA	3.30	111.12	108.27
26	e6	201	PEB	CHA-C1B-NB	-3.30	118.03	124.93
26	bB	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
28	HB	1001	CYC	C4A-C3A-C2A	-3.30	102.72	106.51
26	H3	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	ME	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	fl	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	jA	202	PEB	OD-C4D-ND	-3.30	121.04	125.93
26	s1	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
26	U1	202	PEB	CHC-C4C-C3C	-3.30	124.71	130.34
26	RF	202	PEB	OD-C4D-C3D	-3.30	121.99	129.46
26	HG	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
26	bB	201	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	v1	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
26	A7	302	PEB	CMB-C2B-C1B	3.30	130.14	125.06
26	vE	201	PEB	CAB-CBB-CGB	-3.30	106.51	113.60
27	BA	302	PUB	CHC-C1D-ND	-3.30	109.55	113.72
26	F8	202	PEB	C3B-C4B-NB	3.30	114.85	110.05
26	cG	202	PEB	CHC-C1D-ND	-3.30	110.12	113.95
26	M9	202	PEB	CHB-C4B-NB	-3.30	124.25	128.83
26	O6	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
26	OG	202	PEB	CHB-C4B-C3B	-3.30	117.70	125.32
26	V1	202	PEB	CHA-C1B-NB	-3.30	118.04	124.93
26	R2	203	PEB	CAB-CBB-CGB	3.30	120.70	113.60
26	KG	203	PEB	CMB-C2B-C1B	3.30	130.14	125.06
26	V3	202	PEB	OD-C4D-ND	-3.30	121.05	125.93
26	CE	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
26	AG	202	PEB	OD-C4D-ND	-3.30	121.05	125.93
26	mI	201	PEB	OD-C4D-ND	-3.30	121.05	125.93
26	U1	202	PEB	CHA-C1B-NB	-3.30	118.04	124.93
26	L2	1002	PEB	CHB-C4B-NB	-3.30	124.25	128.83
26	V1	201	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
26	L9	203	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
28	J2	1001	CYC	C4A-C3A-C2A	-3.30	102.72	106.51
26	V1	202	PEB	C3B-C4B-NB	3.30	114.84	110.05
26	n4	201	PEB	CBC-CAC-C2C	-3.30	107.00	112.62
26	H4	203	PEB	CMB-C2B-C1B	3.30	130.14	125.06
28	BB	1001	CYC	C2B-C1B-NB	3.30	111.81	106.99
26	SI	201	PEB	C4B-NB-C1B	-3.30	100.30	106.51
26	Z7	201	PEB	C2A-C1A-NA	3.30	111.11	108.27
26	a8	201	PEB	C2A-C1A-NA	3.30	111.11	108.27
26	YG	202	PEB	C2A-C1A-NA	3.30	111.11	108.27
26	YE	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	FJ	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
26	R4	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	D8	202	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	S4	201	PEB	CAB-C3B-C4B	3.29	130.84	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q6	201	PEB	OD-C4D-ND	-3.29	121.05	125.93
26	BE	202	PEB	OD-C4D-ND	-3.29	121.05	125.93
26	I1	201	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	ZG	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	Y2	203	PEB	CAB-CBB-CGB	3.29	120.69	113.60
26	hG	201	PEB	OD-C4D-ND	-3.29	121.05	125.93
26	WG	202	PEB	CHC-C1D-ND	-3.29	110.12	113.95
26	Z1	202	PEB	CHB-C4B-C3B	-3.29	117.71	125.32
26	k6	201	PEB	CHB-C4B-NB	-3.29	124.26	128.83
26	SD	202	PEB	C3D-C4D-ND	3.29	113.72	107.26
26	qE	203	PEB	CHA-C1B-NB	-3.29	118.04	124.93
26	g7	201	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	jI	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	hB	202	PEB	CHC-C1D-ND	-3.29	110.12	113.95
26	LD	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	HF	1002	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	S7	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06
26	p1	202	PEB	CHB-C4B-C3B	3.29	132.93	125.32
26	N4	202	PEB	OD-C4D-ND	-3.29	121.05	125.93
26	AF	302	PEB	OA-C1A-C2A	-3.29	123.56	126.17
26	TE	202	PEB	CHB-C4B-C3B	-3.29	117.71	125.32
26	CG	201	PEB	CHA-C1B-NB	-3.29	118.05	124.93
26	Y1	202	PEB	CHB-C4B-NB	-3.29	124.26	128.83
26	YA	203	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	AF	305	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	c6	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	Q9	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	MA	201	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
26	IE	202	PEB	C3D-C4D-ND	3.29	113.72	107.26
26	gB	201	PEB	CHA-C1B-NB	-3.29	118.05	124.93
26	rE	202	PEB	CHB-C4B-C3B	-3.29	117.72	125.32
26	F1	203	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	a8	203	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	D1	203	PEB	OD-C4D-ND	-3.29	121.05	125.93
26	ZG	201	PEB	OD-C4D-ND	-3.29	121.05	125.93
26	yE	301	PEB	CHA-C1B-NB	-3.29	118.05	124.93
26	eB	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	OD	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	z4	201	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
26	W9	202	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
26	SB	201	PEB	C3B-C4B-NB	3.29	114.84	110.05
26	UB	202	PEB	CHB-C4B-NB	-3.29	124.26	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J7	1001	CYC	CHA-C1A-NA	-3.29	124.26	128.83
26	PE	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	pE	201	PEB	CHC-C1D-ND	-3.29	110.13	113.95
26	S1	202	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
26	H9	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	c2	202	PEB	OD-C4D-C3D	-3.29	122.00	129.46
26	BG	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	M1	401	PEB	CHA-C1B-NB	-3.29	118.05	124.93
26	b7	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	E8	201	PEB	CBC-CAC-C2C	-3.29	107.01	112.62
26	i2	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06
26	OI	201	PEB	CHA-C1B-NB	-3.29	118.05	124.93
26	DG	201	PEB	C3B-C4B-NB	3.29	114.83	110.05
26	A1	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
26	d6	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
26	J4	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	Z8	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	WE	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	HJ	203	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	A7	305	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	YA	201	PEB	CHB-C4B-NB	-3.29	124.26	128.83
26	HA	202	PEB	CAB-C3B-C4B	3.29	130.83	125.01
26	TF	201	PEB	CHC-C1D-ND	-3.29	110.13	113.95
26	B9	203	PEB	OA-C1A-C2A	-3.29	123.56	126.17
26	P9	203	PEB	C3B-C4B-NB	3.29	114.83	110.05
26	W1	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	F8	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
27	Y3	302	PUB	OD-C4D-ND	-3.29	121.06	125.93
26	J5	201	PEB	CHB-C4B-NB	-3.29	124.27	128.83
26	G8	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	GB	1002	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	V3	201	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
26	CA	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
26	JD	203	PEB	CHC-C1D-ND	-3.29	110.13	113.95
26	U1	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	L5	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	c1	201	PEB	CMB-C2B-C1B	3.29	130.13	125.06
26	eG	201	PEB	CHA-C1B-NB	-3.29	118.06	124.93
28	E2	1001	CYC	CHB-C4A-NA	-3.29	118.06	124.93
26	F5	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	mG	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	IJ	201	PEB	C2A-C1A-NA	3.29	111.11	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UB	201	PEB	CBC-CAC-C2C	-3.29	107.01	112.62
28	IB	1001	CYC	C2A-C1A-NA	3.29	114.83	110.05
26	GG	203	PEB	C3D-C4D-ND	3.29	113.71	107.26
26	WG	203	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
26	vG	201	PEB	CHC-C4C-C3C	-3.29	124.73	130.34
26	e2	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
26	oE	203	PEB	OA-C1A-C2A	-3.29	123.56	126.17
26	hI	201	PEB	OA-C1A-C2A	-3.29	123.56	126.17
26	FG	202	PEB	CAB-C3B-C4B	3.29	130.82	125.01
26	L3	202	PEB	CHC-C1D-ND	-3.29	110.13	113.95
26	j2	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	fG	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	T7	201	PEB	CBC-CAC-C2C	-3.29	107.01	112.62
28	D2	1001	CYC	C2A-C1A-NA	3.29	114.83	110.05
26	aA	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	j7	201	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
28	J7	1003	CYC	CMA-C3A-C4A	3.29	130.12	125.06
26	sG	203	PEB	C4B-C3B-C2B	-3.29	103.15	106.78
26	P1	203	PEB	CHC-C4C-C3C	-3.29	124.73	130.34
28	CF	1001	CYC	CMB-C2B-C1B	3.29	128.27	124.17
26	jG	202	PEB	OD-C4D-ND	-3.29	121.06	125.93
26	XD	203	PEB	CMB-C2B-C1B	3.29	130.12	125.06
26	fA	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
26	Y2	202	PEB	C3B-C4B-NB	3.28	114.83	110.05
26	jA	202	PEB	CMD-C2D-C3D	3.28	134.70	130.06
26	O7	203	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
28	C6	1001	CYC	C1B-C2B-C3B	-3.28	104.44	107.87
26	dI	201	PEB	OD-C4D-ND	-3.28	121.06	125.93
26	I5	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	w4	204	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	CC	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	PF	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	wE	303	PEB	C3B-C4B-NB	3.28	114.83	110.05
26	iA	201	PEB	CBC-CAC-C2C	-3.28	107.02	112.62
26	i6	201	PEB	OA-C1A-C2A	-3.28	123.56	126.17
28	PH	1001	CYC	OC-C1C-C2C	-3.28	123.56	126.17
26	GB	1002	PEB	OD-C4D-C3D	-3.28	122.02	129.46
26	j2	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
26	SA	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
26	l8	203	PEB	C3B-C4B-NB	3.28	114.83	110.05
26	ME	201	PEB	CHA-C1B-NB	-3.28	118.06	124.93
26	EE	202	PEB	C1C-CHB-C4B	3.28	132.73	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K9	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06
26	i1	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	b6	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	VB	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	K9	202	PEB	CHC-C1D-ND	-3.28	110.14	113.95
28	JI	1001	CYC	C2C-C1C-NC	3.28	111.10	108.27
28	K7	1001	CYC	CBD-CAD-C3D	-3.28	107.02	112.62
26	F5	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	UG	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	bI	201	PEB	CAB-CBB-CGB	-3.28	106.54	113.60
26	hA	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	j2	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06
26	WD	202	PEB	C3D-C4D-ND	3.28	113.70	107.26
26	g4	203	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	HE	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	UE	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	UF	202	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
26	ZA	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	V8	201	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	lA	203	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	RJ	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	YA	203	PEB	OD-C4D-C3D	-3.28	122.02	129.46
26	P4	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	g2	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
26	AF	302	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
26	sG	201	PEB	C1C-CHB-C4B	3.28	132.73	128.81
26	k8	202	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
26	V2	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	Q6	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	h7	203	PEB	C3D-C4D-ND	3.28	113.70	107.26
26	H8	201	PEB	C3B-C4B-NB	3.28	114.82	110.05
28	IF	1001	CYC	C2A-C1A-NA	3.28	114.82	110.05
26	UE	201	PEB	CMB-C2B-C3B	-3.28	117.21	126.12
26	WF	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	e1	202	PEB	CMC-C3C-C2C	3.28	131.13	124.94
26	d2	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	SF	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	VJ	203	PEB	CHC-C1D-ND	-3.28	110.14	113.95
26	dB	203	PEB	OA-C1A-C2A	-3.28	123.56	126.17
26	j4	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	bE	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	K8	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	iF	201	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
26	S8	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
28	B6	1001	CYC	C2B-C1B-NB	3.28	111.79	106.99
26	PI	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	RJ	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	I8	201	PEB	CHC-C1D-ND	-3.28	110.14	113.95
26	H9	203	PEB	CMB-C2B-C1B	3.28	130.11	125.06
28	E7	1001	CYC	CHA-C1A-NA	-3.28	124.28	128.83
26	OD	201	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	QD	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	M4	402	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	C8	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	T9	201	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
26	m1	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	BJ	203	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	11	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
26	AG	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
26	CJ	201	PEB	C1B-C2B-C3B	-3.28	102.75	106.51
26	xG	304	PEB	OD-C4D-ND	-3.28	121.08	125.93
26	L5	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
26	R3	202	PEB	CHA-C1B-NB	-3.28	118.08	124.93
26	b2	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	c2	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	L5	203	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	EA	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	14	202	PEB	C4B-C3B-C2B	-3.28	103.16	106.78
26	L7	1002	PEB	C4B-C3B-C2B	-3.28	103.16	106.78
26	dB	202	PEB	CHA-C1B-NB	-3.28	118.08	124.93
26	VD	202	PEB	OD-C4D-ND	-3.28	121.08	125.93
26	jE	201	PEB	OA-C1A-NA	3.28	128.91	124.94
26	h6	202	PEB	C3B-C4B-NB	3.28	114.81	110.05
26	qE	202	PEB	CAB-C3B-C4B	3.28	130.81	125.01
26	SF	202	PEB	CHA-C1B-NB	-3.28	118.08	124.93
26	T1	203	PEB	CMB-C2B-C1B	3.28	130.11	125.06
26	mE	201	PEB	CHC-C1D-ND	-3.28	110.14	113.95
26	e2	201	PEB	C2A-C1A-NA	3.28	111.10	108.27
26	yE	301	PEB	C4B-C3B-C2B	-3.28	103.16	106.78
26	FD	201	PEB	CHB-C4B-NB	-3.28	124.28	128.83
26	cE	201	PEB	CAB-C3B-C4B	3.28	130.80	125.01
26	h7	201	PEB	CHA-C1B-NB	-3.28	118.08	124.93
26	G6	1002	PEB	CHC-C1D-ND	-3.28	110.14	113.95
26	XA	201	PEB	CHC-C1D-ND	3.28	117.75	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HB	1002	PEB	OA-C1A-C2A	-3.28	123.57	126.17
26	S3	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
28	EB	1001	CYC	C2A-C1A-NA	3.27	114.81	110.05
26	GA	203	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	U4	201	PEB	C2A-C1A-NA	3.27	111.10	108.27
26	x4	202	PEB	C2A-C1A-NA	3.27	111.10	108.27
26	CG	203	PEB	C2A-C1A-NA	3.27	111.10	108.27
26	J7	1002	PEB	C3B-C4B-NB	3.27	114.81	110.05
28	H2	1001	CYC	CMA-C3A-C4A	3.27	130.11	125.06
26	l7	203	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	UB	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	J9	202	PEB	CHC-C4C-C3C	-3.27	124.75	130.34
27	yE	302	PUB	CHA-C1B-C2B	-3.27	124.75	130.34
26	aG	201	PEB	OA-C1A-C2A	-3.27	123.57	126.17
26	d8	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
28	DI	1001	CYC	C4A-C3A-C2A	-3.27	102.75	106.51
26	fG	202	PEB	CHC-C1D-ND	3.27	117.75	113.95
26	d7	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	oE	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
26	Q1	201	PEB	CBC-CAC-C2C	-3.27	107.03	112.62
26	QA	203	PEB	CHA-C1B-NB	-3.27	118.09	124.93
26	XE	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
28	qH	1001	CYC	OC-C1C-C2C	-3.27	123.57	126.17
26	DG	203	PEB	OD-C4D-ND	-3.27	121.08	125.93
26	FJ	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
26	eE	202	PEB	CAA-C3A-C4A	3.27	121.08	112.67
26	F3	203	PEB	C2A-C1A-NA	3.27	111.09	108.27
26	W6	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
26	h6	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
26	gB	202	PEB	CHA-C1B-NB	-3.27	118.09	124.93
26	L5	203	PEB	C3B-C4B-NB	3.27	114.81	110.05
26	Y3	304	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	jB	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	U1	201	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
26	fA	201	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
26	O3	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
26	AJ	303	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
26	uE	203	PEB	CHA-C1B-NB	-3.27	118.09	124.93
26	X8	201	PEB	C3B-C4B-NB	3.27	114.81	110.05
26	MA	202	PEB	CMA-C2A-C1A	-3.27	105.35	112.40
26	O8	203	PEB	CHA-C1B-NB	-3.27	118.09	124.93
26	mE	203	PEB	CHA-C1B-NB	-3.27	118.09	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D3	203	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	e2	202	PEB	OA-C1A-C2A	-3.27	123.57	126.17
26	EJ	201	PEB	OA-C1A-C2A	-3.27	123.57	126.17
27	KD	203	PUB	OD-C4D-ND	-3.27	121.08	125.93
26	W7	203	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
28	N2	1001	CYC	CMA-C3A-C4A	3.27	130.10	125.06
26	PE	202	PEB	CHB-C4B-C3B	-3.27	117.76	125.32
26	CA	202	PEB	OD-C4D-ND	-3.27	121.08	125.93
26	D1	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	XG	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
26	jI	202	PEB	CMB-C2B-C1B	3.27	130.10	125.06
26	S7	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
26	QF	202	PEB	OA-C1A-C2A	-3.27	123.57	126.17
26	B4	201	PEB	CHB-C4B-C3B	-3.27	117.77	125.32
26	nG	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
26	OD	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
26	U6	202	PEB	CHB-C4B-NB	-3.27	124.29	128.83
26	A6	304	PEB	C1C-CHB-C4B	-3.27	124.90	128.81
26	V1	203	PEB	CMC-C3C-C2C	-3.27	118.78	124.94
26	FE	202	PEB	OA-C1A-C2A	-3.27	123.57	126.17
26	ZF	203	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
26	uG	202	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
26	V1	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
26	R2	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
28	DF	1003	CYC	CMA-C3A-C4A	3.27	130.10	125.06
26	Q3	202	PEB	C3D-C4D-ND	3.27	113.67	107.26
28	L6	1001	CYC	OB-C4B-C3B	-3.27	124.49	128.04
26	gI	201	PEB	C2A-C1A-NA	3.27	111.09	108.27
26	U2	201	PEB	OD-C4D-C3D	-3.27	122.06	129.46
26	N2	1002	PEB	CMB-C2B-C1B	3.27	130.10	125.06
26	Y9	202	PEB	C3B-C4B-NB	3.27	114.80	110.05
26	G4	201	PEB	CHB-C4B-C3B	-3.27	117.77	125.32
26	b6	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
26	IG	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
26	MG	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
26	Y1	201	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
26	GE	203	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
26	IG	202	PEB	C3D-C4D-ND	3.27	113.67	107.26
26	HG	201	PEB	CMA-C2A-C1A	-3.27	105.36	112.40
26	IE	201	PEB	CMA-C2A-C1A	3.27	119.44	112.40
26	G8	202	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
26	S8	203	PEB	C1B-C2B-C3B	-3.27	102.76	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	cI	201	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
26	jI	202	PEB	OD-C4D-C3D	-3.27	122.06	129.46
27	AA	304	PUB	OA-C1A-NA	-3.27	121.09	125.93
26	pE	201	PEB	CHC-C4C-C3C	-3.27	124.77	130.34
28	K7	1001	CYC	CMA-C3A-C4A	3.27	130.09	125.06
26	UE	202	PEB	CHC-C1D-ND	-3.27	110.16	113.95
26	qG	203	PEB	CHB-C4B-NB	-3.27	124.30	128.83
26	R2	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
26	j1	201	PEB	CAB-C3B-C2B	3.27	133.96	127.88
26	e8	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
26	24	405	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
26	g7	202	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
28	B6	1002	CYC	C4A-C3A-C2A	-3.27	102.76	106.51
26	DI	1002	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
26	wE	302	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	Y2	201	PEB	OD-C4D-ND	-3.26	121.09	125.93
26	dG	201	PEB	OD-C4D-ND	-3.26	121.09	125.93
26	J3	201	PEB	C2A-C1A-NA	3.26	111.09	108.27
28	D7	1001	CYC	C2C-C1C-NC	3.26	111.09	108.27
26	i1	202	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
26	k4	201	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
26	dB	201	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
26	O3	201	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	H5	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
26	YI	201	PEB	C3B-C4B-NB	3.26	114.80	110.05
28	II	1001	CYC	C2A-C1A-NA	3.26	114.80	110.05
26	D1	201	PEB	C2A-C1A-NA	3.26	111.09	108.27
26	c1	203	PEB	C2A-C1A-NA	3.26	111.09	108.27
26	GJ	201	PEB	C2A-C1A-NA	3.26	111.09	108.27
26	Z4	201	PEB	CMB-C2B-C1B	3.26	130.09	125.06
26	dA	201	PEB	CHC-C1D-ND	-3.26	110.16	113.95
26	Y4	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
26	j1	202	PEB	CHA-C4A-NA	-3.26	121.33	125.20
26	jI	202	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
26	h4	203	PEB	CMB-C2B-C1B	3.26	130.09	125.06
26	FA	202	PEB	C3B-C4B-NB	3.26	114.79	110.05
26	RG	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
28	KF	1001	CYC	C2C-C1C-NC	3.26	111.08	108.27
26	AI	301	PEB	OD-C4D-ND	-3.26	121.10	125.93
28	E2	1001	CYC	CBD-CAD-C3D	-3.26	107.05	112.62
26	q1	203	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
26	ED	202	PEB	C1B-C2B-C3B	-3.26	102.76	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aE	203	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
26	cI	202	PEB	OD-C4D-C3D	-3.26	122.07	129.46
26	QG	201	PEB	CHC-C1D-ND	-3.26	110.16	113.95
26	iA	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
28	NI	1001	CYC	C2A-C1A-NA	3.26	114.79	110.05
28	H2	1001	CYC	O2A-CGA-CBA	3.26	124.51	114.03
26	cB	201	PEB	CMB-C2B-C1B	3.26	130.09	125.06
26	t4	201	PEB	OD-C4D-ND	-3.26	121.10	125.93
26	L8	202	PEB	CHA-C1B-NB	-3.26	118.11	124.93
26	X4	201	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	bI	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	g4	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
26	Y7	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
26	X4	203	PEB	C2A-C3A-C4A	-3.26	96.46	101.34
26	BA	301	PEB	CMB-C2B-C1B	3.26	130.09	125.06
26	J4	201	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	m7	201	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	PA	202	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	YA	203	PEB	CAB-CBB-CGB	-3.26	106.59	113.60
26	R6	201	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
26	r1	201	PEB	CMC-C3C-C2C	3.26	131.09	124.94
28	MI	1001	CYC	CHA-C1A-NA	-3.26	124.31	128.83
28	E7	1001	CYC	C4A-C3A-C2A	-3.26	102.77	106.51
28	EI	1001	CYC	C4A-C3A-C2A	-3.26	102.77	106.51
26	A8	302	PEB	C4B-C3B-C2B	-3.26	103.18	106.78
26	OE	201	PEB	C4B-C3B-C2B	-3.26	103.18	106.78
26	e4	201	PEB	OD-C4D-ND	-3.26	121.10	125.93
26	eB	201	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
26	H1	203	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
26	D4	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
26	M4	403	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
26	JC	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
26	OI	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
26	z1	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
26	P2	201	PEB	C4B-C3B-C2B	-3.26	103.18	106.78
26	U1	201	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	GA	203	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	vE	201	PEB	CHC-C1D-ND	-3.26	110.17	113.95
28	FF	1001	CYC	C1B-NB-C4B	-3.26	106.52	110.67
26	O8	202	PEB	OD-C4D-C3D	-3.26	122.08	129.46
26	AJ	301	PEB	OD-C4D-C3D	-3.26	122.08	129.46
28	HI	1001	CYC	O2A-CGA-CBA	3.26	124.49	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HJ	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
26	B9	202	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
26	d1	203	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	d4	203	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	u1	201	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	BG	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	cI	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
26	L5	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
26	h4	202	PEB	C3B-C4B-NB	3.26	114.78	110.05
26	O8	202	PEB	C3B-C4B-NB	3.26	114.78	110.05
26	T1	201	PEB	CHC-C4C-C3C	3.26	135.89	130.34
26	A2	304	PEB	OD-C4D-ND	-3.26	121.11	125.93
26	JG	202	PEB	CHA-C1B-NB	-3.26	118.12	124.93
26	E4	202	PEB	CHB-C4B-NB	-3.26	124.31	128.83
26	S4	202	PEB	CMB-C2B-C1B	3.26	130.08	125.06
26	a8	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
26	U4	201	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
26	P1	201	PEB	C3B-C4B-NB	3.26	114.78	110.05
26	DA	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
26	GE	203	PEB	C2A-C1A-NA	3.25	111.08	108.27
26	AJ	304	PEB	C2A-C1A-NA	3.25	111.08	108.27
26	W4	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
26	uE	203	PEB	CMB-C2B-C1B	3.25	130.08	125.06
26	IJ	202	PEB	CHC-C1D-ND	-3.25	110.17	113.95
26	c2	203	PEB	C3B-C4B-NB	3.25	114.78	110.05
26	K4	201	PEB	C3B-C4B-NB	3.25	114.78	110.05
28	BB	1001	CYC	C1B-C2B-C3B	-3.25	104.47	107.87
26	AC	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
26	YB	202	PEB	CMC-C3C-C2C	3.25	131.08	124.94
26	A9	303	PEB	CMB-C2B-C1B	3.25	130.07	125.06
26	cB	202	PEB	C1C-CHB-C4B	-3.25	124.92	128.81
26	24	404	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
26	e6	202	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
26	eE	203	PEB	OA-C1A-C2A	-3.25	123.59	126.17
26	K8	203	PEB	OD-C4D-ND	-3.25	121.11	125.93
26	dA	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
27	yG	303	PUB	OA-C1A-NA	-3.25	121.11	125.93
26	Q9	201	PEB	CHC-C1D-ND	-3.25	110.17	113.95
26	PG	202	PEB	CHB-C4B-C3B	-3.25	117.80	125.32
26	R3	203	PEB	CHC-C4C-C3C	-3.25	124.79	130.34
26	mB	201	PEB	CHC-C4C-C3C	-3.25	124.79	130.34
26	Y2	201	PEB	C4B-C3B-C2B	-3.25	103.18	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	dF	202	PEB	C1C-CHB-C4B	3.25	132.69	128.81
26	S6	201	PEB	C3B-C4B-NB	3.25	114.78	110.05
26	ZF	203	PEB	C3B-C4B-NB	3.25	114.78	110.05
26	fF	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
27	A9	302	PUB	OA-C1A-NA	-3.25	121.11	125.93
26	W3	202	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
26	U3	202	PEB	C3D-C4D-ND	3.25	113.64	107.26
26	WE	201	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
26	mG	203	PEB	C3B-C4B-NB	3.25	114.78	110.05
26	JJ	202	PEB	CHC-C4C-C3C	-3.25	124.79	130.34
26	j4	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
26	aA	204	PEB	CMB-C2B-C1B	3.25	130.07	125.06
26	V1	202	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
26	M4	401	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
26	M8	201	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
26	b2	201	PEB	CAB-CBB-CGB	-3.25	106.61	113.60
26	H1	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
26	iI	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
28	B6	1002	CYC	C2C-C1C-NC	3.25	111.08	108.27
26	c1	203	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
26	Z4	202	PEB	CHB-C4B-C3B	-3.25	117.81	125.32
26	R9	203	PEB	OA-C1A-C2A	-3.25	123.59	126.17
26	WG	201	PEB	OA-C1A-C2A	-3.25	123.59	126.17
28	LH	1001	CYC	CHA-C1A-NA	-3.25	124.32	128.83
28	CF	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
26	FJ	202	PEB	CHC-C1D-ND	-3.25	110.17	113.95
26	O1	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
26	O4	201	PEB	CHA-C4A-NA	3.25	129.07	125.20
28	PH	1001	CYC	C4D-CHA-C1A	3.25	132.69	128.81
26	R6	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
26	YI	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
26	PI	203	PEB	CHC-C1D-ND	-3.25	110.17	113.95
26	f8	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	h6	203	PEB	OD-C4D-ND	-3.25	121.12	125.93
26	O4	202	PEB	OD-C4D-C3D	-3.25	122.10	129.46
26	e6	203	PEB	CHA-C1B-C2B	3.25	133.25	124.90
26	hG	202	PEB	CHB-C4B-NB	-3.25	124.32	128.83
26	H5	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
26	S6	203	PEB	OD-C4D-ND	-3.25	121.12	125.93
26	z1	201	PEB	CAA-C3A-C2A	-3.25	106.14	114.26
26	H5	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	mG	203	PEB	C4B-C3B-C2B	-3.25	103.19	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k1	202	PEB	CHC-C4C-C3C	-3.25	124.80	130.34
26	u4	203	PEB	CHC-C1D-ND	-3.25	110.17	113.95
26	Y7	202	PEB	CHC-C1D-ND	-3.25	110.17	113.95
26	cE	203	PEB	OD-C4D-C3D	-3.25	122.10	129.46
26	M4	403	PEB	C2A-C1A-NA	3.25	111.07	108.27
26	k7	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	T4	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
26	VF	201	PEB	CHC-C4C-C3C	-3.25	124.80	130.34
26	V4	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	g4	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	KJ	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	y1	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
26	AJ	303	PEB	CMB-C2B-C1B	3.25	130.06	125.06
26	k8	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
28	L2	1001	CYC	C2A-C1A-NA	3.25	114.77	110.05
26	dI	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
26	EJ	202	PEB	OD-C4D-ND	-3.25	121.12	125.93
26	U9	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
26	aA	202	PEB	C3B-C4B-NB	3.25	114.77	110.05
28	F7	1001	CYC	CHA-C1A-NA	-3.25	124.32	128.83
26	dG	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	QJ	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	SA	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
26	LD	201	PEB	C2A-C1A-NA	3.25	111.07	108.27
26	R3	201	PEB	CMA-C2A-C1A	-3.25	105.41	112.40
26	i7	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
26	u4	202	PEB	OD-C4D-C3D	-3.25	122.11	129.46
26	j8	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
26	l8	203	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
26	s4	202	PEB	CMB-C2B-C1B	3.24	130.06	125.06
26	NI	1002	PEB	CMB-C2B-C1B	3.24	130.06	125.06
26	s4	203	PEB	OD-C4D-ND	-3.24	121.12	125.93
26	U6	201	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	WG	202	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	Q7	203	PEB	C2A-C1A-NA	3.24	111.07	108.27
26	oE	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
26	JJ	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
28	QH	1001	CYC	C1A-C2A-C3A	-3.24	103.19	106.78
26	J9	201	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
26	WB	202	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
26	eE	203	PEB	C3D-C4D-ND	3.24	113.62	107.26
26	L3	201	PEB	CHA-C1B-C2B	3.24	133.24	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	XE	201	PEB	C1C-CHB-C4B	3.24	132.68	128.81
26	UE	203	PEB	CAA-C3A-C2A	3.24	122.36	114.26
26	S3	202	PEB	C3D-C4D-ND	3.24	113.62	107.26
26	eA	202	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	B3	203	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
26	xE	303	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
26	m4	201	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
26	C9	202	PEB	CHB-C4B-NB	-3.24	124.33	128.83
26	GJ	201	PEB	CAB-CBB-CGB	-3.24	106.62	113.60
26	24	405	PEB	CMB-C2B-C1B	3.24	130.06	125.06
26	K4	202	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	fA	201	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	WG	203	PEB	C3D-C4D-ND	3.24	113.62	107.26
26	c8	201	PEB	CHC-C1D-ND	3.24	117.71	113.95
26	P4	203	PEB	OA-C1A-C2A	-3.24	123.59	126.17
26	bB	202	PEB	OA-C1A-C2A	-3.24	123.59	126.17
26	h1	202	PEB	CMB-C2B-C1B	3.24	130.06	125.06
26	r4	202	PEB	C2A-C1A-NA	3.24	111.07	108.27
26	VI	201	PEB	OD-C4D-ND	-3.24	121.13	125.93
26	k4	203	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	z4	201	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	aI	203	PEB	C3B-C4B-NB	3.24	114.77	110.05
26	S8	203	PEB	CHB-C4B-NB	-3.24	124.33	128.83
26	iE	203	PEB	CMB-C2B-C1B	3.24	130.06	125.06
26	O2	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
26	gI	203	PEB	C1C-CHB-C4B	-3.24	124.94	128.81
28	K6	202	CYC	C1B-NB-C4B	-3.24	106.54	110.67
28	KB	202	CYC	C1B-NB-C4B	-3.24	106.54	110.67
26	gI	202	PEB	CMB-C2B-C1B	3.24	130.06	125.06
26	Q1	201	PEB	OD-C4D-ND	-3.24	121.13	125.93
26	JG	201	PEB	OD-C4D-ND	-3.24	121.13	125.93
27	xE	301	PUB	OD-C4D-ND	-3.24	121.13	125.93
26	Q8	204	PEB	OD-C4D-C3D	-3.24	122.12	129.46
26	J3	202	PEB	CHA-C1B-NB	-3.24	118.15	124.93
26	N4	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
26	JD	203	PEB	C3B-C4B-NB	3.24	114.76	110.05
26	W1	202	PEB	CMB-C2B-C1B	3.24	130.05	125.06
26	EA	203	PEB	CMB-C2B-C1B	3.24	130.05	125.06
28	CB	1001	CYC	C1B-C2B-C3B	-3.24	104.49	107.87
26	JC	202	PEB	C3B-C4B-NB	3.24	114.76	110.05
28	DI	1001	CYC	C2A-C1A-NA	3.24	114.76	110.05
26	SA	202	PEB	C2A-C1A-NA	3.24	111.07	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K8	203	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	dF	201	PEB	CHA-C1B-NB	-3.24	118.16	124.93
26	a8	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
26	Y2	201	PEB	CHB-C4B-NB	-3.24	124.33	128.83
26	u1	201	PEB	OD-C4D-ND	-3.24	121.13	125.93
26	AE	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
26	R4	201	PEB	CHC-C4C-C3C	-3.24	124.81	130.34
26	A6	304	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
26	xG	302	PEB	OD-C4D-ND	-3.24	121.13	125.93
26	D9	201	PEB	C2A-C1A-NA	3.24	111.06	108.27
26	cA	201	PEB	C2A-C1A-NA	3.24	111.06	108.27
26	WB	202	PEB	C2A-C1A-NA	3.24	111.06	108.27
27	xG	305	PUB	CHA-C1B-C2B	-3.24	124.81	130.34
26	aA	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	V4	201	PEB	CAA-C3A-C2A	-3.24	106.17	114.26
26	MG	202	PEB	CHC-C4C-C3C	-3.24	124.81	130.34
26	BJ	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
26	T1	203	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
26	BJ	201	PEB	C1C-CHB-C4B	3.24	132.68	128.81
26	XA	201	PEB	C3B-C4B-NB	3.24	114.76	110.05
26	TG	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
28	G2	1001	CYC	C1A-C2A-C3A	-3.24	103.20	106.78
26	p4	202	PEB	CHB-C4B-C3B	3.24	132.80	125.32
26	V9	202	PEB	C2A-C1A-NA	3.24	111.06	108.27
26	MJ	202	PEB	CHC-C4C-C3C	-3.24	124.81	130.34
28	NI	1001	CYC	C2B-C1B-NB	3.24	111.73	106.99
26	J1	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
26	N9	202	PEB	CHC-C4C-C3C	-3.24	124.82	130.34
26	C1	202	PEB	OD-C4D-ND	-3.24	121.14	125.93
26	O2	201	PEB	OD-C4D-ND	-3.24	121.14	125.93
26	Y8	201	PEB	OD-C4D-ND	-3.24	121.14	125.93
26	P1	202	PEB	C3B-C4B-NB	3.24	114.76	110.05
26	V3	202	PEB	C2A-C1A-NA	3.24	111.06	108.27
26	Q8	204	PEB	CHC-C1D-ND	-3.24	110.19	113.95
26	OB	201	PEB	CHB-C4B-C3B	-3.24	117.84	125.32
26	l1	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
26	P2	202	PEB	OD-C4D-ND	-3.24	121.14	125.93
26	Q2	202	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	F2	1002	PEB	CHB-C4B-NB	-3.24	124.34	128.83
28	EI	1001	CYC	CBD-CAD-C3D	-3.24	107.10	112.62
26	lA	203	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
26	YE	203	PEB	C1B-C2B-C3B	-3.24	102.79	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aA	201	PEB	C2A-C1A-NA	3.24	111.06	108.27
26	O6	202	PEB	CHC-C4C-C3C	-3.24	124.82	130.34
26	m4	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
26	C5	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
26	J8	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
28	CH	1001	CYC	C1A-C2A-C3A	-3.24	103.20	106.78
26	kB	201	PEB	C3B-C4B-NB	3.24	114.75	110.05
26	WG	203	PEB	C3B-C4B-NB	3.24	114.75	110.05
26	G6	1002	PEB	OD-C4D-C3D	-3.23	122.13	129.46
26	hI	201	PEB	CHB-C4B-C3B	-3.23	117.85	125.32
26	U7	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	LG	202	PEB	OD-C4D-ND	-3.23	121.14	125.93
26	OI	201	PEB	OD-C4D-ND	-3.23	121.14	125.93
26	PI	202	PEB	OD-C4D-ND	-3.23	121.14	125.93
26	fB	203	PEB	C1B-C2B-C3B	-3.23	102.79	106.51
26	j4	201	PEB	CHB-C4B-NB	-3.23	124.34	128.83
26	z4	202	PEB	CHA-C1B-NB	-3.23	118.17	124.93
26	a8	203	PEB	CMC-C3C-C2C	3.23	131.04	124.94
26	U4	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	R8	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	11	202	PEB	CBC-CAC-C2C	3.23	118.14	112.62
28	JF	1001	CYC	C1B-NB-C4B	-3.23	106.55	110.67
26	kG	202	PEB	CHC-C4C-C3C	-3.23	124.82	130.34
26	C1	201	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
26	cB	202	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
26	R4	202	PEB	OD-C4D-ND	-3.23	121.14	125.93
26	bF	203	PEB	CMB-C2B-C1B	3.23	130.04	125.06
26	WF	201	PEB	C3B-C4B-NB	3.23	114.75	110.05
26	UG	201	PEB	CHA-C1B-NB	-3.23	118.17	124.93
26	Z6	203	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	NJ	203	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	G9	202	PEB	CHC-C4C-C3C	-3.23	124.82	130.34
26	UF	203	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
28	DF	1001	CYC	CMB-C2B-C1B	3.23	128.20	124.17
26	m7	201	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
26	gB	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	TG	202	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	G4	201	PEB	CHC-C1D-ND	-3.23	110.19	113.95
26	JE	201	PEB	OD-C4D-ND	-3.23	121.14	125.93
26	dF	203	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
26	i1	201	PEB	OD-C4D-C3D	-3.23	122.14	129.46
26	I9	202	PEB	CMB-C2B-C1B	3.23	130.04	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	jA	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	p1	201	PEB	CHB-C4B-NB	-3.23	124.34	128.83
26	d1	202	PEB	CAA-C3A-C4A	-3.23	104.38	112.67
26	p4	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	K5	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	T7	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	aI	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
27	wE	304	PUB	OD-C4D-ND	-3.23	121.14	125.93
26	A6	304	PEB	CHA-C1B-NB	-3.23	118.17	124.93
26	lE	201	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
26	kB	202	PEB	OA-C1A-C2A	-3.23	123.60	126.17
28	I6	1001	CYC	C2A-C1A-NA	3.23	114.75	110.05
26	IG	201	PEB	CAC-C2C-C3C	3.23	136.53	127.25
26	RA	202	PEB	O2B-CGB-CBB	3.23	124.41	114.03
26	Y3	301	PEB	OD-C4D-ND	-3.23	121.14	125.93
26	k8	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	VA	201	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	iB	201	PEB	CAB-CBB-CGB	-3.23	106.65	113.60
26	GG	203	PEB	CHC-C1D-ND	-3.23	110.20	113.95
26	O1	202	PEB	OD-C4D-C3D	-3.23	122.14	129.46
26	eE	201	PEB	CBC-CAC-C2C	3.23	118.13	112.62
26	DE	202	PEB	C3B-C4B-NB	3.23	114.75	110.05
26	fI	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	l7	203	PEB	CHC-C4C-C3C	-3.23	124.83	130.34
26	wE	302	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
26	SF	201	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
26	a4	201	PEB	OD-C4D-ND	-3.23	121.15	125.93
26	P1	201	PEB	OD-C4D-ND	-3.23	121.15	125.93
26	w1	201	PEB	OA-C1A-C2A	-3.23	123.61	126.17
26	F5	203	PEB	OA-C1A-C2A	-3.23	123.61	126.17
26	KG	203	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
26	d6	202	PEB	CHA-C1B-NB	-3.23	118.18	124.93
26	I3	201	PEB	CAB-CBB-CGB	-3.23	106.66	113.60
26	BJ	201	PEB	CMB-C2B-C1B	3.23	130.03	125.06
26	QD	201	PEB	CHA-C4A-NA	3.23	129.04	125.20
26	E9	202	PEB	OD-C4D-ND	-3.23	121.15	125.93
26	PB	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	eG	202	PEB	CHA-C1B-NB	-3.23	118.18	124.93
26	AJ	304	PEB	CHC-C4C-C3C	-3.23	124.83	130.34
26	J3	201	PEB	OA-C1A-C2A	-3.23	123.61	126.17
26	RE	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
26	Y8	203	PEB	C4B-C3B-C2B	-3.23	103.21	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	uG	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	L4	201	PEB	C3B-C4B-NB	3.23	114.74	110.05
26	gI	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
26	PD	202	PEB	OD-C4D-ND	-3.23	121.15	125.93
26	KE	202	PEB	OD-C4D-ND	-3.23	121.15	125.93
26	X8	201	PEB	CHA-C1B-C2B	3.23	133.20	124.90
26	Y6	201	PEB	C1C-CHB-C4B	3.23	132.66	128.81
26	R9	202	PEB	C3D-C4D-ND	3.23	113.59	107.26
26	P2	202	PEB	C3B-C4B-NB	3.23	114.74	110.05
26	P4	201	PEB	C3B-C4B-NB	3.23	114.74	110.05
26	p1	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	CG	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	BD	202	PEB	CMB-C2B-C1B	3.23	130.03	125.06
26	J3	203	PEB	C2A-C1A-NA	3.23	111.05	108.27
26	hA	202	PEB	C2A-C1A-NA	3.23	111.05	108.27
26	VI	202	PEB	C2A-C1A-NA	3.23	111.05	108.27
26	HD	202	PEB	CHB-C4B-NB	-3.23	124.35	128.83
28	H6	1001	CYC	C4A-C3A-C2A	-3.23	102.80	106.51
26	c7	202	PEB	OD-C4D-C3D	-3.23	122.15	129.46
26	B5	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	j7	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
26	d4	202	PEB	C3B-C4B-NB	3.22	114.74	110.05
26	g2	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	V1	201	PEB	CMB-C2B-C1B	3.22	130.03	125.06
26	wE	301	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	h6	203	PEB	CHC-C4C-C3C	-3.22	124.84	130.34
26	M9	201	PEB	OD-C4D-ND	-3.22	121.15	125.93
26	V3	202	PEB	C4B-C3B-C2B	-3.22	103.21	106.78
26	V6	201	PEB	C4B-C3B-C2B	-3.22	103.21	106.78
26	wE	301	PEB	C3B-C4B-NB	3.22	114.74	110.05
26	iI	202	PEB	C3B-C4B-NB	3.22	114.74	110.05
26	BJ	203	PEB	CBC-CAC-C2C	3.22	118.12	112.62
26	lA	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
28	MI	1001	CYC	C4A-C3A-C2A	-3.22	102.81	106.51
26	AD	202	PEB	CMB-C2B-C1B	3.22	130.03	125.06
26	HC	203	PEB	OD-C4D-ND	-3.22	121.15	125.93
26	dI	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	lF	203	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	QD	201	PEB	CBB-CAB-C3B	-3.22	103.67	112.63
26	f2	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	F2	1002	PEB	CMD-C2D-C3D	3.22	134.61	130.06
26	N4	202	PEB	C3B-C4B-NB	3.22	114.74	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	EF	1001	CYC	CHB-C4A-C3A	3.22	133.19	124.90
26	H4	203	PEB	CHC-C1D-ND	-3.22	110.20	113.95
26	T1	201	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	qG	203	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	PJ	203	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	l6	203	PEB	OD-C4D-ND	-3.22	121.16	125.93
26	s4	201	PEB	CHC-C4C-C3C	-3.22	124.84	130.34
26	eI	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
28	K6	202	CYC	C1A-C2A-C3A	-3.22	103.22	106.78
26	C3	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	M3	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	A6	304	PEB	C3B-C4B-NB	3.22	114.73	110.05
26	OB	201	PEB	C3B-C4B-NB	3.22	114.73	110.05
26	Z2	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	HF	1002	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	NF	1002	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	U6	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	P7	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	EG	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
27	AB	302	PUB	OD-C4D-ND	-3.22	121.16	125.93
26	w1	201	PEB	CAB-C3B-C4B	3.22	130.71	125.01
26	QB	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
28	EB	1001	CYC	CHA-C1A-NA	-3.22	124.36	128.83
26	d2	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
26	KJ	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
26	g8	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	NB	1002	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
28	G6	1001	CYC	C1A-C2A-C3A	-3.22	103.22	106.78
26	R1	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	a4	201	PEB	CHA-C1B-C2B	3.22	133.18	124.90
26	O3	201	PEB	C3B-C4B-NB	3.22	114.73	110.05
26	L4	201	PEB	CHC-C1D-ND	-3.22	110.21	113.95
26	VB	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	lB	203	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	IC	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	ND	203	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	YF	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	G8	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
27	YD	302	PUB	C1C-C2C-C3C	-3.22	103.22	106.78
26	YG	201	PEB	CMB-C2B-C1B	3.22	130.02	125.06
26	P7	201	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	PF	201	PEB	C1B-C2B-C3B	-3.22	102.81	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	NF	1001	CYC	C4A-C3A-C2A	-3.22	102.81	106.51
28	I2	1001	CYC	C2A-C1A-NA	3.22	114.73	110.05
26	m1	203	PEB	CBC-CAC-C2C	3.22	118.11	112.62
26	O2	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	QE	201	PEB	C2A-C1A-NA	-3.22	105.50	108.27
26	SI	201	PEB	CHC-C1D-ND	-3.22	110.21	113.95
26	YI	203	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	W1	201	PEB	OD-C4D-ND	-3.22	121.16	125.93
26	O6	202	PEB	OD-C4D-ND	-3.22	121.16	125.93
26	G8	201	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	I5	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	FD	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	BJ	203	PEB	CHA-C1B-NB	-3.22	118.20	124.93
26	H8	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	gB	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	ME	202	PEB	OD-C4D-ND	-3.22	121.17	125.93
26	TA	202	PEB	OD-C4D-C3D	-3.22	122.17	129.46
26	b2	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
26	MJ	201	PEB	C1C-CHB-C4B	3.22	132.65	128.81
26	B3	203	PEB	C1C-CHB-C4B	-3.22	124.97	128.81
26	N3	202	PEB	CHA-C4A-NA	3.22	129.03	125.20
26	e1	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	F4	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	T6	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	T1	203	PEB	C2A-C1A-NA	3.22	111.05	108.27
26	R9	201	PEB	C1B-C2B-C3B	-3.22	102.82	106.51
26	OE	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	YE	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
26	HA	201	PEB	C3B-C4B-NB	3.22	114.73	110.05
26	JD	202	PEB	C3B-C4B-NB	3.22	114.73	110.05
26	YG	203	PEB	OD-C4D-ND	-3.22	121.17	125.93
26	eB	203	PEB	CHC-C1D-ND	-3.21	110.21	113.95
27	21	402	PUB	CHA-C4A-NA	-3.21	110.21	113.95
26	F9	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	Z7	201	PEB	CHA-C4A-NA	3.21	129.03	125.20
26	f6	203	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
26	y1	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	w4	202	PEB	C4B-C3B-C2B	-3.21	103.22	106.78
28	HI	1001	CYC	C2C-C1C-NC	3.21	111.04	108.27
26	k1	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	C1	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
27	AA	304	PUB	OD-C4D-ND	-3.21	121.17	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O8	203	PEB	CHB-C4B-NB	-3.21	124.37	128.83
26	e3	401	PEB	OD-C4D-C3D	-3.21	122.18	129.46
26	M1	403	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	iE	202	PEB	CHB-C4B-C3B	-3.21	117.90	125.32
26	mG	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	hF	201	PEB	OD-C4D-ND	-3.21	121.17	125.93
26	T6	202	PEB	C1C-CHB-C4B	-3.21	124.97	128.81
26	W6	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
26	bI	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
26	QF	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	M4	402	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	yG	301	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	PI	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	a1	201	PEB	CAB-CBB-CGB	-3.21	106.69	113.60
26	qE	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	YI	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	P9	203	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
28	D2	1001	CYC	C4A-C3A-C2A	-3.21	102.82	106.51
26	JA	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	wG	303	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	CA	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	SF	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	JJ	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	hI	201	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	a6	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	QE	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	cG	203	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	F5	203	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	S8	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	J8	201	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	fF	201	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
28	B6	1002	CYC	CMB-C2B-C1B	3.21	128.18	124.17
26	a2	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
28	M6	1001	CYC	C1A-C2A-C3A	-3.21	103.23	106.78
26	LJ	201	PEB	OD-C4D-ND	-3.21	121.17	125.93
26	BC	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	PA	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
28	M6	1001	CYC	C2A-C1A-NA	3.21	114.72	110.05
26	oG	203	PEB	CHA-C1B-NB	-3.21	118.22	124.93
26	I8	203	PEB	CBC-CAC-C2C	-3.21	107.14	112.62
28	CI	1001	CYC	CHA-C1A-NA	-3.21	124.38	128.83
26	BJ	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	bE	202	PEB	CMB-C2B-C1B	3.21	130.01	125.06
26	jF	201	PEB	OD-C4D-ND	-3.21	121.18	125.93
26	J3	203	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	eG	203	PEB	C3D-C4D-ND	3.21	113.56	107.26
26	QE	201	PEB	CHC-C1D-ND	-3.21	110.22	113.95
26	OA	203	PEB	CHB-C4B-NB	-3.21	124.38	128.83
26	uG	202	PEB	CHB-C4B-NB	-3.21	124.38	128.83
26	O3	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	M8	203	PEB	OD-C4D-ND	-3.21	121.18	125.93
26	L4	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	gE	203	PEB	OA-C1A-C2A	-3.21	123.62	126.17
27	K4	203	PUB	CHA-C1B-C2B	-3.21	124.86	130.34
26	XA	202	PEB	CHA-C1B-NB	-3.21	118.22	124.93
26	kB	201	PEB	CHA-C1B-NB	-3.21	118.22	124.93
26	iI	201	PEB	CHC-C1D-ND	-3.21	110.22	113.95
26	eF	202	PEB	CMB-C2B-C1B	3.21	130.00	125.06
26	xG	304	PEB	C1C-CHB-C4B	-3.21	124.98	128.81
26	EE	201	PEB	OD-C4D-ND	-3.21	121.18	125.93
26	L7	1002	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	gG	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
26	E3	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	V7	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	xE	302	PEB	C2A-C1A-NA	3.21	111.04	108.27
26	KG	203	PEB	C3D-C4D-ND	3.21	113.55	107.26
26	GJ	202	PEB	CAC-C2C-C3C	3.21	136.46	127.25
26	iI	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	T4	203	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	O6	202	PEB	CHC-C1D-ND	-3.21	110.22	113.95
26	UF	203	PEB	CHC-C4C-C3C	-3.21	124.87	130.34
26	W3	202	PEB	C3B-C4B-NB	3.21	114.71	110.05
26	kF	201	PEB	C3B-C4B-NB	3.21	114.71	110.05
26	WA	202	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
26	MD	202	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
26	jA	202	PEB	CBC-CAC-C2C	-3.21	107.15	112.62
26	iE	202	PEB	CBC-CAC-C2C	-3.21	107.15	112.62
26	iE	202	PEB	CHC-C4C-C3C	-3.21	124.87	130.34
26	h6	201	PEB	OD-C4D-C3D	-3.21	122.19	129.46
26	h6	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	IJ	201	PEB	C1C-CHB-C4B	3.21	132.64	128.81
26	YD	303	PEB	CMB-C2B-C1B	3.21	130.00	125.06
26	P4	201	PEB	CMD-C2D-C3D	-3.21	125.54	130.06
26	B3	201	PEB	OD-C4D-ND	-3.21	121.18	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	yE	301	PEB	C3B-C4B-NB	3.21	114.71	110.05
26	g2	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
26	UE	202	PEB	C3D-C4D-ND	3.21	113.55	107.26
26	w4	204	PEB	C3B-C4B-NB	3.20	114.71	110.05
28	KF	1001	CYC	CMA-C3A-C4A	3.20	130.00	125.06
26	M1	401	PEB	OD-C4D-C3D	-3.20	122.20	129.46
26	eD	401	PEB	OD-C4D-C3D	-3.20	122.20	129.46
26	V2	202	PEB	CMB-C2B-C1B	3.20	130.00	125.06
26	UG	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	s4	201	PEB	OD-C4D-ND	-3.20	121.18	125.93
26	KG	201	PEB	OD-C4D-ND	-3.20	121.18	125.93
27	xG	305	PUB	OA-C1A-NA	-3.20	121.18	125.93
26	XD	203	PEB	CAC-CBC-CGC	-3.20	104.78	113.76
26	N3	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	MJ	202	PEB	CHB-C4B-NB	-3.20	124.38	128.83
26	d2	202	PEB	CHC-C4C-C3C	-3.20	124.87	130.34
26	dA	201	PEB	C3B-C4B-NB	3.20	114.71	110.05
26	iI	203	PEB	C3B-C4B-NB	3.20	114.71	110.05
26	A1	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	iF	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	dF	201	PEB	CMB-C2B-C1B	3.20	130.00	125.06
26	j6	201	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
26	CJ	201	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	SB	202	PEB	CBA-CAA-C3A	-3.20	106.34	113.47
28	rH	1001	CYC	C4D-CHA-C1A	3.20	132.63	128.81
26	wG	303	PEB	C3B-C4B-NB	3.20	114.71	110.05
26	LJ	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	NA	201	PEB	CBC-CAC-C2C	-3.20	107.16	112.62
26	Y9	201	PEB	CHC-C4C-C3C	-3.20	124.88	130.34
26	AE	201	PEB	CHC-C4C-C3C	-3.20	124.88	130.34
26	u1	201	PEB	CAA-C3A-C2A	-3.20	106.26	114.26
26	L1	201	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
26	L3	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
26	KD	201	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
26	C1	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	M8	203	PEB	CMB-C2B-C1B	3.20	130.00	125.06
28	HI	1001	CYC	CMA-C3A-C4A	3.20	130.00	125.06
26	g7	201	PEB	C1C-CHB-C4B	3.20	132.63	128.81
26	Y6	202	PEB	CHC-C1D-ND	-3.20	110.23	113.95
28	IB	1001	CYC	C1A-C2A-C3A	-3.20	103.24	106.78
26	MA	203	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	YD	301	PEB	C1B-C2B-C3B	-3.20	102.83	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	GB	1001	CYC	C2A-C1A-NA	3.20	114.71	110.05
26	b1	501	PEB	OD-C4D-C3D	-3.20	122.21	129.46
26	u1	202	PEB	OD-C4D-C3D	-3.20	122.21	129.46
26	WB	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	R3	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	RF	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	SJ	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	xE	302	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	Q6	203	PEB	CBA-CAA-C3A	-3.20	106.34	113.47
26	I5	203	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
26	WB	201	PEB	OD-C4D-C3D	-3.20	122.21	129.46
26	m4	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	j8	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	RB	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	k8	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
26	PF	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
26	U4	201	PEB	C3B-C4B-NB	3.20	114.70	110.05
26	BJ	201	PEB	C3B-C4B-NB	3.20	114.70	110.05
26	LI	1002	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	A4	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	H8	202	PEB	C3B-C4B-NB	3.20	114.70	110.05
26	IA	201	PEB	C3B-C4B-NB	3.20	114.70	110.05
26	W8	201	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	IC	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	OG	203	PEB	CHB-C4B-NB	-3.20	124.39	128.83
26	S7	202	PEB	C3D-C4D-ND	3.20	113.54	107.26
26	WD	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
26	Q9	201	PEB	CHC-C4C-C3C	-3.20	124.88	130.34
26	OE	202	PEB	CHC-C1D-ND	-3.20	110.23	113.95
26	PF	201	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	O7	202	PEB	C3D-C4D-ND	3.20	113.53	107.26
26	c2	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	gI	203	PEB	CAB-C3B-C2B	3.20	133.83	127.88
26	GD	201	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
26	AI	304	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	RD	203	PEB	CMB-C2B-C1B	3.20	129.99	125.06
26	gF	202	PEB	CAA-C3A-C4A	3.20	120.88	112.67
26	O7	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
26	T1	203	PEB	CHA-C1B-NB	-3.20	118.25	124.93
26	WF	202	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
26	e1	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
26	M9	202	PEB	C2A-C1A-NA	3.20	111.03	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	dE	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
27	KD	203	PUB	OA-C1A-NA	-3.20	121.19	125.93
26	f7	202	PEB	CHA-C4A-NA	-3.20	121.40	125.20
26	aA	202	PEB	CHC-C1D-ND	-3.20	110.23	113.95
26	mE	202	PEB	C3B-C4B-NB	3.20	114.70	110.05
28	tH	1001	CYC	CAB-C3B-C4B	3.20	126.43	121.38
26	21	404	PEB	C4B-C3B-C2B	-3.20	103.25	106.78
26	D4	203	PEB	C4B-C3B-C2B	-3.20	103.25	106.78
28	I6	1001	CYC	C1A-C2A-C3A	-3.20	103.25	106.78
26	l7	201	PEB	CHA-C1B-NB	-3.20	118.25	124.93
26	P1	203	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	jE	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
26	f4	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
26	J8	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
26	ZE	202	PEB	C3B-C4B-NB	3.20	114.70	110.05
26	lB	201	PEB	C4B-C3B-C2B	-3.20	103.25	106.78
28	jH	1001	CYC	CAA-C2A-C1A	3.20	130.66	125.01
26	g4	203	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
26	BG	202	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
26	GB	1002	PEB	CHC-C1D-ND	-3.19	110.24	113.95
26	KC	202	PEB	CHC-C1D-ND	-3.19	110.24	113.95
26	AF	305	PEB	OD-C4D-ND	-3.19	121.20	125.93
26	rE	201	PEB	OA-C1A-NA	3.19	128.81	124.94
26	F3	202	PEB	C3B-C4B-NB	3.19	114.70	110.05
26	A7	301	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	TE	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	21	401	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
26	Y7	201	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
26	VI	202	PEB	CMB-C2B-C1B	3.19	129.98	125.06
26	TF	201	PEB	CHB-C4B-NB	-3.19	124.40	128.83
26	TG	201	PEB	CHB-C4B-NB	-3.19	124.40	128.83
26	cI	201	PEB	CHB-C4B-NB	-3.19	124.40	128.83
26	UD	202	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
26	iE	203	PEB	C3D-C4D-ND	3.19	113.53	107.26
26	U6	201	PEB	CBC-CAC-C2C	-3.19	107.17	112.62
26	A2	304	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	Q7	202	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
26	P7	202	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
26	W6	201	PEB	OD-C4D-C3D	-3.19	122.22	129.46
26	dB	202	PEB	C2A-C1A-NA	3.19	111.03	108.27
26	fB	203	PEB	C2A-C1A-NA	3.19	111.03	108.27
26	fE	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UG	201	PEB	CAC-C2C-C3C	3.19	136.42	127.25
26	A2	304	PEB	CMB-C2B-C1B	3.19	129.98	125.06
26	ZI	202	PEB	CMB-C2B-C1B	3.19	129.98	125.06
26	AI	304	PEB	CHA-C1B-NB	-3.19	118.25	124.93
28	HB	1001	CYC	CHA-C1A-NA	-3.19	124.40	128.83
26	R6	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
27	Q8	201	PUB	C2C-C1C-NC	3.19	114.69	110.05
26	DA	202	PEB	CHC-C1D-ND	-3.19	110.24	113.95
26	C5	204	PEB	C2A-C1A-NA	3.19	111.03	108.27
26	U3	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
26	gA	201	PEB	OD-C4D-ND	-3.19	121.20	125.93
28	H7	1001	CYC	CHA-C1A-NA	-3.19	124.40	128.83
26	TA	202	PEB	CHA-C1B-NB	-3.19	118.26	124.93
26	jB	201	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
26	DF	1002	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
28	M2	1001	CYC	C2A-C1A-NA	3.19	114.69	110.05
26	T4	203	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	tE	201	PEB	CHC-C1D-ND	-3.19	110.24	113.95
26	W6	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
26	R9	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
26	IE	203	PEB	C2A-C1A-NA	3.19	111.02	108.27
26	d7	201	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
26	W1	201	PEB	CHA-C1B-NB	-3.19	118.26	124.93
26	Y7	201	PEB	CMB-C2B-C1B	3.19	129.98	125.06
26	f8	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	RD	203	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	DD	201	PEB	CHA-C1B-C2B	3.19	133.10	124.90
26	eA	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
26	C9	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	O9	201	PEB	C2A-C1A-NA	3.19	111.02	108.27
26	WJ	201	PEB	CHB-C4B-C3B	-3.19	117.95	125.32
26	V7	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
26	SA	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
26	MA	201	PEB	CMB-C2B-C1B	3.19	129.98	125.06
26	VB	202	PEB	CMB-C2B-C1B	3.19	129.98	125.06
26	NA	201	PEB	CHA-C1B-C2B	3.19	133.10	124.90
28	KI	1001	CYC	CBC-CAC-C3C	-3.19	106.37	113.47
26	N2	1002	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	G8	203	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	X9	203	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	G4	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
26	l6	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b6	201	PEB	CHC-C4C-C3C	-3.19	124.90	130.34
26	LI	1002	PEB	OD-C4D-C3D	-3.19	122.23	129.46
26	H4	202	PEB	CHA-C1B-NB	-3.19	118.26	124.93
26	A5	202	PEB	C1C-CHB-C4B	3.19	132.62	128.81
26	iA	202	PEB	C1C-CHB-C4B	-3.19	125.00	128.81
26	IG	203	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
26	kA	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
26	rE	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
26	R4	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	ZE	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	aE	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
26	VE	201	PEB	CAB-C3B-C4B	3.19	130.65	125.01
26	S1	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
26	OA	201	PEB	C2A-C1A-NA	3.19	111.02	108.27
26	b7	203	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
26	qG	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
26	R2	203	PEB	CHC-C1D-ND	-3.19	110.25	113.95
26	L9	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
26	l6	201	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
26	IE	202	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
26	AI	304	PEB	C2A-C1A-NA	3.19	111.02	108.27
26	lF	201	PEB	C3D-C4D-ND	3.19	113.51	107.26
26	O3	201	PEB	C4B-C3B-C2B	-3.19	103.26	106.78
26	V4	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
26	TB	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
26	XG	201	PEB	OD-C4D-ND	-3.19	121.21	125.93
26	T7	201	PEB	C1C-CHB-C4B	3.19	132.62	128.81
26	JC	201	PEB	CHC-C4C-C3C	-3.19	124.90	130.34
26	M4	402	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
28	G7	1001	CYC	C4A-C3A-C2A	-3.19	102.85	106.51
26	M1	402	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	V3	202	PEB	C3B-C4B-NB	3.19	114.68	110.05
26	AB	304	PEB	C3B-C4B-NB	3.19	114.68	110.05
26	H4	201	PEB	CHC-C1D-ND	-3.19	110.25	113.95
26	k6	202	PEB	C4B-C3B-C2B	-3.19	103.26	106.78
26	X3	203	PEB	CAC-CBC-CGC	-3.19	104.83	113.76
26	e4	202	PEB	C2A-C1A-NA	3.19	111.02	108.27
26	KG	203	PEB	C2A-C1A-NA	3.19	111.02	108.27
26	i1	203	PEB	CHA-C1B-NB	-3.18	118.27	124.93
26	14	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
26	H6	1002	PEB	OA-C1A-C2A	-3.18	123.64	126.17
28	B6	1001	CYC	C1B-C2B-C3B	-3.18	104.55	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g1	203	PEB	OD-C4D-C3D	-3.18	122.25	129.46
26	AA	301	PEB	C2A-C1A-NA	3.18	111.02	108.27
26	UE	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
26	R6	201	PEB	OD-C4D-ND	-3.18	121.21	125.93
26	T3	202	PEB	C2B-C1B-NB	3.18	117.33	110.53
26	w4	201	PEB	CHB-C4B-NB	-3.18	124.41	128.83
26	cE	203	PEB	CHC-C1D-ND	3.18	117.64	113.95
26	R7	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
26	k7	202	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
26	FJ	202	PEB	OD-C4D-ND	-3.18	121.21	125.93
26	k1	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
26	QF	201	PEB	CHA-C1B-NB	-3.18	118.28	124.93
26	N6	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
28	KB	202	CYC	C1A-C2A-C3A	-3.18	103.26	106.78
26	e8	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	WI	201	PEB	CHA-C4A-NA	3.18	128.99	125.20
26	F1	201	PEB	CMB-C2B-C1B	3.18	129.97	125.06
26	FE	202	PEB	CAB-C3B-C4B	3.18	130.64	125.01
26	iI	202	PEB	C1B-C2B-C3B	-3.18	102.85	106.51
26	J3	203	PEB	CHC-C1D-ND	-3.18	110.25	113.95
27	xG	305	PUB	CHA-C4A-NA	-3.18	110.25	113.95
26	HC	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	Y2	201	PEB	CMB-C2B-C1B	3.18	129.96	125.06
26	HC	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
26	XG	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
26	Y9	201	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
26	WA	201	PEB	OD-C4D-C3D	-3.18	122.25	129.46
26	k6	201	PEB	CHA-C1B-NB	-3.18	118.28	124.93
26	w4	204	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	UI	202	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	AF	301	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	L4	201	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
26	V6	202	PEB	CHC-C1D-ND	-3.18	110.25	113.95
26	AB	304	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
28	J7	1001	CYC	CHB-C1B-NB	-3.18	119.23	126.06
26	j7	201	PEB	C3B-C4B-NB	3.18	114.68	110.05
28	DB	1001	CYC	CAB-C3B-C4B	3.18	126.40	121.38
28	LF	1001	CYC	CHA-C1A-C2A	-3.18	117.97	125.32
26	L6	1002	PEB	C2A-C1A-NA	3.18	111.02	108.27
26	ZI	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	B5	201	PEB	CMB-C2B-C1B	3.18	129.96	125.06
26	M8	201	PEB	CMB-C2B-C1B	3.18	129.96	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KC	203	PEB	CMB-C2B-C1B	3.18	129.96	125.06
26	F7	1002	PEB	C3B-C4B-NB	3.18	114.67	110.05
28	F2	1001	CYC	C1A-C2A-C3A	-3.18	103.26	106.78
26	UA	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	WA	203	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	N9	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	wE	303	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	DB	1002	PEB	C2A-C1A-NA	3.18	111.01	108.27
26	j7	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	KB	201	PEB	C1C-CHB-C4B	3.18	132.61	128.81
26	21	404	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	H3	202	PEB	CHB-C4B-NB	-3.18	124.42	128.83
26	hE	201	PEB	OA-C1A-NA	3.18	128.79	124.94
26	nG	202	PEB	CHB-C4B-C3B	-3.18	117.98	125.32
28	L6	1001	CYC	CMB-C2B-C1B	3.18	128.14	124.17
26	QD	201	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	c1	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
26	j6	202	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
28	EF	1001	CYC	C1A-C2A-C3A	-3.18	103.27	106.78
26	j7	202	PEB	C3B-C4B-NB	3.18	114.67	110.05
26	E4	201	PEB	CHC-C4C-C3C	-3.18	124.92	130.34
28	pH	1001	CYC	C4D-CHA-C1A	3.18	132.60	128.81
26	AJ	305	PEB	OD-C4D-C3D	-3.18	122.26	129.46
26	HC	202	PEB	CHB-C4B-NB	-3.18	124.42	128.83
26	w4	202	PEB	CAB-CBB-CGB	-3.18	106.77	113.60
26	X4	201	PEB	C3B-C4B-NB	3.18	114.67	110.05
26	W6	202	PEB	C3B-C4B-NB	3.18	114.67	110.05
26	i8	201	PEB	C3B-C4B-NB	3.18	114.67	110.05
26	dB	204	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
26	FC	203	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
26	Z2	202	PEB	CMB-C2B-C1B	3.18	129.96	125.06
26	R8	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	f8	201	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	b6	202	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	mI	201	PEB	CHA-C1B-NB	-3.18	118.29	124.93
26	b6	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
28	K2	1001	CYC	CBC-CAC-C3C	-3.18	106.39	113.47
26	ED	201	PEB	C2A-C1A-NA	3.18	111.01	108.27
26	K3	201	PEB	C1C-CHB-C4B	3.18	132.60	128.81
26	WB	202	PEB	C3B-C4B-NB	3.18	114.67	110.05
26	e2	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
26	G5	201	PEB	OD-C4D-ND	-3.18	121.22	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h8	202	PEB	CAB-CBB-CGB	-3.18	106.77	113.60
26	y4	202	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	z1	404	PEB	CMB-C2B-C1B	3.18	129.95	125.06
26	n4	202	PEB	CMB-C2B-C1B	3.18	129.95	125.06
26	j7	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
26	q1	201	PEB	OD-C4D-ND	-3.18	121.23	125.93
26	JD	203	PEB	OD-C4D-ND	-3.18	121.23	125.93
26	EG	202	PEB	OD-C4D-ND	-3.18	121.23	125.93
26	P1	203	PEB	CHC-C1D-ND	-3.18	110.26	113.95
26	E3	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	S8	203	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	ZE	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	ME	202	PEB	CHC-C4C-C3C	-3.17	124.92	130.34
26	B9	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
26	XJ	201	PEB	CHB-C4B-NB	-3.17	124.42	128.83
26	H7	1002	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
26	FC	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
26	Z2	202	PEB	C3B-C4B-NB	3.17	114.67	110.05
26	U8	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	d8	202	PEB	CHC-C4C-C3C	-3.17	124.92	130.34
26	MA	203	PEB	CHA-C1B-NB	-3.17	118.29	124.93
26	JE	201	PEB	CHA-C1B-NB	-3.17	118.29	124.93
26	I9	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	CA	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	ED	202	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	vE	201	PEB	CHC-C4C-C3C	-3.17	124.92	130.34
26	AE	202	PEB	CHC-C1D-ND	-3.17	110.26	113.95
26	EE	202	PEB	CHC-C1D-ND	-3.17	110.26	113.95
26	mG	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
26	K9	201	PEB	C3B-C4B-NB	3.17	114.67	110.05
26	ME	202	PEB	C3B-C4B-NB	3.17	114.67	110.05
26	G1	201	PEB	CHC-C4C-C3C	-3.17	124.92	130.34
28	YH	1003	CYC	CAA-C2A-C1A	3.17	130.62	125.01
26	E1	202	PEB	C1B-C2B-C3B	-3.17	102.86	106.51
26	v1	202	PEB	C1C-CHB-C4B	3.17	132.60	128.81
26	A2	301	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	I4	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	TA	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	dB	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	SE	203	PEB	C3B-C4B-NB	3.17	114.66	110.05
26	IJ	201	PEB	CHC-C4C-C3C	-3.17	124.93	130.34
26	VA	202	PEB	CBB-CAB-C3B	3.17	121.44	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l2	202	PEB	CMB-C2B-C1B	3.17	129.95	125.06
26	SB	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
27	xG	301	PUB	CMD-C2D-C3D	3.17	132.53	127.77
26	BC	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
26	JC	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
26	KA	203	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	UE	201	PEB	CAC-CBC-CGC	3.17	122.65	113.76
26	GC	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	Q6	203	PEB	C1C-CHB-C4B	3.17	132.60	128.81
26	g1	203	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	F4	201	PEB	CAB-CBB-CGB	-3.17	106.78	113.60
26	J9	201	PEB	CMB-C2B-C1B	3.17	129.95	125.06
26	ZE	202	PEB	CMB-C2B-C1B	3.17	129.95	125.06
26	b4	501	PEB	OD-C4D-C3D	-3.17	122.27	129.46
26	Y7	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	sE	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
26	F3	203	PEB	CHA-C1B-NB	-3.17	118.30	124.93
26	X9	202	PEB	CHA-C1B-NB	-3.17	118.30	124.93
26	o1	501	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	W3	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	DE	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	N1	202	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	Q2	201	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	D3	203	PEB	CHC-C1D-ND	-3.17	110.27	113.95
26	r4	202	PEB	CHA-C4A-NA	-3.17	121.44	125.20
26	W3	202	PEB	C3D-C4D-ND	3.17	113.48	107.26
26	P8	202	PEB	OD-C4D-C3D	-3.17	122.28	129.46
26	K1	201	PEB	C3B-C4B-NB	3.17	114.66	110.05
26	bG	202	PEB	CHB-C4B-C3B	-3.17	118.00	125.32
26	CC	203	PEB	C2A-C1A-NA	3.17	111.01	108.27
28	B6	1001	CYC	OB-C4B-C3B	-3.17	124.60	128.04
26	OD	202	PEB	C3D-C4D-ND	3.17	113.48	107.26
26	R3	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	f4	201	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	Z6	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
26	ZG	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	g1	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
26	Z2	202	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	OE	203	PEB	OD-C4D-ND	-3.17	121.23	125.93
26	OD	201	PEB	C2A-C1A-NA	3.17	111.00	108.27
26	Q3	201	PEB	OD-C4D-ND	-3.17	121.24	125.93
26	ZI	201	PEB	CHA-C1B-NB	-3.17	118.31	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M4	401	PEB	OD-C4D-C3D	-3.17	122.28	129.46
26	s4	203	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	Q9	202	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	AI	304	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
26	YI	201	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
26	FJ	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	k7	202	PEB	C2A-C1A-NA	3.17	111.00	108.27
26	bF	201	PEB	OD-C4D-C3D	-3.17	122.28	129.46
26	LC	202	PEB	OD-C4D-ND	-3.17	121.24	125.93
26	SG	201	PEB	OD-C4D-ND	-3.17	121.24	125.93
26	Q7	201	PEB	C3B-C4B-NB	3.17	114.66	110.05
26	kG	201	PEB	C3B-C4B-NB	3.17	114.66	110.05
26	B9	202	PEB	C1C-CHB-C4B	3.17	132.59	128.81
26	l4	201	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
26	aI	203	PEB	CAC-CBC-CGC	-3.17	104.88	113.76
26	c8	201	PEB	C2A-C1A-NA	3.17	111.00	108.27
26	O4	201	PEB	CBC-CAC-C2C	-3.17	107.22	112.62
26	m2	201	PEB	CHA-C1B-NB	-3.17	118.31	124.93
26	A3	201	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	XA	201	PEB	CHA-C1B-C2B	3.17	133.04	124.90
26	aA	203	PEB	OD-C4D-ND	-3.17	121.24	125.93
26	JG	202	PEB	OD-C4D-ND	-3.17	121.24	125.93
26	KC	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
26	mI	201	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
28	K6	202	CYC	C2A-C1A-NA	3.17	114.66	110.05
26	HG	201	PEB	CAA-C3A-C2A	3.17	122.17	114.26
26	cG	202	PEB	CHA-C1B-NB	-3.17	118.31	124.93
26	O2	202	PEB	CHC-C4C-C3C	-3.17	124.94	130.34
26	X1	202	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
26	gE	202	PEB	CHC-C1D-ND	-3.17	110.27	113.95
26	B9	203	PEB	C2A-C1A-NA	3.17	111.00	108.27
26	g1	203	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
26	wG	303	PEB	OD-C4D-ND	-3.17	121.24	125.93
26	o1	501	PEB	CBA-CAA-C3A	-3.17	106.42	113.47
26	Z4	201	PEB	CAB-CBB-CGB	-3.17	106.79	113.60
26	R4	202	PEB	C3B-C4B-NB	3.17	114.65	110.05
26	j8	203	PEB	OD-C4D-ND	-3.16	121.24	125.93
26	P4	201	PEB	CMC-C3C-C2C	-3.16	118.98	124.94
26	w4	204	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	TB	202	PEB	C1C-CHB-C4B	-3.16	125.03	128.81
26	B9	202	PEB	CHC-C1D-ND	-3.16	110.27	113.95
26	I5	201	PEB	CHB-C4B-NB	-3.16	124.44	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s1	201	PEB	OD-C4D-ND	-3.16	121.24	125.93
26	SB	202	PEB	CMB-C2B-C1B	3.16	129.94	125.06
26	YI	201	PEB	CMB-C2B-C1B	3.16	129.94	125.06
26	A5	201	PEB	CHC-C4C-C3C	-3.16	124.94	130.34
26	DB	1002	PEB	C3B-C4B-NB	3.16	114.65	110.05
27	A4	203	PUB	OA-C1A-NA	-3.16	121.24	125.93
26	mG	203	PEB	CHC-C1D-ND	-3.16	110.27	113.95
26	gI	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	L5	203	PEB	OD-C4D-C3D	-3.16	122.29	129.46
26	O6	201	PEB	C3B-C4B-NB	3.16	114.65	110.05
26	H1	203	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
26	A6	304	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
26	G9	201	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
28	MI	1001	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
26	YG	201	PEB	CHA-C1B-NB	-3.16	118.32	124.93
28	EB	1001	CYC	C1B-NB-C4B	-3.16	106.64	110.67
26	B3	201	PEB	C1C-CHB-C4B	-3.16	125.03	128.81
26	Y2	202	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	QE	202	PEB	CHC-C4C-C3C	-3.16	124.94	130.34
26	F3	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	yE	301	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	l1	202	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
26	b1	501	PEB	CMD-C2D-C3D	3.16	134.52	130.06
26	YE	203	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	dI	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	W7	202	PEB	CHC-C4C-C3C	-3.16	124.94	130.34
26	d7	202	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	g1	201	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
26	B5	203	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	U8	203	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	VJ	202	PEB	C3D-C4D-ND	3.16	113.46	107.26
26	a2	203	PEB	CAB-CBB-CGB	3.16	120.41	113.60
26	r4	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	TE	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	O8	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	kE	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	k6	201	PEB	C3B-C4B-NB	3.16	114.65	110.05
28	KB	202	CYC	C2A-C1A-NA	3.16	114.65	110.05
26	e1	202	PEB	C1C-CHB-C4B	-3.16	125.03	128.81
26	L1	201	PEB	CHC-C4C-C3C	-3.16	124.95	130.34
26	i4	202	PEB	CHC-C4C-C3C	-3.16	124.95	130.34
26	h2	201	PEB	CHB-C4B-C3B	-3.16	118.02	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B5	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	h6	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	l7	203	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	h4	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	N1	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
28	EF	1001	CYC	C4A-C3A-C2A	-3.16	102.88	106.51
26	m2	201	PEB	CHC-C4C-C3C	-3.16	124.95	130.34
26	u4	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	I5	202	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	Y8	203	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	dB	201	PEB	CHA-C1B-NB	-3.16	118.32	124.93
26	P7	201	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	GE	203	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	DI	1002	PEB	CMB-C2B-C1B	3.16	129.93	125.06
26	i2	202	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	VF	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	s4	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	II	201	PEB	C4B-NB-C1B	-3.16	100.56	106.51
26	M8	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	TB	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	NJ	204	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	TE	201	PEB	CHB-C4B-NB	-3.16	124.45	128.83
28	mH	1001	CYC	OC-C1C-C2C	-3.16	123.66	126.17
26	C9	202	PEB	CHC-C1D-ND	-3.16	110.28	113.95
26	AI	304	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	d6	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	Q8	202	PEB	C2A-C1A-NA	3.16	111.00	108.27
26	CC	201	PEB	CAA-C3A-C2A	-3.16	106.37	114.26
26	J3	201	PEB	OD-C4D-C3D	-3.16	122.31	129.46
26	mE	203	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	M3	201	PEB	CAB-C3B-C4B	3.16	130.59	125.01
26	H7	1002	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	F4	201	PEB	C1C-CHB-C4B	3.16	132.58	128.81
26	kI	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	TJ	203	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	ZI	202	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
26	i2	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	Y6	202	PEB	CMC-C3C-C2C	3.16	130.89	124.94
26	RB	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
26	a7	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	WD	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
26	yG	301	PEB	CHA-C1B-NB	-3.16	118.33	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z2	201	PEB	C2B-C1B-NB	3.16	117.27	110.53
26	L8	202	PEB	CHC-C4C-C3C	-3.16	124.95	130.34
26	g6	202	PEB	CHC-C1D-ND	-3.16	110.28	113.95
26	DA	201	PEB	C3B-C4B-NB	3.16	114.64	110.05
26	uE	201	PEB	C1B-C2B-C3B	-3.16	102.89	106.51
26	rE	201	PEB	C2A-C1A-NA	3.16	110.99	108.27
28	J2	1001	CYC	C2C-C1C-NC	3.16	110.99	108.27
26	dE	201	PEB	OD-C4D-ND	-3.16	121.26	125.93
26	r1	201	PEB	CHC-C4C-C3C	-3.15	124.96	130.34
26	R1	203	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	hG	202	PEB	C3B-C4B-NB	3.15	114.64	110.05
26	A9	301	PEB	OD-C4D-C3D	-3.15	122.31	129.46
26	hF	201	PEB	CHA-C1B-NB	-3.15	118.33	124.93
26	jB	202	PEB	CMB-C2B-C1B	3.15	129.92	125.06
26	l8	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	gE	201	PEB	CBC-CAC-C2C	-3.15	107.24	112.62
26	F9	202	PEB	C3D-C4D-ND	3.15	113.45	107.26
26	aB	201	PEB	C1C-CHB-C4B	3.15	132.58	128.81
26	T4	203	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	BE	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	AG	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	PG	202	PEB	C3B-C4B-NB	3.15	114.64	110.05
26	B8	301	PEB	CMB-C2B-C1B	3.15	129.92	125.06
26	S9	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	cB	201	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	JJ	202	PEB	OD-C4D-C3D	-3.15	122.31	129.46
26	T2	201	PEB	CHA-C1B-NB	-3.15	118.34	124.93
26	I8	201	PEB	CHA-C1B-NB	-3.15	118.34	124.93
26	YE	201	PEB	CHA-C1B-NB	-3.15	118.34	124.93
26	h6	203	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	eB	201	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	F5	203	PEB	C3B-C4B-NB	3.15	114.64	110.05
26	m4	203	PEB	CMB-C2B-C1B	3.15	129.92	125.06
26	n1	201	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	f4	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	i2	202	PEB	OD-C4D-C3D	-3.15	122.32	129.46
26	j8	201	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	VG	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	m6	201	PEB	CMB-C2B-C1B	3.15	129.92	125.06
26	WB	201	PEB	CHC-C4C-C3C	-3.15	124.96	130.34
27	24	403	PUB	OD-C4D-ND	-3.15	121.26	125.93
26	JD	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OF	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	TI	201	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
26	fA	202	PEB	OD-C4D-C3D	-3.15	122.32	129.46
26	F9	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
26	RF	201	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	H4	203	PEB	CHA-C1B-NB	-3.15	118.34	124.93
26	R4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	P9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	hG	201	PEB	OA-C1A-NA	3.15	128.76	124.94
26	E4	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	U6	201	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	OB	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	OG	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
26	Y4	202	PEB	CHB-C4B-NB	-3.15	124.45	128.83
26	V9	201	PEB	OD-C4D-C3D	-3.15	122.32	129.46
26	Y6	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
26	fE	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	P8	201	PEB	CMB-C2B-C1B	3.15	129.92	125.06
26	A1	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
26	N3	203	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	gE	203	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	FC	203	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	eE	201	PEB	CAC-CBC-CGC	-3.15	104.93	113.76
28	qH	1002	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
26	n4	201	PEB	CHB-C4B-NB	-3.15	124.46	128.83
28	K2	1001	CYC	CHA-C1A-NA	-3.15	124.46	128.83
26	I4	202	PEB	CHC-C4C-C3C	-3.15	124.96	130.34
26	Q2	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	iG	201	PEB	OD-C4D-ND	-3.15	121.26	125.93
26	HC	202	PEB	C1C-CHB-C4B	3.15	132.57	128.81
26	VJ	203	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	J4	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	P4	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
26	P8	201	PEB	C3B-C4B-NB	3.15	114.63	110.05
28	QH	1001	CYC	CHB-C4A-C3A	3.15	133.00	124.90
26	cG	203	PEB	CHC-C1D-ND	-3.15	110.29	113.95
28	D6	1001	CYC	CAB-C3B-C4B	3.15	126.35	121.38
26	K4	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
26	q4	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	CE	201	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	hE	201	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	hI	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	ZI	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
28	BB	1001	CYC	OB-C4B-C3B	-3.15	124.62	128.04
26	A2	301	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	gA	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	QB	203	PEB	CHC-C4C-C3C	-3.15	124.97	130.34
27	A7	304	PUB	OA-C1A-NA	-3.15	121.27	125.93
26	b7	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
26	LD	201	PEB	CAB-CBB-CGB	-3.15	106.83	113.60
26	R8	202	PEB	O2B-CGB-CBB	3.15	124.14	114.03
26	s1	201	PEB	CHC-C4C-C3C	-3.15	124.97	130.34
26	21	401	PEB	C3B-C4B-NB	3.15	114.63	110.05
26	k7	201	PEB	C3B-C4B-NB	3.15	114.63	110.05
26	EA	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
26	J1	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
26	YG	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
26	AJ	303	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
26	21	405	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
26	O2	201	PEB	CHA-C1B-NB	-3.15	118.35	124.93
26	AA	301	PEB	C3B-C4B-NB	3.15	114.63	110.05
26	EJ	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
28	MB	1001	CYC	C2A-C1A-NA	3.15	114.63	110.05
26	jI	201	PEB	C4B-NB-C1B	-3.15	100.58	106.51
26	T4	203	PEB	OD-C4D-ND	-3.15	121.27	125.93
26	UB	203	PEB	OD-C4D-ND	-3.15	121.27	125.93
26	i2	201	PEB	CMB-C2B-C1B	3.15	129.91	125.06
26	B9	203	PEB	CHA-C1B-NB	-3.15	118.35	124.93
26	j8	201	PEB	OD-C4D-C3D	-3.15	122.33	129.46
26	U8	203	PEB	C3B-C4B-NB	3.15	114.62	110.05
26	w4	201	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
26	f7	202	PEB	C1B-C2B-C3B	-3.15	102.90	106.51
26	U6	203	PEB	OD-C4D-ND	-3.15	121.27	125.93
26	A4	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	mH	1001	CYC	CHA-C1A-NA	-3.15	124.46	128.83
26	T6	202	PEB	C3B-C4B-NB	3.15	114.62	110.05
26	k1	201	PEB	CHC-C1D-ND	-3.15	110.30	113.95
26	iB	201	PEB	CMB-C2B-C1B	3.14	129.91	125.06
26	A9	301	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
28	YH	1003	CYC	C1A-C2A-C3A	-3.14	103.30	106.78
26	b7	201	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
26	hB	203	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	ZI	201	PEB	C2B-C1B-NB	3.14	117.24	110.53
26	A8	301	PEB	C3B-C4B-NB	3.14	114.62	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	YI	202	PEB	OD-C4D-ND	-3.14	121.27	125.93
26	k1	201	PEB	C1C-CHB-C4B	3.14	132.56	128.81
28	LI	1001	CYC	C4D-CHA-C1A	3.14	132.56	128.81
26	Y9	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	S2	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
26	a2	202	PEB	CAB-C3B-C4B	3.14	130.57	125.01
26	b7	201	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
26	YB	202	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
26	XA	202	PEB	O2B-CGB-CBB	3.14	124.13	114.03
26	M1	401	PEB	CHC-C4C-C3C	-3.14	124.97	130.34
26	a2	203	PEB	CAC-CBC-CGC	-3.14	104.95	113.76
28	H6	1001	CYC	CHA-C1A-NA	-3.14	124.47	128.83
26	u4	203	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	KC	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	SI	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	MA	203	PEB	CMB-C2B-C1B	3.14	129.91	125.06
26	Y3	303	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
26	YJ	201	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
26	SB	203	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	aA	203	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	v1	202	PEB	OD-C4D-ND	-3.14	121.27	125.93
26	H4	202	PEB	OD-C4D-ND	-3.14	121.27	125.93
26	VF	201	PEB	OD-C4D-ND	-3.14	121.27	125.93
26	NG	201	PEB	OD-C4D-ND	-3.14	121.27	125.93
26	s1	201	PEB	CAA-C3A-C2A	-3.14	106.41	114.26
26	J2	1002	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	Y2	202	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	RD	202	PEB	CHA-C1B-NB	-3.14	118.36	124.93
26	m2	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	IA	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	PA	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	R1	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	d7	202	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	P6	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
26	SG	203	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	B5	202	PEB	OD-C4D-C3D	-3.14	122.34	129.46
26	II	202	PEB	OD-C4D-C3D	-3.14	122.34	129.46
26	M4	402	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	AI	305	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	K1	202	PEB	C3B-C4B-NB	3.14	114.62	110.05
26	m2	201	PEB	CHB-C4B-NB	-3.14	124.47	128.83
26	T4	203	PEB	CHC-C4C-C3C	-3.14	124.98	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	JD	202	PEB	CHC-C1D-ND	-3.14	110.30	113.95
26	QG	201	PEB	CAB-C3B-C4B	3.14	130.56	125.01
26	A3	201	PEB	C3D-C4D-ND	3.14	113.42	107.26
26	y1	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
26	xE	304	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
26	HJ	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
28	gH	1001	CYC	OC-C1C-C2C	-3.14	123.68	126.17
28	oH	1001	CYC	OC-C1C-C2C	-3.14	123.68	126.17
26	T2	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	TJ	203	PEB	CHA-C1B-NB	-3.14	118.36	124.93
27	yE	303	PUB	OA-C1A-NA	-3.14	121.28	125.93
26	KD	202	PEB	OD-C4D-C3D	-3.14	122.34	129.46
26	VF	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	z4	201	PEB	CBA-CAA-C3A	3.14	120.46	113.47
26	M1	401	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
28	RH	1001	CYC	C4A-C3A-C2A	-3.14	102.90	106.51
26	ZE	202	PEB	CAB-C3B-C4B	3.14	130.56	125.01
26	KC	203	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	RI	203	PEB	CAB-CBB-CGB	3.14	120.36	113.60
26	UA	203	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	bG	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	FF	1002	PEB	C3B-C4B-NB	3.14	114.61	110.05
26	eA	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
26	t4	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
28	N7	1001	CYC	C4A-C3A-C2A	-3.14	102.90	106.51
26	AG	201	PEB	CHA-C1B-C2B	3.14	132.97	124.90
26	Y8	203	PEB	CAB-CBB-CGB	-3.14	106.85	113.60
26	l6	202	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
28	UH	1001	CYC	CAA-C2A-C1A	3.14	130.56	125.01
26	d6	201	PEB	C3B-C4B-NB	3.14	114.61	110.05
26	T6	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
26	oG	203	PEB	OD-C4D-C3D	-3.14	122.35	129.46
26	nE	201	PEB	CHB-C4B-NB	-3.14	124.47	128.83
26	fG	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
28	K7	1001	CYC	C2C-C1C-NC	3.14	110.98	108.27
26	mG	202	PEB	CMB-C2B-C1B	3.14	129.90	125.06
26	w4	203	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	PB	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	E8	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
27	A1	203	PUB	OA-C1A-NA	-3.14	121.28	125.93
26	Z4	202	PEB	C3B-C4B-NB	3.14	114.61	110.05
26	F5	202	PEB	C3B-C4B-NB	3.14	114.61	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TI	201	PEB	CHA-C1B-NB	-3.14	118.37	124.93
26	uG	202	PEB	CHA-C1B-C2B	3.14	132.97	124.90
26	MA	202	PEB	OD-C4D-C3D	-3.14	122.35	129.46
26	H9	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
26	fF	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
26	ZB	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
28	NB	1001	CYC	CBD-CAD-C3D	3.14	117.97	112.62
26	H4	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	W7	203	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	wG	303	PEB	CHA-C1B-C2B	3.14	132.97	124.90
26	AF	301	PEB	CMB-C2B-C1B	3.14	129.89	125.06
26	HE	201	PEB	CAA-C3A-C2A	3.14	122.09	114.26
26	S2	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
26	i4	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
26	H1	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
26	V4	202	PEB	C3B-C4B-NB	3.14	114.61	110.05
26	TJ	203	PEB	C3B-C4B-NB	3.14	114.61	110.05
26	R1	203	PEB	C1C-CHB-C4B	-3.14	125.06	128.81
26	W2	201	PEB	C2B-C1B-NB	3.14	117.22	110.53
26	uG	203	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	CJ	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
26	jA	201	PEB	OD-C4D-C3D	-3.14	122.36	129.46
26	b1	501	PEB	CHC-C4C-C3C	-3.14	124.99	130.34
26	Q4	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
26	O6	202	PEB	CHA-C1B-NB	-3.14	118.38	124.93
26	aG	203	PEB	C3B-C4B-NB	3.13	114.61	110.05
26	ZI	202	PEB	C3B-C4B-NB	3.13	114.61	110.05
26	S1	201	PEB	CAB-C3B-C4B	3.13	130.55	125.01
26	CE	202	PEB	C2A-C1A-NA	-3.13	105.57	108.27
26	YB	201	PEB	C1C-CHB-C4B	3.13	132.55	128.81
26	i2	201	PEB	C4B-C3B-C2B	-3.13	103.31	106.78
28	jH	1001	CYC	C1A-C2A-C3A	-3.13	103.31	106.78
26	ID	201	PEB	OD-C4D-C3D	-3.13	122.36	129.46
26	uE	201	PEB	CHC-C1D-ND	-3.13	110.31	113.95
26	R7	201	PEB	CMB-C2B-C1B	3.13	129.89	125.06
26	a1	201	PEB	CHC-C4C-C3C	-3.13	124.99	130.34
26	h8	202	PEB	CHA-C1B-NB	-3.13	118.38	124.93
26	T4	203	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
26	YG	202	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
26	qG	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
27	A9	302	PUB	OD-C4D-ND	-3.13	121.29	125.93
26	gB	202	PEB	C3B-C4B-NB	3.13	114.61	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J7	1003	CYC	C4D-CHA-C1A	3.13	132.55	128.81
26	RI	203	PEB	CHC-C1D-ND	-3.13	110.31	113.95
26	d2	202	PEB	CHB-C4B-NB	-3.13	124.48	128.83
26	uE	202	PEB	OD-C4D-ND	-3.13	121.29	125.93
28	JF	1003	CYC	C2A-C1A-NA	3.13	114.61	110.05
26	S6	201	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
26	WE	203	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
26	G9	202	PEB	CAC-CBC-CGC	-3.13	104.98	113.76
26	AA	302	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
26	XG	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
26	P2	202	PEB	CAB-C3B-C4B	3.13	130.55	125.01
26	i8	202	PEB	C3B-C4B-NB	3.13	114.61	110.05
26	i4	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
26	WG	202	PEB	CHC-C4C-C3C	-3.13	125.00	130.34
26	K4	202	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
26	I4	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
26	YI	201	PEB	CHB-C4B-NB	-3.13	124.48	128.83
26	GA	201	PEB	C3B-C4B-NB	3.13	114.60	110.05
26	E4	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
26	NI	1002	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
26	VI	202	PEB	CHC-C1D-ND	-3.13	110.31	113.95
28	N7	1001	CYC	CHB-C4A-NA	-3.13	118.38	124.93
26	vE	202	PEB	CMB-C2B-C1B	3.13	129.89	125.06
26	VF	203	PEB	C1C-CHB-C4B	3.13	132.55	128.81
26	A2	304	PEB	C2A-C1A-NA	3.13	110.97	108.27
26	LJ	203	PEB	C2A-C1A-NA	3.13	110.97	108.27
26	J4	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
26	TB	202	PEB	OD-C4D-ND	-3.13	121.29	125.93
26	b2	201	PEB	C2B-C1B-NB	3.13	117.21	110.53
26	FC	203	PEB	C3B-C4B-NB	3.13	114.60	110.05
26	Q3	201	PEB	CHA-C4A-NA	3.13	128.93	125.20
27	Y3	302	PUB	CHA-C4A-NA	-3.13	110.31	113.95
26	FG	201	PEB	CAB-C3B-C4B	3.13	130.55	125.01
28	MB	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
26	q1	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	h8	203	PEB	OD-C4D-ND	-3.13	121.29	125.93
26	hA	203	PEB	C1B-C2B-C3B	-3.13	102.91	106.51
26	cE	202	PEB	OD-C4D-C3D	-3.13	122.37	129.46
26	vG	202	PEB	CMB-C2B-C1B	3.13	129.88	125.06
26	R8	202	PEB	CAB-C3B-C4B	3.13	130.55	125.01
28	EB	1001	CYC	C1B-C2B-C3B	-3.13	104.61	107.87
26	QA	202	PEB	C2A-C1A-NA	3.13	110.97	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	dG	201	PEB	CMB-C2B-C1B	3.13	129.88	125.06
26	S8	202	PEB	CHB-C4B-NB	-3.13	124.49	128.83
26	jE	201	PEB	C3B-C4B-NB	3.13	114.60	110.05
26	h8	201	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
26	Q9	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	fI	202	PEB	CHC-C4C-C3C	-3.13	125.00	130.34
26	BJ	202	PEB	CHC-C4C-C3C	-3.13	125.00	130.34
28	HF	1001	CYC	CHB-C4A-NA	-3.13	118.39	124.93
28	N7	1001	CYC	CHB-C1B-NB	-3.13	119.34	126.06
26	D2	1002	PEB	C3B-C4B-NB	3.13	114.60	110.05
26	gB	201	PEB	CHB-C4B-NB	-3.13	124.49	128.83
26	GD	201	PEB	C2A-C1A-NA	3.13	110.97	108.27
26	F3	201	PEB	C1C-CHB-C4B	3.13	132.55	128.81
27	AA	303	PUB	OD-C4D-ND	-3.13	121.30	125.93
26	B5	203	PEB	CMB-C2B-C1B	3.13	129.88	125.06
26	OB	203	PEB	CHA-C1B-NB	-3.13	118.39	124.93
26	LE	201	PEB	CHA-C1B-NB	-3.13	118.39	124.93
26	UF	203	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	IE	203	PEB	CMA-C2A-C1A	-3.13	105.66	112.40
26	e3	401	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
26	OB	203	PEB	C2A-C1A-NA	3.13	110.97	108.27
28	G6	1001	CYC	C2A-C1A-NA	3.13	114.60	110.05
26	mB	203	PEB	CHB-C4B-NB	-3.13	124.49	128.83
28	CH	1001	CYC	CBD-CAD-C3D	-3.13	107.28	112.62
28	GI	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
26	oG	202	PEB	OD-C4D-ND	-3.13	121.30	125.93
26	d4	201	PEB	CHC-C4C-C3C	-3.13	125.00	130.34
26	dB	203	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
26	aG	203	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
26	QA	203	PEB	C3B-C4B-NB	3.13	114.60	110.05
26	hB	201	PEB	OD-C4D-C3D	-3.13	122.38	129.46
26	O8	201	PEB	CAB-CBB-CGB	-3.13	106.88	113.60
26	MG	203	PEB	C2A-C1A-NA	3.13	110.97	108.27
28	DI	1001	CYC	C2C-C1C-NC	3.13	110.97	108.27
26	e7	202	PEB	CHA-C1B-C2B	3.13	132.94	124.90
26	hA	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
26	MJ	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
26	T2	202	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
27	A6	303	PUB	CHB-C1C-NC	-3.13	124.49	128.83
26	j2	202	PEB	CHC-C4C-C3C	-3.13	125.01	130.34
26	U3	201	PEB	C3B-C4B-NB	3.13	114.59	110.05
26	C5	204	PEB	C1C-CHB-C4B	3.12	132.54	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g6	201	PEB	CHB-C4B-NB	-3.12	124.49	128.83
26	X4	203	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
26	SI	202	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
26	P7	201	PEB	CMB-C2B-C1B	3.12	129.88	125.06
26	A7	302	PEB	CHA-C1B-NB	-3.12	118.40	124.93
26	a8	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	N9	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	zE	501	PEB	CHC-C4C-C3C	-3.12	125.01	130.34
26	Q4	201	PEB	OD-C4D-ND	-3.12	121.30	125.93
26	g1	201	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
28	F7	1001	CYC	C4A-C3A-C2A	-3.12	102.92	106.51
26	Y6	202	PEB	CBC-CAC-C2C	3.12	117.95	112.62
26	Y6	201	PEB	CHC-C4C-C3C	-3.12	125.01	130.34
26	Q6	203	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	cA	203	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	S4	202	PEB	CHA-C1B-NB	-3.12	118.40	124.93
26	fE	202	PEB	OD-C4D-ND	-3.12	121.30	125.93
26	cF	202	PEB	CHC-C4C-C3C	-3.12	125.01	130.34
28	NF	1001	CYC	CHB-C4A-NA	-3.12	118.40	124.93
26	M8	202	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
28	eH	1001	CYC	C1B-C2B-C3B	-3.12	104.61	107.87
26	z4	202	PEB	C2A-C1A-NA	3.12	110.97	108.27
26	O7	201	PEB	C2A-C1A-NA	3.12	110.97	108.27
26	jE	202	PEB	C2A-C1A-NA	3.12	110.97	108.27
26	SF	201	PEB	OD-C4D-ND	-3.12	121.30	125.93
26	QJ	202	PEB	CMB-C2B-C1B	3.12	129.87	125.06
26	YA	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	QB	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	I1	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	FC	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	WB	203	PEB	CHA-C1B-NB	-3.12	118.40	124.93
26	K8	201	PEB	CBB-CAB-C3B	-3.12	103.95	112.63
26	A6	301	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
26	Q8	203	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
26	k1	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	D7	1002	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	A8	302	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	lF	202	PEB	CMB-C2B-C1B	3.12	129.87	125.06
28	RH	1001	CYC	C4D-CHA-C1A	3.12	132.54	128.81
26	WE	201	PEB	OD-C4D-C3D	-3.12	122.39	129.46
26	Q3	202	PEB	CBA-CAA-C3A	-3.12	106.52	113.47
26	g6	202	PEB	OD-C4D-ND	-3.12	121.31	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fB	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	OF	203	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	A1	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	YE	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	T3	203	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
27	K4	203	PUB	C4B-CHB-C1C	-3.12	125.08	128.81
26	DA	201	PEB	OD-C4D-C3D	-3.12	122.39	129.46
26	U2	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	R7	201	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	h8	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	R9	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
28	NB	1001	CYC	CHB-C1B-NB	-3.12	119.36	126.06
26	X4	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	B8	301	PEB	C2A-C1A-NA	3.12	110.96	108.27
26	PJ	202	PEB	CHB-C4B-NB	-3.12	124.50	128.83
26	g6	202	PEB	C3B-C4B-NB	3.12	114.59	110.05
26	H7	1002	PEB	CMB-C2B-C1B	3.12	129.87	125.06
28	II	1001	CYC	CHB-C4A-NA	-3.12	118.41	124.93
26	C4	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	U9	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	FE	201	PEB	CAB-C3B-C4B	3.12	130.53	125.01
26	YI	203	PEB	CAB-CBB-CGB	3.12	120.31	113.60
26	R8	202	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
26	YD	301	PEB	C3B-C4B-NB	3.12	114.58	110.05
26	24	404	PEB	C2A-C1A-NA	3.12	110.96	108.27
26	g4	203	PEB	OD-C4D-C3D	-3.12	122.39	129.46
26	d6	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	B3	203	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	V4	201	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	H3	203	PEB	CHA-C4A-NA	-3.12	121.50	125.20
26	U3	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	mF	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
28	M2	1001	CYC	C1A-C2A-C3A	-3.12	103.33	106.78
26	KA	201	PEB	CBB-CAB-C3B	-3.12	103.97	112.63
26	PE	202	PEB	C3B-C4B-NB	3.12	114.58	110.05
26	OG	203	PEB	C1C-CHB-C4B	3.12	132.53	128.81
26	d8	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	SI	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	eE	202	PEB	CHA-C1B-C2B	3.12	132.92	124.90
26	k4	201	PEB	CAB-CBB-CGB	-3.12	106.89	113.60
28	LI	1001	CYC	CHB-C1B-NB	-3.12	119.37	126.06
26	G8	203	PEB	C1B-C2B-C3B	-3.12	102.93	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	YB	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	G8	201	PEB	CHA-C4A-NA	3.12	128.91	125.20
26	11	203	PEB	C2A-C1A-NA	3.12	110.96	108.27
26	d6	204	PEB	C2A-C1A-NA	3.12	110.96	108.27
26	f7	203	PEB	C2A-C1A-NA	3.12	110.96	108.27
26	cE	202	PEB	CHA-C1B-NB	-3.12	118.41	124.93
26	P6	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	GA	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	M1	402	PEB	OD-C4D-C3D	-3.12	122.40	129.46
26	gA	202	PEB	CMB-C2B-C1B	3.12	129.86	125.06
26	a1	203	PEB	CHB-C4B-NB	-3.12	124.50	128.83
26	A9	303	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	jB	202	PEB	CHA-C1B-NB	-3.12	118.42	124.93
26	A9	303	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	hG	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	w4	201	PEB	C2A-C1A-NA	3.12	110.96	108.27
28	JF	1001	CYC	C2A-C1A-NA	3.12	114.58	110.05
26	QI	201	PEB	CHA-C4A-NA	3.12	128.91	125.20
26	YA	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
26	I4	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
26	M1	402	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
26	ED	202	PEB	CMB-C2B-C1B	3.11	129.86	125.06
26	DG	201	PEB	CHC-C4C-C3C	-3.11	125.02	130.34
26	j7	201	PEB	C1C-CHB-C4B	3.11	132.53	128.81
26	AG	201	PEB	CHC-C1D-ND	-3.11	110.33	113.95
26	i4	201	PEB	C3B-C4B-NB	3.11	114.58	110.05
26	B9	201	PEB	C3B-C4B-NB	3.11	114.58	110.05
26	XE	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
26	IA	203	PEB	OD-C4D-C3D	-3.11	122.40	129.46
26	YD	301	PEB	OD-C4D-C3D	-3.11	122.40	129.46
27	AJ	302	PUB	CBB-CAB-C3B	3.11	117.94	112.62
26	Y3	304	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
26	C8	202	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
26	dI	202	PEB	CMB-C2B-C1B	3.11	129.86	125.06
26	L1	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	T8	201	PEB	C3B-C4B-NB	3.11	114.58	110.05
26	jA	203	PEB	CHA-C1B-NB	-3.11	118.42	124.93
28	TH	1001	CYC	OC-C1C-C2C	-3.11	123.70	126.17
26	C5	203	PEB	OD-C4D-ND	-3.11	121.32	125.93
26	J7	1002	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
26	Q2	201	PEB	CHA-C1B-NB	-3.11	118.42	124.93
26	cE	202	PEB	C1B-C2B-C3B	-3.11	102.93	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lA	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
27	N9	201	PUB	C1C-C2C-C3C	-3.11	103.34	106.78
26	A1	202	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
26	VB	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
26	U1	201	PEB	CHC-C1D-ND	-3.11	110.33	113.95
26	T1	202	PEB	CMB-C2B-C1B	3.11	129.86	125.06
26	aE	202	PEB	CAB-C3B-C4B	3.11	130.52	125.01
28	MH	1001	CYC	CAA-C2A-C1A	3.11	130.52	125.01
26	fA	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	hG	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	O3	201	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
26	OG	203	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
26	hA	203	PEB	OD-C4D-ND	-3.11	121.32	125.93
26	EE	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
26	O3	202	PEB	C3D-C4D-ND	3.11	113.37	107.26
28	E6	1001	CYC	C1B-C2B-C3B	-3.11	104.62	107.87
26	WB	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	YG	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	t1	202	PEB	C2A-C1A-NA	3.11	110.96	108.27
26	Z7	202	PEB	C2A-C1A-NA	3.11	110.96	108.27
26	N2	1002	PEB	C3B-C4B-NB	3.11	114.58	110.05
26	R7	201	PEB	CHB-C4B-NB	-3.11	124.51	128.83
26	O1	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
26	YD	304	PEB	CHA-C1B-C2B	3.11	132.90	124.90
26	N1	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	Z1	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	K6	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
27	24	403	PUB	C2C-C1C-NC	3.11	114.58	110.05
26	kB	201	PEB	CAB-C3B-C4B	3.11	130.51	125.01
26	YI	202	PEB	CHA-C1B-NB	-3.11	118.42	124.93
26	14	203	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	u4	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
26	dB	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
26	T4	203	PEB	CHA-C1B-NB	-3.11	118.43	124.93
26	24	401	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	a8	204	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	ZE	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	Y8	202	PEB	OD-C4D-ND	-3.11	121.32	125.93
26	r4	201	PEB	CMB-C2B-C1B	3.11	129.85	125.06
26	BA	301	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	PJ	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	C4	202	PEB	C3B-C4B-NB	3.11	114.57	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l8	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	PA	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	HC	203	PEB	C2A-C1A-NA	3.11	110.95	108.27
27	YD	302	PUB	OD-C4D-ND	-3.11	121.32	125.93
26	IA	201	PEB	CHC-C1D-ND	-3.11	110.34	113.95
26	R4	201	PEB	CHA-C1B-NB	-3.11	118.43	124.93
26	gE	202	PEB	CHA-C1B-NB	-3.11	118.43	124.93
26	kA	202	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
28	D7	1001	CYC	CHA-C1A-NA	-3.11	124.51	128.83
26	iF	201	PEB	C1C-CHB-C4B	3.11	132.52	128.81
26	g2	203	PEB	CAB-C3B-C2B	3.11	133.67	127.88
26	UF	201	PEB	OD-C4D-C3D	-3.11	122.42	129.46
26	T9	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	BA	301	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	JG	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	V4	203	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	mA	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	B1	201	PEB	CHB-C4B-C3B	-3.11	118.14	125.32
26	CC	203	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
26	K8	203	PEB	CHC-C1D-ND	-3.11	110.34	113.95
26	sG	203	PEB	CHC-C1D-ND	-3.11	110.34	113.95
26	UF	202	PEB	C3B-C4B-NB	3.11	114.57	110.05
28	NB	1001	CYC	C2A-C1A-NA	3.11	114.57	110.05
26	f7	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
26	j7	201	PEB	CMB-C2B-C1B	3.11	129.85	125.06
26	x4	202	PEB	CHA-C1B-NB	-3.11	118.43	124.93
26	lE	201	PEB	CHA-C1B-NB	-3.11	118.43	124.93
26	E1	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	XG	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	a7	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
26	U4	201	PEB	CHB-C4B-NB	-3.11	124.52	128.83
26	E9	201	PEB	OD-C4D-C3D	-3.11	122.42	129.46
26	LC	203	PEB	OD-C4D-C3D	-3.11	122.42	129.46
26	N1	203	PEB	CMD-C2D-C3D	-3.11	125.68	130.06
26	U7	201	PEB	CHC-C1D-ND	-3.11	110.34	113.95
26	Z6	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
28	HF	1001	CYC	C1B-NB-C4B	-3.11	106.71	110.67
26	l8	201	PEB	CMB-C2B-C1B	3.11	129.85	125.06
26	hE	201	PEB	CMB-C2B-C1B	3.11	129.85	125.06
26	QA	203	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
26	mI	203	PEB	CBB-CAB-C3B	3.11	121.26	112.63
26	PD	201	PEB	CHA-C1B-NB	-3.11	118.44	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	QI	202	PEB	CHB-C4B-NB	-3.11	124.52	128.83
26	kF	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
26	b2	201	PEB	C4B-NB-C1B	-3.11	100.66	106.51
26	fF	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
26	UG	202	PEB	C3D-C4D-ND	3.11	113.35	107.26
26	G1	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	d4	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	IG	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	I1	202	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
26	kF	202	PEB	CAA-C3A-C4A	3.11	120.65	112.67
26	D8	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
26	jA	203	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	kI	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
26	O8	202	PEB	C4B-C3B-C2B	-3.11	103.35	106.78
26	kG	202	PEB	C4B-C3B-C2B	-3.11	103.35	106.78
26	HI	1002	PEB	C1C-CHB-C4B	3.10	132.52	128.81
26	RJ	202	PEB	C3D-C4D-ND	3.10	113.35	107.26
26	I8	203	PEB	OD-C4D-C3D	-3.10	122.42	129.46
26	AJ	305	PEB	CHB-C4B-NB	-3.10	124.52	128.83
26	aB	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	WI	201	PEB	C2B-C1B-NB	3.10	117.16	110.53
26	hG	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	g4	202	PEB	C2A-C1A-NA	3.10	110.95	108.27
26	YD	303	PEB	C2A-C1A-NA	3.10	110.95	108.27
28	J2	1001	CYC	CHA-C1A-NA	-3.10	124.52	128.83
26	Y3	303	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
26	v1	202	PEB	CAB-C3B-C4B	3.10	130.50	125.01
26	AG	201	PEB	CAB-C3B-C4B	3.10	130.50	125.01
26	tG	202	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
26	F5	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	g8	201	PEB	OD-C4D-ND	-3.10	121.33	125.93
26	LC	201	PEB	OD-C4D-ND	-3.10	121.33	125.93
26	UJ	201	PEB	CHC-C1D-ND	-3.10	110.34	113.95
26	lF	203	PEB	CHA-C1B-C2B	3.10	132.88	124.90
26	T9	201	PEB	CHA-C1B-NB	-3.10	118.44	124.93
26	S7	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	ID	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	G1	201	PEB	OD-C4D-ND	-3.10	121.33	125.93
26	k4	201	PEB	OD-C4D-ND	-3.10	121.33	125.93
26	KE	201	PEB	OD-C4D-ND	-3.10	121.33	125.93
27	A8	303	PUB	OD-C4D-ND	-3.10	121.33	125.93
26	M4	402	PEB	OD-C4D-C3D	-3.10	122.43	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mB	201	PEB	CAA-C3A-C2A	-3.10	106.51	114.26
26	L4	201	PEB	CHA-C1B-NB	-3.10	118.44	124.93
26	M1	403	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
26	sE	201	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
26	QI	201	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
26	P1	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	Q6	203	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	OB	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	V6	202	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	UI	202	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	P9	203	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
28	F7	1001	CYC	C1A-C2A-C3A	-3.10	103.35	106.78
26	AJ	301	PEB	C2A-C1A-NA	3.10	110.95	108.27
26	iB	202	PEB	OD-C4D-ND	-3.10	121.33	125.93
26	OA	203	PEB	CHA-C1B-NB	-3.10	118.44	124.93
26	HE	201	PEB	C1C-CHB-C4B	3.10	132.51	128.81
26	NG	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	v4	201	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	cF	202	PEB	OD-C4D-C3D	-3.10	122.43	129.46
26	H4	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	c7	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	w4	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	C5	204	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	KD	202	PEB	C2A-C1A-NA	3.10	110.95	108.27
26	B1	203	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	C1	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	K4	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
26	iI	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
26	WG	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	oG	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	dB	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	WF	203	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	p1	202	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	M4	403	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	RA	202	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
27	yG	303	PUB	CHA-C1B-C2B	-3.10	125.05	130.34
26	ID	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	gE	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	VJ	203	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	Q4	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	A2	304	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	h8	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r1	201	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	J8	201	PEB	CHA-C4A-NA	3.10	128.89	125.20
26	M4	401	PEB	CHA-C1B-NB	-3.10	118.45	124.93
26	mI	201	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
26	X1	201	PEB	CAC-CBC-CGC	-3.10	105.07	113.76
26	m8	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
27	21	403	PUB	OD-C4D-ND	-3.10	121.34	125.93
26	a6	202	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	Y9	201	PEB	CHB-C4B-NB	-3.10	124.53	128.83
26	GE	203	PEB	OA-C1A-C2A	-3.10	123.71	126.17
28	oH	1001	CYC	CAA-C2A-C1A	3.10	130.49	125.01
26	K9	201	PEB	CMB-C2B-C1B	3.10	129.84	125.06
26	L9	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	cE	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	U4	201	PEB	CHC-C1D-ND	-3.10	110.35	113.95
26	OE	202	PEB	CHA-C1B-C2B	3.10	132.87	124.90
26	PG	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	A2	305	PEB	C2A-C1A-NA	3.10	110.94	108.27
26	E8	202	PEB	C2A-C1A-NA	3.10	110.94	108.27
26	eG	203	PEB	C3B-C4B-NB	3.10	114.56	110.05
26	N4	203	PEB	CMC-C3C-C2C	-3.10	119.10	124.94
26	aG	203	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
26	HC	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	ND	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	gI	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
26	V1	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	CC	202	PEB	OD-C4D-ND	-3.10	121.34	125.93
28	KI	1001	CYC	CHA-C1A-NA	-3.10	124.53	128.83
26	R9	202	PEB	CMB-C2B-C1B	3.10	129.83	125.06
26	TB	201	PEB	C1C-CHB-C4B	3.10	132.51	128.81
26	JD	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	kF	202	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	Z2	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	d2	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	YB	202	PEB	CHC-C1D-ND	-3.10	110.35	113.95
26	j6	202	PEB	CMB-C2B-C1B	3.10	129.83	125.06
28	C2	1001	CYC	CHA-C1A-NA	-3.10	124.53	128.83
27	A2	302	PUB	C4B-CHB-C1C	-3.10	125.11	128.81
26	pE	202	PEB	CAB-C3B-C4B	3.10	130.49	125.01
26	C8	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
26	dF	202	PEB	C3B-C4B-NB	3.10	114.55	110.05
26	MJ	201	PEB	C3B-C4B-NB	3.10	114.55	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A9	303	PEB	CHC-C4C-C3C	-3.10	125.06	130.34
26	LA	202	PEB	CHC-C4C-C3C	-3.10	125.06	130.34
26	h4	202	PEB	C2A-C1A-NA	3.10	110.94	108.27
26	J1	202	PEB	CAB-C3B-C4B	3.10	130.49	125.01
26	WG	202	PEB	CAA-C3A-C2A	-3.10	106.52	114.26
26	K6	201	PEB	C1C-CHB-C4B	3.10	132.51	128.81
26	aA	203	PEB	C3B-C4B-NB	3.10	114.55	110.05
26	W4	202	PEB	CMB-C2B-C1B	3.10	129.83	125.06
26	B5	203	PEB	CHA-C1B-NB	-3.10	118.46	124.93
26	aG	202	PEB	CHB-C4B-NB	-3.10	124.53	128.83
26	YB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
26	xE	303	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	J1	201	PEB	CHC-C1D-ND	-3.10	110.35	113.95
27	A7	303	PUB	OA-C1A-NA	-3.09	121.34	125.93
26	gI	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
26	h8	203	PEB	C2A-C1A-NA	3.09	110.94	108.27
26	LE	202	PEB	CAA-C3A-C4A	-3.09	104.73	112.67
26	JI	1002	PEB	CAB-C3B-C4B	3.09	130.48	125.01
26	S9	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
26	s1	203	PEB	CHB-C4B-NB	-3.09	124.53	128.83
26	c7	202	PEB	CHB-C4B-NB	-3.09	124.53	128.83
26	v1	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
26	e7	202	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
26	D3	201	PEB	C1B-C2B-C3B	-3.09	102.95	106.51
26	Y1	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	Q3	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	V7	201	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	aB	201	PEB	CBC-CAC-C2C	3.09	117.90	112.62
26	JC	201	PEB	CMA-C2A-C1A	-3.09	105.73	112.40
26	N9	203	PEB	C2A-C1A-NA	3.09	110.94	108.27
26	T6	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
27	A2	303	PUB	OD-C4D-ND	-3.09	121.35	125.93
26	L2	1002	PEB	CMB-C2B-C1B	3.09	129.83	125.06
26	JI	1002	PEB	CMB-C2B-C1B	3.09	129.83	125.06
26	D4	203	PEB	CHA-C1B-NB	-3.09	118.46	124.93
26	t1	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	JC	201	PEB	CHB-C4B-NB	-3.09	124.54	128.83
26	d7	203	PEB	CHA-C1B-C2B	3.09	132.85	124.90
26	U8	203	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	T4	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
26	M9	202	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
26	gB	201	PEB	C2A-C1A-NA	3.09	110.94	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GC	203	PEB	C2A-C1A-NA	3.09	110.94	108.27
27	xE	301	PUB	CHA-C4A-NA	-3.09	110.36	113.95
26	PA	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
26	KB	201	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	kB	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	EA	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	J5	201	PEB	CAA-C3A-C4A	-3.09	104.73	112.67
26	kB	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
26	sG	201	PEB	OD-C4D-C3D	-3.09	122.45	129.46
26	KG	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	LJ	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	HG	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	O6	201	PEB	CHB-C4B-C3B	-3.09	118.18	125.32
26	H4	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
26	VA	202	PEB	OA-C1A-NA	3.09	128.69	124.94
26	UA	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
26	i7	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
26	V6	202	PEB	CHA-C1B-NB	-3.09	118.47	124.93
26	c6	201	PEB	CHB-C4B-NB	-3.09	124.54	128.83
26	MA	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	EG	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	T1	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
26	Q8	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
26	Y9	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
26	c6	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	l8	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	OG	201	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	W8	201	PEB	OD-C4D-C3D	-3.09	122.46	129.46
26	G1	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	SG	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	I1	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
26	d4	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	W7	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	a6	201	PEB	CBC-CAC-C2C	3.09	117.89	112.62
26	M4	401	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	h7	203	PEB	CMB-C2B-C1B	3.09	129.82	125.06
26	I5	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	OI	202	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
26	b7	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	O2	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
26	TI	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
26	k2	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mE	203	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	IC	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	ED	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	TD	203	PEB	CHB-C4B-C3B	-3.09	118.19	125.32
26	d7	203	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	k4	202	PEB	CHB-C4B-NB	-3.09	124.54	128.83
26	T8	202	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
26	U1	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
26	m2	202	PEB	C2A-C1A-NA	3.09	110.94	108.27
26	O6	202	PEB	C2A-C1A-NA	3.09	110.94	108.27
26	W4	201	PEB	CHA-C1B-NB	-3.09	118.47	124.93
26	S8	203	PEB	CMB-C2B-C1B	3.09	129.82	125.06
26	aA	201	PEB	CMB-C2B-C1B	3.09	129.82	125.06
26	N8	201	PEB	CHA-C1B-C2B	3.09	132.84	124.90
28	KF	1001	CYC	CBD-CAD-C3D	-3.09	107.35	112.62
26	j1	201	PEB	OD-C4D-ND	-3.09	121.36	125.93
26	x1	201	PEB	CHB-C4B-NB	-3.09	124.54	128.83
26	QB	203	PEB	CBA-CAA-C3A	-3.09	106.59	113.47
26	TB	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	I4	202	PEB	C3B-C4B-NB	3.09	114.54	110.05
26	lA	203	PEB	OD-C4D-C3D	-3.09	122.47	129.46
26	c2	203	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
26	C3	202	PEB	CHA-C1B-NB	-3.09	118.48	124.93
26	qE	203	PEB	C2A-C1A-NA	3.09	110.93	108.27
28	NB	1001	CYC	CHA-C1A-NA	-3.09	124.55	128.83
28	iH	1001	CYC	C1B-C2B-C3B	-3.09	104.65	107.87
26	Y7	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
26	VD	203	PEB	CHC-C1D-ND	-3.09	110.36	113.95
26	q1	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
26	L3	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	W1	201	PEB	CAB-C3B-C4B	3.09	130.47	125.01
26	SA	202	PEB	OD-C4D-ND	-3.09	121.36	125.93
26	IE	201	PEB	OD-C4D-ND	-3.09	121.36	125.93
27	24	403	PUB	OA-C1A-NA	-3.09	121.36	125.93
26	a2	202	PEB	OD-C4D-ND	-3.09	121.36	125.93
26	U2	201	PEB	C2B-C1B-NB	3.09	117.11	110.53
26	RA	202	PEB	C3B-C4B-NB	3.09	114.54	110.05
26	LI	1002	PEB	C3B-C4B-NB	3.09	114.54	110.05
26	KG	202	PEB	CBC-CAC-C2C	-3.09	107.36	112.62
26	GA	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	RD	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	KA	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TB	202	PEB	C3B-C4B-NB	3.08	114.54	110.05
26	MG	203	PEB	C3B-C4B-NB	3.08	114.54	110.05
26	P3	203	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	O4	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
28	KF	1001	CYC	C1A-C2A-C3A	-3.08	103.37	106.78
26	TG	202	PEB	CAB-C3B-C4B	3.08	130.47	125.01
26	g2	203	PEB	C1C-CHB-C4B	-3.08	125.12	128.81
26	vE	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	QA	203	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	UE	202	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	B3	202	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	QD	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	D1	203	PEB	CHA-C1B-NB	-3.08	118.48	124.93
26	xG	304	PEB	CHC-C4C-C3C	-3.08	125.08	130.34
26	L3	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	KC	203	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	U6	203	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	WE	203	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	xG	302	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	nE	201	PEB	CMB-C2B-C1B	3.08	129.81	125.06
26	C9	202	PEB	C1C-CHB-C4B	3.08	132.49	128.81
26	pG	201	PEB	CHC-C1D-ND	-3.08	110.37	113.95
26	O6	203	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	P1	202	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	I8	203	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	Y3	301	PEB	CMD-C2D-C3D	3.08	134.41	130.06
26	sE	201	PEB	OD-C4D-C3D	-3.08	122.48	129.46
26	O2	202	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	P7	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	TI	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
26	X1	203	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	m6	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	Y3	303	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
27	yG	302	PUB	CAC-CBC-CGC	-3.08	106.97	113.60
26	bI	202	PEB	CHC-C1D-ND	-3.08	110.37	113.95
26	l2	201	PEB	CMA-C2A-C1A	-3.08	105.76	112.40
26	lE	201	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	L9	203	PEB	CHC-C4C-C3C	-3.08	125.08	130.34
26	iG	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	uG	203	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	k2	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	N8	202	PEB	OD-C4D-ND	-3.08	121.37	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KG	203	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
26	w1	203	PEB	CBC-CAC-C2C	-3.08	107.36	112.62
26	GC	203	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	BC	203	PEB	CMB-C2B-C1B	3.08	129.81	125.06
26	l8	201	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
26	mA	201	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
26	t4	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	cG	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	OB	201	PEB	CHC-C4C-C3C	-3.08	125.08	130.34
26	D9	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	XJ	203	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	VA	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	jG	201	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	M1	401	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
26	N1	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
26	ZG	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
28	nH	1001	CYC	OC-C1C-C2C	-3.08	123.72	126.17
27	AI	303	PUB	OD-C4D-ND	-3.08	121.37	125.93
28	IF	1001	CYC	CHA-C1A-NA	-3.08	124.56	128.83
26	b1	501	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
28	E2	1001	CYC	C4A-C3A-C2A	-3.08	102.97	106.51
26	Y4	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	H7	1002	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	WB	203	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	lA	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
26	JE	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	Y7	201	PEB	CHC-C4C-C3C	-3.08	125.09	130.34
28	NB	1001	CYC	CMB-C2B-C1B	3.08	128.01	124.17
28	CI	1001	CYC	C1A-C2A-C3A	-3.08	103.38	106.78
26	N9	204	PEB	CHC-C1D-ND	-3.08	110.37	113.95
26	C4	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	OD	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
26	aG	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	F1	203	PEB	C2A-C1A-NA	3.08	110.93	108.27
26	cA	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	u4	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
26	m2	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
26	E8	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	24	401	PEB	CHA-C1B-NB	-3.08	118.50	124.93
26	z1	202	PEB	CHA-C1B-C2B	3.08	132.81	124.90
26	WG	202	PEB	CHA-C1B-C2B	3.08	132.81	124.90
26	PG	202	PEB	CBC-CAC-C2C	3.08	117.87	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E6	1001	CYC	C1B-NB-C4B	-3.08	106.75	110.67
26	PD	201	PEB	C2A-C1A-NA	3.08	110.92	108.27
26	G5	202	PEB	OA-C1A-C2A	-3.08	123.73	126.17
26	b6	202	PEB	OA-C1A-C2A	-3.08	123.73	126.17
26	a4	201	PEB	CHC-C4C-C3C	-3.08	125.09	130.34
27	xE	301	PUB	CBA-CAA-C3A	-3.08	108.31	112.98
26	CG	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
28	E7	1001	CYC	CMB-C2B-C1B	3.08	128.01	124.17
26	II	201	PEB	C2B-C1B-NB	3.08	117.09	110.53
26	L3	203	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	Q6	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	UA	203	PEB	OD-C4D-ND	-3.08	121.37	125.93
26	N4	203	PEB	CMD-C2D-C3D	-3.08	125.73	130.06
26	Q8	204	PEB	CBC-CAC-C2C	-3.08	107.37	112.62
26	T7	201	PEB	OD-C4D-C3D	-3.07	122.49	129.46
26	HJ	202	PEB	OD-C4D-ND	-3.07	121.38	125.93
26	W3	202	PEB	CMB-C2B-C1B	3.07	129.80	125.06
26	MD	202	PEB	CHC-C4C-C3C	-3.07	125.09	130.34
26	BJ	202	PEB	CHC-C1D-ND	-3.07	110.38	113.95
27	AI	302	PUB	CHA-C4A-NA	-3.07	110.38	113.95
26	RJ	203	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	H3	201	PEB	CHA-C1B-NB	-3.07	118.50	124.93
26	X9	202	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
26	OI	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
26	a6	201	PEB	C1C-CHB-C4B	3.07	132.48	128.81
26	mE	201	PEB	CHA-C1B-C2B	3.07	132.80	124.90
26	AB	301	PEB	C3B-C4B-NB	3.07	114.52	110.05
26	W7	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	SA	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	AC	203	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	wE	302	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	w1	203	PEB	CMB-C2B-C1B	3.07	129.80	125.06
26	z4	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
26	GC	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
28	RH	1001	CYC	C1B-NB-C4B	-3.07	106.76	110.67
26	AE	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
26	JI	1002	PEB	C3B-C4B-NB	3.07	114.52	110.05
26	DD	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
26	UB	203	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
26	NG	201	PEB	CHC-C1D-ND	-3.07	110.38	113.95
26	kE	203	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	Y3	301	PEB	C1B-C2B-C3B	-3.07	102.98	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lB	201	PEB	CHA-C1B-NB	-3.07	118.51	124.93
26	OD	202	PEB	C1C-CHB-C4B	3.07	132.48	128.81
26	dE	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
26	SD	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
26	g2	202	PEB	CHA-C1B-NB	-3.07	118.51	124.93
26	z1	202	PEB	OD-C4D-C3D	-3.07	122.50	129.46
26	l8	203	PEB	OD-C4D-C3D	-3.07	122.50	129.46
26	M1	403	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	GA	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
26	p4	201	PEB	CMB-C2B-C1B	3.07	129.79	125.06
26	Q8	202	PEB	CHC-C1D-ND	-3.07	110.38	113.95
26	G9	202	PEB	CHC-C1D-ND	-3.07	110.38	113.95
26	E8	203	PEB	C3B-C4B-NB	3.07	114.52	110.05
26	R9	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
26	R9	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	iG	203	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	XJ	203	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
26	V1	203	PEB	OD-C4D-ND	-3.07	121.38	125.93
26	e1	201	PEB	OD-C4D-ND	-3.07	121.38	125.93
26	eB	203	PEB	OD-C4D-ND	-3.07	121.38	125.93
26	S2	202	PEB	C2A-C1A-NA	3.07	110.92	108.27
26	i7	201	PEB	CHC-C1D-ND	-3.07	110.38	113.95
26	M1	402	PEB	CHA-C1B-NB	-3.07	118.51	124.93
26	d6	203	PEB	OD-C4D-ND	-3.07	121.38	125.93
26	ZE	201	PEB	OD-C4D-ND	-3.07	121.38	125.93
27	AF	303	PUB	OA-C1A-NA	-3.07	121.38	125.93
28	yH	1001	CYC	OC-C1C-C2C	-3.07	123.73	126.17
26	J9	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	MA	202	PEB	CHA-C4A-NA	3.07	128.85	125.20
26	21	404	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
26	f6	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
26	WG	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
26	Y3	303	PEB	C2A-C1A-NA	3.07	110.92	108.27
26	cA	202	PEB	CHC-C1D-ND	-3.07	110.38	113.95
26	C5	204	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
26	G5	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
26	f6	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	f7	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	jI	201	PEB	C2B-C1B-NB	3.07	117.08	110.53
28	E2	1001	CYC	C2A-C1A-NA	3.07	114.51	110.05
26	k1	203	PEB	CHB-C4B-NB	-3.07	124.57	128.83
26	X9	201	PEB	CHB-C4B-NB	-3.07	124.57	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B1	203	PEB	OD-C4D-ND	-3.07	121.38	125.93
26	RG	202	PEB	OD-C4D-C3D	-3.07	122.51	129.46
26	eE	202	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
26	g2	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
28	kH	1001	CYC	CHA-C1A-NA	-3.07	124.57	128.83
26	f2	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	QJ	201	PEB	CHC-C4C-C3C	-3.07	125.11	130.34
26	jB	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
26	WD	201	PEB	OD-C4D-C3D	-3.07	122.51	129.46
26	eD	401	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
26	fA	201	PEB	OD-C4D-ND	-3.07	121.39	125.93
26	iE	202	PEB	OD-C4D-ND	-3.07	121.39	125.93
26	SJ	201	PEB	OD-C4D-ND	-3.07	121.39	125.93
26	l6	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	AE	201	PEB	CAB-C3B-C4B	3.07	130.44	125.01
26	LJ	201	PEB	C2A-C1A-NA	3.07	110.92	108.27
26	X8	202	PEB	O2B-CGB-CBB	3.07	123.88	114.03
26	LI	1002	PEB	CMB-C2B-C1B	3.07	129.79	125.06
26	Y2	202	PEB	CHA-C1B-NB	-3.07	118.52	124.93
26	b4	501	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
26	l7	202	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
26	AJ	305	PEB	C1B-C2B-C3B	-3.07	102.99	106.51
26	QA	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	P2	201	PEB	OD-C4D-ND	-3.07	121.39	125.93
26	hF	203	PEB	CHB-C4B-NB	-3.07	124.57	128.83
26	EA	201	PEB	CMB-C2B-C1B	3.07	129.78	125.06
26	bE	202	PEB	CHB-C4B-C3B	-3.07	118.24	125.32
28	J7	1003	CYC	CHB-C1B-NB	-3.07	119.48	126.06
26	L9	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	hA	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	hG	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
26	c1	203	PEB	C3B-C4B-NB	3.07	114.51	110.05
26	k4	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
26	PI	201	PEB	CHB-C4B-NB	-3.07	124.58	128.83
26	ZB	203	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	gG	203	PEB	C2A-C1A-NA	3.06	110.92	108.27
26	fE	202	PEB	CMC-C3C-C2C	-3.06	119.16	124.94
28	lH	1001	CYC	C1B-C2B-C3B	-3.06	104.67	107.87
26	KE	203	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
26	mB	202	PEB	CHB-C4B-C3B	-3.06	118.24	125.32
26	eI	202	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	AI	301	PEB	CMB-C2B-C1B	3.06	129.78	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q8	203	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
26	F3	202	PEB	OD-C4D-C3D	-3.06	122.52	129.46
26	YD	304	PEB	C3B-C4B-NB	3.06	114.50	110.05
26	HD	203	PEB	CHA-C4A-NA	-3.06	121.56	125.20
26	H5	201	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	yG	301	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	F4	201	PEB	CHB-C4B-NB	-3.06	124.58	128.83
26	fB	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
26	aI	202	PEB	CAB-C3B-C4B	3.06	130.43	125.01
26	RA	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
26	mG	203	PEB	CAA-C3A-C4A	3.06	120.54	112.67
26	HF	1002	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	NJ	204	PEB	CMB-C2B-C1B	3.06	129.78	125.06
26	VI	202	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	HD	202	PEB	OD-C4D-ND	-3.06	121.39	125.93
26	tE	201	PEB	OD-C4D-ND	-3.06	121.39	125.93
26	N8	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
26	AC	201	PEB	CHB-C4B-NB	-3.06	124.58	128.83
26	NE	201	PEB	OD-C4D-ND	-3.06	121.39	125.93
26	M9	201	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	UB	201	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	qG	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	SE	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	QE	203	PEB	OD-C4D-C3D	-3.06	122.52	129.46
26	E9	201	PEB	CHA-C1B-NB	-3.06	118.53	124.93
26	eA	201	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
26	S6	202	PEB	CHB-C4B-NB	-3.06	124.58	128.83
26	A1	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	M8	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	i7	201	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
26	G9	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	UI	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	d1	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	S4	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	i8	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	MA	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	KE	203	PEB	C1C-CHB-C4B	3.06	132.46	128.81
26	e6	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	HF	1002	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	t1	202	PEB	OD-C4D-C3D	-3.06	122.53	129.46
26	D6	1002	PEB	OD-C4D-C3D	-3.06	122.53	129.46
26	h8	202	PEB	OD-C4D-C3D	-3.06	122.53	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m2	203	PEB	CBB-CAB-C3B	3.06	121.13	112.63
26	T2	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	U4	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
26	EE	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	E4	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	W9	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	gI	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
28	L2	1001	CYC	CHB-C1B-NB	-3.06	119.49	126.06
26	B8	301	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	iG	203	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	vG	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
27	A6	302	PUB	OD-C4D-ND	-3.06	121.40	125.93
26	O9	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
28	lH	1001	CYC	CBD-CAD-C3D	-3.06	107.40	112.62
26	T2	201	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	M8	202	PEB	CHA-C4A-NA	3.06	128.84	125.20
26	Q7	203	PEB	C1C-CHB-C4B	-3.06	125.16	128.81
26	lG	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	g2	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	cI	203	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	S7	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	dA	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	xG	303	PEB	OD-C4D-C3D	-3.06	122.53	129.46
26	bB	201	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
26	jF	202	PEB	CHA-C4A-NA	-3.06	121.57	125.20
26	SA	203	PEB	CMB-C2B-C1B	3.06	129.77	125.06
26	gB	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	SG	203	PEB	C1C-CHB-C4B	3.06	132.46	128.81
26	Z4	202	PEB	CAA-C3A-C4A	3.06	120.52	112.67
26	CE	203	PEB	C3B-C4B-NB	3.06	114.50	110.05
26	iF	201	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
26	e1	202	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	L5	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	C9	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	IE	203	PEB	OD-C4D-C3D	-3.06	122.53	129.46
26	P2	201	PEB	CHB-C4B-NB	-3.06	124.59	128.83
26	I4	202	PEB	CHB-C4B-NB	-3.06	124.59	128.83
26	g2	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
26	AI	304	PEB	CHC-C1D-ND	-3.06	110.40	113.95
27	K1	203	PUB	CHA-C1B-C2B	-3.06	125.12	130.34
26	SB	201	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	XE	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	hE	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	H4	203	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	LA	202	PEB	CBC-CAC-C2C	3.06	117.83	112.62
26	l6	201	PEB	CHA-C1B-NB	-3.06	118.54	124.93
26	D1	203	PEB	C3B-C4B-NB	3.06	114.49	110.05
26	UI	202	PEB	C3B-C4B-NB	3.06	114.49	110.05
26	t4	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	j7	203	PEB	C2A-C1A-NA	3.06	110.91	108.27
26	E1	201	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	S1	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	Q3	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	c7	201	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	DD	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	VJ	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
26	D9	203	PEB	C3D-C4D-ND	3.06	113.25	107.26
26	cA	201	PEB	CAB-C3B-C4B	3.06	130.41	125.01
26	rG	202	PEB	CHA-C1B-NB	-3.06	118.54	124.93
26	c6	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
26	L4	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	OE	203	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	JJ	201	PEB	C1B-C2B-C3B	-3.06	103.00	106.51
26	f6	202	PEB	C3B-C4B-NB	3.06	114.49	110.05
26	FF	1002	PEB	CHB-C4B-NB	-3.05	124.59	128.83
28	I2	1001	CYC	CHB-C4A-NA	-3.05	118.54	124.93
26	Q6	203	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
28	qH	1002	CYC	C1B-NB-C4B	-3.05	106.78	110.67
26	Y1	202	PEB	C2A-C1A-NA	3.05	110.91	108.27
26	aB	202	PEB	C2A-C1A-NA	3.05	110.91	108.27
26	YE	202	PEB	C2A-C1A-NA	3.05	110.91	108.27
28	hH	1001	CYC	CHA-C1A-NA	-3.05	124.59	128.83
26	a4	203	PEB	C1B-C2B-C3B	-3.05	103.00	106.51
26	EJ	201	PEB	OD-C4D-C3D	-3.05	122.54	129.46
26	e6	201	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
26	MD	201	PEB	CMB-C2B-C1B	3.05	129.77	125.06
26	CE	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	I3	202	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
26	M3	202	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
26	e4	201	PEB	C1B-C2B-C3B	-3.05	103.00	106.51
26	DA	202	PEB	CMB-C2B-C1B	3.05	129.77	125.06
26	x1	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	a6	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	cB	201	PEB	OD-C4D-ND	-3.05	121.41	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AJ	304	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	NJ	202	PEB	CHB-C4B-NB	-3.05	124.59	128.83
26	OF	201	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
26	I5	203	PEB	CMB-C2B-C1B	3.05	129.76	125.06
26	UA	203	PEB	C1B-C2B-C3B	-3.05	103.00	106.51
26	T2	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	a8	203	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	fF	203	PEB	CHC-C1D-ND	-3.05	110.40	113.95
28	EH	1001	CYC	C1B-NB-C4B	-3.05	106.78	110.67
26	YE	202	PEB	C1B-C2B-C3B	-3.05	103.00	106.51
26	jF	202	PEB	C1B-C2B-C3B	-3.05	103.00	106.51
26	H5	202	PEB	C3B-C4B-NB	3.05	114.49	110.05
26	cI	201	PEB	C3B-C4B-NB	3.05	114.49	110.05
26	L2	1002	PEB	OD-C4D-C3D	-3.05	122.55	129.46
26	mG	202	PEB	CHA-C1B-NB	-3.05	118.55	124.93
26	U7	203	PEB	C3D-C4D-ND	3.05	113.25	107.26
28	nH	1001	CYC	C4D-CHA-C1A	3.05	132.45	128.81
26	d1	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	Q8	203	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	R4	203	PEB	OD-C4D-C3D	-3.05	122.55	129.46
26	A2	301	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	N4	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	LG	202	PEB	CAB-C3B-C4B	3.05	130.41	125.01
26	R8	201	PEB	CMB-C2B-C1B	3.05	129.76	125.06
26	l8	203	PEB	CMB-C2B-C1B	3.05	129.76	125.06
26	tG	202	PEB	OD-C4D-C3D	-3.05	122.55	129.46
27	AF	304	PUB	CMA-C2A-C3A	3.05	135.94	129.67
26	s1	203	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	S2	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
26	IJ	203	PEB	CBC-CAC-C2C	-3.05	107.42	112.62
26	B4	203	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
26	WF	203	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
26	E4	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	OB	202	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	M8	202	PEB	OD-C4D-C3D	-3.05	122.55	129.46
26	mE	202	PEB	C1C-CHB-C4B	3.05	132.45	128.81
26	PB	201	PEB	C2A-C1A-NA	3.05	110.90	108.27
26	iB	201	PEB	C3B-C4B-NB	3.05	114.48	110.05
26	AE	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
27	xG	301	PUB	CAC-CBC-CGC	-3.05	107.04	113.60
26	FF	1002	PEB	OD-C4D-ND	-3.05	121.41	125.93
28	RH	1001	CYC	CAB-C3B-C4B	3.05	126.19	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a8	204	PEB	CHA-C1B-NB	-3.05	118.56	124.93
28	F7	1001	CYC	C2A-C1A-NA	3.05	114.48	110.05
26	C1	201	PEB	CMB-C2B-C1B	3.05	129.76	125.06
26	QA	204	PEB	CMB-C2B-C1B	3.05	129.76	125.06
26	OI	202	PEB	CMB-C2B-C1B	3.05	129.76	125.06
26	QD	202	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	j4	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
26	L8	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	PE	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
26	L1	201	PEB	OD-C4D-C3D	-3.05	122.55	129.46
26	D3	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	E3	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	B4	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	PF	201	PEB	CHC-C4C-C3C	-3.05	125.14	130.34
26	BC	203	PEB	CHA-C1B-NB	-3.05	118.56	124.93
26	WG	201	PEB	CMA-C2A-C1A	-3.05	105.83	112.40
26	K9	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
26	A2	304	PEB	CHC-C1D-ND	-3.05	110.41	113.95
26	TD	203	PEB	CAB-C3B-C2B	3.05	133.55	127.88
28	LI	1001	CYC	OB-C4B-C3B	-3.05	124.73	128.04
26	iI	201	PEB	C3B-C4B-NB	3.05	114.48	110.05
26	K5	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	R1	201	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
26	DA	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
26	EA	202	PEB	OD-C4D-ND	-3.05	121.42	125.93
26	f4	202	PEB	CHC-C4C-C3C	-3.05	125.14	130.34
26	L2	1002	PEB	C3B-C4B-NB	3.05	114.48	110.05
26	LC	202	PEB	C3B-C4B-NB	3.05	114.48	110.05
28	H6	1001	CYC	C2A-C1A-NA	3.05	114.48	110.05
26	l2	201	PEB	C4B-NB-C1B	-3.05	100.77	106.51
26	PJ	201	PEB	C1B-C2B-C3B	-3.05	103.01	106.51
26	aB	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
26	L1	201	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	E4	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	U9	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	PJ	203	PEB	CHA-C1B-NB	-3.05	118.56	124.93
26	o1	501	PEB	CMB-C2B-C1B	3.05	129.75	125.06
26	l6	202	PEB	OD-C4D-C3D	-3.05	122.56	129.46
26	I5	201	PEB	C2A-C1A-NA	3.05	110.90	108.27
28	CB	1001	CYC	C2A-C1A-NA	3.05	114.48	110.05
28	JI	1001	CYC	C2A-C1A-NA	3.05	114.48	110.05
26	A4	201	PEB	OD-C4D-ND	-3.05	121.42	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C8	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
26	c4	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	hE	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
26	vG	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
28	K7	1001	CYC	C2A-C1A-NA	3.05	114.48	110.05
26	KB	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
26	T4	202	PEB	OD-C4D-ND	-3.05	121.42	125.93
27	K4	203	PUB	OD-C4D-ND	-3.05	121.42	125.93
28	1H	1000	CYC	CHA-C1A-NA	-3.04	124.60	128.83
26	II	201	PEB	OA-C1A-C2A	-3.04	123.75	126.17
26	f7	201	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
26	F1	203	PEB	CHC-C4C-C3C	-3.04	125.14	130.34
26	W6	203	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
26	W7	202	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
26	J8	202	PEB	OD-C4D-ND	-3.04	121.42	125.93
26	P3	203	PEB	C3B-C4B-NB	3.04	114.48	110.05
28	D6	1001	CYC	C2A-C1A-NA	3.04	114.48	110.05
26	b7	201	PEB	C2A-C1A-NA	3.04	110.90	108.27
26	SA	203	PEB	C2A-C1A-NA	3.04	110.90	108.27
26	A7	302	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
28	G2	1001	CYC	C4A-C3A-C2A	-3.04	103.01	106.51
26	C5	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
26	A9	303	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
26	Z7	202	PEB	OA-C1A-C2A	-3.04	123.75	126.17
26	IC	203	PEB	OA-C1A-C2A	-3.04	123.75	126.17
26	11	203	PEB	CHC-C1D-ND	-3.04	110.41	113.95
26	DE	201	PEB	C3B-C4B-NB	3.04	114.48	110.05
26	QD	201	PEB	OD-C4D-C3D	-3.04	122.56	129.46
26	S9	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
26	k7	201	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
26	CC	202	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
26	e4	202	PEB	CMC-C3C-C2C	3.04	130.68	124.94
26	EG	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	d8	203	PEB	CHB-C4B-NB	-3.04	124.61	128.83
26	kI	203	PEB	CHB-C4B-NB	-3.04	124.61	128.83
26	J4	201	PEB	C2A-C1A-NA	3.04	110.90	108.27
26	mB	201	PEB	OA-C1A-C2A	-3.04	123.75	126.17
26	OD	201	PEB	OA-C1A-C2A	-3.04	123.75	126.17
26	D8	201	PEB	OD-C4D-C3D	-3.04	122.57	129.46
26	C5	203	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	MA	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	CD	202	PEB	CHB-C4B-NB	-3.04	124.61	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E6	1001	CYC	CHA-C1A-NA	-3.04	124.61	128.83
26	hA	203	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	DB	1002	PEB	OD-C4D-C3D	-3.04	122.57	129.46
26	T1	201	PEB	CHC-C1D-ND	-3.04	110.42	113.95
26	nE	202	PEB	C2A-C1A-NA	3.04	110.89	108.27
26	K4	202	PEB	CHB-C4B-NB	-3.04	124.61	128.83
26	KA	202	PEB	CBC-CAC-C2C	-3.04	107.43	112.62
26	2I	404	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
28	hH	1001	CYC	OC-C1C-C2C	-3.04	123.75	126.17
26	TG	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
26	U9	202	PEB	CMB-C2B-C1B	3.04	129.75	125.06
26	U4	201	PEB	CHA-C1B-NB	-3.04	118.57	124.93
26	YF	202	PEB	CHB-C4B-C3B	-3.04	118.30	125.32
26	h7	202	PEB	CAB-CBB-CGB	-3.04	107.06	113.60
26	N4	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	14	203	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	iB	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	HC	201	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	kE	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	S7	203	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	RD	203	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	VF	201	PEB	CHC-C1D-ND	-3.04	110.42	113.95
26	I1	202	PEB	CHC-C4C-C3C	-3.04	125.15	130.34
26	14	203	PEB	CHC-C4C-C3C	-3.04	125.15	130.34
26	d2	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	NI	1002	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	BC	201	PEB	CMB-C2B-C1B	3.04	129.75	125.06
26	dF	203	PEB	CMB-C2B-C1B	3.04	129.75	125.06
26	D4	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	g8	202	PEB	C2A-C1A-NA	3.04	110.89	108.27
26	vE	202	PEB	C2A-C1A-NA	3.04	110.89	108.27
26	K6	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
26	DD	203	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	MG	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	MJ	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	f4	202	PEB	CAB-C3B-C4B	3.04	130.38	125.01
26	uG	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
26	k8	202	PEB	OA-C1A-C2A	-3.04	123.76	126.17
28	C7	1001	CYC	CHB-C1B-NB	-3.04	119.53	126.06
26	P6	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	QI	201	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	h7	202	PEB	CHA-C1B-NB	-3.04	118.58	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	GI	1001	CYC	CHB-C4A-NA	-3.04	118.58	124.93
26	A6	301	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	GA	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	G5	201	PEB	CAA-C3A-C2A	-3.04	106.67	114.26
26	K4	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	m7	201	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	lA	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
26	z1	202	PEB	CHB-C4B-C3B	3.04	132.34	125.32
26	Y1	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
26	W3	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
28	WH	1001	CYC	OC-C1C-C2C	-3.04	123.76	126.17
26	v4	202	PEB	CAB-C3B-C4B	3.04	130.38	125.01
26	HA	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	dI	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	V3	202	PEB	CAA-C3A-C2A	-3.04	106.67	114.26
28	YH	1002	CYC	CHA-C1A-NA	-3.04	124.61	128.83
26	F5	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
26	rE	202	PEB	C2A-C1A-NA	3.04	110.89	108.27
26	pG	202	PEB	C2A-C1A-NA	3.04	110.89	108.27
26	l6	203	PEB	CHC-C1D-ND	-3.04	110.42	113.95
26	RD	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	SG	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
26	A7	305	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
26	YD	303	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
26	R2	201	PEB	CHB-C4B-C3B	-3.04	118.31	125.32
26	AB	304	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
28	CH	1001	CYC	C1B-C2B-C3B	-3.04	104.70	107.87
26	WD	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
28	IB	1001	CYC	C1B-NB-C4B	-3.04	106.80	110.67
27	21	402	PUB	CHA-C1B-C2B	-3.04	125.16	130.34
26	R7	202	PEB	OD-C4D-C3D	-3.04	122.58	129.46
26	OD	202	PEB	C1B-C2B-C3B	-3.04	103.02	106.51
28	BB	1001	CYC	C4A-C3A-C2A	-3.04	103.02	106.51
26	PD	203	PEB	C3B-C4B-NB	3.04	114.46	110.05
26	J2	1002	PEB	CAB-C3B-C4B	3.03	130.38	125.01
26	l8	202	PEB	OD-C4D-ND	-3.03	121.43	125.93
26	MG	203	PEB	OD-C4D-ND	-3.03	121.43	125.93
26	QG	203	PEB	OD-C4D-ND	-3.03	121.43	125.93
26	eF	201	PEB	CHC-C1D-ND	-3.03	110.42	113.95
26	F1	203	PEB	OA-C1A-C2A	-3.03	123.76	126.17
26	OA	202	PEB	OD-C4D-C3D	-3.03	122.58	129.46
26	C3	202	PEB	C2A-C1A-NA	3.03	110.89	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lB	202	PEB	C2A-C1A-NA	3.03	110.89	108.27
26	qE	202	PEB	CAB-CBB-CGB	-3.03	107.07	113.60
26	W4	201	PEB	CAB-C3B-C4B	3.03	130.38	125.01
26	HI	1002	PEB	C1B-C2B-C3B	-3.03	103.02	106.51
28	I6	1001	CYC	C1B-NB-C4B	-3.03	106.81	110.67
26	K9	202	PEB	C4B-C3B-C2B	-3.03	103.42	106.78
26	bF	203	PEB	C3B-C4B-NB	3.03	114.46	110.05
26	HG	201	PEB	C3B-C4B-NB	3.03	114.46	110.05
26	Y2	203	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	xE	302	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	K9	201	PEB	CHC-C4C-C3C	-3.03	125.16	130.34
26	xG	302	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
26	CJ	202	PEB	OD-C4D-C3D	-3.03	122.59	129.46
26	LG	201	PEB	CAB-C3B-C4B	3.03	130.38	125.01
26	T4	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
26	hB	201	PEB	CMB-C2B-C1B	3.03	129.74	125.06
26	r1	201	PEB	CHB-C4B-C3B	-3.03	118.31	125.32
26	R1	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	JE	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	f6	201	PEB	CAB-CBB-CGB	-3.03	107.08	113.60
26	E3	202	PEB	CMB-C2B-C1B	3.03	129.73	125.06
26	D1	202	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
26	JI	1002	PEB	CAC-CBC-CGC	-3.03	105.26	113.76
26	RB	201	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
26	Z1	202	PEB	C2A-C1A-NA	3.03	110.89	108.27
26	y4	201	PEB	C1C-CHB-C4B	3.03	132.43	128.81
28	B6	1002	CYC	CAB-C3B-C4B	3.03	126.17	121.38
26	wG	302	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	H6	1002	PEB	OD-C4D-C3D	-3.03	122.59	129.46
26	Q2	201	PEB	C2B-C1B-NB	3.03	117.00	110.53
28	GI	1001	CYC	CMA-C3A-C4A	3.03	129.73	125.06
26	tE	202	PEB	OD-C4D-C3D	-3.03	122.59	129.46
26	D6	1002	PEB	C2A-C1A-NA	3.03	110.89	108.27
26	SA	202	PEB	OA-C1A-C2A	-3.03	123.76	126.17
26	cA	202	PEB	OA-C1A-C2A	-3.03	123.76	126.17
28	eH	1001	CYC	OC-C1C-C2C	-3.03	123.76	126.17
26	BJ	202	PEB	C3B-C4B-NB	3.03	114.46	110.05
26	Z2	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
26	LC	202	PEB	CMB-C2B-C1B	3.03	129.73	125.06
26	UI	201	PEB	C2B-C1B-NB	3.03	117.00	110.53
26	w1	202	PEB	CAB-C3B-C4B	3.03	130.37	125.01
26	SE	202	PEB	C1C-CHB-C4B	3.03	132.43	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HA	201	PEB	OD-C4D-C3D	-3.03	122.59	129.46
26	ZB	202	PEB	C3B-C4B-NB	3.03	114.46	110.05
26	gB	201	PEB	OD-C4D-ND	-3.03	121.44	125.93
27	AA	303	PUB	OD-C4D-C3D	-3.03	124.75	128.04
26	pG	201	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
26	Y9	201	PEB	C2A-C1A-NA	3.03	110.89	108.27
26	BC	203	PEB	C2A-C1A-NA	3.03	110.89	108.27
26	CA	202	PEB	CHA-C1B-NB	-3.03	118.59	124.93
26	XJ	203	PEB	CHA-C1B-NB	-3.03	118.59	124.93
26	OG	202	PEB	CHC-C1D-ND	-3.03	110.43	113.95
26	PB	202	PEB	CMC-C3C-C2C	3.03	130.65	124.94
26	hE	202	PEB	C3B-C4B-NB	3.03	114.46	110.05
26	PI	201	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	n1	201	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
26	B3	201	PEB	CMB-C2B-C1B	3.03	129.73	125.06
26	m8	201	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	lE	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	AC	202	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
26	hA	202	PEB	CAB-CBB-CGB	-3.03	107.08	113.60
26	D2	1002	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	D3	202	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	CC	201	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	D4	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
26	FI	1002	PEB	CMD-C2D-C3D	3.03	134.34	130.06
26	VF	201	PEB	CAB-CBB-CGB	-3.03	107.09	113.60
27	yE	302	PUB	CAC-CBC-CGC	-3.03	107.09	113.60
26	e8	201	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	X9	203	PEB	C3B-C4B-NB	3.03	114.45	110.05
27	A6	303	PUB	OA-C1A-NA	-3.03	121.44	125.93
28	N2	1001	CYC	C4A-C3A-C2A	-3.03	103.03	106.51
27	AF	303	PUB	CHA-C4A-NA	-3.03	110.43	113.95
26	RD	202	PEB	CHA-C4A-NA	3.03	128.81	125.20
26	C8	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	OF	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	dF	203	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	WD	201	PEB	OD-C4D-ND	-3.03	121.44	125.93
26	p1	201	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
28	DF	1001	CYC	C1B-CHB-C4A	-3.03	120.69	128.08
26	U8	203	PEB	CHA-C1B-NB	-3.03	118.60	124.93
26	GB	1002	PEB	C1C-CHB-C4B	3.03	132.43	128.81
26	YF	201	PEB	CAB-CBB-CGB	-3.03	107.09	113.60
26	LJ	203	PEB	OD-C4D-ND	-3.03	121.45	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lG	201	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	J9	202	PEB	OD-C4D-C3D	-3.03	122.60	129.46
26	FG	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
26	d2	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
26	j6	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
26	eB	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
26	m4	201	PEB	OD-C4D-C3D	-3.03	122.60	129.46
28	I7	1001	CYC	CHA-C1A-NA	-3.03	124.63	128.83
26	E9	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	TA	201	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	NJ	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
26	l7	203	PEB	CMB-C2B-C1B	3.03	129.72	125.06
26	f7	202	PEB	OA-C1A-C2A	-3.03	123.77	126.17
26	DG	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
26	CA	203	PEB	OD-C4D-ND	-3.03	121.45	125.93
26	d6	204	PEB	OD-C4D-C3D	-3.03	122.61	129.46
26	n1	201	PEB	CMB-C2B-C1B	3.03	129.72	125.06
26	Q7	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
26	Q1	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
26	F5	201	PEB	OD-C4D-C3D	-3.02	122.61	129.46
26	T2	203	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	T9	202	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	mB	203	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	f8	201	PEB	C3B-C4B-NB	3.02	114.45	110.05
26	JG	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	H2	1002	PEB	C1B-C2B-C3B	-3.02	103.03	106.51
26	h8	202	PEB	C1C-CHB-C4B	3.02	132.42	128.81
26	A7	302	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	L9	203	PEB	CMB-C2B-C1B	3.02	129.72	125.06
26	Q8	202	PEB	C3B-C4B-NB	3.02	114.45	110.05
26	TD	202	PEB	C2B-C1B-NB	3.02	116.98	110.53
26	Z4	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
28	M2	1001	CYC	C4A-C3A-C2A	-3.02	103.04	106.51
26	k7	201	PEB	OD-C4D-C3D	-3.02	122.61	129.46
26	B3	203	PEB	CHA-C4A-NA	-3.02	121.61	125.20
26	kI	202	PEB	C3B-C4B-NB	3.02	114.45	110.05
26	E1	201	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	K3	201	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	QG	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	T6	202	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
26	eF	202	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
26	G5	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m4	202	PEB	CHC-C4C-C3C	-3.02	125.18	130.34
26	Y8	203	PEB	CHC-C4C-C3C	-3.02	125.18	130.34
26	RD	201	PEB	CMA-C2A-C1A	-3.02	105.89	112.40
26	B9	201	PEB	C1C-CHB-C4B	3.02	132.42	128.81
28	MH	1001	CYC	C4D-CHA-C1A	3.02	132.42	128.81
26	A7	305	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	NA	202	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	b7	201	PEB	OD-C4D-C3D	-3.02	122.61	129.46
26	ZG	201	PEB	CAB-CBB-CGB	-3.02	107.10	113.60
26	c8	201	PEB	OD-C4D-C3D	-3.02	122.61	129.46
26	PF	202	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	x4	201	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
26	b4	501	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	R8	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	ED	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	d8	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	P9	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	AC	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
28	D2	1001	CYC	C1A-C2A-C3A	-3.02	103.44	106.78
28	JF	1003	CYC	CMB-C2B-C1B	3.02	127.94	124.17
26	XG	203	PEB	CBC-CAC-C2C	3.02	117.78	112.62
26	kG	203	PEB	CHA-C4A-NA	-3.02	121.61	125.20
26	fB	201	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	UF	201	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	u4	201	PEB	OD-C4D-ND	-3.02	121.45	125.93
26	NA	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	j6	202	PEB	CHA-C1B-NB	-3.02	118.61	124.93
26	GA	203	PEB	CHA-C1B-NB	-3.02	118.61	124.93
26	SB	202	PEB	OA-C1A-C2A	-3.02	123.77	126.17
28	L2	1001	CYC	OB-C4B-C3B	-3.02	124.76	128.04
26	lA	201	PEB	CHA-C1B-NB	-3.02	118.61	124.93
26	T3	201	PEB	OD-C4D-ND	-3.02	121.45	125.93
27	K4	203	PUB	C1D-CHC-C4C	-3.02	106.80	113.37
26	M3	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	I4	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	k4	201	PEB	CMB-C2B-C1B	3.02	129.72	125.06
26	WA	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
26	gF	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
27	A8	304	PUB	CAC-CBC-CGC	-3.02	107.10	113.60
26	B3	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	x1	202	PEB	CAA-C3A-C2A	-3.02	106.71	114.26
26	QB	203	PEB	OA-C1A-C2A	-3.02	123.77	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	RE	202	PEB	OD-C4D-C3D	-3.02	122.62	129.46
26	R1	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	P6	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
26	YF	201	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
26	NG	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	IG	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	g6	202	PEB	CHA-C1B-NB	-3.02	118.62	124.93
26	b6	202	PEB	CHC-C4C-C3C	-3.02	125.19	130.34
26	N9	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	m7	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	T8	201	PEB	OD-C4D-ND	-3.02	121.46	125.93
27	A2	302	PUB	OD-C4D-ND	-3.02	121.46	125.93
26	SA	202	PEB	CHA-C4A-NA	-3.02	121.62	125.20
28	EH	1001	CYC	OC-C1C-C2C	-3.02	123.77	126.17
28	RH	1001	CYC	OC-C1C-C2C	-3.02	123.77	126.17
26	Q1	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	J3	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	TF	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	WF	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	j2	201	PEB	CMA-C2A-C1A	-3.02	105.90	112.40
26	gE	203	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	SD	201	PEB	CBB-CAB-C3B	-3.02	104.24	112.63
26	iA	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	BE	201	PEB	C3B-C4B-NB	3.02	114.44	110.05
26	N6	201	PEB	CHA-C1B-NB	-3.02	118.62	124.93
26	H9	201	PEB	OD-C4D-C3D	-3.02	122.62	129.46
26	Z7	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	HI	1002	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	V8	202	PEB	C2A-C1A-NA	3.02	110.87	108.27
26	L7	1002	PEB	OD-C4D-C3D	-3.02	122.62	129.46
26	KE	203	PEB	CHB-C4B-NB	-3.02	124.64	128.83
26	mI	201	PEB	CHB-C4B-NB	-3.02	124.64	128.83
26	lA	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	lB	203	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
26	QA	202	PEB	CMB-C2B-C1B	3.02	129.71	125.06
26	hA	202	PEB	C1C-CHB-C4B	3.02	132.41	128.81
26	F8	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	G9	202	PEB	OD-C4D-ND	-3.02	121.46	125.93
26	Z6	201	PEB	C1B-C2B-C3B	-3.02	103.05	106.51
28	JH	1001	CYC	C1B-C2B-C3B	-3.02	104.72	107.87
26	F9	203	PEB	CHB-C4B-C3B	3.02	132.29	125.32
28	FH	1001	CYC	CHA-C1A-NA	-3.02	124.64	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	cE	203	PEB	C3D-C4D-ND	3.02	113.17	107.26
26	h2	201	PEB	C2B-C1B-NB	3.02	116.97	110.53
26	D4	202	PEB	OD-C4D-C3D	-3.01	122.63	129.46
26	d1	202	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	Q8	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	A4	202	PEB	CHC-C4C-C3C	-3.01	125.19	130.34
26	m6	203	PEB	OD-C4D-ND	-3.01	121.46	125.93
26	LA	202	PEB	CHA-C1B-NB	-3.01	118.63	124.93
26	R6	202	PEB	C1C-CHB-C4B	-3.01	125.21	128.81
26	k1	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	k6	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	AI	304	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	GA	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	ZB	201	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	aB	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	cI	201	PEB	CHA-C1B-NB	-3.01	118.63	124.93
26	tE	202	PEB	CHB-C4B-C3B	-3.01	118.36	125.32
26	m1	203	PEB	CHB-C4B-NB	-3.01	124.65	128.83
26	c1	201	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	gI	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	AJ	305	PEB	CBC-CAC-C2C	-3.01	107.48	112.62
28	cH	1001	CYC	C2C-C1C-NC	3.01	110.87	108.27
27	A8	303	PUB	OD-C4D-C3D	-3.01	124.77	128.04
26	T8	202	PEB	OD-C4D-C3D	-3.01	122.63	129.46
26	D1	201	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	UA	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	IJ	201	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	CD	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	Z2	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	24	405	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	T6	201	PEB	C1C-CHB-C4B	3.01	132.41	128.81
26	dG	202	PEB	C1C-CHB-C4B	3.01	132.41	128.81
26	q1	201	PEB	CBC-CAC-C2C	-3.01	107.48	112.62
26	IC	201	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	RJ	201	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	CE	203	PEB	CHC-C1D-ND	-3.01	110.45	113.95
26	L4	201	PEB	CMB-C2B-C1B	3.01	129.70	125.06
26	GE	203	PEB	CMB-C2B-C1B	3.01	129.70	125.06
26	FJ	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	A5	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	CA	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	i7	201	PEB	CMB-C2B-C1B	3.01	129.70	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H1	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	M3	201	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	PD	203	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	J9	203	PEB	OD-C4D-C3D	-3.01	122.64	129.46
26	PB	202	PEB	CHA-C1B-NB	-3.01	118.63	124.93
26	hI	202	PEB	CHC-C4C-C3C	-3.01	125.20	130.34
28	PH	1001	CYC	C1B-NB-C4B	-3.01	106.83	110.67
26	HC	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	QF	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
28	IH	1001	CYC	C1B-C2B-C3B	-3.01	104.73	107.87
26	cI	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	gI	203	PEB	CBB-CAB-C3B	3.01	120.99	112.63
26	S7	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	WF	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	kF	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	YI	203	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	lB	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
26	T7	202	PEB	OD-C4D-C3D	-3.01	122.64	129.46
26	p4	201	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	h7	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	s4	201	PEB	CHB-C4B-C3B	-3.01	118.37	125.32
26	F4	202	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	P3	203	PEB	OD-C4D-C3D	-3.01	122.64	129.46
26	iA	202	PEB	OD-C4D-C3D	-3.01	122.64	129.46
26	P2	203	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	W8	203	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	mI	203	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	IE	203	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	E1	201	PEB	OA-C1A-C2A	-3.01	123.78	126.17
26	QD	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	D8	201	PEB	CHA-C1B-NB	-3.01	118.64	124.93
26	e7	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	AC	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	T4	201	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	fE	202	PEB	C2A-C1A-NA	3.01	110.87	108.27
26	BE	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
26	I3	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
26	FI	1002	PEB	CHB-C4B-NB	-3.01	124.65	128.83
26	c4	202	PEB	CHC-C4C-C3C	-3.01	125.20	130.34
26	q1	203	PEB	C1C-CHB-C4B	-3.01	125.22	128.81
26	P4	203	PEB	CMB-C2B-C1B	3.01	129.70	125.06
26	BD	203	PEB	CMB-C2B-C1B	3.01	129.70	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GG	201	PEB	CAC-CBC-CGC	-3.01	105.33	113.76
26	WG	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	PJ	203	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	YJ	201	PEB	C3B-C4B-NB	3.01	114.42	110.05
26	IC	201	PEB	CHC-C4C-C3C	-3.01	125.21	130.34
26	F7	1002	PEB	CHC-C1D-ND	-3.01	110.45	113.95
26	cA	201	PEB	CHC-C1D-ND	3.01	117.44	113.95
26	AA	302	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	mF	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	X9	201	PEB	CHA-C1B-NB	-3.01	118.64	124.93
26	H8	201	PEB	OD-C4D-C3D	-3.01	122.64	129.46
26	RI	201	PEB	CHB-C4B-C3B	-3.01	118.37	125.32
26	kG	203	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
26	GG	203	PEB	CBB-CAB-C3B	3.01	120.98	112.63
26	CC	201	PEB	CBA-CAA-C3A	3.01	120.16	113.47
26	Q9	202	PEB	CHB-C4B-NB	-3.01	124.66	128.83
26	FD	202	PEB	OD-C4D-C3D	-3.01	122.65	129.46
26	q1	203	PEB	CHC-C1D-ND	-3.01	110.45	113.95
26	e6	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
26	m1	201	PEB	CMB-C2B-C1B	3.01	129.69	125.06
26	a8	201	PEB	CMB-C2B-C1B	3.01	129.69	125.06
26	fB	201	PEB	CHC-C4C-C3C	-3.01	125.21	130.34
26	R1	202	PEB	C3B-C4B-NB	3.01	114.42	110.05
26	jI	202	PEB	C3B-C4B-NB	3.01	114.42	110.05
26	m1	203	PEB	CMC-C3C-C2C	3.01	130.61	124.94
26	e2	202	PEB	C2A-C1A-NA	3.01	110.86	108.27
26	v4	201	PEB	OD-C4D-ND	-3.01	121.48	125.93
26	U8	203	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
26	F9	203	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
26	c4	201	PEB	CHB-C4B-C3B	-3.01	118.38	125.32
26	A2	301	PEB	C3B-C4B-NB	3.01	114.42	110.05
26	g2	201	PEB	C3B-C4B-NB	3.01	114.42	110.05
26	cF	202	PEB	CAC-CBC-CGC	-3.01	105.33	113.76
26	J5	201	PEB	CHC-C4C-C3C	-3.01	125.21	130.34
26	W6	202	PEB	CMB-C2B-C1B	3.01	129.69	125.06
26	vG	202	PEB	OA-C1A-C2A	-3.01	123.78	126.17
26	iB	201	PEB	OD-C4D-C3D	-3.01	122.65	129.46
26	C5	201	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
26	CG	201	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
26	S6	201	PEB	CMB-C2B-C1B	3.01	129.69	125.06
26	CJ	202	PEB	CHB-C4B-NB	-3.01	124.66	128.83
26	LA	201	PEB	OD-C4D-ND	-3.01	121.48	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fG	201	PEB	OD-C4D-ND	-3.01	121.48	125.93
26	CJ	201	PEB	CHA-C1B-NB	-3.01	118.65	124.93
28	EI	1001	CYC	C2A-C1A-NA	3.00	114.42	110.05
26	L1	201	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	NJ	202	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	r4	201	PEB	CHA-C1B-NB	-3.00	118.65	124.93
26	XG	203	PEB	CAB-C3B-C4B	3.00	130.32	125.01
26	z1	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	u4	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	uG	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	L3	201	PEB	CAB-CBB-CGB	-3.00	107.14	113.60
26	O4	201	PEB	CHC-C4C-C3C	-3.00	125.21	130.34
26	O6	201	PEB	CHC-C4C-C3C	-3.00	125.21	130.34
26	D3	201	PEB	C3B-C4B-NB	3.00	114.42	110.05
26	H9	201	PEB	C3B-C4B-NB	3.00	114.42	110.05
26	lA	203	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	c2	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
26	C5	202	PEB	OD-C4D-ND	-3.00	121.48	125.93
26	TB	202	PEB	CBC-CAC-C2C	3.00	117.75	112.62
26	JG	201	PEB	CHA-C1B-NB	-3.00	118.65	124.93
26	R7	202	PEB	CHC-C4C-C3C	-3.00	125.21	130.34
26	R3	203	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	B9	202	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	W6	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	g6	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
26	VD	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
26	K3	201	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	DJ	202	PEB	C3B-C4B-NB	3.00	114.42	110.05
26	mB	203	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	T3	202	PEB	CBC-CAC-C2C	3.00	117.74	112.62
26	iG	201	PEB	CHA-C1B-C2B	3.00	132.62	124.90
26	G4	201	PEB	CHC-C4C-C3C	-3.00	125.22	130.34
26	g6	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
26	QA	204	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
26	eI	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
26	wG	301	PEB	OA-C1A-C2A	-3.00	123.79	126.17
26	P4	202	PEB	CHC-C1D-ND	-3.00	110.46	113.95
26	Y4	201	PEB	CHC-C1D-ND	-3.00	110.46	113.95
26	QE	203	PEB	CHC-C1D-ND	-3.00	110.46	113.95
26	ID	202	PEB	C3B-C4B-NB	3.00	114.42	110.05
26	P1	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	gA	202	PEB	C2A-C1A-NA	3.00	110.86	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d4	203	PEB	OD-C4D-C3D	-3.00	122.66	129.46
26	11	203	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	V1	202	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	AI	304	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	QI	201	PEB	C2B-C1B-NB	3.00	116.94	110.53
26	Q9	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
26	HF	1002	PEB	CMB-C2B-C1B	3.00	129.69	125.06
26	OA	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
26	k6	201	PEB	CHC-C4C-C3C	-3.00	125.22	130.34
26	s1	203	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	YD	304	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	MD	201	PEB	CAB-C3B-C4B	3.00	130.32	125.01
26	GG	201	PEB	CAA-C3A-C2A	3.00	121.76	114.26
26	eG	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	EJ	201	PEB	CAB-CBB-CGB	-3.00	107.15	113.60
26	J1	201	PEB	OD-C4D-ND	-3.00	121.48	125.93
26	WE	202	PEB	CAB-C3B-C4B	3.00	130.32	125.01
28	tH	1001	CYC	CAB-C3B-C2B	3.00	132.66	127.53
26	HD	203	PEB	CAB-C3B-C2B	-3.00	122.29	127.88
27	xE	305	PUB	CBA-CAA-C3A	-3.00	108.43	112.98
26	YE	201	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	m4	203	PEB	CMC-C3C-C2C	3.00	130.60	124.94
26	d4	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	lE	201	PEB	CBB-CAB-C3B	3.00	120.96	112.63
26	O9	201	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	AB	301	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
28	vH	1001	CYC	C4A-C3A-C2A	-3.00	103.06	106.51
26	KA	201	PEB	OD-C4D-C3D	-3.00	122.66	129.46
26	l7	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
27	24	402	PUB	CHC-C1D-ND	-3.00	109.93	113.72
26	xG	304	PEB	CHA-C1B-NB	-3.00	118.66	124.93
26	Z1	201	PEB	CMB-C2B-C1B	3.00	129.68	125.06
26	L5	202	PEB	CMB-C2B-C1B	3.00	129.68	125.06
26	JD	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	T1	202	PEB	C1C-CHB-C4B	3.00	132.39	128.81
26	v1	201	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	KC	201	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	hG	202	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
26	DE	202	PEB	OD-C4D-C3D	-3.00	122.67	129.46
26	X4	201	PEB	CAC-CBC-CGC	-3.00	105.35	113.76
26	A7	305	PEB	CHA-C1B-NB	-3.00	118.66	124.93
26	DJ	203	PEB	C3D-C4D-ND	3.00	113.14	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fA	201	PEB	OA-C1A-C2A	-3.00	123.79	126.17
26	S1	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
26	N2	1002	PEB	CHC-C1D-ND	-3.00	110.47	113.95
26	j6	201	PEB	CAB-CBB-CGB	-3.00	107.15	113.60
26	P3	202	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
28	L6	1001	CYC	C4A-C3A-C2A	-3.00	103.07	106.51
28	LH	1001	CYC	C4A-C3A-C2A	-3.00	103.07	106.51
26	h7	202	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
26	F4	203	PEB	CMB-C2B-C1B	3.00	129.68	125.06
26	XG	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
26	g2	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
26	m4	202	PEB	OD-C4D-ND	-3.00	121.49	125.93
26	E4	202	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
26	u4	203	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
26	PD	203	PEB	OD-C4D-C3D	-3.00	122.67	129.46
26	X3	201	PEB	CBC-CAC-C2C	3.00	117.73	112.62
28	DI	1001	CYC	C1A-C2A-C3A	-3.00	103.47	106.78
27	A8	304	PUB	CHB-C1C-NC	-3.00	124.67	128.83
26	G8	201	PEB	C3B-C4B-NB	3.00	114.41	110.05
26	S8	201	PEB	C3B-C4B-NB	3.00	114.41	110.05
26	uE	201	PEB	C3B-C4B-NB	3.00	114.41	110.05
26	FD	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
26	D4	203	PEB	C2A-C1A-NA	3.00	110.86	108.27
28	J7	1001	CYC	C2C-C1C-NC	3.00	110.86	108.27
27	YD	302	PUB	CBB-CAB-C3B	-3.00	107.51	112.62
26	QE	201	PEB	CAB-C3B-C4B	3.00	130.31	125.01
26	R4	202	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
26	SI	201	PEB	CHA-C4A-NA	3.00	128.77	125.20
26	vE	202	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
26	MG	203	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
28	K2	1001	CYC	C1A-C2A-C3A	-3.00	103.47	106.78
26	CG	203	PEB	OD-C4D-ND	-3.00	121.49	125.93
26	DD	203	PEB	CMB-C2B-C1B	3.00	129.68	125.06
26	y1	201	PEB	CHA-C1B-C2B	-3.00	117.20	124.90
26	A4	201	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
26	D3	203	PEB	CMB-C2B-C1B	2.99	129.68	125.06
26	RF	201	PEB	CHC-C4C-C3C	-2.99	125.23	130.34
26	h7	202	PEB	OA-C1A-C2A	-2.99	123.79	126.17
26	F3	203	PEB	OD-C4D-C3D	-2.99	122.67	129.46
26	xE	303	PEB	C3B-C4B-NB	2.99	114.41	110.05
26	e3	401	PEB	C1C-CHB-C4B	2.99	132.39	128.81
26	g7	202	PEB	CHC-C1D-ND	-2.99	110.47	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	WD	202	PEB	CMB-C2B-C1B	2.99	129.68	125.06
28	L2	1001	CYC	CAB-C3B-C4B	2.99	126.11	121.38
26	A9	304	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	C4	202	PEB	OD-C4D-ND	-2.99	121.50	125.93
26	W2	201	PEB	OD-C4D-C3D	-2.99	122.68	129.46
26	SA	201	PEB	OD-C4D-C3D	-2.99	122.68	129.46
26	NB	1002	PEB	OD-C4D-C3D	-2.99	122.68	129.46
26	K4	201	PEB	CHC-C4C-C3C	-2.99	125.23	130.34
26	aI	202	PEB	C1B-C2B-C3B	-2.99	103.07	106.51
28	fH	1001	CYC	OC-C1C-C2C	-2.99	123.79	126.17
26	mE	201	PEB	OD-C4D-C3D	-2.99	122.68	129.46
26	d6	204	PEB	C3B-C4B-NB	2.99	114.40	110.05
26	MJ	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
26	A7	302	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
26	VD	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
26	fB	202	PEB	OD-C4D-ND	-2.99	121.50	125.93
26	YA	203	PEB	CHC-C4C-C3C	-2.99	125.23	130.34
28	B6	1002	CYC	CHA-C1A-NA	-2.99	124.67	128.83
28	MH	1001	CYC	C1B-C2B-C3B	-2.99	104.75	107.87
26	z4	202	PEB	CAB-C3B-C4B	2.99	130.30	125.01
26	a4	203	PEB	CMB-C2B-C1B	2.99	129.67	125.06
26	TF	201	PEB	CMB-C2B-C1B	2.99	129.67	125.06
26	ZF	202	PEB	OD-C4D-ND	-2.99	121.50	125.93
28	K7	1001	CYC	CHB-C4A-NA	-2.99	118.67	124.93
28	NB	1001	CYC	C2C-C1C-NC	2.99	110.85	108.27
26	BJ	202	PEB	CBC-CAC-C2C	-2.99	107.52	112.62
26	SD	201	PEB	CMA-C2A-C1A	-2.99	105.95	112.40
26	BC	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
26	d6	203	PEB	CHC-C4C-C3C	-2.99	125.23	130.34
26	YG	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
26	k1	202	PEB	OD-C4D-C3D	-2.99	122.68	129.46
26	A1	201	PEB	CAA-C3A-C2A	-2.99	106.79	114.26
26	j2	201	PEB	C4B-NB-C1B	-2.99	100.88	106.51
26	WA	202	PEB	CBC-CAC-C2C	-2.99	107.52	112.62
26	a4	203	PEB	OA-C1A-C2A	-2.99	123.80	126.17
26	F1	201	PEB	CHA-C1B-NB	-2.99	118.68	124.93
26	V2	202	PEB	CHA-C1B-NB	-2.99	118.68	124.93
26	K5	201	PEB	C1B-C2B-C3B	-2.99	103.07	106.51
26	Z4	202	PEB	OD-C4D-C3D	-2.99	122.68	129.46
26	hA	203	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	nG	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	I5	201	PEB	C3B-C4B-NB	2.99	114.40	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j6	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
26	iA	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
26	RF	201	PEB	CMB-C2B-C1B	2.99	129.67	125.06
28	fH	1001	CYC	CAA-C2A-C1A	2.99	130.30	125.01
26	e8	202	PEB	CHA-C1B-NB	-2.99	118.68	124.93
26	F8	202	PEB	O2B-CGB-CBB	2.99	123.64	114.03
26	NB	1002	PEB	CHA-C1B-NB	-2.99	118.68	124.93
26	FA	202	PEB	OD-C4D-ND	-2.99	121.50	125.93
26	T7	201	PEB	OA-C1A-C2A	-2.99	123.80	126.17
26	l4	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	sE	203	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	bE	201	PEB	CHA-C1B-NB	-2.99	118.68	124.93
26	WD	201	PEB	CHA-C4A-NA	2.99	128.76	125.20
26	L4	203	PEB	CHC-C4C-C3C	-2.99	125.24	130.34
26	PF	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
26	P3	203	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
26	T3	201	PEB	C1C-CHB-C4B	2.99	132.38	128.81
26	L1	202	PEB	CAC-CBC-CGC	-2.99	105.38	113.76
26	A3	201	PEB	CAB-CBB-CGB	-2.99	107.17	113.60
26	B5	202	PEB	CMB-C2B-C1B	2.99	129.67	125.06
26	HB	1002	PEB	OD-C4D-C3D	-2.99	122.69	129.46
28	cH	1001	CYC	OC-C1C-C2C	-2.99	123.80	126.17
26	bB	201	PEB	C2A-C1A-NA	2.99	110.85	108.27
28	NI	1001	CYC	CHB-C1B-NB	-2.99	119.64	126.06
26	l4	202	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
26	QE	202	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
28	LB	1001	CYC	C4A-C3A-C2A	-2.99	103.08	106.51
26	f2	202	PEB	CHC-C4C-C3C	-2.99	125.24	130.34
26	HG	201	PEB	CHA-C1B-C2B	2.99	132.58	124.90
26	K4	201	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
26	T3	201	PEB	CMA-C2A-C1A	-2.99	105.96	112.40
28	B6	1001	CYC	C4A-C3A-C2A	-2.99	103.08	106.51
26	AF	305	PEB	CHC-C4C-C3C	-2.99	125.24	130.34
27	Y3	302	PUB	OA-C1A-NA	-2.99	121.50	125.93
26	Q3	202	PEB	OA-C1A-C2A	-2.99	123.80	126.17
28	MH	1001	CYC	OC-C1C-C2C	-2.99	123.80	126.17
26	f7	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	kA	202	PEB	C3B-C4B-NB	2.99	114.39	110.05
28	BB	1001	CYC	C2A-C1A-NA	2.99	114.39	110.05
26	l1	203	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
26	P1	202	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
26	x1	201	PEB	C1B-C2B-C3B	-2.99	103.08	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a7	201	PEB	OD-C4D-ND	-2.99	121.51	125.93
28	LB	1001	CYC	OB-C4B-C3B	-2.99	124.80	128.04
26	u1	203	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
26	k1	201	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	AC	203	PEB	C2A-C1A-NA	2.99	110.85	108.27
26	G9	201	PEB	CHB-C4B-NB	-2.99	124.69	128.83
26	dB	203	PEB	OD-C4D-ND	-2.99	121.51	125.93
26	G9	201	PEB	C3B-C4B-NB	2.99	114.39	110.05
26	d6	201	PEB	CHA-C1B-NB	-2.99	118.69	124.93
26	N6	201	PEB	CMB-C2B-C1B	2.99	129.66	125.06
28	IH	1001	CYC	CHA-C1A-NA	-2.99	124.69	128.83
26	q4	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	SA	201	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	ME	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
27	QA	201	PUB	C2C-C1C-NC	2.98	114.39	110.05
26	dB	204	PEB	OD-C4D-C3D	-2.98	122.70	129.46
26	eF	201	PEB	C2A-C1A-NA	2.98	110.85	108.27
26	aG	203	PEB	C2A-C1A-NA	2.98	110.85	108.27
26	A4	202	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
26	H7	1002	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
26	EA	203	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
26	cA	202	PEB	CHB-C4B-NB	-2.98	124.69	128.83
26	GC	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
26	i6	202	PEB	CHC-C4C-C3C	-2.98	125.25	130.34
26	L4	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	R4	203	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	t1	201	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
26	d6	201	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
28	GI	1001	CYC	C4A-C3A-C2A	-2.98	103.08	106.51
26	w1	201	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	Z7	203	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	hF	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	NG	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	jA	201	PEB	CHA-C1B-NB	-2.98	118.69	124.93
26	cB	202	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
26	U7	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
26	O4	202	PEB	CHA-C1B-NB	-2.98	118.69	124.93
26	P4	202	PEB	CHC-C4C-C3C	-2.98	125.25	130.34
26	D1	203	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	U6	203	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	R9	201	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	l1	201	PEB	OD-C4D-ND	-2.98	121.51	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O1	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	n4	202	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	D1	201	PEB	CHA-C1B-NB	-2.98	118.69	124.93
26	BJ	202	PEB	OA-C1A-C2A	-2.98	123.80	126.17
26	a8	201	PEB	CHC-C4C-C3C	-2.98	125.25	130.34
26	d2	202	PEB	OD-C4D-ND	-2.98	121.51	125.93
27	A2	302	PUB	OA-C1A-NA	-2.98	121.51	125.93
26	E4	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
26	T1	201	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
28	CB	1001	CYC	C1B-NB-C4B	-2.98	106.87	110.67
26	Y3	301	PEB	CMB-C2B-C1B	2.98	129.66	125.06
28	B6	1001	CYC	CMB-C2B-C1B	2.98	127.89	124.17
26	M9	202	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
26	m1	203	PEB	C1C-CHB-C4B	2.98	132.37	128.81
26	E8	203	PEB	OD-C4D-ND	-2.98	121.51	125.93
26	P6	202	PEB	CMC-C3C-C2C	2.98	130.56	124.94
26	d7	201	PEB	C3B-C4B-NB	2.98	114.39	110.05
26	x1	201	PEB	OA-C1A-C2A	-2.98	123.80	126.17
26	z1	201	PEB	CHC-C1D-ND	-2.98	110.49	113.95
26	D4	203	PEB	CHC-C1D-ND	-2.98	110.49	113.95
26	P7	202	PEB	CHC-C1D-ND	-2.98	110.49	113.95
26	f1	201	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	F8	201	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	GA	201	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
26	lB	202	PEB	OD-C4D-C3D	-2.98	122.71	129.46
26	A2	305	PEB	OD-C4D-ND	-2.98	121.52	125.93
28	RH	1001	CYC	C1B-C2B-C3B	-2.98	104.76	107.87
26	q1	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	l8	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	NB	1002	PEB	CMB-C2B-C1B	2.98	129.65	125.06
26	CJ	201	PEB	C4B-NB-C1B	-2.98	100.90	106.51
26	N1	202	PEB	CHA-C1B-NB	-2.98	118.70	124.93
26	eI	201	PEB	OD-C4D-ND	-2.98	121.52	125.93
26	S3	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	y1	201	PEB	C1C-CHB-C4B	2.98	132.37	128.81
26	MG	203	PEB	CBC-CAC-C2C	2.98	117.70	112.62
26	ED	201	PEB	CHA-C1B-C2B	2.98	132.56	124.90
26	i6	201	PEB	OD-C4D-C3D	-2.98	122.71	129.46
26	R8	202	PEB	CAA-C3A-C2A	-2.98	106.82	114.26
26	Z8	202	PEB	O2B-CGB-CBB	2.98	123.60	114.03
26	C1	201	PEB	OD-C4D-ND	-2.98	121.52	125.93
26	VF	202	PEB	OD-C4D-ND	-2.98	121.52	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F1	202	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	M1	402	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	YE	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	tE	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	lF	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	TG	201	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	S2	202	PEB	OD-C4D-C3D	-2.98	122.71	129.46
26	e2	201	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
26	VI	201	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
26	Y8	203	PEB	CMB-C2B-C1B	2.98	129.65	125.06
26	m4	203	PEB	CBC-CAC-C2C	2.98	117.70	112.62
26	W6	202	PEB	C1C-CHB-C4B	2.98	132.37	128.81
28	kH	1001	CYC	C1B-C2B-C3B	-2.98	104.76	107.87
26	fA	203	PEB	CHA-C1B-NB	-2.98	118.70	124.93
27	AJ	302	PUB	OA-C1A-NA	-2.98	121.52	125.93
26	y1	201	PEB	CAA-C3A-C2A	-2.98	106.82	114.26
26	D8	202	PEB	CAA-C3A-C4A	2.98	120.32	112.67
28	C6	1001	CYC	C2A-C1A-NA	2.98	114.38	110.05
26	UA	203	PEB	CHA-C1B-NB	-2.98	118.70	124.93
26	DJ	203	PEB	C1C-CHB-C4B	2.98	132.37	128.81
26	J8	201	PEB	CBC-CAC-C2C	-2.98	107.54	112.62
26	DD	202	PEB	CHA-C4A-NA	2.98	128.75	125.20
26	E3	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	cE	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
27	KD	203	PUB	CHA-C1B-C2B	-2.98	125.26	130.34
26	hI	201	PEB	C2B-C1B-NB	2.98	116.88	110.53
26	AF	301	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
26	fG	201	PEB	CMB-C2B-C1B	2.98	129.65	125.06
28	HB	1001	CYC	C2A-C1A-NA	2.98	114.38	110.05
26	Q9	201	PEB	C2A-C1A-NA	2.98	110.84	108.27
26	bI	201	PEB	OD-C4D-C3D	-2.98	122.72	129.46
26	fA	202	PEB	CBC-CAC-C2C	-2.98	107.54	112.62
26	c8	202	PEB	OD-C4D-ND	-2.98	121.52	125.93
26	fB	203	PEB	OD-C4D-ND	-2.98	121.52	125.93
26	w1	202	PEB	OD-C4D-C3D	-2.98	122.72	129.46
26	C9	202	PEB	OD-C4D-C3D	-2.98	122.72	129.46
26	pG	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	R4	201	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
28	TH	1001	CYC	C4A-C3A-C2A	-2.98	103.09	106.51
28	VH	1001	CYC	C1B-NB-C4B	-2.98	106.88	110.67
26	s4	203	PEB	CHB-C4B-NB	-2.98	124.70	128.83
28	JH	1001	CYC	CBD-CAD-C3D	-2.98	107.54	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A5	201	PEB	OD-C4D-C3D	-2.98	122.72	129.46
26	fE	201	PEB	CMB-C2B-C1B	2.98	129.65	125.06
26	i1	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
26	N9	204	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
26	ID	202	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
27	NJ	201	PUB	CMD-C2D-C3D	2.97	132.23	127.77
26	Q7	202	PEB	CHA-C4A-NA	2.97	128.74	125.20
26	CD	201	PEB	C3B-C4B-NB	2.97	114.38	110.05
26	a1	201	PEB	CHC-C1D-ND	-2.97	110.49	113.95
26	T1	201	PEB	C2A-C1A-NA	2.97	110.84	108.27
26	d6	203	PEB	C2A-C1A-NA	2.97	110.84	108.27
26	O6	203	PEB	OD-C4D-ND	-2.97	121.52	125.93
26	IC	202	PEB	OD-C4D-ND	-2.97	121.52	125.93
26	Z6	203	PEB	C1B-C2B-C3B	-2.97	103.09	106.51
26	FA	201	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
26	KB	201	PEB	OD-C4D-C3D	-2.97	122.72	129.46
26	AI	301	PEB	CHC-C1D-ND	-2.97	110.49	113.95
28	NH	1001	CYC	C1B-C2B-C3B	-2.97	104.77	107.87
26	B3	203	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	l7	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	M9	201	PEB	CBC-CAC-C2C	2.97	117.69	112.62
26	G3	201	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
26	P3	201	PEB	C2A-C1A-NA	2.97	110.84	108.27
26	v4	202	PEB	C2A-C1A-NA	2.97	110.84	108.27
26	U9	201	PEB	CHA-C1B-NB	-2.97	118.71	124.93
26	W3	202	PEB	CHB-C4B-NB	-2.97	124.70	128.83
26	h4	201	PEB	C1B-C2B-C3B	-2.97	103.09	106.51
26	v4	202	PEB	C1B-C2B-C3B	-2.97	103.09	106.51
26	VE	202	PEB	C1B-C2B-C3B	-2.97	103.09	106.51
26	e7	202	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
26	FJ	201	PEB	CHC-C1D-ND	-2.97	110.50	113.95
26	aE	203	PEB	OA-C1A-C2A	-2.97	123.81	126.17
26	B1	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	mE	203	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
28	L6	1001	CYC	C1B-NB-C4B	-2.97	106.89	110.67
26	T3	201	PEB	CAB-C3B-C4B	2.97	130.27	125.01
28	uH	1001	CYC	C1B-C2B-C3B	-2.97	104.77	107.87
26	VB	202	PEB	CHA-C1B-NB	-2.97	118.72	124.93
26	E1	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
26	c7	201	PEB	CHB-C4B-NB	-2.97	124.70	128.83
26	N7	1002	PEB	C3B-C4B-NB	2.97	114.37	110.05
26	OD	202	PEB	C3B-C4B-NB	2.97	114.37	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mE	202	PEB	CHA-C1B-NB	-2.97	118.72	124.93
26	NI	1002	PEB	CHC-C1D-ND	-2.97	110.50	113.95
26	RJ	203	PEB	CHC-C1D-ND	-2.97	110.50	113.95
26	AB	304	PEB	C1C-CHB-C4B	-2.97	125.26	128.81
26	C4	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	u4	203	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	gA	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	d6	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	T1	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
28	SH	1001	CYC	CHA-C1A-NA	-2.97	124.71	128.83
26	FD	203	PEB	CHA-C4A-NA	-2.97	121.67	125.20
26	qE	201	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	A7	302	PEB	C3B-C4B-NB	2.97	114.37	110.05
26	UD	202	PEB	C3B-C4B-NB	2.97	114.37	110.05
26	p4	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
26	R4	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	R7	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	GE	203	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
26	q4	203	PEB	CAB-C3B-C4B	2.97	130.26	125.01
26	cA	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	cF	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	h7	203	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
26	h2	201	PEB	CMB-C2B-C1B	2.97	129.64	125.06
26	R4	203	PEB	CMB-C2B-C1B	2.97	129.64	125.06
26	H2	1002	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	WE	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	RI	203	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	W3	201	PEB	OD-C4D-C3D	-2.97	122.73	129.46
26	eB	203	PEB	CHA-C1B-NB	-2.97	118.72	124.93
26	F1	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
26	E4	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
26	W9	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
26	QB	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	I4	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
26	oE	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
26	pG	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
26	IG	201	PEB	CAB-C3B-C4B	2.97	130.26	125.01
26	AI	305	PEB	CHA-C1B-NB	-2.97	118.72	124.93
26	F1	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	LD	203	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	c4	202	PEB	OD-C4D-C3D	-2.97	122.73	129.46
26	M3	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J4	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	aA	202	PEB	CMB-C2B-C1B	2.97	129.63	125.06
26	eG	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
26	i4	201	PEB	CHB-C4B-C3B	-2.97	118.47	125.32
26	AD	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	BD	201	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	X9	203	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
26	BC	203	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
26	ZF	203	PEB	CHA-C1B-C2B	2.97	132.53	124.90
26	F1	203	PEB	CMB-C2B-C1B	2.97	129.63	125.06
26	h4	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	aF	201	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	F1	203	PEB	CHA-C1B-NB	-2.97	118.73	124.93
26	hA	202	PEB	CHA-C1B-NB	-2.97	118.73	124.93
26	gG	202	PEB	C1C-CHB-C4B	2.97	132.35	128.81
26	TF	202	PEB	OD-C4D-C3D	-2.97	122.74	129.46
28	H6	1001	CYC	CHB-C1B-NB	-2.97	119.69	126.06
26	EJ	201	PEB	CHA-C1B-NB	-2.97	118.73	124.93
26	oE	203	PEB	OD-C4D-C3D	-2.97	122.74	129.46
28	KB	202	CYC	CHA-C1A-NA	-2.97	124.71	128.83
26	G5	203	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	B9	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	IG	203	PEB	C2A-C1A-NA	2.97	110.83	108.27
26	24	405	PEB	OD-C4D-ND	-2.97	121.54	125.93
26	VF	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	iI	201	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
28	GH	1001	CYC	C1B-C2B-C3B	-2.97	104.78	107.87
26	I1	201	PEB	OA-C1A-C2A	-2.97	123.81	126.17
26	S6	201	PEB	CHB-C4B-NB	-2.97	124.71	128.83
28	DF	1003	CYC	CHA-C1A-NA	-2.97	124.71	128.83
26	XA	202	PEB	CHC-C4C-C3C	-2.97	125.28	130.34
26	hA	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
27	AB	303	PUB	OA-C1A-NA	-2.97	121.54	125.93
26	I1	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	T1	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	xG	303	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
26	FC	201	PEB	C2A-C1A-NA	2.96	110.83	108.27
27	xE	301	PUB	CHA-C1B-C2B	-2.96	125.28	130.34
28	uH	1001	CYC	C2C-C3C-C4C	2.96	105.78	101.34
26	DE	201	PEB	C1C-CHB-C4B	2.96	132.35	128.81
26	WJ	202	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
26	T2	203	PEB	CHC-C1D-ND	-2.96	110.50	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q3	201	PEB	OD-C4D-C3D	-2.96	122.74	129.46
26	Y3	304	PEB	OD-C4D-C3D	-2.96	122.74	129.46
26	f4	202	PEB	OD-C4D-C3D	-2.96	122.74	129.46
26	TD	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
26	AG	201	PEB	CBC-CAC-C2C	-2.96	107.56	112.62
26	R7	201	PEB	C2A-C1A-NA	2.96	110.83	108.27
26	LA	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
28	DF	1003	CYC	CHB-C4A-NA	-2.96	118.73	124.93
26	TE	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
26	VG	201	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
28	1H	1000	CYC	C1B-NB-C4B	-2.96	106.90	110.67
26	DJ	203	PEB	C2B-C1B-NB	2.96	116.85	110.53
26	U3	202	PEB	CMB-C2B-C1B	2.96	129.63	125.06
26	RD	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
26	a8	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
26	m4	202	PEB	CMB-C2B-C1B	2.96	129.63	125.06
26	Q9	202	PEB	C3B-C4B-NB	2.96	114.36	110.05
28	J7	1003	CYC	C2A-C1A-NA	2.96	114.36	110.05
26	WA	202	PEB	CMA-C2A-C1A	-2.96	106.02	112.40
26	N8	202	PEB	CHA-C1B-NB	-2.96	118.74	124.93
26	gI	202	PEB	OD-C4D-ND	-2.96	121.54	125.93
27	N9	201	PUB	OD-C4D-ND	-2.96	121.54	125.93
28	NH	1001	CYC	CHA-C1A-NA	-2.96	124.72	128.83
26	Q8	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
26	A2	304	PEB	C3B-C4B-NB	2.96	114.36	110.05
26	Y4	202	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
28	iH	1001	CYC	C1A-C2A-C3A	-2.96	103.50	106.78
26	k4	203	PEB	OD-C4D-C3D	-2.96	122.75	129.46
26	cB	201	PEB	CHB-C4B-NB	-2.96	124.72	128.83
26	B5	203	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
26	b6	201	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
26	A7	305	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
26	Y8	203	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
28	HB	1001	CYC	CHB-C1B-NB	-2.96	119.70	126.06
26	r4	201	PEB	CMC-C3C-C2C	2.96	130.52	124.94
26	hI	202	PEB	OD-C4D-ND	-2.96	121.54	125.93
26	JC	201	PEB	CBB-CAB-C3B	-2.96	104.40	112.63
26	j8	203	PEB	CHA-C1B-NB	-2.96	118.74	124.93
26	k4	203	PEB	CMB-C2B-C1B	2.96	129.62	125.06
26	jF	203	PEB	C2A-C1A-NA	2.96	110.83	108.27
26	wG	303	PEB	CAB-C3B-C2B	2.96	133.39	127.88
28	J2	1001	CYC	O1A-CGA-CBA	-2.96	113.57	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	hH	1001	CYC	C4D-CHA-C1A	2.96	132.34	128.81
26	m1	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
26	j7	202	PEB	CHC-C1D-ND	-2.96	110.51	113.95
26	b7	203	PEB	CHB-C4B-NB	-2.96	124.72	128.83
26	j1	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
26	fE	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
26	L9	203	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
26	M1	403	PEB	C3B-C4B-NB	2.96	114.35	110.05
28	VH	1001	CYC	CMC-C2C-C3C	2.96	125.77	113.83
26	L3	202	PEB	OA-C1A-NA	2.96	128.53	124.94
26	QF	201	PEB	OD-C4D-ND	-2.96	121.55	125.93
26	sG	201	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
26	H8	202	PEB	CMA-C2A-C1A	-2.96	106.02	112.40
28	LI	1001	CYC	CAB-C3B-C4B	2.96	126.05	121.38
26	C4	202	PEB	C2A-C1A-NA	2.96	110.82	108.27
26	e8	201	PEB	CAB-CBB-CGB	-2.96	107.23	113.60
26	h6	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
26	gE	201	PEB	CMB-C2B-C3B	-2.96	118.08	126.12
26	cG	202	PEB	C3D-C4D-ND	2.96	113.06	107.26
26	l2	201	PEB	C2B-C1B-NB	2.96	116.84	110.53
26	N6	201	PEB	OD-C4D-C3D	-2.96	122.76	129.46
26	E4	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	V1	201	PEB	CHA-C1B-NB	-2.96	118.74	124.93
26	D4	201	PEB	CHA-C1B-NB	-2.96	118.74	124.93
26	X9	201	PEB	OD-C4D-ND	-2.96	121.55	125.93
26	vE	201	PEB	OD-C4D-ND	-2.96	121.55	125.93
28	qH	1002	CYC	CHA-C1A-C2A	-2.96	118.49	125.32
26	L9	201	PEB	OA-C1A-C2A	-2.96	123.82	126.17
26	k2	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	lB	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	iE	201	PEB	C2A-C1A-NA	2.96	110.82	108.27
26	MD	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
26	Y7	201	PEB	CAB-CBB-CGB	-2.96	107.24	113.60
26	fA	202	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
26	T6	202	PEB	CBC-CAC-C2C	2.96	117.67	112.62
26	g2	203	PEB	C2A-C1A-NA	2.96	110.82	108.27
26	B4	202	PEB	C2A-C1A-NA	2.96	110.82	108.27
26	J9	202	PEB	C2A-C1A-NA	2.96	110.82	108.27
26	wE	303	PEB	OA-C1A-C2A	-2.96	123.82	126.17
27	xE	306	PUB	C4B-CHB-C1C	2.96	132.34	128.81
26	Q4	202	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	P7	202	PEB	OD-C4D-ND	-2.96	121.55	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AF	302	PEB	OD-C4D-ND	-2.96	121.55	125.93
26	g2	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
26	M8	203	PEB	OD-C4D-C3D	-2.96	122.76	129.46
26	L4	201	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
26	T9	203	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
26	sE	201	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
26	R3	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	q4	203	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	L8	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	AG	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
28	B6	1001	CYC	C2A-C1A-NA	2.96	114.35	110.05
26	P4	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
26	j7	203	PEB	OD-C4D-ND	-2.96	121.55	125.93
26	R1	202	PEB	C1C-CHB-C4B	2.96	132.34	128.81
26	KG	201	PEB	CHA-C1B-NB	-2.96	118.75	124.93
26	B1	202	PEB	OD-C4D-C3D	-2.96	122.76	129.46
26	S7	202	PEB	C2A-C1A-NA	2.96	110.82	108.27
26	C9	201	PEB	OA-C1A-C2A	-2.96	123.82	126.17
26	SG	203	PEB	CHA-C4A-NA	2.96	128.72	125.20
26	kG	201	PEB	CHA-C1B-C2B	2.96	132.50	124.90
26	YF	202	PEB	CHA-C1B-NB	-2.96	118.75	124.93
26	d4	201	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	xE	302	PEB	C3B-C4B-NB	2.96	114.35	110.05
26	XG	202	PEB	OD-C4D-C3D	-2.96	122.76	129.46
26	UI	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
28	KI	1001	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
26	WE	201	PEB	CMA-C2A-C1A	-2.96	106.03	112.40
26	O1	201	PEB	C1C-CHB-C4B	2.96	132.34	128.81
26	R4	203	PEB	C1C-CHB-C4B	-2.96	125.28	128.81
28	M2	1001	CYC	CHA-C1A-NA	-2.95	124.73	128.83
28	HF	1001	CYC	CMC-C2C-C1C	-2.95	106.03	112.40
26	j2	201	PEB	C2B-C1B-NB	2.95	116.84	110.53
26	PB	202	PEB	C3B-C4B-NB	2.95	114.35	110.05
26	eF	201	PEB	OD-C4D-ND	-2.95	121.55	125.93
26	aI	203	PEB	OD-C4D-ND	-2.95	121.55	125.93
26	c6	201	PEB	CHA-C1B-NB	-2.95	118.75	124.93
26	iG	202	PEB	CHA-C1B-NB	-2.95	118.75	124.93
28	K6	202	CYC	CHA-C1A-NA	-2.95	124.73	128.83
26	c7	201	PEB	OD-C4D-ND	-2.95	121.55	125.93
26	WF	201	PEB	CAC-CBC-CGC	2.95	122.04	113.76
26	Q6	201	PEB	CHA-C1B-NB	-2.95	118.75	124.93
26	R3	202	PEB	CHA-C4A-NA	2.95	128.72	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U2	202	PEB	OD-C4D-C3D	-2.95	122.77	129.46
26	K4	201	PEB	CHA-C1B-NB	-2.95	118.75	124.93
28	mH	1001	CYC	C1B-C2B-C3B	-2.95	104.79	107.87
26	gG	203	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
28	G7	1001	CYC	C1A-C2A-C3A	-2.95	103.51	106.78
26	a4	203	PEB	C2A-C1A-NA	2.95	110.82	108.27
26	t1	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
27	BA	302	PUB	OA-C1A-NA	-2.95	121.56	125.93
26	x4	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	JE	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	kB	201	PEB	OD-C4D-C3D	-2.95	122.77	129.46
26	J9	202	PEB	CBC-CAC-C2C	-2.95	107.58	112.62
26	eI	203	PEB	CMB-C2B-C1B	2.95	129.61	125.06
28	MH	1001	CYC	CHA-C1A-NA	-2.95	124.73	128.83
26	B4	203	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	TD	203	PEB	CHC-C4C-C3C	-2.95	125.30	130.34
26	Q2	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	HG	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	l4	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	SB	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
28	C6	1001	CYC	C1B-NB-C4B	-2.95	106.91	110.67
26	K3	201	PEB	CMB-C2B-C1B	2.95	129.61	125.06
26	k2	203	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	l4	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	l6	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	N9	203	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	wG	302	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	U2	201	PEB	CMA-C2A-C1A	-2.95	106.04	112.40
26	gA	202	PEB	CAB-C3B-C4B	2.95	130.23	125.01
26	QA	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	jA	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
27	A7	303	PUB	OD-C4D-ND	-2.95	121.56	125.93
26	OA	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	V6	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	I5	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	l7	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	wE	302	PEB	C3B-C4B-NB	2.95	114.34	110.05
28	G2	1001	CYC	C2A-C1A-NA	2.95	114.34	110.05
26	jB	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
26	TD	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
26	cA	203	PEB	OD-C4D-ND	-2.95	121.56	125.93
26	DI	1002	PEB	OD-C4D-ND	-2.95	121.56	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V2	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	t4	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	y4	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	DG	203	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	TI	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	XJ	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
28	JF	1003	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
26	G5	203	PEB	CHC-C1D-ND	-2.95	110.52	113.95
26	a8	202	PEB	CMB-C2B-C1B	2.95	129.61	125.06
28	G7	1001	CYC	CMA-C3A-C4A	2.95	129.61	125.06
26	b1	501	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	h2	202	PEB	CHC-C4C-C3C	-2.95	125.31	130.34
26	V2	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	Y7	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
28	E7	1001	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
26	mB	202	PEB	CMB-C2B-C1B	2.95	129.60	125.06
26	k6	201	PEB	CBC-CAC-C2C	2.95	117.65	112.62
26	C4	201	PEB	CHA-C1B-NB	-2.95	118.77	124.93
26	UI	201	PEB	CMA-C2A-C1A	-2.95	106.05	112.40
28	DB	1001	CYC	CHB-C1B-NB	-2.95	119.73	126.06
26	kB	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
28	G7	1001	CYC	C2A-C1A-NA	2.95	114.34	110.05
28	BB	1001	CYC	CMB-C2B-C1B	2.95	127.85	124.17
26	B9	203	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	ZI	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	d1	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
26	HG	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
26	m7	201	PEB	CHC-C4C-C3C	-2.95	125.31	130.34
26	Y2	203	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	Q7	203	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	M9	202	PEB	C3B-C4B-NB	2.95	114.34	110.05
26	iG	203	PEB	C2A-C1A-NA	2.95	110.81	108.27
26	iI	201	PEB	CMB-C2B-C1B	2.95	129.60	125.06
26	cB	201	PEB	CHA-C1B-NB	-2.95	118.77	124.93
26	mG	203	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	VB	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	FE	202	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
28	eH	1001	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
28	JF	1003	CYC	CHB-C1B-NB	-2.95	119.73	126.06
26	YE	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
27	K4	203	PUB	OA-C1A-NA	-2.95	121.56	125.93
27	xG	301	PUB	C2C-C1C-NC	2.95	114.33	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	MJ	201	PEB	CBC-CAC-C2C	2.95	117.65	112.62
26	s1	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
26	w1	203	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
26	bF	203	PEB	CHB-C4B-NB	-2.95	124.74	128.83
26	u1	201	PEB	CHC-C1D-ND	-2.95	110.53	113.95
26	TF	202	PEB	CAA-C3A-C4A	2.95	120.24	112.67
28	FH	1001	CYC	CMB-C2B-C1B	2.95	127.84	124.17
26	s1	203	PEB	CMB-C2B-C1B	2.95	129.60	125.06
26	M9	202	PEB	CMB-C2B-C1B	2.95	129.60	125.06
26	LD	203	PEB	CMB-C2B-C1B	2.95	129.60	125.06
26	e2	201	PEB	CHC-C4C-C3C	-2.95	125.31	130.34
26	k6	202	PEB	C1B-C2B-C3B	-2.95	103.13	106.51
26	l2	202	PEB	CHA-C1B-NB	-2.95	118.77	124.93
26	GC	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
26	JF	1002	PEB	CAB-CBB-CGB	-2.95	107.27	113.60
26	m2	203	PEB	OD-C4D-ND	-2.95	121.57	125.93
26	d7	202	PEB	C3B-C4B-NB	2.95	114.33	110.05
26	AJ	305	PEB	C3B-C4B-NB	2.95	114.33	110.05
28	LB	1001	CYC	CMC-C2C-C1C	-2.94	106.06	112.40
26	y4	203	PEB	OD-C4D-C3D	-2.94	122.79	129.46
26	PB	201	PEB	CAB-C3B-C4B	2.94	130.22	125.01
26	D8	202	PEB	OD-C4D-C3D	-2.94	122.79	129.46
26	i8	202	PEB	OA-C1A-C2A	-2.94	123.83	126.17
26	i8	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
28	B6	1002	CYC	CAD-CBD-CGD	-2.94	105.51	113.76
27	AI	302	PUB	OD-C4D-ND	-2.94	121.57	125.93
26	B5	201	PEB	OD-C4D-C3D	-2.94	122.79	129.46
26	XJ	201	PEB	OD-C4D-C3D	-2.94	122.79	129.46
26	y4	203	PEB	CHA-C4A-NA	-2.94	121.70	125.20
28	rH	1001	CYC	C4A-C3A-C2A	-2.94	103.13	106.51
26	P7	202	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	RJ	202	PEB	CMB-C2B-C1B	2.94	129.60	125.06
26	d7	201	PEB	CHC-C1D-ND	-2.94	110.53	113.95
26	jF	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
26	c6	202	PEB	OD-C4D-C3D	-2.94	122.79	129.46
26	GE	202	PEB	OD-C4D-C3D	-2.94	122.79	129.46
26	X1	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	QA	202	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	k4	203	PEB	CHA-C4A-NA	2.94	128.70	125.20
26	IC	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
26	LC	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
26	VD	202	PEB	CHC-C1D-ND	-2.94	110.53	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	xG	301	PUB	CHA-C4A-NA	-2.94	110.53	113.95
26	aB	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
26	i6	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
26	h8	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
28	tH	1001	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
26	SB	201	PEB	CHB-C4B-NB	-2.94	124.75	128.83
26	BC	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
26	TI	203	PEB	CHC-C1D-ND	-2.94	110.53	113.95
26	m6	201	PEB	OD-C4D-ND	-2.94	121.57	125.93
26	J7	1002	PEB	OD-C4D-ND	-2.94	121.57	125.93
26	JD	201	PEB	C2A-C1A-NA	2.94	110.81	108.27
26	mF	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
26	e4	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	R3	203	PEB	OD-C4D-ND	-2.94	121.57	125.93
26	B1	203	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	TI	202	PEB	OA-C1A-C2A	-2.94	123.83	126.17
26	kI	201	PEB	OD-C4D-ND	-2.94	121.57	125.93
26	Z7	203	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
26	B9	202	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	cG	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
26	f1	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
26	aI	203	PEB	CAB-CBB-CGB	2.94	119.93	113.60
26	Z7	201	PEB	OA-C1A-NA	2.94	128.50	124.94
26	QJ	202	PEB	C3B-C4B-NB	2.94	114.33	110.05
26	z1	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
26	QF	201	PEB	C2A-C1A-NA	2.94	110.81	108.27
26	fA	203	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
26	S6	203	PEB	OA-C1A-C2A	-2.94	123.84	126.17
26	AD	202	PEB	OA-C1A-C2A	-2.94	123.84	126.17
26	i2	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
26	eI	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
28	BB	1001	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
26	P6	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
26	V3	203	PEB	C1C-CHB-C4B	2.94	132.32	128.81
28	JH	1001	CYC	C4D-CHA-C1A	2.94	132.32	128.81
26	dE	201	PEB	C2A-C1A-NA	2.94	110.81	108.27
26	aB	201	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
27	A7	303	PUB	CHC-C1D-ND	-2.94	110.01	113.72
26	ZA	202	PEB	O2B-CGB-CBB	2.94	123.47	114.03
26	O7	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	KG	203	PEB	OA-C1A-C2A	-2.94	123.84	126.17
26	D1	202	PEB	CBC-CAC-C2C	-2.94	107.61	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	QE	203	PEB	CHA-C1B-C2B	2.94	132.45	124.90
26	K6	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	T9	203	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	KB	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	aE	203	PEB	OD-C4D-C3D	-2.94	122.81	129.46
26	uE	201	PEB	OD-C4D-C3D	-2.94	122.81	129.46
26	c1	201	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
26	cF	201	PEB	CHB-C4B-C3B	-2.94	118.53	125.32
26	C1	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	G8	201	PEB	OA-C1A-C2A	-2.94	123.84	126.17
28	K2	1001	CYC	C4A-C3A-C2A	-2.94	103.14	106.51
26	M4	403	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
26	gE	202	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
26	Q4	202	PEB	CHB-C4B-NB	-2.94	124.75	128.83
26	J7	1002	PEB	CMB-C2B-C1B	2.94	129.59	125.06
26	LJ	203	PEB	CMB-C2B-C1B	2.94	129.59	125.06
26	fA	202	PEB	CHA-C1B-NB	-2.94	118.79	124.93
26	dA	201	PEB	OA-C1A-C2A	-2.94	123.84	126.17
26	V3	201	PEB	OD-C4D-C3D	-2.94	122.81	129.46
26	aA	201	PEB	OD-C4D-C3D	-2.94	122.81	129.46
26	V1	203	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	M9	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	VD	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
26	mA	202	PEB	CBB-CAB-C3B	2.94	120.78	112.63
26	F1	202	PEB	CMB-C2B-C1B	2.94	129.58	125.06
26	GA	202	PEB	OD-C4D-C3D	-2.93	122.81	129.46
26	AA	302	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
26	oE	203	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
28	lH	1001	CYC	C1B-NB-C4B	-2.93	106.93	110.67
26	L1	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	I3	201	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	aG	201	PEB	C3B-C4B-NB	2.93	114.32	110.05
26	WA	202	PEB	CMC-C3C-C2C	2.93	130.47	124.94
26	d1	201	PEB	CMB-C2B-C1B	2.93	129.58	125.06
26	gB	201	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
26	uE	203	PEB	OD-C4D-ND	-2.93	121.58	125.93
27	Q8	201	PUB	OD-C4D-ND	-2.93	121.58	125.93
26	Y1	202	PEB	CHA-C1B-NB	-2.93	118.80	124.93
26	V1	201	PEB	CMA-C2A-C1A	-2.93	106.08	112.40
26	e6	201	PEB	OA-C1A-C2A	-2.93	123.84	126.17
26	OE	202	PEB	OA-C1A-C2A	-2.93	123.84	126.17
26	lI	202	PEB	CHB-C4B-NB	-2.93	124.76	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	JA	202	PEB	OD-C4D-ND	-2.93	121.58	125.93
26	LD	202	PEB	OD-C4D-ND	-2.93	121.58	125.93
26	QJ	201	PEB	OD-C4D-ND	-2.93	121.58	125.93
26	H3	203	PEB	OD-C4D-C3D	-2.93	122.81	129.46
26	D8	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	dB	201	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	O2	201	PEB	C2B-C1B-NB	2.93	116.79	110.53
26	RJ	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
28	rH	1001	CYC	C1B-NB-C4B	-2.93	106.93	110.67
26	a8	202	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
26	WA	203	PEB	CHC-C1D-ND	-2.93	110.54	113.95
26	nG	202	PEB	OD-C4D-C3D	-2.93	122.81	129.46
26	SJ	202	PEB	OD-C4D-C3D	-2.93	122.81	129.46
26	D3	202	PEB	CHA-C4A-NA	2.93	128.69	125.20
26	a6	201	PEB	CHC-C4C-C3C	-2.93	125.33	130.34
26	NE	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
28	N2	1001	CYC	CHA-C1A-NA	-2.93	124.76	128.83
26	NA	202	PEB	CHA-C1B-NB	-2.93	118.80	124.93
26	WI	201	PEB	OD-C4D-C3D	-2.93	122.82	129.46
26	d6	203	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
26	jB	202	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
26	lA	201	PEB	CHB-C4B-C3B	-2.93	118.55	125.32
26	y4	203	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	X9	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	D9	201	PEB	OD-C4D-C3D	-2.93	122.82	129.46
26	hA	202	PEB	OD-C4D-C3D	-2.93	122.82	129.46
26	R2	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	l6	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	A3	201	PEB	OA-C1A-C2A	-2.93	123.84	126.17
26	D3	203	PEB	OD-C4D-ND	-2.93	121.59	125.93
26	LE	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
26	SF	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	G5	203	PEB	C3B-C4B-NB	2.93	114.31	110.05
27	A6	302	PUB	OA-C1A-NA	-2.93	121.59	125.93
26	PD	201	PEB	CHB-C4B-NB	-2.93	124.76	128.83
26	jI	202	PEB	CHC-C4C-C3C	-2.93	125.34	130.34
26	AD	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	fE	202	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	L3	203	PEB	CMB-C2B-C1B	2.93	129.58	125.06
26	t4	202	PEB	CHB-C4B-C3B	2.93	132.09	125.32
26	F4	201	PEB	OA-C1A-C2A	-2.93	123.84	126.17
27	AA	304	PUB	CHC-C1D-ND	-2.93	110.02	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V9	201	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	w4	203	PEB	OD-C4D-C3D	-2.93	122.82	129.46
26	Y8	201	PEB	CAA-C3A-C4A	-2.93	105.15	112.67
26	VF	202	PEB	CMB-C2B-C1B	2.93	129.58	125.06
26	G4	202	PEB	C1C-CHB-C4B	2.93	132.31	128.81
26	BA	301	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	fA	203	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	GG	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	UJ	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	e1	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	k1	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	fG	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	PI	202	PEB	CAB-C3B-C4B	2.93	130.19	125.01
26	N6	201	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
26	RD	203	PEB	OD-C4D-C3D	-2.93	122.82	129.46
26	U6	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
26	wE	302	PEB	OD-C4D-ND	-2.93	121.59	125.93
26	DE	201	PEB	CHA-C1B-NB	-2.93	118.81	124.93
26	CD	201	PEB	CHA-C4A-NA	2.93	128.69	125.20
26	H6	1002	PEB	CAA-C3A-C4A	-2.93	105.15	112.67
26	X8	202	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	c8	202	PEB	OA-C1A-C2A	-2.93	123.84	126.17
26	Q7	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	S8	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	E4	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
26	z4	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
26	eF	201	PEB	CBA-CAA-C3A	-2.93	106.95	113.47
26	DE	203	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
26	KE	203	PEB	CMB-C2B-C1B	2.93	129.57	125.06
26	FI	1002	PEB	CMB-C2B-C1B	2.93	129.57	125.06
26	JD	203	PEB	CHC-C4C-C3C	-2.93	125.34	130.34
26	G8	202	PEB	OD-C4D-C3D	-2.93	122.83	129.46
26	14	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
27	NJ	201	PUB	OA-C1A-NA	-2.93	121.59	125.93
26	14	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	A5	202	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
26	OJ	201	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
28	KI	1001	CYC	C4A-C3A-C2A	-2.93	103.15	106.51
26	K5	203	PEB	CMB-C2B-C1B	2.93	129.57	125.06
26	K5	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	O6	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	eI	202	PEB	C2A-C1A-NA	2.93	110.80	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mI	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
28	F7	1001	CYC	C2C-C1C-NC	2.93	110.80	108.27
26	eF	202	PEB	CHA-C4A-NA	2.93	128.69	125.20
26	gE	203	PEB	OD-C4D-C3D	-2.93	122.83	129.46
26	R6	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	W9	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	bI	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	D4	203	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	P7	201	PEB	CHC-C4C-C3C	-2.93	125.34	130.34
26	cE	202	PEB	CMB-C2B-C1B	2.93	129.57	125.06
26	E1	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	W7	202	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	PJ	203	PEB	C2A-C1A-NA	2.93	110.80	108.27
26	c8	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
26	QA	202	PEB	CBC-CAC-C2C	-2.93	107.63	112.62
26	G9	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
26	jG	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
28	C2	1001	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
27	24	402	PUB	OA-C1A-NA	-2.93	121.59	125.93
26	aB	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
26	R2	203	PEB	OD-C4D-ND	-2.93	121.60	125.93
26	z4	202	PEB	OD-C4D-ND	-2.93	121.60	125.93
26	fG	202	PEB	OD-C4D-ND	-2.93	121.60	125.93
26	H4	202	PEB	CHC-C1D-ND	-2.93	110.55	113.95
26	DF	1002	PEB	CHC-C1D-ND	-2.93	110.55	113.95
26	JA	202	PEB	CAA-C3A-C2A	-2.93	106.95	114.26
26	L9	203	PEB	CHB-C4B-NB	-2.93	124.77	128.83
28	DI	1001	CYC	CHA-C1A-NA	-2.93	124.77	128.83
26	VE	201	PEB	C3B-C4B-NB	2.93	114.30	110.05
26	VJ	202	PEB	C3B-C4B-NB	2.93	114.30	110.05
26	E3	201	PEB	CMD-C2D-C3D	2.92	134.19	130.06
26	YF	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
26	P6	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
27	AI	302	PUB	OA-C1A-NA	-2.92	121.60	125.93
26	DG	203	PEB	CMB-C2B-C1B	2.92	129.57	125.06
26	MD	201	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	g4	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
26	GD	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
26	X3	203	PEB	OD-C4D-C3D	-2.92	122.83	129.46
26	QB	203	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	dB	204	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	UJ	202	PEB	C2A-C1A-NA	2.92	110.79	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V4	202	PEB	CHA-C1B-NB	-2.92	118.82	124.93
26	d4	202	PEB	OA-C1A-C2A	-2.92	123.85	126.17
26	d7	202	PEB	OA-C1A-C2A	-2.92	123.85	126.17
26	A9	301	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
26	OG	202	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
28	iH	1001	CYC	CHA-C1A-NA	-2.92	124.77	128.83
28	FI	1001	CYC	CAB-C3B-C4B	2.92	126.00	121.38
26	qE	202	PEB	CHC-C1D-ND	-2.92	110.55	113.95
26	U6	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	i6	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	KD	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	iI	201	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	EE	201	PEB	CAB-C3B-C4B	2.92	130.18	125.01
26	uG	203	PEB	OD-C4D-ND	-2.92	121.60	125.93
26	OE	202	PEB	OD-C4D-C3D	-2.92	122.84	129.46
26	rE	201	PEB	CAB-CBB-CGB	-2.92	107.31	113.60
28	qH	1001	CYC	C4D-CHA-C1A	2.92	132.30	128.81
26	s4	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	Q1	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	lB	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	bI	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
26	U6	202	PEB	CHC-C1D-ND	-2.92	110.55	113.95
26	e7	201	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	f8	203	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	MG	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
28	OH	1001	CYC	CHA-C1A-NA	-2.92	124.77	128.83
26	B3	202	PEB	CMB-C2B-C1B	2.92	129.56	125.06
26	N8	202	PEB	CHC-C1D-ND	-2.92	110.55	113.95
26	YE	203	PEB	CHA-C1B-NB	-2.92	118.82	124.93
26	j6	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	ZB	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	TF	201	PEB	CBB-CAB-C3B	2.92	120.75	112.63
28	hH	1001	CYC	C1B-C2B-C3B	-2.92	104.82	107.87
26	i7	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	cA	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	WB	203	PEB	OD-C4D-ND	-2.92	121.60	125.93
26	mG	203	PEB	OD-C4D-ND	-2.92	121.60	125.93
26	F4	201	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	I8	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	mB	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	LC	201	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
26	QG	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K5	203	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	kE	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	PG	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	NJ	203	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	JJ	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	KA	201	PEB	OD-C4D-ND	-2.92	121.60	125.93
28	JI	1001	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
28	GH	1001	CYC	C1B-NB-C4B	-2.92	106.95	110.67
26	kA	202	PEB	OD-C4D-C3D	-2.92	122.84	129.46
26	B3	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	a6	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
26	j8	201	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
28	L2	1001	CYC	C4A-C3A-C2A	-2.92	103.16	106.51
26	V7	202	PEB	CAB-CBB-CGB	-2.92	107.32	113.60
26	H1	203	PEB	CHA-C1B-NB	-2.92	118.83	124.93
26	b1	501	PEB	CHA-C1B-NB	-2.92	118.83	124.93
26	24	405	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	cF	201	PEB	CHC-C4C-C3C	-2.92	125.36	130.34
26	eG	202	PEB	CHC-C4C-C3C	-2.92	125.36	130.34
26	R1	203	PEB	OD-C4D-C3D	-2.92	122.84	129.46
26	g2	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
28	C2	1001	CYC	C4A-C3A-C2A	-2.92	103.16	106.51
26	U2	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
26	V3	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
26	IC	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	hG	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
26	DD	202	PEB	CMB-C2B-C1B	2.92	129.56	125.06
26	g8	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	C9	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	IE	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	YG	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	pG	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	OI	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	L4	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
28	YH	1001	CYC	CAA-C2A-C1A	2.92	130.17	125.01
26	QD	202	PEB	CBA-CAA-C3A	-2.92	106.97	113.47
26	YA	201	PEB	CAA-C3A-C4A	-2.92	105.18	112.67
26	bF	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
26	L1	201	PEB	OA-C1A-C2A	-2.92	123.85	126.17
26	a6	201	PEB	CAB-CBB-CGB	-2.92	107.32	113.60
26	tG	201	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
26	QB	203	PEB	C2A-C1A-NA	2.92	110.79	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	dB	203	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	XE	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	i7	202	PEB	OD-C4D-C3D	-2.92	122.85	129.46
26	RD	201	PEB	CHB-C4B-NB	-2.92	124.78	128.83
26	SD	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
26	M4	403	PEB	C3B-C4B-NB	2.92	114.29	110.05
26	Y7	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	H9	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
26	L5	203	PEB	CAC-CBC-CGC	-2.92	105.58	113.76
26	w1	203	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
26	h6	202	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
26	IA	202	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
26	iE	201	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
26	oE	202	PEB	OA-C1A-C2A	-2.92	123.85	126.17
28	qH	1002	CYC	CHB-C4A-C3A	-2.92	117.40	124.90
26	ND	203	PEB	OD-C4D-C3D	-2.92	122.85	129.46
26	OG	202	PEB	OD-C4D-C3D	-2.92	122.85	129.46
26	gG	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
26	jF	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
26	ZG	202	PEB	CHB-C4B-C3B	-2.92	118.58	125.32
26	d8	201	PEB	CAA-C3A-C4A	-2.92	105.19	112.67
26	OD	202	PEB	CMB-C2B-C1B	2.92	129.55	125.06
27	AB	302	PUB	OA-C1A-NA	-2.92	121.61	125.93
26	FA	202	PEB	O2B-CGB-CBB	2.92	123.40	114.03
28	NF	1001	CYC	C1B-C2B-C3B	-2.92	104.83	107.87
26	N1	203	PEB	C1B-C2B-C3B	-2.91	103.16	106.51
28	LF	1001	CYC	C4A-C3A-C2A	-2.91	103.16	106.51
26	BD	202	PEB	OA-C1A-NA	2.91	128.47	124.94
26	C4	201	PEB	C3B-C4B-NB	2.91	114.29	110.05
26	TE	202	PEB	CHA-C1B-NB	-2.91	118.84	124.93
26	f7	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
26	Z7	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
27	Y3	302	PUB	C1C-C2C-C3C	-2.91	103.56	106.78
26	D1	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
26	k2	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
26	fA	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
26	R3	201	PEB	CHA-C1B-NB	-2.91	118.84	124.93
26	HB	1002	PEB	CAA-C3A-C4A	-2.91	105.19	112.67
26	GE	202	PEB	CBC-CAC-C2C	-2.91	107.65	112.62
26	S4	201	PEB	C1C-CHB-C4B	2.91	132.29	128.81
26	V7	201	PEB	CHC-C4C-C3C	-2.91	125.37	130.34
26	O9	201	PEB	OD-C4D-C3D	-2.91	122.86	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R9	201	PEB	OD-C4D-C3D	-2.91	122.86	129.46
28	G2	1001	CYC	CHB-C4A-NA	-2.91	118.84	124.93
26	UD	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
26	d1	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	bB	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	vE	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	QG	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	L9	203	PEB	OD-C4D-ND	-2.91	121.61	125.93
26	L1	202	PEB	OD-C4D-C3D	-2.91	122.86	129.46
26	K3	202	PEB	OD-C4D-C3D	-2.91	122.86	129.46
26	KG	203	PEB	CHB-C4B-NB	-2.91	124.79	128.83
26	A6	301	PEB	OD-C4D-ND	-2.91	121.61	125.93
27	K1	203	PUB	OD-C4D-ND	-2.91	121.61	125.93
26	A5	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	j2	202	PEB	C3B-C4B-NB	2.91	114.29	110.05
26	CG	203	PEB	C3B-C4B-NB	2.91	114.29	110.05
26	KB	201	PEB	CHC-C1D-ND	-2.91	110.56	113.95
26	iI	202	PEB	CHA-C1B-NB	-2.91	118.84	124.93
26	IJ	201	PEB	CHA-C1B-NB	-2.91	118.84	124.93
26	i6	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	iF	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	gG	202	PEB	CHA-C1B-NB	-2.91	118.84	124.93
26	FD	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	YE	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	dI	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	Q6	203	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	QD	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	k1	201	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
26	H4	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
26	P3	201	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	j7	201	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	c4	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
26	CC	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
26	OF	203	PEB	C3B-C4B-NB	2.91	114.28	110.05
26	YF	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
26	PE	202	PEB	CBC-CAC-C2C	2.91	117.59	112.62
26	a7	202	PEB	OD-C4D-C3D	-2.91	122.86	129.46
26	B4	201	PEB	CMB-C2B-C1B	2.91	129.55	125.06
26	E8	201	PEB	CMB-C2B-C1B	2.91	129.55	125.06
26	SA	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	hI	202	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	YE	203	PEB	CHC-C1D-ND	-2.91	110.57	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L3	201	PEB	OD-C4D-C3D	-2.91	122.86	129.46
26	W8	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
26	z4	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	TJ	203	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	PD	201	PEB	CAB-CBB-CGB	-2.91	107.34	113.60
26	WG	203	PEB	OA-C1A-C2A	-2.91	123.86	126.17
27	B8	302	PUB	OA-C1A-NA	-2.91	121.62	125.93
26	SJ	202	PEB	CHA-C4A-NA	-2.91	121.75	125.20
26	RB	202	PEB	CAC-CBC-CGC	-2.91	105.60	113.76
26	O7	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
26	d1	201	PEB	C1C-CHB-C4B	-2.91	125.33	128.81
26	t4	201	PEB	C1C-CHB-C4B	2.91	132.28	128.81
26	T3	203	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
26	N9	204	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	tE	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	F3	202	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	G8	202	PEB	CHA-C1B-NB	-2.91	118.85	124.93
26	L6	1002	PEB	OD-C4D-C3D	-2.91	122.87	129.46
26	jF	201	PEB	CHB-C4B-C3B	-2.91	118.60	125.32
26	HD	201	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
26	PB	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	A3	201	PEB	CAA-C3A-C4A	-2.91	105.20	112.67
26	bF	202	PEB	CMD-C2D-C3D	2.91	134.17	130.06
26	m4	201	PEB	CHA-C4A-NA	-2.91	121.75	125.20
26	B9	202	PEB	CBC-CAC-C2C	-2.91	107.66	112.62
26	S3	201	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
26	B1	203	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	O8	201	PEB	OD-C4D-C3D	-2.91	122.87	129.46
26	P4	203	PEB	OD-C4D-ND	-2.91	121.62	125.93
27	xE	301	PUB	OA-C1A-NA	-2.91	121.62	125.93
26	b4	501	PEB	CHA-C1B-NB	-2.91	118.85	124.93
26	h6	201	PEB	CHB-C4B-NB	-2.91	124.79	128.83
26	cF	202	PEB	CHB-C4B-NB	-2.91	124.79	128.83
26	aF	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
28	LB	1001	CYC	C2A-C1A-NA	2.91	114.28	110.05
26	e4	202	PEB	OA-C1A-C2A	-2.91	123.86	126.17
26	b6	202	PEB	CBC-CAC-C2C	-2.91	107.66	112.62
28	N7	1001	CYC	C1B-NB-C4B	-2.91	106.97	110.67
26	B5	203	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	hB	203	PEB	CAB-C3B-C4B	2.91	130.15	125.01
28	nH	1001	CYC	C4A-C3A-C2A	-2.91	103.17	106.51
28	NI	1001	CYC	C4A-C3A-C2A	-2.91	103.17	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t1	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	D7	1002	PEB	C2A-C1A-NA	2.91	110.78	108.27
26	B1	202	PEB	CBA-CAA-C3A	2.91	119.94	113.47
26	l1	202	PEB	OD-C4D-C3D	-2.91	122.87	129.46
26	V6	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	d8	201	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	AD	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	QE	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
28	LH	1001	CYC	C1B-NB-C4B	-2.91	106.97	110.67
26	v4	201	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
26	KJ	202	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
26	P9	201	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
26	eA	201	PEB	CAB-CBB-CGB	-2.91	107.35	113.60
26	OG	203	PEB	OD-C4D-ND	-2.91	121.62	125.93
26	eI	201	PEB	CHB-C4B-C3B	-2.91	118.61	125.32
26	GA	201	PEB	CHA-C4A-NA	2.91	128.66	125.20
26	vG	201	PEB	CAA-C3A-C2A	-2.91	107.00	114.26
28	qH	1001	CYC	CHA-C1A-NA	-2.91	124.80	128.83
26	j6	201	PEB	CHA-C1B-NB	-2.91	118.86	124.93
26	e4	201	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
28	NB	1001	CYC	C1A-C2A-C3A	-2.91	103.57	106.78
28	YH	1002	CYC	C1B-C2B-C3B	-2.91	104.84	107.87
26	e4	202	PEB	OD-C4D-C3D	-2.91	122.88	129.46
26	V6	201	PEB	OD-C4D-ND	-2.91	121.63	125.93
26	J8	202	PEB	CAA-C3A-C2A	-2.91	107.00	114.26
28	hH	1001	CYC	C1B-CHB-C4A	2.91	135.18	128.08
26	xE	304	PEB	C3B-C4B-NB	2.91	114.28	110.05
26	UE	201	PEB	CAC-C2C-C3C	2.91	135.59	127.25
26	eI	201	PEB	CAB-CBB-CGB	-2.90	107.35	113.60
26	TJ	201	PEB	CHA-C1B-NB	-2.90	118.86	124.93
26	V9	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
26	I3	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
26	NE	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
26	A1	201	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
26	p4	201	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
26	g8	201	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
26	f8	203	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	U4	202	PEB	CHC-C4C-C3C	-2.90	125.38	130.34
26	I9	201	PEB	CAB-C3B-C2B	-2.90	122.47	127.88
26	K6	201	PEB	OD-C4D-C3D	-2.90	122.88	129.46
26	z4	202	PEB	OA-C1A-C2A	-2.90	123.86	126.17
26	k7	202	PEB	OD-C4D-ND	-2.90	121.63	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	NE	201	PEB	CHC-C1D-ND	-2.90	110.58	113.95
26	Y3	304	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	TE	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	cG	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
28	HF	1001	CYC	C2A-C1A-NA	2.90	114.27	110.05
26	JA	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
26	YJ	202	PEB	OD-C4D-C3D	-2.90	122.88	129.46
26	Y6	201	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
26	m4	202	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
26	KC	203	PEB	C3B-C4B-NB	2.90	114.27	110.05
28	K2	1001	CYC	C2A-C1A-NA	2.90	114.27	110.05
26	N3	202	PEB	CBC-CAC-C2C	2.90	117.57	112.62
26	MA	203	PEB	OD-C4D-C3D	-2.90	122.88	129.46
26	hB	202	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
26	hE	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
26	B8	301	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	fB	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	eI	202	PEB	CHA-C1B-NB	-2.90	118.86	124.93
26	wG	302	PEB	CHC-C4C-C3C	-2.90	125.39	130.34
26	PB	201	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
26	D1	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
26	X4	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
26	XD	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
26	gF	201	PEB	OD-C4D-C3D	-2.90	122.89	129.46
26	U8	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	KB	201	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
28	FF	1001	CYC	C4A-C3A-C2A	-2.90	103.18	106.51
26	DI	1002	PEB	CAC-CBC-CGC	-2.90	105.62	113.76
28	oH	1001	CYC	C1B-C2B-C3B	-2.90	104.84	107.87
26	dG	201	PEB	OA-C1A-NA	2.90	128.46	124.94
26	P3	201	PEB	CAB-CBB-CGB	-2.90	107.36	113.60
26	XJ	203	PEB	CHC-C4C-C3C	-2.90	125.39	130.34
26	W6	203	PEB	CHB-C4B-NB	-2.90	124.80	128.83
26	f4	202	PEB	CHA-C1B-NB	-2.90	118.86	124.93
26	uE	202	PEB	CHA-C1B-NB	-2.90	118.86	124.93
26	v1	201	PEB	CHC-C1D-ND	-2.90	110.58	113.95
26	f6	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
26	GG	202	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
28	LB	1001	CYC	C1B-NB-C4B	-2.90	106.97	110.67
27	AA	304	PUB	CAB-CBB-CGB	-2.90	105.63	113.76
27	xE	301	PUB	CMD-C2D-C3D	2.90	132.12	127.77
26	J2	1002	PEB	C3B-C4B-NB	2.90	114.27	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mI	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	J5	201	PEB	CMA-C2A-C1A	-2.90	106.15	112.40
26	HE	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
26	P6	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
28	DB	1001	CYC	C2A-C1A-NA	2.90	114.27	110.05
26	P6	201	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
26	L4	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
26	S8	202	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
28	B6	1001	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
26	N1	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
28	tH	1001	CYC	CHA-C1A-NA	-2.90	124.80	128.83
26	MJ	201	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
26	qG	202	PEB	CAB-CBB-CGB	-2.90	107.36	113.60
26	D1	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	QE	203	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	a7	201	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
26	g7	201	PEB	OD-C4D-C3D	-2.90	122.89	129.46
26	N4	203	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	m4	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	hE	201	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
28	F6	1001	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
26	11	201	PEB	OA-C1A-C2A	-2.90	123.87	126.17
26	B5	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
26	f6	201	PEB	C1C-CHB-C4B	2.90	132.27	128.81
26	W4	201	PEB	CBC-CAC-C2C	2.90	117.57	112.62
26	d4	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
26	U6	203	PEB	CMB-C2B-C1B	2.90	129.53	125.06
26	dI	202	PEB	OD-C4D-ND	-2.90	121.64	125.93
27	B8	302	PUB	OD-C4D-ND	-2.90	121.64	125.93
26	j1	202	PEB	CAA-C3A-C4A	2.90	120.12	112.67
28	KH	1001	CYC	C1A-NA-C4A	2.90	111.97	106.51
26	g1	202	PEB	CHA-C1B-NB	-2.90	118.87	124.93
26	e2	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	e4	202	PEB	CBC-CAC-C2C	2.90	117.57	112.62
26	S3	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
26	G5	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
26	Q8	204	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
26	F2	1002	PEB	CMB-C2B-C1B	2.90	129.53	125.06
26	PJ	202	PEB	CHC-C1D-ND	-2.90	110.58	113.95
27	AI	302	PUB	CHC-C1D-ND	-2.90	110.06	113.72
26	V2	203	PEB	OA-C1A-C2A	-2.90	123.87	126.17
26	DI	1002	PEB	CBC-CAC-C2C	2.90	117.56	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A8	301	PEB	C2A-C1A-NA	2.90	110.77	108.27
26	hB	201	PEB	C2A-C1A-NA	2.90	110.77	108.27
26	24	401	PEB	C3B-C4B-NB	2.90	114.26	110.05
26	L3	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
26	W9	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
26	bB	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
26	YB	201	PEB	CAB-CBB-CGB	-2.90	107.37	113.60
26	k1	203	PEB	OD-C4D-ND	-2.90	121.64	125.93
26	kA	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
26	I9	202	PEB	OD-C4D-C3D	-2.90	122.90	129.46
28	LF	1001	CYC	CHB-C1B-C2B	2.90	132.69	126.95
26	bG	201	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	j7	202	PEB	OD-C4D-ND	-2.90	121.64	125.93
27	YD	302	PUB	OA-C1A-NA	-2.90	121.64	125.93
26	RD	201	PEB	CHA-C1B-NB	-2.90	118.87	124.93
26	h6	203	PEB	C2A-C1A-NA	2.90	110.77	108.27
28	RH	1001	CYC	CAB-C3B-C2B	2.90	132.48	127.53
26	dB	203	PEB	CHC-C4C-C3C	-2.90	125.40	130.34
26	GD	202	PEB	C3B-C4B-NB	2.90	114.26	110.05
28	I7	1001	CYC	C2A-C1A-NA	2.90	114.26	110.05
26	K8	202	PEB	CBC-CAC-C2C	-2.90	107.68	112.62
26	DJ	203	PEB	CBC-CAC-C2C	-2.90	107.68	112.62
26	L6	1002	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
26	e6	203	PEB	CHC-C4C-C3C	-2.90	125.40	130.34
26	E9	202	PEB	CHA-C1B-NB	-2.90	118.88	124.93
26	qG	203	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
28	I7	1001	CYC	C1A-C2A-C3A	-2.90	103.58	106.78
26	nG	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
26	W1	201	PEB	CHB-C4B-C3B	-2.90	118.63	125.32
26	Q9	201	PEB	CHB-C4B-C3B	-2.90	118.63	125.32
26	i2	203	PEB	OD-C4D-C3D	-2.90	122.90	129.46
26	xE	303	PEB	OD-C4D-ND	-2.90	121.64	125.93
26	cI	203	PEB	OD-C4D-ND	-2.90	121.64	125.93
26	dF	202	PEB	CAB-CBB-CGB	-2.90	107.37	113.60
26	R4	203	PEB	C1B-C2B-C3B	-2.89	103.18	106.51
26	j4	202	PEB	C1B-C2B-C3B	-2.89	103.18	106.51
26	A3	202	PEB	OD-C4D-C3D	-2.89	122.90	129.46
26	KJ	202	PEB	OD-C4D-ND	-2.89	121.64	125.93
26	h8	201	PEB	OD-C4D-C3D	-2.89	122.90	129.46
26	iG	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
26	hI	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
26	P6	201	PEB	C2A-C1A-NA	2.89	110.77	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I4	201	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
26	U7	201	PEB	OD-C4D-C3D	-2.89	122.90	129.46
26	k8	201	PEB	OD-C4D-ND	-2.89	121.64	125.93
26	gI	202	PEB	CHA-C1B-NB	-2.89	118.88	124.93
26	I8	202	PEB	CHA-C1B-C2B	2.89	132.34	124.90
26	F5	202	PEB	OD-C4D-C3D	-2.89	122.90	129.46
26	WG	201	PEB	OD-C4D-C3D	-2.89	122.91	129.46
26	jF	201	PEB	C2A-C1A-NA	2.89	110.77	108.27
26	cG	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
26	IJ	202	PEB	CMB-C2B-C1B	2.89	129.52	125.06
26	B5	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
28	RH	1001	CYC	CHA-C1A-NA	-2.89	124.81	128.83
26	K5	202	PEB	OD-C4D-ND	-2.89	121.64	125.93
26	G4	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
26	GG	201	PEB	CMB-C2B-C1B	2.89	129.52	125.06
26	K3	201	PEB	CHA-C1B-NB	-2.89	118.88	124.93
26	h7	201	PEB	OD-C4D-C3D	-2.89	122.91	129.46
26	bF	201	PEB	C2A-C1A-NA	2.89	110.77	108.27
26	TJ	201	PEB	C2A-C1A-NA	2.89	110.77	108.27
26	B4	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	n4	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
28	1H	1000	CYC	C2B-C1B-NB	2.89	111.22	106.99
26	bE	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
26	IJ	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
26	i2	201	PEB	CHB-C4B-NB	-2.89	124.82	128.83
26	P7	202	PEB	CHA-C1B-NB	-2.89	118.89	124.93
26	t1	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
26	v1	202	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
26	F1	201	PEB	CHC-C4C-C3C	-2.89	125.41	130.34
26	S7	203	PEB	CMB-C2B-C1B	2.89	129.52	125.06
26	a8	204	PEB	CHB-C4B-NB	-2.89	124.82	128.83
26	Q4	201	PEB	C1C-CHB-C4B	2.89	132.26	128.81
26	AC	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	rE	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	RI	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
26	A1	201	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
26	UB	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	fF	203	PEB	OD-C4D-C3D	-2.89	122.91	129.46
26	IJ	203	PEB	OD-C4D-C3D	-2.89	122.91	129.46
26	hG	202	PEB	CMB-C2B-C1B	2.89	129.51	125.06
26	dB	204	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
26	I5	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q6	203	PEB	CMB-C2B-C1B	2.89	129.51	125.06
26	J3	203	PEB	CHA-C1B-NB	-2.89	118.89	124.93
26	Z8	202	PEB	CHA-C1B-NB	-2.89	118.89	124.93
26	X3	203	PEB	CHC-C4C-C3C	-2.89	125.41	130.34
26	uE	203	PEB	CHC-C4C-C3C	-2.89	125.41	130.34
26	nG	201	PEB	CAB-CBB-CGB	-2.89	107.39	113.60
26	b2	202	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	M4	403	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	Q7	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	KC	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	TG	202	PEB	CHA-C1B-NB	-2.89	118.89	124.93
26	G5	201	PEB	CHC-C1D-ND	-2.89	110.59	113.95
26	LC	202	PEB	CHC-C1D-ND	-2.89	110.59	113.95
26	XD	203	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
26	GJ	202	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
28	pH	1001	CYC	C1B-C2B-C3B	-2.89	104.86	107.87
26	S7	201	PEB	C1C-CHB-C4B	2.89	132.26	128.81
26	lG	201	PEB	CAB-CBB-CGB	-2.89	107.39	113.60
26	aE	202	PEB	CHC-C4C-C3C	-2.89	125.41	130.34
26	WF	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	AI	305	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	rE	202	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	e6	203	PEB	OD-C4D-C3D	-2.89	122.92	129.46
26	eF	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
26	JJ	202	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
26	CC	203	PEB	CMB-C2B-C1B	2.89	129.51	125.06
26	mI	203	PEB	OA-C1A-C2A	-2.89	123.88	126.17
26	XE	202	PEB	CAB-C3B-C4B	2.89	130.12	125.01
26	z1	202	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
26	w4	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
26	jF	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	cG	203	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	AI	301	PEB	C2A-C1A-NA	2.89	110.76	108.27
26	J3	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
26	AB	304	PEB	CHA-C1B-NB	-2.89	118.89	124.93
26	GA	203	PEB	OD-C4D-C3D	-2.89	122.92	129.46
26	aG	203	PEB	OA-C1A-C2A	-2.89	123.88	126.17
26	QI	201	PEB	OA-C1A-C2A	-2.89	123.88	126.17
28	OH	1001	CYC	OC-C1C-C2C	-2.89	123.88	126.17
26	ND	202	PEB	CHB-C4B-NB	-2.89	124.82	128.83
28	uH	1001	CYC	CHA-C1A-NA	-2.89	124.82	128.83
26	K3	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	uE	202	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
26	AJ	305	PEB	C2A-C1A-NA	2.89	110.76	108.27
26	Y4	201	PEB	CHB-C4B-C3B	-2.89	118.65	125.32
26	GG	203	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	XJ	203	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	LB	1002	PEB	OD-C4D-ND	-2.89	121.66	125.93
26	T1	202	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
26	g8	201	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
26	C9	201	PEB	CHA-C1B-NB	-2.89	118.90	124.93
26	V1	201	PEB	CHB-C4B-NB	-2.89	124.82	128.83
26	X3	201	PEB	CMA-C2A-C1A	-2.89	106.18	112.40
26	BJ	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
26	ED	201	PEB	CMD-C2D-C3D	2.89	134.13	130.06
26	v4	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	AI	301	PEB	C3B-C4B-NB	2.89	114.25	110.05
26	B3	201	PEB	CHA-C1B-NB	-2.89	118.90	124.93
27	A6	303	PUB	CHA-C4A-NA	-2.88	110.60	113.95
26	BJ	202	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
26	iI	203	PEB	OD-C4D-C3D	-2.88	122.92	129.46
26	C8	201	PEB	CMA-C2A-C1A	-2.88	106.19	112.40
26	D1	201	PEB	CMB-C2B-C1B	2.88	129.51	125.06
26	RB	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
26	B9	202	PEB	CHA-C1B-NB	-2.88	118.90	124.93
26	M1	402	PEB	CHC-C1D-ND	-2.88	110.60	113.95
26	S6	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
26	GC	202	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
26	G1	202	PEB	C2A-C1A-NA	2.88	110.76	108.27
26	KE	203	PEB	C2A-C1A-NA	2.88	110.76	108.27
26	QG	203	PEB	CAA-C3A-C2A	2.88	121.46	114.26
26	L1	202	PEB	CBC-CAC-C2C	2.88	117.54	112.62
26	f8	202	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	Q8	203	PEB	CAB-CBB-CGB	-2.88	107.40	113.60
26	V3	202	PEB	OA-C1A-NA	2.88	128.43	124.94
26	TA	202	PEB	CHC-C4C-C3C	-2.88	125.42	130.34
26	cB	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	IE	201	PEB	CAC-C2C-C3C	2.88	135.53	127.25
26	C4	202	PEB	CHC-C4C-C3C	-2.88	125.42	130.34
26	SA	201	PEB	CHA-C1B-NB	-2.88	118.90	124.93
26	iA	201	PEB	CAA-C3A-C2A	-2.88	107.06	114.26
26	O8	201	PEB	CMB-C2B-C1B	2.88	129.50	125.06
26	QA	203	PEB	CAB-CBB-CGB	-2.88	107.40	113.60
26	B4	202	PEB	C3B-C4B-NB	2.88	114.24	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K1	203	PUB	OA-C1A-NA	-2.88	121.66	125.93
26	D1	203	PEB	CHC-C1D-ND	-2.88	110.60	113.95
26	wE	302	PEB	CHC-C4C-C3C	-2.88	125.42	130.34
26	f2	201	PEB	OD-C4D-C3D	-2.88	122.93	129.46
26	V7	201	PEB	CAB-CBB-CGB	-2.88	107.40	113.60
28	LF	1001	CYC	OB-C4B-C3B	-2.88	124.91	128.04
26	y4	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	11	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
26	PJ	201	PEB	CHC-C1D-ND	2.88	117.29	113.95
26	XJ	202	PEB	OA-C1A-C2A	-2.88	123.88	126.17
26	IE	201	PEB	CAB-C3B-C4B	2.88	130.11	125.01
26	N3	202	PEB	CHB-C4B-NB	-2.88	124.83	128.83
26	T4	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
26	h2	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	fE	201	PEB	OD-C4D-ND	-2.88	121.66	125.93
26	mA	202	PEB	OD-C4D-C3D	-2.88	122.93	129.46
26	F4	203	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	SF	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
26	m7	202	PEB	CHA-C1B-NB	-2.88	118.91	124.93
26	BJ	201	PEB	OD-C4D-C3D	-2.88	122.93	129.46
26	jI	201	PEB	OA-C1A-C2A	-2.88	123.88	126.17
26	h8	202	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	OB	203	PEB	CMB-C2B-C1B	2.88	129.50	125.06
26	aA	201	PEB	CHC-C4C-C3C	-2.88	125.42	130.34
26	FD	201	PEB	CHA-C1B-NB	-2.88	118.91	124.93
26	CG	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	aG	203	PEB	CHA-C1B-C2B	2.88	132.31	124.90
26	EA	203	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
26	CC	203	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
28	C6	1001	CYC	C1A-C2A-C3A	-2.88	103.60	106.78
26	WB	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
26	UJ	202	PEB	CMB-C2B-C1B	2.88	129.50	125.06
26	AE	202	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	Q3	202	PEB	C2A-C1A-NA	2.88	110.75	108.27
26	I1	202	PEB	OD-C4D-ND	-2.88	121.67	125.93
26	a7	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	MG	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	L4	201	PEB	CAA-C3A-C2A	-2.88	107.07	114.26
26	LD	201	PEB	CHA-C1B-C2B	2.88	132.30	124.90
26	bF	203	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
26	i2	202	PEB	CHA-C1B-NB	-2.88	118.91	124.93
26	a4	201	PEB	C1B-C2B-C3B	-2.88	103.20	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CA	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
26	HA	202	PEB	CMA-C2A-C1A	-2.88	106.20	112.40
27	AB	303	PUB	CHA-C4A-NA	-2.88	110.61	113.95
26	X1	202	PEB	OD-C4D-C3D	-2.88	122.94	129.46
26	F1	201	PEB	C2A-C1A-NA	2.88	110.75	108.27
26	ZB	203	PEB	OD-C4D-ND	-2.88	121.67	125.93
26	O6	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
28	I2	1001	CYC	CHA-C1A-NA	-2.88	124.83	128.83
26	j1	201	PEB	OA-C1A-C2A	-2.88	123.89	126.17
28	FB	1001	CYC	C1A-C2A-C3A	-2.88	103.60	106.78
26	e4	201	PEB	CHC-C4C-C3C	-2.88	125.43	130.34
26	LB	1002	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	i1	202	PEB	CHA-C1B-NB	-2.88	118.91	124.93
26	i6	201	PEB	CAB-CBB-CGB	-2.88	107.41	113.60
26	Q6	202	PEB	CBC-CAC-C2C	-2.88	107.71	112.62
26	YF	201	PEB	OD-C4D-ND	-2.88	121.67	125.93
27	xG	306	PUB	OD-C4D-ND	-2.88	121.67	125.93
28	KI	1001	CYC	C2A-C1A-NA	2.88	114.23	110.05
26	T8	201	PEB	CAB-CBB-CGB	-2.88	107.41	113.60
26	iB	202	PEB	CHC-C4C-C3C	-2.88	125.43	130.34
26	d4	203	PEB	C2A-C1A-NA	2.88	110.75	108.27
26	a8	204	PEB	OD-C4D-C3D	-2.88	122.94	129.46
26	GG	202	PEB	OD-C4D-C3D	-2.88	122.94	129.46
26	T3	203	PEB	CMA-C2A-C1A	-2.88	106.20	112.40
26	L4	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	L5	202	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	mE	202	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	ZF	202	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
26	s4	202	PEB	CHB-C4B-NB	-2.88	124.84	128.83
26	k6	201	PEB	CAB-C3B-C4B	2.88	130.10	125.01
26	YB	202	PEB	CMB-C2B-C1B	2.88	129.49	125.06
26	fE	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
26	aF	202	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
26	K3	202	PEB	C2A-C1A-NA	2.88	110.75	108.27
26	TI	202	PEB	C2A-C1A-NA	2.88	110.75	108.27
28	C7	1001	CYC	C2C-C1C-NC	2.88	110.75	108.27
26	EG	201	PEB	CHB-C4B-C3B	-2.88	118.68	125.32
26	A1	202	PEB	C1C-CHB-C4B	2.88	132.24	128.81
26	m1	203	PEB	CHC-C1D-ND	-2.88	110.61	113.95
26	SA	201	PEB	CMB-C2B-C1B	2.88	129.49	125.06
26	a6	201	PEB	CAB-C3B-C4B	2.88	130.09	125.01
26	V1	201	PEB	OD-C4D-C3D	-2.87	122.95	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W6	201	PEB	CBA-CAA-C3A	-2.87	107.07	113.47
28	B6	1002	CYC	C2A-C1A-NA	2.87	114.23	110.05
28	D6	1001	CYC	CHB-C1B-NB	-2.87	119.89	126.06
26	cB	201	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	AJ	304	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	UJ	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
28	D6	1001	CYC	C1A-C2A-C3A	-2.87	103.60	106.78
26	b7	203	PEB	CMB-C2B-C1B	2.87	129.49	125.06
26	IC	203	PEB	CMB-C2B-C1B	2.87	129.49	125.06
26	T3	203	PEB	OD-C4D-C3D	-2.87	122.95	129.46
26	T3	202	PEB	CAB-C3B-C4B	2.87	130.09	125.01
26	K9	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
26	UJ	201	PEB	C2A-C1A-NA	2.87	110.75	108.27
26	zE	501	PEB	C3B-C4B-NB	2.87	114.23	110.05
26	g4	202	PEB	OD-C4D-C3D	-2.87	122.95	129.46
26	B5	202	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	j8	202	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	nE	201	PEB	CHC-C4C-C3C	-2.87	125.44	130.34
26	J1	202	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	RD	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	KE	201	PEB	CHA-C1B-C2B	2.87	132.29	124.90
26	k8	202	PEB	OD-C4D-C3D	-2.87	122.95	129.46
26	rG	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
26	fI	201	PEB	C2A-C1A-NA	2.87	110.75	108.27
26	r4	202	PEB	CHB-C4B-C3B	2.87	131.96	125.32
26	q1	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	RB	202	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	aE	203	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	fE	202	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	DG	203	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	bG	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	BD	201	PEB	CHC-C1D-ND	-2.87	110.61	113.95
26	eI	203	PEB	C3B-C4B-NB	2.87	114.23	110.05
26	dE	201	PEB	OA-C1A-NA	2.87	128.42	124.94
26	Q4	201	PEB	CHB-C4B-NB	-2.87	124.84	128.83
28	II	1001	CYC	CHA-C1A-NA	-2.87	124.84	128.83
26	I5	203	PEB	OD-C4D-ND	-2.87	121.67	125.93
26	mG	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
26	o1	501	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	Q6	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	PD	202	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	XD	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W7	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
26	b6	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	WB	202	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
26	UD	201	PEB	C4B-C3B-C2B	-2.87	103.60	106.78
28	CB	1001	CYC	C1A-C2A-C3A	-2.87	103.60	106.78
26	D7	1002	PEB	CHC-C1D-ND	-2.87	110.61	113.95
26	h2	201	PEB	C4B-NB-C1B	-2.87	101.10	106.51
26	f4	201	PEB	CMB-C2B-C1B	2.87	129.49	125.06
26	RA	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
26	AF	302	PEB	C3B-C4B-NB	2.87	114.23	110.05
26	nE	202	PEB	CBC-CAC-C2C	2.87	117.52	112.62
26	A4	201	PEB	CHC-C1D-ND	-2.87	110.61	113.95
26	cI	202	PEB	CHC-C1D-ND	-2.87	110.61	113.95
26	dB	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
26	cA	201	PEB	OD-C4D-C3D	-2.87	122.95	129.46
26	K8	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
26	V8	201	PEB	C2A-C1A-NA	2.87	110.75	108.27
26	U9	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
26	h1	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
27	yG	303	PUB	OD-C4D-ND	-2.87	121.68	125.93
26	X3	202	PEB	CMB-C2B-C1B	2.87	129.49	125.06
26	FD	202	PEB	CMB-C2B-C1B	2.87	129.49	125.06
26	XE	202	PEB	CBC-CAC-C2C	2.87	117.52	112.62
26	BC	201	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	k7	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
28	mH	1001	CYC	C1A-C2A-C3A	-2.87	103.61	106.78
26	eG	201	PEB	CMB-C2B-C1B	2.87	129.48	125.06
26	f8	202	PEB	OD-C4D-C3D	-2.87	122.96	129.46
26	X9	202	PEB	OD-C4D-C3D	-2.87	122.96	129.46
26	FC	201	PEB	CAB-CBB-CGB	-2.87	107.43	113.60
26	V7	202	PEB	CHC-C4C-C3C	-2.87	125.44	130.34
27	A7	303	PUB	CHA-C1B-C2B	-2.87	125.44	130.34
26	M4	403	PEB	CHA-C1B-NB	-2.87	118.93	124.93
26	kF	201	PEB	OD-C4D-C3D	-2.87	122.96	129.46
26	kG	201	PEB	OD-C4D-C3D	-2.87	122.96	129.46
26	DD	201	PEB	CHA-C4A-NA	2.87	128.62	125.20
26	Q8	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
26	D4	201	PEB	CMB-C2B-C1B	2.87	129.48	125.06
26	j7	203	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
26	aA	203	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
26	H3	201	PEB	CHB-C4B-NB	-2.87	124.85	128.83
26	W6	203	PEB	OD-C4D-ND	-2.87	121.68	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	WF	201	PEB	OD-C4D-C3D	-2.87	122.96	129.46
26	U8	201	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
26	V4	203	PEB	C3B-C4B-NB	2.87	114.22	110.05
26	W8	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
26	AF	302	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
26	VI	203	PEB	OD-C4D-C3D	-2.87	122.96	129.46
26	n4	201	PEB	CAB-C3B-C2B	2.87	133.22	127.88
26	BC	202	PEB	CMB-C2B-C1B	2.87	129.48	125.06
26	B3	202	PEB	OA-C1A-NA	2.87	128.41	124.94
26	W7	203	PEB	OD-C4D-ND	-2.87	121.68	125.93
26	fl	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
26	kE	202	PEB	CHC-C4C-C3C	-2.87	125.45	130.34
26	G3	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
26	GJ	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
28	G2	1001	CYC	CMA-C3A-C4A	2.87	129.48	125.06
26	B3	203	PEB	CAC-CBC-CGC	-2.87	105.72	113.76
26	T4	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
26	l8	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
27	B8	302	PUB	C2C-C1C-NC	2.87	114.22	110.05
28	KF	1001	CYC	CHB-C1B-NB	-2.87	119.90	126.06
26	FD	202	PEB	CHA-C1B-NB	-2.87	118.94	124.93
26	P7	201	PEB	C2A-C1A-NA	2.87	110.74	108.27
26	CC	201	PEB	C2A-C1A-NA	2.87	110.74	108.27
26	ZB	202	PEB	CHC-C4C-C3C	-2.87	125.45	130.34
26	C4	202	PEB	OA-C1A-C2A	-2.87	123.89	126.17
26	U6	203	PEB	OA-C1A-C2A	-2.87	123.89	126.17
28	IH	1001	CYC	OC-C1C-C2C	-2.87	123.89	126.17
26	O8	203	PEB	OD-C4D-ND	-2.87	121.68	125.93
26	h1	201	PEB	CBC-CAC-C2C	-2.87	107.73	112.62
26	C5	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
26	iE	203	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
27	yE	303	PUB	OD-C4D-ND	-2.87	121.69	125.93
26	K1	201	PEB	CHA-C1B-NB	-2.87	118.94	124.93
26	GE	202	PEB	CAC-CBC-CGC	2.87	121.79	113.76
26	C4	201	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
26	VB	201	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
26	kI	201	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
26	MA	203	PEB	C3B-C4B-NB	2.87	114.22	110.05
28	YH	1003	CYC	C1B-C2B-C3B	-2.87	104.88	107.87
26	W6	202	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
26	VF	202	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
26	cI	202	PEB	C4B-C3B-C2B	-2.86	103.61	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E1	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
26	J3	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
28	FI	1001	CYC	CAB-C3B-C2B	2.86	132.43	127.53
26	H2	1002	PEB	C1C-CHB-C4B	2.86	132.23	128.81
26	h4	203	PEB	CHC-C4C-C3C	-2.86	125.45	130.34
26	xG	304	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
26	e6	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
26	N8	201	PEB	CMC-C3C-C2C	-2.86	119.54	124.94
26	lF	202	PEB	CHA-C1B-NB	-2.86	118.94	124.93
26	aF	201	PEB	C2A-C1A-NA	2.86	110.74	108.27
26	YG	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
26	XD	203	PEB	CHC-C4C-C3C	-2.86	125.45	130.34
26	dI	202	PEB	CHC-C4C-C3C	-2.86	125.45	130.34
26	jE	202	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
26	QE	202	PEB	CHB-C4B-NB	-2.86	124.85	128.83
26	U6	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
26	S4	201	PEB	OD-C4D-C3D	-2.86	122.97	129.46
26	PF	202	PEB	CHC-C4C-C3C	-2.86	125.45	130.34
26	E1	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	C3	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	IC	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	b2	201	PEB	OD-C4D-C3D	-2.86	122.97	129.46
26	aG	203	PEB	OD-C4D-C3D	-2.86	122.97	129.46
28	wH	1001	CYC	C1A-C2A-C3A	-2.86	103.61	106.78
26	GE	203	PEB	CAB-CBB-CGB	-2.86	107.44	113.60
26	w4	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
26	WB	201	PEB	CBA-CAA-C3A	-2.86	107.09	113.47
26	UB	202	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
28	J7	1001	CYC	C2A-C1A-NA	2.86	114.21	110.05
26	gG	201	PEB	CMB-C2B-C3B	-2.86	118.35	126.12
26	mB	201	PEB	OD-C4D-C3D	-2.86	122.97	129.46
26	J1	201	PEB	CHB-C4B-C3B	-2.86	118.71	125.32
26	e2	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
26	i4	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	hA	203	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	e1	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
26	d6	203	PEB	CHC-C1D-ND	-2.86	110.62	113.95
26	j2	202	PEB	OD-C4D-C3D	-2.86	122.98	129.46
26	d6	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	lF	201	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	SA	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	AF	305	PEB	C3B-C4B-NB	2.86	114.21	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	cG	203	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
26	f2	202	PEB	OD-C4D-C3D	-2.86	122.98	129.46
26	k6	202	PEB	OD-C4D-C3D	-2.86	122.98	129.46
26	J3	202	PEB	CBC-CAC-C2C	2.86	117.50	112.62
26	U2	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	WD	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	bI	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	EA	201	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	H3	203	PEB	CAB-C3B-C2B	-2.86	122.55	127.88
26	T9	203	PEB	CHA-C1B-NB	-2.86	118.95	124.93
26	aB	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
26	j8	202	PEB	OA-C1A-C2A	-2.86	123.90	126.17
26	s4	203	PEB	CMB-C2B-C1B	2.86	129.47	125.06
26	VB	201	PEB	CAB-C3B-C4B	2.86	130.07	125.01
26	A8	302	PEB	C3B-C4B-NB	2.86	114.21	110.05
26	YJ	201	PEB	CHA-C1B-NB	-2.86	118.95	124.93
26	cG	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	f1	201	PEB	C2A-C1A-NA	2.86	110.74	108.27
26	B5	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
26	E8	203	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
26	oG	202	PEB	CHC-C1D-ND	-2.86	110.63	113.95
26	VD	201	PEB	OD-C4D-C3D	-2.86	122.98	129.46
26	C5	203	PEB	CHA-C1B-NB	-2.86	118.95	124.93
26	z1	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
26	AA	301	PEB	OD-C4D-ND	-2.86	121.69	125.93
26	N3	201	PEB	CHA-C4A-NA	2.86	128.60	125.20
26	SB	201	PEB	CHA-C1B-NB	-2.86	118.95	124.93
26	Z1	201	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
26	O3	201	PEB	CMA-C2A-C1A	-2.86	106.24	112.40
26	B4	203	PEB	C1C-CHB-C4B	2.86	132.22	128.81
26	QB	202	PEB	CBC-CAC-C2C	-2.86	107.74	112.62
26	M9	201	PEB	CHB-C4B-C3B	-2.86	118.72	125.32
26	gG	203	PEB	OA-C1A-C2A	-2.86	123.90	126.17
26	OD	202	PEB	OD-C4D-ND	-2.86	121.70	125.93
26	DJ	203	PEB	CHA-C1B-NB	-2.86	118.96	124.93
26	OA	203	PEB	CBC-CAC-C2C	-2.86	107.74	112.62
26	Q2	202	PEB	OD-C4D-ND	-2.86	121.70	125.93
26	w4	204	PEB	OD-C4D-ND	-2.86	121.70	125.93
26	IC	201	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	f8	203	PEB	CHA-C1B-NB	-2.86	118.96	124.93
26	I5	201	PEB	CHC-C4C-C3C	-2.86	125.47	130.34
26	SF	201	PEB	C3B-C4B-NB	2.86	114.20	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UG	202	PEB	OA-C1A-C2A	-2.86	123.90	126.17
26	11	203	PEB	OD-C4D-C3D	-2.86	122.99	129.46
26	P4	202	PEB	OD-C4D-C3D	-2.86	122.99	129.46
26	i4	201	PEB	CMB-C2B-C1B	2.86	129.46	125.06
26	e4	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	P8	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
26	K6	201	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
26	AF	301	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
26	mB	201	PEB	CHC-C1D-ND	-2.86	110.63	113.95
26	k4	202	PEB	OD-C4D-C3D	-2.86	122.99	129.46
26	OA	201	PEB	OD-C4D-C3D	-2.86	122.99	129.46
26	G6	1002	PEB	C1C-CHB-C4B	2.86	132.22	128.81
26	K5	203	PEB	OD-C4D-ND	-2.86	121.70	125.93
26	XJ	203	PEB	CMB-C2B-C1B	2.86	129.46	125.06
26	WF	203	PEB	C4B-C3B-C2B	-2.85	103.62	106.78
26	e2	201	PEB	CHB-C4B-C3B	-2.85	118.72	125.32
27	A4	203	PUB	OD-C4D-ND	-2.85	121.70	125.93
27	QA	201	PUB	OA-C1A-NA	-2.85	121.70	125.93
26	QB	201	PEB	CBC-CAC-C2C	2.85	117.49	112.62
26	YE	202	PEB	OD-C4D-C3D	-2.85	122.99	129.46
26	x4	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
26	NJ	202	PEB	C4B-C3B-C2B	-2.85	103.62	106.78
26	Z7	203	PEB	CHC-C1D-ND	-2.85	110.63	113.95
26	HC	202	PEB	CMB-C2B-C1B	2.85	129.46	125.06
26	t4	202	PEB	OD-C4D-C3D	-2.85	122.99	129.46
26	KJ	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	R6	202	PEB	OD-C4D-ND	-2.85	121.70	125.93
28	FB	1001	CYC	CMA-C3A-C4A	2.85	129.46	125.06
26	UF	202	PEB	CAB-CBB-CGB	-2.85	107.46	113.60
26	M4	402	PEB	CHC-C4C-C3C	-2.85	125.47	130.34
26	UJ	201	PEB	CHC-C4C-C3C	-2.85	125.47	130.34
26	rG	201	PEB	OA-C1A-NA	2.85	128.40	124.94
26	H3	202	PEB	OD-C4D-ND	-2.85	121.70	125.93
27	A7	304	PUB	OD-C4D-ND	-2.85	121.70	125.93
26	A6	304	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	VF	201	PEB	CHB-C4B-C3B	-2.85	118.73	125.32
26	w1	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
26	Y6	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
26	AD	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
26	VF	203	PEB	C3B-C4B-NB	2.85	114.20	110.05
26	Z8	201	PEB	CMA-C2A-C1A	-2.85	106.25	112.40
26	b7	203	PEB	OD-C4D-ND	-2.85	121.70	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mI	202	PEB	CAB-C3B-C4B	2.85	130.05	125.01
26	PF	202	PEB	CAC-CBC-CGC	-2.85	105.77	113.76
26	i4	202	PEB	CMB-C2B-C1B	2.85	129.46	125.06
26	Z7	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
26	EA	202	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
26	pG	201	PEB	CAB-CBB-CGB	-2.85	107.47	113.60
26	qG	203	PEB	CAB-C3B-C4B	2.85	130.05	125.01
26	oG	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	N4	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	j4	201	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	YD	304	PEB	OD-C4D-C3D	-2.85	123.00	129.46
27	xG	305	PUB	C2C-C1C-NC	2.85	114.20	110.05
26	a4	203	PEB	OD-C4D-C3D	-2.85	123.00	129.46
26	K3	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
26	V6	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
26	UA	201	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
26	11	203	PEB	C3B-C4B-NB	2.85	114.19	110.05
26	O3	202	PEB	C3B-C4B-NB	2.85	114.19	110.05
26	P9	203	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	TA	201	PEB	CAB-CBB-CGB	-2.85	107.47	113.60
26	A2	301	PEB	CHC-C4C-C3C	-2.85	125.48	130.34
26	T7	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	UF	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	ZG	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
26	U6	203	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
26	bG	202	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
26	PG	201	PEB	C1C-CHB-C4B	2.85	132.21	128.81
28	KH	1001	CYC	CHB-C1B-C2B	-2.85	121.30	126.95
26	V1	203	PEB	CAC-CBC-CGC	-2.85	105.77	113.76
26	V1	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	N4	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	f6	201	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	NA	202	PEB	CHC-C1D-ND	-2.85	110.64	113.95
28	NF	1001	CYC	C2B-C1B-NB	2.85	111.16	106.99
26	BC	203	PEB	OD-C4D-ND	-2.85	121.71	125.93
26	PJ	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
27	21	402	PUB	CMD-C2D-C3D	2.85	132.04	127.77
26	f4	202	PEB	CMA-C2A-C1A	-2.85	106.26	112.40
26	c1	202	PEB	CMC-C3C-C2C	2.85	130.31	124.94
26	m1	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06
28	oH	1001	CYC	CHA-C1A-NA	-2.85	124.88	128.83
26	O7	203	PEB	OD-C4D-ND	-2.85	121.71	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TI	202	PEB	OD-C4D-ND	-2.85	121.71	125.93
28	E7	1001	CYC	CHB-C1B-NB	-2.85	119.94	126.06
26	G5	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	I7	201	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
26	B9	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
26	MA	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
26	f6	203	PEB	OD-C4D-C3D	-2.85	123.01	129.46
26	OJ	201	PEB	CHC-C4C-C3C	-2.85	125.48	130.34
26	e1	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	S8	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	QB	202	PEB	OA-C1A-C2A	-2.85	123.91	126.17
26	A7	305	PEB	C3B-C4B-NB	2.85	114.19	110.05
28	CI	1001	CYC	C2A-C1A-NA	2.85	114.19	110.05
26	i4	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
26	A7	301	PEB	OD-C4D-ND	-2.85	121.71	125.93
26	l2	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
26	Y9	202	PEB	OD-C4D-C3D	-2.85	123.01	129.46
26	S3	201	PEB	CMA-C2A-C1A	-2.85	106.27	112.40
26	jA	202	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
28	qH	1001	CYC	C4A-C3A-C2A	-2.85	103.24	106.51
26	R1	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06
26	TF	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
26	kF	201	PEB	CAB-C3B-C4B	2.85	130.04	125.01
28	LB	1001	CYC	C1A-C2A-C3A	-2.85	103.63	106.78
26	J1	201	PEB	CAB-CBB-CGB	-2.85	107.48	113.60
26	K3	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
26	aE	203	PEB	C2A-C1A-NA	2.85	110.73	108.27
26	U4	201	PEB	C1C-CHB-C4B	2.85	132.21	128.81
26	e8	202	PEB	CAC-CBC-CGC	-2.85	105.78	113.76
26	TE	202	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
28	nH	1001	CYC	C1B-C2B-C3B	-2.85	104.90	107.87
27	wE	304	PUB	OA-C1A-NA	-2.85	121.71	125.93
26	EE	202	PEB	CHB-C4B-NB	-2.85	124.88	128.83
26	RJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
26	fG	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
26	hI	201	PEB	C4B-NB-C1B	-2.85	101.15	106.51
26	DA	202	PEB	OD-C4D-C3D	-2.85	123.01	129.46
26	S6	201	PEB	CHA-C1B-NB	-2.85	118.98	124.93
28	G7	1001	CYC	CHB-C4A-NA	-2.85	118.98	124.93
26	11	201	PEB	C3B-C4B-NB	2.85	114.19	110.05
26	m6	201	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
26	S9	202	PEB	C1B-C2B-C3B	-2.85	103.24	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S8	201	PEB	CHC-C4C-C3C	-2.85	125.48	130.34
26	X3	203	PEB	C4B-C3B-C2B	-2.84	103.63	106.78
26	lF	203	PEB	C4B-C3B-C2B	-2.84	103.63	106.78
26	OA	201	PEB	CAB-CBB-CGB	-2.84	107.48	113.60
28	NH	1001	CYC	C4D-CHA-C1A	2.84	132.21	128.81
27	YD	302	PUB	CHA-C4A-NA	-2.84	110.64	113.95
26	SE	202	PEB	CAC-CBC-CGC	2.84	121.73	113.76
28	LI	1001	CYC	C4A-C3A-C2A	-2.84	103.24	106.51
26	hA	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	k4	203	PEB	CHA-C1B-NB	-2.84	118.98	124.93
26	P6	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
26	k8	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	LG	202	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	FC	202	PEB	CHC-C1D-ND	-2.84	110.64	113.95
26	eA	202	PEB	CAC-CBC-CGC	-2.84	105.79	113.76
26	14	201	PEB	C2A-C1A-NA	2.84	110.72	108.27
26	hG	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
28	DF	1001	CYC	CHA-C1A-NA	-2.84	124.88	128.83
26	AC	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
26	A4	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	H4	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	U9	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
26	TG	202	PEB	CAA-C3A-C4A	-2.84	105.37	112.67
26	iG	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	lA	201	PEB	CMB-C2B-C1B	2.84	129.44	125.06
26	WE	202	PEB	CHA-C1B-NB	-2.84	118.99	124.93
26	U7	203	PEB	C2A-C1A-NA	2.84	110.72	108.27
26	R8	202	PEB	CHA-C4A-NA	-2.84	121.83	125.20
26	m1	203	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	T8	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	h7	203	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	PB	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	AG	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	NJ	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	OB	201	PEB	CAA-C3A-C2A	-2.84	107.16	114.26
26	G8	203	PEB	OD-C4D-C3D	-2.84	123.02	129.46
26	gE	203	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	u1	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
26	m6	203	PEB	CAB-C3B-C4B	2.84	130.03	125.01
26	YJ	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	H3	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	VJ	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	PD	203	PEB	CHB-C4B-C3B	-2.84	118.76	125.32
26	S7	203	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	jA	201	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	a4	201	PEB	C2A-C1A-NA	2.84	110.72	108.27
26	CE	203	PEB	CMB-C2B-C1B	2.84	129.44	125.06
26	tG	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	ME	203	PEB	CHA-C1B-C2B	2.84	132.20	124.90
28	qH	1001	CYC	C1B-C2B-C3B	-2.84	104.91	107.87
26	i2	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	hE	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	kE	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	A2	305	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	P2	203	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	Q2	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	w4	201	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	AE	202	PEB	CHC-C4C-C3C	-2.84	125.50	130.34
26	g8	201	PEB	CHA-C1B-C2B	2.84	132.20	124.90
26	OA	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	T6	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
26	h8	201	PEB	CHC-C1D-ND	-2.84	110.65	113.95
26	SJ	202	PEB	CHB-C4B-C3B	-2.84	118.76	125.32
26	LE	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	AF	305	PEB	CHA-C1B-NB	-2.84	119.00	124.93
26	h2	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	b2	202	PEB	CMB-C2B-C1B	2.84	129.43	125.06
26	iG	202	PEB	CHB-C4B-C3B	-2.84	118.77	125.32
26	K9	202	PEB	OD-C4D-C3D	-2.84	123.03	129.46
26	m1	203	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	r4	201	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	A5	201	PEB	CAB-CBB-CGB	-2.84	107.50	113.60
26	TF	201	PEB	OA-C1A-C2A	-2.84	123.92	126.17
26	uG	202	PEB	CBA-CAA-C3A	2.84	119.78	113.47
26	U4	202	PEB	OD-C4D-ND	-2.84	121.73	125.93
26	LE	201	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	WE	201	PEB	C3B-C4B-NB	2.84	114.18	110.05
26	O9	202	PEB	CHC-C4C-C3C	-2.84	125.50	130.34
26	D4	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	M8	203	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	UJ	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
26	bI	201	PEB	CMA-C2A-C1A	-2.84	106.29	112.40
26	Q3	201	PEB	CAB-C3B-C4B	2.84	130.03	125.01
26	AF	305	PEB	C1B-C2B-C3B	-2.84	103.25	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	jE	201	PEB	OD-C4D-ND	-2.84	121.73	125.93
26	VI	203	PEB	C3B-C4B-NB	2.84	114.17	110.05
26	GG	202	PEB	CAC-C2C-C3C	2.84	135.40	127.25
26	r1	201	PEB	C2A-C1A-NA	2.84	110.72	108.27
26	Z7	202	PEB	CBC-CAC-C2C	-2.84	107.78	112.62
26	P3	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
26	UI	202	PEB	OD-C4D-C3D	-2.84	123.03	129.46
26	mB	203	PEB	C1C-CHB-C4B	2.84	132.20	128.81
26	V2	203	PEB	CAB-C3B-C4B	2.84	130.03	125.01
26	H1	203	PEB	CHC-C1D-ND	-2.84	110.65	113.95
28	F6	1001	CYC	CMA-C3A-C4A	2.84	129.43	125.06
26	NI	1002	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
26	hB	202	PEB	CHA-C1B-NB	-2.84	119.00	124.93
26	VF	203	PEB	CHA-C1B-NB	-2.84	119.00	124.93
26	h1	202	PEB	OD-C4D-C3D	-2.84	123.04	129.46
26	AC	201	PEB	OD-C4D-C3D	-2.84	123.04	129.46
26	g1	201	PEB	OD-C4D-ND	-2.84	121.73	125.93
26	W3	202	PEB	OD-C4D-ND	-2.84	121.73	125.93
26	f8	201	PEB	CMB-C2B-C1B	2.84	129.43	125.06
28	L6	1001	CYC	C1A-C2A-C3A	-2.84	103.64	106.78
26	H3	203	PEB	CHC-C1D-ND	-2.84	110.66	113.95
26	j4	202	PEB	OA-C1A-C2A	-2.83	123.92	126.17
26	DJ	202	PEB	OA-C1A-C2A	-2.83	123.92	126.17
26	RB	202	PEB	C1C-CHB-C4B	-2.83	125.42	128.81
28	E7	1001	CYC	CHB-C4A-C3A	2.83	132.19	124.90
26	l7	203	PEB	OD-C4D-C3D	-2.83	123.04	129.46
26	H9	203	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	gI	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	X3	203	PEB	CHB-C4B-C3B	-2.83	118.77	125.32
26	aI	202	PEB	OD-C4D-ND	-2.83	121.73	125.93
26	FC	203	PEB	CHA-C1B-NB	-2.83	119.01	124.93
26	A3	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	MG	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	AI	301	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	P4	201	PEB	CMB-C2B-C1B	2.83	129.43	125.06
26	A6	304	PEB	OD-C4D-ND	-2.83	121.73	125.93
26	AI	305	PEB	OD-C4D-ND	-2.83	121.73	125.93
26	dI	202	PEB	OD-C4D-C3D	-2.83	123.04	129.46
26	G3	202	PEB	C3B-C4B-NB	2.83	114.17	110.05
26	eE	203	PEB	C2A-C1A-NA	2.83	110.72	108.27
26	NA	201	PEB	CAB-C3B-C4B	2.83	130.02	125.01
26	jI	201	PEB	OD-C4D-C3D	-2.83	123.04	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HE	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
28	YH	1002	CYC	C1A-C2A-C3A	-2.83	103.65	106.78
26	N6	201	PEB	CHC-C4C-C3C	-2.83	125.51	130.34
26	hI	202	PEB	C3B-C4B-NB	2.83	114.17	110.05
26	sG	202	PEB	CHB-C4B-NB	-2.83	124.90	128.83
26	YA	201	PEB	CHA-C1B-NB	-2.83	119.01	124.93
26	O9	202	PEB	C1C-CHB-C4B	-2.83	125.43	128.81
26	QF	202	PEB	CHA-C4A-NA	2.83	128.57	125.20
26	b2	202	PEB	C3B-C4B-NB	2.83	114.17	110.05
26	vG	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
26	l1	202	PEB	CHB-C4B-NB	-2.83	124.90	128.83
26	W4	201	PEB	CHB-C4B-C3B	-2.83	118.78	125.32
26	a4	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	j8	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
28	CI	1001	CYC	C4A-C3A-C2A	-2.83	103.26	106.51
26	NJ	203	PEB	CHC-C4C-C3C	-2.83	125.51	130.34
26	fF	202	PEB	OA-C1A-C2A	-2.83	123.92	126.17
26	C4	202	PEB	CHA-C4A-NA	-2.83	121.84	125.20
26	qG	201	PEB	CHA-C1B-C2B	2.83	132.18	124.90
26	fG	202	PEB	C3B-C4B-NB	2.83	114.17	110.05
26	JI	1002	PEB	OD-C4D-C3D	-2.83	123.05	129.46
26	TG	202	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
28	tH	1001	CYC	C1B-NB-C4B	-2.83	107.06	110.67
26	R4	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
26	eE	201	PEB	C2A-C1A-NA	2.83	110.71	108.27
26	E3	202	PEB	OD-C4D-C3D	-2.83	123.05	129.46
26	XJ	202	PEB	OD-C4D-C3D	-2.83	123.05	129.46
26	P1	202	PEB	CHC-C4C-C3C	-2.83	125.51	130.34
26	JC	201	PEB	CHC-C1D-ND	-2.83	110.66	113.95
26	WJ	202	PEB	CHC-C1D-ND	-2.83	110.66	113.95
28	qH	1001	CYC	CAA-C2A-C1A	2.83	130.01	125.01
26	qG	202	PEB	CAB-C3B-C2B	-2.83	122.61	127.88
26	J4	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
28	LH	1001	CYC	C2B-C1B-NB	2.83	111.13	106.99
26	V2	203	PEB	C3B-C4B-NB	2.83	114.17	110.05
26	YJ	201	PEB	C2A-C1A-NA	2.83	110.71	108.27
26	M1	403	PEB	OD-C4D-C3D	-2.83	123.05	129.46
26	AD	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
26	PI	203	PEB	OD-C4D-ND	-2.83	121.74	125.93
26	iB	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	T7	201	PEB	CHA-C1B-NB	-2.83	119.02	124.93
26	L1	203	PEB	OD-C4D-C3D	-2.83	123.05	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g4	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
26	V2	202	PEB	CAB-C3B-C4B	2.83	130.01	125.01
26	C5	203	PEB	C3B-C4B-NB	2.83	114.16	110.05
26	PB	202	PEB	CMB-C2B-C1B	2.83	129.42	125.06
26	uE	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
26	fl	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
26	j8	202	PEB	OD-C4D-ND	-2.83	121.74	125.93
26	QJ	201	PEB	CHB-C4B-C3B	-2.83	118.79	125.32
28	qH	1002	CYC	CAA-C2A-C3A	-2.83	122.61	127.88
26	h4	203	PEB	C3B-C4B-NB	2.83	114.16	110.05
26	A4	201	PEB	CHC-C4C-C3C	-2.83	125.52	130.34
26	CC	202	PEB	C3B-C4B-NB	2.83	114.16	110.05
26	c2	201	PEB	CMB-C2B-C1B	2.83	129.42	125.06
26	HJ	203	PEB	CBA-CAA-C3A	-2.83	107.17	113.47
26	A8	301	PEB	CHC-C1D-ND	-2.83	110.67	113.95
26	ZG	202	PEB	CHC-C1D-ND	2.83	117.23	113.95
27	KD	203	PUB	CAC-CBC-CGC	-2.83	107.52	113.60
26	x1	202	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
26	X3	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
28	J7	1003	CYC	C4A-C3A-C2A	-2.83	103.26	106.51
26	k4	202	PEB	CMB-C2B-C1B	2.83	129.42	125.06
26	U4	202	PEB	CAB-C3B-C4B	2.83	130.01	125.01
26	QG	201	PEB	C2A-C1A-NA	-2.83	105.84	108.27
28	mH	1001	CYC	C2C-C3C-C4C	2.83	105.57	101.34
26	Y7	202	PEB	CHA-C1B-NB	-2.83	119.02	124.93
26	TE	202	PEB	CAB-C3B-C4B	2.83	130.01	125.01
26	LJ	203	PEB	CHC-C4C-C3C	-2.83	125.52	130.34
26	NB	1002	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
26	fl	201	PEB	OD-C4D-ND	-2.83	121.75	125.93
26	p1	201	PEB	OA-C1A-C2A	-2.82	123.93	126.17
26	cB	202	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	LD	201	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	FC	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
26	iG	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
26	hE	202	PEB	CHB-C4B-NB	-2.82	124.91	128.83
26	P3	201	PEB	CHC-C4C-C3C	-2.82	125.52	130.34
28	1H	1000	CYC	C1B-C2B-C3B	-2.82	104.92	107.87
26	YD	303	PEB	OD-C4D-C3D	-2.82	123.06	129.46
26	B4	202	PEB	CAA-C3A-C4A	-2.82	105.42	112.67
26	O6	203	PEB	CHA-C1B-NB	-2.82	119.03	124.93
26	O3	202	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	UB	201	PEB	OD-C4D-ND	-2.82	121.75	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	xG	301	PUB	OA-C1A-NA	-2.82	121.75	125.93
26	g7	201	PEB	CHC-C4C-C3C	-2.82	125.52	130.34
26	S3	202	PEB	CMB-C2B-C1B	2.82	129.41	125.06
26	u1	203	PEB	C3B-C4B-NB	2.82	114.16	110.05
26	OI	201	PEB	C2B-C1B-NB	2.82	116.55	110.53
26	q1	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
28	gH	1001	CYC	C1B-NB-C4B	-2.82	107.08	110.67
26	H9	203	PEB	CHA-C1B-NB	-2.82	119.03	124.93
26	d4	203	PEB	CHC-C4C-C3C	-2.82	125.52	130.34
27	xG	301	PUB	CBA-CAA-C3A	-2.82	108.70	112.98
26	l2	202	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	Z6	203	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	oE	202	PEB	C2A-C1A-NA	2.82	110.71	108.27
28	CB	1001	CYC	CHB-C1B-NB	-2.82	120.00	126.06
26	O8	203	PEB	CBC-CAC-C2C	-2.82	107.80	112.62
26	OJ	201	PEB	CHA-C1B-NB	-2.82	119.03	124.93
26	eA	201	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	W1	201	PEB	C1C-CHB-C4B	2.82	132.18	128.81
26	W4	201	PEB	C1C-CHB-C4B	2.82	132.18	128.81
28	YH	1002	CYC	C1B-CHB-C4A	2.82	134.97	128.08
26	VD	202	PEB	CHA-C4A-NA	2.82	128.56	125.20
26	hF	201	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
26	eE	201	PEB	CMB-C2B-C1B	2.82	129.41	125.06
26	j8	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	WJ	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	qG	203	PEB	C2A-C1A-NA	2.82	110.70	108.27
26	v1	202	PEB	OA-C1A-C2A	-2.82	123.93	126.17
26	TD	203	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	m8	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
26	KJ	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
28	YH	1004	CYC	CHA-C1A-NA	-2.82	124.91	128.83
26	s1	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
26	M8	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	S8	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	a2	203	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	l6	201	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	Q7	202	PEB	OD-C4D-C3D	-2.82	123.07	129.46
26	mA	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
28	JF	1003	CYC	C4A-C3A-C2A	-2.82	103.27	106.51
26	BC	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
26	FJ	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
26	g1	202	PEB	C3B-C4B-NB	2.82	114.15	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e7	202	PEB	OD-C4D-C3D	-2.82	123.07	129.46
26	fG	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
26	AI	305	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
26	PJ	202	PEB	CAB-C3B-C4B	2.82	130.00	125.01
26	JJ	201	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	lE	201	PEB	CMB-C2B-C3B	2.82	133.77	126.12
26	yE	301	PEB	CAA-C3A-C4A	-2.82	105.43	112.67
26	b6	201	PEB	CHB-C4B-NB	-2.82	124.92	128.83
26	m7	201	PEB	CHB-C4B-NB	-2.82	124.92	128.83
26	bG	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	jB	202	PEB	CBC-CAC-C2C	-2.82	107.81	112.62
28	DF	1001	CYC	CHB-C4A-NA	-2.82	119.04	124.93
26	mA	202	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
26	KD	202	PEB	CMB-C2B-C1B	2.82	129.41	125.06
26	qE	203	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
26	G5	202	PEB	OD-C4D-C3D	-2.82	123.07	129.46
26	B4	202	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	OB	203	PEB	OD-C4D-ND	-2.82	121.75	125.93
26	M1	402	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
26	IA	201	PEB	CHA-C1B-NB	-2.82	119.04	124.93
26	KD	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
26	tE	202	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
28	UH	1001	CYC	C1A-C2A-C3A	-2.82	103.66	106.78
28	JI	1001	CYC	C1B-NB-C4B	-2.82	107.08	110.67
28	LB	1001	CYC	CMB-C2B-C1B	2.82	127.69	124.17
26	G6	1002	PEB	CBB-CAB-C3B	2.82	120.46	112.63
26	mI	202	PEB	OD-C4D-C3D	-2.82	123.08	129.46
26	c2	201	PEB	OD-C4D-ND	-2.82	121.76	125.93
26	Q6	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
26	SF	202	PEB	C3D-C4D-ND	2.82	112.79	107.26
26	x1	202	PEB	OA-C1A-C2A	-2.82	123.93	126.17
26	J9	203	PEB	OA-C1A-C2A	-2.82	123.93	126.17
26	O1	202	PEB	CHA-C1B-NB	-2.82	119.04	124.93
26	bG	201	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	RD	201	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
26	eE	203	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
26	A4	202	PEB	CHB-C4B-NB	-2.82	124.92	128.83
26	W7	203	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
28	DB	1001	CYC	C1A-C2A-C3A	-2.82	103.67	106.78
26	S9	202	PEB	CMB-C2B-C1B	2.82	129.40	125.06
26	lA	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
26	OD	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fA	201	PEB	C2A-C1A-NA	2.82	110.70	108.27
26	14	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
26	V4	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
26	CG	201	PEB	CMB-C2B-C1B	2.82	129.40	125.06
26	p1	202	PEB	CHA-C1B-C2B	2.82	132.14	124.90
26	k4	202	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
26	fB	203	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
26	H1	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
26	m4	202	PEB	C3B-C4B-NB	2.82	114.14	110.05
26	G8	202	PEB	C3B-C4B-NB	2.82	114.14	110.05
26	j7	202	PEB	CHA-C1B-NB	-2.82	119.04	124.93
26	EA	201	PEB	CBC-CAC-C2C	-2.82	107.81	112.62
26	N2	1002	PEB	C1B-C2B-C3B	-2.82	103.28	106.51
26	nG	201	PEB	OD-C4D-ND	-2.82	121.76	125.93
26	V7	202	PEB	OD-C4D-C3D	-2.82	123.08	129.46
26	H1	201	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
26	O6	201	PEB	CAA-C3A-C2A	-2.82	107.22	114.26
26	X1	203	PEB	C2A-C3A-C4A	-2.82	97.12	101.34
26	k1	202	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
26	UB	202	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
26	A9	303	PEB	C3B-C4B-NB	2.82	114.14	110.05
26	lE	202	PEB	C3B-C4B-NB	2.82	114.14	110.05
26	c1	202	PEB	CMB-C2B-C1B	2.81	129.40	125.06
26	WD	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
26	T4	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	C8	201	PEB	CAB-CBB-CGB	-2.81	107.55	113.60
26	f1	202	PEB	OD-C4D-C3D	-2.81	123.08	129.46
26	eD	401	PEB	C1C-CHB-C4B	2.81	132.17	128.81
26	b2	202	PEB	CHC-C1D-ND	-2.81	110.68	113.95
26	v4	202	PEB	CMB-C2B-C1B	2.81	129.40	125.06
28	J7	1003	CYC	C1A-C2A-C3A	-2.81	103.67	106.78
26	IC	203	PEB	OD-C4D-ND	-2.81	121.76	125.93
26	DF	1002	PEB	OD-C4D-ND	-2.81	121.76	125.93
26	W1	201	PEB	CHA-C4A-NA	2.81	128.55	125.20
26	s1	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
26	JE	202	PEB	CHB-C4B-C3B	-2.81	118.82	125.32
26	e6	202	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
26	O8	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
26	hB	202	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
26	iF	201	PEB	CHB-C4B-C3B	-2.81	118.82	125.32
26	I3	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
28	nH	1001	CYC	C1B-NB-C4B	-2.81	107.09	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L9	201	PEB	CMB-C2B-C1B	2.81	129.40	125.06
26	lA	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
26	m4	203	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	R6	201	PEB	CHC-C4C-C3C	-2.81	125.54	130.34
26	A8	301	PEB	OD-C4D-ND	-2.81	121.76	125.93
26	QA	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
26	KG	202	PEB	OD-C4D-C3D	-2.81	123.09	129.46
26	aG	203	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
28	H6	1001	CYC	C1A-C2A-C3A	-2.81	103.67	106.78
26	J3	203	PEB	CHC-C4C-C3C	-2.81	125.54	130.34
26	D9	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	e8	201	PEB	CAB-C3B-C4B	2.81	129.98	125.01
26	w1	203	PEB	C3B-C4B-NB	2.81	114.14	110.05
26	F5	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
26	G5	201	PEB	CBC-CAC-C2C	-2.81	107.82	112.62
26	CE	203	PEB	CHB-C4B-NB	-2.81	124.93	128.83
26	eB	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	gI	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
26	Q7	202	PEB	C2A-C1A-NA	2.81	110.70	108.27
26	GD	202	PEB	C2A-C1A-NA	2.81	110.70	108.27
26	X9	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
26	gI	203	PEB	OD-C4D-C3D	-2.81	123.09	129.46
26	kI	202	PEB	CMB-C2B-C1B	2.81	129.39	125.06
26	G1	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	k2	203	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	lE	201	PEB	CAB-C3B-C2B	2.81	133.11	127.88
26	X3	203	PEB	CBA-CAA-C3A	2.81	119.72	113.47
26	Q1	201	PEB	C1C-CHB-C4B	2.81	132.17	128.81
26	NJ	204	PEB	OD-C4D-C3D	-2.81	123.09	129.46
26	H9	202	PEB	CHC-C1D-ND	-2.81	110.68	113.95
26	I1	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	A1	202	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	e6	201	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	hE	201	PEB	OD-C4D-C3D	-2.81	123.09	129.46
26	PE	201	PEB	C3B-C4B-NB	2.81	114.14	110.05
26	YF	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
26	QG	203	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
26	U2	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
26	PB	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
26	aA	204	PEB	OD-C4D-C3D	-2.81	123.10	129.46
28	uH	1001	CYC	C4A-C3A-C2A	-2.81	103.28	106.51
26	VE	201	PEB	CAA-C3A-C2A	-2.81	107.24	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m7	202	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	GG	203	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	jG	202	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	j8	203	PEB	C3B-C4B-NB	2.81	114.13	110.05
26	L4	202	PEB	CHA-C1B-NB	-2.81	119.06	124.93
26	dI	201	PEB	CAB-CBB-CGB	-2.81	107.56	113.60
28	cH	1001	CYC	C1A-C2A-C3A	-2.81	103.67	106.78
26	WG	203	PEB	CMB-C2B-C1B	2.81	129.39	125.06
26	P2	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	G3	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	a6	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	GC	202	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
28	SH	1001	CYC	C1B-C2B-C3B	-2.81	104.94	107.87
26	Q7	201	PEB	CHA-C1B-NB	-2.81	119.06	124.93
26	Q7	202	PEB	C3B-C4B-NB	2.81	114.13	110.05
26	gF	201	PEB	C3B-C4B-NB	2.81	114.13	110.05
26	LF	1002	PEB	CHA-C4A-NA	2.81	128.54	125.20
26	N3	202	PEB	CHB-C4B-C3B	-2.81	118.83	125.32
26	LE	202	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	P1	203	PEB	OA-C1A-C2A	-2.81	123.94	126.17
26	X9	202	PEB	CHC-C4C-C3C	-2.81	125.55	130.34
26	y1	202	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
26	A9	304	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
26	jA	203	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
28	1H	1000	CYC	C4A-C3A-C2A	-2.81	103.28	106.51
26	G1	201	PEB	C3B-C4B-NB	2.81	114.13	110.05
26	oE	203	PEB	CHB-C4B-NB	-2.81	124.93	128.83
26	YB	202	PEB	C3B-C4B-NB	2.81	114.13	110.05
26	c2	203	PEB	OD-C4D-ND	-2.81	121.77	125.93
26	j6	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
26	GE	202	PEB	CAB-C3B-C4B	2.81	129.97	125.01
26	OF	201	PEB	C2A-C1A-NA	2.81	110.69	108.27
26	l1	202	PEB	CHC-C4C-C3C	-2.81	125.55	130.34
26	g4	201	PEB	CMB-C2B-C1B	2.81	129.38	125.06
26	BC	201	PEB	OD-C4D-C3D	-2.81	123.10	129.46
26	f8	202	PEB	C3B-C4B-NB	2.81	114.13	110.05
26	d7	203	PEB	OD-C4D-C3D	-2.81	123.10	129.46
26	Z4	201	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
26	u1	201	PEB	C1B-C2B-C3B	-2.81	103.29	106.51
26	Y9	202	PEB	C1B-C2B-C3B	-2.81	103.29	106.51
26	vG	202	PEB	C1B-C2B-C3B	-2.81	103.29	106.51
26	l8	201	PEB	CHB-C4B-C3B	-2.81	118.84	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LE	202	PEB	CAB-C3B-C4B	2.80	129.97	125.01
28	rH	1001	CYC	C1B-C2B-C3B	-2.80	104.94	107.87
26	O9	202	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	GJ	202	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	L3	202	PEB	C3B-C4B-NB	2.80	114.13	110.05
27	yG	302	PUB	CAD-C3D-C4D	2.80	125.81	121.38
26	y1	201	PEB	O2B-CGB-CBB	2.80	123.04	114.03
26	OG	202	PEB	CHA-C1B-C2B	2.80	132.11	124.90
26	FC	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	b7	203	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
26	r4	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	m8	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	Y9	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	TE	201	PEB	CHA-C1B-NB	-2.80	119.07	124.93
26	p1	202	PEB	OD-C4D-ND	-2.80	121.78	125.93
27	xE	306	PUB	OD-C4D-ND	-2.80	121.78	125.93
26	C5	201	PEB	C3B-C4B-NB	2.80	114.13	110.05
26	OJ	201	PEB	CHC-C1D-ND	-2.80	110.69	113.95
26	k6	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	FD	203	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	uG	203	PEB	CHC-C4C-C3C	-2.80	125.56	130.34
26	m2	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	B9	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
28	MB	1001	CYC	C4A-C3A-C2A	-2.80	103.29	106.51
26	F3	202	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
26	KG	202	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	k1	201	PEB	C3B-C4B-NB	2.80	114.13	110.05
26	g7	201	PEB	C3B-C4B-NB	2.80	114.13	110.05
26	j2	201	PEB	OA-C1A-C2A	-2.80	123.94	126.17
26	sE	203	PEB	CHC-C1D-ND	-2.80	110.69	113.95
26	kE	203	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	Y6	201	PEB	CAB-CBB-CGB	-2.80	107.57	113.60
26	hB	202	PEB	C3B-C4B-NB	2.80	114.13	110.05
26	DD	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	QI	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	VJ	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	kI	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	H4	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	d2	201	PEB	CAB-CBB-CGB	-2.80	107.57	113.60
26	U9	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	rG	201	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	WB	202	PEB	C1C-CHB-C4B	2.80	132.16	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fB	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
28	cH	1001	CYC	C4A-C3A-C2A	-2.80	103.29	106.51
26	24	404	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
26	F7	1002	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	QG	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	h2	201	PEB	CHA-C1B-NB	-2.80	119.07	124.93
26	ZA	202	PEB	CHA-C1B-NB	-2.80	119.07	124.93
26	D3	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
26	h8	203	PEB	OA-C1A-C2A	-2.80	123.95	126.17
26	H5	202	PEB	CHB-C4B-NB	-2.80	124.94	128.83
28	eH	1001	CYC	C2B-C1B-NB	2.80	111.09	106.99
26	C5	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	J3	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	j7	201	PEB	CHA-C1B-NB	-2.80	119.08	124.93
28	H7	1001	CYC	CHB-C4A-NA	-2.80	119.08	124.93
26	J3	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	TI	203	PEB	CAB-CBB-CGB	2.80	119.63	113.60
26	PD	201	PEB	CBC-CAC-C2C	-2.80	107.84	112.62
26	X8	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	g7	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
26	IC	203	PEB	CHA-C1B-NB	-2.80	119.08	124.93
26	B1	203	PEB	CHB-C4B-NB	-2.80	124.94	128.83
28	KF	1001	CYC	CHA-C1A-C2A	-2.80	118.85	125.32
28	hH	1001	CYC	C1A-C2A-C3A	-2.80	103.69	106.78
26	lE	202	PEB	CHC-C4C-C3C	-2.80	125.56	130.34
28	UH	1001	CYC	C1B-CHB-C4A	2.80	134.92	128.08
26	H8	202	PEB	O2B-CGB-CBB	2.80	123.02	114.03
26	W6	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	IA	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	eB	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	kB	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	FC	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	H9	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
28	LF	1001	CYC	C1B-CHB-C4A	-2.80	121.24	128.08
26	i2	203	PEB	OA-C1A-C2A	-2.80	123.95	126.17
26	B1	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
26	kG	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
26	WB	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
26	MG	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	RG	201	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	J2	1002	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	a8	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m8	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	NE	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	Z6	202	PEB	CHC-C4C-C3C	-2.80	125.56	130.34
26	YI	202	PEB	CAB-C3B-C4B	2.80	129.96	125.01
26	C8	203	PEB	CMB-C2B-C1B	2.80	129.37	125.06
26	h7	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	S7	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
28	YH	1004	CYC	C1B-C2B-C3B	-2.80	104.95	107.87
26	AC	202	PEB	CHA-C1B-NB	-2.80	119.08	124.93
26	H4	203	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
26	e6	203	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
26	U7	201	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
26	jI	202	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
26	K1	202	PEB	OA-C1A-C2A	-2.80	123.95	126.17
28	LH	1001	CYC	CAA-C2A-C1A	2.80	129.96	125.01
28	MB	1001	CYC	CMB-C2B-C1B	2.80	127.66	124.17
26	uE	203	PEB	CBC-CAC-C2C	2.80	117.39	112.62
26	OA	203	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	DG	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	N6	201	PEB	C1C-CHB-C4B	-2.80	125.47	128.81
26	d7	203	PEB	CMB-C2B-C1B	2.80	129.37	125.06
26	bI	202	PEB	CMB-C2B-C1B	2.80	129.37	125.06
26	a4	203	PEB	CHC-C4C-C3C	-2.80	125.57	130.34
26	XG	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	G9	202	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
26	BC	202	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
26	MJ	201	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
26	lI	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
26	e6	203	PEB	CMC-C3C-C2C	2.80	130.21	124.94
26	aE	201	PEB	OD-C4D-ND	-2.80	121.79	125.93
26	e8	201	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	W9	202	PEB	C3B-C4B-NB	2.80	114.12	110.05
26	V9	202	PEB	OA-C1A-C2A	-2.80	123.95	126.17
26	R4	203	PEB	CHA-C1B-NB	-2.80	119.08	124.93
26	w4	201	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
26	BD	201	PEB	OD-C4D-C3D	-2.80	123.13	129.46
26	uE	202	PEB	CHB-C4B-NB	-2.80	124.95	128.83
28	EF	1001	CYC	CHA-C1A-NA	-2.80	124.95	128.83
26	SJ	202	PEB	CAA-C3A-C4A	2.80	119.85	112.67
26	lB	202	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
26	uE	203	PEB	C4B-C3B-C2B	-2.80	103.69	106.78
26	kG	203	PEB	C3B-C4B-NB	2.80	114.11	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y1	203	PEB	OD-C4D-C3D	-2.80	123.13	129.46
26	B1	202	PEB	CMB-C2B-C1B	2.79	129.37	125.06
26	X9	202	PEB	CMB-C2B-C1B	2.79	129.37	125.06
26	fI	201	PEB	CMB-C2B-C1B	2.79	129.37	125.06
28	L7	1001	CYC	C4A-C3A-C2A	-2.79	103.30	106.51
26	K3	201	PEB	OD-C4D-C3D	-2.79	123.13	129.46
26	kI	202	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	VJ	202	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	sG	203	PEB	OD-C4D-ND	-2.79	121.79	125.93
26	e4	202	PEB	CHA-C4A-NA	-2.79	121.88	125.20
27	KD	203	PUB	CBB-CAB-C3B	-2.79	107.85	112.62
26	TJ	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
26	Y8	201	PEB	CHA-C1B-NB	-2.79	119.09	124.93
26	VB	201	PEB	CHA-C1B-NB	-2.79	119.09	124.93
26	i1	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
26	SA	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
26	bE	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
28	YH	1002	CYC	C4D-CHA-C1A	2.79	132.15	128.81
26	G3	202	PEB	OD-C4D-C3D	-2.79	123.13	129.46
28	IH	1001	CYC	C2B-C1B-NB	2.79	111.08	106.99
26	H4	203	PEB	OD-C4D-ND	-2.79	121.79	125.93
26	VE	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
26	dF	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
26	J1	201	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	iI	201	PEB	OD-C4D-C3D	-2.79	123.13	129.46
26	hG	202	PEB	CHA-C1B-NB	-2.79	119.09	124.93
26	mE	202	PEB	OD-C4D-ND	-2.79	121.79	125.93
26	R1	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
28	VH	1001	CYC	C1B-C2B-C3B	-2.79	104.96	107.87
26	S9	202	PEB	CAA-C3A-C4A	2.79	119.84	112.67
26	EG	202	PEB	CMB-C2B-C1B	2.79	129.36	125.06
26	NE	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
26	uE	203	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	sG	201	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	PJ	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
26	iG	203	PEB	CHC-C4C-C3C	-2.79	125.58	130.34
26	s4	202	PEB	CMA-C2A-C1A	-2.79	106.39	112.40
26	fB	201	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
26	XA	201	PEB	OD-C4D-C3D	-2.79	123.14	129.46
28	wH	1001	CYC	C1B-CHB-C4A	2.79	134.90	128.08
26	TG	201	PEB	CHA-C1B-NB	-2.79	119.09	124.93
26	m8	202	PEB	OD-C4D-C3D	-2.79	123.14	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	uG	202	PEB	OD-C4D-C3D	-2.79	123.14	129.46
26	LJ	202	PEB	CHC-C1D-ND	-2.79	110.71	113.95
26	hE	202	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	GG	203	PEB	CMA-C2A-C1A	-2.79	106.39	112.40
26	YG	203	PEB	C4B-C3B-C2B	-2.79	103.69	106.78
26	d4	202	PEB	CHA-C4A-NA	-2.79	121.89	125.20
26	B9	202	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	FC	203	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	V4	203	PEB	CAC-CBC-CGC	-2.79	105.94	113.76
26	lE	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	lB	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
26	KD	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
26	TD	203	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
26	l4	203	PEB	OD-C4D-C3D	-2.79	123.14	129.46
26	RB	202	PEB	OD-C4D-C3D	-2.79	123.14	129.46
26	L2	1002	PEB	CAB-C3B-C4B	2.79	129.94	125.01
26	R4	201	PEB	CHB-C4B-C3B	-2.79	118.88	125.32
26	M3	202	PEB	CMB-C2B-C1B	2.79	129.36	125.06
26	F1	202	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
26	aE	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
28	FF	1001	CYC	C2A-C1A-NA	2.79	114.11	110.05
26	L4	201	PEB	C2A-C1A-NA	2.79	110.68	108.27
26	fl	202	PEB	CHA-C1B-NB	-2.79	119.10	124.93
26	P1	202	PEB	OD-C4D-C3D	-2.79	123.14	129.46
26	r1	201	PEB	OD-C4D-C3D	-2.79	123.14	129.46
26	f2	202	PEB	CMB-C2B-C1B	2.79	129.36	125.06
26	d6	201	PEB	CHC-C4C-C3C	-2.79	125.58	130.34
26	TJ	202	PEB	OA-C1A-C2A	-2.79	123.96	126.17
27	yG	303	PUB	C2C-C1C-NC	2.79	114.11	110.05
28	NH	1001	CYC	C1A-C2A-C3A	-2.79	103.70	106.78
26	KC	202	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	MA	203	PEB	CBA-CAA-C3A	-2.79	107.26	113.47
26	A8	302	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
26	q4	202	PEB	CMB-C2B-C1B	2.79	129.36	125.06
26	F1	203	PEB	CHC-C1D-ND	-2.79	110.71	113.95
26	i6	202	PEB	C3B-C4B-NB	2.79	114.10	110.05
26	AJ	303	PEB	C3B-C4B-NB	2.79	114.10	110.05
26	U1	201	PEB	CHB-C4B-NB	-2.79	124.96	128.83
26	eG	202	PEB	CAB-C3B-C4B	2.79	129.94	125.01
26	b2	202	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
26	D3	203	PEB	CHC-C4C-C3C	-2.79	125.58	130.34
26	L3	203	PEB	OA-C1A-C2A	-2.79	123.96	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k8	201	PEB	OA-C1A-C2A	-2.79	123.96	126.17
26	R9	202	PEB	OA-C1A-C2A	-2.79	123.96	126.17
26	gA	201	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
26	VF	202	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
26	AA	301	PEB	CHC-C1D-ND	-2.79	110.71	113.95
26	OG	202	PEB	CMB-C2B-C3B	-2.79	118.55	126.12
28	OH	1001	CYC	C1B-C2B-C3B	-2.79	104.96	107.87
26	kG	203	PEB	OD-C4D-C3D	-2.79	123.15	129.46
26	b6	202	PEB	C2A-C1A-NA	2.79	110.67	108.27
26	L1	202	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
26	fA	202	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
26	BG	202	PEB	C4B-C3B-C2B	-2.79	103.70	106.78
26	K4	201	PEB	CMA-C2A-C1A	-2.79	106.40	112.40
28	L6	1001	CYC	C2A-C1A-NA	2.79	114.10	110.05
26	LE	202	PEB	CHA-C1B-NB	-2.79	119.11	124.93
26	q4	203	PEB	CHC-C1D-ND	-2.79	110.71	113.95
26	i4	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	H9	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	eE	203	PEB	CHA-C4A-NA	2.79	128.52	125.20
26	O4	201	PEB	CHB-C4B-C3B	-2.79	118.89	125.32
26	HJ	203	PEB	C3B-C4B-NB	2.79	114.10	110.05
26	U8	201	PEB	CHB-C4B-NB	-2.79	124.96	128.83
26	O7	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	Q7	203	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	WE	203	PEB	OD-C4D-ND	-2.79	121.80	125.93
26	d4	202	PEB	CHA-C1B-NB	-2.78	119.11	124.93
26	J9	201	PEB	OD-C4D-C3D	-2.78	123.15	129.46
26	YE	201	PEB	OA-C1A-C2A	-2.78	123.96	126.17
26	OD	202	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
26	WA	201	PEB	C3B-C4B-NB	2.78	114.10	110.05
26	QF	202	PEB	OD-C4D-C3D	-2.78	123.15	129.46
26	W1	201	PEB	CMC-C3C-C2C	2.78	130.19	124.94
26	l4	201	PEB	CAB-CBB-CGB	-2.78	107.61	113.60
26	h6	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	WI	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	P9	202	PEB	OD-C4D-C3D	-2.78	123.15	129.46
26	eF	201	PEB	CHC-C4C-C3C	-2.78	125.59	130.34
26	UF	201	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
26	T9	202	PEB	C3B-C4B-NB	2.78	114.10	110.05
26	JJ	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
27	24	403	PUB	CAB-CBB-CGB	-2.78	105.96	113.76
26	Q9	202	PEB	OD-C4D-C3D	-2.78	123.15	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F4	201	PEB	C3B-C4B-NB	2.78	114.10	110.05
26	b7	203	PEB	C3B-C4B-NB	2.78	114.10	110.05
26	G3	202	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
26	d4	203	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
26	Z6	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
26	lB	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
26	DD	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
26	hE	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
27	xG	306	PUB	OA-C1A-NA	-2.78	121.81	125.93
27	A7	304	PUB	CHA-C1B-C2B	-2.78	125.59	130.34
26	UJ	202	PEB	CHB-C4B-NB	-2.78	124.97	128.83
26	D3	203	PEB	OA-C1A-C2A	-2.78	123.96	126.17
26	NJ	202	PEB	OD-C4D-C3D	-2.78	123.16	129.46
26	jB	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	lB	203	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	FD	203	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	DE	203	PEB	C4B-C3B-C2B	-2.78	103.70	106.78
26	SB	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
26	kE	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
26	WF	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
26	dE	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
26	r4	202	PEB	CBA-CAA-C3A	-2.78	107.27	113.47
26	h1	201	PEB	OD-C4D-C3D	-2.78	123.16	129.46
26	h4	201	PEB	C3B-C4B-NB	2.78	114.09	110.05
26	YI	203	PEB	C3B-C4B-NB	2.78	114.09	110.05
26	F5	203	PEB	CHA-C1B-NB	-2.78	119.12	124.93
26	FE	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
26	PB	202	PEB	CHC-C1D-ND	-2.78	110.72	113.95
26	JJ	203	PEB	OA-C1A-C2A	-2.78	123.96	126.17
26	Q3	201	PEB	CBB-CAB-C3B	-2.78	104.90	112.63
26	21	404	PEB	C3B-C4B-NB	2.78	114.09	110.05
26	SI	202	PEB	C3B-C4B-NB	2.78	114.09	110.05
28	qH	1002	CYC	CAB-C3B-C4B	2.78	125.77	121.38
26	T7	202	PEB	CMB-C2B-C1B	2.78	129.35	125.06
26	B5	202	PEB	C2A-C1A-NA	2.78	110.67	108.27
26	iB	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
26	UF	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
28	YH	1004	CYC	C2C-C1C-NC	2.78	110.67	108.27
26	bF	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	kG	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	EA	203	PEB	CHB-C4B-C3B	-2.78	118.90	125.32
26	TD	203	PEB	C1C-CHB-C4B	2.78	132.13	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P6	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	j7	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	i8	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	d7	202	PEB	CHA-C1B-NB	-2.78	119.12	124.93
26	N4	203	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	I8	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
28	C2	1001	CYC	CBC-CAC-C3C	-2.78	107.28	113.47
28	YH	1004	CYC	C1B-CHB-C4A	2.78	134.87	128.08
26	a4	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	FG	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	G8	201	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
26	FG	201	PEB	CHA-C1B-NB	-2.78	119.12	124.93
26	HJ	203	PEB	CHA-C1B-NB	-2.78	119.12	124.93
26	Q1	202	PEB	CHB-C4B-NB	-2.78	124.97	128.83
26	SE	202	PEB	CAC-C2C-C3C	2.78	135.23	127.25
26	L1	203	PEB	C3B-C4B-NB	2.78	114.09	110.05
26	Z6	203	PEB	C3B-C4B-NB	2.78	114.09	110.05
26	JF	1002	PEB	CMB-C2B-C1B	2.78	129.34	125.06
26	V8	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
26	x4	201	PEB	OA-C1A-C2A	-2.78	123.96	126.17
26	v4	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	eF	201	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	G1	202	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
26	VG	201	PEB	CAA-C3A-C2A	-2.78	107.32	114.26
26	JI	1002	PEB	CHA-C1B-NB	-2.78	119.12	124.93
26	N4	202	PEB	CMB-C2B-C1B	2.78	129.34	125.06
26	ZI	201	PEB	OA-C1A-NA	2.78	128.31	124.94
26	M1	403	PEB	CBC-CAC-C2C	-2.78	107.88	112.62
26	eA	201	PEB	OD-C4D-C3D	-2.78	123.17	129.46
26	HD	201	PEB	CMB-C2B-C1B	2.78	129.34	125.06
26	R1	203	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
26	U9	201	PEB	CHC-C4C-C3C	-2.78	125.60	130.34
28	1H	1000	CYC	C1B-CHB-C4A	2.78	134.87	128.08
26	CJ	201	PEB	OA-C1A-C2A	-2.78	123.97	126.17
26	K1	201	PEB	OD-C4D-C3D	-2.78	123.17	129.46
26	L4	202	PEB	OD-C4D-C3D	-2.78	123.17	129.46
26	aE	202	PEB	OD-C4D-ND	-2.78	121.82	125.93
26	jB	201	PEB	CMB-C2B-C1B	2.78	129.34	125.06
28	D2	1001	CYC	CHA-C1A-NA	-2.78	124.98	128.83
26	MD	202	PEB	C3B-C4B-NB	2.78	114.09	110.05
26	Y7	202	PEB	CHB-C4B-C3B	-2.78	118.91	125.32
26	K6	201	PEB	CHC-C1D-ND	-2.78	110.72	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BC	201	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
26	BE	202	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
26	cF	201	PEB	C4B-C3B-C2B	-2.78	103.71	106.78
26	S4	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
26	lE	202	PEB	OD-C4D-ND	-2.78	121.82	125.93
26	QF	203	PEB	OD-C4D-ND	-2.78	121.82	125.93
26	aI	201	PEB	CHC-C4C-C3C	-2.77	125.60	130.34
26	V7	201	PEB	OD-C4D-C3D	-2.77	123.17	129.46
26	GC	202	PEB	OD-C4D-C3D	-2.77	123.17	129.46
26	PB	201	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
28	AH	1001	CYC	C4A-C3A-C2A	-2.77	103.32	106.51
26	Z7	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
28	FB	1001	CYC	C2A-C1A-NA	2.77	114.08	110.05
28	YH	1001	CYC	CHA-C1A-NA	-2.77	124.98	128.83
27	24	403	PUB	CAC-C2C-C1C	2.77	129.92	125.01
26	h4	203	PEB	OD-C4D-ND	-2.77	121.82	125.93
26	BC	203	PEB	CBC-CAC-C2C	-2.77	107.89	112.62
26	z4	202	PEB	CAA-C3A-C2A	-2.77	107.33	114.26
26	A6	304	PEB	CHC-C1D-ND	-2.77	110.73	113.95
26	W8	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	PI	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	FC	202	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
26	HC	202	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
26	QF	202	PEB	OD-C4D-ND	-2.77	121.82	125.93
26	eI	203	PEB	OD-C4D-ND	-2.77	121.82	125.93
26	UD	201	PEB	CBB-CAB-C3B	-2.77	104.92	112.63
26	AD	201	PEB	CMB-C2B-C1B	2.77	129.34	125.06
26	N1	203	PEB	CHA-C1B-NB	-2.77	119.13	124.93
26	d1	203	PEB	OD-C4D-ND	-2.77	121.82	125.93
26	V2	201	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
26	xG	304	PEB	CAB-C3B-C4B	2.77	129.91	125.01
26	eF	201	PEB	CMB-C2B-C1B	2.77	129.33	125.06
26	Z1	201	PEB	C4B-C3B-C2B	-2.77	103.71	106.78
26	c4	201	PEB	C4B-C3B-C2B	-2.77	103.71	106.78
26	v4	202	PEB	C4B-C3B-C2B	-2.77	103.71	106.78
26	GC	203	PEB	C4B-C3B-C2B	-2.77	103.71	106.78
26	21	401	PEB	OD-C4D-C3D	-2.77	123.18	129.46
26	YB	202	PEB	OD-C4D-C3D	-2.77	123.18	129.46
26	a2	201	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
26	KG	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
28	YH	1004	CYC	C1B-NB-C4B	-2.77	107.14	110.67
26	QJ	201	PEB	CHA-C1B-NB	-2.77	119.13	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lF	202	PEB	OD-C4D-C3D	-2.77	123.18	129.46
28	OH	1001	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
26	U8	203	PEB	OA-C1A-C2A	-2.77	123.97	126.17
26	S9	202	PEB	OA-C1A-C2A	-2.77	123.97	126.17
26	A2	301	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	CC	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	QD	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	N4	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	T3	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46
26	N3	203	PEB	OD-C4D-ND	-2.77	121.82	125.93
26	GG	202	PEB	OD-C4D-ND	-2.77	121.82	125.93
26	o1	501	PEB	CHB-C4B-C3B	-2.77	118.92	125.32
26	RB	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	G8	201	PEB	CHC-C1D-ND	-2.77	110.73	113.95
26	AF	302	PEB	C2A-C1A-NA	2.77	110.66	108.27
26	LJ	202	PEB	C2A-C1A-NA	2.77	110.66	108.27
26	c2	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	g8	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	YD	303	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	KC	201	PEB	OD-C4D-ND	-2.77	121.83	125.93
26	jB	201	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	Y7	202	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
26	iF	201	PEB	OA-C1A-C2A	-2.77	123.97	126.17
26	Q2	202	PEB	OD-C4D-C3D	-2.77	123.18	129.46
26	fF	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46
26	D3	201	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	Z7	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	AG	201	PEB	C1C-CHB-C4B	2.77	132.12	128.81
26	cI	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	g2	203	PEB	CBB-CAB-C3B	2.77	120.32	112.63
26	u4	203	PEB	CMB-C2B-C1B	2.77	129.33	125.06
26	D1	201	PEB	CHB-C4B-NB	-2.77	124.98	128.83
26	eF	202	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	L3	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	y4	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	FC	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	c7	202	PEB	CAC-CBC-CGC	-2.77	106.00	113.76
26	P6	201	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	lA	201	PEB	CMA-C2A-C1A	-2.77	106.44	112.40
26	H1	201	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	CC	201	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	ZG	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	SH	1001	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
26	f7	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	ZF	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	11	203	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
28	OH	1001	CYC	C1B-NB-C4B	-2.77	107.14	110.67
26	B1	201	PEB	OD-C4D-ND	-2.77	121.83	125.93
26	h1	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	e2	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	d6	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	AC	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	IJ	203	PEB	CMB-C2B-C1B	2.77	129.33	125.06
26	j2	202	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	A4	202	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	PB	202	PEB	CAC-C2C-C3C	2.77	135.20	127.25
26	x1	202	PEB	CHC-C1D-ND	-2.77	110.73	113.95
26	kF	201	PEB	CHC-C1D-ND	-2.77	110.73	113.95
28	1H	1000	CYC	C2C-C1C-NC	2.77	110.66	108.27
26	FI	1002	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	PI	201	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	VB	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
26	s1	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
26	V4	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
28	GI	1001	CYC	C2A-C1A-NA	2.77	114.08	110.05
26	R4	202	PEB	CHA-C1B-NB	-2.77	119.14	124.93
26	UB	201	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	L3	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	M9	202	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	iI	201	PEB	CHB-C4B-NB	-2.77	124.99	128.83
26	k7	202	PEB	C3B-C4B-NB	2.77	114.07	110.05
26	SJ	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
28	C6	1001	CYC	CHB-C1B-NB	-2.77	120.12	126.06
26	cG	201	PEB	C1C-CHB-C4B	2.77	132.11	128.81
26	UA	201	PEB	CHB-C4B-NB	-2.77	124.99	128.83
26	h4	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
26	24	404	PEB	OD-C4D-ND	-2.77	121.83	125.93
26	XA	201	PEB	OD-C4D-ND	-2.77	121.83	125.93
26	K5	202	PEB	C3B-C4B-NB	2.77	114.07	110.05
26	a8	202	PEB	CHC-C1D-ND	-2.77	110.73	113.95
26	lB	201	PEB	CHC-C1D-ND	-2.77	110.73	113.95
26	U1	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	g6	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	e2	202	PEB	C3B-C4B-NB	2.77	114.07	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	XD	203	PEB	C3B-C4B-NB	2.77	114.07	110.05
26	x4	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	i8	202	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	OJ	201	PEB	OD-C4D-C3D	-2.77	123.19	129.46
26	U7	201	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
26	QB	203	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
28	I7	1001	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
26	WE	203	PEB	CHA-C1B-NB	-2.77	119.15	124.93
26	QF	202	PEB	CAB-CBB-CGB	-2.76	107.65	113.60
26	sE	201	PEB	C3B-C4B-NB	2.76	114.07	110.05
28	F6	1001	CYC	C2A-C1A-NA	2.76	114.07	110.05
26	11	201	PEB	CAB-C3B-C4B	2.76	129.90	125.01
26	J4	201	PEB	CHA-C1B-NB	-2.76	119.15	124.93
26	J4	203	PEB	C4B-C3B-C2B	-2.76	103.72	106.78
27	xG	301	PUB	CHA-C1B-C2B	-2.76	125.62	130.34
26	DD	202	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	OI	202	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	Z4	201	PEB	C1B-C2B-C3B	-2.76	103.33	106.51
26	r1	202	PEB	CHB-C4B-C3B	2.76	131.71	125.32
26	SE	202	PEB	C2A-C3A-C4A	-2.76	97.20	101.34
26	l8	201	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	Q9	202	PEB	C4B-C3B-C2B	-2.76	103.72	106.78
26	A3	201	PEB	CHA-C1B-NB	-2.76	119.15	124.93
26	D9	203	PEB	C2B-C1B-NB	2.76	116.43	110.53
26	PJ	202	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	a6	201	PEB	C1B-C2B-C3B	-2.76	103.33	106.51
26	LJ	201	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	D9	203	PEB	CHA-C1B-NB	-2.76	119.15	124.93
26	J9	201	PEB	C2A-C1A-NA	2.76	110.66	108.27
26	S8	201	PEB	CMA-C2A-C1A	-2.76	106.45	112.40
26	A2	301	PEB	CMB-C2B-C1B	2.76	129.32	125.06
26	nG	202	PEB	CMB-C2B-C1B	2.76	129.32	125.06
26	I9	201	PEB	CBC-CAC-C2C	2.76	117.33	112.62
26	DI	1002	PEB	C3B-C4B-NB	2.76	114.07	110.05
26	R3	201	PEB	C4B-C3B-C2B	-2.76	103.72	106.78
26	CE	203	PEB	C4B-C3B-C2B	-2.76	103.72	106.78
26	hI	201	PEB	CHA-C1B-NB	-2.76	119.15	124.93
26	k7	202	PEB	CAA-C3A-C4A	2.76	119.77	112.67
26	q4	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
26	g7	202	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	l8	201	PEB	CHA-C4A-NA	2.76	128.49	125.20
26	R9	202	PEB	C2A-C1A-NA	2.76	110.65	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q2	202	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
26	OD	201	PEB	CHC-C1D-ND	-2.76	110.74	113.95
26	C5	204	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	S7	203	PEB	OD-C4D-C3D	-2.76	123.20	129.46
26	V9	202	PEB	CMB-C2B-C1B	2.76	129.32	125.06
26	D7	1002	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
26	NF	1002	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	J4	202	PEB	CAB-C3B-C4B	2.76	129.89	125.01
26	YG	201	PEB	CHC-C4C-C3C	-2.76	125.63	130.34
26	O4	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
28	IF	1001	CYC	C4A-C3A-C2A	-2.76	103.34	106.51
26	AB	304	PEB	OA-C1A-C2A	-2.76	123.98	126.17
28	uH	1001	CYC	OC-C1C-C2C	-2.76	123.98	126.17
26	e6	203	PEB	CBC-CAC-C2C	2.76	117.33	112.62
26	XD	203	PEB	CHB-C4B-C3B	-2.76	118.94	125.32
26	bF	203	PEB	CAA-C3A-C4A	-2.76	105.58	112.67
26	W2	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	q4	201	PEB	C3B-C4B-NB	2.76	114.06	110.05
26	ME	201	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
26	Q1	201	PEB	CHB-C4B-C3B	-2.76	118.94	125.32
26	j6	202	PEB	CBC-CAC-C2C	-2.76	107.91	112.62
26	fB	203	PEB	CHA-C1B-NB	-2.76	119.16	124.93
26	VJ	201	PEB	CHA-C1B-NB	-2.76	119.16	124.93
26	G3	202	PEB	CMB-C2B-C1B	2.76	129.31	125.06
26	e4	201	PEB	CMB-C2B-C1B	2.76	129.31	125.06
26	B1	202	PEB	CAB-C3B-C4B	2.76	129.89	125.01
26	oE	203	PEB	C2A-C1A-NA	2.76	110.65	108.27
26	11	201	PEB	CHC-C1D-ND	-2.76	110.74	113.95
26	uG	203	PEB	CHC-C1D-ND	-2.76	110.74	113.95
26	J3	202	PEB	CHB-C4B-C3B	-2.76	118.95	125.32
26	aA	202	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
26	N1	203	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	dF	203	PEB	OD-C4D-ND	-2.76	121.84	125.93
28	YH	1001	CYC	C1B-C2B-C3B	-2.76	104.99	107.87
26	T6	201	PEB	CHB-C4B-NB	-2.76	125.00	128.83
26	FD	203	PEB	CHC-C4C-C3C	-2.76	125.63	130.34
26	AB	301	PEB	CHA-C1B-NB	-2.76	119.16	124.93
26	UI	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	RJ	202	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	L4	203	PEB	C3B-C4B-NB	2.76	114.06	110.05
26	XD	201	PEB	CMA-C2A-C1A	-2.76	106.46	112.40
26	hI	202	PEB	CHA-C1B-NB	-2.76	119.16	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LE	202	PEB	OD-C4D-C3D	-2.76	123.21	129.46
26	d7	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
26	A2	305	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
26	H3	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
26	S6	203	PEB	C2A-C1A-NA	2.76	110.65	108.27
28	PH	1001	CYC	C4A-C3A-C2A	-2.76	103.34	106.51
26	T4	203	PEB	CMB-C2B-C1B	2.76	129.31	125.06
26	TD	202	PEB	CHA-C4A-NA	2.76	128.48	125.20
26	oE	202	PEB	OD-C4D-ND	-2.76	121.85	125.93
26	u1	201	PEB	OA-C1A-C2A	-2.76	123.98	126.17
28	MB	1001	CYC	CBC-CAC-C3C	-2.76	107.33	113.47
26	S2	201	PEB	C2B-C1B-NB	2.76	116.41	110.53
26	P1	202	PEB	CBC-CAC-C2C	-2.76	107.92	112.62
26	lA	201	PEB	CBC-CAC-C2C	-2.76	107.92	112.62
26	l6	202	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
28	OH	1001	CYC	CAA-C2A-C1A	2.76	129.88	125.01
26	W9	202	PEB	OD-C4D-C3D	-2.76	123.22	129.46
26	b7	202	PEB	CMD-C2D-C3D	2.76	133.95	130.06
26	M1	402	PEB	C2A-C1A-NA	2.76	110.65	108.27
26	jA	203	PEB	C3B-C4B-NB	2.76	114.06	110.05
26	ZB	203	PEB	C3B-C4B-NB	2.76	114.06	110.05
26	oE	201	PEB	OD-C4D-C3D	-2.76	123.22	129.46
26	VJ	202	PEB	OA-C1A-C2A	-2.76	123.98	126.17
26	K1	201	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
26	eG	203	PEB	C4B-C3B-C2B	-2.76	103.73	106.78
27	BA	302	PUB	OD-C4D-ND	-2.76	121.85	125.93
27	xE	306	PUB	OA-C1A-NA	-2.76	121.85	125.93
26	R9	203	PEB	OD-C4D-C3D	-2.76	123.22	129.46
26	q1	201	PEB	C3B-C4B-NB	2.76	114.06	110.05
26	v4	202	PEB	CAA-C3A-C2A	-2.76	107.38	114.26
26	U1	201	PEB	CHA-C1B-NB	-2.76	119.17	124.93
28	qH	1001	CYC	C1B-NB-C4B	-2.76	107.16	110.67
26	M4	402	PEB	CHC-C1D-ND	-2.75	110.75	113.95
26	N8	202	PEB	O2B-CGB-CBB	2.75	122.88	114.03
26	A7	302	PEB	OD-C4D-ND	-2.75	121.85	125.93
26	c2	201	PEB	CHA-C1B-NB	-2.75	119.17	124.93
26	H9	202	PEB	C3B-C4B-NB	2.75	114.06	110.05
26	gA	202	PEB	C3B-C4B-NB	2.75	114.06	110.05
26	A1	201	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	TJ	202	PEB	CAA-C3A-C2A	-2.75	107.38	114.26
27	NJ	201	PUB	CHA-C1B-C2B	-2.75	125.64	130.34
26	Q2	201	PEB	OA-C1A-C2A	-2.75	123.98	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	iI	203	PEB	OA-C1A-C2A	-2.75	123.98	126.17
26	H1	203	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	a1	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	N7	1002	PEB	OD-C4D-C3D	-2.75	123.22	129.46
28	LH	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
28	jH	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
26	QJ	202	PEB	CHC-C1D-ND	-2.75	110.75	113.95
26	JF	1002	PEB	CHC-C4C-C3C	-2.75	125.64	130.34
26	RF	201	PEB	CBA-CAA-C3A	-2.75	107.34	113.47
26	eA	201	PEB	CAB-C3B-C4B	2.75	129.88	125.01
26	qE	201	PEB	CMB-C2B-C1B	2.75	129.30	125.06
26	T1	202	PEB	C2A-C3A-C4A	-2.75	97.22	101.34
26	kA	201	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	N1	203	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	g2	203	PEB	CHC-C1D-ND	-2.75	110.75	113.95
26	e2	202	PEB	CHA-C1B-NB	-2.75	119.17	124.93
26	r1	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	UB	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
28	GH	1001	CYC	CHA-C1A-NA	-2.75	125.01	128.83
26	OA	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
26	OF	201	PEB	OD-C4D-ND	-2.75	121.85	125.93
26	k2	203	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	V8	201	PEB	OD-C4D-C3D	-2.75	123.22	129.46
28	AH	1001	CYC	C2C-C1C-NC	2.75	110.65	108.27
26	BC	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	s4	201	PEB	CHA-C1B-C2B	2.75	131.98	124.90
26	Q8	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	FA	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	VJ	202	PEB	CHA-C1B-NB	-2.75	119.18	124.93
26	e2	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
26	hB	202	PEB	OD-C4D-ND	-2.75	121.85	125.93
26	lG	201	PEB	OA-C1A-NA	2.75	128.28	124.94
26	XE	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	UB	203	PEB	CMB-C2B-C1B	2.75	129.30	125.06
26	lA	202	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
26	HE	202	PEB	OD-C4D-C3D	-2.75	123.22	129.46
26	T7	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	UD	201	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	V2	201	PEB	CHB-C4B-C3B	-2.75	118.96	125.32
26	WJ	201	PEB	C1C-CHB-C4B	2.75	132.10	128.81
26	gF	201	PEB	CHC-C1D-ND	-2.75	110.75	113.95
26	W4	202	PEB	CMA-C2A-C1A	-2.75	106.47	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	NA	201	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	B3	202	PEB	CHB-C4B-NB	-2.75	125.01	128.83
28	JF	1001	CYC	CHA-C1A-NA	-2.75	125.01	128.83
26	R1	203	PEB	CHA-C1B-NB	-2.75	119.18	124.93
26	O6	201	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	VI	201	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	UB	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	T3	202	PEB	CHA-C4A-NA	2.75	128.48	125.20
26	W4	201	PEB	CHA-C4A-NA	2.75	128.48	125.20
26	E8	203	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
26	DF	1002	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
26	UB	203	PEB	CBA-CAA-C3A	-2.75	107.34	113.47
26	VG	201	PEB	CAB-CBB-CGB	-2.75	107.68	113.60
26	CC	201	PEB	C1C-CHB-C4B	-2.75	125.52	128.81
26	hE	202	PEB	CMB-C2B-C1B	2.75	129.30	125.06
26	AB	304	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	kA	202	PEB	OA-C1A-C2A	-2.75	123.99	126.17
26	VI	201	PEB	CHB-C4B-C3B	-2.75	118.97	125.32
26	hF	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
28	C2	1001	CYC	C2A-C1A-NA	2.75	114.05	110.05
26	w1	202	PEB	C2A-C1A-NA	2.75	110.64	108.27
26	O1	202	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	l6	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	W3	201	PEB	CHA-C1B-NB	-2.75	119.18	124.93
26	L6	1002	PEB	CAC-CBC-CGC	-2.75	106.05	113.76
26	JG	202	PEB	CAB-C3B-C4B	2.75	129.87	125.01
26	F1	201	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
26	Y1	202	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	G3	201	PEB	OD-C4D-ND	-2.75	121.86	125.93
28	fH	1001	CYC	CHA-C1A-NA	-2.75	125.01	128.83
26	hG	202	PEB	CHC-C1D-ND	-2.75	110.75	113.95
28	nH	1001	CYC	C1B-CHB-C4A	2.75	134.80	128.08
26	F5	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	bB	201	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
26	SB	202	PEB	C4B-C3B-C2B	-2.75	103.74	106.78
26	x1	202	PEB	C2A-C1A-NA	2.75	110.64	108.27
26	NG	201	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	OE	203	PEB	CHC-C4C-C3C	-2.75	125.65	130.34
26	VI	202	PEB	CAB-C3B-C4B	2.75	129.87	125.01
26	U3	202	PEB	C3B-C4B-NB	2.75	114.05	110.05
26	NF	1002	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	M3	202	PEB	C4B-C3B-C2B	-2.75	103.74	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AA	301	PEB	CBC-CAC-C2C	-2.75	107.93	112.62
26	aI	203	PEB	OA-C1A-C2A	-2.75	123.99	126.17
26	d7	201	PEB	CHA-C1B-NB	-2.75	119.19	124.93
26	v4	201	PEB	CHC-C4C-C3C	-2.75	125.65	130.34
26	E1	202	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	R6	202	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	b7	202	PEB	OD-C4D-C3D	-2.75	123.23	129.46
26	eB	202	PEB	CMB-C2B-C1B	2.75	129.29	125.06
26	Z1	202	PEB	OD-C4D-ND	-2.75	121.86	125.93
26	G8	202	PEB	OD-C4D-ND	-2.75	121.86	125.93
26	f2	201	PEB	C2B-C1B-NB	2.75	116.39	110.53
26	GE	201	PEB	CAC-CBC-CGC	-2.75	106.06	113.76
26	k4	202	PEB	CHA-C1B-NB	-2.75	119.19	124.93
26	DJ	201	PEB	CHA-C1B-NB	-2.75	119.19	124.93
28	kH	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
26	PG	202	PEB	CAB-C3B-C4B	2.75	129.87	125.01
26	R3	202	PEB	C2B-C1B-NB	2.75	116.39	110.53
26	n4	202	PEB	OD-C4D-ND	-2.75	121.86	125.93
26	CC	203	PEB	CHC-C4C-C3C	-2.75	125.65	130.34
26	tE	201	PEB	CAA-C3A-C4A	-2.75	105.62	112.67
26	X3	201	PEB	CAC-CBC-CGC	-2.75	106.06	113.76
28	IH	1001	CYC	C4D-CHA-C1A	2.75	132.09	128.81
26	FE	201	PEB	CHA-C1B-NB	-2.75	119.19	124.93
26	bF	201	PEB	CHA-C1B-NB	-2.75	119.19	124.93
28	IH	1001	CYC	CHA-C1A-NA	-2.75	125.02	128.83
26	XJ	202	PEB	CMB-C2B-C1B	2.75	129.29	125.06
26	J9	203	PEB	C1B-C2B-C3B	-2.75	103.36	106.51
26	E9	201	PEB	CAB-CBB-CGB	-2.75	107.69	113.60
26	Y9	201	PEB	OD-C4D-C3D	-2.75	123.24	129.46
26	bF	203	PEB	OD-C4D-C3D	-2.75	123.24	129.46
26	JJ	203	PEB	C2A-C1A-NA	2.75	110.64	108.27
28	G6	1001	CYC	CHA-C1A-NA	-2.75	125.02	128.83
26	Y2	202	PEB	CAB-C3B-C4B	2.75	129.87	125.01
26	S9	202	PEB	CHC-C4C-C3C	-2.75	125.65	130.34
26	HA	202	PEB	O2B-CGB-CBB	2.75	122.85	114.03
26	Y1	201	PEB	CHA-C1B-NB	-2.75	119.19	124.93
26	P8	202	PEB	CHA-C1B-C2B	2.75	131.96	124.90
26	H1	203	PEB	OD-C4D-ND	-2.75	121.86	125.93
26	aI	202	PEB	OD-C4D-C3D	-2.75	123.24	129.46
26	HC	203	PEB	C1B-C2B-C3B	-2.75	103.36	106.51
26	hG	201	PEB	C1B-C2B-C3B	-2.75	103.36	106.51
26	oG	202	PEB	C1B-C2B-C3B	-2.75	103.36	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HF	1002	PEB	C3B-C4B-NB	2.74	114.04	110.05
26	c4	201	PEB	CHC-C4C-C3C	-2.74	125.66	130.34
26	VA	202	PEB	OD-C4D-C3D	-2.74	123.24	129.46
26	c7	202	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	Y3	304	PEB	CHA-C1B-C2B	2.74	131.96	124.90
26	lA	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
26	wG	302	PEB	C2A-C1A-NA	2.74	110.64	108.27
26	z4	202	PEB	CHB-C4B-C3B	2.74	131.66	125.32
26	W4	201	PEB	CMC-C3C-C2C	2.74	130.12	124.94
26	lF	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
26	nE	202	PEB	CMB-C2B-C1B	2.74	129.29	125.06
26	bI	201	PEB	C4B-NB-C1B	-2.74	101.34	106.51
26	m6	202	PEB	OD-C4D-ND	-2.74	121.86	125.93
27	A8	303	PUB	OA-C1A-NA	-2.74	121.86	125.93
27	AA	303	PUB	OA-C1A-NA	-2.74	121.86	125.93
28	UH	1001	CYC	C1B-NB-C4B	-2.74	107.17	110.67
28	K7	1001	CYC	C1A-C2A-C3A	-2.74	103.75	106.78
26	jF	203	PEB	CHC-C1D-ND	-2.74	110.76	113.95
26	AF	301	PEB	CHA-C4A-NA	2.74	128.47	125.20
26	xG	304	PEB	CHA-C4A-NA	2.74	128.47	125.20
26	c7	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
26	sE	203	PEB	OD-C4D-ND	-2.74	121.87	125.93
26	VG	201	PEB	OD-C4D-ND	-2.74	121.87	125.93
26	E8	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
26	BJ	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
26	N9	203	PEB	CHA-C1B-NB	-2.74	119.19	124.93
26	k2	203	PEB	CAB-CBB-CGB	2.74	119.51	113.60
26	N1	201	PEB	OA-C1A-NA	2.74	128.26	124.94
26	jB	201	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	QB	203	PEB	CMB-C2B-C1B	2.74	129.29	125.06
26	p1	201	PEB	OD-C4D-C3D	-2.74	123.25	129.46
26	eE	202	PEB	CMB-C2B-C3B	-2.74	118.67	126.12
26	bE	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
28	eH	1001	CYC	C1B-NB-C4B	-2.74	107.18	110.67
26	N6	201	PEB	C3B-C4B-NB	2.74	114.04	110.05
26	JA	202	PEB	C3B-C4B-NB	2.74	114.04	110.05
26	k8	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
26	X1	203	PEB	CHA-C1B-C2B	2.74	131.95	124.90
26	dE	202	PEB	CHB-C4B-C3B	-2.74	118.99	125.32
26	qE	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
26	P1	203	PEB	C1C-CHB-C4B	2.74	132.08	128.81
27	xE	305	PUB	C2C-C1C-NC	2.74	114.04	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	GB	1001	CYC	CHA-C1A-NA	-2.74	125.02	128.83
26	P8	201	PEB	CBC-CAC-C2C	-2.74	107.94	112.62
26	P6	202	PEB	CAC-C2C-C3C	2.74	135.12	127.25
26	i8	201	PEB	OD-C4D-C3D	-2.74	123.25	129.46
26	TI	202	PEB	OD-C4D-C3D	-2.74	123.25	129.46
26	W7	202	PEB	C3B-C4B-NB	2.74	114.04	110.05
26	xG	304	PEB	C3B-C4B-NB	2.74	114.04	110.05
26	OF	203	PEB	CHA-C1B-NB	-2.74	119.20	124.93
26	B9	203	PEB	CBC-CAC-C2C	2.74	117.30	112.62
26	A7	301	PEB	OD-C4D-C3D	-2.74	123.25	129.46
26	V6	201	PEB	CHC-C4C-C3C	-2.74	125.66	130.34
26	d7	202	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	sE	202	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	cA	203	PEB	OD-C4D-C3D	-2.74	123.25	129.46
26	sE	202	PEB	C2A-C1A-NA	2.74	110.64	108.27
26	T2	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
28	DI	1001	CYC	CHB-C1B-NB	-2.74	120.18	126.06
26	H1	203	PEB	C3B-C4B-NB	2.74	114.03	110.05
26	gA	201	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	F4	202	PEB	CHA-C1B-C2B	2.74	131.94	124.90
26	F2	1002	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
28	nH	1001	CYC	CAA-C2A-C1A	2.74	129.85	125.01
28	L7	1001	CYC	CAA-CBA-CGA	-2.74	107.71	113.60
27	xG	306	PUB	CHB-C1C-C2C	-2.74	118.99	125.32
26	K5	201	PEB	OD-C4D-C3D	-2.74	123.25	129.46
26	YF	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
26	LD	203	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	UE	201	PEB	CHA-C1B-NB	-2.74	119.20	124.93
26	b2	201	PEB	CBC-CAC-C2C	-2.74	107.95	112.62
26	e1	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	HD	203	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	P4	203	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
26	UF	201	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
26	Z2	201	PEB	OA-C1A-NA	2.74	128.26	124.94
26	S8	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
26	AI	301	PEB	CHA-C1B-NB	-2.74	119.21	124.93
26	LJ	201	PEB	CAB-C3B-C4B	2.74	129.85	125.01
26	G3	201	PEB	C2A-C1A-NA	2.74	110.63	108.27
26	fF	202	PEB	C2A-C1A-NA	2.74	110.63	108.27
26	I4	201	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	V9	202	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
26	l7	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TD	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	lB	201	PEB	OD-C4D-ND	-2.74	121.88	125.93
26	Z6	201	PEB	CMB-C2B-C1B	2.74	129.28	125.06
28	SH	1001	CYC	C1B-NB-C4B	-2.74	107.18	110.67
26	B5	203	PEB	C4B-C3B-C2B	-2.74	103.75	106.78
28	FF	1001	CYC	C1A-C2A-C3A	-2.74	103.75	106.78
26	IA	202	PEB	CHA-C1B-C2B	2.74	131.94	124.90
26	f7	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	PJ	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	fF	203	PEB	C2A-C1A-NA	2.74	110.63	108.27
26	F1	203	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
26	RB	202	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
26	VB	202	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
26	SG	202	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
28	M6	1001	CYC	CBC-CAC-C3C	-2.74	107.38	113.47
26	k4	201	PEB	CHC-C4C-C3C	-2.74	125.67	130.34
26	F8	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	JJ	203	PEB	CHA-C1B-NB	-2.74	119.21	124.93
26	W3	201	PEB	CMB-C2B-C1B	2.74	129.28	125.06
26	P7	201	PEB	CAB-CBB-CGB	-2.74	107.72	113.60
26	l4	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	hB	202	PEB	OD-C4D-C3D	-2.74	123.26	129.46
26	d4	203	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
26	RE	202	PEB	C1B-C2B-C3B	-2.74	103.37	106.51
26	ZG	202	PEB	CAB-C3B-C4B	2.74	129.85	125.01
26	J8	202	PEB	CHA-C1B-NB	-2.74	119.21	124.93
26	UB	203	PEB	OA-C1A-C2A	-2.74	124.00	126.17
28	M6	1001	CYC	CMB-C2B-C1B	2.74	127.58	124.17
26	l1	202	PEB	C2A-C1A-NA	2.74	110.63	108.27
26	f1	201	PEB	C2B-C1B-NB	2.74	116.37	110.53
26	K1	202	PEB	C2A-C3A-C4A	-2.74	97.24	101.34
26	QJ	202	PEB	CBC-CAC-C2C	-2.73	107.95	112.62
28	AH	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
28	SH	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
26	N4	201	PEB	OA-C1A-NA	2.73	128.25	124.94
26	jF	201	PEB	CAB-CBB-CGB	-2.73	107.72	113.60
26	iG	203	PEB	C3B-C4B-NB	2.73	114.03	110.05
26	kE	201	PEB	OD-C4D-ND	-2.73	121.88	125.93
26	YJ	201	PEB	OD-C4D-ND	-2.73	121.88	125.93
26	Z6	201	PEB	CHA-C1B-NB	-2.73	119.21	124.93
26	fA	202	PEB	CMB-C2B-C1B	2.73	129.28	125.06
26	QA	203	PEB	CHC-C4C-C3C	-2.73	125.67	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	iI	203	PEB	CBB-CAB-C3B	2.73	120.22	112.63
26	hE	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	qE	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	ZB	202	PEB	CAC-CBC-CGC	-2.73	106.09	113.76
26	k2	203	PEB	OD-C4D-ND	-2.73	121.88	125.93
26	tG	202	PEB	CAC-C2C-C3C	2.73	135.10	127.25
26	HD	201	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
26	a1	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	d1	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	ED	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	c6	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
26	sE	202	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
26	11	201	PEB	OD-C4D-ND	-2.73	121.88	125.93
26	p4	201	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
28	SH	1001	CYC	CAA-C2A-C1A	2.73	129.84	125.01
26	QF	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
26	ND	201	PEB	CHA-C4A-NA	2.73	128.45	125.20
26	h7	203	PEB	CHA-C1B-C2B	2.73	131.93	124.90
26	Y4	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	uG	203	PEB	C1C-CHB-C4B	-2.73	125.55	128.81
28	HB	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
26	N4	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	VF	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
27	21	403	PUB	CAB-CBB-CGB	-2.73	106.10	113.76
26	iB	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
26	eB	202	PEB	OD-C4D-ND	-2.73	121.88	125.93
26	FD	203	PEB	CAA-C3A-C4A	-2.73	105.66	112.67
26	t1	202	PEB	CMB-C2B-C1B	2.73	129.27	125.06
26	VJ	201	PEB	OA-C1A-C2A	-2.73	124.00	126.17
26	OE	202	PEB	CAB-C3B-C4B	2.73	129.84	125.01
26	XG	203	PEB	CAA-C3A-C4A	-2.73	105.66	112.67
26	P4	202	PEB	CBC-CAC-C2C	-2.73	107.96	112.62
26	hB	202	PEB	CBC-CAC-C2C	-2.73	107.96	112.62
26	h7	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
26	dE	201	PEB	CMB-C2B-C1B	2.73	129.27	125.06
26	CC	203	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	eE	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
26	Q1	202	PEB	CHA-C1B-NB	-2.73	119.22	124.93
26	eB	203	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
26	T9	202	PEB	OD-C4D-C3D	-2.73	123.27	129.46
28	IB	1001	CYC	CBC-CAC-C3C	-2.73	107.39	113.47
26	n4	202	PEB	CHC-C4C-C3C	-2.73	125.68	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c2	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
26	FG	202	PEB	CHA-C1B-NB	-2.73	119.22	124.93
26	G8	203	PEB	C3B-C4B-NB	2.73	114.02	110.05
28	sH	1001	CYC	CHA-C1A-NA	-2.73	125.04	128.83
26	J4	203	PEB	CHC-C4C-C3C	-2.73	125.68	130.34
26	C1	202	PEB	C2A-C1A-NA	2.73	110.63	108.27
26	k8	201	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
26	l1	202	PEB	OD-C4D-C3D	-2.73	123.28	129.46
26	h1	202	PEB	C4B-C3B-C2B	-2.73	103.76	106.78
26	OI	201	PEB	CHA-C4A-NA	2.73	128.45	125.20
26	mA	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
26	kG	201	PEB	CHC-C4C-C3C	-2.73	125.68	130.34
26	Y6	202	PEB	OD-C4D-C3D	-2.73	123.28	129.46
26	TD	201	PEB	CMA-C2A-C1A	-2.73	106.52	112.40
26	wE	303	PEB	CAB-C3B-C2B	2.73	132.96	127.88
26	Z8	202	PEB	CAB-CBB-CGB	2.73	119.47	113.60
26	K1	201	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
26	O4	202	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
26	R6	202	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
26	AA	301	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
26	I3	201	PEB	OD-C4D-ND	-2.73	121.89	125.93
26	O4	202	PEB	CAC-CBC-CGC	-2.73	106.11	113.76
26	A9	303	PEB	C2A-C1A-NA	2.73	110.62	108.27
28	dH	1001	CYC	C2C-C1C-NC	2.73	110.62	108.27
28	IH	1001	CYC	C1B-NB-C4B	-2.73	107.19	110.67
26	F1	201	PEB	CAB-CBB-CGB	-2.73	107.73	113.60
26	X4	202	PEB	CHC-C4C-C3C	-2.73	125.68	130.34
26	h7	203	PEB	OD-C4D-ND	-2.73	121.89	125.93
26	CA	201	PEB	CMA-C2A-C1A	-2.73	106.52	112.40
26	Q1	201	PEB	CHB-C4B-NB	-2.73	125.04	128.83
26	YE	201	PEB	C2A-C1A-NA	2.73	110.62	108.27
28	FF	1001	CYC	C2C-C1C-NC	2.73	110.62	108.27
26	t1	202	PEB	CHB-C4B-C3B	2.73	131.62	125.32
26	Z7	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
26	J8	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
26	EJ	202	PEB	CAC-CBC-CGC	-2.73	106.11	113.76
26	W1	202	PEB	CMA-C2A-C1A	-2.73	106.53	112.40
26	n4	201	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
26	t4	201	PEB	CHC-C4C-C3C	-2.73	125.69	130.34
26	MG	203	PEB	OD-C4D-C3D	-2.73	123.28	129.46
26	Z6	202	PEB	OA-C1A-C2A	-2.73	124.00	126.17
26	eE	202	PEB	OA-C1A-C2A	-2.73	124.00	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	VG	202	PEB	C4B-NB-C1B	-2.73	101.37	106.51
26	F8	202	PEB	CHC-C1D-ND	-2.73	110.78	113.95
28	OH	1001	CYC	C2B-C1B-NB	2.73	110.98	106.99
26	OD	201	PEB	CMA-C2A-C1A	-2.73	106.53	112.40
26	Q1	202	PEB	CAB-CBB-CGB	-2.73	107.74	113.60
26	y1	201	PEB	CHB-C4B-NB	-2.73	125.05	128.83
26	PJ	202	PEB	CHA-C1B-C2B	2.73	131.91	124.90
26	A3	202	PEB	C3B-C4B-NB	2.73	114.01	110.05
26	kE	202	PEB	C3B-C4B-NB	2.73	114.01	110.05
26	AA	302	PEB	CHA-C1B-C2B	2.73	131.91	124.90
26	K1	202	PEB	CHA-C1B-NB	-2.73	119.23	124.93
26	X4	201	PEB	CMB-C2B-C1B	2.73	129.26	125.06
26	hB	203	PEB	C1B-C2B-C3B	-2.73	103.38	106.51
26	FJ	201	PEB	C3B-C4B-NB	2.73	114.01	110.05
26	N3	203	PEB	OD-C4D-C3D	-2.72	123.29	129.46
26	h6	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
26	j7	201	PEB	CAB-CBB-CGB	-2.72	107.74	113.60
26	J5	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
26	QE	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
26	a7	202	PEB	C2A-C1A-NA	2.72	110.62	108.27
26	wE	302	PEB	C2A-C1A-NA	2.72	110.62	108.27
26	f6	203	PEB	CHA-C1B-NB	-2.72	119.23	124.93
26	L3	202	PEB	OD-C4D-ND	-2.72	121.89	125.93
26	C1	202	PEB	CHC-C4C-C3C	-2.72	125.69	130.34
26	dB	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
26	P8	202	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
28	EB	1001	CYC	C4A-C3A-C2A	-2.72	103.38	106.51
26	H2	1002	PEB	CMB-C2B-C1B	2.72	129.26	125.06
26	iF	201	PEB	CHB-C4B-NB	-2.72	125.05	128.83
26	GA	202	PEB	OD-C4D-ND	-2.72	121.89	125.93
26	NA	202	PEB	O2B-CGB-CBB	2.72	122.78	114.03
28	RH	1001	CYC	C2B-C1B-NB	2.72	110.97	106.99
26	YF	202	PEB	CHC-C4C-C3C	-2.72	125.69	130.34
26	d6	203	PEB	CAB-CBB-CGB	-2.72	107.74	113.60
26	FD	201	PEB	C3B-C4B-NB	2.72	114.01	110.05
26	l2	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
26	J5	202	PEB	OD-C4D-C3D	-2.72	123.29	129.46
26	l1	202	PEB	C2A-C1A-NA	2.72	110.62	108.27
26	G4	202	PEB	C2A-C1A-NA	2.72	110.62	108.27
26	J1	203	PEB	CAB-C3B-C4B	2.72	129.82	125.01
26	Z2	201	PEB	OD-C4D-C3D	-2.72	123.29	129.46
26	xE	303	PEB	OD-C4D-C3D	-2.72	123.29	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	eG	201	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
26	k6	202	PEB	CHA-C1B-NB	-2.72	119.24	124.93
26	Q8	202	PEB	CBC-CAC-C2C	-2.72	107.97	112.62
26	VE	202	PEB	CBC-CAC-C2C	2.72	117.27	112.62
28	nH	1001	CYC	C2B-C1B-NB	2.72	110.97	106.99
26	XD	203	PEB	OA-C1A-C2A	-2.72	124.01	126.17
26	R7	202	PEB	CHA-C1B-NB	-2.72	119.24	124.93
26	S2	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
26	v1	201	PEB	CHB-C4B-C3B	-2.72	119.03	125.32
26	S1	201	PEB	OD-C4D-C3D	-2.72	123.29	129.46
26	SB	203	PEB	C2A-C1A-NA	2.72	110.62	108.27
26	T9	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
26	WA	201	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
26	Q3	202	PEB	CHA-C1B-NB	-2.72	119.24	124.93
26	FD	203	PEB	CHA-C1B-NB	-2.72	119.24	124.93
26	X8	201	PEB	OD-C4D-ND	-2.72	121.90	125.93
26	AG	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
26	24	401	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
26	K9	202	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
26	uG	201	PEB	C1B-C2B-C3B	-2.72	103.38	106.51
26	j8	203	PEB	CAA-C3A-C4A	-2.72	105.69	112.67
26	GE	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
26	ZF	203	PEB	OA-C1A-C2A	-2.72	124.01	126.17
26	FG	202	PEB	CBC-CAC-C2C	2.72	117.26	112.62
26	f8	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	F9	202	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	m8	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
26	aI	201	PEB	CHB-C4B-NB	-2.72	125.05	128.83
28	HF	1001	CYC	CHA-C1A-NA	-2.72	125.05	128.83
28	UH	1001	CYC	C1B-C2B-C3B	-2.72	105.03	107.87
26	CA	201	PEB	CAB-CBB-CGB	-2.72	107.75	113.60
26	lE	202	PEB	OD-C4D-C3D	-2.72	123.30	129.46
26	AJ	303	PEB	OD-C4D-C3D	-2.72	123.30	129.46
26	OG	203	PEB	CHC-C4C-C3C	-2.72	125.70	130.34
26	U9	201	PEB	CHA-C4A-NA	2.72	128.44	125.20
26	iG	202	PEB	OA-C1A-C2A	-2.72	124.01	126.17
28	DB	1001	CYC	C2C-C1C-NC	2.72	110.62	108.27
26	P2	201	PEB	CBC-CAC-C2C	-2.72	107.98	112.62
26	BC	202	PEB	CHA-C1B-NB	-2.72	119.25	124.93
26	LD	201	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
26	oE	202	PEB	C4B-C3B-C2B	-2.72	103.77	106.78
28	B6	1002	CYC	CBD-CAD-C3D	2.72	117.26	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	JI	1001	CYC	CHB-C1B-NB	-2.72	120.22	126.06
26	i7	201	PEB	CHB-C4B-NB	-2.72	125.06	128.83
26	RI	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	j8	202	PEB	CMD-C2D-C3D	2.72	133.90	130.06
26	a7	201	PEB	CHC-C1D-ND	-2.72	110.79	113.95
26	kA	202	PEB	C2A-C1A-NA	2.72	110.62	108.27
26	X3	203	PEB	OA-C1A-C2A	-2.72	124.01	126.17
26	i1	202	PEB	CBC-CAC-C2C	-2.72	107.98	112.62
26	d2	202	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
26	G4	202	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
28	GH	1001	CYC	C1A-C2A-C3A	-2.72	103.78	106.78
26	c7	201	PEB	CMB-C2B-C1B	2.72	129.25	125.06
26	x1	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
26	21	405	PEB	OD-C4D-C3D	-2.72	123.30	129.46
26	TA	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
26	TJ	202	PEB	OD-C4D-C3D	-2.72	123.30	129.46
26	a4	201	PEB	C3B-C4B-NB	2.72	114.00	110.05
28	NF	1001	CYC	C2A-C1A-NA	2.72	114.00	110.05
26	VE	202	PEB	CAB-C3B-C4B	2.72	129.82	125.01
26	F9	202	PEB	CBC-CAC-C2C	-2.72	107.98	112.62
26	e6	203	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	T9	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
27	21	402	PUB	OA-C1A-NA	-2.72	121.91	125.93
26	LD	202	PEB	CHB-C4B-NB	-2.72	125.06	128.83
26	UB	203	PEB	C2A-C1A-NA	2.72	110.61	108.27
26	eI	203	PEB	OD-C4D-C3D	-2.72	123.31	129.46
26	F4	203	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	GJ	202	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	DE	203	PEB	CMB-C2B-C1B	2.72	129.25	125.06
26	NB	1002	PEB	CHC-C4C-C3C	-2.72	125.70	130.34
26	A3	201	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
26	O6	202	PEB	C4B-C3B-C2B	-2.72	103.78	106.78
28	PH	1001	CYC	C1B-C2B-C3B	-2.72	105.04	107.87
26	B9	201	PEB	OD-C4D-C3D	-2.72	123.31	129.46
26	Y6	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
26	cG	201	PEB	OD-C4D-ND	-2.72	121.91	125.93
28	uH	1001	CYC	C2B-C1B-NB	2.72	110.96	106.99
26	m7	201	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	PA	202	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	XJ	202	PEB	C1B-C2B-C3B	-2.72	103.39	106.51
26	i6	201	PEB	C3B-C4B-NB	2.72	114.00	110.05
26	pE	201	PEB	C3B-C4B-NB	2.72	114.00	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	eI	202	PEB	C3B-C4B-NB	2.72	114.00	110.05
26	N9	202	PEB	OD-C4D-C3D	-2.72	123.31	129.46
26	jG	201	PEB	OD-C4D-ND	-2.72	121.91	125.93
26	d2	201	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	IC	203	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	AI	305	PEB	OD-C4D-C3D	-2.71	123.31	129.46
26	DG	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	U7	201	PEB	C3B-C4B-NB	2.71	114.00	110.05
26	DA	202	PEB	O2B-CGB-CBB	2.71	122.75	114.03
26	LI	1002	PEB	CHB-C4B-NB	-2.71	125.06	128.83
26	CG	202	PEB	CHC-C1D-ND	-2.71	110.80	113.95
26	e8	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
26	i6	201	PEB	C2A-C1A-NA	2.71	110.61	108.27
26	i1	203	PEB	OD-C4D-ND	-2.71	121.91	125.93
26	I3	201	PEB	CMB-C2B-C1B	2.71	129.24	125.06
26	QE	202	PEB	CMB-C2B-C1B	2.71	129.24	125.06
26	AC	201	PEB	C3B-C4B-NB	2.71	114.00	110.05
26	JJ	201	PEB	CAB-C3B-C4B	2.71	129.81	125.01
26	E8	201	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	dE	202	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	a2	202	PEB	OD-C4D-C3D	-2.71	123.31	129.46
26	D3	203	PEB	CHB-C4B-NB	-2.71	125.06	128.83
26	bF	201	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	LJ	202	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	WJ	201	PEB	CMD-C2D-C3D	2.71	133.89	130.06
26	CA	203	PEB	CAA-C3A-C4A	-2.71	105.70	112.67
26	11	202	PEB	CMC-C3C-C2C	2.71	130.06	124.94
26	J8	202	PEB	C3B-C4B-NB	2.71	114.00	110.05
26	m4	203	PEB	CHB-C4B-NB	-2.71	125.06	128.83
26	U6	202	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	LF	1002	PEB	CMB-C2B-C1B	2.71	129.24	125.06
26	Q9	201	PEB	CHA-C1B-NB	-2.71	119.26	124.93
26	P1	203	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	K1	202	PEB	CBA-CAA-C3A	2.71	119.51	113.47
26	R3	201	PEB	CHC-C4C-C3C	-2.71	125.71	130.34
26	RE	201	PEB	C3B-C4B-NB	2.71	114.00	110.05
26	SG	202	PEB	C3B-C4B-NB	2.71	114.00	110.05
26	x4	202	PEB	OD-C4D-ND	-2.71	121.91	125.93
26	i1	203	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	CA	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
26	NF	1002	PEB	C2A-C1A-NA	2.71	110.61	108.27
26	U6	201	PEB	CHA-C1B-NB	-2.71	119.26	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	z4	201	PEB	CAA-C3A-C2A	-2.71	107.48	114.26
26	B4	202	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	C3	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	j6	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	Y7	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	T6	202	PEB	CAC-CBC-CGC	-2.71	106.16	113.76
26	Z6	202	PEB	CAC-CBC-CGC	-2.71	106.16	113.76
26	cA	201	PEB	OD-C4D-ND	-2.71	121.91	125.93
26	tG	202	PEB	OD-C4D-ND	-2.71	121.91	125.93
28	YH	1001	CYC	OC-C1C-C2C	-2.71	124.02	126.17
26	XD	201	PEB	CBC-CAC-C2C	2.71	117.25	112.62
26	dG	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	g2	201	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
26	XG	201	PEB	C3B-C4B-NB	2.71	113.99	110.05
26	T9	202	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	uG	203	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	PI	202	PEB	C1B-C2B-C3B	-2.71	103.39	106.51
26	P9	203	PEB	CHA-C1B-NB	-2.71	119.26	124.93
26	ED	202	PEB	CHA-C1B-NB	-2.71	119.26	124.93
26	q1	201	PEB	CHC-C1D-ND	-2.71	110.80	113.95
26	S8	202	PEB	C2A-C1A-NA	2.71	110.61	108.27
26	L8	202	PEB	OA-C1A-NA	2.71	128.22	124.94
26	vE	201	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
26	W1	201	PEB	CBC-CAC-C2C	2.71	117.25	112.62
26	VE	202	PEB	C4B-NB-C1B	-2.71	101.40	106.51
28	rH	1001	CYC	C1B-CHB-C4A	2.71	134.70	128.08
26	W7	201	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	H9	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	TD	203	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	AC	203	PEB	CMB-C2B-C1B	2.71	129.24	125.06
26	ZA	201	PEB	CMA-C2A-C1A	-2.71	106.56	112.40
26	SI	202	PEB	C4B-C3B-C2B	-2.71	103.78	106.78
28	hH	1001	CYC	C1B-NB-C4B	-2.71	107.22	110.67
26	N9	204	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
26	U1	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
26	N9	203	PEB	CHC-C4C-C3C	-2.71	125.72	130.34
26	g7	201	PEB	CMB-C2B-C1B	2.71	129.24	125.06
26	KA	201	PEB	OA-C1A-C2A	-2.71	124.02	126.17
26	IG	203	PEB	CBC-CAC-C2C	2.71	117.24	112.62
26	h7	202	PEB	OD-C4D-ND	-2.71	121.92	125.93
26	m6	201	PEB	CHA-C1B-NB	-2.71	119.27	124.93
26	K3	202	PEB	C4B-C3B-C2B	-2.71	103.78	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a4	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
28	DF	1003	CYC	C4A-C3A-C2A	-2.71	103.40	106.51
26	T1	203	PEB	CHC-C1D-ND	-2.71	110.80	113.95
26	V2	203	PEB	OD-C4D-C3D	-2.71	123.32	129.46
26	JD	203	PEB	CHA-C4A-NA	-2.71	121.98	125.20
26	R3	201	PEB	CHB-C4B-NB	-2.71	125.07	128.83
26	J1	201	PEB	CHC-C4C-C3C	-2.71	125.72	130.34
28	qH	1001	CYC	C2B-C1B-NB	2.71	110.95	106.99
26	K8	201	PEB	OA-C1A-C2A	-2.71	124.02	126.17
26	FA	201	PEB	CHA-C1B-C2B	2.71	131.86	124.90
26	LA	202	PEB	CAA-C3A-C2A	-2.71	107.50	114.26
26	OA	201	PEB	CMB-C2B-C1B	2.71	129.23	125.06
26	cB	202	PEB	CMB-C2B-C1B	2.71	129.23	125.06
26	AA	302	PEB	C3B-C4B-NB	2.71	113.99	110.05
26	mB	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
26	i2	201	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
26	j8	201	PEB	OA-C1A-C2A	-2.71	124.02	126.17
26	fB	202	PEB	OA-C1A-C2A	-2.71	124.02	126.17
26	b7	201	PEB	C3B-C4B-NB	2.71	113.99	110.05
26	J1	203	PEB	OD-C4D-C3D	-2.71	123.33	129.46
26	rG	202	PEB	OD-C4D-C3D	-2.71	123.33	129.46
26	I1	201	PEB	OD-C4D-ND	-2.71	121.92	125.93
26	N8	201	PEB	CAB-C3B-C4B	2.71	129.80	125.01
26	G5	202	PEB	C1B-C2B-C3B	-2.71	103.40	106.51
26	ZE	201	PEB	C4B-C3B-C2B	-2.71	103.79	106.78
26	ZE	201	PEB	CAB-CBB-CGB	-2.71	107.78	113.60
26	21	405	PEB	CHC-C4C-C3C	-2.71	125.72	130.34
26	FC	203	PEB	OD-C4D-C3D	-2.71	123.33	129.46
26	Z7	201	PEB	OD-C4D-ND	-2.71	121.92	125.93
26	lF	203	PEB	OD-C4D-ND	-2.71	121.92	125.93
26	MG	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	f8	202	PEB	CBC-CAC-C2C	-2.71	108.00	112.62
26	TE	202	PEB	CAA-C3A-C4A	-2.71	105.73	112.67
26	SG	203	PEB	CHA-C1B-NB	-2.71	119.27	124.93
26	i8	202	PEB	CAA-C3A-C2A	-2.71	107.50	114.26
26	W3	201	PEB	C3B-C4B-NB	2.71	113.98	110.05
26	BG	201	PEB	C3B-C4B-NB	2.71	113.98	110.05
26	i7	202	PEB	CHC-C4C-C3C	-2.71	125.72	130.34
26	iB	201	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
26	HJ	203	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
26	W6	203	PEB	CHA-C1B-NB	-2.70	119.28	124.93
26	RF	201	PEB	OD-C4D-C3D	-2.70	123.33	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B9	203	PEB	CMB-C2B-C1B	2.70	129.23	125.06
26	wE	303	PEB	CMB-C2B-C1B	2.70	129.23	125.06
26	ZA	202	PEB	CAB-CBB-CGB	2.70	119.42	113.60
26	EA	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
26	lG	202	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
26	bE	201	PEB	CMB-C2B-C1B	2.70	129.23	125.06
26	a8	203	PEB	CHA-C1B-NB	-2.70	119.28	124.93
26	x4	201	PEB	CHC-C4C-C3C	-2.70	125.72	130.34
26	b2	202	PEB	OD-C4D-C3D	-2.70	123.33	129.46
26	Y7	202	PEB	C3B-C4B-NB	2.70	113.98	110.05
26	BC	201	PEB	OD-C4D-ND	-2.70	121.92	125.93
26	jA	203	PEB	CAA-C3A-C4A	-2.70	105.73	112.67
26	g2	203	PEB	OD-C4D-C3D	-2.70	123.33	129.46
28	EF	1001	CYC	CMB-C2B-C1B	2.70	127.54	124.17
26	L1	203	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
26	G4	201	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
26	gF	201	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
26	VG	202	PEB	C1B-C2B-C3B	-2.70	103.40	106.51
26	m4	202	PEB	CHC-C1D-ND	-2.70	110.81	113.95
26	g7	201	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
26	K4	201	PEB	CHB-C4B-NB	-2.70	125.08	128.83
26	J9	203	PEB	C3B-C4B-NB	2.70	113.98	110.05
26	aI	202	PEB	C3B-C4B-NB	2.70	113.98	110.05
26	K5	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	c8	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	i1	203	PEB	CMB-C2B-C1B	2.70	129.23	125.06
26	D3	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	BA	301	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
26	TB	201	PEB	CHB-C4B-NB	-2.70	125.08	128.83
26	FA	202	PEB	CHC-C1D-ND	-2.70	110.81	113.95
26	OJ	201	PEB	OD-C4D-ND	-2.70	121.93	125.93
26	HJ	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	xG	303	PEB	C3B-C4B-NB	2.70	113.98	110.05
26	IG	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	fA	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
26	OD	202	PEB	CHC-C1D-ND	-2.70	110.81	113.95
26	O1	201	PEB	CHA-C4A-NA	2.70	128.42	125.20
26	mA	202	PEB	CHA-C1B-C2B	2.70	131.85	124.90
26	V7	201	PEB	CHB-C4B-NB	-2.70	125.08	128.83
26	II	201	PEB	CMA-C2A-C1A	-2.70	106.58	112.40
26	M1	403	PEB	OD-C4D-ND	-2.70	121.93	125.93
27	xE	305	PUB	OD-C4D-ND	-2.70	121.93	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	pH	1001	CYC	C4A-C3A-C2A	-2.70	103.41	106.51
26	eE	202	PEB	CHC-C1D-ND	-2.70	110.81	113.95
26	IG	202	PEB	CHB-C4B-C3B	-2.70	119.08	125.32
26	kG	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	GA	202	PEB	C3B-C4B-NB	2.70	113.98	110.05
26	IC	201	PEB	OD-C4D-ND	-2.70	121.93	125.93
26	VF	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
26	M1	401	PEB	CMB-C2B-C1B	2.70	129.22	125.06
26	F5	201	PEB	CAB-CBB-CGB	-2.70	107.79	113.60
26	LJ	201	PEB	CAB-CBB-CGB	-2.70	107.79	113.60
26	R2	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
26	YA	203	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
26	Q8	204	PEB	CHA-C1B-NB	-2.70	119.29	124.93
26	T1	201	PEB	C3D-C4D-ND	2.70	112.56	107.26
26	F1	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
26	II	202	PEB	CMB-C2B-C1B	2.70	129.22	125.06
26	iG	201	PEB	C2A-C1A-NA	2.70	110.60	108.27
26	aF	202	PEB	OD-C4D-C3D	-2.70	123.34	129.46
26	E1	201	PEB	CHC-C1D-ND	-2.70	110.81	113.95
26	OE	201	PEB	CHA-C4A-NA	2.70	128.41	125.20
26	IC	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
27	yG	302	PUB	OA-C1A-NA	-2.70	121.93	125.93
28	wH	1001	CYC	CHA-C1A-NA	-2.70	125.08	128.83
26	OJ	201	PEB	CMA-C2A-C1A	-2.70	106.59	112.40
26	gF	201	PEB	CHB-C4B-C3B	-2.70	119.09	125.32
26	O1	202	PEB	C3B-C4B-NB	2.70	113.97	110.05
26	H7	1002	PEB	C3B-C4B-NB	2.70	113.97	110.05
26	LC	203	PEB	CHA-C1B-NB	-2.70	119.29	124.93
28	IH	1001	CYC	C1B-CHB-C4A	2.70	134.67	128.08
26	g2	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
26	b2	201	PEB	C2A-C1A-NA	2.70	110.60	108.27
26	TB	202	PEB	C2A-C1A-NA	2.70	110.60	108.27
26	OI	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
26	c1	202	PEB	C4B-C3B-C2B	-2.70	103.80	106.78
26	LC	203	PEB	CAB-C3B-C4B	2.70	129.78	125.01
26	AB	304	PEB	OD-C4D-ND	-2.70	121.93	125.93
26	dB	201	PEB	CHC-C4C-C3C	-2.70	125.74	130.34
26	O1	202	PEB	CAC-CBC-CGC	-2.70	106.20	113.76
26	S8	202	PEB	CHA-C4A-NA	-2.70	122.00	125.20
26	x4	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
26	UB	202	PEB	CHC-C1D-ND	-2.70	110.81	113.95
26	r4	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	JF	1003	CYC	C2C-C1C-NC	2.70	110.60	108.27
28	D2	1001	CYC	CHB-C1B-NB	-2.70	120.27	126.06
28	kH	1001	CYC	C1B-NB-C4B	-2.70	107.23	110.67
26	GG	202	PEB	CMB-C2B-C3B	-2.70	118.80	126.12
26	V8	201	PEB	OD-C4D-ND	-2.70	121.94	125.93
26	Q6	201	PEB	CBC-CAC-C2C	2.70	117.22	112.62
26	RF	201	PEB	CHB-C4B-NB	-2.70	125.09	128.83
28	tH	1001	CYC	C1B-C2B-C3B	-2.70	105.06	107.87
26	SD	201	PEB	CAB-C3B-C4B	2.70	129.78	125.01
26	G4	202	PEB	CHA-C4A-NA	-2.70	122.00	125.20
26	F8	201	PEB	CHA-C1B-C2B	2.70	131.83	124.90
26	P2	202	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
26	RA	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
26	PI	201	PEB	CHC-C4C-C3C	-2.70	125.74	130.34
26	a2	203	PEB	C3B-C4B-NB	2.70	113.97	110.05
26	L9	202	PEB	C3B-C4B-NB	2.70	113.97	110.05
26	F3	203	PEB	CMB-C2B-C1B	2.70	129.22	125.06
26	N4	203	PEB	CMB-C2B-C1B	2.70	129.22	125.06
28	JF	1001	CYC	CHB-C1B-NB	-2.70	120.27	126.06
26	c2	203	PEB	OD-C4D-C3D	-2.70	123.35	129.46
26	k8	202	PEB	C2A-C1A-NA	2.70	110.60	108.27
26	SG	201	PEB	C2A-C1A-NA	2.70	110.60	108.27
28	IH	1001	CYC	C2B-C1B-NB	2.70	110.93	106.99
26	WA	201	PEB	CHA-C4A-NA	2.70	128.41	125.20
26	d7	203	PEB	C3B-C4B-NB	2.70	113.97	110.05
26	KC	202	PEB	C3B-C4B-NB	2.70	113.97	110.05
26	DJ	201	PEB	C1B-C2B-C3B	-2.70	103.41	106.51
28	uH	1001	CYC	CAA-C2A-C1A	2.70	129.78	125.01
26	VE	202	PEB	CHC-C4C-C3C	-2.70	125.74	130.34
26	m4	203	PEB	OD-C4D-C3D	-2.70	123.35	129.46
26	GD	202	PEB	OD-C4D-C3D	-2.70	123.35	129.46
26	kB	201	PEB	CBC-CAC-C2C	2.69	117.22	112.62
26	UB	201	PEB	CMB-C2B-C1B	2.69	129.21	125.06
26	a1	202	PEB	C3B-C4B-NB	2.69	113.97	110.05
26	E9	201	PEB	C2A-C1A-NA	2.69	110.60	108.27
26	NG	202	PEB	C1B-C2B-C3B	-2.69	103.41	106.51
26	A8	301	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	TB	202	PEB	CAC-CBC-CGC	-2.69	106.20	113.76
28	NB	1001	CYC	CAD-CBD-CGD	-2.69	106.20	113.76
26	c7	201	PEB	CHC-C4C-C3C	-2.69	125.74	130.34
26	L8	202	PEB	CAA-C3A-C2A	-2.69	107.53	114.26
26	vG	201	PEB	CAB-CBB-CGB	-2.69	107.81	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R8	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	M3	202	PEB	C3B-C4B-NB	2.69	113.97	110.05
26	b1	501	PEB	CHA-C4A-NA	2.69	128.41	125.20
26	eE	202	PEB	CHB-C4B-C3B	-2.69	119.10	125.32
26	h1	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	C9	202	PEB	C3B-C4B-NB	2.69	113.97	110.05
26	D9	202	PEB	C4B-C3B-C2B	-2.69	103.80	106.78
26	N1	201	PEB	C4B-NB-C1B	-2.69	101.44	106.51
26	o1	501	PEB	CHB-C4B-NB	-2.69	125.09	128.83
26	b2	201	PEB	CMA-C2A-C1A	-2.69	106.60	112.40
26	Y7	201	PEB	CHA-C1B-NB	-2.69	119.30	124.93
26	VA	201	PEB	CHA-C1B-C2B	2.69	131.82	124.90
26	aI	203	PEB	CBB-CAB-C3B	2.69	120.11	112.63
28	M6	1001	CYC	C4A-C3A-C2A	-2.69	103.42	106.51
26	QA	202	PEB	OD-C4D-ND	-2.69	121.94	125.93
26	TJ	202	PEB	OD-C4D-ND	-2.69	121.94	125.93
26	UA	203	PEB	OA-C1A-C2A	-2.69	124.03	126.17
26	m1	202	PEB	CAB-C3B-C4B	2.69	129.77	125.01
26	T3	201	PEB	CHA-C1B-C2B	2.69	131.82	124.90
26	OE	202	PEB	CHB-C4B-C3B	-2.69	119.10	125.32
26	C8	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
28	IH	1001	CYC	C1A-C2A-C3A	-2.69	103.80	106.78
26	NB	1002	PEB	C3B-C4B-NB	2.69	113.97	110.05
26	U9	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	l6	202	PEB	CAB-CBB-CGB	-2.69	107.81	113.60
26	J4	203	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	F7	1002	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	i2	203	PEB	CBB-CAB-C3B	2.69	120.11	112.63
26	cI	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	U7	203	PEB	OA-C1A-C2A	-2.69	124.03	126.17
26	dI	201	PEB	C4B-C3B-C2B	-2.69	103.80	106.78
26	U1	201	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	cF	201	PEB	C2A-C1A-NA	2.69	110.59	108.27
28	qH	1002	CYC	C2C-C1C-NC	2.69	110.59	108.27
26	P4	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	14	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	PE	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	OG	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	KA	202	PEB	CHA-C1B-NB	-2.69	119.30	124.93
26	mF	201	PEB	CHB-C4B-C3B	-2.69	119.10	125.32
26	W8	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
26	Q7	202	PEB	CAB-CBB-CGB	-2.69	107.81	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N9	203	PEB	CMB-C2B-C1B	2.69	129.21	125.06
26	jA	201	PEB	CMB-C2B-C1B	2.69	129.21	125.06
28	kH	1001	CYC	C4A-C3A-C2A	-2.69	103.42	106.51
26	W7	203	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	kE	202	PEB	OD-C4D-C3D	-2.69	123.36	129.46
26	jB	202	PEB	OD-C4D-ND	-2.69	121.94	125.93
26	FG	202	PEB	C2A-C1A-NA	2.69	110.59	108.27
26	n4	202	PEB	CAC-CBC-CGC	-2.69	106.22	113.76
26	fG	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	I1	201	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
26	qG	201	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
26	q4	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
26	W1	201	PEB	CHB-C4B-NB	-2.69	125.10	128.83
26	J8	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	m6	203	PEB	C3B-C4B-NB	2.69	113.96	110.05
26	cA	203	PEB	C2A-C1A-NA	2.69	110.59	108.27
26	wE	303	PEB	C2A-C1A-NA	2.69	110.59	108.27
26	D9	203	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	pG	201	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	AJ	305	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
26	EA	203	PEB	OD-C4D-ND	-2.69	121.95	125.93
26	Q4	202	PEB	CHA-C1B-NB	-2.69	119.31	124.93
26	dI	202	PEB	CHA-C1B-NB	-2.69	119.31	124.93
26	F3	202	PEB	CHC-C1D-ND	-2.69	110.83	113.95
26	gB	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	lE	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
28	VH	1001	CYC	C4A-C3A-C2A	-2.69	103.42	106.51
28	iH	1001	CYC	C1B-NB-C4B	-2.69	107.25	110.67
26	j1	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	lA	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	YD	303	PEB	C3B-C4B-NB	2.69	113.96	110.05
26	pE	201	PEB	CAB-CBB-CGB	-2.69	107.82	113.60
26	t4	202	PEB	CMB-C2B-C1B	2.69	129.20	125.06
26	jE	202	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	JA	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
28	uH	1001	CYC	C1B-NB-C4B	-2.69	107.25	110.67
26	WB	201	PEB	CMA-C2A-C1A	-2.69	106.61	112.40
26	A1	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
26	i1	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
26	JA	201	PEB	CHA-C4A-NA	2.69	128.40	125.20
26	V6	201	PEB	CAB-C3B-C4B	2.69	129.76	125.01
26	EJ	202	PEB	CHA-C1B-NB	-2.69	119.31	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M3	202	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	g8	201	PEB	C3B-C4B-NB	2.69	113.96	110.05
26	Y4	202	PEB	CAB-CBB-CGB	-2.69	107.82	113.60
26	d1	202	PEB	CAC-CBC-CGC	-2.69	106.23	113.76
26	bF	202	PEB	CHA-C4A-NA	-2.69	122.01	125.20
26	11	201	PEB	CHC-C4C-C3C	-2.69	125.75	130.34
26	iA	201	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	RI	203	PEB	OD-C4D-C3D	-2.69	123.37	129.46
26	L3	203	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
26	Z7	203	PEB	OD-C4D-ND	-2.69	121.95	125.93
26	m1	202	PEB	OD-C4D-C3D	-2.69	123.38	129.46
26	VF	203	PEB	OD-C4D-C3D	-2.69	123.38	129.46
26	s1	202	PEB	OD-C4D-ND	-2.69	121.95	125.93
26	mE	202	PEB	OD-C4D-C3D	-2.69	123.38	129.46
26	w4	203	PEB	C3B-C4B-NB	2.69	113.95	110.05
26	V8	201	PEB	CHA-C1B-C2B	2.69	131.81	124.90
27	Q8	201	PUB	CHA-C1B-C2B	-2.69	125.76	130.34
26	gF	201	PEB	C4B-C3B-C2B	-2.69	103.81	106.78
26	gF	201	PEB	CMB-C2B-C1B	2.69	129.20	125.06
26	NJ	204	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
26	l6	203	PEB	CBC-CAC-C2C	-2.68	108.04	112.62
26	dF	201	PEB	OD-C4D-C3D	-2.68	123.38	129.46
26	kG	203	PEB	CHB-C4B-C3B	-2.68	119.12	125.32
26	F4	203	PEB	OD-C4D-ND	-2.68	121.95	125.93
26	eE	201	PEB	OD-C4D-ND	-2.68	121.95	125.93
26	uG	203	PEB	CHA-C4A-NA	2.68	128.40	125.20
26	KE	202	PEB	CHC-C4C-C3C	-2.68	125.76	130.34
26	SD	201	PEB	C3B-C4B-NB	2.68	113.95	110.05
26	OF	201	PEB	CBC-CAC-C2C	-2.68	108.04	112.62
26	q4	201	PEB	CHC-C1D-ND	-2.68	110.83	113.95
26	mE	203	PEB	C4B-C3B-C2B	-2.68	103.81	106.78
26	F7	1002	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
26	LE	202	PEB	C4B-NB-C1B	-2.68	101.45	106.51
26	fA	201	PEB	CAB-C3B-C4B	2.68	129.76	125.01
26	VA	202	PEB	OD-C4D-ND	-2.68	121.95	125.93
26	Y4	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
26	ff	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
26	CG	203	PEB	CMB-C2B-C1B	2.68	129.20	125.06
26	iG	203	PEB	CMB-C2B-C1B	2.68	129.20	125.06
26	JE	202	PEB	CHA-C4A-NA	2.68	128.40	125.20
27	Y3	302	PUB	CAC-CBC-CGC	-2.68	107.83	113.60
26	cF	202	PEB	C4B-C3B-C2B	-2.68	103.81	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D8	201	PEB	CMB-C2B-C1B	2.68	129.20	125.06
26	D3	203	PEB	C2A-C1A-NA	2.68	110.59	108.27
26	TF	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
26	fI	202	PEB	OD-C4D-C3D	-2.68	123.38	129.46
27	AF	304	PUB	OD-C4D-ND	-2.68	121.96	125.93
28	qH	1001	CYC	C1B-CHB-C4A	2.68	134.63	128.08
26	a4	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
26	h8	203	PEB	CHA-C1B-NB	-2.68	119.32	124.93
26	w4	201	PEB	CAA-C3A-C2A	-2.68	107.56	114.26
26	D3	203	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
26	D4	203	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
26	h2	202	PEB	OD-C4D-C3D	-2.68	123.38	129.46
26	W8	201	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	WJ	202	PEB	CBC-CAC-C2C	-2.68	108.04	112.62
26	Q7	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
26	Y9	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
26	MD	202	PEB	CMB-C2B-C1B	2.68	129.19	125.06
26	O2	201	PEB	OD-C4D-C3D	-2.68	123.38	129.46
26	DF	1002	PEB	C3B-C4B-NB	2.68	113.95	110.05
26	KJ	201	PEB	C3B-C4B-NB	2.68	113.95	110.05
26	UI	201	PEB	C4B-C3B-C2B	-2.68	103.81	106.78
26	FE	202	PEB	CHA-C1B-NB	-2.68	119.33	124.93
26	H8	201	PEB	CBC-CAC-C2C	-2.68	108.05	112.62
26	hF	201	PEB	CBC-CAC-C2C	2.68	117.19	112.62
26	FC	202	PEB	C2A-C1A-NA	2.68	110.58	108.27
28	IH	1001	CYC	C2C-C1C-NC	2.68	110.58	108.27
26	LI	1002	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
26	S2	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
26	DJ	202	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
26	ZB	201	PEB	CMB-C2B-C1B	2.68	129.19	125.06
26	k1	201	PEB	CMA-C2A-C1A	-2.68	106.62	112.40
28	OH	1001	CYC	C4D-CHA-C1A	2.68	132.01	128.81
26	C4	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
26	f8	201	PEB	OA-C1A-C2A	-2.68	124.04	126.17
26	NE	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
26	kB	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
26	j2	201	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
28	E2	1001	CYC	C1A-C2A-C3A	-2.68	103.82	106.78
26	14	201	PEB	C3B-C4B-NB	2.68	113.95	110.05
26	FD	202	PEB	C3B-C4B-NB	2.68	113.95	110.05
26	O2	201	PEB	CHA-C4A-NA	2.68	128.39	125.20
26	XG	201	PEB	CAB-C3B-C4B	2.68	129.75	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R1	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
26	eG	203	PEB	CHC-C4C-C3C	-2.68	125.77	130.34
26	AJ	303	PEB	CMA-C2A-C1A	-2.68	106.63	112.40
26	f2	202	PEB	CHA-C1B-NB	-2.68	119.33	124.93
26	V6	202	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
26	i7	201	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
26	f6	201	PEB	OD-C4D-C3D	-2.68	123.39	129.46
26	DD	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
26	PI	201	PEB	CBC-CAC-C2C	-2.68	108.05	112.62
28	LF	1001	CYC	O2D-CGD-CBD	2.68	122.64	114.03
26	OF	201	PEB	C3B-C4B-NB	2.68	113.94	110.05
26	A8	302	PEB	CHA-C1B-C2B	2.68	131.79	124.90
26	OA	202	PEB	OD-C4D-ND	-2.68	121.96	125.93
26	W8	201	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
26	eE	201	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
26	H5	201	PEB	OD-C4D-C3D	-2.68	123.39	129.46
26	PJ	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
26	ZB	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
26	X3	203	PEB	C3B-C4B-NB	2.68	113.94	110.05
26	UJ	202	PEB	C3B-C4B-NB	2.68	113.94	110.05
26	D9	203	PEB	CBC-CAC-C2C	-2.68	108.05	112.62
26	BJ	202	PEB	CMB-C2B-C1B	2.68	129.19	125.06
26	q1	201	PEB	CAB-CBB-CGB	-2.68	107.84	113.60
27	yE	302	PUB	CAD-C3D-C4D	2.68	125.61	121.38
27	A6	302	PUB	CMD-C2D-C3D	2.68	131.78	127.77
26	oE	201	PEB	OD-C4D-ND	-2.68	121.97	125.93
26	BJ	201	PEB	CHC-C1D-ND	-2.68	110.84	113.95
26	24	404	PEB	OD-C4D-C3D	-2.68	123.40	129.46
26	g4	201	PEB	C1B-C2B-C3B	-2.68	103.44	106.51
26	S1	201	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	rG	201	PEB	CAB-CBB-CGB	-2.68	107.84	113.60
26	NJ	203	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
26	vE	202	PEB	CHB-C4B-C3B	-2.68	119.14	125.32
26	L4	203	PEB	OD-C4D-C3D	-2.68	123.40	129.46
26	b7	202	PEB	OD-C4D-ND	-2.68	121.97	125.93
27	A6	302	PUB	CHA-C4A-NA	-2.68	110.84	113.95
26	dB	203	PEB	CAB-CBB-CGB	-2.68	107.84	113.60
26	R1	201	PEB	CHB-C4B-C3B	-2.68	119.14	125.32
26	A1	201	PEB	CAB-C3B-C4B	2.68	129.74	125.01
26	14	201	PEB	CAB-C3B-C4B	2.68	129.74	125.01
26	21	405	PEB	C3B-C4B-NB	2.68	113.94	110.05
26	Y1	201	PEB	C1C-CHB-C4B	2.68	132.00	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C1	201	PEB	C1B-C2B-C3B	-2.68	103.44	106.51
26	JD	202	PEB	CMB-C2B-C1B	2.68	129.18	125.06
26	N8	201	PEB	OD-C4D-ND	-2.68	121.97	125.93
26	e8	202	PEB	OA-C1A-C2A	-2.68	124.05	126.17
26	Y1	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	l1	201	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	g4	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	V9	203	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	l7	202	PEB	CHA-C1B-NB	-2.67	119.34	124.93
28	mH	1001	CYC	C4D-CHA-C1A	2.67	132.00	128.81
26	FD	203	PEB	C4B-C3B-C2B	-2.67	103.82	106.78
26	gF	202	PEB	C4B-C3B-C2B	-2.67	103.82	106.78
26	ZI	201	PEB	OD-C4D-C3D	-2.67	123.40	129.46
26	RD	202	PEB	C2B-C1B-NB	2.67	116.24	110.53
26	l6	203	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	CC	203	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	HJ	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	KE	203	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
26	WG	203	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
26	a6	202	PEB	CHC-C1D-ND	-2.67	110.84	113.95
26	b4	501	PEB	OD-C4D-ND	-2.67	121.97	125.93
26	K8	201	PEB	OD-C4D-ND	-2.67	121.97	125.93
26	AB	301	PEB	OD-C4D-ND	-2.67	121.97	125.93
26	gI	203	PEB	C2A-C1A-NA	2.67	110.58	108.27
26	D2	1002	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
26	U6	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	T2	202	PEB	OD-C4D-C3D	-2.67	123.40	129.46
26	bE	202	PEB	CMC-C3C-C2C	-2.67	119.90	124.94
26	V2	203	PEB	OD-C4D-ND	-2.67	121.97	125.93
26	H4	202	PEB	CAA-C3A-C4A	-2.67	105.81	112.67
26	I4	201	PEB	CHB-C4B-NB	-2.67	125.12	128.83
26	A5	202	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	J9	203	PEB	C2A-C1A-NA	2.67	110.58	108.27
26	W7	202	PEB	OA-C1A-C2A	-2.67	124.05	126.17
26	OI	201	PEB	OA-C1A-C2A	-2.67	124.05	126.17
26	G8	203	PEB	CHA-C1B-NB	-2.67	119.34	124.93
26	wE	301	PEB	CBC-CAC-C2C	-2.67	108.06	112.62
26	j6	201	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	YE	203	PEB	C3B-C4B-NB	2.67	113.94	110.05
26	s4	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	PB	201	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	Q2	201	PEB	CHA-C4A-NA	2.67	128.38	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N4	201	PEB	CHA-C4A-NA	2.67	128.38	125.20
26	24	405	PEB	CHA-C1B-C2B	2.67	131.77	124.90
26	N1	203	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	g8	202	PEB	CMB-C2B-C1B	2.67	129.18	125.06
26	BD	201	PEB	CMB-C2B-C1B	2.67	129.18	125.06
27	BA	302	PUB	C2C-C1C-NC	2.67	113.94	110.05
26	l8	202	PEB	CAA-C3A-C2A	-2.67	107.58	114.26
26	JF	1002	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	M1	402	PEB	OD-C4D-ND	-2.67	121.97	125.93
28	OH	1001	CYC	C1B-CHB-C4A	2.67	134.61	128.08
26	eE	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	bF	201	PEB	C3B-C4B-NB	2.67	113.93	110.05
26	N4	201	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
26	jE	201	PEB	CHC-C1D-ND	-2.67	110.85	113.95
26	G1	202	PEB	CAB-C3B-C4B	2.67	129.73	125.01
26	F3	201	PEB	CMB-C2B-C1B	2.67	129.18	125.06
26	Q4	201	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
26	JJ	201	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	K5	201	PEB	OD-C4D-ND	-2.67	121.97	125.93
26	R2	203	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	LJ	202	PEB	C3B-C4B-NB	2.67	113.93	110.05
26	r1	201	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
26	rG	201	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
26	P2	201	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
26	UF	201	PEB	CHB-C4B-NB	-2.67	125.12	128.83
26	Y7	202	PEB	C2A-C1A-NA	2.67	110.57	108.27
26	W8	201	PEB	OD-C4D-ND	-2.67	121.98	125.93
28	FB	1001	CYC	CHB-C1B-NB	-2.67	120.33	126.06
26	YG	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	ZI	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	f2	202	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
26	I1	202	PEB	OD-C4D-C3D	-2.67	123.41	129.46
26	EE	201	PEB	CHB-C4B-NB	-2.67	125.12	128.83
26	J1	203	PEB	CHC-C4C-C3C	-2.67	125.79	130.34
26	SG	203	PEB	CHC-C4C-C3C	-2.67	125.79	130.34
26	H4	203	PEB	OD-C4D-C3D	-2.67	123.42	129.46
26	bI	202	PEB	OD-C4D-C3D	-2.67	123.42	129.46
26	GJ	202	PEB	OD-C4D-C3D	-2.67	123.42	129.46
26	Y4	201	PEB	CHA-C1B-NB	-2.67	119.35	124.93
26	H4	203	PEB	C2A-C1A-NA	2.67	110.57	108.27
26	y4	202	PEB	C2A-C1A-NA	2.67	110.57	108.27
27	yE	302	PUB	OA-C1A-NA	-2.67	121.98	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J8	201	PEB	OD-C4D-C3D	-2.67	123.42	129.46
27	21	402	PUB	C2C-C1C-NC	2.67	113.93	110.05
26	VE	202	PEB	CAC-CBC-CGC	-2.67	106.28	113.76
26	SE	203	PEB	CHB-C4B-NB	-2.67	125.13	128.83
26	G1	202	PEB	CHA-C4A-NA	-2.67	122.03	125.20
26	f2	201	PEB	C2A-C1A-NA	2.67	110.57	108.27
28	HI	1001	CYC	C4A-C3A-C2A	-2.67	103.45	106.51
26	iI	201	PEB	OD-C4D-ND	-2.67	121.98	125.93
26	Q6	202	PEB	OA-C1A-C2A	-2.67	124.05	126.17
26	J1	203	PEB	CMB-C2B-C1B	2.67	129.17	125.06
26	TF	201	PEB	CBC-CAC-C2C	-2.67	108.07	112.62
26	ME	203	PEB	C4B-C3B-C2B	-2.67	103.83	106.78
26	H5	201	PEB	CHA-C1B-C2B	2.67	131.76	124.90
28	NI	1001	CYC	CAA-C2A-C3A	2.67	132.84	127.88
26	A7	302	PEB	OD-C4D-C3D	-2.67	123.42	129.46
26	G8	203	PEB	OD-C4D-ND	-2.67	121.98	125.93
26	W9	202	PEB	OD-C4D-ND	-2.67	121.98	125.93
26	ZA	201	PEB	CMD-C2D-C3D	2.67	133.82	130.06
26	VG	201	PEB	OD-C4D-C3D	-2.67	123.42	129.46
26	YG	201	PEB	OD-C4D-C3D	-2.67	123.42	129.46
28	tH	1001	CYC	C4D-CHA-C1A	2.67	131.99	128.81
26	IC	203	PEB	C3B-C4B-NB	2.67	113.93	110.05
26	Y7	202	PEB	OD-C4D-ND	-2.67	121.98	125.93
26	kG	203	PEB	OD-C4D-ND	-2.67	121.98	125.93
26	mB	203	PEB	CAB-CBB-CGB	-2.66	107.87	113.60
26	AD	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
28	J7	1001	CYC	CAC-C3C-C4C	-2.66	105.83	112.67
26	Q8	204	PEB	CMD-C2D-C3D	2.66	133.82	130.06
26	cE	201	PEB	CHC-C4C-C3C	-2.66	125.79	130.34
26	O2	202	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	ZF	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
26	K1	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
26	B8	301	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
26	J5	202	PEB	CHC-C4C-C3C	2.66	134.88	130.34
26	h7	201	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	FJ	202	PEB	CHA-C1B-C2B	2.66	131.75	124.90
26	l7	201	PEB	CMB-C2B-C1B	2.66	129.17	125.06
26	P9	202	PEB	C4B-C3B-C2B	-2.66	103.83	106.78
26	nE	201	PEB	C4B-C3B-C2B	-2.66	103.83	106.78
26	j6	202	PEB	C2A-C1A-NA	2.66	110.57	108.27
26	UD	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	kG	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d8	201	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	dG	202	PEB	OD-C4D-ND	-2.66	121.98	125.93
26	JI	1002	PEB	OD-C4D-ND	-2.66	121.98	125.93
26	gE	202	PEB	CMB-C2B-C1B	2.66	129.16	125.06
26	c1	201	PEB	CHB-C4B-C3B	-2.66	119.17	125.32
26	Q2	201	PEB	CMD-C2D-C3D	2.66	133.82	130.06
26	S2	202	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	Z6	202	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	jI	201	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	S1	202	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	VJ	201	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	WA	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
26	aB	202	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	YF	202	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	ZA	202	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
28	VH	1001	CYC	C2B-C1B-NB	2.66	110.89	106.99
26	L5	203	PEB	CAB-C3B-C4B	2.66	129.72	125.01
26	PF	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	LJ	203	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	V8	202	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	S3	202	PEB	CHA-C1B-NB	-2.66	119.36	124.93
26	R1	203	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	M4	401	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	JA	201	PEB	CAB-CBB-CGB	-2.66	107.88	113.60
26	YB	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	E3	201	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	TI	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
26	N4	203	PEB	CHA-C1B-NB	-2.66	119.37	124.93
26	cG	201	PEB	OA-C1A-C2A	-2.66	124.06	126.17
26	F8	201	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	OE	202	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
26	r4	201	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	CC	203	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	f8	201	PEB	C2A-C1A-NA	2.66	110.57	108.27
26	i1	203	PEB	OD-C4D-C3D	-2.66	123.43	129.46
28	YH	1004	CYC	C2B-C1B-NB	2.66	110.88	106.99
26	m1	203	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	C5	204	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	PG	202	PEB	CHC-C4C-C3C	2.66	134.87	130.34
26	ME	201	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	MD	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	S8	202	PEB	OD-C4D-C3D	-2.66	123.43	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LG	202	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
28	PH	1001	CYC	C1A-C2A-C3A	-2.66	103.84	106.78
26	SG	202	PEB	CBB-CAB-C3B	-2.66	105.24	112.63
26	D4	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
26	G5	202	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	X9	203	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	JA	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	VE	201	PEB	OD-C4D-C3D	-2.66	123.43	129.46
26	NB	1002	PEB	CAC-CBC-CGC	-2.66	106.30	113.76
28	mH	1001	CYC	C1B-CHB-C4A	2.66	134.58	128.08
26	e2	203	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	H4	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	KD	201	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	sE	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	w4	203	PEB	CMB-C2B-C1B	2.66	129.16	125.06
26	R7	202	PEB	CMB-C2B-C1B	2.66	129.16	125.06
28	NH	1001	CYC	C1B-NB-C4B	-2.66	107.28	110.67
26	p1	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	14	201	PEB	O2B-CGB-CBB	2.66	122.57	114.03
26	W1	201	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
26	y4	203	PEB	CAB-C3B-C4B	2.66	129.71	125.01
26	KA	202	PEB	CBA-CAA-C3A	-2.66	107.55	113.47
26	SB	202	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
26	BD	203	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
26	l8	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	KC	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
27	wG	304	PUB	OA-C1A-NA	-2.66	121.99	125.93
26	R6	202	PEB	C3B-C4B-NB	2.66	113.92	110.05
26	N4	202	PEB	CBA-CAA-C3A	-2.66	107.55	113.47
26	nE	201	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	A8	301	PEB	CBC-CAC-C2C	-2.66	108.08	112.62
26	P1	201	PEB	CMB-C2B-C1B	2.66	129.16	125.06
26	v1	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	V1	202	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	J2	1002	PEB	OD-C4D-ND	-2.66	121.99	125.93
26	TI	203	PEB	C3B-C4B-NB	2.66	113.91	110.05
28	CF	1001	CYC	C2A-C1A-NA	2.66	113.91	110.05
26	A4	202	PEB	CHA-C4A-NA	-2.66	122.05	125.20
26	TA	201	PEB	CMB-C2B-C1B	2.66	129.16	125.06
26	bI	201	PEB	C2B-C1B-NB	2.66	116.20	110.53
26	RD	203	PEB	C2A-C1A-NA	2.66	110.56	108.27
26	XG	202	PEB	CHA-C1B-C2B	2.66	131.73	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OE	201	PEB	C3B-C4B-NB	2.66	113.91	110.05
26	eG	201	PEB	C3B-C4B-NB	2.66	113.91	110.05
28	NB	1001	CYC	C4A-C3A-C2A	-2.66	103.46	106.51
26	kG	203	PEB	OA-C1A-C2A	-2.66	124.06	126.17
26	tG	201	PEB	C4B-C3B-C2B	-2.66	103.84	106.78
26	BC	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	IC	203	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	iF	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	ZB	202	PEB	CHA-C1B-C2B	2.66	131.73	124.90
26	d2	201	PEB	C2B-C1B-NB	2.66	116.20	110.53
26	DG	202	PEB	CMB-C2B-C1B	2.66	129.15	125.06
26	HI	1002	PEB	CMB-C2B-C1B	2.66	129.15	125.06
26	JC	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	I5	203	PEB	CAC-CBC-CGC	-2.66	106.31	113.76
26	J1	203	PEB	OD-C4D-ND	-2.66	122.00	125.93
26	h2	202	PEB	OD-C4D-ND	-2.66	122.00	125.93
26	uG	202	PEB	OD-C4D-ND	-2.66	122.00	125.93
26	GC	202	PEB	C3B-C4B-NB	2.66	113.91	110.05
26	L5	201	PEB	CHA-C1B-C2B	2.66	131.73	124.90
26	S4	202	PEB	C1B-C2B-C3B	-2.66	103.46	106.51
26	j8	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
26	bE	202	PEB	OD-C4D-C3D	-2.66	123.44	129.46
28	JH	1001	CYC	C1B-NB-C4B	-2.66	107.29	110.67
26	oG	201	PEB	CMB-C2B-C1B	2.66	129.15	125.06
26	K1	201	PEB	CMA-C2A-C1A	-2.65	106.68	112.40
26	T2	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
26	h8	201	PEB	C3B-C4B-NB	2.65	113.91	110.05
26	FA	201	PEB	C3B-C4B-NB	2.65	113.91	110.05
26	A1	202	PEB	CHB-C4B-C3B	-2.65	119.19	125.32
26	B4	202	PEB	CAB-C3B-C4B	2.65	129.71	125.01
26	R8	202	PEB	C4B-C3B-C2B	-2.65	103.84	106.78
26	a2	203	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	m8	202	PEB	CBB-CAB-C3B	2.65	120.00	112.63
26	LC	203	PEB	CBB-CAB-C3B	-2.65	105.25	112.63
26	sE	202	PEB	C3B-C4B-NB	2.65	113.91	110.05
26	a2	201	PEB	CHB-C4B-NB	-2.65	125.14	128.83
26	f4	201	PEB	CHC-C4C-C3C	-2.65	125.81	130.34
26	Q7	202	PEB	CHA-C1B-C2B	2.65	131.72	124.90
26	W1	201	PEB	O2B-CGB-CBB	2.65	122.56	114.03
26	lB	203	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	H5	202	PEB	CMB-C2B-C1B	2.65	129.15	125.06
26	FF	1002	PEB	C1B-C2B-C3B	-2.65	103.46	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	hF	202	PEB	OD-C4D-ND	-2.65	122.00	125.93
26	P8	201	PEB	CAB-C3B-C4B	2.65	129.70	125.01
26	WJ	201	PEB	C3B-C4B-NB	2.65	113.91	110.05
26	rE	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	s4	202	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
26	e2	203	PEB	CMB-C2B-C1B	2.65	129.15	125.06
26	F4	202	PEB	CMB-C2B-C1B	2.65	129.15	125.06
26	J9	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
27	xG	305	PUB	OD-C4D-ND	-2.65	122.00	125.93
26	c7	202	PEB	CHA-C1B-C2B	2.65	131.72	124.90
26	nE	201	PEB	C3B-C4B-NB	2.65	113.91	110.05
28	D7	1001	CYC	CHB-C4A-NA	-2.65	119.38	124.93
26	Z6	203	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
26	R1	201	PEB	OA-C1A-C2A	-2.65	124.06	126.17
26	a4	202	PEB	CHC-C1D-ND	-2.65	110.87	113.95
26	O9	202	PEB	CHC-C1D-ND	-2.65	110.87	113.95
26	jA	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
26	O6	203	PEB	CMB-C2B-C1B	2.65	129.15	125.06
26	PF	201	PEB	CHB-C4B-NB	-2.65	125.15	128.83
26	D2	1002	PEB	CAB-C3B-C4B	2.65	129.70	125.01
26	BG	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
26	f6	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	LB	1002	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	YB	201	PEB	CMA-C2A-C1A	-2.65	106.69	112.40
26	gG	201	PEB	CHC-C4C-C3C	-2.65	125.81	130.34
26	D2	1002	PEB	CHA-C1B-NB	-2.65	119.39	124.93
26	QG	202	PEB	CMB-C2B-C1B	2.65	129.15	125.06
26	B4	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	Y8	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
28	wH	1001	CYC	C1B-NB-C4B	-2.65	107.29	110.67
28	UH	1001	CYC	C2B-C1B-NB	2.65	110.87	106.99
26	FD	203	PEB	OA-C1A-C2A	-2.65	124.06	126.17
26	h4	203	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	J8	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	HG	202	PEB	OD-C4D-C3D	-2.65	123.45	129.46
26	GC	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
26	lE	202	PEB	CMB-C2B-C1B	2.65	129.15	125.06
26	DD	203	PEB	CHB-C4B-NB	-2.65	125.15	128.83
26	CG	202	PEB	CBB-CAB-C3B	-2.65	105.26	112.63
28	I2	1001	CYC	CBC-CAC-C3C	-2.65	107.57	113.47
26	I8	202	PEB	CMA-C2A-C1A	-2.65	106.69	112.40
26	K5	203	PEB	CAC-CBC-CGC	-2.65	106.33	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aB	201	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
28	KH	1001	CYC	C4A-C3A-C2A	-2.65	103.47	106.51
26	Y3	303	PEB	CHA-C1B-C2B	2.65	131.72	124.90
26	M4	403	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	AF	301	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	g4	201	PEB	CHB-C4B-NB	-2.65	125.15	128.83
26	I8	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
26	aE	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	eA	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
26	T8	202	PEB	CMA-C2A-C1A	-2.65	106.69	112.40
26	HE	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
26	YI	201	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
26	TA	202	PEB	CAB-CBB-CGB	2.65	119.30	113.60
26	H2	1002	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	Z7	201	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
26	eG	201	PEB	OD-C4D-ND	-2.65	122.01	125.93
26	GC	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	JD	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	ZF	203	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
28	EH	1001	CYC	C4A-C3A-C2A	-2.65	103.47	106.51
26	A6	304	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	KC	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
26	d4	203	PEB	CHC-C1D-ND	-2.65	110.87	113.95
26	eI	202	PEB	CHC-C1D-ND	-2.65	110.87	113.95
26	A1	202	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
28	F6	1001	CYC	CHB-C1B-NB	-2.65	120.37	126.06
26	v1	201	PEB	C3B-C4B-NB	2.65	113.90	110.05
26	F3	201	PEB	C3B-C4B-NB	2.65	113.90	110.05
26	rE	201	PEB	C3B-C4B-NB	2.65	113.90	110.05
26	PE	202	PEB	CAB-C3B-C4B	2.65	129.69	125.01
26	IE	201	PEB	CAC-CBC-CGC	2.65	121.18	113.76
26	W4	201	PEB	O2B-CGB-CBB	2.65	122.54	114.03
27	AA	303	PUB	CHA-C1B-C2B	-2.65	125.82	130.34
26	j4	201	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
26	M1	401	PEB	C3B-C4B-NB	2.65	113.90	110.05
26	AC	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
26	c4	202	PEB	CMC-C3C-C2C	2.65	129.93	124.94
26	O3	202	PEB	C4B-C3B-C2B	-2.65	103.85	106.78
28	FI	1001	CYC	C1A-C2A-C3A	-2.65	103.85	106.78
26	JJ	201	PEB	C2A-C1A-NA	2.65	110.56	108.27
26	T2	201	PEB	CHC-C4C-C3C	-2.65	125.82	130.34
26	f8	203	PEB	CAA-C3A-C4A	-2.65	105.88	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	gE	202	PEB	OD-C4D-ND	-2.65	122.01	125.93
26	w4	202	PEB	C1B-C2B-C3B	-2.65	103.47	106.51
26	S9	202	PEB	CMA-C2A-C1A	-2.65	106.70	112.40
26	kF	201	PEB	CAA-C3A-C4A	2.65	119.47	112.67
28	mH	1001	CYC	C1B-NB-C4B	-2.65	107.30	110.67
26	AB	301	PEB	OD-C4D-C3D	-2.65	123.46	129.46
28	kH	1001	CYC	C1A-C2A-C3A	-2.65	103.85	106.78
26	cF	201	PEB	OD-C4D-ND	-2.65	122.01	125.93
26	bI	202	PEB	CHA-C1B-NB	-2.65	119.40	124.93
27	AF	304	PUB	CHC-C1D-ND	-2.65	110.38	113.72
26	SI	201	PEB	C2B-C1B-NB	2.65	116.18	110.53
26	mB	202	PEB	OD-C4D-C3D	-2.65	123.47	129.46
26	p4	201	PEB	OD-C4D-ND	-2.65	122.01	125.93
26	S9	201	PEB	CMB-C2B-C1B	2.65	129.14	125.06
26	QF	202	PEB	C3B-C4B-NB	2.65	113.90	110.05
26	m1	202	PEB	CMA-C2A-C1A	-2.65	106.70	112.40
26	Q4	202	PEB	CAB-CBB-CGB	-2.65	107.91	113.60
26	X9	202	PEB	OD-C4D-ND	-2.64	122.01	125.93
26	O3	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
26	PF	202	PEB	C3B-C4B-NB	2.64	113.90	110.05
26	VE	201	PEB	CBB-CAB-C3B	2.64	119.97	112.63
26	GB	1002	PEB	CBB-CAB-C3B	2.64	119.97	112.63
26	YA	202	PEB	OD-C4D-C3D	-2.64	123.47	129.46
26	R9	201	PEB	CHA-C1B-NB	-2.64	119.40	124.93
26	J7	1002	PEB	CAB-CBB-CGB	-2.64	107.91	113.60
26	mB	203	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
26	sG	202	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
26	yE	301	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
26	wG	302	PEB	OD-C4D-ND	-2.64	122.01	125.93
26	VI	203	PEB	CAB-C3B-C4B	2.64	129.69	125.01
26	gI	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
26	N4	201	PEB	C4B-NB-C1B	-2.64	101.53	106.51
26	L1	201	PEB	CAA-C3A-C2A	-2.64	107.66	114.26
28	EI	1001	CYC	CHB-C1B-NB	-2.64	120.38	126.06
26	g4	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
26	K5	203	PEB	OD-C4D-C3D	-2.64	123.47	129.46
26	cB	202	PEB	OD-C4D-C3D	-2.64	123.47	129.46
26	k4	203	PEB	C1B-C2B-C3B	-2.64	103.47	106.51
26	c1	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
26	l1	202	PEB	C1C-CHB-C4B	2.64	131.97	128.81
26	B5	201	PEB	C3B-C4B-NB	2.64	113.89	110.05
26	Y1	201	PEB	CHA-C4A-NA	2.64	128.35	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	NE	202	PEB	CHC-C4C-C3C	2.64	134.84	130.34
26	a2	202	PEB	C1B-C2B-C3B	-2.64	103.47	106.51
26	RI	202	PEB	C1B-C2B-C3B	-2.64	103.47	106.51
26	N7	1002	PEB	CBA-CAA-C3A	-2.64	107.59	113.47
26	R1	203	PEB	CMD-C2D-C3D	-2.64	126.34	130.06
26	PE	201	PEB	CAB-CBB-CGB	-2.64	107.92	113.60
26	f8	202	PEB	CHC-C1D-ND	-2.64	110.88	113.95
26	g8	201	PEB	CHC-C1D-ND	2.64	117.01	113.95
26	aE	201	PEB	CHA-C1B-C2B	2.64	131.69	124.90
26	f1	201	PEB	C3B-C4B-NB	2.64	113.89	110.05
26	eB	202	PEB	CBC-CAC-C2C	-2.64	108.11	112.62
26	Y1	201	PEB	CHB-C4B-C3B	-2.64	119.22	125.32
26	f7	203	PEB	CMB-C2B-C1B	2.64	129.13	125.06
26	j6	201	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
26	DE	201	PEB	CAB-CBB-CGB	-2.64	107.92	113.60
27	wG	304	PUB	CMD-C2D-C3D	2.64	131.73	127.77
26	R7	202	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
26	A8	301	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
26	OB	201	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
26	v4	202	PEB	CHB-C4B-C3B	2.64	131.42	125.32
26	D7	1002	PEB	C3B-C4B-NB	2.64	113.89	110.05
28	tH	1001	CYC	C2A-C1A-NA	2.64	113.89	110.05
26	z4	201	PEB	CHA-C1B-C2B	-2.64	118.11	124.90
26	Q6	203	PEB	CHB-C4B-NB	-2.64	125.16	128.83
26	U4	202	PEB	CAC-CBC-CGC	-2.64	106.36	113.76
27	AF	303	PUB	CHC-C1D-ND	-2.64	110.38	113.72
26	RB	201	PEB	CBB-CAB-C3B	2.64	119.96	112.63
26	o1	501	PEB	CHA-C1B-NB	-2.64	119.41	124.93
26	cE	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
26	NE	201	PEB	C3B-C4B-NB	2.64	113.89	110.05
26	T4	201	PEB	CHB-C4B-NB	-2.64	125.17	128.83
26	GE	201	PEB	C2B-C1B-NB	2.64	116.16	110.53
26	U3	201	PEB	CHC-C1D-ND	-2.64	110.88	113.95
26	FC	201	PEB	OD-C4D-ND	-2.64	122.02	125.93
27	K1	203	PUB	C1D-CHC-C4C	-2.64	107.62	113.37
26	XD	201	PEB	CAC-CBC-CGC	-2.64	106.36	113.76
26	RA	202	PEB	CAB-CBB-CGB	2.64	119.28	113.60
26	c7	202	PEB	CHC-C1D-ND	-2.64	110.88	113.95
26	e6	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
26	V6	201	PEB	CHA-C1B-NB	-2.64	119.41	124.93
26	R1	203	PEB	OD-C4D-ND	-2.64	122.02	125.93
26	f2	202	PEB	OD-C4D-ND	-2.64	122.02	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AF	303	PUB	OD-C4D-ND	-2.64	122.02	125.93
26	PI	203	PEB	OD-C4D-C3D	-2.64	123.48	129.46
26	K9	201	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
26	f2	201	PEB	C4B-NB-C1B	-2.64	101.54	106.51
26	l4	201	PEB	CMB-C2B-C1B	2.64	129.13	125.06
26	KC	201	PEB	C4B-C3B-C2B	-2.64	103.86	106.78
28	uH	1001	CYC	C1A-C2A-C3A	-2.64	103.86	106.78
28	uH	1001	CYC	C1B-CHB-C4A	2.64	134.52	128.08
28	H2	1001	CYC	C4A-C3A-C2A	-2.64	103.48	106.51
26	Y6	202	PEB	CMB-C2B-C1B	2.64	129.12	125.06
26	cB	202	PEB	CHA-C1B-NB	-2.64	119.42	124.93
26	J4	201	PEB	CHB-C4B-NB	-2.64	125.17	128.83
26	Y1	202	PEB	OD-C4D-ND	-2.64	122.02	125.93
26	Y4	202	PEB	OD-C4D-ND	-2.64	122.02	125.93
26	XJ	203	PEB	OD-C4D-ND	-2.64	122.02	125.93
26	L1	201	PEB	C2A-C1A-NA	2.64	110.55	108.27
26	ID	201	PEB	C2A-C1A-NA	2.64	110.55	108.27
26	DF	1002	PEB	C2A-C1A-NA	2.64	110.55	108.27
26	MD	201	PEB	CAB-CBB-CGB	-2.64	107.93	113.60
27	K1	203	PUB	C2C-C1C-NC	2.64	113.88	110.05
26	K5	203	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
26	a1	202	PEB	OD-C4D-ND	-2.64	122.03	125.93
26	i8	202	PEB	OD-C4D-ND	-2.64	122.03	125.93
26	I1	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
26	W8	203	PEB	OD-C4D-C3D	-2.64	123.49	129.46
26	DD	201	PEB	C3B-C4B-NB	2.64	113.88	110.05
28	SH	1001	CYC	C2B-C1B-NB	2.64	110.85	106.99
26	RF	201	PEB	CHA-C1B-NB	-2.64	119.42	124.93
26	c1	201	PEB	C2A-C1A-NA	2.64	110.55	108.27
26	HG	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
28	YH	1004	CYC	C4A-C3A-C2A	-2.64	103.48	106.51
26	PB	202	PEB	CAC-CBC-CGC	-2.64	106.37	113.76
26	W4	201	PEB	CHC-C4C-C3C	-2.64	125.84	130.34
26	u1	202	PEB	CHC-C1D-ND	-2.64	110.89	113.95
26	c2	202	PEB	CHC-C1D-ND	-2.64	110.89	113.95
26	kE	201	PEB	CHC-C1D-ND	2.64	117.01	113.95
26	O3	202	PEB	CMB-C2B-C1B	2.64	129.12	125.06
26	k8	202	PEB	C3B-C4B-NB	2.63	113.88	110.05
28	GH	1001	CYC	C2B-C1B-NB	2.63	110.84	106.99
26	SB	202	PEB	OD-C4D-ND	-2.63	122.03	125.93
26	EA	202	PEB	OD-C4D-C3D	-2.63	123.49	129.46
28	K6	202	CYC	CMB-C2B-C1B	2.63	127.46	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	RG	201	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
26	Q9	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
26	UA	203	PEB	CMB-C2B-C1B	2.63	129.12	125.06
26	TD	202	PEB	CAB-C3B-C4B	2.63	129.67	125.01
26	VB	202	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	QF	203	PEB	CHC-C1D-ND	-2.63	110.89	113.95
28	DF	1003	CYC	C2C-C1C-NC	2.63	110.54	108.27
26	FG	202	PEB	C4B-NB-C1B	-2.63	101.55	106.51
26	d6	203	PEB	CAB-C3B-C4B	2.63	129.67	125.01
28	KB	202	CYC	CMB-C2B-C1B	2.63	127.45	124.17
26	T3	202	PEB	C4B-NB-C1B	-2.63	101.55	106.51
26	X9	202	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
26	m2	201	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
26	N7	1002	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
28	YH	1001	CYC	C4A-C3A-C2A	-2.63	103.48	106.51
26	r1	201	PEB	OD-C4D-ND	-2.63	122.03	125.93
26	g1	202	PEB	OD-C4D-C3D	-2.63	123.49	129.46
26	W6	201	PEB	CMA-C2A-C1A	-2.63	106.73	112.40
26	n1	201	PEB	C3B-C4B-NB	2.63	113.88	110.05
26	fl	202	PEB	C3B-C4B-NB	2.63	113.88	110.05
26	u1	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
26	W7	201	PEB	OD-C4D-ND	-2.63	122.03	125.93
26	21	405	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	w1	202	PEB	CHA-C4A-NA	-2.63	122.08	125.20
26	Q4	202	PEB	CAC-CBC-CGC	-2.63	106.38	113.76
26	J8	201	PEB	CAB-CBB-CGB	-2.63	107.94	113.60
26	p4	201	PEB	CHB-C4B-NB	-2.63	125.17	128.83
26	O3	202	PEB	CBA-CAA-C3A	-2.63	107.61	113.47
28	CI	1001	CYC	CBC-CAC-C3C	-2.63	107.61	113.47
26	l4	201	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
26	KG	203	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
26	cB	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	UJ	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	14	203	PEB	CBC-CAC-C2C	-2.63	108.13	112.62
26	w1	203	PEB	C2A-C1A-NA	2.63	110.54	108.27
28	eH	1001	CYC	C2C-C1C-NC	2.63	110.54	108.27
26	U6	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	R2	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
28	gH	1001	CYC	C4A-C3A-C2A	-2.63	103.49	106.51
26	h2	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
26	gG	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
26	K5	201	PEB	CHC-C1D-ND	-2.63	110.89	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GG	202	PEB	CAC-CBC-CGC	2.63	121.14	113.76
26	XD	203	PEB	CBA-CAA-C3A	2.63	119.33	113.47
26	D1	201	PEB	CHB-C4B-C3B	-2.63	119.24	125.32
26	JJ	203	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	VB	201	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
26	D9	202	PEB	OA-C1A-C2A	-2.63	124.08	126.17
26	BC	203	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	GC	201	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
28	fH	1001	CYC	C1A-C2A-C3A	-2.63	103.87	106.78
26	i1	202	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	b7	203	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	YG	202	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	P7	202	PEB	C2A-C1A-NA	2.63	110.54	108.27
26	I8	203	PEB	CMC-C3C-C2C	2.63	129.90	124.94
26	QA	204	PEB	C2B-C1B-NB	2.63	116.14	110.53
26	M4	402	PEB	OD-C4D-ND	-2.63	122.03	125.93
26	H4	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	S8	201	PEB	CMB-C2B-C1B	2.63	129.12	125.06
26	hF	202	PEB	CMB-C2B-C1B	2.63	129.12	125.06
26	tE	202	PEB	C3B-C4B-NB	2.63	113.88	110.05
26	k4	202	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	I5	203	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
26	PG	202	PEB	C4B-C3B-C2B	-2.63	103.87	106.78
26	W9	201	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
26	TI	201	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
26	RA	201	PEB	CHA-C1B-C2B	2.63	131.66	124.90
26	J1	201	PEB	OA-C1A-C2A	-2.63	124.08	126.17
26	mE	202	PEB	OA-C1A-C2A	-2.63	124.08	126.17
26	wG	303	PEB	OA-C1A-C2A	-2.63	124.08	126.17
26	jB	202	PEB	C2A-C1A-NA	2.63	110.54	108.27
26	p4	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	a6	202	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	AA	302	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	KJ	202	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	a7	201	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
26	q4	201	PEB	CAB-CBB-CGB	-2.63	107.94	113.60
26	N8	202	PEB	CAB-CBB-CGB	2.63	119.26	113.60
26	P6	202	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	dB	203	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	VG	202	PEB	CAC-CBC-CGC	-2.63	106.39	113.76
26	mG	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	GE	202	PEB	CAC-C2C-C3C	2.63	134.80	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	YJ	202	PEB	OD-C4D-ND	-2.63	122.04	125.93
28	oH	1001	CYC	C4D-CHA-C1A	2.63	131.95	128.81
28	pH	1001	CYC	C1B-NB-C4B	-2.63	107.32	110.67
28	eH	1001	CYC	C2C-C3C-C4C	2.63	105.28	101.34
26	RJ	203	PEB	OD-C4D-C3D	-2.63	123.50	129.46
26	L9	202	PEB	CHC-C1D-ND	-2.63	110.89	113.95
26	QI	201	PEB	CMD-C2D-C3D	2.63	133.77	130.06
26	K1	201	PEB	CHC-C4C-C3C	-2.63	125.86	130.34
28	NH	1001	CYC	C4A-C3A-C2A	-2.63	103.49	106.51
26	bG	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
26	XE	201	PEB	C3B-C4B-NB	2.63	113.87	110.05
26	K4	202	PEB	C2A-C1A-NA	2.63	110.54	108.27
28	fH	1001	CYC	C2C-C3C-C4C	2.63	105.27	101.34
26	FG	202	PEB	CAA-C3A-C4A	-2.63	105.93	112.67
26	W6	203	PEB	OD-C4D-C3D	-2.63	123.51	129.46
26	QF	202	PEB	C4B-C3B-C2B	-2.63	103.88	106.78
26	P9	202	PEB	CAA-C3A-C2A	-2.63	107.70	114.26
26	F5	202	PEB	C2A-C1A-NA	2.63	110.54	108.27
26	h4	203	PEB	C1C-CHB-C4B	-2.63	125.67	128.81
28	iH	1001	CYC	C2B-C1B-NB	2.63	110.83	106.99
26	PJ	202	PEB	CAA-C3A-C2A	-2.63	107.70	114.26
26	FI	1002	PEB	CAB-CBB-CGB	-2.63	107.95	113.60
26	M3	202	PEB	OD-C4D-ND	-2.63	122.04	125.93
26	cG	202	PEB	CHC-C4C-C3C	-2.63	125.86	130.34
26	Y6	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
26	PG	202	PEB	C1B-C2B-C3B	-2.63	103.49	106.51
26	d7	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
26	EG	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
26	RA	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
26	AC	201	PEB	OD-C4D-ND	-2.63	122.04	125.93
26	m8	202	PEB	CAA-C3A-C2A	-2.63	107.70	114.26
26	i1	201	PEB	C1B-C2B-C3B	-2.62	103.49	106.51
26	ZE	202	PEB	C1B-C2B-C3B	-2.62	103.49	106.51
28	GB	1001	CYC	C4A-C3A-C2A	-2.62	103.49	106.51
26	a7	202	PEB	CHC-C1D-ND	-2.62	110.90	113.95
26	Q7	201	PEB	OD-C4D-C3D	-2.62	123.51	129.46
26	BE	202	PEB	OD-C4D-C3D	-2.62	123.51	129.46
26	DI	1002	PEB	CAB-C3B-C4B	2.62	129.65	125.01
26	R4	202	PEB	CMB-C2B-C1B	2.62	129.11	125.06
26	DJ	201	PEB	CMB-C2B-C1B	2.62	129.11	125.06
26	G9	202	PEB	C3B-C4B-NB	2.62	113.87	110.05
26	J4	201	PEB	CHB-C4B-C3B	-2.62	119.26	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T1	201	PEB	CHB-C4B-NB	-2.62	125.19	128.83
26	l6	201	PEB	OD-C4D-C3D	-2.62	123.51	129.46
26	Z8	202	PEB	CHC-C4C-C3C	-2.62	125.86	130.34
26	V2	201	PEB	CAB-CBB-CGB	-2.62	107.96	113.60
26	NA	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	J4	203	PEB	OD-C4D-ND	-2.62	122.04	125.93
26	E9	202	PEB	CAC-CBC-CGC	-2.62	106.40	113.76
26	B9	203	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	DI	1002	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	cA	203	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	aE	201	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	OE	202	PEB	CMB-C2B-C3B	-2.62	119.00	126.12
26	P1	201	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
26	g4	201	PEB	CHA-C1B-NB	-2.62	119.45	124.93
26	IE	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	cG	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	C9	201	PEB	CHC-C4C-C3C	-2.62	125.86	130.34
26	U2	201	PEB	C4B-C3B-C2B	-2.62	103.88	106.78
28	wH	1001	CYC	C1B-C2B-C3B	-2.62	105.13	107.87
26	GD	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	l6	202	PEB	C2A-C1A-NA	2.62	110.53	108.27
26	Y3	303	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	l1	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
28	E6	1001	CYC	CMB-C2B-C1B	2.62	127.44	124.17
26	F5	202	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
26	UB	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	M8	203	PEB	CBA-CAA-C3A	-2.62	107.63	113.47
26	JE	201	PEB	CAB-C3B-C4B	2.62	129.65	125.01
26	RB	202	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	L6	1002	PEB	OD-C4D-ND	-2.62	122.05	125.93
26	B9	203	PEB	OD-C4D-ND	-2.62	122.05	125.93
26	T1	203	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	a4	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	I5	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	c6	201	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	F4	201	PEB	CHA-C1B-NB	-2.62	119.45	124.93
26	XD	202	PEB	CHA-C4A-NA	2.62	128.32	125.20
26	QD	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	UD	202	PEB	C4B-C3B-C2B	-2.62	103.88	106.78
26	WJ	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	v1	202	PEB	C2A-C1A-NA	2.62	110.53	108.27
26	DD	203	PEB	CHA-C1B-NB	-2.62	119.45	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y4	202	PEB	CAB-C3B-C4B	2.62	129.64	125.01
26	g1	203	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	gE	202	PEB	CHC-C4C-C3C	-2.62	125.87	130.34
26	A8	302	PEB	OD-C4D-C3D	-2.62	123.52	129.46
26	T2	201	PEB	CAB-CBB-CGB	-2.62	107.97	113.60
26	VD	201	PEB	CAB-CBB-CGB	-2.62	107.97	113.60
26	F1	201	PEB	C3B-C4B-NB	2.62	113.86	110.05
28	II	1001	CYC	CBC-CAC-C3C	-2.62	107.63	113.47
26	wE	301	PEB	CHA-C1B-NB	-2.62	119.45	124.93
26	WG	201	PEB	C2A-C3A-C4A	-2.62	97.42	101.34
26	A2	305	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	c2	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	V4	202	PEB	CMB-C2B-C1B	2.62	129.10	125.06
26	j7	202	PEB	C2A-C1A-NA	2.62	110.53	108.27
26	LD	203	PEB	C2A-C1A-NA	2.62	110.53	108.27
26	DD	202	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	S7	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	NG	202	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	cG	203	PEB	CBC-CAC-C2C	2.62	117.09	112.62
26	P7	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
28	PH	1001	CYC	C2B-C1B-NB	2.62	110.82	106.99
26	y1	202	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	VG	202	PEB	C4B-C3B-C2B	-2.62	103.89	106.78
26	m2	201	PEB	CAB-CBB-CGB	-2.62	107.97	113.60
26	l4	201	PEB	CHC-C1D-ND	-2.62	110.91	113.95
28	IH	1001	CYC	C4A-C3A-C2A	-2.62	103.50	106.51
26	J2	1002	PEB	CHA-C1B-NB	-2.62	119.46	124.93
26	j4	202	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	SI	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	XJ	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
26	AJ	305	PEB	CAA-C3A-C2A	-2.62	107.72	114.26
26	YG	203	PEB	CBA-CAA-C3A	-2.62	107.64	113.47
26	h4	201	PEB	CAC-CBC-CGC	-2.62	106.42	113.76
26	a7	201	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	AF	301	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	j7	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	N8	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	BD	201	PEB	OD-C4D-ND	-2.62	122.05	125.93
26	B3	201	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	BG	202	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	BC	203	PEB	C3B-C4B-NB	2.62	113.86	110.05
26	PA	202	PEB	CAB-C3B-C4B	2.62	129.64	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BG	202	PEB	CAA-C3A-C4A	-2.62	105.95	112.67
26	P9	202	PEB	OD-C4D-ND	-2.62	122.06	125.93
26	bI	201	PEB	C4B-C3B-C2B	-2.62	103.89	106.78
26	IA	202	PEB	CMA-C2A-C1A	-2.62	106.77	112.40
26	m6	202	PEB	CHB-C4B-C3B	-2.62	119.28	125.32
26	OI	201	PEB	CHC-C1D-ND	-2.62	110.91	113.95
26	W9	202	PEB	CBC-CAC-C2C	-2.62	108.16	112.62
26	f6	202	PEB	CAB-C3B-C4B	2.62	129.63	125.01
26	IG	203	PEB	OD-C4D-C3D	-2.62	123.53	129.46
26	YD	304	PEB	OD-C4D-ND	-2.62	122.06	125.93
26	gG	202	PEB	OD-C4D-ND	-2.62	122.06	125.93
26	sG	202	PEB	OD-C4D-ND	-2.62	122.06	125.93
26	HC	201	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	DF	1002	PEB	OD-C4D-C3D	-2.61	123.54	129.46
27	A7	304	PUB	CBB-CAB-C3B	-2.61	108.16	112.62
26	DG	203	PEB	C2A-C1A-NA	2.61	110.53	108.27
26	j2	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	eB	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	MD	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	pG	202	PEB	CHA-C1B-NB	-2.61	119.47	124.93
26	qG	203	PEB	CHA-C4A-NA	2.61	128.31	125.20
26	Q2	201	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	VE	202	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
26	KC	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
26	mA	201	PEB	C3B-C4B-NB	2.61	113.85	110.05
26	HC	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
26	VJ	201	PEB	C1C-CHB-C4B	2.61	131.93	128.81
26	ZG	201	PEB	C2A-C1A-NA	2.61	110.53	108.27
26	I5	202	PEB	CAB-C3B-C4B	2.61	129.63	125.01
26	wG	303	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	FC	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	V4	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	L9	201	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	jF	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
26	QE	201	PEB	CBC-CAC-C2C	-2.61	108.16	112.62
28	DB	1001	CYC	CAA-C2A-C1A	2.61	129.63	125.01
26	A1	201	PEB	CHA-C1B-C2B	2.61	131.62	124.90
27	AB	302	PUB	CMD-C2D-C3D	2.61	131.69	127.77
26	WJ	202	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	YJ	202	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	P9	201	PEB	C3B-C4B-NB	2.61	113.85	110.05
26	TE	201	PEB	OD-C4D-C3D	-2.61	123.54	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mA	202	PEB	CHC-C1D-ND	-2.61	110.91	113.95
26	i4	202	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
26	UI	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	O8	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
26	h2	202	PEB	CHA-C1B-NB	-2.61	119.47	124.93
26	j8	201	PEB	CHA-C1B-NB	-2.61	119.47	124.93
26	g1	201	PEB	CHB-C4B-C3B	-2.61	119.29	125.32
26	TI	201	PEB	CHB-C4B-C3B	-2.61	119.29	125.32
26	Q2	201	PEB	CHC-C1D-ND	-2.61	110.92	113.95
27	yG	302	PUB	CHA-C4A-NA	-2.61	110.92	113.95
26	WJ	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	W8	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
26	ZF	202	PEB	CMB-C2B-C1B	2.61	129.09	125.06
26	IA	203	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
26	I3	201	PEB	C3B-C4B-NB	2.61	113.85	110.05
26	IE	202	PEB	CHB-C4B-NB	-2.61	125.20	128.83
26	c1	201	PEB	CHC-C4C-C3C	-2.61	125.88	130.34
26	VI	201	PEB	CAB-CBB-CGB	-2.61	107.98	113.60
26	j4	202	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	cI	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	RJ	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	V1	201	PEB	C3B-C4B-NB	2.61	113.85	110.05
26	U9	202	PEB	CHB-C4B-NB	-2.61	125.21	128.83
26	w4	203	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	KC	202	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	mI	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	O6	203	PEB	CAB-C3B-C4B	2.61	129.63	125.01
26	VB	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	d2	201	PEB	C4B-NB-C1B	-2.61	101.59	106.51
26	P4	201	PEB	CHA-C1B-NB	-2.61	119.47	124.93
26	G4	201	PEB	OA-C1A-C2A	-2.61	124.10	126.17
26	p1	201	PEB	C3B-C4B-NB	2.61	113.84	110.05
26	Z2	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	U4	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	N1	201	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
26	k1	201	PEB	C4B-C3B-C2B	-2.61	103.89	106.78
26	W3	201	PEB	CAB-CBB-CGB	-2.61	107.99	113.60
26	RF	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	II	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
26	CE	202	PEB	CAB-C3B-C4B	2.61	129.62	125.01
28	EB	1001	CYC	CMB-C2B-C1B	2.61	127.42	124.17
26	L3	203	PEB	CHC-C4C-C3C	-2.61	125.89	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I9	202	PEB	C3B-C4B-NB	2.61	113.84	110.05
26	X4	201	PEB	CMD-C2D-C3D	-2.61	126.39	130.06
28	JF	1001	CYC	CAD-CBD-CGD	-2.61	106.45	113.76
26	I8	202	PEB	CHC-C1D-ND	-2.61	110.92	113.95
26	VA	201	PEB	CHC-C1D-ND	2.61	116.98	113.95
26	L7	1002	PEB	CMB-C2B-C1B	2.61	129.08	125.06
26	XD	202	PEB	CMB-C2B-C1B	2.61	129.08	125.06
26	VD	203	PEB	C1C-CHB-C4B	2.61	131.93	128.81
26	Y2	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	MJ	202	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	u4	201	PEB	C4B-C3B-C2B	-2.61	103.90	106.78
26	R6	202	PEB	CHA-C1B-NB	-2.61	119.48	124.93
26	RD	203	PEB	CAC-CBC-CGC	-2.61	106.45	113.76
26	R1	201	PEB	CMA-C2A-C1A	-2.61	106.78	112.40
26	N1	201	PEB	CHA-C4A-NA	2.61	128.31	125.20
26	QJ	202	PEB	CHA-C4A-NA	-2.61	122.10	125.20
26	g1	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	ID	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	WF	203	PEB	C2A-C1A-NA	2.61	110.52	108.27
28	MH	1001	CYC	C2B-C1B-NB	2.61	110.81	106.99
26	c4	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
26	K3	202	PEB	C3B-C4B-NB	2.61	113.84	110.05
26	H9	202	PEB	C4B-C3B-C2B	-2.61	103.90	106.78
26	VF	201	PEB	C4B-C3B-C2B	-2.61	103.90	106.78
26	HD	202	PEB	CBB-CAB-C3B	-2.61	105.38	112.63
26	N8	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	DJ	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
28	kH	1001	CYC	OC-C1C-C2C	-2.61	124.10	126.17
26	LF	1002	PEB	CAB-CBB-CGB	-2.61	107.99	113.60
26	N2	1002	PEB	C1C-CHB-C4B	2.61	131.92	128.81
26	LA	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
26	aG	201	PEB	OD-C4D-ND	-2.61	122.07	125.93
27	xE	305	PUB	OA-C1A-NA	-2.61	122.07	125.93
26	m2	202	PEB	CAB-C3B-C4B	2.61	129.62	125.01
26	SB	202	PEB	C3B-C4B-NB	2.61	113.84	110.05
26	h1	202	PEB	OA-C1A-C2A	-2.61	124.10	126.17
26	T8	201	PEB	CMB-C2B-C1B	2.61	129.08	125.06
26	sE	202	PEB	OD-C4D-C3D	-2.61	123.56	129.46
26	T3	203	PEB	OD-C4D-ND	-2.61	122.07	125.93
26	NA	201	PEB	OD-C4D-ND	-2.61	122.07	125.93
28	NH	1001	CYC	C2B-C1B-NB	2.61	110.80	106.99
26	UB	201	PEB	CHA-C1B-NB	-2.61	119.48	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	tG	202	PEB	C3B-C4B-NB	2.61	113.84	110.05
26	oE	201	PEB	C2A-C1A-NA	2.61	110.52	108.27
26	t1	201	PEB	CAB-CBB-CGB	-2.61	108.00	113.60
28	I6	1001	CYC	CBC-CAC-C3C	-2.61	107.67	113.47
26	L5	203	PEB	OD-C4D-ND	-2.61	122.07	125.93
27	A2	303	PUB	OA-C1A-NA	-2.61	122.07	125.93
26	l7	201	PEB	OD-C4D-C3D	-2.61	123.56	129.46
26	a1	203	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
28	hH	1001	CYC	C2B-C1B-NB	2.60	110.80	106.99
26	G5	201	PEB	C4B-C3B-C2B	-2.60	103.90	106.78
26	21	401	PEB	CMB-C2B-C1B	2.60	129.07	125.06
26	x4	202	PEB	CAA-C3A-C2A	-2.60	107.75	114.26
26	jB	201	PEB	C3B-C4B-NB	2.60	113.84	110.05
26	a4	203	PEB	CHA-C1B-NB	-2.60	119.49	124.93
26	O7	201	PEB	CMB-C2B-C1B	2.60	129.07	125.06
28	JF	1001	CYC	C1A-C2A-C3A	-2.60	103.90	106.78
26	IE	202	PEB	CHB-C4B-C3B	-2.60	119.31	125.32
26	LB	1002	PEB	CAC-CBC-CGC	-2.60	106.46	113.76
26	iE	201	PEB	CHA-C1B-C2B	2.60	131.59	124.90
26	cA	202	PEB	C3B-C4B-NB	2.60	113.84	110.05
26	qE	201	PEB	C3B-C4B-NB	2.60	113.84	110.05
26	H5	202	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
26	eI	201	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
26	I9	201	PEB	CHA-C1B-NB	-2.60	119.49	124.93
26	GB	1002	PEB	CAA-C3A-C4A	-2.60	105.99	112.67
26	Y1	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
26	AA	301	PEB	OD-C4D-C3D	-2.60	123.56	129.46
26	HG	202	PEB	CAB-C3B-C4B	2.60	129.61	125.01
26	L8	202	PEB	O2B-CGB-CBB	2.60	122.39	114.03
26	eB	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
26	O9	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	AJ	303	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	R3	201	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
26	fF	203	PEB	C4B-C3B-C2B	-2.60	103.90	106.78
26	j8	201	PEB	C1C-CHB-C4B	-2.60	125.70	128.81
26	I5	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	i7	202	PEB	CHA-C1B-NB	-2.60	119.49	124.93
26	RE	202	PEB	CHC-C1D-ND	-2.60	110.93	113.95
26	b6	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
26	f8	203	PEB	OD-C4D-C3D	-2.60	123.57	129.46
26	lG	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
26	G1	201	PEB	CAB-CBB-CGB	-2.60	108.00	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BD	203	PEB	CAB-CBB-CGB	-2.60	108.00	113.60
26	x1	202	PEB	C2B-C1B-NB	2.60	116.08	110.53
26	JF	1002	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	RG	201	PEB	CAB-CBB-CGB	-2.60	108.01	113.60
26	u1	203	PEB	C2A-C1A-NA	2.60	110.52	108.27
26	m4	201	PEB	CMB-C2B-C1B	2.60	129.07	125.06
26	FE	202	PEB	CBC-CAC-C2C	2.60	117.06	112.62
26	k4	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	pG	201	PEB	OA-C1A-NA	2.60	128.09	124.94
27	Q8	201	PUB	CMD-C2D-C3D	2.60	131.67	127.77
26	y1	201	PEB	CBA-CAA-C3A	2.60	119.26	113.47
27	A9	302	PUB	CBB-CAB-C3B	2.60	117.06	112.62
26	Y4	202	PEB	C3B-C4B-NB	2.60	113.83	110.05
26	GA	202	PEB	CHC-C1D-ND	-2.60	110.93	113.95
28	F2	1001	CYC	CAA-C2A-C3A	-2.60	123.04	127.88
26	E3	202	PEB	CHA-C1B-NB	-2.60	119.50	124.93
26	I8	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
26	ZF	201	PEB	C1B-C2B-C3B	-2.60	103.52	106.51
26	jF	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
26	11	201	PEB	CMB-C2B-C1B	2.60	129.07	125.06
28	J7	1003	CYC	CHA-C1A-NA	-2.60	125.22	128.83
26	N6	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	24	401	PEB	CBC-CAC-C2C	-2.60	108.19	112.62
26	A4	201	PEB	CAB-C3B-C4B	-2.60	120.41	125.01
26	C5	204	PEB	C3B-C4B-NB	2.60	113.83	110.05
26	IA	203	PEB	CMC-C3C-C2C	2.60	129.84	124.94
26	NA	201	PEB	CMC-C3C-C2C	-2.60	120.04	124.94
26	Y3	304	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	s1	201	PEB	CHB-C4B-C3B	-2.60	119.32	125.32
26	T2	201	PEB	CHB-C4B-C3B	-2.60	119.32	125.32
26	VA	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
26	WB	203	PEB	OD-C4D-C3D	-2.60	123.57	129.46
26	QB	201	PEB	C1B-C2B-C3B	-2.60	103.53	106.51
26	h8	203	PEB	C3B-C4B-NB	2.60	113.83	110.05
26	OA	201	PEB	C3B-C4B-NB	2.60	113.83	110.05
27	AF	303	PUB	CHA-C1B-C2B	-2.60	125.91	130.34
26	DD	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	gE	202	PEB	OD-C4D-C3D	-2.60	123.58	129.46
26	jA	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
26	i2	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
26	kI	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
26	zE	501	PEB	C1B-C2B-C3B	-2.60	103.53	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SG	201	PEB	CMB-C2B-C1B	2.60	129.06	125.06
27	A7	304	PUB	CHC-C1D-ND	-2.60	110.44	113.72
26	I8	203	PEB	C4B-C3B-C2B	-2.60	103.91	106.78
26	dF	202	PEB	C4B-C3B-C2B	-2.60	103.91	106.78
26	l2	202	PEB	C3B-C4B-NB	2.60	113.83	110.05
26	g8	202	PEB	C3B-C4B-NB	2.60	113.83	110.05
26	C8	202	PEB	CHA-C1B-NB	-2.60	119.50	124.93
26	hB	202	PEB	C1C-CHB-C4B	2.60	131.91	128.81
26	uE	202	PEB	OA-C1A-C2A	-2.60	124.11	126.17
26	j2	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
26	FD	203	PEB	CAC-CBC-CGC	-2.60	106.48	113.76
26	K5	201	PEB	C4B-C3B-C2B	-2.60	103.91	106.78
28	UH	1001	CYC	CHA-C1A-NA	-2.60	125.23	128.83
26	aF	202	PEB	OD-C4D-ND	-2.60	122.08	125.93
26	D3	202	PEB	CMB-C2B-C1B	2.60	129.06	125.06
26	R9	201	PEB	CAB-C3B-C4B	2.60	129.60	125.01
26	Q1	202	PEB	CAC-CBC-CGC	-2.60	106.48	113.76
26	JA	201	PEB	CHA-C1B-C2B	2.60	131.57	124.90
26	PF	201	PEB	CAB-CBB-CGB	-2.60	108.02	113.60
26	D3	203	PEB	CHA-C1B-NB	-2.59	119.50	124.93
26	F4	201	PEB	C4B-C3B-C2B	-2.59	103.91	106.78
28	N2	1001	CYC	C1B-NB-C4B	-2.59	107.36	110.67
26	D9	201	PEB	CHC-C1D-ND	-2.59	110.93	113.95
26	XG	203	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	jG	201	PEB	OD-C4D-C3D	-2.59	123.58	129.46
26	KG	202	PEB	C1C-CHB-C4B	2.59	131.91	128.81
26	N3	201	PEB	CHA-C1B-C2B	2.59	131.57	124.90
28	C7	1001	CYC	CHB-C4A-NA	-2.59	119.51	124.93
26	mA	201	PEB	OD-C4D-C3D	-2.59	123.58	129.46
26	LD	202	PEB	OD-C4D-C3D	-2.59	123.58	129.46
26	CD	201	PEB	C4B-C3B-C2B	-2.59	103.91	106.78
26	kF	202	PEB	C4B-C3B-C2B	-2.59	103.91	106.78
26	X3	201	PEB	CHA-C4A-NA	2.59	128.29	125.20
26	P4	203	PEB	C2A-C1A-NA	2.59	110.51	108.27
26	a1	201	PEB	CMA-C2A-C1A	-2.59	106.81	112.40
26	q4	202	PEB	C3B-C4B-NB	2.59	113.82	110.05
26	kE	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	K5	203	PEB	CMA-C2A-C1A	-2.59	106.81	112.40
26	c1	201	PEB	OD-C4D-C3D	-2.59	123.58	129.46
26	R8	202	PEB	OD-C4D-C3D	-2.59	123.58	129.46
26	JA	202	PEB	CHA-C1B-NB	-2.59	119.51	124.93
28	IH	1001	CYC	C1A-C2A-C3A	-2.59	103.91	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j6	201	PEB	CBC-CAC-C2C	-2.59	108.19	112.62
26	T8	202	PEB	CAB-CBB-CGB	2.59	119.18	113.60
26	Q4	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	aE	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	jG	201	PEB	CHA-C1B-C2B	2.59	131.57	124.90
26	XG	201	PEB	CBC-CAC-C2C	-2.59	108.20	112.62
26	c6	202	PEB	C3B-C4B-NB	2.59	113.82	110.05
26	MA	202	PEB	CAA-C3A-C2A	-2.59	107.78	114.26
26	N9	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	RA	201	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	S1	201	PEB	CHA-C4A-NA	2.59	128.29	125.20
26	s4	201	PEB	CHA-C4A-NA	2.59	128.29	125.20
26	m6	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	R1	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
28	JH	1001	CYC	C2C-C1C-NC	2.59	110.51	108.27
26	YA	201	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	jA	201	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	gB	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	c2	202	PEB	CAB-C3B-C4B	2.59	129.59	125.01
26	L4	203	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	TD	201	PEB	CHA-C1B-C2B	2.59	131.56	124.90
26	IA	203	PEB	CBC-CAC-C2C	-2.59	108.20	112.62
26	aG	203	PEB	CHB-C4B-NB	-2.59	125.23	128.83
26	H4	202	PEB	CAB-C3B-C4B	2.59	129.59	125.01
26	SE	201	PEB	C2A-C1A-NA	2.59	110.51	108.27
26	m4	201	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	JG	202	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	jB	201	PEB	CBC-CAC-C2C	-2.59	108.20	112.62
26	JE	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	L7	1002	PEB	CAB-CBB-CGB	-2.59	108.03	113.60
26	N1	203	PEB	CMB-C2B-C1B	2.59	129.05	125.06
26	sG	203	PEB	OA-C1A-C2A	-2.59	124.11	126.17
26	EJ	201	PEB	CMA-C2A-C1A	-2.59	106.82	112.40
26	eE	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
28	CB	1001	CYC	CHA-C1A-C2A	-2.59	119.34	125.32
26	c6	202	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	X8	202	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	tE	202	PEB	C1B-C2B-C3B	-2.59	103.53	106.51
26	m7	201	PEB	C2A-C1A-NA	2.59	110.50	108.27
26	TJ	202	PEB	C2A-C1A-NA	2.59	110.50	108.27
26	VJ	201	PEB	C2A-C1A-NA	2.59	110.50	108.27
26	e7	201	PEB	CMB-C2B-C1B	2.59	129.05	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E2	1001	CYC	CHB-C1B-NB	-2.59	120.50	126.06
26	GA	203	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	kB	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	mI	202	PEB	OD-C4D-ND	-2.59	122.09	125.93
26	e2	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	gG	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
26	YF	201	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
26	FC	202	PEB	CMB-C2B-C1B	2.59	129.05	125.06
26	KC	203	PEB	C1B-C2B-C3B	-2.59	103.54	106.51
26	CD	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	f8	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	fE	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	sG	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	eE	202	PEB	CBC-CAC-C2C	-2.59	108.20	112.62
26	X9	202	PEB	C1C-CHB-C4B	2.59	131.90	128.81
26	VI	203	PEB	OD-C4D-ND	-2.59	122.10	125.93
28	GH	1001	CYC	C4A-C3A-C2A	-2.59	103.54	106.51
26	I3	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	MJ	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
28	fH	1001	CYC	C1B-C2B-C3B	-2.59	105.17	107.87
26	x1	201	PEB	CHC-C1D-ND	-2.59	110.94	113.95
26	t1	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	T7	201	PEB	CAB-C3B-C4B	2.59	129.59	125.01
26	RJ	203	PEB	OD-C4D-ND	-2.59	122.10	125.93
26	L8	201	PEB	CHA-C1B-C2B	2.59	131.55	124.90
26	IA	202	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
28	EI	1001	CYC	C1A-C2A-C3A	-2.59	103.92	106.78
26	m2	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	XJ	201	PEB	CMB-C2B-C1B	2.59	129.05	125.06
26	F4	203	PEB	CHC-C1D-ND	-2.59	110.94	113.95
26	I4	202	PEB	CHC-C1D-ND	-2.59	110.94	113.95
26	K4	202	PEB	OD-C4D-ND	-2.59	122.10	125.93
26	S9	201	PEB	C1C-CHB-C4B	2.59	131.90	128.81
26	YJ	201	PEB	C4B-C3B-C2B	-2.59	103.92	106.78
26	O9	202	PEB	C1B-C2B-C3B	-2.59	103.54	106.51
26	D2	1002	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	X4	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	IC	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	OI	202	PEB	C3B-C4B-NB	2.59	113.81	110.05
28	NI	1001	CYC	CAD-CBD-CGD	-2.59	106.51	113.76
26	O2	201	PEB	CHC-C1D-ND	-2.59	110.94	113.95
26	S2	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	lE	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
26	D3	202	PEB	C3B-C4B-NB	2.58	113.81	110.05
26	UA	203	PEB	OD-C4D-C3D	-2.58	123.60	129.46
26	s4	203	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	kB	201	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	g8	202	PEB	CHC-C4C-C3C	-2.58	125.93	130.34
26	L8	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	LD	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
27	A2	303	PUB	CHC-C1D-ND	-2.58	110.45	113.72
26	H3	202	PEB	C4B-C3B-C2B	-2.58	103.92	106.78
26	CG	203	PEB	C4B-C3B-C2B	-2.58	103.92	106.78
26	X1	201	PEB	CMD-C2D-C3D	-2.58	126.42	130.06
26	g8	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	G4	202	PEB	CAB-C3B-C4B	2.58	129.58	125.01
26	j2	202	PEB	OD-C4D-ND	-2.58	122.10	125.93
26	i7	202	PEB	OD-C4D-ND	-2.58	122.10	125.93
26	Z1	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	GC	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	QF	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	M4	401	PEB	C1C-CHB-C4B	-2.58	125.72	128.81
28	E6	1001	CYC	C4A-C3A-C2A	-2.58	103.54	106.51
28	LF	1001	CYC	CHB-C4A-NA	-2.58	119.53	124.93
26	i2	202	PEB	CAB-C3B-C4B	2.58	129.58	125.01
26	lB	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	HC	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
27	AI	303	PUB	OA-C1A-NA	-2.58	122.10	125.93
26	a2	202	PEB	C3B-C4B-NB	2.58	113.81	110.05
26	IA	202	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	N9	204	PEB	CMB-C2B-C1B	2.58	129.04	125.06
26	QJ	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	UJ	202	PEB	C1B-C2B-C3B	-2.58	103.54	106.51
26	q1	201	PEB	C2A-C1A-NA	2.58	110.50	108.27
26	D9	201	PEB	CHA-C1B-NB	-2.58	119.53	124.93
26	GE	202	PEB	CHA-C4A-NA	-2.58	122.14	125.20
26	MG	201	PEB	CBC-CAC-C2C	-2.58	108.21	112.62
26	MG	202	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	mB	203	PEB	CAB-C3B-C4B	2.58	129.58	125.01
28	GB	1001	CYC	CMB-C2B-C1B	2.58	127.39	124.17
26	GC	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
26	RE	201	PEB	C1B-C2B-C3B	-2.58	103.54	106.51
28	G6	1001	CYC	C4A-C3A-C2A	-2.58	103.54	106.51
26	LG	201	PEB	C3B-C4B-NB	2.58	113.80	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A6	302	PUB	CAC-C2C-C1C	2.58	129.57	125.01
26	R4	201	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
26	WD	201	PEB	C4B-C3B-C2B	-2.58	103.93	106.78
26	Q3	202	PEB	CMB-C2B-C1B	2.58	129.04	125.06
26	m2	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	KC	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	mI	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	V4	201	PEB	CHA-C1B-NB	-2.58	119.53	124.93
26	DJ	202	PEB	CBB-CAB-C3B	-2.58	105.46	112.63
26	f6	202	PEB	OD-C4D-ND	-2.58	122.11	125.93
26	VG	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
26	CJ	202	PEB	C3B-C4B-NB	2.58	113.80	110.05
26	H3	201	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
26	W8	201	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
26	d2	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	ND	201	PEB	CHA-C1B-C2B	2.58	131.53	124.90
26	hG	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
26	A2	301	PEB	C2A-C1A-NA	2.58	110.50	108.27
26	L7	1002	PEB	CHA-C4A-NA	2.58	128.27	125.20
26	m2	203	PEB	OA-C1A-C2A	-2.58	124.12	126.17
26	Y1	202	PEB	CAB-CBB-CGB	-2.58	108.05	113.60
28	D6	1001	CYC	CAB-C3B-C2B	2.58	131.94	127.53
28	EH	1001	CYC	C1B-CHB-C4A	2.58	134.38	128.08
26	A5	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
26	V7	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
26	Q4	201	PEB	CMA-C2A-C1A	-2.58	106.84	112.40
26	A1	202	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	IA	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	sE	203	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	HI	1002	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	T9	201	PEB	CAC-CBC-CGC	-2.58	106.53	113.76
26	b1	501	PEB	OD-C4D-ND	-2.58	122.11	125.93
26	R6	202	PEB	CAC-CBC-CGC	-2.58	106.53	113.76
26	d4	203	PEB	C3B-C4B-NB	2.58	113.80	110.05
26	M4	403	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	W8	203	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	gI	203	PEB	CHC-C1D-ND	-2.58	110.95	113.95
26	c6	201	PEB	C1C-CHB-C4B	2.58	131.89	128.81
26	SB	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	M3	201	PEB	C3B-C4B-NB	2.58	113.80	110.05
27	wG	304	PUB	C2C-C1C-NC	2.58	113.80	110.05
26	I1	201	PEB	CHB-C4B-NB	-2.58	125.25	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	jE	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	DA	202	PEB	O1B-CGB-CBB	-2.58	114.80	123.08
27	A7	303	PUB	CMD-C2D-C3D	2.58	131.64	127.77
26	ND	202	PEB	CHB-C4B-C3B	-2.58	119.37	125.32
27	Q8	201	PUB	OA-C1A-NA	-2.58	122.11	125.93
26	BC	201	PEB	C3B-C4B-NB	2.58	113.80	110.05
26	G1	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	YE	201	PEB	CAB-CBB-CGB	-2.58	108.06	113.60
26	LD	202	PEB	OA-C1A-NA	2.58	128.06	124.94
26	jG	202	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
26	FJ	202	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
26	z4	201	PEB	OA-C1A-C2A	-2.58	124.12	126.17
26	mI	201	PEB	CAB-CBB-CGB	-2.58	108.06	113.60
26	L7	1002	PEB	OD-C4D-ND	-2.58	122.11	125.93
26	N3	202	PEB	C2B-C1B-NB	2.58	116.03	110.53
26	FE	202	PEB	C2A-C1A-NA	2.58	110.49	108.27
26	m2	203	PEB	CAB-C3B-C2B	2.58	132.68	127.88
26	y4	201	PEB	CHB-C4B-NB	-2.58	125.25	128.83
26	T7	202	PEB	CHC-C4C-C3C	-2.58	125.94	130.34
26	A7	301	PEB	C3B-C4B-NB	2.58	113.80	110.05
26	YI	201	PEB	CHA-C1B-NB	-2.58	119.55	124.93
26	g1	202	PEB	C1C-CHB-C4B	-2.58	125.73	128.81
26	gA	201	PEB	CHC-C1D-ND	2.58	116.94	113.95
28	NI	1001	CYC	CHA-C1A-NA	-2.58	125.25	128.83
26	A1	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
26	S6	203	PEB	CMB-C2B-C1B	2.58	129.03	125.06
28	mH	1001	CYC	C2C-C1C-NC	2.58	110.49	108.27
26	l6	201	PEB	C3B-C4B-NB	2.58	113.80	110.05
26	bB	201	PEB	OD-C4D-C3D	-2.58	123.63	129.46
26	SE	201	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	YE	201	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	d1	202	PEB	C3B-C4B-NB	2.57	113.79	110.05
28	EF	1001	CYC	CHB-C1B-NB	-2.57	120.53	126.06
28	YH	1002	CYC	C1B-NB-C4B	-2.57	107.39	110.67
26	V1	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	gG	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	iF	201	PEB	C2A-C1A-NA	2.57	110.49	108.27
28	oH	1001	CYC	C2C-C1C-NC	2.57	110.49	108.27
27	AJ	302	PUB	OD-C4D-ND	-2.57	122.12	125.93
26	N6	201	PEB	CAC-CBC-CGC	-2.57	106.54	113.76
26	VB	202	PEB	C3B-C4B-NB	2.57	113.79	110.05
26	dE	201	PEB	C3B-C4B-NB	2.57	113.79	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T1	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	aI	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	LA	201	PEB	CHA-C1B-C2B	2.57	131.52	124.90
26	RG	201	PEB	CMB-C2B-C1B	2.57	129.03	125.06
26	GB	1002	PEB	CAC-CBC-CGC	-2.57	106.55	113.76
26	P6	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	m4	203	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
26	WE	201	PEB	CAA-C3A-C2A	2.57	120.69	114.26
26	K5	202	PEB	C1B-C2B-C3B	-2.57	103.55	106.51
26	fE	201	PEB	C1B-C2B-C3B	-2.57	103.55	106.51
28	IB	1001	CYC	C4A-C3A-C2A	-2.57	103.55	106.51
26	q1	201	PEB	CHB-C4B-NB	-2.57	125.26	128.83
26	cF	202	PEB	C3B-C4B-NB	2.57	113.79	110.05
26	iG	201	PEB	C3B-C4B-NB	2.57	113.79	110.05
26	Q7	203	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
26	SD	201	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
26	ZF	201	PEB	OA-C1A-NA	2.57	128.06	124.94
26	xG	303	PEB	OA-C1A-C2A	-2.57	124.13	126.17
26	o1	501	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
26	NB	1002	PEB	OD-C4D-ND	-2.57	122.12	125.93
27	B8	302	PUB	CBA-CAA-C3A	-2.57	109.08	112.98
26	IJ	203	PEB	C3B-C4B-NB	2.57	113.79	110.05
26	SA	203	PEB	CAB-C3B-C4B	2.57	129.56	125.01
26	fE	202	PEB	C1C-CHB-C4B	2.57	131.88	128.81
26	m7	201	PEB	CHC-C1D-ND	-2.57	110.96	113.95
26	EA	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
26	XE	202	PEB	CAA-C3A-C4A	-2.57	106.07	112.67
26	L4	201	PEB	CHB-C4B-C3B	-2.57	119.38	125.32
26	I5	201	PEB	CBC-CAC-C2C	-2.57	108.23	112.62
28	I2	1001	CYC	CBD-CAD-C3D	-2.57	108.23	112.62
28	gH	1001	CYC	C1B-CHB-C4A	2.57	134.36	128.08
26	HA	201	PEB	CHA-C1B-C2B	2.57	131.51	124.90
26	s1	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
26	XJ	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
26	k6	202	PEB	OD-C4D-ND	-2.57	122.12	125.93
26	TD	203	PEB	CMA-C2A-C1A	-2.57	106.86	112.40
26	c4	202	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
26	T3	202	PEB	CMB-C2B-C1B	2.57	129.02	125.06
26	m4	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
26	TG	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
26	YA	203	PEB	CAB-C3B-C4B	2.57	129.56	125.01
26	YD	303	PEB	CAB-C3B-C4B	2.57	129.56	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D6	1002	PEB	CAA-C3A-C4A	-2.57	106.07	112.67
26	w4	202	PEB	CHC-C1D-ND	-2.57	110.96	113.95
28	E2	1001	CYC	CMB-C2B-C1B	2.57	127.38	124.17
26	QE	202	PEB	C3B-C4B-NB	2.57	113.79	110.05
26	t4	202	PEB	CHA-C1B-C2B	2.57	131.51	124.90
26	R2	201	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
26	b7	202	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
26	hA	203	PEB	CHA-C1B-NB	-2.57	119.56	124.93
26	lB	203	PEB	CBC-CAC-C2C	-2.57	108.23	112.62
26	I5	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
26	BJ	202	PEB	OD-C4D-ND	-2.57	122.12	125.93
26	YE	201	PEB	CHC-C4C-C3C	-2.57	125.96	130.34
26	j7	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
26	q1	203	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
26	AC	201	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
26	EG	202	PEB	CHB-C4B-NB	-2.57	125.26	128.83
26	qG	201	PEB	CBA-CAA-C3A	2.57	119.19	113.47
26	eF	202	PEB	OA-C1A-C2A	-2.57	124.13	126.17
28	EH	1001	CYC	C1B-C2B-C3B	-2.57	105.19	107.87
26	U1	202	PEB	CAB-C3B-C4B	2.57	129.55	125.01
26	u4	202	PEB	C3B-C4B-NB	2.57	113.78	110.05
26	uG	203	PEB	C3B-C4B-NB	2.57	113.78	110.05
26	E8	203	PEB	CHB-C4B-NB	-2.57	125.27	128.83
26	J4	203	PEB	C1B-C2B-C3B	-2.57	103.56	106.51
26	lA	201	PEB	OD-C4D-ND	-2.57	122.13	125.93
26	F8	202	PEB	CHA-C1B-NB	-2.57	119.56	124.93
26	k1	202	PEB	CBC-CAC-C2C	-2.57	108.24	112.62
26	CC	202	PEB	CHC-C1D-ND	-2.57	110.97	113.95
26	Y8	202	PEB	C2A-C1A-NA	2.57	110.49	108.27
28	YH	1001	CYC	C1A-C2A-C3A	-2.57	103.94	106.78
26	A2	304	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
26	GG	202	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
26	c6	202	PEB	OD-C4D-ND	-2.57	122.13	125.93
26	CA	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
27	xE	301	PUB	CAB-CBB-CGB	-2.57	106.56	113.76
26	WF	202	PEB	CMC-C3C-C2C	2.57	129.78	124.94
26	I4	201	PEB	CHA-C4A-NA	2.57	128.26	125.20
26	21	405	PEB	C2A-C1A-NA	2.57	110.48	108.27
26	DE	203	PEB	C2A-C1A-NA	2.57	110.48	108.27
26	l6	202	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
26	oG	203	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
26	e1	201	PEB	OD-C4D-C3D	-2.57	123.65	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	PI	203	PEB	CMB-C2B-C1B	2.57	129.01	125.06
26	tG	201	PEB	CAB-CBB-CGB	-2.57	108.08	113.60
26	E8	201	PEB	C3B-C4B-NB	2.57	113.78	110.05
26	Q7	203	PEB	CHC-C1D-ND	-2.57	110.97	113.95
26	L1	201	PEB	CHB-C4B-NB	-2.57	125.27	128.83
26	C1	201	PEB	OD-C4D-C3D	-2.57	123.65	129.46
26	d2	201	PEB	OD-C4D-C3D	-2.57	123.65	129.46
26	fE	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
26	l8	201	PEB	OD-C4D-ND	-2.57	122.13	125.93
28	KH	1001	CYC	C1B-CHB-C4A	2.57	134.35	128.08
26	P3	201	PEB	CHA-C1B-C2B	2.56	131.50	124.90
26	N3	203	PEB	CMB-C2B-C1B	2.56	129.01	125.06
26	R4	201	PEB	CMA-C2A-C1A	-2.56	106.87	112.40
26	j4	202	PEB	C3B-C4B-NB	2.56	113.78	110.05
26	YE	201	PEB	C3B-C4B-NB	2.56	113.78	110.05
26	N1	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	tG	201	PEB	CHA-C1B-NB	-2.56	119.57	124.93
26	RF	201	PEB	CHB-C4B-C3B	-2.56	119.39	125.32
26	I5	201	PEB	C1B-C2B-C3B	-2.56	103.56	106.51
26	FE	202	PEB	CAA-C3A-C4A	-2.56	106.09	112.67
26	hA	203	PEB	OA-C1A-C2A	-2.56	124.13	126.17
26	U8	203	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	z1	202	PEB	CMB-C2B-C1B	2.56	129.01	125.06
26	j7	203	PEB	CMB-C2B-C1B	2.56	129.01	125.06
26	mB	202	PEB	C4B-C3B-C2B	-2.56	103.94	106.78
28	L7	1001	CYC	C1A-C2A-C3A	-2.56	103.94	106.78
26	e8	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	HG	202	PEB	C1B-C2B-C3B	-2.56	103.56	106.51
28	YH	1002	CYC	C2B-C1B-NB	2.56	110.74	106.99
26	VJ	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
26	Z6	202	PEB	CHA-C1B-C2B	2.56	131.49	124.90
28	FB	1001	CYC	CAD-CBD-CGD	-2.56	106.57	113.76
26	R6	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
26	eA	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	PB	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	s4	201	PEB	C3B-C4B-NB	2.56	113.78	110.05
27	AI	303	PUB	C2C-C1C-NC	2.56	113.78	110.05
26	mI	203	PEB	CAB-C3B-C2B	2.56	132.65	127.88
26	U1	202	PEB	OD-C4D-ND	-2.56	122.13	125.93
26	TB	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	dE	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	a8	201	PEB	CHC-C1D-ND	-2.56	110.97	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	z1	202	PEB	CAA-C3A-C2A	-2.56	107.86	114.26
26	B4	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
26	pG	202	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	jI	201	PEB	OD-C4D-ND	-2.56	122.13	125.93
26	HF	1002	PEB	CHA-C1B-C2B	2.56	131.49	124.90
26	bF	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	PE	201	PEB	CMA-C2A-C1A	-2.56	106.88	112.40
26	g8	202	PEB	CAB-C3B-C4B	2.56	129.54	125.01
26	L1	203	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	Z4	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	IJ	203	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	Y3	301	PEB	CHA-C1B-NB	-2.56	119.58	124.93
26	PE	202	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
26	B5	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	Y6	201	PEB	CMA-C2A-C1A	-2.56	106.88	112.40
26	lF	201	PEB	CMB-C2B-C1B	2.56	129.01	125.06
27	K1	203	PUB	CAC-CBC-CGC	-2.56	108.09	113.60
26	n4	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	AC	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	dI	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	dF	202	PEB	CMA-C2A-C1A	-2.56	106.88	112.40
26	QB	202	PEB	C3B-C4B-NB	2.56	113.77	110.05
26	GC	203	PEB	CHB-C4B-C3B	-2.56	119.41	125.32
26	Q1	202	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
26	N1	202	PEB	CMB-C2B-C1B	2.56	129.01	125.06
26	L9	201	PEB	CAB-C3B-C4B	2.56	129.54	125.01
28	lH	1001	CYC	CAB-C3B-C2B	2.56	131.91	127.53
26	cE	203	PEB	CHA-C4A-NA	2.56	128.25	125.20
26	fB	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	SF	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	x1	201	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	eE	202	PEB	CAB-C3B-C4B	2.56	129.54	125.01
26	ND	203	PEB	CMB-C2B-C1B	2.56	129.01	125.06
26	DE	202	PEB	CMB-C2B-C1B	2.56	129.01	125.06
26	V7	202	PEB	CHA-C1B-NB	-2.56	119.58	124.93
28	WH	1001	CYC	C1B-CHB-C4A	2.56	134.33	128.08
26	i8	202	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	P6	202	PEB	CAC-CBC-CGC	-2.56	106.58	113.76
26	wE	301	PEB	C2A-C1A-NA	2.56	110.48	108.27
26	e2	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
26	E8	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	S4	202	PEB	C3B-C4B-NB	2.56	113.77	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c7	202	PEB	C3B-C4B-NB	2.56	113.77	110.05
28	FI	1001	CYC	C2A-C1A-NA	2.56	113.77	110.05
26	n4	201	PEB	CBB-CAB-C3B	2.56	119.74	112.63
28	wH	1001	CYC	C2B-C1B-NB	2.56	110.73	106.99
26	s1	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
26	m8	201	PEB	CAB-C3B-C4B	2.56	129.53	125.01
26	R9	203	PEB	C3B-C4B-NB	2.56	113.77	110.05
26	E8	202	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
26	LC	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
26	mE	203	PEB	CHC-C1D-ND	-2.56	110.98	113.95
28	LH	1001	CYC	C1B-CHB-C4A	2.56	134.33	128.08
26	m8	201	PEB	C3B-C4B-NB	2.56	113.77	110.05
26	gA	201	PEB	C3B-C4B-NB	2.56	113.77	110.05
26	RI	203	PEB	C3B-C4B-NB	2.56	113.77	110.05
26	EE	202	PEB	CMB-C2B-C1B	2.56	129.00	125.06
26	w4	203	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	nG	202	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	f6	202	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
26	A5	202	PEB	OD-C4D-C3D	-2.56	123.67	129.46
26	iA	202	PEB	CHC-C1D-ND	-2.56	110.98	113.95
26	UB	203	PEB	CHC-C1D-ND	-2.56	110.98	113.95
26	sE	202	PEB	CHB-C4B-NB	-2.56	125.28	128.83
26	B4	203	PEB	C2A-C1A-NA	2.56	110.48	108.27
26	iE	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
26	m2	202	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	g7	202	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	iE	203	PEB	OD-C4D-ND	-2.56	122.14	125.93
26	O8	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
26	BD	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
28	qH	1002	CYC	CAB-C3B-C2B	2.56	131.90	127.53
26	U6	203	PEB	CBA-CAA-C3A	-2.56	107.78	113.47
26	ZA	202	PEB	OD-C4D-C3D	-2.56	123.67	129.46
26	nE	201	PEB	CHC-C1D-ND	-2.56	110.98	113.95
26	G1	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
26	j4	202	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
26	ZB	203	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
26	U6	201	PEB	CMB-C2B-C1B	2.56	129.00	125.06
26	vE	202	PEB	CAB-C3B-C4B	2.56	129.53	125.01
26	cE	201	PEB	CAC-C2C-C3C	2.56	134.59	127.25
26	b7	203	PEB	OD-C4D-C3D	-2.56	123.67	129.46
26	WA	203	PEB	OD-C4D-C3D	-2.56	123.67	129.46
26	eI	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A5	201	PEB	CAB-C3B-C4B	2.56	129.53	125.01
26	11	201	PEB	OD-C4D-C3D	-2.56	123.67	129.46
26	TD	201	PEB	C1C-CHB-C4B	2.55	131.86	128.81
26	Q2	201	PEB	OA-C1A-NA	2.55	128.04	124.94
28	D6	1001	CYC	CAA-C2A-C1A	2.55	129.53	125.01
26	1F	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
26	DG	202	PEB	CBD-CAD-C3D	-2.55	114.91	127.62
26	JJ	203	PEB	C3B-C4B-NB	2.55	113.77	110.05
26	g8	201	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	x4	201	PEB	CHC-C1D-ND	-2.55	110.98	113.95
26	E8	201	PEB	OD-C4D-C3D	-2.55	123.67	129.46
26	f7	203	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
26	HJ	203	PEB	CMD-C2D-C3D	2.55	133.67	130.06
26	OE	203	PEB	CHB-C4B-C3B	-2.55	119.42	125.32
26	m6	202	PEB	CMB-C2B-C1B	2.55	129.00	125.06
26	fA	201	PEB	CMB-C2B-C1B	2.55	129.00	125.06
26	QI	201	PEB	OA-C1A-NA	2.55	128.03	124.94
26	W6	201	PEB	CHB-C4B-NB	-2.55	125.28	128.83
26	cI	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
26	aA	201	PEB	CBC-CAC-C2C	-2.55	108.26	112.62
28	C7	1001	CYC	CHD-C4C-NC	2.55	128.24	125.20
26	YI	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
26	u4	203	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
27	A8	304	PUB	C2C-C1C-NC	2.55	113.76	110.05
26	QA	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	V1	201	PEB	OA-C1A-C2A	-2.55	124.14	126.17
26	l2	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
26	j2	202	PEB	CHA-C1B-NB	-2.55	119.59	124.93
26	GG	203	PEB	CAB-C3B-C2B	-2.55	123.12	127.88
26	Q8	203	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	AI	305	PEB	CHC-C1D-ND	-2.55	110.98	113.95
26	dG	202	PEB	C3B-C4B-NB	2.55	113.76	110.05
26	zG	501	PEB	C3B-C4B-NB	2.55	113.76	110.05
26	24	401	PEB	OD-C4D-ND	-2.55	122.15	125.93
27	YD	302	PUB	CAC-CBC-CGC	-2.55	108.11	113.60
26	fA	201	PEB	OD-C4D-C3D	-2.55	123.68	129.46
26	T6	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	jB	201	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	NJ	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	TA	201	PEB	CHA-C1B-NB	-2.55	119.59	124.93
26	T6	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
28	JH	1001	CYC	C1A-C2A-C3A	-2.55	103.96	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	NF	1001	CYC	CAD-CBD-CGD	-2.55	106.61	113.76
26	YF	201	PEB	CHA-C4A-NA	2.55	128.24	125.20
26	IJ	201	PEB	CHB-C4B-C3B	-2.55	119.43	125.32
26	IC	202	PEB	CAB-C3B-C4B	2.55	129.52	125.01
26	K4	201	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
26	VF	203	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
26	B5	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
27	wG	304	PUB	CHB-C1C-C2C	-2.55	119.43	125.32
26	FF	1002	PEB	OD-C4D-C3D	-2.55	123.68	129.46
28	HF	1001	CYC	OB-C4B-C3B	-2.55	125.27	128.04
26	OB	201	PEB	CMA-C2A-C1A	-2.55	106.91	112.40
26	b7	202	PEB	C3B-C4B-NB	2.55	113.76	110.05
26	gI	203	PEB	OD-C4D-ND	-2.55	122.15	125.93
28	EH	1001	CYC	C2B-C1B-NB	2.55	110.72	106.99
26	S7	201	PEB	CMB-C2B-C1B	2.55	128.99	125.06
28	JF	1003	CYC	CHB-C4A-NA	-2.55	119.60	124.93
26	QF	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	j8	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	f8	201	PEB	CAB-C3B-C4B	2.55	129.52	125.01
26	d1	203	PEB	C3B-C4B-NB	2.55	113.76	110.05
28	SH	1001	CYC	C2A-C1A-NA	2.55	113.76	110.05
26	k2	203	PEB	CAC-CBC-CGC	-2.55	106.61	113.76
26	mB	203	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
26	KC	201	PEB	CHC-C1D-ND	-2.55	110.99	113.95
26	J1	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
28	WH	1001	CYC	C1B-C2B-C3B	-2.55	105.21	107.87
27	KD	203	PUB	C2C-C1C-NC	2.55	113.75	110.05
26	JG	202	PEB	OD-C4D-C3D	-2.55	123.69	129.46
26	AJ	301	PEB	CHA-C1B-NB	-2.55	119.60	124.93
26	S9	202	PEB	CHB-C4B-NB	-2.55	125.29	128.83
26	hG	201	PEB	CHC-C1D-ND	-2.55	110.99	113.95
26	j8	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	B5	203	PEB	CBC-CAC-C2C	-2.55	108.27	112.62
26	G5	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
26	qG	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
26	F5	201	PEB	CHA-C1B-NB	-2.55	119.61	124.93
26	M8	202	PEB	CAA-C3A-C2A	-2.55	107.89	114.26
28	yH	1001	CYC	C1B-C2B-C3B	-2.55	105.21	107.87
26	S3	201	PEB	OD-C4D-ND	-2.55	122.16	125.93
26	hE	201	PEB	C3B-C4B-NB	2.55	113.75	110.05
26	OI	201	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
26	aG	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k7	201	PEB	CAB-CBB-CGB	-2.55	108.12	113.60
28	G6	1001	CYC	CMB-C2B-C1B	2.55	127.35	124.17
28	J7	1001	CYC	CHB-C4A-C3A	2.55	131.45	124.90
26	G1	202	PEB	C3B-C4B-NB	2.55	113.75	110.05
26	L9	201	PEB	C2A-C1A-NA	2.55	110.47	108.27
26	G9	202	PEB	CMB-C2B-C1B	2.55	128.99	125.06
26	SB	203	PEB	CMB-C2B-C1B	2.55	128.99	125.06
26	h2	202	PEB	C4B-C3B-C2B	-2.55	103.97	106.78
26	kB	201	PEB	CAC-CBC-CGC	-2.55	106.62	113.76
26	NJ	204	PEB	CHC-C1D-ND	-2.55	110.99	113.95
26	t1	202	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
28	tH	1001	CYC	C4A-C3A-C2A	-2.55	103.58	106.51
26	k4	201	PEB	C3B-C4B-NB	2.55	113.75	110.05
26	X9	203	PEB	CHC-C4C-C3C	-2.55	126.00	130.34
26	R4	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
26	Z8	202	PEB	OD-C4D-C3D	-2.55	123.69	129.46
26	FG	202	PEB	OD-C4D-C3D	-2.55	123.69	129.46
26	oG	202	PEB	C4B-C3B-C2B	-2.55	103.97	106.78
26	C3	201	PEB	CHA-C4A-NA	2.55	128.23	125.20
26	MD	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
26	Y6	202	PEB	CHA-C1B-NB	-2.54	119.61	124.93
26	z1	405	PEB	CHA-C1B-C2B	2.54	131.44	124.90
26	fF	203	PEB	CHA-C1B-NB	-2.54	119.61	124.93
26	QJ	201	PEB	CAA-C3A-C2A	-2.54	107.90	114.26
26	n4	202	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
26	Y8	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
28	kH	1001	CYC	C1B-CHB-C4A	2.54	134.30	128.08
26	PA	202	PEB	O2B-CGB-CBB	2.54	122.20	114.03
26	T2	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
26	a8	201	PEB	OD-C4D-ND	-2.54	122.16	125.93
26	W6	201	PEB	CHA-C1B-C2B	2.54	131.44	124.90
26	bF	202	PEB	CMB-C2B-C1B	2.54	128.98	125.06
26	HE	202	PEB	CAB-C3B-C4B	2.54	129.51	125.01
26	K8	203	PEB	OD-C4D-C3D	-2.54	123.70	129.46
26	JD	202	PEB	OD-C4D-C3D	-2.54	123.70	129.46
26	B3	202	PEB	CBA-CAA-C3A	-2.54	107.81	113.47
26	k2	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
26	YI	202	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
26	lB	203	PEB	CMB-C2B-C1B	2.54	128.98	125.06
26	aE	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
26	S8	203	PEB	CAB-C3B-C4B	2.54	129.51	125.01
26	gA	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W4	201	PEB	CHB-C4B-NB	-2.54	125.30	128.83
26	hE	202	PEB	CAB-C3B-C4B	2.54	129.51	125.01
26	TD	202	PEB	CMB-C2B-C1B	2.54	128.98	125.06
26	N3	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
27	A2	303	PUB	C2C-C1C-NC	2.54	113.75	110.05
26	DI	1002	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
28	lH	1001	CYC	C4A-C3A-C2A	-2.54	103.59	106.51
26	k7	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	Q1	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
27	K4	203	PUB	CAB-CBB-CGB	-2.54	106.63	113.76
28	F2	1001	CYC	CMB-C2B-C3B	2.54	133.02	126.12
26	y1	203	PEB	CAB-C3B-C4B	2.54	129.50	125.01
26	fF	201	PEB	OD-C4D-ND	-2.54	122.17	125.93
26	f2	202	PEB	C3B-C4B-NB	2.54	113.75	110.05
26	hB	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
26	lF	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
26	vG	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
26	QG	203	PEB	CHC-C1D-ND	-2.54	111.00	113.95
28	II	1001	CYC	C4A-C3A-C2A	-2.54	103.59	106.51
26	QG	202	PEB	OD-C4D-C3D	-2.54	123.70	129.46
26	k1	203	PEB	CHA-C1B-NB	-2.54	119.62	124.93
26	j1	202	PEB	OD-C4D-ND	-2.54	122.17	125.93
26	N7	1002	PEB	OD-C4D-ND	-2.54	122.17	125.93
26	V7	202	PEB	OD-C4D-ND	-2.54	122.17	125.93
28	IB	1001	CYC	CHA-C1A-NA	-2.54	125.30	128.83
27	xE	301	PUB	C2C-C1C-NC	2.54	113.75	110.05
26	iF	202	PEB	OA-C1A-NA	2.54	128.02	124.94
26	WJ	202	PEB	OA-C1A-C2A	-2.54	124.15	126.17
26	iE	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
26	xG	303	PEB	C2A-C1A-NA	2.54	110.46	108.27
26	TJ	201	PEB	CAB-C3B-C4B	2.54	129.50	125.01
26	J1	201	PEB	CAA-C3A-C2A	-2.54	107.91	114.26
26	k4	203	PEB	CHB-C4B-C3B	-2.54	119.45	125.32
26	i1	202	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
26	Q3	202	PEB	CHC-C1D-ND	-2.54	111.00	113.95
28	CB	1001	CYC	C4A-C3A-C2A	-2.54	103.59	106.51
26	RJ	201	PEB	CHA-C1B-NB	-2.54	119.62	124.93
28	N7	1001	CYC	C2A-C1A-NA	2.54	113.74	110.05
26	M9	201	PEB	OA-C1A-C2A	-2.54	124.15	126.17
26	UB	201	PEB	C2A-C1A-NA	2.54	110.46	108.27
28	uH	1001	CYC	CHB-C1B-C2B	-2.54	121.92	126.95
27	A6	303	PUB	OD-C4D-ND	-2.54	122.17	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z6	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
26	KA	202	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
28	RH	1001	CYC	C2A-C1A-NA	2.54	113.74	110.05
26	X3	201	PEB	CAA-C3A-C2A	-2.54	107.92	114.26
26	L9	202	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
28	JH	1001	CYC	C2B-C1B-NB	2.54	110.70	106.99
26	NA	202	PEB	CAB-CBB-CGB	2.54	119.07	113.60
26	JC	202	PEB	CAB-CBB-CGB	-2.54	108.14	113.60
26	R1	202	PEB	CHA-C1B-NB	-2.54	119.62	124.93
28	TH	1001	CYC	C1B-C2B-C3B	-2.54	105.22	107.87
26	H5	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
26	TI	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
26	OA	202	PEB	CMB-C2B-C1B	2.54	128.97	125.06
28	F6	1001	CYC	CAD-CBD-CGD	-2.54	106.64	113.76
26	LA	202	PEB	O2B-CGB-CBB	2.54	122.19	114.03
27	AB	303	PUB	OD-C4D-ND	-2.54	122.17	125.93
26	B4	201	PEB	C2A-C1A-NA	2.54	110.46	108.27
26	jI	201	PEB	C2A-C1A-NA	2.54	110.46	108.27
26	dB	204	PEB	CHA-C1B-NB	-2.54	119.62	124.93
26	A9	304	PEB	C3B-C4B-NB	2.54	113.74	110.05
26	c4	202	PEB	CMB-C2B-C1B	2.54	128.97	125.06
26	Q9	201	PEB	CBA-CAA-C3A	-2.54	107.82	113.47
26	C5	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
26	uE	203	PEB	CHA-C4A-NA	2.54	128.22	125.20
26	L3	201	PEB	C1C-CHB-C4B	-2.54	125.78	128.81
28	L7	1001	CYC	CHA-C1A-NA	-2.54	125.31	128.83
26	d4	201	PEB	CAB-C3B-C4B	2.54	129.50	125.01
26	Q4	201	PEB	CHB-C4B-C3B	-2.54	119.46	125.32
26	m1	202	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
26	a7	202	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
28	D6	1001	CYC	C2C-C1C-NC	2.54	110.46	108.27
26	x4	201	PEB	C3B-C4B-NB	2.54	113.74	110.05
28	iH	1001	CYC	C2A-C1A-NA	2.54	113.74	110.05
26	a8	203	PEB	OD-C4D-C3D	-2.54	123.71	129.46
26	EE	201	PEB	CHC-C1D-ND	-2.54	111.00	113.95
26	C9	202	PEB	OD-C4D-ND	-2.54	122.17	125.93
26	Q9	202	PEB	OD-C4D-ND	-2.54	122.17	125.93
26	YA	202	PEB	CBB-CAB-C3B	-2.54	105.58	112.63
26	K1	201	PEB	CHB-C4B-NB	-2.54	125.31	128.83
26	m6	201	PEB	C2A-C1A-NA	2.54	110.46	108.27
26	EA	201	PEB	OD-C4D-C3D	-2.54	123.72	129.46
28	AH	1001	CYC	C1B-CHB-C4A	2.54	134.28	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	UH	1001	CYC	CHB-C1B-C2B	-2.54	121.92	126.95
26	W8	201	PEB	CAA-C3A-C2A	-2.54	107.92	114.26
26	R2	203	PEB	C3B-C4B-NB	2.54	113.74	110.05
26	c1	201	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
26	YE	201	PEB	CMB-C2B-C1B	2.54	128.97	125.06
26	Z6	201	PEB	CAB-C3B-C4B	2.53	129.49	125.01
26	VJ	203	PEB	CBD-CAD-C3D	-2.53	115.01	127.62
26	h1	201	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	eG	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	G1	201	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
26	KJ	201	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
26	B3	202	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
26	SA	201	PEB	OD-C4D-ND	-2.53	122.18	125.93
26	gB	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	mF	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	XG	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	Y2	201	PEB	CHA-C1B-NB	-2.53	119.63	124.93
26	QJ	201	PEB	C1B-C2B-C3B	-2.53	103.60	106.51
26	mB	201	PEB	CAB-C3B-C4B	2.53	129.49	125.01
26	K8	201	PEB	CMA-C2A-C1A	-2.53	106.94	112.40
28	EI	1001	CYC	CMB-C2B-C1B	2.53	127.33	124.17
26	f7	203	PEB	CHA-C1B-NB	-2.53	119.64	124.93
26	aB	202	PEB	CHC-C1D-ND	-2.53	111.01	113.95
26	B1	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	D1	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	P2	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	kA	202	PEB	OD-C4D-ND	-2.53	122.18	125.93
26	W8	201	PEB	CAB-C3B-C4B	2.53	129.49	125.01
26	kF	201	PEB	CAB-CBB-CGB	-2.53	108.15	113.60
26	AF	301	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	PF	201	PEB	CHB-C4B-C3B	-2.53	119.47	125.32
28	BB	1001	CYC	CHB-C4A-C3A	2.53	131.41	124.90
28	N2	1001	CYC	CAD-CBD-CGD	-2.53	106.66	113.76
26	l4	201	PEB	CHA-C1B-NB	-2.53	119.64	124.93
26	Y6	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	m6	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
26	TI	201	PEB	CAB-CBB-CGB	-2.53	108.16	113.60
26	A9	304	PEB	CHA-C4A-NA	-2.53	122.19	125.20
26	I9	202	PEB	OD-C4D-ND	-2.53	122.18	125.93
26	B1	201	PEB	CMB-C2B-C1B	2.53	128.96	125.06
26	XE	202	PEB	OD-C4D-C3D	-2.53	123.73	129.46
26	E1	202	PEB	CHB-C4B-NB	-2.53	125.32	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C3	202	PEB	OD-C4D-ND	-2.53	122.18	125.93
26	L3	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
26	NG	202	PEB	CMC-C3C-C2C	-2.53	120.17	124.94
26	f7	201	PEB	C3B-C4B-NB	2.53	113.73	110.05
26	d1	201	PEB	CAB-C3B-C4B	2.53	129.49	125.01
26	WA	201	PEB	CMA-C2A-C1A	-2.53	106.95	112.40
26	ME	201	PEB	OA-C1A-NA	2.53	128.01	124.94
26	IE	203	PEB	CHA-C1B-C2B	2.53	131.41	124.90
26	eB	203	PEB	C2A-C1A-NA	2.53	110.45	108.27
26	fF	202	PEB	CHA-C4A-NA	-2.53	122.20	125.20
26	I8	202	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
26	D4	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	BD	203	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	R4	201	PEB	CBB-CAB-C3B	-2.53	105.60	112.63
26	C5	204	PEB	OD-C4D-ND	-2.53	122.18	125.93
26	J1	201	PEB	CAB-C3B-C4B	2.53	129.48	125.01
26	RJ	201	PEB	CAB-C3B-C4B	2.53	129.48	125.01
26	g6	201	PEB	OD-C4D-C3D	-2.53	123.73	129.46
26	L3	203	PEB	C3B-C4B-NB	2.53	113.73	110.05
26	dG	201	PEB	C3B-C4B-NB	2.53	113.73	110.05
26	K9	201	PEB	OD-C4D-C3D	-2.53	123.73	129.46
26	kI	202	PEB	OD-C4D-C3D	-2.53	123.73	129.46
26	HC	201	PEB	CHA-C1B-C2B	2.53	131.40	124.90
26	HE	201	PEB	CAB-C3B-C4B	2.53	129.48	125.01
26	hE	201	PEB	CHA-C1B-C2B	2.53	131.40	124.90
26	i7	202	PEB	C4B-C3B-C2B	-2.53	103.98	106.78
26	LD	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
26	i1	202	PEB	C2A-C1A-NA	2.53	110.45	108.27
26	OE	201	PEB	CAB-C3B-C4B	2.53	129.48	125.01
26	U9	201	PEB	CHC-C1D-ND	-2.53	111.01	113.95
28	J2	1001	CYC	CHB-C1B-NB	-2.53	120.63	126.06
26	Y1	201	PEB	C1B-C2B-C3B	-2.53	103.61	106.51
26	E8	203	PEB	CMB-C2B-C1B	2.53	128.96	125.06
26	V3	203	PEB	CAC-CBC-CGC	-2.53	106.67	113.76
26	DJ	202	PEB	CMD-C2D-C3D	2.53	133.63	130.06
26	m6	202	PEB	C4B-C3B-C2B	-2.53	103.99	106.78
26	h4	201	PEB	CAB-CBB-CGB	-2.53	108.17	113.60
26	K9	202	PEB	OD-C4D-ND	-2.53	122.19	125.93
26	Y1	201	PEB	CHC-C1D-ND	-2.53	111.01	113.95
26	J8	202	PEB	OA-C1A-C2A	-2.53	124.16	126.17
26	W7	201	PEB	CHA-C1B-NB	-2.53	119.65	124.93
26	RD	201	PEB	C1B-C2B-C3B	-2.53	103.61	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e6	202	PEB	C3B-C4B-NB	2.53	113.72	110.05
26	kF	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	rH	1001	CYC	C1A-C2A-C3A	-2.53	103.99	106.78
26	D4	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
26	V6	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
26	pG	202	PEB	CBB-CAB-C3B	2.53	119.64	112.63
26	x4	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
26	GD	201	PEB	OD-C4D-ND	-2.53	122.19	125.93
26	RJ	202	PEB	C2A-C1A-NA	2.53	110.45	108.27
28	WH	1001	CYC	C2C-C1C-NC	2.53	110.45	108.27
26	hI	201	PEB	C4B-C3B-C2B	-2.53	103.99	106.78
28	SH	1001	CYC	C1B-CHB-C4A	2.53	134.25	128.08
26	A7	305	PEB	CHC-C1D-ND	-2.52	111.02	113.95
26	i6	202	PEB	C1C-CHB-C4B	-2.52	125.79	128.81
26	Q4	201	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
26	aF	201	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
26	CA	203	PEB	CMB-C2B-C1B	2.52	128.95	125.06
26	B9	201	PEB	OD-C4D-ND	-2.52	122.19	125.93
26	l7	201	PEB	C3B-C4B-NB	2.52	113.72	110.05
26	ID	201	PEB	CAB-CBB-CGB	-2.52	108.17	113.60
26	A1	201	PEB	OA-C1A-C2A	-2.52	124.17	126.17
26	SJ	201	PEB	CMB-C2B-C1B	2.52	128.95	125.06
26	f1	202	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
26	P9	202	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
26	kF	201	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
26	f1	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	z4	202	PEB	OD-C4D-C3D	-2.52	123.74	129.46
26	O8	203	PEB	OD-C4D-C3D	-2.52	123.74	129.46
26	IC	202	PEB	OD-C4D-C3D	-2.52	123.74	129.46
26	U8	201	PEB	CHB-C4B-C3B	-2.52	119.49	125.32
26	F3	203	PEB	C4B-C3B-C2B	-2.52	103.99	106.78
26	j4	201	PEB	CMB-C2B-C1B	2.52	128.95	125.06
26	O1	201	PEB	CBA-CAA-C3A	2.52	119.08	113.47
26	h7	202	PEB	CBC-CAC-C2C	-2.52	108.31	112.62
26	EG	202	PEB	CAA-C3A-C4A	-2.52	106.19	112.67
26	wE	303	PEB	CHA-C1B-C2B	2.52	131.39	124.90
26	A6	301	PEB	CHA-C1B-NB	-2.52	119.66	124.93
26	ZB	201	PEB	CAB-C3B-C4B	2.52	129.47	125.01
26	hA	201	PEB	CHC-C1D-ND	-2.52	111.02	113.95
26	H3	202	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	OA	201	PEB	OD-C4D-ND	-2.52	122.19	125.93
26	kA	202	PEB	CAB-C3B-C4B	2.52	129.47	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BD	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
26	eB	203	PEB	C4B-C3B-C2B	-2.52	103.99	106.78
26	hA	203	PEB	CMB-C2B-C1B	2.52	128.95	125.06
26	iI	201	PEB	C1C-CHB-C4B	2.52	131.82	128.81
26	y4	203	PEB	OD-C4D-ND	-2.52	122.19	125.93
26	O7	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	YF	201	PEB	CHB-C4B-C3B	-2.52	119.50	125.32
26	J9	201	PEB	CHA-C1B-C2B	2.52	131.38	124.90
28	SH	1001	CYC	CHB-C1B-C2B	-2.52	121.95	126.95
26	SF	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	ND	201	PEB	C3B-C4B-NB	2.52	113.72	110.05
26	JG	201	PEB	CAB-C3B-C4B	2.52	129.47	125.01
26	C4	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	d7	202	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	AC	202	PEB	CHC-C1D-ND	-2.52	111.02	113.95
26	U2	202	PEB	OD-C4D-ND	-2.52	122.20	125.93
26	W6	201	PEB	CHA-C4A-NA	2.52	128.20	125.20
26	N9	202	PEB	C1C-CHB-C4B	2.52	131.82	128.81
26	R7	202	PEB	CAB-CBB-CGB	-2.52	108.18	113.60
28	II	1001	CYC	CBD-CAD-C3D	-2.52	108.32	112.62
26	V9	202	PEB	C3B-C4B-NB	2.52	113.72	110.05
28	NB	1001	CYC	CMC-C2C-C1C	-2.52	106.97	112.40
26	Y2	203	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	Y8	202	PEB	CBB-CAB-C3B	-2.52	105.63	112.63
26	f7	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	d1	203	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
26	24	401	PEB	C2A-C1A-NA	2.52	110.44	108.27
26	JC	201	PEB	C3B-C4B-NB	2.52	113.71	110.05
28	PH	1001	CYC	C2A-C1A-NA	2.52	113.71	110.05
26	T4	202	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	EE	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	cF	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	w4	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	C5	201	PEB	CHA-C1B-NB	-2.52	119.66	124.93
26	FJ	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
26	FE	202	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	CJ	201	PEB	C2B-C1B-NB	2.52	115.90	110.53
26	i4	201	PEB	CHC-C1D-ND	-2.52	111.02	113.95
26	Q9	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
26	vG	202	PEB	CHB-C4B-C3B	-2.52	119.50	125.32
26	W3	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
26	gG	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UA	201	PEB	CHB-C4B-C3B	-2.52	119.50	125.32
26	jB	202	PEB	OD-C4D-C3D	-2.52	123.76	129.46
26	K5	202	PEB	CMB-C2B-C1B	2.52	128.94	125.06
26	T7	201	PEB	CMB-C2B-C1B	2.52	128.94	125.06
26	UF	203	PEB	CMB-C2B-C1B	2.52	128.94	125.06
26	X8	202	PEB	CBC-CAC-C2C	-2.52	108.32	112.62
26	WF	203	PEB	CAB-CBB-CGB	-2.52	108.19	113.60
26	O6	203	PEB	OD-C4D-C3D	-2.52	123.76	129.46
26	sG	202	PEB	OD-C4D-C3D	-2.52	123.76	129.46
28	oH	1001	CYC	C1A-C2A-C3A	-2.52	104.00	106.78
26	Y1	202	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
26	tE	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
26	cE	203	PEB	C3B-C4B-NB	2.52	113.71	110.05
26	d4	201	PEB	CAA-C3A-C2A	-2.52	107.97	114.26
26	i8	202	PEB	CHA-C4A-NA	-2.52	122.21	125.20
26	D4	201	PEB	CHB-C4B-C3B	-2.52	119.51	125.32
26	JC	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
26	aG	202	PEB	CBC-CAC-C2C	-2.52	108.33	112.62
27	A4	203	PUB	CBB-CAB-C3B	-2.52	108.33	112.62
26	H5	203	PEB	CHA-C1B-NB	-2.52	119.67	124.93
26	B1	203	PEB	OD-C4D-C3D	-2.52	123.76	129.46
26	M9	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
26	AF	302	PEB	OD-C4D-C3D	-2.52	123.76	129.46
26	M4	403	PEB	C1C-CHB-C4B	-2.52	125.80	128.81
26	R3	203	PEB	CAC-CBC-CGC	-2.52	106.71	113.76
26	HD	203	PEB	C3B-C4B-NB	2.52	113.71	110.05
26	C3	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
26	ND	203	PEB	OD-C4D-ND	-2.52	122.20	125.93
26	Q1	201	PEB	CMA-C2A-C1A	-2.51	106.98	112.40
26	kA	201	PEB	CHA-C1B-C2B	2.51	131.37	124.90
26	O1	201	PEB	C4B-NB-C1B	-2.51	101.77	106.51
26	G5	201	PEB	C1C-CHB-C4B	2.51	131.81	128.81
26	JJ	203	PEB	OD-C4D-ND	-2.51	122.20	125.93
26	ZB	201	PEB	OD-C4D-C3D	-2.51	123.76	129.46
26	p1	201	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
26	HJ	202	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
28	MH	1001	CYC	C1A-C2A-C3A	-2.51	104.00	106.78
26	F4	203	PEB	OD-C4D-C3D	-2.51	123.76	129.46
26	VF	201	PEB	OD-C4D-C3D	-2.51	123.76	129.46
26	h1	201	PEB	CAC-CBC-CGC	-2.51	106.71	113.76
26	eD	401	PEB	C3B-C4B-NB	2.51	113.71	110.05
27	AB	303	PUB	C2C-C1C-NC	2.51	113.71	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F9	201	PEB	CHC-C1D-ND	-2.51	111.03	113.95
28	CF	1001	CYC	C2C-C1C-NC	2.51	110.44	108.27
26	jB	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	GC	201	PEB	CAA-C3A-C2A	-2.51	107.98	114.26
26	MG	201	PEB	CHB-C4B-NB	-2.51	125.34	128.83
26	HE	201	PEB	C3B-C4B-NB	2.51	113.70	110.05
26	M1	403	PEB	C1C-CHB-C4B	-2.51	125.81	128.81
27	AI	302	PUB	C4B-CHB-C1C	-2.51	125.81	128.81
26	bF	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	hE	202	PEB	CHA-C1B-NB	-2.51	119.68	124.93
26	P1	202	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
26	ED	201	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
26	ZI	201	PEB	C4B-C3B-C2B	-2.51	104.00	106.78
28	dH	1001	CYC	C1A-C2A-C3A	-2.51	104.00	106.78
26	CJ	201	PEB	CAC-C2C-C3C	2.51	134.47	127.25
26	kG	202	PEB	OD-C4D-ND	-2.51	122.21	125.93
26	D1	203	PEB	C1B-C2B-C3B	-2.51	103.62	106.51
26	G9	201	PEB	C1B-C2B-C3B	-2.51	103.62	106.51
27	BA	302	PUB	CBA-CAA-C3A	-2.51	109.17	112.98
26	s1	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	TB	201	PEB	CAB-C3B-C4B	2.51	129.45	125.01
26	aF	201	PEB	CHB-C4B-C3B	-2.51	119.52	125.32
26	g2	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	JC	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	HJ	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	Q7	201	PEB	CMB-C2B-C1B	2.51	128.93	125.06
26	LD	201	PEB	C1B-C2B-C3B	-2.51	103.62	106.51
26	H3	202	PEB	CBB-CAB-C3B	-2.51	105.65	112.63
28	CI	1001	CYC	CMB-C2B-C1B	2.51	127.30	124.17
26	XE	201	PEB	CAB-C3B-C4B	2.51	129.45	125.01
26	SA	202	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	l1	201	PEB	CHA-C1B-NB	-2.51	119.68	124.93
26	JA	202	PEB	CAB-C3B-C4B	2.51	129.45	125.01
26	H5	203	PEB	OD-C4D-C3D	-2.51	123.77	129.46
26	A5	201	PEB	CHA-C4A-NA	2.51	128.19	125.20
28	L7	1001	CYC	C2A-C1A-NA	2.51	113.70	110.05
26	v4	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
28	I6	1001	CYC	C4A-C3A-C2A	-2.51	103.63	106.51
26	P1	201	PEB	CHA-C1B-NB	-2.51	119.68	124.93
26	c4	201	PEB	OD-C4D-ND	-2.51	122.21	125.93
26	WB	201	PEB	CHA-C1B-C2B	2.51	131.35	124.90
26	rE	202	PEB	CMC-C3C-C2C	-2.51	120.21	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	eB	203	PEB	OD-C4D-C3D	-2.51	123.78	129.46
26	KJ	201	PEB	CBC-CAC-C2C	-2.51	108.34	112.62
26	B1	202	PEB	OD-C4D-ND	-2.51	122.21	125.93
28	rH	1001	CYC	CHA-C1A-NA	-2.51	125.35	128.83
26	ZB	202	PEB	OA-C1A-C2A	-2.51	124.18	126.17
26	qG	202	PEB	C1B-C2B-C3B	-2.51	103.63	106.51
26	TJ	201	PEB	C1B-C2B-C3B	-2.51	103.63	106.51
26	uG	202	PEB	C4B-C3B-C2B	-2.51	104.01	106.78
26	T1	202	PEB	CHA-C4A-NA	-2.51	122.22	125.20
26	kF	201	PEB	CMB-C2B-C1B	2.51	128.93	125.06
26	LC	203	PEB	CAC-CBC-CGC	-2.51	106.73	113.76
26	WB	201	PEB	CHB-C4B-C3B	-2.51	119.53	125.32
26	RJ	201	PEB	CAA-C3A-C4A	-2.51	106.23	112.67
26	h4	202	PEB	CAC-CBC-CGC	-2.51	106.73	113.76
26	fl	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
26	d1	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
26	aA	204	PEB	OD-C4D-ND	-2.51	122.22	125.93
26	J1	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
26	B1	202	PEB	C3B-C4B-NB	2.51	113.70	110.05
28	I6	1001	CYC	CHA-C1A-NA	-2.51	125.35	128.83
26	QA	204	PEB	CBC-CAC-C2C	-2.51	108.34	112.62
26	Y2	202	PEB	C1B-C2B-C3B	-2.51	103.63	106.51
26	N7	1002	PEB	CAB-C3B-C4B	2.51	129.44	125.01
26	OG	202	PEB	CAB-C3B-C4B	2.51	129.44	125.01
28	M2	1001	CYC	CMB-C2B-C1B	2.51	127.30	124.17
26	s1	201	PEB	C4B-C3B-C2B	-2.51	104.01	106.78
26	FC	201	PEB	C4B-C3B-C2B	-2.51	104.01	106.78
26	YA	203	PEB	CMB-C2B-C1B	2.51	128.93	125.06
26	TI	203	PEB	OD-C4D-C3D	-2.51	123.78	129.46
26	W2	201	PEB	CHC-C1D-ND	-2.51	111.04	113.95
26	l7	202	PEB	CAA-C3A-C2A	-2.51	108.00	114.26
28	RH	1001	CYC	C1B-CHB-C4A	2.51	134.20	128.08
26	BD	201	PEB	CAB-CBB-CGB	-2.51	108.21	113.60
26	RE	201	PEB	CMB-C2B-C1B	2.51	128.92	125.06
28	K2	1001	CYC	CMB-C2B-C1B	2.51	127.30	124.17
26	jF	201	PEB	CHB-C4B-NB	-2.51	125.35	128.83
26	l2	201	PEB	C4B-C3B-C2B	-2.51	104.01	106.78
28	GH	1001	CYC	C1B-CHB-C4A	2.51	134.20	128.08
26	e7	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
26	dF	203	PEB	OD-C4D-C3D	-2.51	123.78	129.46
26	U7	203	PEB	CHC-C1D-ND	-2.51	111.04	113.95
26	ID	202	PEB	OD-C4D-ND	-2.51	122.22	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	mF	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	H7	1001	CYC	C2A-C1A-NA	2.51	113.69	110.05
26	I3	201	PEB	CAB-C3B-C4B	2.50	129.44	125.01
26	N9	202	PEB	CAB-C3B-C4B	2.50	129.44	125.01
26	PF	202	PEB	CAB-C3B-C4B	2.50	129.44	125.01
28	VH	1001	CYC	C1B-CHB-C4A	2.50	134.20	128.08
26	kE	201	PEB	OD-C4D-C3D	-2.50	123.78	129.46
26	x4	201	PEB	CHB-C4B-NB	-2.50	125.35	128.83
26	S4	201	PEB	CHA-C4A-NA	2.50	128.18	125.20
26	WB	201	PEB	CHA-C4A-NA	2.50	128.18	125.20
26	FA	202	PEB	CHA-C1B-NB	-2.50	119.69	124.93
26	f2	201	PEB	C4B-C3B-C2B	-2.50	104.01	106.78
26	m1	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	g6	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	iE	203	PEB	C3B-C4B-NB	2.50	113.69	110.05
26	mG	203	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	Q1	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	rH	1001	CYC	C2B-C1B-NB	2.50	110.65	106.99
26	f4	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	CC	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	hG	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	nG	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	dG	202	PEB	CHB-C4B-C3B	-2.50	119.54	125.32
26	RG	201	PEB	CBC-CAC-C2C	-2.50	108.35	112.62
26	DB	1002	PEB	CAA-C3A-C4A	-2.50	106.25	112.67
26	N8	201	PEB	CMA-C2A-C1A	-2.50	107.01	112.40
26	Q7	203	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	e1	201	PEB	C3B-C4B-NB	2.50	113.69	110.05
26	G4	202	PEB	C3B-C4B-NB	2.50	113.69	110.05
26	K9	202	PEB	C3B-C4B-NB	2.50	113.69	110.05
28	QH	1001	CYC	C2C-C3C-C4C	2.50	105.09	101.34
27	QA	201	PUB	CMD-C2D-C3D	2.50	131.52	127.77
26	ZB	202	PEB	C4B-C3B-C2B	-2.50	104.01	106.78
28	N2	1001	CYC	CAA-C2A-C3A	2.50	132.54	127.88
26	aB	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	KJ	201	PEB	CMB-C2B-C1B	2.50	128.92	125.06
26	p1	201	PEB	OD-C4D-ND	-2.50	122.22	125.93
26	BJ	201	PEB	CHA-C1B-C2B	2.50	131.34	124.90
28	rH	1001	CYC	C2A-C1A-NA	2.50	113.69	110.05
28	EH	1001	CYC	C1A-C2A-C3A	-2.50	104.01	106.78
26	L5	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	YJ	201	PEB	CHC-C1D-ND	-2.50	111.04	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E3	201	PEB	CHA-C1B-C2B	2.50	131.33	124.90
26	dB	202	PEB	CAA-C3A-C4A	-2.50	106.25	112.67
26	f8	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
26	fF	203	PEB	CMB-C2B-C1B	2.50	128.92	125.06
26	MJ	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
26	dB	202	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	Z7	202	PEB	C1C-CHB-C4B	2.50	131.80	128.81
26	W8	201	PEB	CHA-C4A-NA	2.50	128.18	125.20
26	R4	203	PEB	C3B-C4B-NB	2.50	113.69	110.05
26	X9	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
26	q1	202	PEB	C4B-C3B-C2B	-2.50	104.02	106.78
26	TJ	202	PEB	CHA-C1B-C2B	-2.50	118.47	124.90
28	M6	1001	CYC	CHA-C1A-NA	-2.50	125.36	128.83
26	v1	202	PEB	CAB-CBB-CGB	-2.50	108.22	113.60
26	W7	201	PEB	C1C-CHB-C4B	2.50	131.80	128.81
26	HG	201	PEB	CAB-C3B-C4B	2.50	129.43	125.01
26	KG	203	PEB	CAB-C3B-C4B	2.50	129.43	125.01
26	T2	203	PEB	OD-C4D-C3D	-2.50	123.80	129.46
26	U9	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	eF	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
27	24	402	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
26	R9	201	PEB	OD-C4D-ND	-2.50	122.23	125.93
26	iA	202	PEB	OD-C4D-ND	-2.50	122.23	125.93
26	eA	202	PEB	O2B-CGB-CBB	2.50	122.06	114.03
26	V4	203	PEB	OD-C4D-C3D	-2.50	123.80	129.46
26	QD	201	PEB	C4B-C3B-C2B	-2.50	104.02	106.78
28	HF	1001	CYC	C1A-C2A-C3A	-2.50	104.02	106.78
26	RI	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	d4	201	PEB	C2A-C1A-NA	2.50	110.43	108.27
28	B6	1001	CYC	CHB-C4A-C3A	2.50	131.33	124.90
26	OE	201	PEB	OD-C4D-C3D	-2.50	123.80	129.46
26	V6	202	PEB	C3B-C4B-NB	2.50	113.69	110.05
28	I2	1001	CYC	C4A-C3A-C2A	-2.50	103.64	106.51
26	C9	202	PEB	CMB-C2B-C1B	2.50	128.91	125.06
26	PG	201	PEB	CAB-CBB-CGB	-2.50	108.22	113.60
28	JF	1003	CYC	CHA-C1A-C2A	-2.50	119.55	125.32
26	NI	1002	PEB	CMD-C2D-C3D	2.50	133.59	130.06
26	JE	202	PEB	CAB-C3B-C4B	2.50	129.43	125.01
26	AC	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
26	kB	202	PEB	C2A-C1A-NA	2.50	110.43	108.27
28	KF	1001	CYC	CMB-C2B-C1B	2.50	127.29	124.17
28	YH	1001	CYC	C2B-C1B-NB	2.50	110.64	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d4	201	PEB	CHC-C1D-ND	-2.50	111.05	113.95
27	yE	303	PUB	C2C-C1C-NC	2.50	113.68	110.05
26	RE	201	PEB	CAB-CBB-CGB	-2.50	108.23	113.60
26	LC	201	PEB	CHA-C1B-C2B	2.50	131.32	124.90
26	NI	1002	PEB	C1C-CHB-C4B	2.50	131.79	128.81
26	Q6	202	PEB	CBB-CAB-C3B	-2.50	105.69	112.63
26	H5	203	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
26	X3	203	PEB	OD-C4D-ND	-2.50	122.23	125.93
26	fl	201	PEB	CAB-CBB-CGB	-2.50	108.23	113.60
26	OB	203	PEB	CAB-C3B-C4B	2.50	129.43	125.01
26	CG	203	PEB	CHB-C4B-NB	-2.50	125.36	128.83
26	TB	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	sE	203	PEB	C3B-C4B-NB	2.50	113.68	110.05
26	C9	202	PEB	CBC-CAC-C2C	-2.50	108.36	112.62
26	MG	202	PEB	CMB-C2B-C1B	2.50	128.91	125.06
26	V1	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
26	m6	203	PEB	CAB-CBB-CGB	-2.50	108.23	113.60
26	J3	202	PEB	CHA-C4A-NA	2.50	128.17	125.20
28	iH	1001	CYC	CAB-C3B-C2B	2.50	131.80	127.53
26	mB	202	PEB	OD-C4D-ND	-2.50	122.23	125.93
26	T8	201	PEB	CHA-C1B-NB	-2.50	119.71	124.93
26	k1	203	PEB	CMB-C2B-C1B	2.50	128.91	125.06
26	FE	201	PEB	CMA-C2A-C1A	-2.50	107.02	112.40
26	P7	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
26	I8	201	PEB	OD-C4D-C3D	-2.50	123.80	129.46
28	PH	1001	CYC	C1B-CHB-C4A	2.50	134.18	128.08
28	yH	1001	CYC	C1B-CHB-C4A	2.50	134.18	128.08
26	a4	203	PEB	OD-C4D-ND	-2.50	122.23	125.93
26	DD	203	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	A6	304	PEB	C2A-C1A-NA	2.50	110.42	108.27
26	w4	203	PEB	CBC-CAC-C2C	-2.50	108.36	112.62
26	S2	201	PEB	CHA-C4A-NA	2.50	128.17	125.20
26	IG	202	PEB	CHB-C4B-NB	-2.50	125.36	128.83
26	Y8	201	PEB	CMB-C2B-C1B	2.50	128.91	125.06
26	a8	202	PEB	OD-C4D-C3D	-2.50	123.81	129.46
26	d8	202	PEB	OD-C4D-C3D	-2.50	123.81	129.46
26	P9	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
26	LC	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
28	C2	1001	CYC	CMB-C2B-C1B	2.50	127.28	124.17
26	F2	1002	PEB	CAB-CBB-CGB	-2.50	108.23	113.60
26	B5	202	PEB	OD-C4D-ND	-2.50	122.23	125.93
26	VD	201	PEB	OD-C4D-ND	-2.50	122.23	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a6	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
26	b7	202	PEB	CMB-C2B-C1B	2.50	128.91	125.06
26	i6	202	PEB	OD-C4D-C3D	-2.50	123.81	129.46
26	e7	201	PEB	C2A-C1A-NA	2.50	110.42	108.27
26	BJ	202	PEB	C2A-C1A-NA	2.50	110.42	108.27
28	KB	202	CYC	C4A-C3A-C2A	-2.50	103.64	106.51
26	D9	202	PEB	CBB-CAB-C3B	-2.49	105.69	112.63
26	C5	202	PEB	CAA-C3A-C4A	-2.49	106.27	112.67
26	24	401	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	G4	201	PEB	CBC-CAC-C2C	-2.49	108.36	112.62
26	a4	203	PEB	CBC-CAC-C2C	-2.49	108.36	112.62
26	k4	202	PEB	CBC-CAC-C2C	-2.49	108.36	112.62
26	J3	202	PEB	C2B-C1B-NB	2.49	115.85	110.53
28	vH	1001	CYC	C1B-C2B-C3B	-2.49	105.27	107.87
26	fG	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	T6	201	PEB	C1B-C2B-C3B	-2.49	103.64	106.51
26	BG	201	PEB	CAB-C3B-C4B	2.49	129.42	125.01
26	W1	202	PEB	C3B-C4B-NB	2.49	113.68	110.05
26	jF	201	PEB	CHC-C1D-ND	-2.49	111.05	113.95
26	WI	201	PEB	CHC-C1D-ND	-2.49	111.05	113.95
26	AB	304	PEB	CBC-CAC-C2C	-2.49	108.36	112.62
26	S6	203	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	Z2	201	PEB	C4B-C3B-C2B	-2.49	104.02	106.78
28	KI	1001	CYC	CMB-C2B-C1B	2.49	127.28	124.17
26	e4	201	PEB	CHA-C1B-NB	-2.49	119.72	124.93
26	p4	201	PEB	CHA-C1B-NB	-2.49	119.72	124.93
28	yH	1001	CYC	C1B-NB-C4B	-2.49	107.49	110.67
26	OB	203	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	eI	202	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	H8	201	PEB	CHA-C1B-C2B	2.49	131.31	124.90
26	m4	203	PEB	OD-C4D-ND	-2.49	122.24	125.93
26	G6	1002	PEB	OD-C4D-ND	-2.49	122.24	125.93
26	oG	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	GJ	202	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	f8	203	PEB	OD-C4D-ND	-2.49	122.24	125.93
26	JE	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
26	X8	202	PEB	O1B-CGB-CBB	-2.49	115.08	123.08
26	O8	201	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	H9	203	PEB	CBA-CAA-C3A	-2.49	107.92	113.47
26	T8	202	PEB	C1B-C2B-C3B	-2.49	103.65	106.51
26	a1	203	PEB	OD-C4D-ND	-2.49	122.24	125.93
26	Y9	201	PEB	CMB-C2B-C1B	2.49	128.90	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G6	1002	PEB	CHA-C1B-NB	-2.49	119.72	124.93
26	jI	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
26	jI	201	PEB	CMA-C2A-C1A	-2.49	107.03	112.40
26	bB	201	PEB	CHB-C4B-NB	-2.49	125.37	128.83
26	j6	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	OF	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	JG	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	vE	201	PEB	C3B-C4B-NB	2.49	113.67	110.05
28	yH	1001	CYC	C2C-C1C-NC	2.49	110.42	108.27
26	G6	1002	PEB	CAC-CBC-CGC	-2.49	106.78	113.76
26	H5	203	PEB	C1C-CHB-C4B	2.49	131.78	128.81
27	YD	302	PUB	CHB-C1C-C2C	-2.49	119.57	125.32
26	fG	202	PEB	CAB-C3B-C4B	2.49	129.41	125.01
26	V6	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	j6	202	PEB	OD-C4D-ND	-2.49	122.24	125.93
26	fB	202	PEB	CAA-C3A-C2A	-2.49	108.04	114.26
26	gF	201	PEB	CAB-CBB-CGB	-2.49	108.24	113.60
26	jI	201	PEB	CAB-CBB-CGB	-2.49	108.24	113.60
26	D9	202	PEB	CAA-C3A-C4A	-2.49	106.28	112.67
26	qG	203	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	jE	201	PEB	CHA-C1B-C2B	2.49	131.30	124.90
27	A4	203	PUB	C2C-C1C-NC	2.49	113.67	110.05
26	A3	201	PEB	CMB-C2B-C1B	2.49	128.90	125.06
26	C5	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	e6	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	AE	201	PEB	CHA-C1B-NB	-2.49	119.73	124.93
26	dB	203	PEB	CAB-C3B-C4B	2.49	129.41	125.01
26	W8	201	PEB	CMA-C2A-C1A	-2.49	107.04	112.40
26	uE	202	PEB	C4B-C3B-C2B	-2.49	104.03	106.78
26	z1	202	PEB	C1B-C2B-C3B	-2.49	103.65	106.51
26	eG	202	PEB	CBC-CAC-C2C	-2.49	108.37	112.62
26	Q4	201	PEB	CAB-C3B-C4B	2.49	129.41	125.01
26	kB	202	PEB	CAB-C3B-C4B	2.49	129.41	125.01
26	F1	203	PEB	OD-C4D-C3D	-2.49	123.82	129.46
26	jF	202	PEB	OD-C4D-ND	-2.49	122.25	125.93
26	YG	202	PEB	OD-C4D-ND	-2.49	122.25	125.93
26	n4	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	LD	203	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	I8	201	PEB	C2B-C1B-NB	2.49	115.84	110.53
26	bG	202	PEB	C4B-C3B-C2B	-2.49	104.03	106.78
26	fI	202	PEB	C4B-C3B-C2B	-2.49	104.03	106.78
26	f4	202	PEB	C1B-C2B-C3B	-2.49	103.65	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H3	201	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	m6	202	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	YG	203	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	Z7	202	PEB	CHC-C1D-ND	-2.49	111.06	113.95
26	r1	202	PEB	CBA-CAA-C3A	-2.49	107.93	113.47
26	FG	201	PEB	CMA-C2A-C1A	-2.49	107.04	112.40
26	DG	201	PEB	CAB-CBB-CGB	-2.49	108.25	113.60
26	FD	203	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	JA	201	PEB	C1B-C2B-C3B	-2.49	103.65	106.51
26	J9	202	PEB	CMB-C2B-C1B	2.49	128.89	125.06
26	T9	202	PEB	CHA-C4A-NA	2.49	128.16	125.20
26	AJ	303	PEB	C2A-C1A-NA	2.49	110.42	108.27
26	OG	201	PEB	C3B-C4B-NB	2.49	113.67	110.05
26	K8	203	PEB	C2B-C1B-NB	2.49	115.83	110.53
26	O2	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
26	L1	203	PEB	C1C-CHB-C4B	-2.49	125.84	128.81
26	Z6	202	PEB	CHB-C4B-NB	-2.49	125.38	128.83
26	OG	201	PEB	CHA-C4A-NA	2.49	128.16	125.20
28	hH	1001	CYC	CAA-C2A-C1A	2.49	129.41	125.01
26	g8	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
26	lF	202	PEB	CBB-CAB-C3B	-2.48	105.72	112.63
26	rG	201	PEB	C2A-C1A-NA	2.48	110.42	108.27
26	l1	201	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	y1	202	PEB	CHB-C4B-NB	-2.48	125.38	128.83
26	A4	202	PEB	OD-C4D-C3D	-2.48	123.83	129.46
26	jE	201	PEB	CMB-C2B-C1B	2.48	128.89	125.06
26	UJ	201	PEB	OD-C4D-ND	-2.48	122.25	125.93
26	f4	201	PEB	CHA-C1B-NB	-2.48	119.74	124.93
26	c1	202	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	H7	1002	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	lG	202	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	AJ	301	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	R8	202	PEB	OA-C1A-C2A	-2.48	124.20	126.17
26	A7	305	PEB	CMB-C2B-C1B	2.48	128.89	125.06
26	tE	201	PEB	OA-C1A-NA	2.48	127.95	124.94
26	TF	202	PEB	C3B-C4B-NB	2.48	113.66	110.05
26	xE	303	PEB	CHC-C1D-ND	-2.48	111.06	113.95
28	UH	1001	CYC	C2C-C1C-NC	2.48	110.41	108.27
26	X1	202	PEB	CAA-C3A-C2A	2.48	120.46	114.26
26	eG	202	PEB	OD-C4D-C3D	-2.48	123.83	129.46
26	aI	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
26	PD	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L3	203	PEB	CAC-CBC-CGC	-2.48	106.80	113.76
27	Y3	302	PUB	CHC-C1D-ND	-2.48	110.58	113.72
26	cE	201	PEB	OD-C4D-ND	-2.48	122.25	125.93
26	z4	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
26	mG	202	PEB	OD-C4D-C3D	-2.48	123.83	129.46
26	s1	202	PEB	CAA-C3A-C4A	-2.48	106.30	112.67
26	FE	202	PEB	C4B-NB-C1B	-2.48	101.83	106.51
28	B6	1001	CYC	C1B-NB-C4B	-2.48	107.51	110.67
26	AA	302	PEB	CAB-C3B-C4B	2.48	129.40	125.01
26	KA	203	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	qG	203	PEB	OD-C4D-ND	-2.48	122.25	125.93
26	j1	202	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	eE	203	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	U9	202	PEB	C1C-CHB-C4B	2.48	131.77	128.81
26	z1	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	P2	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06
26	eI	202	PEB	CMB-C2B-C1B	2.48	128.89	125.06
26	fE	202	PEB	CAB-C3B-C4B	2.48	129.40	125.01
28	sH	1001	CYC	C2A-C1A-NA	2.48	113.66	110.05
26	ZF	202	PEB	CBC-CAC-C2C	-2.48	108.39	112.62
26	ZF	203	PEB	CAA-C3A-C4A	2.48	119.05	112.67
26	E4	202	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	PE	201	PEB	C1C-CHB-C4B	2.48	131.77	128.81
26	j8	202	PEB	CMB-C2B-C1B	2.48	128.88	125.06
26	Q1	201	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	N3	203	PEB	CMA-C2A-C1A	-2.48	107.06	112.40
26	p4	202	PEB	CHA-C1B-C2B	2.48	131.28	124.90
26	W6	202	PEB	CHB-C4B-C3B	-2.48	119.59	125.32
26	D9	201	PEB	CMB-C2B-C1B	2.48	128.88	125.06
26	QJ	201	PEB	CBB-CAB-C3B	2.48	119.52	112.63
26	O7	201	PEB	CBC-CAC-C2C	-2.48	108.39	112.62
28	fH	1001	CYC	C1B-CHB-C4A	2.48	134.14	128.08
26	W4	202	PEB	C1C-CHB-C4B	2.48	131.77	128.81
26	S1	202	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	V9	201	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	F3	202	PEB	OD-C4D-ND	-2.48	122.26	125.93
26	CE	202	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	FA	202	PEB	CAB-CBB-CGB	2.48	118.94	113.60
26	U2	201	PEB	CBA-CAA-C3A	-2.48	107.95	113.47
26	uE	202	PEB	C3B-C4B-NB	2.48	113.66	110.05
28	C7	1001	CYC	C1B-CHB-C4A	-2.48	122.02	128.08
26	c8	201	PEB	OD-C4D-ND	-2.48	122.26	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g2	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	l6	203	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	qE	202	PEB	C3B-C4B-NB	2.48	113.66	110.05
26	iI	203	PEB	OD-C4D-ND	-2.48	122.26	125.93
26	a2	201	PEB	CHB-C4B-C3B	-2.48	119.59	125.32
26	T2	203	PEB	C1B-C2B-C3B	-2.48	103.66	106.51
26	PD	201	PEB	CAB-C3B-C4B	2.48	129.39	125.01
26	d1	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	YJ	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
26	u1	202	PEB	C3B-C4B-NB	2.48	113.65	110.05
26	bE	202	PEB	C3B-C4B-NB	2.48	113.65	110.05
28	PH	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
26	CJ	202	PEB	CMB-C2B-C1B	2.48	128.88	125.06
26	PG	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
26	U7	201	PEB	C2A-C1A-NA	2.48	110.41	108.27
28	BB	1001	CYC	C1B-NB-C4B	-2.48	107.51	110.67
26	LD	203	PEB	C3B-C4B-NB	2.48	113.65	110.05
26	l2	201	PEB	CHA-C1B-NB	-2.48	119.75	124.93
26	M4	401	PEB	OD-C4D-ND	-2.48	122.26	125.93
26	dB	203	PEB	OD-C4D-C3D	-2.48	123.85	129.46
26	PE	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
26	kA	202	PEB	CBB-CAB-C3B	2.48	119.51	112.63
26	LG	202	PEB	C4B-NB-C1B	-2.48	101.84	106.51
26	nG	202	PEB	C4B-C3B-C2B	-2.48	104.04	106.78
26	i4	201	PEB	OD-C4D-C3D	-2.48	123.85	129.46
26	ZE	202	PEB	OD-C4D-C3D	-2.48	123.85	129.46
28	VH	1001	CYC	CAA-C2A-C1A	2.48	129.39	125.01
26	ZE	201	PEB	C3B-C4B-NB	2.48	113.65	110.05
28	E2	1001	CYC	CHA-C1A-NA	-2.48	125.39	128.83
26	J8	202	PEB	CAB-C3B-C4B	2.48	129.39	125.01
28	pH	1001	CYC	C1A-C2A-C3A	-2.48	104.04	106.78
26	bI	201	PEB	OD-C4D-ND	-2.48	122.26	125.93
28	NH	1001	CYC	C2C-C1C-NC	2.48	110.41	108.27
26	R1	202	PEB	CMB-C2B-C1B	2.48	128.88	125.06
26	d7	201	PEB	CMB-C2B-C1B	2.48	128.88	125.06
26	wE	303	PEB	OD-C4D-C3D	-2.48	123.85	129.46
26	O2	201	PEB	OA-C1A-C2A	-2.48	124.20	126.17
26	WG	202	PEB	OA-C1A-C2A	-2.48	124.20	126.17
26	LD	203	PEB	C1B-C2B-C3B	-2.48	103.67	106.51
26	RG	202	PEB	C1B-C2B-C3B	-2.48	103.67	106.51
26	F8	202	PEB	CAB-CBB-CGB	2.47	118.93	113.60
26	BJ	202	PEB	OD-C4D-C3D	-2.47	123.85	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	kE	203	PEB	OD-C4D-ND	-2.47	122.26	125.93
26	YA	201	PEB	CMB-C2B-C1B	2.47	128.88	125.06
26	s1	203	PEB	C4B-C3B-C2B	-2.47	104.04	106.78
26	N3	201	PEB	CMA-C2A-C1A	-2.47	107.07	112.40
26	W9	202	PEB	CHA-C1B-NB	-2.47	119.76	124.93
28	EB	1001	CYC	CHB-C1B-NB	-2.47	120.75	126.06
26	f6	202	PEB	CAA-C3A-C2A	-2.47	108.08	114.26
26	P9	202	PEB	CHC-C1D-ND	-2.47	111.07	113.95
26	KD	201	PEB	CHA-C1B-NB	-2.47	119.76	124.93
26	W3	202	PEB	CBA-CAA-C3A	-2.47	107.96	113.47
26	wG	302	PEB	CBA-CAA-C3A	-2.47	107.96	113.47
26	WB	201	PEB	CHB-C4B-NB	-2.47	125.39	128.83
28	RH	1001	CYC	C1A-C2A-C3A	-2.47	104.05	106.78
26	XE	201	PEB	CBC-CAC-C2C	-2.47	108.40	112.62
26	NJ	204	PEB	CBA-CAA-C3A	-2.47	107.96	113.47
26	fF	201	PEB	C3B-C4B-NB	2.47	113.65	110.05
26	A6	301	PEB	CMB-C2B-C1B	2.47	128.87	125.06
26	WA	201	PEB	CAA-C3A-C2A	-2.47	108.08	114.26
26	GA	202	PEB	CHA-C1B-NB	-2.47	119.76	124.93
26	J3	201	PEB	CHC-C4C-C3C	-2.47	126.12	130.34
26	O8	203	PEB	CMB-C2B-C1B	2.47	128.87	125.06
26	f7	201	PEB	OD-C4D-ND	-2.47	122.27	125.93
26	h8	201	PEB	OD-C4D-ND	-2.47	122.27	125.93
26	RI	202	PEB	CMA-C2A-C1A	-2.47	107.07	112.40
26	14	201	PEB	OA-C1A-C2A	-2.47	124.21	126.17
26	F8	201	PEB	CMD-C2D-C3D	2.47	133.55	130.06
26	eD	401	PEB	CHB-C4B-NB	-2.47	125.40	128.83
26	T9	201	PEB	CAB-C3B-C4B	2.47	129.38	125.01
26	mA	201	PEB	CAB-C3B-C4B	2.47	129.38	125.01
26	UB	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
28	C6	1001	CYC	CHA-C1A-C2A	-2.47	119.61	125.32
26	GJ	202	PEB	C1C-CHB-C4B	-2.47	125.86	128.81
26	oG	201	PEB	O1C-CGC-CBC	-2.47	115.14	123.08
26	C5	201	PEB	CHC-C1D-ND	-2.47	111.08	113.95
26	GA	201	PEB	CHC-C1D-ND	-2.47	111.08	113.95
28	F2	1001	CYC	C2A-C1A-NA	2.47	113.64	110.05
26	AD	201	PEB	OA-C1A-C2A	-2.47	124.21	126.17
28	BB	1001	CYC	CHA-C1A-C2A	-2.47	119.61	125.32
26	F9	201	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	X9	201	PEB	CMB-C2B-C1B	2.47	128.87	125.06
26	V9	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
26	O8	201	PEB	OD-C4D-ND	-2.47	122.27	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l6	202	PEB	CHA-C1B-NB	-2.47	119.77	124.93
26	A9	301	PEB	CHA-C1B-NB	-2.47	119.77	124.93
28	FF	1001	CYC	CHB-C1B-C2B	2.47	131.84	126.95
26	HC	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
26	H8	201	PEB	CMC-C3C-C2C	-2.47	120.28	124.94
26	F5	202	PEB	OD-C4D-ND	-2.47	122.27	125.93
26	HD	203	PEB	OD-C4D-ND	-2.47	122.27	125.93
26	c4	203	PEB	C3B-C4B-NB	2.47	113.64	110.05
26	dG	202	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
26	v4	202	PEB	CAB-CBB-CGB	-2.47	108.29	113.60
26	aA	203	PEB	CHA-C1B-NB	-2.47	119.77	124.93
26	p4	201	PEB	CAA-C3A-C2A	-2.47	108.09	114.26
26	Y4	201	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
26	Z8	202	PEB	CBA-CAA-C3A	-2.47	107.97	113.47
26	R6	202	PEB	CAB-C3B-C4B	2.47	129.38	125.01
27	N9	201	PUB	CHB-C1C-C2C	-2.47	119.62	125.32
27	yG	302	PUB	C4B-CHB-C1C	2.47	131.76	128.81
28	uH	1001	CYC	C2A-C1A-NA	2.47	113.64	110.05
26	E1	201	PEB	CBA-CAA-C3A	-2.47	107.97	113.47
26	F8	201	PEB	CMA-C2A-C1A	-2.47	107.08	112.40
26	LE	202	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	DI	1002	PEB	CHA-C1B-NB	-2.47	119.77	124.93
26	X3	202	PEB	C2B-C1B-NB	2.47	115.80	110.53
26	HA	201	PEB	CBC-CAC-C2C	-2.47	108.41	112.62
26	CC	203	PEB	CHC-C1D-ND	-2.47	111.08	113.95
26	I9	201	PEB	C1B-C2B-C3B	-2.47	103.67	106.51
26	C3	201	PEB	CBA-CAA-C3A	-2.47	107.97	113.47
26	S6	201	PEB	CAB-CBB-CGB	-2.47	108.29	113.60
26	d6	203	PEB	C3B-C4B-NB	2.47	113.64	110.05
27	AI	302	PUB	C2C-C1C-NC	2.47	113.64	110.05
26	aF	202	PEB	C1C-CHB-C4B	-2.47	125.86	128.81
26	R7	201	PEB	OD-C4D-C3D	-2.47	123.87	129.46
26	FD	201	PEB	OD-C4D-C3D	-2.47	123.87	129.46
26	I8	203	PEB	CAB-C3B-C4B	2.47	129.37	125.01
26	V9	201	PEB	OA-C1A-C2A	-2.47	124.21	126.17
26	U3	202	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	k4	201	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	eE	203	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	SG	202	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	Z6	203	PEB	OD-C4D-C3D	-2.47	123.87	129.46
26	d6	202	PEB	OD-C4D-C3D	-2.47	123.87	129.46
26	bF	203	PEB	OD-C4D-ND	-2.47	122.28	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OJ	201	PEB	C2A-C1A-NA	2.47	110.40	108.27
26	g4	203	PEB	C3B-C4B-NB	2.47	113.64	110.05
26	bB	202	PEB	C3B-C4B-NB	2.47	113.64	110.05
26	VF	202	PEB	C3B-C4B-NB	2.47	113.64	110.05
28	wH	1001	CYC	C2A-C1A-NA	2.47	113.64	110.05
26	fI	201	PEB	CBC-CAC-C2C	-2.47	108.41	112.62
26	Q3	201	PEB	CBA-CAA-C3A	-2.47	107.98	113.47
26	N8	201	PEB	C1C-CHB-C4B	-2.47	125.86	128.81
26	N4	201	PEB	OD-C4D-C3D	-2.47	123.87	129.46
26	xE	304	PEB	CAA-C3A-C4A	-2.47	106.34	112.67
26	pG	202	PEB	CHB-C4B-NB	-2.47	125.41	128.83
28	JH	1001	CYC	C1B-CHB-C4A	2.47	134.10	128.08
26	i4	201	PEB	C4B-C3B-C2B	-2.47	104.05	106.78
26	a2	201	PEB	C1B-C2B-C3B	-2.47	103.68	106.51
26	cI	202	PEB	CAB-C3B-C4B	2.47	129.37	125.01
26	hA	201	PEB	OD-C4D-ND	-2.47	122.28	125.93
26	I4	201	PEB	OD-C4D-C3D	-2.47	123.88	129.46
26	h2	202	PEB	CBB-CAB-C3B	-2.47	105.78	112.63
26	tG	202	PEB	CHA-C1B-C2B	-2.47	118.56	124.90
26	G9	202	PEB	CAC-C2C-C3C	2.46	134.33	127.25
26	B3	203	PEB	CAB-C3B-C4B	2.46	129.37	125.01
26	jA	203	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	G6	1002	PEB	C1B-C2B-C3B	-2.46	103.68	106.51
26	UG	201	PEB	CHA-C1B-C2B	2.46	131.24	124.90
27	QA	201	PUB	CHA-C1B-C2B	-2.46	126.13	130.34
26	P9	201	PEB	OD-C4D-ND	-2.46	122.28	125.93
26	T2	202	PEB	C3B-C4B-NB	2.46	113.63	110.05
26	fI	201	PEB	C4B-NB-C1B	-2.46	101.87	106.51
26	lF	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	K9	202	PEB	CHC-C4C-C3C	-2.46	126.13	130.34
26	E4	201	PEB	CHA-C1B-NB	-2.46	119.78	124.93
26	C5	203	PEB	CHC-C1D-ND	-2.46	111.09	113.95
26	A6	301	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	aG	201	PEB	C2A-C1A-NA	2.46	110.40	108.27
26	I5	203	PEB	C3B-C4B-NB	2.46	113.63	110.05
26	U1	202	PEB	C1B-C2B-C3B	-2.46	103.68	106.51
28	F2	1001	CYC	C4A-C3A-C2A	-2.46	103.68	106.51
26	C3	202	PEB	CMB-C2B-C1B	2.46	128.86	125.06
26	CC	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
28	FF	1001	CYC	CHA-C1A-C2A	-2.46	119.63	125.32
26	LE	202	PEB	C2B-C1B-NB	2.46	115.79	110.53
26	J4	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CH	1001	CYC	C2B-C1B-NB	2.46	110.59	106.99
26	h4	201	PEB	C1C-CHB-C4B	-2.46	125.87	128.81
26	J5	201	PEB	C1C-CHB-C4B	-2.46	125.87	128.81
26	a2	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
28	PH	1001	CYC	CHA-C1A-NA	-2.46	125.41	128.83
28	oH	1001	CYC	C2B-C1B-NB	2.46	110.59	106.99
26	GG	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	j4	201	PEB	CAB-CBB-CGB	-2.46	108.31	113.60
26	QD	201	PEB	C3B-C4B-NB	2.46	113.63	110.05
26	AA	302	PEB	CBC-CAC-C2C	-2.46	108.42	112.62
26	i4	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	m7	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	NG	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
26	ZE	202	PEB	CHB-C4B-C3B	-2.46	119.63	125.32
26	NB	1002	PEB	C1C-CHB-C4B	-2.46	125.87	128.81
26	k7	202	PEB	CMA-C2A-C1A	-2.46	107.10	112.40
26	OJ	201	PEB	CBA-CAA-C3A	2.46	118.95	113.47
26	Q6	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46
26	L1	203	PEB	OD-C4D-ND	-2.46	122.28	125.93
27	AA	303	PUB	CMC-C3C-C4C	2.46	133.74	126.37
26	L1	203	PEB	CMB-C2B-C1B	2.46	128.85	125.06
26	c6	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
26	N1	201	PEB	CHA-C1B-C2B	2.46	131.23	124.90
28	E6	1001	CYC	CHB-C1B-NB	-2.46	120.78	126.06
26	aA	203	PEB	OD-C4D-C3D	-2.46	123.89	129.46
26	SB	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
26	k2	203	PEB	CHA-C1B-NB	-2.46	119.79	124.93
26	P3	202	PEB	CHA-C4A-NA	2.46	128.13	125.20
27	Q8	201	PUB	C1D-CHC-C4C	-2.46	108.02	113.37
26	d8	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
26	hI	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
28	TH	1001	CYC	C1B-NB-C4B	-2.46	107.54	110.67
28	lH	1001	CYC	C1B-CHB-C4A	2.46	134.09	128.08
27	xG	301	PUB	CAB-CBB-CGB	-2.46	106.86	113.76
26	kA	201	PEB	C1B-C2B-C3B	-2.46	103.68	106.51
26	I4	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46
26	W4	201	PEB	O1B-CGB-CBB	-2.46	115.18	123.08
26	g1	202	PEB	OD-C4D-ND	-2.46	122.29	125.93
26	GB	1002	PEB	OD-C4D-ND	-2.46	122.29	125.93
26	f6	203	PEB	C3B-C4B-NB	2.46	113.63	110.05
27	A6	303	PUB	C2C-C1C-NC	2.46	113.63	110.05
26	C1	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d4	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
26	U8	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
28	PH	1001	CYC	CHB-C1B-C2B	-2.46	122.08	126.95
26	G4	202	PEB	CBC-CAC-C2C	-2.46	108.42	112.62
28	MB	1001	CYC	CHA-C1A-NA	-2.46	125.42	128.83
26	24	405	PEB	CHC-C1D-ND	-2.46	111.09	113.95
28	sH	1001	CYC	C1B-C2B-C3B	-2.46	105.31	107.87
26	W3	201	PEB	O2C-CGC-CBC	2.46	121.93	114.03
26	T2	202	PEB	CHC-C1D-ND	-2.46	111.09	113.95
26	T9	202	PEB	CHA-C1B-NB	-2.46	119.79	124.93
26	RA	201	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
26	B3	203	PEB	CHC-C4C-C3C	-2.46	126.14	130.34
28	pH	1001	CYC	C2B-C1B-NB	2.46	110.58	106.99
28	fH	1001	CYC	C1B-NB-C4B	-2.46	107.54	110.67
26	f7	203	PEB	OD-C4D-ND	-2.46	122.29	125.93
26	QG	202	PEB	OD-C4D-ND	-2.46	122.29	125.93
26	e2	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
26	W4	202	PEB	C3B-C4B-NB	2.46	113.62	110.05
26	m1	202	PEB	C2A-C1A-NA	2.46	110.39	108.27
26	S3	202	PEB	C2B-C1B-NB	2.46	115.77	110.53
26	r1	202	PEB	CAB-C3B-C4B	2.46	129.35	125.01
26	J1	203	PEB	CAB-CBB-CGB	-2.46	108.32	113.60
26	O3	201	PEB	CHC-C1D-ND	-2.46	111.09	113.95
26	V8	201	PEB	CHC-C1D-ND	2.46	116.80	113.95
28	mH	1001	CYC	C2B-C1B-NB	2.46	110.58	106.99
26	eF	202	PEB	OD-C4D-ND	-2.46	122.29	125.93
28	B6	1001	CYC	CHA-C1A-C2A	-2.46	119.65	125.32
26	EA	202	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
26	TB	201	PEB	CHB-C4B-C3B	-2.46	119.65	125.32
26	aI	201	PEB	CHB-C4B-C3B	-2.46	119.65	125.32
26	M1	403	PEB	CHC-C1D-ND	-2.46	111.10	113.95
26	ZB	203	PEB	CHC-C1D-ND	-2.46	111.10	113.95
26	XD	203	PEB	OD-C4D-ND	-2.46	122.29	125.93
26	dB	203	PEB	C3B-C4B-NB	2.45	113.62	110.05
26	L5	201	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
26	P9	202	PEB	CAB-C3B-C4B	2.45	129.35	125.01
28	L7	1001	CYC	C1B-CHB-C4A	-2.45	122.08	128.08
28	C6	1001	CYC	C4A-C3A-C2A	-2.45	103.69	106.51
26	A5	201	PEB	C3B-C4B-NB	2.45	113.62	110.05
26	J7	1002	PEB	OD-C4D-C3D	-2.45	123.90	129.46
26	uE	202	PEB	OD-C4D-C3D	-2.45	123.90	129.46
26	CG	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	uG	203	PEB	CHA-C1B-NB	-2.45	119.80	124.93
28	YH	1003	CYC	C2B-C1B-NB	2.45	110.58	106.99
26	ND	202	PEB	CBC-CAC-C2C	2.45	116.81	112.62
26	IE	201	PEB	CBC-CAC-C2C	-2.45	108.43	112.62
26	P9	202	PEB	C3B-C4B-NB	2.45	113.62	110.05
26	KJ	202	PEB	C3B-C4B-NB	2.45	113.62	110.05
26	LJ	201	PEB	C3B-C4B-NB	2.45	113.62	110.05
26	gA	202	PEB	CHA-C1B-NB	-2.45	119.80	124.93
26	FD	202	PEB	OD-C4D-ND	-2.45	122.30	125.93
26	ZI	202	PEB	CHA-C1B-NB	-2.45	119.80	124.93
26	X1	202	PEB	CHC-C4C-C3C	-2.45	126.15	130.34
26	C5	203	PEB	OD-C4D-C3D	-2.45	123.90	129.46
26	U6	202	PEB	OD-C4D-C3D	-2.45	123.90	129.46
26	C8	202	PEB	OD-C4D-C3D	-2.45	123.90	129.46
26	W6	201	PEB	CHB-C4B-C3B	-2.45	119.65	125.32
26	C8	203	PEB	CAA-C3A-C4A	-2.45	106.38	112.67
26	i2	203	PEB	CHC-C1D-ND	-2.45	111.10	113.95
26	H1	201	PEB	OD-C4D-ND	-2.45	122.30	125.93
26	SJ	202	PEB	OA-C1A-C2A	-2.45	124.22	126.17
26	ZE	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46
26	BD	201	PEB	CAB-C3B-C2B	2.45	132.44	127.88
26	BJ	202	PEB	CHA-C1B-NB	-2.45	119.80	124.93
26	OA	201	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
26	R7	201	PEB	CHA-C1B-NB	-2.45	119.81	124.93
26	gA	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	KD	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	m1	203	PEB	C3B-C4B-NB	2.45	113.61	110.05
26	BE	201	PEB	OD-C4D-ND	2.45	129.56	125.93
26	aI	203	PEB	C2A-C1A-NA	2.45	110.39	108.27
26	TE	201	PEB	CAB-CBB-CGB	-2.45	108.33	113.60
28	yH	1001	CYC	C4A-C3A-C2A	-2.45	103.69	106.51
26	b6	202	PEB	CMB-C2B-C1B	2.45	128.84	125.06
26	m6	203	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	EE	201	PEB	CHB-C4B-C3B	-2.45	119.66	125.32
26	fB	201	PEB	CAB-CBB-CGB	-2.45	108.33	113.60
26	P1	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	TI	202	PEB	C3B-C4B-NB	2.45	113.61	110.05
26	pG	201	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
26	L8	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	aB	202	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
28	WH	1001	CYC	C1B-NB-C4B	-2.45	107.55	110.67
26	F9	202	PEB	CMB-C2B-C1B	2.45	128.84	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HJ	201	PEB	CMB-C2B-C1B	2.45	128.84	125.06
26	S7	201	PEB	C3B-C4B-NB	2.45	113.61	110.05
26	PE	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	PF	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	e4	201	PEB	CHC-C1D-ND	-2.45	111.10	113.95
26	N4	201	PEB	CHA-C1B-C2B	2.45	131.20	124.90
26	e7	202	PEB	CAA-C3A-C2A	-2.45	108.14	114.26
26	NA	201	PEB	CMA-C2A-C1A	-2.45	107.12	112.40
26	k7	201	PEB	OD-C4D-ND	-2.45	122.30	125.93
26	f6	202	PEB	C2A-C3A-C4A	-2.45	97.67	101.34
26	A2	301	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	QB	202	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	VD	203	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
26	X9	203	PEB	CHA-C1B-NB	-2.45	119.81	124.93
26	N9	204	PEB	OD-C4D-C3D	-2.45	123.91	129.46
26	BE	201	PEB	CAB-C3B-C4B	2.45	129.34	125.01
26	a8	204	PEB	OD-C4D-ND	-2.45	122.30	125.93
26	HB	1002	PEB	OD-C4D-ND	-2.45	122.30	125.93
26	j2	201	PEB	CHA-C1B-NB	-2.45	119.81	124.93
26	F4	202	PEB	CBC-CAC-C2C	-2.45	108.44	112.62
26	GC	201	PEB	C3B-C4B-NB	2.45	113.61	110.05
26	kB	201	PEB	C1B-C2B-C3B	-2.45	103.70	106.51
26	SD	201	PEB	OD-C4D-ND	-2.45	122.31	125.93
26	SB	201	PEB	CAB-CBB-CGB	-2.45	108.34	113.60
28	CH	1001	CYC	C4D-CHA-C1A	2.45	131.73	128.81
26	dG	202	PEB	C4B-C3B-C2B	-2.45	104.08	106.78
26	c4	201	PEB	OD-C4D-C3D	-2.45	123.92	129.46
26	NE	201	PEB	OD-C4D-C3D	-2.45	123.92	129.46
26	i2	203	PEB	OD-C4D-ND	-2.45	122.31	125.93
26	nE	201	PEB	OD-C4D-ND	-2.45	122.31	125.93
26	V3	202	PEB	C2B-C1B-NB	2.45	115.75	110.53
26	Y7	201	PEB	OD-C4D-C3D	-2.45	123.92	129.46
26	YD	301	PEB	CMB-C2B-C1B	2.45	128.83	125.06
26	c6	202	PEB	CHA-C4A-NA	-2.45	122.30	125.20
28	NF	1001	CYC	C1A-C2A-C3A	-2.45	104.08	106.78
26	QF	203	PEB	OD-C4D-C3D	-2.45	123.92	129.46
26	DG	203	PEB	OD-C4D-C3D	-2.45	123.92	129.46
26	P4	202	PEB	CHB-C4B-NB	-2.45	125.43	128.83
26	Y3	303	PEB	CAB-C3B-C4B	2.45	129.34	125.01
26	A5	201	PEB	CBA-CAA-C3A	-2.45	108.02	113.47
28	MH	1001	CYC	C4A-C3A-C2A	-2.45	103.70	106.51
26	kE	203	PEB	CMB-C2B-C1B	2.45	128.83	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	MH	1001	CYC	C1B-NB-C4B	-2.45	107.56	110.67
26	h1	202	PEB	C2A-C1A-NA	2.45	110.38	108.27
26	F3	203	PEB	OD-C4D-ND	-2.45	122.31	125.93
26	jG	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
26	k4	203	PEB	OD-C4D-ND	-2.44	122.31	125.93
26	m6	203	PEB	CMB-C2B-C1B	2.44	128.83	125.06
26	I4	202	PEB	C2A-C1A-NA	2.44	110.38	108.27
26	Z7	202	PEB	OD-C4D-C3D	-2.44	123.92	129.46
26	J9	201	PEB	C3B-C4B-NB	2.44	113.60	110.05
27	K3	203	PUB	C2C-C1C-NC	2.44	113.60	110.05
26	U4	202	PEB	C1B-C2B-C3B	-2.44	103.70	106.51
26	K6	201	PEB	OD-C4D-ND	-2.44	122.31	125.93
26	k8	202	PEB	CAA-C3A-C4A	2.44	118.95	112.67
26	Z7	203	PEB	OD-C4D-C3D	-2.44	123.92	129.46
26	CD	201	PEB	CMA-C2A-C1A	-2.44	107.14	112.40
26	B9	202	PEB	OD-C4D-C3D	-2.44	123.92	129.46
26	l7	202	PEB	OD-C4D-ND	-2.44	122.31	125.93
26	Q4	202	PEB	C1B-C2B-C3B	-2.44	103.70	106.51
27	xE	301	PUB	CAC-CBC-CGC	-2.44	108.35	113.60
26	iE	202	PEB	CAB-C3B-C4B	2.44	129.33	125.01
26	RG	201	PEB	CAB-C3B-C4B	2.44	129.33	125.01
26	P1	202	PEB	CHB-C4B-C3B	-2.44	119.68	125.32
26	v4	201	PEB	CHB-C4B-C3B	-2.44	119.68	125.32
28	MB	1001	CYC	CHB-C1B-NB	-2.44	120.81	126.06
26	e3	401	PEB	C3B-C4B-NB	2.44	113.60	110.05
26	gG	203	PEB	C3B-C4B-NB	2.44	113.60	110.05
26	Z2	202	PEB	CHA-C1B-NB	-2.44	119.82	124.93
26	N1	201	PEB	CAB-C3B-C4B	2.44	129.33	125.01
26	MG	201	PEB	CAB-C3B-C4B	2.44	129.33	125.01
26	c7	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46
28	CF	1001	CYC	CHA-C1A-NA	-2.44	125.44	128.83
26	QJ	202	PEB	C1B-C2B-C3B	-2.44	103.70	106.51
26	F1	202	PEB	C3B-C4B-NB	2.44	113.60	110.05
26	oE	203	PEB	C3B-C4B-NB	2.44	113.60	110.05
26	k1	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46
26	mG	201	PEB	OD-C4D-ND	-2.44	122.31	125.93
26	KA	201	PEB	CMA-C2A-C1A	-2.44	107.14	112.40
26	ZG	202	PEB	OD-C4D-C3D	-2.44	123.93	129.46
26	v1	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
26	J5	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
26	k8	202	PEB	O2B-CGB-CBB	2.44	121.87	114.03
26	sG	202	PEB	C1B-C2B-C3B	-2.44	103.70	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	DG	203	PEB	C2B-C1B-NB	2.44	115.74	110.53
26	MD	202	PEB	C1C-CHB-C4B	-2.44	125.89	128.81
26	jF	203	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	mB	203	PEB	OD-C4D-C3D	-2.44	123.93	129.46
26	F4	202	PEB	CMA-C2A-C1A	-2.44	107.14	112.40
26	QD	201	PEB	C2A-C1A-NA	2.44	110.38	108.27
26	RF	201	PEB	C2B-C1B-NB	2.44	115.74	110.53
26	e8	202	PEB	CHC-C1D-ND	-2.44	111.11	113.95
26	T6	201	PEB	CAB-C3B-C4B	2.44	129.33	125.01
26	LA	202	PEB	OD-C4D-C3D	-2.44	123.93	129.46
26	SB	203	PEB	OD-C4D-C3D	-2.44	123.93	129.46
26	O2	202	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
26	A1	201	PEB	OD-C4D-ND	-2.44	122.31	125.93
26	a2	203	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	a1	202	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
26	UF	202	PEB	C1C-CHB-C4B	2.44	131.72	128.81
26	s4	202	PEB	C3B-C4B-NB	2.44	113.60	110.05
26	WA	201	PEB	OD-C4D-ND	-2.44	122.32	125.93
26	mB	201	PEB	OD-C4D-ND	-2.44	122.32	125.93
26	J9	203	PEB	CHA-C1B-NB	-2.44	119.83	124.93
26	YB	201	PEB	OD-C4D-C3D	-2.44	123.93	129.46
26	f6	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
28	uH	1001	CYC	CAC-C3C-C2C	2.44	120.35	114.26
26	Y7	201	PEB	CHB-C4B-NB	-2.44	125.44	128.83
26	KE	202	PEB	CAC-C2C-C3C	2.44	134.25	127.25
26	U8	203	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	cG	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
28	tH	1001	CYC	C2B-C1B-NB	2.44	110.56	106.99
28	D7	1001	CYC	C2A-C1A-NA	2.44	113.60	110.05
26	21	405	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	H3	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	JJ	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	h1	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
26	e6	203	PEB	OD-C4D-ND	-2.44	122.32	125.93
26	y4	202	PEB	CAA-C3A-C2A	-2.44	108.17	114.26
26	T3	203	PEB	CAB-C3B-C2B	2.44	132.42	127.88
26	Q9	202	PEB	CHA-C4A-NA	-2.44	122.31	125.20
26	R9	203	PEB	CHA-C1B-C2B	2.44	131.17	124.90
26	P4	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	G1	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	c8	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	VD	203	PEB	C1B-C2B-C3B	-2.44	103.71	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X1	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	m7	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	F4	203	PEB	CHA-C1B-NB	-2.44	119.83	124.93
26	Y8	203	PEB	CAB-C3B-C4B	2.44	129.32	125.01
26	FD	203	PEB	CHC-C1D-ND	-2.44	111.12	113.95
26	RB	201	PEB	C2A-C1A-NA	2.44	110.37	108.27
26	v1	202	PEB	CAA-C3A-C2A	-2.44	108.17	114.26
26	I5	202	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	FG	202	PEB	C2B-C1B-NB	2.44	115.73	110.53
26	nG	201	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
26	DF	1002	PEB	CHA-C1B-C2B	2.44	131.17	124.90
26	RB	202	PEB	CAB-C3B-C4B	2.44	129.32	125.01
26	BJ	201	PEB	CAB-C3B-C4B	2.44	129.32	125.01
26	S6	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	AF	305	PEB	CMB-C2B-C1B	2.44	128.82	125.06
26	J8	202	PEB	C2A-C1A-NA	2.44	110.37	108.27
26	R3	203	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
26	RD	203	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
26	SG	203	PEB	C1B-C2B-C3B	-2.44	103.71	106.51
26	T1	201	PEB	CHB-C4B-C3B	-2.44	119.69	125.32
26	S2	202	PEB	CBA-CAA-C3A	-2.44	108.04	113.47
26	w4	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
26	LC	203	PEB	OD-C4D-ND	-2.44	122.32	125.93
26	cA	202	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	yG	301	PEB	CHC-C1D-ND	-2.44	111.12	113.95
26	D6	1002	PEB	O2B-CGB-CBB	2.44	121.85	114.03
26	U9	201	PEB	OD-C4D-C3D	-2.44	123.94	129.46
26	d6	202	PEB	CAA-C3A-C4A	-2.44	106.42	112.67
28	WH	1001	CYC	C4A-C3A-C2A	-2.44	103.71	106.51
28	DI	1001	CYC	CBB-CAB-C3B	-2.44	105.72	112.43
26	l1	202	PEB	C4B-C3B-C2B	-2.43	104.09	106.78
26	MA	202	PEB	C4B-C3B-C2B	-2.43	104.09	106.78
26	m4	203	PEB	C3B-C4B-NB	2.43	113.59	110.05
26	wG	302	PEB	OD-C4D-C3D	-2.43	123.94	129.46
26	AI	304	PEB	OD-C4D-C3D	-2.43	123.94	129.46
26	d2	201	PEB	CHC-C1D-ND	-2.43	111.12	113.95
26	qG	203	PEB	CHA-C1B-NB	-2.43	119.84	124.93
26	D7	1002	PEB	CHA-C1B-C2B	2.43	131.16	124.90
26	lF	202	PEB	OD-C4D-ND	-2.43	122.32	125.93
26	XG	202	PEB	CBC-CAC-C2C	-2.43	108.47	112.62
26	z1	201	PEB	C1B-C2B-C3B	-2.43	103.71	106.51
26	eA	201	PEB	C1B-C2B-C3B	-2.43	103.71	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	gI	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
26	S3	201	PEB	O2C-CGC-CBC	2.43	121.85	114.03
26	HB	1002	PEB	C2A-C1A-NA	2.43	110.37	108.27
26	EG	201	PEB	CBC-CAC-C2C	-2.43	108.47	112.62
26	P4	203	PEB	OD-C4D-C3D	-2.43	123.95	129.46
26	BE	202	PEB	CHA-C1B-NB	-2.43	119.84	124.93
26	e8	201	PEB	C1B-C2B-C3B	-2.43	103.71	106.51
26	J9	201	PEB	CAB-C3B-C4B	2.43	129.31	125.01
26	KD	201	PEB	CAA-C3A-C4A	-2.43	106.42	112.67
26	II	201	PEB	C4B-C3B-C2B	-2.43	104.09	106.78
26	b6	202	PEB	CAB-CBB-CGB	-2.43	108.37	113.60
26	oG	201	PEB	O2C-CGC-CBC	2.43	121.85	114.03
26	IC	203	PEB	CAC-CBC-CGC	-2.43	106.94	113.76
26	A7	305	PEB	OD-C4D-C3D	-2.43	123.95	129.46
26	ZF	201	PEB	OD-C4D-C3D	-2.43	123.95	129.46
26	T8	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
26	RJ	203	PEB	CHA-C1B-C2B	2.43	131.16	124.90
26	c6	201	PEB	CAB-C3B-C4B	2.43	129.31	125.01
26	j7	203	PEB	CAB-CBB-CGB	-2.43	108.37	113.60
26	BE	202	PEB	CAA-C3A-C4A	-2.43	106.43	112.67
26	RF	202	PEB	CHC-C4C-C3C	-2.43	126.19	130.34
27	AI	303	PUB	CMD-C2D-C3D	2.43	131.42	127.77
27	A8	303	PUB	CHA-C1B-C2B	-2.43	126.19	130.34
26	kA	202	PEB	CAA-C3A-C4A	2.43	118.92	112.67
26	SJ	201	PEB	OD-C4D-C3D	-2.43	123.95	129.46
26	KJ	202	PEB	CHA-C1B-C2B	2.43	131.15	124.90
26	P7	202	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
26	e8	202	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
26	YA	202	PEB	C2A-C1A-NA	2.43	110.37	108.27
26	wG	303	PEB	C2A-C1A-NA	2.43	110.37	108.27
26	J1	201	PEB	CHB-C4B-NB	-2.43	125.45	128.83
28	EB	1001	CYC	CBD-CAD-C3D	-2.43	108.47	112.62
26	C1	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
26	I9	201	PEB	CHA-C4A-NA	2.43	128.09	125.20
26	RA	202	PEB	CHA-C4A-NA	-2.43	122.31	125.20
28	JH	1001	CYC	CAB-C3B-C2B	2.43	131.69	127.53
26	R8	202	PEB	C3B-C4B-NB	2.43	113.58	110.05
26	ZA	201	PEB	CHA-C1B-C2B	2.43	131.15	124.90
26	MD	202	PEB	CHA-C1B-NB	-2.43	119.85	124.93
26	iB	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
26	aG	202	PEB	OA-C1A-C2A	-2.43	124.24	126.17
26	SI	202	PEB	OD-C4D-ND	-2.43	122.33	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	QF	203	PEB	C4B-C3B-C2B	-2.43	104.09	106.78
26	O6	201	PEB	CMA-C2A-C1A	-2.43	107.17	112.40
26	dA	201	PEB	CBC-CAC-C2C	-2.43	108.47	112.62
26	gA	202	PEB	CHC-C4C-C3C	-2.43	126.19	130.34
26	yG	301	PEB	CHC-C4C-C3C	-2.43	126.19	130.34
26	iB	202	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	lE	202	PEB	CHB-C4B-C3B	-2.43	119.71	125.32
26	ZF	202	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	Q8	204	PEB	C2B-C1B-NB	2.43	115.71	110.53
26	ZG	202	PEB	C2B-C1B-NB	2.43	115.71	110.53
28	NH	1001	CYC	C1B-CHB-C4A	2.43	134.01	128.08
26	OB	202	PEB	C3B-C4B-NB	2.43	113.58	110.05
26	G9	202	PEB	CMC-C3C-C2C	2.43	129.52	124.94
26	C3	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	j8	203	PEB	OD-C4D-C3D	-2.43	123.96	129.46
27	yE	302	PUB	CHA-C4A-NA	-2.43	111.13	113.95
28	EI	1001	CYC	CHA-C1A-NA	-2.43	125.46	128.83
26	wE	303	PEB	CBB-CAB-C3B	2.43	119.37	112.63
26	S9	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	fG	201	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
26	bG	201	PEB	CBA-CAA-C3A	-2.43	108.06	113.47
26	uG	202	PEB	C3B-C4B-NB	2.43	113.58	110.05
26	OE	203	PEB	CAA-C3A-C2A	-2.43	108.19	114.26
26	k1	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
27	xG	305	PUB	CAC-C2C-C1C	2.43	129.30	125.01
26	RE	202	PEB	CAB-C3B-C4B	2.43	129.30	125.01
26	I8	203	PEB	C2B-C1B-NB	2.43	115.71	110.53
26	G5	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
26	hA	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
26	U7	203	PEB	CMB-C2B-C1B	2.43	128.80	125.06
26	l8	201	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
26	k7	202	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
26	aA	202	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	ZB	203	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	YI	202	PEB	OD-C4D-C3D	-2.43	123.96	129.46
28	M2	1001	CYC	CBD-CAD-C3D	-2.43	108.48	112.62
26	k6	202	PEB	C1C-CHB-C4B	-2.43	125.91	128.81
26	FD	202	PEB	CAB-C3B-C4B	2.43	129.30	125.01
26	e4	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
26	YD	301	PEB	CMC-C3C-C2C	-2.43	120.37	124.94
26	y1	203	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
26	C9	202	PEB	C1B-C2B-C3B	-2.43	103.72	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P2	203	PEB	CAB-CBB-CGB	2.43	118.82	113.60
26	A4	201	PEB	CHB-C4B-C3B	-2.43	119.72	125.32
27	A2	303	PUB	CMD-C2D-C3D	2.42	131.41	127.77
27	AJ	302	PUB	CMD-C2D-C3D	2.42	131.41	127.77
26	f6	202	PEB	OA-C1A-C2A	-2.42	124.25	126.17
26	e7	201	PEB	CHC-C4C-C3C	-2.42	126.20	130.34
26	xE	304	PEB	CHA-C4A-NA	2.42	128.09	125.20
26	J3	201	PEB	CAB-CBB-CGB	-2.42	108.39	113.60
28	IH	1001	CYC	C2A-C1A-NA	2.42	113.58	110.05
26	LD	202	PEB	CHB-C4B-C3B	-2.42	119.72	125.32
26	kG	201	PEB	C1B-C2B-C3B	-2.42	103.72	106.51
26	F1	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	e2	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	J5	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	PF	201	PEB	C2A-C1A-NA	2.42	110.36	108.27
26	E8	203	PEB	CMD-C2D-C3D	2.42	133.48	130.06
26	lB	202	PEB	OD-C4D-ND	-2.42	122.34	125.93
28	CH	1001	CYC	C2A-C1A-NA	2.42	113.58	110.05
26	TI	203	PEB	C1B-C2B-C3B	-2.42	103.72	106.51
26	l1	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	xG	304	PEB	OD-C4D-C3D	-2.42	123.97	129.46
27	A6	303	PUB	CMD-C2D-C3D	2.42	131.41	127.77
26	YB	202	PEB	CAC-C2C-C3C	2.42	134.21	127.25
26	FA	201	PEB	CMA-C2A-C1A	-2.42	107.18	112.40
26	U7	203	PEB	OD-C4D-ND	-2.42	122.34	125.93
26	uE	201	PEB	OD-C4D-ND	-2.42	122.34	125.93
26	cI	203	PEB	CHC-C1D-ND	-2.42	111.13	113.95
26	k2	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	BD	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	mB	201	PEB	C2A-C1A-NA	2.42	110.36	108.27
26	OE	201	PEB	CAC-CBC-CGC	-2.42	106.97	113.76
26	U6	202	PEB	CAB-CBB-CGB	-2.42	108.39	113.60
26	I3	202	PEB	OD-C4D-ND	-2.42	122.34	125.93
26	VG	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	OE	201	PEB	CMB-C2B-C1B	2.42	128.79	125.06
26	uE	203	PEB	C3B-C4B-NB	2.42	113.57	110.05
26	GC	201	PEB	CHC-C1D-ND	-2.42	111.13	113.95
26	MJ	201	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
26	k6	201	PEB	OD-C4D-ND	-2.42	122.34	125.93
26	OF	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
26	eI	203	PEB	CAB-CBB-CGB	2.42	118.81	113.60
26	OE	203	PEB	CHB-C4B-NB	-2.42	125.47	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F5	203	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	O1	201	PEB	C2B-C1B-NB	2.42	115.70	110.53
26	BD	202	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
26	f8	202	PEB	CAB-C3B-C4B	2.42	129.29	125.01
26	Q1	201	PEB	O2B-CGB-CBB	2.42	121.81	114.03
26	P8	202	PEB	C3B-C4B-NB	2.42	113.57	110.05
26	PG	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	PI	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
26	e2	201	PEB	C1C-CHB-C4B	2.42	131.70	128.81
26	ZF	203	PEB	C2A-C1A-NA	2.42	110.36	108.27
26	ME	203	PEB	CMD-C2D-C3D	-2.42	126.65	130.06
26	OA	201	PEB	CAA-C3A-C4A	-2.42	106.46	112.67
26	G4	201	PEB	C4B-C3B-C2B	-2.42	104.10	106.78
26	SI	202	PEB	CBA-CAA-C3A	-2.42	108.08	113.47
26	UJ	201	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
26	D3	203	PEB	OD-C4D-C3D	-2.42	123.98	129.46
26	NJ	202	PEB	CBC-CAC-C2C	-2.42	108.49	112.62
26	H3	203	PEB	C3B-C4B-NB	2.42	113.57	110.05
26	e2	201	PEB	CHA-C4A-NA	2.42	128.08	125.20
26	i6	201	PEB	C4B-C3B-C2B	-2.42	104.11	106.78
26	T1	201	PEB	CHA-C1B-NB	-2.42	119.87	124.93
26	j8	201	PEB	CMB-C2B-C1B	2.42	128.79	125.06
26	P7	202	PEB	CAC-CBC-CGC	-2.42	106.98	113.76
26	M8	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
26	UA	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
28	NH	1001	CYC	CAC-C3C-C4C	2.42	118.89	112.67
26	d1	203	PEB	CHA-C1B-C2B	2.42	131.12	124.90
26	P3	201	PEB	CAB-C3B-C4B	2.42	129.29	125.01
26	L1	201	PEB	CHB-C4B-C3B	-2.42	119.73	125.32
26	X1	201	PEB	CMB-C2B-C1B	2.42	128.79	125.06
26	v1	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
26	h4	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
26	SG	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
26	D3	201	PEB	OD-C4D-ND	-2.42	122.35	125.93
26	X4	202	PEB	CAA-C3A-C2A	2.42	120.30	114.26
26	z4	202	PEB	C3B-C4B-NB	2.42	113.57	110.05
26	SA	201	PEB	CMA-C2A-C1A	-2.42	107.19	112.40
26	NI	1002	PEB	CAB-CBB-CGB	-2.42	108.40	113.60
26	DA	202	PEB	OD-C4D-ND	-2.42	122.35	125.93
28	J7	1003	CYC	C1B-CHB-C4A	-2.42	122.17	128.08
26	aB	201	PEB	CHA-C1B-NB	-2.42	119.88	124.93
26	aE	201	PEB	C2A-C1A-NA	2.42	110.36	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	QH	1001	CYC	C2C-C1C-NC	2.42	110.36	108.27
26	R8	201	PEB	OD-C4D-ND	-2.42	122.35	125.93
28	pH	1001	CYC	C1B-CHB-C4A	2.42	133.99	128.08
26	JA	202	PEB	OA-C1A-C2A	-2.42	124.25	126.17
26	PA	201	PEB	CHA-C1B-C2B	2.42	131.12	124.90
26	K8	202	PEB	CHA-C1B-NB	-2.42	119.88	124.93
26	y4	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
28	J7	1001	CYC	C1A-C2A-C3A	-2.42	104.11	106.78
26	T1	202	PEB	CAB-CBB-CGB	-2.42	108.40	113.60
26	R7	202	PEB	OD-C4D-ND	-2.42	122.35	125.93
26	OA	202	PEB	CHA-C1B-NB	-2.42	119.88	124.93
26	FC	201	PEB	CHA-C1B-NB	-2.42	119.88	124.93
26	M1	401	PEB	CHC-C1D-ND	-2.42	111.14	113.95
26	G6	1002	PEB	CAA-C3A-C4A	-2.42	106.47	112.67
26	D9	203	PEB	CBA-CAA-C3A	-2.42	108.09	113.47
26	BD	202	PEB	C3B-C4B-NB	2.42	113.56	110.05
26	lF	203	PEB	C2A-C1A-NA	2.42	110.36	108.27
26	jE	202	PEB	OD-C4D-C3D	-2.42	123.99	129.46
26	KJ	201	PEB	OD-C4D-C3D	-2.42	123.99	129.46
26	lA	203	PEB	CHA-C1B-NB	-2.42	119.88	124.93
26	W9	201	PEB	C1C-CHB-C4B	2.42	131.69	128.81
26	N2	1002	PEB	CMD-C2D-C3D	2.42	133.47	130.06
26	KA	202	PEB	CMD-C2D-C3D	2.42	133.47	130.06
28	NH	1001	CYC	C2A-C1A-NA	2.42	113.56	110.05
26	BJ	203	PEB	CMB-C2B-C1B	2.42	128.78	125.06
26	KE	203	PEB	C2B-C1B-NB	2.42	115.68	110.53
26	PI	202	PEB	OD-C4D-C3D	-2.42	123.99	129.46
26	r4	202	PEB	CAB-C3B-C4B	2.42	129.28	125.01
28	M6	1001	CYC	CHB-C1B-NB	-2.42	120.87	126.06
26	A1	201	PEB	CBA-CAA-C3A	-2.42	108.09	113.47
26	J1	202	PEB	C3B-C4B-NB	2.41	113.56	110.05
26	f4	202	PEB	C3B-C4B-NB	2.41	113.56	110.05
26	YG	202	PEB	CMB-C2B-C1B	2.41	128.78	125.06
26	J5	201	PEB	CHC-C1D-ND	-2.41	111.14	113.95
26	UI	201	PEB	OA-C1A-C2A	-2.41	124.25	126.17
26	X1	203	PEB	CHA-C4A-NA	2.41	128.08	125.20
26	AJ	304	PEB	CHA-C4A-NA	-2.41	122.33	125.20
26	V2	201	PEB	OD-C4D-C3D	-2.41	123.99	129.46
26	Q4	201	PEB	O2B-CGB-CBB	2.41	121.79	114.03
26	F8	201	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
28	fH	1001	CYC	C4A-C3A-C2A	-2.41	103.74	106.51
26	F9	202	PEB	OD-C4D-ND	-2.41	122.35	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	HA	201	PEB	C2A-C1A-NA	2.41	110.35	108.27
26	J1	203	PEB	C3B-C4B-NB	2.41	113.56	110.05
26	fG	201	PEB	CAB-CBB-CGB	-2.41	108.41	113.60
26	W1	201	PEB	O1B-CGB-CBB	-2.41	115.33	123.08
26	U3	201	PEB	OD-C4D-C3D	-2.41	123.99	129.46
26	YF	201	PEB	OD-C4D-C3D	-2.41	123.99	129.46
26	O3	201	PEB	O2C-CGC-CBC	2.41	121.78	114.03
26	y4	201	PEB	O2B-CGB-CBB	2.41	121.78	114.03
26	x4	201	PEB	C1C-CHB-C4B	2.41	131.69	128.81
26	Y7	201	PEB	CHB-C4B-C3B	-2.41	119.75	125.32
26	Z8	201	PEB	CHA-C1B-C2B	2.41	131.11	124.90
26	O1	201	PEB	CMC-C3C-C2C	2.41	129.49	124.94
26	b2	202	PEB	CHA-C1B-NB	-2.41	119.89	124.93
26	jI	201	PEB	CHA-C1B-NB	-2.41	119.89	124.93
26	B9	201	PEB	CMA-C2A-C1A	-2.41	107.20	112.40
26	FA	201	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
26	K4	201	PEB	OD-C4D-C3D	-2.41	123.99	129.46
26	fB	201	PEB	CMD-C2D-C3D	2.41	133.47	130.06
26	WB	202	PEB	CHB-C4B-C3B	-2.41	119.75	125.32
26	LG	201	PEB	CBA-CAA-C3A	2.41	118.84	113.47
26	H1	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
26	WJ	201	PEB	CHC-C4C-C3C	-2.41	126.22	130.34
26	NF	1002	PEB	CMB-C2B-C1B	2.41	128.78	125.06
26	J4	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	k4	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	e1	202	PEB	OD-C4D-ND	-2.41	122.36	125.93
26	gF	201	PEB	CHC-C4C-C3C	-2.41	126.22	130.34
26	H5	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	DD	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	T2	203	PEB	CAB-CBB-CGB	2.41	118.79	113.60
26	P3	203	PEB	CMB-C2B-C1B	2.41	128.78	125.06
26	F5	203	PEB	C2A-C1A-NA	2.41	110.35	108.27
26	mE	203	PEB	C3B-C4B-NB	2.41	113.56	110.05
26	k6	201	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
28	B6	1001	CYC	CHB-C1B-NB	-2.41	120.88	126.06
26	B5	201	PEB	CHA-C1B-NB	-2.41	119.89	124.93
26	fB	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	J3	201	PEB	CHA-C4A-NA	-2.41	122.34	125.20
26	vG	202	PEB	CHB-C4B-NB	-2.41	125.48	128.83
26	lA	202	PEB	CAA-C3A-C2A	-2.41	108.23	114.26
26	J8	202	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
26	XJ	201	PEB	C4B-C3B-C2B	-2.41	104.11	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V7	201	PEB	CHA-C4A-NA	2.41	128.07	125.20
28	LF	1001	CYC	O2A-CGA-O1A	-2.41	117.29	123.30
26	j7	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	L4	203	PEB	CAC-CBC-CGC	-2.41	107.00	113.76
28	kH	1001	CYC	C2A-C1A-NA	2.41	113.56	110.05
26	D2	1002	PEB	C1C-CHB-C4B	2.41	131.69	128.81
26	EA	203	PEB	C1C-CHB-C4B	2.41	131.69	128.81
26	LG	201	PEB	C1C-CHB-C4B	2.41	131.69	128.81
26	R3	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	dB	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	WF	201	PEB	OD-C4D-ND	-2.41	122.36	125.93
26	TJ	203	PEB	CMB-C2B-C1B	2.41	128.78	125.06
26	k1	201	PEB	CHB-C4B-NB	-2.41	125.48	128.83
26	VI	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	EG	202	PEB	CHB-C4B-C3B	-2.41	119.75	125.32
28	YH	1003	CYC	C1B-NB-C4B	-2.41	107.60	110.67
26	DG	202	PEB	OD-C4D-ND	-2.41	122.36	125.93
26	aI	201	PEB	CAB-C3B-C4B	2.41	129.27	125.01
26	L2	1002	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
26	Y4	202	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
27	yE	302	PUB	CBD-CAD-C3D	2.41	119.07	112.43
26	UA	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
26	u4	203	PEB	CAA-C3A-C4A	-2.41	106.49	112.67
26	F4	201	PEB	CAA-C3A-C2A	-2.41	108.24	114.26
26	fA	202	PEB	C1C-CHB-C4B	2.41	131.69	128.81
26	L3	201	PEB	OD-C4D-ND	-2.41	122.36	125.93
28	NI	1001	CYC	CHB-C4A-C3A	2.41	131.09	124.90
26	T4	201	PEB	CBC-CAC-C2C	-2.41	108.51	112.62
26	fG	201	PEB	CHA-C1B-C2B	2.41	131.09	124.90
26	o1	501	PEB	OD-C4D-C3D	-2.41	124.01	129.46
26	R2	202	PEB	CMA-C2A-C1A	-2.41	107.21	112.40
28	KH	1001	CYC	OC-C1C-C2C	-2.41	124.26	126.17
26	OG	201	PEB	CMB-C2B-C1B	2.41	128.77	125.06
26	mB	201	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
26	hI	201	PEB	C2A-C1A-NA	2.41	110.35	108.27
26	HD	202	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
26	VF	202	PEB	CHB-C4B-NB	-2.41	125.49	128.83
26	W8	202	PEB	CMA-C2A-C1A	-2.41	107.22	112.40
26	O3	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
28	H2	1001	CYC	O1A-CGA-CBA	-2.41	115.35	123.08
26	b7	203	PEB	CHA-C1B-NB	-2.41	119.90	124.93
26	l1	201	PEB	CHC-C4C-C3C	-2.41	126.23	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	fE	201	PEB	CHA-C1B-C2B	2.41	131.09	124.90
26	A8	302	PEB	CBC-CAC-C2C	-2.41	108.51	112.62
26	VB	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
26	iA	202	PEB	O2B-CGB-CBB	2.41	121.76	114.03
26	ND	202	PEB	C2B-C1B-NB	2.41	115.66	110.53
26	y1	203	PEB	OD-C4D-ND	-2.41	122.37	125.93
26	U8	202	PEB	CMA-C2A-C1A	-2.41	107.22	112.40
26	x1	201	PEB	C2A-C1A-NA	2.41	110.35	108.27
26	aI	201	PEB	C1B-C2B-C3B	-2.41	103.75	106.51
28	YH	1002	CYC	C4A-C3A-C2A	-2.41	103.75	106.51
28	NI	1001	CYC	C1B-NB-C4B	-2.41	107.61	110.67
28	EF	1001	CYC	CHA-C1A-C2A	-2.41	119.76	125.32
26	vG	201	PEB	C1C-CHB-C4B	2.41	131.68	128.81
26	CJ	201	PEB	CMA-C2A-C1A	-2.40	107.22	112.40
26	R4	201	PEB	CBC-CAC-C2C	-2.40	108.52	112.62
26	XA	202	PEB	CAB-CBB-CGB	2.40	118.78	113.60
26	h2	201	PEB	OD-C4D-C3D	-2.40	124.01	129.46
26	g1	203	PEB	C3B-C4B-NB	2.40	113.55	110.05
26	F3	203	PEB	CAA-C3A-C2A	-2.40	108.25	114.26
28	K6	202	CYC	C4A-C3A-C2A	-2.40	103.75	106.51
26	fB	202	PEB	CAB-C3B-C4B	2.40	129.26	125.01
26	ZF	202	PEB	CAB-C3B-C4B	2.40	129.26	125.01
26	E8	203	PEB	OD-C4D-C3D	-2.40	124.01	129.46
26	mA	202	PEB	CAA-C3A-C2A	-2.40	108.25	114.26
26	F9	201	PEB	C3B-C4B-NB	2.40	113.55	110.05
26	hA	201	PEB	C3B-C4B-NB	2.40	113.55	110.05
26	u1	201	PEB	OD-C4D-C3D	-2.40	124.01	129.46
26	a7	201	PEB	OD-C4D-C3D	-2.40	124.01	129.46
26	S9	202	PEB	CHB-C4B-C3B	-2.40	119.77	125.32
26	d6	204	PEB	CBC-CAC-C2C	-2.40	108.52	112.62
28	iH	1001	CYC	C4A-C3A-C2A	-2.40	103.75	106.51
28	oH	1001	CYC	C4A-C3A-C2A	-2.40	103.75	106.51
27	N9	201	PUB	CMD-C2D-C3D	2.40	131.38	127.77
27	A2	302	PUB	CHA-C4A-NA	-2.40	111.16	113.95
26	TF	202	PEB	OA-C1A-C2A	-2.40	124.26	126.17
26	RB	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
26	P9	201	PEB	CHA-C1B-NB	-2.40	119.91	124.93
26	iB	201	PEB	CHC-C1D-ND	-2.40	111.16	113.95
26	X1	202	PEB	C1C-CHB-C4B	2.40	131.68	128.81
26	xE	302	PEB	OD-C4D-C3D	-2.40	124.02	129.46
26	ZE	201	PEB	CBA-CAA-C3A	2.40	118.82	113.47
27	YD	302	PUB	CHC-C1D-ND	-2.40	110.69	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FI	1002	PEB	CAA-C3A-C2A	-2.40	108.26	114.26
26	MA	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
26	ID	202	PEB	CHA-C4A-NA	-2.40	122.35	125.20
26	O7	201	PEB	C1C-CHB-C4B	2.40	131.68	128.81
26	GE	203	PEB	CAB-C3B-C4B	2.40	129.26	125.01
26	NE	201	PEB	CAB-C3B-C4B	2.40	129.26	125.01
26	mE	201	PEB	C4B-C3B-C2B	-2.40	104.12	106.78
26	GJ	201	PEB	CAA-C3A-C4A	-2.40	106.51	112.67
26	R8	201	PEB	CHA-C4A-NA	2.40	128.06	125.20
26	eD	401	PEB	OD-C4D-ND	-2.40	122.37	125.93
26	XG	202	PEB	OD-C4D-ND	-2.40	122.37	125.93
28	cH	1001	CYC	C1B-CHB-C4A	2.40	133.95	128.08
26	q4	203	PEB	CHA-C1B-NB	-2.40	119.91	124.93
26	I5	203	PEB	CMA-C2A-C1A	-2.40	107.23	112.40
28	jH	1001	CYC	C1B-NB-C4B	-2.40	107.61	110.67
26	K1	201	PEB	OD-C4D-ND	-2.40	122.37	125.93
26	C3	201	PEB	CAB-C3B-C4B	2.40	129.25	125.01
28	JH	1001	CYC	C4A-C3A-C2A	-2.40	103.75	106.51
26	TD	202	PEB	CBC-CAC-C2C	2.40	116.72	112.62
26	RF	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
26	bB	201	PEB	CHB-C4B-C3B	-2.40	119.78	125.32
26	J4	202	PEB	C3B-C4B-NB	2.40	113.54	110.05
26	Z7	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
26	CJ	202	PEB	OD-C4D-ND	-2.40	122.38	125.93
26	l2	202	PEB	C4B-C3B-C2B	-2.40	104.13	106.78
26	L5	201	PEB	CAC-CBC-CGC	-2.40	107.03	113.76
26	XE	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
26	ND	201	PEB	CMA-C2A-C1A	-2.40	107.23	112.40
26	h4	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
26	n4	202	PEB	C3B-C4B-NB	2.40	113.54	110.05
26	f1	202	PEB	C3B-C4B-NB	2.40	113.54	110.05
26	oG	202	PEB	C3B-C4B-NB	2.40	113.54	110.05
26	VG	202	PEB	CHC-C4C-C3C	-2.40	126.25	130.34
26	cE	202	PEB	CAB-CBB-CGB	-2.40	108.44	113.60
26	j1	201	PEB	C2B-C1B-NB	2.40	115.65	110.53
26	e1	202	PEB	CHA-C4A-NA	-2.40	122.35	125.20
26	G3	202	PEB	C2A-C1A-NA	2.40	110.34	108.27
26	K5	202	PEB	C1C-CHB-C4B	2.40	131.67	128.81
26	xG	303	PEB	C1C-CHB-C4B	-2.40	125.94	128.81
26	k2	203	PEB	CBB-CAB-C3B	2.40	119.29	112.63
26	J3	203	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	mF	202	PEB	CHA-C4A-NA	2.40	128.06	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UB	202	PEB	CAB-CBB-CGB	-2.40	108.44	113.60
26	KE	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	VE	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	X3	201	PEB	CHA-C1B-C2B	2.40	131.06	124.90
26	P2	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	AJ	304	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	TJ	202	PEB	C2B-C1B-NB	2.40	115.64	110.53
26	L5	203	PEB	CMA-C2A-C1A	-2.40	107.24	112.40
26	YG	202	PEB	CHA-C1B-NB	-2.40	119.92	124.93
26	HC	203	PEB	C1C-CHB-C4B	2.40	131.67	128.81
26	HA	201	PEB	CMC-C3C-C2C	-2.40	120.42	124.94
26	T6	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	k7	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	NB	1002	PEB	CAB-C3B-C4B	2.40	129.25	125.01
26	B3	202	PEB	C3B-C4B-NB	2.40	113.53	110.05
26	RD	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
26	GD	201	PEB	C1C-CHB-C4B	2.40	131.67	128.81
26	VI	202	PEB	CBC-CAC-C2C	-2.39	108.53	112.62
26	UA	202	PEB	CMA-C2A-C1A	-2.39	107.24	112.40
26	Q6	202	PEB	C3B-C4B-NB	2.39	113.53	110.05
28	CF	1001	CYC	CHB-C4A-C3A	2.39	131.06	124.90
26	b7	201	PEB	CAA-C3A-C4A	-2.39	106.53	112.67
26	lB	201	PEB	CMB-C2B-C1B	2.39	128.75	125.06
28	eH	1001	CYC	C4D-CHA-C1A	2.39	131.67	128.81
26	f1	201	PEB	C1B-C2B-C3B	-2.39	103.76	106.51
26	L3	203	PEB	C1B-C2B-C3B	-2.39	103.76	106.51
26	eD	401	PEB	CBA-CAA-C3A	-2.39	108.14	113.47
26	T1	203	PEB	OD-C4D-ND	-2.39	122.38	125.93
26	YD	303	PEB	CMC-C3C-C2C	2.39	129.46	124.94
26	y1	202	PEB	CAC-CBC-CGC	-2.39	107.05	113.76
26	WJ	201	PEB	C4B-C3B-C2B	-2.39	104.13	106.78
28	gH	1001	CYC	C1A-C2A-C3A	-2.39	104.13	106.78
26	D1	203	PEB	C1C-CHB-C4B	-2.39	125.95	128.81
26	lI	202	PEB	OD-C4D-ND	-2.39	122.39	125.93
26	bE	201	PEB	C3B-C4B-NB	2.39	113.53	110.05
28	DB	1001	CYC	CAB-C3B-C2B	2.39	131.62	127.53
28	B6	1002	CYC	CMC-C2C-C1C	-2.39	107.25	112.40
26	i4	201	PEB	C2B-C1B-NB	2.39	115.64	110.53
26	CG	202	PEB	OD-C4D-C3D	-2.39	124.04	129.46
26	I3	202	PEB	CHA-C1B-NB	-2.39	119.93	124.93
26	M8	202	PEB	C4B-C3B-C2B	-2.39	104.14	106.78
26	O7	202	PEB	OD-C4D-ND	-2.39	122.39	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l8	203	PEB	CHA-C1B-NB	-2.39	119.93	124.93
26	T4	201	PEB	C3D-C4D-ND	2.39	111.95	107.26
27	Q8	201	PUB	CAC-CBC-CGC	-2.39	108.45	113.60
26	e3	401	PEB	CBA-CAA-C3A	-2.39	108.14	113.47
26	DE	203	PEB	OD-C4D-C3D	-2.39	124.04	129.46
26	MJ	202	PEB	C1C-CHB-C4B	2.39	131.67	128.81
26	s4	203	PEB	C4B-C3B-C2B	-2.39	104.14	106.78
26	kE	201	PEB	CHA-C1B-C2B	2.39	131.05	124.90
26	OA	201	PEB	CHC-C1D-ND	-2.39	111.17	113.95
26	A2	304	PEB	OD-C4D-C3D	-2.39	124.04	129.46
28	iH	1001	CYC	CBD-CAD-C3D	-2.39	108.54	112.62
26	xG	304	PEB	CAB-CBB-CGB	-2.39	108.46	113.60
26	NJ	204	PEB	CAB-CBB-CGB	-2.39	108.46	113.60
28	NB	1001	CYC	CBB-CAB-C3B	-2.39	105.84	112.43
26	W1	201	PEB	OD-C4D-C3D	-2.39	124.04	129.46
26	u4	203	PEB	OD-C4D-C3D	-2.39	124.04	129.46
26	gF	201	PEB	CAA-C3A-C2A	-2.39	108.28	114.26
27	yG	303	PUB	CMD-C2D-C3D	2.39	131.36	127.77
26	fF	201	PEB	CMB-C2B-C1B	2.39	128.75	125.06
26	J4	203	PEB	C3B-C4B-NB	2.39	113.53	110.05
26	IA	202	PEB	C3B-C4B-NB	2.39	113.53	110.05
26	L3	203	PEB	CAB-CBB-CGB	-2.39	108.46	113.60
26	aI	203	PEB	C1C-CHB-C4B	2.39	131.66	128.81
28	TH	1001	CYC	C1A-C2A-C3A	-2.39	104.14	106.78
26	J1	202	PEB	OD-C4D-C3D	-2.39	124.04	129.46
26	h2	202	PEB	O2B-CGB-CBB	2.39	121.71	114.03
26	U4	201	PEB	O2B-CGB-CBB	2.39	121.71	114.03
26	A3	202	PEB	OD-C4D-ND	-2.39	122.39	125.93
27	AB	303	PUB	CMD-C2D-C3D	2.39	131.35	127.77
26	UI	201	PEB	CBA-CAA-C3A	-2.39	108.14	113.47
26	I4	201	PEB	CAB-C3B-C4B	2.39	129.24	125.01
26	w4	204	PEB	OD-C4D-C3D	-2.39	124.05	129.46
26	XG	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
28	QH	1001	CYC	C1B-C2B-C3B	-2.39	105.38	107.87
26	e6	202	PEB	CHC-C1D-ND	-2.39	111.17	113.95
26	QD	202	PEB	CHC-C1D-ND	-2.39	111.17	113.95
26	eG	201	PEB	C2A-C1A-NA	2.39	110.33	108.27
26	IA	203	PEB	CAB-C3B-C4B	2.39	129.24	125.01
26	VD	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
26	L8	201	PEB	CHC-C1D-ND	2.39	116.72	113.95
26	P3	201	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
26	RE	201	PEB	CAB-C3B-C4B	2.39	129.23	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h1	201	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
26	V6	202	PEB	CMC-C3C-C2C	2.39	129.44	124.94
26	h1	202	PEB	CHA-C1B-NB	-2.39	119.94	124.93
26	h1	202	PEB	C3B-C4B-NB	2.39	113.52	110.05
26	d4	203	PEB	CAC-CBC-CGC	-2.39	107.07	113.76
26	gB	201	PEB	CHC-C1D-ND	-2.39	111.17	113.95
28	NB	1001	CYC	OB-C4B-C3B	-2.39	125.45	128.04
26	W6	201	PEB	C4B-C3B-C2B	-2.39	104.14	106.78
26	OB	201	PEB	C4B-C3B-C2B	-2.39	104.14	106.78
26	KG	202	PEB	C4B-C3B-C2B	-2.39	104.14	106.78
26	W1	202	PEB	OD-C4D-C3D	-2.39	124.05	129.46
26	NA	202	PEB	CAA-C3A-C2A	-2.39	108.30	114.26
26	DD	203	PEB	CHB-C4B-C3B	-2.39	119.81	125.32
26	XD	201	PEB	CHA-C4A-NA	2.39	128.04	125.20
26	a7	201	PEB	CBC-CAC-C2C	-2.39	108.55	112.62
26	CG	202	PEB	CAC-C2C-C3C	2.39	134.10	127.25
26	i6	201	PEB	CHC-C1D-ND	-2.39	111.18	113.95
28	LF	1001	CYC	C2B-C1B-NB	2.39	110.48	106.99
26	lB	203	PEB	CBA-CAA-C3A	-2.39	108.15	113.47
26	DE	201	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
26	J5	202	PEB	CMC-C3C-C2C	-2.39	120.44	124.94
26	E1	202	PEB	CHB-C4B-C3B	-2.39	119.81	125.32
26	a2	201	PEB	CAB-C3B-C4B	2.39	129.23	125.01
26	S8	201	PEB	OD-C4D-C3D	-2.39	124.06	129.46
26	t4	202	PEB	OD-C4D-ND	-2.39	122.40	125.93
26	U7	201	PEB	CHB-C4B-C3B	-2.39	119.81	125.32
26	lE	201	PEB	OA-C1A-NA	2.39	127.83	124.94
26	t1	201	PEB	C3B-C4B-NB	2.39	113.52	110.05
26	H5	202	PEB	CAA-C3A-C2A	-2.39	108.30	114.26
26	N8	202	PEB	CAA-C3A-C2A	-2.39	108.30	114.26
28	HI	1001	CYC	CHB-C4A-C3A	2.39	131.03	124.90
26	eI	201	PEB	CHA-C4A-NA	2.39	128.04	125.20
26	e6	202	PEB	CHA-C1B-NB	-2.39	119.94	124.93
26	L4	203	PEB	CMB-C2B-C1B	2.39	128.74	125.06
26	D1	202	PEB	CAB-C3B-C4B	2.38	129.23	125.01
28	JF	1001	CYC	CAC-C3C-C4C	-2.38	106.55	112.67
26	YI	201	PEB	CHA-C4A-NA	2.38	128.04	125.20
27	K4	203	PUB	C2C-C1C-NC	2.38	113.52	110.05
26	i6	202	PEB	CMB-C2B-C1B	2.38	128.74	125.06
26	nE	201	PEB	CHA-C1B-C2B	2.38	131.03	124.90
26	TB	201	PEB	C1B-C2B-C3B	-2.38	103.77	106.51
26	cB	201	PEB	CHA-C4A-NA	2.38	128.04	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aG	202	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
26	f8	202	PEB	CAB-CBB-CGB	-2.38	108.47	113.60
26	OD	201	PEB	CMD-C2D-C3D	2.38	133.43	130.06
26	V1	202	PEB	CBA-CAA-C3A	-2.38	108.16	113.47
26	TI	201	PEB	CHB-C4B-NB	-2.38	125.52	128.83
26	eA	202	PEB	CHC-C1D-ND	-2.38	111.18	113.95
26	E9	202	PEB	C1B-C2B-C3B	-2.38	103.77	106.51
28	UH	1001	CYC	C4A-C3A-C2A	-2.38	103.77	106.51
26	IA	203	PEB	C2B-C1B-NB	2.38	115.61	110.53
26	ZG	201	PEB	CMB-C2B-C1B	2.38	128.73	125.06
26	h4	203	PEB	CAB-C3B-C4B	2.38	129.22	125.01
26	n4	202	PEB	CHA-C1B-NB	-2.38	119.95	124.93
26	J9	201	PEB	CMA-C2A-C1A	-2.38	107.27	112.40
26	I8	201	PEB	CAA-C3A-C4A	-2.38	106.56	112.67
26	TG	202	PEB	C2B-C1B-NB	2.38	115.61	110.53
26	r1	202	PEB	C3B-C4B-NB	2.38	113.51	110.05
28	eH	1001	CYC	C4A-C3A-C2A	-2.38	103.77	106.51
26	k1	203	PEB	CHA-C4A-NA	2.38	128.04	125.20
26	l7	202	PEB	CMB-C2B-C1B	2.38	128.73	125.06
27	AI	303	PUB	CHC-C1D-ND	-2.38	110.71	113.72
26	WI	201	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
26	k1	202	PEB	OD-C4D-ND	-2.38	122.40	125.93
26	e7	202	PEB	OD-C4D-ND	-2.38	122.40	125.93
26	O3	201	PEB	CBC-CAC-C2C	2.38	116.68	112.62
26	Y2	202	PEB	OD-C4D-C3D	-2.38	124.06	129.46
26	lG	201	PEB	CBB-CAB-C3B	2.38	119.24	112.63
26	cE	203	PEB	CMD-C2D-C3D	-2.38	126.71	130.06
26	a4	202	PEB	C1B-C2B-C3B	-2.38	103.77	106.51
26	IC	201	PEB	CBC-CAC-C2C	-2.38	108.56	112.62
26	hB	203	PEB	CHC-C4C-C3C	-2.38	126.28	130.34
28	TH	1001	CYC	CHB-C1B-C2B	-2.38	122.23	126.95
26	hF	202	PEB	OD-C4D-C3D	-2.38	124.07	129.46
26	W9	202	PEB	CHC-C1D-ND	-2.38	111.18	113.95
26	AD	201	PEB	C2A-C1A-NA	2.38	110.33	108.27
26	A1	202	PEB	C2B-C1B-NB	2.38	115.61	110.53
26	eE	203	PEB	C3B-C4B-NB	2.38	113.51	110.05
26	XD	202	PEB	C2B-C1B-NB	2.38	115.61	110.53
26	c1	202	PEB	OD-C4D-C3D	-2.38	124.07	129.46
26	dI	201	PEB	CHC-C1D-ND	-2.38	111.18	113.95
28	YH	1002	CYC	C2A-C1A-NA	2.38	113.51	110.05
26	SD	201	PEB	O2C-CGC-CBC	2.38	121.67	114.03
26	O9	202	PEB	C2A-C1A-NA	2.38	110.32	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	KG	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
26	J2	1002	PEB	CAC-CBC-CGC	-2.38	107.09	113.76
26	NG	201	PEB	CMB-C2B-C1B	2.38	128.73	125.06
26	k6	201	PEB	CHC-C1D-ND	-2.38	111.19	113.95
26	f7	201	PEB	CBC-CAC-C2C	-2.38	108.56	112.62
26	kA	202	PEB	CHA-C4A-NA	-2.38	122.38	125.20
26	X4	203	PEB	CHA-C4A-NA	2.38	128.03	125.20
26	T3	203	PEB	CAC-CBC-CGC	-2.38	107.09	113.76
26	B9	201	PEB	CAB-C3B-C4B	2.38	129.22	125.01
26	xG	303	PEB	CHA-C1B-NB	-2.38	119.96	124.93
26	NJ	202	PEB	OD-C4D-ND	-2.38	122.41	125.93
26	DJ	203	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
26	WB	201	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
28	YH	1004	CYC	C1A-C2A-C3A	-2.38	104.15	106.78
26	HA	201	PEB	CMA-C2A-C1A	-2.38	107.28	112.40
26	CJ	201	PEB	CBC-CAC-C2C	2.38	116.68	112.62
26	KA	203	PEB	C2B-C1B-NB	2.38	115.60	110.53
26	B3	202	PEB	OD-C4D-C3D	-2.38	124.07	129.46
26	SG	202	PEB	OD-C4D-C3D	-2.38	124.07	129.46
26	V7	201	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
26	JA	201	PEB	CBC-CAC-C2C	-2.38	108.56	112.62
26	T2	201	PEB	CHB-C4B-NB	-2.38	125.53	128.83
26	H4	203	PEB	C3B-C4B-NB	2.38	113.51	110.05
26	K1	202	PEB	OD-C4D-C3D	-2.38	124.08	129.46
26	aG	201	PEB	C2B-C1B-NB	2.38	115.60	110.53
26	LA	201	PEB	CHC-C1D-ND	2.38	116.71	113.95
26	m4	202	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
28	IF	1001	CYC	CBD-CAD-C3D	-2.38	108.56	112.62
27	A4	203	PUB	CAC-C2C-C1C	2.38	129.21	125.01
26	AG	202	PEB	CHC-C4C-C3C	-2.38	126.28	130.34
26	j1	202	PEB	C3B-C4B-NB	2.38	113.51	110.05
28	JF	1003	CYC	C1B-CHB-C4A	-2.38	122.28	128.08
26	KB	201	PEB	OD-C4D-ND	-2.38	122.41	125.93
26	hI	202	PEB	OD-C4D-C3D	-2.38	124.08	129.46
26	IG	203	PEB	CMB-C2B-C1B	2.38	128.72	125.06
26	y1	203	PEB	CHA-C4A-NA	-2.38	122.38	125.20
26	KC	201	PEB	C3B-C4B-NB	2.38	113.50	110.05
26	mG	203	PEB	C2A-C1A-NA	2.38	110.32	108.27
26	LD	202	PEB	C2B-C1B-NB	2.38	115.60	110.53
26	V3	201	PEB	C4B-C3B-C2B	-2.38	104.15	106.78
26	R3	203	PEB	O1B-CGB-CBB	-2.38	115.45	123.08
26	G5	203	PEB	OD-C4D-C3D	-2.38	124.08	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R6	201	PEB	OD-C4D-C3D	-2.38	124.08	129.46
26	qE	202	PEB	CHC-C4C-C3C	-2.37	126.29	130.34
26	YA	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	S2	201	PEB	OA-C1A-C2A	-2.37	124.28	126.17
26	M3	202	PEB	CHC-C1D-ND	-2.37	111.19	113.95
26	WE	202	PEB	CHC-C1D-ND	-2.37	111.19	113.95
26	E3	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	O7	202	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	d4	201	PEB	C1C-CHB-C4B	-2.37	125.97	128.81
26	Z1	201	PEB	CHA-C1B-C2B	2.37	131.00	124.90
26	fB	202	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	n4	201	PEB	CHB-C4B-C3B	-2.37	119.84	125.32
26	eE	202	PEB	CHA-C4A-NA	-2.37	122.38	125.20
26	14	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	eF	201	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	CG	203	PEB	OD-C4D-C3D	-2.37	124.08	129.46
26	a2	203	PEB	C1C-CHB-C4B	2.37	131.64	128.81
28	BB	1001	CYC	CHB-C1B-NB	-2.37	120.96	126.06
26	WG	202	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
26	E9	202	PEB	CHC-C4C-C3C	-2.37	126.29	130.34
26	RB	202	PEB	CAB-CBB-CGB	-2.37	108.50	113.60
26	YJ	201	PEB	CHB-C4B-C3B	-2.37	119.84	125.32
26	TG	202	PEB	C4B-NB-C1B	-2.37	102.04	106.51
26	VG	201	PEB	C3B-C4B-NB	2.37	113.50	110.05
26	F5	201	PEB	OD-C4D-ND	-2.37	122.42	125.93
26	BJ	201	PEB	OD-C4D-ND	-2.37	122.42	125.93
28	iH	1001	CYC	C1B-CHB-C4A	2.37	133.88	128.08
26	g4	202	PEB	CHA-C1B-NB	-2.37	119.97	124.93
26	RG	202	PEB	CHC-C1D-ND	-2.37	111.19	113.95
26	O9	202	PEB	CMB-C2B-C1B	2.37	128.72	125.06
26	XD	201	PEB	CHA-C1B-C2B	2.37	131.00	124.90
26	RG	201	PEB	OD-C4D-C3D	-2.37	124.09	129.46
26	H9	202	PEB	OA-C1A-C2A	-2.37	124.29	126.17
26	hF	202	PEB	OA-C1A-C2A	-2.37	124.29	126.17
26	FA	201	PEB	CMD-C2D-C3D	2.37	133.41	130.06
26	hB	201	PEB	CAA-C3A-C2A	-2.37	108.33	114.26
26	E1	201	PEB	CHA-C1B-NB	-2.37	119.97	124.93
26	QA	202	PEB	CHC-C1D-ND	-2.37	111.19	113.95
26	JJ	201	PEB	C3B-C4B-NB	2.37	113.50	110.05
26	Q1	201	PEB	CAB-C3B-C4B	2.37	129.20	125.01
26	NG	201	PEB	CAB-C3B-C4B	2.37	129.20	125.01
26	LC	202	PEB	OD-C4D-C3D	-2.37	124.09	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P1	202	PEB	CHB-C4B-NB	-2.37	125.54	128.83
26	TB	202	PEB	CMC-C3C-C2C	2.37	129.41	124.94
26	EE	202	PEB	CAA-C3A-C4A	-2.37	106.58	112.67
26	PG	201	PEB	CMA-C2A-C1A	-2.37	107.29	112.40
27	A1	203	PUB	CMD-C2D-C3D	2.37	131.33	127.77
26	L3	203	PEB	C2A-C1A-NA	2.37	110.32	108.27
26	L4	202	PEB	C3B-C4B-NB	2.37	113.50	110.05
27	xG	306	PUB	C2C-C1C-NC	2.37	113.50	110.05
26	l6	201	PEB	CMB-C2B-C1B	2.37	128.72	125.06
26	n1	201	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
26	OD	202	PEB	CBA-CAA-C3A	-2.37	108.19	113.47
26	b7	201	PEB	CAB-CBB-CGB	-2.37	108.50	113.60
26	x1	201	PEB	C3B-C4B-NB	2.37	113.50	110.05
26	r4	201	PEB	C2A-C1A-NA	2.37	110.32	108.27
26	a6	201	PEB	CHA-C1B-NB	-2.37	119.98	124.93
28	LF	1001	CYC	CMA-C3A-C2A	-2.37	119.68	126.12
26	z4	202	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
28	HI	1001	CYC	O1A-CGA-CBA	-2.37	115.47	123.08
26	U1	201	PEB	O2B-CGB-CBB	2.37	121.64	114.03
26	TE	202	PEB	CHC-C4C-C3C	2.37	134.38	130.34
28	1H	1000	CYC	C1A-C2A-C3A	-2.37	104.16	106.78
26	SA	203	PEB	CAB-CBB-CGB	-2.37	108.50	113.60
26	n4	202	PEB	OD-C4D-C3D	-2.37	124.09	129.46
26	aG	202	PEB	OD-C4D-C3D	-2.37	124.09	129.46
27	21	403	PUB	C2C-C1C-NC	2.37	113.50	110.05
26	C5	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
26	UB	203	PEB	CAB-C3B-C4B	2.37	129.20	125.01
28	JH	1001	CYC	CHA-C1A-NA	-2.37	125.54	128.83
26	cA	201	PEB	CHA-C1B-NB	-2.37	119.98	124.93
26	WG	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
26	AB	304	PEB	CHC-C1D-ND	-2.37	111.20	113.95
26	VE	202	PEB	CHC-C1D-ND	-2.37	111.20	113.95
26	s4	203	PEB	C3B-C4B-NB	2.37	113.49	110.05
27	A6	302	PUB	C2C-C1C-NC	2.37	113.49	110.05
26	jA	202	PEB	CMB-C2B-C1B	2.37	128.71	125.06
26	y4	201	PEB	CAA-C3A-C4A	-2.37	106.59	112.67
26	L4	202	PEB	OD-C4D-ND	-2.37	122.42	125.93
28	hH	1001	CYC	C2C-C3C-C4C	2.37	104.89	101.34
26	X8	202	PEB	CAA-C3A-C2A	-2.37	108.34	114.26
26	j8	202	PEB	CMC-C3C-C2C	2.37	129.41	124.94
26	DA	201	PEB	CMB-C2B-C1B	2.37	128.71	125.06
26	FD	203	PEB	C2A-C1A-NA	2.37	110.31	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S8	203	PEB	CAB-CBB-CGB	-2.37	108.51	113.60
27	K1	203	PUB	CMD-C2D-C3D	2.37	131.32	127.77
26	V4	202	PEB	CBA-CAA-C3A	-2.37	108.20	113.47
26	BD	203	PEB	OA-C1A-C2A	-2.37	124.29	126.17
28	wH	1001	CYC	CAA-C2A-C1A	2.37	129.19	125.01
26	MJ	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
26	OI	202	PEB	C4B-C3B-C2B	-2.37	104.16	106.78
26	xE	303	PEB	CBA-CAA-C3A	-2.37	108.20	113.47
26	RF	202	PEB	CAB-C3B-C4B	2.37	129.19	125.01
28	H7	1001	CYC	CBA-CAA-C2A	-2.37	106.05	112.63
26	F9	202	PEB	CHC-C1D-ND	-2.37	111.20	113.95
26	IG	202	PEB	CHC-C1D-ND	-2.37	111.20	113.95
26	C9	201	PEB	C4B-NB-C1B	-2.37	102.05	106.51
26	TE	202	PEB	CMC-C3C-C2C	-2.37	120.48	124.94
26	SJ	202	PEB	CMA-C2A-C1A	-2.37	107.30	112.40
26	E9	201	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
26	oG	203	PEB	CBA-CAA-C3A	-2.37	108.20	113.47
26	cA	203	PEB	CHC-C1D-ND	-2.36	111.20	113.95
26	KA	202	PEB	C3B-C4B-NB	2.36	113.49	110.05
26	H6	1002	PEB	OD-C4D-ND	-2.36	122.43	125.93
26	qE	201	PEB	OD-C4D-C3D	-2.36	124.10	129.46
26	F2	1002	PEB	CAA-C3A-C2A	-2.36	108.35	114.26
26	d6	203	PEB	OD-C4D-C3D	-2.36	124.10	129.46
26	oE	202	PEB	OD-C4D-C3D	-2.36	124.10	129.46
26	YA	203	PEB	OD-C4D-ND	-2.36	122.43	125.93
26	l1	202	PEB	CHA-C1B-NB	-2.36	119.99	124.93
26	XD	201	PEB	CAA-C3A-C2A	-2.36	108.35	114.26
26	d1	201	PEB	C1B-C2B-C3B	-2.36	103.79	106.51
26	LG	202	PEB	C1B-C2B-C3B	-2.36	103.79	106.51
26	R7	202	PEB	CHA-C4A-NA	2.36	128.01	125.20
26	HF	1002	PEB	CHC-C4C-C3C	-2.36	126.31	130.34
26	21	404	PEB	CHC-C1D-ND	-2.36	111.20	113.95
27	24	402	PUB	CMD-C2D-C3D	2.36	131.31	127.77
26	hF	201	PEB	CMB-C2B-C1B	2.36	128.70	125.06
26	iG	201	PEB	CMB-C2B-C1B	2.36	128.70	125.06
28	YH	1001	CYC	C1B-NB-C4B	-2.36	107.66	110.67
26	11	203	PEB	OD-C4D-ND	-2.36	122.43	125.93
26	aG	202	PEB	CHC-C1D-ND	-2.36	111.20	113.95
26	D8	202	PEB	OD-C4D-ND	-2.36	122.43	125.93
26	11	202	PEB	C3B-C4B-NB	2.36	113.48	110.05
26	kE	203	PEB	C3B-C4B-NB	2.36	113.48	110.05
28	YH	1001	CYC	C2A-C1A-NA	2.36	113.48	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LD	203	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
26	HB	1002	PEB	O2B-CGB-CBB	2.36	121.62	114.03
26	X8	202	PEB	OD-C4D-C3D	-2.36	124.11	129.46
26	lB	202	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
26	QB	201	PEB	CMB-C2B-C1B	2.36	128.70	125.06
26	q4	203	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
26	a8	201	PEB	CBC-CAC-C2C	-2.36	108.59	112.62
26	JA	201	PEB	C3B-C4B-NB	2.36	113.48	110.05
28	lB	1001	CYC	CHA-C1A-C2A	-2.36	119.87	125.32
26	p1	201	PEB	CHC-C1D-ND	-2.36	111.21	113.95
26	T3	201	PEB	CMC-C3C-C2C	2.36	129.39	124.94
26	WG	201	PEB	CBA-CAA-C3A	2.36	118.72	113.47
26	rE	201	PEB	OD-C4D-C3D	-2.36	124.11	129.46
26	c2	203	PEB	CHA-C4A-NA	-2.36	122.40	125.20
26	AJ	301	PEB	CHA-C4A-NA	-2.36	122.40	125.20
26	qE	203	PEB	C3B-C4B-NB	2.36	113.48	110.05
28	H7	1001	CYC	CAC-C3C-C2C	-2.36	108.36	114.26
27	21	403	PUB	CAC-C2C-C1C	2.36	129.18	125.01
26	D4	202	PEB	CBC-CAC-C2C	-2.36	108.59	112.62
26	N2	1002	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
27	AF	304	PUB	CHA-C1B-C2B	-2.36	126.31	130.34
26	AD	201	PEB	CBB-CAB-C3B	2.36	119.18	112.63
26	X4	203	PEB	OA-C1A-C2A	-2.36	124.30	126.17
26	JI	1002	PEB	CBA-CAA-C3A	-2.36	108.21	113.47
26	FD	201	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
26	qE	203	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
26	K3	202	PEB	CMC-C3C-C2C	2.36	129.39	124.94
26	FE	202	PEB	C2B-C1B-NB	2.36	115.56	110.53
26	S2	201	PEB	C4B-C3B-C2B	-2.36	104.17	106.78
26	a7	201	PEB	C4B-C3B-C2B	-2.36	104.17	106.78
26	P2	202	PEB	OD-C4D-C3D	-2.36	124.12	129.46
26	iA	201	PEB	CHA-C1B-NB	-2.36	120.00	124.93
26	G3	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
26	HC	203	PEB	CAB-C3B-C4B	2.36	129.18	125.01
28	GH	1001	CYC	C2A-C1A-NA	2.36	113.48	110.05
26	k4	203	PEB	CAA-C3A-C2A	-2.36	108.37	114.26
26	RI	203	PEB	CMB-C2B-C1B	2.36	128.70	125.06
28	eH	1001	CYC	C1B-CHB-C4A	2.36	133.84	128.08
26	YI	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
26	m7	201	PEB	CHB-C4B-C3B	-2.36	119.87	125.32
26	JD	202	PEB	C2B-C1B-NB	2.36	115.56	110.53
26	oE	203	PEB	C4B-C3B-C2B	-2.36	104.17	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F1	201	PEB	CMC-C3C-C2C	2.36	129.39	124.94
26	O8	201	PEB	CAA-C3A-C4A	-2.36	106.62	112.67
26	U6	202	PEB	CAA-C3A-C2A	-2.36	108.37	114.26
26	g8	202	PEB	OA-C1A-NA	2.36	127.80	124.94
28	gH	1001	CYC	C1B-C2B-C3B	-2.36	105.41	107.87
26	21	405	PEB	OD-C4D-ND	-2.36	122.44	125.93
26	g7	202	PEB	C4B-C3B-C2B	-2.36	104.17	106.78
26	sG	202	PEB	C3B-C4B-NB	2.36	113.48	110.05
26	A4	202	PEB	C2A-C1A-NA	2.36	110.31	108.27
26	c8	202	PEB	C2A-C1A-NA	2.36	110.31	108.27
26	d6	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
26	L9	202	PEB	OD-C4D-C3D	-2.36	124.12	129.46
26	XA	202	PEB	OA-C1A-NA	2.36	127.80	124.94
26	qG	203	PEB	C3B-C4B-NB	2.36	113.48	110.05
26	LJ	201	PEB	CMB-C2B-C1B	2.36	128.69	125.06
26	H1	202	PEB	CBC-CAC-C2C	2.36	116.64	112.62
26	PE	202	PEB	CHC-C4C-C3C	2.36	134.35	130.34
26	GA	201	PEB	C2A-C1A-NA	2.36	110.30	108.27
26	vE	201	PEB	CMB-C2B-C1B	2.36	128.69	125.06
26	mB	203	PEB	C3B-C4B-NB	2.36	113.48	110.05
26	iG	203	PEB	CAB-C3B-C4B	2.36	129.18	125.01
26	CJ	202	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
26	ZA	202	PEB	CBA-CAA-C3A	-2.36	108.22	113.47
26	KE	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
26	CA	203	PEB	OD-C4D-C3D	-2.36	124.12	129.46
26	I1	201	PEB	CAB-C3B-C4B	2.36	129.18	125.01
26	A8	302	PEB	CAB-C3B-C4B	2.36	129.18	125.01
26	T4	201	PEB	CHB-C4B-C3B	-2.35	119.88	125.32
26	y4	201	PEB	CHB-C4B-C3B	-2.35	119.88	125.32
28	jH	1001	CYC	C2B-C1B-NB	2.35	110.44	106.99
26	mF	202	PEB	C2A-C1A-NA	2.35	110.30	108.27
26	T6	202	PEB	CHC-C1D-ND	-2.35	111.21	113.95
26	WF	203	PEB	CHC-C1D-ND	-2.35	111.21	113.95
26	bF	203	PEB	CHC-C1D-ND	-2.35	111.21	113.95
26	MG	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	j1	201	PEB	CHC-C4C-C3C	-2.35	126.32	130.34
26	QJ	201	PEB	CBA-CAA-C3A	-2.35	108.22	113.47
28	hH	1001	CYC	C4A-C3A-C2A	-2.35	103.81	106.51
26	lF	203	PEB	CHB-C4B-C3B	2.35	130.76	125.32
26	BC	201	PEB	CHA-C1B-NB	-2.35	120.01	124.93
26	xE	304	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	L1	202	PEB	C3B-C4B-NB	2.35	113.47	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W7	203	PEB	C3B-C4B-NB	2.35	113.47	110.05
26	DJ	202	PEB	C2A-C1A-NA	2.35	110.30	108.27
28	fH	1001	CYC	C2C-C1C-NC	2.35	110.30	108.27
26	N4	201	PEB	CAB-C3B-C4B	2.35	129.17	125.01
26	gF	202	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	SJ	202	PEB	CMB-C2B-C1B	2.35	128.69	125.06
27	A8	303	PUB	CMC-C3C-C4C	2.35	133.42	126.37
26	D1	202	PEB	CHA-C4A-NA	-2.35	122.41	125.20
28	mH	1001	CYC	C4A-C3A-C2A	-2.35	103.81	106.51
26	XA	202	PEB	O1B-CGB-CBB	-2.35	115.52	123.08
26	R6	201	PEB	CBB-CAB-C3B	2.35	119.17	112.63
26	KE	202	PEB	CAC-CBC-CGC	2.35	120.35	113.76
26	RJ	202	PEB	OA-C1A-C2A	-2.35	124.30	126.17
26	E1	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	R3	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	dA	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	G8	203	PEB	CBA-CAA-C3A	-2.35	108.23	113.47
26	RF	202	PEB	C4B-C3B-C2B	-2.35	104.18	106.78
26	O3	202	PEB	CHC-C1D-ND	-2.35	111.22	113.95
26	gB	202	PEB	CMB-C2B-C1B	2.35	128.69	125.06
26	aA	201	PEB	OD-C4D-ND	-2.35	122.44	125.93
26	TB	202	PEB	CAA-C3A-C4A	-2.35	106.63	112.67
27	21	403	PUB	CMB-C2B-C3B	2.35	129.38	124.94
26	F4	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	q4	202	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	nE	202	PEB	CMD-C2D-C3D	2.35	133.38	130.06
26	X9	203	PEB	OD-C4D-ND	-2.35	122.45	125.93
26	YB	201	PEB	C4B-NB-C1B	-2.35	102.08	106.51
26	i7	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	S1	202	PEB	CHA-C1B-NB	-2.35	120.01	124.93
26	l8	201	PEB	CMA-C2A-C1A	-2.35	107.33	112.40
26	KG	203	PEB	CAA-C3A-C4A	-2.35	106.64	112.67
26	QF	201	PEB	CMB-C2B-C1B	2.35	128.69	125.06
26	Y8	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	h7	201	PEB	OD-C4D-ND	-2.35	122.45	125.93
26	RB	201	PEB	CMA-C2A-C1A	-2.35	107.33	112.40
26	PJ	202	PEB	C3B-C4B-NB	2.35	113.47	110.05
26	O6	201	PEB	C4B-C3B-C2B	-2.35	104.18	106.78
26	IA	201	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	ZB	202	PEB	OD-C4D-C3D	-2.35	124.13	129.46
26	N6	201	PEB	CAB-C3B-C4B	2.35	129.17	125.01
26	iA	202	PEB	CAB-C3B-C4B	2.35	129.17	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c8	202	PEB	CHA-C4A-NA	-2.35	122.41	125.20
28	KF	1001	CYC	CHB-C4A-NA	-2.35	120.02	124.93
26	H3	203	PEB	OD-C4D-ND	-2.35	122.45	125.93
28	LI	1001	CYC	C1B-NB-C4B	-2.35	107.68	110.67
28	CF	1001	CYC	CHB-C1B-NB	-2.35	121.01	126.06
26	a8	202	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
26	aG	202	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
26	2I	401	PEB	CBC-CAC-C2C	-2.35	108.61	112.62
26	a1	202	PEB	CHA-C1B-NB	-2.35	120.02	124.93
26	k1	203	PEB	OD-C4D-C3D	-2.35	124.14	129.46
26	b2	201	PEB	OD-C4D-ND	-2.35	122.45	125.93
26	JG	202	PEB	CHA-C4A-NA	2.35	128.00	125.20
27	BA	302	PUB	CBC-CAC-C2C	-2.35	106.10	112.63
26	k8	201	PEB	CHA-C1B-C2B	2.35	130.94	124.90
26	UF	201	PEB	CHA-C1B-C2B	2.35	130.94	124.90
26	YI	201	PEB	CHC-C4C-C3C	-2.35	126.33	130.34
26	k6	202	PEB	CAC-CBC-CGC	-2.35	107.17	113.76
26	IJ	203	PEB	CBB-CAB-C3B	2.35	119.15	112.63
26	cG	203	PEB	OD-C4D-C3D	-2.35	124.14	129.46
26	V9	201	PEB	OD-C4D-ND	-2.35	122.45	125.93
28	DF	1001	CYC	C2A-C1A-NA	2.35	113.47	110.05
28	vH	1001	CYC	C2A-C1A-NA	2.35	113.47	110.05
26	mI	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
26	oE	202	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
26	JF	1002	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
26	GD	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
26	hF	201	PEB	C3B-C4B-NB	2.35	113.46	110.05
26	X4	203	PEB	CHA-C1B-C2B	2.35	130.94	124.90
26	U2	201	PEB	CHC-C1D-ND	-2.35	111.22	113.95
26	mB	201	PEB	CMB-C2B-C1B	2.35	128.68	125.06
26	dI	201	PEB	C2B-C1B-NB	2.35	115.54	110.53
26	aE	203	PEB	CHA-C4A-NA	2.35	128.00	125.20
26	jG	202	PEB	OD-C4D-C3D	-2.35	124.14	129.46
26	QA	204	PEB	C1C-CHB-C4B	2.35	131.61	128.81
26	V4	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
26	JG	201	PEB	CAA-C3A-C4A	-2.35	106.65	112.67
26	24	404	PEB	C3B-C4B-NB	2.35	113.46	110.05
26	K5	201	PEB	CBC-CAC-C2C	-2.35	108.61	112.62
26	H3	202	PEB	CHA-C1B-NB	-2.35	120.02	124.93
26	ZG	201	PEB	CHA-C4A-NA	2.35	128.00	125.20
26	m2	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
26	QG	201	PEB	CBC-CAC-C2C	-2.35	108.62	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	QH	1001	CYC	C2A-C1A-NA	2.35	113.46	110.05
28	tH	1001	CYC	C1B-CHB-C4A	2.35	133.81	128.08
26	tG	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
26	TD	203	PEB	CAC-CBC-CGC	-2.35	107.18	113.76
27	AI	302	PUB	CMD-C2D-C3D	2.35	131.29	127.77
28	vH	1001	CYC	C1B-NB-C4B	-2.35	107.68	110.67
26	S3	201	PEB	CHA-C4A-NA	2.35	127.99	125.20
26	U1	202	PEB	CAC-CBC-CGC	-2.35	107.18	113.76
26	24	405	PEB	C3B-C4B-NB	2.35	113.46	110.05
26	eE	203	PEB	CHB-C4B-NB	-2.35	125.57	128.83
26	SI	202	PEB	CHA-C1B-NB	-2.35	120.03	124.93
26	gI	201	PEB	CHA-C1B-NB	-2.35	120.03	124.93
28	I6	1001	CYC	CHA-C1A-C2A	-2.35	119.90	125.32
26	14	203	PEB	OD-C4D-ND	-2.35	122.46	125.93
26	D7	1002	PEB	OD-C4D-C3D	-2.35	124.15	129.46
26	XA	202	PEB	OD-C4D-C3D	-2.35	124.15	129.46
26	xE	304	PEB	CAB-C3B-C4B	2.35	129.16	125.01
26	VE	202	PEB	C2B-C1B-NB	2.35	115.53	110.53
28	HB	1001	CYC	CMC-C2C-C1C	-2.35	107.35	112.40
26	T6	201	PEB	CHB-C4B-C3B	-2.34	119.90	125.32
26	O7	202	PEB	CMB-C2B-C1B	2.34	128.68	125.06
28	I7	1001	CYC	CHB-C1B-NB	-2.34	121.02	126.06
26	A4	202	PEB	C1C-CHB-C4B	2.34	131.61	128.81
26	mG	201	PEB	CBA-CAA-C3A	-2.34	108.25	113.47
26	TD	202	PEB	C4B-NB-C1B	-2.34	102.09	106.51
26	pE	202	PEB	CAA-C3A-C4A	2.34	118.69	112.67
26	H6	1002	PEB	O2B-CGB-CBB	2.34	121.56	114.03
26	h2	201	PEB	OA-C1A-C2A	-2.34	124.31	126.17
26	Z6	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
26	O9	201	PEB	CAA-C3A-C2A	-2.34	108.40	114.26
26	X9	203	PEB	CMB-C2B-C1B	2.34	128.67	125.06
26	YA	202	PEB	C3B-C4B-NB	2.34	113.46	110.05
26	YD	301	PEB	CHA-C4A-NA	2.34	127.99	125.20
26	jA	202	PEB	CHA-C4A-NA	-2.34	122.42	125.20
26	GC	201	PEB	C1C-CHB-C4B	2.34	131.61	128.81
26	NG	202	PEB	C1C-CHB-C4B	2.34	131.61	128.81
26	OG	201	PEB	CAC-CBC-CGC	-2.34	107.19	113.76
26	TB	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
26	jF	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
26	CJ	201	PEB	CMC-C3C-C2C	2.34	129.36	124.94
26	f4	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
26	T3	203	PEB	CHA-C1B-NB	-2.34	120.03	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	LC	201	PEB	CAC-CBC-CGC	-2.34	107.19	113.76
26	U7	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
26	pE	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
26	KD	201	PEB	CHB-C4B-C3B	-2.34	119.91	125.32
26	c1	203	PEB	C2B-C1B-NB	2.34	115.53	110.53
26	EJ	201	PEB	C2A-C1A-NA	2.34	110.29	108.27
26	fA	201	PEB	CHA-C4A-NA	-2.34	122.42	125.20
26	LG	201	PEB	O2B-CGB-CBB	2.34	121.56	114.03
26	FJ	201	PEB	C1C-CHB-C4B	2.34	131.61	128.81
26	bB	202	PEB	CHA-C1B-NB	-2.34	120.03	124.93
26	l4	202	PEB	C4B-C3B-C2B	-2.34	104.19	106.78
26	XA	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
28	wH	1001	CYC	C4A-C3A-C2A	-2.34	103.82	106.51
26	iE	203	PEB	CHA-C1B-NB	-2.34	120.03	124.93
26	ME	202	PEB	OD-C4D-C3D	-2.34	124.15	129.46
27	AF	304	PUB	CHB-C1C-C2C	2.34	130.73	125.32
26	Y8	202	PEB	C3B-C4B-NB	2.34	113.46	110.05
26	e3	401	PEB	OD-C4D-ND	-2.34	122.46	125.93
26	V3	201	PEB	OD-C4D-ND	-2.34	122.46	125.93
26	jI	202	PEB	OD-C4D-ND	-2.34	122.46	125.93
26	D7	1002	PEB	CAB-CBB-CGB	-2.34	108.56	113.60
26	iF	201	PEB	C2B-C1B-NB	2.34	115.53	110.53
26	kG	202	PEB	CAB-C3B-C4B	2.34	129.15	125.01
26	mE	201	PEB	OD-C4D-ND	-2.34	122.46	125.93
26	T3	202	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
26	i1	202	PEB	CHB-C4B-C3B	-2.34	119.91	125.32
26	GC	201	PEB	CBC-CAC-C2C	-2.34	108.63	112.62
26	sE	202	PEB	CHA-C4A-NA	2.34	127.99	125.20
28	LH	1001	CYC	CAC-C3C-C2C	-2.34	108.41	114.26
26	P4	202	PEB	CHB-C4B-C3B	-2.34	119.92	125.32
26	k7	202	PEB	CHB-C4B-NB	-2.34	125.58	128.83
26	z4	201	PEB	C2B-C1B-NB	2.34	115.52	110.53
26	ME	202	PEB	C2B-C1B-NB	2.34	115.52	110.53
26	qE	201	PEB	CHA-C1B-C2B	2.34	130.92	124.90
26	W4	202	PEB	OD-C4D-C3D	-2.34	124.16	129.46
28	D2	1001	CYC	CBB-CAB-C3B	-2.34	105.98	112.43
28	H7	1001	CYC	C1A-C2A-C3A	-2.34	104.19	106.78
26	WA	203	PEB	C2B-C1B-NB	2.34	115.52	110.53
26	y1	201	PEB	CAB-C3B-C4B	2.34	129.15	125.01
28	J7	1001	CYC	CBB-CAB-C3B	-2.34	105.98	112.43
26	LI	1002	PEB	CMC-C3C-C2C	2.34	129.35	124.94
26	XD	202	PEB	OA-C1A-NA	2.34	127.77	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q9	201	PEB	CBB-CAB-C3B	2.34	119.12	112.63
26	V3	203	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
26	YE	202	PEB	CMB-C2B-C1B	2.34	128.66	125.06
26	rE	202	PEB	C4B-C3B-C2B	-2.34	104.19	106.78
26	J3	202	PEB	CHB-C4B-NB	-2.34	125.58	128.83
26	L9	203	PEB	OD-C4D-C3D	-2.34	124.16	129.46
26	ZB	202	PEB	CHB-C4B-C3B	-2.34	119.92	125.32
26	eF	202	PEB	C3B-C4B-NB	2.34	113.45	110.05
26	kB	202	PEB	CMC-C3C-C2C	2.34	129.35	124.94
26	A3	202	PEB	CHC-C4C-C3C	-2.34	126.35	130.34
26	x1	202	PEB	OD-C4D-C3D	-2.34	124.16	129.46
28	DF	1003	CYC	CAC-C3C-C2C	-2.34	108.42	114.26
26	AB	304	PEB	C2A-C1A-NA	2.34	110.29	108.27
26	G5	202	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
27	K3	203	PUB	CAC-CBC-CGC	-2.34	108.57	113.60
28	EH	1001	CYC	CHB-C1B-C2B	-2.34	122.32	126.95
26	C5	202	PEB	C1C-CHB-C4B	-2.34	126.02	128.81
26	d4	203	PEB	OD-C4D-ND	-2.34	122.47	125.93
26	WB	202	PEB	CHB-C4B-NB	-2.34	125.58	128.83
26	jA	202	PEB	OD-C4D-C3D	-2.34	124.17	129.46
26	tE	202	PEB	CAB-C3B-C4B	2.34	129.14	125.01
26	GC	203	PEB	C1B-C2B-C3B	-2.34	103.83	106.51
26	tG	201	PEB	C3B-C4B-NB	2.34	113.45	110.05
26	T4	202	PEB	CAB-CBB-CGB	-2.34	108.58	113.60
26	GD	202	PEB	CAB-CBB-CGB	-2.34	108.58	113.60
26	WD	201	PEB	CAB-CBB-CGB	-2.34	108.58	113.60
26	G4	202	PEB	CMB-C2B-C1B	2.34	128.66	125.06
28	M6	1001	CYC	CHA-C1A-C2A	-2.34	119.92	125.32
26	i2	203	PEB	C2A-C1A-NA	2.34	110.29	108.27
26	N2	1002	PEB	OD-C4D-C3D	-2.34	124.17	129.46
26	JD	203	PEB	CHA-C1B-NB	-2.34	120.05	124.93
26	NE	201	PEB	CMB-C2B-C1B	2.34	128.66	125.06
26	KC	203	PEB	CAC-CBC-CGC	-2.34	107.21	113.76
26	R8	202	PEB	CHC-C1D-ND	-2.34	111.23	113.95
26	ED	202	PEB	CMC-C3C-C2C	2.34	129.34	124.94
26	RA	201	PEB	CMA-C2A-C1A	-2.34	107.37	112.40
26	nE	202	PEB	OD-C4D-C3D	-2.34	124.17	129.46
26	PF	202	PEB	OD-C4D-C3D	-2.34	124.17	129.46
26	z1	201	PEB	C4B-C3B-C2B	-2.33	104.20	106.78
26	iF	202	PEB	C4B-C3B-C2B	-2.33	104.20	106.78
26	g7	202	PEB	C3B-C4B-NB	2.33	113.44	110.05
26	jF	202	PEB	CHB-C4B-C3B	2.33	130.71	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	hA	203	PEB	OD-C4D-C3D	-2.33	124.17	129.46
26	RE	201	PEB	OD-C4D-C3D	-2.33	124.17	129.46
26	zG	501	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
26	OA	202	PEB	CBC-CAC-C2C	-2.33	108.64	112.62
28	GH	1001	CYC	CBD-CAD-C3D	-2.33	108.64	112.62
26	QA	204	PEB	CHA-C1B-NB	-2.33	120.05	124.93
26	FC	203	PEB	C2A-C1A-NA	2.33	110.28	108.27
26	eG	202	PEB	C1C-CHB-C4B	-2.33	126.02	128.81
26	QG	203	PEB	CHB-C4B-C3B	2.33	130.71	125.32
26	R2	202	PEB	OD-C4D-C3D	-2.33	124.17	129.46
26	Y2	201	PEB	OD-C4D-C3D	-2.33	124.17	129.46
26	l1	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
26	HJ	201	PEB	CAA-C3A-C4A	-2.33	106.68	112.67
26	lG	201	PEB	OD-C4D-C3D	-2.33	124.18	129.46
28	fH	1001	CYC	C2B-C1B-NB	2.33	110.40	106.99
26	eA	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
26	jE	201	PEB	CBC-CAC-C2C	-2.33	108.64	112.62
28	L7	1001	CYC	CAA-C2A-C1A	2.33	129.13	125.01
26	I8	203	PEB	CHC-C1D-ND	-2.33	111.24	113.95
26	KE	203	PEB	CHB-C4B-C3B	-2.33	119.93	125.32
28	mH	1001	CYC	C2A-C1A-NA	2.33	113.44	110.05
26	YG	201	PEB	CAB-CBB-CGB	-2.33	108.59	113.60
28	H2	1001	CYC	CHB-C4A-C3A	2.33	130.90	124.90
26	W4	201	PEB	OD-C4D-C3D	-2.33	124.18	129.46
26	MJ	201	PEB	CHC-C4C-C3C	-2.33	126.36	130.34
26	G1	201	PEB	CHB-C4B-C3B	-2.33	119.94	125.32
26	XG	203	PEB	C4B-NB-C1B	-2.33	102.12	106.51
26	J2	1002	PEB	CBA-CAA-C3A	-2.33	108.28	113.47
26	U9	202	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
28	CH	1001	CYC	C2C-C1C-NC	2.33	110.28	108.27
26	Z6	202	PEB	CHB-C4B-C3B	-2.33	119.94	125.32
26	i1	201	PEB	CMC-C3C-C2C	2.33	129.34	124.94
26	jG	201	PEB	CAB-CBB-CGB	-2.33	108.59	113.60
26	cB	201	PEB	C1C-CHB-C4B	2.33	131.59	128.81
26	Y8	203	PEB	OD-C4D-ND	-2.33	122.48	125.93
26	G1	201	PEB	CHC-C1D-ND	-2.33	111.24	113.95
26	n4	201	PEB	O2B-CGB-CBB	2.33	121.51	114.03
26	VI	203	PEB	CBB-CAB-C3B	2.33	119.10	112.63
26	iE	202	PEB	OD-C4D-C3D	-2.33	124.18	129.46
26	Z7	202	PEB	CMB-C2B-C1B	2.33	128.65	125.06
26	X3	202	PEB	CHA-C1B-NB	-2.33	120.06	124.93
28	C7	1001	CYC	C2A-C1A-NA	2.33	113.44	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	MG	203	PEB	CHA-C1B-C2B	2.33	130.89	124.90
26	Y1	201	PEB	CHB-C4B-NB	-2.33	125.60	128.83
26	ZB	202	PEB	CHB-C4B-NB	-2.33	125.60	128.83
26	HG	202	PEB	CHA-C4A-NA	-2.33	122.44	125.20
26	QA	203	PEB	OD-C4D-C3D	-2.33	124.18	129.46
26	AI	301	PEB	OD-C4D-C3D	-2.33	124.18	129.46
26	F3	201	PEB	CHA-C1B-NB	-2.33	120.06	124.93
26	m6	202	PEB	CHC-C1D-ND	-2.33	111.24	113.95
26	S1	201	PEB	CMC-C3C-C2C	2.33	129.33	124.94
26	O7	203	PEB	OD-C4D-C3D	-2.33	124.19	129.46
28	H6	1001	CYC	CMC-C2C-C1C	-2.33	107.38	112.40
26	U8	202	PEB	C3B-C4B-NB	2.33	113.44	110.05
26	y4	203	PEB	CHA-C1B-NB	-2.33	120.06	124.93
26	U1	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
26	d7	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
26	dA	201	PEB	C1C-CHB-C4B	-2.33	126.03	128.81
26	T8	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
26	CJ	201	PEB	CHB-C4B-NB	-2.33	125.60	128.83
26	i4	202	PEB	C2B-C1B-NB	2.33	115.50	110.53
28	wH	1001	CYC	CHB-C1B-C2B	-2.33	122.34	126.95
28	eH	1001	CYC	C2A-C1A-NA	2.33	113.43	110.05
26	t4	202	PEB	CAA-C3A-C2A	-2.33	108.44	114.26
26	S9	201	PEB	CHC-C4C-C3C	-2.33	126.37	130.34
28	BB	1001	CYC	O2D-CGD-CBD	2.33	121.50	114.03
26	pG	201	PEB	CAA-C3A-C2A	-2.33	108.45	114.26
26	GC	203	PEB	CAB-C3B-C4B	2.33	129.12	125.01
26	iE	201	PEB	C3B-C4B-NB	2.33	113.43	110.05
26	dE	201	PEB	OD-C4D-C3D	-2.33	124.19	129.46
26	lE	202	PEB	CAC-CBC-CGC	-2.33	107.24	113.76
26	P7	202	PEB	CAB-C3B-C4B	2.33	129.12	125.01
26	L5	203	PEB	CMC-C3C-C2C	-2.33	120.56	124.94
26	H6	1002	PEB	C2A-C1A-NA	2.33	110.28	108.27
26	fG	202	PEB	CHC-C4C-C3C	2.33	134.30	130.34
27	yG	302	PUB	C2C-C1C-NC	2.33	113.43	110.05
26	h7	202	PEB	CMB-C2B-C1B	2.33	128.65	125.06
26	SE	201	PEB	CMB-C2B-C1B	2.33	128.65	125.06
26	Y3	301	PEB	OD-C4D-C3D	-2.33	124.19	129.46
26	IA	203	PEB	OD-C4D-ND	-2.32	122.49	125.93
26	K5	201	PEB	C3B-C4B-NB	2.32	113.43	110.05
27	KD	203	PUB	C1D-CHC-C4C	-2.32	108.31	113.37
26	I1	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	dB	204	PEB	OD-C4D-ND	-2.32	122.49	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a4	201	PEB	CMA-C2A-C1A	-2.32	107.39	112.40
28	NI	1001	CYC	CHA-C1A-C2A	-2.32	119.95	125.32
26	c4	203	PEB	CMB-C2B-C1B	2.32	128.64	125.06
26	P4	202	PEB	C4B-C3B-C2B	-2.32	104.21	106.78
26	ZF	201	PEB	CAA-C3A-C2A	-2.32	108.45	114.26
26	l6	202	PEB	OD-C4D-ND	-2.32	122.49	125.93
26	mI	203	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
28	D2	1001	CYC	CAD-CBD-CGD	-2.32	107.25	113.76
26	YI	203	PEB	CMB-C2B-C1B	2.32	128.64	125.06
26	z1	202	PEB	CHC-C4C-C3C	-2.32	126.37	130.34
27	xG	301	PUB	CAC-C2C-C1C	2.32	129.12	125.01
28	kH	1001	CYC	C4D-CHA-C1A	2.32	131.58	128.81
26	B8	301	PEB	C1C-CHB-C4B	-2.32	126.03	128.81
26	F3	203	PEB	C3B-C4B-NB	2.32	113.43	110.05
26	mG	203	PEB	CMB-C2B-C1B	2.32	128.64	125.06
26	y1	202	PEB	OD-C4D-C3D	-2.32	124.20	129.46
26	O3	202	PEB	CHA-C1B-NB	-2.32	120.08	124.93
26	F9	202	PEB	OD-C4D-C3D	-2.32	124.20	129.46
28	J7	1001	CYC	C4D-CHA-C1A	2.32	131.58	128.81
26	O8	202	PEB	CHA-C1B-NB	-2.32	120.08	124.93
26	xE	304	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	iG	202	PEB	CHB-C4B-NB	-2.32	125.61	128.83
26	R6	202	PEB	CAB-CBB-CGB	-2.32	108.61	113.60
26	F5	203	PEB	CMC-C3C-C2C	-2.32	120.56	124.94
26	TG	202	PEB	CMC-C3C-C2C	-2.32	120.56	124.94
26	R9	203	PEB	CMB-C2B-C1B	2.32	128.64	125.06
27	AB	302	PUB	CAC-C2C-C1C	2.32	129.12	125.01
28	MB	1001	CYC	CHA-C1A-C2A	-2.32	119.96	125.32
26	a1	201	PEB	C4B-C3B-C2B	-2.32	104.21	106.78
26	CA	201	PEB	C4B-C3B-C2B	-2.32	104.21	106.78
26	W6	203	PEB	CAB-CBB-CGB	-2.32	108.61	113.60
26	h7	201	PEB	CAB-CBB-CGB	-2.32	108.61	113.60
26	DG	203	PEB	C4B-NB-C1B	-2.32	102.14	106.51
26	QA	204	PEB	CAB-C3B-C4B	2.32	129.11	125.01
26	F9	201	PEB	CHA-C4A-NA	2.32	127.96	125.20
26	OB	202	PEB	OD-C4D-C3D	-2.32	124.20	129.46
26	CC	201	PEB	CAB-C3B-C4B	2.32	129.11	125.01
26	c1	203	PEB	CMB-C2B-C1B	2.32	128.64	125.06
26	fG	201	PEB	C3B-C4B-NB	2.32	113.42	110.05
26	C8	203	PEB	OD-C4D-C3D	-2.32	124.20	129.46
28	NH	1001	CYC	CBD-CAD-C3D	-2.32	108.66	112.62
26	W1	202	PEB	C1C-CHB-C4B	2.32	131.58	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j8	202	PEB	CHA-C1B-NB	-2.32	120.08	124.93
26	fE	202	PEB	CHA-C1B-NB	-2.32	120.08	124.93
26	M9	202	PEB	OD-C4D-C3D	-2.32	124.20	129.46
26	P9	202	PEB	CMA-C2A-C1A	-2.32	107.40	112.40
26	ME	201	PEB	CHB-C4B-NB	-2.32	125.61	128.83
26	A4	202	PEB	CMB-C2B-C1B	2.32	128.64	125.06
26	V2	201	PEB	CHC-C4C-C3C	-2.32	126.38	130.34
26	AC	201	PEB	CMB-C2B-C1B	2.32	128.63	125.06
28	YH	1003	CYC	C2A-C1A-NA	2.32	113.42	110.05
26	c4	203	PEB	OD-C4D-C3D	-2.32	124.21	129.46
26	O9	201	PEB	CHB-C4B-C3B	-2.32	119.96	125.32
28	vH	1001	CYC	C1A-C2A-C3A	-2.32	104.22	106.78
26	Z8	201	PEB	CMD-C2D-C3D	2.32	133.33	130.06
26	Y4	201	PEB	OD-C4D-C3D	-2.32	124.21	129.46
26	AG	201	PEB	OD-C4D-C3D	-2.32	124.21	129.46
26	ZG	201	PEB	OD-C4D-C3D	-2.32	124.21	129.46
26	RI	202	PEB	OD-C4D-C3D	-2.32	124.21	129.46
26	YE	202	PEB	CHA-C1B-NB	-2.32	120.08	124.93
26	F5	201	PEB	CMA-C2A-C1A	-2.32	107.41	112.40
26	kB	201	PEB	OD-C4D-ND	-2.32	122.50	125.93
26	C5	204	PEB	CHC-C4C-C3C	-2.32	126.38	130.34
26	vG	202	PEB	CHC-C4C-C3C	-2.32	126.38	130.34
26	HG	202	PEB	CHC-C1D-ND	-2.32	111.26	113.95
28	AH	1001	CYC	CHB-C1B-C2B	-2.32	122.36	126.95
26	S7	203	PEB	CHB-C4B-NB	-2.32	125.61	128.83
26	rG	202	PEB	C4B-C3B-C2B	-2.32	104.22	106.78
26	TA	202	PEB	C1B-C2B-C3B	-2.32	103.85	106.51
28	B6	1002	CYC	CAB-C3B-C2B	2.32	131.49	127.53
26	vG	202	PEB	CAB-C3B-C4B	2.32	129.11	125.01
26	B5	202	PEB	CHA-C1B-NB	-2.32	120.09	124.93
26	QJ	201	PEB	CHA-C4A-NA	2.32	127.96	125.20
26	a7	202	PEB	OD-C4D-ND	-2.32	122.50	125.93
26	FJ	201	PEB	OD-C4D-C3D	-2.32	124.21	129.46
26	J5	201	PEB	C3B-C4B-NB	2.32	113.42	110.05
26	GD	202	PEB	CAB-C3B-C4B	2.32	129.10	125.01
26	TE	201	PEB	C1B-C2B-C3B	-2.32	103.85	106.51
28	N7	1001	CYC	C1A-C2A-C3A	-2.32	104.22	106.78
26	a8	204	PEB	CHB-C4B-C3B	-2.32	119.97	125.32
26	JA	202	PEB	C2A-C1A-NA	2.32	110.27	108.27
26	VI	203	PEB	CAC-CBC-CGC	-2.32	107.27	113.76
26	AF	305	PEB	OD-C4D-C3D	-2.32	124.22	129.46
26	GJ	201	PEB	C1B-C2B-C3B	-2.31	103.85	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	HB	1001	CYC	CBD-CAD-C3D	-2.31	108.67	112.62
28	LF	1001	CYC	CBA-CAA-C2A	-2.31	106.20	112.63
26	WF	201	PEB	CAC-C2C-C3C	2.31	133.90	127.25
26	WD	201	PEB	O2C-CGC-CBC	2.31	121.47	114.03
26	O4	201	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	PD	202	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	T7	201	PEB	C2A-C1A-NA	2.31	110.27	108.27
26	U9	202	PEB	CHA-C4A-NA	-2.31	122.45	125.20
26	d4	201	PEB	CMB-C2B-C1B	2.31	128.63	125.06
26	O1	202	PEB	OD-C4D-ND	-2.31	122.50	125.93
26	aE	203	PEB	CHA-C1B-C2B	2.31	130.85	124.90
26	a1	201	PEB	C3B-C4B-NB	2.31	113.41	110.05
28	TH	1001	CYC	C2A-C1A-NA	2.31	113.41	110.05
26	EG	201	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	U6	202	PEB	CMB-C2B-C1B	2.31	128.63	125.06
26	d1	201	PEB	CAA-C3A-C2A	-2.31	108.48	114.26
26	KA	202	PEB	CAB-C3B-C4B	2.31	129.10	125.01
28	rH	1001	CYC	CAB-C3B-C2B	2.31	131.49	127.53
26	k8	202	PEB	CAB-C3B-C2B	-2.31	123.57	127.88
26	c1	202	PEB	C3B-C4B-NB	2.31	113.41	110.05
26	Q3	201	PEB	C3B-C4B-NB	2.31	113.41	110.05
26	UA	202	PEB	C3B-C4B-NB	2.31	113.41	110.05
26	iG	202	PEB	O1C-CGC-CBC	-2.31	115.65	123.08
26	S2	201	PEB	CMD-C2D-C3D	2.31	133.32	130.06
26	oE	201	PEB	CAB-CBB-CGB	-2.31	108.63	113.60
26	PD	203	PEB	OD-C4D-ND	-2.31	122.50	125.93
26	OG	203	PEB	CAA-C3A-C4A	-2.31	106.74	112.67
26	ED	201	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	LD	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
28	eH	1001	CYC	CHB-C1B-C2B	-2.31	122.37	126.95
26	JJ	202	PEB	C2B-C1B-NB	2.31	115.46	110.53
26	21	404	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	QE	202	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	vE	201	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	U2	201	PEB	OA-C1A-C2A	-2.31	124.33	126.17
26	u1	203	PEB	C1B-C2B-C3B	-2.31	103.85	106.51
26	X3	202	PEB	CHA-C4A-NA	2.31	127.95	125.20
26	WF	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
26	f7	201	PEB	CHA-C1B-NB	-2.31	120.10	124.93
26	iG	203	PEB	CHA-C1B-NB	-2.31	120.10	124.93
26	eE	202	PEB	CHB-C4B-NB	-2.31	125.62	128.83
26	oE	201	PEB	O1C-CGC-CBC	-2.31	115.66	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	u1	201	PEB	CAB-C3B-C4B	2.31	129.10	125.01
26	P1	203	PEB	CHB-C4B-C3B	-2.31	119.98	125.32
26	V7	202	PEB	C4B-C3B-C2B	-2.31	104.23	106.78
28	DF	1001	CYC	C1A-C2A-C3A	-2.31	104.23	106.78
26	iF	202	PEB	CAB-C3B-C4B	2.31	129.09	125.01
26	QI	201	PEB	CAB-C3B-C4B	2.31	129.09	125.01
26	kG	202	PEB	C3B-C4B-NB	2.31	113.41	110.05
26	OE	203	PEB	CMB-C2B-C1B	2.31	128.62	125.06
26	lB	202	PEB	CHA-C1B-NB	-2.31	120.10	124.93
28	L2	1001	CYC	C1B-NB-C4B	-2.31	107.73	110.67
28	vH	1001	CYC	C2C-C1C-NC	2.31	110.26	108.27
26	Y2	201	PEB	CHA-C4A-NA	2.31	127.95	125.20
26	eF	201	PEB	CMA-C2A-C1A	-2.31	107.42	112.40
28	B6	1001	CYC	O2D-CGD-CBD	2.31	121.45	114.03
26	EA	203	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	P3	203	PEB	OD-C4D-ND	-2.31	122.51	125.93
28	UH	1001	CYC	C2C-C3C-C4C	2.31	104.80	101.34
26	u1	203	PEB	CHB-C4B-C3B	-2.31	119.99	125.32
26	uG	203	PEB	OD-C4D-C3D	-2.31	124.23	129.46
26	fG	202	PEB	CAC-CBC-CGC	-2.31	107.29	113.76
26	D4	202	PEB	C3B-C4B-NB	2.31	113.41	110.05
26	a6	201	PEB	CMA-C2A-C1A	-2.31	107.43	112.40
26	B1	203	PEB	CAB-C3B-C4B	2.31	129.09	125.01
26	aA	202	PEB	CMA-C2A-C1A	-2.31	107.43	112.40
26	gE	201	PEB	CHA-C4A-NA	2.31	127.95	125.20
26	CD	201	PEB	CAB-C3B-C4B	2.31	129.09	125.01
28	gH	1001	CYC	C2B-C1B-NB	2.31	110.37	106.99
26	r4	202	PEB	C3B-C4B-NB	2.31	113.41	110.05
26	M8	203	PEB	CBC-CAC-C2C	-2.31	108.68	112.62
26	I8	203	PEB	OD-C4D-ND	-2.31	122.51	125.93
26	W9	201	PEB	CMD-C2D-C3D	2.31	133.32	130.06
26	iE	203	PEB	C2A-C1A-NA	2.31	110.26	108.27
26	y1	201	PEB	OD-C4D-C3D	-2.31	124.23	129.46
26	P3	202	PEB	OD-C4D-C3D	-2.31	124.23	129.46
26	aG	201	PEB	CMB-C2B-C1B	2.31	128.62	125.06
26	mF	201	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
26	gE	201	PEB	O2C-CGC-CBC	2.31	121.44	114.03
26	BE	201	PEB	CMD-C2D-C3D	-2.31	126.81	130.06
26	JE	201	PEB	C3B-C4B-NB	2.31	113.40	110.05
26	DE	203	PEB	C2B-C1B-NB	2.31	115.45	110.53
26	J3	203	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
26	D3	203	PEB	CHB-C4B-C3B	-2.31	119.99	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	MG	202	PEB	OD-C4D-C3D	-2.31	124.24	129.46
26	L5	203	PEB	CHA-C1B-NB	-2.31	120.11	124.93
26	EJ	201	PEB	OD-C4D-ND	-2.31	122.52	125.93
27	A6	303	PUB	CBA-CAA-C3A	-2.31	109.48	112.98
28	nH	1001	CYC	C2C-C3C-C4C	2.31	104.79	101.34
26	Z6	203	PEB	CHA-C4A-NA	2.31	127.95	125.20
26	V8	201	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
26	R1	201	PEB	OD-C4D-C3D	-2.31	124.24	129.46
26	Q6	201	PEB	OD-C4D-C3D	-2.31	124.24	129.46
26	yG	301	PEB	OD-C4D-C3D	-2.31	124.24	129.46
26	kF	202	PEB	C3B-C4B-NB	2.31	113.40	110.05
26	SB	202	PEB	CBC-CAC-C2C	-2.30	108.69	112.62
27	24	402	PUB	CAC-C2C-C1C	2.30	129.09	125.01
26	d4	201	PEB	C1B-C2B-C3B	-2.30	103.86	106.51
26	rE	201	PEB	C1B-C2B-C3B	-2.30	103.86	106.51
26	NI	1002	PEB	OD-C4D-C3D	-2.30	124.24	129.46
26	PA	202	PEB	OD-C4D-ND	-2.30	122.52	125.93
26	JJ	203	PEB	CBD-CAD-C3D	-2.30	116.16	127.62
26	fE	201	PEB	CAB-CBB-CGB	-2.30	108.64	113.60
26	S2	202	PEB	CHA-C1B-NB	-2.30	120.11	124.93
26	m4	201	PEB	CHC-C1D-ND	-2.30	111.27	113.95
28	pH	1001	CYC	C2A-C1A-NA	2.30	113.40	110.05
26	d1	201	PEB	CHC-C4C-C3C	-2.30	126.41	130.34
26	VF	203	PEB	CHC-C4C-C3C	-2.30	126.41	130.34
26	d6	203	PEB	C4B-C3B-C2B	-2.30	104.23	106.78
26	B5	203	PEB	C3B-C4B-NB	2.30	113.40	110.05
26	A9	303	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
26	TA	202	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
26	q1	202	PEB	OD-C4D-C3D	-2.30	124.24	129.46
26	U8	202	PEB	OD-C4D-C3D	-2.30	124.24	129.46
26	F9	201	PEB	OD-C4D-C3D	-2.30	124.24	129.46
26	PG	201	PEB	CMB-C2B-C1B	2.30	128.61	125.06
26	W9	201	PEB	CAB-CBB-CGB	-2.30	108.65	113.60
26	mA	201	PEB	CHA-C1B-C2B	2.30	130.82	124.90
26	mA	201	PEB	CAA-C3A-C4A	-2.30	106.76	112.67
26	jG	201	PEB	CMB-C2B-C1B	2.30	128.61	125.06
26	M8	202	PEB	CAA-C3A-C4A	-2.30	106.76	112.67
26	yE	301	PEB	OD-C4D-C3D	-2.30	124.25	129.46
26	z1	202	PEB	OD-C4D-ND	-2.30	122.52	125.93
26	M3	201	PEB	CAB-CBB-CGB	-2.30	108.65	113.60
26	SA	201	PEB	CAB-CBB-CGB	-2.30	108.65	113.60
26	e8	202	PEB	O2B-CGB-CBB	2.30	121.42	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y1	201	PEB	CAB-C3B-C4B	2.30	129.08	125.01
26	G4	202	PEB	OD-C4D-C3D	-2.30	124.25	129.46
26	W1	202	PEB	CHA-C1B-NB	-2.30	120.12	124.93
26	W6	203	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
26	TJ	201	PEB	CAC-CBC-CGC	-2.30	107.31	113.76
26	y4	202	PEB	CMB-C2B-C1B	2.30	128.61	125.06
26	d4	202	PEB	OD-C4D-ND	-2.30	122.52	125.93
28	NB	1001	CYC	CBA-CAA-C2A	-2.30	106.23	112.63
26	L9	202	PEB	OA-C1A-C2A	-2.30	124.34	126.17
26	A3	201	PEB	C3B-C4B-NB	2.30	113.39	110.05
26	fE	201	PEB	C3B-C4B-NB	2.30	113.39	110.05
26	TF	201	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
26	J7	1002	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
26	N9	202	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
26	mE	203	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
26	g7	201	PEB	OD-C4D-ND	-2.30	122.52	125.93
26	f8	202	PEB	OD-C4D-ND	-2.30	122.52	125.93
26	T4	202	PEB	CHA-C4A-NA	-2.30	122.47	125.20
26	TG	201	PEB	CAB-CBB-CGB	-2.30	108.66	113.60
26	c1	203	PEB	OD-C4D-C3D	-2.30	124.25	129.46
26	H4	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
26	W9	201	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
26	PD	201	PEB	CAA-C3A-C2A	-2.30	108.52	114.26
26	24	405	PEB	OD-C4D-C3D	-2.30	124.25	129.46
26	C8	202	PEB	CBC-CAC-C2C	-2.30	108.70	112.62
26	rE	201	PEB	CBC-CAC-C2C	-2.30	108.70	112.62
27	YD	302	PUB	C2C-C1C-NC	2.30	113.39	110.05
28	dH	1001	CYC	C2A-C1A-NA	2.30	113.39	110.05
26	g4	202	PEB	CMB-C2B-C1B	2.30	128.60	125.06
26	oG	203	PEB	CMA-C2A-C1A	-2.30	107.45	112.40
26	Z4	202	PEB	CHA-C4A-NA	-2.30	122.47	125.20
26	eD	401	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
26	A4	201	PEB	OD-C4D-C3D	-2.30	124.25	129.46
28	II	1001	CYC	CMB-C2B-C1B	2.30	127.04	124.17
26	QB	203	PEB	CHB-C4B-C3B	-2.30	120.01	125.32
26	e1	201	PEB	CMB-C2B-C1B	2.30	128.60	125.06
26	qG	202	PEB	C2A-C1A-NA	2.30	110.25	108.27
26	B4	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
26	TB	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	XE	201	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
26	LC	201	PEB	C3B-C4B-NB	2.30	113.39	110.05
26	f1	202	PEB	OD-C4D-ND	-2.30	122.53	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N7	1002	PEB	CHA-C1B-NB	-2.30	120.13	124.93
26	mG	202	PEB	CAB-C3B-C4B	2.30	129.07	125.01
26	D1	203	PEB	OD-C4D-C3D	-2.30	124.26	129.46
26	WB	202	PEB	OD-C4D-C3D	-2.30	124.26	129.46
26	Q9	201	PEB	CAA-C3A-C2A	-2.30	108.52	114.26
26	N1	201	PEB	CHC-C4C-C3C	-2.30	126.42	130.34
26	A7	301	PEB	CHC-C4C-C3C	-2.30	126.42	130.34
26	t4	202	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
26	L3	201	PEB	C3B-C4B-NB	2.30	113.39	110.05
26	CG	202	PEB	CHA-C1B-NB	-2.30	120.13	124.93
26	B3	203	PEB	OD-C4D-C3D	-2.30	124.26	129.46
26	d7	203	PEB	CBD-CAD-C3D	-2.30	116.19	127.62
28	H6	1001	CYC	CBD-CAD-C3D	-2.30	108.70	112.62
26	s1	203	PEB	C3B-C4B-NB	2.30	113.39	110.05
26	g7	201	PEB	CHB-C4B-C3B	-2.30	120.02	125.32
26	WB	203	PEB	CAB-CBB-CGB	-2.30	108.66	113.60
28	oH	1001	CYC	C2C-C3C-C4C	2.30	104.78	101.34
26	O8	202	PEB	OD-C4D-ND	-2.30	122.53	125.93
28	B6	1002	CYC	C1A-C2A-C3A	-2.30	104.24	106.78
26	p1	201	PEB	CHC-C4C-C3C	-2.30	126.42	130.34
26	LE	201	PEB	CHC-C4C-C3C	-2.30	126.42	130.34
26	n4	201	PEB	CHA-C1B-NB	-2.30	120.13	124.93
26	L2	1002	PEB	CMC-C3C-C2C	2.30	129.27	124.94
26	HD	202	PEB	C3B-C4B-NB	2.30	113.39	110.05
28	H2	1001	CYC	CAB-C3B-C2B	2.30	131.46	127.53
26	YD	303	PEB	OD-C4D-ND	-2.30	122.53	125.93
26	V1	203	PEB	C1B-C2B-C3B	-2.29	103.87	106.51
26	A5	201	PEB	C1B-C2B-C3B	-2.29	103.87	106.51
26	K1	201	PEB	CHB-C4B-C3B	-2.29	120.02	125.32
26	jA	202	PEB	C3B-C4B-NB	2.29	113.39	110.05
26	dG	202	PEB	CHC-C4C-C3C	2.29	134.25	130.34
26	GE	203	PEB	C2B-C1B-NB	2.29	115.43	110.53
26	TE	202	PEB	C2B-C1B-NB	2.29	115.43	110.53
28	KB	202	CYC	CHB-C1B-NB	-2.29	121.13	126.06
26	Q8	203	PEB	C2A-C1A-NA	2.29	110.25	108.27
26	SE	202	PEB	OD-C4D-C3D	-2.29	124.26	129.46
26	TB	202	PEB	CHA-C4A-NA	2.29	127.93	125.20
26	fG	202	PEB	CHA-C1B-NB	-2.29	120.13	124.93
28	yH	1001	CYC	C2B-C1B-NB	2.29	110.35	106.99
26	bE	202	PEB	C4B-C3B-C2B	-2.29	104.24	106.78
26	Z1	201	PEB	CBB-CAB-C3B	2.29	119.00	112.63
26	i1	202	PEB	OD-C4D-C3D	-2.29	124.26	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	xG	305	PUB	CBA-CAA-C3A	-2.29	109.50	112.98
28	yH	1001	CYC	C2C-C3C-C4C	2.29	104.77	101.34
26	fF	203	PEB	OD-C4D-ND	-2.29	122.53	125.93
26	QF	201	PEB	CAB-C3B-C4B	2.29	129.06	125.01
28	uH	1001	CYC	OC-C1C-NC	2.29	127.72	124.94
26	G3	202	PEB	CHA-C1B-NB	-2.29	120.14	124.93
26	UJ	201	PEB	CAB-C3B-C4B	2.29	129.06	125.01
26	GC	203	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	F3	203	PEB	CAB-CBB-CGB	-2.29	108.67	113.60
26	V4	201	PEB	C4B-C3B-C2B	-2.29	104.25	106.78
26	dE	202	PEB	C2A-C1A-NA	2.29	110.25	108.27
26	eB	203	PEB	C3B-C4B-NB	2.29	113.38	110.05
28	C7	1001	CYC	CBD-CAD-C3D	-2.29	108.71	112.62
26	F1	202	PEB	CAC-CBC-CGC	-2.29	107.33	113.76
26	fA	201	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	fF	201	PEB	CAB-C3B-C4B	2.29	129.06	125.01
26	r1	201	PEB	CHB-C4B-NB	-2.29	125.65	128.83
26	V3	201	PEB	CAB-CBB-CGB	-2.29	108.67	113.60
26	B9	201	PEB	CHA-C1B-C2B	2.29	130.79	124.90
26	CE	203	PEB	CHA-C1B-NB	-2.29	120.14	124.93
26	vE	202	PEB	C2B-C1B-NB	2.29	115.42	110.53
26	eG	201	PEB	C2B-C1B-NB	2.29	115.42	110.53
26	KE	202	PEB	CHA-C1B-NB	-2.29	120.14	124.93
26	G9	202	PEB	OD-C4D-C3D	-2.29	124.27	129.46
26	QB	203	PEB	CHB-C4B-NB	-2.29	125.65	128.83
26	GG	203	PEB	O2B-CGB-CBB	2.29	121.39	114.03
26	VI	201	PEB	CHC-C4C-C3C	-2.29	126.43	130.34
26	P8	201	PEB	OD-C4D-C3D	-2.29	124.27	129.46
26	X1	201	PEB	CBC-CAC-C2C	2.29	116.53	112.62
26	U7	201	PEB	CHA-C1B-NB	-2.29	120.14	124.93
26	UI	201	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	N9	202	PEB	CMB-C2B-C1B	2.29	128.59	125.06
26	P1	202	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
26	D9	202	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
26	p1	202	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
26	O6	201	PEB	OD-C4D-C3D	-2.29	124.28	129.46
26	JD	203	PEB	OD-C4D-C3D	-2.29	124.28	129.46
26	k6	202	PEB	CMC-C3C-C2C	2.29	129.26	124.94
26	W1	201	PEB	C2A-C1A-NA	2.29	110.25	108.27
26	jE	202	PEB	CAB-C3B-C4B	2.29	129.06	125.01
26	H9	201	PEB	CMB-C2B-C1B	2.29	128.59	125.06
26	g4	201	PEB	CHB-C4B-C3B	-2.29	120.03	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T7	201	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	TF	201	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
26	k6	201	PEB	CAC-CBC-CGC	-2.29	107.34	113.76
26	aF	202	PEB	C3B-C4B-NB	2.29	113.38	110.05
26	q4	203	PEB	CMB-C2B-C1B	2.29	128.59	125.06
26	I9	202	PEB	CBB-CAB-C3B	2.29	118.98	112.63
26	E9	201	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
26	jG	202	PEB	CAB-C3B-C4B	2.29	129.06	125.01
26	pG	202	PEB	OD-C4D-C3D	-2.29	124.28	129.46
26	AJ	304	PEB	C3B-C4B-NB	2.29	113.38	110.05
27	A9	302	PUB	C2C-C1C-NC	2.29	113.38	110.05
26	h6	203	PEB	CBC-CAC-C2C	-2.29	108.72	112.62
26	aB	201	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
26	d1	202	PEB	OD-C4D-C3D	-2.29	124.28	129.46
26	hB	201	PEB	C4B-C3B-C2B	-2.29	104.25	106.78
26	K5	202	PEB	CAC-CBC-CGC	-2.29	107.35	113.76
26	mF	201	PEB	OD-C4D-C3D	-2.29	124.28	129.46
26	aF	202	PEB	CHC-C4C-C3C	-2.29	126.44	130.34
26	WJ	201	PEB	CAB-CBB-CGB	-2.29	108.68	113.60
26	c8	201	PEB	CHA-C1B-NB	-2.29	120.15	124.93
26	dE	202	PEB	CHA-C1B-NB	-2.29	120.15	124.93
28	IF	1001	CYC	CMC-C2C-C1C	-2.29	107.47	112.40
26	L5	202	PEB	CBA-CAA-C3A	-2.29	108.38	113.47
26	uE	203	PEB	OD-C4D-C3D	-2.29	124.28	129.46
26	eG	202	PEB	CHA-C1B-C2B	2.29	130.78	124.90
28	MI	1001	CYC	CBD-CAD-C3D	-2.29	108.72	112.62
26	Z4	202	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
26	T8	202	PEB	O2B-CGB-CBB	2.29	121.37	114.03
26	KE	202	PEB	OA-C1A-C2A	2.29	127.99	126.17
26	W8	203	PEB	C2B-C1B-NB	2.29	115.41	110.53
26	cF	201	PEB	C2B-C1B-NB	2.29	115.41	110.53
26	B4	203	PEB	CMB-C2B-C1B	2.29	128.58	125.06
26	SI	201	PEB	C4B-C3B-C2B	-2.29	104.25	106.78
26	g4	201	PEB	CMA-C2A-C1A	-2.28	107.48	112.40
26	A2	301	PEB	CHC-C1D-ND	-2.28	111.29	113.95
26	j8	202	PEB	CAB-C3B-C4B	2.28	129.05	125.01
26	lG	202	PEB	CAB-C3B-C4B	2.28	129.05	125.01
27	K4	203	PUB	CMD-C2D-C3D	2.28	131.20	127.77
26	hF	201	PEB	CAB-CBB-CGB	-2.28	108.69	113.60
26	QE	202	PEB	CAA-C3A-C4A	-2.28	106.81	112.67
26	A8	302	PEB	C2A-C1A-NA	2.28	110.24	108.27
27	AF	304	PUB	CMA-C2A-C1A	2.28	126.76	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BC	202	PEB	C1C-CHB-C4B	-2.28	126.08	128.81
28	HF	1001	CYC	OB-C4B-NB	-2.28	119.77	125.08
26	L3	203	PEB	OD-C4D-C3D	-2.28	124.29	129.46
26	WE	203	PEB	OD-C4D-C3D	-2.28	124.29	129.46
26	aA	202	PEB	CHA-C1B-NB	-2.28	120.16	124.93
26	m2	203	PEB	CAB-CBB-CGB	2.28	118.52	113.60
26	q4	203	PEB	OD-C4D-C3D	-2.28	124.29	129.46
26	dG	201	PEB	OD-C4D-C3D	-2.28	124.29	129.46
26	ZE	202	PEB	CHB-C4B-NB	-2.28	125.66	128.83
26	hB	203	PEB	CBC-CAC-C2C	-2.28	108.72	112.62
28	K6	202	CYC	CHB-C1B-NB	-2.28	121.16	126.06
26	J9	202	PEB	C2B-C1B-NB	2.28	115.40	110.53
28	LH	1001	CYC	OC-C1C-NC	2.28	127.71	124.94
26	wE	302	PEB	OD-C4D-C3D	-2.28	124.29	129.46
26	cF	201	PEB	C1C-CHB-C4B	2.28	131.53	128.81
26	MA	203	PEB	CBC-CAC-C2C	-2.28	108.73	112.62
28	NF	1001	CYC	CHA-C1A-C2A	-2.28	120.05	125.32
26	W9	202	PEB	C2A-C1A-NA	2.28	110.24	108.27
26	BJ	201	PEB	C2A-C1A-NA	2.28	110.24	108.27
26	EG	201	PEB	CMB-C2B-C3B	-2.28	119.92	126.12
26	j1	202	PEB	CHA-C1B-C2B	-2.28	119.03	124.90
26	DB	1002	PEB	O2B-CGB-CBB	2.28	121.36	114.03
26	PF	201	PEB	CMA-C2A-C1A	-2.28	107.49	112.40
26	l6	203	PEB	CMB-C2B-C1B	2.28	128.58	125.06
26	QJ	202	PEB	C2A-C1A-NA	2.28	110.24	108.27
26	fA	203	PEB	CAA-C3A-C4A	-2.28	106.82	112.67
26	mE	203	PEB	OD-C4D-C3D	-2.28	124.29	129.46
26	NJ	202	PEB	CAB-C3B-C4B	2.28	129.04	125.01
26	l4	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
26	R2	203	PEB	CMB-C2B-C1B	2.28	128.57	125.06
26	VG	201	PEB	CHB-C4B-NB	-2.28	125.66	128.83
26	UJ	201	PEB	CAB-CBB-CGB	-2.28	108.70	113.60
26	jG	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	L9	202	PEB	C1C-CHB-C4B	2.28	131.53	128.81
26	w1	201	PEB	OD-C4D-C3D	-2.28	124.30	129.46
26	O9	202	PEB	CAA-C3A-C4A	2.28	118.53	112.67
26	GG	202	PEB	CHB-C4B-NB	-2.28	125.67	128.83
26	wG	303	PEB	CBB-CAB-C3B	2.28	118.96	112.63
26	eE	201	PEB	C3B-C4B-NB	2.28	113.36	110.05
26	PD	201	PEB	C4B-C3B-C2B	-2.28	104.26	106.78
26	AB	301	PEB	CMB-C2B-C1B	2.28	128.57	125.06
26	uG	203	PEB	CMB-C2B-C1B	2.28	128.57	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	qH	1002	CYC	CAC-C3C-C2C	-2.28	108.57	114.26
26	mF	201	PEB	CHA-C1B-NB	-2.28	120.17	124.93
26	GJ	202	PEB	CAB-C3B-C4B	2.28	129.04	125.01
26	ED	202	PEB	OD-C4D-ND	-2.28	122.56	125.93
26	UE	201	PEB	CMA-C2A-C1A	2.28	117.31	112.40
26	G8	201	PEB	C2A-C1A-NA	2.28	110.24	108.27
26	h1	202	PEB	CHC-C4C-C3C	-2.28	126.45	130.34
26	M9	201	PEB	CHC-C4C-C3C	-2.28	126.45	130.34
26	Y6	201	PEB	C4B-NB-C1B	-2.28	102.22	106.51
26	cE	203	PEB	CBB-CAB-C3B	2.28	118.96	112.63
26	Y8	201	PEB	CHB-C4B-C3B	-2.28	120.06	125.32
26	j1	202	PEB	C4B-C3B-C2B	-2.28	104.26	106.78
26	WG	201	PEB	OD-C4D-ND	-2.28	122.56	125.93
26	mG	201	PEB	C3B-C4B-NB	2.28	113.36	110.05
26	R8	201	PEB	CMA-C2A-C1A	-2.28	107.49	112.40
26	QD	201	PEB	CAB-C3B-C4B	2.28	129.04	125.01
28	WH	1001	CYC	C2C-C3C-C4C	2.28	104.75	101.34
27	yE	303	PUB	CMD-C2D-C3D	2.28	131.19	127.77
26	gA	201	PEB	C2A-C1A-NA	2.28	110.24	108.27
26	h1	201	PEB	CHA-C4A-NA	2.28	127.91	125.20
26	V2	203	PEB	CMB-C2B-C1B	2.28	128.57	125.06
26	i2	203	PEB	CAB-C3B-C2B	2.28	132.12	127.88
26	u4	202	PEB	CHA-C1B-NB	-2.28	120.17	124.93
27	A8	303	PUB	CMD-C2D-C3D	2.28	131.18	127.77
26	vG	201	PEB	CHA-C1B-NB	-2.28	120.17	124.93
26	SE	201	PEB	CAC-CBC-CGC	-2.28	107.38	113.76
26	jA	202	PEB	C2A-C1A-NA	2.28	110.23	108.27
26	g6	201	PEB	C2B-C1B-NB	2.28	115.39	110.53
26	KC	203	PEB	CHA-C1B-NB	-2.28	120.17	124.93
26	PA	201	PEB	OD-C4D-C3D	-2.28	124.31	129.46
28	hH	1001	CYC	C2A-C1A-NA	2.28	113.36	110.05
26	14	202	PEB	CHA-C1B-NB	-2.28	120.17	124.93
26	hG	202	PEB	CAB-C3B-C4B	2.28	129.03	125.01
26	QJ	202	PEB	CAB-C3B-C4B	2.28	129.03	125.01
26	L3	202	PEB	CHB-C4B-C3B	-2.27	120.06	125.32
26	h7	201	PEB	CMB-C2B-C1B	2.27	128.57	125.06
26	T4	201	PEB	CHA-C1B-NB	-2.27	120.17	124.93
27	24	402	PUB	C2C-C1C-NC	2.27	113.36	110.05
26	L4	202	PEB	CMB-C2B-C1B	2.27	128.57	125.06
26	J3	201	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
26	S7	203	PEB	OD-C4D-ND	-2.27	122.56	125.93
26	PB	201	PEB	CMA-C2A-C1A	-2.27	107.50	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	iI	203	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	b4	501	PEB	CHA-C4A-NA	2.27	127.91	125.20
26	EJ	202	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
26	D9	201	PEB	OD-C4D-ND	-2.27	122.56	125.93
26	YE	202	PEB	OD-C4D-ND	-2.27	122.56	125.93
28	CH	1001	CYC	CAA-C2A-C1A	2.27	129.03	125.01
26	U1	201	PEB	CHB-C4B-C3B	-2.27	120.07	125.32
26	oE	203	PEB	CHA-C4A-NA	2.27	127.91	125.20
26	xE	302	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
26	h2	201	PEB	C2A-C1A-NA	2.27	110.23	108.27
26	B9	201	PEB	C2A-C1A-NA	2.27	110.23	108.27
26	x4	201	PEB	C4B-C3B-C2B	-2.27	104.27	106.78
26	t4	201	PEB	OD-C4D-C3D	-2.27	124.31	129.46
26	C4	201	PEB	CAB-CBB-CGB	-2.27	108.71	113.60
26	L4	201	PEB	CAB-CBB-CGB	-2.27	108.71	113.60
27	AA	303	PUB	CAC-CBC-CGC	-2.27	108.71	113.60
26	J2	1002	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
26	t1	201	PEB	CAA-C3A-C4A	-2.27	106.84	112.67
26	iA	201	PEB	CMD-C2D-C3D	2.27	133.27	130.06
28	JI	1001	CYC	CBD-CAD-C3D	-2.27	108.74	112.62
26	J8	201	PEB	CHA-C1B-C2B	2.27	130.74	124.90
26	U3	201	PEB	CHA-C4A-NA	2.27	127.91	125.20
26	C9	202	PEB	CAB-C3B-C4B	2.27	129.03	125.01
26	II	202	PEB	O2B-CGB-CBB	2.27	121.33	114.03
26	kF	202	PEB	OA-C1A-NA	2.27	127.69	124.94
26	vE	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
26	ME	203	PEB	C3B-C4B-NB	2.27	113.35	110.05
26	l8	201	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
26	W4	201	PEB	C2A-C1A-NA	2.27	110.23	108.27
26	P6	201	PEB	CHB-C4B-NB	-2.27	125.68	128.83
26	XE	202	PEB	C2B-C1B-NB	2.27	115.38	110.53
26	OG	201	PEB	CAB-C3B-C4B	2.27	129.03	125.01
26	TF	201	PEB	CHB-C4B-C3B	-2.27	120.07	125.32
26	kE	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	VJ	203	PEB	CMB-C2B-C1B	2.27	128.56	125.06
26	k6	202	PEB	CBC-CAC-C2C	2.27	116.50	112.62
26	Z1	201	PEB	C3B-C4B-NB	2.27	113.35	110.05
26	VF	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
26	JD	201	PEB	CHC-C4C-C3C	-2.27	126.46	130.34
27	A2	303	PUB	CBA-CAA-C3A	-2.27	109.53	112.98
26	kI	201	PEB	CMB-C2B-C1B	2.27	128.56	125.06
26	TF	201	PEB	CBD-CAD-C3D	-2.27	116.33	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I3	202	PEB	OA-C1A-C2A	-2.27	124.37	126.17
26	h4	203	PEB	C2A-C1A-NA	2.27	110.23	108.27
26	iA	202	PEB	CHA-C4A-NA	-2.27	122.51	125.20
26	pG	201	PEB	CAB-C3B-C4B	2.27	129.02	125.01
28	jH	1001	CYC	C2A-C1A-NA	2.27	113.35	110.05
26	SD	202	PEB	C2B-C1B-NB	2.27	115.37	110.53
26	VA	202	PEB	CHA-C1B-C2B	2.27	130.74	124.90
26	J4	202	PEB	CHA-C1B-NB	-2.27	120.19	124.93
26	KE	202	PEB	CAB-C3B-C4B	2.27	129.02	125.01
26	lF	203	PEB	C3B-C4B-NB	2.27	113.35	110.05
26	K3	201	PEB	CAA-C3A-C4A	-2.27	106.85	112.67
26	N1	201	PEB	CMB-C2B-C3B	-2.27	119.96	126.12
26	LE	202	PEB	CHA-C4A-NA	2.27	127.90	125.20
26	PI	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
26	S4	201	PEB	CMC-C3C-C2C	2.27	129.22	124.94
26	y1	203	PEB	CMB-C2B-C1B	2.27	128.56	125.06
26	U6	203	PEB	CAB-C3B-C4B	2.27	129.02	125.01
26	s4	203	PEB	OD-C4D-C3D	-2.27	124.32	129.46
26	m6	201	PEB	CAA-C3A-C2A	-2.27	108.59	114.26
26	SI	201	PEB	CMD-C2D-C3D	2.27	133.26	130.06
26	c2	203	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	UD	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	i8	202	PEB	CMB-C2B-C1B	2.27	128.56	125.06
26	SJ	202	PEB	CHC-C4C-C3C	-2.27	126.47	130.34
26	z1	201	PEB	CBA-CAA-C3A	-2.27	108.42	113.47
26	DG	201	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
26	Q6	201	PEB	CMB-C2B-C1B	2.27	128.56	125.06
28	KH	1001	CYC	CMA-C3A-C4A	2.27	128.56	125.06
26	q4	201	PEB	CHA-C4A-NA	2.27	127.90	125.20
26	bB	202	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
26	cF	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
26	OD	201	PEB	O2C-CGC-CBC	2.27	121.31	114.03
28	eH	1001	CYC	CAA-C2A-C1A	2.27	129.02	125.01
26	s4	201	PEB	OD-C4D-C3D	-2.27	124.32	129.46
26	QJ	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
26	T6	202	PEB	CMC-C3C-C2C	2.27	129.22	124.94
26	jA	201	PEB	C1C-CHB-C4B	-2.27	126.10	128.81
26	VI	203	PEB	C1C-CHB-C4B	2.27	131.52	128.81
26	i6	201	PEB	OD-C4D-ND	-2.27	122.57	125.93
26	BJ	201	PEB	CBA-CAA-C3A	-2.27	108.42	113.47
26	e1	202	PEB	C3B-C4B-NB	2.27	113.35	110.05
26	HJ	202	PEB	OA-C1A-C2A	-2.27	124.37	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	oE	201	PEB	O2C-CGC-CBC	2.27	121.31	114.03
26	D8	201	PEB	OD-C4D-ND	-2.27	122.57	125.93
26	V8	202	PEB	CMA-C2A-C1A	-2.27	107.52	112.40
26	vE	202	PEB	CHB-C4B-NB	-2.27	125.68	128.83
26	G9	201	PEB	CAA-C3A-C4A	-2.27	106.85	112.67
26	U3	202	PEB	CHC-C1D-ND	-2.27	111.32	113.95
26	P8	201	PEB	CHC-C1D-ND	2.27	116.58	113.95
26	d7	202	PEB	CAB-CBB-CGB	-2.27	108.73	113.60
26	d8	202	PEB	CAB-CBB-CGB	-2.27	108.73	113.60
26	z4	201	PEB	C4B-NB-C1B	-2.27	102.24	106.51
26	V4	201	PEB	CHB-C4B-C3B	-2.27	120.09	125.32
26	WJ	201	PEB	C1B-C2B-C3B	-2.27	103.91	106.51
26	G5	201	PEB	C3B-C4B-NB	2.27	113.34	110.05
26	d8	202	PEB	C2B-C1B-NB	2.27	115.36	110.53
28	oH	1001	CYC	C1B-NB-C4B	-2.26	107.78	110.67
26	LD	202	PEB	CHA-C1B-NB	-2.26	120.20	124.93
26	iE	203	PEB	OD-C4D-C3D	-2.26	124.33	129.46
26	T6	201	PEB	CAC-CBC-CGC	-2.26	107.41	113.76
28	K2	1001	CYC	CHB-C1B-NB	-2.26	121.20	126.06
26	SJ	202	PEB	OD-C4D-ND	-2.26	122.58	125.93
26	P4	203	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	JE	202	PEB	CHB-C4B-NB	-2.26	125.69	128.83
26	p4	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
26	XE	202	PEB	C4B-NB-C1B	-2.26	102.25	106.51
26	BG	201	PEB	CMB-C2B-C1B	2.26	128.55	125.06
26	Z8	201	PEB	OD-C4D-C3D	-2.26	124.33	129.46
26	h4	201	PEB	CHC-C4C-C3C	-2.26	126.48	130.34
26	PF	202	PEB	C1B-C2B-C3B	-2.26	103.91	106.51
26	g1	201	PEB	CHB-C4B-NB	-2.26	125.69	128.83
26	VF	201	PEB	CHA-C1B-C2B	2.26	130.72	124.90
26	Z6	203	PEB	CAB-C3B-C4B	2.26	129.01	125.01
26	H8	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
26	IG	202	PEB	C2B-C1B-NB	2.26	115.36	110.53
26	C4	201	PEB	C2A-C1A-NA	2.26	110.22	108.27
28	LH	1001	CYC	CHB-C1B-C2B	-2.26	122.46	126.95
26	D9	203	PEB	CHC-C4C-C3C	-2.26	126.48	130.34
26	k2	203	PEB	OA-C1A-C2A	-2.26	124.37	126.17
26	dF	202	PEB	OA-C1A-C2A	-2.26	124.37	126.17
28	D7	1001	CYC	C1A-C2A-C3A	-2.26	104.28	106.78
28	OH	1001	CYC	C1A-C2A-C3A	-2.26	104.28	106.78
26	U8	202	PEB	CHA-C4A-NA	2.26	127.89	125.20
28	qH	1002	CYC	C2A-C1A-NA	2.26	113.34	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UJ	201	PEB	CBA-CAA-C3A	2.26	118.50	113.47
28	E2	1001	CYC	CHA-C1A-C2A	-2.26	120.09	125.32
26	RD	203	PEB	CHA-C1B-NB	-2.26	120.20	124.93
26	bE	201	PEB	OD-C4D-C3D	-2.26	124.34	129.46
26	W1	201	PEB	CAA-C3A-C2A	-2.26	108.61	114.26
26	S8	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
26	14	202	PEB	CMC-C3C-C2C	2.26	129.21	124.94
26	GC	203	PEB	CBB-CAB-C3B	-2.26	106.34	112.63
26	U1	201	PEB	OD-C4D-C3D	-2.26	124.34	129.46
26	rE	201	PEB	CHA-C1B-NB	-2.26	120.20	124.93
26	Q2	202	PEB	CMB-C2B-C1B	2.26	128.55	125.06
26	M3	202	PEB	CBA-CAA-C3A	-2.26	108.43	113.47
28	N2	1001	CYC	CHB-C4A-C3A	2.26	130.71	124.90
26	h4	202	PEB	C1B-C2B-C3B	-2.26	103.91	106.51
26	Y6	202	PEB	CMA-C2A-C1A	-2.26	107.53	112.40
27	xG	306	PUB	CMD-C2D-C3D	2.26	131.16	127.77
26	J4	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
28	UH	1001	CYC	C2A-C1A-NA	2.26	113.34	110.05
26	I9	201	PEB	CMC-C3C-C2C	2.26	129.20	124.94
26	H7	1002	PEB	CAC-CBC-CGC	-2.26	107.42	113.76
28	WH	1001	CYC	C2B-C1B-NB	2.26	110.30	106.99
26	OB	202	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
28	GH	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
28	RH	1001	CYC	CHB-C1B-C2B	-2.26	122.47	126.95
27	A1	203	PUB	C1D-CHC-C4C	-2.26	108.45	113.37
26	hG	201	PEB	CHA-C1B-C2B	2.26	130.71	124.90
26	k6	202	PEB	CAB-C3B-C4B	2.26	129.00	125.01
26	GC	201	PEB	CMB-C2B-C1B	2.26	128.54	125.06
27	Y3	302	PUB	CBB-CAB-C3B	-2.26	108.77	112.62
28	QH	1001	CYC	CHA-C1A-NA	-2.26	125.69	128.83
26	Q3	201	PEB	O2C-CGC-CBC	2.26	121.29	114.03
26	U8	201	PEB	CAC-CBC-CGC	-2.26	107.43	113.76
26	V3	201	PEB	CHA-C1B-C2B	2.26	130.71	124.90
26	RD	203	PEB	O1B-CGB-CBB	-2.26	115.83	123.08
26	nE	202	PEB	CMC-C3C-C2C	-2.26	120.68	124.94
26	Y2	201	PEB	CHC-C4C-C3C	-2.26	126.48	130.34
26	B8	301	PEB	CHC-C4C-C3C	-2.26	126.48	130.34
26	24	404	PEB	CHA-C4A-NA	2.26	127.89	125.20
26	u1	201	PEB	CAC-C2C-C3C	2.26	133.74	127.25
26	QI	201	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	C1	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
26	H5	203	PEB	CAB-C3B-C4B	2.26	129.00	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	aE	201	PEB	C2B-C1B-NB	2.26	115.35	110.53
26	lE	201	PEB	C2B-C1B-NB	2.26	115.35	110.53
26	cB	201	PEB	CAB-CBB-CGB	-2.26	108.75	113.60
26	UE	201	PEB	CHA-C4A-NA	2.26	127.89	125.20
26	oE	202	PEB	CHA-C4A-NA	2.26	127.89	125.20
26	lG	202	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	XD	203	PEB	CHA-C1B-NB	-2.26	120.21	124.93
26	zE	501	PEB	OD-C4D-C3D	-2.26	124.35	129.46
26	cA	203	PEB	O2B-CGB-CBB	2.26	121.28	114.03
26	WJ	202	PEB	C1C-CHB-C4B	2.26	131.50	128.81
26	TE	202	PEB	C4B-NB-C1B	-2.26	102.26	106.51
26	YD	303	PEB	CHA-C1B-C2B	2.26	130.70	124.90
26	UB	201	PEB	CAB-CBB-CGB	-2.26	108.75	113.60
26	V2	203	PEB	CAC-CBC-CGC	-2.26	107.43	113.76
26	k4	203	PEB	CHC-C1D-ND	-2.26	111.33	113.95
28	hH	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
26	DE	202	PEB	C2B-C1B-NB	2.26	115.34	110.53
26	H3	201	PEB	CAB-CBB-CGB	-2.26	108.75	113.60
26	S1	202	PEB	CAB-C3B-C4B	2.26	129.00	125.01
26	qE	203	PEB	CAB-C3B-C4B	2.26	129.00	125.01
26	c1	201	PEB	CAA-C3A-C4A	-2.26	106.88	112.67
26	V9	202	PEB	OD-C4D-C3D	-2.26	124.35	129.46
26	U7	202	PEB	CHA-C1B-NB	-2.26	120.22	124.93
26	XD	203	PEB	C2A-C1A-NA	2.26	110.22	108.27
26	cI	201	PEB	CBC-CAC-C2C	-2.25	108.77	112.62
26	o1	501	PEB	CAB-CBB-CGB	-2.25	108.75	113.60
26	SE	202	PEB	CHC-C4C-C3C	-2.25	126.49	130.34
26	21	401	PEB	OD-C4D-ND	-2.25	122.59	125.93
26	T9	202	PEB	CHB-C4B-NB	-2.25	125.70	128.83
26	YJ	201	PEB	CHB-C4B-NB	-2.25	125.70	128.83
27	xE	305	PUB	CAC-C2C-C1C	2.25	129.00	125.01
26	WF	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	i1	202	PEB	CHB-C4B-NB	-2.25	125.70	128.83
26	AC	203	PEB	CHA-C1B-NB	-2.25	120.22	124.93
27	A4	203	PUB	CMD-C2D-C3D	2.25	131.15	127.77
26	f2	201	PEB	OD-C4D-ND	-2.25	122.59	125.93
26	R8	201	PEB	CHA-C1B-C2B	2.25	130.69	124.90
26	YF	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
26	fF	203	PEB	CAB-C3B-C4B	2.25	128.99	125.01
26	i2	201	PEB	CHA-C1B-NB	-2.25	120.22	124.93
26	PE	201	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
26	EJ	201	PEB	C1B-C2B-C3B	-2.25	103.92	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	GA	201	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	dI	201	PEB	C4B-NB-C1B	-2.25	102.27	106.51
26	jE	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	S4	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	kE	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
26	H5	203	PEB	CMA-C2A-C1A	-2.25	107.55	112.40
27	yG	302	PUB	CAC-C2C-C1C	2.25	128.99	125.01
26	xG	303	PEB	OD-C4D-ND	-2.25	122.60	125.93
26	KA	201	PEB	C3B-C4B-NB	2.25	113.32	110.05
26	MA	202	PEB	C3B-C4B-NB	2.25	113.32	110.05
28	EI	1001	CYC	CHA-C1A-C2A	-2.25	120.12	125.32
26	R8	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
26	aF	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
26	T1	201	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	C5	204	PEB	CAB-CBB-CGB	-2.25	108.76	113.60
26	a7	202	PEB	CHC-C4C-C3C	-2.25	126.50	130.34
26	M8	202	PEB	C3B-C4B-NB	2.25	113.32	110.05
26	M3	201	PEB	CHA-C1B-C2B	2.25	130.69	124.90
28	NF	1001	CYC	C1B-NB-C4B	-2.25	107.80	110.67
26	pE	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	bF	201	PEB	CBB-CAB-C3B	-2.25	106.38	112.63
26	jG	201	PEB	CAA-C3A-C2A	-2.25	108.64	114.26
28	TH	1001	CYC	C2B-C1B-NB	2.25	110.28	106.99
26	B1	201	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
26	Q9	201	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
26	zG	501	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	lA	201	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	qG	201	PEB	C3B-C4B-NB	2.25	113.32	110.05
26	GG	203	PEB	O2C-CGC-CBC	2.25	121.26	114.03
26	W6	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
26	AB	301	PEB	CHA-C4A-NA	-2.25	122.53	125.20
26	OE	202	PEB	CHB-C4B-NB	-2.25	125.71	128.83
26	OA	203	PEB	CMB-C2B-C1B	2.25	128.53	125.06
26	m2	203	PEB	C1B-C2B-C3B	-2.25	103.93	106.51
26	LC	203	PEB	C1B-C2B-C3B	-2.25	103.93	106.51
26	VD	203	PEB	C3B-C4B-NB	2.25	113.32	110.05
28	J2	1001	CYC	CAD-CBD-CGD	-2.25	107.45	113.76
28	N7	1001	CYC	CAD-CBD-CGD	-2.25	107.45	113.76
26	e7	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
26	FD	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
26	NG	201	PEB	CMA-C2A-C1A	-2.25	107.56	112.40
26	T4	202	PEB	C2A-C1A-NA	2.25	110.21	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	xE	303	PEB	C2A-C1A-NA	2.25	110.21	108.27
26	PF	202	PEB	C2A-C1A-NA	2.25	110.21	108.27
26	O2	201	PEB	C4B-C3B-C2B	-2.25	104.30	106.78
28	CF	1001	CYC	C1A-C2A-C3A	-2.25	104.30	106.78
26	P8	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
26	KE	203	PEB	CAA-C3A-C4A	-2.25	106.90	112.67
26	X1	203	PEB	CAA-C3A-C2A	-2.25	108.64	114.26
26	OB	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
27	xE	305	PUB	CHA-C4A-NA	-2.25	111.34	113.95
26	E4	201	PEB	OD-C4D-C3D	-2.25	124.37	129.46
26	ZA	201	PEB	OD-C4D-C3D	-2.25	124.37	129.46
26	QG	203	PEB	OD-C4D-C3D	-2.25	124.37	129.46
26	J4	202	PEB	CMB-C2B-C1B	2.25	128.53	125.06
26	F5	202	PEB	CMB-C2B-C1B	2.25	128.53	125.06
26	j2	201	PEB	CAB-C3B-C4B	2.25	128.98	125.01
26	b6	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
26	DJ	202	PEB	CBA-CAA-C3A	2.25	118.47	113.47
26	CC	201	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	FF	1002	PEB	CMB-C2B-C1B	2.25	128.52	125.06
26	I3	201	PEB	C2B-C1B-NB	2.25	115.32	110.53
28	SH	1001	CYC	C2C-C3C-C4C	2.25	104.70	101.34
26	Q4	201	PEB	O1B-CGB-CBB	-2.25	115.86	123.08
26	h6	202	PEB	CBC-CAC-C2C	-2.25	108.79	112.62
26	VJ	202	PEB	C2B-C1B-NB	2.25	115.32	110.53
26	WG	201	PEB	CAA-C3A-C2A	2.25	119.87	114.26
26	PB	201	PEB	CHB-C4B-NB	-2.25	125.71	128.83
26	c8	202	PEB	CBA-CAA-C3A	-2.25	108.47	113.47
26	w1	201	PEB	C1B-C2B-C3B	-2.25	103.93	106.51
26	F5	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	gB	201	PEB	CAB-CBB-CGB	-2.24	108.77	113.60
28	fH	1001	CYC	C2A-C1A-NA	2.24	113.31	110.05
28	IB	1001	CYC	CMC-C2C-C1C	-2.24	107.56	112.40
28	CH	1001	CYC	C1B-NB-C4B	-2.24	107.81	110.67
26	K4	201	PEB	CHB-C4B-C3B	-2.24	120.14	125.32
26	aA	201	PEB	C2B-C1B-NB	2.24	115.32	110.53
26	h8	203	PEB	CHA-C4A-NA	-2.24	122.54	125.20
26	XG	203	PEB	C2B-C1B-NB	2.24	115.32	110.53
26	P8	201	PEB	C1B-C2B-C3B	-2.24	103.93	106.51
26	R3	203	PEB	C2A-C1A-NA	2.24	110.21	108.27
28	YH	1002	CYC	C2C-C1C-NC	2.24	110.21	108.27
28	pH	1001	CYC	C2C-C1C-NC	2.24	110.21	108.27
26	E9	201	PEB	OD-C4D-ND	-2.24	122.61	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	IH	1001	CYC	C2C-C3C-C4C	2.24	104.70	101.34
28	F2	1001	CYC	CHB-C4A-NA	-2.24	120.24	124.93
26	KG	203	PEB	C2B-C1B-NB	2.24	115.32	110.53
26	d7	203	PEB	CHC-C4C-C3C	-2.24	126.51	130.34
26	i8	201	PEB	CMD-C2D-C3D	2.24	133.23	130.06
26	U7	203	PEB	OD-C4D-C3D	-2.24	124.38	129.46
26	PJ	203	PEB	OD-C4D-C3D	-2.24	124.38	129.46
26	RE	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
26	w1	202	PEB	CMB-C2B-C1B	2.24	128.52	125.06
26	U2	202	PEB	CMB-C2B-C1B	2.24	128.52	125.06
26	U9	201	PEB	CAB-CBB-CGB	-2.24	108.78	113.60
26	g6	201	PEB	CHB-C4B-C3B	-2.24	120.14	125.32
26	YA	201	PEB	CHB-C4B-C3B	-2.24	120.14	125.32
26	K3	202	PEB	CHA-C1B-NB	-2.24	120.24	124.93
28	VH	1001	CYC	C1A-C2A-C3A	-2.24	104.30	106.78
26	f2	201	PEB	CAB-CBB-CGB	-2.24	108.78	113.60
26	dG	202	PEB	CHC-C1D-ND	-2.24	111.34	113.95
26	bB	202	PEB	CMB-C2B-C1B	2.24	128.52	125.06
26	UA	202	PEB	CHA-C4A-NA	2.24	127.87	125.20
26	GE	202	PEB	CHC-C4C-C3C	-2.24	126.51	130.34
26	YD	301	PEB	CBA-CAA-C3A	2.24	118.46	113.47
26	ZB	203	PEB	CAB-C3B-C4B	2.24	128.97	125.01
26	ZG	201	PEB	CHA-C1B-C2B	2.24	130.66	124.90
26	L8	201	PEB	OA-C1A-NA	2.24	127.66	124.94
26	eI	201	PEB	C1C-CHB-C4B	2.24	131.49	128.81
26	GE	202	PEB	CHB-C4B-NB	-2.24	125.72	128.83
26	F7	1002	PEB	CMB-C2B-C1B	2.24	128.51	125.06
26	GJ	201	PEB	CBB-CAB-C3B	2.24	118.85	112.63
26	P8	201	PEB	CHA-C1B-C2B	2.24	130.66	124.90
26	HG	201	PEB	CBC-CAC-C2C	-2.24	108.80	112.62
26	hB	201	PEB	CHB-C4B-C3B	-2.24	120.14	125.32
26	LE	201	PEB	O2B-CGB-CBB	2.24	121.23	114.03
28	J7	1001	CYC	CAD-CBD-CGD	-2.24	107.48	113.76
26	lF	201	PEB	OD-C4D-ND	-2.24	122.61	125.93
26	W9	202	PEB	CMA-C2A-C1A	-2.24	107.58	112.40
26	WF	203	PEB	C3B-C4B-NB	2.24	113.31	110.05
26	PJ	201	PEB	C3B-C4B-NB	2.24	113.31	110.05
26	e3	401	PEB	CHB-C4B-NB	-2.24	125.72	128.83
26	l7	202	PEB	CAB-C3B-C4B	2.24	128.97	125.01
26	H5	201	PEB	C1C-CHB-C4B	2.24	131.48	128.81
26	n4	201	PEB	O1B-CGB-CBB	-2.24	115.89	123.08
26	c4	202	PEB	OD-C4D-ND	-2.24	122.61	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b2	201	PEB	CHC-C1D-ND	-2.24	111.35	113.95
26	CA	201	PEB	C3B-C4B-NB	2.24	113.31	110.05
26	T9	203	PEB	CMB-C2B-C1B	2.24	128.51	125.06
26	Q3	201	PEB	C4B-C3B-C2B	-2.24	104.31	106.78
26	W7	203	PEB	CAB-C3B-C4B	2.24	128.97	125.01
26	q1	201	PEB	CHA-C4A-NA	2.24	127.87	125.20
26	P4	202	PEB	C2A-C1A-NA	2.24	110.20	108.27
26	E3	202	PEB	OD-C4D-ND	-2.24	122.61	125.93
26	h2	201	PEB	CBA-CAA-C3A	-2.24	108.48	113.47
26	c8	201	PEB	CAB-CBB-CGB	-2.24	108.79	113.60
26	F2	1002	PEB	CHA-C1B-NB	-2.24	120.25	124.93
26	H1	203	PEB	CMB-C2B-C1B	2.24	128.51	125.06
26	yE	301	PEB	CHC-C1D-ND	-2.24	111.35	113.95
28	KI	1001	CYC	CHB-C1B-NB	-2.24	121.25	126.06
26	R7	202	PEB	C4B-C3B-C2B	-2.24	104.31	106.78
26	RA	201	PEB	CHA-C4A-NA	2.24	127.87	125.20
26	O4	202	PEB	OD-C4D-ND	-2.24	122.61	125.93
26	c6	202	PEB	CAB-C3B-C4B	2.24	128.97	125.01
26	D1	203	PEB	CAA-C3A-C4A	2.24	118.42	112.67
26	14	202	PEB	C3B-C4B-NB	2.24	113.30	110.05
26	pG	202	PEB	CHC-C1D-ND	-2.24	111.35	113.95
26	R1	201	PEB	CHB-C4B-NB	-2.24	125.72	128.83
26	g4	202	PEB	OD-C4D-ND	-2.24	122.62	125.93
26	RE	202	PEB	OD-C4D-ND	-2.24	122.62	125.93
26	qE	203	PEB	OD-C4D-ND	-2.24	122.62	125.93
26	Q2	201	PEB	CAB-C3B-C4B	2.24	128.97	125.01
26	dB	203	PEB	C4B-C3B-C2B	-2.24	104.31	106.78
26	S8	202	PEB	C2B-C1B-NB	2.24	115.30	110.53
26	HD	203	PEB	CAC-CBC-CGC	-2.24	107.49	113.76
26	u1	201	PEB	O2B-CGB-CBB	2.24	121.22	114.03
26	b6	201	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
26	D3	203	PEB	CAC-CBC-CGC	-2.24	107.49	113.76
28	NF	1001	CYC	CMC-C2C-C1C	-2.24	107.58	112.40
26	HE	201	PEB	CBA-CAA-C3A	2.24	118.44	113.47
26	s1	203	PEB	CHC-C1D-ND	-2.24	111.35	113.95
27	QA	201	PUB	CAC-CBC-CGC	-2.24	108.79	113.60
26	aA	204	PEB	C2B-C1B-NB	2.24	115.30	110.53
26	aG	203	PEB	CHB-C4B-C3B	-2.24	120.16	125.32
26	V1	201	PEB	CMC-C3C-C2C	2.24	129.16	124.94
26	e7	201	PEB	C2B-C1B-NB	2.24	115.30	110.53
26	MG	202	PEB	CHA-C1B-NB	-2.24	120.26	124.93
26	gF	202	PEB	CAB-C3B-C4B	2.23	128.96	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I8	202	PEB	C3B-C4B-NB	2.23	113.30	110.05
26	YE	203	PEB	OD-C4D-C3D	-2.23	124.40	129.46
26	JE	201	PEB	CAC-CBC-CGC	-2.23	107.49	113.76
26	x1	201	PEB	C4B-C3B-C2B	-2.23	104.31	106.78
26	F9	203	PEB	C4B-NB-C1B	2.23	110.72	106.51
26	a1	201	PEB	OD-C4D-C3D	-2.23	124.40	129.46
27	A2	302	PUB	CMD-C2D-C3D	2.23	131.12	127.77
26	cA	202	PEB	CHA-C4A-NA	-2.23	122.55	125.20
26	YA	202	PEB	CMA-C2A-C1A	-2.23	107.59	112.40
26	EE	202	PEB	CHB-C4B-C3B	-2.23	120.16	125.32
28	nH	1001	CYC	C1A-C2A-C3A	-2.23	104.31	106.78
26	sG	203	PEB	C3B-C4B-NB	2.23	113.30	110.05
26	RG	201	PEB	CAA-C3A-C2A	-2.23	108.68	114.26
26	A4	202	PEB	CAB-CBB-CGB	-2.23	108.80	113.60
26	Y8	202	PEB	CBC-CAC-C2C	-2.23	108.81	112.62
26	cG	201	PEB	C2B-C1B-NB	2.23	115.30	110.53
26	iB	201	PEB	OD-C4D-ND	-2.23	122.62	125.93
26	LF	1002	PEB	OD-C4D-ND	-2.23	122.62	125.93
26	PD	202	PEB	CHA-C4A-NA	2.23	127.86	125.20
27	A8	304	PUB	CAB-CBB-CGB	-2.23	107.50	113.76
26	Y7	202	PEB	C4B-C3B-C2B	-2.23	104.31	106.78
26	L1	202	PEB	CMB-C2B-C1B	2.23	128.50	125.06
26	O8	201	PEB	CHC-C1D-ND	-2.23	111.36	113.95
26	IA	203	PEB	C3B-C4B-NB	2.23	113.30	110.05
26	nE	202	PEB	C3B-C4B-NB	2.23	113.30	110.05
26	M1	403	PEB	CHA-C1B-C2B	2.23	130.64	124.90
26	N4	201	PEB	CMB-C2B-C3B	-2.23	120.06	126.12
26	IE	201	PEB	CMB-C2B-C3B	-2.23	120.06	126.12
26	x1	202	PEB	CMB-C2B-C3B	2.23	132.18	126.12
26	A3	201	PEB	C2A-C1A-NA	2.23	110.20	108.27
26	h8	202	PEB	OD-C4D-ND	-2.23	122.62	125.93
26	Y2	201	PEB	CAB-C3B-C4B	2.23	128.96	125.01
26	R3	201	PEB	CAC-CBC-CGC	-2.23	107.50	113.76
26	D8	202	PEB	CAA-C3A-C2A	-2.23	108.68	114.26
26	T2	201	PEB	CHA-C4A-NA	2.23	127.86	125.20
26	TA	201	PEB	C1B-C2B-C3B	-2.23	103.95	106.51
26	AE	201	PEB	OA-C1A-C2A	2.23	127.95	126.17
26	F8	202	PEB	OA-C1A-NA	2.23	127.64	124.94
26	D1	202	PEB	OD-C4D-C3D	-2.23	124.41	129.46
26	dF	202	PEB	OD-C4D-C3D	-2.23	124.41	129.46
26	FG	201	PEB	O2B-CGB-CBB	2.23	121.20	114.03
26	eF	202	PEB	CHA-C1B-C2B	2.23	130.64	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M3	201	PEB	O1C-CGC-CBC	-2.23	115.92	123.08
26	v4	201	PEB	CHC-C1D-ND	-2.23	111.36	113.95
26	ME	201	PEB	OD-C4D-C3D	-2.23	124.41	129.46
26	k4	201	PEB	CAB-C3B-C4B	2.23	128.95	125.01
26	X8	201	PEB	C1B-C2B-C3B	-2.23	103.95	106.51
26	DA	202	PEB	CAA-C3A-C2A	-2.23	108.69	114.26
26	Q1	201	PEB	O1B-CGB-CBB	-2.23	115.92	123.08
26	LD	203	PEB	OA-C1A-C2A	-2.23	124.40	126.17
26	BJ	201	PEB	CMA-C2A-C1A	-2.23	107.60	112.40
28	N7	1001	CYC	CHA-C1A-NA	-2.23	125.73	128.83
26	mI	203	PEB	CAB-CBB-CGB	2.23	118.40	113.60
26	V1	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
26	j7	203	PEB	CHC-C1D-ND	-2.23	111.36	113.95
26	oE	202	PEB	C3B-C4B-NB	2.23	113.29	110.05
27	yE	302	PUB	C2C-C1C-NC	2.23	113.29	110.05
26	LA	202	PEB	CAB-CBB-CGB	2.23	118.40	113.60
26	x1	202	PEB	CBC-CAC-C2C	-2.23	108.82	112.62
26	M8	203	PEB	C1C-CHB-C4B	2.23	131.47	128.81
26	m1	202	PEB	C3B-C4B-NB	2.23	113.29	110.05
26	K8	202	PEB	OD-C4D-ND	-2.23	122.63	125.93
26	fA	203	PEB	OD-C4D-ND	-2.23	122.63	125.93
26	UJ	202	PEB	CHC-C4C-C3C	-2.23	126.54	130.34
26	QJ	201	PEB	CAB-CBB-CGB	-2.23	108.81	113.60
26	WA	201	PEB	C1C-CHB-C4B	2.23	131.47	128.81
26	v1	202	PEB	CHA-C1B-C2B	2.23	130.63	124.90
26	h7	203	PEB	OD-C4D-C3D	-2.23	124.41	129.46
26	Z4	202	PEB	OD-C4D-ND	-2.23	122.63	125.93
26	CC	203	PEB	CAB-C3B-C4B	2.23	128.95	125.01
26	FI	1002	PEB	OD-C4D-C3D	-2.23	124.42	129.46
26	GG	203	PEB	C1B-C2B-C3B	-2.23	103.95	106.51
26	U7	202	PEB	C2B-C1B-NB	2.23	115.28	110.53
26	PF	201	PEB	C2B-C1B-NB	2.23	115.28	110.53
26	Q8	204	PEB	CAB-C3B-C4B	2.23	128.95	125.01
26	W2	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
26	C8	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
26	U4	201	PEB	OD-C4D-C3D	-2.23	124.42	129.46
28	sH	1001	CYC	C2C-C1C-NC	2.23	110.19	108.27
26	O7	201	PEB	CAA-C3A-C4A	-2.23	106.96	112.67
26	jF	203	PEB	OD-C4D-C3D	-2.23	124.42	129.46
26	WA	203	PEB	CAB-C3B-C4B	2.23	128.94	125.01
26	g7	202	PEB	OA-C1A-NA	2.23	127.64	124.94
26	mG	202	PEB	CHC-C1D-ND	-2.23	111.36	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	II	202	PEB	C3B-C4B-NB	2.23	113.29	110.05
26	W6	202	PEB	CHB-C4B-NB	-2.23	125.74	128.83
26	m6	202	PEB	CAB-CBB-CGB	-2.22	108.81	113.60
26	RE	201	PEB	CAA-C3A-C2A	-2.22	108.70	114.26
26	z1	202	PEB	CAB-C3B-C4B	2.22	128.94	125.01
26	N9	203	PEB	OD-C4D-C3D	-2.22	124.42	129.46
26	H4	202	PEB	CMB-C2B-C1B	2.22	128.49	125.06
26	bF	202	PEB	C3B-C4B-NB	2.22	113.28	110.05
26	TB	201	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
26	o1	501	PEB	CBC-CAC-C2C	-2.22	108.82	112.62
26	P8	202	PEB	O2B-CGB-CBB	2.22	121.18	114.03
26	gG	201	PEB	CAB-C3B-C4B	2.22	128.94	125.01
26	VD	202	PEB	CMB-C2B-C1B	2.22	128.49	125.06
26	dG	202	PEB	CMA-C2A-C1A	-2.22	107.61	112.40
26	UF	201	PEB	C3B-C4B-NB	2.22	113.28	110.05
26	NJ	204	PEB	C3B-C4B-NB	2.22	113.28	110.05
26	SE	203	PEB	CHB-C4B-C3B	-2.22	120.18	125.32
26	X4	203	PEB	CAA-C3A-C2A	-2.22	108.70	114.26
26	j2	201	PEB	C2A-C1A-NA	2.22	110.19	108.27
26	fB	202	PEB	C2A-C1A-NA	2.22	110.19	108.27
26	t4	201	PEB	C4B-C3B-C2B	-2.22	104.32	106.78
26	WF	202	PEB	OA-C1A-C2A	-2.22	124.41	126.17
26	GJ	202	PEB	CMB-C2B-C1B	2.22	128.49	125.06
26	e2	203	PEB	CAB-CBB-CGB	2.22	118.39	113.60
26	A9	301	PEB	CAC-CBC-CGC	-2.22	107.53	113.76
26	c8	202	PEB	CHC-C1D-ND	-2.22	111.37	113.95
28	L7	1001	CYC	O2D-CGD-CBD	2.22	121.17	114.03
26	OA	201	PEB	CHA-C1B-NB	-2.22	120.28	124.93
26	L9	201	PEB	C3B-C4B-NB	2.22	113.28	110.05
26	GG	202	PEB	CMA-C2A-C3A	-2.22	104.86	113.83
26	MG	201	PEB	CHA-C1B-NB	-2.22	120.28	124.93
26	O9	202	PEB	CHA-C4A-NA	-2.22	122.56	125.20
26	MJ	202	PEB	CBC-CAC-C2C	-2.22	108.83	112.62
26	d1	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
26	IE	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
26	RD	201	PEB	CAC-CBC-CGC	-2.22	107.53	113.76
26	c7	201	PEB	CHB-C4B-C3B	-2.22	120.19	125.32
26	P4	203	PEB	CHB-C4B-NB	-2.22	125.75	128.83
26	T7	201	PEB	CBA-CAA-C3A	-2.22	108.52	113.47
27	N9	201	PUB	CAC-C2C-C1C	2.22	128.94	125.01
26	IG	201	PEB	C1C-CHB-C4B	2.22	131.46	128.81
26	H8	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	tE	201	PEB	CAB-CBB-CGB	-2.22	108.82	113.60
26	VG	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
27	A8	303	PUB	O2B-CGB-CBB	2.22	121.16	114.03
26	TI	202	PEB	CAB-C3B-C4B	2.22	128.94	125.01
26	T7	201	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
26	C9	201	PEB	OD-C4D-C3D	-2.22	124.43	129.46
28	rH	1001	CYC	CBD-CAD-C3D	-2.22	108.83	112.62
28	J2	1001	CYC	CAA-C2A-C3A	2.22	132.01	127.88
26	GE	202	PEB	C4B-NB-C1B	-2.22	102.33	106.51
26	I1	201	PEB	CHB-C4B-C3B	-2.22	120.19	125.32
28	D2	1001	CYC	CHA-C1A-C2A	-2.22	120.19	125.32
26	e1	201	PEB	CHA-C1B-NB	-2.22	120.29	124.93
26	K9	201	PEB	CHA-C1B-NB	-2.22	120.29	124.93
26	j8	203	PEB	CBC-CAC-C2C	-2.22	108.83	112.62
26	cB	202	PEB	CAC-CBC-CGC	-2.22	107.54	113.76
26	mA	202	PEB	CAB-CBB-CGB	2.22	118.38	113.60
26	wG	303	PEB	CHA-C4A-NA	2.22	127.84	125.20
28	DI	1001	CYC	CAD-CBD-CGD	-2.22	107.54	113.76
26	RE	202	PEB	C4B-NB-C1B	-2.22	102.33	106.51
26	j2	201	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
26	D3	203	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
26	D8	202	PEB	O2B-CGB-CBB	2.22	121.16	114.03
26	c7	202	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
26	V9	201	PEB	CAB-C3B-C4B	2.22	128.93	125.01
26	C9	201	PEB	CMA-C2A-C1A	-2.22	107.62	112.40
26	tG	201	PEB	CMA-C2A-C1A	-2.22	107.62	112.40
26	kB	202	PEB	CAC-CBC-CGC	-2.22	107.54	113.76
26	X3	203	PEB	C2A-C1A-NA	2.22	110.19	108.27
28	JF	1001	CYC	C2C-C1C-NC	2.22	110.19	108.27
26	OF	201	PEB	C2B-C1B-NB	2.22	115.26	110.53
26	RG	202	PEB	OD-C4D-ND	-2.22	122.64	125.93
26	K4	202	PEB	CMB-C2B-C1B	2.22	128.48	125.06
26	rG	201	PEB	CBC-CAC-C2C	-2.22	108.84	112.62
26	c2	203	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
26	jG	201	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
26	pG	202	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
28	GI	1001	CYC	CHB-C1B-NB	-2.22	121.30	126.06
26	D8	202	PEB	CBC-CAC-C2C	-2.22	108.84	112.62
26	F5	201	PEB	CHC-C1D-ND	-2.22	111.37	113.95
26	AF	305	PEB	CHC-C1D-ND	-2.22	111.37	113.95
26	D4	203	PEB	OD-C4D-C3D	-2.22	124.44	129.46
26	LG	201	PEB	OD-C4D-C3D	-2.22	124.44	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a8	201	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
26	h4	203	PEB	CAA-C3A-C4A	2.22	118.36	112.67
26	UF	202	PEB	CAB-C3B-C4B	2.22	128.93	125.01
26	A6	301	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
26	P8	202	PEB	C2A-C1A-NA	2.22	110.18	108.27
26	T9	202	PEB	CHB-C4B-C3B	-2.22	120.20	125.32
26	h8	203	PEB	OD-C4D-C3D	-2.22	124.44	129.46
26	V1	203	PEB	CHA-C1B-NB	-2.22	120.30	124.93
26	VJ	202	PEB	CHC-C4C-C3C	-2.22	126.56	130.34
26	SE	202	PEB	CMB-C2B-C3B	-2.22	120.10	126.12
26	w4	203	PEB	CAB-C3B-C4B	2.22	128.93	125.01
26	e7	201	PEB	CAB-C3B-C4B	2.22	128.93	125.01
26	QF	201	PEB	CAC-CBC-CGC	-2.22	107.55	113.76
26	jB	201	PEB	CAB-C3B-C4B	2.21	128.93	125.01
26	Q8	203	PEB	OD-C4D-C3D	-2.21	124.44	129.46
26	V9	203	PEB	CBD-CAD-C3D	-2.21	116.60	127.62
26	Y3	301	PEB	CBC-CAC-C2C	-2.21	108.84	112.62
26	I3	202	PEB	C2A-C1A-NA	2.21	110.18	108.27
26	KG	203	PEB	O2C-CGC-CBC	2.21	121.14	114.03
28	pH	1001	CYC	CHA-C1A-NA	-2.21	125.75	128.83
26	XJ	201	PEB	C3B-C4B-NB	2.21	113.27	110.05
27	A6	303	PUB	CAC-CBC-CGC	-2.21	108.84	113.60
26	X3	202	PEB	CAB-C3B-C4B	2.21	128.93	125.01
26	x4	201	PEB	CAB-C3B-C4B	2.21	128.93	125.01
26	C9	201	PEB	C2B-C1B-NB	2.21	115.25	110.53
26	bF	202	PEB	CHA-C1B-C2B	2.21	130.59	124.90
26	f8	201	PEB	CAB-CBB-CGB	-2.21	108.84	113.60
26	X1	202	PEB	CMB-C2B-C3B	-2.21	120.11	126.12
26	kF	202	PEB	CHB-C4B-C3B	-2.21	120.21	125.32
26	RG	202	PEB	C4B-NB-C1B	-2.21	102.34	106.51
26	dG	202	PEB	C2A-C1A-NA	2.21	110.18	108.27
26	d1	203	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	oE	202	PEB	CHC-C1D-ND	-2.21	111.38	113.95
28	D6	1001	CYC	C1B-CHB-C4A	-2.21	122.67	128.08
26	I9	201	PEB	CBB-CAB-C3B	2.21	118.78	112.63
26	c2	202	PEB	OD-C4D-ND	-2.21	122.65	125.93
26	s4	202	PEB	OD-C4D-ND	-2.21	122.65	125.93
26	T3	201	PEB	C3B-C4B-NB	2.21	113.27	110.05
26	P2	201	PEB	CMA-C2A-C1A	-2.21	107.63	112.40
26	JD	202	PEB	CHA-C4A-NA	2.21	127.84	125.20
26	M4	403	PEB	CBC-CAC-C2C	-2.21	108.84	112.62
26	PI	203	PEB	CAC-CBC-CGC	-2.21	107.56	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O6	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	N3	201	PEB	CAB-C3B-C4B	2.21	128.92	125.01
26	V7	201	PEB	CHB-C4B-C3B	-2.21	120.21	125.32
26	E8	203	PEB	CHB-C4B-C3B	-2.21	120.21	125.32
26	VB	202	PEB	CMC-C3C-C2C	2.21	129.11	124.94
28	HI	1001	CYC	CAB-C3B-C2B	2.21	131.31	127.53
26	dB	204	PEB	C2B-C1B-NB	2.21	115.25	110.53
26	R4	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	WE	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	ND	203	PEB	CMA-C2A-C1A	-2.21	107.64	112.40
27	xG	306	PUB	CHA-C1B-C2B	-2.21	126.56	130.34
26	Z8	201	PEB	CHA-C4A-NA	2.21	127.83	125.20
26	VD	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	CJ	202	PEB	CBC-CAC-C2C	-2.21	108.85	112.62
26	K3	202	PEB	OD-C4D-ND	-2.21	122.66	125.93
26	IG	203	PEB	C2B-C1B-NB	2.21	115.25	110.53
26	c6	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
26	cF	202	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
26	G8	201	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	a7	202	PEB	C1C-CHB-C4B	-2.21	126.17	128.81
26	U9	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	B4	203	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
26	ME	201	PEB	CAB-C3B-C4B	2.21	128.92	125.01
26	pG	202	PEB	CHB-C4B-C3B	-2.21	120.22	125.32
26	j1	201	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
26	M3	201	PEB	CHA-C4A-NA	2.21	127.83	125.20
26	Z4	201	PEB	C3B-C4B-NB	2.21	113.26	110.05
26	AD	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
26	SD	202	PEB	CHA-C1B-NB	-2.21	120.31	124.93
26	EE	201	PEB	CHA-C1B-NB	-2.21	120.31	124.93
26	HC	201	PEB	CBB-CAB-C3B	-2.21	106.49	112.63
26	N8	202	PEB	CMA-C2A-C1A	-2.21	107.64	112.40
26	QB	202	PEB	C4B-C3B-C2B	-2.21	104.34	106.78
26	WF	201	PEB	CMB-C2B-C1B	2.21	128.47	125.06
26	m8	202	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	M8	202	PEB	OA-C1A-NA	2.21	127.62	124.94
26	V8	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
26	KG	203	PEB	CHB-C4B-C3B	-2.21	120.22	125.32
26	H8	202	PEB	CHA-C4A-NA	-2.21	122.58	125.20
26	CC	201	PEB	CMB-C2B-C1B	2.21	128.47	125.06
26	a4	201	PEB	OD-C4D-C3D	-2.21	124.46	129.46
26	f1	202	PEB	CAB-C3B-C4B	2.21	128.91	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	x1	201	PEB	CAB-C3B-C4B	2.21	128.91	125.01
26	i7	202	PEB	CAB-C3B-C4B	2.21	128.91	125.01
26	WE	201	PEB	C1C-CHB-C4B	2.21	131.45	128.81
26	UD	201	PEB	CMA-C2A-C1A	-2.21	107.64	112.40
26	J9	203	PEB	CBD-CAD-C3D	-2.21	116.63	127.62
26	m8	201	PEB	CAA-C3A-C4A	-2.21	107.00	112.67
26	FC	201	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	HA	202	PEB	OD-C4D-C3D	-2.21	124.46	129.46
26	HD	202	PEB	OD-C4D-C3D	-2.21	124.46	129.46
26	XG	201	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
26	PJ	202	PEB	CMA-C2A-C1A	-2.21	107.65	112.40
26	L3	202	PEB	CHA-C1B-NB	-2.21	120.32	124.93
26	h6	202	PEB	CHA-C1B-NB	-2.21	120.32	124.93
26	dA	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
26	TD	201	PEB	C3B-C4B-NB	2.21	113.26	110.05
26	l1	201	PEB	CMB-C2B-C1B	2.21	128.46	125.06
26	i8	202	PEB	O2B-CGB-CBB	2.21	121.12	114.03
26	B4	203	PEB	CHC-C1D-ND	-2.21	111.39	113.95
26	m6	203	PEB	CHC-C1D-ND	-2.21	111.39	113.95
26	vG	201	PEB	OD-C4D-C3D	-2.21	124.46	129.46
26	TA	202	PEB	O2B-CGB-CBB	2.21	121.12	114.03
26	b7	202	PEB	CHA-C4A-NA	-2.21	122.58	125.20
26	RG	202	PEB	C2B-C1B-NB	2.21	115.24	110.53
26	U6	201	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
26	YJ	202	PEB	CAB-C3B-C4B	2.21	128.91	125.01
26	P2	202	PEB	CAC-CBC-CGC	-2.21	107.58	113.76
26	z4	201	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
26	H9	202	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
28	MH	1001	CYC	CAB-C3B-C2B	2.21	131.30	127.53
26	N9	204	PEB	CBA-CAA-C3A	-2.21	108.56	113.47
26	y1	201	PEB	CHB-C4B-C3B	-2.21	120.23	125.32
28	iH	1001	CYC	C2C-C1C-NC	2.21	110.17	108.27
26	F3	202	PEB	C2B-C1B-NB	2.21	115.23	110.53
26	SA	201	PEB	O1C-CGC-CBC	-2.21	116.00	123.08
26	k4	203	PEB	CHB-C4B-NB	-2.20	125.77	128.83
27	xE	306	PUB	C2C-C1C-NC	2.20	113.26	110.05
26	YA	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
26	W3	202	PEB	CHA-C1B-NB	-2.20	120.32	124.93
26	OG	203	PEB	OD-C4D-C3D	-2.20	124.47	129.46
26	f8	201	PEB	CHA-C4A-NA	-2.20	122.58	125.20
26	AI	301	PEB	CAC-CBC-CGC	-2.20	107.58	113.76
28	EH	1001	CYC	C2A-C1A-NA	2.20	113.25	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BG	201	PEB	CMA-C2A-C1A	-2.20	107.65	112.40
26	YG	203	PEB	CMA-C2A-C1A	-2.20	107.65	112.40
26	u4	201	PEB	OD-C4D-C3D	-2.20	124.47	129.46
26	X3	203	PEB	CHA-C1B-NB	-2.20	120.32	124.93
26	i4	201	PEB	CHA-C1B-NB	-2.20	120.32	124.93
26	K3	201	PEB	OA-C1A-C2A	-2.20	124.42	126.17
26	jE	201	PEB	CAB-C3B-C4B	2.20	128.91	125.01
26	L1	201	PEB	CAB-CBB-CGB	-2.20	108.86	113.60
26	dF	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	L1	202	PEB	OD-C4D-ND	-2.20	122.67	125.93
26	D6	1002	PEB	OD-C4D-ND	-2.20	122.67	125.93
26	f1	201	PEB	CAB-C3B-C4B	2.20	128.91	125.01
26	T1	201	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
26	iE	201	PEB	CMB-C2B-C1B	2.20	128.46	125.06
26	L8	202	PEB	CAB-CBB-CGB	2.20	118.34	113.60
26	JD	201	PEB	CAB-CBB-CGB	-2.20	108.86	113.60
26	HD	201	PEB	C3B-C4B-NB	2.20	113.25	110.05
26	vE	202	PEB	CHC-C4C-C3C	-2.20	126.58	130.34
26	ID	202	PEB	CHA-C1B-NB	-2.20	120.33	124.93
26	D8	201	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
28	JF	1001	CYC	OC-C1C-C2C	-2.20	124.42	126.17
28	J2	1001	CYC	CHA-C1A-C2A	-2.20	120.23	125.32
26	HB	1002	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	G9	201	PEB	CHC-C4C-C3C	-2.20	126.58	130.34
26	UE	203	PEB	CHA-C4A-NA	2.20	127.82	125.20
26	y1	202	PEB	CAA-C3A-C4A	-2.20	107.02	112.67
26	WG	202	PEB	C2A-C1A-NA	2.20	110.17	108.27
26	S1	201	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
26	F1	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
26	JE	202	PEB	CAA-C3A-C4A	-2.20	107.02	112.67
26	LA	201	PEB	OA-C1A-NA	2.20	127.61	124.94
26	J4	201	PEB	CAB-CBB-CGB	-2.20	108.87	113.60
26	fE	202	PEB	CAC-CBC-CGC	-2.20	107.59	113.76
26	v4	201	PEB	CAB-C3B-C4B	2.20	128.90	125.01
26	dE	202	PEB	CAB-C3B-C4B	2.20	128.90	125.01
26	eF	201	PEB	CAB-C3B-C4B	2.20	128.90	125.01
26	i1	202	PEB	C2B-C1B-NB	2.20	115.23	110.53
26	W7	201	PEB	CMB-C2B-C1B	2.20	128.45	125.06
26	RB	202	PEB	CMC-C3C-C2C	2.20	129.09	124.94
26	PF	202	PEB	CHA-C1B-NB	-2.20	120.33	124.93
28	cH	1001	CYC	CHB-C1B-C2B	-2.20	122.59	126.95
28	gH	1001	CYC	CHB-C1B-C2B	-2.20	122.59	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q3	201	PEB	C2A-C1A-NA	2.20	110.17	108.27
26	B4	203	PEB	OD-C4D-C3D	-2.20	124.47	129.46
26	k2	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
26	cA	201	PEB	CAB-CBB-CGB	-2.20	108.87	113.60
26	F4	202	PEB	C4B-C3B-C2B	-2.20	104.35	106.78
26	BJ	203	PEB	OD-C4D-C3D	-2.20	124.48	129.46
26	UJ	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
26	KG	202	PEB	OA-C1A-C2A	-2.20	124.42	126.17
28	N2	1001	CYC	CHA-C1A-C2A	-2.20	120.24	125.32
26	H3	202	PEB	C2B-C1B-NB	2.20	115.22	110.53
26	S9	201	PEB	C2A-C1A-NA	2.20	110.17	108.27
26	RJ	203	PEB	C3B-C4B-NB	2.20	113.25	110.05
26	p1	202	PEB	C1C-CHB-C4B	-2.20	126.18	128.81
26	Q6	203	PEB	CHB-C4B-C3B	-2.20	120.24	125.32
26	YD	303	PEB	CHB-C4B-C3B	2.20	130.40	125.32
26	m8	202	PEB	CHA-C1B-C2B	2.20	130.56	124.90
26	f6	201	PEB	C2B-C1B-NB	2.20	115.22	110.53
26	N3	203	PEB	CBA-CAA-C3A	2.20	118.36	113.47
28	M2	1001	CYC	CBC-CAC-C3C	-2.20	108.57	113.47
26	SA	201	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	L1	203	PEB	CMC-C3C-C2C	2.20	129.09	124.94
28	IH	1001	CYC	C2A-C1A-NA	2.20	113.25	110.05
26	BD	202	PEB	CHB-C4B-NB	-2.20	125.78	128.83
26	OE	201	PEB	CAA-C3A-C4A	-2.20	107.03	112.67
26	Z7	202	PEB	C2B-C1B-NB	2.20	115.22	110.53
26	CJ	201	PEB	CAB-C3B-C4B	2.20	128.90	125.01
26	U8	203	PEB	CMD-C2D-C3D	2.20	133.16	130.06
26	VD	203	PEB	CMB-C2B-C1B	2.20	128.45	125.06
26	z4	201	PEB	C4B-C3B-C2B	-2.20	104.35	106.78
26	M9	201	PEB	C4B-C3B-C2B	-2.20	104.35	106.78
26	V4	203	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
26	AC	203	PEB	CHC-C4C-C3C	-2.20	126.59	130.34
27	AI	303	PUB	CBA-CAA-C3A	-2.20	109.65	112.98
28	vH	1001	CYC	C2C-C3C-C4C	2.20	104.63	101.34
26	AB	304	PEB	CMA-C2A-C1A	-2.20	107.67	112.40
26	YE	203	PEB	CMB-C2B-C1B	2.20	128.45	125.06
26	WE	201	PEB	CAB-C3B-C4B	2.20	128.89	125.01
26	yG	301	PEB	CAB-C3B-C4B	2.20	128.89	125.01
26	TJ	202	PEB	CAB-C3B-C4B	2.20	128.89	125.01
28	IH	1001	CYC	CAA-C2A-C1A	2.20	128.89	125.01
26	gG	201	PEB	OD-C4D-C3D	-2.20	124.48	129.46
26	TB	201	PEB	CAC-CBC-CGC	-2.20	107.60	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A1	203	PUB	CHA-C1B-C2B	-2.20	126.59	130.34
26	jA	201	PEB	OD-C4D-ND	-2.20	122.68	125.93
26	f6	201	PEB	CAA-C3A-C4A	-2.20	107.03	112.67
26	UD	202	PEB	CHA-C1B-NB	-2.20	120.34	124.93
28	BB	1001	CYC	CAA-C2A-C3A	2.20	131.97	127.88
26	CG	202	PEB	CAC-CBC-CGC	2.20	119.91	113.76
26	FJ	201	PEB	CAB-C3B-C4B	2.20	128.89	125.01
26	L2	1002	PEB	OD-C4D-ND	-2.20	122.68	125.93
26	H7	1002	PEB	CHA-C1B-C2B	2.20	130.54	124.90
27	xG	301	PUB	CBD-CAD-C3D	-2.19	106.38	112.43
26	MA	202	PEB	OA-C1A-NA	2.19	127.60	124.94
28	JI	1001	CYC	CAD-CBD-CGD	-2.19	107.61	113.76
26	ZI	201	PEB	C2A-C1A-NA	-2.19	106.38	108.27
28	MI	1001	CYC	CBC-CAC-C3C	-2.19	108.58	113.47
26	W8	201	PEB	CAB-CBB-CGB	-2.19	108.88	113.60
28	I2	1001	CYC	CMB-C2B-C1B	2.19	126.91	124.17
26	t4	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06
26	dB	204	PEB	CAA-C3A-C2A	-2.19	108.78	114.26
26	F4	203	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
26	IJ	201	PEB	CBC-CAC-C2C	2.19	116.36	112.62
26	i1	203	PEB	C2B-C1B-NB	2.19	115.21	110.53
26	x1	201	PEB	CHC-C4C-C3C	-2.19	126.59	130.34
26	hG	202	PEB	CHC-C4C-C3C	-2.19	126.59	130.34
26	P6	202	PEB	CAA-C3A-C4A	-2.19	107.04	112.67
28	NB	1001	CYC	CMA-C3A-C2A	-2.19	120.16	126.12
26	V4	201	PEB	CMC-C3C-C2C	2.19	129.08	124.94
26	RF	201	PEB	CAB-C3B-C4B	2.19	128.89	125.01
27	AF	303	PUB	CAC-C2C-C1C	2.19	128.89	125.01
26	L5	202	PEB	OD-C4D-C3D	-2.19	124.49	129.46
26	aE	202	PEB	CMB-C2B-C3B	-2.19	120.16	126.12
26	DJ	202	PEB	CAB-C3B-C4B	2.19	128.89	125.01
26	P6	201	PEB	CMA-C2A-C1A	-2.19	107.68	112.40
26	c4	201	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
28	KB	202	CYC	CBD-CAD-C3D	-2.19	108.88	112.62
26	CJ	202	PEB	CAB-C3B-C4B	2.19	128.89	125.01
26	P9	201	PEB	CHB-C4B-NB	-2.19	125.79	128.83
26	Y6	202	PEB	CAC-C2C-C3C	2.19	133.54	127.25
27	AJ	302	PUB	C2C-C1C-NC	2.19	113.24	110.05
28	D2	1001	CYC	CMC-C2C-C1C	-2.19	107.68	112.40
26	SA	201	PEB	O2C-CGC-CBC	2.19	121.07	114.03
26	qG	203	PEB	C1B-C2B-C3B	-2.19	103.99	106.51
28	JH	1001	CYC	C2C-C3C-C4C	2.19	104.62	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	hI	201	PEB	CBA-CAA-C3A	-2.19	108.59	113.47
26	K8	202	PEB	CAB-C3B-C4B	2.19	128.88	125.01
26	lE	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	VF	201	PEB	CBB-CAB-C3B	2.19	118.71	112.63
26	OB	201	PEB	OD-C4D-C3D	-2.19	124.50	129.46
26	OF	203	PEB	OD-C4D-C3D	-2.19	124.50	129.46
27	21	403	PUB	CMD-C2D-C3D	2.19	131.06	127.77
26	F2	1002	PEB	OD-C4D-C3D	-2.19	124.50	129.46
26	C8	201	PEB	C3B-C4B-NB	2.19	113.23	110.05
26	dG	201	PEB	CAA-C3A-C2A	-2.19	108.79	114.26
26	TF	202	PEB	OD-C4D-ND	-2.19	122.69	125.93
26	s4	201	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
26	FA	202	PEB	OA-C1A-NA	2.19	127.59	124.94
26	eG	201	PEB	CAB-C3B-C4B	2.19	128.88	125.01
26	VF	202	PEB	CMA-C2A-C1A	-2.19	107.68	112.40
26	CE	202	PEB	CAC-C2C-C3C	2.19	133.54	127.25
28	MH	1001	CYC	C2A-C1A-NA	2.19	113.23	110.05
26	wE	301	PEB	OD-C4D-C3D	-2.19	124.50	129.46
26	AA	302	PEB	CHA-C4A-NA	2.19	127.81	125.20
26	TJ	201	PEB	CHC-C1D-ND	2.19	116.49	113.95
26	fG	202	PEB	C1C-CHB-C4B	2.19	131.42	128.81
26	AD	201	PEB	OD-C4D-C3D	-2.19	124.50	129.46
26	AA	302	PEB	C2A-C1A-NA	2.19	110.16	108.27
26	VJ	203	PEB	C2A-C1A-NA	2.19	110.16	108.27
26	L9	201	PEB	CAB-CBB-CGB	-2.19	108.89	113.60
26	V2	203	PEB	CBB-CAB-C3B	2.19	118.71	112.63
26	S1	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
26	V8	202	PEB	CAA-C3A-C2A	-2.19	108.79	114.26
26	OJ	201	PEB	CMB-C2B-C1B	2.19	128.43	125.06
26	U8	201	PEB	CAB-C3B-C2B	2.19	131.95	127.88
27	AJ	302	PUB	CBA-CAA-C3A	-2.19	109.66	112.98
26	Z2	201	PEB	C2A-C1A-NA	-2.19	106.39	108.27
26	L8	201	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
26	BD	201	PEB	CHA-C4A-NA	2.19	127.81	125.20
26	LI	1002	PEB	CHA-C4A-NA	2.19	127.81	125.20
26	v1	202	PEB	CMD-C2D-C3D	2.19	133.15	130.06
26	l7	201	PEB	CBC-CAC-C2C	-2.19	108.89	112.62
28	GB	1001	CYC	CHA-C1A-C2A	-2.19	120.27	125.32
26	l2	201	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	GE	201	PEB	CBA-CAA-C3A	2.19	118.34	113.47
26	P2	201	PEB	CAB-CBB-CGB	-2.19	108.90	113.60
26	KC	202	PEB	CHA-C1B-NB	-2.19	120.36	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	w1	203	PEB	OD-C4D-C3D	-2.19	124.50	129.46
26	j8	203	PEB	CMB-C2B-C1B	2.19	128.43	125.06
26	OG	203	PEB	CHB-C4B-C3B	-2.19	120.27	125.32
26	q1	203	PEB	CBC-CAC-C2C	-2.19	108.89	112.62
26	BG	202	PEB	C2B-C1B-NB	2.19	115.20	110.53
26	R7	201	PEB	CHB-C4B-C3B	-2.19	120.27	125.32
26	S7	203	PEB	CHB-C4B-C3B	-2.19	120.27	125.32
26	XJ	202	PEB	CAB-C3B-C4B	2.19	128.88	125.01
26	v1	201	PEB	CHA-C1B-NB	-2.19	120.36	124.93
26	UB	202	PEB	CAA-C3A-C2A	-2.19	108.80	114.26
26	DA	201	PEB	OD-C4D-ND	-2.19	122.69	125.93
26	UB	203	PEB	OD-C4D-C3D	-2.19	124.51	129.46
26	AC	201	PEB	CAB-CBB-CGB	-2.19	108.90	113.60
26	eB	203	PEB	CAB-C3B-C4B	2.19	128.88	125.01
26	c8	201	PEB	CBC-CAC-C2C	-2.19	108.89	112.62
26	X8	202	PEB	OA-C1A-NA	2.19	127.59	124.94
26	QJ	202	PEB	CHC-C4C-C3C	-2.19	126.61	130.34
28	JF	1001	CYC	CBB-CAB-C3B	-2.19	106.41	112.43
26	HJ	201	PEB	C2B-C1B-NB	2.19	115.19	110.53
26	g6	201	PEB	CAB-CBB-CGB	-2.19	108.90	113.60
26	c4	202	PEB	C3B-C4B-NB	2.19	113.23	110.05
28	GH	1001	CYC	CAA-C2A-C1A	2.19	128.87	125.01
26	ND	201	PEB	CBC-CAC-C2C	-2.19	108.89	112.62
27	A1	203	PUB	CBB-CAB-C3B	2.19	116.35	112.62
26	KE	201	PEB	C2B-C1B-NB	2.18	115.19	110.53
26	H2	1002	PEB	CHA-C1B-NB	-2.18	120.36	124.93
26	X9	202	PEB	C2A-C1A-NA	2.18	110.16	108.27
26	FG	201	PEB	C1C-CHB-C4B	2.18	131.42	128.81
26	G4	201	PEB	CAB-CBB-CGB	-2.18	108.90	113.60
27	A2	302	PUB	C2C-C1C-NC	2.18	113.23	110.05
26	eG	201	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	q1	201	PEB	CAA-C3A-C4A	-2.18	107.06	112.67
26	W8	202	PEB	CHA-C1B-NB	-2.18	120.36	124.93
26	K8	202	PEB	CBB-CAB-C3B	-2.18	106.56	112.63
26	Y9	201	PEB	OD-C4D-ND	-2.18	122.70	125.93
26	d4	203	PEB	CHA-C1B-C2B	2.18	130.51	124.90
26	K9	202	PEB	CHA-C1B-C2B	2.18	130.51	124.90
26	SE	201	PEB	C2B-C1B-NB	2.18	115.19	110.53
26	K6	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
26	MA	202	PEB	CAA-C3A-C4A	-2.18	107.07	112.67
26	AB	301	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
27	A9	302	PUB	CMD-C2D-C3D	2.18	131.04	127.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H8	202	PEB	O1B-CGB-CBB	-2.18	116.07	123.08
26	xE	304	PEB	CMB-C2B-C1B	2.18	128.43	125.06
26	UF	202	PEB	CMB-C2B-C1B	2.18	128.43	125.06
26	iG	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
26	iG	202	PEB	O2C-CGC-CBC	2.18	121.04	114.03
26	DA	202	PEB	CBC-CAC-C2C	-2.18	108.90	112.62
28	L2	1001	CYC	O2A-CGA-CBA	2.18	121.04	114.03
28	EH	1001	CYC	CHA-C1A-NA	-2.18	125.80	128.83
26	A5	202	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
26	O4	201	PEB	C1B-C2B-C3B	-2.18	104.00	106.51
26	S1	201	PEB	O2B-CGB-CBB	2.18	121.04	114.03
26	L1	203	PEB	CHA-C1B-NB	-2.18	120.37	124.93
26	CC	203	PEB	CHA-C1B-NB	-2.18	120.37	124.93
26	k8	201	PEB	CHC-C1D-ND	2.18	116.48	113.95
27	A7	304	PUB	CBA-CAA-C3A	-2.18	109.67	112.98
26	cB	201	PEB	CHB-C4B-C3B	-2.18	120.28	125.32
26	yE	301	PEB	CAB-C3B-C4B	2.18	128.87	125.01
26	qG	202	PEB	C3B-C4B-NB	2.18	113.22	110.05
26	LG	202	PEB	C2B-C1B-NB	2.18	115.18	110.53
26	C4	202	PEB	CHA-C1B-NB	-2.18	120.37	124.93
26	OG	203	PEB	C2B-C1B-NB	2.18	115.18	110.53
26	B4	201	PEB	C1B-C2B-C3B	-2.18	104.00	106.51
26	SF	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
26	m1	203	PEB	OD-C4D-ND	-2.18	122.70	125.93
26	e4	202	PEB	OD-C4D-ND	-2.18	122.70	125.93
26	mB	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	F8	202	PEB	CMA-C2A-C1A	-2.18	107.70	112.40
26	Y4	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
26	CG	202	PEB	CAB-C3B-C4B	2.18	128.87	125.01
26	SD	201	PEB	CHA-C4A-NA	2.18	127.80	125.20
26	JC	202	PEB	CMC-C3C-C2C	-2.18	120.83	124.94
26	TD	202	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
26	dE	201	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	dG	202	PEB	CAB-C3B-C4B	2.18	128.86	125.01
26	f6	201	PEB	CHA-C1B-NB	-2.18	120.37	124.93
26	a8	202	PEB	CHA-C1B-NB	-2.18	120.37	124.93
26	wG	301	PEB	CHA-C1B-NB	-2.18	120.37	124.93
28	E6	1001	CYC	CMC-C2C-C1C	-2.18	107.70	112.40
26	M1	401	PEB	OD-C4D-ND	-2.18	122.70	125.93
26	X4	202	PEB	OA-C1A-NA	2.18	127.58	124.94
26	BA	301	PEB	C1C-CHB-C4B	-2.18	126.21	128.81
27	B8	302	PUB	CAC-C2C-C1C	2.18	128.86	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	II	1001	CYC	CHB-C1B-NB	-2.18	121.38	126.06
26	L3	202	PEB	CHB-C4B-NB	-2.18	125.80	128.83
26	FE	201	PEB	CAA-C3A-C2A	-2.18	108.81	114.26
26	k2	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	gF	202	PEB	CMB-C2B-C1B	2.18	128.42	125.06
28	C7	1001	CYC	CHA-C1A-NA	-2.18	125.81	128.83
26	FI	1002	PEB	CHA-C1B-NB	-2.18	120.38	124.93
26	OE	203	PEB	CAA-C3A-C4A	-2.18	107.08	112.67
26	m7	202	PEB	CBC-CAC-C2C	-2.18	108.90	112.62
26	FA	201	PEB	CAB-CBB-CGB	-2.18	108.92	113.60
26	J5	202	PEB	C2B-C1B-NB	2.18	115.18	110.53
26	fB	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	SI	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
28	LF	1001	CYC	CAA-CBA-CGA	2.18	118.29	113.60
26	H9	201	PEB	C2B-C1B-NB	2.18	115.18	110.53
26	cB	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
26	tG	202	PEB	C1B-C2B-C3B	-2.18	104.01	106.51
26	V4	203	PEB	CHA-C1B-NB	-2.18	120.38	124.93
26	f6	203	PEB	OD-C4D-ND	-2.18	122.70	125.93
26	OB	203	PEB	C2B-C1B-NB	2.18	115.17	110.53
26	i1	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	i8	201	PEB	CHA-C4A-NA	2.18	127.79	125.20
26	x4	202	PEB	CHB-C4B-C3B	2.18	130.35	125.32
26	LA	202	PEB	OA-C1A-NA	2.18	127.58	124.94
26	GA	203	PEB	C2B-C1B-NB	2.18	115.17	110.53
26	V3	201	PEB	C3B-C4B-NB	2.18	113.22	110.05
26	TD	201	PEB	CMC-C3C-C2C	2.18	129.04	124.94
26	B5	202	PEB	C1C-CHB-C4B	-2.18	126.21	128.81
26	LI	1002	PEB	CAB-C3B-C4B	2.18	128.86	125.01
26	TG	202	PEB	CHC-C4C-C3C	2.18	134.05	130.34
26	A9	301	PEB	CMB-C2B-C1B	2.18	128.41	125.06
26	XA	202	PEB	CMB-C2B-C3B	-2.18	120.21	126.12
26	R9	203	PEB	OD-C4D-ND	-2.18	122.71	125.93
26	IG	202	PEB	CAC-CBC-CGC	-2.18	107.66	113.76
26	dE	201	PEB	CAA-C3A-C2A	-2.17	108.83	114.26
26	WD	202	PEB	OD-C4D-C3D	-2.17	124.53	129.46
26	bF	201	PEB	C1C-CHB-C4B	2.17	131.41	128.81
26	F5	203	PEB	CAB-CBB-CGB	-2.17	108.92	113.60
27	AA	303	PUB	CMC-C3C-C2C	-2.17	120.21	126.12
26	U6	203	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	P8	202	PEB	CAC-CBC-CGC	-2.17	107.66	113.76
26	QG	202	PEB	CAA-C3A-C4A	-2.17	107.09	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	gA	201	PEB	CMD-C2D-C3D	2.17	133.13	130.06
26	L5	202	PEB	CBC-CAC-C2C	-2.17	108.91	112.62
28	L6	1001	CYC	CHB-C1B-NB	-2.17	121.39	126.06
26	U4	202	PEB	CHA-C1B-NB	-2.17	120.39	124.93
26	rG	202	PEB	C2A-C1A-NA	2.17	110.15	108.27
26	BA	301	PEB	CHC-C4C-C3C	-2.17	126.63	130.34
26	j8	201	PEB	OD-C4D-ND	-2.17	122.71	125.93
26	fB	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
26	P2	203	PEB	CAC-CBC-CGC	-2.17	107.67	113.76
26	hA	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	EE	202	PEB	OD-C4D-C3D	-2.17	124.54	129.46
26	PF	202	PEB	CBC-CAC-C2C	2.17	116.33	112.62
26	JJ	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	i1	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
26	WE	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
26	I5	202	PEB	C1C-CHB-C4B	2.17	131.41	128.81
26	WF	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
26	R7	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
26	C3	201	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
26	K3	202	PEB	C1C-CHB-C4B	-2.17	126.21	128.81
26	J7	1002	PEB	C1C-CHB-C4B	-2.17	126.21	128.81
26	bE	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
26	qG	201	PEB	CAB-C3B-C4B	2.17	128.85	125.01
26	TF	202	PEB	CHC-C4C-C3C	-2.17	126.63	130.34
26	UB	202	PEB	CHA-C1B-NB	-2.17	120.39	124.93
26	V4	201	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	R4	203	PEB	OD-C4D-ND	-2.17	122.71	125.93
26	D6	1002	PEB	CAA-C3A-C2A	-2.17	108.83	114.26
26	L5	201	PEB	C3B-C4B-NB	2.17	113.21	110.05
26	wG	301	PEB	C2A-C1A-NA	2.17	110.14	108.27
26	J8	201	PEB	CAA-C3A-C4A	-2.17	107.10	112.67
26	w1	202	PEB	CAB-CBB-CGB	-2.17	108.93	113.60
26	I1	202	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	X3	201	PEB	C4B-C3B-C2B	-2.17	104.38	106.78
26	K5	201	PEB	CAA-C3A-C4A	-2.17	107.10	112.67
26	sE	201	PEB	OD-C4D-ND	-2.17	122.71	125.93
26	WF	202	PEB	CHA-C1B-C2B	2.17	130.48	124.90
26	e7	202	PEB	OA-C1A-C2A	-2.17	124.45	126.17
26	OE	201	PEB	C2B-C1B-NB	2.17	115.16	110.53
26	g4	203	PEB	OD-C4D-ND	-2.17	122.72	125.93
26	aF	202	PEB	C2A-C1A-NA	2.17	110.14	108.27
26	V4	201	PEB	CHB-C4B-NB	-2.17	125.82	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K8	202	PEB	C3B-C4B-NB	2.17	113.21	110.05
28	JH	1001	CYC	C2A-C1A-NA	2.17	113.21	110.05
26	d8	201	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	y4	201	PEB	O1B-CGB-CBB	-2.17	116.11	123.08
26	S2	201	PEB	OA-C1A-NA	2.17	127.57	124.94
26	W3	201	PEB	CAA-C3A-C4A	-2.17	107.10	112.67
26	I5	202	PEB	CAC-CBC-CGC	-2.17	107.68	113.76
26	i1	201	PEB	OD-C4D-ND	-2.17	122.72	125.93
26	UI	201	PEB	CMA-C2A-C3A	-2.17	105.08	113.83
26	qG	202	PEB	OD-C4D-C3D	-2.17	124.55	129.46
26	O7	203	PEB	C2B-C1B-NB	2.17	115.16	110.53
26	k7	201	PEB	C2B-C1B-NB	2.17	115.16	110.53
26	W1	202	PEB	C1B-C2B-C3B	-2.17	104.02	106.51
26	PI	203	PEB	CAB-CBB-CGB	2.17	118.27	113.60
26	Q7	201	PEB	C2B-C1B-NB	2.17	115.16	110.53
26	V3	203	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	jA	203	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	bI	201	PEB	CAB-C3B-C4B	2.17	128.84	125.01
26	e6	203	PEB	O2C-CGC-CBC	2.17	121.00	114.03
26	u1	201	PEB	CAB-CBB-CGB	-2.17	108.94	113.60
26	R1	201	PEB	CBB-CAB-C3B	-2.17	106.60	112.63
26	d8	202	PEB	CAA-C3A-C4A	-2.17	107.11	112.67
26	bE	201	PEB	CAB-CBB-CGB	-2.17	108.94	113.60
28	qH	1001	CYC	CHB-C1B-C2B	-2.17	122.65	126.95
26	QG	201	PEB	CMB-C2B-C3B	-2.17	120.23	126.12
26	TF	202	PEB	CAB-CBB-CGB	-2.17	108.94	113.60
26	DB	1002	PEB	OD-C4D-ND	-2.17	122.72	125.93
26	y4	201	PEB	CHA-C1B-NB	2.17	129.47	124.93
26	b2	201	PEB	C4B-C3B-C2B	-2.17	104.38	106.78
26	II	202	PEB	CBA-CAA-C3A	-2.17	108.64	113.47
28	LI	1001	CYC	O2A-CGA-CBA	2.17	120.99	114.03
26	BJ	203	PEB	CBD-CAD-C3D	-2.17	116.84	127.62
26	CE	201	PEB	CBA-CAA-C3A	-2.17	108.64	113.47
26	MJ	201	PEB	OA-C1A-C2A	-2.17	124.45	126.17
26	P9	203	PEB	OD-C4D-C3D	-2.17	124.55	129.46
26	HJ	201	PEB	CHC-C1D-ND	-2.17	111.43	113.95
27	xE	301	PUB	CAC-C2C-C1C	2.17	128.84	125.01
26	U6	203	PEB	OD-C4D-C3D	-2.17	124.55	129.46
28	IH	1001	CYC	C2C-C3C-C4C	2.17	104.58	101.34
26	GC	201	PEB	CAB-CBB-CGB	-2.17	108.94	113.60
26	w4	204	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	N1	201	PEB	C2B-C1B-NB	2.17	115.15	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UF	202	PEB	C2B-C1B-NB	2.17	115.15	110.53
26	h6	203	PEB	OD-C4D-C3D	-2.17	124.55	129.46
26	O7	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	j7	202	PEB	CBC-CAC-C2C	-2.17	108.92	112.62
28	LH	1001	CYC	C1A-C2A-C3A	-2.17	104.39	106.78
28	RH	1001	CYC	C2C-C1C-NC	2.17	110.14	108.27
28	HI	1001	CYC	C1B-CHB-C4A	-2.17	122.79	128.08
26	R9	203	PEB	CAA-C3A-C4A	-2.17	107.11	112.67
26	H7	1002	PEB	OD-C4D-C3D	-2.17	124.55	129.46
26	bG	202	PEB	CHC-C4C-C3C	2.17	134.03	130.34
26	JG	201	PEB	C3B-C4B-NB	2.17	113.20	110.05
26	BG	201	PEB	O2B-CGB-CBB	2.17	120.99	114.03
26	WG	201	PEB	C2B-C1B-NB	2.17	115.15	110.53
26	Q1	202	PEB	OD-C4D-C3D	-2.17	124.56	129.46
26	NA	202	PEB	CMA-C2A-C1A	-2.17	107.74	112.40
26	S4	201	PEB	C1B-C2B-C3B	-2.17	104.02	106.51
26	D4	202	PEB	OD-C4D-ND	-2.17	122.72	125.93
26	hB	203	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	q1	203	PEB	OD-C4D-C3D	-2.16	124.56	129.46
26	AE	201	PEB	OD-C4D-C3D	-2.16	124.56	129.46
26	s1	201	PEB	CBB-CAB-C3B	-2.16	106.61	112.63
26	G3	201	PEB	CBB-CAB-C3B	-2.16	106.61	112.63
26	T2	202	PEB	CAB-C3B-C4B	2.16	128.84	125.01
26	aE	203	PEB	OD-C4D-ND	-2.16	122.72	125.93
26	fB	201	PEB	CHA-C1B-NB	-2.16	120.41	124.93
26	BA	301	PEB	CMD-C2D-C3D	2.16	133.12	130.06
26	KC	201	PEB	CBC-CAC-C2C	-2.16	108.93	112.62
26	O1	201	PEB	CBC-CAC-C2C	-2.16	108.93	112.62
26	O9	201	PEB	C2B-C1B-NB	2.16	115.15	110.53
26	I5	203	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	zG	501	PEB	CAB-C3B-C4B	2.16	128.84	125.01
26	H1	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
26	QB	201	PEB	OD-C4D-C3D	-2.16	124.56	129.46
26	Y8	203	PEB	CHA-C1B-NB	-2.16	120.41	124.93
26	DJ	202	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
26	a1	203	PEB	CHB-C4B-C3B	-2.16	120.32	125.32
26	e4	202	PEB	C3B-C4B-NB	2.16	113.19	110.05
26	N4	201	PEB	CHC-C4C-C3C	-2.16	126.65	130.34
26	KE	203	PEB	O2C-CGC-CBC	2.16	120.98	114.03
26	kF	202	PEB	OD-C4D-C3D	-2.16	124.56	129.46
26	M4	401	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	mB	201	PEB	CHA-C1B-NB	-2.16	120.41	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j4	202	PEB	CHB-C4B-C3B	-2.16	120.33	125.32
26	T7	202	PEB	OD-C4D-ND	-2.16	122.73	125.93
28	K6	202	CYC	CBD-CAD-C3D	-2.16	108.93	112.62
26	P3	201	PEB	C4B-C3B-C2B	-2.16	104.39	106.78
26	T3	202	PEB	CAA-C3A-C2A	-2.16	108.86	114.26
26	B8	301	PEB	CMD-C2D-C3D	2.16	133.11	130.06
26	QJ	202	PEB	OA-C1A-C2A	-2.16	124.45	126.17
26	gB	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
26	GE	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
26	O3	201	PEB	C1C-CHB-C4B	2.16	131.39	128.81
26	VF	202	PEB	CHA-C1B-NB	-2.16	120.41	124.93
26	R9	201	PEB	C3B-C4B-NB	2.16	113.19	110.05
26	HC	201	PEB	C4B-C3B-C2B	-2.16	104.39	106.78
26	X4	202	PEB	CMB-C2B-C3B	-2.16	120.25	126.12
26	CJ	201	PEB	OD-C4D-C3D	-2.16	124.56	129.46
26	P6	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
26	v1	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	V4	201	PEB	C2A-C1A-NA	2.16	110.14	108.27
26	D9	202	PEB	C2A-C1A-NA	2.16	110.14	108.27
26	Q7	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
26	mF	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
28	vH	1001	CYC	C2B-C1B-NB	2.16	110.15	106.99
26	U2	201	PEB	CMA-C2A-C3A	-2.16	105.11	113.83
26	FG	201	PEB	CAA-C3A-C2A	-2.16	108.86	114.26
26	o1	501	PEB	C2B-C1B-NB	2.16	115.14	110.53
26	c6	201	PEB	CHB-C4B-C3B	-2.16	120.33	125.32
26	g8	202	PEB	CHA-C1B-NB	-2.16	120.41	124.93
28	qH	1001	CYC	C1A-C2A-C3A	-2.16	104.39	106.78
26	hB	201	PEB	OD-C4D-ND	-2.16	122.73	125.93
26	HG	202	PEB	C4B-NB-C1B	-2.16	102.44	106.51
26	h6	201	PEB	CHA-C1B-NB	-2.16	120.42	124.93
26	A1	201	PEB	C2A-C1A-NA	2.16	110.14	108.27
26	NJ	203	PEB	OD-C4D-C3D	-2.16	124.57	129.46
26	HI	1002	PEB	CAB-CBB-CGB	-2.16	108.95	113.60
26	VG	202	PEB	CHA-C4A-NA	2.16	127.77	125.20
28	yH	1001	CYC	C1A-C2A-C3A	-2.16	104.39	106.78
26	GA	201	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
26	I5	202	PEB	CHA-C1B-C2B	2.16	130.45	124.90
28	IF	1001	CYC	CAC-C3C-C2C	2.16	119.65	114.26
26	s1	202	PEB	OA-C1A-NA	2.16	127.56	124.94
26	c7	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
26	U3	201	PEB	O2C-CGC-CBC	2.16	120.97	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S7	203	PEB	CHA-C1B-NB	-2.16	120.42	124.93
26	VE	201	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
26	ND	203	PEB	CHC-C4C-C3C	-2.16	126.66	130.34
26	ME	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	N1	201	PEB	OA-C1A-C2A	-2.16	124.46	126.17
26	k2	201	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	zE	501	PEB	CAB-C3B-C4B	2.16	128.83	125.01
26	VF	203	PEB	CAB-C3B-C4B	2.16	128.83	125.01
28	NB	1001	CYC	OB-C4B-NB	-2.16	120.06	125.08
26	RJ	203	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	bB	202	PEB	OD-C4D-C3D	-2.16	124.57	129.46
26	RJ	202	PEB	CBC-CAC-C2C	-2.16	108.94	112.62
26	gI	201	PEB	CAB-CBB-CGB	-2.16	108.96	113.60
26	JE	202	PEB	CHC-C4C-C3C	2.16	134.01	130.34
26	hA	203	PEB	CHA-C4A-NA	-2.16	122.64	125.20
26	UA	203	PEB	CMD-C2D-C3D	2.16	133.11	130.06
26	F9	201	PEB	CAB-C3B-C4B	2.16	128.82	125.01
26	Q4	202	PEB	OD-C4D-C3D	-2.16	124.57	129.46
26	LC	203	PEB	CMC-C3C-C2C	-2.16	120.88	124.94
26	ZI	201	PEB	CHB-C4B-NB	2.16	131.82	128.83
26	QE	203	PEB	CAA-C3A-C2A	2.16	119.65	114.26
26	aE	201	PEB	CAB-C3B-C4B	2.16	128.82	125.01
26	nG	202	PEB	C2B-C1B-NB	2.16	115.13	110.53
26	H2	1002	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	hB	203	PEB	CBA-CAA-C3A	-2.16	108.67	113.47
26	v1	202	PEB	CAA-C3A-C4A	2.16	118.21	112.67
26	PI	202	PEB	CAC-CBC-CGC	-2.16	107.71	113.76
26	u1	203	PEB	CHB-C4B-NB	-2.16	125.84	128.83
26	g7	201	PEB	CHB-C4B-NB	-2.16	125.84	128.83
26	OB	201	PEB	CAC-CBC-CGC	-2.16	107.72	113.76
26	FI	1002	PEB	CHB-C4B-C3B	-2.16	120.34	125.32
27	Y3	302	PUB	CHB-C1C-C2C	-2.16	120.34	125.32
26	g2	201	PEB	CAA-C3A-C4A	-2.16	107.14	112.67
26	IJ	202	PEB	CAC-CBC-CGC	-2.16	107.72	113.76
26	QB	203	PEB	OD-C4D-C3D	-2.16	124.58	129.46
26	ND	201	PEB	OD-C4D-C3D	-2.16	124.58	129.46
26	FJ	202	PEB	OD-C4D-C3D	-2.16	124.58	129.46
28	EF	1001	CYC	CMC-C2C-C1C	-2.16	107.76	112.40
26	l4	201	PEB	OD-C4D-C3D	-2.16	124.58	129.46
26	x1	201	PEB	CMC-C3C-C2C	2.16	129.00	124.94
26	e3	401	PEB	C4B-C3B-C2B	-2.15	104.40	106.78
26	x1	202	PEB	C4B-NB-C1B	-2.15	102.45	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e7	201	PEB	CMD-C2D-C3D	2.15	133.10	130.06
26	TI	201	PEB	CHA-C4A-NA	2.15	127.77	125.20
26	e7	202	PEB	C1B-C2B-C3B	-2.15	104.03	106.51
26	cA	203	PEB	C1B-C2B-C3B	-2.15	104.03	106.51
26	ND	203	PEB	C1B-C2B-C3B	-2.15	104.03	106.51
26	JI	1002	PEB	C1B-C2B-C3B	-2.15	104.03	106.51
26	k7	202	PEB	CHB-C4B-C3B	-2.15	120.34	125.32
27	A2	302	PUB	CAC-C2C-C1C	2.15	128.82	125.01
26	G1	201	PEB	OD-C4D-C3D	-2.15	124.58	129.46
26	lA	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	HI	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	C4	201	PEB	CAA-C3A-C2A	-2.15	108.88	114.26
26	cF	202	PEB	OD-C4D-ND	-2.15	122.74	125.93
26	W4	201	PEB	CAC-C2C-C3C	2.15	133.43	127.25
26	aA	202	PEB	CAB-CBB-CGB	-2.15	108.97	113.60
26	11	203	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	CD	201	PEB	CBA-CAA-C3A	-2.15	108.67	113.47
26	21	401	PEB	CBD-CAD-C3D	-2.15	116.91	127.62
26	HA	201	PEB	CAB-C3B-C4B	2.15	128.82	125.01
26	l7	203	PEB	OD-C4D-ND	-2.15	122.74	125.93
26	eG	202	PEB	CMB-C2B-C3B	-2.15	120.27	126.12
26	M8	201	PEB	CBA-CAA-C3A	-2.15	108.67	113.47
28	B6	1002	CYC	OB-C4B-NB	-2.15	120.08	125.08
26	j8	201	PEB	CAB-C3B-C4B	2.15	128.82	125.01
28	oH	1001	CYC	C2A-C1A-NA	2.15	113.18	110.05
26	m1	202	PEB	CBC-CAC-C2C	-2.15	108.95	112.62
26	cA	203	PEB	CBA-CAA-C3A	-2.15	108.67	113.47
26	U7	203	PEB	CHA-C4A-NA	-2.15	122.65	125.20
26	t1	202	PEB	OD-C4D-ND	-2.15	122.74	125.93
26	NE	201	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
26	C5	203	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	WG	202	PEB	OD-C4D-C3D	-2.15	124.58	129.46
26	DD	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
27	A2	303	PUB	CAC-C2C-C1C	2.15	128.81	125.01
26	CG	203	PEB	CHB-C4B-C3B	-2.15	120.35	125.32
26	LJ	203	PEB	OD-C4D-C3D	-2.15	124.59	129.46
26	L3	201	PEB	CHA-C4A-NA	2.15	127.76	125.20
26	A5	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	rG	202	PEB	CMC-C3C-C2C	-2.15	120.89	124.94
26	m1	201	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
26	T6	202	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
26	v4	202	PEB	C3B-C4B-NB	2.15	113.18	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	PB	201	PEB	C2B-C1B-NB	2.15	115.12	110.53
26	aE	203	PEB	O2C-CGC-CBC	2.15	120.94	114.03
26	Z7	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
28	I6	1001	CYC	CMC-C2C-C1C	-2.15	107.77	112.40
26	CA	201	PEB	C2A-C1A-NA	2.15	110.13	108.27
26	O9	201	PEB	OD-C4D-ND	-2.15	122.75	125.93
26	iI	202	PEB	OD-C4D-ND	-2.15	122.75	125.93
26	UD	202	PEB	C2B-C1B-NB	2.15	115.12	110.53
26	B3	202	PEB	CMC-C3C-C2C	2.15	129.00	124.94
26	Q1	201	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
26	s1	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	X4	201	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
26	N4	201	PEB	OA-C1A-C2A	-2.15	124.46	126.17
28	JF	1003	CYC	CHA-C1A-NA	-2.15	125.84	128.83
26	W2	201	PEB	OA-C1A-NA	2.15	127.55	124.94
26	M9	202	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
26	UJ	202	PEB	C1C-CHB-C4B	2.15	131.38	128.81
26	O1	201	PEB	OD-C4D-C3D	-2.15	124.59	129.46
26	f7	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	h8	203	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	SB	201	PEB	CAC-CBC-CGC	-2.15	107.73	113.76
26	A2	305	PEB	CBA-CAA-C3A	-2.15	108.68	113.47
28	mH	1001	CYC	CAB-C3B-C2B	2.15	131.20	127.53
26	R8	201	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
27	AI	303	PUB	CAC-C2C-C1C	2.15	128.81	125.01
26	e7	202	PEB	OA-C1A-NA	2.15	127.54	124.94
26	t4	201	PEB	CAC-CBC-CGC	-2.15	107.74	113.76
26	w1	201	PEB	C3B-C4B-NB	2.15	113.17	110.05
26	A4	201	PEB	CAA-C3A-C2A	2.15	119.63	114.26
26	h4	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
26	KB	201	PEB	CAB-C3B-C4B	2.15	128.81	125.01
26	c2	202	PEB	CMD-C2D-C3D	2.15	133.09	130.06
26	e7	201	PEB	CBA-CAA-C3A	-2.15	108.69	113.47
26	XD	201	PEB	C4B-C3B-C2B	-2.15	104.41	106.78
26	m7	202	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
26	u1	203	PEB	OD-C4D-C3D	-2.15	124.59	129.46
26	DG	203	PEB	CAB-C3B-C4B	2.15	128.81	125.01
26	PI	201	PEB	CHB-C4B-C3B	-2.15	120.36	125.32
26	K5	201	PEB	CMD-C2D-C3D	2.15	133.09	130.06
26	i1	201	PEB	CHA-C1B-NB	-2.15	120.44	124.93
26	b7	201	PEB	CBC-CAC-C2C	-2.15	108.96	112.62
28	qH	1002	CYC	CMD-C2D-C3D	2.15	128.99	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y1	203	PEB	CHC-C4C-C3C	-2.15	126.67	130.34
26	d6	204	PEB	OD-C4D-ND	-2.15	122.75	125.93
28	II	1001	CYC	CHA-C1A-C2A	-2.15	120.36	125.32
26	GG	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
26	L9	203	PEB	CHB-C4B-C3B	-2.15	120.36	125.32
26	u1	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
26	YB	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
26	wG	301	PEB	C2B-C1B-NB	2.15	115.11	110.53
26	T6	201	PEB	CMA-C2A-C1A	-2.15	107.78	112.40
26	O8	203	PEB	CMA-C2A-C1A	-2.15	107.78	112.40
26	fF	203	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
26	P9	201	PEB	CHB-C4B-C3B	-2.15	120.36	125.32
26	O8	201	PEB	CHA-C1B-NB	-2.15	120.44	124.93
28	G7	1001	CYC	CAC-C3C-C2C	-2.15	108.90	114.26
26	AC	201	PEB	CHC-C1D-ND	-2.15	111.46	113.95
26	y4	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
26	Y9	202	PEB	C2B-C1B-NB	2.15	115.11	110.53
26	WJ	202	PEB	CHA-C1B-NB	-2.15	120.45	124.93
28	L2	1001	CYC	CAB-C3B-C2B	2.15	131.20	127.53
28	OH	1001	CYC	CHB-C1B-C2B	-2.15	122.70	126.95
26	S7	201	PEB	CAA-C3A-C2A	-2.14	108.90	114.26
26	LD	201	PEB	C3B-C4B-NB	2.14	113.17	110.05
26	rE	202	PEB	CHA-C1B-NB	-2.14	120.45	124.93
26	H4	201	PEB	CAB-CBB-CGB	-2.14	108.99	113.60
26	OE	203	PEB	OD-C4D-C3D	-2.14	124.60	129.46
28	NB	1001	CYC	CAD-C3D-C2D	2.14	133.41	127.25
26	g6	201	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	m4	203	PEB	CMA-C2A-C1A	-2.14	107.78	112.40
26	XD	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
26	q1	202	PEB	C3B-C4B-NB	2.14	113.17	110.05
26	I8	203	PEB	C3B-C4B-NB	2.14	113.17	110.05
26	FD	203	PEB	CAB-CBB-CGB	-2.14	108.99	113.60
26	OG	202	PEB	CAB-CBB-CGB	-2.14	108.99	113.60
26	S4	202	PEB	C1C-CHB-C4B	-2.14	126.25	128.81
26	cG	203	PEB	CAC-CBC-CGC	-2.14	107.75	113.76
26	W7	203	PEB	CAB-CBB-CGB	-2.14	108.99	113.60
26	SE	201	PEB	CAB-C3B-C2B	2.14	131.87	127.88
27	A1	203	PUB	CAC-C2C-C1C	2.14	128.80	125.01
26	Q6	202	PEB	C4B-C3B-C2B	-2.14	104.41	106.78
28	I2	1001	CYC	CHB-C1B-NB	-2.14	121.46	126.06
26	A9	303	PEB	CAA-C3A-C4A	2.14	118.18	112.67
26	cA	203	PEB	CHA-C4A-NA	-2.14	122.66	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X9	202	PEB	CAB-C3B-C4B	2.14	128.80	125.01
26	k1	202	PEB	C2B-C1B-NB	2.14	115.10	110.53
26	MD	201	PEB	O1C-CGC-CBC	-2.14	116.20	123.08
26	Z6	203	PEB	CHA-C1B-C2B	2.14	130.41	124.90
26	pE	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
26	l2	202	PEB	O2B-CGB-CBB	2.14	120.91	114.03
28	YH	1003	CYC	CBD-CAD-C3D	-2.14	108.96	112.62
27	wG	304	PUB	CAC-CBC-CGC	-2.14	108.99	113.60
26	xE	302	PEB	CHA-C4A-NA	-2.14	122.66	125.20
26	bG	201	PEB	CHA-C4A-NA	2.14	127.75	125.20
27	A4	203	PUB	CHA-C1B-C2B	-2.14	126.68	130.34
26	HG	201	PEB	CBA-CAA-C3A	2.14	118.24	113.47
26	aF	202	PEB	CHA-C1B-C2B	2.14	130.41	124.90
26	QJ	202	PEB	CHA-C1B-NB	-2.14	120.45	124.93
26	B1	203	PEB	CMB-C2B-C1B	2.14	128.36	125.06
28	F2	1001	CYC	CBB-CAB-C3B	2.14	118.33	112.43
26	fl	202	PEB	CBA-CAA-C3A	-2.14	108.70	113.47
26	R6	201	PEB	CMA-C2A-C1A	-2.14	107.79	112.40
26	XE	202	PEB	CHA-C1B-NB	-2.14	120.45	124.93
26	G1	201	PEB	CHA-C4A-NA	2.14	127.75	125.20
26	i8	202	PEB	CAB-C3B-C4B	2.14	128.80	125.01
26	d2	202	PEB	CHA-C1B-NB	-2.14	120.45	124.93
26	P2	201	PEB	CHB-C4B-C3B	-2.14	120.38	125.32
26	f6	201	PEB	CBC-CAC-C2C	-2.14	108.97	112.62
26	UA	202	PEB	OA-C1A-C2A	-2.14	124.47	126.17
26	b6	202	PEB	C1C-CHB-C4B	-2.14	126.25	128.81
26	P3	202	PEB	C2B-C1B-NB	2.14	115.10	110.53
26	N3	201	PEB	OD-C4D-C3D	-2.14	124.61	129.46
26	b7	201	PEB	CHA-C1B-NB	-2.14	120.46	124.93
26	C1	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	XJ	201	PEB	OD-C4D-ND	-2.14	122.76	125.93
26	LJ	202	PEB	OD-C4D-C3D	-2.14	124.61	129.46
26	L4	201	PEB	CHB-C4B-NB	-2.14	125.86	128.83
28	WH	1001	CYC	C1A-C2A-C3A	-2.14	104.42	106.78
26	JE	202	PEB	C2B-C1B-NB	2.14	115.09	110.53
26	jA	203	PEB	CAB-C3B-C4B	2.14	128.79	125.01
26	L6	1002	PEB	CHA-C1B-NB	-2.14	120.46	124.93
26	f1	202	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
26	H8	201	PEB	OD-C4D-ND	-2.14	122.76	125.93
27	xG	306	PUB	CHC-C1D-ND	-2.14	111.02	113.72
26	H9	201	PEB	CHC-C1D-ND	-2.14	111.46	113.95
28	B6	1002	CYC	CMA-C3A-C2A	-2.14	120.31	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A9	302	PUB	C1D-CHC-C4C	-2.14	108.71	113.37
26	F4	201	PEB	C2A-C1A-NA	2.14	110.12	108.27
28	pH	1001	CYC	CHB-C1B-C2B	-2.14	122.71	126.95
26	m8	201	PEB	CHA-C1B-C2B	2.14	130.40	124.90
28	VH	1001	CYC	OC-C1C-NC	2.14	127.53	124.94
28	GB	1001	CYC	CHB-C1B-NB	-2.14	121.47	126.06
26	A4	201	PEB	CMB-C2B-C3B	2.14	131.92	126.12
26	U8	202	PEB	O1C-CGC-CBC	-2.14	116.21	123.08
26	YJ	201	PEB	CAC-CBC-CGC	-2.14	107.76	113.76
26	h8	202	PEB	CAB-C3B-C4B	2.14	128.79	125.01
26	U9	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
26	Z6	203	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	j1	201	PEB	OD-C4D-C3D	-2.14	124.62	129.46
26	F4	202	PEB	OD-C4D-C3D	-2.14	124.62	129.46
26	cG	202	PEB	OD-C4D-C3D	-2.14	124.62	129.46
26	VG	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
26	dG	201	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
26	J1	203	PEB	CAC-CBC-CGC	-2.14	107.77	113.76
26	CE	201	PEB	OD-C4D-ND	-2.14	122.76	125.93
26	Q6	203	PEB	OD-C4D-C3D	-2.14	124.62	129.46
28	G6	1001	CYC	CHA-C1A-C2A	-2.14	120.38	125.32
26	G8	201	PEB	CAA-C3A-C4A	-2.14	107.18	112.67
26	R6	202	PEB	CMC-C3C-C2C	2.14	128.97	124.94
26	uG	201	PEB	CBA-CAA-C3A	-2.14	108.71	113.47
26	a1	202	PEB	CHC-C1D-ND	-2.14	111.47	113.95
26	D9	202	PEB	CMD-C2D-C3D	2.14	133.08	130.06
26	DE	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
28	FI	1001	CYC	C1B-CHB-C4A	-2.14	122.86	128.08
27	xG	306	PUB	O2B-CGB-CBB	2.14	120.89	114.03
26	p4	201	PEB	CHB-C4B-C3B	-2.14	120.38	125.32
26	U7	201	PEB	OD-C4D-ND	-2.14	122.77	125.93
28	HB	1001	CYC	CBB-CAB-C3B	-2.14	106.54	112.43
28	IF	1001	CYC	CHB-C4A-C3A	2.14	130.39	124.90
26	L3	201	PEB	C1B-C2B-C3B	-2.14	104.06	106.51
26	OG	201	PEB	C2B-C1B-NB	2.14	115.09	110.53
26	I5	202	PEB	CHA-C4A-NA	2.14	127.75	125.20
26	A6	301	PEB	CHA-C4A-NA	-2.14	122.67	125.20
26	ND	203	PEB	CHA-C4A-NA	-2.14	122.67	125.20
26	m8	201	PEB	CHC-C4C-C3C	-2.14	126.69	130.34
26	P1	203	PEB	CBA-CAA-C3A	-2.14	108.71	113.47
26	F9	202	PEB	CBA-CAA-C3A	-2.14	108.71	113.47
26	OF	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k1	201	PEB	CHB-C4B-C3B	-2.14	120.39	125.32
26	R6	201	PEB	C1B-C2B-C3B	-2.14	104.06	106.51
26	c8	201	PEB	C1B-C2B-C3B	-2.14	104.06	106.51
26	ZB	203	PEB	CHA-C4A-NA	2.14	127.74	125.20
26	O4	201	PEB	CAA-C3A-C4A	-2.14	107.19	112.67
26	GE	203	PEB	O2C-CGC-CBC	2.14	120.89	114.03
26	C9	201	PEB	CHB-C4B-NB	-2.13	125.86	128.83
26	K9	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
26	dE	202	PEB	CHC-C1D-ND	2.13	116.43	113.95
26	ME	201	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
26	mF	201	PEB	CAA-C3A-C2A	-2.13	108.93	114.26
26	N8	202	PEB	OA-C1A-NA	2.13	127.53	124.94
26	G3	202	PEB	C2A-C3A-C4A	-2.13	98.14	101.34
26	r4	202	PEB	OD-C4D-C3D	-2.13	124.62	129.46
26	WD	202	PEB	CBA-CAA-C3A	-2.13	108.72	113.47
26	iA	202	PEB	O1B-CGB-CBB	-2.13	116.23	123.08
28	KF	1001	CYC	CHA-C1A-NA	-2.13	125.87	128.83
26	EG	202	PEB	C2B-C1B-NB	2.13	115.08	110.53
26	AJ	301	PEB	C2B-C1B-NB	2.13	115.08	110.53
26	mB	202	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
26	k2	202	PEB	C2A-C1A-NA	2.13	110.11	108.27
26	RD	203	PEB	CBD-CAD-C3D	-2.13	117.01	127.62
26	EG	202	PEB	OD-C4D-C3D	-2.13	124.63	129.46
28	DF	1003	CYC	CHA-C1A-C2A	-2.13	120.39	125.32
26	FE	201	PEB	O2B-CGB-CBB	2.13	120.88	114.03
26	h4	202	PEB	CHA-C1B-NB	-2.13	120.47	124.93
26	VB	201	PEB	C2B-C1B-NB	2.13	115.08	110.53
26	eA	202	PEB	CAA-C3A-C2A	-2.13	108.93	114.26
28	YH	1002	CYC	C2C-C3C-C4C	2.13	104.53	101.34
26	y1	203	PEB	CHA-C1B-NB	-2.13	120.47	124.93
26	21	404	PEB	CHA-C1B-C2B	2.13	130.38	124.90
26	P1	203	PEB	OD-C4D-C3D	-2.13	124.63	129.46
26	E9	202	PEB	OD-C4D-C3D	-2.13	124.63	129.46
26	ZA	201	PEB	CHA-C4A-NA	2.13	127.74	125.20
26	P8	201	PEB	CAB-CBB-CGB	-2.13	109.02	113.60
26	YD	301	PEB	OD-C4D-ND	-2.13	122.77	125.93
26	S4	201	PEB	O2B-CGB-CBB	2.13	120.88	114.03
26	HI	1002	PEB	CHA-C1B-NB	-2.13	120.47	124.93
26	G4	201	PEB	C2A-C3A-C4A	-2.13	98.15	101.34
28	oH	1001	CYC	CAB-C3B-C2B	2.13	131.18	127.53
26	j6	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
26	V6	201	PEB	CAB-CBB-CGB	-2.13	109.02	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W1	201	PEB	CAC-C2C-C3C	2.13	133.37	127.25
26	CG	203	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	RG	201	PEB	CHC-C1D-ND	-2.13	111.47	113.95
27	xG	306	PUB	C4B-CHB-C1C	2.13	131.35	128.81
26	K5	203	PEB	CHA-C1B-NB	-2.13	120.47	124.93
26	HA	201	PEB	OD-C4D-ND	-2.13	122.77	125.93
26	E9	201	PEB	CBC-CAC-C2C	2.13	116.26	112.62
26	F3	203	PEB	OA-C1A-NA	2.13	127.52	124.94
26	LA	201	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
28	tH	1001	CYC	C2C-C1C-NC	2.13	110.11	108.27
26	WA	202	PEB	CMD-C2D-C3D	2.13	133.07	130.06
26	h6	201	PEB	C4B-C3B-C2B	-2.13	104.42	106.78
26	R3	202	PEB	CAB-C3B-C4B	2.13	128.78	125.01
28	NF	1001	CYC	CBC-CAC-C3C	2.13	118.21	113.47
26	UG	201	PEB	O2C-CGC-CBC	2.13	120.87	114.03
26	N3	201	PEB	CBC-CAC-C2C	-2.13	108.98	112.62
26	LI	1002	PEB	CHB-C4B-C3B	-2.13	120.40	125.32
26	F5	201	PEB	CAA-C3A-C4A	-2.13	107.20	112.67
26	h7	202	PEB	CAA-C3A-C2A	-2.13	108.94	114.26
26	11	203	PEB	CHA-C4A-NA	-2.13	122.67	125.20
27	Q8	201	PUB	CAB-CBB-CGB	-2.13	107.79	113.76
26	R2	201	PEB	OD-C4D-C3D	-2.13	124.64	129.46
26	GB	1002	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
26	B3	201	PEB	C2A-C3A-C4A	2.13	104.53	101.34
26	Y4	201	PEB	CMA-C2A-C1A	-2.13	107.81	112.40
27	A7	304	PUB	CHB-C1C-C2C	2.13	130.24	125.32
27	AA	304	PUB	CAC-C2C-C1C	2.13	128.77	125.01
26	D4	202	PEB	CHC-C1D-ND	-2.13	111.48	113.95
26	UF	201	PEB	OD-C4D-ND	-2.13	122.78	125.93
26	FD	201	PEB	CAA-C3A-C4A	-2.13	107.21	112.67
26	mF	201	PEB	CHB-C4B-NB	-2.13	125.88	128.83
26	RA	201	PEB	CBC-CAC-C2C	-2.13	108.99	112.62
26	eG	202	PEB	CAC-C2C-C3C	2.13	133.36	127.25
26	X3	202	PEB	CHB-C4B-C3B	-2.13	120.41	125.32
26	MG	201	PEB	CHB-C4B-C3B	-2.13	120.41	125.32
26	t4	201	PEB	C3B-C4B-NB	2.13	113.14	110.05
26	CG	203	PEB	CHA-C1B-NB	-2.13	120.48	124.93
26	C8	203	PEB	C2B-C1B-NB	2.13	115.07	110.53
26	yG	301	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
26	nE	202	PEB	CHB-C4B-C3B	-2.13	120.41	125.32
28	JF	1001	CYC	CHA-C1A-C2A	-2.13	120.41	125.32
26	H4	201	PEB	C1C-CHB-C4B	2.13	131.35	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L4	203	PEB	C1C-CHB-C4B	-2.13	126.27	128.81
26	AJ	303	PEB	CHA-C1B-C2B	2.13	130.37	124.90
26	VA	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
26	jF	203	PEB	CAB-C3B-C4B	2.13	128.77	125.01
26	A8	302	PEB	CHA-C4A-NA	2.13	127.73	125.20
26	kE	201	PEB	CHA-C4A-NA	2.13	127.73	125.20
26	cI	202	PEB	C3B-C4B-NB	2.13	113.14	110.05
26	Q9	201	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
26	24	405	PEB	CHC-C4C-C3C	-2.13	126.71	130.34
26	Z8	201	PEB	C1B-C2B-C3B	-2.13	104.07	106.51
26	kF	202	PEB	C1B-C2B-C3B	-2.13	104.07	106.51
26	JG	201	PEB	CBC-CAC-C2C	-2.13	108.99	112.62
26	U3	202	PEB	CHA-C1B-NB	-2.13	120.48	124.93
26	k2	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
26	V8	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
26	G4	201	PEB	CHA-C1B-C2B	2.13	130.37	124.90
26	P6	201	PEB	C4B-NB-C1B	-2.13	102.50	106.51
26	M9	201	PEB	C2A-C1A-NA	2.13	110.11	108.27
26	S8	203	PEB	CMA-C2A-C1A	-2.13	107.82	112.40
26	w1	201	PEB	CAA-C3A-C4A	-2.13	107.21	112.67
26	j7	203	PEB	CAB-C3B-C4B	2.13	128.77	125.01
26	QG	201	PEB	OD-C4D-C3D	-2.13	124.64	129.46
26	P3	202	PEB	CAC-CBC-CGC	-2.13	107.80	113.76
26	WE	201	PEB	CAC-CBC-CGC	-2.13	107.80	113.76
26	cA	201	PEB	C1B-C2B-C3B	-2.13	104.07	106.51
28	1H	1000	CYC	CHB-C1B-C2B	-2.13	122.74	126.95
26	WJ	201	PEB	OD-C4D-C3D	-2.13	124.64	129.46
26	I5	203	PEB	OA-C1A-NA	2.13	127.52	124.94
26	gG	201	PEB	CHA-C4A-NA	2.13	127.73	125.20
26	sG	202	PEB	CHA-C4A-NA	2.13	127.73	125.20
28	nH	1001	CYC	C2C-C1C-NC	2.13	110.11	108.27
26	UE	201	PEB	O2C-CGC-CBC	2.12	120.86	114.03
26	h4	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	H1	202	PEB	CHA-C1B-NB	-2.12	120.49	124.93
26	V1	201	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	O4	202	PEB	CAB-C3B-C4B	2.12	128.77	125.01
26	vE	201	PEB	CAA-C3A-C2A	-2.12	108.95	114.26
26	C5	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	g6	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	SB	201	PEB	CHB-C4B-C3B	-2.12	120.41	125.32
26	b7	201	PEB	CMD-C2D-C3D	2.12	133.06	130.06
26	U1	201	PEB	CHA-C4A-NA	2.12	127.73	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	u1	201	PEB	C2B-C1B-NB	2.12	115.06	110.53
26	GG	202	PEB	CHA-C1B-NB	-2.12	120.49	124.93
26	X9	201	PEB	C2B-C1B-NB	2.12	115.06	110.53
26	N9	204	PEB	CAB-CBB-CGB	-2.12	109.03	113.60
28	YH	1002	CYC	CAA-C2A-C1A	2.12	128.76	125.01
28	yH	1001	CYC	CHB-C1B-C2B	-2.12	122.74	126.95
26	O7	201	PEB	C2B-C1B-NB	2.12	115.06	110.53
28	IF	1001	CYC	CHB-C1B-NB	-2.12	121.50	126.06
26	F4	201	PEB	CMC-C3C-C2C	2.12	128.94	124.94
26	FJ	201	PEB	CHA-C4A-NA	2.12	127.73	125.20
26	BC	203	PEB	CAB-C3B-C4B	2.12	128.76	125.01
26	vG	202	PEB	OD-C4D-C3D	-2.12	124.65	129.46
26	BE	201	PEB	O2B-CGB-CBB	2.12	120.85	114.03
26	KA	202	PEB	OD-C4D-ND	-2.12	122.79	125.93
26	WA	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
26	OE	203	PEB	C2B-C1B-NB	2.12	115.06	110.53
26	iI	201	PEB	CHA-C1B-NB	-2.12	120.50	124.93
26	VD	202	PEB	OA-C1A-NA	2.12	127.51	124.94
26	g1	202	PEB	O2C-CGC-CBC	2.12	120.84	114.03
26	l4	202	PEB	CHB-C4B-C3B	-2.12	120.42	125.32
26	S9	202	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	21	405	PEB	CMA-C2A-C1A	-2.12	107.83	112.40
26	H9	202	PEB	CMA-C2A-C1A	-2.12	107.83	112.40
28	J7	1003	CYC	CHA-C1A-C2A	-2.12	120.42	125.32
26	ZB	202	PEB	CBB-CAB-C3B	-2.12	106.73	112.63
26	Y8	202	PEB	CMA-C2A-C1A	-2.12	107.83	112.40
26	C8	201	PEB	C2A-C1A-NA	2.12	110.10	108.27
26	JG	202	PEB	C4B-NB-C1B	-2.12	102.52	106.51
26	TD	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
26	VA	201	PEB	CHA-C4A-NA	2.12	127.73	125.20
26	IJ	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
26	cB	201	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	i1	202	PEB	CMA-C2A-C1A	-2.12	107.83	112.40
26	YG	201	PEB	CAC-C2C-C3C	2.12	133.34	127.25
28	vH	1001	CYC	CHA-C1A-C2A	-2.12	120.42	125.32
26	JE	201	PEB	C1B-C2B-C3B	-2.12	104.07	106.51
26	PD	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	TI	203	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	KA	201	PEB	CHA-C4A-NA	2.12	127.72	125.20
26	X9	202	PEB	C3B-C4B-NB	2.12	113.13	110.05
28	IF	1001	CYC	CAB-C3B-C2B	2.12	131.15	127.53
26	j4	202	PEB	C2A-C1A-NA	2.12	110.10	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I7	1001	CYC	CMB-C2B-C1B	2.12	126.81	124.17
26	D3	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	KC	202	PEB	CAC-CBC-CGC	-2.12	107.82	113.76
26	D4	203	PEB	C1C-CHB-C4B	-2.12	126.28	128.81
26	a8	202	PEB	CMA-C2A-C1A	-2.12	107.84	112.40
27	AA	303	PUB	O2B-CGB-CBB	2.12	120.84	114.03
26	z1	201	PEB	CHB-C4B-NB	2.12	131.76	128.83
26	O4	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83
26	cA	201	PEB	CBC-CAC-C2C	-2.12	109.00	112.62
26	PD	201	PEB	C1B-C2B-C3B	-2.12	104.08	106.51
26	gG	203	PEB	CAB-C3B-C4B	2.12	128.75	125.01
26	QF	203	PEB	C1C-CHB-C4B	-2.12	126.28	128.81
26	eI	202	PEB	CAC-CBC-CGC	-2.12	107.82	113.76
26	E1	202	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	D4	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
26	LG	201	PEB	CHA-C1B-C2B	2.12	130.34	124.90
26	dI	201	PEB	C2A-C1A-NA	2.12	110.10	108.27
26	G5	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	O7	201	PEB	CAB-C3B-C4B	2.12	128.75	125.01
26	mE	202	PEB	CAA-C3A-C2A	-2.12	108.97	114.26
26	iG	203	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
26	Z7	202	PEB	CMD-C2D-C3D	2.12	133.05	130.06
26	TG	201	PEB	C1B-C2B-C3B	-2.12	104.08	106.51
26	OF	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	j4	202	PEB	CHB-C4B-NB	-2.12	125.89	128.83
26	HD	201	PEB	CAB-CBB-CGB	-2.12	109.05	113.60
26	aF	202	PEB	CAA-C3A-C4A	2.12	118.11	112.67
26	T6	201	PEB	CHA-C4A-NA	2.12	127.72	125.20
26	GG	202	PEB	CHA-C4A-NA	-2.12	122.69	125.20
26	g2	201	PEB	CHA-C1B-NB	-2.12	120.51	124.93
26	R8	201	PEB	CBC-CAC-C2C	-2.12	109.01	112.62
26	F3	201	PEB	CMA-C2A-C1A	-2.12	107.84	112.40
26	jA	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
26	T4	203	PEB	OD-C4D-C3D	-2.12	124.67	129.46
26	YJ	202	PEB	CHA-C4A-NA	-2.12	122.69	125.20
26	G9	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
26	NJ	204	PEB	CAB-C3B-C4B	2.12	128.75	125.01
28	I2	1001	CYC	CHA-C1A-C2A	-2.12	120.43	125.32
26	YJ	202	PEB	CHC-C1D-ND	-2.12	111.49	113.95
26	g1	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	nG	202	PEB	CBC-CAC-C2C	2.11	116.23	112.62
26	DJ	203	PEB	CHC-C4C-C3C	-2.11	126.73	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	YI	203	PEB	C1B-C2B-C3B	-2.11	104.08	106.51
26	CE	202	PEB	CAC-CBC-CGC	2.11	119.69	113.76
26	WF	201	PEB	C2B-C1B-NB	2.11	115.04	110.53
26	mI	203	PEB	CHA-C1B-NB	-2.11	120.51	124.93
26	t1	201	PEB	CHC-C4C-C3C	-2.11	126.73	130.34
26	R8	202	PEB	CAB-CBB-CGB	2.11	118.15	113.60
26	i7	202	PEB	OA-C1A-NA	2.11	127.50	124.94
26	XD	202	PEB	CAA-C3A-C2A	-2.11	108.98	114.26
26	EJ	201	PEB	CBC-CAC-C2C	2.11	116.23	112.62
26	tE	202	PEB	CHA-C1B-C2B	-2.11	119.47	124.90
26	S3	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
26	f4	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
26	T1	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
26	A9	301	PEB	OD-C4D-ND	-2.11	122.80	125.93
26	OG	203	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	C5	204	PEB	CAB-C3B-C4B	2.11	128.75	125.01
26	ID	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
28	HI	1001	CYC	CAD-CBD-CGD	-2.11	107.84	113.76
26	K8	201	PEB	C3B-C4B-NB	2.11	113.12	110.05
26	B4	203	PEB	CAB-C3B-C4B	2.11	128.75	125.01
26	W7	202	PEB	OD-C4D-C3D	-2.11	124.67	129.46
26	D1	202	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
26	R1	201	PEB	CBC-CAC-C2C	-2.11	109.02	112.62
26	IE	202	PEB	OD-C4D-C3D	-2.11	124.68	129.46
26	eB	201	PEB	CAB-C3B-C4B	2.11	128.74	125.01
26	24	401	PEB	CHC-C4C-C3C	-2.11	126.73	130.34
26	V6	201	PEB	C2B-C1B-NB	2.11	115.03	110.53
26	pG	202	PEB	CBC-CAC-C2C	-2.11	109.02	112.62
26	gB	201	PEB	CHB-C4B-C3B	-2.11	120.44	125.32
26	mI	201	PEB	CHB-C4B-C3B	-2.11	120.44	125.32
26	gE	203	PEB	C3B-C4B-NB	2.11	113.12	110.05
28	dH	1001	CYC	CHB-C4A-C3A	2.11	130.33	124.90
26	DI	1002	PEB	CHC-C1D-ND	-2.11	111.50	113.95
26	XD	202	PEB	CHA-C1B-NB	-2.11	120.52	124.93
26	kG	202	PEB	CHA-C1B-NB	-2.11	120.52	124.93
27	yE	302	PUB	CBB-CAB-C3B	-2.11	109.02	112.62
26	fA	203	PEB	CAB-C3B-C4B	2.11	128.74	125.01
26	G5	201	PEB	CAB-CBB-CGB	-2.11	109.06	113.60
26	wG	301	PEB	OD-C4D-C3D	-2.11	124.68	129.46
26	v4	202	PEB	CHC-C4C-C3C	-2.11	126.74	130.34
26	Y3	301	PEB	CBA-CAA-C3A	2.11	118.17	113.47
26	WB	203	PEB	C2B-C1B-NB	2.11	115.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BE	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
26	C8	201	PEB	CAA-C3A-C2A	-2.11	108.99	114.26
26	T4	201	PEB	OD-C4D-C3D	-2.11	124.68	129.46
26	K8	202	PEB	CMC-C3C-C2C	2.11	128.92	124.94
27	A7	304	PUB	C2C-C1C-NC	2.11	113.12	110.05
28	jH	1001	CYC	C2C-C3C-C4C	2.11	104.50	101.34
28	RH	1001	CYC	CBD-CAD-C3D	-2.11	109.02	112.62
28	mH	1001	CYC	CBD-CAD-C3D	-2.11	109.02	112.62
26	YJ	201	PEB	CBC-CAC-C2C	2.11	116.22	112.62
26	y4	201	PEB	CHC-C4C-C3C	-2.11	126.74	130.34
28	LB	1001	CYC	OB-C4B-NB	-2.11	120.18	125.08
26	H3	201	PEB	OD-C4D-C3D	-2.11	124.68	129.46
26	y4	202	PEB	OD-C4D-C3D	-2.11	124.68	129.46
26	EE	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
27	yG	302	PUB	CBB-CAB-C3B	-2.11	109.02	112.62
27	A7	303	PUB	CAC-C2C-C1C	2.11	128.74	125.01
26	RI	201	PEB	OD-C4D-C3D	-2.11	124.68	129.46
26	HG	201	PEB	C2B-C1B-NB	2.11	115.03	110.53
26	PI	201	PEB	CMA-C2A-C1A	-2.11	107.86	112.40
27	A7	303	PUB	C2C-C1C-NC	2.11	113.12	110.05
28	KF	1001	CYC	C3A-C4A-NA	2.11	115.03	110.53
26	iI	202	PEB	CHC-C1D-ND	-2.11	111.50	113.95
26	HJ	202	PEB	CMA-C2A-C1A	-2.11	107.86	112.40
26	aI	201	PEB	CAB-CBB-CGB	-2.11	109.07	113.60
26	vG	201	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
26	Y4	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
26	D6	1002	PEB	O1B-CGB-CBB	-2.11	116.31	123.08
26	eI	203	PEB	CBC-CAC-C2C	-2.11	109.02	112.62
26	DE	202	PEB	CMA-C2A-C1A	-2.11	107.86	112.40
26	M3	202	PEB	C1C-CHB-C4B	-2.11	126.29	128.81
26	XD	201	PEB	OD-C4D-C3D	-2.11	124.69	129.46
26	bG	201	PEB	OD-C4D-C3D	-2.11	124.69	129.46
26	HD	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
26	lB	203	PEB	CAB-C3B-C4B	2.11	128.74	125.01
26	14	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	UE	203	PEB	OD-C4D-C3D	-2.11	124.69	129.46
26	eB	202	PEB	CHC-C1D-ND	-2.11	111.50	113.95
28	B6	1001	CYC	CAA-C2A-C3A	2.11	131.80	127.88
26	V3	203	PEB	C3B-C4B-NB	2.11	113.11	110.05
26	wE	301	PEB	C2B-C1B-NB	2.11	115.02	110.53
26	EJ	202	PEB	OD-C4D-C3D	-2.11	124.69	129.46
26	qE	201	PEB	CHA-C4A-NA	2.11	127.71	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	IA	202	PEB	CAB-CBB-CGB	-2.11	109.07	113.60
26	IG	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	D4	201	PEB	C2B-C1B-NB	2.11	115.02	110.53
26	X1	201	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
26	Q6	202	PEB	CHA-C1B-C2B	2.11	130.31	124.90
26	kG	201	PEB	OA-C1A-C2A	-2.11	124.50	126.17
26	EA	203	PEB	CMD-C2D-C3D	2.11	133.03	130.06
26	Y2	203	PEB	CMB-C2B-C1B	2.11	128.31	125.06
28	sH	1001	CYC	C2C-C3C-C4C	2.11	104.49	101.34
26	B1	203	PEB	CAB-CBB-CGB	-2.11	109.07	113.60
26	IG	201	PEB	C1B-C2B-C3B	-2.10	104.09	106.51
26	RF	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
26	IA	201	PEB	C2B-C1B-NB	2.10	115.02	110.53
26	V3	202	PEB	OD-C4D-C3D	-2.10	124.69	129.46
26	h2	201	PEB	CHB-C4B-NB	-2.10	125.91	128.83
26	EJ	202	PEB	CHC-C4C-C3C	-2.10	126.75	130.34
26	u1	201	PEB	C4B-NB-C1B	-2.10	102.55	106.51
26	fB	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
26	f1	201	PEB	OD-C4D-C3D	-2.10	124.69	129.46
26	TA	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
28	C2	1001	CYC	CHB-C1B-NB	-2.10	121.54	126.06
26	H1	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
26	K4	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
26	u4	203	PEB	CAB-C3B-C4B	2.10	128.73	125.01
26	T4	202	PEB	C1C-CHB-C4B	2.10	131.32	128.81
26	NJ	204	PEB	OD-C4D-ND	-2.10	122.81	125.93
28	LI	1001	CYC	CAB-C3B-C2B	2.10	131.13	127.53
28	H6	1001	CYC	CAD-CBD-CGD	-2.10	107.86	113.76
27	wE	304	PUB	CMD-C2D-C3D	2.10	130.92	127.77
26	r1	201	PEB	CAC-C2C-C3C	2.10	133.29	127.25
26	d6	202	PEB	CBC-CAC-C2C	-2.10	109.03	112.62
26	gA	201	PEB	CBC-CAC-C2C	-2.10	109.03	112.62
28	E6	1001	CYC	CBD-CAD-C3D	-2.10	109.03	112.62
26	UF	202	PEB	CHA-C1B-NB	-2.10	120.53	124.93
28	E6	1001	CYC	CHA-C1A-C2A	-2.10	120.46	125.32
28	GI	1001	CYC	CMB-C2B-C1B	2.10	126.79	124.17
26	N1	201	PEB	CBA-CAA-C3A	-2.10	108.78	113.47
26	RA	202	PEB	OA-C1A-C2A	-2.10	124.50	126.17
26	k1	203	PEB	C2B-C1B-NB	2.10	115.02	110.53
26	q1	201	PEB	OD-C4D-C3D	-2.10	124.70	129.46
26	KA	202	PEB	C2A-C3A-C4A	2.10	104.49	101.34
27	xE	306	PUB	O2B-CGB-CBB	2.10	120.78	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	ME	201	PEB	CHB-C4B-C3B	-2.10	120.46	125.32
26	nG	201	PEB	CHC-C1D-ND	-2.10	111.51	113.95
26	i2	201	PEB	C1C-CHB-C4B	2.10	131.32	128.81
26	W4	202	PEB	CHA-C1B-NB	-2.10	120.54	124.93
26	iB	202	PEB	CMA-C2A-C1A	-2.10	107.87	112.40
26	m6	203	PEB	C1B-C2B-C3B	-2.10	104.09	106.51
26	a2	202	PEB	CHA-C1B-C2B	2.10	130.30	124.90
26	y1	201	PEB	O1B-CGB-CBB	-2.10	116.33	123.08
26	DG	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	hI	201	PEB	CAB-CBB-CGB	-2.10	109.08	113.60
28	DI	1001	CYC	CHA-C1A-C2A	-2.10	120.47	125.32
26	I5	201	PEB	CBB-CAB-C3B	-2.10	106.79	112.63
26	HJ	202	PEB	CAB-CBB-CGB	-2.10	109.08	113.60
26	PI	203	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
26	m4	201	PEB	CBA-CAA-C3A	-2.10	108.79	113.47
26	AE	201	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
26	kB	202	PEB	CBC-CAC-C2C	2.10	116.20	112.62
26	PA	201	PEB	CHA-C4A-NA	2.10	127.70	125.20
26	VJ	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	lA	202	PEB	CAB-CBB-CGB	-2.10	109.08	113.60
26	Q9	202	PEB	CHC-C4C-C3C	-2.10	126.75	130.34
26	TI	201	PEB	CAC-CBC-CGC	-2.10	107.87	113.76
28	LB	1001	CYC	CHB-C1B-NB	-2.10	121.55	126.06
26	N4	201	PEB	C2B-C1B-NB	2.10	115.01	110.53
28	cH	1001	CYC	C2C-C3C-C4C	2.10	104.48	101.34
26	A3	201	PEB	CHC-C1D-ND	-2.10	111.51	113.95
26	SJ	202	PEB	CHC-C1D-ND	-2.10	111.51	113.95
26	V8	202	PEB	CAB-CBB-CGB	2.10	118.12	113.60
26	c8	202	PEB	O2B-CGB-CBB	2.10	120.78	114.03
26	F1	201	PEB	OD-C4D-C3D	-2.10	124.70	129.46
26	a2	202	PEB	CMA-C2A-C1A	-2.10	107.88	112.40
26	c1	202	PEB	CAC-C2C-C3C	2.10	133.28	127.25
26	L4	202	PEB	CAB-C3B-C4B	2.10	128.72	125.01
26	iF	201	PEB	C4B-NB-C1B	-2.10	102.56	106.51
26	h4	201	PEB	C2B-C1B-NB	2.10	115.01	110.53
26	fB	202	PEB	C2A-C3A-C4A	-2.10	98.20	101.34
26	B5	203	PEB	CAB-C3B-C4B	2.10	128.72	125.01
26	e6	203	PEB	CAB-C3B-C4B	2.10	128.72	125.01
26	l8	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
26	VI	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
26	JA	202	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
26	GA	203	PEB	CBA-CAA-C3A	-2.10	108.80	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	xG	304	PEB	CHC-C1D-ND	-2.10	111.51	113.95
27	xE	301	PUB	C4B-CHB-C1C	2.10	131.31	128.81
26	AJ	301	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
26	wE	303	PEB	CHA-C4A-NA	2.10	127.70	125.20
26	LC	201	PEB	CBB-CAB-C3B	-2.10	106.80	112.63
26	i8	201	PEB	CAB-CBB-CGB	-2.10	109.09	113.60
26	XD	201	PEB	CAB-CBB-CGB	-2.10	109.09	113.60
27	K4	203	PUB	CAC-CBC-CGC	-2.10	109.09	113.60
26	j1	201	PEB	C4B-NB-C1B	-2.10	102.56	106.51
26	OA	203	PEB	C2B-C1B-NB	2.10	115.00	110.53
26	j7	202	PEB	CMA-C2A-C1A	-2.10	107.88	112.40
26	LB	1002	PEB	CAA-C3A-C4A	-2.10	107.29	112.67
26	H2	1002	PEB	CAB-CBB-CGB	-2.10	109.09	113.60
28	F7	1001	CYC	CBD-CAD-C3D	-2.10	109.04	112.62
26	l2	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
26	Y1	201	PEB	CMA-C2A-C1A	-2.10	107.88	112.40
26	hF	201	PEB	OD-C4D-C3D	-2.10	124.71	129.46
26	p4	202	PEB	C1B-C2B-C3B	-2.10	104.10	106.51
26	iE	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
26	UF	203	PEB	CHA-C4A-NA	-2.10	122.71	125.20
26	jA	202	PEB	CHC-C4C-C3C	-2.10	126.76	130.34
26	GC	203	PEB	CHC-C4C-C3C	-2.10	126.76	130.34
26	S6	201	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
26	oG	201	PEB	C2B-C1B-NB	2.10	115.00	110.53
28	1H	1000	CYC	CBD-CAD-C3D	-2.10	109.04	112.62
26	OD	202	PEB	CBB-CAB-C3B	-2.10	106.81	112.63
26	s1	202	PEB	CAB-C3B-C4B	2.10	128.72	125.01
27	Q8	201	PUB	O2B-CGB-CBB	2.10	120.76	114.03
26	e6	203	PEB	C3B-C4B-NB	2.10	113.10	110.05
26	JC	201	PEB	C1C-CHB-C4B	-2.10	126.31	128.81
28	TH	1001	CYC	CHA-C1A-C2A	-2.10	120.48	125.32
26	jF	203	PEB	CMC-C3C-C2C	2.10	128.89	124.94
26	ZF	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
28	TH	1001	CYC	CAA-C2A-C1A	2.09	128.71	125.01
26	L1	201	PEB	OD-C4D-ND	-2.09	122.83	125.93
26	sG	201	PEB	OD-C4D-ND	-2.09	122.83	125.93
26	BD	203	PEB	OD-C4D-C3D	-2.09	124.72	129.46
26	iE	202	PEB	CHA-C1B-NB	-2.09	120.55	124.93
26	O7	203	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	X3	202	PEB	OA-C1A-NA	2.09	127.48	124.94
26	p4	201	PEB	OA-C1A-NA	2.09	127.48	124.94
26	NA	202	PEB	OA-C1A-NA	2.09	127.48	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T9	201	PEB	C3B-C4B-NB	2.09	113.09	110.05
28	gH	1001	CYC	C2A-C1A-NA	2.09	113.09	110.05
26	g7	201	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
26	HA	202	PEB	O1B-CGB-CBB	-2.09	116.35	123.08
28	pH	1001	CYC	CBD-CAD-C3D	-2.09	109.05	112.62
26	GD	202	PEB	C2B-C1B-NB	2.09	115.00	110.53
26	lB	203	PEB	CHC-C1D-ND	-2.09	111.52	113.95
28	HB	1001	CYC	CAD-CBD-CGD	-2.09	107.89	113.76
26	DE	203	PEB	C4B-NB-C1B	-2.09	102.57	106.51
26	V4	201	PEB	CMA-C2A-C1A	-2.09	107.89	112.40
26	O4	201	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
26	eB	203	PEB	CMC-C3C-C2C	2.09	128.89	124.94
26	OF	203	PEB	C2B-C1B-NB	2.09	115.00	110.53
26	S2	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
26	eB	201	PEB	CBC-CAC-C2C	-2.09	109.05	112.62
26	14	203	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	JD	201	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
26	AD	201	PEB	C3B-C4B-NB	2.09	113.09	110.05
26	B5	203	PEB	CBB-CAB-C3B	-2.09	106.81	112.63
26	p1	202	PEB	CHC-C4C-C3C	-2.09	126.77	130.34
26	eI	202	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
26	k2	203	PEB	C2A-C1A-NA	2.09	110.08	108.27
28	rH	1001	CYC	C2C-C1C-NC	2.09	110.08	108.27
26	G1	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
26	Q2	202	PEB	CBC-CAC-C2C	-2.09	109.05	112.62
26	QE	201	PEB	OD-C4D-C3D	-2.09	124.72	129.46
26	HE	202	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	SE	203	PEB	CAB-C3B-C4B	2.09	128.71	125.01
26	i2	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
26	eA	202	PEB	CAB-CBB-CGB	2.09	118.10	113.60
26	F2	1002	PEB	CHB-C4B-C3B	-2.09	120.49	125.32
26	g2	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
26	sG	203	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	TJ	202	PEB	C1C-CHB-C4B	2.09	131.31	128.81
26	PB	201	PEB	C4B-NB-C1B	-2.09	102.57	106.51
26	hB	203	PEB	OD-C4D-C3D	-2.09	124.72	129.46
28	PH	1001	CYC	CAB-C3B-C2B	2.09	131.10	127.53
26	HC	203	PEB	CBB-CAB-C3B	-2.09	106.82	112.63
26	O6	203	PEB	C2B-C1B-NB	2.09	114.99	110.53
26	V3	201	PEB	O2C-CGC-CBC	2.09	120.74	114.03
26	C5	204	PEB	CHA-C1B-NB	-2.09	120.56	124.93
26	H9	201	PEB	CAA-C3A-C4A	-2.09	107.31	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	iF	201	PEB	CBC-CAC-C2C	2.09	116.19	112.62
26	SE	201	PEB	O1C-CGC-CBC	-2.09	116.37	123.08
28	D6	1001	CYC	C3A-C4A-NA	2.09	114.99	110.53
26	fA	201	PEB	C1C-CHB-C4B	-2.09	126.31	128.81
26	H5	202	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	O9	201	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	cB	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
26	mE	203	PEB	C2A-C1A-NA	2.09	110.07	108.27
26	W1	201	PEB	C4B-NB-C1B	-2.09	102.57	106.51
27	wG	304	PUB	CBB-CAB-C3B	-2.09	109.06	112.62
26	SA	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	lA	203	PEB	OD-C4D-ND	-2.09	122.84	125.93
26	e2	203	PEB	CBC-CAC-C2C	-2.09	109.06	112.62
26	YE	202	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	f8	203	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	e8	201	PEB	CHA-C4A-NA	2.09	127.69	125.20
26	AD	201	PEB	CAB-C3B-C2B	-2.09	123.99	127.88
26	f8	203	PEB	CAB-C3B-C4B	2.09	128.70	125.01
26	cE	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
26	WG	201	PEB	CAB-C3B-C4B	2.09	128.70	125.01
27	21	402	PUB	CAC-C2C-C1C	2.09	128.70	125.01
28	PH	1001	CYC	C2C-C1C-NC	2.09	110.07	108.27
26	j7	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	S7	202	PEB	CHC-C4C-C3C	-2.09	126.78	130.34
26	h6	203	PEB	C2B-C1B-NB	2.09	114.98	110.53
26	A9	303	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	DD	203	PEB	CAC-CBC-CGC	-2.09	107.91	113.76
26	QF	201	PEB	C2B-C1B-NB	2.09	114.98	110.53
26	fA	202	PEB	C3B-C4B-NB	2.09	113.08	110.05
26	S6	201	PEB	CHB-C4B-C3B	-2.09	120.50	125.32
26	m2	203	PEB	CHA-C1B-NB	-2.09	120.57	124.93
26	s1	202	PEB	CBB-CAB-C3B	-2.09	106.83	112.63
28	H6	1001	CYC	CBB-CAB-C3B	-2.09	106.68	112.43
26	FD	202	PEB	CBC-CAC-C2C	2.09	116.18	112.62
26	mI	202	PEB	CMA-C2A-C1A	-2.09	107.91	112.40
26	A4	201	PEB	C2B-C1B-NB	2.09	114.98	110.53
26	fG	202	PEB	C2B-C1B-NB	2.09	114.98	110.53
26	G1	201	PEB	CHB-C4B-NB	-2.09	125.93	128.83
26	LE	201	PEB	CAA-C3A-C2A	-2.09	109.05	114.26
28	JI	1001	CYC	O2A-CGA-CBA	2.09	120.73	114.03
28	LI	1001	CYC	CAD-CBD-CGD	-2.09	107.91	113.76
26	fF	202	PEB	OD-C4D-C3D	-2.09	124.73	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g1	202	PEB	C2B-C1B-NB	2.09	114.98	110.53
26	aG	203	PEB	OD-C4D-ND	-2.09	122.84	125.93
26	VD	203	PEB	CHA-C4A-NA	-2.09	122.72	125.20
26	I4	201	PEB	CHB-C4B-C3B	-2.09	120.50	125.32
28	YH	1003	CYC	C2C-C3C-C4C	2.09	104.46	101.34
26	V7	202	PEB	CAC-CBC-CGC	-2.09	107.91	113.76
26	L5	201	PEB	CMA-C2A-C1A	-2.09	107.91	112.40
26	KE	201	PEB	CAB-C3B-C4B	2.09	128.70	125.01
26	HF	1002	PEB	CAC-CBC-CGC	-2.09	107.91	113.76
26	k8	202	PEB	CHA-C4A-NA	-2.08	122.73	125.20
26	v1	201	PEB	CBA-CAA-C3A	-2.08	108.83	113.47
26	T2	201	PEB	CAC-CBC-CGC	-2.08	107.91	113.76
26	bF	201	PEB	CAB-C3B-C4B	2.08	128.70	125.01
26	VA	202	PEB	O1B-CGB-CBB	-2.08	116.39	123.08
26	V8	201	PEB	CHA-C4A-NA	2.08	127.68	125.20
26	hA	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
26	WE	203	PEB	CHC-C1D-ND	-2.08	111.53	113.95
26	I9	201	PEB	OD-C4D-C3D	-2.08	124.74	129.46
26	KA	202	PEB	CMC-C3C-C2C	2.08	128.87	124.94
26	iI	203	PEB	CAB-C3B-C2B	2.08	131.76	127.88
26	z4	202	PEB	CBC-CAC-C2C	-2.08	109.06	112.62
26	CE	203	PEB	OD-C4D-C3D	-2.08	124.74	129.46
26	aF	201	PEB	OD-C4D-C3D	-2.08	124.74	129.46
26	P4	202	PEB	CMA-C2A-C1A	-2.08	107.91	112.40
26	TD	203	PEB	O1B-CGB-CBB	-2.08	116.39	123.08
26	mA	201	PEB	CHA-C4A-NA	2.08	127.68	125.20
26	G8	201	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
26	g8	201	PEB	CBC-CAC-C2C	-2.08	109.06	112.62
26	VJ	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
28	N7	1001	CYC	CHA-C1A-C2A	-2.08	120.51	125.32
26	RD	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
26	DE	201	PEB	OD-C4D-C3D	-2.08	124.74	129.46
26	S9	202	PEB	OD-C4D-ND	-2.08	122.84	125.93
26	ZB	201	PEB	C2B-C1B-NB	2.08	114.97	110.53
26	QF	202	PEB	CHC-C1D-ND	-2.08	111.53	113.95
26	iF	202	PEB	CHC-C4C-C3C	-2.08	126.78	130.34
26	hE	201	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
26	KG	202	PEB	CBB-CAB-C3B	-2.08	106.84	112.63
26	DG	202	PEB	C2B-C1B-NB	2.08	114.97	110.53
26	B3	203	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
26	m1	203	PEB	CHA-C1B-NB	-2.08	120.58	124.93
26	U4	201	PEB	C1B-C2B-C3B	-2.08	104.12	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	ZF	203	PEB	OD-C4D-C3D	-2.08	124.75	129.46
26	C8	201	PEB	CBA-CAA-C3A	-2.08	108.83	113.47
26	KE	201	PEB	CBA-CAA-C3A	2.08	118.10	113.47
26	H3	203	PEB	CAC-CBC-CGC	-2.08	107.92	113.76
26	S8	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	aF	201	PEB	CHA-C1B-NB	-2.08	120.58	124.93
26	O8	203	PEB	CHB-C4B-C3B	-2.08	120.51	125.32
26	iF	202	PEB	CAC-CBC-CGC	-2.08	107.92	113.76
26	N4	202	PEB	OD-C4D-C3D	-2.08	124.75	129.46
26	f1	201	PEB	CHA-C1B-C2B	2.08	130.25	124.90
26	L6	1002	PEB	CAA-C3A-C4A	-2.08	107.33	112.67
26	DE	203	PEB	CAB-C3B-C4B	2.08	128.69	125.01
26	UE	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
26	tG	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
26	g2	202	PEB	CMD-C2D-C3D	2.08	133.00	130.06
26	S4	202	PEB	CAC-CBC-CGC	-2.08	107.93	113.76
26	U6	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
26	G4	201	PEB	OD-C4D-C3D	-2.08	124.75	129.46
26	fA	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
26	qG	203	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
26	MA	201	PEB	CBA-CAA-C3A	-2.08	108.84	113.47
26	CA	201	PEB	O2C-CGC-CBC	2.08	120.71	114.03
26	f7	203	PEB	C3B-C4B-NB	2.08	113.07	110.05
26	eG	201	PEB	CAC-CBC-CGC	-2.08	107.93	113.76
26	n1	201	PEB	CHA-C1B-NB	-2.08	120.58	124.93
26	rE	202	PEB	C2B-C1B-NB	2.08	114.97	110.53
26	cE	201	PEB	CMB-C2B-C3B	-2.08	120.47	126.12
26	21	401	PEB	CMD-C2D-C3D	2.08	133.00	130.06
26	jF	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
26	ZA	201	PEB	C1B-C2B-C3B	-2.08	104.12	106.51
26	CA	201	PEB	CAA-C3A-C2A	-2.08	109.06	114.26
26	NG	202	PEB	C2A-C1A-NA	2.08	110.06	108.27
26	b7	201	PEB	OD-C4D-ND	-2.08	122.85	125.93
26	21	401	PEB	CAA-C3A-C2A	-2.08	109.07	114.26
26	A4	201	PEB	CHA-C4A-NA	2.08	127.68	125.20
26	Z6	201	PEB	C2B-C1B-NB	2.08	114.96	110.53
26	IE	202	PEB	CHC-C1D-ND	-2.08	111.53	113.95
26	RF	201	PEB	C4B-NB-C1B	-2.08	102.59	106.51
26	W9	201	PEB	OD-C4D-C3D	-2.08	124.75	129.46
26	w1	202	PEB	CBA-CAA-C3A	-2.08	108.84	113.47
26	FE	201	PEB	C1C-CHB-C4B	2.08	131.29	128.81
26	GG	203	PEB	CAA-C3A-C2A	-2.08	109.07	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j7	203	PEB	C3B-C4B-NB	2.08	113.07	110.05
26	S9	202	PEB	CHA-C4A-NA	-2.08	122.73	125.20
26	P3	201	PEB	CBA-CAA-C3A	2.08	118.09	113.47
26	JC	202	PEB	C1C-CHB-C4B	-2.08	126.33	128.81
26	PD	201	PEB	C1C-CHB-C4B	2.08	131.29	128.81
26	XD	202	PEB	CAB-C3B-C4B	2.08	128.68	125.01
26	gE	201	PEB	CAC-CBC-CGC	2.08	119.58	113.76
26	HJ	201	PEB	O2B-CGB-CBB	2.08	120.70	114.03
26	CA	201	PEB	CHC-C1D-ND	-2.08	111.54	113.95
26	F8	201	PEB	CAB-CBB-CGB	-2.08	109.14	113.60
26	iI	201	PEB	CHB-C4B-C3B	-2.08	120.52	125.32
26	xG	302	PEB	OD-C4D-C3D	-2.08	124.76	129.46
26	fE	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
26	SE	202	PEB	CMA-C2A-C1A	2.08	116.88	112.40
26	z4	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	KD	202	PEB	CAA-C3A-C4A	-2.08	107.34	112.67
26	G1	201	PEB	C1C-CHB-C4B	2.08	131.29	128.81
28	NF	1001	CYC	CHA-C1A-NA	-2.08	125.95	128.83
26	RG	201	PEB	CMA-C2A-C1A	-2.08	107.93	112.40
26	F1	203	PEB	CBC-CAC-C2C	-2.07	109.08	112.62
26	Q6	201	PEB	C2B-C1B-NB	2.07	114.96	110.53
28	IH	1001	CYC	CHB-C1B-C2B	-2.07	122.84	126.95
26	KA	203	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
26	LB	1002	PEB	CAB-C3B-C2B	2.07	131.74	127.88
26	sG	203	PEB	CMA-C2A-C1A	-2.07	107.93	112.40
26	DB	1002	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
26	SA	202	PEB	C2B-C1B-NB	2.07	114.96	110.53
26	I5	201	PEB	CHA-C1B-C2B	2.07	130.23	124.90
26	A6	304	PEB	CMA-C2A-C1A	-2.07	107.93	112.40
26	fA	201	PEB	CHA-C1B-NB	-2.07	120.59	124.93
26	m4	202	PEB	CAB-C3B-C4B	2.07	128.68	125.01
26	M1	403	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
26	XA	202	PEB	CHA-C1B-C2B	2.07	130.23	124.90
28	G6	1001	CYC	CHB-C1B-NB	-2.07	121.61	126.06
26	MA	203	PEB	C1C-CHB-C4B	2.07	131.29	128.81
26	YB	202	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
26	II	201	PEB	CAB-C3B-C4B	2.07	128.68	125.01
26	FD	201	PEB	CHA-C4A-NA	2.07	127.67	125.20
26	UA	201	PEB	CAB-C3B-C2B	2.07	131.74	127.88
26	ZF	202	PEB	C2B-C1B-NB	2.07	114.95	110.53
26	dA	201	PEB	C2A-C1A-NA	2.07	110.06	108.27
26	i2	201	PEB	CHB-C4B-C3B	-2.07	120.53	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U8	202	PEB	OA-C1A-C2A	-2.07	124.53	126.17
26	RJ	201	PEB	C3B-C4B-NB	2.07	113.06	110.05
26	wG	301	PEB	CBC-CAC-C2C	-2.07	109.08	112.62
26	ZE	202	PEB	C2B-C1B-NB	2.07	114.95	110.53
26	P8	202	PEB	OD-C4D-ND	-2.07	122.86	125.93
26	KJ	201	PEB	CHA-C1B-NB	-2.07	120.60	124.93
26	uE	202	PEB	C2A-C1A-NA	2.07	110.06	108.27
26	R7	201	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
26	O3	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	kI	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	OE	202	PEB	C1C-CHB-C4B	2.07	131.28	128.81
28	NH	1001	CYC	C2C-C3C-C4C	2.07	104.44	101.34
28	CI	1001	CYC	CHB-C1B-NB	-2.07	121.61	126.06
26	qG	202	PEB	CBC-CAC-C2C	-2.07	109.09	112.62
28	WH	1001	CYC	CHB-C1B-C2B	-2.07	122.84	126.95
26	QE	201	PEB	CMB-C2B-C3B	-2.07	120.50	126.12
26	CA	201	PEB	CBB-CAB-C3B	-2.07	106.87	112.63
27	A2	302	PUB	CBA-CAA-C3A	-2.07	109.84	112.98
28	wH	1001	CYC	C2C-C1C-NC	2.07	110.06	108.27
26	a8	201	PEB	C2B-C1B-NB	2.07	114.95	110.53
26	d6	204	PEB	CAA-C3A-C4A	-2.07	107.36	112.67
26	V2	201	PEB	CHB-C4B-NB	-2.07	125.95	128.83
26	GA	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	jB	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	RI	201	PEB	CMA-C2A-C1A	-2.07	107.94	112.40
26	uG	201	PEB	C3B-C4B-NB	2.07	113.06	110.05
26	iG	202	PEB	C2B-C1B-NB	2.07	114.95	110.53
26	U8	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	21	401	PEB	CHC-C4C-C3C	-2.07	126.81	130.34
26	F7	1002	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
26	nE	202	PEB	CHA-C1B-NB	-2.07	120.61	124.93
26	P3	203	PEB	CAC-CBC-CGC	-2.07	107.96	113.76
26	cF	202	PEB	CHA-C4A-NA	2.07	127.67	125.20
26	AC	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	CA	203	PEB	C2B-C1B-NB	2.07	114.94	110.53
26	EJ	201	PEB	CBD-CAD-C3D	-2.07	117.33	127.62
26	jF	201	PEB	C2B-C1B-NB	2.07	114.94	110.53
26	gE	203	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	pE	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
26	m7	202	PEB	C4B-C3B-C2B	-2.07	104.49	106.78
26	G5	201	PEB	CHA-C1B-NB	-2.07	120.61	124.93
26	dG	201	PEB	CBC-CAC-C2C	-2.07	109.09	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	YH	1004	CYC	CBD-CAD-C3D	-2.07	109.09	112.62
26	XJ	202	PEB	C3B-C4B-NB	2.07	113.06	110.05
26	oE	203	PEB	OD-C4D-ND	-2.07	122.87	125.93
28	vH	1001	CYC	CHB-C1B-C2B	-2.07	122.85	126.95
26	X1	203	PEB	OA-C1A-C2A	-2.07	124.53	126.17
26	I3	202	PEB	C2B-C1B-NB	2.07	114.94	110.53
26	K8	203	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
26	aG	203	PEB	CHA-C4A-NA	2.07	127.66	125.20
26	oG	201	PEB	CMA-C2A-C1A	-2.07	107.95	112.40
26	u4	202	PEB	C2B-C1B-NB	2.07	114.94	110.53
26	A4	202	PEB	CHC-C1D-ND	-2.07	111.55	113.95
26	jE	201	PEB	CAA-C3A-C2A	-2.07	109.09	114.26
26	D9	202	PEB	OD-C4D-C3D	-2.07	124.78	129.46
26	D3	201	PEB	CAA-C3A-C4A	-2.07	107.37	112.67
26	YI	201	PEB	CAB-C3B-C4B	2.07	128.66	125.01
28	KF	1001	CYC	CHD-C4C-NC	2.07	127.66	125.20
26	eG	202	PEB	CHA-C4A-NA	-2.07	122.75	125.20
26	l4	202	PEB	C3B-C4B-NB	2.07	113.06	110.05
26	N1	202	PEB	OD-C4D-C3D	-2.07	124.78	129.46
26	FA	202	PEB	CMA-C2A-C1A	-2.07	107.95	112.40
26	GE	203	PEB	O1C-CGC-CBC	-2.07	116.44	123.08
26	RD	203	PEB	CAB-C3B-C2B	2.07	131.73	127.88
26	gE	201	PEB	OD-C4D-C3D	-2.07	124.78	129.46
26	DG	201	PEB	OD-C4D-C3D	-2.07	124.78	129.46
26	T7	202	PEB	C1B-C2B-C3B	-2.07	104.14	106.51
26	W3	202	PEB	OD-C4D-C3D	-2.07	124.78	129.46
26	RD	203	PEB	OD-C4D-ND	-2.07	122.87	125.93
26	l7	203	PEB	CHC-C1D-ND	-2.07	111.55	113.95
26	II	201	PEB	CHC-C1D-ND	-2.07	111.55	113.95
28	CH	1001	CYC	C2C-C3C-C4C	2.07	104.43	101.34
28	iH	1001	CYC	C2C-C3C-C4C	2.07	104.43	101.34
26	ME	203	PEB	CBD-CAD-C3D	-2.06	117.35	127.62
26	U8	202	PEB	O2C-CGC-CBC	2.06	120.66	114.03
26	N2	1002	PEB	CHA-C1B-NB	-2.06	120.61	124.93
26	Y6	201	PEB	C2B-C1B-NB	2.06	114.94	110.53
26	HE	201	PEB	CAB-CBB-CGB	-2.06	109.16	113.60
28	H2	1001	CYC	C1B-CHB-C4A	-2.06	123.04	128.08
26	JF	1002	PEB	CAA-C3A-C4A	-2.06	107.37	112.67
26	J1	202	PEB	CHA-C1B-NB	-2.06	120.61	124.93
26	q1	203	PEB	CAB-C3B-C4B	2.06	128.66	125.01
26	j8	203	PEB	CAB-C3B-C4B	2.06	128.66	125.01
26	AB	301	PEB	CAB-C3B-C4B	2.06	128.66	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	gA	202	PEB	O2B-CGB-CBB	2.06	120.66	114.03
26	UE	201	PEB	C2A-C3A-C4A	-2.06	98.25	101.34
26	ID	201	PEB	OD-C4D-ND	-2.06	122.87	125.93
26	11	201	PEB	CHA-C1B-NB	-2.06	120.62	124.93
26	TB	202	PEB	CAC-C2C-C3C	2.06	133.18	127.25
26	g2	203	PEB	C1B-C2B-C3B	-2.06	104.14	106.51
26	W4	202	PEB	C1B-C2B-C3B	-2.06	104.14	106.51
26	kA	201	PEB	CHA-C4A-NA	2.06	127.66	125.20
26	l8	203	PEB	OD-C4D-ND	-2.06	122.87	125.93
28	LF	1001	CYC	O1D-CGD-CBD	-2.06	116.45	123.08
26	J4	203	PEB	CAC-CBC-CGC	-2.06	107.98	113.76
26	KJ	201	PEB	CAB-C3B-C4B	2.06	128.66	125.01
26	ID	202	PEB	C2A-C1A-NA	2.06	110.05	108.27
26	hG	201	PEB	C2A-C1A-NA	2.06	110.05	108.27
26	LJ	203	PEB	C2B-C1B-NB	2.06	114.93	110.53
26	x1	202	PEB	CHA-C4A-NA	-2.06	122.75	125.20
26	SA	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
26	g1	203	PEB	CHA-C1B-C2B	2.06	130.20	124.90
26	d8	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
26	LB	1002	PEB	CHA-C1B-NB	-2.06	120.62	124.93
26	R9	202	PEB	CBC-CAC-C2C	-2.06	109.10	112.62
26	NJ	204	PEB	CHA-C1B-C2B	2.06	130.20	124.90
26	O9	201	PEB	CBC-CAC-C2C	-2.06	109.10	112.62
26	KD	201	PEB	C2B-C1B-NB	2.06	114.93	110.53
26	YI	201	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
26	M8	202	PEB	CHC-C1D-ND	-2.06	111.55	113.95
26	xE	302	PEB	CHB-C4B-C3B	2.06	130.08	125.32
26	G4	201	PEB	CHA-C4A-NA	2.06	127.66	125.20
26	i6	202	PEB	CHA-C4A-NA	-2.06	122.75	125.20
26	VA	202	PEB	CAA-C3A-C2A	-2.06	109.11	114.26
26	bF	201	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	z1	202	PEB	C1C-CHB-C4B	2.06	131.27	128.81
26	P7	201	PEB	C2B-C1B-NB	2.06	114.92	110.53
26	AE	202	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
26	a7	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
28	FF	1001	CYC	CBC-CAC-C3C	2.06	118.05	113.47
26	OA	203	PEB	CHB-C4B-C3B	-2.06	120.56	125.32
26	CG	203	PEB	C2B-C1B-NB	2.06	114.92	110.53
26	RJ	201	PEB	C2B-C1B-NB	2.06	114.92	110.53
26	IC	202	PEB	CAC-CBC-CGC	-2.06	107.99	113.76
26	WE	202	PEB	CAC-C2C-C3C	2.06	133.16	127.25
26	T3	203	PEB	CMB-C2B-C1B	2.06	128.24	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	DD	202	PEB	CBD-CAD-C3D	-2.06	117.38	127.62
28	HF	1001	CYC	CBA-CAA-C2A	-2.06	106.91	112.63
26	vG	201	PEB	CAA-C3A-C4A	-2.06	107.39	112.67
26	II	201	PEB	CHA-C1B-NB	-2.06	120.63	124.93
26	c7	201	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
26	dE	201	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
26	h4	202	PEB	CBC-CAC-C2C	-2.06	109.11	112.62
26	H5	202	PEB	CHB-C4B-C3B	-2.06	120.56	125.32
26	EA	203	PEB	CBA-CAA-C3A	-2.06	108.88	113.47
26	B1	201	PEB	C4B-NB-C1B	-2.06	102.63	106.51
26	II	202	PEB	C4B-C3B-C2B	-2.06	104.50	106.78
26	MA	202	PEB	CHA-C1B-C2B	2.06	130.19	124.90
26	m4	203	PEB	CHA-C1B-NB	-2.06	120.63	124.93
28	E6	1001	CYC	OB-C4B-NB	-2.06	120.30	125.08
26	C8	201	PEB	O2C-CGC-CBC	2.06	120.64	114.03
26	OE	202	PEB	CBC-CAC-C2C	-2.06	109.11	112.62
26	YB	201	PEB	CBB-CAB-C3B	2.06	118.34	112.63
26	eF	201	PEB	C2B-C1B-NB	2.06	114.92	110.53
26	KE	203	PEB	OA-C1A-C2A	-2.06	124.54	126.17
26	y1	203	PEB	CAC-CBC-CGC	-2.06	107.99	113.76
26	DA	202	PEB	CAC-CBC-CGC	-2.06	107.99	113.76
28	FI	1001	CYC	CMB-C2B-C1B	2.06	126.73	124.17
26	L3	202	PEB	CAA-C3A-C2A	-2.06	109.12	114.26
26	I1	201	PEB	CHA-C4A-NA	2.06	127.65	125.20
26	PD	201	PEB	OD-C4D-C3D	-2.06	124.80	129.46
26	O7	201	PEB	CAB-CBB-CGB	-2.06	109.18	113.60
26	iA	201	PEB	CAB-CBB-CGB	-2.06	109.18	113.60
26	uE	201	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	T7	202	PEB	CAA-C3A-C4A	2.06	117.95	112.67
28	jH	1001	CYC	C2C-C1C-NC	2.06	110.05	108.27
27	AI	302	PUB	CBA-CAA-C3A	-2.06	109.86	112.98
26	GG	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
26	k7	201	PEB	CAB-C3B-C4B	2.06	128.64	125.01
26	xE	303	PEB	CMB-C2B-C1B	2.06	128.23	125.06
28	BB	1001	CYC	OB-C4B-NB	-2.06	120.30	125.08
26	VI	203	PEB	OA-C1A-C2A	-2.06	124.54	126.17
26	WE	202	PEB	CBC-CAC-C2C	-2.06	109.11	112.62
26	Z4	201	PEB	OD-C4D-C3D	-2.05	124.81	129.46
26	RJ	202	PEB	OD-C4D-C3D	-2.05	124.81	129.46
26	I8	202	PEB	CAB-CBB-CGB	-2.05	109.18	113.60
26	C1	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
26	TB	201	PEB	CHA-C1B-C2B	2.05	130.18	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	w1	203	PEB	CAB-C3B-C4B	2.05	128.64	125.01
26	aI	201	PEB	CMA-C2A-C1A	-2.05	107.97	112.40
26	mG	202	PEB	C1B-C2B-C3B	-2.05	104.15	106.51
26	U8	202	PEB	C4B-C3B-C2B	-2.05	104.51	106.78
26	WG	201	PEB	CHA-C1B-C2B	2.05	130.18	124.90
26	WE	202	PEB	CHB-C4B-NB	-2.05	125.98	128.83
26	Z6	202	PEB	CBB-CAB-C3B	-2.05	106.92	112.63
26	CE	203	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
28	M2	1001	CYC	CHA-C1A-C2A	-2.05	120.58	125.32
26	c8	201	PEB	CHC-C4C-C3C	-2.05	126.83	130.34
26	SG	201	PEB	C2B-C1B-NB	2.05	114.91	110.53
28	GH	1001	CYC	CHB-C1B-C2B	-2.05	122.88	126.95
26	DD	202	PEB	C1C-CHB-C4B	2.05	131.26	128.81
26	eF	202	PEB	C1C-CHB-C4B	-2.05	126.36	128.81
26	ND	201	PEB	CAB-C3B-C4B	2.05	128.64	125.01
26	D4	202	PEB	CHA-C1B-NB	-2.05	120.64	124.93
26	Y9	202	PEB	CHC-C1D-ND	-2.05	111.56	113.95
26	IA	202	PEB	CHA-C4A-NA	2.05	127.64	125.20
26	Z2	201	PEB	CHB-C4B-NB	2.05	131.67	128.83
26	S7	201	PEB	CAB-C3B-C4B	2.05	128.64	125.01
26	MG	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
26	D7	1002	PEB	CBC-CAC-C2C	-2.05	109.12	112.62
28	NB	1001	CYC	CAB-C3B-C2B	2.05	131.04	127.53
26	G4	201	PEB	CMA-C2A-C1A	-2.05	107.98	112.40
26	VF	202	PEB	CAB-C3B-C4B	2.05	128.64	125.01
26	R3	201	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
26	II	202	PEB	CBB-CAB-C3B	-2.05	106.93	112.63
26	a2	201	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
26	iE	201	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
26	W3	202	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
26	CE	203	PEB	C2B-C1B-NB	2.05	114.91	110.53
26	gG	202	PEB	C2B-C1B-NB	2.05	114.91	110.53
26	SE	203	PEB	CAA-C3A-C4A	-2.05	107.41	112.67
26	M1	401	PEB	CAB-C3B-C4B	2.05	128.63	125.01
26	m1	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
26	j4	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
26	DA	201	PEB	C1B-C2B-C3B	-2.05	104.15	106.51
26	NG	201	PEB	C1B-C2B-C3B	-2.05	104.15	106.51
26	e7	201	PEB	CHA-C1B-NB	-2.05	120.64	124.93
26	F3	201	PEB	OD-C4D-C3D	-2.05	124.82	129.46
26	a6	202	PEB	CAC-CBC-CGC	-2.05	108.01	113.76
28	DB	1001	CYC	C1B-CHB-C4A	-2.05	123.07	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X3	201	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
26	PA	202	PEB	C2B-C1B-NB	2.05	114.90	110.53
26	OG	202	PEB	OD-C4D-ND	-2.05	122.89	125.93
26	OF	202	PEB	OD-C4D-C3D	-2.05	124.82	129.46
26	j4	201	PEB	CHC-C4C-C3C	-2.05	126.84	130.34
27	NJ	201	PUB	CMB-C2B-C3B	2.05	128.81	124.94
27	A7	304	PUB	CMD-C2D-C3D	2.05	130.84	127.77
27	AF	303	PUB	CMD-C2D-C3D	2.05	130.84	127.77
26	a6	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	Y8	202	PEB	C4B-C3B-C2B	-2.05	104.52	106.78
26	SE	203	PEB	C1B-C2B-C3B	-2.05	104.16	106.51
26	RE	201	PEB	CBC-CAC-C2C	-2.05	109.12	112.62
26	OD	202	PEB	OD-C4D-C3D	-2.05	124.82	129.46
26	gF	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
26	aB	201	PEB	CHB-C4B-C3B	-2.05	120.59	125.32
26	AG	201	PEB	CMB-C2B-C3B	-2.05	120.56	126.12
26	A9	301	PEB	C2B-C1B-NB	2.05	114.90	110.53
26	JG	202	PEB	C2B-C1B-NB	2.05	114.90	110.53
26	eB	203	PEB	CMD-C2D-C3D	2.05	132.95	130.06
26	B1	201	PEB	C2A-C1A-NA	2.05	110.04	108.27
26	MJ	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
26	AF	305	PEB	CMC-C3C-C2C	2.05	128.80	124.94
26	YA	202	PEB	C4B-C3B-C2B	-2.05	104.52	106.78
28	NF	1001	CYC	CAA-CBA-CGA	2.05	118.01	113.60
27	K3	203	PUB	CBA-CAA-C3A	-2.05	109.87	112.98
26	BD	202	PEB	CBA-CAA-C3A	-2.05	108.91	113.47
26	VI	203	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	h4	203	PEB	CHA-C4A-NA	-2.05	122.77	125.20
26	jF	202	PEB	CHA-C1B-C2B	2.05	130.17	124.90
26	i8	202	PEB	O1B-CGB-CBB	-2.05	116.50	123.08
26	kA	202	PEB	C1B-C2B-C3B	-2.05	104.16	106.51
26	j4	202	PEB	CHC-C1D-ND	-2.05	111.57	113.95
26	e6	201	PEB	CAB-CBB-CGB	-2.05	109.20	113.60
26	AE	202	PEB	OD-C4D-C3D	-2.05	124.82	129.46
26	l8	202	PEB	CBB-CAB-C3B	-2.05	106.94	112.63
26	N8	201	PEB	CAA-C3A-C2A	-2.05	109.14	114.26
26	lB	203	PEB	CAA-C3A-C2A	-2.05	109.14	114.26
26	f2	202	PEB	CBA-CAA-C3A	-2.05	108.91	113.47
26	VI	202	PEB	CAC-CBC-CGC	-2.05	108.02	113.76
26	V8	202	PEB	C1B-C2B-C3B	-2.05	104.16	106.51
28	J7	1001	CYC	O2D-CGD-CBD	2.05	120.61	114.03
28	BB	1001	CYC	CHA-C1A-NA	-2.05	125.99	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a2	203	PEB	OA-C1A-C2A	-2.05	124.55	126.17
26	s4	203	PEB	CHA-C1B-NB	-2.05	120.65	124.93
26	QE	202	PEB	CHA-C1B-NB	-2.05	120.65	124.93
27	AB	303	PUB	CBA-CAA-C3A	-2.05	109.88	112.98
26	UF	203	PEB	C2B-C1B-NB	2.05	114.89	110.53
26	aI	202	PEB	CHA-C1B-C2B	2.05	130.16	124.90
26	g1	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
26	AG	202	PEB	OD-C4D-C3D	-2.05	124.83	129.46
26	A6	304	PEB	CAB-C3B-C4B	2.05	128.63	125.01
27	A8	303	PUB	CAC-CBC-CGC	-2.05	109.20	113.60
26	X8	201	PEB	CBC-CAC-C2C	-2.05	109.13	112.62
26	bI	201	PEB	C2A-C1A-NA	2.05	110.04	108.27
26	DB	1002	PEB	O1B-CGB-CBB	-2.05	116.51	123.08
26	lG	201	PEB	CHA-C1B-NB	-2.04	120.66	124.93
26	11	202	PEB	CAB-C3B-C4B	2.04	128.62	125.01
28	F2	1001	CYC	C1B-CHB-C4A	-2.04	123.09	128.08
26	c2	202	PEB	C3B-C4B-NB	2.04	113.02	110.05
26	H3	201	PEB	CAA-C3A-C2A	-2.04	109.15	114.26
28	M2	1001	CYC	CHB-C1B-NB	-2.04	121.67	126.06
26	G5	203	PEB	CHC-C4C-C3C	-2.04	126.85	130.34
26	gE	201	PEB	CHC-C4C-C3C	-2.04	126.85	130.34
26	iI	203	PEB	C1B-C2B-C3B	-2.04	104.16	106.51
26	f2	201	PEB	CAB-C3B-C4B	2.04	128.62	125.01
26	AC	203	PEB	CAB-C3B-C4B	2.04	128.62	125.01
26	C8	201	PEB	CBB-CAB-C3B	-2.04	106.95	112.63
26	F4	203	PEB	CAB-C3B-C4B	2.04	128.62	125.01
26	H4	201	PEB	CAA-C3A-C4A	-2.04	107.43	112.67
26	W6	201	PEB	C2B-C1B-NB	2.04	114.89	110.53
26	F3	201	PEB	CAA-C3A-C4A	-2.04	107.43	112.67
26	l4	202	PEB	CHA-C1B-NB	-2.04	120.66	124.93
26	t1	202	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
26	wE	302	PEB	CBA-CAA-C3A	-2.04	108.92	113.47
26	V2	203	PEB	C1C-CHB-C4B	2.04	131.25	128.81
26	cE	202	PEB	C1C-CHB-C4B	-2.04	126.37	128.81
26	JE	201	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
26	NI	1002	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
26	u4	203	PEB	C3B-C4B-NB	2.04	113.02	110.05
26	nG	201	PEB	CHA-C1B-C2B	2.04	130.15	124.90
26	24	404	PEB	CAB-C3B-C4B	2.04	128.62	125.01
26	CC	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
28	B6	1001	CYC	OB-C4B-NB	-2.04	120.33	125.08
26	E4	202	PEB	CHC-C4C-C3C	-2.04	126.85	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	OF	202	PEB	C2B-C1B-NB	2.04	114.89	110.53
26	V3	203	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
26	lF	201	PEB	CBC-CAC-C2C	-2.04	109.14	112.62
26	f7	201	PEB	CAB-CBB-CGB	-2.04	109.21	113.60
26	yE	301	PEB	CAB-CBB-CGB	-2.04	109.21	113.60
26	EJ	201	PEB	CBA-CAA-C3A	-2.04	108.92	113.47
28	H2	1001	CYC	CAD-CBD-CGD	-2.04	108.04	113.76
26	e1	201	PEB	CAB-C3B-C4B	2.04	128.62	125.01
26	G5	203	PEB	OA-C1A-NA	2.04	127.41	124.94
26	XG	203	PEB	CHA-C1B-NB	-2.04	120.66	124.93
27	AA	304	PUB	CAC-CBC-CGC	-2.04	109.21	113.60
26	a7	202	PEB	CHA-C1B-C2B	2.04	130.15	124.90
26	U3	202	PEB	C2B-C1B-NB	2.04	114.88	110.53
26	d7	202	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
26	m2	201	PEB	CHB-C4B-C3B	-2.04	120.61	125.32
26	PA	201	PEB	C1B-C2B-C3B	-2.04	104.17	106.51
26	dB	202	PEB	CBC-CAC-C2C	-2.04	109.14	112.62
26	d7	202	PEB	CBB-CAB-C3B	-2.04	106.96	112.63
26	b7	201	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	i8	201	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	C8	201	PEB	CHC-C1D-ND	-2.04	111.58	113.95
26	z1	201	PEB	CMD-C2D-C3D	2.04	132.94	130.06
26	GG	203	PEB	O1B-CGB-CBB	-2.04	116.53	123.08
26	bF	203	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
26	SG	202	PEB	OA-C1A-C2A	-2.04	124.55	126.17
28	B6	1001	CYC	CHA-C1A-NA	-2.04	126.00	128.83
26	HD	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	N3	202	PEB	CAA-C3A-C2A	-2.04	109.16	114.26
26	N3	203	PEB	CHA-C4A-NA	-2.04	122.78	125.20
26	mG	201	PEB	CHA-C4A-NA	2.04	127.63	125.20
26	PD	202	PEB	CAC-CBC-CGC	-2.04	108.04	113.76
26	g8	201	PEB	CAB-CBB-CGB	-2.04	109.21	113.60
26	F3	201	PEB	CAB-C3B-C4B	2.04	128.62	125.01
26	eA	202	PEB	C2A-C1A-NA	2.04	110.03	108.27
26	E9	201	PEB	CBD-CAD-C3D	-2.04	117.47	127.62
26	R2	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
26	NI	1002	PEB	CHA-C1B-NB	-2.04	120.67	124.93
28	K6	202	CYC	CHA-C1A-C2A	-2.04	120.61	125.32
26	I3	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
26	xG	302	PEB	CAB-C3B-C4B	2.04	128.61	125.01
26	hE	201	PEB	O2B-CGB-CBB	2.04	120.58	114.03
26	VJ	202	PEB	CAB-C3B-C4B	2.04	128.61	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	UI	202	PEB	CHA-C1B-NB	-2.04	120.67	124.93
26	Y8	201	PEB	CAA-C3A-C2A	-2.04	109.17	114.26
26	H1	201	PEB	CHC-C1D-ND	-2.04	111.58	113.95
28	G7	1001	CYC	CMD-C2D-C3D	2.04	128.78	124.94
26	j7	201	PEB	CAB-C3B-C4B	2.04	128.61	125.01
26	gF	202	PEB	CAB-CBB-CGB	-2.04	109.22	113.60
26	u4	201	PEB	CHA-C1B-NB	-2.04	120.67	124.93
28	qH	1002	CYC	CHB-C4A-NA	2.04	129.20	124.93
26	l8	201	PEB	C2B-C1B-NB	2.04	114.88	110.53
26	j1	201	PEB	CMC-C3C-C2C	2.04	128.78	124.94
26	tG	202	PEB	CMC-C3C-C2C	2.04	128.78	124.94
26	XE	202	PEB	CAC-CBC-CGC	-2.04	108.05	113.76
26	K8	202	PEB	C4B-C3B-C2B	-2.04	104.53	106.78
26	V2	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
28	wH	1001	CYC	C2C-C3C-C4C	2.04	104.39	101.34
26	hB	202	PEB	CAB-CBB-CGB	-2.04	109.22	113.60
27	AA	303	PUB	C2C-C1C-NC	2.04	113.01	110.05
28	NH	1001	CYC	CHB-C1B-C2B	-2.04	122.91	126.95
26	c2	203	PEB	CAC-CBC-CGC	-2.04	108.05	113.76
26	a1	203	PEB	CMB-C2B-C1B	2.04	128.20	125.06
28	JF	1001	CYC	CBD-CAD-C3D	2.04	116.09	112.62
26	BJ	203	PEB	CAB-C3B-C4B	2.04	128.61	125.01
26	WB	201	PEB	C2B-C1B-NB	2.04	114.87	110.53
26	eB	201	PEB	C2B-C1B-NB	2.04	114.87	110.53
26	O8	202	PEB	CBC-CAC-C2C	-2.04	109.15	112.62
28	C2	1001	CYC	CHB-C4A-C3A	2.03	130.13	124.90
26	zG	501	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
26	VI	201	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
26	M8	202	PEB	CHA-C1B-C2B	2.03	130.13	124.90
26	m2	202	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
26	V7	201	PEB	CHA-C1B-C2B	2.03	130.13	124.90
28	IF	1001	CYC	CHA-C1A-C2A	-2.03	120.62	125.32
28	F2	1001	CYC	CBA-CAA-C2A	2.03	118.28	112.63
26	IC	201	PEB	CBB-CAB-C3B	-2.03	106.98	112.63
26	W7	202	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
26	ZF	202	PEB	C1C-CHB-C4B	2.03	131.24	128.81
26	t4	201	PEB	CHB-C4B-C3B	-2.03	120.62	125.32
26	Q3	202	PEB	C2B-C1B-NB	2.03	114.87	110.53
26	q4	202	PEB	CBA-CAA-C3A	-2.03	108.94	113.47
26	n1	201	PEB	CAB-C3B-C4B	2.03	128.60	125.01
26	w4	203	PEB	CHC-C1D-ND	-2.03	111.59	113.95
26	UA	202	PEB	O1C-CGC-CBC	-2.03	116.55	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	NB	1001	CYC	C1B-NB-C4B	-2.03	108.08	110.67
26	V7	202	PEB	OA-C1A-NA	2.03	127.40	124.94
26	e3	401	PEB	CHB-C4B-C3B	-2.03	120.62	125.32
26	K4	202	PEB	CHB-C4B-C3B	-2.03	120.62	125.32
26	HE	202	PEB	C4B-NB-C1B	-2.03	102.68	106.51
26	E1	202	PEB	C2B-C1B-NB	2.03	114.87	110.53
26	SA	203	PEB	C2B-C1B-NB	2.03	114.87	110.53
26	B3	201	PEB	CAC-CBC-CGC	-2.03	108.06	113.76
26	w4	201	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
26	Y1	202	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
28	LF	1001	CYC	CBC-CAC-C3C	2.03	117.99	113.47
26	HD	202	PEB	CHA-C1B-NB	-2.03	120.68	124.93
28	KB	202	CYC	CHB-C4A-C3A	2.03	130.13	124.90
26	i7	201	PEB	CHB-C4B-C3B	-2.03	120.63	125.32
26	I8	202	PEB	CHA-C4A-NA	2.03	127.62	125.20
28	C6	1001	CYC	CHA-C1A-NA	-2.03	126.01	128.83
26	L3	201	PEB	CAC-CBC-CGC	-2.03	108.06	113.76
26	S3	201	PEB	O1C-CGC-CBC	-2.03	116.55	123.08
26	iE	202	PEB	CAA-C3A-C2A	-2.03	109.18	114.26
26	LB	1002	PEB	CMC-C3C-C2C	-2.03	121.11	124.94
26	h2	202	PEB	C2B-C1B-NB	2.03	114.86	110.53
26	P4	202	PEB	CBB-CAB-C3B	-2.03	106.98	112.63
26	T9	203	PEB	CHC-C4C-C3C	-2.03	126.87	130.34
26	OB	201	PEB	OA-C1A-NA	2.03	127.40	124.94
26	tG	201	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	TF	201	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
27	AB	303	PUB	CAC-CBC-CGC	-2.03	109.23	113.60
26	A1	202	PEB	CHA-C1B-C2B	-2.03	119.68	124.90
26	cI	203	PEB	CBB-CAB-C3B	2.03	118.27	112.63
26	vG	202	PEB	C2B-C1B-NB	2.03	114.86	110.53
26	T7	202	PEB	C1C-CHB-C4B	-2.03	126.38	128.81
26	V1	201	PEB	CBA-CAA-C3A	2.03	117.99	113.47
28	EH	1001	CYC	CAB-C3B-C2B	2.03	131.00	127.53
26	W7	202	PEB	CMC-C3C-C2C	2.03	128.77	124.94
26	x4	202	PEB	O2B-CGB-CBB	2.03	120.55	114.03
26	ZG	202	PEB	C4B-NB-C1B	-2.03	102.69	106.51
26	A9	303	PEB	OD-C4D-C3D	-2.03	124.86	129.46
26	IE	203	PEB	CBC-CAC-C2C	2.03	116.08	112.62
26	14	202	PEB	CHC-C1D-ND	-2.03	111.59	113.95
28	CH	1001	CYC	C1B-CHB-C4A	2.03	133.04	128.08
26	ZA	201	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
26	D1	202	PEB	CMA-C2A-C1A	-2.03	108.03	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R2	203	PEB	CAC-CBC-CGC	-2.03	108.07	113.76
26	A9	304	PEB	OD-C4D-C3D	-2.03	124.86	129.46
26	DB	1002	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
26	CJ	201	PEB	CHC-C4C-C3C	-2.03	126.88	130.34
28	gH	1001	CYC	C2C-C3C-C4C	2.03	104.38	101.34
26	KD	201	PEB	C2A-C1A-NA	2.03	110.02	108.27
26	H1	202	PEB	CMC-C3C-C2C	2.03	128.77	124.94
26	UA	202	PEB	CAB-C3B-C4B	2.03	128.60	125.01
26	l7	203	PEB	CHA-C1B-C2B	2.03	130.12	124.90
26	q1	203	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	C4	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	hE	202	PEB	CHB-C4B-C3B	-2.03	120.63	125.32
26	sE	203	PEB	CAA-C3A-C4A	-2.03	107.46	112.67
26	H8	202	PEB	CBA-CAA-C3A	-2.03	108.95	113.47
26	GG	201	PEB	CAB-C3B-C4B	2.03	128.60	125.01
26	HG	202	PEB	C2B-C1B-NB	2.03	114.86	110.53
26	V1	202	PEB	CHC-C1D-ND	-2.03	111.59	113.95
26	LJ	203	PEB	CHA-C1B-NB	-2.03	120.69	124.93
26	A5	201	PEB	CAC-CBC-CGC	-2.03	108.07	113.76
28	KB	202	CYC	CHA-C1A-C2A	-2.03	120.64	125.32
26	WG	202	PEB	O1C-CGC-CBC	-2.03	116.57	123.08
26	XD	202	PEB	CHC-C1D-ND	-2.03	111.59	113.95
26	W7	202	PEB	CAB-C3B-C4B	2.03	128.59	125.01
26	DD	203	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
26	E4	201	PEB	CBC-CAC-C2C	-2.03	109.16	112.62
26	AJ	301	PEB	CBC-CAC-C2C	2.03	116.08	112.62
26	u4	201	PEB	C2B-C1B-NB	2.03	114.85	110.53
26	hB	201	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
26	QE	203	PEB	CAB-C3B-C4B	2.03	128.59	125.01
26	HJ	201	PEB	CAA-C3A-C2A	-2.03	109.20	114.26
26	BC	201	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
26	V8	202	PEB	CHB-C4B-C3B	2.03	130.00	125.32
28	CF	1001	CYC	CHA-C1A-C2A	-2.03	120.64	125.32
26	14	201	PEB	CMD-C2D-C3D	2.03	132.92	130.06
26	w4	202	PEB	CMC-C3C-C2C	2.03	128.76	124.94
26	U7	202	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
26	IC	203	PEB	CHC-C1D-ND	-2.03	111.59	113.95
26	Z8	202	PEB	OA-C1A-NA	2.03	127.39	124.94
28	qH	1001	CYC	C2C-C1C-NC	2.03	110.02	108.27
26	x4	202	PEB	CAB-C3B-C4B	2.03	128.59	125.01
26	AB	304	PEB	CAB-C3B-C4B	2.03	128.59	125.01
26	rE	201	PEB	CAB-C3B-C4B	2.03	128.59	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AG	202	PEB	CAB-C3B-C4B	2.03	128.59	125.01
26	aG	202	PEB	CAB-C3B-C4B	2.03	128.59	125.01
26	m7	201	PEB	CAB-CBB-CGB	-2.03	109.25	113.60
26	E4	202	PEB	C1C-CHB-C4B	2.02	131.23	128.81
26	iI	203	PEB	CAA-C3A-C2A	-2.02	109.20	114.26
26	R2	201	PEB	CMD-C2D-C3D	2.02	132.92	130.06
26	G3	202	PEB	CAB-C3B-C4B	2.02	128.59	125.01
26	X3	201	PEB	C1B-C2B-C3B	-2.02	104.18	106.51
26	JA	202	PEB	CHC-C1D-ND	-2.02	111.60	113.95
26	W6	201	PEB	OA-C1A-C2A	-2.02	124.56	126.17
26	O3	202	PEB	OD-C4D-C3D	-2.02	124.88	129.46
26	gI	201	PEB	CAA-C3A-C4A	-2.02	107.48	112.67
28	HF	1001	CYC	CHA-C1A-C2A	-2.02	120.65	125.32
26	FD	202	PEB	CBD-CAD-C3D	-2.02	117.55	127.62
26	e8	202	PEB	CAA-C3A-C2A	-2.02	109.20	114.26
26	WJ	202	PEB	CAB-C3B-C4B	2.02	128.59	125.01
26	a8	204	PEB	CAA-C3A-C2A	-2.02	109.20	114.26
26	T2	203	PEB	CMB-C2B-C1B	2.02	128.18	125.06
26	OI	201	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
26	eG	202	PEB	CHB-C4B-C3B	-2.02	120.65	125.32
26	PG	201	PEB	CHA-C1B-C2B	2.02	130.10	124.90
26	X4	202	PEB	C1C-CHB-C4B	2.02	131.22	128.81
26	VD	201	PEB	C3B-C4B-NB	2.02	112.99	110.05
27	xE	306	PUB	CMB-C2B-C3B	2.02	128.75	124.94
26	J7	1002	PEB	CHA-C1B-NB	-2.02	120.70	124.93
26	DF	1002	PEB	CBC-CAC-C2C	-2.02	109.17	112.62
26	w4	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
26	N4	201	PEB	CBA-CAA-C3A	-2.02	108.97	113.47
26	TG	202	PEB	CBD-CAD-C3D	-2.02	117.56	127.62
26	YJ	202	PEB	C1C-CHB-C4B	-2.02	126.39	128.81
26	PD	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
27	AI	302	PUB	C1D-CHC-C4C	-2.02	108.97	113.37
26	y1	201	PEB	C1B-C2B-C3B	-2.02	104.19	106.51
26	HD	201	PEB	OD-C4D-C3D	-2.02	124.88	129.46
26	t4	202	PEB	CHC-C4C-C3C	-2.02	126.89	130.34
26	e3	401	PEB	O2B-CGB-CBB	2.02	120.52	114.03
28	CI	1001	CYC	CMC-C2C-C1C	-2.02	108.05	112.40
26	EA	203	PEB	C2B-C1B-NB	2.02	114.84	110.53
26	jA	203	PEB	CBC-CAC-C2C	-2.02	109.17	112.62
26	A9	301	PEB	CHA-C4A-NA	-2.02	122.80	125.20
26	h6	202	PEB	CAB-CBB-CGB	-2.02	109.25	113.60
26	q4	202	PEB	CAB-C3B-C4B	2.02	128.58	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l6	203	PEB	CAB-C3B-C4B	2.02	128.58	125.01
26	S8	201	PEB	CAB-C3B-C4B	2.02	128.58	125.01
26	JA	201	PEB	CAA-C3A-C4A	-2.02	107.48	112.67
26	RB	201	PEB	C1B-C2B-C3B	-2.02	104.19	106.51
26	VB	201	PEB	CAB-CBB-CGB	-2.02	109.25	113.60
26	YA	201	PEB	CAA-C3A-C2A	-2.02	109.21	114.26
26	UA	202	PEB	C4B-C3B-C2B	-2.02	104.55	106.78
26	KA	202	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
26	YF	201	PEB	CBB-CAB-C3B	2.02	118.24	112.63
26	eA	201	PEB	CHA-C4A-NA	2.02	127.61	125.20
26	h7	203	PEB	CMD-C2D-C3D	2.02	132.91	130.06
26	TI	203	PEB	CAA-C3A-C4A	-2.02	107.49	112.67
26	cI	201	PEB	C1C-CHB-C4B	2.02	131.22	128.81
26	W8	202	PEB	CBD-CAD-C3D	-2.02	117.57	127.62
26	u1	202	PEB	C2B-C1B-NB	2.02	114.84	110.53
26	RF	202	PEB	CAC-CBC-CGC	-2.02	108.10	113.76
26	Z1	202	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
26	FC	203	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
26	l8	202	PEB	CHC-C1D-ND	-2.02	111.60	113.95
26	A2	301	PEB	CBC-CAC-C2C	-2.02	109.17	112.62
26	BC	201	PEB	CBC-CAC-C2C	-2.02	109.17	112.62
26	a6	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
26	A9	304	PEB	CMC-C3C-C2C	2.02	128.75	124.94
26	R9	201	PEB	CAA-C3A-C4A	-2.02	107.49	112.67
26	e2	202	PEB	CAC-CBC-CGC	-2.02	108.10	113.76
26	N2	1002	PEB	CAA-C3A-C2A	-2.02	109.21	114.26
26	f7	201	PEB	CAB-C3B-C4B	2.02	128.58	125.01
27	AA	304	PUB	C2C-C1C-NC	2.02	112.99	110.05
26	AJ	301	PEB	CMB-C2B-C1B	2.02	128.17	125.06
26	a8	204	PEB	C2B-C1B-NB	2.02	114.84	110.53
26	IJ	202	PEB	OD-C4D-C3D	-2.02	124.89	129.46
26	C8	202	PEB	CMC-C3C-C2C	2.02	128.75	124.94
26	U9	202	PEB	CHB-C4B-C3B	-2.02	120.66	125.32
26	eB	201	PEB	CHC-C1D-ND	-2.02	111.60	113.95
26	GC	202	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
26	HE	202	PEB	CHA-C4A-NA	-2.02	122.81	125.20
28	GH	1001	CYC	C2C-C3C-C4C	2.02	104.36	101.34
26	kB	201	PEB	O2B-CGB-CBB	2.02	120.51	114.03
26	VD	202	PEB	CBC-CAC-C2C	2.02	116.06	112.62
26	SJ	201	PEB	CAB-C3B-C4B	2.02	128.58	125.01
26	zG	501	PEB	O1B-CGB-CBB	-2.02	116.60	123.08
26	i7	202	PEB	C1B-C2B-C3B	-2.02	104.19	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	FA	202	PEB	C1B-C2B-C3B	-2.02	104.19	106.51
26	OE	202	PEB	OD-C4D-ND	-2.02	122.94	125.93
28	NF	1001	CYC	CBB-CAB-C3B	-2.02	106.87	112.43
26	f1	202	PEB	CHA-C1B-C2B	-2.02	119.71	124.90
26	k2	201	PEB	C2B-C1B-NB	2.02	114.83	110.53
26	FD	203	PEB	C2B-C1B-NB	2.02	114.83	110.53
26	h2	201	PEB	CHC-C1D-ND	-2.02	111.60	113.95
26	MG	201	PEB	CBB-CAB-C3B	-2.02	107.02	112.63
26	t1	202	PEB	C3B-C4B-NB	2.02	112.98	110.05
26	z1	202	PEB	CBC-CAC-C2C	-2.02	109.18	112.62
26	mF	201	PEB	OA-C1A-C2A	-2.02	124.57	126.17
26	BD	202	PEB	CHB-C4B-C3B	-2.02	120.66	125.32
26	HI	1002	PEB	CAC-CBC-CGC	-2.02	108.10	113.76
26	r1	202	PEB	OD-C4D-C3D	-2.02	124.89	129.46
26	y4	201	PEB	CHC-C1D-ND	-2.02	111.61	113.95
26	S9	201	PEB	CAB-C3B-C4B	2.02	128.58	125.01
26	AJ	301	PEB	OD-C4D-ND	-2.02	122.94	125.93
26	x4	202	PEB	C2B-C1B-NB	2.02	114.83	110.53
26	NA	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
28	E2	1001	CYC	OB-C4B-NB	-2.02	120.39	125.08
26	v1	201	PEB	CAB-C3B-C4B	2.02	128.57	125.01
26	VI	202	PEB	CMA-C2A-C1A	-2.02	108.06	112.40
26	jA	202	PEB	OA-C1A-C2A	-2.02	124.57	126.17
26	R4	203	PEB	CHC-C1D-ND	2.02	116.29	113.95
26	K3	201	PEB	CAC-C2C-C3C	-2.02	121.45	127.25
26	YJ	201	PEB	CAB-C3B-C4B	2.02	128.57	125.01
26	E3	201	PEB	C3B-C4B-NB	2.02	112.98	110.05
27	A6	302	PUB	CBA-CAA-C3A	-2.02	109.92	112.98
26	IJ	201	PEB	OD-C4D-C3D	-2.02	124.89	129.46
26	NF	1002	PEB	CHA-C1B-NB	-2.02	120.72	124.93
26	a8	202	PEB	O1C-CGC-CBC	-2.02	116.61	123.08
28	YH	1003	CYC	C1B-CHB-C4A	2.02	133.00	128.08
26	UG	202	PEB	C2B-C1B-NB	2.02	114.83	110.53
26	O2	202	PEB	O2B-CGB-CBB	2.01	120.50	114.03
26	AG	201	PEB	CMA-C2A-C1A	-2.01	108.06	112.40
26	O6	201	PEB	CAC-CBC-CGC	-2.01	108.11	113.76
26	QB	201	PEB	C2B-C1B-NB	2.01	114.83	110.53
26	I3	202	PEB	CHA-C4A-NA	-2.01	122.81	125.20
26	i6	202	PEB	CMA-C2A-C1A	-2.01	108.06	112.40
26	hB	203	PEB	C2B-C1B-NB	2.01	114.83	110.53
26	gE	201	PEB	O1C-CGC-CBC	-2.01	116.61	123.08
26	YE	201	PEB	CAA-C3A-C2A	-2.01	109.23	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	VA	201	PEB	CAB-CBB-CGB	-2.01	109.27	113.60
26	tE	202	PEB	CAC-C2C-C3C	2.01	133.03	127.25
26	cB	201	PEB	C2B-C1B-NB	2.01	114.83	110.53
28	F7	1001	CYC	C3A-C4A-NA	2.01	114.83	110.53
26	EA	202	PEB	CAB-C3B-C4B	2.01	128.57	125.01
28	qH	1001	CYC	C2C-C3C-C4C	2.01	104.35	101.34
28	G6	1001	CYC	CMC-C2C-C1C	-2.01	108.06	112.40
26	gE	202	PEB	C1C-CHB-C4B	2.01	131.21	128.81
28	gH	1001	CYC	CHA-C1A-NA	-2.01	126.03	128.83
26	lA	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
26	bG	202	PEB	CAB-CBB-CGB	-2.01	109.27	113.60
26	q1	201	PEB	CHA-C1B-NB	-2.01	120.72	124.93
26	r4	201	PEB	CAC-C2C-C3C	2.01	133.03	127.25
26	A7	301	PEB	C2B-C1B-NB	2.01	114.82	110.53
26	PE	201	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	T6	202	PEB	CAC-C2C-C3C	2.01	133.03	127.25
28	gH	1001	CYC	C2C-C1C-NC	2.01	110.01	108.27
26	L6	1002	PEB	CAB-C3B-C2B	2.01	131.62	127.88
26	S1	202	PEB	CAC-CBC-CGC	-2.01	108.12	113.76
26	s1	203	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	UA	201	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	bF	201	PEB	OD-C4D-ND	-2.01	122.95	125.93
26	D3	202	PEB	CBB-CAB-C3B	-2.01	107.04	112.63
26	iI	203	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	q1	201	PEB	CHB-C4B-C3B	-2.01	120.67	125.32
26	i8	202	PEB	CBA-CAA-C3A	-2.01	108.99	113.47
28	DB	1001	CYC	C3A-C4A-NA	2.01	114.82	110.53
26	HJ	203	PEB	OD-C4D-C3D	-2.01	124.91	129.46
26	S1	202	PEB	C1C-CHB-C4B	-2.01	126.41	128.81
28	GI	1001	CYC	OC-C1C-NC	2.01	127.38	124.94
26	X1	201	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	lI	202	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	Z1	201	PEB	OD-C4D-C3D	-2.01	124.91	129.46
26	VA	201	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
26	T4	203	PEB	CAA-C3A-C2A	-2.01	109.24	114.26
26	NE	202	PEB	C2B-C1B-NB	2.01	114.82	110.53
26	G5	203	PEB	CAB-C3B-C4B	2.01	128.56	125.01
26	O7	202	PEB	CBC-CAC-C2C	-2.01	109.19	112.62
26	g7	202	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
26	B1	202	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
26	PJ	202	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
26	ZG	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k4	201	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	QD	201	PEB	OA-C1A-C2A	-2.01	124.58	126.17
26	hE	202	PEB	C2B-C1B-NB	2.01	114.81	110.53
26	g2	203	PEB	CHA-C4A-NA	-2.01	122.82	125.20
26	PE	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
26	gE	201	PEB	CAC-C2C-C3C	2.01	133.02	127.25
26	D6	1002	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
26	OD	201	PEB	C1C-CHB-C4B	2.01	131.21	128.81
26	S6	201	PEB	CBA-CAA-C3A	-2.01	109.00	113.47
26	D1	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
26	d1	203	PEB	CAB-C3B-C4B	2.01	128.56	125.01
26	TB	202	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
26	F8	202	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
26	KD	201	PEB	CHC-C1D-ND	-2.01	111.62	113.95
28	C2	1001	CYC	CMC-C2C-C1C	-2.01	108.08	112.40
28	QH	1001	CYC	CAB-C3B-C2B	2.01	130.96	127.53
26	BD	203	PEB	CHA-C1B-NB	-2.01	120.73	124.93
26	w1	201	PEB	O2B-CGB-CBB	2.01	120.48	114.03
26	M8	202	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
26	j4	201	PEB	CHB-C4B-C3B	-2.01	120.68	125.32
26	hE	201	PEB	CAA-C3A-C2A	-2.01	109.25	114.26
28	SH	1001	CYC	C2C-C1C-NC	2.01	110.00	108.27
26	h1	202	PEB	CAB-C3B-C4B	2.01	128.56	125.01
26	A7	302	PEB	CHC-C1D-ND	-2.01	111.62	113.95
26	h8	202	PEB	CHC-C1D-ND	-2.01	111.62	113.95
26	S8	202	PEB	CHB-C4B-C3B	-2.01	120.69	125.32
26	X1	202	PEB	OA-C1A-NA	2.01	127.37	124.94
26	T4	202	PEB	C2B-C1B-NB	2.01	114.81	110.53
26	LF	1002	PEB	C2B-C1B-NB	2.01	114.81	110.53
26	zG	501	PEB	CHC-C1D-ND	-2.01	111.62	113.95
26	IG	203	PEB	CAC-CBC-CGC	-2.01	108.14	113.76
28	L2	1001	CYC	CAD-CBD-CGD	-2.01	108.14	113.76
26	sG	202	PEB	C2A-C3A-C4A	2.01	104.34	101.34
26	r4	202	PEB	CHC-C4C-C3C	-2.01	126.92	130.34
26	Y8	203	PEB	CMD-C2D-C3D	2.01	132.89	130.06
28	OH	1001	CYC	C2A-C1A-NA	2.01	112.97	110.05
28	EB	1001	CYC	OB-C4B-NB	-2.01	120.42	125.08
26	a6	201	PEB	CHB-C4B-C3B	-2.01	120.69	125.32
26	h2	201	PEB	CAB-CBB-CGB	-2.01	109.29	113.60
26	NE	202	PEB	CHA-C1B-NB	-2.01	120.74	124.93
26	TF	202	PEB	CBD-CAD-C3D	-2.01	117.64	127.62
26	UE	203	PEB	CAB-C3B-C4B	2.01	128.56	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	QD	201	PEB	CBA-CAA-C3A	-2.00	109.00	113.47
26	fF	202	PEB	CHC-C4C-C3C	-2.00	126.92	130.34
26	CA	202	PEB	CMC-C3C-C2C	2.00	128.72	124.94
26	HC	202	PEB	CHC-C1D-ND	-2.00	111.62	113.95
26	K5	201	PEB	CHA-C1B-C2B	2.00	130.06	124.90
26	W3	201	PEB	O1C-CGC-CBC	-2.00	116.64	123.08
26	c4	201	PEB	CAA-C3A-C4A	-2.00	107.53	112.67
28	CI	1001	CYC	CHB-C4A-C3A	2.00	130.05	124.90
26	CA	202	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
26	fF	201	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
26	l7	202	PEB	CBB-CAB-C3B	-2.00	107.06	112.63
26	ZB	201	PEB	CAC-CBC-CGC	-2.00	108.14	113.76
26	LI	1002	PEB	CBD-CAD-C3D	-2.00	117.65	127.62
26	OF	201	PEB	CAB-CBB-CGB	-2.00	109.29	113.60
26	GE	202	PEB	CHA-C1B-NB	-2.00	120.74	124.93
27	B8	302	PUB	CBB-CAB-C3B	-2.00	109.20	112.62
27	KD	203	PUB	CBA-CAA-C3A	-2.00	109.94	112.98
26	e6	201	PEB	CAB-C3B-C4B	2.00	128.55	125.01
26	H4	202	PEB	CMC-C3C-C2C	2.00	128.72	124.94
26	IE	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	y4	201	PEB	C1B-C2B-C3B	-2.00	104.21	106.51
27	xE	306	PUB	CMD-C2D-C3D	2.00	130.77	127.77
28	AH	1001	CYC	CHA-C1A-C2A	2.00	129.95	125.32
26	XD	202	PEB	CHB-C4B-C3B	-2.00	120.69	125.32
26	E4	202	PEB	CHA-C4A-NA	-2.00	122.82	125.20
27	B8	302	PUB	CAB-CBB-CGB	-2.00	108.14	113.76
26	W3	201	PEB	C1C-CHB-C4B	2.00	131.20	128.81
26	lA	201	PEB	OA-C1A-NA	2.00	127.37	124.94
26	x4	202	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
27	BA	302	PUB	CAC-C2C-C1C	2.00	128.55	125.01
26	ZE	201	PEB	C2B-C1B-NB	2.00	114.80	110.53
26	EA	202	PEB	C3B-C4B-NB	2.00	112.96	110.05
26	g7	201	PEB	CAB-C3B-C4B	2.00	128.55	125.01
26	VD	203	PEB	OD-C4D-C3D	-2.00	124.93	129.46
26	OA	202	PEB	C2B-C1B-NB	2.00	114.80	110.53
26	cG	202	PEB	C2B-C1B-NB	2.00	114.80	110.53
26	j6	202	PEB	CAB-C3B-C4B	2.00	128.55	125.01
27	BA	302	PUB	CAB-CBB-CGB	-2.00	108.15	113.76
26	WB	203	PEB	CHB-C4B-C3B	-2.00	120.70	125.32
26	m6	203	PEB	CHA-C4A-NA	-2.00	122.83	125.20
26	HA	201	PEB	CAA-C3A-C2A	-2.00	109.26	114.26
28	GH	1001	CYC	CAB-C3B-C2B	2.00	130.95	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H2	1002	PEB	CAC-CBC-CGC	-2.00	108.15	113.76
26	HE	202	PEB	C2B-C1B-NB	2.00	114.80	110.53
26	W9	202	PEB	CAB-C3B-C4B	2.00	128.55	125.01
26	gA	202	PEB	C1B-C2B-C3B	-2.00	104.21	106.51
26	q1	202	PEB	CBB-CAB-C3B	-2.00	107.07	112.63
27	A8	303	PUB	CBC-CAC-C2C	-2.00	107.07	112.63
26	K5	202	PEB	CHA-C1B-NB	-2.00	120.75	124.93
26	E8	203	PEB	CMC-C3C-C2C	2.00	128.71	124.94
26	S8	203	PEB	C2B-C1B-NB	2.00	114.80	110.53

There are no chirality outliers.

All (14179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A1	201	PEB	ND-C1D-CHC-C4C
26	A1	201	PEB	C2D-C1D-CHC-C4C
26	A1	201	PEB	NB-C1B-CHA-C4A
26	A1	201	PEB	C2B-C1B-CHA-C4A
26	A1	202	PEB	NC-C1C-CHB-C4B
26	A1	202	PEB	C2C-C1C-CHB-C4B
26	A1	202	PEB	C2C-CAC-CBC-CGC
26	A1	202	PEB	NB-C1B-CHA-C4A
26	A1	202	PEB	C2B-C1B-CHA-C4A
26	B1	201	PEB	ND-C1D-CHC-C4C
26	B1	201	PEB	C2A-C3A-CAA-CBA
26	B1	201	PEB	NB-C1B-CHA-C4A
26	B1	201	PEB	C2B-C1B-CHA-C4A
26	B1	202	PEB	C2A-C3A-CAA-CBA
26	B1	202	PEB	C4A-C3A-CAA-CBA
26	B1	202	PEB	NB-C1B-CHA-C4A
26	B1	202	PEB	C2B-C1B-CHA-C4A
26	B1	203	PEB	NC-C1C-CHB-C4B
26	B1	203	PEB	C2C-C1C-CHB-C4B
26	B1	203	PEB	C2A-C3A-CAA-CBA
26	B1	203	PEB	C4A-C3A-CAA-CBA
26	B1	203	PEB	NB-C1B-CHA-C4A
26	B1	203	PEB	C2B-C1B-CHA-C4A
26	C1	201	PEB	NB-C1B-CHA-C4A
26	C1	201	PEB	C2B-C1B-CHA-C4A
26	C1	202	PEB	NC-C1C-CHB-C4B
26	C1	202	PEB	C2C-C1C-CHB-C4B
26	C1	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	C1	202	PEB	C4A-C3A-CAA-CBA
26	C1	202	PEB	NB-C1B-CHA-C4A
26	C1	202	PEB	C2B-C1B-CHA-C4A
26	D1	201	PEB	ND-C1D-CHC-C4C
26	D1	201	PEB	C2D-C1D-CHC-C4C
26	D1	201	PEB	C2C-CAC-CBC-CGC
26	D1	201	PEB	NB-C1B-CHA-C4A
26	D1	201	PEB	C2B-C1B-CHA-C4A
26	D1	202	PEB	NC-C1C-CHB-C4B
26	D1	202	PEB	C2A-C3A-CAA-CBA
26	D1	202	PEB	C4A-C3A-CAA-CBA
26	D1	202	PEB	NB-C1B-CHA-C4A
26	D1	202	PEB	C2B-C1B-CHA-C4A
26	D1	203	PEB	NC-C1C-CHB-C4B
26	D1	203	PEB	C2C-C1C-CHB-C4B
26	D1	203	PEB	C4A-C3A-CAA-CBA
26	D1	203	PEB	NB-C1B-CHA-C4A
26	D1	203	PEB	C2B-C1B-CHA-C4A
26	E1	201	PEB	ND-C1D-CHC-C4C
26	E1	201	PEB	C2A-C3A-CAA-CBA
26	E1	201	PEB	C4A-C3A-CAA-CBA
26	E1	201	PEB	NB-C1B-CHA-C4A
26	E1	201	PEB	C2B-C1B-CHA-C4A
26	E1	202	PEB	NC-C1C-CHB-C4B
26	E1	202	PEB	C2C-C1C-CHB-C4B
26	E1	202	PEB	C2A-C3A-CAA-CBA
26	E1	202	PEB	C4A-C3A-CAA-CBA
26	E1	202	PEB	NB-C1B-CHA-C4A
26	E1	202	PEB	C2B-C1B-CHA-C4A
26	F1	201	PEB	ND-C1D-CHC-C4C
26	F1	201	PEB	C2C-CAC-CBC-CGC
26	F1	201	PEB	NB-C1B-CHA-C4A
26	F1	201	PEB	C2B-C1B-CHA-C4A
26	F1	202	PEB	C2A-C3A-CAA-CBA
26	F1	202	PEB	C4A-C3A-CAA-CBA
26	F1	202	PEB	NB-C1B-CHA-C4A
26	F1	202	PEB	C2B-C1B-CHA-C4A
26	F1	203	PEB	NC-C1C-CHB-C4B
26	F1	203	PEB	C2C-C1C-CHB-C4B
26	F1	203	PEB	NB-C1B-CHA-C4A
26	F1	203	PEB	C2B-C1B-CHA-C4A
26	G1	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	G1	201	PEB	C2C-CAC-CBC-CGC
26	G1	201	PEB	C2A-C3A-CAA-CBA
26	G1	201	PEB	C4A-C3A-CAA-CBA
26	G1	201	PEB	NB-C1B-CHA-C4A
26	G1	201	PEB	C2B-C1B-CHA-C4A
26	G1	202	PEB	NB-C1B-CHA-C4A
26	G1	202	PEB	C2B-C1B-CHA-C4A
26	H1	201	PEB	ND-C1D-CHC-C4C
26	H1	201	PEB	NB-C1B-CHA-C4A
26	H1	201	PEB	C2B-C1B-CHA-C4A
26	H1	201	PEB	C3B-CAB-CBB-CGB
26	H1	202	PEB	NC-C1C-CHB-C4B
26	H1	202	PEB	C4A-C3A-CAA-CBA
26	H1	202	PEB	NB-C1B-CHA-C4A
26	H1	202	PEB	C2B-C1B-CHA-C4A
26	H1	203	PEB	NC-C1C-CHB-C4B
26	H1	203	PEB	C2C-C1C-CHB-C4B
26	H1	203	PEB	NB-C1B-CHA-C4A
26	H1	203	PEB	C2B-C1B-CHA-C4A
26	I1	201	PEB	C2A-C3A-CAA-CBA
26	I1	201	PEB	C4A-C3A-CAA-CBA
26	I1	201	PEB	NB-C1B-CHA-C4A
26	I1	201	PEB	C2B-C1B-CHA-C4A
26	I1	202	PEB	NC-C1C-CHB-C4B
26	I1	202	PEB	C2C-C1C-CHB-C4B
26	I1	202	PEB	NB-C1B-CHA-C4A
26	I1	202	PEB	C2B-C1B-CHA-C4A
26	J1	201	PEB	ND-C1D-CHC-C4C
26	J1	201	PEB	C2D-C1D-CHC-C4C
26	J1	201	PEB	C4A-C3A-CAA-CBA
26	J1	201	PEB	NB-C1B-CHA-C4A
26	J1	201	PEB	C2B-C1B-CHA-C4A
26	J1	202	PEB	C2A-C3A-CAA-CBA
26	J1	202	PEB	C4A-C3A-CAA-CBA
26	J1	202	PEB	NB-C1B-CHA-C4A
26	J1	202	PEB	C2B-C1B-CHA-C4A
26	J1	203	PEB	C2C-CAC-CBC-CGC
26	J1	203	PEB	NB-C1B-CHA-C4A
26	J1	203	PEB	C2B-C1B-CHA-C4A
26	K1	201	PEB	ND-C1D-CHC-C4C
26	K1	201	PEB	C2D-C1D-CHC-C4C
26	K1	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	K1	201	PEB	C2B-C1B-CHA-C4A
26	K1	202	PEB	ND-C1D-CHC-C4C
26	K1	202	PEB	C2D-C1D-CHC-C4C
26	K1	202	PEB	NC-C1C-CHB-C4B
26	K1	202	PEB	C2C-C1C-CHB-C4B
26	K1	202	PEB	C2A-C3A-CAA-CBA
26	K1	202	PEB	NB-C1B-CHA-C4A
26	K1	202	PEB	C2B-C1B-CHA-C4A
26	L1	201	PEB	ND-C1D-CHC-C4C
26	L1	201	PEB	C2D-C1D-CHC-C4C
26	L1	201	PEB	C2C-CAC-CBC-CGC
26	L1	201	PEB	C2D-C3D-CAD-CBD
26	L1	201	PEB	C4D-C3D-CAD-CBD
26	L1	201	PEB	C4A-C3A-CAA-CBA
26	L1	201	PEB	NB-C1B-CHA-C4A
26	L1	201	PEB	C2B-C1B-CHA-C4A
26	L1	202	PEB	C4A-C3A-CAA-CBA
26	L1	202	PEB	NB-C1B-CHA-C4A
26	L1	202	PEB	C2B-C1B-CHA-C4A
26	L1	203	PEB	ND-C1D-CHC-C4C
26	L1	203	PEB	C2D-C1D-CHC-C4C
26	L1	203	PEB	NC-C1C-CHB-C4B
26	L1	203	PEB	C2A-C3A-CAA-CBA
26	L1	203	PEB	C4A-C3A-CAA-CBA
26	L1	203	PEB	NB-C1B-CHA-C4A
26	L1	203	PEB	C2B-C1B-CHA-C4A
26	M1	401	PEB	C2D-C3D-CAD-CBD
26	M1	401	PEB	C4D-C3D-CAD-CBD
26	M1	401	PEB	C2A-C3A-CAA-CBA
26	M1	401	PEB	NB-C1B-CHA-C4A
26	M1	401	PEB	C2B-C1B-CHA-C4A
26	M1	402	PEB	ND-C1D-CHC-C4C
26	M1	402	PEB	NC-C1C-CHB-C4B
26	M1	402	PEB	C2C-C1C-CHB-C4B
26	M1	402	PEB	NB-C1B-CHA-C4A
26	M1	402	PEB	C2B-C1B-CHA-C4A
26	M1	403	PEB	C2A-C3A-CAA-CBA
26	M1	403	PEB	NB-C1B-CHA-C4A
26	M1	403	PEB	C2B-C1B-CHA-C4A
26	N1	201	PEB	NB-C1B-CHA-C4A
26	N1	201	PEB	C2B-C1B-CHA-C4A
26	N1	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	N1	202	PEB	C2C-C1C-CHB-C4B
26	N1	202	PEB	C4A-C3A-CAA-CBA
26	N1	202	PEB	NB-C1B-CHA-C4A
26	N1	202	PEB	C2B-C1B-CHA-C4A
26	N1	203	PEB	ND-C1D-CHC-C4C
26	N1	203	PEB	C2D-C1D-CHC-C4C
26	N1	203	PEB	C4A-C3A-CAA-CBA
26	N1	203	PEB	NB-C1B-CHA-C4A
26	N1	203	PEB	C2B-C1B-CHA-C4A
26	O1	201	PEB	C2C-CAC-CBC-CGC
26	O1	201	PEB	C2A-C3A-CAA-CBA
26	O1	201	PEB	C4A-C3A-CAA-CBA
26	O1	201	PEB	NB-C1B-CHA-C4A
26	O1	201	PEB	C2B-C1B-CHA-C4A
26	O1	202	PEB	NC-C1C-CHB-C4B
26	O1	202	PEB	C2C-C1C-CHB-C4B
26	O1	202	PEB	NB-C1B-CHA-C4A
26	O1	202	PEB	C2B-C1B-CHA-C4A
26	P1	201	PEB	ND-C1D-CHC-C4C
26	P1	201	PEB	C2D-C1D-CHC-C4C
26	P1	201	PEB	C1C-C2C-CAC-CBC
26	P1	201	PEB	C3C-C2C-CAC-CBC
26	P1	201	PEB	C4A-C3A-CAA-CBA
26	P1	201	PEB	NB-C1B-CHA-C4A
26	P1	201	PEB	C2B-C1B-CHA-C4A
26	P1	202	PEB	NB-C1B-CHA-C4A
26	P1	202	PEB	C2B-C1B-CHA-C4A
26	P1	203	PEB	C4A-C3A-CAA-CBA
26	P1	203	PEB	NB-C1B-CHA-C4A
26	P1	203	PEB	C2B-C1B-CHA-C4A
26	P1	203	PEB	C3B-CAB-CBB-CGB
26	Q1	201	PEB	NB-C1B-CHA-C4A
26	Q1	201	PEB	C2B-C1B-CHA-C4A
26	Q1	202	PEB	C2C-C1C-CHB-C4B
26	Q1	202	PEB	NB-C1B-CHA-C4A
26	Q1	202	PEB	C2B-C1B-CHA-C4A
26	R1	201	PEB	C2A-C3A-CAA-CBA
26	R1	201	PEB	C4A-C3A-CAA-CBA
26	R1	201	PEB	NB-C1B-CHA-C4A
26	R1	201	PEB	C2B-C1B-CHA-C4A
26	R1	202	PEB	C4A-C3A-CAA-CBA
26	R1	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	R1	202	PEB	C2B-C1B-CHA-C4A
26	R1	203	PEB	ND-C1D-CHC-C4C
26	R1	203	PEB	C2D-C1D-CHC-C4C
26	R1	203	PEB	NB-C1B-CHA-C4A
26	R1	203	PEB	C2B-C1B-CHA-C4A
26	S1	201	PEB	ND-C1D-CHC-C4C
26	S1	201	PEB	C2D-C1D-CHC-C4C
26	S1	201	PEB	NB-C1B-CHA-C4A
26	S1	201	PEB	C2B-C1B-CHA-C4A
26	S1	202	PEB	NC-C1C-CHB-C4B
26	S1	202	PEB	C2C-C1C-CHB-C4B
26	S1	202	PEB	NB-C1B-CHA-C4A
26	S1	202	PEB	C2B-C1B-CHA-C4A
26	T1	201	PEB	NC-C1C-CHB-C4B
26	T1	201	PEB	C4A-C3A-CAA-CBA
26	T1	201	PEB	NB-C1B-CHA-C4A
26	T1	201	PEB	C2B-C1B-CHA-C4A
26	T1	202	PEB	C2A-C3A-CAA-CBA
26	T1	202	PEB	C4A-C3A-CAA-CBA
26	T1	202	PEB	NB-C1B-CHA-C4A
26	T1	202	PEB	C2B-C1B-CHA-C4A
26	T1	203	PEB	C2A-C3A-CAA-CBA
26	T1	203	PEB	C4A-C3A-CAA-CBA
26	T1	203	PEB	NB-C1B-CHA-C4A
26	T1	203	PEB	C2B-C1B-CHA-C4A
26	U1	201	PEB	NB-C1B-CHA-C4A
26	U1	201	PEB	C2B-C1B-CHA-C4A
26	U1	202	PEB	NB-C1B-CHA-C4A
26	U1	202	PEB	C2B-C1B-CHA-C4A
26	V1	201	PEB	C2A-C3A-CAA-CBA
26	V1	201	PEB	C4A-C3A-CAA-CBA
26	V1	201	PEB	NB-C1B-CHA-C4A
26	V1	201	PEB	C2B-C1B-CHA-C4A
26	V1	202	PEB	C2C-CAC-CBC-CGC
26	V1	202	PEB	C4A-C3A-CAA-CBA
26	V1	202	PEB	NB-C1B-CHA-C4A
26	V1	202	PEB	C2B-C1B-CHA-C4A
26	V1	203	PEB	ND-C1D-CHC-C4C
26	V1	203	PEB	C2D-C1D-CHC-C4C
26	V1	203	PEB	C2A-C3A-CAA-CBA
26	V1	203	PEB	C4A-C3A-CAA-CBA
26	V1	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	V1	203	PEB	C2B-C1B-CHA-C4A
26	W1	201	PEB	C1C-C2C-CAC-CBC
26	W1	201	PEB	C3C-C2C-CAC-CBC
26	W1	201	PEB	NB-C1B-CHA-C4A
26	W1	201	PEB	C2B-C1B-CHA-C4A
26	W1	202	PEB	NB-C1B-CHA-C4A
26	W1	202	PEB	C2B-C1B-CHA-C4A
26	X1	201	PEB	ND-C1D-CHC-C4C
26	X1	201	PEB	C2D-C1D-CHC-C4C
26	X1	201	PEB	C3C-C2C-CAC-CBC
26	X1	201	PEB	C4A-C3A-CAA-CBA
26	X1	201	PEB	NB-C1B-CHA-C4A
26	X1	201	PEB	C2B-C1B-CHA-C4A
26	X1	202	PEB	C2C-C1C-CHB-C4B
26	X1	202	PEB	C2A-C3A-CAA-CBA
26	X1	202	PEB	C4A-C3A-CAA-CBA
26	X1	202	PEB	NB-C1B-CHA-C4A
26	X1	202	PEB	C2B-C1B-CHA-C4A
26	X1	203	PEB	C2C-C1C-CHB-C4B
26	X1	203	PEB	NB-C1B-CHA-C4A
26	X1	203	PEB	C2B-C1B-CHA-C4A
26	Y1	201	PEB	NB-C1B-CHA-C4A
26	Y1	201	PEB	C2B-C1B-CHA-C4A
26	Y1	202	PEB	NB-C1B-CHA-C4A
26	Y1	202	PEB	C2B-C1B-CHA-C4A
26	Z1	201	PEB	NB-C1B-CHA-C4A
26	Z1	201	PEB	C2B-C1B-CHA-C4A
26	Z1	202	PEB	ND-C1D-CHC-C4C
26	Z1	202	PEB	C2D-C1D-CHC-C4C
26	Z1	202	PEB	NC-C1C-CHB-C4B
26	Z1	202	PEB	C2C-C1C-CHB-C4B
26	Z1	202	PEB	C4A-C3A-CAA-CBA
26	Z1	202	PEB	NB-C1B-CHA-C4A
26	Z1	202	PEB	C2B-C1B-CHA-C4A
26	a1	201	PEB	NB-C1B-CHA-C4A
26	a1	201	PEB	C2B-C1B-CHA-C4A
26	a1	202	PEB	NC-C1C-CHB-C4B
26	a1	202	PEB	NB-C1B-CHA-C4A
26	a1	202	PEB	C2B-C1B-CHA-C4A
26	a1	203	PEB	ND-C1D-CHC-C4C
26	a1	203	PEB	C2D-C1D-CHC-C4C
26	a1	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	a1	203	PEB	C2C-C1C-CHB-C4B
26	a1	203	PEB	NB-C1B-CHA-C4A
26	a1	203	PEB	C2B-C1B-CHA-C4A
26	b1	501	PEB	NB-C1B-CHA-C4A
26	b1	501	PEB	C2B-C1B-CHA-C4A
26	c1	201	PEB	NC-C1C-CHB-C4B
26	c1	201	PEB	C2C-C1C-CHB-C4B
26	c1	201	PEB	C2A-C3A-CAA-CBA
26	c1	201	PEB	C4A-C3A-CAA-CBA
26	c1	201	PEB	NB-C1B-CHA-C4A
26	c1	201	PEB	C2B-C1B-CHA-C4A
26	c1	202	PEB	C1C-C2C-CAC-CBC
26	c1	202	PEB	C3C-C2C-CAC-CBC
26	c1	202	PEB	NB-C1B-CHA-C4A
26	c1	202	PEB	C2B-C1B-CHA-C4A
26	c1	203	PEB	C4A-C3A-CAA-CBA
26	c1	203	PEB	NB-C1B-CHA-C4A
26	c1	203	PEB	C2B-C1B-CHA-C4A
26	d1	201	PEB	ND-C1D-CHC-C4C
26	d1	201	PEB	C2D-C1D-CHC-C4C
26	d1	201	PEB	NC-C1C-CHB-C4B
26	d1	201	PEB	C2C-C1C-CHB-C4B
26	d1	201	PEB	NB-C1B-CHA-C4A
26	d1	201	PEB	C2B-C1B-CHA-C4A
26	d1	202	PEB	NB-C1B-CHA-C4A
26	d1	202	PEB	C2B-C1B-CHA-C4A
26	d1	203	PEB	NC-C1C-CHB-C4B
26	d1	203	PEB	C2C-C1C-CHB-C4B
26	d1	203	PEB	NB-C1B-CHA-C4A
26	d1	203	PEB	C2B-C1B-CHA-C4A
26	e1	201	PEB	ND-C1D-CHC-C4C
26	e1	201	PEB	C2D-C1D-CHC-C4C
26	e1	201	PEB	NB-C1B-CHA-C4A
26	e1	201	PEB	C2B-C1B-CHA-C4A
26	e1	202	PEB	NC-C1C-CHB-C4B
26	e1	202	PEB	C2C-C1C-CHB-C4B
26	e1	202	PEB	C1C-C2C-CAC-CBC
26	e1	202	PEB	C3C-C2C-CAC-CBC
26	e1	202	PEB	NB-C1B-CHA-C4A
26	e1	202	PEB	C2B-C1B-CHA-C4A
26	f1	201	PEB	ND-C1D-CHC-C4C
26	f1	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	f1	201	PEB	C2B-C1B-CHA-C4A
26	f1	202	PEB	C2C-C1C-CHB-C4B
26	f1	202	PEB	NB-C1B-CHA-C4A
26	f1	202	PEB	C2B-C1B-CHA-C4A
26	g1	201	PEB	ND-C1D-CHC-C4C
26	g1	201	PEB	C2D-C1D-CHC-C4C
26	g1	201	PEB	NB-C1B-CHA-C4A
26	g1	201	PEB	C2B-C1B-CHA-C4A
26	g1	202	PEB	NB-C1B-CHA-C4A
26	g1	202	PEB	C2B-C1B-CHA-C4A
26	g1	203	PEB	ND-C1D-CHC-C4C
26	g1	203	PEB	NC-C1C-CHB-C4B
26	g1	203	PEB	C2C-C1C-CHB-C4B
26	g1	203	PEB	C2D-C3D-CAD-CBD
26	g1	203	PEB	C4D-C3D-CAD-CBD
26	g1	203	PEB	C2A-C3A-CAA-CBA
26	g1	203	PEB	C4A-C3A-CAA-CBA
26	g1	203	PEB	NB-C1B-CHA-C4A
26	g1	203	PEB	C2B-C1B-CHA-C4A
26	h1	201	PEB	ND-C1D-CHC-C4C
26	h1	201	PEB	C2D-C1D-CHC-C4C
26	h1	201	PEB	NB-C1B-CHA-C4A
26	h1	201	PEB	C2B-C1B-CHA-C4A
26	h1	202	PEB	NC-C1C-CHB-C4B
26	h1	202	PEB	C2C-C1C-CHB-C4B
26	h1	202	PEB	NB-C1B-CHA-C4A
26	h1	202	PEB	C2B-C1B-CHA-C4A
26	i1	201	PEB	NC-C1C-CHB-C4B
26	i1	201	PEB	C2C-C1C-CHB-C4B
26	i1	201	PEB	C2A-C3A-CAA-CBA
26	i1	201	PEB	C4A-C3A-CAA-CBA
26	i1	201	PEB	NB-C1B-CHA-C4A
26	i1	201	PEB	C2B-C1B-CHA-C4A
26	i1	202	PEB	C2A-C3A-CAA-CBA
26	i1	202	PEB	C4A-C3A-CAA-CBA
26	i1	202	PEB	NB-C1B-CHA-C4A
26	i1	202	PEB	C2B-C1B-CHA-C4A
26	i1	203	PEB	NC-C1C-CHB-C4B
26	i1	203	PEB	NB-C1B-CHA-C4A
26	i1	203	PEB	C2B-C1B-CHA-C4A
26	j1	201	PEB	ND-C1D-CHC-C4C
26	j1	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	j1	201	PEB	C4A-C3A-CAA-CBA
26	j1	201	PEB	NB-C1B-CHA-C4A
26	j1	201	PEB	C2B-C1B-CHA-C4A
26	j1	201	PEB	C2B-C3B-CAB-CBB
26	j1	202	PEB	NB-C1B-CHA-C4A
26	j1	202	PEB	C2B-C1B-CHA-C4A
26	k1	201	PEB	C4A-C3A-CAA-CBA
26	k1	201	PEB	NB-C1B-CHA-C4A
26	k1	201	PEB	C2B-C1B-CHA-C4A
26	k1	202	PEB	NB-C1B-CHA-C4A
26	k1	202	PEB	C2B-C1B-CHA-C4A
26	k1	203	PEB	C4A-C3A-CAA-CBA
26	k1	203	PEB	NB-C1B-CHA-C4A
26	k1	203	PEB	C2B-C1B-CHA-C4A
26	l1	201	PEB	ND-C1D-CHC-C4C
26	l1	201	PEB	C2D-C1D-CHC-C4C
26	l1	201	PEB	NB-C1B-CHA-C4A
26	l1	201	PEB	C2B-C1B-CHA-C4A
26	l1	202	PEB	ND-C1D-CHC-C4C
26	l1	202	PEB	NC-C1C-CHB-C4B
26	l1	202	PEB	C2C-C1C-CHB-C4B
26	l1	202	PEB	NB-C1B-CHA-C4A
26	l1	202	PEB	C2B-C1B-CHA-C4A
26	m1	201	PEB	NC-C1C-CHB-C4B
26	m1	201	PEB	C2C-C1C-CHB-C4B
26	m1	201	PEB	C2A-C3A-CAA-CBA
26	m1	201	PEB	C4A-C3A-CAA-CBA
26	m1	201	PEB	NB-C1B-CHA-C4A
26	m1	201	PEB	C2B-C1B-CHA-C4A
26	m1	202	PEB	C4A-C3A-CAA-CBA
26	m1	202	PEB	NB-C1B-CHA-C4A
26	m1	202	PEB	C2B-C1B-CHA-C4A
26	m1	203	PEB	C1C-C2C-CAC-CBC
26	m1	203	PEB	C3C-C2C-CAC-CBC
26	m1	203	PEB	NB-C1B-CHA-C4A
26	m1	203	PEB	C2B-C1B-CHA-C4A
26	n1	201	PEB	NC-C1C-CHB-C4B
26	n1	201	PEB	C2C-C1C-CHB-C4B
26	n1	201	PEB	NB-C1B-CHA-C4A
26	n1	201	PEB	C2B-C1B-CHA-C4A
26	o1	501	PEB	C2A-C3A-CAA-CBA
26	o1	501	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	o1	501	PEB	NB-C1B-CHA-C4A
26	o1	501	PEB	C2B-C1B-CHA-C4A
26	p1	201	PEB	ND-C1D-CHC-C4C
26	p1	201	PEB	C2D-C1D-CHC-C4C
26	p1	201	PEB	NC-C1C-CHB-C4B
26	p1	201	PEB	C2C-C1C-CHB-C4B
26	p1	201	PEB	C2D-C3D-CAD-CBD
26	p1	201	PEB	C4D-C3D-CAD-CBD
26	p1	201	PEB	NB-C1B-CHA-C4A
26	p1	201	PEB	C2B-C1B-CHA-C4A
26	p1	202	PEB	ND-C1D-CHC-C4C
26	p1	202	PEB	C2D-C1D-CHC-C4C
26	p1	202	PEB	NC-C1C-CHB-C4B
26	p1	202	PEB	C2C-C1C-CHB-C4B
26	p1	202	PEB	C2A-C3A-CAA-CBA
26	p1	202	PEB	C4A-C3A-CAA-CBA
26	p1	202	PEB	NB-C1B-CHA-C4A
26	p1	202	PEB	C2B-C1B-CHA-C4A
26	q1	201	PEB	ND-C1D-CHC-C4C
26	q1	201	PEB	NC-C1C-CHB-C4B
26	q1	201	PEB	C2C-C1C-CHB-C4B
26	q1	201	PEB	NB-C1B-CHA-C4A
26	q1	201	PEB	C2B-C1B-CHA-C4A
26	q1	202	PEB	C4A-C3A-CAA-CBA
26	q1	202	PEB	NB-C1B-CHA-C4A
26	q1	202	PEB	C2B-C1B-CHA-C4A
26	q1	203	PEB	NB-C1B-CHA-C4A
26	q1	203	PEB	C2B-C1B-CHA-C4A
26	r1	201	PEB	ND-C1D-CHC-C4C
26	r1	201	PEB	C4A-C3A-CAA-CBA
26	r1	201	PEB	NB-C1B-CHA-C4A
26	r1	201	PEB	C2B-C1B-CHA-C4A
26	r1	202	PEB	ND-C1D-CHC-C4C
26	r1	202	PEB	C2D-C1D-CHC-C4C
26	r1	202	PEB	NC-C1C-CHB-C4B
26	r1	202	PEB	C2C-C1C-CHB-C4B
26	r1	202	PEB	C4A-C3A-CAA-CBA
26	r1	202	PEB	NB-C1B-CHA-C4A
26	r1	202	PEB	C2B-C1B-CHA-C4A
26	s1	201	PEB	ND-C1D-CHC-C4C
26	s1	201	PEB	C2D-C1D-CHC-C4C
26	s1	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	s1	201	PEB	C2B-C1B-CHA-C4A
26	s1	202	PEB	NC-C1C-CHB-C4B
26	s1	202	PEB	C2C-C1C-CHB-C4B
26	s1	202	PEB	NB-C1B-CHA-C4A
26	s1	202	PEB	C2B-C1B-CHA-C4A
26	s1	203	PEB	NC-C1C-CHB-C4B
26	s1	203	PEB	C2C-C1C-CHB-C4B
26	s1	203	PEB	NB-C1B-CHA-C4A
26	s1	203	PEB	C2B-C1B-CHA-C4A
26	t1	201	PEB	ND-C1D-CHC-C4C
26	t1	201	PEB	C2A-C3A-CAA-CBA
26	t1	201	PEB	C4A-C3A-CAA-CBA
26	t1	201	PEB	NB-C1B-CHA-C4A
26	t1	201	PEB	C2B-C1B-CHA-C4A
26	t1	202	PEB	ND-C1D-CHC-C4C
26	t1	202	PEB	NC-C1C-CHB-C4B
26	t1	202	PEB	C2C-C1C-CHB-C4B
26	t1	202	PEB	C4D-C3D-CAD-CBD
26	t1	202	PEB	C2A-C3A-CAA-CBA
26	t1	202	PEB	C4A-C3A-CAA-CBA
26	t1	202	PEB	NB-C1B-CHA-C4A
26	t1	202	PEB	C2B-C1B-CHA-C4A
26	u1	201	PEB	NC-C1C-CHB-C4B
26	u1	201	PEB	C2C-C1C-CHB-C4B
26	u1	201	PEB	C2C-CAC-CBC-CGC
26	u1	201	PEB	C4A-C3A-CAA-CBA
26	u1	201	PEB	NB-C1B-CHA-C4A
26	u1	201	PEB	C2B-C1B-CHA-C4A
26	u1	202	PEB	C4A-C3A-CAA-CBA
26	u1	202	PEB	NB-C1B-CHA-C4A
26	u1	202	PEB	C2B-C1B-CHA-C4A
26	u1	203	PEB	NC-C1C-CHB-C4B
26	u1	203	PEB	C2C-C1C-CHB-C4B
26	u1	203	PEB	NB-C1B-CHA-C4A
26	u1	203	PEB	C2B-C1B-CHA-C4A
26	v1	201	PEB	ND-C1D-CHC-C4C
26	v1	201	PEB	C2A-C3A-CAA-CBA
26	v1	201	PEB	C4A-C3A-CAA-CBA
26	v1	201	PEB	NB-C1B-CHA-C4A
26	v1	201	PEB	C2B-C1B-CHA-C4A
26	v1	202	PEB	NC-C1C-CHB-C4B
26	v1	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	v1	202	PEB	NB-C1B-CHA-C4A
26	v1	202	PEB	C2B-C1B-CHA-C4A
26	w1	201	PEB	ND-C1D-CHC-C4C
26	w1	201	PEB	NC-C1C-CHB-C4B
26	w1	201	PEB	C4A-C3A-CAA-CBA
26	w1	201	PEB	NB-C1B-CHA-C4A
26	w1	201	PEB	C2B-C1B-CHA-C4A
26	w1	202	PEB	NC-C1C-CHB-C4B
26	w1	202	PEB	C2C-C1C-CHB-C4B
26	w1	202	PEB	C2D-C3D-CAD-CBD
26	w1	202	PEB	C4D-C3D-CAD-CBD
26	w1	202	PEB	C4A-C3A-CAA-CBA
26	w1	202	PEB	NB-C1B-CHA-C4A
26	w1	202	PEB	C2B-C1B-CHA-C4A
26	w1	203	PEB	NC-C1C-CHB-C4B
26	w1	203	PEB	C2C-C1C-CHB-C4B
26	w1	203	PEB	NB-C1B-CHA-C4A
26	w1	203	PEB	C2B-C1B-CHA-C4A
26	x1	201	PEB	ND-C1D-CHC-C4C
26	x1	201	PEB	C2D-C1D-CHC-C4C
26	x1	201	PEB	C2C-CAC-CBC-CGC
26	x1	201	PEB	NB-C1B-CHA-C4A
26	x1	201	PEB	C2B-C1B-CHA-C4A
26	x1	202	PEB	NC-C1C-CHB-C4B
26	x1	202	PEB	C2C-C1C-CHB-C4B
26	x1	202	PEB	NB-C1B-CHA-C4A
26	x1	202	PEB	C2B-C1B-CHA-C4A
26	y1	201	PEB	ND-C1D-CHC-C4C
26	y1	201	PEB	NB-C1B-CHA-C4A
26	y1	201	PEB	C2B-C1B-CHA-C4A
26	y1	202	PEB	NB-C1B-CHA-C4A
26	y1	202	PEB	C2B-C1B-CHA-C4A
26	y1	203	PEB	ND-C1D-CHC-C4C
26	y1	203	PEB	C2D-C1D-CHC-C4C
26	y1	203	PEB	NC-C1C-CHB-C4B
26	y1	203	PEB	C2C-C1C-CHB-C4B
26	y1	203	PEB	NB-C1B-CHA-C4A
26	y1	203	PEB	C2B-C1B-CHA-C4A
26	z1	201	PEB	NC-C1C-CHB-C4B
26	z1	201	PEB	C2C-C1C-CHB-C4B
26	z1	201	PEB	NB-C1B-CHA-C4A
26	z1	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	z1	202	PEB	ND-C1D-CHC-C4C
26	z1	202	PEB	NC-C1C-CHB-C4B
26	z1	202	PEB	C2C-C1C-CHB-C4B
26	z1	202	PEB	NB-C1B-CHA-C4A
26	z1	202	PEB	C2B-C1B-CHA-C4A
26	11	201	PEB	ND-C1D-CHC-C4C
26	11	201	PEB	NC-C1C-CHB-C4B
26	11	201	PEB	NB-C1B-CHA-C4A
26	11	201	PEB	C2B-C1B-CHA-C4A
26	11	202	PEB	C2A-C3A-CAA-CBA
26	11	202	PEB	C4A-C3A-CAA-CBA
26	11	202	PEB	NB-C1B-CHA-C4A
26	11	202	PEB	C2B-C1B-CHA-C4A
26	11	203	PEB	NC-C1C-CHB-C4B
26	11	203	PEB	C2C-C1C-CHB-C4B
26	11	203	PEB	NB-C1B-CHA-C4A
26	11	203	PEB	C2B-C1B-CHA-C4A
26	21	401	PEB	NC-C1C-CHB-C4B
26	21	401	PEB	C2C-C1C-CHB-C4B
26	21	401	PEB	C4D-C3D-CAD-CBD
26	21	401	PEB	C2A-C3A-CAA-CBA
26	21	401	PEB	C4A-C3A-CAA-CBA
26	21	401	PEB	NB-C1B-CHA-C4A
26	21	401	PEB	C2B-C1B-CHA-C4A
26	21	404	PEB	ND-C1D-CHC-C4C
26	21	404	PEB	NB-C1B-CHA-C4A
26	21	404	PEB	C2B-C1B-CHA-C4A
26	21	405	PEB	ND-C1D-CHC-C4C
26	21	405	PEB	C2C-CAC-CBC-CGC
26	21	405	PEB	C2A-C3A-CAA-CBA
26	21	405	PEB	NB-C1B-CHA-C4A
26	21	405	PEB	C2B-C1B-CHA-C4A
26	A2	301	PEB	C2C-CAC-CBC-CGC
26	A2	301	PEB	NB-C1B-CHA-C4A
26	A2	301	PEB	C2B-C1B-CHA-C4A
26	A2	304	PEB	NC-C1C-CHB-C4B
26	A2	304	PEB	C2A-C3A-CAA-CBA
26	A2	304	PEB	C4A-C3A-CAA-CBA
26	A2	304	PEB	NB-C1B-CHA-C4A
26	A2	304	PEB	C2B-C1B-CHA-C4A
26	A2	305	PEB	NC-C1C-CHB-C4B
26	A2	305	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	A2	305	PEB	C2A-C3A-CAA-CBA
26	A2	305	PEB	C4A-C3A-CAA-CBA
26	A2	305	PEB	NB-C1B-CHA-C4A
26	A2	305	PEB	C2B-C1B-CHA-C4A
26	D2	1002	PEB	NB-C1B-CHA-C4A
26	D2	1002	PEB	C2B-C1B-CHA-C4A
26	F2	1002	PEB	C2A-C3A-CAA-CBA
26	F2	1002	PEB	C4A-C3A-CAA-CBA
26	F2	1002	PEB	NB-C1B-CHA-C4A
26	F2	1002	PEB	C2B-C1B-CHA-C4A
26	H2	1002	PEB	C2C-CAC-CBC-CGC
26	H2	1002	PEB	NB-C1B-CHA-C4A
26	H2	1002	PEB	C2B-C1B-CHA-C4A
26	J2	1002	PEB	ND-C1D-CHC-C4C
26	J2	1002	PEB	C2D-C1D-CHC-C4C
26	J2	1002	PEB	C4A-C3A-CAA-CBA
26	J2	1002	PEB	NB-C1B-CHA-C4A
26	J2	1002	PEB	C2B-C1B-CHA-C4A
26	L2	1002	PEB	ND-C1D-CHC-C4C
26	L2	1002	PEB	C2D-C1D-CHC-C4C
26	L2	1002	PEB	C2C-CAC-CBC-CGC
26	L2	1002	PEB	NB-C1B-CHA-C4A
26	L2	1002	PEB	C2B-C1B-CHA-C4A
26	N2	1002	PEB	C4A-C3A-CAA-CBA
26	N2	1002	PEB	NB-C1B-CHA-C4A
26	N2	1002	PEB	C2B-C1B-CHA-C4A
26	O2	201	PEB	C2A-C3A-CAA-CBA
26	O2	201	PEB	C4A-C3A-CAA-CBA
26	O2	201	PEB	NB-C1B-CHA-C4A
26	O2	201	PEB	C2B-C1B-CHA-C4A
26	O2	202	PEB	ND-C1D-CHC-C4C
26	O2	202	PEB	C2A-C3A-CAA-CBA
26	O2	202	PEB	NB-C1B-CHA-C4A
26	O2	202	PEB	C2B-C1B-CHA-C4A
26	P2	201	PEB	NB-C1B-CHA-C4A
26	P2	201	PEB	C2B-C1B-CHA-C4A
26	P2	202	PEB	NB-C1B-CHA-C4A
26	P2	202	PEB	C2B-C1B-CHA-C4A
26	P2	203	PEB	NB-C1B-CHA-C4A
26	P2	203	PEB	C2B-C1B-CHA-C4A
26	Q2	201	PEB	C4A-C3A-CAA-CBA
26	Q2	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	Q2	201	PEB	C2B-C1B-CHA-C4A
26	Q2	202	PEB	ND-C1D-CHC-C4C
26	Q2	202	PEB	NB-C1B-CHA-C4A
26	Q2	202	PEB	C2B-C1B-CHA-C4A
26	R2	201	PEB	NB-C1B-CHA-C4A
26	R2	201	PEB	C2B-C1B-CHA-C4A
26	R2	202	PEB	NB-C1B-CHA-C4A
26	R2	202	PEB	C2B-C1B-CHA-C4A
26	R2	203	PEB	NC-C1C-CHB-C4B
26	R2	203	PEB	C2C-C1C-CHB-C4B
26	R2	203	PEB	NB-C1B-CHA-C4A
26	R2	203	PEB	C2B-C1B-CHA-C4A
26	S2	201	PEB	C2A-C3A-CAA-CBA
26	S2	201	PEB	C4A-C3A-CAA-CBA
26	S2	201	PEB	NB-C1B-CHA-C4A
26	S2	201	PEB	C2B-C1B-CHA-C4A
26	S2	202	PEB	ND-C1D-CHC-C4C
26	S2	202	PEB	C4A-C3A-CAA-CBA
26	S2	202	PEB	NB-C1B-CHA-C4A
26	S2	202	PEB	C2B-C1B-CHA-C4A
26	T2	201	PEB	NB-C1B-CHA-C4A
26	T2	201	PEB	C2B-C1B-CHA-C4A
26	T2	202	PEB	NB-C1B-CHA-C4A
26	T2	202	PEB	C2B-C1B-CHA-C4A
26	T2	203	PEB	NC-C1C-CHB-C4B
26	T2	203	PEB	C2C-C1C-CHB-C4B
26	T2	203	PEB	C2A-C3A-CAA-CBA
26	T2	203	PEB	C4A-C3A-CAA-CBA
26	T2	203	PEB	NB-C1B-CHA-C4A
26	T2	203	PEB	C2B-C1B-CHA-C4A
26	U2	201	PEB	NC-C1C-CHB-C4B
26	U2	201	PEB	C2A-C3A-CAA-CBA
26	U2	201	PEB	C4A-C3A-CAA-CBA
26	U2	201	PEB	NB-C1B-CHA-C4A
26	U2	202	PEB	ND-C1D-CHC-C4C
26	U2	202	PEB	C2D-C1D-CHC-C4C
26	U2	202	PEB	NB-C1B-CHA-C4A
26	U2	202	PEB	C2B-C1B-CHA-C4A
26	V2	201	PEB	C2A-C3A-CAA-CBA
26	V2	201	PEB	C4A-C3A-CAA-CBA
26	V2	201	PEB	NB-C1B-CHA-C4A
26	V2	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	V2	202	PEB	ND-C1D-CHC-C4C
26	V2	202	PEB	C2D-C3D-CAD-CBD
26	V2	202	PEB	C4D-C3D-CAD-CBD
26	V2	202	PEB	C2A-C3A-CAA-CBA
26	V2	202	PEB	NB-C1B-CHA-C4A
26	V2	202	PEB	C2B-C1B-CHA-C4A
26	V2	203	PEB	NC-C1C-CHB-C4B
26	V2	203	PEB	C2C-C1C-CHB-C4B
26	V2	203	PEB	C2A-C3A-CAA-CBA
26	V2	203	PEB	C4A-C3A-CAA-CBA
26	V2	203	PEB	NB-C1B-CHA-C4A
26	V2	203	PEB	C2B-C1B-CHA-C4A
26	V2	203	PEB	C3B-CAB-CBB-CGB
26	W2	201	PEB	NC-C1C-CHB-C4B
26	W2	201	PEB	C4A-C3A-CAA-CBA
26	W2	201	PEB	NB-C1B-CHA-C4A
26	W2	201	PEB	C2B-C1B-CHA-C4A
26	Y2	201	PEB	NB-C1B-CHA-C4A
26	Y2	201	PEB	C2B-C1B-CHA-C4A
26	Y2	202	PEB	NB-C1B-CHA-C4A
26	Y2	202	PEB	C2B-C1B-CHA-C4A
26	Y2	203	PEB	NC-C1C-CHB-C4B
26	Y2	203	PEB	C2C-C1C-CHB-C4B
26	Y2	203	PEB	C2A-C3A-CAA-CBA
26	Y2	203	PEB	C4A-C3A-CAA-CBA
26	Y2	203	PEB	NB-C1B-CHA-C4A
26	Y2	203	PEB	C2B-C1B-CHA-C4A
26	Z2	201	PEB	C4A-C3A-CAA-CBA
26	Z2	201	PEB	NB-C1B-CHA-C4A
26	Z2	201	PEB	C2B-C1B-CHA-C4A
26	Z2	202	PEB	ND-C1D-CHC-C4C
26	Z2	202	PEB	C2D-C1D-CHC-C4C
26	Z2	202	PEB	NB-C1B-CHA-C4A
26	Z2	202	PEB	C2B-C1B-CHA-C4A
26	a2	201	PEB	NB-C1B-CHA-C4A
26	a2	201	PEB	C2B-C1B-CHA-C4A
26	a2	202	PEB	NB-C1B-CHA-C4A
26	a2	202	PEB	C2B-C1B-CHA-C4A
26	a2	203	PEB	C2C-C1C-CHB-C4B
26	a2	203	PEB	C2A-C3A-CAA-CBA
26	a2	203	PEB	C4A-C3A-CAA-CBA
26	a2	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	a2	203	PEB	C2B-C1B-CHA-C4A
26	b2	201	PEB	C4A-C3A-CAA-CBA
26	b2	201	PEB	NB-C1B-CHA-C4A
26	b2	201	PEB	C2B-C1B-CHA-C4A
26	b2	202	PEB	ND-C1D-CHC-C4C
26	b2	202	PEB	NB-C1B-CHA-C4A
26	b2	202	PEB	C2B-C1B-CHA-C4A
26	c2	201	PEB	NB-C1B-CHA-C4A
26	c2	201	PEB	C2B-C1B-CHA-C4A
26	c2	202	PEB	ND-C1D-CHC-C4C
26	c2	202	PEB	C2D-C1D-CHC-C4C
26	c2	202	PEB	NB-C1B-CHA-C4A
26	c2	202	PEB	C2B-C1B-CHA-C4A
26	c2	203	PEB	NC-C1C-CHB-C4B
26	c2	203	PEB	C2C-C1C-CHB-C4B
26	c2	203	PEB	NB-C1B-CHA-C4A
26	c2	203	PEB	C2B-C1B-CHA-C4A
26	d2	201	PEB	C4A-C3A-CAA-CBA
26	d2	201	PEB	NB-C1B-CHA-C4A
26	d2	201	PEB	C2B-C1B-CHA-C4A
26	d2	202	PEB	ND-C1D-CHC-C4C
26	d2	202	PEB	C2D-C1D-CHC-C4C
26	d2	202	PEB	NB-C1B-CHA-C4A
26	d2	202	PEB	C2B-C1B-CHA-C4A
26	e2	201	PEB	NB-C1B-CHA-C4A
26	e2	201	PEB	C2B-C1B-CHA-C4A
26	e2	202	PEB	C2C-CAC-CBC-CGC
26	e2	202	PEB	C2A-C3A-CAA-CBA
26	e2	202	PEB	NB-C1B-CHA-C4A
26	e2	202	PEB	C2B-C1B-CHA-C4A
26	e2	203	PEB	NC-C1C-CHB-C4B
26	e2	203	PEB	C2C-C1C-CHB-C4B
26	e2	203	PEB	NB-C1B-CHA-C4A
26	e2	203	PEB	C2B-C1B-CHA-C4A
26	f2	201	PEB	ND-C1D-CHC-C4C
26	f2	201	PEB	C2D-C1D-CHC-C4C
26	f2	201	PEB	C2A-C3A-CAA-CBA
26	f2	201	PEB	C4A-C3A-CAA-CBA
26	f2	201	PEB	NB-C1B-CHA-C4A
26	f2	201	PEB	C2B-C1B-CHA-C4A
26	f2	202	PEB	ND-C1D-CHC-C4C
26	f2	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	f2	202	PEB	C4A-C3A-CAA-CBA
26	f2	202	PEB	NB-C1B-CHA-C4A
26	f2	202	PEB	C2B-C1B-CHA-C4A
26	g2	201	PEB	NB-C1B-CHA-C4A
26	g2	201	PEB	C2B-C1B-CHA-C4A
26	g2	202	PEB	ND-C1D-CHC-C4C
26	g2	202	PEB	NB-C1B-CHA-C4A
26	g2	202	PEB	C2B-C1B-CHA-C4A
26	g2	203	PEB	NC-C1C-CHB-C4B
26	g2	203	PEB	C2C-C1C-CHB-C4B
26	g2	203	PEB	NB-C1B-CHA-C4A
26	g2	203	PEB	C2B-C1B-CHA-C4A
26	g2	203	PEB	C2B-C3B-CAB-CBB
26	h2	201	PEB	C4A-C3A-CAA-CBA
26	h2	201	PEB	NB-C1B-CHA-C4A
26	h2	201	PEB	C2B-C1B-CHA-C4A
26	h2	202	PEB	ND-C1D-CHC-C4C
26	h2	202	PEB	C4A-C3A-CAA-CBA
26	h2	202	PEB	NB-C1B-CHA-C4A
26	h2	202	PEB	C2B-C1B-CHA-C4A
26	i2	201	PEB	C2A-C3A-CAA-CBA
26	i2	201	PEB	C4A-C3A-CAA-CBA
26	i2	201	PEB	NB-C1B-CHA-C4A
26	i2	201	PEB	C2B-C1B-CHA-C4A
26	i2	202	PEB	ND-C1D-CHC-C4C
26	i2	202	PEB	C2A-C3A-CAA-CBA
26	i2	202	PEB	NB-C1B-CHA-C4A
26	i2	202	PEB	C2B-C1B-CHA-C4A
26	i2	203	PEB	NC-C1C-CHB-C4B
26	i2	203	PEB	C2C-C1C-CHB-C4B
26	i2	203	PEB	C2A-C3A-CAA-CBA
26	i2	203	PEB	C4A-C3A-CAA-CBA
26	i2	203	PEB	NB-C1B-CHA-C4A
26	i2	203	PEB	C2B-C1B-CHA-C4A
26	i2	203	PEB	C2B-C3B-CAB-CBB
26	i2	203	PEB	C4B-C3B-CAB-CBB
26	j2	201	PEB	ND-C1D-CHC-C4C
26	j2	201	PEB	C4A-C3A-CAA-CBA
26	j2	201	PEB	NB-C1B-CHA-C4A
26	j2	201	PEB	C2B-C1B-CHA-C4A
26	j2	202	PEB	ND-C1D-CHC-C4C
26	j2	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	j2	202	PEB	NC-C1C-CHB-C4B
26	j2	202	PEB	C2C-C1C-CHB-C4B
26	j2	202	PEB	NB-C1B-CHA-C4A
26	j2	202	PEB	C2B-C1B-CHA-C4A
26	k2	201	PEB	C2C-CAC-CBC-CGC
26	k2	201	PEB	C4A-C3A-CAA-CBA
26	k2	201	PEB	NB-C1B-CHA-C4A
26	k2	201	PEB	C2B-C1B-CHA-C4A
26	k2	202	PEB	ND-C1D-CHC-C4C
26	k2	202	PEB	NC-C1C-CHB-C4B
26	k2	202	PEB	C2C-CAC-CBC-CGC
26	k2	202	PEB	C2A-C3A-CAA-CBA
26	k2	202	PEB	NB-C1B-CHA-C4A
26	k2	202	PEB	C2B-C1B-CHA-C4A
26	k2	203	PEB	ND-C1D-CHC-C4C
26	k2	203	PEB	C2D-C1D-CHC-C4C
26	k2	203	PEB	NC-C1C-CHB-C4B
26	k2	203	PEB	C2C-C1C-CHB-C4B
26	k2	203	PEB	NB-C1B-CHA-C4A
26	k2	203	PEB	C2B-C1B-CHA-C4A
26	l2	201	PEB	ND-C1D-CHC-C4C
26	l2	201	PEB	C4A-C3A-CAA-CBA
26	l2	201	PEB	NB-C1B-CHA-C4A
26	l2	201	PEB	C2B-C1B-CHA-C4A
26	l2	202	PEB	ND-C1D-CHC-C4C
26	l2	202	PEB	C2D-C1D-CHC-C4C
26	l2	202	PEB	NB-C1B-CHA-C4A
26	l2	202	PEB	C2B-C1B-CHA-C4A
26	m2	201	PEB	C2A-C3A-CAA-CBA
26	m2	201	PEB	C4A-C3A-CAA-CBA
26	m2	201	PEB	NB-C1B-CHA-C4A
26	m2	201	PEB	C2B-C1B-CHA-C4A
26	m2	202	PEB	ND-C1D-CHC-C4C
26	m2	202	PEB	C2D-C1D-CHC-C4C
26	m2	202	PEB	NB-C1B-CHA-C4A
26	m2	202	PEB	C2B-C1B-CHA-C4A
26	m2	203	PEB	NC-C1C-CHB-C4B
26	m2	203	PEB	C2C-C1C-CHB-C4B
26	m2	203	PEB	NB-C1B-CHA-C4A
26	m2	203	PEB	C2B-C1B-CHA-C4A
26	m2	203	PEB	C2B-C3B-CAB-CBB
26	m2	203	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	e3	401	PEB	ND-C1D-CHC-C4C
26	e3	401	PEB	C2D-C1D-CHC-C4C
26	e3	401	PEB	NB-C1B-CHA-C4A
26	e3	401	PEB	C2B-C1B-CHA-C4A
26	A3	201	PEB	ND-C1D-CHC-C4C
26	A3	201	PEB	C2D-C1D-CHC-C4C
26	A3	201	PEB	NB-C1B-CHA-C4A
26	A3	201	PEB	C2B-C1B-CHA-C4A
26	A3	202	PEB	ND-C1D-CHC-C4C
26	A3	202	PEB	C2D-C1D-CHC-C4C
26	A3	202	PEB	C2D-C3D-CAD-CBD
26	A3	202	PEB	C4D-C3D-CAD-CBD
26	A3	202	PEB	C4A-C3A-CAA-CBA
26	A3	202	PEB	NB-C1B-CHA-C4A
26	A3	202	PEB	C2B-C1B-CHA-C4A
26	B3	201	PEB	NB-C1B-CHA-C4A
26	B3	201	PEB	C2B-C1B-CHA-C4A
26	B3	202	PEB	NB-C1B-CHA-C4A
26	B3	202	PEB	C2B-C1B-CHA-C4A
26	B3	203	PEB	NC-C1C-CHB-C4B
26	B3	203	PEB	C2C-C1C-CHB-C4B
26	B3	203	PEB	C2C-CAC-CBC-CGC
26	B3	203	PEB	NB-C1B-CHA-C4A
26	B3	203	PEB	C2B-C1B-CHA-C4A
26	C3	201	PEB	ND-C1D-CHC-C4C
26	C3	201	PEB	NC-C1C-CHB-C4B
26	C3	201	PEB	C2C-C1C-CHB-C4B
26	C3	201	PEB	C4A-C3A-CAA-CBA
26	C3	201	PEB	NB-C1B-CHA-C4A
26	C3	201	PEB	C2B-C1B-CHA-C4A
26	C3	202	PEB	NC-C1C-CHB-C4B
26	C3	202	PEB	C2C-C1C-CHB-C4B
26	C3	202	PEB	C2C-CAC-CBC-CGC
26	C3	202	PEB	C2A-C3A-CAA-CBA
26	C3	202	PEB	C4A-C3A-CAA-CBA
26	C3	202	PEB	NB-C1B-CHA-C4A
26	C3	202	PEB	C2B-C1B-CHA-C4A
26	D3	201	PEB	ND-C1D-CHC-C4C
26	D3	201	PEB	C2D-C1D-CHC-C4C
26	D3	201	PEB	NB-C1B-CHA-C4A
26	D3	201	PEB	C2B-C1B-CHA-C4A
26	D3	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	D3	202	PEB	NC-C1C-CHB-C4B
26	D3	202	PEB	C2C-CAC-CBC-CGC
26	D3	202	PEB	C4A-C3A-CAA-CBA
26	D3	202	PEB	NB-C1B-CHA-C4A
26	D3	202	PEB	C2B-C1B-CHA-C4A
26	D3	203	PEB	ND-C1D-CHC-C4C
26	D3	203	PEB	C2D-C1D-CHC-C4C
26	D3	203	PEB	NC-C1C-CHB-C4B
26	D3	203	PEB	C2C-C1C-CHB-C4B
26	D3	203	PEB	C2C-CAC-CBC-CGC
26	D3	203	PEB	NB-C1B-CHA-C4A
26	D3	203	PEB	C2B-C1B-CHA-C4A
26	E3	201	PEB	C2C-CAC-CBC-CGC
26	E3	201	PEB	NB-C1B-CHA-C4A
26	E3	201	PEB	C2B-C1B-CHA-C4A
26	E3	202	PEB	C4D-C3D-CAD-CBD
26	E3	202	PEB	C4A-C3A-CAA-CBA
26	E3	202	PEB	NB-C1B-CHA-C4A
26	E3	202	PEB	C2B-C1B-CHA-C4A
26	F3	201	PEB	C2C-CAC-CBC-CGC
26	F3	201	PEB	NB-C1B-CHA-C4A
26	F3	201	PEB	C2B-C1B-CHA-C4A
26	F3	202	PEB	C4A-C3A-CAA-CBA
26	F3	202	PEB	NB-C1B-CHA-C4A
26	F3	202	PEB	C2B-C1B-CHA-C4A
26	F3	203	PEB	ND-C1D-CHC-C4C
26	F3	203	PEB	NC-C1C-CHB-C4B
26	F3	203	PEB	C2C-C1C-CHB-C4B
26	F3	203	PEB	C1C-C2C-CAC-CBC
26	F3	203	PEB	C3C-C2C-CAC-CBC
26	F3	203	PEB	NB-C1B-CHA-C4A
26	F3	203	PEB	C2B-C1B-CHA-C4A
26	G3	201	PEB	NC-C1C-CHB-C4B
26	G3	201	PEB	C2C-C1C-CHB-C4B
26	G3	201	PEB	C4A-C3A-CAA-CBA
26	G3	201	PEB	NB-C1B-CHA-C4A
26	G3	201	PEB	C2B-C1B-CHA-C4A
26	G3	202	PEB	NC-C1C-CHB-C4B
26	G3	202	PEB	C2C-C1C-CHB-C4B
26	G3	202	PEB	C2C-CAC-CBC-CGC
26	G3	202	PEB	C2A-C3A-CAA-CBA
26	G3	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	G3	202	PEB	NB-C1B-CHA-C4A
26	G3	202	PEB	C2B-C1B-CHA-C4A
26	H3	201	PEB	NB-C1B-CHA-C4A
26	H3	201	PEB	C2B-C1B-CHA-C4A
26	H3	202	PEB	ND-C1D-CHC-C4C
26	H3	202	PEB	C2D-C1D-CHC-C4C
26	H3	202	PEB	C4A-C3A-CAA-CBA
26	H3	202	PEB	NB-C1B-CHA-C4A
26	H3	202	PEB	C2B-C1B-CHA-C4A
26	H3	203	PEB	NC-C1C-CHB-C4B
26	H3	203	PEB	C2C-C1C-CHB-C4B
26	H3	203	PEB	C2D-C3D-CAD-CBD
26	H3	203	PEB	C4D-C3D-CAD-CBD
26	H3	203	PEB	NB-C1B-CHA-C4A
26	H3	203	PEB	C2B-C1B-CHA-C4A
26	I3	201	PEB	ND-C1D-CHC-C4C
26	I3	201	PEB	C2D-C1D-CHC-C4C
26	I3	201	PEB	NC-C1C-CHB-C4B
26	I3	201	PEB	C2C-C1C-CHB-C4B
26	I3	201	PEB	C2C-CAC-CBC-CGC
26	I3	201	PEB	C2A-C3A-CAA-CBA
26	I3	201	PEB	C4A-C3A-CAA-CBA
26	I3	201	PEB	NB-C1B-CHA-C4A
26	I3	201	PEB	C2B-C1B-CHA-C4A
26	I3	202	PEB	NC-C1C-CHB-C4B
26	I3	202	PEB	C2C-C1C-CHB-C4B
26	I3	202	PEB	C4A-C3A-CAA-CBA
26	I3	202	PEB	NB-C1B-CHA-C4A
26	I3	202	PEB	C2B-C1B-CHA-C4A
26	J3	201	PEB	NB-C1B-CHA-C4A
26	J3	201	PEB	C2B-C1B-CHA-C4A
26	J3	202	PEB	NC-C1C-CHB-C4B
26	J3	202	PEB	C2C-C1C-CHB-C4B
26	J3	202	PEB	C2C-CAC-CBC-CGC
26	J3	202	PEB	C4A-C3A-CAA-CBA
26	J3	202	PEB	NB-C1B-CHA-C4A
26	J3	202	PEB	C2B-C1B-CHA-C4A
26	J3	203	PEB	ND-C1D-CHC-C4C
26	J3	203	PEB	NC-C1C-CHB-C4B
26	J3	203	PEB	C2C-C1C-CHB-C4B
26	J3	203	PEB	NB-C1B-CHA-C4A
26	J3	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	K3	201	PEB	ND-C1D-CHC-C4C
26	K3	201	PEB	C2D-C1D-CHC-C4C
26	K3	201	PEB	C1C-C2C-CAC-CBC
26	K3	201	PEB	C3C-C2C-CAC-CBC
26	K3	201	PEB	NB-C1B-CHA-C4A
26	K3	201	PEB	C2B-C1B-CHA-C4A
26	K3	202	PEB	C2C-CAC-CBC-CGC
26	K3	202	PEB	NB-C1B-CHA-C4A
26	K3	202	PEB	C2B-C1B-CHA-C4A
26	L3	201	PEB	NB-C1B-CHA-C4A
26	L3	201	PEB	C2B-C1B-CHA-C4A
26	L3	202	PEB	C4A-C3A-CAA-CBA
26	L3	202	PEB	NB-C1B-CHA-C4A
26	L3	202	PEB	C2B-C1B-CHA-C4A
26	L3	203	PEB	NC-C1C-CHB-C4B
26	L3	203	PEB	C2C-C1C-CHB-C4B
26	L3	203	PEB	NB-C1B-CHA-C4A
26	L3	203	PEB	C2B-C1B-CHA-C4A
26	M3	201	PEB	NC-C1C-CHB-C4B
26	M3	201	PEB	C2C-C1C-CHB-C4B
26	M3	201	PEB	NB-C1B-CHA-C4A
26	M3	201	PEB	C2B-C1B-CHA-C4A
26	M3	202	PEB	ND-C1D-CHC-C4C
26	M3	202	PEB	C2D-C1D-CHC-C4C
26	M3	202	PEB	NC-C1C-CHB-C4B
26	M3	202	PEB	C2C-C1C-CHB-C4B
26	M3	202	PEB	C4A-C3A-CAA-CBA
26	M3	202	PEB	NB-C1B-CHA-C4A
26	M3	202	PEB	C2B-C1B-CHA-C4A
26	N3	201	PEB	NB-C1B-CHA-C4A
26	N3	201	PEB	C2B-C1B-CHA-C4A
26	N3	202	PEB	C4A-C3A-CAA-CBA
26	N3	202	PEB	NB-C1B-CHA-C4A
26	N3	202	PEB	C2B-C1B-CHA-C4A
26	N3	203	PEB	NC-C1C-CHB-C4B
26	N3	203	PEB	C2C-C1C-CHB-C4B
26	N3	203	PEB	NB-C1B-CHA-C4A
26	N3	203	PEB	C2B-C1B-CHA-C4A
26	O3	201	PEB	NC-C1C-CHB-C4B
26	O3	201	PEB	C2C-C1C-CHB-C4B
26	O3	201	PEB	C2B-C1B-CHA-C4A
26	O3	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	O3	202	PEB	C2A-C3A-CAA-CBA
26	O3	202	PEB	C4A-C3A-CAA-CBA
26	O3	202	PEB	NB-C1B-CHA-C4A
26	O3	202	PEB	C2B-C1B-CHA-C4A
26	P3	201	PEB	C2A-C3A-CAA-CBA
26	P3	201	PEB	C4A-C3A-CAA-CBA
26	P3	201	PEB	NB-C1B-CHA-C4A
26	P3	201	PEB	C2B-C1B-CHA-C4A
26	P3	202	PEB	C4A-C3A-CAA-CBA
26	P3	202	PEB	NB-C1B-CHA-C4A
26	P3	202	PEB	C2B-C1B-CHA-C4A
26	P3	203	PEB	NC-C1C-CHB-C4B
26	P3	203	PEB	C2C-C1C-CHB-C4B
26	P3	203	PEB	NB-C1B-CHA-C4A
26	P3	203	PEB	C2B-C1B-CHA-C4A
26	Q3	201	PEB	NC-C1C-CHB-C4B
26	Q3	201	PEB	C2C-C1C-CHB-C4B
26	Q3	201	PEB	NB-C1B-CHA-C4A
26	Q3	201	PEB	C2B-C1B-CHA-C4A
26	Q3	202	PEB	C4A-C3A-CAA-CBA
26	Q3	202	PEB	NB-C1B-CHA-C4A
26	Q3	202	PEB	C2B-C1B-CHA-C4A
26	R3	201	PEB	NB-C1B-CHA-C4A
26	R3	201	PEB	C2B-C1B-CHA-C4A
26	R3	202	PEB	C4A-C3A-CAA-CBA
26	R3	202	PEB	NB-C1B-CHA-C4A
26	R3	202	PEB	C2B-C1B-CHA-C4A
26	R3	203	PEB	NC-C1C-CHB-C4B
26	R3	203	PEB	C2C-C1C-CHB-C4B
26	R3	203	PEB	C2A-C3A-CAA-CBA
26	R3	203	PEB	NB-C1B-CHA-C4A
26	R3	203	PEB	C2B-C1B-CHA-C4A
26	S3	201	PEB	NC-C1C-CHB-C4B
26	S3	201	PEB	C2C-C1C-CHB-C4B
26	S3	202	PEB	C4A-C3A-CAA-CBA
26	S3	202	PEB	NB-C1B-CHA-C4A
26	S3	202	PEB	C2B-C1B-CHA-C4A
26	T3	201	PEB	NB-C1B-CHA-C4A
26	T3	201	PEB	C2B-C1B-CHA-C4A
26	T3	202	PEB	C4A-C3A-CAA-CBA
26	T3	202	PEB	NB-C1B-CHA-C4A
26	T3	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	T3	203	PEB	NB-C1B-CHA-C4A
26	T3	203	PEB	C2B-C1B-CHA-C4A
26	U3	201	PEB	NB-C1B-CHA-C4A
26	U3	202	PEB	NC-C1C-CHB-C4B
26	U3	202	PEB	C2C-C1C-CHB-C4B
26	U3	202	PEB	C2C-CAC-CBC-CGC
26	U3	202	PEB	C4A-C3A-CAA-CBA
26	U3	202	PEB	NB-C1B-CHA-C4A
26	U3	202	PEB	C2B-C1B-CHA-C4A
26	V3	201	PEB	ND-C1D-CHC-C4C
26	V3	201	PEB	C2D-C1D-CHC-C4C
26	V3	201	PEB	C2A-C3A-CAA-CBA
26	V3	201	PEB	C4A-C3A-CAA-CBA
26	V3	201	PEB	NB-C1B-CHA-C4A
26	V3	201	PEB	C2B-C1B-CHA-C4A
26	V3	202	PEB	C2A-C3A-CAA-CBA
26	V3	202	PEB	C4A-C3A-CAA-CBA
26	V3	202	PEB	NB-C1B-CHA-C4A
26	V3	202	PEB	C2B-C1B-CHA-C4A
26	V3	203	PEB	NC-C1C-CHB-C4B
26	V3	203	PEB	C2C-C1C-CHB-C4B
26	V3	203	PEB	NB-C1B-CHA-C4A
26	V3	203	PEB	C2B-C1B-CHA-C4A
26	W3	201	PEB	NB-C1B-CHA-C4A
26	W3	201	PEB	C2B-C1B-CHA-C4A
26	W3	202	PEB	NC-C1C-CHB-C4B
26	W3	202	PEB	C2C-C1C-CHB-C4B
26	W3	202	PEB	C4A-C3A-CAA-CBA
26	W3	202	PEB	NB-C1B-CHA-C4A
26	W3	202	PEB	C2B-C1B-CHA-C4A
26	X3	201	PEB	C2C-C1C-CHB-C4B
26	X3	201	PEB	NB-C1B-CHA-C4A
26	X3	201	PEB	C2B-C1B-CHA-C4A
26	X3	202	PEB	C2C-CAC-CBC-CGC
26	X3	202	PEB	C4A-C3A-CAA-CBA
26	X3	202	PEB	NB-C1B-CHA-C4A
26	X3	202	PEB	C2B-C1B-CHA-C4A
26	X3	203	PEB	NC-C1C-CHB-C4B
26	X3	203	PEB	C2C-C1C-CHB-C4B
26	X3	203	PEB	C1C-C2C-CAC-CBC
26	X3	203	PEB	C3C-C2C-CAC-CBC
26	X3	203	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	X3	203	PEB	NB-C1B-CHA-C4A
26	X3	203	PEB	C2B-C1B-CHA-C4A
26	Y3	301	PEB	ND-C1D-CHC-C4C
26	Y3	301	PEB	C2D-C1D-CHC-C4C
26	Y3	301	PEB	NC-C1C-CHB-C4B
26	Y3	301	PEB	C2C-C1C-CHB-C4B
26	Y3	301	PEB	C2A-C3A-CAA-CBA
26	Y3	301	PEB	NB-C1B-CHA-C4A
26	Y3	301	PEB	C2B-C1B-CHA-C4A
26	Y3	303	PEB	ND-C1D-CHC-C4C
26	Y3	303	PEB	NC-C1C-CHB-C4B
26	Y3	303	PEB	C2C-C1C-CHB-C4B
26	Y3	303	PEB	C2C-CAC-CBC-CGC
26	Y3	303	PEB	C4D-C3D-CAD-CBD
26	Y3	303	PEB	C2A-C3A-CAA-CBA
26	Y3	303	PEB	NB-C1B-CHA-C4A
26	Y3	303	PEB	C2B-C1B-CHA-C4A
26	Y3	304	PEB	ND-C1D-CHC-C4C
26	Y3	304	PEB	C2D-C1D-CHC-C4C
26	Y3	304	PEB	NC-C1C-CHB-C4B
26	Y3	304	PEB	C2C-C1C-CHB-C4B
26	Y3	304	PEB	NB-C1B-CHA-C4A
26	Y3	304	PEB	C2B-C1B-CHA-C4A
26	A4	201	PEB	ND-C1D-CHC-C4C
26	A4	201	PEB	C2D-C1D-CHC-C4C
26	A4	201	PEB	C2A-C3A-CAA-CBA
26	A4	201	PEB	C4A-C3A-CAA-CBA
26	A4	201	PEB	NB-C1B-CHA-C4A
26	A4	201	PEB	C2B-C1B-CHA-C4A
26	A4	201	PEB	C4B-C3B-CAB-CBB
26	A4	202	PEB	NC-C1C-CHB-C4B
26	A4	202	PEB	C2C-C1C-CHB-C4B
26	A4	202	PEB	C2C-CAC-CBC-CGC
26	A4	202	PEB	C2A-C3A-CAA-CBA
26	A4	202	PEB	NB-C1B-CHA-C4A
26	A4	202	PEB	C2B-C1B-CHA-C4A
26	B4	201	PEB	ND-C1D-CHC-C4C
26	B4	201	PEB	C2A-C3A-CAA-CBA
26	B4	201	PEB	C4A-C3A-CAA-CBA
26	B4	201	PEB	NB-C1B-CHA-C4A
26	B4	201	PEB	C2B-C1B-CHA-C4A
26	B4	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	B4	202	PEB	NB-C1B-CHA-C4A
26	B4	202	PEB	C2B-C1B-CHA-C4A
26	B4	203	PEB	NC-C1C-CHB-C4B
26	B4	203	PEB	C2C-C1C-CHB-C4B
26	B4	203	PEB	C2A-C3A-CAA-CBA
26	B4	203	PEB	C4A-C3A-CAA-CBA
26	B4	203	PEB	NB-C1B-CHA-C4A
26	B4	203	PEB	C2B-C1B-CHA-C4A
26	C4	201	PEB	ND-C1D-CHC-C4C
26	C4	201	PEB	NB-C1B-CHA-C4A
26	C4	201	PEB	C2B-C1B-CHA-C4A
26	C4	202	PEB	NC-C1C-CHB-C4B
26	C4	202	PEB	C2C-C1C-CHB-C4B
26	C4	202	PEB	NB-C1B-CHA-C4A
26	C4	202	PEB	C2B-C1B-CHA-C4A
26	D4	201	PEB	C2C-CAC-CBC-CGC
26	D4	201	PEB	NB-C1B-CHA-C4A
26	D4	201	PEB	C2B-C1B-CHA-C4A
26	D4	202	PEB	NC-C1C-CHB-C4B
26	D4	202	PEB	C2A-C3A-CAA-CBA
26	D4	202	PEB	C4A-C3A-CAA-CBA
26	D4	202	PEB	NB-C1B-CHA-C4A
26	D4	202	PEB	C2B-C1B-CHA-C4A
26	D4	203	PEB	NC-C1C-CHB-C4B
26	D4	203	PEB	C2C-C1C-CHB-C4B
26	D4	203	PEB	NB-C1B-CHA-C4A
26	D4	203	PEB	C2B-C1B-CHA-C4A
26	E4	201	PEB	ND-C1D-CHC-C4C
26	E4	201	PEB	C2A-C3A-CAA-CBA
26	E4	201	PEB	C4A-C3A-CAA-CBA
26	E4	201	PEB	NB-C1B-CHA-C4A
26	E4	201	PEB	C2B-C1B-CHA-C4A
26	E4	202	PEB	NC-C1C-CHB-C4B
26	E4	202	PEB	C2C-C1C-CHB-C4B
26	E4	202	PEB	NB-C1B-CHA-C4A
26	E4	202	PEB	C2B-C1B-CHA-C4A
26	F4	201	PEB	ND-C1D-CHC-C4C
26	F4	201	PEB	C2C-CAC-CBC-CGC
26	F4	201	PEB	NB-C1B-CHA-C4A
26	F4	201	PEB	C2B-C1B-CHA-C4A
26	F4	202	PEB	C2A-C3A-CAA-CBA
26	F4	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	F4	202	PEB	NB-C1B-CHA-C4A
26	F4	202	PEB	C2B-C1B-CHA-C4A
26	F4	203	PEB	NC-C1C-CHB-C4B
26	F4	203	PEB	C2C-C1C-CHB-C4B
26	F4	203	PEB	NB-C1B-CHA-C4A
26	F4	203	PEB	C2B-C1B-CHA-C4A
26	G4	201	PEB	C2A-C3A-CAA-CBA
26	G4	201	PEB	C4A-C3A-CAA-CBA
26	G4	201	PEB	NB-C1B-CHA-C4A
26	G4	201	PEB	C2B-C1B-CHA-C4A
26	G4	202	PEB	NC-C1C-CHB-C4B
26	G4	202	PEB	C2C-C1C-CHB-C4B
26	G4	202	PEB	NB-C1B-CHA-C4A
26	G4	202	PEB	C2B-C1B-CHA-C4A
26	H4	201	PEB	ND-C1D-CHC-C4C
26	H4	201	PEB	NB-C1B-CHA-C4A
26	H4	201	PEB	C2B-C1B-CHA-C4A
26	H4	202	PEB	NC-C1C-CHB-C4B
26	H4	202	PEB	C2C-C1C-CHB-C4B
26	H4	202	PEB	C4A-C3A-CAA-CBA
26	H4	202	PEB	NB-C1B-CHA-C4A
26	H4	202	PEB	C2B-C1B-CHA-C4A
26	H4	203	PEB	NC-C1C-CHB-C4B
26	H4	203	PEB	C2C-C1C-CHB-C4B
26	H4	203	PEB	NB-C1B-CHA-C4A
26	H4	203	PEB	C2B-C1B-CHA-C4A
26	I4	201	PEB	C2A-C3A-CAA-CBA
26	I4	201	PEB	C4A-C3A-CAA-CBA
26	I4	201	PEB	NB-C1B-CHA-C4A
26	I4	201	PEB	C2B-C1B-CHA-C4A
26	I4	202	PEB	NC-C1C-CHB-C4B
26	I4	202	PEB	C2C-C1C-CHB-C4B
26	I4	202	PEB	NB-C1B-CHA-C4A
26	I4	202	PEB	C2B-C1B-CHA-C4A
26	J4	201	PEB	C4A-C3A-CAA-CBA
26	J4	201	PEB	NB-C1B-CHA-C4A
26	J4	201	PEB	C2B-C1B-CHA-C4A
26	J4	202	PEB	C2A-C3A-CAA-CBA
26	J4	202	PEB	C4A-C3A-CAA-CBA
26	J4	202	PEB	NB-C1B-CHA-C4A
26	J4	202	PEB	C2B-C1B-CHA-C4A
26	J4	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	J4	203	PEB	C2B-C1B-CHA-C4A
26	K4	201	PEB	NB-C1B-CHA-C4A
26	K4	201	PEB	C2B-C1B-CHA-C4A
26	K4	202	PEB	ND-C1D-CHC-C4C
26	K4	202	PEB	C2D-C1D-CHC-C4C
26	K4	202	PEB	NC-C1C-CHB-C4B
26	K4	202	PEB	C2C-C1C-CHB-C4B
26	K4	202	PEB	C2C-CAC-CBC-CGC
26	K4	202	PEB	C2A-C3A-CAA-CBA
26	K4	202	PEB	NB-C1B-CHA-C4A
26	K4	202	PEB	C2B-C1B-CHA-C4A
26	K4	202	PEB	C3B-CAB-CBB-CGB
26	L4	201	PEB	ND-C1D-CHC-C4C
26	L4	201	PEB	C2C-CAC-CBC-CGC
26	L4	201	PEB	C2D-C3D-CAD-CBD
26	L4	201	PEB	C4D-C3D-CAD-CBD
26	L4	201	PEB	C2A-C3A-CAA-CBA
26	L4	201	PEB	C4A-C3A-CAA-CBA
26	L4	201	PEB	NB-C1B-CHA-C4A
26	L4	201	PEB	C2B-C1B-CHA-C4A
26	L4	202	PEB	C4A-C3A-CAA-CBA
26	L4	202	PEB	NB-C1B-CHA-C4A
26	L4	202	PEB	C2B-C1B-CHA-C4A
26	L4	203	PEB	ND-C1D-CHC-C4C
26	L4	203	PEB	C2D-C1D-CHC-C4C
26	L4	203	PEB	NC-C1C-CHB-C4B
26	L4	203	PEB	C2C-C1C-CHB-C4B
26	L4	203	PEB	C2A-C3A-CAA-CBA
26	L4	203	PEB	C4A-C3A-CAA-CBA
26	L4	203	PEB	NB-C1B-CHA-C4A
26	L4	203	PEB	C2B-C1B-CHA-C4A
26	M4	401	PEB	C2D-C3D-CAD-CBD
26	M4	401	PEB	C4D-C3D-CAD-CBD
26	M4	401	PEB	C2A-C3A-CAA-CBA
26	M4	401	PEB	NB-C1B-CHA-C4A
26	M4	401	PEB	C2B-C1B-CHA-C4A
26	M4	402	PEB	ND-C1D-CHC-C4C
26	M4	402	PEB	C2D-C1D-CHC-C4C
26	M4	402	PEB	NC-C1C-CHB-C4B
26	M4	402	PEB	C2C-C1C-CHB-C4B
26	M4	402	PEB	NB-C1B-CHA-C4A
26	M4	402	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	M4	403	PEB	NB-C1B-CHA-C4A
26	M4	403	PEB	C2B-C1B-CHA-C4A
26	N4	201	PEB	NB-C1B-CHA-C4A
26	N4	201	PEB	C2B-C1B-CHA-C4A
26	N4	202	PEB	NC-C1C-CHB-C4B
26	N4	202	PEB	C2C-C1C-CHB-C4B
26	N4	202	PEB	C4A-C3A-CAA-CBA
26	N4	202	PEB	NB-C1B-CHA-C4A
26	N4	202	PEB	C2B-C1B-CHA-C4A
26	N4	203	PEB	ND-C1D-CHC-C4C
26	N4	203	PEB	C2D-C1D-CHC-C4C
26	N4	203	PEB	C4A-C3A-CAA-CBA
26	N4	203	PEB	NB-C1B-CHA-C4A
26	N4	203	PEB	C2B-C1B-CHA-C4A
26	O4	201	PEB	C2C-CAC-CBC-CGC
26	O4	201	PEB	NB-C1B-CHA-C4A
26	O4	201	PEB	C2B-C1B-CHA-C4A
26	O4	202	PEB	NC-C1C-CHB-C4B
26	O4	202	PEB	C2C-C1C-CHB-C4B
26	O4	202	PEB	NB-C1B-CHA-C4A
26	O4	202	PEB	C2B-C1B-CHA-C4A
26	P4	201	PEB	ND-C1D-CHC-C4C
26	P4	201	PEB	C2D-C1D-CHC-C4C
26	P4	201	PEB	C1C-C2C-CAC-CBC
26	P4	201	PEB	C3C-C2C-CAC-CBC
26	P4	201	PEB	C4A-C3A-CAA-CBA
26	P4	201	PEB	NB-C1B-CHA-C4A
26	P4	201	PEB	C2B-C1B-CHA-C4A
26	P4	202	PEB	NB-C1B-CHA-C4A
26	P4	202	PEB	C2B-C1B-CHA-C4A
26	P4	203	PEB	NC-C1C-CHB-C4B
26	P4	203	PEB	C2C-C1C-CHB-C4B
26	P4	203	PEB	C2C-CAC-CBC-CGC
26	P4	203	PEB	C2A-C3A-CAA-CBA
26	P4	203	PEB	C4A-C3A-CAA-CBA
26	P4	203	PEB	NB-C1B-CHA-C4A
26	P4	203	PEB	C2B-C1B-CHA-C4A
26	Q4	201	PEB	NB-C1B-CHA-C4A
26	Q4	201	PEB	C2B-C1B-CHA-C4A
26	Q4	202	PEB	C2C-C1C-CHB-C4B
26	Q4	202	PEB	NB-C1B-CHA-C4A
26	Q4	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	R4	201	PEB	C2A-C3A-CAA-CBA
26	R4	201	PEB	C4A-C3A-CAA-CBA
26	R4	201	PEB	NB-C1B-CHA-C4A
26	R4	201	PEB	C2B-C1B-CHA-C4A
26	R4	202	PEB	C2C-CAC-CBC-CGC
26	R4	202	PEB	C4A-C3A-CAA-CBA
26	R4	202	PEB	NB-C1B-CHA-C4A
26	R4	202	PEB	C2B-C1B-CHA-C4A
26	R4	203	PEB	ND-C1D-CHC-C4C
26	R4	203	PEB	C2D-C1D-CHC-C4C
26	R4	203	PEB	NB-C1B-CHA-C4A
26	R4	203	PEB	C2B-C1B-CHA-C4A
26	S4	201	PEB	ND-C1D-CHC-C4C
26	S4	201	PEB	NB-C1B-CHA-C4A
26	S4	201	PEB	C2B-C1B-CHA-C4A
26	S4	202	PEB	C2C-C1C-CHB-C4B
26	S4	202	PEB	NB-C1B-CHA-C4A
26	S4	202	PEB	C2B-C1B-CHA-C4A
26	T4	201	PEB	NC-C1C-CHB-C4B
26	T4	201	PEB	C4A-C3A-CAA-CBA
26	T4	201	PEB	NB-C1B-CHA-C4A
26	T4	201	PEB	C2B-C1B-CHA-C4A
26	T4	202	PEB	C4A-C3A-CAA-CBA
26	T4	202	PEB	NB-C1B-CHA-C4A
26	T4	202	PEB	C2B-C1B-CHA-C4A
26	T4	203	PEB	C2A-C3A-CAA-CBA
26	T4	203	PEB	C4A-C3A-CAA-CBA
26	T4	203	PEB	NB-C1B-CHA-C4A
26	T4	203	PEB	C2B-C1B-CHA-C4A
26	U4	201	PEB	NB-C1B-CHA-C4A
26	U4	201	PEB	C2B-C1B-CHA-C4A
26	U4	202	PEB	C2C-C1C-CHB-C4B
26	U4	202	PEB	C4A-C3A-CAA-CBA
26	U4	202	PEB	NB-C1B-CHA-C4A
26	U4	202	PEB	C2B-C1B-CHA-C4A
26	V4	201	PEB	C2A-C3A-CAA-CBA
26	V4	201	PEB	C4A-C3A-CAA-CBA
26	V4	201	PEB	NB-C1B-CHA-C4A
26	V4	201	PEB	C2B-C1B-CHA-C4A
26	V4	201	PEB	C3B-CAB-CBB-CGB
26	V4	202	PEB	C2C-CAC-CBC-CGC
26	V4	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	V4	202	PEB	NB-C1B-CHA-C4A
26	V4	202	PEB	C2B-C1B-CHA-C4A
26	V4	203	PEB	ND-C1D-CHC-C4C
26	V4	203	PEB	C2D-C1D-CHC-C4C
26	V4	203	PEB	C2A-C3A-CAA-CBA
26	V4	203	PEB	C4A-C3A-CAA-CBA
26	V4	203	PEB	NB-C1B-CHA-C4A
26	V4	203	PEB	C2B-C1B-CHA-C4A
26	W4	201	PEB	C1C-C2C-CAC-CBC
26	W4	201	PEB	C3C-C2C-CAC-CBC
26	W4	201	PEB	NB-C1B-CHA-C4A
26	W4	201	PEB	C2B-C1B-CHA-C4A
26	W4	202	PEB	NB-C1B-CHA-C4A
26	W4	202	PEB	C2B-C1B-CHA-C4A
26	X4	201	PEB	ND-C1D-CHC-C4C
26	X4	201	PEB	C2D-C1D-CHC-C4C
26	X4	201	PEB	C4A-C3A-CAA-CBA
26	X4	201	PEB	NB-C1B-CHA-C4A
26	X4	201	PEB	C2B-C1B-CHA-C4A
26	X4	202	PEB	C2C-C1C-CHB-C4B
26	X4	202	PEB	C2A-C3A-CAA-CBA
26	X4	202	PEB	C4A-C3A-CAA-CBA
26	X4	202	PEB	NB-C1B-CHA-C4A
26	X4	202	PEB	C2B-C1B-CHA-C4A
26	X4	203	PEB	C2C-C1C-CHB-C4B
26	X4	203	PEB	NB-C1B-CHA-C4A
26	X4	203	PEB	C2B-C1B-CHA-C4A
26	Y4	201	PEB	NB-C1B-CHA-C4A
26	Y4	201	PEB	C2B-C1B-CHA-C4A
26	Y4	202	PEB	NB-C1B-CHA-C4A
26	Y4	202	PEB	C2B-C1B-CHA-C4A
26	Z4	201	PEB	NB-C1B-CHA-C4A
26	Z4	201	PEB	C2B-C1B-CHA-C4A
26	Z4	202	PEB	ND-C1D-CHC-C4C
26	Z4	202	PEB	C2D-C1D-CHC-C4C
26	Z4	202	PEB	NC-C1C-CHB-C4B
26	Z4	202	PEB	C2C-C1C-CHB-C4B
26	Z4	202	PEB	C2D-C3D-CAD-CBD
26	Z4	202	PEB	C4D-C3D-CAD-CBD
26	Z4	202	PEB	NB-C1B-CHA-C4A
26	Z4	202	PEB	C2B-C1B-CHA-C4A
26	a4	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	a4	201	PEB	C2B-C1B-CHA-C4A
26	a4	202	PEB	NB-C1B-CHA-C4A
26	a4	202	PEB	C2B-C1B-CHA-C4A
26	a4	203	PEB	ND-C1D-CHC-C4C
26	a4	203	PEB	NC-C1C-CHB-C4B
26	a4	203	PEB	C2C-C1C-CHB-C4B
26	a4	203	PEB	NB-C1B-CHA-C4A
26	a4	203	PEB	C2B-C1B-CHA-C4A
26	b4	501	PEB	NB-C1B-CHA-C4A
26	b4	501	PEB	C2B-C1B-CHA-C4A
26	c4	201	PEB	NC-C1C-CHB-C4B
26	c4	201	PEB	C2C-C1C-CHB-C4B
26	c4	201	PEB	NB-C1B-CHA-C4A
26	c4	201	PEB	C2B-C1B-CHA-C4A
26	c4	202	PEB	C1C-C2C-CAC-CBC
26	c4	202	PEB	C3C-C2C-CAC-CBC
26	c4	202	PEB	NB-C1B-CHA-C4A
26	c4	202	PEB	C2B-C1B-CHA-C4A
26	c4	203	PEB	NC-C1C-CHB-C4B
26	c4	203	PEB	C2C-C1C-CHB-C4B
26	c4	203	PEB	C4A-C3A-CAA-CBA
26	c4	203	PEB	NB-C1B-CHA-C4A
26	c4	203	PEB	C2B-C1B-CHA-C4A
26	d4	201	PEB	NC-C1C-CHB-C4B
26	d4	201	PEB	C2C-C1C-CHB-C4B
26	d4	201	PEB	NB-C1B-CHA-C4A
26	d4	201	PEB	C2B-C1B-CHA-C4A
26	d4	202	PEB	C4A-C3A-CAA-CBA
26	d4	202	PEB	NB-C1B-CHA-C4A
26	d4	202	PEB	C2B-C1B-CHA-C4A
26	d4	203	PEB	ND-C1D-CHC-C4C
26	d4	203	PEB	C2D-C1D-CHC-C4C
26	d4	203	PEB	NC-C1C-CHB-C4B
26	d4	203	PEB	C2C-C1C-CHB-C4B
26	d4	203	PEB	NB-C1B-CHA-C4A
26	d4	203	PEB	C2B-C1B-CHA-C4A
26	e4	201	PEB	ND-C1D-CHC-C4C
26	e4	201	PEB	C2D-C1D-CHC-C4C
26	e4	201	PEB	C4A-C3A-CAA-CBA
26	e4	201	PEB	NB-C1B-CHA-C4A
26	e4	201	PEB	C2B-C1B-CHA-C4A
26	e4	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	e4	202	PEB	C2B-C1B-CHA-C4A
26	f4	201	PEB	ND-C1D-CHC-C4C
26	f4	201	PEB	C2D-C1D-CHC-C4C
26	f4	201	PEB	C2C-CAC-CBC-CGC
26	f4	201	PEB	NB-C1B-CHA-C4A
26	f4	201	PEB	C2B-C1B-CHA-C4A
26	f4	202	PEB	C2C-CAC-CBC-CGC
26	f4	202	PEB	NB-C1B-CHA-C4A
26	f4	202	PEB	C2B-C1B-CHA-C4A
26	g4	201	PEB	ND-C1D-CHC-C4C
26	g4	201	PEB	C2D-C1D-CHC-C4C
26	g4	201	PEB	NB-C1B-CHA-C4A
26	g4	201	PEB	C2B-C1B-CHA-C4A
26	g4	202	PEB	NB-C1B-CHA-C4A
26	g4	202	PEB	C2B-C1B-CHA-C4A
26	g4	203	PEB	NC-C1C-CHB-C4B
26	g4	203	PEB	C2C-C1C-CHB-C4B
26	g4	203	PEB	C4A-C3A-CAA-CBA
26	g4	203	PEB	NB-C1B-CHA-C4A
26	g4	203	PEB	C2B-C1B-CHA-C4A
26	h4	201	PEB	ND-C1D-CHC-C4C
26	h4	201	PEB	NB-C1B-CHA-C4A
26	h4	201	PEB	C2B-C1B-CHA-C4A
26	h4	202	PEB	ND-C1D-CHC-C4C
26	h4	202	PEB	C2D-C1D-CHC-C4C
26	h4	202	PEB	NC-C1C-CHB-C4B
26	h4	202	PEB	C2C-C1C-CHB-C4B
26	h4	202	PEB	C2C-CAC-CBC-CGC
26	h4	202	PEB	NB-C1B-CHA-C4A
26	h4	202	PEB	C2B-C1B-CHA-C4A
26	h4	203	PEB	NC-C1C-CHB-C4B
26	h4	203	PEB	C2C-C1C-CHB-C4B
26	h4	203	PEB	NB-C1B-CHA-C4A
26	h4	203	PEB	C2B-C1B-CHA-C4A
26	i4	201	PEB	C4A-C3A-CAA-CBA
26	i4	201	PEB	NB-C1B-CHA-C4A
26	i4	201	PEB	C2B-C1B-CHA-C4A
26	i4	202	PEB	NC-C1C-CHB-C4B
26	i4	202	PEB	NB-C1B-CHA-C4A
26	i4	202	PEB	C2B-C1B-CHA-C4A
26	j4	201	PEB	ND-C1D-CHC-C4C
26	j4	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	j4	201	PEB	C2A-C3A-CAA-CBA
26	j4	201	PEB	C4A-C3A-CAA-CBA
26	j4	201	PEB	NB-C1B-CHA-C4A
26	j4	201	PEB	C2B-C1B-CHA-C4A
26	j4	202	PEB	C2C-CAC-CBC-CGC
26	j4	202	PEB	NB-C1B-CHA-C4A
26	j4	202	PEB	C2B-C1B-CHA-C4A
26	k4	201	PEB	NB-C1B-CHA-C4A
26	k4	201	PEB	C2B-C1B-CHA-C4A
26	k4	202	PEB	NB-C1B-CHA-C4A
26	k4	202	PEB	C2B-C1B-CHA-C4A
26	k4	203	PEB	NC-C1C-CHB-C4B
26	k4	203	PEB	C4A-C3A-CAA-CBA
26	k4	203	PEB	NB-C1B-CHA-C4A
26	k4	203	PEB	C2B-C1B-CHA-C4A
26	l4	201	PEB	ND-C1D-CHC-C4C
26	l4	201	PEB	C2D-C1D-CHC-C4C
26	l4	201	PEB	NB-C1B-CHA-C4A
26	l4	201	PEB	C2B-C1B-CHA-C4A
26	l4	202	PEB	NC-C1C-CHB-C4B
26	l4	202	PEB	C2C-C1C-CHB-C4B
26	l4	202	PEB	NB-C1B-CHA-C4A
26	l4	202	PEB	C2B-C1B-CHA-C4A
26	m4	201	PEB	NC-C1C-CHB-C4B
26	m4	201	PEB	C2C-C1C-CHB-C4B
26	m4	201	PEB	C4A-C3A-CAA-CBA
26	m4	201	PEB	NB-C1B-CHA-C4A
26	m4	201	PEB	C2B-C1B-CHA-C4A
26	m4	202	PEB	C4A-C3A-CAA-CBA
26	m4	202	PEB	NB-C1B-CHA-C4A
26	m4	202	PEB	C2B-C1B-CHA-C4A
26	m4	203	PEB	C1C-C2C-CAC-CBC
26	m4	203	PEB	C3C-C2C-CAC-CBC
26	m4	203	PEB	C2D-C3D-CAD-CBD
26	m4	203	PEB	C4D-C3D-CAD-CBD
26	m4	203	PEB	NB-C1B-CHA-C4A
26	m4	203	PEB	C2B-C1B-CHA-C4A
26	n4	201	PEB	NC-C1C-CHB-C4B
26	n4	201	PEB	C2C-C1C-CHB-C4B
26	n4	201	PEB	C2A-C3A-CAA-CBA
26	n4	201	PEB	C4A-C3A-CAA-CBA
26	n4	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	n4	201	PEB	C2B-C1B-CHA-C4A
26	n4	202	PEB	NC-C1C-CHB-C4B
26	n4	202	PEB	C2C-C1C-CHB-C4B
26	n4	202	PEB	NB-C1B-CHA-C4A
26	n4	202	PEB	C2B-C1B-CHA-C4A
26	p4	201	PEB	ND-C1D-CHC-C4C
26	p4	201	PEB	C2D-C1D-CHC-C4C
26	p4	201	PEB	NC-C1C-CHB-C4B
26	p4	201	PEB	C2C-C1C-CHB-C4B
26	p4	201	PEB	C4A-C3A-CAA-CBA
26	p4	201	PEB	NB-C1B-CHA-C4A
26	p4	201	PEB	C2B-C1B-CHA-C4A
26	p4	202	PEB	NC-C1C-CHB-C4B
26	p4	202	PEB	C2C-C1C-CHB-C4B
26	p4	202	PEB	C2A-C3A-CAA-CBA
26	p4	202	PEB	C4A-C3A-CAA-CBA
26	p4	202	PEB	NB-C1B-CHA-C4A
26	p4	202	PEB	C2B-C1B-CHA-C4A
26	q4	201	PEB	ND-C1D-CHC-C4C
26	q4	201	PEB	NC-C1C-CHB-C4B
26	q4	201	PEB	NB-C1B-CHA-C4A
26	q4	201	PEB	C2B-C1B-CHA-C4A
26	q4	202	PEB	C4A-C3A-CAA-CBA
26	q4	202	PEB	NB-C1B-CHA-C4A
26	q4	202	PEB	C2B-C1B-CHA-C4A
26	q4	203	PEB	NB-C1B-CHA-C4A
26	q4	203	PEB	C2B-C1B-CHA-C4A
26	r4	201	PEB	ND-C1D-CHC-C4C
26	r4	201	PEB	C2D-C1D-CHC-C4C
26	r4	201	PEB	NC-C1C-CHB-C4B
26	r4	201	PEB	NB-C1B-CHA-C4A
26	r4	201	PEB	C2B-C1B-CHA-C4A
26	r4	202	PEB	ND-C1D-CHC-C4C
26	r4	202	PEB	C2D-C1D-CHC-C4C
26	r4	202	PEB	NC-C1C-CHB-C4B
26	r4	202	PEB	C2C-C1C-CHB-C4B
26	r4	202	PEB	C4A-C3A-CAA-CBA
26	r4	202	PEB	NB-C1B-CHA-C4A
26	r4	202	PEB	C2B-C1B-CHA-C4A
26	s4	201	PEB	ND-C1D-CHC-C4C
26	s4	201	PEB	NB-C1B-CHA-C4A
26	s4	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	s4	202	PEB	C2A-C3A-CAA-CBA
26	s4	202	PEB	C4A-C3A-CAA-CBA
26	s4	202	PEB	NB-C1B-CHA-C4A
26	s4	202	PEB	C2B-C1B-CHA-C4A
26	s4	203	PEB	NC-C1C-CHB-C4B
26	s4	203	PEB	C2C-C1C-CHB-C4B
26	s4	203	PEB	C2C-CAC-CBC-CGC
26	s4	203	PEB	NB-C1B-CHA-C4A
26	s4	203	PEB	C2B-C1B-CHA-C4A
26	t4	201	PEB	ND-C1D-CHC-C4C
26	t4	201	PEB	NB-C1B-CHA-C4A
26	t4	201	PEB	C2B-C1B-CHA-C4A
26	t4	202	PEB	ND-C1D-CHC-C4C
26	t4	202	PEB	NC-C1C-CHB-C4B
26	t4	202	PEB	C2C-C1C-CHB-C4B
26	t4	202	PEB	C2C-CAC-CBC-CGC
26	t4	202	PEB	C2D-C3D-CAD-CBD
26	t4	202	PEB	C4D-C3D-CAD-CBD
26	t4	202	PEB	C2A-C3A-CAA-CBA
26	t4	202	PEB	C4A-C3A-CAA-CBA
26	t4	202	PEB	NB-C1B-CHA-C4A
26	t4	202	PEB	C2B-C1B-CHA-C4A
26	u4	201	PEB	NC-C1C-CHB-C4B
26	u4	201	PEB	C2C-C1C-CHB-C4B
26	u4	201	PEB	C4A-C3A-CAA-CBA
26	u4	201	PEB	NB-C1B-CHA-C4A
26	u4	201	PEB	C2B-C1B-CHA-C4A
26	u4	202	PEB	C4A-C3A-CAA-CBA
26	u4	202	PEB	NB-C1B-CHA-C4A
26	u4	202	PEB	C2B-C1B-CHA-C4A
26	u4	203	PEB	NB-C1B-CHA-C4A
26	u4	203	PEB	C2B-C1B-CHA-C4A
26	v4	201	PEB	ND-C1D-CHC-C4C
26	v4	201	PEB	C2D-C1D-CHC-C4C
26	v4	201	PEB	C2A-C3A-CAA-CBA
26	v4	201	PEB	C4A-C3A-CAA-CBA
26	v4	201	PEB	NB-C1B-CHA-C4A
26	v4	201	PEB	C2B-C1B-CHA-C4A
26	v4	202	PEB	NC-C1C-CHB-C4B
26	v4	202	PEB	C2C-C1C-CHB-C4B
26	v4	202	PEB	C4A-C3A-CAA-CBA
26	v4	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	v4	202	PEB	C2B-C1B-CHA-C4A
26	w4	201	PEB	ND-C1D-CHC-C4C
26	w4	201	PEB	C2D-C1D-CHC-C4C
26	w4	201	PEB	NC-C1C-CHB-C4B
26	w4	201	PEB	C2C-C1C-CHB-C4B
26	w4	201	PEB	C2A-C3A-CAA-CBA
26	w4	201	PEB	C4A-C3A-CAA-CBA
26	w4	201	PEB	NB-C1B-CHA-C4A
26	w4	201	PEB	C2B-C1B-CHA-C4A
26	w4	202	PEB	C4A-C3A-CAA-CBA
26	w4	202	PEB	NB-C1B-CHA-C4A
26	w4	202	PEB	C2B-C1B-CHA-C4A
26	w4	202	PEB	C3B-CAB-CBB-CGB
26	w4	203	PEB	NC-C1C-CHB-C4B
26	w4	203	PEB	C2C-C1C-CHB-C4B
26	w4	203	PEB	NB-C1B-CHA-C4A
26	w4	203	PEB	C2B-C1B-CHA-C4A
26	w4	204	PEB	NC-C1C-CHB-C4B
26	w4	204	PEB	C2C-C1C-CHB-C4B
26	w4	204	PEB	C2A-C3A-CAA-CBA
26	w4	204	PEB	C4A-C3A-CAA-CBA
26	w4	204	PEB	NB-C1B-CHA-C4A
26	w4	204	PEB	C2B-C1B-CHA-C4A
26	x4	201	PEB	ND-C1D-CHC-C4C
26	x4	201	PEB	C2D-C1D-CHC-C4C
26	x4	201	PEB	C2C-CAC-CBC-CGC
26	x4	201	PEB	C4A-C3A-CAA-CBA
26	x4	201	PEB	NB-C1B-CHA-C4A
26	x4	201	PEB	C2B-C1B-CHA-C4A
26	x4	202	PEB	ND-C1D-CHC-C4C
26	x4	202	PEB	C2D-C1D-CHC-C4C
26	x4	202	PEB	NC-C1C-CHB-C4B
26	x4	202	PEB	C2C-C1C-CHB-C4B
26	x4	202	PEB	C4A-C3A-CAA-CBA
26	x4	202	PEB	NB-C1B-CHA-C4A
26	x4	202	PEB	C2B-C1B-CHA-C4A
26	x4	202	PEB	C3B-C4B-CHB-C1C
26	y4	201	PEB	ND-C1D-CHC-C4C
26	y4	201	PEB	C2C-CAC-CBC-CGC
26	y4	201	PEB	C2A-C3A-CAA-CBA
26	y4	201	PEB	C4A-C3A-CAA-CBA
26	y4	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	y4	201	PEB	C2B-C1B-CHA-C4A
26	y4	202	PEB	C2C-C1C-CHB-C4B
26	y4	202	PEB	C2A-C3A-CAA-CBA
26	y4	202	PEB	C4A-C3A-CAA-CBA
26	y4	202	PEB	NB-C1B-CHA-C4A
26	y4	202	PEB	C2B-C1B-CHA-C4A
26	y4	203	PEB	ND-C1D-CHC-C4C
26	y4	203	PEB	NC-C1C-CHB-C4B
26	y4	203	PEB	C2C-C1C-CHB-C4B
26	y4	203	PEB	NB-C1B-CHA-C4A
26	y4	203	PEB	C2B-C1B-CHA-C4A
26	z4	201	PEB	NC-C1C-CHB-C4B
26	z4	201	PEB	C2C-C1C-CHB-C4B
26	z4	201	PEB	C4A-C3A-CAA-CBA
26	z4	201	PEB	NB-C1B-CHA-C4A
26	z4	201	PEB	C2B-C1B-CHA-C4A
26	z4	202	PEB	NC-C1C-CHB-C4B
26	z4	202	PEB	C2C-C1C-CHB-C4B
26	z4	202	PEB	NB-C1B-CHA-C4A
26	z4	202	PEB	C2B-C1B-CHA-C4A
26	14	201	PEB	ND-C1D-CHC-C4C
26	14	201	PEB	C2D-C1D-CHC-C4C
26	14	201	PEB	NC-C1C-CHB-C4B
26	14	201	PEB	C2A-C3A-CAA-CBA
26	14	201	PEB	C4A-C3A-CAA-CBA
26	14	201	PEB	NB-C1B-CHA-C4A
26	14	201	PEB	C2B-C1B-CHA-C4A
26	14	201	PEB	C3B-CAB-CBB-CGB
26	14	202	PEB	C2A-C3A-CAA-CBA
26	14	202	PEB	C4A-C3A-CAA-CBA
26	14	202	PEB	NB-C1B-CHA-C4A
26	14	202	PEB	C2B-C1B-CHA-C4A
26	14	203	PEB	ND-C1D-CHC-C4C
26	14	203	PEB	C2D-C1D-CHC-C4C
26	14	203	PEB	NC-C1C-CHB-C4B
26	14	203	PEB	C2C-C1C-CHB-C4B
26	14	203	PEB	NB-C1B-CHA-C4A
26	14	203	PEB	C2B-C1B-CHA-C4A
26	24	401	PEB	NC-C1C-CHB-C4B
26	24	401	PEB	C2C-C1C-CHB-C4B
26	24	401	PEB	C2D-C3D-CAD-CBD
26	24	401	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
26	24	401	PEB	C4A-C3A-CAA-CBA
26	24	401	PEB	NB-C1B-CHA-C4A
26	24	401	PEB	C2B-C1B-CHA-C4A
26	24	404	PEB	ND-C1D-CHC-C4C
26	24	404	PEB	C2D-C1D-CHC-C4C
26	24	404	PEB	NC-C1C-CHB-C4B
26	24	404	PEB	C2C-C1C-CHB-C4B
26	24	404	PEB	NB-C1B-CHA-C4A
26	24	404	PEB	C2B-C1B-CHA-C4A
26	24	405	PEB	ND-C1D-CHC-C4C
26	24	405	PEB	NB-C1B-CHA-C4A
26	24	405	PEB	C2B-C1B-CHA-C4A
26	A5	201	PEB	NC-C1C-CHB-C4B
26	A5	201	PEB	C2C-C1C-CHB-C4B
26	A5	201	PEB	C2A-C3A-CAA-CBA
26	A5	201	PEB	C4A-C3A-CAA-CBA
26	A5	201	PEB	NB-C1B-CHA-C4A
26	A5	201	PEB	C2B-C1B-CHA-C4A
26	A5	202	PEB	ND-C1D-CHC-C4C
26	A5	202	PEB	C2D-C1D-CHC-C4C
26	A5	202	PEB	NC-C1C-CHB-C4B
26	A5	202	PEB	C2C-C1C-CHB-C4B
26	A5	202	PEB	NB-C1B-CHA-C4A
26	A5	202	PEB	C2B-C1B-CHA-C4A
26	B5	201	PEB	C2A-C3A-CAA-CBA
26	B5	201	PEB	C4A-C3A-CAA-CBA
26	B5	201	PEB	NB-C1B-CHA-C4A
26	B5	201	PEB	C2B-C1B-CHA-C4A
26	B5	202	PEB	ND-C1D-CHC-C4C
26	B5	202	PEB	C2D-C1D-CHC-C4C
26	B5	202	PEB	NB-C1B-CHA-C4A
26	B5	202	PEB	C2B-C1B-CHA-C4A
26	B5	203	PEB	ND-C1D-CHC-C4C
26	B5	203	PEB	C2D-C1D-CHC-C4C
26	B5	203	PEB	NC-C1C-CHB-C4B
26	B5	203	PEB	C2C-C1C-CHB-C4B
26	B5	203	PEB	NB-C1B-CHA-C4A
26	B5	203	PEB	C2B-C1B-CHA-C4A
26	C5	201	PEB	NB-C1B-CHA-C4A
26	C5	201	PEB	C2B-C1B-CHA-C4A
26	C5	202	PEB	NB-C1B-CHA-C4A
26	C5	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	C5	203	PEB	ND-C1D-CHC-C4C
26	C5	203	PEB	NB-C1B-CHA-C4A
26	C5	203	PEB	C2B-C1B-CHA-C4A
26	C5	204	PEB	ND-C1D-CHC-C4C
26	C5	204	PEB	C2D-C1D-CHC-C4C
26	C5	204	PEB	NC-C1C-CHB-C4B
26	C5	204	PEB	C2C-C1C-CHB-C4B
26	C5	204	PEB	NB-C1B-CHA-C4A
26	C5	204	PEB	C2B-C1B-CHA-C4A
26	F5	201	PEB	NB-C1B-CHA-C4A
26	F5	201	PEB	C2B-C1B-CHA-C4A
26	F5	202	PEB	ND-C1D-CHC-C4C
26	F5	202	PEB	C2D-C1D-CHC-C4C
26	F5	202	PEB	C2A-C3A-CAA-CBA
26	F5	202	PEB	C4A-C3A-CAA-CBA
26	F5	202	PEB	NB-C1B-CHA-C4A
26	F5	202	PEB	C2B-C1B-CHA-C4A
26	F5	203	PEB	ND-C1D-CHC-C4C
26	F5	203	PEB	NC-C1C-CHB-C4B
26	F5	203	PEB	C2C-C1C-CHB-C4B
26	F5	203	PEB	NB-C1B-CHA-C4A
26	F5	203	PEB	C2B-C1B-CHA-C4A
26	G5	201	PEB	ND-C1D-CHC-C4C
26	G5	201	PEB	C2D-C1D-CHC-C4C
26	G5	201	PEB	C2A-C3A-CAA-CBA
26	G5	201	PEB	C4A-C3A-CAA-CBA
26	G5	201	PEB	NB-C1B-CHA-C4A
26	G5	201	PEB	C2B-C1B-CHA-C4A
26	G5	202	PEB	NB-C1B-CHA-C4A
26	G5	202	PEB	C2B-C1B-CHA-C4A
26	G5	203	PEB	ND-C1D-CHC-C4C
26	G5	203	PEB	NC-C1C-CHB-C4B
26	G5	203	PEB	C2C-C1C-CHB-C4B
26	G5	203	PEB	C2C-CAC-CBC-CGC
26	G5	203	PEB	NB-C1B-CHA-C4A
26	G5	203	PEB	C2B-C1B-CHA-C4A
26	H5	201	PEB	C2A-C3A-CAA-CBA
26	H5	201	PEB	C4A-C3A-CAA-CBA
26	H5	201	PEB	NB-C1B-CHA-C4A
26	H5	201	PEB	C2B-C1B-CHA-C4A
26	H5	202	PEB	C2A-C3A-CAA-CBA
26	H5	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	H5	202	PEB	NB-C1B-CHA-C4A
26	H5	202	PEB	C2B-C1B-CHA-C4A
26	H5	203	PEB	ND-C1D-CHC-C4C
26	H5	203	PEB	C2D-C1D-CHC-C4C
26	H5	203	PEB	NC-C1C-CHB-C4B
26	H5	203	PEB	C2C-C1C-CHB-C4B
26	H5	203	PEB	C2C-CAC-CBC-CGC
26	H5	203	PEB	NB-C1B-CHA-C4A
26	H5	203	PEB	C2B-C1B-CHA-C4A
26	I5	201	PEB	NB-C1B-CHA-C4A
26	I5	201	PEB	C2B-C1B-CHA-C4A
26	I5	202	PEB	C2C-CAC-CBC-CGC
26	I5	202	PEB	NB-C1B-CHA-C4A
26	I5	202	PEB	C2B-C1B-CHA-C4A
26	I5	203	PEB	ND-C1D-CHC-C4C
26	I5	203	PEB	C2D-C1D-CHC-C4C
26	I5	203	PEB	NC-C1C-CHB-C4B
26	I5	203	PEB	C2C-C1C-CHB-C4B
26	I5	203	PEB	C1C-C2C-CAC-CBC
26	I5	203	PEB	C3C-C2C-CAC-CBC
26	I5	203	PEB	NB-C1B-CHA-C4A
26	I5	203	PEB	C2B-C1B-CHA-C4A
26	J5	201	PEB	NC-C1C-CHB-C4B
26	J5	201	PEB	C2C-C1C-CHB-C4B
26	J5	202	PEB	ND-C1D-CHC-C4C
26	J5	202	PEB	NB-C1B-CHA-C4A
26	J5	202	PEB	C2B-C1B-CHA-C4A
26	K5	201	PEB	NB-C1B-CHA-C4A
26	K5	201	PEB	C2B-C1B-CHA-C4A
26	K5	202	PEB	C2A-C3A-CAA-CBA
26	K5	202	PEB	C4A-C3A-CAA-CBA
26	K5	202	PEB	NB-C1B-CHA-C4A
26	K5	202	PEB	C2B-C1B-CHA-C4A
26	K5	203	PEB	NC-C1C-CHB-C4B
26	K5	203	PEB	C2C-C1C-CHB-C4B
26	K5	203	PEB	NB-C1B-CHA-C4A
26	K5	203	PEB	C2B-C1B-CHA-C4A
26	L5	201	PEB	NB-C1B-CHA-C4A
26	L5	201	PEB	C2B-C1B-CHA-C4A
26	L5	202	PEB	C2A-C3A-CAA-CBA
26	L5	202	PEB	C4A-C3A-CAA-CBA
26	L5	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	L5	202	PEB	C2B-C1B-CHA-C4A
26	L5	203	PEB	ND-C1D-CHC-C4C
26	L5	203	PEB	NC-C1C-CHB-C4B
26	L5	203	PEB	C2C-C1C-CHB-C4B
26	L5	203	PEB	NB-C1B-CHA-C4A
26	L5	203	PEB	C2B-C1B-CHA-C4A
26	A6	301	PEB	NC-C1C-CHB-C4B
26	A6	301	PEB	C2C-C1C-CHB-C4B
26	A6	301	PEB	NB-C1B-CHA-C4A
26	A6	301	PEB	C2B-C1B-CHA-C4A
26	A6	304	PEB	NB-C1B-CHA-C4A
26	A6	304	PEB	C2B-C1B-CHA-C4A
26	D6	1002	PEB	NB-C1B-CHA-C4A
26	D6	1002	PEB	C2B-C1B-CHA-C4A
26	G6	1002	PEB	C2D-C3D-CAD-CBD
26	G6	1002	PEB	C4D-C3D-CAD-CBD
26	G6	1002	PEB	NB-C1B-CHA-C4A
26	G6	1002	PEB	C2B-C1B-CHA-C4A
26	G6	1002	PEB	C2B-C3B-CAB-CBB
26	H6	1002	PEB	NB-C1B-CHA-C4A
26	H6	1002	PEB	C2B-C1B-CHA-C4A
26	K6	201	PEB	NB-C1B-CHA-C4A
26	K6	201	PEB	C2B-C1B-CHA-C4A
26	L6	1002	PEB	ND-C1D-CHC-C4C
26	L6	1002	PEB	C2D-C1D-CHC-C4C
26	L6	1002	PEB	NB-C1B-CHA-C4A
26	L6	1002	PEB	C2B-C1B-CHA-C4A
26	N6	201	PEB	ND-C1D-CHC-C4C
26	N6	201	PEB	C2D-C1D-CHC-C4C
26	N6	201	PEB	NC-C1C-CHB-C4B
26	N6	201	PEB	C2C-C1C-CHB-C4B
26	N6	201	PEB	NB-C1B-CHA-C4A
26	N6	201	PEB	C2B-C1B-CHA-C4A
26	O6	201	PEB	C4A-C3A-CAA-CBA
26	O6	201	PEB	NB-C1B-CHA-C4A
26	O6	201	PEB	C2B-C1B-CHA-C4A
26	O6	202	PEB	C4A-C3A-CAA-CBA
26	O6	202	PEB	NB-C1B-CHA-C4A
26	O6	202	PEB	C2B-C1B-CHA-C4A
26	O6	203	PEB	C4A-C3A-CAA-CBA
26	O6	203	PEB	NB-C1B-CHA-C4A
26	O6	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	P6	201	PEB	NB-C1B-CHA-C4A
26	P6	201	PEB	C2B-C1B-CHA-C4A
26	P6	202	PEB	NC-C1C-CHB-C4B
26	P6	202	PEB	C2C-C1C-CHB-C4B
26	P6	202	PEB	C1C-C2C-CAC-CBC
26	P6	202	PEB	C3C-C2C-CAC-CBC
26	P6	202	PEB	C2C-CAC-CBC-CGC
26	P6	202	PEB	NB-C1B-CHA-C4A
26	P6	202	PEB	C2B-C1B-CHA-C4A
26	Q6	201	PEB	C4A-C3A-CAA-CBA
26	Q6	201	PEB	NB-C1B-CHA-C4A
26	Q6	201	PEB	C2B-C1B-CHA-C4A
26	Q6	202	PEB	ND-C1D-CHC-C4C
26	Q6	202	PEB	C2A-C3A-CAA-CBA
26	Q6	202	PEB	C4A-C3A-CAA-CBA
26	Q6	202	PEB	NB-C1B-CHA-C4A
26	Q6	202	PEB	C2B-C1B-CHA-C4A
26	Q6	202	PEB	C3B-CAB-CBB-CGB
26	Q6	203	PEB	C2C-CAC-CBC-CGC
26	Q6	203	PEB	NB-C1B-CHA-C4A
26	Q6	203	PEB	C2B-C1B-CHA-C4A
26	R6	201	PEB	C2A-C3A-CAA-CBA
26	R6	201	PEB	C4A-C3A-CAA-CBA
26	R6	201	PEB	NB-C1B-CHA-C4A
26	R6	201	PEB	C2B-C1B-CHA-C4A
26	R6	202	PEB	NC-C1C-CHB-C4B
26	R6	202	PEB	C2C-C1C-CHB-C4B
26	R6	202	PEB	C2A-C3A-CAA-CBA
26	R6	202	PEB	C4A-C3A-CAA-CBA
26	R6	202	PEB	NB-C1B-CHA-C4A
26	R6	202	PEB	C2B-C1B-CHA-C4A
26	S6	201	PEB	C4A-C3A-CAA-CBA
26	S6	201	PEB	NB-C1B-CHA-C4A
26	S6	201	PEB	C2B-C1B-CHA-C4A
26	S6	202	PEB	C2A-C3A-CAA-CBA
26	S6	202	PEB	C4A-C3A-CAA-CBA
26	S6	202	PEB	NB-C1B-CHA-C4A
26	S6	202	PEB	C2B-C1B-CHA-C4A
26	S6	202	PEB	C3B-CAB-CBB-CGB
26	S6	203	PEB	C4A-C3A-CAA-CBA
26	S6	203	PEB	NB-C1B-CHA-C4A
26	S6	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	T6	201	PEB	NB-C1B-CHA-C4A
26	T6	201	PEB	C2B-C1B-CHA-C4A
26	T6	202	PEB	NC-C1C-CHB-C4B
26	T6	202	PEB	C2C-C1C-CHB-C4B
26	T6	202	PEB	C1C-C2C-CAC-CBC
26	T6	202	PEB	C3C-C2C-CAC-CBC
26	T6	202	PEB	NB-C1B-CHA-C4A
26	T6	202	PEB	C2B-C1B-CHA-C4A
26	U6	201	PEB	C2A-C3A-CAA-CBA
26	U6	201	PEB	C4A-C3A-CAA-CBA
26	U6	201	PEB	NB-C1B-CHA-C4A
26	U6	201	PEB	C2B-C1B-CHA-C4A
26	U6	202	PEB	NB-C1B-CHA-C4A
26	U6	202	PEB	C2B-C1B-CHA-C4A
26	U6	203	PEB	C2C-C1C-CHB-C4B
26	U6	203	PEB	C4A-C3A-CAA-CBA
26	U6	203	PEB	NB-C1B-CHA-C4A
26	U6	203	PEB	C2B-C1B-CHA-C4A
26	V6	201	PEB	NB-C1B-CHA-C4A
26	V6	201	PEB	C2B-C1B-CHA-C4A
26	V6	202	PEB	ND-C1D-CHC-C4C
26	V6	202	PEB	C2D-C1D-CHC-C4C
26	V6	202	PEB	NC-C1C-CHB-C4B
26	V6	202	PEB	C2C-C1C-CHB-C4B
26	V6	202	PEB	NB-C1B-CHA-C4A
26	V6	202	PEB	C2B-C1B-CHA-C4A
26	W6	201	PEB	NB-C1B-CHA-C4A
26	W6	201	PEB	C2B-C1B-CHA-C4A
26	W6	202	PEB	NB-C1B-CHA-C4A
26	W6	202	PEB	C2B-C1B-CHA-C4A
26	W6	203	PEB	C2A-C3A-CAA-CBA
26	W6	203	PEB	C4A-C3A-CAA-CBA
26	W6	203	PEB	NB-C1B-CHA-C4A
26	W6	203	PEB	C2B-C1B-CHA-C4A
26	Y6	201	PEB	C1C-C2C-CAC-CBC
26	Y6	201	PEB	C3C-C2C-CAC-CBC
26	Y6	201	PEB	C2A-C3A-CAA-CBA
26	Y6	201	PEB	C4A-C3A-CAA-CBA
26	Y6	201	PEB	NB-C1B-CHA-C4A
26	Y6	201	PEB	C2B-C1B-CHA-C4A
26	Y6	202	PEB	NC-C1C-CHB-C4B
26	Y6	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	Y6	202	PEB	C1C-C2C-CAC-CBC
26	Y6	202	PEB	C3C-C2C-CAC-CBC
26	Y6	202	PEB	C2C-CAC-CBC-CGC
26	Y6	202	PEB	NB-C1B-CHA-C4A
26	Y6	202	PEB	C2B-C1B-CHA-C4A
26	Z6	201	PEB	C2C-CAC-CBC-CGC
26	Z6	201	PEB	C2A-C3A-CAA-CBA
26	Z6	201	PEB	C4A-C3A-CAA-CBA
26	Z6	201	PEB	NB-C1B-CHA-C4A
26	Z6	201	PEB	C2B-C1B-CHA-C4A
26	Z6	202	PEB	C2A-C3A-CAA-CBA
26	Z6	202	PEB	C4A-C3A-CAA-CBA
26	Z6	202	PEB	NB-C1B-CHA-C4A
26	Z6	202	PEB	C2B-C1B-CHA-C4A
26	Z6	203	PEB	NC-C1C-CHB-C4B
26	Z6	203	PEB	C2C-C1C-CHB-C4B
26	Z6	203	PEB	NB-C1B-CHA-C4A
26	Z6	203	PEB	C2B-C1B-CHA-C4A
26	a6	201	PEB	C1C-C2C-CAC-CBC
26	a6	201	PEB	C3C-C2C-CAC-CBC
26	a6	201	PEB	NB-C1B-CHA-C4A
26	a6	201	PEB	C2B-C1B-CHA-C4A
26	a6	202	PEB	NC-C1C-CHB-C4B
26	a6	202	PEB	C2C-C1C-CHB-C4B
26	a6	202	PEB	NB-C1B-CHA-C4A
26	a6	202	PEB	C2B-C1B-CHA-C4A
26	b6	201	PEB	NB-C1B-CHA-C4A
26	b6	201	PEB	C2B-C1B-CHA-C4A
26	b6	202	PEB	ND-C1D-CHC-C4C
26	b6	202	PEB	C2D-C1D-CHC-C4C
26	b6	202	PEB	C2C-CAC-CBC-CGC
26	b6	202	PEB	NB-C1B-CHA-C4A
26	b6	202	PEB	C2B-C1B-CHA-C4A
26	c6	201	PEB	NB-C1B-CHA-C4A
26	c6	201	PEB	C2B-C1B-CHA-C4A
26	c6	202	PEB	ND-C1D-CHC-C4C
26	c6	202	PEB	C2D-C1D-CHC-C4C
26	c6	202	PEB	NC-C1C-CHB-C4B
26	c6	202	PEB	C2C-C1C-CHB-C4B
26	c6	202	PEB	NB-C1B-CHA-C4A
26	c6	202	PEB	C2B-C1B-CHA-C4A
26	d6	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	d6	201	PEB	C2B-C1B-CHA-C4A
26	d6	202	PEB	C4A-C3A-CAA-CBA
26	d6	202	PEB	NB-C1B-CHA-C4A
26	d6	202	PEB	C2B-C1B-CHA-C4A
26	d6	203	PEB	NB-C1B-CHA-C4A
26	d6	203	PEB	C2B-C1B-CHA-C4A
26	d6	204	PEB	NC-C1C-CHB-C4B
26	d6	204	PEB	C2C-C1C-CHB-C4B
26	d6	204	PEB	C2A-C3A-CAA-CBA
26	d6	204	PEB	C4A-C3A-CAA-CBA
26	d6	204	PEB	NB-C1B-CHA-C4A
26	d6	204	PEB	C2B-C1B-CHA-C4A
26	e6	201	PEB	ND-C1D-CHC-C4C
26	e6	201	PEB	C2D-C1D-CHC-C4C
26	e6	201	PEB	C2C-CAC-CBC-CGC
26	e6	201	PEB	NB-C1B-CHA-C4A
26	e6	201	PEB	C2B-C1B-CHA-C4A
26	e6	202	PEB	C2C-CAC-CBC-CGC
26	e6	202	PEB	C2A-C3A-CAA-CBA
26	e6	202	PEB	C4A-C3A-CAA-CBA
26	e6	202	PEB	NB-C1B-CHA-C4A
26	e6	202	PEB	C2B-C1B-CHA-C4A
26	e6	203	PEB	ND-C1D-CHC-C4C
26	e6	203	PEB	C2D-C1D-CHC-C4C
26	e6	203	PEB	NC-C1C-CHB-C4B
26	e6	203	PEB	C2C-C1C-CHB-C4B
26	e6	203	PEB	C1C-C2C-CAC-CBC
26	e6	203	PEB	C3C-C2C-CAC-CBC
26	e6	203	PEB	NB-C1B-CHA-C4A
26	e6	203	PEB	C2B-C1B-CHA-C4A
26	f6	201	PEB	ND-C1D-CHC-C4C
26	f6	201	PEB	C2D-C1D-CHC-C4C
26	f6	201	PEB	NB-C1B-CHA-C4A
26	f6	201	PEB	C2B-C1B-CHA-C4A
26	f6	202	PEB	NB-C1B-CHA-C4A
26	f6	202	PEB	C2B-C1B-CHA-C4A
26	f6	203	PEB	C2A-C3A-CAA-CBA
26	f6	203	PEB	C4A-C3A-CAA-CBA
26	f6	203	PEB	NB-C1B-CHA-C4A
26	f6	203	PEB	C2B-C1B-CHA-C4A
26	g6	201	PEB	NB-C1B-CHA-C4A
26	g6	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	g6	202	PEB	ND-C1D-CHC-C4C
26	g6	202	PEB	C2D-C1D-CHC-C4C
26	g6	202	PEB	NC-C1C-CHB-C4B
26	g6	202	PEB	C2C-C1C-CHB-C4B
26	g6	202	PEB	NB-C1B-CHA-C4A
26	g6	202	PEB	C2B-C1B-CHA-C4A
26	g6	202	PEB	C3B-CAB-CBB-CGB
26	h6	201	PEB	ND-C1D-CHC-C4C
26	h6	201	PEB	C2D-C1D-CHC-C4C
26	h6	201	PEB	C2A-C3A-CAA-CBA
26	h6	201	PEB	C4A-C3A-CAA-CBA
26	h6	201	PEB	NB-C1B-CHA-C4A
26	h6	201	PEB	C2B-C1B-CHA-C4A
26	h6	202	PEB	ND-C1D-CHC-C4C
26	h6	202	PEB	C2D-C1D-CHC-C4C
26	h6	202	PEB	C4A-C3A-CAA-CBA
26	h6	202	PEB	NB-C1B-CHA-C4A
26	h6	202	PEB	C2B-C1B-CHA-C4A
26	h6	203	PEB	NB-C1B-CHA-C4A
26	h6	203	PEB	C2B-C1B-CHA-C4A
26	i6	201	PEB	ND-C1D-CHC-C4C
26	i6	201	PEB	C2D-C1D-CHC-C4C
26	i6	201	PEB	C2C-CAC-CBC-CGC
26	i6	201	PEB	NB-C1B-CHA-C4A
26	i6	201	PEB	C2B-C1B-CHA-C4A
26	i6	202	PEB	NC-C1C-CHB-C4B
26	i6	202	PEB	C2C-C1C-CHB-C4B
26	i6	202	PEB	NB-C1B-CHA-C4A
26	i6	202	PEB	C2B-C1B-CHA-C4A
26	j6	201	PEB	C4A-C3A-CAA-CBA
26	j6	201	PEB	NB-C1B-CHA-C4A
26	j6	201	PEB	C2B-C1B-CHA-C4A
26	j6	202	PEB	NB-C1B-CHA-C4A
26	j6	202	PEB	C2B-C1B-CHA-C4A
26	k6	201	PEB	C1C-C2C-CAC-CBC
26	k6	201	PEB	C3C-C2C-CAC-CBC
26	k6	201	PEB	NB-C1B-CHA-C4A
26	k6	201	PEB	C2B-C1B-CHA-C4A
26	k6	202	PEB	NC-C1C-CHB-C4B
26	k6	202	PEB	C2C-C1C-CHB-C4B
26	k6	202	PEB	C1C-C2C-CAC-CBC
26	k6	202	PEB	C3C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	k6	202	PEB	C2C-CAC-CBC-CGC
26	k6	202	PEB	NB-C1B-CHA-C4A
26	k6	202	PEB	C2B-C1B-CHA-C4A
26	l6	201	PEB	C2A-C3A-CAA-CBA
26	l6	201	PEB	C4A-C3A-CAA-CBA
26	l6	201	PEB	NB-C1B-CHA-C4A
26	l6	201	PEB	C2B-C1B-CHA-C4A
26	l6	202	PEB	ND-C1D-CHC-C4C
26	l6	202	PEB	C2D-C1D-CHC-C4C
26	l6	202	PEB	C4A-C3A-CAA-CBA
26	l6	202	PEB	NB-C1B-CHA-C4A
26	l6	202	PEB	C2B-C1B-CHA-C4A
26	l6	203	PEB	NB-C1B-CHA-C4A
26	l6	203	PEB	C2B-C1B-CHA-C4A
26	m6	201	PEB	ND-C1D-CHC-C4C
26	m6	201	PEB	C2D-C1D-CHC-C4C
26	m6	201	PEB	NB-C1B-CHA-C4A
26	m6	201	PEB	C2B-C1B-CHA-C4A
26	m6	202	PEB	C2A-C3A-CAA-CBA
26	m6	202	PEB	C4A-C3A-CAA-CBA
26	m6	202	PEB	NB-C1B-CHA-C4A
26	m6	202	PEB	C2B-C1B-CHA-C4A
26	m6	203	PEB	NC-C1C-CHB-C4B
26	m6	203	PEB	C2C-C1C-CHB-C4B
26	m6	203	PEB	NB-C1B-CHA-C4A
26	m6	203	PEB	C2B-C1B-CHA-C4A
26	A7	301	PEB	NC-C1C-CHB-C4B
26	A7	301	PEB	C2C-C1C-CHB-C4B
26	A7	301	PEB	NB-C1B-CHA-C4A
26	A7	301	PEB	C2B-C1B-CHA-C4A
26	A7	302	PEB	C4A-C3A-CAA-CBA
26	A7	302	PEB	NB-C1B-CHA-C4A
26	A7	302	PEB	C2B-C1B-CHA-C4A
26	A7	305	PEB	ND-C1D-CHC-C4C
26	A7	305	PEB	C2D-C1D-CHC-C4C
26	A7	305	PEB	NC-C1C-CHB-C4B
26	A7	305	PEB	C2C-C1C-CHB-C4B
26	A7	305	PEB	C2A-C3A-CAA-CBA
26	A7	305	PEB	C4A-C3A-CAA-CBA
26	A7	305	PEB	NB-C1B-CHA-C4A
26	A7	305	PEB	C2B-C1B-CHA-C4A
26	D7	1002	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	D7	1002	PEB	C2A-C3A-CAA-CBA
26	D7	1002	PEB	C4A-C3A-CAA-CBA
26	D7	1002	PEB	NB-C1B-CHA-C4A
26	D7	1002	PEB	C2B-C1B-CHA-C4A
26	F7	1002	PEB	NB-C1B-CHA-C4A
26	F7	1002	PEB	C2B-C1B-CHA-C4A
26	H7	1002	PEB	C2A-C3A-CAA-CBA
26	H7	1002	PEB	C4A-C3A-CAA-CBA
26	H7	1002	PEB	NB-C1B-CHA-C4A
26	H7	1002	PEB	C2B-C1B-CHA-C4A
26	J7	1002	PEB	NB-C1B-CHA-C4A
26	J7	1002	PEB	C2B-C1B-CHA-C4A
26	L7	1002	PEB	C2A-C3A-CAA-CBA
26	L7	1002	PEB	C4A-C3A-CAA-CBA
26	L7	1002	PEB	NB-C1B-CHA-C4A
26	L7	1002	PEB	C2B-C1B-CHA-C4A
26	N7	1002	PEB	NB-C1B-CHA-C4A
26	N7	1002	PEB	C2B-C1B-CHA-C4A
26	O7	201	PEB	ND-C1D-CHC-C4C
26	O7	201	PEB	C2D-C1D-CHC-C4C
26	O7	201	PEB	NB-C1B-CHA-C4A
26	O7	201	PEB	C2B-C1B-CHA-C4A
26	O7	202	PEB	NB-C1B-CHA-C4A
26	O7	202	PEB	C2B-C1B-CHA-C4A
26	O7	203	PEB	C2C-CAC-CBC-CGC
26	O7	203	PEB	C2A-C3A-CAA-CBA
26	O7	203	PEB	NB-C1B-CHA-C4A
26	O7	203	PEB	C2B-C1B-CHA-C4A
26	P7	201	PEB	NB-C1B-CHA-C4A
26	P7	201	PEB	C2B-C1B-CHA-C4A
26	P7	202	PEB	NC-C1C-CHB-C4B
26	P7	202	PEB	C2C-C1C-CHB-C4B
26	P7	202	PEB	NB-C1B-CHA-C4A
26	P7	202	PEB	C2B-C1B-CHA-C4A
26	Q7	201	PEB	C2A-C3A-CAA-CBA
26	Q7	201	PEB	NB-C1B-CHA-C4A
26	Q7	201	PEB	C2B-C1B-CHA-C4A
26	Q7	202	PEB	NB-C1B-CHA-C4A
26	Q7	202	PEB	C2B-C1B-CHA-C4A
26	Q7	203	PEB	C2C-CAC-CBC-CGC
26	Q7	203	PEB	C2A-C3A-CAA-CBA
26	Q7	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	Q7	203	PEB	C2B-C1B-CHA-C4A
26	R7	201	PEB	NB-C1B-CHA-C4A
26	R7	201	PEB	C2B-C1B-CHA-C4A
26	R7	202	PEB	ND-C1D-CHC-C4C
26	R7	202	PEB	C2D-C1D-CHC-C4C
26	R7	202	PEB	NC-C1C-CHB-C4B
26	R7	202	PEB	C2C-C1C-CHB-C4B
26	R7	202	PEB	NB-C1B-CHA-C4A
26	R7	202	PEB	C2B-C1B-CHA-C4A
26	S7	201	PEB	C2A-C3A-CAA-CBA
26	S7	201	PEB	C4A-C3A-CAA-CBA
26	S7	201	PEB	NB-C1B-CHA-C4A
26	S7	201	PEB	C2B-C1B-CHA-C4A
26	S7	202	PEB	NB-C1B-CHA-C4A
26	S7	202	PEB	C2B-C1B-CHA-C4A
26	S7	203	PEB	NB-C1B-CHA-C4A
26	S7	203	PEB	C2B-C1B-CHA-C4A
26	T7	201	PEB	ND-C1D-CHC-C4C
26	T7	201	PEB	C2D-C1D-CHC-C4C
26	T7	201	PEB	C4A-C3A-CAA-CBA
26	T7	201	PEB	NB-C1B-CHA-C4A
26	T7	201	PEB	C2B-C1B-CHA-C4A
26	T7	202	PEB	ND-C1D-CHC-C4C
26	T7	202	PEB	C2D-C1D-CHC-C4C
26	T7	202	PEB	NC-C1C-CHB-C4B
26	T7	202	PEB	C2C-C1C-CHB-C4B
26	T7	202	PEB	NB-C1B-CHA-C4A
26	T7	202	PEB	C2B-C1B-CHA-C4A
26	U7	201	PEB	NC-C1C-CHB-C4B
26	U7	201	PEB	C2C-C1C-CHB-C4B
26	U7	201	PEB	C2A-C3A-CAA-CBA
26	U7	201	PEB	C4A-C3A-CAA-CBA
26	U7	201	PEB	NB-C1B-CHA-C4A
26	U7	201	PEB	C2B-C1B-CHA-C4A
26	U7	202	PEB	C4A-C3A-CAA-CBA
26	U7	202	PEB	NB-C1B-CHA-C4A
26	U7	202	PEB	C2B-C1B-CHA-C4A
26	U7	203	PEB	C2A-C3A-CAA-CBA
26	U7	203	PEB	NB-C1B-CHA-C4A
26	U7	203	PEB	C2B-C1B-CHA-C4A
26	V7	201	PEB	NB-C1B-CHA-C4A
26	V7	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	V7	202	PEB	ND-C1D-CHC-C4C
26	V7	202	PEB	C2D-C1D-CHC-C4C
26	V7	202	PEB	NC-C1C-CHB-C4B
26	V7	202	PEB	C2C-C1C-CHB-C4B
26	V7	202	PEB	NB-C1B-CHA-C4A
26	V7	202	PEB	C2B-C1B-CHA-C4A
26	W7	201	PEB	ND-C1D-CHC-C4C
26	W7	201	PEB	C2D-C1D-CHC-C4C
26	W7	201	PEB	C4A-C3A-CAA-CBA
26	W7	201	PEB	NB-C1B-CHA-C4A
26	W7	201	PEB	C2B-C1B-CHA-C4A
26	W7	202	PEB	NC-C1C-CHB-C4B
26	W7	202	PEB	C2C-C1C-CHB-C4B
26	W7	202	PEB	NB-C1B-CHA-C4A
26	W7	202	PEB	C2B-C1B-CHA-C4A
26	W7	203	PEB	C2A-C3A-CAA-CBA
26	W7	203	PEB	NB-C1B-CHA-C4A
26	W7	203	PEB	C2B-C1B-CHA-C4A
26	Y7	201	PEB	NB-C1B-CHA-C4A
26	Y7	201	PEB	C2B-C1B-CHA-C4A
26	Y7	202	PEB	NB-C1B-CHA-C4A
26	Y7	202	PEB	C2B-C1B-CHA-C4A
26	Z7	201	PEB	C4A-C3A-CAA-CBA
26	Z7	201	PEB	NB-C1B-CHA-C4A
26	Z7	201	PEB	C2B-C1B-CHA-C4A
26	Z7	202	PEB	ND-C1D-CHC-C4C
26	Z7	202	PEB	C2D-C1D-CHC-C4C
26	Z7	202	PEB	C2A-C3A-CAA-CBA
26	Z7	202	PEB	C4A-C3A-CAA-CBA
26	Z7	202	PEB	NB-C1B-CHA-C4A
26	Z7	202	PEB	C2B-C1B-CHA-C4A
26	Z7	203	PEB	NB-C1B-CHA-C4A
26	Z7	203	PEB	C2B-C1B-CHA-C4A
26	a7	201	PEB	NB-C1B-CHA-C4A
26	a7	201	PEB	C2B-C1B-CHA-C4A
26	a7	202	PEB	ND-C1D-CHC-C4C
26	a7	202	PEB	C2D-C1D-CHC-C4C
26	a7	202	PEB	C2C-CAC-CBC-CGC
26	a7	202	PEB	NB-C1B-CHA-C4A
26	a7	202	PEB	C2B-C1B-CHA-C4A
26	b7	201	PEB	ND-C1D-CHC-C4C
26	b7	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	b7	201	PEB	C4D-C3D-CAD-CBD
26	b7	201	PEB	C2A-C3A-CAA-CBA
26	b7	201	PEB	C4A-C3A-CAA-CBA
26	b7	201	PEB	NB-C1B-CHA-C4A
26	b7	201	PEB	C2B-C1B-CHA-C4A
26	b7	202	PEB	NB-C1B-CHA-C4A
26	b7	202	PEB	C2B-C1B-CHA-C4A
26	b7	203	PEB	C2A-C3A-CAA-CBA
26	b7	203	PEB	C4A-C3A-CAA-CBA
26	b7	203	PEB	NB-C1B-CHA-C4A
26	b7	203	PEB	C2B-C1B-CHA-C4A
26	c7	201	PEB	NB-C1B-CHA-C4A
26	c7	201	PEB	C2B-C1B-CHA-C4A
26	c7	202	PEB	NC-C1C-CHB-C4B
26	c7	202	PEB	C2C-C1C-CHB-C4B
26	c7	202	PEB	NB-C1B-CHA-C4A
26	c7	202	PEB	C2B-C1B-CHA-C4A
26	d7	201	PEB	NC-C1C-CHB-C4B
26	d7	201	PEB	NB-C1B-CHA-C4A
26	d7	201	PEB	C2B-C1B-CHA-C4A
26	d7	202	PEB	ND-C1D-CHC-C4C
26	d7	202	PEB	C4A-C3A-CAA-CBA
26	d7	202	PEB	NB-C1B-CHA-C4A
26	d7	202	PEB	C2B-C1B-CHA-C4A
26	d7	203	PEB	C2C-CAC-CBC-CGC
26	d7	203	PEB	C2D-C3D-CAD-CBD
26	d7	203	PEB	C4D-C3D-CAD-CBD
26	d7	203	PEB	NB-C1B-CHA-C4A
26	d7	203	PEB	C2B-C1B-CHA-C4A
26	e7	201	PEB	NB-C1B-CHA-C4A
26	e7	201	PEB	C2B-C1B-CHA-C4A
26	e7	202	PEB	ND-C1D-CHC-C4C
26	e7	202	PEB	C2D-C1D-CHC-C4C
26	e7	202	PEB	NC-C1C-CHB-C4B
26	e7	202	PEB	C2C-C1C-CHB-C4B
26	e7	202	PEB	NB-C1B-CHA-C4A
26	e7	202	PEB	C2B-C1B-CHA-C4A
26	f7	201	PEB	ND-C1D-CHC-C4C
26	f7	201	PEB	NB-C1B-CHA-C4A
26	f7	201	PEB	C2B-C1B-CHA-C4A
26	f7	202	PEB	C2C-CAC-CBC-CGC
26	f7	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	f7	202	PEB	C2B-C1B-CHA-C4A
26	f7	203	PEB	NC-C1C-CHB-C4B
26	f7	203	PEB	C2C-C1C-CHB-C4B
26	f7	203	PEB	C2C-CAC-CBC-CGC
26	f7	203	PEB	NB-C1B-CHA-C4A
26	f7	203	PEB	C2B-C1B-CHA-C4A
26	g7	201	PEB	NC-C1C-CHB-C4B
26	g7	201	PEB	NB-C1B-CHA-C4A
26	g7	201	PEB	C2B-C1B-CHA-C4A
26	g7	202	PEB	NC-C1C-CHB-C4B
26	g7	202	PEB	NB-C1B-CHA-C4A
26	g7	202	PEB	C2B-C1B-CHA-C4A
26	h7	201	PEB	NB-C1B-CHA-C4A
26	h7	201	PEB	C2B-C1B-CHA-C4A
26	h7	202	PEB	ND-C1D-CHC-C4C
26	h7	202	PEB	C2D-C1D-CHC-C4C
26	h7	202	PEB	NC-C1C-CHB-C4B
26	h7	202	PEB	C2C-C1C-CHB-C4B
26	h7	202	PEB	C2A-C3A-CAA-CBA
26	h7	202	PEB	C4A-C3A-CAA-CBA
26	h7	202	PEB	NB-C1B-CHA-C4A
26	h7	202	PEB	C2B-C1B-CHA-C4A
26	h7	203	PEB	C2A-C3A-CAA-CBA
26	h7	203	PEB	NB-C1B-CHA-C4A
26	h7	203	PEB	C2B-C1B-CHA-C4A
26	h7	203	PEB	C3B-CAB-CBB-CGB
26	i7	201	PEB	NB-C1B-CHA-C4A
26	i7	201	PEB	C2B-C1B-CHA-C4A
26	i7	202	PEB	ND-C1D-CHC-C4C
26	i7	202	PEB	C2D-C1D-CHC-C4C
26	i7	202	PEB	NC-C1C-CHB-C4B
26	i7	202	PEB	C2C-C1C-CHB-C4B
26	i7	202	PEB	NB-C1B-CHA-C4A
26	i7	202	PEB	C2B-C1B-CHA-C4A
26	j7	201	PEB	ND-C1D-CHC-C4C
26	j7	201	PEB	C2D-C1D-CHC-C4C
26	j7	201	PEB	C2A-C3A-CAA-CBA
26	j7	201	PEB	C4A-C3A-CAA-CBA
26	j7	201	PEB	NB-C1B-CHA-C4A
26	j7	201	PEB	C2B-C1B-CHA-C4A
26	j7	202	PEB	NB-C1B-CHA-C4A
26	j7	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	j7	203	PEB	NB-C1B-CHA-C4A
26	j7	203	PEB	C2B-C1B-CHA-C4A
26	k7	201	PEB	ND-C1D-CHC-C4C
26	k7	201	PEB	C2D-C1D-CHC-C4C
26	k7	201	PEB	NC-C1C-CHB-C4B
26	k7	201	PEB	C2C-C1C-CHB-C4B
26	k7	201	PEB	C2A-C3A-CAA-CBA
26	k7	201	PEB	NB-C1B-CHA-C4A
26	k7	201	PEB	C2B-C1B-CHA-C4A
26	k7	202	PEB	NC-C1C-CHB-C4B
26	k7	202	PEB	C2C-C1C-CHB-C4B
26	k7	202	PEB	C2C-CAC-CBC-CGC
26	k7	202	PEB	C2A-C3A-CAA-CBA
26	k7	202	PEB	C4A-C3A-CAA-CBA
26	k7	202	PEB	NB-C1B-CHA-C4A
26	k7	202	PEB	C2B-C1B-CHA-C4A
26	l7	201	PEB	C2D-C3D-CAD-CBD
26	l7	201	PEB	C4D-C3D-CAD-CBD
26	l7	201	PEB	NB-C1B-CHA-C4A
26	l7	201	PEB	C2B-C1B-CHA-C4A
26	l7	202	PEB	ND-C1D-CHC-C4C
26	l7	202	PEB	NB-C1B-CHA-C4A
26	l7	202	PEB	C2B-C1B-CHA-C4A
26	l7	203	PEB	NB-C1B-CHA-C4A
26	l7	203	PEB	C2B-C1B-CHA-C4A
26	m7	201	PEB	NC-C1C-CHB-C4B
26	m7	201	PEB	C2C-C1C-CHB-C4B
26	m7	201	PEB	NB-C1B-CHA-C4A
26	m7	201	PEB	C2B-C1B-CHA-C4A
26	m7	202	PEB	NC-C1C-CHB-C4B
26	m7	202	PEB	C2A-C3A-CAA-CBA
26	m7	202	PEB	C4A-C3A-CAA-CBA
26	m7	202	PEB	NB-C1B-CHA-C4A
26	m7	202	PEB	C2B-C1B-CHA-C4A
26	A8	301	PEB	ND-C1D-CHC-C4C
26	A8	301	PEB	C2D-C1D-CHC-C4C
26	A8	301	PEB	NC-C1C-CHB-C4B
26	A8	301	PEB	C2C-C1C-CHB-C4B
26	A8	301	PEB	C2A-C3A-CAA-CBA
26	A8	301	PEB	C4A-C3A-CAA-CBA
26	A8	301	PEB	NB-C1B-CHA-C4A
26	A8	301	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	A8	302	PEB	ND-C1D-CHC-C4C
26	A8	302	PEB	NC-C1C-CHB-C4B
26	A8	302	PEB	C2C-C1C-CHB-C4B
26	A8	302	PEB	NB-C1B-CHA-C4A
26	A8	302	PEB	C2B-C1B-CHA-C4A
26	B8	301	PEB	NC-C1C-CHB-C4B
26	B8	301	PEB	C2C-C1C-CHB-C4B
26	B8	301	PEB	NB-C1B-CHA-C4A
26	B8	301	PEB	C2B-C1B-CHA-C4A
26	C8	201	PEB	NB-C1B-CHA-C4A
26	C8	201	PEB	C2B-C1B-CHA-C4A
26	C8	202	PEB	NC-C1C-CHB-C4B
26	C8	202	PEB	C2C-C1C-CHB-C4B
26	C8	202	PEB	C2C-CAC-CBC-CGC
26	C8	202	PEB	NB-C1B-CHA-C4A
26	C8	202	PEB	C2B-C1B-CHA-C4A
26	C8	203	PEB	NB-C1B-CHA-C4A
26	C8	203	PEB	C2B-C1B-CHA-C4A
26	D8	201	PEB	ND-C1D-CHC-C4C
26	D8	201	PEB	C2D-C1D-CHC-C4C
26	D8	201	PEB	NC-C1C-CHB-C4B
26	D8	201	PEB	C2C-C1C-CHB-C4B
26	D8	201	PEB	NB-C1B-CHA-C4A
26	D8	201	PEB	C2B-C1B-CHA-C4A
26	D8	202	PEB	NC-C1C-CHB-C4B
26	D8	202	PEB	C2C-C1C-CHB-C4B
26	D8	202	PEB	NB-C1B-CHA-C4A
26	D8	202	PEB	C2B-C1B-CHA-C4A
26	E8	201	PEB	C2A-C3A-CAA-CBA
26	E8	201	PEB	NB-C1B-CHA-C4A
26	E8	201	PEB	C2B-C1B-CHA-C4A
26	E8	202	PEB	C2A-C3A-CAA-CBA
26	E8	202	PEB	C4A-C3A-CAA-CBA
26	E8	202	PEB	NB-C1B-CHA-C4A
26	E8	202	PEB	C2B-C1B-CHA-C4A
26	E8	203	PEB	C4A-C3A-CAA-CBA
26	E8	203	PEB	NB-C1B-CHA-C4A
26	E8	203	PEB	C2B-C1B-CHA-C4A
26	F8	201	PEB	ND-C1D-CHC-C4C
26	F8	201	PEB	C2D-C1D-CHC-C4C
26	F8	201	PEB	C2C-C1C-CHB-C4B
26	F8	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	F8	201	PEB	C2B-C1B-CHA-C4A
26	F8	202	PEB	NC-C1C-CHB-C4B
26	F8	202	PEB	C2C-C1C-CHB-C4B
26	F8	202	PEB	NB-C1B-CHA-C4A
26	F8	202	PEB	C2B-C1B-CHA-C4A
26	G8	201	PEB	C2A-C3A-CAA-CBA
26	G8	201	PEB	C4A-C3A-CAA-CBA
26	G8	202	PEB	C2C-CAC-CBC-CGC
26	G8	202	PEB	NB-C1B-CHA-C4A
26	G8	202	PEB	C2B-C1B-CHA-C4A
26	G8	203	PEB	C4A-C3A-CAA-CBA
26	G8	203	PEB	NB-C1B-CHA-C4A
26	G8	203	PEB	C2B-C1B-CHA-C4A
26	H8	201	PEB	ND-C1D-CHC-C4C
26	H8	201	PEB	NB-C1B-CHA-C4A
26	H8	201	PEB	C2B-C1B-CHA-C4A
26	H8	202	PEB	NC-C1C-CHB-C4B
26	H8	202	PEB	C2C-C1C-CHB-C4B
26	H8	202	PEB	C2C-CAC-CBC-CGC
26	H8	202	PEB	NB-C1B-CHA-C4A
26	H8	202	PEB	C2B-C1B-CHA-C4A
26	I8	201	PEB	C4A-C3A-CAA-CBA
26	I8	201	PEB	NB-C1B-CHA-C4A
26	I8	201	PEB	C2B-C1B-CHA-C4A
26	I8	202	PEB	NB-C1B-CHA-C4A
26	I8	202	PEB	C2B-C1B-CHA-C4A
26	I8	203	PEB	NC-C1C-CHB-C4B
26	I8	203	PEB	C2C-C1C-CHB-C4B
26	I8	203	PEB	C2A-C3A-CAA-CBA
26	I8	203	PEB	C4A-C3A-CAA-CBA
26	I8	203	PEB	NB-C1B-CHA-C4A
26	I8	203	PEB	C2B-C1B-CHA-C4A
26	J8	201	PEB	ND-C1D-CHC-C4C
26	J8	201	PEB	C2D-C1D-CHC-C4C
26	J8	201	PEB	NC-C1C-CHB-C4B
26	J8	201	PEB	C2C-C1C-CHB-C4B
26	J8	201	PEB	C2A-C3A-CAA-CBA
26	J8	201	PEB	NB-C1B-CHA-C4A
26	J8	201	PEB	C2B-C1B-CHA-C4A
26	J8	202	PEB	NC-C1C-CHB-C4B
26	J8	202	PEB	C2C-C1C-CHB-C4B
26	J8	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	J8	202	PEB	NB-C1B-CHA-C4A
26	J8	202	PEB	C2B-C1B-CHA-C4A
26	K8	201	PEB	C2A-C3A-CAA-CBA
26	K8	201	PEB	C4A-C3A-CAA-CBA
26	K8	202	PEB	NB-C1B-CHA-C4A
26	K8	202	PEB	C2B-C1B-CHA-C4A
26	K8	203	PEB	C4A-C3A-CAA-CBA
26	K8	203	PEB	NB-C1B-CHA-C4A
26	K8	203	PEB	C2B-C1B-CHA-C4A
26	L8	201	PEB	ND-C1D-CHC-C4C
26	L8	201	PEB	NB-C1B-CHA-C4A
26	L8	201	PEB	C2B-C1B-CHA-C4A
26	L8	202	PEB	NC-C1C-CHB-C4B
26	L8	202	PEB	C2C-C1C-CHB-C4B
26	L8	202	PEB	NB-C1B-CHA-C4A
26	L8	202	PEB	C2B-C1B-CHA-C4A
26	M8	201	PEB	C4A-C3A-CAA-CBA
26	M8	201	PEB	NB-C1B-CHA-C4A
26	M8	201	PEB	C2B-C1B-CHA-C4A
26	M8	202	PEB	NB-C1B-CHA-C4A
26	M8	202	PEB	C2B-C1B-CHA-C4A
26	M8	203	PEB	C2A-C3A-CAA-CBA
26	M8	203	PEB	C4A-C3A-CAA-CBA
26	M8	203	PEB	NB-C1B-CHA-C4A
26	M8	203	PEB	C2B-C1B-CHA-C4A
26	N8	201	PEB	ND-C1D-CHC-C4C
26	N8	201	PEB	NB-C1B-CHA-C4A
26	N8	201	PEB	C2B-C1B-CHA-C4A
26	N8	202	PEB	NC-C1C-CHB-C4B
26	N8	202	PEB	C2C-C1C-CHB-C4B
26	N8	202	PEB	NB-C1B-CHA-C4A
26	N8	202	PEB	C2B-C1B-CHA-C4A
26	O8	201	PEB	C2A-C3A-CAA-CBA
26	O8	201	PEB	C4A-C3A-CAA-CBA
26	O8	201	PEB	NB-C1B-CHA-C4A
26	O8	201	PEB	C2B-C1B-CHA-C4A
26	O8	202	PEB	C2C-CAC-CBC-CGC
26	O8	202	PEB	NB-C1B-CHA-C4A
26	O8	202	PEB	C2B-C1B-CHA-C4A
26	O8	203	PEB	C2A-C3A-CAA-CBA
26	O8	203	PEB	C4A-C3A-CAA-CBA
26	O8	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	O8	203	PEB	C2B-C1B-CHA-C4A
26	P8	201	PEB	ND-C1D-CHC-C4C
26	P8	201	PEB	C2D-C1D-CHC-C4C
26	P8	201	PEB	NC-C1C-CHB-C4B
26	P8	201	PEB	NB-C1B-CHA-C4A
26	P8	201	PEB	C2B-C1B-CHA-C4A
26	P8	202	PEB	NC-C1C-CHB-C4B
26	P8	202	PEB	C2C-C1C-CHB-C4B
26	P8	202	PEB	NB-C1B-CHA-C4A
26	P8	202	PEB	C2B-C1B-CHA-C4A
26	Q8	202	PEB	NB-C1B-CHA-C4A
26	Q8	202	PEB	C2B-C1B-CHA-C4A
26	Q8	203	PEB	NB-C1B-CHA-C4A
26	Q8	203	PEB	C2B-C1B-CHA-C4A
26	Q8	204	PEB	ND-C1D-CHC-C4C
26	Q8	204	PEB	C2D-C1D-CHC-C4C
26	Q8	204	PEB	NC-C1C-CHB-C4B
26	Q8	204	PEB	C2C-C1C-CHB-C4B
26	Q8	204	PEB	NB-C1B-CHA-C4A
26	Q8	204	PEB	C2B-C1B-CHA-C4A
26	R8	201	PEB	ND-C1D-CHC-C4C
26	R8	201	PEB	C2D-C1D-CHC-C4C
26	R8	201	PEB	NB-C1B-CHA-C4A
26	R8	201	PEB	C2B-C1B-CHA-C4A
26	R8	202	PEB	ND-C1D-CHC-C4C
26	R8	202	PEB	C2D-C1D-CHC-C4C
26	R8	202	PEB	NC-C1C-CHB-C4B
26	R8	202	PEB	C2C-C1C-CHB-C4B
26	R8	202	PEB	NB-C1B-CHA-C4A
26	R8	202	PEB	C2B-C1B-CHA-C4A
26	S8	201	PEB	C2A-C3A-CAA-CBA
26	S8	201	PEB	C4A-C3A-CAA-CBA
26	S8	201	PEB	NB-C1B-CHA-C4A
26	S8	201	PEB	C2B-C1B-CHA-C4A
26	S8	202	PEB	C2A-C3A-CAA-CBA
26	S8	202	PEB	C4A-C3A-CAA-CBA
26	S8	202	PEB	NB-C1B-CHA-C4A
26	S8	202	PEB	C2B-C1B-CHA-C4A
26	S8	203	PEB	C2A-C3A-CAA-CBA
26	S8	203	PEB	C4A-C3A-CAA-CBA
26	S8	203	PEB	NB-C1B-CHA-C4A
26	S8	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	T8	201	PEB	ND-C1D-CHC-C4C
26	T8	201	PEB	C2D-C1D-CHC-C4C
26	T8	201	PEB	NB-C1B-CHA-C4A
26	T8	201	PEB	C2B-C1B-CHA-C4A
26	T8	202	PEB	C2C-CAC-CBC-CGC
26	T8	202	PEB	NB-C1B-CHA-C4A
26	T8	202	PEB	C2B-C1B-CHA-C4A
26	U8	201	PEB	C2A-C3A-CAA-CBA
26	U8	201	PEB	C4A-C3A-CAA-CBA
26	U8	201	PEB	NB-C1B-CHA-C4A
26	U8	201	PEB	C2B-C1B-CHA-C4A
26	U8	203	PEB	C2C-CAC-CBC-CGC
26	U8	203	PEB	NB-C1B-CHA-C4A
26	U8	203	PEB	C2B-C1B-CHA-C4A
26	V8	201	PEB	ND-C1D-CHC-C4C
26	V8	201	PEB	C2D-C1D-CHC-C4C
26	V8	201	PEB	NC-C1C-CHB-C4B
26	V8	201	PEB	C2C-C1C-CHB-C4B
26	V8	201	PEB	NB-C1B-CHA-C4A
26	V8	201	PEB	C2B-C1B-CHA-C4A
26	V8	202	PEB	NC-C1C-CHB-C4B
26	V8	202	PEB	C2C-C1C-CHB-C4B
26	V8	202	PEB	C2C-CAC-CBC-CGC
26	V8	202	PEB	NB-C1B-CHA-C4A
26	V8	202	PEB	C2B-C1B-CHA-C4A
26	V8	202	PEB	C2B-C3B-CAB-CBB
26	W8	201	PEB	NB-C1B-CHA-C4A
26	W8	202	PEB	NC-C1C-CHB-C4B
26	W8	202	PEB	C2C-C1C-CHB-C4B
26	W8	202	PEB	C2C-CAC-CBC-CGC
26	W8	202	PEB	NB-C1B-CHA-C4A
26	W8	202	PEB	C2B-C1B-CHA-C4A
26	W8	203	PEB	C4A-C3A-CAA-CBA
26	W8	203	PEB	NB-C1B-CHA-C4A
26	W8	203	PEB	C2B-C1B-CHA-C4A
26	X8	201	PEB	ND-C1D-CHC-C4C
26	X8	201	PEB	C2D-C1D-CHC-C4C
26	X8	201	PEB	C2A-C3A-CAA-CBA
26	X8	201	PEB	C4A-C3A-CAA-CBA
26	X8	201	PEB	NB-C1B-CHA-C4A
26	X8	201	PEB	C2B-C1B-CHA-C4A
26	X8	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	X8	202	PEB	C2C-C1C-CHB-C4B
26	X8	202	PEB	NB-C1B-CHA-C4A
26	X8	202	PEB	C2B-C1B-CHA-C4A
26	Y8	201	PEB	C4A-C3A-CAA-CBA
26	Y8	201	PEB	NB-C1B-CHA-C4A
26	Y8	201	PEB	C2B-C1B-CHA-C4A
26	Y8	202	PEB	NB-C1B-CHA-C4A
26	Y8	203	PEB	NB-C1B-CHA-C4A
26	Y8	203	PEB	C2B-C1B-CHA-C4A
26	Z8	201	PEB	ND-C1D-CHC-C4C
26	Z8	201	PEB	C2D-C1D-CHC-C4C
26	Z8	201	PEB	NB-C1B-CHA-C4A
26	Z8	201	PEB	C2B-C1B-CHA-C4A
26	Z8	202	PEB	C2C-CAC-CBC-CGC
26	Z8	202	PEB	NB-C1B-CHA-C4A
26	Z8	202	PEB	C2B-C1B-CHA-C4A
26	a8	201	PEB	NC-C1C-CHB-C4B
26	a8	201	PEB	C2C-C1C-CHB-C4B
26	a8	201	PEB	C2A-C3A-CAA-CBA
26	a8	201	PEB	C4A-C3A-CAA-CBA
26	a8	201	PEB	NB-C1B-CHA-C4A
26	a8	201	PEB	C2B-C1B-CHA-C4A
26	a8	202	PEB	NB-C1B-CHA-C4A
26	a8	202	PEB	C2B-C1B-CHA-C4A
26	a8	203	PEB	NC-C1C-CHB-C4B
26	a8	203	PEB	C2C-C1C-CHB-C4B
26	a8	203	PEB	NB-C1B-CHA-C4A
26	a8	203	PEB	C2B-C1B-CHA-C4A
26	a8	204	PEB	C2A-C3A-CAA-CBA
26	a8	204	PEB	C4A-C3A-CAA-CBA
26	a8	204	PEB	NB-C1B-CHA-C4A
26	a8	204	PEB	C2B-C1B-CHA-C4A
26	c8	201	PEB	ND-C1D-CHC-C4C
26	c8	201	PEB	C2D-C1D-CHC-C4C
26	c8	201	PEB	NC-C1C-CHB-C4B
26	c8	201	PEB	C2C-C1C-CHB-C4B
26	c8	201	PEB	NB-C1B-CHA-C4A
26	c8	201	PEB	C2B-C1B-CHA-C4A
26	c8	202	PEB	NC-C1C-CHB-C4B
26	c8	202	PEB	C2C-C1C-CHB-C4B
26	c8	202	PEB	C2C-CAC-CBC-CGC
26	c8	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	c8	202	PEB	C2B-C1B-CHA-C4A
26	d8	201	PEB	C2C-CAC-CBC-CGC
26	d8	201	PEB	C4A-C3A-CAA-CBA
26	d8	201	PEB	NB-C1B-CHA-C4A
26	d8	201	PEB	C2B-C1B-CHA-C4A
26	d8	202	PEB	NB-C1B-CHA-C4A
26	d8	202	PEB	C2B-C1B-CHA-C4A
26	d8	203	PEB	ND-C1D-CHC-C4C
26	d8	203	PEB	C2A-C3A-CAA-CBA
26	d8	203	PEB	C4A-C3A-CAA-CBA
26	d8	203	PEB	NB-C1B-CHA-C4A
26	d8	203	PEB	C2B-C1B-CHA-C4A
26	d8	203	PEB	C3B-CAB-CBB-CGB
26	e8	201	PEB	ND-C1D-CHC-C4C
26	e8	201	PEB	C2D-C1D-CHC-C4C
26	e8	201	PEB	NB-C1B-CHA-C4A
26	e8	201	PEB	C2B-C1B-CHA-C4A
26	e8	202	PEB	NC-C1C-CHB-C4B
26	e8	202	PEB	C2C-C1C-CHB-C4B
26	e8	202	PEB	C2C-CAC-CBC-CGC
26	e8	202	PEB	NB-C1B-CHA-C4A
26	e8	202	PEB	C2B-C1B-CHA-C4A
26	f8	201	PEB	ND-C1D-CHC-C4C
26	f8	201	PEB	NC-C1C-CHB-C4B
26	f8	201	PEB	C2C-C1C-CHB-C4B
26	f8	201	PEB	NB-C1B-CHA-C4A
26	f8	201	PEB	C2B-C1B-CHA-C4A
26	f8	202	PEB	C4A-C3A-CAA-CBA
26	f8	202	PEB	NB-C1B-CHA-C4A
26	f8	202	PEB	C2B-C1B-CHA-C4A
26	f8	203	PEB	NB-C1B-CHA-C4A
26	f8	203	PEB	C2B-C1B-CHA-C4A
26	g8	201	PEB	ND-C1D-CHC-C4C
26	g8	201	PEB	C2D-C1D-CHC-C4C
26	g8	201	PEB	NC-C1C-CHB-C4B
26	g8	201	PEB	C2C-C1C-CHB-C4B
26	g8	201	PEB	C2C-CAC-CBC-CGC
26	g8	201	PEB	NB-C1B-CHA-C4A
26	g8	201	PEB	C2B-C1B-CHA-C4A
26	g8	202	PEB	NC-C1C-CHB-C4B
26	g8	202	PEB	C2C-C1C-CHB-C4B
26	g8	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	g8	202	PEB	NB-C1B-CHA-C4A
26	g8	202	PEB	C2B-C1B-CHA-C4A
26	h8	201	PEB	ND-C1D-CHC-C4C
26	h8	201	PEB	C2D-C1D-CHC-C4C
26	h8	201	PEB	C2A-C3A-CAA-CBA
26	h8	201	PEB	C4A-C3A-CAA-CBA
26	h8	201	PEB	NB-C1B-CHA-C4A
26	h8	201	PEB	C2B-C1B-CHA-C4A
26	h8	202	PEB	NB-C1B-CHA-C4A
26	h8	202	PEB	C2B-C1B-CHA-C4A
26	h8	203	PEB	C2C-CAC-CBC-CGC
26	h8	203	PEB	NB-C1B-CHA-C4A
26	h8	203	PEB	C2B-C1B-CHA-C4A
26	i8	201	PEB	ND-C1D-CHC-C4C
26	i8	201	PEB	C2D-C1D-CHC-C4C
26	i8	201	PEB	NB-C1B-CHA-C4A
26	i8	201	PEB	C2B-C1B-CHA-C4A
26	i8	202	PEB	NC-C1C-CHB-C4B
26	i8	202	PEB	C2C-C1C-CHB-C4B
26	i8	202	PEB	NB-C1B-CHA-C4A
26	i8	202	PEB	C2B-C1B-CHA-C4A
26	j8	201	PEB	ND-C1D-CHC-C4C
26	j8	201	PEB	NB-C1B-CHA-C4A
26	j8	201	PEB	C2B-C1B-CHA-C4A
26	j8	202	PEB	NC-C1C-CHB-C4B
26	j8	202	PEB	C2C-C1C-CHB-C4B
26	j8	202	PEB	C1C-C2C-CAC-CBC
26	j8	202	PEB	C3C-C2C-CAC-CBC
26	j8	202	PEB	NB-C1B-CHA-C4A
26	j8	202	PEB	C2B-C1B-CHA-C4A
26	j8	203	PEB	C2A-C3A-CAA-CBA
26	j8	203	PEB	C4A-C3A-CAA-CBA
26	j8	203	PEB	NB-C1B-CHA-C4A
26	j8	203	PEB	C2B-C1B-CHA-C4A
26	k8	201	PEB	ND-C1D-CHC-C4C
26	k8	201	PEB	C2D-C1D-CHC-C4C
26	k8	201	PEB	NC-C1C-CHB-C4B
26	k8	201	PEB	C2C-C1C-CHB-C4B
26	k8	201	PEB	C2A-C3A-CAA-CBA
26	k8	201	PEB	C4A-C3A-CAA-CBA
26	k8	201	PEB	NB-C1B-CHA-C4A
26	k8	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	k8	202	PEB	ND-C1D-CHC-C4C
26	k8	202	PEB	C2D-C1D-CHC-C4C
26	k8	202	PEB	NC-C1C-CHB-C4B
26	k8	202	PEB	C2C-C1C-CHB-C4B
26	k8	202	PEB	NB-C1B-CHA-C4A
26	k8	202	PEB	C2B-C1B-CHA-C4A
26	l8	201	PEB	NC-C1C-CHB-C4B
26	l8	201	PEB	C2C-C1C-CHB-C4B
26	l8	201	PEB	C2A-C3A-CAA-CBA
26	l8	201	PEB	C4A-C3A-CAA-CBA
26	l8	201	PEB	NB-C1B-CHA-C4A
26	l8	201	PEB	C2B-C1B-CHA-C4A
26	l8	202	PEB	NB-C1B-CHA-C4A
26	l8	202	PEB	C2B-C1B-CHA-C4A
26	l8	203	PEB	NC-C1C-CHB-C4B
26	l8	203	PEB	C2C-C1C-CHB-C4B
26	l8	203	PEB	C2A-C3A-CAA-CBA
26	l8	203	PEB	C4A-C3A-CAA-CBA
26	l8	203	PEB	NB-C1B-CHA-C4A
26	l8	203	PEB	C2B-C1B-CHA-C4A
26	m8	201	PEB	ND-C1D-CHC-C4C
26	m8	201	PEB	C2D-C1D-CHC-C4C
26	m8	201	PEB	NC-C1C-CHB-C4B
26	m8	201	PEB	C2C-C1C-CHB-C4B
26	m8	201	PEB	NB-C1B-CHA-C4A
26	m8	201	PEB	C2B-C1B-CHA-C4A
26	m8	202	PEB	NC-C1C-CHB-C4B
26	m8	202	PEB	C2C-C1C-CHB-C4B
26	m8	202	PEB	NB-C1B-CHA-C4A
26	m8	202	PEB	C2B-C1B-CHA-C4A
26	m8	202	PEB	C2B-C3B-CAB-CBB
26	A9	301	PEB	C2C-CAC-CBC-CGC
26	A9	301	PEB	NB-C1B-CHA-C4A
26	A9	301	PEB	C2B-C1B-CHA-C4A
26	A9	303	PEB	ND-C1D-CHC-C4C
26	A9	303	PEB	C2A-C3A-CAA-CBA
26	A9	303	PEB	NB-C1B-CHA-C4A
26	A9	303	PEB	C2B-C1B-CHA-C4A
26	A9	304	PEB	NC-C1C-CHB-C4B
26	A9	304	PEB	C2C-C1C-CHB-C4B
26	A9	304	PEB	NB-C1B-CHA-C4A
26	A9	304	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	B9	201	PEB	ND-C1D-CHC-C4C
26	B9	201	PEB	C2D-C1D-CHC-C4C
26	B9	201	PEB	NC-C1C-CHB-C4B
26	B9	201	PEB	C2C-C1C-CHB-C4B
26	B9	201	PEB	NB-C1B-CHA-C4A
26	B9	201	PEB	C2B-C1B-CHA-C4A
26	B9	202	PEB	NC-C1C-CHB-C4B
26	B9	202	PEB	C2C-C1C-CHB-C4B
26	B9	202	PEB	C2A-C3A-CAA-CBA
26	B9	202	PEB	C4A-C3A-CAA-CBA
26	B9	202	PEB	NB-C1B-CHA-C4A
26	B9	202	PEB	C2B-C1B-CHA-C4A
26	B9	203	PEB	C2D-C3D-CAD-CBD
26	B9	203	PEB	C4D-C3D-CAD-CBD
26	B9	203	PEB	C4A-C3A-CAA-CBA
26	B9	203	PEB	NB-C1B-CHA-C4A
26	B9	203	PEB	C2B-C1B-CHA-C4A
26	C9	201	PEB	NB-C1B-CHA-C4A
26	C9	201	PEB	C2B-C1B-CHA-C4A
26	C9	202	PEB	NB-C1B-CHA-C4A
26	C9	202	PEB	C2B-C1B-CHA-C4A
26	D9	201	PEB	C2D-C3D-CAD-CBD
26	D9	201	PEB	C4D-C3D-CAD-CBD
26	D9	201	PEB	C4A-C3A-CAA-CBA
26	D9	201	PEB	NB-C1B-CHA-C4A
26	D9	201	PEB	C2B-C1B-CHA-C4A
26	D9	202	PEB	ND-C1D-CHC-C4C
26	D9	202	PEB	C2D-C1D-CHC-C4C
26	D9	202	PEB	NC-C1C-CHB-C4B
26	D9	202	PEB	C2C-C1C-CHB-C4B
26	D9	202	PEB	C3B-CAB-CBB-CGB
26	D9	203	PEB	NC-C1C-CHB-C4B
26	D9	203	PEB	C2C-C1C-CHB-C4B
26	D9	203	PEB	C4A-C3A-CAA-CBA
26	D9	203	PEB	NB-C1B-CHA-C4A
26	D9	203	PEB	C2B-C1B-CHA-C4A
26	E9	201	PEB	ND-C1D-CHC-C4C
26	E9	201	PEB	C1C-C2C-CAC-CBC
26	E9	201	PEB	C3C-C2C-CAC-CBC
26	E9	201	PEB	C2D-C3D-CAD-CBD
26	E9	201	PEB	C4D-C3D-CAD-CBD
26	E9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	E9	201	PEB	C2B-C1B-CHA-C4A
26	E9	202	PEB	NB-C1B-CHA-C4A
26	E9	202	PEB	C2B-C1B-CHA-C4A
26	F9	201	PEB	ND-C1D-CHC-C4C
26	F9	201	PEB	C2D-C1D-CHC-C4C
26	F9	201	PEB	NC-C1C-CHB-C4B
26	F9	201	PEB	C2C-C1C-CHB-C4B
26	F9	201	PEB	C2D-C3D-CAD-CBD
26	F9	201	PEB	C4D-C3D-CAD-CBD
26	F9	201	PEB	NB-C1B-CHA-C4A
26	F9	201	PEB	C2B-C1B-CHA-C4A
26	F9	202	PEB	NC-C1C-CHB-C4B
26	F9	202	PEB	C2C-C1C-CHB-C4B
26	F9	202	PEB	C2A-C3A-CAA-CBA
26	F9	202	PEB	C4A-C3A-CAA-CBA
26	F9	202	PEB	NB-C1B-CHA-C4A
26	F9	202	PEB	C2B-C1B-CHA-C4A
26	F9	203	PEB	C4A-C3A-CAA-CBA
26	F9	203	PEB	NB-C1B-CHA-C4A
26	F9	203	PEB	C2B-C1B-CHA-C4A
26	G9	201	PEB	NB-C1B-CHA-C4A
26	G9	201	PEB	C2B-C1B-CHA-C4A
26	G9	202	PEB	NC-C1C-CHB-C4B
26	G9	202	PEB	C2C-C1C-CHB-C4B
26	G9	202	PEB	C1C-C2C-CAC-CBC
26	G9	202	PEB	C3C-C2C-CAC-CBC
26	G9	202	PEB	C2A-C3A-CAA-CBA
26	G9	202	PEB	C4A-C3A-CAA-CBA
26	G9	202	PEB	NB-C1B-CHA-C4A
26	G9	202	PEB	C2B-C1B-CHA-C4A
26	H9	201	PEB	NC-C1C-CHB-C4B
26	H9	201	PEB	C4A-C3A-CAA-CBA
26	H9	201	PEB	NB-C1B-CHA-C4A
26	H9	201	PEB	C2B-C1B-CHA-C4A
26	H9	202	PEB	ND-C1D-CHC-C4C
26	H9	202	PEB	C2D-C1D-CHC-C4C
26	H9	202	PEB	NC-C1C-CHB-C4B
26	H9	202	PEB	C2C-C1C-CHB-C4B
26	H9	202	PEB	NB-C1B-CHA-C4A
26	H9	203	PEB	ND-C1D-CHC-C4C
26	H9	203	PEB	NC-C1C-CHB-C4B
26	H9	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	H9	203	PEB	C4A-C3A-CAA-CBA
26	H9	203	PEB	NB-C1B-CHA-C4A
26	H9	203	PEB	C2B-C1B-CHA-C4A
26	I9	201	PEB	C1C-C2C-CAC-CBC
26	I9	201	PEB	C3C-C2C-CAC-CBC
26	I9	201	PEB	NB-C1B-CHA-C4A
26	I9	201	PEB	C2B-C1B-CHA-C4A
26	I9	202	PEB	NB-C1B-CHA-C4A
26	I9	202	PEB	C2B-C1B-CHA-C4A
26	J9	201	PEB	ND-C1D-CHC-C4C
26	J9	201	PEB	NC-C1C-CHB-C4B
26	J9	201	PEB	C2C-C1C-CHB-C4B
26	J9	201	PEB	NB-C1B-CHA-C4A
26	J9	201	PEB	C2B-C1B-CHA-C4A
26	J9	202	PEB	NC-C1C-CHB-C4B
26	J9	202	PEB	C2C-C1C-CHB-C4B
26	J9	202	PEB	C4A-C3A-CAA-CBA
26	J9	202	PEB	NB-C1B-CHA-C4A
26	J9	202	PEB	C2B-C1B-CHA-C4A
26	J9	203	PEB	C2D-C3D-CAD-CBD
26	J9	203	PEB	C4D-C3D-CAD-CBD
26	J9	203	PEB	C4A-C3A-CAA-CBA
26	J9	203	PEB	NB-C1B-CHA-C4A
26	J9	203	PEB	C2B-C1B-CHA-C4A
26	K9	201	PEB	ND-C1D-CHC-C4C
26	K9	201	PEB	C2A-C3A-CAA-CBA
26	K9	201	PEB	C4A-C3A-CAA-CBA
26	K9	201	PEB	NB-C1B-CHA-C4A
26	K9	201	PEB	C2B-C1B-CHA-C4A
26	K9	202	PEB	ND-C1D-CHC-C4C
26	K9	202	PEB	NC-C1C-CHB-C4B
26	K9	202	PEB	C2C-C1C-CHB-C4B
26	K9	202	PEB	C2C-CAC-CBC-CGC
26	K9	202	PEB	C2D-C3D-CAD-CBD
26	K9	202	PEB	C4D-C3D-CAD-CBD
26	K9	202	PEB	NB-C1B-CHA-C4A
26	K9	202	PEB	C2B-C1B-CHA-C4A
26	L9	201	PEB	C4A-C3A-CAA-CBA
26	L9	201	PEB	NB-C1B-CHA-C4A
26	L9	201	PEB	C2B-C1B-CHA-C4A
26	L9	202	PEB	ND-C1D-CHC-C4C
26	L9	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	L9	202	PEB	C2B-C1B-CHA-C4A
26	L9	203	PEB	NC-C1C-CHB-C4B
26	L9	203	PEB	C2C-C1C-CHB-C4B
26	L9	203	PEB	C2A-C3A-CAA-CBA
26	L9	203	PEB	C4A-C3A-CAA-CBA
26	L9	203	PEB	NB-C1B-CHA-C4A
26	L9	203	PEB	C2B-C1B-CHA-C4A
26	M9	201	PEB	C1C-C2C-CAC-CBC
26	M9	201	PEB	C3C-C2C-CAC-CBC
26	M9	201	PEB	NB-C1B-CHA-C4A
26	M9	201	PEB	C2B-C1B-CHA-C4A
26	M9	202	PEB	NC-C1C-CHB-C4B
26	M9	202	PEB	C2C-C1C-CHB-C4B
26	M9	202	PEB	NB-C1B-CHA-C4A
26	M9	202	PEB	C2B-C1B-CHA-C4A
26	N9	202	PEB	ND-C1D-CHC-C4C
26	N9	202	PEB	C2D-C1D-CHC-C4C
26	N9	202	PEB	C2A-C3A-CAA-CBA
26	N9	202	PEB	C4A-C3A-CAA-CBA
26	N9	202	PEB	NB-C1B-CHA-C4A
26	N9	202	PEB	C2B-C1B-CHA-C4A
26	N9	203	PEB	ND-C1D-CHC-C4C
26	N9	203	PEB	C2D-C1D-CHC-C4C
26	N9	203	PEB	NC-C1C-CHB-C4B
26	N9	203	PEB	C2C-C1C-CHB-C4B
26	N9	203	PEB	C4A-C3A-CAA-CBA
26	N9	203	PEB	NB-C1B-CHA-C4A
26	N9	203	PEB	C2B-C1B-CHA-C4A
26	N9	204	PEB	NC-C1C-CHB-C4B
26	N9	204	PEB	C2C-C1C-CHB-C4B
26	N9	204	PEB	C4A-C3A-CAA-CBA
26	N9	204	PEB	NB-C1B-CHA-C4A
26	N9	204	PEB	C2B-C1B-CHA-C4A
26	O9	201	PEB	NB-C1B-CHA-C4A
26	O9	201	PEB	C2B-C1B-CHA-C4A
26	O9	202	PEB	NC-C1C-CHB-C4B
26	O9	202	PEB	C2C-C1C-CHB-C4B
26	O9	202	PEB	C2D-C3D-CAD-CBD
26	O9	202	PEB	C4D-C3D-CAD-CBD
26	O9	202	PEB	NB-C1B-CHA-C4A
26	O9	202	PEB	C2B-C1B-CHA-C4A
26	P9	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	P9	201	PEB	C4A-C3A-CAA-CBA
26	P9	201	PEB	NB-C1B-CHA-C4A
26	P9	201	PEB	C2B-C1B-CHA-C4A
26	P9	202	PEB	ND-C1D-CHC-C4C
26	P9	202	PEB	C2D-C1D-CHC-C4C
26	P9	202	PEB	NC-C1C-CHB-C4B
26	P9	202	PEB	C2C-C1C-CHB-C4B
26	P9	202	PEB	NB-C1B-CHA-C4A
26	P9	202	PEB	C2B-C1B-CHA-C4A
26	P9	203	PEB	ND-C1D-CHC-C4C
26	P9	203	PEB	C2D-C1D-CHC-C4C
26	P9	203	PEB	NC-C1C-CHB-C4B
26	P9	203	PEB	C2C-C1C-CHB-C4B
26	P9	203	PEB	C2A-C3A-CAA-CBA
26	P9	203	PEB	C4A-C3A-CAA-CBA
26	P9	203	PEB	NB-C1B-CHA-C4A
26	P9	203	PEB	C2B-C1B-CHA-C4A
26	Q9	201	PEB	NB-C1B-CHA-C4A
26	Q9	201	PEB	C2B-C1B-CHA-C4A
26	Q9	202	PEB	ND-C1D-CHC-C4C
26	Q9	202	PEB	C2C-C1C-CHB-C4B
26	Q9	202	PEB	NB-C1B-CHA-C4A
26	Q9	202	PEB	C2B-C1B-CHA-C4A
26	R9	201	PEB	ND-C1D-CHC-C4C
26	R9	201	PEB	C2D-C1D-CHC-C4C
26	R9	201	PEB	NC-C1C-CHB-C4B
26	R9	201	PEB	NB-C1B-CHA-C4A
26	R9	201	PEB	C2B-C1B-CHA-C4A
26	R9	202	PEB	NC-C1C-CHB-C4B
26	R9	202	PEB	C2C-C1C-CHB-C4B
26	R9	202	PEB	C4A-C3A-CAA-CBA
26	R9	202	PEB	NB-C1B-CHA-C4A
26	R9	202	PEB	C2B-C1B-CHA-C4A
26	R9	203	PEB	C2A-C3A-CAA-CBA
26	R9	203	PEB	C4A-C3A-CAA-CBA
26	R9	203	PEB	NB-C1B-CHA-C4A
26	R9	203	PEB	C2B-C1B-CHA-C4A
26	S9	201	PEB	NC-C1C-CHB-C4B
26	S9	201	PEB	C2C-C1C-CHB-C4B
26	S9	201	PEB	NB-C1B-CHA-C4A
26	S9	201	PEB	C2B-C1B-CHA-C4A
26	S9	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	S9	202	PEB	C2B-C1B-CHA-C4A
26	T9	201	PEB	C2D-C3D-CAD-CBD
26	T9	201	PEB	C4D-C3D-CAD-CBD
26	T9	201	PEB	C4A-C3A-CAA-CBA
26	T9	201	PEB	NB-C1B-CHA-C4A
26	T9	201	PEB	C2B-C1B-CHA-C4A
26	T9	202	PEB	ND-C1D-CHC-C4C
26	T9	202	PEB	C2D-C1D-CHC-C4C
26	T9	202	PEB	C2A-C3A-CAA-CBA
26	T9	202	PEB	C4A-C3A-CAA-CBA
26	T9	202	PEB	NB-C1B-CHA-C4A
26	T9	202	PEB	C2B-C1B-CHA-C4A
26	T9	202	PEB	C3B-CAB-CBB-CGB
26	T9	203	PEB	ND-C1D-CHC-C4C
26	T9	203	PEB	C2D-C1D-CHC-C4C
26	T9	203	PEB	NC-C1C-CHB-C4B
26	T9	203	PEB	C2C-C1C-CHB-C4B
26	T9	203	PEB	C2A-C3A-CAA-CBA
26	T9	203	PEB	C4A-C3A-CAA-CBA
26	T9	203	PEB	NB-C1B-CHA-C4A
26	T9	203	PEB	C2B-C1B-CHA-C4A
26	U9	201	PEB	ND-C1D-CHC-C4C
26	U9	201	PEB	C2D-C1D-CHC-C4C
26	U9	201	PEB	NB-C1B-CHA-C4A
26	U9	201	PEB	C2B-C1B-CHA-C4A
26	U9	202	PEB	C2C-C1C-CHB-C4B
26	U9	202	PEB	NB-C1B-CHA-C4A
26	U9	202	PEB	C2B-C1B-CHA-C4A
26	V9	201	PEB	ND-C1D-CHC-C4C
26	V9	201	PEB	C2D-C1D-CHC-C4C
26	V9	201	PEB	NC-C1C-CHB-C4B
26	V9	201	PEB	C2C-C1C-CHB-C4B
26	V9	201	PEB	C2D-C3D-CAD-CBD
26	V9	201	PEB	C4D-C3D-CAD-CBD
26	V9	201	PEB	NB-C1B-CHA-C4A
26	V9	201	PEB	C2B-C1B-CHA-C4A
26	V9	202	PEB	ND-C1D-CHC-C4C
26	V9	202	PEB	C2D-C1D-CHC-C4C
26	V9	202	PEB	NC-C1C-CHB-C4B
26	V9	202	PEB	C2C-C1C-CHB-C4B
26	V9	202	PEB	C4A-C3A-CAA-CBA
26	V9	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	V9	202	PEB	C2B-C1B-CHA-C4A
26	V9	203	PEB	NC-C1C-CHB-C4B
26	V9	203	PEB	C2C-C1C-CHB-C4B
26	V9	203	PEB	C2C-CAC-CBC-CGC
26	V9	203	PEB	C4D-C3D-CAD-CBD
26	V9	203	PEB	C4A-C3A-CAA-CBA
26	V9	203	PEB	NB-C1B-CHA-C4A
26	V9	203	PEB	C2B-C1B-CHA-C4A
26	W9	201	PEB	NB-C1B-CHA-C4A
26	W9	201	PEB	C2B-C1B-CHA-C4A
26	W9	202	PEB	NC-C1C-CHB-C4B
26	W9	202	PEB	C2C-C1C-CHB-C4B
26	W9	202	PEB	NB-C1B-CHA-C4A
26	W9	202	PEB	C2B-C1B-CHA-C4A
26	X9	201	PEB	C2C-CAC-CBC-CGC
26	X9	201	PEB	C4A-C3A-CAA-CBA
26	X9	201	PEB	NB-C1B-CHA-C4A
26	X9	201	PEB	C2B-C1B-CHA-C4A
26	X9	202	PEB	ND-C1D-CHC-C4C
26	X9	202	PEB	NB-C1B-CHA-C4A
26	X9	202	PEB	C2B-C1B-CHA-C4A
26	X9	203	PEB	NC-C1C-CHB-C4B
26	X9	203	PEB	C2C-C1C-CHB-C4B
26	X9	203	PEB	C4A-C3A-CAA-CBA
26	X9	203	PEB	NB-C1B-CHA-C4A
26	X9	203	PEB	C2B-C1B-CHA-C4A
26	Y9	201	PEB	NB-C1B-CHA-C4A
26	Y9	201	PEB	C2B-C1B-CHA-C4A
26	Y9	202	PEB	C2C-CAC-CBC-CGC
26	Y9	202	PEB	NB-C1B-CHA-C4A
26	Y9	202	PEB	C2B-C1B-CHA-C4A
26	AA	301	PEB	ND-C1D-CHC-C4C
26	AA	301	PEB	C2D-C1D-CHC-C4C
26	AA	301	PEB	NC-C1C-CHB-C4B
26	AA	301	PEB	C2C-C1C-CHB-C4B
26	AA	301	PEB	C2A-C3A-CAA-CBA
26	AA	301	PEB	C4A-C3A-CAA-CBA
26	AA	301	PEB	NB-C1B-CHA-C4A
26	AA	301	PEB	C2B-C1B-CHA-C4A
26	AA	302	PEB	ND-C1D-CHC-C4C
26	AA	302	PEB	NC-C1C-CHB-C4B
26	AA	302	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	AA	302	PEB	NB-C1B-CHA-C4A
26	AA	302	PEB	C2B-C1B-CHA-C4A
26	BA	301	PEB	NC-C1C-CHB-C4B
26	BA	301	PEB	C2C-C1C-CHB-C4B
26	BA	301	PEB	C2A-C3A-CAA-CBA
26	BA	301	PEB	C4A-C3A-CAA-CBA
26	BA	301	PEB	NB-C1B-CHA-C4A
26	BA	301	PEB	C2B-C1B-CHA-C4A
26	CA	201	PEB	NB-C1B-CHA-C4A
26	CA	201	PEB	C2B-C1B-CHA-C4A
26	CA	202	PEB	NC-C1C-CHB-C4B
26	CA	202	PEB	C2C-C1C-CHB-C4B
26	CA	202	PEB	C2C-CAC-CBC-CGC
26	CA	202	PEB	NB-C1B-CHA-C4A
26	CA	202	PEB	C2B-C1B-CHA-C4A
26	CA	203	PEB	NB-C1B-CHA-C4A
26	CA	203	PEB	C2B-C1B-CHA-C4A
26	DA	201	PEB	ND-C1D-CHC-C4C
26	DA	201	PEB	C2D-C1D-CHC-C4C
26	DA	201	PEB	NC-C1C-CHB-C4B
26	DA	201	PEB	C2C-C1C-CHB-C4B
26	DA	201	PEB	NB-C1B-CHA-C4A
26	DA	201	PEB	C2B-C1B-CHA-C4A
26	DA	202	PEB	NC-C1C-CHB-C4B
26	DA	202	PEB	C2C-C1C-CHB-C4B
26	DA	202	PEB	NB-C1B-CHA-C4A
26	DA	202	PEB	C2B-C1B-CHA-C4A
26	EA	201	PEB	C2A-C3A-CAA-CBA
26	EA	201	PEB	NB-C1B-CHA-C4A
26	EA	201	PEB	C2B-C1B-CHA-C4A
26	EA	202	PEB	ND-C1D-CHC-C4C
26	EA	202	PEB	C2A-C3A-CAA-CBA
26	EA	202	PEB	C4A-C3A-CAA-CBA
26	EA	202	PEB	NB-C1B-CHA-C4A
26	EA	203	PEB	C2A-C3A-CAA-CBA
26	EA	203	PEB	C4A-C3A-CAA-CBA
26	EA	203	PEB	NB-C1B-CHA-C4A
26	EA	203	PEB	C2B-C1B-CHA-C4A
26	FA	201	PEB	ND-C1D-CHC-C4C
26	FA	201	PEB	C2D-C1D-CHC-C4C
26	FA	201	PEB	C2C-C1C-CHB-C4B
26	FA	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	FA	201	PEB	C2B-C1B-CHA-C4A
26	FA	202	PEB	NC-C1C-CHB-C4B
26	FA	202	PEB	C2C-C1C-CHB-C4B
26	FA	202	PEB	NB-C1B-CHA-C4A
26	FA	202	PEB	C2B-C1B-CHA-C4A
26	GA	201	PEB	C2A-C3A-CAA-CBA
26	GA	201	PEB	C4A-C3A-CAA-CBA
26	GA	202	PEB	C2C-CAC-CBC-CGC
26	GA	202	PEB	NB-C1B-CHA-C4A
26	GA	202	PEB	C2B-C1B-CHA-C4A
26	GA	203	PEB	C4A-C3A-CAA-CBA
26	GA	203	PEB	NB-C1B-CHA-C4A
26	GA	203	PEB	C2B-C1B-CHA-C4A
26	HA	201	PEB	ND-C1D-CHC-C4C
26	HA	201	PEB	NB-C1B-CHA-C4A
26	HA	201	PEB	C2B-C1B-CHA-C4A
26	HA	202	PEB	NC-C1C-CHB-C4B
26	HA	202	PEB	C2C-C1C-CHB-C4B
26	HA	202	PEB	C2C-CAC-CBC-CGC
26	HA	202	PEB	NB-C1B-CHA-C4A
26	HA	202	PEB	C2B-C1B-CHA-C4A
26	IA	201	PEB	C4A-C3A-CAA-CBA
26	IA	201	PEB	NB-C1B-CHA-C4A
26	IA	201	PEB	C2B-C1B-CHA-C4A
26	IA	202	PEB	NB-C1B-CHA-C4A
26	IA	202	PEB	C2B-C1B-CHA-C4A
26	IA	203	PEB	NC-C1C-CHB-C4B
26	IA	203	PEB	C2C-C1C-CHB-C4B
26	IA	203	PEB	C4A-C3A-CAA-CBA
26	IA	203	PEB	NB-C1B-CHA-C4A
26	IA	203	PEB	C2B-C1B-CHA-C4A
26	JA	201	PEB	ND-C1D-CHC-C4C
26	JA	201	PEB	C2D-C1D-CHC-C4C
26	JA	201	PEB	NC-C1C-CHB-C4B
26	JA	201	PEB	C2C-C1C-CHB-C4B
26	JA	201	PEB	C2A-C3A-CAA-CBA
26	JA	201	PEB	C4A-C3A-CAA-CBA
26	JA	201	PEB	NB-C1B-CHA-C4A
26	JA	201	PEB	C2B-C1B-CHA-C4A
26	JA	202	PEB	NC-C1C-CHB-C4B
26	JA	202	PEB	C2C-C1C-CHB-C4B
26	JA	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	JA	202	PEB	NB-C1B-CHA-C4A
26	JA	202	PEB	C2B-C1B-CHA-C4A
26	KA	201	PEB	C2A-C3A-CAA-CBA
26	KA	201	PEB	C4A-C3A-CAA-CBA
26	KA	202	PEB	NB-C1B-CHA-C4A
26	KA	202	PEB	C2B-C1B-CHA-C4A
26	KA	203	PEB	C4A-C3A-CAA-CBA
26	KA	203	PEB	NB-C1B-CHA-C4A
26	KA	203	PEB	C2B-C1B-CHA-C4A
26	LA	201	PEB	ND-C1D-CHC-C4C
26	LA	201	PEB	NB-C1B-CHA-C4A
26	LA	201	PEB	C2B-C1B-CHA-C4A
26	LA	202	PEB	NC-C1C-CHB-C4B
26	LA	202	PEB	C2C-C1C-CHB-C4B
26	LA	202	PEB	C1C-C2C-CAC-CBC
26	LA	202	PEB	C3C-C2C-CAC-CBC
26	LA	202	PEB	NB-C1B-CHA-C4A
26	LA	202	PEB	C2B-C1B-CHA-C4A
26	MA	201	PEB	C4A-C3A-CAA-CBA
26	MA	201	PEB	NB-C1B-CHA-C4A
26	MA	201	PEB	C2B-C1B-CHA-C4A
26	MA	202	PEB	NB-C1B-CHA-C4A
26	MA	202	PEB	C2B-C1B-CHA-C4A
26	MA	203	PEB	C4A-C3A-CAA-CBA
26	MA	203	PEB	NB-C1B-CHA-C4A
26	MA	203	PEB	C2B-C1B-CHA-C4A
26	NA	201	PEB	ND-C1D-CHC-C4C
26	NA	201	PEB	NB-C1B-CHA-C4A
26	NA	201	PEB	C2B-C1B-CHA-C4A
26	NA	202	PEB	NC-C1C-CHB-C4B
26	NA	202	PEB	C2C-C1C-CHB-C4B
26	NA	202	PEB	NB-C1B-CHA-C4A
26	NA	202	PEB	C2B-C1B-CHA-C4A
26	OA	201	PEB	C4A-C3A-CAA-CBA
26	OA	201	PEB	NB-C1B-CHA-C4A
26	OA	201	PEB	C2B-C1B-CHA-C4A
26	OA	202	PEB	NB-C1B-CHA-C4A
26	OA	202	PEB	C2B-C1B-CHA-C4A
26	OA	203	PEB	C2A-C3A-CAA-CBA
26	OA	203	PEB	C4A-C3A-CAA-CBA
26	OA	203	PEB	NB-C1B-CHA-C4A
26	OA	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	PA	201	PEB	ND-C1D-CHC-C4C
26	PA	201	PEB	C2D-C1D-CHC-C4C
26	PA	201	PEB	NB-C1B-CHA-C4A
26	PA	201	PEB	C2B-C1B-CHA-C4A
26	PA	202	PEB	NC-C1C-CHB-C4B
26	PA	202	PEB	C2C-C1C-CHB-C4B
26	PA	202	PEB	NB-C1B-CHA-C4A
26	PA	202	PEB	C2B-C1B-CHA-C4A
26	QA	202	PEB	C2A-C3A-CAA-CBA
26	QA	202	PEB	NB-C1B-CHA-C4A
26	QA	202	PEB	C2B-C1B-CHA-C4A
26	QA	203	PEB	NB-C1B-CHA-C4A
26	QA	203	PEB	C2B-C1B-CHA-C4A
26	QA	204	PEB	NC-C1C-CHB-C4B
26	QA	204	PEB	C2C-C1C-CHB-C4B
26	QA	204	PEB	NB-C1B-CHA-C4A
26	QA	204	PEB	C2B-C1B-CHA-C4A
26	RA	201	PEB	ND-C1D-CHC-C4C
26	RA	201	PEB	C2D-C1D-CHC-C4C
26	RA	201	PEB	NB-C1B-CHA-C4A
26	RA	201	PEB	C2B-C1B-CHA-C4A
26	RA	202	PEB	ND-C1D-CHC-C4C
26	RA	202	PEB	C2D-C1D-CHC-C4C
26	RA	202	PEB	NC-C1C-CHB-C4B
26	RA	202	PEB	C2C-C1C-CHB-C4B
26	RA	202	PEB	NB-C1B-CHA-C4A
26	RA	202	PEB	C2B-C1B-CHA-C4A
26	SA	201	PEB	C2A-C3A-CAA-CBA
26	SA	201	PEB	C4A-C3A-CAA-CBA
26	SA	201	PEB	NB-C1B-CHA-C4A
26	SA	201	PEB	C2B-C1B-CHA-C4A
26	SA	202	PEB	C2A-C3A-CAA-CBA
26	SA	202	PEB	C4A-C3A-CAA-CBA
26	SA	202	PEB	NB-C1B-CHA-C4A
26	SA	202	PEB	C2B-C1B-CHA-C4A
26	SA	203	PEB	C2A-C3A-CAA-CBA
26	SA	203	PEB	C4A-C3A-CAA-CBA
26	SA	203	PEB	NB-C1B-CHA-C4A
26	SA	203	PEB	C2B-C1B-CHA-C4A
26	TA	201	PEB	ND-C1D-CHC-C4C
26	TA	201	PEB	C2D-C1D-CHC-C4C
26	TA	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	TA	201	PEB	C2B-C1B-CHA-C4A
26	TA	202	PEB	NC-C1C-CHB-C4B
26	TA	202	PEB	C2C-CAC-CBC-CGC
26	TA	202	PEB	NB-C1B-CHA-C4A
26	TA	202	PEB	C2B-C1B-CHA-C4A
26	UA	201	PEB	C2A-C3A-CAA-CBA
26	UA	201	PEB	C4A-C3A-CAA-CBA
26	UA	201	PEB	NB-C1B-CHA-C4A
26	UA	201	PEB	C2B-C1B-CHA-C4A
26	UA	203	PEB	C2C-CAC-CBC-CGC
26	UA	203	PEB	NB-C1B-CHA-C4A
26	UA	203	PEB	C2B-C1B-CHA-C4A
26	VA	201	PEB	ND-C1D-CHC-C4C
26	VA	201	PEB	C2D-C1D-CHC-C4C
26	VA	201	PEB	NC-C1C-CHB-C4B
26	VA	201	PEB	C2C-C1C-CHB-C4B
26	VA	201	PEB	NB-C1B-CHA-C4A
26	VA	201	PEB	C2B-C1B-CHA-C4A
26	VA	202	PEB	NC-C1C-CHB-C4B
26	VA	202	PEB	C2C-C1C-CHB-C4B
26	VA	202	PEB	C2C-CAC-CBC-CGC
26	VA	202	PEB	NB-C1B-CHA-C4A
26	VA	202	PEB	C2B-C1B-CHA-C4A
26	VA	202	PEB	C4B-C3B-CAB-CBB
26	WA	201	PEB	NB-C1B-CHA-C4A
26	WA	202	PEB	NC-C1C-CHB-C4B
26	WA	202	PEB	C2C-C1C-CHB-C4B
26	WA	202	PEB	NB-C1B-CHA-C4A
26	WA	202	PEB	C2B-C1B-CHA-C4A
26	WA	203	PEB	C4A-C3A-CAA-CBA
26	WA	203	PEB	NB-C1B-CHA-C4A
26	WA	203	PEB	C2B-C1B-CHA-C4A
26	XA	201	PEB	ND-C1D-CHC-C4C
26	XA	201	PEB	C2D-C1D-CHC-C4C
26	XA	201	PEB	C2A-C3A-CAA-CBA
26	XA	201	PEB	C4A-C3A-CAA-CBA
26	XA	201	PEB	NB-C1B-CHA-C4A
26	XA	201	PEB	C2B-C1B-CHA-C4A
26	XA	202	PEB	ND-C1D-CHC-C4C
26	XA	202	PEB	NC-C1C-CHB-C4B
26	XA	202	PEB	C2C-C1C-CHB-C4B
26	XA	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	XA	202	PEB	C2B-C1B-CHA-C4A
26	YA	201	PEB	C4A-C3A-CAA-CBA
26	YA	201	PEB	NB-C1B-CHA-C4A
26	YA	201	PEB	C2B-C1B-CHA-C4A
26	YA	202	PEB	NB-C1B-CHA-C4A
26	YA	203	PEB	C2A-C3A-CAA-CBA
26	YA	203	PEB	C4A-C3A-CAA-CBA
26	YA	203	PEB	NB-C1B-CHA-C4A
26	YA	203	PEB	C2B-C1B-CHA-C4A
26	ZA	201	PEB	ND-C1D-CHC-C4C
26	ZA	201	PEB	C2D-C1D-CHC-C4C
26	ZA	201	PEB	NB-C1B-CHA-C4A
26	ZA	201	PEB	C2B-C1B-CHA-C4A
26	ZA	202	PEB	C2C-CAC-CBC-CGC
26	ZA	202	PEB	NB-C1B-CHA-C4A
26	ZA	202	PEB	C2B-C1B-CHA-C4A
26	aA	201	PEB	NC-C1C-CHB-C4B
26	aA	201	PEB	C2C-C1C-CHB-C4B
26	aA	201	PEB	NB-C1B-CHA-C4A
26	aA	201	PEB	C2B-C1B-CHA-C4A
26	aA	202	PEB	NB-C1B-CHA-C4A
26	aA	202	PEB	C2B-C1B-CHA-C4A
26	aA	203	PEB	NC-C1C-CHB-C4B
26	aA	203	PEB	C2C-C1C-CHB-C4B
26	aA	203	PEB	C1C-C2C-CAC-CBC
26	aA	203	PEB	C3C-C2C-CAC-CBC
26	aA	203	PEB	NB-C1B-CHA-C4A
26	aA	203	PEB	C2B-C1B-CHA-C4A
26	aA	204	PEB	C2A-C3A-CAA-CBA
26	aA	204	PEB	C4A-C3A-CAA-CBA
26	aA	204	PEB	NB-C1B-CHA-C4A
26	aA	204	PEB	C2B-C1B-CHA-C4A
26	cA	201	PEB	ND-C1D-CHC-C4C
26	cA	201	PEB	C2D-C1D-CHC-C4C
26	cA	201	PEB	NC-C1C-CHB-C4B
26	cA	201	PEB	C2C-C1C-CHB-C4B
26	cA	201	PEB	NB-C1B-CHA-C4A
26	cA	201	PEB	C2B-C1B-CHA-C4A
26	cA	202	PEB	C2A-C3A-CAA-CBA
26	cA	202	PEB	C4A-C3A-CAA-CBA
26	cA	202	PEB	NB-C1B-CHA-C4A
26	cA	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	cA	203	PEB	NC-C1C-CHB-C4B
26	cA	203	PEB	C2C-C1C-CHB-C4B
26	cA	203	PEB	C2C-CAC-CBC-CGC
26	cA	203	PEB	NB-C1B-CHA-C4A
26	cA	203	PEB	C2B-C1B-CHA-C4A
26	dA	201	PEB	NB-C1B-CHA-C4A
26	dA	201	PEB	C2B-C1B-CHA-C4A
26	eA	201	PEB	ND-C1D-CHC-C4C
26	eA	201	PEB	C2D-C1D-CHC-C4C
26	eA	201	PEB	NB-C1B-CHA-C4A
26	eA	201	PEB	C2B-C1B-CHA-C4A
26	eA	202	PEB	NC-C1C-CHB-C4B
26	eA	202	PEB	C2C-C1C-CHB-C4B
26	eA	202	PEB	C2C-CAC-CBC-CGC
26	eA	202	PEB	NB-C1B-CHA-C4A
26	eA	202	PEB	C2B-C1B-CHA-C4A
26	fA	201	PEB	ND-C1D-CHC-C4C
26	fA	201	PEB	NC-C1C-CHB-C4B
26	fA	201	PEB	C2C-C1C-CHB-C4B
26	fA	201	PEB	NB-C1B-CHA-C4A
26	fA	201	PEB	C2B-C1B-CHA-C4A
26	fA	202	PEB	NC-C1C-CHB-C4B
26	fA	202	PEB	C2C-C1C-CHB-C4B
26	fA	202	PEB	C4A-C3A-CAA-CBA
26	fA	202	PEB	NB-C1B-CHA-C4A
26	fA	202	PEB	C2B-C1B-CHA-C4A
26	fA	203	PEB	NB-C1B-CHA-C4A
26	fA	203	PEB	C2B-C1B-CHA-C4A
26	gA	201	PEB	ND-C1D-CHC-C4C
26	gA	201	PEB	C2D-C1D-CHC-C4C
26	gA	201	PEB	NC-C1C-CHB-C4B
26	gA	201	PEB	C2C-C1C-CHB-C4B
26	gA	201	PEB	C2C-CAC-CBC-CGC
26	gA	201	PEB	C2A-C3A-CAA-CBA
26	gA	201	PEB	C4A-C3A-CAA-CBA
26	gA	201	PEB	NB-C1B-CHA-C4A
26	gA	201	PEB	C2B-C1B-CHA-C4A
26	gA	202	PEB	NC-C1C-CHB-C4B
26	gA	202	PEB	C2C-C1C-CHB-C4B
26	gA	202	PEB	C2C-CAC-CBC-CGC
26	gA	202	PEB	NB-C1B-CHA-C4A
26	gA	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hA	201	PEB	ND-C1D-CHC-C4C
26	hA	201	PEB	C2D-C1D-CHC-C4C
26	hA	201	PEB	C2A-C3A-CAA-CBA
26	hA	201	PEB	C4A-C3A-CAA-CBA
26	hA	201	PEB	NB-C1B-CHA-C4A
26	hA	201	PEB	C2B-C1B-CHA-C4A
26	hA	202	PEB	NB-C1B-CHA-C4A
26	hA	202	PEB	C2B-C1B-CHA-C4A
26	hA	203	PEB	C2C-CAC-CBC-CGC
26	hA	203	PEB	NB-C1B-CHA-C4A
26	hA	203	PEB	C2B-C1B-CHA-C4A
26	iA	201	PEB	ND-C1D-CHC-C4C
26	iA	201	PEB	C2D-C1D-CHC-C4C
26	iA	201	PEB	C2C-C1C-CHB-C4B
26	iA	201	PEB	C4A-C3A-CAA-CBA
26	iA	201	PEB	NB-C1B-CHA-C4A
26	iA	201	PEB	C2B-C1B-CHA-C4A
26	iA	202	PEB	NC-C1C-CHB-C4B
26	iA	202	PEB	C2C-C1C-CHB-C4B
26	iA	202	PEB	NB-C1B-CHA-C4A
26	iA	202	PEB	C2B-C1B-CHA-C4A
26	jA	201	PEB	ND-C1D-CHC-C4C
26	jA	201	PEB	NB-C1B-CHA-C4A
26	jA	201	PEB	C2B-C1B-CHA-C4A
26	jA	202	PEB	NB-C1B-CHA-C4A
26	jA	202	PEB	C2B-C1B-CHA-C4A
26	jA	203	PEB	C2A-C3A-CAA-CBA
26	jA	203	PEB	C4A-C3A-CAA-CBA
26	jA	203	PEB	NB-C1B-CHA-C4A
26	jA	203	PEB	C2B-C1B-CHA-C4A
26	kA	201	PEB	ND-C1D-CHC-C4C
26	kA	201	PEB	C2D-C1D-CHC-C4C
26	kA	201	PEB	NC-C1C-CHB-C4B
26	kA	201	PEB	C2C-C1C-CHB-C4B
26	kA	201	PEB	NB-C1B-CHA-C4A
26	kA	201	PEB	C2B-C1B-CHA-C4A
26	kA	202	PEB	ND-C1D-CHC-C4C
26	kA	202	PEB	C2D-C1D-CHC-C4C
26	kA	202	PEB	NC-C1C-CHB-C4B
26	kA	202	PEB	C2C-C1C-CHB-C4B
26	kA	202	PEB	NB-C1B-CHA-C4A
26	kA	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	kA	202	PEB	C3B-CAB-CBB-CGB
26	lA	201	PEB	NC-C1C-CHB-C4B
26	lA	201	PEB	C2C-C1C-CHB-C4B
26	lA	201	PEB	NB-C1B-CHA-C4A
26	lA	201	PEB	C2B-C1B-CHA-C4A
26	lA	202	PEB	NB-C1B-CHA-C4A
26	lA	202	PEB	C2B-C1B-CHA-C4A
26	lA	203	PEB	NC-C1C-CHB-C4B
26	lA	203	PEB	C2C-C1C-CHB-C4B
26	lA	203	PEB	C2A-C3A-CAA-CBA
26	lA	203	PEB	C4A-C3A-CAA-CBA
26	lA	203	PEB	NB-C1B-CHA-C4A
26	lA	203	PEB	C2B-C1B-CHA-C4A
26	mA	201	PEB	ND-C1D-CHC-C4C
26	mA	201	PEB	C2D-C1D-CHC-C4C
26	mA	201	PEB	NC-C1C-CHB-C4B
26	mA	201	PEB	C2C-C1C-CHB-C4B
26	mA	201	PEB	NB-C1B-CHA-C4A
26	mA	201	PEB	C2B-C1B-CHA-C4A
26	mA	202	PEB	NC-C1C-CHB-C4B
26	mA	202	PEB	C2C-C1C-CHB-C4B
26	mA	202	PEB	NB-C1B-CHA-C4A
26	mA	202	PEB	C2B-C1B-CHA-C4A
26	mA	202	PEB	C2B-C3B-CAB-CBB
26	mA	202	PEB	C4B-C3B-CAB-CBB
26	AB	301	PEB	NC-C1C-CHB-C4B
26	AB	301	PEB	C2C-C1C-CHB-C4B
26	AB	301	PEB	NB-C1B-CHA-C4A
26	AB	301	PEB	C2B-C1B-CHA-C4A
26	AB	304	PEB	NB-C1B-CHA-C4A
26	AB	304	PEB	C2B-C1B-CHA-C4A
26	DB	1002	PEB	NB-C1B-CHA-C4A
26	DB	1002	PEB	C2B-C1B-CHA-C4A
26	GB	1002	PEB	C2D-C3D-CAD-CBD
26	GB	1002	PEB	C4D-C3D-CAD-CBD
26	GB	1002	PEB	NB-C1B-CHA-C4A
26	GB	1002	PEB	C2B-C1B-CHA-C4A
26	GB	1002	PEB	C2B-C3B-CAB-CBB
26	HB	1002	PEB	NB-C1B-CHA-C4A
26	HB	1002	PEB	C2B-C1B-CHA-C4A
26	KB	201	PEB	NB-C1B-CHA-C4A
26	KB	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	LB	1002	PEB	ND-C1D-CHC-C4C
26	LB	1002	PEB	C2D-C1D-CHC-C4C
26	LB	1002	PEB	C2A-C3A-CAA-CBA
26	LB	1002	PEB	C4A-C3A-CAA-CBA
26	LB	1002	PEB	NB-C1B-CHA-C4A
26	LB	1002	PEB	C2B-C1B-CHA-C4A
26	NB	1002	PEB	ND-C1D-CHC-C4C
26	NB	1002	PEB	C2D-C1D-CHC-C4C
26	NB	1002	PEB	NC-C1C-CHB-C4B
26	NB	1002	PEB	C2C-C1C-CHB-C4B
26	NB	1002	PEB	NB-C1B-CHA-C4A
26	NB	1002	PEB	C2B-C1B-CHA-C4A
26	OB	201	PEB	C4A-C3A-CAA-CBA
26	OB	201	PEB	NB-C1B-CHA-C4A
26	OB	201	PEB	C2B-C1B-CHA-C4A
26	OB	202	PEB	C2A-C3A-CAA-CBA
26	OB	202	PEB	C4A-C3A-CAA-CBA
26	OB	202	PEB	NB-C1B-CHA-C4A
26	OB	202	PEB	C2B-C1B-CHA-C4A
26	OB	203	PEB	C4A-C3A-CAA-CBA
26	OB	203	PEB	NB-C1B-CHA-C4A
26	OB	203	PEB	C2B-C1B-CHA-C4A
26	PB	201	PEB	NB-C1B-CHA-C4A
26	PB	201	PEB	C2B-C1B-CHA-C4A
26	PB	202	PEB	NC-C1C-CHB-C4B
26	PB	202	PEB	C2C-C1C-CHB-C4B
26	PB	202	PEB	C1C-C2C-CAC-CBC
26	PB	202	PEB	C3C-C2C-CAC-CBC
26	PB	202	PEB	C2C-CAC-CBC-CGC
26	PB	202	PEB	NB-C1B-CHA-C4A
26	PB	202	PEB	C2B-C1B-CHA-C4A
26	QB	201	PEB	C2A-C3A-CAA-CBA
26	QB	201	PEB	C4A-C3A-CAA-CBA
26	QB	201	PEB	NB-C1B-CHA-C4A
26	QB	201	PEB	C2B-C1B-CHA-C4A
26	QB	202	PEB	ND-C1D-CHC-C4C
26	QB	202	PEB	C2D-C1D-CHC-C4C
26	QB	202	PEB	NB-C1B-CHA-C4A
26	QB	202	PEB	C2B-C1B-CHA-C4A
26	QB	203	PEB	C2C-CAC-CBC-CGC
26	QB	203	PEB	C4A-C3A-CAA-CBA
26	QB	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	QB	203	PEB	C2B-C1B-CHA-C4A
26	RB	201	PEB	C2A-C3A-CAA-CBA
26	RB	201	PEB	C4A-C3A-CAA-CBA
26	RB	201	PEB	NB-C1B-CHA-C4A
26	RB	201	PEB	C2B-C1B-CHA-C4A
26	RB	202	PEB	NC-C1C-CHB-C4B
26	RB	202	PEB	C2C-C1C-CHB-C4B
26	RB	202	PEB	C2A-C3A-CAA-CBA
26	RB	202	PEB	C4A-C3A-CAA-CBA
26	RB	202	PEB	NB-C1B-CHA-C4A
26	RB	202	PEB	C2B-C1B-CHA-C4A
26	SB	201	PEB	C4A-C3A-CAA-CBA
26	SB	201	PEB	NB-C1B-CHA-C4A
26	SB	201	PEB	C2B-C1B-CHA-C4A
26	SB	202	PEB	C2A-C3A-CAA-CBA
26	SB	202	PEB	C4A-C3A-CAA-CBA
26	SB	202	PEB	NB-C1B-CHA-C4A
26	SB	202	PEB	C2B-C1B-CHA-C4A
26	SB	203	PEB	C2A-C3A-CAA-CBA
26	SB	203	PEB	C4A-C3A-CAA-CBA
26	SB	203	PEB	NB-C1B-CHA-C4A
26	SB	203	PEB	C2B-C1B-CHA-C4A
26	TB	201	PEB	NB-C1B-CHA-C4A
26	TB	201	PEB	C2B-C1B-CHA-C4A
26	TB	202	PEB	NC-C1C-CHB-C4B
26	TB	202	PEB	C2C-C1C-CHB-C4B
26	TB	202	PEB	C1C-C2C-CAC-CBC
26	TB	202	PEB	C3C-C2C-CAC-CBC
26	TB	202	PEB	NB-C1B-CHA-C4A
26	TB	202	PEB	C2B-C1B-CHA-C4A
26	UB	201	PEB	C2A-C3A-CAA-CBA
26	UB	201	PEB	C4A-C3A-CAA-CBA
26	UB	201	PEB	NB-C1B-CHA-C4A
26	UB	201	PEB	C2B-C1B-CHA-C4A
26	UB	202	PEB	C2A-C3A-CAA-CBA
26	UB	202	PEB	C4A-C3A-CAA-CBA
26	UB	202	PEB	NB-C1B-CHA-C4A
26	UB	202	PEB	C2B-C1B-CHA-C4A
26	UB	203	PEB	C2C-C1C-CHB-C4B
26	UB	203	PEB	C4A-C3A-CAA-CBA
26	UB	203	PEB	NB-C1B-CHA-C4A
26	UB	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	VB	201	PEB	NB-C1B-CHA-C4A
26	VB	201	PEB	C2B-C1B-CHA-C4A
26	VB	202	PEB	ND-C1D-CHC-C4C
26	VB	202	PEB	C2D-C1D-CHC-C4C
26	VB	202	PEB	NC-C1C-CHB-C4B
26	VB	202	PEB	C2C-C1C-CHB-C4B
26	VB	202	PEB	NB-C1B-CHA-C4A
26	VB	202	PEB	C2B-C1B-CHA-C4A
26	WB	201	PEB	NB-C1B-CHA-C4A
26	WB	201	PEB	C2B-C1B-CHA-C4A
26	WB	202	PEB	NB-C1B-CHA-C4A
26	WB	202	PEB	C2B-C1B-CHA-C4A
26	WB	203	PEB	C2A-C3A-CAA-CBA
26	WB	203	PEB	C4A-C3A-CAA-CBA
26	WB	203	PEB	NB-C1B-CHA-C4A
26	WB	203	PEB	C2B-C1B-CHA-C4A
26	YB	201	PEB	C1C-C2C-CAC-CBC
26	YB	201	PEB	C3C-C2C-CAC-CBC
26	YB	201	PEB	C2A-C3A-CAA-CBA
26	YB	201	PEB	C4A-C3A-CAA-CBA
26	YB	201	PEB	NB-C1B-CHA-C4A
26	YB	201	PEB	C2B-C1B-CHA-C4A
26	YB	202	PEB	NC-C1C-CHB-C4B
26	YB	202	PEB	C2C-C1C-CHB-C4B
26	YB	202	PEB	C1C-C2C-CAC-CBC
26	YB	202	PEB	C3C-C2C-CAC-CBC
26	YB	202	PEB	C2C-CAC-CBC-CGC
26	YB	202	PEB	NB-C1B-CHA-C4A
26	YB	202	PEB	C2B-C1B-CHA-C4A
26	ZB	201	PEB	C2C-CAC-CBC-CGC
26	ZB	201	PEB	C2A-C3A-CAA-CBA
26	ZB	201	PEB	C4A-C3A-CAA-CBA
26	ZB	201	PEB	NB-C1B-CHA-C4A
26	ZB	201	PEB	C2B-C1B-CHA-C4A
26	ZB	202	PEB	C2A-C3A-CAA-CBA
26	ZB	202	PEB	C4A-C3A-CAA-CBA
26	ZB	202	PEB	NB-C1B-CHA-C4A
26	ZB	202	PEB	C2B-C1B-CHA-C4A
26	ZB	203	PEB	NC-C1C-CHB-C4B
26	ZB	203	PEB	C2C-C1C-CHB-C4B
26	ZB	203	PEB	NB-C1B-CHA-C4A
26	ZB	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	aB	201	PEB	C1C-C2C-CAC-CBC
26	aB	201	PEB	C3C-C2C-CAC-CBC
26	aB	201	PEB	NB-C1B-CHA-C4A
26	aB	201	PEB	C2B-C1B-CHA-C4A
26	aB	202	PEB	NC-C1C-CHB-C4B
26	aB	202	PEB	C2C-C1C-CHB-C4B
26	aB	202	PEB	NB-C1B-CHA-C4A
26	aB	202	PEB	C2B-C1B-CHA-C4A
26	bB	201	PEB	NB-C1B-CHA-C4A
26	bB	201	PEB	C2B-C1B-CHA-C4A
26	bB	202	PEB	NB-C1B-CHA-C4A
26	bB	202	PEB	C2B-C1B-CHA-C4A
26	cB	201	PEB	NB-C1B-CHA-C4A
26	cB	201	PEB	C2B-C1B-CHA-C4A
26	cB	202	PEB	ND-C1D-CHC-C4C
26	cB	202	PEB	C2D-C1D-CHC-C4C
26	cB	202	PEB	NC-C1C-CHB-C4B
26	cB	202	PEB	C2C-C1C-CHB-C4B
26	cB	202	PEB	NB-C1B-CHA-C4A
26	cB	202	PEB	C2B-C1B-CHA-C4A
26	dB	201	PEB	ND-C1D-CHC-C4C
26	dB	201	PEB	NB-C1B-CHA-C4A
26	dB	201	PEB	C2B-C1B-CHA-C4A
26	dB	202	PEB	C4A-C3A-CAA-CBA
26	dB	202	PEB	NB-C1B-CHA-C4A
26	dB	202	PEB	C2B-C1B-CHA-C4A
26	dB	203	PEB	NB-C1B-CHA-C4A
26	dB	203	PEB	C2B-C1B-CHA-C4A
26	dB	204	PEB	NC-C1C-CHB-C4B
26	dB	204	PEB	C2C-C1C-CHB-C4B
26	dB	204	PEB	NB-C1B-CHA-C4A
26	dB	204	PEB	C2B-C1B-CHA-C4A
26	eB	201	PEB	ND-C1D-CHC-C4C
26	eB	201	PEB	C2D-C1D-CHC-C4C
26	eB	201	PEB	C2C-CAC-CBC-CGC
26	eB	201	PEB	NB-C1B-CHA-C4A
26	eB	201	PEB	C2B-C1B-CHA-C4A
26	eB	202	PEB	C2A-C3A-CAA-CBA
26	eB	202	PEB	C4A-C3A-CAA-CBA
26	eB	202	PEB	NB-C1B-CHA-C4A
26	eB	202	PEB	C2B-C1B-CHA-C4A
26	eB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	eB	203	PEB	C2D-C1D-CHC-C4C
26	eB	203	PEB	NC-C1C-CHB-C4B
26	eB	203	PEB	C2C-C1C-CHB-C4B
26	eB	203	PEB	C2C-CAC-CBC-CGC
26	eB	203	PEB	C2A-C3A-CAA-CBA
26	eB	203	PEB	C4A-C3A-CAA-CBA
26	eB	203	PEB	NB-C1B-CHA-C4A
26	eB	203	PEB	C2B-C1B-CHA-C4A
26	fB	201	PEB	NC-C1C-CHB-C4B
26	fB	201	PEB	C2C-C1C-CHB-C4B
26	fB	201	PEB	C2A-C3A-CAA-CBA
26	fB	201	PEB	C4A-C3A-CAA-CBA
26	fB	201	PEB	NB-C1B-CHA-C4A
26	fB	201	PEB	C2B-C1B-CHA-C4A
26	fB	202	PEB	NB-C1B-CHA-C4A
26	fB	202	PEB	C2B-C1B-CHA-C4A
26	fB	202	PEB	C3B-CAB-CBB-CGB
26	fB	203	PEB	C4A-C3A-CAA-CBA
26	fB	203	PEB	NB-C1B-CHA-C4A
26	fB	203	PEB	C2B-C1B-CHA-C4A
26	gB	201	PEB	NB-C1B-CHA-C4A
26	gB	201	PEB	C2B-C1B-CHA-C4A
26	gB	202	PEB	ND-C1D-CHC-C4C
26	gB	202	PEB	C2D-C1D-CHC-C4C
26	gB	202	PEB	NC-C1C-CHB-C4B
26	gB	202	PEB	C2C-C1C-CHB-C4B
26	gB	202	PEB	NB-C1B-CHA-C4A
26	gB	202	PEB	C2B-C1B-CHA-C4A
26	hB	201	PEB	ND-C1D-CHC-C4C
26	hB	201	PEB	C2D-C1D-CHC-C4C
26	hB	201	PEB	C2A-C3A-CAA-CBA
26	hB	201	PEB	C4A-C3A-CAA-CBA
26	hB	201	PEB	NB-C1B-CHA-C4A
26	hB	201	PEB	C2B-C1B-CHA-C4A
26	hB	202	PEB	ND-C1D-CHC-C4C
26	hB	202	PEB	C2D-C1D-CHC-C4C
26	hB	202	PEB	C4A-C3A-CAA-CBA
26	hB	202	PEB	NB-C1B-CHA-C4A
26	hB	202	PEB	C2B-C1B-CHA-C4A
26	hB	203	PEB	C2A-C3A-CAA-CBA
26	hB	203	PEB	C4A-C3A-CAA-CBA
26	hB	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hB	203	PEB	C2B-C1B-CHA-C4A
26	iB	201	PEB	ND-C1D-CHC-C4C
26	iB	201	PEB	C2D-C1D-CHC-C4C
26	iB	201	PEB	NB-C1B-CHA-C4A
26	iB	201	PEB	C2B-C1B-CHA-C4A
26	iB	201	PEB	C3B-CAB-CBB-CGB
26	iB	202	PEB	NC-C1C-CHB-C4B
26	iB	202	PEB	C2C-C1C-CHB-C4B
26	iB	202	PEB	NB-C1B-CHA-C4A
26	iB	202	PEB	C2B-C1B-CHA-C4A
26	jB	201	PEB	C2A-C3A-CAA-CBA
26	jB	201	PEB	C4A-C3A-CAA-CBA
26	jB	201	PEB	NB-C1B-CHA-C4A
26	jB	201	PEB	C2B-C1B-CHA-C4A
26	jB	202	PEB	NB-C1B-CHA-C4A
26	jB	202	PEB	C2B-C1B-CHA-C4A
26	kB	201	PEB	C1C-C2C-CAC-CBC
26	kB	201	PEB	C3C-C2C-CAC-CBC
26	kB	201	PEB	NB-C1B-CHA-C4A
26	kB	201	PEB	C2B-C1B-CHA-C4A
26	kB	202	PEB	NC-C1C-CHB-C4B
26	kB	202	PEB	C2C-C1C-CHB-C4B
26	kB	202	PEB	C1C-C2C-CAC-CBC
26	kB	202	PEB	C2C-CAC-CBC-CGC
26	kB	202	PEB	NB-C1B-CHA-C4A
26	kB	202	PEB	C2B-C1B-CHA-C4A
26	lB	201	PEB	C2A-C3A-CAA-CBA
26	lB	201	PEB	C4A-C3A-CAA-CBA
26	lB	201	PEB	NB-C1B-CHA-C4A
26	lB	201	PEB	C2B-C1B-CHA-C4A
26	lB	202	PEB	ND-C1D-CHC-C4C
26	lB	202	PEB	C2D-C1D-CHC-C4C
26	lB	202	PEB	C4A-C3A-CAA-CBA
26	lB	202	PEB	NB-C1B-CHA-C4A
26	lB	202	PEB	C2B-C1B-CHA-C4A
26	lB	203	PEB	NB-C1B-CHA-C4A
26	lB	203	PEB	C2B-C1B-CHA-C4A
26	lB	203	PEB	C3B-CAB-CBB-CGB
26	mB	201	PEB	ND-C1D-CHC-C4C
26	mB	201	PEB	C2D-C1D-CHC-C4C
26	mB	201	PEB	NB-C1B-CHA-C4A
26	mB	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	mB	202	PEB	C2A-C3A-CAA-CBA
26	mB	202	PEB	C4A-C3A-CAA-CBA
26	mB	202	PEB	NB-C1B-CHA-C4A
26	mB	202	PEB	C2B-C1B-CHA-C4A
26	mB	203	PEB	NC-C1C-CHB-C4B
26	mB	203	PEB	C2C-C1C-CHB-C4B
26	mB	203	PEB	NB-C1B-CHA-C4A
26	mB	203	PEB	C2B-C1B-CHA-C4A
26	AC	201	PEB	NC-C1C-CHB-C4B
26	AC	201	PEB	C2C-C1C-CHB-C4B
26	AC	201	PEB	NB-C1B-CHA-C4A
26	AC	201	PEB	C2B-C1B-CHA-C4A
26	AC	202	PEB	NB-C1B-CHA-C4A
26	AC	202	PEB	C2B-C1B-CHA-C4A
26	AC	203	PEB	ND-C1D-CHC-C4C
26	AC	203	PEB	C2D-C1D-CHC-C4C
26	AC	203	PEB	NC-C1C-CHB-C4B
26	AC	203	PEB	C2C-C1C-CHB-C4B
26	AC	203	PEB	NB-C1B-CHA-C4A
26	AC	203	PEB	C2B-C1B-CHA-C4A
26	BC	201	PEB	NB-C1B-CHA-C4A
26	BC	201	PEB	C2B-C1B-CHA-C4A
26	BC	202	PEB	NC-C1C-CHB-C4B
26	BC	202	PEB	C2C-C1C-CHB-C4B
26	BC	202	PEB	NB-C1B-CHA-C4A
26	BC	202	PEB	C2B-C1B-CHA-C4A
26	BC	203	PEB	ND-C1D-CHC-C4C
26	BC	203	PEB	C2D-C1D-CHC-C4C
26	BC	203	PEB	NC-C1C-CHB-C4B
26	BC	203	PEB	C2C-C1C-CHB-C4B
26	BC	203	PEB	NB-C1B-CHA-C4A
26	BC	203	PEB	C2B-C1B-CHA-C4A
26	CC	201	PEB	NC-C1C-CHB-C4B
26	CC	201	PEB	C2C-C1C-CHB-C4B
26	CC	201	PEB	NB-C1B-CHA-C4A
26	CC	201	PEB	C2B-C1B-CHA-C4A
26	CC	202	PEB	NB-C1B-CHA-C4A
26	CC	202	PEB	C2B-C1B-CHA-C4A
26	CC	203	PEB	ND-C1D-CHC-C4C
26	CC	203	PEB	C2D-C1D-CHC-C4C
26	CC	203	PEB	NC-C1C-CHB-C4B
26	CC	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	CC	203	PEB	NB-C1B-CHA-C4A
26	CC	203	PEB	C2B-C1B-CHA-C4A
26	FC	201	PEB	NB-C1B-CHA-C4A
26	FC	201	PEB	C2B-C1B-CHA-C4A
26	FC	202	PEB	ND-C1D-CHC-C4C
26	FC	202	PEB	C2A-C3A-CAA-CBA
26	FC	202	PEB	C4A-C3A-CAA-CBA
26	FC	202	PEB	NB-C1B-CHA-C4A
26	FC	202	PEB	C2B-C1B-CHA-C4A
26	FC	203	PEB	ND-C1D-CHC-C4C
26	FC	203	PEB	C2D-C1D-CHC-C4C
26	FC	203	PEB	NC-C1C-CHB-C4B
26	FC	203	PEB	C2C-C1C-CHB-C4B
26	FC	203	PEB	NB-C1B-CHA-C4A
26	FC	203	PEB	C2B-C1B-CHA-C4A
26	GC	201	PEB	ND-C1D-CHC-C4C
26	GC	201	PEB	C2D-C1D-CHC-C4C
26	GC	201	PEB	C2A-C3A-CAA-CBA
26	GC	201	PEB	C4A-C3A-CAA-CBA
26	GC	201	PEB	NB-C1B-CHA-C4A
26	GC	201	PEB	C2B-C1B-CHA-C4A
26	GC	202	PEB	NB-C1B-CHA-C4A
26	GC	202	PEB	C2B-C1B-CHA-C4A
26	GC	203	PEB	ND-C1D-CHC-C4C
26	GC	203	PEB	C2D-C1D-CHC-C4C
26	GC	203	PEB	NC-C1C-CHB-C4B
26	GC	203	PEB	C2C-C1C-CHB-C4B
26	GC	203	PEB	C2C-CAC-CBC-CGC
26	GC	203	PEB	C2A-C3A-CAA-CBA
26	GC	203	PEB	C4A-C3A-CAA-CBA
26	GC	203	PEB	NB-C1B-CHA-C4A
26	GC	203	PEB	C2B-C1B-CHA-C4A
26	HC	201	PEB	C2A-C3A-CAA-CBA
26	HC	201	PEB	C4A-C3A-CAA-CBA
26	HC	201	PEB	NB-C1B-CHA-C4A
26	HC	201	PEB	C2B-C1B-CHA-C4A
26	HC	202	PEB	C4A-C3A-CAA-CBA
26	HC	202	PEB	NB-C1B-CHA-C4A
26	HC	202	PEB	C2B-C1B-CHA-C4A
26	HC	203	PEB	ND-C1D-CHC-C4C
26	HC	203	PEB	C2D-C1D-CHC-C4C
26	HC	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	HC	203	PEB	C2C-C1C-CHB-C4B
26	HC	203	PEB	C2C-CAC-CBC-CGC
26	HC	203	PEB	NB-C1B-CHA-C4A
26	HC	203	PEB	C2B-C1B-CHA-C4A
26	IC	201	PEB	NB-C1B-CHA-C4A
26	IC	201	PEB	C2B-C1B-CHA-C4A
26	IC	202	PEB	C2C-CAC-CBC-CGC
26	IC	202	PEB	NB-C1B-CHA-C4A
26	IC	202	PEB	C2B-C1B-CHA-C4A
26	IC	203	PEB	ND-C1D-CHC-C4C
26	IC	203	PEB	C2D-C1D-CHC-C4C
26	IC	203	PEB	NC-C1C-CHB-C4B
26	IC	203	PEB	C2C-C1C-CHB-C4B
26	IC	203	PEB	C2C-CAC-CBC-CGC
26	IC	203	PEB	NB-C1B-CHA-C4A
26	IC	203	PEB	C2B-C1B-CHA-C4A
26	JC	201	PEB	NC-C1C-CHB-C4B
26	JC	201	PEB	C2C-C1C-CHB-C4B
26	JC	201	PEB	C2A-C3A-CAA-CBA
26	JC	201	PEB	C4A-C3A-CAA-CBA
26	JC	202	PEB	ND-C1D-CHC-C4C
26	JC	202	PEB	C2D-C1D-CHC-C4C
26	JC	202	PEB	NB-C1B-CHA-C4A
26	JC	202	PEB	C2B-C1B-CHA-C4A
26	JC	202	PEB	C3B-CAB-CBB-CGB
26	KC	201	PEB	C2A-C3A-CAA-CBA
26	KC	201	PEB	C4A-C3A-CAA-CBA
26	KC	201	PEB	NB-C1B-CHA-C4A
26	KC	201	PEB	C2B-C1B-CHA-C4A
26	KC	202	PEB	C2A-C3A-CAA-CBA
26	KC	202	PEB	C4A-C3A-CAA-CBA
26	KC	202	PEB	NB-C1B-CHA-C4A
26	KC	202	PEB	C2B-C1B-CHA-C4A
26	KC	203	PEB	NC-C1C-CHB-C4B
26	KC	203	PEB	C2C-C1C-CHB-C4B
26	KC	203	PEB	NB-C1B-CHA-C4A
26	KC	203	PEB	C2B-C1B-CHA-C4A
26	LC	201	PEB	NB-C1B-CHA-C4A
26	LC	201	PEB	C2B-C1B-CHA-C4A
26	LC	202	PEB	C2A-C3A-CAA-CBA
26	LC	202	PEB	C4A-C3A-CAA-CBA
26	LC	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	LC	202	PEB	C2B-C1B-CHA-C4A
26	LC	203	PEB	ND-C1D-CHC-C4C
26	LC	203	PEB	C2D-C1D-CHC-C4C
26	LC	203	PEB	NC-C1C-CHB-C4B
26	LC	203	PEB	C2C-C1C-CHB-C4B
26	LC	203	PEB	NB-C1B-CHA-C4A
26	LC	203	PEB	C2B-C1B-CHA-C4A
26	eD	401	PEB	ND-C1D-CHC-C4C
26	eD	401	PEB	C2D-C1D-CHC-C4C
26	eD	401	PEB	NB-C1B-CHA-C4A
26	eD	401	PEB	C2B-C1B-CHA-C4A
26	AD	201	PEB	ND-C1D-CHC-C4C
26	AD	201	PEB	C2D-C1D-CHC-C4C
26	AD	201	PEB	NB-C1B-CHA-C4A
26	AD	201	PEB	C2B-C1B-CHA-C4A
26	AD	202	PEB	C2D-C3D-CAD-CBD
26	AD	202	PEB	C4D-C3D-CAD-CBD
26	AD	202	PEB	C2A-C3A-CAA-CBA
26	AD	202	PEB	C4A-C3A-CAA-CBA
26	AD	202	PEB	NB-C1B-CHA-C4A
26	AD	202	PEB	C2B-C1B-CHA-C4A
26	BD	201	PEB	ND-C1D-CHC-C4C
26	BD	201	PEB	NB-C1B-CHA-C4A
26	BD	201	PEB	C2B-C1B-CHA-C4A
26	BD	202	PEB	C2A-C3A-CAA-CBA
26	BD	202	PEB	C4A-C3A-CAA-CBA
26	BD	202	PEB	NB-C1B-CHA-C4A
26	BD	202	PEB	C2B-C1B-CHA-C4A
26	BD	203	PEB	NC-C1C-CHB-C4B
26	BD	203	PEB	C2C-C1C-CHB-C4B
26	BD	203	PEB	C2C-CAC-CBC-CGC
26	BD	203	PEB	C2A-C3A-CAA-CBA
26	BD	203	PEB	NB-C1B-CHA-C4A
26	BD	203	PEB	C2B-C1B-CHA-C4A
26	CD	201	PEB	ND-C1D-CHC-C4C
26	CD	201	PEB	NC-C1C-CHB-C4B
26	CD	201	PEB	C2C-C1C-CHB-C4B
26	CD	201	PEB	NB-C1B-CHA-C4A
26	CD	201	PEB	C2B-C1B-CHA-C4A
26	CD	202	PEB	NC-C1C-CHB-C4B
26	CD	202	PEB	C2C-C1C-CHB-C4B
26	CD	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	CD	202	PEB	C3C-C2C-CAC-CBC
26	CD	202	PEB	C2A-C3A-CAA-CBA
26	CD	202	PEB	C4A-C3A-CAA-CBA
26	CD	202	PEB	NB-C1B-CHA-C4A
26	CD	202	PEB	C2B-C1B-CHA-C4A
26	CD	202	PEB	NB-C4B-CHB-C1C
26	DD	201	PEB	ND-C1D-CHC-C4C
26	DD	201	PEB	C2D-C1D-CHC-C4C
26	DD	201	PEB	NB-C1B-CHA-C4A
26	DD	201	PEB	C2B-C1B-CHA-C4A
26	DD	202	PEB	ND-C1D-CHC-C4C
26	DD	202	PEB	NC-C1C-CHB-C4B
26	DD	202	PEB	C2C-C1C-CHB-C4B
26	DD	202	PEB	C2C-CAC-CBC-CGC
26	DD	202	PEB	C4A-C3A-CAA-CBA
26	DD	202	PEB	NB-C1B-CHA-C4A
26	DD	202	PEB	C2B-C1B-CHA-C4A
26	DD	203	PEB	ND-C1D-CHC-C4C
26	DD	203	PEB	C2D-C1D-CHC-C4C
26	DD	203	PEB	NC-C1C-CHB-C4B
26	DD	203	PEB	C2C-C1C-CHB-C4B
26	DD	203	PEB	NB-C1B-CHA-C4A
26	DD	203	PEB	C2B-C1B-CHA-C4A
26	ED	201	PEB	NB-C1B-CHA-C4A
26	ED	201	PEB	C2B-C1B-CHA-C4A
26	ED	202	PEB	C4A-C3A-CAA-CBA
26	ED	202	PEB	NB-C1B-CHA-C4A
26	ED	202	PEB	C2B-C1B-CHA-C4A
26	FD	201	PEB	C2C-CAC-CBC-CGC
26	FD	201	PEB	NB-C1B-CHA-C4A
26	FD	201	PEB	C2B-C1B-CHA-C4A
26	FD	202	PEB	C4A-C3A-CAA-CBA
26	FD	202	PEB	NB-C1B-CHA-C4A
26	FD	202	PEB	C2B-C1B-CHA-C4A
26	FD	203	PEB	ND-C1D-CHC-C4C
26	FD	203	PEB	NC-C1C-CHB-C4B
26	FD	203	PEB	C2C-C1C-CHB-C4B
26	FD	203	PEB	C2C-CAC-CBC-CGC
26	FD	203	PEB	C2A-C3A-CAA-CBA
26	FD	203	PEB	C4A-C3A-CAA-CBA
26	FD	203	PEB	NB-C1B-CHA-C4A
26	FD	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	GD	201	PEB	C2A-C3A-CAA-CBA
26	GD	201	PEB	C4A-C3A-CAA-CBA
26	GD	201	PEB	NB-C1B-CHA-C4A
26	GD	201	PEB	C2B-C1B-CHA-C4A
26	GD	202	PEB	NC-C1C-CHB-C4B
26	GD	202	PEB	C2C-C1C-CHB-C4B
26	GD	202	PEB	C2C-CAC-CBC-CGC
26	GD	202	PEB	C2A-C3A-CAA-CBA
26	GD	202	PEB	C4A-C3A-CAA-CBA
26	GD	202	PEB	NB-C1B-CHA-C4A
26	GD	202	PEB	C2B-C1B-CHA-C4A
26	HD	201	PEB	NB-C1B-CHA-C4A
26	HD	201	PEB	C2B-C1B-CHA-C4A
26	HD	202	PEB	ND-C1D-CHC-C4C
26	HD	202	PEB	C2D-C1D-CHC-C4C
26	HD	202	PEB	C4A-C3A-CAA-CBA
26	HD	202	PEB	NB-C1B-CHA-C4A
26	HD	202	PEB	C2B-C1B-CHA-C4A
26	HD	203	PEB	NC-C1C-CHB-C4B
26	HD	203	PEB	C2C-C1C-CHB-C4B
26	HD	203	PEB	NB-C1B-CHA-C4A
26	HD	203	PEB	C2B-C1B-CHA-C4A
26	HD	203	PEB	C2B-C3B-CAB-CBB
26	ID	201	PEB	ND-C1D-CHC-C4C
26	ID	201	PEB	C2D-C1D-CHC-C4C
26	ID	201	PEB	NC-C1C-CHB-C4B
26	ID	201	PEB	C2C-C1C-CHB-C4B
26	ID	201	PEB	C2A-C3A-CAA-CBA
26	ID	201	PEB	C4A-C3A-CAA-CBA
26	ID	201	PEB	NB-C1B-CHA-C4A
26	ID	201	PEB	C2B-C1B-CHA-C4A
26	ID	202	PEB	NC-C1C-CHB-C4B
26	ID	202	PEB	C2C-C1C-CHB-C4B
26	ID	202	PEB	C2A-C3A-CAA-CBA
26	ID	202	PEB	C4A-C3A-CAA-CBA
26	ID	202	PEB	NB-C1B-CHA-C4A
26	ID	202	PEB	C2B-C1B-CHA-C4A
26	JD	201	PEB	NB-C1B-CHA-C4A
26	JD	201	PEB	C2B-C1B-CHA-C4A
26	JD	202	PEB	NC-C1C-CHB-C4B
26	JD	202	PEB	C2C-C1C-CHB-C4B
26	JD	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	JD	202	PEB	NB-C1B-CHA-C4A
26	JD	202	PEB	C2B-C1B-CHA-C4A
26	JD	203	PEB	ND-C1D-CHC-C4C
26	JD	203	PEB	NC-C1C-CHB-C4B
26	JD	203	PEB	C2C-C1C-CHB-C4B
26	JD	203	PEB	C2A-C3A-CAA-CBA
26	JD	203	PEB	C4A-C3A-CAA-CBA
26	JD	203	PEB	NB-C1B-CHA-C4A
26	JD	203	PEB	C2B-C1B-CHA-C4A
26	KD	201	PEB	C1C-C2C-CAC-CBC
26	KD	201	PEB	C3C-C2C-CAC-CBC
26	KD	201	PEB	NB-C1B-CHA-C4A
26	KD	201	PEB	C2B-C1B-CHA-C4A
26	KD	202	PEB	C2C-CAC-CBC-CGC
26	KD	202	PEB	C2D-C3D-CAD-CBD
26	KD	202	PEB	C4D-C3D-CAD-CBD
26	KD	202	PEB	NB-C1B-CHA-C4A
26	KD	202	PEB	C2B-C1B-CHA-C4A
26	LD	201	PEB	NB-C1B-CHA-C4A
26	LD	201	PEB	C2B-C1B-CHA-C4A
26	LD	202	PEB	C2C-CAC-CBC-CGC
26	LD	202	PEB	C4A-C3A-CAA-CBA
26	LD	202	PEB	NB-C1B-CHA-C4A
26	LD	202	PEB	C2B-C1B-CHA-C4A
26	LD	203	PEB	NC-C1C-CHB-C4B
26	LD	203	PEB	C2C-C1C-CHB-C4B
26	LD	203	PEB	NB-C1B-CHA-C4A
26	LD	203	PEB	C2B-C1B-CHA-C4A
26	MD	201	PEB	NC-C1C-CHB-C4B
26	MD	201	PEB	C2C-C1C-CHB-C4B
26	MD	201	PEB	NB-C1B-CHA-C4A
26	MD	201	PEB	C2B-C1B-CHA-C4A
26	MD	202	PEB	ND-C1D-CHC-C4C
26	MD	202	PEB	C2D-C1D-CHC-C4C
26	MD	202	PEB	NC-C1C-CHB-C4B
26	MD	202	PEB	C2C-C1C-CHB-C4B
26	MD	202	PEB	C4A-C3A-CAA-CBA
26	MD	202	PEB	NB-C1B-CHA-C4A
26	MD	202	PEB	C2B-C1B-CHA-C4A
26	ND	201	PEB	NB-C1B-CHA-C4A
26	ND	201	PEB	C2B-C1B-CHA-C4A
26	ND	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	ND	202	PEB	NB-C1B-CHA-C4A
26	ND	202	PEB	C2B-C1B-CHA-C4A
26	ND	203	PEB	NC-C1C-CHB-C4B
26	ND	203	PEB	C2C-C1C-CHB-C4B
26	ND	203	PEB	NB-C1B-CHA-C4A
26	ND	203	PEB	C2B-C1B-CHA-C4A
26	OD	201	PEB	NC-C1C-CHB-C4B
26	OD	201	PEB	C2C-C1C-CHB-C4B
26	OD	201	PEB	C2B-C1B-CHA-C4A
26	OD	202	PEB	NC-C1C-CHB-C4B
26	OD	202	PEB	C2C-C1C-CHB-C4B
26	OD	202	PEB	C2A-C3A-CAA-CBA
26	OD	202	PEB	C4A-C3A-CAA-CBA
26	OD	202	PEB	NB-C1B-CHA-C4A
26	OD	202	PEB	C2B-C1B-CHA-C4A
26	PD	201	PEB	NB-C1B-CHA-C4A
26	PD	201	PEB	C2B-C1B-CHA-C4A
26	PD	202	PEB	C4A-C3A-CAA-CBA
26	PD	202	PEB	NB-C1B-CHA-C4A
26	PD	202	PEB	C2B-C1B-CHA-C4A
26	PD	203	PEB	NC-C1C-CHB-C4B
26	PD	203	PEB	C2C-C1C-CHB-C4B
26	PD	203	PEB	NB-C1B-CHA-C4A
26	PD	203	PEB	C2B-C1B-CHA-C4A
26	QD	201	PEB	NC-C1C-CHB-C4B
26	QD	201	PEB	C2C-C1C-CHB-C4B
26	QD	201	PEB	NB-C1B-CHA-C4A
26	QD	201	PEB	C2B-C1B-CHA-C4A
26	QD	202	PEB	C4A-C3A-CAA-CBA
26	QD	202	PEB	NB-C1B-CHA-C4A
26	QD	202	PEB	C2B-C1B-CHA-C4A
26	RD	201	PEB	NB-C1B-CHA-C4A
26	RD	201	PEB	C2B-C1B-CHA-C4A
26	RD	202	PEB	C4A-C3A-CAA-CBA
26	RD	202	PEB	NB-C1B-CHA-C4A
26	RD	202	PEB	C2B-C1B-CHA-C4A
26	RD	203	PEB	NC-C1C-CHB-C4B
26	RD	203	PEB	C2C-C1C-CHB-C4B
26	RD	203	PEB	C2D-C3D-CAD-CBD
26	RD	203	PEB	C4D-C3D-CAD-CBD
26	RD	203	PEB	NB-C1B-CHA-C4A
26	RD	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	SD	201	PEB	NC-C1C-CHB-C4B
26	SD	201	PEB	C2C-C1C-CHB-C4B
26	SD	202	PEB	C4A-C3A-CAA-CBA
26	SD	202	PEB	NB-C1B-CHA-C4A
26	SD	202	PEB	C2B-C1B-CHA-C4A
26	TD	201	PEB	NB-C1B-CHA-C4A
26	TD	201	PEB	C2B-C1B-CHA-C4A
26	TD	202	PEB	C4A-C3A-CAA-CBA
26	TD	202	PEB	NB-C1B-CHA-C4A
26	TD	202	PEB	C2B-C1B-CHA-C4A
26	TD	203	PEB	NB-C1B-CHA-C4A
26	TD	203	PEB	C2B-C1B-CHA-C4A
26	UD	201	PEB	NB-C1B-CHA-C4A
26	UD	202	PEB	NC-C1C-CHB-C4B
26	UD	202	PEB	C2C-C1C-CHB-C4B
26	UD	202	PEB	C4A-C3A-CAA-CBA
26	UD	202	PEB	NB-C1B-CHA-C4A
26	UD	202	PEB	C2B-C1B-CHA-C4A
26	VD	201	PEB	ND-C1D-CHC-C4C
26	VD	201	PEB	C2D-C1D-CHC-C4C
26	VD	201	PEB	C2A-C3A-CAA-CBA
26	VD	201	PEB	C4A-C3A-CAA-CBA
26	VD	201	PEB	NB-C1B-CHA-C4A
26	VD	201	PEB	C2B-C1B-CHA-C4A
26	VD	202	PEB	C2C-CAC-CBC-CGC
26	VD	202	PEB	C2A-C3A-CAA-CBA
26	VD	202	PEB	C4A-C3A-CAA-CBA
26	VD	202	PEB	NB-C1B-CHA-C4A
26	VD	202	PEB	C2B-C1B-CHA-C4A
26	VD	203	PEB	NC-C1C-CHB-C4B
26	VD	203	PEB	C2C-C1C-CHB-C4B
26	VD	203	PEB	NB-C1B-CHA-C4A
26	VD	203	PEB	C2B-C1B-CHA-C4A
26	WD	201	PEB	NB-C1B-CHA-C4A
26	WD	201	PEB	C2B-C1B-CHA-C4A
26	WD	202	PEB	NC-C1C-CHB-C4B
26	WD	202	PEB	C2C-C1C-CHB-C4B
26	WD	202	PEB	C2A-C3A-CAA-CBA
26	WD	202	PEB	C4A-C3A-CAA-CBA
26	WD	202	PEB	NB-C1B-CHA-C4A
26	WD	202	PEB	C2B-C1B-CHA-C4A
26	XD	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	XD	201	PEB	C2B-C1B-CHA-C4A
26	XD	202	PEB	C2C-CAC-CBC-CGC
26	XD	202	PEB	C4A-C3A-CAA-CBA
26	XD	202	PEB	NB-C1B-CHA-C4A
26	XD	202	PEB	C2B-C1B-CHA-C4A
26	XD	203	PEB	NC-C1C-CHB-C4B
26	XD	203	PEB	C2C-C1C-CHB-C4B
26	XD	203	PEB	C1C-C2C-CAC-CBC
26	XD	203	PEB	C3C-C2C-CAC-CBC
26	XD	203	PEB	C2A-C3A-CAA-CBA
26	XD	203	PEB	NB-C1B-CHA-C4A
26	XD	203	PEB	C2B-C1B-CHA-C4A
26	YD	301	PEB	ND-C1D-CHC-C4C
26	YD	301	PEB	NC-C1C-CHB-C4B
26	YD	301	PEB	C2C-C1C-CHB-C4B
26	YD	301	PEB	C2A-C3A-CAA-CBA
26	YD	301	PEB	C4A-C3A-CAA-CBA
26	YD	301	PEB	NB-C1B-CHA-C4A
26	YD	301	PEB	C2B-C1B-CHA-C4A
26	YD	303	PEB	ND-C1D-CHC-C4C
26	YD	303	PEB	NC-C1C-CHB-C4B
26	YD	303	PEB	C2C-C1C-CHB-C4B
26	YD	303	PEB	C2A-C3A-CAA-CBA
26	YD	303	PEB	NB-C1B-CHA-C4A
26	YD	303	PEB	C2B-C1B-CHA-C4A
26	YD	304	PEB	ND-C1D-CHC-C4C
26	YD	304	PEB	C2D-C1D-CHC-C4C
26	YD	304	PEB	NC-C1C-CHB-C4B
26	YD	304	PEB	C2C-C1C-CHB-C4B
26	YD	304	PEB	C2A-C3A-CAA-CBA
26	YD	304	PEB	NB-C1B-CHA-C4A
26	YD	304	PEB	C2B-C1B-CHA-C4A
26	AE	201	PEB	C2A-C3A-CAA-CBA
26	AE	201	PEB	C4A-C3A-CAA-CBA
26	AE	201	PEB	NB-C1B-CHA-C4A
26	AE	201	PEB	C2B-C1B-CHA-C4A
26	AE	202	PEB	NC-C1C-CHB-C4B
26	AE	202	PEB	C2C-C1C-CHB-C4B
26	AE	202	PEB	C2C-CAC-CBC-CGC
26	AE	202	PEB	C4A-C3A-CAA-CBA
26	AE	202	PEB	NB-C1B-CHA-C4A
26	AE	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	BE	201	PEB	NC-C1C-CHB-C4B
26	BE	201	PEB	C2C-C1C-CHB-C4B
26	BE	201	PEB	NB-C1B-CHA-C4A
26	BE	201	PEB	C2B-C1B-CHA-C4A
26	BE	202	PEB	ND-C1D-CHC-C4C
26	BE	202	PEB	C2D-C1D-CHC-C4C
26	BE	202	PEB	NC-C1C-CHB-C4B
26	BE	202	PEB	C2C-C1C-CHB-C4B
26	BE	202	PEB	C2C-CAC-CBC-CGC
26	BE	202	PEB	C2A-C3A-CAA-CBA
26	BE	202	PEB	C4A-C3A-CAA-CBA
26	BE	202	PEB	NB-C1B-CHA-C4A
26	BE	202	PEB	C2B-C1B-CHA-C4A
26	CE	201	PEB	C2D-C1D-CHC-C4C
26	CE	201	PEB	C2C-CAC-CBC-CGC
26	CE	201	PEB	C2A-C3A-CAA-CBA
26	CE	201	PEB	C4A-C3A-CAA-CBA
26	CE	201	PEB	NB-C1B-CHA-C4A
26	CE	201	PEB	C2B-C1B-CHA-C4A
26	CE	202	PEB	C2A-C3A-CAA-CBA
26	CE	202	PEB	C4A-C3A-CAA-CBA
26	CE	202	PEB	NB-C1B-CHA-C4A
26	CE	202	PEB	C2B-C1B-CHA-C4A
26	CE	203	PEB	NC-C1C-CHB-C4B
26	CE	203	PEB	C2C-C1C-CHB-C4B
26	CE	203	PEB	C2C-CAC-CBC-CGC
26	CE	203	PEB	NB-C1B-CHA-C4A
26	CE	203	PEB	C2B-C1B-CHA-C4A
26	DE	201	PEB	NB-C1B-CHA-C4A
26	DE	201	PEB	C2B-C1B-CHA-C4A
26	DE	202	PEB	C2D-C3D-CAD-CBD
26	DE	202	PEB	C4D-C3D-CAD-CBD
26	DE	202	PEB	C4A-C3A-CAA-CBA
26	DE	202	PEB	NB-C1B-CHA-C4A
26	DE	202	PEB	C2B-C1B-CHA-C4A
26	DE	203	PEB	ND-C1D-CHC-C4C
26	DE	203	PEB	C2D-C1D-CHC-C4C
26	DE	203	PEB	NC-C1C-CHB-C4B
26	DE	203	PEB	C2C-C1C-CHB-C4B
26	DE	203	PEB	NB-C1B-CHA-C4A
26	DE	203	PEB	C2B-C1B-CHA-C4A
26	EE	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	EE	201	PEB	C4A-C3A-CAA-CBA
26	EE	201	PEB	NB-C1B-CHA-C4A
26	EE	201	PEB	C2B-C1B-CHA-C4A
26	EE	202	PEB	NC-C1C-CHB-C4B
26	EE	202	PEB	C2C-C1C-CHB-C4B
26	EE	202	PEB	C2C-CAC-CBC-CGC
26	EE	202	PEB	NB-C1B-CHA-C4A
26	EE	202	PEB	C2B-C1B-CHA-C4A
26	FE	201	PEB	NB-C1B-CHA-C4A
26	FE	201	PEB	C2B-C1B-CHA-C4A
26	FE	202	PEB	ND-C1D-CHC-C4C
26	FE	202	PEB	C2D-C1D-CHC-C4C
26	FE	202	PEB	NC-C1C-CHB-C4B
26	FE	202	PEB	C2C-C1C-CHB-C4B
26	FE	202	PEB	C2C-CAC-CBC-CGC
26	FE	202	PEB	NB-C1B-CHA-C4A
26	FE	202	PEB	C2B-C1B-CHA-C4A
26	GE	201	PEB	C2A-C3A-CAA-CBA
26	GE	201	PEB	C4A-C3A-CAA-CBA
26	GE	201	PEB	NB-C1B-CHA-C4A
26	GE	201	PEB	C2B-C1B-CHA-C4A
26	GE	202	PEB	C4A-C3A-CAA-CBA
26	GE	202	PEB	NB-C1B-CHA-C4A
26	GE	202	PEB	C2B-C1B-CHA-C4A
26	GE	203	PEB	NC-C1C-CHB-C4B
26	GE	203	PEB	C2C-C1C-CHB-C4B
26	GE	203	PEB	C2C-CAC-CBC-CGC
26	GE	203	PEB	NB-C1B-CHA-C4A
26	GE	203	PEB	C2B-C1B-CHA-C4A
26	HE	201	PEB	NC-C1C-CHB-C4B
26	HE	201	PEB	C2D-C3D-CAD-CBD
26	HE	201	PEB	C4D-C3D-CAD-CBD
26	HE	201	PEB	C2A-C3A-CAA-CBA
26	HE	201	PEB	C4A-C3A-CAA-CBA
26	HE	201	PEB	NB-C1B-CHA-C4A
26	HE	201	PEB	C2B-C1B-CHA-C4A
26	HE	202	PEB	ND-C1D-CHC-C4C
26	HE	202	PEB	C2D-C1D-CHC-C4C
26	HE	202	PEB	NC-C1C-CHB-C4B
26	HE	202	PEB	C2C-C1C-CHB-C4B
26	HE	202	PEB	C2C-CAC-CBC-CGC
26	HE	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	HE	202	PEB	C2B-C1B-CHA-C4A
26	IE	201	PEB	C2A-C3A-CAA-CBA
26	IE	201	PEB	C4A-C3A-CAA-CBA
26	IE	201	PEB	NB-C1B-CHA-C4A
26	IE	201	PEB	C2B-C1B-CHA-C4A
26	IE	201	PEB	C3B-CAB-CBB-CGB
26	IE	202	PEB	C2C-CAC-CBC-CGC
26	IE	202	PEB	C4A-C3A-CAA-CBA
26	IE	202	PEB	NB-C1B-CHA-C4A
26	IE	202	PEB	C2B-C1B-CHA-C4A
26	IE	203	PEB	C4A-C3A-CAA-CBA
26	IE	203	PEB	NB-C1B-CHA-C4A
26	IE	203	PEB	C2B-C1B-CHA-C4A
26	JE	201	PEB	NB-C1B-CHA-C4A
26	JE	201	PEB	C2B-C1B-CHA-C4A
26	JE	202	PEB	ND-C1D-CHC-C4C
26	JE	202	PEB	C2D-C1D-CHC-C4C
26	JE	202	PEB	NC-C1C-CHB-C4B
26	JE	202	PEB	C2C-C1C-CHB-C4B
26	JE	202	PEB	NB-C1B-CHA-C4A
26	JE	202	PEB	C2B-C1B-CHA-C4A
26	KE	201	PEB	C2A-C3A-CAA-CBA
26	KE	201	PEB	C4A-C3A-CAA-CBA
26	KE	201	PEB	NB-C1B-CHA-C4A
26	KE	201	PEB	C2B-C1B-CHA-C4A
26	KE	202	PEB	C2A-C3A-CAA-CBA
26	KE	202	PEB	C4A-C3A-CAA-CBA
26	KE	202	PEB	NB-C1B-CHA-C4A
26	KE	202	PEB	C2B-C1B-CHA-C4A
26	KE	203	PEB	C2C-CAC-CBC-CGC
26	KE	203	PEB	NB-C1B-CHA-C4A
26	KE	203	PEB	C2B-C1B-CHA-C4A
26	LE	201	PEB	NB-C1B-CHA-C4A
26	LE	201	PEB	C2B-C1B-CHA-C4A
26	LE	202	PEB	ND-C1D-CHC-C4C
26	LE	202	PEB	C2D-C1D-CHC-C4C
26	LE	202	PEB	NC-C1C-CHB-C4B
26	LE	202	PEB	C2C-C1C-CHB-C4B
26	LE	202	PEB	C1C-C2C-CAC-CBC
26	LE	202	PEB	C3C-C2C-CAC-CBC
26	LE	202	PEB	C2C-CAC-CBC-CGC
26	LE	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	LE	202	PEB	C2B-C1B-CHA-C4A
26	ME	201	PEB	NB-C1B-CHA-C4A
26	ME	201	PEB	C2B-C1B-CHA-C4A
26	ME	202	PEB	C2C-CAC-CBC-CGC
26	ME	202	PEB	C2A-C3A-CAA-CBA
26	ME	202	PEB	C4A-C3A-CAA-CBA
26	ME	202	PEB	NB-C1B-CHA-C4A
26	ME	202	PEB	C2B-C1B-CHA-C4A
26	ME	203	PEB	NB-C1B-CHA-C4A
26	ME	203	PEB	C2B-C1B-CHA-C4A
26	NE	201	PEB	NB-C1B-CHA-C4A
26	NE	201	PEB	C2B-C1B-CHA-C4A
26	NE	202	PEB	ND-C1D-CHC-C4C
26	NE	202	PEB	C2D-C1D-CHC-C4C
26	NE	202	PEB	NC-C1C-CHB-C4B
26	NE	202	PEB	C2C-C1C-CHB-C4B
26	NE	202	PEB	NB-C1B-CHA-C4A
26	NE	202	PEB	C2B-C1B-CHA-C4A
26	OE	201	PEB	NB-C1B-CHA-C4A
26	OE	201	PEB	C2B-C1B-CHA-C4A
26	OE	202	PEB	ND-C1D-CHC-C4C
26	OE	202	PEB	NB-C1B-CHA-C4A
26	OE	202	PEB	C2B-C1B-CHA-C4A
26	OE	203	PEB	NC-C1C-CHB-C4B
26	OE	203	PEB	C2C-C1C-CHB-C4B
26	OE	203	PEB	C4A-C3A-CAA-CBA
26	OE	203	PEB	NB-C1B-CHA-C4A
26	OE	203	PEB	C2B-C1B-CHA-C4A
26	PE	201	PEB	NB-C1B-CHA-C4A
26	PE	201	PEB	C2B-C1B-CHA-C4A
26	PE	202	PEB	ND-C1D-CHC-C4C
26	PE	202	PEB	C2D-C1D-CHC-C4C
26	PE	202	PEB	NC-C1C-CHB-C4B
26	PE	202	PEB	C2C-C1C-CHB-C4B
26	PE	202	PEB	C2C-CAC-CBC-CGC
26	PE	202	PEB	NB-C1B-CHA-C4A
26	PE	202	PEB	C2B-C1B-CHA-C4A
26	PE	202	PEB	C3B-CAB-CBB-CGB
26	QE	201	PEB	C2A-C3A-CAA-CBA
26	QE	201	PEB	C4A-C3A-CAA-CBA
26	QE	201	PEB	NB-C1B-CHA-C4A
26	QE	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	QE	202	PEB	NC-C1C-CHB-C4B
26	QE	202	PEB	C2C-C1C-CHB-C4B
26	QE	202	PEB	C2C-CAC-CBC-CGC
26	QE	202	PEB	NB-C1B-CHA-C4A
26	QE	202	PEB	C2B-C1B-CHA-C4A
26	QE	203	PEB	NB-C1B-CHA-C4A
26	QE	203	PEB	C2B-C1B-CHA-C4A
26	RE	201	PEB	NB-C1B-CHA-C4A
26	RE	201	PEB	C2B-C1B-CHA-C4A
26	RE	202	PEB	ND-C1D-CHC-C4C
26	RE	202	PEB	C2D-C1D-CHC-C4C
26	RE	202	PEB	NC-C1C-CHB-C4B
26	RE	202	PEB	C2C-C1C-CHB-C4B
26	RE	202	PEB	C2A-C3A-CAA-CBA
26	RE	202	PEB	C4A-C3A-CAA-CBA
26	RE	202	PEB	NB-C1B-CHA-C4A
26	RE	202	PEB	C2B-C1B-CHA-C4A
26	SE	201	PEB	C2A-C3A-CAA-CBA
26	SE	201	PEB	C4A-C3A-CAA-CBA
26	SE	201	PEB	NB-C1B-CHA-C4A
26	SE	201	PEB	C2B-C1B-CHA-C4A
26	SE	202	PEB	C2A-C3A-CAA-CBA
26	SE	202	PEB	C4A-C3A-CAA-CBA
26	SE	202	PEB	NB-C1B-CHA-C4A
26	SE	202	PEB	C2B-C1B-CHA-C4A
26	SE	202	PEB	C3B-CAB-CBB-CGB
26	SE	203	PEB	NC-C1C-CHB-C4B
26	SE	203	PEB	C2C-C1C-CHB-C4B
26	SE	203	PEB	C2C-CAC-CBC-CGC
26	SE	203	PEB	NB-C1B-CHA-C4A
26	SE	203	PEB	C2B-C1B-CHA-C4A
26	TE	201	PEB	NB-C1B-CHA-C4A
26	TE	201	PEB	C2B-C1B-CHA-C4A
26	TE	202	PEB	ND-C1D-CHC-C4C
26	TE	202	PEB	C2D-C1D-CHC-C4C
26	TE	202	PEB	NC-C1C-CHB-C4B
26	TE	202	PEB	C2C-C1C-CHB-C4B
26	TE	202	PEB	C2D-C3D-CAD-CBD
26	TE	202	PEB	C4D-C3D-CAD-CBD
26	TE	202	PEB	NB-C1B-CHA-C4A
26	TE	202	PEB	C2B-C1B-CHA-C4A
26	UE	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	UE	201	PEB	C4A-C3A-CAA-CBA
26	UE	201	PEB	NB-C1B-CHA-C4A
26	UE	201	PEB	C2B-C1B-CHA-C4A
26	UE	202	PEB	C2C-CAC-CBC-CGC
26	UE	202	PEB	C2A-C3A-CAA-CBA
26	UE	202	PEB	NB-C1B-CHA-C4A
26	UE	202	PEB	C2B-C1B-CHA-C4A
26	UE	203	PEB	C2A-C3A-CAA-CBA
26	UE	203	PEB	C4A-C3A-CAA-CBA
26	UE	203	PEB	NB-C1B-CHA-C4A
26	UE	203	PEB	C2B-C1B-CHA-C4A
26	VE	201	PEB	C2A-C3A-CAA-CBA
26	VE	201	PEB	C4A-C3A-CAA-CBA
26	VE	201	PEB	NB-C1B-CHA-C4A
26	VE	201	PEB	C2B-C1B-CHA-C4A
26	VE	202	PEB	ND-C1D-CHC-C4C
26	VE	202	PEB	C2D-C1D-CHC-C4C
26	VE	202	PEB	NC-C1C-CHB-C4B
26	VE	202	PEB	C2C-C1C-CHB-C4B
26	VE	202	PEB	C2C-CAC-CBC-CGC
26	VE	202	PEB	NB-C1B-CHA-C4A
26	VE	202	PEB	C2B-C1B-CHA-C4A
26	WE	201	PEB	C2D-C3D-CAD-CBD
26	WE	201	PEB	C4D-C3D-CAD-CBD
26	WE	201	PEB	C2A-C3A-CAA-CBA
26	WE	201	PEB	C4A-C3A-CAA-CBA
26	WE	201	PEB	NB-C1B-CHA-C4A
26	WE	201	PEB	C2B-C1B-CHA-C4A
26	WE	202	PEB	C2A-C3A-CAA-CBA
26	WE	202	PEB	C4A-C3A-CAA-CBA
26	WE	202	PEB	NB-C1B-CHA-C4A
26	WE	202	PEB	C2B-C1B-CHA-C4A
26	WE	203	PEB	NC-C1C-CHB-C4B
26	WE	203	PEB	C2C-C1C-CHB-C4B
26	WE	203	PEB	C2C-CAC-CBC-CGC
26	WE	203	PEB	NB-C1B-CHA-C4A
26	WE	203	PEB	C2B-C1B-CHA-C4A
26	XE	201	PEB	NB-C1B-CHA-C4A
26	XE	201	PEB	C2B-C1B-CHA-C4A
26	XE	202	PEB	ND-C1D-CHC-C4C
26	XE	202	PEB	C2D-C1D-CHC-C4C
26	XE	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	XE	202	PEB	C2C-C1C-CHB-C4B
26	XE	202	PEB	C2C-CAC-CBC-CGC
26	XE	202	PEB	NB-C1B-CHA-C4A
26	XE	202	PEB	C2B-C1B-CHA-C4A
26	YE	201	PEB	ND-C1D-CHC-C4C
26	YE	201	PEB	C2A-C3A-CAA-CBA
26	YE	201	PEB	C4A-C3A-CAA-CBA
26	YE	201	PEB	NB-C1B-CHA-C4A
26	YE	201	PEB	C2B-C1B-CHA-C4A
26	YE	202	PEB	NC-C1C-CHB-C4B
26	YE	202	PEB	C2C-C1C-CHB-C4B
26	YE	202	PEB	NB-C1B-CHA-C4A
26	YE	202	PEB	C2B-C1B-CHA-C4A
26	YE	203	PEB	NC-C1C-CHB-C4B
26	YE	203	PEB	C2C-C1C-CHB-C4B
26	YE	203	PEB	C4A-C3A-CAA-CBA
26	YE	203	PEB	NB-C1B-CHA-C4A
26	YE	203	PEB	C2B-C1B-CHA-C4A
26	ZE	201	PEB	ND-C1D-CHC-C4C
26	ZE	201	PEB	C2D-C1D-CHC-C4C
26	ZE	201	PEB	C2A-C3A-CAA-CBA
26	ZE	201	PEB	C4A-C3A-CAA-CBA
26	ZE	201	PEB	NB-C1B-CHA-C4A
26	ZE	201	PEB	C2B-C1B-CHA-C4A
26	ZE	202	PEB	ND-C1D-CHC-C4C
26	ZE	202	PEB	C2D-C1D-CHC-C4C
26	ZE	202	PEB	NC-C1C-CHB-C4B
26	ZE	202	PEB	C2C-C1C-CHB-C4B
26	ZE	202	PEB	NB-C1B-CHA-C4A
26	ZE	202	PEB	C2B-C1B-CHA-C4A
26	aE	201	PEB	NB-C1B-CHA-C4A
26	aE	201	PEB	C2B-C1B-CHA-C4A
26	aE	202	PEB	C2A-C3A-CAA-CBA
26	aE	202	PEB	C4A-C3A-CAA-CBA
26	aE	202	PEB	NB-C1B-CHA-C4A
26	aE	202	PEB	C2B-C1B-CHA-C4A
26	aE	203	PEB	NC-C1C-CHB-C4B
26	aE	203	PEB	C2C-C1C-CHB-C4B
26	aE	203	PEB	C2C-CAC-CBC-CGC
26	aE	203	PEB	NB-C1B-CHA-C4A
26	aE	203	PEB	C2B-C1B-CHA-C4A
26	bE	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	bE	201	PEB	C4A-C3A-CAA-CBA
26	bE	201	PEB	NB-C1B-CHA-C4A
26	bE	201	PEB	C2B-C1B-CHA-C4A
26	bE	202	PEB	ND-C1D-CHC-C4C
26	bE	202	PEB	C2D-C1D-CHC-C4C
26	bE	202	PEB	NC-C1C-CHB-C4B
26	bE	202	PEB	C2C-C1C-CHB-C4B
26	bE	202	PEB	NB-C1B-CHA-C4A
26	bE	202	PEB	C2B-C1B-CHA-C4A
26	cE	201	PEB	ND-C1D-CHC-C4C
26	cE	201	PEB	C2C-CAC-CBC-CGC
26	cE	201	PEB	C2A-C3A-CAA-CBA
26	cE	201	PEB	C4A-C3A-CAA-CBA
26	cE	201	PEB	NB-C1B-CHA-C4A
26	cE	201	PEB	C2B-C1B-CHA-C4A
26	cE	202	PEB	NC-C1C-CHB-C4B
26	cE	202	PEB	C2C-C1C-CHB-C4B
26	cE	202	PEB	C2C-CAC-CBC-CGC
26	cE	202	PEB	NB-C1B-CHA-C4A
26	cE	202	PEB	C2B-C1B-CHA-C4A
26	cE	203	PEB	ND-C1D-CHC-C4C
26	cE	203	PEB	C2D-C1D-CHC-C4C
26	cE	203	PEB	C2A-C3A-CAA-CBA
26	cE	203	PEB	NB-C1B-CHA-C4A
26	dE	201	PEB	NB-C1B-CHA-C4A
26	dE	201	PEB	C2B-C1B-CHA-C4A
26	dE	202	PEB	ND-C1D-CHC-C4C
26	dE	202	PEB	C2D-C1D-CHC-C4C
26	dE	202	PEB	NC-C1C-CHB-C4B
26	dE	202	PEB	C2C-C1C-CHB-C4B
26	dE	202	PEB	C2C-CAC-CBC-CGC
26	dE	202	PEB	NB-C1B-CHA-C4A
26	dE	202	PEB	C2B-C1B-CHA-C4A
26	eE	201	PEB	NC-C1C-CHB-C4B
26	eE	201	PEB	C2C-C1C-CHB-C4B
26	eE	201	PEB	NB-C1B-CHA-C4A
26	eE	201	PEB	C2B-C1B-CHA-C4A
26	eE	202	PEB	ND-C1D-CHC-C4C
26	eE	202	PEB	C2D-C1D-CHC-C4C
26	eE	202	PEB	C2A-C3A-CAA-CBA
26	eE	202	PEB	C4A-C3A-CAA-CBA
26	eE	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	eE	202	PEB	C2B-C1B-CHA-C4A
26	eE	203	PEB	NC-C1C-CHB-C4B
26	eE	203	PEB	C2C-C1C-CHB-C4B
26	fE	201	PEB	NC-C1C-CHB-C4B
26	fE	201	PEB	C4A-C3A-CAA-CBA
26	fE	201	PEB	NB-C1B-CHA-C4A
26	fE	201	PEB	C2B-C1B-CHA-C4A
26	fE	202	PEB	ND-C1D-CHC-C4C
26	fE	202	PEB	NC-C1C-CHB-C4B
26	fE	202	PEB	C2C-C1C-CHB-C4B
26	fE	202	PEB	NB-C1B-CHA-C4A
26	fE	202	PEB	C2B-C1B-CHA-C4A
26	gE	201	PEB	NC-C1C-CHB-C4B
26	gE	201	PEB	C2C-C1C-CHB-C4B
26	gE	202	PEB	NC-C1C-CHB-C4B
26	gE	202	PEB	C2C-C1C-CHB-C4B
26	gE	202	PEB	C2C-CAC-CBC-CGC
26	gE	202	PEB	NB-C1B-CHA-C4A
26	gE	202	PEB	C2B-C1B-CHA-C4A
26	gE	203	PEB	NC-C1C-CHB-C4B
26	gE	203	PEB	C2C-C1C-CHB-C4B
26	gE	203	PEB	C2A-C3A-CAA-CBA
26	gE	203	PEB	NB-C1B-CHA-C4A
26	gE	203	PEB	C2B-C1B-CHA-C4A
26	hE	201	PEB	NC-C1C-CHB-C4B
26	hE	201	PEB	C2C-C1C-CHB-C4B
26	hE	201	PEB	NB-C1B-CHA-C4A
26	hE	201	PEB	C2B-C1B-CHA-C4A
26	hE	202	PEB	ND-C1D-CHC-C4C
26	hE	202	PEB	C2D-C1D-CHC-C4C
26	hE	202	PEB	NC-C1C-CHB-C4B
26	hE	202	PEB	C2C-C1C-CHB-C4B
26	hE	202	PEB	NB-C1B-CHA-C4A
26	hE	202	PEB	C2B-C1B-CHA-C4A
26	iE	201	PEB	C2A-C3A-CAA-CBA
26	iE	201	PEB	C4A-C3A-CAA-CBA
26	iE	201	PEB	NB-C1B-CHA-C4A
26	iE	201	PEB	C2B-C1B-CHA-C4A
26	iE	202	PEB	ND-C1D-CHC-C4C
26	iE	202	PEB	C2D-C1D-CHC-C4C
26	iE	202	PEB	C4A-C3A-CAA-CBA
26	iE	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	iE	202	PEB	C2B-C1B-CHA-C4A
26	iE	203	PEB	NC-C1C-CHB-C4B
26	iE	203	PEB	C2C-C1C-CHB-C4B
26	iE	203	PEB	C2C-CAC-CBC-CGC
26	iE	203	PEB	NB-C1B-CHA-C4A
26	iE	203	PEB	C2B-C1B-CHA-C4A
26	jE	201	PEB	NB-C1B-CHA-C4A
26	jE	201	PEB	C2B-C1B-CHA-C4A
26	jE	202	PEB	ND-C1D-CHC-C4C
26	jE	202	PEB	C2D-C1D-CHC-C4C
26	jE	202	PEB	NC-C1C-CHB-C4B
26	jE	202	PEB	C2C-C1C-CHB-C4B
26	jE	202	PEB	NB-C1B-CHA-C4A
26	jE	202	PEB	C2B-C1B-CHA-C4A
26	kE	201	PEB	ND-C1D-CHC-C4C
26	kE	201	PEB	C2D-C1D-CHC-C4C
26	kE	201	PEB	NC-C1C-CHB-C4B
26	kE	201	PEB	C2C-C1C-CHB-C4B
26	kE	201	PEB	NB-C1B-CHA-C4A
26	kE	201	PEB	C2B-C1B-CHA-C4A
26	kE	202	PEB	NC-C1C-CHB-C4B
26	kE	202	PEB	C2C-C1C-CHB-C4B
26	kE	202	PEB	C2C-CAC-CBC-CGC
26	kE	202	PEB	NB-C1B-CHA-C4A
26	kE	202	PEB	C2B-C1B-CHA-C4A
26	kE	203	PEB	NB-C1B-CHA-C4A
26	kE	203	PEB	C2B-C1B-CHA-C4A
26	lE	201	PEB	NB-C1B-CHA-C4A
26	lE	201	PEB	C2B-C1B-CHA-C4A
26	lE	201	PEB	C2B-C3B-CAB-CBB
26	lE	201	PEB	C4B-C3B-CAB-CBB
26	lE	201	PEB	C3B-CAB-CBB-CGB
26	lE	202	PEB	ND-C1D-CHC-C4C
26	lE	202	PEB	C2D-C1D-CHC-C4C
26	lE	202	PEB	NC-C1C-CHB-C4B
26	lE	202	PEB	C2C-C1C-CHB-C4B
26	lE	202	PEB	C4A-C3A-CAA-CBA
26	lE	202	PEB	NB-C1B-CHA-C4A
26	lE	202	PEB	C2B-C1B-CHA-C4A
26	mE	201	PEB	NB-C1B-CHA-C4A
26	mE	201	PEB	C2B-C1B-CHA-C4A
26	mE	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	mE	202	PEB	C2D-C1D-CHC-C4C
26	mE	202	PEB	NC-C1C-CHB-C4B
26	mE	202	PEB	C2C-C1C-CHB-C4B
26	mE	202	PEB	C2A-C3A-CAA-CBA
26	mE	202	PEB	C4A-C3A-CAA-CBA
26	mE	202	PEB	NB-C1B-CHA-C4A
26	mE	202	PEB	C2B-C1B-CHA-C4A
26	mE	203	PEB	ND-C1D-CHC-C4C
26	mE	203	PEB	NC-C1C-CHB-C4B
26	mE	203	PEB	C2C-C1C-CHB-C4B
26	mE	203	PEB	C2C-CAC-CBC-CGC
26	mE	203	PEB	NB-C1B-CHA-C4A
26	mE	203	PEB	C2B-C1B-CHA-C4A
26	nE	201	PEB	NC-C1C-CHB-C4B
26	nE	201	PEB	C2C-C1C-CHB-C4B
26	nE	201	PEB	NB-C1B-CHA-C4A
26	nE	202	PEB	ND-C1D-CHC-C4C
26	nE	202	PEB	C2D-C1D-CHC-C4C
26	nE	202	PEB	NC-C1C-CHB-C4B
26	nE	202	PEB	C2C-C1C-CHB-C4B
26	nE	202	PEB	C2C-CAC-CBC-CGC
26	nE	202	PEB	NB-C1B-CHA-C4A
26	nE	202	PEB	C2B-C1B-CHA-C4A
26	oE	201	PEB	ND-C1D-CHC-C4C
26	oE	201	PEB	NC-C1C-CHB-C4B
26	oE	201	PEB	C2C-C1C-CHB-C4B
26	oE	202	PEB	NB-C1B-CHA-C4A
26	oE	202	PEB	C2B-C1B-CHA-C4A
26	oE	203	PEB	NC-C1C-CHB-C4B
26	oE	203	PEB	C2C-C1C-CHB-C4B
26	oE	203	PEB	C2D-C3D-CAD-CBD
26	oE	203	PEB	C4D-C3D-CAD-CBD
26	oE	203	PEB	NB-C1B-CHA-C4A
26	pE	201	PEB	NC-C1C-CHB-C4B
26	pE	201	PEB	C2C-C1C-CHB-C4B
26	pE	201	PEB	C2A-C3A-CAA-CBA
26	pE	201	PEB	C4A-C3A-CAA-CBA
26	pE	201	PEB	NB-C1B-CHA-C4A
26	pE	201	PEB	C2B-C1B-CHA-C4A
26	pE	202	PEB	ND-C1D-CHC-C4C
26	pE	202	PEB	C2D-C1D-CHC-C4C
26	pE	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	pE	202	PEB	C2C-C1C-CHB-C4B
26	pE	202	PEB	C2C-CAC-CBC-CGC
26	pE	202	PEB	NB-C1B-CHA-C4A
26	pE	202	PEB	C2B-C1B-CHA-C4A
26	qE	201	PEB	NC-C1C-CHB-C4B
26	qE	201	PEB	C2C-C1C-CHB-C4B
26	qE	201	PEB	C4A-C3A-CAA-CBA
26	qE	201	PEB	NB-C1B-CHA-C4A
26	qE	201	PEB	C2B-C1B-CHA-C4A
26	qE	202	PEB	C4A-C3A-CAA-CBA
26	qE	202	PEB	NB-C1B-CHA-C4A
26	qE	202	PEB	C2B-C1B-CHA-C4A
26	qE	203	PEB	NC-C1C-CHB-C4B
26	qE	203	PEB	C2C-C1C-CHB-C4B
26	qE	203	PEB	NB-C1B-CHA-C4A
26	qE	203	PEB	C2B-C1B-CHA-C4A
26	rE	201	PEB	C2A-C3A-CAA-CBA
26	rE	201	PEB	C4A-C3A-CAA-CBA
26	rE	201	PEB	NB-C1B-CHA-C4A
26	rE	201	PEB	C2B-C1B-CHA-C4A
26	rE	202	PEB	ND-C1D-CHC-C4C
26	rE	202	PEB	C2D-C1D-CHC-C4C
26	rE	202	PEB	NC-C1C-CHB-C4B
26	rE	202	PEB	C2C-C1C-CHB-C4B
26	rE	202	PEB	NB-C1B-CHA-C4A
26	rE	202	PEB	C2B-C1B-CHA-C4A
26	sE	201	PEB	ND-C1D-CHC-C4C
26	sE	201	PEB	C2D-C1D-CHC-C4C
26	sE	201	PEB	C2C-CAC-CBC-CGC
26	sE	201	PEB	C4A-C3A-CAA-CBA
26	sE	201	PEB	NB-C1B-CHA-C4A
26	sE	201	PEB	C2B-C1B-CHA-C4A
26	sE	202	PEB	NC-C1C-CHB-C4B
26	sE	202	PEB	C2C-C1C-CHB-C4B
26	sE	202	PEB	C2C-CAC-CBC-CGC
26	sE	202	PEB	NB-C1B-CHA-C4A
26	sE	202	PEB	C2B-C1B-CHA-C4A
26	sE	203	PEB	C2A-C3A-CAA-CBA
26	sE	203	PEB	C4A-C3A-CAA-CBA
26	sE	203	PEB	NB-C1B-CHA-C4A
26	sE	203	PEB	C2B-C1B-CHA-C4A
26	tE	201	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	tE	201	PEB	C2C-CAC-CBC-CGC
26	tE	201	PEB	NB-C1B-CHA-C4A
26	tE	201	PEB	C2B-C1B-CHA-C4A
26	tE	202	PEB	ND-C1D-CHC-C4C
26	tE	202	PEB	C2D-C1D-CHC-C4C
26	tE	202	PEB	NC-C1C-CHB-C4B
26	tE	202	PEB	C2C-C1C-CHB-C4B
26	tE	202	PEB	NB-C1B-CHA-C4A
26	tE	202	PEB	C2B-C1B-CHA-C4A
26	uE	201	PEB	NC-C1C-CHB-C4B
26	uE	201	PEB	C2C-C1C-CHB-C4B
26	uE	201	PEB	C2C-CAC-CBC-CGC
26	uE	201	PEB	C2A-C3A-CAA-CBA
26	uE	201	PEB	C4A-C3A-CAA-CBA
26	uE	201	PEB	NB-C1B-CHA-C4A
26	uE	201	PEB	C2B-C1B-CHA-C4A
26	uE	202	PEB	ND-C1D-CHC-C4C
26	uE	202	PEB	C4A-C3A-CAA-CBA
26	uE	202	PEB	NB-C1B-CHA-C4A
26	uE	202	PEB	C2B-C1B-CHA-C4A
26	uE	203	PEB	NC-C1C-CHB-C4B
26	uE	203	PEB	C2C-C1C-CHB-C4B
26	uE	203	PEB	NB-C1B-CHA-C4A
26	uE	203	PEB	C2B-C1B-CHA-C4A
26	vE	201	PEB	NC-C1C-CHB-C4B
26	vE	201	PEB	C2C-C1C-CHB-C4B
26	vE	201	PEB	NB-C1B-CHA-C4A
26	vE	201	PEB	C2B-C1B-CHA-C4A
26	vE	202	PEB	ND-C1D-CHC-C4C
26	vE	202	PEB	NC-C1C-CHB-C4B
26	vE	202	PEB	C2C-C1C-CHB-C4B
26	vE	202	PEB	C2C-CAC-CBC-CGC
26	vE	202	PEB	NB-C1B-CHA-C4A
26	vE	202	PEB	C2B-C1B-CHA-C4A
26	wE	301	PEB	NC-C1C-CHB-C4B
26	wE	301	PEB	C2C-C1C-CHB-C4B
26	wE	301	PEB	C2A-C3A-CAA-CBA
26	wE	301	PEB	NB-C1B-CHA-C4A
26	wE	301	PEB	C2B-C1B-CHA-C4A
26	wE	302	PEB	C2A-C3A-CAA-CBA
26	wE	302	PEB	C4A-C3A-CAA-CBA
26	wE	302	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	wE	302	PEB	C2B-C1B-CHA-C4A
26	wE	303	PEB	NB-C1B-CHA-C4A
26	wE	303	PEB	C2B-C1B-CHA-C4A
26	xE	302	PEB	ND-C1D-CHC-C4C
26	xE	302	PEB	NC-C1C-CHB-C4B
26	xE	302	PEB	C2C-C1C-CHB-C4B
26	xE	302	PEB	C4A-C3A-CAA-CBA
26	xE	302	PEB	NB-C1B-CHA-C4A
26	xE	302	PEB	C2B-C1B-CHA-C4A
26	xE	303	PEB	ND-C1D-CHC-C4C
26	xE	303	PEB	C2D-C1D-CHC-C4C
26	xE	303	PEB	C4A-C3A-CAA-CBA
26	xE	303	PEB	NB-C1B-CHA-C4A
26	xE	303	PEB	C2B-C1B-CHA-C4A
26	xE	304	PEB	NC-C1C-CHB-C4B
26	xE	304	PEB	C2C-C1C-CHB-C4B
26	xE	304	PEB	NB-C1B-CHA-C4A
26	xE	304	PEB	C2B-C1B-CHA-C4A
26	yE	301	PEB	C4A-C3A-CAA-CBA
26	yE	301	PEB	NB-C1B-CHA-C4A
26	yE	301	PEB	C2B-C1B-CHA-C4A
26	zE	501	PEB	NB-C1B-CHA-C4A
26	zE	501	PEB	C2B-C1B-CHA-C4A
26	AF	301	PEB	NB-C1B-CHA-C4A
26	AF	301	PEB	C2B-C1B-CHA-C4A
26	AF	302	PEB	C4A-C3A-CAA-CBA
26	AF	302	PEB	NB-C1B-CHA-C4A
26	AF	302	PEB	C2B-C1B-CHA-C4A
26	AF	305	PEB	ND-C1D-CHC-C4C
26	AF	305	PEB	C2D-C1D-CHC-C4C
26	AF	305	PEB	NC-C1C-CHB-C4B
26	AF	305	PEB	C2C-C1C-CHB-C4B
26	AF	305	PEB	C2A-C3A-CAA-CBA
26	AF	305	PEB	C4A-C3A-CAA-CBA
26	AF	305	PEB	NB-C1B-CHA-C4A
26	AF	305	PEB	C2B-C1B-CHA-C4A
26	DF	1002	PEB	ND-C1D-CHC-C4C
26	DF	1002	PEB	C2D-C1D-CHC-C4C
26	DF	1002	PEB	C2A-C3A-CAA-CBA
26	DF	1002	PEB	C4A-C3A-CAA-CBA
26	DF	1002	PEB	NB-C1B-CHA-C4A
26	DF	1002	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	FF	1002	PEB	C4A-C3A-CAA-CBA
26	FF	1002	PEB	NB-C1B-CHA-C4A
26	FF	1002	PEB	C2B-C1B-CHA-C4A
26	HF	1002	PEB	C4A-C3A-CAA-CBA
26	HF	1002	PEB	NB-C1B-CHA-C4A
26	HF	1002	PEB	C2B-C1B-CHA-C4A
26	JF	1002	PEB	NB-C1B-CHA-C4A
26	JF	1002	PEB	C2B-C1B-CHA-C4A
26	LF	1002	PEB	C2A-C3A-CAA-CBA
26	LF	1002	PEB	C4A-C3A-CAA-CBA
26	LF	1002	PEB	NB-C1B-CHA-C4A
26	LF	1002	PEB	C2B-C1B-CHA-C4A
26	LF	1002	PEB	C3B-CAB-CBB-CGB
26	NF	1002	PEB	C2A-C3A-CAA-CBA
26	NF	1002	PEB	C4A-C3A-CAA-CBA
26	NF	1002	PEB	NB-C1B-CHA-C4A
26	NF	1002	PEB	C2B-C1B-CHA-C4A
26	OF	201	PEB	ND-C1D-CHC-C4C
26	OF	201	PEB	C2D-C1D-CHC-C4C
26	OF	201	PEB	C2A-C3A-CAA-CBA
26	OF	201	PEB	C4A-C3A-CAA-CBA
26	OF	201	PEB	NB-C1B-CHA-C4A
26	OF	201	PEB	C2B-C1B-CHA-C4A
26	OF	202	PEB	NB-C1B-CHA-C4A
26	OF	202	PEB	C2B-C1B-CHA-C4A
26	OF	203	PEB	C2C-CAC-CBC-CGC
26	OF	203	PEB	C2A-C3A-CAA-CBA
26	OF	203	PEB	NB-C1B-CHA-C4A
26	OF	203	PEB	C2B-C1B-CHA-C4A
26	PF	201	PEB	NB-C1B-CHA-C4A
26	PF	201	PEB	C2B-C1B-CHA-C4A
26	PF	202	PEB	NB-C1B-CHA-C4A
26	PF	202	PEB	C2B-C1B-CHA-C4A
26	QF	201	PEB	NB-C1B-CHA-C4A
26	QF	201	PEB	C2B-C1B-CHA-C4A
26	QF	202	PEB	NC-C1C-CHB-C4B
26	QF	202	PEB	C2C-C1C-CHB-C4B
26	QF	202	PEB	C2A-C3A-CAA-CBA
26	QF	202	PEB	C4A-C3A-CAA-CBA
26	QF	203	PEB	C2C-CAC-CBC-CGC
26	QF	203	PEB	NB-C1B-CHA-C4A
26	QF	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	QF	203	PEB	C3B-CAB-CBB-CGB
26	RF	201	PEB	C2A-C3A-CAA-CBA
26	RF	201	PEB	C4A-C3A-CAA-CBA
26	RF	201	PEB	NB-C1B-CHA-C4A
26	RF	201	PEB	C2B-C1B-CHA-C4A
26	RF	202	PEB	ND-C1D-CHC-C4C
26	RF	202	PEB	C2D-C1D-CHC-C4C
26	RF	202	PEB	NC-C1C-CHB-C4B
26	RF	202	PEB	C2C-C1C-CHB-C4B
26	RF	202	PEB	NB-C1B-CHA-C4A
26	RF	202	PEB	C2B-C1B-CHA-C4A
26	SF	201	PEB	NB-C1B-CHA-C4A
26	SF	201	PEB	C2B-C1B-CHA-C4A
26	SF	202	PEB	NB-C1B-CHA-C4A
26	SF	202	PEB	C2B-C1B-CHA-C4A
26	TF	201	PEB	ND-C1D-CHC-C4C
26	TF	201	PEB	C2D-C1D-CHC-C4C
26	TF	201	PEB	NB-C1B-CHA-C4A
26	TF	201	PEB	C2B-C1B-CHA-C4A
26	TF	202	PEB	ND-C1D-CHC-C4C
26	TF	202	PEB	C2D-C1D-CHC-C4C
26	TF	202	PEB	NC-C1C-CHB-C4B
26	TF	202	PEB	C2C-C1C-CHB-C4B
26	TF	202	PEB	C4D-C3D-CAD-CBD
26	TF	202	PEB	NB-C1B-CHA-C4A
26	TF	202	PEB	C2B-C1B-CHA-C4A
26	UF	201	PEB	C2A-C3A-CAA-CBA
26	UF	201	PEB	C4A-C3A-CAA-CBA
26	UF	201	PEB	NB-C1B-CHA-C4A
26	UF	201	PEB	C2B-C1B-CHA-C4A
26	UF	202	PEB	C4A-C3A-CAA-CBA
26	UF	202	PEB	NB-C1B-CHA-C4A
26	UF	202	PEB	C2B-C1B-CHA-C4A
26	UF	203	PEB	C2A-C3A-CAA-CBA
26	UF	203	PEB	NB-C1B-CHA-C4A
26	UF	203	PEB	C2B-C1B-CHA-C4A
26	VF	201	PEB	NB-C1B-CHA-C4A
26	VF	202	PEB	NB-C1B-CHA-C4A
26	VF	202	PEB	C2B-C1B-CHA-C4A
26	VF	203	PEB	ND-C1D-CHC-C4C
26	VF	203	PEB	C2D-C1D-CHC-C4C
26	VF	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	VF	203	PEB	C2C-C1C-CHB-C4B
26	VF	203	PEB	NB-C1B-CHA-C4A
26	VF	203	PEB	C2B-C1B-CHA-C4A
26	WF	201	PEB	ND-C1D-CHC-C4C
26	WF	201	PEB	C2D-C1D-CHC-C4C
26	WF	201	PEB	C4A-C3A-CAA-CBA
26	WF	201	PEB	NB-C1B-CHA-C4A
26	WF	201	PEB	C2B-C1B-CHA-C4A
26	WF	202	PEB	NB-C1B-CHA-C4A
26	WF	202	PEB	C2B-C1B-CHA-C4A
26	WF	203	PEB	C2A-C3A-CAA-CBA
26	WF	203	PEB	NB-C1B-CHA-C4A
26	WF	203	PEB	C2B-C1B-CHA-C4A
26	YF	201	PEB	C2A-C3A-CAA-CBA
26	YF	201	PEB	C4A-C3A-CAA-CBA
26	YF	201	PEB	NB-C1B-CHA-C4A
26	YF	201	PEB	C2B-C1B-CHA-C4A
26	YF	202	PEB	NB-C1B-CHA-C4A
26	YF	202	PEB	C2B-C1B-CHA-C4A
26	ZF	201	PEB	C2A-C3A-CAA-CBA
26	ZF	201	PEB	C4A-C3A-CAA-CBA
26	ZF	201	PEB	NB-C1B-CHA-C4A
26	ZF	201	PEB	C2B-C1B-CHA-C4A
26	ZF	202	PEB	ND-C1D-CHC-C4C
26	ZF	202	PEB	C2D-C1D-CHC-C4C
26	ZF	202	PEB	C2A-C3A-CAA-CBA
26	ZF	202	PEB	C4A-C3A-CAA-CBA
26	ZF	202	PEB	NB-C1B-CHA-C4A
26	ZF	202	PEB	C2B-C1B-CHA-C4A
26	ZF	203	PEB	NB-C1B-CHA-C4A
26	ZF	203	PEB	C2B-C1B-CHA-C4A
26	aF	201	PEB	NB-C1B-CHA-C4A
26	aF	201	PEB	C2B-C1B-CHA-C4A
26	aF	202	PEB	ND-C1D-CHC-C4C
26	aF	202	PEB	C2D-C1D-CHC-C4C
26	aF	202	PEB	C2C-CAC-CBC-CGC
26	aF	202	PEB	NB-C1B-CHA-C4A
26	aF	202	PEB	C2B-C1B-CHA-C4A
26	bF	201	PEB	ND-C1D-CHC-C4C
26	bF	201	PEB	C2D-C1D-CHC-C4C
26	bF	201	PEB	NB-C1B-CHA-C4A
26	bF	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bF	202	PEB	NB-C1B-CHA-C4A
26	bF	202	PEB	C2B-C1B-CHA-C4A
26	bF	203	PEB	C4A-C3A-CAA-CBA
26	bF	203	PEB	NB-C1B-CHA-C4A
26	bF	203	PEB	C2B-C1B-CHA-C4A
26	cF	201	PEB	C2A-C3A-CAA-CBA
26	cF	201	PEB	C4A-C3A-CAA-CBA
26	cF	201	PEB	NB-C1B-CHA-C4A
26	cF	201	PEB	C2B-C1B-CHA-C4A
26	cF	202	PEB	NC-C1C-CHB-C4B
26	cF	202	PEB	C2C-C1C-CHB-C4B
26	cF	202	PEB	C4A-C3A-CAA-CBA
26	cF	202	PEB	NB-C1B-CHA-C4A
26	dF	201	PEB	NC-C1C-CHB-C4B
26	dF	201	PEB	C2C-C1C-CHB-C4B
26	dF	201	PEB	NB-C1B-CHA-C4A
26	dF	201	PEB	C2B-C1B-CHA-C4A
26	dF	202	PEB	ND-C1D-CHC-C4C
26	dF	202	PEB	C4A-C3A-CAA-CBA
26	dF	202	PEB	NB-C1B-CHA-C4A
26	dF	202	PEB	C2B-C1B-CHA-C4A
26	dF	203	PEB	C2C-CAC-CBC-CGC
26	dF	203	PEB	C2A-C3A-CAA-CBA
26	dF	203	PEB	NB-C1B-CHA-C4A
26	dF	203	PEB	C2B-C1B-CHA-C4A
26	eF	201	PEB	ND-C1D-CHC-C4C
26	eF	201	PEB	NB-C1B-CHA-C4A
26	eF	201	PEB	C2B-C1B-CHA-C4A
26	eF	202	PEB	ND-C1D-CHC-C4C
26	eF	202	PEB	C2D-C1D-CHC-C4C
26	eF	202	PEB	NC-C1C-CHB-C4B
26	eF	202	PEB	C2C-C1C-CHB-C4B
26	eF	202	PEB	NB-C1B-CHA-C4A
26	eF	202	PEB	C2B-C1B-CHA-C4A
26	fF	201	PEB	ND-C1D-CHC-C4C
26	fF	201	PEB	C2D-C1D-CHC-C4C
26	fF	201	PEB	NB-C1B-CHA-C4A
26	fF	201	PEB	C2B-C1B-CHA-C4A
26	fF	202	PEB	C2C-CAC-CBC-CGC
26	fF	202	PEB	C2A-C3A-CAA-CBA
26	fF	202	PEB	NB-C1B-CHA-C4A
26	fF	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	fF	203	PEB	NC-C1C-CHB-C4B
26	fF	203	PEB	C2C-C1C-CHB-C4B
26	fF	203	PEB	C2C-CAC-CBC-CGC
26	fF	203	PEB	C2A-C3A-CAA-CBA
26	fF	203	PEB	NB-C1B-CHA-C4A
26	fF	203	PEB	C2B-C1B-CHA-C4A
26	gF	201	PEB	NC-C1C-CHB-C4B
26	gF	201	PEB	NB-C1B-CHA-C4A
26	gF	201	PEB	C2B-C1B-CHA-C4A
26	gF	202	PEB	NC-C1C-CHB-C4B
26	gF	202	PEB	C2C-C1C-CHB-C4B
26	gF	202	PEB	NB-C1B-CHA-C4A
26	gF	202	PEB	C2B-C1B-CHA-C4A
26	hF	201	PEB	C2C-CAC-CBC-CGC
26	hF	201	PEB	NB-C1B-CHA-C4A
26	hF	201	PEB	C2B-C1B-CHA-C4A
26	hF	202	PEB	ND-C1D-CHC-C4C
26	hF	202	PEB	C2A-C3A-CAA-CBA
26	hF	202	PEB	C4A-C3A-CAA-CBA
26	hF	202	PEB	NB-C1B-CHA-C4A
26	hF	202	PEB	C2B-C1B-CHA-C4A
26	hF	202	PEB	C3B-CAB-CBB-CGB
26	hF	203	PEB	NC-C1C-CHB-C4B
26	hF	203	PEB	NA-C4A-CHA-C1B
26	hF	203	PEB	C3A-C4A-CHA-C1B
26	hF	203	PEB	NB-C1B-CHA-C4A
26	hF	203	PEB	C2B-C1B-CHA-C4A
26	iF	201	PEB	NC-C1C-CHB-C4B
26	iF	201	PEB	NB-C1B-CHA-C4A
26	iF	201	PEB	C2B-C1B-CHA-C4A
26	iF	202	PEB	ND-C1D-CHC-C4C
26	iF	202	PEB	C2D-C1D-CHC-C4C
26	iF	202	PEB	NC-C1C-CHB-C4B
26	iF	202	PEB	C2C-C1C-CHB-C4B
26	iF	202	PEB	NB-C1B-CHA-C4A
26	iF	202	PEB	C2B-C1B-CHA-C4A
26	jF	201	PEB	ND-C1D-CHC-C4C
26	jF	201	PEB	C2D-C1D-CHC-C4C
26	jF	201	PEB	NB-C1B-CHA-C4A
26	jF	201	PEB	C2B-C1B-CHA-C4A
26	jF	202	PEB	NB-C1B-CHA-C4A
26	jF	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	jF	203	PEB	C2A-C3A-CAA-CBA
26	jF	203	PEB	NB-C1B-CHA-C4A
26	jF	203	PEB	C2B-C1B-CHA-C4A
26	kF	201	PEB	ND-C1D-CHC-C4C
26	kF	201	PEB	C4A-C3A-CAA-CBA
26	kF	201	PEB	NB-C1B-CHA-C4A
26	kF	201	PEB	C2B-C1B-CHA-C4A
26	kF	202	PEB	NC-C1C-CHB-C4B
26	kF	202	PEB	C2C-C1C-CHB-C4B
26	kF	202	PEB	C2C-CAC-CBC-CGC
26	kF	202	PEB	NB-C1B-CHA-C4A
26	kF	202	PEB	C2B-C1B-CHA-C4A
26	lF	201	PEB	NB-C1B-CHA-C4A
26	lF	201	PEB	C2B-C1B-CHA-C4A
26	lF	202	PEB	ND-C1D-CHC-C4C
26	lF	202	PEB	C2D-C1D-CHC-C4C
26	lF	202	PEB	C2D-C3D-CAD-CBD
26	lF	202	PEB	C4D-C3D-CAD-CBD
26	lF	202	PEB	NB-C1B-CHA-C4A
26	lF	202	PEB	C2B-C1B-CHA-C4A
26	lF	203	PEB	NC-C1C-CHB-C4B
26	lF	203	PEB	C2C-C1C-CHB-C4B
26	lF	203	PEB	C2A-C3A-CAA-CBA
26	lF	203	PEB	NB-C1B-CHA-C4A
26	lF	203	PEB	C2B-C1B-CHA-C4A
26	mF	201	PEB	NC-C1C-CHB-C4B
26	mF	201	PEB	C2C-C1C-CHB-C4B
26	mF	201	PEB	NB-C1B-CHA-C4A
26	mF	201	PEB	C2B-C1B-CHA-C4A
26	mF	202	PEB	NC-C1C-CHB-C4B
26	mF	202	PEB	C2C-C1C-CHB-C4B
26	mF	202	PEB	NB-C1B-CHA-C4A
26	mF	202	PEB	C2B-C1B-CHA-C4A
26	mF	202	PEB	C3B-CAB-CBB-CGB
26	AG	201	PEB	ND-C1D-CHC-C4C
26	AG	201	PEB	NB-C1B-CHA-C4A
26	AG	201	PEB	C2B-C1B-CHA-C4A
26	AG	202	PEB	NC-C1C-CHB-C4B
26	AG	202	PEB	C2C-C1C-CHB-C4B
26	AG	202	PEB	C2C-CAC-CBC-CGC
26	AG	202	PEB	C2A-C3A-CAA-CBA
26	AG	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	AG	202	PEB	NB-C1B-CHA-C4A
26	AG	202	PEB	C2B-C1B-CHA-C4A
26	BG	201	PEB	NC-C1C-CHB-C4B
26	BG	201	PEB	C2C-C1C-CHB-C4B
26	BG	201	PEB	NB-C1B-CHA-C4A
26	BG	201	PEB	C2B-C1B-CHA-C4A
26	BG	202	PEB	ND-C1D-CHC-C4C
26	BG	202	PEB	C2D-C1D-CHC-C4C
26	BG	202	PEB	NC-C1C-CHB-C4B
26	BG	202	PEB	C2C-C1C-CHB-C4B
26	BG	202	PEB	C2C-CAC-CBC-CGC
26	BG	202	PEB	C2A-C3A-CAA-CBA
26	BG	202	PEB	C4A-C3A-CAA-CBA
26	BG	202	PEB	NB-C1B-CHA-C4A
26	BG	202	PEB	C2B-C1B-CHA-C4A
26	CG	201	PEB	NB-C1B-CHA-C4A
26	CG	201	PEB	C2B-C1B-CHA-C4A
26	CG	202	PEB	C4A-C3A-CAA-CBA
26	CG	202	PEB	NB-C1B-CHA-C4A
26	CG	202	PEB	C2B-C1B-CHA-C4A
26	CG	203	PEB	NC-C1C-CHB-C4B
26	CG	203	PEB	C2C-C1C-CHB-C4B
26	CG	203	PEB	C2C-CAC-CBC-CGC
26	CG	203	PEB	NB-C1B-CHA-C4A
26	CG	203	PEB	C2B-C1B-CHA-C4A
26	DG	201	PEB	NB-C1B-CHA-C4A
26	DG	201	PEB	C2B-C1B-CHA-C4A
26	DG	202	PEB	C2D-C3D-CAD-CBD
26	DG	202	PEB	C4D-C3D-CAD-CBD
26	DG	202	PEB	C4A-C3A-CAA-CBA
26	DG	202	PEB	NB-C1B-CHA-C4A
26	DG	202	PEB	C2B-C1B-CHA-C4A
26	DG	203	PEB	ND-C1D-CHC-C4C
26	DG	203	PEB	C2D-C1D-CHC-C4C
26	DG	203	PEB	NC-C1C-CHB-C4B
26	DG	203	PEB	C2C-C1C-CHB-C4B
26	DG	203	PEB	NB-C1B-CHA-C4A
26	DG	203	PEB	C2B-C1B-CHA-C4A
26	EG	201	PEB	C2A-C3A-CAA-CBA
26	EG	201	PEB	C4A-C3A-CAA-CBA
26	EG	201	PEB	NB-C1B-CHA-C4A
26	EG	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	EG	202	PEB	NC-C1C-CHB-C4B
26	EG	202	PEB	C2C-C1C-CHB-C4B
26	EG	202	PEB	C2C-CAC-CBC-CGC
26	EG	202	PEB	NB-C1B-CHA-C4A
26	EG	202	PEB	C2B-C1B-CHA-C4A
26	FG	201	PEB	NB-C1B-CHA-C4A
26	FG	201	PEB	C2B-C1B-CHA-C4A
26	FG	202	PEB	ND-C1D-CHC-C4C
26	FG	202	PEB	C2D-C1D-CHC-C4C
26	FG	202	PEB	NC-C1C-CHB-C4B
26	FG	202	PEB	C2C-C1C-CHB-C4B
26	FG	202	PEB	C2C-CAC-CBC-CGC
26	FG	202	PEB	NB-C1B-CHA-C4A
26	FG	202	PEB	C2B-C1B-CHA-C4A
26	GG	201	PEB	C2A-C3A-CAA-CBA
26	GG	201	PEB	C4A-C3A-CAA-CBA
26	GG	201	PEB	NB-C1B-CHA-C4A
26	GG	201	PEB	C2B-C1B-CHA-C4A
26	GG	202	PEB	C2A-C3A-CAA-CBA
26	GG	202	PEB	C4A-C3A-CAA-CBA
26	GG	202	PEB	NB-C1B-CHA-C4A
26	GG	202	PEB	C2B-C1B-CHA-C4A
26	GG	203	PEB	C2C-CAC-CBC-CGC
26	GG	203	PEB	NB-C1B-CHA-C4A
26	GG	203	PEB	C2B-C1B-CHA-C4A
26	HG	201	PEB	C2A-C3A-CAA-CBA
26	HG	201	PEB	C4A-C3A-CAA-CBA
26	HG	201	PEB	NB-C1B-CHA-C4A
26	HG	201	PEB	C2B-C1B-CHA-C4A
26	HG	202	PEB	ND-C1D-CHC-C4C
26	HG	202	PEB	C2D-C1D-CHC-C4C
26	HG	202	PEB	NC-C1C-CHB-C4B
26	HG	202	PEB	C2C-C1C-CHB-C4B
26	HG	202	PEB	C2C-CAC-CBC-CGC
26	HG	202	PEB	NB-C1B-CHA-C4A
26	HG	202	PEB	C2B-C1B-CHA-C4A
26	IG	201	PEB	C4A-C3A-CAA-CBA
26	IG	201	PEB	NB-C1B-CHA-C4A
26	IG	201	PEB	C2B-C1B-CHA-C4A
26	IG	202	PEB	C2C-CAC-CBC-CGC
26	IG	202	PEB	C4A-C3A-CAA-CBA
26	IG	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	IG	202	PEB	C2B-C1B-CHA-C4A
26	IG	203	PEB	C4A-C3A-CAA-CBA
26	IG	203	PEB	NB-C1B-CHA-C4A
26	IG	203	PEB	C2B-C1B-CHA-C4A
26	JG	201	PEB	C2A-C3A-CAA-CBA
26	JG	201	PEB	NB-C1B-CHA-C4A
26	JG	201	PEB	C2B-C1B-CHA-C4A
26	JG	202	PEB	ND-C1D-CHC-C4C
26	JG	202	PEB	C2D-C1D-CHC-C4C
26	JG	202	PEB	NC-C1C-CHB-C4B
26	JG	202	PEB	C2C-C1C-CHB-C4B
26	JG	202	PEB	C4A-C3A-CAA-CBA
26	JG	202	PEB	NB-C1B-CHA-C4A
26	JG	202	PEB	C2B-C1B-CHA-C4A
26	KG	201	PEB	C4A-C3A-CAA-CBA
26	KG	201	PEB	NB-C1B-CHA-C4A
26	KG	201	PEB	C2B-C1B-CHA-C4A
26	KG	202	PEB	NB-C1B-CHA-C4A
26	KG	202	PEB	C2B-C1B-CHA-C4A
26	KG	203	PEB	C2C-CAC-CBC-CGC
26	KG	203	PEB	NB-C1B-CHA-C4A
26	KG	203	PEB	C2B-C1B-CHA-C4A
26	LG	201	PEB	C2A-C3A-CAA-CBA
26	LG	201	PEB	C4A-C3A-CAA-CBA
26	LG	201	PEB	NB-C1B-CHA-C4A
26	LG	201	PEB	C2B-C1B-CHA-C4A
26	LG	202	PEB	ND-C1D-CHC-C4C
26	LG	202	PEB	C2D-C1D-CHC-C4C
26	LG	202	PEB	NC-C1C-CHB-C4B
26	LG	202	PEB	C2C-C1C-CHB-C4B
26	LG	202	PEB	C1C-C2C-CAC-CBC
26	LG	202	PEB	C3C-C2C-CAC-CBC
26	LG	202	PEB	NB-C1B-CHA-C4A
26	LG	202	PEB	C2B-C1B-CHA-C4A
26	MG	201	PEB	ND-C1D-CHC-C4C
26	MG	201	PEB	C2D-C1D-CHC-C4C
26	MG	201	PEB	NB-C1B-CHA-C4A
26	MG	201	PEB	C2B-C1B-CHA-C4A
26	MG	202	PEB	NC-C1C-CHB-C4B
26	MG	202	PEB	C2C-C1C-CHB-C4B
26	MG	202	PEB	C2C-CAC-CBC-CGC
26	MG	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	MG	202	PEB	C2B-C1B-CHA-C4A
26	MG	203	PEB	C4A-C3A-CAA-CBA
26	MG	203	PEB	NB-C1B-CHA-C4A
26	MG	203	PEB	C2B-C1B-CHA-C4A
26	NG	201	PEB	NB-C1B-CHA-C4A
26	NG	201	PEB	C2B-C1B-CHA-C4A
26	NG	202	PEB	ND-C1D-CHC-C4C
26	NG	202	PEB	NC-C1C-CHB-C4B
26	NG	202	PEB	C2C-C1C-CHB-C4B
26	NG	202	PEB	NB-C1B-CHA-C4A
26	NG	202	PEB	C2B-C1B-CHA-C4A
26	OG	201	PEB	NB-C1B-CHA-C4A
26	OG	201	PEB	C2B-C1B-CHA-C4A
26	OG	202	PEB	ND-C1D-CHC-C4C
26	OG	202	PEB	NB-C1B-CHA-C4A
26	OG	202	PEB	C2B-C1B-CHA-C4A
26	OG	203	PEB	NC-C1C-CHB-C4B
26	OG	203	PEB	C2C-C1C-CHB-C4B
26	OG	203	PEB	NB-C1B-CHA-C4A
26	OG	203	PEB	C2B-C1B-CHA-C4A
26	PG	201	PEB	NB-C1B-CHA-C4A
26	PG	201	PEB	C2B-C1B-CHA-C4A
26	PG	202	PEB	ND-C1D-CHC-C4C
26	PG	202	PEB	NC-C1C-CHB-C4B
26	PG	202	PEB	C2C-C1C-CHB-C4B
26	PG	202	PEB	C2C-CAC-CBC-CGC
26	PG	202	PEB	NB-C1B-CHA-C4A
26	PG	202	PEB	C2B-C1B-CHA-C4A
26	QG	201	PEB	C2A-C3A-CAA-CBA
26	QG	201	PEB	C4A-C3A-CAA-CBA
26	QG	201	PEB	NB-C1B-CHA-C4A
26	QG	201	PEB	C2B-C1B-CHA-C4A
26	QG	202	PEB	C2C-CAC-CBC-CGC
26	QG	202	PEB	NB-C1B-CHA-C4A
26	QG	202	PEB	C2B-C1B-CHA-C4A
26	QG	203	PEB	NB-C1B-CHA-C4A
26	QG	203	PEB	C2B-C1B-CHA-C4A
26	RG	201	PEB	NB-C1B-CHA-C4A
26	RG	201	PEB	C2B-C1B-CHA-C4A
26	RG	202	PEB	ND-C1D-CHC-C4C
26	RG	202	PEB	C2D-C1D-CHC-C4C
26	RG	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	RG	202	PEB	C2C-C1C-CHB-C4B
26	RG	202	PEB	C2A-C3A-CAA-CBA
26	RG	202	PEB	C4A-C3A-CAA-CBA
26	RG	202	PEB	NB-C1B-CHA-C4A
26	RG	202	PEB	C2B-C1B-CHA-C4A
26	SG	201	PEB	C2A-C3A-CAA-CBA
26	SG	201	PEB	C4A-C3A-CAA-CBA
26	SG	201	PEB	NB-C1B-CHA-C4A
26	SG	201	PEB	C2B-C1B-CHA-C4A
26	SG	202	PEB	NB-C1B-CHA-C4A
26	SG	203	PEB	NC-C1C-CHB-C4B
26	SG	203	PEB	C2C-C1C-CHB-C4B
26	SG	203	PEB	C2C-CAC-CBC-CGC
26	SG	203	PEB	NB-C1B-CHA-C4A
26	SG	203	PEB	C2B-C1B-CHA-C4A
26	TG	201	PEB	NB-C1B-CHA-C4A
26	TG	201	PEB	C2B-C1B-CHA-C4A
26	TG	202	PEB	ND-C1D-CHC-C4C
26	TG	202	PEB	C2D-C1D-CHC-C4C
26	TG	202	PEB	NC-C1C-CHB-C4B
26	TG	202	PEB	C2C-C1C-CHB-C4B
26	TG	202	PEB	C2D-C3D-CAD-CBD
26	TG	202	PEB	C4D-C3D-CAD-CBD
26	TG	202	PEB	C4A-C3A-CAA-CBA
26	TG	202	PEB	NB-C1B-CHA-C4A
26	TG	202	PEB	C2B-C1B-CHA-C4A
26	UG	201	PEB	C4A-C3A-CAA-CBA
26	UG	201	PEB	NB-C1B-CHA-C4A
26	UG	201	PEB	C2B-C1B-CHA-C4A
26	UG	202	PEB	C2C-CAC-CBC-CGC
26	UG	202	PEB	C2A-C3A-CAA-CBA
26	UG	202	PEB	NB-C1B-CHA-C4A
26	UG	202	PEB	C2B-C1B-CHA-C4A
26	VG	201	PEB	C2A-C3A-CAA-CBA
26	VG	201	PEB	C4A-C3A-CAA-CBA
26	VG	201	PEB	NB-C1B-CHA-C4A
26	VG	201	PEB	C2B-C1B-CHA-C4A
26	VG	202	PEB	ND-C1D-CHC-C4C
26	VG	202	PEB	C2D-C1D-CHC-C4C
26	VG	202	PEB	NC-C1C-CHB-C4B
26	VG	202	PEB	C2C-C1C-CHB-C4B
26	VG	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	VG	202	PEB	NB-C1B-CHA-C4A
26	VG	202	PEB	C2B-C1B-CHA-C4A
26	WG	201	PEB	C2D-C3D-CAD-CBD
26	WG	201	PEB	C4D-C3D-CAD-CBD
26	WG	201	PEB	NB-C1B-CHA-C4A
26	WG	201	PEB	C2B-C1B-CHA-C4A
26	WG	202	PEB	C2A-C3A-CAA-CBA
26	WG	202	PEB	C4A-C3A-CAA-CBA
26	WG	202	PEB	NB-C1B-CHA-C4A
26	WG	202	PEB	C2B-C1B-CHA-C4A
26	WG	203	PEB	NC-C1C-CHB-C4B
26	WG	203	PEB	C2C-C1C-CHB-C4B
26	WG	203	PEB	C2C-CAC-CBC-CGC
26	WG	203	PEB	C2A-C3A-CAA-CBA
26	WG	203	PEB	NB-C1B-CHA-C4A
26	WG	203	PEB	C2B-C1B-CHA-C4A
26	XG	201	PEB	NB-C1B-CHA-C4A
26	XG	201	PEB	C2B-C1B-CHA-C4A
26	XG	202	PEB	C2A-C3A-CAA-CBA
26	XG	202	PEB	C4A-C3A-CAA-CBA
26	XG	202	PEB	NB-C1B-CHA-C4A
26	XG	202	PEB	C2B-C1B-CHA-C4A
26	XG	203	PEB	ND-C1D-CHC-C4C
26	XG	203	PEB	C2D-C1D-CHC-C4C
26	XG	203	PEB	NC-C1C-CHB-C4B
26	XG	203	PEB	C2C-C1C-CHB-C4B
26	XG	203	PEB	C2C-CAC-CBC-CGC
26	XG	203	PEB	NB-C1B-CHA-C4A
26	XG	203	PEB	C2B-C1B-CHA-C4A
26	YG	201	PEB	ND-C1D-CHC-C4C
26	YG	201	PEB	NB-C1B-CHA-C4A
26	YG	201	PEB	C2B-C1B-CHA-C4A
26	YG	202	PEB	NC-C1C-CHB-C4B
26	YG	202	PEB	C2C-C1C-CHB-C4B
26	YG	202	PEB	NB-C1B-CHA-C4A
26	YG	202	PEB	C2B-C1B-CHA-C4A
26	YG	203	PEB	NC-C1C-CHB-C4B
26	YG	203	PEB	C2C-C1C-CHB-C4B
26	YG	203	PEB	NB-C1B-CHA-C4A
26	YG	203	PEB	C2B-C1B-CHA-C4A
26	ZG	201	PEB	ND-C1D-CHC-C4C
26	ZG	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	ZG	201	PEB	NB-C1B-CHA-C4A
26	ZG	201	PEB	C2B-C1B-CHA-C4A
26	ZG	202	PEB	C2D-C1D-CHC-C4C
26	ZG	202	PEB	NC-C1C-CHB-C4B
26	ZG	202	PEB	C2C-C1C-CHB-C4B
26	ZG	202	PEB	NB-C1B-CHA-C4A
26	ZG	202	PEB	C2B-C1B-CHA-C4A
26	aG	201	PEB	C2A-C3A-CAA-CBA
26	aG	201	PEB	C4A-C3A-CAA-CBA
26	aG	201	PEB	NB-C1B-CHA-C4A
26	aG	201	PEB	C2B-C1B-CHA-C4A
26	aG	202	PEB	C2A-C3A-CAA-CBA
26	aG	202	PEB	C4A-C3A-CAA-CBA
26	aG	202	PEB	NB-C1B-CHA-C4A
26	aG	202	PEB	C2B-C1B-CHA-C4A
26	aG	203	PEB	NC-C1C-CHB-C4B
26	aG	203	PEB	C2C-C1C-CHB-C4B
26	aG	203	PEB	C2C-CAC-CBC-CGC
26	aG	203	PEB	C2A-C3A-CAA-CBA
26	aG	203	PEB	NB-C1B-CHA-C4A
26	aG	203	PEB	C2B-C1B-CHA-C4A
26	bG	201	PEB	C2A-C3A-CAA-CBA
26	bG	201	PEB	C4A-C3A-CAA-CBA
26	bG	201	PEB	NB-C1B-CHA-C4A
26	bG	201	PEB	C2B-C1B-CHA-C4A
26	bG	202	PEB	ND-C1D-CHC-C4C
26	bG	202	PEB	NC-C1C-CHB-C4B
26	bG	202	PEB	C2C-C1C-CHB-C4B
26	bG	202	PEB	NB-C1B-CHA-C4A
26	bG	202	PEB	C2B-C1B-CHA-C4A
26	cG	201	PEB	ND-C1D-CHC-C4C
26	cG	201	PEB	C2D-C1D-CHC-C4C
26	cG	201	PEB	NB-C1B-CHA-C4A
26	cG	201	PEB	C2B-C1B-CHA-C4A
26	cG	202	PEB	NC-C1C-CHB-C4B
26	cG	202	PEB	C2C-C1C-CHB-C4B
26	cG	202	PEB	C2C-CAC-CBC-CGC
26	cG	202	PEB	NB-C1B-CHA-C4A
26	cG	202	PEB	C2B-C1B-CHA-C4A
26	cG	203	PEB	C2A-C3A-CAA-CBA
26	cG	203	PEB	NB-C1B-CHA-C4A
26	cG	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dG	201	PEB	NC-C1C-CHB-C4B
26	dG	201	PEB	NB-C1B-CHA-C4A
26	dG	201	PEB	C2B-C1B-CHA-C4A
26	dG	202	PEB	ND-C1D-CHC-C4C
26	dG	202	PEB	C2D-C1D-CHC-C4C
26	dG	202	PEB	NC-C1C-CHB-C4B
26	dG	202	PEB	C2C-C1C-CHB-C4B
26	dG	202	PEB	NB-C1B-CHA-C4A
26	dG	202	PEB	C2B-C1B-CHA-C4A
26	eG	201	PEB	NC-C1C-CHB-C4B
26	eG	201	PEB	C2C-C1C-CHB-C4B
26	eG	201	PEB	C2C-CAC-CBC-CGC
26	eG	201	PEB	NB-C1B-CHA-C4A
26	eG	201	PEB	C2B-C1B-CHA-C4A
26	eG	202	PEB	ND-C1D-CHC-C4C
26	eG	202	PEB	C2D-C1D-CHC-C4C
26	eG	202	PEB	C4A-C3A-CAA-CBA
26	eG	202	PEB	NB-C1B-CHA-C4A
26	eG	202	PEB	C2B-C1B-CHA-C4A
26	eG	203	PEB	NC-C1C-CHB-C4B
26	eG	203	PEB	C2C-C1C-CHB-C4B
26	eG	203	PEB	C2C-CAC-CBC-CGC
26	eG	203	PEB	NB-C1B-CHA-C4A
26	eG	203	PEB	C2B-C1B-CHA-C4A
26	fG	201	PEB	NC-C1C-CHB-C4B
26	fG	201	PEB	C4A-C3A-CAA-CBA
26	fG	201	PEB	NB-C1B-CHA-C4A
26	fG	201	PEB	C2B-C1B-CHA-C4A
26	fG	202	PEB	ND-C1D-CHC-C4C
26	fG	202	PEB	NC-C1C-CHB-C4B
26	fG	202	PEB	C2C-C1C-CHB-C4B
26	fG	202	PEB	NB-C1B-CHA-C4A
26	fG	202	PEB	C2B-C1B-CHA-C4A
26	gG	201	PEB	NB-C1B-CHA-C4A
26	gG	202	PEB	NC-C1C-CHB-C4B
26	gG	202	PEB	C2C-C1C-CHB-C4B
26	gG	202	PEB	NB-C1B-CHA-C4A
26	gG	202	PEB	C2B-C1B-CHA-C4A
26	gG	203	PEB	NC-C1C-CHB-C4B
26	gG	203	PEB	C2A-C3A-CAA-CBA
26	gG	203	PEB	NB-C1B-CHA-C4A
26	gG	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hG	201	PEB	NC-C1C-CHB-C4B
26	hG	201	PEB	C2C-C1C-CHB-C4B
26	hG	201	PEB	NB-C1B-CHA-C4A
26	hG	201	PEB	C2B-C1B-CHA-C4A
26	hG	202	PEB	ND-C1D-CHC-C4C
26	hG	202	PEB	C2D-C1D-CHC-C4C
26	hG	202	PEB	NC-C1C-CHB-C4B
26	hG	202	PEB	C2C-C1C-CHB-C4B
26	hG	202	PEB	NB-C1B-CHA-C4A
26	hG	202	PEB	C2B-C1B-CHA-C4A
26	iG	201	PEB	NC-C1C-CHB-C4B
26	iG	201	PEB	C2C-C1C-CHB-C4B
26	iG	201	PEB	C4A-C3A-CAA-CBA
26	iG	201	PEB	NB-C1B-CHA-C4A
26	iG	201	PEB	C2B-C1B-CHA-C4A
26	iG	202	PEB	ND-C1D-CHC-C4C
26	iG	202	PEB	C2D-C1D-CHC-C4C
26	iG	202	PEB	NC-C1C-CHB-C4B
26	iG	202	PEB	C2C-C1C-CHB-C4B
26	iG	202	PEB	C4A-C3A-CAA-CBA
26	iG	202	PEB	NB-C1B-CHA-C4A
26	iG	202	PEB	C2B-C1B-CHA-C4A
26	iG	203	PEB	NC-C1C-CHB-C4B
26	iG	203	PEB	C2C-C1C-CHB-C4B
26	iG	203	PEB	C4A-C3A-CAA-CBA
26	iG	203	PEB	NB-C1B-CHA-C4A
26	iG	203	PEB	C2B-C1B-CHA-C4A
26	jG	201	PEB	NB-C1B-CHA-C4A
26	jG	202	PEB	ND-C1D-CHC-C4C
26	jG	202	PEB	C2D-C1D-CHC-C4C
26	jG	202	PEB	NC-C1C-CHB-C4B
26	jG	202	PEB	C2C-C1C-CHB-C4B
26	jG	202	PEB	NB-C1B-CHA-C4A
26	jG	202	PEB	C2B-C1B-CHA-C4A
26	kG	201	PEB	ND-C1D-CHC-C4C
26	kG	201	PEB	NC-C1C-CHB-C4B
26	kG	201	PEB	C2C-C1C-CHB-C4B
26	kG	201	PEB	C4A-C3A-CAA-CBA
26	kG	201	PEB	NB-C1B-CHA-C4A
26	kG	201	PEB	C2B-C1B-CHA-C4A
26	kG	201	PEB	C3B-CAB-CBB-CGB
26	kG	202	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	kG	202	PEB	C2C-C1C-CHB-C4B
26	kG	202	PEB	C2C-CAC-CBC-CGC
26	kG	202	PEB	C2A-C3A-CAA-CBA
26	kG	202	PEB	NB-C1B-CHA-C4A
26	kG	202	PEB	C2B-C1B-CHA-C4A
26	kG	203	PEB	C2A-C3A-CAA-CBA
26	kG	203	PEB	C4A-C3A-CAA-CBA
26	kG	203	PEB	NB-C1B-CHA-C4A
26	kG	203	PEB	C2B-C1B-CHA-C4A
26	lG	201	PEB	C2A-C3A-CAA-CBA
26	lG	201	PEB	C4A-C3A-CAA-CBA
26	lG	201	PEB	NB-C1B-CHA-C4A
26	lG	201	PEB	C2B-C1B-CHA-C4A
26	lG	202	PEB	ND-C1D-CHC-C4C
26	lG	202	PEB	C2D-C1D-CHC-C4C
26	lG	202	PEB	NC-C1C-CHB-C4B
26	lG	202	PEB	C2C-C1C-CHB-C4B
26	lG	202	PEB	NB-C1B-CHA-C4A
26	lG	202	PEB	C2B-C1B-CHA-C4A
26	mG	201	PEB	C2C-CAC-CBC-CGC
26	mG	201	PEB	C2A-C3A-CAA-CBA
26	mG	201	PEB	C4A-C3A-CAA-CBA
26	mG	201	PEB	NB-C1B-CHA-C4A
26	mG	201	PEB	C2B-C1B-CHA-C4A
26	mG	202	PEB	NC-C1C-CHB-C4B
26	mG	202	PEB	C2C-C1C-CHB-C4B
26	mG	202	PEB	NB-C1B-CHA-C4A
26	mG	202	PEB	C2B-C1B-CHA-C4A
26	mG	203	PEB	C2A-C3A-CAA-CBA
26	mG	203	PEB	C4A-C3A-CAA-CBA
26	mG	203	PEB	NB-C1B-CHA-C4A
26	mG	203	PEB	C2B-C1B-CHA-C4A
26	mG	203	PEB	C3B-CAB-CBB-CGB
26	nG	201	PEB	NB-C1B-CHA-C4A
26	nG	201	PEB	C2B-C1B-CHA-C4A
26	nG	202	PEB	ND-C1D-CHC-C4C
26	nG	202	PEB	C2D-C1D-CHC-C4C
26	nG	202	PEB	NC-C1C-CHB-C4B
26	nG	202	PEB	C2C-C1C-CHB-C4B
26	nG	202	PEB	C2C-CAC-CBC-CGC
26	nG	202	PEB	NB-C1B-CHA-C4A
26	nG	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	oG	201	PEB	ND-C1D-CHC-C4C
26	oG	201	PEB	C2D-C1D-CHC-C4C
26	oG	201	PEB	NC-C1C-CHB-C4B
26	oG	201	PEB	C2C-C1C-CHB-C4B
26	oG	201	PEB	C2A-C3A-CAA-CBA
26	oG	201	PEB	C4A-C3A-CAA-CBA
26	oG	201	PEB	NB-C1B-CHA-C4A
26	oG	201	PEB	C2B-C1B-CHA-C4A
26	oG	202	PEB	NB-C1B-CHA-C4A
26	oG	202	PEB	C2B-C1B-CHA-C4A
26	oG	203	PEB	ND-C1D-CHC-C4C
26	oG	203	PEB	NC-C1C-CHB-C4B
26	oG	203	PEB	C2C-C1C-CHB-C4B
26	oG	203	PEB	C2D-C3D-CAD-CBD
26	oG	203	PEB	C4D-C3D-CAD-CBD
26	oG	203	PEB	C2A-C3A-CAA-CBA
26	oG	203	PEB	C4A-C3A-CAA-CBA
26	oG	203	PEB	NB-C1B-CHA-C4A
26	oG	203	PEB	C2B-C1B-CHA-C4A
26	pG	201	PEB	NC-C1C-CHB-C4B
26	pG	201	PEB	C2C-C1C-CHB-C4B
26	pG	201	PEB	C2A-C3A-CAA-CBA
26	pG	201	PEB	C4A-C3A-CAA-CBA
26	pG	201	PEB	NB-C1B-CHA-C4A
26	pG	201	PEB	C2B-C1B-CHA-C4A
26	pG	202	PEB	ND-C1D-CHC-C4C
26	pG	202	PEB	C2D-C1D-CHC-C4C
26	pG	202	PEB	NC-C1C-CHB-C4B
26	pG	202	PEB	C2C-C1C-CHB-C4B
26	pG	202	PEB	NB-C1B-CHA-C4A
26	pG	202	PEB	C2B-C1B-CHA-C4A
26	qG	201	PEB	NC-C1C-CHB-C4B
26	qG	201	PEB	C2A-C3A-CAA-CBA
26	qG	201	PEB	C4A-C3A-CAA-CBA
26	qG	201	PEB	NB-C1B-CHA-C4A
26	qG	201	PEB	C2B-C1B-CHA-C4A
26	qG	202	PEB	C1C-C2C-CAC-CBC
26	qG	202	PEB	C3C-C2C-CAC-CBC
26	qG	202	PEB	C4A-C3A-CAA-CBA
26	qG	202	PEB	NB-C1B-CHA-C4A
26	qG	202	PEB	C2B-C1B-CHA-C4A
26	qG	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	qG	203	PEB	C2C-C1C-CHB-C4B
26	qG	203	PEB	C4A-C3A-CAA-CBA
26	qG	203	PEB	NB-C1B-CHA-C4A
26	qG	203	PEB	C2B-C1B-CHA-C4A
26	rG	201	PEB	ND-C1D-CHC-C4C
26	rG	201	PEB	C2D-C1D-CHC-C4C
26	rG	201	PEB	C2A-C3A-CAA-CBA
26	rG	201	PEB	C4A-C3A-CAA-CBA
26	rG	201	PEB	NB-C1B-CHA-C4A
26	rG	201	PEB	C2B-C1B-CHA-C4A
26	rG	202	PEB	ND-C1D-CHC-C4C
26	rG	202	PEB	C2D-C1D-CHC-C4C
26	rG	202	PEB	NC-C1C-CHB-C4B
26	rG	202	PEB	C2C-C1C-CHB-C4B
26	rG	202	PEB	NB-C1B-CHA-C4A
26	rG	202	PEB	C2B-C1B-CHA-C4A
26	sG	201	PEB	ND-C1D-CHC-C4C
26	sG	201	PEB	C2D-C1D-CHC-C4C
26	sG	201	PEB	C2C-CAC-CBC-CGC
26	sG	201	PEB	C4A-C3A-CAA-CBA
26	sG	201	PEB	NB-C1B-CHA-C4A
26	sG	201	PEB	C2B-C1B-CHA-C4A
26	sG	202	PEB	NC-C1C-CHB-C4B
26	sG	202	PEB	C2C-C1C-CHB-C4B
26	sG	202	PEB	C2C-CAC-CBC-CGC
26	sG	202	PEB	NB-C1B-CHA-C4A
26	sG	202	PEB	C2B-C1B-CHA-C4A
26	sG	203	PEB	NB-C1B-CHA-C4A
26	sG	203	PEB	C2B-C1B-CHA-C4A
26	tG	201	PEB	NC-C1C-CHB-C4B
26	tG	201	PEB	C2C-C1C-CHB-C4B
26	tG	201	PEB	NB-C1B-CHA-C4A
26	tG	201	PEB	C2B-C1B-CHA-C4A
26	tG	202	PEB	ND-C1D-CHC-C4C
26	tG	202	PEB	C2D-C1D-CHC-C4C
26	tG	202	PEB	C1C-C2C-CAC-CBC
26	tG	202	PEB	C3C-C2C-CAC-CBC
26	tG	202	PEB	NB-C1B-CHA-C4A
26	tG	202	PEB	C2B-C1B-CHA-C4A
26	tG	202	PEB	C3B-CAB-CBB-CGB
26	uG	201	PEB	NC-C1C-CHB-C4B
26	uG	201	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	uG	201	PEB	C4A-C3A-CAA-CBA
26	uG	201	PEB	NB-C1B-CHA-C4A
26	uG	201	PEB	C2B-C1B-CHA-C4A
26	uG	202	PEB	ND-C1D-CHC-C4C
26	uG	202	PEB	C2A-C3A-CAA-CBA
26	uG	202	PEB	C4A-C3A-CAA-CBA
26	uG	202	PEB	NB-C1B-CHA-C4A
26	uG	202	PEB	C2B-C1B-CHA-C4A
26	uG	203	PEB	NC-C1C-CHB-C4B
26	uG	203	PEB	C2C-C1C-CHB-C4B
26	uG	203	PEB	NB-C1B-CHA-C4A
26	uG	203	PEB	C2B-C1B-CHA-C4A
26	vG	201	PEB	NC-C1C-CHB-C4B
26	vG	201	PEB	C2C-C1C-CHB-C4B
26	vG	201	PEB	NB-C1B-CHA-C4A
26	vG	201	PEB	C2B-C1B-CHA-C4A
26	vG	202	PEB	ND-C1D-CHC-C4C
26	vG	202	PEB	NC-C1C-CHB-C4B
26	vG	202	PEB	C2C-C1C-CHB-C4B
26	vG	202	PEB	NB-C1B-CHA-C4A
26	vG	202	PEB	C2B-C1B-CHA-C4A
26	wG	301	PEB	NC-C1C-CHB-C4B
26	wG	301	PEB	C2C-C1C-CHB-C4B
26	wG	301	PEB	C2A-C3A-CAA-CBA
26	wG	301	PEB	NB-C1B-CHA-C4A
26	wG	301	PEB	C2B-C1B-CHA-C4A
26	wG	302	PEB	C2A-C3A-CAA-CBA
26	wG	302	PEB	C4A-C3A-CAA-CBA
26	wG	302	PEB	NB-C1B-CHA-C4A
26	wG	302	PEB	C2B-C1B-CHA-C4A
26	wG	303	PEB	NB-C1B-CHA-C4A
26	wG	303	PEB	C2B-C1B-CHA-C4A
26	xG	302	PEB	ND-C1D-CHC-C4C
26	xG	302	PEB	C2D-C1D-CHC-C4C
26	xG	302	PEB	NC-C1C-CHB-C4B
26	xG	302	PEB	C2C-C1C-CHB-C4B
26	xG	302	PEB	NB-C1B-CHA-C4A
26	xG	302	PEB	C2B-C1B-CHA-C4A
26	xG	303	PEB	ND-C1D-CHC-C4C
26	xG	303	PEB	C4A-C3A-CAA-CBA
26	xG	303	PEB	NB-C1B-CHA-C4A
26	xG	303	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	xG	304	PEB	NC-C1C-CHB-C4B
26	xG	304	PEB	C2C-C1C-CHB-C4B
26	xG	304	PEB	NB-C1B-CHA-C4A
26	xG	304	PEB	C2B-C1B-CHA-C4A
26	yG	301	PEB	C4A-C3A-CAA-CBA
26	yG	301	PEB	NB-C1B-CHA-C4A
26	yG	301	PEB	C2B-C1B-CHA-C4A
26	zG	501	PEB	NB-C1B-CHA-C4A
26	zG	501	PEB	C2B-C1B-CHA-C4A
26	AI	301	PEB	NB-C1B-CHA-C4A
26	AI	301	PEB	C2B-C1B-CHA-C4A
26	AI	304	PEB	C2A-C3A-CAA-CBA
26	AI	304	PEB	C4A-C3A-CAA-CBA
26	AI	304	PEB	NB-C1B-CHA-C4A
26	AI	304	PEB	C2B-C1B-CHA-C4A
26	AI	305	PEB	NC-C1C-CHB-C4B
26	AI	305	PEB	C4A-C3A-CAA-CBA
26	AI	305	PEB	NB-C1B-CHA-C4A
26	AI	305	PEB	C2B-C1B-CHA-C4A
26	DI	1002	PEB	C4A-C3A-CAA-CBA
26	DI	1002	PEB	NB-C1B-CHA-C4A
26	DI	1002	PEB	C2B-C1B-CHA-C4A
26	FI	1002	PEB	C2A-C3A-CAA-CBA
26	FI	1002	PEB	C4A-C3A-CAA-CBA
26	FI	1002	PEB	NB-C1B-CHA-C4A
26	FI	1002	PEB	C2B-C1B-CHA-C4A
26	FI	1002	PEB	C3B-CAB-CBB-CGB
26	HI	1002	PEB	C2C-CAC-CBC-CGC
26	HI	1002	PEB	NB-C1B-CHA-C4A
26	HI	1002	PEB	C2B-C1B-CHA-C4A
26	JI	1002	PEB	ND-C1D-CHC-C4C
26	JI	1002	PEB	C2D-C1D-CHC-C4C
26	JI	1002	PEB	NC-C1C-CHB-C4B
26	JI	1002	PEB	C4A-C3A-CAA-CBA
26	JI	1002	PEB	NB-C1B-CHA-C4A
26	JI	1002	PEB	C2B-C1B-CHA-C4A
26	LI	1002	PEB	ND-C1D-CHC-C4C
26	LI	1002	PEB	C2D-C1D-CHC-C4C
26	LI	1002	PEB	NC-C1C-CHB-C4B
26	LI	1002	PEB	C2C-CAC-CBC-CGC
26	LI	1002	PEB	NB-C1B-CHA-C4A
26	LI	1002	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	NI	1002	PEB	C4A-C3A-CAA-CBA
26	NI	1002	PEB	NB-C1B-CHA-C4A
26	NI	1002	PEB	C2B-C1B-CHA-C4A
26	OI	201	PEB	NC-C1C-CHB-C4B
26	OI	201	PEB	C2A-C3A-CAA-CBA
26	OI	201	PEB	C4A-C3A-CAA-CBA
26	OI	201	PEB	NB-C1B-CHA-C4A
26	OI	201	PEB	C2B-C1B-CHA-C4A
26	OI	202	PEB	ND-C1D-CHC-C4C
26	OI	202	PEB	NB-C1B-CHA-C4A
26	OI	202	PEB	C2B-C1B-CHA-C4A
26	PI	201	PEB	NB-C1B-CHA-C4A
26	PI	201	PEB	C2B-C1B-CHA-C4A
26	PI	202	PEB	NB-C1B-CHA-C4A
26	PI	202	PEB	C2B-C1B-CHA-C4A
26	PI	203	PEB	NB-C1B-CHA-C4A
26	PI	203	PEB	C2B-C1B-CHA-C4A
26	QI	201	PEB	C4A-C3A-CAA-CBA
26	QI	201	PEB	NB-C1B-CHA-C4A
26	QI	201	PEB	C2B-C1B-CHA-C4A
26	QI	202	PEB	C4A-C3A-CAA-CBA
26	QI	202	PEB	NB-C1B-CHA-C4A
26	QI	202	PEB	C2B-C1B-CHA-C4A
26	RI	201	PEB	NB-C1B-CHA-C4A
26	RI	201	PEB	C2B-C1B-CHA-C4A
26	RI	202	PEB	C2A-C3A-CAA-CBA
26	RI	202	PEB	NB-C1B-CHA-C4A
26	RI	202	PEB	C2B-C1B-CHA-C4A
26	RI	203	PEB	NC-C1C-CHB-C4B
26	RI	203	PEB	C2C-C1C-CHB-C4B
26	RI	203	PEB	NB-C1B-CHA-C4A
26	RI	203	PEB	C2B-C1B-CHA-C4A
26	SI	201	PEB	NC-C1C-CHB-C4B
26	SI	201	PEB	C2A-C3A-CAA-CBA
26	SI	201	PEB	C4A-C3A-CAA-CBA
26	SI	201	PEB	NB-C1B-CHA-C4A
26	SI	201	PEB	C2B-C1B-CHA-C4A
26	SI	202	PEB	ND-C1D-CHC-C4C
26	SI	202	PEB	C2D-C1D-CHC-C4C
26	SI	202	PEB	C4A-C3A-CAA-CBA
26	SI	202	PEB	NB-C1B-CHA-C4A
26	SI	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	TI	201	PEB	NB-C1B-CHA-C4A
26	TI	201	PEB	C2B-C1B-CHA-C4A
26	TI	202	PEB	NB-C1B-CHA-C4A
26	TI	202	PEB	C2B-C1B-CHA-C4A
26	TI	203	PEB	NC-C1C-CHB-C4B
26	TI	203	PEB	C2C-C1C-CHB-C4B
26	TI	203	PEB	C2A-C3A-CAA-CBA
26	TI	203	PEB	C4A-C3A-CAA-CBA
26	TI	203	PEB	NB-C1B-CHA-C4A
26	TI	203	PEB	C2B-C1B-CHA-C4A
26	UI	201	PEB	NC-C1C-CHB-C4B
26	UI	201	PEB	C2A-C3A-CAA-CBA
26	UI	201	PEB	C4A-C3A-CAA-CBA
26	UI	202	PEB	ND-C1D-CHC-C4C
26	UI	202	PEB	C2D-C1D-CHC-C4C
26	UI	202	PEB	C2A-C3A-CAA-CBA
26	UI	202	PEB	C4A-C3A-CAA-CBA
26	UI	202	PEB	NB-C1B-CHA-C4A
26	UI	202	PEB	C2B-C1B-CHA-C4A
26	VI	201	PEB	C2A-C3A-CAA-CBA
26	VI	201	PEB	C4A-C3A-CAA-CBA
26	VI	201	PEB	NB-C1B-CHA-C4A
26	VI	201	PEB	C2B-C1B-CHA-C4A
26	VI	202	PEB	ND-C1D-CHC-C4C
26	VI	202	PEB	C2D-C3D-CAD-CBD
26	VI	202	PEB	C4D-C3D-CAD-CBD
26	VI	202	PEB	C2A-C3A-CAA-CBA
26	VI	202	PEB	NB-C1B-CHA-C4A
26	VI	202	PEB	C2B-C1B-CHA-C4A
26	VI	203	PEB	NC-C1C-CHB-C4B
26	VI	203	PEB	C2C-C1C-CHB-C4B
26	VI	203	PEB	C2A-C3A-CAA-CBA
26	VI	203	PEB	NB-C1B-CHA-C4A
26	VI	203	PEB	C2B-C1B-CHA-C4A
26	VI	203	PEB	C3B-CAB-CBB-CGB
26	WI	201	PEB	NC-C1C-CHB-C4B
26	WI	201	PEB	C4A-C3A-CAA-CBA
26	WI	201	PEB	NB-C1B-CHA-C4A
26	WI	201	PEB	C2B-C1B-CHA-C4A
26	YI	201	PEB	NB-C1B-CHA-C4A
26	YI	201	PEB	C2B-C1B-CHA-C4A
26	YI	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	YI	202	PEB	C2B-C1B-CHA-C4A
26	YI	203	PEB	NC-C1C-CHB-C4B
26	YI	203	PEB	C2C-C1C-CHB-C4B
26	YI	203	PEB	C2A-C3A-CAA-CBA
26	YI	203	PEB	C4A-C3A-CAA-CBA
26	YI	203	PEB	NB-C1B-CHA-C4A
26	YI	203	PEB	C2B-C1B-CHA-C4A
26	ZI	201	PEB	C4A-C3A-CAA-CBA
26	ZI	201	PEB	NB-C1B-CHA-C4A
26	ZI	201	PEB	C2B-C1B-CHA-C4A
26	ZI	202	PEB	ND-C1D-CHC-C4C
26	ZI	202	PEB	C2D-C1D-CHC-C4C
26	ZI	202	PEB	NB-C1B-CHA-C4A
26	ZI	202	PEB	C2B-C1B-CHA-C4A
26	aI	201	PEB	NB-C1B-CHA-C4A
26	aI	201	PEB	C2B-C1B-CHA-C4A
26	aI	202	PEB	NB-C1B-CHA-C4A
26	aI	202	PEB	C2B-C1B-CHA-C4A
26	aI	203	PEB	C2C-C1C-CHB-C4B
26	aI	203	PEB	C2A-C3A-CAA-CBA
26	aI	203	PEB	C4A-C3A-CAA-CBA
26	aI	203	PEB	NB-C1B-CHA-C4A
26	aI	203	PEB	C2B-C1B-CHA-C4A
26	bI	201	PEB	C4A-C3A-CAA-CBA
26	bI	201	PEB	NB-C1B-CHA-C4A
26	bI	201	PEB	C2B-C1B-CHA-C4A
26	bI	202	PEB	ND-C1D-CHC-C4C
26	bI	202	PEB	NB-C1B-CHA-C4A
26	bI	202	PEB	C2B-C1B-CHA-C4A
26	cI	201	PEB	NB-C1B-CHA-C4A
26	cI	201	PEB	C2B-C1B-CHA-C4A
26	cI	202	PEB	ND-C1D-CHC-C4C
26	cI	202	PEB	C2D-C1D-CHC-C4C
26	cI	202	PEB	NB-C1B-CHA-C4A
26	cI	202	PEB	C2B-C1B-CHA-C4A
26	cI	203	PEB	C2C-C1C-CHB-C4B
26	cI	203	PEB	NB-C1B-CHA-C4A
26	cI	203	PEB	C2B-C1B-CHA-C4A
26	dI	201	PEB	C2A-C3A-CAA-CBA
26	dI	201	PEB	C4A-C3A-CAA-CBA
26	dI	201	PEB	NB-C1B-CHA-C4A
26	dI	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dI	202	PEB	ND-C1D-CHC-C4C
26	dI	202	PEB	C2D-C1D-CHC-C4C
26	dI	202	PEB	NC-C1C-CHB-C4B
26	dI	202	PEB	NB-C1B-CHA-C4A
26	dI	202	PEB	C2B-C1B-CHA-C4A
26	eI	201	PEB	NB-C1B-CHA-C4A
26	eI	201	PEB	C2B-C1B-CHA-C4A
26	eI	202	PEB	C2C-CAC-CBC-CGC
26	eI	202	PEB	C2A-C3A-CAA-CBA
26	eI	202	PEB	NB-C1B-CHA-C4A
26	eI	202	PEB	C2B-C1B-CHA-C4A
26	eI	203	PEB	NC-C1C-CHB-C4B
26	eI	203	PEB	C2C-C1C-CHB-C4B
26	eI	203	PEB	NB-C1B-CHA-C4A
26	eI	203	PEB	C2B-C1B-CHA-C4A
26	fI	201	PEB	ND-C1D-CHC-C4C
26	fI	201	PEB	C2D-C1D-CHC-C4C
26	fI	201	PEB	C4A-C3A-CAA-CBA
26	fI	201	PEB	NB-C1B-CHA-C4A
26	fI	201	PEB	C2B-C1B-CHA-C4A
26	fI	202	PEB	ND-C1D-CHC-C4C
26	fI	202	PEB	C4A-C3A-CAA-CBA
26	fI	202	PEB	NB-C1B-CHA-C4A
26	fI	202	PEB	C2B-C1B-CHA-C4A
26	gI	201	PEB	NB-C1B-CHA-C4A
26	gI	201	PEB	C2B-C1B-CHA-C4A
26	gI	202	PEB	ND-C1D-CHC-C4C
26	gI	202	PEB	C2A-C3A-CAA-CBA
26	gI	202	PEB	NB-C1B-CHA-C4A
26	gI	202	PEB	C2B-C1B-CHA-C4A
26	gI	203	PEB	NC-C1C-CHB-C4B
26	gI	203	PEB	C2C-C1C-CHB-C4B
26	gI	203	PEB	NB-C1B-CHA-C4A
26	gI	203	PEB	C2B-C1B-CHA-C4A
26	gI	203	PEB	C2B-C3B-CAB-CBB
26	hI	201	PEB	C4A-C3A-CAA-CBA
26	hI	201	PEB	NB-C1B-CHA-C4A
26	hI	201	PEB	C2B-C1B-CHA-C4A
26	hI	202	PEB	ND-C1D-CHC-C4C
26	hI	202	PEB	NB-C1B-CHA-C4A
26	hI	202	PEB	C2B-C1B-CHA-C4A
26	iI	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	iI	201	PEB	C4A-C3A-CAA-CBA
26	iI	201	PEB	NB-C1B-CHA-C4A
26	iI	201	PEB	C2B-C1B-CHA-C4A
26	iI	202	PEB	ND-C1D-CHC-C4C
26	iI	202	PEB	C2D-C1D-CHC-C4C
26	iI	202	PEB	C2A-C3A-CAA-CBA
26	iI	202	PEB	NB-C1B-CHA-C4A
26	iI	202	PEB	C2B-C1B-CHA-C4A
26	iI	203	PEB	NC-C1C-CHB-C4B
26	iI	203	PEB	C2C-C1C-CHB-C4B
26	iI	203	PEB	NB-C1B-CHA-C4A
26	iI	203	PEB	C2B-C1B-CHA-C4A
26	iI	203	PEB	C2B-C3B-CAB-CBB
26	iI	203	PEB	C4B-C3B-CAB-CBB
26	jI	201	PEB	C4A-C3A-CAA-CBA
26	jI	201	PEB	NB-C1B-CHA-C4A
26	jI	201	PEB	C2B-C1B-CHA-C4A
26	jI	202	PEB	ND-C1D-CHC-C4C
26	jI	202	PEB	C2D-C1D-CHC-C4C
26	jI	202	PEB	NC-C1C-CHB-C4B
26	jI	202	PEB	C2C-C1C-CHB-C4B
26	jI	202	PEB	NB-C1B-CHA-C4A
26	jI	202	PEB	C2B-C1B-CHA-C4A
26	kI	201	PEB	NC-C1C-CHB-C4B
26	kI	201	PEB	C4A-C3A-CAA-CBA
26	kI	201	PEB	NB-C1B-CHA-C4A
26	kI	201	PEB	C2B-C1B-CHA-C4A
26	kI	202	PEB	NC-C1C-CHB-C4B
26	kI	202	PEB	C2A-C3A-CAA-CBA
26	kI	202	PEB	NB-C1B-CHA-C4A
26	kI	202	PEB	C2B-C1B-CHA-C4A
26	kI	203	PEB	C2A-C3A-CAA-CBA
26	kI	203	PEB	C4A-C3A-CAA-CBA
26	kI	203	PEB	NB-C1B-CHA-C4A
26	kI	203	PEB	C2B-C1B-CHA-C4A
26	kI	203	PEB	C4B-C3B-CAB-CBB
26	lI	201	PEB	ND-C1D-CHC-C4C
26	lI	201	PEB	C4A-C3A-CAA-CBA
26	lI	201	PEB	NB-C1B-CHA-C4A
26	lI	201	PEB	C2B-C1B-CHA-C4A
26	lI	202	PEB	ND-C1D-CHC-C4C
26	lI	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	II	202	PEB	C4A-C3A-CAA-CBA
26	II	202	PEB	NB-C1B-CHA-C4A
26	II	202	PEB	C2B-C1B-CHA-C4A
26	mI	201	PEB	C2A-C3A-CAA-CBA
26	mI	201	PEB	C4A-C3A-CAA-CBA
26	mI	201	PEB	NB-C1B-CHA-C4A
26	mI	201	PEB	C2B-C1B-CHA-C4A
26	mI	202	PEB	NB-C1B-CHA-C4A
26	mI	202	PEB	C2B-C1B-CHA-C4A
26	mI	203	PEB	NC-C1C-CHB-C4B
26	mI	203	PEB	C2C-C1C-CHB-C4B
26	mI	203	PEB	NB-C1B-CHA-C4A
26	mI	203	PEB	C2B-C1B-CHA-C4A
26	mI	203	PEB	C2B-C3B-CAB-CBB
26	mI	203	PEB	C4B-C3B-CAB-CBB
26	AJ	301	PEB	C2C-CAC-CBC-CGC
26	AJ	301	PEB	NB-C1B-CHA-C4A
26	AJ	301	PEB	C2B-C1B-CHA-C4A
26	AJ	303	PEB	ND-C1D-CHC-C4C
26	AJ	303	PEB	C2D-C1D-CHC-C4C
26	AJ	303	PEB	C2A-C3A-CAA-CBA
26	AJ	303	PEB	NB-C1B-CHA-C4A
26	AJ	303	PEB	C2B-C1B-CHA-C4A
26	AJ	304	PEB	NC-C1C-CHB-C4B
26	AJ	304	PEB	C2C-C1C-CHB-C4B
26	AJ	304	PEB	NB-C1B-CHA-C4A
26	AJ	304	PEB	C2B-C1B-CHA-C4A
26	AJ	305	PEB	NB-C1B-CHA-C4A
26	AJ	305	PEB	C2B-C1B-CHA-C4A
26	BJ	201	PEB	ND-C1D-CHC-C4C
26	BJ	201	PEB	C2D-C1D-CHC-C4C
26	BJ	201	PEB	NC-C1C-CHB-C4B
26	BJ	201	PEB	C2C-C1C-CHB-C4B
26	BJ	201	PEB	NB-C1B-CHA-C4A
26	BJ	201	PEB	C2B-C1B-CHA-C4A
26	BJ	202	PEB	NC-C1C-CHB-C4B
26	BJ	202	PEB	C2C-C1C-CHB-C4B
26	BJ	202	PEB	C4A-C3A-CAA-CBA
26	BJ	202	PEB	NB-C1B-CHA-C4A
26	BJ	202	PEB	C2B-C1B-CHA-C4A
26	BJ	203	PEB	C2D-C3D-CAD-CBD
26	BJ	203	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
26	BJ	203	PEB	C4A-C3A-CAA-CBA
26	BJ	203	PEB	NB-C1B-CHA-C4A
26	BJ	203	PEB	C2B-C1B-CHA-C4A
26	CJ	201	PEB	ND-C1D-CHC-C4C
26	CJ	201	PEB	NB-C1B-CHA-C4A
26	CJ	201	PEB	C2B-C1B-CHA-C4A
26	CJ	202	PEB	NC-C1C-CHB-C4B
26	CJ	202	PEB	NB-C1B-CHA-C4A
26	CJ	202	PEB	C2B-C1B-CHA-C4A
26	DJ	201	PEB	C2D-C3D-CAD-CBD
26	DJ	201	PEB	C4A-C3A-CAA-CBA
26	DJ	201	PEB	NB-C1B-CHA-C4A
26	DJ	201	PEB	C2B-C1B-CHA-C4A
26	DJ	202	PEB	ND-C1D-CHC-C4C
26	DJ	202	PEB	NC-C1C-CHB-C4B
26	DJ	202	PEB	C2C-C1C-CHB-C4B
26	DJ	202	PEB	C2A-C3A-CAA-CBA
26	DJ	202	PEB	C4A-C3A-CAA-CBA
26	DJ	202	PEB	C3B-CAB-CBB-CGB
26	DJ	203	PEB	NC-C1C-CHB-C4B
26	DJ	203	PEB	C2C-C1C-CHB-C4B
26	DJ	203	PEB	C4A-C3A-CAA-CBA
26	DJ	203	PEB	NB-C1B-CHA-C4A
26	DJ	203	PEB	C2B-C1B-CHA-C4A
26	EJ	201	PEB	ND-C1D-CHC-C4C
26	EJ	201	PEB	C1C-C2C-CAC-CBC
26	EJ	201	PEB	C3C-C2C-CAC-CBC
26	EJ	201	PEB	C2D-C3D-CAD-CBD
26	EJ	201	PEB	C4D-C3D-CAD-CBD
26	EJ	201	PEB	NB-C1B-CHA-C4A
26	EJ	201	PEB	C2B-C1B-CHA-C4A
26	EJ	202	PEB	NB-C1B-CHA-C4A
26	EJ	202	PEB	C2B-C1B-CHA-C4A
26	FJ	201	PEB	ND-C1D-CHC-C4C
26	FJ	201	PEB	C2D-C1D-CHC-C4C
26	FJ	201	PEB	NC-C1C-CHB-C4B
26	FJ	201	PEB	C2D-C3D-CAD-CBD
26	FJ	201	PEB	C4D-C3D-CAD-CBD
26	FJ	201	PEB	NB-C1B-CHA-C4A
26	FJ	201	PEB	C2B-C1B-CHA-C4A
26	FJ	202	PEB	NC-C1C-CHB-C4B
26	FJ	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	FJ	202	PEB	NB-C1B-CHA-C4A
26	FJ	202	PEB	C2B-C1B-CHA-C4A
26	GJ	201	PEB	NB-C1B-CHA-C4A
26	GJ	201	PEB	C2B-C1B-CHA-C4A
26	GJ	202	PEB	NC-C1C-CHB-C4B
26	GJ	202	PEB	C2C-C1C-CHB-C4B
26	GJ	202	PEB	C1C-C2C-CAC-CBC
26	GJ	202	PEB	C3C-C2C-CAC-CBC
26	GJ	202	PEB	NB-C1B-CHA-C4A
26	GJ	202	PEB	C2B-C1B-CHA-C4A
26	HJ	201	PEB	NC-C1C-CHB-C4B
26	HJ	201	PEB	C2C-C1C-CHB-C4B
26	HJ	201	PEB	C2D-C3D-CAD-CBD
26	HJ	201	PEB	C4D-C3D-CAD-CBD
26	HJ	201	PEB	C4A-C3A-CAA-CBA
26	HJ	201	PEB	NB-C1B-CHA-C4A
26	HJ	201	PEB	C2B-C1B-CHA-C4A
26	HJ	202	PEB	ND-C1D-CHC-C4C
26	HJ	202	PEB	C2D-C1D-CHC-C4C
26	HJ	202	PEB	NC-C1C-CHB-C4B
26	HJ	202	PEB	C2C-C1C-CHB-C4B
26	HJ	202	PEB	NB-C1B-CHA-C4A
26	HJ	202	PEB	C3B-CAB-CBB-CGB
26	HJ	203	PEB	ND-C1D-CHC-C4C
26	HJ	203	PEB	C2D-C1D-CHC-C4C
26	HJ	203	PEB	NC-C1C-CHB-C4B
26	HJ	203	PEB	C2C-C1C-CHB-C4B
26	HJ	203	PEB	C4A-C3A-CAA-CBA
26	HJ	203	PEB	NB-C1B-CHA-C4A
26	HJ	203	PEB	C2B-C1B-CHA-C4A
26	IJ	201	PEB	C1C-C2C-CAC-CBC
26	IJ	201	PEB	C3C-C2C-CAC-CBC
26	IJ	201	PEB	NB-C1B-CHA-C4A
26	IJ	201	PEB	C2B-C1B-CHA-C4A
26	IJ	202	PEB	C2C-CAC-CBC-CGC
26	IJ	202	PEB	C4A-C3A-CAA-CBA
26	IJ	202	PEB	NB-C1B-CHA-C4A
26	IJ	202	PEB	C2B-C1B-CHA-C4A
26	IJ	203	PEB	C2D-C3D-CAD-CBD
26	IJ	203	PEB	C4D-C3D-CAD-CBD
26	IJ	203	PEB	NB-C1B-CHA-C4A
26	IJ	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	JJ	201	PEB	ND-C1D-CHC-C4C
26	JJ	201	PEB	NC-C1C-CHB-C4B
26	JJ	201	PEB	C2C-C1C-CHB-C4B
26	JJ	201	PEB	NB-C1B-CHA-C4A
26	JJ	201	PEB	C2B-C1B-CHA-C4A
26	JJ	202	PEB	NC-C1C-CHB-C4B
26	JJ	202	PEB	C2C-C1C-CHB-C4B
26	JJ	202	PEB	C4A-C3A-CAA-CBA
26	JJ	202	PEB	NB-C1B-CHA-C4A
26	JJ	202	PEB	C2B-C1B-CHA-C4A
26	JJ	203	PEB	C2D-C3D-CAD-CBD
26	JJ	203	PEB	C4D-C3D-CAD-CBD
26	JJ	203	PEB	C4A-C3A-CAA-CBA
26	JJ	203	PEB	NB-C1B-CHA-C4A
26	JJ	203	PEB	C2B-C1B-CHA-C4A
26	KJ	201	PEB	C2C-CAC-CBC-CGC
26	KJ	201	PEB	C2A-C3A-CAA-CBA
26	KJ	201	PEB	C4A-C3A-CAA-CBA
26	KJ	201	PEB	NB-C1B-CHA-C4A
26	KJ	201	PEB	C2B-C1B-CHA-C4A
26	KJ	202	PEB	ND-C1D-CHC-C4C
26	KJ	202	PEB	NC-C1C-CHB-C4B
26	KJ	202	PEB	C2C-CAC-CBC-CGC
26	KJ	202	PEB	NB-C1B-CHA-C4A
26	KJ	202	PEB	C2B-C1B-CHA-C4A
26	LJ	201	PEB	C4A-C3A-CAA-CBA
26	LJ	201	PEB	NB-C1B-CHA-C4A
26	LJ	201	PEB	C2B-C1B-CHA-C4A
26	LJ	202	PEB	ND-C1D-CHC-C4C
26	LJ	202	PEB	NB-C1B-CHA-C4A
26	LJ	202	PEB	C2B-C1B-CHA-C4A
26	LJ	203	PEB	NC-C1C-CHB-C4B
26	LJ	203	PEB	C2C-C1C-CHB-C4B
26	LJ	203	PEB	NB-C1B-CHA-C4A
26	LJ	203	PEB	C2B-C1B-CHA-C4A
26	MJ	201	PEB	C1C-C2C-CAC-CBC
26	MJ	201	PEB	C3C-C2C-CAC-CBC
26	MJ	201	PEB	NB-C1B-CHA-C4A
26	MJ	201	PEB	C2B-C1B-CHA-C4A
26	MJ	202	PEB	NC-C1C-CHB-C4B
26	MJ	202	PEB	C2C-C1C-CHB-C4B
26	MJ	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	MJ	202	PEB	NB-C1B-CHA-C4A
26	MJ	202	PEB	C2B-C1B-CHA-C4A
26	NJ	202	PEB	ND-C1D-CHC-C4C
26	NJ	202	PEB	C2D-C1D-CHC-C4C
26	NJ	202	PEB	C4A-C3A-CAA-CBA
26	NJ	202	PEB	NB-C1B-CHA-C4A
26	NJ	202	PEB	C2B-C1B-CHA-C4A
26	NJ	203	PEB	ND-C1D-CHC-C4C
26	NJ	203	PEB	C2D-C1D-CHC-C4C
26	NJ	203	PEB	NC-C1C-CHB-C4B
26	NJ	203	PEB	C2C-C1C-CHB-C4B
26	NJ	203	PEB	C4A-C3A-CAA-CBA
26	NJ	203	PEB	NB-C1B-CHA-C4A
26	NJ	203	PEB	C2B-C1B-CHA-C4A
26	NJ	204	PEB	NC-C1C-CHB-C4B
26	NJ	204	PEB	C2C-C1C-CHB-C4B
26	NJ	204	PEB	C4A-C3A-CAA-CBA
26	NJ	204	PEB	NB-C1B-CHA-C4A
26	NJ	204	PEB	C2B-C1B-CHA-C4A
26	OJ	201	PEB	ND-C1D-CHC-C4C
26	OJ	201	PEB	C2D-C1D-CHC-C4C
26	OJ	201	PEB	NC-C1C-CHB-C4B
26	OJ	201	PEB	C2C-C1C-CHB-C4B
26	OJ	201	PEB	C2D-C3D-CAD-CBD
26	OJ	201	PEB	C4D-C3D-CAD-CBD
26	OJ	201	PEB	C2A-C3A-CAA-CBA
26	OJ	201	PEB	C4A-C3A-CAA-CBA
26	OJ	201	PEB	NB-C1B-CHA-C4A
26	OJ	201	PEB	C2B-C1B-CHA-C4A
26	PJ	201	PEB	C2A-C3A-CAA-CBA
26	PJ	201	PEB	C4A-C3A-CAA-CBA
26	PJ	201	PEB	NB-C1B-CHA-C4A
26	PJ	201	PEB	C2B-C1B-CHA-C4A
26	PJ	202	PEB	ND-C1D-CHC-C4C
26	PJ	202	PEB	C2D-C1D-CHC-C4C
26	PJ	202	PEB	NC-C1C-CHB-C4B
26	PJ	202	PEB	C2C-C1C-CHB-C4B
26	PJ	202	PEB	NB-C1B-CHA-C4A
26	PJ	202	PEB	C2B-C1B-CHA-C4A
26	PJ	203	PEB	ND-C1D-CHC-C4C
26	PJ	203	PEB	C2D-C1D-CHC-C4C
26	PJ	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
26	PJ	203	PEB	C2C-C1C-CHB-C4B
26	PJ	203	PEB	C2A-C3A-CAA-CBA
26	PJ	203	PEB	C4A-C3A-CAA-CBA
26	PJ	203	PEB	NB-C1B-CHA-C4A
26	PJ	203	PEB	C2B-C1B-CHA-C4A
26	QJ	201	PEB	NB-C1B-CHA-C4A
26	QJ	201	PEB	C2B-C1B-CHA-C4A
26	QJ	202	PEB	ND-C1D-CHC-C4C
26	QJ	202	PEB	NC-C1C-CHB-C4B
26	QJ	202	PEB	C2C-C1C-CHB-C4B
26	QJ	202	PEB	NB-C1B-CHA-C4A
26	QJ	202	PEB	C2B-C1B-CHA-C4A
26	RJ	201	PEB	ND-C1D-CHC-C4C
26	RJ	201	PEB	C2D-C1D-CHC-C4C
26	RJ	201	PEB	NC-C1C-CHB-C4B
26	RJ	201	PEB	NB-C1B-CHA-C4A
26	RJ	201	PEB	C2B-C1B-CHA-C4A
26	RJ	202	PEB	NC-C1C-CHB-C4B
26	RJ	202	PEB	C2C-C1C-CHB-C4B
26	RJ	202	PEB	C4A-C3A-CAA-CBA
26	RJ	202	PEB	NB-C1B-CHA-C4A
26	RJ	202	PEB	C2B-C1B-CHA-C4A
26	RJ	203	PEB	NB-C1B-CHA-C4A
26	RJ	203	PEB	C2B-C1B-CHA-C4A
26	SJ	201	PEB	NC-C1C-CHB-C4B
26	SJ	201	PEB	C2C-C1C-CHB-C4B
26	SJ	201	PEB	NB-C1B-CHA-C4A
26	SJ	201	PEB	C2B-C1B-CHA-C4A
26	SJ	202	PEB	NB-C1B-CHA-C4A
26	SJ	202	PEB	C2B-C1B-CHA-C4A
26	TJ	201	PEB	C2D-C3D-CAD-CBD
26	TJ	201	PEB	C4D-C3D-CAD-CBD
26	TJ	201	PEB	C4A-C3A-CAA-CBA
26	TJ	201	PEB	NB-C1B-CHA-C4A
26	TJ	201	PEB	C2B-C1B-CHA-C4A
26	TJ	202	PEB	ND-C1D-CHC-C4C
26	TJ	202	PEB	C2D-C1D-CHC-C4C
26	TJ	202	PEB	C2C-CAC-CBC-CGC
26	TJ	202	PEB	C4A-C3A-CAA-CBA
26	TJ	202	PEB	NB-C1B-CHA-C4A
26	TJ	202	PEB	C2B-C1B-CHA-C4A
26	TJ	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	TJ	203	PEB	C2D-C1D-CHC-C4C
26	TJ	203	PEB	NC-C1C-CHB-C4B
26	TJ	203	PEB	C2C-C1C-CHB-C4B
26	TJ	203	PEB	NB-C1B-CHA-C4A
26	TJ	203	PEB	C2B-C1B-CHA-C4A
26	UJ	201	PEB	ND-C1D-CHC-C4C
26	UJ	201	PEB	C2D-C1D-CHC-C4C
26	UJ	201	PEB	C2A-C3A-CAA-CBA
26	UJ	201	PEB	C4A-C3A-CAA-CBA
26	UJ	201	PEB	NB-C1B-CHA-C4A
26	UJ	201	PEB	C2B-C1B-CHA-C4A
26	UJ	202	PEB	NC-C1C-CHB-C4B
26	UJ	202	PEB	C2C-C1C-CHB-C4B
26	UJ	202	PEB	NB-C1B-CHA-C4A
26	UJ	202	PEB	C2B-C1B-CHA-C4A
26	VJ	201	PEB	C4A-C3A-CAA-CBA
26	VJ	201	PEB	NB-C1B-CHA-C4A
26	VJ	201	PEB	C2B-C1B-CHA-C4A
26	VJ	202	PEB	NC-C1C-CHB-C4B
26	VJ	202	PEB	C2C-C1C-CHB-C4B
26	VJ	202	PEB	C4A-C3A-CAA-CBA
26	VJ	202	PEB	NB-C1B-CHA-C4A
26	VJ	202	PEB	C2B-C1B-CHA-C4A
26	VJ	203	PEB	NC-C1C-CHB-C4B
26	VJ	203	PEB	C2C-C1C-CHB-C4B
26	VJ	203	PEB	C2C-CAC-CBC-CGC
26	VJ	203	PEB	C2D-C3D-CAD-CBD
26	VJ	203	PEB	C4D-C3D-CAD-CBD
26	VJ	203	PEB	C4A-C3A-CAA-CBA
26	VJ	203	PEB	NB-C1B-CHA-C4A
26	VJ	203	PEB	C2B-C1B-CHA-C4A
26	WJ	201	PEB	NB-C1B-CHA-C4A
26	WJ	201	PEB	C2B-C1B-CHA-C4A
26	WJ	202	PEB	NC-C1C-CHB-C4B
26	WJ	202	PEB	C2C-C1C-CHB-C4B
26	WJ	202	PEB	NB-C1B-CHA-C4A
26	WJ	202	PEB	C2B-C1B-CHA-C4A
26	XJ	201	PEB	C2C-CAC-CBC-CGC
26	XJ	201	PEB	C4A-C3A-CAA-CBA
26	XJ	201	PEB	NB-C1B-CHA-C4A
26	XJ	201	PEB	C2B-C1B-CHA-C4A
26	XJ	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	XJ	202	PEB	C2D-C1D-CHC-C4C
26	XJ	202	PEB	NB-C1B-CHA-C4A
26	XJ	202	PEB	C2B-C1B-CHA-C4A
26	XJ	203	PEB	NC-C1C-CHB-C4B
26	XJ	203	PEB	C2C-C1C-CHB-C4B
26	XJ	203	PEB	C2A-C3A-CAA-CBA
26	XJ	203	PEB	C4A-C3A-CAA-CBA
26	XJ	203	PEB	NB-C1B-CHA-C4A
26	XJ	203	PEB	C2B-C1B-CHA-C4A
26	YJ	201	PEB	NB-C1B-CHA-C4A
26	YJ	201	PEB	C2B-C1B-CHA-C4A
26	YJ	202	PEB	C2C-CAC-CBC-CGC
26	YJ	202	PEB	NB-C1B-CHA-C4A
26	YJ	202	PEB	C2B-C1B-CHA-C4A
27	A1	203	PUB	ND-C1D-CHC-C4C
27	A1	203	PUB	NB-C4B-CHB-C1C
27	A1	203	PUB	C3B-C4B-CHB-C1C
27	K1	203	PUB	NA-C4A-CHA-C1B
27	K1	203	PUB	C2B-C3B-CAB-CBB
27	K1	203	PUB	C4B-C3B-CAB-CBB
27	21	402	PUB	NC-C4C-CHC-C1D
27	21	402	PUB	ND-C1D-CHC-C4C
27	21	402	PUB	C2D-C1D-CHC-C4C
27	21	402	PUB	NA-C4A-CHA-C1B
27	21	403	PUB	C3C-C4C-CHC-C1D
27	21	403	PUB	ND-C1D-CHC-C4C
27	21	403	PUB	NA-C4A-CHA-C1B
27	21	403	PUB	C3A-C4A-CHA-C1B
27	21	403	PUB	NB-C4B-CHB-C1C
27	21	403	PUB	C3B-C4B-CHB-C1C
27	A2	302	PUB	C3C-C4C-CHC-C1D
27	A2	302	PUB	NA-C4A-CHA-C1B
27	A2	302	PUB	C3A-C4A-CHA-C1B
27	A2	303	PUB	C3C-C4C-CHC-C1D
27	K3	203	PUB	C3C-C4C-CHC-C1D
27	K3	203	PUB	NA-C4A-CHA-C1B
27	K3	203	PUB	C3A-C4A-CHA-C1B
27	K3	203	PUB	NB-C4B-CHB-C1C
27	K3	203	PUB	C3B-C4B-CHB-C1C
27	Y3	302	PUB	ND-C1D-CHC-C4C
27	A4	203	PUB	NB-C4B-CHB-C1C
27	A4	203	PUB	C3B-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
27	K4	203	PUB	NA-C4A-CHA-C1B
27	K4	203	PUB	C2B-C3B-CAB-CBB
27	K4	203	PUB	C4B-C3B-CAB-CBB
27	24	402	PUB	NC-C4C-CHC-C1D
27	24	402	PUB	ND-C1D-CHC-C4C
27	24	402	PUB	NA-C4A-CHA-C1B
27	24	403	PUB	ND-C1D-CHC-C4C
27	24	403	PUB	NA-C4A-CHA-C1B
27	24	403	PUB	NB-C4B-CHB-C1C
27	24	403	PUB	C3B-C4B-CHB-C1C
27	A6	302	PUB	C3C-C4C-CHC-C1D
27	A6	302	PUB	C3B-CAB-CBB-CGB
27	A6	303	PUB	NC-C4C-CHC-C1D
27	A7	303	PUB	NA-C4A-CHA-C1B
27	A7	303	PUB	C3A-C4A-CHA-C1B
27	A7	303	PUB	C2B-C3B-CAB-CBB
27	A7	303	PUB	C4B-C3B-CAB-CBB
27	A7	304	PUB	C3C-C4C-CHC-C1D
27	A7	304	PUB	ND-C1D-CHC-C4C
27	A7	304	PUB	NA-C4A-CHA-C1B
27	A7	304	PUB	C3A-C4A-CHA-C1B
27	A7	304	PUB	NB-C4B-CHB-C1C
27	A7	304	PUB	C3B-C4B-CHB-C1C
27	A8	303	PUB	C3C-C4C-CHC-C1D
27	A8	303	PUB	NA-C4A-CHA-C1B
27	A8	303	PUB	C2B-C3B-CAB-CBB
27	A8	303	PUB	C4B-C3B-CAB-CBB
27	A8	304	PUB	NC-C4C-CHC-C1D
27	A8	304	PUB	ND-C1D-CHC-C4C
27	A8	304	PUB	NA-C4A-CHA-C1B
27	Q8	201	PUB	NC-C4C-CHC-C1D
27	Q8	201	PUB	ND-C1D-CHC-C4C
27	Q8	201	PUB	NA-C4A-CHA-C1B
27	Q8	201	PUB	C3A-C4A-CHA-C1B
27	Q8	201	PUB	NB-C4B-CHB-C1C
27	A9	302	PUB	C3C-C4C-CHC-C1D
27	A9	302	PUB	ND-C1D-CHC-C4C
27	A9	302	PUB	C2D-C1D-CHC-C4C
27	AA	303	PUB	NC-C4C-CHC-C1D
27	AA	303	PUB	C3C-C4C-CHC-C1D
27	AA	303	PUB	NA-C4A-CHA-C1B
27	AA	303	PUB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	AA	303	PUB	C4B-C3B-CAB-CBB
27	AA	304	PUB	NC-C4C-CHC-C1D
27	AA	304	PUB	ND-C1D-CHC-C4C
27	AA	304	PUB	NA-C4A-CHA-C1B
27	BA	302	PUB	NC-C4C-CHC-C1D
27	QA	201	PUB	ND-C1D-CHC-C4C
27	QA	201	PUB	NA-C4A-CHA-C1B
27	QA	201	PUB	C3A-C4A-CHA-C1B
27	QA	201	PUB	C2B-C3B-CAB-CBB
27	QA	201	PUB	C4B-C3B-CAB-CBB
27	AB	302	PUB	C2C-CAC-CBC-CGC
27	AB	302	PUB	C3B-CAB-CBB-CGB
27	AB	303	PUB	NC-C4C-CHC-C1D
27	AB	303	PUB	NB-C4B-CHB-C1C
27	KD	203	PUB	C3C-C4C-CHC-C1D
27	KD	203	PUB	NA-C4A-CHA-C1B
27	KD	203	PUB	C3A-C4A-CHA-C1B
27	YD	302	PUB	ND-C1D-CHC-C4C
27	wE	304	PUB	C3C-C4C-CHC-C1D
27	wE	304	PUB	ND-C1D-CHC-C4C
27	wE	304	PUB	C2D-C1D-CHC-C4C
27	wE	304	PUB	NA-C4A-CHA-C1B
27	wE	304	PUB	C3A-C4A-CHA-C1B
27	xE	301	PUB	NC-C4C-CHC-C1D
27	xE	301	PUB	ND-C1D-CHC-C4C
27	xE	301	PUB	C2D-C1D-CHC-C4C
27	xE	301	PUB	NB-C4B-CHB-C1C
27	xE	305	PUB	ND-C1D-CHC-C4C
27	xE	305	PUB	C2D-C1D-CHC-C4C
27	xE	305	PUB	C2C-CAC-CBC-CGC
27	xE	305	PUB	C3B-CAB-CBB-CGB
27	xE	306	PUB	C3C-C4C-CHC-C1D
27	xE	306	PUB	ND-C1D-CHC-C4C
27	yE	302	PUB	C4D-C3D-CAD-CBD
27	AF	303	PUB	NA-C4A-CHA-C1B
27	AF	303	PUB	C2B-C3B-CAB-CBB
27	AF	303	PUB	C4B-C3B-CAB-CBB
27	AF	304	PUB	C3C-C4C-CHC-C1D
27	AF	304	PUB	ND-C1D-CHC-C4C
27	AF	304	PUB	C2A-C3A-CAA-CBA
27	AF	304	PUB	NA-C4A-CHA-C1B
27	AF	304	PUB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
27	AF	304	PUB	NB-C4B-CHB-C1C
27	AF	304	PUB	C3B-C4B-CHB-C1C
27	wG	304	PUB	C3C-C4C-CHC-C1D
27	wG	304	PUB	NA-C4A-CHA-C1B
27	wG	304	PUB	C3B-CAB-CBB-CGB
27	xG	301	PUB	ND-C1D-CHC-C4C
27	xG	301	PUB	C2D-C1D-CHC-C4C
27	xG	301	PUB	NB-C4B-CHB-C1C
27	xG	301	PUB	C3B-C4B-CHB-C1C
27	xG	305	PUB	ND-C1D-CHC-C4C
27	xG	305	PUB	C2D-C1D-CHC-C4C
27	xG	305	PUB	NA-C4A-CHA-C1B
27	xG	305	PUB	C3A-C4A-CHA-C1B
27	xG	306	PUB	ND-C1D-CHC-C4C
27	xG	306	PUB	C2D-C1D-CHC-C4C
27	yG	302	PUB	C4D-C3D-CAD-CBD
27	yG	303	PUB	C3B-CAB-CBB-CGB
27	AI	303	PUB	C3C-C4C-CHC-C1D
27	AJ	302	PUB	C3C-C4C-CHC-C1D
27	AJ	302	PUB	ND-C1D-CHC-C4C
27	AJ	302	PUB	C2D-C1D-CHC-C4C
27	NJ	201	PUB	NA-C4A-CHA-C1B
27	NJ	201	PUB	C3A-C4A-CHA-C1B
28	C2	1001	CYC	NA-C4A-CHB-C1B
28	C2	1001	CYC	C3A-C4A-CHB-C1B
28	C2	1001	CYC	C2C-C3C-CAC-CBC
28	C2	1001	CYC	C4C-C3C-CAC-CBC
28	D2	1001	CYC	NA-C4A-CHB-C1B
28	D2	1001	CYC	C3A-C4A-CHB-C1B
28	D2	1001	CYC	ND-C1D-CHD-C4C
28	E2	1001	CYC	NA-C4A-CHB-C1B
28	E2	1001	CYC	C3A-C4A-CHB-C1B
28	F2	1001	CYC	NA-C4A-CHB-C1B
28	F2	1001	CYC	C3A-C4A-CHB-C1B
28	F2	1001	CYC	C2C-C3C-CAC-CBC
28	F2	1001	CYC	C4C-C3C-CAC-CBC
28	G2	1001	CYC	NA-C4A-CHB-C1B
28	G2	1001	CYC	C3A-C4A-CHB-C1B
28	H2	1001	CYC	NA-C4A-CHB-C1B
28	H2	1001	CYC	C3A-C4A-CHB-C1B
28	H2	1001	CYC	C2C-C3C-CAC-CBC
28	H2	1001	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	H2	1001	CYC	ND-C1D-CHD-C4C
28	I2	1001	CYC	NA-C4A-CHB-C1B
28	I2	1001	CYC	C3A-C4A-CHB-C1B
28	I2	1001	CYC	C2C-C3C-CAC-CBC
28	I2	1001	CYC	C4C-C3C-CAC-CBC
28	J2	1001	CYC	C2C-C3C-CAC-CBC
28	J2	1001	CYC	C4C-C3C-CAC-CBC
28	K2	1001	CYC	NA-C4A-CHB-C1B
28	K2	1001	CYC	C3A-C4A-CHB-C1B
28	K2	1001	CYC	C2C-C3C-CAC-CBC
28	K2	1001	CYC	C4C-C3C-CAC-CBC
28	L2	1001	CYC	ND-C1D-CHD-C4C
28	M2	1001	CYC	NA-C4A-CHB-C1B
28	M2	1001	CYC	C3A-C4A-CHB-C1B
28	M2	1001	CYC	C2C-C3C-CAC-CBC
28	M2	1001	CYC	C4C-C3C-CAC-CBC
28	N2	1001	CYC	NA-C4A-CHB-C1B
28	N2	1001	CYC	C3A-C4A-CHB-C1B
28	N2	1001	CYC	C2C-C3C-CAC-CBC
28	N2	1001	CYC	C4C-C3C-CAC-CBC
28	B6	1001	CYC	NA-C4A-CHB-C1B
28	B6	1001	CYC	C3A-C4A-CHB-C1B
28	B6	1001	CYC	C2C-C3C-CAC-CBC
28	B6	1001	CYC	C4C-C3C-CAC-CBC
28	B6	1001	CYC	ND-C1D-CHD-C4C
28	C6	1001	CYC	NA-C4A-CHB-C1B
28	C6	1001	CYC	C3A-C4A-CHB-C1B
28	D6	1001	CYC	NA-C4A-CHB-C1B
28	D6	1001	CYC	C3A-C4A-CHB-C1B
28	D6	1001	CYC	C2C-C3C-CAC-CBC
28	D6	1001	CYC	C4C-C3C-CAC-CBC
28	E6	1001	CYC	NA-C4A-CHB-C1B
28	E6	1001	CYC	C3A-C4A-CHB-C1B
28	F6	1001	CYC	NA-C4A-CHB-C1B
28	F6	1001	CYC	C3A-C4A-CHB-C1B
28	F6	1001	CYC	C2C-C3C-CAC-CBC
28	F6	1001	CYC	C4C-C3C-CAC-CBC
28	G6	1001	CYC	NA-C4A-CHB-C1B
28	G6	1001	CYC	C3A-C4A-CHB-C1B
28	G6	1001	CYC	C2C-C3C-CAC-CBC
28	G6	1001	CYC	C4C-C3C-CAC-CBC
28	H6	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
28	H6	1001	CYC	C3A-C4A-CHB-C1B
28	H6	1001	CYC	ND-C1D-CHD-C4C
28	I6	1001	CYC	NA-C4A-CHB-C1B
28	I6	1001	CYC	C3A-C4A-CHB-C1B
28	I6	1001	CYC	C2C-C3C-CAC-CBC
28	I6	1001	CYC	C4C-C3C-CAC-CBC
28	K6	202	CYC	NA-C4A-CHB-C1B
28	K6	202	CYC	C3A-C4A-CHB-C1B
28	L6	1001	CYC	ND-C4D-CHA-C1A
28	L6	1001	CYC	C2C-C3C-CAC-CBC
28	L6	1001	CYC	C4C-C3C-CAC-CBC
28	L6	1001	CYC	C2D-C3D-CAD-CBD
28	L6	1001	CYC	C4D-C3D-CAD-CBD
28	M6	1001	CYC	NA-C4A-CHB-C1B
28	M6	1001	CYC	C3A-C4A-CHB-C1B
28	M6	1001	CYC	C2C-C3C-CAC-CBC
28	M6	1001	CYC	C4C-C3C-CAC-CBC
28	C7	1001	CYC	NA-C4A-CHB-C1B
28	C7	1001	CYC	C3A-C4A-CHB-C1B
28	C7	1001	CYC	C2C-C3C-CAC-CBC
28	C7	1001	CYC	C4C-C3C-CAC-CBC
28	D7	1001	CYC	NA-C4A-CHB-C1B
28	D7	1001	CYC	C3A-C4A-CHB-C1B
28	E7	1001	CYC	NA-C4A-CHB-C1B
28	E7	1001	CYC	C3A-C4A-CHB-C1B
28	F7	1001	CYC	NA-C4A-CHB-C1B
28	F7	1001	CYC	C3A-C4A-CHB-C1B
28	F7	1001	CYC	C2C-C3C-CAC-CBC
28	F7	1001	CYC	C4C-C3C-CAC-CBC
28	G7	1001	CYC	NA-C4A-CHB-C1B
28	G7	1001	CYC	C3A-C4A-CHB-C1B
28	G7	1001	CYC	C2C-C3C-CAC-CBC
28	G7	1001	CYC	C4C-C3C-CAC-CBC
28	G7	1001	CYC	ND-C1D-CHD-C4C
28	G7	1001	CYC	C2D-C1D-CHD-C4C
28	H7	1001	CYC	NA-C4A-CHB-C1B
28	H7	1001	CYC	C3A-C4A-CHB-C1B
28	H7	1001	CYC	C2D-C1D-CHD-C4C
28	I7	1001	CYC	NA-C4A-CHB-C1B
28	I7	1001	CYC	C3A-C4A-CHB-C1B
28	I7	1001	CYC	C2C-C3C-CAC-CBC
28	I7	1001	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	I7	1001	CYC	ND-C1D-CHD-C4C
28	I7	1001	CYC	C2D-C1D-CHD-C4C
28	J7	1001	CYC	NA-C4A-CHB-C1B
28	J7	1001	CYC	C3A-C4A-CHB-C1B
28	J7	1001	CYC	C2D-C3D-CAD-CBD
28	J7	1003	CYC	NA-C4A-CHB-C1B
28	J7	1003	CYC	C3A-C4A-CHB-C1B
28	K7	1001	CYC	NA-C4A-CHB-C1B
28	K7	1001	CYC	C3A-C4A-CHB-C1B
28	K7	1001	CYC	C4C-C3C-CAC-CBC
28	L7	1001	CYC	ND-C4D-CHA-C1A
28	L7	1001	CYC	NA-C4A-CHB-C1B
28	L7	1001	CYC	C3A-C4A-CHB-C1B
28	L7	1001	CYC	C2C-C3C-CAC-CBC
28	L7	1001	CYC	C4C-C3C-CAC-CBC
28	N7	1001	CYC	NA-C4A-CHB-C1B
28	N7	1001	CYC	C3A-C4A-CHB-C1B
28	N7	1001	CYC	C2C-C3C-CAC-CBC
28	N7	1001	CYC	C4C-C3C-CAC-CBC
28	BB	1001	CYC	NA-C4A-CHB-C1B
28	BB	1001	CYC	C3A-C4A-CHB-C1B
28	BB	1001	CYC	C2C-C3C-CAC-CBC
28	BB	1001	CYC	C4C-C3C-CAC-CBC
28	BB	1001	CYC	ND-C1D-CHD-C4C
28	CB	1001	CYC	NA-C4A-CHB-C1B
28	CB	1001	CYC	C3A-C4A-CHB-C1B
28	DB	1001	CYC	NA-C4A-CHB-C1B
28	DB	1001	CYC	C3A-C4A-CHB-C1B
28	DB	1001	CYC	C2C-C3C-CAC-CBC
28	DB	1001	CYC	C4C-C3C-CAC-CBC
28	EB	1001	CYC	NA-C4A-CHB-C1B
28	EB	1001	CYC	C3A-C4A-CHB-C1B
28	FB	1001	CYC	NA-C4A-CHB-C1B
28	FB	1001	CYC	C3A-C4A-CHB-C1B
28	FB	1001	CYC	C2C-C3C-CAC-CBC
28	FB	1001	CYC	C4C-C3C-CAC-CBC
28	GB	1001	CYC	NA-C4A-CHB-C1B
28	GB	1001	CYC	C3A-C4A-CHB-C1B
28	GB	1001	CYC	C2C-C3C-CAC-CBC
28	GB	1001	CYC	C4C-C3C-CAC-CBC
28	HB	1001	CYC	NA-C4A-CHB-C1B
28	HB	1001	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
28	HB	1001	CYC	ND-C1D-CHD-C4C
28	IB	1001	CYC	NA-C4A-CHB-C1B
28	IB	1001	CYC	C3A-C4A-CHB-C1B
28	IB	1001	CYC	C2C-C3C-CAC-CBC
28	IB	1001	CYC	C4C-C3C-CAC-CBC
28	KB	202	CYC	NA-C4A-CHB-C1B
28	KB	202	CYC	C3A-C4A-CHB-C1B
28	LB	1001	CYC	C2D-C3D-CAD-CBD
28	LB	1001	CYC	C4D-C3D-CAD-CBD
28	MB	1001	CYC	NA-C4A-CHB-C1B
28	MB	1001	CYC	C3A-C4A-CHB-C1B
28	MB	1001	CYC	C2C-C3C-CAC-CBC
28	MB	1001	CYC	C4C-C3C-CAC-CBC
28	NB	1001	CYC	C3A-C4A-CHB-C1B
28	CF	1001	CYC	ND-C4D-CHA-C1A
28	CF	1001	CYC	NA-C4A-CHB-C1B
28	CF	1001	CYC	C3A-C4A-CHB-C1B
28	CF	1001	CYC	C2C-C3C-CAC-CBC
28	CF	1001	CYC	C4C-C3C-CAC-CBC
28	CF	1001	CYC	ND-C1D-CHD-C4C
28	CF	1001	CYC	C2D-C1D-CHD-C4C
28	DF	1001	CYC	NA-C4A-CHB-C1B
28	DF	1001	CYC	C3A-C4A-CHB-C1B
28	DF	1003	CYC	NA-C4A-CHB-C1B
28	DF	1003	CYC	C3A-C4A-CHB-C1B
28	DF	1003	CYC	C2C-C3C-CAC-CBC
28	DF	1003	CYC	C4C-C3C-CAC-CBC
28	DF	1003	CYC	ND-C1D-CHD-C4C
28	DF	1003	CYC	C2D-C1D-CHD-C4C
28	EF	1001	CYC	NA-C4A-CHB-C1B
28	EF	1001	CYC	C3A-C4A-CHB-C1B
28	FF	1001	CYC	NA-C4A-CHB-C1B
28	FF	1001	CYC	C3A-C4A-CHB-C1B
28	FF	1001	CYC	C2C-C3C-CAC-CBC
28	FF	1001	CYC	C4C-C3C-CAC-CBC
28	HF	1001	CYC	NA-C4A-CHB-C1B
28	HF	1001	CYC	C3A-C4A-CHB-C1B
28	HF	1001	CYC	C2D-C1D-CHD-C4C
28	IF	1001	CYC	NA-C4A-CHB-C1B
28	IF	1001	CYC	C3A-C4A-CHB-C1B
28	IF	1001	CYC	C2C-C3C-CAC-CBC
28	IF	1001	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	IF	1001	CYC	ND-C1D-CHD-C4C
28	IF	1001	CYC	C2D-C1D-CHD-C4C
28	JF	1001	CYC	NA-C4A-CHB-C1B
28	JF	1001	CYC	C3A-C4A-CHB-C1B
28	JF	1003	CYC	NA-C4A-CHB-C1B
28	JF	1003	CYC	C3A-C4A-CHB-C1B
28	KF	1001	CYC	NA-C4A-CHB-C1B
28	KF	1001	CYC	C3A-C4A-CHB-C1B
28	KF	1001	CYC	C2C-C3C-CAC-CBC
28	KF	1001	CYC	C4C-C3C-CAC-CBC
28	KF	1001	CYC	ND-C1D-CHD-C4C
28	LF	1001	CYC	NA-C4A-CHB-C1B
28	LF	1001	CYC	C3A-C4A-CHB-C1B
28	LF	1001	CYC	C2C-C3C-CAC-CBC
28	LF	1001	CYC	C4C-C3C-CAC-CBC
28	NF	1001	CYC	NA-C4A-CHB-C1B
28	NF	1001	CYC	C3A-C4A-CHB-C1B
28	NF	1001	CYC	C2C-C3C-CAC-CBC
28	NF	1001	CYC	C4C-C3C-CAC-CBC
28	AH	1001	CYC	ND-C1D-CHD-C4C
28	AH	1001	CYC	C2D-C1D-CHD-C4C
28	CH	1001	CYC	C4B-C3B-CAB-CBB
28	CH	1001	CYC	ND-C1D-CHD-C4C
28	CH	1001	CYC	C2D-C1D-CHD-C4C
28	FH	1001	CYC	NA-C4A-CHB-C1B
28	FH	1001	CYC	C3A-C4A-CHB-C1B
28	EH	1001	CYC	ND-C1D-CHD-C4C
28	EH	1001	CYC	C2D-C1D-CHD-C4C
28	GH	1001	CYC	C2C-C3C-CAC-CBC
28	GH	1001	CYC	ND-C1D-CHD-C4C
28	GH	1001	CYC	C2D-C1D-CHD-C4C
28	IH	1001	CYC	C3A-C4A-CHB-C1B
28	IH	1001	CYC	ND-C1D-CHD-C4C
28	IH	1001	CYC	C2D-C1D-CHD-C4C
28	JH	1001	CYC	ND-C1D-CHD-C4C
28	JH	1001	CYC	C2D-C1D-CHD-C4C
28	KH	1001	CYC	C2A-C1A-CHA-C4D
28	KH	1001	CYC	ND-C4D-CHA-C1A
28	KH	1001	CYC	C3D-C4D-CHA-C1A
28	KH	1001	CYC	C4C-C3C-CAC-CBC
28	KH	1001	CYC	NC-C4C-CHD-C1D
28	KH	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
28	KH	1001	CYC	C2D-C1D-CHD-C4C
28	LH	1001	CYC	ND-C1D-CHD-C4C
28	LH	1001	CYC	C2D-C1D-CHD-C4C
28	MH	1001	CYC	NA-C4A-CHB-C1B
28	MH	1001	CYC	C4C-C3C-CAC-CBC
28	MH	1001	CYC	ND-C1D-CHD-C4C
28	MH	1001	CYC	C2D-C1D-CHD-C4C
28	NH	1001	CYC	ND-C1D-CHD-C4C
28	NH	1001	CYC	C2D-C1D-CHD-C4C
28	OH	1001	CYC	NA-C4A-CHB-C1B
28	OH	1001	CYC	C3A-C4A-CHB-C1B
28	OH	1001	CYC	ND-C1D-CHD-C4C
28	OH	1001	CYC	C2D-C1D-CHD-C4C
28	PH	1001	CYC	ND-C1D-CHD-C4C
28	PH	1001	CYC	C2D-C1D-CHD-C4C
28	QH	1001	CYC	NA-C4A-CHB-C1B
28	QH	1001	CYC	ND-C1D-CHD-C4C
28	QH	1001	CYC	C2D-C1D-CHD-C4C
28	RH	1001	CYC	ND-C1D-CHD-C4C
28	RH	1001	CYC	C2D-C1D-CHD-C4C
28	SH	1001	CYC	ND-C1D-CHD-C4C
28	SH	1001	CYC	C2D-C1D-CHD-C4C
28	TH	1001	CYC	NA-C4A-CHB-C1B
28	TH	1001	CYC	C4C-C3C-CAC-CBC
28	TH	1001	CYC	ND-C1D-CHD-C4C
28	TH	1001	CYC	C2D-C1D-CHD-C4C
28	UH	1001	CYC	ND-C1D-CHD-C4C
28	UH	1001	CYC	C2D-C1D-CHD-C4C
28	VH	1001	CYC	C3A-C4A-CHB-C1B
28	VH	1001	CYC	C2A-CAA-CBA-CGA
28	VH	1001	CYC	C2C-C3C-CAC-CBC
28	VH	1001	CYC	ND-C1D-CHD-C4C
28	VH	1001	CYC	C2D-C1D-CHD-C4C
28	WH	1001	CYC	ND-C1D-CHD-C4C
28	WH	1001	CYC	C2D-C1D-CHD-C4C
28	YH	1001	CYC	NA-C4A-CHB-C1B
28	YH	1001	CYC	ND-C1D-CHD-C4C
28	YH	1001	CYC	C2D-C1D-CHD-C4C
28	YH	1002	CYC	NA-C4A-CHB-C1B
28	YH	1002	CYC	C3A-C4A-CHB-C1B
28	YH	1002	CYC	ND-C1D-CHD-C4C
28	YH	1002	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
28	YH	1003	CYC	ND-C1D-CHD-C4C
28	YH	1003	CYC	C2D-C1D-CHD-C4C
28	YH	1004	CYC	NA-C4A-CHB-C1B
28	YH	1004	CYC	C3A-C4A-CHB-C1B
28	cH	1001	CYC	ND-C1D-CHD-C4C
28	cH	1001	CYC	C2D-C1D-CHD-C4C
28	dH	1001	CYC	NA-C4A-CHB-C1B
28	dH	1001	CYC	ND-C1D-CHD-C4C
28	dH	1001	CYC	C2D-C1D-CHD-C4C
28	eH	1001	CYC	C4B-C3B-CAB-CBB
28	eH	1001	CYC	ND-C1D-CHD-C4C
28	eH	1001	CYC	C2D-C1D-CHD-C4C
28	fH	1001	CYC	ND-C1D-CHD-C4C
28	fH	1001	CYC	C2D-C1D-CHD-C4C
28	gH	1001	CYC	ND-C1D-CHD-C4C
28	gH	1001	CYC	C2D-C1D-CHD-C4C
28	hH	1001	CYC	NA-C4A-CHB-C1B
28	hH	1001	CYC	C3A-C4A-CHB-C1B
28	hH	1001	CYC	ND-C1D-CHD-C4C
28	hH	1001	CYC	C2D-C1D-CHD-C4C
28	iH	1001	CYC	C2C-C3C-CAC-CBC
28	iH	1001	CYC	ND-C1D-CHD-C4C
28	iH	1001	CYC	C2D-C1D-CHD-C4C
28	jH	1001	CYC	NA-C4A-CHB-C1B
28	jH	1001	CYC	ND-C1D-CHD-C4C
28	jH	1001	CYC	C2D-C1D-CHD-C4C
28	kH	1001	CYC	ND-C1D-CHD-C4C
28	kH	1001	CYC	C2D-C1D-CHD-C4C
28	lH	1001	CYC	ND-C1D-CHD-C4C
28	lH	1001	CYC	C2D-C1D-CHD-C4C
28	mH	1001	CYC	ND-C1D-CHD-C4C
28	mH	1001	CYC	C2D-C1D-CHD-C4C
28	nH	1001	CYC	ND-C1D-CHD-C4C
28	nH	1001	CYC	C2D-C1D-CHD-C4C
28	oH	1001	CYC	NA-C4A-CHB-C1B
28	oH	1001	CYC	ND-C1D-CHD-C4C
28	oH	1001	CYC	C2D-C1D-CHD-C4C
28	pH	1001	CYC	ND-C1D-CHD-C4C
28	pH	1001	CYC	C2D-C1D-CHD-C4C
28	qH	1001	CYC	NA-C4A-CHB-C1B
28	qH	1001	CYC	C3A-C4A-CHB-C1B
28	qH	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
28	qH	1001	CYC	C2D-C1D-CHD-C4C
28	qH	1002	CYC	ND-C4D-CHA-C1A
28	qH	1002	CYC	C3D-C4D-CHA-C1A
28	qH	1002	CYC	ND-C1D-CHD-C4C
28	qH	1002	CYC	C2D-C1D-CHD-C4C
28	qH	1002	CYC	C3D-CAD-CBD-CGD
28	rH	1001	CYC	ND-C1D-CHD-C4C
28	rH	1001	CYC	C2D-C1D-CHD-C4C
28	sH	1001	CYC	NA-C4A-CHB-C1B
28	sH	1001	CYC	ND-C1D-CHD-C4C
28	sH	1001	CYC	C2D-C1D-CHD-C4C
28	tH	1001	CYC	C2C-C3C-CAC-CBC
28	tH	1001	CYC	ND-C1D-CHD-C4C
28	tH	1001	CYC	C2D-C1D-CHD-C4C
28	uH	1001	CYC	C2C-C3C-CAC-CBC
28	uH	1001	CYC	C4C-C3C-CAC-CBC
28	uH	1001	CYC	ND-C1D-CHD-C4C
28	uH	1001	CYC	C2D-C1D-CHD-C4C
28	vH	1001	CYC	NA-C4A-CHB-C1B
28	vH	1001	CYC	ND-C1D-CHD-C4C
28	vH	1001	CYC	C2D-C1D-CHD-C4C
28	wH	1001	CYC	ND-C1D-CHD-C4C
28	wH	1001	CYC	C2D-C1D-CHD-C4C
28	yH	1001	CYC	ND-C1D-CHD-C4C
28	yH	1001	CYC	C2D-C1D-CHD-C4C
28	lH	1000	CYC	C3A-C4A-CHB-C1B
28	CI	1001	CYC	NA-C4A-CHB-C1B
28	CI	1001	CYC	C3A-C4A-CHB-C1B
28	CI	1001	CYC	C2C-C3C-CAC-CBC
28	CI	1001	CYC	C4C-C3C-CAC-CBC
28	DI	1001	CYC	NA-C4A-CHB-C1B
28	DI	1001	CYC	C3A-C4A-CHB-C1B
28	DI	1001	CYC	C2C-C3C-CAC-CBC
28	DI	1001	CYC	C4C-C3C-CAC-CBC
28	DI	1001	CYC	ND-C1D-CHD-C4C
28	EI	1001	CYC	NA-C4A-CHB-C1B
28	EI	1001	CYC	C3A-C4A-CHB-C1B
28	FI	1001	CYC	NA-C4A-CHB-C1B
28	FI	1001	CYC	C3A-C4A-CHB-C1B
28	FI	1001	CYC	C2C-C3C-CAC-CBC
28	FI	1001	CYC	C4C-C3C-CAC-CBC
28	GI	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
28	GI	1001	CYC	C3A-C4A-CHB-C1B
28	HI	1001	CYC	NA-C4A-CHB-C1B
28	HI	1001	CYC	C3A-C4A-CHB-C1B
28	HI	1001	CYC	C2C-C3C-CAC-CBC
28	HI	1001	CYC	C4C-C3C-CAC-CBC
28	HI	1001	CYC	ND-C1D-CHD-C4C
28	II	1001	CYC	NA-C4A-CHB-C1B
28	II	1001	CYC	C3A-C4A-CHB-C1B
28	II	1001	CYC	C2C-C3C-CAC-CBC
28	II	1001	CYC	C4C-C3C-CAC-CBC
28	JI	1001	CYC	C2C-C3C-CAC-CBC
28	JI	1001	CYC	C4C-C3C-CAC-CBC
28	KI	1001	CYC	NA-C4A-CHB-C1B
28	KI	1001	CYC	C3A-C4A-CHB-C1B
28	KI	1001	CYC	C2C-C3C-CAC-CBC
28	KI	1001	CYC	C4C-C3C-CAC-CBC
28	LI	1001	CYC	ND-C1D-CHD-C4C
28	MI	1001	CYC	NA-C4A-CHB-C1B
28	MI	1001	CYC	C3A-C4A-CHB-C1B
28	MI	1001	CYC	C2C-C3C-CAC-CBC
28	MI	1001	CYC	C4C-C3C-CAC-CBC
28	NI	1001	CYC	NA-C4A-CHB-C1B
28	NI	1001	CYC	C3A-C4A-CHB-C1B
28	NI	1001	CYC	C2C-C3C-CAC-CBC
28	NI	1001	CYC	C4C-C3C-CAC-CBC
28	YH	1001	CYC	C2B-C3B-CAB-CBB
27	yE	302	PUB	C2D-C3D-CAD-CBD
28	CH	1001	CYC	C2B-C3B-CAB-CBB
28	F2	1001	CYC	C2B-C3B-CAB-CBB
28	eH	1001	CYC	C2B-C3B-CAB-CBB
27	yG	302	PUB	C2D-C3D-CAD-CBD
28	E6	1001	CYC	C2B-C3B-CAB-CBB
26	H3	203	PEB	C2B-C3B-CAB-CBB
26	A4	201	PEB	C2B-C3B-CAB-CBB
26	VA	202	PEB	C2B-C3B-CAB-CBB
26	kI	203	PEB	C2B-C3B-CAB-CBB
28	EB	1001	CYC	C2B-C3B-CAB-CBB
28	B6	1001	CYC	C2B-C3B-CAB-CBB
28	BB	1001	CYC	C2B-C3B-CAB-CBB
26	j1	201	PEB	C4B-C3B-CAB-CBB
26	g2	203	PEB	C4B-C3B-CAB-CBB
26	H3	203	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	G6	1002	PEB	C4B-C3B-CAB-CBB
26	V8	202	PEB	C4B-C3B-CAB-CBB
26	m8	202	PEB	C4B-C3B-CAB-CBB
26	GB	1002	PEB	C4B-C3B-CAB-CBB
26	HD	203	PEB	C4B-C3B-CAB-CBB
26	gI	203	PEB	C4B-C3B-CAB-CBB
28	qH	1002	CYC	C2B-C3B-CAB-CBB
28	qH	1002	CYC	C2B-C1B-CHB-C4A
27	AF	304	PUB	C4A-C3A-CAA-CBA
28	C6	1001	CYC	C2B-C3B-CAB-CBB
28	NI	1001	CYC	C3A-C2A-CAA-CBA
28	CB	1001	CYC	C2B-C3B-CAB-CBB
26	D1	203	PEB	C3B-CAB-CBB-CGB
26	F1	202	PEB	C3B-CAB-CBB-CGB
26	J1	202	PEB	C3B-CAB-CBB-CGB
26	J1	203	PEB	C3B-CAB-CBB-CGB
26	R1	202	PEB	C3B-CAB-CBB-CGB
26	m1	202	PEB	C3B-CAB-CBB-CGB
26	q1	201	PEB	C3B-CAB-CBB-CGB
26	t1	201	PEB	C3B-CAB-CBB-CGB
26	w1	203	PEB	C3B-CAB-CBB-CGB
26	21	401	PEB	C3B-CAB-CBB-CGB
26	A2	305	PEB	C3B-CAB-CBB-CGB
26	F2	1002	PEB	C3B-CAB-CBB-CGB
26	H2	1002	PEB	C3B-CAB-CBB-CGB
26	J2	1002	PEB	C3B-CAB-CBB-CGB
26	R2	203	PEB	C3B-CAB-CBB-CGB
26	f2	201	PEB	C3B-CAB-CBB-CGB
26	E3	201	PEB	C3B-CAB-CBB-CGB
26	O3	201	PEB	C3B-CAB-CBB-CGB
26	T3	203	PEB	C3B-CAB-CBB-CGB
26	A4	202	PEB	C3B-CAB-CBB-CGB
26	E4	202	PEB	C3B-CAB-CBB-CGB
26	F4	202	PEB	C3B-CAB-CBB-CGB
26	H4	201	PEB	C3B-CAB-CBB-CGB
26	j4	202	PEB	C3B-CAB-CBB-CGB
26	s4	202	PEB	C3B-CAB-CBB-CGB
26	14	202	PEB	C3B-CAB-CBB-CGB
26	24	401	PEB	C3B-CAB-CBB-CGB
26	F5	203	PEB	C3B-CAB-CBB-CGB
26	L5	203	PEB	C3B-CAB-CBB-CGB
26	O6	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	P6	202	PEB	C3B-CAB-CBB-CGB
26	Q6	203	PEB	C3B-CAB-CBB-CGB
26	W6	203	PEB	C3B-CAB-CBB-CGB
26	f6	202	PEB	C3B-CAB-CBB-CGB
26	h6	202	PEB	C3B-CAB-CBB-CGB
26	l6	202	PEB	C3B-CAB-CBB-CGB
26	A7	301	PEB	C3B-CAB-CBB-CGB
26	A7	302	PEB	C3B-CAB-CBB-CGB
26	F7	1002	PEB	C3B-CAB-CBB-CGB
26	J7	1002	PEB	C3B-CAB-CBB-CGB
26	L7	1002	PEB	C3B-CAB-CBB-CGB
26	N7	1002	PEB	C3B-CAB-CBB-CGB
26	P7	202	PEB	C3B-CAB-CBB-CGB
26	R7	202	PEB	C3B-CAB-CBB-CGB
26	c7	202	PEB	C3B-CAB-CBB-CGB
26	f7	203	PEB	C3B-CAB-CBB-CGB
26	g7	201	PEB	C3B-CAB-CBB-CGB
26	g7	202	PEB	C3B-CAB-CBB-CGB
26	h7	202	PEB	C3B-CAB-CBB-CGB
26	E8	202	PEB	C3B-CAB-CBB-CGB
26	E8	203	PEB	C3B-CAB-CBB-CGB
26	I8	203	PEB	C3B-CAB-CBB-CGB
26	a8	202	PEB	C3B-CAB-CBB-CGB
26	l8	203	PEB	C3B-CAB-CBB-CGB
26	A9	304	PEB	C3B-CAB-CBB-CGB
26	H9	202	PEB	C3B-CAB-CBB-CGB
26	M9	202	PEB	C3B-CAB-CBB-CGB
26	N9	202	PEB	C3B-CAB-CBB-CGB
26	WA	202	PEB	C3B-CAB-CBB-CGB
26	lA	203	PEB	C3B-CAB-CBB-CGB
26	mA	202	PEB	C3B-CAB-CBB-CGB
26	OB	202	PEB	C3B-CAB-CBB-CGB
26	WB	202	PEB	C3B-CAB-CBB-CGB
26	WB	203	PEB	C3B-CAB-CBB-CGB
26	gB	202	PEB	C3B-CAB-CBB-CGB
26	lB	202	PEB	C3B-CAB-CBB-CGB
26	FC	203	PEB	C3B-CAB-CBB-CGB
26	ED	201	PEB	C3B-CAB-CBB-CGB
26	OD	201	PEB	C3B-CAB-CBB-CGB
26	YD	301	PEB	C3B-CAB-CBB-CGB
26	DE	203	PEB	C3B-CAB-CBB-CGB
26	GE	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	GE	203	PEB	C3B-CAB-CBB-CGB
26	KE	201	PEB	C3B-CAB-CBB-CGB
26	ZE	201	PEB	C3B-CAB-CBB-CGB
26	gE	203	PEB	C3B-CAB-CBB-CGB
26	hE	201	PEB	C3B-CAB-CBB-CGB
26	jE	201	PEB	C3B-CAB-CBB-CGB
26	kE	201	PEB	C3B-CAB-CBB-CGB
26	oE	203	PEB	C3B-CAB-CBB-CGB
26	rE	202	PEB	C3B-CAB-CBB-CGB
26	tE	201	PEB	C3B-CAB-CBB-CGB
26	wE	302	PEB	C3B-CAB-CBB-CGB
26	DF	1002	PEB	C3B-CAB-CBB-CGB
26	FF	1002	PEB	C3B-CAB-CBB-CGB
26	JF	1002	PEB	C3B-CAB-CBB-CGB
26	OF	202	PEB	C3B-CAB-CBB-CGB
26	QF	202	PEB	C3B-CAB-CBB-CGB
26	gF	201	PEB	C3B-CAB-CBB-CGB
26	hF	201	PEB	C3B-CAB-CBB-CGB
26	iF	202	PEB	C3B-CAB-CBB-CGB
26	lF	203	PEB	C3B-CAB-CBB-CGB
26	DG	203	PEB	C3B-CAB-CBB-CGB
26	GG	202	PEB	C3B-CAB-CBB-CGB
26	IG	201	PEB	C3B-CAB-CBB-CGB
26	KG	203	PEB	C3B-CAB-CBB-CGB
26	OG	201	PEB	C3B-CAB-CBB-CGB
26	PG	201	PEB	C3B-CAB-CBB-CGB
26	ZG	201	PEB	C3B-CAB-CBB-CGB
26	aG	201	PEB	C3B-CAB-CBB-CGB
26	dG	202	PEB	C3B-CAB-CBB-CGB
26	jG	201	PEB	C3B-CAB-CBB-CGB
26	lG	201	PEB	C3B-CAB-CBB-CGB
26	mG	201	PEB	C3B-CAB-CBB-CGB
26	qG	202	PEB	C3B-CAB-CBB-CGB
26	rG	202	PEB	C3B-CAB-CBB-CGB
26	wG	302	PEB	C3B-CAB-CBB-CGB
26	AI	305	PEB	C3B-CAB-CBB-CGB
26	HI	1002	PEB	C3B-CAB-CBB-CGB
26	JI	1002	PEB	C3B-CAB-CBB-CGB
26	RI	203	PEB	C3B-CAB-CBB-CGB
26	YI	203	PEB	C3B-CAB-CBB-CGB
26	iI	203	PEB	C3B-CAB-CBB-CGB
26	AJ	304	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	LJ	202	PEB	C3B-CAB-CBB-CGB
26	YJ	202	PEB	C3B-CAB-CBB-CGB
27	A6	302	PUB	C2C-CAC-CBC-CGC
27	AA	304	PUB	C2C-CAC-CBC-CGC
27	xE	306	PUB	C2C-CAC-CBC-CGC
28	NB	1001	CYC	C2A-CAA-CBA-CGA
28	LF	1001	CYC	C2A-CAA-CBA-CGA
28	KH	1001	CYC	C2A-CAA-CBA-CGA
28	QH	1001	CYC	C2A-CAA-CBA-CGA
28	pH	1001	CYC	C2A-CAA-CBA-CGA
26	Y8	202	PEB	C2B-C1B-CHA-C4A
26	H9	202	PEB	C2B-C1B-CHA-C4A
26	EA	202	PEB	C2B-C1B-CHA-C4A
26	YA	202	PEB	C2B-C1B-CHA-C4A
26	nE	201	PEB	C2B-C1B-CHA-C4A
26	VF	201	PEB	C2B-C1B-CHA-C4A
26	cF	202	PEB	C2B-C1B-CHA-C4A
26	gG	201	PEB	C2B-C1B-CHA-C4A
26	jG	201	PEB	C2B-C1B-CHA-C4A
28	QH	1001	CYC	C3A-C4A-CHB-C1B
28	E2	1001	CYC	C2B-C3B-CAB-CBB
28	EI	1001	CYC	C2B-C3B-CAB-CBB
28	NI	1001	CYC	C1A-C2A-CAA-CBA
28	G2	1001	CYC	C2B-C3B-CAB-CBB
28	I6	1001	CYC	C2B-C3B-CAB-CBB
28	KB	202	CYC	C2B-C3B-CAB-CBB
28	GI	1001	CYC	C2B-C3B-CAB-CBB
28	K6	202	CYC	C2B-C3B-CAB-CBB
28	IB	1001	CYC	C2B-C3B-CAB-CBB
28	oH	1001	CYC	C2B-C3B-CAB-CBB
26	A1	201	PEB	C2C-CAC-CBC-CGC
26	B1	203	PEB	C2C-CAC-CBC-CGC
26	C1	202	PEB	C2C-CAC-CBC-CGC
26	D1	202	PEB	C2C-CAC-CBC-CGC
26	D1	203	PEB	C2C-CAC-CBC-CGC
26	E1	201	PEB	C2C-CAC-CBC-CGC
26	F1	202	PEB	C2C-CAC-CBC-CGC
26	H1	201	PEB	C2C-CAC-CBC-CGC
26	I1	201	PEB	C2C-CAC-CBC-CGC
26	I1	202	PEB	C2C-CAC-CBC-CGC
26	J1	201	PEB	C2C-CAC-CBC-CGC
26	J1	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	K1	202	PEB	C2C-CAC-CBC-CGC
26	L1	203	PEB	C2C-CAC-CBC-CGC
26	M1	401	PEB	C2C-CAC-CBC-CGC
26	N1	203	PEB	C2C-CAC-CBC-CGC
26	R1	202	PEB	C2C-CAC-CBC-CGC
26	U1	202	PEB	C2C-CAC-CBC-CGC
26	X1	201	PEB	C2C-CAC-CBC-CGC
26	c1	201	PEB	C2C-CAC-CBC-CGC
26	e1	201	PEB	C2C-CAC-CBC-CGC
26	f1	201	PEB	C2C-CAC-CBC-CGC
26	f1	202	PEB	C2C-CAC-CBC-CGC
26	h1	202	PEB	C2C-CAC-CBC-CGC
26	i1	201	PEB	C2C-CAC-CBC-CGC
26	j1	202	PEB	C2C-CAC-CBC-CGC
26	l1	202	PEB	C2C-CAC-CBC-CGC
26	m1	202	PEB	C2C-CAC-CBC-CGC
26	q1	201	PEB	C2C-CAC-CBC-CGC
26	q1	202	PEB	C2C-CAC-CBC-CGC
26	r1	202	PEB	C2C-CAC-CBC-CGC
26	t1	201	PEB	C2C-CAC-CBC-CGC
26	v1	202	PEB	C2C-CAC-CBC-CGC
26	w1	202	PEB	C2C-CAC-CBC-CGC
26	11	202	PEB	C2C-CAC-CBC-CGC
26	21	404	PEB	C2C-CAC-CBC-CGC
26	D2	1002	PEB	C2C-CAC-CBC-CGC
26	J2	1002	PEB	C2C-CAC-CBC-CGC
26	V2	202	PEB	C2C-CAC-CBC-CGC
26	B3	201	PEB	C2C-CAC-CBC-CGC
26	E3	202	PEB	C2C-CAC-CBC-CGC
26	F3	203	PEB	C2C-CAC-CBC-CGC
26	J3	203	PEB	C2C-CAC-CBC-CGC
26	M3	202	PEB	C2C-CAC-CBC-CGC
26	P3	202	PEB	C2C-CAC-CBC-CGC
26	R3	202	PEB	C2C-CAC-CBC-CGC
26	T3	201	PEB	C2C-CAC-CBC-CGC
26	T3	203	PEB	C2C-CAC-CBC-CGC
26	V3	202	PEB	C2C-CAC-CBC-CGC
26	V3	203	PEB	C2C-CAC-CBC-CGC
26	W3	202	PEB	C2C-CAC-CBC-CGC
26	A4	201	PEB	C2C-CAC-CBC-CGC
26	B4	202	PEB	C2C-CAC-CBC-CGC
26	B4	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	C4	201	PEB	C2C-CAC-CBC-CGC
26	C4	202	PEB	C2C-CAC-CBC-CGC
26	D4	203	PEB	C2C-CAC-CBC-CGC
26	E4	201	PEB	C2C-CAC-CBC-CGC
26	E4	202	PEB	C2C-CAC-CBC-CGC
26	F4	202	PEB	C2C-CAC-CBC-CGC
26	H4	201	PEB	C2C-CAC-CBC-CGC
26	I4	201	PEB	C2C-CAC-CBC-CGC
26	I4	202	PEB	C2C-CAC-CBC-CGC
26	J4	203	PEB	C2C-CAC-CBC-CGC
26	L4	202	PEB	C2C-CAC-CBC-CGC
26	M4	401	PEB	C2C-CAC-CBC-CGC
26	N4	201	PEB	C2C-CAC-CBC-CGC
26	N4	203	PEB	C2C-CAC-CBC-CGC
26	T4	203	PEB	C2C-CAC-CBC-CGC
26	X4	201	PEB	C2C-CAC-CBC-CGC
26	Y4	201	PEB	C2C-CAC-CBC-CGC
26	a4	203	PEB	C2C-CAC-CBC-CGC
26	b4	501	PEB	C2C-CAC-CBC-CGC
26	c4	201	PEB	C2C-CAC-CBC-CGC
26	d4	202	PEB	C2C-CAC-CBC-CGC
26	e4	201	PEB	C2C-CAC-CBC-CGC
26	h4	203	PEB	C2C-CAC-CBC-CGC
26	k4	201	PEB	C2C-CAC-CBC-CGC
26	m4	202	PEB	C2C-CAC-CBC-CGC
26	q4	202	PEB	C2C-CAC-CBC-CGC
26	r4	202	PEB	C2C-CAC-CBC-CGC
26	t4	201	PEB	C2C-CAC-CBC-CGC
26	v4	202	PEB	C2C-CAC-CBC-CGC
26	y4	202	PEB	C2C-CAC-CBC-CGC
26	y4	203	PEB	C2C-CAC-CBC-CGC
26	24	405	PEB	C2C-CAC-CBC-CGC
26	A5	201	PEB	C2C-CAC-CBC-CGC
26	F5	203	PEB	C2C-CAC-CBC-CGC
26	G5	202	PEB	C2C-CAC-CBC-CGC
26	I5	203	PEB	C2C-CAC-CBC-CGC
26	J5	202	PEB	C2C-CAC-CBC-CGC
26	K5	201	PEB	C2C-CAC-CBC-CGC
26	L5	201	PEB	C2C-CAC-CBC-CGC
26	D6	1002	PEB	C2C-CAC-CBC-CGC
26	K6	201	PEB	C2C-CAC-CBC-CGC
26	L6	1002	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	N6	201	PEB	C2C-CAC-CBC-CGC
26	Q6	201	PEB	C2C-CAC-CBC-CGC
26	W6	201	PEB	C2C-CAC-CBC-CGC
26	d6	202	PEB	C2C-CAC-CBC-CGC
26	e6	203	PEB	C2C-CAC-CBC-CGC
26	f6	201	PEB	C2C-CAC-CBC-CGC
26	f6	202	PEB	C2C-CAC-CBC-CGC
26	f6	203	PEB	C2C-CAC-CBC-CGC
26	g6	201	PEB	C2C-CAC-CBC-CGC
26	i6	202	PEB	C2C-CAC-CBC-CGC
26	J7	1002	PEB	C2C-CAC-CBC-CGC
26	R7	201	PEB	C2C-CAC-CBC-CGC
26	S7	202	PEB	C2C-CAC-CBC-CGC
26	Z7	201	PEB	C2C-CAC-CBC-CGC
26	h7	203	PEB	C2C-CAC-CBC-CGC
26	j7	201	PEB	C2C-CAC-CBC-CGC
26	j7	203	PEB	C2C-CAC-CBC-CGC
26	k7	201	PEB	C2C-CAC-CBC-CGC
26	E8	203	PEB	C2C-CAC-CBC-CGC
26	F8	201	PEB	C2C-CAC-CBC-CGC
26	K8	202	PEB	C2C-CAC-CBC-CGC
26	L8	202	PEB	C2C-CAC-CBC-CGC
26	P8	202	PEB	C2C-CAC-CBC-CGC
26	R8	201	PEB	C2C-CAC-CBC-CGC
26	U8	201	PEB	C2C-CAC-CBC-CGC
26	V8	201	PEB	C2C-CAC-CBC-CGC
26	Y8	203	PEB	C2C-CAC-CBC-CGC
26	a8	202	PEB	C2C-CAC-CBC-CGC
26	a8	203	PEB	C2C-CAC-CBC-CGC
26	i8	201	PEB	C2C-CAC-CBC-CGC
26	i8	202	PEB	C2C-CAC-CBC-CGC
26	B9	203	PEB	C2C-CAC-CBC-CGC
26	E9	201	PEB	C2C-CAC-CBC-CGC
26	E9	202	PEB	C2C-CAC-CBC-CGC
26	G9	201	PEB	C2C-CAC-CBC-CGC
26	H9	201	PEB	C2C-CAC-CBC-CGC
26	H9	202	PEB	C2C-CAC-CBC-CGC
26	J9	201	PEB	C2C-CAC-CBC-CGC
26	J9	203	PEB	C2C-CAC-CBC-CGC
26	M9	201	PEB	C2C-CAC-CBC-CGC
26	M9	202	PEB	C2C-CAC-CBC-CGC
26	S9	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	S9	202	PEB	C2C-CAC-CBC-CGC
26	T9	201	PEB	C2C-CAC-CBC-CGC
26	T9	203	PEB	C2C-CAC-CBC-CGC
26	EA	203	PEB	C2C-CAC-CBC-CGC
26	FA	201	PEB	C2C-CAC-CBC-CGC
26	JA	201	PEB	C2C-CAC-CBC-CGC
26	PA	202	PEB	C2C-CAC-CBC-CGC
26	RA	201	PEB	C2C-CAC-CBC-CGC
26	WA	202	PEB	C2C-CAC-CBC-CGC
26	YA	203	PEB	C2C-CAC-CBC-CGC
26	aA	202	PEB	C2C-CAC-CBC-CGC
26	cA	202	PEB	C2C-CAC-CBC-CGC
26	iA	201	PEB	C2C-CAC-CBC-CGC
26	iA	202	PEB	C2C-CAC-CBC-CGC
26	mA	201	PEB	C2C-CAC-CBC-CGC
26	DB	1002	PEB	C2C-CAC-CBC-CGC
26	KB	201	PEB	C2C-CAC-CBC-CGC
26	LB	1002	PEB	C2C-CAC-CBC-CGC
26	NB	1002	PEB	C2C-CAC-CBC-CGC
26	QB	201	PEB	C2C-CAC-CBC-CGC
26	UB	203	PEB	C2C-CAC-CBC-CGC
26	WB	201	PEB	C2C-CAC-CBC-CGC
26	dB	201	PEB	C2C-CAC-CBC-CGC
26	dB	202	PEB	C2C-CAC-CBC-CGC
26	eB	202	PEB	C2C-CAC-CBC-CGC
26	fB	201	PEB	C2C-CAC-CBC-CGC
26	fB	202	PEB	C2C-CAC-CBC-CGC
26	gB	201	PEB	C2C-CAC-CBC-CGC
26	iB	201	PEB	C2C-CAC-CBC-CGC
26	iB	202	PEB	C2C-CAC-CBC-CGC
26	kB	201	PEB	C2C-CAC-CBC-CGC
26	AC	201	PEB	C2C-CAC-CBC-CGC
26	FC	203	PEB	C2C-CAC-CBC-CGC
26	GC	202	PEB	C2C-CAC-CBC-CGC
26	IC	201	PEB	C2C-CAC-CBC-CGC
26	KC	201	PEB	C2C-CAC-CBC-CGC
26	LC	201	PEB	C2C-CAC-CBC-CGC
26	AD	202	PEB	C2C-CAC-CBC-CGC
26	CD	202	PEB	C2C-CAC-CBC-CGC
26	DD	203	PEB	C2C-CAC-CBC-CGC
26	ED	201	PEB	C2C-CAC-CBC-CGC
26	ED	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	ID	201	PEB	C2C-CAC-CBC-CGC
26	JD	202	PEB	C2C-CAC-CBC-CGC
26	JD	203	PEB	C2C-CAC-CBC-CGC
26	KD	201	PEB	C2C-CAC-CBC-CGC
26	LD	201	PEB	C2C-CAC-CBC-CGC
26	MD	202	PEB	C2C-CAC-CBC-CGC
26	TD	201	PEB	C2C-CAC-CBC-CGC
26	UD	202	PEB	C2C-CAC-CBC-CGC
26	VD	201	PEB	C2C-CAC-CBC-CGC
26	VD	203	PEB	C2C-CAC-CBC-CGC
26	WD	202	PEB	C2C-CAC-CBC-CGC
26	YD	301	PEB	C2C-CAC-CBC-CGC
26	DE	202	PEB	C2C-CAC-CBC-CGC
26	DE	203	PEB	C2C-CAC-CBC-CGC
26	NE	202	PEB	C2C-CAC-CBC-CGC
26	OE	203	PEB	C2C-CAC-CBC-CGC
26	QE	203	PEB	C2C-CAC-CBC-CGC
26	RE	202	PEB	C2C-CAC-CBC-CGC
26	ZE	202	PEB	C2C-CAC-CBC-CGC
26	bE	202	PEB	C2C-CAC-CBC-CGC
26	eE	203	PEB	C2C-CAC-CBC-CGC
26	gE	201	PEB	C2C-CAC-CBC-CGC
26	hE	202	PEB	C2C-CAC-CBC-CGC
26	jE	202	PEB	C2C-CAC-CBC-CGC
26	kE	203	PEB	C2C-CAC-CBC-CGC
26	lE	202	PEB	C2C-CAC-CBC-CGC
26	mE	201	PEB	C2C-CAC-CBC-CGC
26	qE	203	PEB	C2C-CAC-CBC-CGC
26	tE	202	PEB	C2C-CAC-CBC-CGC
26	wE	303	PEB	C2C-CAC-CBC-CGC
26	xE	304	PEB	C2C-CAC-CBC-CGC
26	FF	1002	PEB	C2C-CAC-CBC-CGC
26	JF	1002	PEB	C2C-CAC-CBC-CGC
26	QF	201	PEB	C2C-CAC-CBC-CGC
26	RF	201	PEB	C2C-CAC-CBC-CGC
26	RF	202	PEB	C2C-CAC-CBC-CGC
26	SF	202	PEB	C2C-CAC-CBC-CGC
26	TF	202	PEB	C2C-CAC-CBC-CGC
26	UF	203	PEB	C2C-CAC-CBC-CGC
26	ZF	201	PEB	C2C-CAC-CBC-CGC
26	ZF	203	PEB	C2C-CAC-CBC-CGC
26	hF	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	jF	201	PEB	C2C-CAC-CBC-CGC
26	jF	202	PEB	C2C-CAC-CBC-CGC
26	jF	203	PEB	C2C-CAC-CBC-CGC
26	kF	201	PEB	C2C-CAC-CBC-CGC
26	lF	201	PEB	C2C-CAC-CBC-CGC
26	DG	202	PEB	C2C-CAC-CBC-CGC
26	DG	203	PEB	C2C-CAC-CBC-CGC
26	JG	201	PEB	C2C-CAC-CBC-CGC
26	LG	202	PEB	C2C-CAC-CBC-CGC
26	OG	203	PEB	C2C-CAC-CBC-CGC
26	QG	203	PEB	C2C-CAC-CBC-CGC
26	RG	202	PEB	C2C-CAC-CBC-CGC
26	ZG	202	PEB	C2C-CAC-CBC-CGC
26	bG	202	PEB	C2C-CAC-CBC-CGC
26	gG	202	PEB	C2C-CAC-CBC-CGC
26	hG	202	PEB	C2C-CAC-CBC-CGC
26	iG	201	PEB	C2C-CAC-CBC-CGC
26	iG	203	PEB	C2C-CAC-CBC-CGC
26	jG	202	PEB	C2C-CAC-CBC-CGC
26	oG	203	PEB	C2C-CAC-CBC-CGC
26	pG	202	PEB	C2C-CAC-CBC-CGC
26	tG	201	PEB	C2C-CAC-CBC-CGC
26	uG	201	PEB	C2C-CAC-CBC-CGC
26	uG	203	PEB	C2C-CAC-CBC-CGC
26	wG	303	PEB	C2C-CAC-CBC-CGC
26	xG	302	PEB	C2C-CAC-CBC-CGC
26	xG	303	PEB	C2C-CAC-CBC-CGC
26	xG	304	PEB	C2C-CAC-CBC-CGC
26	AI	301	PEB	C2C-CAC-CBC-CGC
26	NI	1002	PEB	C2C-CAC-CBC-CGC
26	VI	202	PEB	C2C-CAC-CBC-CGC
26	hI	202	PEB	C2C-CAC-CBC-CGC
26	kI	202	PEB	C2C-CAC-CBC-CGC
26	EJ	201	PEB	C2C-CAC-CBC-CGC
26	EJ	202	PEB	C2C-CAC-CBC-CGC
26	GJ	201	PEB	C2C-CAC-CBC-CGC
26	GJ	202	PEB	C2C-CAC-CBC-CGC
26	HJ	202	PEB	C2C-CAC-CBC-CGC
26	JJ	201	PEB	C2C-CAC-CBC-CGC
26	JJ	203	PEB	C2C-CAC-CBC-CGC
26	MJ	201	PEB	C2C-CAC-CBC-CGC
26	SJ	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	SJ	202	PEB	C2C-CAC-CBC-CGC
26	TJ	201	PEB	C2C-CAC-CBC-CGC
26	TJ	203	PEB	C2C-CAC-CBC-CGC
27	K1	203	PUB	C3B-CAB-CBB-CGB
27	K4	203	PUB	C3B-CAB-CBB-CGB
27	QA	201	PUB	C3B-CAB-CBB-CGB
27	wE	304	PUB	C3B-CAB-CBB-CGB
27	xG	305	PUB	C3B-CAB-CBB-CGB
28	FH	1001	CYC	C2B-C3B-CAB-CBB
28	NI	1001	CYC	C2B-C3B-CAB-CBB
26	kI	203	PEB	NB-C4B-CHB-C1C
28	F2	1001	CYC	C4B-C3B-CAB-CBB
28	B6	1001	CYC	C4B-C3B-CAB-CBB
28	E6	1001	CYC	C4B-C3B-CAB-CBB
28	BB	1001	CYC	C4B-C3B-CAB-CBB
28	EB	1001	CYC	C4B-C3B-CAB-CBB
28	YH	1001	CYC	C4B-C3B-CAB-CBB
28	qH	1002	CYC	C4B-C3B-CAB-CBB
26	n4	201	PEB	C4B-C3B-CAB-CBB
28	FH	1001	CYC	NB-C1B-CHB-C4A
26	E1	202	PEB	C3B-CAB-CBB-CGB
26	F1	203	PEB	C3B-CAB-CBB-CGB
26	G1	202	PEB	C3B-CAB-CBB-CGB
26	H1	203	PEB	C3B-CAB-CBB-CGB
26	J1	201	PEB	C3B-CAB-CBB-CGB
26	M1	401	PEB	C3B-CAB-CBB-CGB
26	S1	202	PEB	C3B-CAB-CBB-CGB
26	U1	202	PEB	C3B-CAB-CBB-CGB
26	a1	203	PEB	C3B-CAB-CBB-CGB
26	c1	202	PEB	C3B-CAB-CBB-CGB
26	f1	202	PEB	C3B-CAB-CBB-CGB
26	g1	202	PEB	C3B-CAB-CBB-CGB
26	i1	203	PEB	C3B-CAB-CBB-CGB
26	j1	202	PEB	C3B-CAB-CBB-CGB
26	k1	202	PEB	C3B-CAB-CBB-CGB
26	l1	201	PEB	C3B-CAB-CBB-CGB
26	u1	201	PEB	C3B-CAB-CBB-CGB
26	u1	203	PEB	C3B-CAB-CBB-CGB
26	w1	202	PEB	C3B-CAB-CBB-CGB
26	y1	201	PEB	C3B-CAB-CBB-CGB
26	L2	1002	PEB	C3B-CAB-CBB-CGB
26	Y2	203	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	c2	203	PEB	C3B-CAB-CBB-CGB
26	k2	202	PEB	C3B-CAB-CBB-CGB
26	k2	203	PEB	C3B-CAB-CBB-CGB
26	W3	202	PEB	C3B-CAB-CBB-CGB
26	Y3	301	PEB	C3B-CAB-CBB-CGB
26	Y3	303	PEB	C3B-CAB-CBB-CGB
26	D4	203	PEB	C3B-CAB-CBB-CGB
26	G4	202	PEB	C3B-CAB-CBB-CGB
26	J4	201	PEB	C3B-CAB-CBB-CGB
26	M4	401	PEB	C3B-CAB-CBB-CGB
26	P4	203	PEB	C3B-CAB-CBB-CGB
26	U4	202	PEB	C3B-CAB-CBB-CGB
26	c4	202	PEB	C3B-CAB-CBB-CGB
26	e4	202	PEB	C3B-CAB-CBB-CGB
26	g4	202	PEB	C3B-CAB-CBB-CGB
26	i4	202	PEB	C3B-CAB-CBB-CGB
26	k4	202	PEB	C3B-CAB-CBB-CGB
26	w4	203	PEB	C3B-CAB-CBB-CGB
26	G5	203	PEB	C3B-CAB-CBB-CGB
26	U6	203	PEB	C3B-CAB-CBB-CGB
26	W6	202	PEB	C3B-CAB-CBB-CGB
26	Z6	203	PEB	C3B-CAB-CBB-CGB
26	a6	202	PEB	C3B-CAB-CBB-CGB
26	i6	202	PEB	C3B-CAB-CBB-CGB
26	l6	203	PEB	C3B-CAB-CBB-CGB
26	D7	1002	PEB	C3B-CAB-CBB-CGB
26	Q7	203	PEB	C3B-CAB-CBB-CGB
26	S7	202	PEB	C3B-CAB-CBB-CGB
26	Y7	202	PEB	C3B-CAB-CBB-CGB
26	b7	202	PEB	C3B-CAB-CBB-CGB
26	b7	203	PEB	C3B-CAB-CBB-CGB
26	e7	202	PEB	C3B-CAB-CBB-CGB
26	h7	201	PEB	C3B-CAB-CBB-CGB
26	j7	203	PEB	C3B-CAB-CBB-CGB
26	k7	202	PEB	C3B-CAB-CBB-CGB
26	l7	203	PEB	C3B-CAB-CBB-CGB
26	m7	202	PEB	C3B-CAB-CBB-CGB
26	B8	301	PEB	C3B-CAB-CBB-CGB
26	O8	202	PEB	C3B-CAB-CBB-CGB
26	j8	202	PEB	C3B-CAB-CBB-CGB
26	L9	202	PEB	C3B-CAB-CBB-CGB
26	U9	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	Y9	201	PEB	C3B-CAB-CBB-CGB
26	Y9	202	PEB	C3B-CAB-CBB-CGB
26	BA	301	PEB	C3B-CAB-CBB-CGB
26	EA	202	PEB	C3B-CAB-CBB-CGB
26	EA	203	PEB	C3B-CAB-CBB-CGB
26	OA	202	PEB	C3B-CAB-CBB-CGB
26	QA	203	PEB	C3B-CAB-CBB-CGB
26	jA	202	PEB	C3B-CAB-CBB-CGB
26	PB	202	PEB	C3B-CAB-CBB-CGB
26	QB	203	PEB	C3B-CAB-CBB-CGB
26	UB	203	PEB	C3B-CAB-CBB-CGB
26	ZB	203	PEB	C3B-CAB-CBB-CGB
26	aB	202	PEB	C3B-CAB-CBB-CGB
26	hB	203	PEB	C3B-CAB-CBB-CGB
26	iB	202	PEB	C3B-CAB-CBB-CGB
26	LC	203	PEB	C3B-CAB-CBB-CGB
26	AD	201	PEB	C3B-CAB-CBB-CGB
26	BD	201	PEB	C3B-CAB-CBB-CGB
26	DD	202	PEB	C3B-CAB-CBB-CGB
26	YD	303	PEB	C3B-CAB-CBB-CGB
26	EE	202	PEB	C3B-CAB-CBB-CGB
26	HE	202	PEB	C3B-CAB-CBB-CGB
26	KE	203	PEB	C3B-CAB-CBB-CGB
26	LE	201	PEB	C3B-CAB-CBB-CGB
26	OE	202	PEB	C3B-CAB-CBB-CGB
26	PE	201	PEB	C3B-CAB-CBB-CGB
26	YE	201	PEB	C3B-CAB-CBB-CGB
26	aE	201	PEB	C3B-CAB-CBB-CGB
26	cE	201	PEB	C3B-CAB-CBB-CGB
26	cE	202	PEB	C3B-CAB-CBB-CGB
26	eE	201	PEB	C3B-CAB-CBB-CGB
26	gE	202	PEB	C3B-CAB-CBB-CGB
26	iE	202	PEB	C3B-CAB-CBB-CGB
26	jE	202	PEB	C3B-CAB-CBB-CGB
26	nE	201	PEB	C3B-CAB-CBB-CGB
26	sE	201	PEB	C3B-CAB-CBB-CGB
26	wE	301	PEB	C3B-CAB-CBB-CGB
26	xE	303	PEB	C3B-CAB-CBB-CGB
26	AF	302	PEB	C3B-CAB-CBB-CGB
26	RF	202	PEB	C3B-CAB-CBB-CGB
26	SF	202	PEB	C3B-CAB-CBB-CGB
26	YF	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	bF	202	PEB	C3B-CAB-CBB-CGB
26	cF	202	PEB	C3B-CAB-CBB-CGB
26	kF	202	PEB	C3B-CAB-CBB-CGB
26	EG	202	PEB	C3B-CAB-CBB-CGB
26	HG	202	PEB	C3B-CAB-CBB-CGB
26	LG	201	PEB	C3B-CAB-CBB-CGB
26	MG	202	PEB	C3B-CAB-CBB-CGB
26	UG	201	PEB	C3B-CAB-CBB-CGB
26	WG	201	PEB	C3B-CAB-CBB-CGB
26	WG	203	PEB	C3B-CAB-CBB-CGB
26	ZG	202	PEB	C3B-CAB-CBB-CGB
26	cG	201	PEB	C3B-CAB-CBB-CGB
26	eG	201	PEB	C3B-CAB-CBB-CGB
26	jG	202	PEB	C3B-CAB-CBB-CGB
26	nG	201	PEB	C3B-CAB-CBB-CGB
26	oG	201	PEB	C3B-CAB-CBB-CGB
26	qG	201	PEB	C3B-CAB-CBB-CGB
26	sG	201	PEB	C3B-CAB-CBB-CGB
26	wG	301	PEB	C3B-CAB-CBB-CGB
26	xG	303	PEB	C3B-CAB-CBB-CGB
26	LI	1002	PEB	C3B-CAB-CBB-CGB
26	aI	203	PEB	C3B-CAB-CBB-CGB
26	cI	203	PEB	C3B-CAB-CBB-CGB
26	iI	202	PEB	C3B-CAB-CBB-CGB
26	kI	202	PEB	C3B-CAB-CBB-CGB
26	JJ	201	PEB	C3B-CAB-CBB-CGB
26	UJ	202	PEB	C3B-CAB-CBB-CGB
28	AH	1001	CYC	C2A-CAA-CBA-CGA
28	EH	1001	CYC	C2A-CAA-CBA-CGA
28	GH	1001	CYC	C2A-CAA-CBA-CGA
28	TH	1001	CYC	C2A-CAA-CBA-CGA
28	cH	1001	CYC	C2A-CAA-CBA-CGA
28	dH	1001	CYC	C2A-CAA-CBA-CGA
28	gH	1001	CYC	C2A-CAA-CBA-CGA
28	vH	1001	CYC	C2A-CAA-CBA-CGA
28	I7	1001	CYC	C2B-C3B-CAB-CBB
26	D9	202	PEB	C2B-C1B-CHA-C4A
26	KA	201	PEB	C2B-C1B-CHA-C4A
28	J2	1001	CYC	C3A-C4A-CHB-C1B
28	UH	1001	CYC	C3A-C4A-CHB-C1B
28	fH	1001	CYC	C3A-C4A-CHB-C1B
28	kH	1001	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
28	mH	1001	CYC	C3A-C4A-CHB-C1B
28	nH	1001	CYC	C3A-C4A-CHB-C1B
28	qH	1002	CYC	C3A-C4A-CHB-C1B
28	rH	1001	CYC	C3A-C4A-CHB-C1B
28	wH	1001	CYC	C3A-C4A-CHB-C1B
27	B8	302	PUB	C2D-C3D-CAD-CBD
28	HF	1001	CYC	C2B-C3B-CAB-CBB
28	jH	1001	CYC	C2B-C3B-CAB-CBB
28	MI	1001	CYC	C2B-C3B-CAB-CBB
26	p1	202	PEB	C3B-C4B-CHB-C1C
26	r1	202	PEB	C3B-C4B-CHB-C1C
26	t1	202	PEB	C3B-C4B-CHB-C1C
26	v1	202	PEB	C3B-C4B-CHB-C1C
26	x1	202	PEB	C3B-C4B-CHB-C1C
26	z1	202	PEB	C3B-C4B-CHB-C1C
26	p4	202	PEB	C3B-C4B-CHB-C1C
26	r4	202	PEB	C3B-C4B-CHB-C1C
26	t4	202	PEB	C3B-C4B-CHB-C1C
26	v4	202	PEB	C3B-C4B-CHB-C1C
26	z4	202	PEB	C3B-C4B-CHB-C1C
26	qE	202	PEB	C3B-C4B-CHB-C1C
26	qG	202	PEB	C3B-C4B-CHB-C1C
27	BA	302	PUB	C2D-C3D-CAD-CBD
28	YH	1003	CYC	C2B-C3B-CAB-CBB
26	k2	203	PEB	C2B-C3B-CAB-CBB
28	MH	1001	CYC	C2B-C3B-CAB-CBB
26	AD	201	PEB	C2B-C3B-CAB-CBB
28	F2	1001	CYC	C3A-C2A-CAA-CBA
28	N2	1001	CYC	C3A-C2A-CAA-CBA
28	F2	1001	CYC	C1A-C2A-CAA-CBA
28	N2	1001	CYC	C1A-C2A-CAA-CBA
26	A1	202	PEB	C3B-CAB-CBB-CGB
26	E1	201	PEB	C3B-CAB-CBB-CGB
26	M1	403	PEB	C3B-CAB-CBB-CGB
26	V1	201	PEB	C3B-CAB-CBB-CGB
26	V1	202	PEB	C3B-CAB-CBB-CGB
26	e1	201	PEB	C3B-CAB-CBB-CGB
26	11	202	PEB	C3B-CAB-CBB-CGB
26	e2	202	PEB	C3B-CAB-CBB-CGB
26	g2	202	PEB	C3B-CAB-CBB-CGB
26	O3	201	PEB	NB-C1B-CHA-C4A
26	S3	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	E4	201	PEB	C3B-CAB-CBB-CGB
26	k4	201	PEB	C3B-CAB-CBB-CGB
26	k4	203	PEB	C3B-CAB-CBB-CGB
26	v4	202	PEB	C3B-CAB-CBB-CGB
26	J5	201	PEB	NB-C1B-CHA-C4A
26	K6	201	PEB	C3B-CAB-CBB-CGB
26	N6	201	PEB	C3B-CAB-CBB-CGB
26	m6	203	PEB	C3B-CAB-CBB-CGB
26	O7	202	PEB	C3B-CAB-CBB-CGB
26	a7	202	PEB	C3B-CAB-CBB-CGB
26	G8	201	PEB	NB-C1B-CHA-C4A
26	K8	201	PEB	NB-C1B-CHA-C4A
26	Q8	202	PEB	C3B-CAB-CBB-CGB
26	U8	202	PEB	NB-C1B-CHA-C4A
26	D9	202	PEB	NB-C1B-CHA-C4A
26	F9	201	PEB	C3B-CAB-CBB-CGB
26	GA	201	PEB	NB-C1B-CHA-C4A
26	KA	201	PEB	NB-C1B-CHA-C4A
26	QA	202	PEB	C3B-CAB-CBB-CGB
26	UA	202	PEB	NB-C1B-CHA-C4A
26	DB	1002	PEB	C3B-CAB-CBB-CGB
26	KB	201	PEB	C3B-CAB-CBB-CGB
26	NB	1002	PEB	C3B-CAB-CBB-CGB
26	hB	201	PEB	C3B-CAB-CBB-CGB
26	mB	203	PEB	C3B-CAB-CBB-CGB
26	JC	201	PEB	NB-C1B-CHA-C4A
26	OD	201	PEB	NB-C1B-CHA-C4A
26	SD	201	PEB	NB-C1B-CHA-C4A
26	KE	202	PEB	C3B-CAB-CBB-CGB
26	QE	201	PEB	C3B-CAB-CBB-CGB
26	UE	201	PEB	C3B-CAB-CBB-CGB
26	WE	201	PEB	C3B-CAB-CBB-CGB
26	eE	203	PEB	NB-C1B-CHA-C4A
26	gE	201	PEB	NB-C1B-CHA-C4A
26	mE	203	PEB	C3B-CAB-CBB-CGB
26	oE	201	PEB	NB-C1B-CHA-C4A
26	qE	202	PEB	C3B-CAB-CBB-CGB
26	qE	203	PEB	C3B-CAB-CBB-CGB
26	QF	202	PEB	NB-C1B-CHA-C4A
26	fF	203	PEB	C3B-CAB-CBB-CGB
26	OG	202	PEB	C3B-CAB-CBB-CGB
26	QG	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	cG	202	PEB	C3B-CAB-CBB-CGB
26	AI	304	PEB	C3B-CAB-CBB-CGB
26	UI	201	PEB	NB-C1B-CHA-C4A
26	eI	202	PEB	C3B-CAB-CBB-CGB
26	fI	201	PEB	C3B-CAB-CBB-CGB
26	gI	202	PEB	C3B-CAB-CBB-CGB
26	kI	203	PEB	C3B-CAB-CBB-CGB
26	DJ	202	PEB	NB-C1B-CHA-C4A
26	FJ	201	PEB	C3B-CAB-CBB-CGB
26	MJ	202	PEB	C3B-CAB-CBB-CGB
26	VJ	201	PEB	C3B-CAB-CBB-CGB
28	E2	1001	CYC	C2A-CAA-CBA-CGA
28	J2	1001	CYC	NA-C4A-CHB-C1B
28	L2	1001	CYC	NA-C4A-CHB-C1B
28	N2	1001	CYC	C2A-CAA-CBA-CGA
28	B6	1002	CYC	NA-C4A-CHB-C1B
28	B6	1002	CYC	C2A-CAA-CBA-CGA
28	L6	1001	CYC	NA-C4A-CHB-C1B
28	LB	1001	CYC	NA-C4A-CHB-C1B
28	NB	1001	CYC	NA-C4A-CHB-C1B
28	JF	1003	CYC	C2A-CAA-CBA-CGA
28	AH	1001	CYC	NA-C4A-CHB-C1B
28	CH	1001	CYC	NA-C4A-CHB-C1B
28	EH	1001	CYC	NA-C4A-CHB-C1B
28	GH	1001	CYC	NA-C4A-CHB-C1B
28	IH	1001	CYC	NA-C4A-CHB-C1B
28	JH	1001	CYC	NA-C4A-CHB-C1B
28	KH	1001	CYC	NA-C4A-CHB-C1B
28	LH	1001	CYC	NA-C4A-CHB-C1B
28	NH	1001	CYC	NA-C4A-CHB-C1B
28	PH	1001	CYC	NA-C4A-CHB-C1B
28	RH	1001	CYC	NA-C4A-CHB-C1B
28	SH	1001	CYC	NA-C4A-CHB-C1B
28	UH	1001	CYC	NA-C4A-CHB-C1B
28	VH	1001	CYC	NA-C4A-CHB-C1B
28	WH	1001	CYC	NA-C4A-CHB-C1B
28	YH	1003	CYC	NA-C4A-CHB-C1B
28	cH	1001	CYC	NA-C4A-CHB-C1B
28	eH	1001	CYC	NA-C4A-CHB-C1B
28	fH	1001	CYC	NA-C4A-CHB-C1B
28	gH	1001	CYC	NA-C4A-CHB-C1B
28	iH	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
28	kH	1001	CYC	NA-C4A-CHB-C1B
28	lH	1001	CYC	NA-C4A-CHB-C1B
28	mH	1001	CYC	NA-C4A-CHB-C1B
28	nH	1001	CYC	NA-C4A-CHB-C1B
28	pH	1001	CYC	NA-C4A-CHB-C1B
28	rH	1001	CYC	NA-C4A-CHB-C1B
28	tH	1001	CYC	NA-C4A-CHB-C1B
28	uH	1001	CYC	NA-C4A-CHB-C1B
28	wH	1001	CYC	NA-C4A-CHB-C1B
28	yH	1001	CYC	NA-C4A-CHB-C1B
28	1H	1000	CYC	NA-C4A-CHB-C1B
28	EI	1001	CYC	C2A-CAA-CBA-CGA
28	JI	1001	CYC	NA-C4A-CHB-C1B
28	LI	1001	CYC	NA-C4A-CHB-C1B
26	U2	201	PEB	C2B-C1B-CHA-C4A
26	S3	201	PEB	C2B-C1B-CHA-C4A
26	U3	201	PEB	C2B-C1B-CHA-C4A
26	J5	201	PEB	C2B-C1B-CHA-C4A
26	G8	201	PEB	C2B-C1B-CHA-C4A
26	K8	201	PEB	C2B-C1B-CHA-C4A
26	U8	202	PEB	C2B-C1B-CHA-C4A
26	W8	201	PEB	C2B-C1B-CHA-C4A
26	GA	201	PEB	C2B-C1B-CHA-C4A
26	UA	202	PEB	C2B-C1B-CHA-C4A
26	WA	201	PEB	C2B-C1B-CHA-C4A
26	JC	201	PEB	C2B-C1B-CHA-C4A
26	SD	201	PEB	C2B-C1B-CHA-C4A
26	UD	201	PEB	C2B-C1B-CHA-C4A
26	cE	203	PEB	C2B-C1B-CHA-C4A
26	eE	203	PEB	C2B-C1B-CHA-C4A
26	gE	201	PEB	C2B-C1B-CHA-C4A
26	oE	201	PEB	C2B-C1B-CHA-C4A
26	oE	203	PEB	C2B-C1B-CHA-C4A
26	QF	202	PEB	C2B-C1B-CHA-C4A
26	SG	202	PEB	C2B-C1B-CHA-C4A
26	UI	201	PEB	C2B-C1B-CHA-C4A
26	DJ	202	PEB	C2B-C1B-CHA-C4A
26	HJ	202	PEB	C2B-C1B-CHA-C4A
28	L2	1001	CYC	C3A-C4A-CHB-C1B
28	B6	1002	CYC	C3A-C4A-CHB-C1B
28	L6	1001	CYC	C3A-C4A-CHB-C1B
28	LB	1001	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
28	AH	1001	CYC	C3A-C4A-CHB-C1B
28	CH	1001	CYC	C3A-C4A-CHB-C1B
28	EH	1001	CYC	C3A-C4A-CHB-C1B
28	GH	1001	CYC	C3A-C4A-CHB-C1B
28	JH	1001	CYC	C3A-C4A-CHB-C1B
28	KH	1001	CYC	C3A-C4A-CHB-C1B
28	LH	1001	CYC	C3A-C4A-CHB-C1B
28	MH	1001	CYC	C3A-C4A-CHB-C1B
28	NH	1001	CYC	C3A-C4A-CHB-C1B
28	PH	1001	CYC	C3A-C4A-CHB-C1B
28	RH	1001	CYC	C3A-C4A-CHB-C1B
28	SH	1001	CYC	C3A-C4A-CHB-C1B
28	TH	1001	CYC	C3A-C4A-CHB-C1B
28	WH	1001	CYC	C3A-C4A-CHB-C1B
28	YH	1001	CYC	C3A-C4A-CHB-C1B
28	YH	1003	CYC	C3A-C4A-CHB-C1B
28	cH	1001	CYC	C3A-C4A-CHB-C1B
28	dH	1001	CYC	C3A-C4A-CHB-C1B
28	eH	1001	CYC	C3A-C4A-CHB-C1B
28	gH	1001	CYC	C3A-C4A-CHB-C1B
28	iH	1001	CYC	C3A-C4A-CHB-C1B
28	jH	1001	CYC	C3A-C4A-CHB-C1B
28	lH	1001	CYC	C3A-C4A-CHB-C1B
28	oH	1001	CYC	C3A-C4A-CHB-C1B
28	pH	1001	CYC	C3A-C4A-CHB-C1B
28	sH	1001	CYC	C3A-C4A-CHB-C1B
28	tH	1001	CYC	C3A-C4A-CHB-C1B
28	uH	1001	CYC	C3A-C4A-CHB-C1B
28	vH	1001	CYC	C3A-C4A-CHB-C1B
28	yH	1001	CYC	C3A-C4A-CHB-C1B
28	JI	1001	CYC	C3A-C4A-CHB-C1B
28	LI	1001	CYC	C3A-C4A-CHB-C1B
28	K2	1001	CYC	C2B-C3B-CAB-CBB
28	KI	1001	CYC	C2B-C3B-CAB-CBB
28	FH	1001	CYC	C2B-C1B-CHB-C4A
27	AF	304	PUB	C3C-C2C-CAC-CBC
28	M2	1001	CYC	C2B-C3B-CAB-CBB
26	B1	202	PEB	C2C-CAC-CBC-CGC
26	N1	201	PEB	C2C-CAC-CBC-CGC
26	Y1	201	PEB	C2C-CAC-CBC-CGC
26	k1	201	PEB	C2C-CAC-CBC-CGC
26	k1	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	l1	201	PEB	C2C-CAC-CBC-CGC
26	p1	201	PEB	C2C-CAC-CBC-CGC
26	y1	202	PEB	C2C-CAC-CBC-CGC
26	P2	201	PEB	C2C-CAC-CBC-CGC
26	T2	201	PEB	C2C-CAC-CBC-CGC
26	e3	401	PEB	C2C-CAC-CBC-CGC
26	N3	201	PEB	C2C-CAC-CBC-CGC
26	V3	201	PEB	C2C-CAC-CBC-CGC
26	D4	202	PEB	C2C-CAC-CBC-CGC
26	J4	201	PEB	C2C-CAC-CBC-CGC
26	J4	202	PEB	C2C-CAC-CBC-CGC
26	T4	202	PEB	C2C-CAC-CBC-CGC
26	k4	203	PEB	C2C-CAC-CBC-CGC
26	l4	201	PEB	C2C-CAC-CBC-CGC
26	p4	201	PEB	C2C-CAC-CBC-CGC
26	q4	203	PEB	C2C-CAC-CBC-CGC
26	s4	202	PEB	C2C-CAC-CBC-CGC
26	I5	201	PEB	C2C-CAC-CBC-CGC
26	k6	201	PEB	C2C-CAC-CBC-CGC
26	P7	201	PEB	C2C-CAC-CBC-CGC
26	U7	203	PEB	C2C-CAC-CBC-CGC
26	l7	201	PEB	C2C-CAC-CBC-CGC
26	m7	201	PEB	C2C-CAC-CBC-CGC
26	J8	201	PEB	C2C-CAC-CBC-CGC
26	m8	201	PEB	C2C-CAC-CBC-CGC
26	G9	202	PEB	C2C-CAC-CBC-CGC
26	K9	201	PEB	C2C-CAC-CBC-CGC
26	N9	202	PEB	C2C-CAC-CBC-CGC
26	KA	202	PEB	C2C-CAC-CBC-CGC
26	lA	201	PEB	C2C-CAC-CBC-CGC
26	mA	202	PEB	C2C-CAC-CBC-CGC
26	eD	401	PEB	C2C-CAC-CBC-CGC
26	ND	201	PEB	C2C-CAC-CBC-CGC
26	PD	202	PEB	C2C-CAC-CBC-CGC
26	RD	202	PEB	C2C-CAC-CBC-CGC
26	TE	202	PEB	C2C-CAC-CBC-CGC
26	XE	201	PEB	C2C-CAC-CBC-CGC
26	gE	203	PEB	C2C-CAC-CBC-CGC
26	rE	202	PEB	C2C-CAC-CBC-CGC
26	sE	203	PEB	C2C-CAC-CBC-CGC
26	PF	201	PEB	C2C-CAC-CBC-CGC
26	PF	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	eF	201	PEB	C2C-CAC-CBC-CGC
26	iF	201	PEB	C2C-CAC-CBC-CGC
26	mF	201	PEB	C2C-CAC-CBC-CGC
26	JG	202	PEB	C2C-CAC-CBC-CGC
26	NG	202	PEB	C2C-CAC-CBC-CGC
26	TG	202	PEB	C2C-CAC-CBC-CGC
26	VG	201	PEB	C2C-CAC-CBC-CGC
26	XG	201	PEB	C2C-CAC-CBC-CGC
26	gG	203	PEB	C2C-CAC-CBC-CGC
26	kG	201	PEB	C2C-CAC-CBC-CGC
26	qG	203	PEB	C2C-CAC-CBC-CGC
26	PI	201	PEB	C2C-CAC-CBC-CGC
26	TI	201	PEB	C2C-CAC-CBC-CGC
26	HJ	201	PEB	C2C-CAC-CBC-CGC
26	XJ	202	PEB	C2C-CAC-CBC-CGC
26	XJ	203	PEB	C2C-CAC-CBC-CGC
27	xE	301	PUB	C3B-CAB-CBB-CGB
27	xG	301	PUB	C3B-CAB-CBB-CGB
28	D6	1001	CYC	C4B-C3B-CAB-CBB
28	FI	1001	CYC	C4B-C3B-CAB-CBB
26	k2	203	PEB	C4B-C3B-CAB-CBB
28	qH	1002	CYC	NB-C1B-CHB-C4A
26	K1	201	PEB	C4D-C3D-CAD-CBD
26	L1	203	PEB	C4D-C3D-CAD-CBD
26	M1	402	PEB	C4D-C3D-CAD-CBD
26	i1	201	PEB	C4D-C3D-CAD-CBD
26	L2	1002	PEB	C4D-C3D-CAD-CBD
26	c2	202	PEB	C4D-C3D-CAD-CBD
26	i2	202	PEB	C4D-C3D-CAD-CBD
26	E3	201	PEB	C4D-C3D-CAD-CBD
26	G3	202	PEB	C4D-C3D-CAD-CBD
26	L3	202	PEB	C4D-C3D-CAD-CBD
26	P3	201	PEB	C4D-C3D-CAD-CBD
26	U3	201	PEB	C4D-C3D-CAD-CBD
26	V3	201	PEB	C4D-C3D-CAD-CBD
26	X3	202	PEB	C4D-C3D-CAD-CBD
26	M4	402	PEB	C4D-C3D-CAD-CBD
26	c4	202	PEB	C4D-C3D-CAD-CBD
26	f4	202	PEB	C4D-C3D-CAD-CBD
26	g4	202	PEB	C4D-C3D-CAD-CBD
26	h4	202	PEB	C4D-C3D-CAD-CBD
26	y4	203	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
26	l6	202	PEB	C4D-C3D-CAD-CBD
26	T7	202	PEB	C4D-C3D-CAD-CBD
26	U7	201	PEB	C4D-C3D-CAD-CBD
26	f7	201	PEB	C4D-C3D-CAD-CBD
26	h7	201	PEB	C4D-C3D-CAD-CBD
26	l7	202	PEB	C4D-C3D-CAD-CBD
26	W8	202	PEB	C4D-C3D-CAD-CBD
26	A9	301	PEB	C4D-C3D-CAD-CBD
26	H9	202	PEB	C4D-C3D-CAD-CBD
26	Q9	202	PEB	C4D-C3D-CAD-CBD
26	TA	202	PEB	C4D-C3D-CAD-CBD
26	WA	202	PEB	C4D-C3D-CAD-CBD
26	lB	202	PEB	C4D-C3D-CAD-CBD
26	GD	202	PEB	C4D-C3D-CAD-CBD
26	ID	201	PEB	C4D-C3D-CAD-CBD
26	YD	301	PEB	C4D-C3D-CAD-CBD
26	ME	203	PEB	C4D-C3D-CAD-CBD
26	OE	202	PEB	C4D-C3D-CAD-CBD
26	RE	202	PEB	C4D-C3D-CAD-CBD
26	aE	201	PEB	C4D-C3D-CAD-CBD
26	cE	202	PEB	C4D-C3D-CAD-CBD
26	cE	203	PEB	C4D-C3D-CAD-CBD
26	sE	201	PEB	C4D-C3D-CAD-CBD
26	TF	201	PEB	C4D-C3D-CAD-CBD
26	WF	201	PEB	C4D-C3D-CAD-CBD
26	bF	201	PEB	C4D-C3D-CAD-CBD
26	OG	202	PEB	C4D-C3D-CAD-CBD
26	RG	202	PEB	C4D-C3D-CAD-CBD
26	cG	202	PEB	C4D-C3D-CAD-CBD
26	oG	202	PEB	C4D-C3D-CAD-CBD
26	xG	303	PEB	C4D-C3D-CAD-CBD
26	LI	1002	PEB	C4D-C3D-CAD-CBD
26	cI	202	PEB	C4D-C3D-CAD-CBD
26	AJ	301	PEB	C4D-C3D-CAD-CBD
26	AJ	305	PEB	C4D-C3D-CAD-CBD
26	DJ	201	PEB	C4D-C3D-CAD-CBD
26	DJ	202	PEB	C4D-C3D-CAD-CBD
26	HJ	202	PEB	C4D-C3D-CAD-CBD
26	RJ	203	PEB	C4D-C3D-CAD-CBD
26	XJ	201	PEB	C4D-C3D-CAD-CBD
26	N1	202	PEB	C3B-CAB-CBB-CGB
26	T1	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	n1	201	PEB	C3B-CAB-CBB-CGB
26	A2	304	PEB	C3B-CAB-CBB-CGB
26	H3	203	PEB	C3B-CAB-CBB-CGB
26	I3	202	PEB	C3B-CAB-CBB-CGB
26	J3	203	PEB	C3B-CAB-CBB-CGB
26	X3	202	PEB	C3B-CAB-CBB-CGB
26	H4	203	PEB	C3B-CAB-CBB-CGB
26	T4	201	PEB	C3B-CAB-CBB-CGB
26	e4	201	PEB	C3B-CAB-CBB-CGB
26	s4	201	PEB	C3B-CAB-CBB-CGB
26	y4	201	PEB	C3B-CAB-CBB-CGB
26	D6	1002	PEB	C3B-CAB-CBB-CGB
26	d6	203	PEB	C3B-CAB-CBB-CGB
26	Q7	202	PEB	C3B-CAB-CBB-CGB
26	Z7	202	PEB	C3B-CAB-CBB-CGB
26	d7	203	PEB	C3B-CAB-CBB-CGB
26	A8	301	PEB	C3B-CAB-CBB-CGB
26	K8	202	PEB	C3B-CAB-CBB-CGB
26	M8	201	PEB	C3B-CAB-CBB-CGB
26	U9	201	PEB	C3B-CAB-CBB-CGB
26	AA	301	PEB	C3B-CAB-CBB-CGB
26	IA	203	PEB	C3B-CAB-CBB-CGB
26	aA	202	PEB	C3B-CAB-CBB-CGB
26	dB	203	PEB	C3B-CAB-CBB-CGB
26	tE	202	PEB	C3B-CAB-CBB-CGB
26	uE	203	PEB	C3B-CAB-CBB-CGB
26	ZF	202	PEB	C3B-CAB-CBB-CGB
26	hF	203	PEB	C3B-CAB-CBB-CGB
26	jF	203	PEB	C3B-CAB-CBB-CGB
26	HG	201	PEB	C3B-CAB-CBB-CGB
26	KG	201	PEB	C3B-CAB-CBB-CGB
26	PG	202	PEB	C3B-CAB-CBB-CGB
26	XG	201	PEB	C3B-CAB-CBB-CGB
26	YG	202	PEB	C3B-CAB-CBB-CGB
26	lG	202	PEB	C3B-CAB-CBB-CGB
26	qG	203	PEB	C3B-CAB-CBB-CGB
26	cI	202	PEB	C3B-CAB-CBB-CGB
26	TJ	202	PEB	C3B-CAB-CBB-CGB
27	xG	305	PUB	C2C-CAC-CBC-CGC
28	tH	1001	CYC	C2A-CAA-CBA-CGA
28	D6	1001	CYC	C2B-C3B-CAB-CBB
28	LB	1001	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	vH	1001	CYC	C2B-C3B-CAB-CBB
26	AD	201	PEB	C4B-C3B-CAB-CBB
26	wE	303	PEB	C4B-C3B-CAB-CBB
26	wG	303	PEB	C4B-C3B-CAB-CBB
27	A7	304	PUB	C1C-C2C-CAC-CBC
27	AF	304	PUB	C1C-C2C-CAC-CBC
28	GB	1001	CYC	C2B-C3B-CAB-CBB
27	A7	304	PUB	C3C-C2C-CAC-CBC
28	G6	1001	CYC	C2B-C3B-CAB-CBB
26	K1	201	PEB	C2D-C3D-CAD-CBD
26	L1	203	PEB	C2D-C3D-CAD-CBD
26	M1	402	PEB	C2D-C3D-CAD-CBD
26	i1	201	PEB	C2D-C3D-CAD-CBD
26	t1	202	PEB	C2D-C3D-CAD-CBD
26	21	401	PEB	C2D-C3D-CAD-CBD
26	L2	1002	PEB	C2D-C3D-CAD-CBD
26	c2	202	PEB	C2D-C3D-CAD-CBD
26	i2	202	PEB	C2D-C3D-CAD-CBD
26	E3	201	PEB	C2D-C3D-CAD-CBD
26	E3	202	PEB	C2D-C3D-CAD-CBD
26	G3	202	PEB	C2D-C3D-CAD-CBD
26	L3	202	PEB	C2D-C3D-CAD-CBD
26	P3	201	PEB	C2D-C3D-CAD-CBD
26	U3	201	PEB	C2D-C3D-CAD-CBD
26	V3	201	PEB	C2D-C3D-CAD-CBD
26	X3	202	PEB	C2D-C3D-CAD-CBD
26	Y3	303	PEB	C2D-C3D-CAD-CBD
26	M4	402	PEB	C2D-C3D-CAD-CBD
26	c4	202	PEB	C2D-C3D-CAD-CBD
26	f4	202	PEB	C2D-C3D-CAD-CBD
26	g4	202	PEB	C2D-C3D-CAD-CBD
26	h4	202	PEB	C2D-C3D-CAD-CBD
26	y4	203	PEB	C2D-C3D-CAD-CBD
26	l6	202	PEB	C2D-C3D-CAD-CBD
26	U7	201	PEB	C2D-C3D-CAD-CBD
26	b7	201	PEB	C2D-C3D-CAD-CBD
26	f7	201	PEB	C2D-C3D-CAD-CBD
26	h7	201	PEB	C2D-C3D-CAD-CBD
26	l7	202	PEB	C2D-C3D-CAD-CBD
26	W8	202	PEB	C2D-C3D-CAD-CBD
26	A9	301	PEB	C2D-C3D-CAD-CBD
26	H9	201	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
26	H9	202	PEB	C2D-C3D-CAD-CBD
26	J9	201	PEB	C2D-C3D-CAD-CBD
26	Q9	202	PEB	C2D-C3D-CAD-CBD
26	V9	203	PEB	C2D-C3D-CAD-CBD
26	Y9	201	PEB	C2D-C3D-CAD-CBD
26	TA	202	PEB	C2D-C3D-CAD-CBD
26	WA	202	PEB	C2D-C3D-CAD-CBD
26	IB	202	PEB	C2D-C3D-CAD-CBD
26	FD	202	PEB	C2D-C3D-CAD-CBD
26	GD	202	PEB	C2D-C3D-CAD-CBD
26	ID	201	PEB	C2D-C3D-CAD-CBD
26	YD	301	PEB	C2D-C3D-CAD-CBD
26	ME	203	PEB	C2D-C3D-CAD-CBD
26	OE	202	PEB	C2D-C3D-CAD-CBD
26	RE	202	PEB	C2D-C3D-CAD-CBD
26	aE	201	PEB	C2D-C3D-CAD-CBD
26	cE	202	PEB	C2D-C3D-CAD-CBD
26	cE	203	PEB	C2D-C3D-CAD-CBD
26	sE	201	PEB	C2D-C3D-CAD-CBD
26	TF	201	PEB	C2D-C3D-CAD-CBD
26	TF	202	PEB	C2D-C3D-CAD-CBD
26	WF	201	PEB	C2D-C3D-CAD-CBD
26	bF	201	PEB	C2D-C3D-CAD-CBD
26	eF	202	PEB	C2D-C3D-CAD-CBD
26	OG	202	PEB	C2D-C3D-CAD-CBD
26	RG	202	PEB	C2D-C3D-CAD-CBD
26	cG	202	PEB	C2D-C3D-CAD-CBD
26	oG	202	PEB	C2D-C3D-CAD-CBD
26	xG	303	PEB	C2D-C3D-CAD-CBD
26	LI	1002	PEB	C2D-C3D-CAD-CBD
26	cI	202	PEB	C2D-C3D-CAD-CBD
26	AJ	301	PEB	C2D-C3D-CAD-CBD
26	AJ	305	PEB	C2D-C3D-CAD-CBD
26	DJ	202	PEB	C2D-C3D-CAD-CBD
26	HJ	202	PEB	C2D-C3D-CAD-CBD
26	RJ	203	PEB	C2D-C3D-CAD-CBD
26	XJ	201	PEB	C2D-C3D-CAD-CBD
28	TH	1001	CYC	C2B-C3B-CAB-CBB
26	CD	202	PEB	C3B-C4B-CHB-C1C
26	TD	203	PEB	C4B-C3B-CAB-CBB
26	GG	203	PEB	C4B-C3B-CAB-CBB
28	II	1001	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	I2	1001	CYC	C2B-C3B-CAB-CBB
26	O1	201	PEB	C3B-CAB-CBB-CGB
26	B4	201	PEB	C3B-CAB-CBB-CGB
26	K4	201	PEB	C3B-CAB-CBB-CGB
26	O4	201	PEB	C3B-CAB-CBB-CGB
26	V4	202	PEB	C3B-CAB-CBB-CGB
26	H6	1002	PEB	C3B-CAB-CBB-CGB
26	h6	201	PEB	C3B-CAB-CBB-CGB
26	V7	202	PEB	C3B-CAB-CBB-CGB
26	MA	201	PEB	C3B-CAB-CBB-CGB
26	HB	1002	PEB	C3B-CAB-CBB-CGB
26	JD	203	PEB	C3B-CAB-CBB-CGB
26	WD	202	PEB	C3B-CAB-CBB-CGB
26	XD	202	PEB	C3B-CAB-CBB-CGB
26	HE	201	PEB	C3B-CAB-CBB-CGB
26	QE	203	PEB	C3B-CAB-CBB-CGB
26	XE	201	PEB	C3B-CAB-CBB-CGB
26	gE	201	PEB	C3B-CAB-CBB-CGB
26	VF	203	PEB	C3B-CAB-CBB-CGB
26	bF	203	PEB	C3B-CAB-CBB-CGB
26	AG	201	PEB	C3B-CAB-CBB-CGB
26	VG	201	PEB	C3B-CAB-CBB-CGB
26	YG	203	PEB	C3B-CAB-CBB-CGB
26	gG	201	PEB	C3B-CAB-CBB-CGB
26	hG	201	PEB	C3B-CAB-CBB-CGB
26	YJ	201	PEB	C3B-CAB-CBB-CGB
27	A8	304	PUB	C2C-CAC-CBC-CGC
28	NI	1001	CYC	C2A-CAA-CBA-CGA
28	FI	1001	CYC	C2B-C3B-CAB-CBB
26	H1	202	PEB	C2A-C3A-CAA-CBA
26	J1	201	PEB	C2A-C3A-CAA-CBA
26	L1	201	PEB	C2A-C3A-CAA-CBA
26	L1	202	PEB	C2A-C3A-CAA-CBA
26	M1	403	PEB	C2C-CAC-CBC-CGC
26	N1	202	PEB	C2A-C3A-CAA-CBA
26	N1	203	PEB	C2A-C3A-CAA-CBA
26	P1	201	PEB	C2A-C3A-CAA-CBA
26	P1	203	PEB	C2A-C3A-CAA-CBA
26	R1	202	PEB	C2A-C3A-CAA-CBA
26	R1	203	PEB	C2A-C3A-CAA-CBA
26	T1	201	PEB	C2A-C3A-CAA-CBA
26	V1	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	X1	201	PEB	C2A-C3A-CAA-CBA
26	c1	203	PEB	C2A-C3A-CAA-CBA
26	j1	201	PEB	C2A-C3A-CAA-CBA
26	k1	201	PEB	C2A-C3A-CAA-CBA
26	k1	203	PEB	C2A-C3A-CAA-CBA
26	l1	201	PEB	C2A-C3A-CAA-CBA
26	m1	202	PEB	C2A-C3A-CAA-CBA
26	q1	202	PEB	C2A-C3A-CAA-CBA
26	q1	203	PEB	C2C-CAC-CBC-CGC
26	r1	202	PEB	C2A-C3A-CAA-CBA
26	u1	202	PEB	C2A-C3A-CAA-CBA
26	w1	201	PEB	C2A-C3A-CAA-CBA
26	w1	202	PEB	C2A-C3A-CAA-CBA
26	z1	201	PEB	C2A-C3A-CAA-CBA
26	J2	1002	PEB	C2A-C3A-CAA-CBA
26	N2	1002	PEB	C2A-C3A-CAA-CBA
26	Q2	201	PEB	C2A-C3A-CAA-CBA
26	Q2	202	PEB	C2C-CAC-CBC-CGC
26	R2	202	PEB	C2A-C3A-CAA-CBA
26	S2	202	PEB	C2A-C3A-CAA-CBA
26	W2	201	PEB	C2A-C3A-CAA-CBA
26	Z2	201	PEB	C2A-C3A-CAA-CBA
26	b2	201	PEB	C2A-C3A-CAA-CBA
26	d2	201	PEB	C2A-C3A-CAA-CBA
26	f2	202	PEB	C2A-C3A-CAA-CBA
26	g2	202	PEB	C2A-C3A-CAA-CBA
26	h2	201	PEB	C2A-C3A-CAA-CBA
26	h2	202	PEB	C2A-C3A-CAA-CBA
26	j2	201	PEB	C2A-C3A-CAA-CBA
26	k2	201	PEB	C2A-C3A-CAA-CBA
26	l2	201	PEB	C2A-C3A-CAA-CBA
26	A3	202	PEB	C2A-C3A-CAA-CBA
26	B3	202	PEB	C2A-C3A-CAA-CBA
26	C3	201	PEB	C2A-C3A-CAA-CBA
26	D3	202	PEB	C2A-C3A-CAA-CBA
26	E3	202	PEB	C2A-C3A-CAA-CBA
26	F3	202	PEB	C2A-C3A-CAA-CBA
26	G3	201	PEB	C2A-C3A-CAA-CBA
26	H3	202	PEB	C2A-C3A-CAA-CBA
26	I3	202	PEB	C2A-C3A-CAA-CBA
26	J3	202	PEB	C2A-C3A-CAA-CBA
26	L3	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	M3	202	PEB	C2A-C3A-CAA-CBA
26	N3	202	PEB	C2A-C3A-CAA-CBA
26	P3	202	PEB	C2A-C3A-CAA-CBA
26	Q3	202	PEB	C2A-C3A-CAA-CBA
26	R3	202	PEB	C2A-C3A-CAA-CBA
26	S3	202	PEB	C2A-C3A-CAA-CBA
26	T3	202	PEB	C2A-C3A-CAA-CBA
26	U3	202	PEB	C2A-C3A-CAA-CBA
26	W3	202	PEB	C2A-C3A-CAA-CBA
26	X3	202	PEB	C2A-C3A-CAA-CBA
26	B4	202	PEB	C2A-C3A-CAA-CBA
26	F4	201	PEB	C2A-C3A-CAA-CBA
26	H4	202	PEB	C2A-C3A-CAA-CBA
26	J4	201	PEB	C2A-C3A-CAA-CBA
26	L4	202	PEB	C2A-C3A-CAA-CBA
26	N4	202	PEB	C2A-C3A-CAA-CBA
26	N4	203	PEB	C2A-C3A-CAA-CBA
26	P4	201	PEB	C2A-C3A-CAA-CBA
26	R4	202	PEB	C2A-C3A-CAA-CBA
26	S4	201	PEB	C2A-C3A-CAA-CBA
26	T4	201	PEB	C2A-C3A-CAA-CBA
26	T4	202	PEB	C2A-C3A-CAA-CBA
26	V4	202	PEB	C2A-C3A-CAA-CBA
26	X4	201	PEB	C2A-C3A-CAA-CBA
26	b4	501	PEB	C2A-C3A-CAA-CBA
26	c4	203	PEB	C2A-C3A-CAA-CBA
26	d4	202	PEB	C2A-C3A-CAA-CBA
26	d4	203	PEB	C2C-CAC-CBC-CGC
26	e4	201	PEB	C2A-C3A-CAA-CBA
26	g4	203	PEB	C2A-C3A-CAA-CBA
26	i4	201	PEB	C2A-C3A-CAA-CBA
26	k4	203	PEB	C2A-C3A-CAA-CBA
26	m4	201	PEB	C2A-C3A-CAA-CBA
26	m4	202	PEB	C2A-C3A-CAA-CBA
26	p4	201	PEB	C2A-C3A-CAA-CBA
26	q4	202	PEB	C2A-C3A-CAA-CBA
26	r4	202	PEB	C2A-C3A-CAA-CBA
26	u4	202	PEB	C2A-C3A-CAA-CBA
26	v4	202	PEB	C2A-C3A-CAA-CBA
26	w4	202	PEB	C2A-C3A-CAA-CBA
26	x4	201	PEB	C2A-C3A-CAA-CBA
26	x4	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	24	401	PEB	C2A-C3A-CAA-CBA
26	24	405	PEB	C2A-C3A-CAA-CBA
26	J5	201	PEB	C2A-C3A-CAA-CBA
26	L6	1002	PEB	C2A-C3A-CAA-CBA
26	O6	201	PEB	C2A-C3A-CAA-CBA
26	O6	202	PEB	C2A-C3A-CAA-CBA
26	O6	203	PEB	C2A-C3A-CAA-CBA
26	Q6	201	PEB	C2A-C3A-CAA-CBA
26	S6	201	PEB	C2A-C3A-CAA-CBA
26	S6	203	PEB	C2A-C3A-CAA-CBA
26	U6	202	PEB	C2A-C3A-CAA-CBA
26	U6	203	PEB	C2A-C3A-CAA-CBA
26	a6	202	PEB	C2C-CAC-CBC-CGC
26	d6	202	PEB	C2A-C3A-CAA-CBA
26	f6	201	PEB	C2A-C3A-CAA-CBA
26	h6	202	PEB	C2A-C3A-CAA-CBA
26	j6	201	PEB	C2A-C3A-CAA-CBA
26	l6	202	PEB	C2A-C3A-CAA-CBA
26	A7	302	PEB	C2A-C3A-CAA-CBA
26	P7	202	PEB	C2C-CAC-CBC-CGC
26	T7	201	PEB	C2A-C3A-CAA-CBA
26	U7	202	PEB	C2A-C3A-CAA-CBA
26	W7	201	PEB	C2A-C3A-CAA-CBA
26	Y7	201	PEB	C2A-C3A-CAA-CBA
26	Y7	202	PEB	C2C-CAC-CBC-CGC
26	Z7	201	PEB	C2A-C3A-CAA-CBA
26	c7	201	PEB	C2A-C3A-CAA-CBA
26	f7	202	PEB	C2A-C3A-CAA-CBA
26	j7	203	PEB	C2A-C3A-CAA-CBA
26	E8	203	PEB	C2A-C3A-CAA-CBA
26	G8	203	PEB	C2A-C3A-CAA-CBA
26	I8	201	PEB	C2A-C3A-CAA-CBA
26	K8	203	PEB	C2A-C3A-CAA-CBA
26	M8	201	PEB	C2A-C3A-CAA-CBA
26	Q8	202	PEB	C2A-C3A-CAA-CBA
26	W8	203	PEB	C2A-C3A-CAA-CBA
26	Y8	201	PEB	C2A-C3A-CAA-CBA
26	Z8	202	PEB	C2A-C3A-CAA-CBA
26	d8	201	PEB	C2A-C3A-CAA-CBA
26	f8	202	PEB	C2A-C3A-CAA-CBA
26	B9	203	PEB	C2A-C3A-CAA-CBA
26	D9	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	D9	203	PEB	C2A-C3A-CAA-CBA
26	F9	203	PEB	C2A-C3A-CAA-CBA
26	H9	201	PEB	C2A-C3A-CAA-CBA
26	H9	203	PEB	C2A-C3A-CAA-CBA
26	J9	202	PEB	C2A-C3A-CAA-CBA
26	J9	203	PEB	C2A-C3A-CAA-CBA
26	L9	201	PEB	C2A-C3A-CAA-CBA
26	N9	203	PEB	C2A-C3A-CAA-CBA
26	N9	204	PEB	C2A-C3A-CAA-CBA
26	R9	201	PEB	C2A-C3A-CAA-CBA
26	R9	202	PEB	C2A-C3A-CAA-CBA
26	T9	201	PEB	C2A-C3A-CAA-CBA
26	V9	202	PEB	C2A-C3A-CAA-CBA
26	V9	203	PEB	C2A-C3A-CAA-CBA
26	X9	201	PEB	C2A-C3A-CAA-CBA
26	X9	203	PEB	C2A-C3A-CAA-CBA
26	GA	203	PEB	C2A-C3A-CAA-CBA
26	IA	201	PEB	C2A-C3A-CAA-CBA
26	IA	203	PEB	C2A-C3A-CAA-CBA
26	KA	203	PEB	C2A-C3A-CAA-CBA
26	MA	201	PEB	C2A-C3A-CAA-CBA
26	MA	203	PEB	C2A-C3A-CAA-CBA
26	OA	201	PEB	C2A-C3A-CAA-CBA
26	PA	202	PEB	C2A-C3A-CAA-CBA
26	QA	204	PEB	C2A-C3A-CAA-CBA
26	WA	203	PEB	C2A-C3A-CAA-CBA
26	YA	201	PEB	C2A-C3A-CAA-CBA
26	ZA	202	PEB	C2A-C3A-CAA-CBA
26	fA	202	PEB	C2A-C3A-CAA-CBA
26	iA	201	PEB	C2A-C3A-CAA-CBA
26	OB	201	PEB	C2A-C3A-CAA-CBA
26	OB	203	PEB	C2A-C3A-CAA-CBA
26	QB	203	PEB	C2A-C3A-CAA-CBA
26	SB	201	PEB	C2A-C3A-CAA-CBA
26	TB	202	PEB	C2C-CAC-CBC-CGC
26	UB	203	PEB	C2A-C3A-CAA-CBA
26	dB	202	PEB	C2A-C3A-CAA-CBA
26	fB	203	PEB	C2A-C3A-CAA-CBA
26	hB	202	PEB	C2A-C3A-CAA-CBA
26	lB	202	PEB	C2A-C3A-CAA-CBA
26	BC	201	PEB	C2A-C3A-CAA-CBA
26	HC	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	JC	202	PEB	C2C-CAC-CBC-CGC
26	DD	202	PEB	C2A-C3A-CAA-CBA
26	ED	202	PEB	C2A-C3A-CAA-CBA
26	FD	202	PEB	C2A-C3A-CAA-CBA
26	HD	202	PEB	C2A-C3A-CAA-CBA
26	JD	202	PEB	C2A-C3A-CAA-CBA
26	LD	202	PEB	C2A-C3A-CAA-CBA
26	MD	202	PEB	C2A-C3A-CAA-CBA
26	ND	202	PEB	C2A-C3A-CAA-CBA
26	PD	202	PEB	C2A-C3A-CAA-CBA
26	QD	202	PEB	C2A-C3A-CAA-CBA
26	RD	202	PEB	C2A-C3A-CAA-CBA
26	SD	202	PEB	C2A-C3A-CAA-CBA
26	TD	202	PEB	C2A-C3A-CAA-CBA
26	UD	202	PEB	C2A-C3A-CAA-CBA
26	XD	202	PEB	C2A-C3A-CAA-CBA
26	AE	202	PEB	C2A-C3A-CAA-CBA
26	DE	202	PEB	C2A-C3A-CAA-CBA
26	GE	202	PEB	C2A-C3A-CAA-CBA
26	IE	202	PEB	C2A-C3A-CAA-CBA
26	IE	203	PEB	C2A-C3A-CAA-CBA
26	JE	201	PEB	C2C-CAC-CBC-CGC
26	JE	202	PEB	C2C-CAC-CBC-CGC
26	OE	203	PEB	C2A-C3A-CAA-CBA
26	YE	203	PEB	C2A-C3A-CAA-CBA
26	aE	201	PEB	C2A-C3A-CAA-CBA
26	eE	201	PEB	C2C-CAC-CBC-CGC
26	fE	201	PEB	C2A-C3A-CAA-CBA
26	iE	201	PEB	C2C-CAC-CBC-CGC
26	iE	202	PEB	C2A-C3A-CAA-CBA
26	qE	201	PEB	C2A-C3A-CAA-CBA
26	qE	202	PEB	C2A-C3A-CAA-CBA
26	sE	201	PEB	C2A-C3A-CAA-CBA
26	uE	202	PEB	C2A-C3A-CAA-CBA
26	xE	302	PEB	C2A-C3A-CAA-CBA
26	xE	303	PEB	C2A-C3A-CAA-CBA
26	yE	301	PEB	C2A-C3A-CAA-CBA
26	AF	302	PEB	C2A-C3A-CAA-CBA
26	FF	1002	PEB	C2A-C3A-CAA-CBA
26	HF	1002	PEB	C2A-C3A-CAA-CBA
26	QF	203	PEB	C2A-C3A-CAA-CBA
26	TF	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	UF	202	PEB	C2A-C3A-CAA-CBA
26	WF	201	PEB	C2A-C3A-CAA-CBA
26	WF	202	PEB	C2A-C3A-CAA-CBA
26	YF	202	PEB	C2C-CAC-CBC-CGC
26	bF	203	PEB	C2A-C3A-CAA-CBA
26	dF	202	PEB	C2A-C3A-CAA-CBA
26	eF	201	PEB	C2A-C3A-CAA-CBA
26	eF	202	PEB	C2C-CAC-CBC-CGC
26	gF	201	PEB	C2A-C3A-CAA-CBA
26	CG	202	PEB	C2A-C3A-CAA-CBA
26	CG	203	PEB	C2A-C3A-CAA-CBA
26	DG	202	PEB	C2A-C3A-CAA-CBA
26	IG	201	PEB	C2A-C3A-CAA-CBA
26	IG	202	PEB	C2A-C3A-CAA-CBA
26	IG	203	PEB	C2A-C3A-CAA-CBA
26	JG	202	PEB	C2A-C3A-CAA-CBA
26	KG	201	PEB	C2A-C3A-CAA-CBA
26	MG	203	PEB	C2A-C3A-CAA-CBA
26	TG	202	PEB	C2A-C3A-CAA-CBA
26	UG	201	PEB	C2A-C3A-CAA-CBA
26	dG	202	PEB	C2C-CAC-CBC-CGC
26	eG	202	PEB	C2A-C3A-CAA-CBA
26	fG	201	PEB	C2A-C3A-CAA-CBA
26	iG	201	PEB	C2A-C3A-CAA-CBA
26	iG	202	PEB	C2A-C3A-CAA-CBA
26	iG	203	PEB	C2A-C3A-CAA-CBA
26	kG	201	PEB	C2A-C3A-CAA-CBA
26	lG	202	PEB	C2C-CAC-CBC-CGC
26	qG	202	PEB	C2A-C3A-CAA-CBA
26	qG	203	PEB	C2A-C3A-CAA-CBA
26	sG	201	PEB	C2A-C3A-CAA-CBA
26	uG	201	PEB	C2A-C3A-CAA-CBA
26	wG	302	PEB	C2C-CAC-CBC-CGC
26	xG	303	PEB	C2A-C3A-CAA-CBA
26	yG	301	PEB	C2A-C3A-CAA-CBA
26	AI	305	PEB	C2A-C3A-CAA-CBA
26	DI	1002	PEB	C2A-C3A-CAA-CBA
26	JI	1002	PEB	C2A-C3A-CAA-CBA
26	NI	1002	PEB	C2A-C3A-CAA-CBA
26	QI	201	PEB	C2A-C3A-CAA-CBA
26	SI	202	PEB	C2A-C3A-CAA-CBA
26	TI	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	WI	201	PEB	C2A-C3A-CAA-CBA
26	ZI	201	PEB	C2A-C3A-CAA-CBA
26	ZI	202	PEB	C2C-CAC-CBC-CGC
26	bI	201	PEB	C2A-C3A-CAA-CBA
26	fI	201	PEB	C2A-C3A-CAA-CBA
26	fI	202	PEB	C2A-C3A-CAA-CBA
26	hI	201	PEB	C2A-C3A-CAA-CBA
26	jI	201	PEB	C2A-C3A-CAA-CBA
26	kI	201	PEB	C2A-C3A-CAA-CBA
26	lI	201	PEB	C2A-C3A-CAA-CBA
26	lI	202	PEB	C2A-C3A-CAA-CBA
26	BJ	202	PEB	C2A-C3A-CAA-CBA
26	BJ	203	PEB	C2C-CAC-CBC-CGC
26	BJ	203	PEB	C2A-C3A-CAA-CBA
26	DJ	201	PEB	C2A-C3A-CAA-CBA
26	DJ	203	PEB	C2A-C3A-CAA-CBA
26	GJ	202	PEB	C2A-C3A-CAA-CBA
26	HJ	201	PEB	C2A-C3A-CAA-CBA
26	HJ	203	PEB	C2A-C3A-CAA-CBA
26	IJ	201	PEB	C2C-CAC-CBC-CGC
26	IJ	202	PEB	C2A-C3A-CAA-CBA
26	JJ	202	PEB	C2A-C3A-CAA-CBA
26	JJ	203	PEB	C2A-C3A-CAA-CBA
26	LJ	201	PEB	C2A-C3A-CAA-CBA
26	LJ	203	PEB	C2A-C3A-CAA-CBA
26	NJ	202	PEB	C2A-C3A-CAA-CBA
26	NJ	203	PEB	C2A-C3A-CAA-CBA
26	NJ	204	PEB	C2A-C3A-CAA-CBA
26	RJ	201	PEB	C2A-C3A-CAA-CBA
26	RJ	202	PEB	C2A-C3A-CAA-CBA
26	TJ	201	PEB	C2A-C3A-CAA-CBA
26	TJ	202	PEB	C2A-C3A-CAA-CBA
26	VJ	201	PEB	C2A-C3A-CAA-CBA
26	VJ	202	PEB	C2A-C3A-CAA-CBA
26	VJ	203	PEB	C2A-C3A-CAA-CBA
26	XJ	201	PEB	C2A-C3A-CAA-CBA
27	K3	203	PUB	C3B-CAB-CBB-CGB
27	AB	303	PUB	C3B-CAB-CBB-CGB
27	KD	203	PUB	C3B-CAB-CBB-CGB
27	yE	303	PUB	C3B-CAB-CBB-CGB
28	K6	202	CYC	C2C-C3C-CAC-CBC
28	K7	1001	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	KB	202	CYC	C2C-C3C-CAC-CBC
28	JF	1003	CYC	C2C-C3C-CAC-CBC
28	MH	1001	CYC	C2C-C3C-CAC-CBC
28	RH	1001	CYC	C2C-C3C-CAC-CBC
28	TH	1001	CYC	C2C-C3C-CAC-CBC
28	vH	1001	CYC	C2C-C3C-CAC-CBC
26	QI	202	PEB	NB-C4B-CHB-C1C
26	I8	201	PEB	C4B-C3B-CAB-CBB
26	PA	201	PEB	C4B-C3B-CAB-CBB
26	cA	202	PEB	C4B-C3B-CAB-CBB
26	aI	203	PEB	C4B-C3B-CAB-CBB
26	IJ	203	PEB	C4B-C3B-CAB-CBB
28	sH	1001	CYC	C1A-C2A-CAA-CBA
28	NH	1001	CYC	C2B-C3B-CAB-CBB
28	sH	1001	CYC	C2B-C3B-CAB-CBB
26	n4	201	PEB	C2B-C3B-CAB-CBB
26	TD	203	PEB	C2B-C3B-CAB-CBB
26	aI	203	PEB	C2B-C3B-CAB-CBB
28	sH	1001	CYC	C3A-C2A-CAA-CBA
26	x1	202	PEB	C4B-C3B-CAB-CBB
26	c2	203	PEB	C4B-C3B-CAB-CBB
26	J3	203	PEB	C4B-C3B-CAB-CBB
26	LB	1002	PEB	C4B-C3B-CAB-CBB
26	cI	203	PEB	C4B-C3B-CAB-CBB
26	C1	202	PEB	C3B-CAB-CBB-CGB
26	L1	202	PEB	C3B-CAB-CBB-CGB
26	L1	203	PEB	C3B-CAB-CBB-CGB
26	a1	202	PEB	C3B-CAB-CBB-CGB
26	11	201	PEB	C3B-CAB-CBB-CGB
26	a2	203	PEB	C3B-CAB-CBB-CGB
26	T3	202	PEB	C3B-CAB-CBB-CGB
26	L4	202	PEB	C3B-CAB-CBB-CGB
26	a4	203	PEB	C3B-CAB-CBB-CGB
26	y4	202	PEB	C3B-CAB-CBB-CGB
26	H5	203	PEB	C3B-CAB-CBB-CGB
26	G6	1002	PEB	C3B-CAB-CBB-CGB
26	GB	1002	PEB	C3B-CAB-CBB-CGB
26	RD	203	PEB	C3B-CAB-CBB-CGB
26	YE	203	PEB	C3B-CAB-CBB-CGB
26	cE	203	PEB	C3B-CAB-CBB-CGB
26	dE	201	PEB	C3B-CAB-CBB-CGB
26	WF	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	aF	202	PEB	C3B-CAB-CBB-CGB
26	QG	203	PEB	C3B-CAB-CBB-CGB
26	NJ	204	PEB	C3B-CAB-CBB-CGB
28	IH	1001	CYC	C2A-CAA-CBA-CGA
28	qH	1002	CYC	NA-C4A-CHB-C1B
28	qH	1002	CYC	C2A-CAA-CBA-CGA
28	yH	1001	CYC	C2B-C3B-CAB-CBB
26	wE	303	PEB	C2B-C3B-CAB-CBB
26	GG	203	PEB	C2B-C3B-CAB-CBB
26	wG	303	PEB	C2B-C3B-CAB-CBB
28	N2	1001	CYC	C2B-C3B-CAB-CBB
26	A1	202	PEB	NA-C4A-CHA-C1B
26	C1	202	PEB	NA-C4A-CHA-C1B
26	E1	202	PEB	NA-C4A-CHA-C1B
26	G1	202	PEB	NA-C4A-CHA-C1B
26	I1	202	PEB	NA-C4A-CHA-C1B
26	K1	202	PEB	NA-C4A-CHA-C1B
26	p1	202	PEB	NA-C4A-CHA-C1B
26	r1	202	PEB	NA-C4A-CHA-C1B
26	t1	202	PEB	NA-C4A-CHA-C1B
26	v1	202	PEB	NA-C4A-CHA-C1B
26	x1	202	PEB	NA-C4A-CHA-C1B
26	z1	202	PEB	NA-C4A-CHA-C1B
26	A4	202	PEB	NA-C4A-CHA-C1B
26	C4	202	PEB	NA-C4A-CHA-C1B
26	E4	202	PEB	NA-C4A-CHA-C1B
26	G4	202	PEB	NA-C4A-CHA-C1B
26	I4	202	PEB	NA-C4A-CHA-C1B
26	K4	202	PEB	NA-C4A-CHA-C1B
26	p4	202	PEB	NA-C4A-CHA-C1B
26	r4	202	PEB	NA-C4A-CHA-C1B
26	t4	202	PEB	NA-C4A-CHA-C1B
26	v4	202	PEB	NA-C4A-CHA-C1B
26	x4	202	PEB	NA-C4A-CHA-C1B
26	z4	202	PEB	NA-C4A-CHA-C1B
26	GG	203	PEB	NA-C4A-CHA-C1B
26	mG	203	PEB	NA-C4A-CHA-C1B
26	B1	201	PEB	C2D-C1D-CHC-C4C
26	C1	201	PEB	C2D-C1D-CHC-C4C
26	C1	202	PEB	C2D-C1D-CHC-C4C
26	E1	201	PEB	C2D-C1D-CHC-C4C
26	F1	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	G1	201	PEB	C2D-C1D-CHC-C4C
26	G1	202	PEB	C2D-C1D-CHC-C4C
26	H1	201	PEB	C2D-C1D-CHC-C4C
26	H1	203	PEB	C2D-C1D-CHC-C4C
26	J1	203	PEB	C2D-C1D-CHC-C4C
26	M1	402	PEB	C2D-C1D-CHC-C4C
26	R1	201	PEB	C2D-C1D-CHC-C4C
26	T1	203	PEB	C2D-C1D-CHC-C4C
26	Z1	201	PEB	C2D-C1D-CHC-C4C
26	d1	203	PEB	C2D-C1D-CHC-C4C
26	f1	201	PEB	C2D-C1D-CHC-C4C
26	g1	203	PEB	C2D-C1D-CHC-C4C
26	h1	202	PEB	C2D-C1D-CHC-C4C
26	i1	203	PEB	C2D-C1D-CHC-C4C
26	j1	202	PEB	C2D-C1D-CHC-C4C
26	k1	201	PEB	C2D-C1D-CHC-C4C
26	l1	202	PEB	C2D-C1D-CHC-C4C
26	m1	202	PEB	C2D-C1D-CHC-C4C
26	q1	201	PEB	C2D-C1D-CHC-C4C
26	q1	203	PEB	C2D-C1D-CHC-C4C
26	r1	201	PEB	C2D-C1D-CHC-C4C
26	s1	202	PEB	C2D-C1D-CHC-C4C
26	t1	201	PEB	C2D-C1D-CHC-C4C
26	t1	202	PEB	C2D-C1D-CHC-C4C
26	v1	201	PEB	C2D-C1D-CHC-C4C
26	w1	201	PEB	C2D-C1D-CHC-C4C
26	y1	201	PEB	C2D-C1D-CHC-C4C
26	z1	202	PEB	C2D-C1D-CHC-C4C
26	11	201	PEB	C2D-C1D-CHC-C4C
26	21	401	PEB	C2D-C1D-CHC-C4C
26	21	404	PEB	C2D-C1D-CHC-C4C
26	21	405	PEB	C2D-C1D-CHC-C4C
26	O2	202	PEB	C2D-C1D-CHC-C4C
26	Q2	202	PEB	C2D-C1D-CHC-C4C
26	S2	202	PEB	C2D-C1D-CHC-C4C
26	V2	202	PEB	C2D-C1D-CHC-C4C
26	b2	201	PEB	C2D-C1D-CHC-C4C
26	b2	202	PEB	C2D-C1D-CHC-C4C
26	c2	203	PEB	C2D-C1D-CHC-C4C
26	g2	202	PEB	C2D-C1D-CHC-C4C
26	h2	201	PEB	C2D-C1D-CHC-C4C
26	h2	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	i2	202	PEB	C2D-C1D-CHC-C4C
26	j2	201	PEB	C2D-C1D-CHC-C4C
26	k2	202	PEB	C2D-C1D-CHC-C4C
26	l2	201	PEB	C2D-C1D-CHC-C4C
26	C3	201	PEB	C2D-C1D-CHC-C4C
26	D3	202	PEB	C2D-C1D-CHC-C4C
26	E3	202	PEB	C2D-C1D-CHC-C4C
26	F3	203	PEB	C2D-C1D-CHC-C4C
26	J3	201	PEB	C2D-C1D-CHC-C4C
26	J3	203	PEB	C2D-C1D-CHC-C4C
26	P3	201	PEB	C2D-C1D-CHC-C4C
26	Y3	303	PEB	C2D-C1D-CHC-C4C
26	B4	201	PEB	C2D-C1D-CHC-C4C
26	C4	201	PEB	C2D-C1D-CHC-C4C
26	D4	201	PEB	C2D-C1D-CHC-C4C
26	E4	201	PEB	C2D-C1D-CHC-C4C
26	F4	201	PEB	C2D-C1D-CHC-C4C
26	F4	202	PEB	C2D-C1D-CHC-C4C
26	H4	201	PEB	C2D-C1D-CHC-C4C
26	H4	203	PEB	C2D-C1D-CHC-C4C
26	J4	201	PEB	C2D-C1D-CHC-C4C
26	J4	203	PEB	C2D-C1D-CHC-C4C
26	K4	201	PEB	C2D-C1D-CHC-C4C
26	L4	201	PEB	C2D-C1D-CHC-C4C
26	R4	201	PEB	C2D-C1D-CHC-C4C
26	S4	201	PEB	C2D-C1D-CHC-C4C
26	a4	203	PEB	C2D-C1D-CHC-C4C
26	c4	203	PEB	C2D-C1D-CHC-C4C
26	d4	201	PEB	C2D-C1D-CHC-C4C
26	h4	201	PEB	C2D-C1D-CHC-C4C
26	i4	202	PEB	C2D-C1D-CHC-C4C
26	k4	201	PEB	C2D-C1D-CHC-C4C
26	l4	202	PEB	C2D-C1D-CHC-C4C
26	m4	202	PEB	C2D-C1D-CHC-C4C
26	p4	202	PEB	C2D-C1D-CHC-C4C
26	q4	201	PEB	C2D-C1D-CHC-C4C
26	s4	201	PEB	C2D-C1D-CHC-C4C
26	t4	201	PEB	C2D-C1D-CHC-C4C
26	t4	202	PEB	C2D-C1D-CHC-C4C
26	w4	204	PEB	C2D-C1D-CHC-C4C
26	y4	201	PEB	C2D-C1D-CHC-C4C
26	y4	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	z4	202	PEB	C2D-C1D-CHC-C4C
26	24	401	PEB	C2D-C1D-CHC-C4C
26	24	405	PEB	C2D-C1D-CHC-C4C
26	C5	201	PEB	C2D-C1D-CHC-C4C
26	C5	202	PEB	C2D-C1D-CHC-C4C
26	C5	203	PEB	C2D-C1D-CHC-C4C
26	F5	203	PEB	C2D-C1D-CHC-C4C
26	G5	203	PEB	C2D-C1D-CHC-C4C
26	J5	202	PEB	C2D-C1D-CHC-C4C
26	L5	203	PEB	C2D-C1D-CHC-C4C
26	A6	301	PEB	C2D-C1D-CHC-C4C
26	Q6	202	PEB	C2D-C1D-CHC-C4C
26	S6	201	PEB	C2D-C1D-CHC-C4C
26	U6	203	PEB	C2D-C1D-CHC-C4C
26	a6	202	PEB	C2D-C1D-CHC-C4C
26	d6	201	PEB	C2D-C1D-CHC-C4C
26	l6	201	PEB	C2D-C1D-CHC-C4C
26	m6	203	PEB	C2D-C1D-CHC-C4C
26	D7	1002	PEB	C2D-C1D-CHC-C4C
26	P7	201	PEB	C2D-C1D-CHC-C4C
26	Q7	202	PEB	C2D-C1D-CHC-C4C
26	Z7	201	PEB	C2D-C1D-CHC-C4C
26	c7	201	PEB	C2D-C1D-CHC-C4C
26	d7	202	PEB	C2D-C1D-CHC-C4C
26	d7	203	PEB	C2D-C1D-CHC-C4C
26	f7	201	PEB	C2D-C1D-CHC-C4C
26	f7	202	PEB	C2D-C1D-CHC-C4C
26	g7	201	PEB	C2D-C1D-CHC-C4C
26	l7	202	PEB	C2D-C1D-CHC-C4C
26	m7	201	PEB	C2D-C1D-CHC-C4C
26	A8	302	PEB	C2D-C1D-CHC-C4C
26	B8	301	PEB	C2D-C1D-CHC-C4C
26	E8	202	PEB	C2D-C1D-CHC-C4C
26	H8	201	PEB	C2D-C1D-CHC-C4C
26	L8	201	PEB	C2D-C1D-CHC-C4C
26	N8	201	PEB	C2D-C1D-CHC-C4C
26	S8	201	PEB	C2D-C1D-CHC-C4C
26	U8	201	PEB	C2D-C1D-CHC-C4C
26	U8	202	PEB	C2D-C1D-CHC-C4C
26	V8	202	PEB	C2D-C1D-CHC-C4C
26	X8	202	PEB	C2D-C1D-CHC-C4C
26	Y8	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	d8	203	PEB	C2D-C1D-CHC-C4C
26	f8	201	PEB	C2D-C1D-CHC-C4C
26	j8	201	PEB	C2D-C1D-CHC-C4C
26	j8	202	PEB	C2D-C1D-CHC-C4C
26	A9	303	PEB	C2D-C1D-CHC-C4C
26	E9	201	PEB	C2D-C1D-CHC-C4C
26	H9	203	PEB	C2D-C1D-CHC-C4C
26	I9	201	PEB	C2D-C1D-CHC-C4C
26	J9	201	PEB	C2D-C1D-CHC-C4C
26	J9	202	PEB	C2D-C1D-CHC-C4C
26	J9	203	PEB	C2D-C1D-CHC-C4C
26	K9	201	PEB	C2D-C1D-CHC-C4C
26	K9	202	PEB	C2D-C1D-CHC-C4C
26	L9	202	PEB	C2D-C1D-CHC-C4C
26	O9	201	PEB	C2D-C1D-CHC-C4C
26	O9	202	PEB	C2D-C1D-CHC-C4C
26	Q9	202	PEB	C2D-C1D-CHC-C4C
26	R9	203	PEB	C2D-C1D-CHC-C4C
26	X9	202	PEB	C2D-C1D-CHC-C4C
26	AA	302	PEB	C2D-C1D-CHC-C4C
26	BA	301	PEB	C2D-C1D-CHC-C4C
26	EA	202	PEB	C2D-C1D-CHC-C4C
26	HA	201	PEB	C2D-C1D-CHC-C4C
26	LA	201	PEB	C2D-C1D-CHC-C4C
26	NA	201	PEB	C2D-C1D-CHC-C4C
26	QA	204	PEB	C2D-C1D-CHC-C4C
26	SA	201	PEB	C2D-C1D-CHC-C4C
26	SA	202	PEB	C2D-C1D-CHC-C4C
26	UA	201	PEB	C2D-C1D-CHC-C4C
26	UA	202	PEB	C2D-C1D-CHC-C4C
26	XA	202	PEB	C2D-C1D-CHC-C4C
26	fA	201	PEB	C2D-C1D-CHC-C4C
26	jA	201	PEB	C2D-C1D-CHC-C4C
26	jA	202	PEB	C2D-C1D-CHC-C4C
26	AB	301	PEB	C2D-C1D-CHC-C4C
26	SB	201	PEB	C2D-C1D-CHC-C4C
26	UB	203	PEB	C2D-C1D-CHC-C4C
26	dB	201	PEB	C2D-C1D-CHC-C4C
26	lB	201	PEB	C2D-C1D-CHC-C4C
26	AC	202	PEB	C2D-C1D-CHC-C4C
26	CC	201	PEB	C2D-C1D-CHC-C4C
26	CC	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	FC	202	PEB	C2D-C1D-CHC-C4C
26	LC	202	PEB	C2D-C1D-CHC-C4C
26	AD	202	PEB	C2D-C1D-CHC-C4C
26	BD	201	PEB	C2D-C1D-CHC-C4C
26	CD	201	PEB	C2D-C1D-CHC-C4C
26	DD	202	PEB	C2D-C1D-CHC-C4C
26	ED	202	PEB	C2D-C1D-CHC-C4C
26	FD	203	PEB	C2D-C1D-CHC-C4C
26	JD	201	PEB	C2D-C1D-CHC-C4C
26	JD	203	PEB	C2D-C1D-CHC-C4C
26	YD	301	PEB	C2D-C1D-CHC-C4C
26	YD	303	PEB	C2D-C1D-CHC-C4C
26	AE	201	PEB	C2D-C1D-CHC-C4C
26	CE	202	PEB	C2D-C1D-CHC-C4C
26	ME	201	PEB	C2D-C1D-CHC-C4C
26	OE	202	PEB	C2D-C1D-CHC-C4C
26	SE	202	PEB	C2D-C1D-CHC-C4C
26	YE	201	PEB	C2D-C1D-CHC-C4C
26	cE	201	PEB	C2D-C1D-CHC-C4C
26	dE	201	PEB	C2D-C1D-CHC-C4C
26	fE	202	PEB	C2D-C1D-CHC-C4C
26	gE	202	PEB	C2D-C1D-CHC-C4C
26	mE	203	PEB	C2D-C1D-CHC-C4C
26	oE	201	PEB	C2D-C1D-CHC-C4C
26	uE	202	PEB	C2D-C1D-CHC-C4C
26	vE	202	PEB	C2D-C1D-CHC-C4C
26	wE	302	PEB	C2D-C1D-CHC-C4C
26	xE	302	PEB	C2D-C1D-CHC-C4C
26	ZF	201	PEB	C2D-C1D-CHC-C4C
26	dF	202	PEB	C2D-C1D-CHC-C4C
26	eF	201	PEB	C2D-C1D-CHC-C4C
26	hF	202	PEB	C2D-C1D-CHC-C4C
26	kF	201	PEB	C2D-C1D-CHC-C4C
26	mF	201	PEB	C2D-C1D-CHC-C4C
26	mF	202	PEB	C2D-C1D-CHC-C4C
26	AG	201	PEB	C2D-C1D-CHC-C4C
26	BG	201	PEB	C2D-C1D-CHC-C4C
26	NG	202	PEB	C2D-C1D-CHC-C4C
26	OG	202	PEB	C2D-C1D-CHC-C4C
26	PG	202	PEB	C2D-C1D-CHC-C4C
26	SG	202	PEB	C2D-C1D-CHC-C4C
26	YG	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	bG	202	PEB	C2D-C1D-CHC-C4C
26	dG	201	PEB	C2D-C1D-CHC-C4C
26	fG	202	PEB	C2D-C1D-CHC-C4C
26	kG	201	PEB	C2D-C1D-CHC-C4C
26	kG	203	PEB	C2D-C1D-CHC-C4C
26	oG	203	PEB	C2D-C1D-CHC-C4C
26	uG	201	PEB	C2D-C1D-CHC-C4C
26	uG	202	PEB	C2D-C1D-CHC-C4C
26	vG	202	PEB	C2D-C1D-CHC-C4C
26	wG	302	PEB	C2D-C1D-CHC-C4C
26	xG	303	PEB	C2D-C1D-CHC-C4C
26	OI	202	PEB	C2D-C1D-CHC-C4C
26	VI	202	PEB	C2D-C1D-CHC-C4C
26	bI	202	PEB	C2D-C1D-CHC-C4C
26	cI	203	PEB	C2D-C1D-CHC-C4C
26	fI	202	PEB	C2D-C1D-CHC-C4C
26	gI	202	PEB	C2D-C1D-CHC-C4C
26	gI	203	PEB	C2D-C1D-CHC-C4C
26	hI	201	PEB	C2D-C1D-CHC-C4C
26	hI	202	PEB	C2D-C1D-CHC-C4C
26	jI	201	PEB	C2D-C1D-CHC-C4C
26	kI	202	PEB	C2D-C1D-CHC-C4C
26	kI	203	PEB	C2D-C1D-CHC-C4C
26	lI	201	PEB	C2D-C1D-CHC-C4C
26	AJ	305	PEB	C2D-C1D-CHC-C4C
26	CJ	201	PEB	C2D-C1D-CHC-C4C
26	DJ	202	PEB	C2D-C1D-CHC-C4C
26	EJ	201	PEB	C2D-C1D-CHC-C4C
26	FJ	202	PEB	C2D-C1D-CHC-C4C
26	JJ	201	PEB	C2D-C1D-CHC-C4C
26	JJ	202	PEB	C2D-C1D-CHC-C4C
26	KJ	202	PEB	C2D-C1D-CHC-C4C
26	LJ	202	PEB	C2D-C1D-CHC-C4C
26	PJ	201	PEB	C2D-C1D-CHC-C4C
26	QJ	202	PEB	C2D-C1D-CHC-C4C
26	RJ	203	PEB	C2D-C1D-CHC-C4C
26	TJ	201	PEB	C2D-C1D-CHC-C4C
26	VJ	201	PEB	C2D-C1D-CHC-C4C
27	K1	203	PUB	C3A-C4A-CHA-C1B
27	21	402	PUB	C3A-C4A-CHA-C1B
27	K4	203	PUB	C3A-C4A-CHA-C1B
27	24	402	PUB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
27	24	403	PUB	C3A-C4A-CHA-C1B
27	A6	303	PUB	C3A-C4A-CHA-C1B
27	A8	303	PUB	C3A-C4A-CHA-C1B
27	A8	304	PUB	C3A-C4A-CHA-C1B
27	AA	303	PUB	C3A-C4A-CHA-C1B
27	AA	304	PUB	C3A-C4A-CHA-C1B
27	AB	303	PUB	C3A-C4A-CHA-C1B
27	xE	305	PUB	C3A-C4A-CHA-C1B
27	yE	303	PUB	C3A-C4A-CHA-C1B
27	AF	303	PUB	C3A-C4A-CHA-C1B
27	wG	304	PUB	C3A-C4A-CHA-C1B
27	AI	302	PUB	C3A-C4A-CHA-C1B
26	L6	1002	PEB	C4B-C3B-CAB-CBB
26	d6	204	PEB	C4B-C3B-CAB-CBB
26	U8	201	PEB	C4B-C3B-CAB-CBB
26	ZG	201	PEB	C4B-C3B-CAB-CBB
26	lG	201	PEB	C4B-C3B-CAB-CBB
28	B6	1001	CYC	C1A-C2A-CAA-CBA
28	BB	1001	CYC	C1A-C2A-CAA-CBA
28	L6	1001	CYC	C2B-C3B-CAB-CBB
26	c2	203	PEB	C2B-C3B-CAB-CBB
26	I8	201	PEB	C2B-C3B-CAB-CBB
26	c8	201	PEB	C2B-C3B-CAB-CBB
26	PA	201	PEB	C2B-C3B-CAB-CBB
26	cA	202	PEB	C2B-C3B-CAB-CBB
26	LB	1002	PEB	C2B-C3B-CAB-CBB
26	QB	201	PEB	C2B-C3B-CAB-CBB
26	cI	203	PEB	C2B-C3B-CAB-CBB
26	IJ	203	PEB	C2B-C3B-CAB-CBB
26	kI	203	PEB	C3B-C4B-CHB-C1C
26	H1	203	PEB	C2C-CAC-CBC-CGC
26	V1	203	PEB	C2C-CAC-CBC-CGC
26	W1	201	PEB	C2C-CAC-CBC-CGC
26	X1	202	PEB	C2C-CAC-CBC-CGC
26	e1	202	PEB	C2C-CAC-CBC-CGC
26	y1	201	PEB	C2C-CAC-CBC-CGC
26	R2	202	PEB	C2C-CAC-CBC-CGC
26	G3	201	PEB	C2C-CAC-CBC-CGC
26	Q3	201	PEB	C2C-CAC-CBC-CGC
26	P4	202	PEB	C2C-CAC-CBC-CGC
26	W4	201	PEB	C2C-CAC-CBC-CGC
26	X4	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	p4	202	PEB	C2C-CAC-CBC-CGC
26	24	404	PEB	C2C-CAC-CBC-CGC
26	L7	1002	PEB	C2C-CAC-CBC-CGC
26	N7	1002	PEB	C2C-CAC-CBC-CGC
26	Z7	203	PEB	C2C-CAC-CBC-CGC
26	W8	203	PEB	C2C-CAC-CBC-CGC
26	m8	202	PEB	C2C-CAC-CBC-CGC
26	I9	201	PEB	C2C-CAC-CBC-CGC
26	RA	202	PEB	C2C-CAC-CBC-CGC
26	TA	201	PEB	C2C-CAC-CBC-CGC
26	VA	201	PEB	C2C-CAC-CBC-CGC
26	kA	201	PEB	C2C-CAC-CBC-CGC
26	OB	202	PEB	C2C-CAC-CBC-CGC
26	wE	302	PEB	C2C-CAC-CBC-CGC
26	QF	202	PEB	C2C-CAC-CBC-CGC
26	kG	203	PEB	C2C-CAC-CBC-CGC
26	NJ	202	PEB	C2C-CAC-CBC-CGC
26	QJ	201	PEB	C2C-CAC-CBC-CGC
27	AI	303	PUB	C3B-CAB-CBB-CGB
26	Q1	202	PEB	C3B-CAB-CBB-CGB
26	p1	202	PEB	C3B-CAB-CBB-CGB
26	c2	202	PEB	C3B-CAB-CBB-CGB
26	i2	202	PEB	C3B-CAB-CBB-CGB
26	D3	202	PEB	C3B-CAB-CBB-CGB
26	L3	203	PEB	C3B-CAB-CBB-CGB
26	M3	201	PEB	C3B-CAB-CBB-CGB
26	O3	202	PEB	C3B-CAB-CBB-CGB
26	R3	203	PEB	C3B-CAB-CBB-CGB
26	B4	203	PEB	C3B-CAB-CBB-CGB
26	D4	202	PEB	C3B-CAB-CBB-CGB
26	J4	203	PEB	C3B-CAB-CBB-CGB
26	n4	202	PEB	C3B-CAB-CBB-CGB
26	U6	201	PEB	C3B-CAB-CBB-CGB
26	b6	202	PEB	C3B-CAB-CBB-CGB
26	T7	202	PEB	C3B-CAB-CBB-CGB
26	W7	202	PEB	C3B-CAB-CBB-CGB
26	W8	202	PEB	C3B-CAB-CBB-CGB
26	W8	203	PEB	C3B-CAB-CBB-CGB
26	Y8	201	PEB	C3B-CAB-CBB-CGB
26	j8	203	PEB	C3B-CAB-CBB-CGB
26	B9	201	PEB	C3B-CAB-CBB-CGB
26	D9	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	J9	203	PEB	C3B-CAB-CBB-CGB
26	N9	204	PEB	C3B-CAB-CBB-CGB
26	O9	202	PEB	C3B-CAB-CBB-CGB
26	R9	201	PEB	C3B-CAB-CBB-CGB
26	W9	202	PEB	C3B-CAB-CBB-CGB
26	KA	202	PEB	C3B-CAB-CBB-CGB
26	KA	203	PEB	C3B-CAB-CBB-CGB
26	WA	203	PEB	C3B-CAB-CBB-CGB
26	YA	201	PEB	C3B-CAB-CBB-CGB
26	jA	203	PEB	C3B-CAB-CBB-CGB
26	UB	201	PEB	C3B-CAB-CBB-CGB
26	dB	202	PEB	C3B-CAB-CBB-CGB
26	dB	204	PEB	C3B-CAB-CBB-CGB
26	eB	202	PEB	C3B-CAB-CBB-CGB
26	ID	202	PEB	C3B-CAB-CBB-CGB
26	JD	202	PEB	C3B-CAB-CBB-CGB
26	LD	203	PEB	C3B-CAB-CBB-CGB
26	OD	202	PEB	C3B-CAB-CBB-CGB
26	RD	202	PEB	C3B-CAB-CBB-CGB
26	TD	202	PEB	C3B-CAB-CBB-CGB
26	GE	201	PEB	C3B-CAB-CBB-CGB
26	LE	202	PEB	C3B-CAB-CBB-CGB
26	ME	202	PEB	C3B-CAB-CBB-CGB
26	OE	201	PEB	C3B-CAB-CBB-CGB
26	pE	202	PEB	C3B-CAB-CBB-CGB
26	wE	303	PEB	C3B-CAB-CBB-CGB
26	NF	1002	PEB	C3B-CAB-CBB-CGB
26	TF	202	PEB	C3B-CAB-CBB-CGB
26	DG	202	PEB	C3B-CAB-CBB-CGB
26	LG	202	PEB	C3B-CAB-CBB-CGB
26	cG	203	PEB	C3B-CAB-CBB-CGB
26	fG	202	PEB	C3B-CAB-CBB-CGB
26	gG	202	PEB	C3B-CAB-CBB-CGB
26	BJ	201	PEB	C3B-CAB-CBB-CGB
26	DJ	201	PEB	C3B-CAB-CBB-CGB
26	JJ	203	PEB	C3B-CAB-CBB-CGB
26	RJ	201	PEB	C3B-CAB-CBB-CGB
26	XJ	202	PEB	C3B-CAB-CBB-CGB
27	A7	303	PUB	C2C-CAC-CBC-CGC
27	AF	303	PUB	C2C-CAC-CBC-CGC
27	xG	306	PUB	C2C-CAC-CBC-CGC
28	B6	1001	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	BB	1001	CYC	C2A-CAA-CBA-CGA
28	PH	1001	CYC	C2A-CAA-CBA-CGA
28	kH	1001	CYC	C2A-CAA-CBA-CGA
26	p1	202	PEB	NB-C4B-CHB-C1C
26	r1	202	PEB	NB-C4B-CHB-C1C
26	t1	202	PEB	NB-C4B-CHB-C1C
26	v1	202	PEB	NB-C4B-CHB-C1C
26	x1	202	PEB	NB-C4B-CHB-C1C
26	z1	202	PEB	NB-C4B-CHB-C1C
26	p4	202	PEB	NB-C4B-CHB-C1C
26	r4	202	PEB	NB-C4B-CHB-C1C
26	t4	202	PEB	NB-C4B-CHB-C1C
26	v4	202	PEB	NB-C4B-CHB-C1C
26	x4	202	PEB	NB-C4B-CHB-C1C
26	z4	202	PEB	NB-C4B-CHB-C1C
26	qE	202	PEB	NB-C4B-CHB-C1C
26	qG	202	PEB	NB-C4B-CHB-C1C
28	KH	1001	CYC	NA-C1A-CHA-C4D
28	E2	1001	CYC	C4B-C3B-CAB-CBB
28	C6	1001	CYC	C4B-C3B-CAB-CBB
28	CB	1001	CYC	C4B-C3B-CAB-CBB
28	DB	1001	CYC	C4B-C3B-CAB-CBB
28	oH	1001	CYC	C4B-C3B-CAB-CBB
28	EI	1001	CYC	C4B-C3B-CAB-CBB
28	WH	1001	CYC	C2B-C3B-CAB-CBB
26	J3	203	PEB	C2B-C3B-CAB-CBB
26	Q6	201	PEB	C2B-C3B-CAB-CBB
26	RB	201	PEB	C2B-C3B-CAB-CBB
26	DD	201	PEB	C2B-C3B-CAB-CBB
28	SH	1001	CYC	C2B-C3B-CAB-CBB
28	DB	1001	CYC	C2B-C3B-CAB-CBB
26	U8	201	PEB	C2B-C3B-CAB-CBB
26	c8	201	PEB	C4B-C3B-CAB-CBB
26	QB	201	PEB	C4B-C3B-CAB-CBB
28	QH	1001	CYC	C2B-C3B-CAB-CBB
26	S9	202	PEB	C4D-C3D-CAD-CBD
26	FD	202	PEB	C4D-C3D-CAD-CBD
26	eF	202	PEB	C4D-C3D-CAD-CBD
27	wE	304	PUB	C2D-C3D-CAD-CBD
28	L7	1001	CYC	C2B-C3B-CAB-CBB
27	QA	201	PUB	C4A-C3A-CAA-CBA
28	C2	1001	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	B1	201	PEB	C4A-C3A-CAA-CBA
26	K1	202	PEB	C4A-C3A-CAA-CBA
26	l1	201	PEB	C4A-C3A-CAA-CBA
26	y1	201	PEB	C4A-C3A-CAA-CBA
26	z1	202	PEB	C4A-C3A-CAA-CBA
26	21	405	PEB	C4A-C3A-CAA-CBA
26	O2	202	PEB	C4A-C3A-CAA-CBA
26	Q2	202	PEB	C4A-C3A-CAA-CBA
26	e2	202	PEB	C4A-C3A-CAA-CBA
26	B3	202	PEB	C4A-C3A-CAA-CBA
26	E3	201	PEB	C4A-C3A-CAA-CBA
26	R3	203	PEB	C4A-C3A-CAA-CBA
26	X3	203	PEB	C4A-C3A-CAA-CBA
26	Y3	301	PEB	C4A-C3A-CAA-CBA
26	P4	202	PEB	C4A-C3A-CAA-CBA
26	S4	201	PEB	C4A-C3A-CAA-CBA
26	Z4	202	PEB	C4A-C3A-CAA-CBA
26	b4	501	PEB	C4A-C3A-CAA-CBA
26	P6	202	PEB	C4A-C3A-CAA-CBA
26	Q6	203	PEB	C4A-C3A-CAA-CBA
26	T7	202	PEB	C4A-C3A-CAA-CBA
26	h7	203	PEB	C4A-C3A-CAA-CBA
26	l7	202	PEB	C4A-C3A-CAA-CBA
26	J8	201	PEB	C4A-C3A-CAA-CBA
26	Z8	202	PEB	C4A-C3A-CAA-CBA
26	k8	202	PEB	C4A-C3A-CAA-CBA
26	R9	201	PEB	C4A-C3A-CAA-CBA
26	QA	204	PEB	C4A-C3A-CAA-CBA
26	BC	201	PEB	C4A-C3A-CAA-CBA
26	ED	201	PEB	C4A-C3A-CAA-CBA
26	YD	303	PEB	C4A-C3A-CAA-CBA
26	XE	202	PEB	C4A-C3A-CAA-CBA
26	aE	201	PEB	C4A-C3A-CAA-CBA
26	gE	203	PEB	C4A-C3A-CAA-CBA
26	wE	301	PEB	C4A-C3A-CAA-CBA
26	TF	201	PEB	C4A-C3A-CAA-CBA
26	TF	202	PEB	C4A-C3A-CAA-CBA
26	WF	203	PEB	C4A-C3A-CAA-CBA
26	dF	203	PEB	C4A-C3A-CAA-CBA
26	mF	202	PEB	C4A-C3A-CAA-CBA
26	CG	203	PEB	C4A-C3A-CAA-CBA
26	cG	203	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	gG	203	PEB	C4A-C3A-CAA-CBA
26	lG	202	PEB	C4A-C3A-CAA-CBA
26	wG	301	PEB	C4A-C3A-CAA-CBA
26	VI	203	PEB	C4A-C3A-CAA-CBA
26	eI	202	PEB	C4A-C3A-CAA-CBA
26	LJ	203	PEB	C4A-C3A-CAA-CBA
28	K6	202	CYC	C4C-C3C-CAC-CBC
28	KB	202	CYC	C4C-C3C-CAC-CBC
28	cH	1001	CYC	C4C-C3C-CAC-CBC
28	mH	1001	CYC	C4C-C3C-CAC-CBC
26	D1	201	PEB	C3B-CAB-CBB-CGB
26	v1	202	PEB	C3B-CAB-CBB-CGB
26	D2	1002	PEB	C3B-CAB-CBB-CGB
26	i2	203	PEB	C3B-CAB-CBB-CGB
26	J3	202	PEB	C3B-CAB-CBB-CGB
26	K3	201	PEB	C3B-CAB-CBB-CGB
26	R3	202	PEB	C3B-CAB-CBB-CGB
26	V3	202	PEB	C3B-CAB-CBB-CGB
26	Y3	304	PEB	C3B-CAB-CBB-CGB
26	D4	201	PEB	C3B-CAB-CBB-CGB
26	Q4	202	PEB	C3B-CAB-CBB-CGB
26	S4	202	PEB	C3B-CAB-CBB-CGB
26	l6	201	PEB	C3B-CAB-CBB-CGB
26	K8	203	PEB	C3B-CAB-CBB-CGB
26	Q9	202	PEB	C3B-CAB-CBB-CGB
26	CA	202	PEB	C3B-CAB-CBB-CGB
26	GC	203	PEB	C3B-CAB-CBB-CGB
26	MD	201	PEB	C3B-CAB-CBB-CGB
26	FE	201	PEB	C3B-CAB-CBB-CGB
26	RE	201	PEB	C3B-CAB-CBB-CGB
26	YE	202	PEB	C3B-CAB-CBB-CGB
26	aE	203	PEB	C3B-CAB-CBB-CGB
26	fE	202	PEB	C3B-CAB-CBB-CGB
26	dF	201	PEB	C3B-CAB-CBB-CGB
26	FG	201	PEB	C3B-CAB-CBB-CGB
26	GG	203	PEB	C3B-CAB-CBB-CGB
26	TG	201	PEB	C3B-CAB-CBB-CGB
26	pG	202	PEB	C3B-CAB-CBB-CGB
26	SI	201	PEB	C3B-CAB-CBB-CGB
26	UJ	201	PEB	C3B-CAB-CBB-CGB
28	D6	1001	CYC	C2A-CAA-CBA-CGA
28	RH	1001	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	x1	202	PEB	C2B-C3B-CAB-CBB
26	I9	202	PEB	C2B-C3B-CAB-CBB
27	A1	203	PUB	C2D-C1D-CHC-C4C
27	21	403	PUB	C2D-C1D-CHC-C4C
27	24	402	PUB	C2D-C1D-CHC-C4C
27	A6	302	PUB	C2D-C1D-CHC-C4C
27	A7	304	PUB	C2D-C1D-CHC-C4C
27	A8	304	PUB	C2D-C1D-CHC-C4C
27	Q8	201	PUB	C2D-C1D-CHC-C4C
27	AA	304	PUB	C2D-C1D-CHC-C4C
27	QA	201	PUB	C2D-C1D-CHC-C4C
27	AB	302	PUB	C2D-C1D-CHC-C4C
27	xE	306	PUB	C2D-C1D-CHC-C4C
26	L6	1002	PEB	C2B-C3B-CAB-CBB
26	d6	204	PEB	C2B-C3B-CAB-CBB
26	E1	202	PEB	C2C-CAC-CBC-CGC
26	G1	202	PEB	C2C-CAC-CBC-CGC
26	P1	202	PEB	C2C-CAC-CBC-CGC
26	i1	202	PEB	C2C-CAC-CBC-CGC
26	s1	203	PEB	C2C-CAC-CBC-CGC
26	m2	202	PEB	C2C-CAC-CBC-CGC
26	A3	202	PEB	C2C-CAC-CBC-CGC
26	X3	201	PEB	C2C-CAC-CBC-CGC
26	Y3	304	PEB	C2C-CAC-CBC-CGC
26	i4	201	PEB	C2C-CAC-CBC-CGC
26	G6	1002	PEB	C2C-CAC-CBC-CGC
26	T6	202	PEB	C2C-CAC-CBC-CGC
26	f8	201	PEB	C2C-CAC-CBC-CGC
26	GA	201	PEB	C2C-CAC-CBC-CGC
26	jA	201	PEB	C2C-CAC-CBC-CGC
26	mB	201	PEB	C2C-CAC-CBC-CGC
26	TD	203	PEB	C2C-CAC-CBC-CGC
26	YD	304	PEB	C2C-CAC-CBC-CGC
26	iI	203	PEB	C2C-CAC-CBC-CGC
26	mI	202	PEB	C2C-CAC-CBC-CGC
27	AJ	302	PUB	C3B-CAB-CBB-CGB
28	CI	1001	CYC	C2B-C3B-CAB-CBB
26	L1	202	PEB	C2D-C3D-CAD-CBD
26	O1	202	PEB	C2D-C3D-CAD-CBD
26	k2	202	PEB	C2D-C3D-CAD-CBD
26	F3	202	PEB	C2D-C3D-CAD-CBD
26	X3	203	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
26	O4	202	PEB	C2D-C3D-CAD-CBD
26	T7	202	PEB	C2D-C3D-CAD-CBD
26	S9	202	PEB	C2D-C3D-CAD-CBD
26	X9	202	PEB	C2D-C3D-CAD-CBD
26	iE	201	PEB	C2D-C3D-CAD-CBD
26	bF	202	PEB	C2D-C3D-CAD-CBD
26	cF	202	PEB	C2D-C3D-CAD-CBD
26	fF	201	PEB	C2D-C3D-CAD-CBD
26	JJ	201	PEB	C2D-C3D-CAD-CBD
28	F6	1001	CYC	C2B-C3B-CAB-CBB
28	G2	1001	CYC	C4B-C3B-CAB-CBB
28	I6	1001	CYC	C4B-C3B-CAB-CBB
28	K6	202	CYC	C4B-C3B-CAB-CBB
28	KB	202	CYC	C4B-C3B-CAB-CBB
28	GI	1001	CYC	C4B-C3B-CAB-CBB
26	Q6	201	PEB	C4B-C3B-CAB-CBB
26	m4	202	PEB	C3B-CAB-CBB-CGB
26	dE	202	PEB	C3B-CAB-CBB-CGB
27	Q8	201	PUB	C4A-C3A-CAA-CBA
28	dH	1001	CYC	C2B-C3B-CAB-CBB
26	I9	202	PEB	C4B-C3B-CAB-CBB
26	UA	201	PEB	C2B-C3B-CAB-CBB
26	cA	201	PEB	C2B-C3B-CAB-CBB
26	JD	203	PEB	C2B-C3B-CAB-CBB
28	BB	1001	CYC	C3A-C2A-CAA-CBA
28	E7	1001	CYC	C2B-C3B-CAB-CBB
26	L4	203	PEB	C3B-CAB-CBB-CGB
26	RA	202	PEB	C3B-CAB-CBB-CGB
26	TE	201	PEB	C3B-CAB-CBB-CGB
26	ZE	202	PEB	C3B-CAB-CBB-CGB
26	RG	201	PEB	C3B-CAB-CBB-CGB
26	YG	201	PEB	C3B-CAB-CBB-CGB
26	iG	202	PEB	C3B-CAB-CBB-CGB
26	DI	1002	PEB	C3B-CAB-CBB-CGB
26	kA	202	PEB	C2B-C3B-CAB-CBB
26	SE	201	PEB	C2B-C3B-CAB-CBB
28	QH	1001	CYC	C3A-C2A-CAA-CBA
26	JD	203	PEB	C4B-C3B-CAB-CBB
28	J2	1001	CYC	C2B-C3B-CAB-CBB
26	C1	202	PEB	ND-C1D-CHC-C4C
26	F1	201	PEB	C2A-C3A-CAA-CBA
26	G1	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	J1	203	PEB	ND-C1D-CHC-C4C
26	M1	401	PEB	ND-C1D-CHC-C4C
26	Q1	202	PEB	C2C-CAC-CBC-CGC
26	c1	203	PEB	C2C-CAC-CBC-CGC
26	d1	203	PEB	C2C-CAC-CBC-CGC
26	j1	202	PEB	ND-C1D-CHC-C4C
26	q1	203	PEB	ND-C1D-CHC-C4C
26	r1	201	PEB	C2A-C3A-CAA-CBA
26	u1	201	PEB	ND-C1D-CHC-C4C
26	u1	201	PEB	C2A-C3A-CAA-CBA
26	v1	201	PEB	C2C-CAC-CBC-CGC
26	z1	202	PEB	C2A-C3A-CAA-CBA
26	21	401	PEB	ND-C1D-CHC-C4C
26	H2	1002	PEB	C2A-C3A-CAA-CBA
26	N2	1002	PEB	C2C-CAC-CBC-CGC
26	a2	202	PEB	C2A-C3A-CAA-CBA
26	c2	203	PEB	ND-C1D-CHC-C4C
26	i2	203	PEB	C2C-CAC-CBC-CGC
26	E3	202	PEB	ND-C1D-CHC-C4C
26	P3	203	PEB	C2C-CAC-CBC-CGC
26	R3	201	PEB	C2C-CAC-CBC-CGC
26	Y3	304	PEB	C2A-C3A-CAA-CBA
26	C4	202	PEB	ND-C1D-CHC-C4C
26	D4	201	PEB	C2A-C3A-CAA-CBA
26	F4	202	PEB	ND-C1D-CHC-C4C
26	G4	202	PEB	ND-C1D-CHC-C4C
26	J4	201	PEB	ND-C1D-CHC-C4C
26	M4	403	PEB	C2C-CAC-CBC-CGC
26	P4	202	PEB	C2A-C3A-CAA-CBA
26	Q4	202	PEB	C2C-CAC-CBC-CGC
26	V4	203	PEB	C2C-CAC-CBC-CGC
26	c4	201	PEB	ND-C1D-CHC-C4C
26	i4	202	PEB	ND-C1D-CHC-C4C
26	j4	202	PEB	ND-C1D-CHC-C4C
26	m4	202	PEB	ND-C1D-CHC-C4C
26	m4	203	PEB	ND-C1D-CHC-C4C
26	p4	202	PEB	ND-C1D-CHC-C4C
26	w4	204	PEB	ND-C1D-CHC-C4C
26	z4	202	PEB	ND-C1D-CHC-C4C
26	24	401	PEB	ND-C1D-CHC-C4C
26	A6	301	PEB	ND-C1D-CHC-C4C
26	O6	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	P6	202	PEB	C2A-C3A-CAA-CBA
26	Q6	203	PEB	C2A-C3A-CAA-CBA
26	R6	202	PEB	C2C-CAC-CBC-CGC
26	f6	203	PEB	ND-C1D-CHC-C4C
26	J7	1002	PEB	ND-C1D-CHC-C4C
26	O7	201	PEB	C2A-C3A-CAA-CBA
26	S7	203	PEB	ND-C1D-CHC-C4C
26	Y7	201	PEB	C2C-CAC-CBC-CGC
26	Z7	201	PEB	ND-C1D-CHC-C4C
26	d7	202	PEB	C2A-C3A-CAA-CBA
26	e7	201	PEB	C2A-C3A-CAA-CBA
26	f7	202	PEB	ND-C1D-CHC-C4C
26	f7	203	PEB	ND-C1D-CHC-C4C
26	h7	201	PEB	C2C-CAC-CBC-CGC
26	m7	201	PEB	ND-C1D-CHC-C4C
26	B8	301	PEB	ND-C1D-CHC-C4C
26	B8	301	PEB	C2A-C3A-CAA-CBA
26	G8	201	PEB	C2C-CAC-CBC-CGC
26	K8	202	PEB	ND-C1D-CHC-C4C
26	S8	202	PEB	ND-C1D-CHC-C4C
26	T8	201	PEB	C2C-CAC-CBC-CGC
26	Y8	203	PEB	ND-C1D-CHC-C4C
26	a8	203	PEB	ND-C1D-CHC-C4C
26	j8	202	PEB	ND-C1D-CHC-C4C
26	A9	301	PEB	ND-C1D-CHC-C4C
26	C9	201	PEB	ND-C1D-CHC-C4C
26	E9	201	PEB	C2A-C3A-CAA-CBA
26	F9	203	PEB	C2C-CAC-CBC-CGC
26	I9	202	PEB	C2C-CAC-CBC-CGC
26	J9	202	PEB	ND-C1D-CHC-C4C
26	J9	203	PEB	ND-C1D-CHC-C4C
26	N9	204	PEB	ND-C1D-CHC-C4C
26	O9	201	PEB	ND-C1D-CHC-C4C
26	O9	202	PEB	ND-C1D-CHC-C4C
26	O9	202	PEB	C2C-CAC-CBC-CGC
26	R9	203	PEB	ND-C1D-CHC-C4C
26	T9	201	PEB	ND-C1D-CHC-C4C
26	V9	203	PEB	ND-C1D-CHC-C4C
26	W9	202	PEB	C2A-C3A-CAA-CBA
26	BA	301	PEB	ND-C1D-CHC-C4C
26	KA	202	PEB	ND-C1D-CHC-C4C
26	QA	204	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	SA	201	PEB	ND-C1D-CHC-C4C
26	SA	202	PEB	ND-C1D-CHC-C4C
26	YA	203	PEB	ND-C1D-CHC-C4C
26	aA	203	PEB	C2C-CAC-CBC-CGC
26	hA	203	PEB	ND-C1D-CHC-C4C
26	jA	202	PEB	ND-C1D-CHC-C4C
26	lA	201	PEB	C2A-C3A-CAA-CBA
26	AB	301	PEB	ND-C1D-CHC-C4C
26	GB	1002	PEB	C2C-CAC-CBC-CGC
26	HB	1002	PEB	C2C-CAC-CBC-CGC
26	OB	203	PEB	C2C-CAC-CBC-CGC
26	RB	202	PEB	C2C-CAC-CBC-CGC
26	aB	202	PEB	C2C-CAC-CBC-CGC
26	bB	202	PEB	C2C-CAC-CBC-CGC
26	fB	203	PEB	ND-C1D-CHC-C4C
26	CC	201	PEB	ND-C1D-CHC-C4C
26	HD	203	PEB	C2C-CAC-CBC-CGC
26	PD	203	PEB	C2C-CAC-CBC-CGC
26	RD	201	PEB	C2C-CAC-CBC-CGC
26	XD	201	PEB	C2C-CAC-CBC-CGC
26	CE	201	PEB	ND-C1D-CHC-C4C
26	ME	203	PEB	ND-C1D-CHC-C4C
26	QE	203	PEB	ND-C1D-CHC-C4C
26	SE	203	PEB	C2A-C3A-CAA-CBA
26	cE	202	PEB	C2A-C3A-CAA-CBA
26	gE	203	PEB	ND-C1D-CHC-C4C
26	kE	203	PEB	ND-C1D-CHC-C4C
26	kE	203	PEB	C2A-C3A-CAA-CBA
26	oE	203	PEB	C2C-CAC-CBC-CGC
26	pE	201	PEB	C2C-CAC-CBC-CGC
26	qE	202	PEB	ND-C1D-CHC-C4C
26	JF	1002	PEB	ND-C1D-CHC-C4C
26	QF	201	PEB	C2A-C3A-CAA-CBA
26	VF	202	PEB	ND-C1D-CHC-C4C
26	WF	202	PEB	C2C-CAC-CBC-CGC
26	ZF	201	PEB	ND-C1D-CHC-C4C
26	fF	203	PEB	ND-C1D-CHC-C4C
26	kF	202	PEB	ND-C1D-CHC-C4C
26	lF	201	PEB	ND-C1D-CHC-C4C
26	lF	203	PEB	ND-C1D-CHC-C4C
26	BG	201	PEB	ND-C1D-CHC-C4C
26	OG	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	ZG	202	PEB	ND-C1D-CHC-C4C
26	aG	201	PEB	ND-C1D-CHC-C4C
26	cG	202	PEB	C2A-C3A-CAA-CBA
26	cG	203	PEB	C2C-CAC-CBC-CGC
26	eG	201	PEB	ND-C1D-CHC-C4C
26	iG	203	PEB	ND-C1D-CHC-C4C
26	kG	203	PEB	ND-C1D-CHC-C4C
26	uG	201	PEB	ND-C1D-CHC-C4C
26	HI	1002	PEB	C2A-C3A-CAA-CBA
26	RI	202	PEB	C2C-CAC-CBC-CGC
26	aI	202	PEB	C2A-C3A-CAA-CBA
26	hI	201	PEB	ND-C1D-CHC-C4C
26	jI	201	PEB	ND-C1D-CHC-C4C
26	AJ	305	PEB	ND-C1D-CHC-C4C
26	FJ	202	PEB	ND-C1D-CHC-C4C
26	JJ	202	PEB	ND-C1D-CHC-C4C
26	KJ	201	PEB	ND-C1D-CHC-C4C
26	RJ	202	PEB	ND-C1D-CHC-C4C
26	RJ	203	PEB	ND-C1D-CHC-C4C
26	TJ	201	PEB	ND-C1D-CHC-C4C
26	VJ	202	PEB	ND-C1D-CHC-C4C
26	VJ	203	PEB	ND-C1D-CHC-C4C
26	XJ	201	PEB	ND-C1D-CHC-C4C
26	XJ	203	PEB	ND-C1D-CHC-C4C
27	A2	303	PUB	C3B-CAB-CBB-CGB
27	A6	303	PUB	C3B-CAB-CBB-CGB
27	N9	201	PUB	C3C-C4C-CHC-C1D
27	AB	303	PUB	NA-C4A-CHA-C1B
27	YD	302	PUB	C3B-CAB-CBB-CGB
27	xE	305	PUB	NA-C4A-CHA-C1B
27	xG	306	PUB	C3C-C4C-CHC-C1D
27	AI	302	PUB	NA-C4A-CHA-C1B
28	EF	1001	CYC	C2C-C3C-CAC-CBC
28	JF	1003	CYC	C3D-CAD-CBD-CGD
28	EH	1001	CYC	C3D-CAD-CBD-CGD
28	kH	1001	CYC	C2C-C3C-CAC-CBC
28	IF	1001	CYC	C2B-C3B-CAB-CBB
28	dH	1001	CYC	NB-C1B-CHB-C4A
26	lG	201	PEB	C2B-C3B-CAB-CBB
28	B6	1001	CYC	C3A-C2A-CAA-CBA
26	X1	201	PEB	C1C-C2C-CAC-CBC
26	11	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	11	202	PEB	C3C-C2C-CAC-CBC
26	J2	1002	PEB	C3C-C2C-CAC-CBC
26	X4	201	PEB	C3C-C2C-CAC-CBC
26	e4	202	PEB	C1C-C2C-CAC-CBC
26	e4	202	PEB	C3C-C2C-CAC-CBC
26	K5	203	PEB	C3C-C2C-CAC-CBC
26	L6	1002	PEB	C3C-C2C-CAC-CBC
26	V6	201	PEB	C3C-C2C-CAC-CBC
26	d6	201	PEB	C1C-C2C-CAC-CBC
26	d6	201	PEB	C3C-C2C-CAC-CBC
26	W7	202	PEB	C1C-C2C-CAC-CBC
26	W7	202	PEB	C3C-C2C-CAC-CBC
26	k7	201	PEB	C1C-C2C-CAC-CBC
26	k7	201	PEB	C3C-C2C-CAC-CBC
26	LB	1002	PEB	C1C-C2C-CAC-CBC
26	LB	1002	PEB	C3C-C2C-CAC-CBC
26	VB	201	PEB	C1C-C2C-CAC-CBC
26	VB	201	PEB	C3C-C2C-CAC-CBC
26	kB	202	PEB	C3C-C2C-CAC-CBC
26	IC	203	PEB	C3C-C2C-CAC-CBC
26	eE	201	PEB	C1C-C2C-CAC-CBC
26	qE	202	PEB	C3C-C2C-CAC-CBC
26	tE	202	PEB	C1C-C2C-CAC-CBC
26	tE	202	PEB	C3C-C2C-CAC-CBC
26	VG	202	PEB	C1C-C2C-CAC-CBC
26	DI	1002	PEB	C3C-C2C-CAC-CBC
26	AJ	301	PEB	C3C-C2C-CAC-CBC
27	A9	302	PUB	C2B-C3B-CAB-CBB
27	AJ	302	PUB	C2B-C3B-CAB-CBB
28	J7	1001	CYC	C4D-C3D-CAD-CBD
28	NB	1001	CYC	C4D-C3D-CAD-CBD
28	FH	1001	CYC	C4B-C3B-CAB-CBB
28	YH	1004	CYC	C4B-C3B-CAB-CBB
26	IA	201	PEB	C4B-C3B-CAB-CBB
26	UA	201	PEB	C4B-C3B-CAB-CBB
26	SE	201	PEB	C4B-C3B-CAB-CBB
28	D7	1001	CYC	C2B-C3B-CAB-CBB
28	H7	1001	CYC	C2B-C3B-CAB-CBB
28	PH	1001	CYC	C2B-C3B-CAB-CBB
28	IH	1001	CYC	C2B-C3B-CAB-CBB
28	MB	1001	CYC	C2B-C3B-CAB-CBB
26	pG	202	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	B1	203	PEB	C3B-CAB-CBB-CGB
26	W1	202	PEB	C3B-CAB-CBB-CGB
26	m1	201	PEB	C3B-CAB-CBB-CGB
26	f4	202	PEB	C3B-CAB-CBB-CGB
26	u4	201	PEB	C3B-CAB-CBB-CGB
26	L5	202	PEB	C3B-CAB-CBB-CGB
26	k8	202	PEB	C3B-CAB-CBB-CGB
26	VD	202	PEB	C3B-CAB-CBB-CGB
26	vG	201	PEB	C3B-CAB-CBB-CGB
26	BJ	203	PEB	C3B-CAB-CBB-CGB
27	Y3	302	PUB	C2C-CAC-CBC-CGC
28	NB	1001	CYC	C2B-C3B-CAB-CBB
28	M6	1001	CYC	C2B-C3B-CAB-CBB
28	DF	1001	CYC	C2B-C3B-CAB-CBB
28	IH	1001	CYC	C2B-C3B-CAB-CBB
26	F3	202	PEB	C4D-C3D-CAD-CBD
26	X3	203	PEB	C4D-C3D-CAD-CBD
26	H9	201	PEB	C4D-C3D-CAD-CBD
26	J9	201	PEB	C4D-C3D-CAD-CBD
26	X9	202	PEB	C4D-C3D-CAD-CBD
26	Y9	201	PEB	C4D-C3D-CAD-CBD
26	iE	201	PEB	C4D-C3D-CAD-CBD
26	JJ	201	PEB	C4D-C3D-CAD-CBD
28	JI	1001	CYC	C2B-C3B-CAB-CBB
26	d8	201	PEB	C2B-C3B-CAB-CBB
26	IA	201	PEB	C2B-C3B-CAB-CBB
26	dB	204	PEB	C2B-C3B-CAB-CBB
28	YH	1003	CYC	C3A-C2A-CAA-CBA
28	jH	1001	CYC	C3A-C2A-CAA-CBA
26	L1	201	PEB	C3B-CAB-CBB-CGB
26	w1	201	PEB	C3B-CAB-CBB-CGB
26	A4	201	PEB	C3B-CAB-CBB-CGB
26	L4	201	PEB	C3B-CAB-CBB-CGB
26	r4	201	PEB	C3B-CAB-CBB-CGB
26	HC	203	PEB	C3B-CAB-CBB-CGB
26	vE	201	PEB	C3B-CAB-CBB-CGB
26	rG	201	PEB	C3B-CAB-CBB-CGB
26	GJ	201	PEB	C3B-CAB-CBB-CGB
26	WJ	202	PEB	C3B-CAB-CBB-CGB
28	DB	1001	CYC	C2A-CAA-CBA-CGA
28	GH	1001	CYC	C2B-C3B-CAB-CBB
26	L1	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	U4	202	PEB	C2C-CAC-CBC-CGC
26	14	202	PEB	C2C-CAC-CBC-CGC
26	l6	202	PEB	C2C-CAC-CBC-CGC
26	DD	201	PEB	C2C-CAC-CBC-CGC
26	YE	201	PEB	C2C-CAC-CBC-CGC
26	oE	202	PEB	C2C-CAC-CBC-CGC
26	oG	202	PEB	C2C-CAC-CBC-CGC
26	IJ	203	PEB	C2C-CAC-CBC-CGC
27	NJ	201	PUB	C3B-CAB-CBB-CGB
26	d8	203	PEB	NB-C4B-CHB-C1C
27	B8	302	PUB	C4D-C3D-CAD-CBD
28	IB	1001	CYC	C4B-C3B-CAB-CBB
28	YH	1003	CYC	C4B-C3B-CAB-CBB
28	jH	1001	CYC	C4B-C3B-CAB-CBB
26	d8	201	PEB	C4B-C3B-CAB-CBB
26	kA	202	PEB	C4B-C3B-CAB-CBB
26	dB	204	PEB	C4B-C3B-CAB-CBB
28	YH	1003	CYC	C1A-C2A-CAA-CBA
28	jH	1001	CYC	C1A-C2A-CAA-CBA
26	j1	201	PEB	CAC-CBC-CGC-O1C
26	h2	201	PEB	CAB-CBB-CGB-O1B
26	m2	201	PEB	CAC-CBC-CGC-O1C
26	R3	202	PEB	CAC-CBC-CGC-O1C
26	T3	201	PEB	CAC-CBC-CGC-O1C
26	eB	201	PEB	CAB-CBB-CGB-O1B
26	fF	201	PEB	CAC-CBC-CGC-O1C
26	YG	203	PEB	CAC-CBC-CGC-O1C
26	v4	201	PEB	CAC-CBC-CGC-O1C
26	l7	203	PEB	CAC-CBC-CGC-O1C
26	VI	203	PEB	CAB-CBB-CGB-O1B
27	AB	303	PUB	CAC-CBC-CGC-O1C
26	NA	201	PEB	C2B-C3B-CAB-CBB
26	ZG	201	PEB	C2B-C3B-CAB-CBB
26	oG	203	PEB	C2B-C3B-CAB-CBB
26	RI	202	PEB	C2B-C3B-CAB-CBB
26	O7	201	PEB	CAB-CBB-CGB-O2B
26	X9	203	PEB	CAB-CBB-CGB-O1B
26	hB	202	PEB	CAB-CBB-CGB-O1B
26	KC	202	PEB	CAC-CBC-CGC-O1C
26	YE	201	PEB	CAC-CBC-CGC-O2C
26	FF	1002	PEB	CAC-CBC-CGC-O2C
28	DB	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	wG	304	PUB	C2D-C3D-CAD-CBD
26	HD	203	PEB	C2D-C3D-CAD-CBD
26	XD	202	PEB	C2D-C3D-CAD-CBD
26	s1	201	PEB	C3B-CAB-CBB-CGB
26	P2	203	PEB	C3B-CAB-CBB-CGB
26	I4	202	PEB	C3B-CAB-CBB-CGB
26	z4	201	PEB	C3B-CAB-CBB-CGB
26	24	404	PEB	C3B-CAB-CBB-CGB
26	F5	201	PEB	C3B-CAB-CBB-CGB
26	d6	204	PEB	C3B-CAB-CBB-CGB
26	h8	203	PEB	C3B-CAB-CBB-CGB
26	B9	203	PEB	C3B-CAB-CBB-CGB
26	S9	201	PEB	C3B-CAB-CBB-CGB
26	mB	201	PEB	C3B-CAB-CBB-CGB
26	GC	201	PEB	C3B-CAB-CBB-CGB
26	LC	202	PEB	C3B-CAB-CBB-CGB
26	ME	201	PEB	C3B-CAB-CBB-CGB
26	oE	201	PEB	C3B-CAB-CBB-CGB
26	NG	201	PEB	C3B-CAB-CBB-CGB
26	aG	203	PEB	C3B-CAB-CBB-CGB
27	YD	302	PUB	C2C-CAC-CBC-CGC
26	L1	201	PEB	CAC-CBC-CGC-O2C
26	T1	203	PEB	CAC-CBC-CGC-O2C
26	a1	201	PEB	CAB-CBB-CGB-O1B
26	b1	501	PEB	CAB-CBB-CGB-O2B
26	h1	201	PEB	CAC-CBC-CGC-O2C
26	k1	201	PEB	CAB-CBB-CGB-O2B
26	r1	201	PEB	CAB-CBB-CGB-O2B
26	F2	1002	PEB	CAC-CBC-CGC-O2C
26	P2	203	PEB	CAB-CBB-CGB-O2B
26	l2	202	PEB	CAC-CBC-CGC-O2C
26	A3	202	PEB	CAB-CBB-CGB-O2B
26	L3	202	PEB	CAC-CBC-CGC-O2C
26	V3	202	PEB	CAB-CBB-CGB-O2B
26	B4	201	PEB	CAC-CBC-CGC-O2C
26	N4	202	PEB	CAB-CBB-CGB-O2B
26	P4	201	PEB	CAB-CBB-CGB-O1B
26	d4	202	PEB	CAC-CBC-CGC-O2C
26	h4	203	PEB	CAB-CBB-CGB-O2B
26	y4	201	PEB	CAC-CBC-CGC-O2C
26	C5	202	PEB	CAB-CBB-CGB-O2B
26	L5	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	Q6	201	PEB	CAC-CBC-CGC-O2C
26	g6	201	PEB	CAC-CBC-CGC-O2C
26	k6	202	PEB	CAB-CBB-CGB-O1B
26	P7	202	PEB	CAB-CBB-CGB-O2B
26	l7	202	PEB	CAC-CBC-CGC-O2C
26	G8	202	PEB	CAC-CBC-CGC-O2C
26	B9	201	PEB	CAB-CBB-CGB-O1B
26	E9	202	PEB	CAB-CBB-CGB-O2B
26	J9	202	PEB	CAB-CBB-CGB-O2B
26	K9	201	PEB	CAC-CBC-CGC-O2C
26	EA	202	PEB	CAC-CBC-CGC-O1C
26	GA	201	PEB	CAC-CBC-CGC-O2C
26	IA	203	PEB	CAC-CBC-CGC-O2C
26	UA	203	PEB	CAB-CBB-CGB-O2B
26	aA	202	PEB	CAC-CBC-CGC-O2C
26	aA	203	PEB	CAC-CBC-CGC-O2C
26	cA	203	PEB	CAC-CBC-CGC-O2C
26	RB	202	PEB	CAC-CBC-CGC-O2C
26	fB	201	PEB	CAB-CBB-CGB-O1B
26	gB	201	PEB	CAC-CBC-CGC-O2C
26	AD	201	PEB	CAC-CBC-CGC-O2C
26	ED	202	PEB	CAB-CBB-CGB-O2B
26	HD	203	PEB	CAB-CBB-CGB-O2B
26	MD	201	PEB	CAC-CBC-CGC-O2C
26	GE	202	PEB	CAC-CBC-CGC-O2C
26	IE	201	PEB	CAC-CBC-CGC-O2C
26	cE	202	PEB	CAC-CBC-CGC-O2C
26	xE	304	PEB	CAC-CBC-CGC-O2C
26	ZF	203	PEB	CAC-CBC-CGC-O2C
26	cF	201	PEB	CAC-CBC-CGC-O2C
26	hF	202	PEB	CAC-CBC-CGC-O2C
26	AG	202	PEB	CAB-CBB-CGB-O1B
26	KG	203	PEB	CAC-CBC-CGC-O2C
26	jG	202	PEB	CAB-CBB-CGB-O2B
26	kG	203	PEB	CAC-CBC-CGC-O1C
26	qG	201	PEB	CAC-CBC-CGC-O2C
26	rG	201	PEB	CAB-CBB-CGB-O2B
26	vG	202	PEB	CAB-CBB-CGB-O2B
26	PI	202	PEB	CAB-CBB-CGB-O1B
26	aI	202	PEB	CAB-CBB-CGB-O1B
26	aI	203	PEB	CAC-CBC-CGC-O1C
26	bI	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	bI	202	PEB	CAC-CBC-CGC-O2C
26	mI	201	PEB	CAC-CBC-CGC-O1C
26	GJ	202	PEB	CAC-CBC-CGC-O1C
26	VJ	202	PEB	CAC-CBC-CGC-O2C
27	AF	304	PUB	CAB-CBB-CGB-O2B
28	D6	1001	CYC	CAD-CBD-CGD-O1D
26	M1	401	PEB	C2D-C1D-CHC-C4C
26	i1	201	PEB	C2D-C1D-CHC-C4C
26	u1	201	PEB	C2D-C1D-CHC-C4C
26	m2	201	PEB	C2D-C1D-CHC-C4C
26	C4	202	PEB	C2D-C1D-CHC-C4C
26	D4	202	PEB	C2D-C1D-CHC-C4C
26	G4	201	PEB	C2D-C1D-CHC-C4C
26	M4	403	PEB	C2D-C1D-CHC-C4C
26	N4	201	PEB	C2D-C1D-CHC-C4C
26	c4	201	PEB	C2D-C1D-CHC-C4C
26	g4	203	PEB	C2D-C1D-CHC-C4C
26	q4	203	PEB	C2D-C1D-CHC-C4C
26	L5	202	PEB	C2D-C1D-CHC-C4C
26	O6	201	PEB	C2D-C1D-CHC-C4C
26	S6	202	PEB	C2D-C1D-CHC-C4C
26	d6	203	PEB	C2D-C1D-CHC-C4C
26	f6	203	PEB	C2D-C1D-CHC-C4C
26	A7	302	PEB	C2D-C1D-CHC-C4C
26	j7	203	PEB	C2D-C1D-CHC-C4C
26	m7	202	PEB	C2D-C1D-CHC-C4C
26	O8	201	PEB	C2D-C1D-CHC-C4C
26	d8	202	PEB	C2D-C1D-CHC-C4C
26	T9	201	PEB	C2D-C1D-CHC-C4C
26	YA	203	PEB	C2D-C1D-CHC-C4C
26	OB	201	PEB	C2D-C1D-CHC-C4C
26	SB	202	PEB	C2D-C1D-CHC-C4C
26	ZB	202	PEB	C2D-C1D-CHC-C4C
26	aB	202	PEB	C2D-C1D-CHC-C4C
26	dB	203	PEB	C2D-C1D-CHC-C4C
26	aE	203	PEB	C2D-C1D-CHC-C4C
26	AF	302	PEB	C2D-C1D-CHC-C4C
26	QF	202	PEB	C2D-C1D-CHC-C4C
26	fF	203	PEB	C2D-C1D-CHC-C4C
26	EG	201	PEB	C2D-C1D-CHC-C4C
26	gG	201	PEB	C2D-C1D-CHC-C4C
26	mI	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	IJ	201	PEB	C2D-C1D-CHC-C4C
26	JJ	203	PEB	C2D-C1D-CHC-C4C
26	KJ	201	PEB	C2D-C1D-CHC-C4C
26	SJ	202	PEB	C2D-C1D-CHC-C4C
26	XJ	203	PEB	C2D-C1D-CHC-C4C
27	A6	302	PUB	C3A-C4A-CHA-C1B
26	RB	201	PEB	C4B-C3B-CAB-CBB
26	DD	201	PEB	C4B-C3B-CAB-CBB
26	N1	202	PEB	CAC-CBC-CGC-O2C
26	R1	203	PEB	CAB-CBB-CGB-O1B
26	V1	203	PEB	CAB-CBB-CGB-O2B
26	g1	202	PEB	CAC-CBC-CGC-O1C
26	i1	203	PEB	CAB-CBB-CGB-O2B
26	A2	305	PEB	CAC-CBC-CGC-O1C
26	J2	1002	PEB	CAB-CBB-CGB-O1B
26	P2	202	PEB	CAB-CBB-CGB-O1B
26	a2	202	PEB	CAB-CBB-CGB-O1B
26	W3	201	PEB	CAC-CBC-CGC-O1C
26	G4	202	PEB	CAB-CBB-CGB-O2B
26	e4	201	PEB	CAB-CBB-CGB-O2B
26	g4	203	PEB	CAC-CBC-CGC-O2C
26	24	401	PEB	CAB-CBB-CGB-O1B
26	B5	202	PEB	CAC-CBC-CGC-O2C
26	Q6	203	PEB	CAB-CBB-CGB-O2B
26	O7	202	PEB	CAC-CBC-CGC-O2C
26	g7	201	PEB	CAB-CBB-CGB-O1B
26	S8	202	PEB	CAC-CBC-CGC-O2C
26	f8	203	PEB	CAC-CBC-CGC-O2C
26	l8	201	PEB	CAC-CBC-CGC-O2C
26	B9	202	PEB	CAC-CBC-CGC-O2C
26	P9	202	PEB	CAB-CBB-CGB-O2B
26	R9	203	PEB	CAC-CBC-CGC-O2C
26	T9	203	PEB	CAB-CBB-CGB-O2B
26	W9	202	PEB	CAC-CBC-CGC-O1C
26	SA	203	PEB	CAC-CBC-CGC-O2C
26	AB	301	PEB	CAC-CBC-CGC-O2C
26	QB	202	PEB	CAB-CBB-CGB-O1B
26	BD	202	PEB	CAB-CBB-CGB-O2B
26	OD	202	PEB	CAC-CBC-CGC-O1C
26	HE	201	PEB	CAC-CBC-CGC-O1C
26	JE	202	PEB	CAB-CBB-CGB-O2B
26	KE	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	OE	201	PEB	CAC-CBC-CGC-O1C
26	eE	202	PEB	CAC-CBC-CGC-O2C
26	qE	201	PEB	CAC-CBC-CGC-O2C
26	AF	302	PEB	CAB-CBB-CGB-O2B
26	VF	202	PEB	CAC-CBC-CGC-O2C
26	VF	203	PEB	CAB-CBB-CGB-O2B
26	CG	203	PEB	CAB-CBB-CGB-O2B
26	JG	202	PEB	CAB-CBB-CGB-O2B
26	SG	202	PEB	CAC-CBC-CGC-O2C
26	PI	202	PEB	CAC-CBC-CGC-O1C
26	II	202	PEB	CAC-CBC-CGC-O2C
26	BJ	201	PEB	CAB-CBB-CGB-O1B
26	BJ	202	PEB	CAC-CBC-CGC-O2C
26	FJ	202	PEB	CAB-CBB-CGB-O2B
26	NJ	203	PEB	CAB-CBB-CGB-O2B
26	XJ	202	PEB	CAB-CBB-CGB-O1B
26	YJ	202	PEB	CAC-CBC-CGC-O1C
28	K2	1001	CYC	CAA-CBA-CGA-O2A
28	D6	1001	CYC	CAA-CBA-CGA-O1A
28	F7	1001	CYC	CAA-CBA-CGA-O2A
28	LF	1001	CYC	CAD-CBD-CGD-O1D
28	KH	1001	CYC	CAA-CBA-CGA-O2A
28	VH	1001	CYC	CAA-CBA-CGA-O1A
28	KI	1001	CYC	CAA-CBA-CGA-O2A
28	NI	1001	CYC	CAD-CBD-CGD-O1D
28	qH	1001	CYC	C2B-C3B-CAB-CBB
26	A1	202	PEB	CAC-CBC-CGC-O2C
26	T1	202	PEB	CAC-CBC-CGC-O2C
26	Z1	201	PEB	CAB-CBB-CGB-O1B
26	a1	203	PEB	CAB-CBB-CGB-O2B
26	d1	202	PEB	CAC-CBC-CGC-O2C
26	m1	203	PEB	CAC-CBC-CGC-O2C
26	O2	201	PEB	CAB-CBB-CGB-O1B
26	O2	202	PEB	CAB-CBB-CGB-O2B
26	P2	202	PEB	CAC-CBC-CGC-O1C
26	a2	202	PEB	CAC-CBC-CGC-O1C
26	a2	203	PEB	CAC-CBC-CGC-O1C
26	A3	202	PEB	CAC-CBC-CGC-O1C
26	G3	201	PEB	CAC-CBC-CGC-O2C
26	H3	203	PEB	CAC-CBC-CGC-O2C
26	M3	201	PEB	CAC-CBC-CGC-O2C
26	X3	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	H4	203	PEB	CAC-CBC-CGC-O1C
26	Q4	202	PEB	CAB-CBB-CGB-O2B
26	S4	202	PEB	CAB-CBB-CGB-O2B
26	V4	201	PEB	CAC-CBC-CGC-O2C
26	a4	202	PEB	CAC-CBC-CGC-O1C
26	l4	201	PEB	CAC-CBC-CGC-O1C
26	v4	201	PEB	CAB-CBB-CGB-O2B
26	A5	201	PEB	CAC-CBC-CGC-O2C
26	C5	201	PEB	CAC-CBC-CGC-O2C
26	I5	203	PEB	CAB-CBB-CGB-O2B
26	J5	202	PEB	CAB-CBB-CGB-O1B
26	D6	1002	PEB	CAC-CBC-CGC-O1C
26	S6	201	PEB	CAB-CBB-CGB-O2B
26	e6	201	PEB	CAB-CBB-CGB-O1B
26	R7	201	PEB	CAB-CBB-CGB-O2B
26	V7	202	PEB	CAB-CBB-CGB-O2B
26	j7	201	PEB	CAC-CBC-CGC-O2C
26	l7	201	PEB	CAB-CBB-CGB-O2B
26	S8	201	PEB	CAB-CBB-CGB-O2B
26	S8	203	PEB	CAC-CBC-CGC-O2C
26	B9	202	PEB	CAB-CBB-CGB-O2B
26	D9	203	PEB	CAB-CBB-CGB-O1B
26	U9	201	PEB	CAC-CBC-CGC-O2C
26	Y9	201	PEB	CAC-CBC-CGC-O2C
26	Y9	202	PEB	CAC-CBC-CGC-O1C
26	TA	202	PEB	CAC-CBC-CGC-O2C
26	cA	201	PEB	CAB-CBB-CGB-O2B
26	fA	203	PEB	CAC-CBC-CGC-O2C
26	jA	202	PEB	CAC-CBC-CGC-O2C
26	CC	202	PEB	CAC-CBC-CGC-O2C
26	TD	201	PEB	CAC-CBC-CGC-O1C
26	SE	202	PEB	CAC-CBC-CGC-O2C
26	iE	203	PEB	CAB-CBB-CGB-O1B
26	cF	202	PEB	CAC-CBC-CGC-O2C
26	gF	201	PEB	CAB-CBB-CGB-O1B
26	lF	201	PEB	CAB-CBB-CGB-O2B
26	jG	201	PEB	CAC-CBC-CGC-O2C
26	oG	203	PEB	CAB-CBB-CGB-O2B
26	AI	305	PEB	CAB-CBB-CGB-O2B
26	OI	201	PEB	CAB-CBB-CGB-O1B
26	eI	201	PEB	CAC-CBC-CGC-O2C
26	hI	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	MJ	202	PEB	CAC-CBC-CGC-O1C
27	A6	303	PUB	CAC-CBC-CGC-O1C
27	A6	303	PUB	CAB-CBB-CGB-O2B
28	DB	1001	CYC	CAD-CBD-CGD-O1D
28	UH	1001	CYC	CAD-CBD-CGD-O1D
28	OH	1001	CYC	C2B-C3B-CAB-CBB
28	cH	1001	CYC	C3A-C2A-CAA-CBA
26	F1	202	PEB	CAC-CBC-CGC-O1C
26	J1	202	PEB	CAB-CBB-CGB-O2B
26	L1	203	PEB	CAB-CBB-CGB-O1B
26	S1	202	PEB	CAB-CBB-CGB-O2B
26	T1	201	PEB	CAB-CBB-CGB-O1B
26	V1	203	PEB	CAB-CBB-CGB-O1B
26	X1	203	PEB	CAB-CBB-CGB-O2B
26	i1	203	PEB	CAC-CBC-CGC-O1C
26	r1	202	PEB	CAB-CBB-CGB-O2B
26	s1	203	PEB	CAB-CBB-CGB-O2B
26	t1	201	PEB	CAB-CBB-CGB-O1B
26	w1	201	PEB	CAC-CBC-CGC-O1C
26	z1	201	PEB	CAC-CBC-CGC-O1C
26	21	404	PEB	CAB-CBB-CGB-O2B
26	f2	202	PEB	CAB-CBB-CGB-O1B
26	h2	201	PEB	CAC-CBC-CGC-O2C
26	m2	201	PEB	CAB-CBB-CGB-O2B
26	B3	203	PEB	CAC-CBC-CGC-O1C
26	E3	201	PEB	CAC-CBC-CGC-O1C
26	T3	203	PEB	CAB-CBB-CGB-O1B
26	A4	201	PEB	CAB-CBB-CGB-O1B
26	J4	202	PEB	CAB-CBB-CGB-O2B
26	L4	201	PEB	CAC-CBC-CGC-O2C
26	M4	402	PEB	CAB-CBB-CGB-O1B
26	N4	202	PEB	CAC-CBC-CGC-O1C
26	N4	202	PEB	CAC-CBC-CGC-O2C
26	c4	202	PEB	CAB-CBB-CGB-O1B
26	j4	201	PEB	CAB-CBB-CGB-O2B
26	C5	203	PEB	CAC-CBC-CGC-O2C
26	G5	202	PEB	CAC-CBC-CGC-O2C
26	L5	203	PEB	CAC-CBC-CGC-O1C
26	R6	202	PEB	CAC-CBC-CGC-O2C
26	f6	203	PEB	CAC-CBC-CGC-O1C
26	i6	202	PEB	CAB-CBB-CGB-O1B
26	A7	302	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	P7	202	PEB	CAB-CBB-CGB-O1B
26	Q7	201	PEB	CAC-CBC-CGC-O1C
26	Y7	202	PEB	CAB-CBB-CGB-O1B
26	d7	202	PEB	CAB-CBB-CGB-O1B
26	f7	201	PEB	CAC-CBC-CGC-O1C
26	f7	203	PEB	CAC-CBC-CGC-O1C
26	h7	202	PEB	CAC-CBC-CGC-O2C
26	D8	202	PEB	CAC-CBC-CGC-O1C
26	E8	201	PEB	CAB-CBB-CGB-O2B
26	E8	203	PEB	CAC-CBC-CGC-O1C
26	V8	202	PEB	CAC-CBC-CGC-O1C
26	O9	201	PEB	CAC-CBC-CGC-O1C
26	Y9	202	PEB	CAB-CBB-CGB-O1B
26	MA	203	PEB	CAC-CBC-CGC-O1C
26	OA	201	PEB	CAC-CBC-CGC-O2C
26	QA	204	PEB	CAC-CBC-CGC-O1C
26	UA	202	PEB	CAC-CBC-CGC-O1C
26	VA	202	PEB	CAC-CBC-CGC-O2C
26	jA	201	PEB	CAC-CBC-CGC-O1C
26	cB	202	PEB	CAC-CBC-CGC-O2C
26	fB	201	PEB	CAC-CBC-CGC-O1C
26	hB	203	PEB	CAC-CBC-CGC-O1C
26	iB	202	PEB	CAB-CBB-CGB-O1B
26	mB	201	PEB	CAC-CBC-CGC-O2C
26	AC	202	PEB	CAC-CBC-CGC-O2C
26	IC	203	PEB	CAB-CBB-CGB-O2B
26	KD	202	PEB	CAC-CBC-CGC-O2C
26	OD	201	PEB	CAC-CBC-CGC-O2C
26	UD	201	PEB	CAC-CBC-CGC-O2C
26	YD	301	PEB	CAC-CBC-CGC-O2C
26	AE	201	PEB	CAB-CBB-CGB-O1B
26	ME	202	PEB	CAC-CBC-CGC-O1C
26	WE	202	PEB	CAC-CBC-CGC-O1C
26	dE	202	PEB	CAB-CBB-CGB-O2B
26	eE	203	PEB	CAB-CBB-CGB-O2B
26	jE	201	PEB	CAC-CBC-CGC-O2C
26	jE	202	PEB	CAB-CBB-CGB-O2B
26	lE	202	PEB	CAB-CBB-CGB-O1B
26	oE	201	PEB	CAC-CBC-CGC-O2C
26	tE	202	PEB	CAB-CBB-CGB-O1B
26	OF	201	PEB	CAC-CBC-CGC-O2C
26	VF	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	YF	202	PEB	CAB-CBB-CGB-01B
26	lF	202	PEB	CAC-CBC-CGC-02C
26	CG	202	PEB	CAC-CBC-CGC-02C
26	MG	202	PEB	CAC-CBC-CGC-01C
26	WG	203	PEB	CAB-CBB-CGB-01B
26	lG	202	PEB	CAC-CBC-CGC-02C
26	wG	301	PEB	CAC-CBC-CGC-02C
26	xG	302	PEB	CAC-CBC-CGC-02C
26	WI	201	PEB	CAC-CBC-CGC-02C
26	cI	201	PEB	CAC-CBC-CGC-01C
26	jI	201	PEB	CAC-CBC-CGC-02C
26	mI	201	PEB	CAB-CBB-CGB-02B
26	AJ	303	PEB	CAC-CBC-CGC-01C
26	DJ	202	PEB	CAC-CBC-CGC-01C
26	EJ	202	PEB	CAB-CBB-CGB-02B
26	SJ	202	PEB	CAC-CBC-CGC-02C
26	TJ	202	PEB	CAC-CBC-CGC-02C
26	TJ	203	PEB	CAC-CBC-CGC-02C
26	XJ	201	PEB	CAC-CBC-CGC-01C
27	A8	304	PUB	CAB-CBB-CGB-02B
27	AA	304	PUB	CAB-CBB-CGB-02B
28	N7	1001	CYC	CAA-CBA-CGA-02A
28	DF	1001	CYC	CAA-CBA-CGA-01A
26	D1	203	PEB	CAC-CBC-CGC-02C
26	J1	201	PEB	CAC-CBC-CGC-02C
26	M1	401	PEB	CAC-CBC-CGC-01C
26	c1	201	PEB	CAC-CBC-CGC-01C
26	c1	203	PEB	CAC-CBC-CGC-01C
26	m1	201	PEB	CAC-CBC-CGC-01C
26	v1	201	PEB	CAC-CBC-CGC-01C
26	x1	202	PEB	CAC-CBC-CGC-01C
26	x1	202	PEB	CAC-CBC-CGC-02C
26	x1	202	PEB	CAB-CBB-CGB-01B
26	Y2	203	PEB	CAC-CBC-CGC-01C
26	f2	202	PEB	CAC-CBC-CGC-01C
26	m2	203	PEB	CAC-CBC-CGC-01C
26	B3	202	PEB	CAC-CBC-CGC-02C
26	G3	202	PEB	CAC-CBC-CGC-01C
26	N3	203	PEB	CAB-CBB-CGB-01B
26	W3	201	PEB	CAB-CBB-CGB-01B
26	W3	202	PEB	CAC-CBC-CGC-02C
26	Y3	304	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	B4	202	PEB	CAC-CBC-CGC-O1C
26	B4	203	PEB	CAB-CBB-CGB-O2B
26	H4	201	PEB	CAC-CBC-CGC-O1C
26	L4	203	PEB	CAB-CBB-CGB-O2B
26	T4	201	PEB	CAB-CBB-CGB-O1B
26	a4	203	PEB	CAB-CBB-CGB-O1B
26	c4	201	PEB	CAC-CBC-CGC-O1C
26	c4	202	PEB	CAC-CBC-CGC-O1C
26	d4	201	PEB	CAC-CBC-CGC-O1C
26	h4	201	PEB	CAC-CBC-CGC-O1C
26	i4	202	PEB	CAC-CBC-CGC-O1C
26	q4	202	PEB	CAB-CBB-CGB-O1B
26	r4	202	PEB	CAC-CBC-CGC-O1C
26	r4	202	PEB	CAB-CBB-CGB-O2B
26	s4	203	PEB	CAB-CBB-CGB-O1B
26	x4	201	PEB	CAC-CBC-CGC-O1C
26	x4	202	PEB	CAB-CBB-CGB-O2B
26	y4	201	PEB	CAB-CBB-CGB-O1B
26	z4	201	PEB	CAC-CBC-CGC-O2C
26	A5	202	PEB	CAC-CBC-CGC-O1C
26	A6	301	PEB	CAB-CBB-CGB-O1B
26	Q6	202	PEB	CAC-CBC-CGC-O2C
26	U6	203	PEB	CAC-CBC-CGC-O1C
26	W6	203	PEB	CAC-CBC-CGC-O1C
26	a6	202	PEB	CAB-CBB-CGB-O1B
26	d6	201	PEB	CAC-CBC-CGC-O2C
26	e6	203	PEB	CAC-CBC-CGC-O1C
26	f6	201	PEB	CAC-CBC-CGC-O1C
26	f6	202	PEB	CAC-CBC-CGC-O1C
26	h6	202	PEB	CAB-CBB-CGB-O1B
26	l6	202	PEB	CAC-CBC-CGC-O1C
26	F7	1002	PEB	CAC-CBC-CGC-O1C
26	P7	202	PEB	CAC-CBC-CGC-O1C
26	Q7	202	PEB	CAC-CBC-CGC-O1C
26	U7	201	PEB	CAC-CBC-CGC-O2C
26	c7	201	PEB	CAC-CBC-CGC-O1C
26	d7	203	PEB	CAC-CBC-CGC-O1C
26	f7	202	PEB	CAC-CBC-CGC-O1C
26	k7	202	PEB	CAB-CBB-CGB-O1B
26	l7	202	PEB	CAC-CBC-CGC-O1C
26	D8	201	PEB	CAC-CBC-CGC-O1C
26	M8	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	Q8	204	PEB	CAC-CBC-CGC-O1C
26	S8	201	PEB	CAC-CBC-CGC-O1C
26	U8	202	PEB	CAC-CBC-CGC-O1C
26	l8	201	PEB	CAB-CBB-CGB-O1B
26	D9	202	PEB	CAC-CBC-CGC-O2C
26	D9	203	PEB	CAC-CBC-CGC-O1C
26	J9	203	PEB	CAC-CBC-CGC-O1C
26	O9	202	PEB	CAC-CBC-CGC-O1C
26	P9	202	PEB	CAC-CBC-CGC-O2C
26	Q9	202	PEB	CAB-CBB-CGB-O1B
26	CA	202	PEB	CAC-CBC-CGC-O1C
26	DA	202	PEB	CAC-CBC-CGC-O1C
26	EA	203	PEB	CAB-CBB-CGB-O1B
26	SA	201	PEB	CAC-CBC-CGC-O2C
26	VA	202	PEB	CAC-CBC-CGC-O1C
26	AB	301	PEB	CAB-CBB-CGB-O1B
26	OB	202	PEB	CAB-CBB-CGB-O2B
26	SB	202	PEB	CAC-CBC-CGC-O2C
26	WB	203	PEB	CAC-CBC-CGC-O1C
26	ZB	203	PEB	CAC-CBC-CGC-O1C
26	ZB	203	PEB	CAB-CBB-CGB-O2B
26	gB	202	PEB	CAC-CBC-CGC-O1C
26	HC	201	PEB	CAB-CBB-CGB-O1B
26	LC	203	PEB	CAC-CBC-CGC-O1C
26	GD	202	PEB	CAB-CBB-CGB-O2B
26	JD	202	PEB	CAC-CBC-CGC-O2C
26	ND	203	PEB	CAB-CBB-CGB-O1B
26	SD	202	PEB	CAC-CBC-CGC-O1C
26	UD	202	PEB	CAC-CBC-CGC-O1C
26	YD	301	PEB	CAB-CBB-CGB-O1B
26	CE	203	PEB	CAC-CBC-CGC-O1C
26	SE	203	PEB	CAB-CBB-CGB-O1B
26	VE	202	PEB	CAB-CBB-CGB-O1B
26	WE	203	PEB	CAB-CBB-CGB-O1B
26	aE	203	PEB	CAC-CBC-CGC-O1C
26	aE	203	PEB	CAB-CBB-CGB-O1B
26	bE	202	PEB	CAB-CBB-CGB-O1B
26	oE	201	PEB	CAC-CBC-CGC-O1C
26	qE	202	PEB	CAC-CBC-CGC-O1C
26	sE	202	PEB	CAC-CBC-CGC-O1C
26	xE	302	PEB	CAB-CBB-CGB-O1B
26	zE	501	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	QF	202	PEB	CAC-CBC-CGC-O1C
26	UF	201	PEB	CAC-CBC-CGC-O1C
26	hF	203	PEB	CAC-CBC-CGC-O1C
26	kF	202	PEB	CAB-CBB-CGB-O1B
26	lF	201	PEB	CAC-CBC-CGC-O1C
26	EG	202	PEB	CAB-CBB-CGB-O1B
26	SG	203	PEB	CAB-CBB-CGB-O1B
26	VG	202	PEB	CAB-CBB-CGB-O1B
26	YG	202	PEB	CAB-CBB-CGB-O1B
26	lG	201	PEB	CAC-CBC-CGC-O1C
26	oG	201	PEB	CAB-CBB-CGB-O1B
26	yG	301	PEB	CAB-CBB-CGB-O1B
26	AI	301	PEB	CAC-CBC-CGC-O1C
26	AI	304	PEB	CAB-CBB-CGB-O1B
26	YI	203	PEB	CAC-CBC-CGC-O1C
26	eI	203	PEB	CAC-CBC-CGC-O1C
26	fI	202	PEB	CAC-CBC-CGC-O1C
26	hI	202	PEB	CAC-CBC-CGC-O1C
26	kI	203	PEB	CAC-CBC-CGC-O1C
26	mI	203	PEB	CAC-CBC-CGC-O1C
26	AJ	303	PEB	CAB-CBB-CGB-O1B
26	IJ	202	PEB	CAB-CBB-CGB-O1B
26	LJ	203	PEB	CAC-CBC-CGC-O2C
26	RJ	202	PEB	CAC-CBC-CGC-O2C
26	TJ	201	PEB	CAB-CBB-CGB-O1B
27	A6	302	PUB	CAC-CBC-CGC-O1C
27	yG	303	PUB	CAB-CBB-CGB-O1B
28	C2	1001	CYC	CAA-CBA-CGA-O1A
28	J7	1003	CYC	CAA-CBA-CGA-O1A
28	qH	1002	CYC	CAD-CBD-CGD-O1D
26	G1	201	PEB	CAC-CBC-CGC-O1C
26	T1	203	PEB	CAC-CBC-CGC-O1C
26	T1	203	PEB	CAB-CBB-CGB-O1B
26	U1	202	PEB	CAB-CBB-CGB-O2B
26	X1	203	PEB	CAB-CBB-CGB-O1B
26	d1	202	PEB	CAC-CBC-CGC-O1C
26	h1	202	PEB	CAB-CBB-CGB-O2B
26	p1	201	PEB	CAC-CBC-CGC-O2C
26	r1	201	PEB	CAC-CBC-CGC-O1C
26	r1	202	PEB	CAC-CBC-CGC-O2C
26	s1	201	PEB	CAB-CBB-CGB-O1B
26	y1	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	z1	202	PEB	CAC-CBC-CGC-O1C
26	21	404	PEB	CAB-CBB-CGB-O1B
26	A2	305	PEB	CAB-CBB-CGB-O2B
26	F2	1002	PEB	CAB-CBB-CGB-O1B
26	T2	202	PEB	CAC-CBC-CGC-O2C
26	V2	203	PEB	CAC-CBC-CGC-O1C
26	d2	201	PEB	CAB-CBB-CGB-O1B
26	e2	201	PEB	CAC-CBC-CGC-O2C
26	j2	201	PEB	CAC-CBC-CGC-O1C
26	D3	203	PEB	CAB-CBB-CGB-O1B
26	F3	202	PEB	CAC-CBC-CGC-O1C
26	J3	203	PEB	CAB-CBB-CGB-O2B
26	L3	203	PEB	CAC-CBC-CGC-O1C
26	L3	203	PEB	CAB-CBB-CGB-O1B
26	A4	202	PEB	CAC-CBC-CGC-O2C
26	D4	203	PEB	CAB-CBB-CGB-O1B
26	J4	202	PEB	CAC-CBC-CGC-O2C
26	P4	203	PEB	CAB-CBB-CGB-O1B
26	R4	202	PEB	CAC-CBC-CGC-O2C
26	S4	202	PEB	CAB-CBB-CGB-O1B
26	V4	203	PEB	CAB-CBB-CGB-O2B
26	Y4	202	PEB	CAB-CBB-CGB-O1B
26	a4	202	PEB	CAB-CBB-CGB-O1B
26	b4	501	PEB	CAB-CBB-CGB-O1B
26	m4	201	PEB	CAC-CBC-CGC-O1C
26	m4	202	PEB	CAB-CBB-CGB-O1B
26	m4	203	PEB	CAC-CBC-CGC-O2C
26	p4	201	PEB	CAC-CBC-CGC-O1C
26	x4	201	PEB	CAB-CBB-CGB-O1B
26	24	404	PEB	CAC-CBC-CGC-O2C
26	C5	202	PEB	CAC-CBC-CGC-O1C
26	C5	203	PEB	CAB-CBB-CGB-O1B
26	L5	203	PEB	CAC-CBC-CGC-O2C
26	H6	1002	PEB	CAC-CBC-CGC-O1C
26	K6	201	PEB	CAC-CBC-CGC-O1C
26	O6	202	PEB	CAC-CBC-CGC-O2C
26	Q6	203	PEB	CAB-CBB-CGB-O1B
26	U6	203	PEB	CAB-CBB-CGB-O2B
26	Z6	203	PEB	CAC-CBC-CGC-O1C
26	b6	202	PEB	CAB-CBB-CGB-O1B
26	c6	201	PEB	CAC-CBC-CGC-O1C
26	g6	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	h6	202	PEB	CAC-CBC-CGC-O1C
26	l6	202	PEB	CAB-CBB-CGB-O2B
26	D7	1002	PEB	CAC-CBC-CGC-O1C
26	O7	202	PEB	CAC-CBC-CGC-O1C
26	Q7	201	PEB	CAB-CBB-CGB-O2B
26	b7	203	PEB	CAC-CBC-CGC-O1C
26	d7	202	PEB	CAB-CBB-CGB-O2B
26	d7	203	PEB	CAB-CBB-CGB-O1B
26	l7	202	PEB	CAB-CBB-CGB-O2B
26	E8	203	PEB	CAB-CBB-CGB-O2B
26	I8	203	PEB	CAC-CBC-CGC-O2C
26	T8	202	PEB	CAC-CBC-CGC-O2C
26	a8	201	PEB	CAB-CBB-CGB-O1B
26	a8	202	PEB	CAC-CBC-CGC-O2C
26	j8	203	PEB	CAC-CBC-CGC-O2C
26	D9	201	PEB	CAC-CBC-CGC-O1C
26	E9	202	PEB	CAB-CBB-CGB-O1B
26	G9	202	PEB	CAC-CBC-CGC-O1C
26	J9	202	PEB	CAC-CBC-CGC-O1C
26	L9	202	PEB	CAB-CBB-CGB-O2B
26	P9	203	PEB	CAC-CBC-CGC-O1C
26	S9	202	PEB	CAC-CBC-CGC-O2C
26	T9	203	PEB	CAC-CBC-CGC-O1C
26	V9	201	PEB	CAB-CBB-CGB-O1B
26	X9	203	PEB	CAC-CBC-CGC-O1C
26	Y9	202	PEB	CAB-CBB-CGB-O2B
26	AA	301	PEB	CAB-CBB-CGB-O1B
26	DA	201	PEB	CAC-CBC-CGC-O1C
26	EA	203	PEB	CAC-CBC-CGC-O2C
26	SA	202	PEB	CAB-CBB-CGB-O1B
26	gA	202	PEB	CAC-CBC-CGC-O1C
26	lA	201	PEB	CAC-CBC-CGC-O1C
26	AB	304	PEB	CAB-CBB-CGB-O1B
26	OB	202	PEB	CAC-CBC-CGC-O1C
26	QB	201	PEB	CAC-CBC-CGC-O2C
26	WB	201	PEB	CAB-CBB-CGB-O2B
26	cB	201	PEB	CAC-CBC-CGC-O1C
26	fB	202	PEB	CAC-CBC-CGC-O1C
26	AC	201	PEB	CAB-CBB-CGB-O1B
26	AC	202	PEB	CAB-CBB-CGB-O1B
26	GC	202	PEB	CAC-CBC-CGC-O1C
26	AD	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	BD	201	PEB	CAC-CBC-CGC-O1C
26	OD	202	PEB	CAB-CBB-CGB-O1B
26	PD	201	PEB	CAC-CBC-CGC-O2C
26	QD	201	PEB	CAC-CBC-CGC-O1C
26	SD	201	PEB	CAC-CBC-CGC-O2C
26	WD	202	PEB	CAC-CBC-CGC-O1C
26	ME	201	PEB	CAC-CBC-CGC-O1C
26	eE	202	PEB	CAC-CBC-CGC-O1C
26	nE	202	PEB	CAB-CBB-CGB-O1B
26	oE	202	PEB	CAC-CBC-CGC-O1C
26	pE	201	PEB	CAC-CBC-CGC-O1C
26	wE	303	PEB	CAC-CBC-CGC-O2C
26	AF	302	PEB	CAB-CBB-CGB-O1B
26	HF	1002	PEB	CAC-CBC-CGC-O1C
26	OF	201	PEB	CAB-CBB-CGB-O2B
26	OF	202	PEB	CAB-CBB-CGB-O1B
26	QF	203	PEB	CAC-CBC-CGC-O2C
26	UF	203	PEB	CAC-CBC-CGC-O2C
26	ZF	203	PEB	CAC-CBC-CGC-O1C
26	jF	201	PEB	CAC-CBC-CGC-O1C
26	mF	201	PEB	CAB-CBB-CGB-O1B
26	CG	203	PEB	CAC-CBC-CGC-O1C
26	EG	201	PEB	CAC-CBC-CGC-O2C
26	QG	202	PEB	CAB-CBB-CGB-O1B
26	SG	202	PEB	CAC-CBC-CGC-O1C
26	dG	201	PEB	CAC-CBC-CGC-O2C
26	mG	202	PEB	CAC-CBC-CGC-O2C
26	oG	202	PEB	CAC-CBC-CGC-O1C
26	FI	1002	PEB	CAC-CBC-CGC-O1C
26	FI	1002	PEB	CAB-CBB-CGB-O1B
26	VI	202	PEB	CAC-CBC-CGC-O1C
26	VI	203	PEB	CAC-CBC-CGC-O1C
26	aI	202	PEB	CAC-CBC-CGC-O1C
26	cI	202	PEB	CAC-CBC-CGC-O1C
26	mI	202	PEB	CAC-CBC-CGC-O1C
26	LJ	202	PEB	CAC-CBC-CGC-O2C
26	LJ	202	PEB	CAB-CBB-CGB-O2B
26	OJ	201	PEB	CAB-CBB-CGB-O2B
26	PJ	202	PEB	CAB-CBB-CGB-O1B
26	PJ	203	PEB	CAB-CBB-CGB-O1B
26	SJ	202	PEB	CAB-CBB-CGB-O1B
27	K1	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
27	K3	203	PUB	CAB-CBB-CGB-O1B
27	AA	303	PUB	CAB-CBB-CGB-O2B
27	AI	303	PUB	CAB-CBB-CGB-O2B
28	I2	1001	CYC	CAA-CBA-CGA-O1A
28	J2	1001	CYC	CAA-CBA-CGA-O2A
28	H7	1001	CYC	CAA-CBA-CGA-O1A
28	J7	1001	CYC	CAD-CBD-CGD-O1D
28	CI	1001	CYC	CAA-CBA-CGA-O1A
28	GI	1001	CYC	CAA-CBA-CGA-O2A
28	II	1001	CYC	CAA-CBA-CGA-O1A
26	cE	203	PEB	C4B-C3B-CAB-CBB
26	h2	202	PEB	C2C-CAC-CBC-CGC
26	A3	201	PEB	C2C-CAC-CBC-CGC
26	I3	202	PEB	C2C-CAC-CBC-CGC
26	R3	203	PEB	C2C-CAC-CBC-CGC
26	B4	201	PEB	C2C-CAC-CBC-CGC
26	e4	202	PEB	C2C-CAC-CBC-CGC
26	U6	203	PEB	C2C-CAC-CBC-CGC
26	e7	202	PEB	C2C-CAC-CBC-CGC
26	j7	202	PEB	C2C-CAC-CBC-CGC
26	cE	203	PEB	C2C-CAC-CBC-CGC
27	Y3	302	PUB	C3B-CAB-CBB-CGB
27	AA	303	PUB	C3B-CAB-CBB-CGB
28	DF	1001	CYC	C3D-CAD-CBD-CGD
26	B1	201	PEB	CAC-CBC-CGC-O1C
26	H1	203	PEB	CAB-CBB-CGB-O2B
26	Y1	202	PEB	CAB-CBB-CGB-O1B
26	b1	501	PEB	CAB-CBB-CGB-O1B
26	e1	202	PEB	CAC-CBC-CGC-O1C
26	e1	202	PEB	CAC-CBC-CGC-O2C
26	e1	202	PEB	CAB-CBB-CGB-O2B
26	g1	203	PEB	CAB-CBB-CGB-O1B
26	i1	201	PEB	CAC-CBC-CGC-O1C
26	21	401	PEB	CAB-CBB-CGB-O1B
26	A2	305	PEB	CAB-CBB-CGB-O1B
26	D2	1002	PEB	CAB-CBB-CGB-O1B
26	F2	1002	PEB	CAC-CBC-CGC-O1C
26	P2	203	PEB	CAB-CBB-CGB-O1B
26	V2	203	PEB	CAB-CBB-CGB-O1B
26	k2	203	PEB	CAC-CBC-CGC-O1C
26	B3	202	PEB	CAB-CBB-CGB-O1B
26	B3	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	D3	203	PEB	CAC-CBC-CGC-O2C
26	G3	202	PEB	CAB-CBB-CGB-O2B
26	H3	203	PEB	CAB-CBB-CGB-O1B
26	O3	202	PEB	CAC-CBC-CGC-O1C
26	Q3	202	PEB	CAC-CBC-CGC-O2C
26	U3	201	PEB	CAC-CBC-CGC-O2C
26	V3	202	PEB	CAB-CBB-CGB-O1B
26	M4	401	PEB	CAB-CBB-CGB-O2B
26	U4	202	PEB	CAC-CBC-CGC-O1C
26	c4	202	PEB	CAC-CBC-CGC-O2C
26	d4	202	PEB	CAC-CBC-CGC-O1C
26	f4	201	PEB	CAC-CBC-CGC-O2C
26	g4	203	PEB	CAC-CBC-CGC-O1C
26	y4	202	PEB	CAC-CBC-CGC-O1C
26	B5	203	PEB	CAC-CBC-CGC-O1C
26	L5	203	PEB	CAB-CBB-CGB-O1B
26	A6	301	PEB	CAB-CBB-CGB-O2B
26	Q6	203	PEB	CAC-CBC-CGC-O2C
26	S6	201	PEB	CAC-CBC-CGC-O1C
26	f6	201	PEB	CAB-CBB-CGB-O1B
26	g6	202	PEB	CAB-CBB-CGB-O1B
26	i6	202	PEB	CAB-CBB-CGB-O2B
26	m6	201	PEB	CAC-CBC-CGC-O1C
26	D7	1002	PEB	CAB-CBB-CGB-O1B
26	O7	202	PEB	CAB-CBB-CGB-O1B
26	U7	203	PEB	CAB-CBB-CGB-O2B
26	Z7	201	PEB	CAC-CBC-CGC-O1C
26	c7	202	PEB	CAC-CBC-CGC-O2C
26	h7	203	PEB	CAB-CBB-CGB-O1B
26	j7	202	PEB	CAB-CBB-CGB-O1B
26	I8	201	PEB	CAC-CBC-CGC-O1C
26	S8	201	PEB	CAB-CBB-CGB-O1B
26	S8	202	PEB	CAB-CBB-CGB-O1B
26	U8	201	PEB	CAC-CBC-CGC-O1C
26	Y8	203	PEB	CAC-CBC-CGC-O1C
26	A9	304	PEB	CAC-CBC-CGC-O1C
26	B9	203	PEB	CAC-CBC-CGC-O1C
26	K9	202	PEB	CAC-CBC-CGC-O1C
26	L9	201	PEB	CAC-CBC-CGC-O2C
26	L9	203	PEB	CAC-CBC-CGC-O1C
26	N9	203	PEB	CAC-CBC-CGC-O2C
26	P9	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	P9	202	PEB	CAB-CBB-CGB-01B
26	P9	203	PEB	CAB-CBB-CGB-01B
26	T9	201	PEB	CAC-CBC-CGC-01C
26	V9	202	PEB	CAB-CBB-CGB-02B
26	X9	202	PEB	CAC-CBC-CGC-01C
26	X9	202	PEB	CAB-CBB-CGB-01B
26	EA	201	PEB	CAB-CBB-CGB-02B
26	KA	202	PEB	CAC-CBC-CGC-01C
26	SA	202	PEB	CAB-CBB-CGB-02B
26	aA	201	PEB	CAC-CBC-CGC-01C
26	fA	202	PEB	CAC-CBC-CGC-01C
26	fA	202	PEB	CAC-CBC-CGC-02C
26	hA	203	PEB	CAC-CBC-CGC-02C
26	jA	201	PEB	CAC-CBC-CGC-02C
26	jA	202	PEB	CAC-CBC-CGC-01C
26	kA	202	PEB	CAC-CBC-CGC-01C
26	AB	301	PEB	CAC-CBC-CGC-01C
26	DB	1002	PEB	CAC-CBC-CGC-01C
26	HB	1002	PEB	CAC-CBC-CGC-01C
26	KB	201	PEB	CAC-CBC-CGC-01C
26	QB	203	PEB	CAC-CBC-CGC-02C
26	SB	201	PEB	CAC-CBC-CGC-01C
26	UB	202	PEB	CAC-CBC-CGC-01C
26	YB	201	PEB	CAC-CBC-CGC-01C
26	ZB	203	PEB	CAB-CBB-CGB-01B
26	bB	202	PEB	CAC-CBC-CGC-02C
26	bB	202	PEB	CAB-CBB-CGB-01B
26	mB	203	PEB	CAB-CBB-CGB-01B
26	AC	201	PEB	CAC-CBC-CGC-01C
26	BC	201	PEB	CAC-CBC-CGC-01C
26	CC	201	PEB	CAC-CBC-CGC-01C
26	BD	202	PEB	CAB-CBB-CGB-01B
26	BD	203	PEB	CAC-CBC-CGC-01C
26	DD	202	PEB	CAC-CBC-CGC-02C
26	ED	201	PEB	CAC-CBC-CGC-01C
26	ED	201	PEB	CAC-CBC-CGC-02C
26	HD	201	PEB	CAC-CBC-CGC-01C
26	MD	202	PEB	CAC-CBC-CGC-01C
26	OD	201	PEB	CAB-CBB-CGB-01B
26	PD	203	PEB	CAB-CBB-CGB-01B
26	RD	202	PEB	CAC-CBC-CGC-01C
26	YD	304	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	AE	202	PEB	CAB-CBB-CGB-01B
26	EE	202	PEB	CAC-CBC-CGC-02C
26	JE	202	PEB	CAB-CBB-CGB-01B
26	KE	203	PEB	CAB-CBB-CGB-02B
26	OE	202	PEB	CAC-CBC-CGC-01C
26	OE	203	PEB	CAB-CBB-CGB-02B
26	SE	203	PEB	CAB-CBB-CGB-02B
26	YE	201	PEB	CAC-CBC-CGC-01C
26	YE	203	PEB	CAC-CBC-CGC-01C
26	eE	203	PEB	CAB-CBB-CGB-01B
26	fE	202	PEB	CAB-CBB-CGB-02B
26	xE	303	PEB	CAC-CBC-CGC-01C
26	yE	301	PEB	CAB-CBB-CGB-01B
26	JF	1002	PEB	CAC-CBC-CGC-02C
26	JF	1002	PEB	CAB-CBB-CGB-01B
26	bF	202	PEB	CAC-CBC-CGC-01C
26	cF	202	PEB	CAC-CBC-CGC-01C
26	fF	203	PEB	CAC-CBC-CGC-02C
26	hF	201	PEB	CAB-CBB-CGB-01B
26	EG	202	PEB	CAC-CBC-CGC-02C
26	MG	201	PEB	CAC-CBC-CGC-01C
26	OG	203	PEB	CAC-CBC-CGC-01C
26	ZG	202	PEB	CAB-CBB-CGB-01B
26	bG	202	PEB	CAB-CBB-CGB-01B
26	mG	201	PEB	CAB-CBB-CGB-01B
26	qG	203	PEB	CAC-CBC-CGC-02C
26	sG	202	PEB	CAC-CBC-CGC-02C
26	uG	202	PEB	CAC-CBC-CGC-02C
26	wG	301	PEB	CAB-CBB-CGB-01B
26	wG	303	PEB	CAC-CBC-CGC-02C
26	xG	302	PEB	CAB-CBB-CGB-01B
26	xG	304	PEB	CAB-CBB-CGB-01B
26	AI	304	PEB	CAC-CBC-CGC-01C
26	PI	203	PEB	CAC-CBC-CGC-01C
26	TI	202	PEB	CAC-CBC-CGC-01C
26	cI	203	PEB	CAC-CBC-CGC-01C
26	iI	202	PEB	CAC-CBC-CGC-01C
26	AJ	304	PEB	CAC-CBC-CGC-01C
26	JJ	202	PEB	CAC-CBC-CGC-01C
26	KJ	202	PEB	CAC-CBC-CGC-01C
26	LJ	201	PEB	CAC-CBC-CGC-02C
26	NJ	202	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	NJ	204	PEB	CAC-CBC-CGC-O1C
26	PJ	203	PEB	CAC-CBC-CGC-O1C
26	QJ	202	PEB	CAB-CBB-CGB-O2B
26	TJ	201	PEB	CAC-CBC-CGC-O1C
26	UJ	202	PEB	CAC-CBC-CGC-O1C
26	VJ	203	PEB	CAC-CBC-CGC-O2C
27	xE	301	PUB	CAB-CBB-CGB-O1B
27	AF	304	PUB	CAC-CBC-CGC-O1C
27	xG	301	PUB	CAB-CBB-CGB-O1B
28	B6	1002	CYC	CAA-CBA-CGA-O1A
28	KH	1001	CYC	CAD-CBD-CGD-O1D
26	R2	202	PEB	C2B-C3B-CAB-CBB
26	B1	202	PEB	CAC-CBC-CGC-O2C
26	B1	203	PEB	CAB-CBB-CGB-O1B
26	F1	203	PEB	CAB-CBB-CGB-O2B
26	G1	202	PEB	CAB-CBB-CGB-O2B
26	H1	201	PEB	CAC-CBC-CGC-O2C
26	N1	202	PEB	CAC-CBC-CGC-O1C
26	Q1	202	PEB	CAB-CBB-CGB-O2B
26	R1	201	PEB	CAC-CBC-CGC-O1C
26	S1	202	PEB	CAC-CBC-CGC-O2C
26	c1	202	PEB	CAC-CBC-CGC-O1C
26	c1	202	PEB	CAC-CBC-CGC-O2C
26	d1	203	PEB	CAB-CBB-CGB-O1B
26	e1	202	PEB	CAB-CBB-CGB-O1B
26	g1	203	PEB	CAC-CBC-CGC-O2C
26	k1	201	PEB	CAB-CBB-CGB-O1B
26	l1	201	PEB	CAB-CBB-CGB-O1B
26	p1	201	PEB	CAC-CBC-CGC-O1C
26	r1	201	PEB	CAB-CBB-CGB-O1B
26	v1	202	PEB	CAC-CBC-CGC-O2C
26	w1	201	PEB	CAC-CBC-CGC-O2C
26	x1	202	PEB	CAB-CBB-CGB-O2B
26	A2	304	PEB	CAC-CBC-CGC-O1C
26	R2	202	PEB	CAB-CBB-CGB-O1B
26	T2	203	PEB	CAB-CBB-CGB-O2B
26	U2	202	PEB	CAC-CBC-CGC-O2C
26	c2	202	PEB	CAB-CBB-CGB-O2B
26	h2	202	PEB	CAC-CBC-CGC-O2C
26	h2	202	PEB	CAB-CBB-CGB-O2B
26	i2	203	PEB	CAC-CBC-CGC-O1C
26	k2	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	E3	202	PEB	CAC-CBC-CGC-O1C
26	H3	201	PEB	CAC-CBC-CGC-O1C
26	Q3	201	PEB	CAC-CBC-CGC-O2C
26	R3	201	PEB	CAB-CBB-CGB-O1B
26	S3	201	PEB	CAC-CBC-CGC-O1C
26	T3	203	PEB	CAB-CBB-CGB-O2B
26	Y3	303	PEB	CAC-CBC-CGC-O2C
26	F4	202	PEB	CAC-CBC-CGC-O2C
26	H4	201	PEB	CAC-CBC-CGC-O2C
26	J4	201	PEB	CAC-CBC-CGC-O2C
26	M4	401	PEB	CAC-CBC-CGC-O1C
26	P4	201	PEB	CAC-CBC-CGC-O2C
26	P4	202	PEB	CAC-CBC-CGC-O1C
26	R4	203	PEB	CAB-CBB-CGB-O1B
26	T4	203	PEB	CAC-CBC-CGC-O2C
26	T4	203	PEB	CAB-CBB-CGB-O1B
26	c4	202	PEB	CAB-CBB-CGB-O2B
26	m4	201	PEB	CAB-CBB-CGB-O1B
26	r4	201	PEB	CAC-CBC-CGC-O2C
26	v4	202	PEB	CAC-CBC-CGC-O2C
26	z4	201	PEB	CAC-CBC-CGC-O1C
26	G5	202	PEB	CAC-CBC-CGC-O1C
26	G5	203	PEB	CAB-CBB-CGB-O1B
26	H5	201	PEB	CAB-CBB-CGB-O1B
26	H5	202	PEB	CAB-CBB-CGB-O1B
26	O6	201	PEB	CAB-CBB-CGB-O1B
26	O6	202	PEB	CAB-CBB-CGB-O2B
26	Z6	203	PEB	CAB-CBB-CGB-O1B
26	Z6	203	PEB	CAB-CBB-CGB-O2B
26	d6	201	PEB	CAC-CBC-CGC-O1C
26	d6	201	PEB	CAB-CBB-CGB-O1B
26	e6	203	PEB	CAB-CBB-CGB-O1B
26	h6	203	PEB	CAC-CBC-CGC-O2C
26	H7	1002	PEB	CAC-CBC-CGC-O1C
26	J7	1002	PEB	CAC-CBC-CGC-O2C
26	J7	1002	PEB	CAB-CBB-CGB-O1B
26	O7	201	PEB	CAB-CBB-CGB-O1B
26	Q7	201	PEB	CAC-CBC-CGC-O2C
26	U7	202	PEB	CAC-CBC-CGC-O1C
26	W7	203	PEB	CAC-CBC-CGC-O1C
26	Y7	202	PEB	CAB-CBB-CGB-O2B
26	b7	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	c7	202	PEB	CAC-CBC-CGC-O1C
26	h7	202	PEB	CAC-CBC-CGC-O1C
26	k7	202	PEB	CAB-CBB-CGB-O2B
26	m7	201	PEB	CAB-CBB-CGB-O2B
26	G8	202	PEB	CAC-CBC-CGC-O1C
26	O8	201	PEB	CAC-CBC-CGC-O2C
26	O8	202	PEB	CAC-CBC-CGC-O2C
26	S8	202	PEB	CAB-CBB-CGB-O2B
26	c8	202	PEB	CAC-CBC-CGC-O2C
26	j8	201	PEB	CAC-CBC-CGC-O2C
26	j8	202	PEB	CAB-CBB-CGB-O1B
26	j8	203	PEB	CAC-CBC-CGC-O1C
26	k8	202	PEB	CAC-CBC-CGC-O1C
26	k8	202	PEB	CAC-CBC-CGC-O2C
26	A9	303	PEB	CAB-CBB-CGB-O2B
26	F9	202	PEB	CAC-CBC-CGC-O1C
26	F9	203	PEB	CAB-CBB-CGB-O2B
26	N9	202	PEB	CAB-CBB-CGB-O2B
26	Q9	202	PEB	CAC-CBC-CGC-O1C
26	U9	202	PEB	CAC-CBC-CGC-O1C
26	CA	201	PEB	CAC-CBC-CGC-O2C
26	DA	201	PEB	CAC-CBC-CGC-O2C
26	GA	202	PEB	CAC-CBC-CGC-O1C
26	GA	202	PEB	CAC-CBC-CGC-O2C
26	HA	202	PEB	CAB-CBB-CGB-O1B
26	LA	202	PEB	CAB-CBB-CGB-O1B
26	LA	202	PEB	CAB-CBB-CGB-O2B
26	ZA	202	PEB	CAB-CBB-CGB-O1B
26	lA	201	PEB	CAB-CBB-CGB-O2B
26	AB	301	PEB	CAB-CBB-CGB-O2B
26	OB	202	PEB	CAC-CBC-CGC-O2C
26	QB	203	PEB	CAB-CBB-CGB-O2B
26	UB	203	PEB	CAB-CBB-CGB-O2B
26	dB	201	PEB	CAB-CBB-CGB-O1B
26	eB	201	PEB	CAC-CBC-CGC-O1C
26	lB	202	PEB	CAB-CBB-CGB-O2B
26	AC	201	PEB	CAC-CBC-CGC-O2C
26	BC	203	PEB	CAC-CBC-CGC-O2C
26	FC	201	PEB	CAB-CBB-CGB-O2B
26	GC	202	PEB	CAC-CBC-CGC-O2C
26	HC	201	PEB	CAC-CBC-CGC-O1C
26	DD	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	ED	202	PEB	CAC-CBC-CGC-O1C
26	FD	203	PEB	CAC-CBC-CGC-O2C
26	ID	201	PEB	CAC-CBC-CGC-O1C
26	ND	203	PEB	CAB-CBB-CGB-O2B
26	QD	202	PEB	CAC-CBC-CGC-O2C
26	WD	202	PEB	CAC-CBC-CGC-O2C
26	YD	301	PEB	CAB-CBB-CGB-O2B
26	GE	201	PEB	CAC-CBC-CGC-O1C
26	YE	202	PEB	CAB-CBB-CGB-O1B
26	dE	201	PEB	CAC-CBC-CGC-O2C
26	eE	203	PEB	CAC-CBC-CGC-O2C
26	kE	203	PEB	CAC-CBC-CGC-O1C
26	mE	203	PEB	CAC-CBC-CGC-O2C
26	oE	203	PEB	CAC-CBC-CGC-O1C
26	qE	202	PEB	CAC-CBC-CGC-O2C
26	wE	301	PEB	CAB-CBB-CGB-O2B
26	xE	302	PEB	CAB-CBB-CGB-O2B
26	FF	1002	PEB	CAC-CBC-CGC-O1C
26	YF	202	PEB	CAB-CBB-CGB-O2B
26	bF	203	PEB	CAC-CBC-CGC-O2C
26	dF	202	PEB	CAB-CBB-CGB-O2B
26	jF	203	PEB	CAC-CBC-CGC-O2C
26	kF	202	PEB	CAB-CBB-CGB-O2B
26	lF	203	PEB	CAC-CBC-CGC-O1C
26	AG	201	PEB	CAC-CBC-CGC-O2C
26	AG	201	PEB	CAB-CBB-CGB-O2B
26	EG	201	PEB	CAB-CBB-CGB-O2B
26	EG	202	PEB	CAB-CBB-CGB-O2B
26	GG	201	PEB	CAC-CBC-CGC-O2C
26	JG	202	PEB	CAB-CBB-CGB-O1B
26	MG	202	PEB	CAB-CBB-CGB-O2B
26	OG	203	PEB	CAC-CBC-CGC-O2C
26	OG	203	PEB	CAB-CBB-CGB-O2B
26	ZG	202	PEB	CAB-CBB-CGB-O2B
26	bG	202	PEB	CAB-CBB-CGB-O2B
26	eG	203	PEB	CAB-CBB-CGB-O2B
26	fG	202	PEB	CAB-CBB-CGB-O2B
26	gG	202	PEB	CAC-CBC-CGC-O2C
26	kG	201	PEB	CAC-CBC-CGC-O1C
26	oG	203	PEB	CAC-CBC-CGC-O1C
26	qG	202	PEB	CAC-CBC-CGC-O1C
26	sG	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	uG	203	PEB	CAC-CBC-CGC-O2C
26	vG	201	PEB	CAB-CBB-CGB-O2B
26	wG	301	PEB	CAC-CBC-CGC-O1C
26	wG	301	PEB	CAB-CBB-CGB-O2B
26	YI	203	PEB	CAB-CBB-CGB-O1B
26	iI	203	PEB	CAC-CBC-CGC-O1C
26	EJ	202	PEB	CAB-CBB-CGB-O1B
26	FJ	202	PEB	CAC-CBC-CGC-O2C
26	HJ	202	PEB	CAC-CBC-CGC-O2C
26	KJ	201	PEB	CAC-CBC-CGC-O1C
26	LJ	202	PEB	CAC-CBC-CGC-O1C
26	LJ	202	PEB	CAB-CBB-CGB-O1B
26	LJ	203	PEB	CAC-CBC-CGC-O1C
26	NJ	203	PEB	CAC-CBC-CGC-O2C
26	PJ	201	PEB	CAC-CBC-CGC-O1C
26	UJ	201	PEB	CAC-CBC-CGC-O2C
26	VJ	202	PEB	CAC-CBC-CGC-O1C
26	XJ	202	PEB	CAC-CBC-CGC-O1C
26	XJ	203	PEB	CAB-CBB-CGB-O1B
27	A4	203	PUB	CAB-CBB-CGB-O2B
27	A6	302	PUB	CAB-CBB-CGB-O2B
27	A8	304	PUB	CAC-CBC-CGC-O1C
28	E2	1001	CYC	CAA-CBA-CGA-O1A
28	E2	1001	CYC	CAA-CBA-CGA-O2A
28	G2	1001	CYC	CAA-CBA-CGA-O1A
28	G2	1001	CYC	CAA-CBA-CGA-O2A
28	C7	1001	CYC	CAD-CBD-CGD-O1D
28	YH	1004	CYC	CAD-CBD-CGD-O1D
28	qH	1002	CYC	CAA-CBA-CGA-O2A
28	wH	1001	CYC	CAA-CBA-CGA-O2A
28	EI	1001	CYC	CAA-CBA-CGA-O2A
27	yE	303	PUB	C4A-C3A-CAA-CBA
26	W1	201	PEB	C3B-CAB-CBB-CGB
26	N2	1002	PEB	C3B-CAB-CBB-CGB
26	C3	201	PEB	C3B-CAB-CBB-CGB
26	F3	201	PEB	C3B-CAB-CBB-CGB
26	I3	201	PEB	C3B-CAB-CBB-CGB
26	W4	201	PEB	C3B-CAB-CBB-CGB
26	q4	201	PEB	C3B-CAB-CBB-CGB
26	G5	201	PEB	C3B-CAB-CBB-CGB
26	e6	202	PEB	C3B-CAB-CBB-CGB
26	m6	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	Y7	201	PEB	C3B-CAB-CBB-CGB
26	W8	201	PEB	C3B-CAB-CBB-CGB
26	G9	201	PEB	C3B-CAB-CBB-CGB
26	WA	201	PEB	C3B-CAB-CBB-CGB
26	CD	201	PEB	C3B-CAB-CBB-CGB
26	WD	201	PEB	C3B-CAB-CBB-CGB
26	BE	201	PEB	C3B-CAB-CBB-CGB
26	DE	201	PEB	C3B-CAB-CBB-CGB
26	JE	201	PEB	C3B-CAB-CBB-CGB
26	NE	201	PEB	C3B-CAB-CBB-CGB
26	bE	201	PEB	C3B-CAB-CBB-CGB
26	rE	201	PEB	C3B-CAB-CBB-CGB
26	OF	201	PEB	C3B-CAB-CBB-CGB
26	SF	201	PEB	C3B-CAB-CBB-CGB
26	BG	201	PEB	C3B-CAB-CBB-CGB
26	DG	201	PEB	C3B-CAB-CBB-CGB
26	dG	201	PEB	C3B-CAB-CBB-CGB
26	pG	201	PEB	C3B-CAB-CBB-CGB
26	NI	1002	PEB	C3B-CAB-CBB-CGB
26	mI	203	PEB	C3B-CAB-CBB-CGB
26	NJ	202	PEB	C3B-CAB-CBB-CGB
26	F1	203	PEB	CAB-CBB-CGB-O1B
26	G1	202	PEB	CAC-CBC-CGC-O2C
26	K1	202	PEB	CAC-CBC-CGC-O2C
26	M1	401	PEB	CAB-CBB-CGB-O1B
26	N1	203	PEB	CAB-CBB-CGB-O1B
26	P1	201	PEB	CAC-CBC-CGC-O2C
26	P1	202	PEB	CAC-CBC-CGC-O2C
26	S1	202	PEB	CAB-CBB-CGB-O1B
26	T1	201	PEB	CAB-CBB-CGB-O2B
26	a1	202	PEB	CAB-CBB-CGB-O1B
26	c1	203	PEB	CAC-CBC-CGC-O2C
26	s1	201	PEB	CAB-CBB-CGB-O2B
26	s1	203	PEB	CAB-CBB-CGB-O1B
26	z1	202	PEB	CAC-CBC-CGC-O2C
26	21	405	PEB	CAB-CBB-CGB-O1B
26	R2	203	PEB	CAB-CBB-CGB-O2B
26	S2	202	PEB	CAB-CBB-CGB-O2B
26	Z2	201	PEB	CAC-CBC-CGC-O2C
26	c2	202	PEB	CAB-CBB-CGB-O1B
26	c2	203	PEB	CAC-CBC-CGC-O1C
26	g2	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	i2	202	PEB	CAC-CBC-CGC-O1C
26	J3	203	PEB	CAB-CBB-CGB-O1B
26	N3	203	PEB	CAB-CBB-CGB-O2B
26	P3	203	PEB	CAB-CBB-CGB-O1B
26	U3	202	PEB	CAC-CBC-CGC-O2C
26	X3	203	PEB	CAB-CBB-CGB-O1B
26	B4	201	PEB	CAC-CBC-CGC-O1C
26	C4	202	PEB	CAB-CBB-CGB-O1B
26	G4	202	PEB	CAB-CBB-CGB-O1B
26	P4	203	PEB	CAB-CBB-CGB-O2B
26	S4	202	PEB	CAC-CBC-CGC-O2C
26	T4	201	PEB	CAB-CBB-CGB-O2B
26	U4	202	PEB	CAB-CBB-CGB-O1B
26	U4	202	PEB	CAB-CBB-CGB-O2B
26	V4	203	PEB	CAB-CBB-CGB-O1B
26	a4	203	PEB	CAB-CBB-CGB-O2B
26	e4	202	PEB	CAC-CBC-CGC-O1C
26	f4	201	PEB	CAC-CBC-CGC-O1C
26	h4	201	PEB	CAC-CBC-CGC-O2C
26	r4	202	PEB	CAC-CBC-CGC-O2C
26	t4	201	PEB	CAB-CBB-CGB-O1B
26	w4	201	PEB	CAC-CBC-CGC-O1C
26	w4	201	PEB	CAC-CBC-CGC-O2C
26	24	404	PEB	CAC-CBC-CGC-O1C
26	24	405	PEB	CAC-CBC-CGC-O1C
26	A5	202	PEB	CAC-CBC-CGC-O2C
26	B5	203	PEB	CAC-CBC-CGC-O2C
26	H5	201	PEB	CAC-CBC-CGC-O1C
26	K5	202	PEB	CAC-CBC-CGC-O1C
26	R6	202	PEB	CAB-CBB-CGB-O1B
26	U6	203	PEB	CAB-CBB-CGB-O1B
26	V6	202	PEB	CAB-CBB-CGB-O1B
26	W6	201	PEB	CAB-CBB-CGB-O2B
26	Y6	202	PEB	CAB-CBB-CGB-O2B
26	a6	202	PEB	CAB-CBB-CGB-O2B
26	f6	201	PEB	CAC-CBC-CGC-O2C
26	A7	305	PEB	CAC-CBC-CGC-O1C
26	H7	1002	PEB	CAC-CBC-CGC-O2C
26	a7	202	PEB	CAC-CBC-CGC-O1C
26	d7	202	PEB	CAC-CBC-CGC-O1C
26	f7	203	PEB	CAC-CBC-CGC-O2C
26	l7	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	D8	202	PEB	CAB-CBB-CGB-O2B
26	H8	202	PEB	CAC-CBC-CGC-O2C
26	K8	201	PEB	CAC-CBC-CGC-O1C
26	N8	201	PEB	CAC-CBC-CGC-O1C
26	Q8	204	PEB	CAC-CBC-CGC-O2C
26	U8	201	PEB	CAB-CBB-CGB-O2B
26	V8	202	PEB	CAC-CBC-CGC-O2C
26	a8	203	PEB	CAC-CBC-CGC-O2C
26	d8	201	PEB	CAC-CBC-CGC-O2C
26	h8	203	PEB	CAC-CBC-CGC-O2C
26	j8	202	PEB	CAB-CBB-CGB-O2B
26	H9	202	PEB	CAC-CBC-CGC-O2C
26	L9	202	PEB	CAC-CBC-CGC-O2C
26	N9	203	PEB	CAC-CBC-CGC-O1C
26	O9	201	PEB	CAC-CBC-CGC-O2C
26	Q9	202	PEB	CAB-CBB-CGB-O2B
26	V9	202	PEB	CAC-CBC-CGC-O2C
26	X9	201	PEB	CAC-CBC-CGC-O2C
26	CA	201	PEB	CAC-CBC-CGC-O1C
26	dA	201	PEB	CAC-CBC-CGC-O2C
26	fA	201	PEB	CAC-CBC-CGC-O2C
26	OB	202	PEB	CAB-CBB-CGB-O1B
26	QB	203	PEB	CAB-CBB-CGB-O1B
26	UB	203	PEB	CAC-CBC-CGC-O1C
26	UB	203	PEB	CAB-CBB-CGB-O1B
26	hB	203	PEB	CAB-CBB-CGB-O2B
26	kB	202	PEB	CAC-CBC-CGC-O2C
26	kB	202	PEB	CAB-CBB-CGB-O1B
26	lB	202	PEB	CAB-CBB-CGB-O1B
26	FC	201	PEB	CAC-CBC-CGC-O1C
26	GC	202	PEB	CAB-CBB-CGB-O2B
26	LC	203	PEB	CAC-CBC-CGC-O2C
26	DD	202	PEB	CAC-CBC-CGC-O1C
26	DD	203	PEB	CAB-CBB-CGB-O1B
26	DD	203	PEB	CAB-CBB-CGB-O2B
26	QD	202	PEB	CAC-CBC-CGC-O1C
26	UD	202	PEB	CAC-CBC-CGC-O2C
26	CE	202	PEB	CAC-CBC-CGC-O1C
26	CE	202	PEB	CAC-CBC-CGC-O2C
26	EE	201	PEB	CAC-CBC-CGC-O1C
26	EE	202	PEB	CAB-CBB-CGB-O1B
26	EE	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	GE	203	PEB	CAC-CBC-CGC-O2C
26	GE	203	PEB	CAB-CBB-CGB-O1B
26	KE	203	PEB	CAB-CBB-CGB-O1B
26	ME	202	PEB	CAC-CBC-CGC-O2C
26	OE	203	PEB	CAC-CBC-CGC-O2C
26	VE	202	PEB	CAB-CBB-CGB-O2B
26	aE	203	PEB	CAB-CBB-CGB-O2B
26	fE	202	PEB	CAC-CBC-CGC-O2C
26	hE	201	PEB	CAC-CBC-CGC-O1C
26	mE	203	PEB	CAC-CBC-CGC-O1C
26	sE	201	PEB	CAC-CBC-CGC-O2C
26	sE	202	PEB	CAB-CBB-CGB-O1B
26	tE	202	PEB	CAB-CBB-CGB-O2B
26	wE	301	PEB	CAB-CBB-CGB-O1B
26	wE	302	PEB	CAB-CBB-CGB-O1B
26	xE	304	PEB	CAC-CBC-CGC-O1C
26	AF	302	PEB	CAC-CBC-CGC-O2C
26	hF	203	PEB	CAB-CBB-CGB-O1B
26	kF	201	PEB	CAB-CBB-CGB-O1B
26	EG	201	PEB	CAC-CBC-CGC-O1C
26	EG	202	PEB	CAC-CBC-CGC-O1C
26	KG	202	PEB	CAC-CBC-CGC-O2C
26	TG	202	PEB	CAB-CBB-CGB-O1B
26	iG	203	PEB	CAC-CBC-CGC-O2C
26	kG	202	PEB	CAB-CBB-CGB-O1B
26	sG	202	PEB	CAC-CBC-CGC-O1C
26	AI	305	PEB	CAB-CBB-CGB-O1B
26	RI	202	PEB	CAB-CBB-CGB-O1B
26	TI	202	PEB	CAC-CBC-CGC-O2C
26	TI	203	PEB	CAB-CBB-CGB-O2B
26	ZI	201	PEB	CAC-CBC-CGC-O2C
26	eI	202	PEB	CAC-CBC-CGC-O1C
26	eI	203	PEB	CAC-CBC-CGC-O2C
26	hI	201	PEB	CAB-CBB-CGB-O1B
26	kI	202	PEB	CAB-CBB-CGB-O1B
26	lI	201	PEB	CAC-CBC-CGC-O1C
26	mI	202	PEB	CAC-CBC-CGC-O2C
26	mI	203	PEB	CAC-CBC-CGC-O2C
26	AJ	301	PEB	CAB-CBB-CGB-O1B
26	BJ	203	PEB	CAC-CBC-CGC-O1C
26	HJ	201	PEB	CAB-CBB-CGB-O1B
26	JJ	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	LJ	201	PEB	CAC-CBC-CGC-O1C
26	PJ	202	PEB	CAB-CBB-CGB-O2B
26	PJ	203	PEB	CAB-CBB-CGB-O2B
26	RJ	201	PEB	CAB-CBB-CGB-O1B
26	WJ	201	PEB	CAC-CBC-CGC-O2C
27	wE	304	PUB	CAB-CBB-CGB-O1B
28	C2	1001	CYC	CAA-CBA-CGA-O2A
28	N2	1001	CYC	CAD-CBD-CGD-O1D
28	H7	1001	CYC	CAA-CBA-CGA-O2A
28	JH	1001	CYC	CAA-CBA-CGA-O2A
28	VH	1001	CYC	CAD-CBD-CGD-O1D
28	WH	1001	CYC	CAD-CBD-CGD-O1D
28	IH	1001	CYC	CAA-CBA-CGA-O2A
28	wH	1001	CYC	CAA-CBA-CGA-O1A
28	yH	1001	CYC	CAD-CBD-CGD-O1D
28	lH	1000	CYC	CAD-CBD-CGD-O1D
28	GI	1001	CYC	CAA-CBA-CGA-O1A
28	EF	1001	CYC	C2B-C3B-CAB-CBB
28	rH	1001	CYC	C2B-C3B-CAB-CBB
26	B1	201	PEB	CAC-CBC-CGC-O2C
26	G1	201	PEB	CAC-CBC-CGC-O2C
26	G1	202	PEB	CAB-CBB-CGB-O1B
26	H1	201	PEB	CAC-CBC-CGC-O1C
26	H1	202	PEB	CAB-CBB-CGB-O1B
26	K1	202	PEB	CAC-CBC-CGC-O1C
26	L1	203	PEB	CAB-CBB-CGB-O2B
26	N1	202	PEB	CAB-CBB-CGB-O1B
26	S1	202	PEB	CAC-CBC-CGC-O1C
26	W1	202	PEB	CAB-CBB-CGB-O1B
26	d1	201	PEB	CAC-CBC-CGC-O1C
26	l1	201	PEB	CAC-CBC-CGC-O2C
26	m1	203	PEB	CAC-CBC-CGC-O1C
26	p1	201	PEB	CAB-CBB-CGB-O1B
26	q1	202	PEB	CAC-CBC-CGC-O1C
26	q1	202	PEB	CAB-CBB-CGB-O1B
26	r1	202	PEB	CAC-CBC-CGC-O1C
26	r1	202	PEB	CAB-CBB-CGB-O1B
26	t1	201	PEB	CAB-CBB-CGB-O2B
26	v1	202	PEB	CAC-CBC-CGC-O1C
26	x1	201	PEB	CAC-CBC-CGC-O1C
26	x1	201	PEB	CAC-CBC-CGC-O2C
26	x1	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	A2	301	PEB	CAB-CBB-CGB-O2B
26	A2	304	PEB	CAB-CBB-CGB-O1B
26	A2	305	PEB	CAC-CBC-CGC-O2C
26	Q2	202	PEB	CAC-CBC-CGC-O1C
26	T2	202	PEB	CAC-CBC-CGC-O1C
26	c2	201	PEB	CAC-CBC-CGC-O1C
26	e2	202	PEB	CAC-CBC-CGC-O1C
26	e2	203	PEB	CAC-CBC-CGC-O2C
26	m2	202	PEB	CAC-CBC-CGC-O1C
26	B3	201	PEB	CAC-CBC-CGC-O2C
26	D3	203	PEB	CAC-CBC-CGC-O1C
26	E3	202	PEB	CAB-CBB-CGB-O1B
26	Q3	201	PEB	CAC-CBC-CGC-O1C
26	U3	201	PEB	CAC-CBC-CGC-O1C
26	Y3	301	PEB	CAC-CBC-CGC-O2C
26	C4	201	PEB	CAB-CBB-CGB-O1B
26	K4	201	PEB	CAC-CBC-CGC-O1C
26	L4	203	PEB	CAB-CBB-CGB-O1B
26	R4	201	PEB	CAC-CBC-CGC-O1C
26	R4	202	PEB	CAB-CBB-CGB-O2B
26	T4	203	PEB	CAB-CBB-CGB-O2B
26	X4	203	PEB	CAB-CBB-CGB-O2B
26	a4	202	PEB	CAC-CBC-CGC-O2C
26	i4	202	PEB	CAB-CBB-CGB-O1B
26	m4	202	PEB	CAB-CBB-CGB-O2B
26	q4	202	PEB	CAB-CBB-CGB-O2B
26	r4	201	PEB	CAC-CBC-CGC-O1C
26	v4	202	PEB	CAC-CBC-CGC-O1C
26	x4	201	PEB	CAC-CBC-CGC-O2C
26	y4	201	PEB	CAC-CBC-CGC-O1C
26	24	405	PEB	CAC-CBC-CGC-O2C
26	A5	201	PEB	CAC-CBC-CGC-O1C
26	B5	202	PEB	CAB-CBB-CGB-O1B
26	F5	202	PEB	CAB-CBB-CGB-O2B
26	G5	201	PEB	CAC-CBC-CGC-O2C
26	A6	301	PEB	CAC-CBC-CGC-O1C
26	N6	201	PEB	CAC-CBC-CGC-O1C
26	O6	202	PEB	CAC-CBC-CGC-O1C
26	O6	202	PEB	CAB-CBB-CGB-O1B
26	U6	202	PEB	CAC-CBC-CGC-O1C
26	W6	201	PEB	CAB-CBB-CGB-O1B
26	Y6	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	f6	202	PEB	CAB-CBB-CGB-O2B
26	f6	203	PEB	CAC-CBC-CGC-O2C
26	j6	201	PEB	CAB-CBB-CGB-O2B
26	k6	201	PEB	CAB-CBB-CGB-O1B
26	k6	202	PEB	CAC-CBC-CGC-O2C
26	l6	202	PEB	CAB-CBB-CGB-O1B
26	A7	302	PEB	CAB-CBB-CGB-O1B
26	N7	1002	PEB	CAC-CBC-CGC-O2C
26	Q7	202	PEB	CAB-CBB-CGB-O1B
26	R7	201	PEB	CAB-CBB-CGB-O1B
26	S7	203	PEB	CAB-CBB-CGB-O2B
26	b7	202	PEB	CAB-CBB-CGB-O2B
26	j7	201	PEB	CAC-CBC-CGC-O1C
26	l7	202	PEB	CAB-CBB-CGB-O1B
26	m7	202	PEB	CAB-CBB-CGB-O1B
26	A8	301	PEB	CAB-CBB-CGB-O2B
26	D8	202	PEB	CAB-CBB-CGB-O1B
26	E8	203	PEB	CAB-CBB-CGB-O1B
26	F8	202	PEB	CAC-CBC-CGC-O2C
26	L8	202	PEB	CAC-CBC-CGC-O1C
26	O8	202	PEB	CAC-CBC-CGC-O1C
26	P8	202	PEB	CAC-CBC-CGC-O2C
26	S8	201	PEB	CAC-CBC-CGC-O2C
26	Z8	202	PEB	CAC-CBC-CGC-O1C
26	g8	202	PEB	CAC-CBC-CGC-O1C
26	h8	203	PEB	CAC-CBC-CGC-O1C
26	i8	202	PEB	CAC-CBC-CGC-O1C
26	A9	303	PEB	CAB-CBB-CGB-O1B
26	A9	304	PEB	CAB-CBB-CGB-O1B
26	B9	203	PEB	CAB-CBB-CGB-O2B
26	F9	202	PEB	CAC-CBC-CGC-O2C
26	F9	203	PEB	CAB-CBB-CGB-O1B
26	H9	201	PEB	CAB-CBB-CGB-O1B
26	H9	202	PEB	CAC-CBC-CGC-O1C
26	K9	201	PEB	CAC-CBC-CGC-O1C
26	L9	201	PEB	CAC-CBC-CGC-O1C
26	M9	202	PEB	CAC-CBC-CGC-O2C
26	V9	202	PEB	CAC-CBC-CGC-O1C
26	X9	201	PEB	CAC-CBC-CGC-O1C
26	DA	202	PEB	CAC-CBC-CGC-O2C
26	FA	202	PEB	CAC-CBC-CGC-O2C
26	MA	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	PA	202	PEB	CAC-CBC-CGC-O1C
26	QA	204	PEB	CAC-CBC-CGC-O2C
26	SA	201	PEB	CAB-CBB-CGB-O1B
26	SA	201	PEB	CAB-CBB-CGB-O2B
26	UA	201	PEB	CAB-CBB-CGB-O1B
26	YA	201	PEB	CAC-CBC-CGC-O2C
26	dA	201	PEB	CAC-CBC-CGC-O1C
26	hA	201	PEB	CAC-CBC-CGC-O2C
26	PB	202	PEB	CAB-CBB-CGB-O2B
26	QB	203	PEB	CAC-CBC-CGC-O1C
26	YB	202	PEB	CAB-CBB-CGB-O2B
26	aB	202	PEB	CAB-CBB-CGB-O1B
26	fB	201	PEB	CAC-CBC-CGC-O2C
26	fB	202	PEB	CAB-CBB-CGB-O2B
26	fB	203	PEB	CAC-CBC-CGC-O1C
26	hB	203	PEB	CAC-CBC-CGC-O2C
26	kB	201	PEB	CAB-CBB-CGB-O1B
26	lB	203	PEB	CAB-CBB-CGB-O2B
26	mB	201	PEB	CAC-CBC-CGC-O1C
26	GC	201	PEB	CAC-CBC-CGC-O2C
26	GC	203	PEB	CAB-CBB-CGB-O2B
26	HC	202	PEB	CAB-CBB-CGB-O1B
26	JC	201	PEB	CAC-CBC-CGC-O2C
26	KC	202	PEB	CAC-CBC-CGC-O2C
26	BD	202	PEB	CAC-CBC-CGC-O1C
26	DD	203	PEB	CAC-CBC-CGC-O1C
26	ED	202	PEB	CAB-CBB-CGB-O1B
26	FD	203	PEB	CAC-CBC-CGC-O1C
26	GD	202	PEB	CAC-CBC-CGC-O1C
26	GD	202	PEB	CAB-CBB-CGB-O1B
26	QD	201	PEB	CAC-CBC-CGC-O2C
26	SD	201	PEB	CAC-CBC-CGC-O1C
26	VD	202	PEB	CAB-CBB-CGB-O1B
26	WD	201	PEB	CAB-CBB-CGB-O1B
26	CE	203	PEB	CAC-CBC-CGC-O2C
26	EE	201	PEB	CAC-CBC-CGC-O2C
26	LE	201	PEB	CAC-CBC-CGC-O1C
26	ME	202	PEB	CAB-CBB-CGB-O1B
26	OE	203	PEB	CAC-CBC-CGC-O1C
26	OE	203	PEB	CAB-CBB-CGB-O1B
26	UE	202	PEB	CAB-CBB-CGB-O1B
26	fE	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	iE	203	PEB	CAB-CBB-CGB-O2B
26	kE	201	PEB	CAC-CBC-CGC-O1C
26	lE	202	PEB	CAB-CBB-CGB-O2B
26	sE	201	PEB	CAB-CBB-CGB-O1B
26	wE	303	PEB	CAC-CBC-CGC-O1C
26	xE	303	PEB	CAB-CBB-CGB-O1B
26	AF	305	PEB	CAB-CBB-CGB-O2B
26	DF	1002	PEB	CAC-CBC-CGC-O1C
26	NF	1002	PEB	CAC-CBC-CGC-O2C
26	NF	1002	PEB	CAB-CBB-CGB-O1B
26	QF	202	PEB	CAB-CBB-CGB-O1B
26	TF	202	PEB	CAC-CBC-CGC-O2C
26	ZF	201	PEB	CAC-CBC-CGC-O1C
26	hF	201	PEB	CAC-CBC-CGC-O1C
26	hF	203	PEB	CAC-CBC-CGC-O2C
26	jF	202	PEB	CAC-CBC-CGC-O1C
26	DG	201	PEB	CAB-CBB-CGB-O2B
26	MG	202	PEB	CAC-CBC-CGC-O2C
26	MG	202	PEB	CAB-CBB-CGB-O1B
26	OG	202	PEB	CAC-CBC-CGC-O1C
26	VG	202	PEB	CAB-CBB-CGB-O2B
26	XG	201	PEB	CAC-CBC-CGC-O1C
26	aG	203	PEB	CAB-CBB-CGB-O1B
26	eG	201	PEB	CAB-CBB-CGB-O1B
26	fG	202	PEB	CAC-CBC-CGC-O1C
26	gG	202	PEB	CAC-CBC-CGC-O1C
26	gG	202	PEB	CAB-CBB-CGB-O2B
26	iG	202	PEB	CAC-CBC-CGC-O2C
26	mG	203	PEB	CAC-CBC-CGC-O1C
26	qG	202	PEB	CAC-CBC-CGC-O2C
26	tG	201	PEB	CAC-CBC-CGC-O2C
26	uG	202	PEB	CAC-CBC-CGC-O1C
26	wG	303	PEB	CAC-CBC-CGC-O1C
26	yG	301	PEB	CAC-CBC-CGC-O1C
26	zG	501	PEB	CAB-CBB-CGB-O1B
26	AI	301	PEB	CAB-CBB-CGB-O2B
26	QI	201	PEB	CAC-CBC-CGC-O2C
26	RI	203	PEB	CAB-CBB-CGB-O1B
26	bI	201	PEB	CAB-CBB-CGB-O2B
26	gI	203	PEB	CAC-CBC-CGC-O1C
26	AJ	304	PEB	CAB-CBB-CGB-O2B
26	BJ	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	BJ	203	PEB	CAB-CBB-CGB-O2B
26	DJ	203	PEB	CAB-CBB-CGB-O1B
26	HJ	201	PEB	CAB-CBB-CGB-O2B
26	HJ	202	PEB	CAC-CBC-CGC-O1C
26	JJ	203	PEB	CAB-CBB-CGB-O2B
26	OJ	201	PEB	CAC-CBC-CGC-O1C
26	RJ	201	PEB	CAC-CBC-CGC-O2C
26	TJ	203	PEB	CAC-CBC-CGC-O1C
26	XJ	203	PEB	CAC-CBC-CGC-O1C
26	XJ	203	PEB	CAC-CBC-CGC-O2C
27	K1	203	PUB	CAB-CBB-CGB-O1B
27	A2	303	PUB	CAB-CBB-CGB-O1B
27	A4	203	PUB	CAB-CBB-CGB-O1B
27	K4	203	PUB	CAC-CBC-CGC-O1C
27	A7	304	PUB	CAB-CBB-CGB-O1B
28	K2	1001	CYC	CAA-CBA-CGA-O1A
28	H6	1001	CYC	CAA-CBA-CGA-O2A
28	C7	1001	CYC	CAA-CBA-CGA-O2A
28	D7	1001	CYC	CAA-CBA-CGA-O2A
28	J7	1003	CYC	CAA-CBA-CGA-O2A
28	DF	1001	CYC	CAA-CBA-CGA-O2A
28	JF	1003	CYC	CAA-CBA-CGA-O1A
28	WH	1001	CYC	CAA-CBA-CGA-O1A
28	EI	1001	CYC	CAA-CBA-CGA-O1A
27	BA	302	PUB	C4D-C3D-CAD-CBD
28	NI	1001	CYC	C4B-C3B-CAB-CBB
28	pH	1001	CYC	C2B-C3B-CAB-CBB
26	C1	201	PEB	CAB-CBB-CGB-O1B
26	H1	203	PEB	CAB-CBB-CGB-O1B
26	J1	201	PEB	CAC-CBC-CGC-O1C
26	N1	203	PEB	CAB-CBB-CGB-O2B
26	P1	201	PEB	CAC-CBC-CGC-O1C
26	P1	202	PEB	CAC-CBC-CGC-O1C
26	P1	203	PEB	CAC-CBC-CGC-O1C
26	R1	202	PEB	CAB-CBB-CGB-O1B
26	U1	202	PEB	CAB-CBB-CGB-O1B
26	V1	201	PEB	CAC-CBC-CGC-O1C
26	V1	203	PEB	CAC-CBC-CGC-O1C
26	c1	201	PEB	CAC-CBC-CGC-O2C
26	m1	201	PEB	CAB-CBB-CGB-O2B
26	t1	201	PEB	CAC-CBC-CGC-O1C
26	z1	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	R2	202	PEB	CAC-CBC-CGC-O1C
26	Y2	203	PEB	CAB-CBB-CGB-O1B
26	c2	202	PEB	CAC-CBC-CGC-O1C
26	k2	201	PEB	CAC-CBC-CGC-O1C
26	m2	203	PEB	CAC-CBC-CGC-O2C
26	e3	401	PEB	CAB-CBB-CGB-O2B
26	E3	201	PEB	CAC-CBC-CGC-O2C
26	E3	202	PEB	CAB-CBB-CGB-O2B
26	G3	202	PEB	CAB-CBB-CGB-O1B
26	L3	203	PEB	CAB-CBB-CGB-O2B
26	O3	201	PEB	CAB-CBB-CGB-O1B
26	O3	202	PEB	CAB-CBB-CGB-O1B
26	Q3	202	PEB	CAC-CBC-CGC-O1C
26	U3	202	PEB	CAC-CBC-CGC-O1C
26	W3	201	PEB	CAB-CBB-CGB-O2B
26	W3	202	PEB	CAC-CBC-CGC-O1C
26	X3	203	PEB	CAB-CBB-CGB-O2B
26	F4	202	PEB	CAC-CBC-CGC-O1C
26	F4	203	PEB	CAC-CBC-CGC-O1C
26	J4	201	PEB	CAC-CBC-CGC-O1C
26	J4	202	PEB	CAC-CBC-CGC-O1C
26	J4	203	PEB	CAB-CBB-CGB-O1B
26	K4	202	PEB	CAC-CBC-CGC-O1C
26	N4	201	PEB	CAC-CBC-CGC-O1C
26	P4	201	PEB	CAC-CBC-CGC-O1C
26	T4	203	PEB	CAC-CBC-CGC-O1C
26	e4	202	PEB	CAC-CBC-CGC-O2C
26	f4	202	PEB	CAB-CBB-CGB-O1B
26	h4	202	PEB	CAC-CBC-CGC-O1C
26	k4	203	PEB	CAC-CBC-CGC-O1C
26	m4	203	PEB	CAC-CBC-CGC-O1C
26	p4	201	PEB	CAC-CBC-CGC-O2C
26	p4	201	PEB	CAB-CBB-CGB-O1B
26	r4	201	PEB	CAB-CBB-CGB-O1B
26	r4	202	PEB	CAB-CBB-CGB-O1B
26	v4	201	PEB	CAC-CBC-CGC-O2C
26	x4	202	PEB	CAB-CBB-CGB-O1B
26	24	405	PEB	CAB-CBB-CGB-O1B
26	B5	201	PEB	CAB-CBB-CGB-O1B
26	C5	201	PEB	CAB-CBB-CGB-O2B
26	G5	203	PEB	CAB-CBB-CGB-O2B
26	L5	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	A6	304	PEB	CAB-CBB-CGB-O1B
26	O6	201	PEB	CAB-CBB-CGB-O2B
26	Q6	203	PEB	CAC-CBC-CGC-O1C
26	V6	202	PEB	CAC-CBC-CGC-O2C
26	Z6	202	PEB	CAC-CBC-CGC-O1C
26	c6	202	PEB	CAB-CBB-CGB-O2B
26	d6	203	PEB	CAB-CBB-CGB-O1B
26	e6	201	PEB	CAC-CBC-CGC-O1C
26	h6	203	PEB	CAC-CBC-CGC-O1C
26	A7	301	PEB	CAB-CBB-CGB-O2B
26	F7	1002	PEB	CAB-CBB-CGB-O1B
26	J7	1002	PEB	CAC-CBC-CGC-O1C
26	O7	203	PEB	CAC-CBC-CGC-O1C
26	Q7	203	PEB	CAC-CBC-CGC-O1C
26	S7	202	PEB	CAC-CBC-CGC-O2C
26	U7	201	PEB	CAC-CBC-CGC-O1C
26	b7	201	PEB	CAB-CBB-CGB-O1B
26	c7	201	PEB	CAC-CBC-CGC-O2C
26	f7	202	PEB	CAC-CBC-CGC-O2C
26	j7	203	PEB	CAC-CBC-CGC-O1C
26	l7	201	PEB	CAC-CBC-CGC-O2C
26	l7	203	PEB	CAB-CBB-CGB-O1B
26	D8	202	PEB	CAC-CBC-CGC-O2C
26	E8	202	PEB	CAC-CBC-CGC-O1C
26	H8	202	PEB	CAB-CBB-CGB-O1B
26	K8	202	PEB	CAC-CBC-CGC-O1C
26	M8	203	PEB	CAC-CBC-CGC-O2C
26	N8	202	PEB	CAC-CBC-CGC-O1C
26	P8	202	PEB	CAC-CBC-CGC-O1C
26	P8	202	PEB	CAB-CBB-CGB-O1B
26	Q8	204	PEB	CAB-CBB-CGB-O1B
26	Y8	201	PEB	CAC-CBC-CGC-O2C
26	Z8	202	PEB	CAB-CBB-CGB-O1B
26	a8	201	PEB	CAC-CBC-CGC-O1C
26	a8	204	PEB	CAC-CBC-CGC-O1C
26	e8	202	PEB	CAB-CBB-CGB-O2B
26	h8	202	PEB	CAC-CBC-CGC-O2C
26	D9	202	PEB	CAC-CBC-CGC-O1C
26	J9	203	PEB	CAB-CBB-CGB-O1B
26	L9	202	PEB	CAC-CBC-CGC-O1C
26	L9	202	PEB	CAB-CBB-CGB-O1B
26	R9	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	V9	201	PEB	CAC-CBC-CGC-O1C
26	V9	203	PEB	CAB-CBB-CGB-O1B
26	V9	203	PEB	CAB-CBB-CGB-O2B
26	CA	202	PEB	CAC-CBC-CGC-O2C
26	EA	201	PEB	CAC-CBC-CGC-O2C
26	IA	203	PEB	CAB-CBB-CGB-O2B
26	KA	202	PEB	CAC-CBC-CGC-O2C
26	MA	201	PEB	CAC-CBC-CGC-O1C
26	cA	202	PEB	CAC-CBC-CGC-O1C
26	fA	201	PEB	CAC-CBC-CGC-O1C
26	gA	202	PEB	CAC-CBC-CGC-O2C
26	hA	202	PEB	CAC-CBC-CGC-O1C
26	hA	203	PEB	CAC-CBC-CGC-O1C
26	jA	202	PEB	CAB-CBB-CGB-O1B
26	jA	203	PEB	CAC-CBC-CGC-O2C
26	lA	201	PEB	CAB-CBB-CGB-O1B
26	OB	201	PEB	CAB-CBB-CGB-O1B
26	VB	202	PEB	CAB-CBB-CGB-O1B
26	bB	202	PEB	CAC-CBC-CGC-O1C
26	dB	201	PEB	CAB-CBB-CGB-O2B
26	eB	201	PEB	CAC-CBC-CGC-O2C
26	gB	202	PEB	CAB-CBB-CGB-O2B
26	iB	202	PEB	CAB-CBB-CGB-O2B
26	jB	202	PEB	CAC-CBC-CGC-O1C
26	jB	202	PEB	CAB-CBB-CGB-O1B
26	lB	202	PEB	CAC-CBC-CGC-O1C
26	AC	203	PEB	CAB-CBB-CGB-O1B
26	BC	203	PEB	CAC-CBC-CGC-O1C
26	CC	202	PEB	CAB-CBB-CGB-O1B
26	FC	201	PEB	CAB-CBB-CGB-O1B
26	AD	202	PEB	CAC-CBC-CGC-O1C
26	HD	203	PEB	CAC-CBC-CGC-O1C
26	UD	201	PEB	CAC-CBC-CGC-O1C
26	VD	201	PEB	CAC-CBC-CGC-O1C
26	XD	203	PEB	CAC-CBC-CGC-O1C
26	XD	203	PEB	CAB-CBB-CGB-O2B
26	AE	201	PEB	CAB-CBB-CGB-O2B
26	DE	201	PEB	CAB-CBB-CGB-O2B
26	HE	202	PEB	CAB-CBB-CGB-O2B
26	aE	203	PEB	CAC-CBC-CGC-O2C
26	dE	202	PEB	CAC-CBC-CGC-O2C
26	eE	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	fE	202	PEB	CAB-CBB-CGB-01B
26	gE	203	PEB	CAC-CBC-CGC-01C
26	iE	202	PEB	CAC-CBC-CGC-01C
26	mE	202	PEB	CAB-CBB-CGB-01B
26	pE	201	PEB	CAC-CBC-CGC-02C
26	zE	501	PEB	CAB-CBB-CGB-02B
26	JF	1002	PEB	CAB-CBB-CGB-02B
26	OF	201	PEB	CAB-CBB-CGB-01B
26	OF	202	PEB	CAB-CBB-CGB-02B
26	PF	202	PEB	CAC-CBC-CGC-02C
26	WF	203	PEB	CAC-CBC-CGC-01C
26	bF	203	PEB	CAC-CBC-CGC-01C
26	hF	202	PEB	CAB-CBB-CGB-01B
26	lF	202	PEB	CAB-CBB-CGB-01B
26	AG	201	PEB	CAC-CBC-CGC-01C
26	AG	201	PEB	CAB-CBB-CGB-01B
26	EG	201	PEB	CAB-CBB-CGB-01B
26	GG	201	PEB	CAC-CBC-CGC-01C
26	GG	202	PEB	CAC-CBC-CGC-02C
26	KG	202	PEB	CAC-CBC-CGC-01C
26	OG	203	PEB	CAB-CBB-CGB-01B
26	QG	202	PEB	CAB-CBB-CGB-02B
26	WG	203	PEB	CAC-CBC-CGC-01C
26	WG	203	PEB	CAB-CBB-CGB-02B
26	cG	201	PEB	CAB-CBB-CGB-01B
26	fG	202	PEB	CAB-CBB-CGB-01B
26	gG	201	PEB	CAC-CBC-CGC-01C
26	gG	201	PEB	CAC-CBC-CGC-02C
26	jG	201	PEB	CAC-CBC-CGC-01C
26	lG	202	PEB	CAB-CBB-CGB-01B
26	mG	202	PEB	CAC-CBC-CGC-01C
26	oG	201	PEB	CAB-CBB-CGB-02B
26	pG	202	PEB	CAB-CBB-CGB-01B
26	rG	202	PEB	CAB-CBB-CGB-01B
26	sG	203	PEB	CAC-CBC-CGC-01C
26	xG	302	PEB	CAC-CBC-CGC-01C
26	AI	301	PEB	CAC-CBC-CGC-02C
26	DI	1002	PEB	CAB-CBB-CGB-01B
26	FI	1002	PEB	CAC-CBC-CGC-02C
26	JI	1002	PEB	CAC-CBC-CGC-01C
26	RI	202	PEB	CAC-CBC-CGC-01C
26	RI	203	PEB	CAB-CBB-CGB-02B

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Mol	Chain	Res	Type	Atoms
26	SI	202	PEB	CAB-CBB-CGB-O2B
26	cI	201	PEB	CAC-CBC-CGC-O2C
26	AJ	303	PEB	CAB-CBB-CGB-O2B
26	BJ	203	PEB	CAB-CBB-CGB-O1B
26	DJ	201	PEB	CAC-CBC-CGC-O1C
26	DJ	202	PEB	CAC-CBC-CGC-O2C
26	FJ	202	PEB	CAC-CBC-CGC-O1C
26	NJ	203	PEB	CAC-CBC-CGC-O1C
26	NJ	203	PEB	CAB-CBB-CGB-O1B
26	NJ	204	PEB	CAB-CBB-CGB-O2B
26	TJ	201	PEB	CAB-CBB-CGB-O2B
27	A6	302	PUB	CAB-CBB-CGB-O1B
27	AA	303	PUB	CAB-CBB-CGB-O1B
27	AB	302	PUB	CAC-CBC-CGC-O1C
27	yG	303	PUB	CAB-CBB-CGB-O2B
28	J2	1001	CYC	CAA-CBA-CGA-O1A
28	C7	1001	CYC	CAA-CBA-CGA-O1A
28	D7	1001	CYC	CAA-CBA-CGA-O1A
28	qH	1002	CYC	CAD-CBD-CGD-O2D
28	CI	1001	CYC	CAA-CBA-CGA-O2A
28	FI	1001	CYC	CAA-CBA-CGA-O1A
28	JI	1001	CYC	CAA-CBA-CGA-O1A
28	JI	1001	CYC	CAA-CBA-CGA-O2A
28	KI	1001	CYC	CAA-CBA-CGA-O1A
26	R6	201	PEB	C2B-C3B-CAB-CBB
26	N8	201	PEB	C2B-C3B-CAB-CBB
26	D1	203	PEB	CAC-CBC-CGC-O1C
26	E1	201	PEB	CAB-CBB-CGB-O1B
26	F1	202	PEB	CAC-CBC-CGC-O2C
26	J1	202	PEB	CAC-CBC-CGC-O1C
26	N1	201	PEB	CAC-CBC-CGC-O1C
26	Q1	202	PEB	CAC-CBC-CGC-O1C
26	V1	202	PEB	CAB-CBB-CGB-O2B
26	X1	203	PEB	CAC-CBC-CGC-O1C
26	f1	201	PEB	CAC-CBC-CGC-O1C
26	f1	201	PEB	CAB-CBB-CGB-O1B
26	g1	203	PEB	CAC-CBC-CGC-O1C
26	n1	201	PEB	CAB-CBB-CGB-O1B
26	p1	202	PEB	CAB-CBB-CGB-O1B
26	q1	203	PEB	CAB-CBB-CGB-O1B
26	P2	203	PEB	CAC-CBC-CGC-O1C
26	R2	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	R2	203	PEB	CAC-CBC-CGC-O1C
26	a2	203	PEB	CAB-CBB-CGB-O1B
26	c2	202	PEB	CAC-CBC-CGC-O2C
26	j2	201	PEB	CAB-CBB-CGB-O1B
26	F3	202	PEB	CAC-CBC-CGC-O2C
26	G3	202	PEB	CAC-CBC-CGC-O2C
26	I3	202	PEB	CAC-CBC-CGC-O2C
26	I3	202	PEB	CAB-CBB-CGB-O1B
26	Y3	301	PEB	CAC-CBC-CGC-O1C
26	Y3	304	PEB	CAB-CBB-CGB-O2B
26	B4	202	PEB	CAC-CBC-CGC-O2C
26	B4	203	PEB	CAB-CBB-CGB-O1B
26	K4	202	PEB	CAB-CBB-CGB-O1B
26	M4	401	PEB	CAB-CBB-CGB-O1B
26	N4	203	PEB	CAB-CBB-CGB-O1B
26	P4	202	PEB	CAC-CBC-CGC-O2C
26	Q4	202	PEB	CAC-CBC-CGC-O1C
26	R4	202	PEB	CAC-CBC-CGC-O1C
26	S4	202	PEB	CAC-CBC-CGC-O1C
26	X4	203	PEB	CAC-CBC-CGC-O1C
26	b4	501	PEB	CAC-CBC-CGC-O1C
26	d4	203	PEB	CAB-CBB-CGB-O2B
26	g4	203	PEB	CAB-CBB-CGB-O2B
26	t4	202	PEB	CAC-CBC-CGC-O1C
26	t4	202	PEB	CAC-CBC-CGC-O2C
26	x4	202	PEB	CAC-CBC-CGC-O2C
26	C5	204	PEB	CAC-CBC-CGC-O1C
26	F5	201	PEB	CAC-CBC-CGC-O1C
26	J5	201	PEB	CAC-CBC-CGC-O2C
26	R6	202	PEB	CAB-CBB-CGB-O2B
26	U6	203	PEB	CAC-CBC-CGC-O2C
26	W6	202	PEB	CAC-CBC-CGC-O1C
26	e6	203	PEB	CAC-CBC-CGC-O2C
26	j6	202	PEB	CAB-CBB-CGB-O2B
26	l6	203	PEB	CAB-CBB-CGB-O1B
26	m6	203	PEB	CAB-CBB-CGB-O1B
26	A7	305	PEB	CAB-CBB-CGB-O2B
26	O7	202	PEB	CAB-CBB-CGB-O2B
26	Q7	201	PEB	CAB-CBB-CGB-O1B
26	S7	201	PEB	CAC-CBC-CGC-O2C
26	S7	202	PEB	CAB-CBB-CGB-O1B
26	U7	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	U7	203	PEB	CAB-CBB-CGB-01B
26	Z7	203	PEB	CAC-CBC-CGC-02C
26	b7	202	PEB	CAC-CBC-CGC-01C
26	h7	203	PEB	CAC-CBC-CGC-01C
26	j7	202	PEB	CAC-CBC-CGC-01C
26	l7	201	PEB	CAC-CBC-CGC-01C
26	m7	201	PEB	CAB-CBB-CGB-01B
26	A8	301	PEB	CAC-CBC-CGC-01C
26	D8	201	PEB	CAC-CBC-CGC-02C
26	I8	203	PEB	CAB-CBB-CGB-01B
26	I8	203	PEB	CAB-CBB-CGB-02B
26	J8	202	PEB	CAC-CBC-CGC-01C
26	M8	201	PEB	CAC-CBC-CGC-01C
26	M8	201	PEB	CAC-CBC-CGC-02C
26	X8	202	PEB	CAC-CBC-CGC-01C
26	X8	202	PEB	CAC-CBC-CGC-02C
26	Y8	201	PEB	CAB-CBB-CGB-01B
26	Y8	202	PEB	CAC-CBC-CGC-01C
26	Y8	203	PEB	CAC-CBC-CGC-02C
26	h8	201	PEB	CAC-CBC-CGC-02C
26	h8	202	PEB	CAC-CBC-CGC-01C
26	l8	201	PEB	CAB-CBB-CGB-02B
26	F9	201	PEB	CAB-CBB-CGB-01B
26	H9	201	PEB	CAB-CBB-CGB-02B
26	J9	203	PEB	CAC-CBC-CGC-02C
26	L9	203	PEB	CAC-CBC-CGC-02C
26	N9	203	PEB	CAB-CBB-CGB-01B
26	R9	201	PEB	CAC-CBC-CGC-01C
26	T9	201	PEB	CAB-CBB-CGB-02B
26	V9	203	PEB	CAC-CBC-CGC-01C
26	EA	203	PEB	CAB-CBB-CGB-02B
26	IA	201	PEB	CAC-CBC-CGC-01C
26	NA	202	PEB	CAC-CBC-CGC-01C
26	XA	202	PEB	CAC-CBC-CGC-01C
26	YA	201	PEB	CAB-CBB-CGB-01B
26	YA	203	PEB	CAC-CBC-CGC-01C
26	ZA	202	PEB	CAC-CBC-CGC-01C
26	aA	201	PEB	CAB-CBB-CGB-02B
26	hA	201	PEB	CAC-CBC-CGC-01C
26	iA	202	PEB	CAC-CBC-CGC-01C
26	WB	201	PEB	CAB-CBB-CGB-01B
26	fB	202	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
26	gB	202	PEB	CAB-CBB-CGB-01B
26	hB	202	PEB	CAC-CBC-CGC-01C
26	AC	203	PEB	CAC-CBC-CGC-01C
26	CC	203	PEB	CAC-CBC-CGC-01C
26	BD	202	PEB	CAC-CBC-CGC-02C
26	BD	203	PEB	CAB-CBB-CGB-02B
26	ID	202	PEB	CAC-CBC-CGC-02C
26	MD	202	PEB	CAC-CBC-CGC-02C
26	ND	203	PEB	CAC-CBC-CGC-01C
26	RD	201	PEB	CAB-CBB-CGB-01B
26	WD	201	PEB	CAC-CBC-CGC-01C
26	XD	203	PEB	CAB-CBB-CGB-01B
26	YD	303	PEB	CAB-CBB-CGB-01B
26	EE	202	PEB	CAC-CBC-CGC-01C
26	PE	202	PEB	CAB-CBB-CGB-01B
26	QE	202	PEB	CAB-CBB-CGB-01B
26	VE	201	PEB	CAB-CBB-CGB-01B
26	cE	202	PEB	CAB-CBB-CGB-02B
26	dE	201	PEB	CAB-CBB-CGB-01B
26	eE	201	PEB	CAB-CBB-CGB-01B
26	gE	202	PEB	CAB-CBB-CGB-01B
26	hE	201	PEB	CAC-CBC-CGC-02C
26	mE	201	PEB	CAC-CBC-CGC-01C
26	yE	301	PEB	CAC-CBC-CGC-01C
26	FF	1002	PEB	CAB-CBB-CGB-01B
26	JF	1002	PEB	CAC-CBC-CGC-01C
26	OF	202	PEB	CAC-CBC-CGC-02C
26	PF	202	PEB	CAB-CBB-CGB-01B
26	QF	201	PEB	CAB-CBB-CGB-02B
26	SF	202	PEB	CAC-CBC-CGC-01C
26	UF	203	PEB	CAB-CBB-CGB-02B
26	aF	201	PEB	CAB-CBB-CGB-01B
26	aF	202	PEB	CAB-CBB-CGB-01B
26	bF	201	PEB	CAB-CBB-CGB-01B
26	fF	202	PEB	CAC-CBC-CGC-01C
26	hF	201	PEB	CAC-CBC-CGC-02C
26	lF	203	PEB	CAB-CBB-CGB-01B
26	HG	202	PEB	CAB-CBB-CGB-02B
26	PG	202	PEB	CAB-CBB-CGB-01B
26	SG	203	PEB	CAB-CBB-CGB-02B
26	UG	202	PEB	CAB-CBB-CGB-01B
26	eG	202	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	eG	203	PEB	CAB-CBB-CGB-O1B
26	qG	201	PEB	CAB-CBB-CGB-O2B
26	tG	202	PEB	CAC-CBC-CGC-O1C
26	xG	304	PEB	CAC-CBC-CGC-O2C
26	xG	304	PEB	CAB-CBB-CGB-O2B
26	AI	304	PEB	CAB-CBB-CGB-O2B
26	JI	1002	PEB	CAB-CBB-CGB-O1B
26	PI	202	PEB	CAC-CBC-CGC-O2C
26	fl	201	PEB	CAC-CBC-CGC-O1C
26	fl	201	PEB	CAB-CBB-CGB-O1B
26	mI	201	PEB	CAC-CBC-CGC-O2C
26	BJ	202	PEB	CAB-CBB-CGB-O2B
26	IJ	201	PEB	CAB-CBB-CGB-O1B
26	JJ	203	PEB	CAB-CBB-CGB-O1B
26	KJ	202	PEB	CAC-CBC-CGC-O2C
26	QJ	202	PEB	CAB-CBB-CGB-O1B
26	VJ	203	PEB	CAB-CBB-CGB-O1B
26	XJ	201	PEB	CAC-CBC-CGC-O2C
27	B8	302	PUB	CAB-CBB-CGB-O1B
27	AB	302	PUB	CAC-CBC-CGC-O2C
27	AB	302	PUB	CAB-CBB-CGB-O2B
27	AB	303	PUB	CAC-CBC-CGC-O2C
27	wG	304	PUB	CAB-CBB-CGB-O1B
28	D2	1001	CYC	CAA-CBA-CGA-O1A
28	N2	1001	CYC	CAD-CBD-CGD-O2D
28	CH	1001	CYC	CAA-CBA-CGA-O1A
28	GH	1001	CYC	CAA-CBA-CGA-O2A
28	JH	1001	CYC	CAA-CBA-CGA-O1A
26	B1	203	PEB	CAB-CBB-CGB-O2B
26	D1	203	PEB	CAB-CBB-CGB-O1B
26	J1	202	PEB	CAB-CBB-CGB-O1B
26	N1	202	PEB	CAB-CBB-CGB-O2B
26	U1	202	PEB	CAC-CBC-CGC-O1C
26	V1	202	PEB	CAB-CBB-CGB-O1B
26	X1	203	PEB	CAC-CBC-CGC-O2C
26	c1	202	PEB	CAB-CBB-CGB-O2B
26	g1	203	PEB	CAB-CBB-CGB-O2B
26	k1	203	PEB	CAB-CBB-CGB-O2B
26	q1	202	PEB	CAB-CBB-CGB-O2B
26	t1	202	PEB	CAC-CBC-CGC-O2C
26	A2	301	PEB	CAC-CBC-CGC-O1C
26	T2	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	b2	201	PEB	CAB-CBB-CGB-O1B
26	d2	202	PEB	CAB-CBB-CGB-O2B
26	h2	202	PEB	CAC-CBC-CGC-O1C
26	k2	203	PEB	CAC-CBC-CGC-O2C
26	l2	202	PEB	CAB-CBB-CGB-O1B
26	D3	203	PEB	CAB-CBB-CGB-O2B
26	I3	201	PEB	CAC-CBC-CGC-O1C
26	L3	203	PEB	CAC-CBC-CGC-O2C
26	M3	202	PEB	CAC-CBC-CGC-O2C
26	R3	203	PEB	CAC-CBC-CGC-O2C
26	S3	202	PEB	CAC-CBC-CGC-O1C
26	T3	201	PEB	CAC-CBC-CGC-O2C
26	V3	201	PEB	CAC-CBC-CGC-O2C
26	Y3	303	PEB	CAB-CBB-CGB-O1B
26	D4	203	PEB	CAC-CBC-CGC-O1C
26	D4	203	PEB	CAC-CBC-CGC-O2C
26	H4	203	PEB	CAC-CBC-CGC-O2C
26	O4	202	PEB	CAB-CBB-CGB-O2B
26	V4	202	PEB	CAB-CBB-CGB-O1B
26	W4	202	PEB	CAB-CBB-CGB-O2B
26	X4	203	PEB	CAC-CBC-CGC-O2C
26	X4	203	PEB	CAB-CBB-CGB-O1B
26	a4	202	PEB	CAB-CBB-CGB-O2B
26	d4	203	PEB	CAB-CBB-CGB-O1B
26	n4	201	PEB	CAB-CBB-CGB-O1B
26	n4	201	PEB	CAB-CBB-CGB-O2B
26	s4	203	PEB	CAB-CBB-CGB-O2B
26	x4	201	PEB	CAB-CBB-CGB-O2B
26	x4	202	PEB	CAC-CBC-CGC-O1C
26	l4	201	PEB	CAB-CBB-CGB-O2B
26	J5	201	PEB	CAC-CBC-CGC-O1C
26	P6	202	PEB	CAB-CBB-CGB-O2B
26	V6	202	PEB	CAC-CBC-CGC-O1C
26	c6	202	PEB	CAC-CBC-CGC-O2C
26	f6	201	PEB	CAB-CBB-CGB-O2B
26	i6	201	PEB	CAC-CBC-CGC-O1C
26	j6	201	PEB	CAC-CBC-CGC-O2C
26	l6	202	PEB	CAC-CBC-CGC-O2C
26	D7	1002	PEB	CAB-CBB-CGB-O2B
26	F7	1002	PEB	CAC-CBC-CGC-O2C
26	J7	1002	PEB	CAB-CBB-CGB-O2B
26	O7	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	S7	202	PEB	CAC-CBC-CGC-O1C
26	U7	203	PEB	CAC-CBC-CGC-O1C
26	Z7	201	PEB	CAC-CBC-CGC-O2C
26	Z7	203	PEB	CAC-CBC-CGC-O1C
26	b7	201	PEB	CAB-CBB-CGB-O2B
26	d7	201	PEB	CAC-CBC-CGC-O1C
26	d7	201	PEB	CAC-CBC-CGC-O2C
26	f7	201	PEB	CAB-CBB-CGB-O1B
26	j7	203	PEB	CAC-CBC-CGC-O2C
26	m7	202	PEB	CAB-CBB-CGB-O2B
26	C8	201	PEB	CAC-CBC-CGC-O2C
26	G8	201	PEB	CAC-CBC-CGC-O2C
26	J8	202	PEB	CAB-CBB-CGB-O2B
26	K8	202	PEB	CAC-CBC-CGC-O2C
26	Q8	203	PEB	CAC-CBC-CGC-O2C
26	R8	202	PEB	CAB-CBB-CGB-O1B
26	Z8	202	PEB	CAB-CBB-CGB-O2B
26	a8	204	PEB	CAC-CBC-CGC-O2C
26	c8	201	PEB	CAB-CBB-CGB-O2B
26	d8	202	PEB	CAC-CBC-CGC-O2C
26	f8	201	PEB	CAC-CBC-CGC-O1C
26	f8	201	PEB	CAC-CBC-CGC-O2C
26	f8	202	PEB	CAC-CBC-CGC-O1C
26	A9	303	PEB	CAC-CBC-CGC-O1C
26	A9	304	PEB	CAB-CBB-CGB-O2B
26	B9	201	PEB	CAC-CBC-CGC-O1C
26	B9	201	PEB	CAC-CBC-CGC-O2C
26	G9	202	PEB	CAC-CBC-CGC-O2C
26	J9	203	PEB	CAB-CBB-CGB-O2B
26	O9	202	PEB	CAB-CBB-CGB-O1B
26	P9	201	PEB	CAC-CBC-CGC-O2C
26	P9	203	PEB	CAC-CBC-CGC-O2C
26	Q9	202	PEB	CAC-CBC-CGC-O2C
26	U9	202	PEB	CAB-CBB-CGB-O1B
26	V9	201	PEB	CAC-CBC-CGC-O2C
26	W9	201	PEB	CAC-CBC-CGC-O2C
26	EA	202	PEB	CAC-CBC-CGC-O2C
26	HA	202	PEB	CAC-CBC-CGC-O2C
26	IA	202	PEB	CAC-CBC-CGC-O1C
26	JA	202	PEB	CAC-CBC-CGC-O1C
26	PA	202	PEB	CAC-CBC-CGC-O2C
26	QA	204	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	UA	201	PEB	CAB-CBB-CGB-O2B
26	aA	201	PEB	CAB-CBB-CGB-O1B
26	aA	203	PEB	CAB-CBB-CGB-O1B
26	gA	201	PEB	CAC-CBC-CGC-O1C
26	hA	202	PEB	CAC-CBC-CGC-O2C
26	AB	304	PEB	CAB-CBB-CGB-O2B
26	DB	1002	PEB	CAC-CBC-CGC-O2C
26	NB	1002	PEB	CAC-CBC-CGC-O1C
26	QB	201	PEB	CAC-CBC-CGC-O1C
26	QB	202	PEB	CAC-CBC-CGC-O2C
26	RB	202	PEB	CAB-CBB-CGB-O1B
26	WB	203	PEB	CAC-CBC-CGC-O2C
26	ZB	202	PEB	CAC-CBC-CGC-O1C
26	cB	202	PEB	CAB-CBB-CGB-O2B
26	dB	203	PEB	CAB-CBB-CGB-O1B
26	hB	202	PEB	CAB-CBB-CGB-O2B
26	jB	201	PEB	CAB-CBB-CGB-O1B
26	jB	201	PEB	CAB-CBB-CGB-O2B
26	kB	201	PEB	CAB-CBB-CGB-O2B
26	AC	203	PEB	CAC-CBC-CGC-O2C
26	FC	202	PEB	CAB-CBB-CGB-O1B
26	GC	203	PEB	CAB-CBB-CGB-O1B
26	HC	203	PEB	CAC-CBC-CGC-O2C
26	JC	201	PEB	CAC-CBC-CGC-O1C
26	LC	202	PEB	CAB-CBB-CGB-O2B
26	LD	203	PEB	CAB-CBB-CGB-O1B
26	RD	203	PEB	CAB-CBB-CGB-O2B
26	YD	304	PEB	CAB-CBB-CGB-O1B
26	GE	203	PEB	CAC-CBC-CGC-O1C
26	ME	201	PEB	CAC-CBC-CGC-O2C
26	ME	202	PEB	CAB-CBB-CGB-O2B
26	TE	201	PEB	CAB-CBB-CGB-O2B
26	VE	201	PEB	CAB-CBB-CGB-O2B
26	YE	203	PEB	CAC-CBC-CGC-O2C
26	ZE	202	PEB	CAB-CBB-CGB-O1B
26	bE	202	PEB	CAB-CBB-CGB-O2B
26	dE	201	PEB	CAB-CBB-CGB-O2B
26	dE	202	PEB	CAC-CBC-CGC-O1C
26	fE	202	PEB	CAC-CBC-CGC-O1C
26	vE	202	PEB	CAC-CBC-CGC-O2C
26	xE	303	PEB	CAC-CBC-CGC-O2C
26	AF	305	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	NF	1002	PEB	CAC-CBC-CGC-O1C
26	NF	1002	PEB	CAB-CBB-CGB-O2B
26	OF	203	PEB	CAC-CBC-CGC-O2C
26	RF	202	PEB	CAB-CBB-CGB-O1B
26	TF	202	PEB	CAC-CBC-CGC-O1C
26	UF	202	PEB	CAC-CBC-CGC-O1C
26	WF	203	PEB	CAC-CBC-CGC-O2C
26	ZF	203	PEB	CAB-CBB-CGB-O1B
26	aF	202	PEB	CAB-CBB-CGB-O2B
26	dF	203	PEB	CAB-CBB-CGB-O1B
26	fF	201	PEB	CAC-CBC-CGC-O2C
26	fF	202	PEB	CAC-CBC-CGC-O2C
26	jF	202	PEB	CAC-CBC-CGC-O2C
26	jF	203	PEB	CAC-CBC-CGC-O1C
26	CG	203	PEB	CAC-CBC-CGC-O2C
26	LG	201	PEB	CAC-CBC-CGC-O2C
26	MG	201	PEB	CAC-CBC-CGC-O2C
26	TG	201	PEB	CAB-CBB-CGB-O2B
26	TG	202	PEB	CAC-CBC-CGC-O1C
26	WG	203	PEB	CAC-CBC-CGC-O2C
26	YG	203	PEB	CAC-CBC-CGC-O2C
26	aG	202	PEB	CAB-CBB-CGB-O1B
26	dG	202	PEB	CAB-CBB-CGB-O2B
26	iG	203	PEB	CAC-CBC-CGC-O1C
26	kG	203	PEB	CAC-CBC-CGC-O2C
26	sG	201	PEB	CAB-CBB-CGB-O1B
26	PI	203	PEB	CAB-CBB-CGB-O1B
26	PI	203	PEB	CAB-CBB-CGB-O2B
26	QI	201	PEB	CAC-CBC-CGC-O1C
26	VI	203	PEB	CAB-CBB-CGB-O2B
26	ZI	201	PEB	CAC-CBC-CGC-O1C
26	eI	203	PEB	CAB-CBB-CGB-O2B
26	hI	202	PEB	CAC-CBC-CGC-O2C
26	jI	201	PEB	CAB-CBB-CGB-O1B
26	II	202	PEB	CAB-CBB-CGB-O2B
26	AJ	304	PEB	CAC-CBC-CGC-O2C
26	DJ	203	PEB	CAC-CBC-CGC-O1C
26	FJ	201	PEB	CAC-CBC-CGC-O2C
26	HJ	203	PEB	CAC-CBC-CGC-O1C
26	JJ	202	PEB	CAB-CBB-CGB-O2B
26	VJ	203	PEB	CAB-CBB-CGB-O2B
26	WJ	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
27	A2	303	PUB	CAB-CBB-CGB-O2B
27	K3	203	PUB	CAB-CBB-CGB-O2B
27	xE	301	PUB	CAB-CBB-CGB-O2B
28	D2	1001	CYC	CAA-CBA-CGA-O2A
28	I2	1001	CYC	CAA-CBA-CGA-O2A
28	D6	1001	CYC	CAA-CBA-CGA-O2A
28	H6	1001	CYC	CAA-CBA-CGA-O1A
28	KH	1001	CYC	CAD-CBD-CGD-O2D
28	IH	1001	CYC	CAA-CBA-CGA-O1A
28	DI	1001	CYC	CAA-CBA-CGA-O1A
28	DI	1001	CYC	CAA-CBA-CGA-O2A
28	II	1001	CYC	CAA-CBA-CGA-O2A
26	F1	203	PEB	CAC-CBC-CGC-O1C
26	F1	203	PEB	CAC-CBC-CGC-O2C
26	G1	202	PEB	CAC-CBC-CGC-O1C
26	L1	201	PEB	CAC-CBC-CGC-O1C
26	T1	203	PEB	CAB-CBB-CGB-O2B
26	U1	202	PEB	CAC-CBC-CGC-O2C
26	V1	201	PEB	CAC-CBC-CGC-O2C
26	b1	501	PEB	CAC-CBC-CGC-O1C
26	f1	201	PEB	CAC-CBC-CGC-O2C
26	o1	501	PEB	CAC-CBC-CGC-O2C
26	r1	201	PEB	CAC-CBC-CGC-O2C
26	u1	202	PEB	CAC-CBC-CGC-O1C
26	y1	201	PEB	CAC-CBC-CGC-O1C
26	z1	401	PEB	CAB-CBB-CGB-O2B
26	A2	304	PEB	CAB-CBB-CGB-O2B
26	Q2	201	PEB	CAC-CBC-CGC-O1C
26	Q2	202	PEB	CAC-CBC-CGC-O2C
26	V2	202	PEB	CAC-CBC-CGC-O1C
26	V2	203	PEB	CAB-CBB-CGB-O2B
26	Z2	201	PEB	CAC-CBC-CGC-O1C
26	c2	201	PEB	CAC-CBC-CGC-O2C
26	e2	203	PEB	CAB-CBB-CGB-O1B
26	j2	201	PEB	CAC-CBC-CGC-O2C
26	l2	202	PEB	CAC-CBC-CGC-O1C
26	B3	202	PEB	CAB-CBB-CGB-O2B
26	D3	202	PEB	CAC-CBC-CGC-O1C
26	F3	203	PEB	CAC-CBC-CGC-O1C
26	I3	201	PEB	CAC-CBC-CGC-O2C
26	I3	202	PEB	CAC-CBC-CGC-O1C
26	I3	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	N3	203	PEB	CAC-CBC-CGC-O1C
26	O3	201	PEB	CAC-CBC-CGC-O2C
26	S3	201	PEB	CAC-CBC-CGC-O2C
26	U3	202	PEB	CAB-CBB-CGB-O2B
26	V3	201	PEB	CAC-CBC-CGC-O1C
26	B4	203	PEB	CAC-CBC-CGC-O1C
26	C4	202	PEB	CAC-CBC-CGC-O2C
26	K4	201	PEB	CAC-CBC-CGC-O2C
26	R4	202	PEB	CAB-CBB-CGB-O1B
26	T4	202	PEB	CAC-CBC-CGC-O2C
26	V4	201	PEB	CAC-CBC-CGC-O1C
26	V4	202	PEB	CAC-CBC-CGC-O1C
26	V4	202	PEB	CAC-CBC-CGC-O2C
26	V4	202	PEB	CAB-CBB-CGB-O2B
26	Y4	201	PEB	CAB-CBB-CGB-O1B
26	b4	501	PEB	CAB-CBB-CGB-O2B
26	c4	201	PEB	CAC-CBC-CGC-O2C
26	d4	201	PEB	CAC-CBC-CGC-O2C
26	i4	201	PEB	CAB-CBB-CGB-O1B
26	m4	201	PEB	CAB-CBB-CGB-O2B
26	u4	202	PEB	CAC-CBC-CGC-O1C
26	y4	201	PEB	CAB-CBB-CGB-O2B
26	y4	202	PEB	CAC-CBC-CGC-O2C
26	24	404	PEB	CAB-CBB-CGB-O1B
26	A5	202	PEB	CAB-CBB-CGB-O1B
26	B5	201	PEB	CAC-CBC-CGC-O1C
26	C5	201	PEB	CAB-CBB-CGB-O1B
26	H5	203	PEB	CAB-CBB-CGB-O1B
26	A6	301	PEB	CAC-CBC-CGC-O2C
26	A6	304	PEB	CAB-CBB-CGB-O2B
26	Q6	202	PEB	CAC-CBC-CGC-O1C
26	W6	203	PEB	CAC-CBC-CGC-O2C
26	Y6	202	PEB	CAC-CBC-CGC-O2C
26	Z6	202	PEB	CAB-CBB-CGB-O1B
26	b6	201	PEB	CAC-CBC-CGC-O1C
26	c6	202	PEB	CAC-CBC-CGC-O1C
26	f6	202	PEB	CAC-CBC-CGC-O2C
26	g6	201	PEB	CAC-CBC-CGC-O1C
26	h6	202	PEB	CAC-CBC-CGC-O2C
26	j6	202	PEB	CAC-CBC-CGC-O1C
26	l6	203	PEB	CAB-CBB-CGB-O2B
26	A7	301	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	D7	1002	PEB	CAC-CBC-CGC-O2C
26	N7	1002	PEB	CAC-CBC-CGC-O1C
26	O7	201	PEB	CAC-CBC-CGC-O2C
26	Q7	203	PEB	CAC-CBC-CGC-O2C
26	R7	202	PEB	CAB-CBB-CGB-O2B
26	W7	203	PEB	CAC-CBC-CGC-O2C
26	Z7	203	PEB	CAB-CBB-CGB-O1B
26	Z7	203	PEB	CAB-CBB-CGB-O2B
26	b7	202	PEB	CAB-CBB-CGB-O1B
26	d7	203	PEB	CAC-CBC-CGC-O2C
26	h7	203	PEB	CAC-CBC-CGC-O2C
26	l7	203	PEB	CAC-CBC-CGC-O2C
26	A8	301	PEB	CAB-CBB-CGB-O1B
26	A8	302	PEB	CAC-CBC-CGC-O1C
26	E8	203	PEB	CAC-CBC-CGC-O2C
26	I8	202	PEB	CAC-CBC-CGC-O2C
26	Q8	202	PEB	CAC-CBC-CGC-O2C
26	U8	201	PEB	CAB-CBB-CGB-O1B
26	U8	202	PEB	CAC-CBC-CGC-O2C
26	Z8	202	PEB	CAC-CBC-CGC-O2C
26	a8	202	PEB	CAC-CBC-CGC-O1C
26	d8	201	PEB	CAC-CBC-CGC-O1C
26	e8	202	PEB	CAB-CBB-CGB-O1B
26	f8	202	PEB	CAC-CBC-CGC-O2C
26	g8	202	PEB	CAC-CBC-CGC-O2C
26	g8	202	PEB	CAB-CBB-CGB-O1B
26	m8	201	PEB	CAB-CBB-CGB-O2B
26	A9	303	PEB	CAC-CBC-CGC-O2C
26	H9	203	PEB	CAC-CBC-CGC-O2C
26	H9	203	PEB	CAB-CBB-CGB-O1B
26	H9	203	PEB	CAB-CBB-CGB-O2B
26	J9	202	PEB	CAC-CBC-CGC-O2C
26	R9	202	PEB	CAB-CBB-CGB-O2B
26	T9	201	PEB	CAB-CBB-CGB-O1B
26	T9	203	PEB	CAC-CBC-CGC-O2C
26	V9	201	PEB	CAB-CBB-CGB-O2B
26	V9	203	PEB	CAC-CBC-CGC-O2C
26	AA	301	PEB	CAC-CBC-CGC-O1C
26	EA	203	PEB	CAC-CBC-CGC-O1C
26	FA	202	PEB	CAC-CBC-CGC-O1C
26	HA	202	PEB	CAC-CBC-CGC-O1C
26	KA	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	OA	202	PEB	CAC-CBC-CGC-O1C
26	OA	202	PEB	CAC-CBC-CGC-O2C
26	UA	202	PEB	CAC-CBC-CGC-O2C
26	UA	203	PEB	CAC-CBC-CGC-O1C
26	WA	202	PEB	CAC-CBC-CGC-O1C
26	YA	202	PEB	CAC-CBC-CGC-O1C
26	ZA	202	PEB	CAC-CBC-CGC-O2C
26	ZA	202	PEB	CAB-CBB-CGB-O2B
26	aA	202	PEB	CAC-CBC-CGC-O1C
26	aA	203	PEB	CAC-CBC-CGC-O1C
26	jA	202	PEB	CAB-CBB-CGB-O2B
26	jA	203	PEB	CAC-CBC-CGC-O1C
26	lA	201	PEB	CAC-CBC-CGC-O2C
26	HB	1002	PEB	CAC-CBC-CGC-O2C
26	OB	203	PEB	CAC-CBC-CGC-O1C
26	PB	202	PEB	CAB-CBB-CGB-O1B
26	QB	202	PEB	CAC-CBC-CGC-O1C
26	RB	202	PEB	CAB-CBB-CGB-O2B
26	WB	202	PEB	CAC-CBC-CGC-O1C
26	WB	202	PEB	CAB-CBB-CGB-O2B
26	YB	201	PEB	CAC-CBC-CGC-O2C
26	YB	202	PEB	CAB-CBB-CGB-O1B
26	ZB	202	PEB	CAB-CBB-CGB-O1B
26	aB	202	PEB	CAC-CBC-CGC-O1C
26	aB	202	PEB	CAB-CBB-CGB-O2B
26	fB	202	PEB	CAB-CBB-CGB-O1B
26	fB	203	PEB	CAC-CBC-CGC-O2C
26	lB	202	PEB	CAC-CBC-CGC-O2C
26	BC	201	PEB	CAB-CBB-CGB-O1B
26	CC	202	PEB	CAB-CBB-CGB-O2B
26	FC	201	PEB	CAC-CBC-CGC-O2C
26	GC	201	PEB	CAC-CBC-CGC-O1C
26	HC	203	PEB	CAB-CBB-CGB-O1B
26	LC	203	PEB	CAB-CBB-CGB-O1B
26	AD	201	PEB	CAC-CBC-CGC-O1C
26	BD	201	PEB	CAC-CBC-CGC-O2C
26	DD	202	PEB	CAB-CBB-CGB-O2B
26	FD	202	PEB	CAC-CBC-CGC-O1C
26	ID	201	PEB	CAC-CBC-CGC-O2C
26	ID	202	PEB	CAC-CBC-CGC-O1C
26	ID	202	PEB	CAB-CBB-CGB-O1B
26	ID	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	JD	203	PEB	CAB-CBB-CGB-01B
26	JD	203	PEB	CAB-CBB-CGB-02B
26	PD	201	PEB	CAC-CBC-CGC-01C
26	RD	202	PEB	CAC-CBC-CGC-02C
26	YD	304	PEB	CAB-CBB-CGB-02B
26	GE	202	PEB	CAC-CBC-CGC-01C
26	HE	202	PEB	CAB-CBB-CGB-01B
26	LE	202	PEB	CAC-CBC-CGC-01C
26	NE	201	PEB	CAC-CBC-CGC-02C
26	PE	202	PEB	CAB-CBB-CGB-02B
26	TE	201	PEB	CAB-CBB-CGB-01B
26	TE	202	PEB	CAC-CBC-CGC-01C
26	WE	202	PEB	CAC-CBC-CGC-02C
26	XE	201	PEB	CAC-CBC-CGC-01C
26	XE	201	PEB	CAC-CBC-CGC-02C
26	gE	202	PEB	CAB-CBB-CGB-02B
26	mE	202	PEB	CAB-CBB-CGB-02B
26	qE	203	PEB	CAC-CBC-CGC-01C
26	qE	203	PEB	CAC-CBC-CGC-02C
26	sE	201	PEB	CAC-CBC-CGC-01C
26	xE	303	PEB	CAB-CBB-CGB-02B
26	xE	304	PEB	CAB-CBB-CGB-02B
26	AF	302	PEB	CAC-CBC-CGC-01C
26	OF	203	PEB	CAC-CBC-CGC-01C
26	QF	203	PEB	CAC-CBC-CGC-01C
26	RF	201	PEB	CAB-CBB-CGB-01B
26	RF	202	PEB	CAC-CBC-CGC-01C
26	SF	201	PEB	CAC-CBC-CGC-02C
26	UF	201	PEB	CAC-CBC-CGC-02C
26	ZF	201	PEB	CAB-CBB-CGB-02B
26	bF	201	PEB	CAB-CBB-CGB-02B
26	bF	202	PEB	CAB-CBB-CGB-01B
26	dF	202	PEB	CAC-CBC-CGC-01C
26	gF	201	PEB	CAC-CBC-CGC-01C
26	gF	202	PEB	CAB-CBB-CGB-01B
26	hF	202	PEB	CAB-CBB-CGB-02B
26	jF	202	PEB	CAB-CBB-CGB-01B
26	lF	203	PEB	CAB-CBB-CGB-02B
26	BG	201	PEB	CAC-CBC-CGC-02C
26	CG	202	PEB	CAC-CBC-CGC-01C
26	GG	202	PEB	CAC-CBC-CGC-01C
26	TG	201	PEB	CAB-CBB-CGB-01B

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Mol	Chain	Res	Type	Atoms
26	TG	202	PEB	CAC-CBC-CGC-O2C
26	XG	201	PEB	CAC-CBC-CGC-O2C
26	aG	202	PEB	CAB-CBB-CGB-O2B
26	aG	203	PEB	CAB-CBB-CGB-O2B
26	cG	202	PEB	CAC-CBC-CGC-O2C
26	eG	201	PEB	CAB-CBB-CGB-O2B
26	fG	202	PEB	CAC-CBC-CGC-O2C
26	gG	202	PEB	CAB-CBB-CGB-O1B
26	kG	201	PEB	CAC-CBC-CGC-O2C
26	lG	202	PEB	CAB-CBB-CGB-O2B
26	tG	202	PEB	CAB-CBB-CGB-O2B
26	xG	303	PEB	CAB-CBB-CGB-O2B
26	AI	301	PEB	CAB-CBB-CGB-O1B
26	JI	1002	PEB	CAC-CBC-CGC-O2C
26	RI	203	PEB	CAC-CBC-CGC-O1C
26	aI	202	PEB	CAC-CBC-CGC-O2C
26	bI	202	PEB	CAC-CBC-CGC-O1C
26	dI	201	PEB	CAB-CBB-CGB-O1B
26	dI	201	PEB	CAB-CBB-CGB-O2B
26	eI	201	PEB	CAC-CBC-CGC-O1C
26	kI	202	PEB	CAB-CBB-CGB-O2B
26	II	202	PEB	CAB-CBB-CGB-O1B
26	BJ	201	PEB	CAC-CBC-CGC-O2C
26	DJ	203	PEB	CAC-CBC-CGC-O2C
26	FJ	201	PEB	CAB-CBB-CGB-O2B
26	OJ	201	PEB	CAB-CBB-CGB-O1B
26	PJ	201	PEB	CAC-CBC-CGC-O2C
26	RJ	202	PEB	CAB-CBB-CGB-O1B
26	RJ	202	PEB	CAB-CBB-CGB-O2B
26	RJ	203	PEB	CAC-CBC-CGC-O2C
26	SJ	202	PEB	CAC-CBC-CGC-O1C
26	SJ	202	PEB	CAB-CBB-CGB-O2B
26	YJ	202	PEB	CAC-CBC-CGC-O2C
27	K1	203	PUB	CAC-CBC-CGC-O1C
27	A7	304	PUB	CAC-CBC-CGC-O1C
27	A7	304	PUB	CAC-CBC-CGC-O2C
27	BA	302	PUB	CAB-CBB-CGB-O1B
27	wE	304	PUB	CAB-CBB-CGB-O2B
27	AF	304	PUB	CAC-CBC-CGC-O2C
27	xG	301	PUB	CAB-CBB-CGB-O2B
28	JF	1003	CYC	CAA-CBA-CGA-O2A
28	UH	1001	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	WH	1001	CYC	CAA-CBA-CGA-O2A
28	cH	1001	CYC	CAA-CBA-CGA-O1A
28	eH	1001	CYC	CAA-CBA-CGA-O1A
28	iH	1001	CYC	CAA-CBA-CGA-O2A
28	yH	1001	CYC	CAA-CBA-CGA-O1A
26	A1	202	PEB	CAC-CBC-CGC-O1C
26	C1	202	PEB	CAC-CBC-CGC-O1C
26	M1	401	PEB	CAC-CBC-CGC-O2C
26	Q1	202	PEB	CAB-CBB-CGB-O1B
26	R1	201	PEB	CAC-CBC-CGC-O2C
26	R1	202	PEB	CAB-CBB-CGB-O2B
26	T1	202	PEB	CAC-CBC-CGC-O1C
26	V1	202	PEB	CAC-CBC-CGC-O1C
26	W1	202	PEB	CAB-CBB-CGB-O2B
26	a1	203	PEB	CAB-CBB-CGB-O1B
26	b1	501	PEB	CAC-CBC-CGC-O2C
26	c1	202	PEB	CAB-CBB-CGB-O1B
26	g1	202	PEB	CAC-CBC-CGC-O2C
26	m1	201	PEB	CAC-CBC-CGC-O2C
26	q1	201	PEB	CAC-CBC-CGC-O2C
26	s1	202	PEB	CAC-CBC-CGC-O1C
26	A2	301	PEB	CAC-CBC-CGC-O2C
26	A2	301	PEB	CAB-CBB-CGB-O1B
26	A2	304	PEB	CAC-CBC-CGC-O2C
26	R2	203	PEB	CAB-CBB-CGB-O1B
26	c2	203	PEB	CAC-CBC-CGC-O2C
26	e2	203	PEB	CAB-CBB-CGB-O2B
26	f2	202	PEB	CAB-CBB-CGB-O2B
26	h2	201	PEB	CAB-CBB-CGB-O2B
26	i2	203	PEB	CAC-CBC-CGC-O2C
26	l2	202	PEB	CAB-CBB-CGB-O2B
26	B3	201	PEB	CAC-CBC-CGC-O1C
26	C3	201	PEB	CAC-CBC-CGC-O1C
26	H3	203	PEB	CAB-CBB-CGB-O2B
26	M3	201	PEB	CAC-CBC-CGC-O1C
26	M3	202	PEB	CAC-CBC-CGC-O1C
26	N3	203	PEB	CAC-CBC-CGC-O2C
26	O3	202	PEB	CAB-CBB-CGB-O2B
26	R3	203	PEB	CAB-CBB-CGB-O2B
26	Y3	303	PEB	CAB-CBB-CGB-O2B
26	A4	202	PEB	CAC-CBC-CGC-O1C
26	D4	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	E4	202	PEB	CAB-CBB-CGB-01B
26	F4	203	PEB	CAC-CBC-CGC-02C
26	H4	203	PEB	CAB-CBB-CGB-02B
26	I4	202	PEB	CAC-CBC-CGC-01C
26	I4	202	PEB	CAB-CBB-CGB-01B
26	J4	202	PEB	CAB-CBB-CGB-01B
26	M4	401	PEB	CAC-CBC-CGC-02C
26	R4	201	PEB	CAC-CBC-CGC-02C
26	R4	203	PEB	CAB-CBB-CGB-02B
26	T4	202	PEB	CAC-CBC-CGC-01C
26	V4	203	PEB	CAC-CBC-CGC-01C
26	W4	202	PEB	CAB-CBB-CGB-01B
26	h4	203	PEB	CAB-CBB-CGB-01B
26	j4	201	PEB	CAB-CBB-CGB-01B
26	j4	202	PEB	CAB-CBB-CGB-01B
26	l4	201	PEB	CAC-CBC-CGC-02C
26	24	401	PEB	CAB-CBB-CGB-02B
26	B5	202	PEB	CAC-CBC-CGC-01C
26	B5	203	PEB	CAB-CBB-CGB-01B
26	F5	201	PEB	CAC-CBC-CGC-02C
26	G5	201	PEB	CAC-CBC-CGC-01C
26	H5	201	PEB	CAB-CBB-CGB-02B
26	I5	203	PEB	CAB-CBB-CGB-01B
26	L5	202	PEB	CAC-CBC-CGC-01C
26	L5	202	PEB	CAC-CBC-CGC-02C
26	P6	202	PEB	CAB-CBB-CGB-01B
26	S6	202	PEB	CAB-CBB-CGB-02B
26	W6	202	PEB	CAB-CBB-CGB-01B
26	Z6	203	PEB	CAC-CBC-CGC-02C
26	c6	202	PEB	CAB-CBB-CGB-01B
26	e6	201	PEB	CAC-CBC-CGC-02C
26	f6	202	PEB	CAB-CBB-CGB-01B
26	g6	202	PEB	CAC-CBC-CGC-02C
26	j6	201	PEB	CAB-CBB-CGB-01B
26	A7	305	PEB	CAB-CBB-CGB-01B
26	P7	202	PEB	CAC-CBC-CGC-02C
26	Q7	202	PEB	CAC-CBC-CGC-02C
26	S7	201	PEB	CAC-CBC-CGC-01C
26	S7	203	PEB	CAB-CBB-CGB-01B
26	V7	202	PEB	CAB-CBB-CGB-01B
26	W7	202	PEB	CAC-CBC-CGC-01C
26	e7	201	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
26	j7	202	PEB	CAC-CBC-CGC-O2C
26	j7	202	PEB	CAB-CBB-CGB-O2B
26	C8	201	PEB	CAC-CBC-CGC-O1C
26	C8	202	PEB	CAC-CBC-CGC-O1C
26	E8	202	PEB	CAC-CBC-CGC-O2C
26	H8	202	PEB	CAC-CBC-CGC-O1C
26	U8	201	PEB	CAC-CBC-CGC-O2C
26	X8	202	PEB	CAB-CBB-CGB-O1B
26	a8	201	PEB	CAB-CBB-CGB-O2B
26	c8	201	PEB	CAB-CBB-CGB-O1B
26	c8	202	PEB	CAC-CBC-CGC-O1C
26	d8	202	PEB	CAC-CBC-CGC-O1C
26	B9	203	PEB	CAB-CBB-CGB-O1B
26	D9	201	PEB	CAC-CBC-CGC-O2C
26	F9	201	PEB	CAB-CBB-CGB-O2B
26	N9	202	PEB	CAB-CBB-CGB-O1B
26	O9	202	PEB	CAC-CBC-CGC-O2C
26	O9	202	PEB	CAB-CBB-CGB-O2B
26	P9	202	PEB	CAC-CBC-CGC-O1C
26	R9	201	PEB	CAC-CBC-CGC-O2C
26	R9	202	PEB	CAB-CBB-CGB-O1B
26	S9	202	PEB	CAB-CBB-CGB-O1B
26	S9	202	PEB	CAB-CBB-CGB-O2B
26	W9	202	PEB	CAC-CBC-CGC-O2C
26	X9	202	PEB	CAC-CBC-CGC-O2C
26	X9	202	PEB	CAB-CBB-CGB-O2B
26	EA	201	PEB	CAB-CBB-CGB-O1B
26	IA	202	PEB	CAC-CBC-CGC-O2C
26	SA	201	PEB	CAC-CBC-CGC-O1C
26	TA	202	PEB	CAC-CBC-CGC-O1C
26	UA	203	PEB	CAB-CBB-CGB-O1B
26	cA	203	PEB	CAC-CBC-CGC-O1C
26	iA	202	PEB	CAB-CBB-CGB-O1B
26	cB	202	PEB	CAC-CBC-CGC-O1C
26	cB	202	PEB	CAB-CBB-CGB-O1B
26	gB	201	PEB	CAC-CBC-CGC-O1C
26	hB	203	PEB	CAB-CBB-CGB-O1B
26	iB	201	PEB	CAC-CBC-CGC-O1C
26	jB	201	PEB	CAC-CBC-CGC-O2C
26	jB	202	PEB	CAB-CBB-CGB-O2B
26	CC	201	PEB	CAC-CBC-CGC-O2C
26	FC	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	HC	201	PEB	CAC-CBC-CGC-O2C
26	HC	203	PEB	CAC-CBC-CGC-O1C
26	LC	202	PEB	CAB-CBB-CGB-O1B
26	AD	202	PEB	CAB-CBB-CGB-O2B
26	BD	203	PEB	CAB-CBB-CGB-O1B
26	CD	201	PEB	CAC-CBC-CGC-O1C
26	CD	201	PEB	CAC-CBC-CGC-O2C
26	GD	202	PEB	CAC-CBC-CGC-O2C
26	HD	203	PEB	CAC-CBC-CGC-O2C
26	LD	202	PEB	CAC-CBC-CGC-O1C
26	LD	203	PEB	CAB-CBB-CGB-O2B
26	MD	201	PEB	CAC-CBC-CGC-O1C
26	OD	201	PEB	CAC-CBC-CGC-O1C
26	OD	202	PEB	CAB-CBB-CGB-O2B
26	RD	203	PEB	CAB-CBB-CGB-O1B
26	WD	201	PEB	CAB-CBB-CGB-O2B
26	YD	303	PEB	CAC-CBC-CGC-O1C
26	YD	303	PEB	CAC-CBC-CGC-O2C
26	YD	303	PEB	CAB-CBB-CGB-O2B
26	FE	202	PEB	CAC-CBC-CGC-O1C
26	HE	202	PEB	CAC-CBC-CGC-O2C
26	ME	203	PEB	CAB-CBB-CGB-O1B
26	SE	202	PEB	CAC-CBC-CGC-O1C
26	WE	202	PEB	CAB-CBB-CGB-O2B
26	WE	203	PEB	CAB-CBB-CGB-O2B
26	cE	202	PEB	CAC-CBC-CGC-O1C
26	dE	201	PEB	CAC-CBC-CGC-O1C
26	eE	201	PEB	CAB-CBB-CGB-O2B
26	iE	202	PEB	CAB-CBB-CGB-O2B
26	jE	202	PEB	CAB-CBB-CGB-O1B
26	kE	202	PEB	CAC-CBC-CGC-O2C
26	mE	202	PEB	CAC-CBC-CGC-O2C
26	sE	202	PEB	CAC-CBC-CGC-O2C
26	vE	202	PEB	CAC-CBC-CGC-O1C
26	xE	304	PEB	CAB-CBB-CGB-O1B
26	UF	202	PEB	CAC-CBC-CGC-O2C
26	UF	203	PEB	CAB-CBB-CGB-O1B
26	bF	202	PEB	CAB-CBB-CGB-O2B
26	dF	203	PEB	CAC-CBC-CGC-O1C
26	dF	203	PEB	CAC-CBC-CGC-O2C
26	fF	203	PEB	CAC-CBC-CGC-O1C
26	jF	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	lF	202	PEB	CAC-CBC-CGC-O1C
26	lF	203	PEB	CAC-CBC-CGC-O2C
26	mF	201	PEB	CAB-CBB-CGB-O2B
26	FG	202	PEB	CAC-CBC-CGC-O1C
26	HG	202	PEB	CAB-CBB-CGB-O1B
26	LG	201	PEB	CAC-CBC-CGC-O1C
26	NG	201	PEB	CAC-CBC-CGC-O2C
26	PG	202	PEB	CAB-CBB-CGB-O2B
26	YG	202	PEB	CAB-CBB-CGB-O2B
26	dG	201	PEB	CAC-CBC-CGC-O1C
26	dG	201	PEB	CAB-CBB-CGB-O1B
26	iG	202	PEB	CAC-CBC-CGC-O1C
26	lG	201	PEB	CAC-CBC-CGC-O2C
26	pG	201	PEB	CAB-CBB-CGB-O2B
26	qG	201	PEB	CAB-CBB-CGB-O1B
26	wG	302	PEB	CAB-CBB-CGB-O1B
26	xG	302	PEB	CAB-CBB-CGB-O2B
26	xG	303	PEB	CAB-CBB-CGB-O1B
26	zG	501	PEB	CAB-CBB-CGB-O2B
26	AI	304	PEB	CAC-CBC-CGC-O2C
26	FI	1002	PEB	CAB-CBB-CGB-O2B
26	YI	203	PEB	CAB-CBB-CGB-O2B
26	bI	201	PEB	CAC-CBC-CGC-O1C
26	cI	202	PEB	CAB-CBB-CGB-O1B
26	cI	202	PEB	CAB-CBB-CGB-O2B
26	cI	203	PEB	CAC-CBC-CGC-O2C
26	fI	202	PEB	CAC-CBC-CGC-O2C
26	kI	203	PEB	CAC-CBC-CGC-O2C
26	BJ	201	PEB	CAB-CBB-CGB-O2B
26	DJ	201	PEB	CAC-CBC-CGC-O2C
26	FJ	201	PEB	CAC-CBC-CGC-O1C
26	JJ	202	PEB	CAC-CBC-CGC-O2C
26	KJ	201	PEB	CAC-CBC-CGC-O2C
26	OJ	201	PEB	CAC-CBC-CGC-O2C
26	TJ	202	PEB	CAC-CBC-CGC-O1C
26	TJ	203	PEB	CAB-CBB-CGB-O2B
27	A7	304	PUB	CAB-CBB-CGB-O2B
27	AB	302	PUB	CAB-CBB-CGB-O1B
28	M2	1001	CYC	CAA-CBA-CGA-O1A
28	M2	1001	CYC	CAA-CBA-CGA-O2A
28	B6	1001	CYC	CAD-CBD-CGD-O2D
28	HB	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	HB	1001	CYC	CAA-CBA-CGA-O2A
28	yH	1001	CYC	CAA-CBA-CGA-O2A
28	MI	1001	CYC	CAA-CBA-CGA-O2A
26	GJ	201	PEB	C2B-C3B-CAB-CBB
26	aB	202	PEB	C4B-C3B-CAB-CBB
26	BD	201	PEB	C4B-C3B-CAB-CBB
26	oG	203	PEB	C4B-C3B-CAB-CBB
28	QH	1001	CYC	C1A-C2A-CAA-CBA
26	C1	202	PEB	CAB-CBB-CGB-O1B
26	D1	203	PEB	CAB-CBB-CGB-O2B
26	I1	202	PEB	CAC-CBC-CGC-O1C
26	I1	202	PEB	CAB-CBB-CGB-O1B
26	J1	203	PEB	CAC-CBC-CGC-O2C
26	Q1	202	PEB	CAC-CBC-CGC-O2C
26	Y1	201	PEB	CAB-CBB-CGB-O1B
26	d1	201	PEB	CAC-CBC-CGC-O2C
26	h1	201	PEB	CAC-CBC-CGC-O1C
26	j1	202	PEB	CAB-CBB-CGB-O2B
26	l1	201	PEB	CAC-CBC-CGC-O1C
26	l1	201	PEB	CAB-CBB-CGB-O2B
26	o1	501	PEB	CAC-CBC-CGC-O1C
26	p1	201	PEB	CAB-CBB-CGB-O2B
26	q1	202	PEB	CAC-CBC-CGC-O2C
26	t1	202	PEB	CAC-CBC-CGC-O1C
26	u1	202	PEB	CAC-CBC-CGC-O2C
26	v1	201	PEB	CAC-CBC-CGC-O2C
26	x1	201	PEB	CAB-CBB-CGB-O1B
26	11	201	PEB	CAC-CBC-CGC-O2C
26	F2	1002	PEB	CAB-CBB-CGB-O2B
26	Q2	201	PEB	CAC-CBC-CGC-O2C
26	Y2	203	PEB	CAC-CBC-CGC-O2C
26	Z2	202	PEB	CAC-CBC-CGC-O2C
26	e2	203	PEB	CAC-CBC-CGC-O1C
26	f2	202	PEB	CAC-CBC-CGC-O2C
26	m2	201	PEB	CAC-CBC-CGC-O2C
26	B3	202	PEB	CAC-CBC-CGC-O1C
26	C3	201	PEB	CAC-CBC-CGC-O2C
26	D3	202	PEB	CAC-CBC-CGC-O2C
26	E3	202	PEB	CAC-CBC-CGC-O2C
26	G3	201	PEB	CAC-CBC-CGC-O1C
26	H3	201	PEB	CAC-CBC-CGC-O2C
26	M3	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	O3	201	PEB	CAB-CBB-CGB-O2B
26	R3	202	PEB	CAC-CBC-CGC-O2C
26	R3	203	PEB	CAB-CBB-CGB-O1B
26	S3	202	PEB	CAB-CBB-CGB-O2B
26	V3	202	PEB	CAC-CBC-CGC-O2C
26	W3	201	PEB	CAC-CBC-CGC-O2C
26	Y3	301	PEB	CAB-CBB-CGB-O2B
26	Y3	304	PEB	CAB-CBB-CGB-O1B
26	N4	202	PEB	CAB-CBB-CGB-O1B
26	Q4	202	PEB	CAC-CBC-CGC-O2C
26	Q4	202	PEB	CAB-CBB-CGB-O1B
26	Y4	202	PEB	CAB-CBB-CGB-O2B
26	g4	203	PEB	CAB-CBB-CGB-O1B
26	m4	201	PEB	CAC-CBC-CGC-O2C
26	w4	201	PEB	CAB-CBB-CGB-O1B
26	24	405	PEB	CAB-CBB-CGB-O2B
26	F5	202	PEB	CAB-CBB-CGB-O1B
26	H5	202	PEB	CAB-CBB-CGB-O2B
26	K5	203	PEB	CAC-CBC-CGC-O2C
26	H6	1002	PEB	CAC-CBC-CGC-O2C
26	K6	201	PEB	CAC-CBC-CGC-O2C
26	Q6	201	PEB	CAC-CBC-CGC-O1C
26	W6	202	PEB	CAB-CBB-CGB-O2B
26	e6	203	PEB	CAB-CBB-CGB-O2B
26	j6	202	PEB	CAB-CBB-CGB-O1B
26	k6	202	PEB	CAC-CBC-CGC-O1C
26	A7	301	PEB	CAC-CBC-CGC-O1C
26	A7	302	PEB	CAB-CBB-CGB-O2B
26	O7	201	PEB	CAC-CBC-CGC-O1C
26	R7	202	PEB	CAB-CBB-CGB-O1B
26	e7	201	PEB	CAC-CBC-CGC-O1C
26	A8	302	PEB	CAC-CBC-CGC-O2C
26	C8	202	PEB	CAC-CBC-CGC-O2C
26	F8	202	PEB	CAC-CBC-CGC-O1C
26	W8	201	PEB	CAB-CBB-CGB-O2B
26	Y8	201	PEB	CAC-CBC-CGC-O1C
26	g8	201	PEB	CAC-CBC-CGC-O2C
26	h8	201	PEB	CAC-CBC-CGC-O1C
26	j8	201	PEB	CAC-CBC-CGC-O1C
26	A9	304	PEB	CAC-CBC-CGC-O2C
26	D9	203	PEB	CAC-CBC-CGC-O2C
26	M9	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	M9	202	PEB	CAB-CBB-CGB-01B
26	S9	202	PEB	CAC-CBC-CGC-01C
26	U9	202	PEB	CAC-CBC-CGC-02C
26	V9	202	PEB	CAB-CBB-CGB-01B
26	Y9	201	PEB	CAC-CBC-CGC-01C
26	HA	202	PEB	CAB-CBB-CGB-02B
26	MA	201	PEB	CAC-CBC-CGC-02C
26	OA	201	PEB	CAC-CBC-CGC-01C
26	WA	201	PEB	CAB-CBB-CGB-01B
26	WA	201	PEB	CAB-CBB-CGB-02B
26	YA	201	PEB	CAC-CBC-CGC-01C
26	cA	202	PEB	CAC-CBC-CGC-02C
26	gA	202	PEB	CAB-CBB-CGB-01B
26	KB	201	PEB	CAC-CBC-CGC-02C
26	SB	201	PEB	CAB-CBB-CGB-02B
26	TB	202	PEB	CAC-CBC-CGC-01C
26	UB	203	PEB	CAC-CBC-CGC-02C
26	gB	202	PEB	CAC-CBC-CGC-02C
26	hB	202	PEB	CAC-CBC-CGC-02C
26	iB	201	PEB	CAC-CBC-CGC-02C
26	kB	202	PEB	CAC-CBC-CGC-01C
26	lB	203	PEB	CAB-CBB-CGB-01B
26	GC	203	PEB	CAC-CBC-CGC-01C
26	eD	401	PEB	CAB-CBB-CGB-02B
26	ED	202	PEB	CAC-CBC-CGC-02C
26	JD	202	PEB	CAC-CBC-CGC-01C
26	LD	202	PEB	CAC-CBC-CGC-02C
26	OD	201	PEB	CAB-CBB-CGB-02B
26	SD	202	PEB	CAC-CBC-CGC-02C
26	VD	202	PEB	CAB-CBB-CGB-02B
26	YD	301	PEB	CAC-CBC-CGC-01C
26	GE	201	PEB	CAC-CBC-CGC-02C
26	HE	202	PEB	CAC-CBC-CGC-01C
26	IE	201	PEB	CAC-CBC-CGC-01C
26	JE	201	PEB	CAB-CBB-CGB-01B
26	LE	202	PEB	CAC-CBC-CGC-02C
26	NE	202	PEB	CAB-CBB-CGB-02B
26	OE	202	PEB	CAC-CBC-CGC-02C
26	YE	202	PEB	CAB-CBB-CGB-02B
26	aE	201	PEB	CAC-CBC-CGC-01C
26	cE	201	PEB	CAC-CBC-CGC-01C
26	cE	202	PEB	CAB-CBB-CGB-01B

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Mol	Chain	Res	Type	Atoms
26	dE	202	PEB	CAB-CBB-CGB-01B
26	jE	201	PEB	CAC-CBC-CGC-01C
26	kE	203	PEB	CAC-CBC-CGC-02C
26	lE	202	PEB	CAC-CBC-CGC-02C
26	oE	202	PEB	CAC-CBC-CGC-02C
26	AF	305	PEB	CAB-CBB-CGB-01B
26	DF	1002	PEB	CAC-CBC-CGC-02C
26	PF	202	PEB	CAC-CBC-CGC-01C
26	QF	201	PEB	CAB-CBB-CGB-01B
26	QF	202	PEB	CAC-CBC-CGC-02C
26	QF	202	PEB	CAB-CBB-CGB-02B
26	RF	202	PEB	CAB-CBB-CGB-02B
26	SF	201	PEB	CAC-CBC-CGC-01C
26	ZF	203	PEB	CAB-CBB-CGB-02B
26	bF	201	PEB	CAC-CBC-CGC-02C
26	bF	202	PEB	CAC-CBC-CGC-02C
26	hF	201	PEB	CAB-CBB-CGB-02B
26	AG	202	PEB	CAB-CBB-CGB-02B
26	CG	201	PEB	CAB-CBB-CGB-02B
26	KG	203	PEB	CAC-CBC-CGC-01C
26	KG	203	PEB	CAB-CBB-CGB-02B
26	TG	201	PEB	CAC-CBC-CGC-01C
26	cG	201	PEB	CAC-CBC-CGC-02C
26	dG	202	PEB	CAC-CBC-CGC-01C
26	nG	201	PEB	CAC-CBC-CGC-01C
26	sG	202	PEB	CAB-CBB-CGB-02B
26	tG	202	PEB	CAB-CBB-CGB-01B
26	vG	202	PEB	CAB-CBB-CGB-01B
26	xG	304	PEB	CAC-CBC-CGC-01C
26	TI	203	PEB	CAB-CBB-CGB-01B
26	VI	202	PEB	CAC-CBC-CGC-02C
26	YI	203	PEB	CAC-CBC-CGC-02C
26	bI	202	PEB	CAB-CBB-CGB-02B
26	eI	202	PEB	CAC-CBC-CGC-02C
26	eI	203	PEB	CAB-CBB-CGB-01B
26	gI	203	PEB	CAC-CBC-CGC-02C
26	iI	202	PEB	CAC-CBC-CGC-02C
26	iI	203	PEB	CAC-CBC-CGC-02C
26	AJ	304	PEB	CAB-CBB-CGB-01B
26	DJ	203	PEB	CAB-CBB-CGB-02B
26	FJ	201	PEB	CAB-CBB-CGB-01B
26	GJ	202	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
26	RJ	201	PEB	CAC-CBC-CGC-O1C
26	TJ	201	PEB	CAC-CBC-CGC-O2C
26	UJ	202	PEB	CAC-CBC-CGC-O2C
26	XJ	202	PEB	CAC-CBC-CGC-O2C
26	XJ	203	PEB	CAB-CBB-CGB-O2B
27	A8	304	PUB	CAC-CBC-CGC-O2C
27	A8	304	PUB	CAB-CBB-CGB-O1B
27	AF	304	PUB	CAB-CBB-CGB-O1B
27	AI	303	PUB	CAB-CBB-CGB-O1B
28	B6	1002	CYC	CAA-CBA-CGA-O2A
28	C6	1001	CYC	CAA-CBA-CGA-O2A
28	F7	1001	CYC	CAA-CBA-CGA-O1A
28	J7	1001	CYC	CAD-CBD-CGD-O2D
28	CB	1001	CYC	CAA-CBA-CGA-O2A
28	DB	1001	CYC	CAA-CBA-CGA-O2A
28	VH	1001	CYC	CAD-CBD-CGD-O2D
28	YH	1004	CYC	CAD-CBD-CGD-O2D
28	1H	1000	CYC	CAD-CBD-CGD-O2D
28	MI	1001	CYC	CAA-CBA-CGA-O1A
26	M1	402	PEB	C3B-CAB-CBB-CGB
26	U1	201	PEB	C3B-CAB-CBB-CGB
26	z1	201	PEB	C3B-CAB-CBB-CGB
26	U4	201	PEB	C3B-CAB-CBB-CGB
26	h6	203	PEB	C3B-CAB-CBB-CGB
26	Z7	201	PEB	C3B-CAB-CBB-CGB
26	YB	202	PEB	C3B-CAB-CBB-CGB
26	aG	202	PEB	C3B-CAB-CBB-CGB
26	UI	201	PEB	C3B-CAB-CBB-CGB
26	kI	201	PEB	C3B-CAB-CBB-CGB
27	A4	203	PUB	C2C-CAC-CBC-CGC
27	yG	302	PUB	C2C-CAC-CBC-CGC
26	A1	202	PEB	CAB-CBB-CGB-O2B
26	R1	202	PEB	CAC-CBC-CGC-O1C
26	R1	203	PEB	CAB-CBB-CGB-O2B
26	a1	201	PEB	CAB-CBB-CGB-O2B
26	h1	201	PEB	CAB-CBB-CGB-O2B
26	j1	201	PEB	CAC-CBC-CGC-O2C
26	y1	203	PEB	CAB-CBB-CGB-O2B
26	11	201	PEB	CAB-CBB-CGB-O1B
26	21	405	PEB	CAB-CBB-CGB-O2B
26	J2	1002	PEB	CAB-CBB-CGB-O2B
26	O2	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	P2	202	PEB	CAB-CBB-CGB-O2B
26	R2	202	PEB	CAC-CBC-CGC-O2C
26	Z2	202	PEB	CAC-CBC-CGC-O1C
26	e2	201	PEB	CAC-CBC-CGC-O1C
26	i2	202	PEB	CAC-CBC-CGC-O2C
26	A3	202	PEB	CAC-CBC-CGC-O2C
26	I3	201	PEB	CAB-CBB-CGB-O2B
26	K3	202	PEB	CAC-CBC-CGC-O2C
26	L3	202	PEB	CAC-CBC-CGC-O1C
26	P3	203	PEB	CAB-CBB-CGB-O2B
26	U3	202	PEB	CAB-CBB-CGB-O1B
26	Y3	301	PEB	CAB-CBB-CGB-O1B
26	C4	202	PEB	CAC-CBC-CGC-O1C
26	M4	402	PEB	CAB-CBB-CGB-O2B
26	O4	202	PEB	CAB-CBB-CGB-O1B
26	P4	201	PEB	CAB-CBB-CGB-O2B
26	P4	203	PEB	CAC-CBC-CGC-O1C
26	c4	203	PEB	CAB-CBB-CGB-O2B
26	p4	201	PEB	CAB-CBB-CGB-O2B
26	H5	201	PEB	CAC-CBC-CGC-O2C
26	H5	202	PEB	CAC-CBC-CGC-O1C
26	H5	202	PEB	CAC-CBC-CGC-O2C
26	L5	202	PEB	CAB-CBB-CGB-O1B
26	D6	1002	PEB	CAC-CBC-CGC-O2C
26	b6	202	PEB	CAB-CBB-CGB-O2B
26	e6	201	PEB	CAB-CBB-CGB-O2B
26	Q7	203	PEB	CAB-CBB-CGB-O1B
26	U7	201	PEB	CAB-CBB-CGB-O2B
26	G8	203	PEB	CAC-CBC-CGC-O1C
26	J8	202	PEB	CAB-CBB-CGB-O1B
26	K8	201	PEB	CAC-CBC-CGC-O2C
26	L8	202	PEB	CAB-CBB-CGB-O1B
26	O8	203	PEB	CAC-CBC-CGC-O2C
26	U8	203	PEB	CAC-CBC-CGC-O1C
26	W8	202	PEB	CAC-CBC-CGC-O1C
26	a8	203	PEB	CAC-CBC-CGC-O1C
26	c8	202	PEB	CAB-CBB-CGB-O2B
26	g8	201	PEB	CAC-CBC-CGC-O1C
26	B9	203	PEB	CAC-CBC-CGC-O2C
26	D9	203	PEB	CAB-CBB-CGB-O2B
26	F9	202	PEB	CAB-CBB-CGB-O2B
26	R9	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	X9	203	PEB	CAB-CBB-CGB-O2B
26	CA	202	PEB	CAB-CBB-CGB-O2B
26	DA	202	PEB	CAB-CBB-CGB-O2B
26	GA	201	PEB	CAC-CBC-CGC-O1C
26	IA	203	PEB	CAB-CBB-CGB-O1B
26	WA	203	PEB	CAC-CBC-CGC-O2C
26	cA	203	PEB	CAB-CBB-CGB-O1B
26	kA	202	PEB	CAC-CBC-CGC-O2C
26	ZB	202	PEB	CAC-CBC-CGC-O2C
26	hB	201	PEB	CAC-CBC-CGC-O1C
26	GC	202	PEB	CAB-CBB-CGB-O1B
26	HC	202	PEB	CAB-CBB-CGB-O2B
26	BD	203	PEB	CAC-CBC-CGC-O2C
26	GD	201	PEB	CAC-CBC-CGC-O2C
26	HD	201	PEB	CAC-CBC-CGC-O2C
26	HD	203	PEB	CAB-CBB-CGB-O1B
26	PD	203	PEB	CAB-CBB-CGB-O2B
26	HE	201	PEB	CAC-CBC-CGC-O2C
26	JE	201	PEB	CAB-CBB-CGB-O2B
26	OE	201	PEB	CAC-CBC-CGC-O2C
26	TE	202	PEB	CAB-CBB-CGB-O1B
26	WE	202	PEB	CAB-CBB-CGB-O1B
26	iE	202	PEB	CAB-CBB-CGB-O1B
26	kE	201	PEB	CAC-CBC-CGC-O2C
26	oE	203	PEB	CAC-CBC-CGC-O2C
26	uE	203	PEB	CAC-CBC-CGC-O1C
26	yE	301	PEB	CAB-CBB-CGB-O2B
26	OF	201	PEB	CAC-CBC-CGC-O1C
26	OF	202	PEB	CAC-CBC-CGC-O1C
26	UF	203	PEB	CAC-CBC-CGC-O1C
26	ZF	201	PEB	CAC-CBC-CGC-O2C
26	aF	202	PEB	CAC-CBC-CGC-O2C
26	cF	201	PEB	CAC-CBC-CGC-O1C
26	gF	201	PEB	CAB-CBB-CGB-O2B
26	hF	203	PEB	CAB-CBB-CGB-O2B
26	iF	201	PEB	CAC-CBC-CGC-O1C
26	AG	202	PEB	CAC-CBC-CGC-O1C
26	BG	201	PEB	CAB-CBB-CGB-O1B
26	KG	203	PEB	CAB-CBB-CGB-O1B
26	SG	202	PEB	CAB-CBB-CGB-O1B
26	SG	202	PEB	CAB-CBB-CGB-O2B
26	dG	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	oG	202	PEB	CAC-CBC-CGC-O2C
26	oG	203	PEB	CAC-CBC-CGC-O2C
26	pG	201	PEB	CAB-CBB-CGB-O1B
26	qG	203	PEB	CAC-CBC-CGC-O1C
26	rG	202	PEB	CAB-CBB-CGB-O2B
26	tG	201	PEB	CAC-CBC-CGC-O1C
26	vG	201	PEB	CAB-CBB-CGB-O1B
26	zG	501	PEB	CAC-CBC-CGC-O1C
26	OI	201	PEB	CAB-CBB-CGB-O2B
26	OI	202	PEB	CAB-CBB-CGB-O2B
26	RI	202	PEB	CAC-CBC-CGC-O2C
26	UI	202	PEB	CAC-CBC-CGC-O2C
26	bI	202	PEB	CAB-CBB-CGB-O1B
26	cI	202	PEB	CAC-CBC-CGC-O2C
26	HJ	203	PEB	CAB-CBB-CGB-O2B
26	MJ	202	PEB	CAC-CBC-CGC-O2C
26	PJ	203	PEB	CAC-CBC-CGC-O2C
26	VJ	203	PEB	CAC-CBC-CGC-O1C
26	XJ	202	PEB	CAB-CBB-CGB-O2B
27	A6	302	PUB	CAC-CBC-CGC-O2C
28	E6	1001	CYC	CAA-CBA-CGA-O1A
28	G6	1001	CYC	CAA-CBA-CGA-O1A
28	M6	1001	CYC	CAA-CBA-CGA-O2A
28	C7	1001	CYC	CAD-CBD-CGD-O2D
28	N7	1001	CYC	CAA-CBA-CGA-O1A
28	EB	1001	CYC	CAA-CBA-CGA-O1A
28	GB	1001	CYC	CAA-CBA-CGA-O1A
28	MB	1001	CYC	CAA-CBA-CGA-O2A
28	JF	1003	CYC	CAD-CBD-CGD-O2D
28	KF	1001	CYC	CAA-CBA-CGA-O2A
28	iH	1001	CYC	CAA-CBA-CGA-O1A
28	NI	1001	CYC	CAD-CBD-CGD-O2D
28	uH	1001	CYC	C2B-C3B-CAB-CBB
26	K1	201	PEB	CAC-CBC-CGC-O2C
26	Z1	201	PEB	CAB-CBB-CGB-O2B
26	Z1	202	PEB	CAB-CBB-CGB-O2B
26	k1	202	PEB	CAB-CBB-CGB-O2B
26	p1	202	PEB	CAB-CBB-CGB-O2B
26	s1	201	PEB	CAC-CBC-CGC-O2C
26	v1	201	PEB	CAB-CBB-CGB-O2B
26	z1	202	PEB	CAB-CBB-CGB-O2B
26	11	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	U2	201	PEB	CAC-CBC-CGC-O2C
26	V2	203	PEB	CAC-CBC-CGC-O2C
26	Y2	203	PEB	CAB-CBB-CGB-O2B
26	a2	202	PEB	CAB-CBB-CGB-O2B
26	a2	203	PEB	CAB-CBB-CGB-O2B
26	b2	201	PEB	CAC-CBC-CGC-O2C
26	e2	202	PEB	CAC-CBC-CGC-O2C
26	I3	201	PEB	CAB-CBB-CGB-O1B
26	L3	202	PEB	CAB-CBB-CGB-O2B
26	M3	201	PEB	CAB-CBB-CGB-O1B
26	X3	203	PEB	CAC-CBC-CGC-O2C
26	A4	202	PEB	CAB-CBB-CGB-O2B
26	M4	403	PEB	CAB-CBB-CGB-O2B
26	e4	202	PEB	CAB-CBB-CGB-O1B
26	j4	202	PEB	CAB-CBB-CGB-O2B
26	k4	202	PEB	CAB-CBB-CGB-O2B
26	A5	202	PEB	CAB-CBB-CGB-O2B
26	C5	201	PEB	CAC-CBC-CGC-O1C
26	C5	202	PEB	CAC-CBC-CGC-O2C
26	G5	203	PEB	CAC-CBC-CGC-O1C
26	Z6	202	PEB	CAC-CBC-CGC-O2C
26	h6	201	PEB	CAC-CBC-CGC-O2C
26	k6	202	PEB	CAB-CBB-CGB-O2B
26	L7	1002	PEB	CAC-CBC-CGC-O2C
26	Q7	203	PEB	CAB-CBB-CGB-O2B
26	f7	202	PEB	CAB-CBB-CGB-O2B
26	C8	202	PEB	CAB-CBB-CGB-O2B
26	U8	203	PEB	CAB-CBB-CGB-O2B
26	W8	203	PEB	CAC-CBC-CGC-O2C
26	G9	202	PEB	CAB-CBB-CGB-O2B
26	M9	202	PEB	CAB-CBB-CGB-O2B
26	O9	201	PEB	CAB-CBB-CGB-O2B
26	P9	203	PEB	CAB-CBB-CGB-O2B
26	CA	202	PEB	CAB-CBB-CGB-O1B
26	CA	203	PEB	CAC-CBC-CGC-O2C
26	OA	203	PEB	CAC-CBC-CGC-O2C
26	QA	203	PEB	CAC-CBC-CGC-O1C
26	gA	201	PEB	CAC-CBC-CGC-O2C
26	kA	201	PEB	CAC-CBC-CGC-O2C
26	VB	202	PEB	CAC-CBC-CGC-O2C
26	WB	202	PEB	CAB-CBB-CGB-O1B
26	eB	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	fB	201	PEB	CAB-CBB-CGB-O2B
26	hB	201	PEB	CAC-CBC-CGC-O2C
26	FC	203	PEB	CAC-CBC-CGC-O2C
26	KC	203	PEB	CAC-CBC-CGC-O2C
26	LC	202	PEB	CAC-CBC-CGC-O1C
26	FD	202	PEB	CAB-CBB-CGB-O2B
26	LD	202	PEB	CAB-CBB-CGB-O2B
26	RD	203	PEB	CAC-CBC-CGC-O2C
26	UD	202	PEB	CAB-CBB-CGB-O2B
26	XD	203	PEB	CAC-CBC-CGC-O2C
26	SE	203	PEB	CAC-CBC-CGC-O1C
26	mE	202	PEB	CAC-CBC-CGC-O1C
26	aF	202	PEB	CAC-CBC-CGC-O1C
26	dF	202	PEB	CAC-CBC-CGC-O2C
26	BG	201	PEB	CAB-CBB-CGB-O2B
26	HG	202	PEB	CAC-CBC-CGC-O1C
26	kG	202	PEB	CAC-CBC-CGC-O2C
26	mG	201	PEB	CAB-CBB-CGB-O2B
26	UI	201	PEB	CAC-CBC-CGC-O2C
26	VI	203	PEB	CAC-CBC-CGC-O2C
26	aI	202	PEB	CAB-CBB-CGB-O2B
26	dI	202	PEB	CAB-CBB-CGB-O2B
26	PJ	202	PEB	CAC-CBC-CGC-O2C
26	XJ	201	PEB	CAB-CBB-CGB-O2B
28	D6	1001	CYC	CAD-CBD-CGD-O2D
28	E7	1001	CYC	CAA-CBA-CGA-O2A
28	L7	1001	CYC	CAA-CBA-CGA-O2A
28	MB	1001	CYC	CAA-CBA-CGA-O1A
28	CF	1001	CYC	CAA-CBA-CGA-O1A
28	LF	1001	CYC	CAD-CBD-CGD-O2D
28	AH	1001	CYC	CAA-CBA-CGA-O2A
28	EH	1001	CYC	CAA-CBA-CGA-O2A
28	VH	1001	CYC	CAA-CBA-CGA-O2A
28	YH	1001	CYC	CAA-CBA-CGA-O1A
28	YH	1001	CYC	CAA-CBA-CGA-O2A
28	cH	1001	CYC	CAA-CBA-CGA-O2A
28	1H	1000	CYC	CAA-CBA-CGA-O2A
26	B1	202	PEB	CAC-CBC-CGC-O1C
26	C1	201	PEB	CAB-CBB-CGB-O2B
26	E1	202	PEB	CAC-CBC-CGC-O1C
26	J1	203	PEB	CAB-CBB-CGB-O1B
26	L1	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	P1	203	PEB	CAC-CBC-CGC-O2C
26	Y1	202	PEB	CAB-CBB-CGB-O2B
26	e1	201	PEB	CAB-CBB-CGB-O1B
26	m1	201	PEB	CAB-CBB-CGB-O1B
26	n1	201	PEB	CAB-CBB-CGB-O2B
26	s1	202	PEB	CAC-CBC-CGC-O2C
26	w1	203	PEB	CAB-CBB-CGB-O1B
26	21	405	PEB	CAC-CBC-CGC-O2C
26	S2	202	PEB	CAB-CBB-CGB-O1B
26	W2	201	PEB	CAC-CBC-CGC-O2C
26	h2	202	PEB	CAB-CBB-CGB-O1B
26	k2	202	PEB	CAB-CBB-CGB-O1B
26	m2	202	PEB	CAC-CBC-CGC-O2C
26	V3	202	PEB	CAC-CBC-CGC-O1C
26	Y3	303	PEB	CAC-CBC-CGC-O1C
26	D4	201	PEB	CAC-CBC-CGC-O1C
26	E4	202	PEB	CAB-CBB-CGB-O2B
26	H4	203	PEB	CAB-CBB-CGB-O1B
26	J4	203	PEB	CAB-CBB-CGB-O2B
26	N4	203	PEB	CAB-CBB-CGB-O2B
26	P4	203	PEB	CAC-CBC-CGC-O2C
26	e4	201	PEB	CAB-CBB-CGB-O1B
26	i4	202	PEB	CAC-CBC-CGC-O2C
26	k4	203	PEB	CAC-CBC-CGC-O2C
26	n4	202	PEB	CAB-CBB-CGB-O1B
26	s4	201	PEB	CAC-CBC-CGC-O2C
26	z4	202	PEB	CAC-CBC-CGC-O2C
26	B5	201	PEB	CAB-CBB-CGB-O2B
26	B5	202	PEB	CAB-CBB-CGB-O2B
26	J5	202	PEB	CAB-CBB-CGB-O2B
26	P6	202	PEB	CAC-CBC-CGC-O2C
26	U6	202	PEB	CAC-CBC-CGC-O2C
26	V6	202	PEB	CAB-CBB-CGB-O2B
26	Z6	202	PEB	CAB-CBB-CGB-O2B
26	b6	202	PEB	CAC-CBC-CGC-O2C
26	c6	201	PEB	CAC-CBC-CGC-O2C
26	d6	201	PEB	CAB-CBB-CGB-O2B
26	d6	204	PEB	CAC-CBC-CGC-O2C
26	h6	202	PEB	CAB-CBB-CGB-O2B
26	F7	1002	PEB	CAB-CBB-CGB-O2B
26	S7	202	PEB	CAB-CBB-CGB-O2B
26	U7	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	W7	202	PEB	CAC-CBC-CGC-O2C
26	g7	201	PEB	CAB-CBB-CGB-O2B
26	E8	201	PEB	CAC-CBC-CGC-O2C
26	E8	201	PEB	CAB-CBB-CGB-O1B
26	G8	203	PEB	CAC-CBC-CGC-O2C
26	H8	202	PEB	CAB-CBB-CGB-O2B
26	I8	202	PEB	CAC-CBC-CGC-O1C
26	N8	201	PEB	CAC-CBC-CGC-O2C
26	O8	201	PEB	CAC-CBC-CGC-O1C
26	O8	202	PEB	CAB-CBB-CGB-O1B
26	Q8	203	PEB	CAC-CBC-CGC-O1C
26	Y8	201	PEB	CAB-CBB-CGB-O2B
26	Y8	202	PEB	CAC-CBC-CGC-O2C
26	a8	203	PEB	CAB-CBB-CGB-O2B
26	f8	203	PEB	CAC-CBC-CGC-O1C
26	i8	202	PEB	CAC-CBC-CGC-O2C
26	i8	202	PEB	CAB-CBB-CGB-O1B
26	B9	202	PEB	CAC-CBC-CGC-O1C
26	R9	201	PEB	CAB-CBB-CGB-O2B
26	R9	202	PEB	CAC-CBC-CGC-O2C
26	T9	202	PEB	CAC-CBC-CGC-O2C
26	T9	203	PEB	CAB-CBB-CGB-O1B
26	U9	201	PEB	CAC-CBC-CGC-O1C
26	U9	202	PEB	CAB-CBB-CGB-O2B
26	AA	301	PEB	CAB-CBB-CGB-O2B
26	AA	302	PEB	CAC-CBC-CGC-O1C
26	JA	202	PEB	CAB-CBB-CGB-O1B
26	KA	201	PEB	CAC-CBC-CGC-O2C
26	NA	202	PEB	CAC-CBC-CGC-O2C
26	PA	202	PEB	CAB-CBB-CGB-O1B
26	YA	202	PEB	CAC-CBC-CGC-O2C
26	aA	203	PEB	CAB-CBB-CGB-O2B
26	iA	202	PEB	CAC-CBC-CGC-O2C
26	iA	202	PEB	CAB-CBB-CGB-O2B
26	OB	201	PEB	CAB-CBB-CGB-O2B
26	YB	202	PEB	CAC-CBC-CGC-O1C
26	ZB	202	PEB	CAB-CBB-CGB-O2B
26	jB	202	PEB	CAC-CBC-CGC-O2C
26	mB	203	PEB	CAB-CBB-CGB-O2B
26	FD	202	PEB	CAC-CBC-CGC-O2C
26	KD	202	PEB	CAC-CBC-CGC-O1C
26	LD	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	MD	201	PEB	CAB-CBB-CGB-01B
26	TD	201	PEB	CAC-CBC-CGC-02C
26	YD	304	PEB	CAC-CBC-CGC-02C
26	BE	201	PEB	CAB-CBB-CGB-02B
26	DE	201	PEB	CAB-CBB-CGB-01B
26	QE	202	PEB	CAB-CBB-CGB-02B
26	TE	201	PEB	CAC-CBC-CGC-01C
26	TE	202	PEB	CAB-CBB-CGB-02B
26	WE	203	PEB	CAC-CBC-CGC-02C
26	XE	202	PEB	CAC-CBC-CGC-01C
26	cE	201	PEB	CAC-CBC-CGC-02C
26	mE	201	PEB	CAB-CBB-CGB-01B
26	rE	201	PEB	CAB-CBB-CGB-02B
26	tE	201	PEB	CAC-CBC-CGC-01C
26	aF	201	PEB	CAC-CBC-CGC-01C
26	dF	202	PEB	CAB-CBB-CGB-01B
26	iF	201	PEB	CAC-CBC-CGC-02C
26	jF	202	PEB	CAB-CBB-CGB-02B
26	AG	202	PEB	CAC-CBC-CGC-02C
26	DG	201	PEB	CAB-CBB-CGB-01B
26	DG	202	PEB	CAB-CBB-CGB-01B
26	DG	202	PEB	CAB-CBB-CGB-02B
26	DG	203	PEB	CAC-CBC-CGC-02C
26	HG	202	PEB	CAC-CBC-CGC-02C
26	IG	201	PEB	CAC-CBC-CGC-01C
26	IG	201	PEB	CAC-CBC-CGC-02C
26	TG	202	PEB	CAB-CBB-CGB-02B
26	XG	203	PEB	CAC-CBC-CGC-01C
26	dG	202	PEB	CAC-CBC-CGC-02C
26	hG	201	PEB	CAC-CBC-CGC-01C
26	kG	202	PEB	CAB-CBB-CGB-02B
26	lG	202	PEB	CAC-CBC-CGC-01C
26	nG	201	PEB	CAC-CBC-CGC-02C
26	oG	203	PEB	CAB-CBB-CGB-01B
26	yG	301	PEB	CAC-CBC-CGC-02C
26	zG	501	PEB	CAC-CBC-CGC-02C
26	PI	202	PEB	CAB-CBB-CGB-02B
26	AJ	303	PEB	CAC-CBC-CGC-02C
26	RJ	202	PEB	CAC-CBC-CGC-01C
26	RJ	203	PEB	CAC-CBC-CGC-01C
26	UJ	201	PEB	CAC-CBC-CGC-01C
27	K1	203	PUB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
27	BA	302	PUB	CAB-CBB-CGB-O2B
28	CF	1001	CYC	CAA-CBA-CGA-O2A
28	NF	1001	CYC	CAA-CBA-CGA-O1A
28	NF	1001	CYC	CAA-CBA-CGA-O2A
28	GH	1001	CYC	CAA-CBA-CGA-O1A
26	P2	202	PEB	C2B-C3B-CAB-CBB
26	aB	202	PEB	C2B-C3B-CAB-CBB
26	C1	202	PEB	CAB-CBB-CGB-O2B
26	D1	201	PEB	CAC-CBC-CGC-O2C
26	H1	202	PEB	CAB-CBB-CGB-O2B
26	J1	202	PEB	CAC-CBC-CGC-O2C
26	J1	203	PEB	CAC-CBC-CGC-O1C
26	J1	203	PEB	CAB-CBB-CGB-O2B
26	R1	202	PEB	CAC-CBC-CGC-O2C
26	S1	201	PEB	CAC-CBC-CGC-O2C
26	Y1	201	PEB	CAB-CBB-CGB-O2B
26	i1	203	PEB	CAC-CBC-CGC-O2C
26	k1	203	PEB	CAC-CBC-CGC-O2C
26	D2	1002	PEB	CAB-CBB-CGB-O2B
26	O2	202	PEB	CAB-CBB-CGB-O1B
26	P2	202	PEB	CAC-CBC-CGC-O2C
26	Q2	202	PEB	CAB-CBB-CGB-O2B
26	a2	202	PEB	CAC-CBC-CGC-O2C
26	b2	202	PEB	CAC-CBC-CGC-O2C
26	l2	201	PEB	CAC-CBC-CGC-O1C
26	A3	202	PEB	CAB-CBB-CGB-O1B
26	F3	203	PEB	CAC-CBC-CGC-O2C
26	H3	203	PEB	CAC-CBC-CGC-O1C
26	O3	202	PEB	CAC-CBC-CGC-O2C
26	P3	201	PEB	CAC-CBC-CGC-O2C
26	Y3	304	PEB	CAC-CBC-CGC-O2C
26	A4	201	PEB	CAB-CBB-CGB-O2B
26	J4	203	PEB	CAC-CBC-CGC-O1C
26	L4	201	PEB	CAC-CBC-CGC-O1C
26	b4	501	PEB	CAC-CBC-CGC-O2C
26	e4	202	PEB	CAB-CBB-CGB-O2B
26	g4	201	PEB	CAB-CBB-CGB-O2B
26	h4	202	PEB	CAC-CBC-CGC-O2C
26	y4	203	PEB	CAB-CBB-CGB-O2B
26	z4	202	PEB	CAC-CBC-CGC-O1C
26	C5	203	PEB	CAC-CBC-CGC-O1C
26	C5	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	H5	203	PEB	CAC-CBC-CGC-O2C
26	K5	203	PEB	CAC-CBC-CGC-O1C
26	P6	202	PEB	CAC-CBC-CGC-O1C
26	Y6	201	PEB	CAC-CBC-CGC-O1C
26	d6	204	PEB	CAB-CBB-CGB-O2B
26	j6	202	PEB	CAC-CBC-CGC-O2C
26	A7	301	PEB	CAC-CBC-CGC-O2C
26	L7	1002	PEB	CAC-CBC-CGC-O1C
26	d7	202	PEB	CAC-CBC-CGC-O2C
26	d7	203	PEB	CAB-CBB-CGB-O2B
26	f7	201	PEB	CAC-CBC-CGC-O2C
26	h7	203	PEB	CAB-CBB-CGB-O2B
26	i7	201	PEB	CAC-CBC-CGC-O2C
26	l7	201	PEB	CAB-CBB-CGB-O1B
26	A8	301	PEB	CAC-CBC-CGC-O2C
26	I8	203	PEB	CAC-CBC-CGC-O1C
26	L8	202	PEB	CAB-CBB-CGB-O2B
26	S8	203	PEB	CAC-CBC-CGC-O1C
26	W8	201	PEB	CAB-CBB-CGB-O1B
26	a8	203	PEB	CAB-CBB-CGB-O1B
26	X9	203	PEB	CAC-CBC-CGC-O2C
26	AA	301	PEB	CAC-CBC-CGC-O2C
26	OA	202	PEB	CAB-CBB-CGB-O1B
26	SA	202	PEB	CAC-CBC-CGC-O2C
26	YA	201	PEB	CAB-CBB-CGB-O2B
26	cA	201	PEB	CAB-CBB-CGB-O1B
26	cA	203	PEB	CAB-CBB-CGB-O2B
26	QB	202	PEB	CAB-CBB-CGB-O2B
26	cB	201	PEB	CAC-CBC-CGC-O2C
26	kB	202	PEB	CAB-CBB-CGB-O2B
26	lB	203	PEB	CAC-CBC-CGC-O2C
26	AC	202	PEB	CAC-CBC-CGC-O1C
26	AC	202	PEB	CAB-CBB-CGB-O2B
26	BC	201	PEB	CAB-CBB-CGB-O2B
26	GC	203	PEB	CAC-CBC-CGC-O2C
26	HC	201	PEB	CAB-CBB-CGB-O2B
26	HC	202	PEB	CAC-CBC-CGC-O2C
26	IC	203	PEB	CAB-CBB-CGB-O1B
26	LC	202	PEB	CAC-CBC-CGC-O2C
26	OD	202	PEB	CAC-CBC-CGC-O2C
26	RD	201	PEB	CAB-CBB-CGB-O2B
26	SD	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	BE	201	PEB	CAC-CBC-CGC-O2C
26	NE	201	PEB	CAC-CBC-CGC-O1C
26	aE	202	PEB	CAB-CBB-CGB-O2B
26	fE	201	PEB	CAB-CBB-CGB-O2B
26	lE	201	PEB	CAC-CBC-CGC-O2C
26	nE	201	PEB	CAC-CBC-CGC-O2C
26	nE	202	PEB	CAB-CBB-CGB-O2B
26	oE	202	PEB	CAB-CBB-CGB-O2B
26	rE	201	PEB	CAC-CBC-CGC-O2C
26	zE	501	PEB	CAC-CBC-CGC-O2C
26	QF	203	PEB	CAB-CBB-CGB-O2B
26	RF	202	PEB	CAC-CBC-CGC-O2C
26	gF	201	PEB	CAC-CBC-CGC-O2C
26	lF	201	PEB	CAC-CBC-CGC-O2C
26	lF	201	PEB	CAB-CBB-CGB-O1B
26	LG	202	PEB	CAC-CBC-CGC-O1C
26	LG	202	PEB	CAC-CBC-CGC-O2C
26	mG	203	PEB	CAB-CBB-CGB-O2B
26	rG	202	PEB	CAC-CBC-CGC-O2C
26	uG	202	PEB	CAB-CBB-CGB-O2B
26	wG	302	PEB	CAB-CBB-CGB-O2B
26	yG	301	PEB	CAB-CBB-CGB-O2B
26	QI	202	PEB	CAB-CBB-CGB-O2B
26	SI	202	PEB	CAB-CBB-CGB-O1B
26	bI	201	PEB	CAC-CBC-CGC-O2C
26	fI	202	PEB	CAB-CBB-CGB-O2B
26	mI	201	PEB	CAB-CBB-CGB-O1B
26	AJ	301	PEB	CAB-CBB-CGB-O2B
26	IJ	202	PEB	CAB-CBB-CGB-O2B
26	JJ	203	PEB	CAC-CBC-CGC-O2C
26	NJ	202	PEB	CAC-CBC-CGC-O2C
27	K4	203	PUB	CAB-CBB-CGB-O1B
27	A6	303	PUB	CAC-CBC-CGC-O2C
27	A6	303	PUB	CAB-CBB-CGB-O1B
27	B8	302	PUB	CAB-CBB-CGB-O2B
27	xG	305	PUB	CAB-CBB-CGB-O2B
28	I7	1001	CYC	CAA-CBA-CGA-O2A
28	BB	1001	CYC	CAD-CBD-CGD-O2D
28	DB	1001	CYC	CAD-CBD-CGD-O2D
28	GB	1001	CYC	CAA-CBA-CGA-O2A
28	KB	202	CYC	CAA-CBA-CGA-O2A
28	EF	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	CH	1001	CYC	CAA-CBA-CGA-O2A
28	YH	1004	CYC	CAA-CBA-CGA-O2A
28	qH	1002	CYC	CAA-CBA-CGA-O1A
28	vH	1001	CYC	CAA-CBA-CGA-O2A
26	k2	202	PEB	C4B-C3B-CAB-CBB
27	yG	303	PUB	C4A-C3A-CAA-CBA
26	B1	201	PEB	C2C-CAC-CBC-CGC
26	D1	201	PEB	C2A-C3A-CAA-CBA
26	P1	203	PEB	C2C-CAC-CBC-CGC
26	S1	201	PEB	C2A-C3A-CAA-CBA
26	Q2	202	PEB	C2A-C3A-CAA-CBA
26	U2	202	PEB	C2A-C3A-CAA-CBA
26	M3	201	PEB	C2C-CAC-CBC-CGC
26	g4	201	PEB	C2A-C3A-CAA-CBA
26	u4	201	PEB	C2A-C3A-CAA-CBA
26	F5	202	PEB	C2C-CAC-CBC-CGC
26	F7	1002	PEB	C2C-CAC-CBC-CGC
26	D8	202	PEB	C2C-CAC-CBC-CGC
26	Y8	203	PEB	C2A-C3A-CAA-CBA
26	j8	201	PEB	C2C-CAC-CBC-CGC
26	k8	201	PEB	C2C-CAC-CBC-CGC
26	fA	201	PEB	C2C-CAC-CBC-CGC
26	kA	201	PEB	C2A-C3A-CAA-CBA
26	fB	203	PEB	C2C-CAC-CBC-CGC
26	KD	202	PEB	C2A-C3A-CAA-CBA
26	MD	201	PEB	C2C-CAC-CBC-CGC
26	XE	201	PEB	C2A-C3A-CAA-CBA
26	mF	202	PEB	C2A-C3A-CAA-CBA
26	XG	201	PEB	C2A-C3A-CAA-CBA
26	hG	201	PEB	C2C-CAC-CBC-CGC
26	EJ	201	PEB	C2A-C3A-CAA-CBA
28	E2	1001	CYC	C2C-C3C-CAC-CBC
26	M1	401	PEB	CAB-CBB-CGB-O2B
26	c1	203	PEB	CAB-CBB-CGB-O2B
26	d1	203	PEB	CAB-CBB-CGB-O2B
26	i1	203	PEB	CAB-CBB-CGB-O1B
26	k1	202	PEB	CAB-CBB-CGB-O1B
26	k1	203	PEB	CAB-CBB-CGB-O1B
26	p1	202	PEB	CAC-CBC-CGC-O1C
26	q1	201	PEB	CAC-CBC-CGC-O1C
26	s1	201	PEB	CAC-CBC-CGC-O1C
26	u1	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	11	201	PEB	CAC-CBC-CGC-O1C
26	N2	1002	PEB	CAB-CBB-CGB-O2B
26	P2	203	PEB	CAC-CBC-CGC-O2C
26	U2	202	PEB	CAC-CBC-CGC-O1C
26	b2	202	PEB	CAB-CBB-CGB-O1B
26	d2	201	PEB	CAB-CBB-CGB-O2B
26	g2	203	PEB	CAC-CBC-CGC-O2C
26	h2	201	PEB	CAC-CBC-CGC-O1C
26	j2	202	PEB	CAB-CBB-CGB-O2B
26	l2	201	PEB	CAC-CBC-CGC-O2C
26	e3	401	PEB	CAB-CBB-CGB-O1B
26	K3	202	PEB	CAC-CBC-CGC-O1C
26	O3	201	PEB	CAC-CBC-CGC-O1C
26	F4	203	PEB	CAB-CBB-CGB-O2B
26	T4	201	PEB	CAC-CBC-CGC-O2C
26	Z4	202	PEB	CAC-CBC-CGC-O2C
26	c4	203	PEB	CAC-CBC-CGC-O2C
26	f4	202	PEB	CAB-CBB-CGB-O2B
26	i4	202	PEB	CAB-CBB-CGB-O2B
26	k4	202	PEB	CAB-CBB-CGB-O1B
26	l4	201	PEB	CAB-CBB-CGB-O2B
26	p4	202	PEB	CAB-CBB-CGB-O1B
26	p4	202	PEB	CAB-CBB-CGB-O2B
26	t4	202	PEB	CAB-CBB-CGB-O2B
26	v4	201	PEB	CAB-CBB-CGB-O1B
26	24	404	PEB	CAB-CBB-CGB-O2B
26	C5	202	PEB	CAB-CBB-CGB-O1B
26	H5	203	PEB	CAB-CBB-CGB-O2B
26	K5	203	PEB	CAB-CBB-CGB-O2B
26	R6	202	PEB	CAC-CBC-CGC-O1C
26	S6	201	PEB	CAB-CBB-CGB-O1B
26	T6	202	PEB	CAC-CBC-CGC-O1C
26	g6	202	PEB	CAB-CBB-CGB-O2B
26	l6	203	PEB	CAC-CBC-CGC-O2C
26	A7	302	PEB	CAC-CBC-CGC-O1C
26	A7	305	PEB	CAC-CBC-CGC-O2C
26	T7	202	PEB	CAB-CBB-CGB-O2B
26	Y7	201	PEB	CAB-CBB-CGB-O1B
26	a7	202	PEB	CAB-CBB-CGB-O1B
26	b7	202	PEB	CAC-CBC-CGC-O2C
26	C8	203	PEB	CAC-CBC-CGC-O2C
26	G8	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	S8	202	PEB	CAC-CBC-CGC-O1C
26	W8	202	PEB	CAC-CBC-CGC-O2C
26	c8	202	PEB	CAB-CBB-CGB-O1B
26	l8	201	PEB	CAC-CBC-CGC-O1C
26	l8	202	PEB	CAC-CBC-CGC-O2C
26	A9	301	PEB	CAB-CBB-CGB-O2B
26	B9	201	PEB	CAB-CBB-CGB-O2B
26	G9	202	PEB	CAB-CBB-CGB-O1B
26	H9	203	PEB	CAC-CBC-CGC-O1C
26	W9	201	PEB	CAC-CBC-CGC-O1C
26	Y9	202	PEB	CAC-CBC-CGC-O2C
26	IA	203	PEB	CAC-CBC-CGC-O1C
26	QA	202	PEB	CAC-CBC-CGC-O2C
26	QA	204	PEB	CAB-CBB-CGB-O2B
26	fA	203	PEB	CAC-CBC-CGC-O1C
26	gA	202	PEB	CAB-CBB-CGB-O2B
26	RB	202	PEB	CAC-CBC-CGC-O1C
26	ZB	203	PEB	CAC-CBC-CGC-O2C
26	aB	202	PEB	CAC-CBC-CGC-O2C
26	dB	204	PEB	CAC-CBC-CGC-O2C
26	dB	204	PEB	CAB-CBB-CGB-O2B
26	eB	203	PEB	CAB-CBB-CGB-O2B
26	AC	201	PEB	CAB-CBB-CGB-O2B
26	BC	202	PEB	CAC-CBC-CGC-O2C
26	CC	202	PEB	CAC-CBC-CGC-O1C
26	HC	203	PEB	CAB-CBB-CGB-O2B
26	KC	203	PEB	CAB-CBB-CGB-O2B
26	AD	201	PEB	CAB-CBB-CGB-O1B
26	AE	202	PEB	CAB-CBB-CGB-O2B
26	BE	201	PEB	CAC-CBC-CGC-O1C
26	CE	203	PEB	CAB-CBB-CGB-O2B
26	DE	203	PEB	CAC-CBC-CGC-O1C
26	DE	203	PEB	CAC-CBC-CGC-O2C
26	KE	203	PEB	CAC-CBC-CGC-O1C
26	QE	202	PEB	CAC-CBC-CGC-O2C
26	RE	202	PEB	CAB-CBB-CGB-O2B
26	SE	203	PEB	CAC-CBC-CGC-O2C
26	TE	202	PEB	CAC-CBC-CGC-O2C
26	ZE	202	PEB	CAB-CBB-CGB-O2B
26	gE	203	PEB	CAC-CBC-CGC-O2C
26	iE	203	PEB	CAC-CBC-CGC-O1C
26	iE	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	kE	202	PEB	CAC-CBC-CGC-O1C
26	mE	201	PEB	CAC-CBC-CGC-O2C
26	pE	202	PEB	CAB-CBB-CGB-O1B
26	sE	201	PEB	CAB-CBB-CGB-O2B
26	vE	201	PEB	CAC-CBC-CGC-O2C
26	wE	302	PEB	CAB-CBB-CGB-O2B
26	yE	301	PEB	CAC-CBC-CGC-O2C
26	AF	305	PEB	CAC-CBC-CGC-O2C
26	RF	201	PEB	CAB-CBB-CGB-O2B
26	SF	202	PEB	CAB-CBB-CGB-O2B
26	VF	202	PEB	CAC-CBC-CGC-O1C
26	bF	201	PEB	CAC-CBC-CGC-O1C
26	BG	201	PEB	CAC-CBC-CGC-O1C
26	CG	201	PEB	CAB-CBB-CGB-O1B
26	CG	203	PEB	CAB-CBB-CGB-O1B
26	DG	203	PEB	CAC-CBC-CGC-O1C
26	IG	202	PEB	CAB-CBB-CGB-O2B
26	cG	202	PEB	CAC-CBC-CGC-O1C
26	hG	201	PEB	CAC-CBC-CGC-O2C
26	jG	202	PEB	CAB-CBB-CGB-O1B
26	qG	201	PEB	CAC-CBC-CGC-O1C
26	rG	201	PEB	CAC-CBC-CGC-O2C
26	rG	201	PEB	CAB-CBB-CGB-O1B
26	sG	203	PEB	CAC-CBC-CGC-O2C
26	uG	203	PEB	CAC-CBC-CGC-O1C
26	vG	201	PEB	CAC-CBC-CGC-O2C
26	WI	201	PEB	CAC-CBC-CGC-O1C
26	dI	201	PEB	CAC-CBC-CGC-O2C
26	hI	201	PEB	CAC-CBC-CGC-O1C
26	jI	201	PEB	CAC-CBC-CGC-O1C
26	jI	202	PEB	CAB-CBB-CGB-O2B
26	II	202	PEB	CAC-CBC-CGC-O1C
26	AJ	305	PEB	CAC-CBC-CGC-O2C
26	FJ	202	PEB	CAB-CBB-CGB-O1B
26	HJ	201	PEB	CAC-CBC-CGC-O2C
26	NJ	204	PEB	CAC-CBC-CGC-O2C
26	UJ	202	PEB	CAB-CBB-CGB-O1B
26	UJ	202	PEB	CAB-CBB-CGB-O2B
26	YJ	202	PEB	CAB-CBB-CGB-O1B
27	2I	402	PUB	CAC-CBC-CGC-O2C
27	A4	203	PUB	CAC-CBC-CGC-O2C
27	K4	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
27	wG	304	PUB	CAB-CBB-CGB-O2B
28	E7	1001	CYC	CAA-CBA-CGA-O1A
28	J7	1001	CYC	CAA-CBA-CGA-O2A
28	EF	1001	CYC	CAA-CBA-CGA-O2A
28	KF	1001	CYC	CAA-CBA-CGA-O1A
28	AH	1001	CYC	CAA-CBA-CGA-O1A
28	gH	1001	CYC	CAA-CBA-CGA-O2A
28	tH	1001	CYC	CAA-CBA-CGA-O2A
28	FI	1001	CYC	CAA-CBA-CGA-O2A
26	N1	201	PEB	CAC-CBC-CGC-O2C
26	h1	202	PEB	CAB-CBB-CGB-O1B
26	j1	202	PEB	CAB-CBB-CGB-O1B
26	q1	203	PEB	CAB-CBB-CGB-O2B
26	y1	201	PEB	CAC-CBC-CGC-O2C
26	21	405	PEB	CAC-CBC-CGC-O1C
26	Q2	202	PEB	CAB-CBB-CGB-O1B
26	k2	202	PEB	CAB-CBB-CGB-O2B
26	R3	201	PEB	CAB-CBB-CGB-O2B
26	N4	201	PEB	CAC-CBC-CGC-O2C
26	g4	201	PEB	CAB-CBB-CGB-O1B
26	i4	201	PEB	CAB-CBB-CGB-O2B
26	w4	201	PEB	CAB-CBB-CGB-O2B
26	G5	203	PEB	CAC-CBC-CGC-O2C
26	Y6	202	PEB	CAC-CBC-CGC-O1C
26	d6	204	PEB	CAB-CBB-CGB-O1B
26	i6	201	PEB	CAC-CBC-CGC-O2C
26	a7	202	PEB	CAC-CBC-CGC-O2C
26	f7	201	PEB	CAB-CBB-CGB-O2B
26	O8	203	PEB	CAC-CBC-CGC-O1C
26	Q8	204	PEB	CAB-CBB-CGB-O2B
26	T8	202	PEB	CAC-CBC-CGC-O1C
26	i8	202	PEB	CAB-CBB-CGB-O2B
26	J9	202	PEB	CAB-CBB-CGB-O1B
26	N9	203	PEB	CAB-CBB-CGB-O2B
26	JA	202	PEB	CAC-CBC-CGC-O2C
26	SA	203	PEB	CAC-CBC-CGC-O1C
26	WA	202	PEB	CAC-CBC-CGC-O2C
26	OB	203	PEB	CAC-CBC-CGC-O2C
26	SB	202	PEB	CAC-CBC-CGC-O1C
26	VB	202	PEB	CAB-CBB-CGB-O2B
26	YB	201	PEB	CAB-CBB-CGB-O2B
26	KC	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	AD	202	PEB	CAC-CBC-CGC-O2C
26	DD	201	PEB	CAB-CBB-CGB-O2B
26	FD	202	PEB	CAB-CBB-CGB-O1B
26	FE	201	PEB	CAB-CBB-CGB-O2B
26	NE	202	PEB	CAB-CBB-CGB-O1B
26	TE	201	PEB	CAC-CBC-CGC-O2C
26	UE	201	PEB	CAC-CBC-CGC-O1C
26	mE	201	PEB	CAB-CBB-CGB-O2B
26	pE	201	PEB	CAB-CBB-CGB-O2B
26	qE	201	PEB	CAC-CBC-CGC-O1C
26	SF	202	PEB	CAB-CBB-CGB-O1B
26	hF	202	PEB	CAC-CBC-CGC-O1C
26	FG	201	PEB	CAB-CBB-CGB-O2B
26	NG	201	PEB	CAC-CBC-CGC-O1C
26	VG	202	PEB	CAC-CBC-CGC-O2C
26	dG	201	PEB	CAB-CBB-CGB-O2B
26	fG	201	PEB	CAB-CBB-CGB-O2B
26	rG	201	PEB	CAC-CBC-CGC-O1C
26	sG	201	PEB	CAB-CBB-CGB-O2B
26	fl	201	PEB	CAC-CBC-CGC-O2C
26	II	201	PEB	CAC-CBC-CGC-O2C
26	BJ	202	PEB	CAC-CBC-CGC-O1C
28	K6	202	CYC	CAA-CBA-CGA-O2A
28	M6	1001	CYC	CAA-CBA-CGA-O1A
28	CB	1001	CYC	CAA-CBA-CGA-O1A
28	FF	1001	CYC	CAA-CBA-CGA-O2A
28	LF	1001	CYC	CAA-CBA-CGA-O2A
28	EH	1001	CYC	CAA-CBA-CGA-O1A
28	KH	1001	CYC	CAA-CBA-CGA-O1A
26	L1	202	PEB	C4D-C3D-CAD-CBD
28	iH	1001	CYC	C2B-C3B-CAB-CBB
26	P8	201	PEB	C2B-C3B-CAB-CBB
26	F1	201	PEB	CAC-CBC-CGC-O2C
26	I1	202	PEB	CAC-CBC-CGC-O2C
26	I1	202	PEB	CAB-CBB-CGB-O2B
26	K1	201	PEB	CAC-CBC-CGC-O1C
26	M1	402	PEB	CAB-CBB-CGB-O1B
26	w1	202	PEB	CAC-CBC-CGC-O2C
26	W2	201	PEB	CAC-CBC-CGC-O1C
26	d2	202	PEB	CAB-CBB-CGB-O1B
26	e2	202	PEB	CAB-CBB-CGB-O1B
26	S3	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	A4	202	PEB	CAB-CBB-CGB-01B
26	C4	201	PEB	CAB-CBB-CGB-02B
26	D4	201	PEB	CAB-CBB-CGB-02B
26	E4	201	PEB	CAB-CBB-CGB-01B
26	K4	202	PEB	CAB-CBB-CGB-02B
26	c4	203	PEB	CAB-CBB-CGB-01B
26	j4	201	PEB	CAC-CBC-CGC-01C
26	n4	202	PEB	CAB-CBB-CGB-02B
26	s4	201	PEB	CAC-CBC-CGC-01C
26	s4	202	PEB	CAC-CBC-CGC-02C
26	u4	202	PEB	CAC-CBC-CGC-02C
26	B5	201	PEB	CAC-CBC-CGC-02C
26	W6	201	PEB	CAC-CBC-CGC-01C
26	b6	202	PEB	CAC-CBC-CGC-01C
26	e7	202	PEB	CAB-CBB-CGB-01B
26	e7	202	PEB	CAB-CBB-CGB-02B
26	O8	202	PEB	CAB-CBB-CGB-02B
26	g8	202	PEB	CAB-CBB-CGB-02B
26	F9	202	PEB	CAB-CBB-CGB-01B
26	T9	201	PEB	CAC-CBC-CGC-02C
26	EA	201	PEB	CAC-CBC-CGC-01C
26	IA	201	PEB	CAC-CBC-CGC-02C
26	JA	202	PEB	CAB-CBB-CGB-02B
26	OA	202	PEB	CAB-CBB-CGB-02B
26	XA	202	PEB	CAC-CBC-CGC-02C
26	SB	201	PEB	CAB-CBB-CGB-01B
26	TB	202	PEB	CAC-CBC-CGC-02C
26	UB	202	PEB	CAC-CBC-CGC-02C
26	WB	201	PEB	CAC-CBC-CGC-01C
26	WB	202	PEB	CAC-CBC-CGC-02C
26	IB	203	PEB	CAC-CBC-CGC-01C
26	CC	203	PEB	CAC-CBC-CGC-02C
26	DD	203	PEB	CAC-CBC-CGC-02C
26	GD	201	PEB	CAC-CBC-CGC-01C
26	RD	203	PEB	CAC-CBC-CGC-01C
26	TD	202	PEB	CAC-CBC-CGC-01C
26	VD	201	PEB	CAC-CBC-CGC-02C
26	RE	202	PEB	CAB-CBB-CGB-01B
26	UE	202	PEB	CAB-CBB-CGB-02B
26	ZE	201	PEB	CAB-CBB-CGB-02B
26	iE	202	PEB	CAC-CBC-CGC-02C
26	nE	201	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	tE	201	PEB	CAC-CBC-CGC-O2C
26	uE	203	PEB	CAC-CBC-CGC-O2C
26	uE	203	PEB	CAB-CBB-CGB-O1B
26	FF	1002	PEB	CAB-CBB-CGB-O2B
26	ZF	201	PEB	CAB-CBB-CGB-O1B
26	dF	203	PEB	CAB-CBB-CGB-O2B
26	iF	201	PEB	CAB-CBB-CGB-O1B
26	OG	202	PEB	CAC-CBC-CGC-O2C
26	cG	201	PEB	CAB-CBB-CGB-O2B
26	mG	201	PEB	CAC-CBC-CGC-O1C
26	tG	202	PEB	CAC-CBC-CGC-O2C
26	RI	203	PEB	CAC-CBC-CGC-O2C
26	UI	201	PEB	CAC-CBC-CGC-O1C
26	ZI	202	PEB	CAC-CBC-CGC-O2C
26	aI	203	PEB	CAC-CBC-CGC-O2C
26	dI	202	PEB	CAB-CBB-CGB-O1B
26	fI	201	PEB	CAB-CBB-CGB-O2B
26	fI	202	PEB	CAB-CBB-CGB-O1B
26	BJ	202	PEB	CAB-CBB-CGB-O1B
26	JJ	202	PEB	CAB-CBB-CGB-O1B
26	NJ	204	PEB	CAB-CBB-CGB-O1B
26	TJ	203	PEB	CAB-CBB-CGB-O1B
26	YJ	202	PEB	CAB-CBB-CGB-O2B
27	2I	403	PUB	CAB-CBB-CGB-O2B
28	H6	1001	CYC	CAD-CBD-CGD-O1D
28	L7	1001	CYC	CAD-CBD-CGD-O1D
28	EB	1001	CYC	CAA-CBA-CGA-O2A
26	a1	202	PEB	CAB-CBB-CGB-O2B
26	w1	203	PEB	CAB-CBB-CGB-O2B
26	y1	203	PEB	CAB-CBB-CGB-O1B
26	R2	203	PEB	CAC-CBC-CGC-O2C
26	b2	201	PEB	CAC-CBC-CGC-O1C
26	m2	201	PEB	CAB-CBB-CGB-O1B
26	D3	201	PEB	CAC-CBC-CGC-O1C
26	P3	201	PEB	CAC-CBC-CGC-O1C
26	R3	203	PEB	CAC-CBC-CGC-O1C
26	C4	202	PEB	CAB-CBB-CGB-O2B
26	F4	201	PEB	CAC-CBC-CGC-O2C
26	J4	203	PEB	CAC-CBC-CGC-O2C
26	K4	202	PEB	CAC-CBC-CGC-O2C
26	Q4	201	PEB	CAB-CBB-CGB-O2B
26	X4	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	Y4	201	PEB	CAB-CBB-CGB-O2B
26	14	201	PEB	CAB-CBB-CGB-O1B
26	A5	201	PEB	CAB-CBB-CGB-O2B
26	C5	204	PEB	CAB-CBB-CGB-O1B
26	R6	201	PEB	CAB-CBB-CGB-O1B
26	S6	202	PEB	CAB-CBB-CGB-O1B
26	m6	201	PEB	CAC-CBC-CGC-O2C
26	m6	203	PEB	CAB-CBB-CGB-O2B
26	U7	201	PEB	CAB-CBB-CGB-O1B
26	f7	202	PEB	CAB-CBB-CGB-O1B
26	N8	202	PEB	CAC-CBC-CGC-O2C
26	P8	202	PEB	CAB-CBB-CGB-O2B
26	U8	203	PEB	CAC-CBC-CGC-O2C
26	W8	202	PEB	CAB-CBB-CGB-O2B
26	a8	201	PEB	CAC-CBC-CGC-O2C
26	f8	202	PEB	CAB-CBB-CGB-O2B
26	B9	202	PEB	CAB-CBB-CGB-O1B
26	O9	201	PEB	CAB-CBB-CGB-O1B
26	PA	201	PEB	CAB-CBB-CGB-O2B
26	QA	203	PEB	CAC-CBC-CGC-O2C
26	YA	203	PEB	CAC-CBC-CGC-O2C
26	YB	202	PEB	CAC-CBC-CGC-O2C
26	bB	201	PEB	CAC-CBC-CGC-O1C
26	jB	201	PEB	CAC-CBC-CGC-O1C
26	eD	401	PEB	CAB-CBB-CGB-O1B
26	LD	203	PEB	CAC-CBC-CGC-O1C
26	ND	203	PEB	CAC-CBC-CGC-O2C
26	FE	202	PEB	CAC-CBC-CGC-O2C
26	QE	203	PEB	CAC-CBC-CGC-O2C
26	RE	201	PEB	CAB-CBB-CGB-O2B
26	XE	201	PEB	CAB-CBB-CGB-O2B
26	bE	201	PEB	CAC-CBC-CGC-O2C
26	lE	202	PEB	CAC-CBC-CGC-O1C
26	aF	201	PEB	CAC-CBC-CGC-O2C
26	eF	201	PEB	CAC-CBC-CGC-O2C
26	eF	202	PEB	CAB-CBB-CGB-O2B
26	lF	202	PEB	CAB-CBB-CGB-O2B
26	MG	203	PEB	CAB-CBB-CGB-O2B
26	RG	201	PEB	CAB-CBB-CGB-O2B
26	WG	201	PEB	CAC-CBC-CGC-O1C
26	aG	201	PEB	CAC-CBC-CGC-O2C
26	OI	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	RI	202	PEB	CAB-CBB-CGB-O2B
26	UI	202	PEB	CAC-CBC-CGC-O1C
26	IJ	201	PEB	CAB-CBB-CGB-O2B
26	QJ	202	PEB	CAC-CBC-CGC-O1C
27	A4	203	PUB	CAC-CBC-CGC-O1C
27	AA	304	PUB	CAC-CBC-CGC-O1C
28	B6	1001	CYC	CAD-CBD-CGD-O1D
28	E6	1001	CYC	CAA-CBA-CGA-O2A
28	1H	1000	CYC	CAA-CBA-CGA-O1A
26	j1	202	PEB	C4A-C3A-CAA-CBA
26	s1	201	PEB	C4A-C3A-CAA-CBA
26	z1	201	PEB	C4A-C3A-CAA-CBA
26	U2	202	PEB	C4A-C3A-CAA-CBA
26	k2	202	PEB	C4A-C3A-CAA-CBA
26	Y3	303	PEB	C4A-C3A-CAA-CBA
26	A4	202	PEB	C4A-C3A-CAA-CBA
26	D4	203	PEB	C4A-C3A-CAA-CBA
26	L6	1002	PEB	C4A-C3A-CAA-CBA
26	U6	202	PEB	C4A-C3A-CAA-CBA
26	Y7	201	PEB	C4A-C3A-CAA-CBA
26	A9	303	PEB	C4A-C3A-CAA-CBA
26	EA	201	PEB	C4A-C3A-CAA-CBA
26	BD	203	PEB	C4A-C3A-CAA-CBA
26	XD	203	PEB	C4A-C3A-CAA-CBA
26	YD	304	PEB	C4A-C3A-CAA-CBA
26	cE	203	PEB	C4A-C3A-CAA-CBA
26	OF	203	PEB	C4A-C3A-CAA-CBA
26	UF	203	PEB	C4A-C3A-CAA-CBA
26	fF	203	PEB	C4A-C3A-CAA-CBA
26	gF	201	PEB	C4A-C3A-CAA-CBA
26	jF	203	PEB	C4A-C3A-CAA-CBA
26	lF	203	PEB	C4A-C3A-CAA-CBA
26	JG	201	PEB	C4A-C3A-CAA-CBA
26	UG	202	PEB	C4A-C3A-CAA-CBA
26	WG	203	PEB	C4A-C3A-CAA-CBA
26	XG	201	PEB	C4A-C3A-CAA-CBA
26	sG	203	PEB	C4A-C3A-CAA-CBA
26	AJ	303	PEB	C4A-C3A-CAA-CBA
28	VH	1001	CYC	C4C-C3C-CAC-CBC
28	fH	1001	CYC	C4C-C3C-CAC-CBC
26	B1	201	PEB	C3B-CAB-CBB-CGB
26	H1	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	X1	203	PEB	C3B-CAB-CBB-CGB
26	x1	201	PEB	C3B-CAB-CBB-CGB
26	z1	202	PEB	C3B-CAB-CBB-CGB
26	m2	203	PEB	C3B-CAB-CBB-CGB
26	W3	201	PEB	C3B-CAB-CBB-CGB
26	C4	202	PEB	C3B-CAB-CBB-CGB
26	g4	201	PEB	C3B-CAB-CBB-CGB
26	g4	203	PEB	C3B-CAB-CBB-CGB
26	m4	201	PEB	C3B-CAB-CBB-CGB
26	B5	202	PEB	C3B-CAB-CBB-CGB
26	I5	201	PEB	C3B-CAB-CBB-CGB
26	S6	203	PEB	C3B-CAB-CBB-CGB
26	i6	201	PEB	C3B-CAB-CBB-CGB
26	O7	201	PEB	C3B-CAB-CBB-CGB
26	U8	202	PEB	C3B-CAB-CBB-CGB
26	IA	201	PEB	C3B-CAB-CBB-CGB
26	bB	201	PEB	C3B-CAB-CBB-CGB
26	lB	201	PEB	C3B-CAB-CBB-CGB
26	pE	201	PEB	C3B-CAB-CBB-CGB
26	sG	203	PEB	C3B-CAB-CBB-CGB
26	vG	202	PEB	C3B-CAB-CBB-CGB
26	RJ	203	PEB	C3B-CAB-CBB-CGB
26	TJ	201	PEB	C3B-CAB-CBB-CGB
26	E1	202	PEB	CAC-CBC-CGC-O2C
26	L1	202	PEB	CAC-CBC-CGC-O2C
26	X1	201	PEB	CAB-CBB-CGB-O1B
26	X1	202	PEB	CAC-CBC-CGC-O1C
26	e1	201	PEB	CAB-CBB-CGB-O2B
26	q1	201	PEB	CAB-CBB-CGB-O2B
26	y1	202	PEB	CAC-CBC-CGC-O2C
26	U2	201	PEB	CAC-CBC-CGC-O1C
26	L3	202	PEB	CAB-CBB-CGB-O1B
26	V3	203	PEB	CAB-CBB-CGB-O2B
26	X3	201	PEB	CAC-CBC-CGC-O2C
26	O4	201	PEB	CAB-CBB-CGB-O2B
26	p4	202	PEB	CAC-CBC-CGC-O1C
26	y4	203	PEB	CAB-CBB-CGB-O1B
26	L5	201	PEB	CAB-CBB-CGB-O2B
26	O6	203	PEB	CAC-CBC-CGC-O2C
26	S6	201	PEB	CAC-CBC-CGC-O2C
26	T6	202	PEB	CAC-CBC-CGC-O2C
26	W6	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	j6	201	PEB	CAC-CBC-CGC-O1C
26	N8	202	PEB	CAB-CBB-CGB-O2B
26	Q8	202	PEB	CAC-CBC-CGC-O1C
26	U8	203	PEB	CAB-CBB-CGB-O1B
26	W8	203	PEB	CAC-CBC-CGC-O1C
26	l8	202	PEB	CAC-CBC-CGC-O1C
26	K9	202	PEB	CAC-CBC-CGC-O2C
26	N9	204	PEB	CAB-CBB-CGB-O2B
26	R9	202	PEB	CAC-CBC-CGC-O1C
26	U9	201	PEB	CAB-CBB-CGB-O2B
26	AA	302	PEB	CAC-CBC-CGC-O2C
26	SA	202	PEB	CAC-CBC-CGC-O1C
26	UA	203	PEB	CAC-CBC-CGC-O2C
26	aA	201	PEB	CAC-CBC-CGC-O2C
26	bB	202	PEB	CAB-CBB-CGB-O2B
26	BC	201	PEB	CAC-CBC-CGC-O2C
26	JE	202	PEB	CAC-CBC-CGC-O2C
26	ME	203	PEB	CAB-CBB-CGB-O2B
26	PE	201	PEB	CAB-CBB-CGB-O2B
26	WE	203	PEB	CAC-CBC-CGC-O1C
26	XE	202	PEB	CAC-CBC-CGC-O2C
26	aE	201	PEB	CAC-CBC-CGC-O2C
26	lE	201	PEB	CAC-CBC-CGC-O1C
26	HF	1002	PEB	CAC-CBC-CGC-O2C
26	SF	202	PEB	CAC-CBC-CGC-O2C
26	gF	202	PEB	CAB-CBB-CGB-O2B
26	FG	202	PEB	CAC-CBC-CGC-O2C
26	XG	201	PEB	CAB-CBB-CGB-O2B
26	cG	201	PEB	CAC-CBC-CGC-O1C
26	eG	202	PEB	CAC-CBC-CGC-O2C
26	nG	201	PEB	CAB-CBB-CGB-O2B
26	vG	201	PEB	CAC-CBC-CGC-O1C
26	eI	202	PEB	CAB-CBB-CGB-O1B
26	HJ	201	PEB	CAC-CBC-CGC-O1C
26	HJ	203	PEB	CAC-CBC-CGC-O2C
26	UJ	201	PEB	CAB-CBB-CGB-O2B
27	AA	304	PUB	CAB-CBB-CGB-O1B
28	G6	1001	CYC	CAA-CBA-CGA-O2A
28	L7	1001	CYC	CAA-CBA-CGA-O1A
28	FF	1001	CYC	CAA-CBA-CGA-O1A
28	JF	1003	CYC	CAD-CBD-CGD-O1D
26	cA	201	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	A1	202	PEB	CAB-CBB-CGB-O1B
26	C1	202	PEB	CAC-CBC-CGC-O2C
26	V1	202	PEB	CAC-CBC-CGC-O2C
26	W1	201	PEB	CAB-CBB-CGB-O2B
26	Z1	202	PEB	CAB-CBB-CGB-O1B
26	h1	201	PEB	CAB-CBB-CGB-O1B
26	k1	202	PEB	CAC-CBC-CGC-O2C
26	u1	201	PEB	CAC-CBC-CGC-O1C
26	b2	202	PEB	CAC-CBC-CGC-O1C
26	F4	203	PEB	CAB-CBB-CGB-O1B
26	I4	202	PEB	CAC-CBC-CGC-O2C
26	I4	202	PEB	CAB-CBB-CGB-O2B
26	S4	201	PEB	CAC-CBC-CGC-O2C
26	W4	201	PEB	CAB-CBB-CGB-O2B
26	h4	202	PEB	CAB-CBB-CGB-O2B
26	k6	201	PEB	CAB-CBB-CGB-O2B
26	a7	201	PEB	CAC-CBC-CGC-O2C
26	J8	202	PEB	CAC-CBC-CGC-O2C
26	K8	203	PEB	CAC-CBC-CGC-O2C
26	R8	202	PEB	CAB-CBB-CGB-O2B
26	X8	202	PEB	CAB-CBB-CGB-O2B
26	h8	203	PEB	CAB-CBB-CGB-O2B
26	k8	202	PEB	CAB-CBB-CGB-O2B
26	N9	204	PEB	CAC-CBC-CGC-O2C
26	DA	201	PEB	CAB-CBB-CGB-O2B
26	KA	203	PEB	CAC-CBC-CGC-O2C
26	PA	202	PEB	CAB-CBB-CGB-O2B
26	SA	203	PEB	CAB-CBB-CGB-O2B
26	WA	203	PEB	CAC-CBC-CGC-O1C
26	fA	202	PEB	CAB-CBB-CGB-O2B
26	hA	203	PEB	CAB-CBB-CGB-O2B
26	PB	202	PEB	CAC-CBC-CGC-O2C
26	GC	201	PEB	CAB-CBB-CGB-O2B
26	MD	201	PEB	CAB-CBB-CGB-O2B
26	WD	201	PEB	CAC-CBC-CGC-O2C
26	XD	201	PEB	CAC-CBC-CGC-O2C
26	IE	202	PEB	CAC-CBC-CGC-O2C
26	UE	202	PEB	CAC-CBC-CGC-O2C
26	VE	201	PEB	CAC-CBC-CGC-O2C
26	aE	202	PEB	CAC-CBC-CGC-O2C
26	gE	202	PEB	CAC-CBC-CGC-O2C
26	vE	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	PF	202	PEB	CAB-CBB-CGB-O2B
26	BG	202	PEB	CAC-CBC-CGC-O2C
26	IG	202	PEB	CAC-CBC-CGC-O2C
26	LG	201	PEB	CAB-CBB-CGB-O2B
26	LG	202	PEB	CAB-CBB-CGB-O2B
26	OG	201	PEB	CAC-CBC-CGC-O1C
26	TG	201	PEB	CAC-CBC-CGC-O2C
26	UG	202	PEB	CAB-CBB-CGB-O2B
26	VG	201	PEB	CAC-CBC-CGC-O2C
26	YG	202	PEB	CAC-CBC-CGC-O2C
26	eG	201	PEB	CAC-CBC-CGC-O2C
26	gG	203	PEB	CAC-CBC-CGC-O2C
26	nG	202	PEB	CAB-CBB-CGB-O2B
26	sG	201	PEB	CAC-CBC-CGC-O2C
26	ZI	202	PEB	CAC-CBC-CGC-O1C
26	GJ	202	PEB	CAB-CBB-CGB-O2B
26	PJ	202	PEB	CAC-CBC-CGC-O1C
26	XJ	201	PEB	CAB-CBB-CGB-O1B
28	BB	1001	CYC	CAD-CBD-CGD-O1D
28	NH	1001	CYC	CAA-CBA-CGA-O2A
28	dH	1001	CYC	CAA-CBA-CGA-O2A
28	tH	1001	CYC	CAA-CBA-CGA-O1A
28	tH	1001	CYC	CAD-CBD-CGD-O2D
28	HI	1001	CYC	CAA-CBA-CGA-O2A
28	FB	1001	CYC	C2B-C3B-CAB-CBB
26	k2	202	PEB	C2B-C3B-CAB-CBB
26	C8	203	PEB	C2B-C3B-CAB-CBB
26	CA	203	PEB	C2B-C3B-CAB-CBB
28	dH	1001	CYC	C3A-C2A-CAA-CBA
26	B1	202	PEB	CAB-CBB-CGB-O2B
26	M1	402	PEB	CAC-CBC-CGC-O2C
26	O1	202	PEB	CAC-CBC-CGC-O2C
26	T1	201	PEB	CAC-CBC-CGC-O2C
26	U1	201	PEB	CAB-CBB-CGB-O2B
26	W1	201	PEB	CAB-CBB-CGB-O1B
26	c1	203	PEB	CAB-CBB-CGB-O1B
26	i1	201	PEB	CAC-CBC-CGC-O2C
26	u1	201	PEB	CAB-CBB-CGB-O1B
26	11	202	PEB	CAC-CBC-CGC-O2C
26	T2	201	PEB	CAC-CBC-CGC-O2C
26	d2	202	PEB	CAC-CBC-CGC-O1C
26	f2	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	Q3	202	PEB	CAB-CBB-CGB-O2B
26	W3	202	PEB	CAB-CBB-CGB-O2B
26	D4	201	PEB	CAC-CBC-CGC-O2C
26	G4	202	PEB	CAC-CBC-CGC-O2C
26	Z4	201	PEB	CAB-CBB-CGB-O2B
26	Z4	202	PEB	CAB-CBB-CGB-O2B
26	c4	201	PEB	CAB-CBB-CGB-O2B
26	g4	202	PEB	CAB-CBB-CGB-O2B
26	h4	201	PEB	CAB-CBB-CGB-O2B
26	s4	202	PEB	CAC-CBC-CGC-O1C
26	T6	202	PEB	CAB-CBB-CGB-O2B
26	i7	202	PEB	CAB-CBB-CGB-O2B
26	C8	203	PEB	CAC-CBC-CGC-O1C
26	H8	201	PEB	CAC-CBC-CGC-O2C
26	W8	201	PEB	CAC-CBC-CGC-O2C
26	e8	202	PEB	CAC-CBC-CGC-O1C
26	k8	201	PEB	CAC-CBC-CGC-O2C
26	C9	202	PEB	CAB-CBB-CGB-O2B
26	HA	201	PEB	CAC-CBC-CGC-O2C
26	NA	202	PEB	CAB-CBB-CGB-O2B
26	OA	203	PEB	CAC-CBC-CGC-O1C
26	PA	201	PEB	CAC-CBC-CGC-O2C
26	eA	202	PEB	CAB-CBB-CGB-O2B
26	lA	202	PEB	CAC-CBC-CGC-O1C
26	lA	203	PEB	CAB-CBB-CGB-O2B
26	SB	201	PEB	CAC-CBC-CGC-O2C
26	TB	202	PEB	CAB-CBB-CGB-O2B
26	ZB	201	PEB	CAC-CBC-CGC-O2C
26	dB	204	PEB	CAB-CBB-CGB-O1B
26	BC	202	PEB	CAC-CBC-CGC-O1C
26	DD	201	PEB	CAB-CBB-CGB-O1B
26	MD	202	PEB	CAB-CBB-CGB-O2B
26	VD	201	PEB	CAB-CBB-CGB-O2B
26	AE	202	PEB	CAC-CBC-CGC-O2C
26	CE	203	PEB	CAB-CBB-CGB-O1B
26	DE	202	PEB	CAB-CBB-CGB-O2B
26	FE	201	PEB	CAB-CBB-CGB-O1B
26	LE	201	PEB	CAB-CBB-CGB-O2B
26	PE	201	PEB	CAC-CBC-CGC-O2C
26	QE	201	PEB	CAC-CBC-CGC-O2C
26	oE	202	PEB	CAB-CBB-CGB-O1B
26	rE	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	WF	202	PEB	CAC-CBC-CGC-O2C
26	dF	201	PEB	CAC-CBC-CGC-O2C
26	JG	201	PEB	CAB-CBB-CGB-O2B
26	VG	201	PEB	CAC-CBC-CGC-O1C
26	VG	202	PEB	CAC-CBC-CGC-O1C
26	XG	203	PEB	CAC-CBC-CGC-O2C
26	XG	203	PEB	CAB-CBB-CGB-O2B
26	NI	1002	PEB	CAB-CBB-CGB-O2B
26	OI	201	PEB	CAC-CBC-CGC-O2C
26	PI	203	PEB	CAC-CBC-CGC-O2C
26	jI	202	PEB	CAB-CBB-CGB-O1B
26	CJ	202	PEB	CAB-CBB-CGB-O2B
26	JJ	201	PEB	CAB-CBB-CGB-O2B
28	IF	1001	CYC	CAA-CBA-CGA-O2A
28	eH	1001	CYC	CAA-CBA-CGA-O2A
27	24	403	PUB	C2D-C1D-CHC-C4C
27	yE	302	PUB	C2D-C1D-CHC-C4C
27	AF	304	PUB	C2D-C1D-CHC-C4C
26	F1	201	PEB	CAC-CBC-CGC-O1C
26	c1	201	PEB	CAB-CBB-CGB-O1B
26	k1	203	PEB	CAC-CBC-CGC-O1C
26	l1	202	PEB	CAB-CBB-CGB-O1B
26	z1	202	PEB	CAB-CBB-CGB-O1B
26	H2	1002	PEB	CAB-CBB-CGB-O1B
26	O2	201	PEB	CAC-CBC-CGC-O2C
26	b2	202	PEB	CAB-CBB-CGB-O2B
26	F3	202	PEB	CAB-CBB-CGB-O2B
26	N3	202	PEB	CAB-CBB-CGB-O1B
26	P3	202	PEB	CAB-CBB-CGB-O2B
26	F4	201	PEB	CAC-CBC-CGC-O1C
26	M4	402	PEB	CAC-CBC-CGC-O2C
26	Q4	201	PEB	CAB-CBB-CGB-O1B
26	X4	202	PEB	CAC-CBC-CGC-O1C
26	Z4	202	PEB	CAC-CBC-CGC-O1C
26	d4	201	PEB	CAB-CBB-CGB-O2B
26	g4	202	PEB	CAB-CBB-CGB-O1B
26	u4	201	PEB	CAB-CBB-CGB-O1B
26	14	203	PEB	CAB-CBB-CGB-O2B
26	24	401	PEB	CAC-CBC-CGC-O2C
26	T7	202	PEB	CAB-CBB-CGB-O1B
26	h7	202	PEB	CAB-CBB-CGB-O1B
26	C8	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	M8	203	PEB	CAB-CBB-CGB-O2B
26	P8	201	PEB	CAC-CBC-CGC-O1C
26	S8	203	PEB	CAB-CBB-CGB-O2B
26	DA	202	PEB	CAB-CBB-CGB-O1B
26	MA	203	PEB	CAB-CBB-CGB-O2B
26	NA	202	PEB	CAB-CBB-CGB-O1B
26	WA	201	PEB	CAC-CBC-CGC-O2C
26	eA	202	PEB	CAC-CBC-CGC-O1C
26	eA	202	PEB	CAB-CBB-CGB-O1B
26	fA	202	PEB	CAB-CBB-CGB-O1B
26	hA	203	PEB	CAB-CBB-CGB-O1B
26	HB	1002	PEB	CAB-CBB-CGB-O2B
26	dB	204	PEB	CAC-CBC-CGC-O1C
26	eB	203	PEB	CAC-CBC-CGC-O1C
26	mB	202	PEB	CAC-CBC-CGC-O2C
26	FC	203	PEB	CAC-CBC-CGC-O1C
26	LC	203	PEB	CAB-CBB-CGB-O2B
26	UD	202	PEB	CAB-CBB-CGB-O1B
26	BE	202	PEB	CAB-CBB-CGB-O1B
26	cE	201	PEB	CAB-CBB-CGB-O1B
26	hE	201	PEB	CAB-CBB-CGB-O2B
26	AF	301	PEB	CAB-CBB-CGB-O2B
26	cF	202	PEB	CAB-CBB-CGB-O1B
26	cF	202	PEB	CAB-CBB-CGB-O2B
26	eF	201	PEB	CAC-CBC-CGC-O1C
26	eF	202	PEB	CAB-CBB-CGB-O1B
26	jF	201	PEB	CAB-CBB-CGB-O2B
26	CG	201	PEB	CAC-CBC-CGC-O1C
26	QG	202	PEB	CAC-CBC-CGC-O1C
26	RG	202	PEB	CAC-CBC-CGC-O2C
26	SG	203	PEB	CAC-CBC-CGC-O2C
26	WG	202	PEB	CAB-CBB-CGB-O2B
26	mG	203	PEB	CAC-CBC-CGC-O2C
26	AI	305	PEB	CAC-CBC-CGC-O1C
26	DI	1002	PEB	CAB-CBB-CGB-O2B
26	QI	202	PEB	CAB-CBB-CGB-O1B
26	dI	201	PEB	CAC-CBC-CGC-O1C
26	hI	202	PEB	CAB-CBB-CGB-O2B
26	HJ	203	PEB	CAB-CBB-CGB-O1B
26	LJ	201	PEB	CAB-CBB-CGB-O2B
26	NJ	202	PEB	CAB-CBB-CGB-O2B
27	21	402	PUB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
27	21	402	PUB	CAB-CBB-CGB-01B
27	yE	303	PUB	CAB-CBB-CGB-01B
28	J7	1001	CYC	CAA-CBA-CGA-01A
28	DF	1003	CYC	CAA-CBA-CGA-02A
28	dH	1001	CYC	CAA-CBA-CGA-01A
28	pH	1001	CYC	CAA-CBA-CGA-01A
26	B1	202	PEB	CAB-CBB-CGB-01B
26	L1	203	PEB	CAC-CBC-CGC-02C
26	P1	201	PEB	CAB-CBB-CGB-01B
26	P1	203	PEB	CAB-CBB-CGB-01B
26	S1	201	PEB	CAB-CBB-CGB-01B
26	c1	201	PEB	CAB-CBB-CGB-02B
26	m1	203	PEB	CAB-CBB-CGB-01B
26	o1	501	PEB	CAB-CBB-CGB-02B
26	w1	201	PEB	CAB-CBB-CGB-02B
26	w1	202	PEB	CAC-CBC-CGC-01C
26	11	203	PEB	CAB-CBB-CGB-01B
26	O2	201	PEB	CAC-CBC-CGC-01C
26	a2	203	PEB	CAC-CBC-CGC-02C
26	C3	202	PEB	CAC-CBC-CGC-01C
26	K3	202	PEB	CAB-CBB-CGB-02B
26	P3	202	PEB	CAB-CBB-CGB-01B
26	M4	402	PEB	CAC-CBC-CGC-01C
26	U4	202	PEB	CAC-CBC-CGC-02C
26	C5	204	PEB	CAC-CBC-CGC-02C
26	F5	203	PEB	CAC-CBC-CGC-01C
26	F5	203	PEB	CAC-CBC-CGC-02C
26	H6	1002	PEB	CAB-CBB-CGB-02B
26	d6	204	PEB	CAC-CBC-CGC-01C
26	h6	201	PEB	CAC-CBC-CGC-01C
26	l6	203	PEB	CAC-CBC-CGC-01C
26	Q7	202	PEB	CAB-CBB-CGB-02B
26	i7	201	PEB	CAC-CBC-CGC-01C
26	I8	201	PEB	CAC-CBC-CGC-02C
26	L8	202	PEB	CAC-CBC-CGC-02C
26	k8	201	PEB	CAC-CBC-CGC-01C
26	L9	203	PEB	CAB-CBB-CGB-01B
26	N9	204	PEB	CAC-CBC-CGC-01C
26	AA	302	PEB	CAB-CBB-CGB-01B
26	CA	203	PEB	CAC-CBC-CGC-01C
26	KA	203	PEB	CAC-CBC-CGC-01C
26	WA	201	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	SB	202	PEB	CAB-CBB-CGB-01B
26	ZB	201	PEB	CAC-CBC-CGC-01C
26	AC	203	PEB	CAB-CBB-CGB-02B
26	LC	201	PEB	CAB-CBB-CGB-02B
26	ND	202	PEB	CAB-CBB-CGB-01B
26	QD	202	PEB	CAB-CBB-CGB-01B
26	LE	201	PEB	CAC-CBC-CGC-02C
26	RE	201	PEB	CAC-CBC-CGC-02C
26	SE	201	PEB	CAC-CBC-CGC-01C
26	UE	201	PEB	CAC-CBC-CGC-02C
26	aE	202	PEB	CAC-CBC-CGC-01C
26	gE	202	PEB	CAC-CBC-CGC-01C
26	nE	201	PEB	CAB-CBB-CGB-01B
26	vE	202	PEB	CAB-CBB-CGB-01B
26	vE	202	PEB	CAB-CBB-CGB-02B
26	LF	1002	PEB	CAB-CBB-CGB-01B
26	UF	201	PEB	CAB-CBB-CGB-01B
26	WF	202	PEB	CAC-CBC-CGC-01C
26	CG	201	PEB	CAC-CBC-CGC-02C
26	FG	201	PEB	CAB-CBB-CGB-01B
26	GG	203	PEB	CAC-CBC-CGC-02C
26	LG	202	PEB	CAB-CBB-CGB-01B
26	RG	201	PEB	CAC-CBC-CGC-02C
26	SG	203	PEB	CAC-CBC-CGC-01C
26	UG	202	PEB	CAC-CBC-CGC-01C
26	UG	202	PEB	CAC-CBC-CGC-02C
26	pG	202	PEB	CAB-CBB-CGB-02B
26	PI	201	PEB	CAB-CBB-CGB-02B
26	AJ	305	PEB	CAC-CBC-CGC-01C
26	BJ	203	PEB	CAC-CBC-CGC-02C
26	LJ	201	PEB	CAB-CBB-CGB-01B
26	RJ	201	PEB	CAB-CBB-CGB-02B
28	HB	1001	CYC	CAD-CBD-CGD-01D
28	IF	1001	CYC	CAA-CBA-CGA-01A
28	TH	1001	CYC	CAA-CBA-CGA-01A
28	TH	1001	CYC	CAA-CBA-CGA-02A
28	YH	1004	CYC	CAA-CBA-CGA-01A
28	tH	1001	CYC	CAD-CBD-CGD-01D
28	HI	1001	CYC	CAA-CBA-CGA-01A
28	YH	1004	CYC	C2B-C3B-CAB-CBB
26	RI	202	PEB	C4B-C3B-CAB-CBB
26	O1	202	PEB	CAB-CBB-CGB-01B

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Mol	Chain	Res	Type	Atoms
26	P1	203	PEB	CAB-CBB-CGB-O2B
26	U1	201	PEB	CAB-CBB-CGB-O1B
26	g1	202	PEB	CAB-CBB-CGB-O2B
26	v1	201	PEB	CAB-CBB-CGB-O1B
26	P2	201	PEB	CAB-CBB-CGB-O2B
26	S2	201	PEB	CAC-CBC-CGC-O1C
26	C3	202	PEB	CAC-CBC-CGC-O2C
26	N3	202	PEB	CAB-CBB-CGB-O2B
26	M4	403	PEB	CAB-CBB-CGB-O1B
26	c4	203	PEB	CAC-CBC-CGC-O1C
26	t4	202	PEB	CAB-CBB-CGB-O1B
26	24	401	PEB	CAC-CBC-CGC-O1C
26	L9	201	PEB	CAB-CBB-CGB-O1B
26	TA	201	PEB	CAC-CBC-CGC-O2C
26	aA	204	PEB	CAC-CBC-CGC-O1C
26	VB	202	PEB	CAC-CBC-CGC-O1C
26	HC	202	PEB	CAC-CBC-CGC-O1C
26	PD	202	PEB	CAB-CBB-CGB-O1B
26	QD	202	PEB	CAB-CBB-CGB-O2B
26	QE	201	PEB	CAC-CBC-CGC-O1C
26	SE	201	PEB	CAC-CBC-CGC-O2C
26	VE	201	PEB	CAC-CBC-CGC-O1C
26	aE	202	PEB	CAB-CBB-CGB-O1B
26	cE	201	PEB	CAB-CBB-CGB-O2B
26	QF	203	PEB	CAB-CBB-CGB-O1B
26	GG	203	PEB	CAC-CBC-CGC-O1C
26	QG	201	PEB	CAC-CBC-CGC-O2C
26	QG	202	PEB	CAC-CBC-CGC-O2C
26	RG	201	PEB	CAC-CBC-CGC-O1C
26	UG	201	PEB	CAC-CBC-CGC-O1C
26	YG	202	PEB	CAC-CBC-CGC-O1C
26	eG	203	PEB	CAC-CBC-CGC-O2C
26	fG	201	PEB	CAB-CBB-CGB-O1B
26	lG	201	PEB	CAB-CBB-CGB-O2B
26	sG	201	PEB	CAC-CBC-CGC-O1C
26	OI	201	PEB	CAC-CBC-CGC-O1C
26	cI	203	PEB	CAB-CBB-CGB-O1B
26	NJ	202	PEB	CAB-CBB-CGB-O1B
28	I6	1001	CYC	CAA-CBA-CGA-O2A
28	IB	1001	CYC	CAA-CBA-CGA-O2A
26	D1	202	PEB	CAC-CBC-CGC-O2C
26	M1	402	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	S1	201	PEB	CAC-CBC-CGC-O1C
26	S1	201	PEB	CAB-CBB-CGB-O2B
26	m1	203	PEB	CAB-CBB-CGB-O2B
26	21	401	PEB	CAC-CBC-CGC-O2C
26	S2	201	PEB	CAC-CBC-CGC-O2C
26	Y2	202	PEB	CAB-CBB-CGB-O1B
26	A3	201	PEB	CAC-CBC-CGC-O1C
26	B3	203	PEB	CAB-CBB-CGB-O2B
26	F3	202	PEB	CAB-CBB-CGB-O1B
26	Q3	202	PEB	CAB-CBB-CGB-O1B
26	G4	202	PEB	CAC-CBC-CGC-O1C
26	k4	201	PEB	CAB-CBB-CGB-O1B
26	k4	201	PEB	CAB-CBB-CGB-O2B
26	r4	201	PEB	CAB-CBB-CGB-O2B
26	14	203	PEB	CAB-CBB-CGB-O1B
26	H5	203	PEB	CAC-CBC-CGC-O1C
26	K8	203	PEB	CAC-CBC-CGC-O1C
26	h8	203	PEB	CAB-CBB-CGB-O1B
26	m8	201	PEB	CAB-CBB-CGB-O1B
26	E9	201	PEB	CAB-CBB-CGB-O2B
26	J9	201	PEB	CAB-CBB-CGB-O2B
26	L9	203	PEB	CAB-CBB-CGB-O2B
26	N9	204	PEB	CAB-CBB-CGB-O1B
26	T9	202	PEB	CAC-CBC-CGC-O1C
26	aA	204	PEB	CAC-CBC-CGC-O2C
26	kA	201	PEB	CAC-CBC-CGC-O1C
26	eB	203	PEB	CAC-CBC-CGC-O2C
26	BC	203	PEB	CAB-CBB-CGB-O1B
26	KC	203	PEB	CAC-CBC-CGC-O1C
26	KD	201	PEB	CAC-CBC-CGC-O2C
26	ND	202	PEB	CAB-CBB-CGB-O2B
26	PD	202	PEB	CAB-CBB-CGB-O2B
26	AE	202	PEB	CAC-CBC-CGC-O1C
26	QE	202	PEB	CAC-CBC-CGC-O1C
26	rE	201	PEB	CAC-CBC-CGC-O1C
26	rE	202	PEB	CAB-CBB-CGB-O1B
26	zE	501	PEB	CAC-CBC-CGC-O1C
26	UF	201	PEB	CAB-CBB-CGB-O2B
26	dF	201	PEB	CAC-CBC-CGC-O1C
26	JG	201	PEB	CAB-CBB-CGB-O1B
26	YG	201	PEB	CAC-CBC-CGC-O2C
26	aG	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	eG	201	PEB	CAC-CBC-CGC-O1C
26	kG	202	PEB	CAC-CBC-CGC-O1C
26	mG	203	PEB	CAB-CBB-CGB-O1B
26	nG	202	PEB	CAB-CBB-CGB-O1B
26	rG	202	PEB	CAC-CBC-CGC-O1C
26	GJ	202	PEB	CAB-CBB-CGB-O1B
28	H2	1001	CYC	CAA-CBA-CGA-O2A
28	C6	1001	CYC	CAA-CBA-CGA-O1A
28	NH	1001	CYC	CAA-CBA-CGA-O1A
28	gH	1001	CYC	CAA-CBA-CGA-O1A
28	mH	1001	CYC	CAA-CBA-CGA-O2A
28	pH	1001	CYC	CAA-CBA-CGA-O2A
26	D1	201	PEB	CAC-CBC-CGC-O1C
26	O1	202	PEB	CAB-CBB-CGB-O2B
26	l1	202	PEB	CAB-CBB-CGB-O2B
26	11	203	PEB	CAB-CBB-CGB-O2B
26	A3	201	PEB	CAC-CBC-CGC-O2C
26	O4	201	PEB	CAB-CBB-CGB-O1B
26	O4	202	PEB	CAC-CBC-CGC-O2C
26	S4	201	PEB	CAC-CBC-CGC-O1C
26	U4	201	PEB	CAB-CBB-CGB-O2B
26	Z4	201	PEB	CAB-CBB-CGB-O1B
26	h4	201	PEB	CAB-CBB-CGB-O1B
26	u4	201	PEB	CAB-CBB-CGB-O2B
26	P6	201	PEB	CAB-CBB-CGB-O1B
26	Z6	201	PEB	CAC-CBC-CGC-O1C
26	Z6	201	PEB	CAC-CBC-CGC-O2C
26	N8	202	PEB	CAB-CBB-CGB-O1B
26	T8	201	PEB	CAC-CBC-CGC-O2C
26	W8	201	PEB	CAC-CBC-CGC-O1C
26	h8	202	PEB	CAB-CBB-CGB-O2B
26	l8	203	PEB	CAB-CBB-CGB-O2B
26	A9	301	PEB	CAC-CBC-CGC-O2C
26	E9	202	PEB	CAC-CBC-CGC-O1C
26	J9	201	PEB	CAB-CBB-CGB-O1B
26	AA	302	PEB	CAB-CBB-CGB-O2B
26	PA	201	PEB	CAC-CBC-CGC-O1C
26	WA	202	PEB	CAB-CBB-CGB-O2B
26	eA	201	PEB	CAC-CBC-CGC-O2C
26	PB	201	PEB	CAB-CBB-CGB-O1B
26	SB	202	PEB	CAB-CBB-CGB-O2B
26	eD	401	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	HD	202	PEB	CAC-CBC-CGC-O2C
26	LD	202	PEB	CAB-CBB-CGB-O1B
26	IE	202	PEB	CAB-CBB-CGB-O2B
26	RE	201	PEB	CAC-CBC-CGC-O1C
26	RE	202	PEB	CAC-CBC-CGC-O2C
26	UE	202	PEB	CAC-CBC-CGC-O1C
26	hE	202	PEB	CAB-CBB-CGB-O2B
26	nE	201	PEB	CAB-CBB-CGB-O2B
26	pE	201	PEB	CAB-CBB-CGB-O1B
26	sE	202	PEB	CAB-CBB-CGB-O2B
26	ZF	202	PEB	CAC-CBC-CGC-O2C
26	DG	203	PEB	CAB-CBB-CGB-O1B
26	IG	202	PEB	CAC-CBC-CGC-O1C
26	XG	203	PEB	CAB-CBB-CGB-O1B
26	gG	203	PEB	CAC-CBC-CGC-O1C
26	hG	202	PEB	CAB-CBB-CGB-O2B
26	oG	201	PEB	CAC-CBC-CGC-O2C
26	SI	201	PEB	CAC-CBC-CGC-O2C
26	TI	201	PEB	CAC-CBC-CGC-O2C
26	YI	202	PEB	CAB-CBB-CGB-O1B
26	iI	201	PEB	CAC-CBC-CGC-O2C
26	JJ	201	PEB	CAB-CBB-CGB-O1B
27	2I	402	PUB	CAB-CBB-CGB-O2B
27	yE	303	PUB	CAB-CBB-CGB-O2B
28	L2	1001	CYC	CAA-CBA-CGA-O2A
28	K6	202	CYC	CAA-CBA-CGA-O1A
28	I7	1001	CYC	CAA-CBA-CGA-O1A
28	KB	202	CYC	CAA-CBA-CGA-O1A
28	HF	1001	CYC	CAA-CBA-CGA-O2A
28	JF	1001	CYC	CAA-CBA-CGA-O2A
28	vH	1001	CYC	CAA-CBA-CGA-O1A
26	U2	201	PEB	C3B-CAB-CBB-CGB
26	d6	202	PEB	C3B-CAB-CBB-CGB
26	X9	202	PEB	C3B-CAB-CBB-CGB
26	jB	201	PEB	C3B-CAB-CBB-CGB
26	JG	201	PEB	C3B-CAB-CBB-CGB
28	H6	1001	CYC	C2A-CAA-CBA-CGA
26	E1	202	PEB	CAB-CBB-CGB-O2B
26	O1	201	PEB	CAC-CBC-CGC-O2C
26	T1	201	PEB	CAC-CBC-CGC-O1C
26	Z1	202	PEB	CAC-CBC-CGC-O2C
26	g1	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	d2	201	PEB	CAC-CBC-CGC-O2C
26	d2	202	PEB	CAC-CBC-CGC-O2C
26	m2	202	PEB	CAB-CBB-CGB-O1B
26	T3	202	PEB	CAC-CBC-CGC-O1C
26	X3	202	PEB	CAC-CBC-CGC-O2C
26	D4	201	PEB	CAB-CBB-CGB-O1B
26	S4	201	PEB	CAB-CBB-CGB-O2B
26	U4	201	PEB	CAC-CBC-CGC-O1C
26	O6	201	PEB	CAC-CBC-CGC-O2C
26	T6	202	PEB	CAB-CBB-CGB-O1B
26	l6	201	PEB	CAC-CBC-CGC-O2C
26	a7	201	PEB	CAC-CBC-CGC-O1C
26	c7	202	PEB	CAB-CBB-CGB-O2B
26	h7	201	PEB	CAC-CBC-CGC-O2C
26	P8	201	PEB	CAC-CBC-CGC-O2C
26	L9	201	PEB	CAB-CBB-CGB-O2B
26	hA	202	PEB	CAB-CBB-CGB-O2B
26	lA	202	PEB	CAC-CBC-CGC-O2C
26	OB	201	PEB	CAC-CBC-CGC-O2C
26	RB	201	PEB	CAB-CBB-CGB-O1B
26	YB	201	PEB	CAB-CBB-CGB-O1B
26	CD	202	PEB	CAC-CBC-CGC-O2C
26	VD	202	PEB	CAC-CBC-CGC-O2C
26	XD	202	PEB	CAC-CBC-CGC-O2C
26	DE	202	PEB	CAB-CBB-CGB-O1B
26	IE	202	PEB	CAC-CBC-CGC-O1C
26	IE	202	PEB	CAB-CBB-CGB-O1B
26	KE	202	PEB	CAC-CBC-CGC-O1C
26	PE	202	PEB	CAC-CBC-CGC-O2C
26	ZF	202	PEB	CAC-CBC-CGC-O1C
26	LG	201	PEB	CAB-CBB-CGB-O1B
26	NG	201	PEB	CAB-CBB-CGB-O2B
26	PG	201	PEB	CAB-CBB-CGB-O2B
26	WG	202	PEB	CAC-CBC-CGC-O2C
26	fG	201	PEB	CAC-CBC-CGC-O2C
26	hG	202	PEB	CAB-CBB-CGB-O1B
26	nG	201	PEB	CAB-CBB-CGB-O1B
26	uG	202	PEB	CAB-CBB-CGB-O1B
26	HI	1002	PEB	CAB-CBB-CGB-O1B
27	A1	203	PUB	CAC-CBC-CGC-O1C
28	IB	1001	CYC	CAA-CBA-CGA-O1A
28	JF	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	NF	1001	CYC	CAD-CBD-CGD-O1D
28	MH	1001	CYC	CAA-CBA-CGA-O2A
28	mH	1001	CYC	CAA-CBA-CGA-O1A
26	E1	201	PEB	CAB-CBB-CGB-O2B
26	O1	202	PEB	CAC-CBC-CGC-O1C
26	21	401	PEB	CAC-CBC-CGC-O1C
26	T2	203	PEB	CAC-CBC-CGC-O1C
26	d2	201	PEB	CAC-CBC-CGC-O1C
26	e3	401	PEB	CAC-CBC-CGC-O2C
26	V3	203	PEB	CAB-CBB-CGB-O1B
26	X3	202	PEB	CAC-CBC-CGC-O1C
26	L4	203	PEB	CAC-CBC-CGC-O1C
26	T4	201	PEB	CAC-CBC-CGC-O1C
26	U4	201	PEB	CAC-CBC-CGC-O2C
26	t4	201	PEB	CAC-CBC-CGC-O1C
26	K5	202	PEB	CAC-CBC-CGC-O2C
26	K5	203	PEB	CAB-CBB-CGB-O1B
26	D6	1002	PEB	CAB-CBB-CGB-O2B
26	O6	201	PEB	CAC-CBC-CGC-O1C
26	S6	203	PEB	CAC-CBC-CGC-O2C
26	Y7	202	PEB	CAC-CBC-CGC-O2C
26	a7	201	PEB	CAB-CBB-CGB-O1B
26	Y8	203	PEB	CAB-CBB-CGB-O2B
26	F9	203	PEB	CAC-CBC-CGC-O1C
26	K9	202	PEB	CAB-CBB-CGB-O2B
26	BA	301	PEB	CAC-CBC-CGC-O1C
26	MA	202	PEB	CAC-CBC-CGC-O1C
26	TA	201	PEB	CAC-CBC-CGC-O1C
26	OB	201	PEB	CAC-CBC-CGC-O1C
26	PB	202	PEB	CAC-CBC-CGC-O1C
26	TB	202	PEB	CAB-CBB-CGB-O1B
26	SD	202	PEB	CAB-CBB-CGB-O1B
26	VD	201	PEB	CAB-CBB-CGB-O1B
26	AE	201	PEB	CAC-CBC-CGC-O2C
26	BE	201	PEB	CAB-CBB-CGB-O1B
26	GE	203	PEB	CAB-CBB-CGB-O2B
26	UE	203	PEB	CAC-CBC-CGC-O1C
26	WE	201	PEB	CAC-CBC-CGC-O1C
26	YE	202	PEB	CAC-CBC-CGC-O2C
26	fE	201	PEB	CAC-CBC-CGC-O2C
26	rE	201	PEB	CAB-CBB-CGB-O1B
26	AF	301	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	DF	1002	PEB	CAB-CBB-CGB-O1B
26	QF	201	PEB	CAC-CBC-CGC-O1C
26	WG	202	PEB	CAB-CBB-CGB-O1B
26	YG	201	PEB	CAC-CBC-CGC-O1C
26	aG	203	PEB	CAC-CBC-CGC-O2C
26	SI	201	PEB	CAC-CBC-CGC-O1C
26	gI	201	PEB	CAC-CBC-CGC-O2C
26	hI	201	PEB	CAB-CBB-CGB-O2B
26	IJ	202	PEB	CAC-CBC-CGC-O1C
26	LJ	203	PEB	CAB-CBB-CGB-O2B
26	WJ	202	PEB	CAC-CBC-CGC-O1C
28	I6	1001	CYC	CAA-CBA-CGA-O1A
28	DF	1003	CYC	CAA-CBA-CGA-O1A
26	Y2	201	PEB	C2C-CAC-CBC-CGC
26	Z2	202	PEB	C2C-CAC-CBC-CGC
26	H3	203	PEB	C2C-CAC-CBC-CGC
26	F4	203	PEB	C2C-CAC-CBC-CGC
26	H6	1002	PEB	C2C-CAC-CBC-CGC
26	V7	201	PEB	C2C-CAC-CBC-CGC
26	HE	201	PEB	C2C-CAC-CBC-CGC
26	E1	202	PEB	CAB-CBB-CGB-O1B
26	V2	202	PEB	CAB-CBB-CGB-O1B
26	f2	201	PEB	CAC-CBC-CGC-O1C
26	j2	202	PEB	CAB-CBB-CGB-O1B
26	S3	202	PEB	CAC-CBC-CGC-O2C
26	T3	202	PEB	CAB-CBB-CGB-O2B
26	O4	201	PEB	CAC-CBC-CGC-O2C
26	u4	201	PEB	CAC-CBC-CGC-O2C
26	d6	203	PEB	CAB-CBB-CGB-O2B
26	m6	202	PEB	CAC-CBC-CGC-O2C
26	R7	202	PEB	CAC-CBC-CGC-O2C
26	E8	201	PEB	CAC-CBC-CGC-O1C
26	M8	202	PEB	CAC-CBC-CGC-O1C
26	T8	202	PEB	CAB-CBB-CGB-O1B
26	A9	301	PEB	CAC-CBC-CGC-O1C
26	C9	202	PEB	CAB-CBB-CGB-O1B
26	M9	201	PEB	CAB-CBB-CGB-O2B
26	FA	202	PEB	CAB-CBB-CGB-O2B
26	RA	202	PEB	CAB-CBB-CGB-O1B
26	SA	203	PEB	CAB-CBB-CGB-O1B
26	XA	202	PEB	CAB-CBB-CGB-O2B
26	eA	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	DE	203	PEB	CAB-CBB-CGB-O1B
26	XE	202	PEB	CAB-CBB-CGB-O1B
26	vE	201	PEB	CAB-CBB-CGB-O2B
26	AF	301	PEB	CAC-CBC-CGC-O2C
26	YF	201	PEB	CAC-CBC-CGC-O2C
26	aF	201	PEB	CAB-CBB-CGB-O2B
26	kF	201	PEB	CAB-CBB-CGB-O2B
26	IG	202	PEB	CAB-CBB-CGB-O1B
26	qG	202	PEB	CAB-CBB-CGB-O1B
26	cI	203	PEB	CAB-CBB-CGB-O2B
26	hI	202	PEB	CAB-CBB-CGB-O1B
26	kI	201	PEB	CAC-CBC-CGC-O2C
26	mI	202	PEB	CAB-CBB-CGB-O1B
26	CJ	202	PEB	CAB-CBB-CGB-O1B
26	EJ	202	PEB	CAC-CBC-CGC-O1C
27	A1	203	PUB	CAC-CBC-CGC-O2C
27	21	403	PUB	CAB-CBB-CGB-O1B
27	xG	305	PUB	CAB-CBB-CGB-O1B
28	WH	1001	CYC	CAD-CBD-CGD-O2D
28	yH	1001	CYC	CAD-CBD-CGD-O2D
26	D1	201	PEB	CAB-CBB-CGB-O2B
26	Y1	201	PEB	CAC-CBC-CGC-O2C
26	Z1	202	PEB	CAC-CBC-CGC-O1C
26	l1	202	PEB	CAC-CBC-CGC-O2C
26	w1	201	PEB	CAB-CBB-CGB-O1B
26	b2	201	PEB	CAB-CBB-CGB-O2B
26	H3	202	PEB	CAC-CBC-CGC-O1C
26	J3	203	PEB	CAC-CBC-CGC-O1C
26	R3	202	PEB	CAB-CBB-CGB-O2B
26	T4	202	PEB	CAB-CBB-CGB-O2B
26	m4	203	PEB	CAB-CBB-CGB-O2B
26	q4	202	PEB	CAC-CBC-CGC-O1C
26	t4	201	PEB	CAB-CBB-CGB-O2B
26	z4	201	PEB	CAB-CBB-CGB-O1B
26	l6	201	PEB	CAC-CBC-CGC-O1C
26	A8	302	PEB	CAB-CBB-CGB-O2B
26	A9	301	PEB	CAB-CBB-CGB-O1B
26	DA	201	PEB	CAB-CBB-CGB-O1B
26	YA	203	PEB	CAB-CBB-CGB-O2B
26	mA	201	PEB	CAB-CBB-CGB-O2B
26	DB	1002	PEB	CAB-CBB-CGB-O2B
26	iB	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	mB	203	PEB	CAC-CBC-CGC-O2C
26	KD	201	PEB	CAC-CBC-CGC-O1C
26	WD	202	PEB	CAB-CBB-CGB-O2B
26	AE	201	PEB	CAC-CBC-CGC-O1C
26	IE	201	PEB	CAB-CBB-CGB-O2B
26	hE	202	PEB	CAB-CBB-CGB-O1B
26	jE	201	PEB	CAB-CBB-CGB-O2B
26	pE	202	PEB	CAB-CBB-CGB-O2B
26	HF	1002	PEB	CAB-CBB-CGB-O2B
26	YF	202	PEB	CAC-CBC-CGC-O2C
26	fF	201	PEB	CAB-CBB-CGB-O2B
26	VG	201	PEB	CAB-CBB-CGB-O2B
26	eG	203	PEB	CAC-CBC-CGC-O1C
26	oG	201	PEB	CAC-CBC-CGC-O1C
26	JI	1002	PEB	CAB-CBB-CGB-O2B
27	K4	203	PUB	CAC-CBC-CGC-O2C
28	UH	1001	CYC	CAA-CBA-CGA-O2A
28	LI	1001	CYC	CAA-CBA-CGA-O2A
26	u1	201	PEB	CAC-CBC-CGC-O2C
26	z1	201	PEB	CAB-CBB-CGB-O2B
26	N2	1002	PEB	CAB-CBB-CGB-O1B
26	Z2	202	PEB	CAB-CBB-CGB-O2B
26	g2	201	PEB	CAC-CBC-CGC-O2C
26	W3	202	PEB	CAB-CBB-CGB-O1B
26	W4	201	PEB	CAB-CBB-CGB-O1B
26	Y4	201	PEB	CAC-CBC-CGC-O2C
26	d4	201	PEB	CAB-CBB-CGB-O1B
26	q4	203	PEB	CAB-CBB-CGB-O2B
26	t4	201	PEB	CAC-CBC-CGC-O2C
26	z4	201	PEB	CAB-CBB-CGB-O2B
26	L5	201	PEB	CAB-CBB-CGB-O1B
26	H6	1002	PEB	CAB-CBB-CGB-O1B
26	S6	202	PEB	CAC-CBC-CGC-O2C
26	h6	203	PEB	CAB-CBB-CGB-O2B
26	T7	201	PEB	CAB-CBB-CGB-O1B
26	F8	202	PEB	CAB-CBB-CGB-O2B
26	M8	202	PEB	CAC-CBC-CGC-O2C
26	S8	203	PEB	CAB-CBB-CGB-O1B
26	T8	201	PEB	CAC-CBC-CGC-O1C
26	d8	203	PEB	CAB-CBB-CGB-O2B
26	M9	201	PEB	CAB-CBB-CGB-O1B
26	BA	301	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	MA	202	PEB	CAC-CBC-CGC-O2C
26	PA	201	PEB	CAB-CBB-CGB-O1B
26	UA	201	PEB	CAC-CBC-CGC-O2C
26	SB	203	PEB	CAC-CBC-CGC-O2C
26	dB	201	PEB	CAC-CBC-CGC-O2C
26	iB	202	PEB	CAC-CBC-CGC-O1C
26	mB	202	PEB	CAC-CBC-CGC-O1C
26	BC	202	PEB	CAB-CBB-CGB-O2B
26	JD	203	PEB	CAC-CBC-CGC-O1C
26	PE	201	PEB	CAC-CBC-CGC-O1C
26	UE	203	PEB	CAC-CBC-CGC-O2C
26	XE	202	PEB	CAB-CBB-CGB-O2B
26	hE	201	PEB	CAB-CBB-CGB-O1B
26	uE	203	PEB	CAB-CBB-CGB-O2B
26	OF	203	PEB	CAB-CBB-CGB-O2B
26	jF	201	PEB	CAB-CBB-CGB-O1B
26	BG	202	PEB	CAB-CBB-CGB-O1B
26	DG	202	PEB	CAC-CBC-CGC-O2C
26	JG	202	PEB	CAC-CBC-CGC-O2C
26	PG	201	PEB	CAC-CBC-CGC-O2C
26	RG	202	PEB	CAC-CBC-CGC-O1C
26	UG	201	PEB	CAC-CBC-CGC-O2C
26	fG	201	PEB	CAC-CBC-CGC-O1C
26	jG	201	PEB	CAB-CBB-CGB-O2B
26	gI	202	PEB	CAC-CBC-CGC-O1C
26	iI	203	PEB	CAB-CBB-CGB-O2B
26	IJ	202	PEB	CAC-CBC-CGC-O2C
26	KJ	202	PEB	CAB-CBB-CGB-O2B
26	LJ	203	PEB	CAB-CBB-CGB-O1B
27	24	403	PUB	CAB-CBB-CGB-O2B
27	KD	203	PUB	CAB-CBB-CGB-O2B
28	G7	1001	CYC	CAA-CBA-CGA-O2A
28	K7	1001	CYC	CAA-CBA-CGA-O2A
28	oH	1001	CYC	CAA-CBA-CGA-O2A
26	O1	201	PEB	CAB-CBB-CGB-O2B
26	U1	201	PEB	CAC-CBC-CGC-O2C
26	t1	202	PEB	CAB-CBB-CGB-O1B
26	t1	202	PEB	CAB-CBB-CGB-O2B
26	z1	201	PEB	CAB-CBB-CGB-O1B
26	Q2	201	PEB	CAB-CBB-CGB-O1B
26	S2	202	PEB	CAC-CBC-CGC-O2C
26	Y2	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	c2	203	PEB	CAB-CBB-CGB-01B
26	k2	202	PEB	CAC-CBC-CGC-01C
26	H3	202	PEB	CAC-CBC-CGC-02C
26	L3	201	PEB	CAC-CBC-CGC-02C
26	S4	201	PEB	CAB-CBB-CGB-01B
26	U4	201	PEB	CAB-CBB-CGB-01B
26	X4	201	PEB	CAC-CBC-CGC-01C
26	m4	203	PEB	CAB-CBB-CGB-01B
26	Z7	201	PEB	CAB-CBB-CGB-01B
26	Z7	201	PEB	CAB-CBB-CGB-02B
26	b7	201	PEB	CAC-CBC-CGC-01C
26	b7	201	PEB	CAC-CBC-CGC-02C
26	c7	202	PEB	CAB-CBB-CGB-01B
26	R8	202	PEB	CAC-CBC-CGC-02C
26	T8	202	PEB	CAB-CBB-CGB-02B
26	W8	202	PEB	CAB-CBB-CGB-01B
26	d8	203	PEB	CAB-CBB-CGB-01B
26	f8	202	PEB	CAB-CBB-CGB-01B
26	C9	202	PEB	CAC-CBC-CGC-01C
26	F9	201	PEB	CAC-CBC-CGC-01C
26	F9	203	PEB	CAC-CBC-CGC-02C
26	K9	202	PEB	CAB-CBB-CGB-01B
26	X9	201	PEB	CAB-CBB-CGB-02B
26	RA	202	PEB	CAB-CBB-CGB-02B
26	HB	1002	PEB	CAB-CBB-CGB-01B
26	UB	202	PEB	CAB-CBB-CGB-01B
26	dB	203	PEB	CAB-CBB-CGB-02B
26	CC	201	PEB	CAB-CBB-CGB-01B
26	CC	201	PEB	CAB-CBB-CGB-02B
26	GC	201	PEB	CAB-CBB-CGB-01B
26	eD	401	PEB	CAC-CBC-CGC-01C
26	CD	202	PEB	CAC-CBC-CGC-01C
26	HD	202	PEB	CAC-CBC-CGC-01C
26	LD	201	PEB	CAB-CBB-CGB-01B
26	XD	201	PEB	CAC-CBC-CGC-01C
26	XD	202	PEB	CAC-CBC-CGC-01C
26	PE	201	PEB	CAB-CBB-CGB-01B
26	PE	202	PEB	CAC-CBC-CGC-01C
26	RE	201	PEB	CAB-CBB-CGB-01B
26	RE	202	PEB	CAC-CBC-CGC-01C
26	VE	202	PEB	CAC-CBC-CGC-02C
26	bE	201	PEB	CAB-CBB-CGB-01B

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Mol	Chain	Res	Type	Atoms
26	NG	201	PEB	CAB-CBB-CGB-O1B
26	PG	201	PEB	CAB-CBB-CGB-O1B
26	PG	202	PEB	CAC-CBC-CGC-O1C
26	PG	202	PEB	CAC-CBC-CGC-O2C
26	QG	201	PEB	CAC-CBC-CGC-O1C
26	VG	201	PEB	CAB-CBB-CGB-O1B
26	aG	202	PEB	CAC-CBC-CGC-O2C
26	jG	202	PEB	CAC-CBC-CGC-O2C
26	nG	202	PEB	CAC-CBC-CGC-O2C
26	QI	201	PEB	CAB-CBB-CGB-O2B
26	SI	202	PEB	CAC-CBC-CGC-O2C
26	TI	203	PEB	CAC-CBC-CGC-O1C
26	YI	202	PEB	CAC-CBC-CGC-O1C
26	ZI	202	PEB	CAB-CBB-CGB-O2B
26	dI	202	PEB	CAC-CBC-CGC-O1C
26	MJ	202	PEB	CAB-CBB-CGB-O1B
26	VJ	202	PEB	CAB-CBB-CGB-O1B
27	AB	303	PUB	CAB-CBB-CGB-O2B
28	PH	1001	CYC	CAA-CBA-CGA-O1A
28	gH	1001	CYC	CAD-CBD-CGD-O2D
26	a6	202	PEB	C2B-C3B-CAB-CBB
26	cE	203	PEB	C2B-C3B-CAB-CBB
26	kI	202	PEB	C2B-C3B-CAB-CBB
26	J1	201	PEB	CAB-CBB-CGB-O1B
26	L1	203	PEB	CAC-CBC-CGC-O1C
26	M1	402	PEB	CAB-CBB-CGB-O2B
26	Q1	201	PEB	CAB-CBB-CGB-O1B
26	T1	202	PEB	CAB-CBB-CGB-O2B
26	U1	201	PEB	CAC-CBC-CGC-O1C
26	V1	203	PEB	CAC-CBC-CGC-O2C
26	g1	201	PEB	CAB-CBB-CGB-O1B
26	q1	203	PEB	CAC-CBC-CGC-O2C
26	t1	201	PEB	CAC-CBC-CGC-O2C
26	P2	201	PEB	CAB-CBB-CGB-O1B
26	U2	202	PEB	CAB-CBB-CGB-O1B
26	V2	202	PEB	CAC-CBC-CGC-O2C
26	Z2	202	PEB	CAB-CBB-CGB-O1B
26	i2	201	PEB	CAC-CBC-CGC-O1C
26	j2	201	PEB	CAB-CBB-CGB-O2B
26	e3	401	PEB	CAC-CBC-CGC-O1C
26	J3	202	PEB	CAC-CBC-CGC-O2C
26	K3	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	L3	201	PEB	CAC-CBC-CGC-O1C
26	M3	202	PEB	CAB-CBB-CGB-O2B
26	H4	202	PEB	CAB-CBB-CGB-O1B
26	O4	201	PEB	CAC-CBC-CGC-O1C
26	Z4	202	PEB	CAB-CBB-CGB-O1B
26	c4	201	PEB	CAB-CBB-CGB-O1B
26	l4	202	PEB	CAB-CBB-CGB-O1B
26	l4	202	PEB	CAB-CBB-CGB-O2B
26	q4	203	PEB	CAB-CBB-CGB-O1B
26	B5	203	PEB	CAB-CBB-CGB-O2B
26	G5	202	PEB	CAB-CBB-CGB-O2B
26	D6	1002	PEB	CAB-CBB-CGB-O1B
26	O6	203	PEB	CAC-CBC-CGC-O1C
26	a6	202	PEB	CAC-CBC-CGC-O1C
26	N7	1002	PEB	CAB-CBB-CGB-O1B
26	N7	1002	PEB	CAB-CBB-CGB-O2B
26	P7	201	PEB	CAB-CBB-CGB-O1B
26	S7	203	PEB	CAC-CBC-CGC-O1C
26	S7	203	PEB	CAC-CBC-CGC-O2C
26	R8	202	PEB	CAC-CBC-CGC-O1C
26	e8	201	PEB	CAC-CBC-CGC-O2C
26	U9	201	PEB	CAB-CBB-CGB-O1B
26	FA	202	PEB	CAB-CBB-CGB-O1B
26	GA	203	PEB	CAC-CBC-CGC-O1C
26	GA	203	PEB	CAC-CBC-CGC-O2C
26	QA	202	PEB	CAC-CBC-CGC-O1C
26	TA	202	PEB	CAB-CBB-CGB-O1B
26	XA	202	PEB	CAB-CBB-CGB-O1B
26	mA	201	PEB	CAB-CBB-CGB-O1B
26	UB	202	PEB	CAB-CBB-CGB-O2B
26	VB	201	PEB	CAC-CBC-CGC-O1C
26	eB	203	PEB	CAB-CBB-CGB-O1B
26	DD	201	PEB	CAC-CBC-CGC-O1C
26	KD	202	PEB	CAB-CBB-CGB-O1B
26	LD	201	PEB	CAB-CBB-CGB-O2B
26	TD	202	PEB	CAB-CBB-CGB-O2B
26	VD	203	PEB	CAB-CBB-CGB-O2B
26	DE	201	PEB	CAC-CBC-CGC-O2C
26	GE	201	PEB	CAB-CBB-CGB-O1B
26	KE	202	PEB	CAC-CBC-CGC-O2C
26	LE	202	PEB	CAB-CBB-CGB-O1B
26	NE	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	bE	201	PEB	CAC-CBC-CGC-O1C
26	bE	201	PEB	CAB-CBB-CGB-O2B
26	fE	201	PEB	CAC-CBC-CGC-O1C
26	pE	202	PEB	CAC-CBC-CGC-O1C
26	uE	202	PEB	CAC-CBC-CGC-O1C
26	uE	202	PEB	CAB-CBB-CGB-O2B
26	AF	301	PEB	CAC-CBC-CGC-O1C
26	QF	201	PEB	CAC-CBC-CGC-O2C
26	TF	202	PEB	CAB-CBB-CGB-O2B
26	VF	202	PEB	CAB-CBB-CGB-O1B
26	VF	202	PEB	CAB-CBB-CGB-O2B
26	YF	201	PEB	CAC-CBC-CGC-O1C
26	fF	202	PEB	CAB-CBB-CGB-O2B
26	mF	202	PEB	CAB-CBB-CGB-O1B
26	mF	202	PEB	CAB-CBB-CGB-O2B
26	BG	202	PEB	CAC-CBC-CGC-O1C
26	DG	201	PEB	CAC-CBC-CGC-O1C
26	DG	201	PEB	CAC-CBC-CGC-O2C
26	GG	201	PEB	CAB-CBB-CGB-O1B
26	IG	201	PEB	CAB-CBB-CGB-O2B
26	MG	203	PEB	CAB-CBB-CGB-O1B
26	ZG	201	PEB	CAC-CBC-CGC-O2C
26	aG	202	PEB	CAC-CBC-CGC-O1C
26	iG	202	PEB	CAB-CBB-CGB-O1B
26	iG	202	PEB	CAB-CBB-CGB-O2B
26	UI	202	PEB	CAB-CBB-CGB-O1B
26	ZI	202	PEB	CAB-CBB-CGB-O1B
26	dI	202	PEB	CAC-CBC-CGC-O2C
26	gI	201	PEB	CAC-CBC-CGC-O1C
26	iI	201	PEB	CAC-CBC-CGC-O1C
26	jI	201	PEB	CAB-CBB-CGB-O2B
26	EJ	201	PEB	CAB-CBB-CGB-O1B
26	JJ	201	PEB	CAC-CBC-CGC-O1C
26	UJ	201	PEB	CAB-CBB-CGB-O1B
26	VJ	202	PEB	CAB-CBB-CGB-O2B
26	YJ	201	PEB	CAC-CBC-CGC-O1C
26	YJ	201	PEB	CAC-CBC-CGC-O2C
27	A2	303	PUB	CAC-CBC-CGC-O1C
27	AB	303	PUB	CAB-CBB-CGB-O1B
28	H2	1001	CYC	CAA-CBA-CGA-O1A
28	L2	1001	CYC	CAA-CBA-CGA-O1A
28	HF	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	LF	1001	CYC	CAA-CBA-CGA-O1A
28	rH	1001	CYC	CAA-CBA-CGA-O1A
26	T3	203	PEB	C4B-C3B-CAB-CBB
28	cH	1001	CYC	C1A-C2A-CAA-CBA
26	J1	201	PEB	CAB-CBB-CGB-O2B
26	N1	203	PEB	CAC-CBC-CGC-O2C
26	O1	201	PEB	CAC-CBC-CGC-O1C
26	Q1	201	PEB	CAB-CBB-CGB-O2B
26	R1	201	PEB	CAB-CBB-CGB-O2B
26	X1	201	PEB	CAC-CBC-CGC-O1C
26	X1	201	PEB	CAB-CBB-CGB-O2B
26	l1	202	PEB	CAC-CBC-CGC-O1C
26	q1	201	PEB	CAB-CBB-CGB-O1B
26	q1	203	PEB	CAC-CBC-CGC-O1C
26	l1	202	PEB	CAC-CBC-CGC-O1C
26	S2	202	PEB	CAC-CBC-CGC-O1C
26	T2	201	PEB	CAC-CBC-CGC-O1C
26	U2	202	PEB	CAB-CBB-CGB-O2B
26	Y2	202	PEB	CAC-CBC-CGC-O2C
26	i2	201	PEB	CAC-CBC-CGC-O2C
26	J3	202	PEB	CAC-CBC-CGC-O1C
26	J3	203	PEB	CAC-CBC-CGC-O2C
26	R3	202	PEB	CAB-CBB-CGB-O1B
26	T3	202	PEB	CAB-CBB-CGB-O1B
26	H4	202	PEB	CAB-CBB-CGB-O2B
26	O4	202	PEB	CAC-CBC-CGC-O1C
26	T4	202	PEB	CAB-CBB-CGB-O1B
26	Y4	201	PEB	CAC-CBC-CGC-O1C
26	h4	202	PEB	CAB-CBB-CGB-O1B
26	l4	201	PEB	CAB-CBB-CGB-O1B
26	l4	201	PEB	CAC-CBC-CGC-O1C
26	l4	201	PEB	CAC-CBC-CGC-O2C
26	A5	201	PEB	CAB-CBB-CGB-O1B
26	S6	202	PEB	CAC-CBC-CGC-O1C
26	V6	201	PEB	CAC-CBC-CGC-O1C
26	Y6	201	PEB	CAB-CBB-CGB-O2B
26	a6	202	PEB	CAC-CBC-CGC-O2C
26	b6	201	PEB	CAC-CBC-CGC-O2C
26	L7	1002	PEB	CAB-CBB-CGB-O1B
26	R7	202	PEB	CAC-CBC-CGC-O1C
26	Z7	202	PEB	CAC-CBC-CGC-O2C
26	a7	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	j7	201	PEB	CAB-CBB-CGB-O1B
26	j7	201	PEB	CAB-CBB-CGB-O2B
26	A8	302	PEB	CAB-CBB-CGB-O1B
26	B8	301	PEB	CAC-CBC-CGC-O1C
26	B8	301	PEB	CAC-CBC-CGC-O2C
26	h8	202	PEB	CAB-CBB-CGB-O1B
26	F9	201	PEB	CAC-CBC-CGC-O2C
26	H9	201	PEB	CAC-CBC-CGC-O1C
26	H9	201	PEB	CAC-CBC-CGC-O2C
26	I9	202	PEB	CAC-CBC-CGC-O1C
26	R9	203	PEB	CAB-CBB-CGB-O2B
26	X9	201	PEB	CAB-CBB-CGB-O1B
26	TA	202	PEB	CAB-CBB-CGB-O2B
26	UA	201	PEB	CAC-CBC-CGC-O1C
26	WA	202	PEB	CAB-CBB-CGB-O1B
26	hA	202	PEB	CAB-CBB-CGB-O1B
26	SB	203	PEB	CAC-CBC-CGC-O1C
26	dB	201	PEB	CAC-CBC-CGC-O1C
26	lB	201	PEB	CAC-CBC-CGC-O1C
26	mB	203	PEB	CAC-CBC-CGC-O1C
26	KD	202	PEB	CAB-CBB-CGB-O2B
26	MD	202	PEB	CAB-CBB-CGB-O1B
26	ND	202	PEB	CAC-CBC-CGC-O1C
26	VD	203	PEB	CAB-CBB-CGB-O1B
26	GE	201	PEB	CAB-CBB-CGB-O2B
26	LE	201	PEB	CAB-CBB-CGB-O1B
26	NE	201	PEB	CAB-CBB-CGB-O2B
26	VE	202	PEB	CAC-CBC-CGC-O1C
26	YE	202	PEB	CAC-CBC-CGC-O1C
26	ZE	201	PEB	CAB-CBB-CGB-O1B
26	jE	202	PEB	CAC-CBC-CGC-O1C
26	jE	202	PEB	CAC-CBC-CGC-O2C
26	pE	202	PEB	CAC-CBC-CGC-O2C
26	PF	201	PEB	CAB-CBB-CGB-O1B
26	fF	202	PEB	CAB-CBB-CGB-O1B
26	iF	202	PEB	CAB-CBB-CGB-O1B
26	iF	202	PEB	CAB-CBB-CGB-O2B
26	FG	202	PEB	CAB-CBB-CGB-O2B
26	GG	201	PEB	CAB-CBB-CGB-O2B
26	IG	201	PEB	CAB-CBB-CGB-O1B
26	RG	201	PEB	CAB-CBB-CGB-O1B
26	WG	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	cG	202	PEB	CAB-CBB-CGB-O1B
26	cG	202	PEB	CAB-CBB-CGB-O2B
26	hG	201	PEB	CAB-CBB-CGB-O2B
26	iG	201	PEB	CAC-CBC-CGC-O1C
26	NI	1002	PEB	CAB-CBB-CGB-O1B
26	PI	201	PEB	CAB-CBB-CGB-O1B
26	QI	201	PEB	CAB-CBB-CGB-O1B
26	QI	202	PEB	CAC-CBC-CGC-O2C
26	SI	202	PEB	CAC-CBC-CGC-O1C
26	UI	202	PEB	CAB-CBB-CGB-O2B
26	YI	202	PEB	CAC-CBC-CGC-O2C
26	iI	203	PEB	CAB-CBB-CGB-O1B
26	AJ	301	PEB	CAC-CBC-CGC-O2C
26	EJ	201	PEB	CAB-CBB-CGB-O2B
26	KJ	202	PEB	CAB-CBB-CGB-O1B
26	MJ	202	PEB	CAB-CBB-CGB-O2B
28	G7	1001	CYC	CAA-CBA-CGA-O1A
28	G7	1001	CYC	CAD-CBD-CGD-O1D
28	K7	1001	CYC	CAA-CBA-CGA-O1A
28	DF	1003	CYC	CAD-CBD-CGD-O1D
28	PH	1001	CYC	CAA-CBA-CGA-O2A
28	RH	1001	CYC	CAA-CBA-CGA-O1A
28	RH	1001	CYC	CAA-CBA-CGA-O2A
26	d4	202	PEB	C3B-CAB-CBB-CGB
26	GA	203	PEB	C3B-CAB-CBB-CGB
26	fE	201	PEB	C3B-CAB-CBB-CGB
26	jF	202	PEB	C3B-CAB-CBB-CGB
28	oH	1001	CYC	C2A-CAA-CBA-CGA
26	D1	202	PEB	CAC-CBC-CGC-O1C
26	O1	201	PEB	CAB-CBB-CGB-O1B
26	R1	203	PEB	CAC-CBC-CGC-O1C
26	g1	201	PEB	CAB-CBB-CGB-O2B
26	m1	202	PEB	CAB-CBB-CGB-O1B
26	m1	202	PEB	CAB-CBB-CGB-O2B
26	Q2	201	PEB	CAB-CBB-CGB-O2B
26	g2	201	PEB	CAC-CBC-CGC-O1C
26	X3	201	PEB	CAC-CBC-CGC-O1C
26	E4	201	PEB	CAB-CBB-CGB-O2B
26	L4	203	PEB	CAC-CBC-CGC-O2C
26	u4	201	PEB	CAC-CBC-CGC-O1C
26	Y7	202	PEB	CAC-CBC-CGC-O1C
26	F8	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	k8	202	PEB	CAB-CBB-CGB-O1B
26	R9	203	PEB	CAB-CBB-CGB-O1B
26	DB	1002	PEB	CAB-CBB-CGB-O1B
26	lB	201	PEB	CAC-CBC-CGC-O2C
26	BC	202	PEB	CAB-CBB-CGB-O1B
26	TD	202	PEB	CAB-CBB-CGB-O1B
26	DE	201	PEB	CAC-CBC-CGC-O1C
26	IE	201	PEB	CAB-CBB-CGB-O1B
26	JE	201	PEB	CAC-CBC-CGC-O2C
26	LE	202	PEB	CAB-CBB-CGB-O2B
26	uE	202	PEB	CAC-CBC-CGC-O2C
26	OF	203	PEB	CAB-CBB-CGB-O1B
26	fF	201	PEB	CAB-CBB-CGB-O1B
26	HG	201	PEB	CAC-CBC-CGC-O1C
26	NG	202	PEB	CAB-CBB-CGB-O2B
26	XG	201	PEB	CAB-CBB-CGB-O1B
26	jG	202	PEB	CAC-CBC-CGC-O1C
26	lG	201	PEB	CAB-CBB-CGB-O1B
26	oG	202	PEB	CAB-CBB-CGB-O2B
26	QI	202	PEB	CAC-CBC-CGC-O1C
26	mI	202	PEB	CAB-CBB-CGB-O2B
26	EJ	202	PEB	CAC-CBC-CGC-O2C
27	24	403	PUB	CAB-CBB-CGB-O1B
27	AI	303	PUB	CAC-CBC-CGC-O1C
28	UH	1001	CYC	CAA-CBA-CGA-O1A
28	rH	1001	CYC	CAA-CBA-CGA-O2A
28	LI	1001	CYC	CAA-CBA-CGA-O1A
28	LF	1001	CYC	C2B-C3B-CAB-CBB
26	fI	201	PEB	CAB-CBB-CGB-O2B
26	jI	201	PEB	CAB-CBB-CGB-O1B
26	kI	202	PEB	CAC-CBC-CGC-O1C
26	g2	202	PEB	CAC-CBC-CGC-O1C
26	B4	201	PEB	CAB-CBB-CGB-O2B
26	X4	201	PEB	CAB-CBB-CGB-O2B
26	G5	202	PEB	CAB-CBB-CGB-O1B
26	U6	202	PEB	CAB-CBB-CGB-O1B
26	h6	203	PEB	CAB-CBB-CGB-O1B
26	S7	201	PEB	CAB-CBB-CGB-O2B
26	h7	201	PEB	CAC-CBC-CGC-O1C
26	M8	203	PEB	CAB-CBB-CGB-O1B
26	l8	203	PEB	CAB-CBB-CGB-O1B
26	VB	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	LC	201	PEB	CAB-CBB-CGB-01B
26	DD	201	PEB	CAC-CBC-CGC-02C
26	VD	202	PEB	CAC-CBC-CGC-01C
26	FE	202	PEB	CAB-CBB-CGB-01B
26	FE	202	PEB	CAB-CBB-CGB-02B
26	JE	202	PEB	CAC-CBC-CGC-01C
26	QE	203	PEB	CAC-CBC-CGC-01C
26	BG	202	PEB	CAB-CBB-CGB-02B
26	JG	202	PEB	CAC-CBC-CGC-01C
26	PG	201	PEB	CAC-CBC-CGC-01C
26	ZG	201	PEB	CAC-CBC-CGC-01C
26	oG	202	PEB	CAB-CBB-CGB-01B
26	kI	201	PEB	CAC-CBC-CGC-01C
26	MJ	201	PEB	CAB-CBB-CGB-02B
26	RJ	203	PEB	CAB-CBB-CGB-02B
27	AJ	302	PUB	CAB-CBB-CGB-02B
28	D2	1001	CYC	CAD-CBD-CGD-01D
28	D7	1001	CYC	CAD-CBD-CGD-01D
28	gH	1001	CYC	CAD-CBD-CGD-01D
28	oH	1001	CYC	CAA-CBA-CGA-01A
28	DI	1001	CYC	CAD-CBD-CGD-01D
26	Y1	201	PEB	CAC-CBC-CGC-01C
26	p1	202	PEB	CAC-CBC-CGC-02C
26	y1	202	PEB	CAB-CBB-CGB-02B
26	e2	202	PEB	CAB-CBB-CGB-02B
26	B3	203	PEB	CAB-CBB-CGB-01B
26	M3	202	PEB	CAB-CBB-CGB-01B
26	N3	202	PEB	CAC-CBC-CGC-01C
26	X4	201	PEB	CAC-CBC-CGC-02C
26	q4	202	PEB	CAC-CBC-CGC-02C
26	G5	201	PEB	CAB-CBB-CGB-02B
26	N6	201	PEB	CAC-CBC-CGC-02C
26	S6	203	PEB	CAC-CBC-CGC-01C
26	m6	202	PEB	CAC-CBC-CGC-01C
26	T7	201	PEB	CAB-CBB-CGB-02B
26	Y7	201	PEB	CAB-CBB-CGB-02B
26	Y8	203	PEB	CAB-CBB-CGB-01B
26	E9	201	PEB	CAB-CBB-CGB-01B
26	J9	201	PEB	CAC-CBC-CGC-01C
26	JD	203	PEB	CAC-CBC-CGC-02C
26	RD	202	PEB	CAB-CBB-CGB-02B
26	ME	203	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
26	XE	201	PEB	CAB-CBB-CGB-01B
26	kE	202	PEB	CAB-CBB-CGB-01B
26	HF	1002	PEB	CAB-CBB-CGB-01B
26	PF	201	PEB	CAB-CBB-CGB-02B
26	TF	202	PEB	CAB-CBB-CGB-01B
26	WF	202	PEB	CAB-CBB-CGB-01B
26	YF	202	PEB	CAC-CBC-CGC-01C
26	iF	201	PEB	CAB-CBB-CGB-02B
26	CJ	202	PEB	CAC-CBC-CGC-01C
27	A2	303	PUB	CAC-CBC-CGC-02C
28	I2	1001	CYC	CAD-CBD-CGD-02D
28	H6	1001	CYC	CAD-CBD-CGD-02D
28	DF	1003	CYC	CAD-CBD-CGD-02D
28	II	1001	CYC	CAD-CBD-CGD-02D
26	n1	201	PEB	CAC-CBC-CGC-02C
26	T2	203	PEB	CAC-CBC-CGC-02C
26	k2	202	PEB	CAC-CBC-CGC-02C
26	T3	202	PEB	CAC-CBC-CGC-02C
26	N4	203	PEB	CAC-CBC-CGC-02C
26	V6	201	PEB	CAC-CBC-CGC-02C
26	Y6	201	PEB	CAB-CBB-CGB-01B
26	O7	203	PEB	CAB-CBB-CGB-02B
26	Z7	202	PEB	CAC-CBC-CGC-01C
26	H8	201	PEB	CAC-CBC-CGC-01C
26	e8	201	PEB	CAC-CBC-CGC-01C
26	C9	202	PEB	CAC-CBC-CGC-02C
26	E9	202	PEB	CAC-CBC-CGC-02C
26	NB	1002	PEB	CAC-CBC-CGC-02C
26	TD	202	PEB	CAC-CBC-CGC-02C
26	WD	202	PEB	CAB-CBB-CGB-01B
26	BE	202	PEB	CAC-CBC-CGC-02C
26	WE	201	PEB	CAC-CBC-CGC-02C
26	sE	203	PEB	CAB-CBB-CGB-02B
26	uE	202	PEB	CAB-CBB-CGB-01B
26	FG	202	PEB	CAB-CBB-CGB-01B
26	NG	202	PEB	CAB-CBB-CGB-01B
26	aG	203	PEB	CAC-CBC-CGC-01C
26	nG	202	PEB	CAC-CBC-CGC-01C
26	TI	201	PEB	CAC-CBC-CGC-01C
26	TI	203	PEB	CAC-CBC-CGC-02C
26	AJ	301	PEB	CAC-CBC-CGC-01C
26	JJ	201	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
26	WJ	202	PEB	CAC-CBC-CGC-O2C
27	KD	203	PUB	CAB-CBB-CGB-O1B
28	G7	1001	CYC	CAD-CBD-CGD-O2D
28	L7	1001	CYC	CAD-CBD-CGD-O2D
26	R2	202	PEB	C4B-C3B-CAB-CBB
26	NA	201	PEB	C4B-C3B-CAB-CBB
26	C1	201	PEB	CAC-CBC-CGC-O2C
26	y1	201	PEB	CAB-CBB-CGB-O1B
26	J3	201	PEB	CAB-CBB-CGB-O1B
26	F4	201	PEB	CAB-CBB-CGB-O1B
26	L4	202	PEB	CAC-CBC-CGC-O1C
26	V4	203	PEB	CAC-CBC-CGC-O2C
26	L7	1002	PEB	CAB-CBB-CGB-O2B
26	W7	202	PEB	CAB-CBB-CGB-O1B
26	lA	203	PEB	CAB-CBB-CGB-O1B
26	ND	202	PEB	CAC-CBC-CGC-O2C
26	TD	203	PEB	CAB-CBB-CGB-O1B
26	tE	201	PEB	CAB-CBB-CGB-O2B
26	iG	203	PEB	CAB-CBB-CGB-O1B
26	cI	201	PEB	CAB-CBB-CGB-O1B
26	gI	202	PEB	CAC-CBC-CGC-O2C
27	A8	303	PUB	CAB-CBB-CGB-O1B
26	a2	202	PEB	C2B-C3B-CAB-CBB
26	T3	203	PEB	C2B-C3B-CAB-CBB
26	TF	201	PEB	C2B-C3B-CAB-CBB
26	j1	201	PEB	CAB-CBB-CGB-O2B
26	a4	201	PEB	CAB-CBB-CGB-O1B
26	j4	201	PEB	CAC-CBC-CGC-O2C
26	C5	204	PEB	CAB-CBB-CGB-O2B
26	P6	201	PEB	CAB-CBB-CGB-O2B
26	W6	201	PEB	CAC-CBC-CGC-O2C
26	B8	301	PEB	CAB-CBB-CGB-O1B
26	e8	202	PEB	CAC-CBC-CGC-O2C
26	I9	202	PEB	CAC-CBC-CGC-O2C
26	eA	202	PEB	CAC-CBC-CGC-O2C
26	PB	201	PEB	CAB-CBB-CGB-O2B
26	RB	201	PEB	CAB-CBB-CGB-O2B
26	BE	202	PEB	CAB-CBB-CGB-O2B
26	HI	1002	PEB	CAB-CBB-CGB-O2B
28	L6	1001	CYC	CAA-CBA-CGA-O1A
26	V2	202	PEB	CAB-CBB-CGB-O2B
26	Y6	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	a7	201	PEB	CAB-CBB-CGB-O2B
26	i7	202	PEB	CAB-CBB-CGB-O1B
26	BA	301	PEB	CAB-CBB-CGB-O1B
26	YA	203	PEB	CAB-CBB-CGB-O1B
26	WB	201	PEB	CAC-CBC-CGC-O2C
26	mB	201	PEB	CAB-CBB-CGB-O2B
26	AD	201	PEB	CAB-CBB-CGB-O2B
26	DE	202	PEB	CAC-CBC-CGC-O2C
26	DE	203	PEB	CAB-CBB-CGB-O2B
26	DF	1002	PEB	CAB-CBB-CGB-O2B
26	DG	203	PEB	CAB-CBB-CGB-O2B
26	mG	201	PEB	CAC-CBC-CGC-O2C
26	SI	201	PEB	CAB-CBB-CGB-O2B
26	QJ	202	PEB	CAC-CBC-CGC-O2C
28	MH	1001	CYC	CAA-CBA-CGA-O1A
28	CI	1001	CYC	CAD-CBD-CGD-O2D
26	N1	203	PEB	CAC-CBC-CGC-O1C
26	X1	202	PEB	CAC-CBC-CGC-O2C
26	D3	201	PEB	CAC-CBC-CGC-O2C
26	B4	203	PEB	CAC-CBC-CGC-O2C
26	p4	202	PEB	CAC-CBC-CGC-O2C
26	i6	202	PEB	CAC-CBC-CGC-O2C
26	Y7	201	PEB	CAC-CBC-CGC-O2C
26	HA	201	PEB	CAC-CBC-CGC-O1C
26	MA	203	PEB	CAB-CBB-CGB-O1B
26	mA	202	PEB	CAC-CBC-CGC-O1C
26	bB	201	PEB	CAC-CBC-CGC-O2C
26	vE	201	PEB	CAB-CBB-CGB-O1B
26	DG	202	PEB	CAC-CBC-CGC-O1C
26	eI	202	PEB	CAB-CBB-CGB-O2B
26	IJ	203	PEB	CAC-CBC-CGC-O1C
28	L2	1001	CYC	CAD-CBD-CGD-O2D
28	EF	1001	CYC	CAD-CBD-CGD-O2D
28	NF	1001	CYC	CAD-CBD-CGD-O2D
26	T1	203	PEB	C2C-CAC-CBC-CGC
26	m1	203	PEB	C2C-CAC-CBC-CGC
26	p1	202	PEB	C2C-CAC-CBC-CGC
26	w1	201	PEB	C2C-CAC-CBC-CGC
26	Y3	301	PEB	C2C-CAC-CBC-CGC
26	u4	201	PEB	C2C-CAC-CBC-CGC
26	B5	203	PEB	C2C-CAC-CBC-CGC
26	F5	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	V6	201	PEB	C2C-CAC-CBC-CGC
26	W6	202	PEB	C2C-CAC-CBC-CGC
26	U7	201	PEB	C2C-CAC-CBC-CGC
26	W7	203	PEB	C2C-CAC-CBC-CGC
26	WB	202	PEB	C2C-CAC-CBC-CGC
26	ID	202	PEB	C2C-CAC-CBC-CGC
26	QD	202	PEB	C2C-CAC-CBC-CGC
26	UD	201	PEB	C2C-CAC-CBC-CGC
26	UF	201	PEB	C2C-CAC-CBC-CGC
26	QG	201	PEB	C2C-CAC-CBC-CGC
26	YG	202	PEB	C2C-CAC-CBC-CGC
26	cG	201	PEB	C2C-CAC-CBC-CGC
26	mG	203	PEB	C2C-CAC-CBC-CGC
27	A9	302	PUB	C3B-CAB-CBB-CGB
27	N9	201	PUB	C3B-CAB-CBB-CGB
26	a6	202	PEB	C4B-C3B-CAB-CBB
28	dH	1001	CYC	C1A-C2A-CAA-CBA
26	Z1	202	PEB	C3B-CAB-CBB-CGB
26	A2	301	PEB	C3B-CAB-CBB-CGB
26	S2	201	PEB	C3B-CAB-CBB-CGB
26	g2	203	PEB	C3B-CAB-CBB-CGB
26	N4	202	PEB	C3B-CAB-CBB-CGB
26	W4	202	PEB	C3B-CAB-CBB-CGB
26	I8	201	PEB	C3B-CAB-CBB-CGB
26	m8	202	PEB	C3B-CAB-CBB-CGB
26	C9	202	PEB	C3B-CAB-CBB-CGB
26	J9	201	PEB	C3B-CAB-CBB-CGB
26	ZB	201	PEB	C3B-CAB-CBB-CGB
26	dF	203	PEB	C3B-CAB-CBB-CGB
26	OG	203	PEB	C3B-CAB-CBB-CGB
26	VG	202	PEB	C3B-CAB-CBB-CGB
26	fG	201	PEB	C3B-CAB-CBB-CGB
26	TI	203	PEB	C3B-CAB-CBB-CGB
26	gI	203	PEB	C3B-CAB-CBB-CGB
28	rH	1001	CYC	C2A-CAA-CBA-CGA
26	P1	201	PEB	CAB-CBB-CGB-O2B
26	i2	203	PEB	CAB-CBB-CGB-O1B
26	R6	201	PEB	CAB-CBB-CGB-O2B
26	m8	202	PEB	CAC-CBC-CGC-O1C
26	jE	201	PEB	CAB-CBB-CGB-O1B
26	YI	202	PEB	CAB-CBB-CGB-O2B
26	kI	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
27	AA	304	PUB	CAC-CBC-CGC-O2C
28	HB	1001	CYC	CAD-CBD-CGD-O2D
26	D1	201	PEB	CAB-CBB-CGB-O1B
26	R1	201	PEB	CAB-CBB-CGB-O1B
26	o1	501	PEB	CAB-CBB-CGB-O1B
26	H2	1002	PEB	CAB-CBB-CGB-O2B
26	X4	202	PEB	CAC-CBC-CGC-O2C
26	P7	201	PEB	CAB-CBB-CGB-O2B
26	S7	201	PEB	CAB-CBB-CGB-O1B
26	WG	201	PEB	CAC-CBC-CGC-O2C
26	qG	202	PEB	CAB-CBB-CGB-O2B
26	uG	201	PEB	CAC-CBC-CGC-O1C
27	A9	302	PUB	CAC-CBC-CGC-O2C
28	LB	1001	CYC	CAA-CBA-CGA-O1A
28	IH	1001	CYC	CAA-CBA-CGA-O2A
26	T1	202	PEB	CAB-CBB-CGB-O1B
26	iB	201	PEB	CAB-CBB-CGB-O1B
27	24	403	PUB	CAC-CBC-CGC-O2C
27	AJ	302	PUB	CAB-CBB-CGB-O1B
26	X1	201	PEB	CAC-CBC-CGC-O2C
26	y1	201	PEB	CAB-CBB-CGB-O2B
26	c2	203	PEB	CAB-CBB-CGB-O2B
26	m2	202	PEB	CAB-CBB-CGB-O2B
26	h7	202	PEB	CAB-CBB-CGB-O2B
26	I9	201	PEB	CAC-CBC-CGC-O1C
26	BC	203	PEB	CAB-CBB-CGB-O2B
26	RD	202	PEB	CAB-CBB-CGB-O1B
26	eE	201	PEB	CAC-CBC-CGC-O2C
26	OG	201	PEB	CAC-CBC-CGC-O2C
26	aI	203	PEB	CAB-CBB-CGB-O1B
26	RJ	203	PEB	CAB-CBB-CGB-O1B
28	HF	1001	CYC	C4B-C3B-CAB-CBB
28	MH	1001	CYC	C4B-C3B-CAB-CBB
26	n1	201	PEB	CAC-CBC-CGC-O1C
26	Y2	202	PEB	CAB-CBB-CGB-O2B
26	R4	203	PEB	CAC-CBC-CGC-O2C
26	n4	201	PEB	CAC-CBC-CGC-O1C
26	L5	201	PEB	CAC-CBC-CGC-O2C
26	W7	203	PEB	CAB-CBB-CGB-O2B
26	D8	201	PEB	CAB-CBB-CGB-O2B
26	xE	302	PEB	CAC-CBC-CGC-O2C
26	VI	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	C6	1001	CYC	CAD-CBD-CGD-O2D
28	CB	1001	CYC	CAD-CBD-CGD-O2D
28	SH	1001	CYC	CAA-CBA-CGA-O2A
28	II	1001	CYC	CAD-CBD-CGD-O1D
26	M1	403	PEB	C2D-C1D-CHC-C4C
26	N1	201	PEB	C2D-C1D-CHC-C4C
26	11	203	PEB	C2D-C1D-CHC-C4C
26	B3	201	PEB	C2D-C1D-CHC-C4C
26	L3	201	PEB	C2D-C1D-CHC-C4C
26	A4	202	PEB	C2D-C1D-CHC-C4C
26	Q4	202	PEB	C2D-C1D-CHC-C4C
26	U6	202	PEB	C2D-C1D-CHC-C4C
26	Z6	202	PEB	C2D-C1D-CHC-C4C
26	j6	201	PEB	C2D-C1D-CHC-C4C
26	K8	202	PEB	C2D-C1D-CHC-C4C
26	O8	202	PEB	C2D-C1D-CHC-C4C
26	S8	202	PEB	C2D-C1D-CHC-C4C
26	a8	203	PEB	C2D-C1D-CHC-C4C
26	c8	202	PEB	C2D-C1D-CHC-C4C
26	l8	202	PEB	C2D-C1D-CHC-C4C
26	C9	201	PEB	C2D-C1D-CHC-C4C
26	KA	202	PEB	C2D-C1D-CHC-C4C
26	OA	201	PEB	C2D-C1D-CHC-C4C
26	cA	203	PEB	C2D-C1D-CHC-C4C
26	lA	202	PEB	C2D-C1D-CHC-C4C
26	UB	202	PEB	C2D-C1D-CHC-C4C
26	fB	203	PEB	C2D-C1D-CHC-C4C
26	jB	201	PEB	C2D-C1D-CHC-C4C
26	BD	203	PEB	C2D-C1D-CHC-C4C
26	EE	201	PEB	C2D-C1D-CHC-C4C
26	ME	203	PEB	C2D-C1D-CHC-C4C
26	UE	201	PEB	C2D-C1D-CHC-C4C
26	kE	203	PEB	C2D-C1D-CHC-C4C
26	FF	1002	PEB	C2D-C1D-CHC-C4C
26	lF	203	PEB	C2D-C1D-CHC-C4C
26	UG	201	PEB	C2D-C1D-CHC-C4C
26	WG	203	PEB	C2D-C1D-CHC-C4C
26	fG	201	PEB	C2D-C1D-CHC-C4C
26	gG	202	PEB	C2D-C1D-CHC-C4C
26	pG	201	PEB	C2D-C1D-CHC-C4C
26	qG	202	PEB	C2D-C1D-CHC-C4C
26	QI	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	VJ	202	PEB	C2D-C1D-CHC-C4C
26	XJ	201	PEB	C2D-C1D-CHC-C4C
27	A2	303	PUB	C3A-C4A-CHA-C1B
27	N9	201	PUB	C3A-C4A-CHA-C1B
27	yG	303	PUB	C3A-C4A-CHA-C1B
27	AI	303	PUB	C3A-C4A-CHA-C1B
26	N8	201	PEB	C4B-C3B-CAB-CBB
26	H1	203	PEB	CAC-CBC-CGC-O2C
26	M1	403	PEB	CAC-CBC-CGC-O2C
26	I4	201	PEB	CAB-CBB-CGB-O2B
26	d6	203	PEB	CAC-CBC-CGC-O2C
26	k6	201	PEB	CAC-CBC-CGC-O2C
26	O7	203	PEB	CAB-CBB-CGB-O1B
26	JC	201	PEB	CAB-CBB-CGB-O2B
26	gE	201	PEB	CAC-CBC-CGC-O2C
26	sE	203	PEB	CAB-CBB-CGB-O1B
26	uE	201	PEB	CAC-CBC-CGC-O2C
26	LF	1002	PEB	CAB-CBB-CGB-O2B
26	WF	203	PEB	CAB-CBB-CGB-O2B
26	hG	201	PEB	CAB-CBB-CGB-O1B
26	AI	305	PEB	CAC-CBC-CGC-O2C
27	K3	203	PUB	CAC-CBC-CGC-O2C
28	KF	1001	CYC	CAD-CBD-CGD-O2D
28	DI	1001	CYC	CAD-CBD-CGD-O2D
26	i2	203	PEB	CAB-CBB-CGB-O2B
26	J3	201	PEB	CAC-CBC-CGC-O2C
26	G4	201	PEB	CAC-CBC-CGC-O2C
26	NE	202	PEB	CAC-CBC-CGC-O2C
28	I2	1001	CYC	CAD-CBD-CGD-O1D
26	C1	201	PEB	CAC-CBC-CGC-O1C
26	U6	202	PEB	CAB-CBB-CGB-O2B
26	V7	201	PEB	CAB-CBB-CGB-O2B
26	Y7	201	PEB	CAC-CBC-CGC-O1C
26	LA	202	PEB	CAC-CBC-CGC-O2C
26	VB	201	PEB	CAB-CBB-CGB-O2B
26	cB	201	PEB	CAB-CBB-CGB-O2B
26	HG	201	PEB	CAC-CBC-CGC-O2C
26	iG	201	PEB	CAC-CBC-CGC-O2C
27	A8	303	PUB	CAB-CBB-CGB-O2B
27	AI	303	PUB	CAC-CBC-CGC-O2C
28	K7	1001	CYC	CAD-CBD-CGD-O2D
26	B3	203	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	f8	203	PEB	C3B-CAB-CBB-CGB
26	A9	303	PEB	C3B-CAB-CBB-CGB
26	fA	203	PEB	C3B-CAB-CBB-CGB
26	SB	203	PEB	C3B-CAB-CBB-CGB
26	PF	202	PEB	C3B-CAB-CBB-CGB
26	J5	201	PEB	CAB-CBB-CGB-O2B
26	a6	201	PEB	CAB-CBB-CGB-O2B
26	i6	201	PEB	CAB-CBB-CGB-O2B
26	P8	201	PEB	CAB-CBB-CGB-O2B
26	aB	201	PEB	CAB-CBB-CGB-O2B
26	mB	201	PEB	CAB-CBB-CGB-O1B
26	JC	201	PEB	CAB-CBB-CGB-O1B
26	BE	202	PEB	CAC-CBC-CGC-O1C
26	jG	201	PEB	CAB-CBB-CGB-O1B
28	uH	1001	CYC	CAA-CBA-CGA-O2A
26	H1	203	PEB	CAC-CBC-CGC-O1C
26	R1	203	PEB	CAC-CBC-CGC-O2C
26	J3	201	PEB	CAC-CBC-CGC-O1C
26	N4	203	PEB	CAC-CBC-CGC-O1C
26	a4	201	PEB	CAB-CBB-CGB-O2B
26	T6	201	PEB	CAB-CBB-CGB-O2B
26	i6	201	PEB	CAB-CBB-CGB-O1B
26	W7	202	PEB	CAB-CBB-CGB-O2B
26	W7	203	PEB	CAB-CBB-CGB-O1B
26	e7	201	PEB	CAB-CBB-CGB-O2B
26	B8	301	PEB	CAB-CBB-CGB-O2B
26	PB	201	PEB	CAC-CBC-CGC-O2C
26	TB	201	PEB	CAB-CBB-CGB-O2B
26	aB	201	PEB	CAB-CBB-CGB-O1B
26	JE	201	PEB	CAC-CBC-CGC-O1C
26	kE	202	PEB	CAB-CBB-CGB-O2B
26	cI	201	PEB	CAB-CBB-CGB-O2B
26	MJ	201	PEB	CAB-CBB-CGB-O1B
28	L6	1001	CYC	CAA-CBA-CGA-O2A
28	D7	1001	CYC	CAD-CBD-CGD-O2D
28	K7	1001	CYC	CAD-CBD-CGD-O1D
28	IH	1001	CYC	CAA-CBA-CGA-O1A
28	JI	1001	CYC	CAD-CBD-CGD-O2D
26	P2	202	PEB	C4B-C3B-CAB-CBB
26	y1	202	PEB	CAB-CBB-CGB-O1B
26	g2	202	PEB	CAC-CBC-CGC-O2C
26	F4	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	R4	203	PEB	CAC-CBC-CGC-O1C
26	G5	201	PEB	CAB-CBB-CGB-O1B
26	TD	203	PEB	CAB-CBB-CGB-O2B
26	ME	203	PEB	CAC-CBC-CGC-O2C
26	tE	201	PEB	CAB-CBB-CGB-O1B
26	WF	202	PEB	CAB-CBB-CGB-O2B
26	iG	203	PEB	CAB-CBB-CGB-O2B
26	SI	201	PEB	CAB-CBB-CGB-O1B
26	aI	203	PEB	CAB-CBB-CGB-O2B
26	CJ	202	PEB	CAC-CBC-CGC-O2C
28	D2	1001	CYC	CAD-CBD-CGD-O2D
28	J7	1003	CYC	CAD-CBD-CGD-O2D
28	kH	1001	CYC	CAA-CBA-CGA-O2A
28	CI	1001	CYC	CAD-CBD-CGD-O1D
26	N3	202	PEB	CAC-CBC-CGC-O2C
26	I4	201	PEB	CAB-CBB-CGB-O1B
26	BA	301	PEB	CAB-CBB-CGB-O2B
26	VB	201	PEB	CAB-CBB-CGB-O1B
26	gB	201	PEB	CAB-CBB-CGB-O1B
26	KE	201	PEB	CAC-CBC-CGC-O1C
26	mE	203	PEB	CAB-CBB-CGB-O1B
26	KG	201	PEB	CAC-CBC-CGC-O2C
26	c2	201	PEB	CAB-CBB-CGB-O2B
26	k2	203	PEB	CAB-CBB-CGB-O2B
26	J3	201	PEB	CAB-CBB-CGB-O2B
26	G4	201	PEB	CAC-CBC-CGC-O1C
26	L4	201	PEB	CAB-CBB-CGB-O2B
26	J5	201	PEB	CAB-CBB-CGB-O1B
26	d6	203	PEB	CAC-CBC-CGC-O1C
26	J9	201	PEB	CAC-CBC-CGC-O2C
26	QG	203	PEB	CAC-CBC-CGC-O2C
28	F2	1001	CYC	CAD-CBD-CGD-O1D
28	L2	1001	CYC	CAD-CBD-CGD-O1D
26	B1	202	PEB	ND-C1D-CHC-C4C
26	I1	201	PEB	ND-C1D-CHC-C4C
26	J1	202	PEB	ND-C1D-CHC-C4C
26	R1	201	PEB	ND-C1D-CHC-C4C
26	b1	501	PEB	C2A-C3A-CAA-CBA
26	i1	203	PEB	ND-C1D-CHC-C4C
26	k1	202	PEB	ND-C1D-CHC-C4C
26	u1	202	PEB	ND-C1D-CHC-C4C
26	w1	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	T2	202	PEB	C2A-C3A-CAA-CBA
26	e2	201	PEB	ND-C1D-CHC-C4C
26	h2	201	PEB	ND-C1D-CHC-C4C
26	Q3	202	PEB	C2C-CAC-CBC-CGC
26	A4	202	PEB	ND-C1D-CHC-C4C
26	I4	201	PEB	ND-C1D-CHC-C4C
26	M4	401	PEB	ND-C1D-CHC-C4C
26	R4	201	PEB	ND-C1D-CHC-C4C
26	R4	203	PEB	C2A-C3A-CAA-CBA
26	d4	201	PEB	ND-C1D-CHC-C4C
26	k4	201	PEB	ND-C1D-CHC-C4C
26	u4	202	PEB	ND-C1D-CHC-C4C
26	z4	201	PEB	C2A-C3A-CAA-CBA
26	C5	201	PEB	ND-C1D-CHC-C4C
26	C5	202	PEB	ND-C1D-CHC-C4C
26	S6	201	PEB	ND-C1D-CHC-C4C
26	U6	203	PEB	ND-C1D-CHC-C4C
26	c6	201	PEB	C2A-C3A-CAA-CBA
26	d6	201	PEB	ND-C1D-CHC-C4C
26	g6	201	PEB	C2A-C3A-CAA-CBA
26	l6	201	PEB	ND-C1D-CHC-C4C
26	O7	203	PEB	ND-C1D-CHC-C4C
26	c7	201	PEB	ND-C1D-CHC-C4C
26	h7	201	PEB	ND-C1D-CHC-C4C
26	h7	202	PEB	C2C-CAC-CBC-CGC
26	k7	202	PEB	ND-C1D-CHC-C4C
26	l7	203	PEB	C2A-C3A-CAA-CBA
26	C8	203	PEB	ND-C1D-CHC-C4C
26	E8	202	PEB	ND-C1D-CHC-C4C
26	I8	203	PEB	ND-C1D-CHC-C4C
26	M8	203	PEB	C2C-CAC-CBC-CGC
26	O8	202	PEB	ND-C1D-CHC-C4C
26	S8	201	PEB	C2C-CAC-CBC-CGC
26	U8	201	PEB	ND-C1D-CHC-C4C
26	U8	202	PEB	ND-C1D-CHC-C4C
26	W8	202	PEB	ND-C1D-CHC-C4C
26	a8	204	PEB	C2C-CAC-CBC-CGC
26	f8	203	PEB	ND-C1D-CHC-C4C
26	f8	203	PEB	C2A-C3A-CAA-CBA
26	h8	203	PEB	ND-C1D-CHC-C4C
26	D9	201	PEB	ND-C1D-CHC-C4C
26	L9	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
26	L9	203	PEB	ND-C1D-CHC-C4C
26	P9	201	PEB	ND-C1D-CHC-C4C
26	MA	203	PEB	C2C-CAC-CBC-CGC
26	UA	202	PEB	ND-C1D-CHC-C4C
26	UA	203	PEB	ND-C1D-CHC-C4C
26	SB	201	PEB	ND-C1D-CHC-C4C
26	VB	201	PEB	C2C-CAC-CBC-CGC
26	IB	202	PEB	C2C-CAC-CBC-CGC
26	AC	202	PEB	ND-C1D-CHC-C4C
26	BC	203	PEB	C2C-CAC-CBC-CGC
26	ED	202	PEB	ND-C1D-CHC-C4C
26	IE	203	PEB	ND-C1D-CHC-C4C
26	QE	201	PEB	C2C-CAC-CBC-CGC
26	XE	202	PEB	C2A-C3A-CAA-CBA
26	aE	201	PEB	ND-C1D-CHC-C4C
26	dE	201	PEB	ND-C1D-CHC-C4C
26	eE	201	PEB	ND-C1D-CHC-C4C
26	mE	201	PEB	ND-C1D-CHC-C4C
26	uE	203	PEB	C2A-C3A-CAA-CBA
26	wE	302	PEB	ND-C1D-CHC-C4C
26	AF	301	PEB	C2C-CAC-CBC-CGC
26	AF	302	PEB	C2C-CAC-CBC-CGC
26	OF	203	PEB	ND-C1D-CHC-C4C
26	YF	201	PEB	C2C-CAC-CBC-CGC
26	aF	201	PEB	C2C-CAC-CBC-CGC
26	fF	202	PEB	ND-C1D-CHC-C4C
26	hF	201	PEB	ND-C1D-CHC-C4C
26	hF	203	PEB	C2A-C3A-CAA-CBA
26	QG	203	PEB	ND-C1D-CHC-C4C
26	QG	203	PEB	C2A-C3A-CAA-CBA
26	cG	201	PEB	C2A-C3A-CAA-CBA
26	dG	201	PEB	ND-C1D-CHC-C4C
26	gG	203	PEB	ND-C1D-CHC-C4C
26	qG	202	PEB	ND-C1D-CHC-C4C
26	xG	302	PEB	C2A-C3A-CAA-CBA
26	cI	201	PEB	C2A-C3A-CAA-CBA
26	cI	203	PEB	ND-C1D-CHC-C4C
26	eI	201	PEB	ND-C1D-CHC-C4C
26	jI	201	PEB	C2C-CAC-CBC-CGC
26	mI	202	PEB	C2A-C3A-CAA-CBA
26	AJ	301	PEB	ND-C1D-CHC-C4C
26	CJ	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
26	DJ	201	PEB	ND-C1D-CHC-C4C
26	HJ	201	PEB	ND-C1D-CHC-C4C
26	JJ	203	PEB	ND-C1D-CHC-C4C
26	LJ	203	PEB	ND-C1D-CHC-C4C
26	LJ	203	PEB	C2C-CAC-CBC-CGC
26	NJ	204	PEB	ND-C1D-CHC-C4C
26	PJ	201	PEB	ND-C1D-CHC-C4C
26	VJ	201	PEB	ND-C1D-CHC-C4C
27	A6	303	PUB	NA-C4A-CHA-C1B
27	A9	302	PUB	NA-C4A-CHA-C1B
27	yE	303	PUB	NA-C4A-CHA-C1B
28	D7	1001	CYC	C3D-CAD-CBD-CGD
28	EH	1001	CYC	C2C-C3C-CAC-CBC
28	sH	1001	CYC	C2C-C3C-CAC-CBC
28	wH	1001	CYC	C2C-C3C-CAC-CBC
28	EI	1001	CYC	C2C-C3C-CAC-CBC
26	U2	201	PEB	CAB-CBB-CGB-O2B
26	B4	201	PEB	CAB-CBB-CGB-O1B
26	H4	201	PEB	CAB-CBB-CGB-O2B
26	R6	201	PEB	CAC-CBC-CGC-O1C
26	V6	201	PEB	CAB-CBB-CGB-O1B
26	V7	201	PEB	CAB-CBB-CGB-O1B
26	D8	201	PEB	CAB-CBB-CGB-O1B
26	LA	202	PEB	CAC-CBC-CGC-O1C
26	cB	201	PEB	CAB-CBB-CGB-O1B
26	CC	203	PEB	CAB-CBB-CGB-O1B
26	FC	202	PEB	CAC-CBC-CGC-O2C
26	gE	201	PEB	CAC-CBC-CGC-O1C
26	uE	201	PEB	CAC-CBC-CGC-O1C
26	VI	202	PEB	CAB-CBB-CGB-O2B
26	ZI	201	PEB	CAB-CBB-CGB-O2B
28	LB	1001	CYC	CAA-CBA-CGA-O2A
28	SH	1001	CYC	CAA-CBA-CGA-O1A
28	JI	1001	CYC	CAD-CBD-CGD-O1D
28	MI	1001	CYC	CAD-CBD-CGD-O2D
26	H1	201	PEB	CAB-CBB-CGB-O1B
26	V3	203	PEB	CAC-CBC-CGC-O1C
26	J4	201	PEB	CAB-CBB-CGB-O1B
26	F5	202	PEB	CAC-CBC-CGC-O1C
26	L5	201	PEB	CAC-CBC-CGC-O1C
26	b6	201	PEB	CAB-CBB-CGB-O1B
26	i6	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	N9	202	PEB	CAC-CBC-CGC-O1C
26	FC	203	PEB	CAB-CBB-CGB-O1B
26	WF	203	PEB	CAB-CBB-CGB-O1B
26	NG	202	PEB	CAC-CBC-CGC-O2C
26	XG	202	PEB	CAC-CBC-CGC-O1C
27	A9	302	PUB	CAC-CBC-CGC-O1C
27	xG	306	PUB	CAB-CBB-CGB-O1B
28	CB	1001	CYC	CAD-CBD-CGD-O1D
28	NB	1001	CYC	CAA-CBA-CGA-O2A
28	FI	1001	CYC	CAD-CBD-CGD-O1D
26	h1	201	PEB	C4B-C3B-CAB-CBB
26	t1	201	PEB	C4B-C3B-CAB-CBB
26	C8	203	PEB	C4B-C3B-CAB-CBB
26	CA	203	PEB	C4B-C3B-CAB-CBB
26	kI	202	PEB	C4B-C3B-CAB-CBB
26	g2	202	PEB	CAB-CBB-CGB-O2B
26	L4	202	PEB	CAC-CBC-CGC-O2C
26	f4	201	PEB	CAB-CBB-CGB-O2B
26	m8	202	PEB	CAC-CBC-CGC-O2C
26	mA	202	PEB	CAC-CBC-CGC-O2C
26	FC	202	PEB	CAC-CBC-CGC-O1C
26	DE	202	PEB	CAC-CBC-CGC-O1C
26	mE	203	PEB	CAB-CBB-CGB-O2B
26	wE	301	PEB	CAC-CBC-CGC-O1C
26	kI	202	PEB	CAC-CBC-CGC-O2C
26	IJ	203	PEB	CAC-CBC-CGC-O2C
27	xG	306	PUB	CAB-CBB-CGB-O2B
28	C6	1001	CYC	CAD-CBD-CGD-O1D
28	F7	1001	CYC	CAD-CBD-CGD-O2D
27	K4	203	PUB	C2D-C3D-CAD-CBD
26	e1	202	PEB	C2B-C3B-CAB-CBB
26	VI	203	PEB	C2B-C3B-CAB-CBB
26	B1	202	PEB	C3B-CAB-CBB-CGB
26	b2	202	PEB	C3B-CAB-CBB-CGB
26	Y6	202	PEB	C3B-CAB-CBB-CGB
26	Z6	201	PEB	C3B-CAB-CBB-CGB
26	d6	201	PEB	C3B-CAB-CBB-CGB
26	F8	202	PEB	C3B-CAB-CBB-CGB
26	R8	202	PEB	C3B-CAB-CBB-CGB
26	UA	202	PEB	C3B-CAB-CBB-CGB
26	OE	203	PEB	C3B-CAB-CBB-CGB
26	WE	202	PEB	C3B-CAB-CBB-CGB

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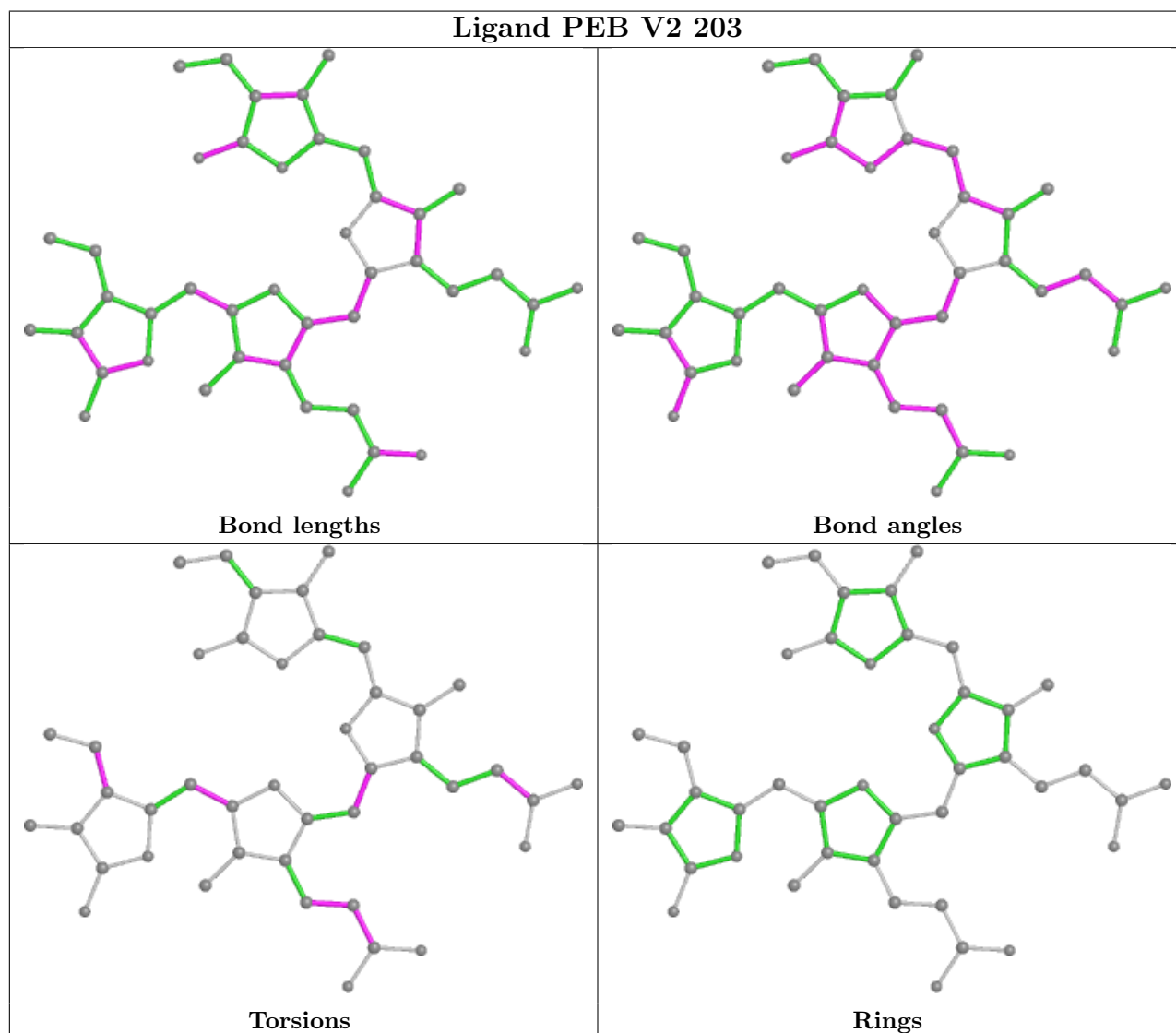
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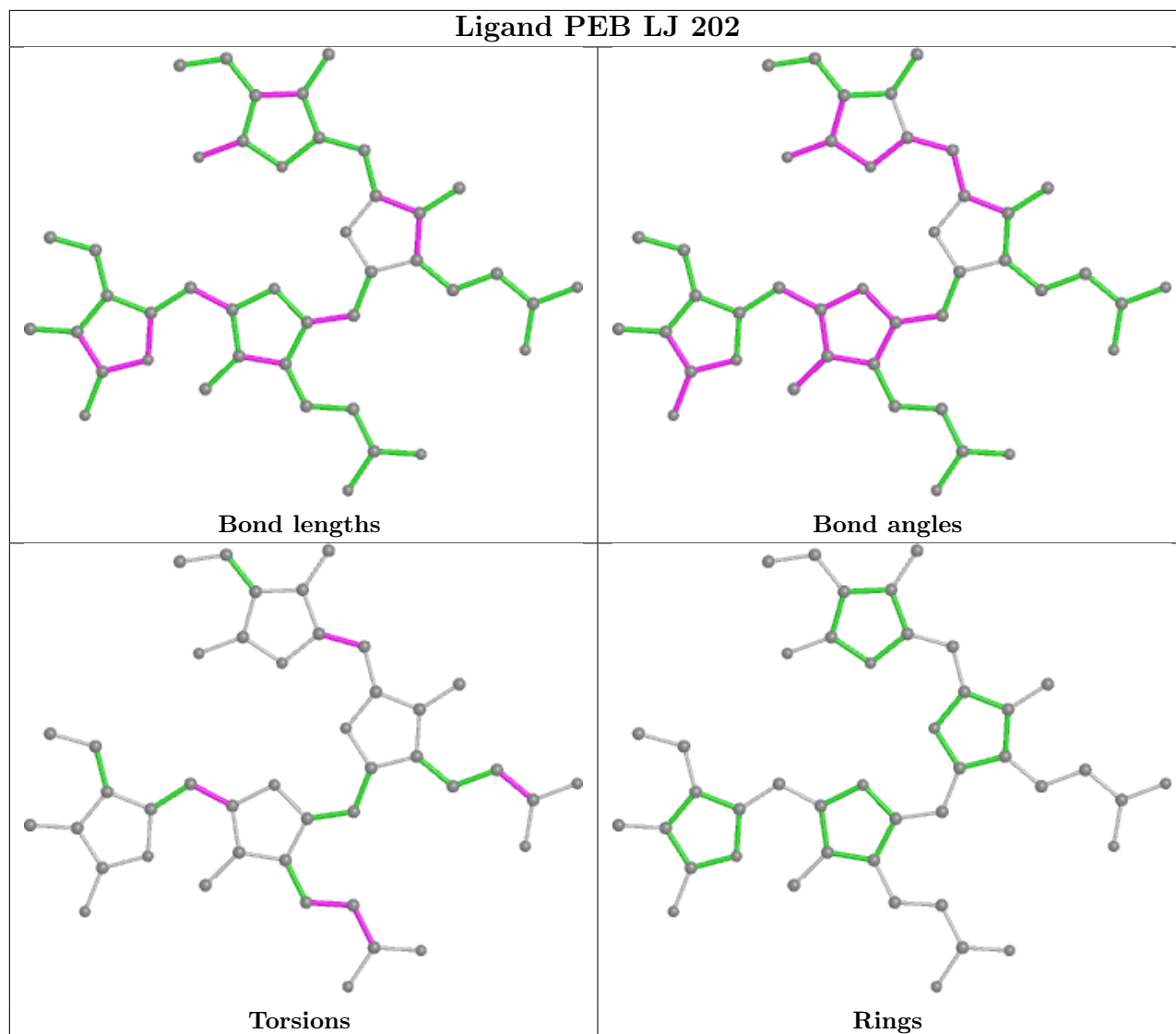
Mol	Chain	Res	Type	Atoms
26	lE	202	PEB	C3B-CAB-CBB-CGB
28	J7	1003	CYC	C2A-CAA-CBA-CGA
28	YH	1001	CYC	C2A-CAA-CBA-CGA
26	Z2	201	PEB	CAB-CBB-CGB-O2B
26	f4	201	PEB	CAB-CBB-CGB-O1B
26	G6	1002	PEB	CAC-CBC-CGC-O1C
26	V6	201	PEB	CAB-CBB-CGB-O2B
26	PB	201	PEB	CAC-CBC-CGC-O1C
26	RB	201	PEB	CAC-CBC-CGC-O1C
26	aB	201	PEB	CAC-CBC-CGC-O2C
26	JC	202	PEB	CAB-CBB-CGB-O2B
26	LC	201	PEB	CAC-CBC-CGC-O2C
26	wE	302	PEB	CAC-CBC-CGC-O1C
26	uG	203	PEB	CAB-CBB-CGB-O1B
26	UI	201	PEB	CAB-CBB-CGB-O2B
26	IJ	201	PEB	CAC-CBC-CGC-O1C
28	J2	1001	CYC	CAD-CBD-CGD-O2D
28	kH	1001	CYC	CAA-CBA-CGA-O1A
26	W2	201	PEB	CAB-CBB-CGB-O2B
26	g2	202	PEB	CAB-CBB-CGB-O1B
26	g2	203	PEB	CAB-CBB-CGB-O2B
26	Z4	201	PEB	CAC-CBC-CGC-O2C
26	n4	201	PEB	CAC-CBC-CGC-O2C
26	F5	202	PEB	CAC-CBC-CGC-O2C
26	b6	201	PEB	CAB-CBB-CGB-O2B
26	P8	201	PEB	CAB-CBB-CGB-O1B
26	dB	203	PEB	CAC-CBC-CGC-O1C
26	gB	201	PEB	CAB-CBB-CGB-O2B
26	iB	201	PEB	CAB-CBB-CGB-O2B
26	CC	203	PEB	CAB-CBB-CGB-O2B
26	LD	201	PEB	CAC-CBC-CGC-O2C
26	NE	202	PEB	CAC-CBC-CGC-O1C
26	eE	201	PEB	CAC-CBC-CGC-O1C
26	uE	201	PEB	CAB-CBB-CGB-O1B
26	uG	203	PEB	CAB-CBB-CGB-O2B
28	K6	202	CYC	CAD-CBD-CGD-O2D
28	N7	1001	CYC	CAD-CBD-CGD-O1D
28	KB	202	CYC	CAD-CBD-CGD-O2D
28	KF	1001	CYC	CAD-CBD-CGD-O1D

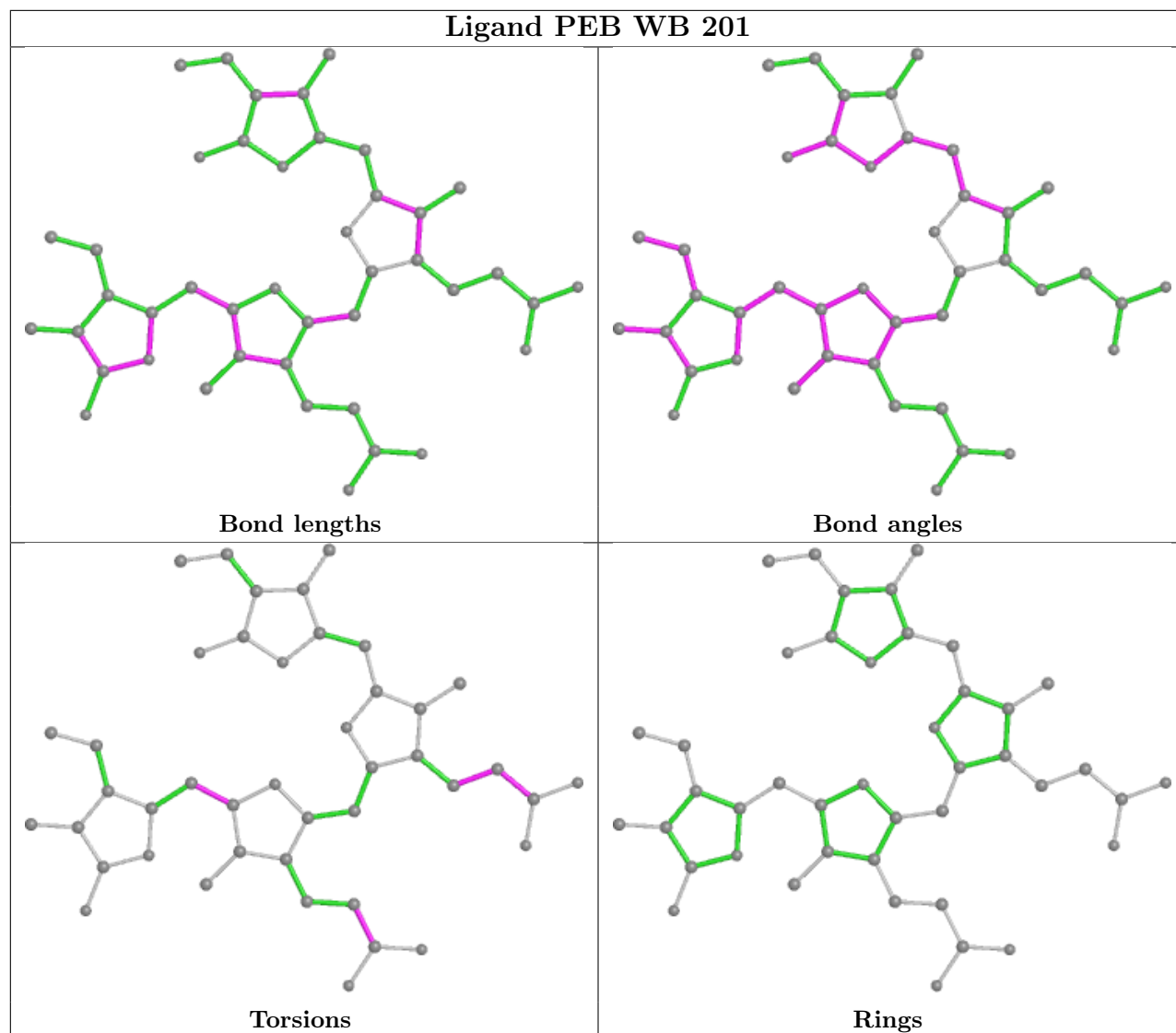
There are no ring outliers.

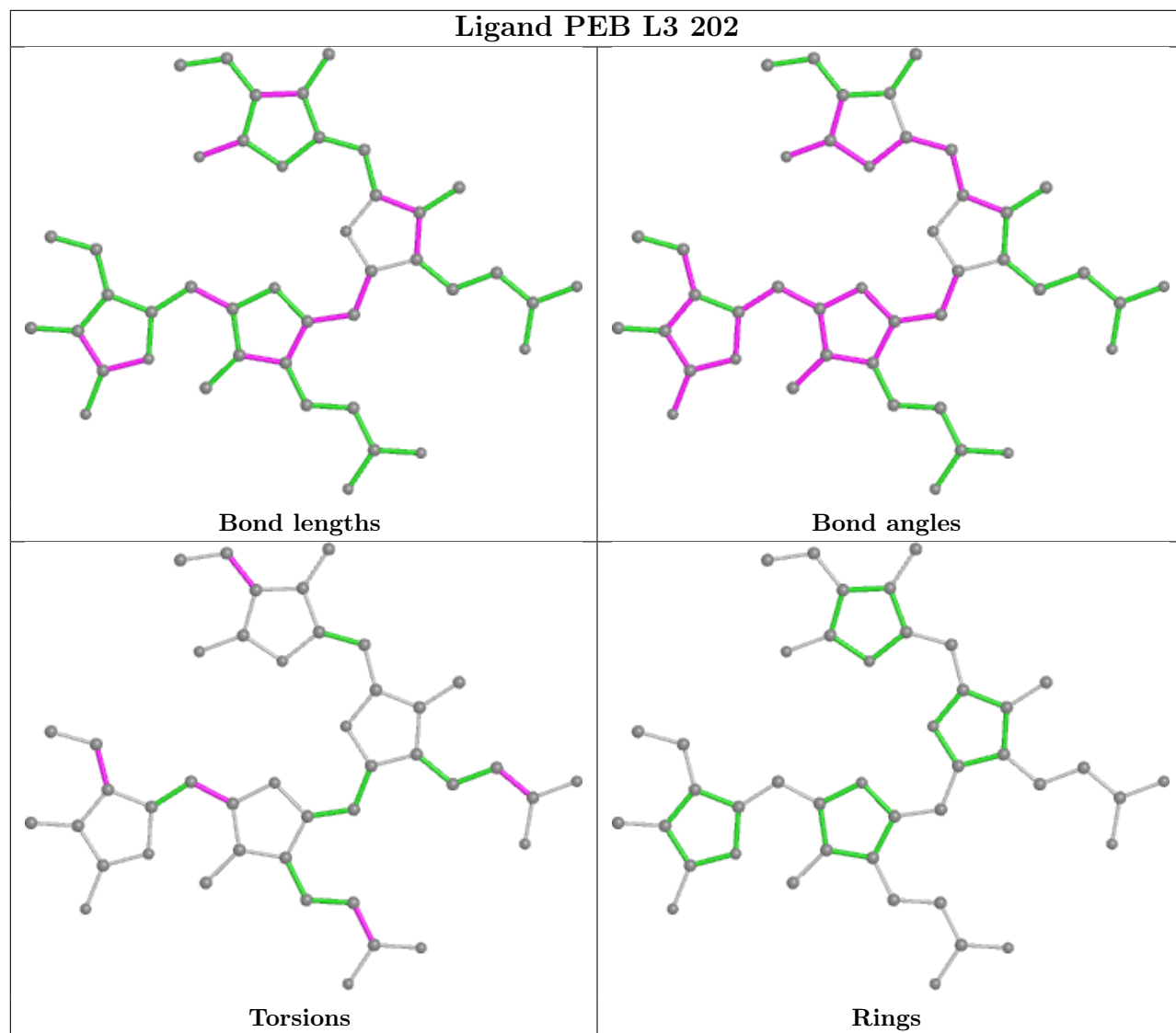
No monomer is involved in short contacts.

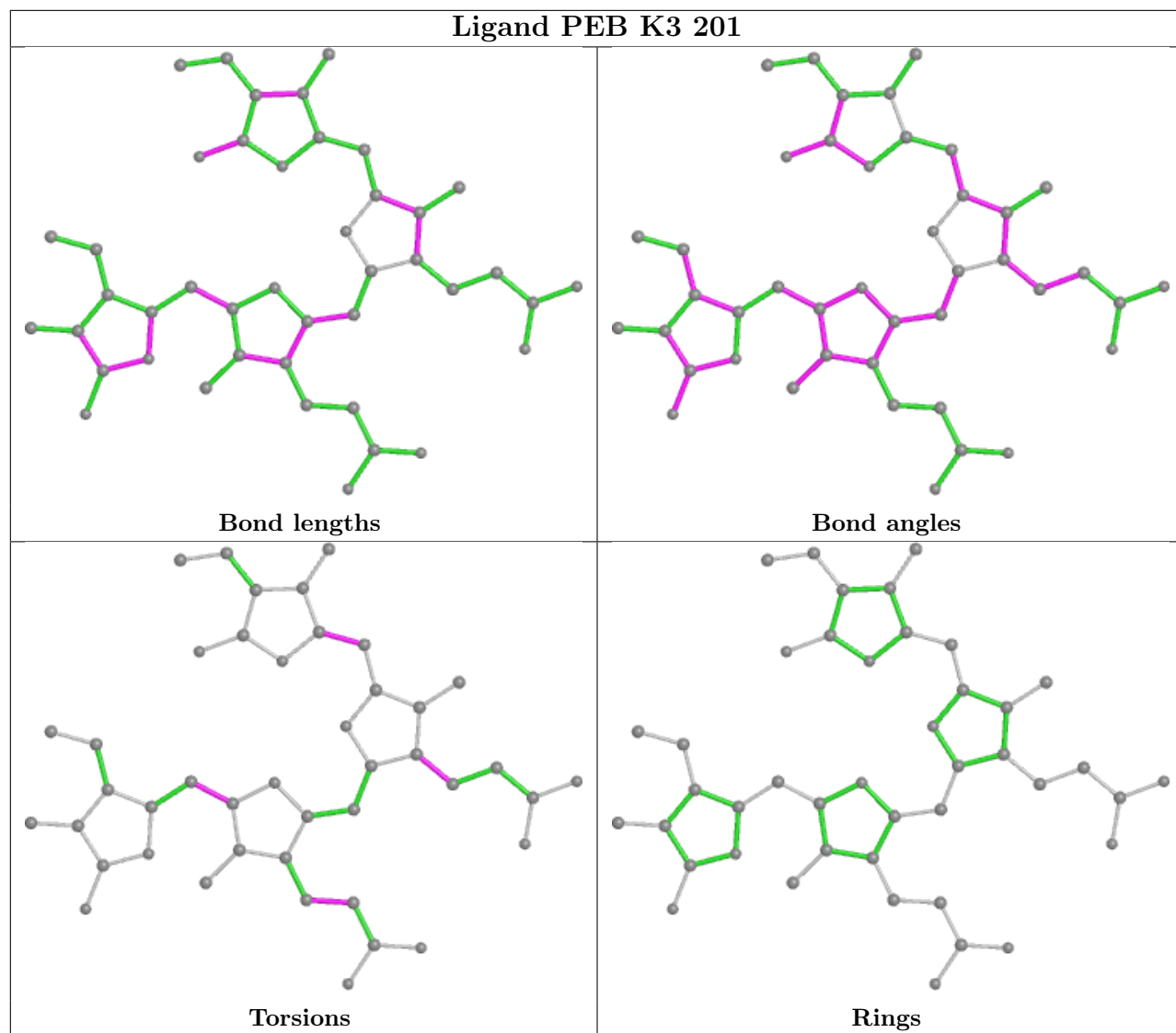
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

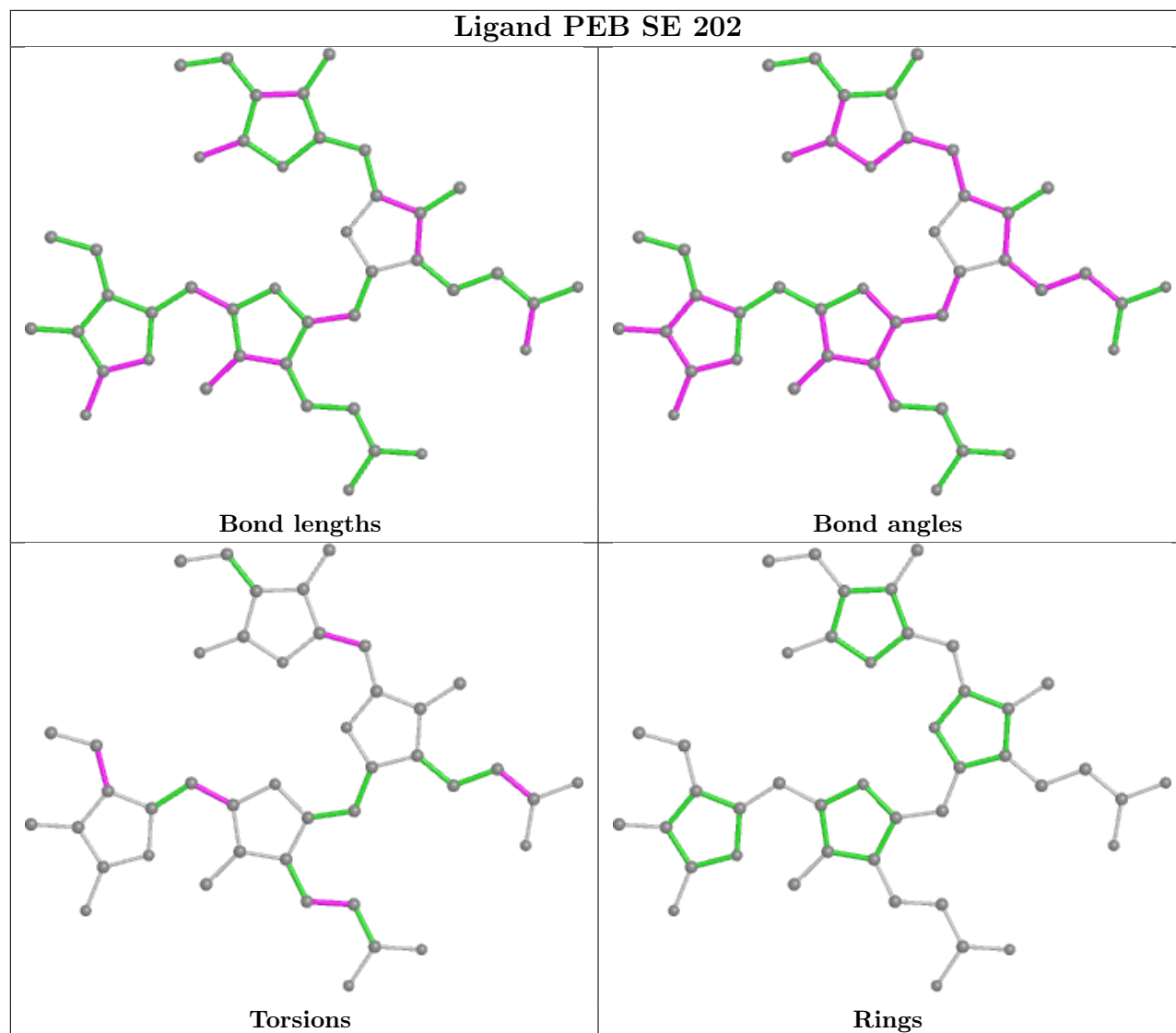


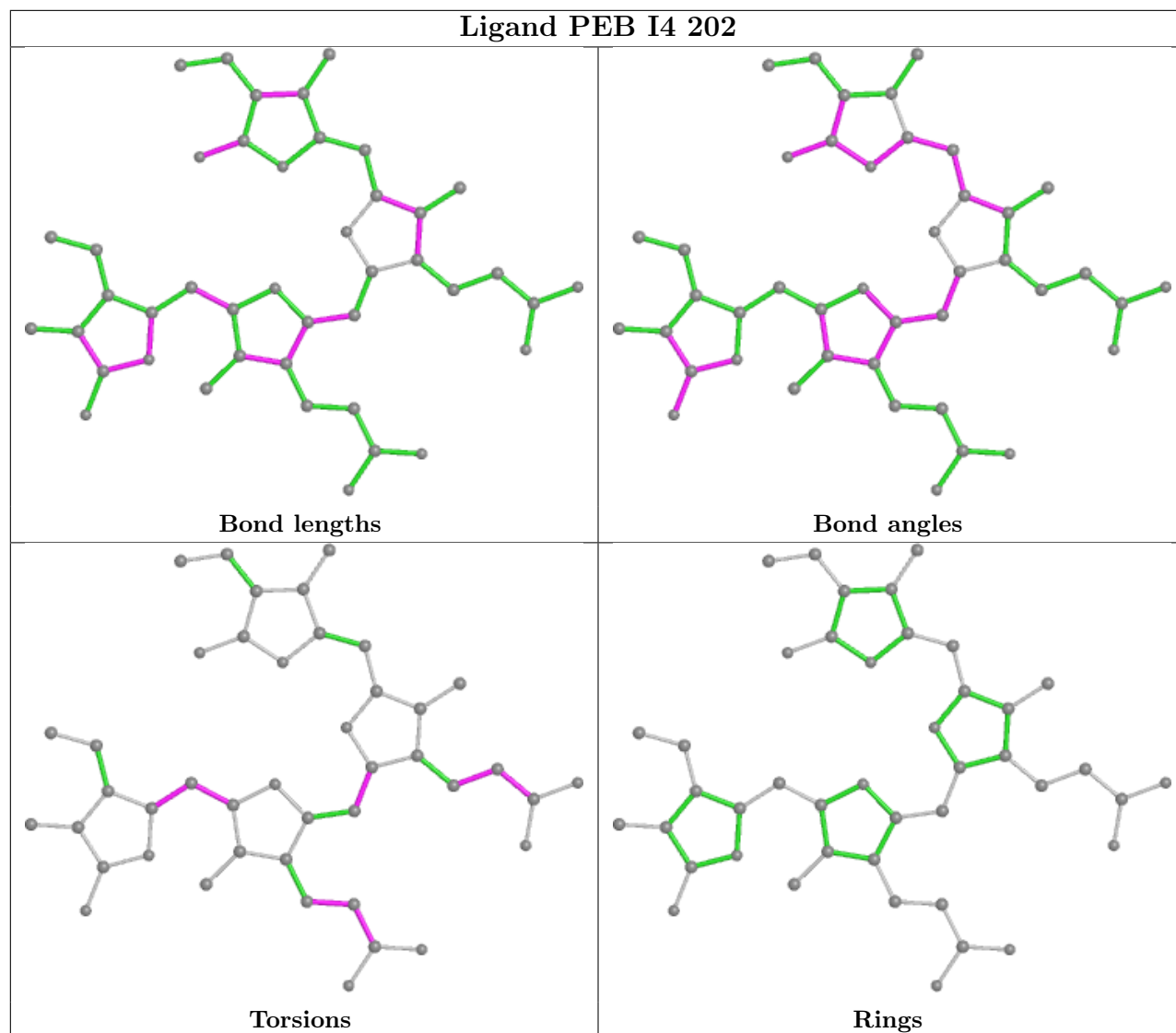


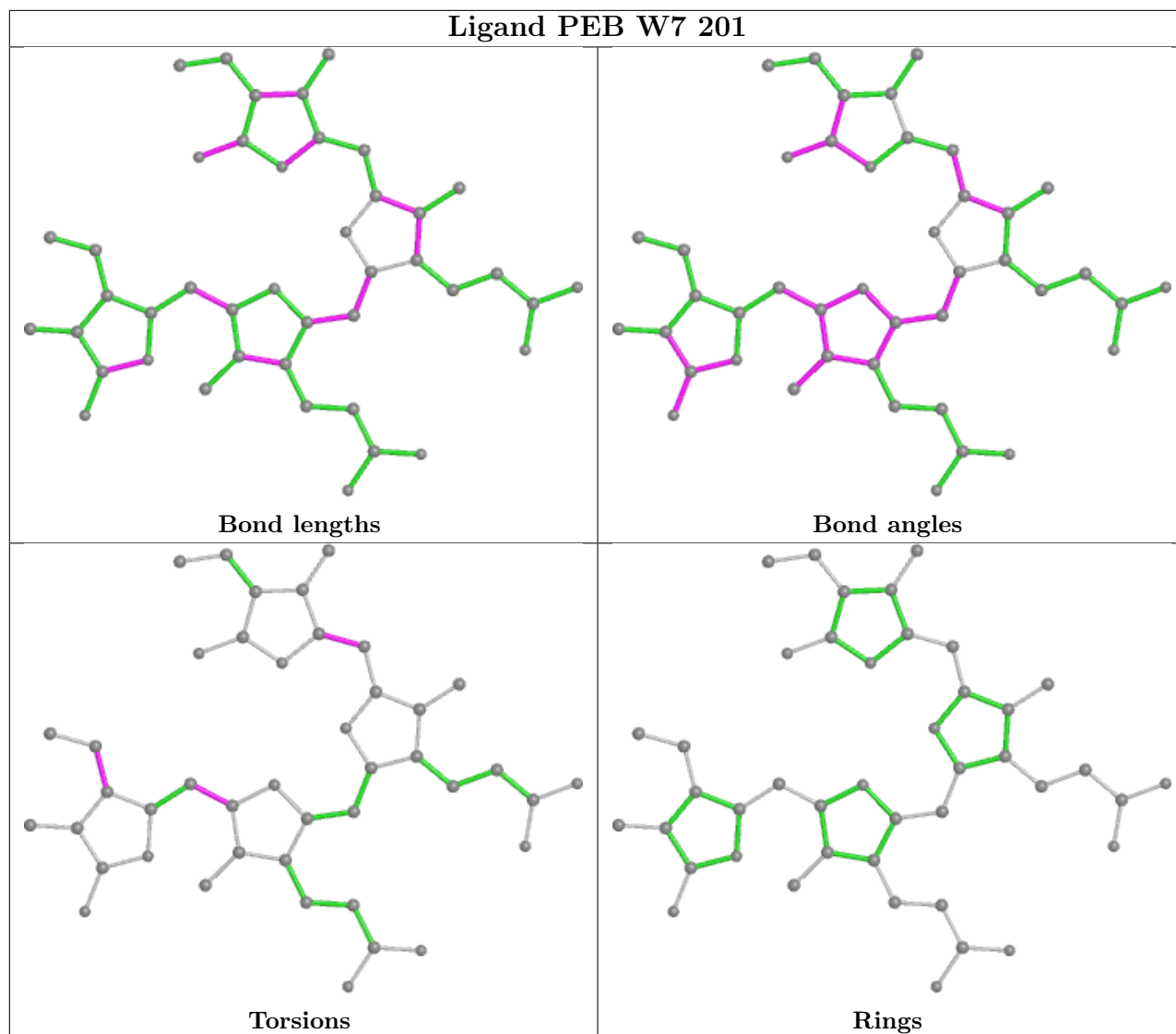


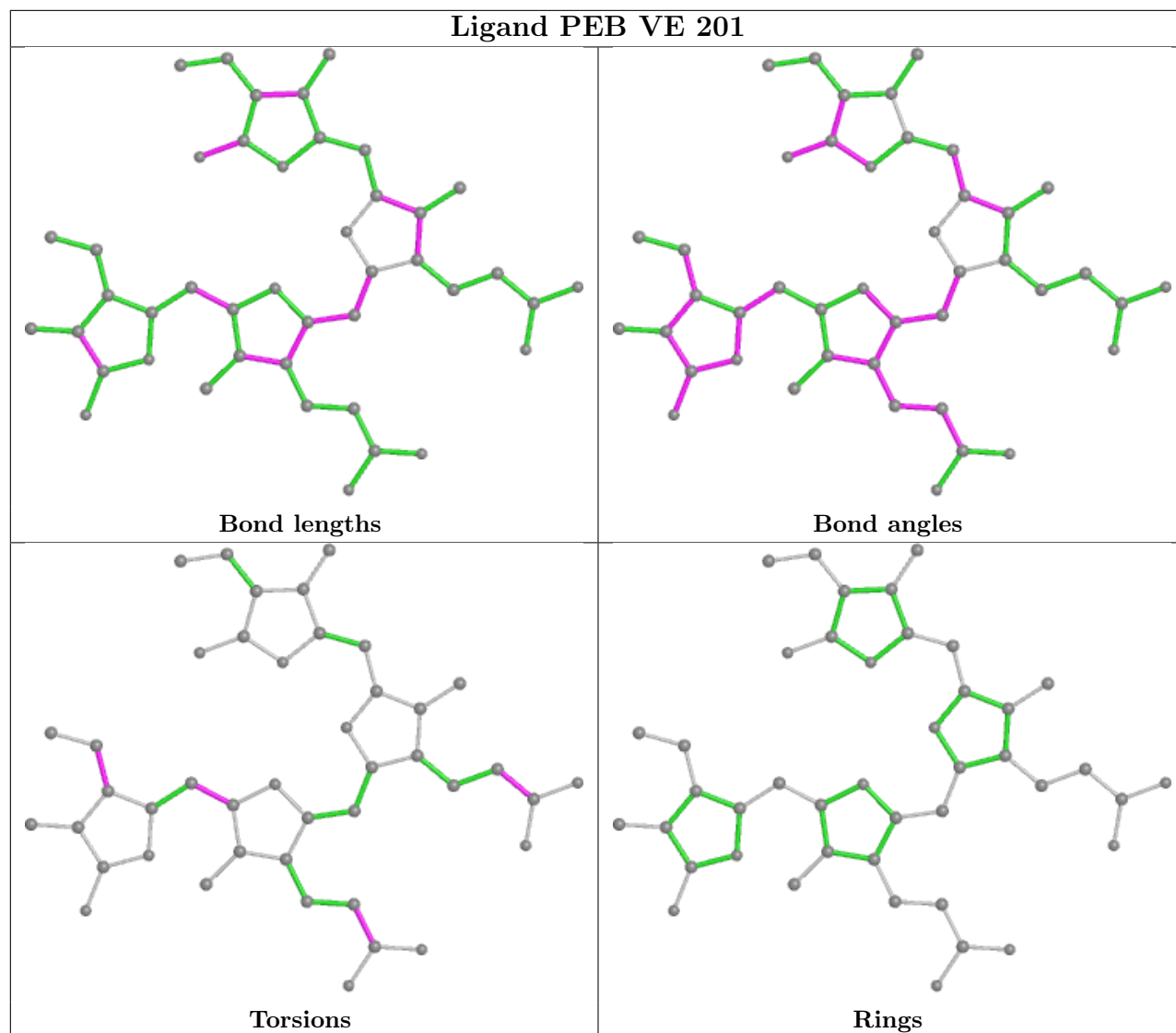


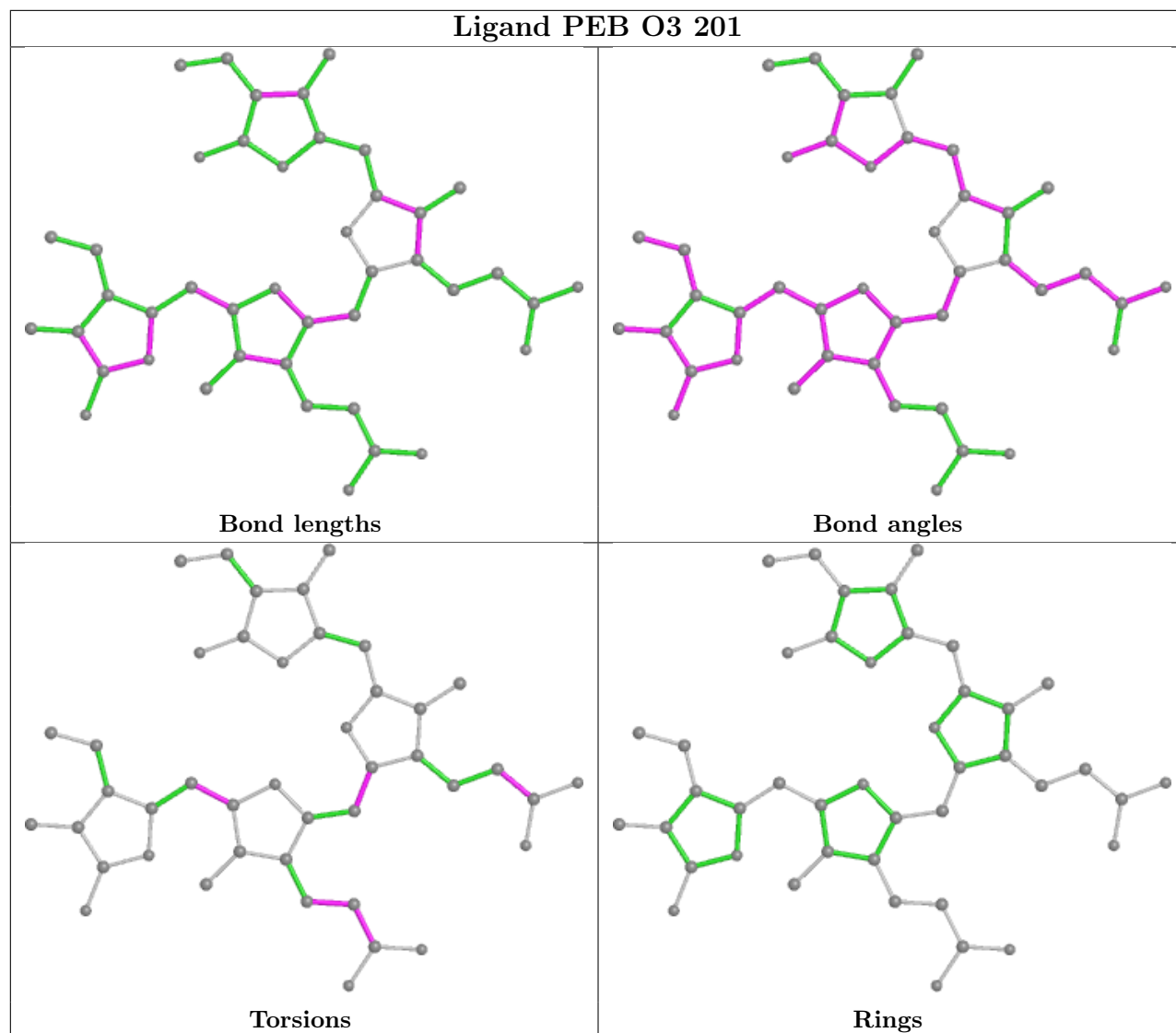


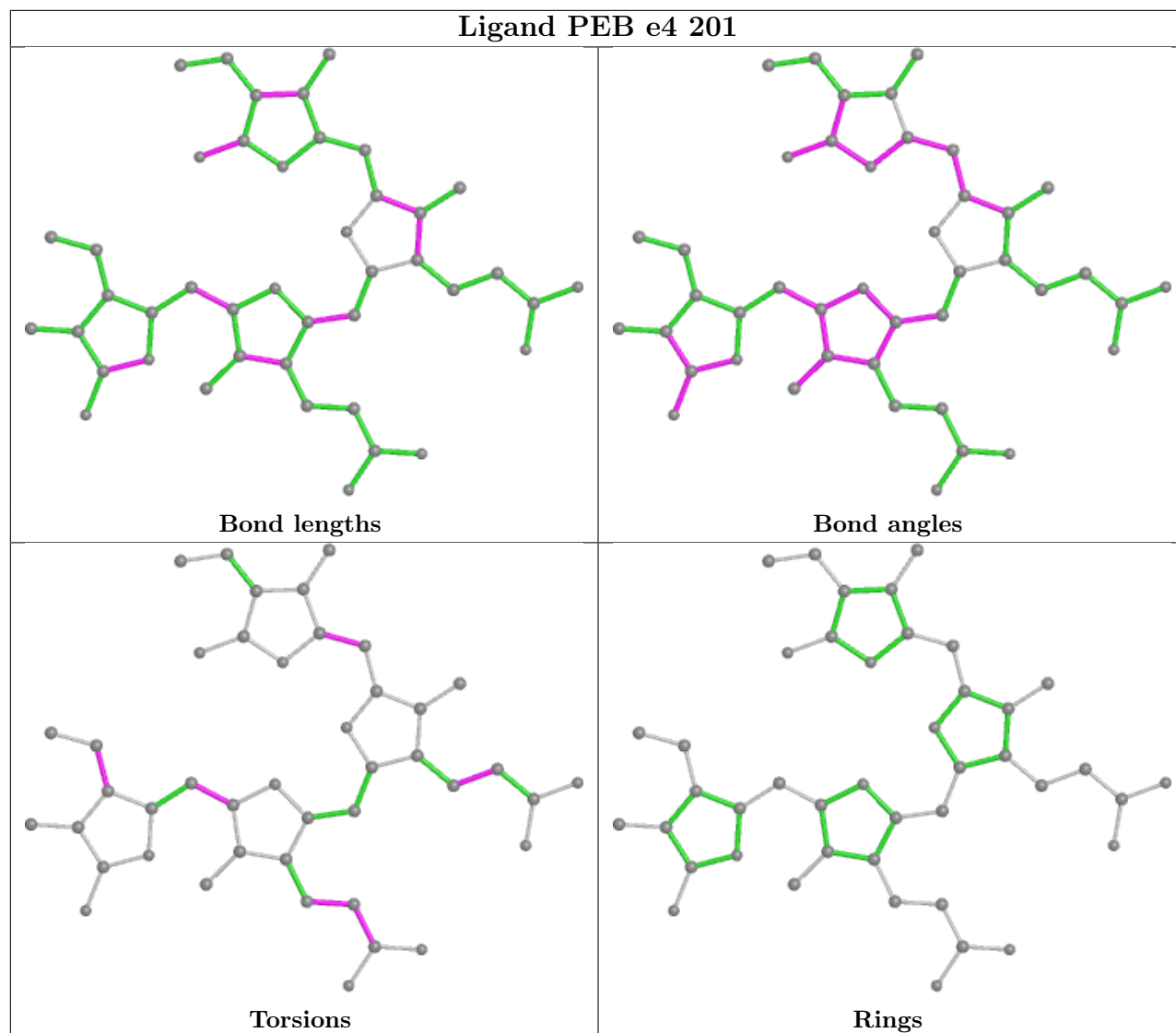


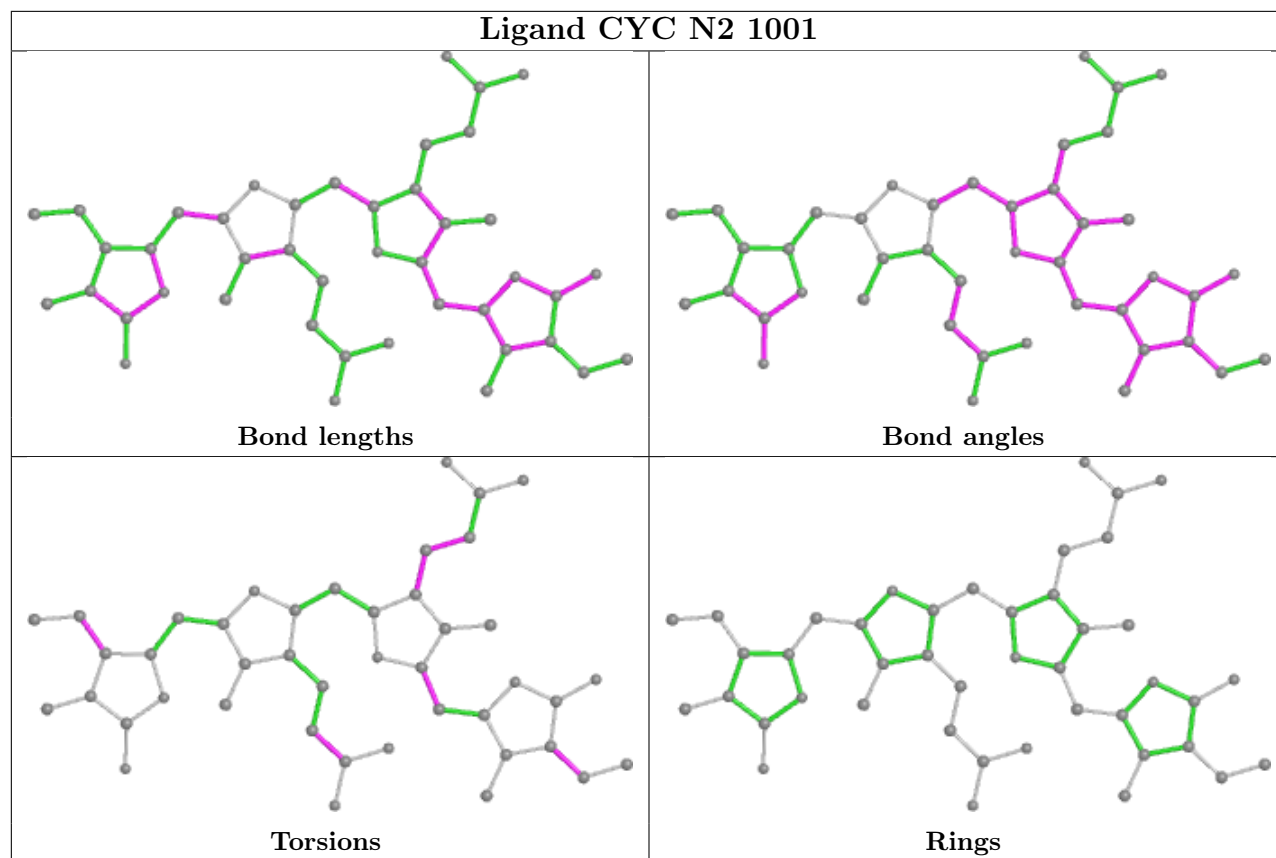


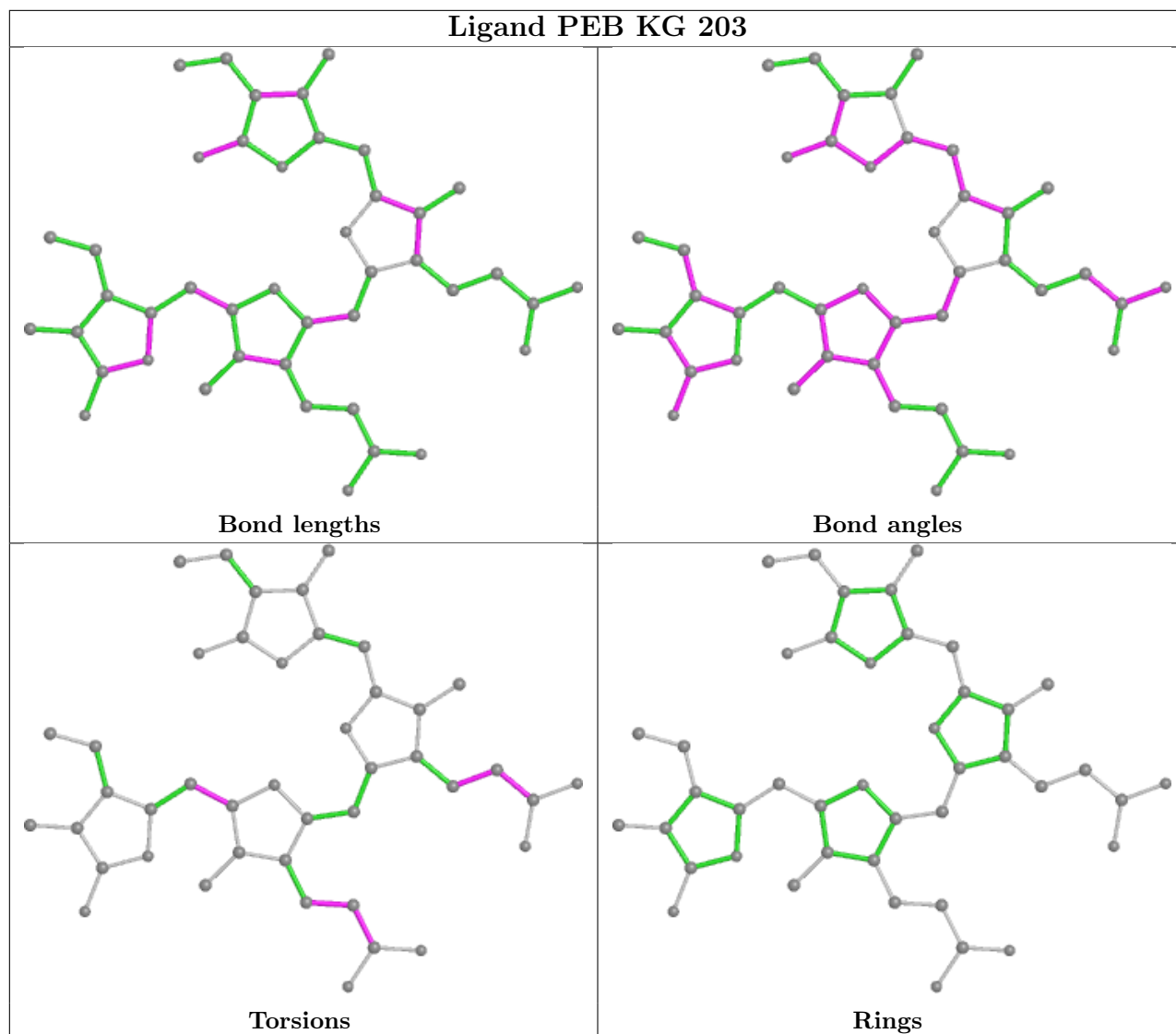


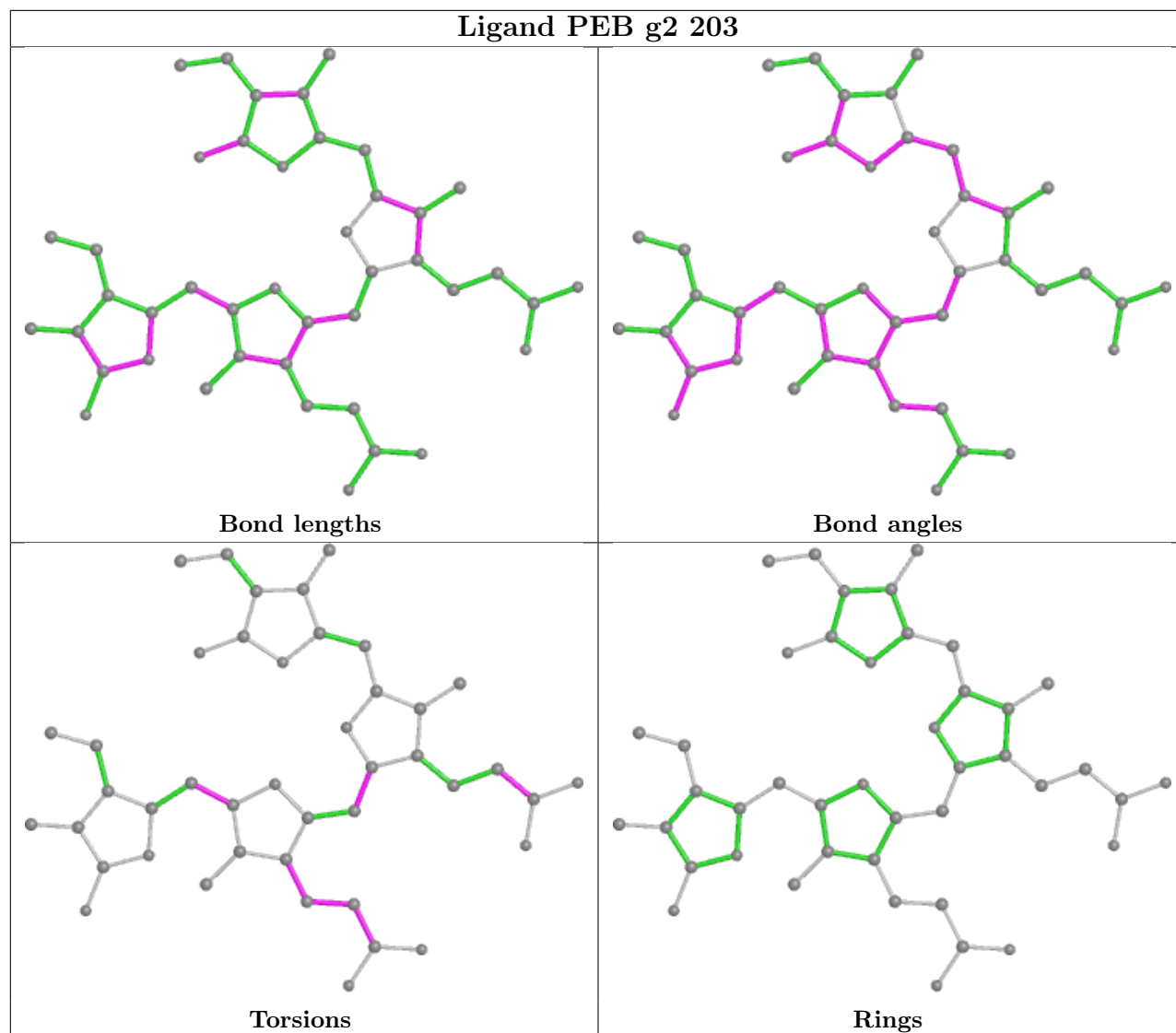


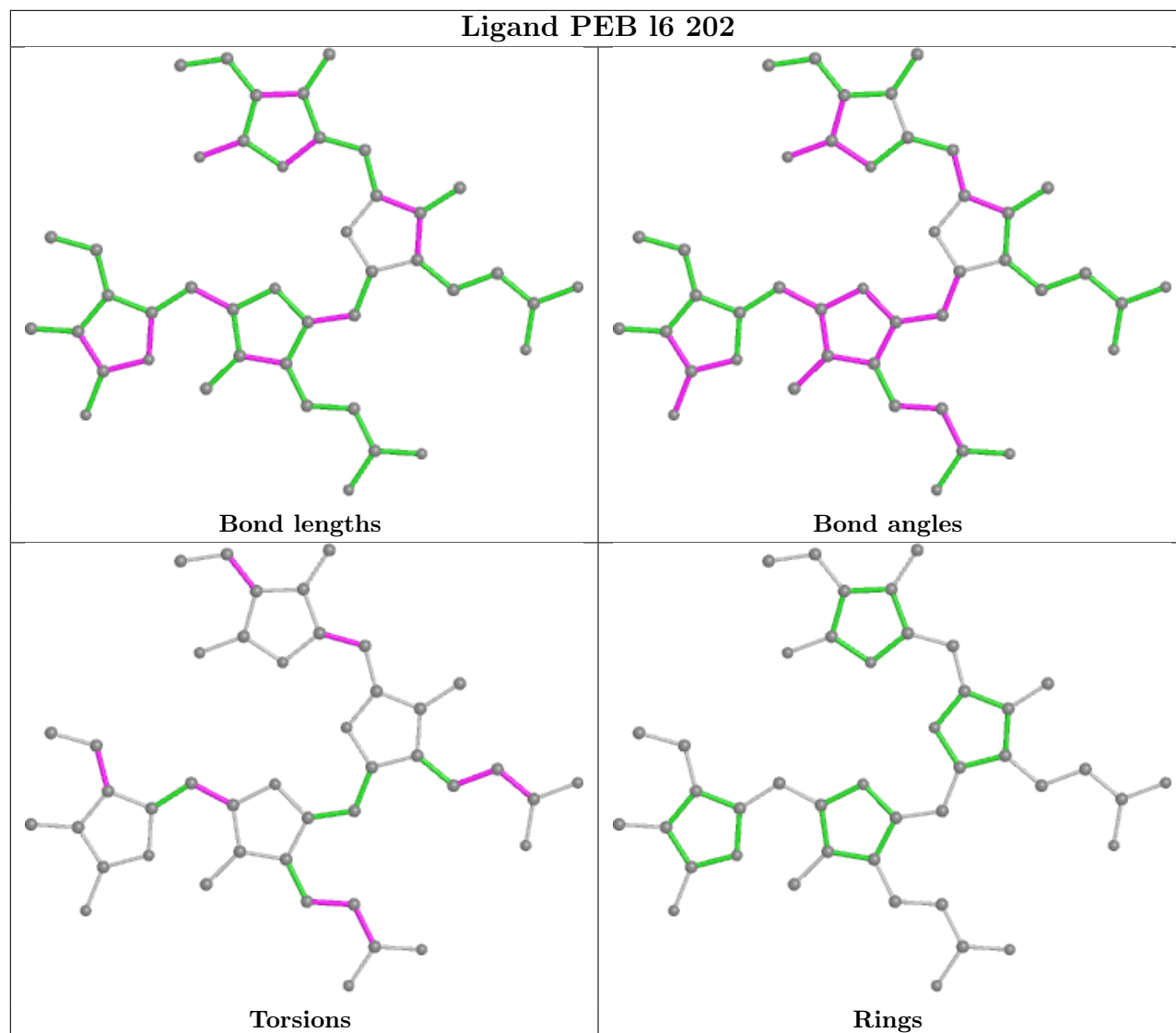


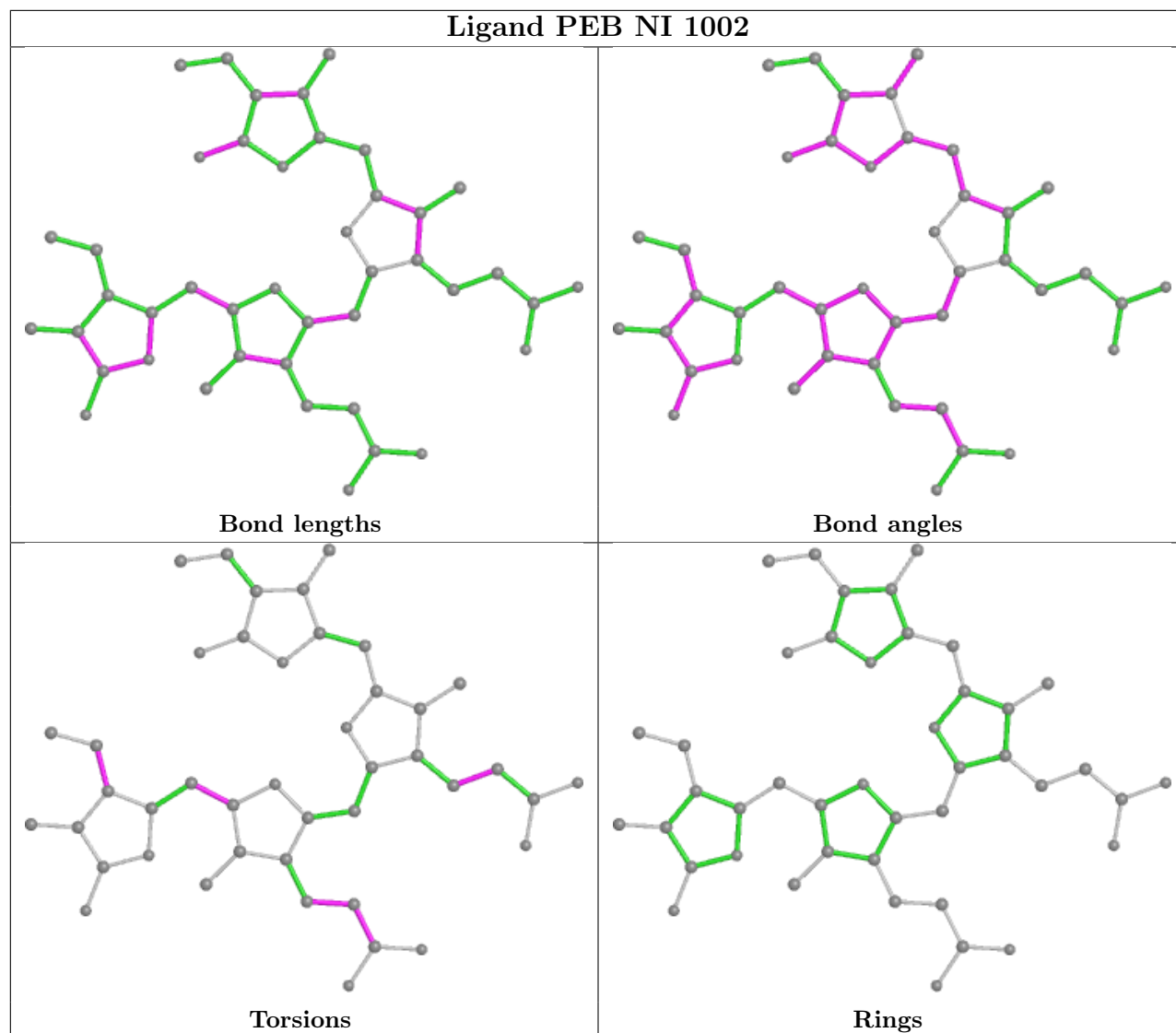


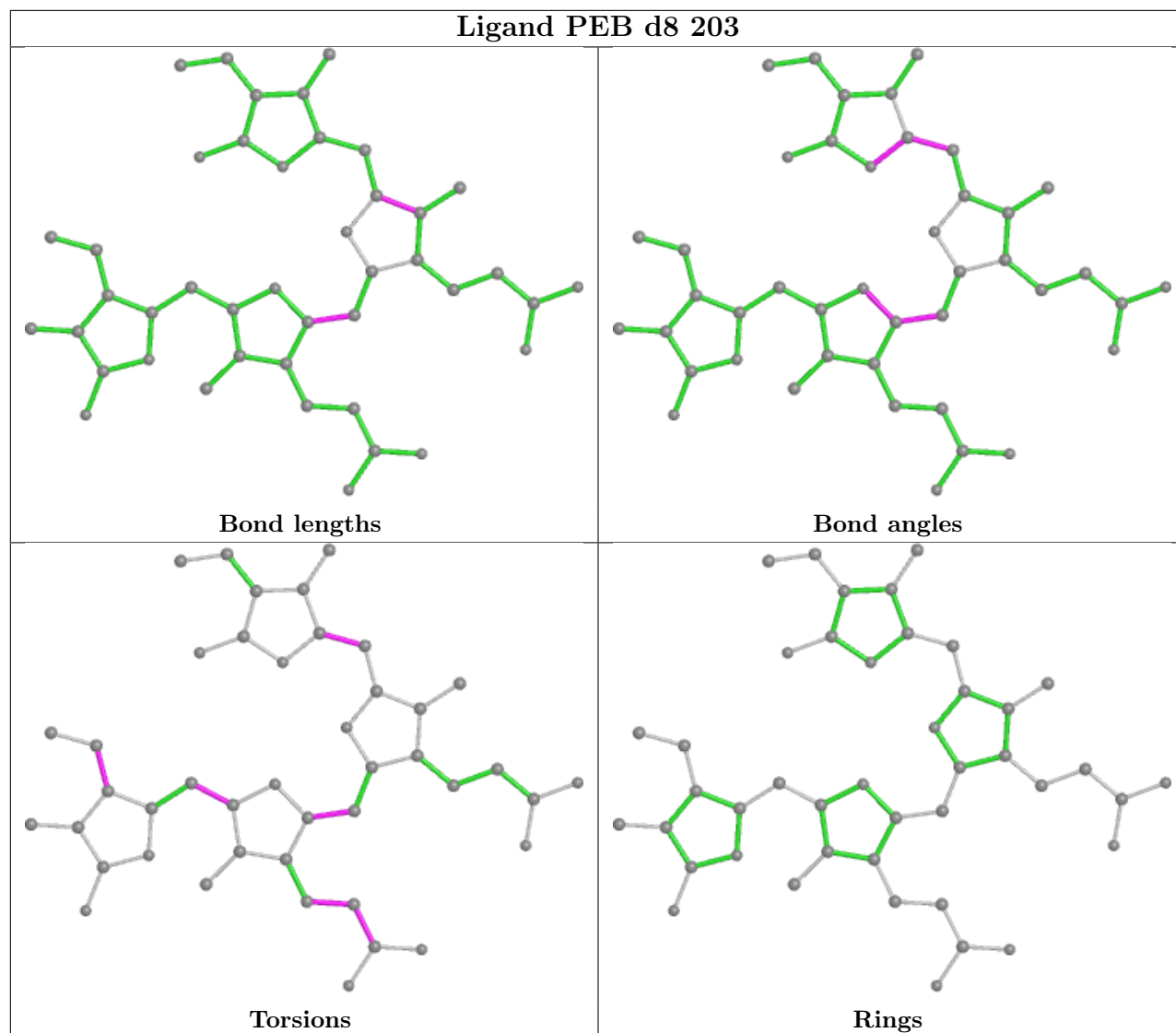


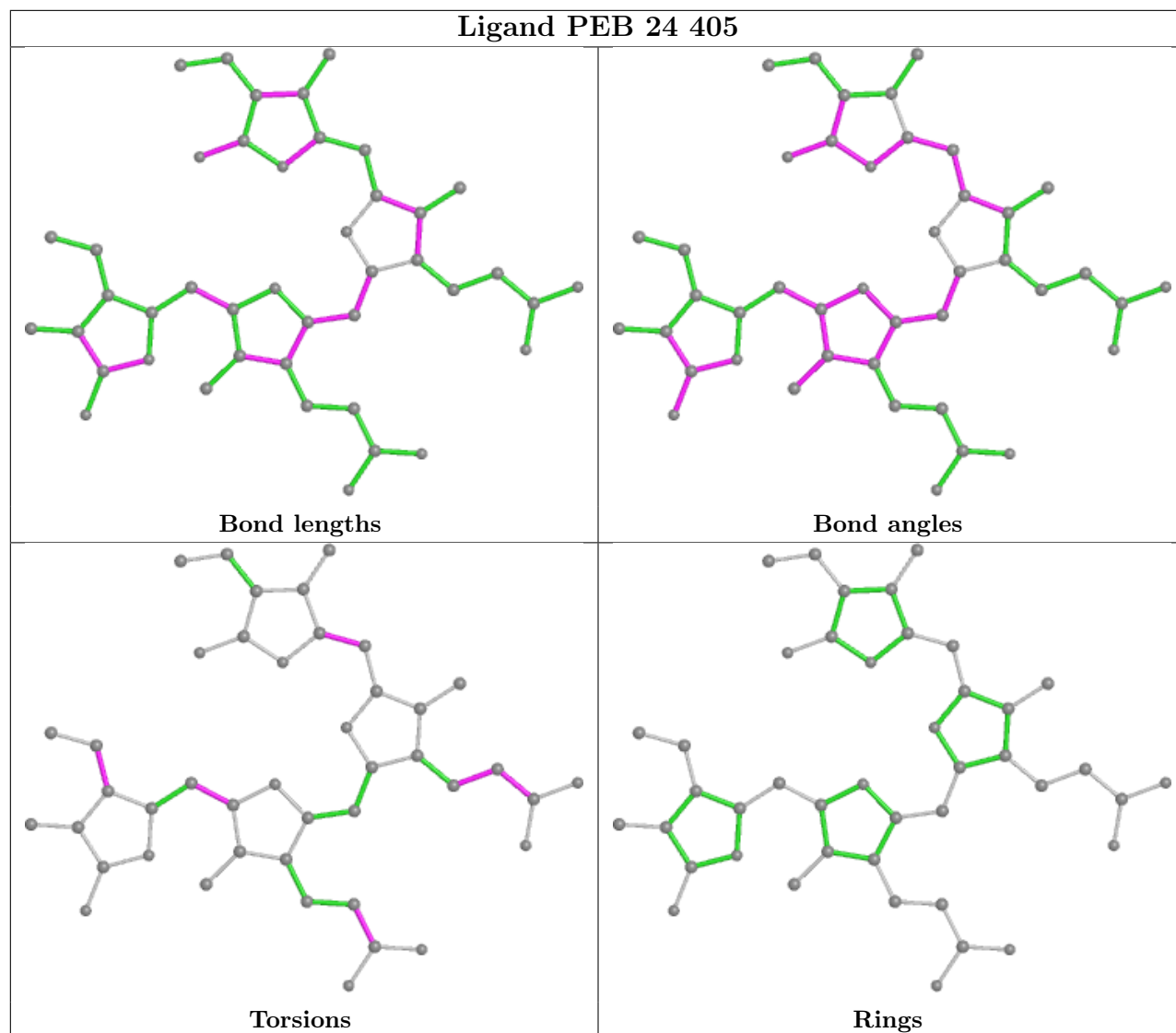


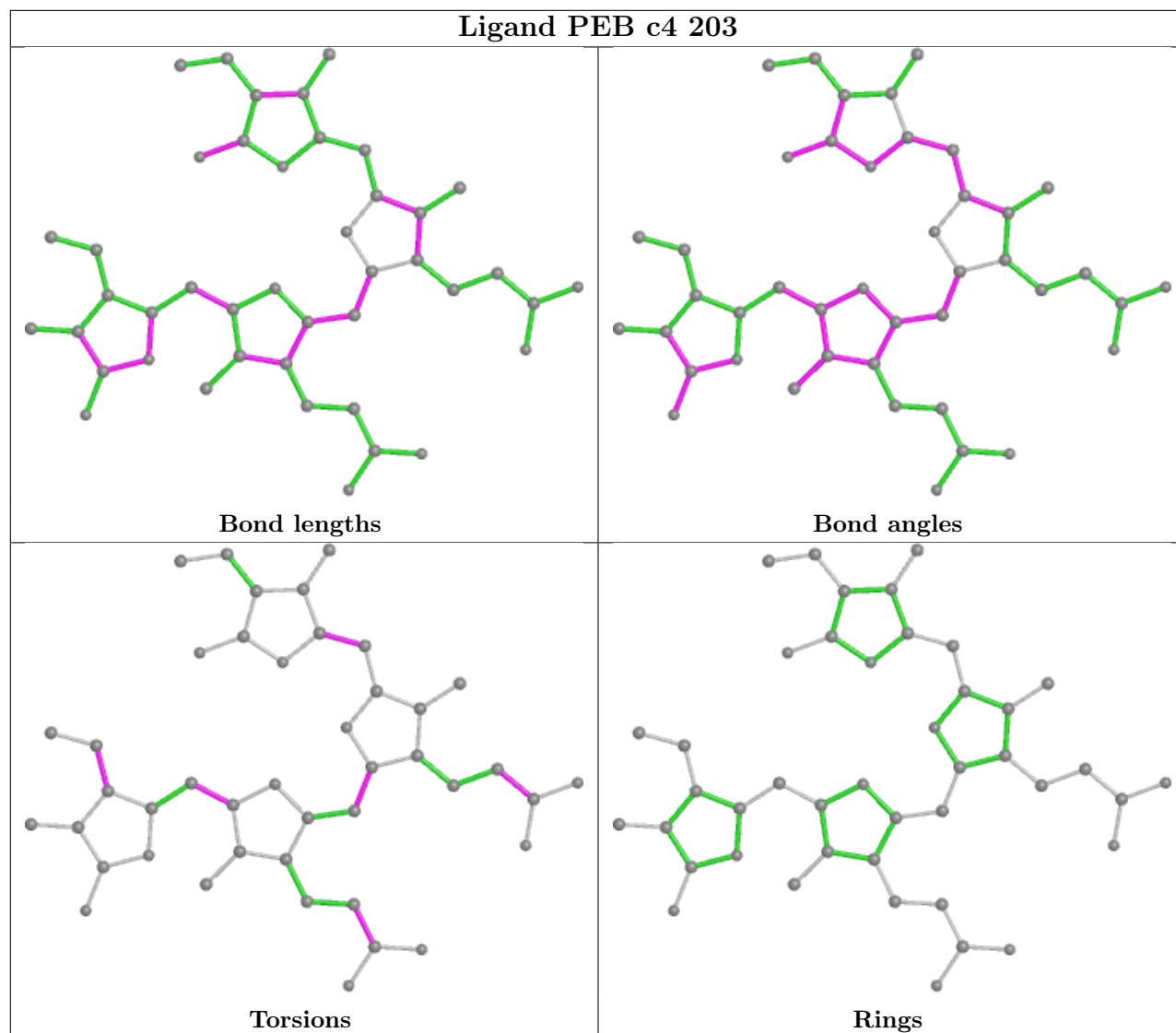


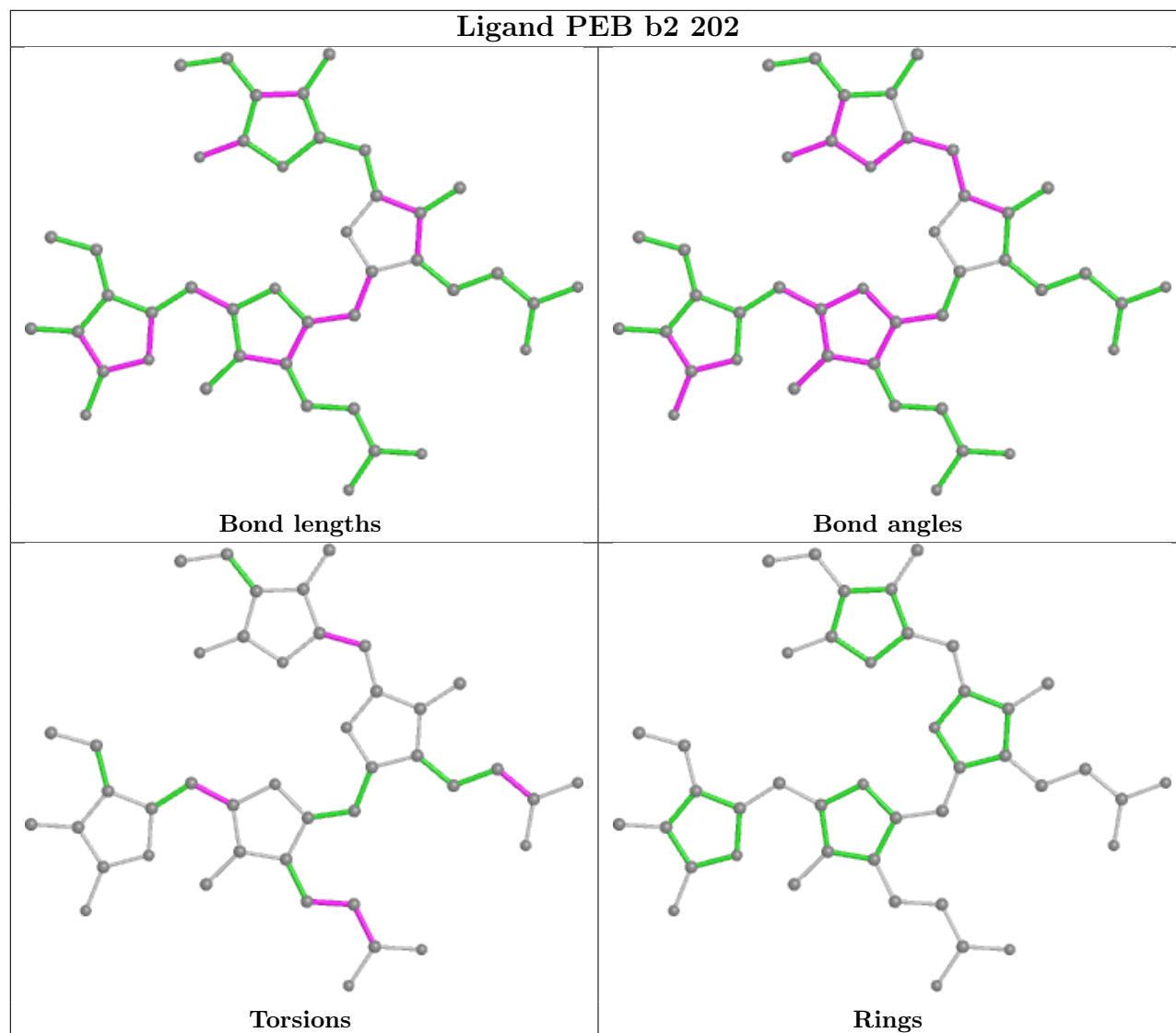


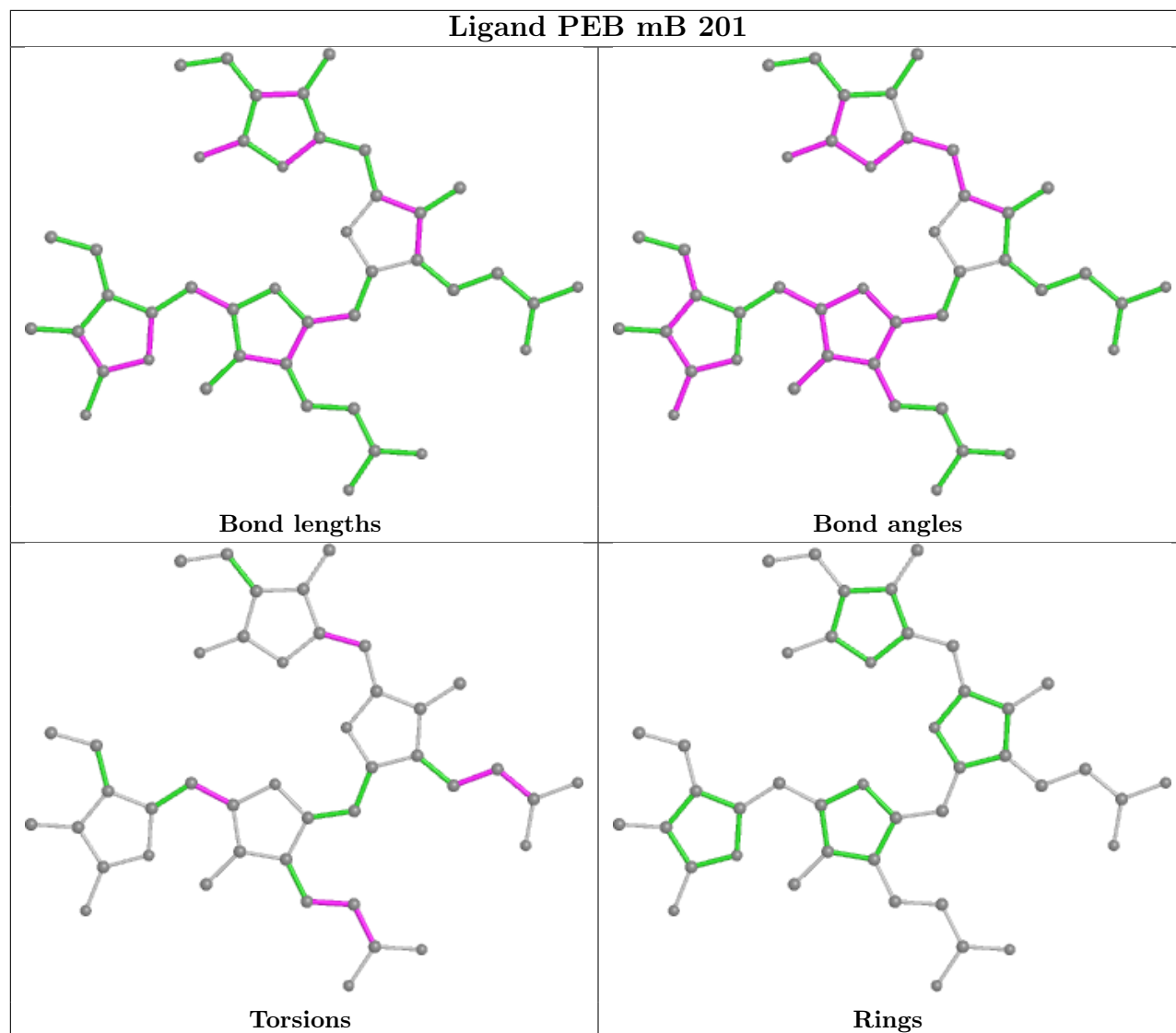


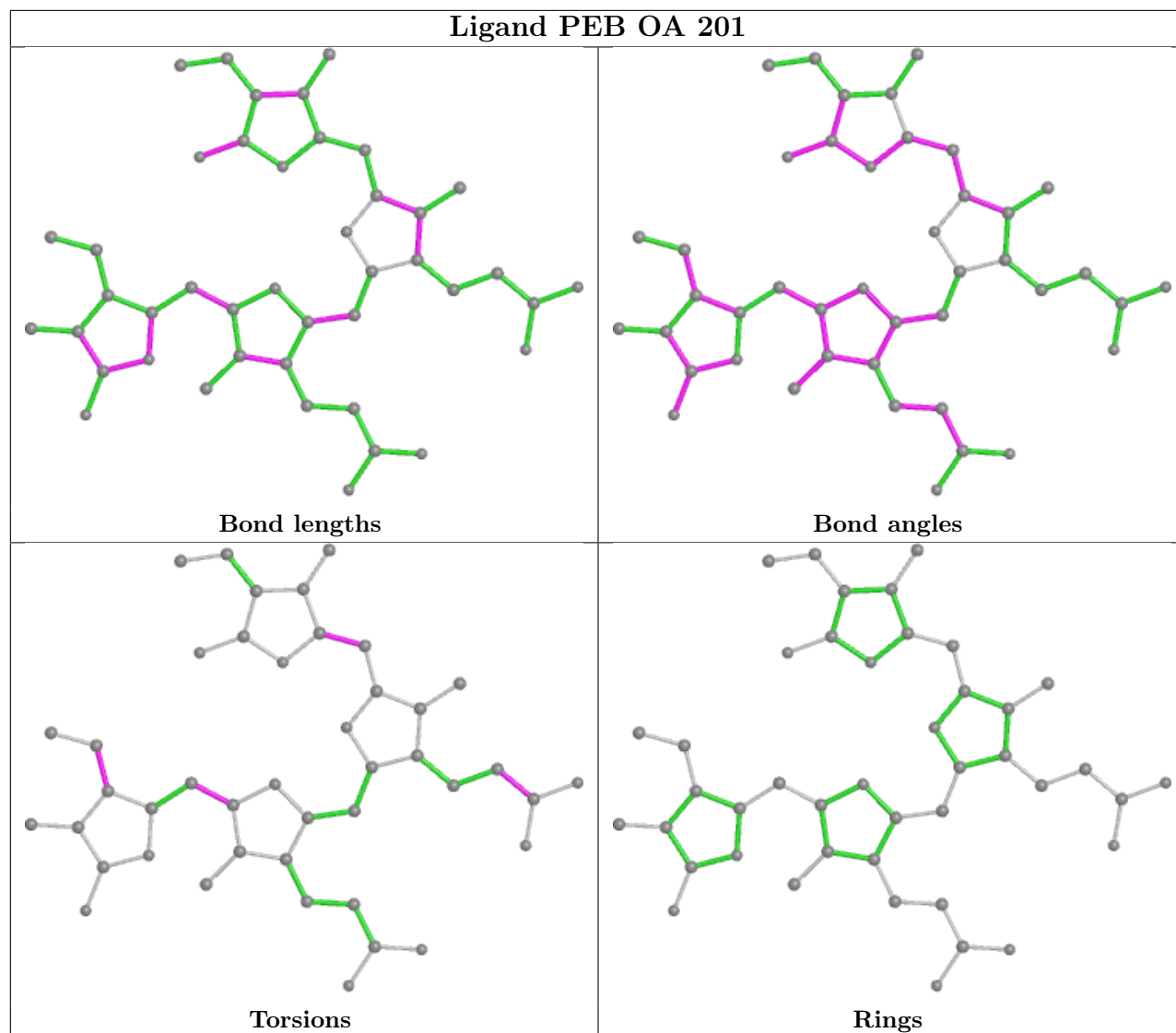


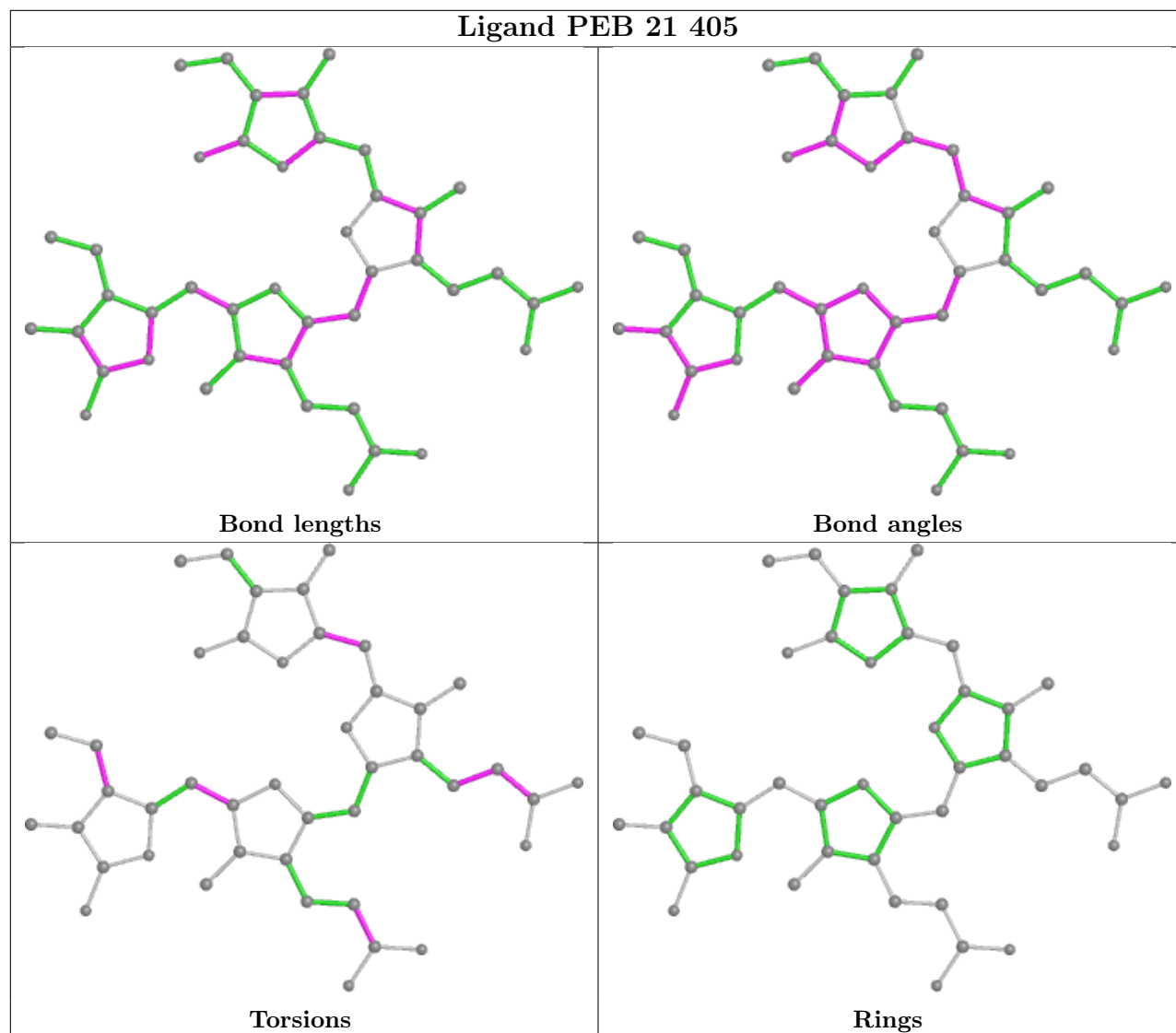


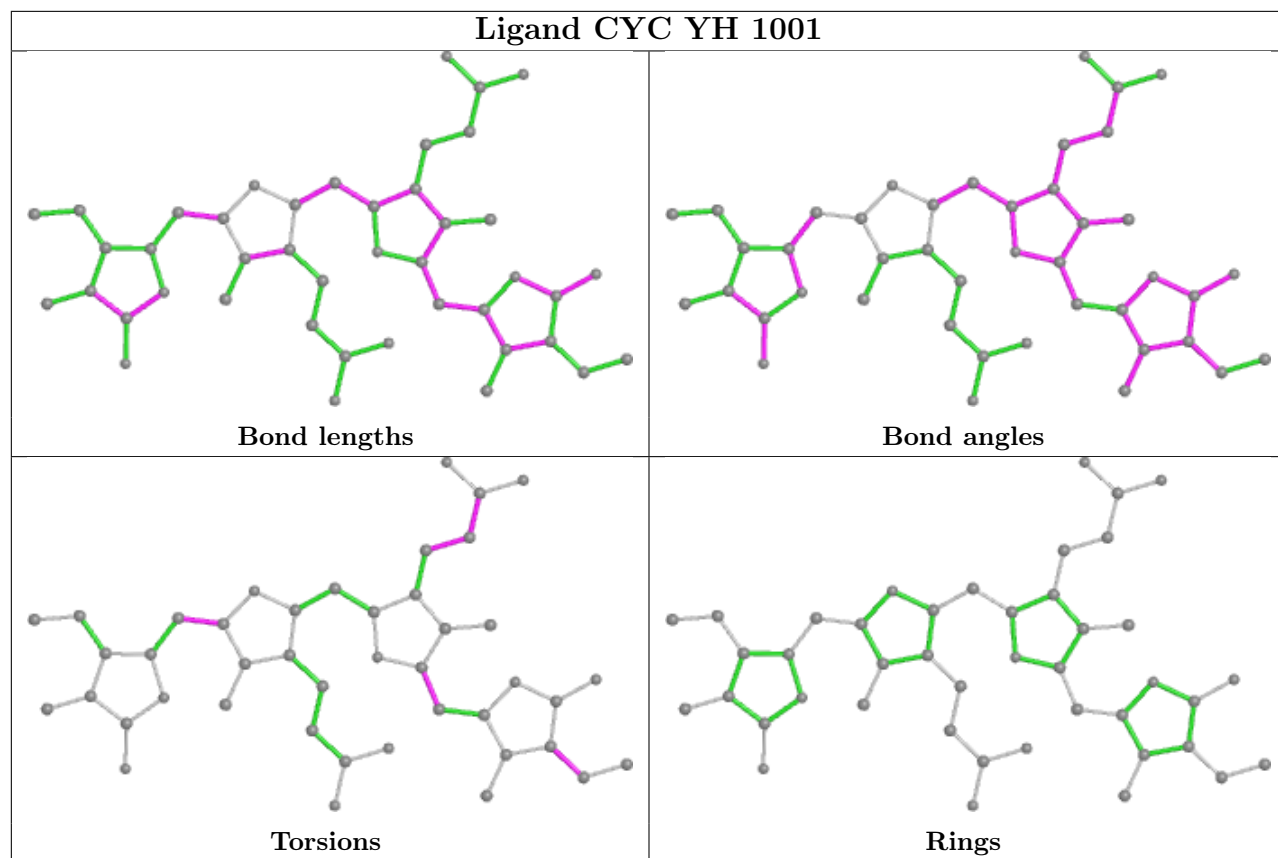


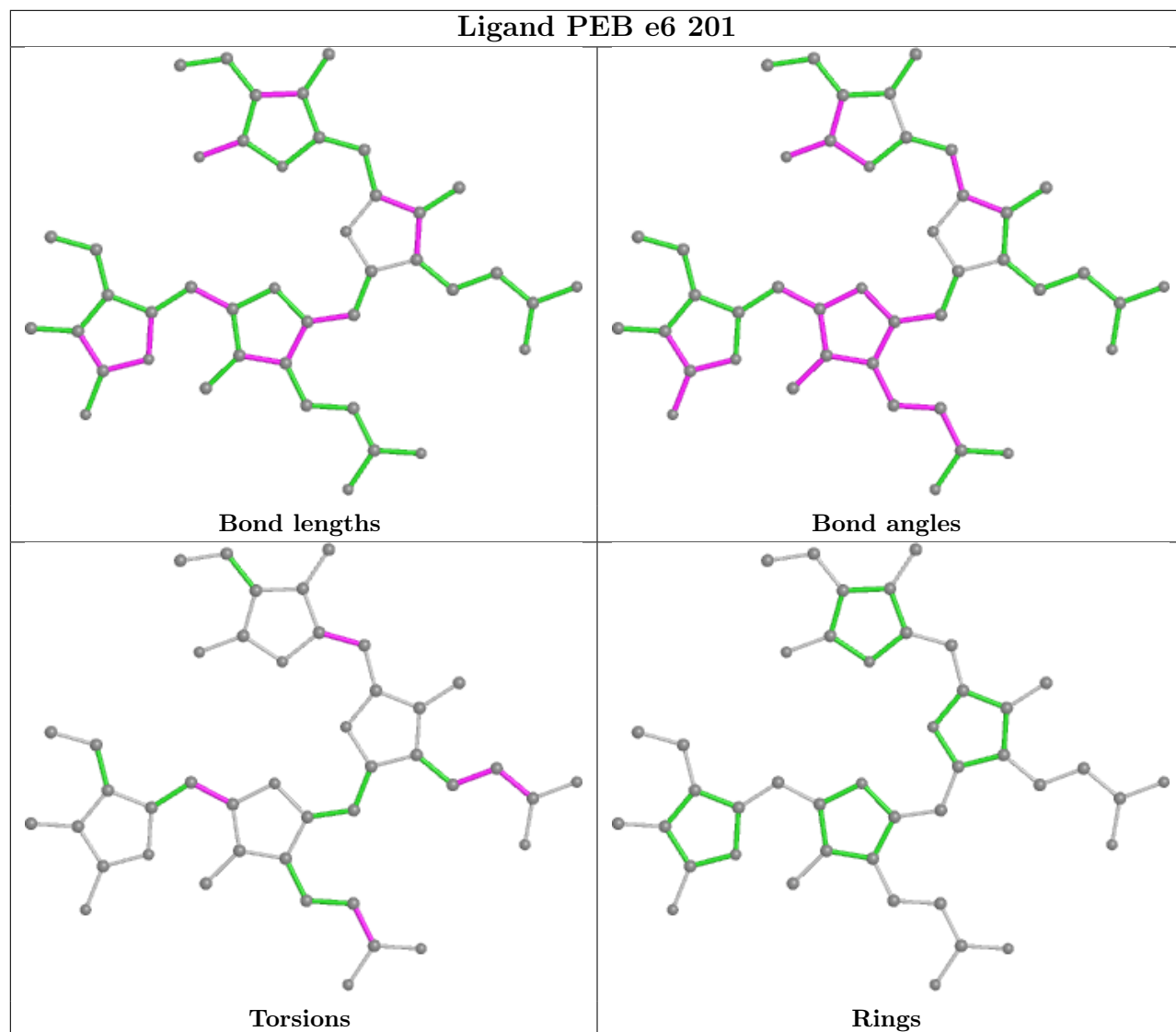


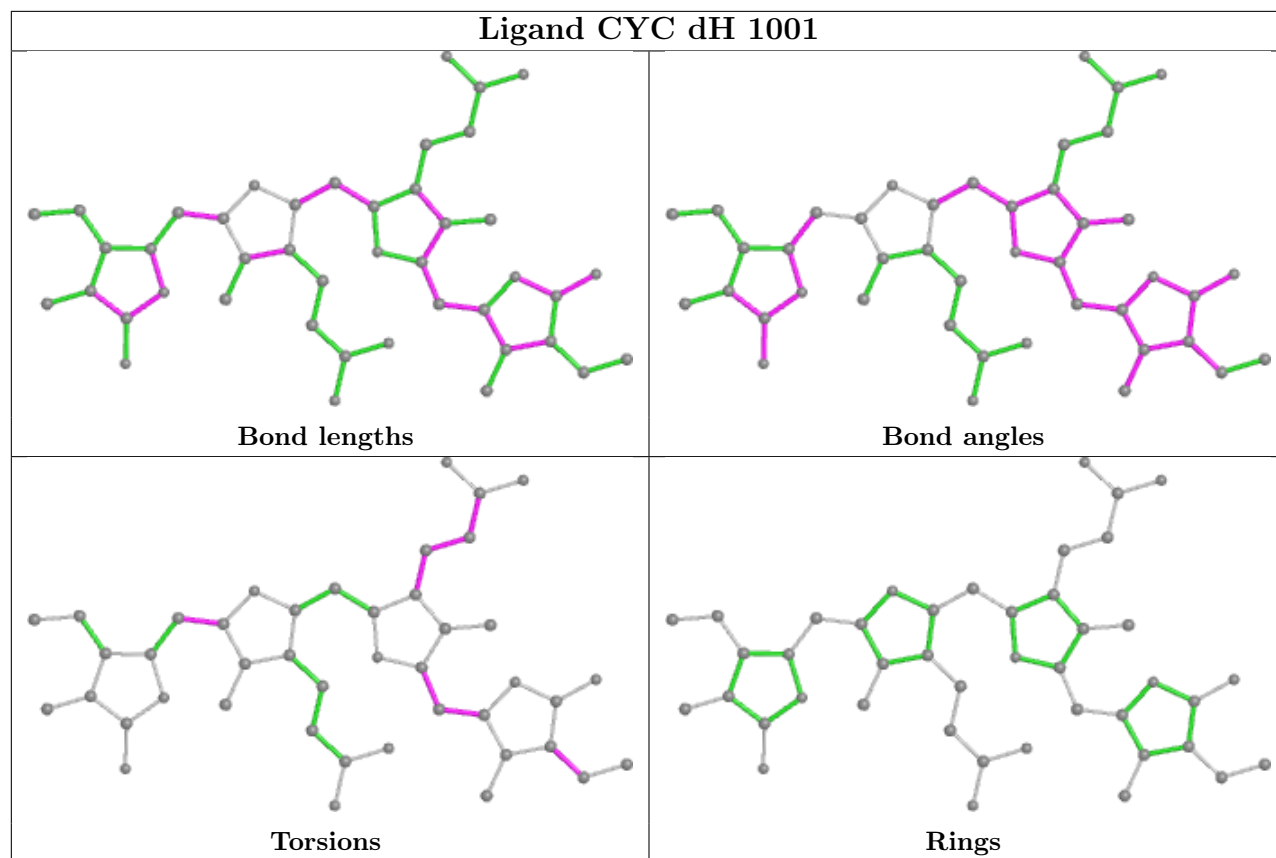


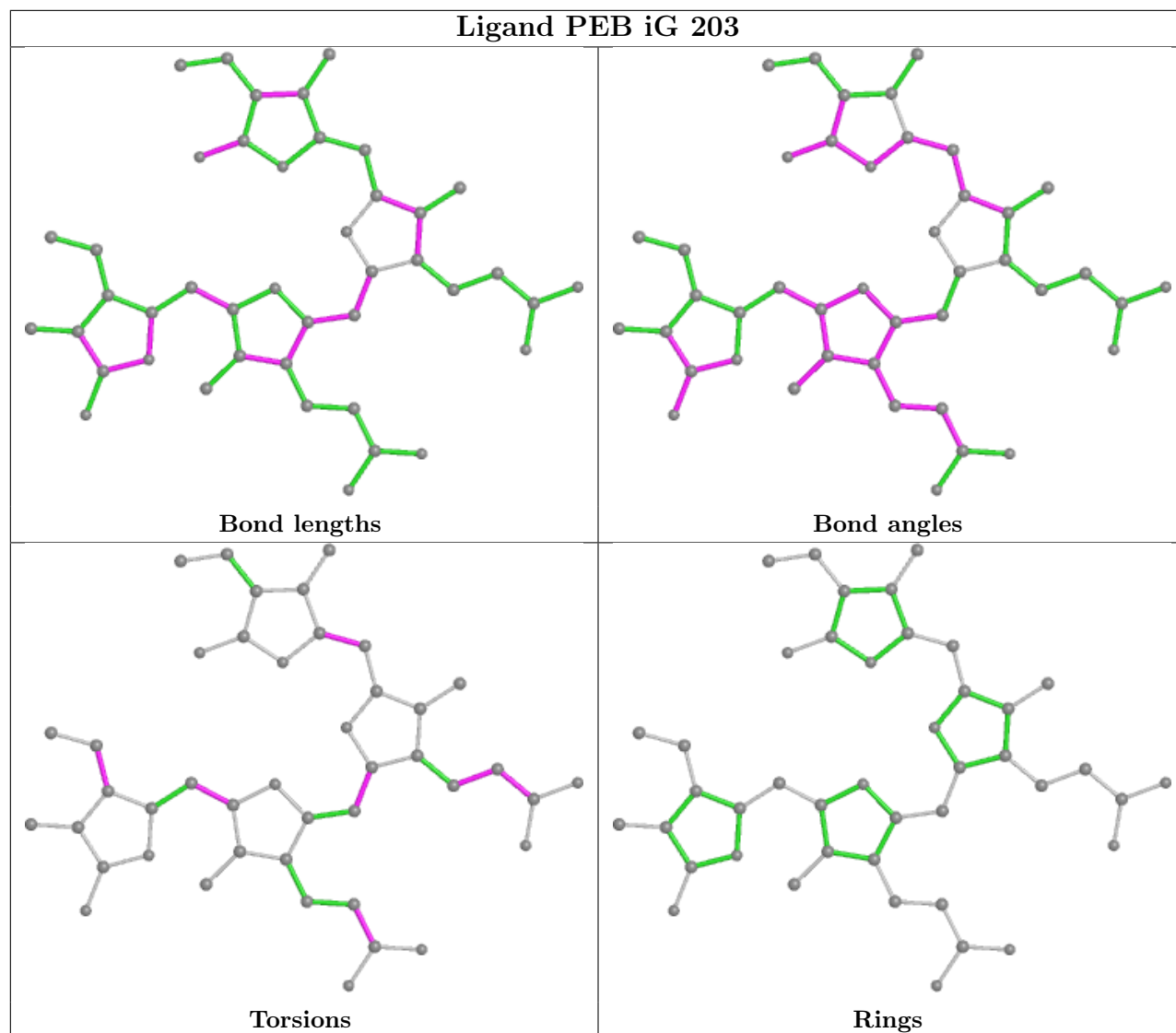


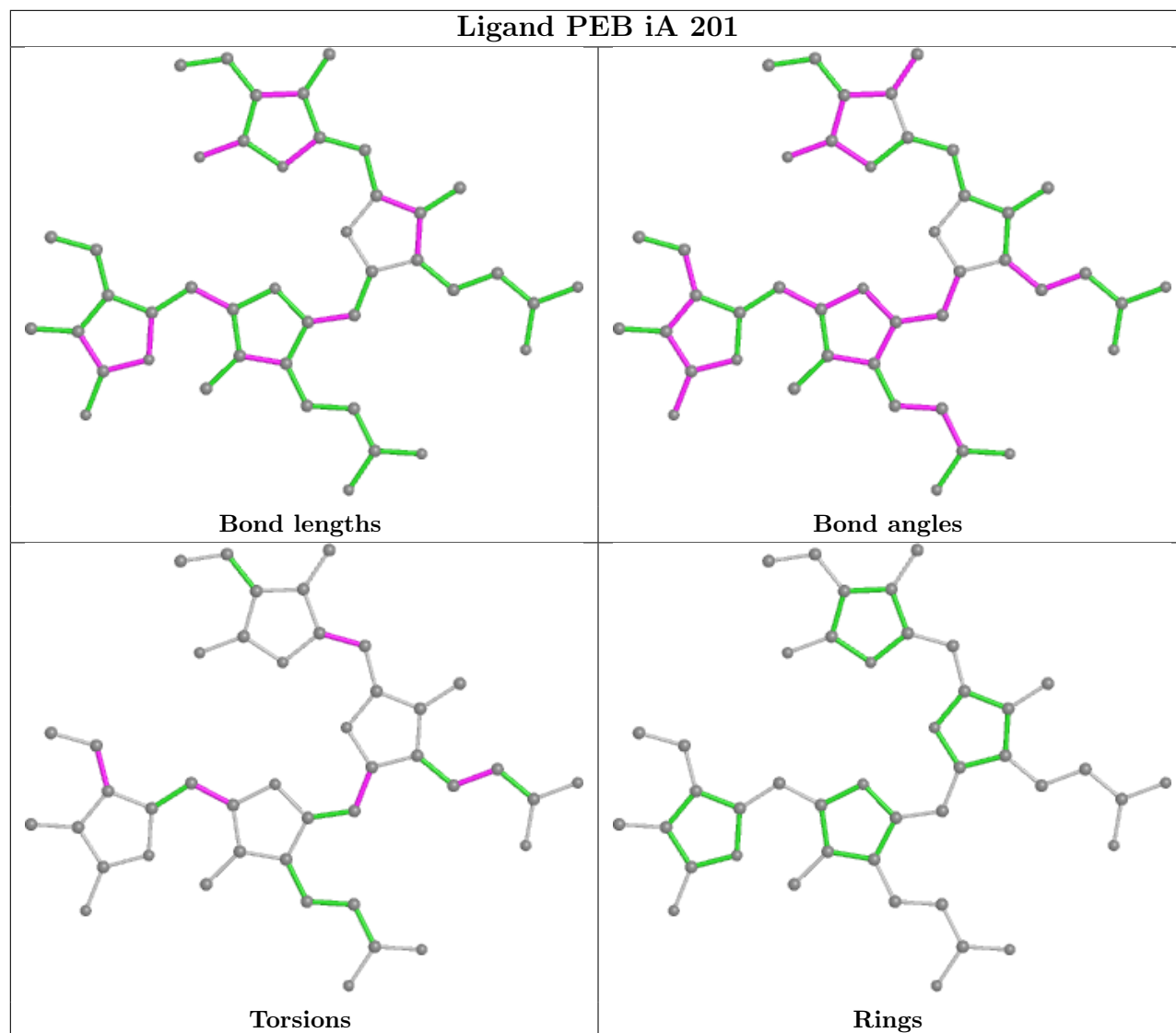


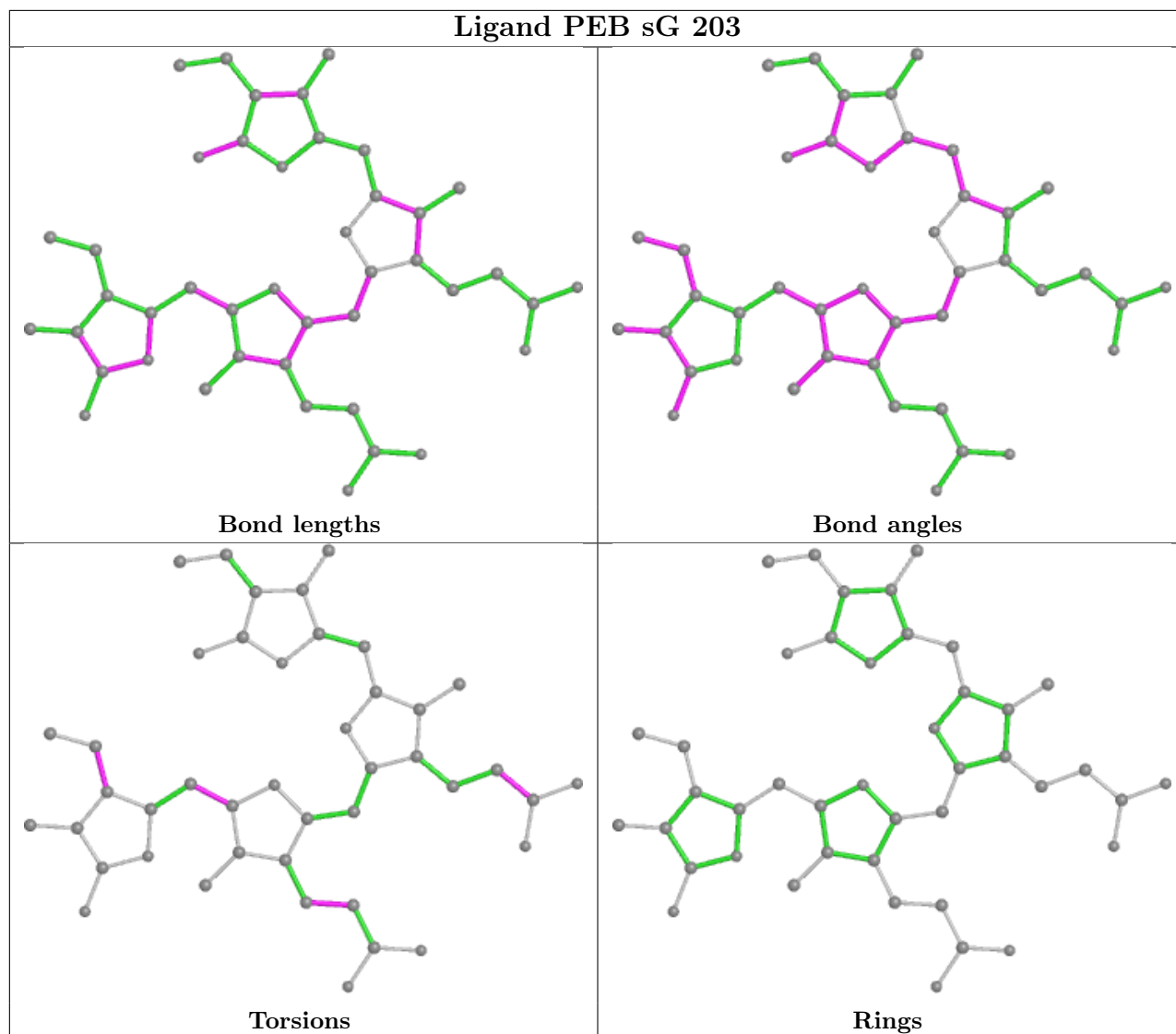


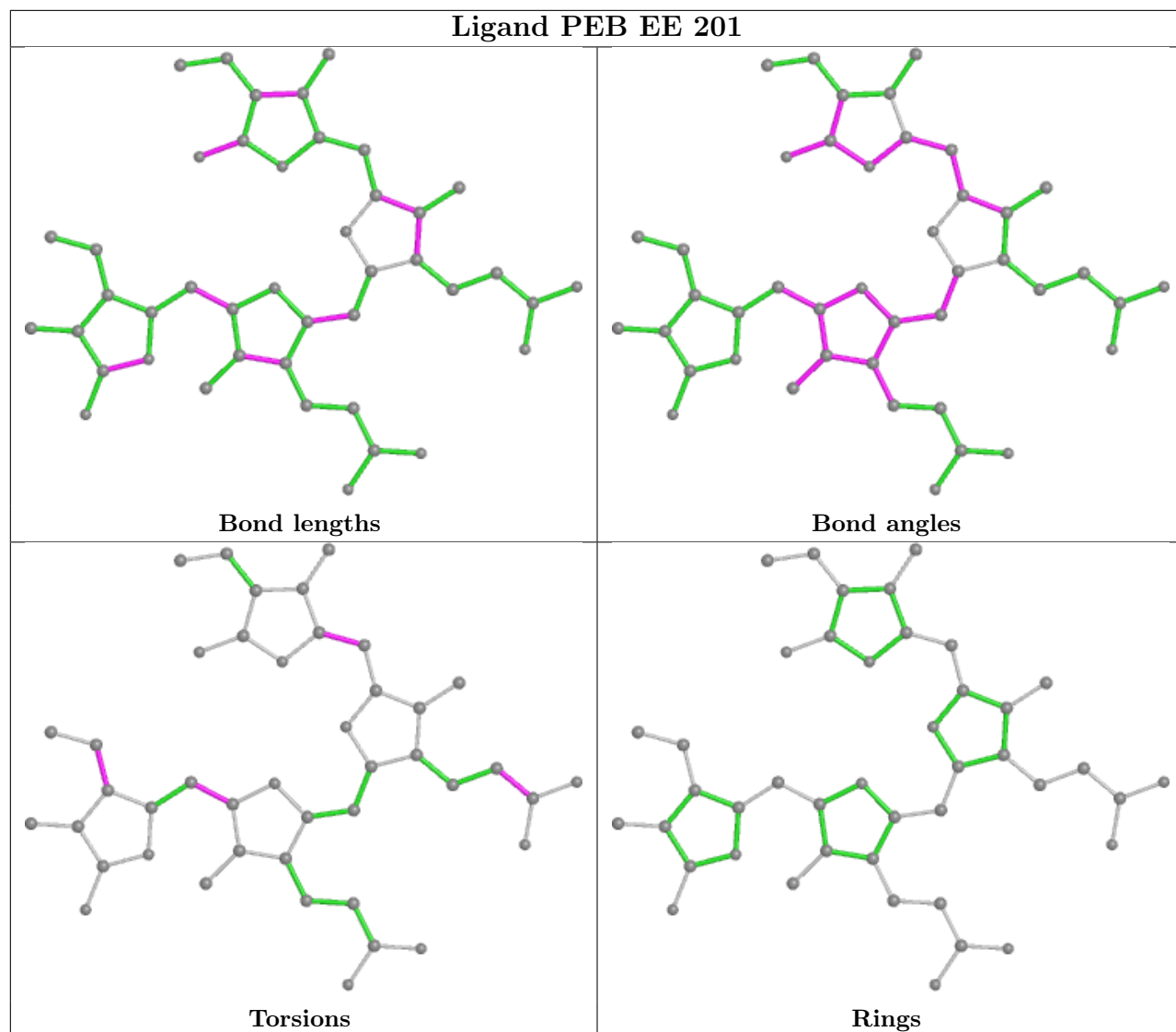


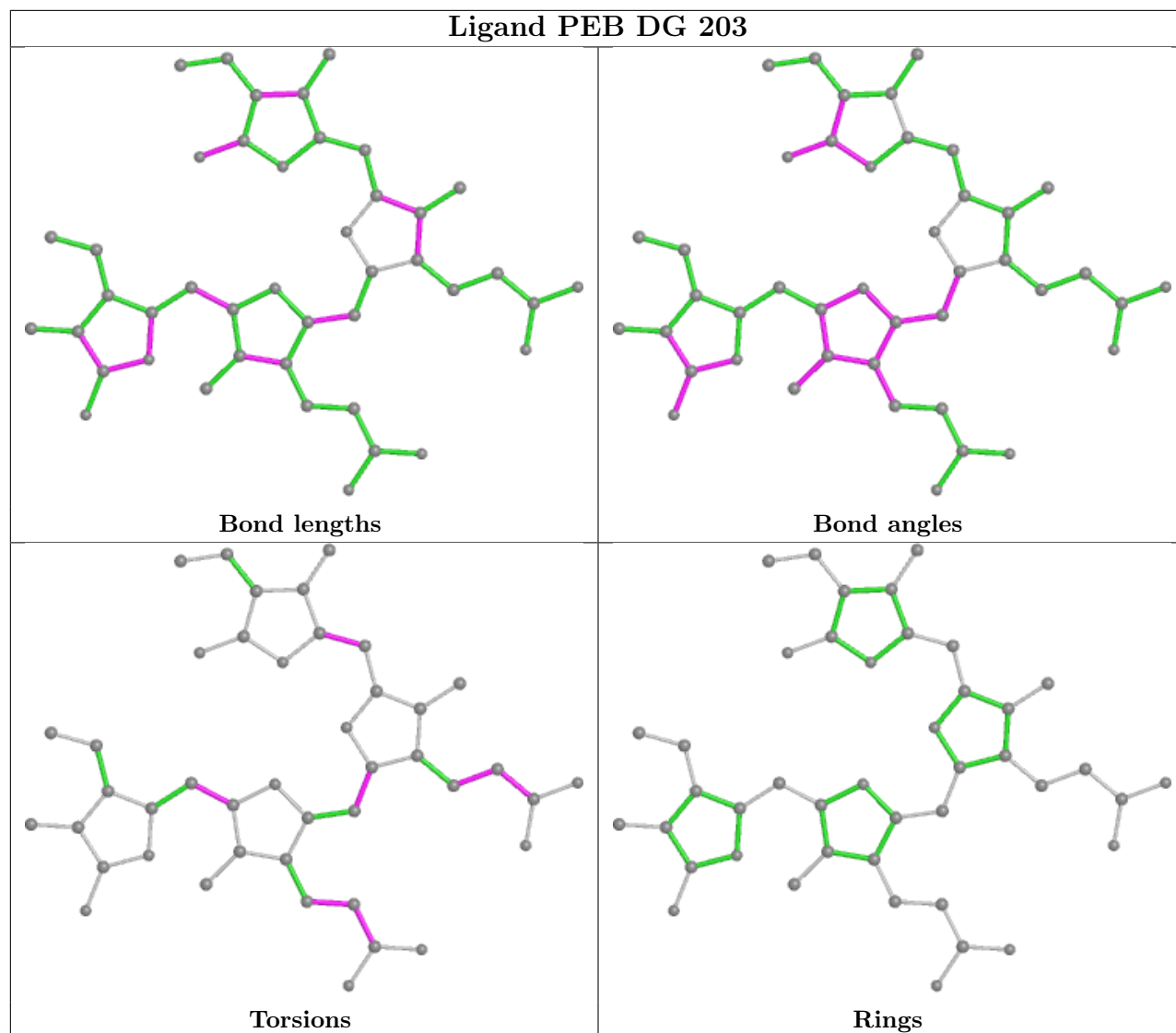


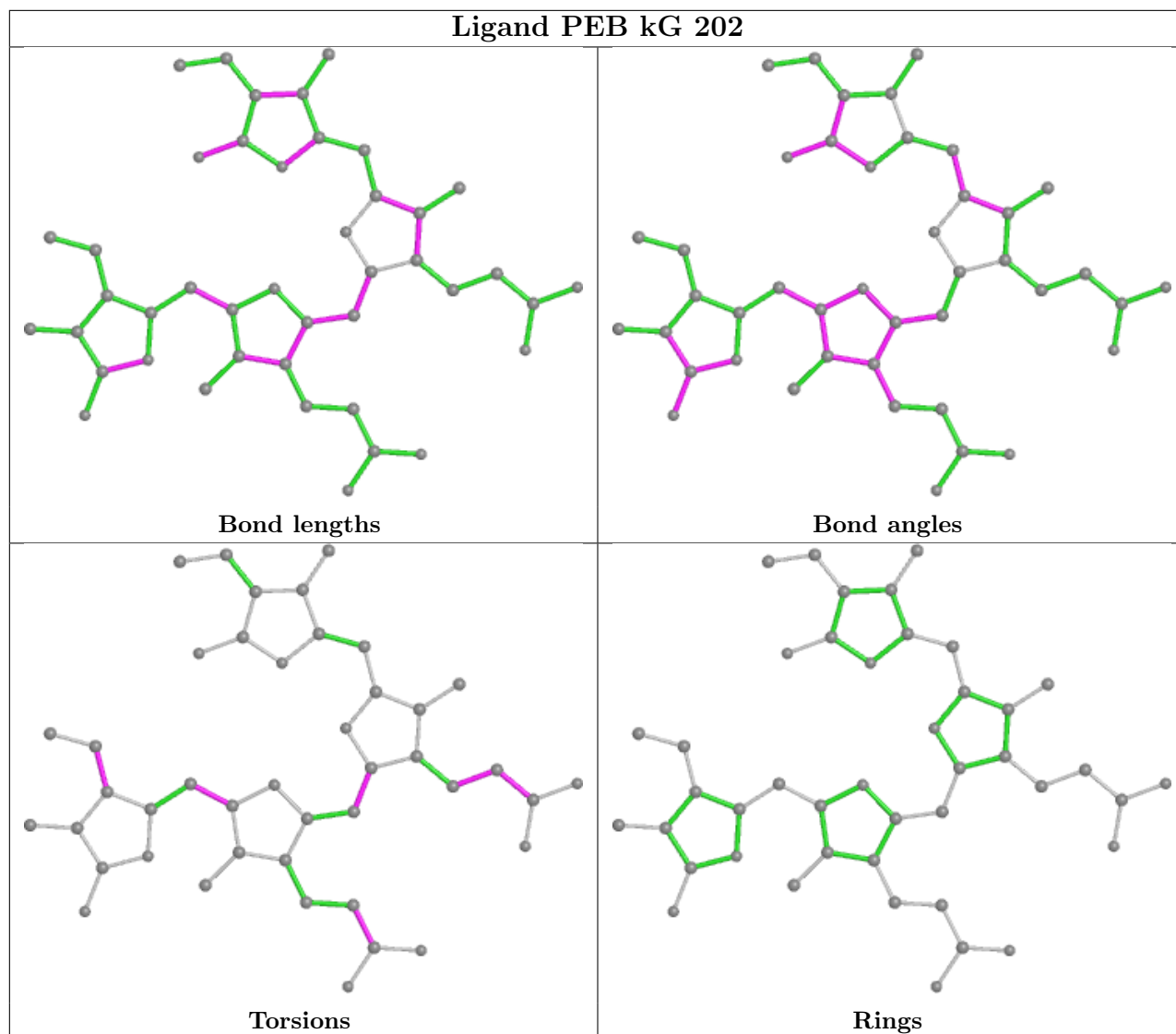


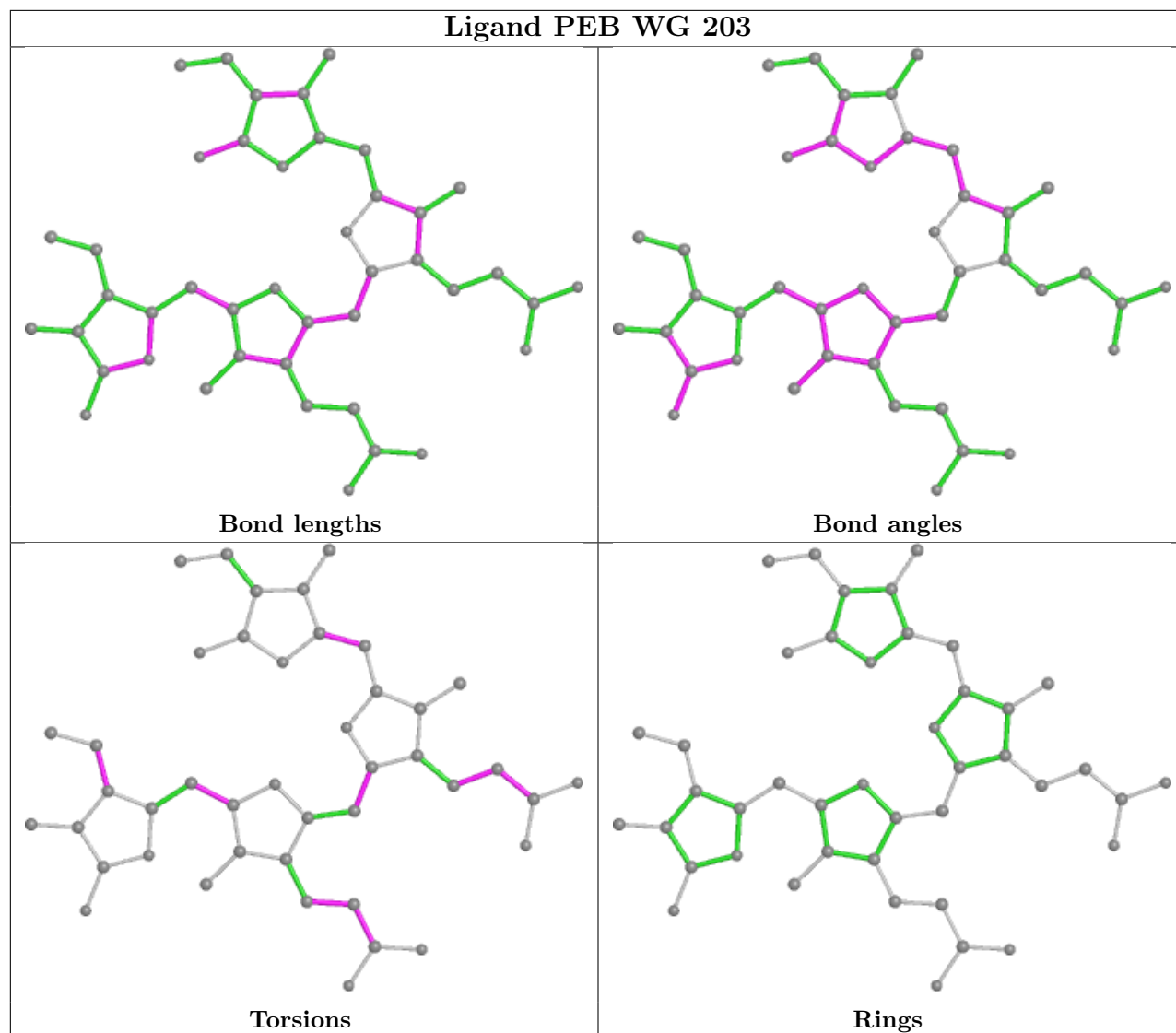


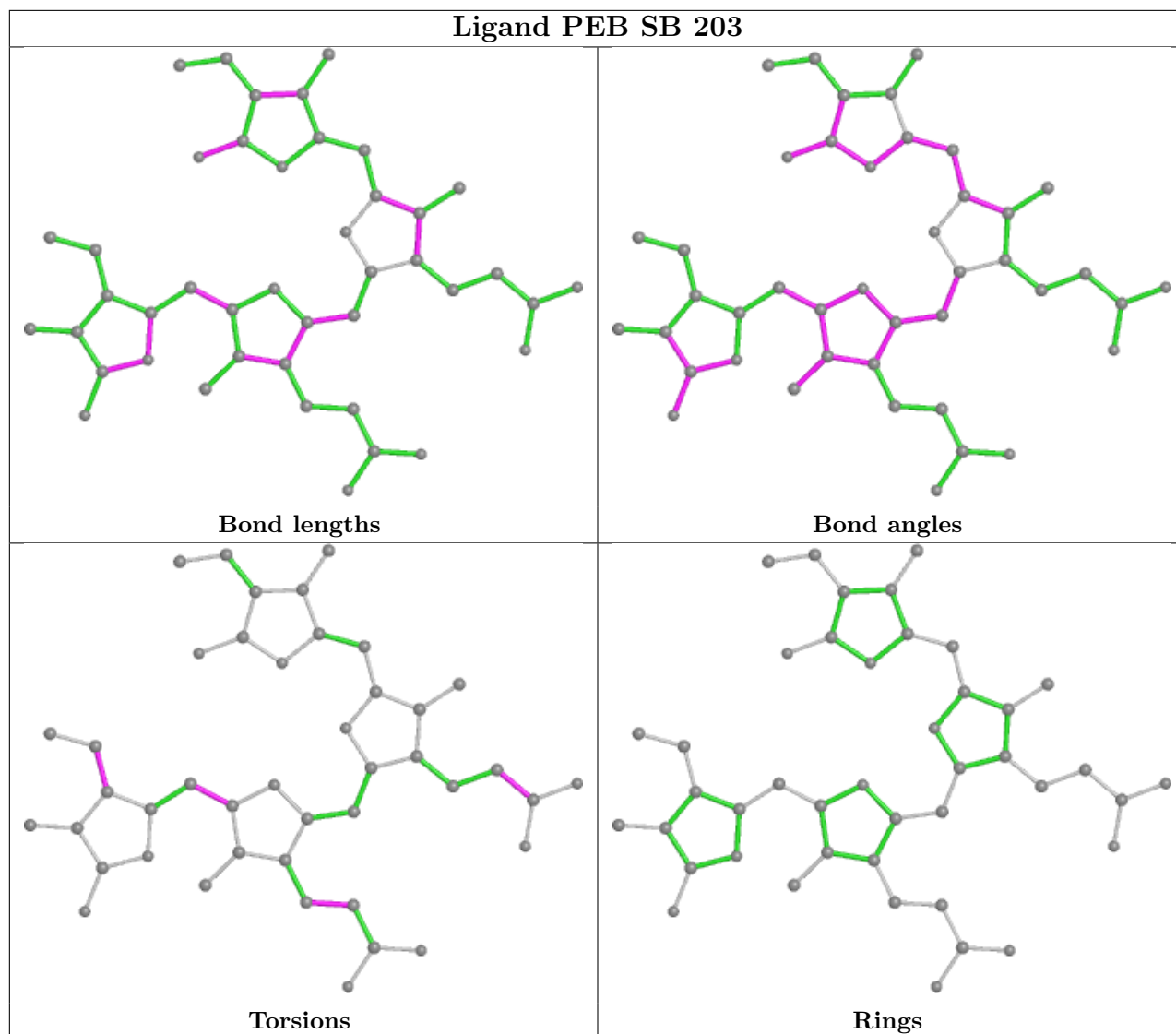


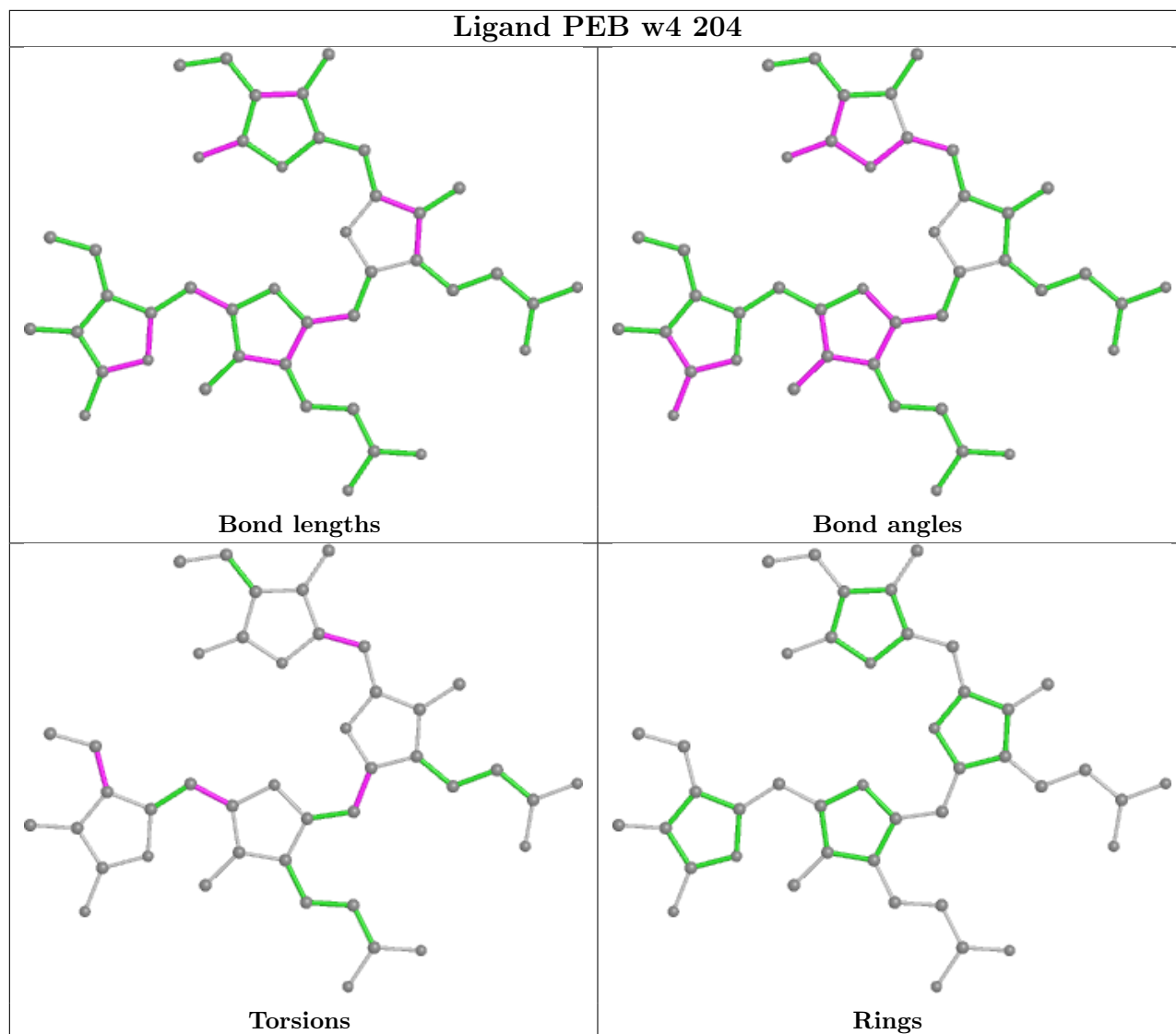


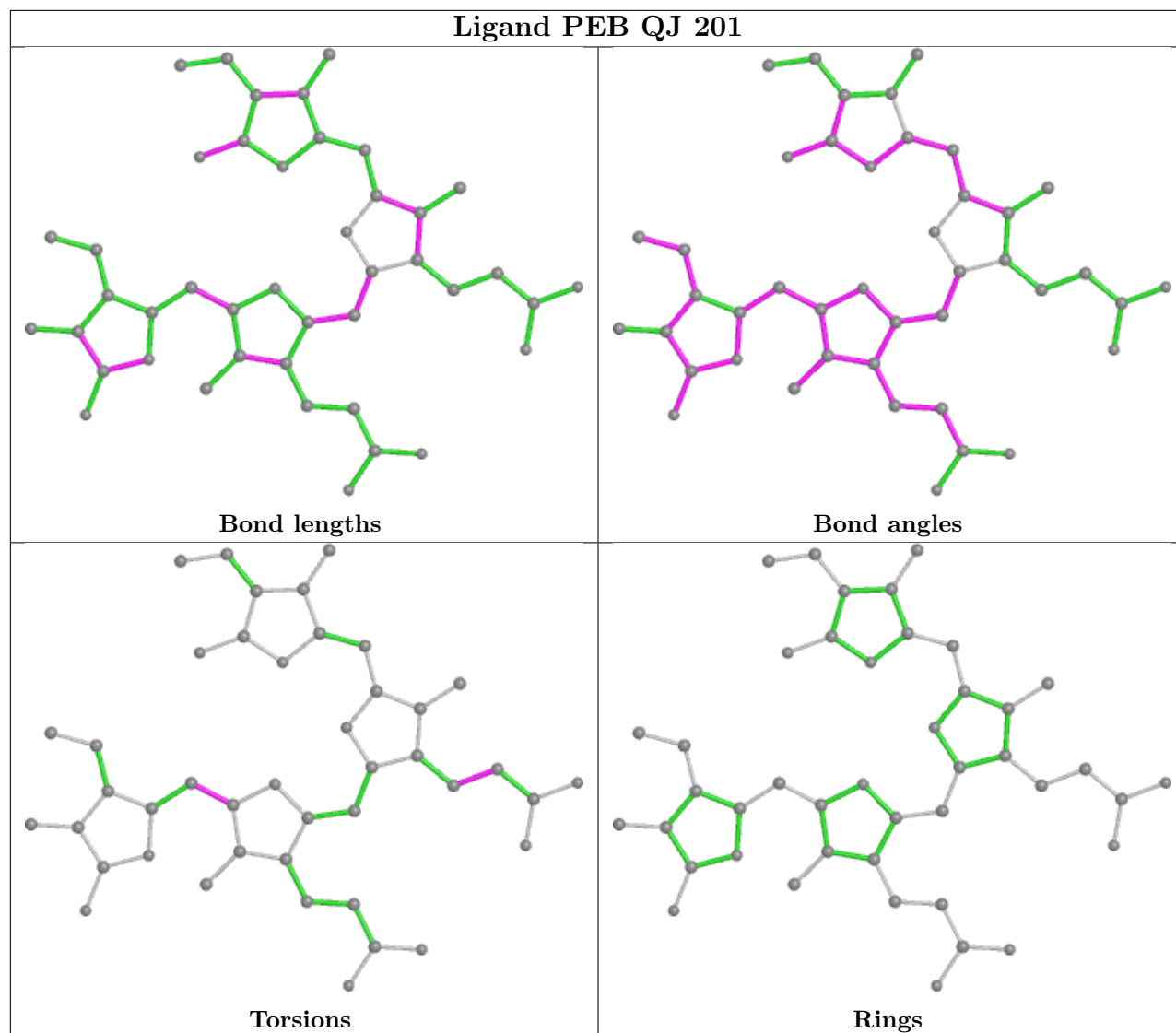


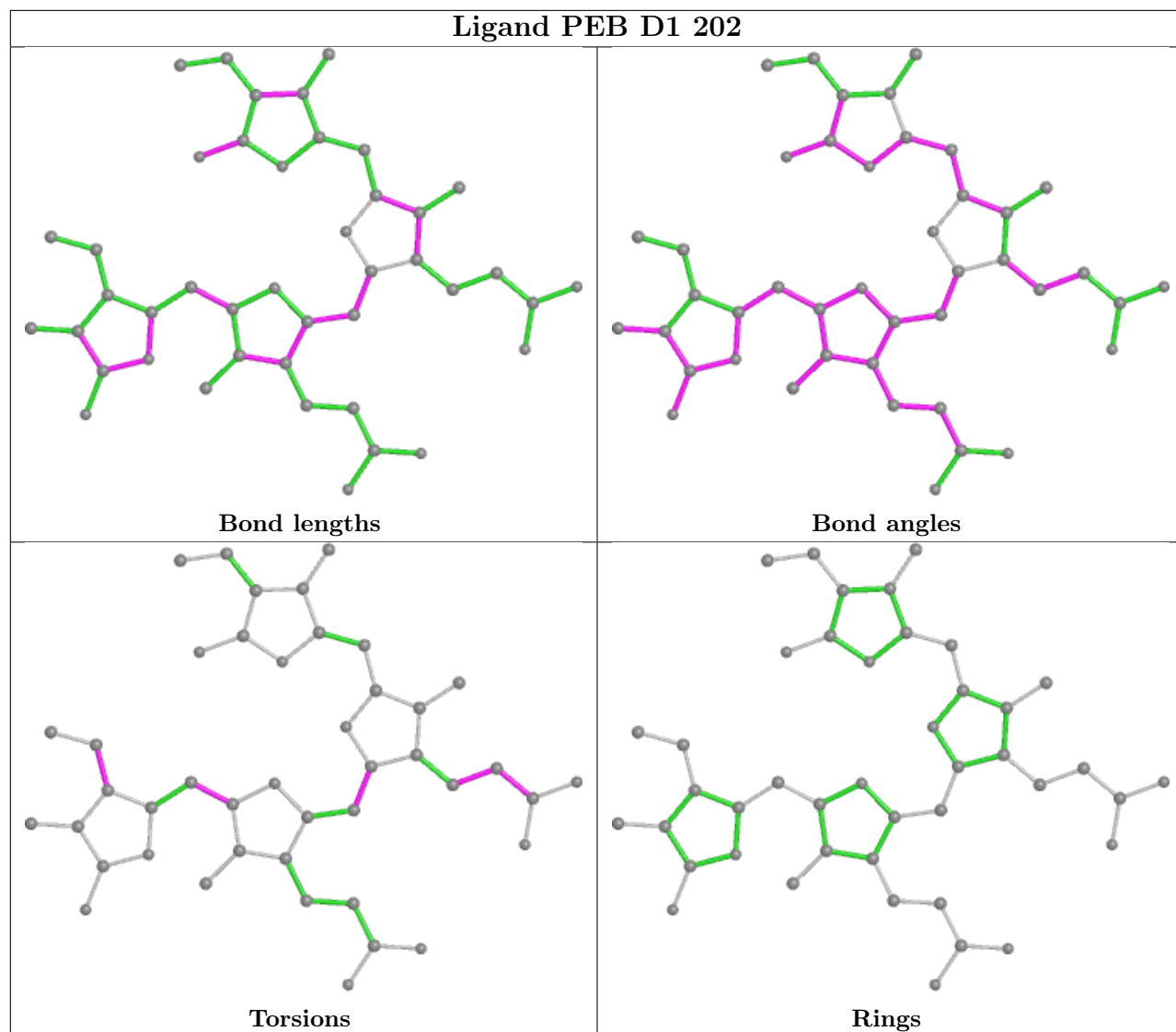


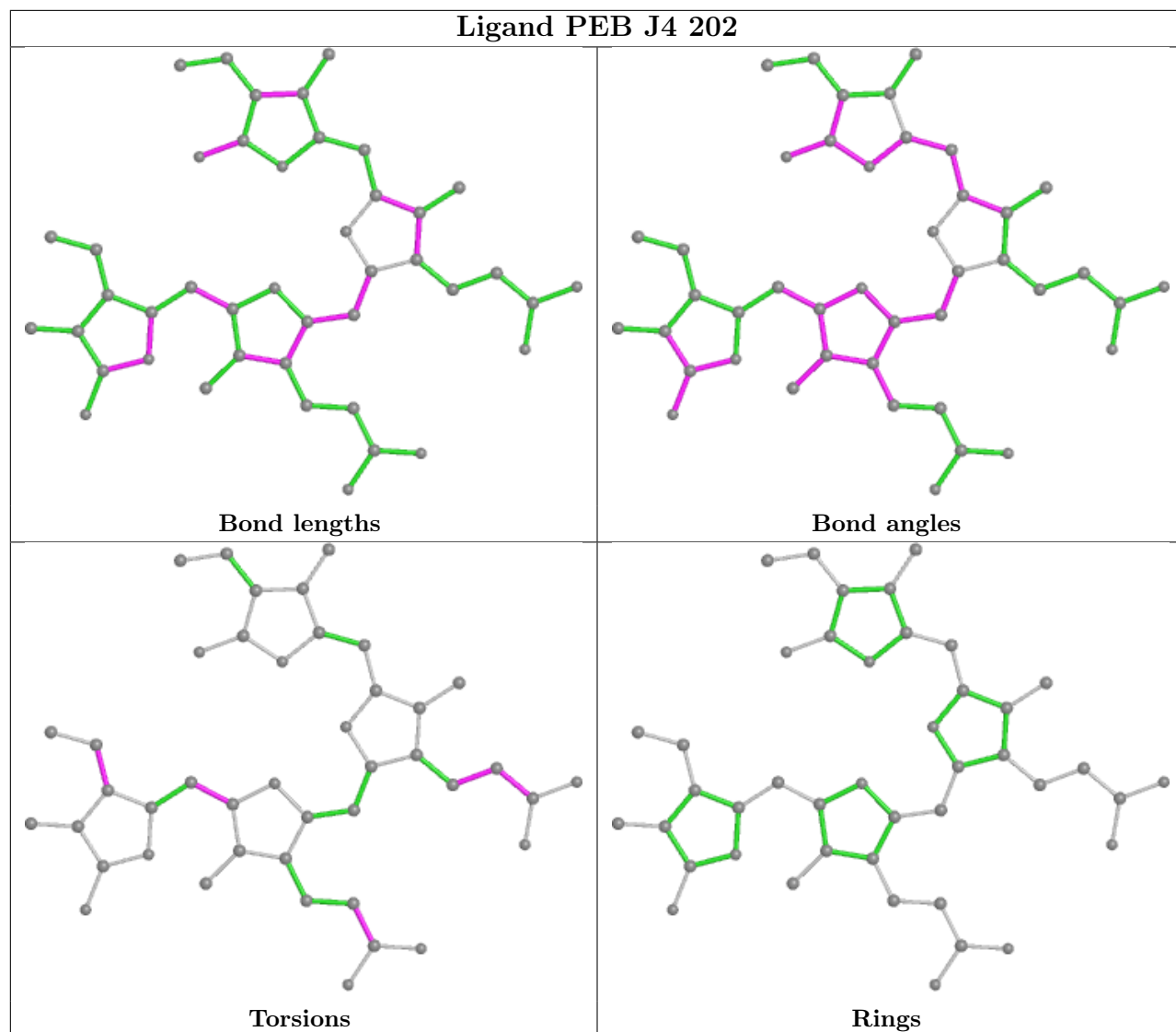


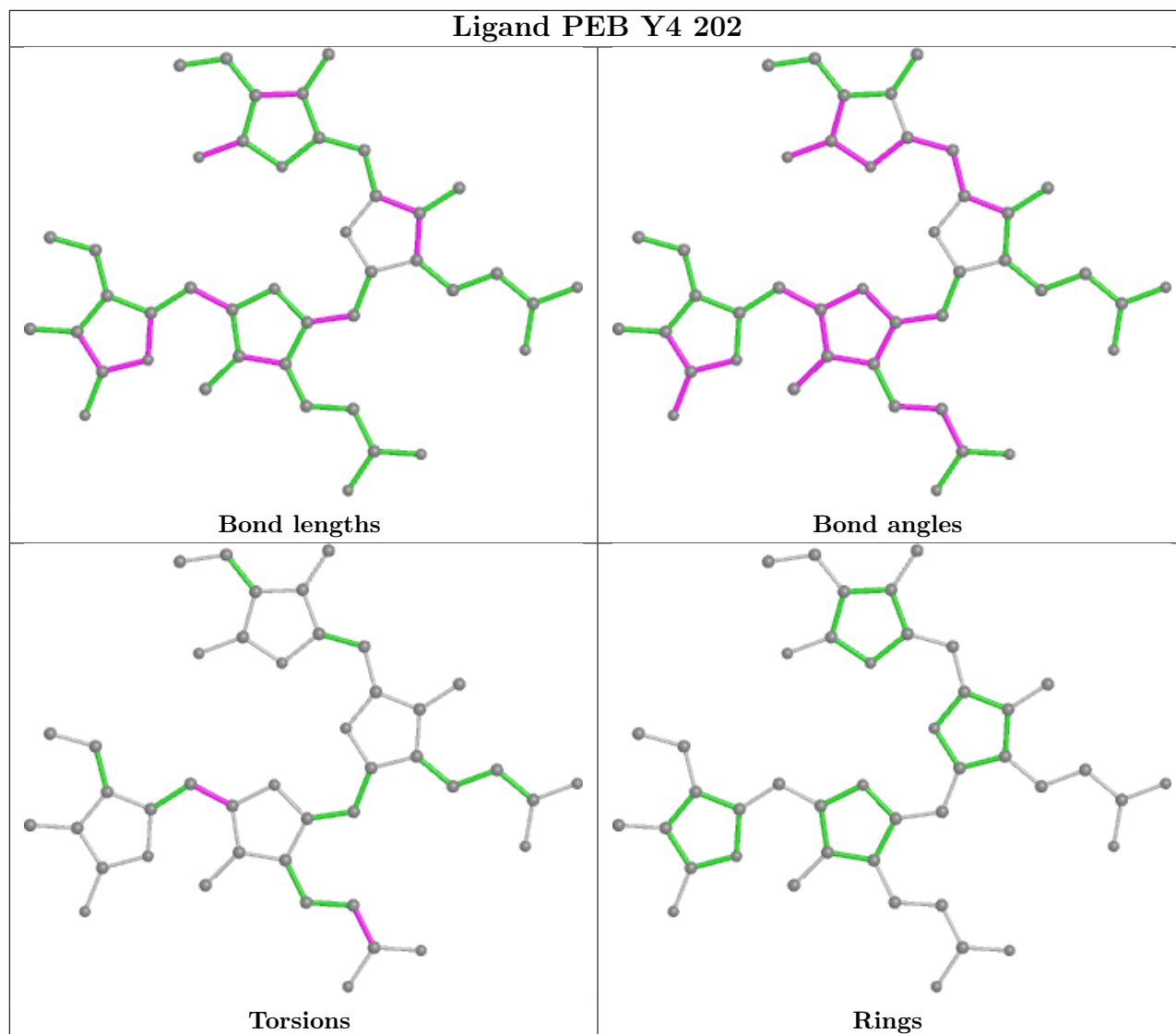


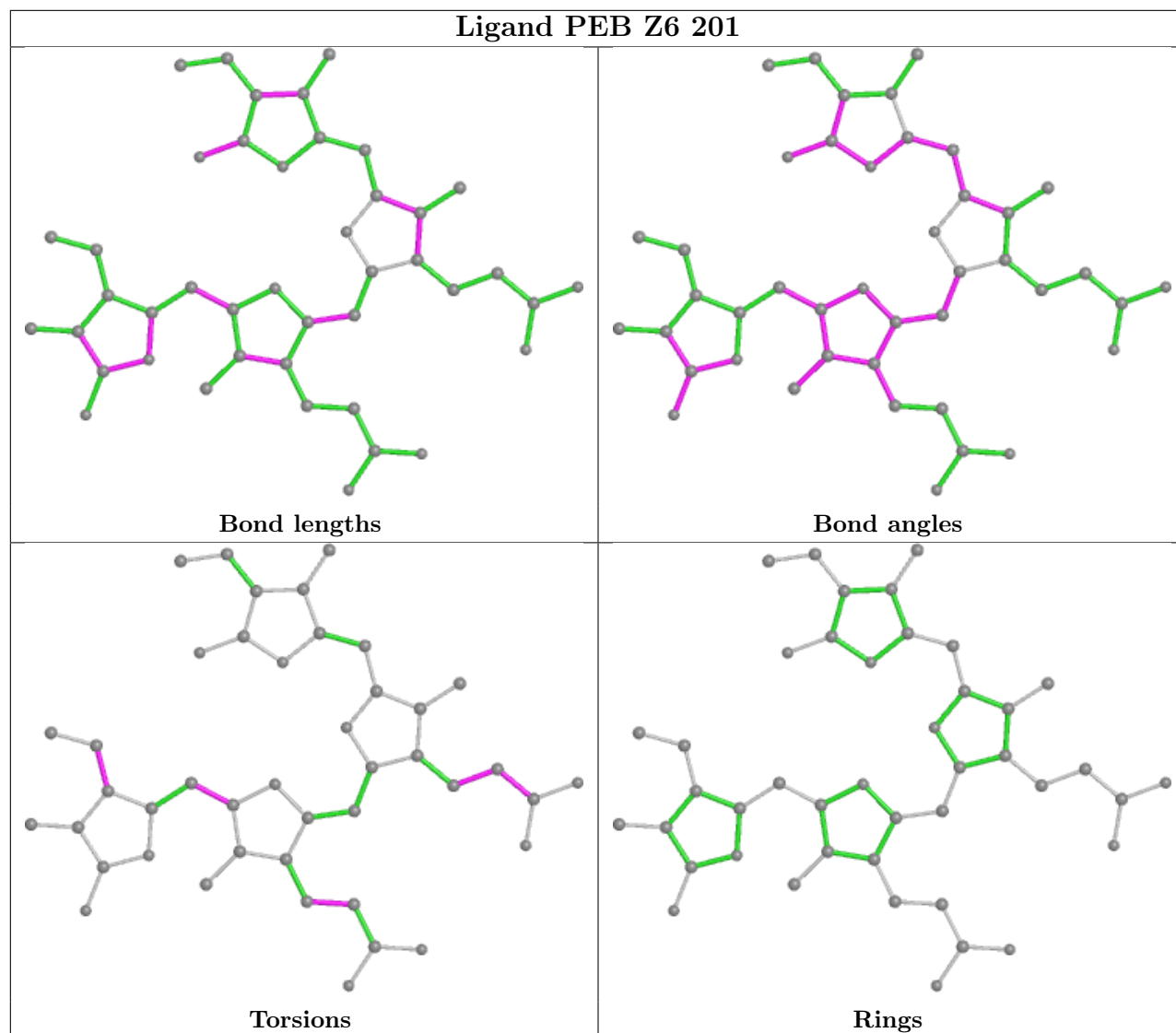


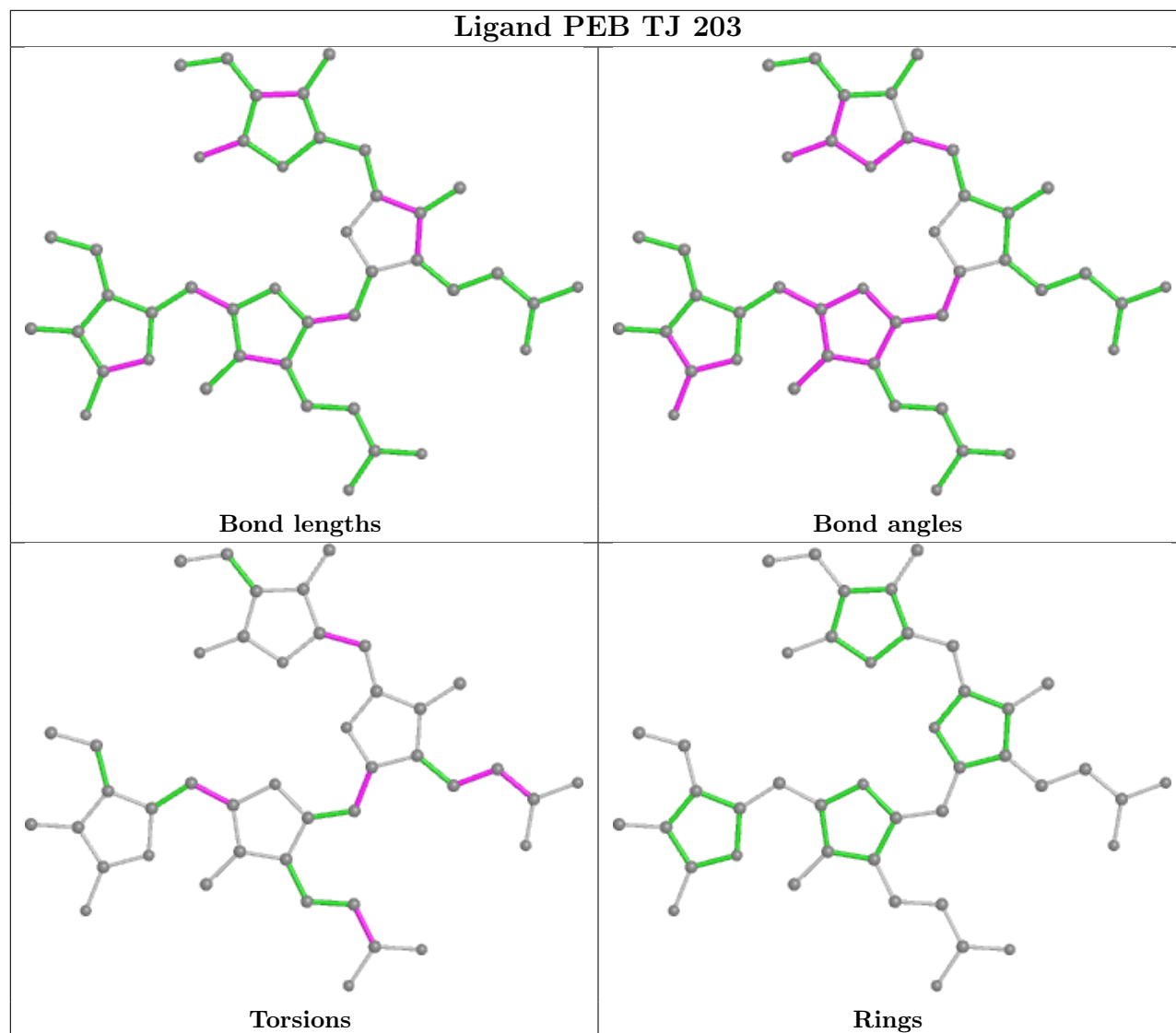


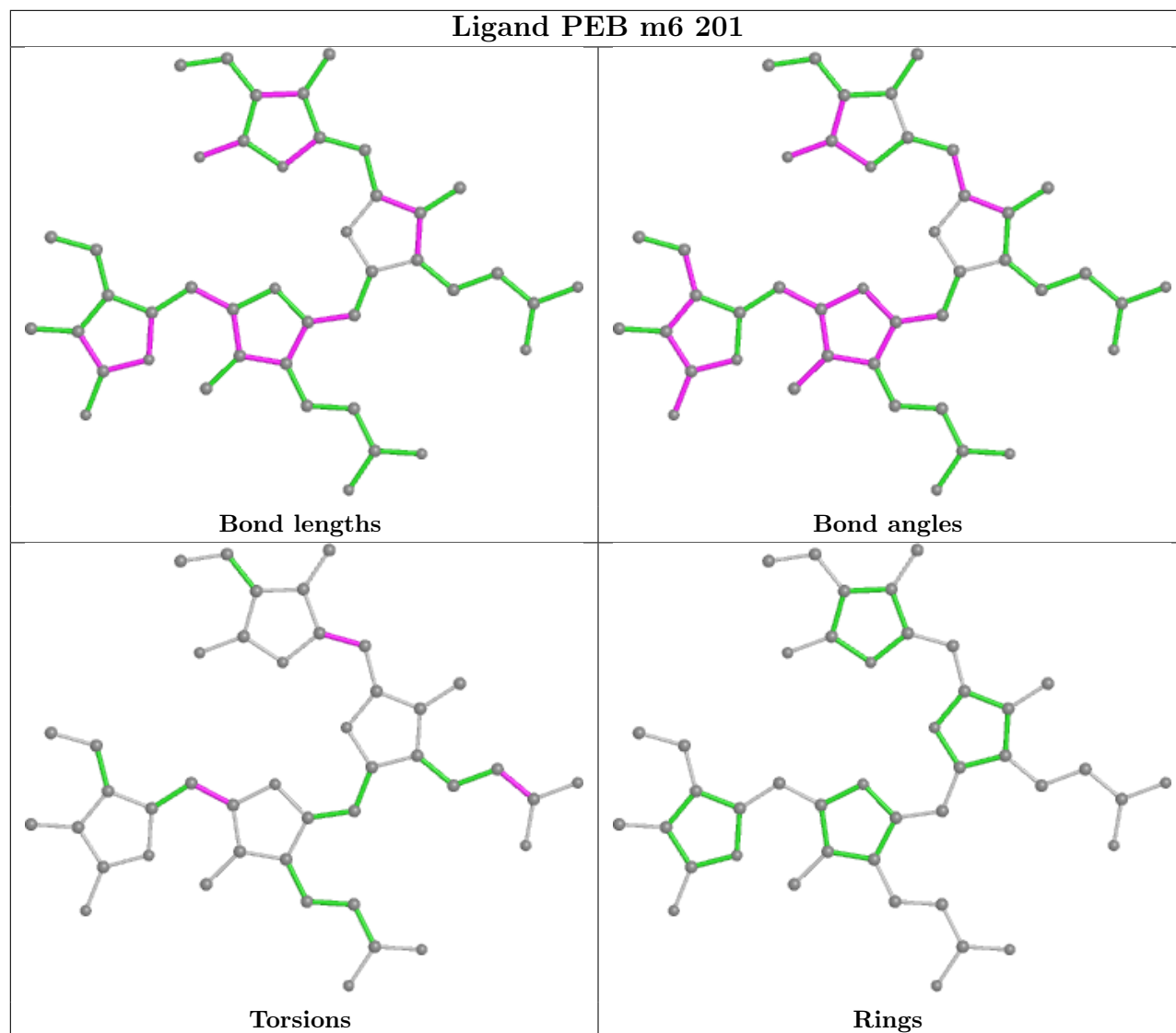


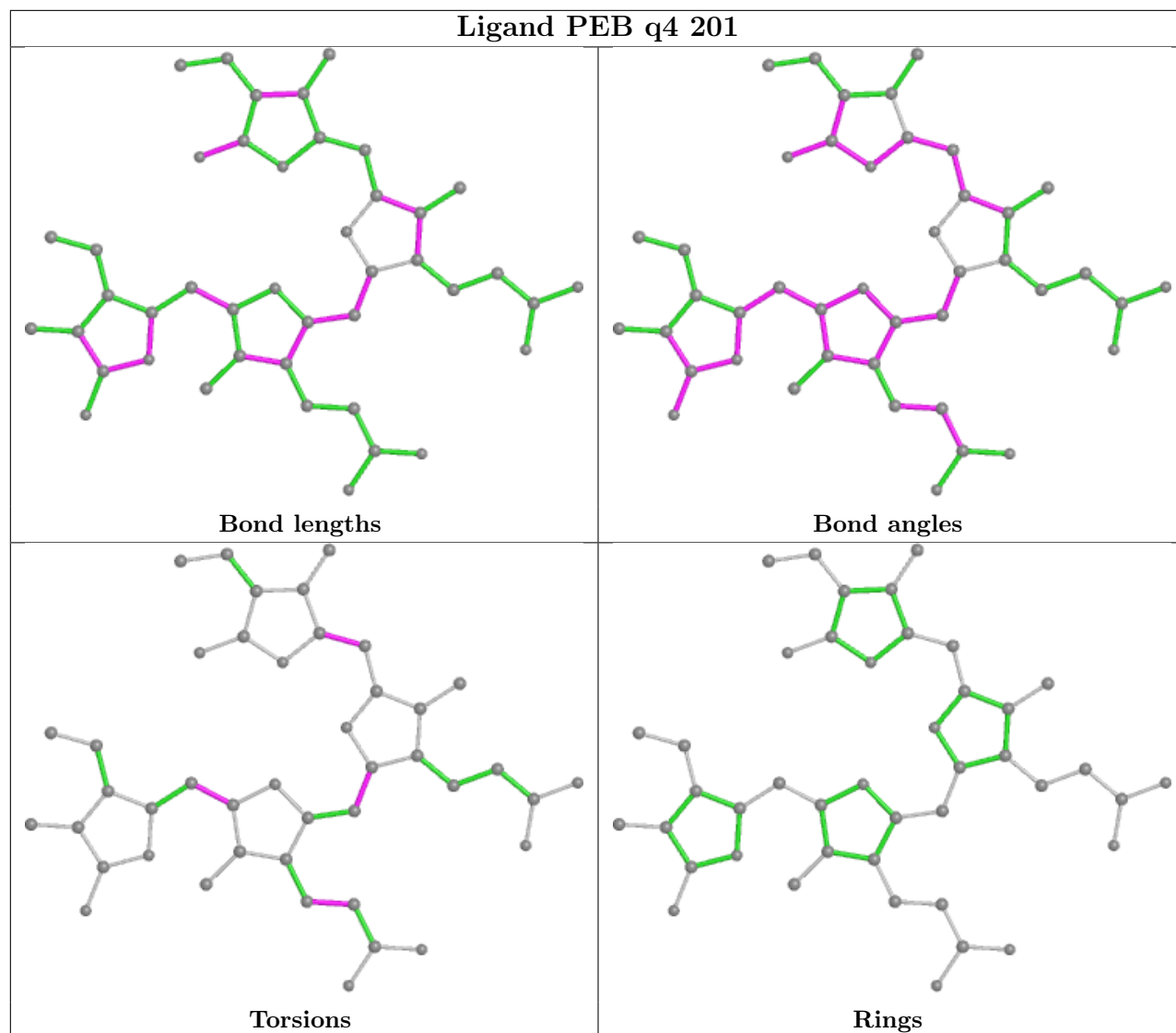


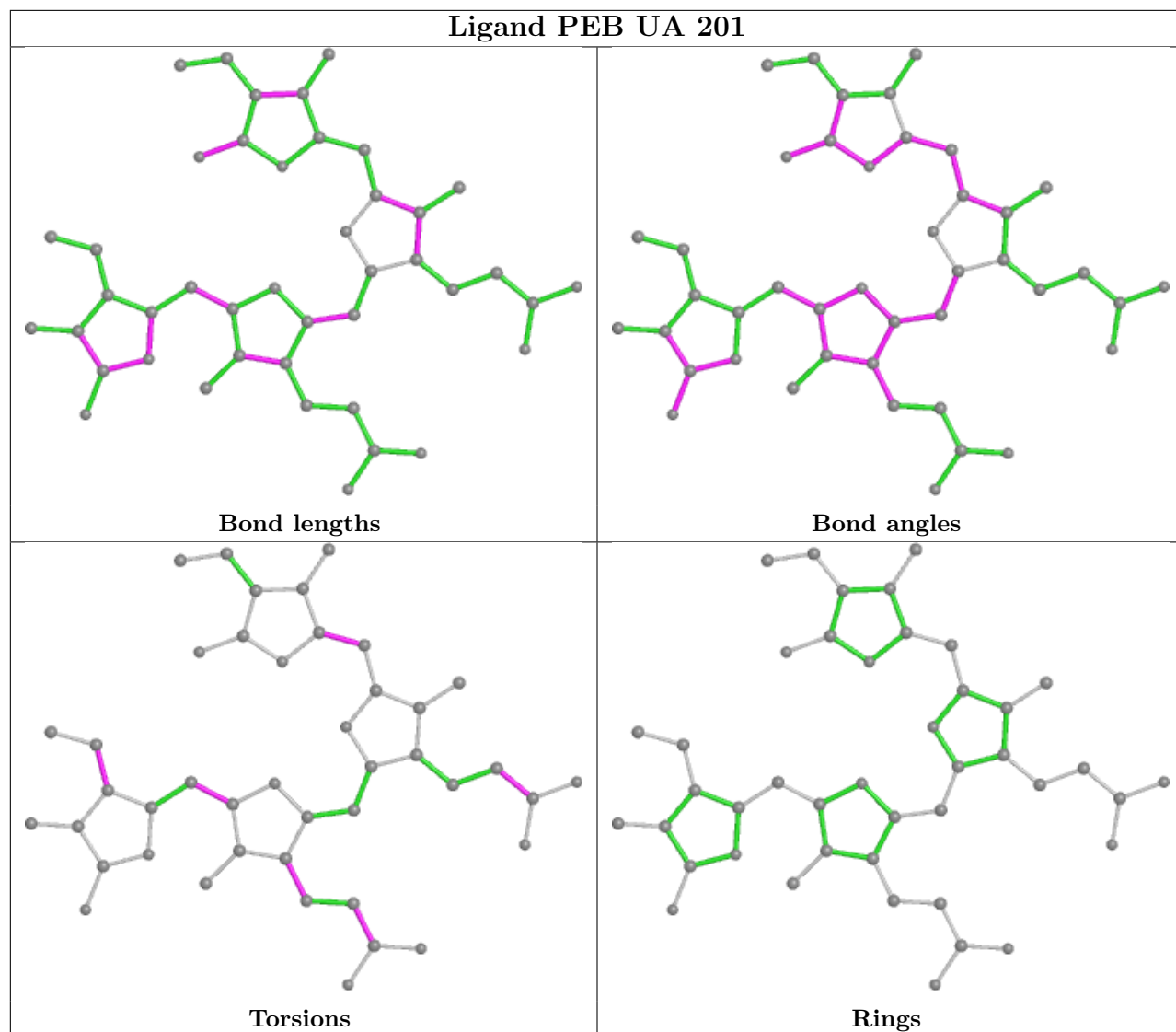


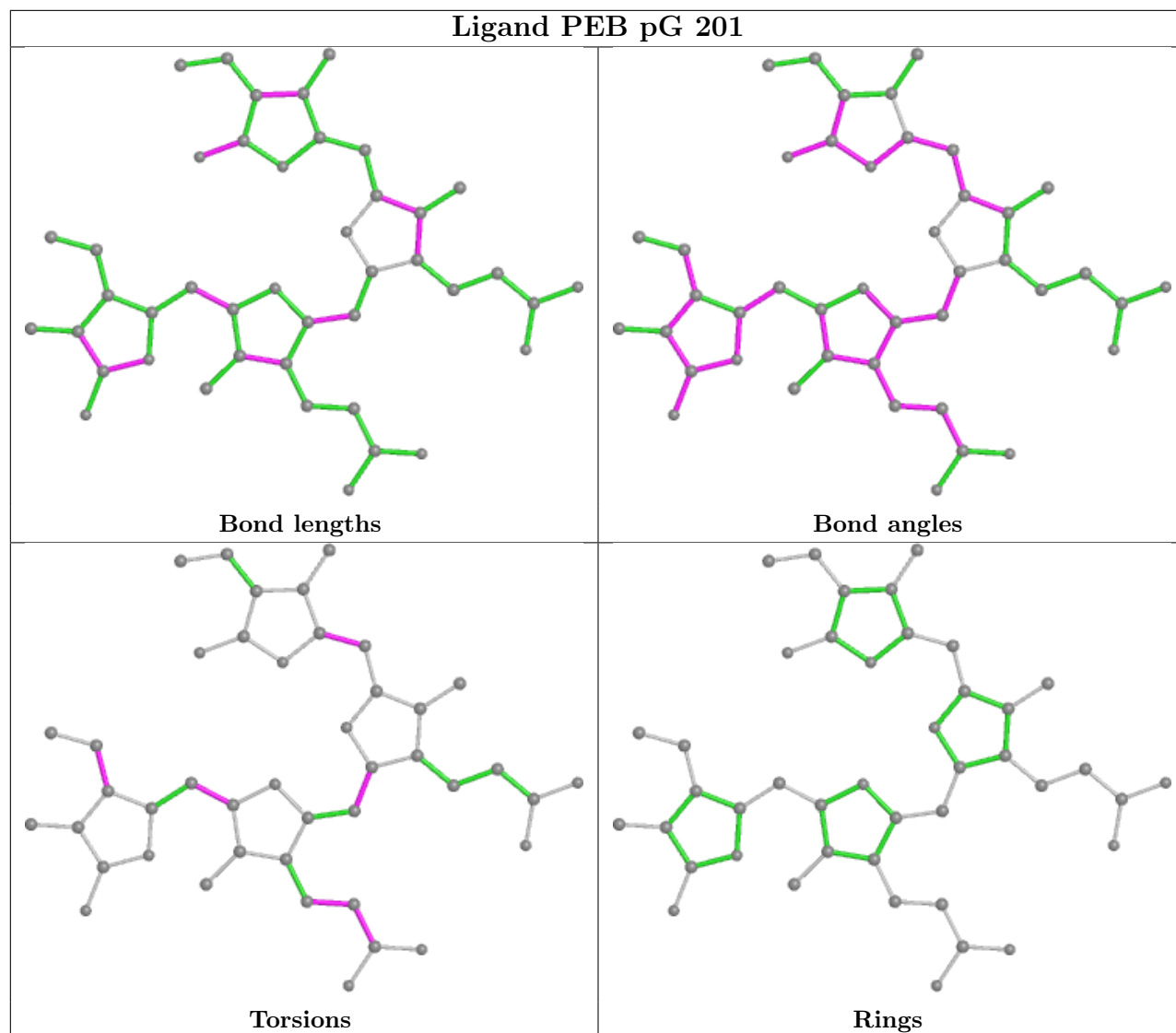


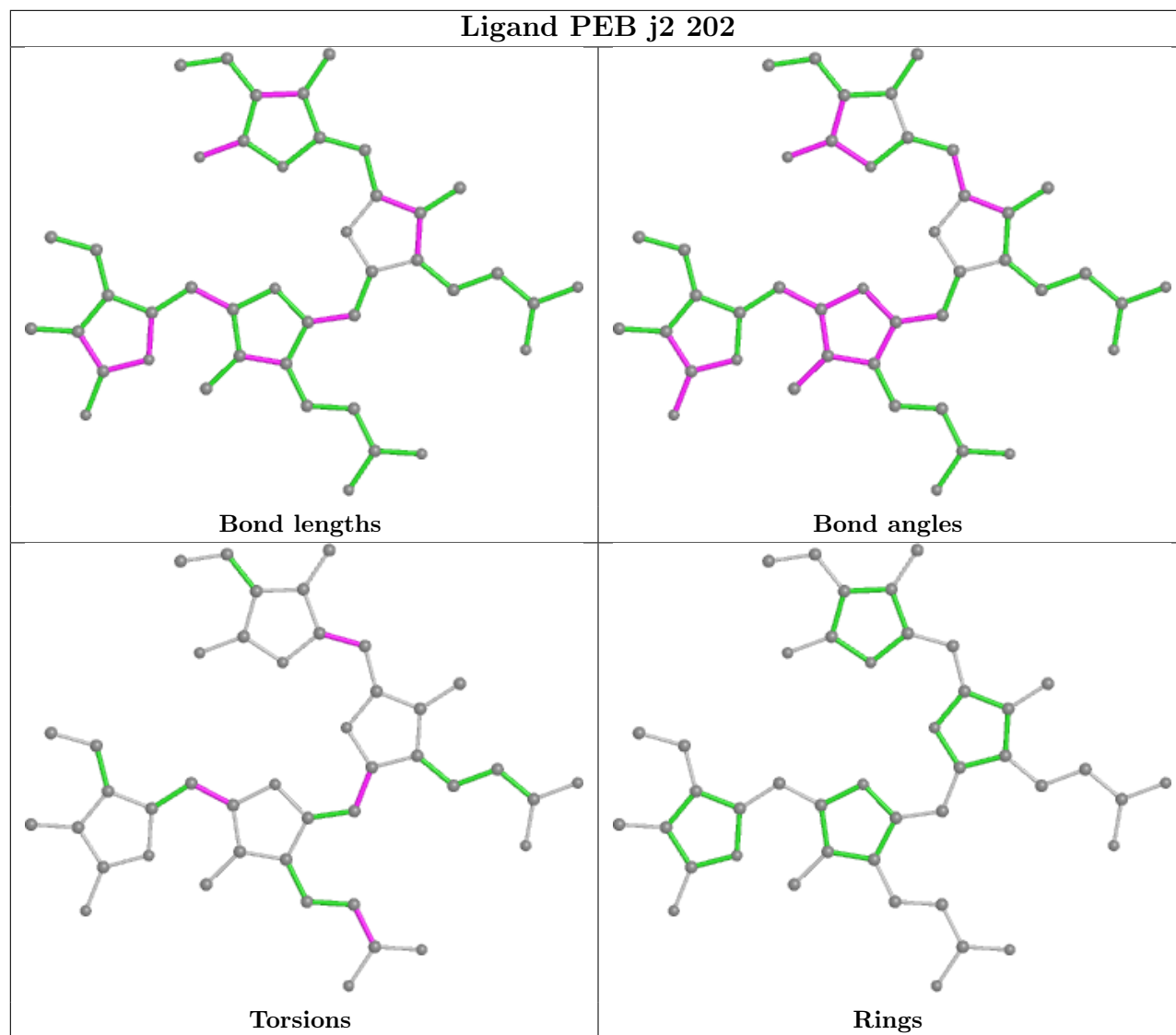


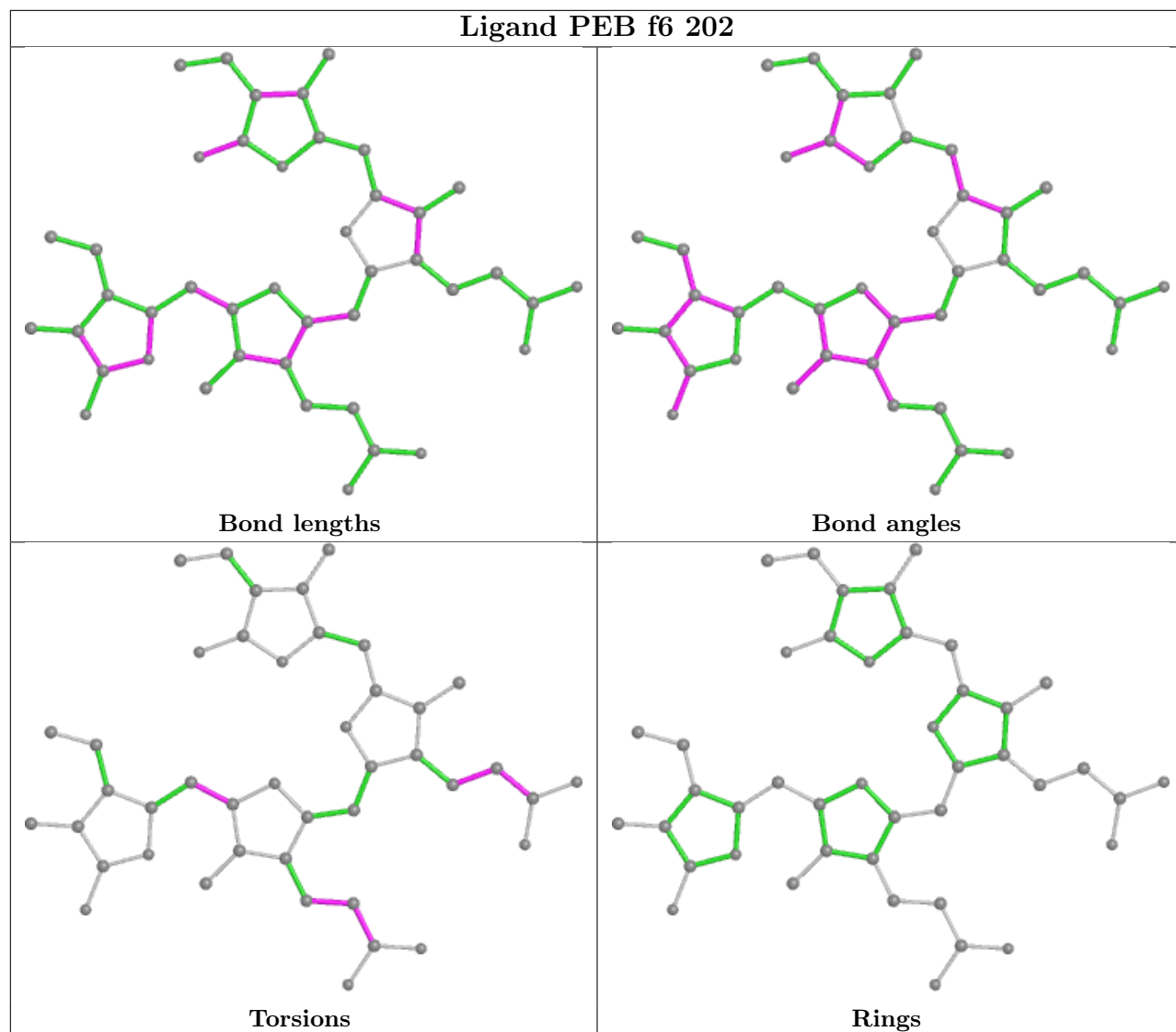


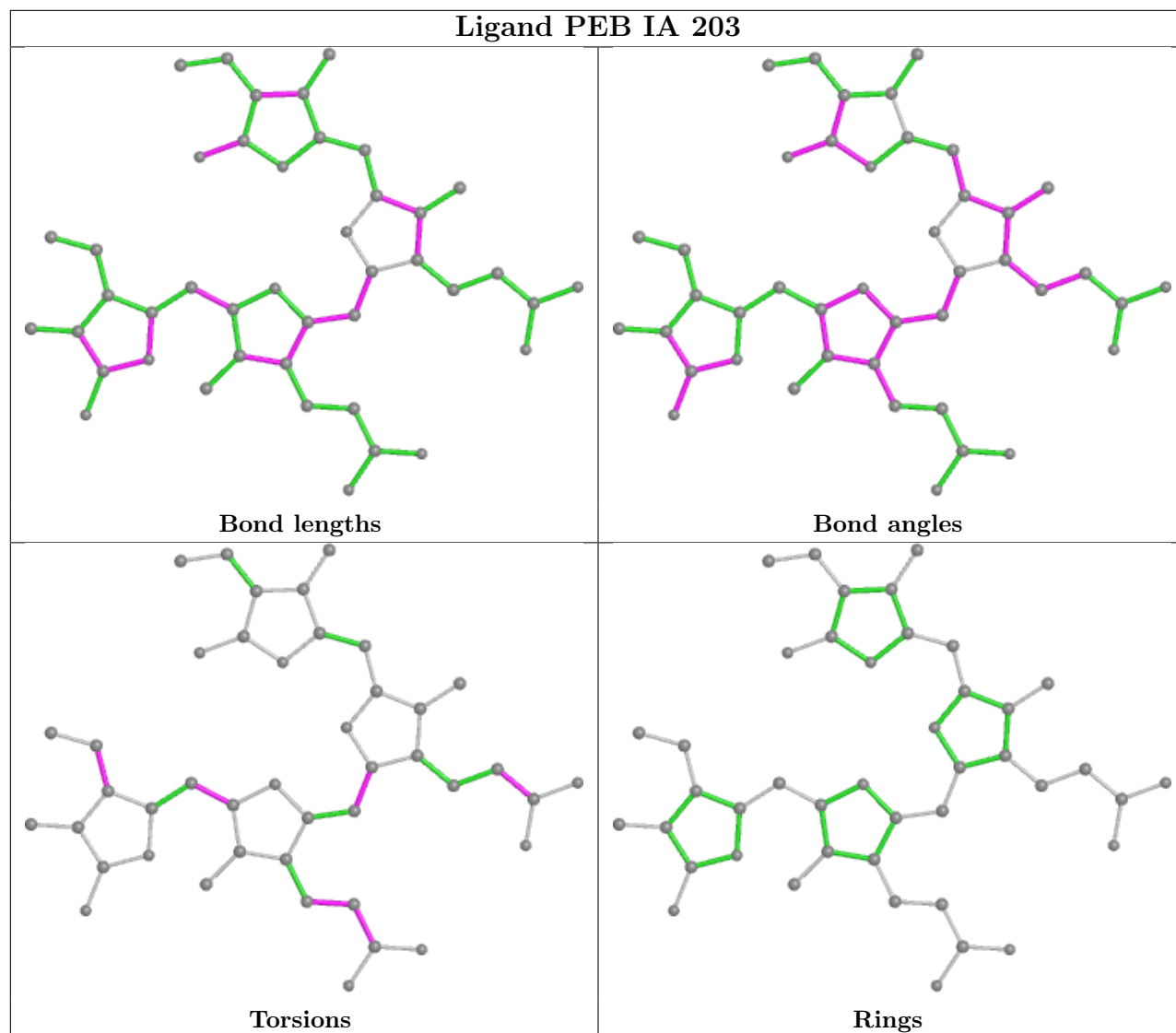


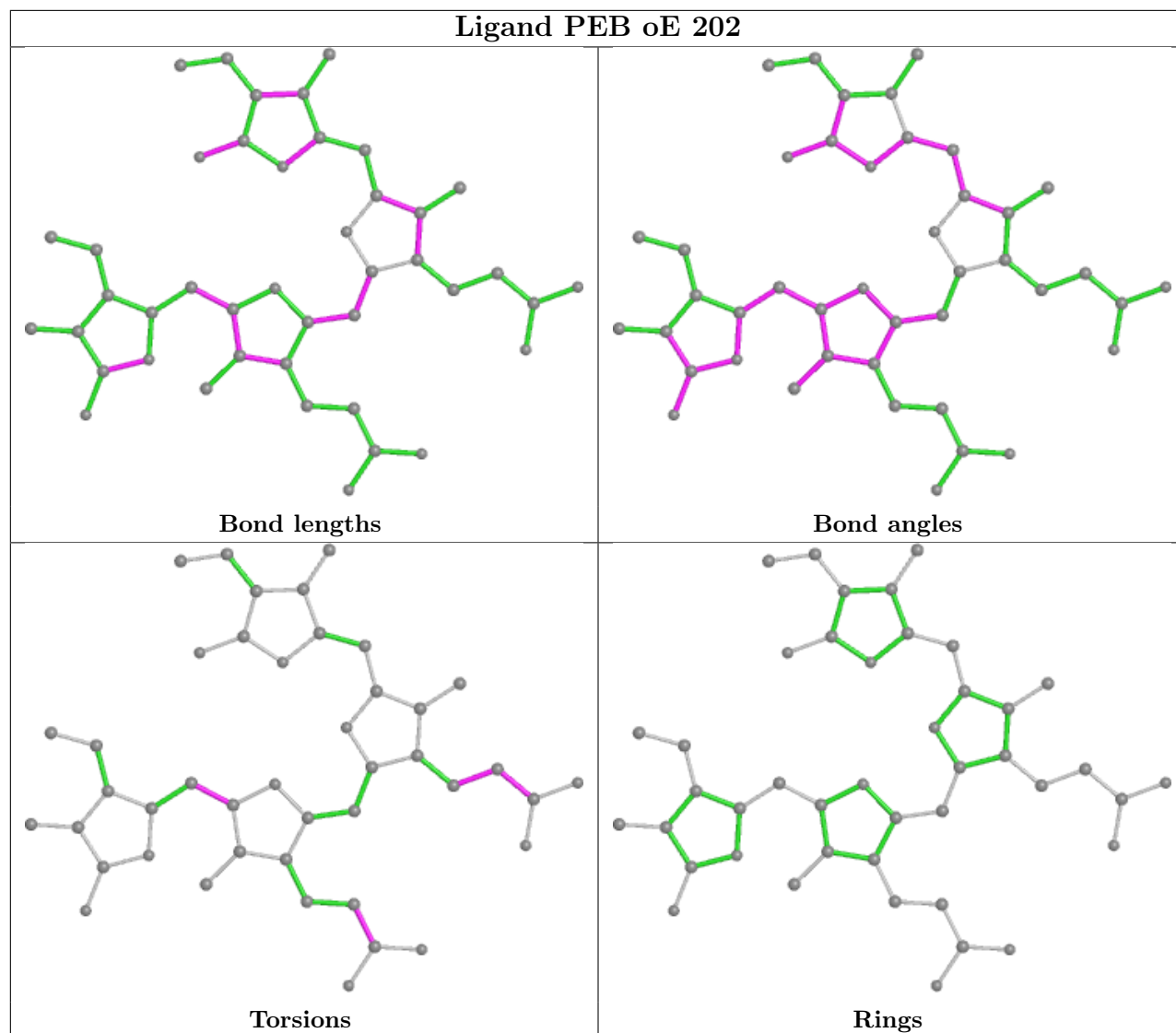


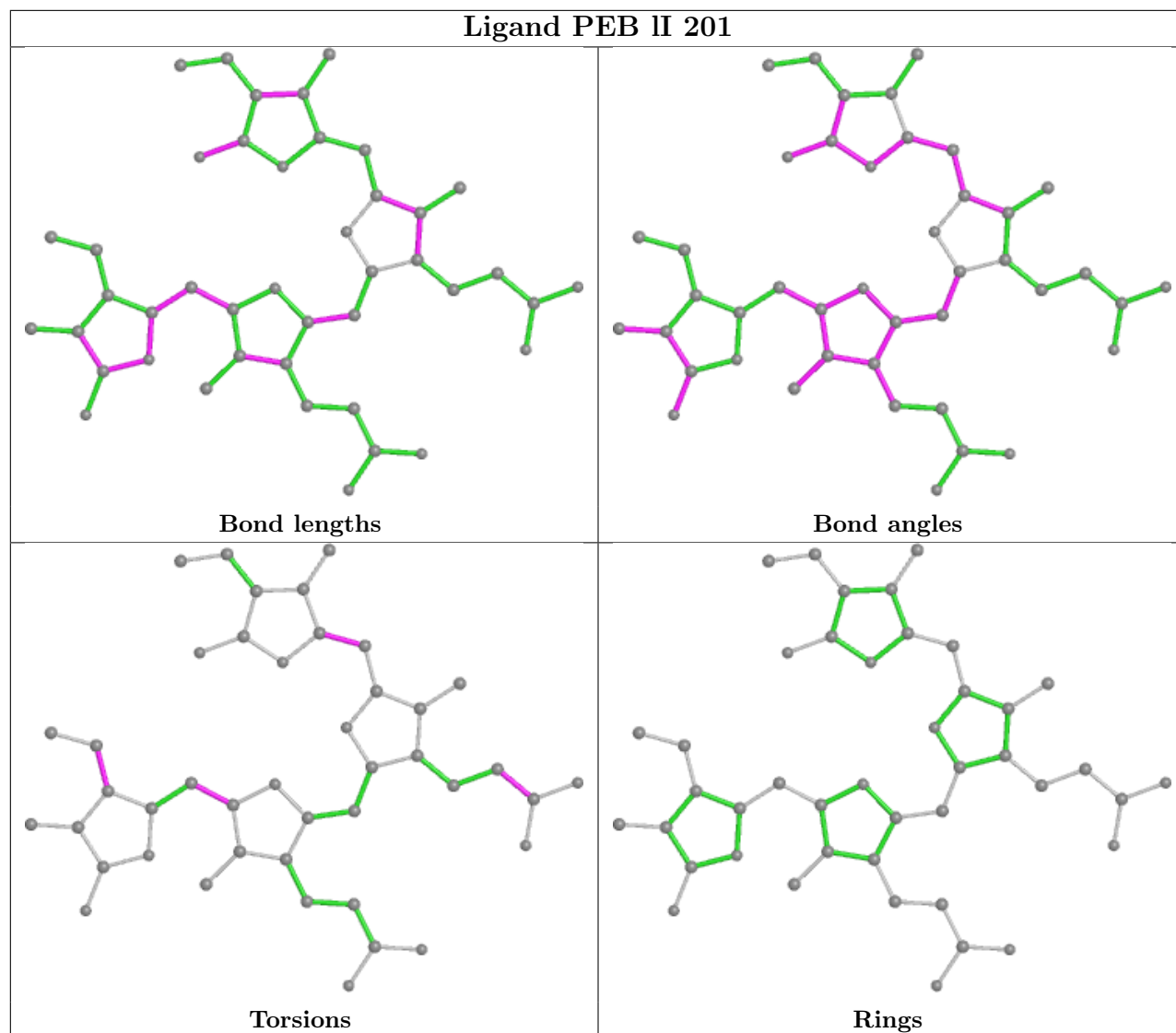


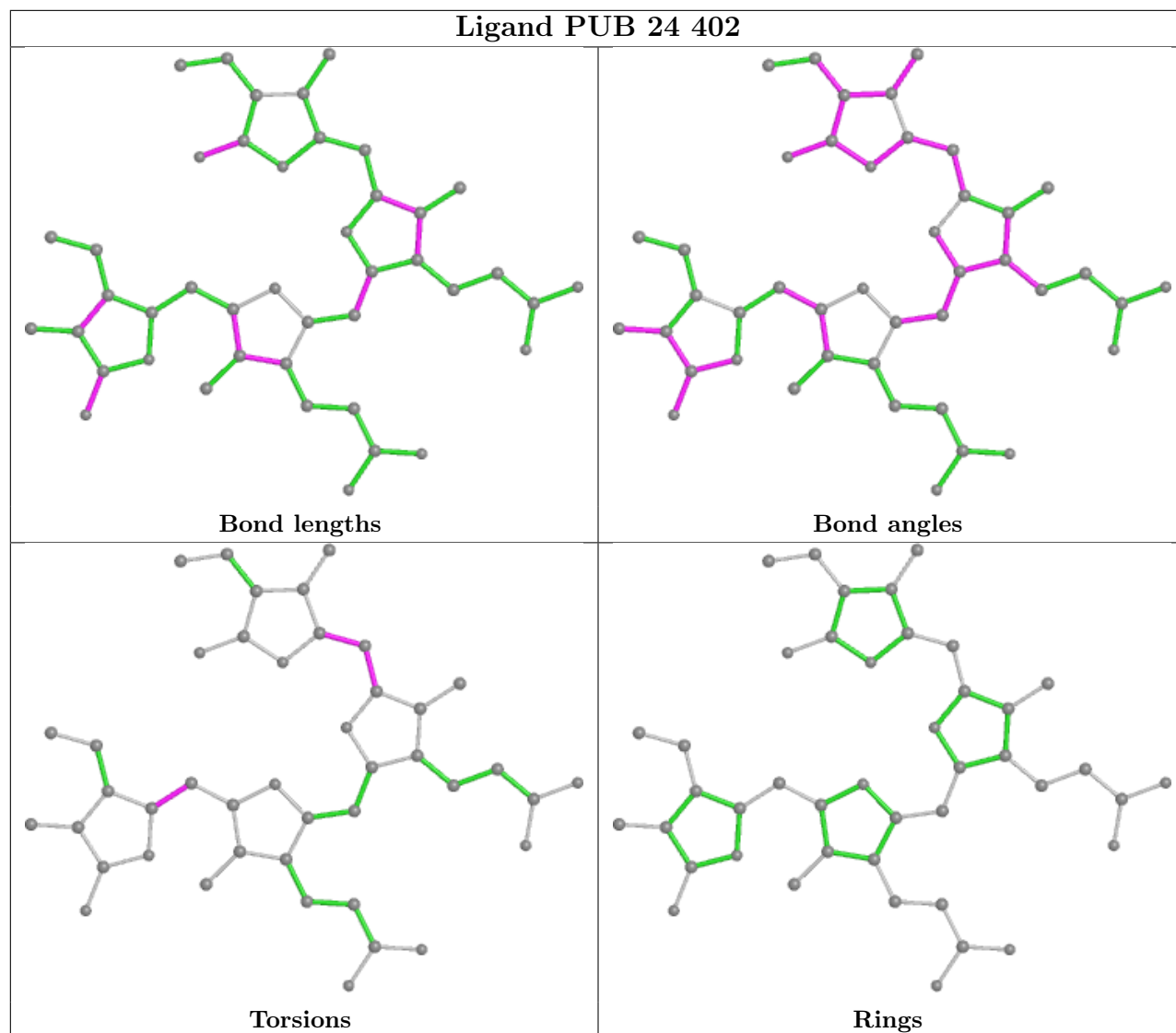


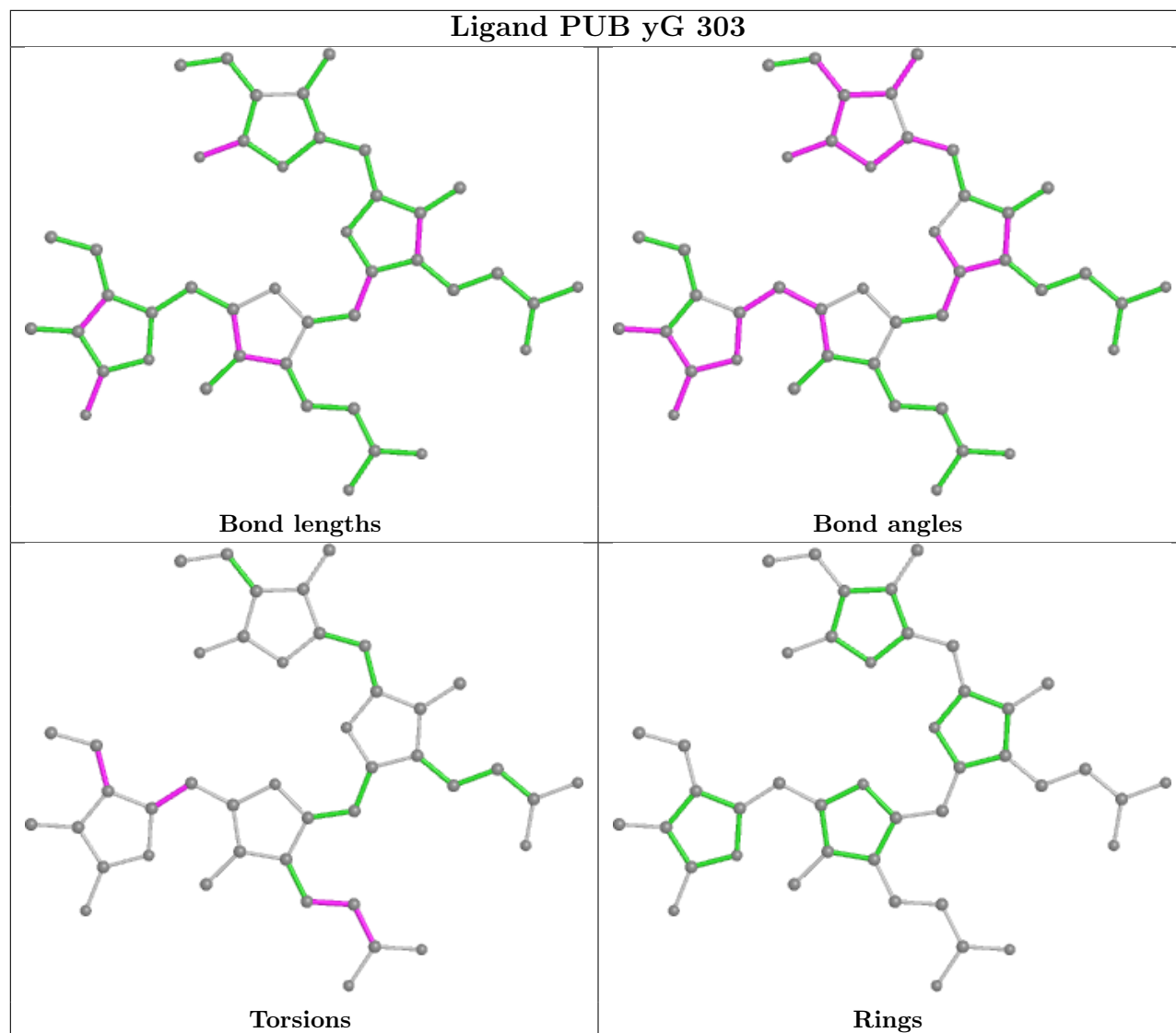


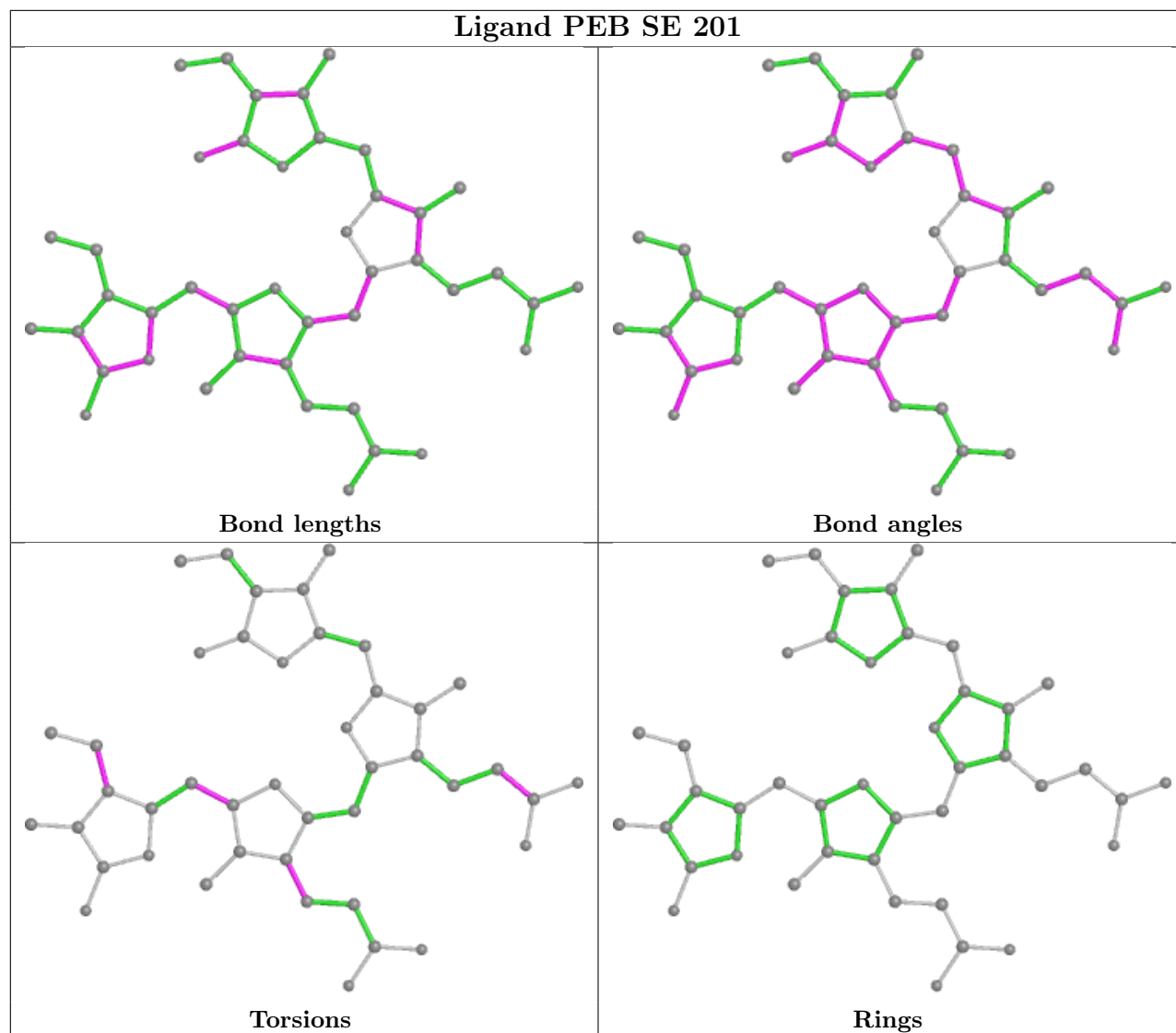


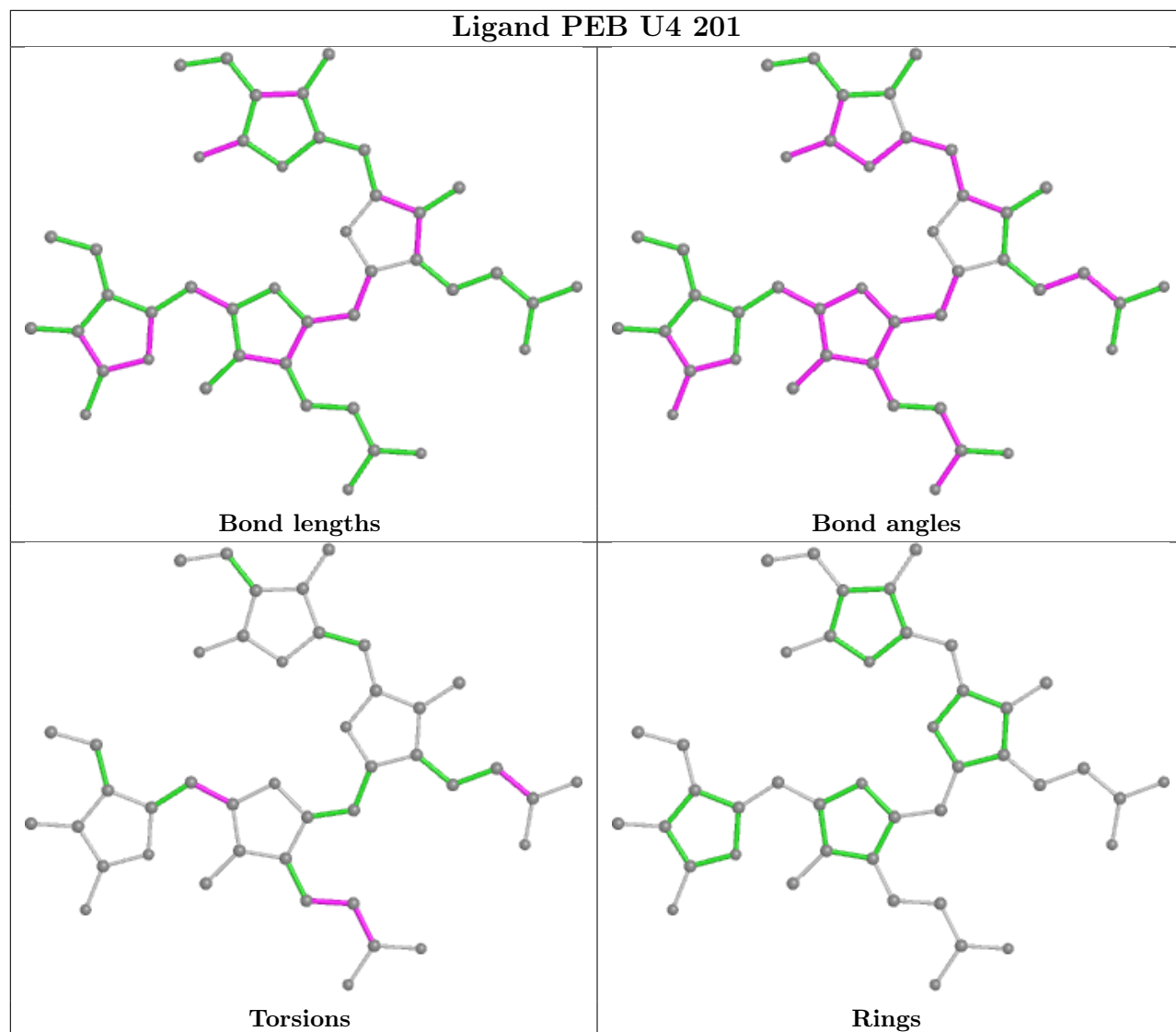


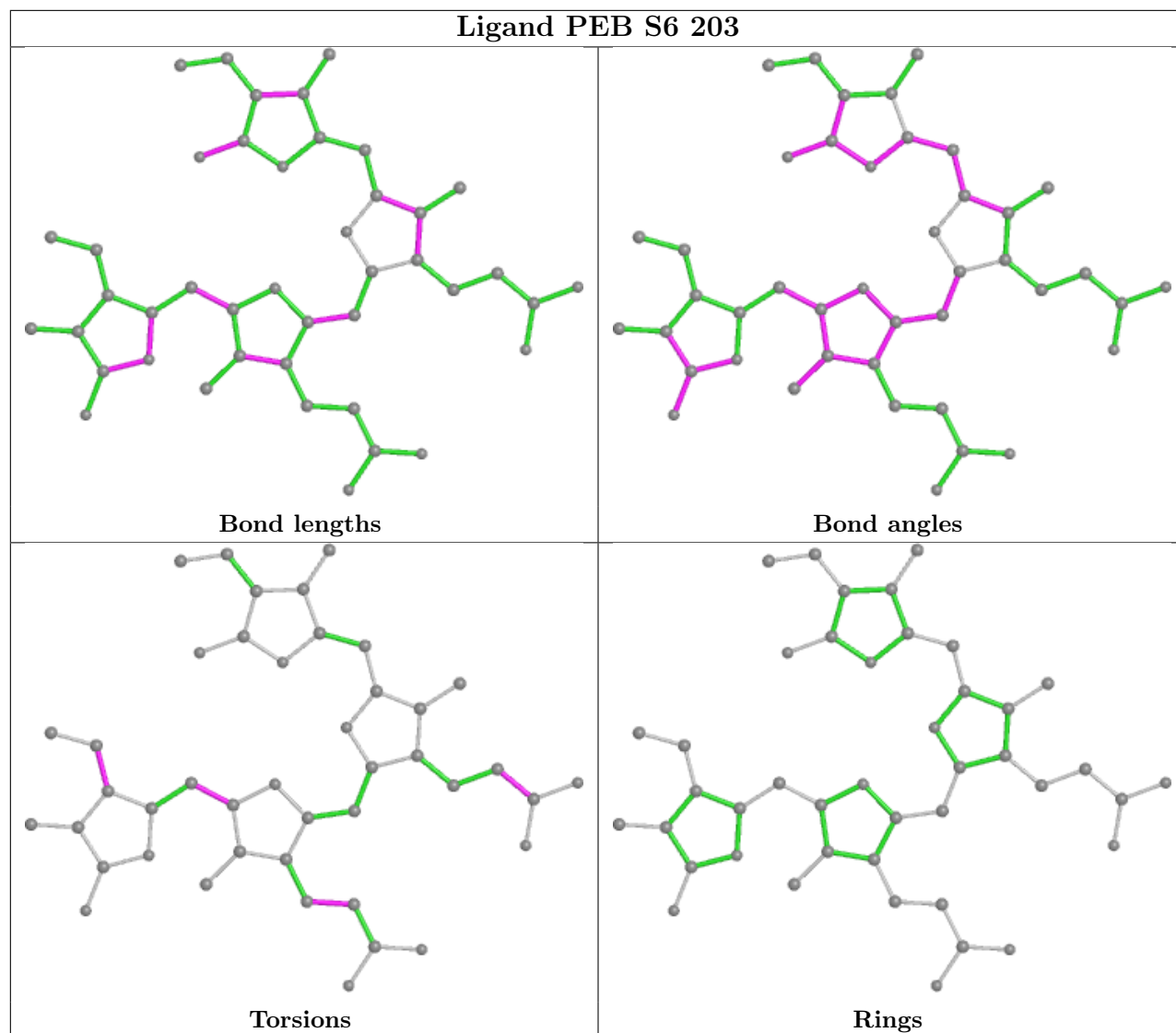


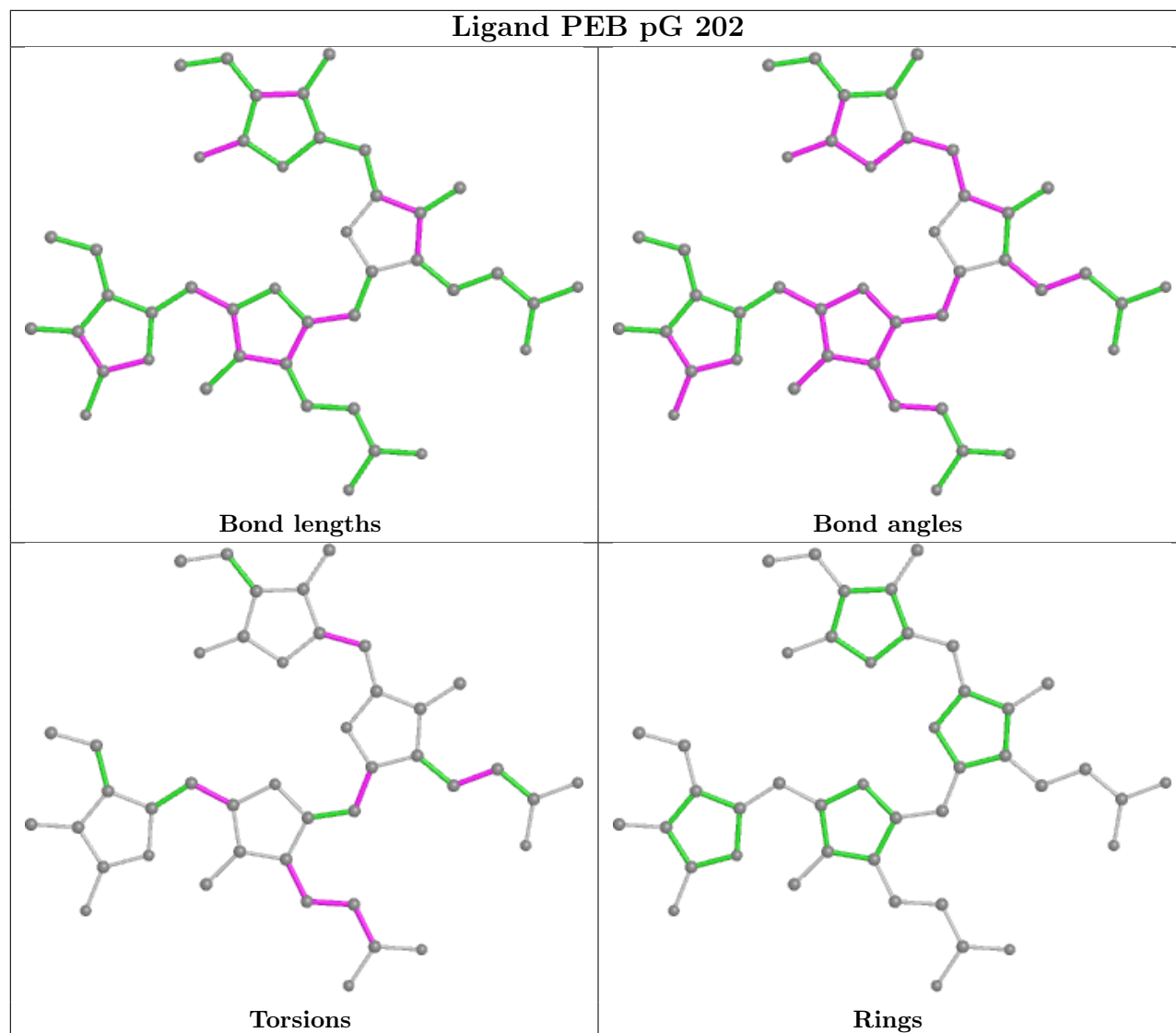


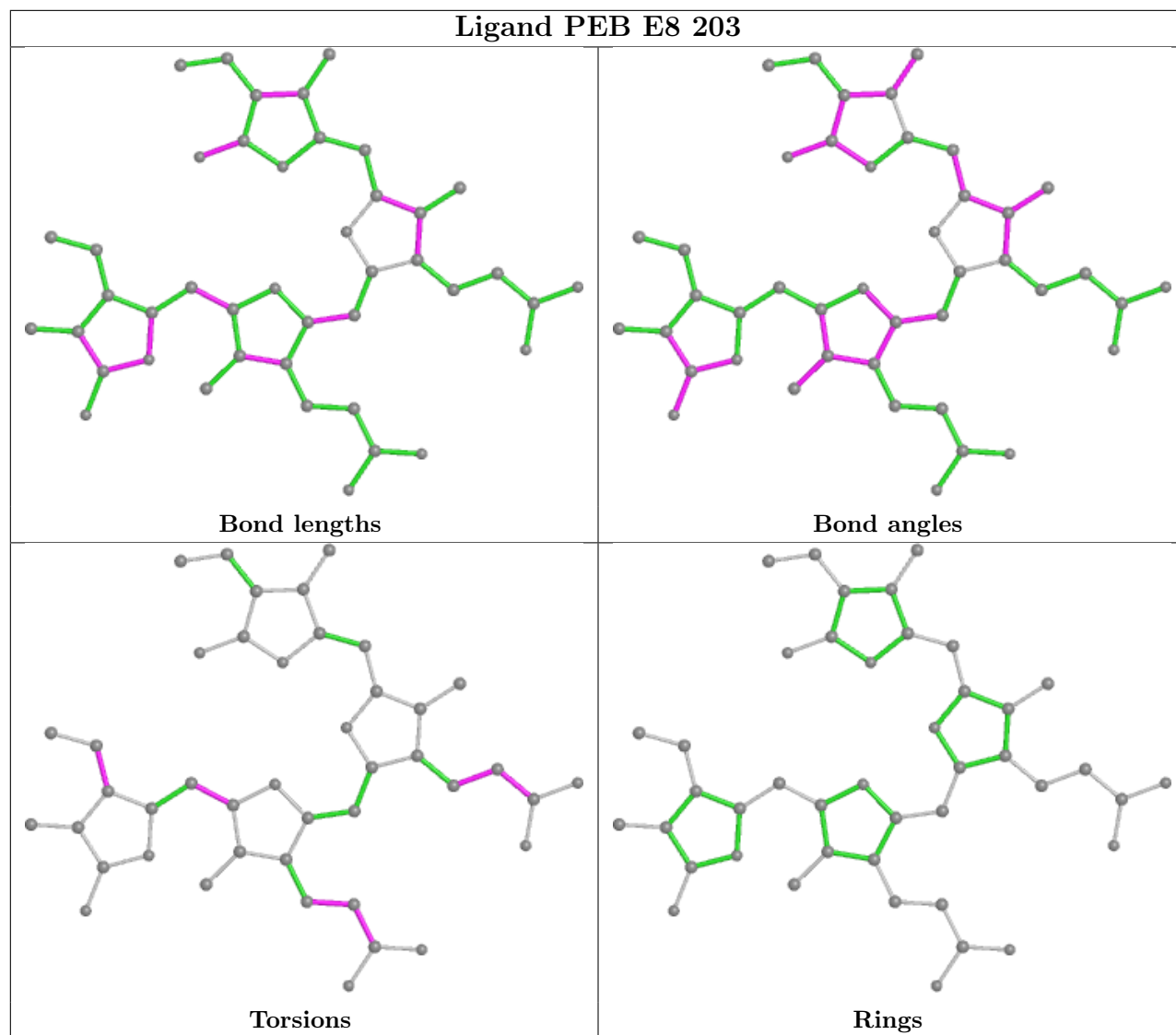


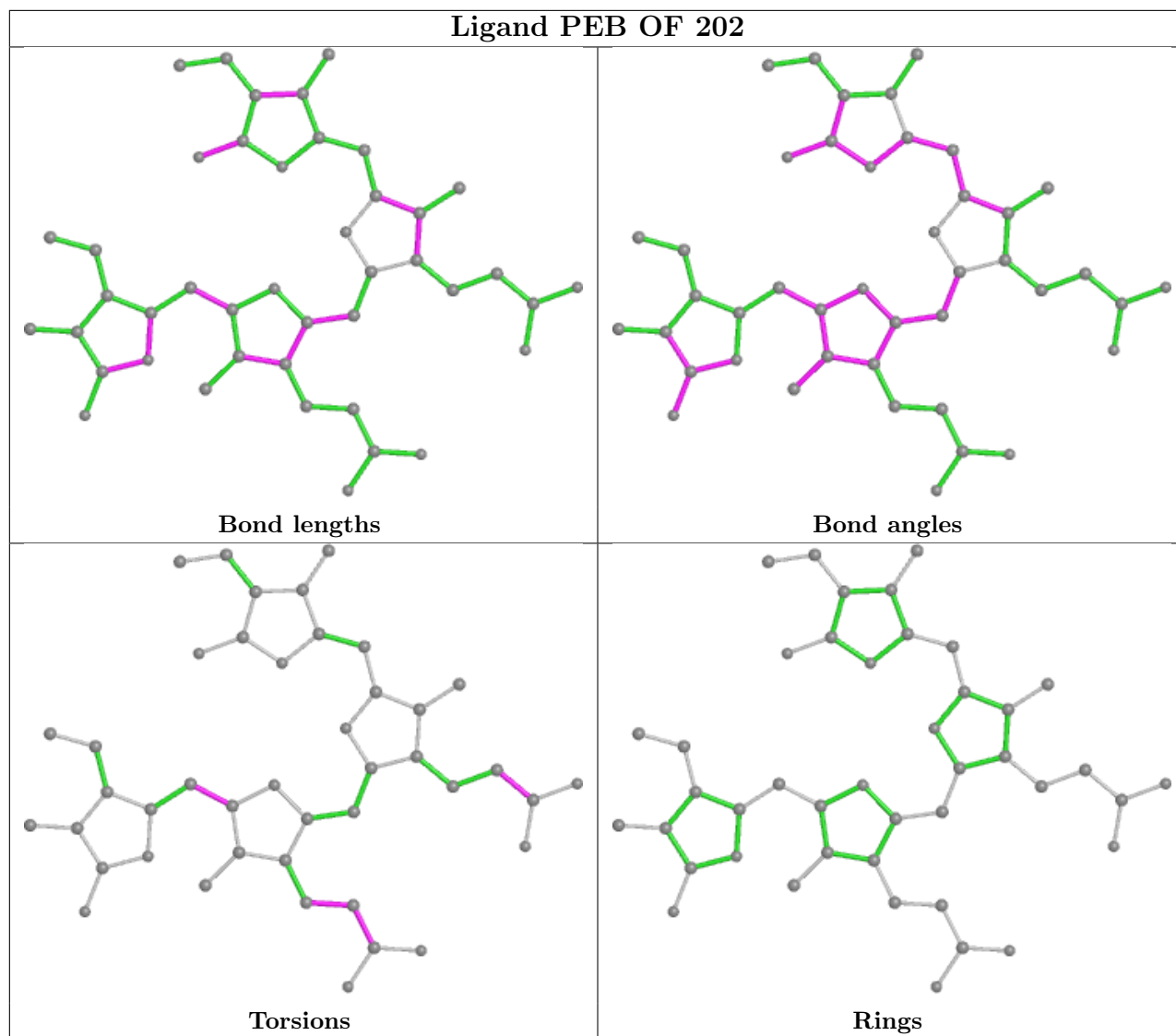


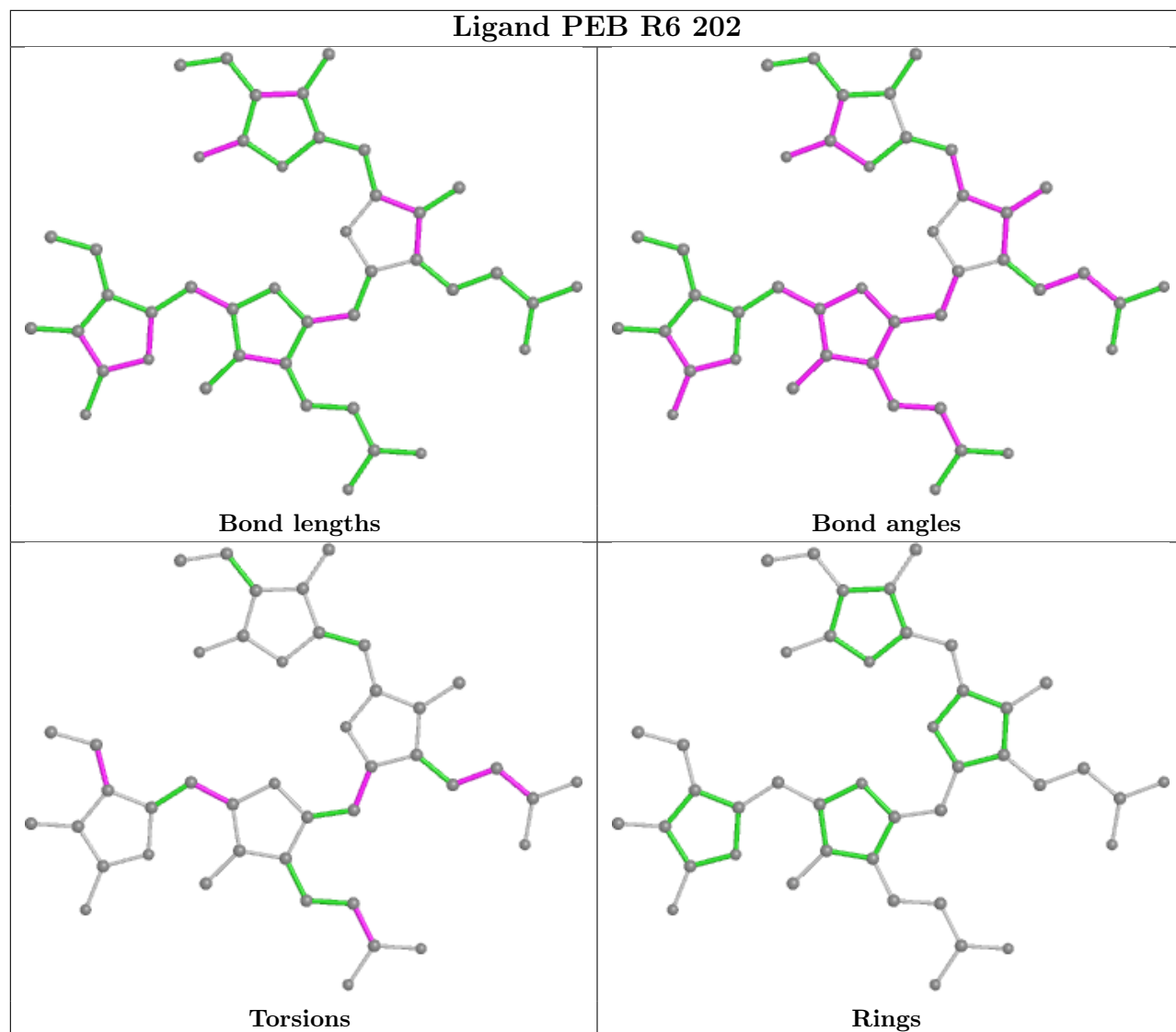


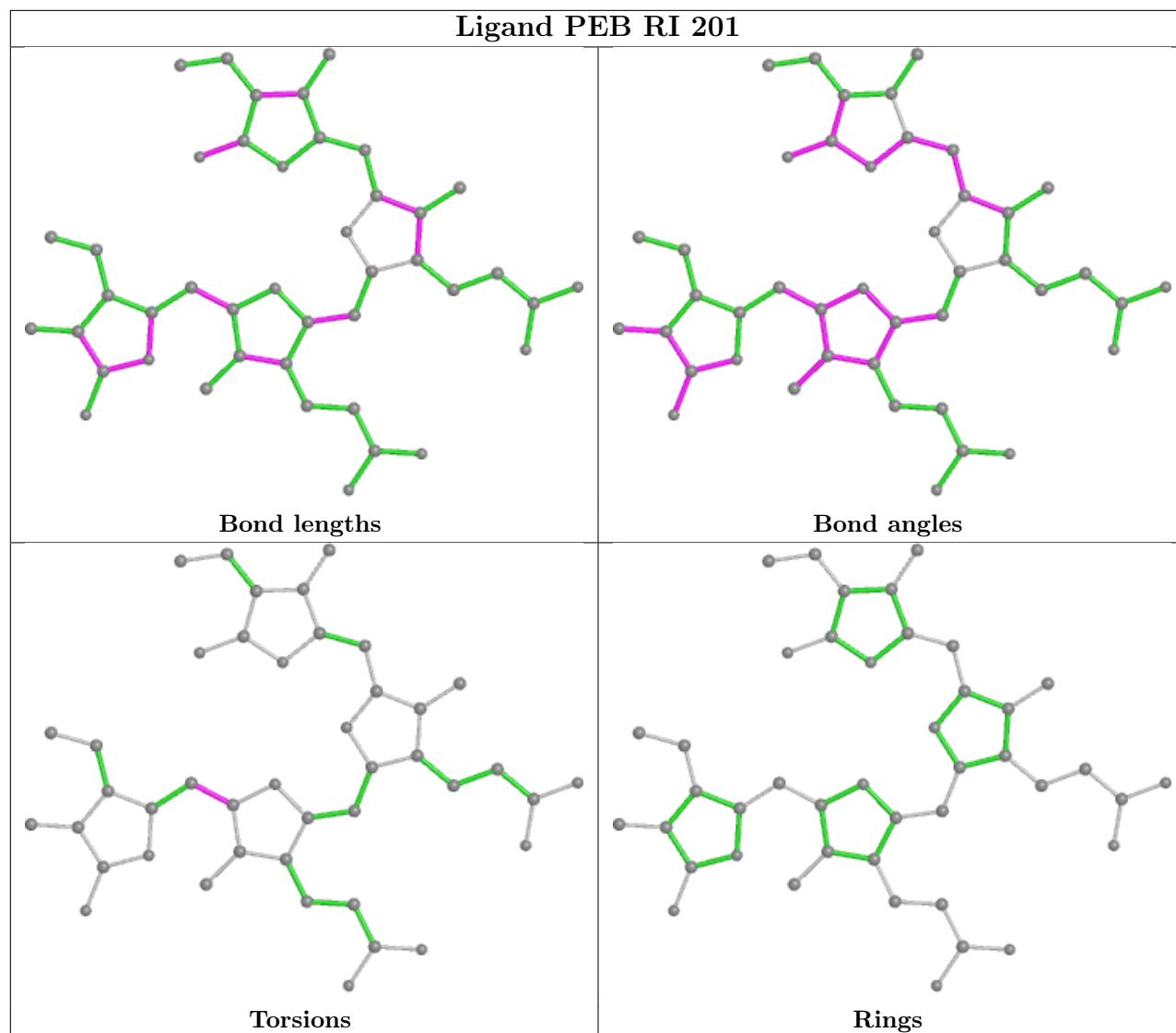


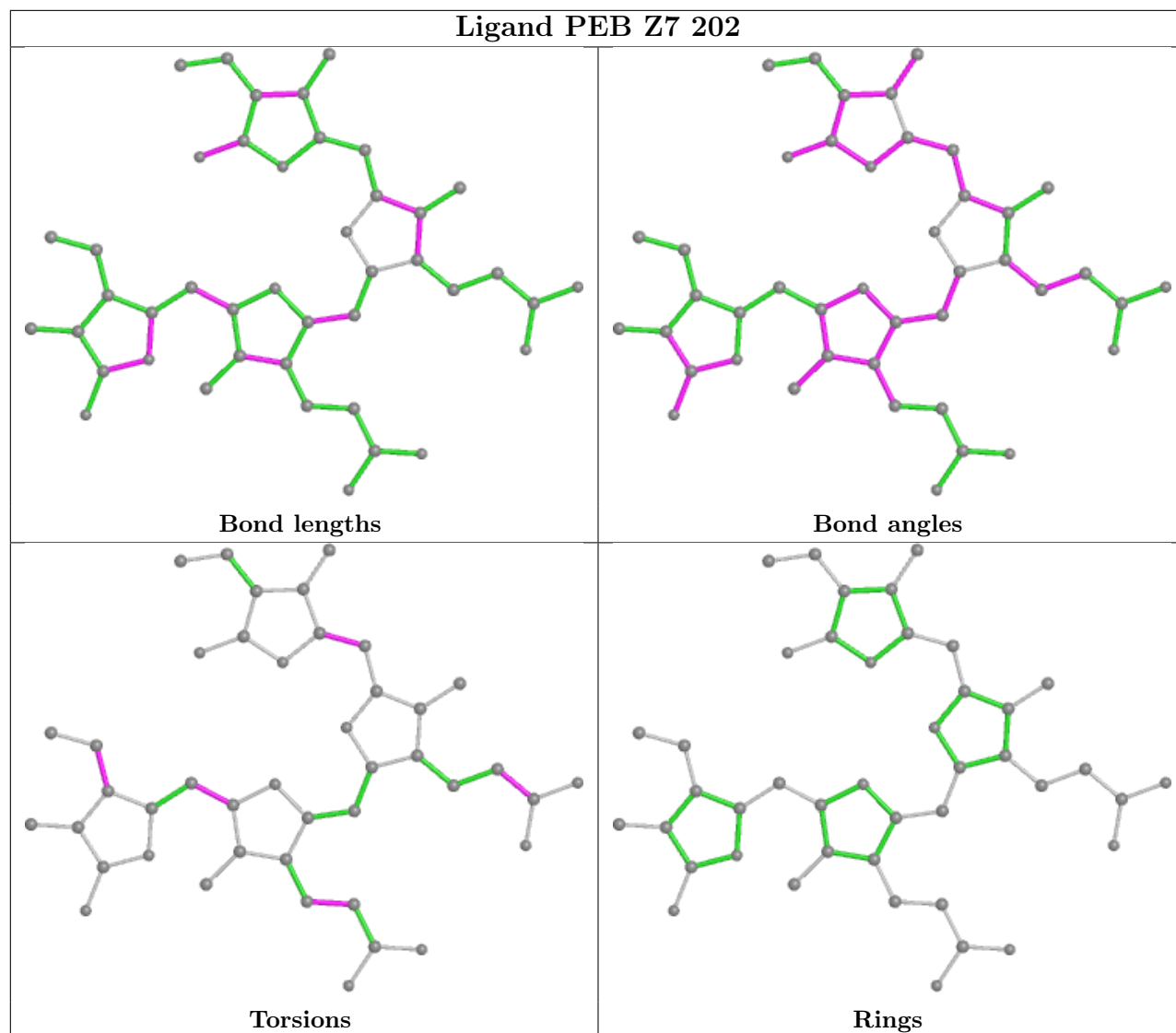


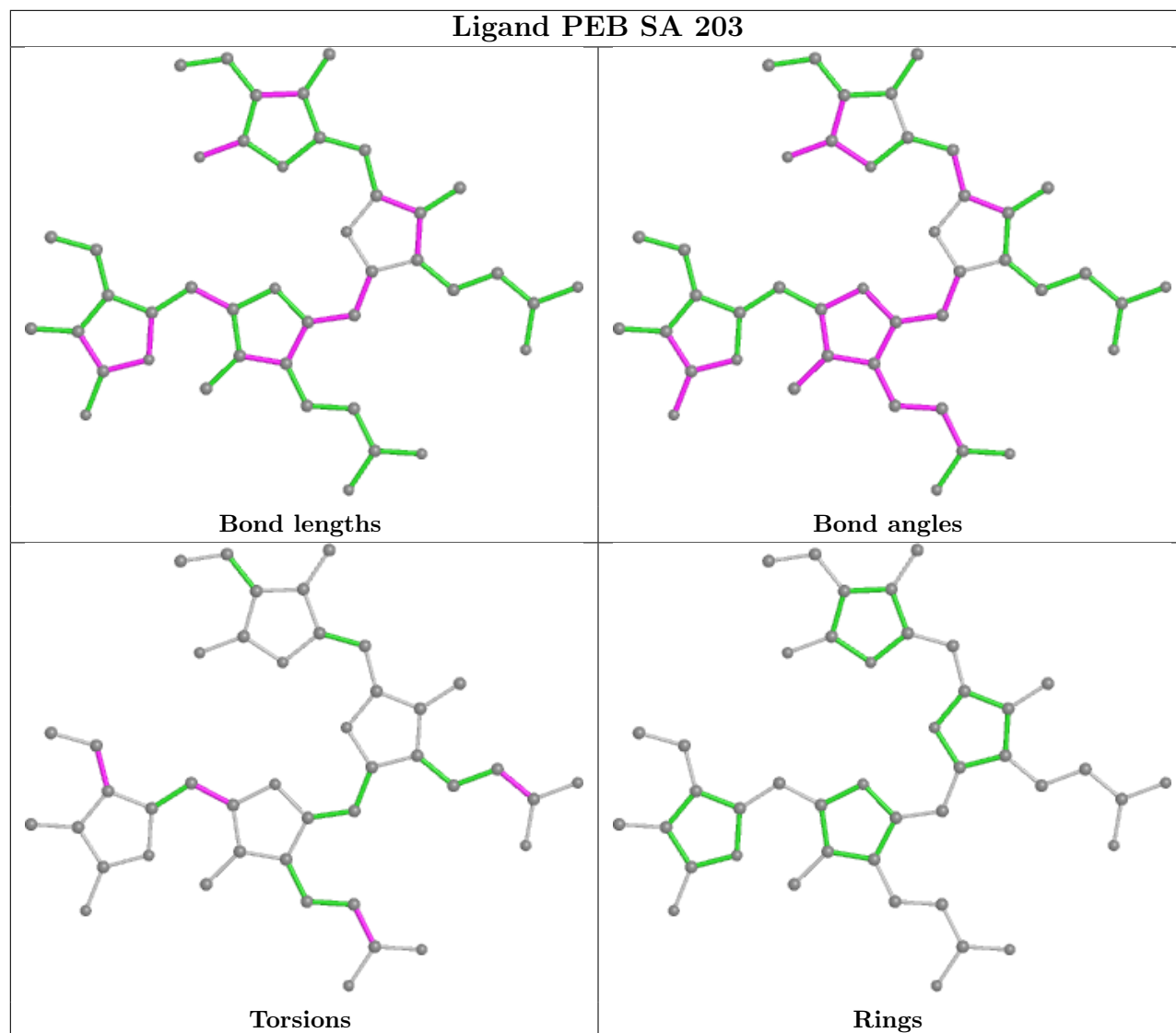


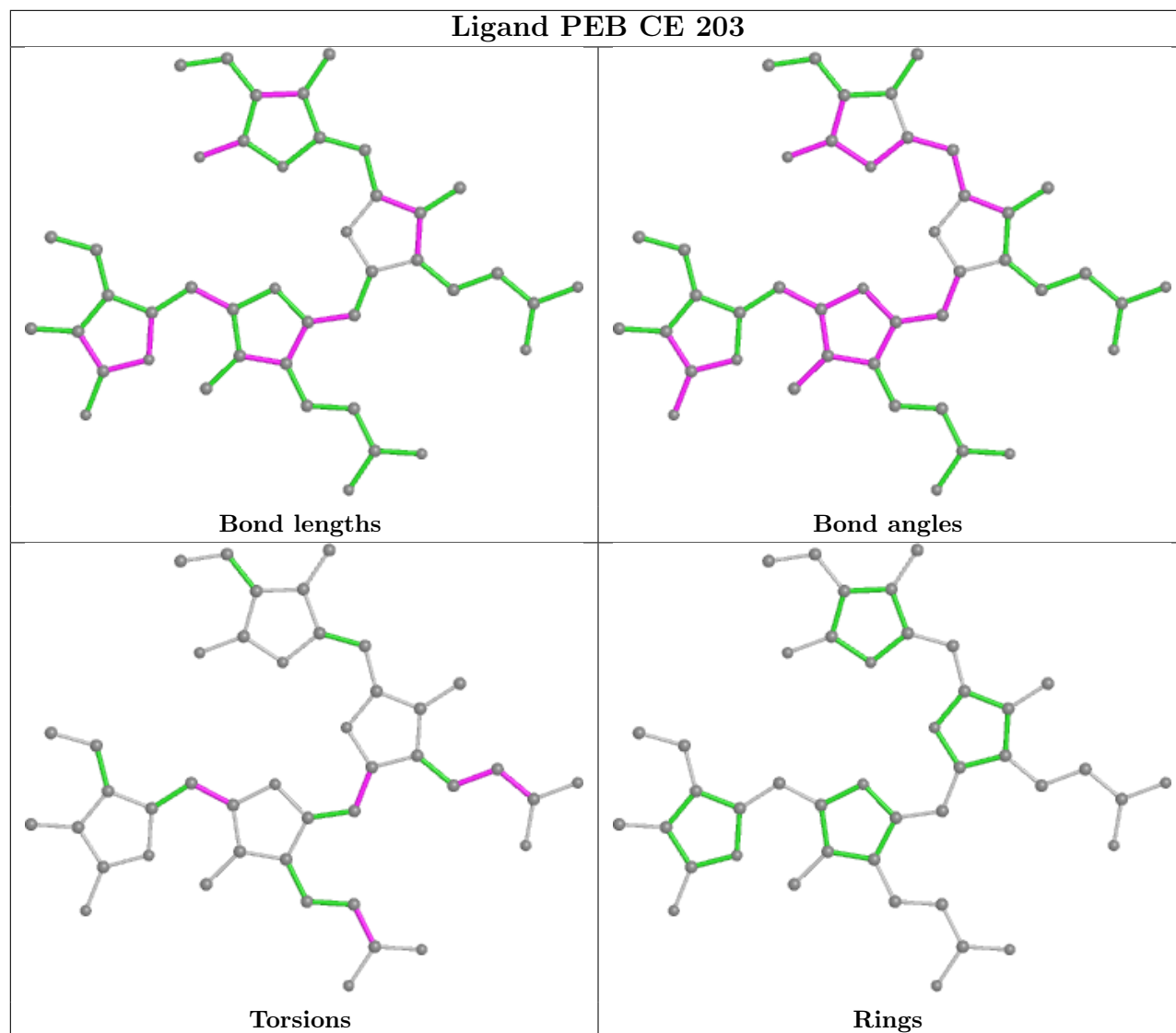


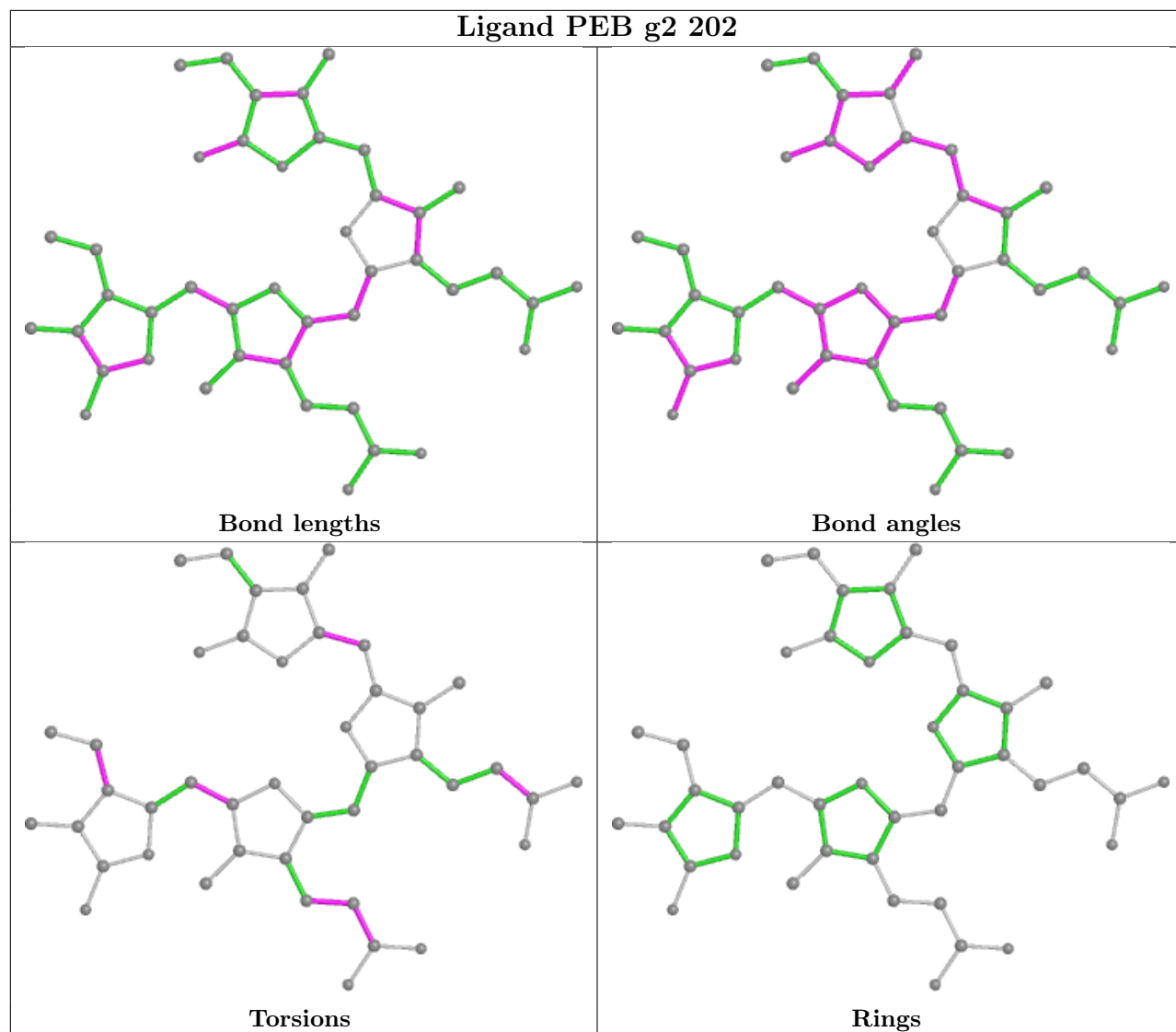


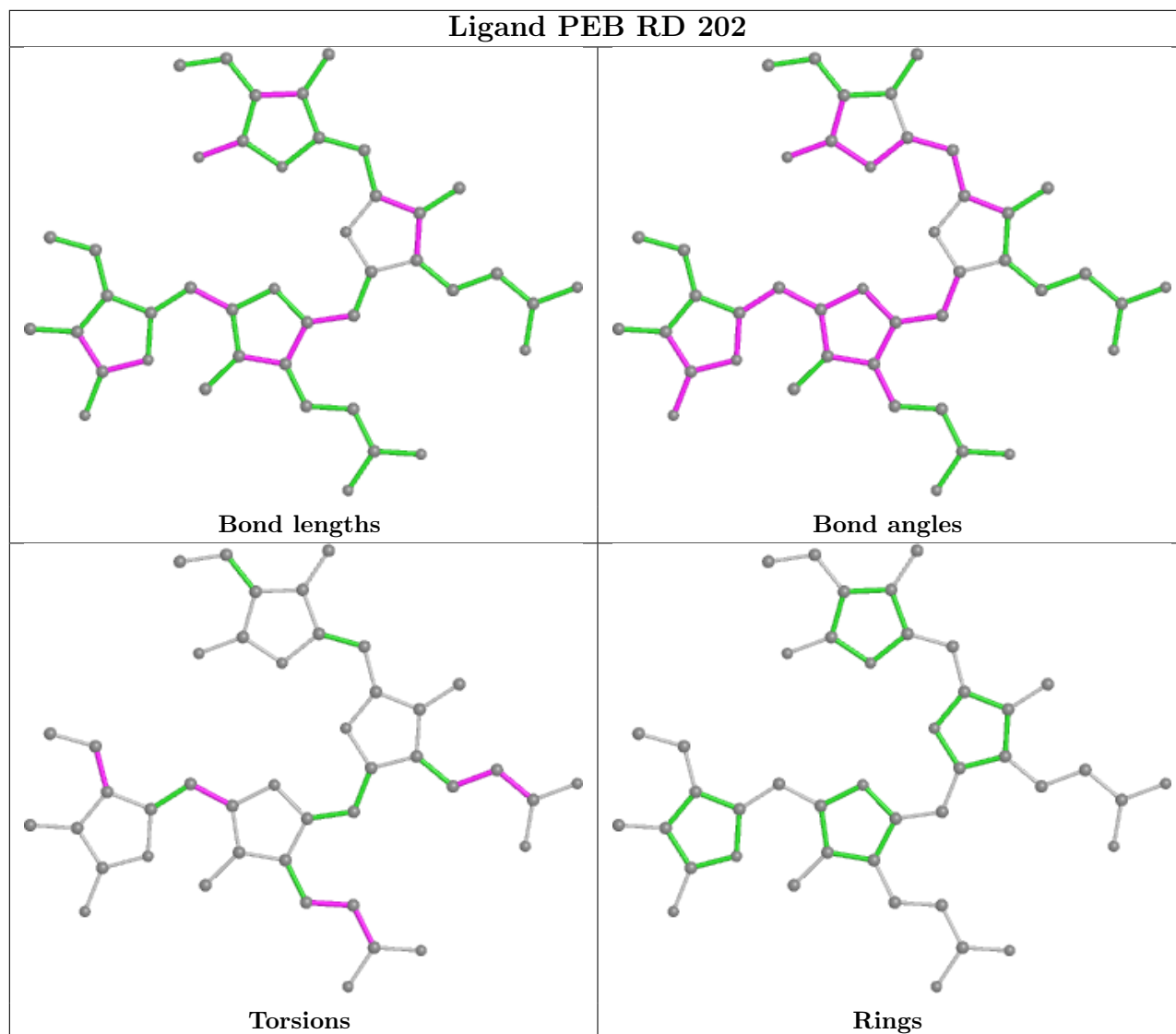


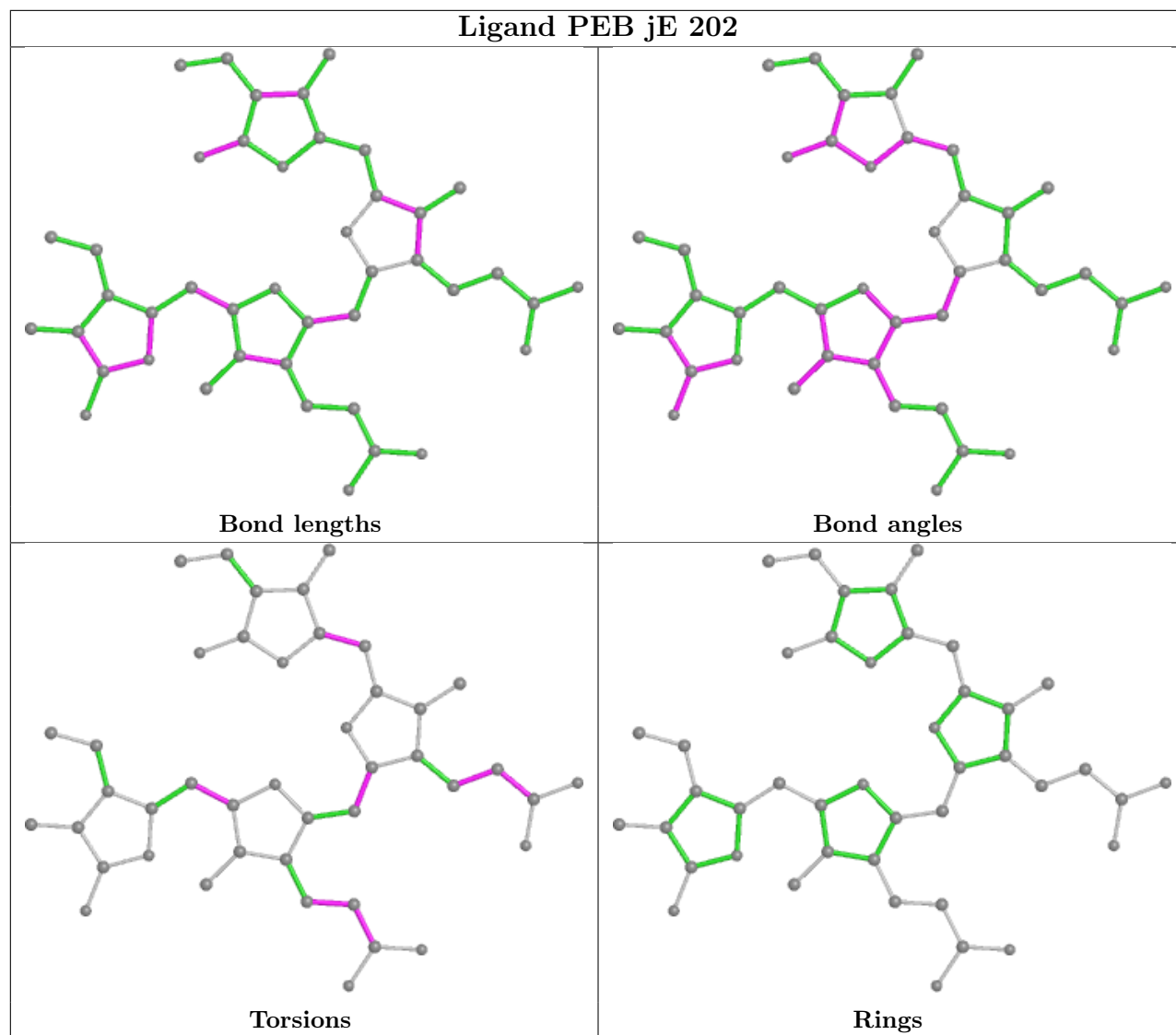


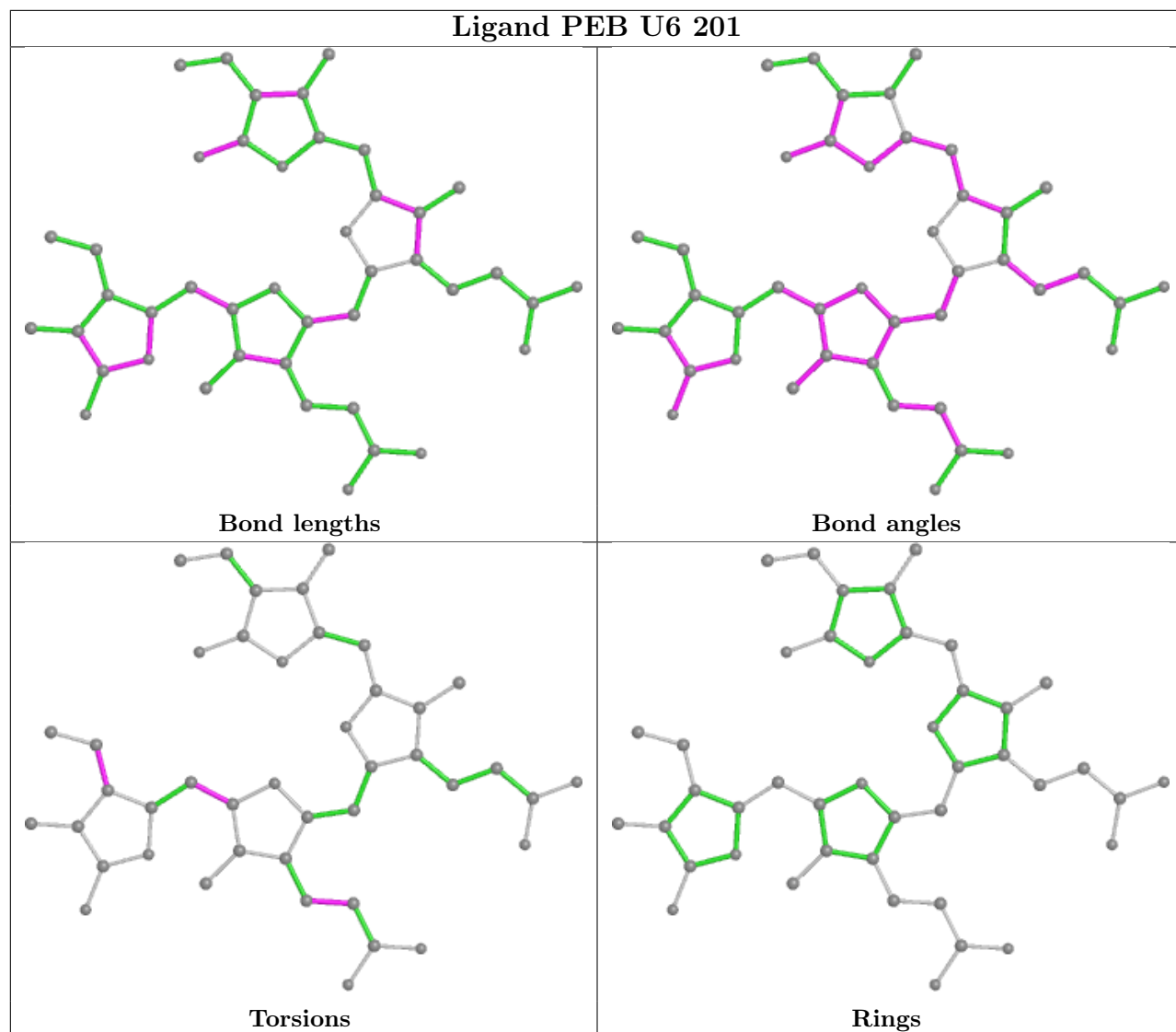


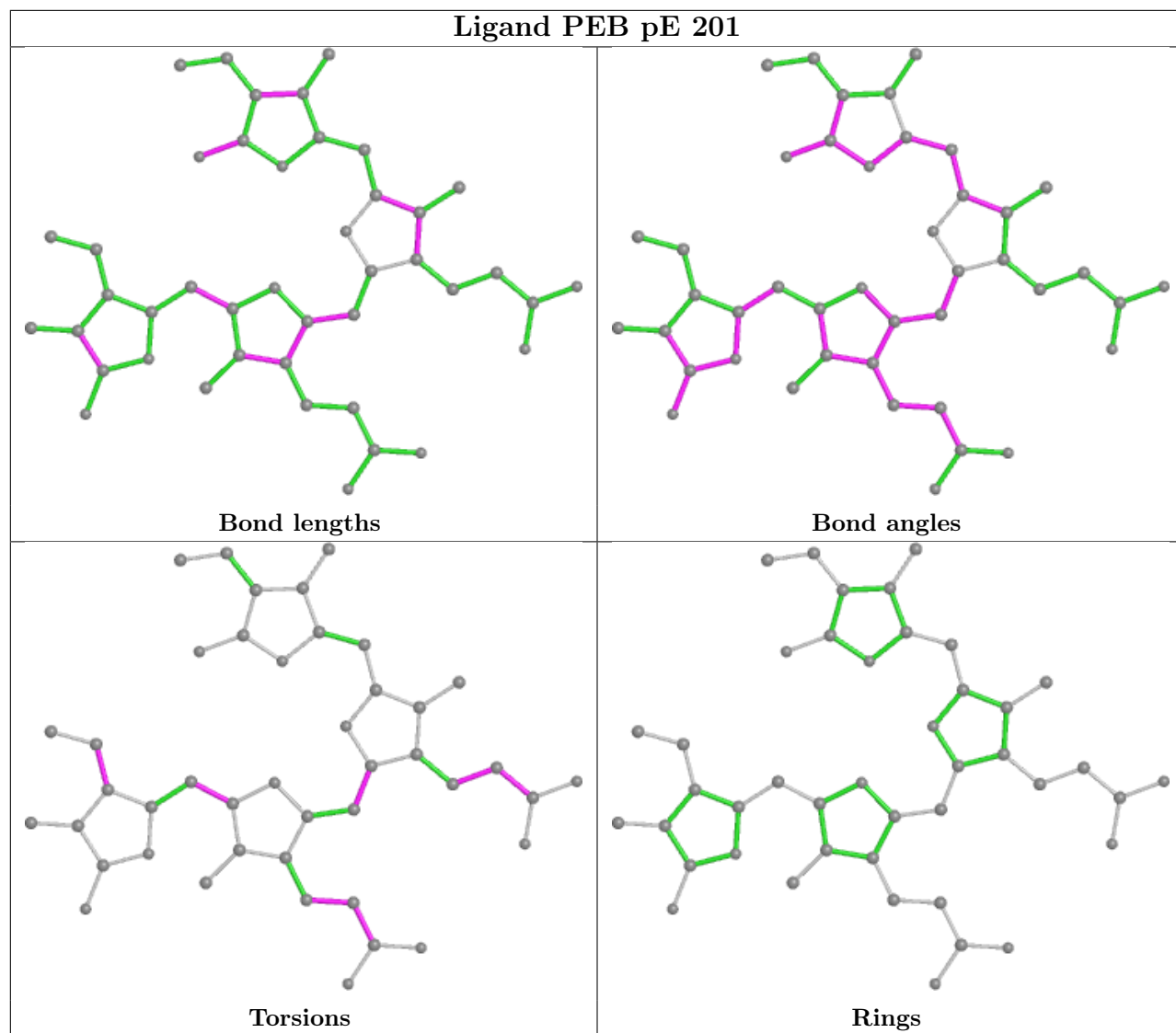


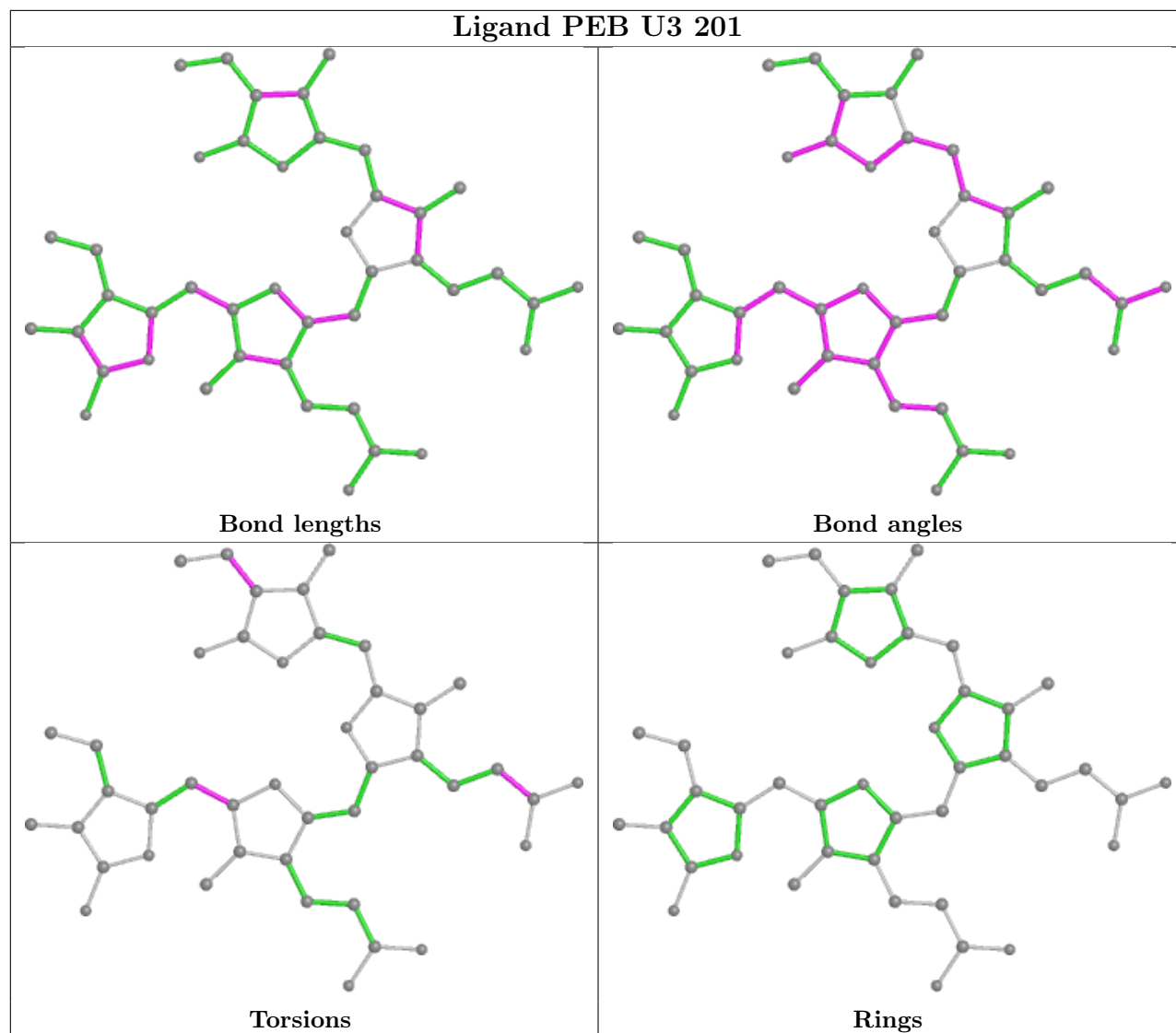


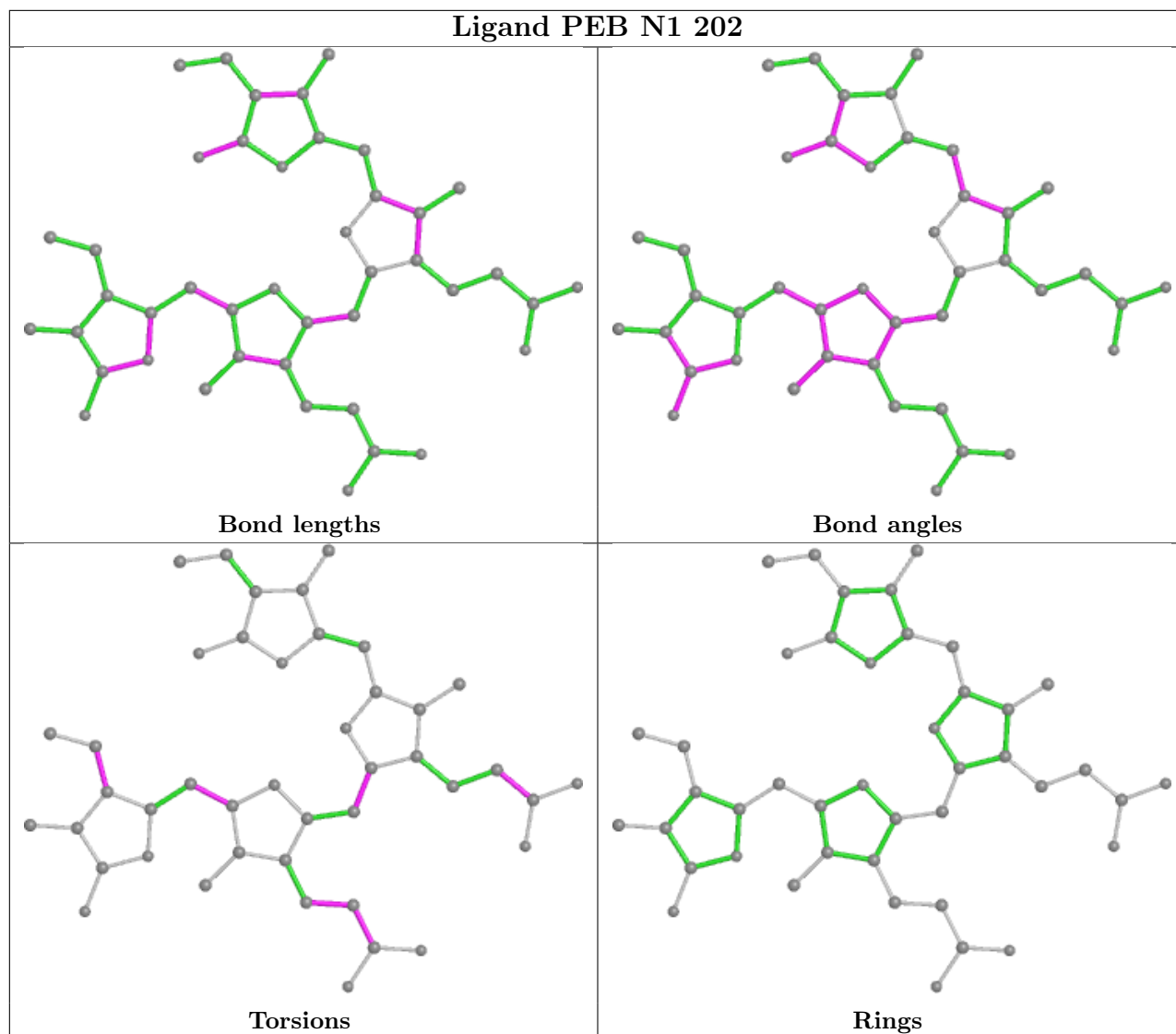


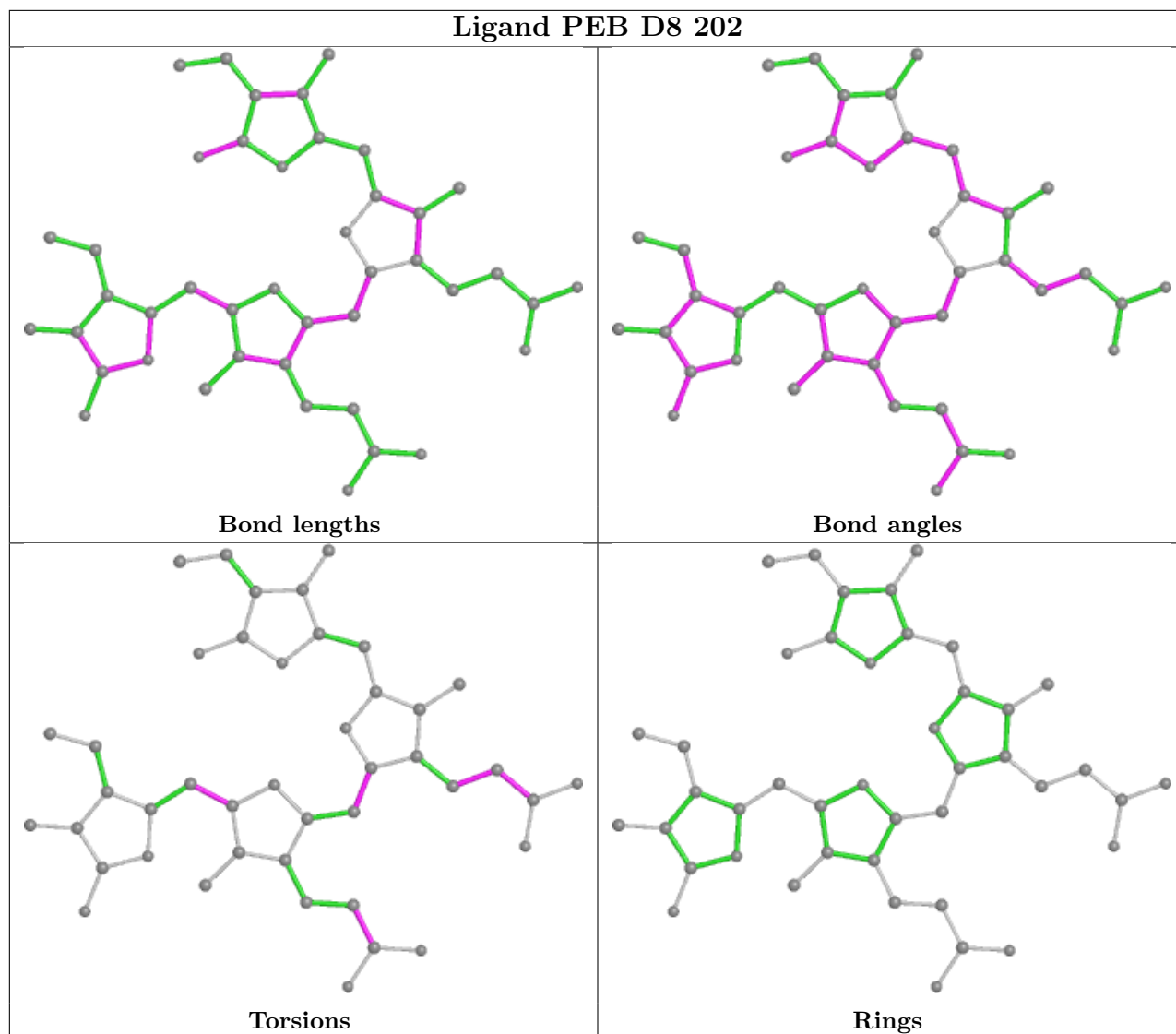


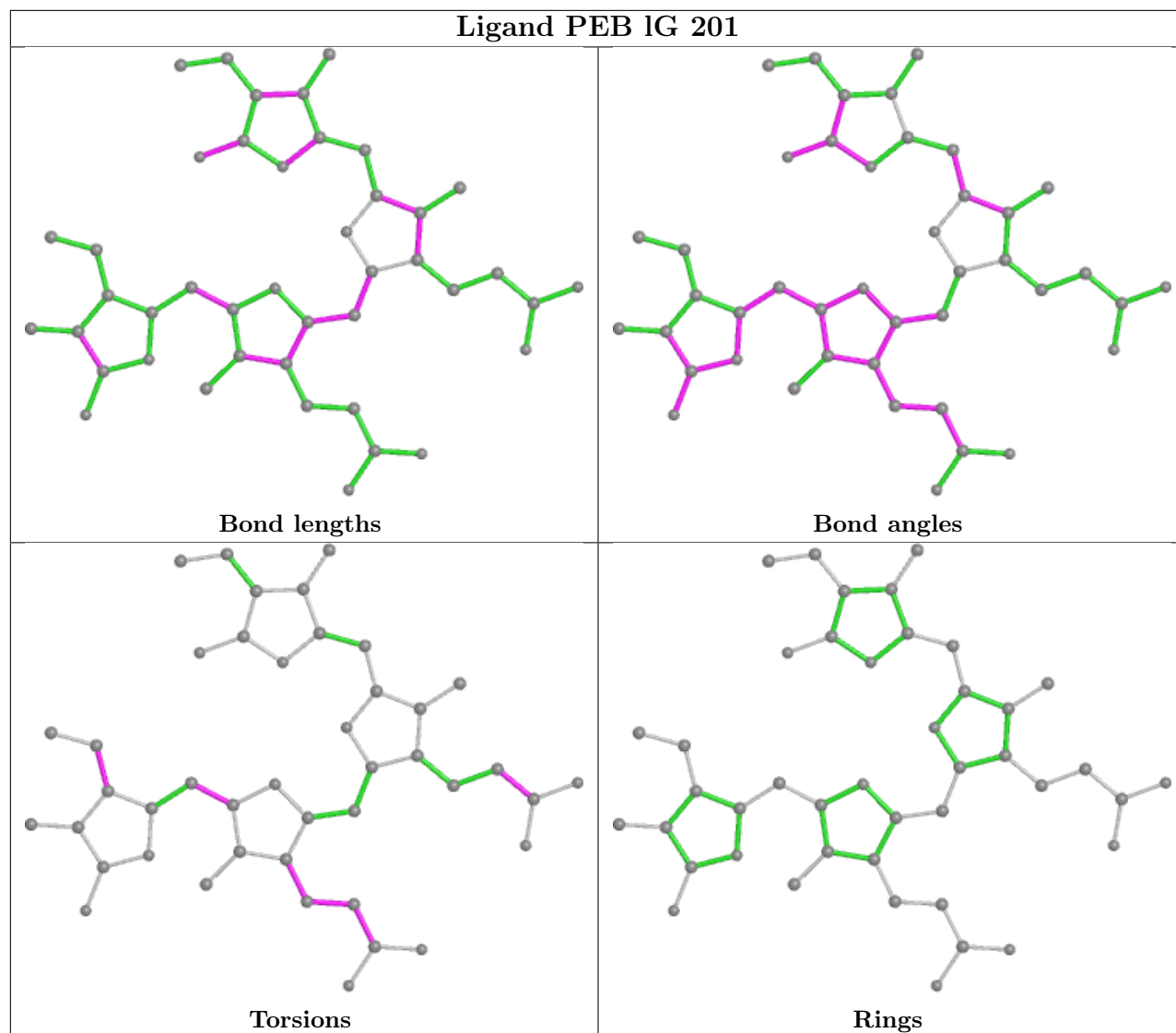


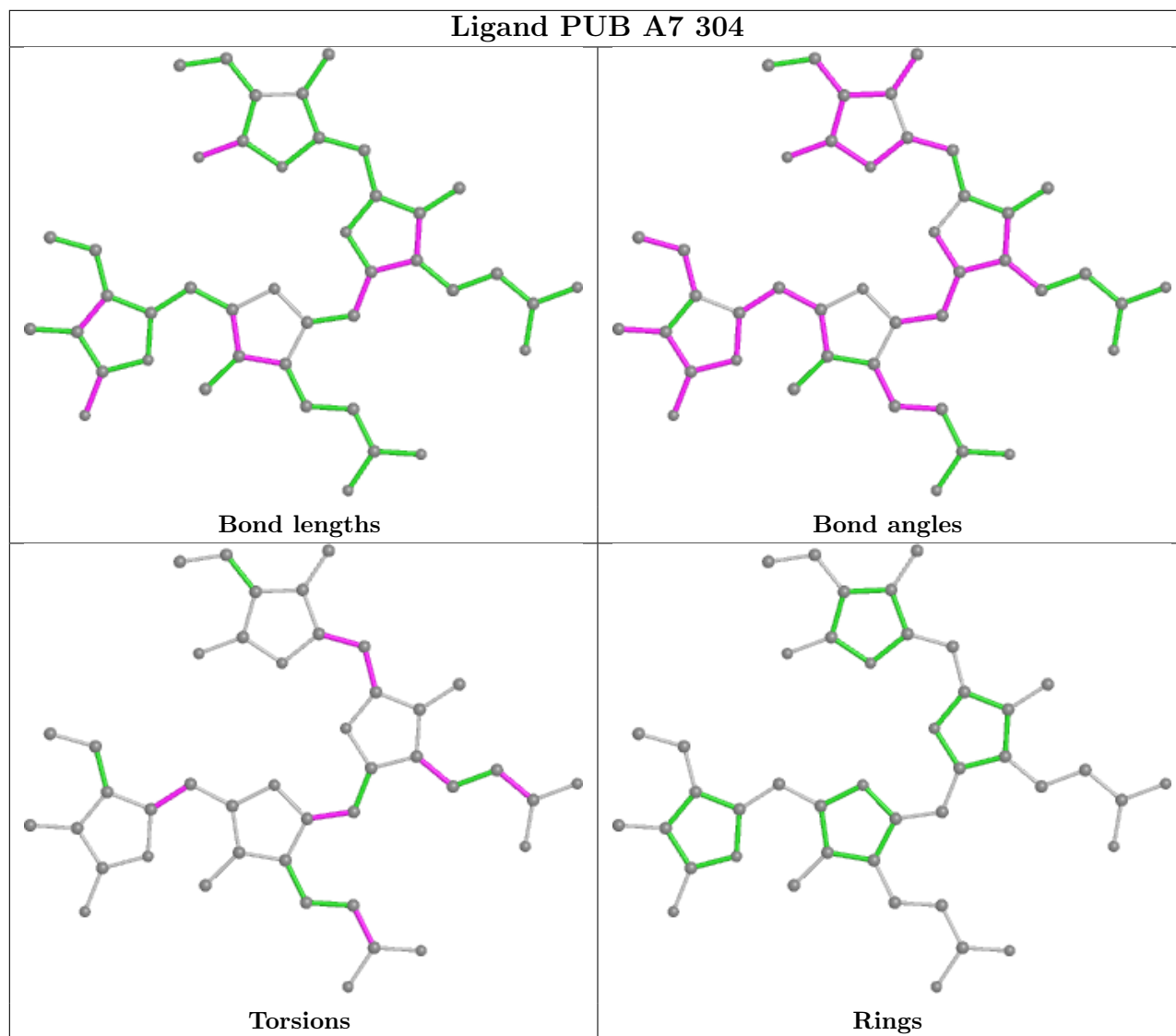


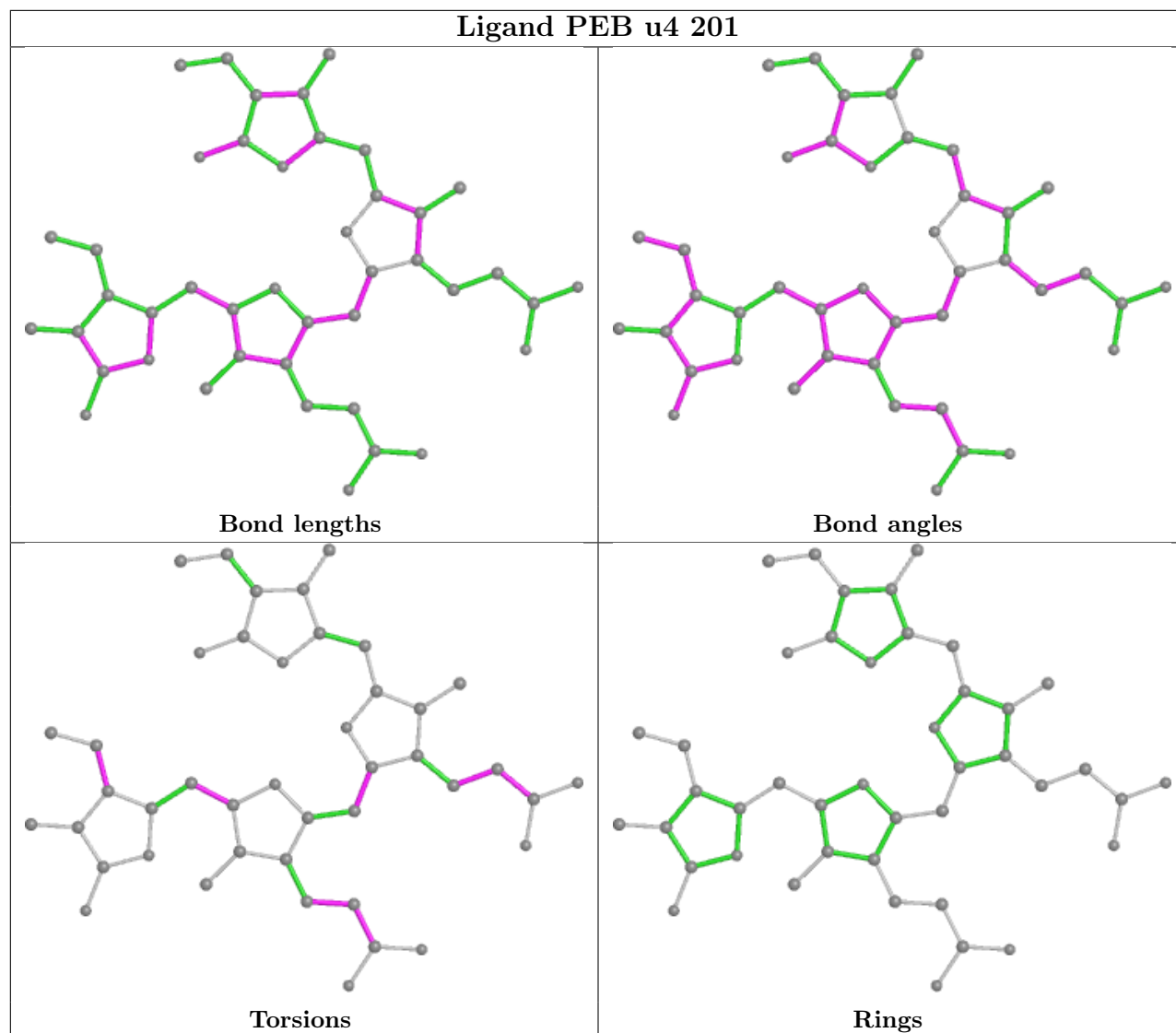


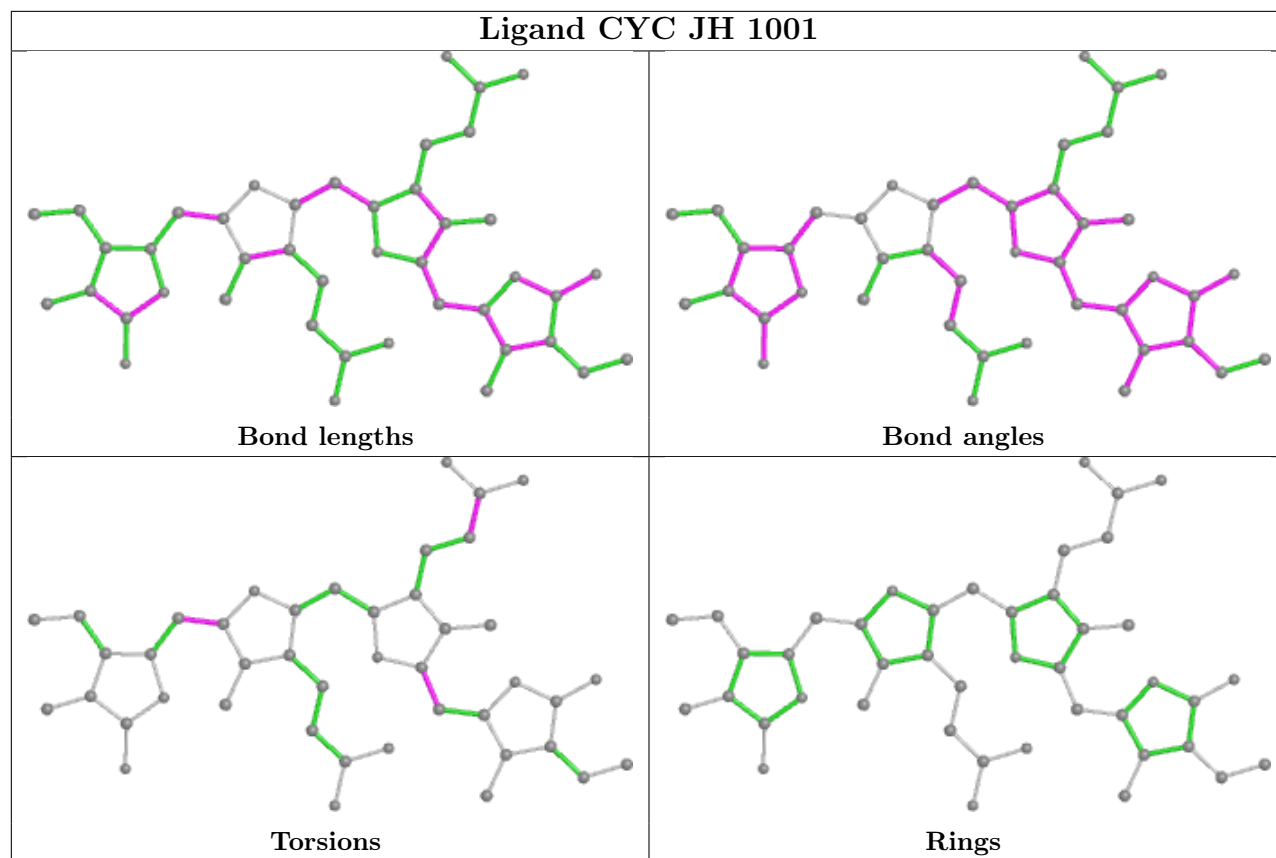


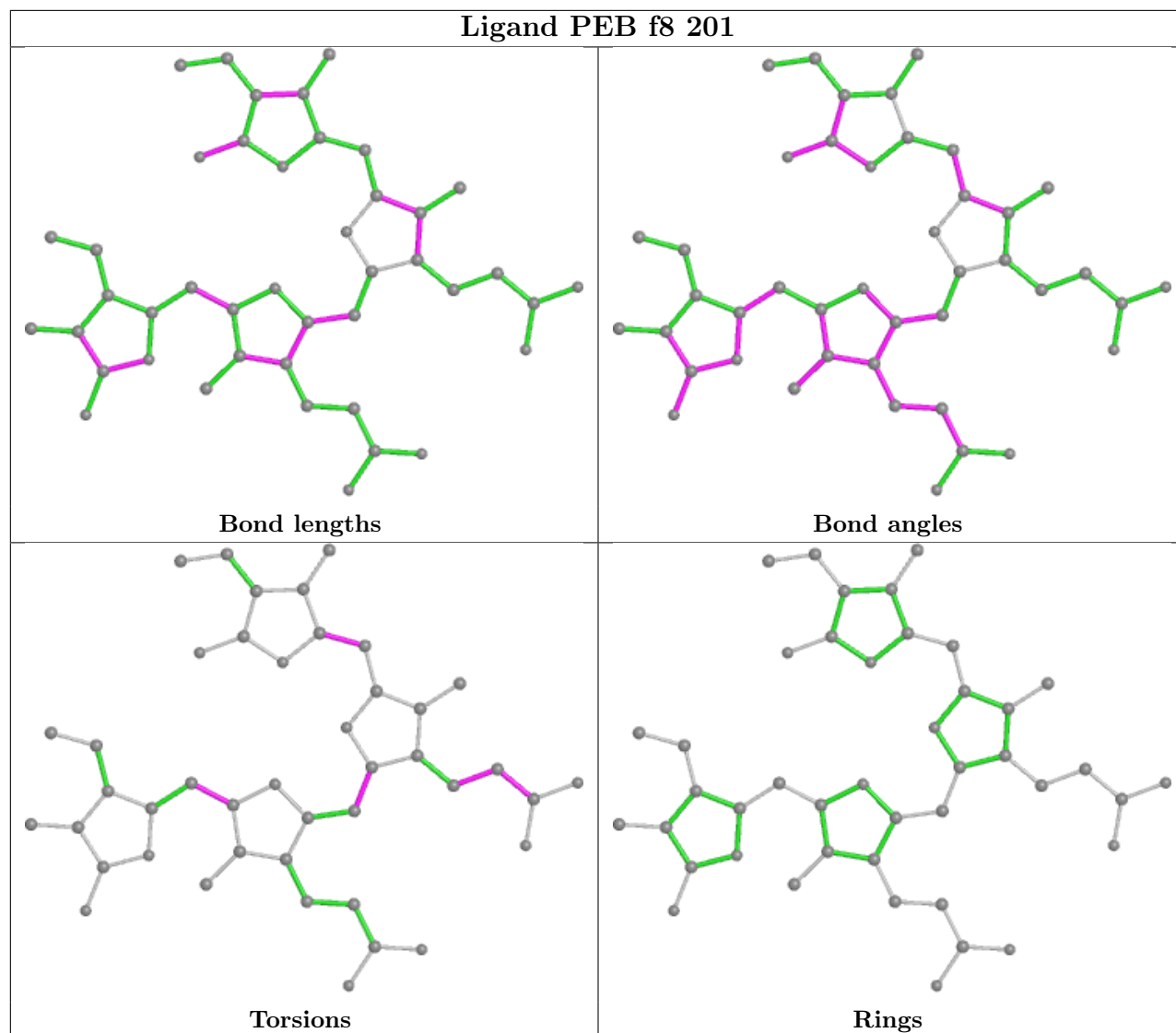


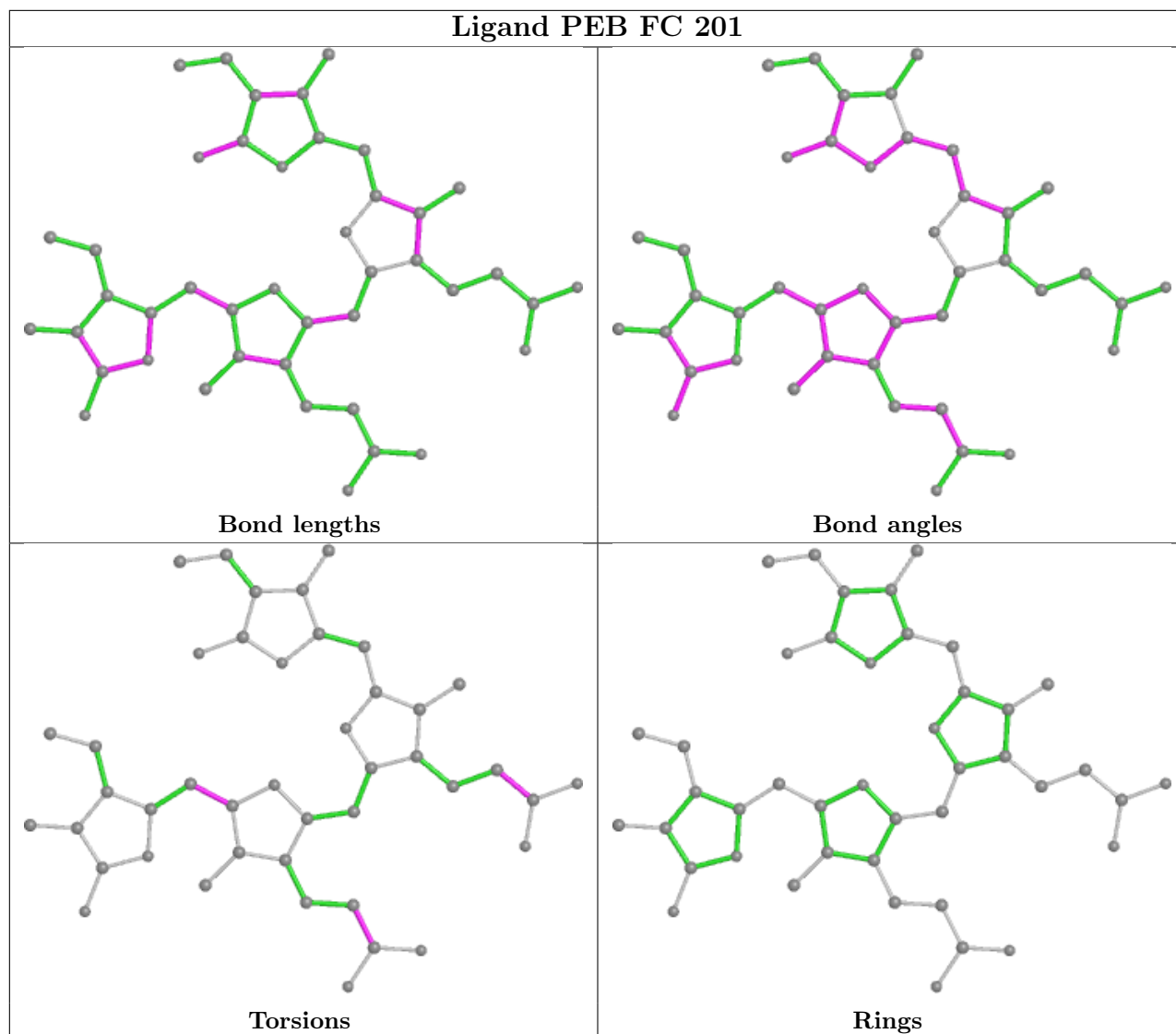


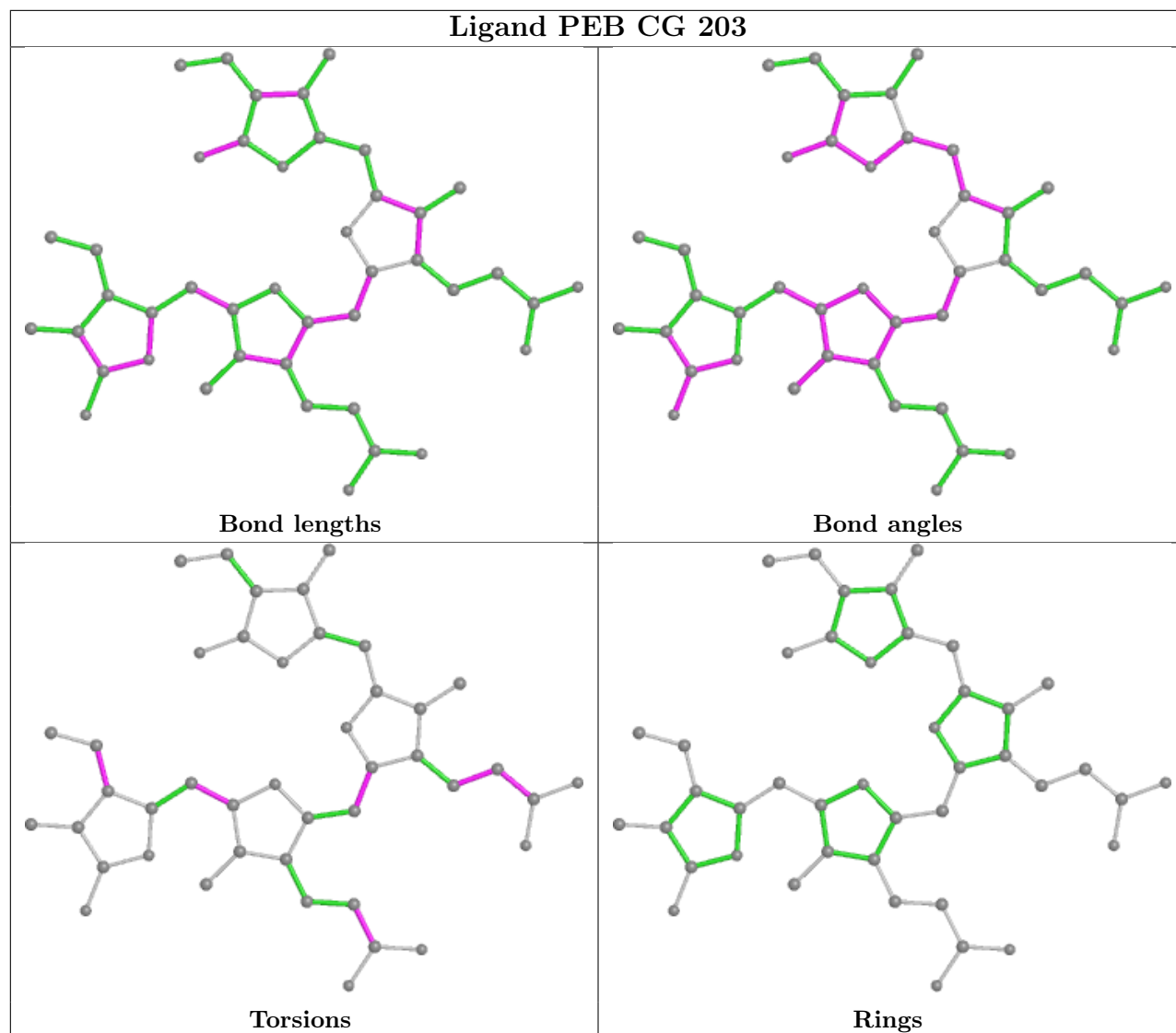


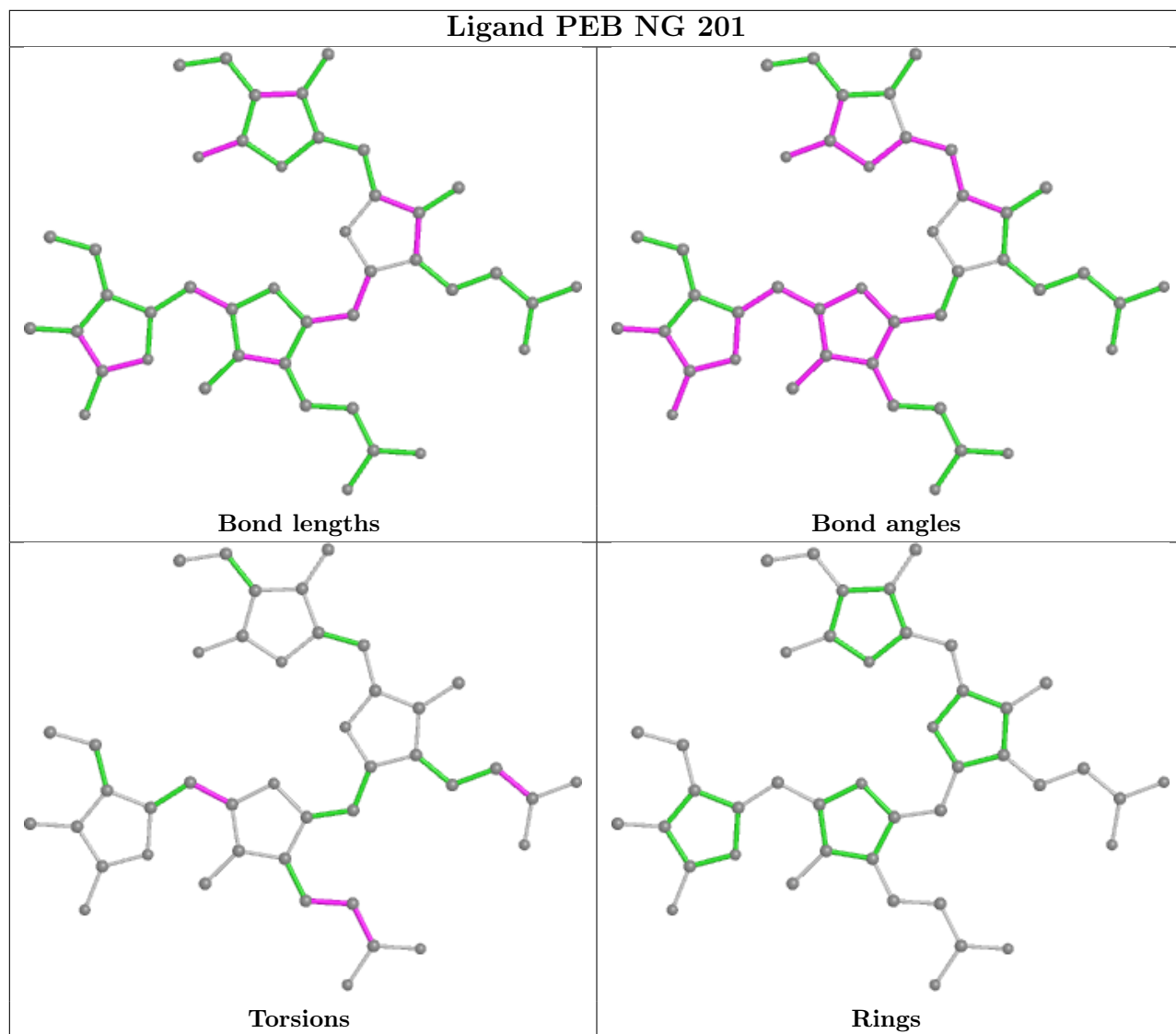


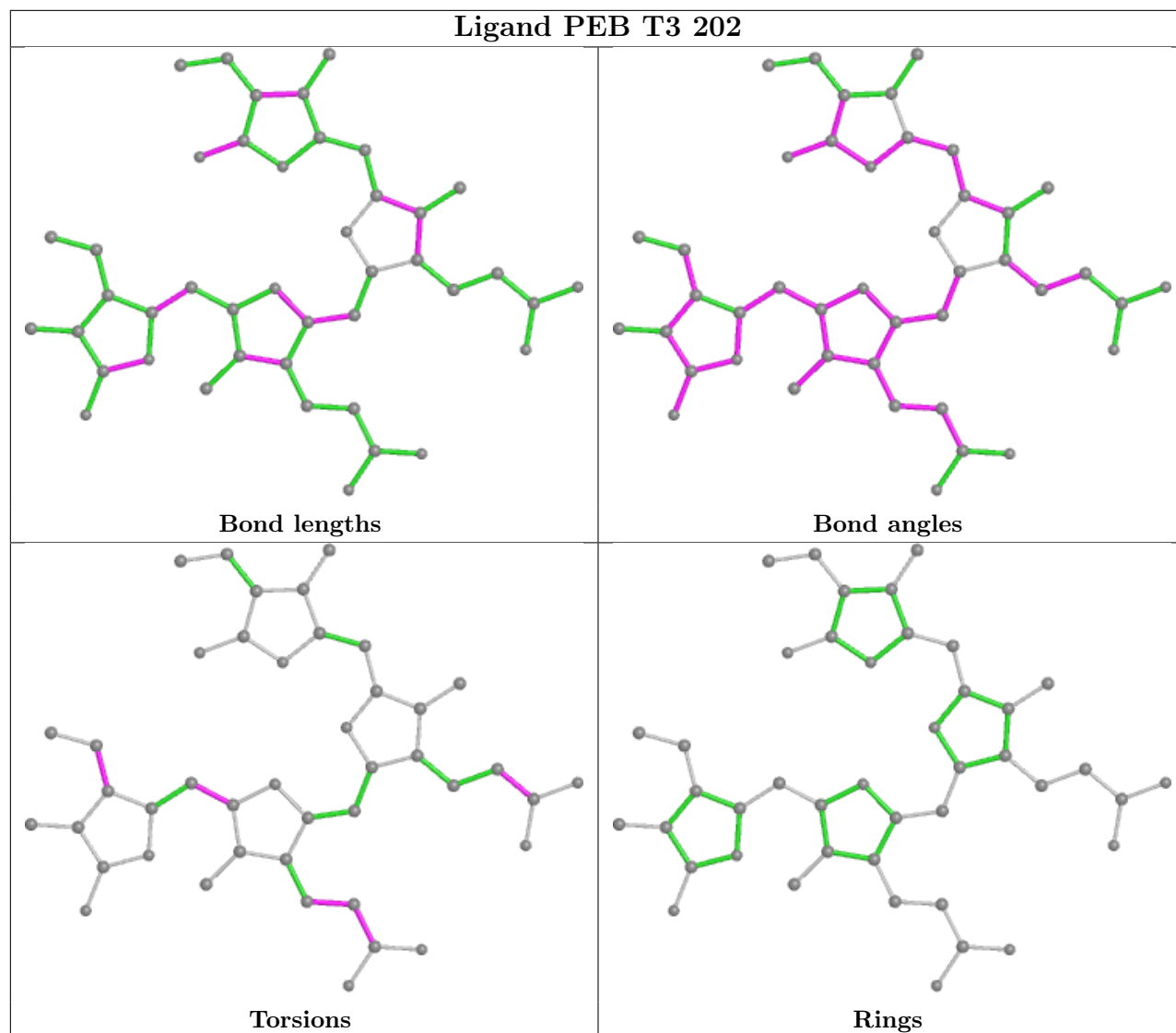


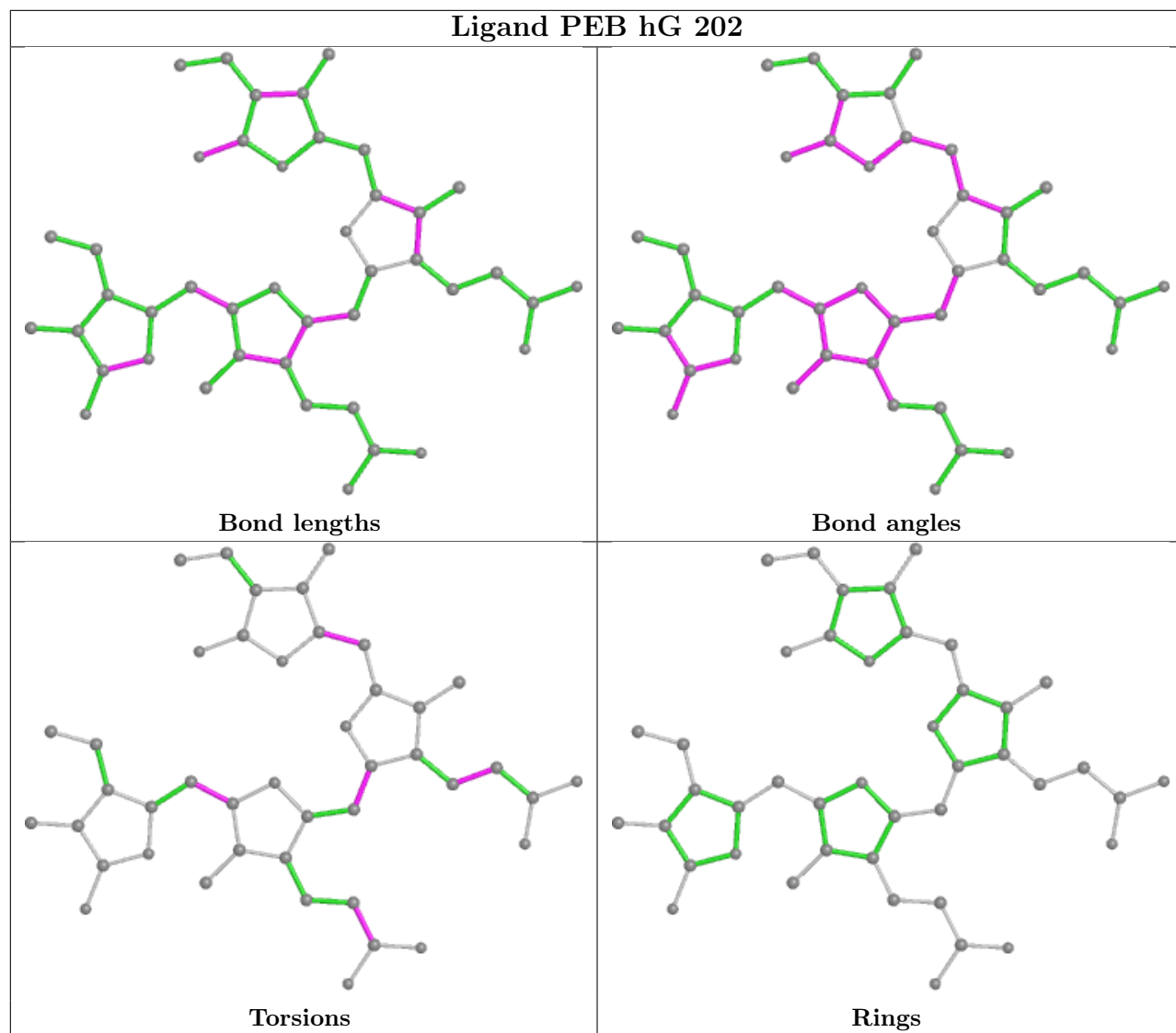


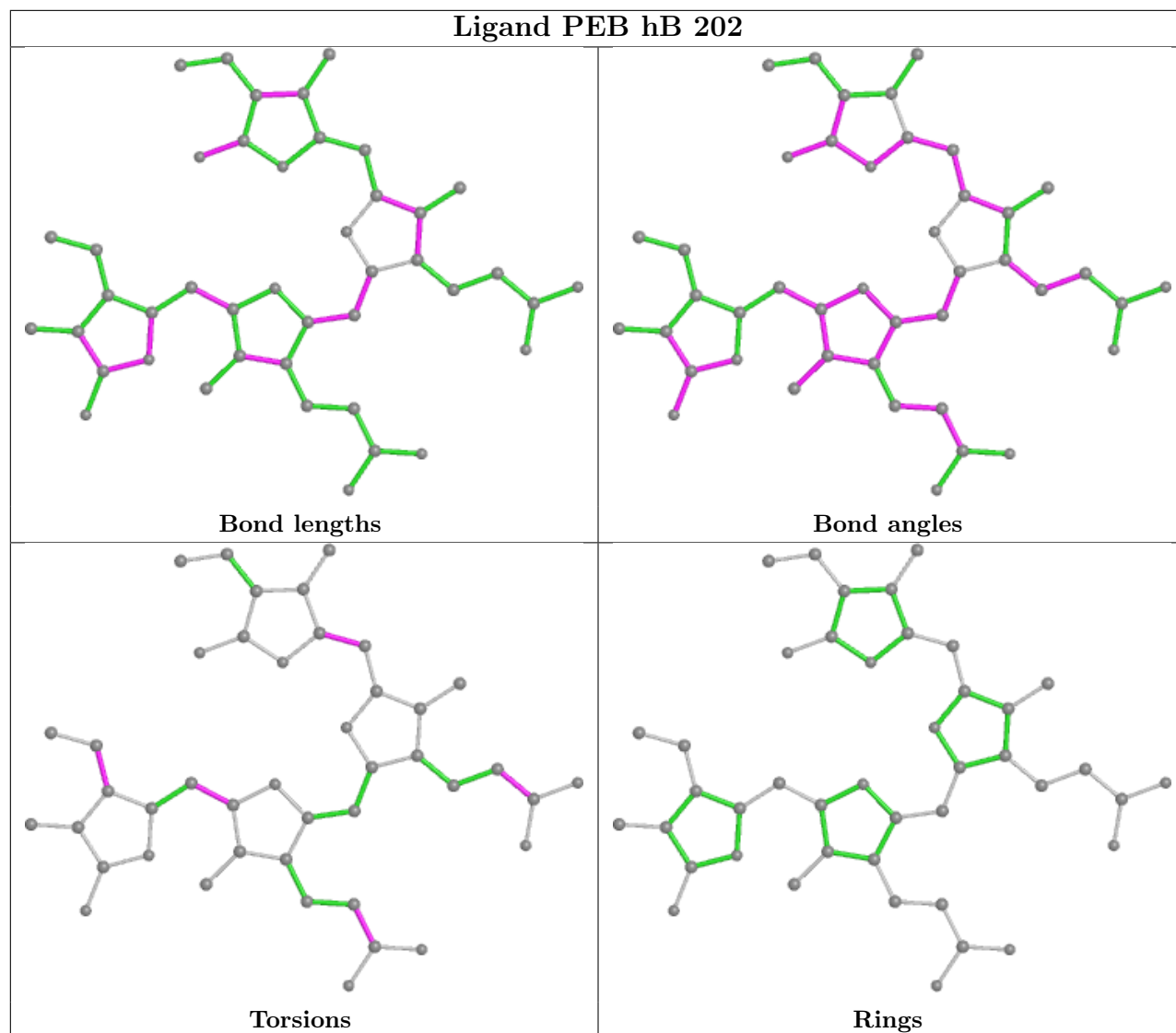


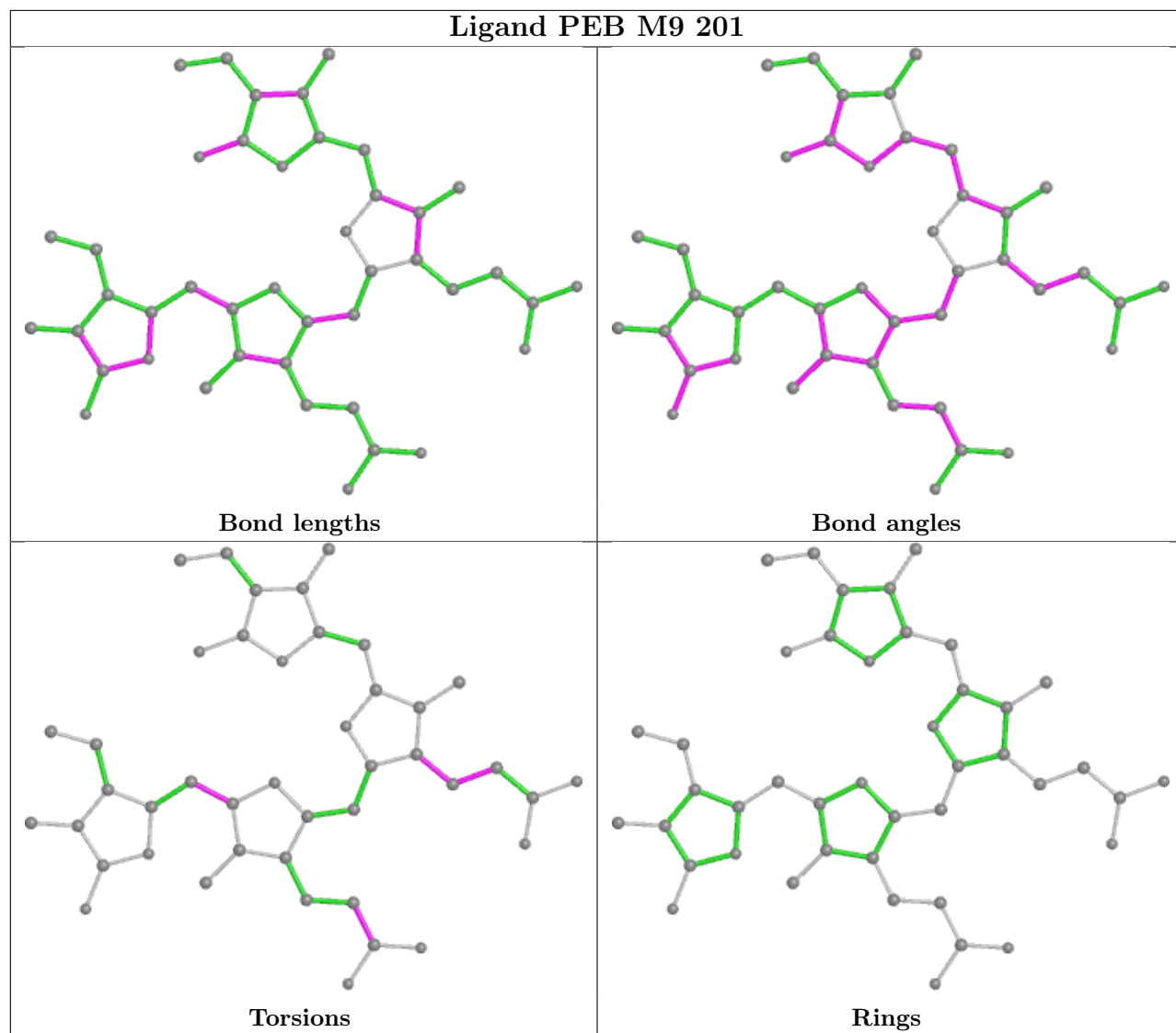


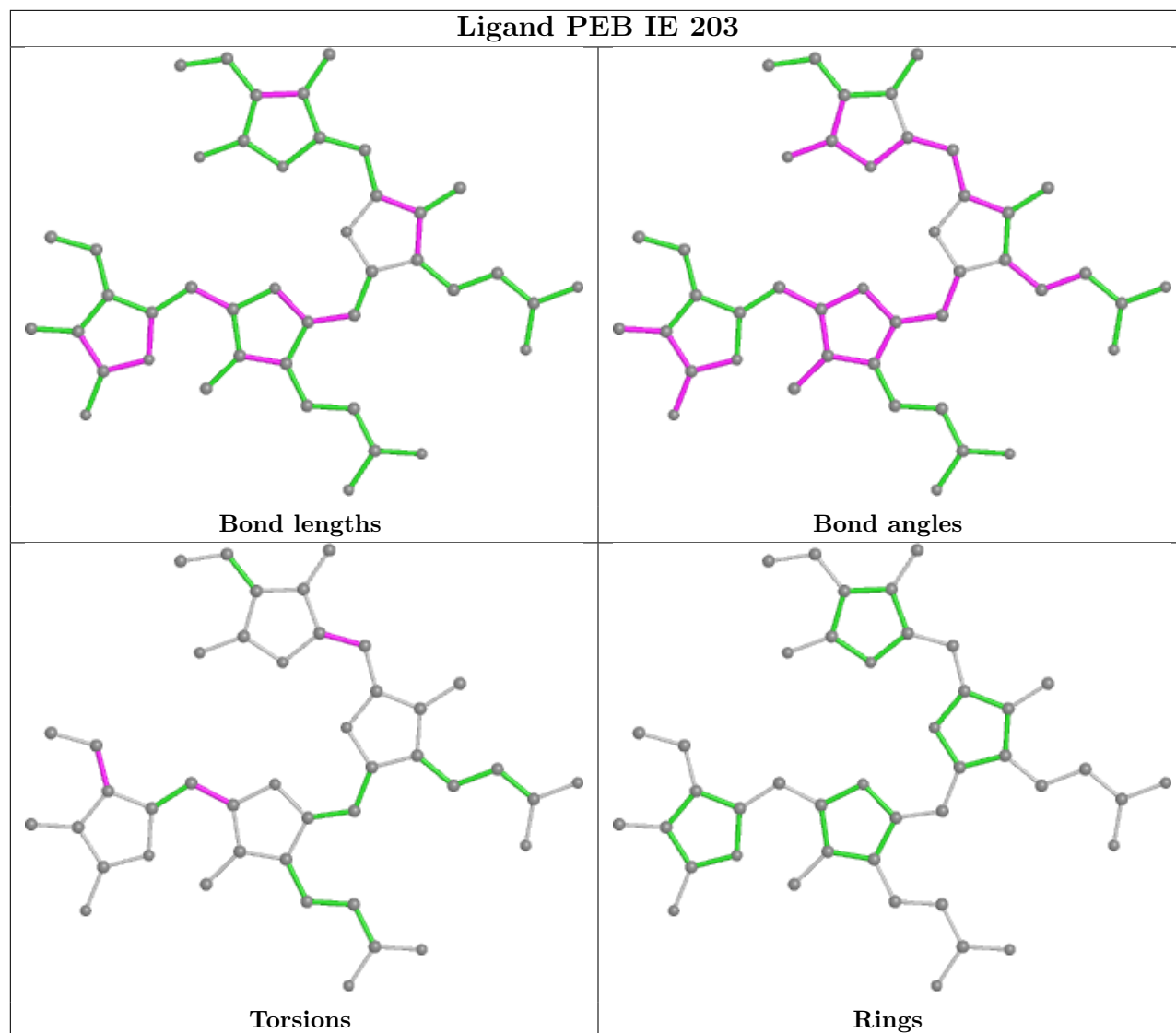


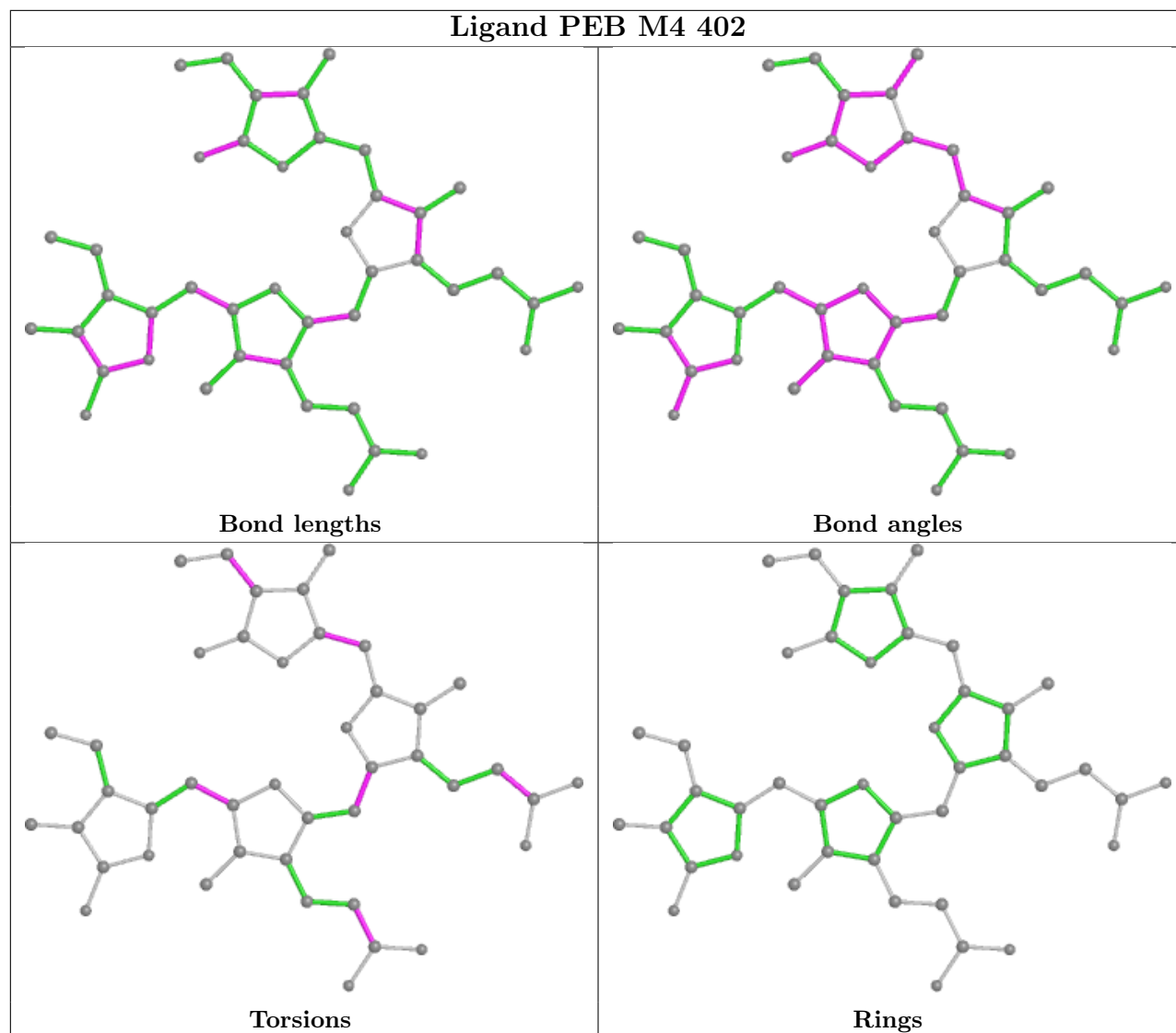


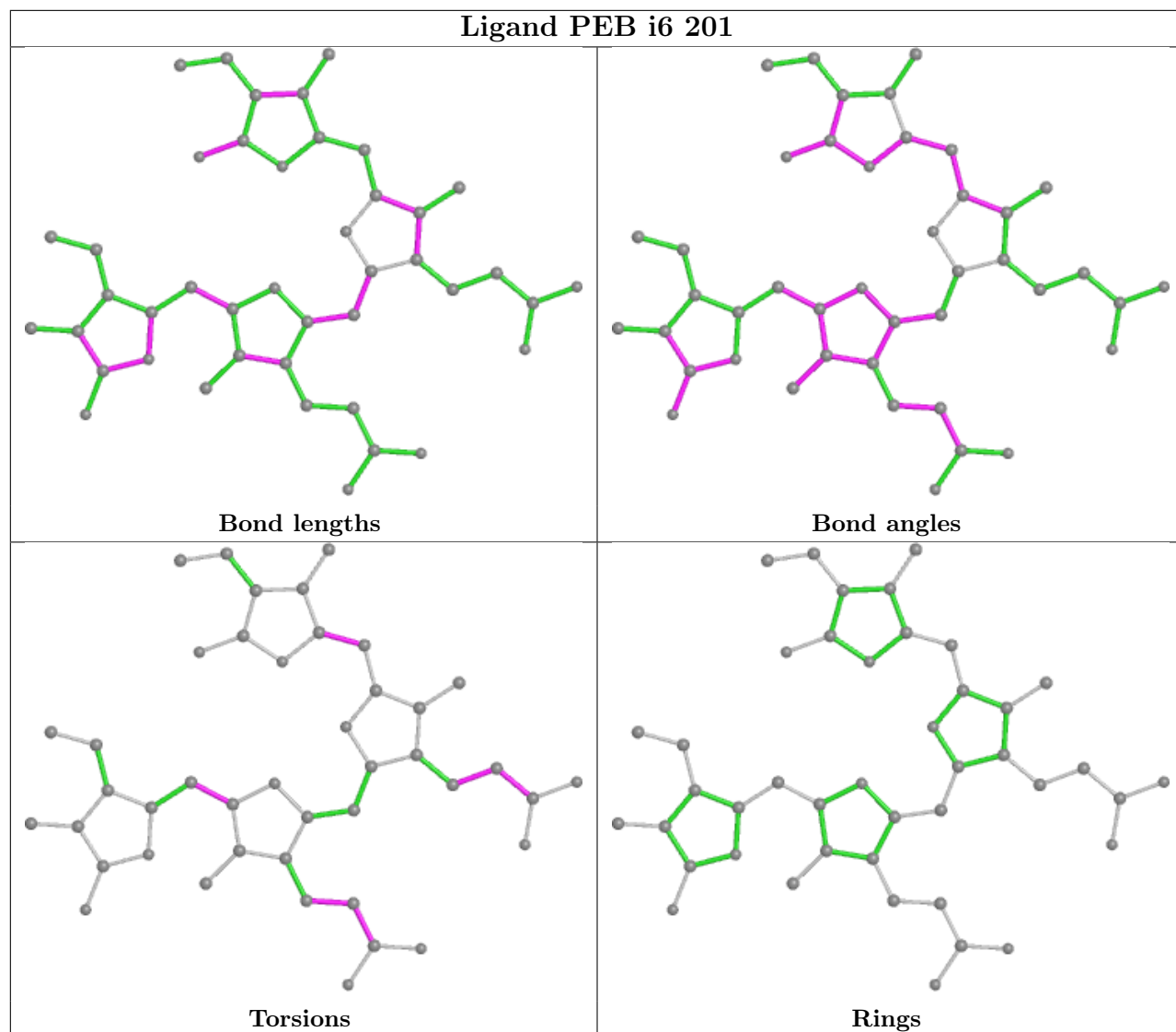


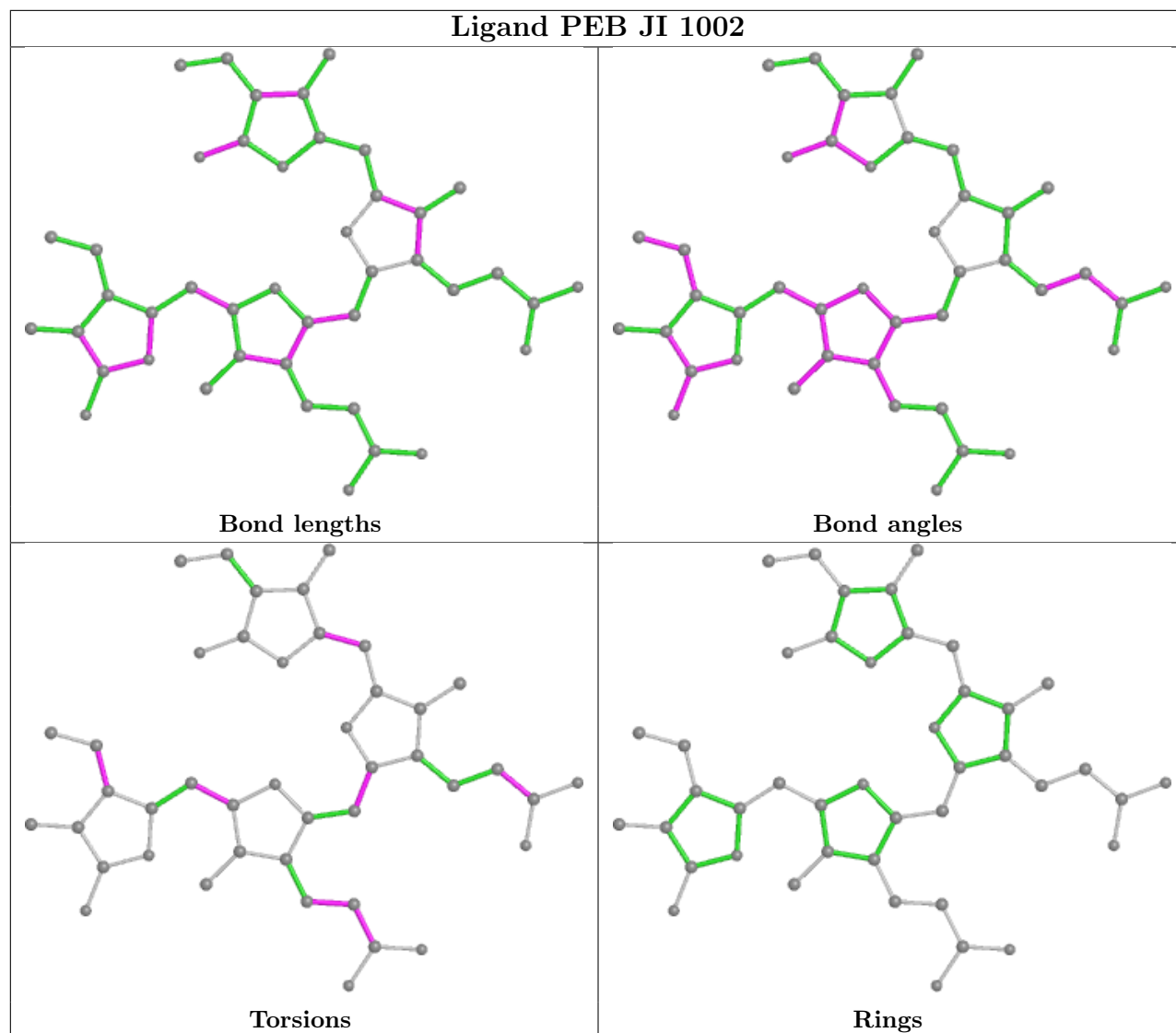


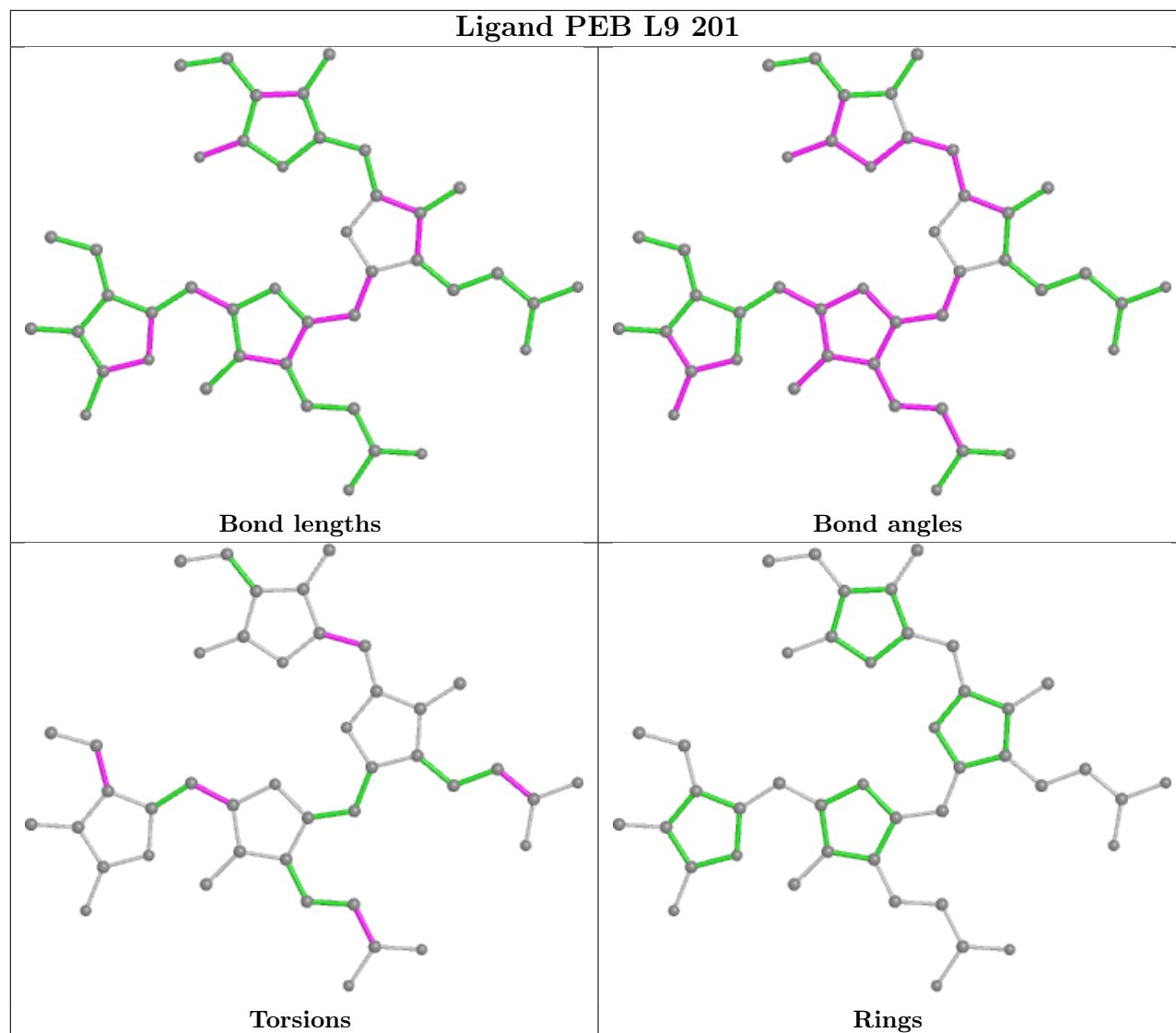


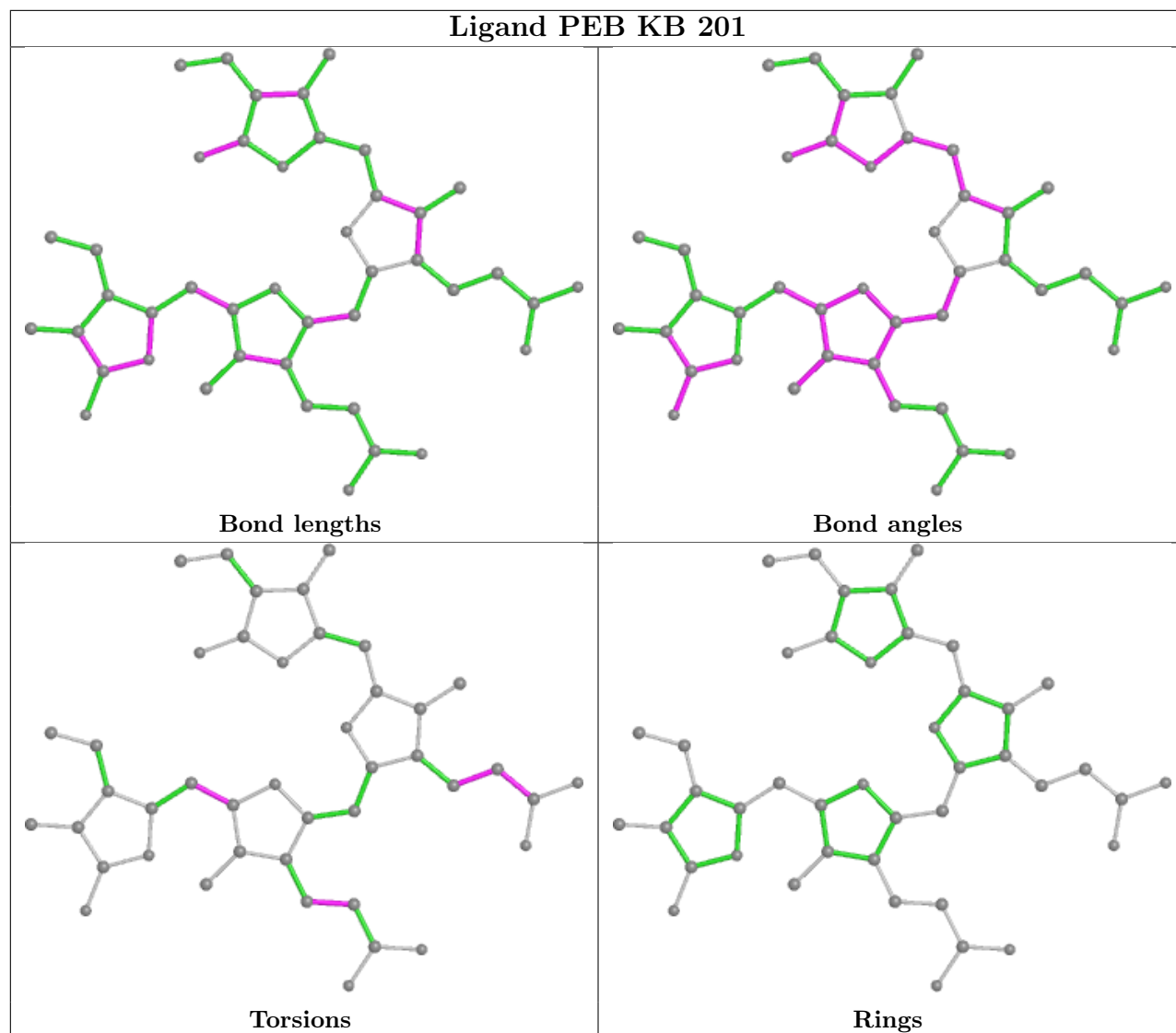


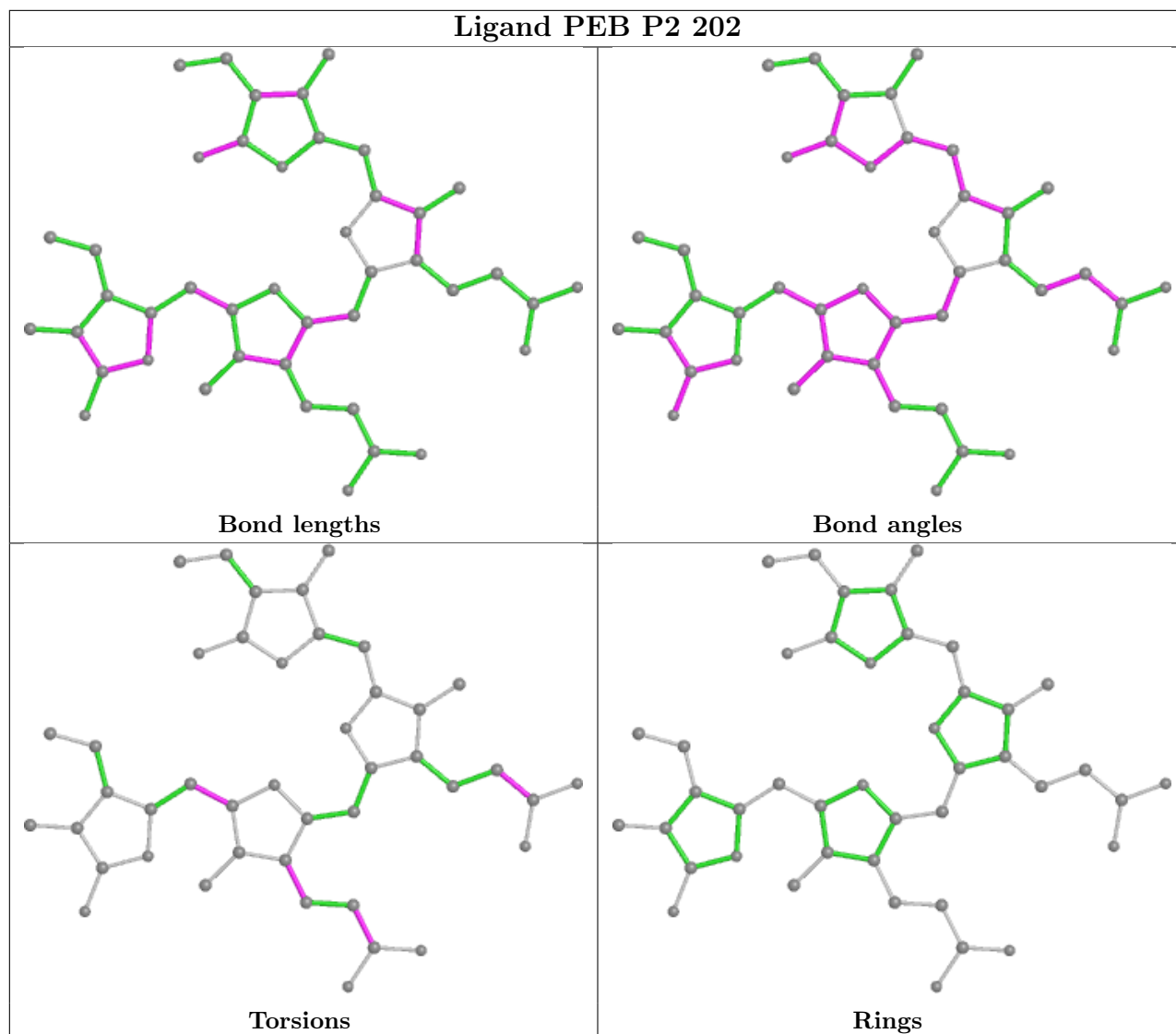


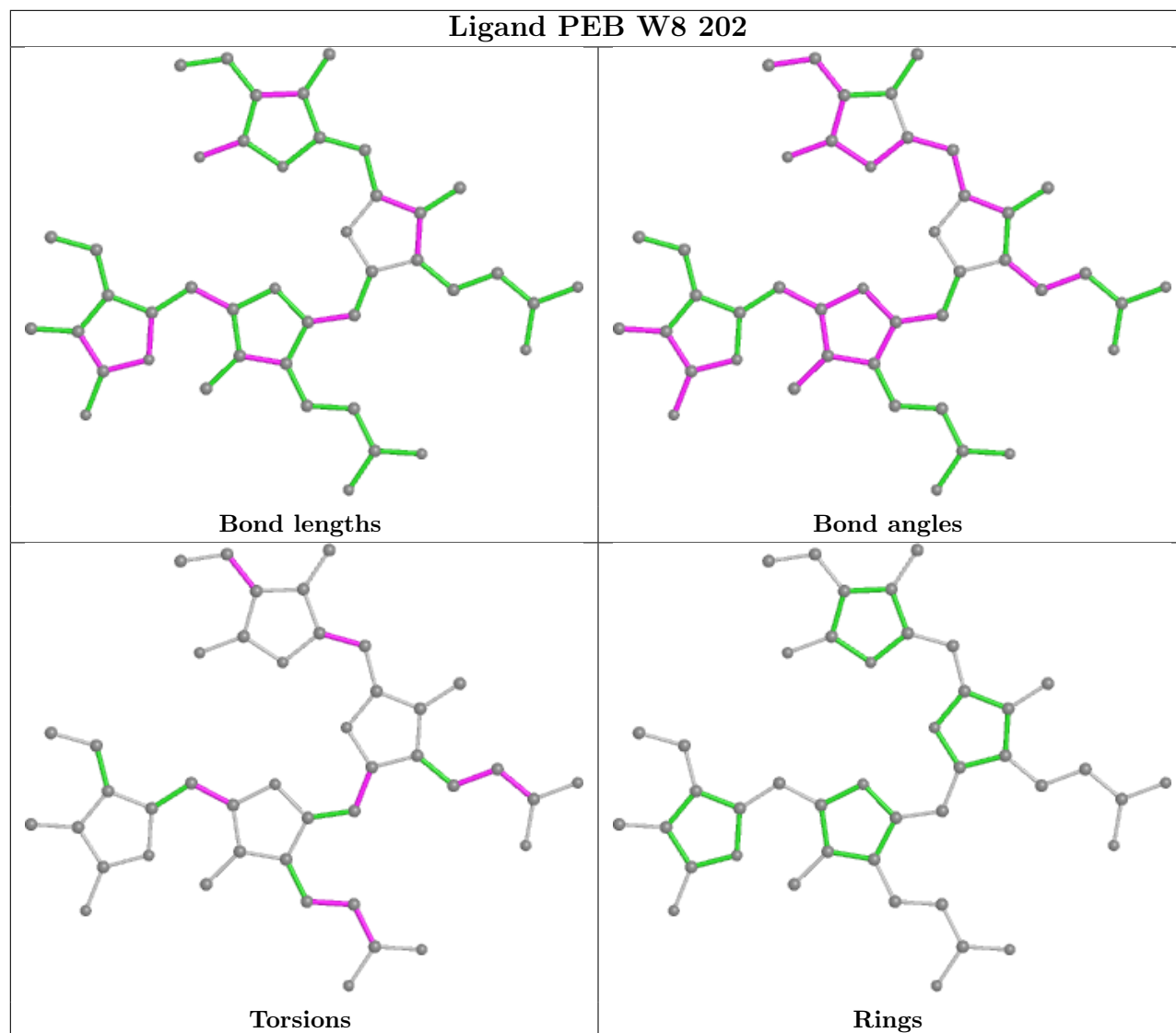


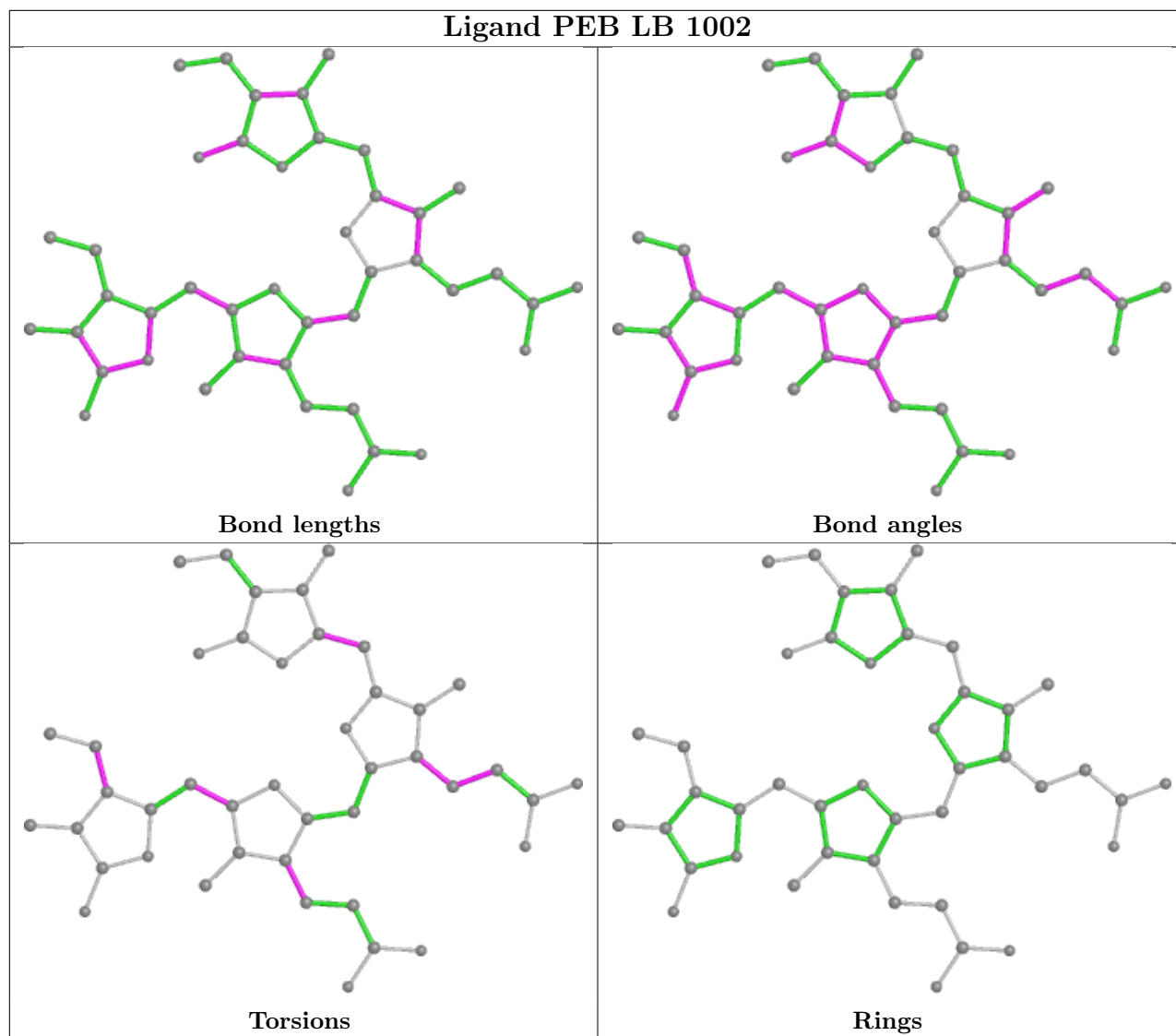


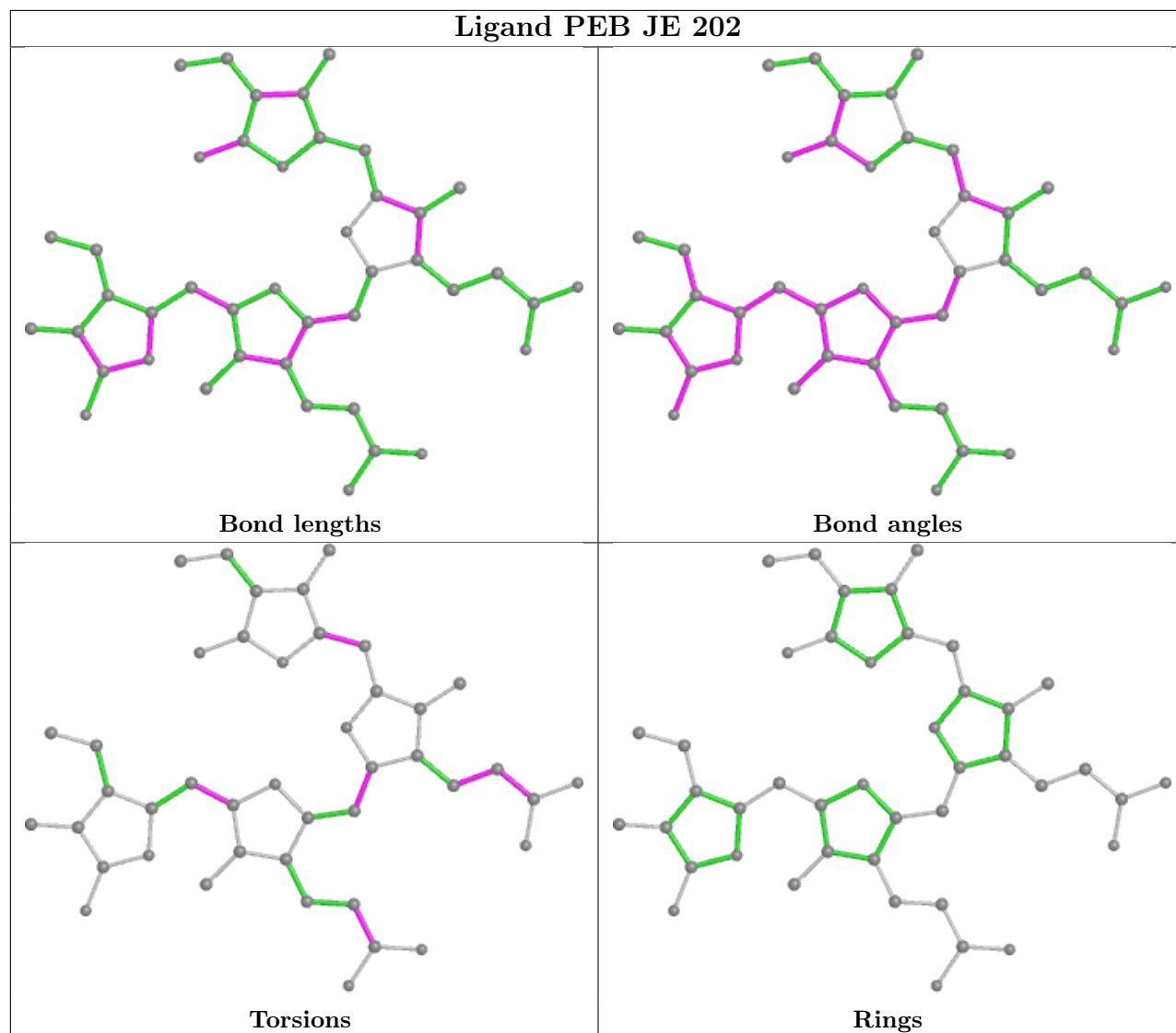


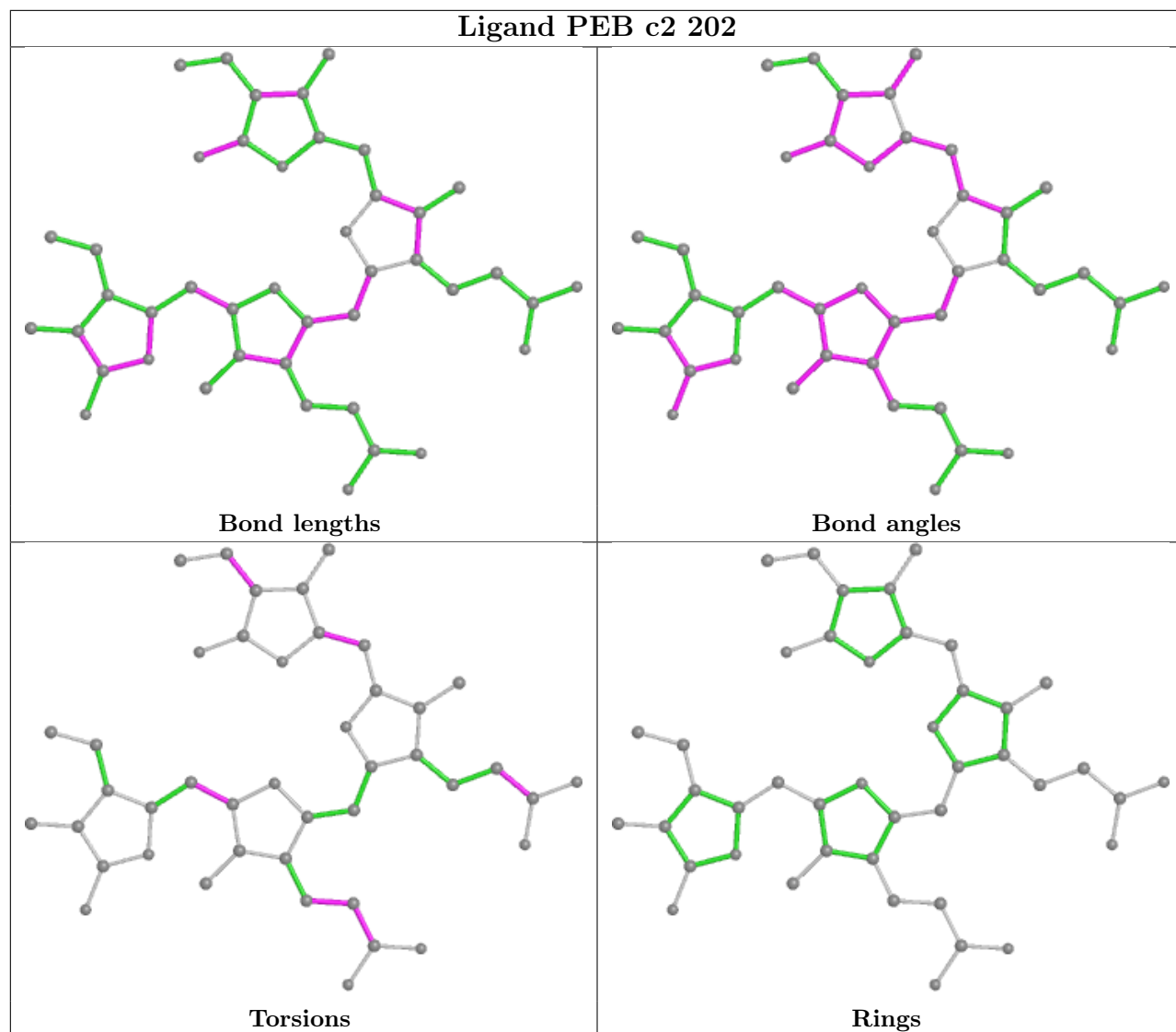


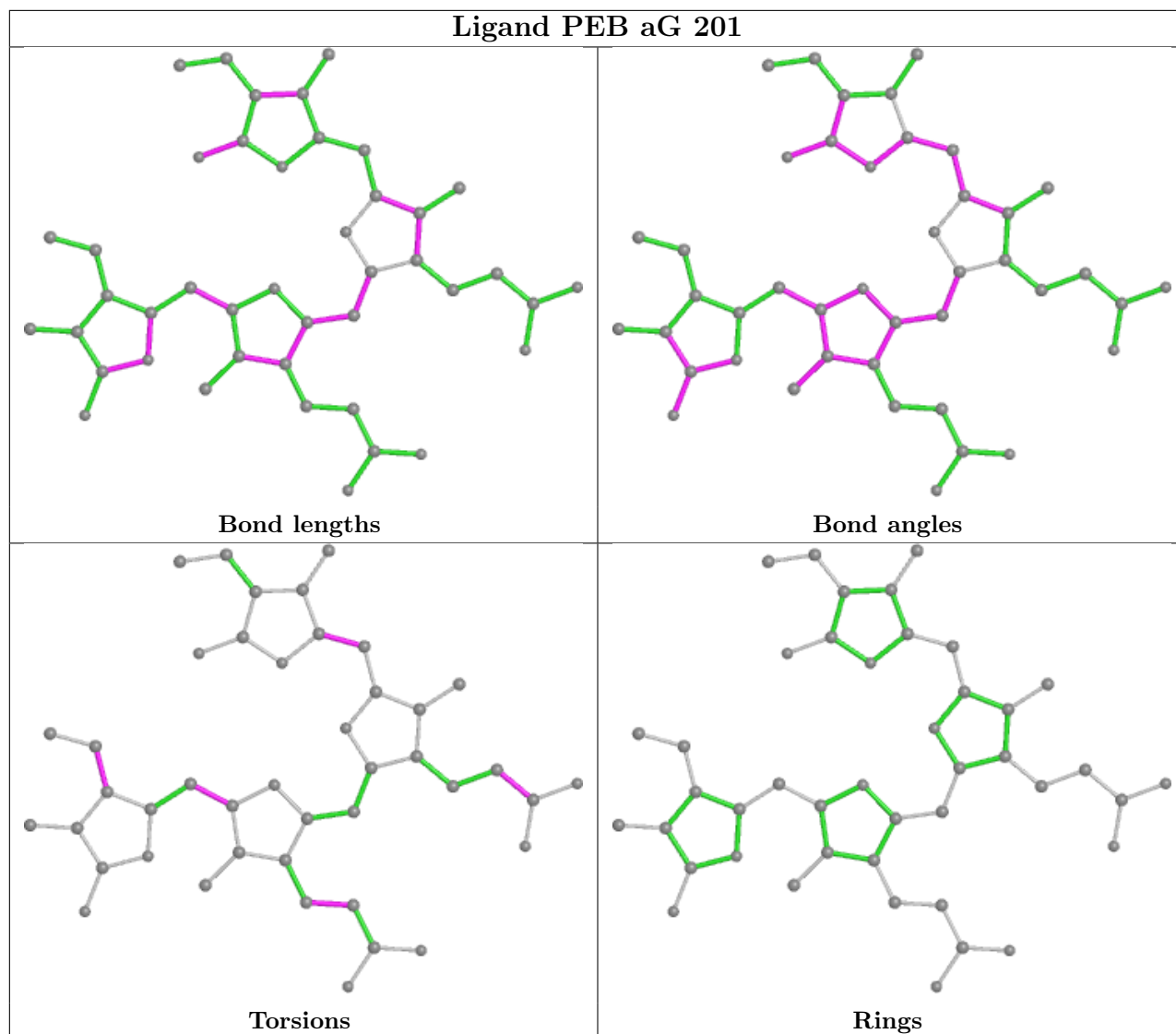


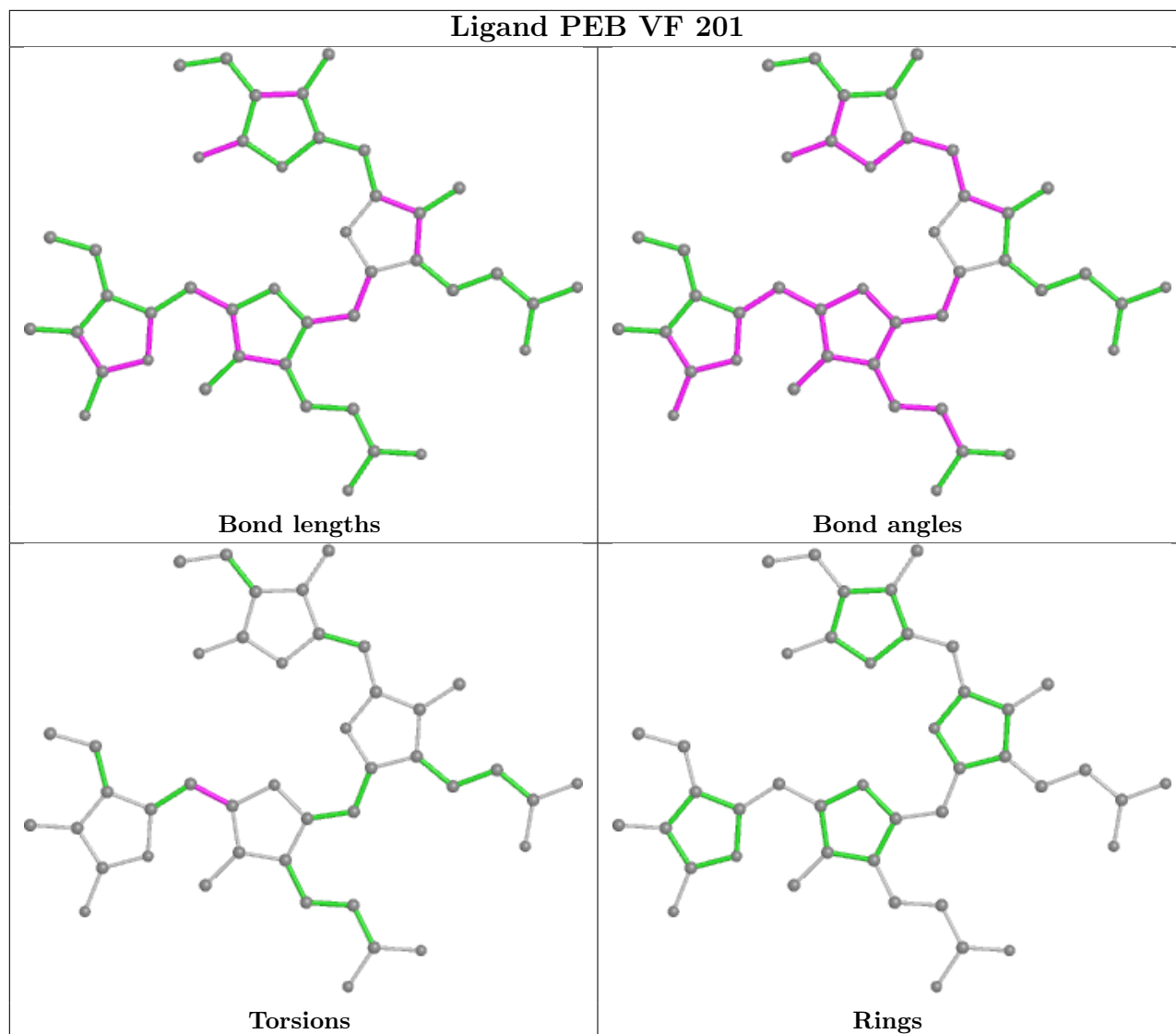


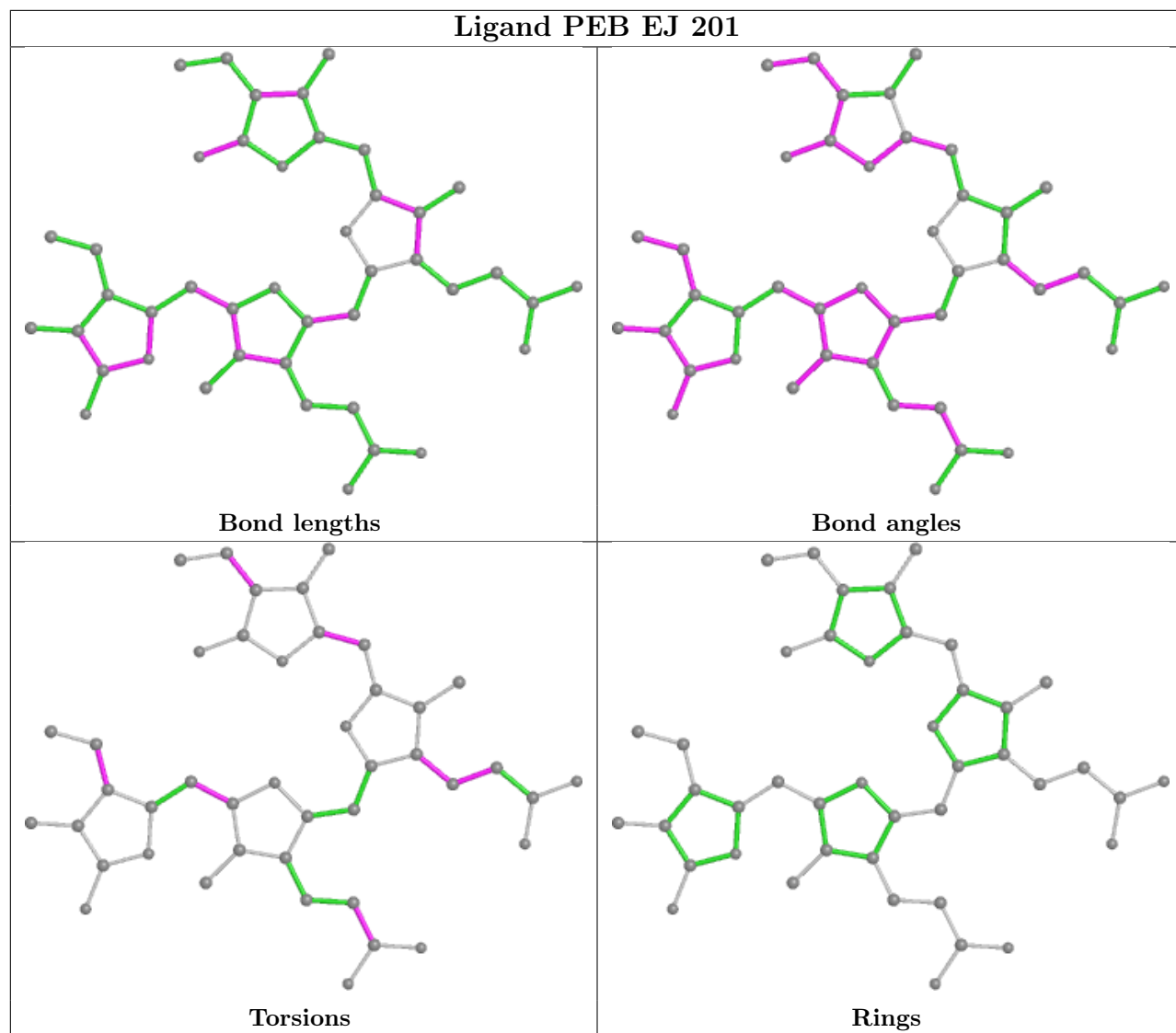


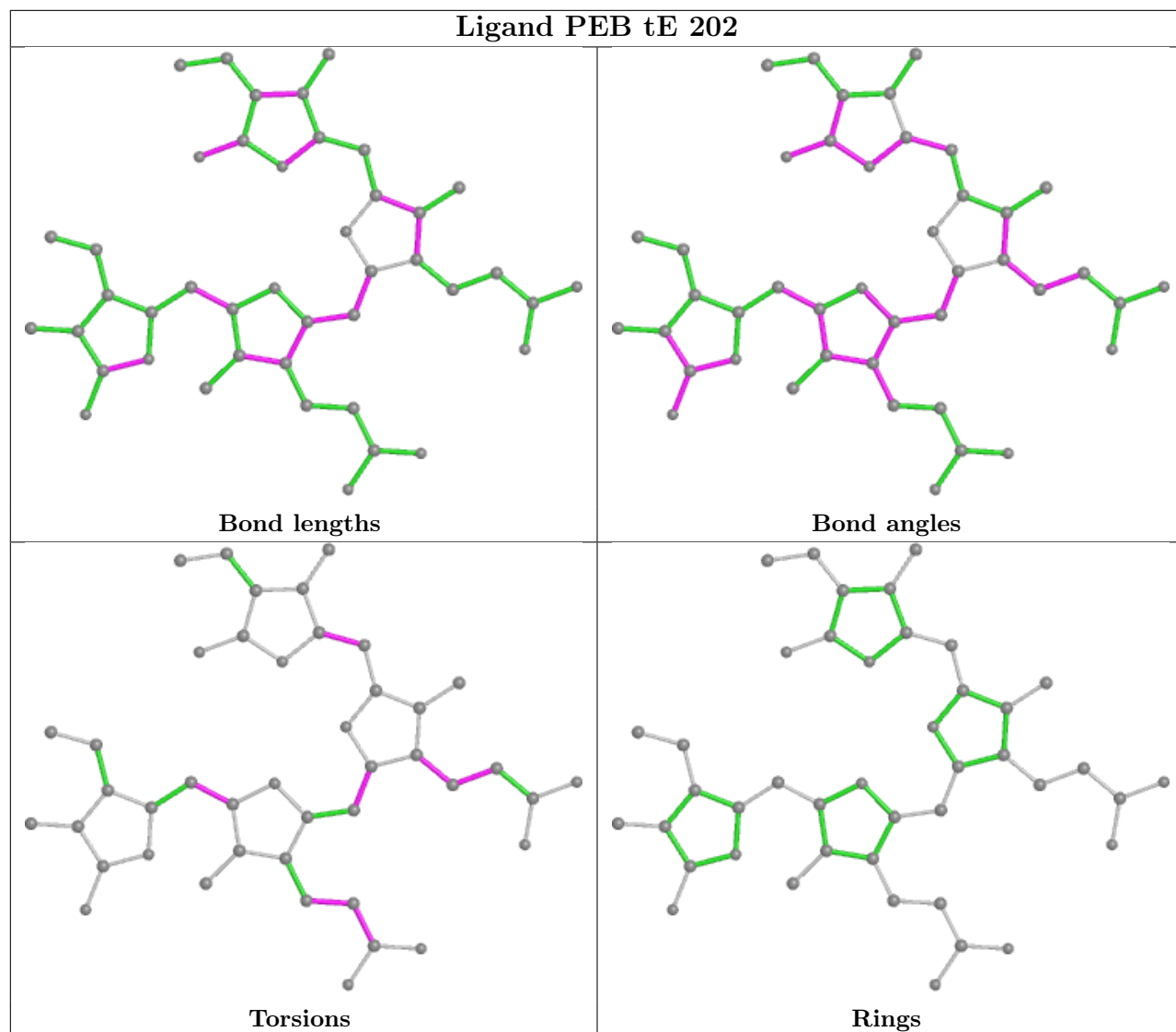


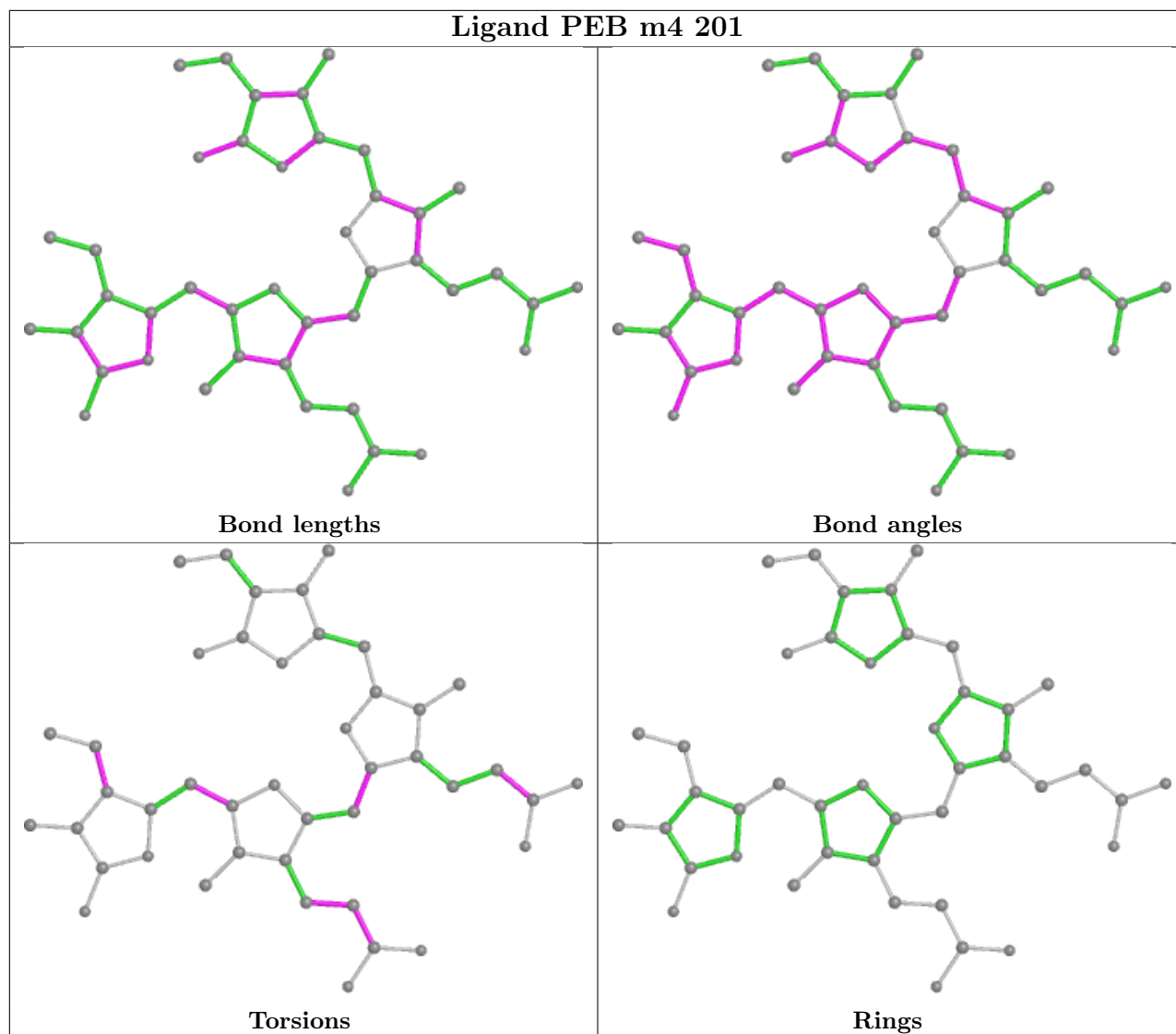


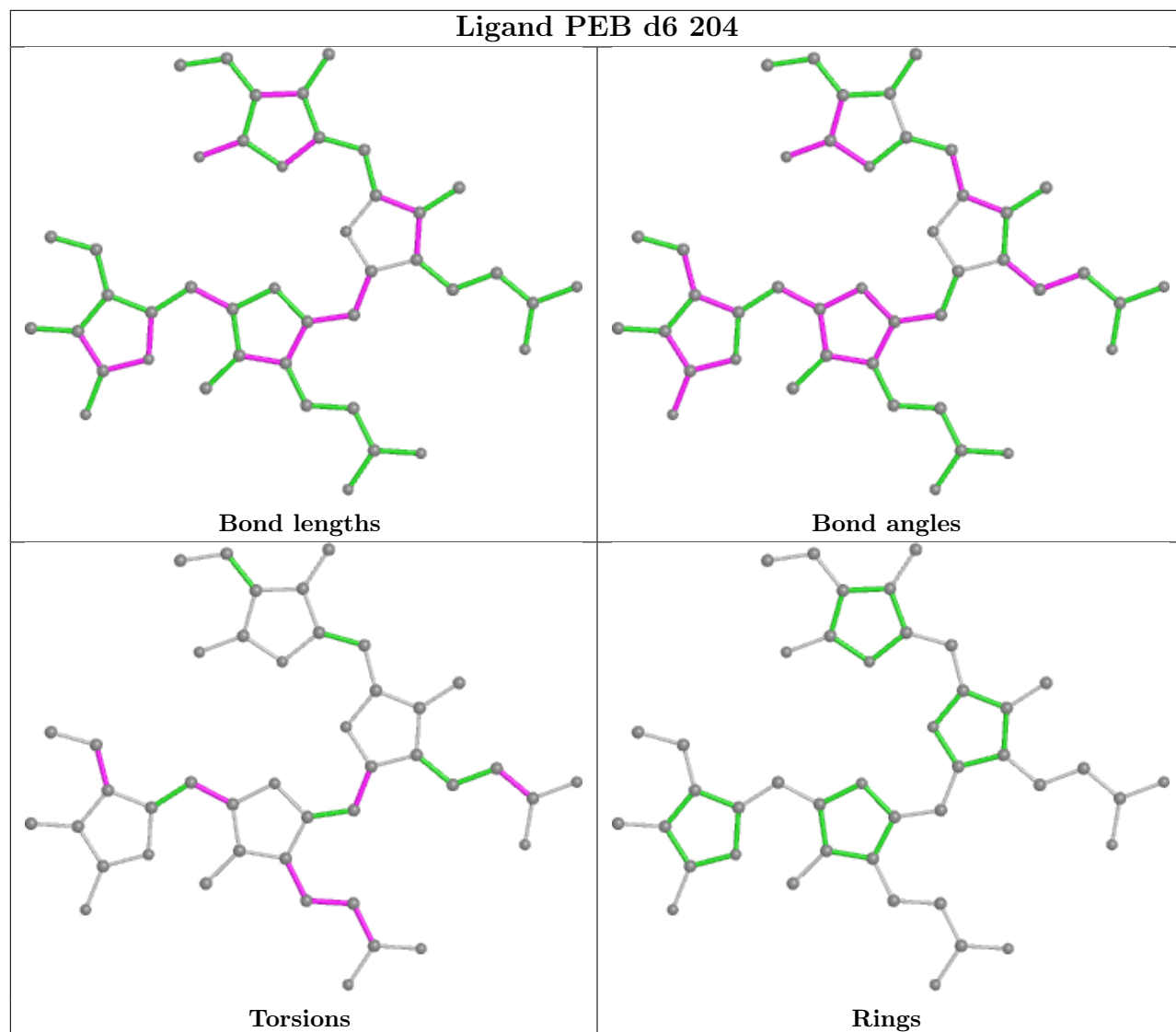


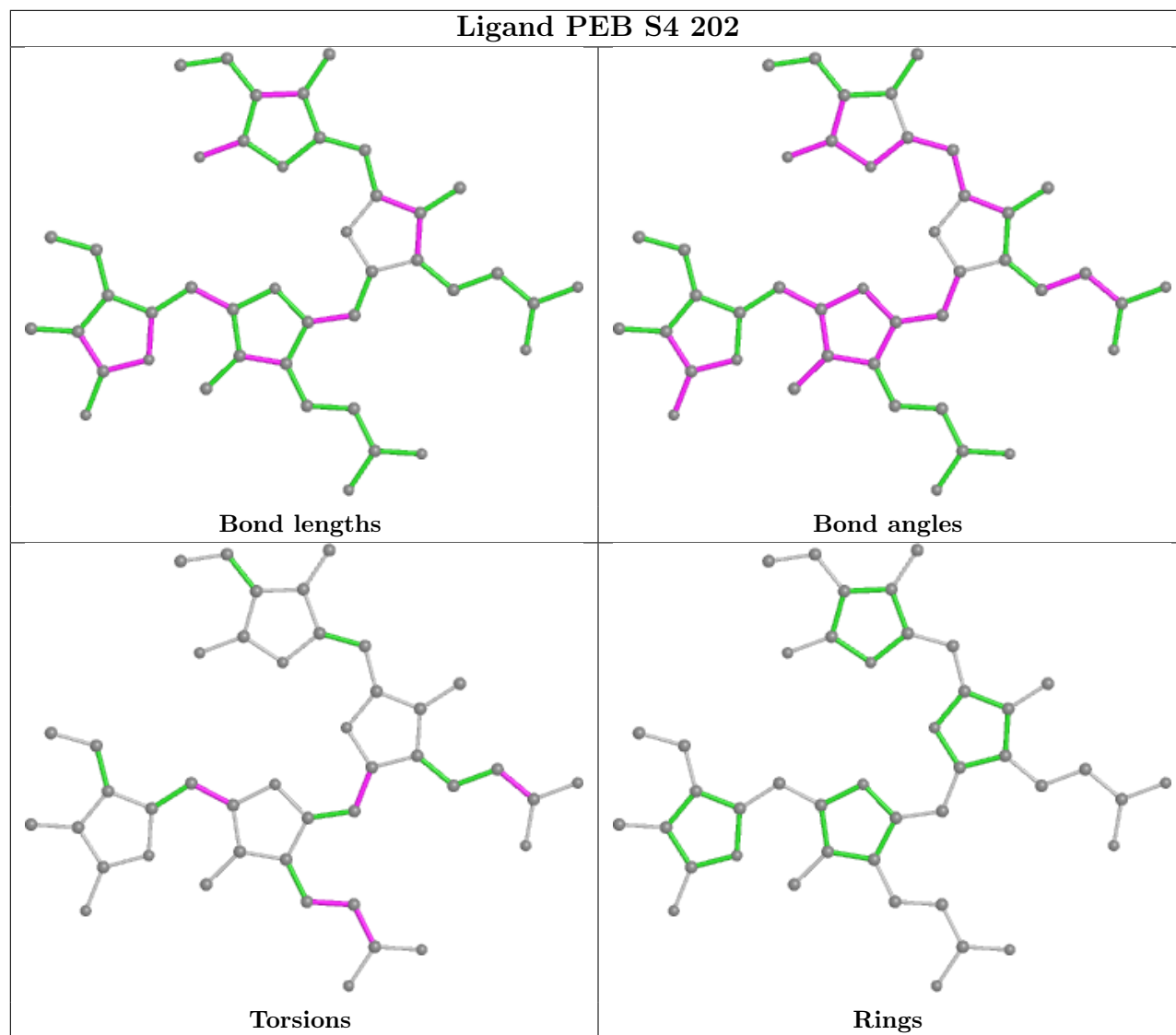


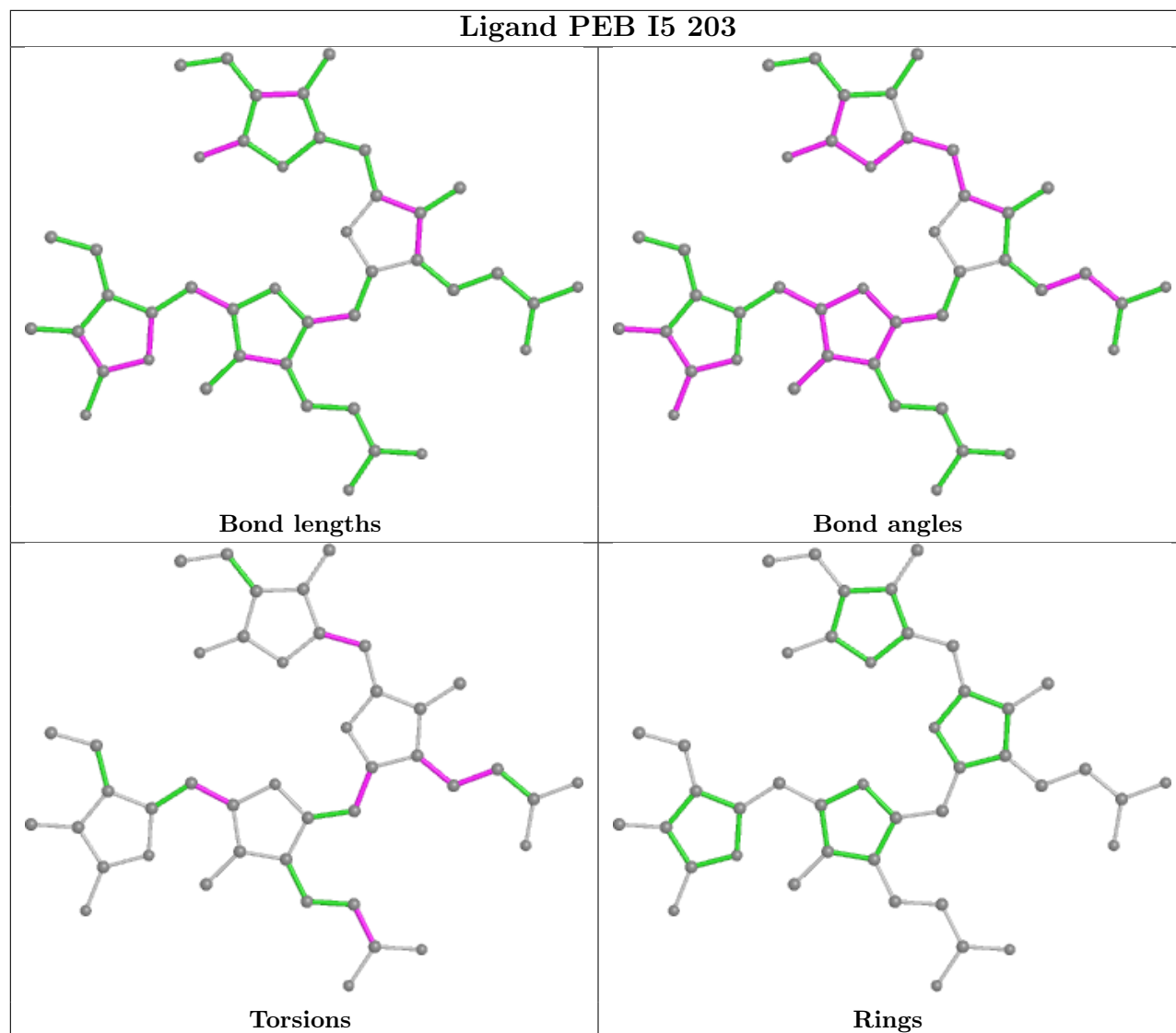


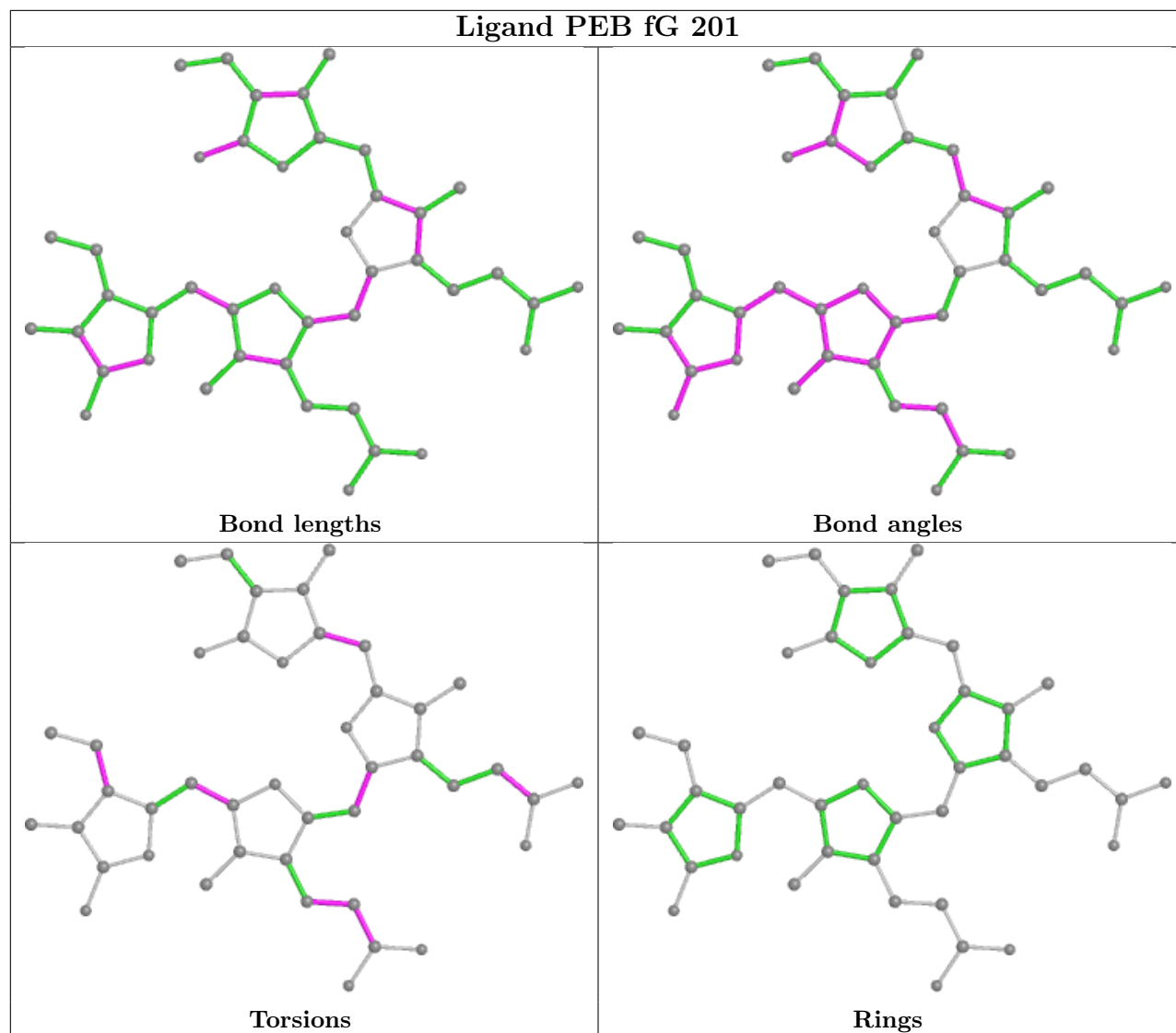


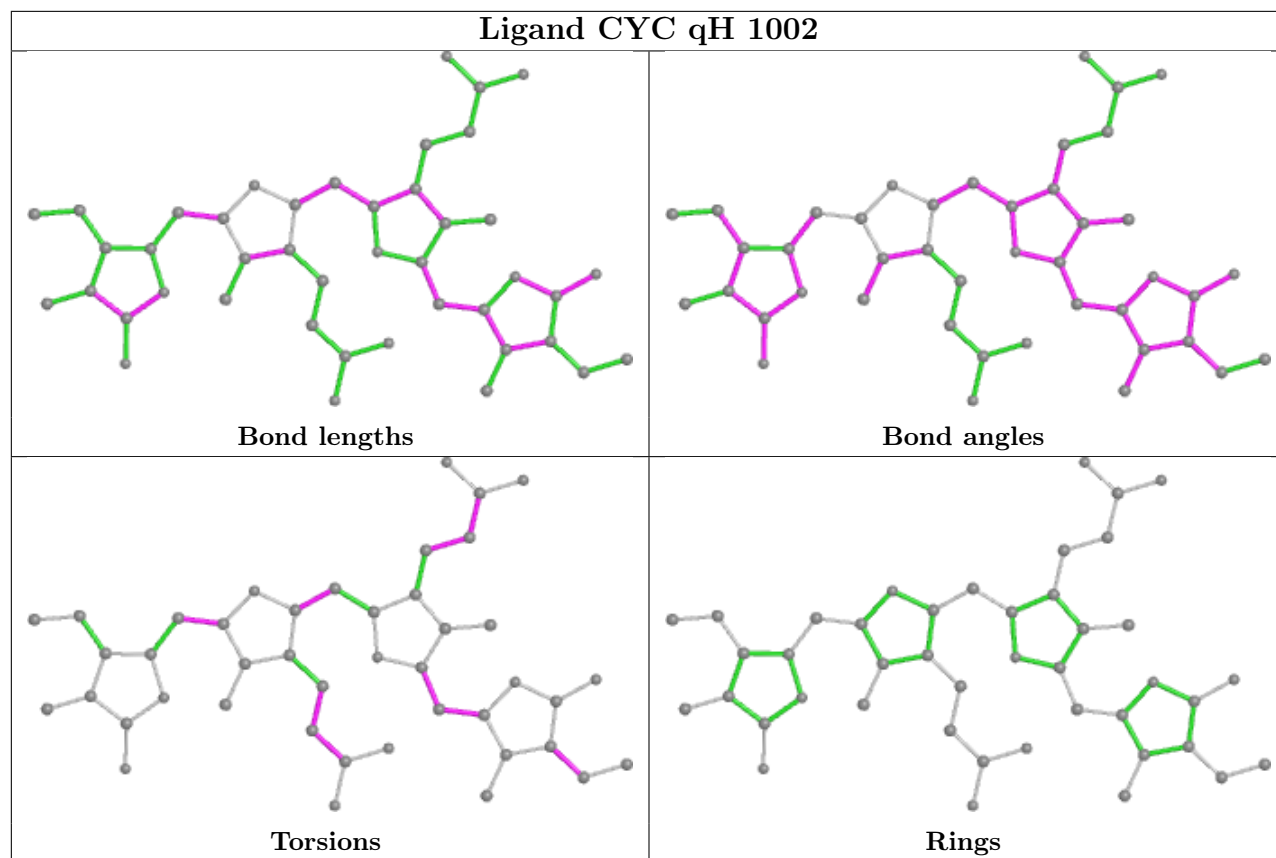


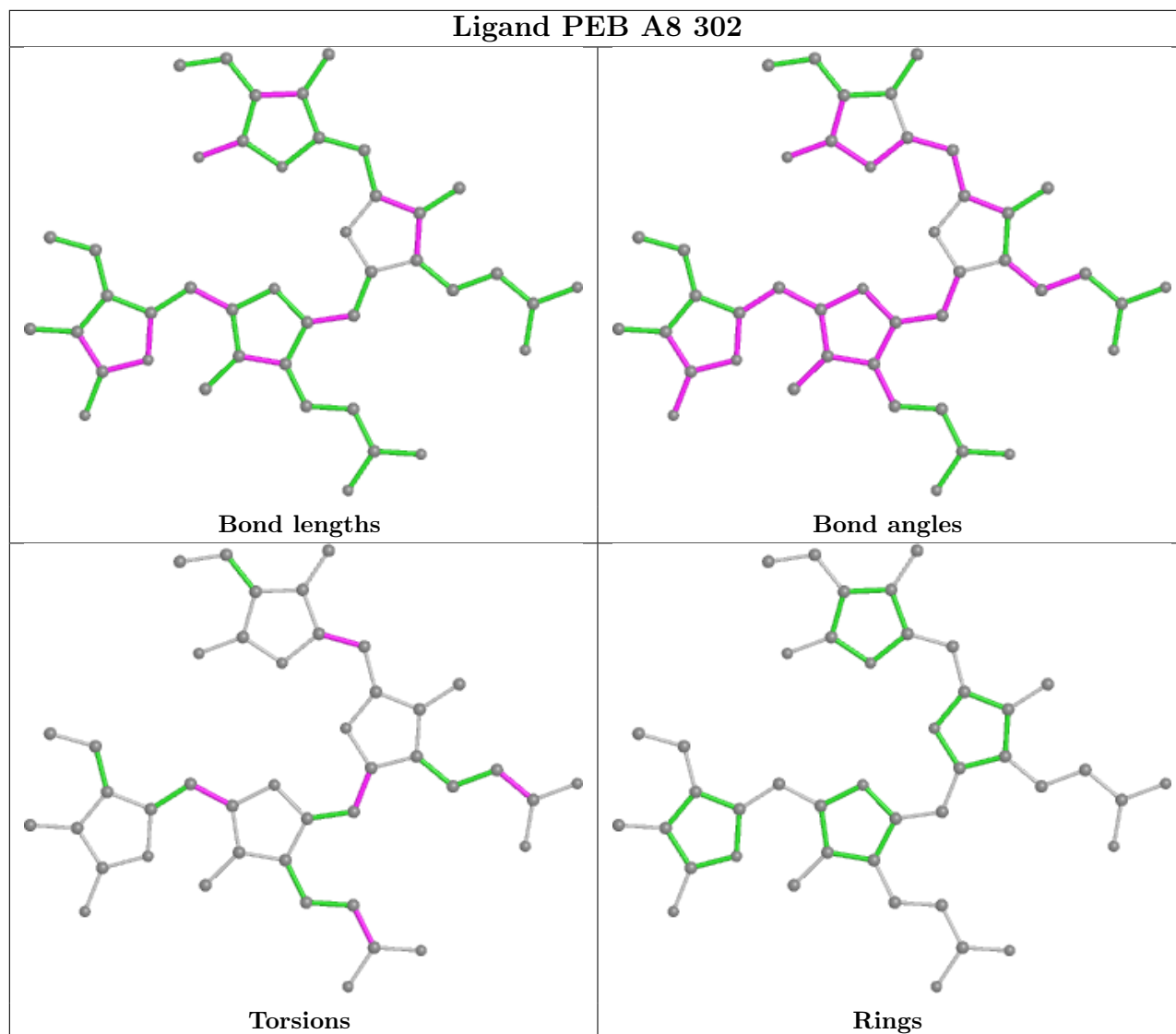


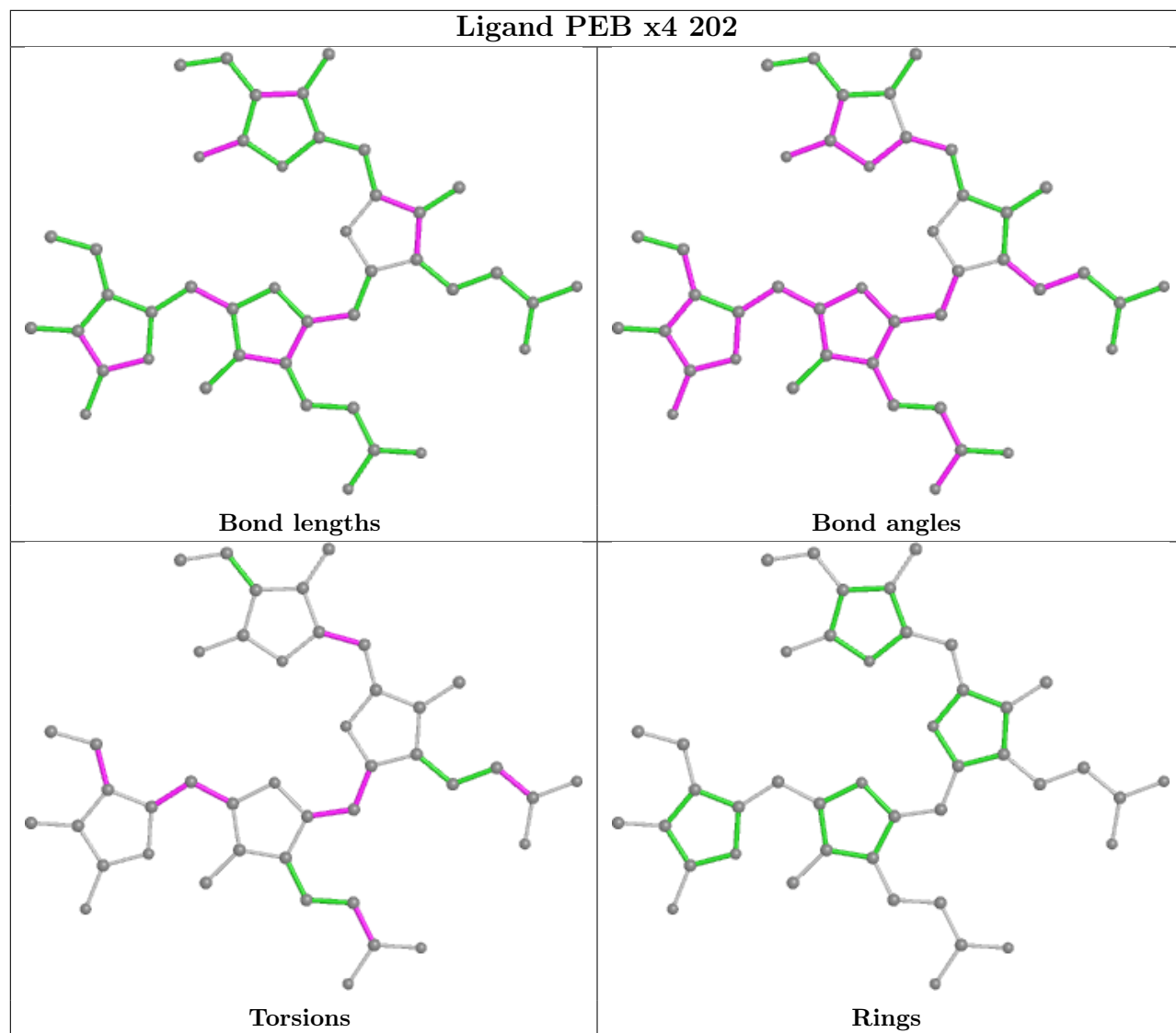


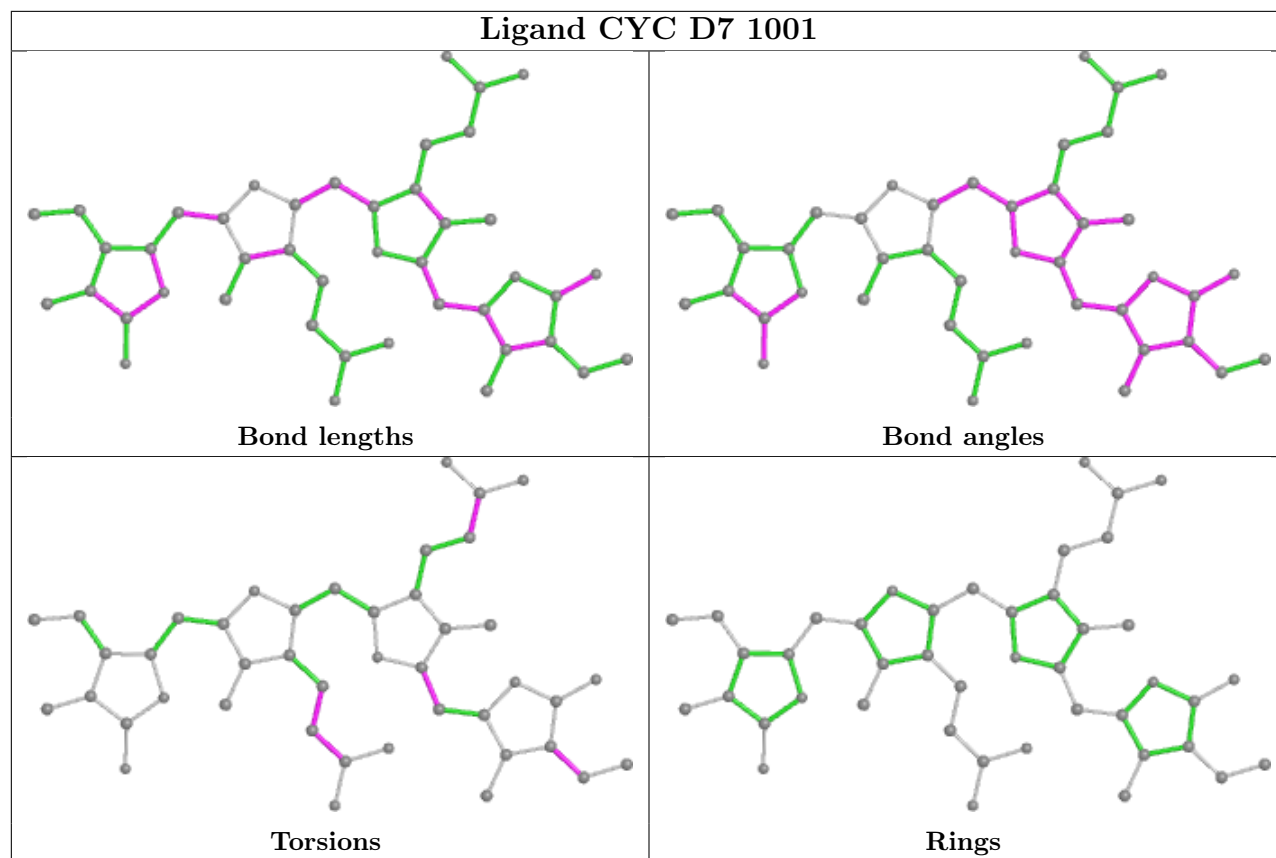


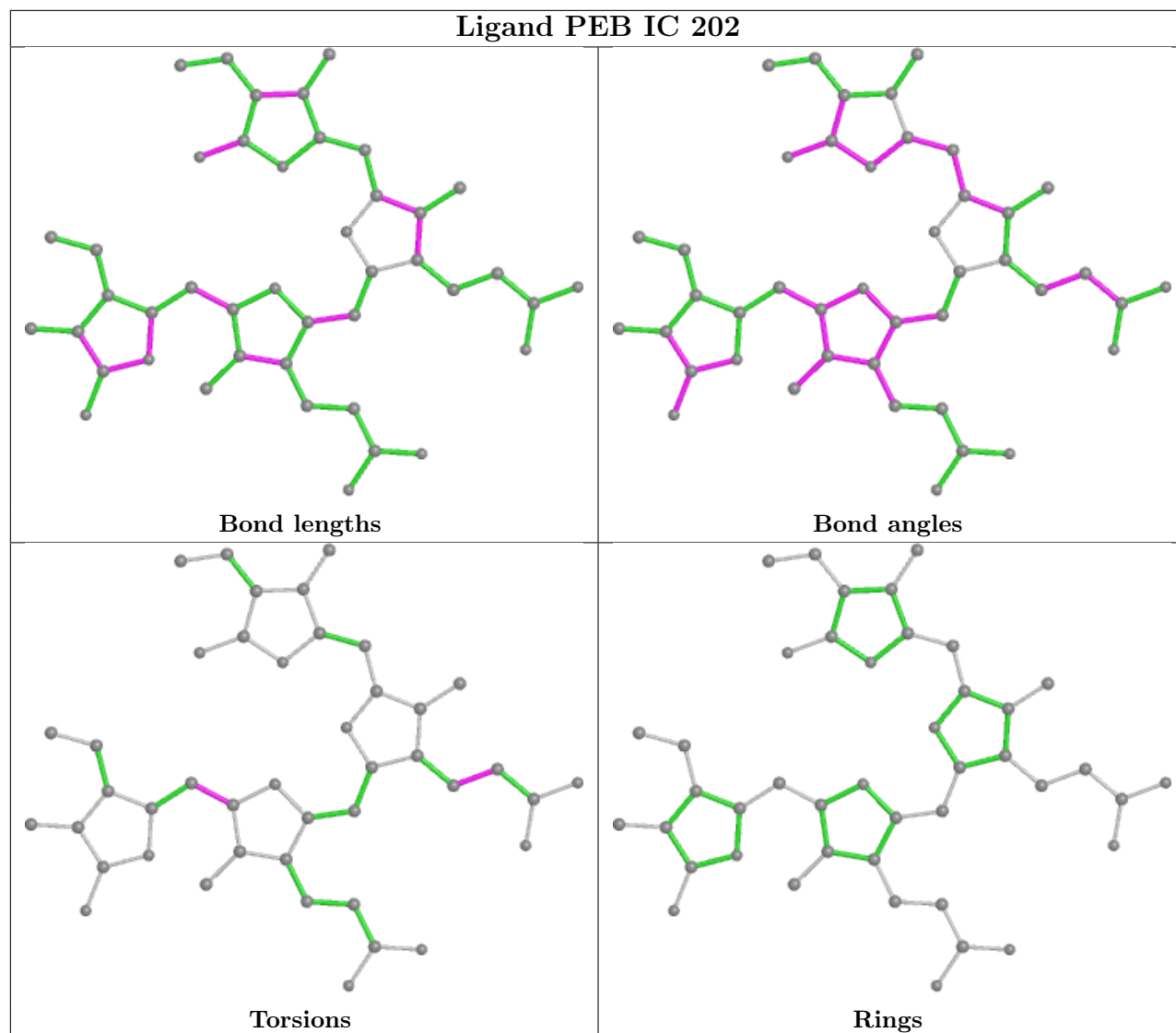


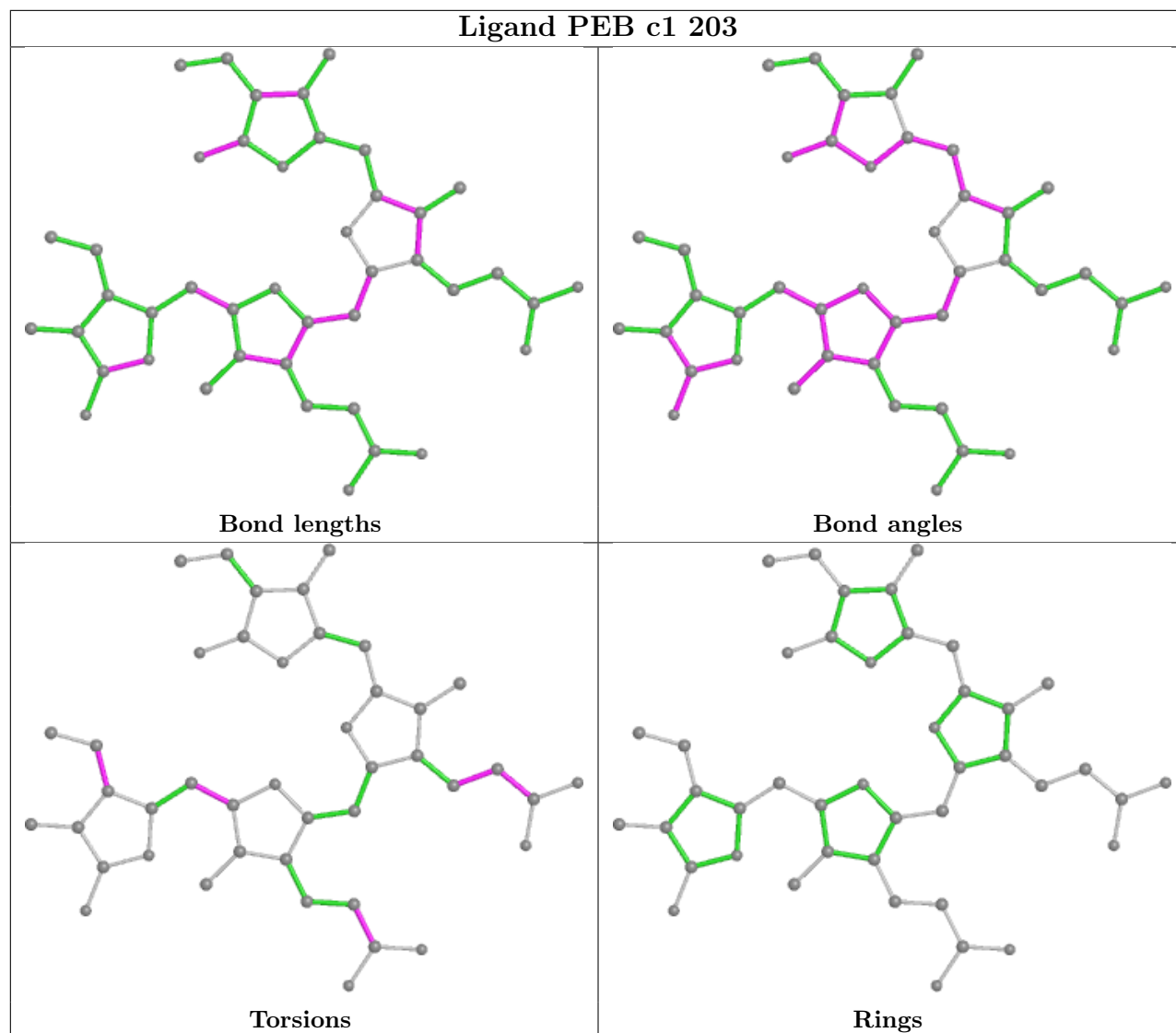


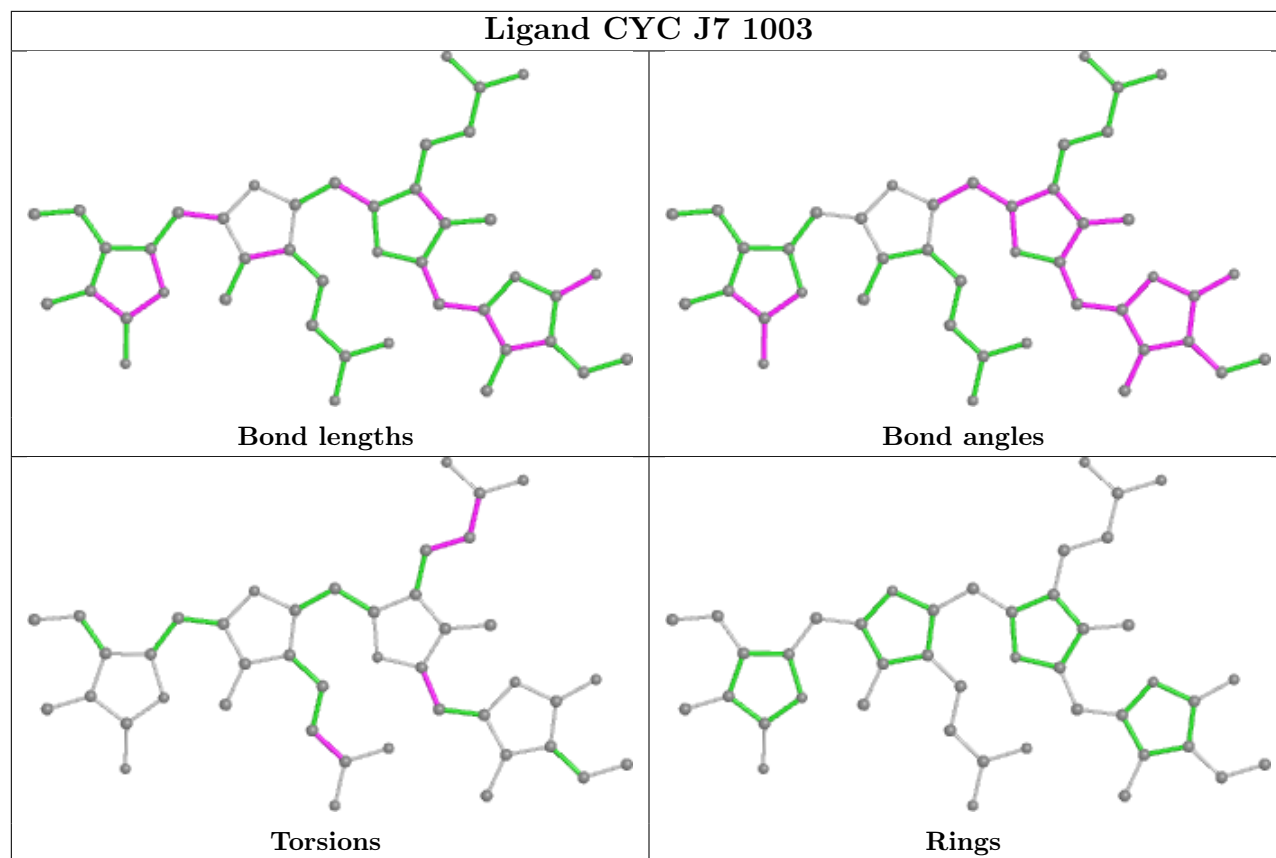


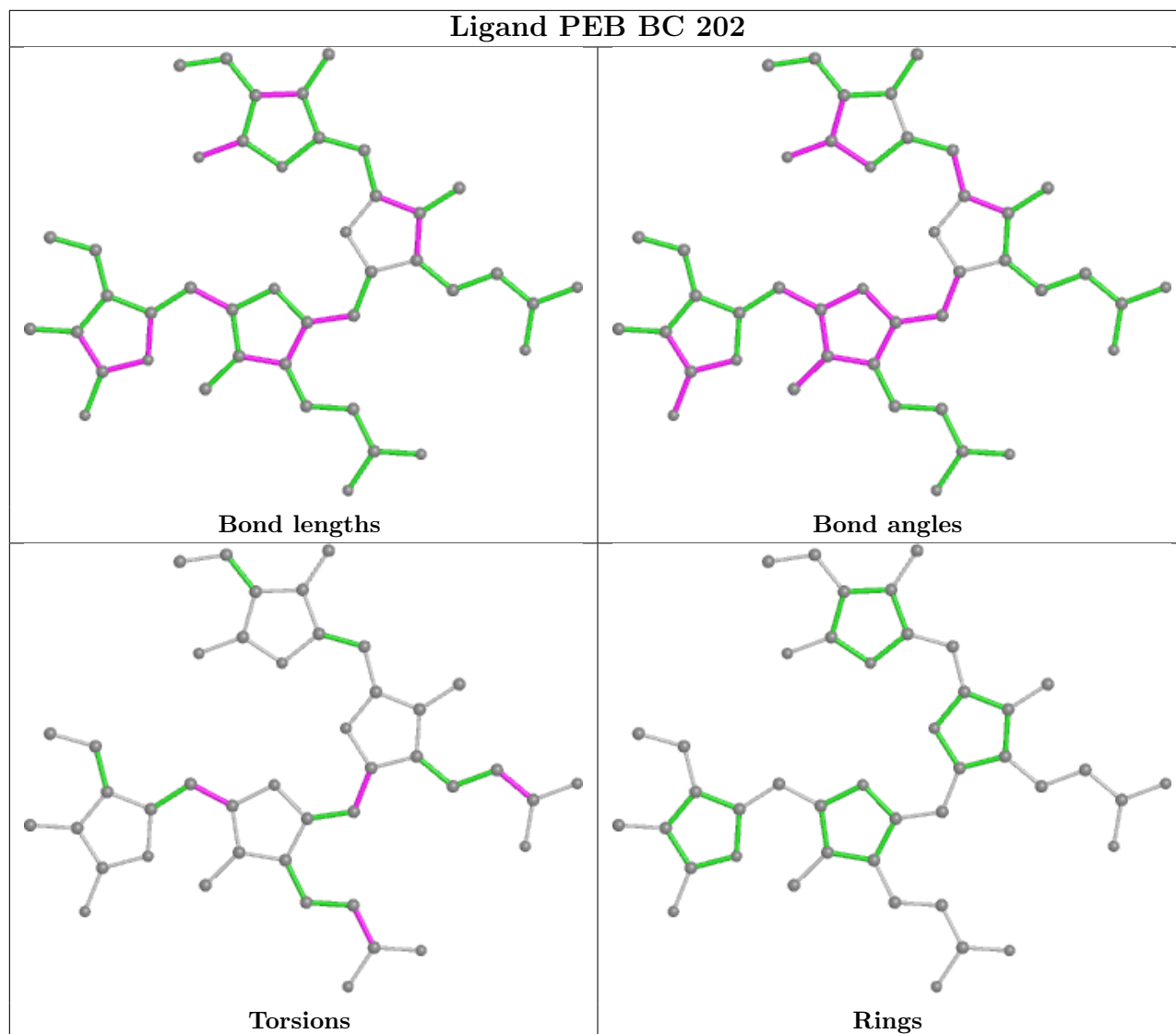


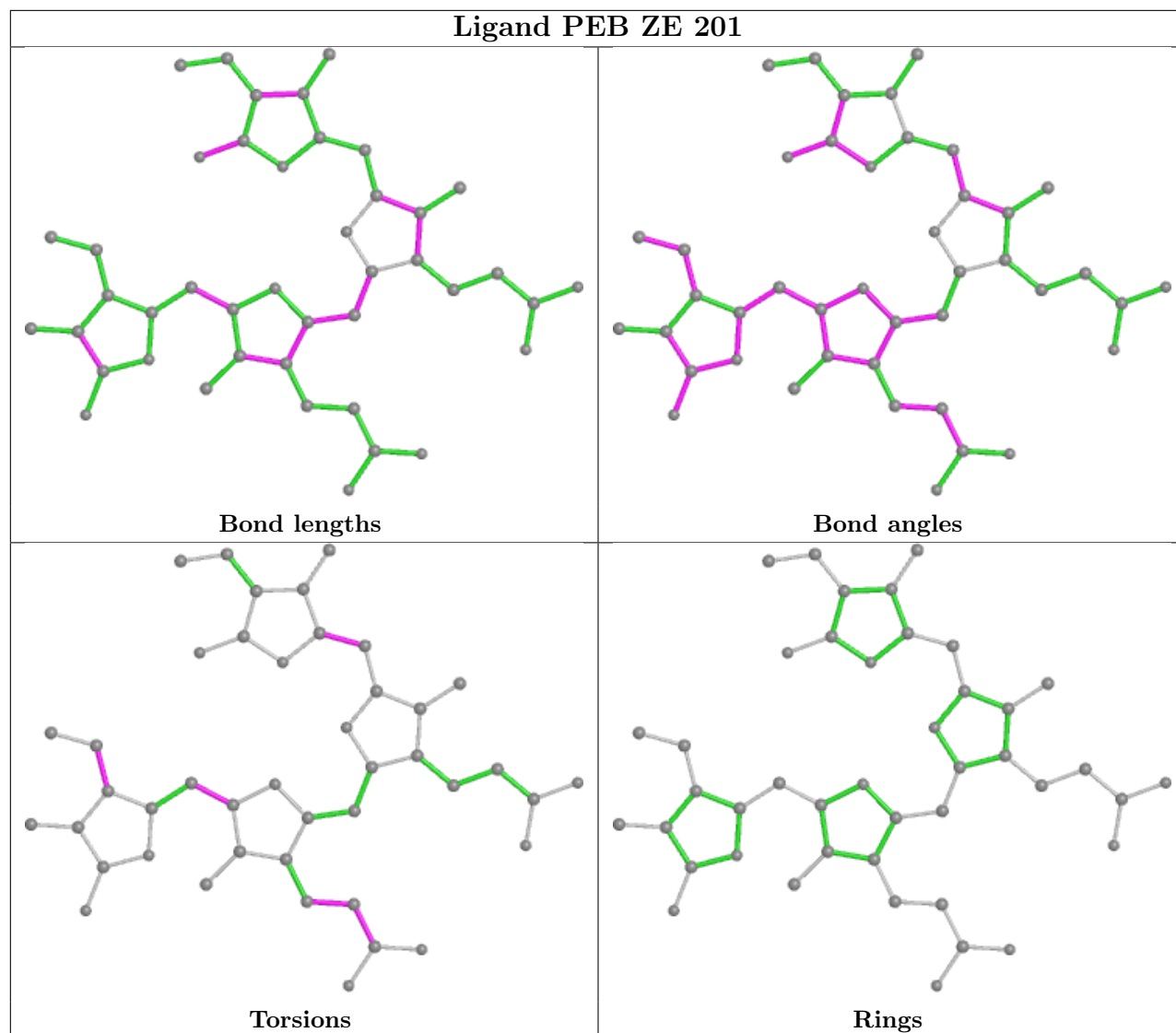


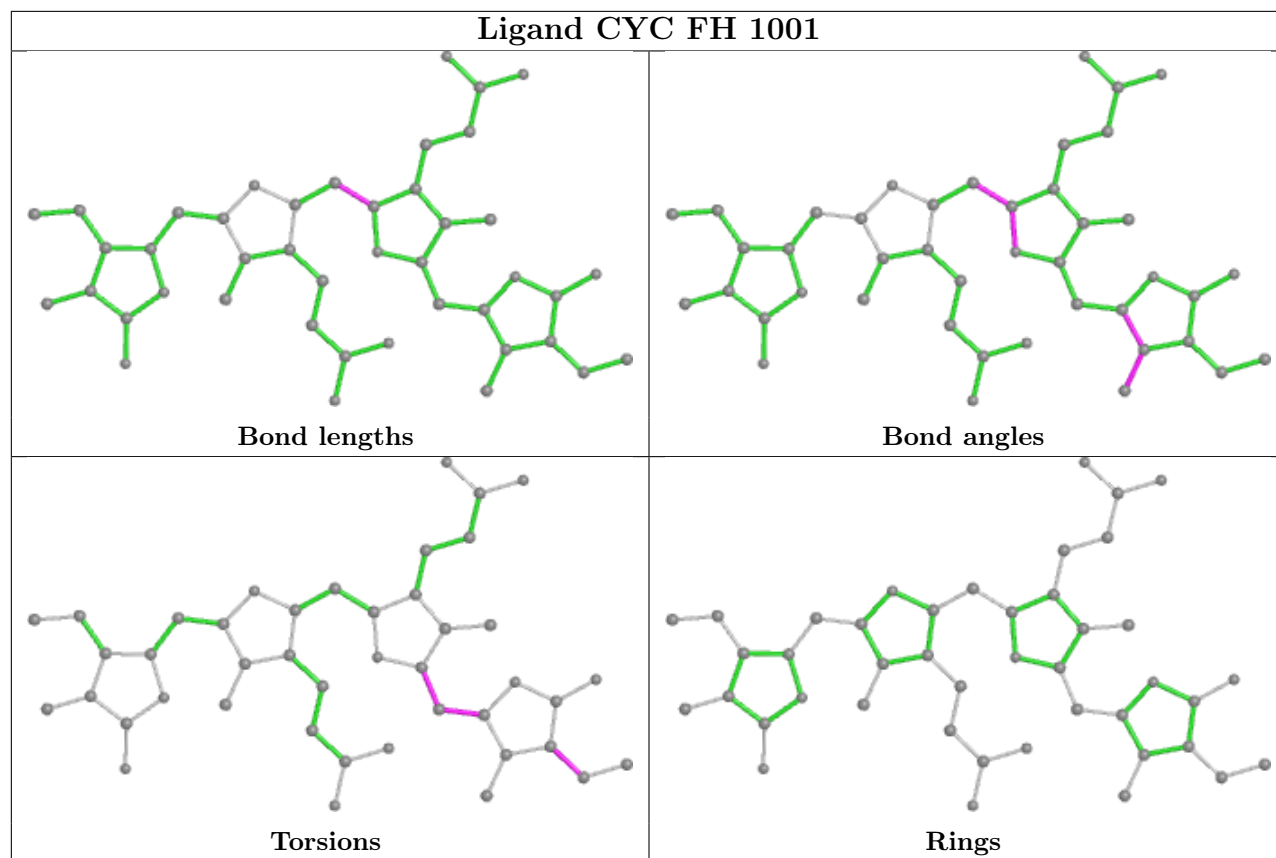


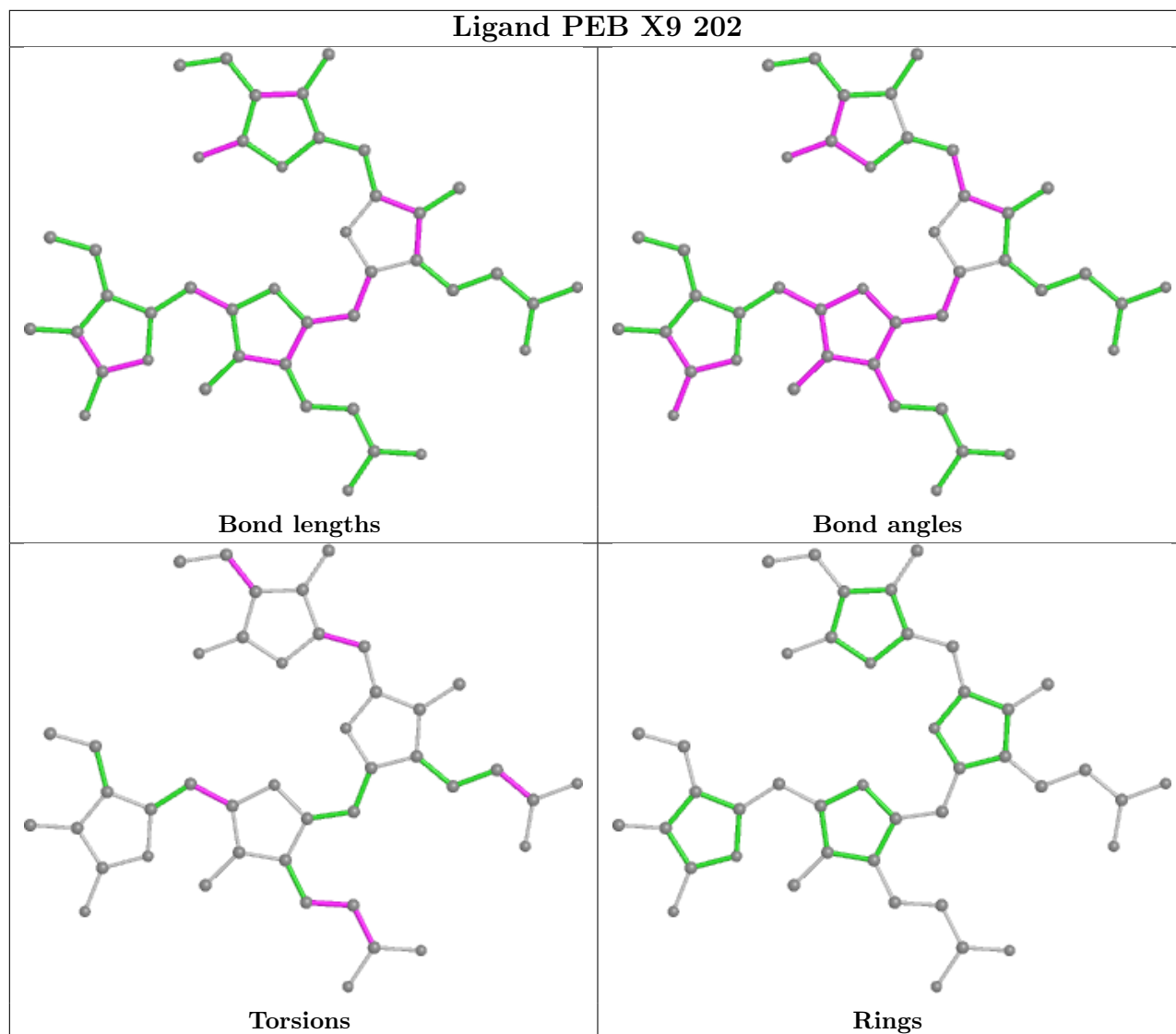


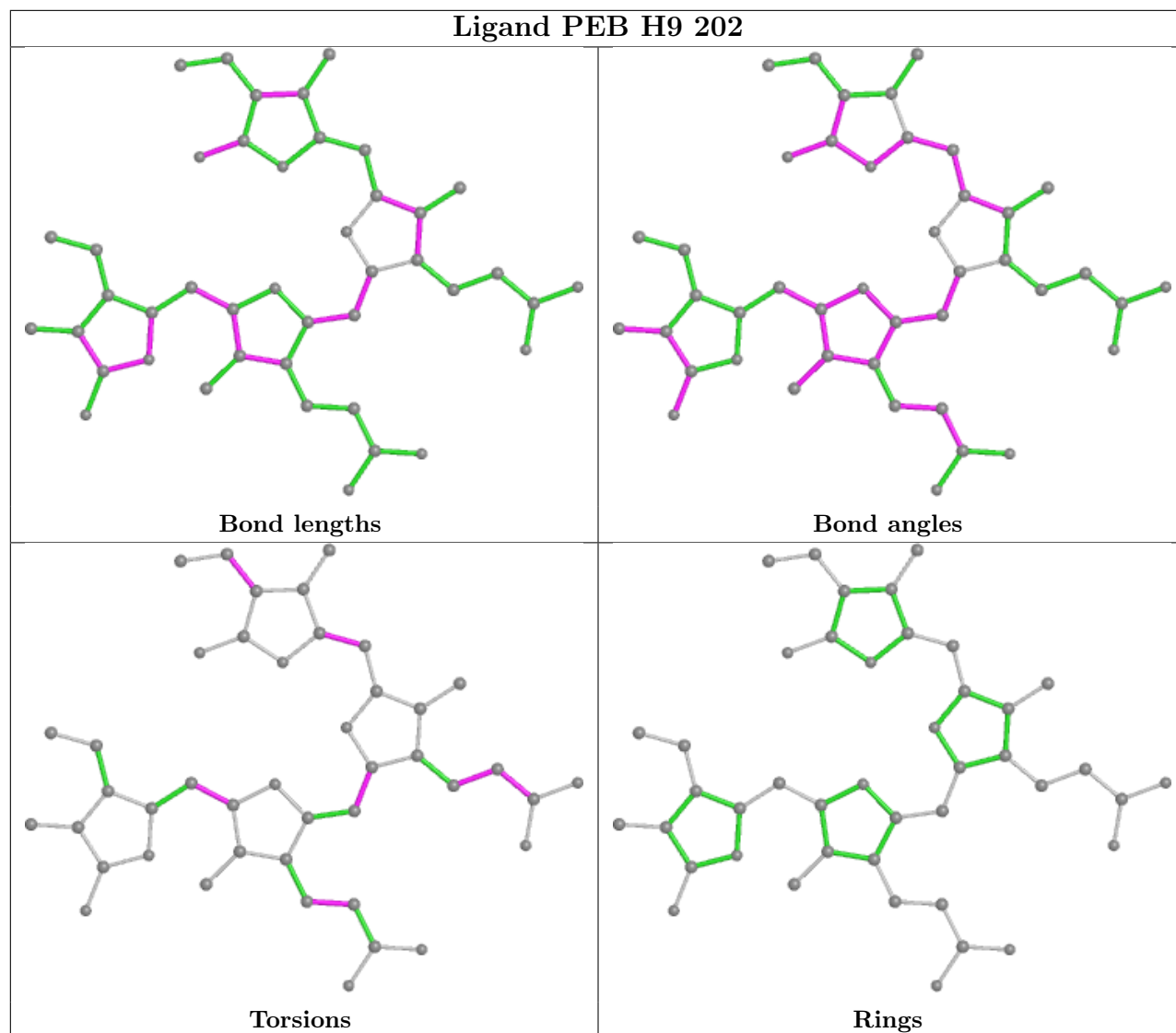


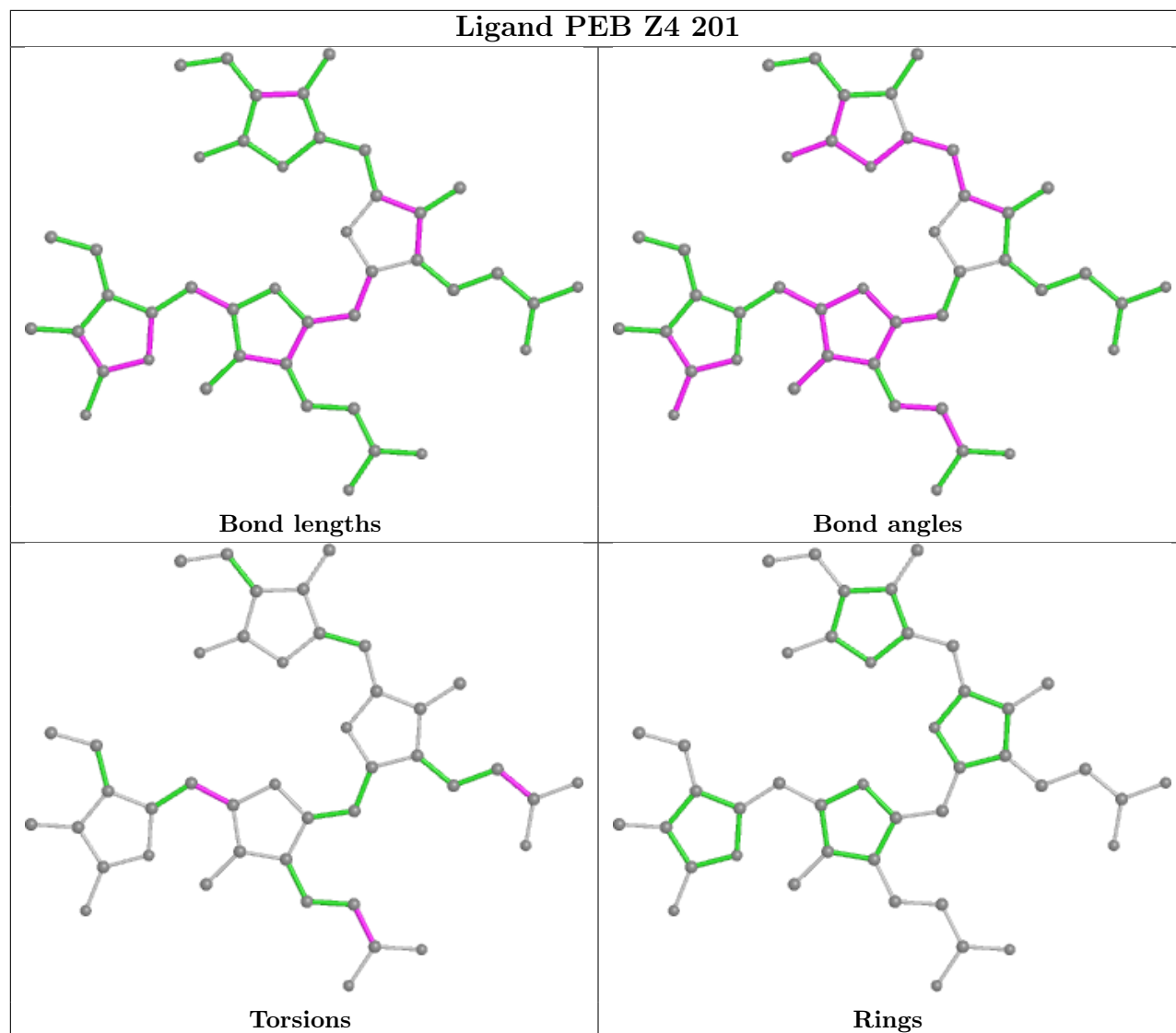


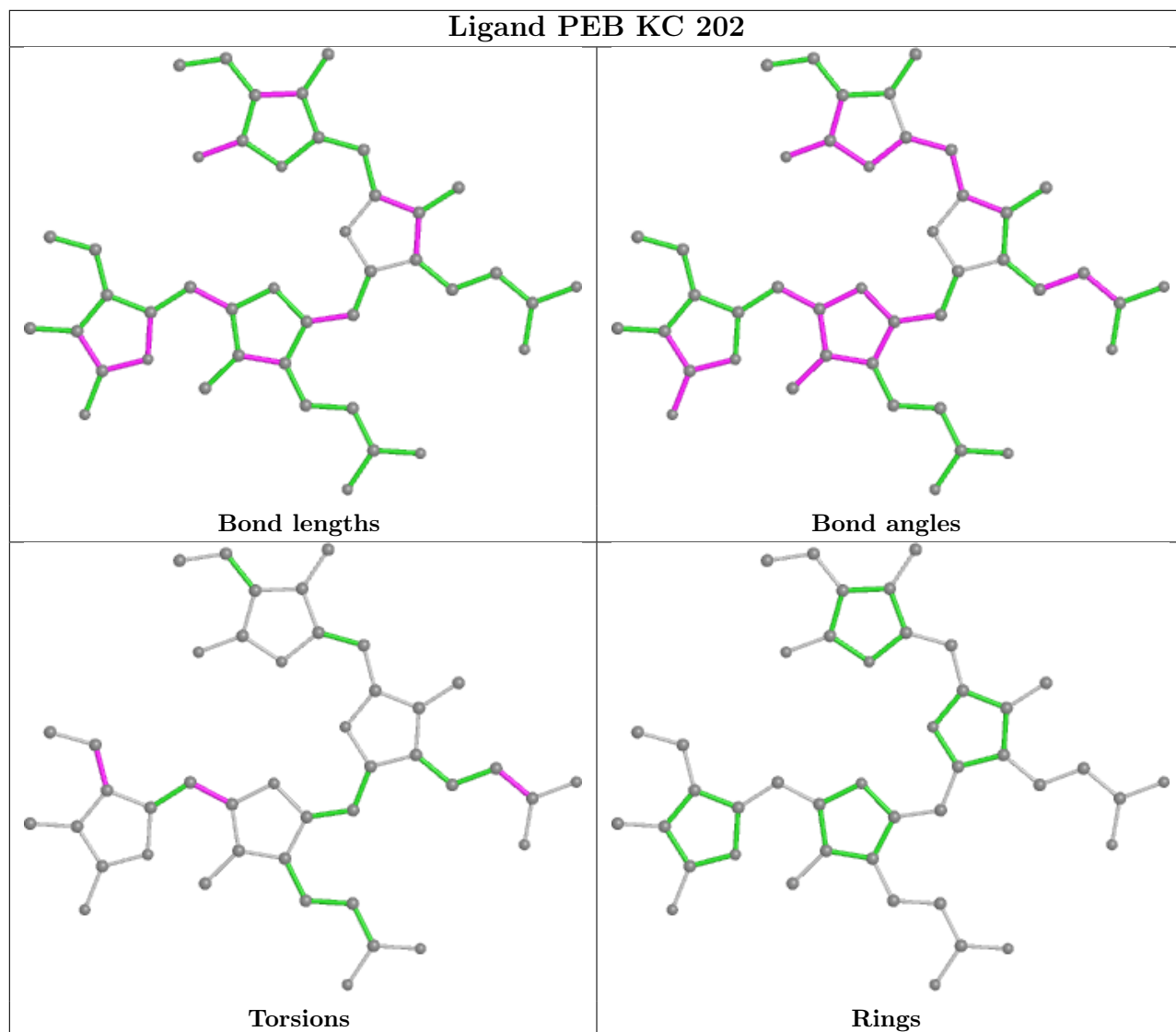


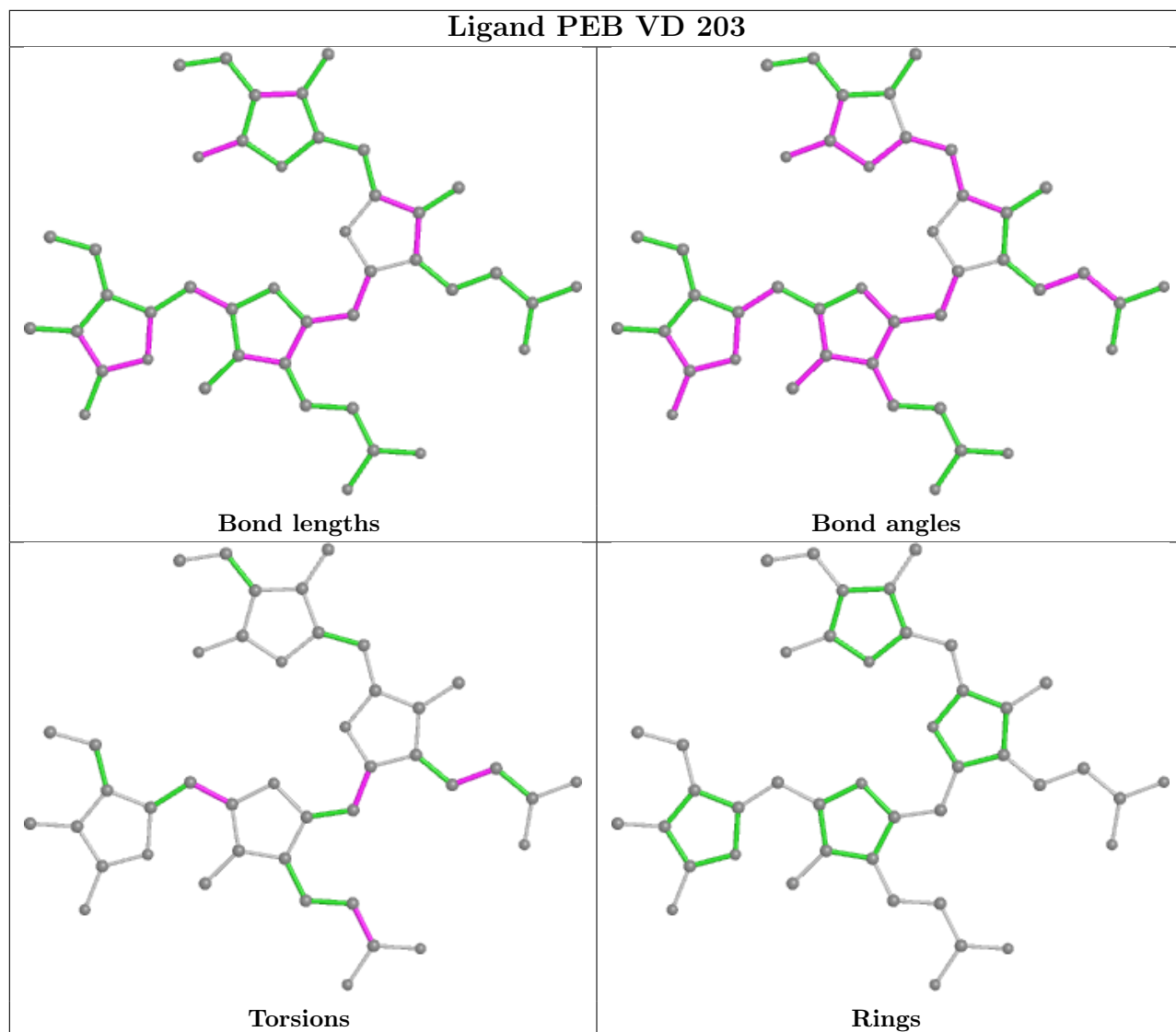


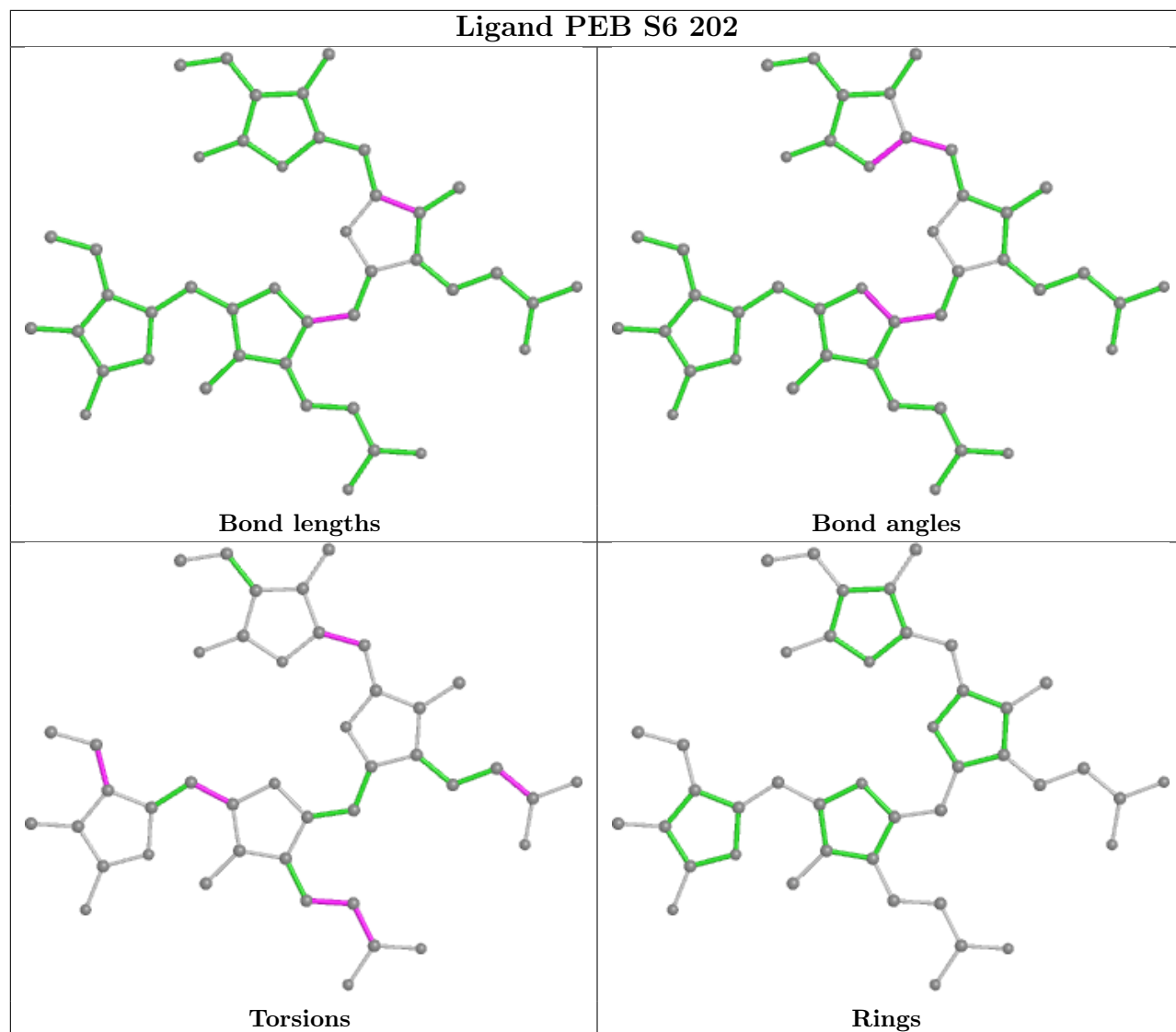


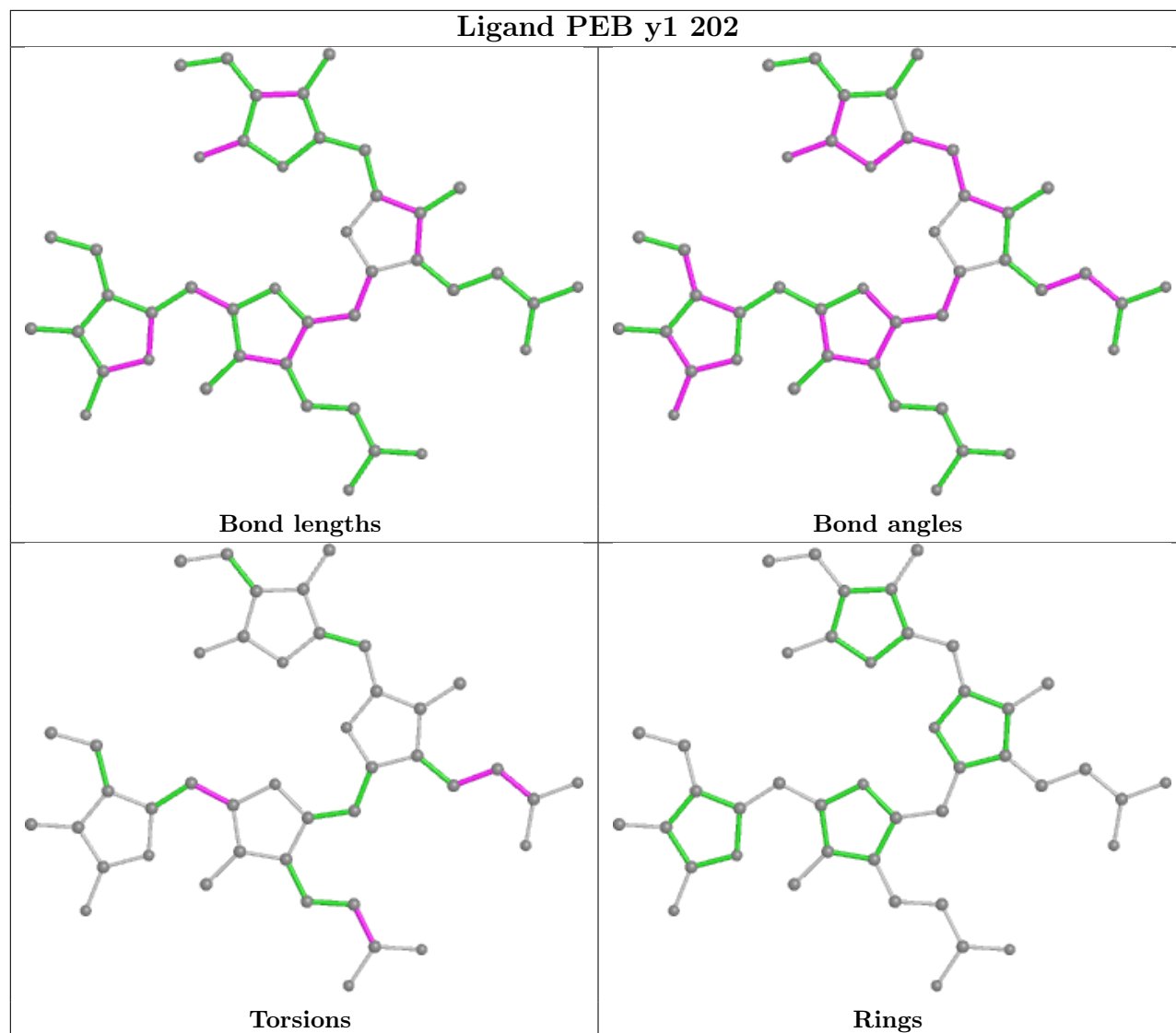


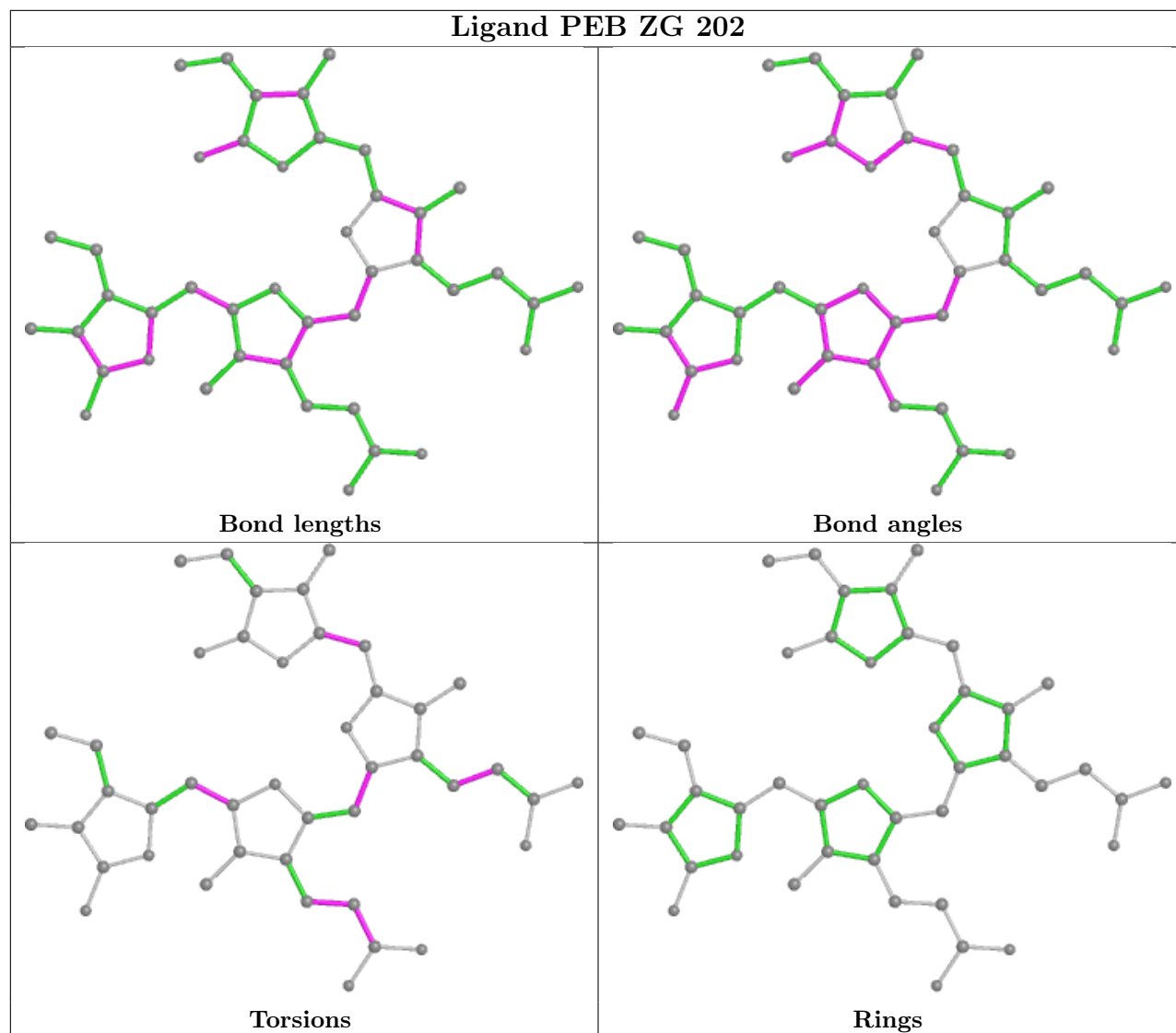


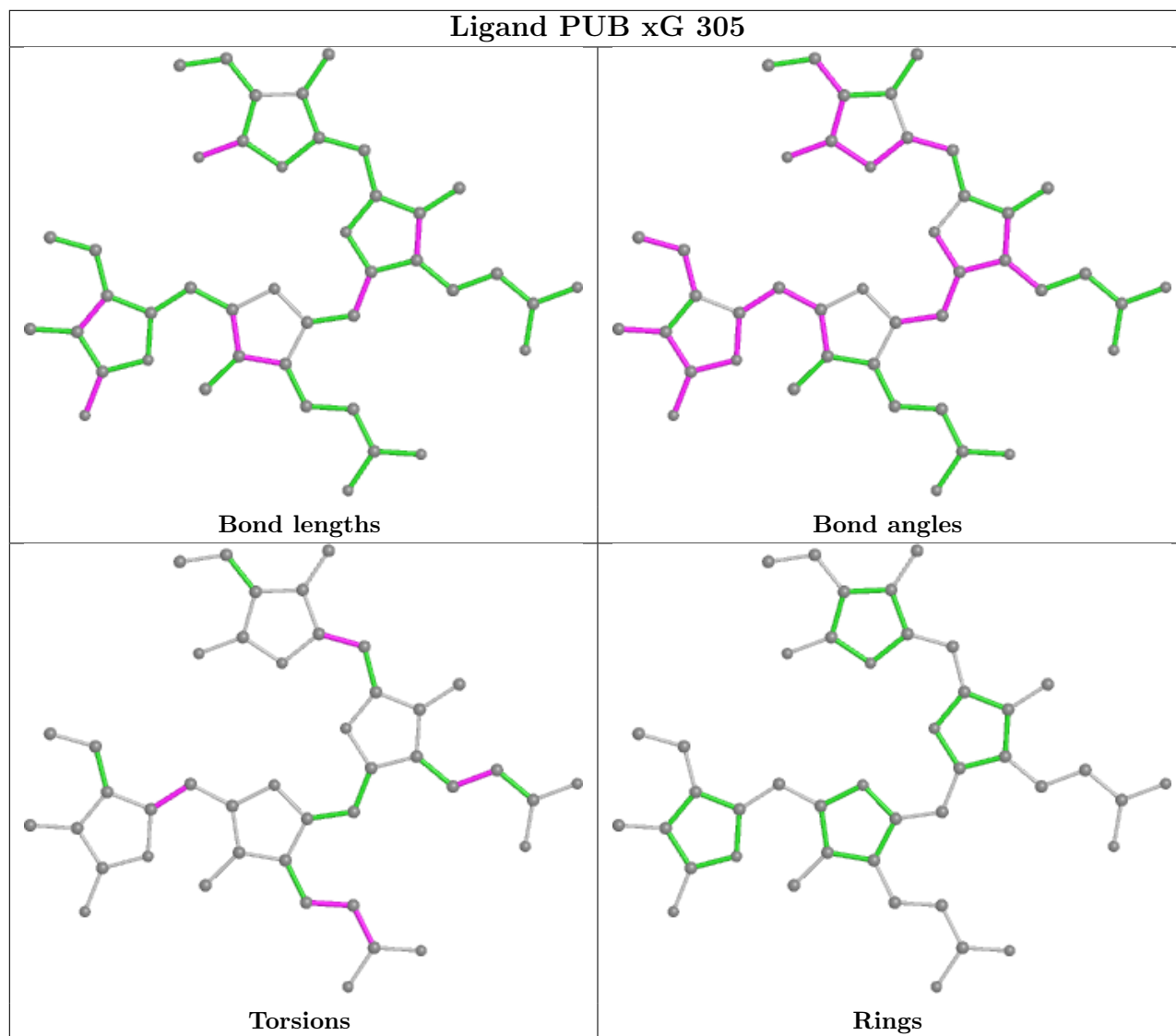


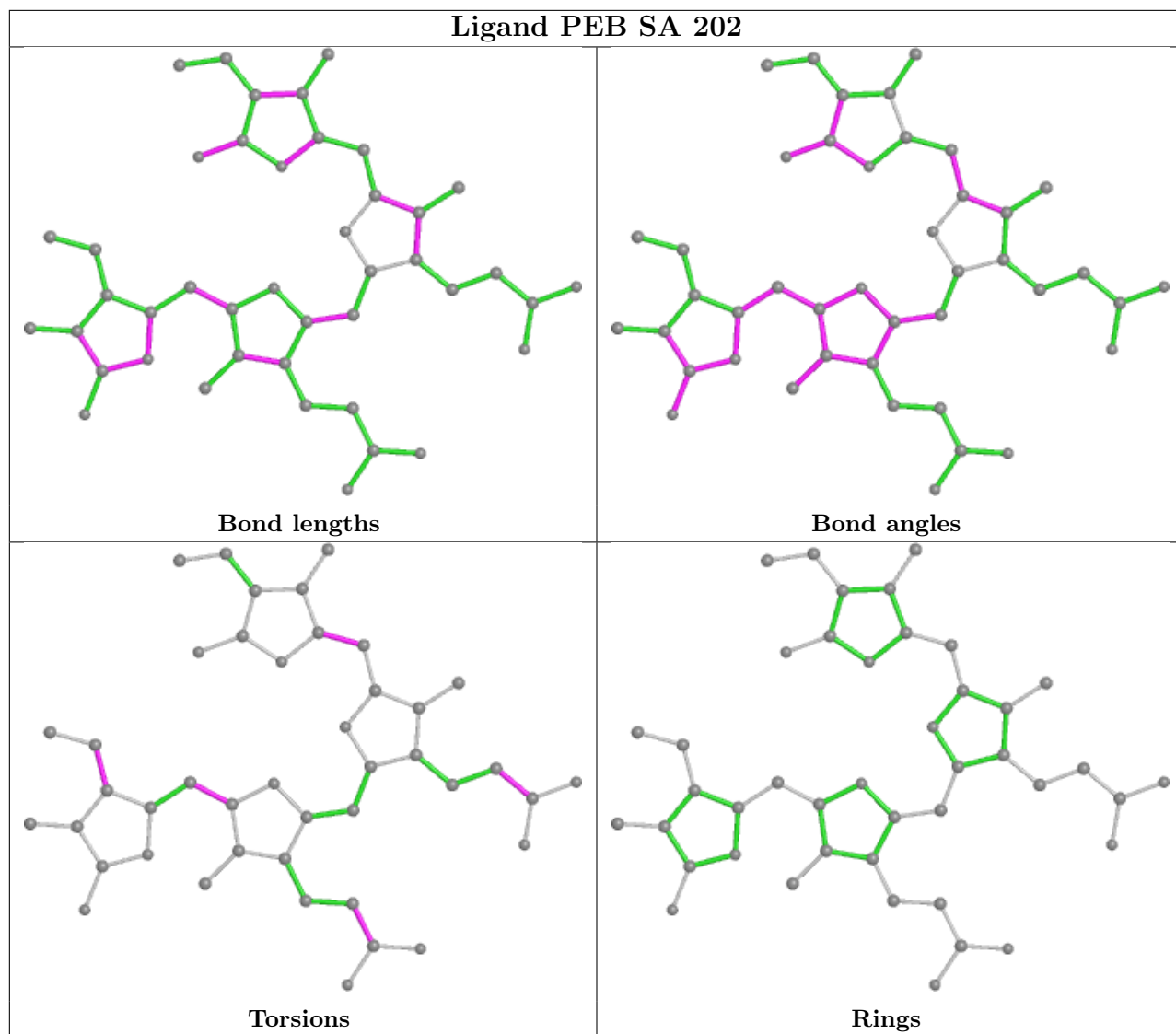


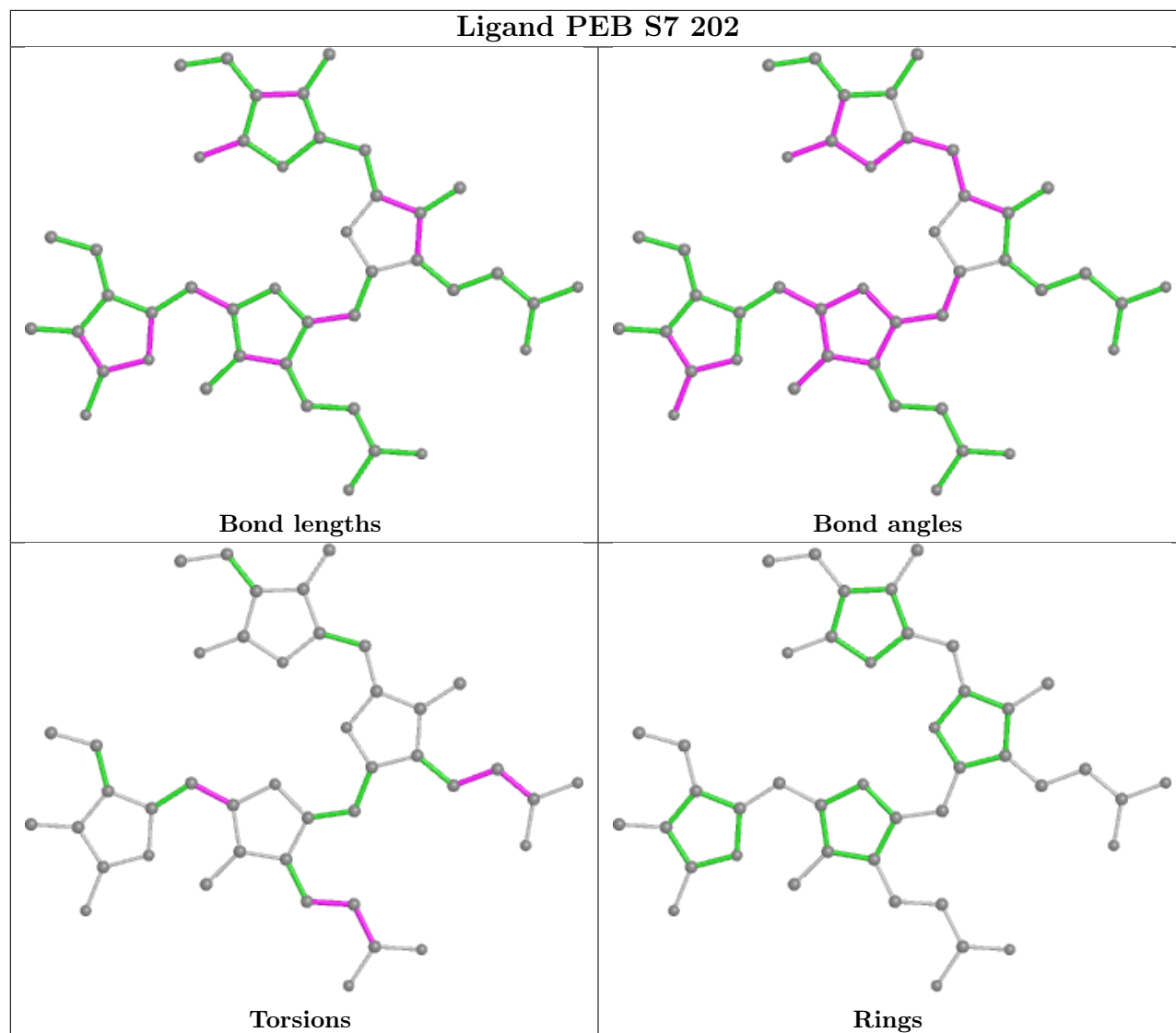


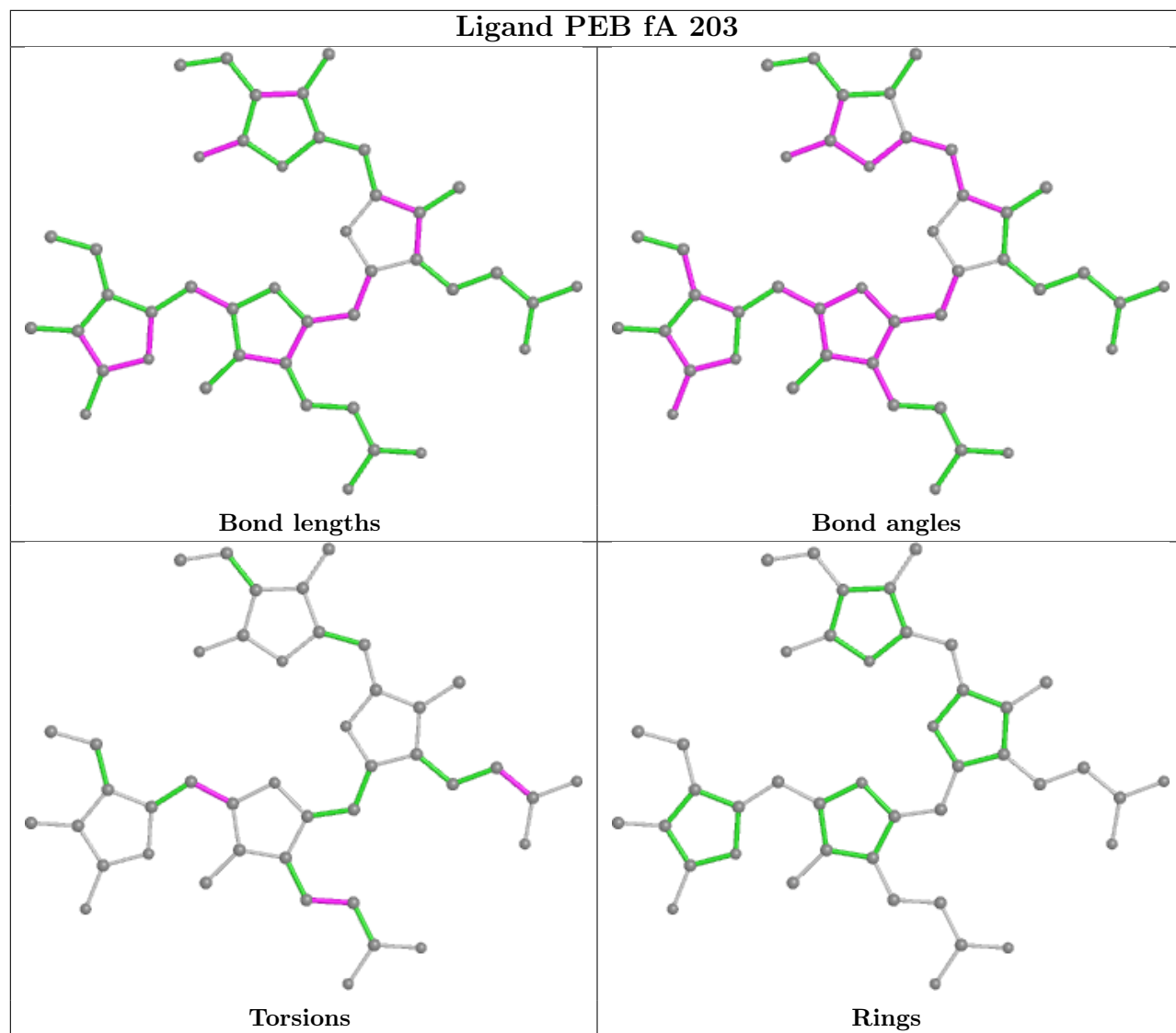


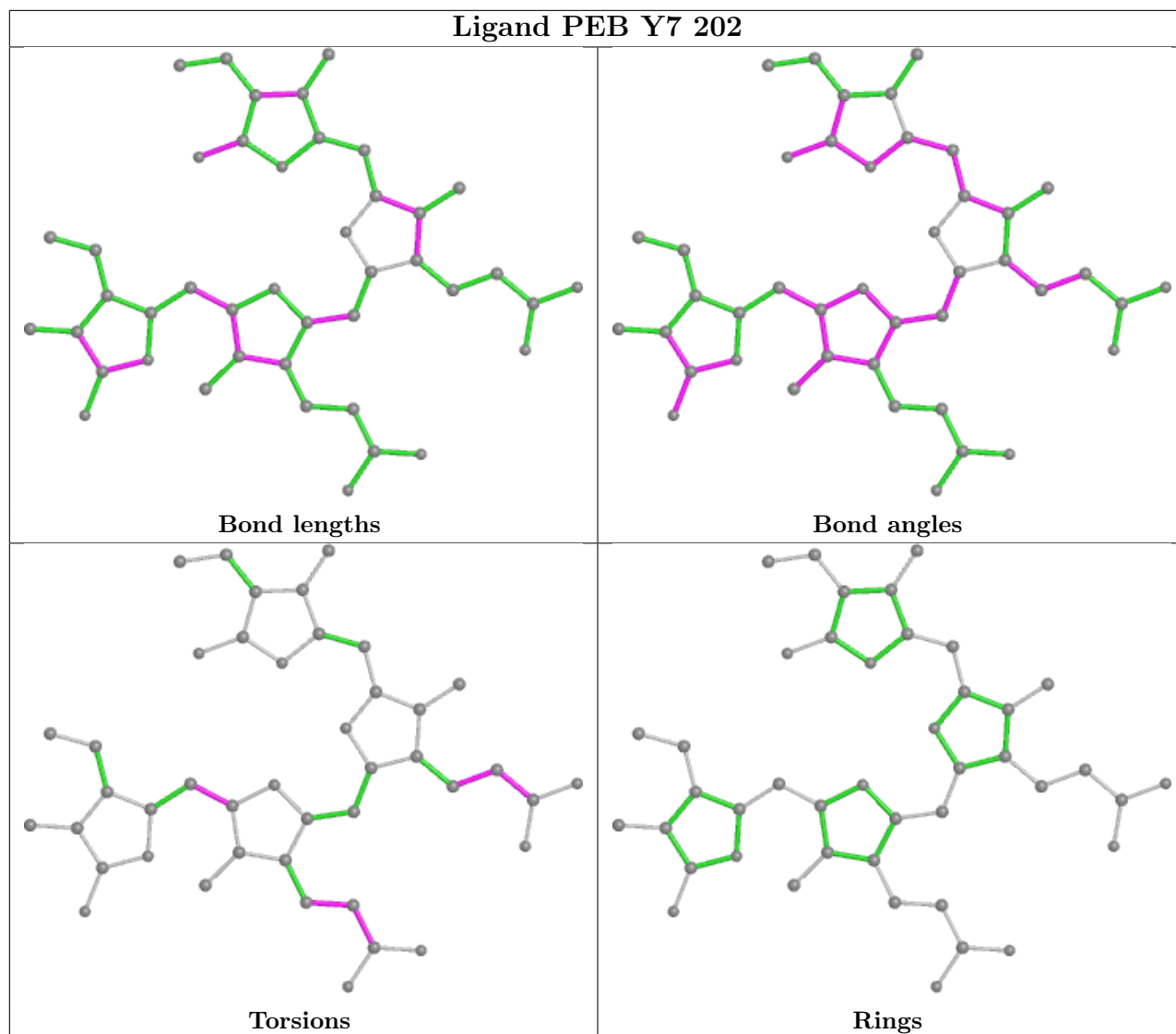


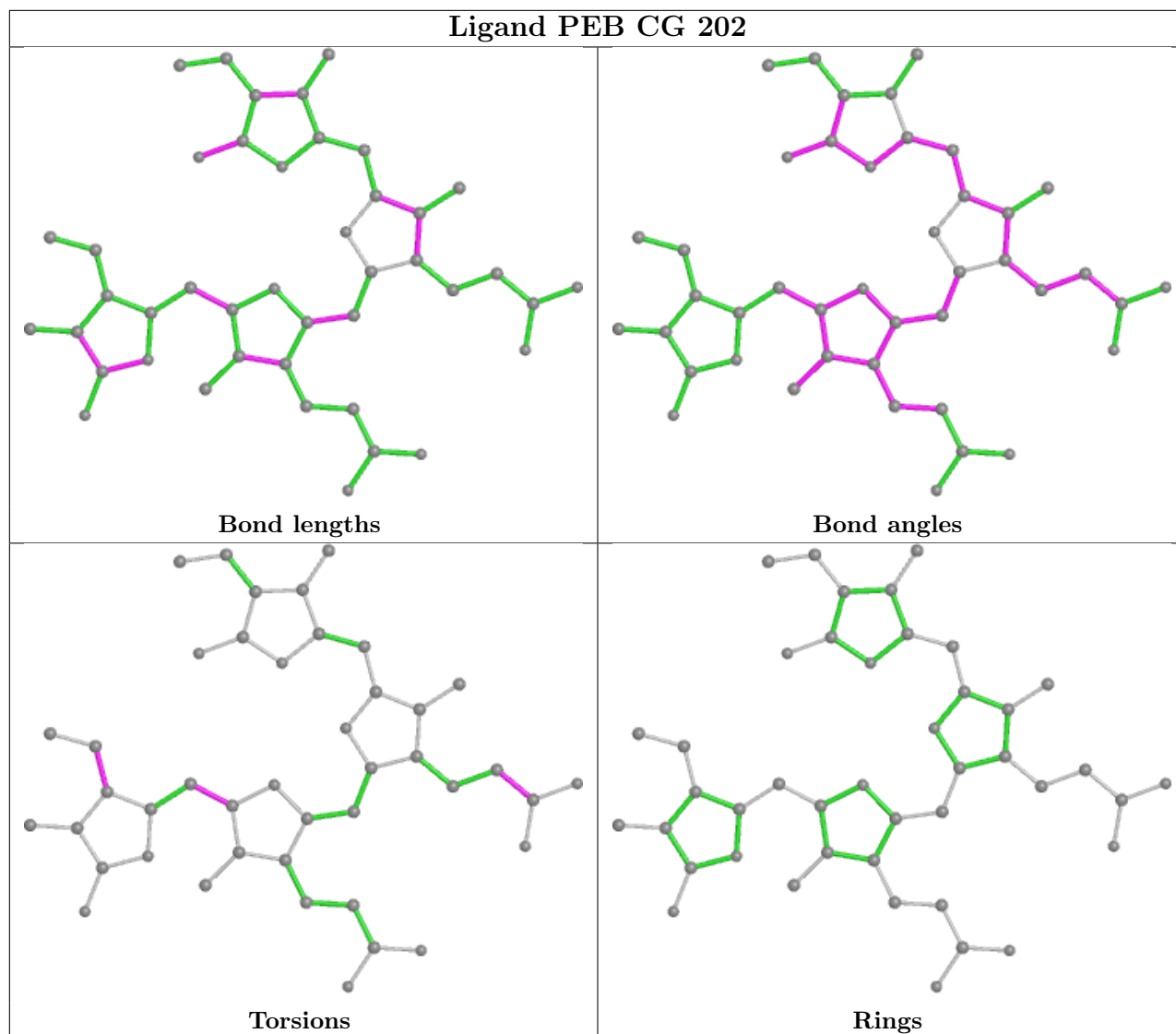


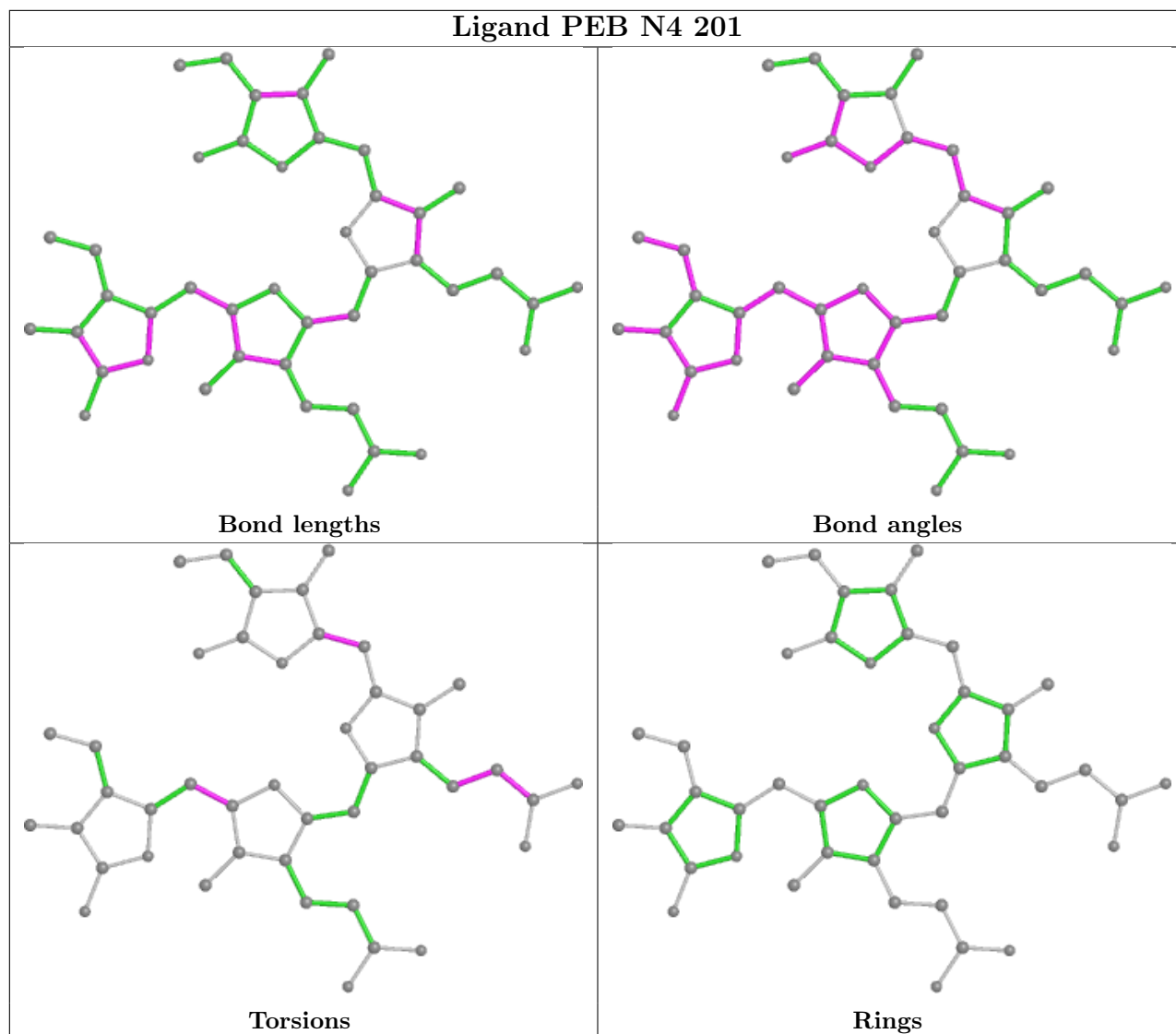


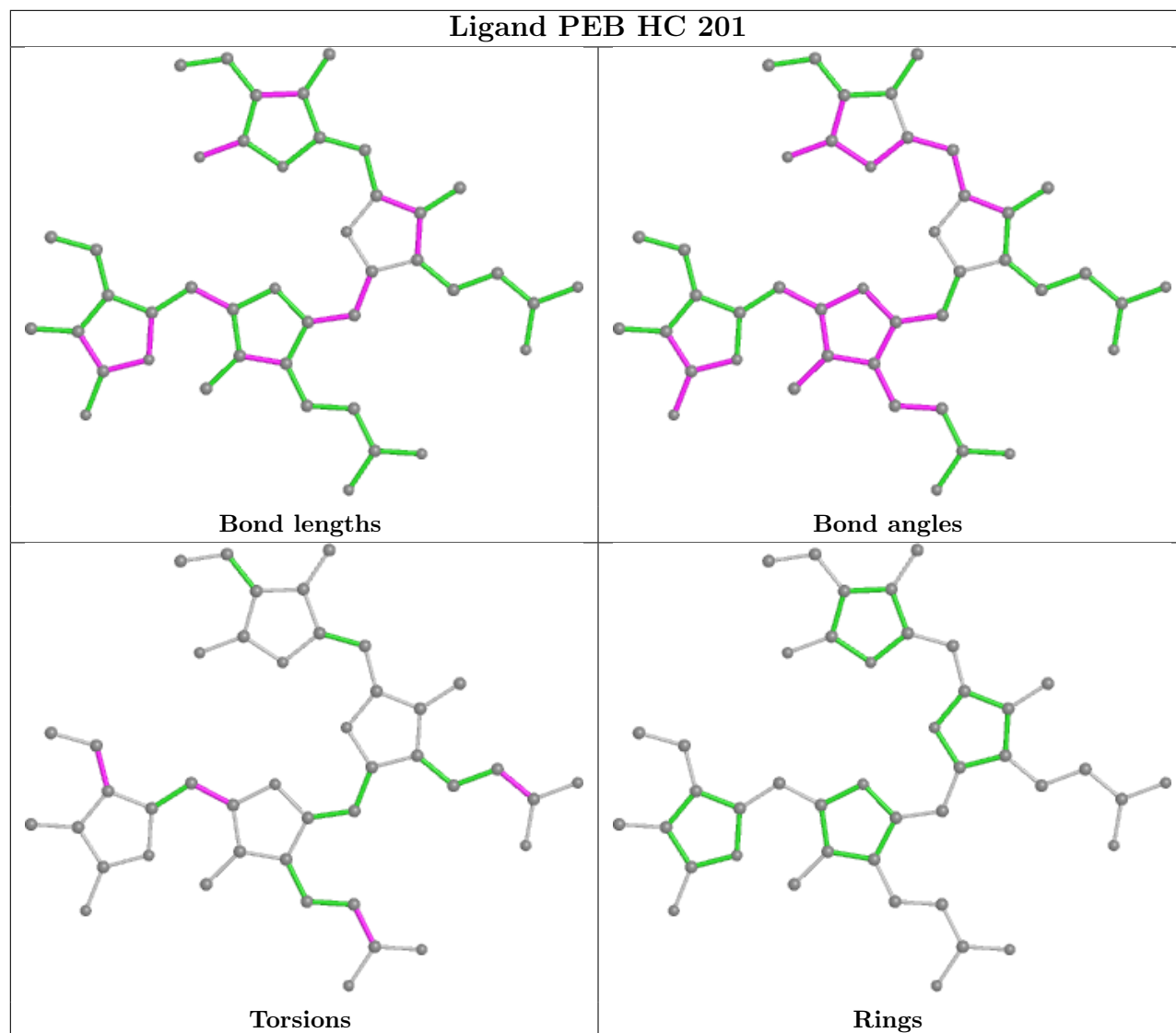


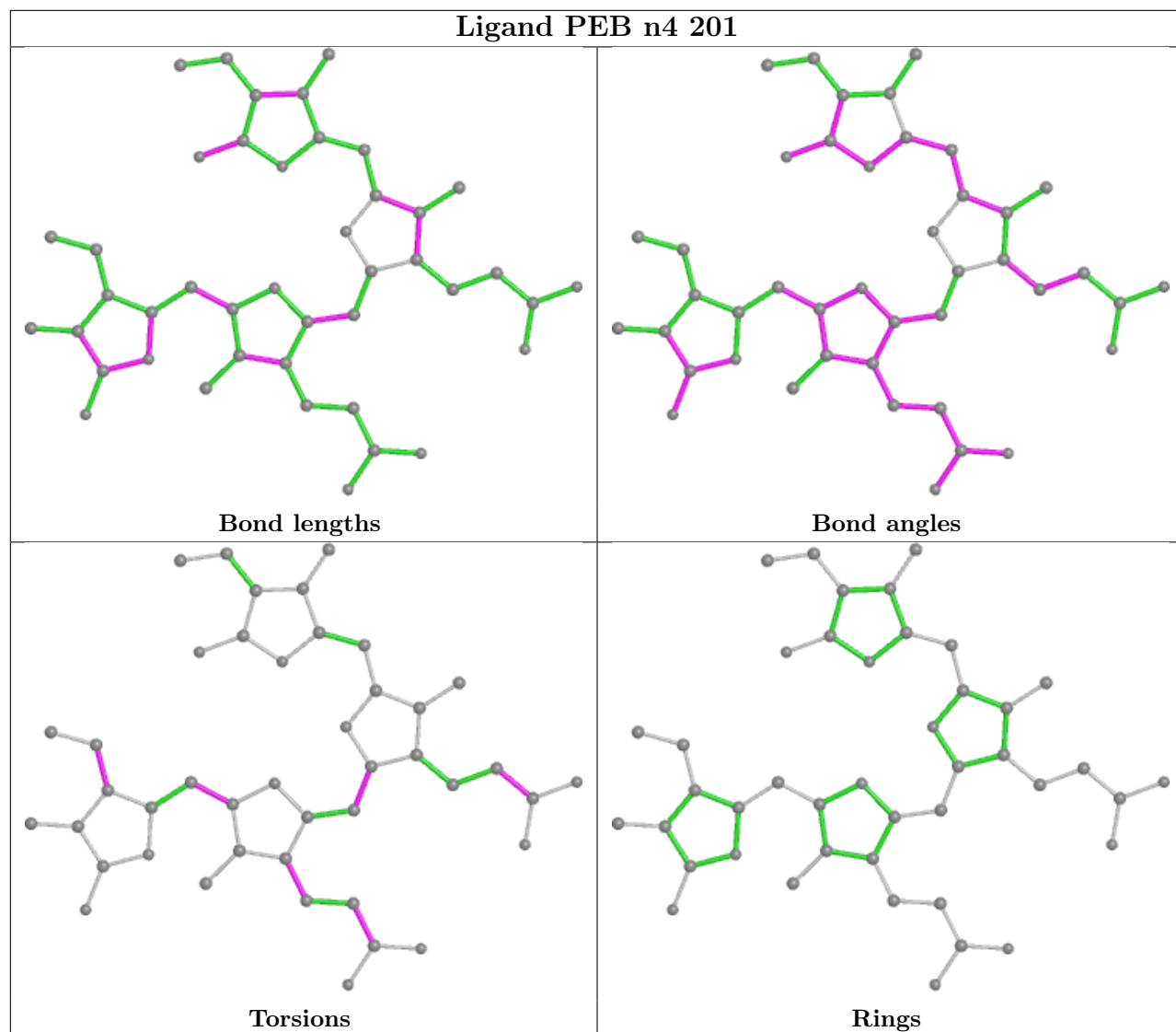


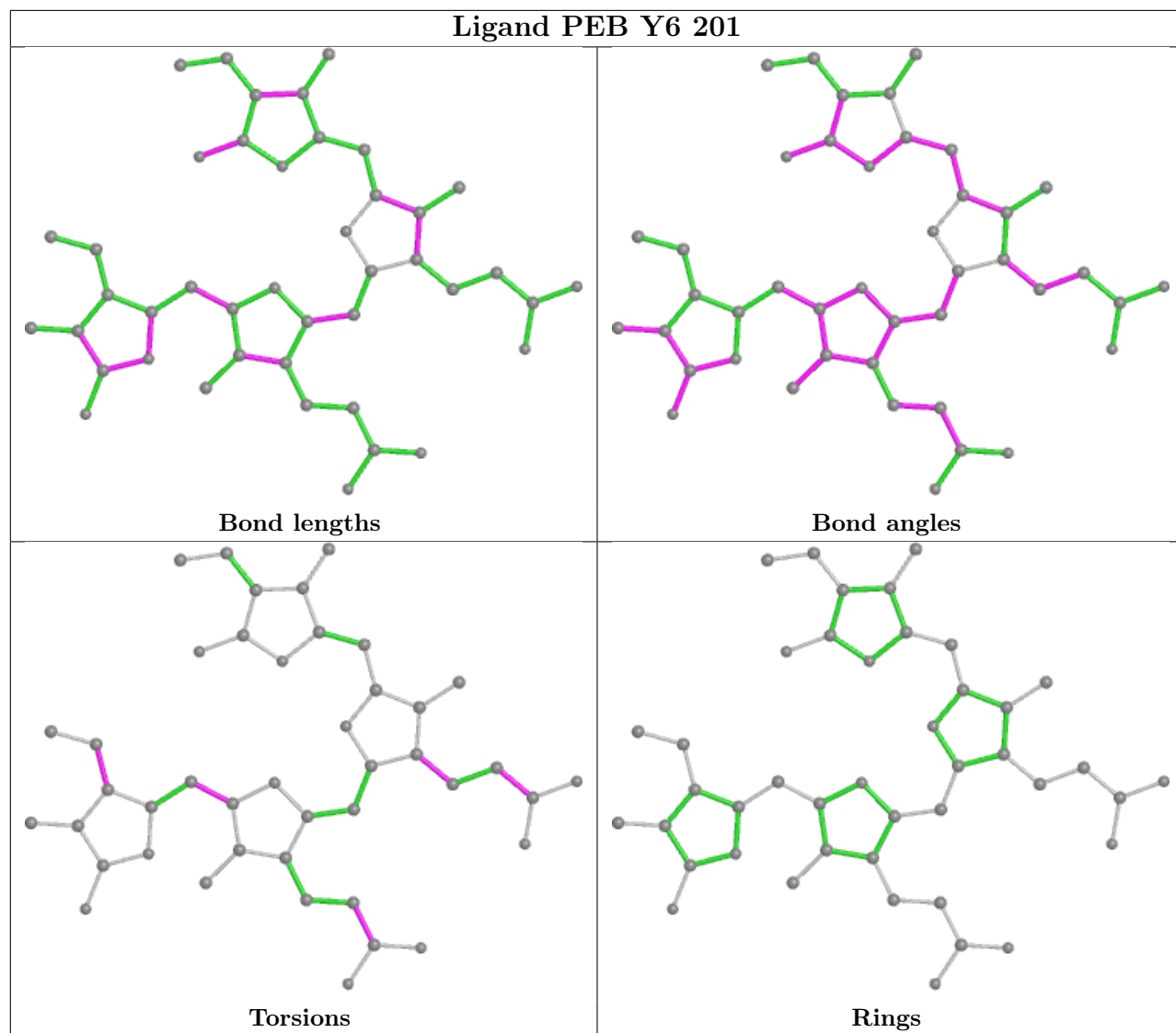


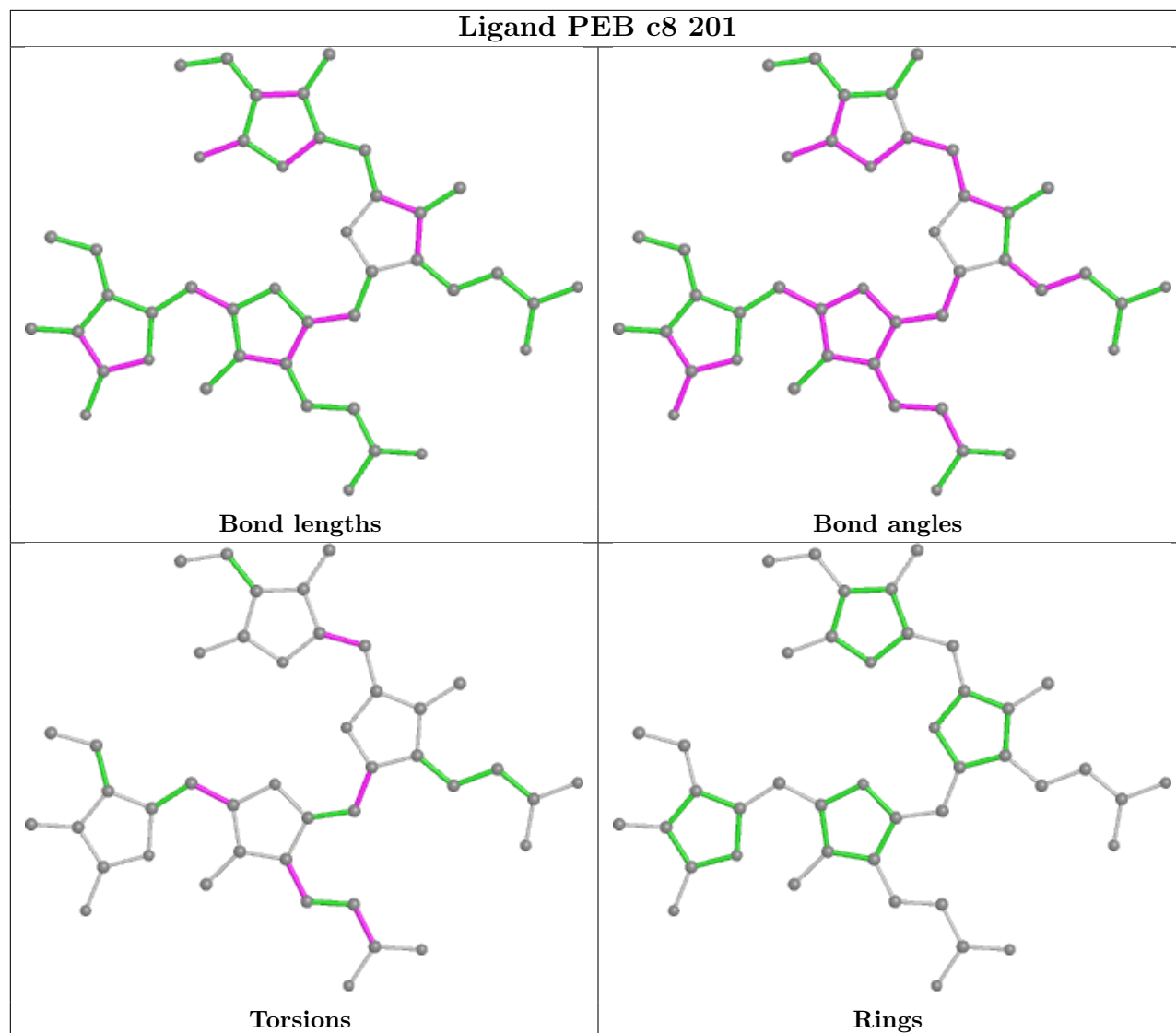


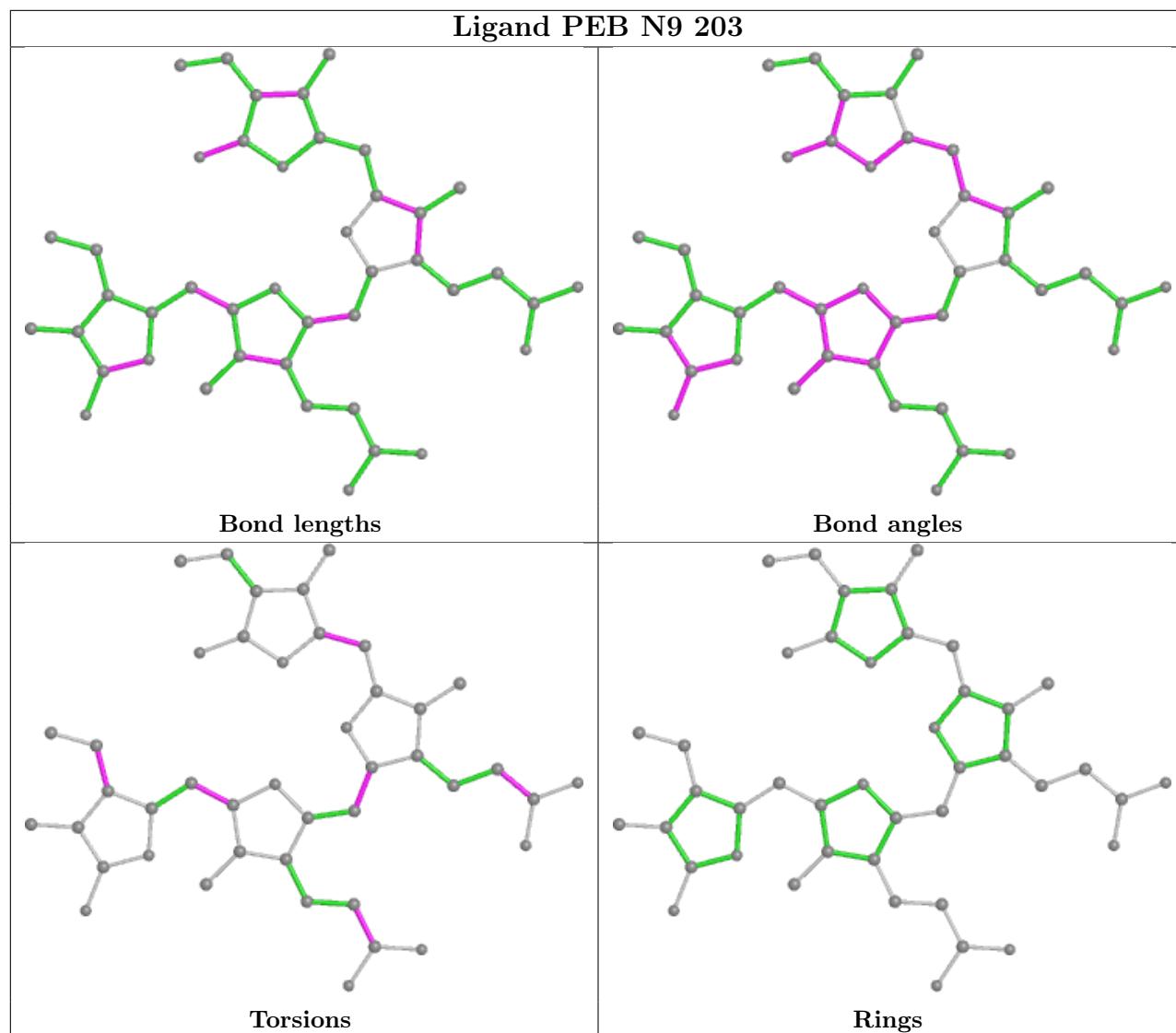


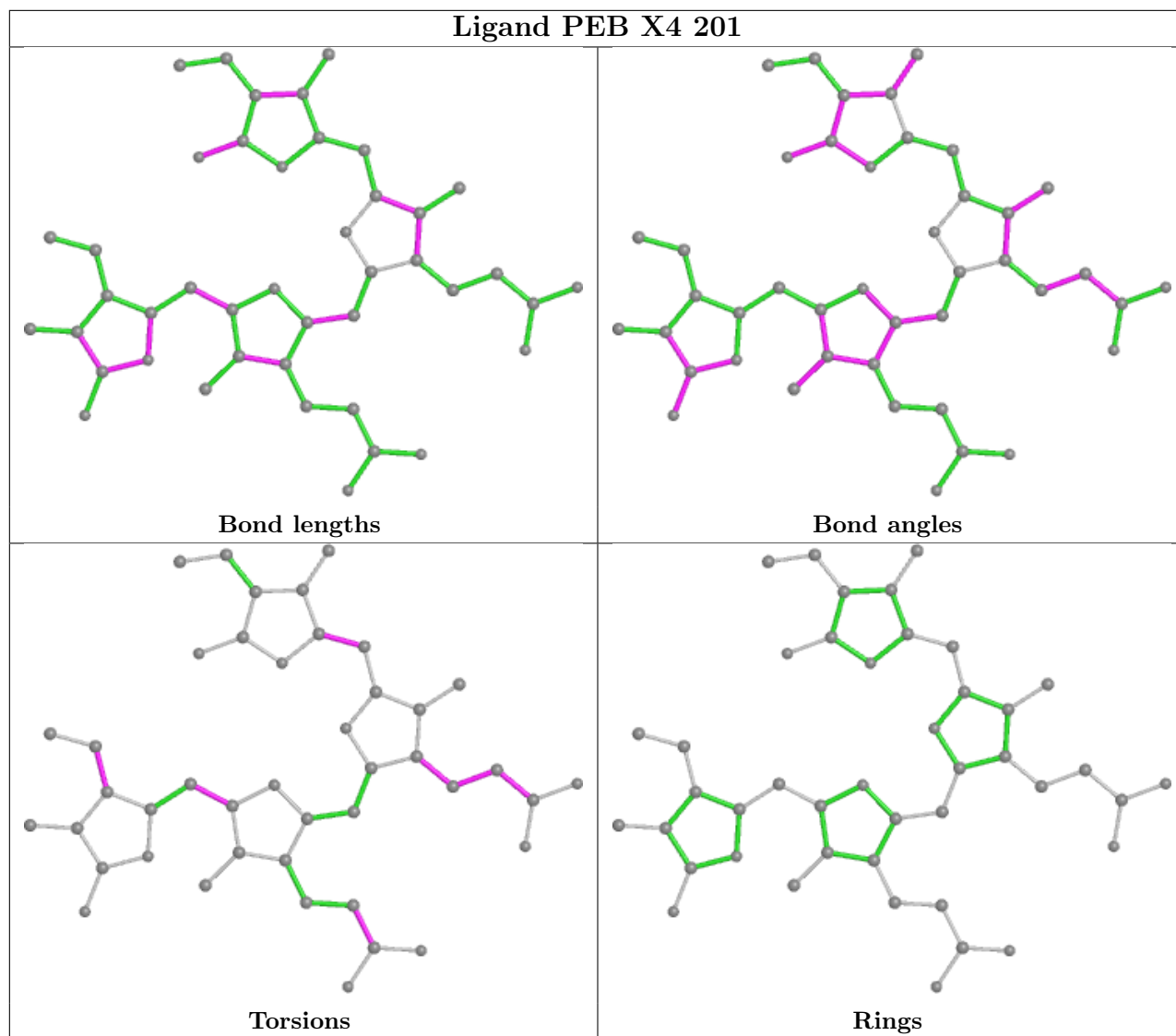


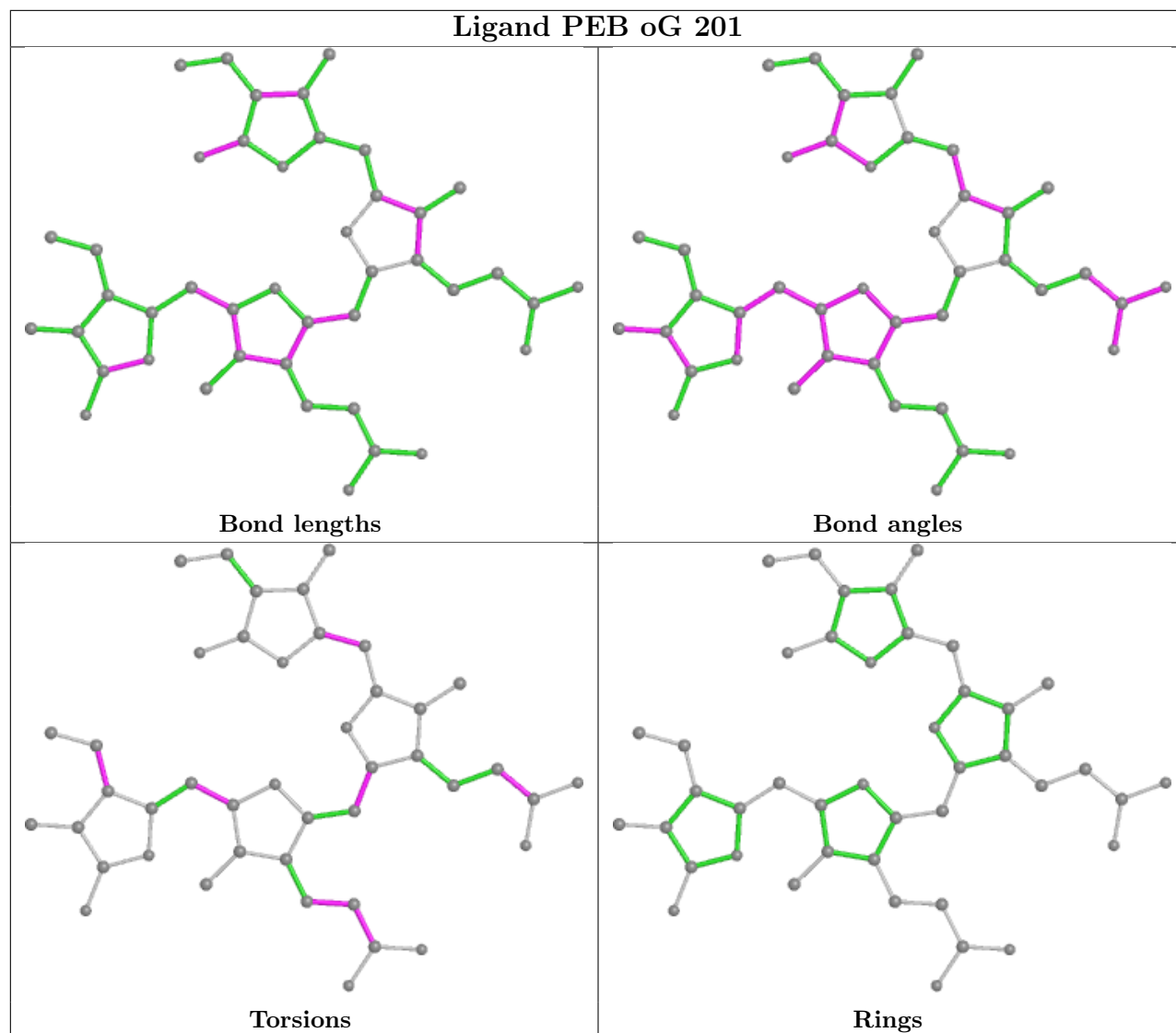


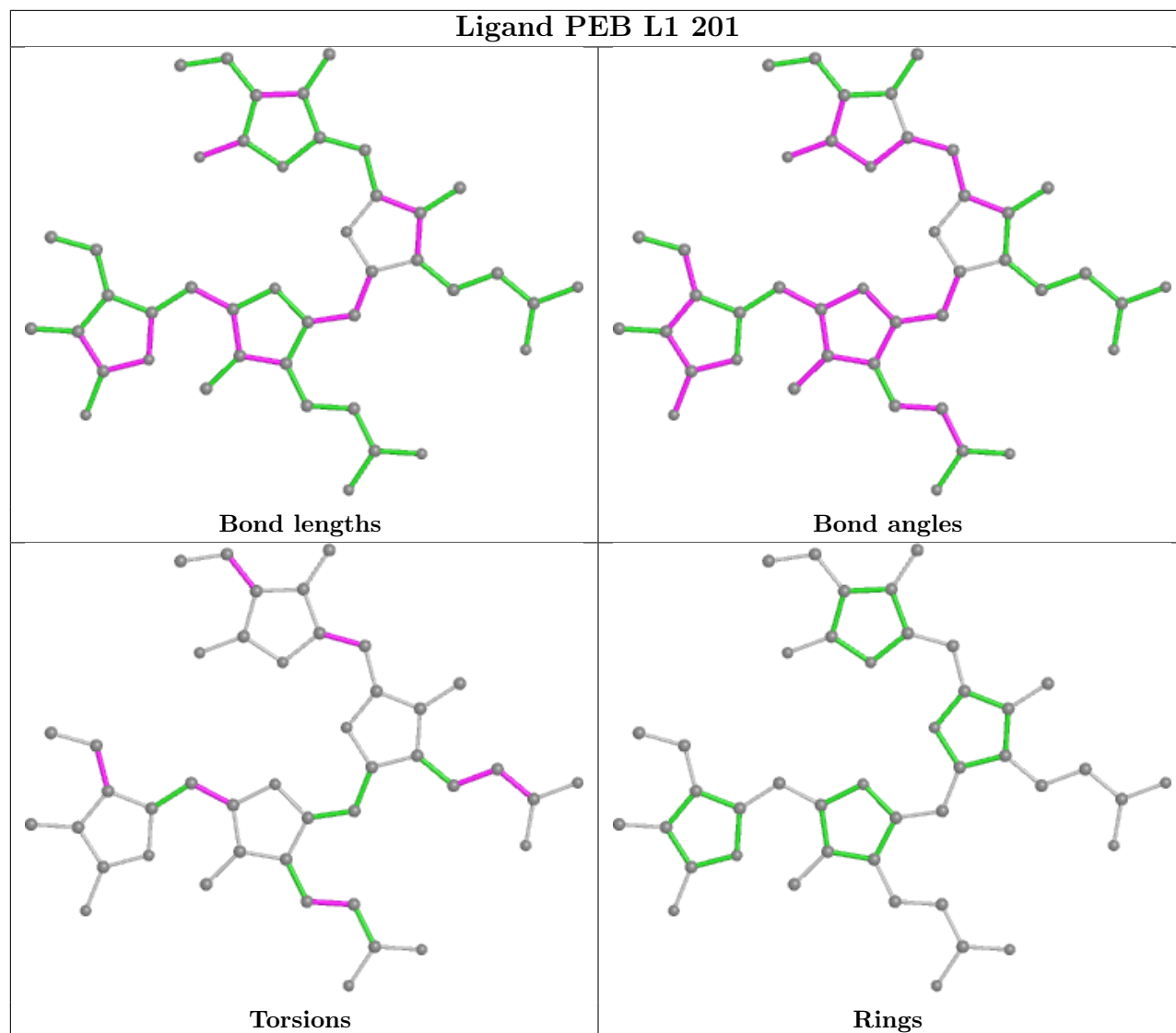


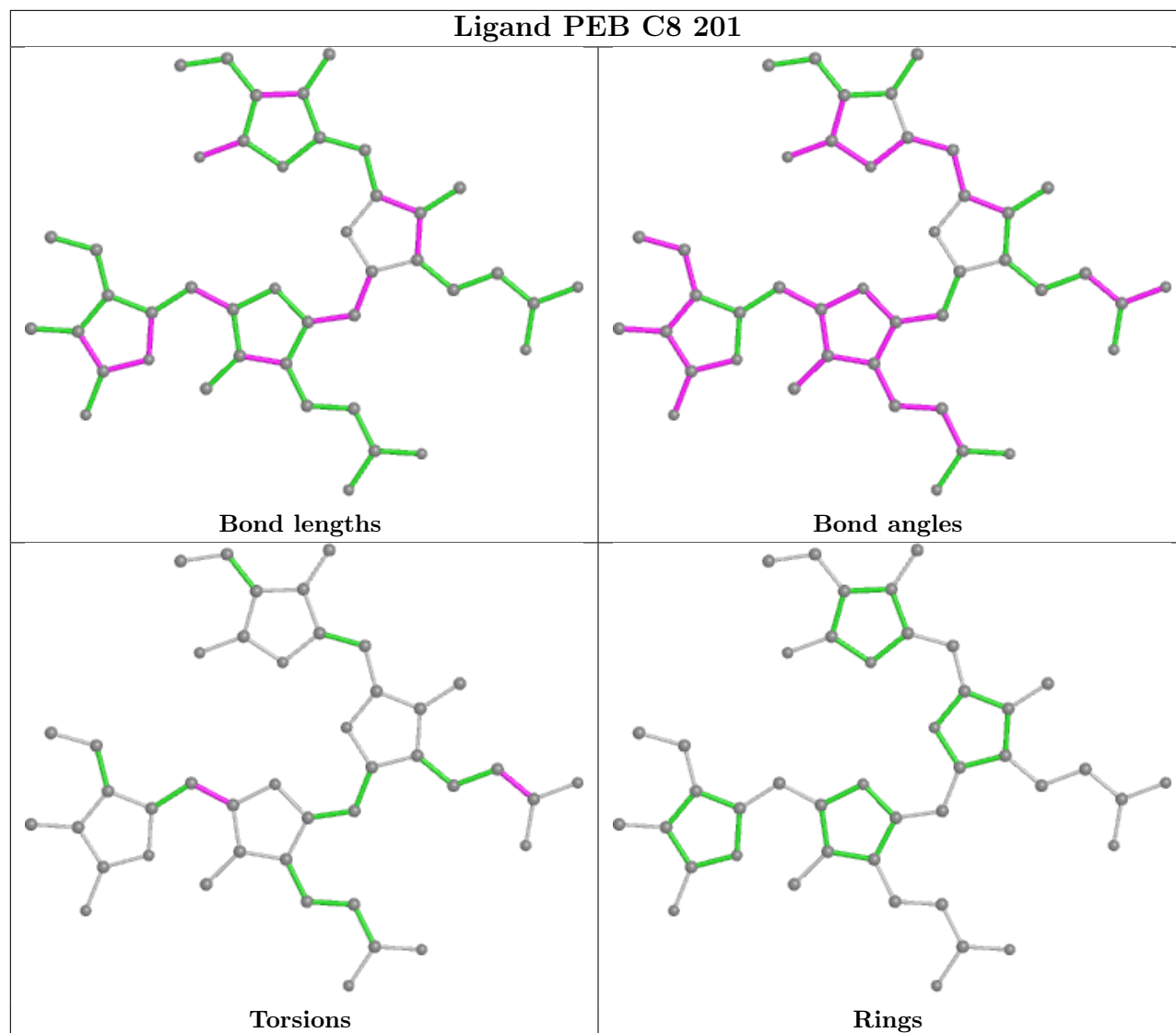


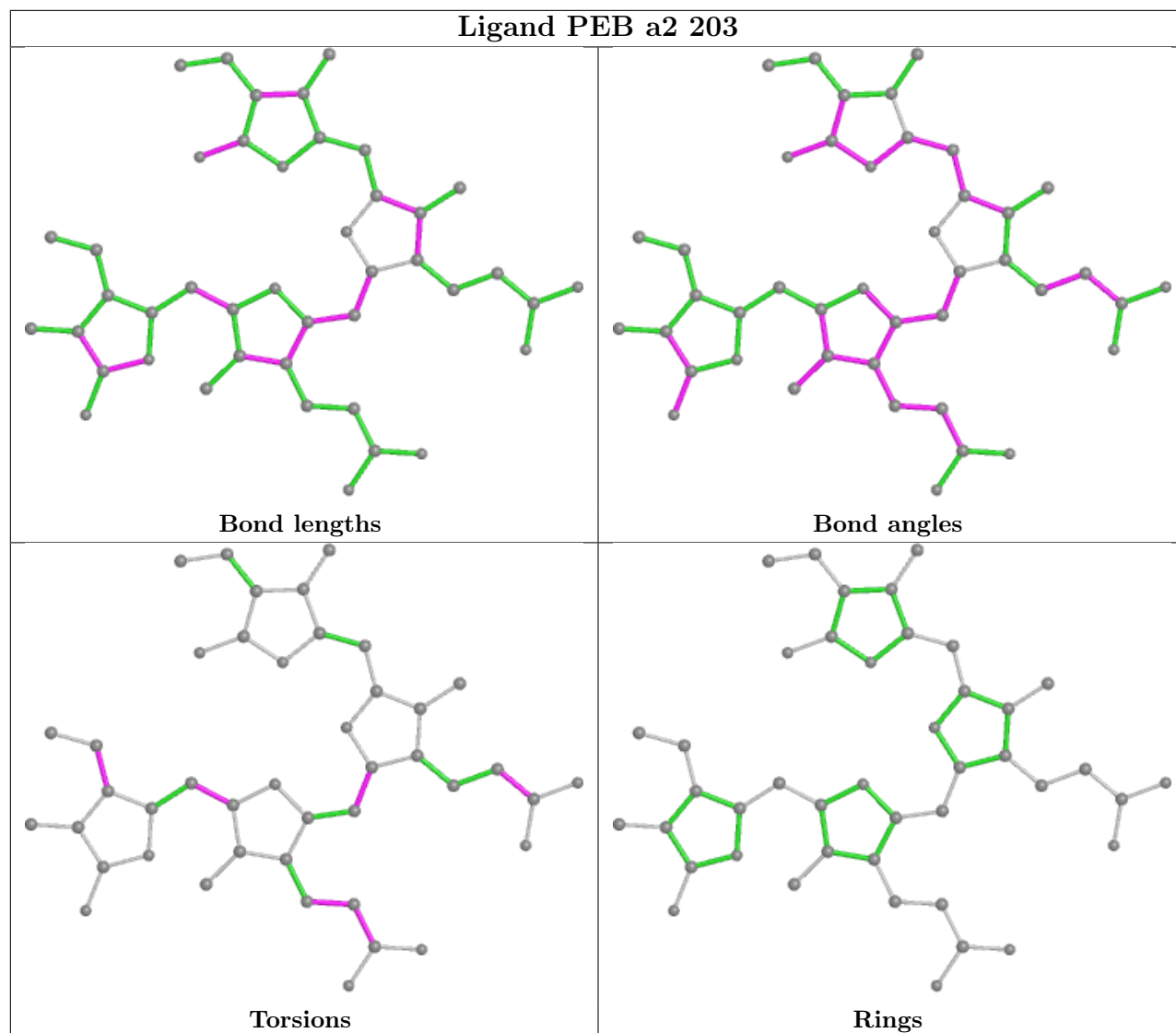


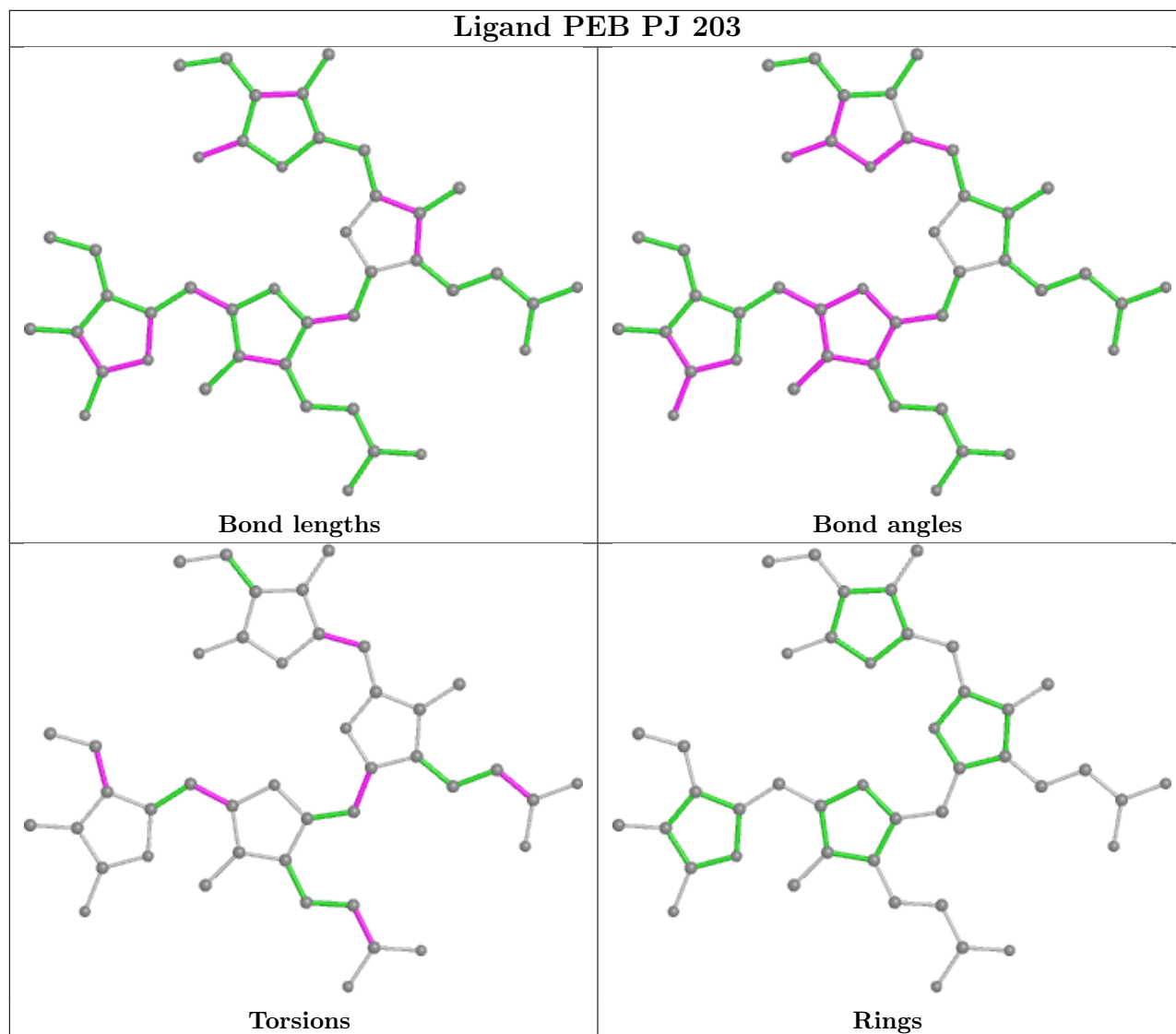


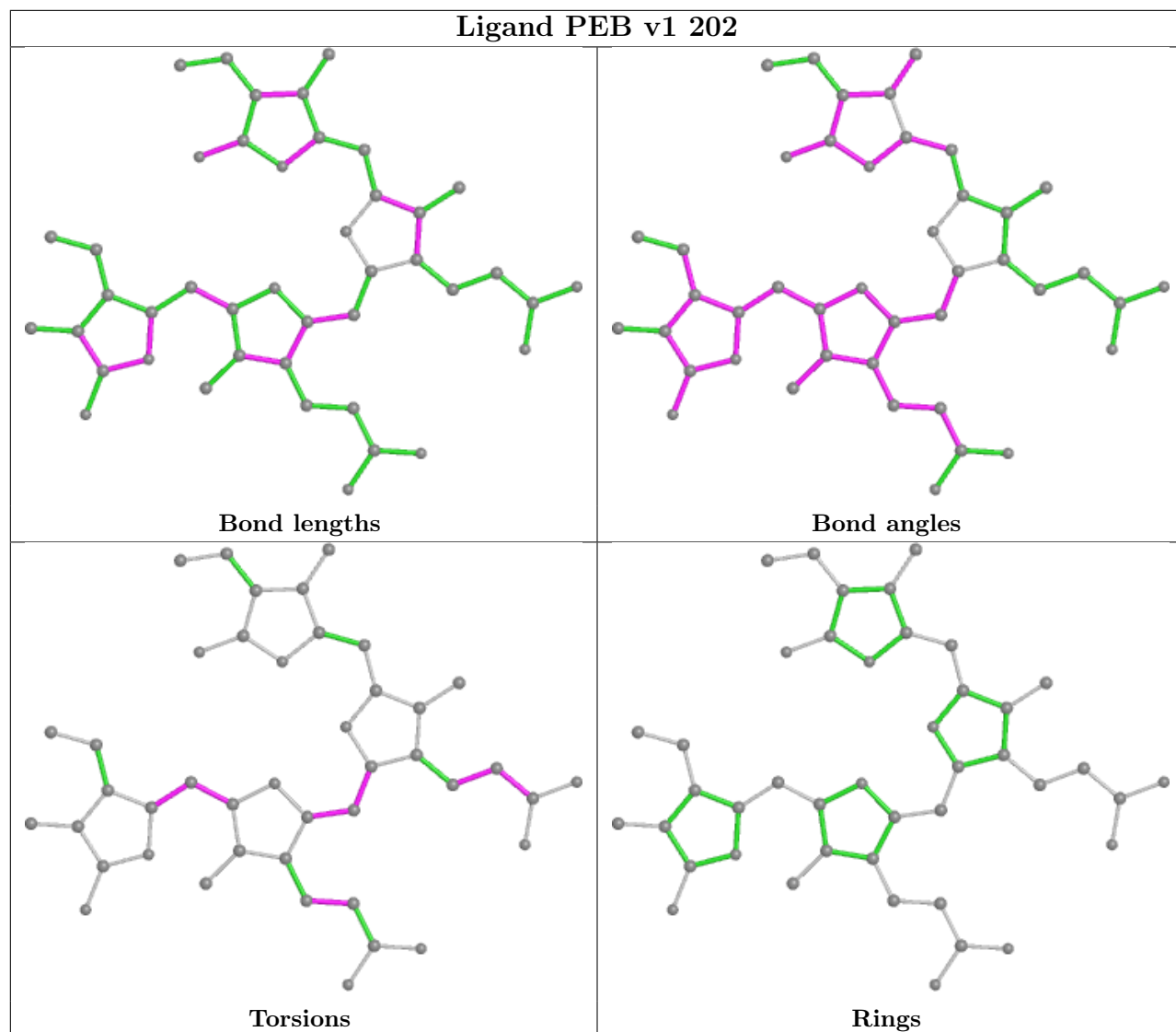


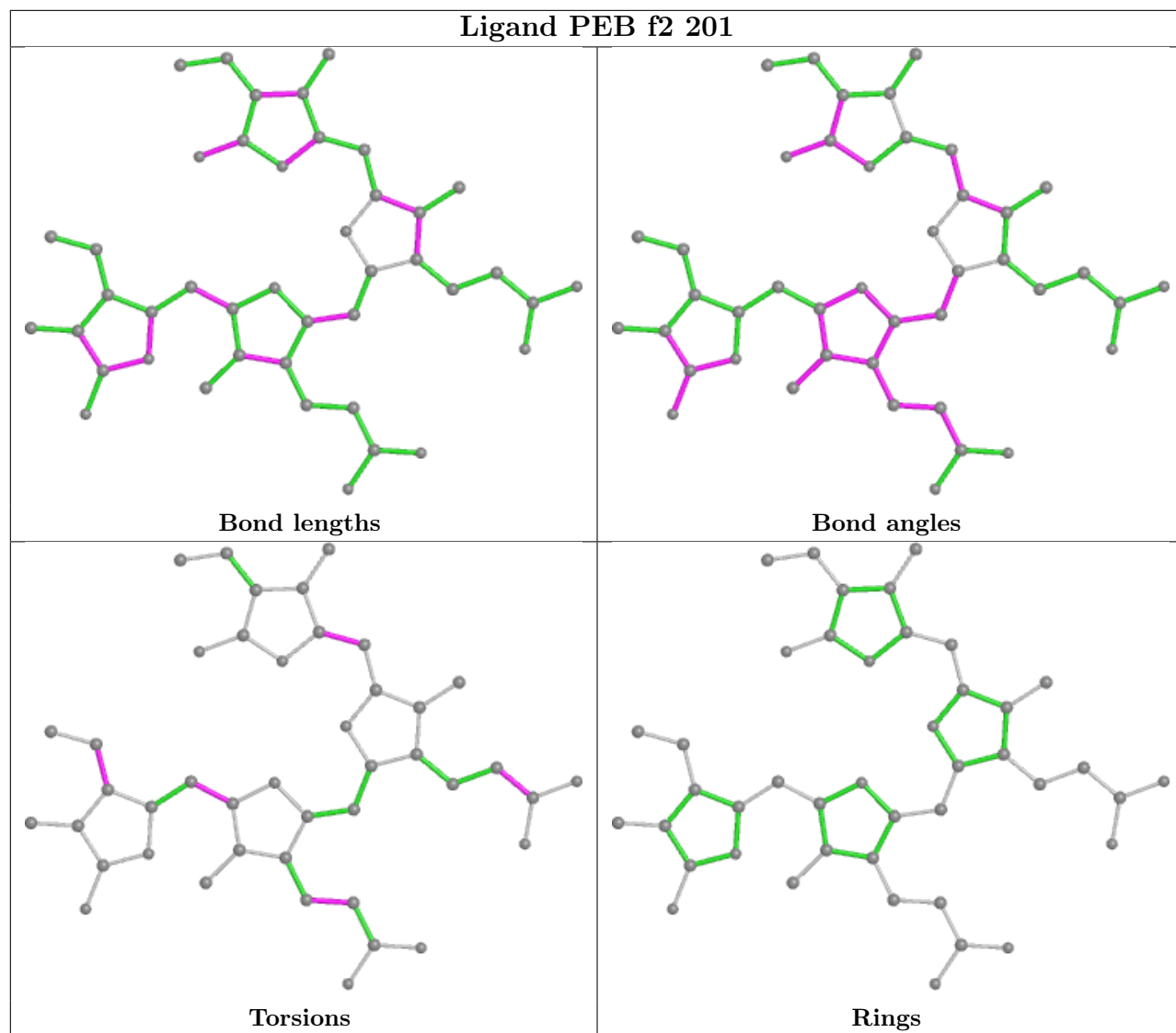


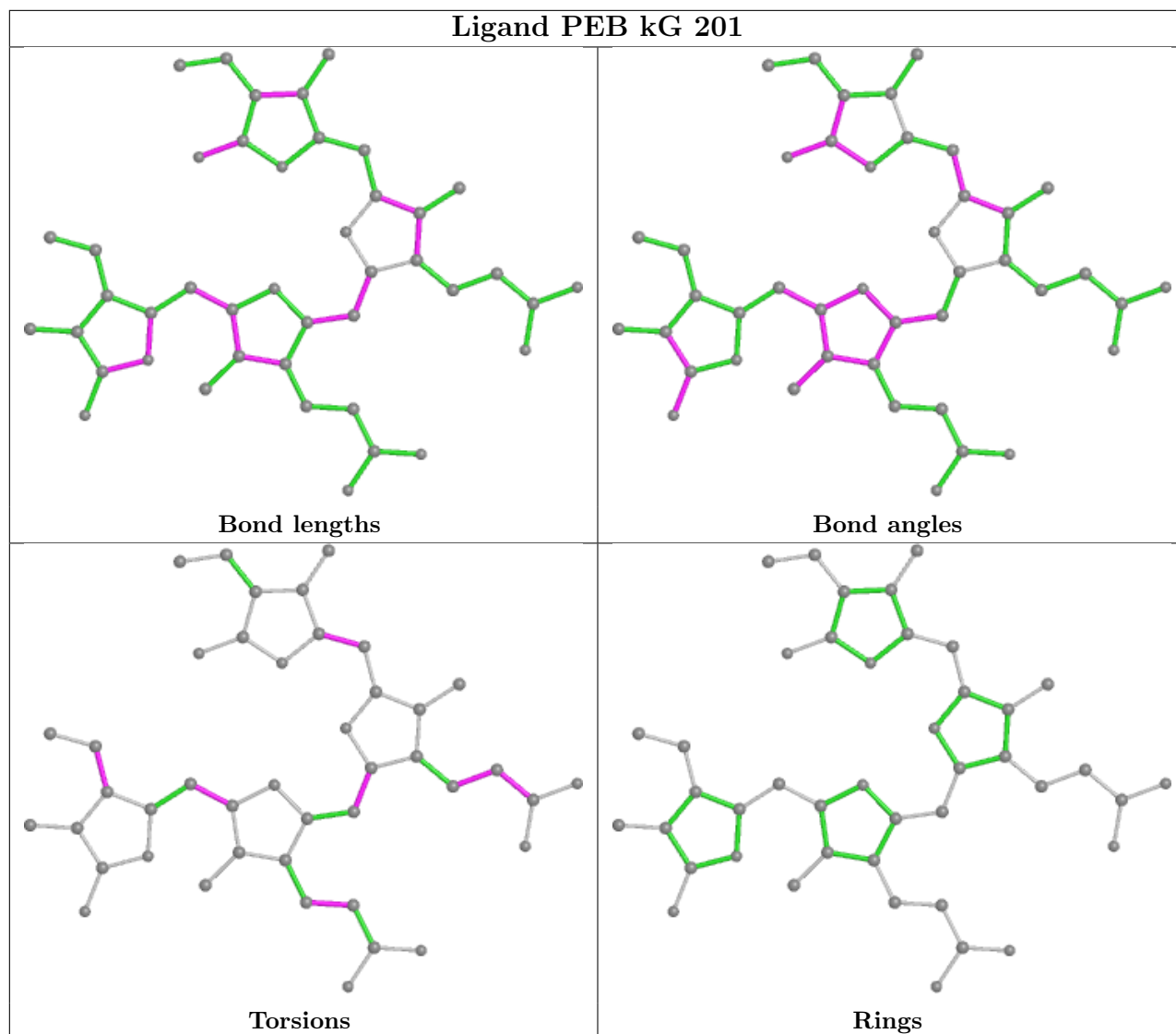


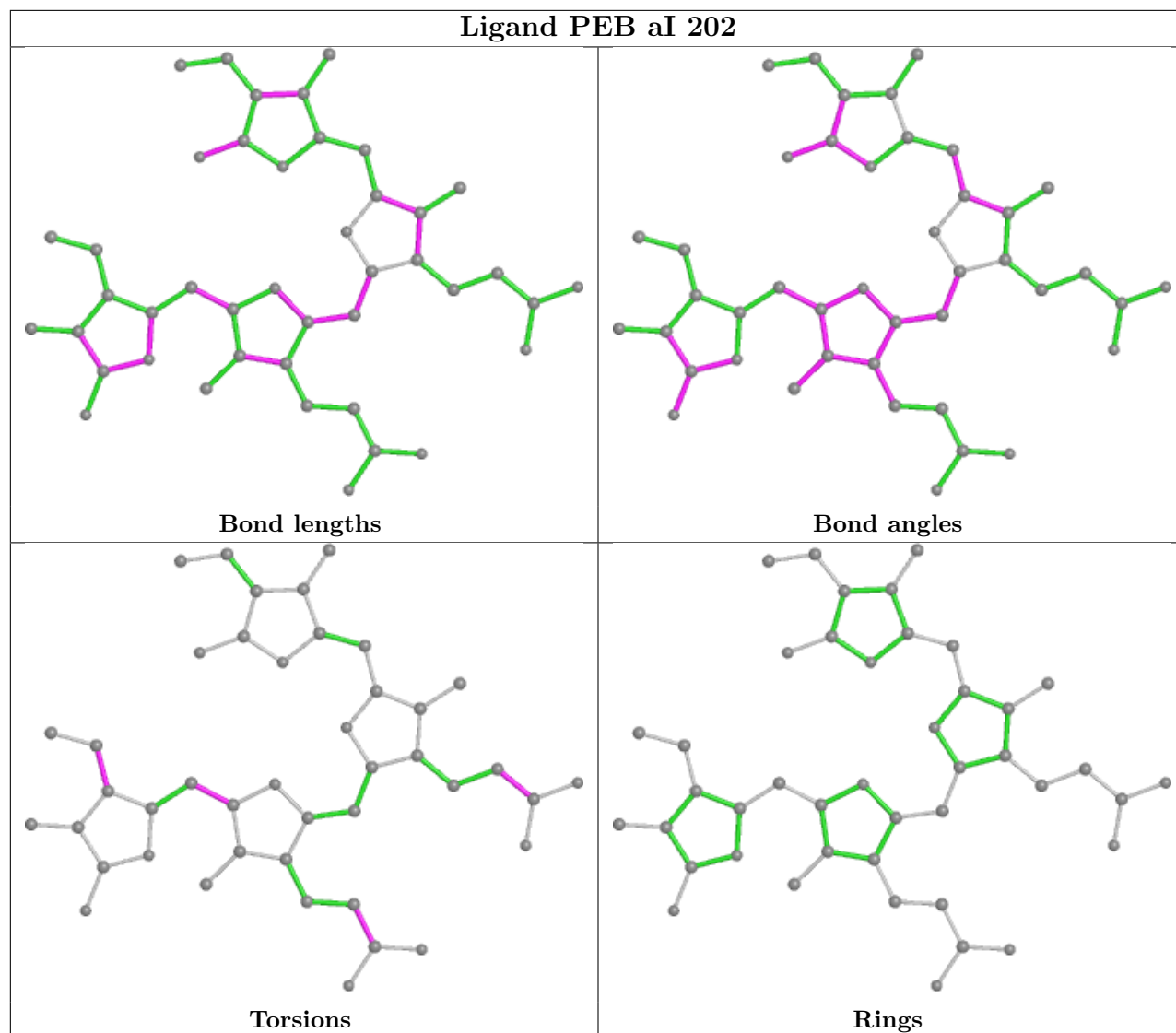


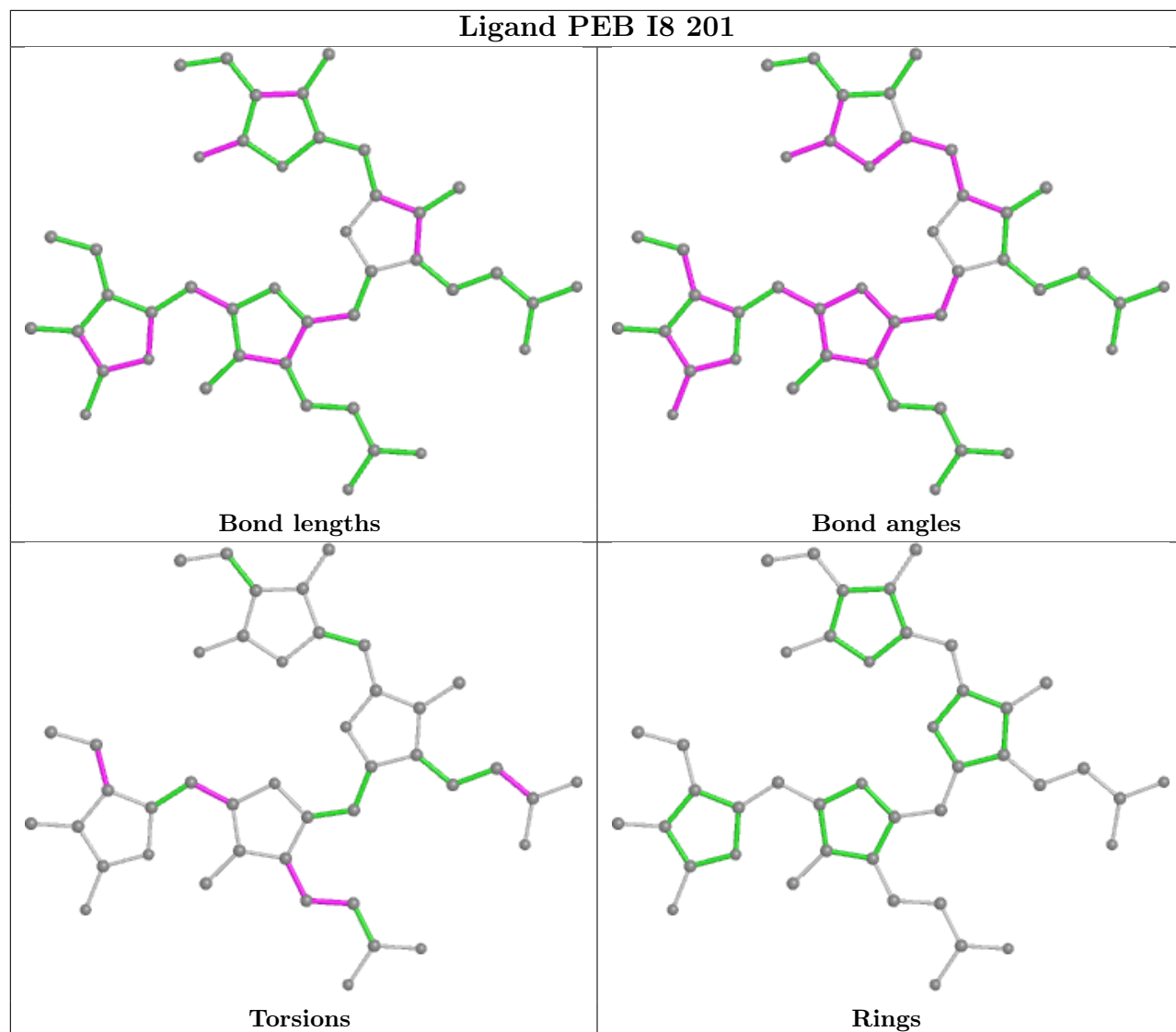


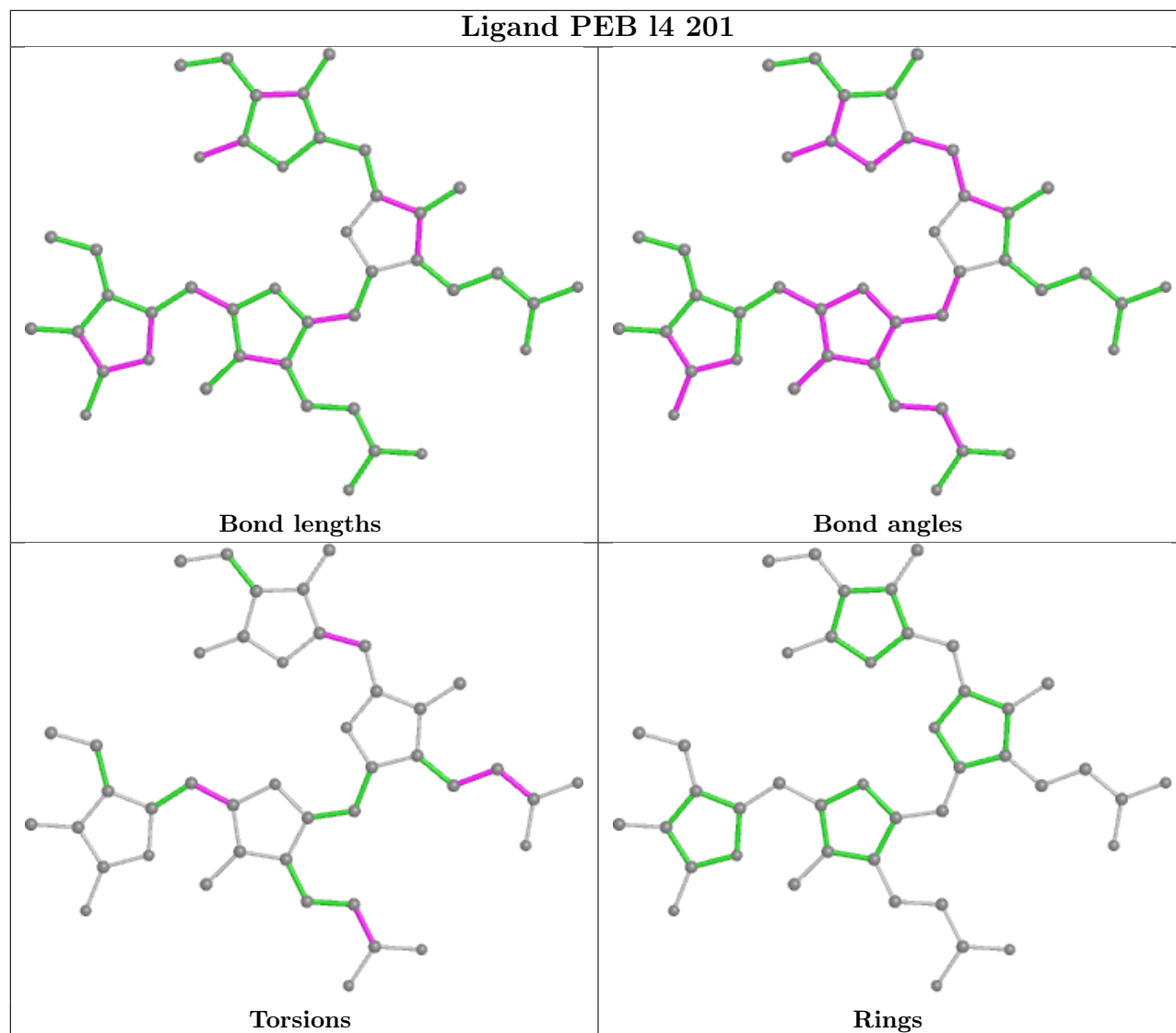


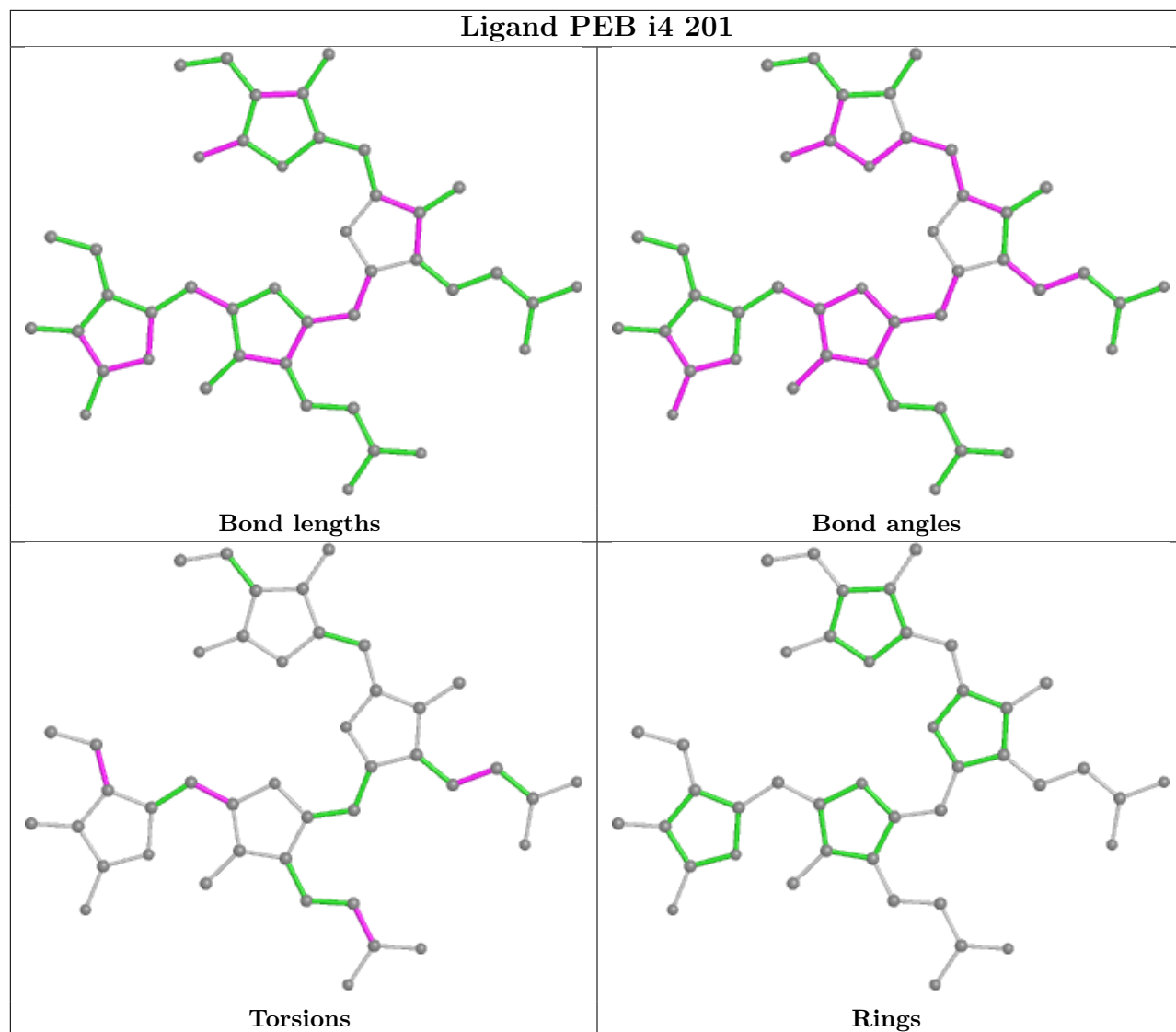


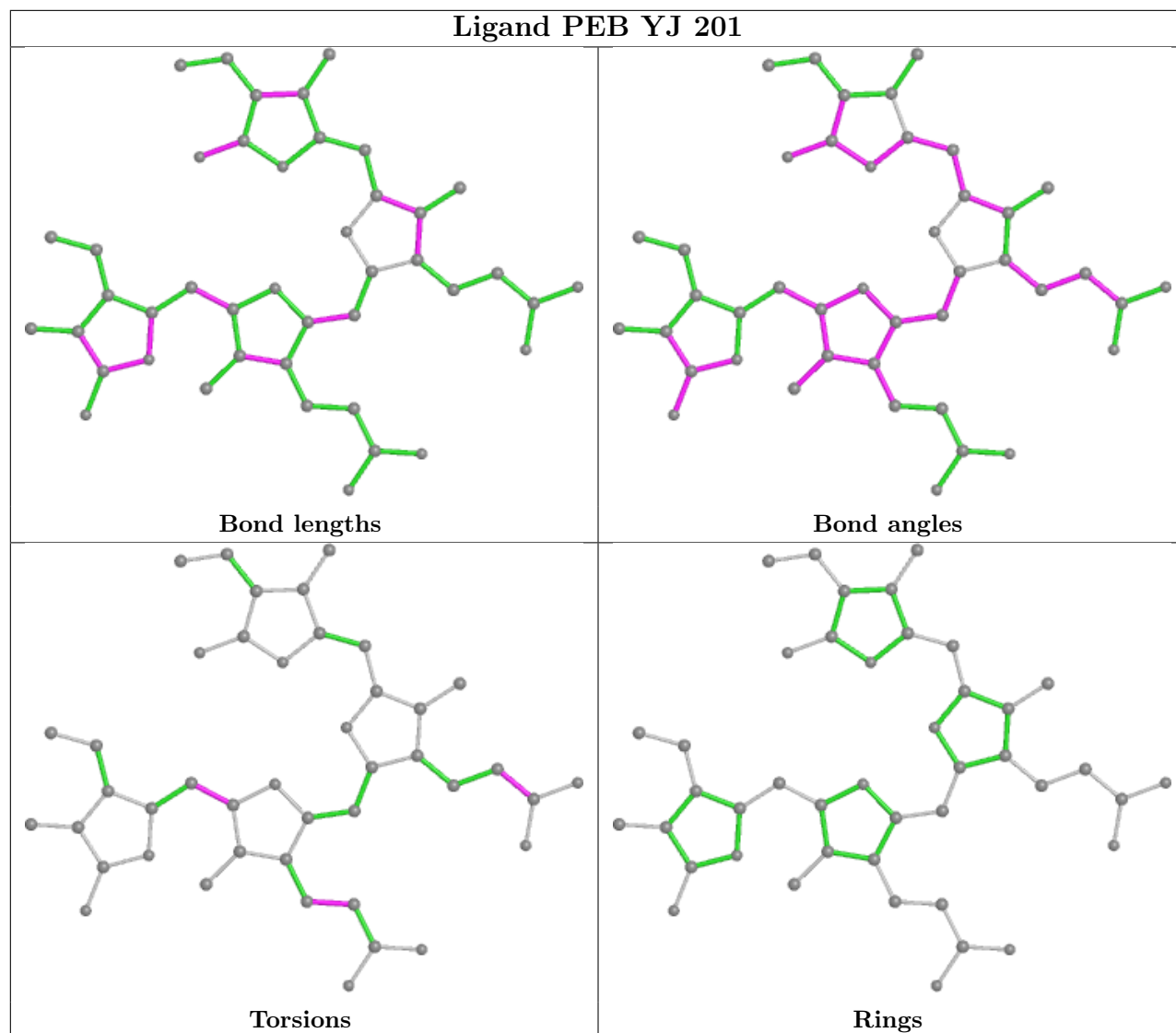


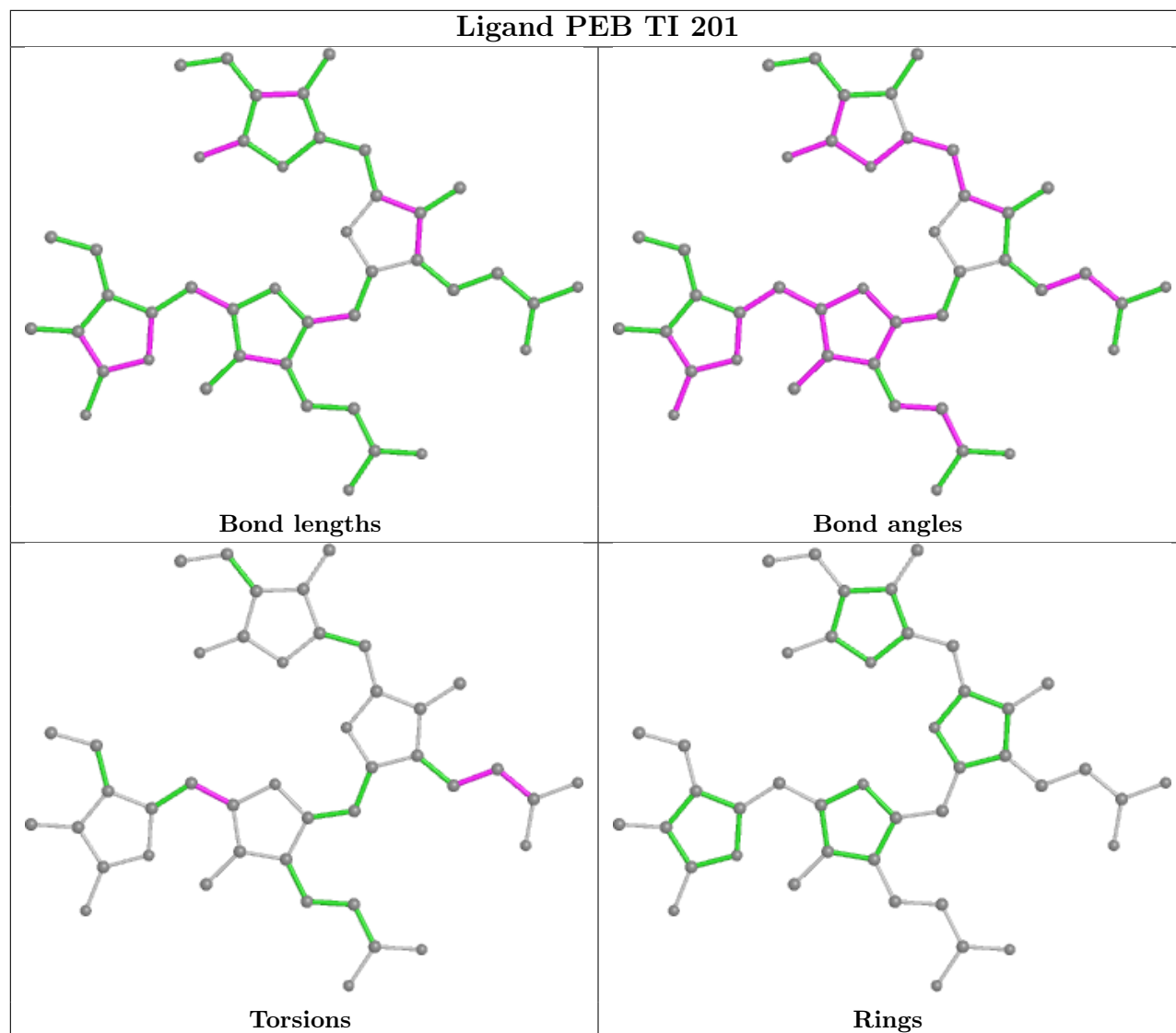


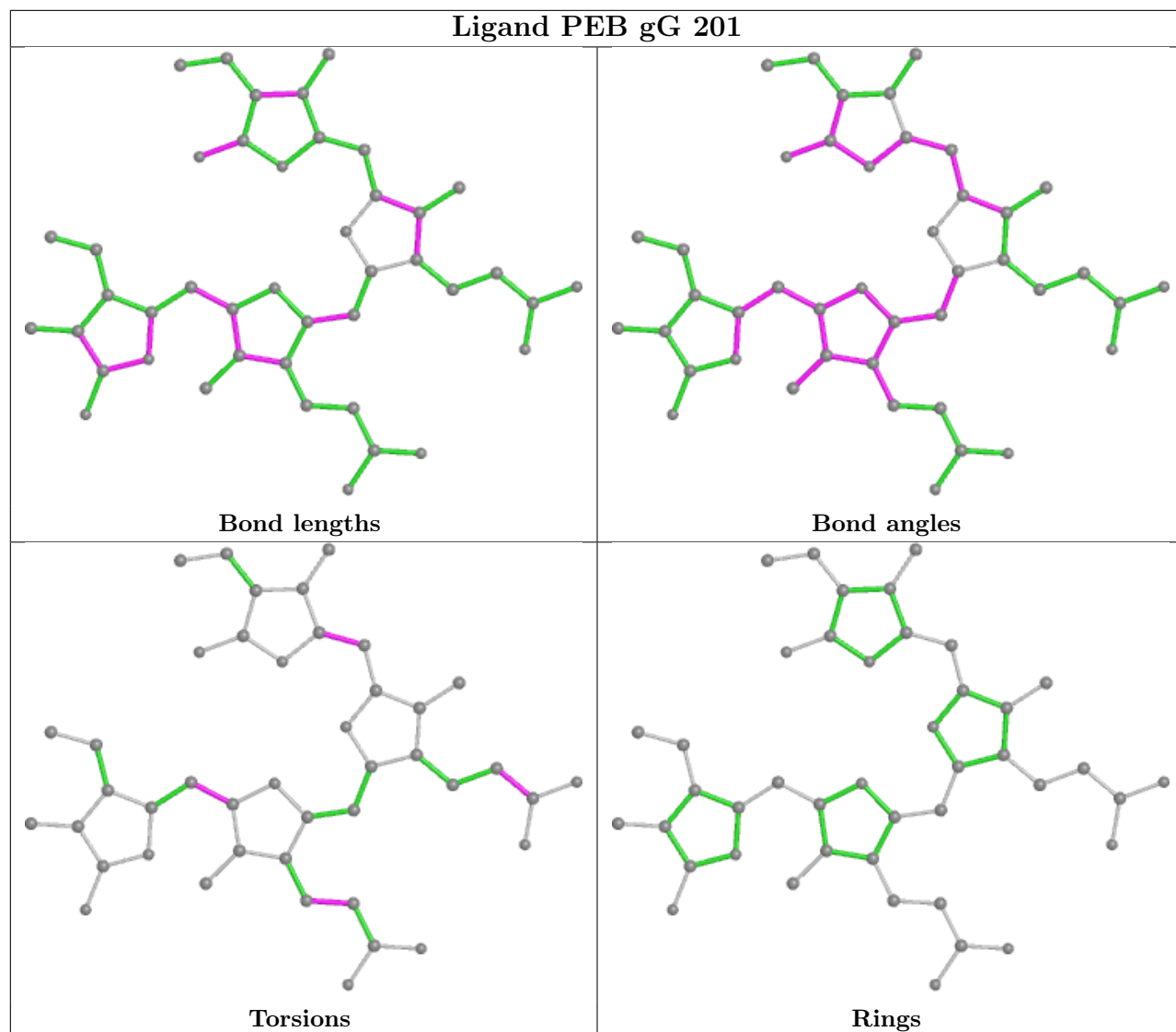


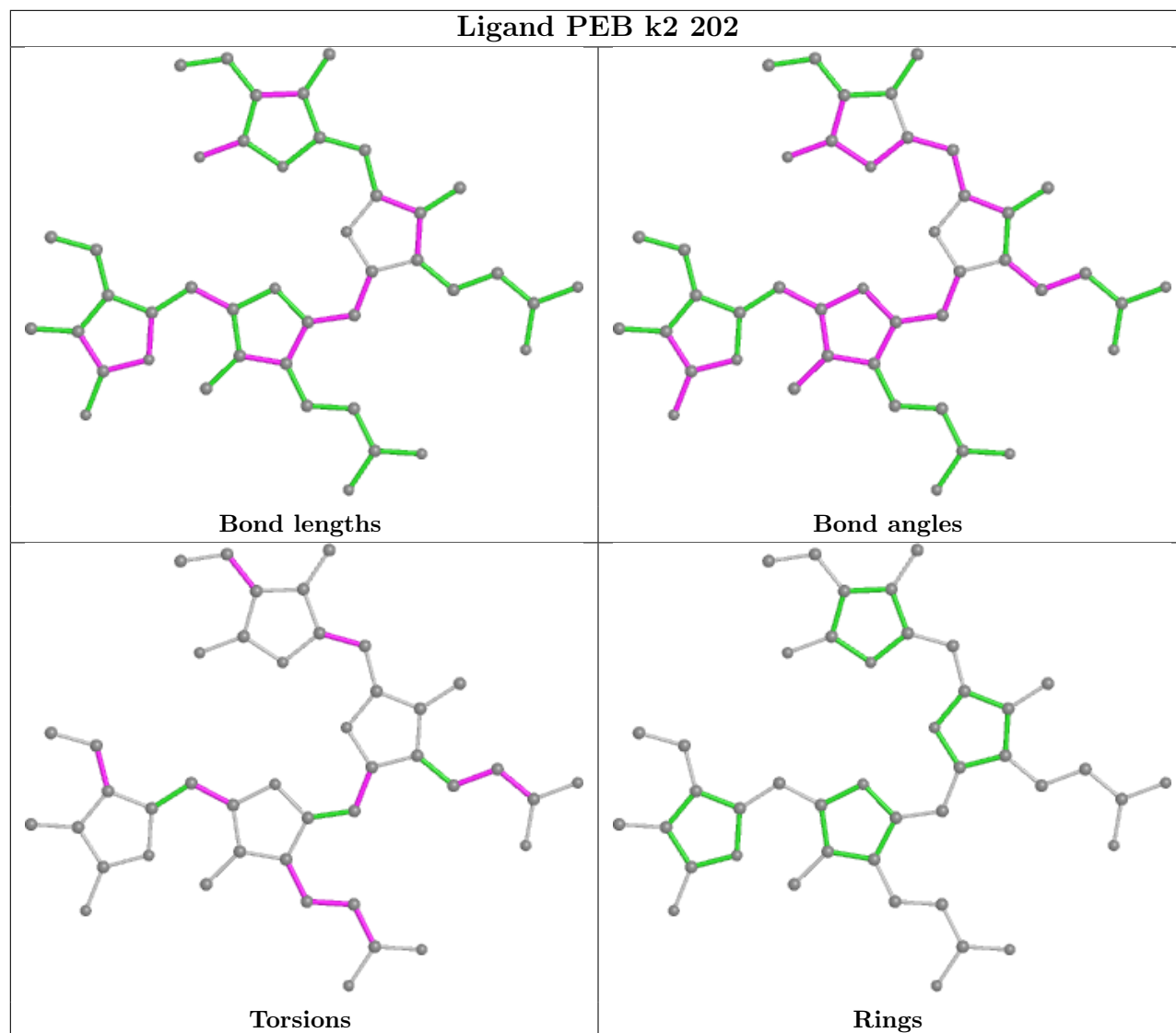


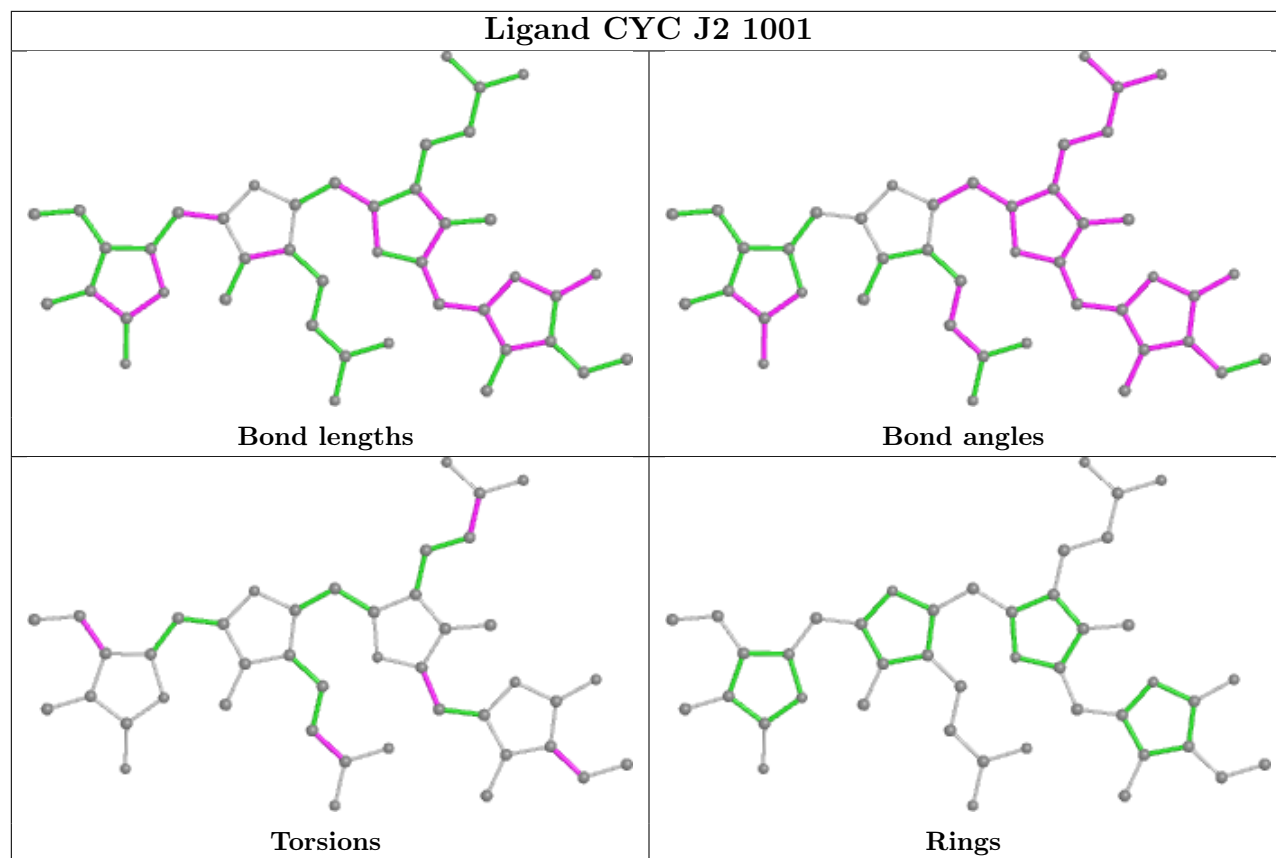


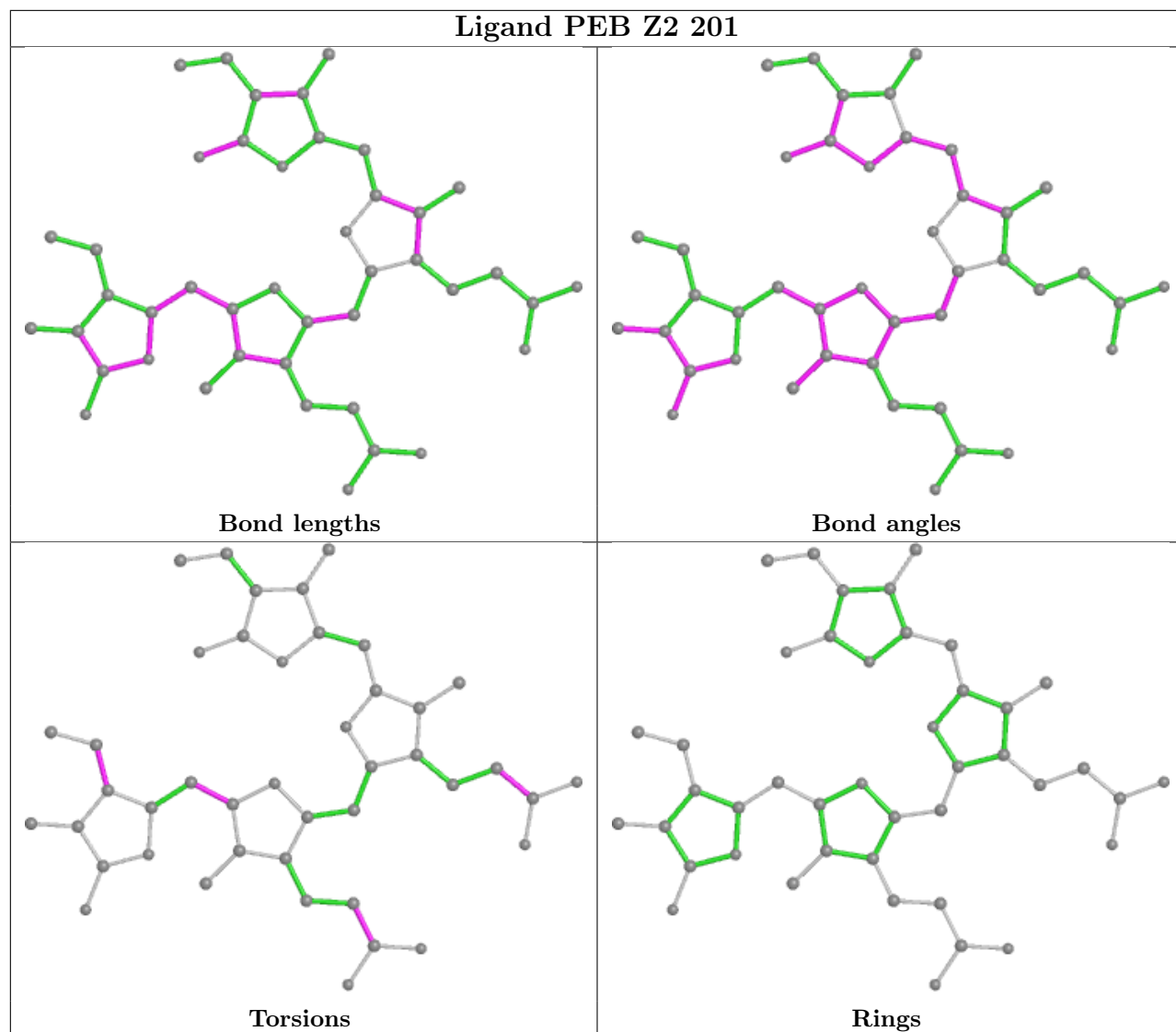


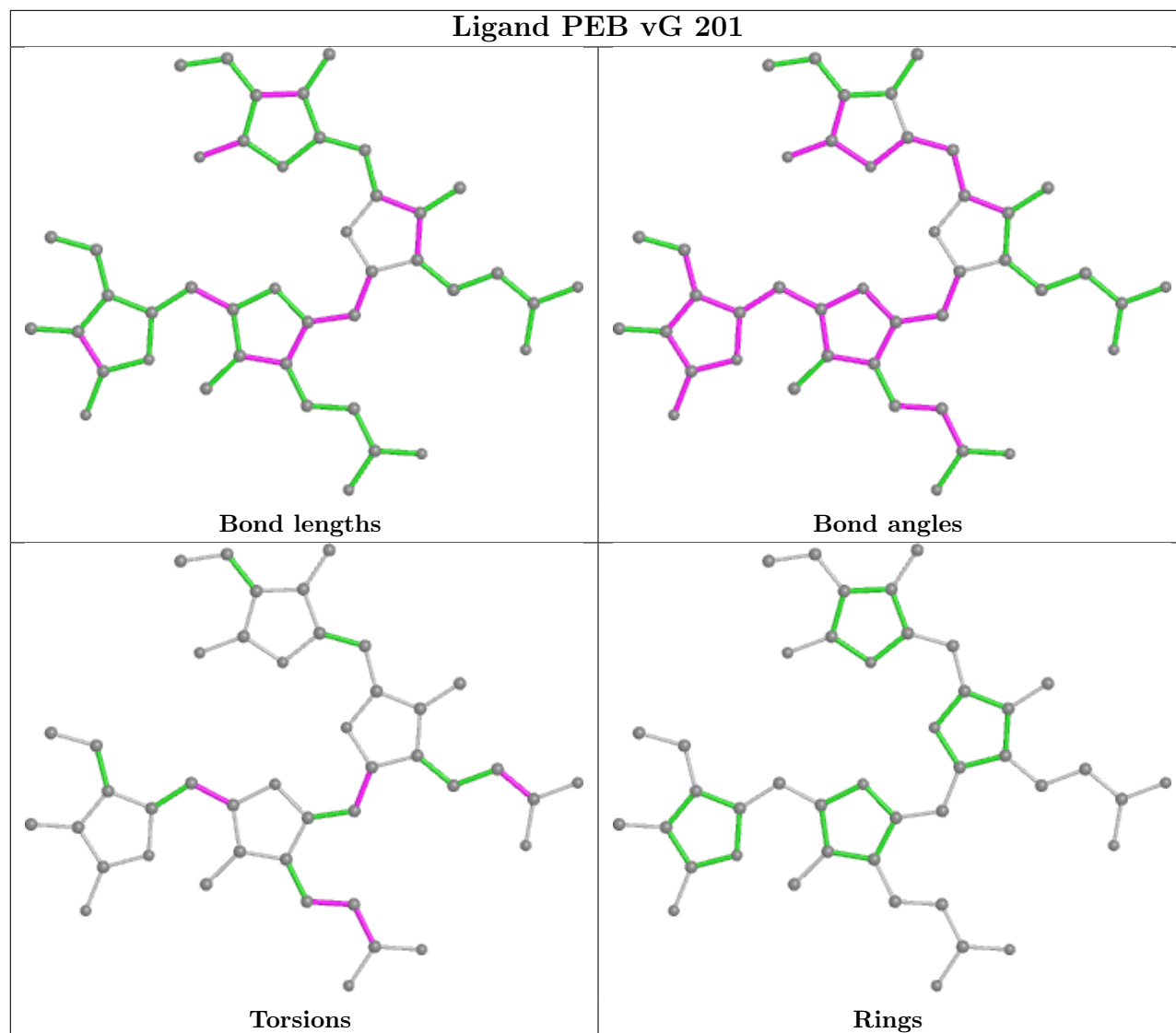


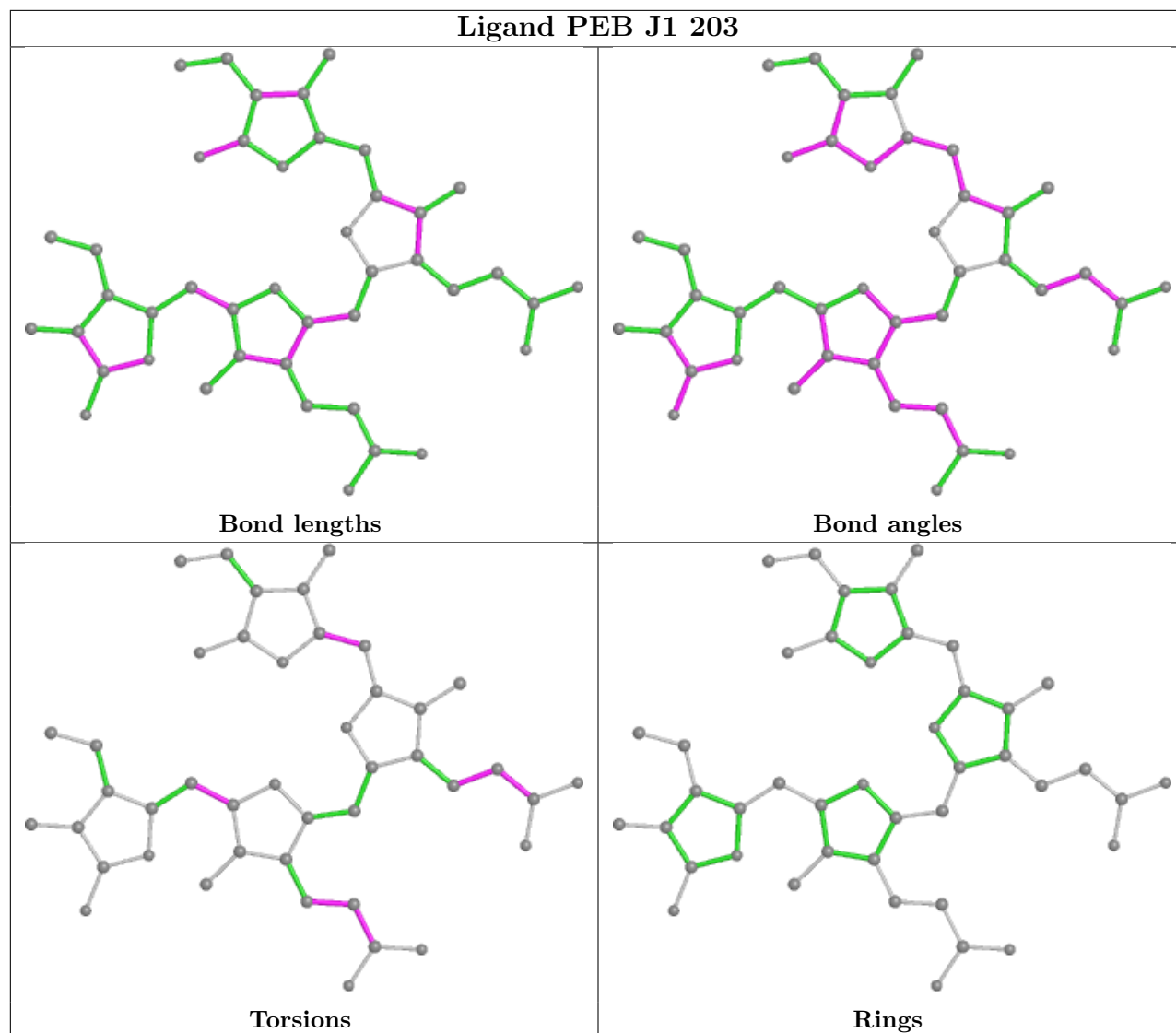


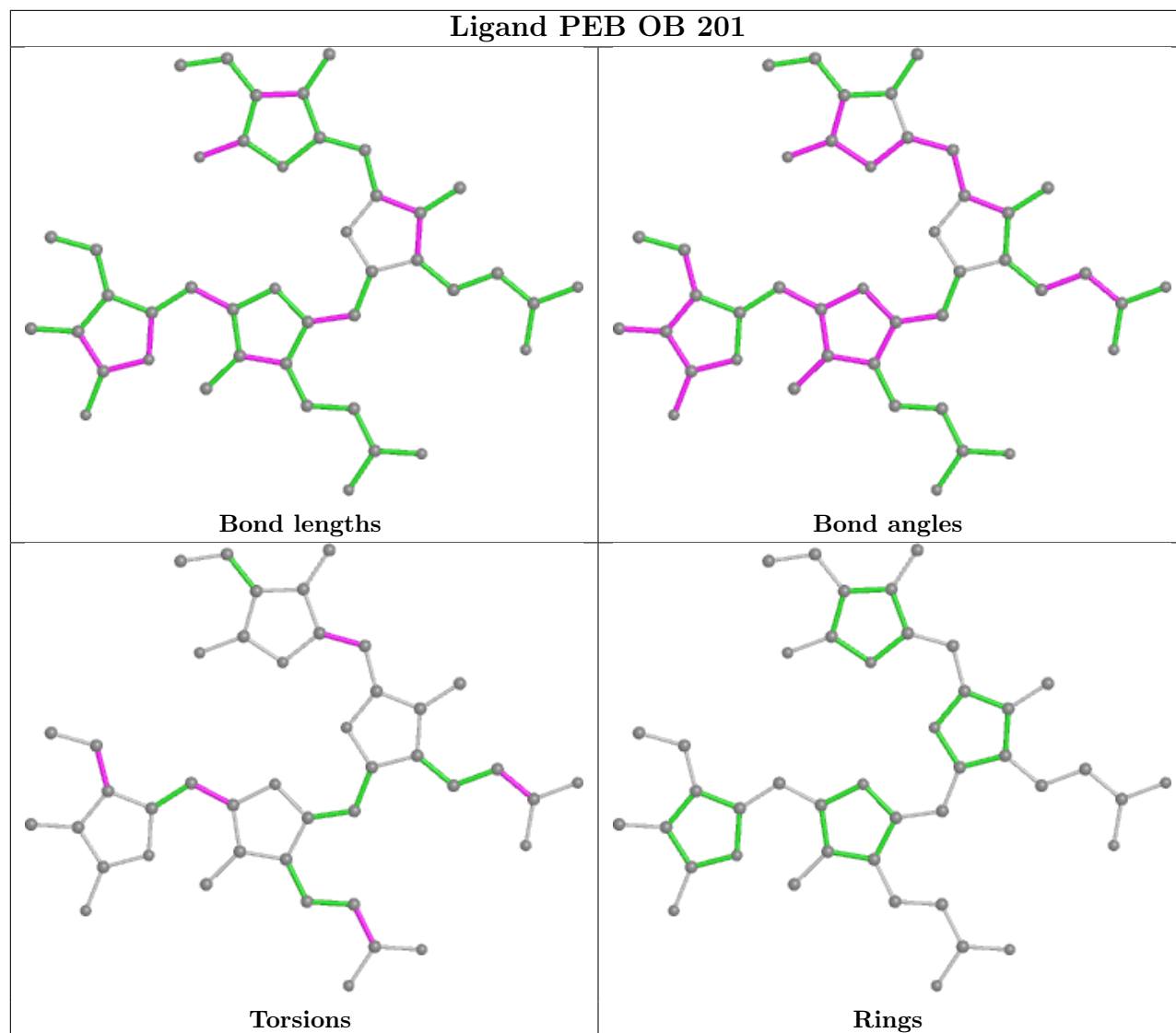


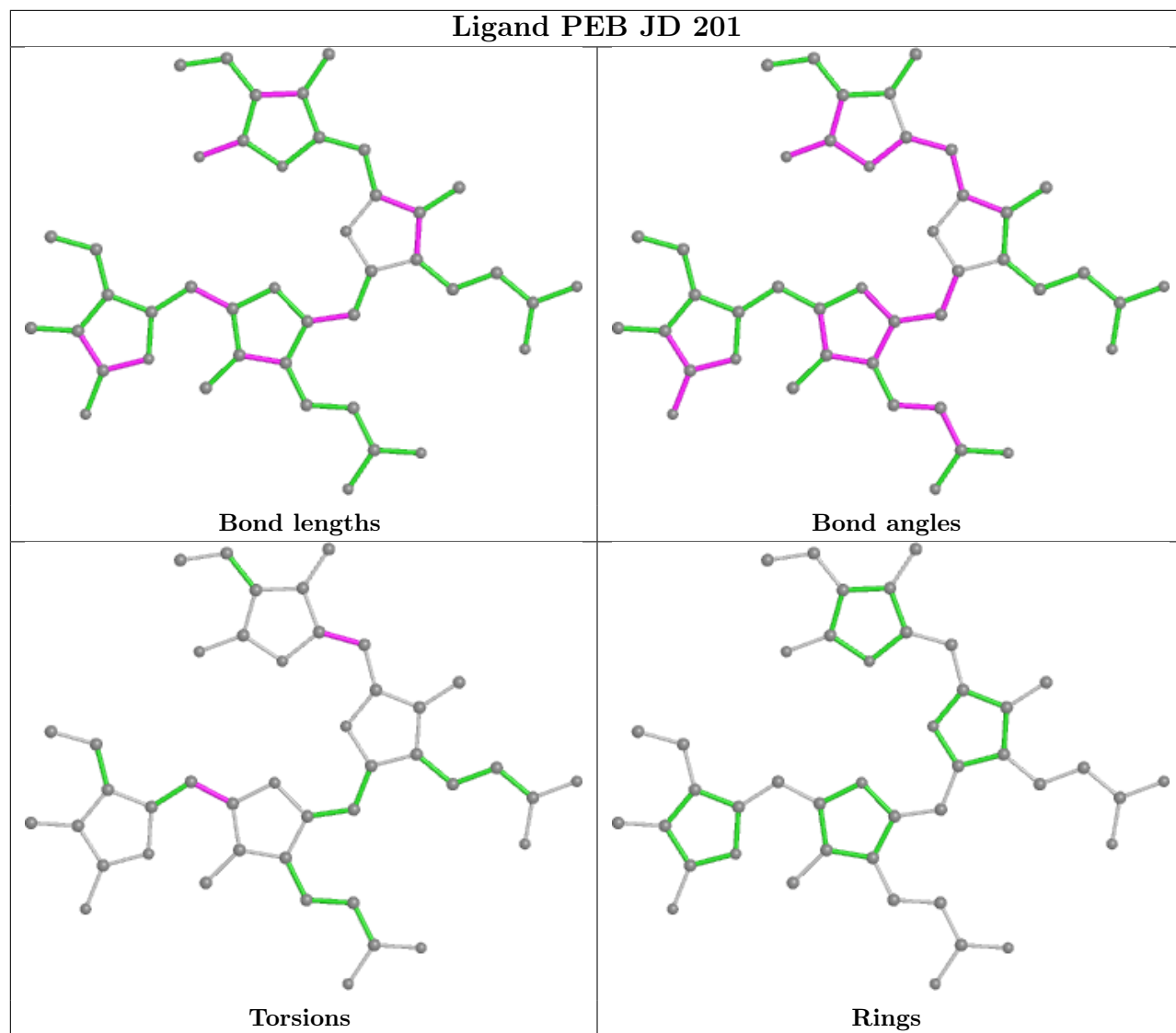


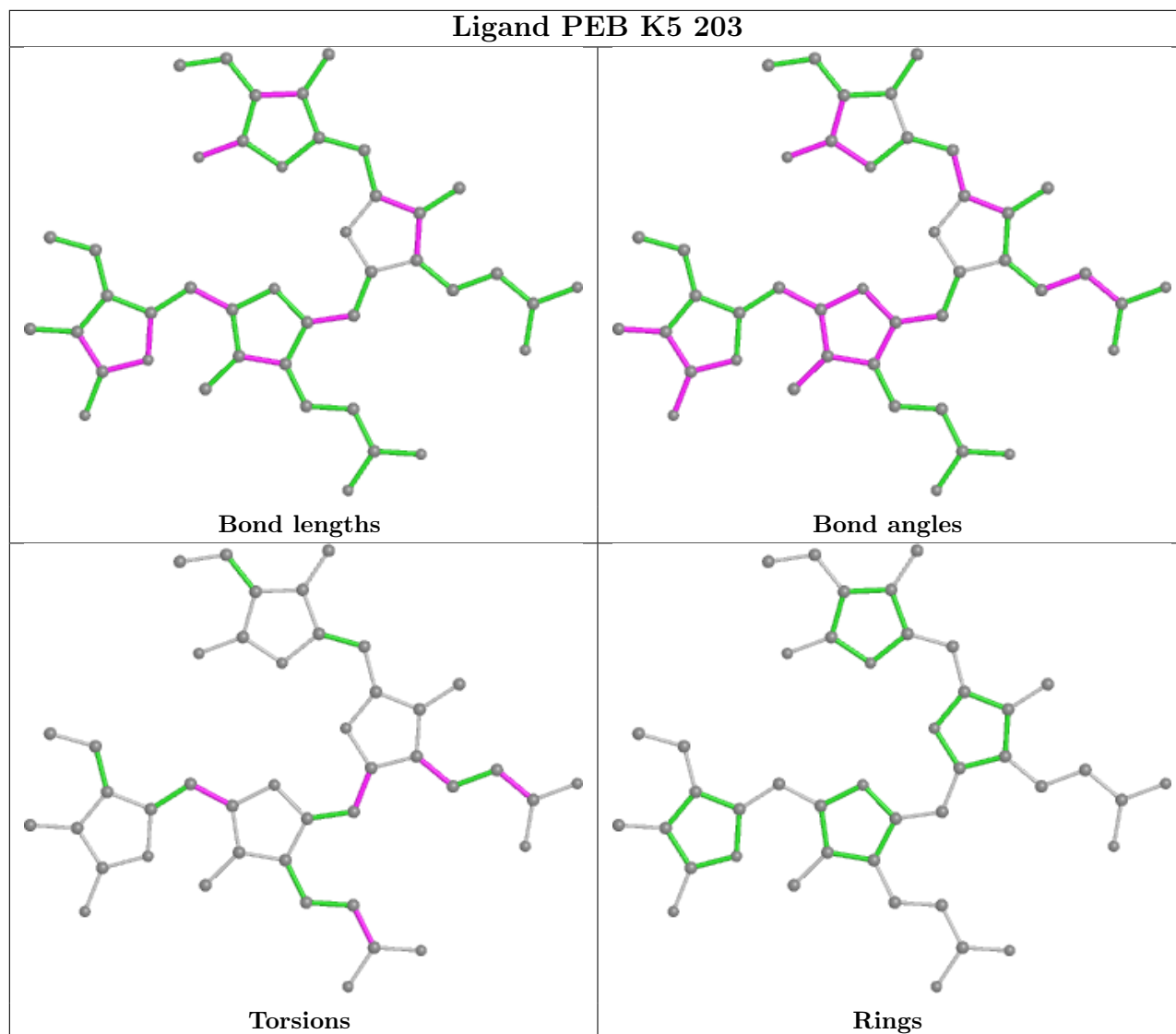


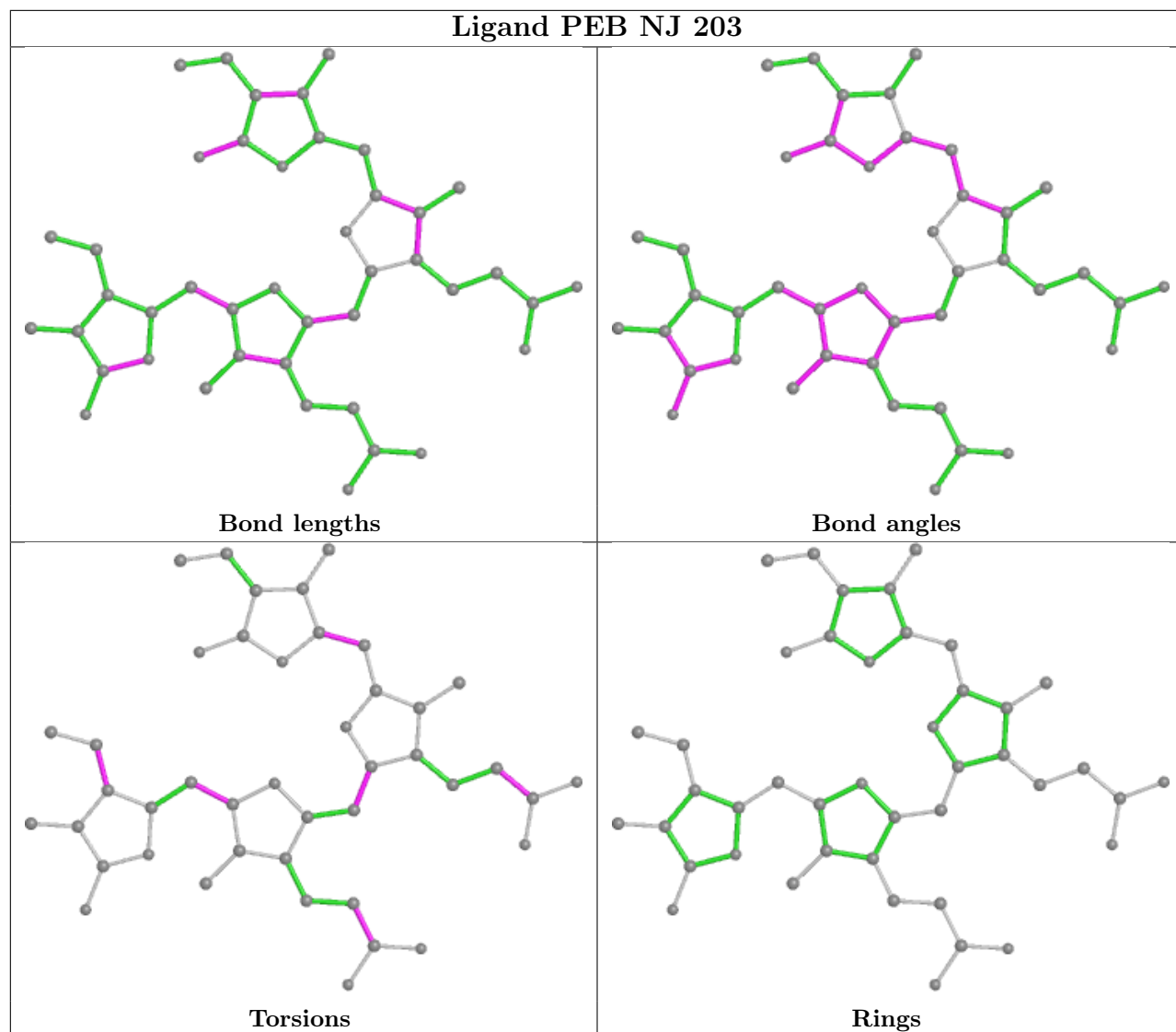


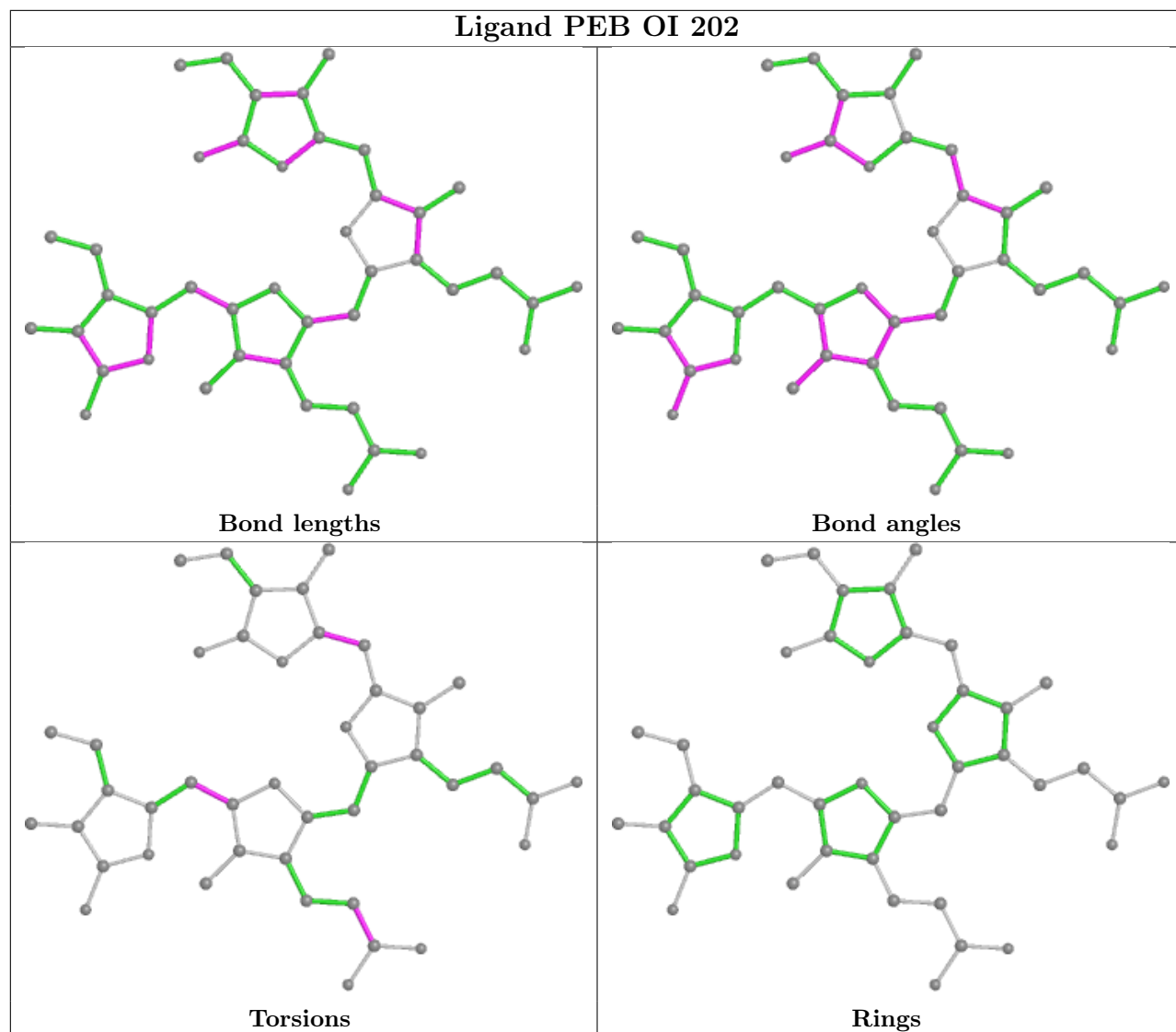


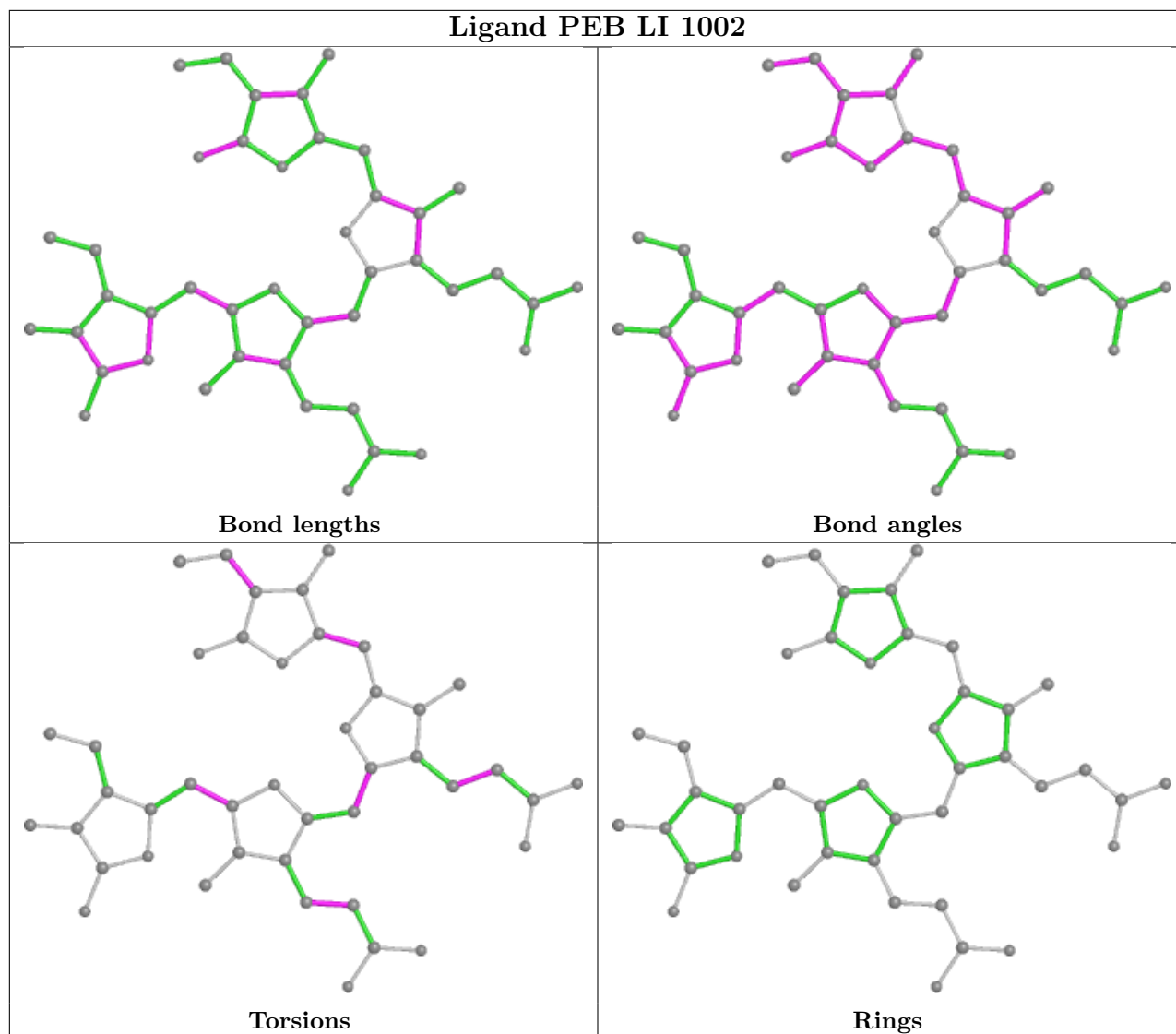


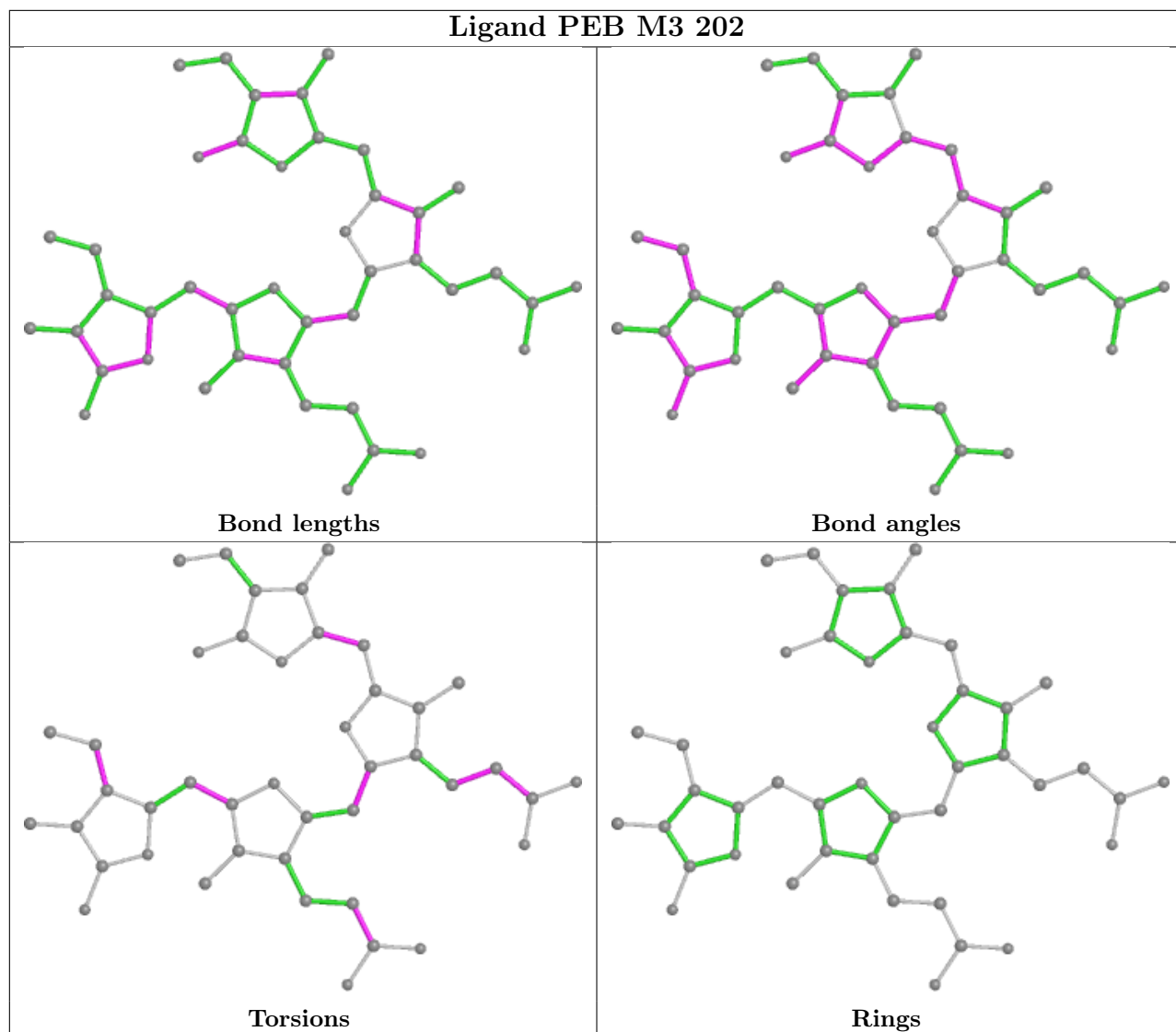


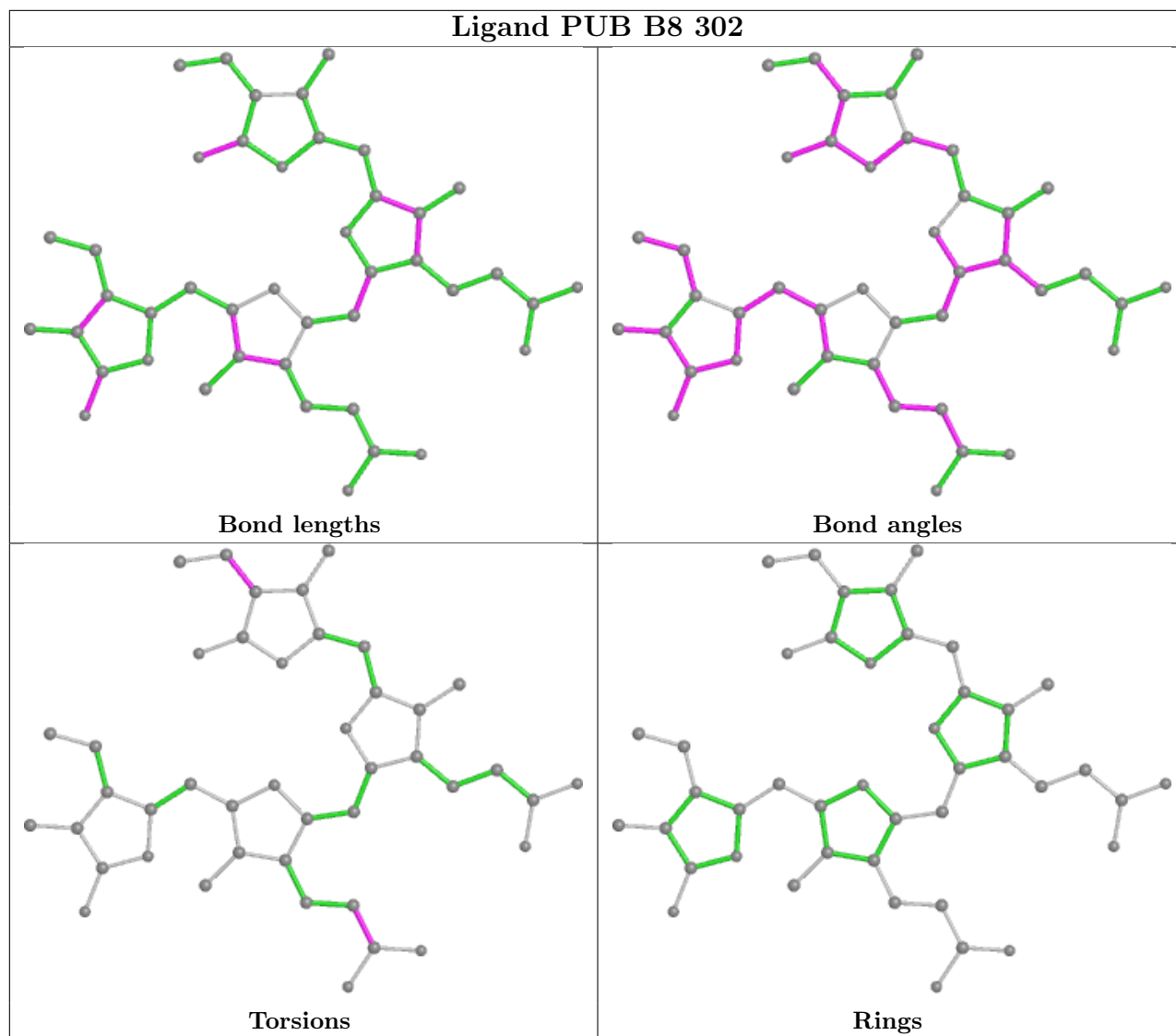


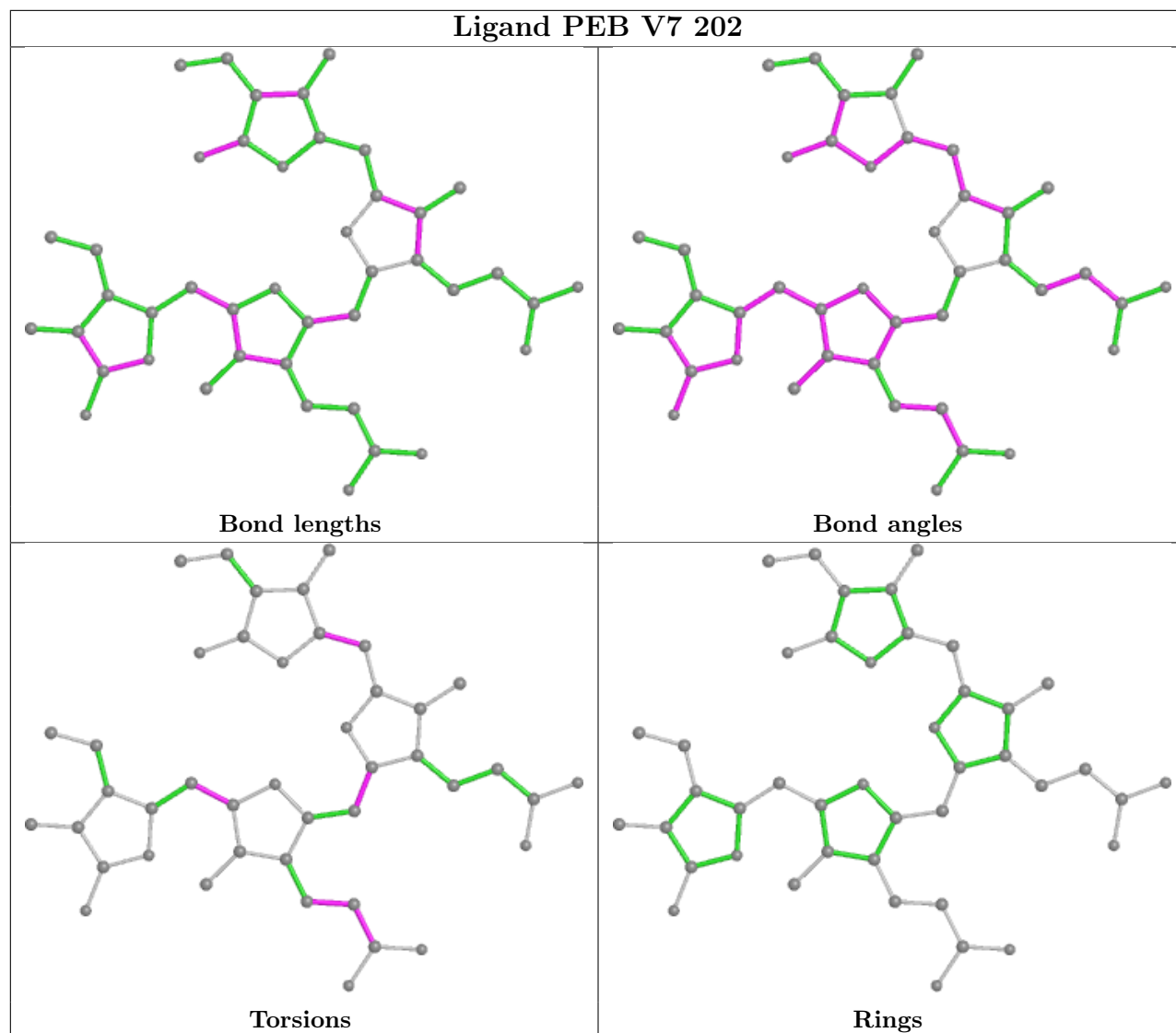


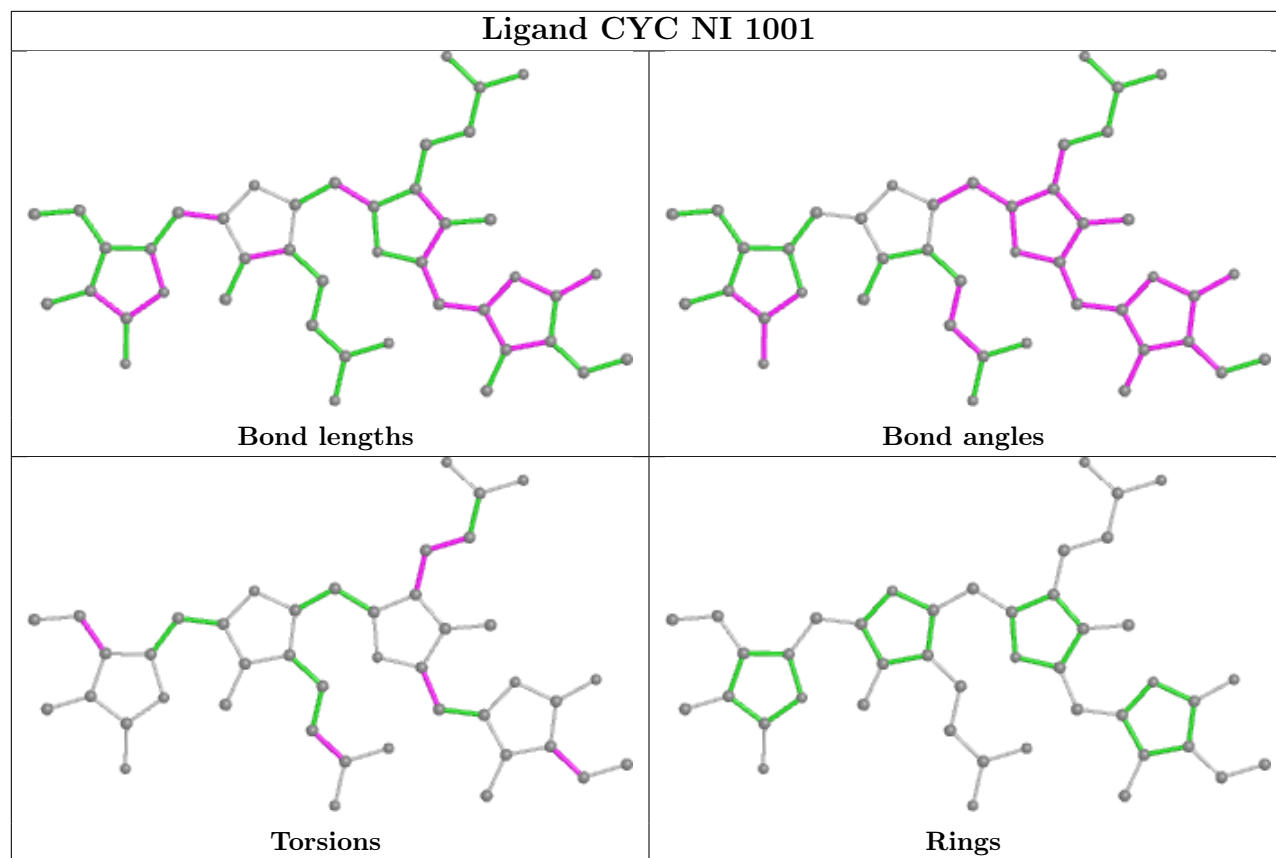


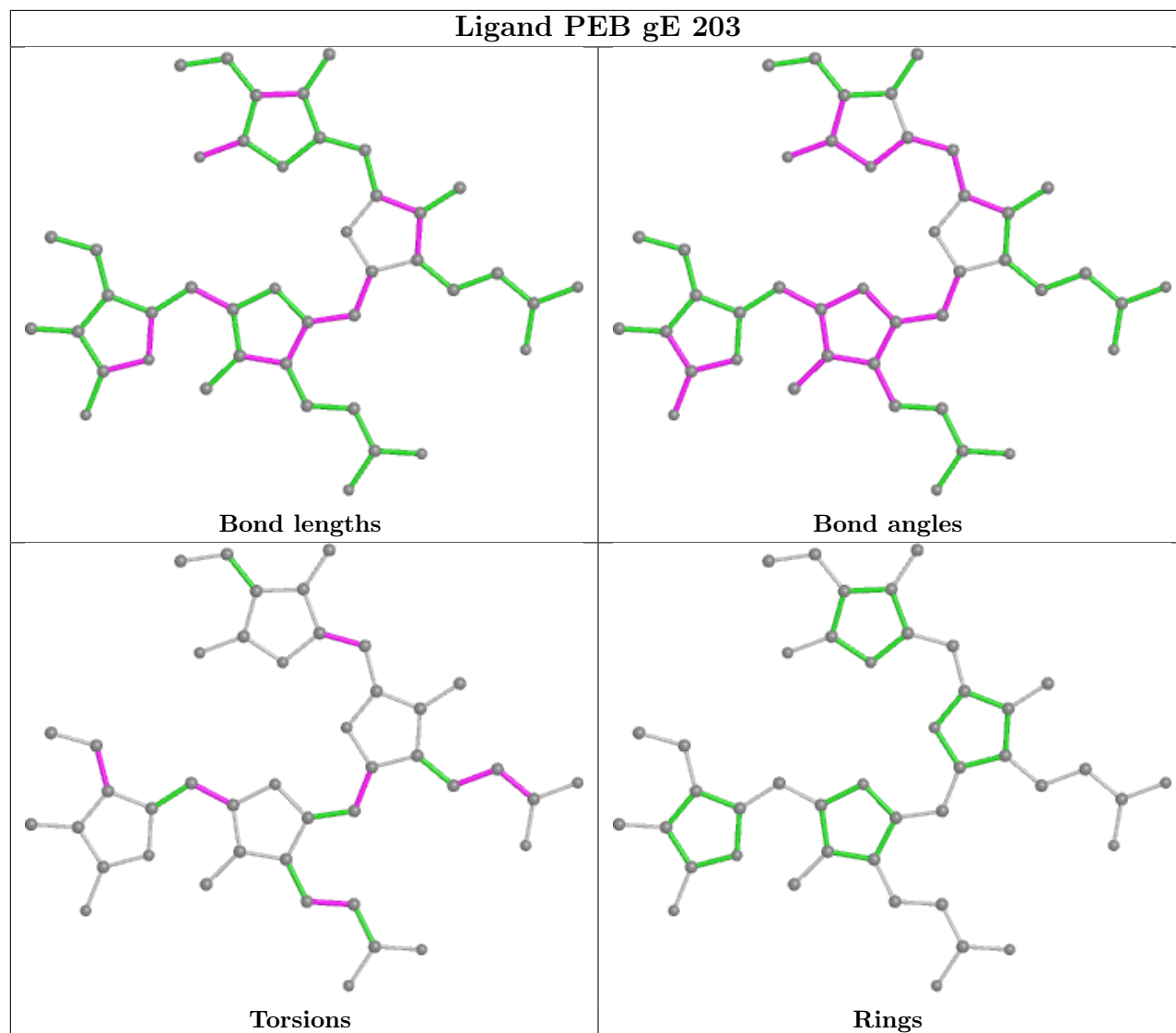


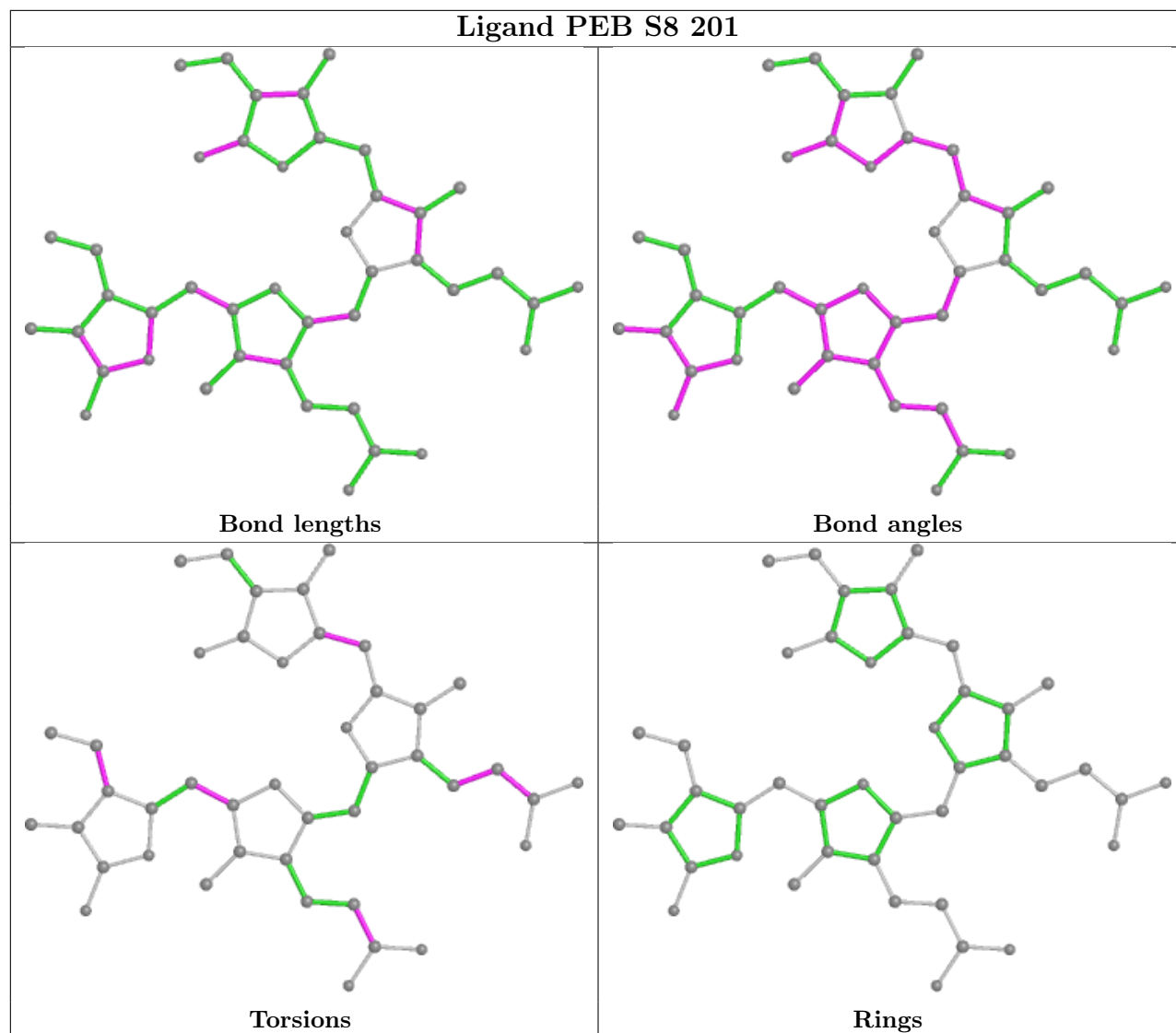


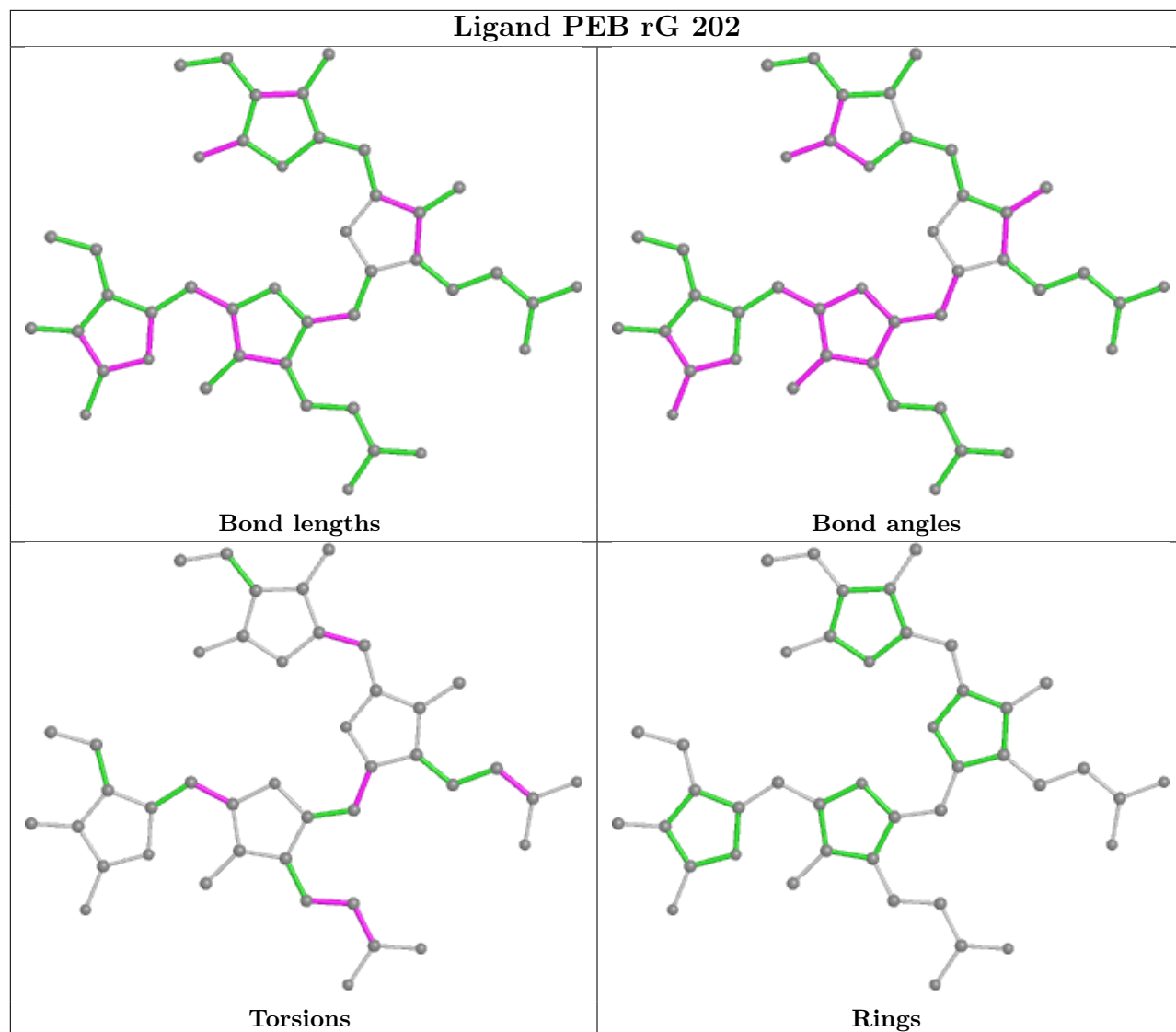


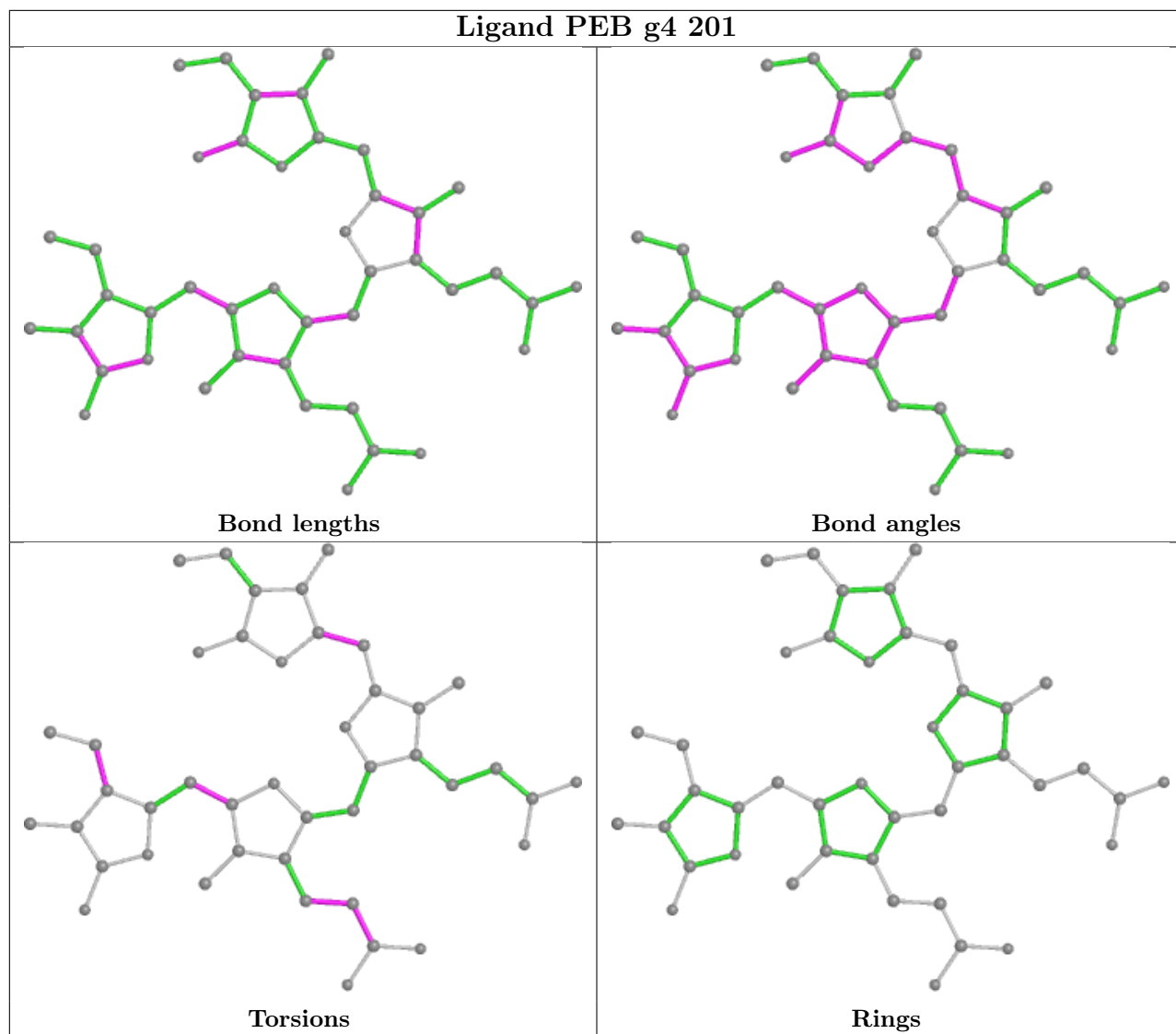


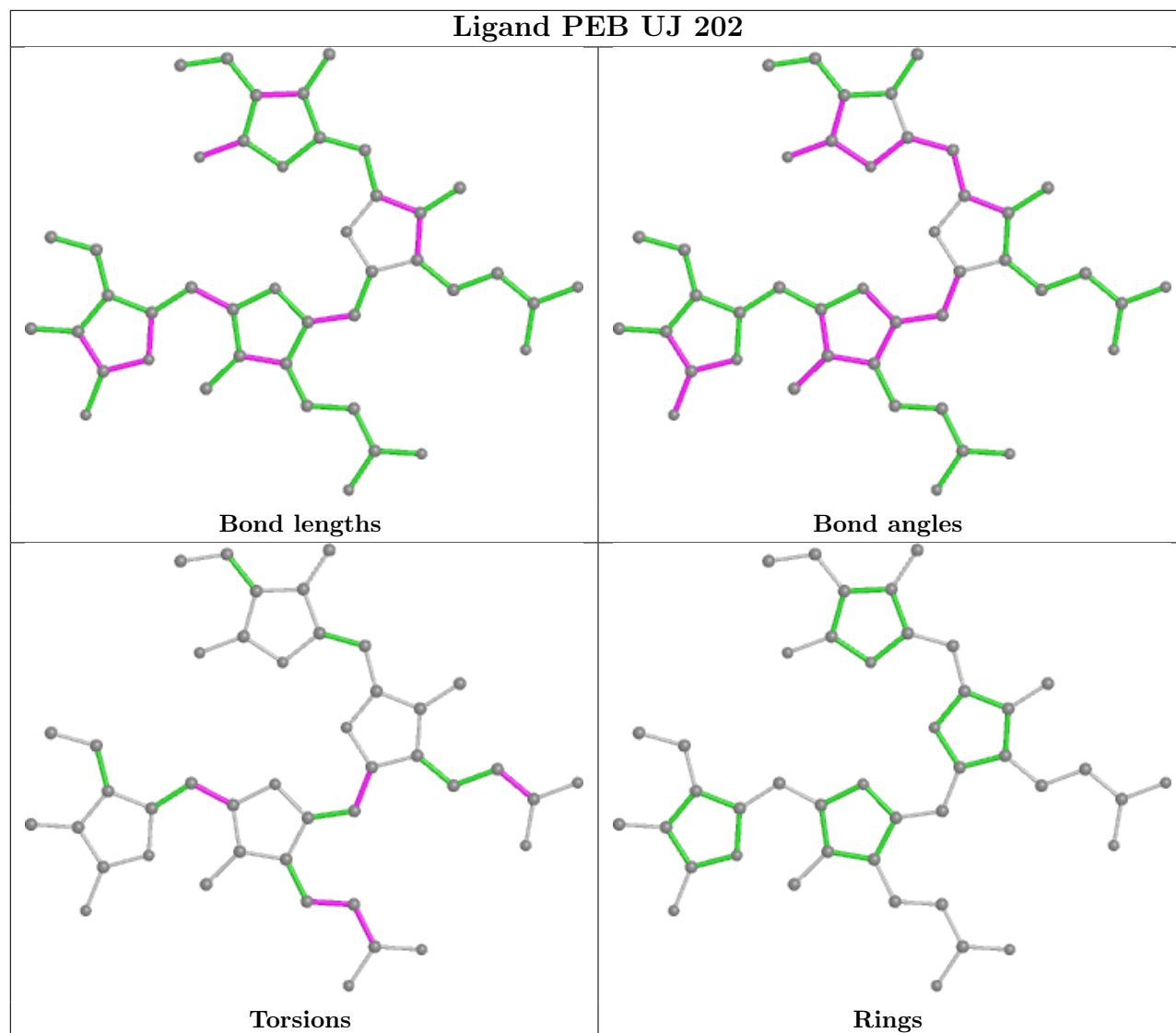


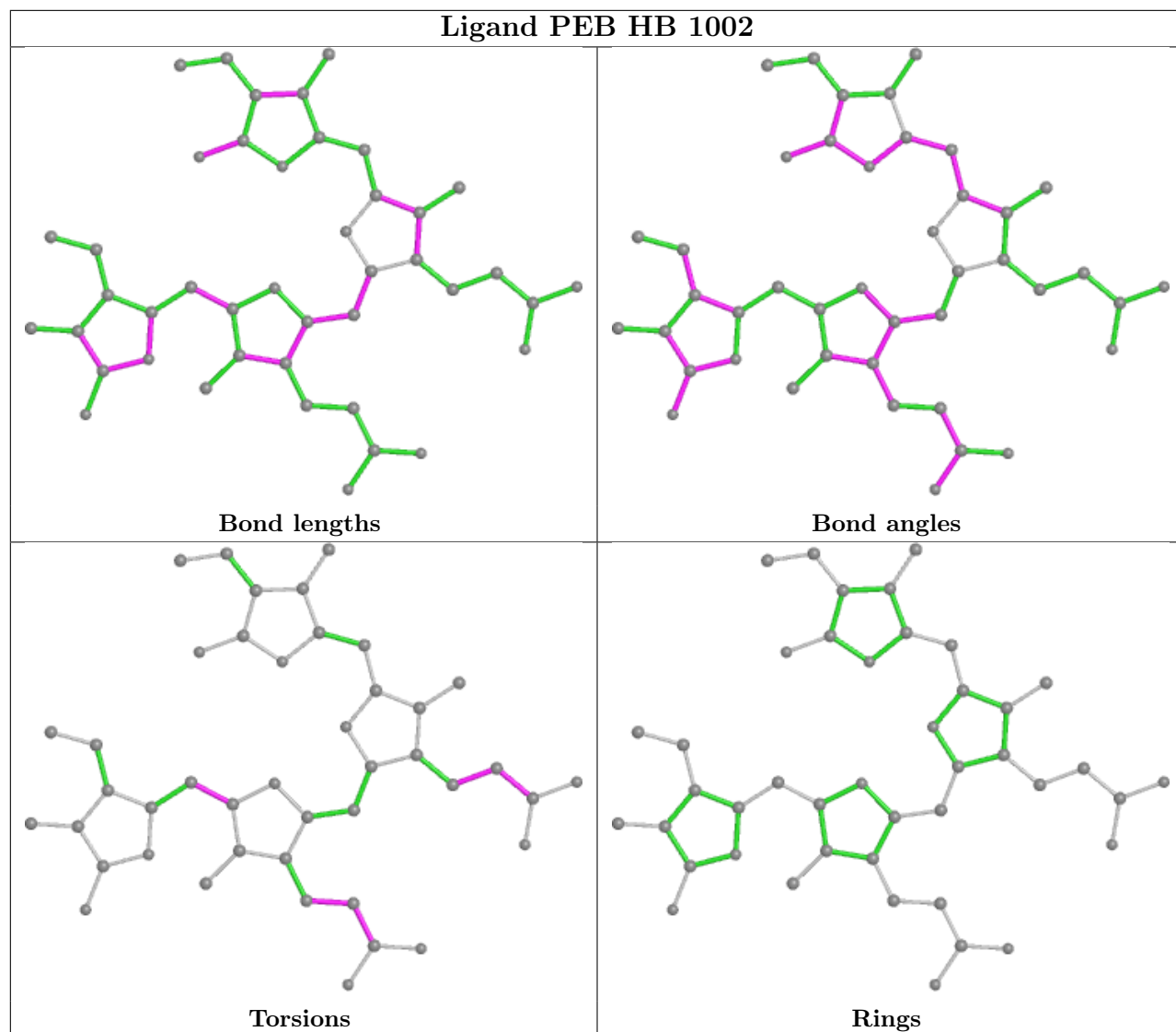


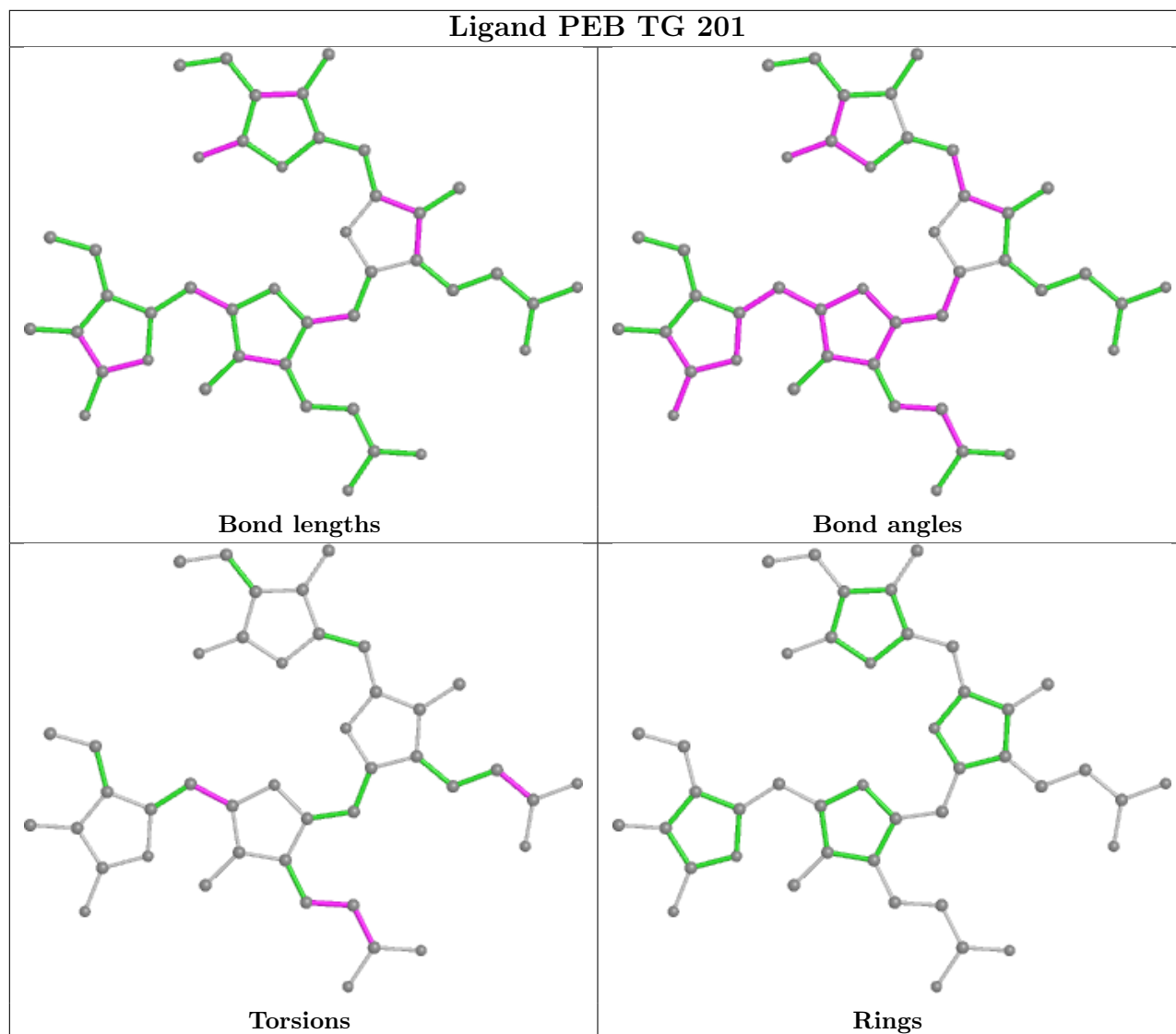


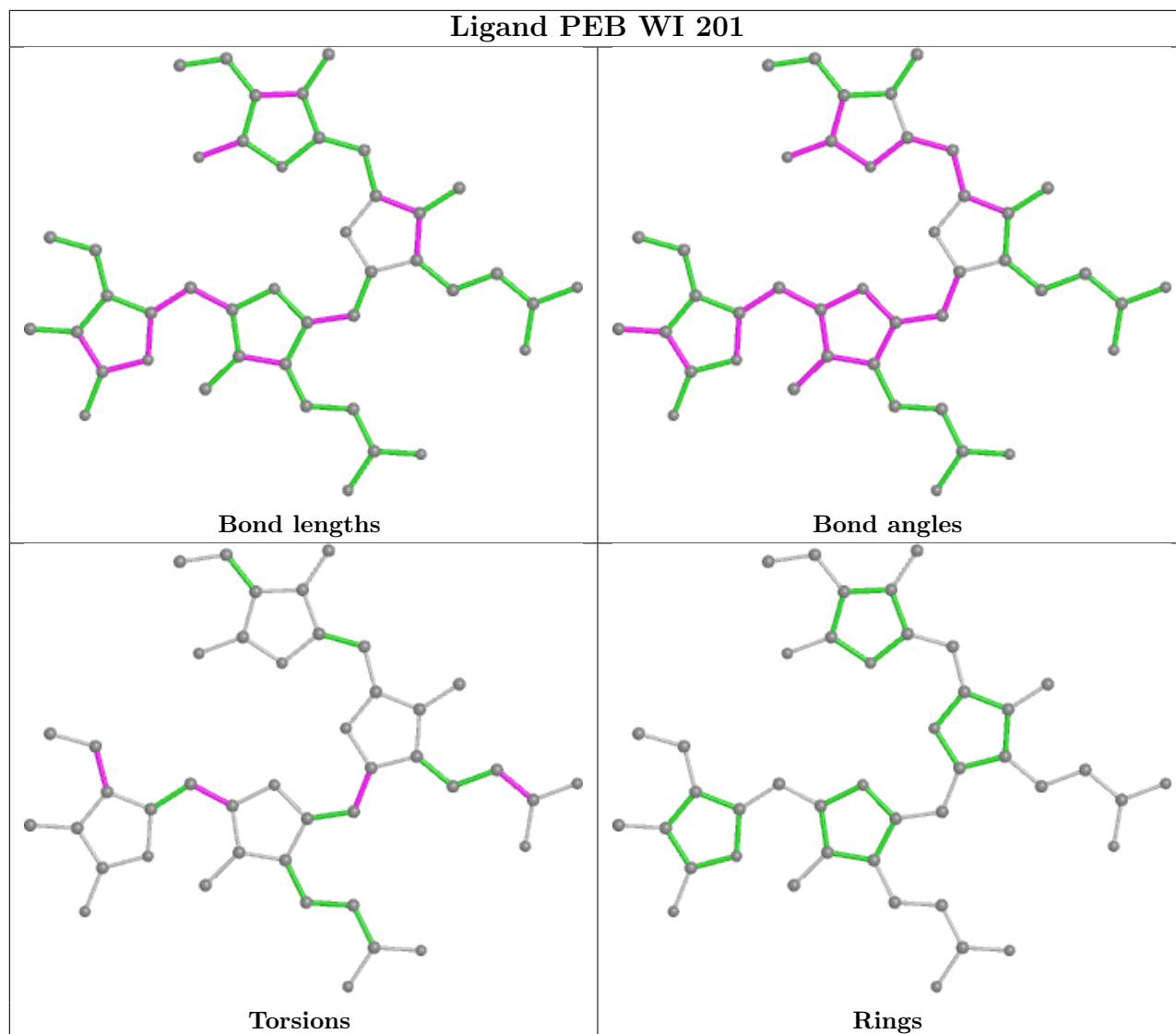


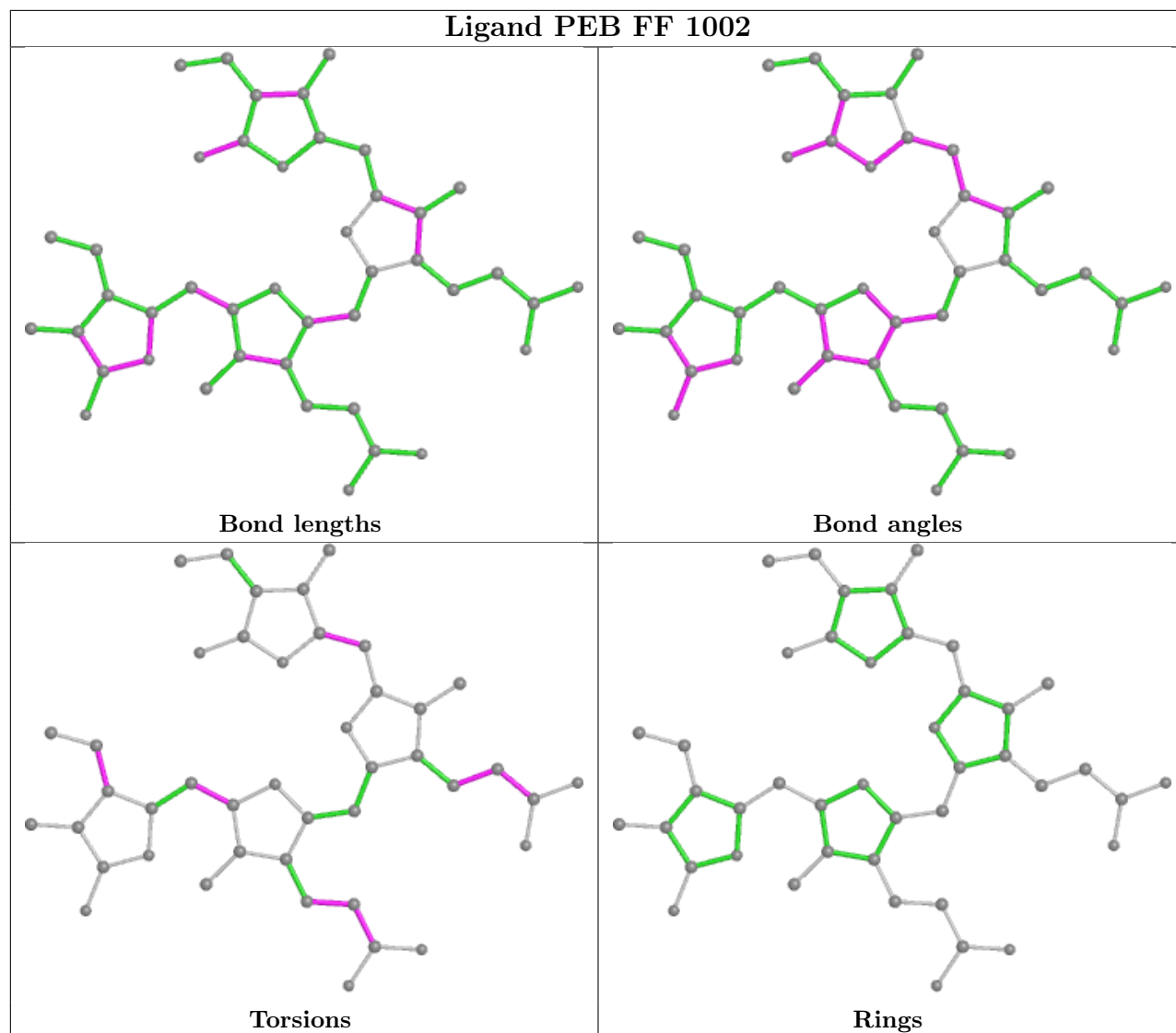


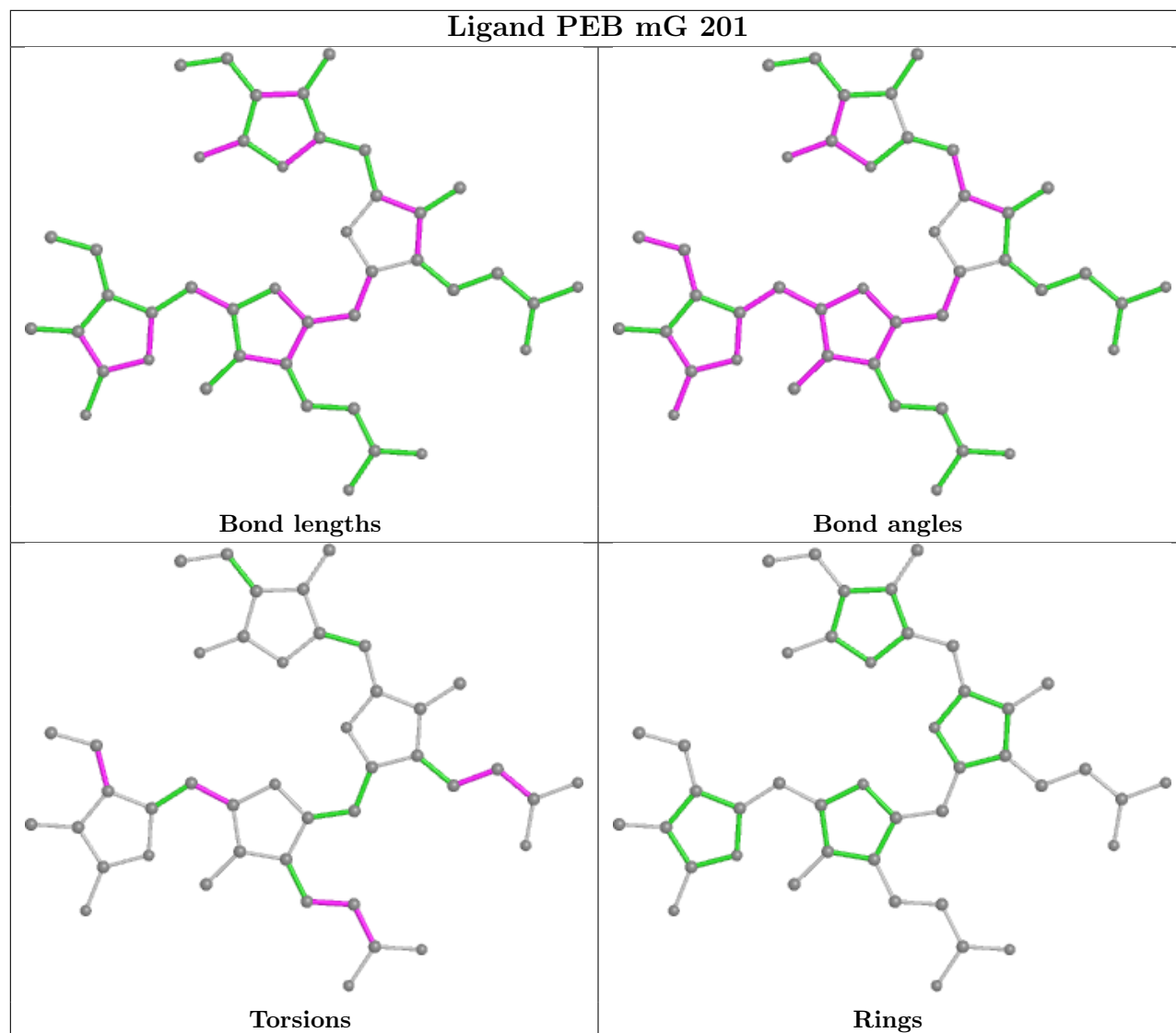


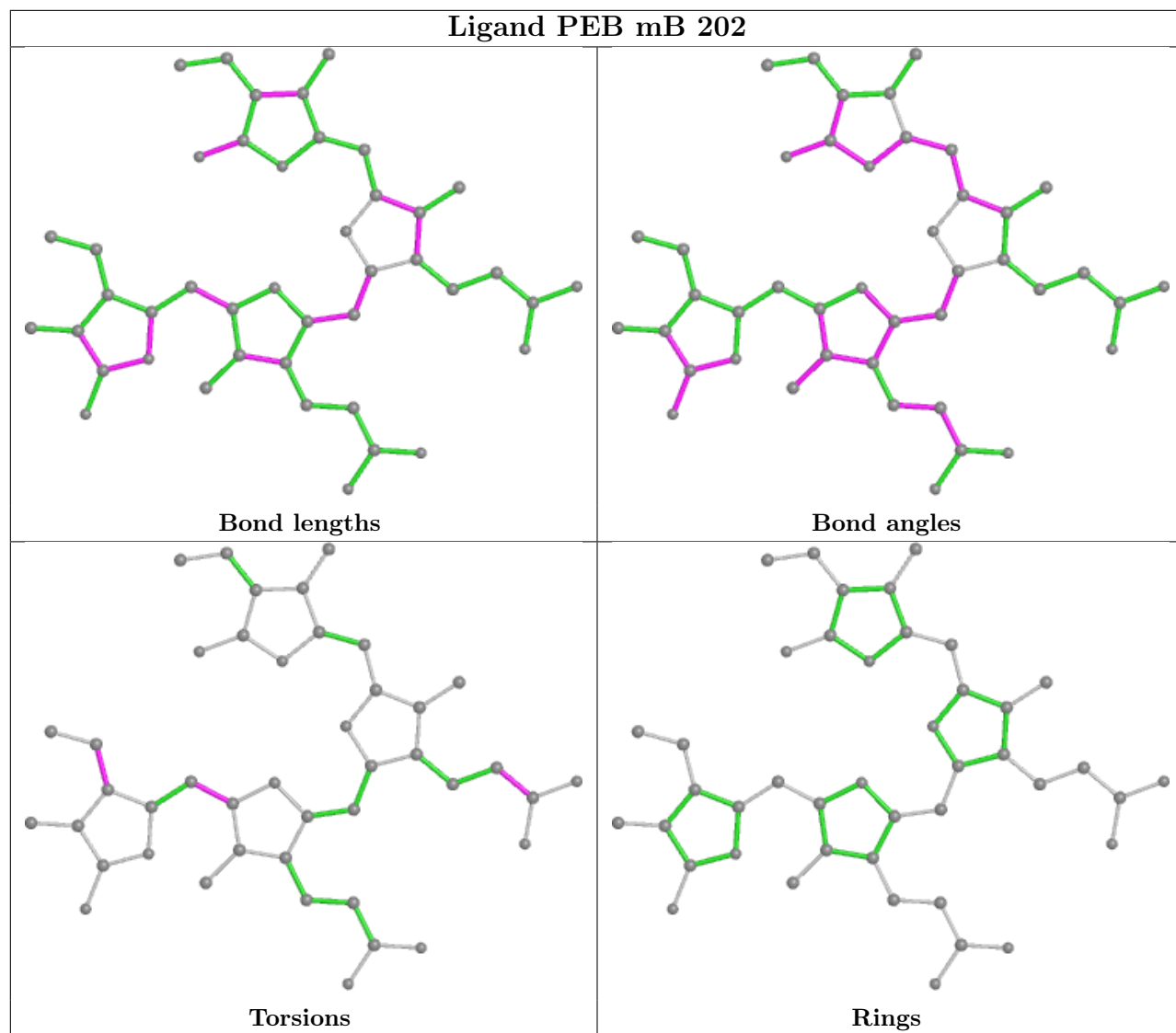


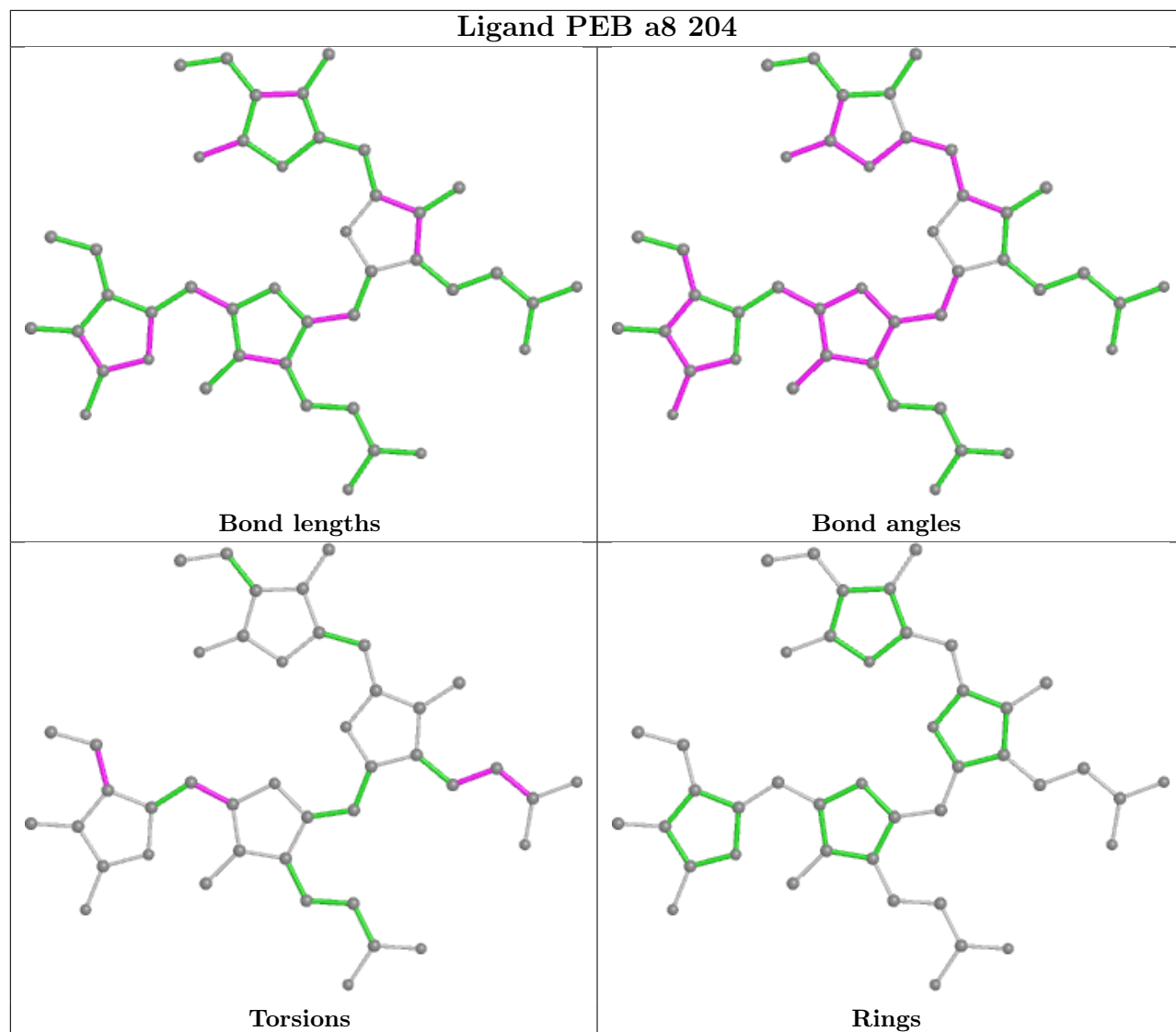


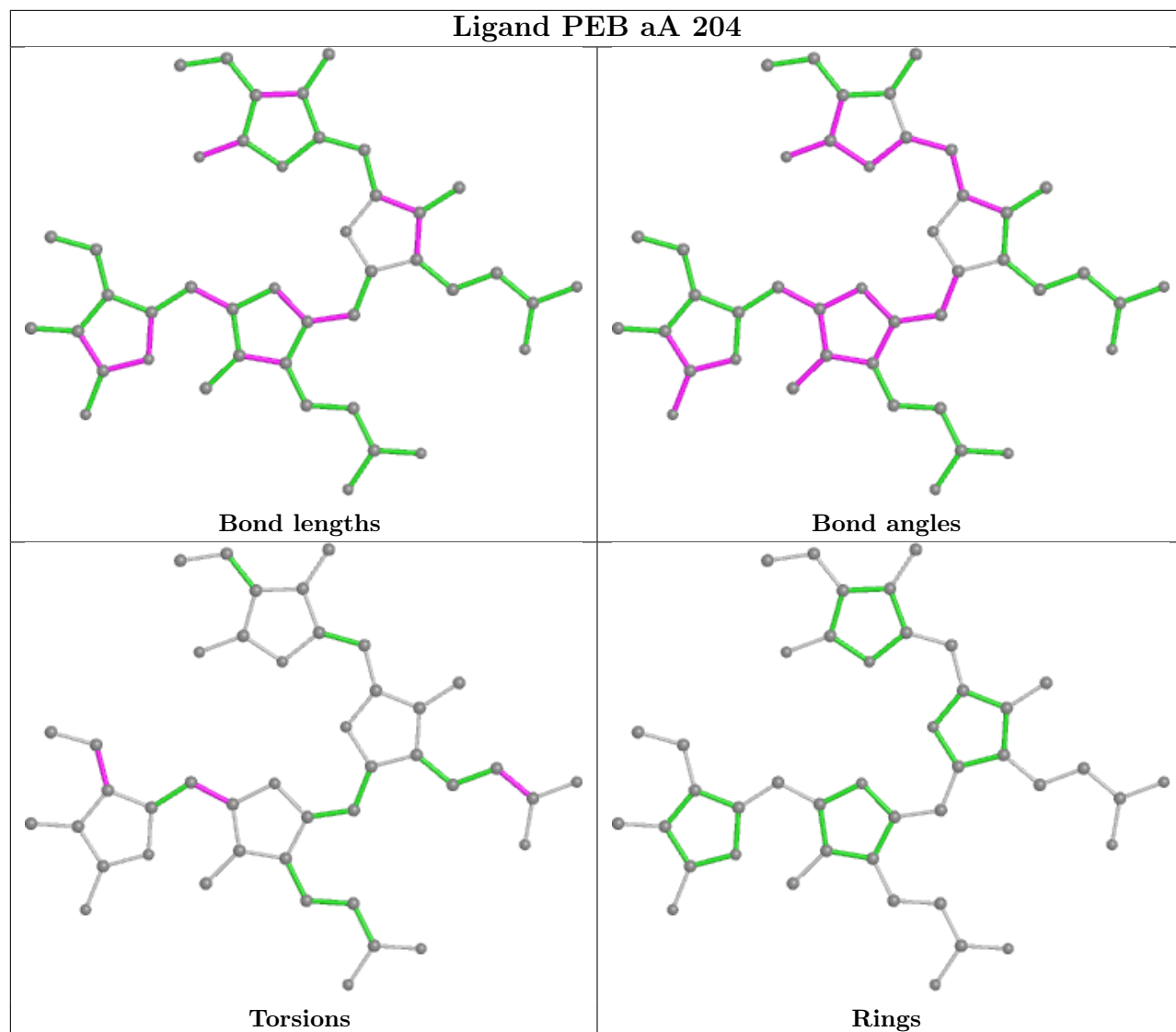


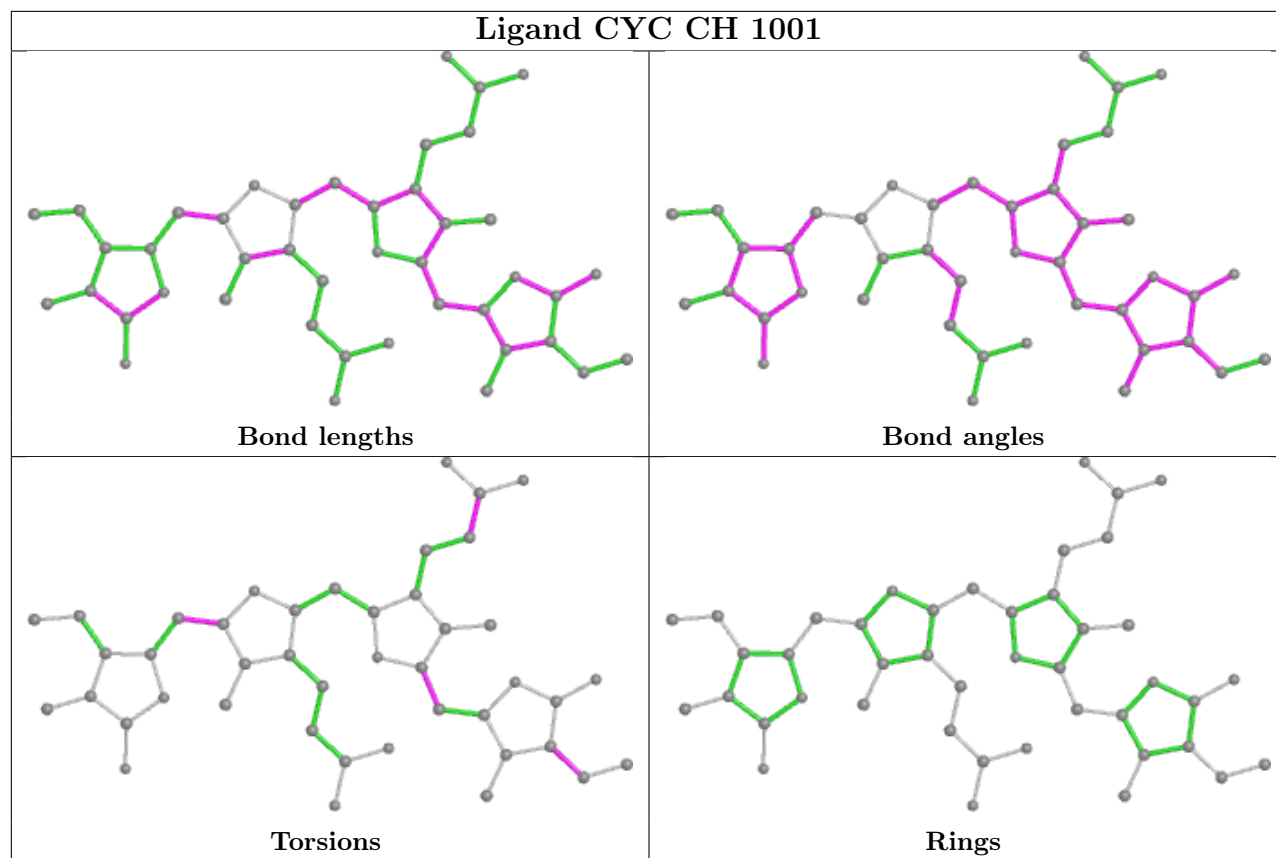


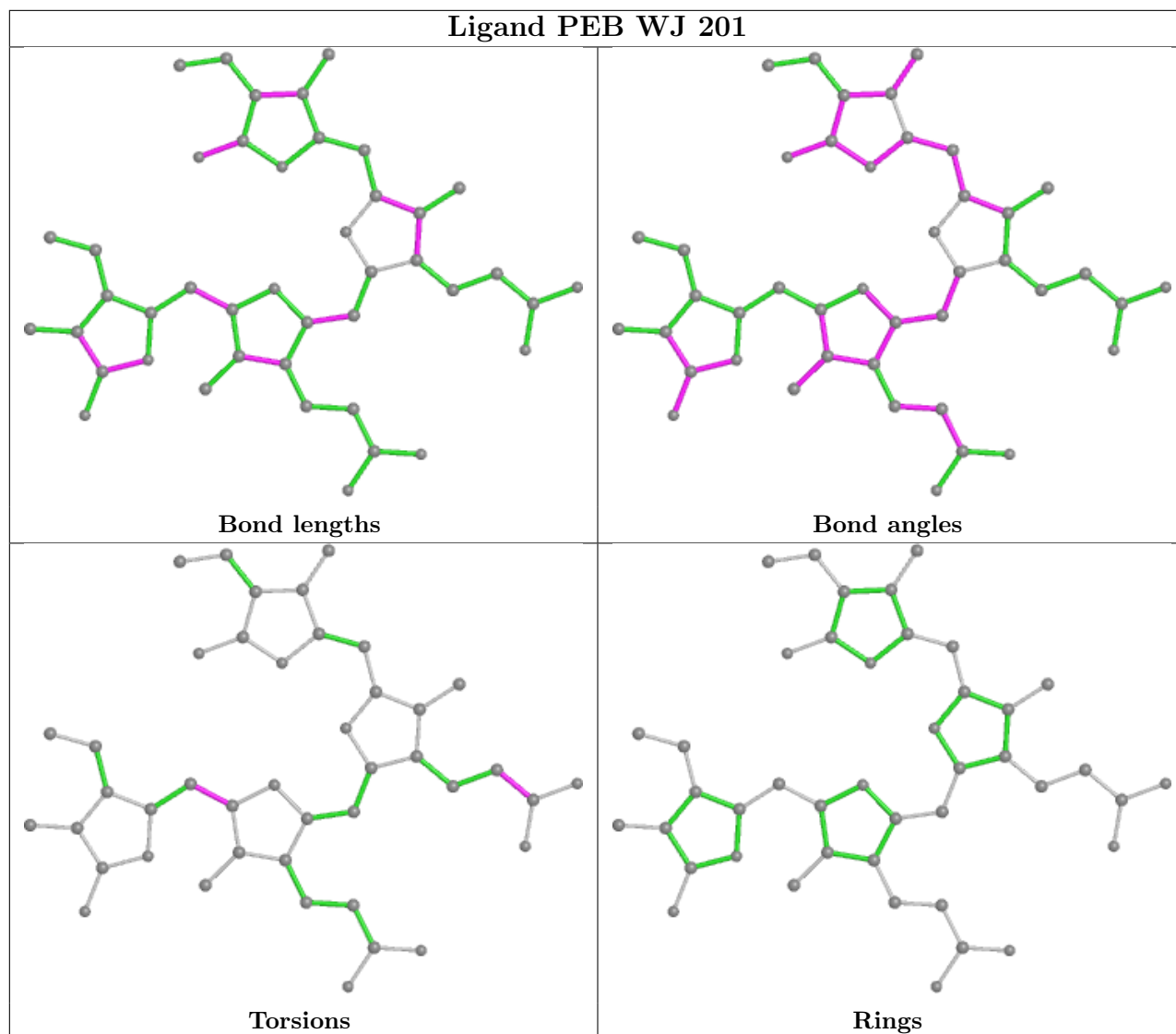


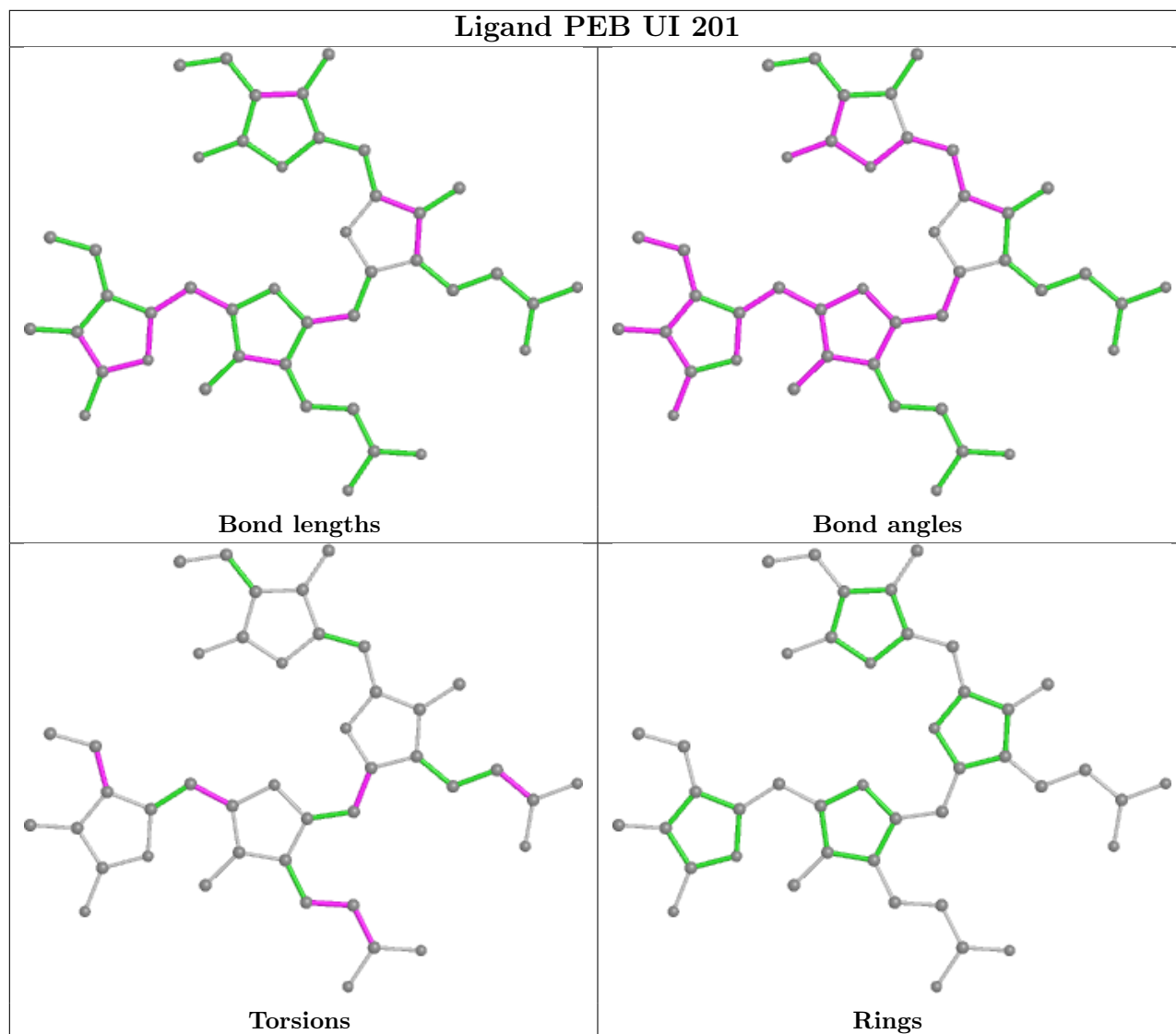


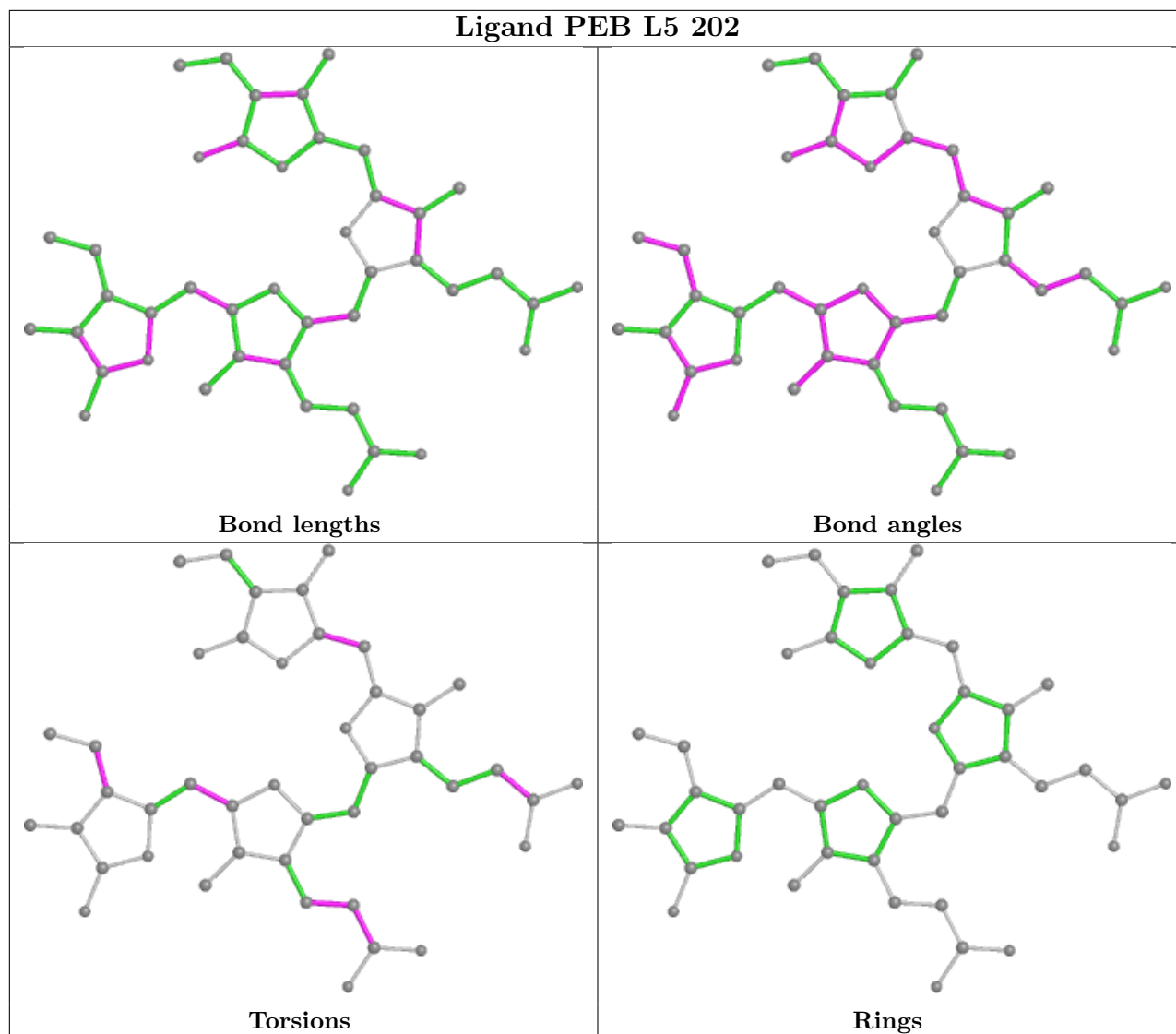


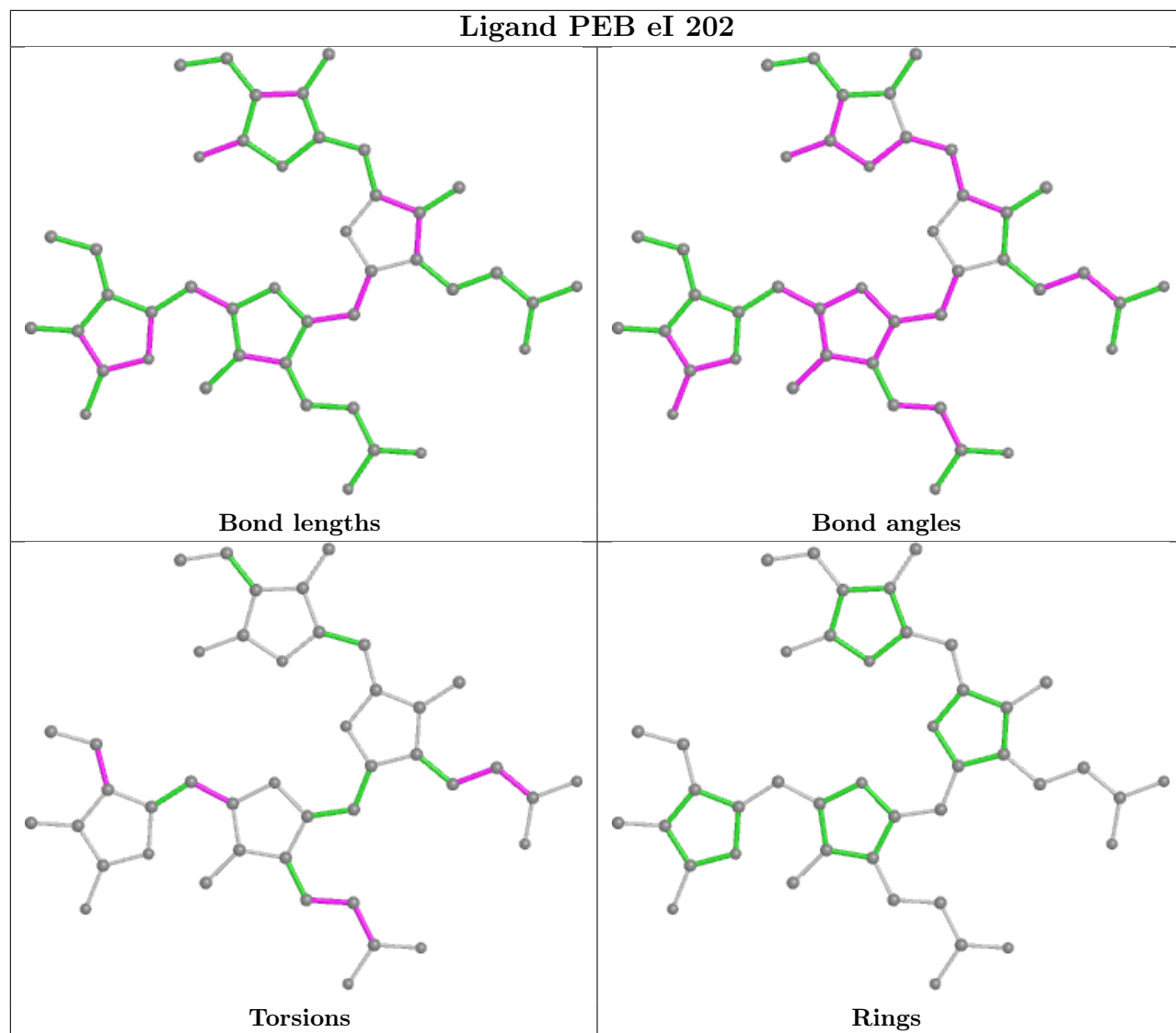


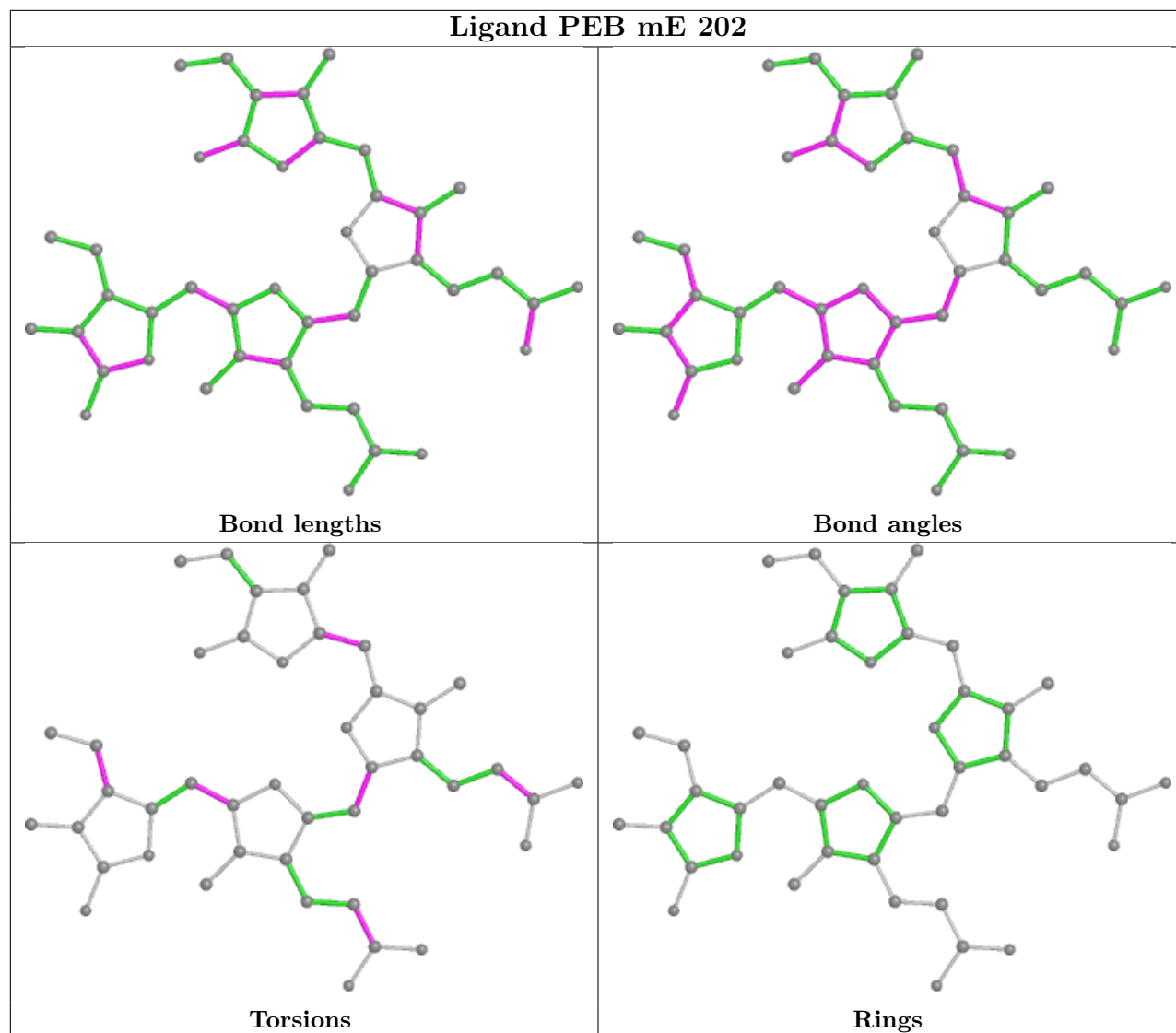


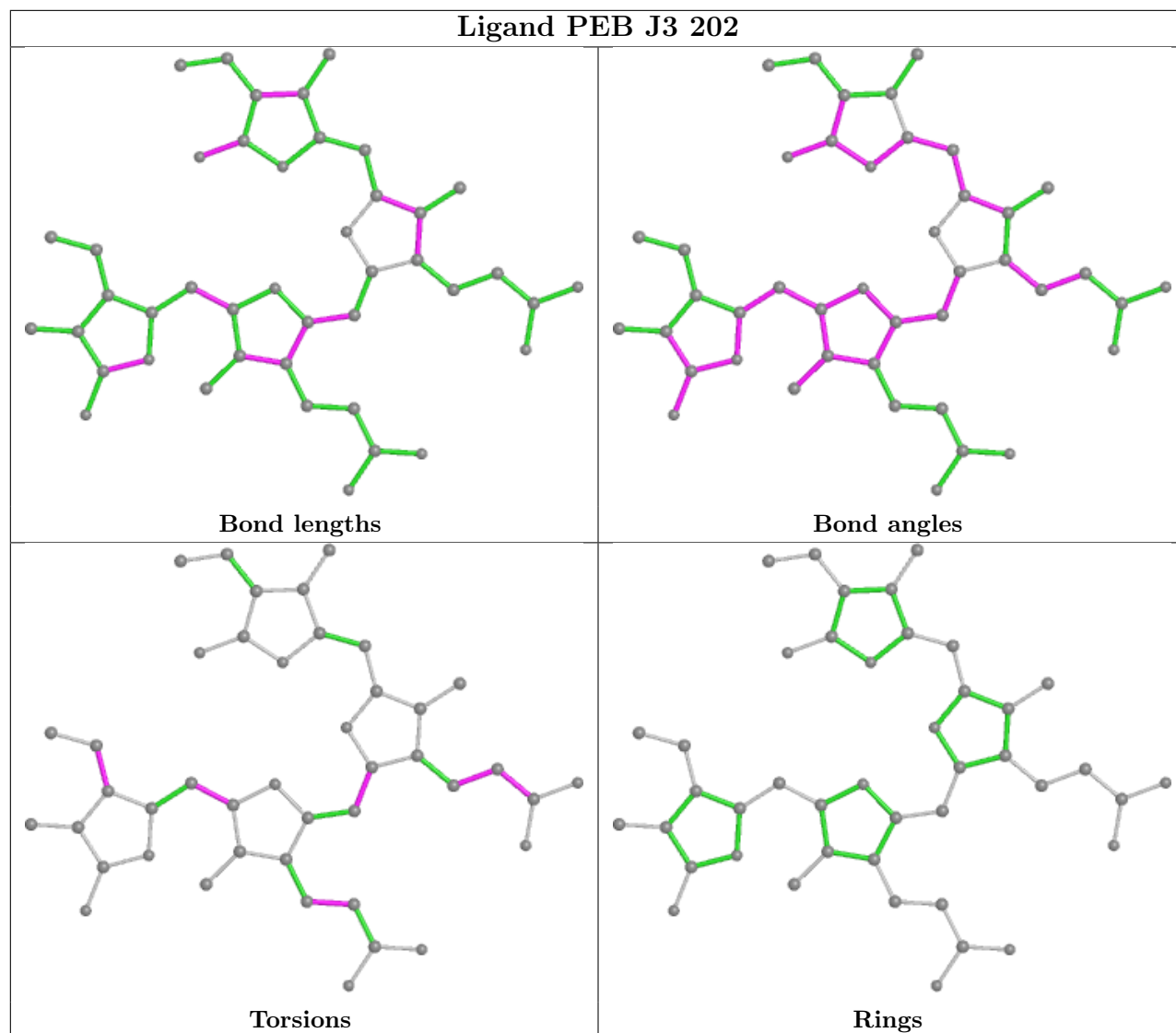


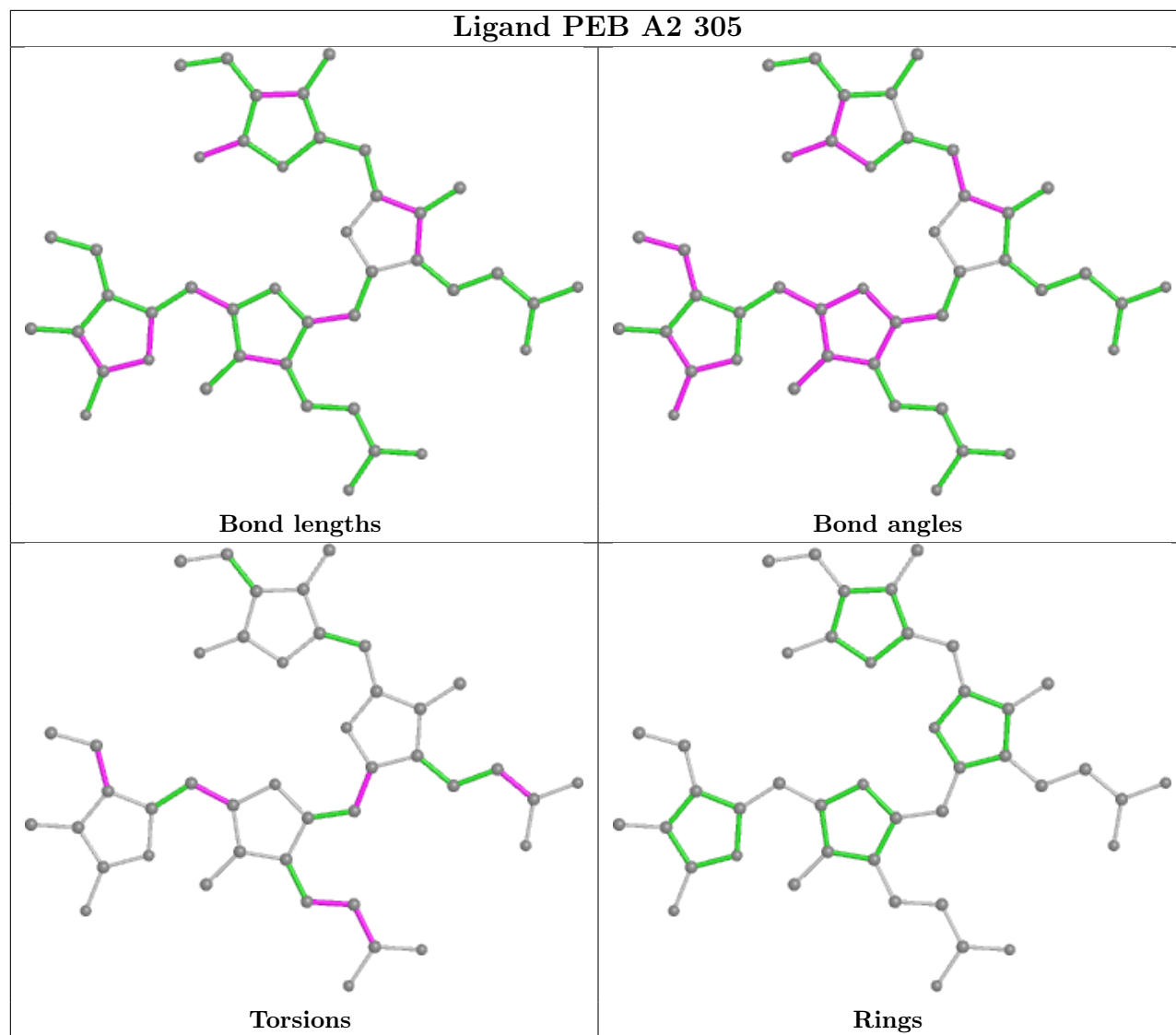


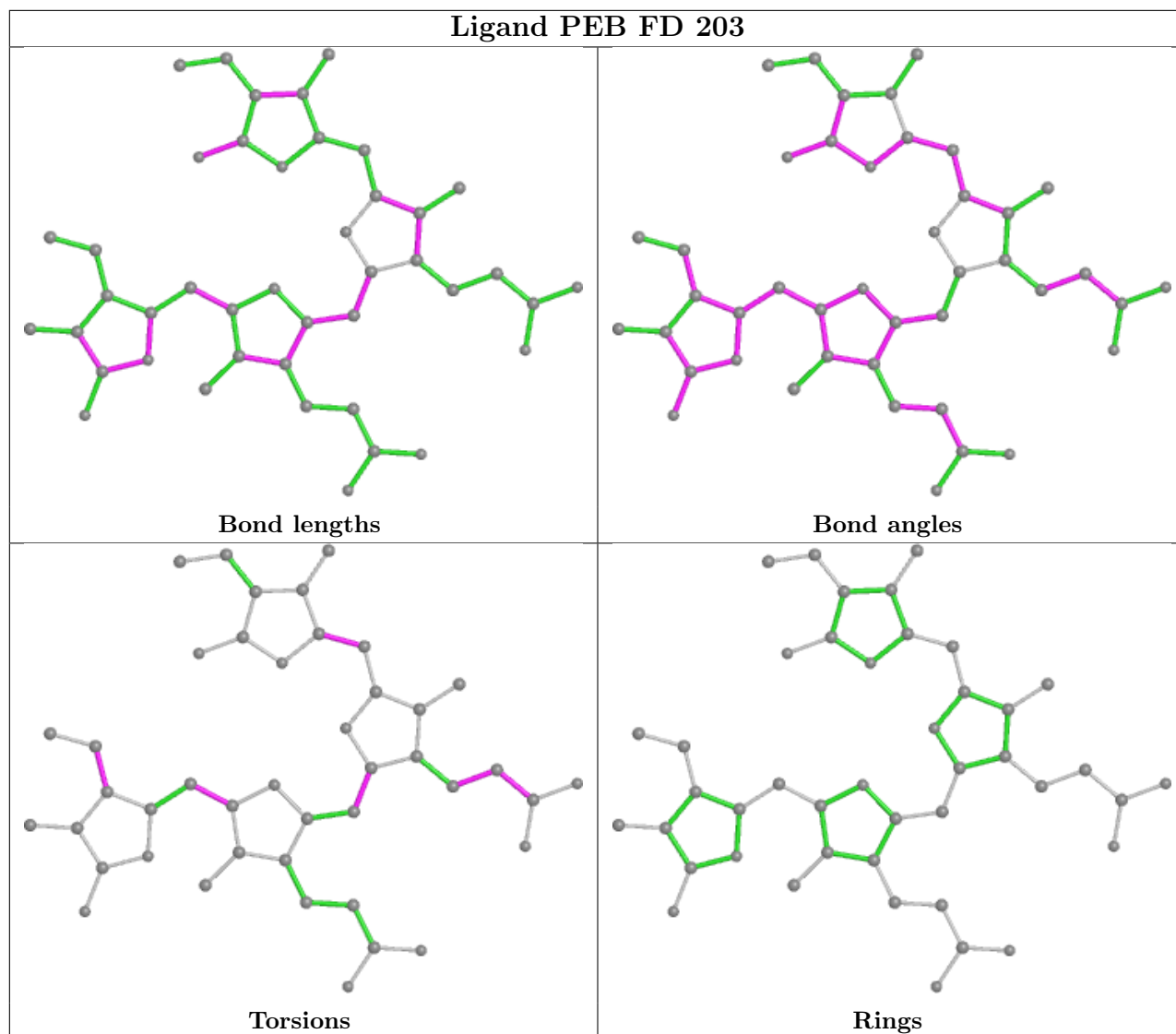


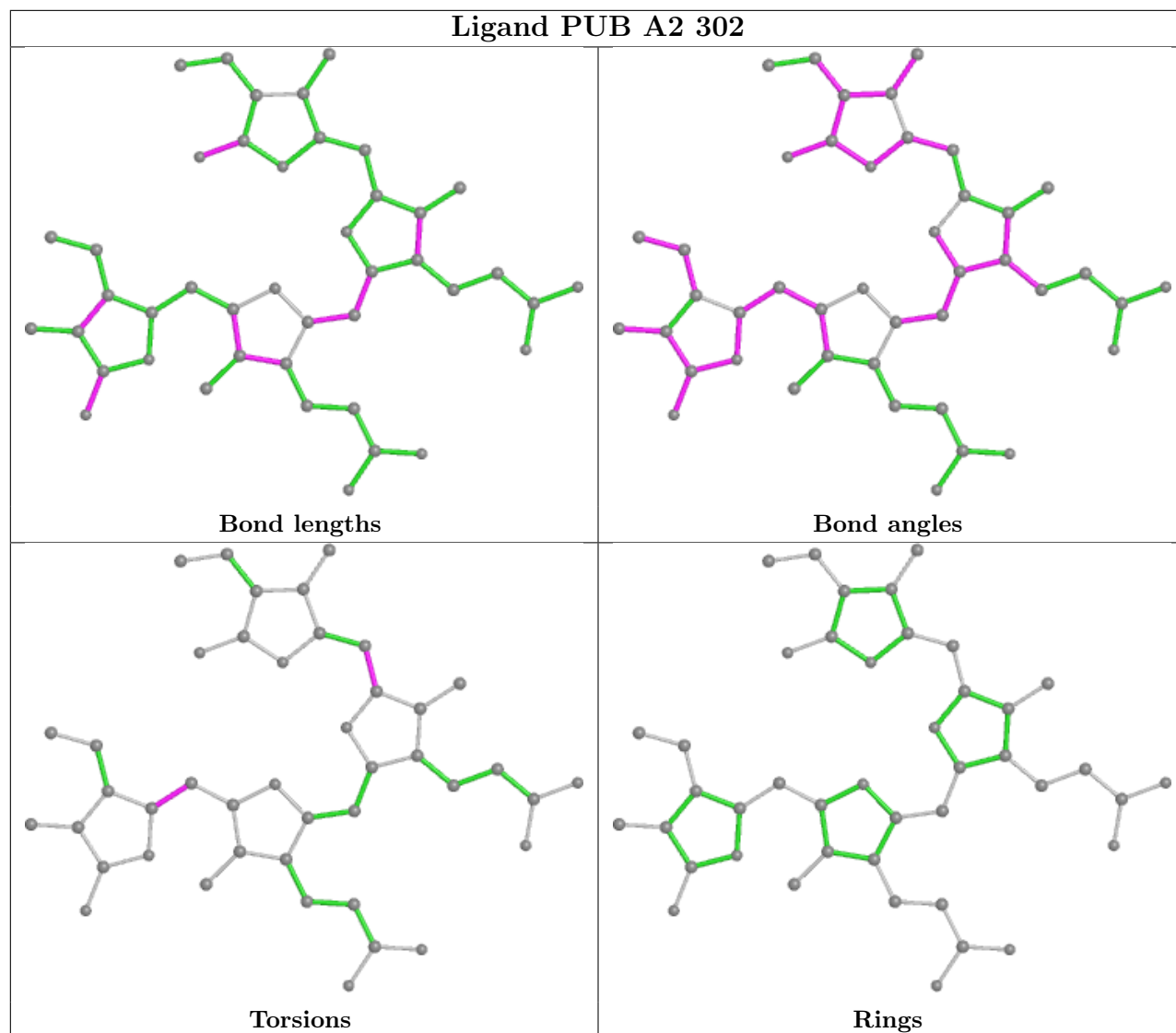


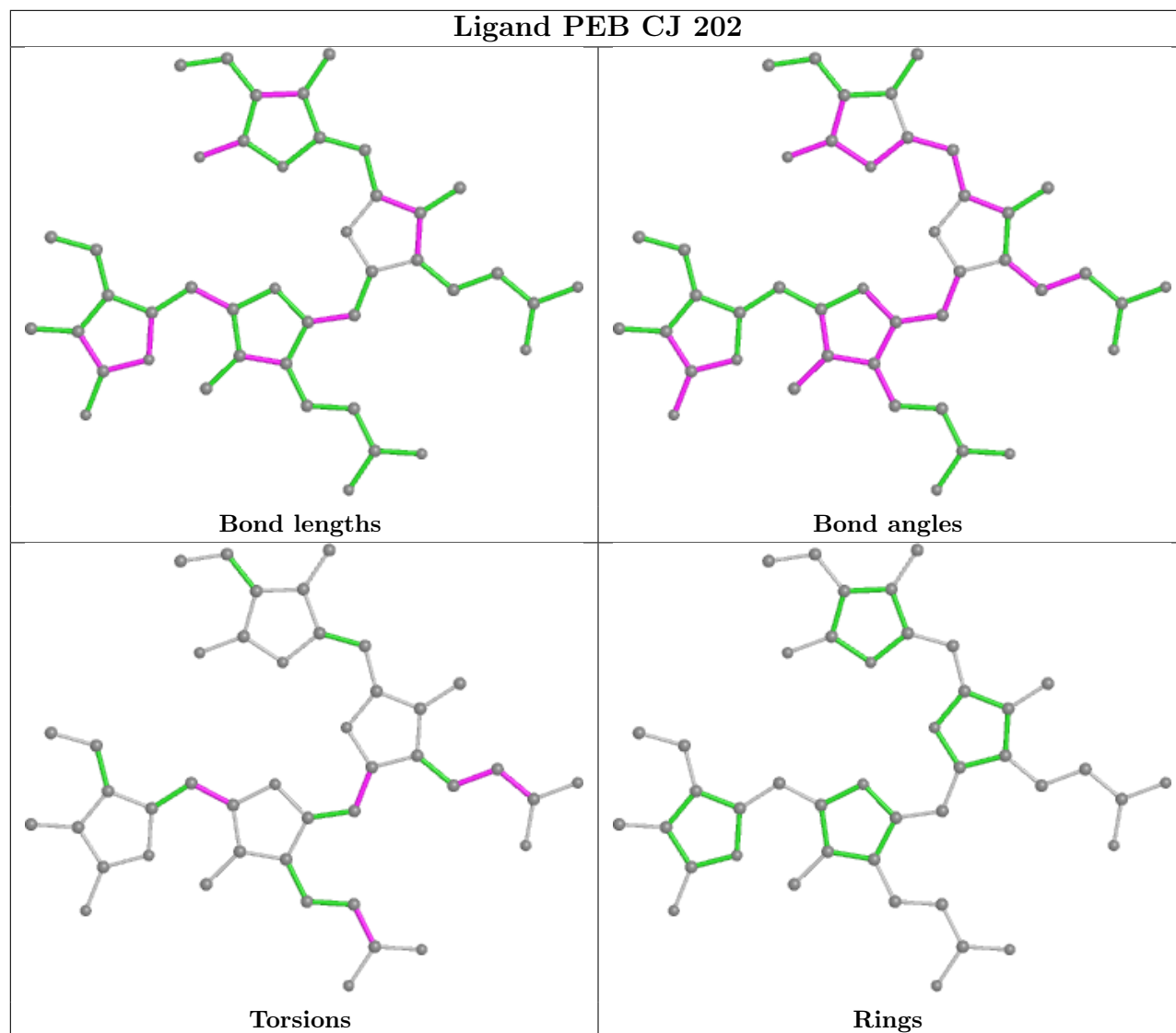


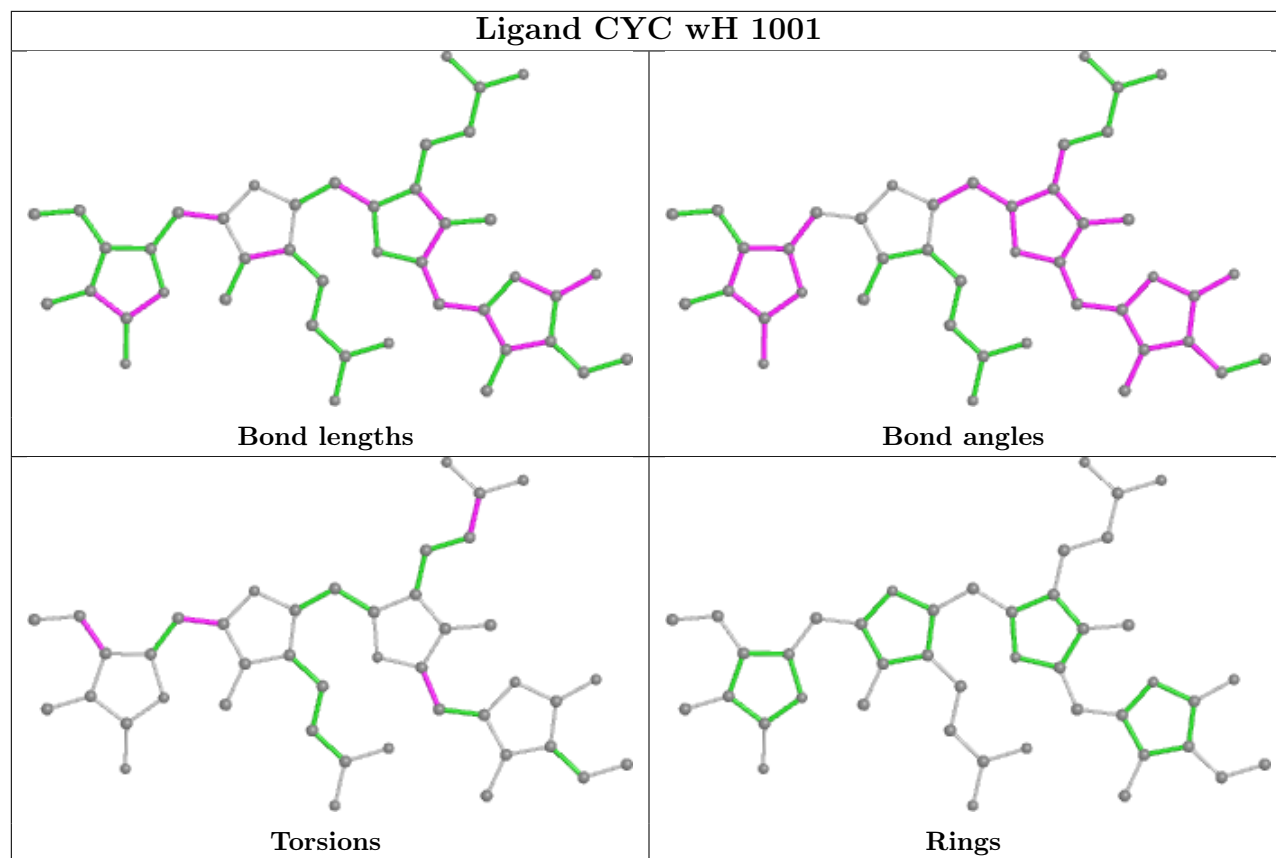


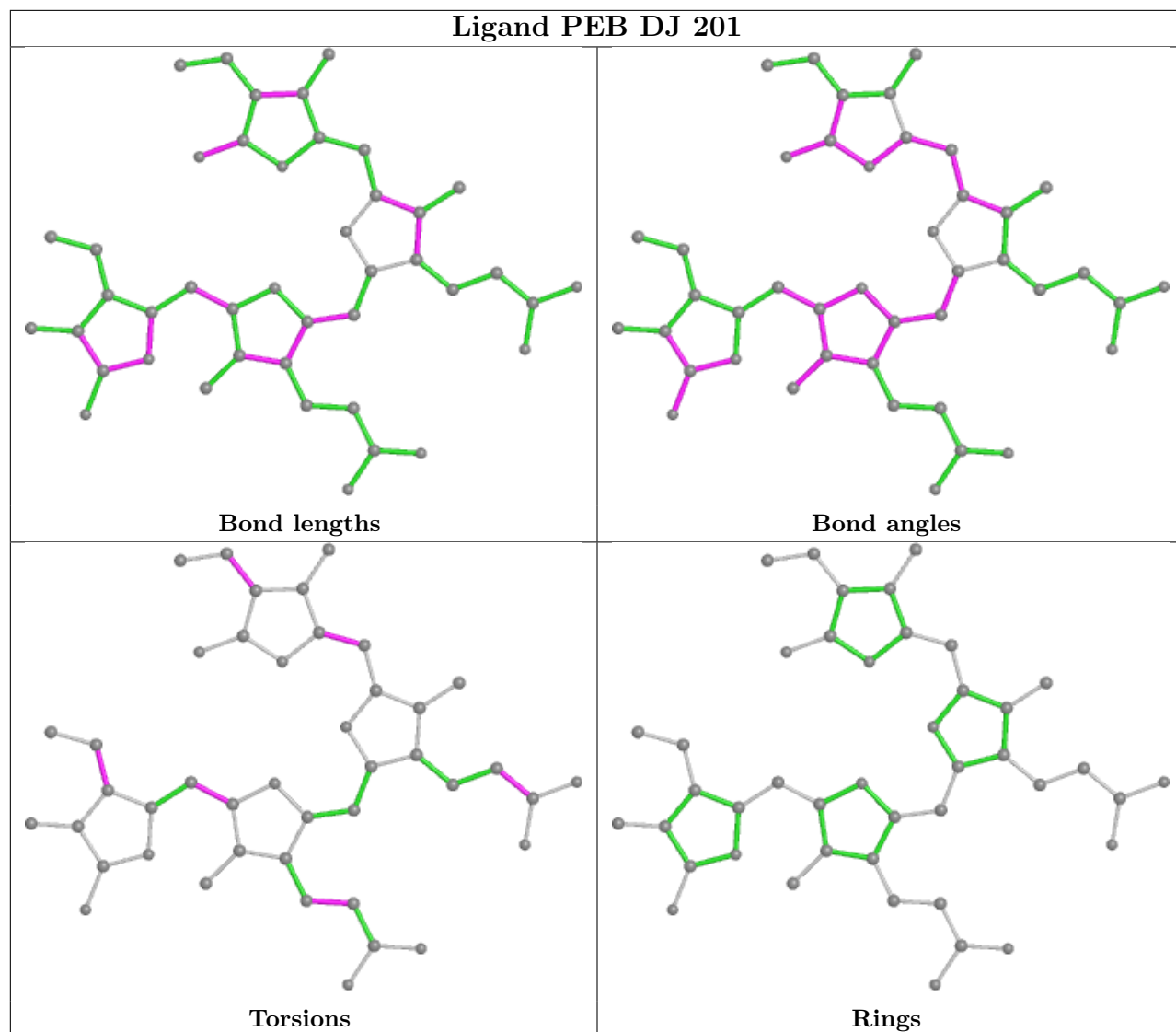


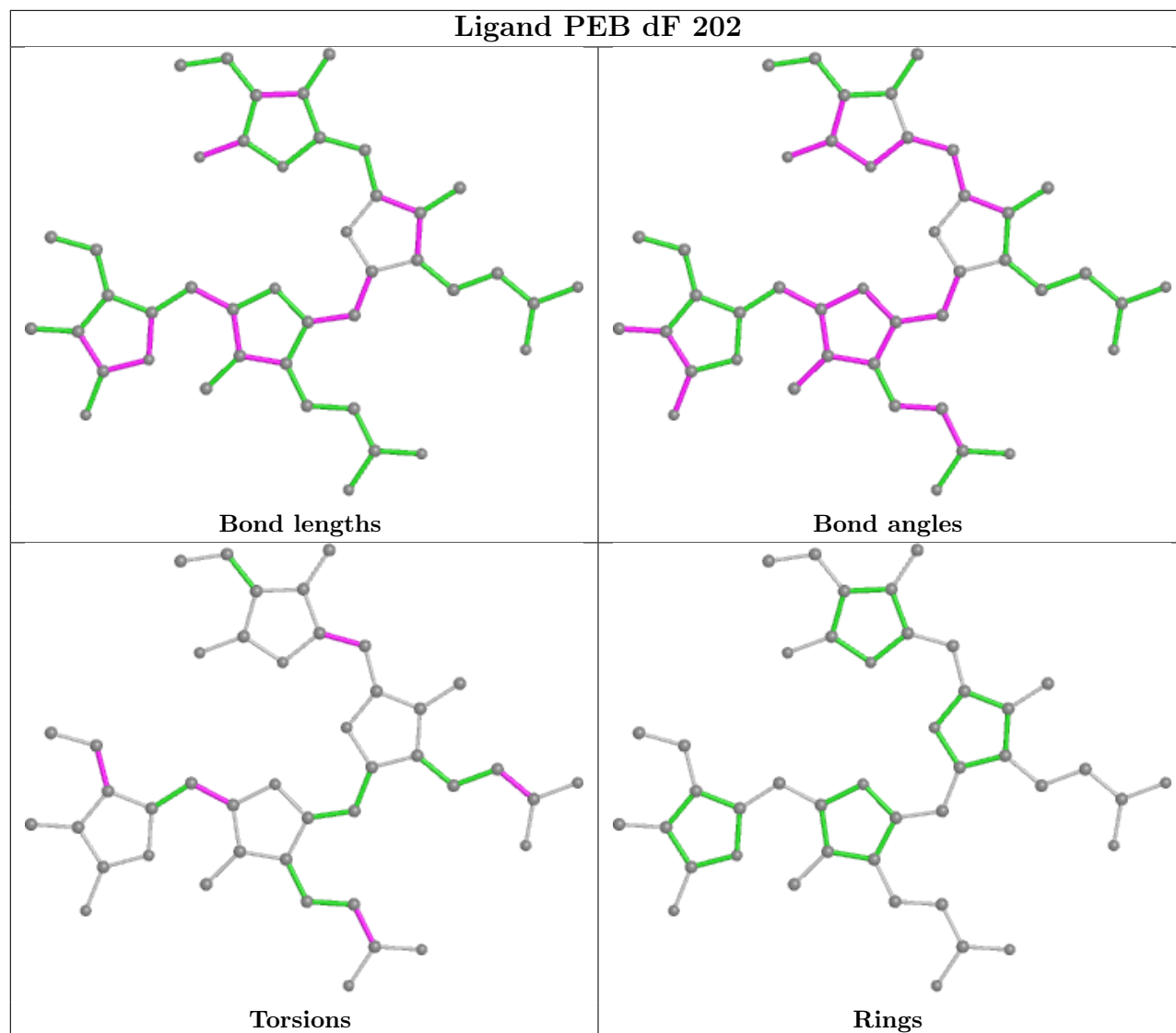


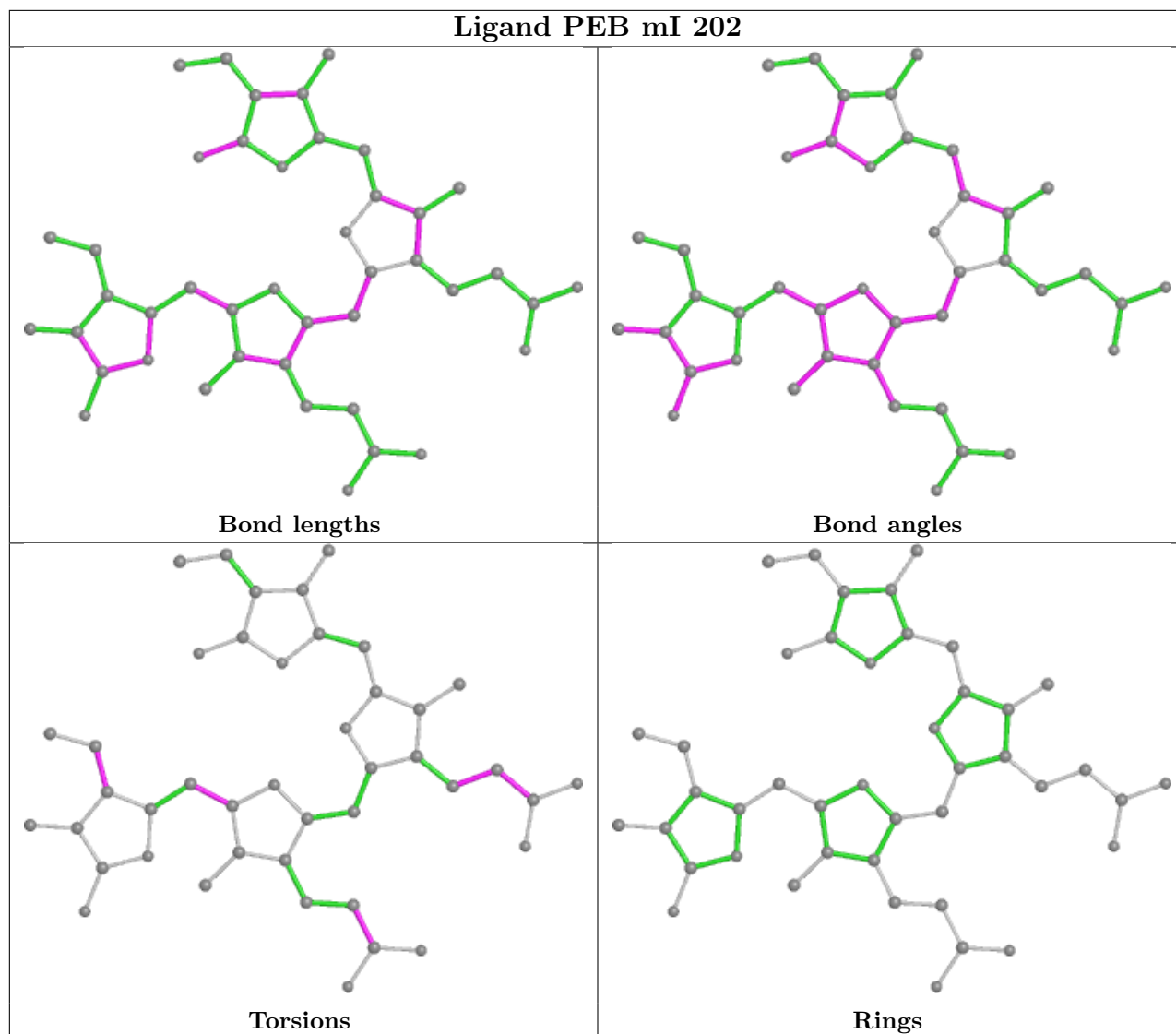


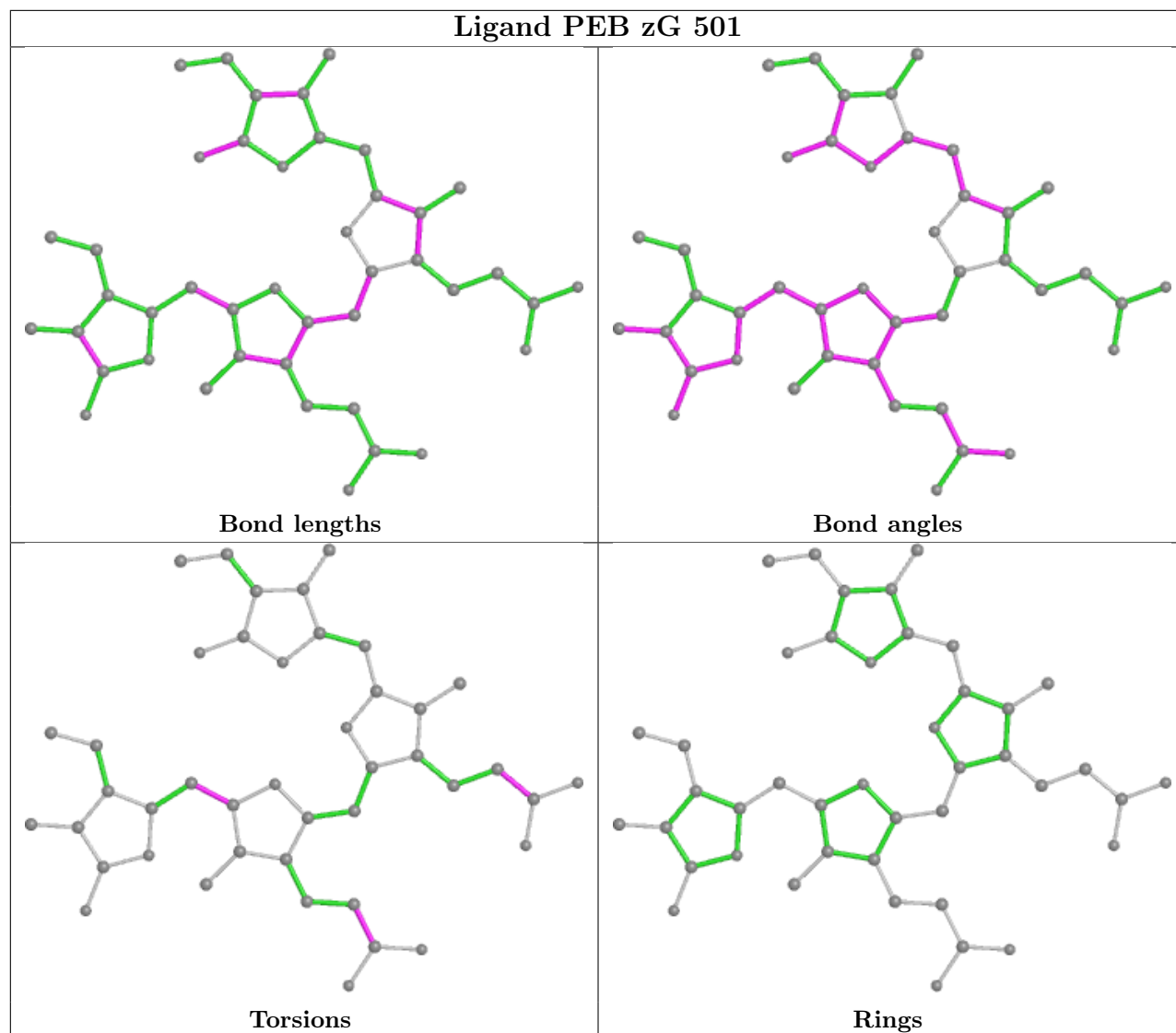


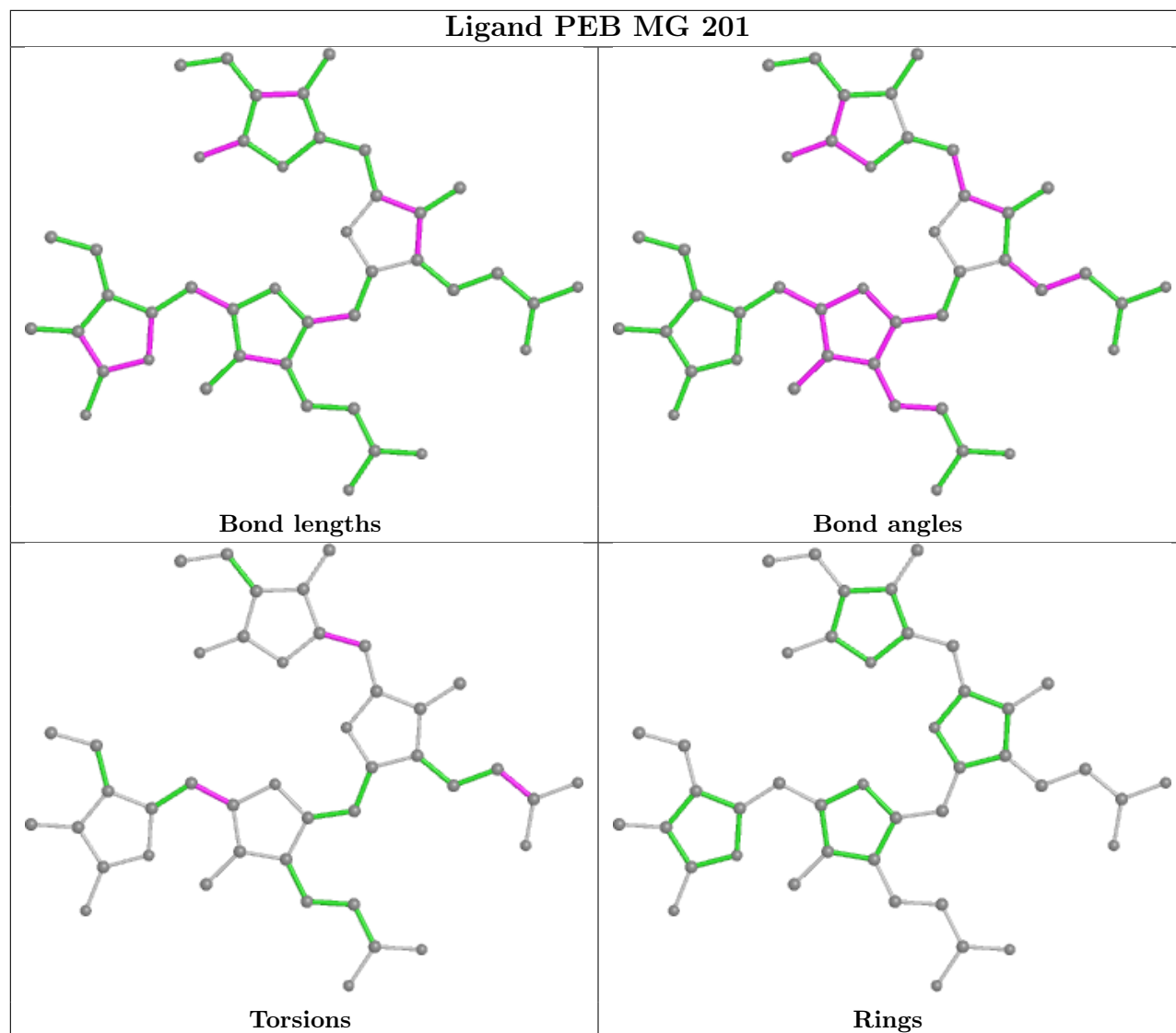


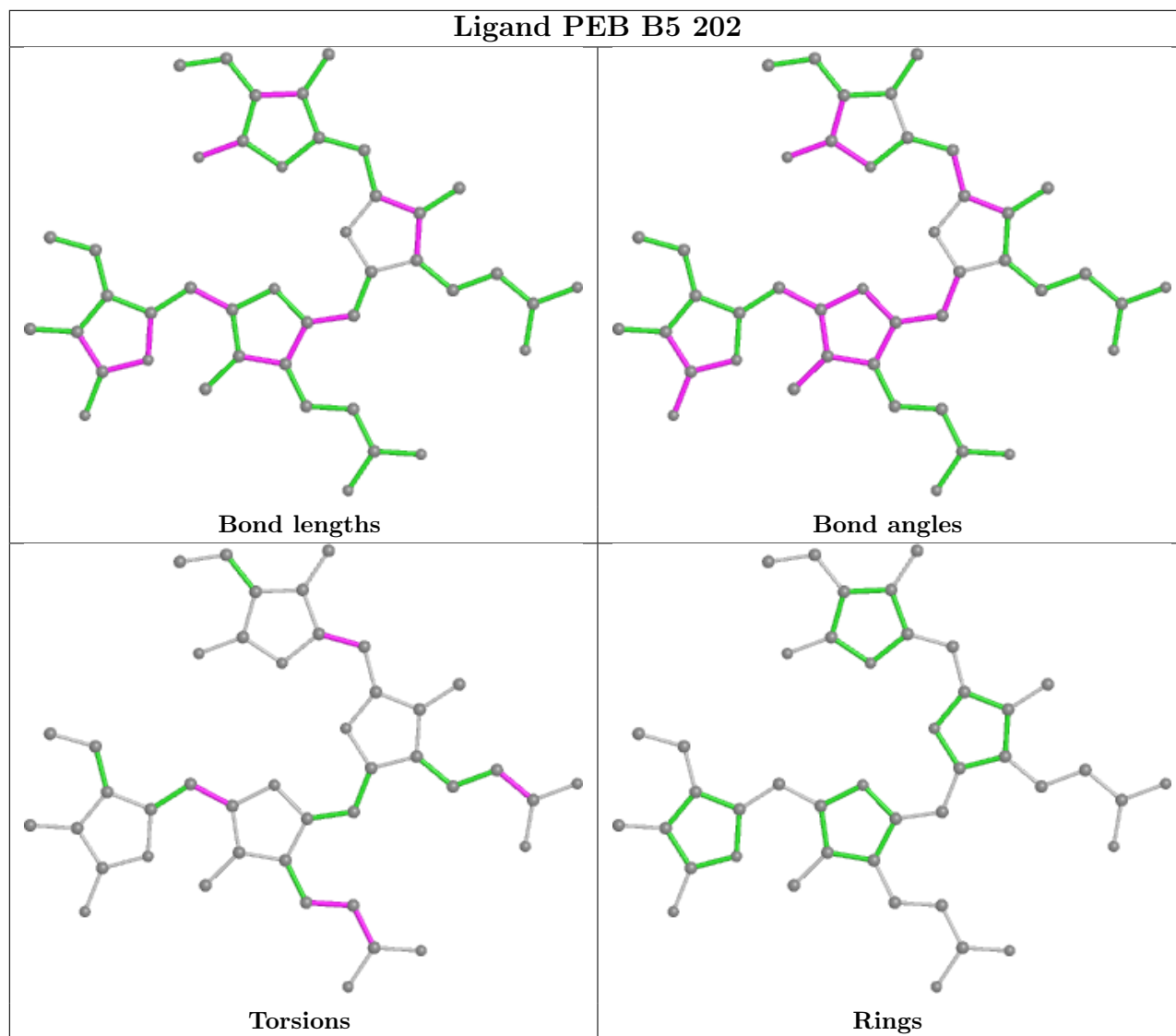


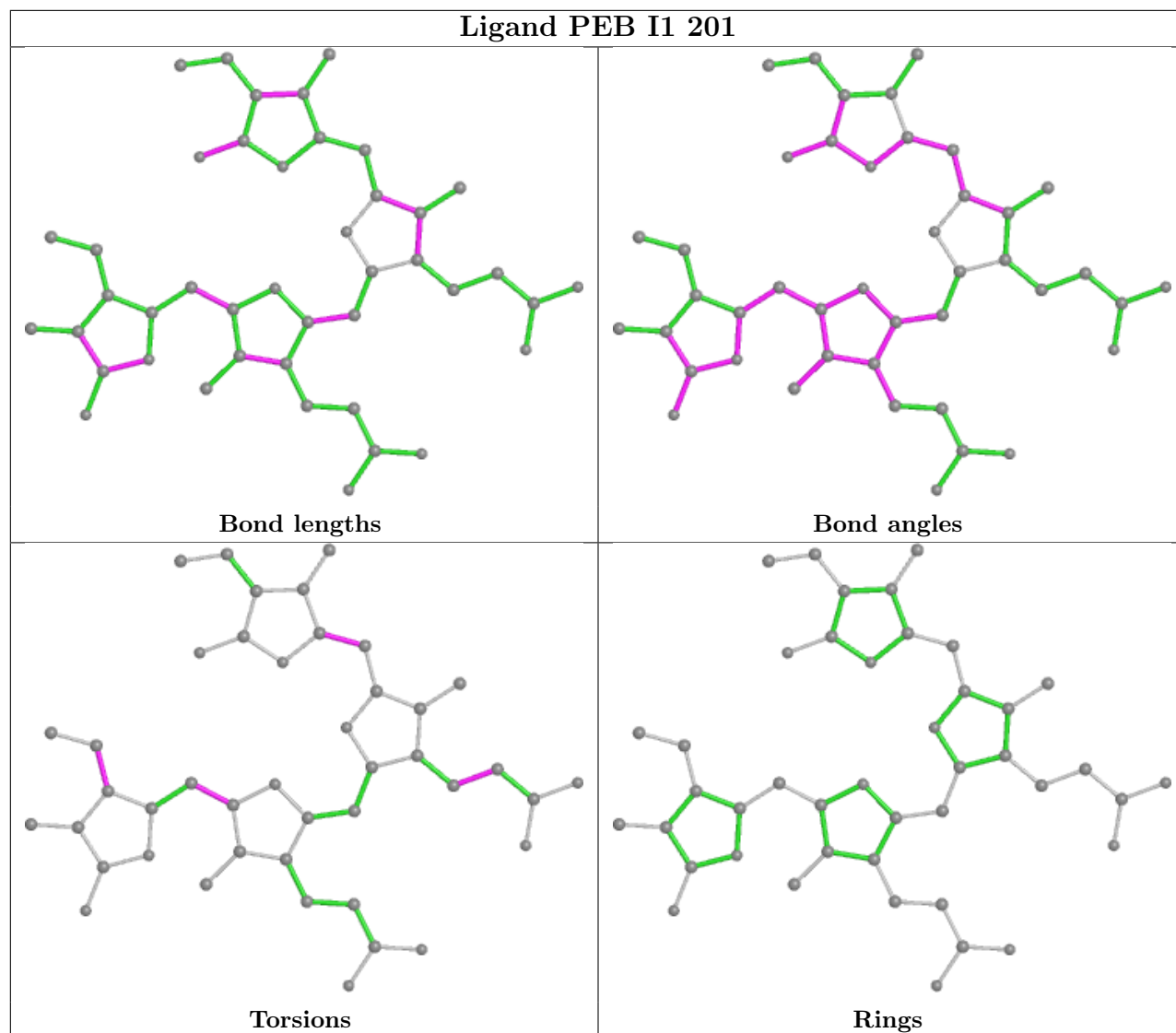


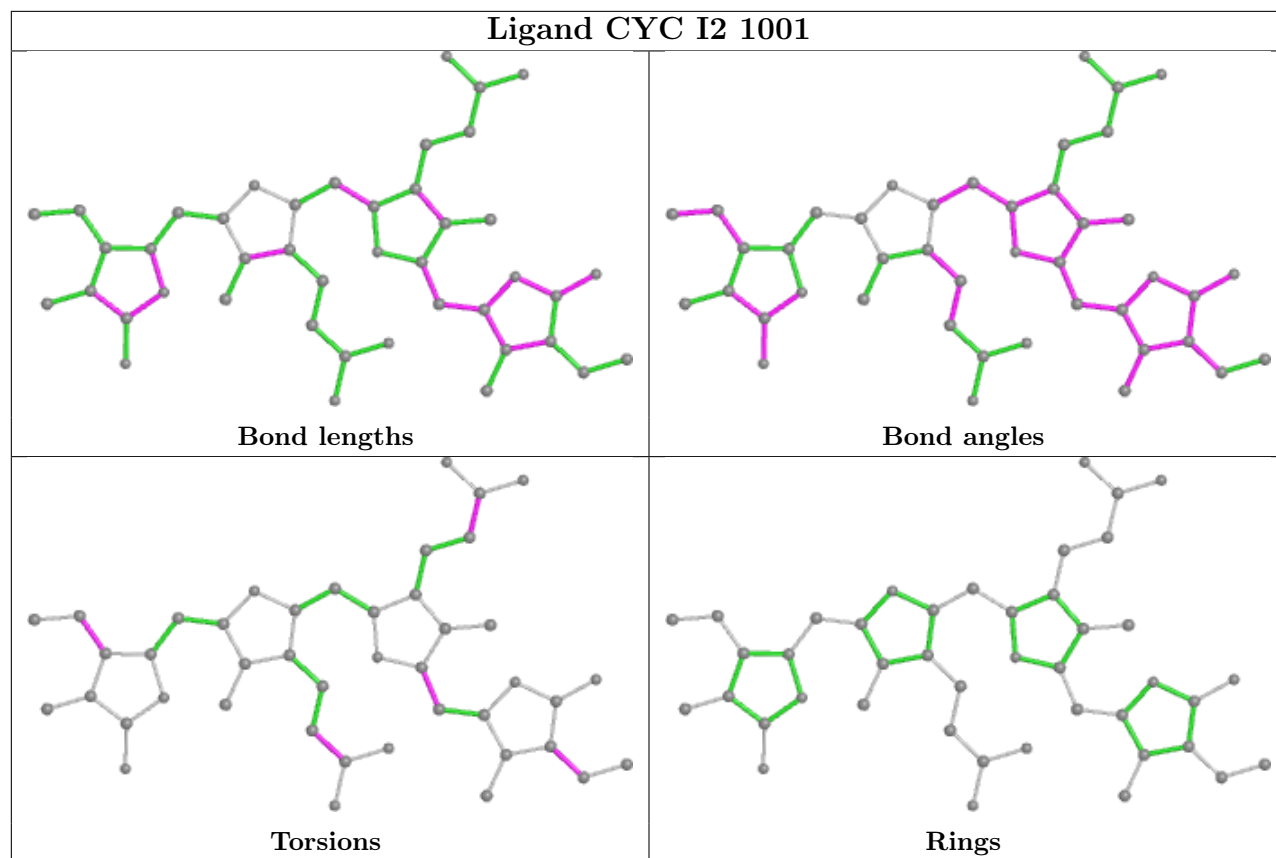


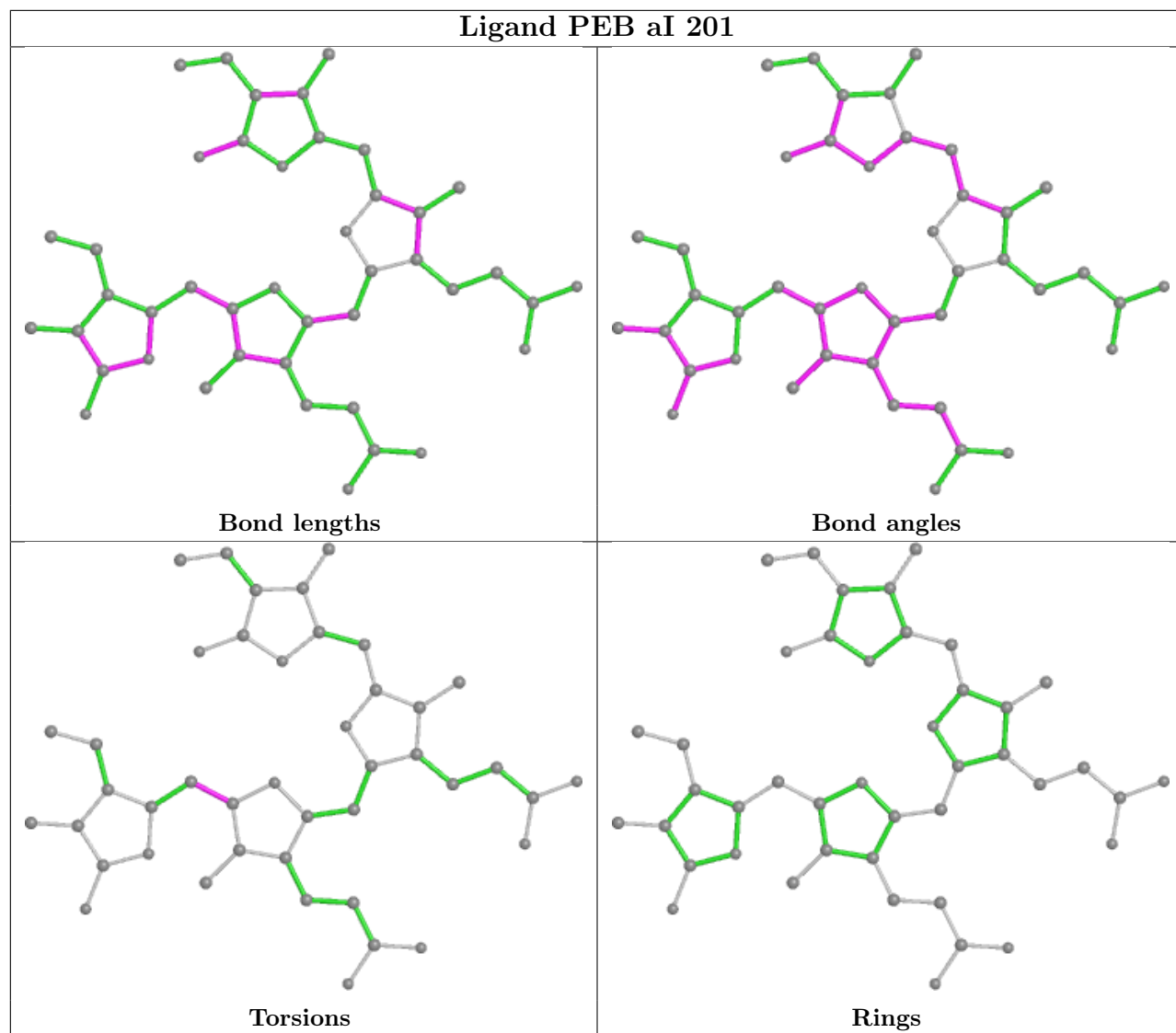


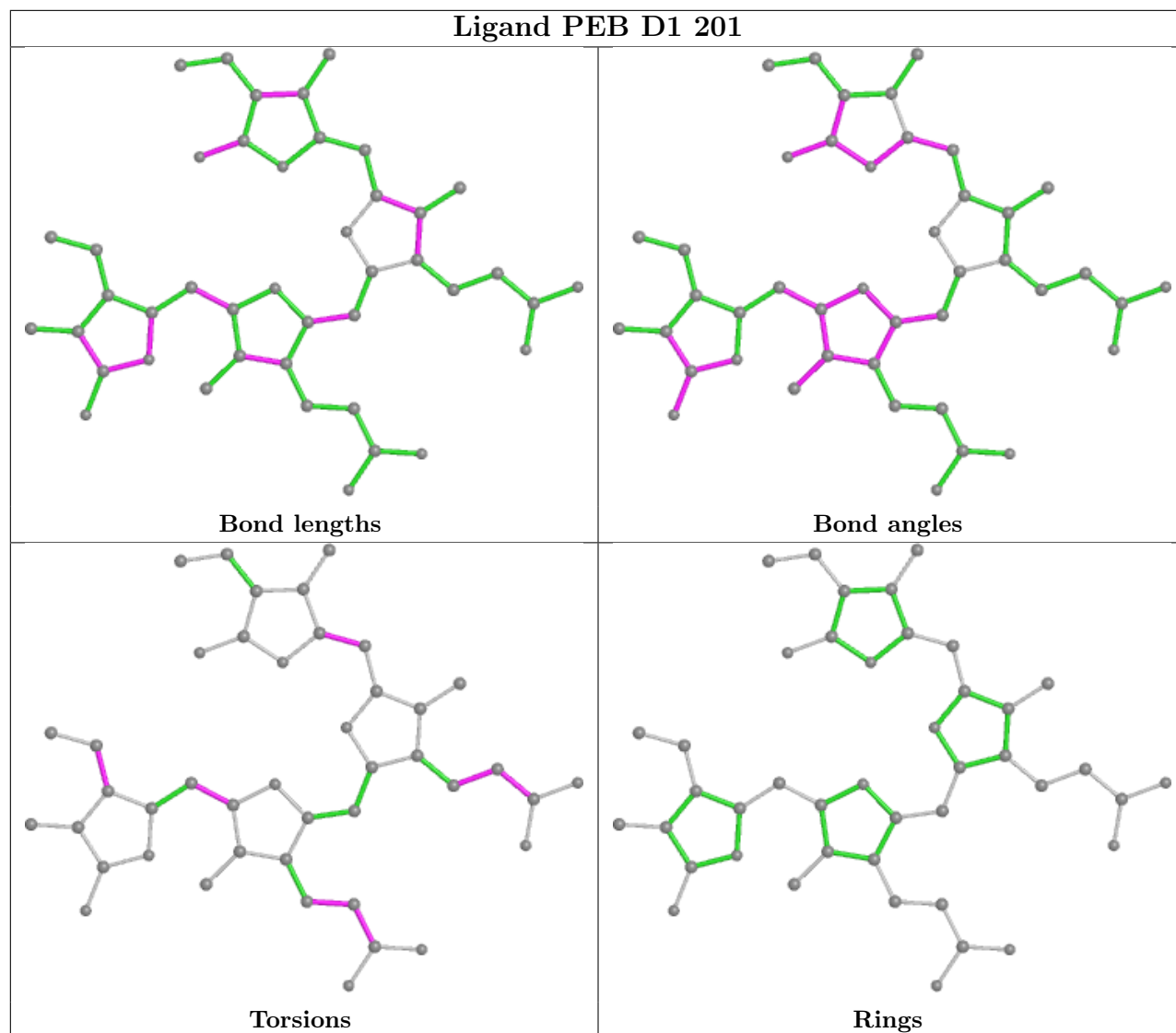


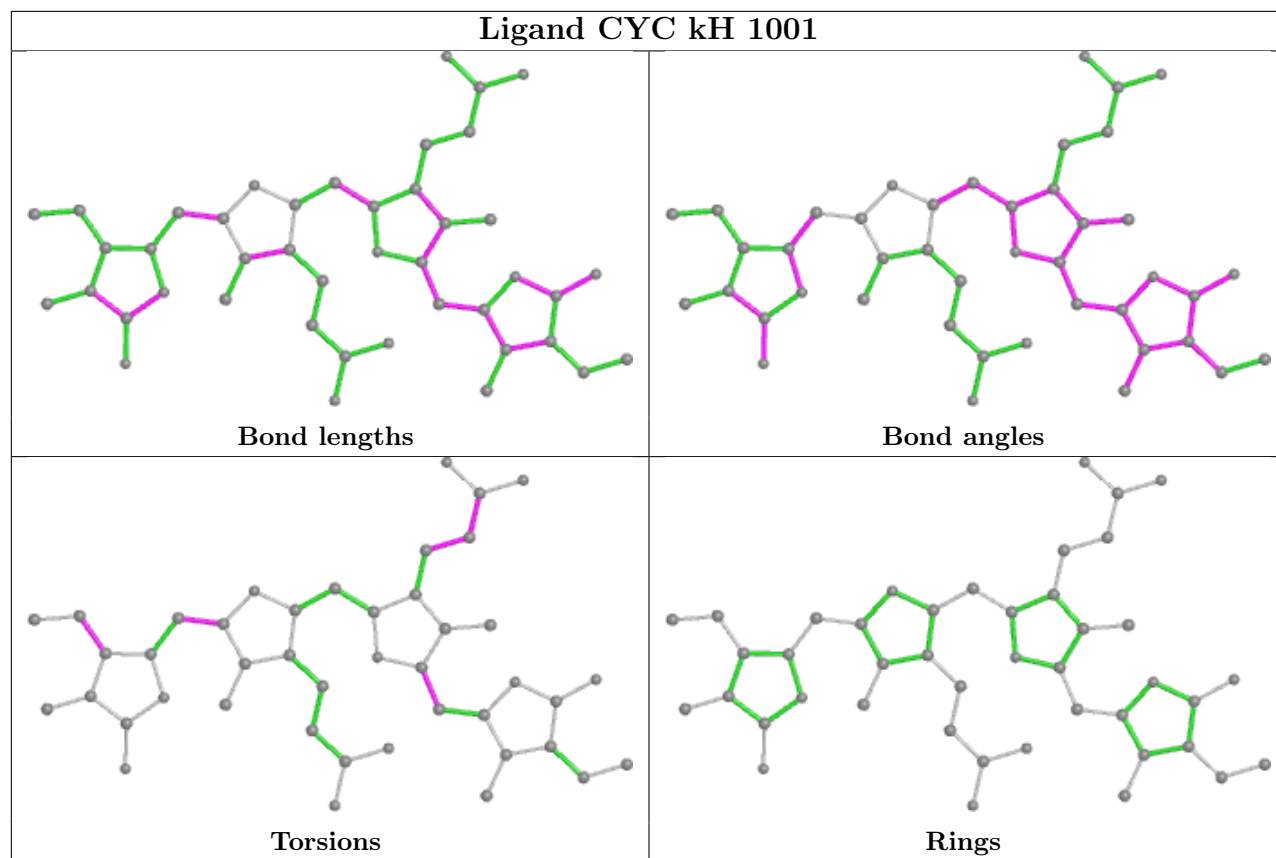


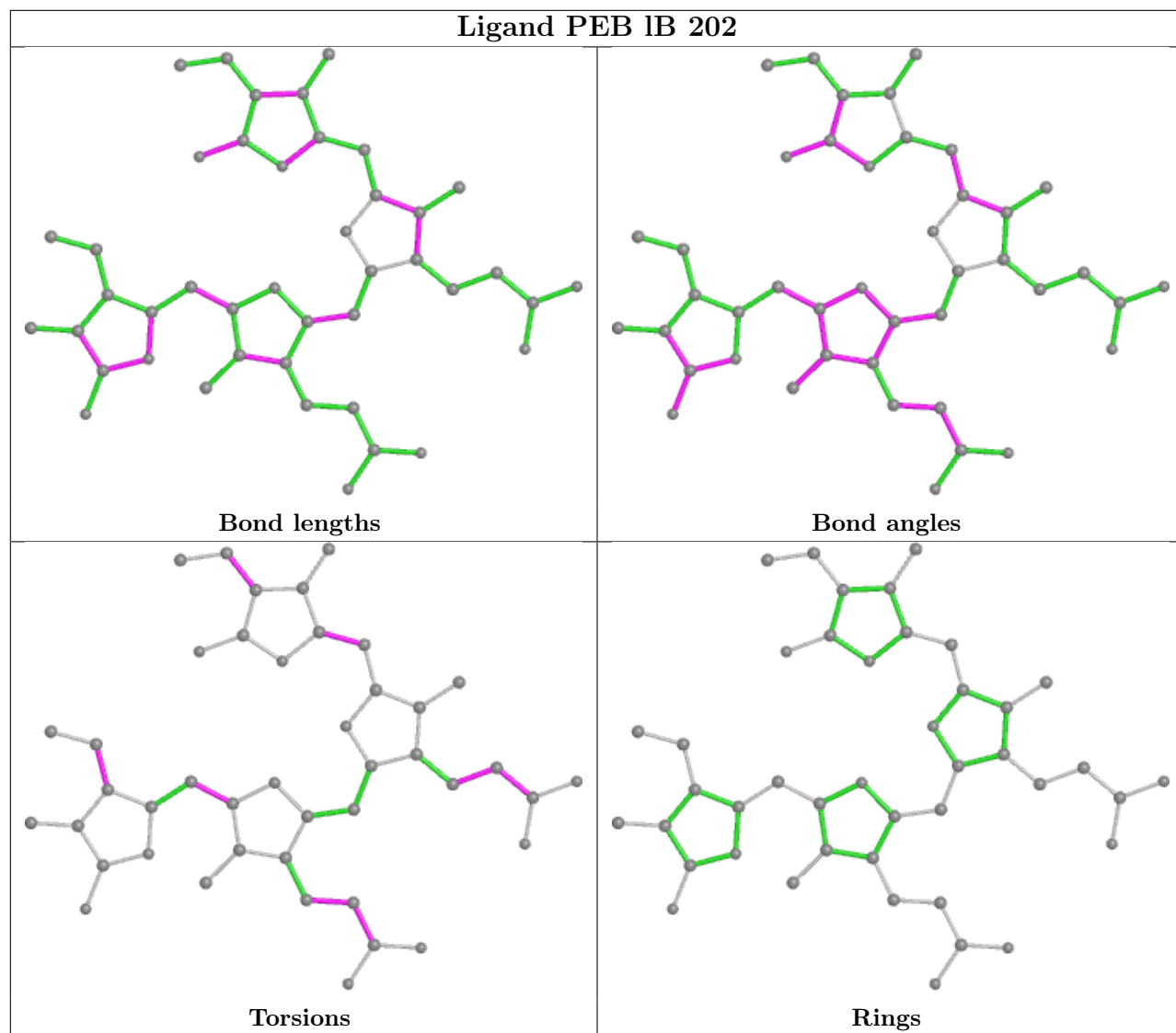


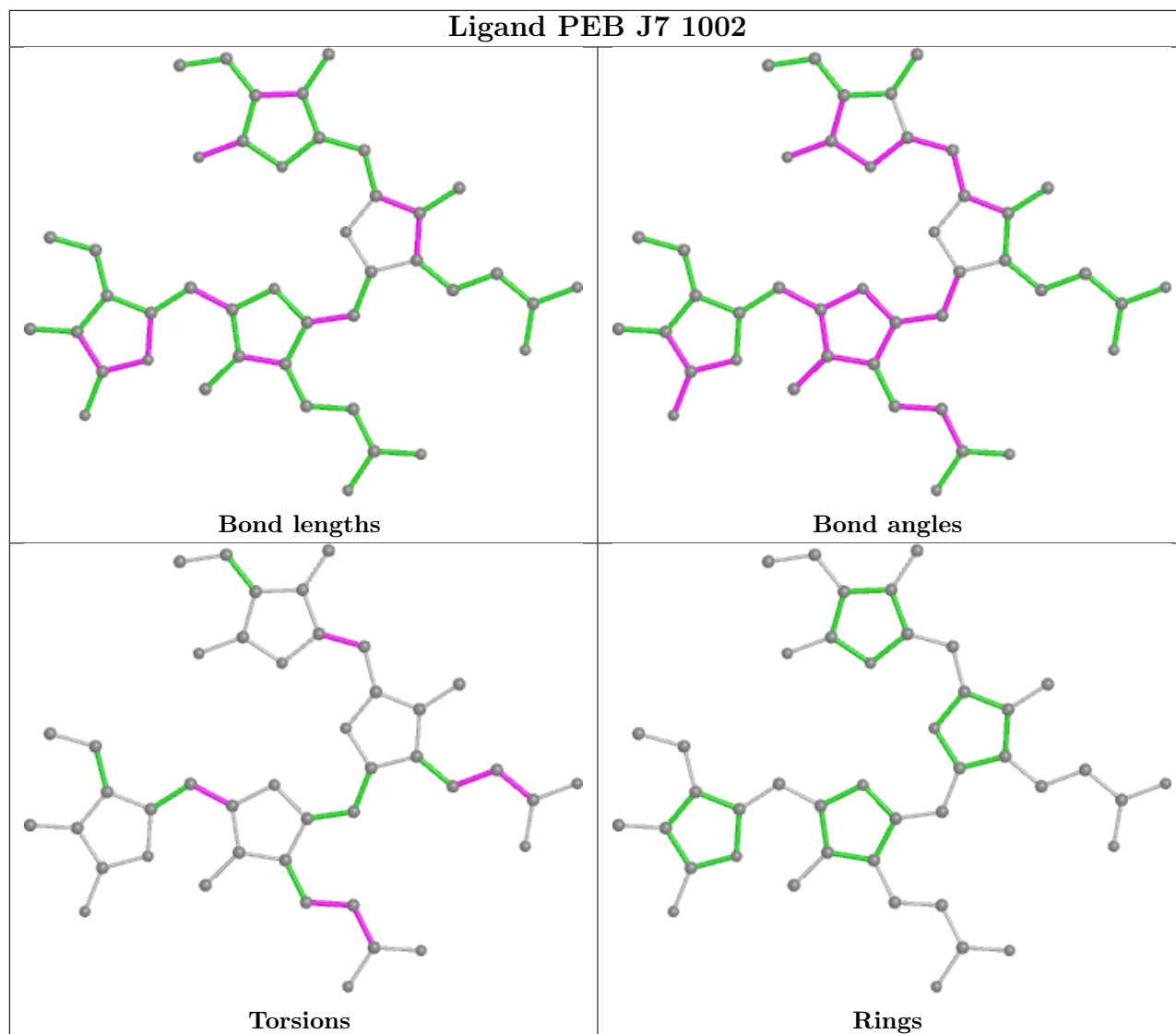


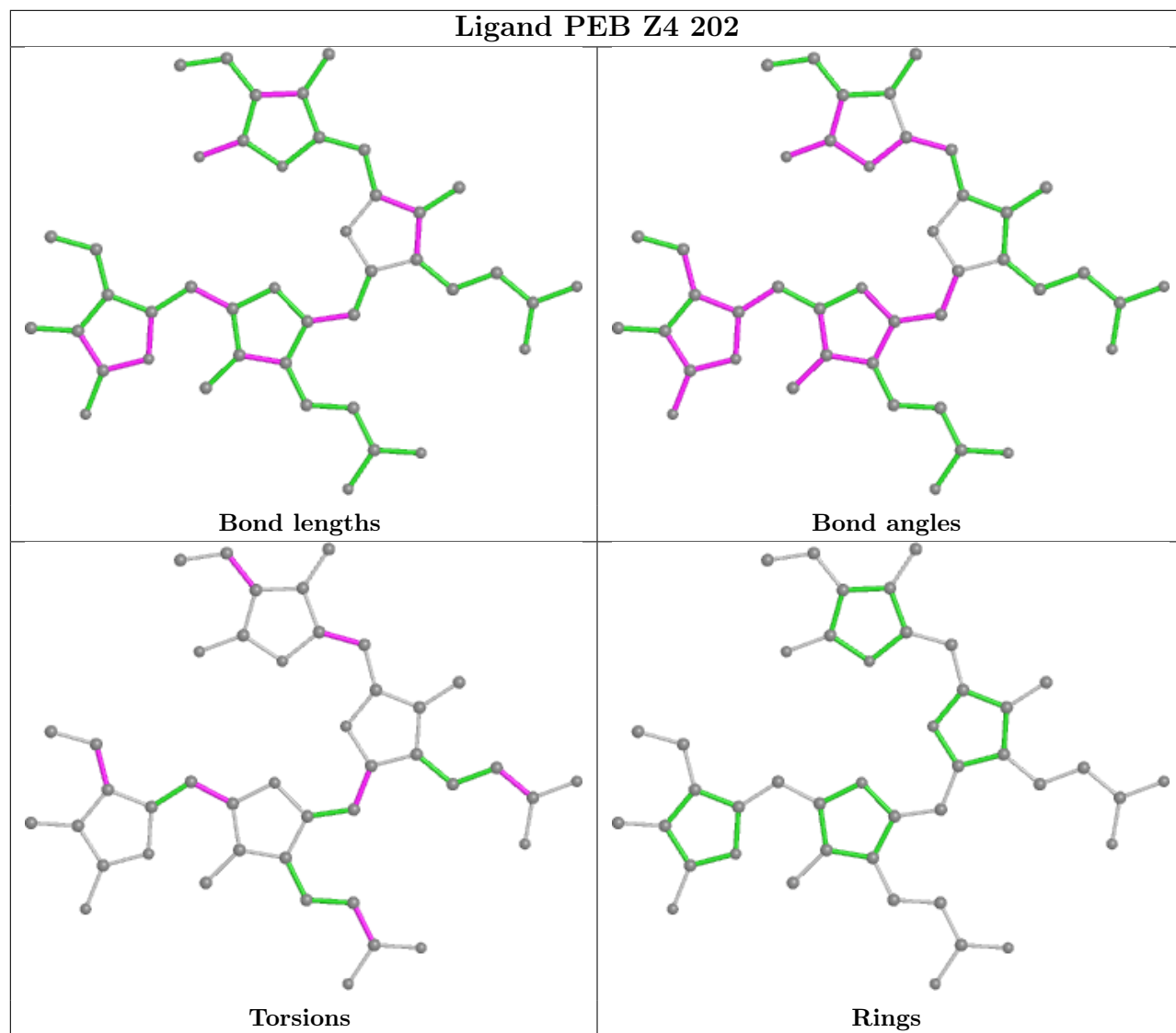


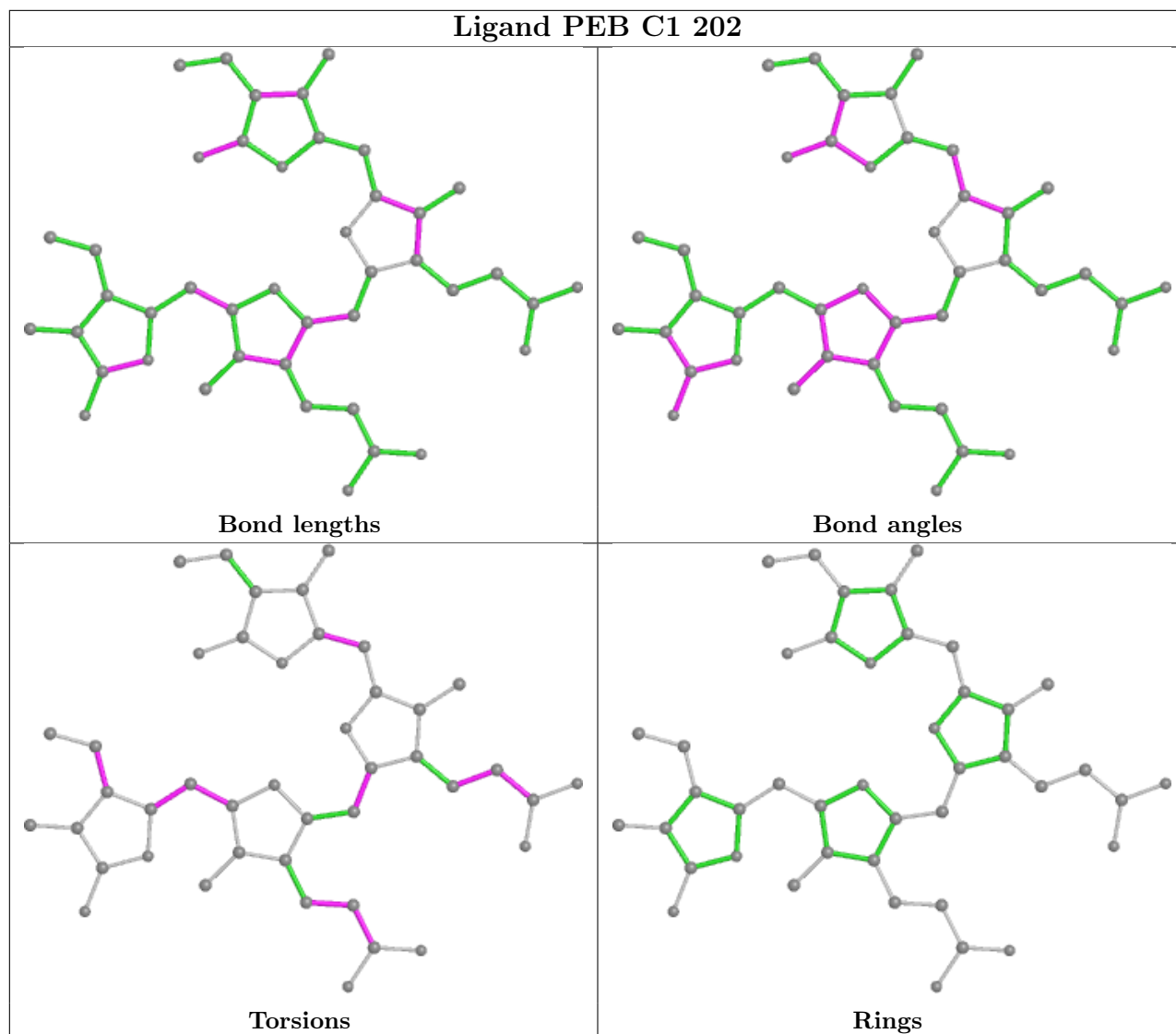


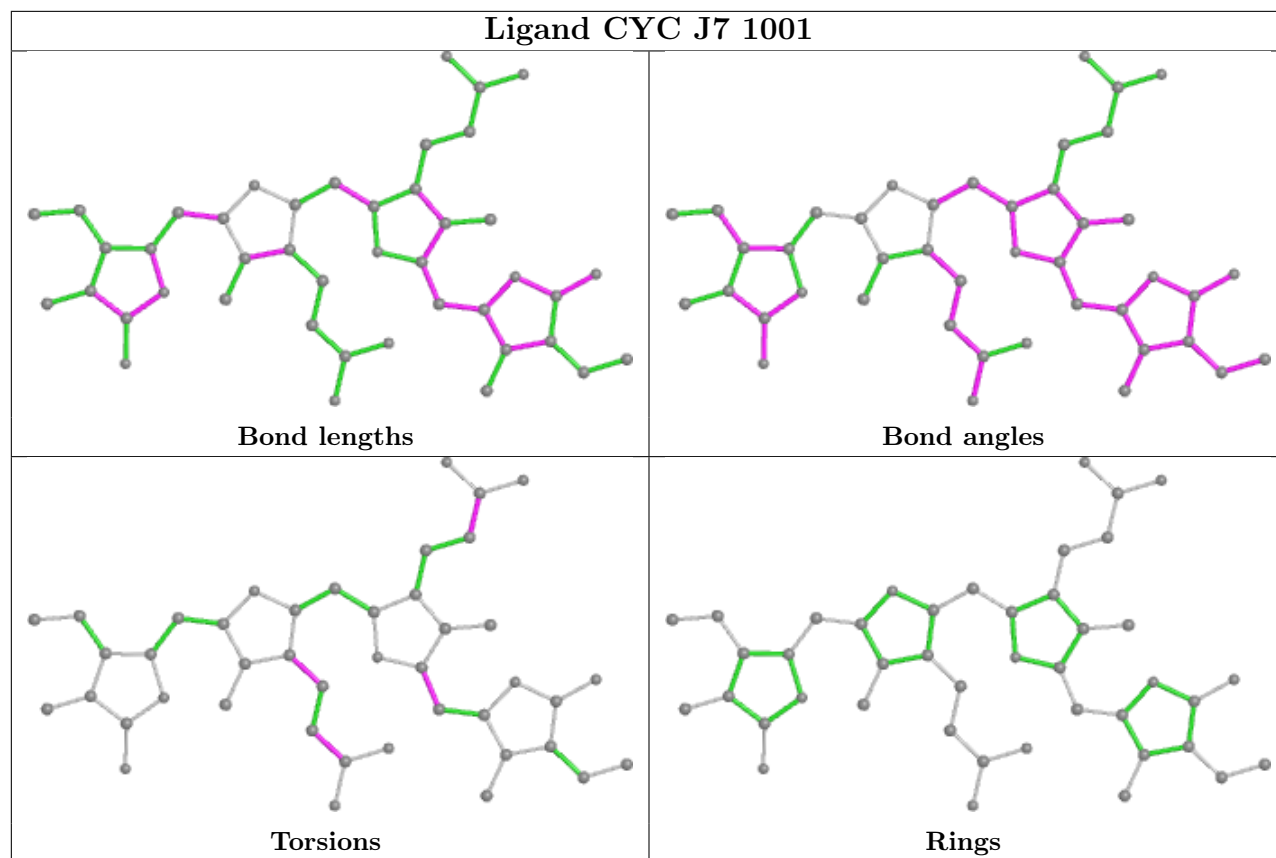


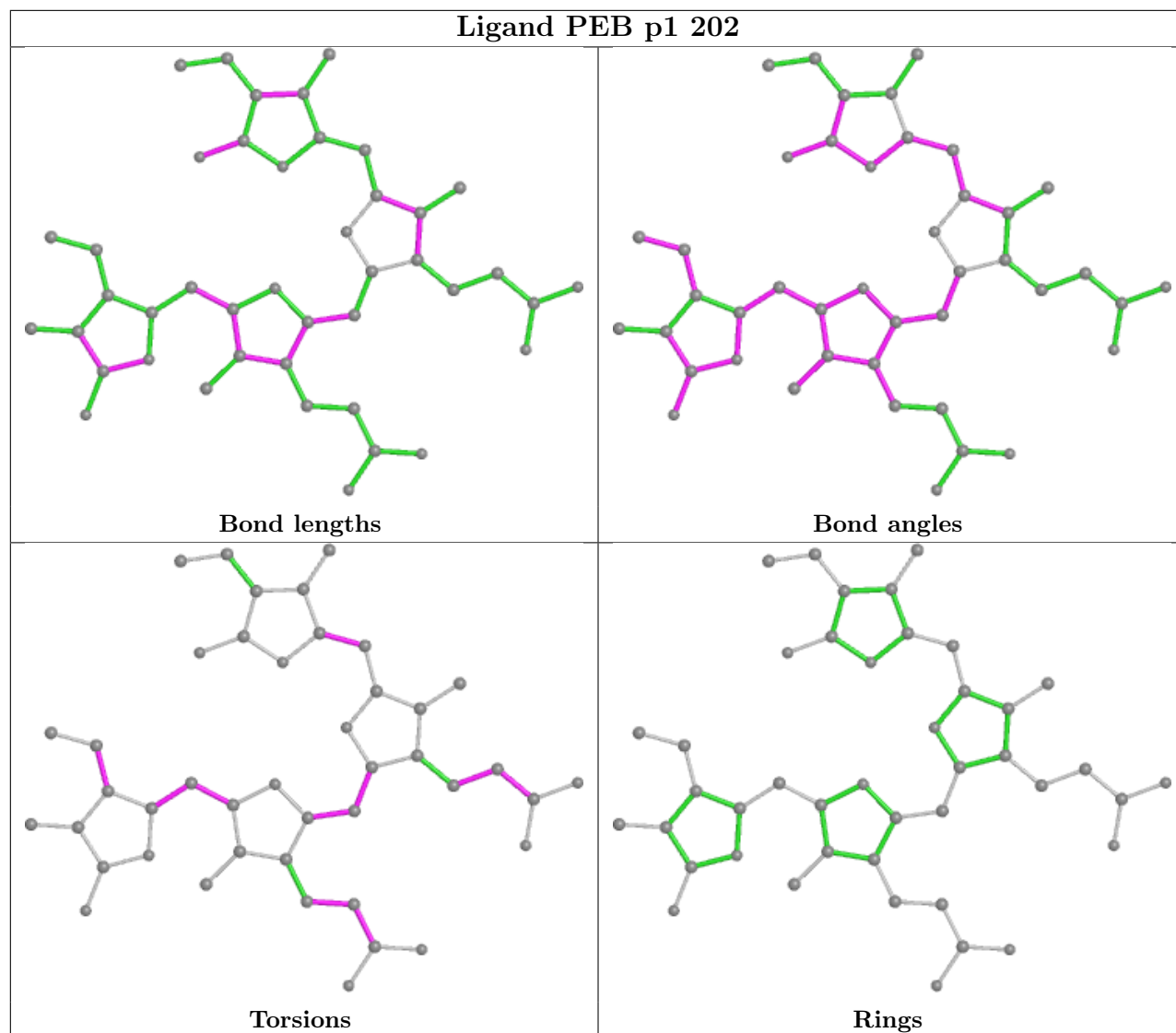


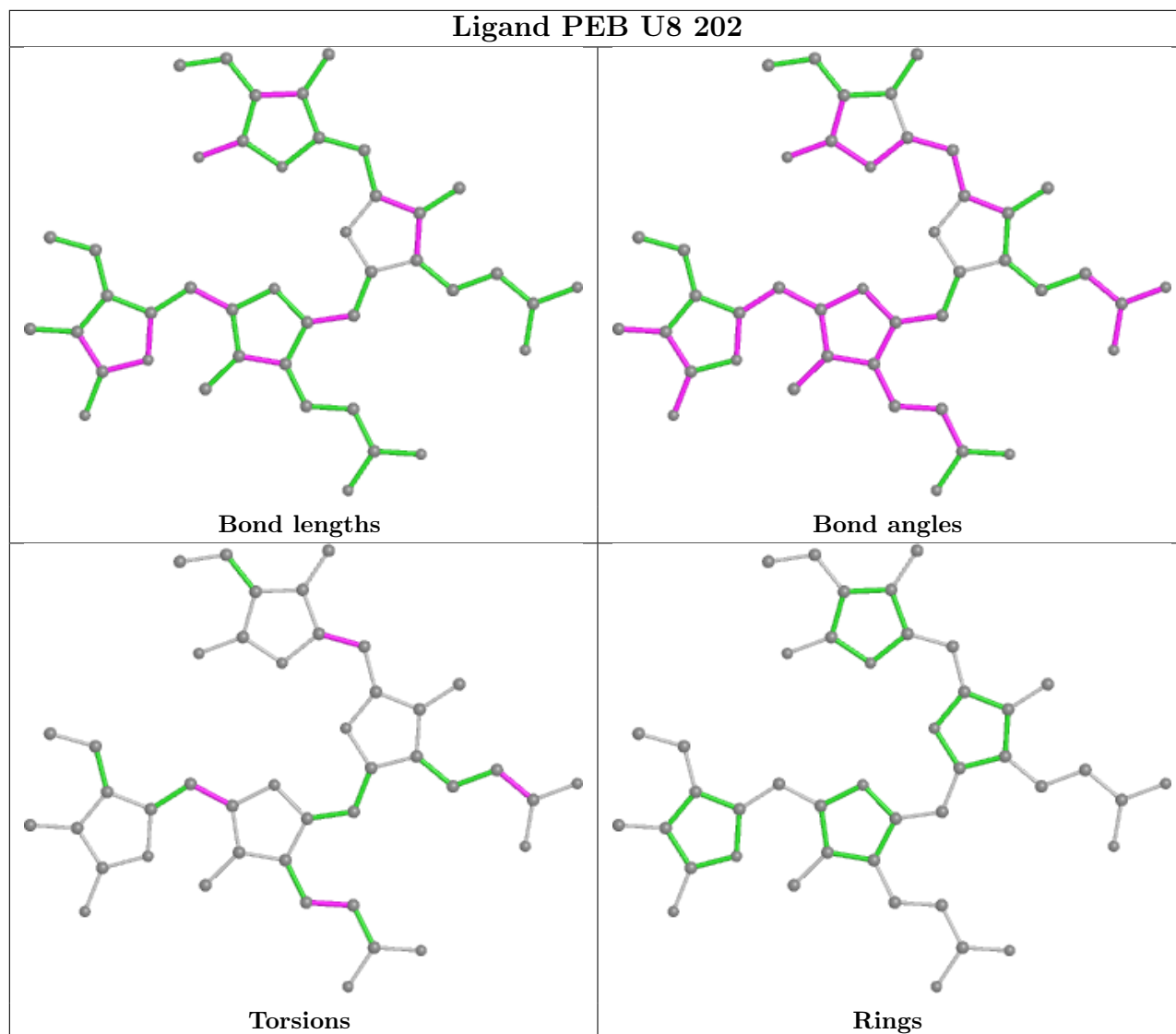


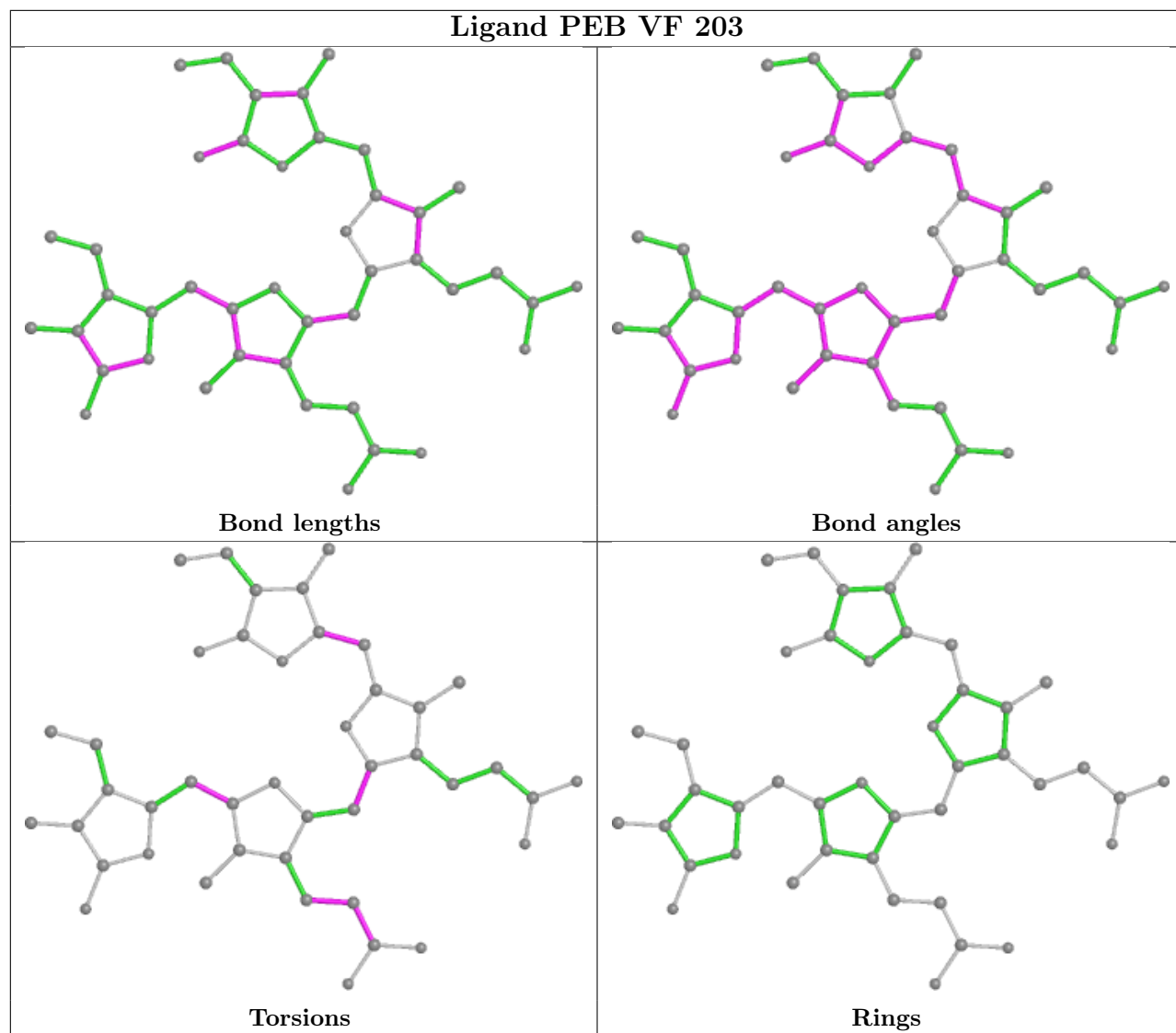


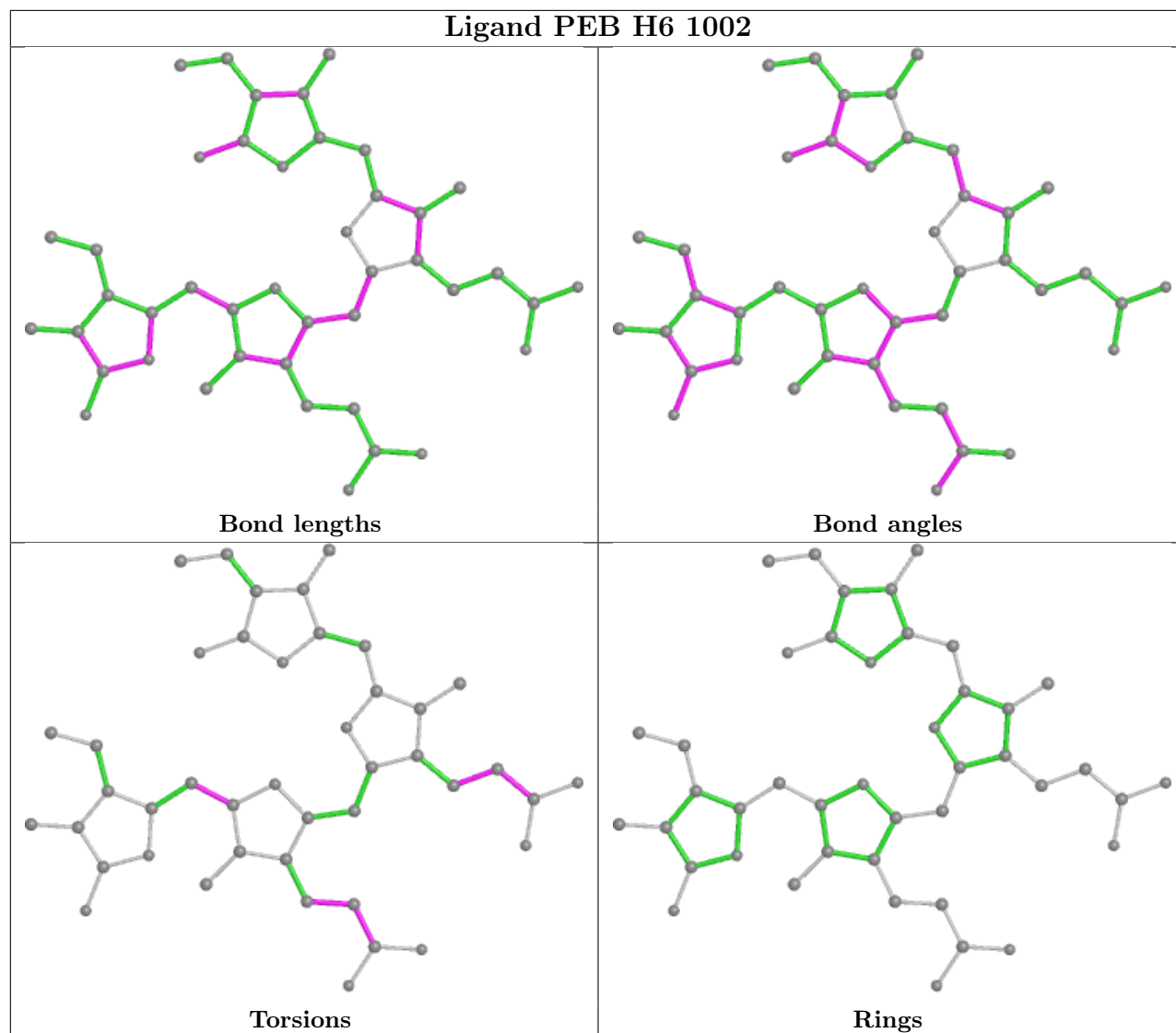


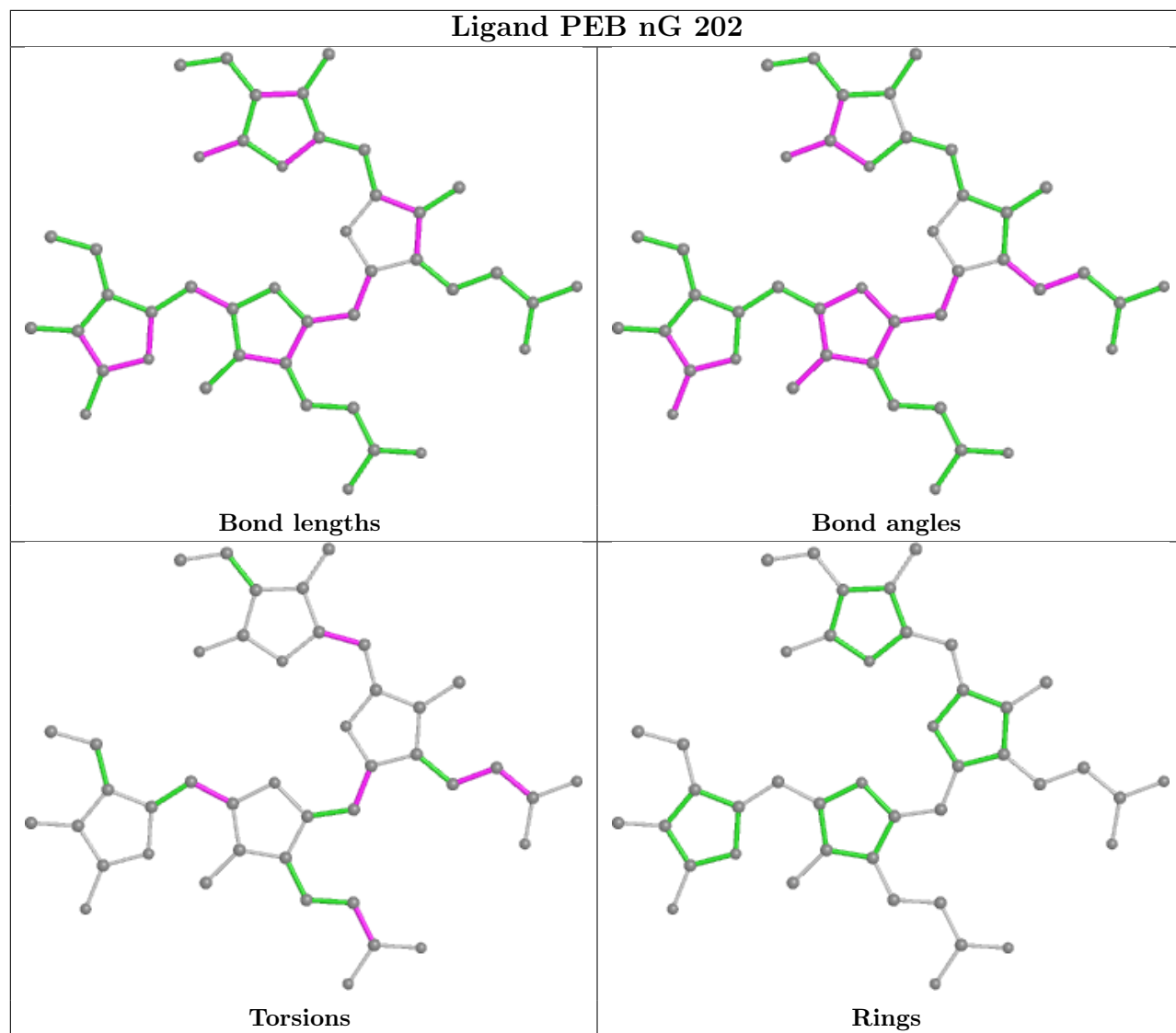


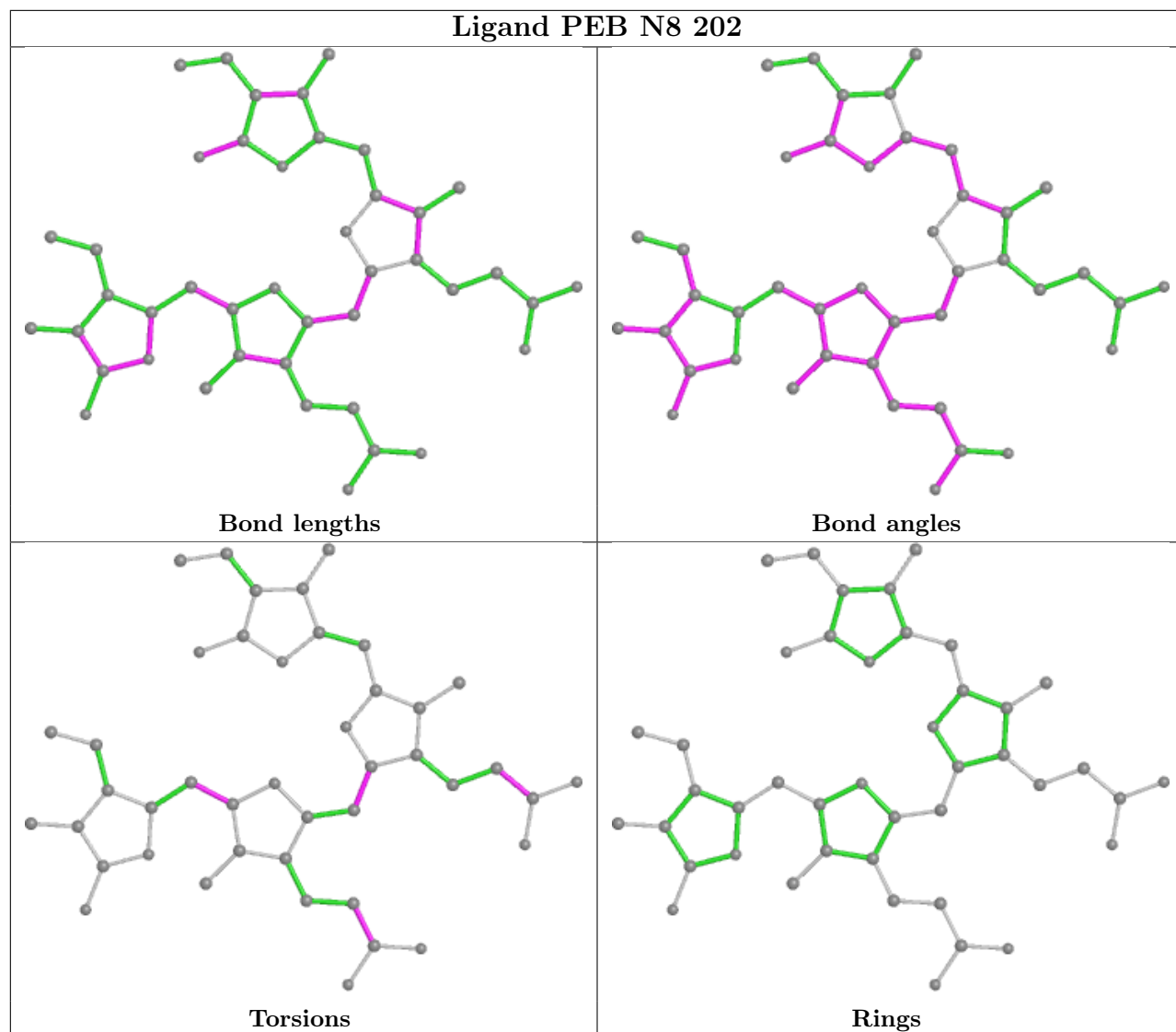


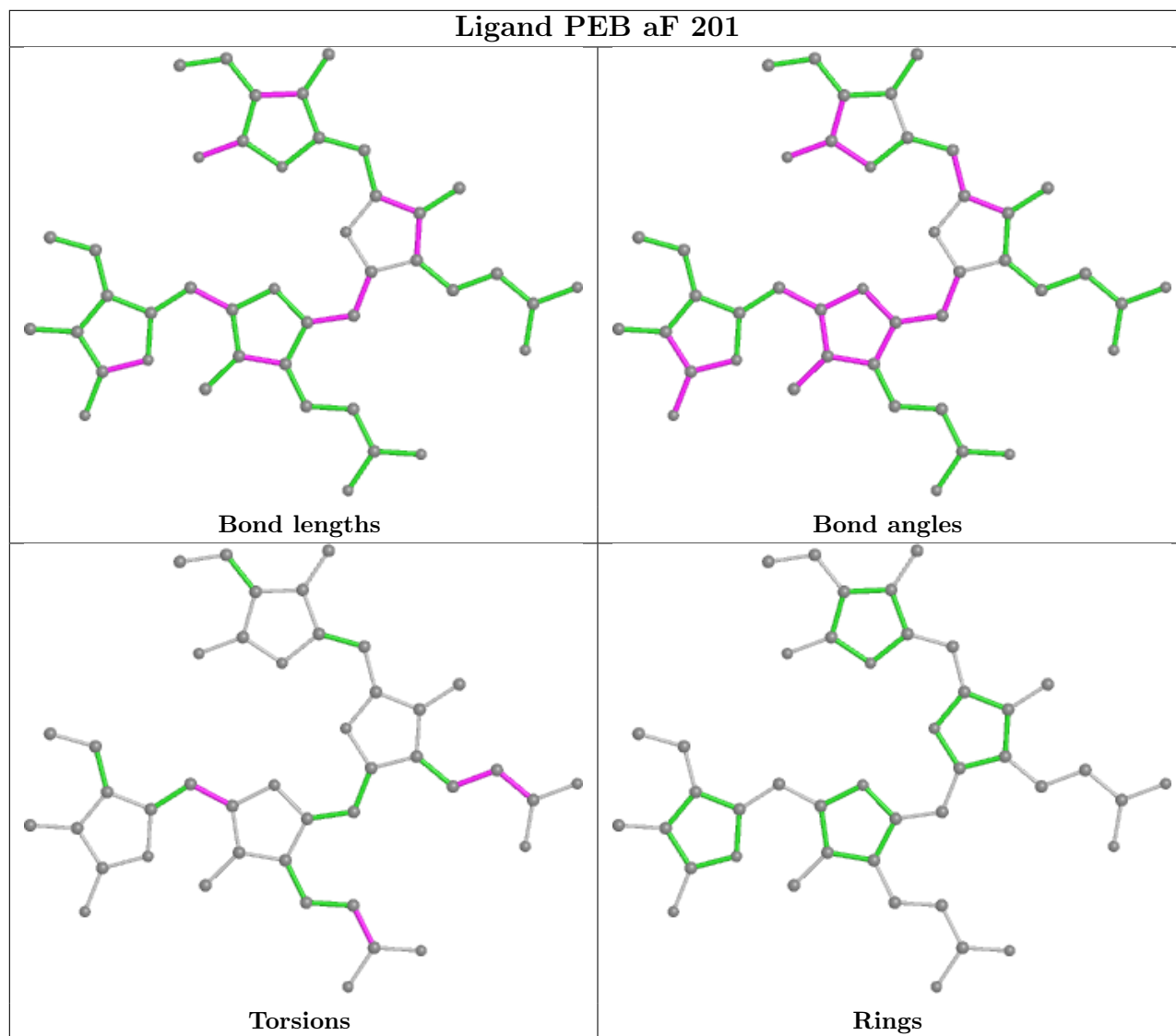


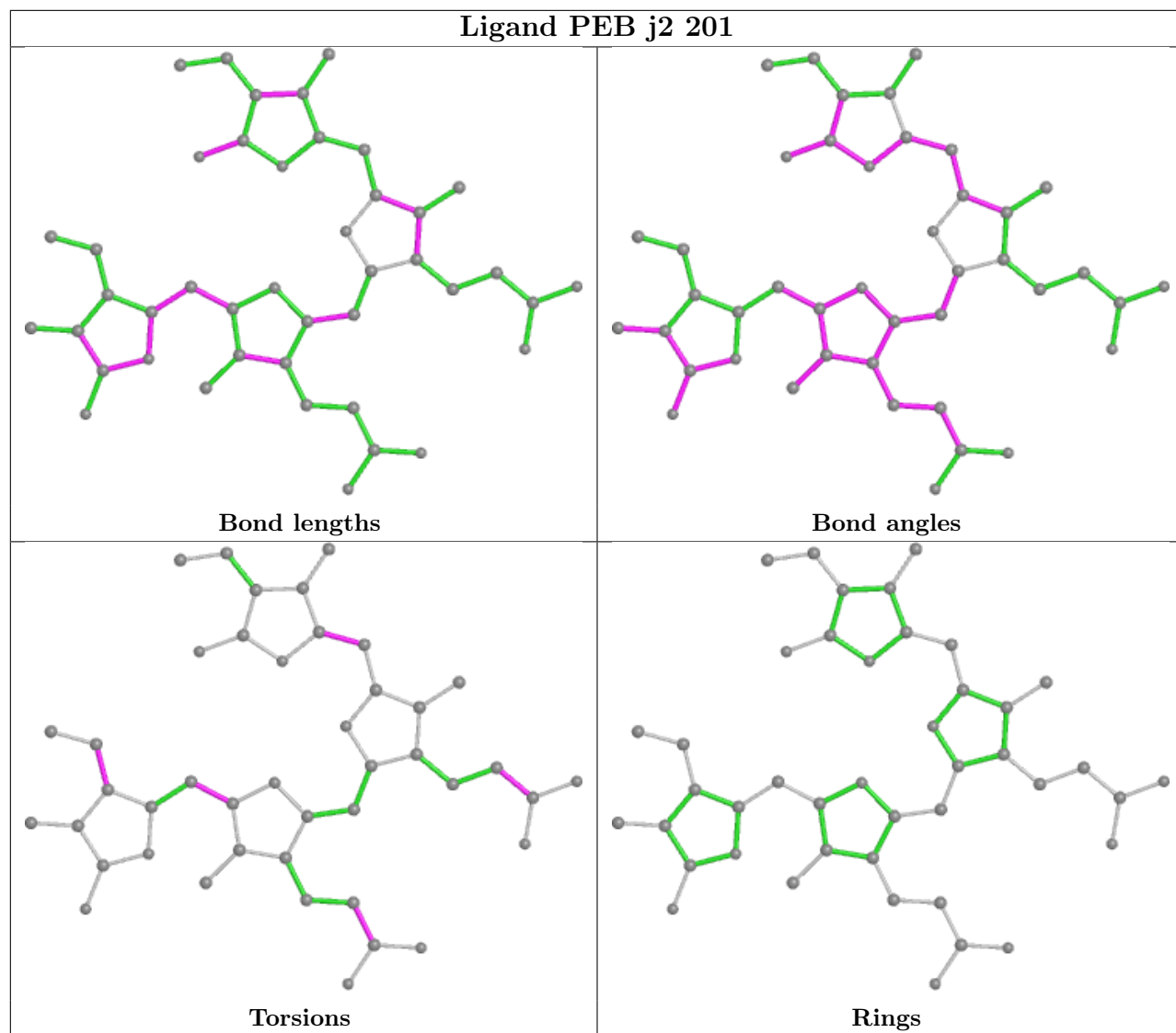


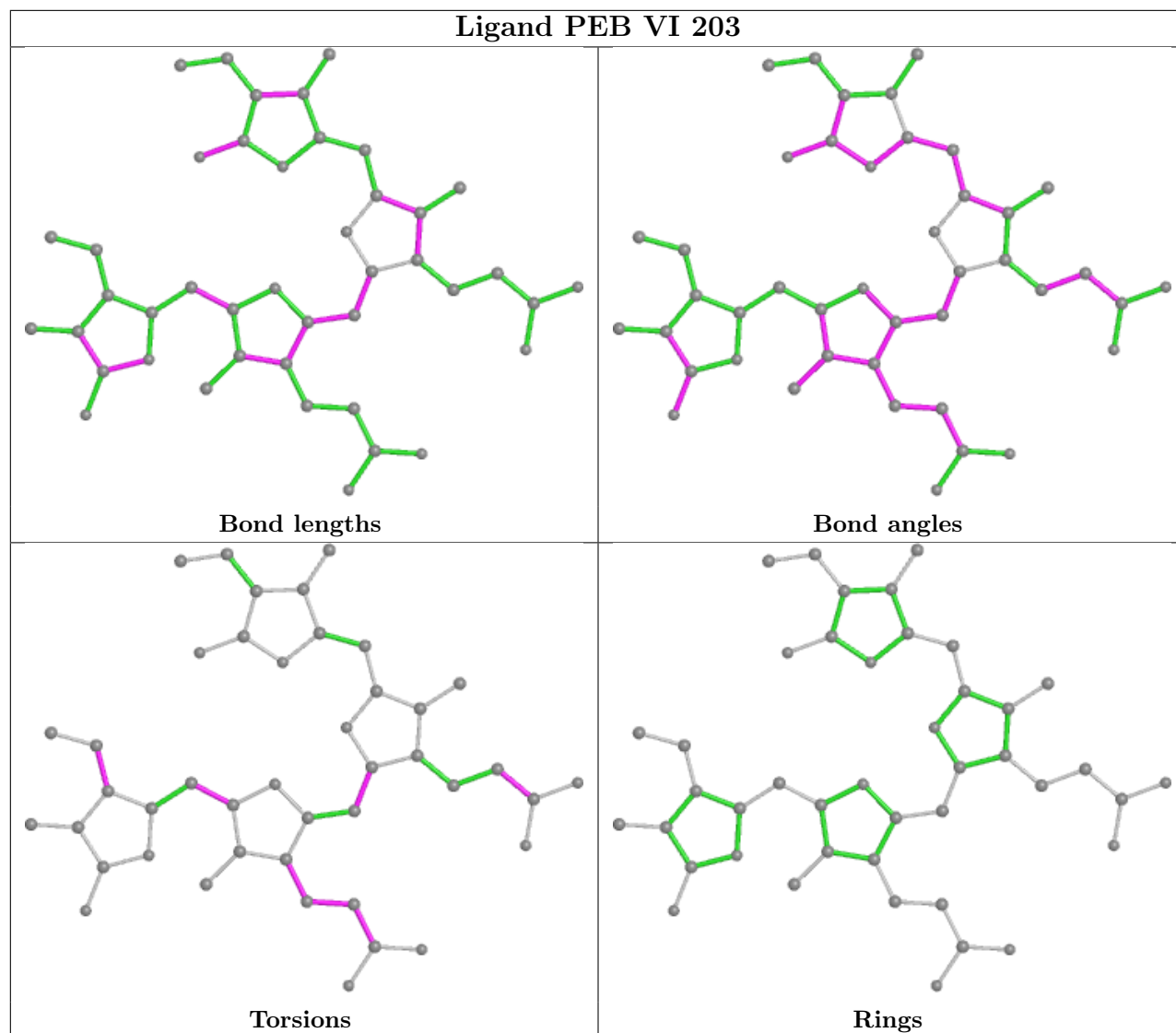


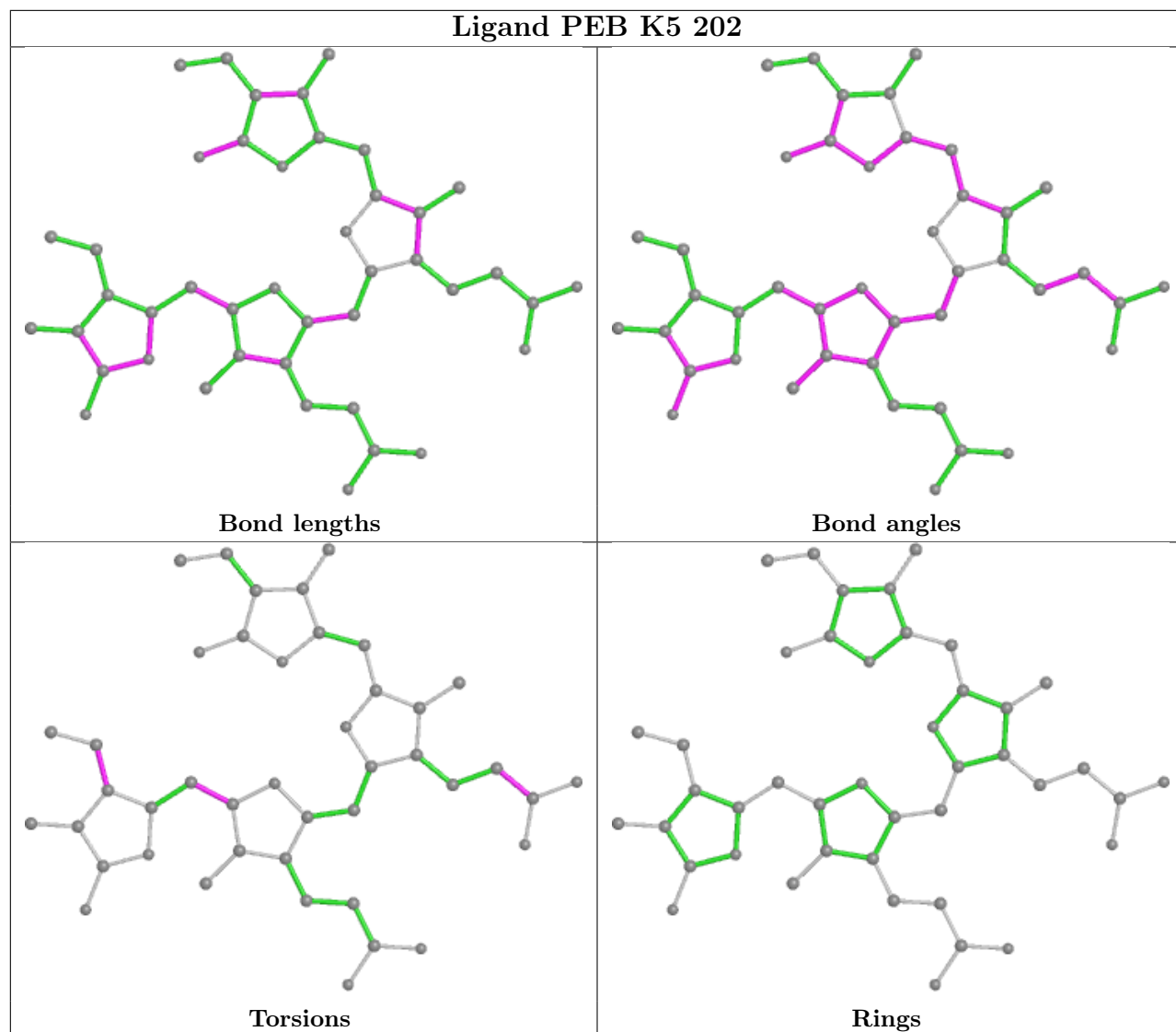


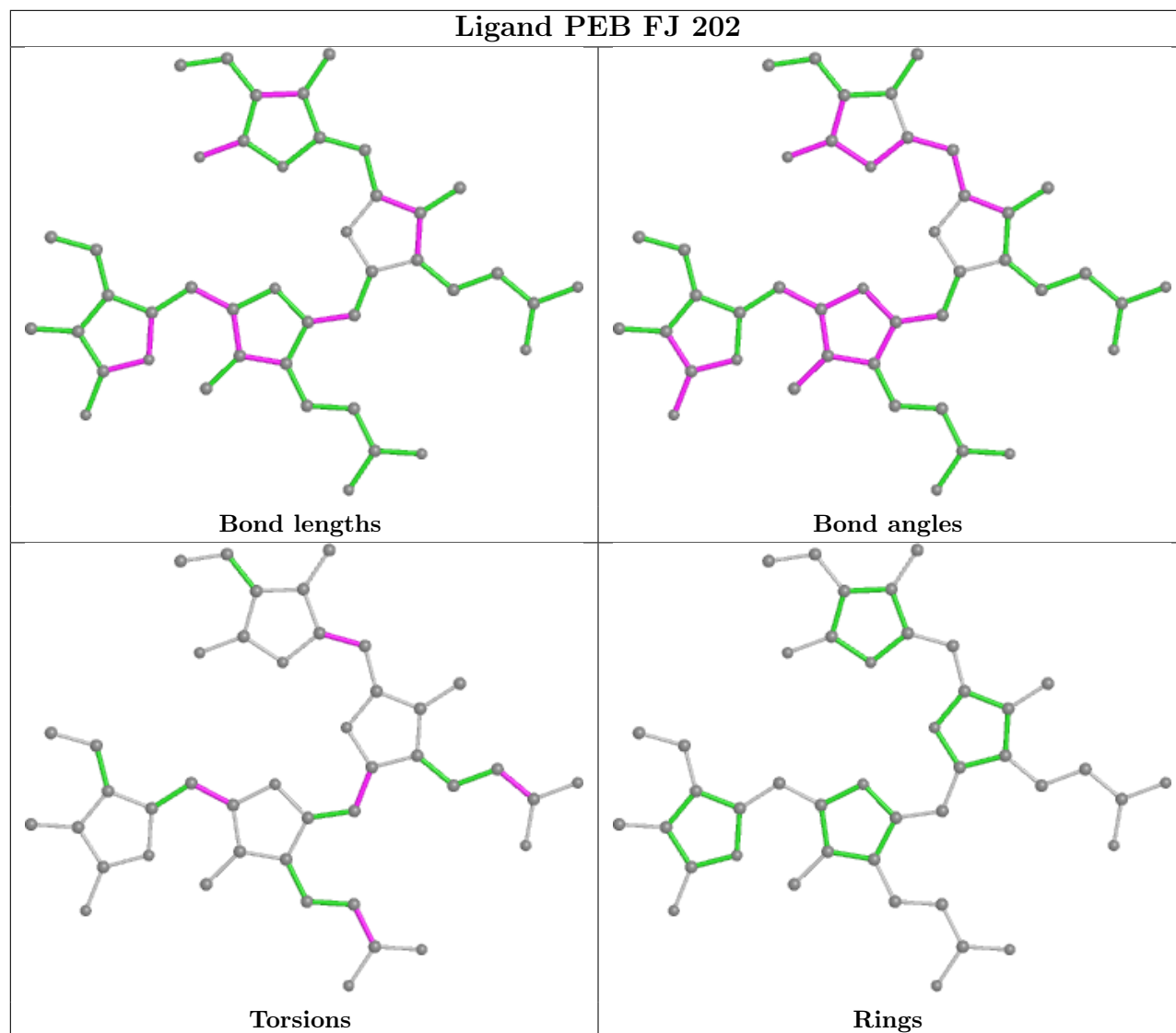


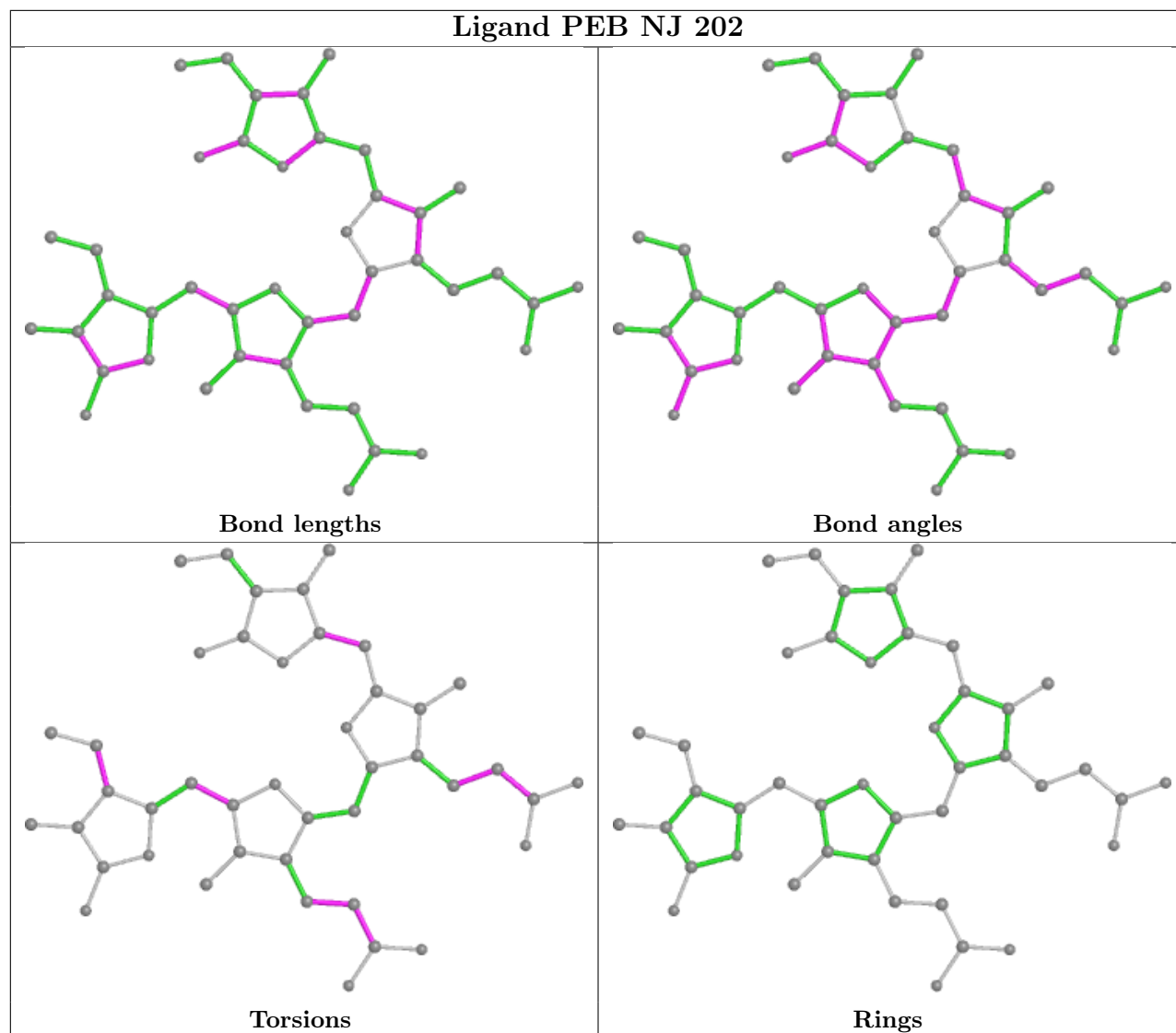


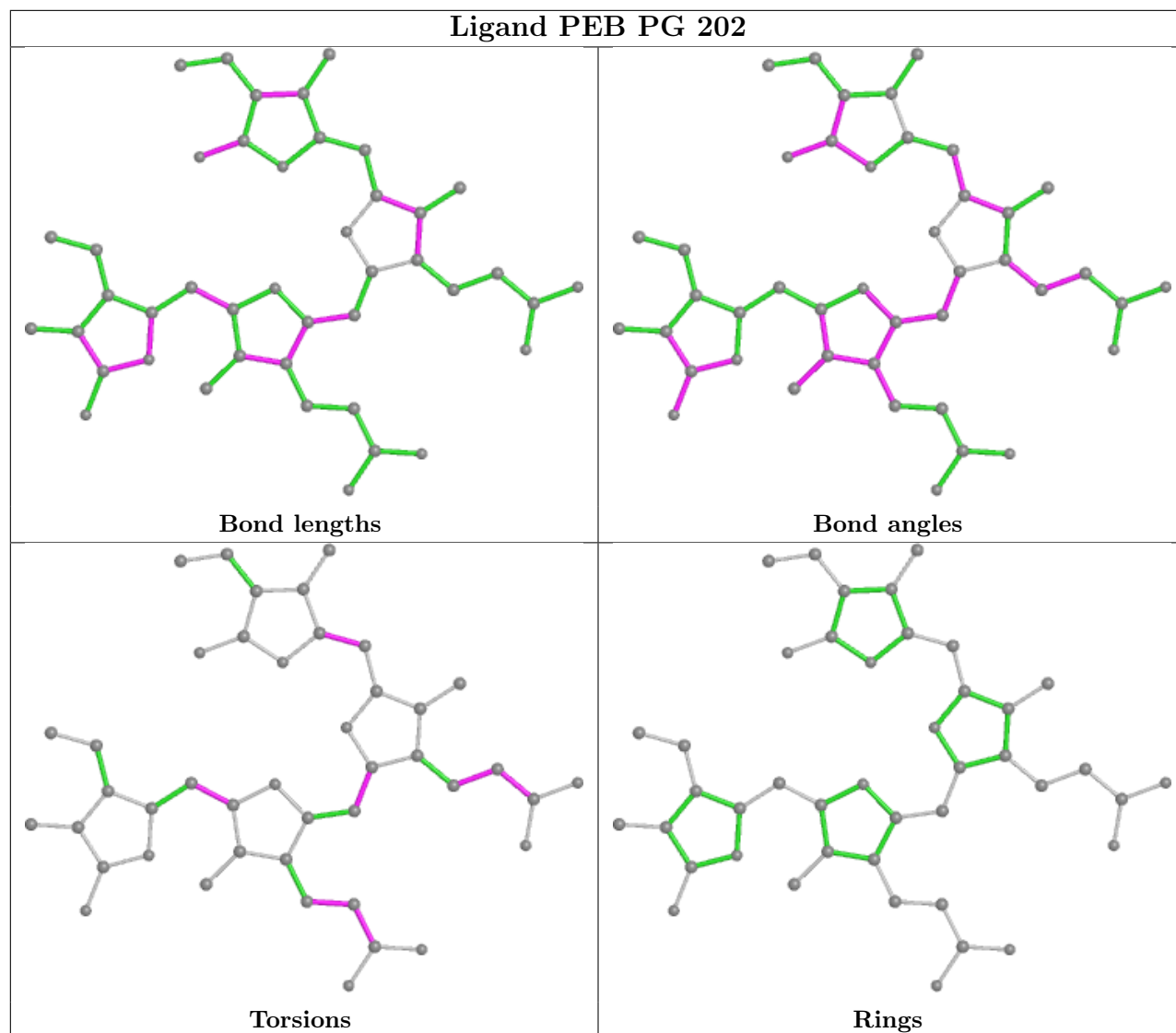


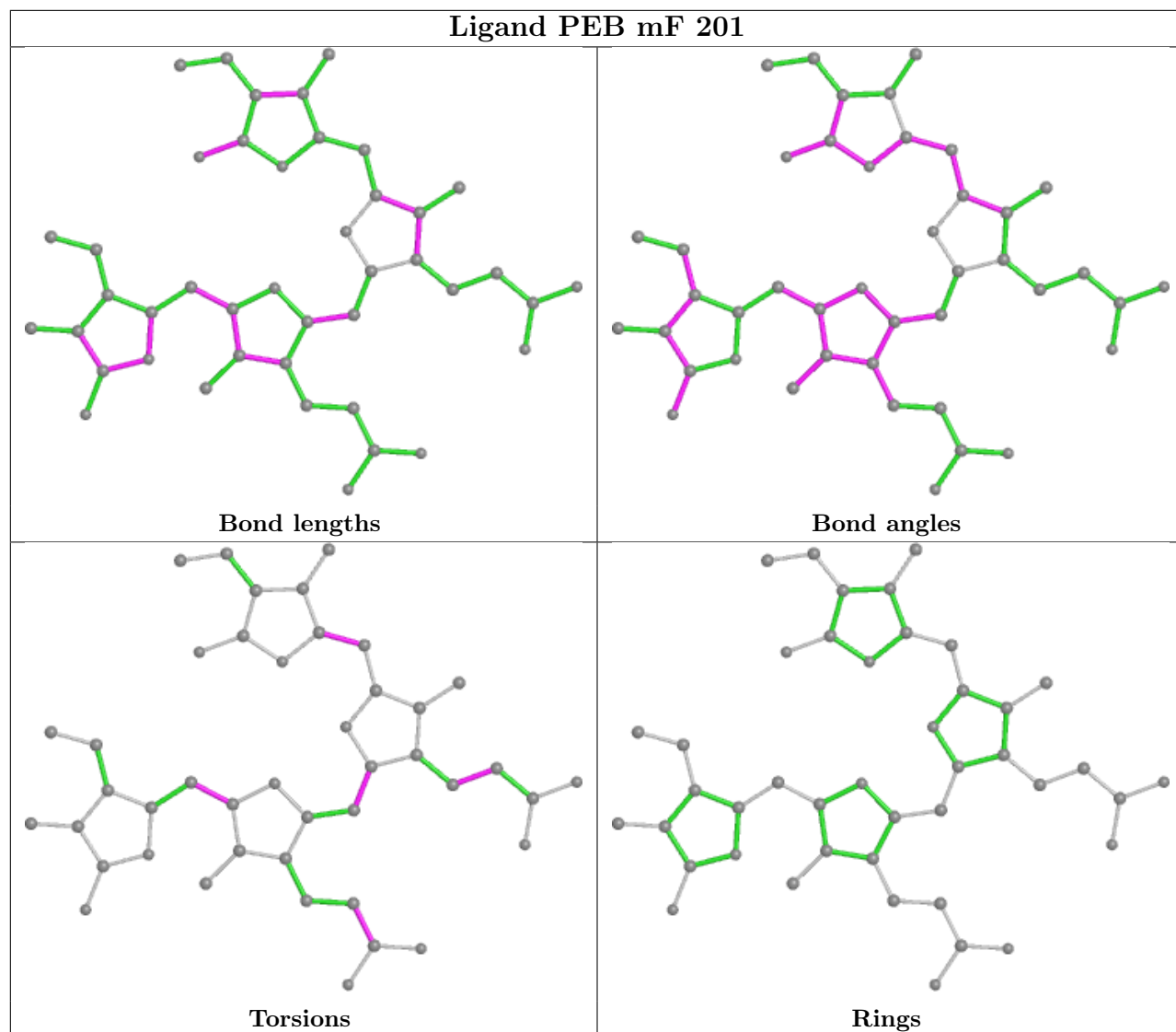


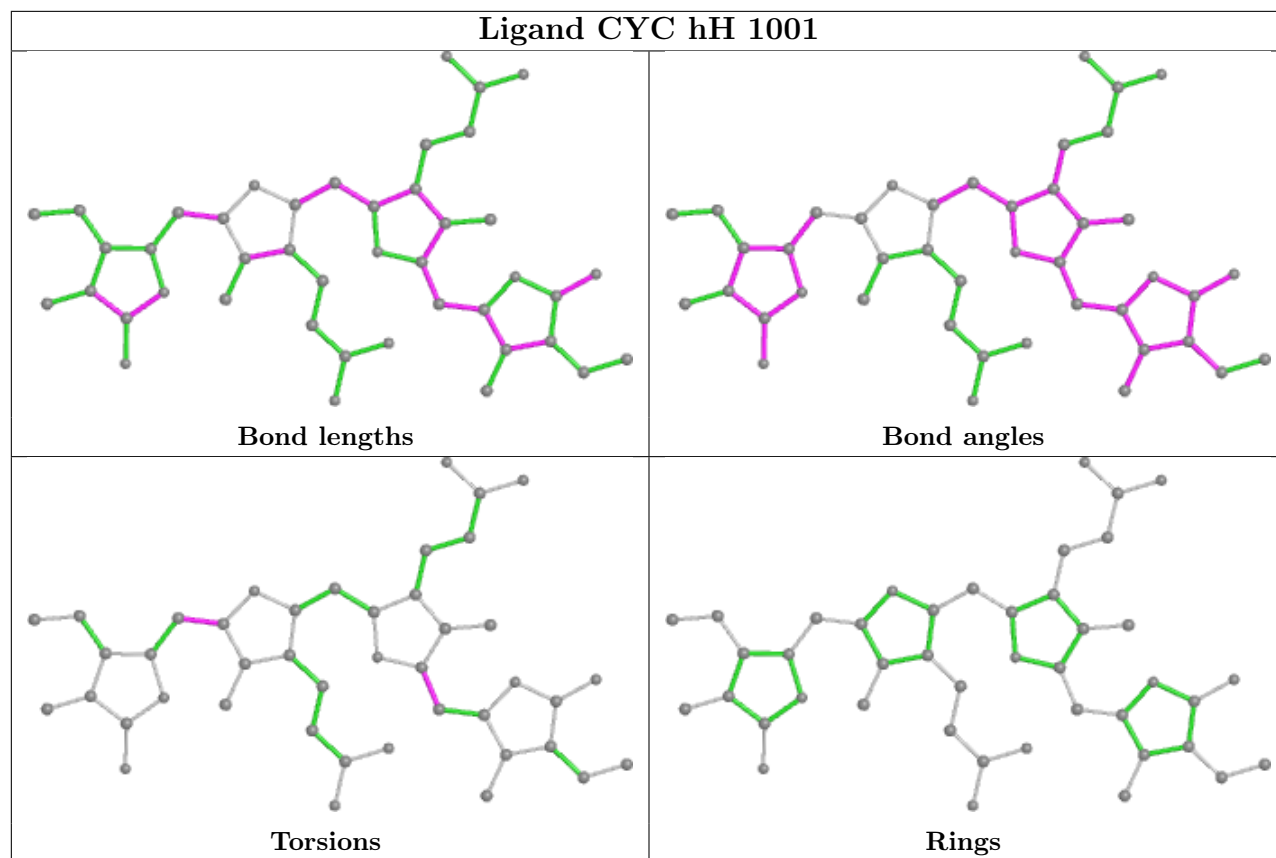


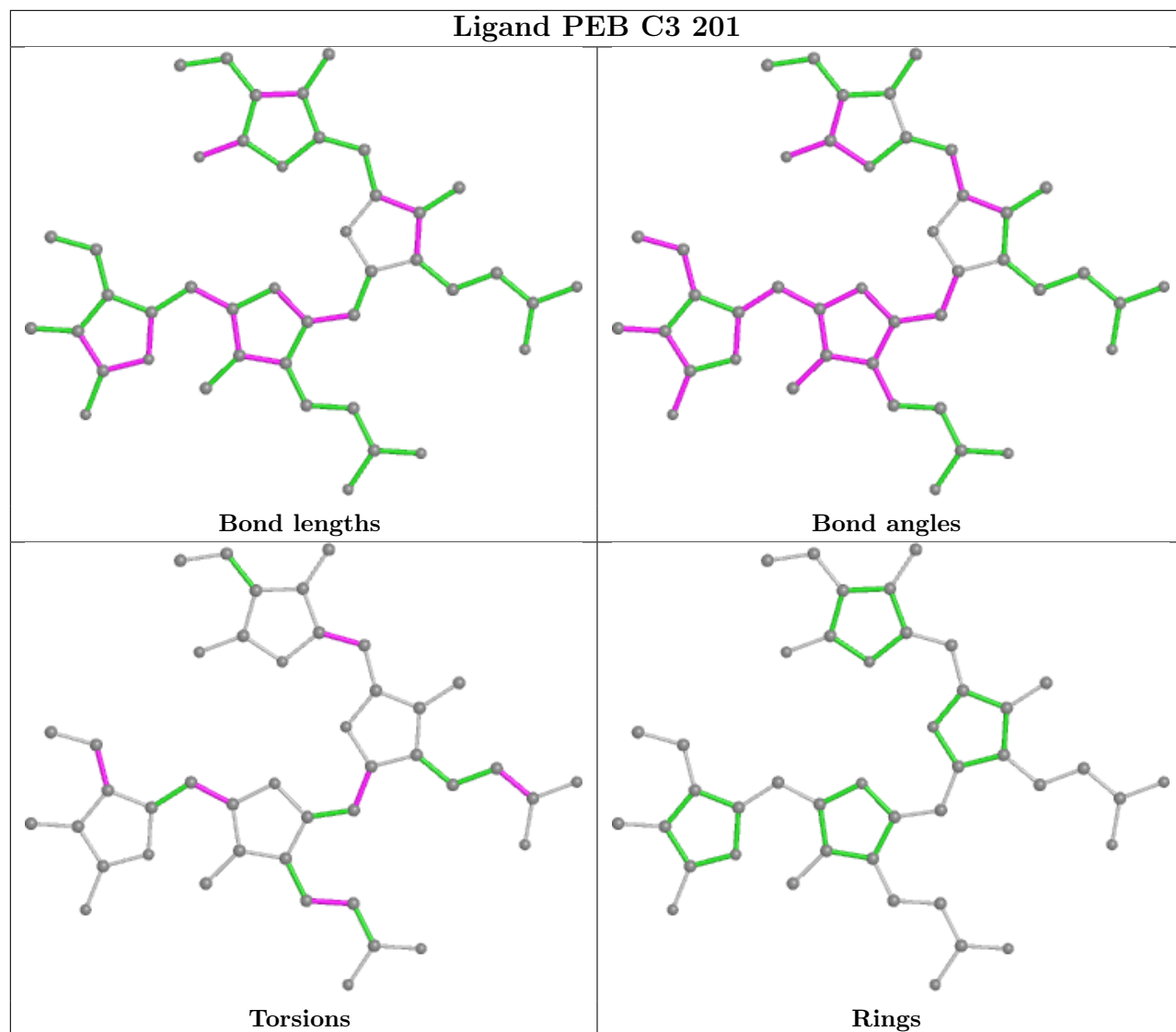


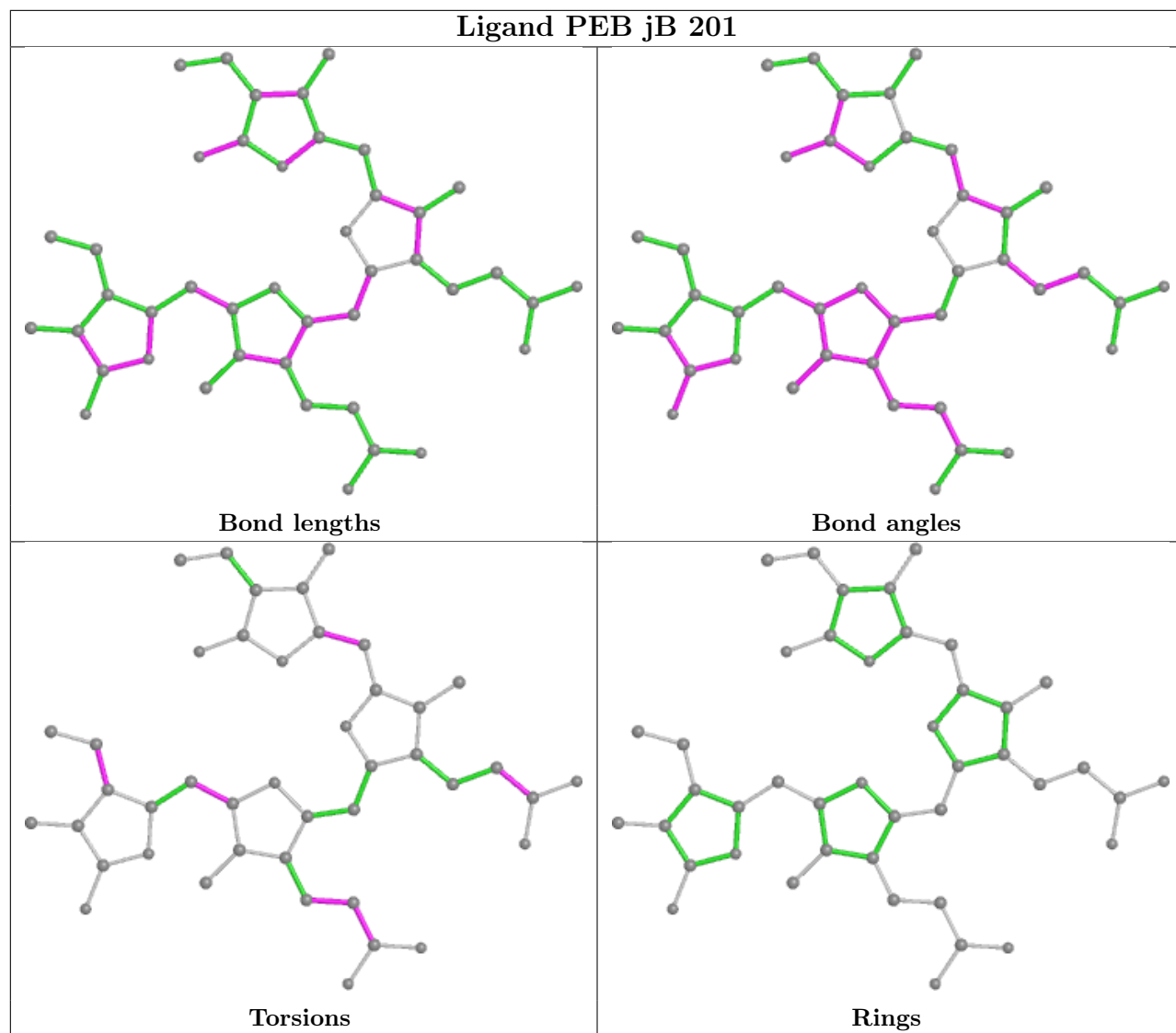


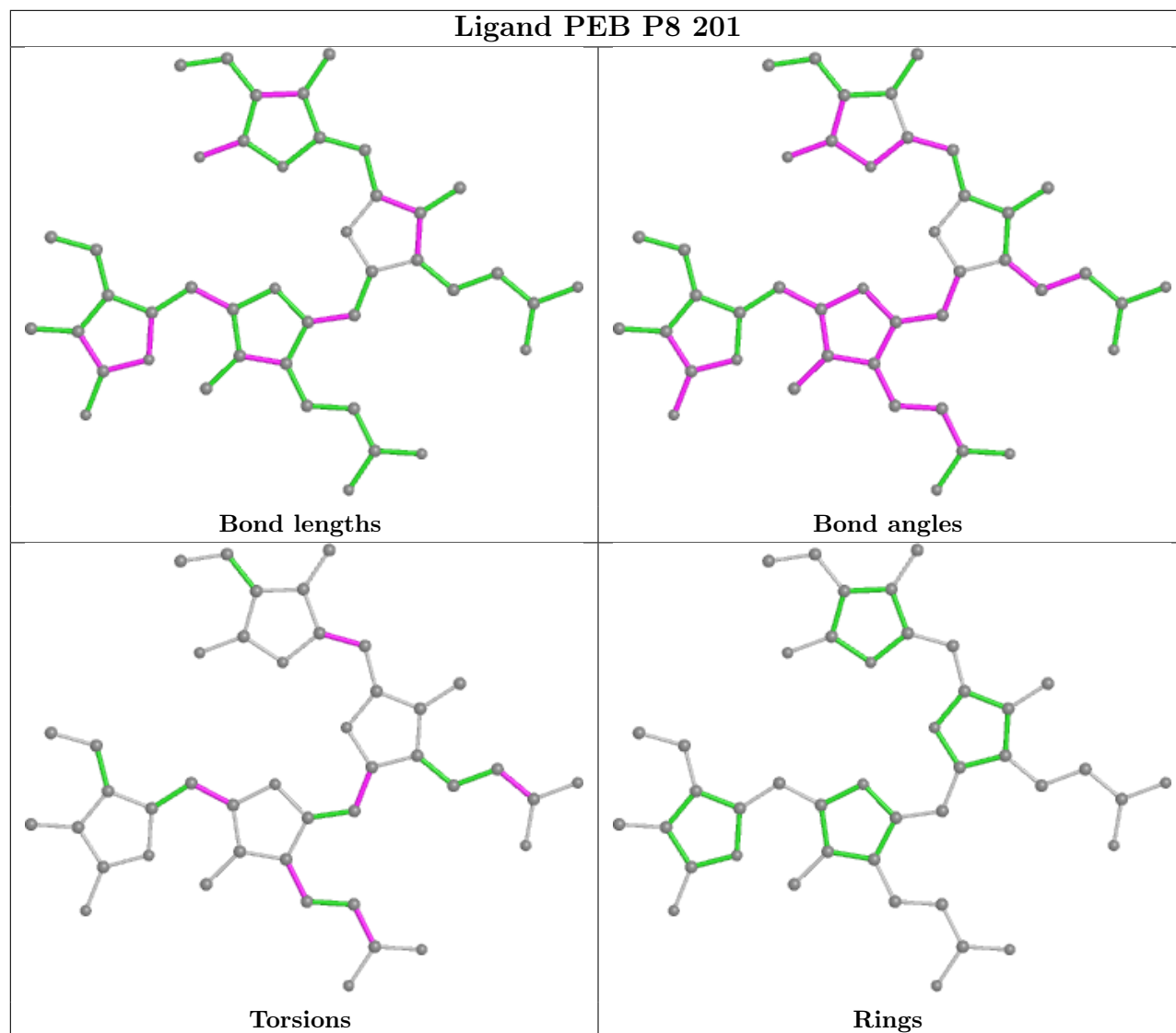


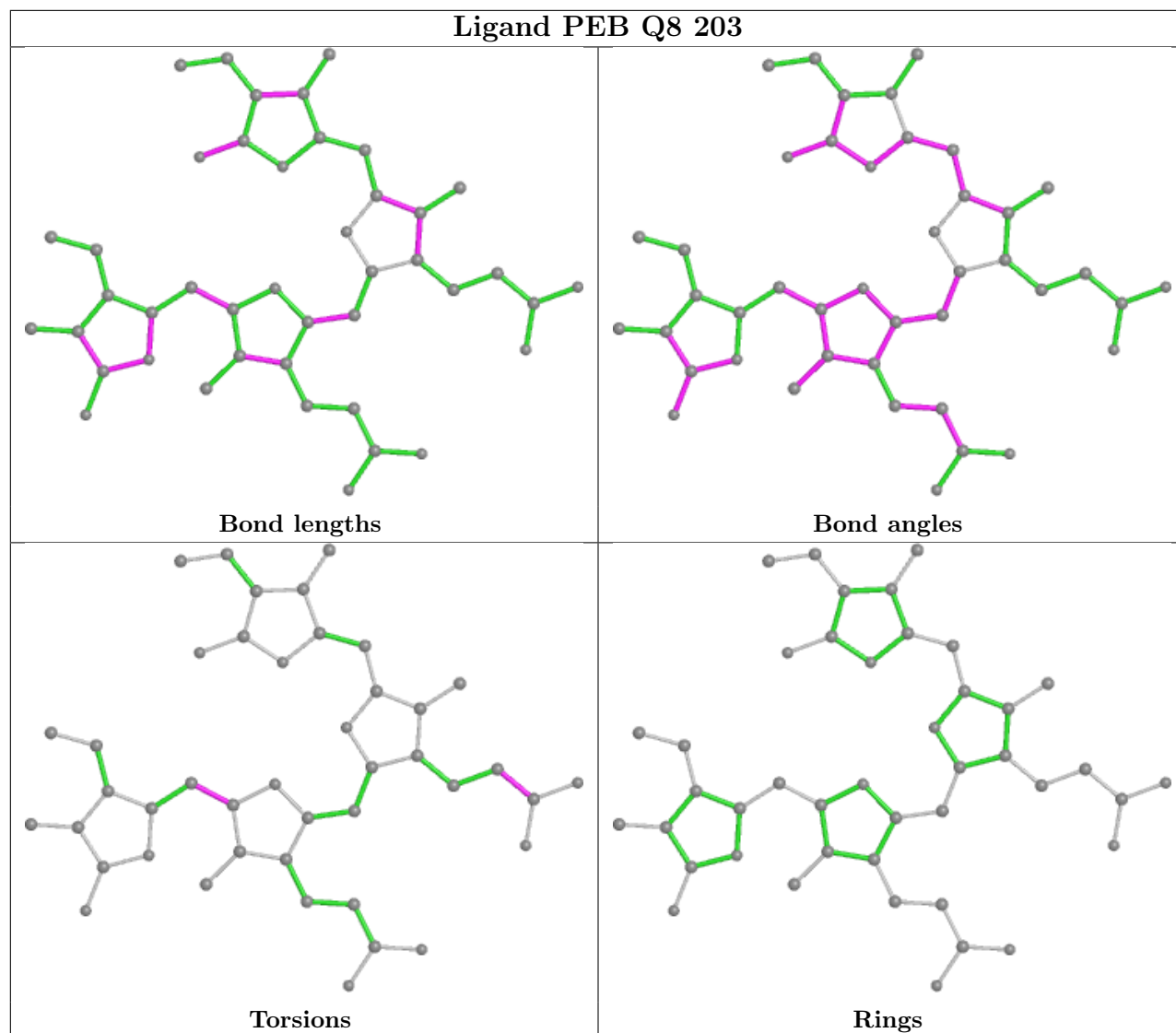


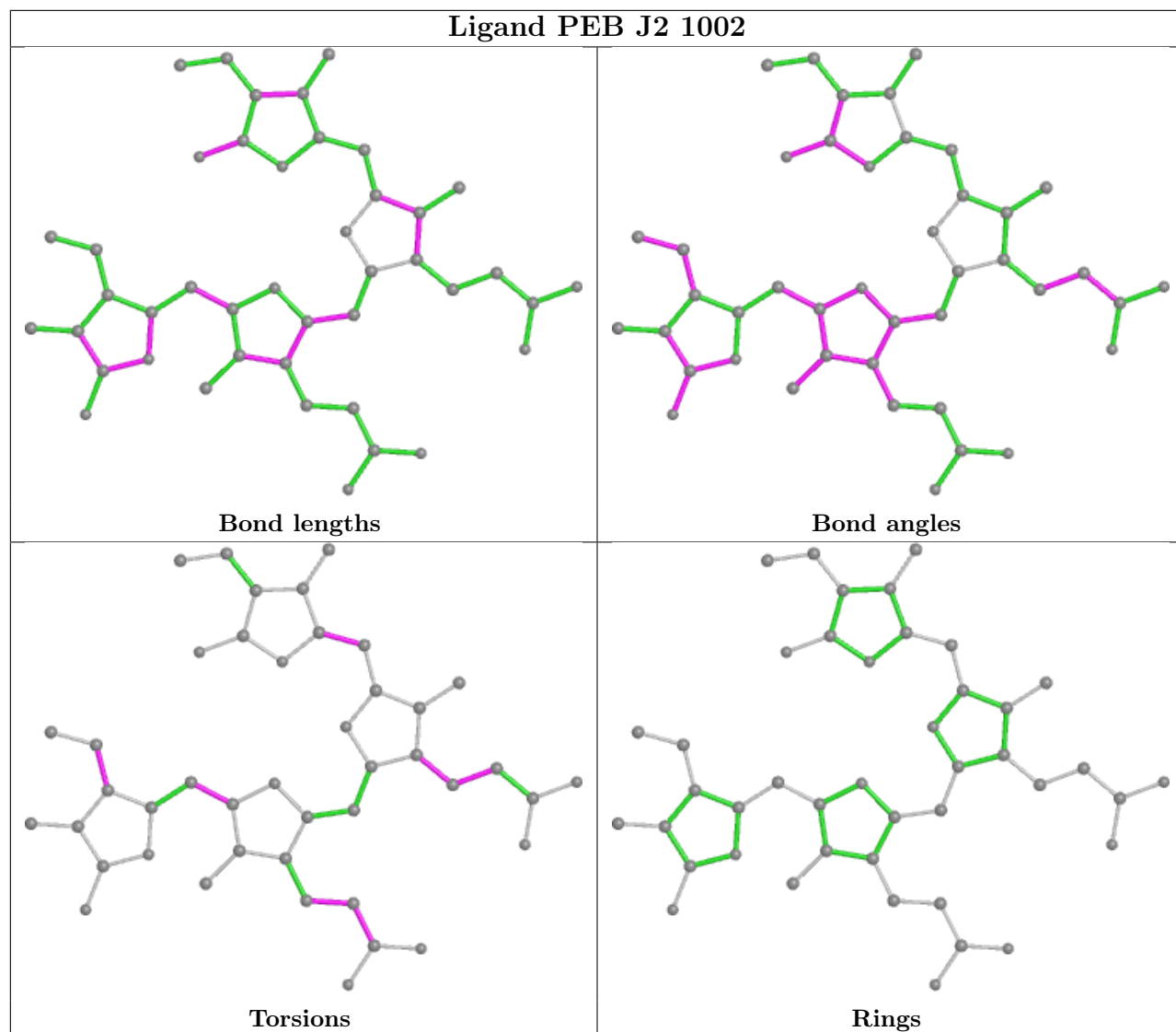


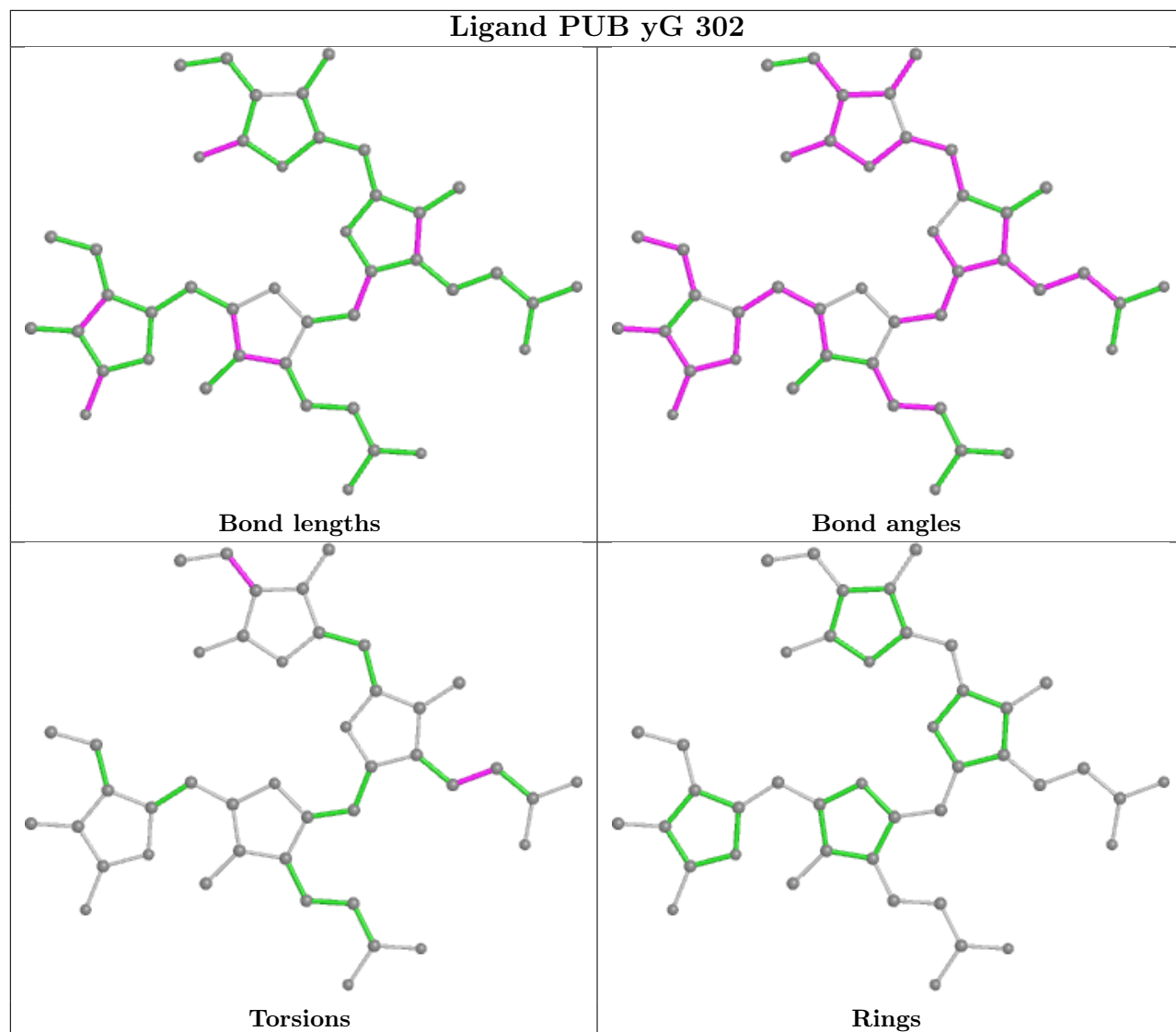


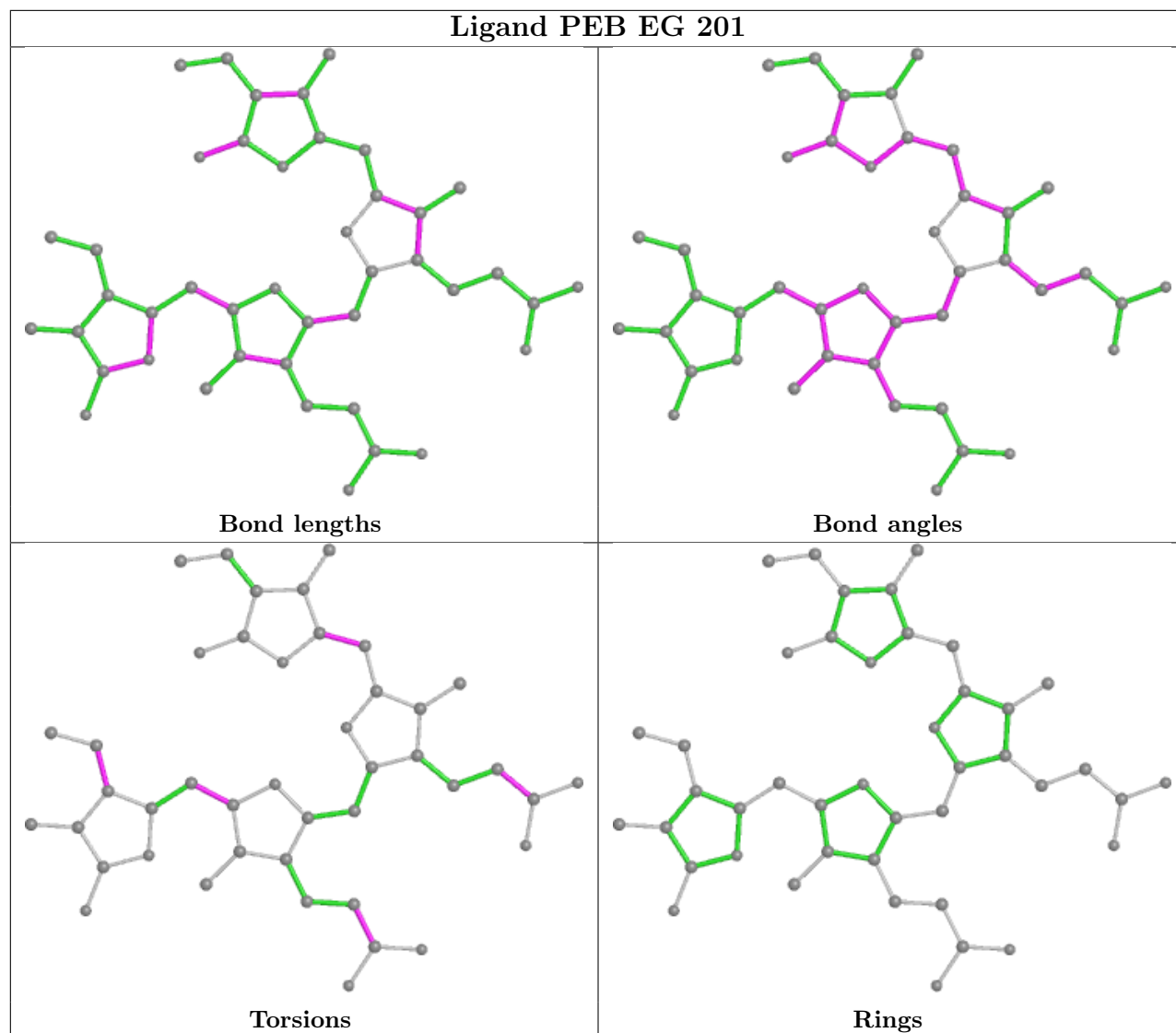


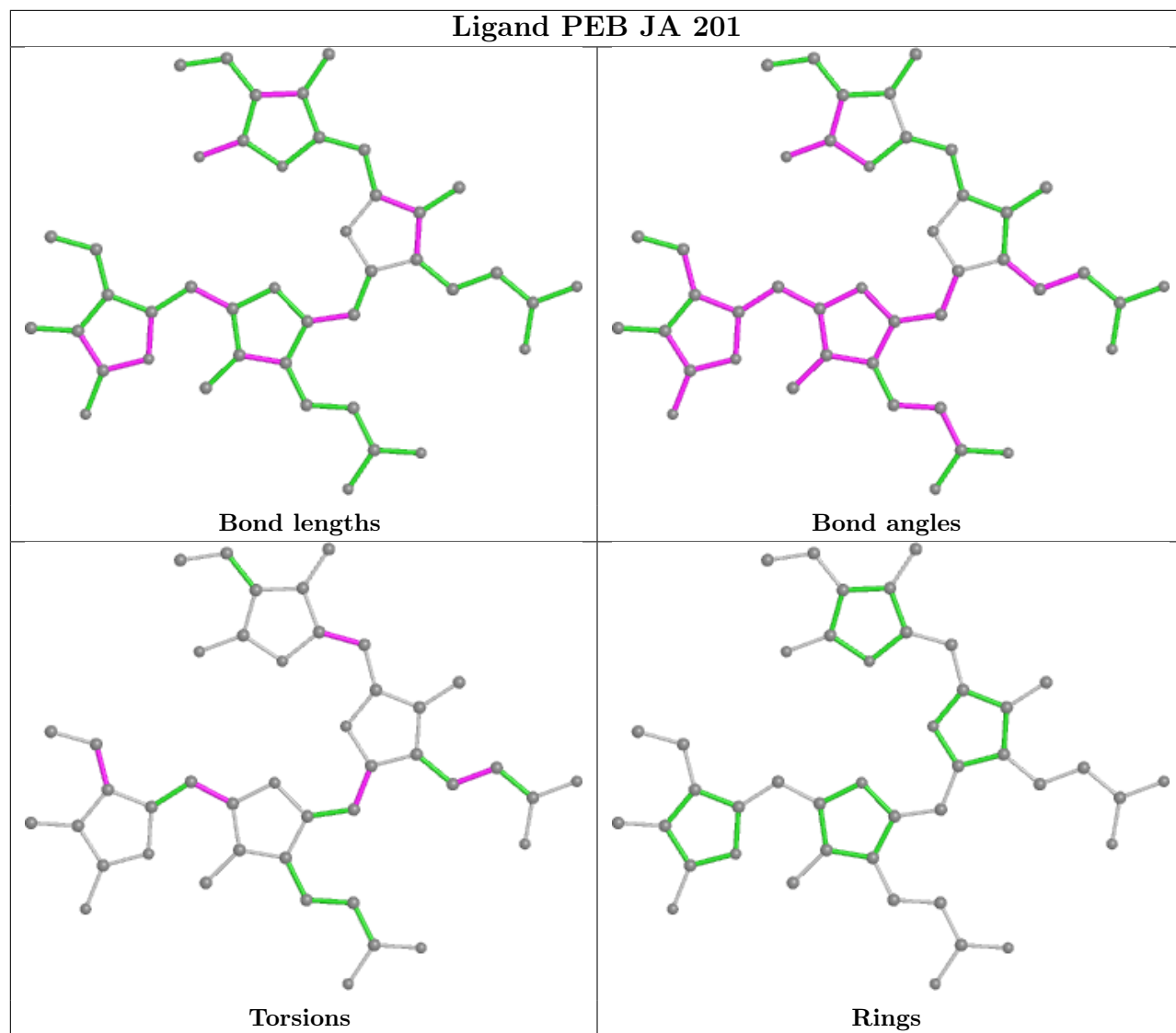


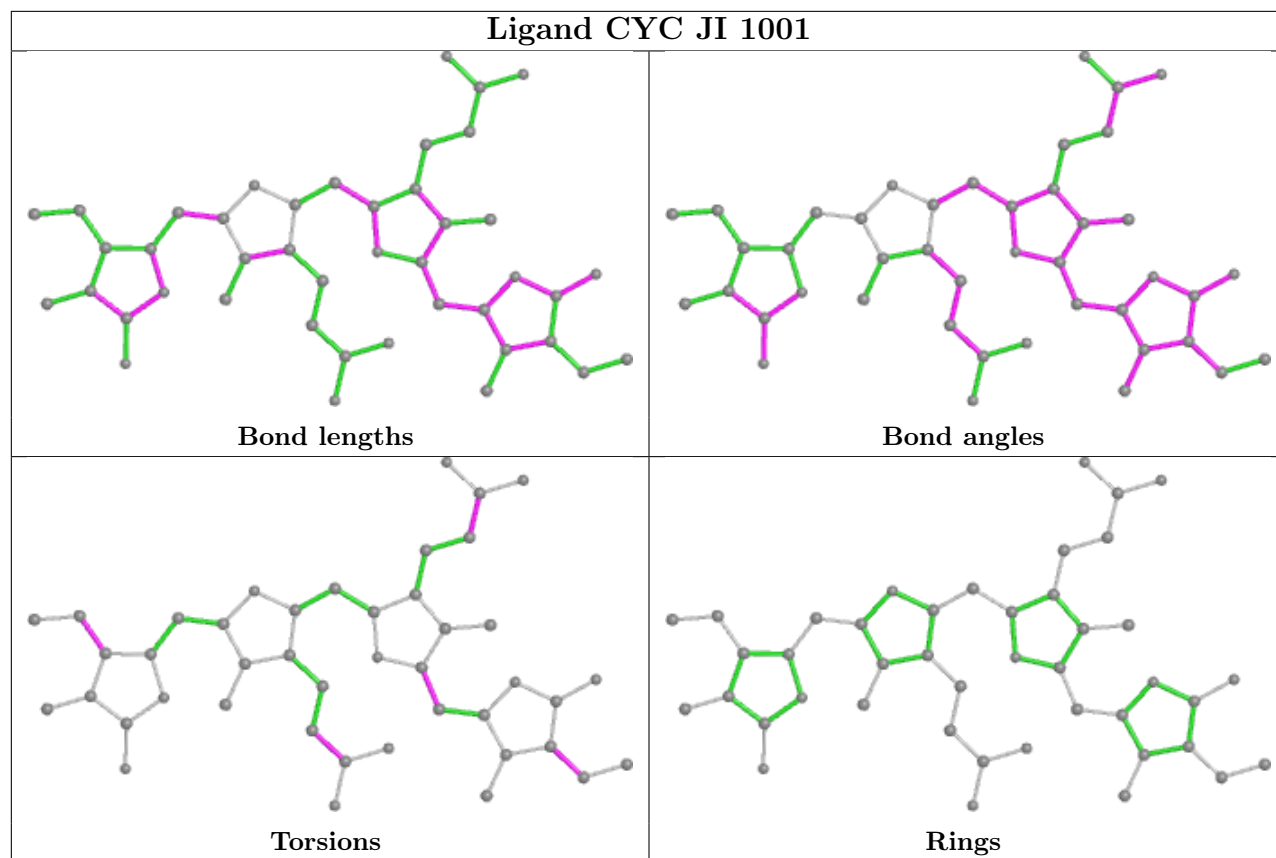


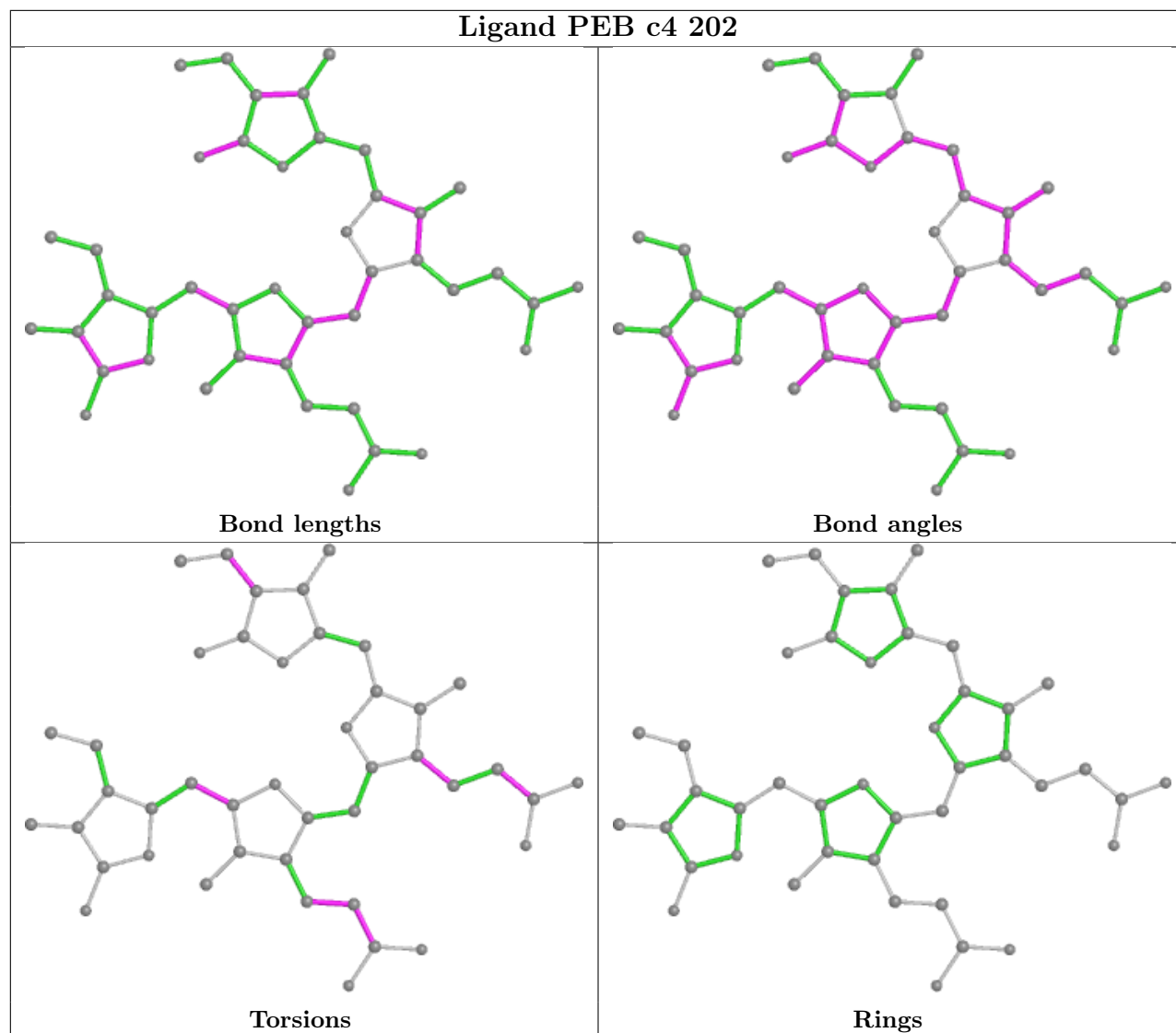


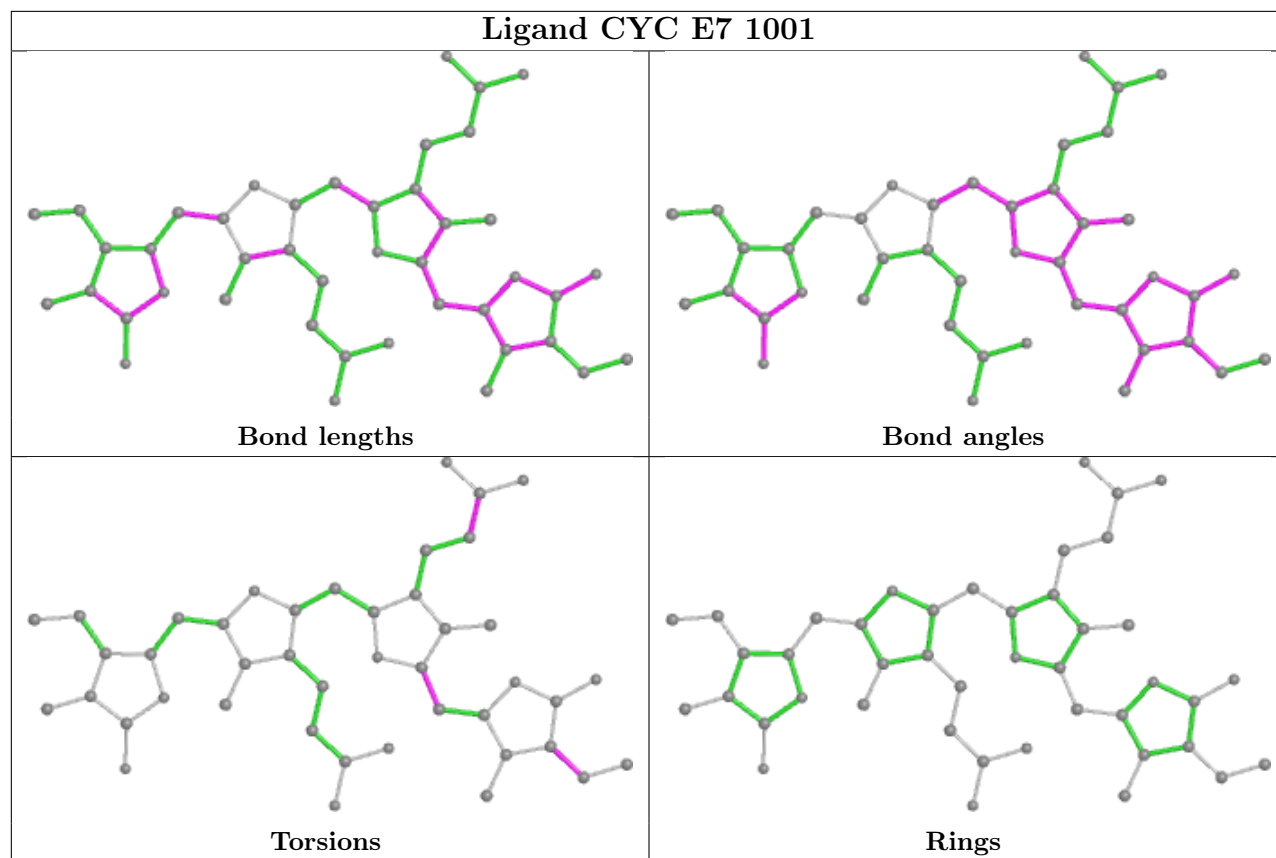


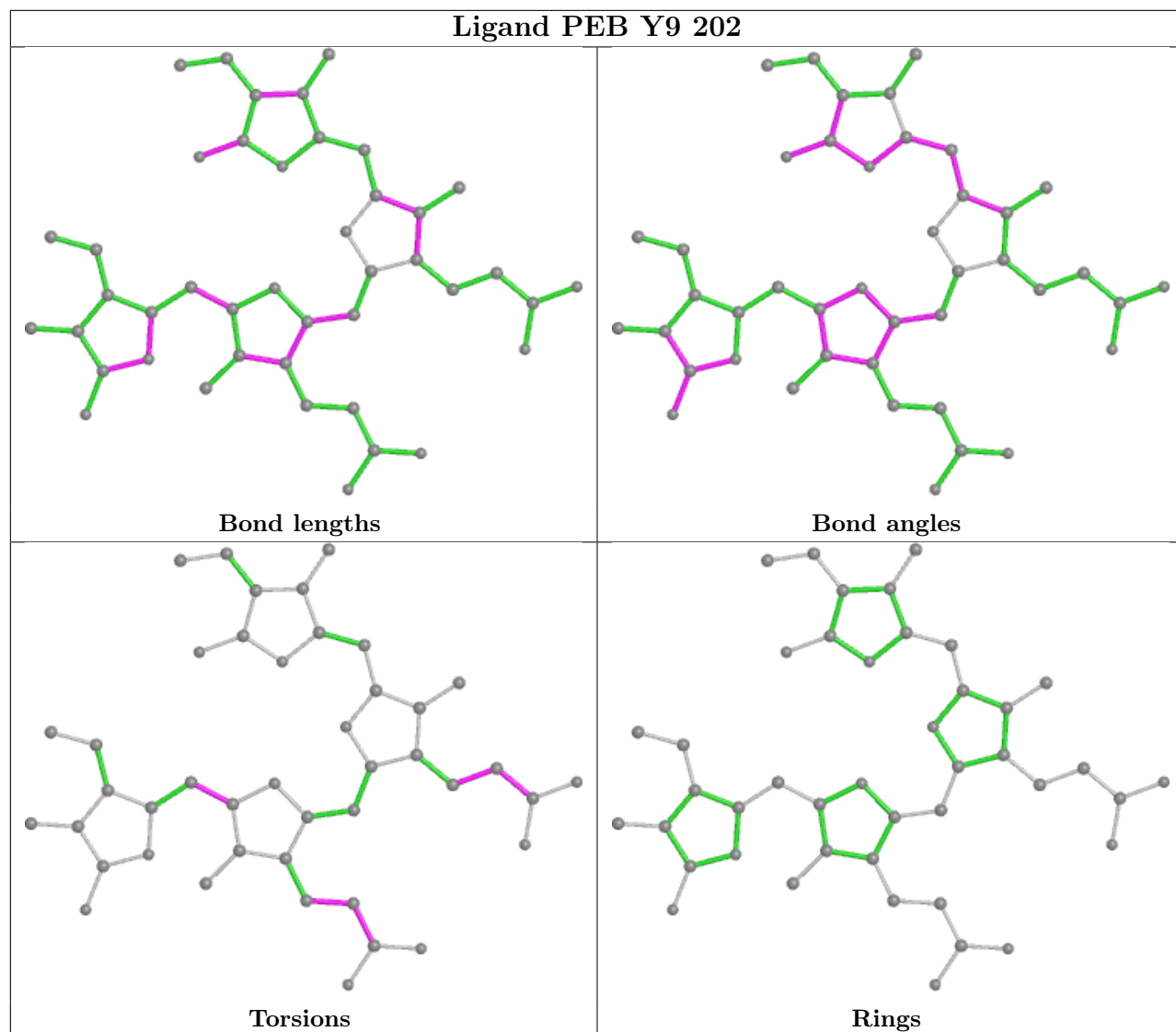


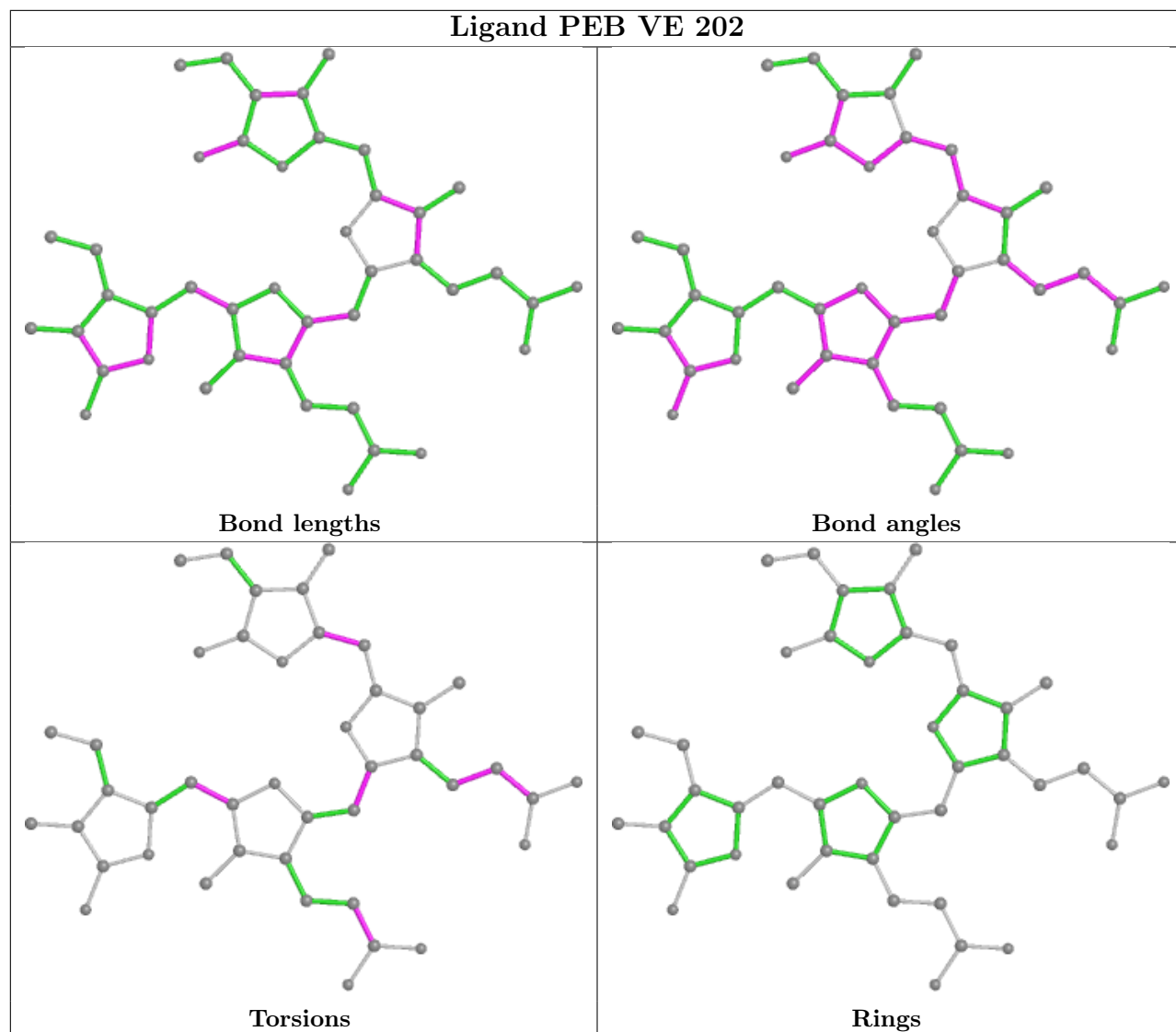


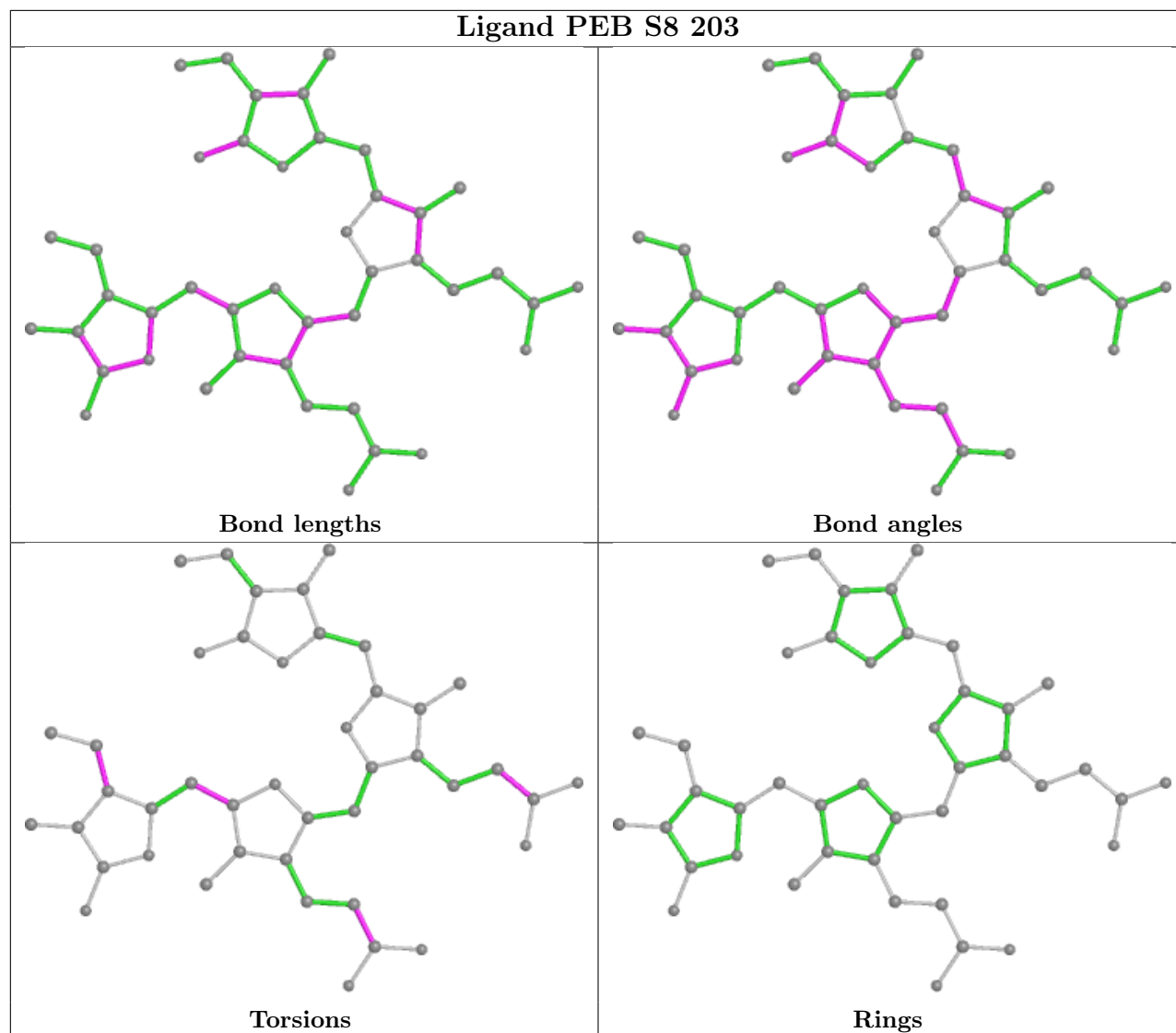


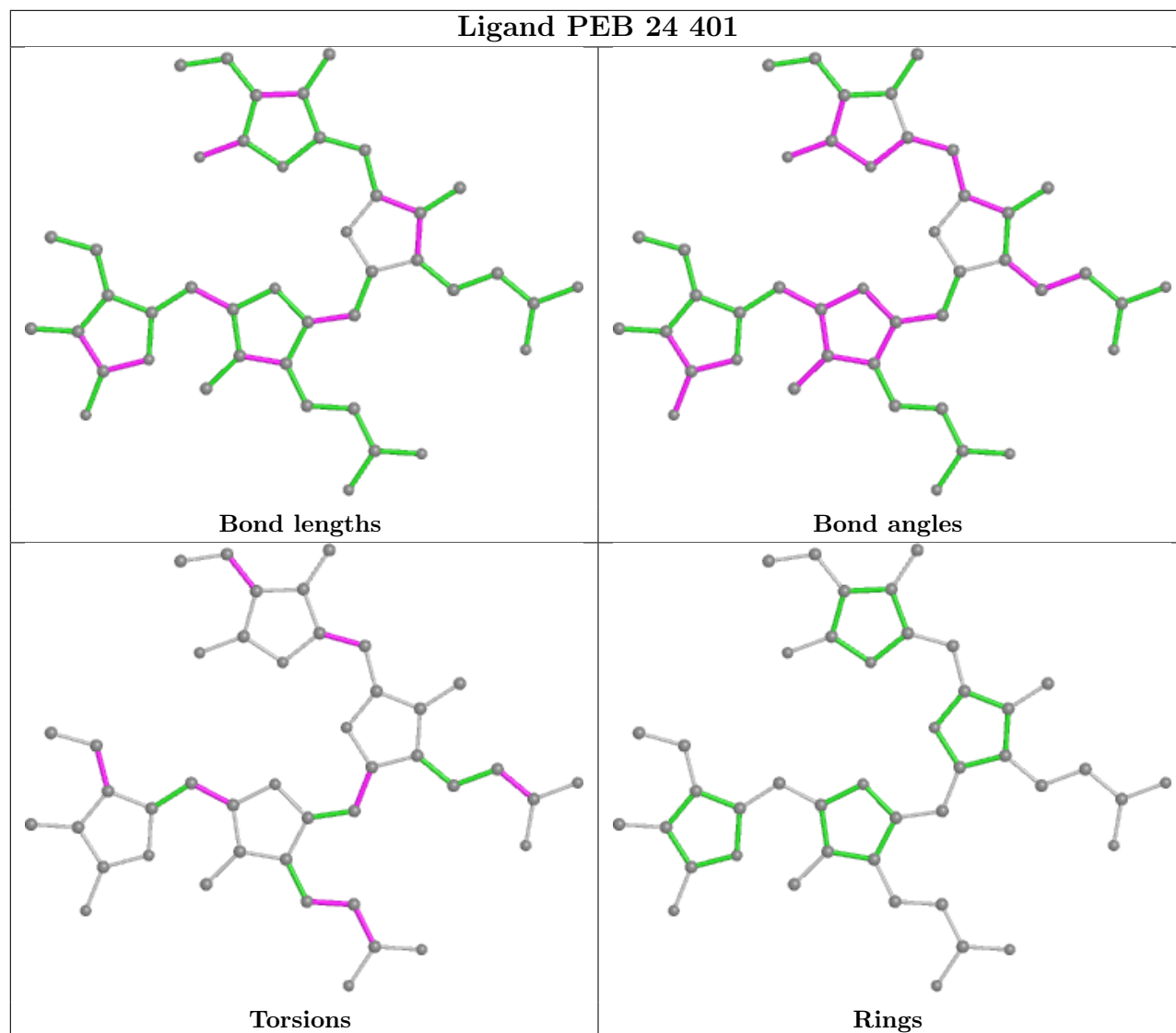


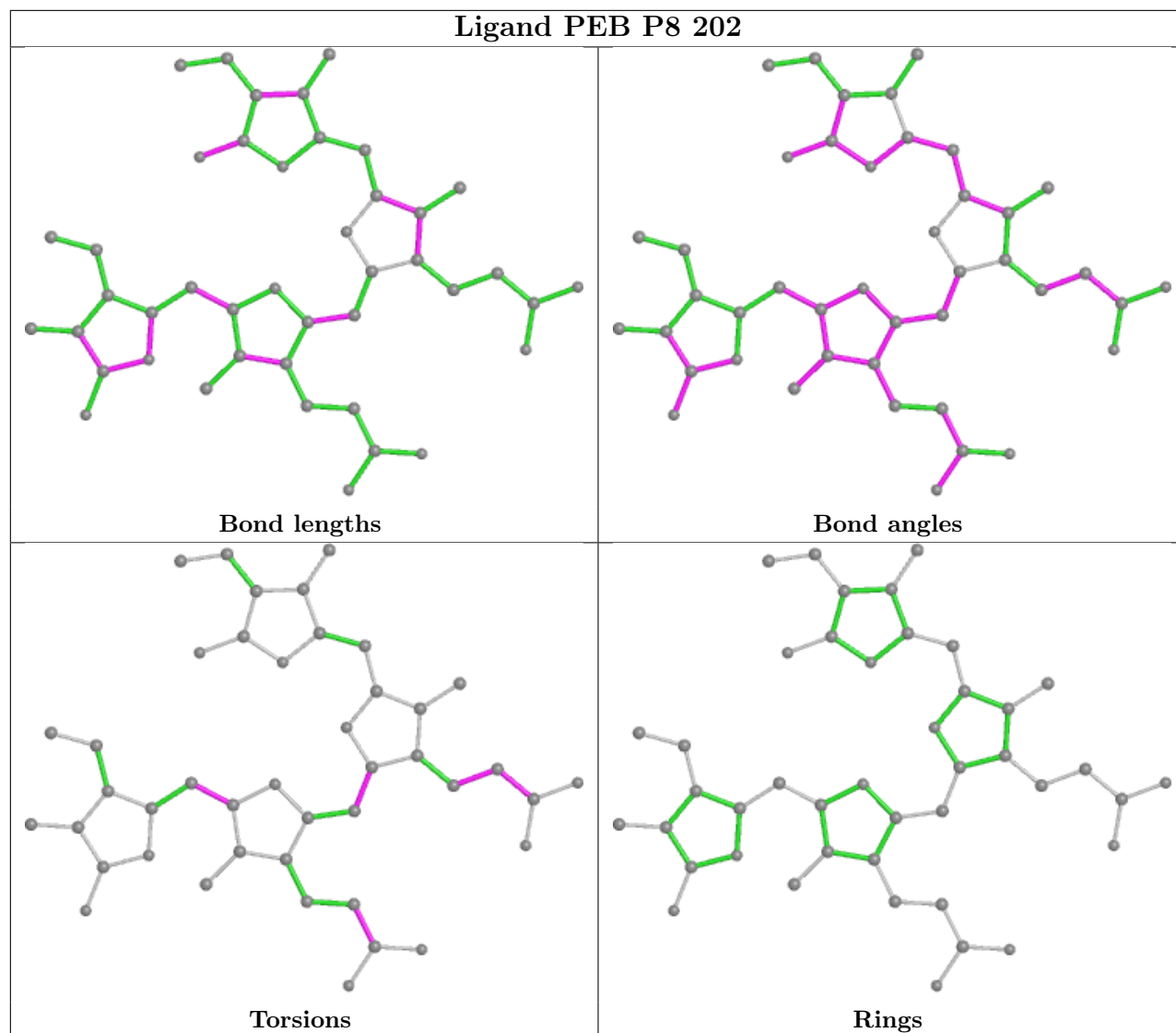


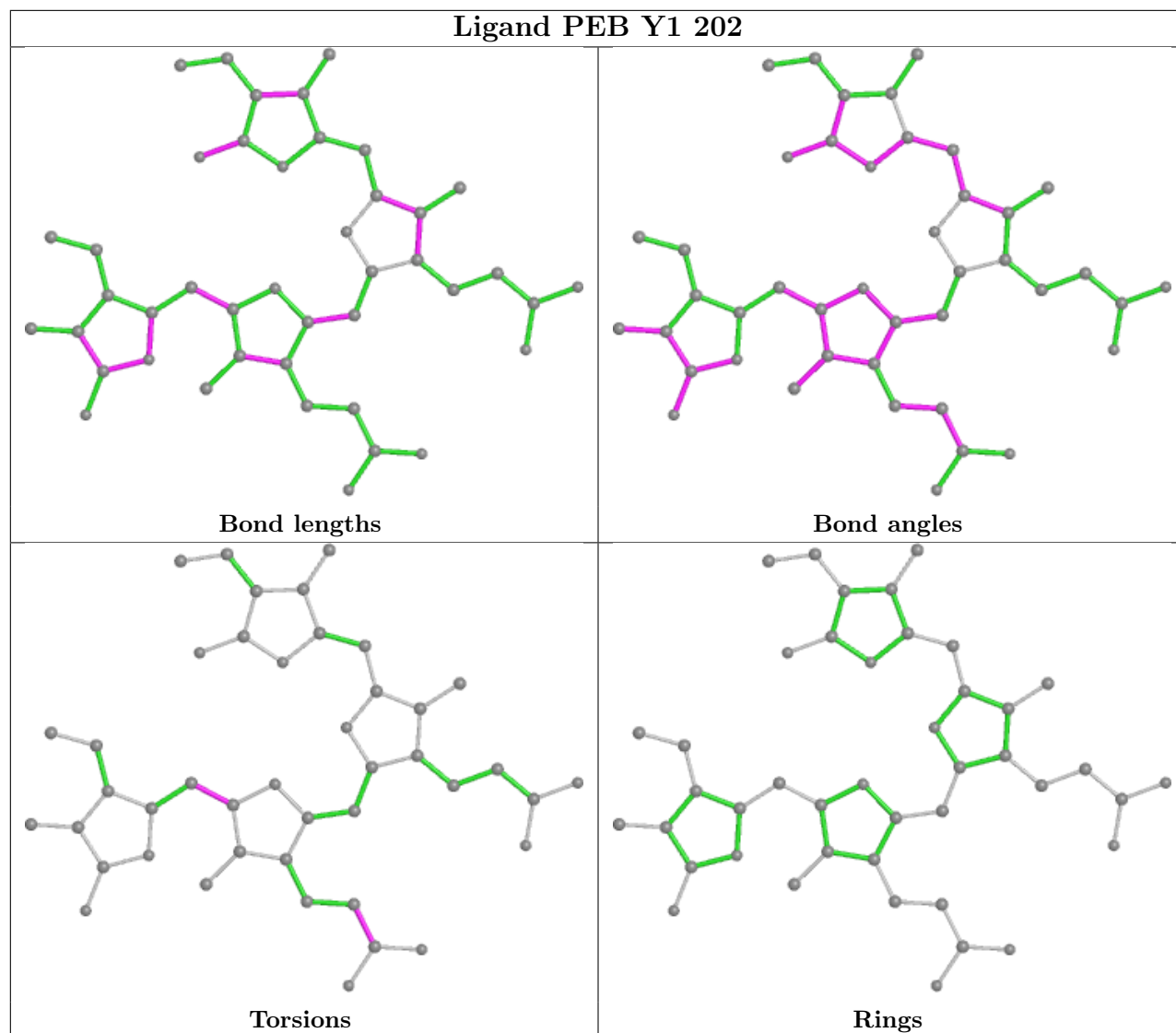


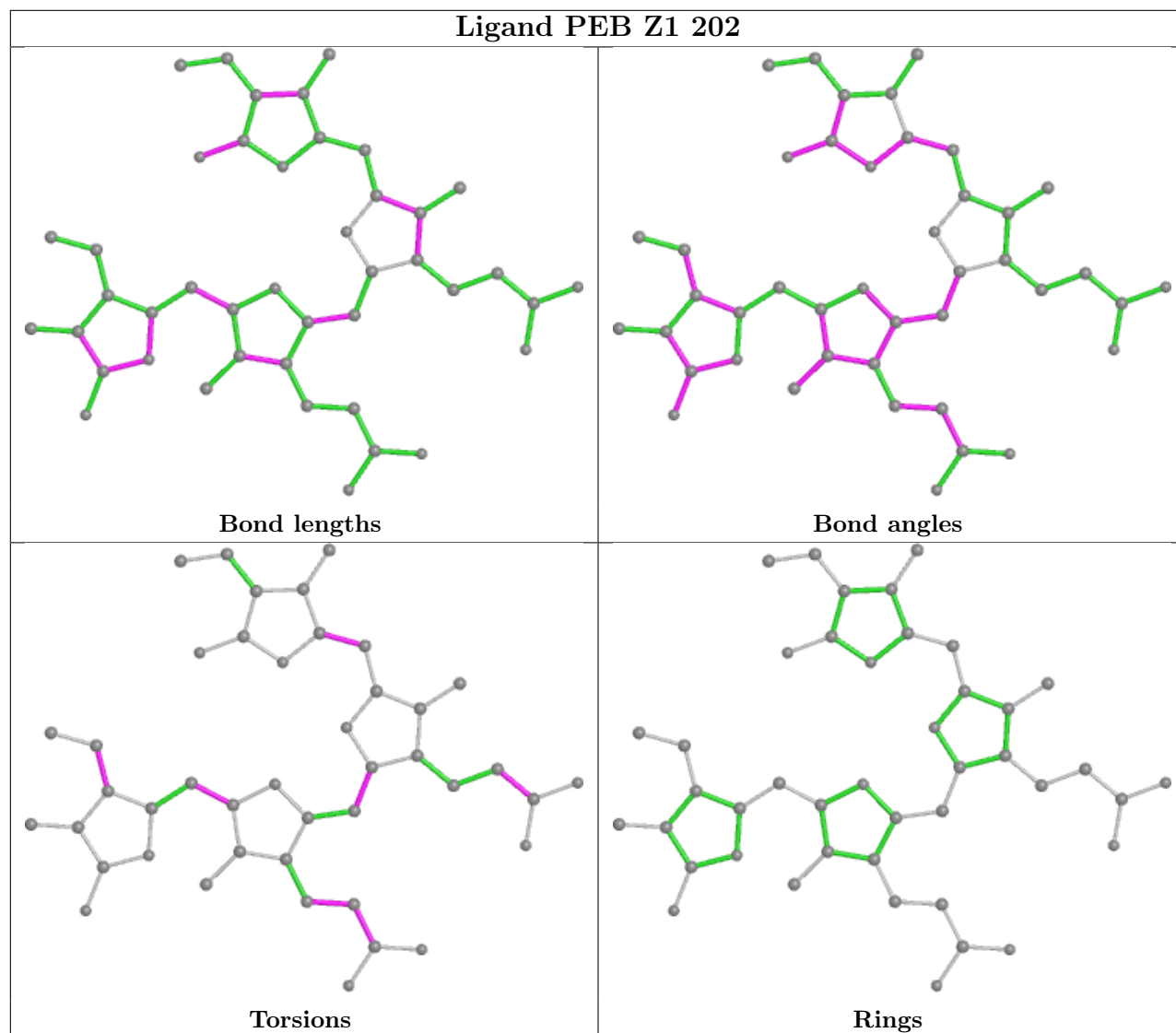


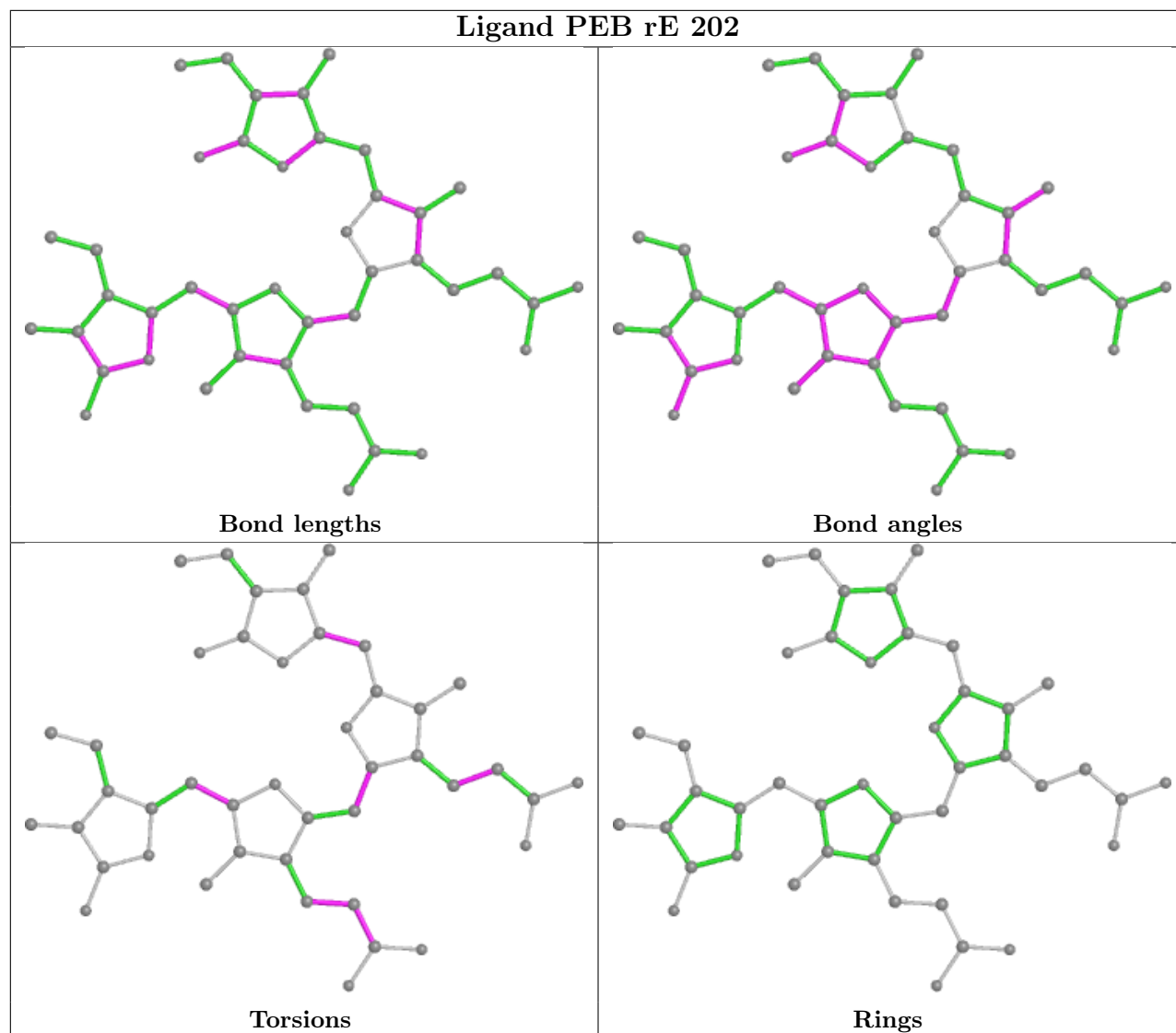


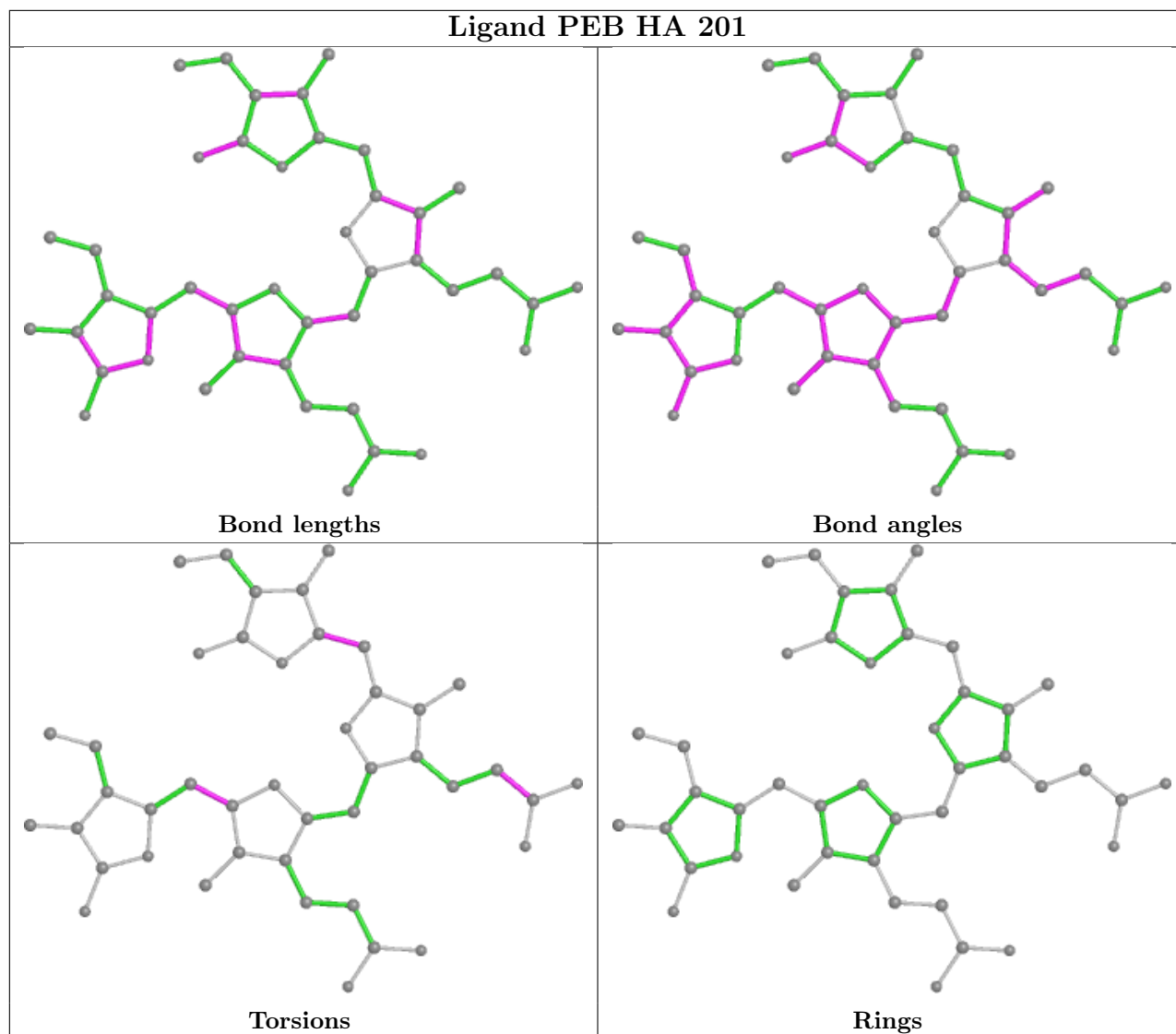


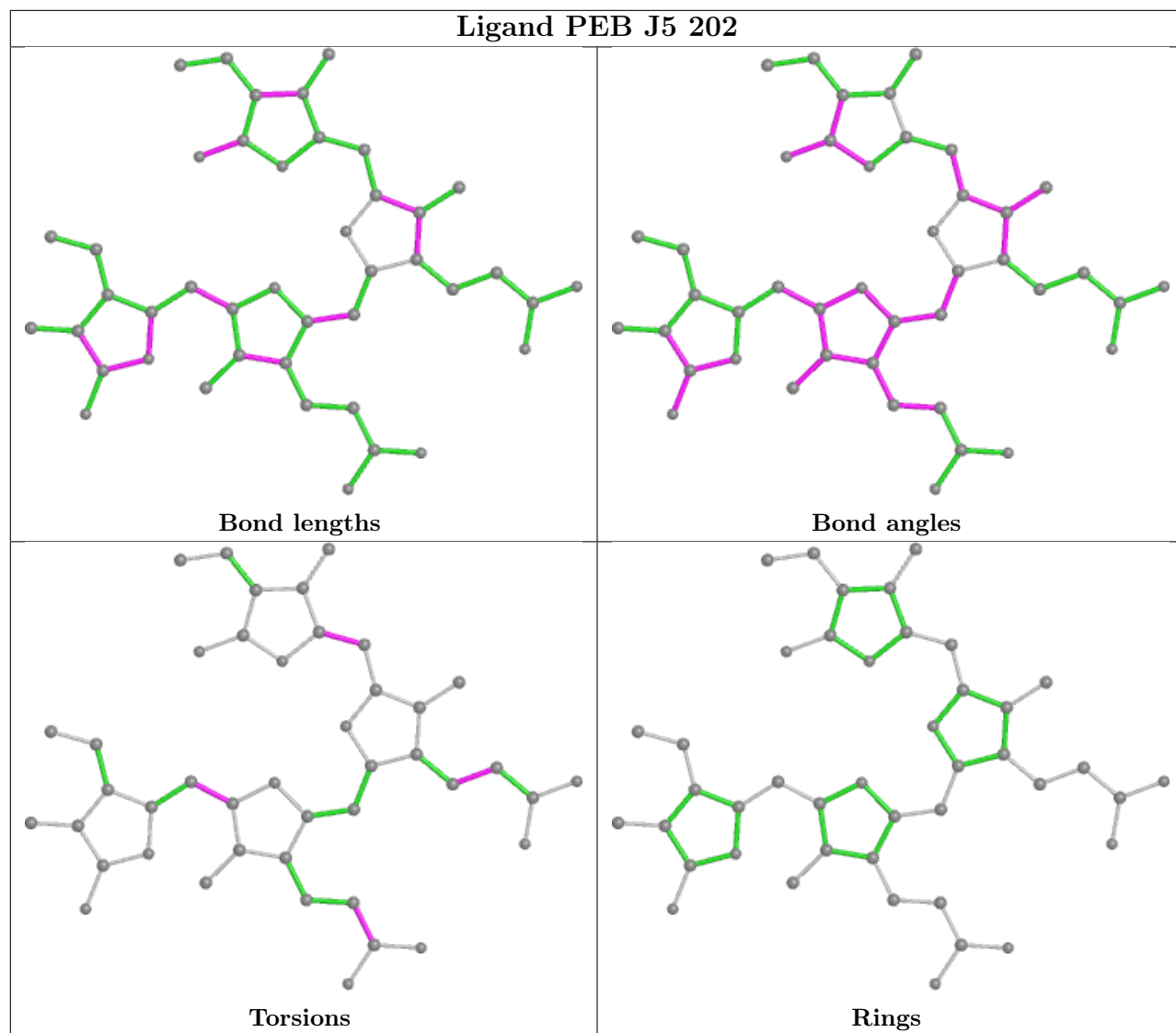


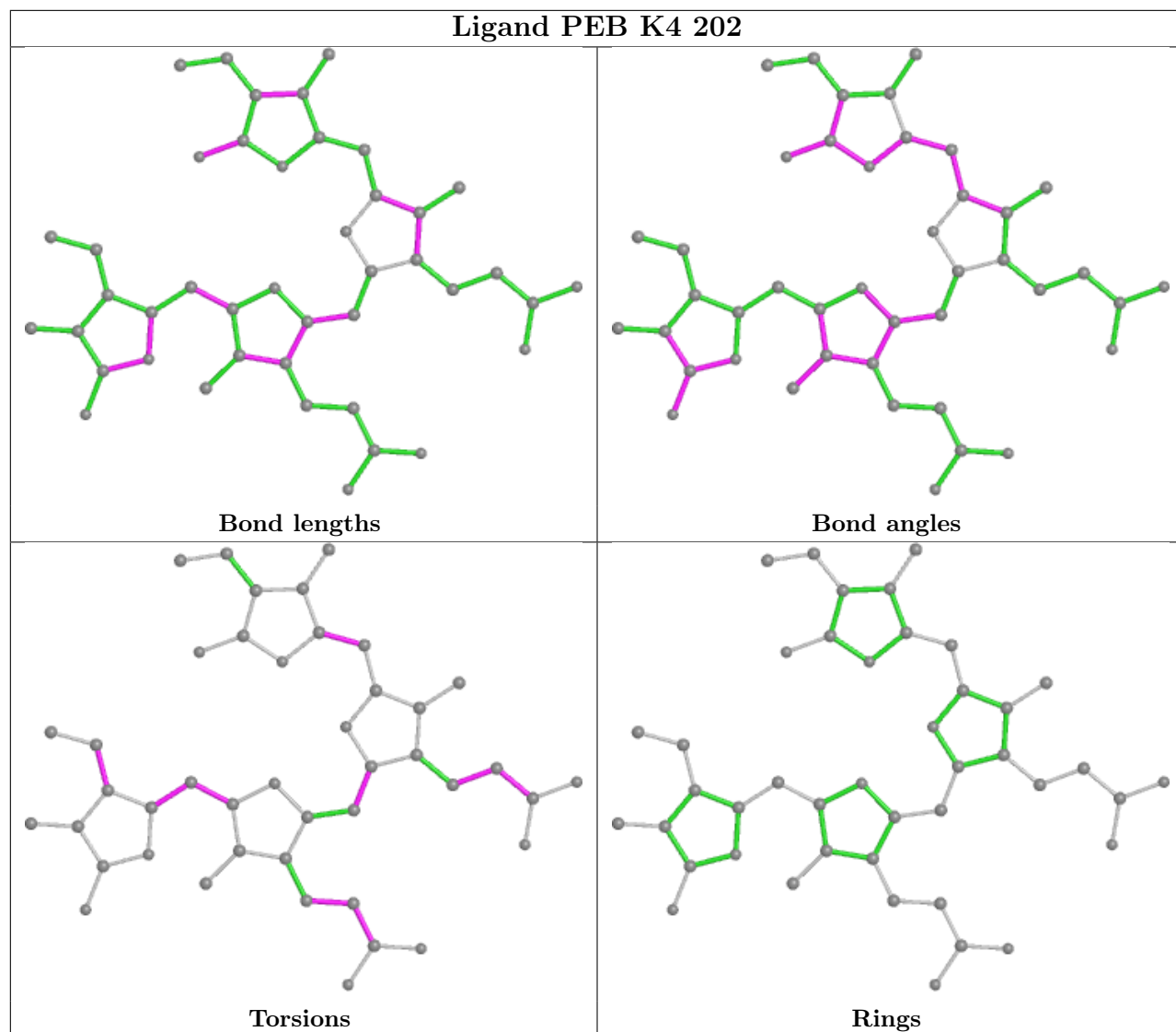


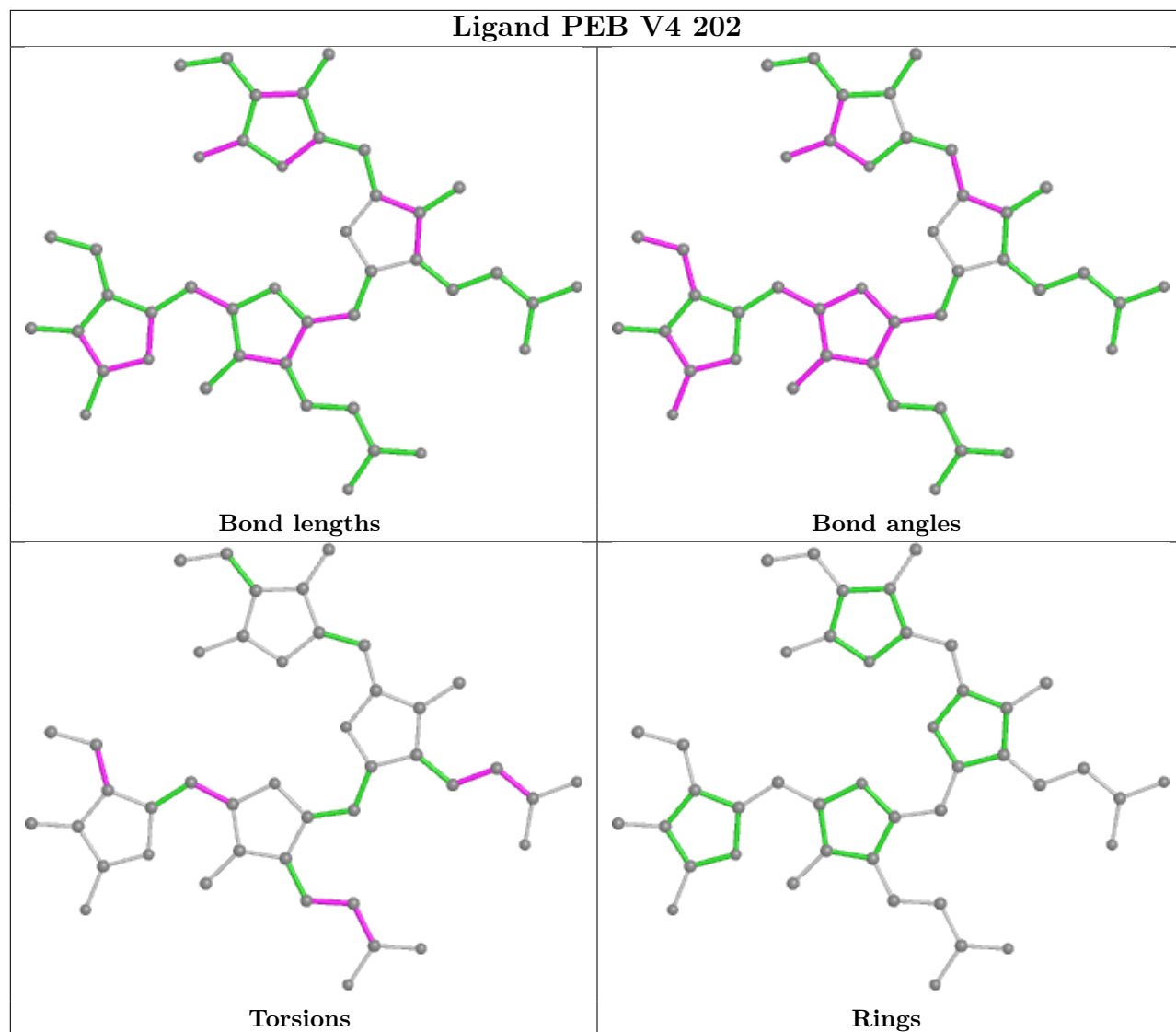


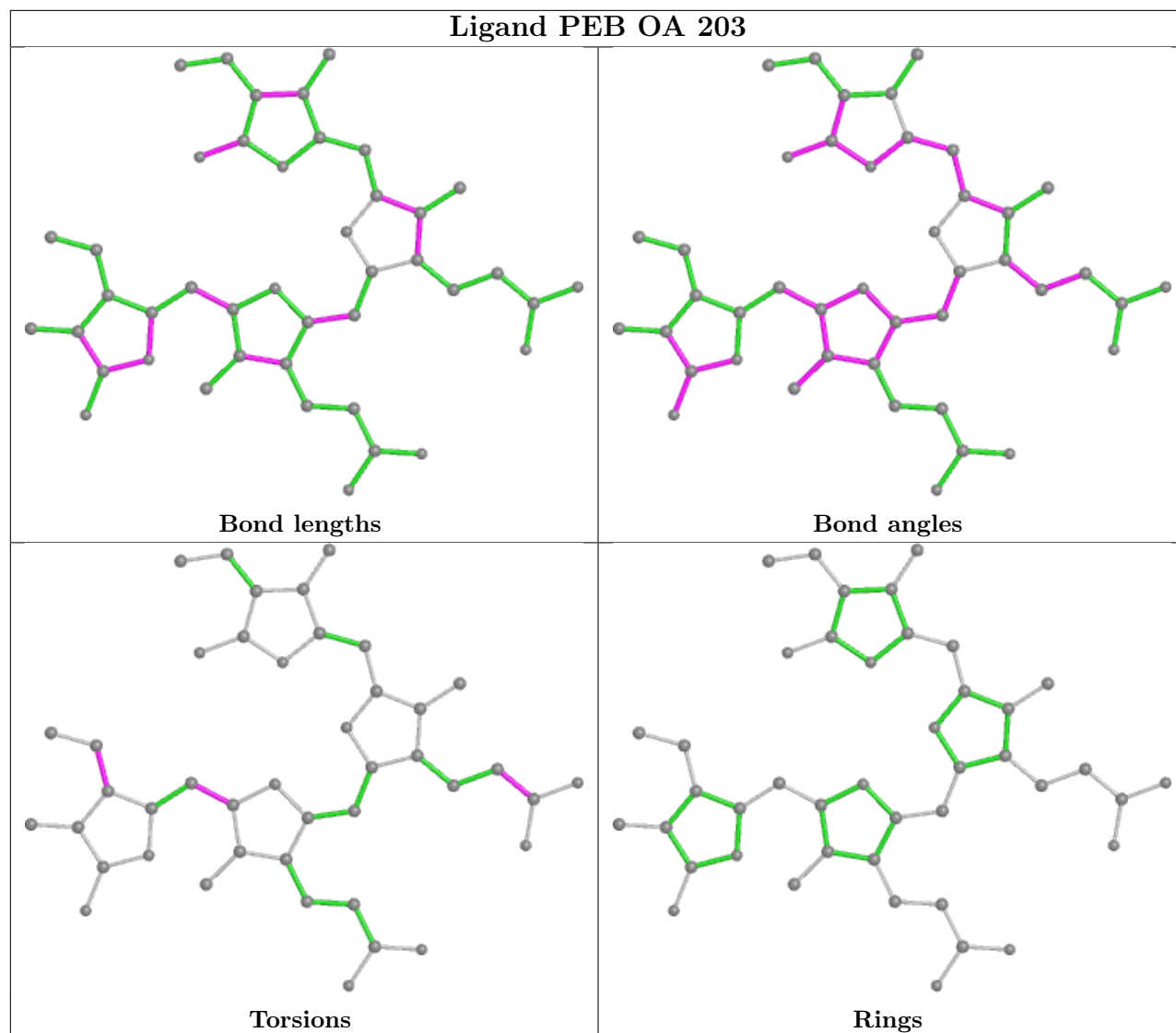


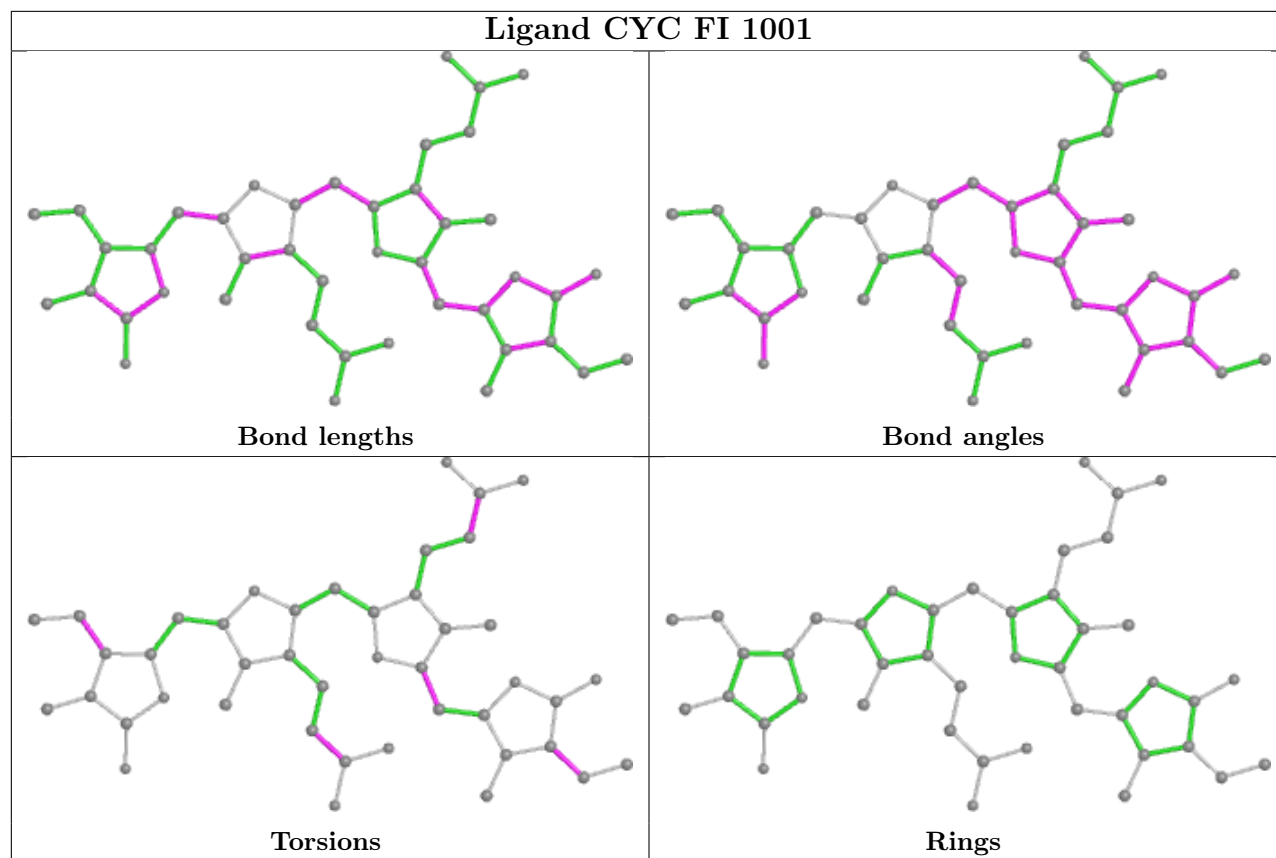


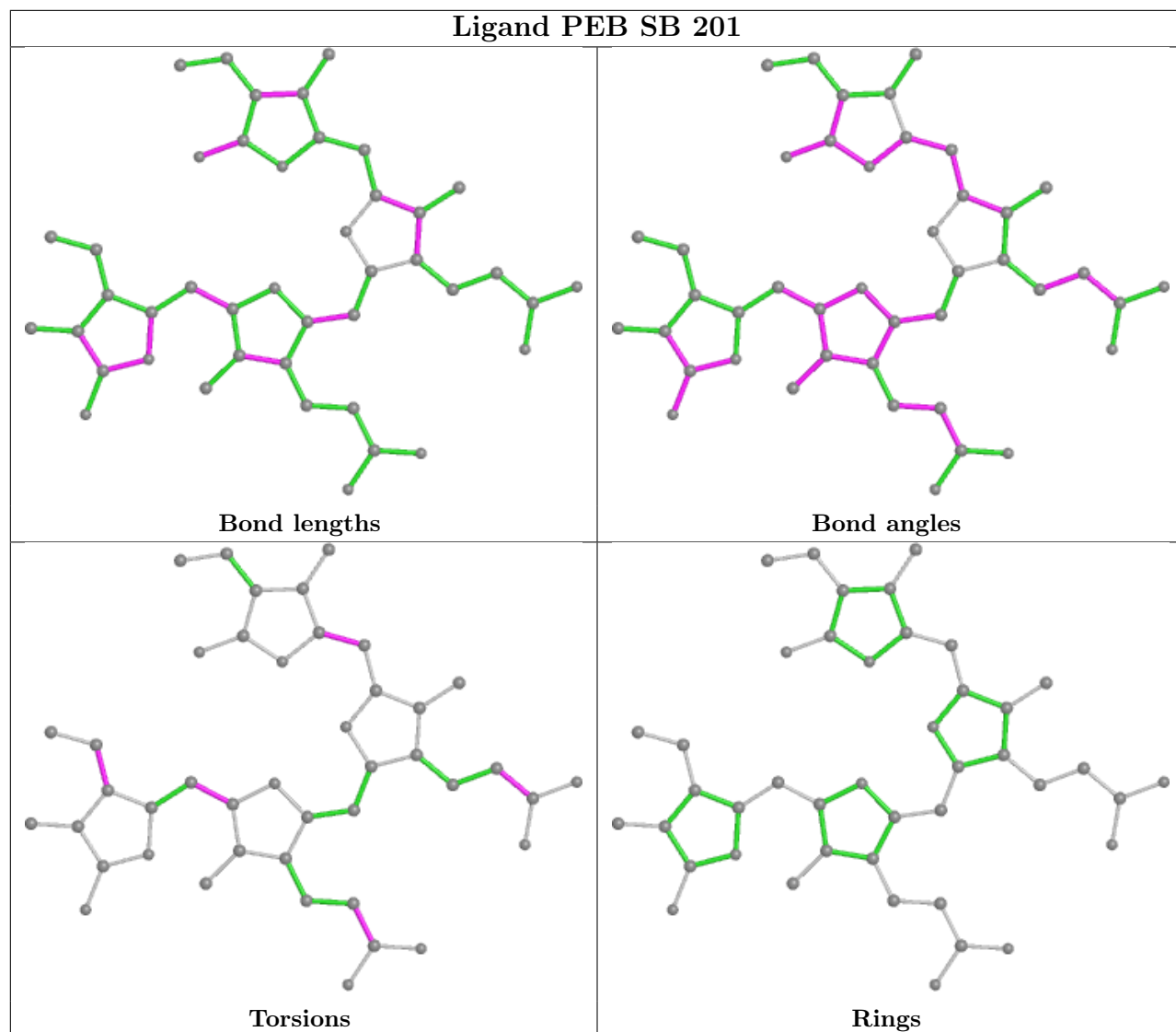


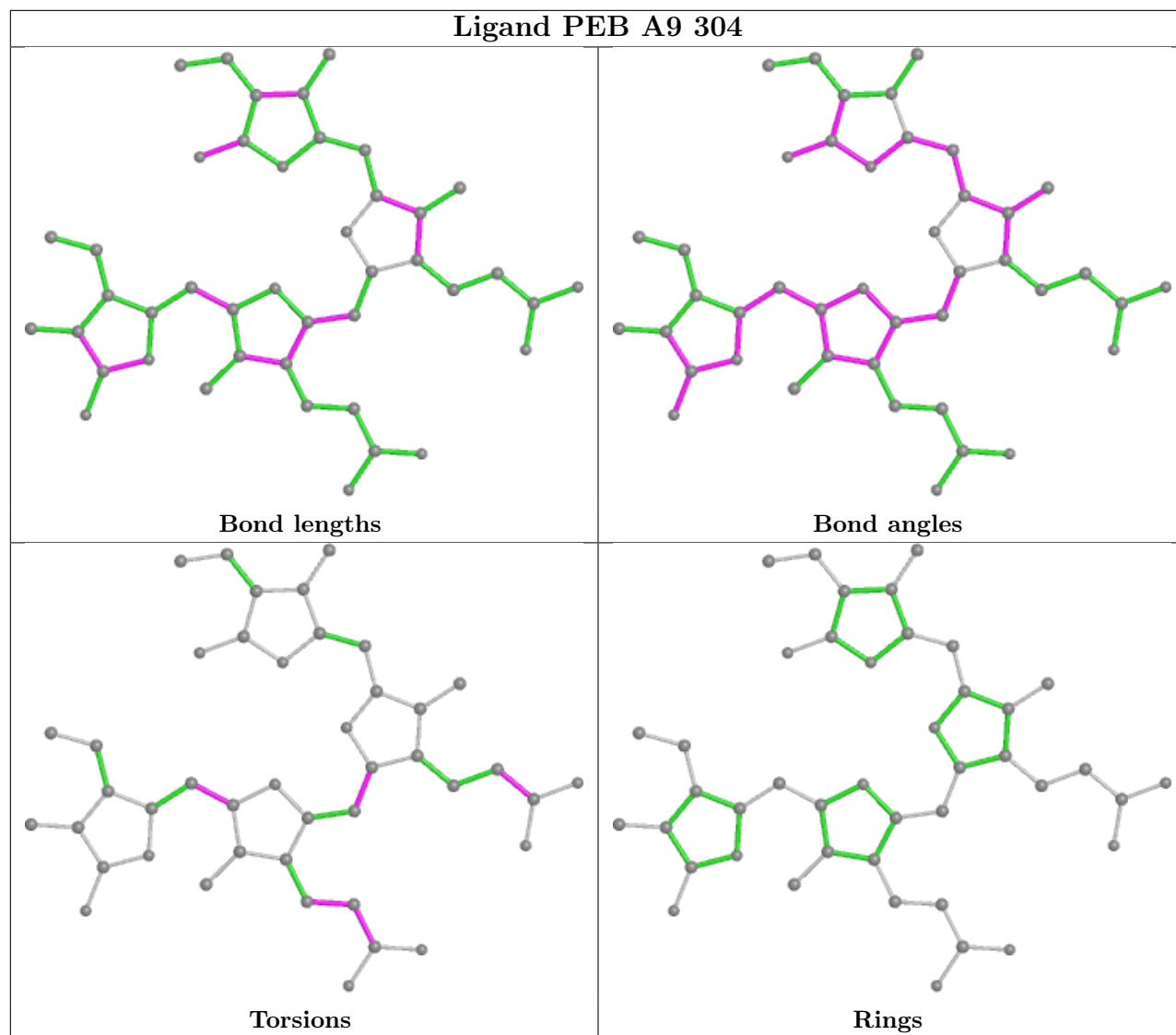


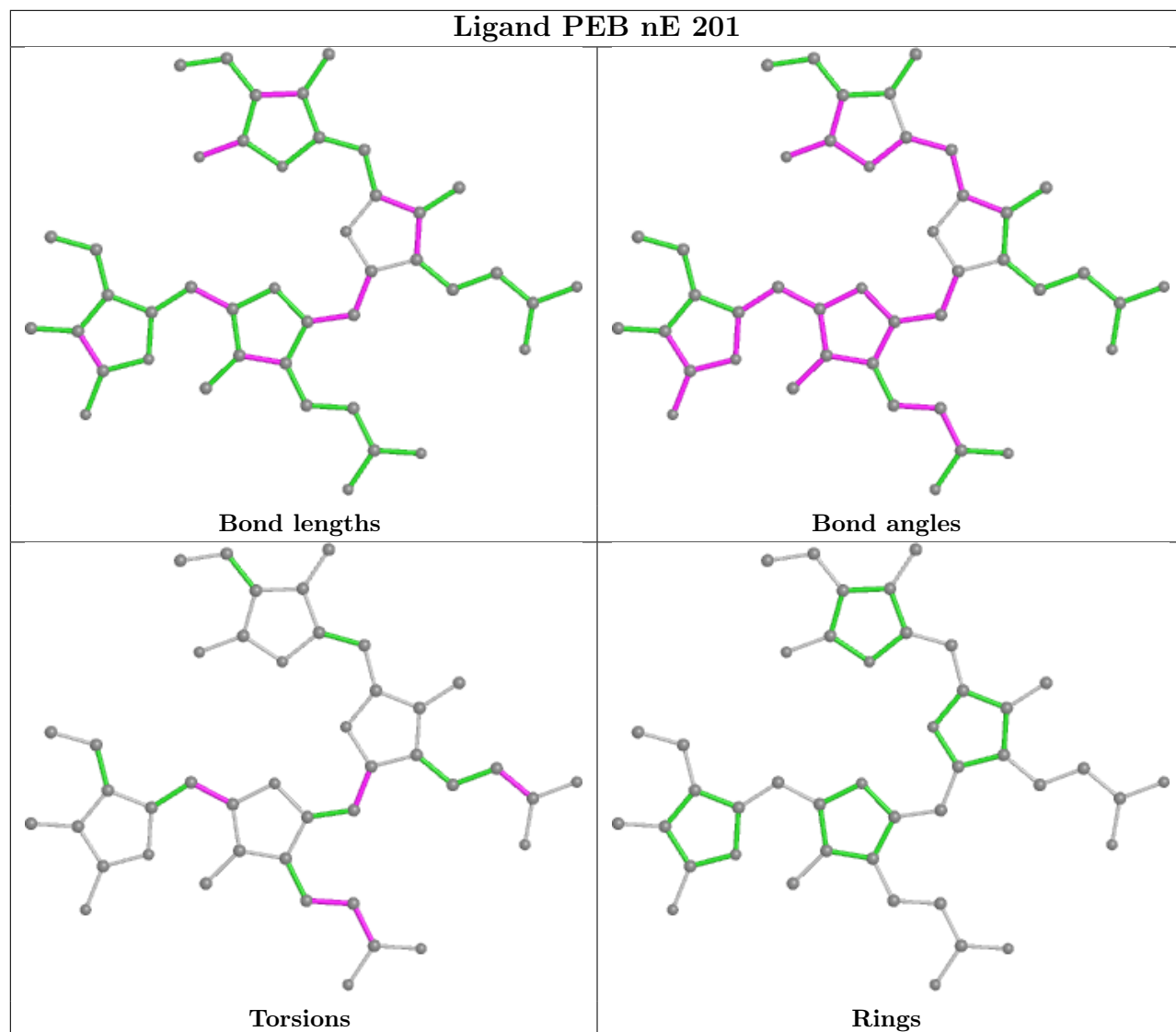


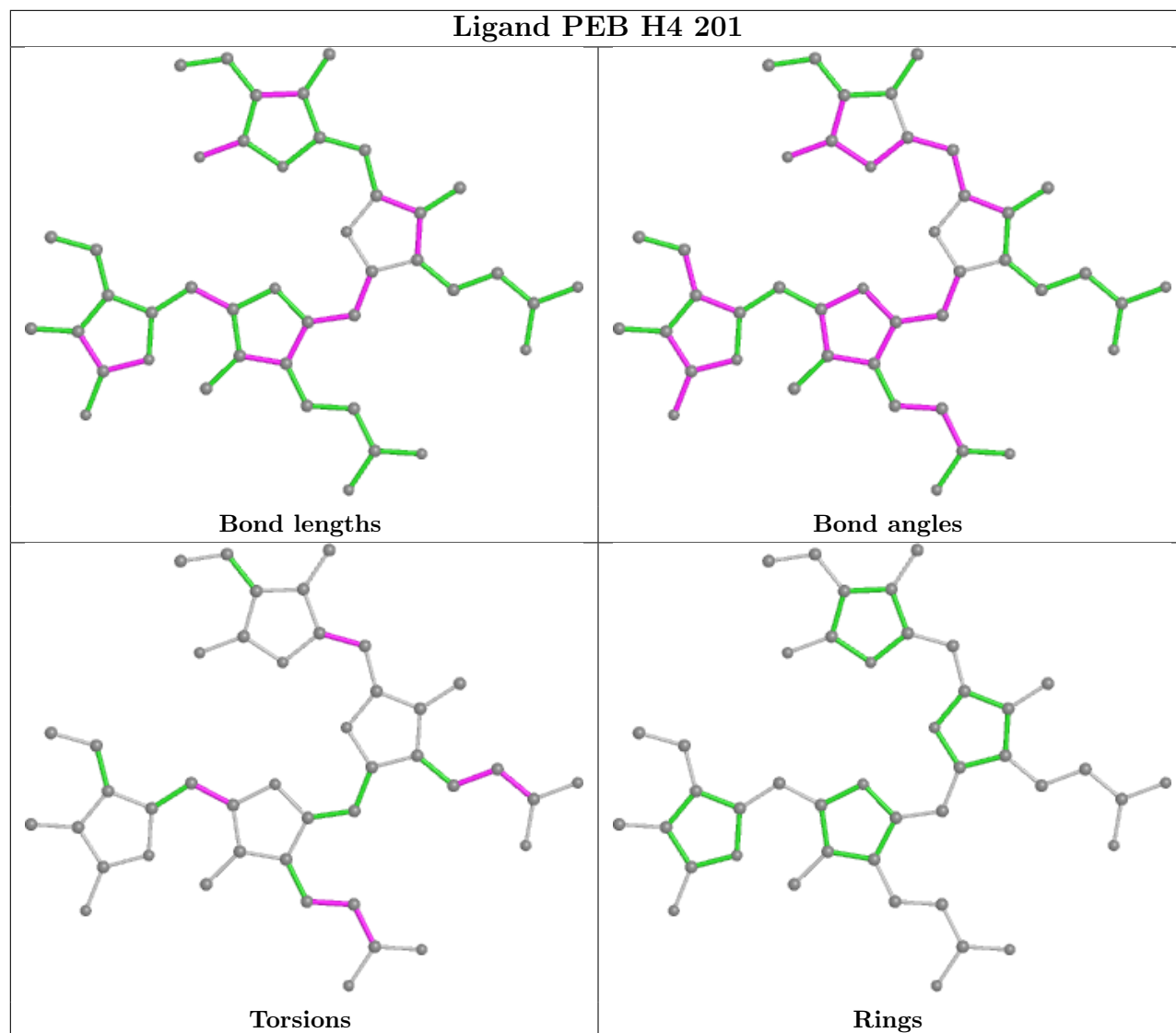


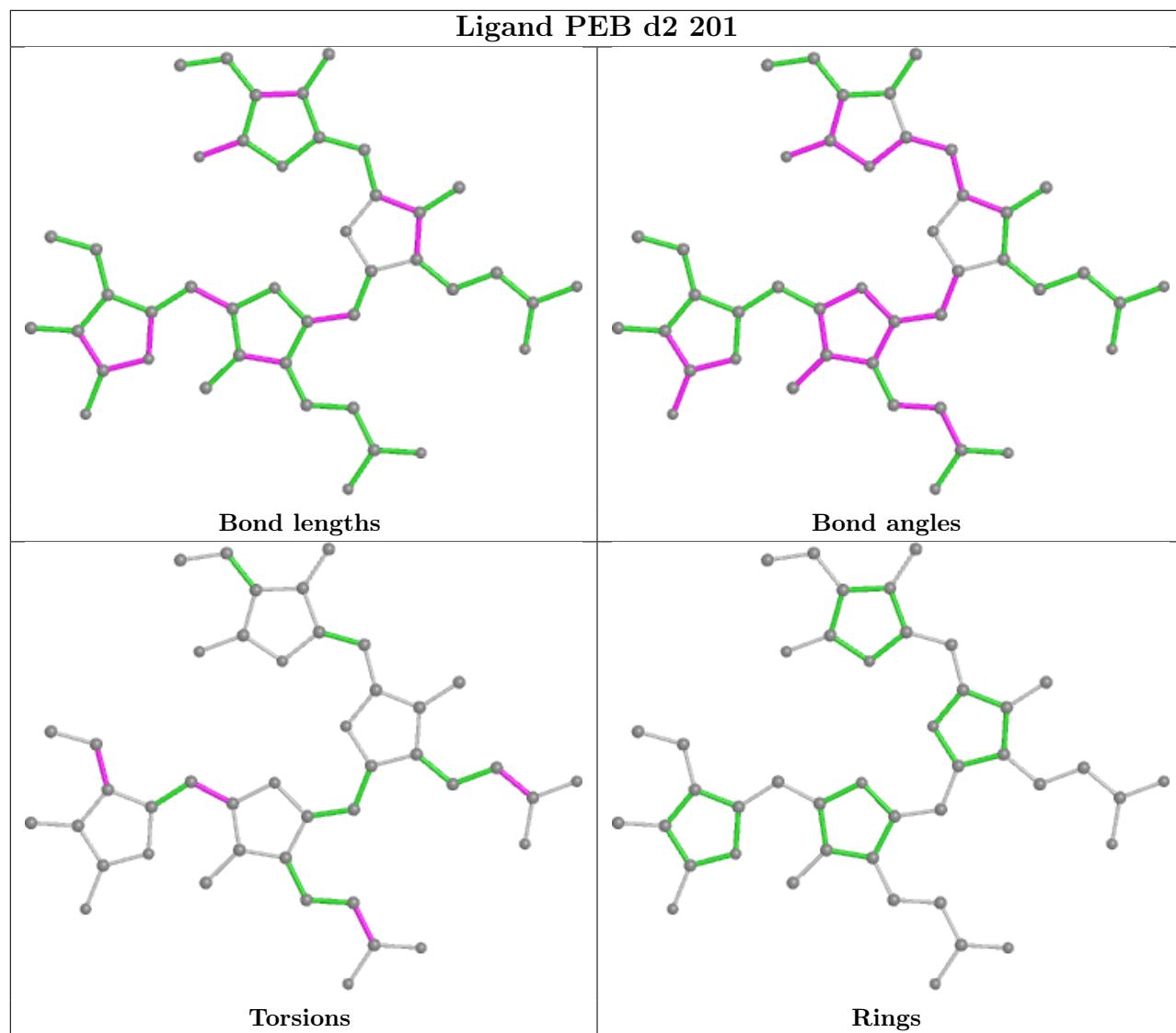


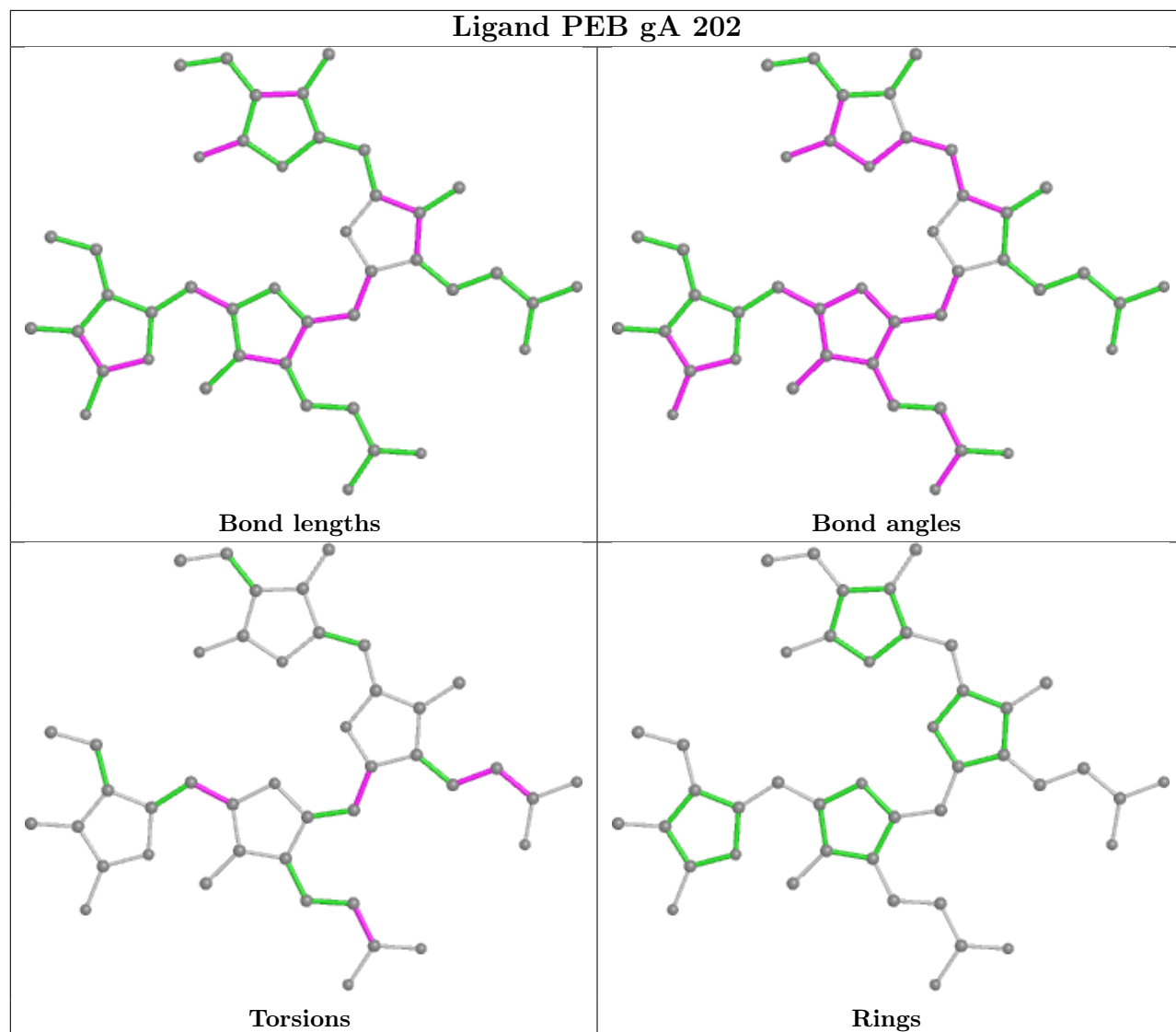


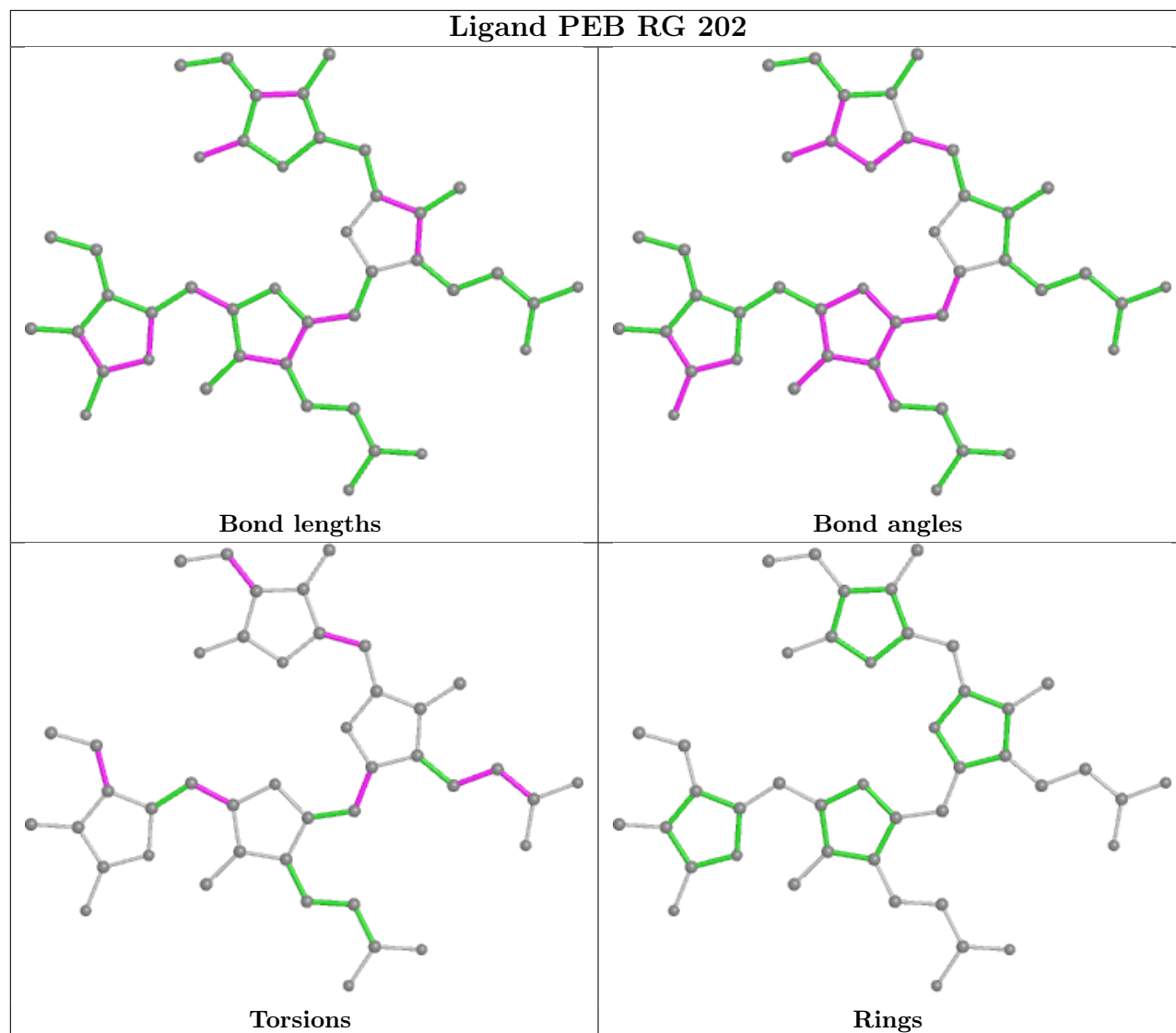


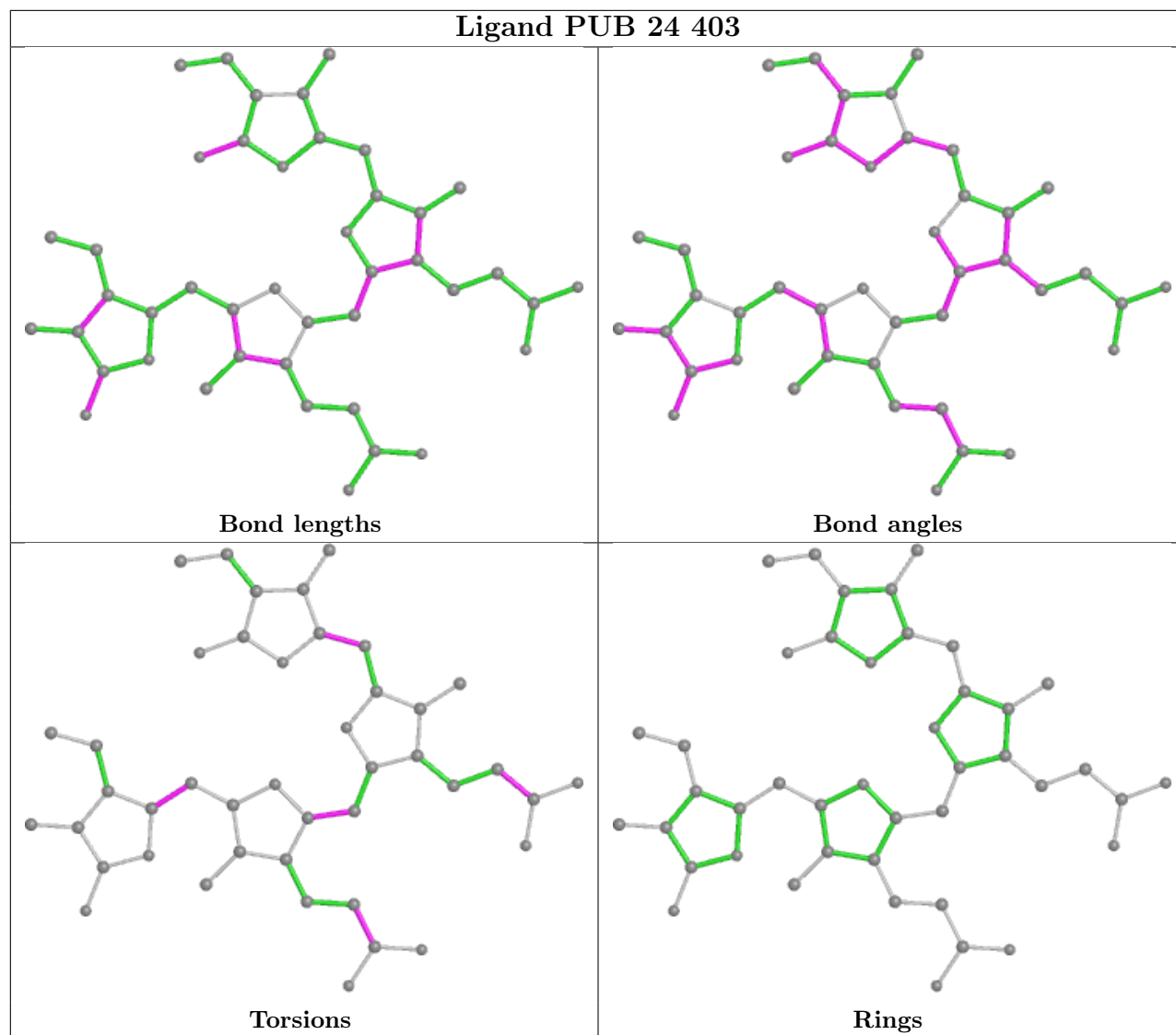


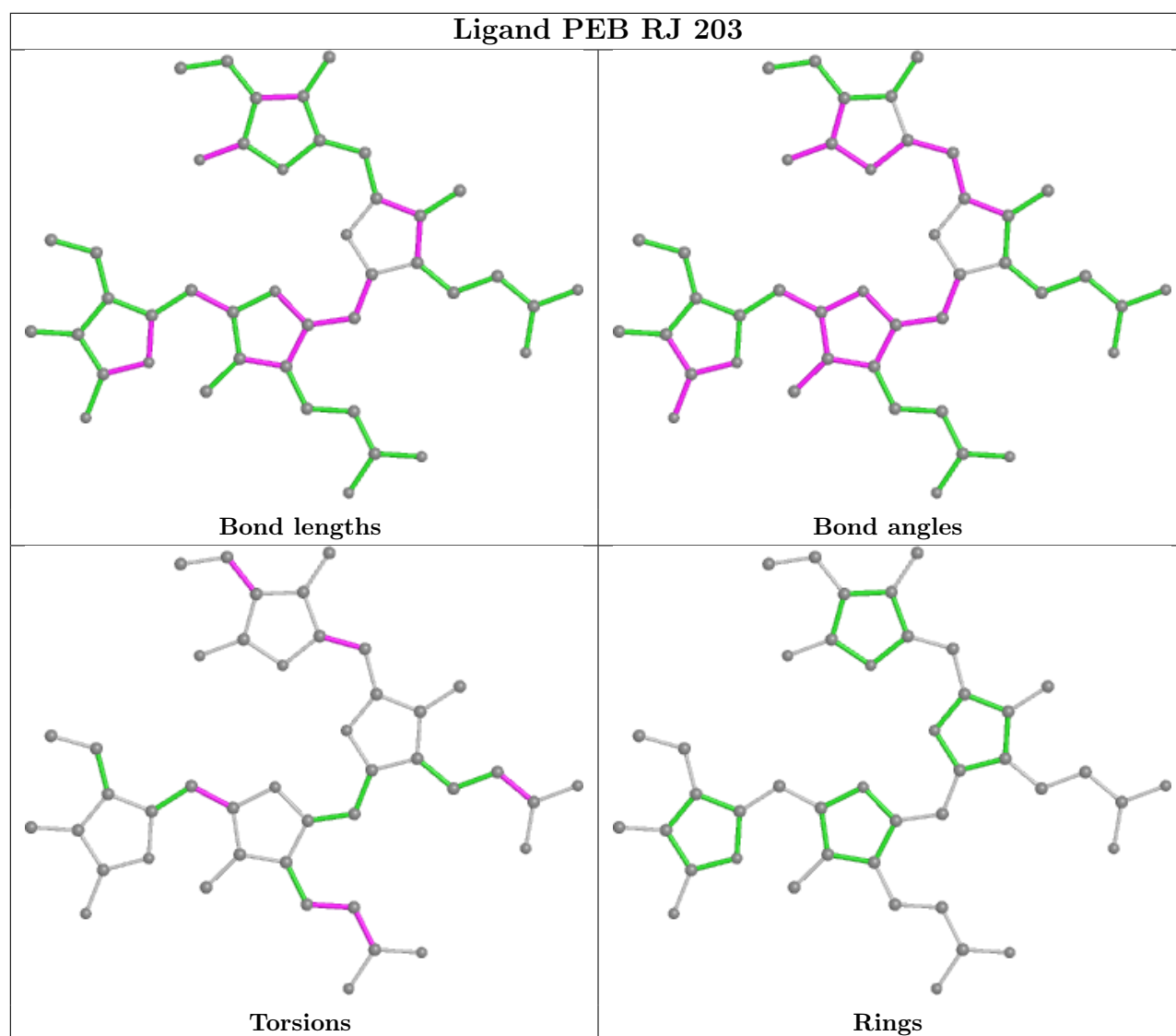


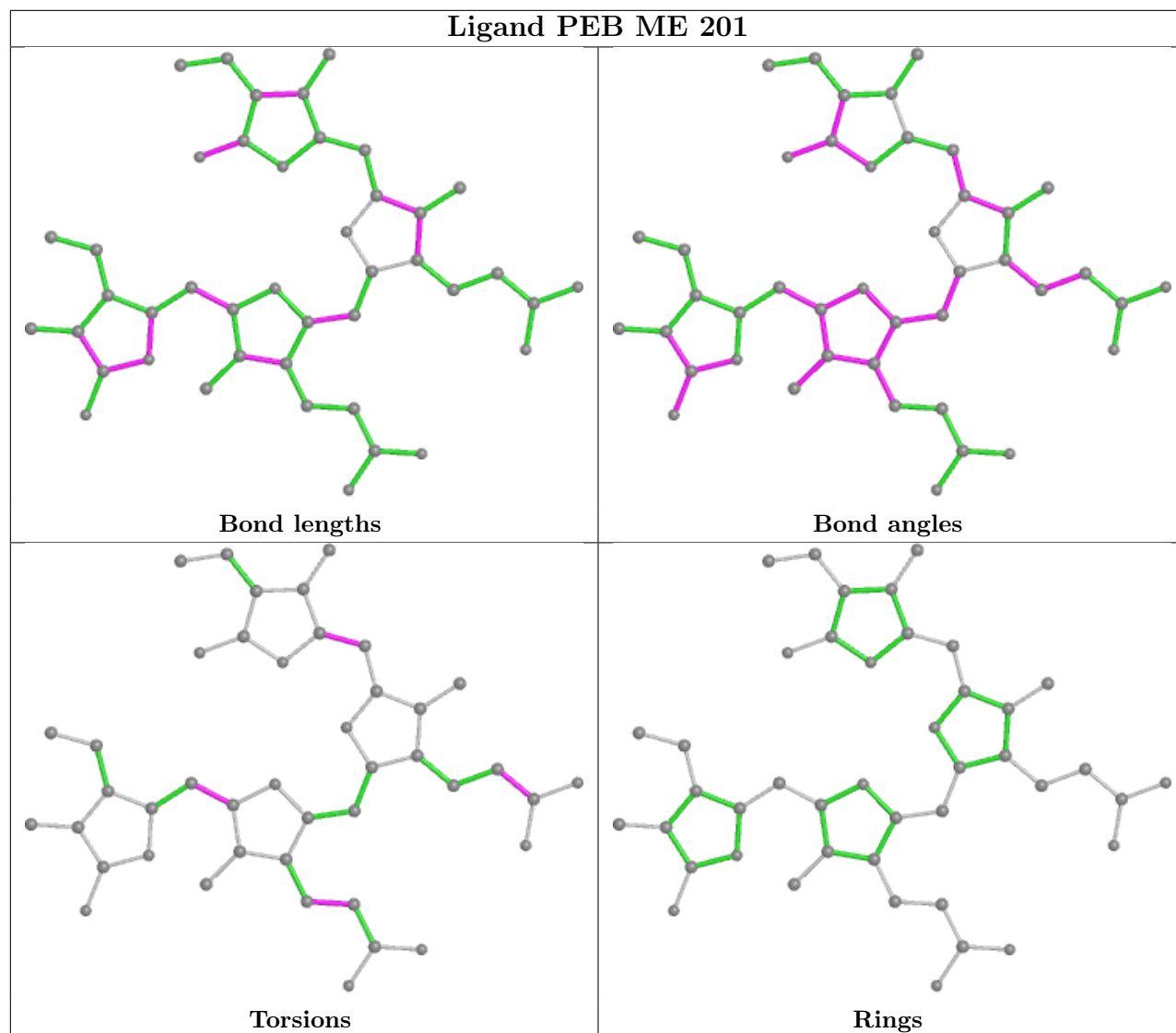


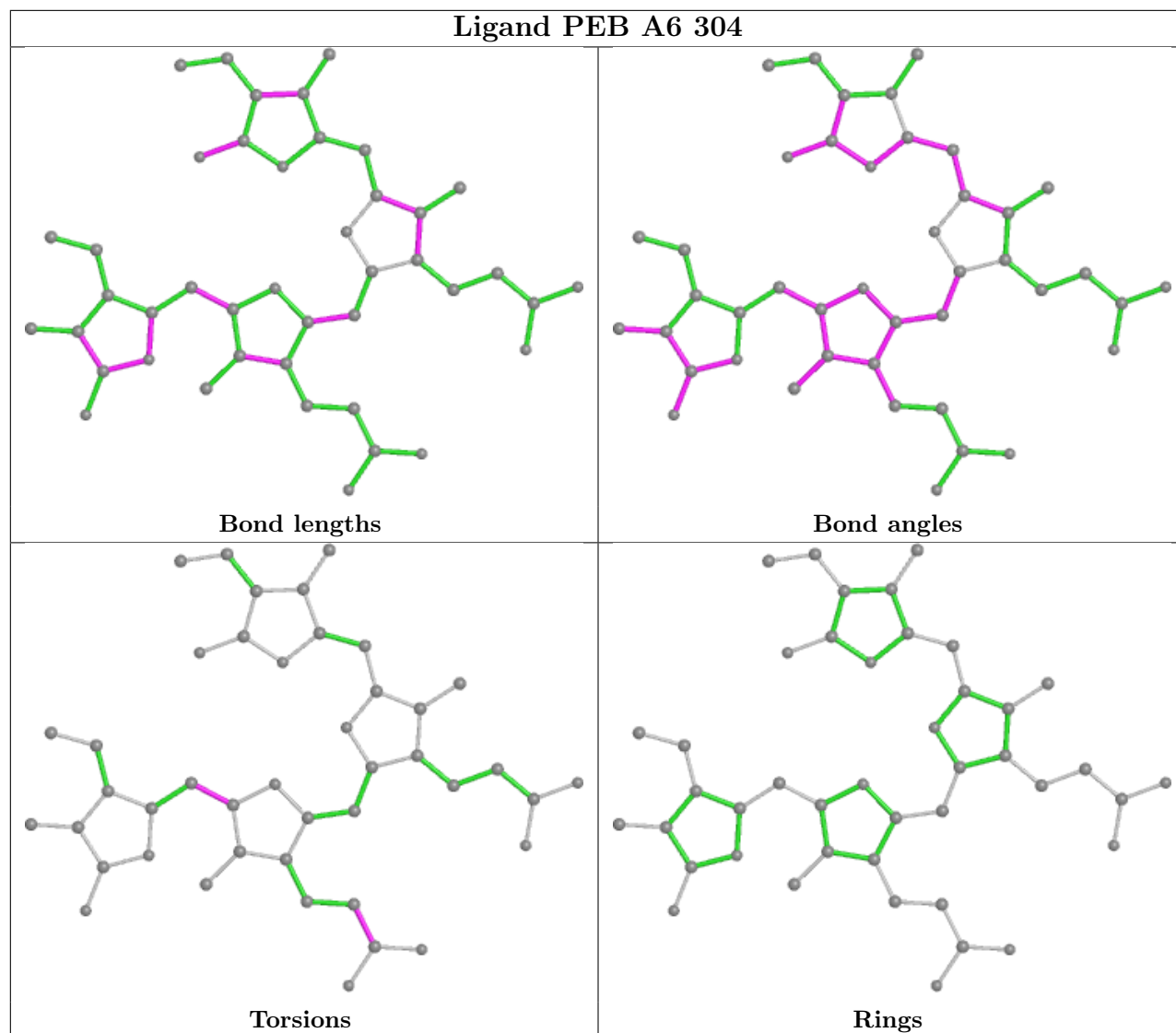


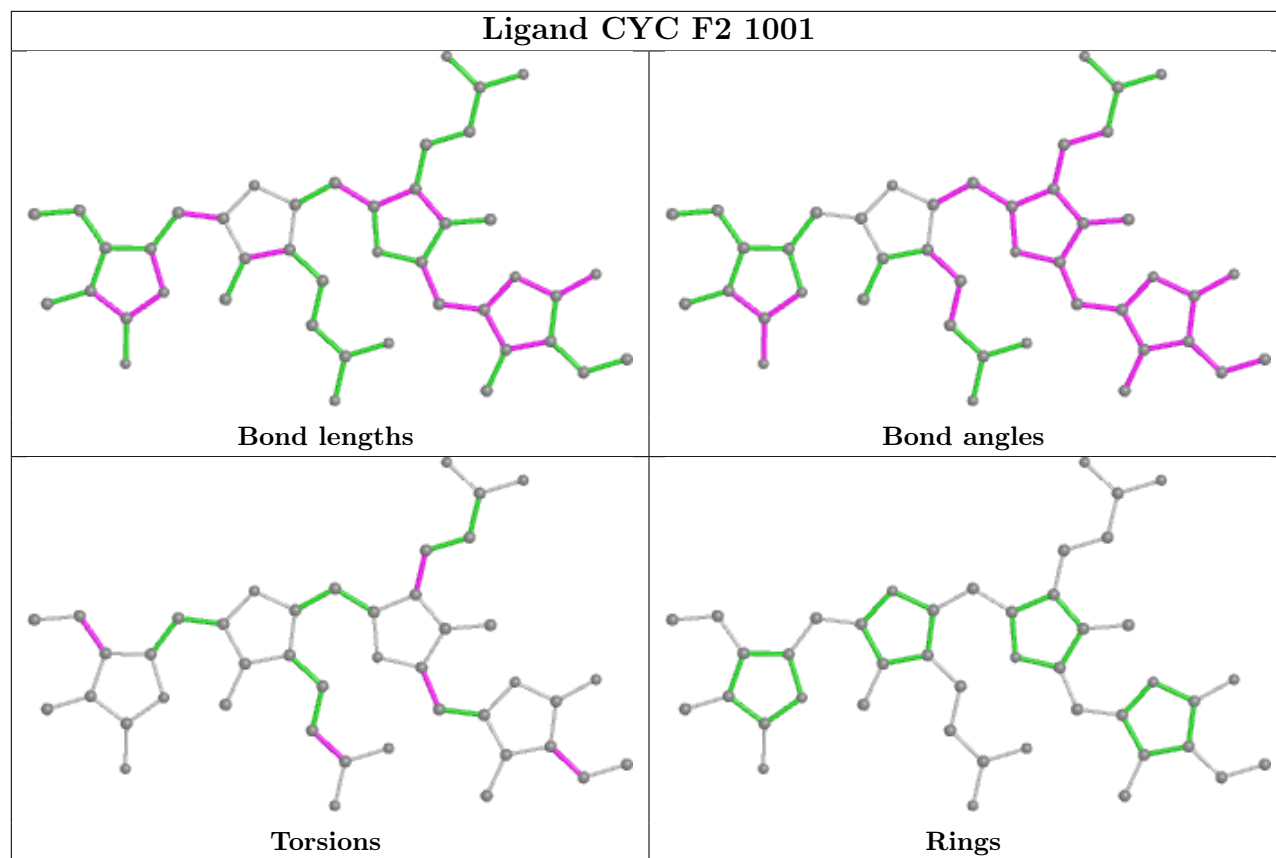


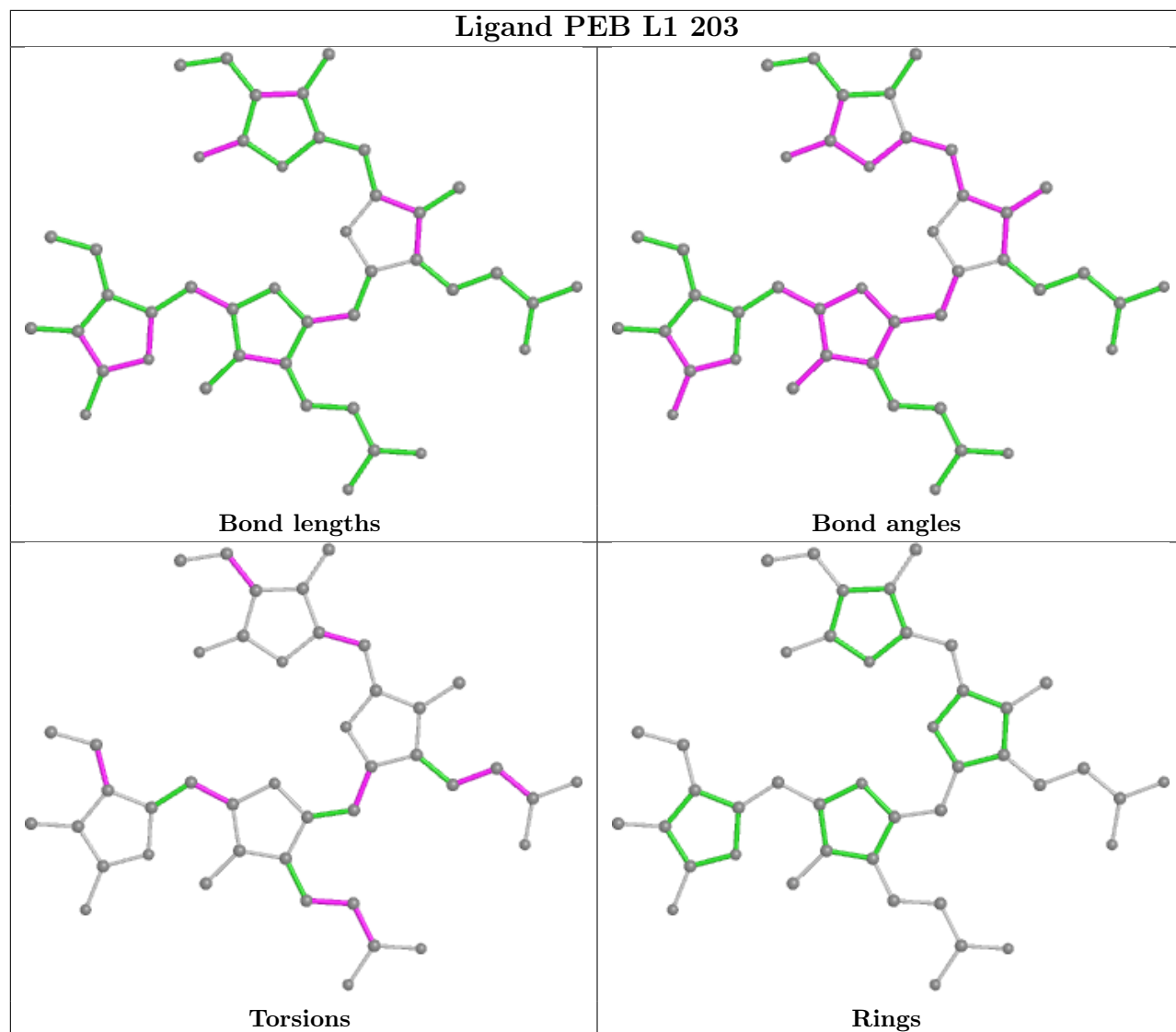


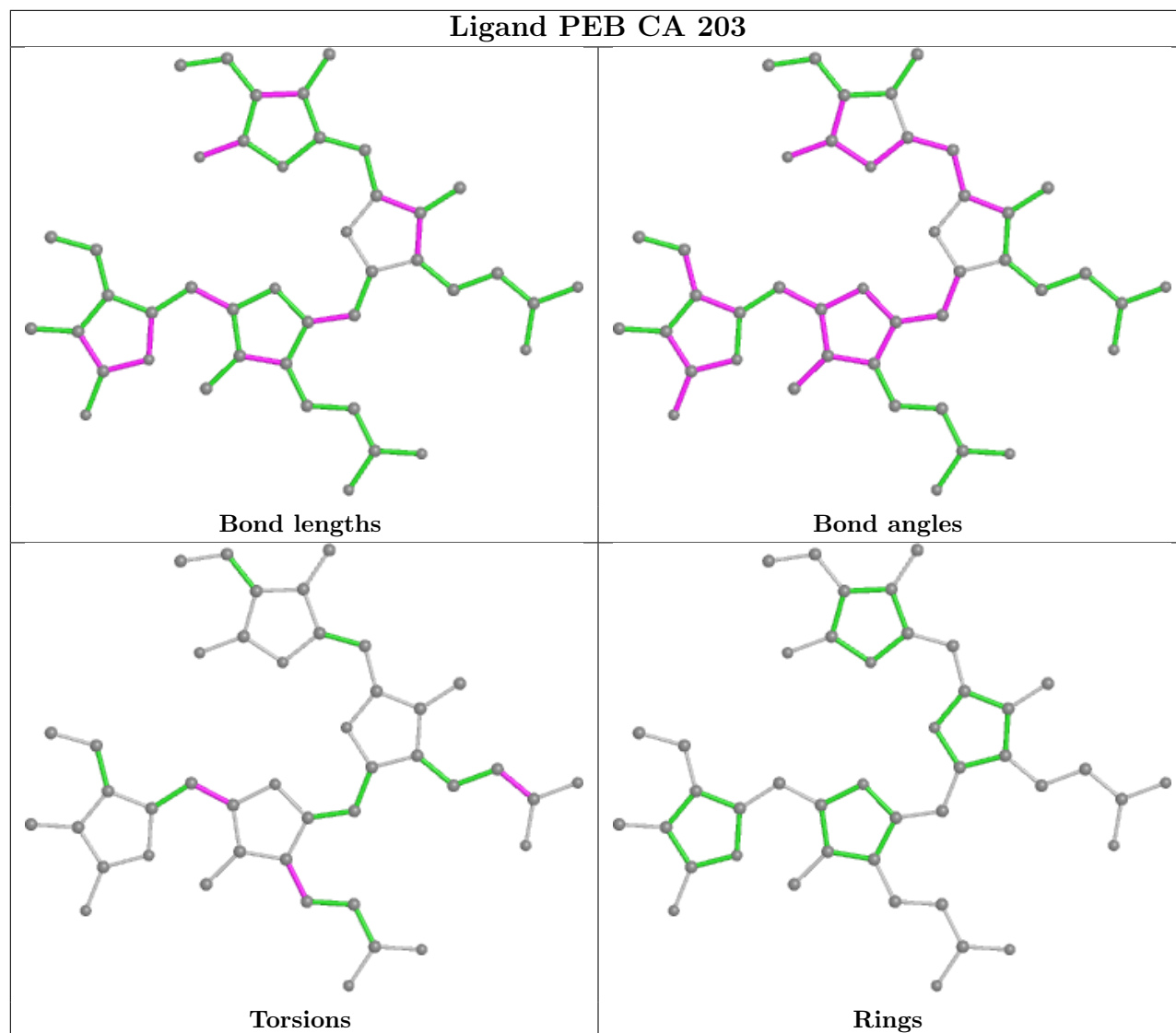


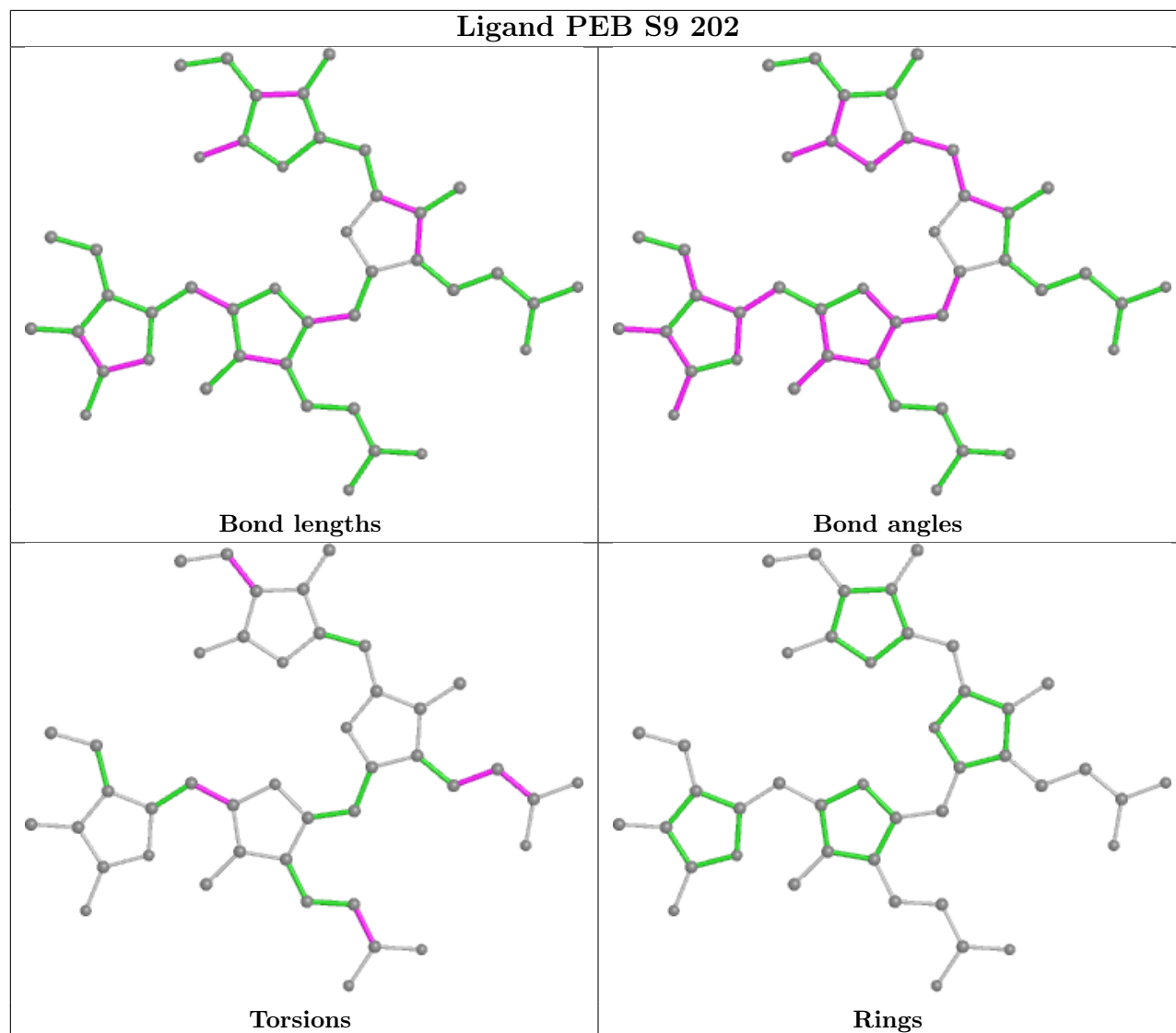


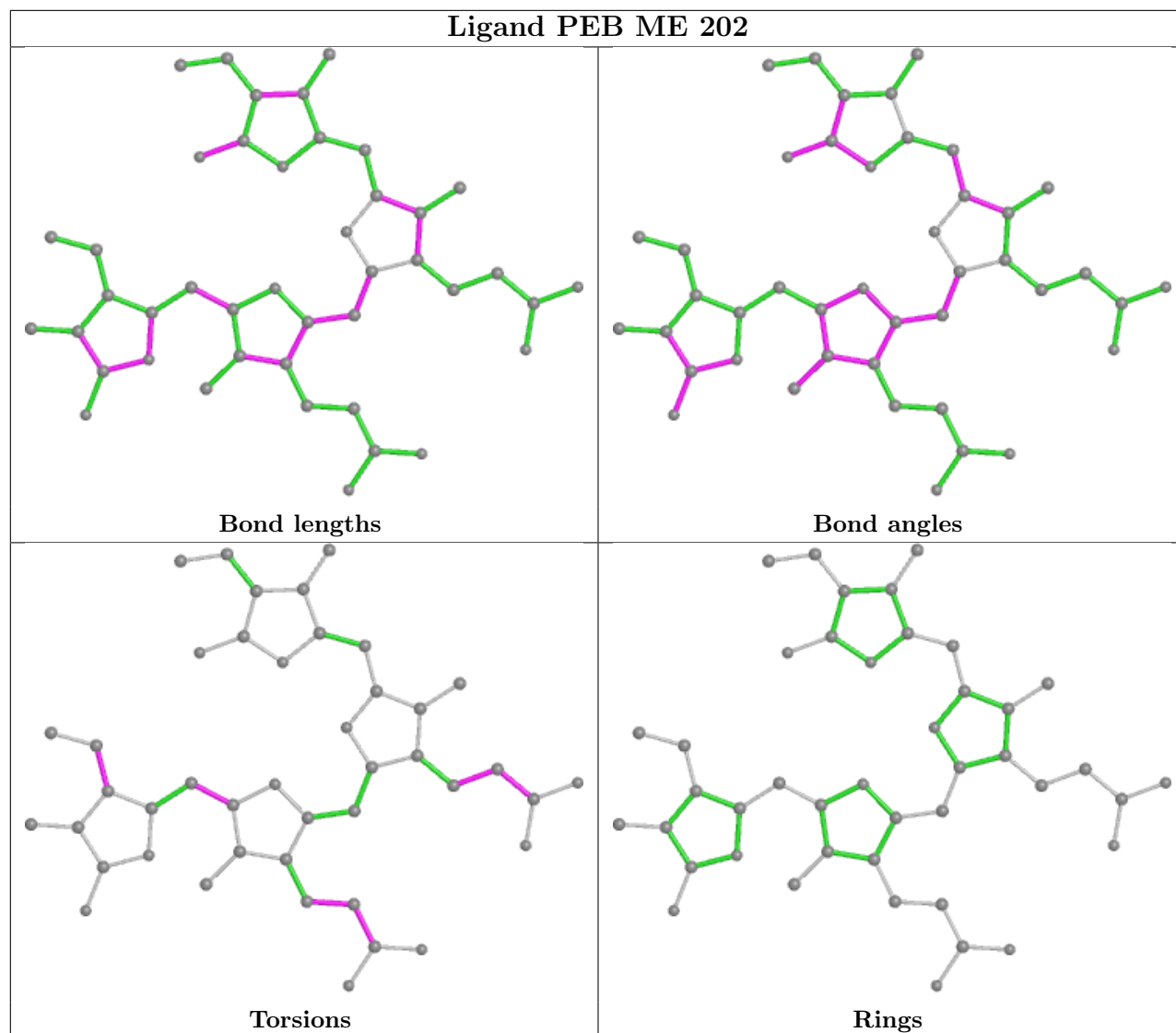


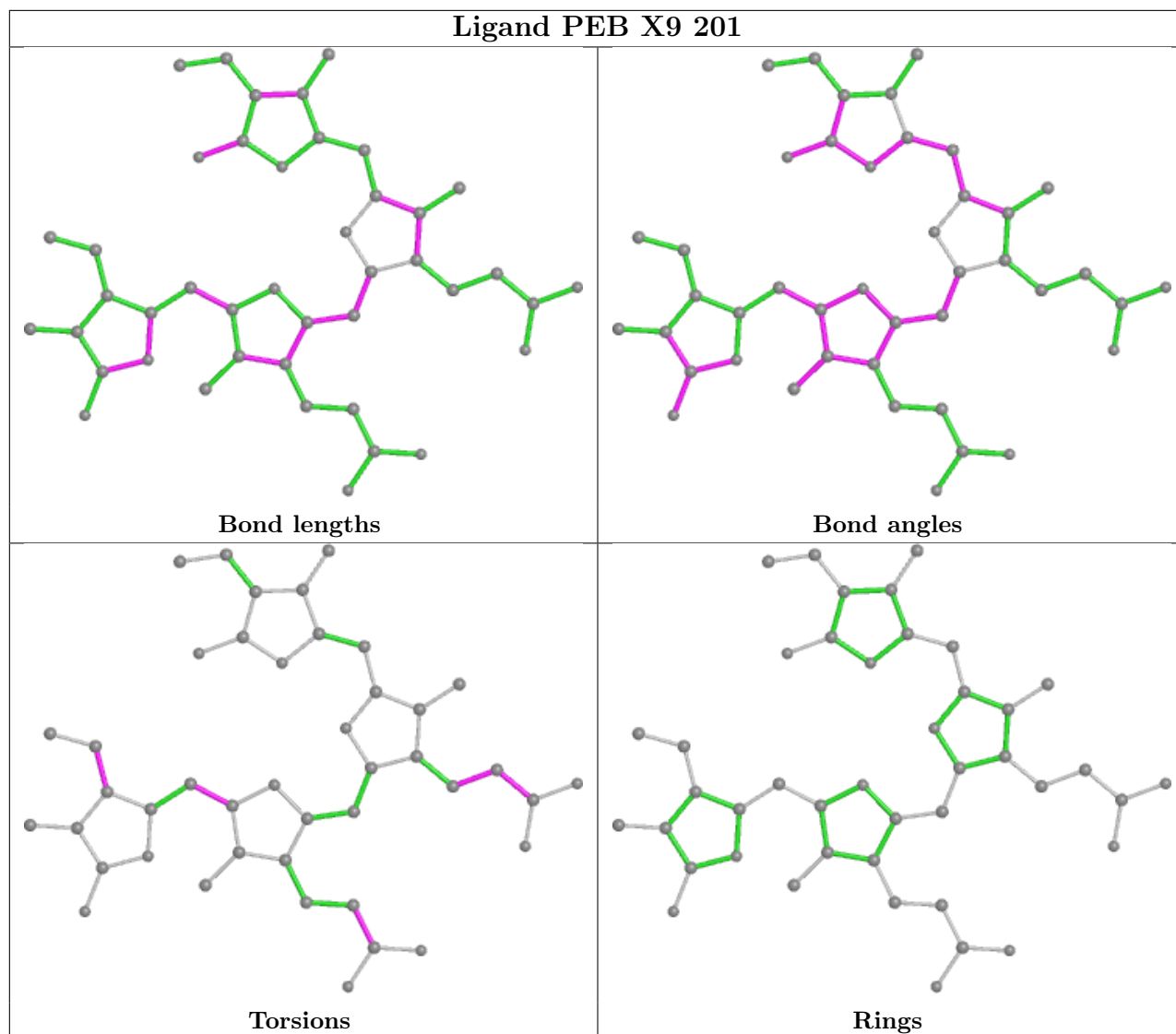


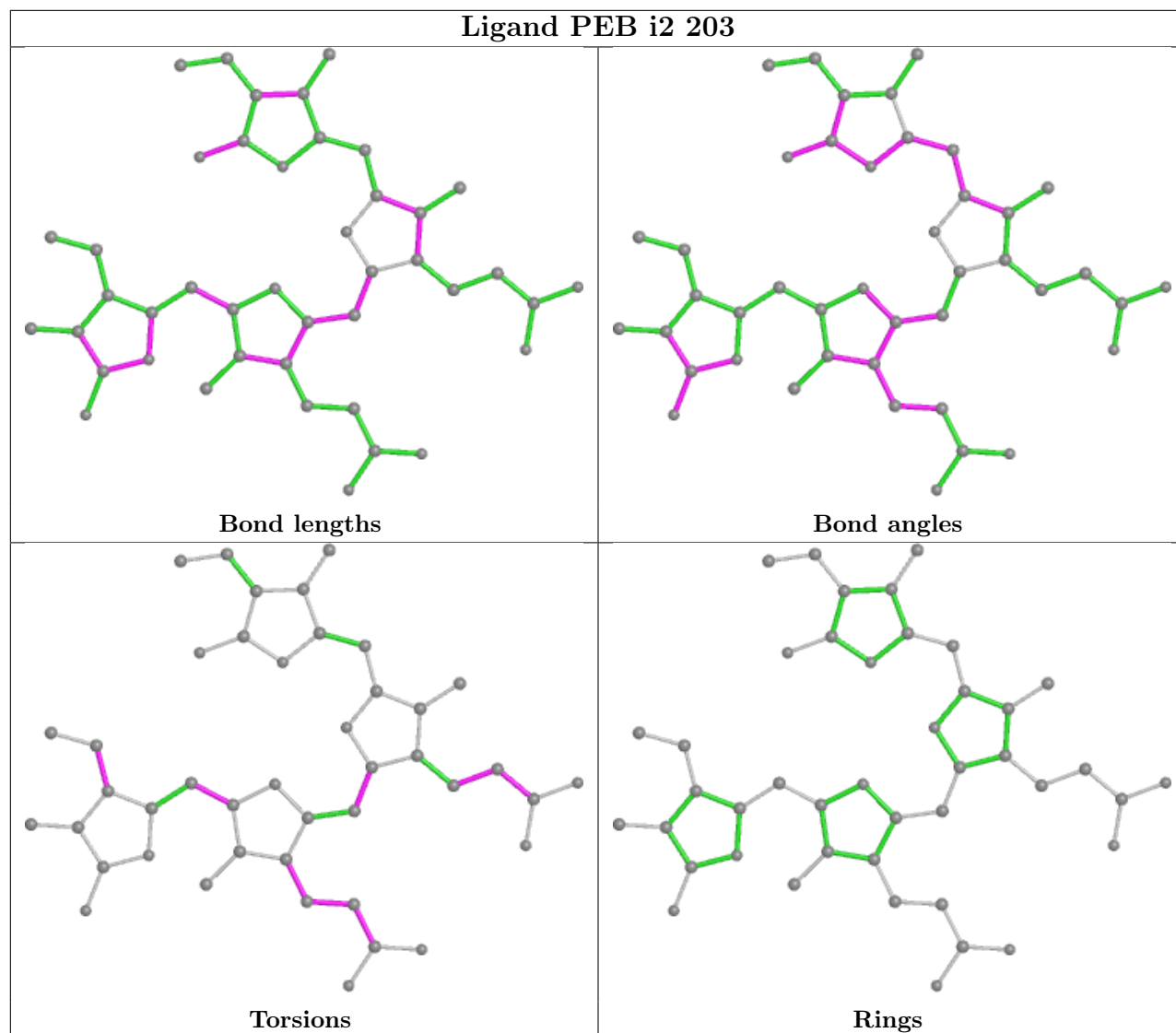


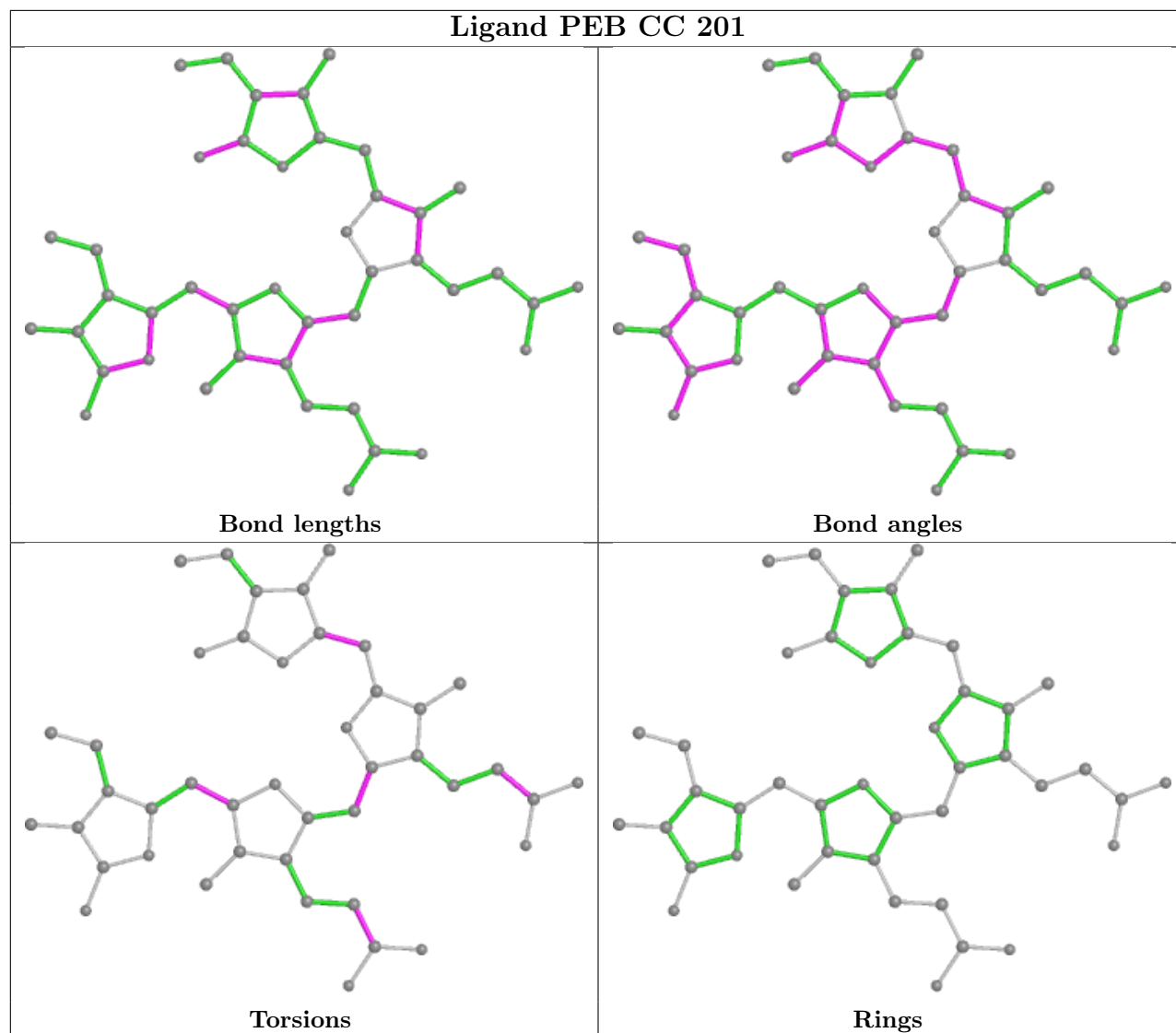


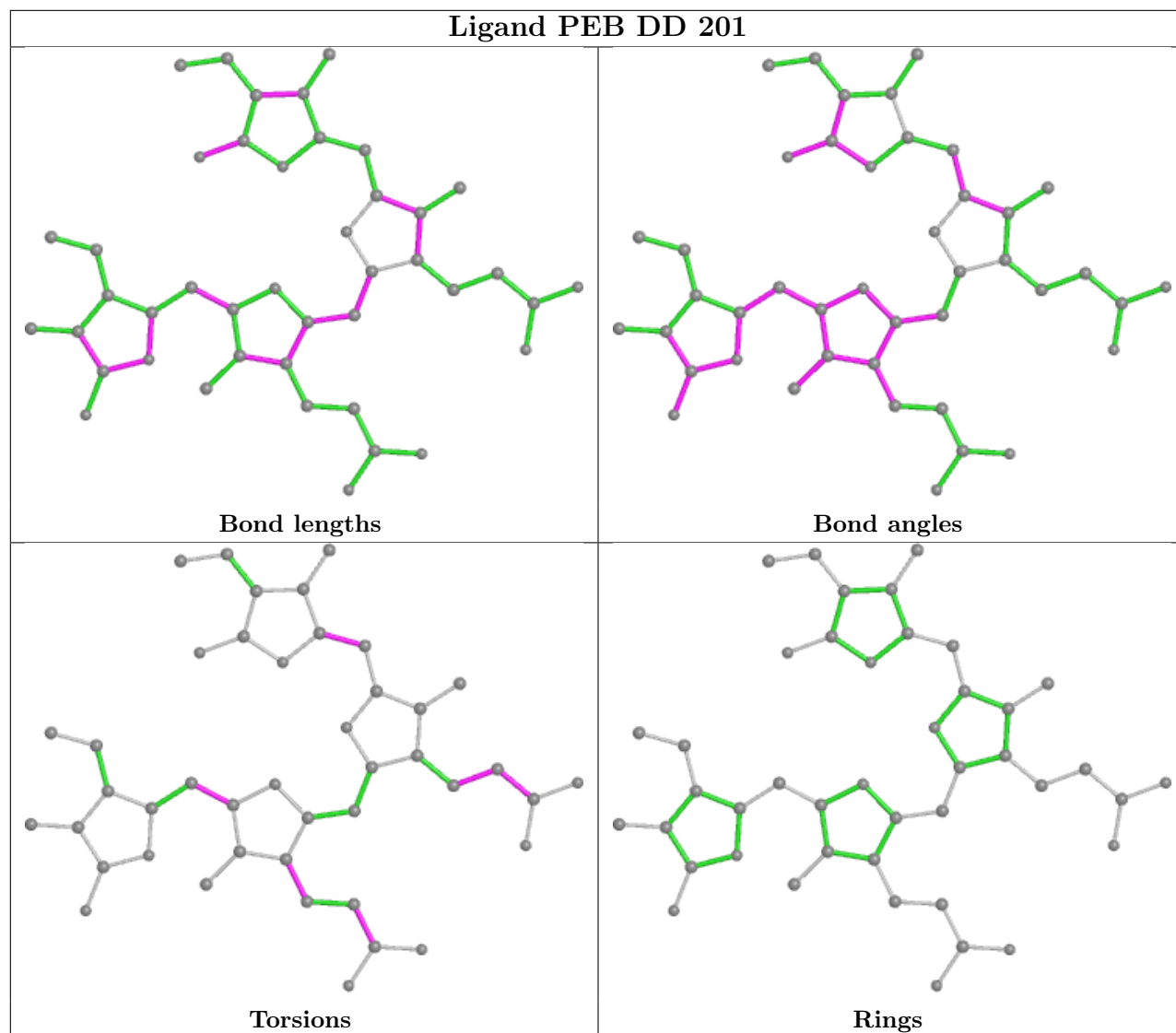


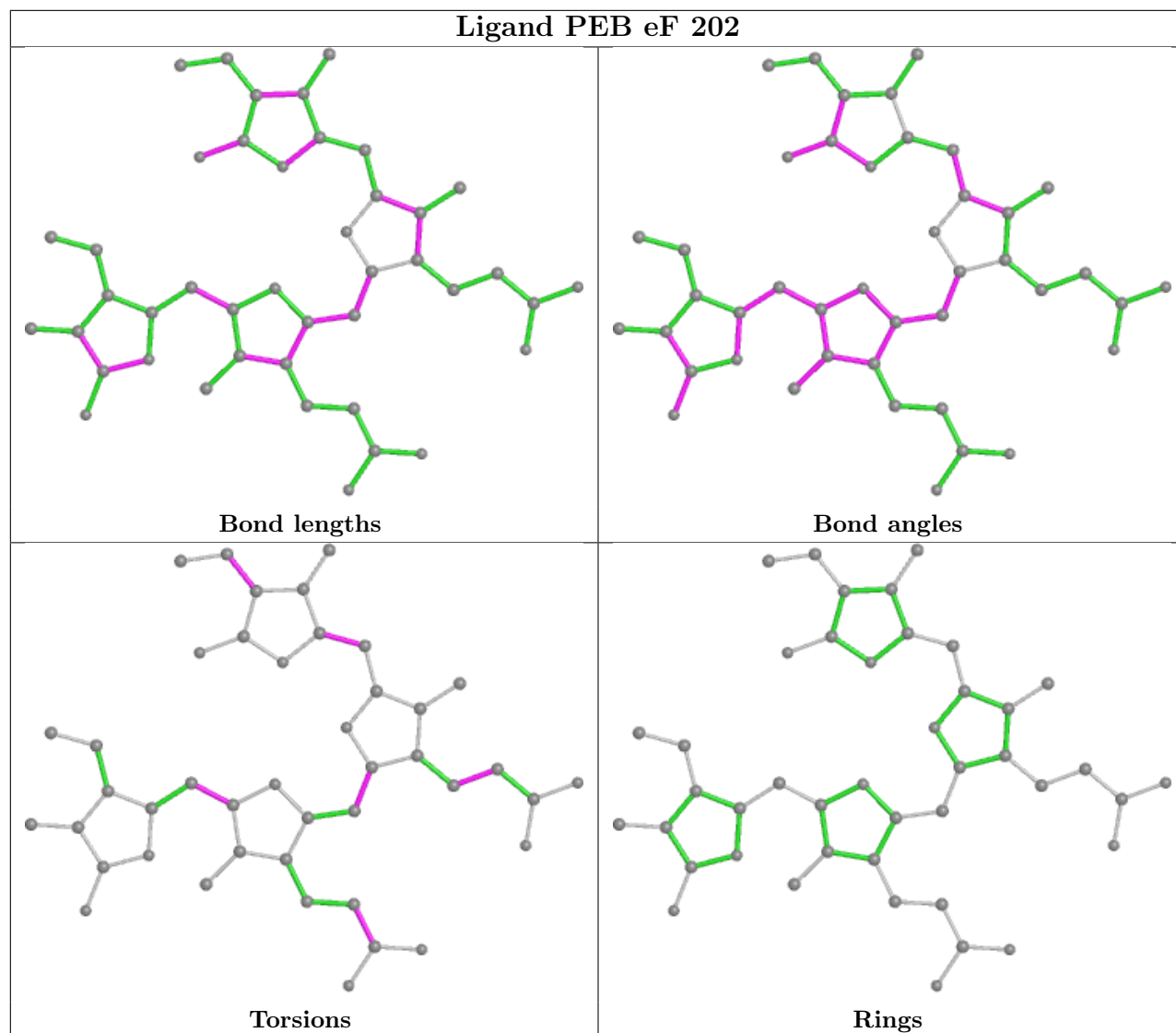


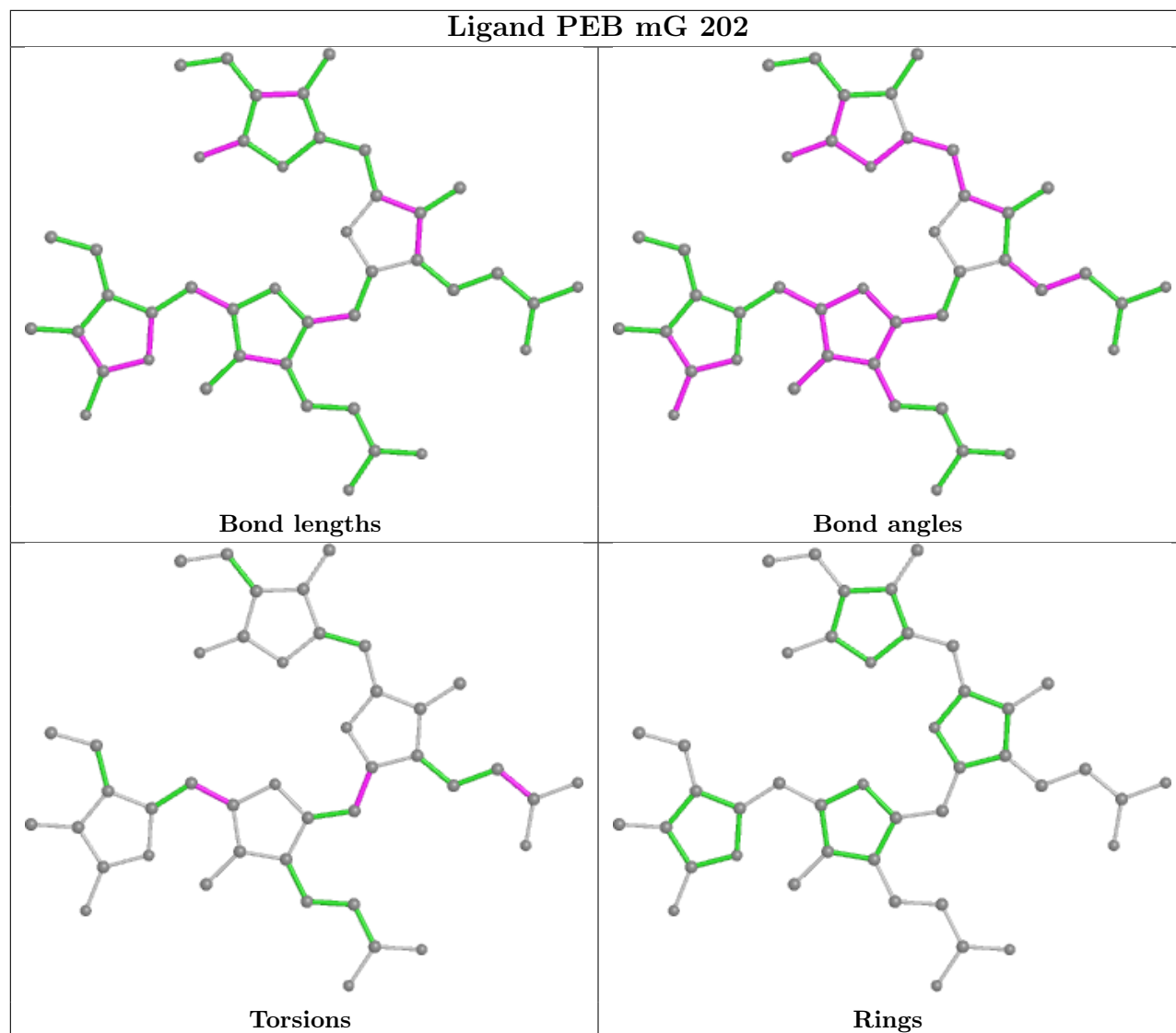


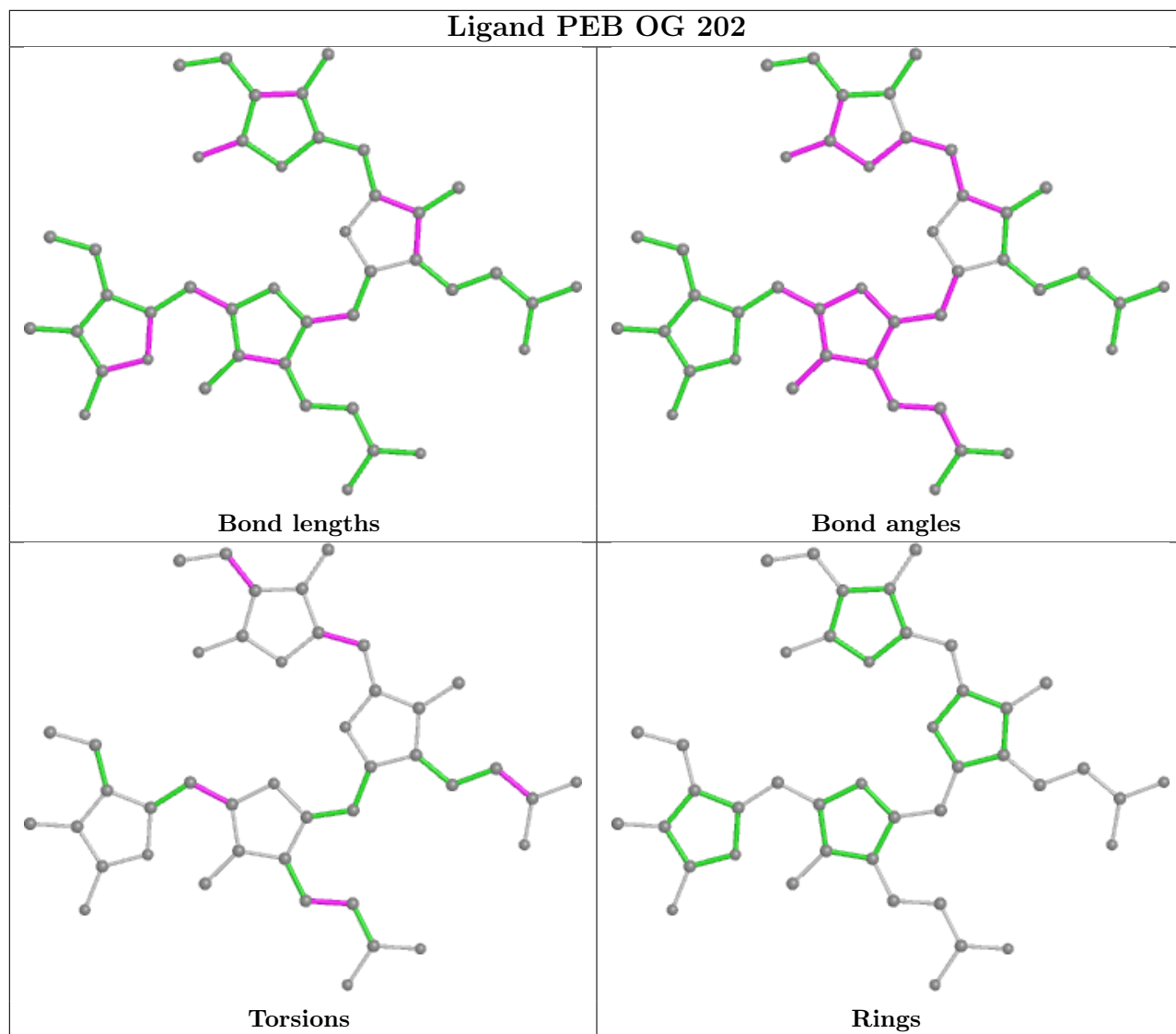


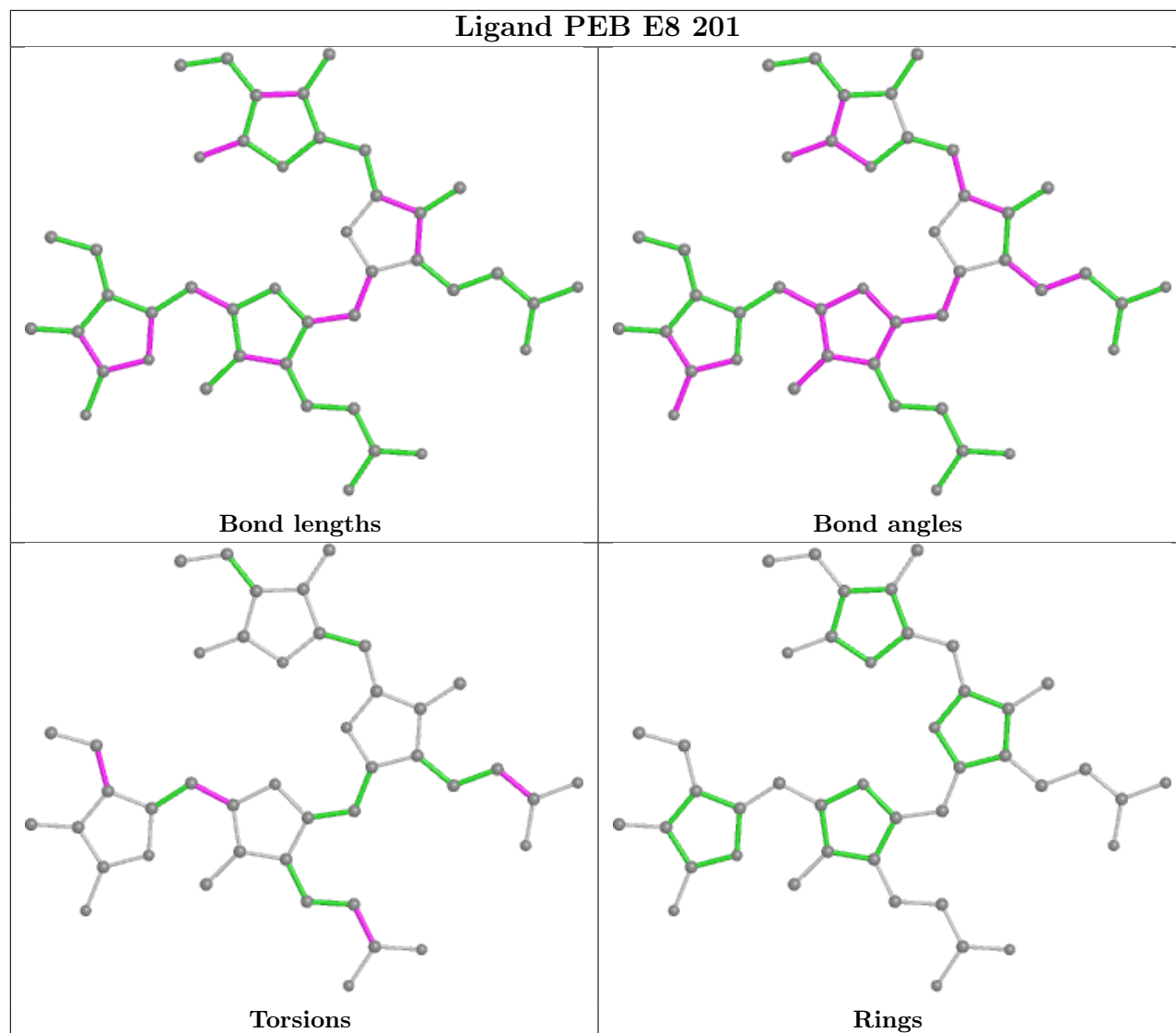


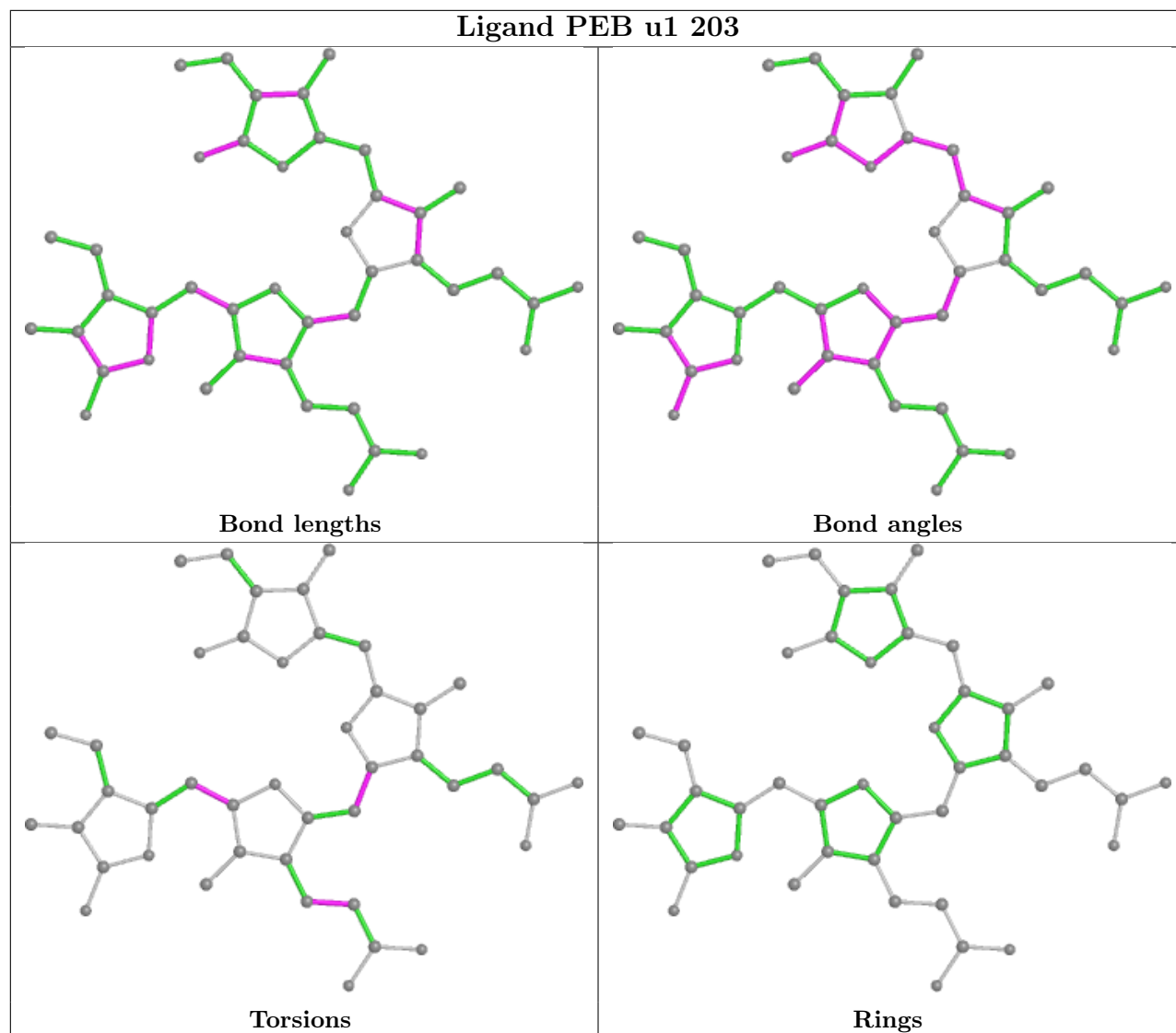


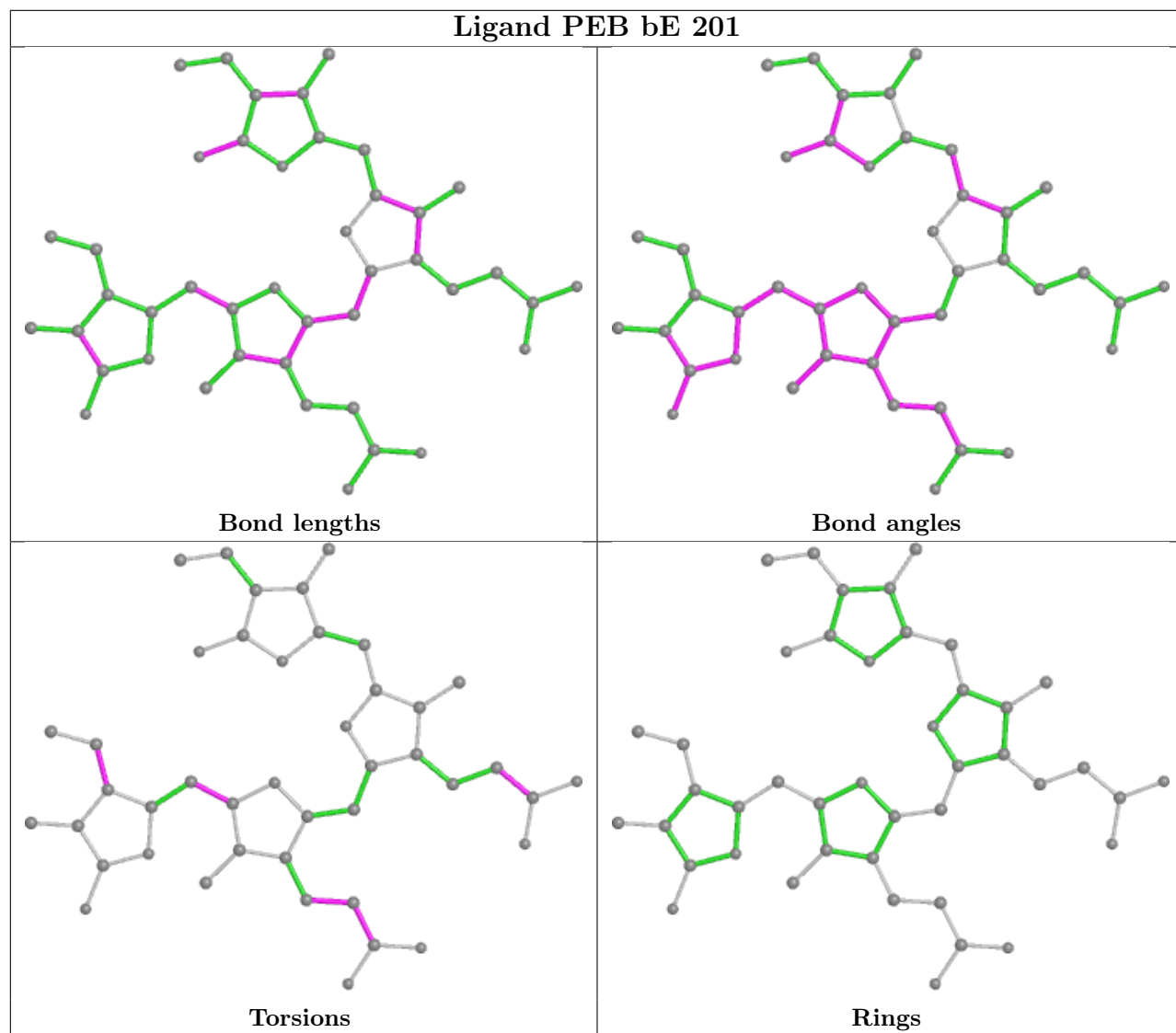


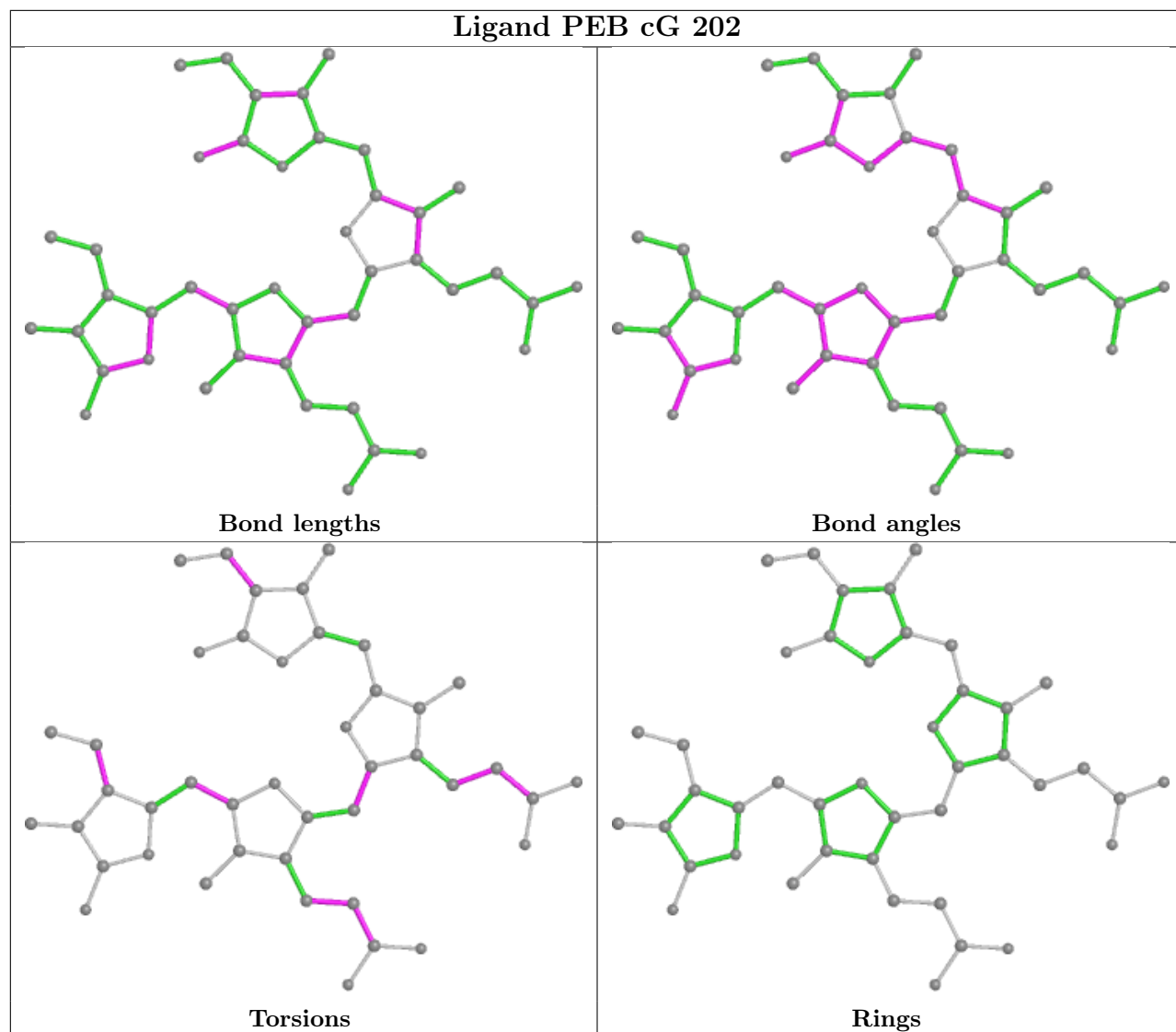


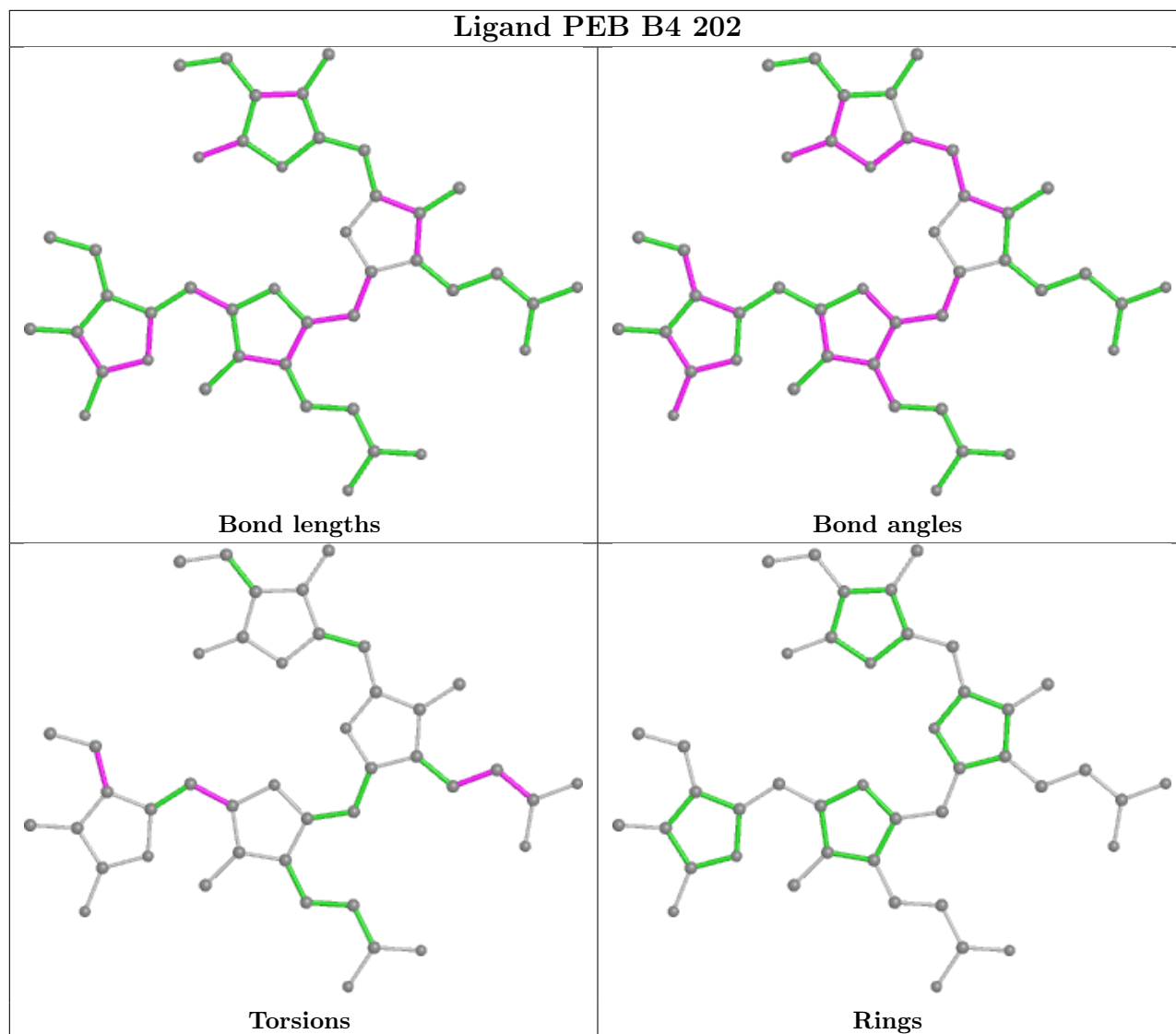


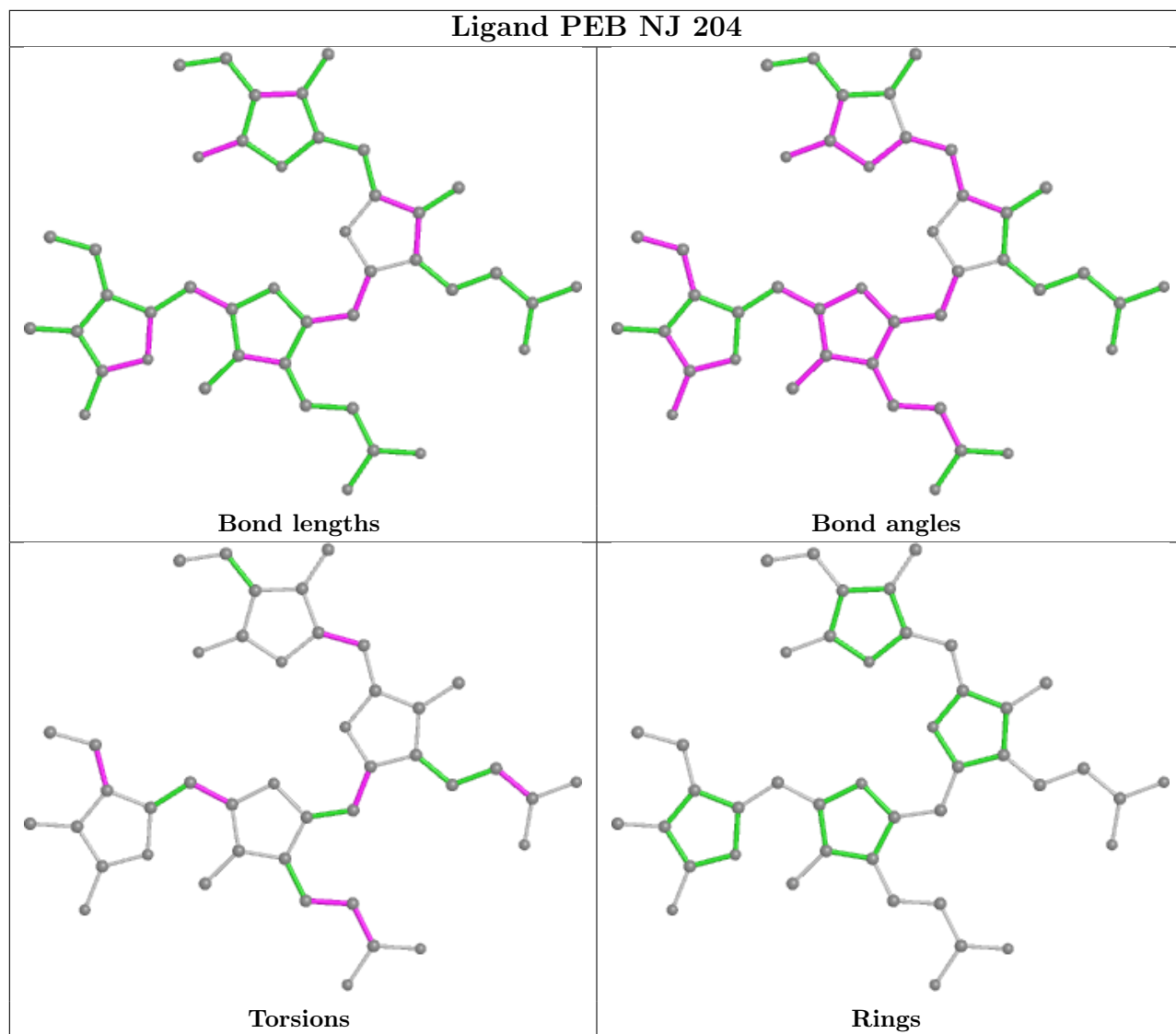


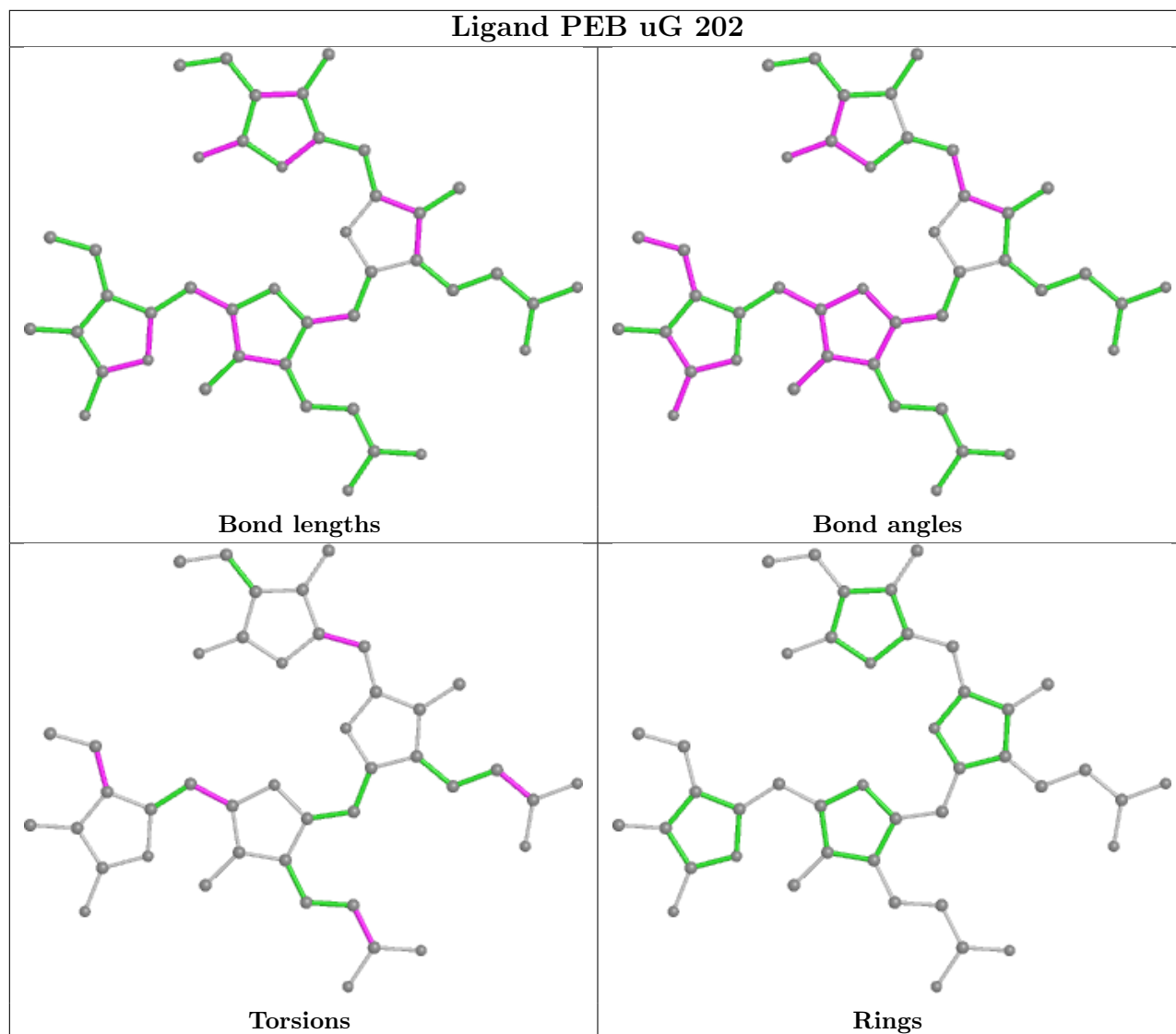


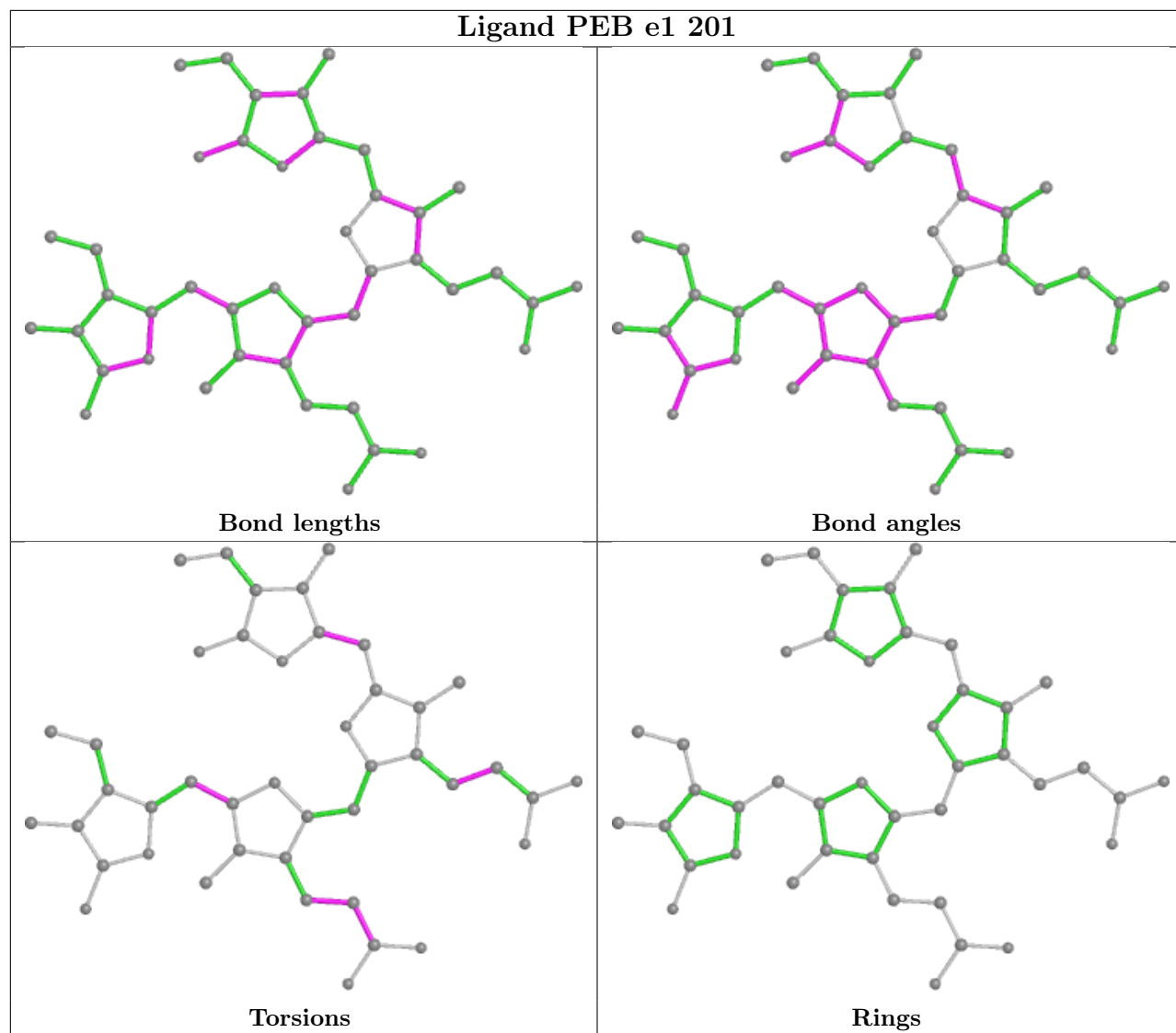


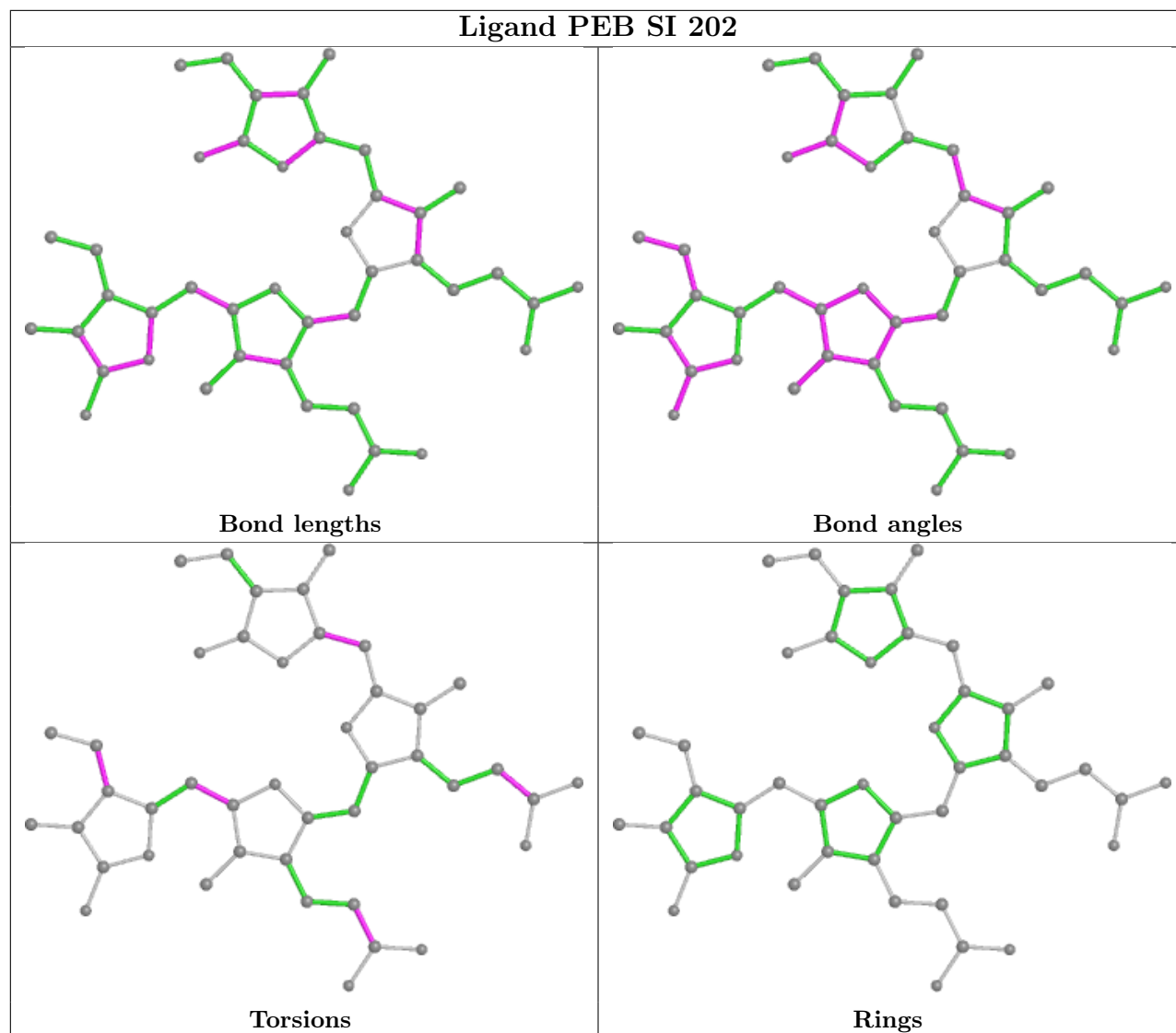


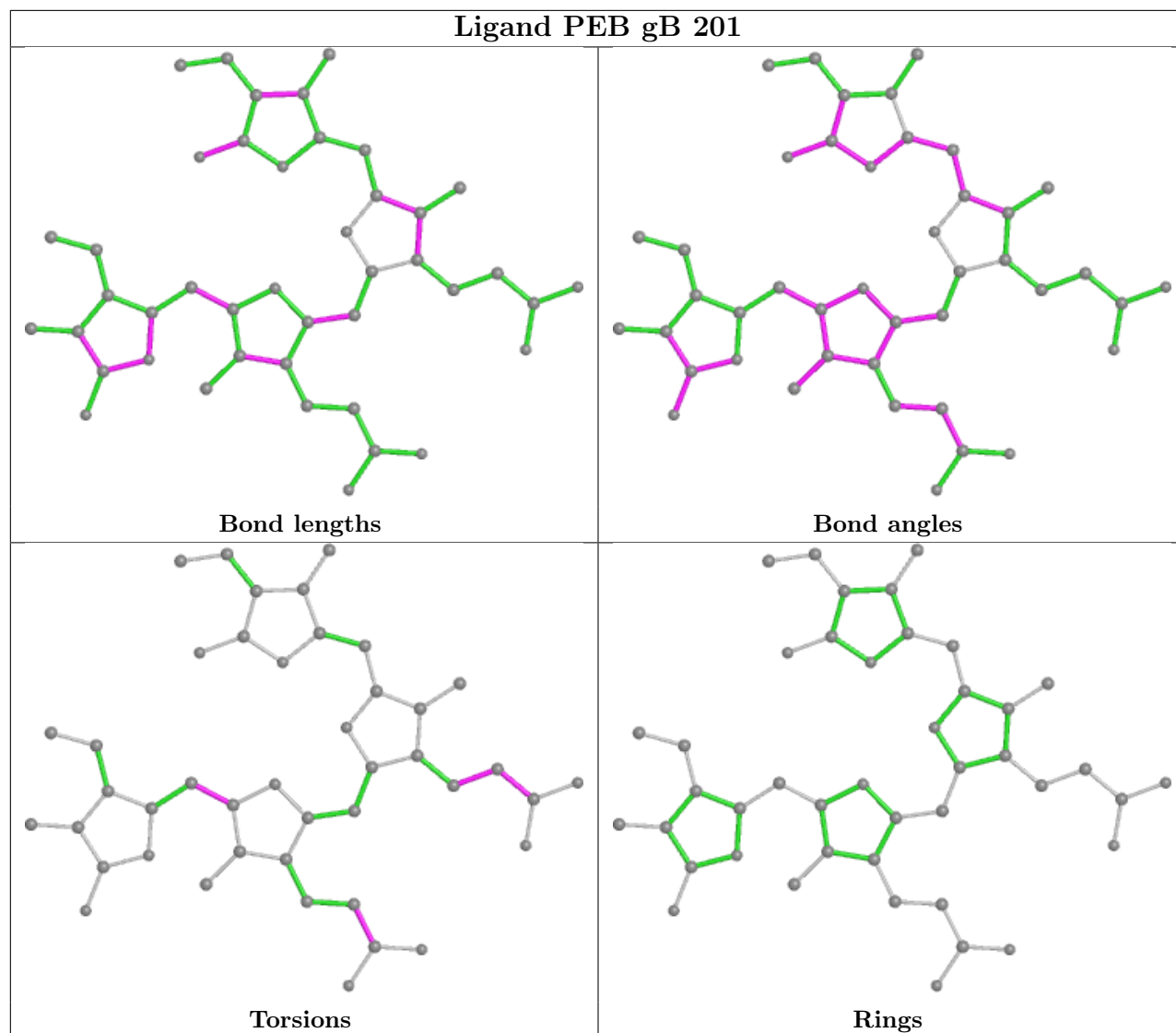


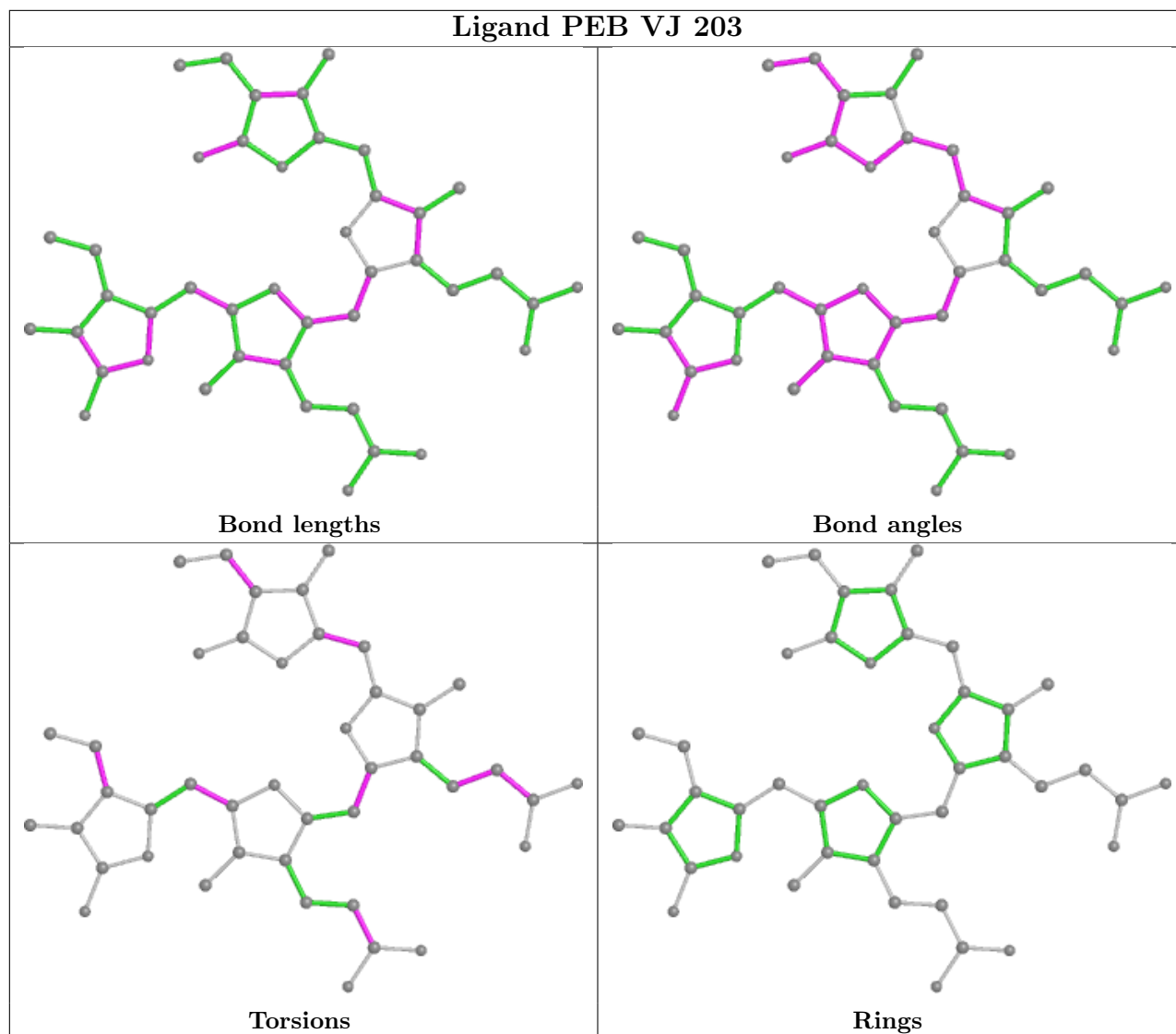


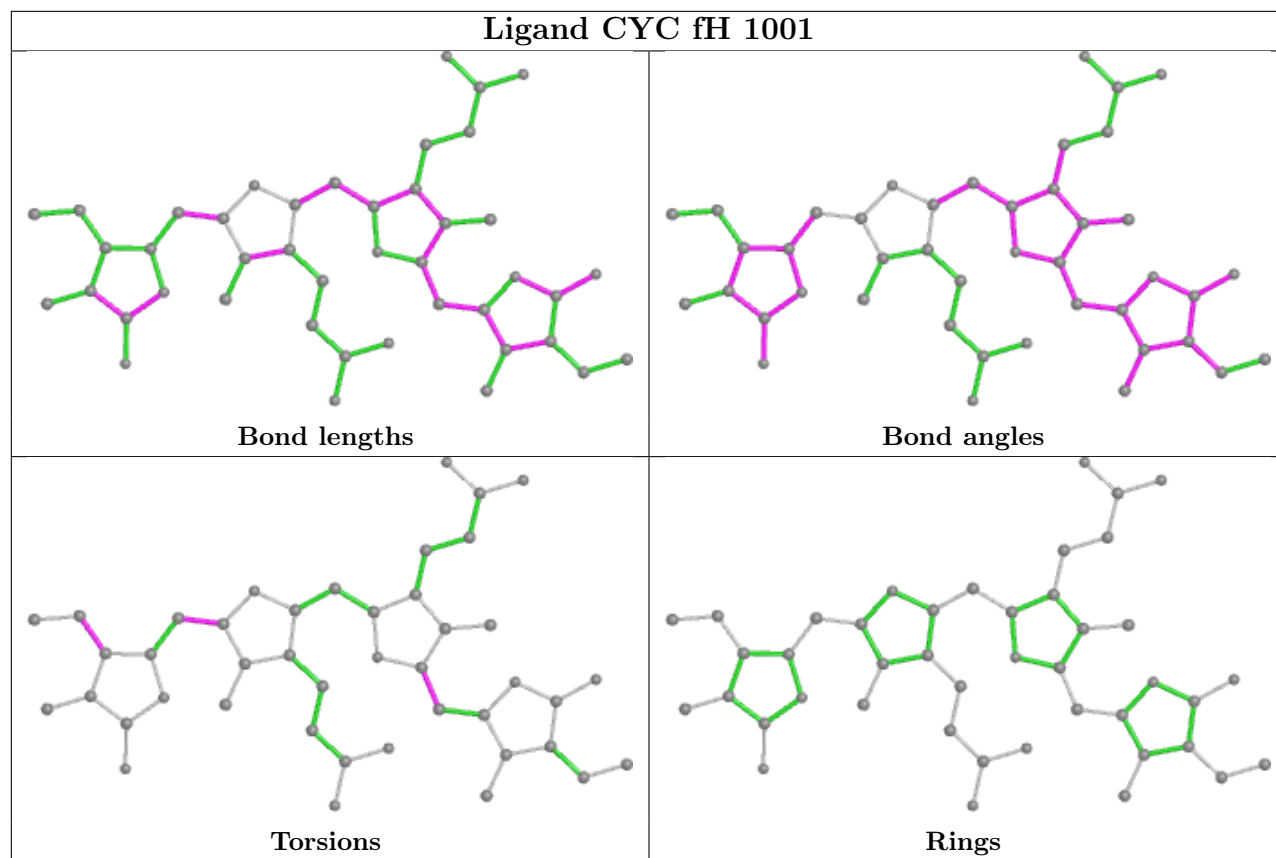


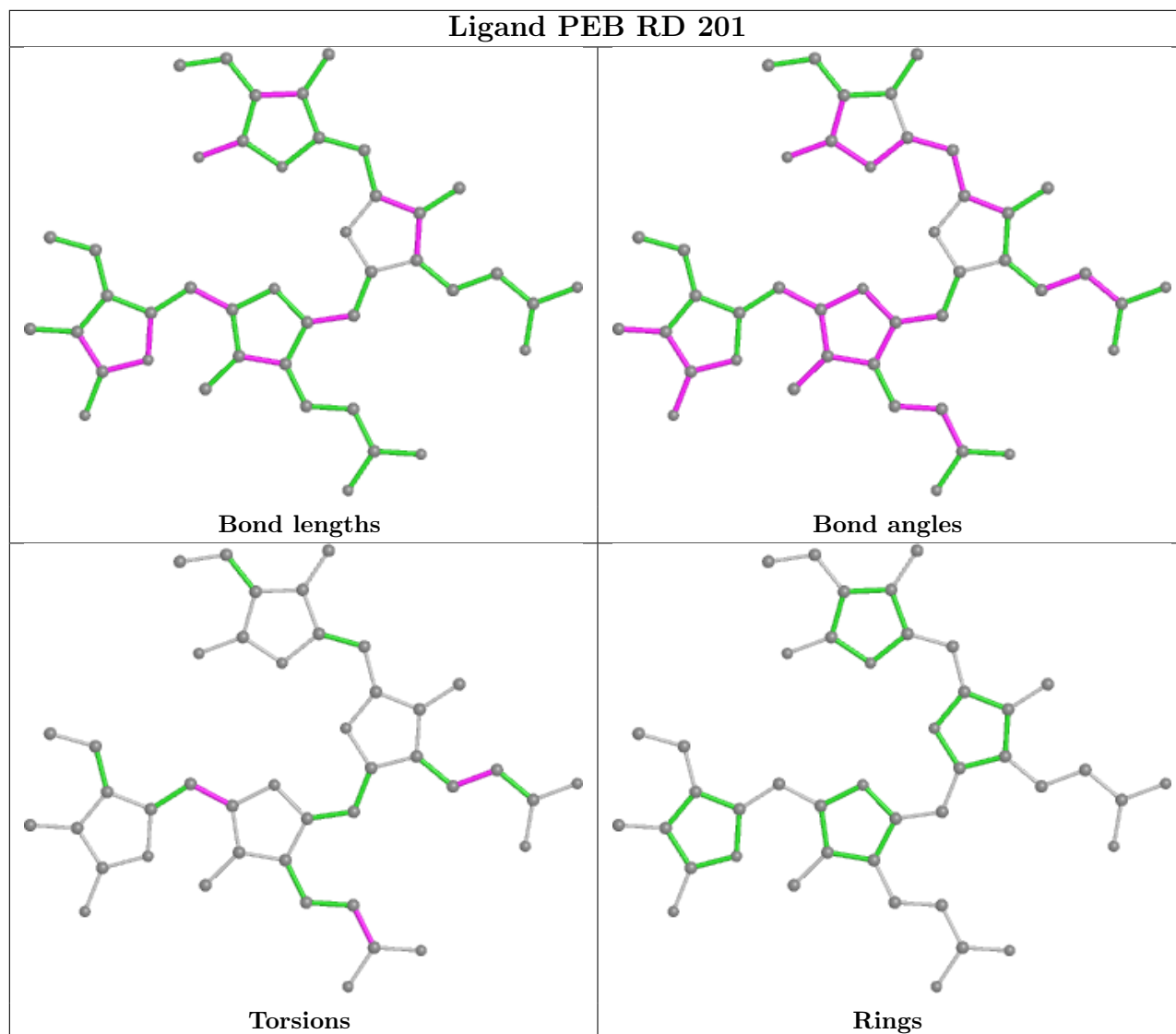


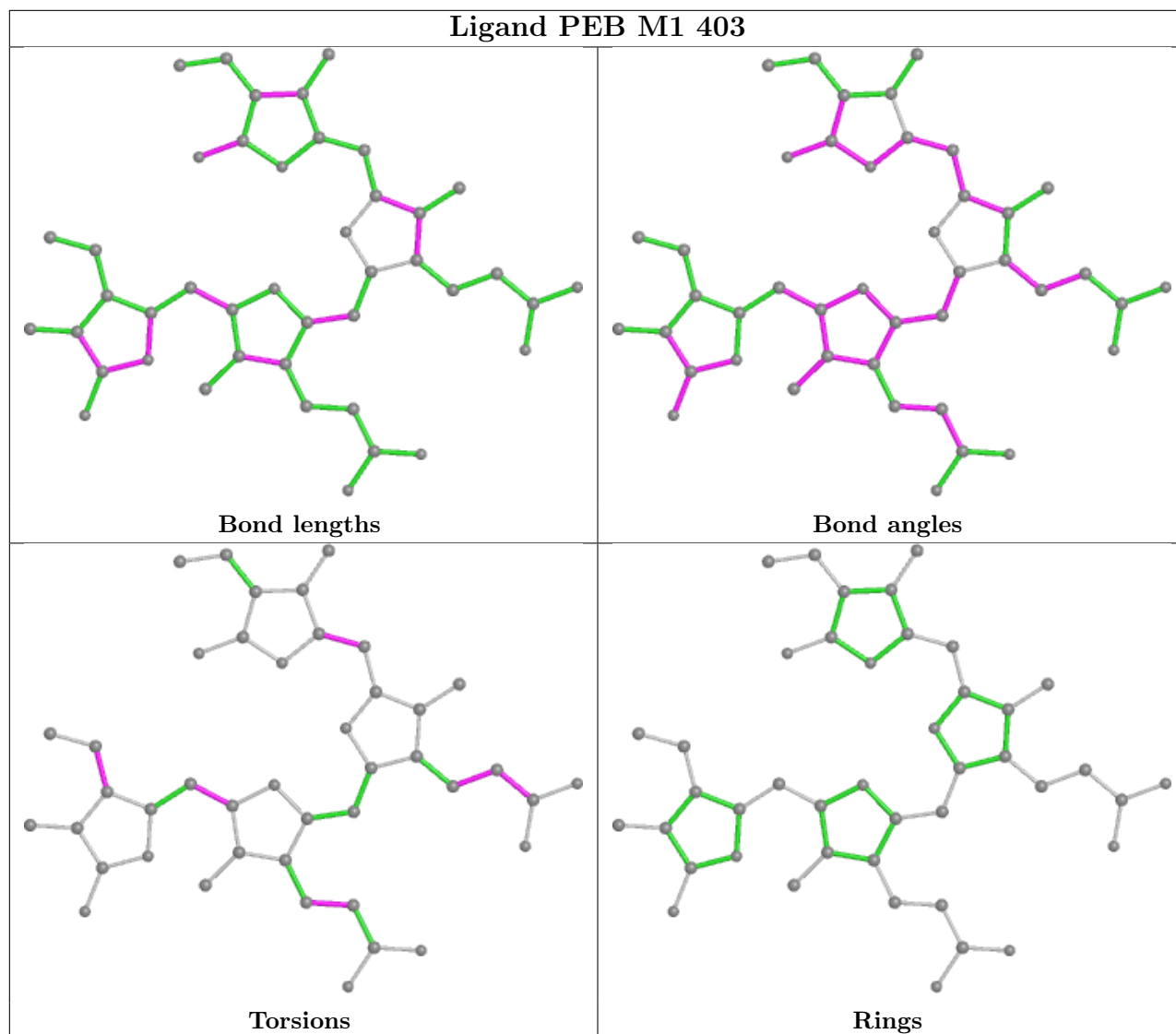


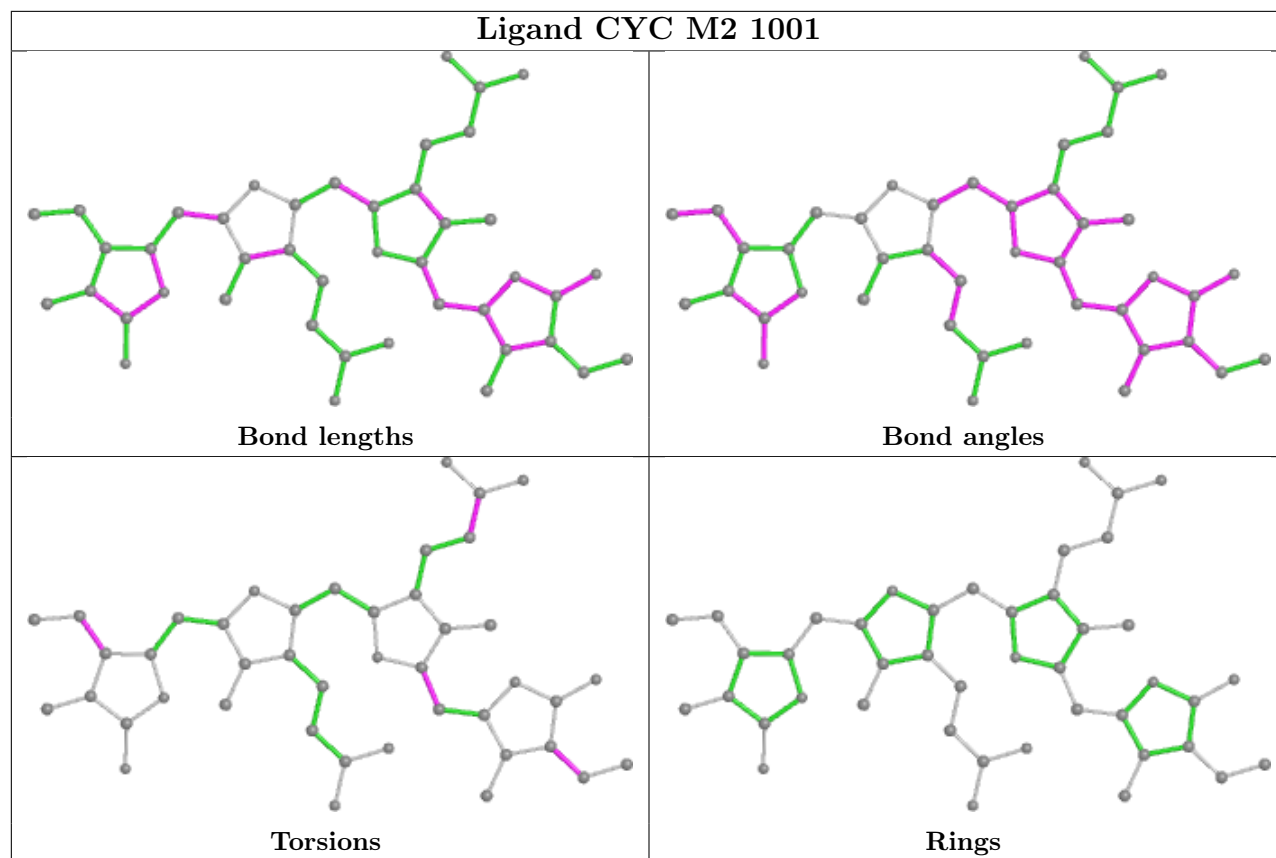


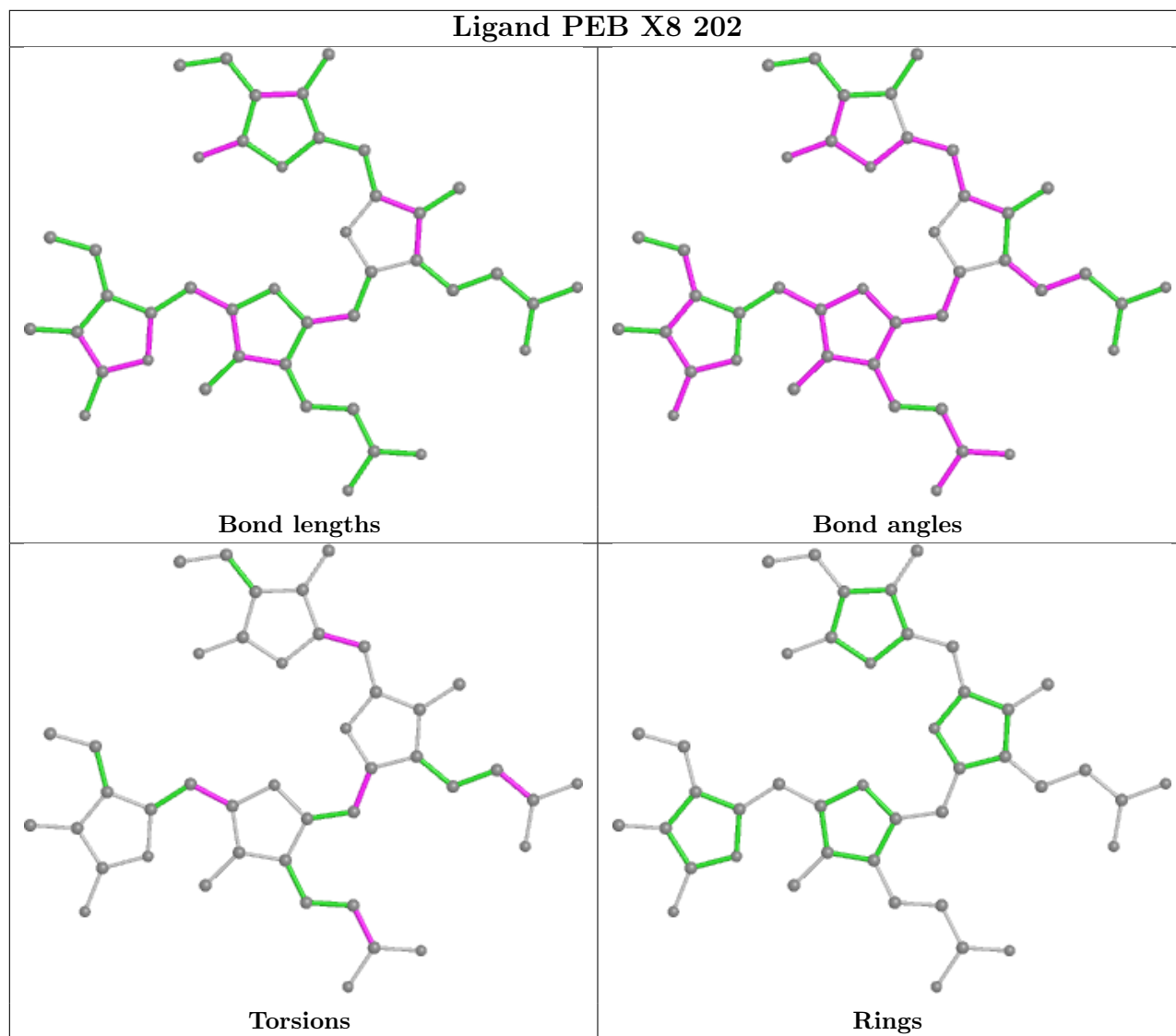


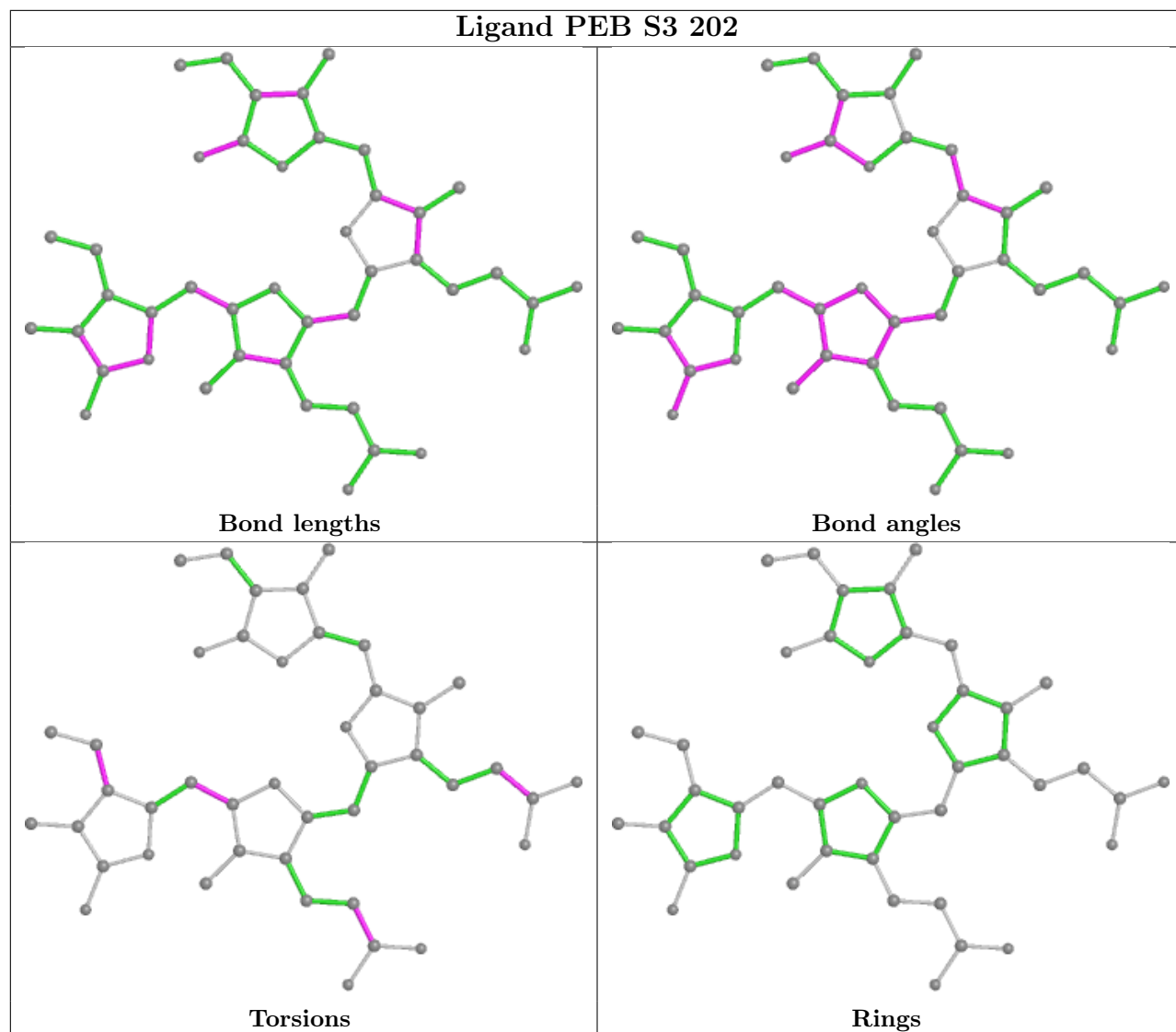


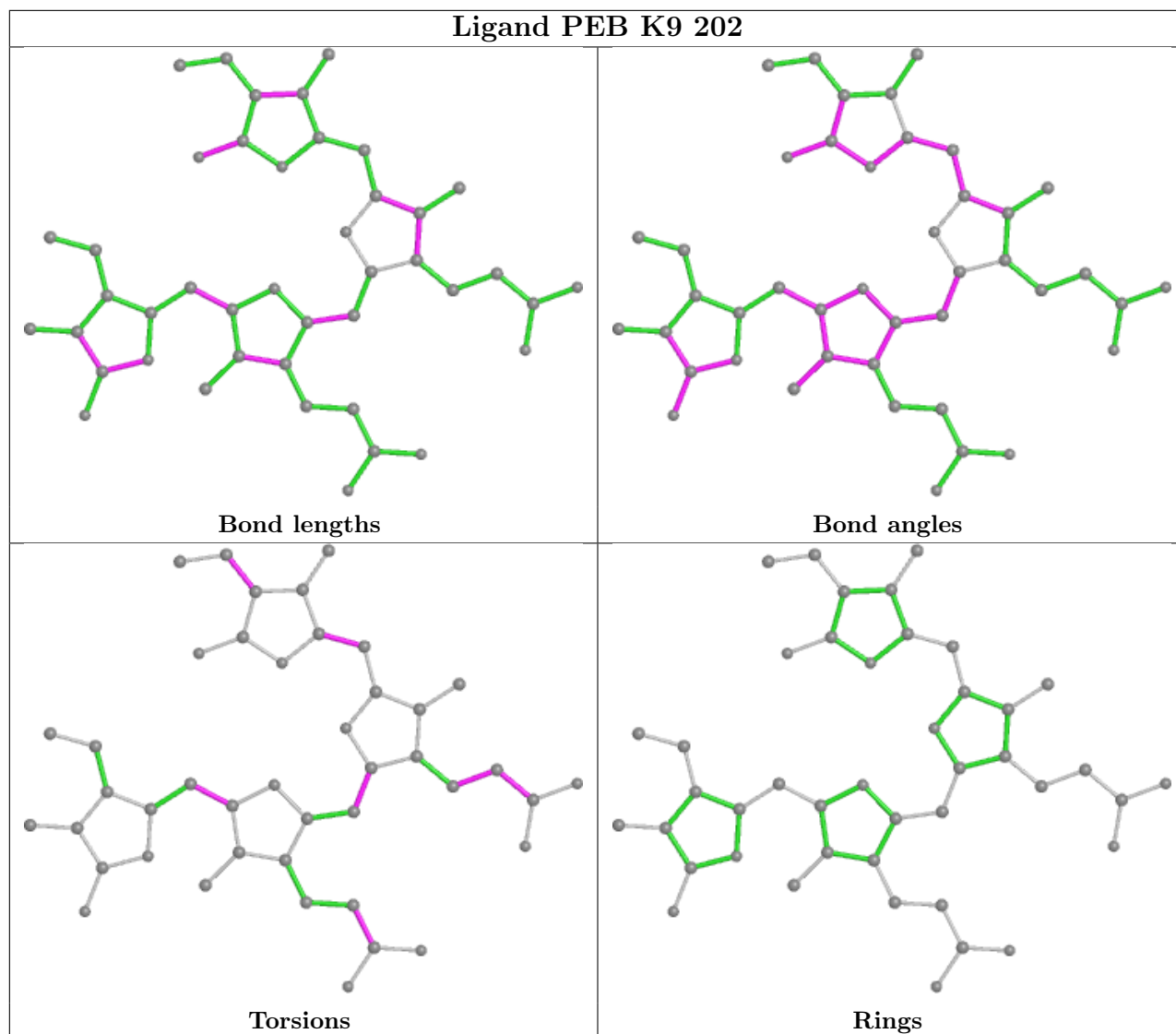


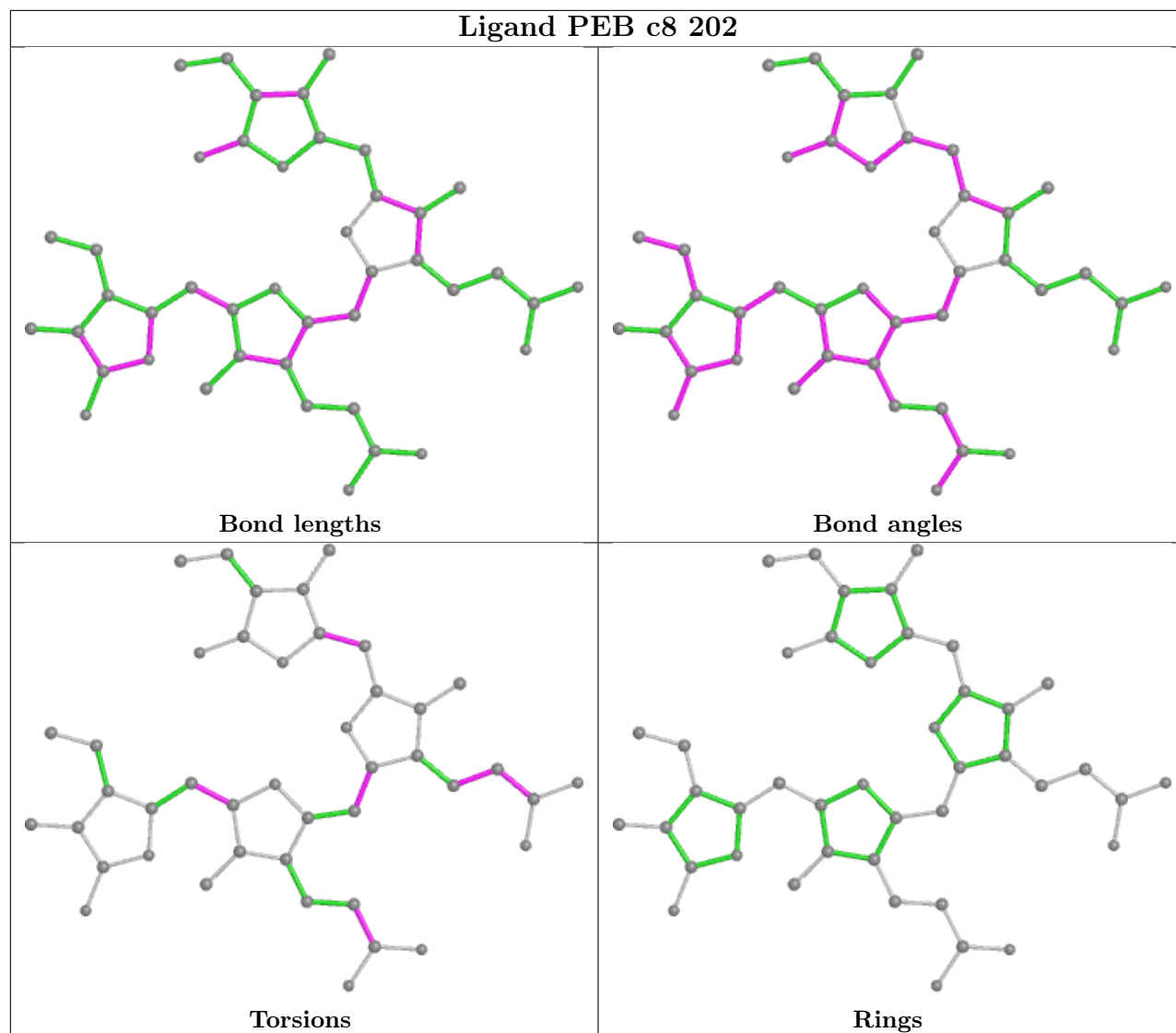


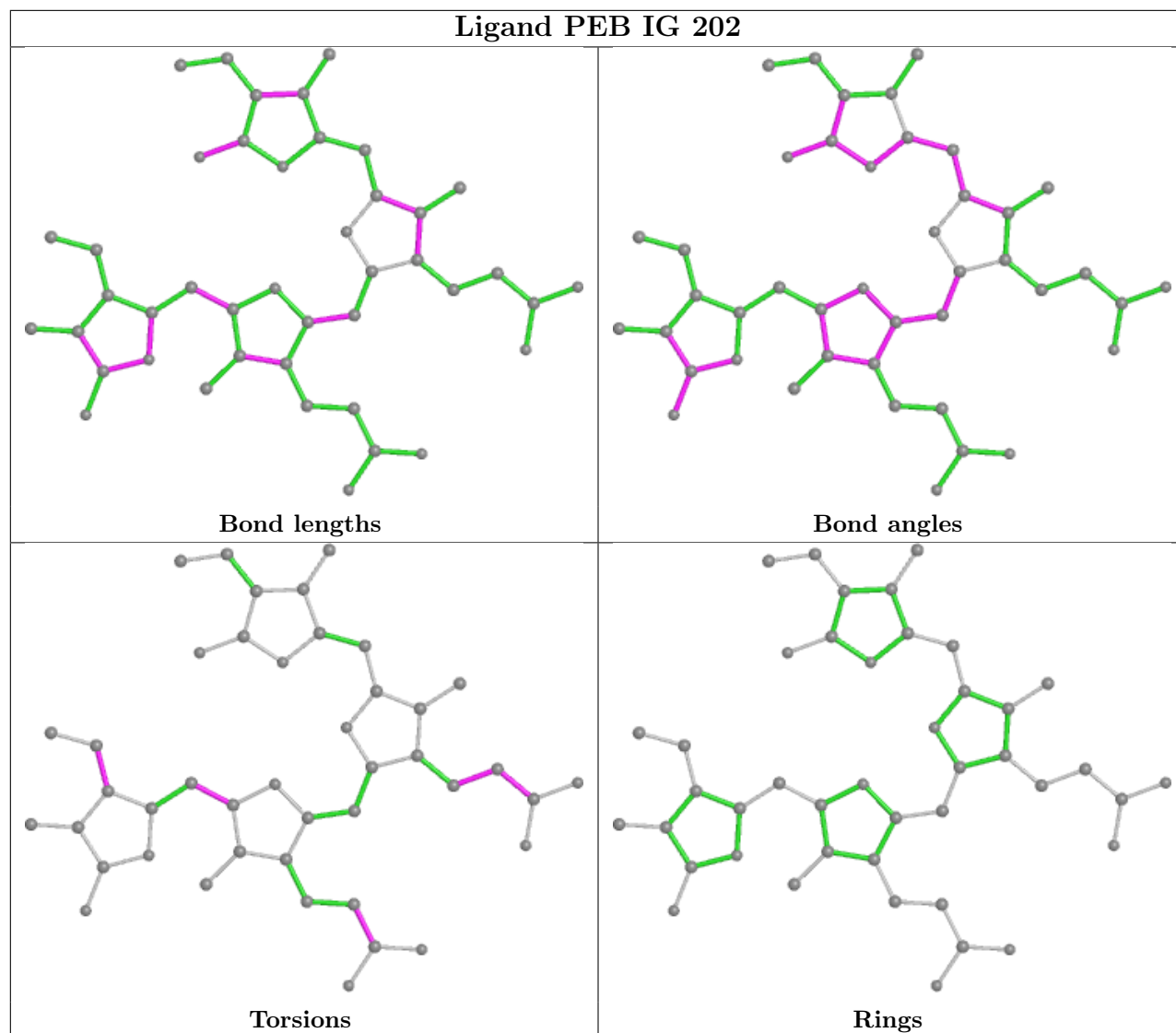


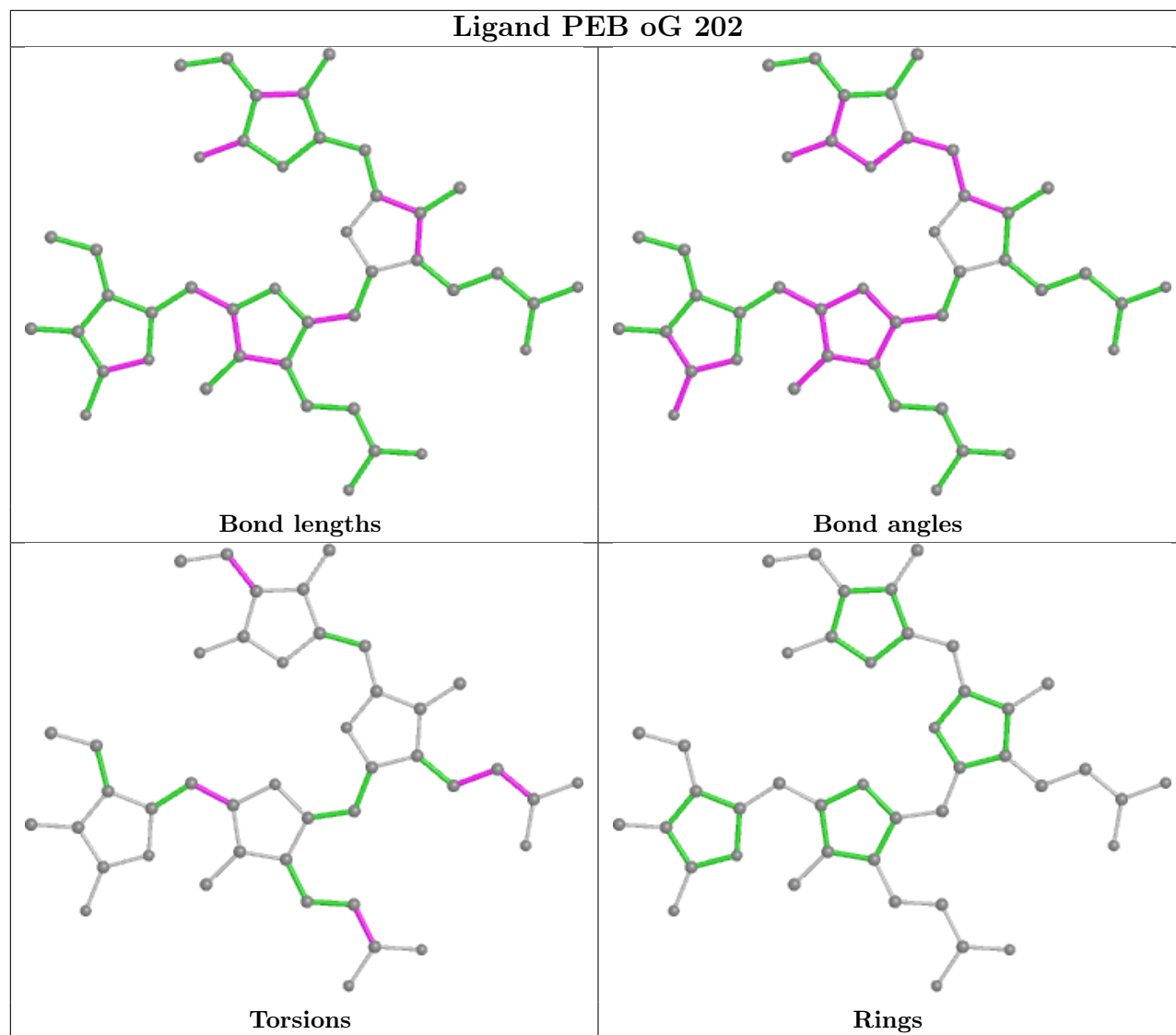


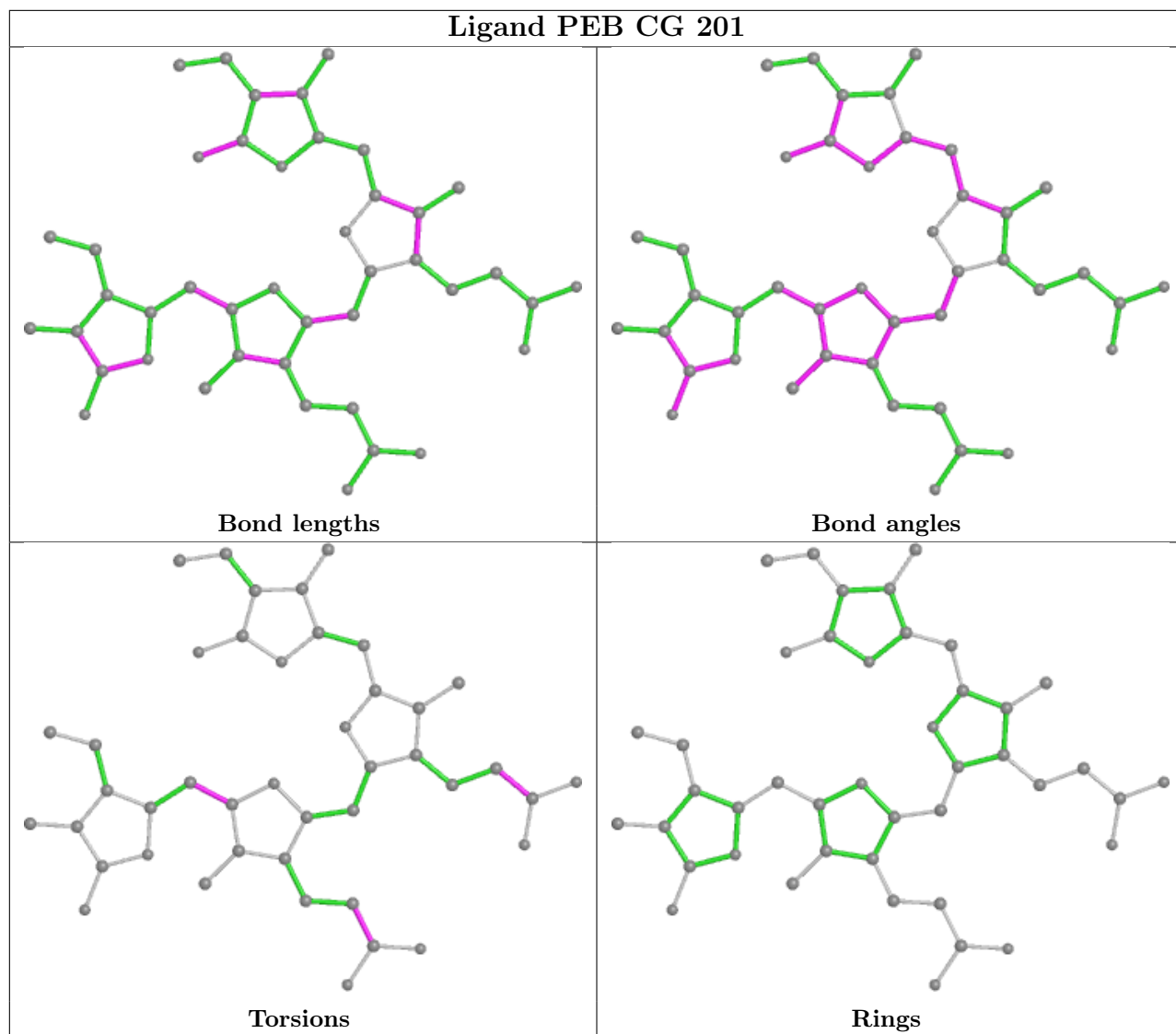


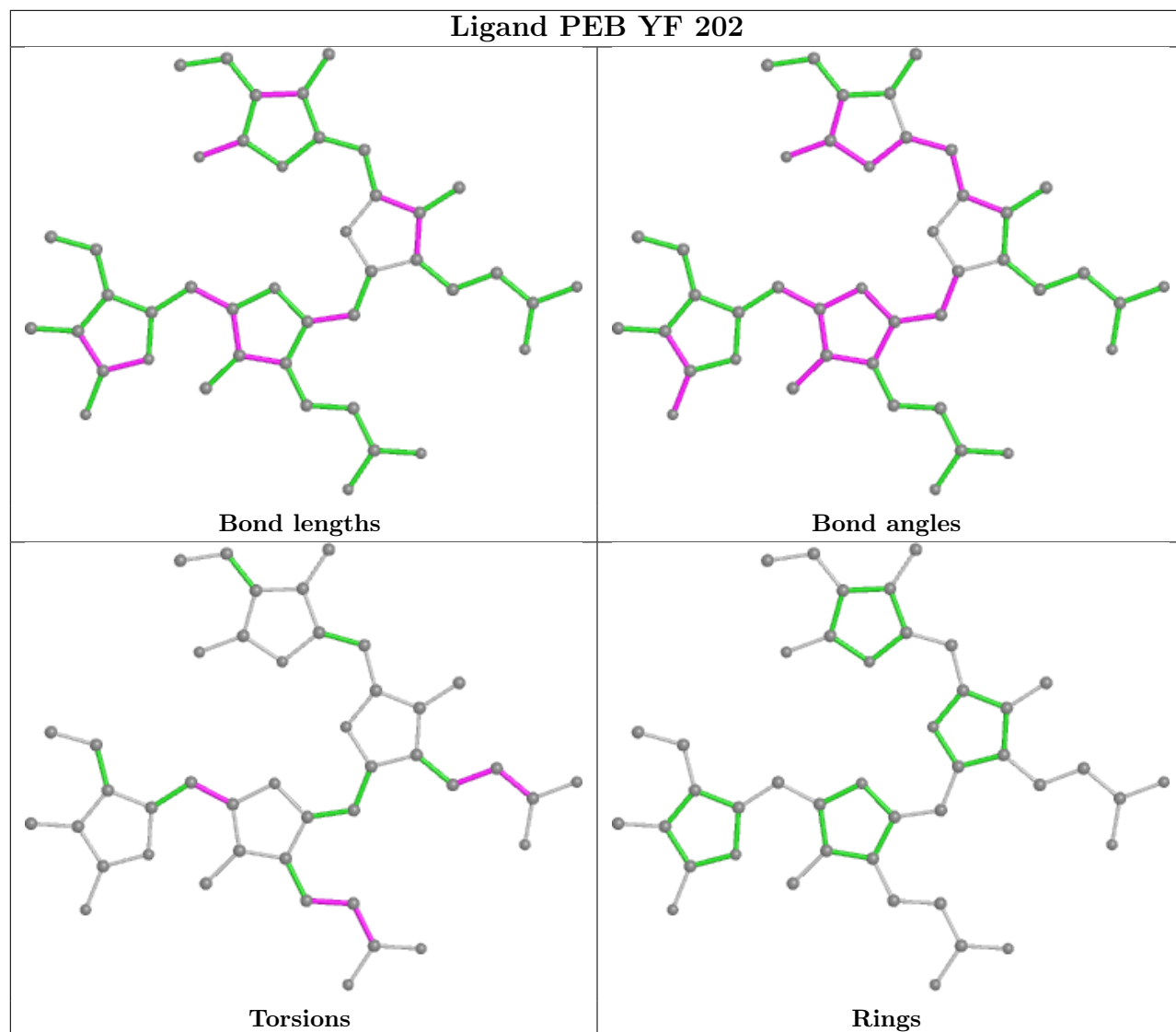


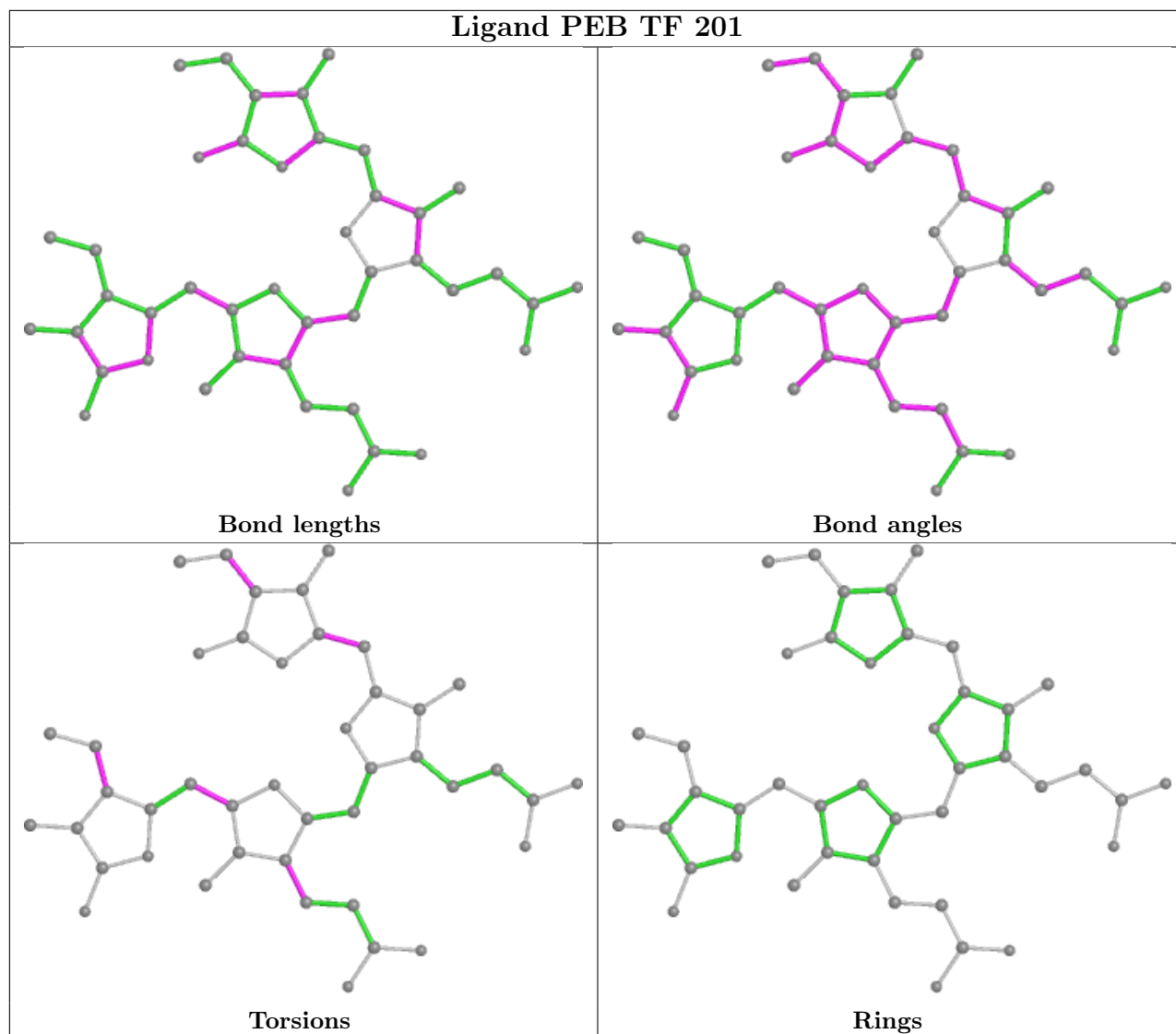


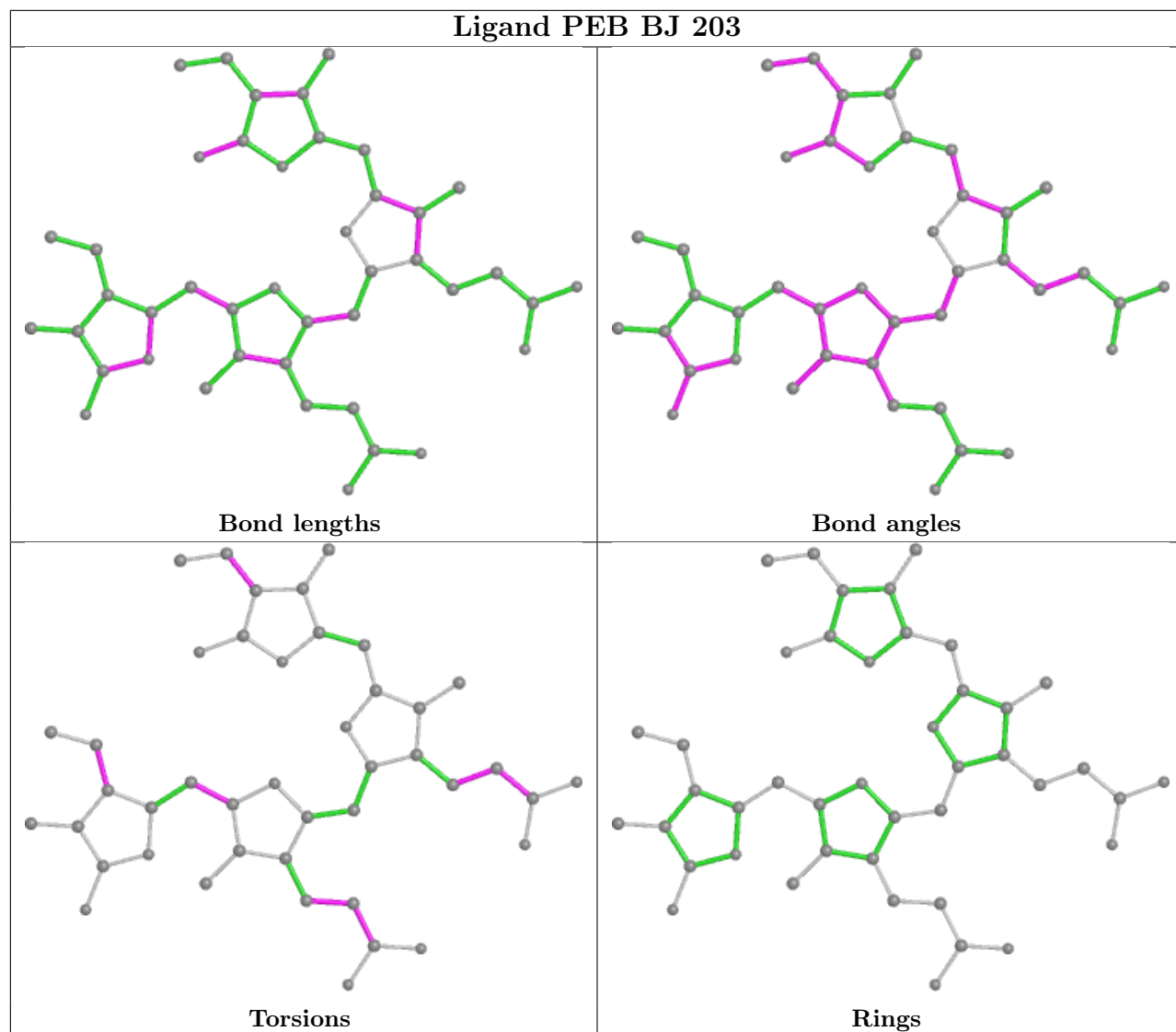


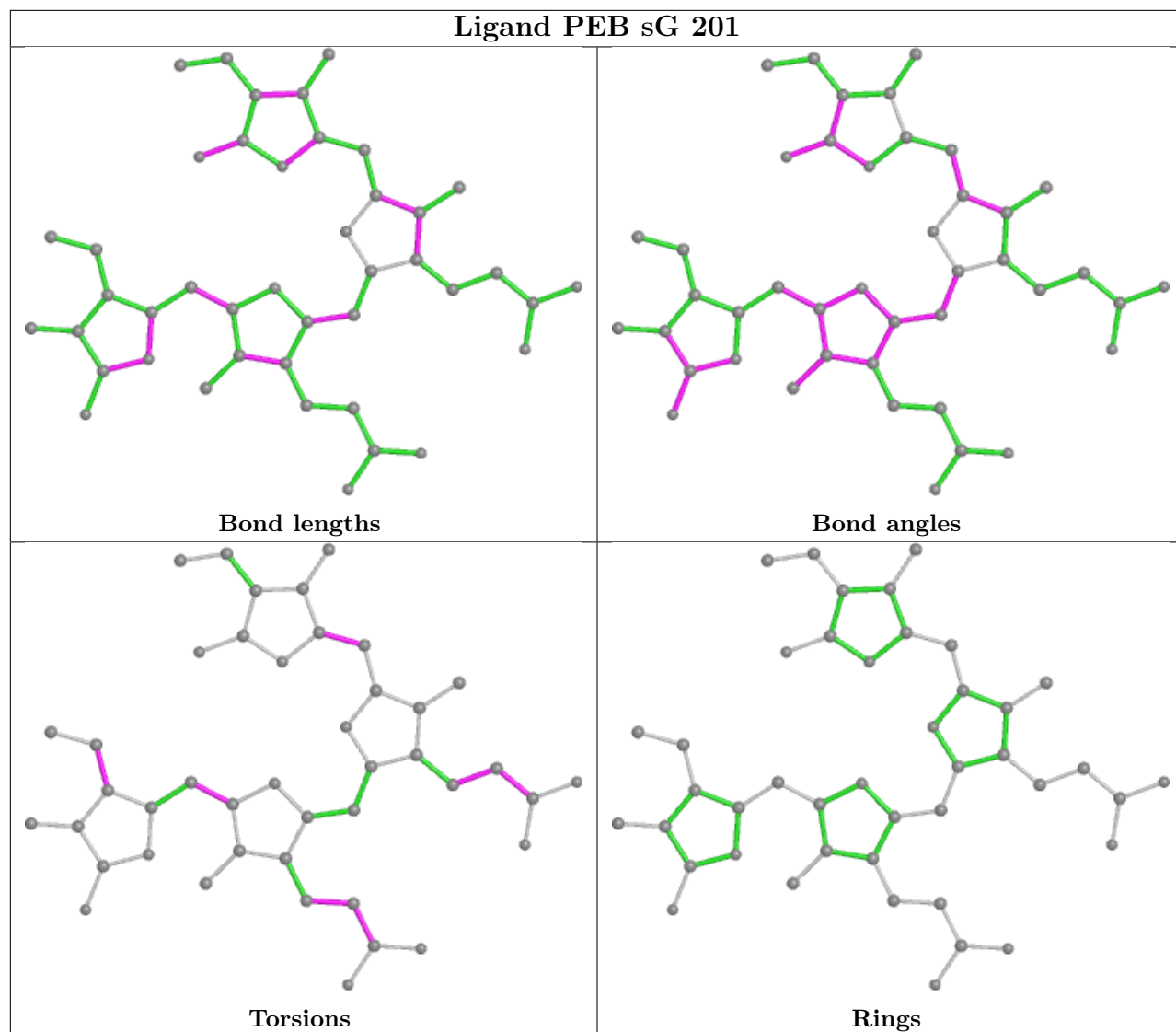


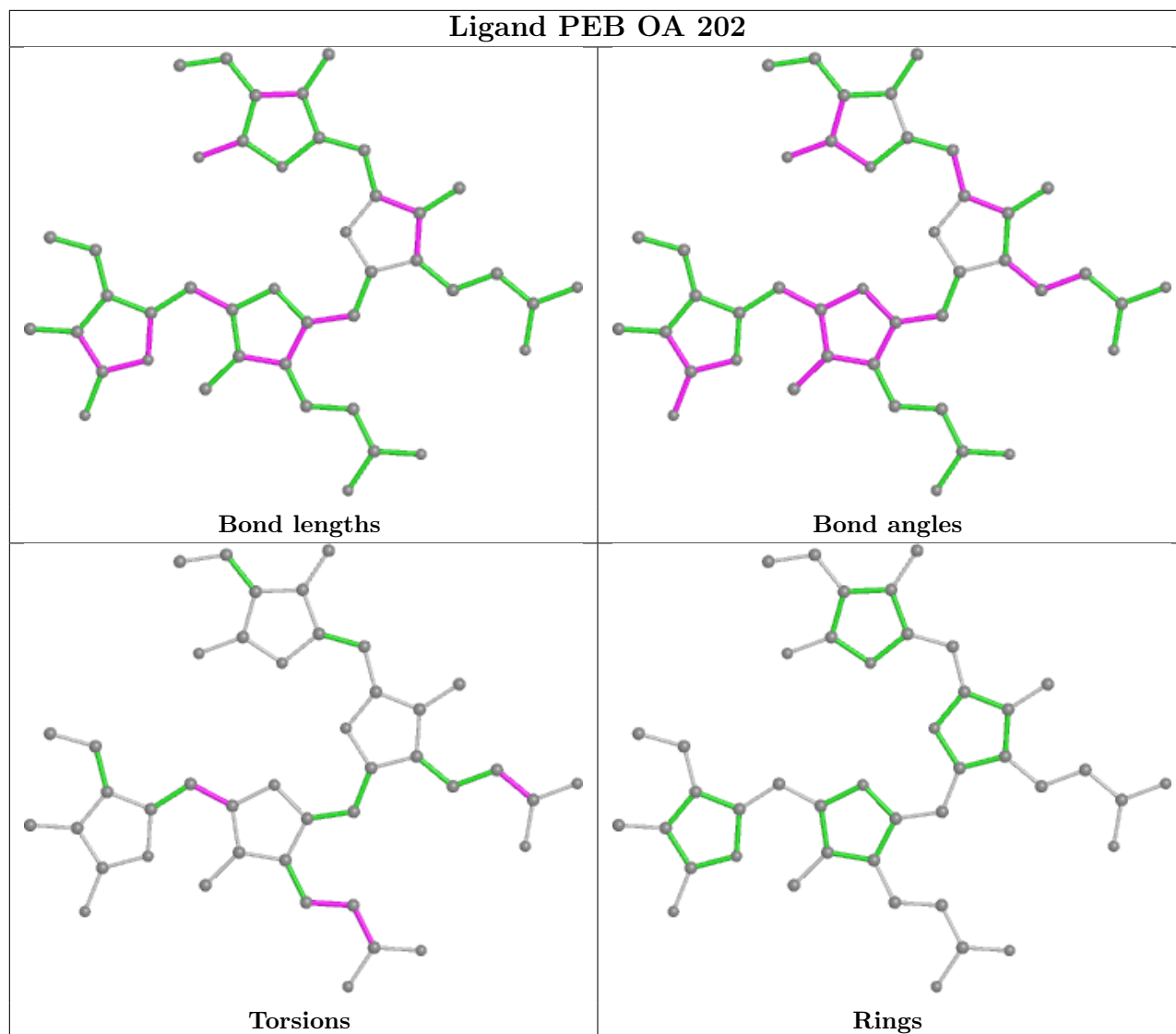


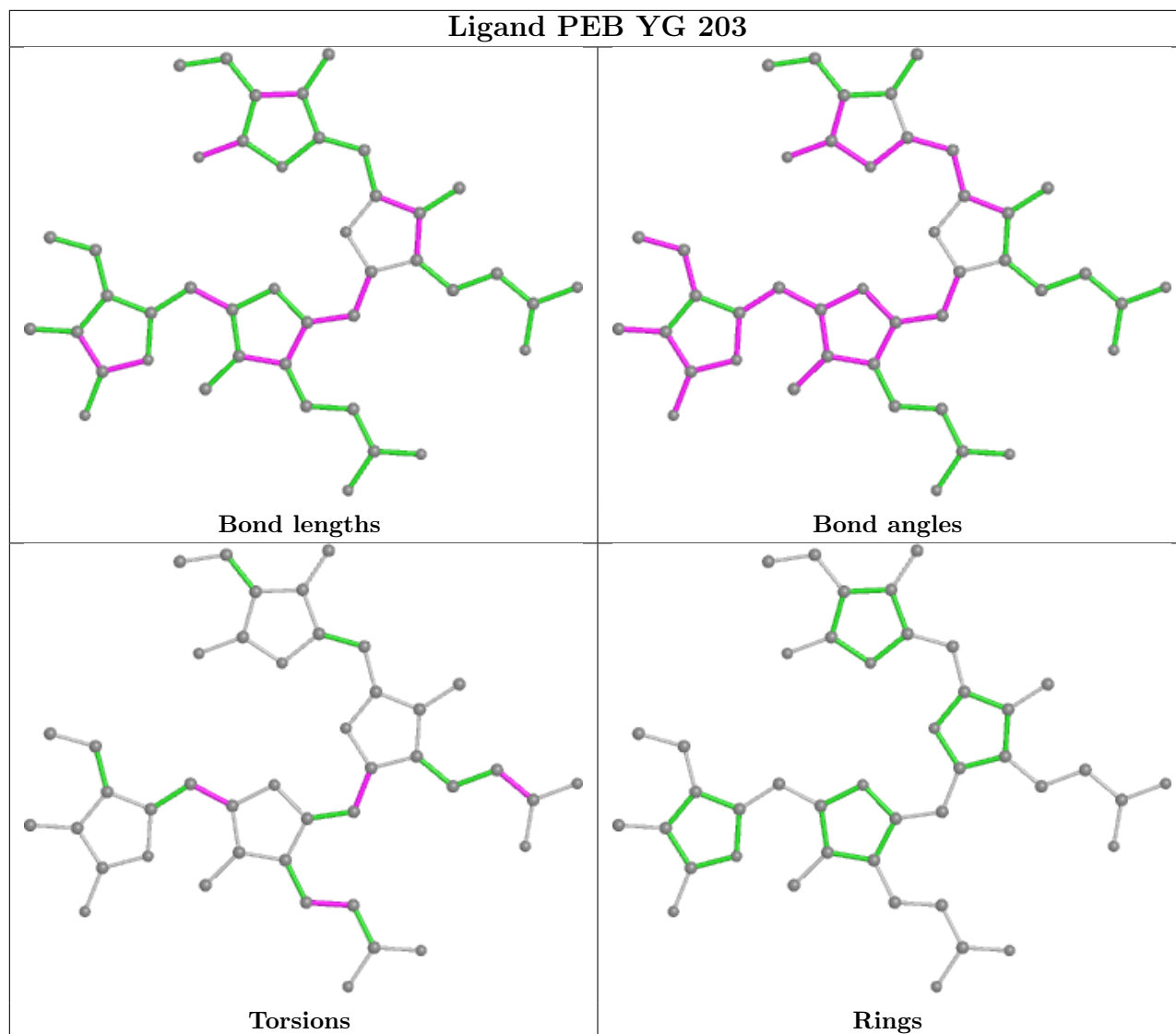


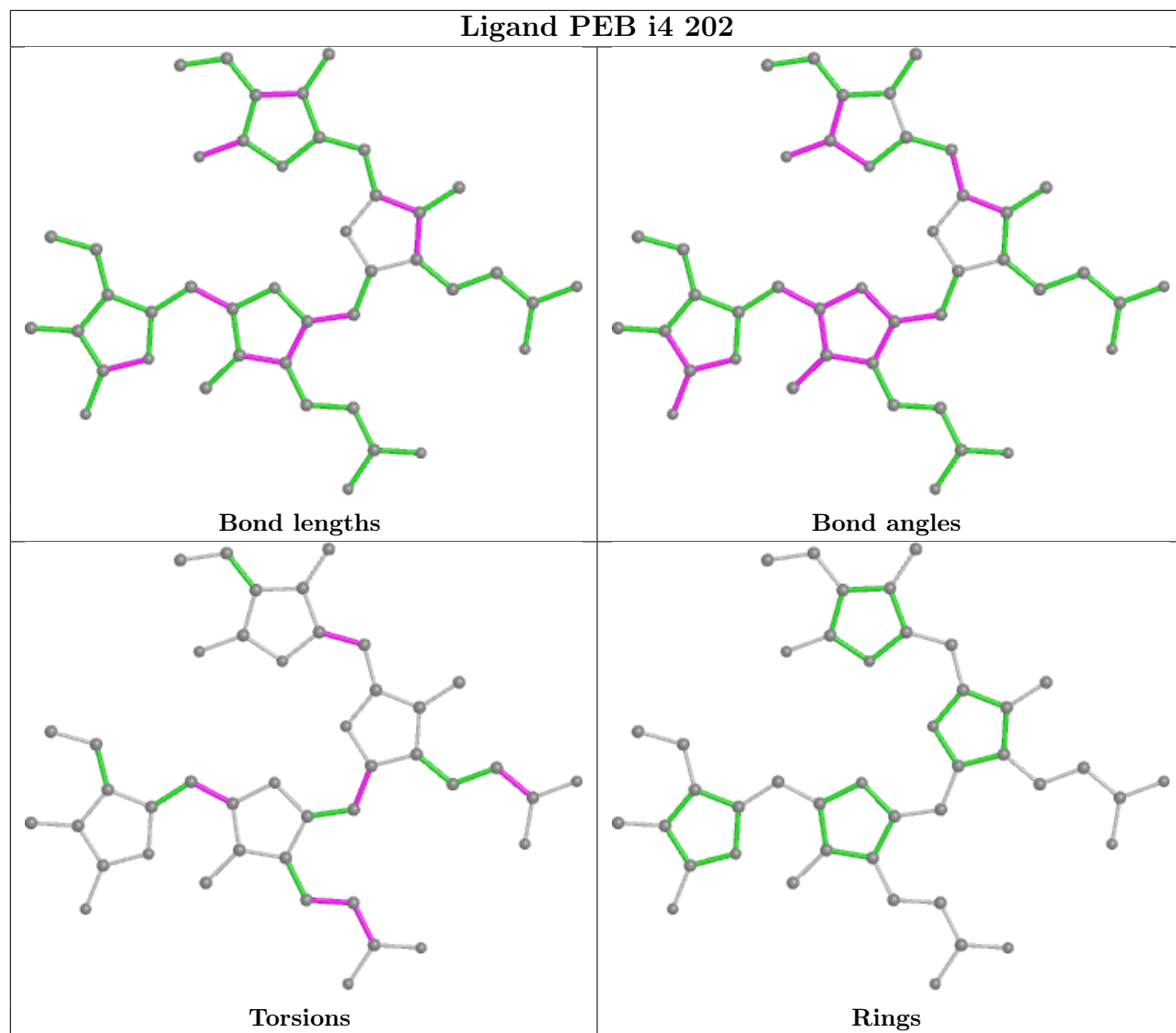


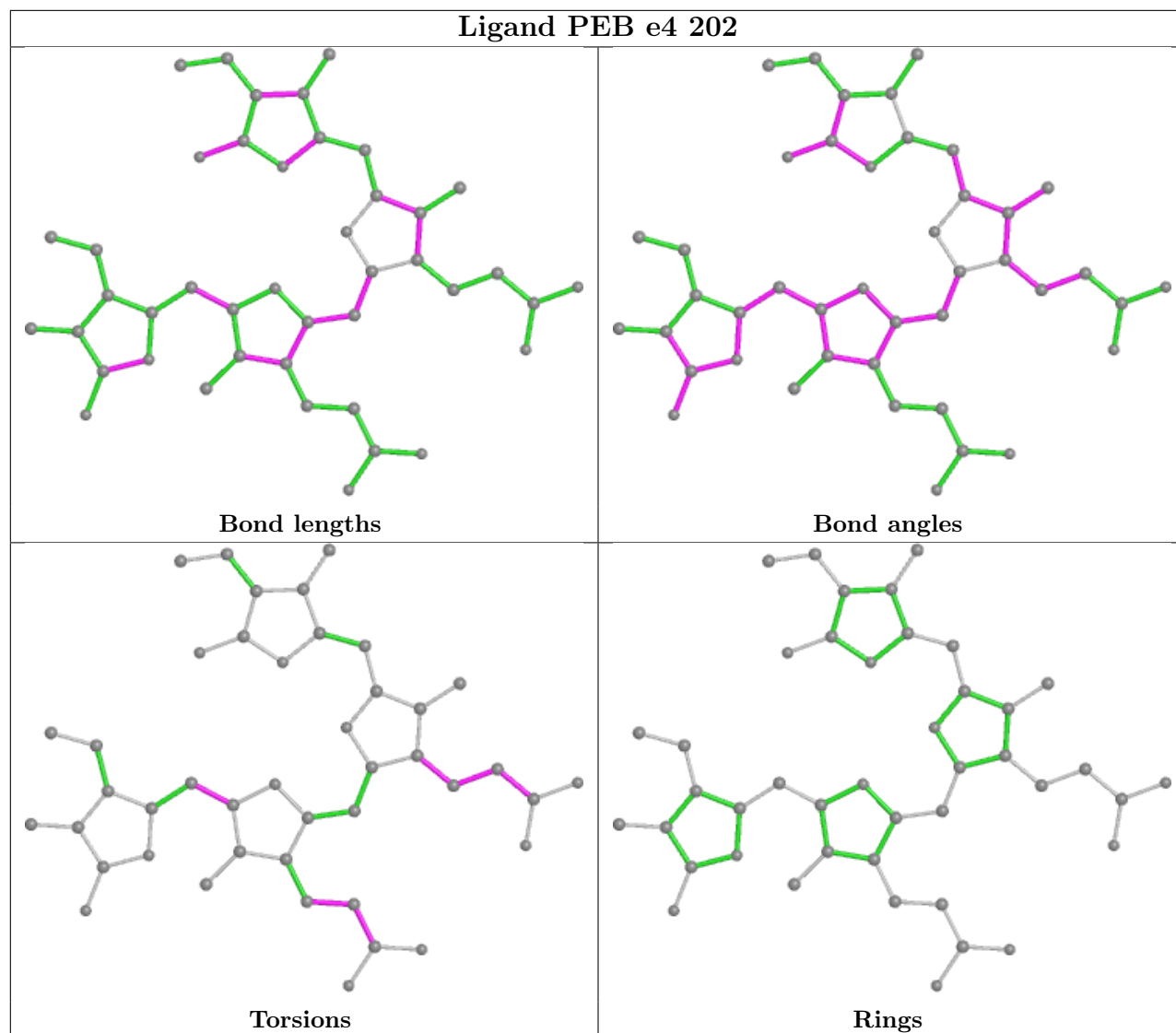


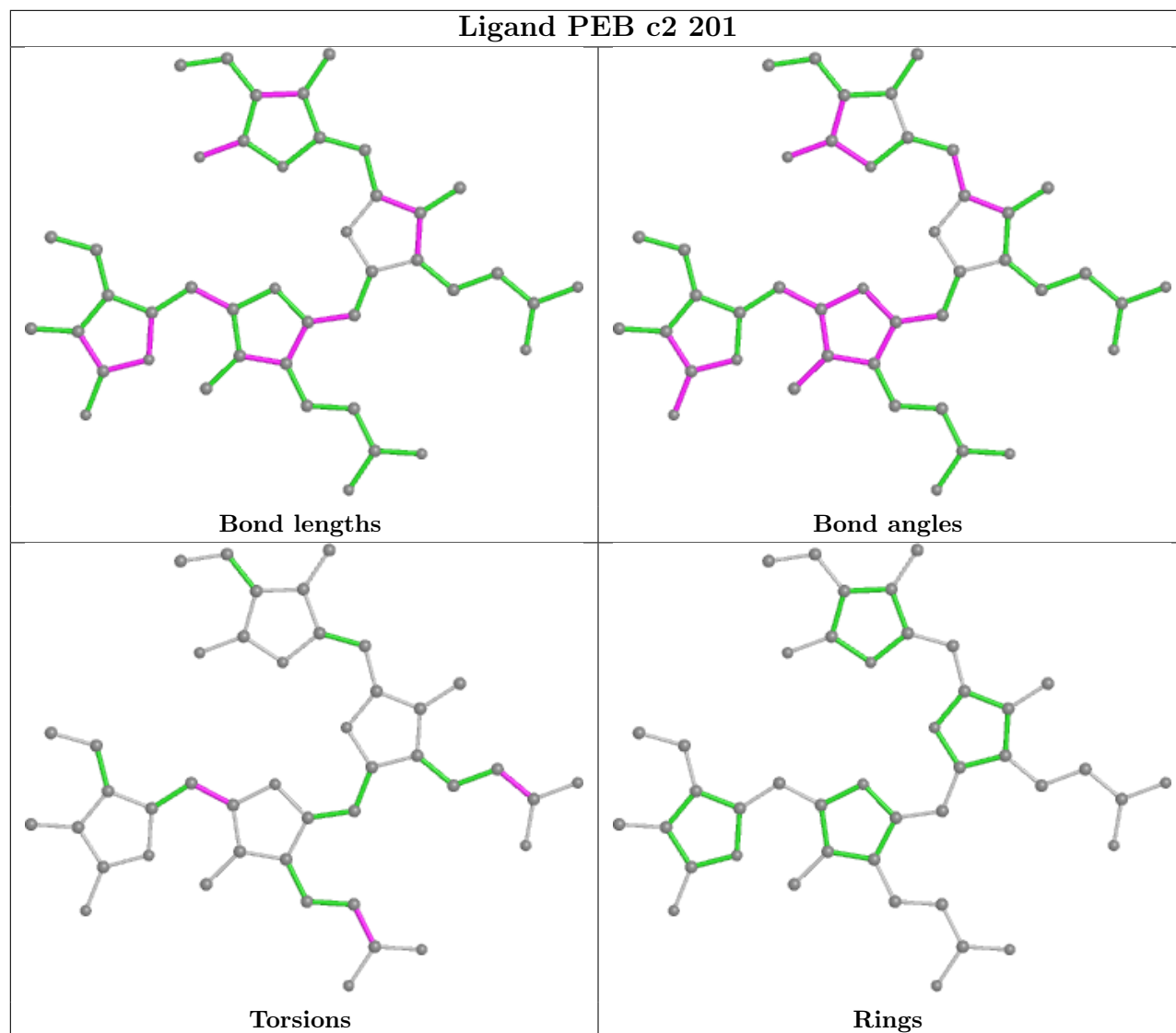


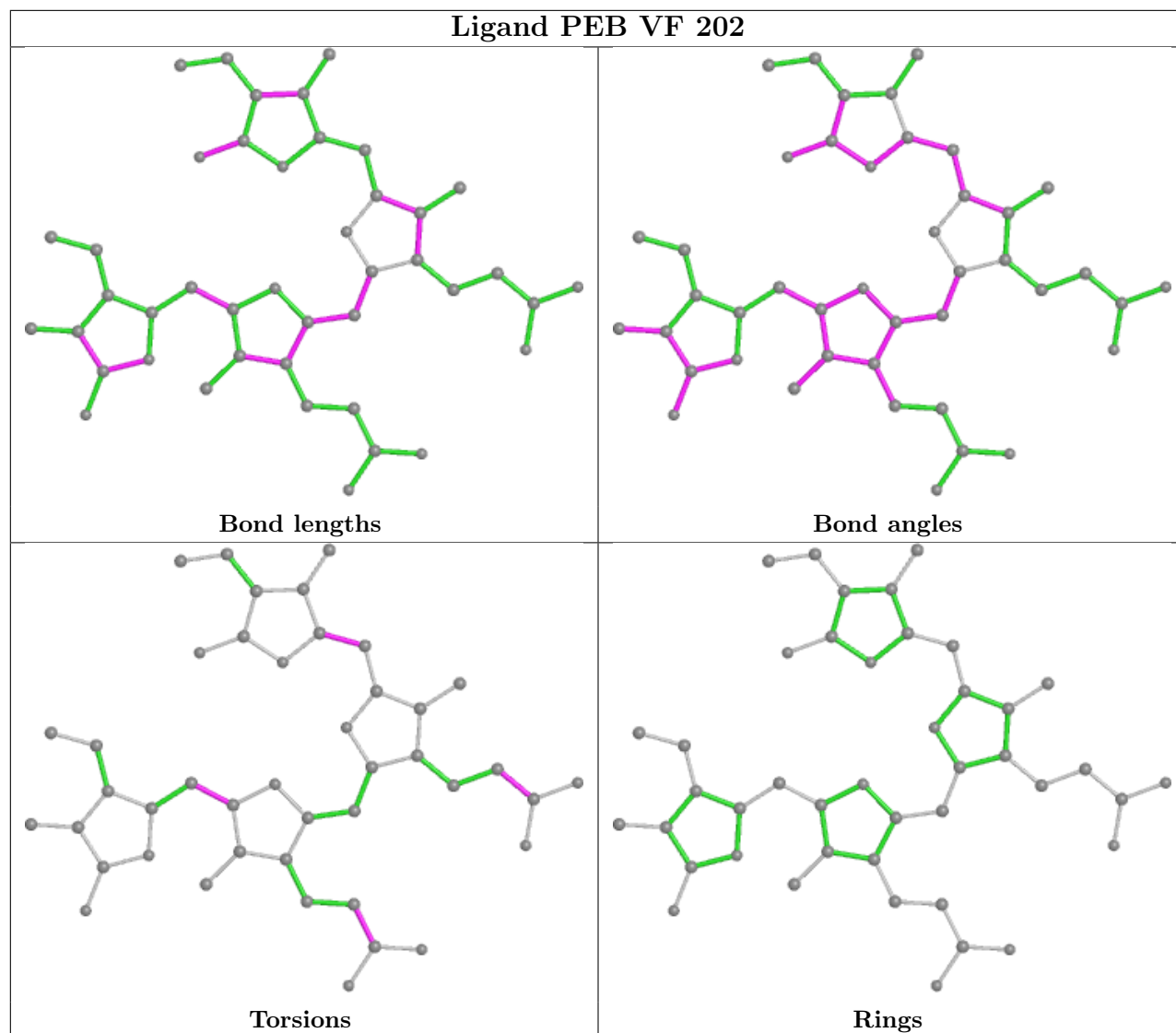


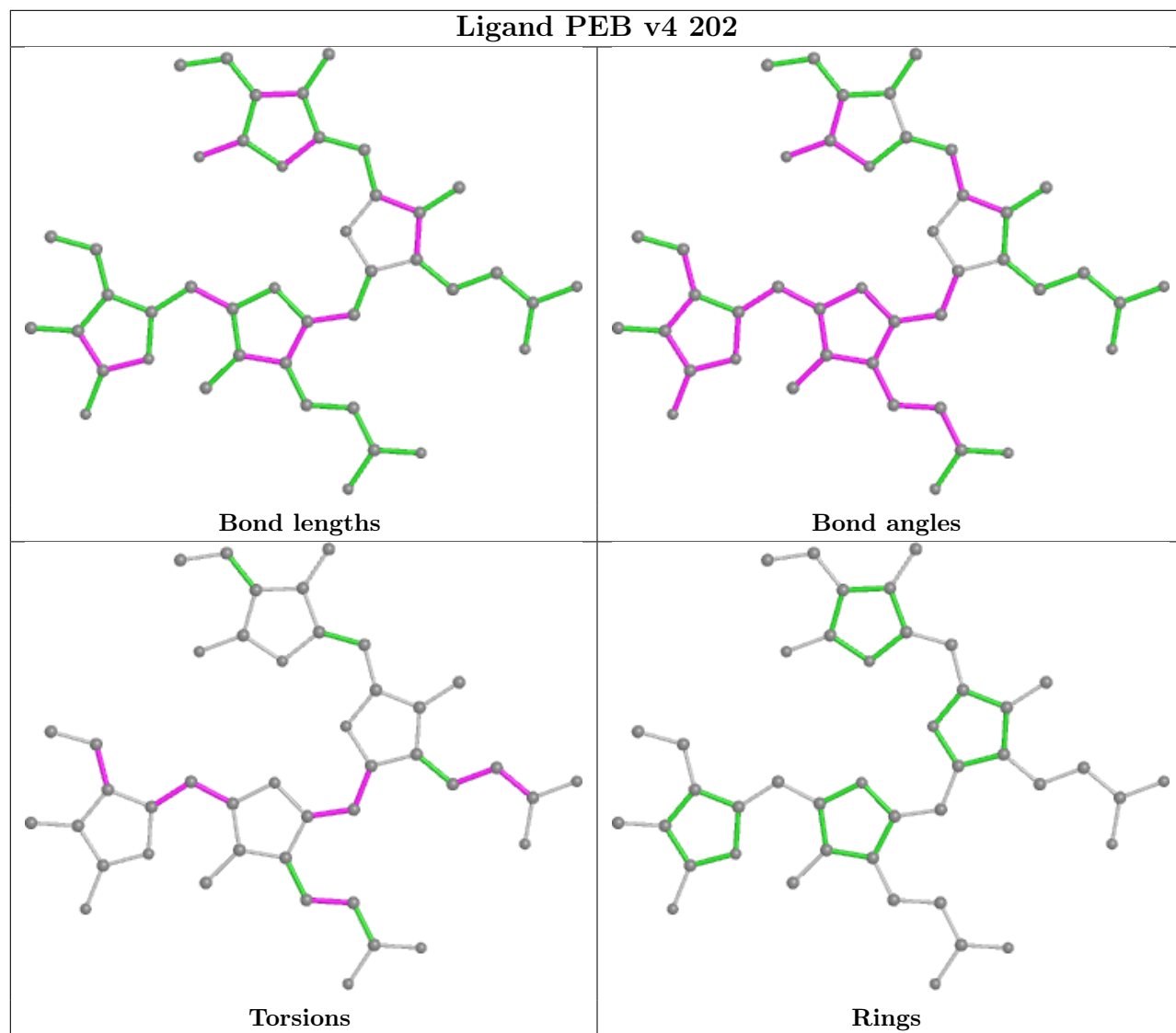


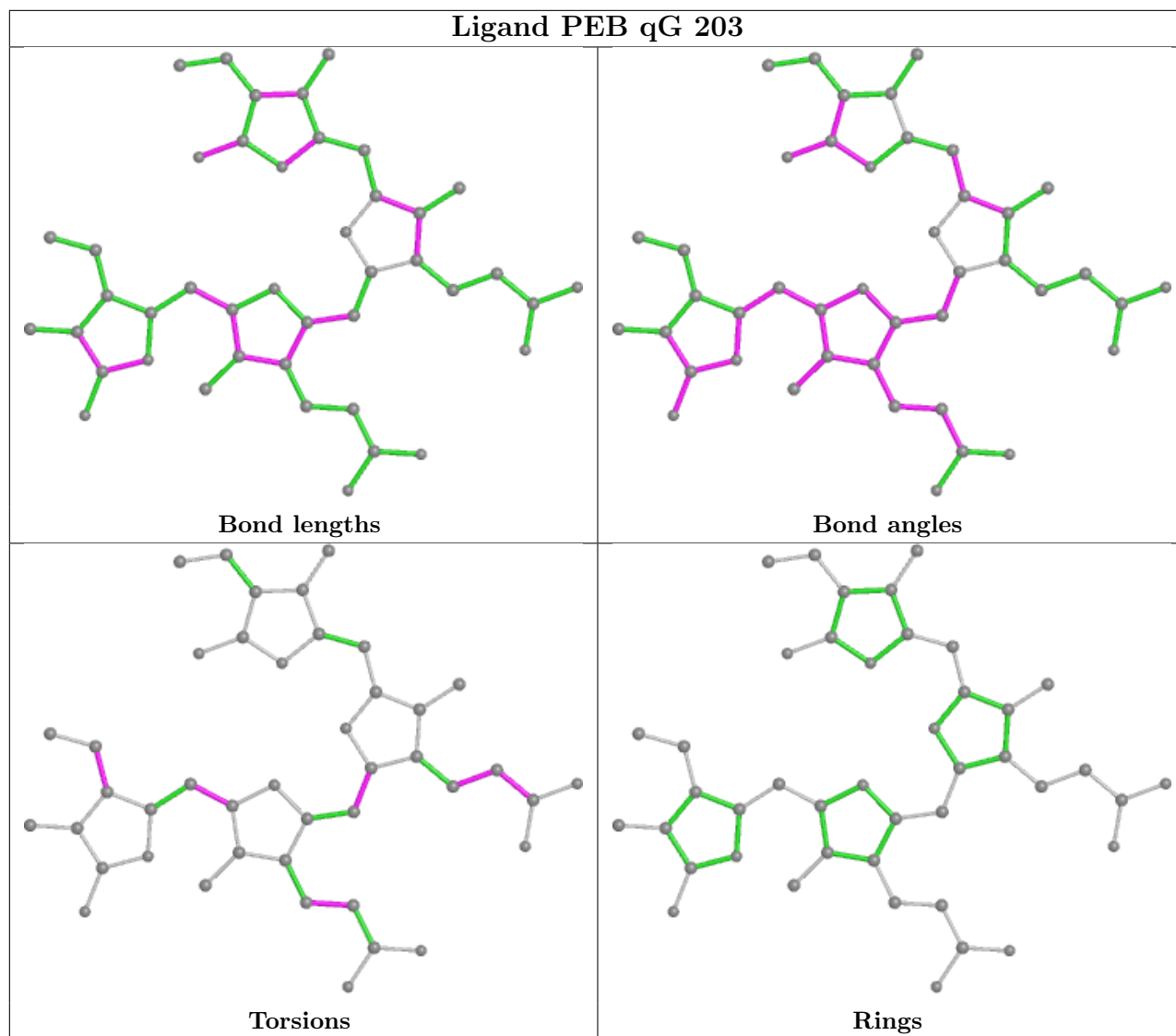


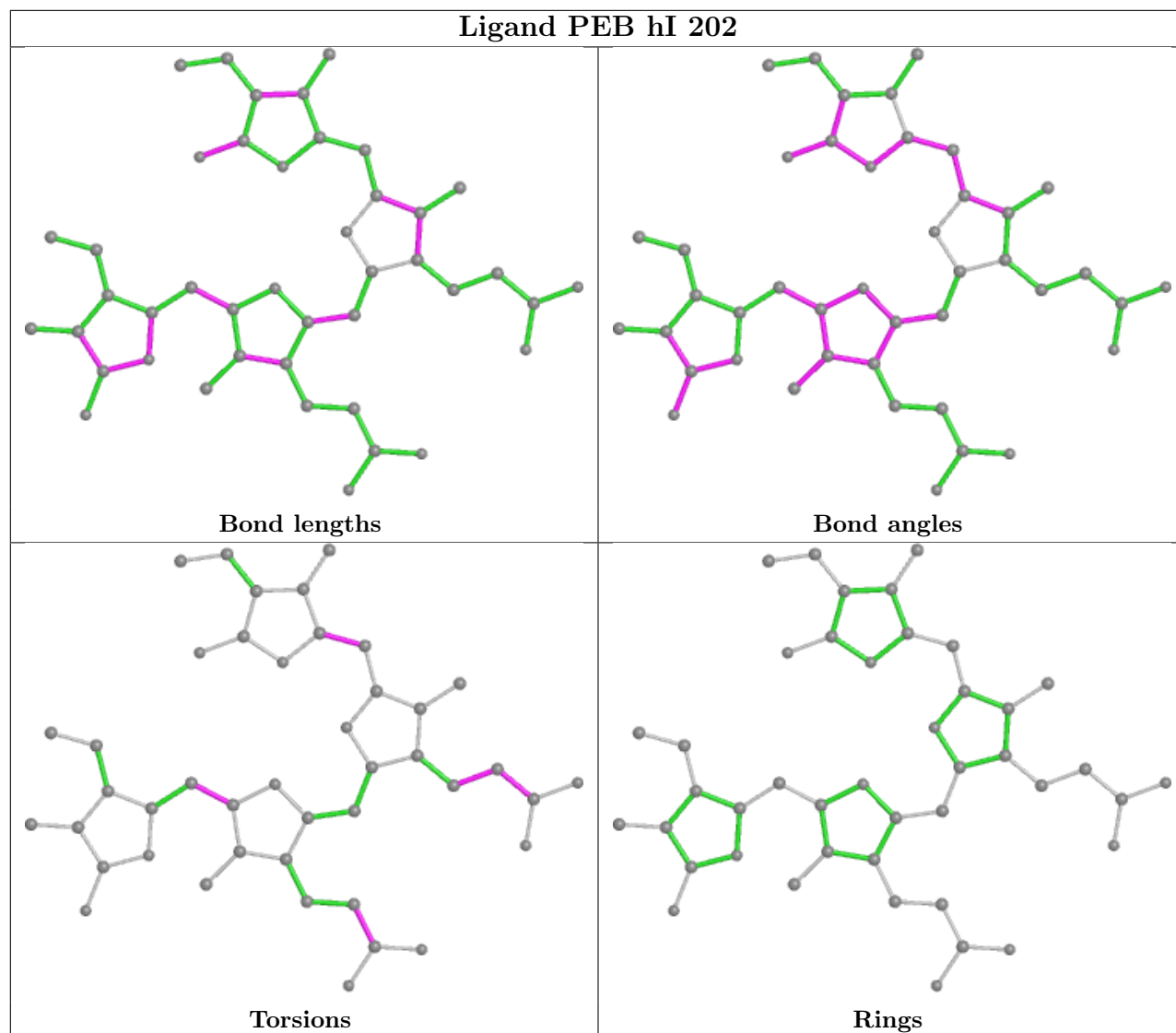


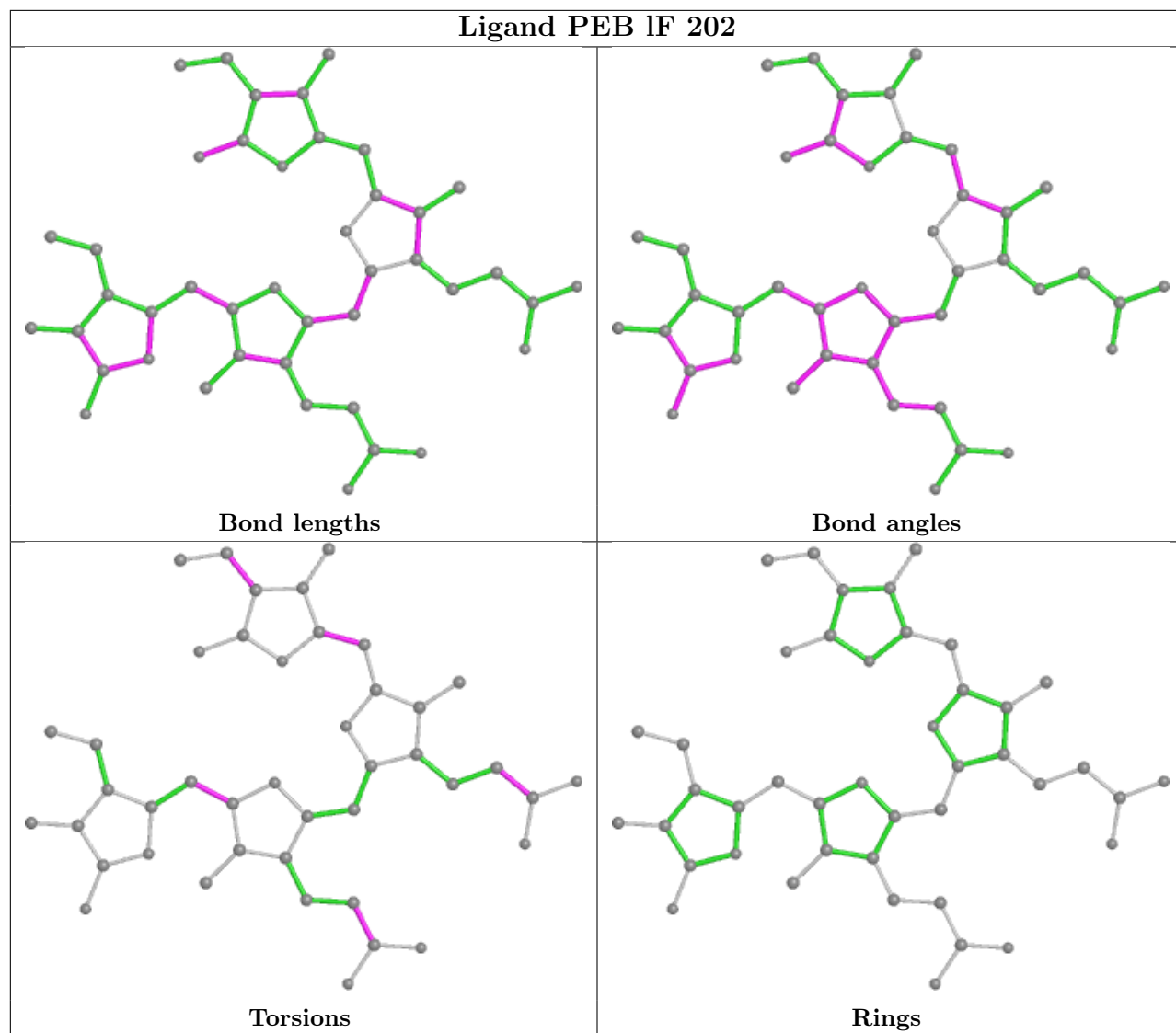


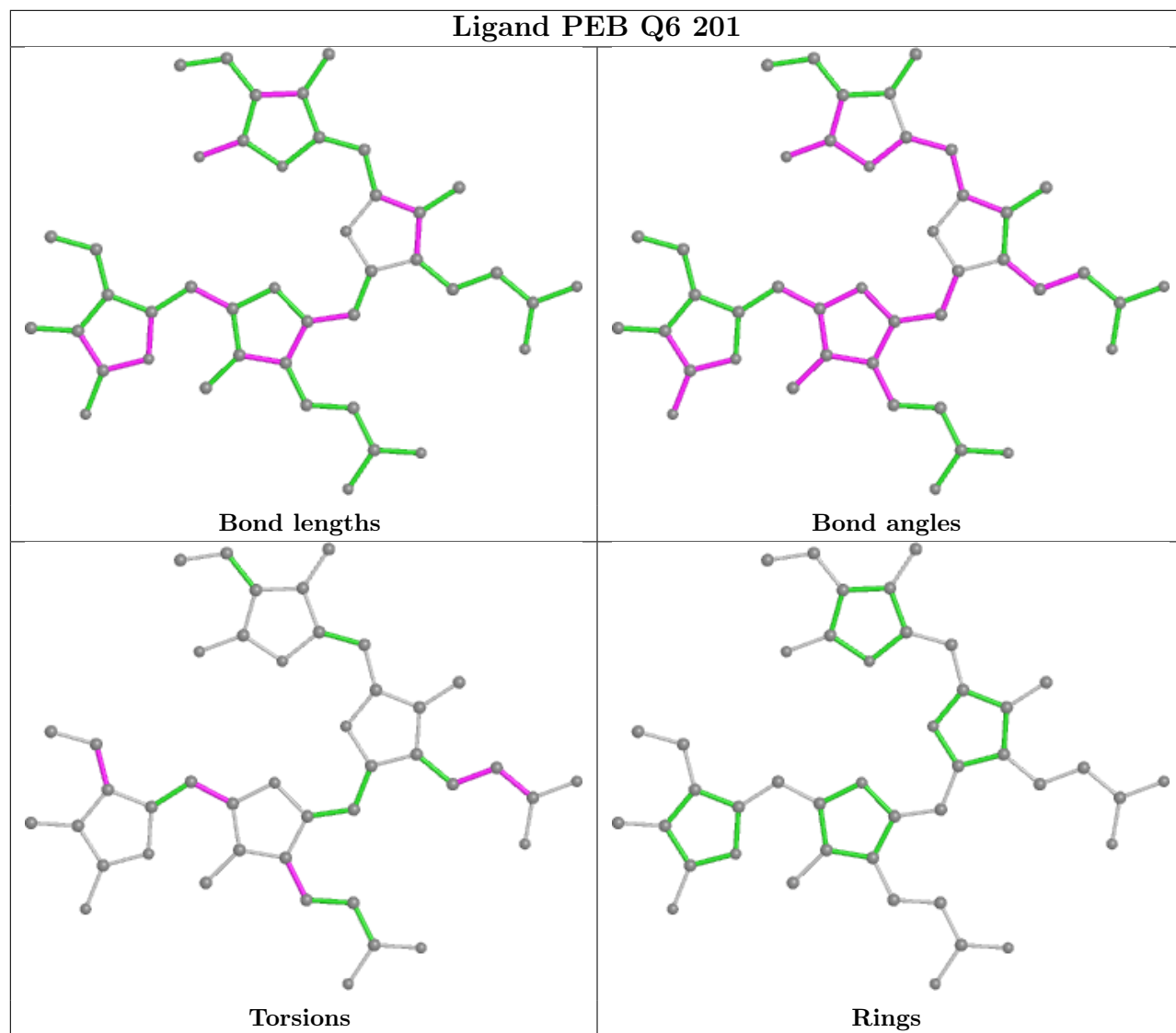


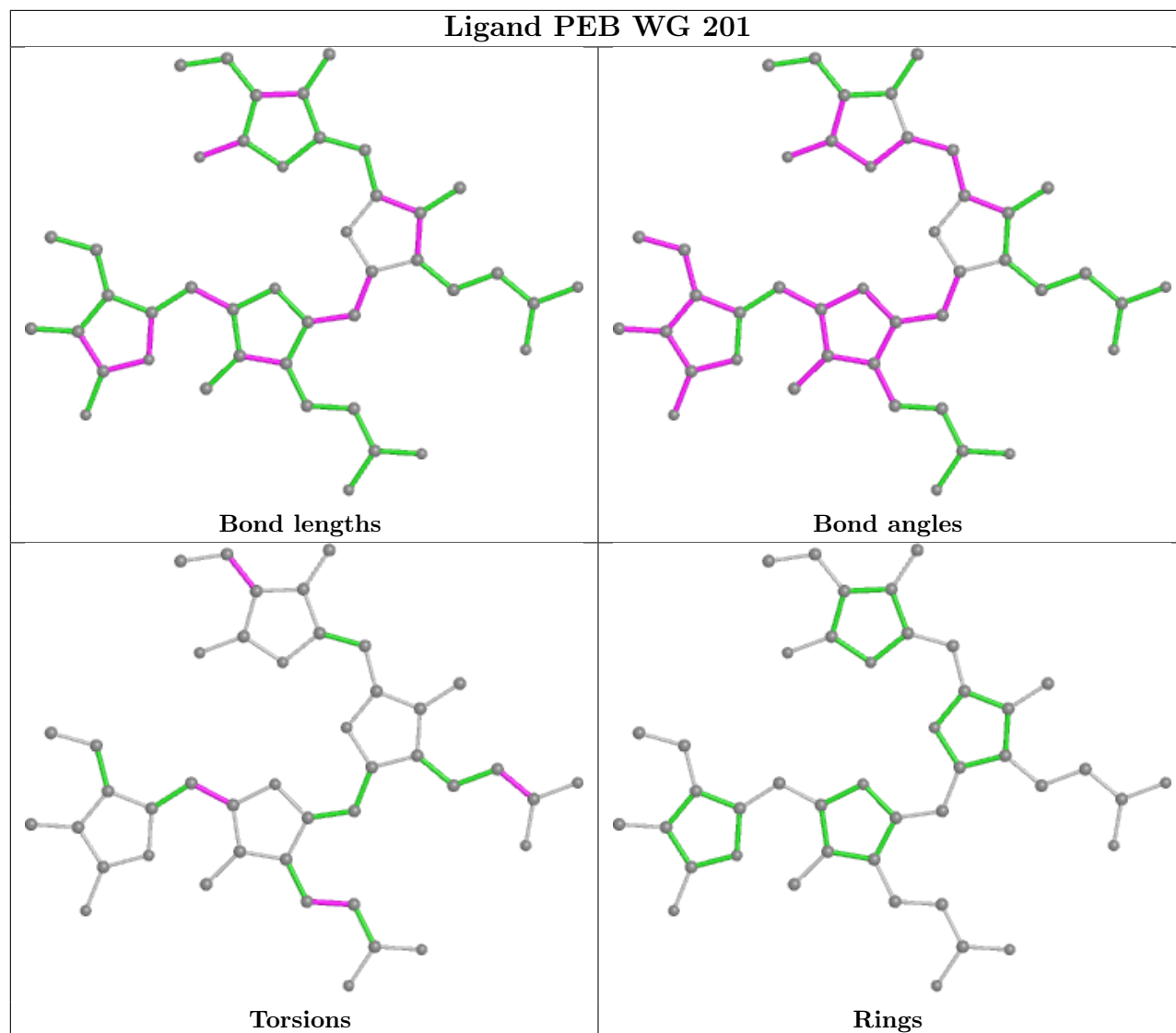


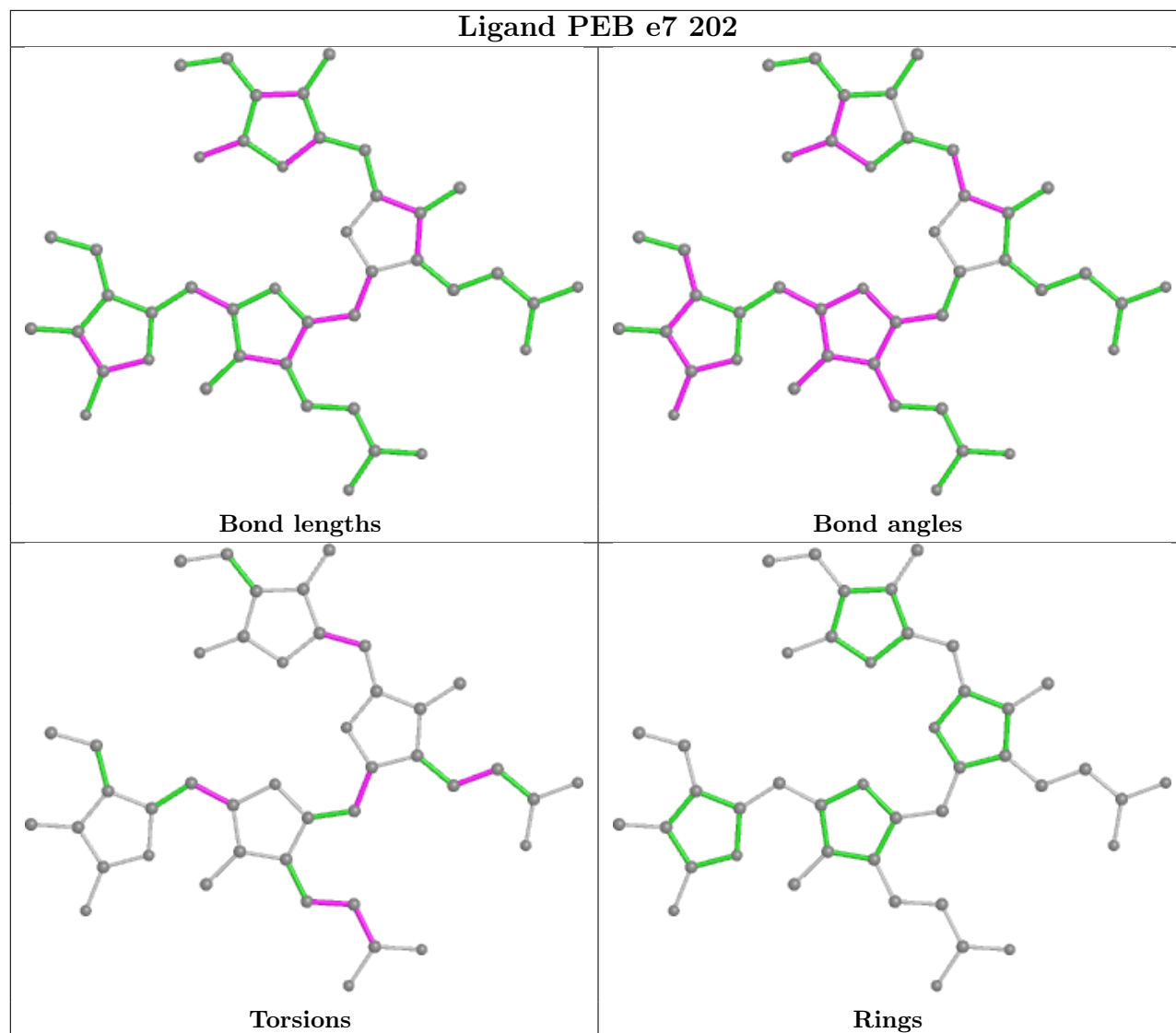


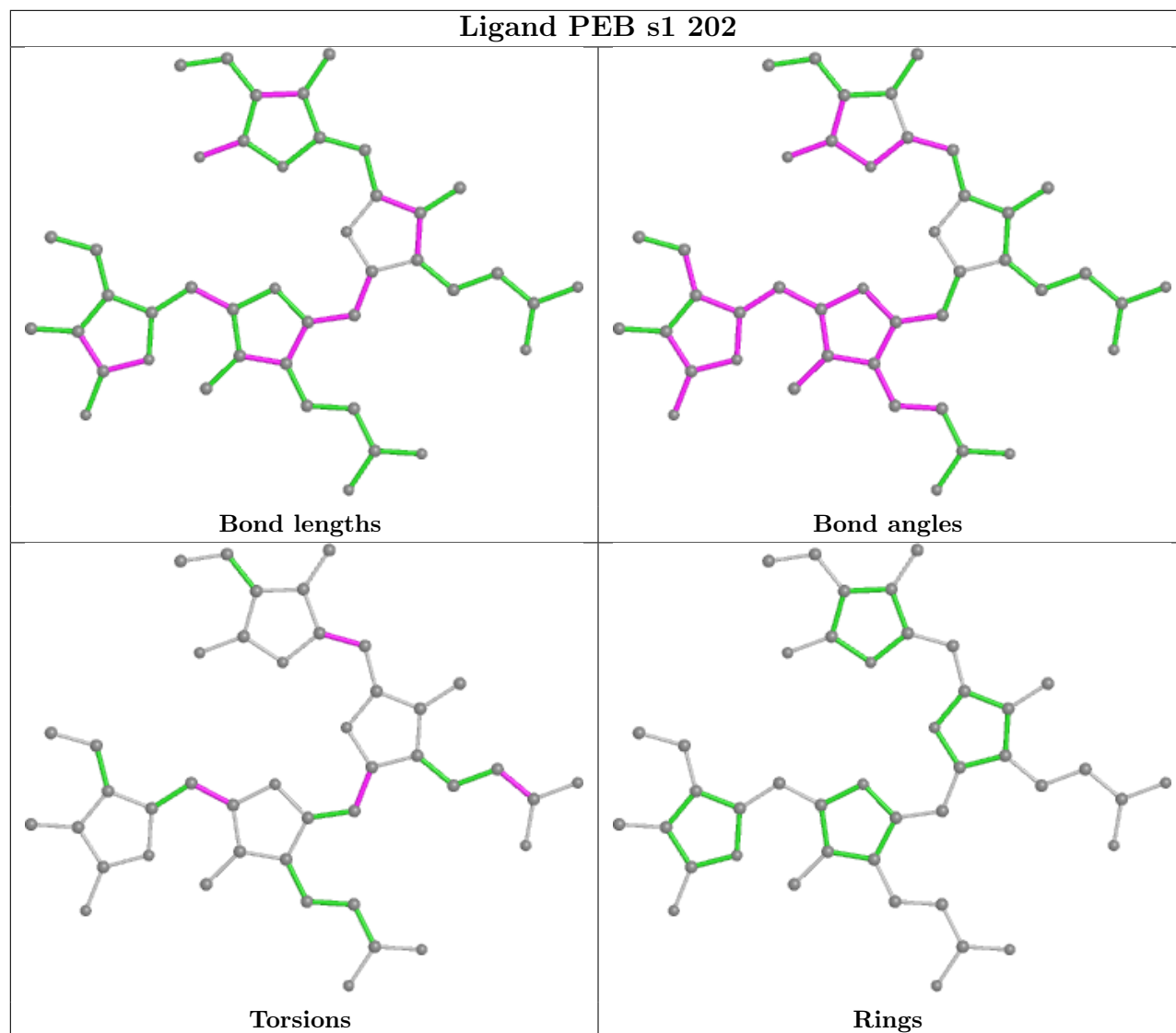


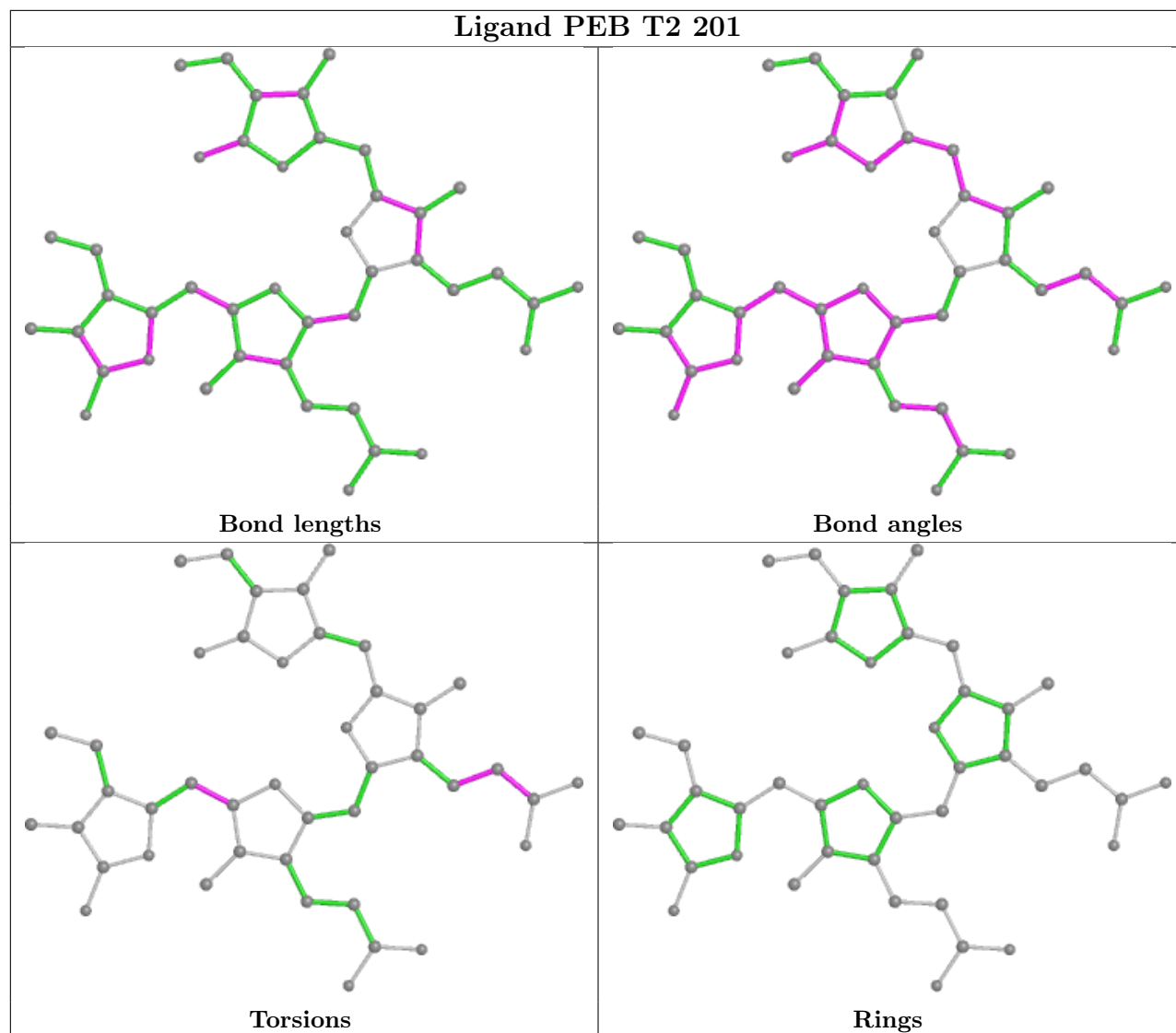


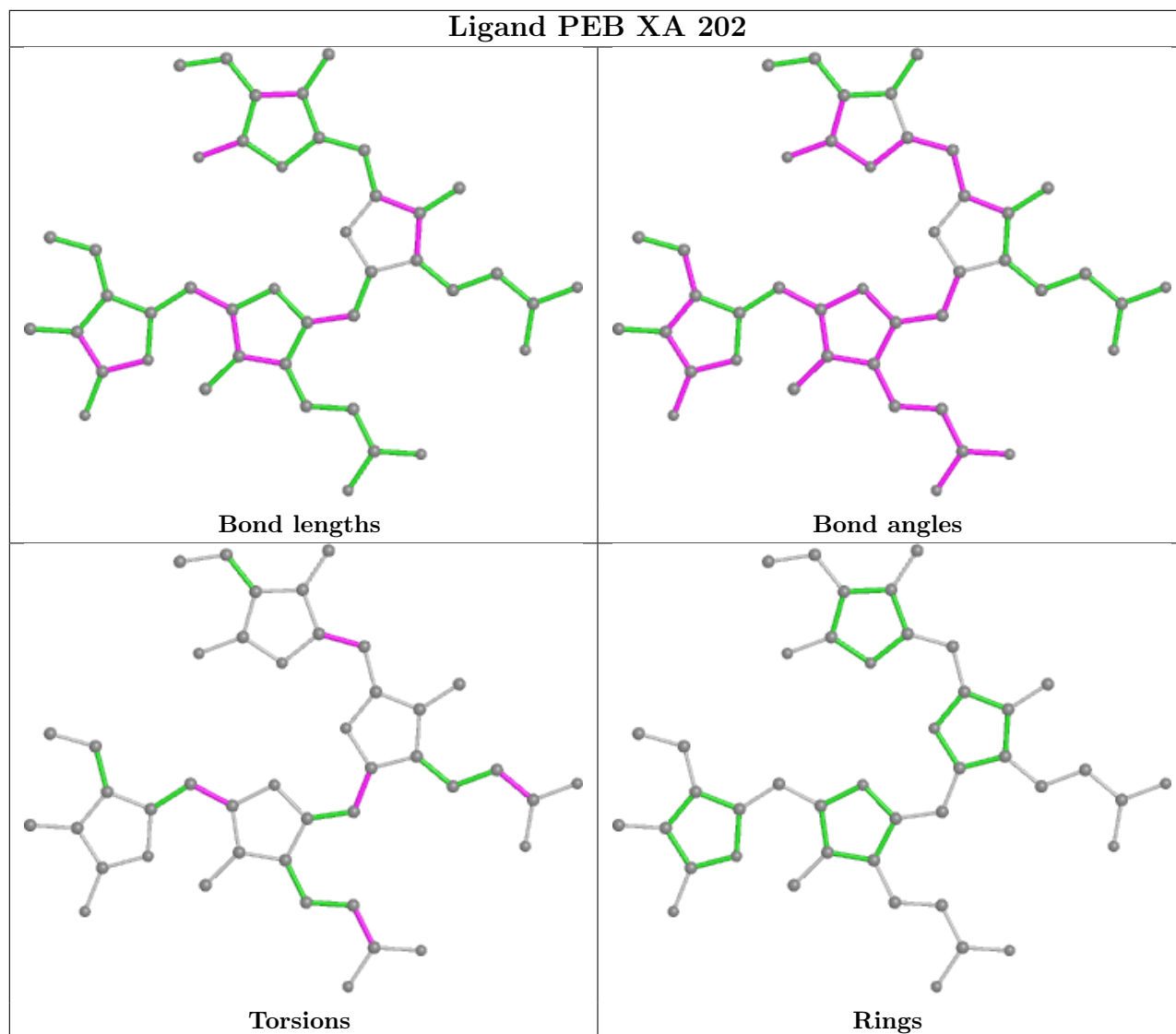


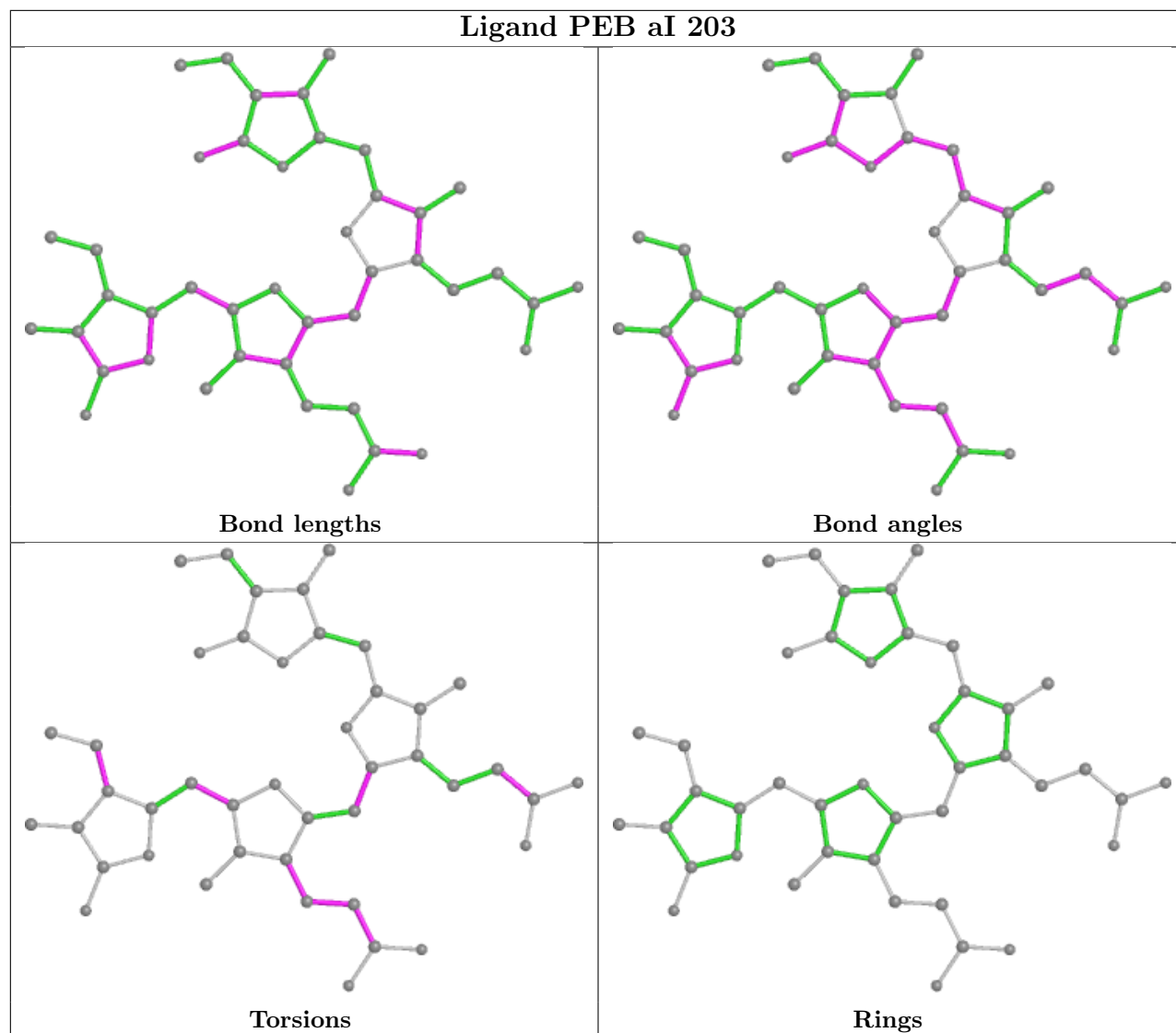


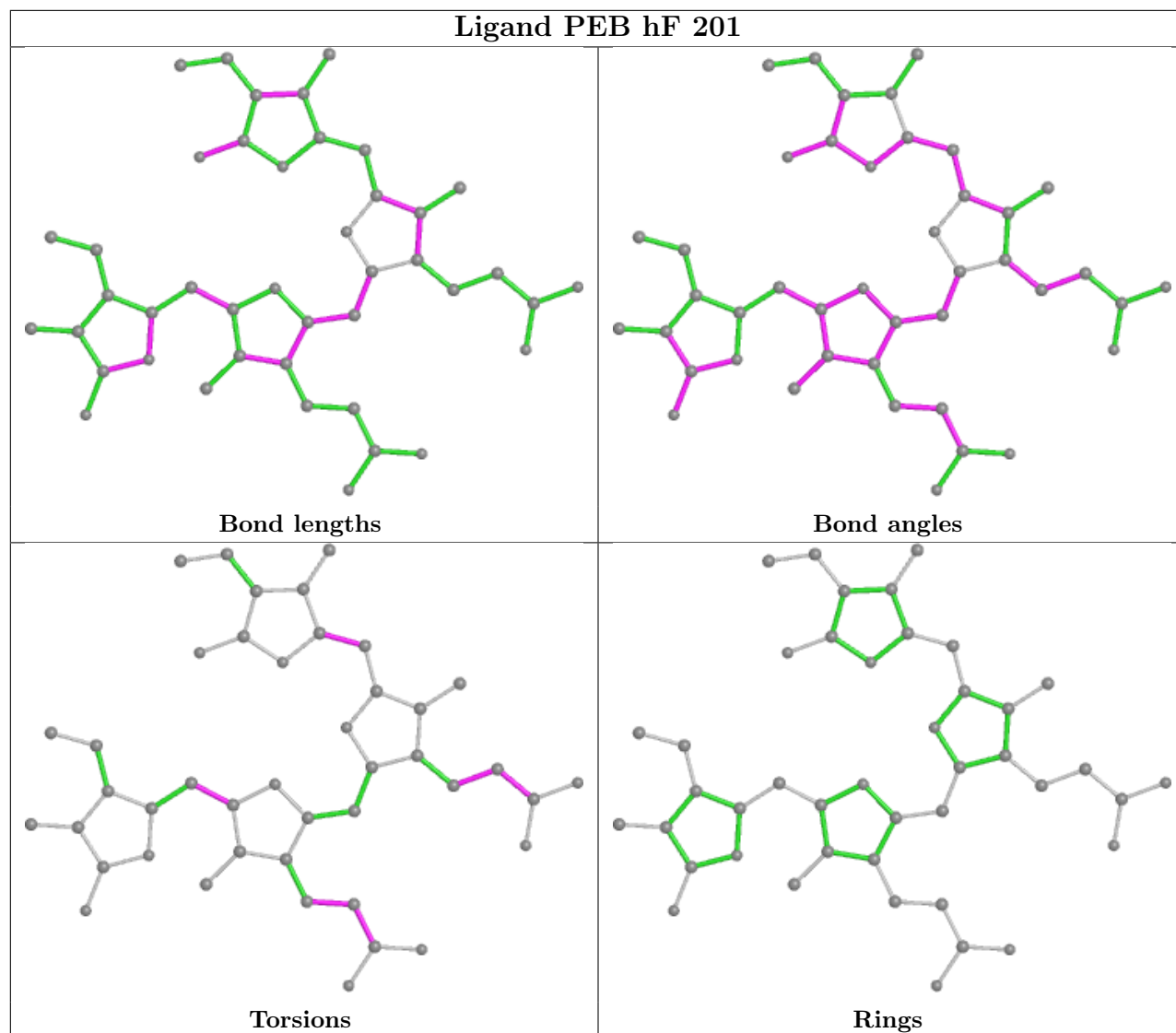


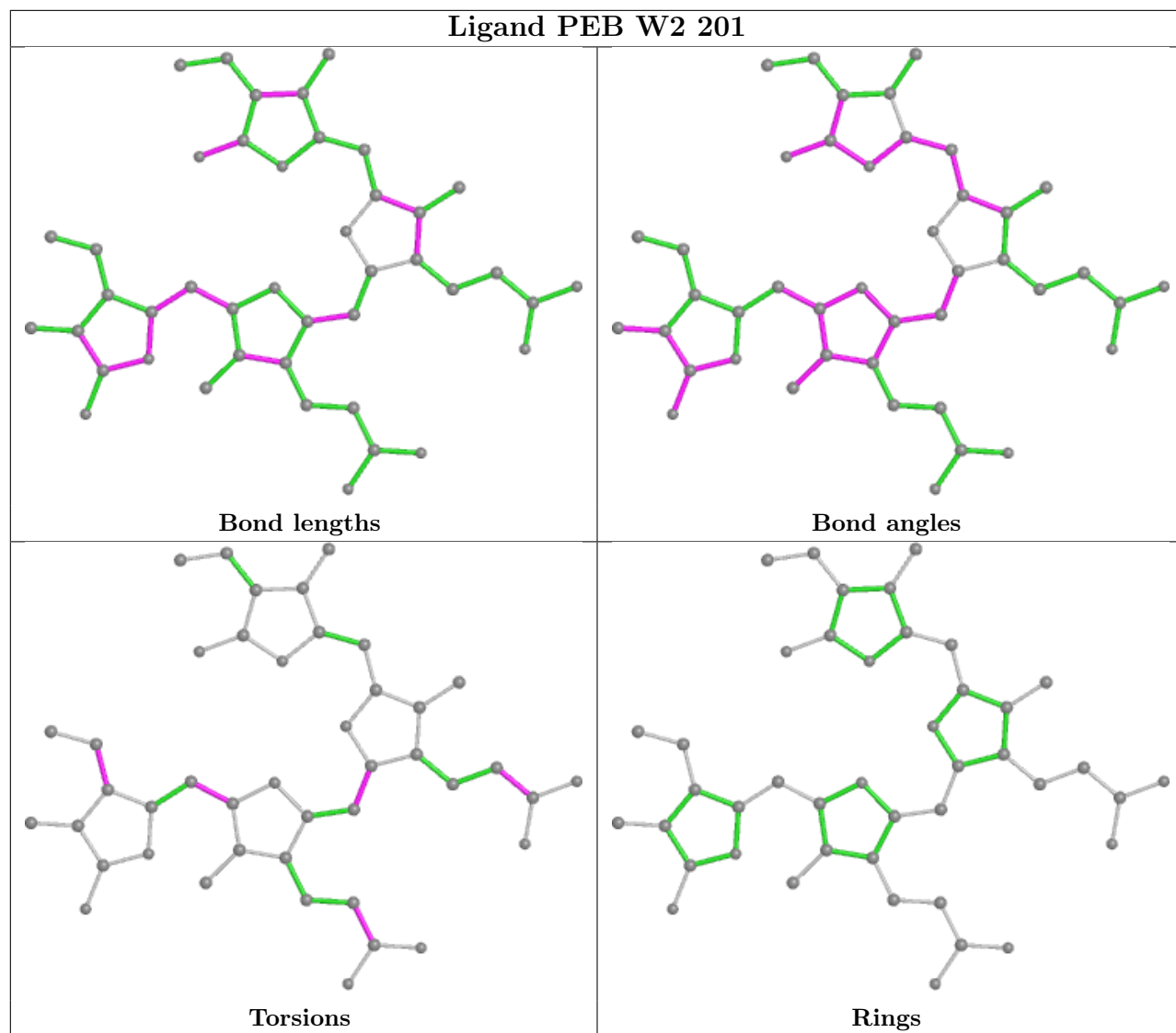


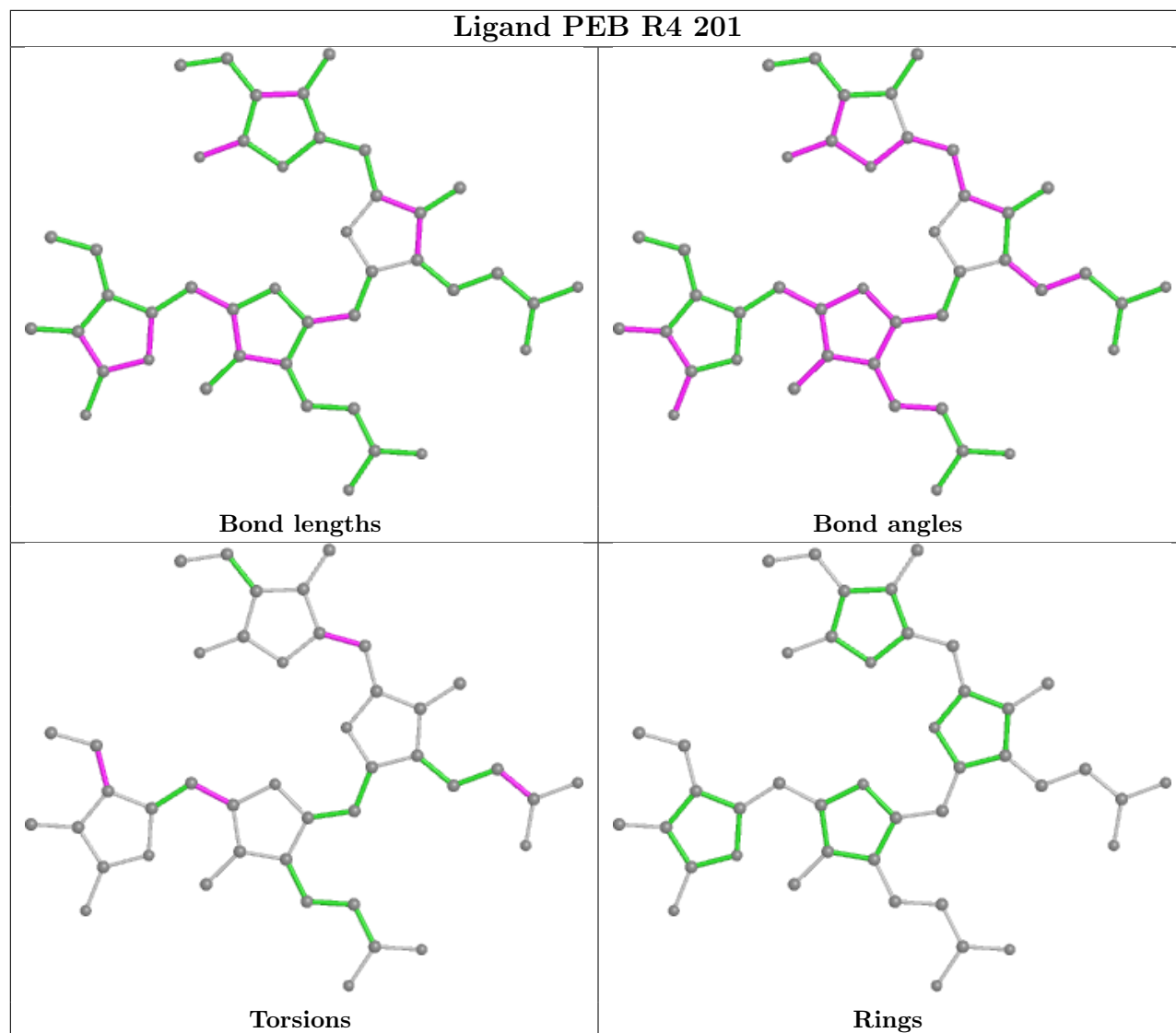


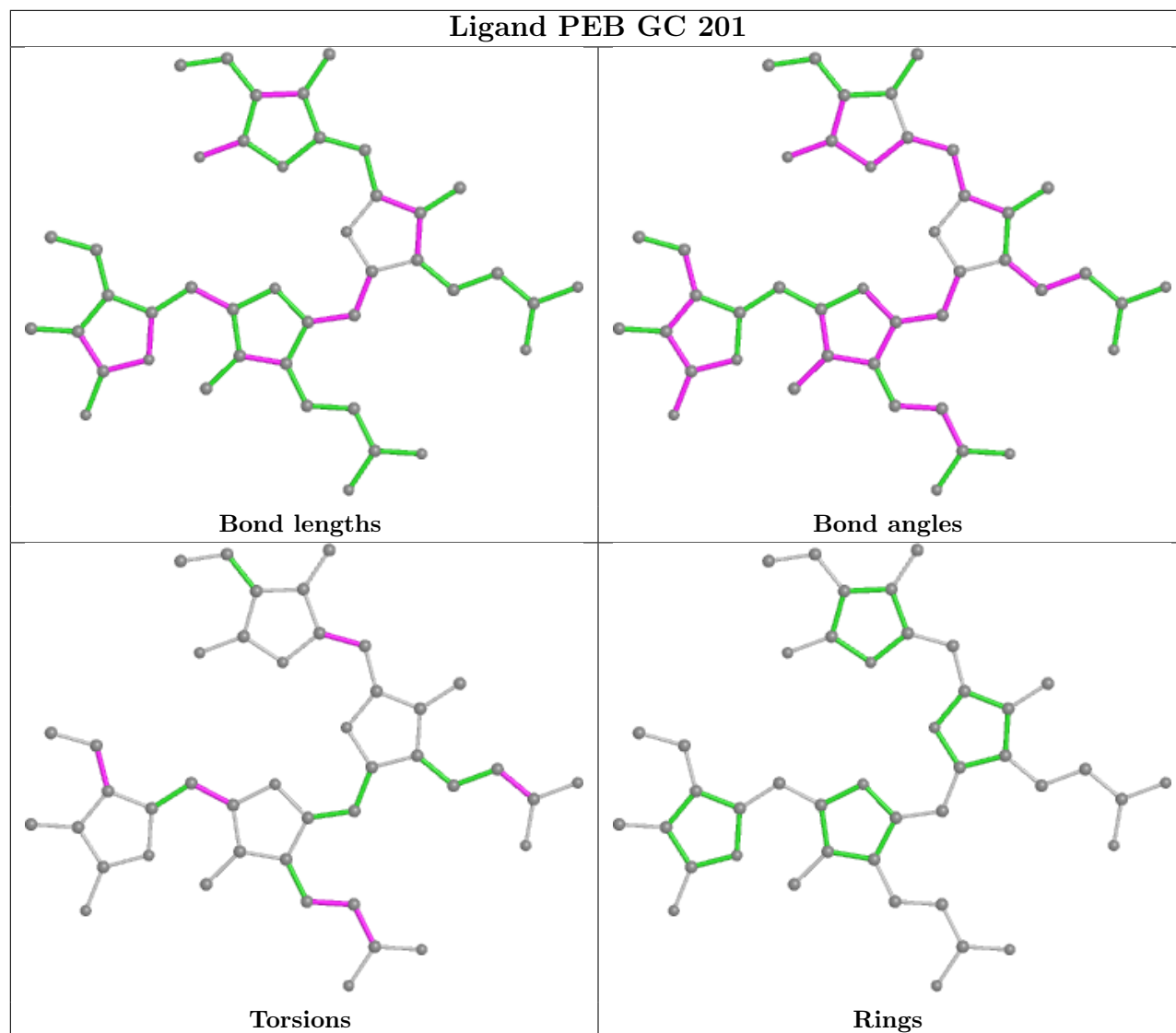


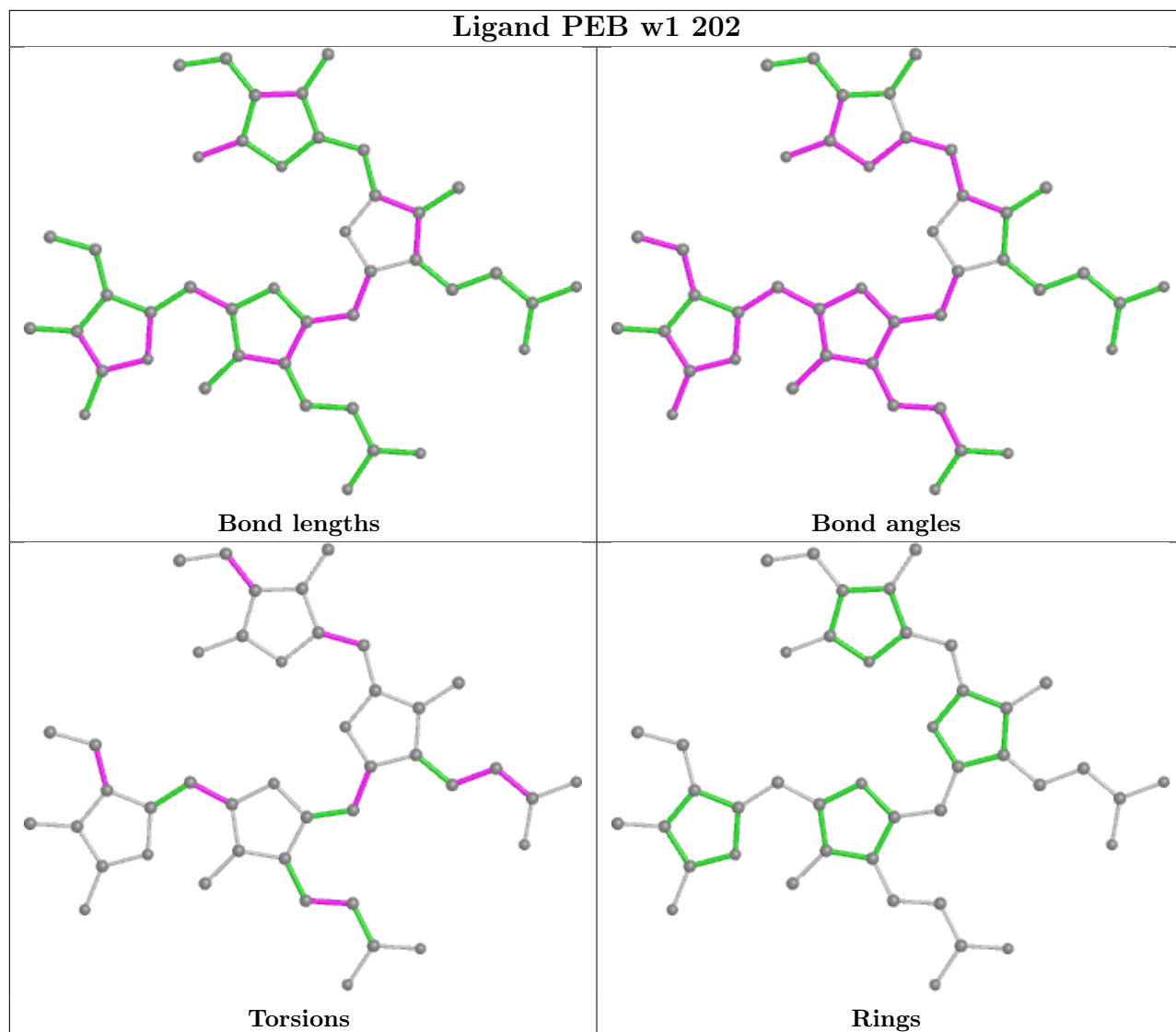


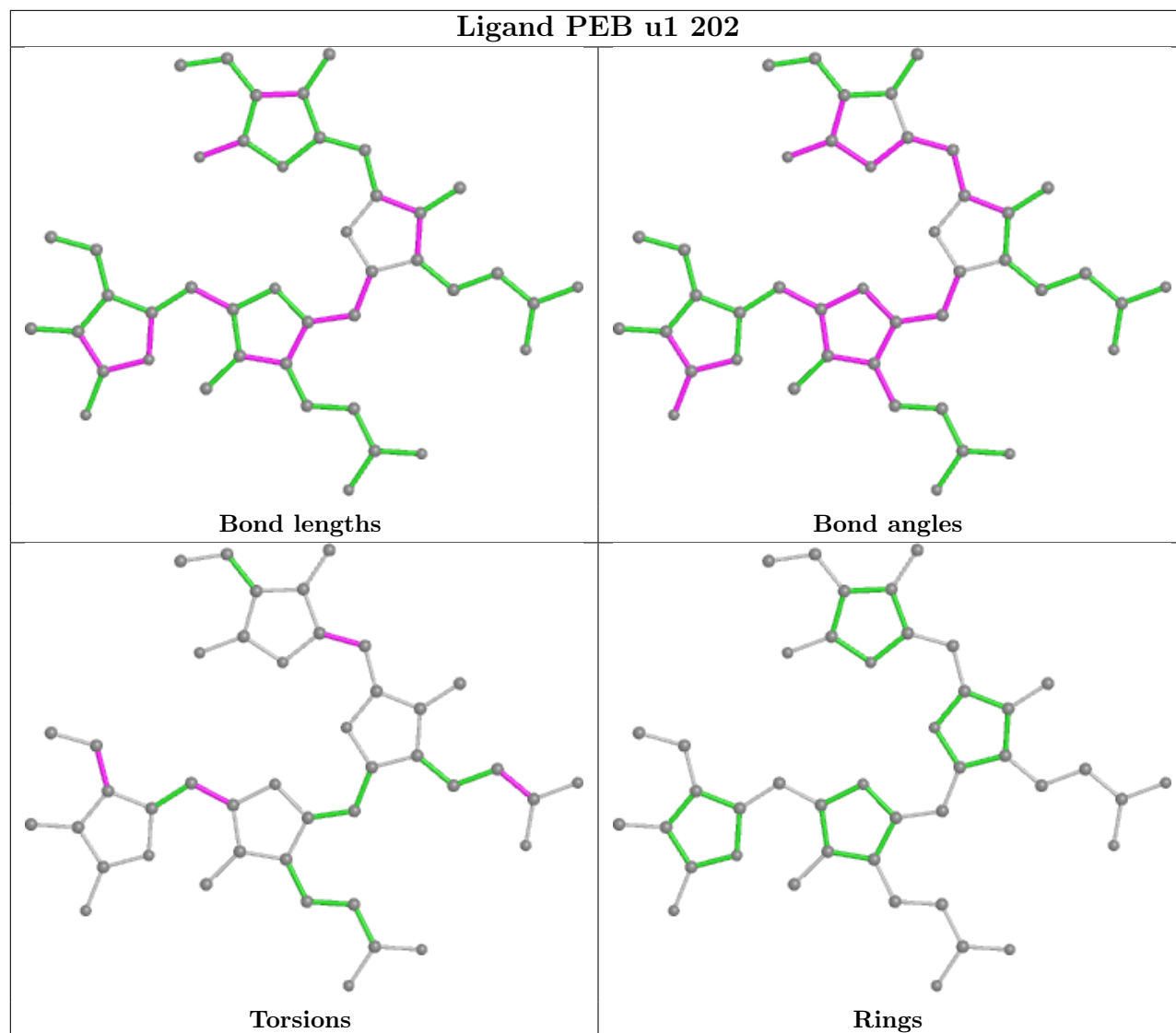


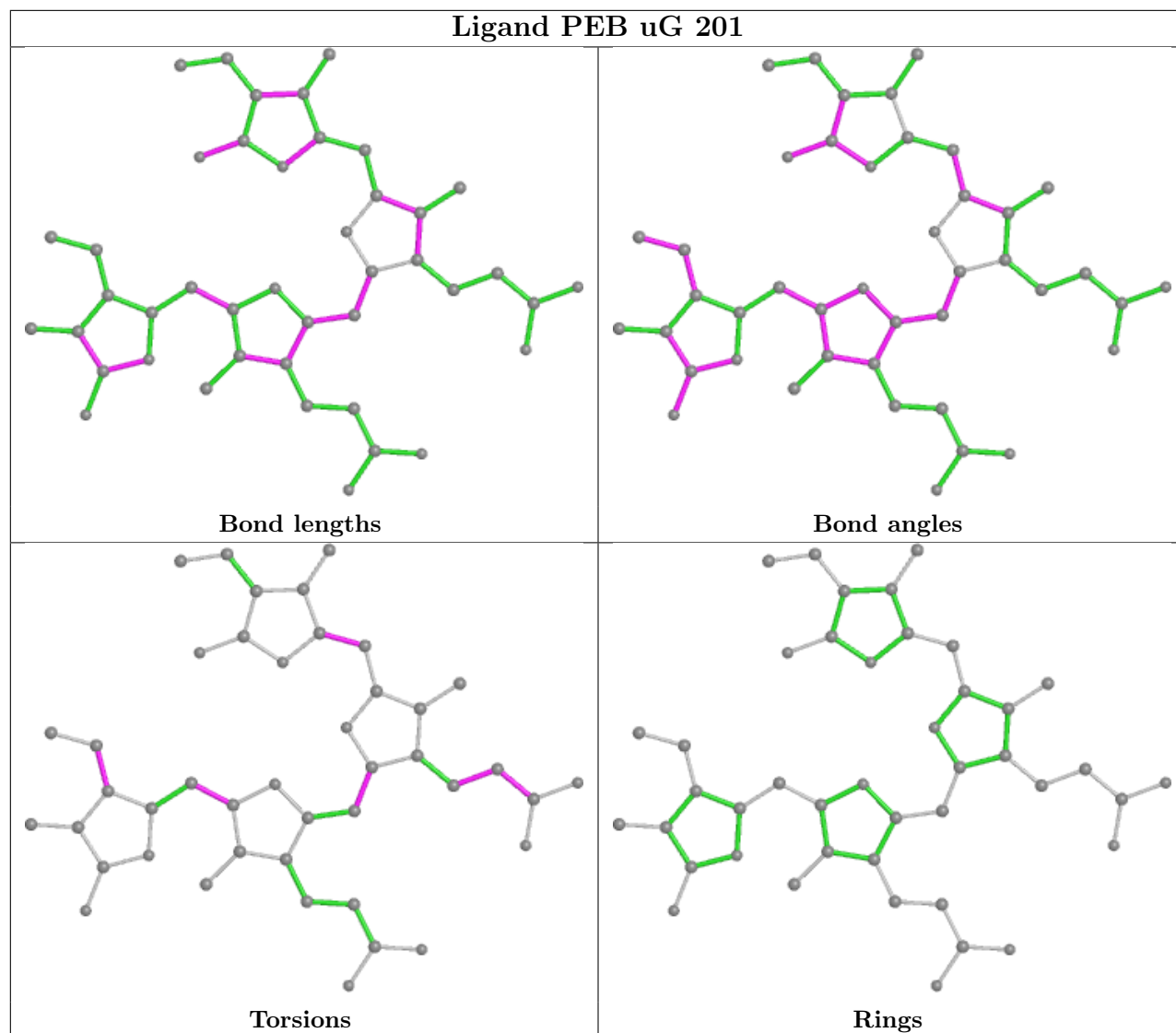


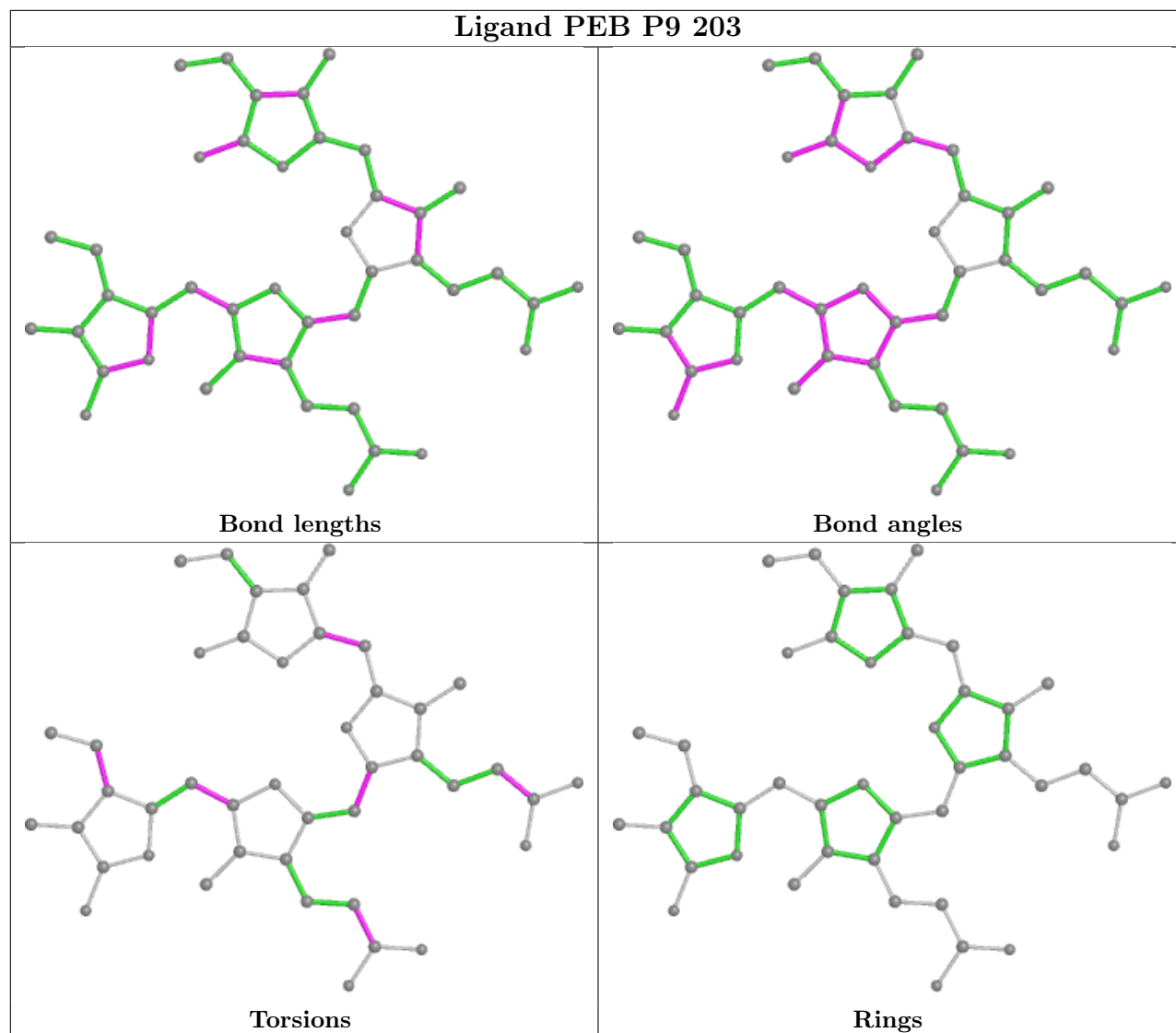


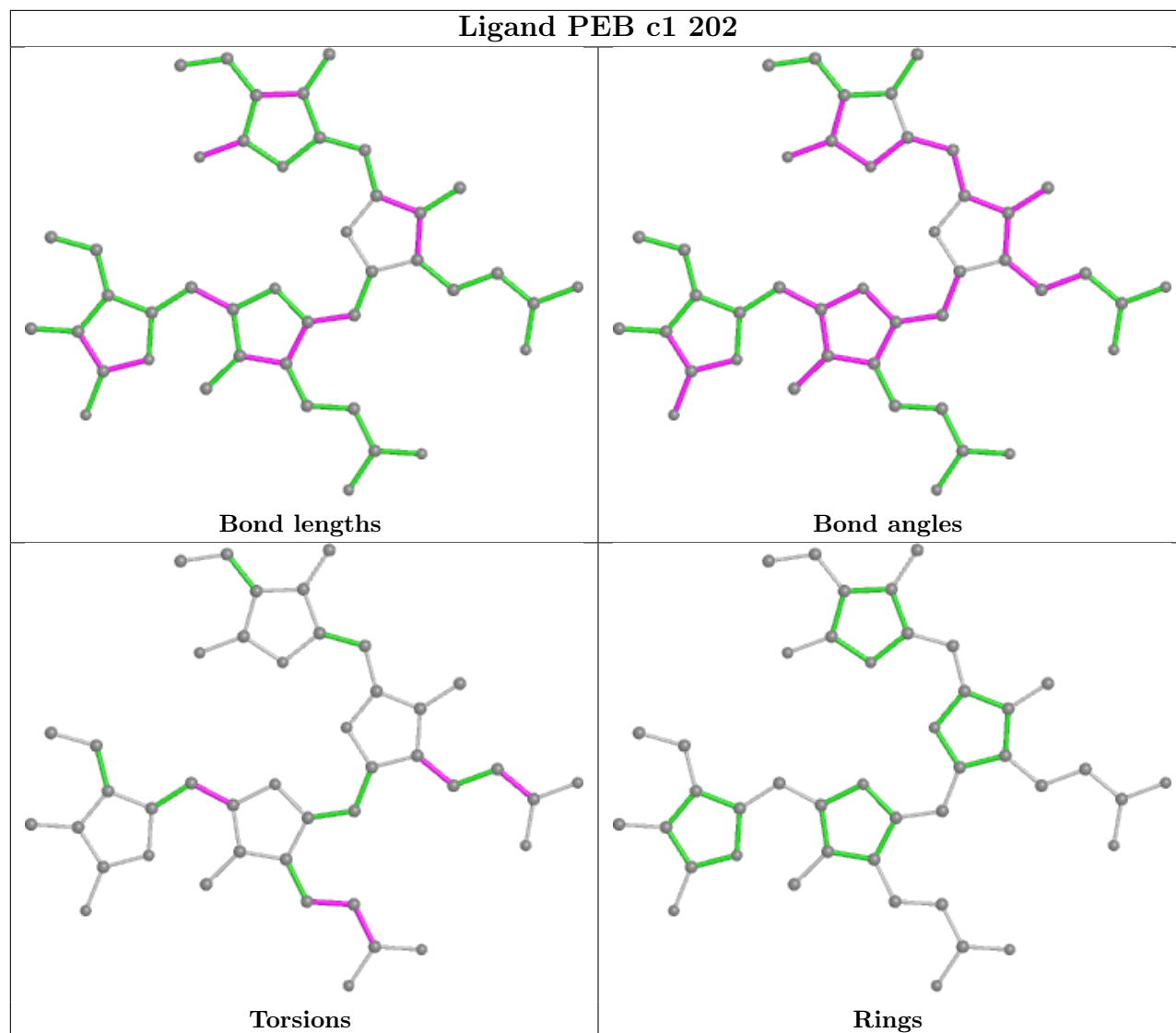


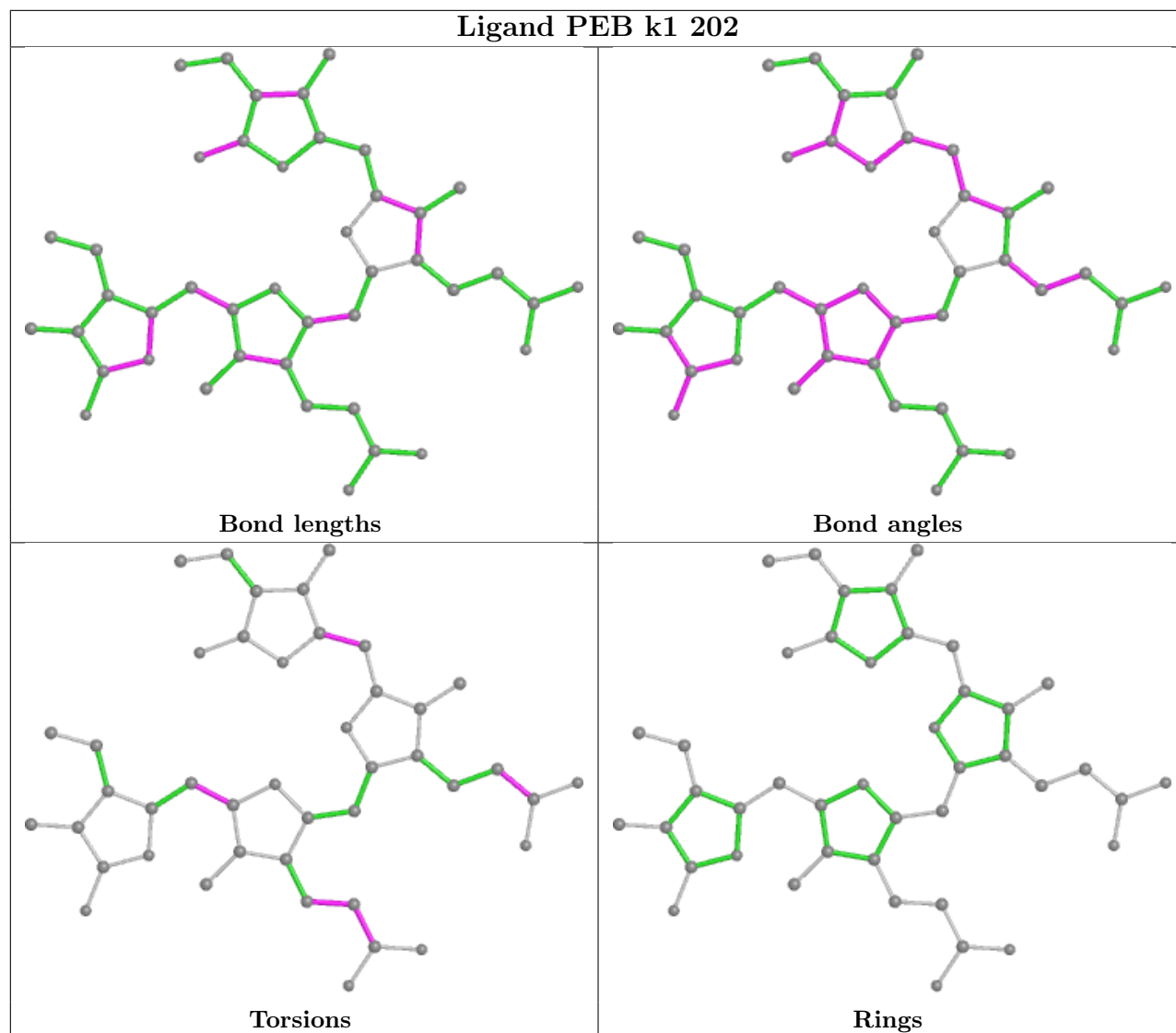


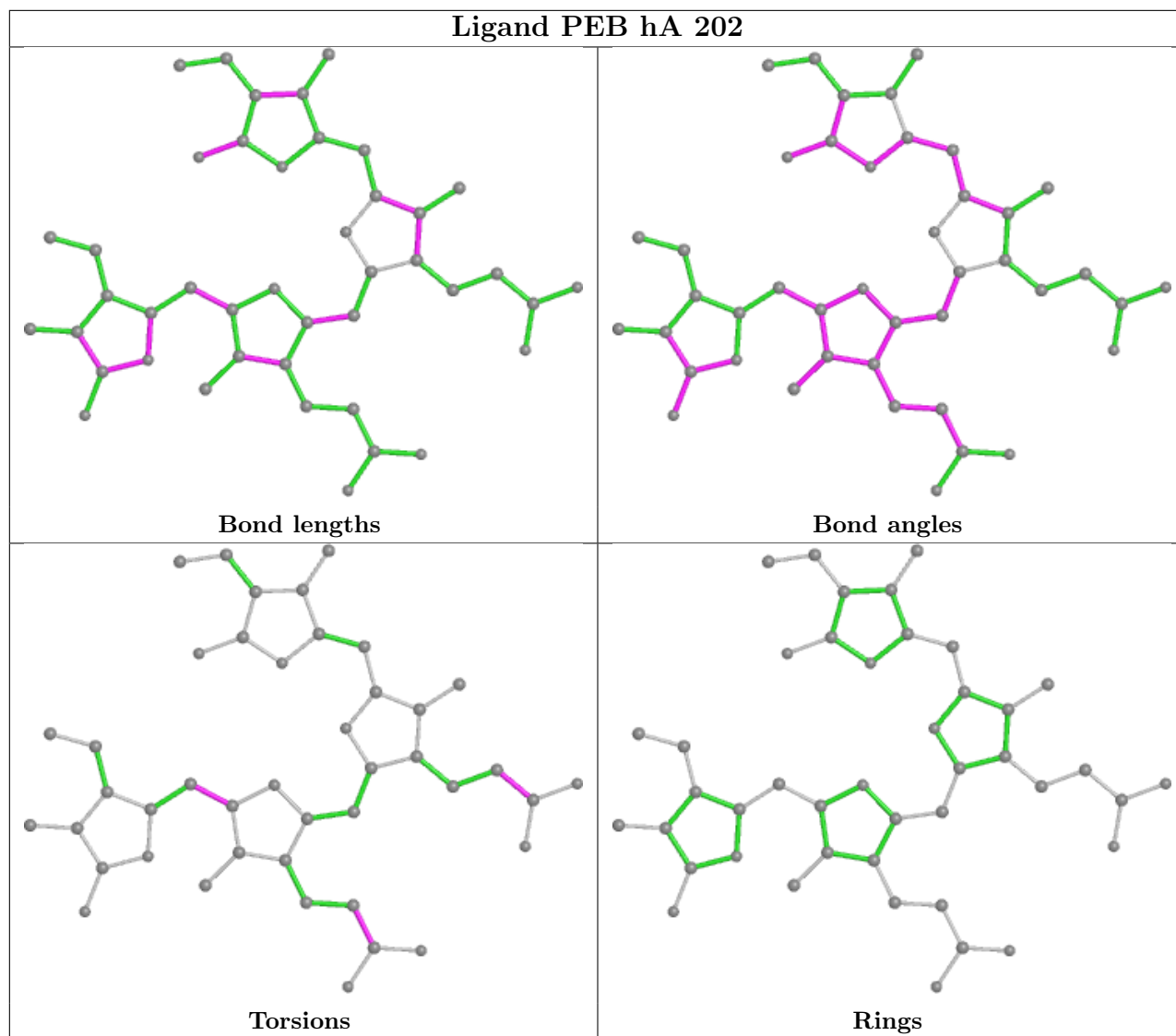


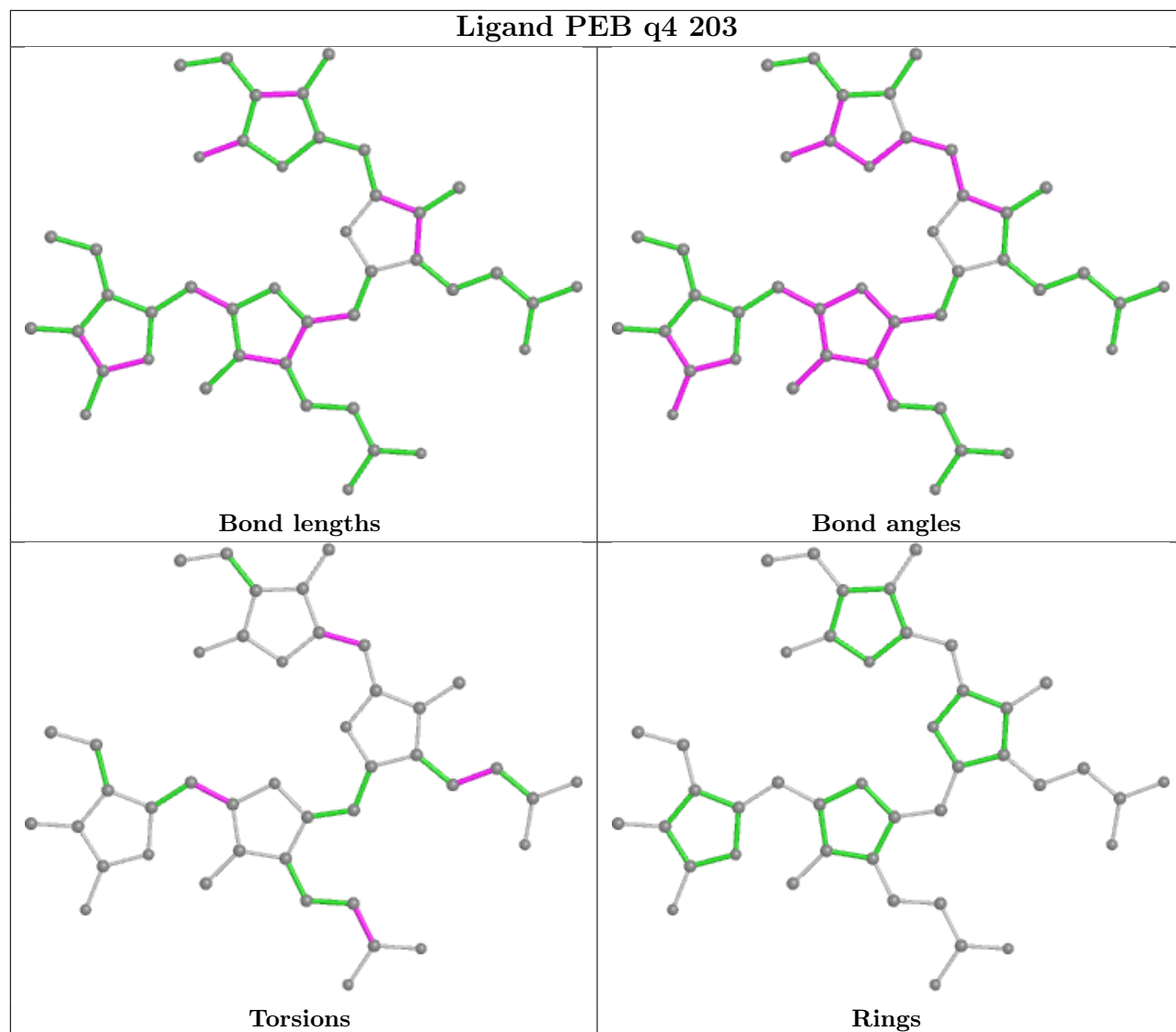


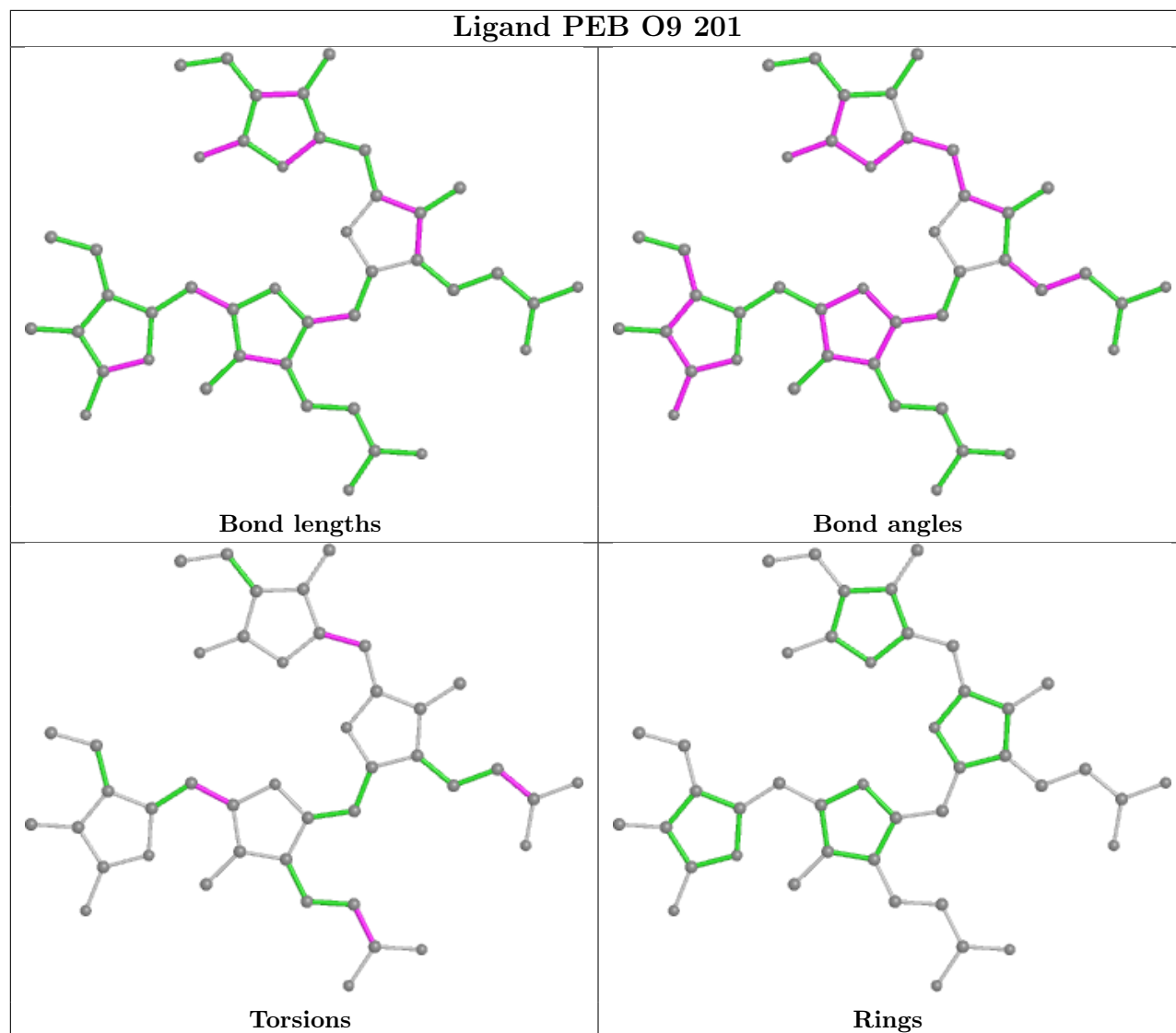


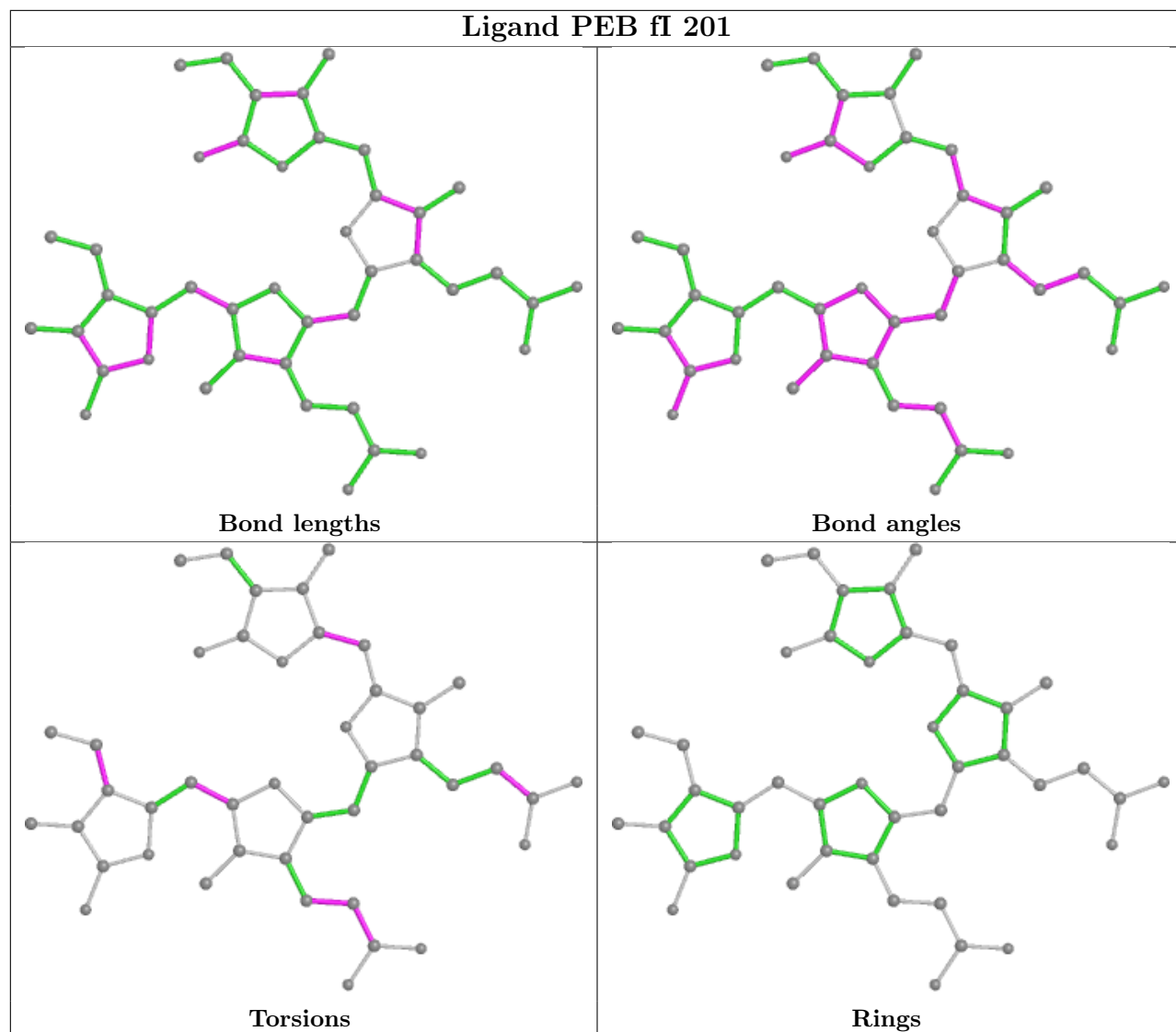


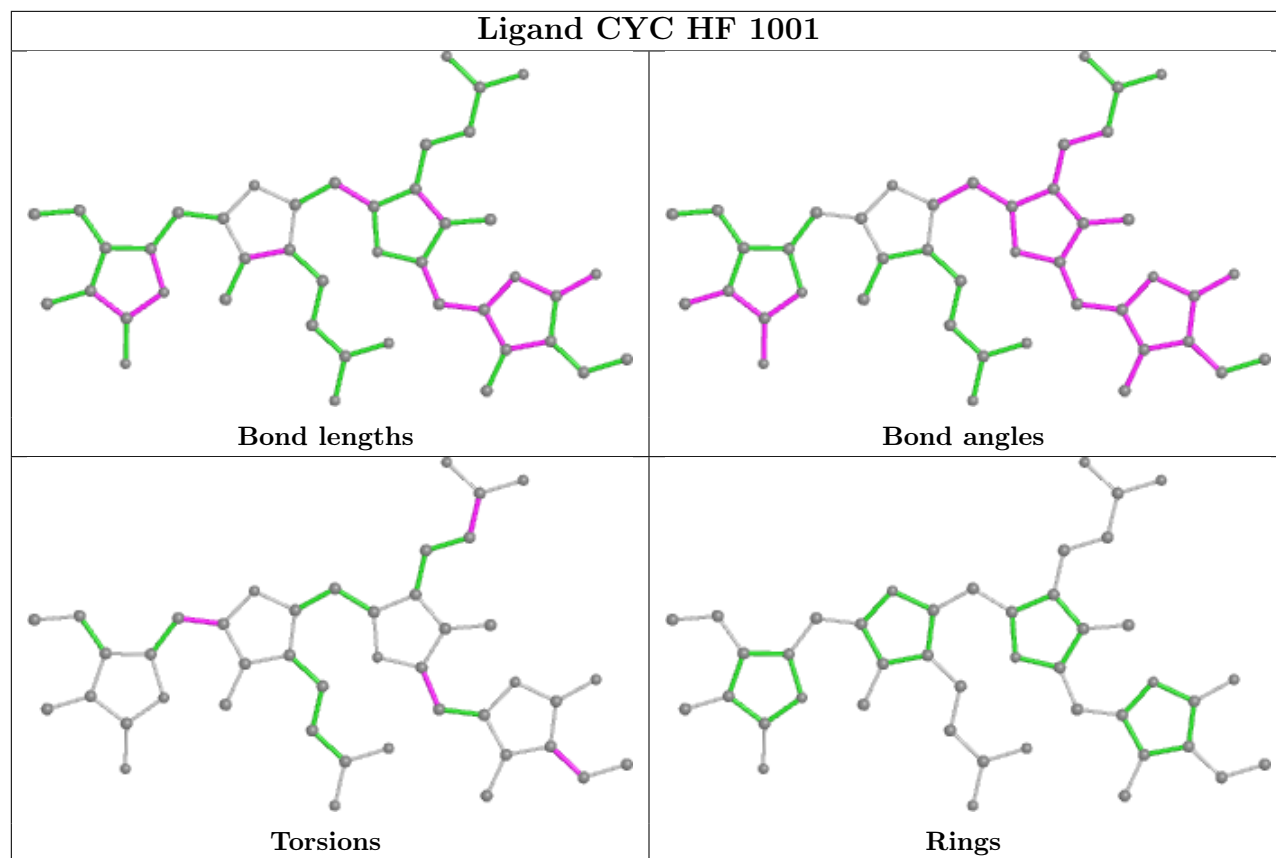


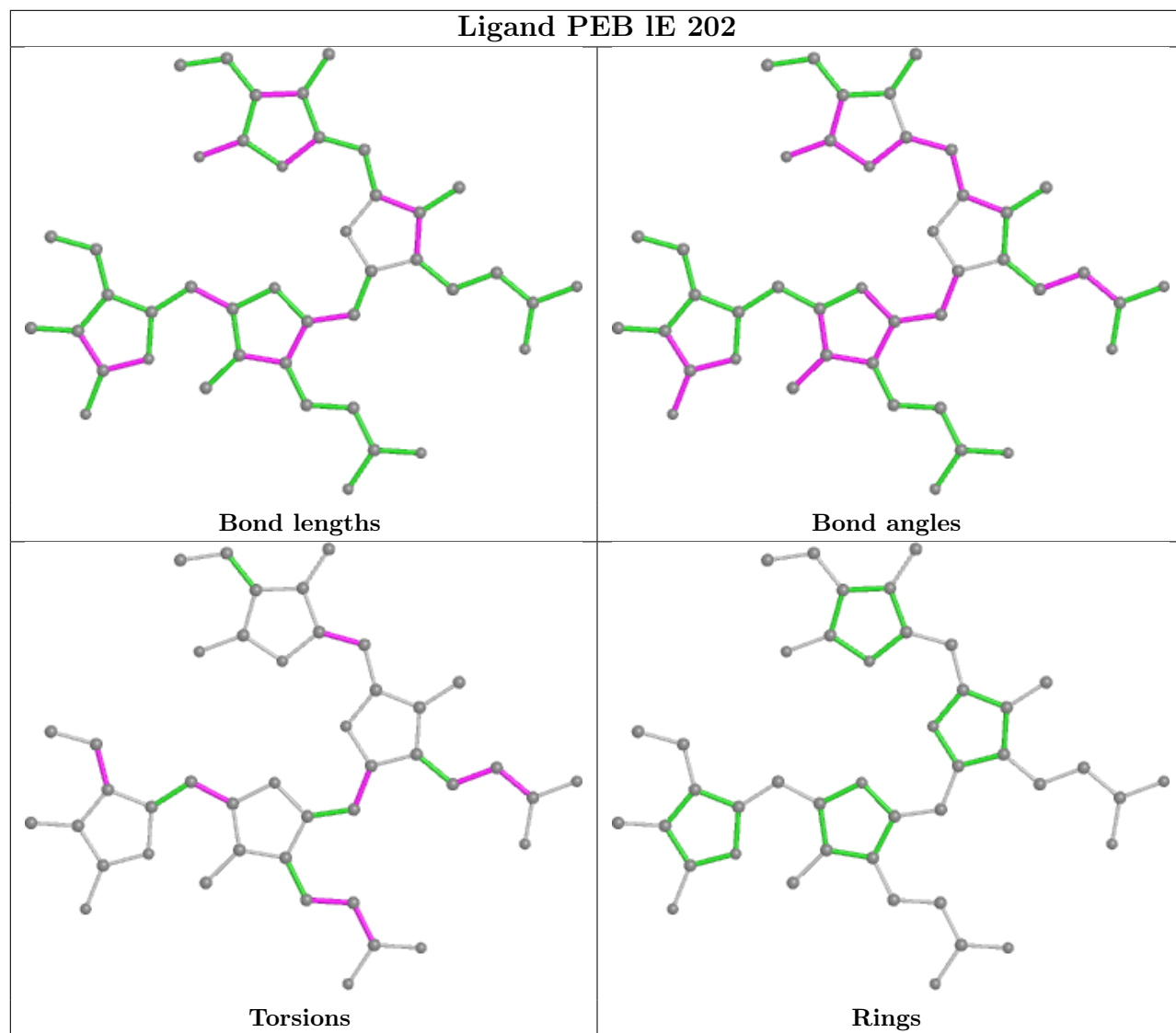


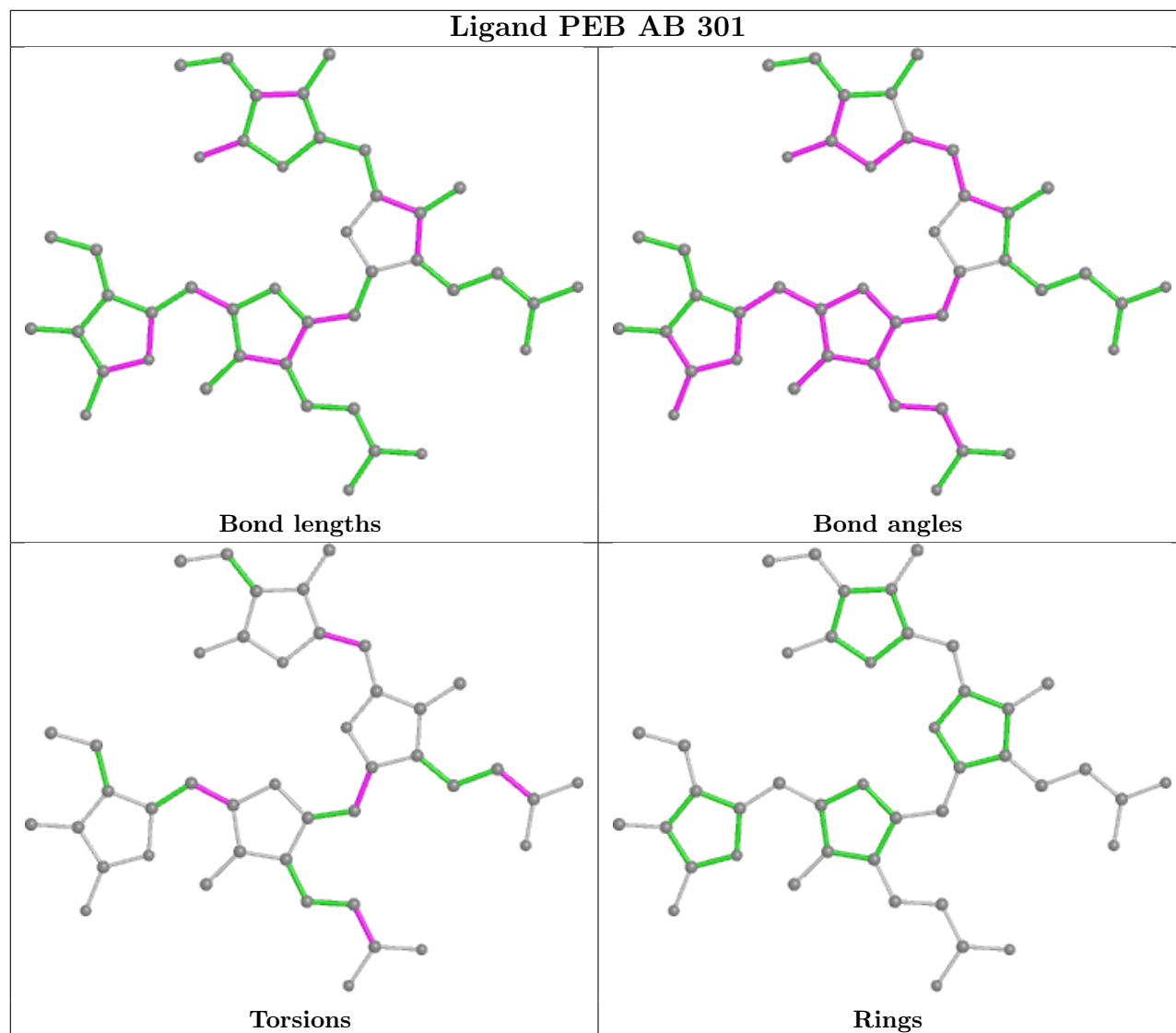


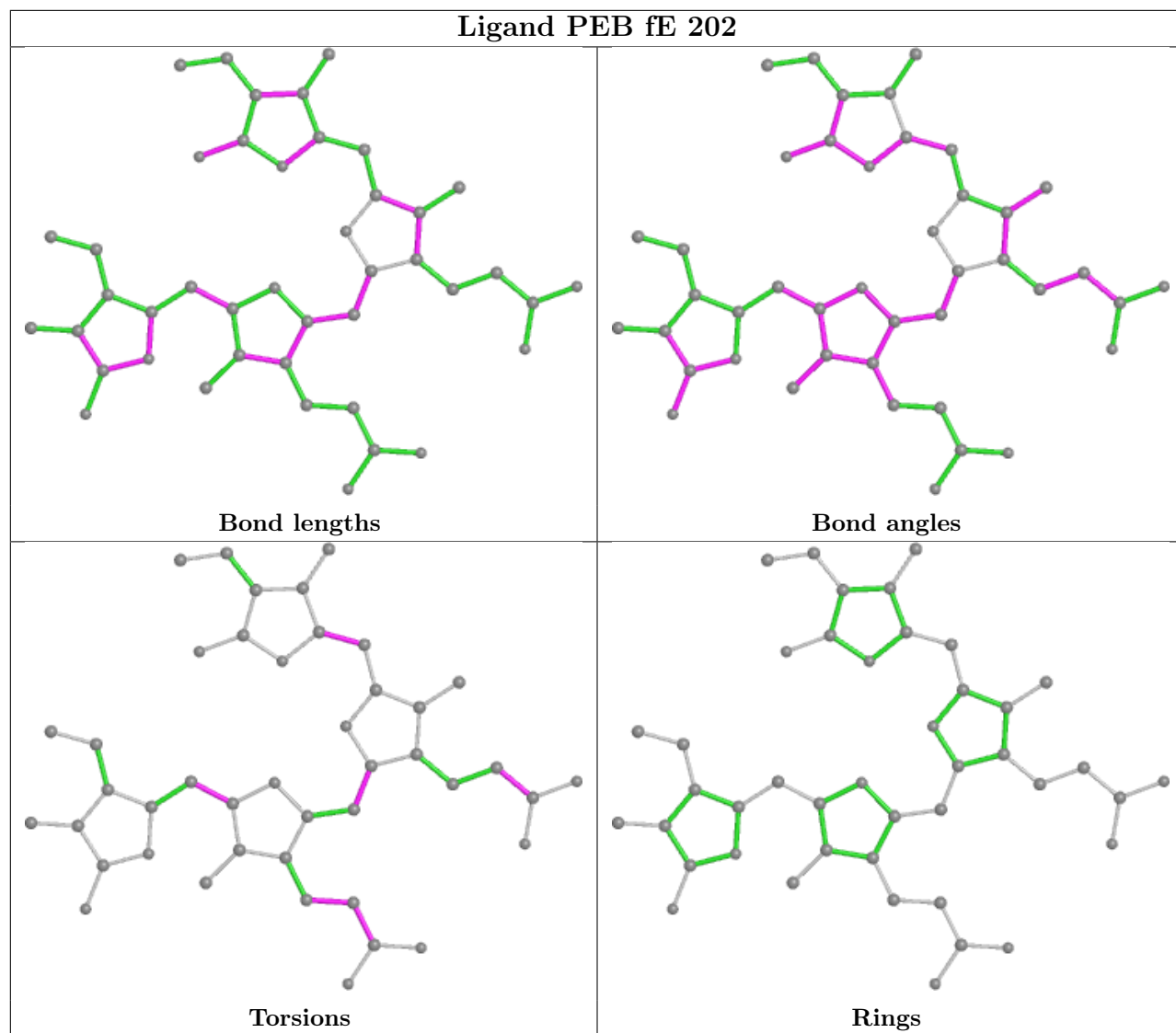


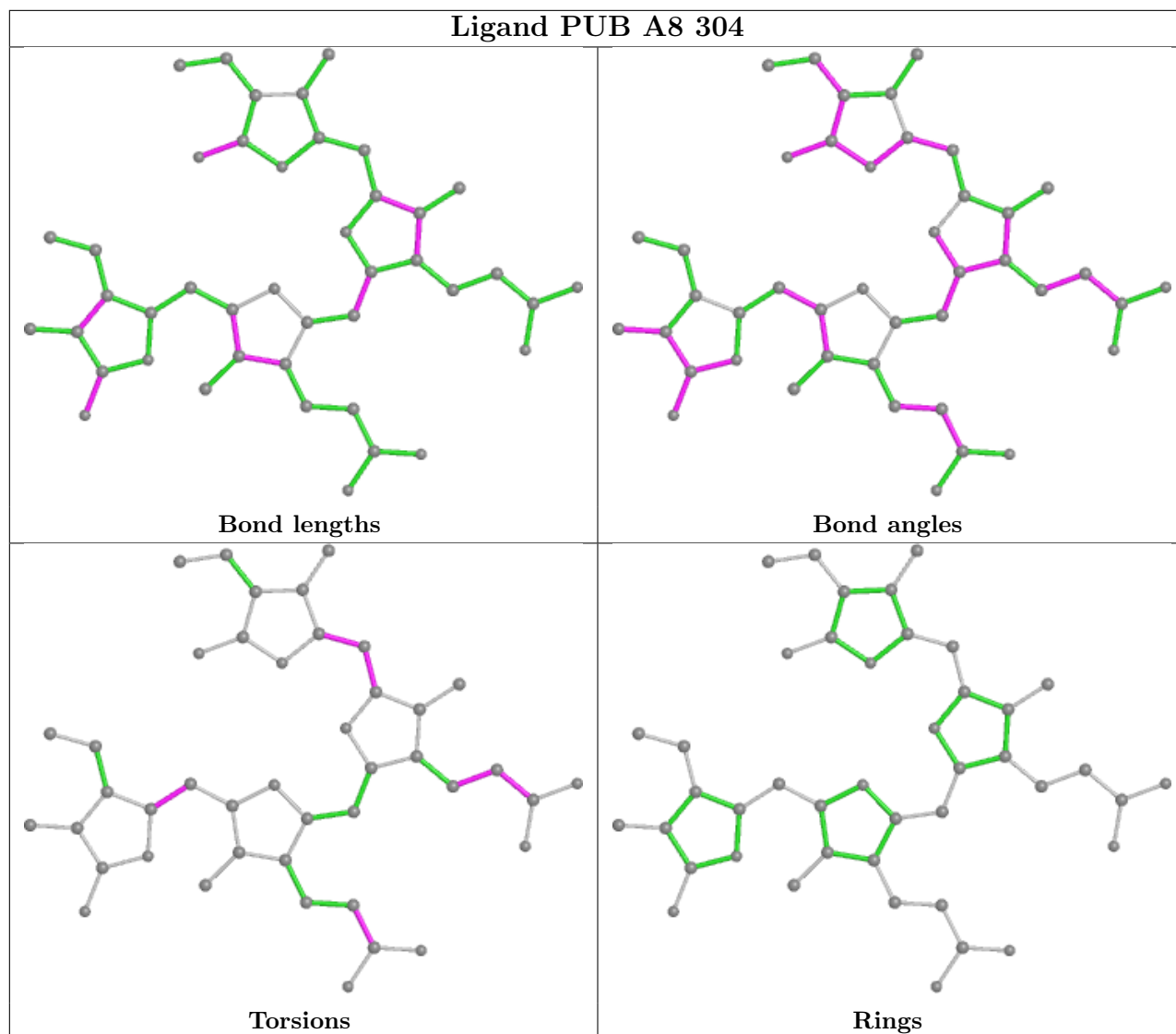


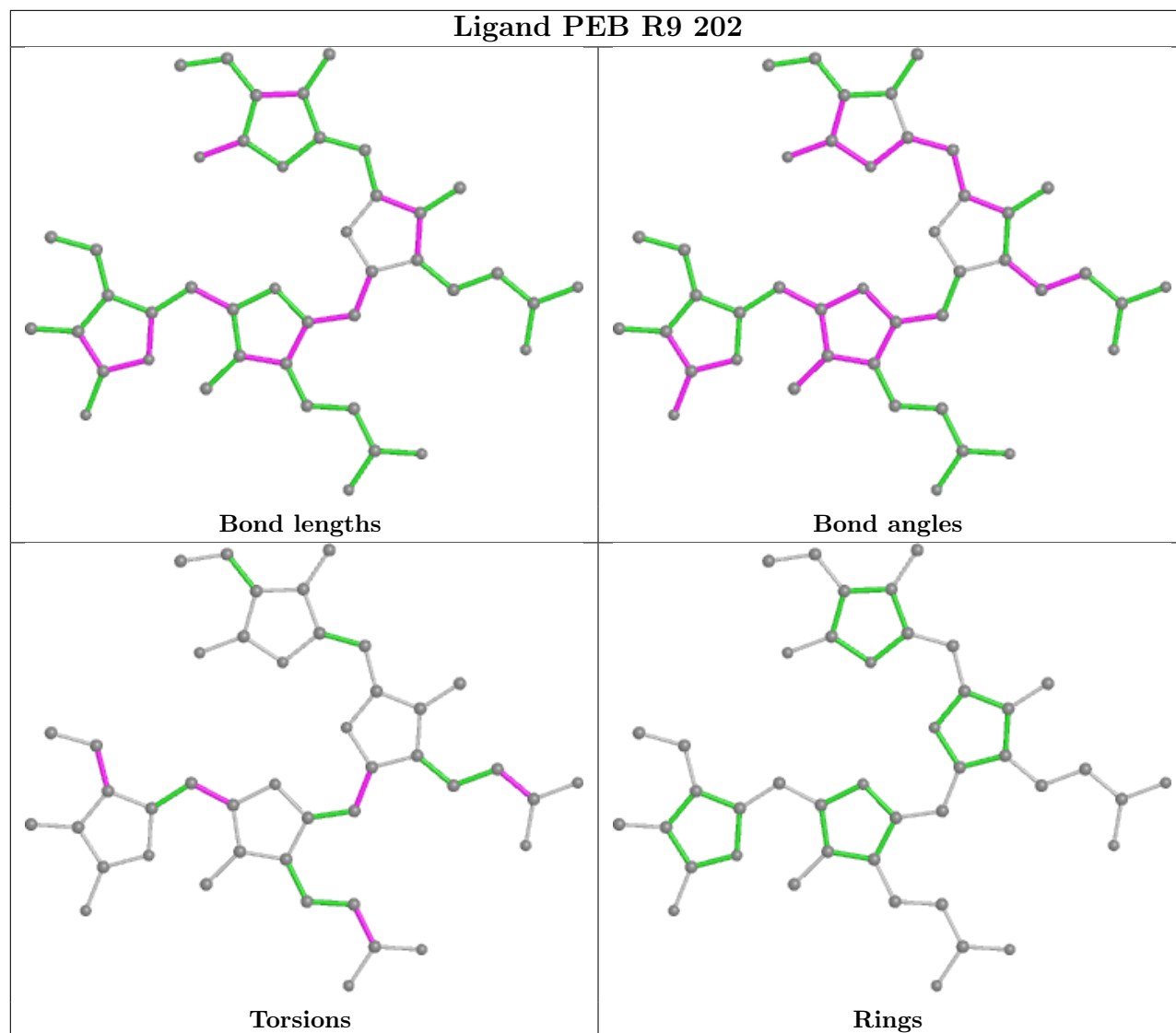


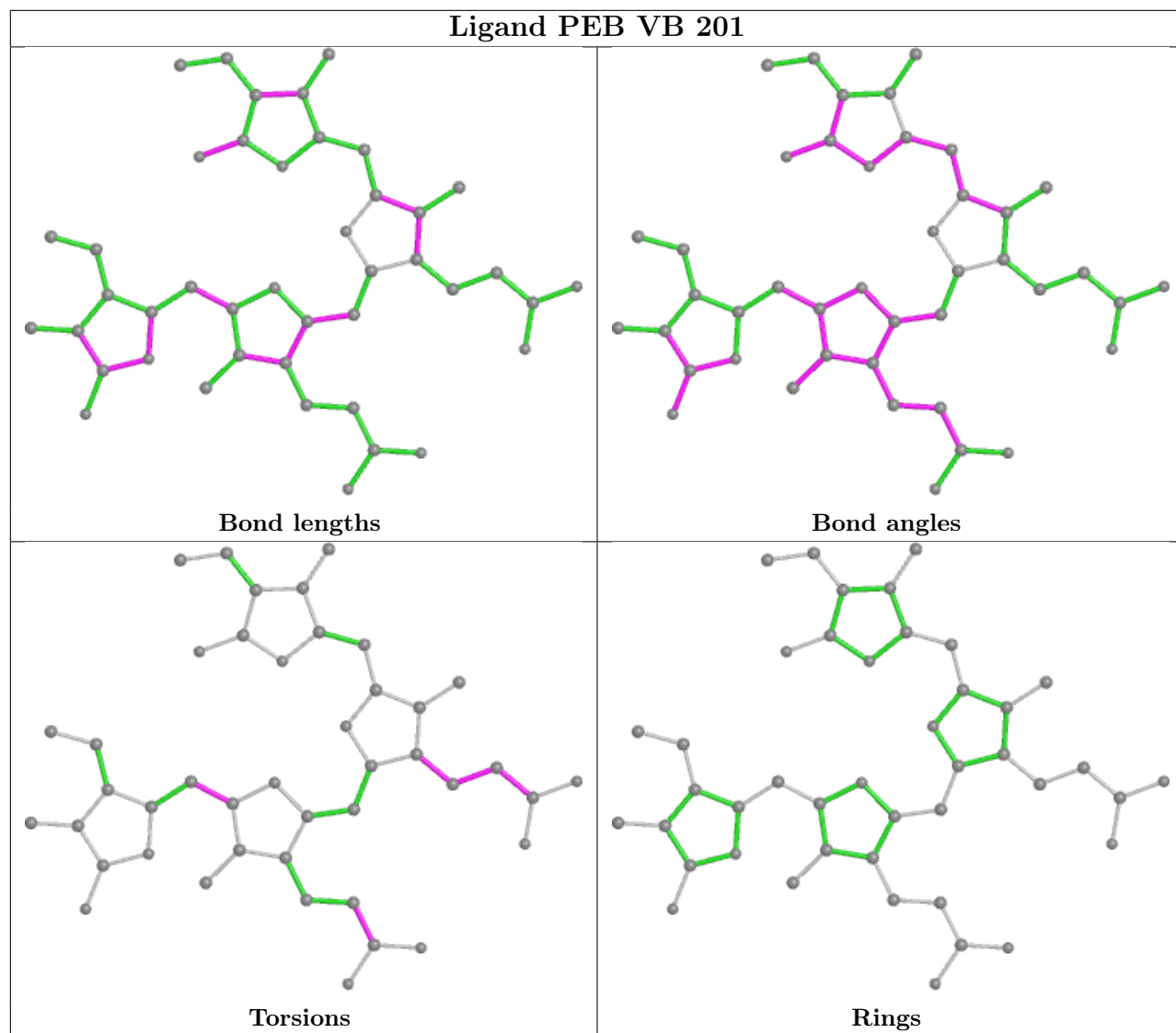


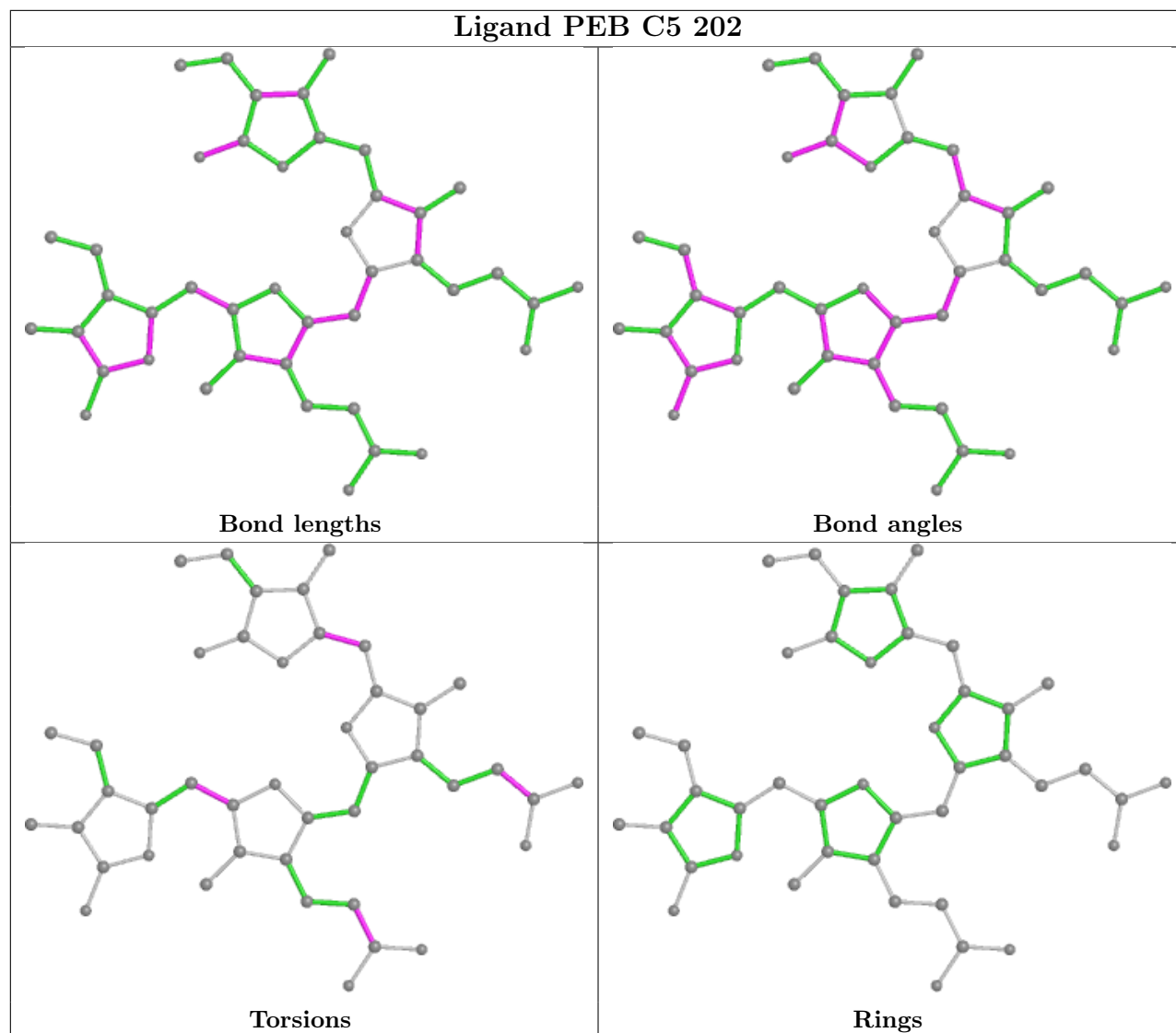


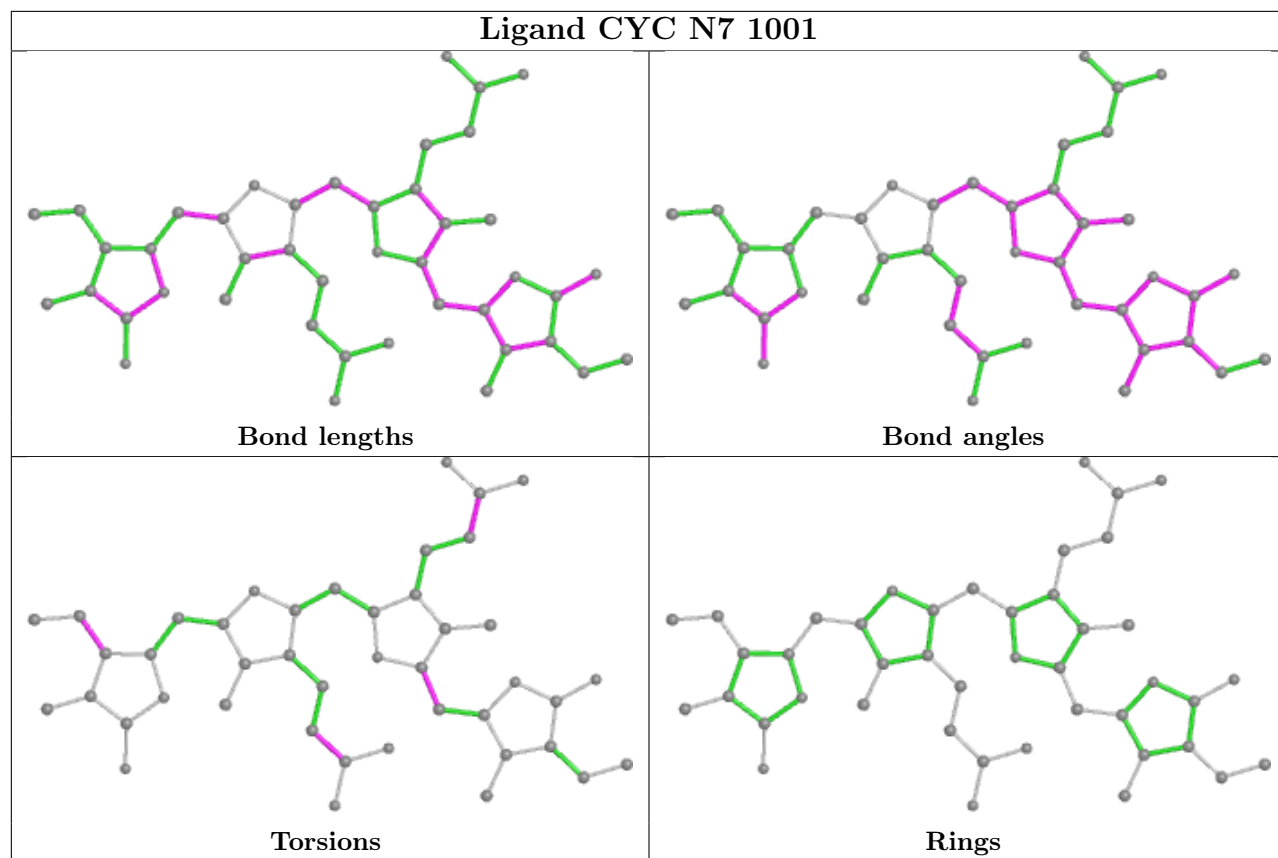


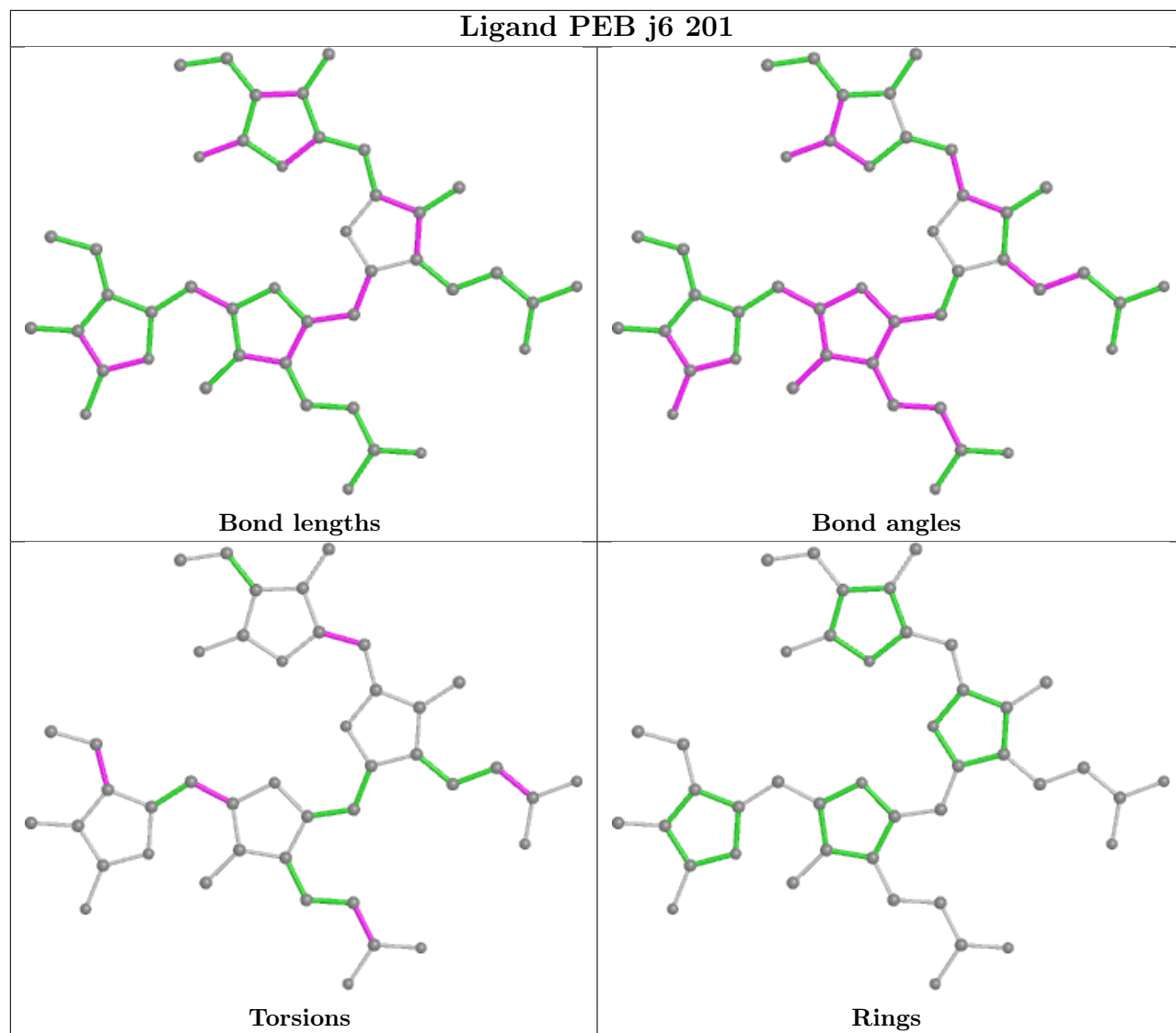


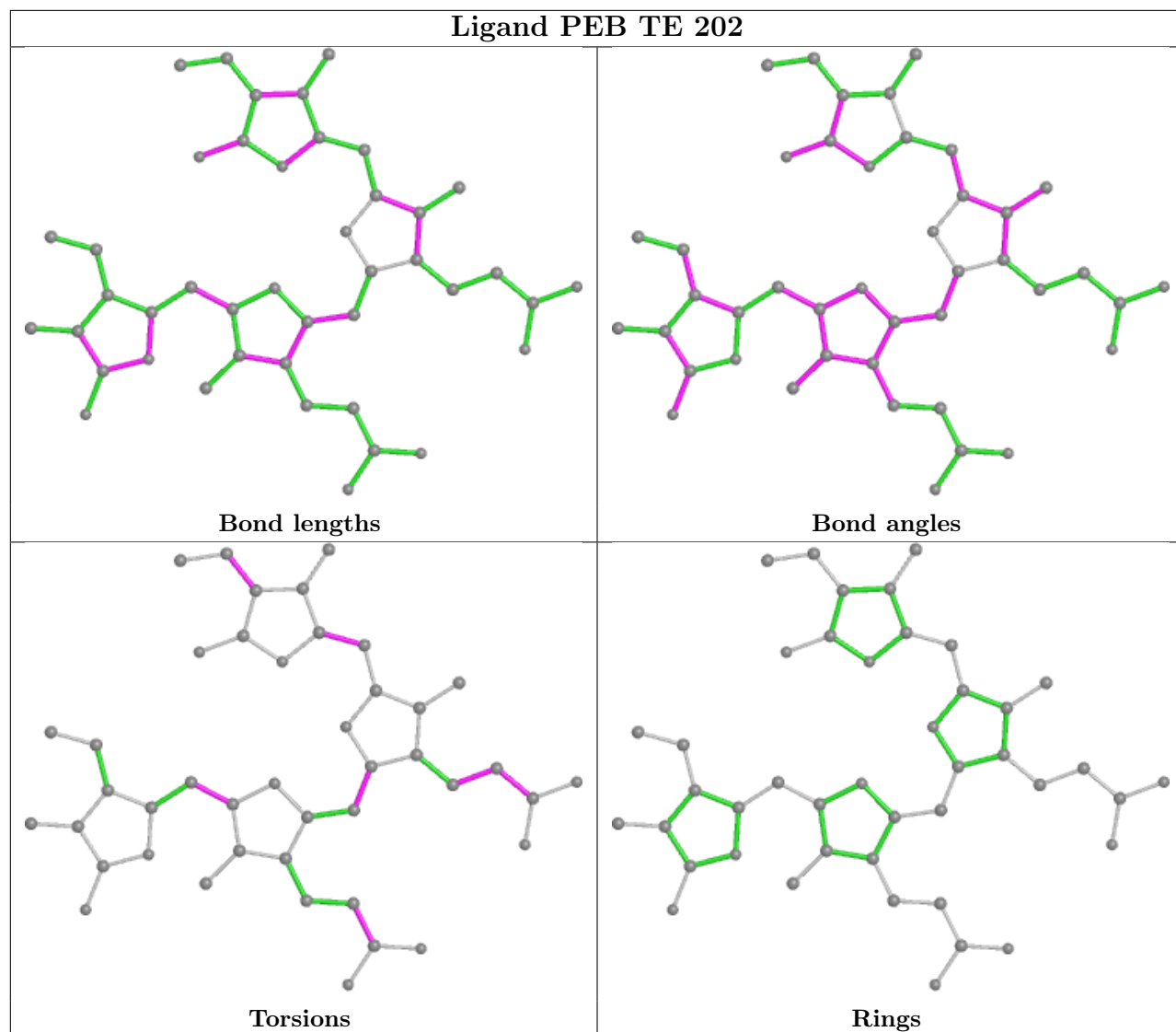


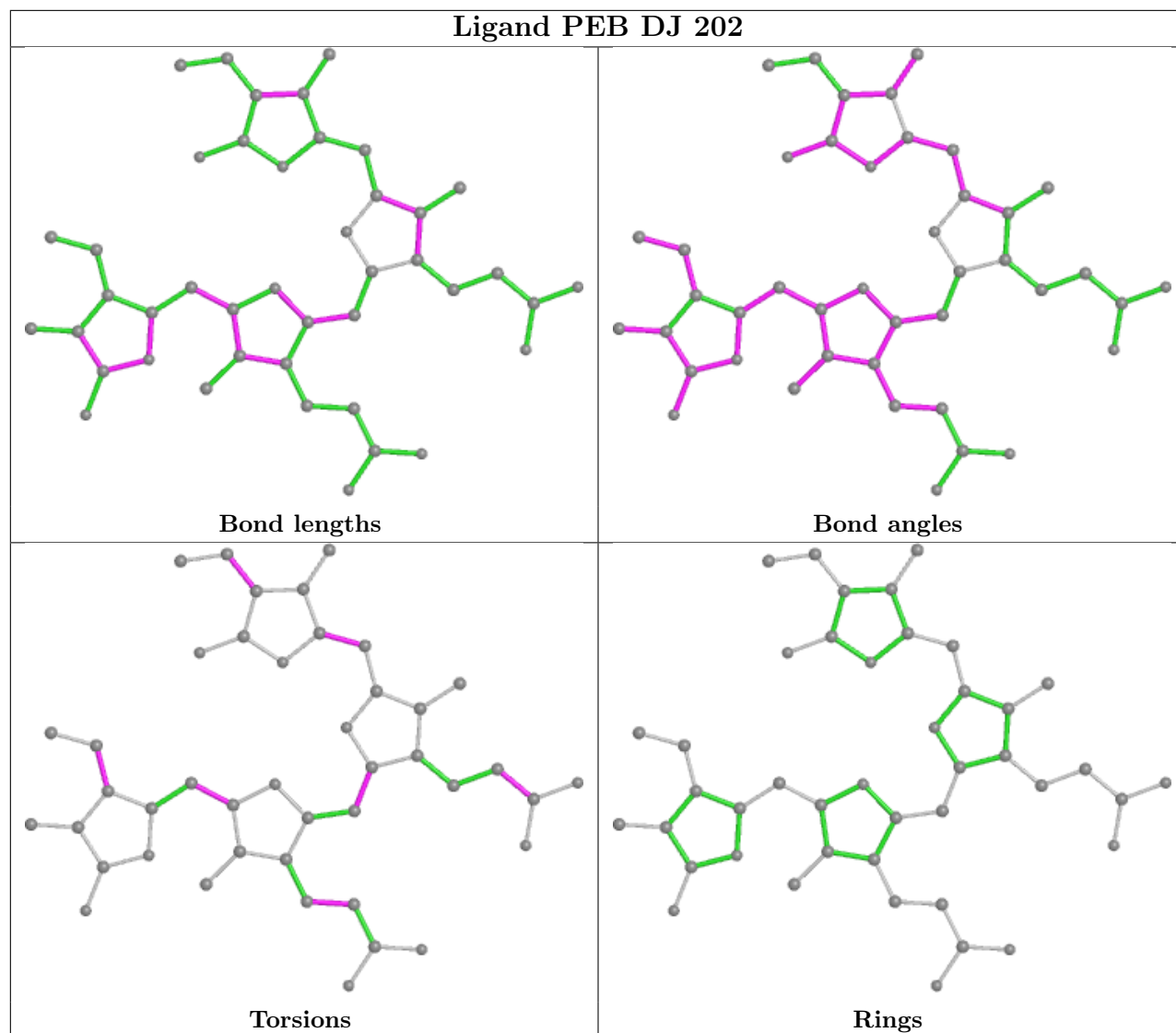


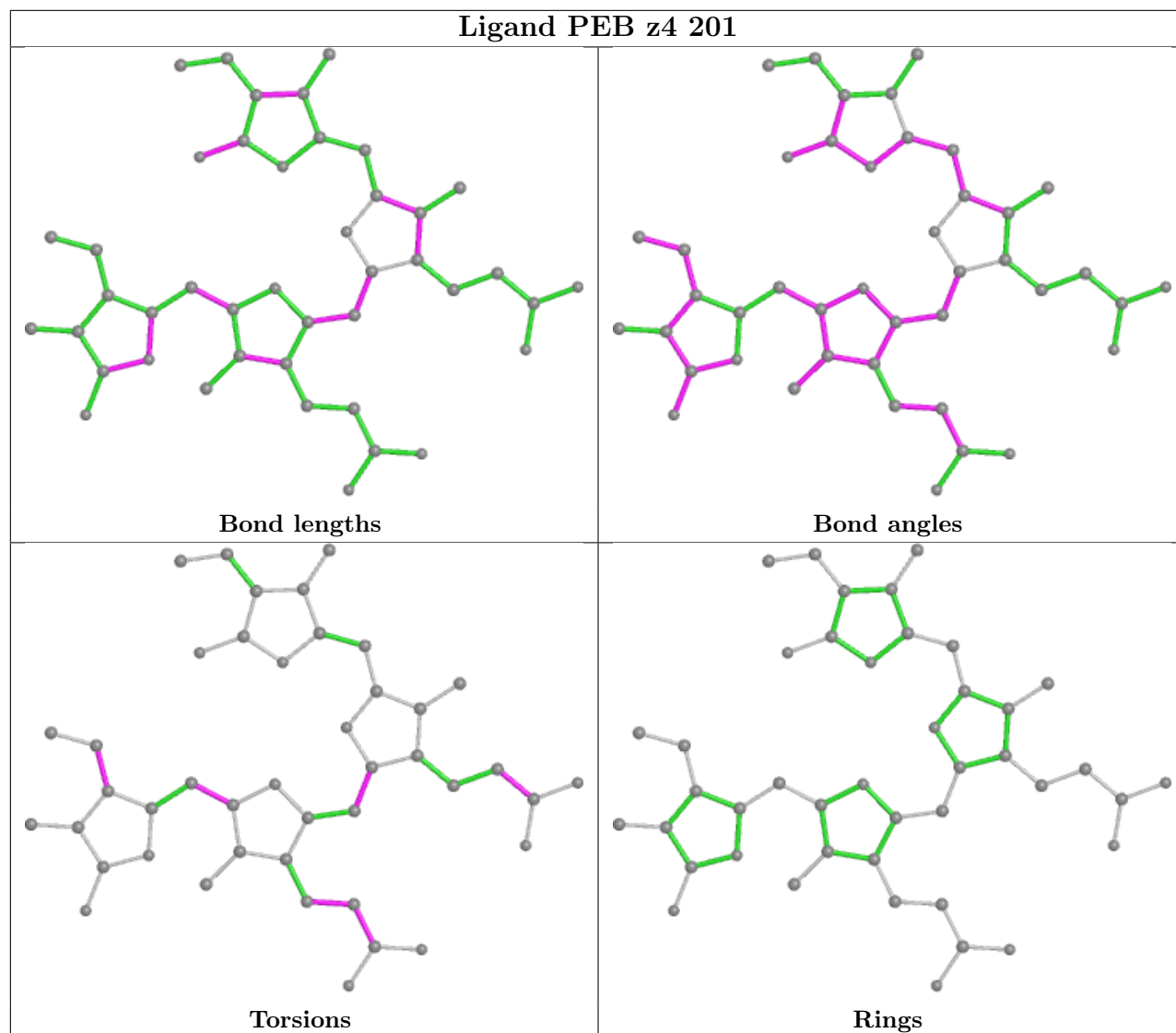


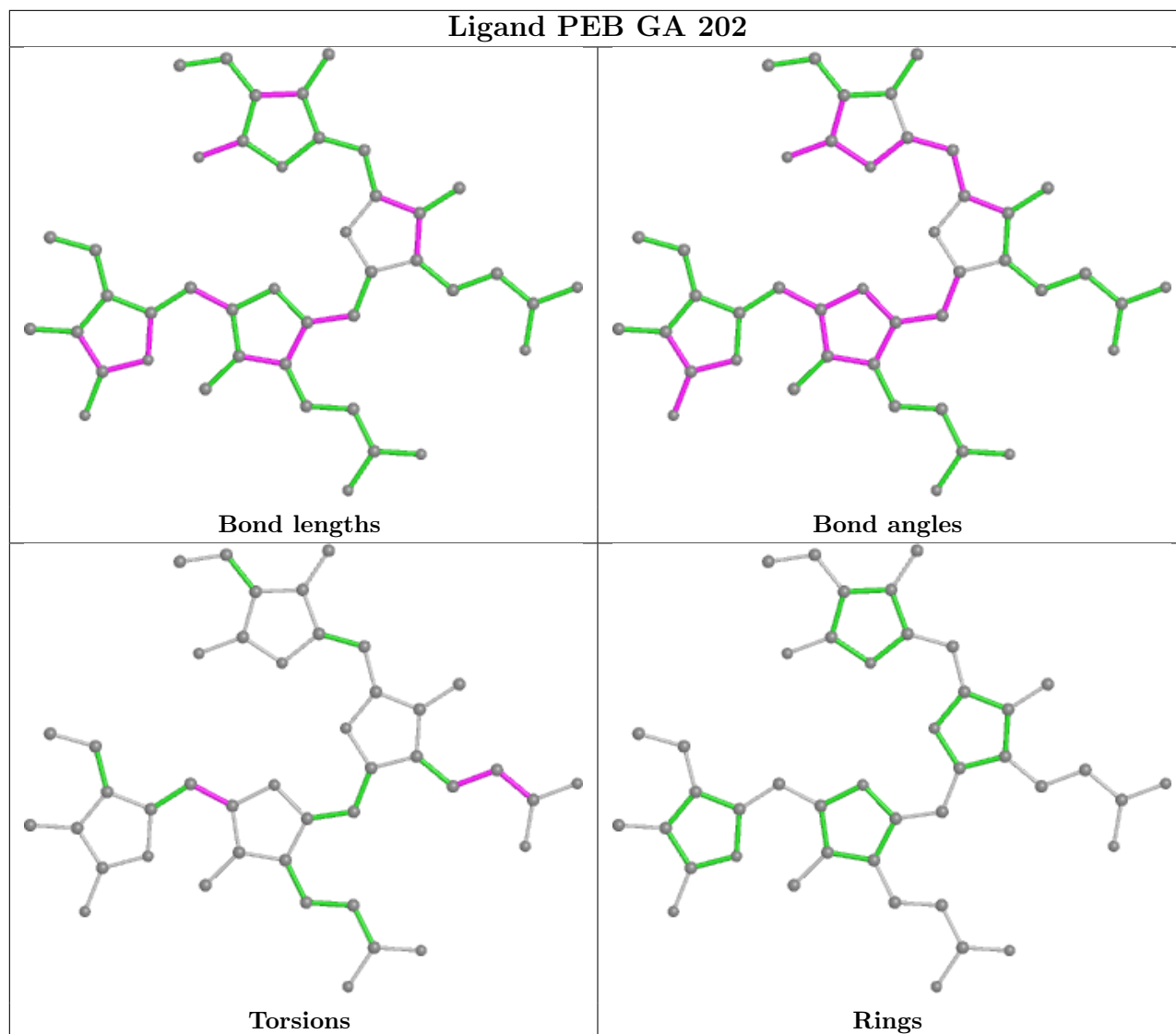


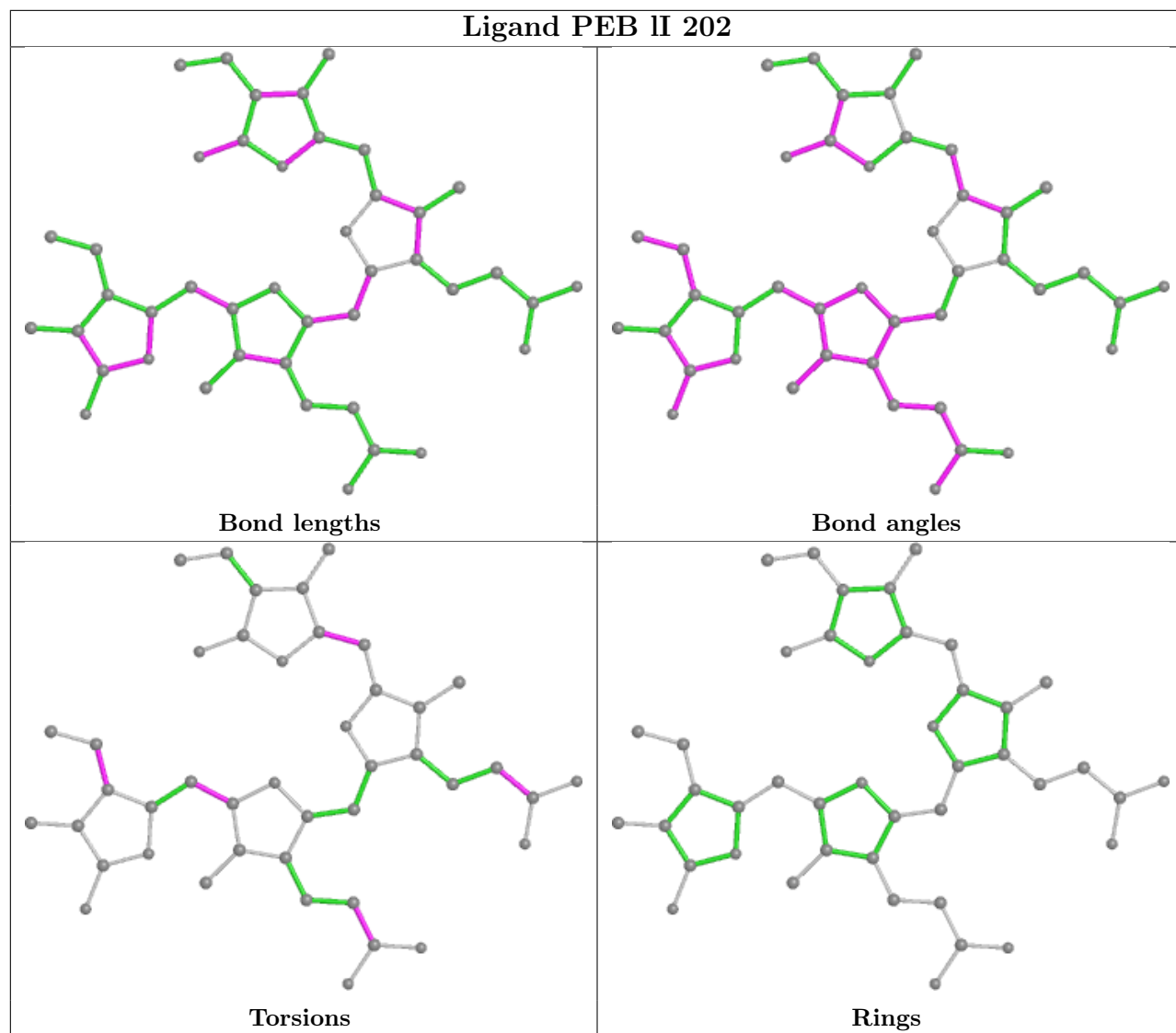


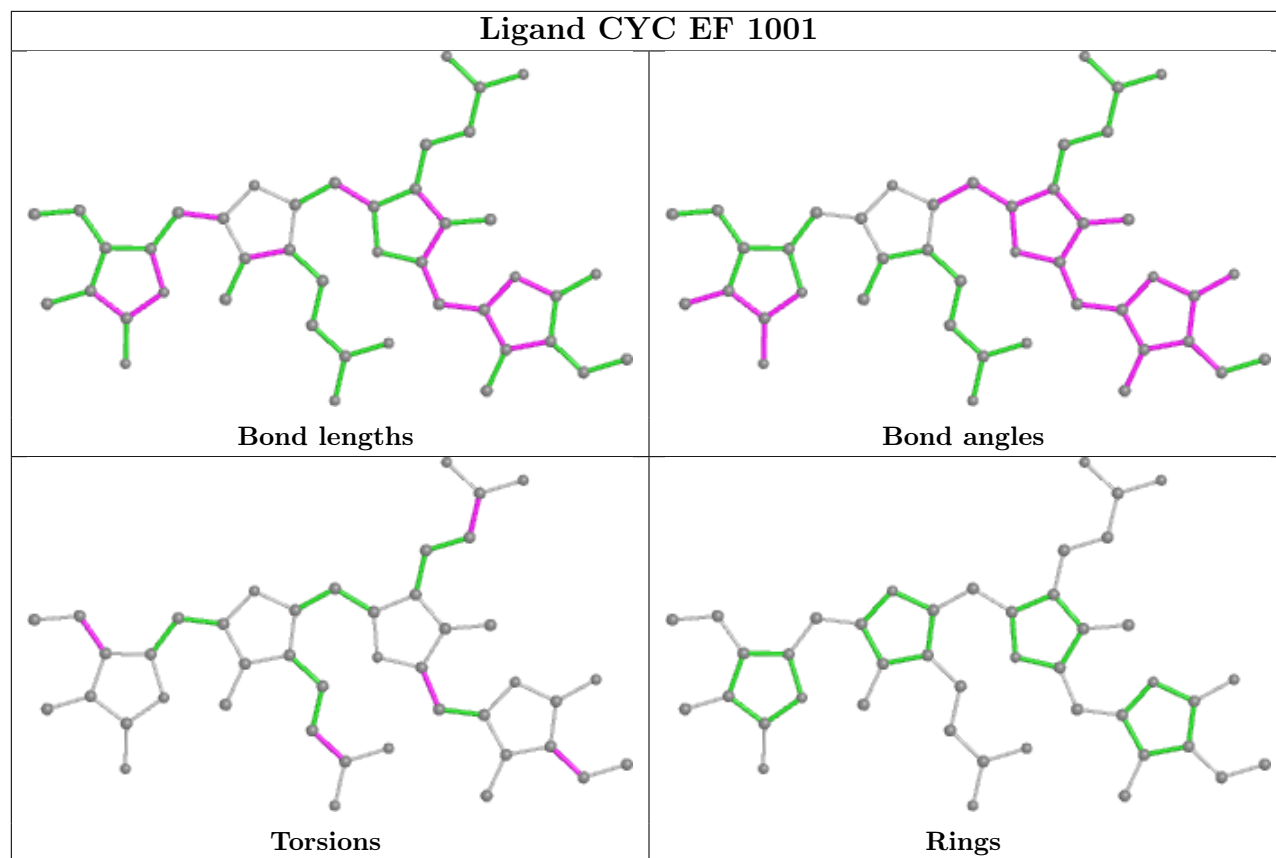


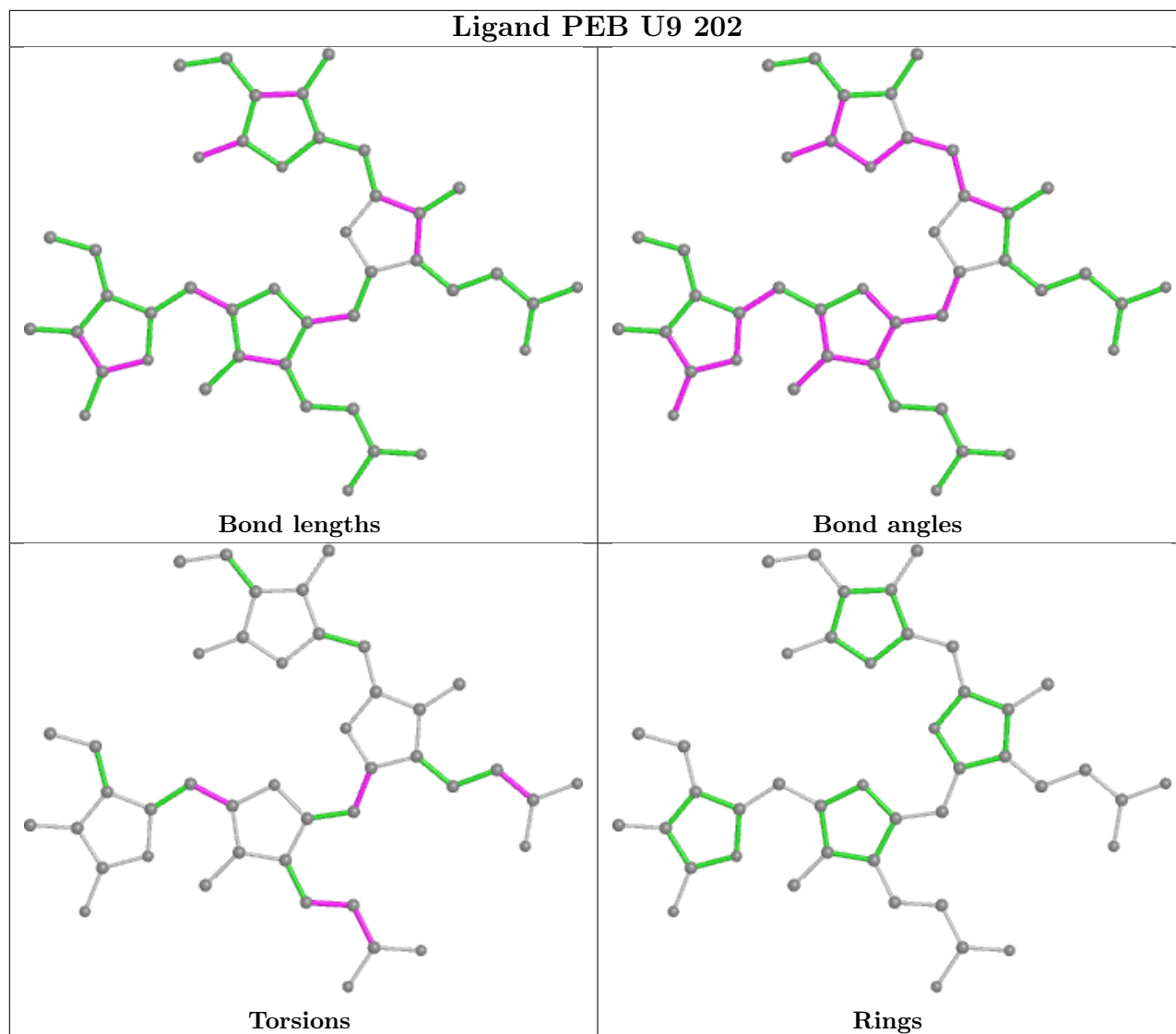


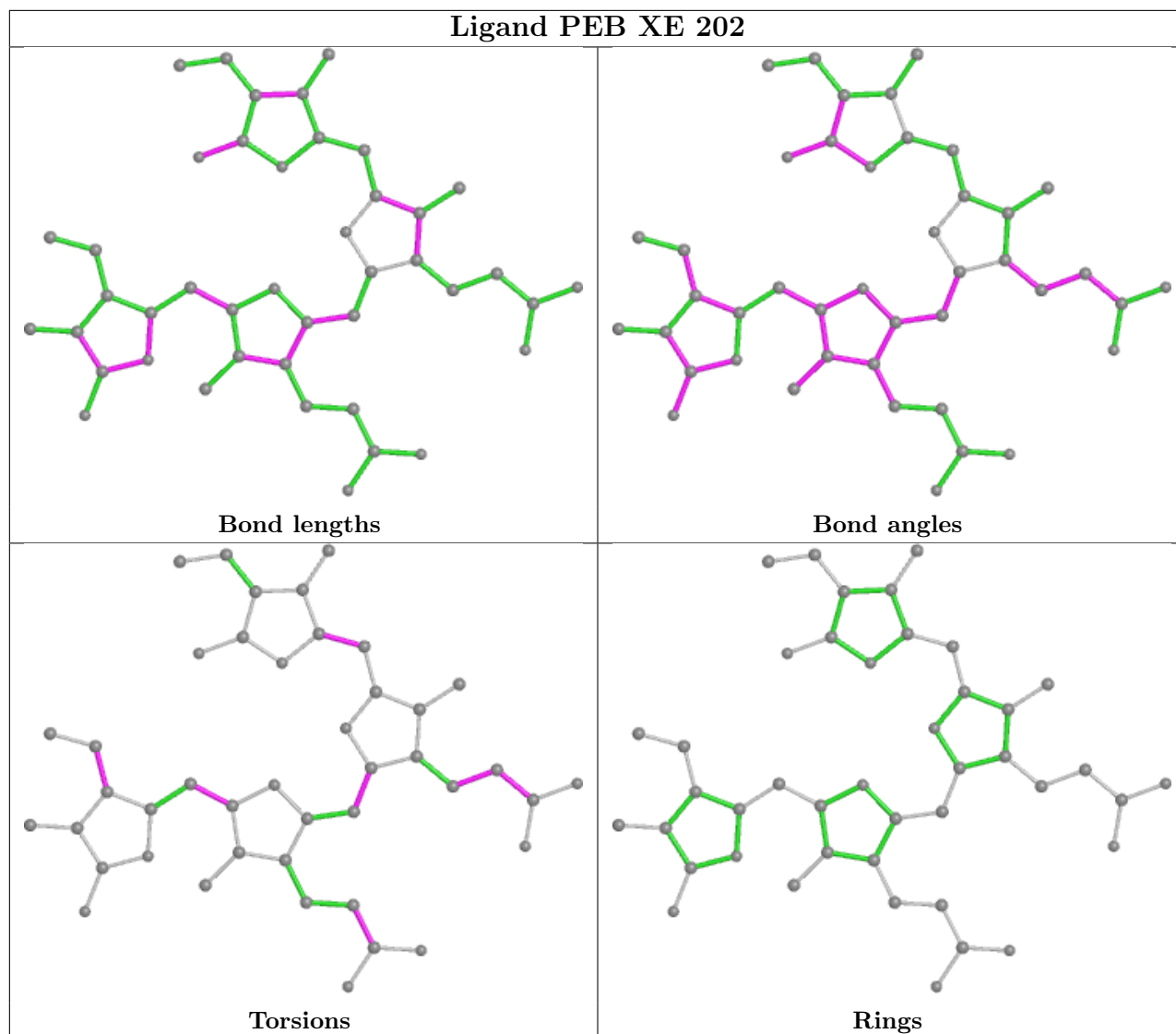


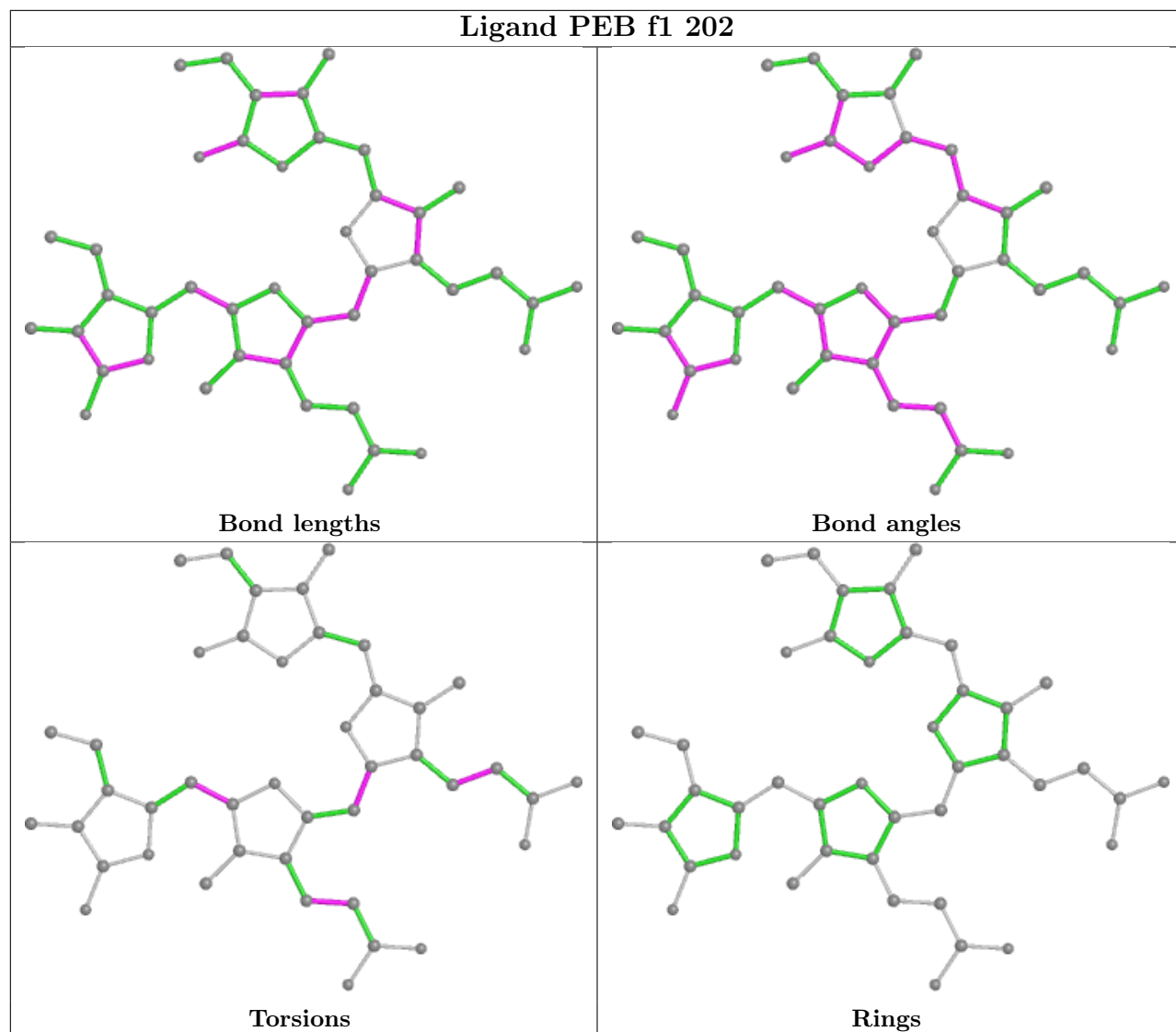


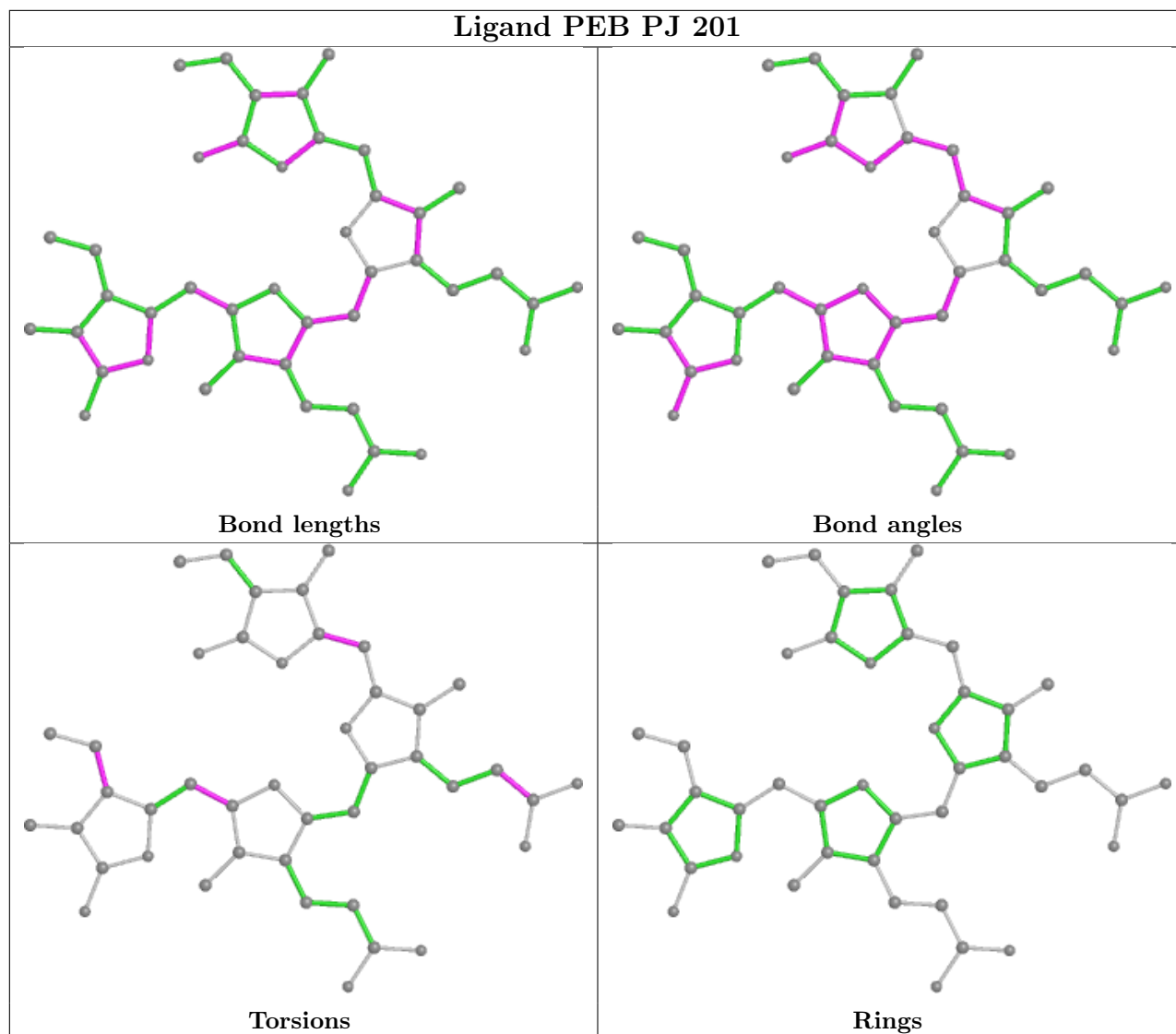


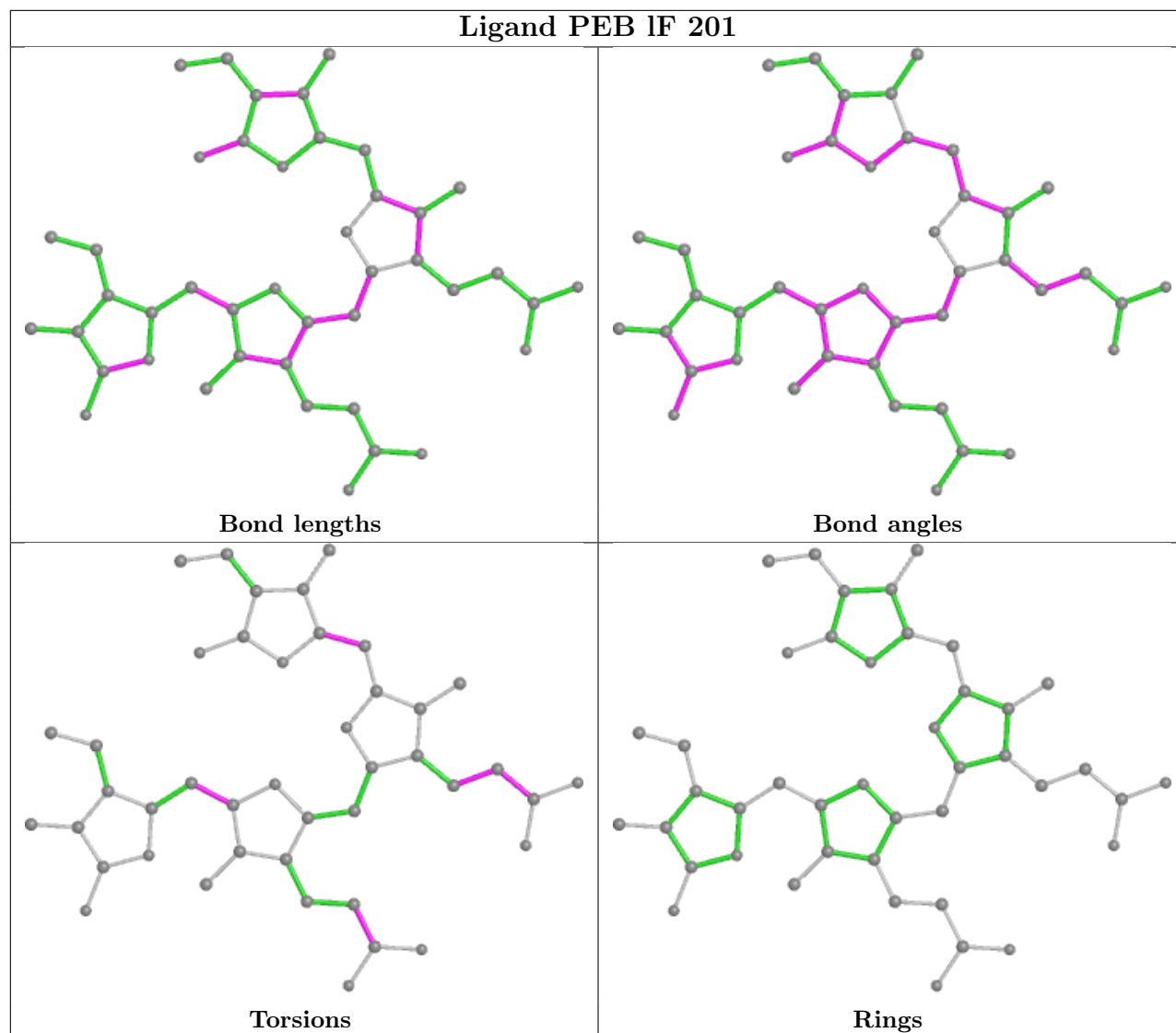


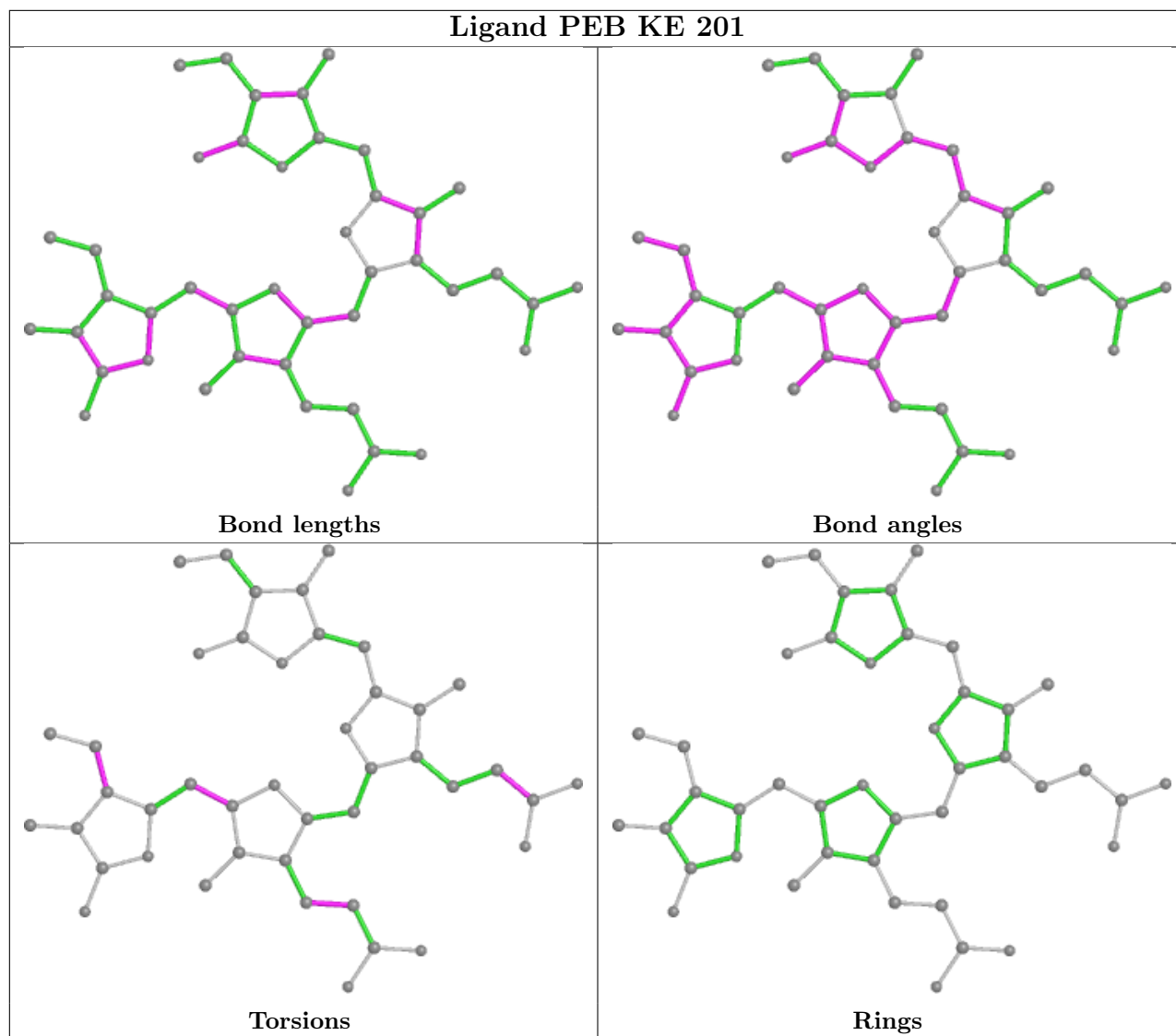


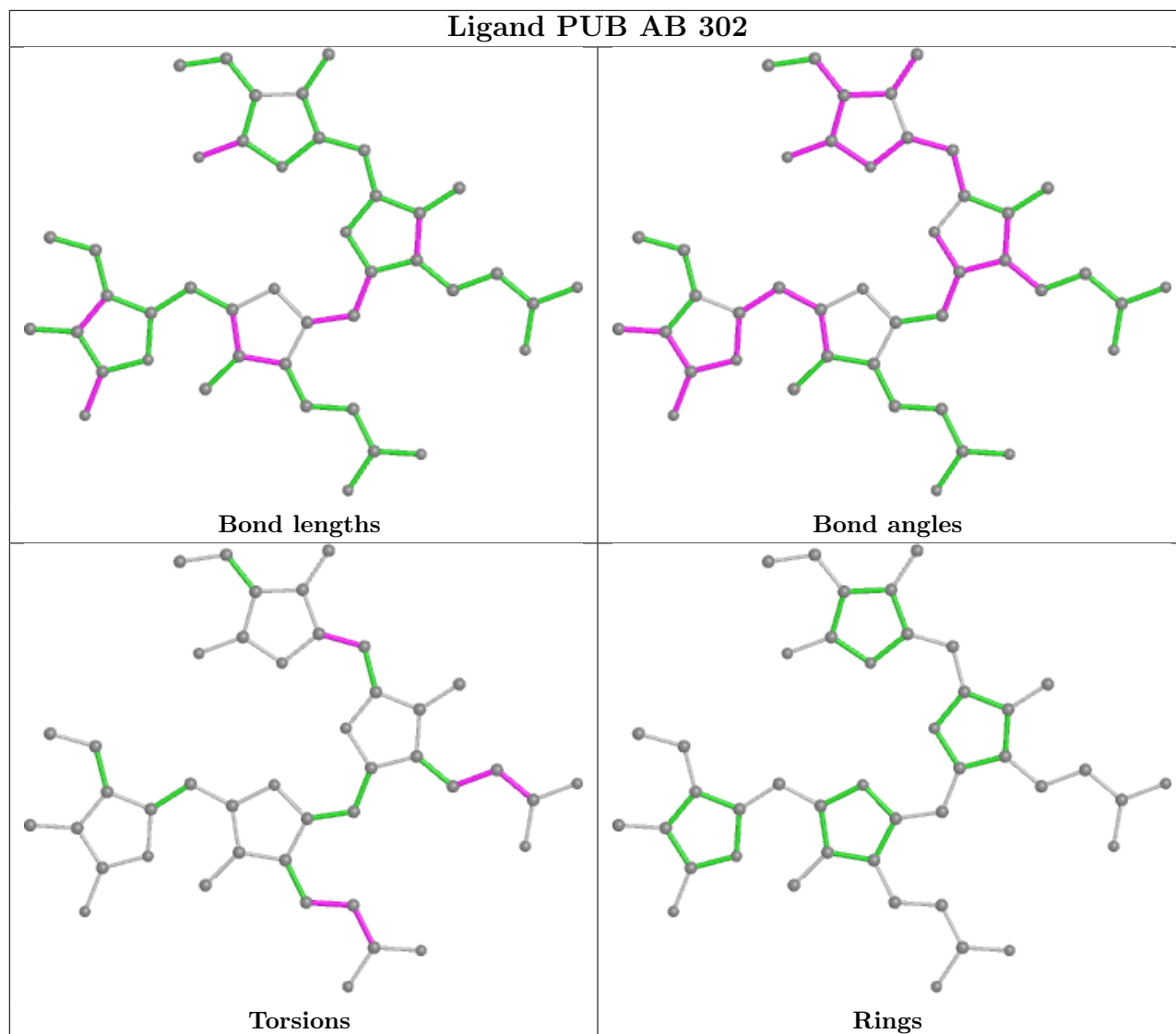


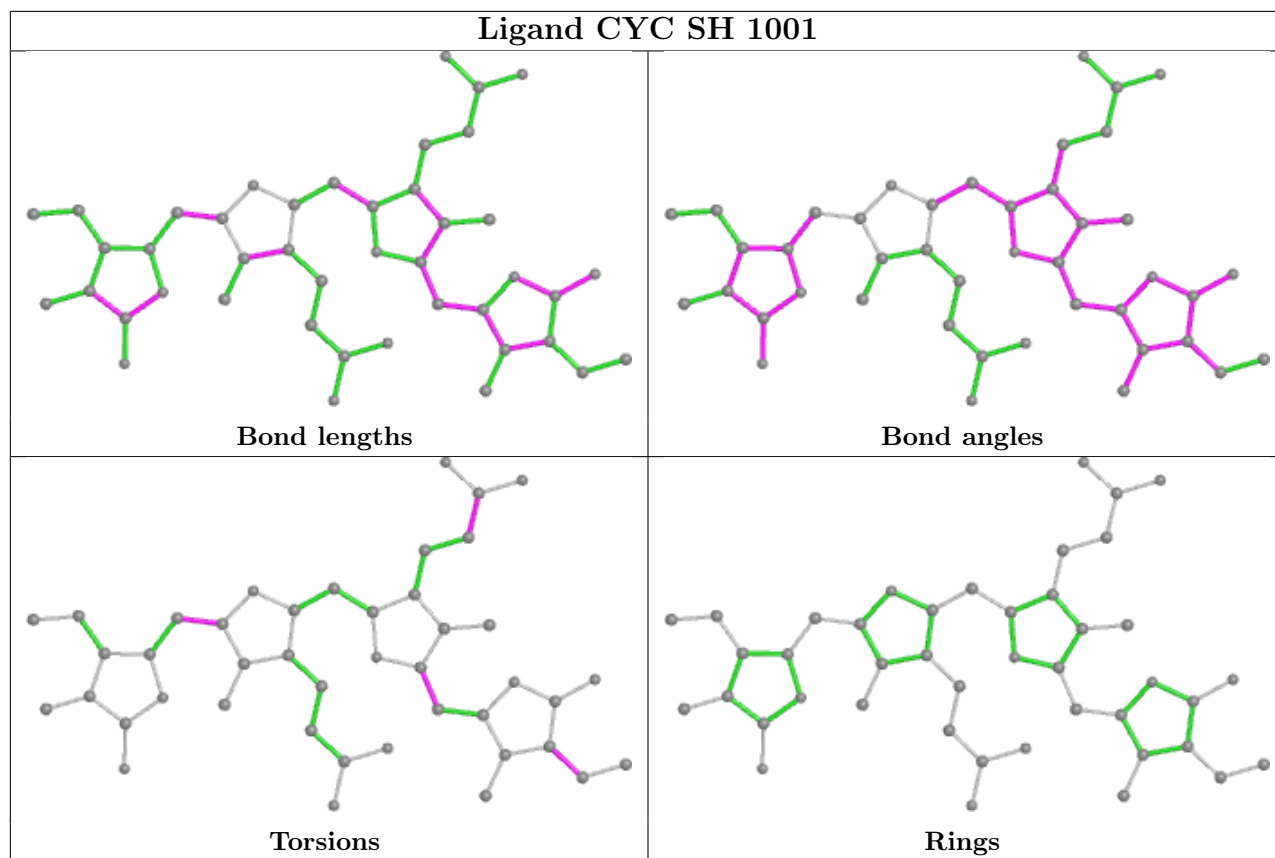


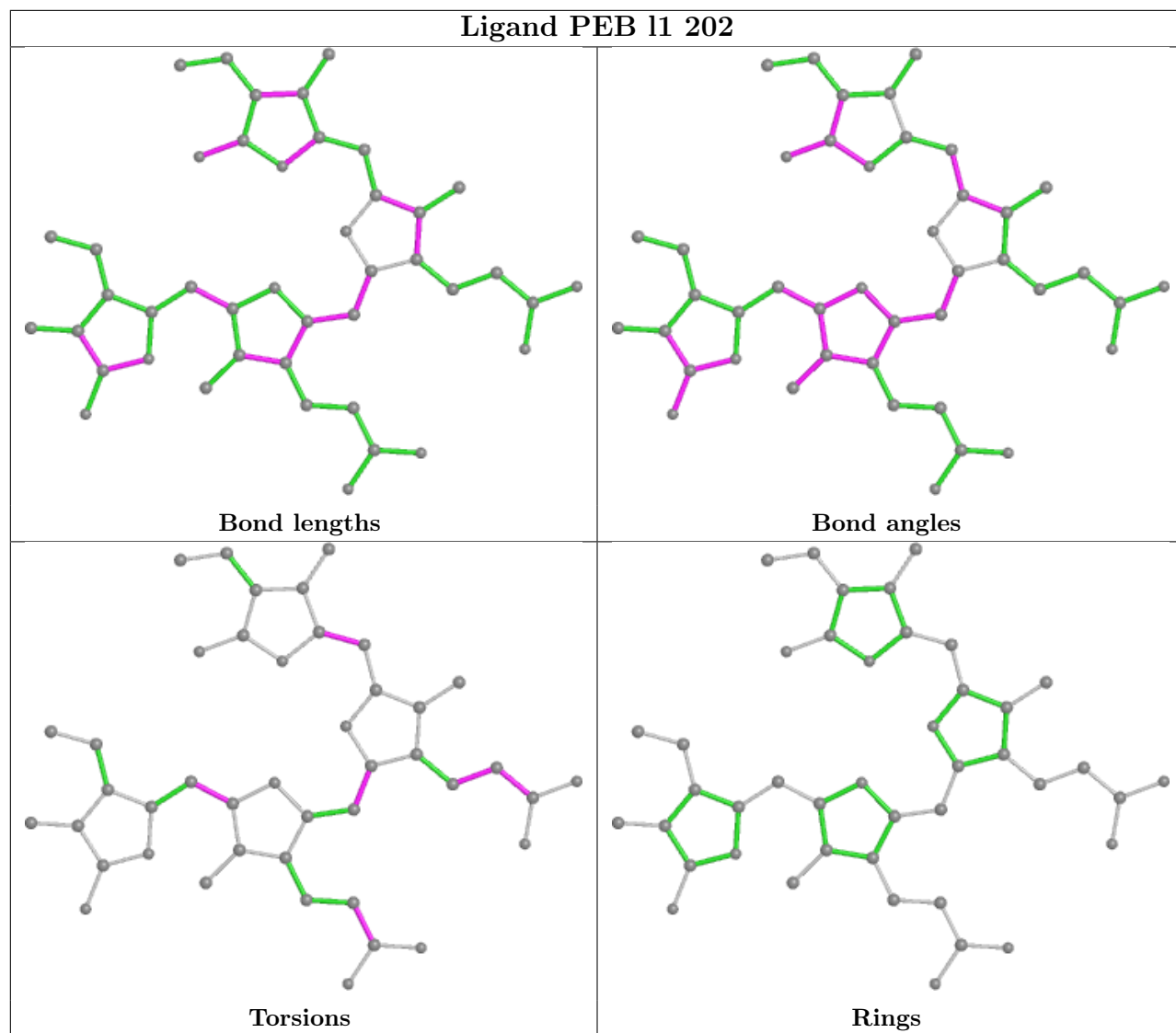


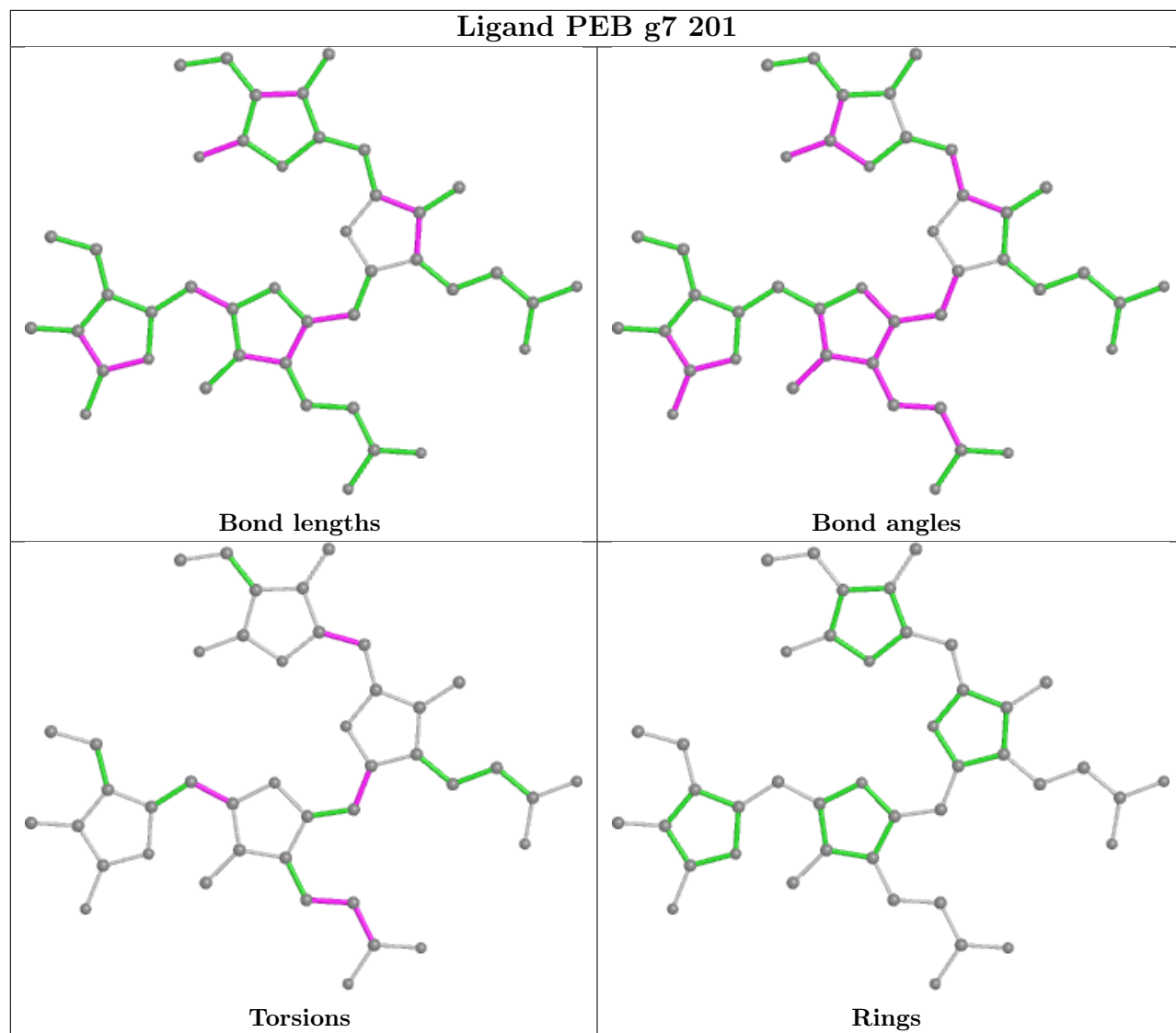


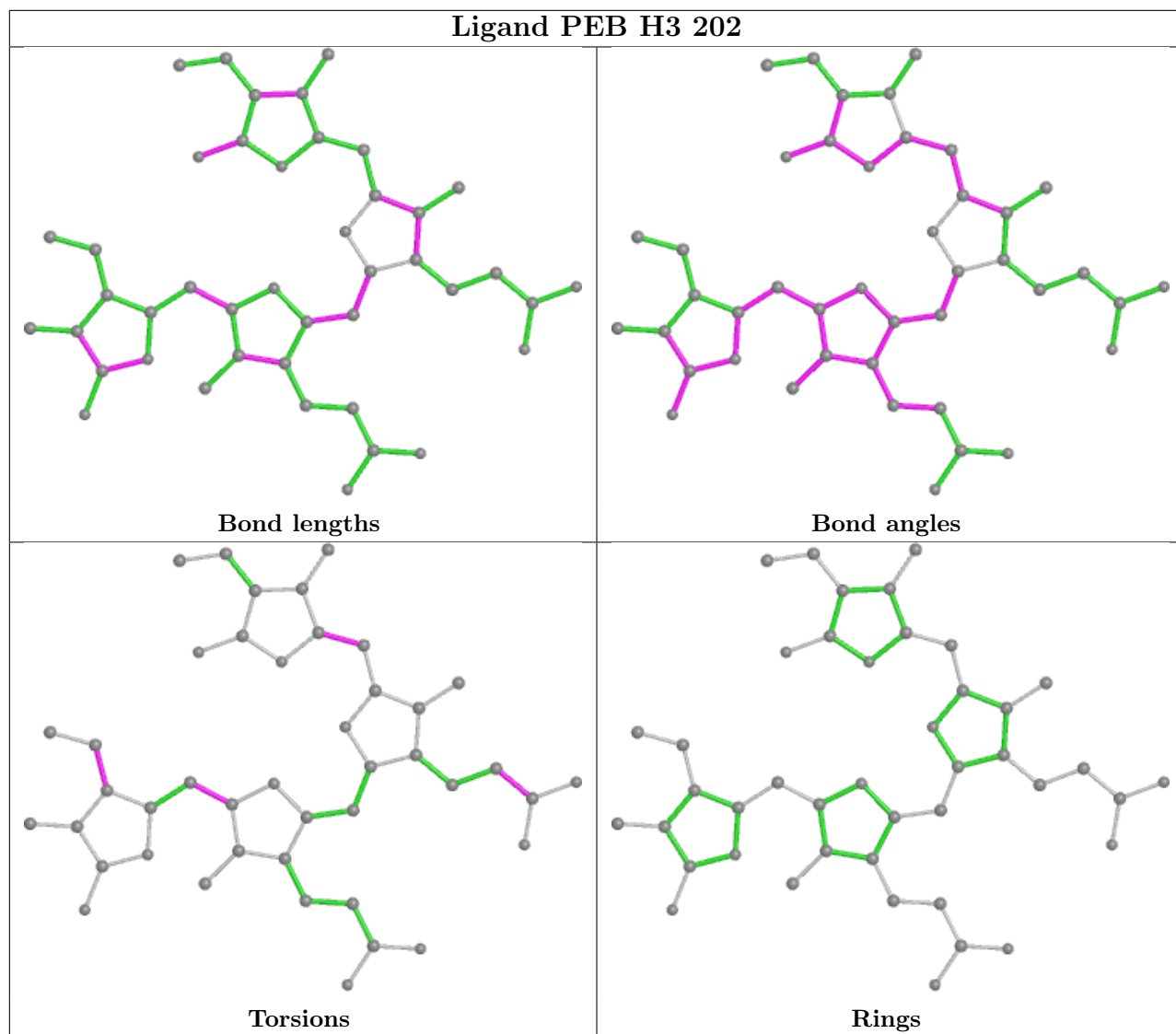


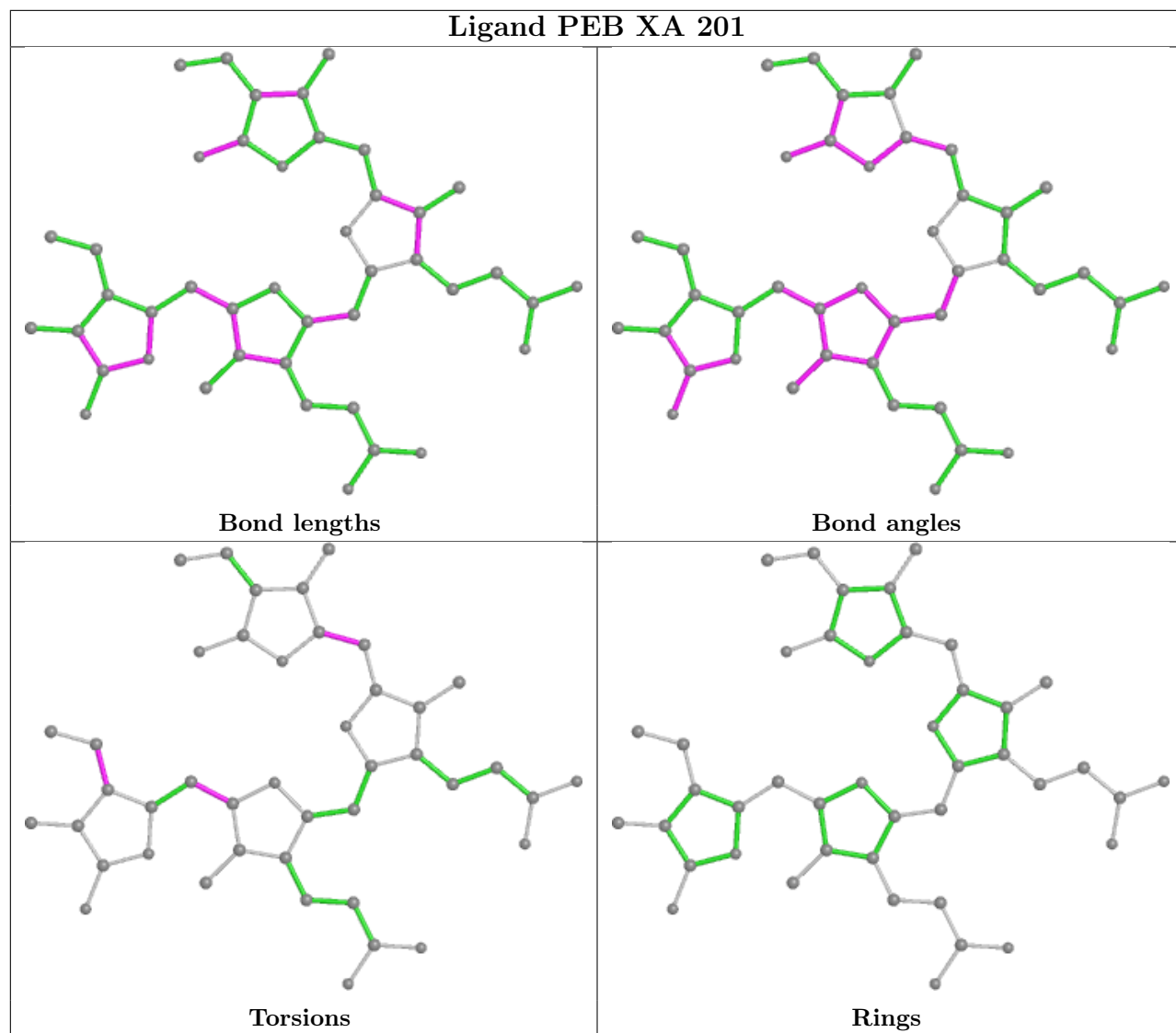


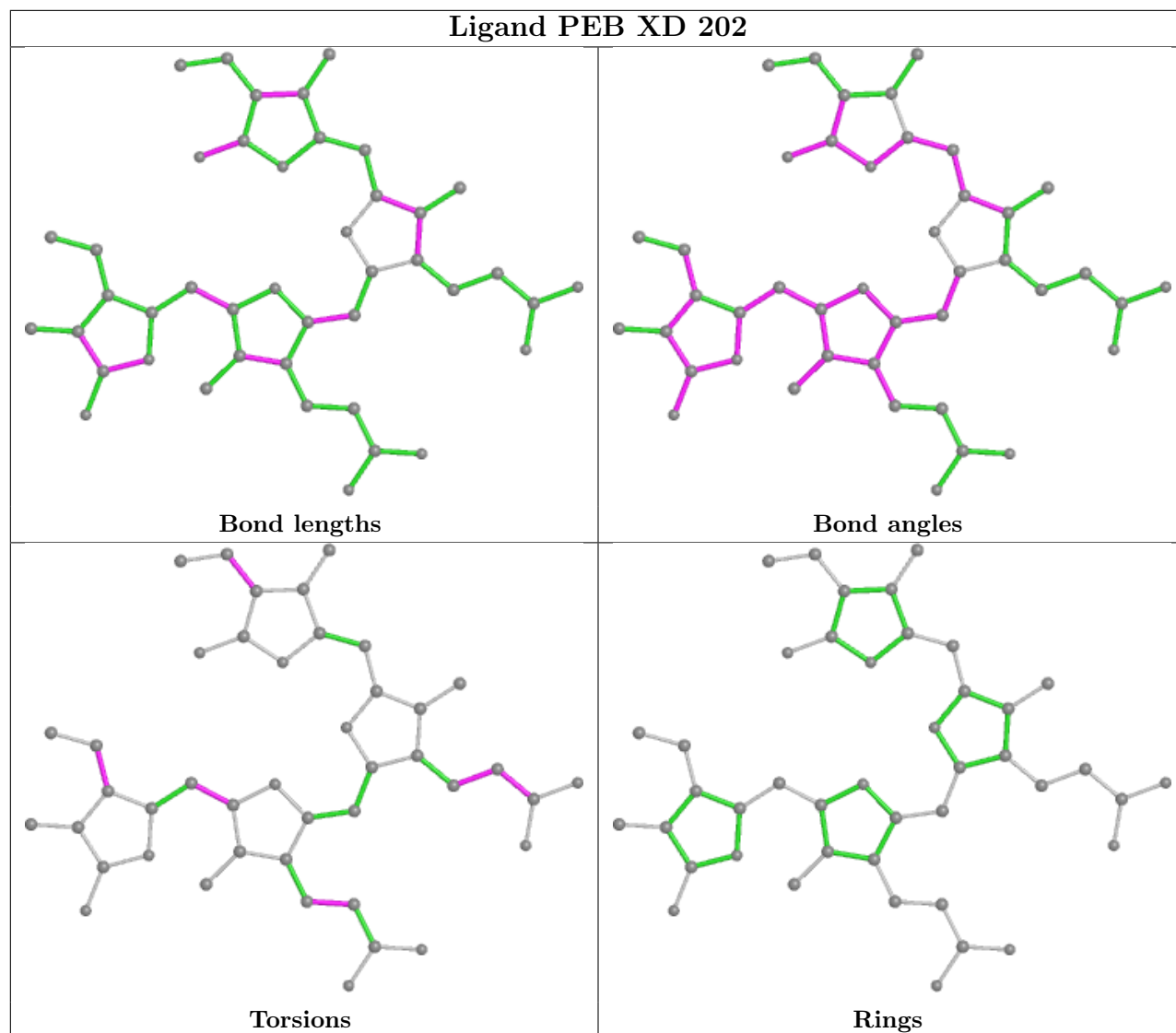


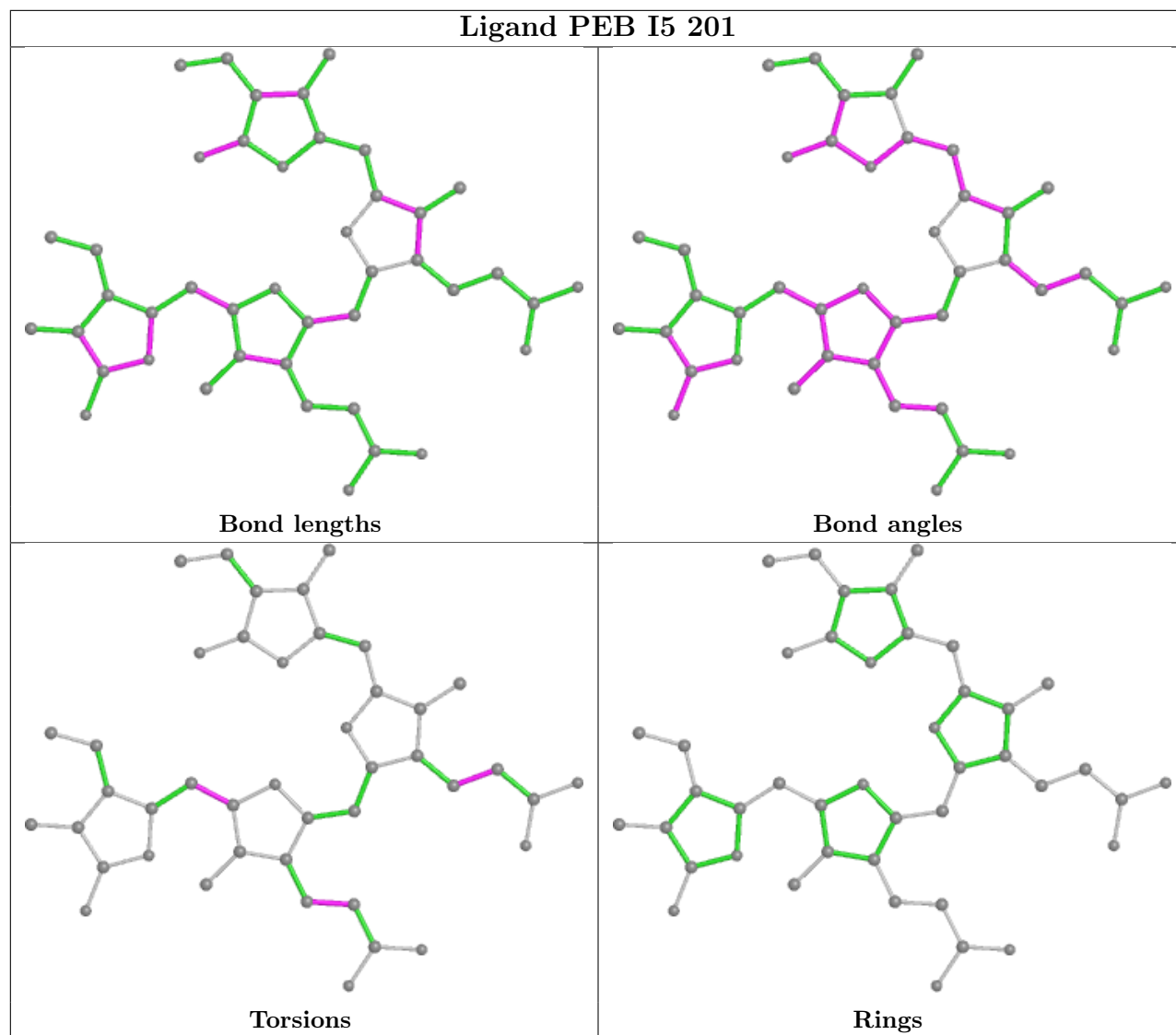


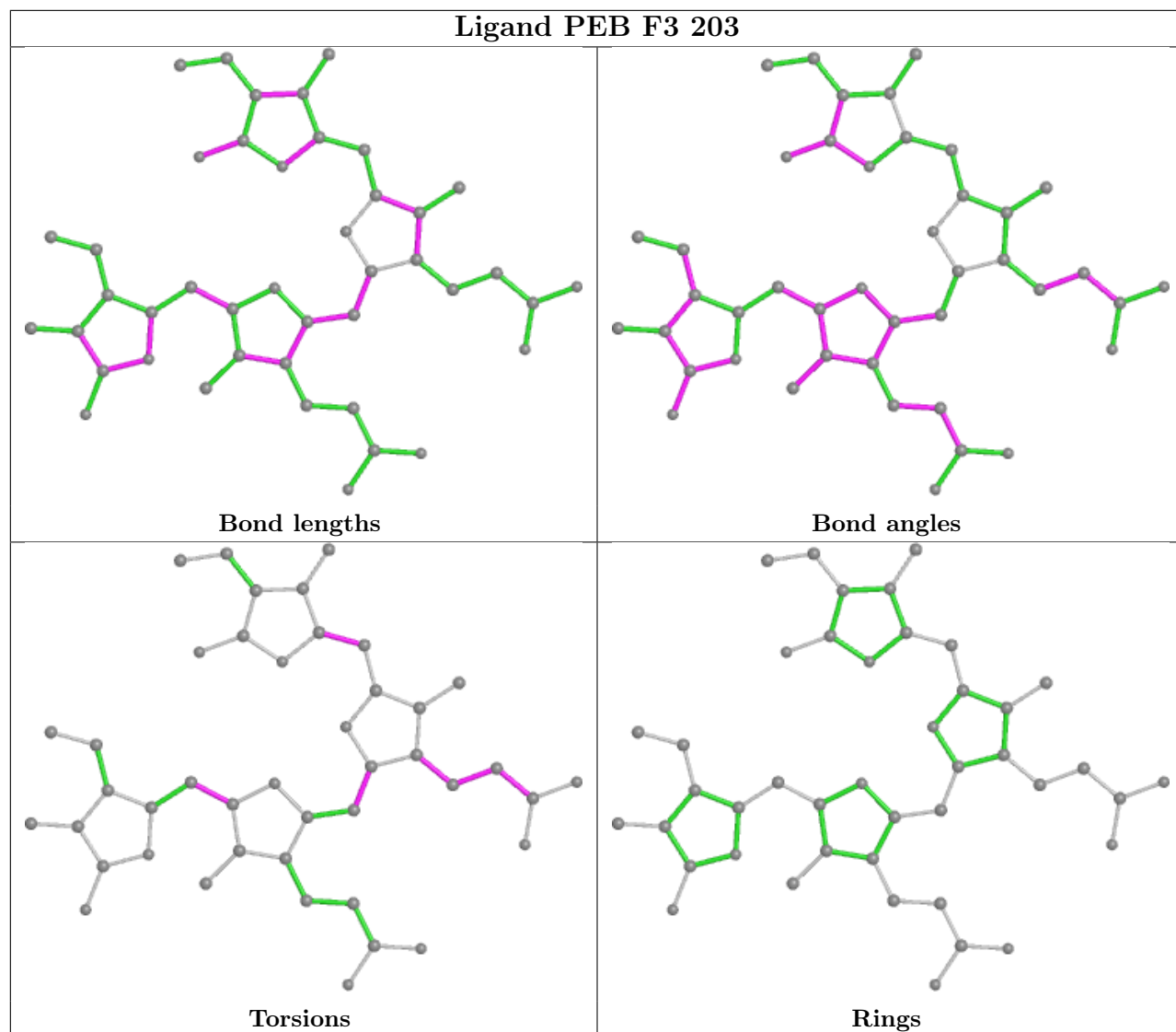


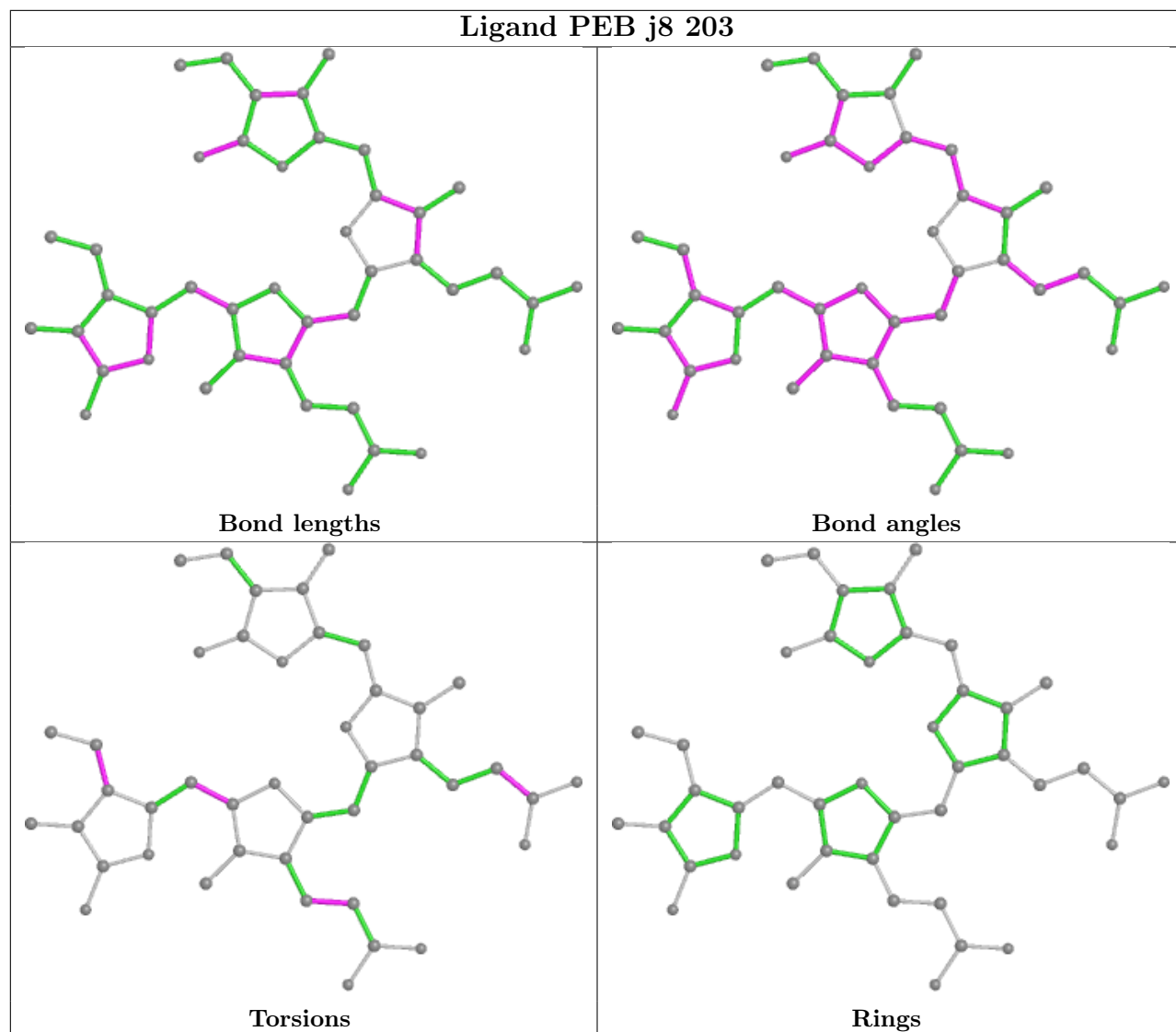


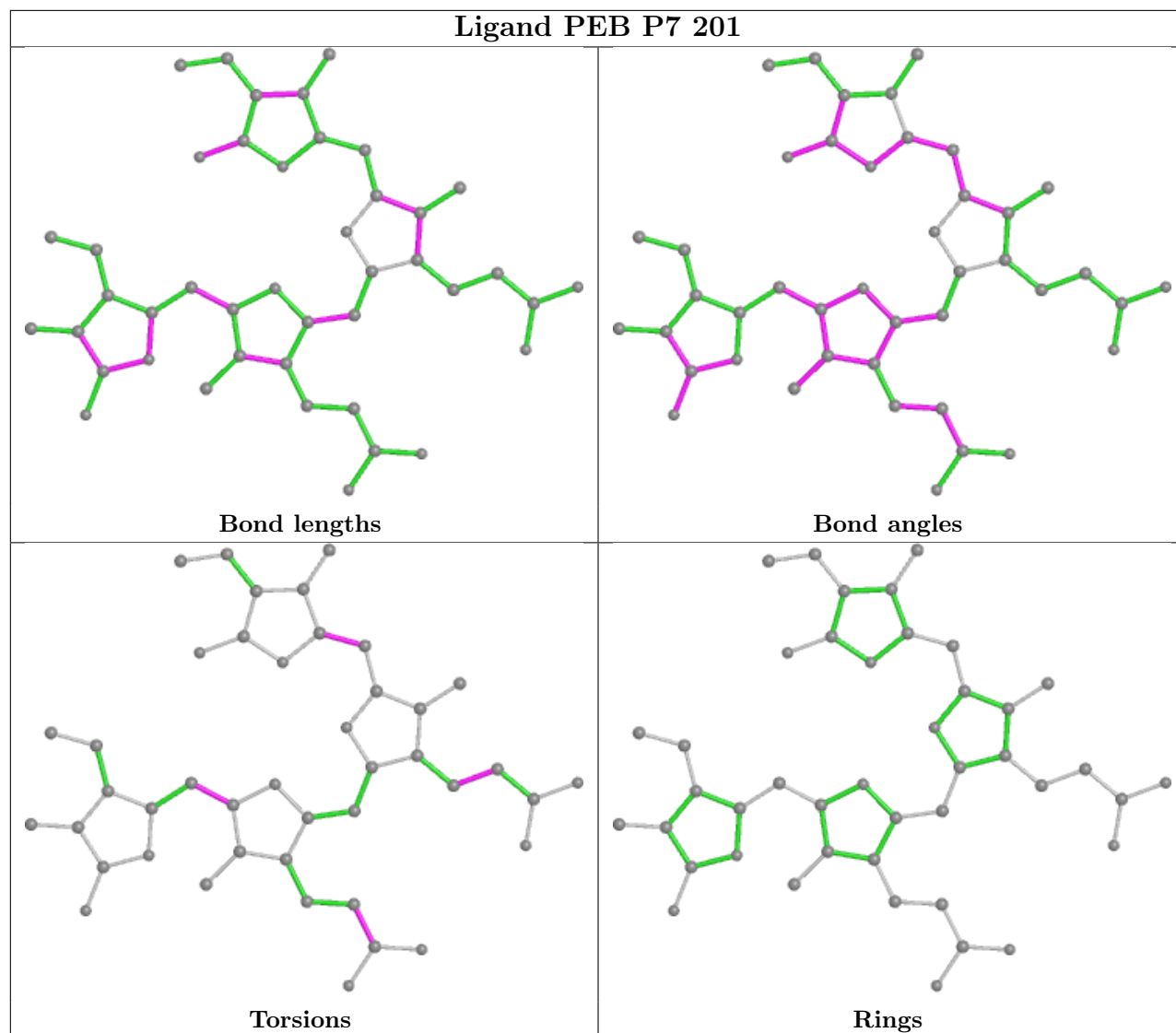


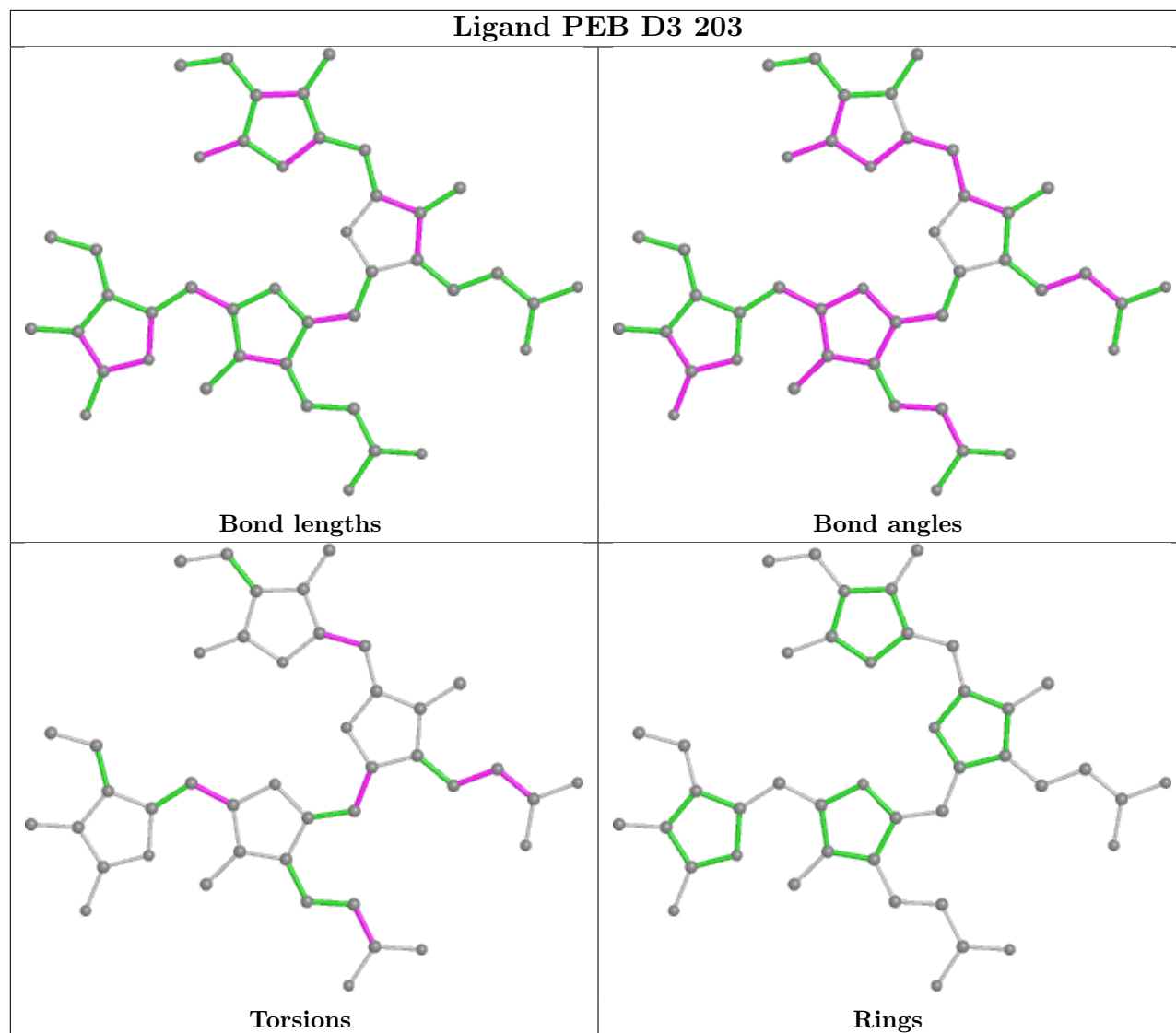


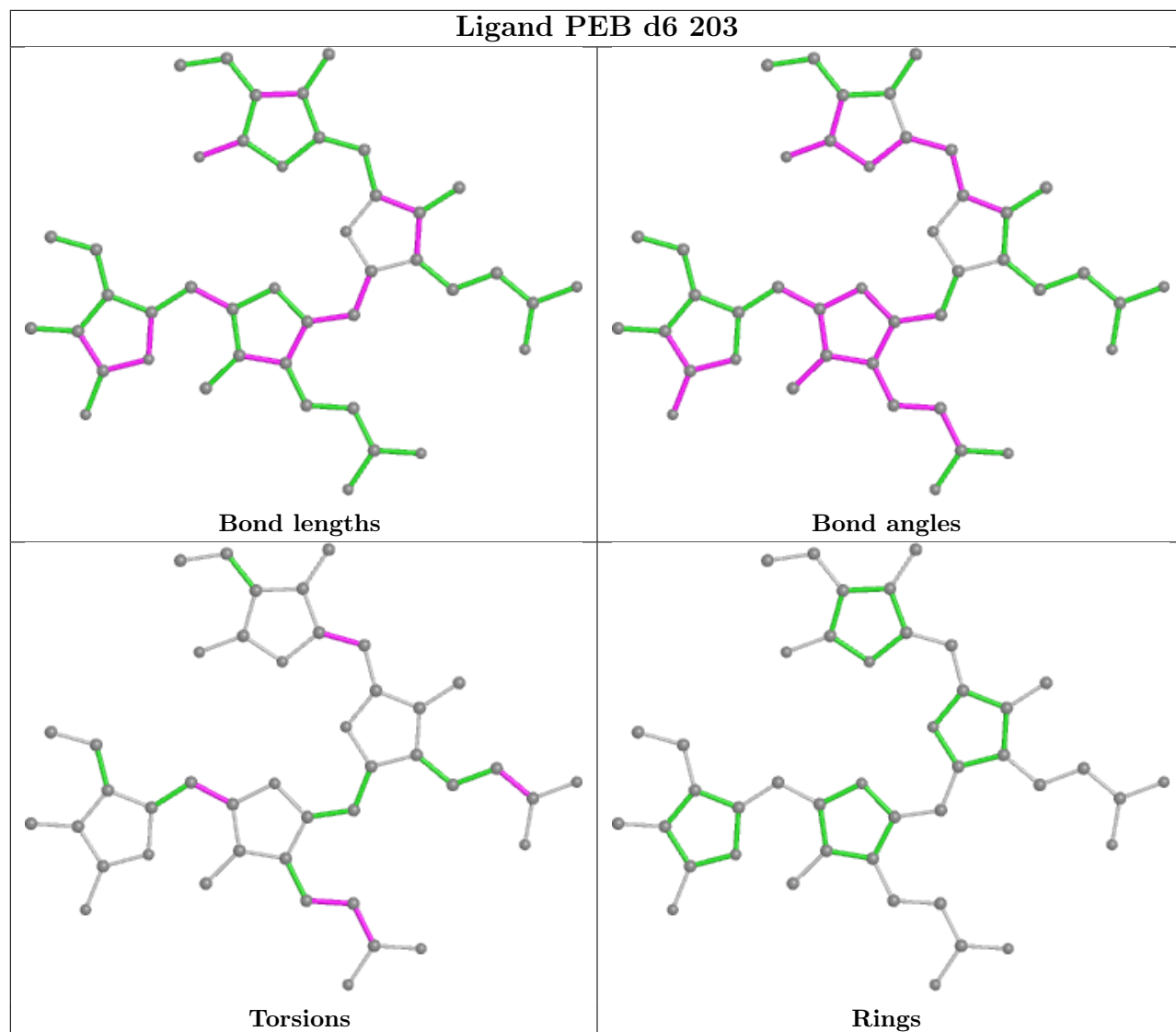


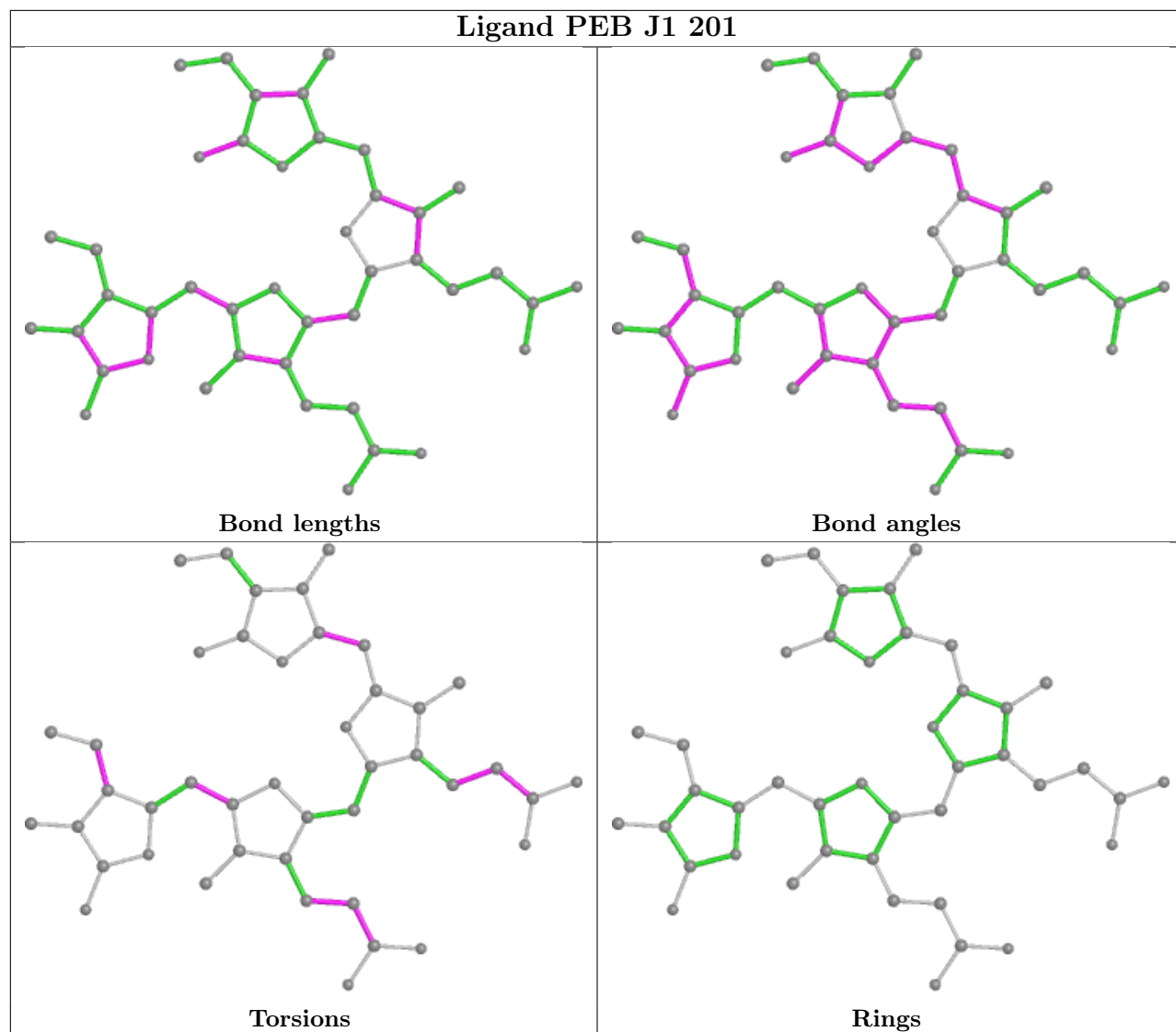


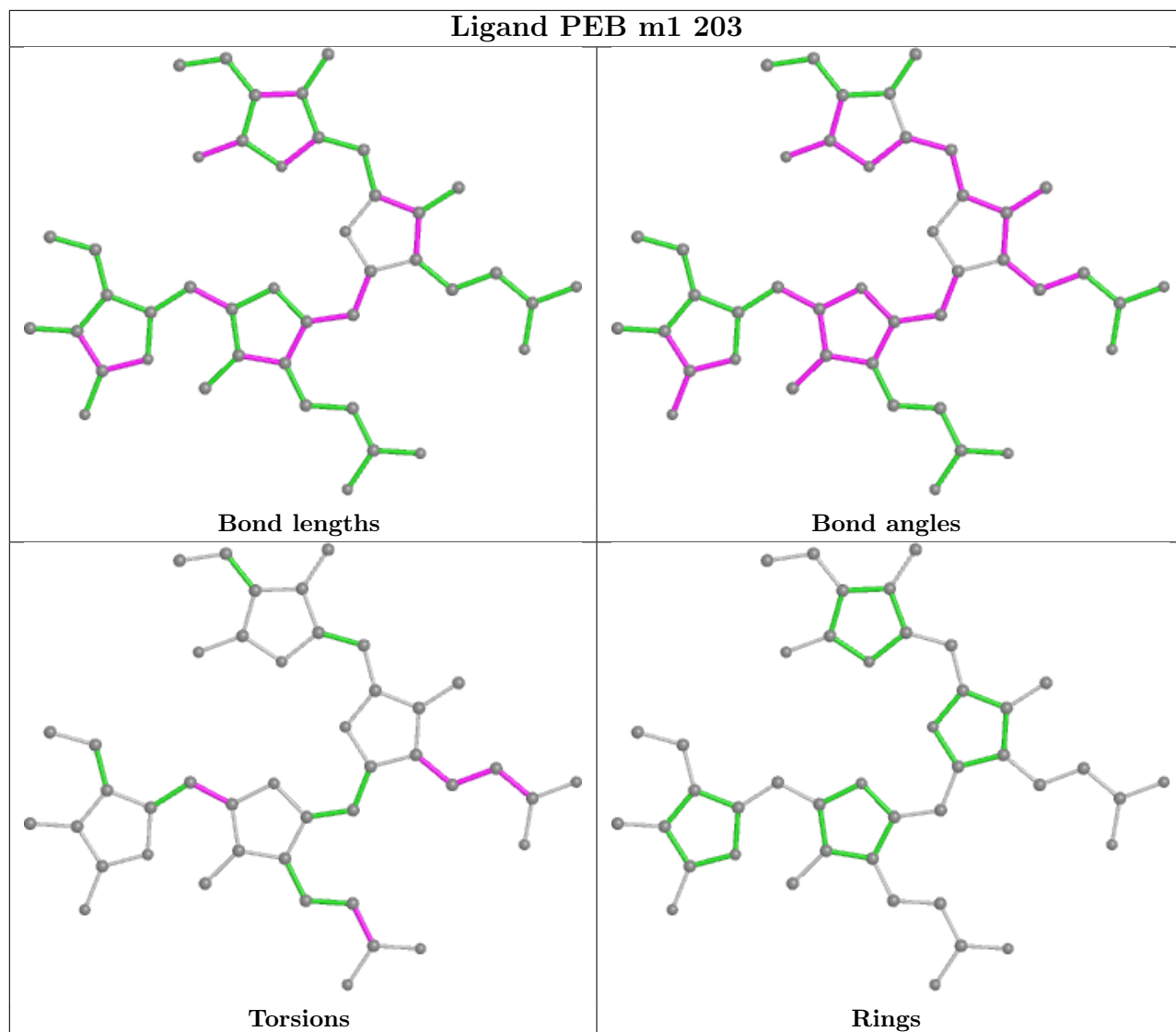


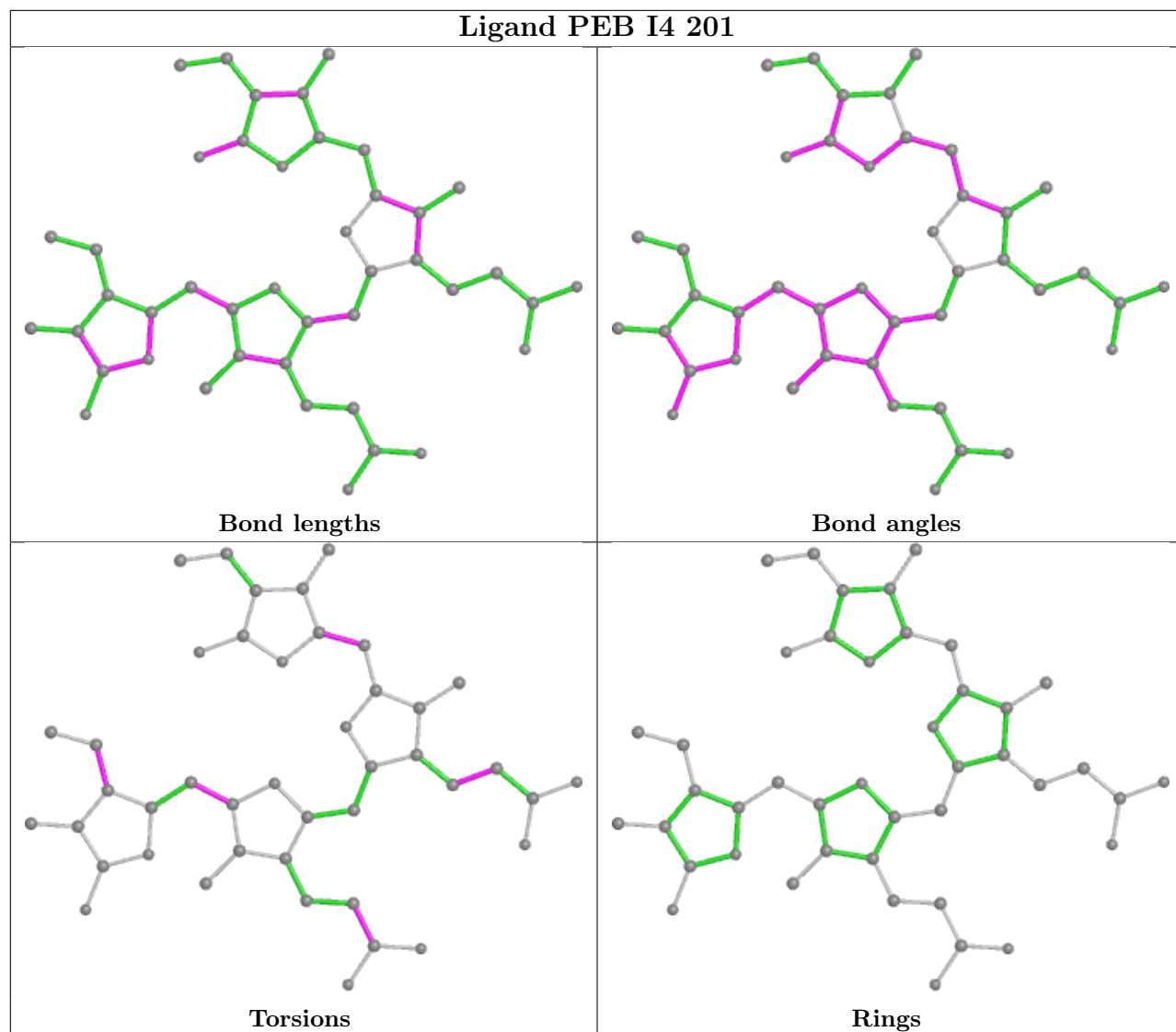


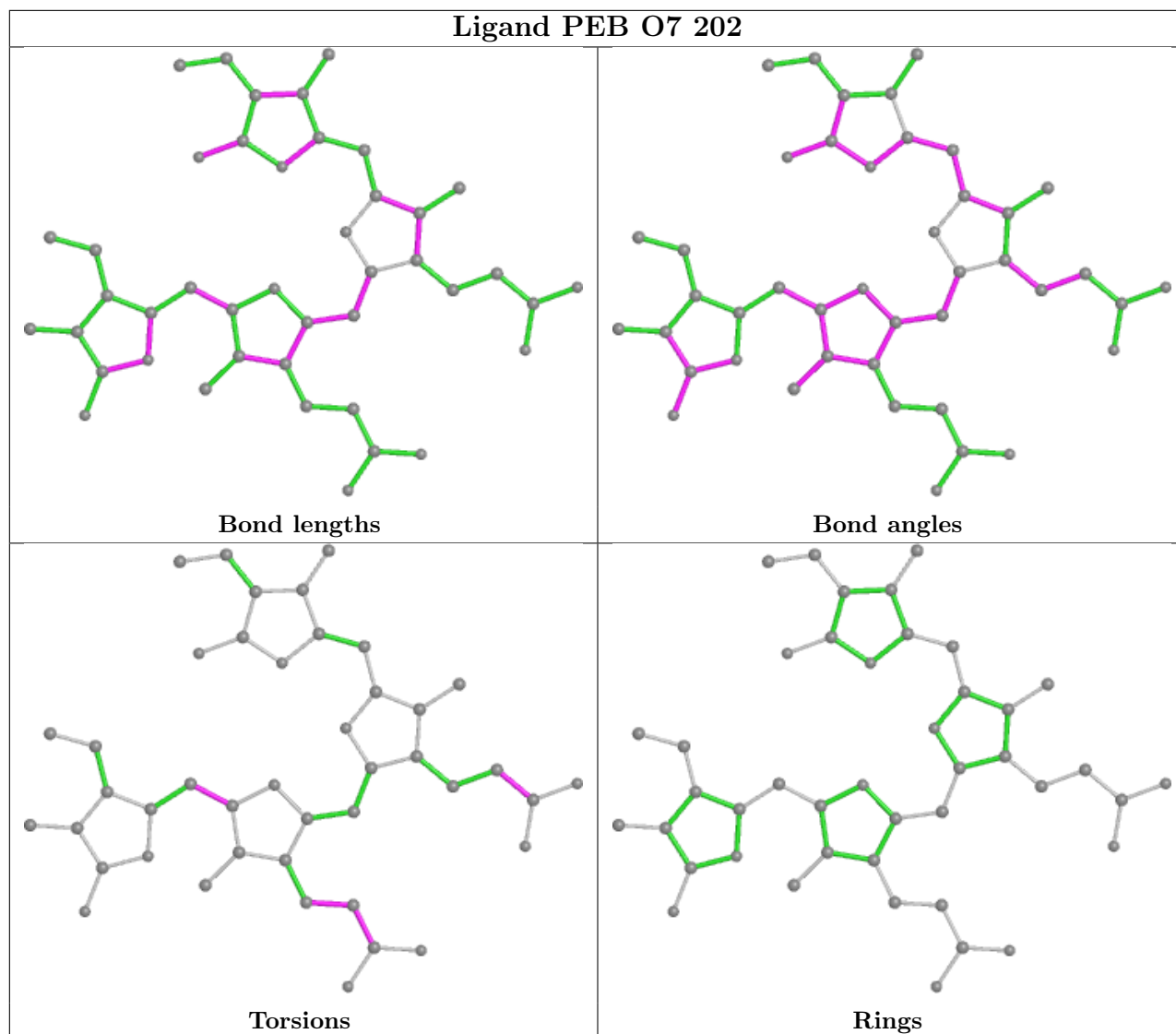


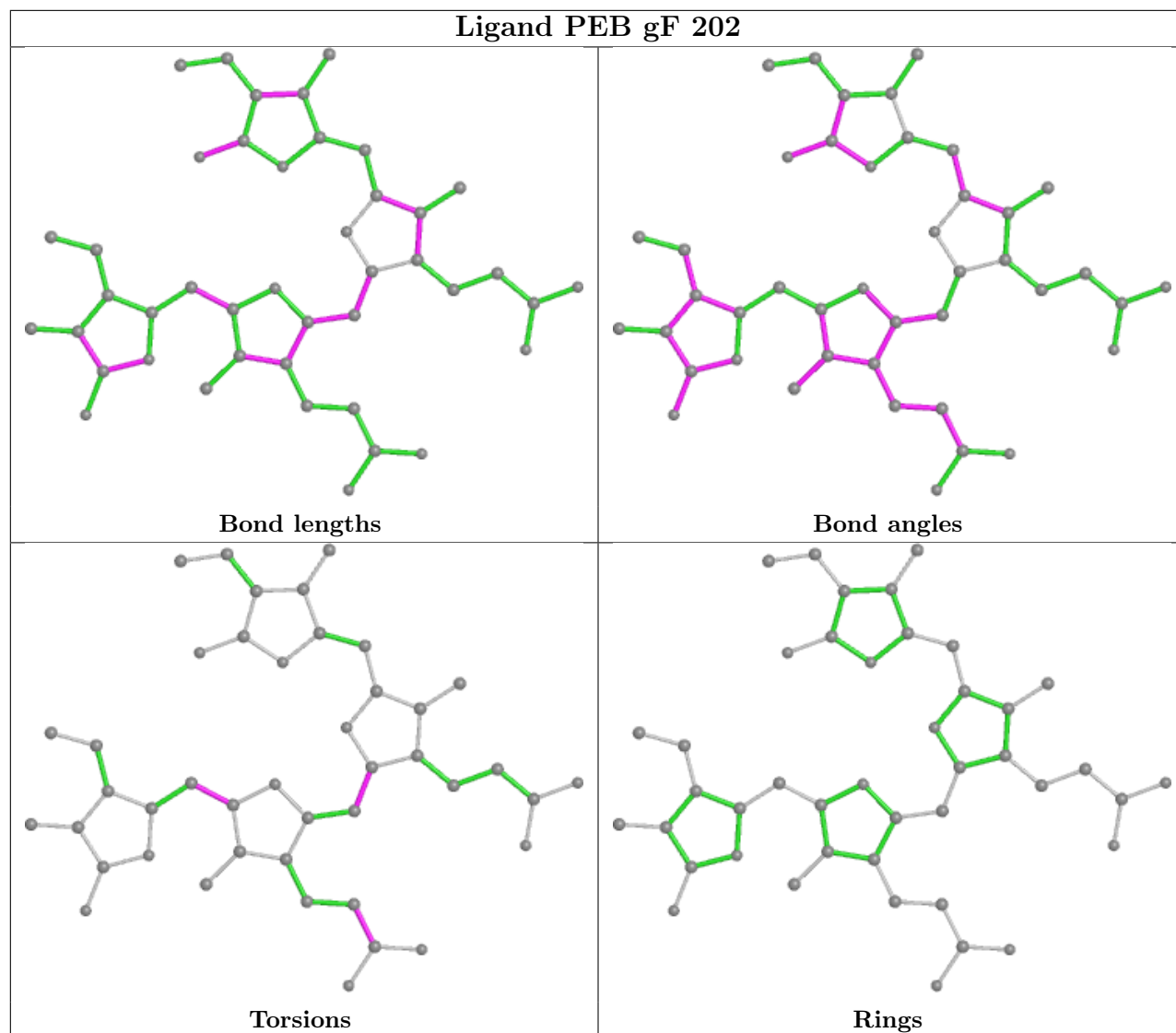


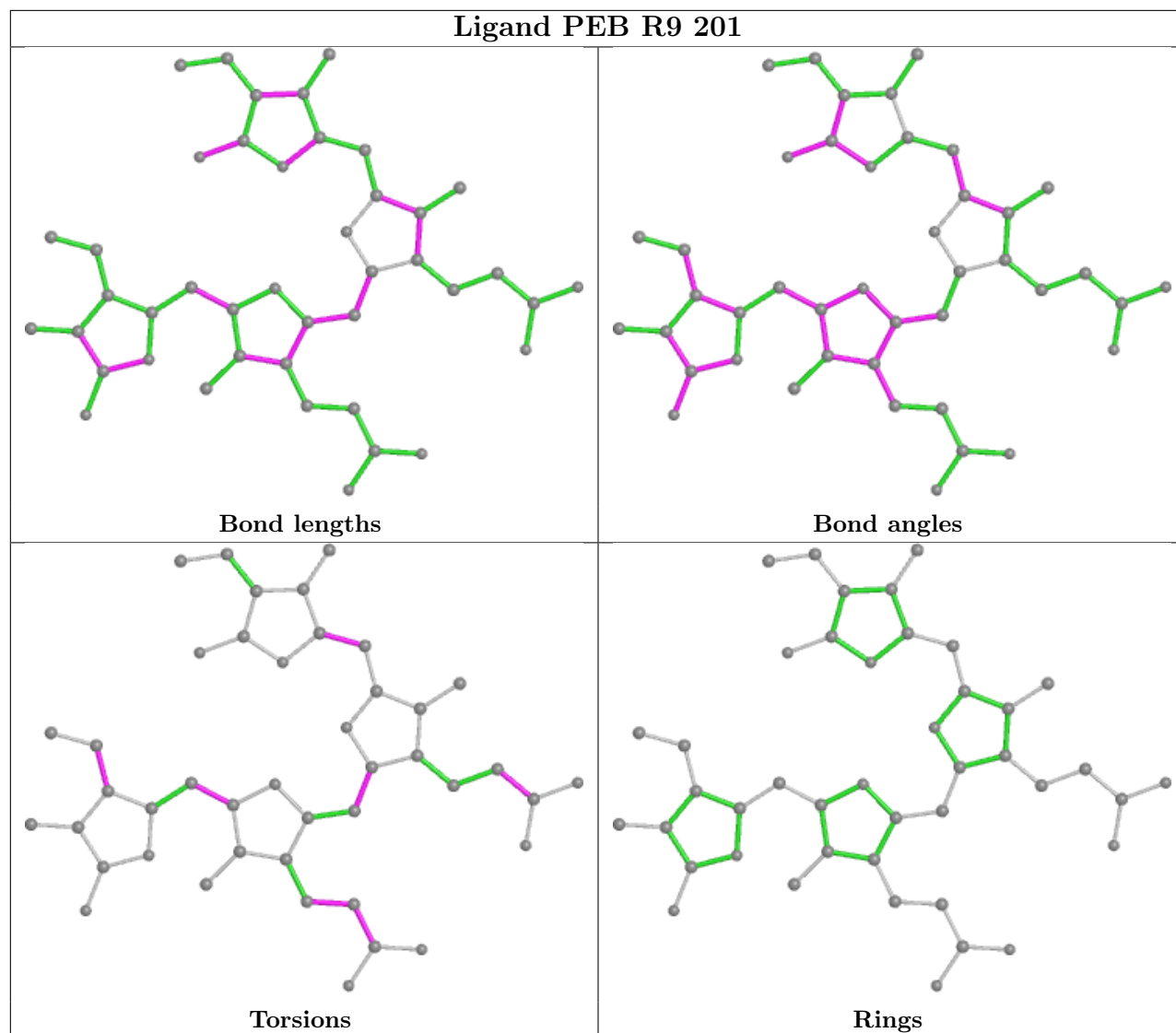


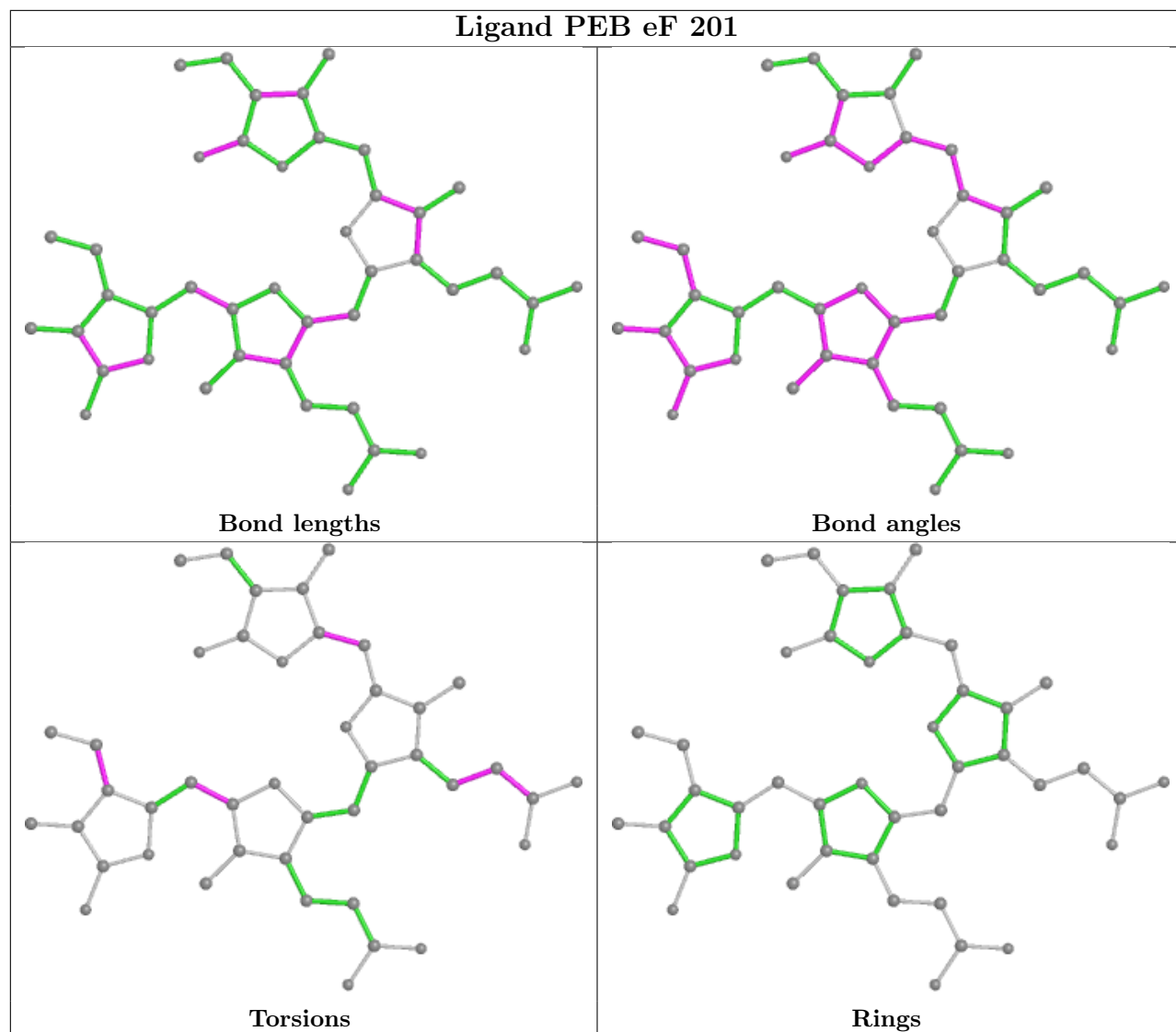


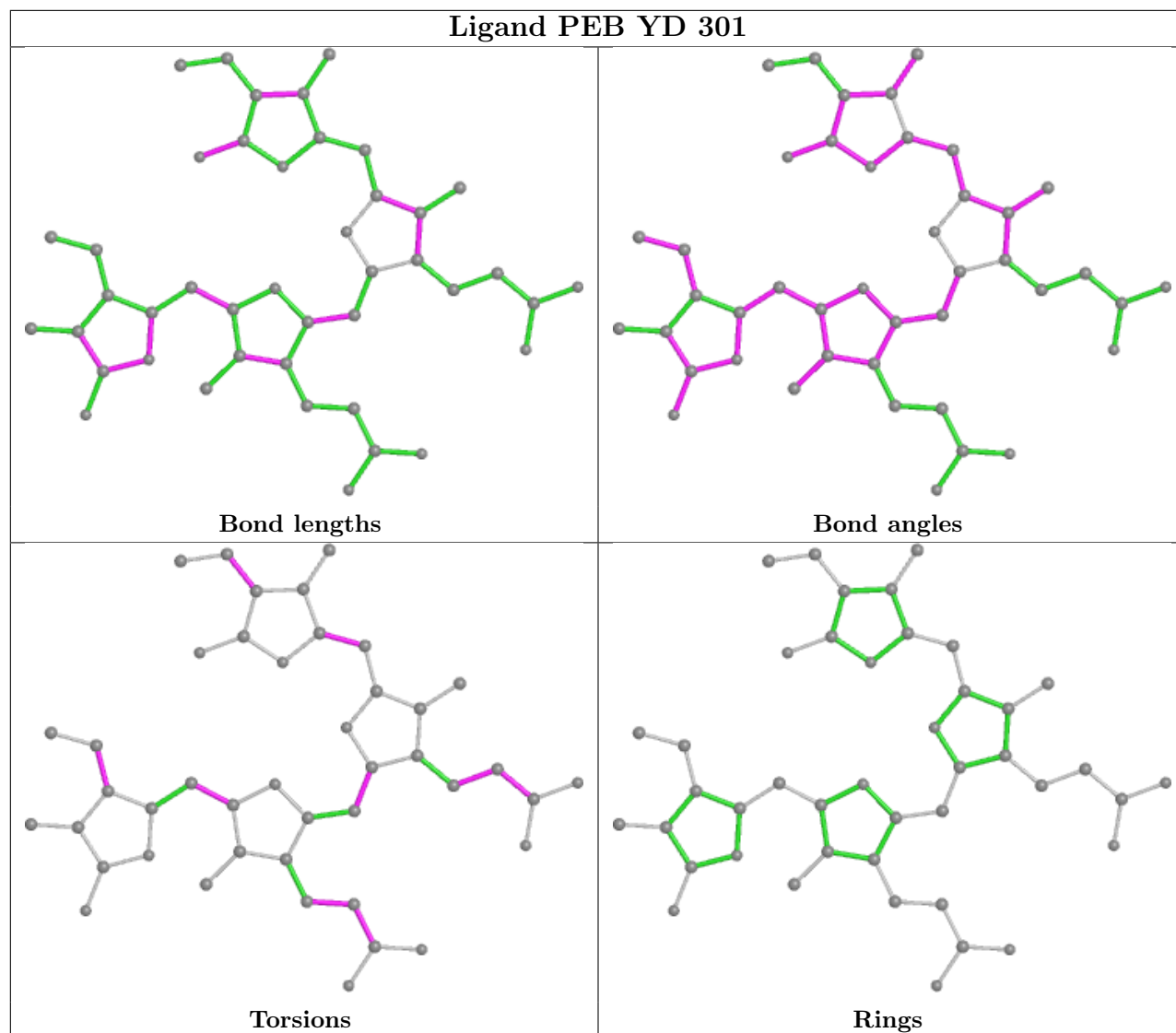


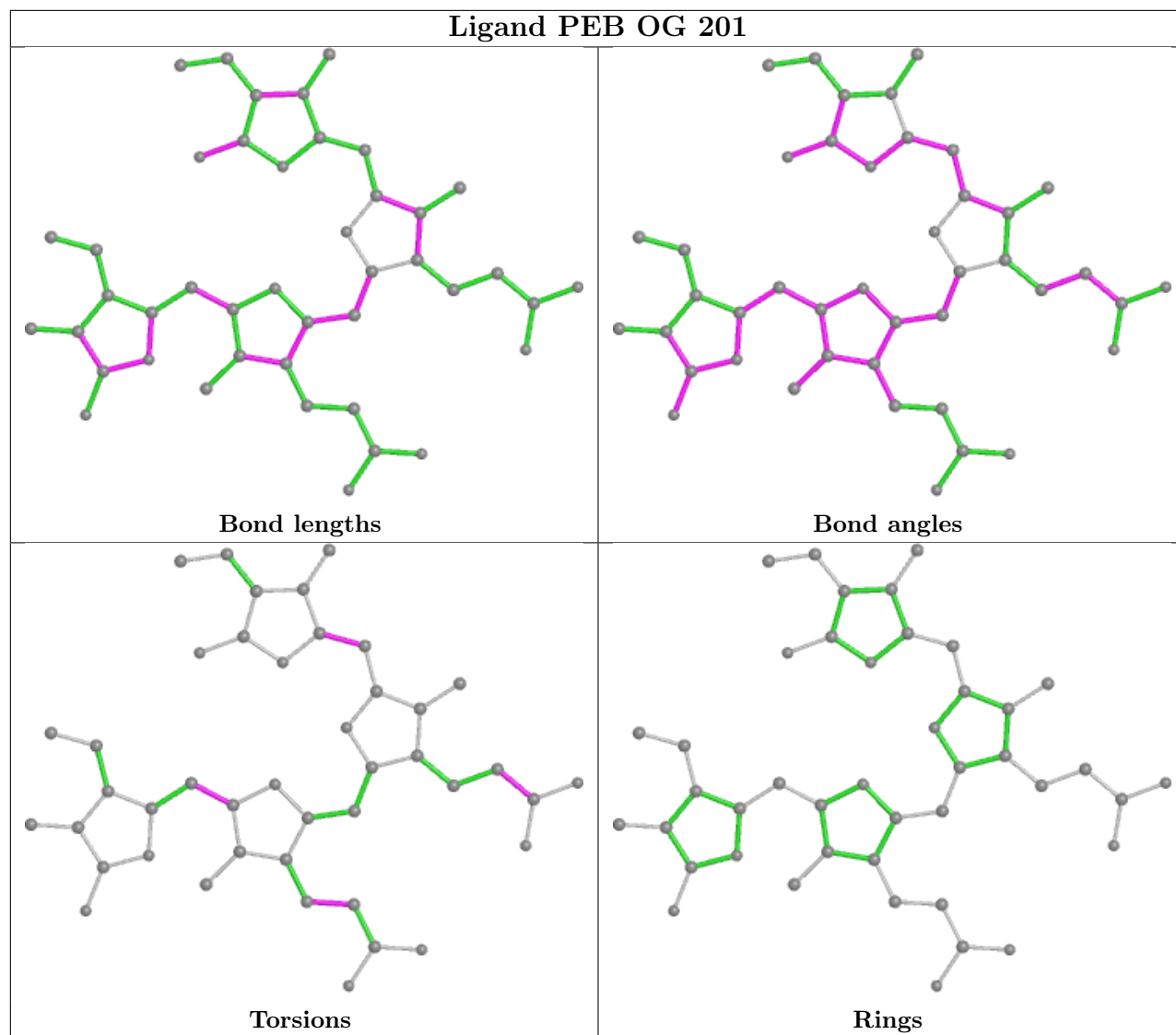


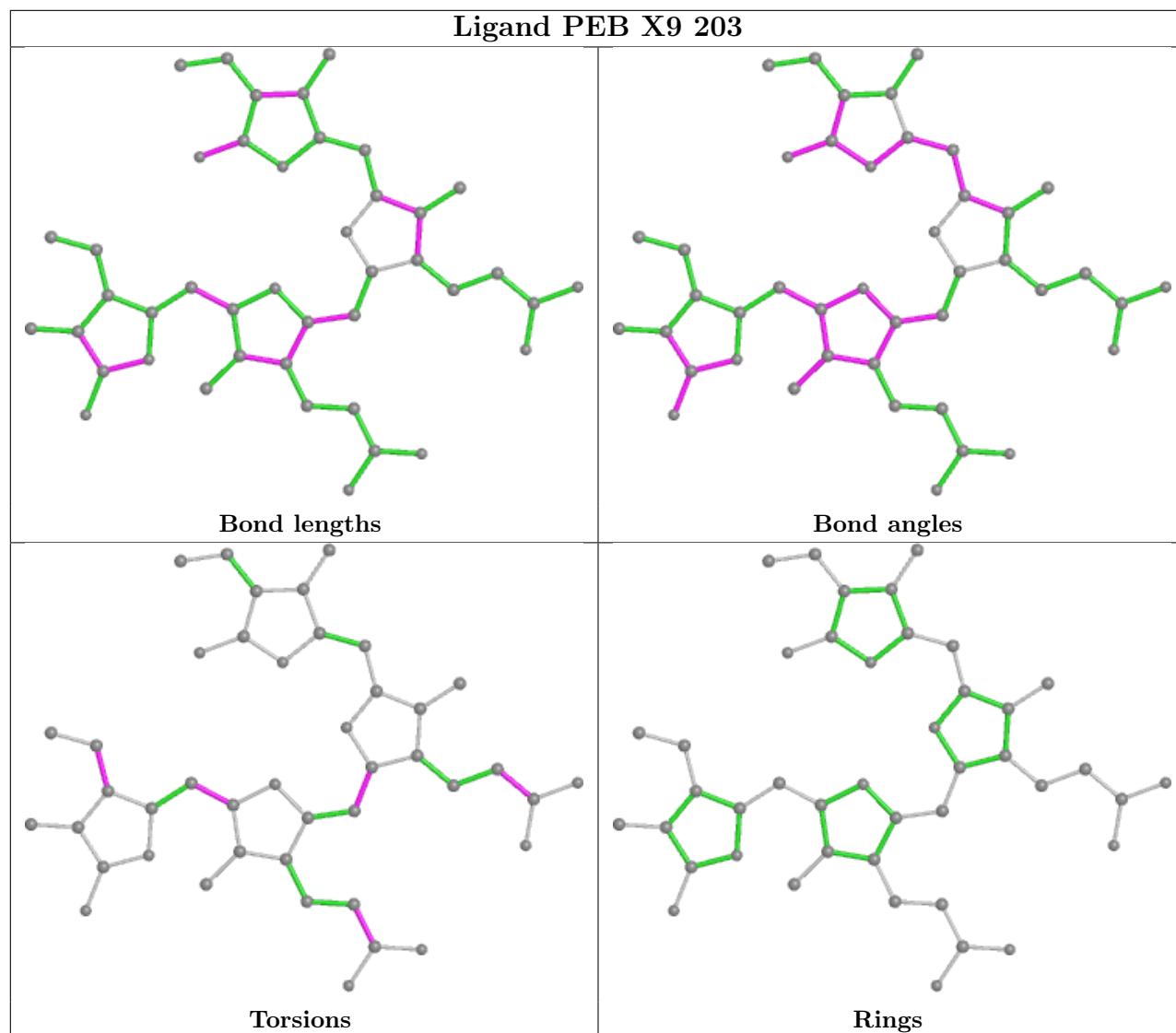


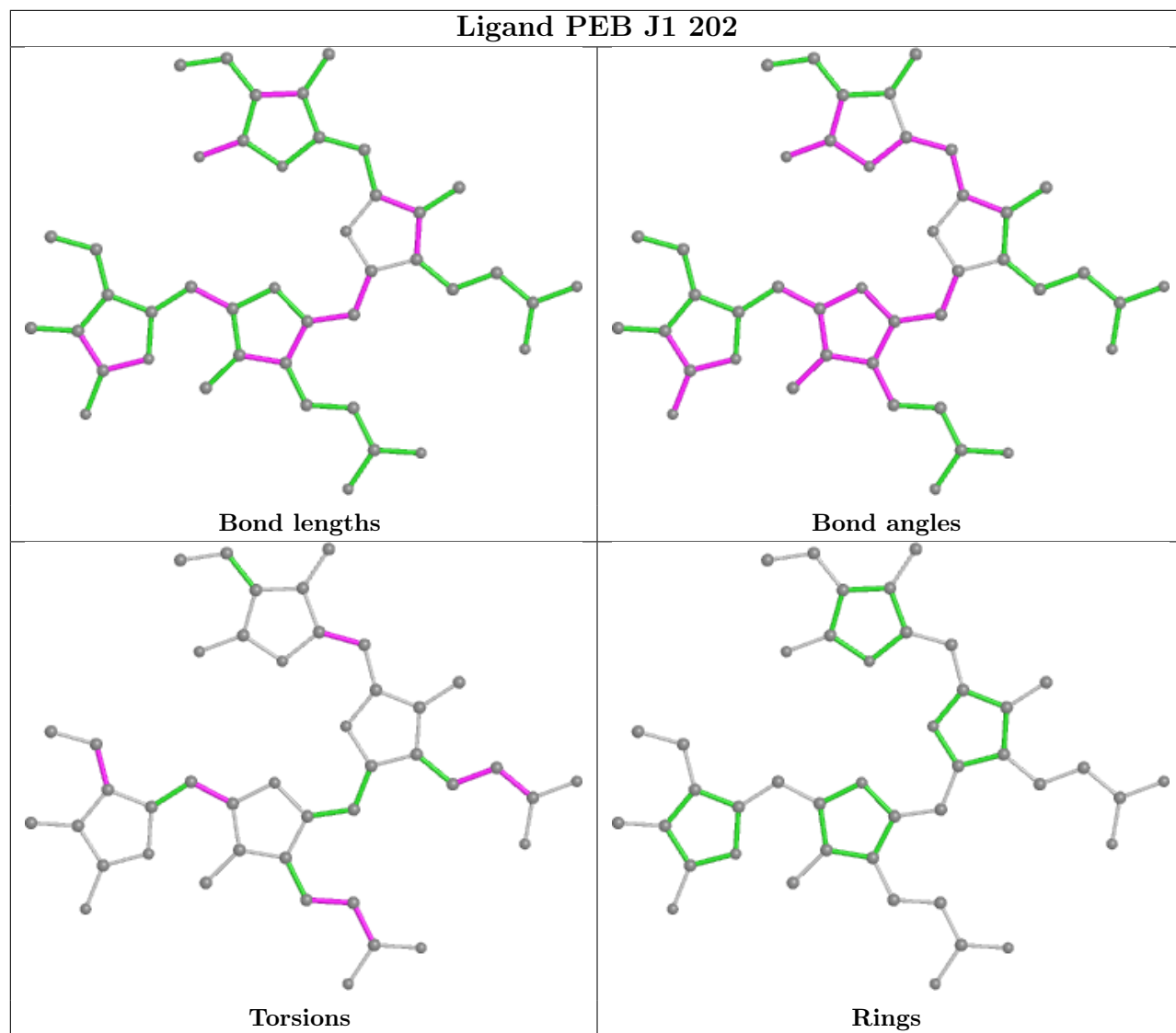


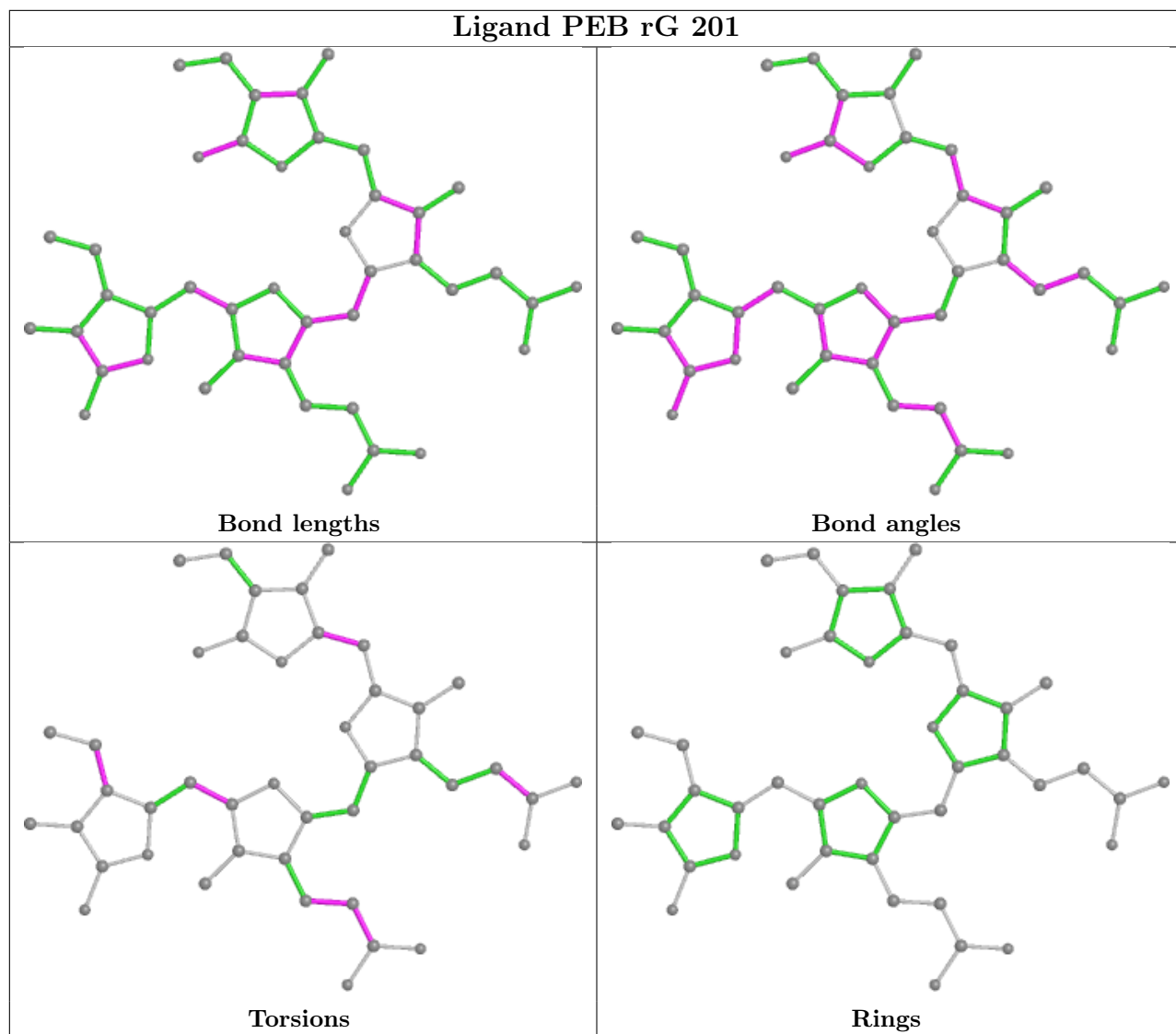


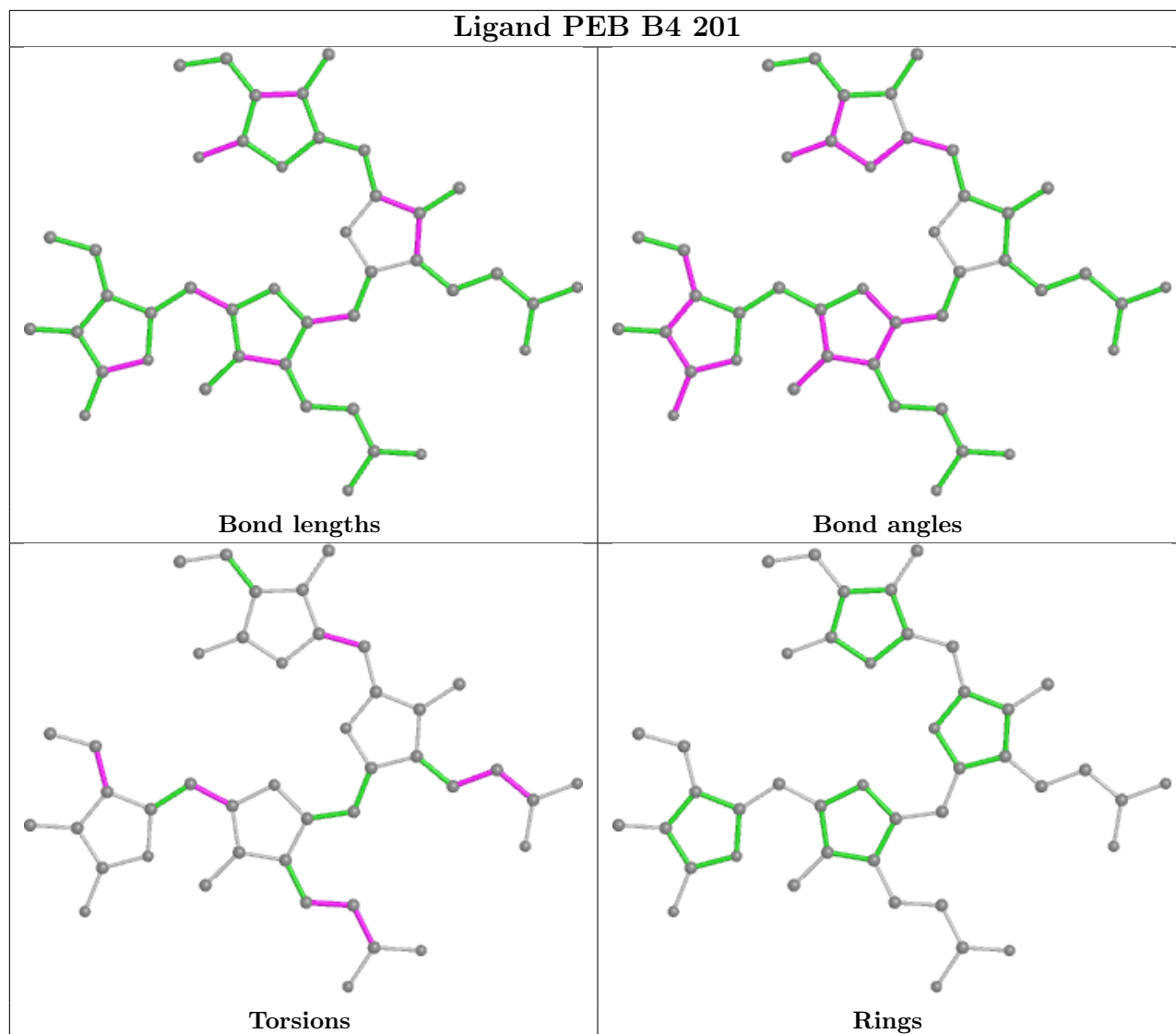


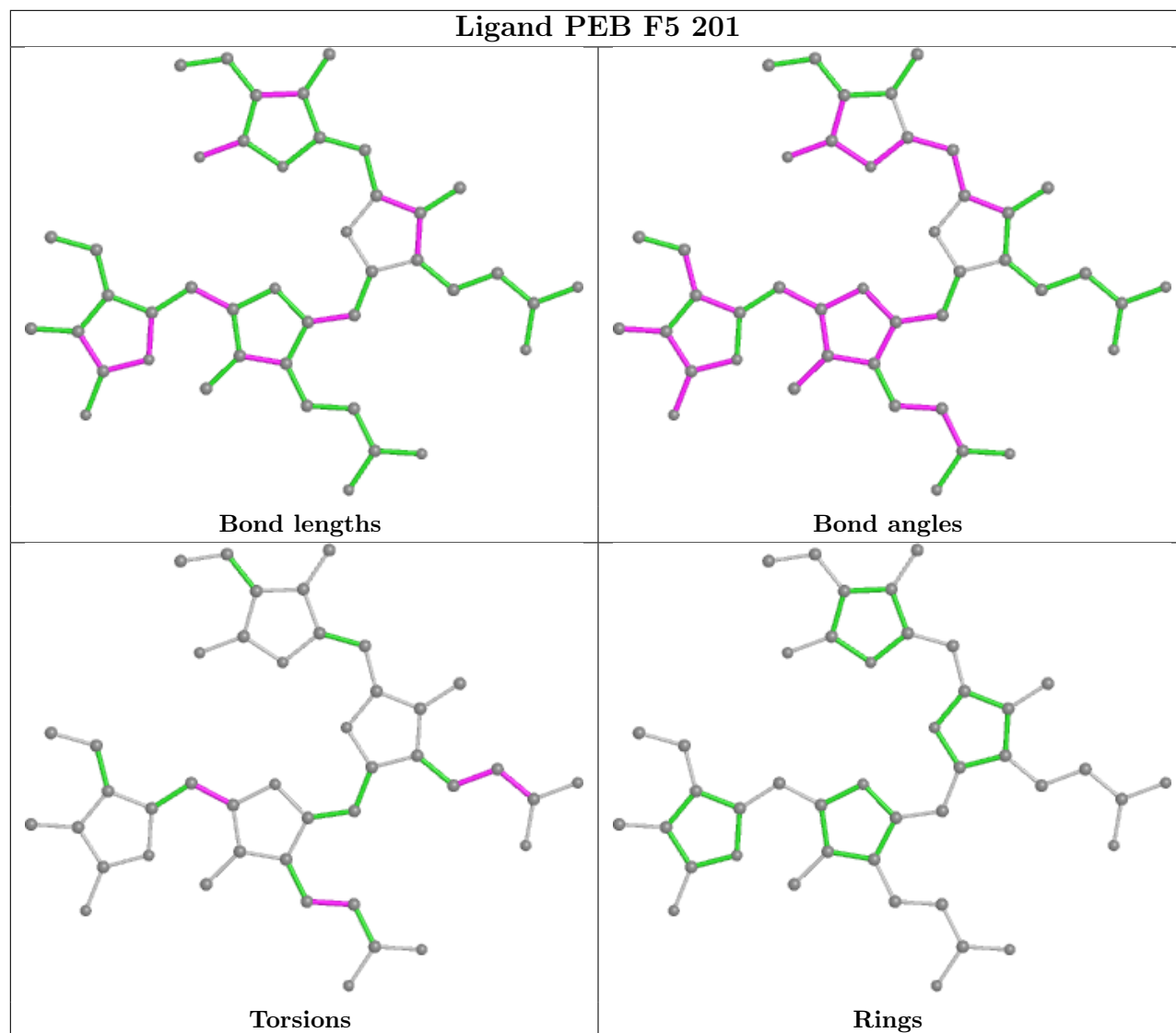


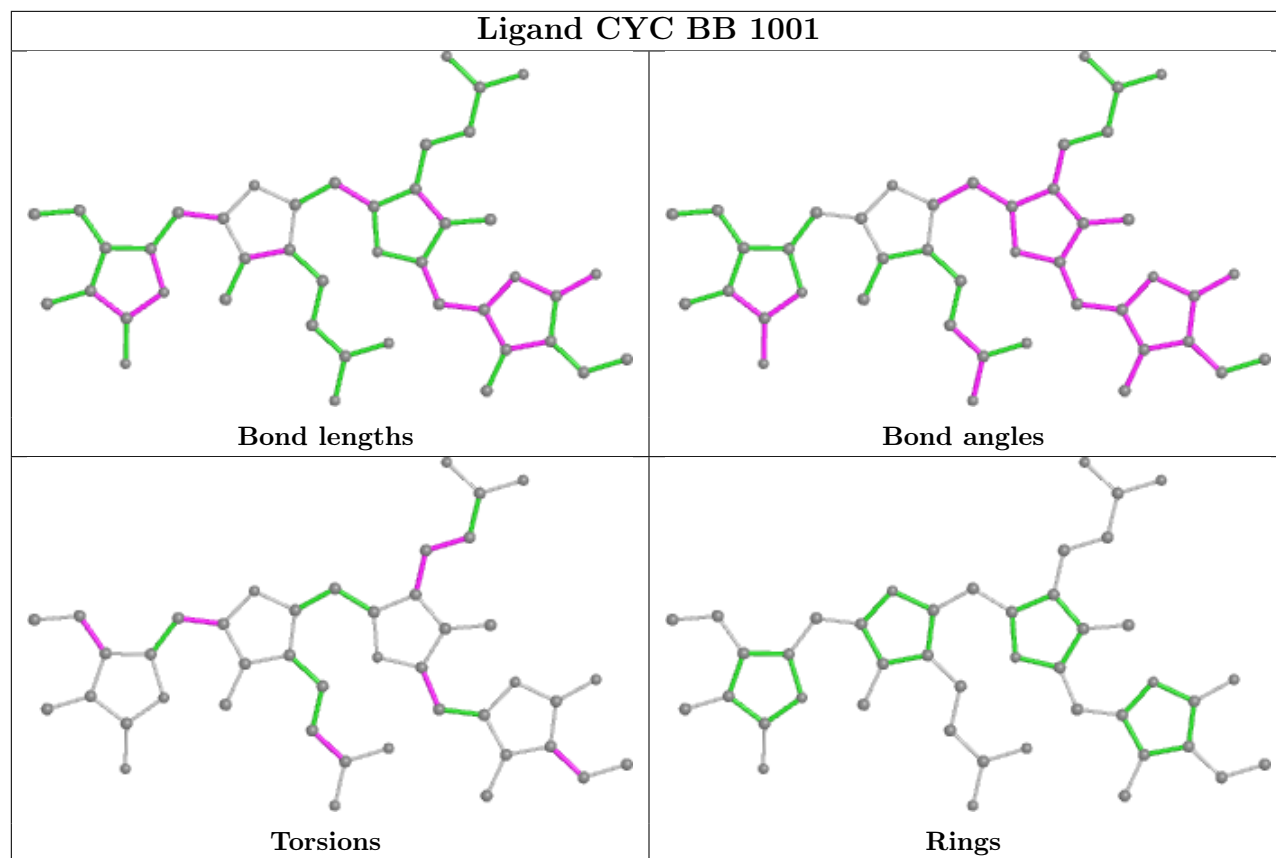


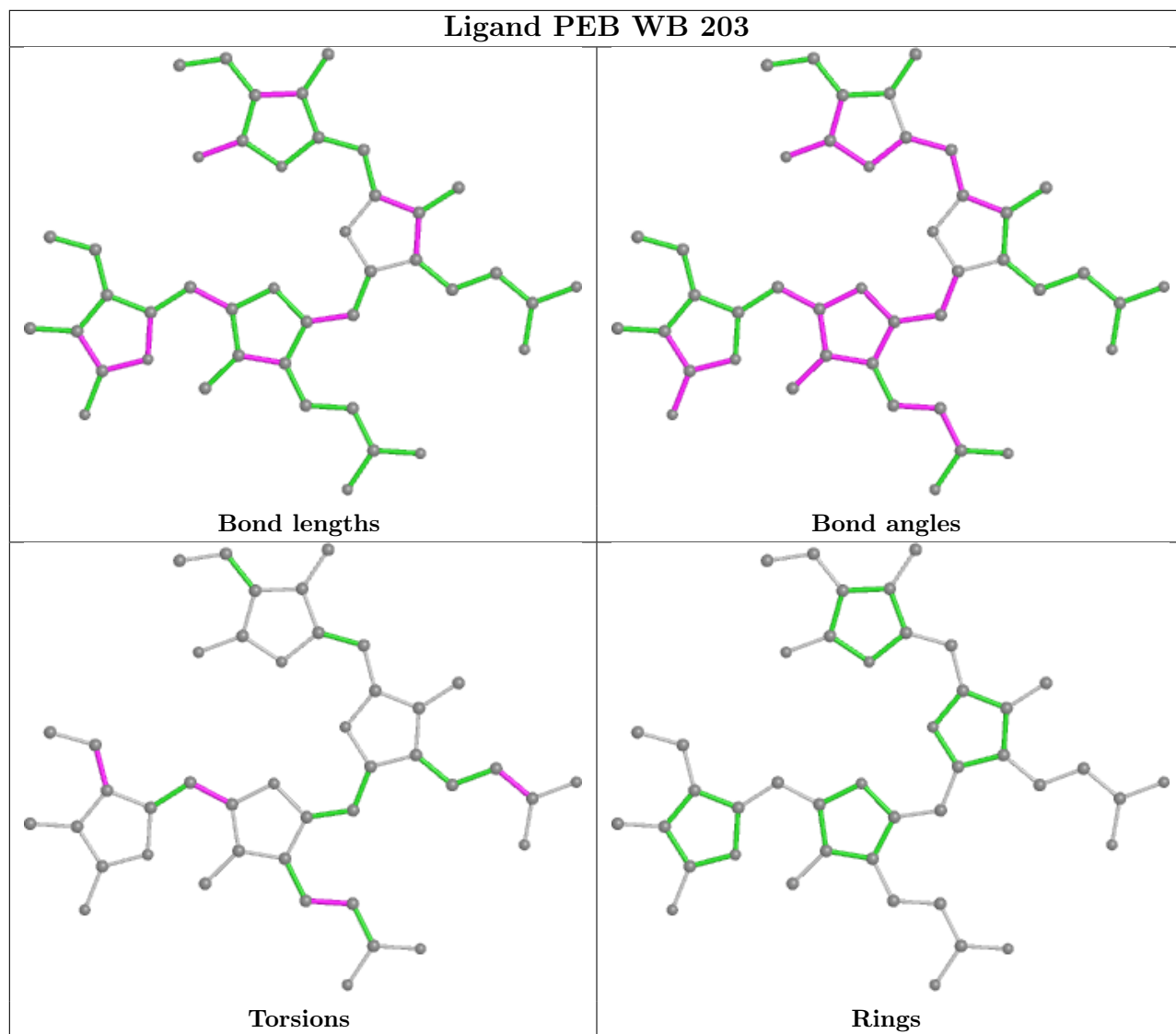


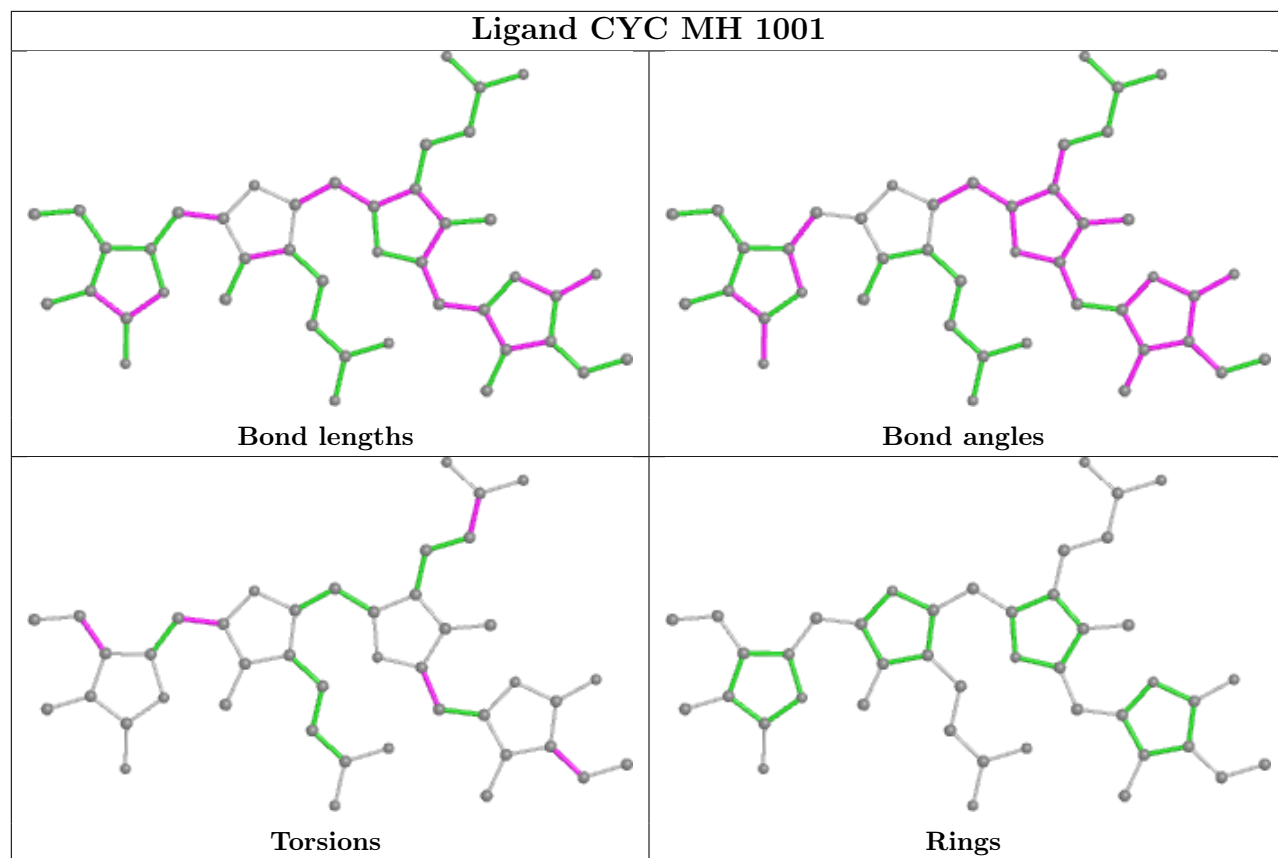


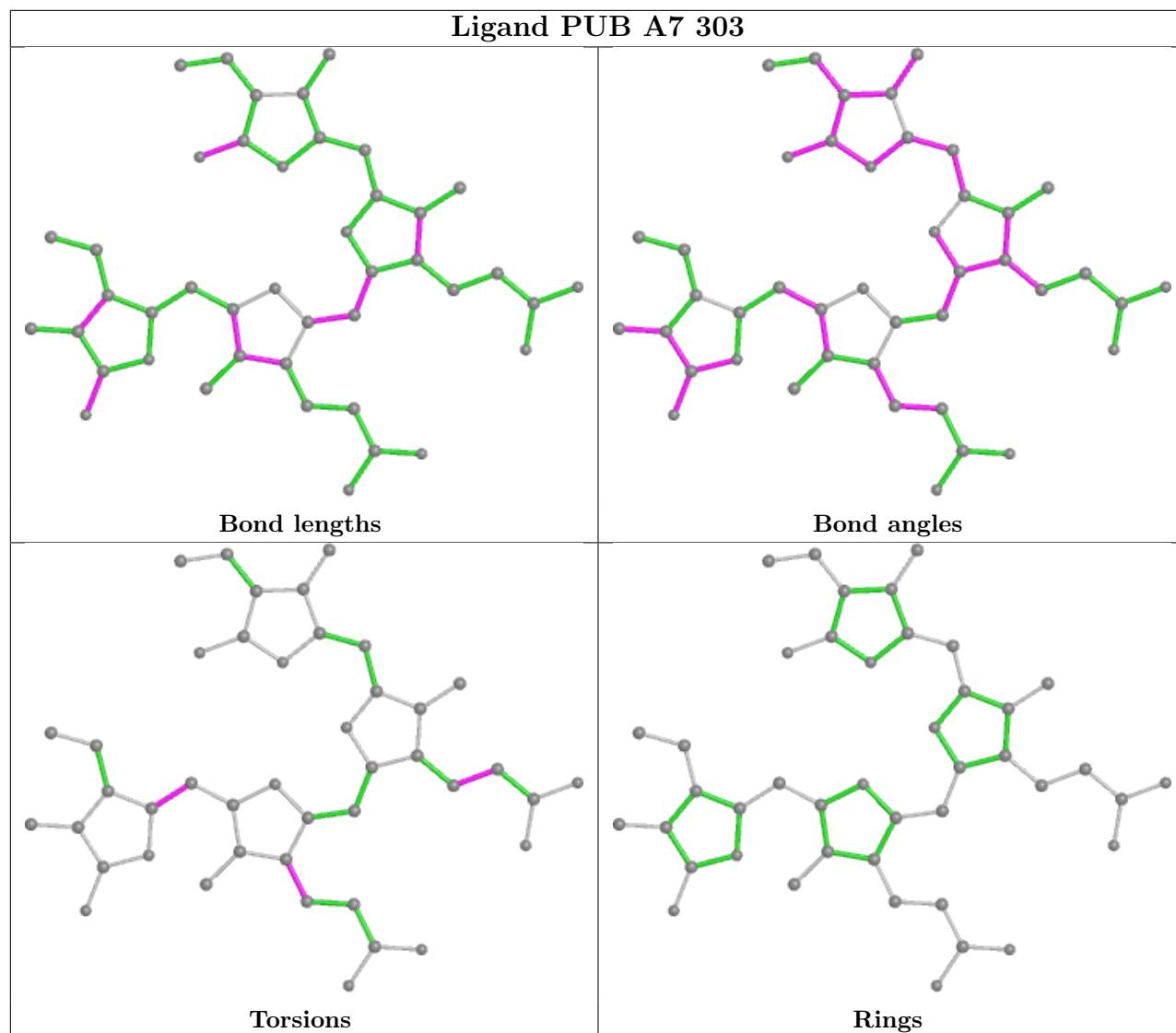


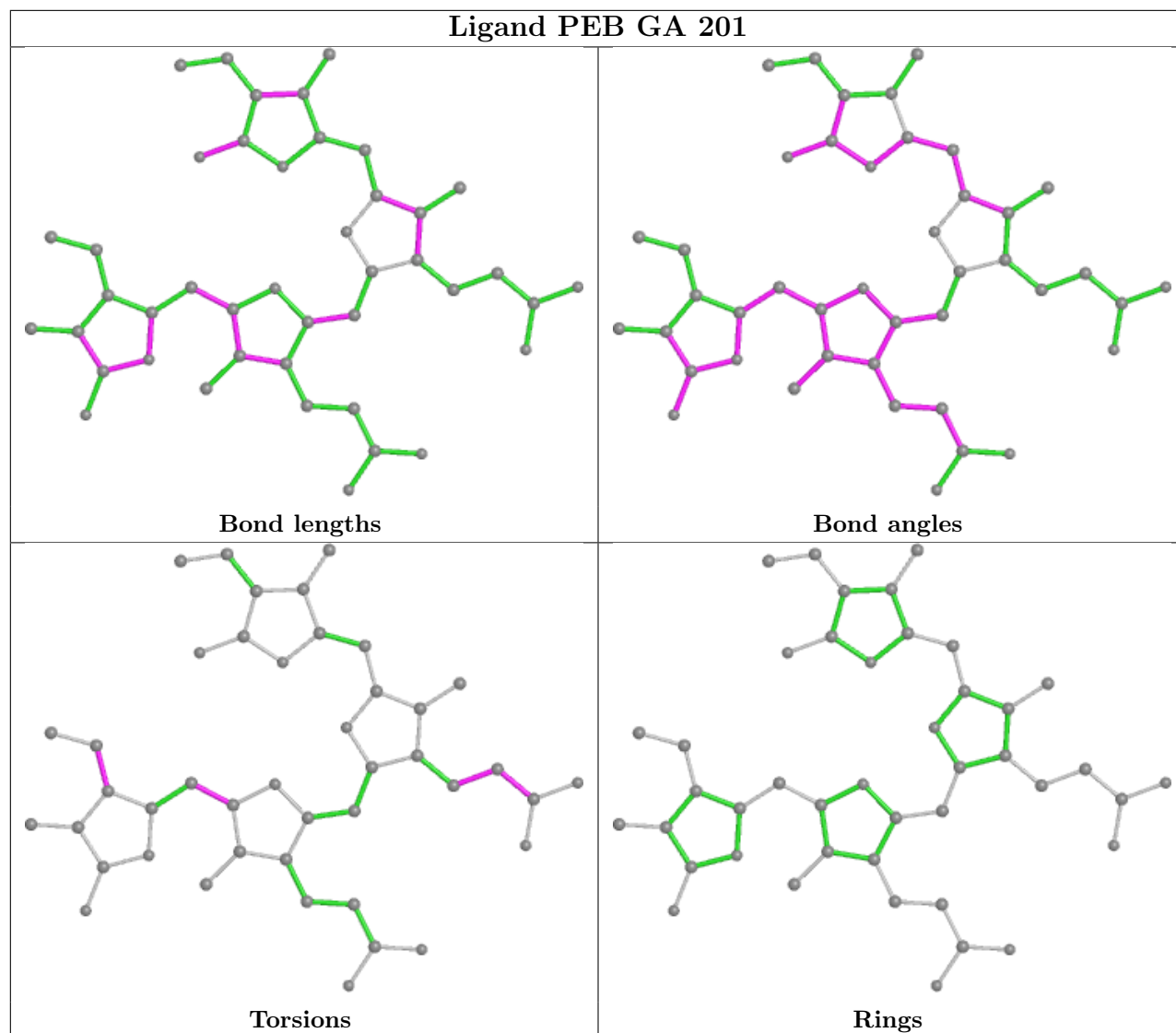


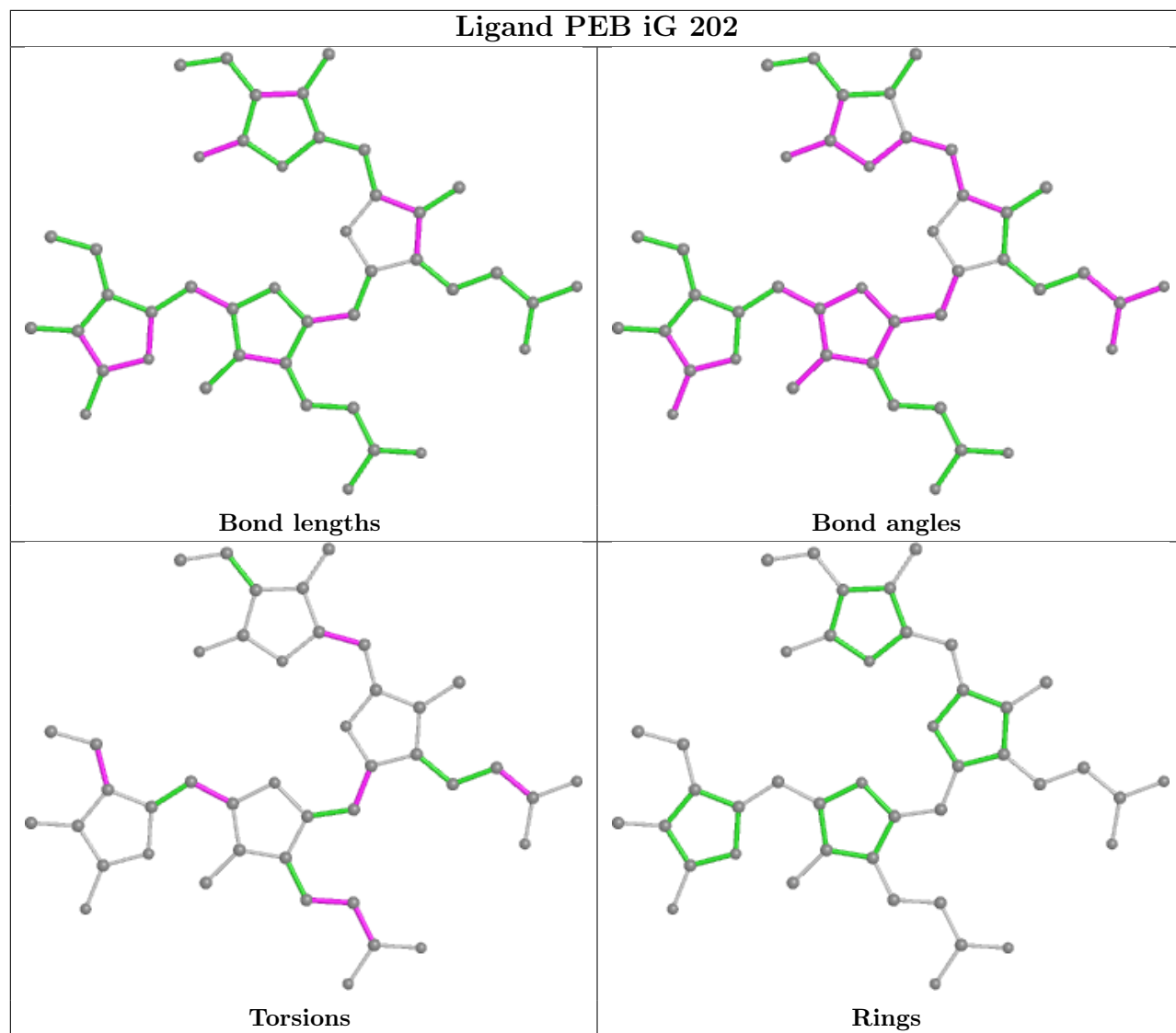


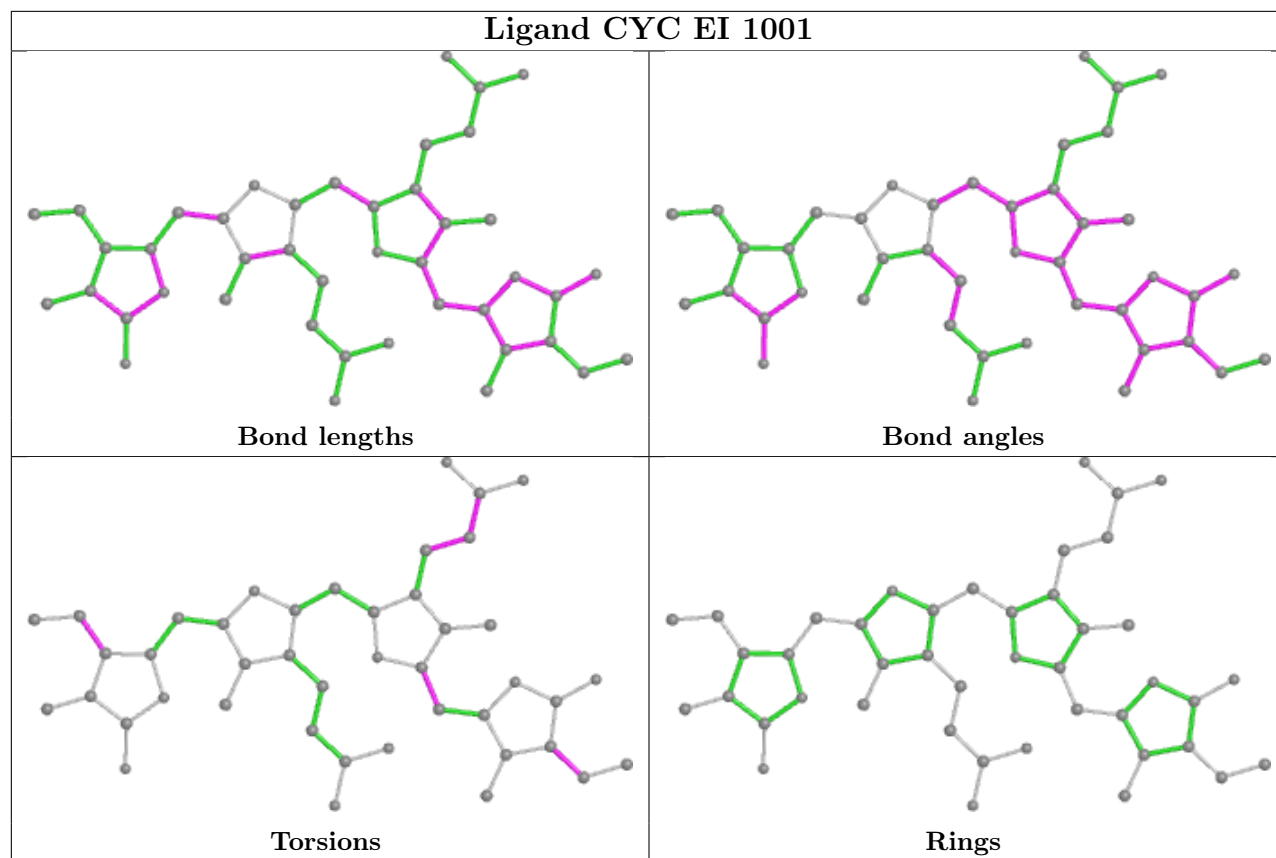


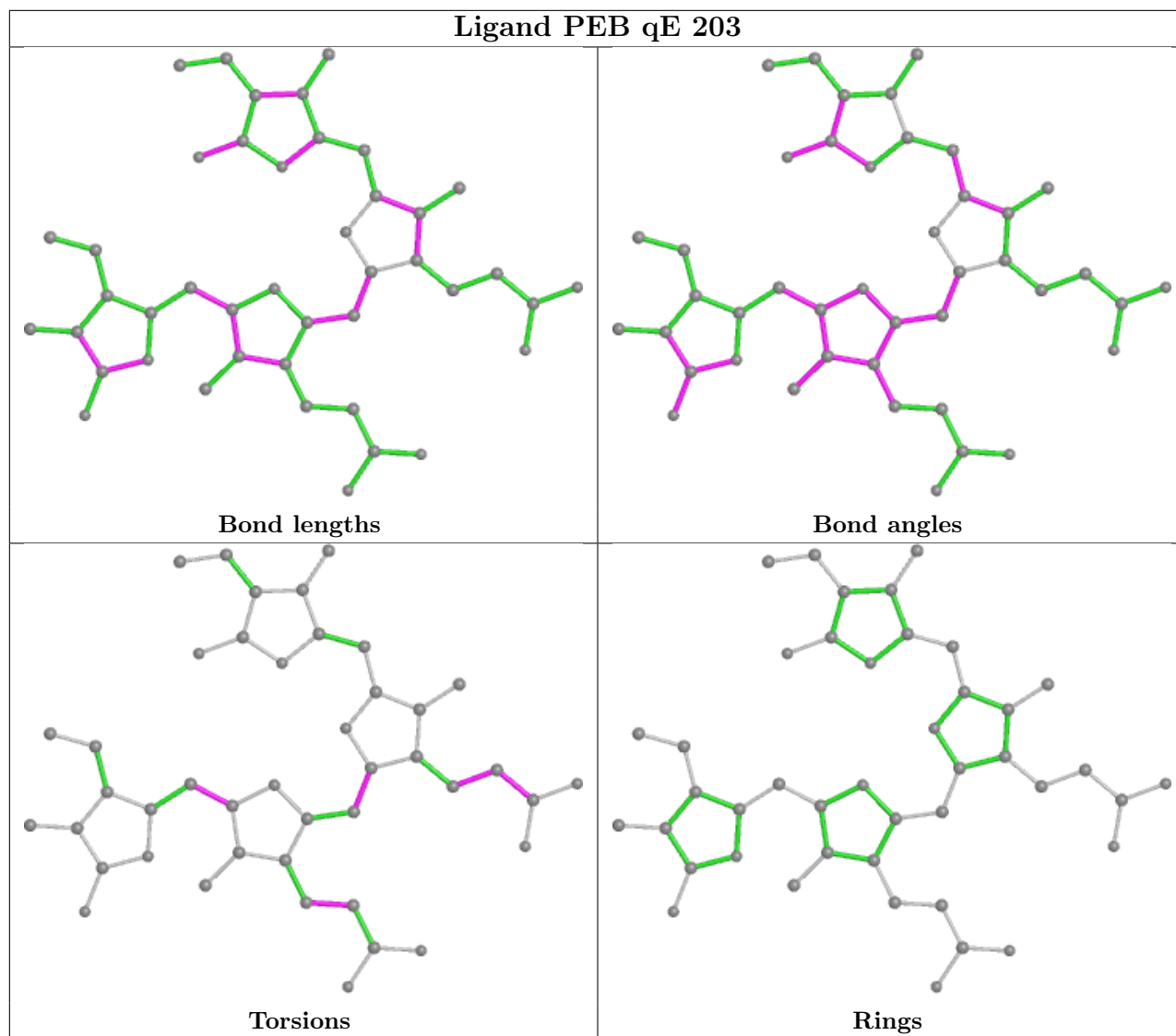


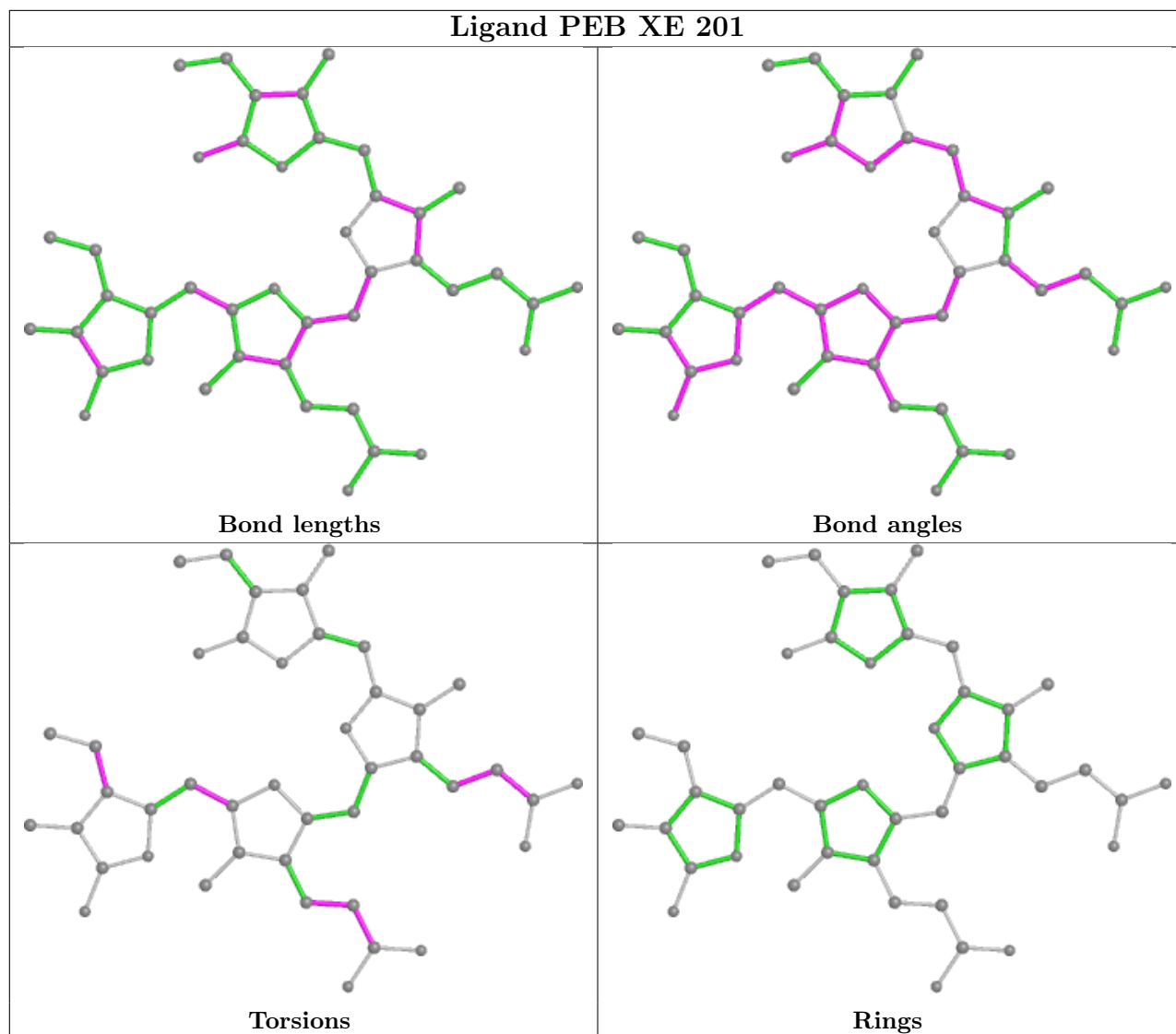


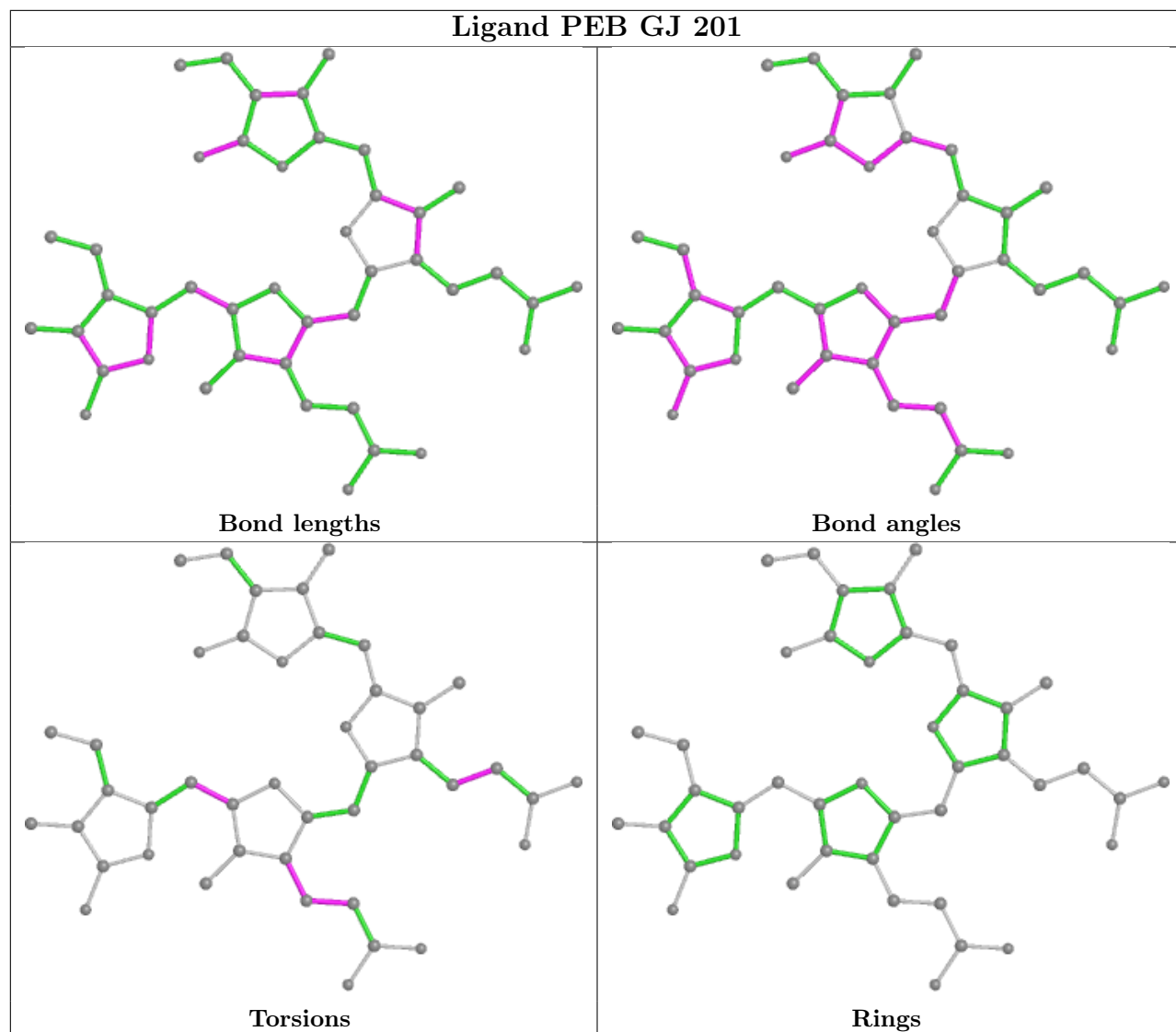


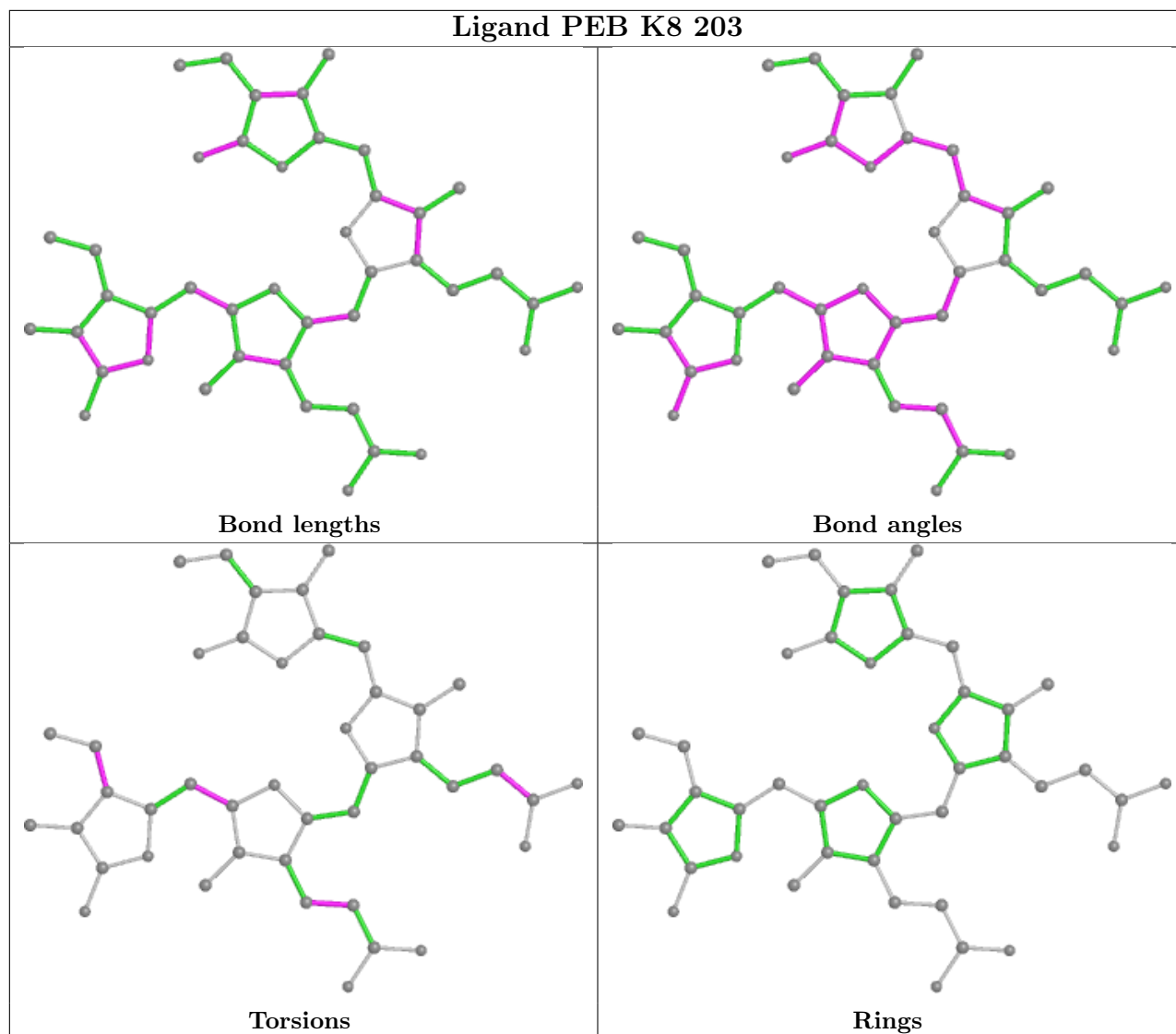


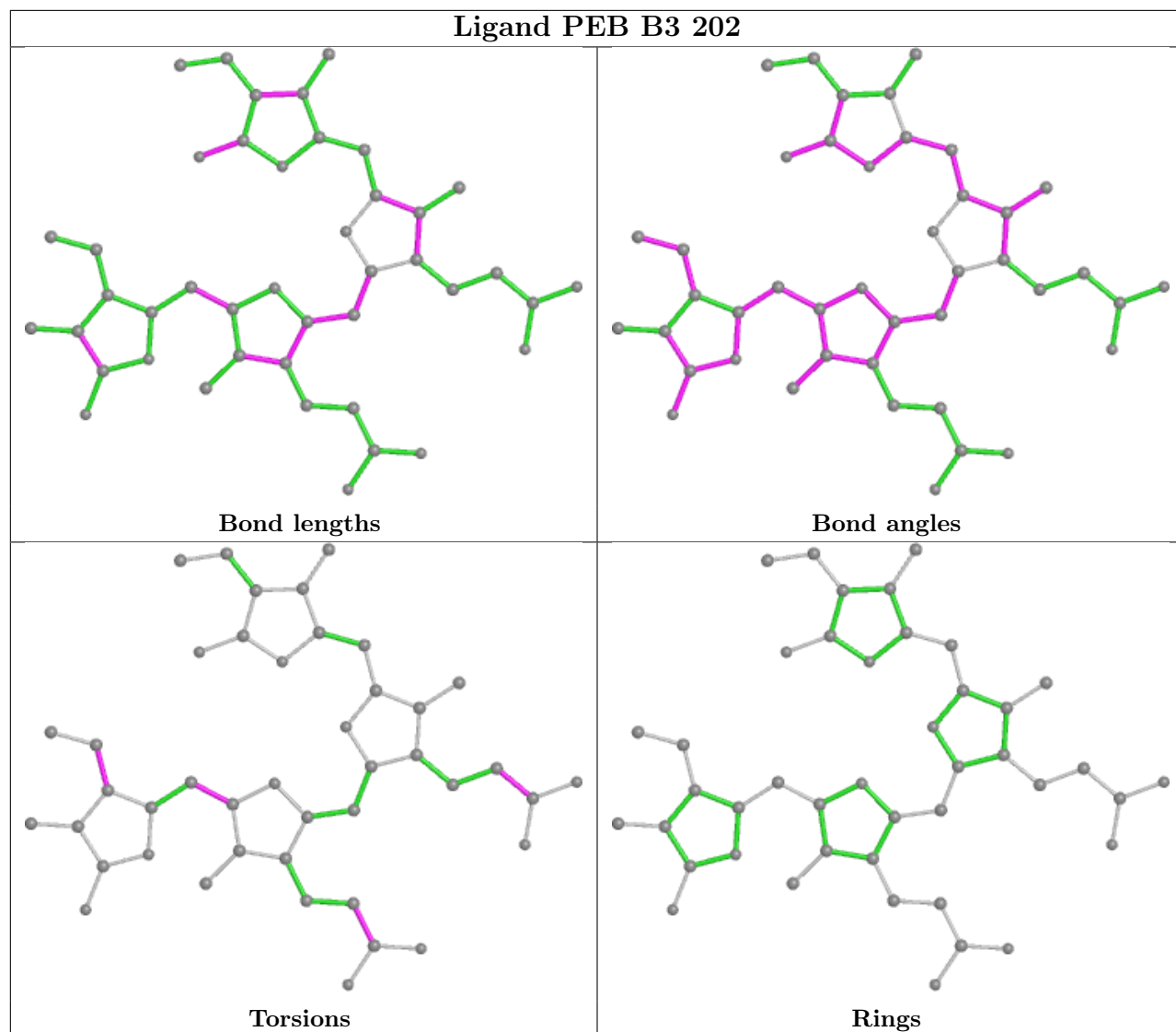


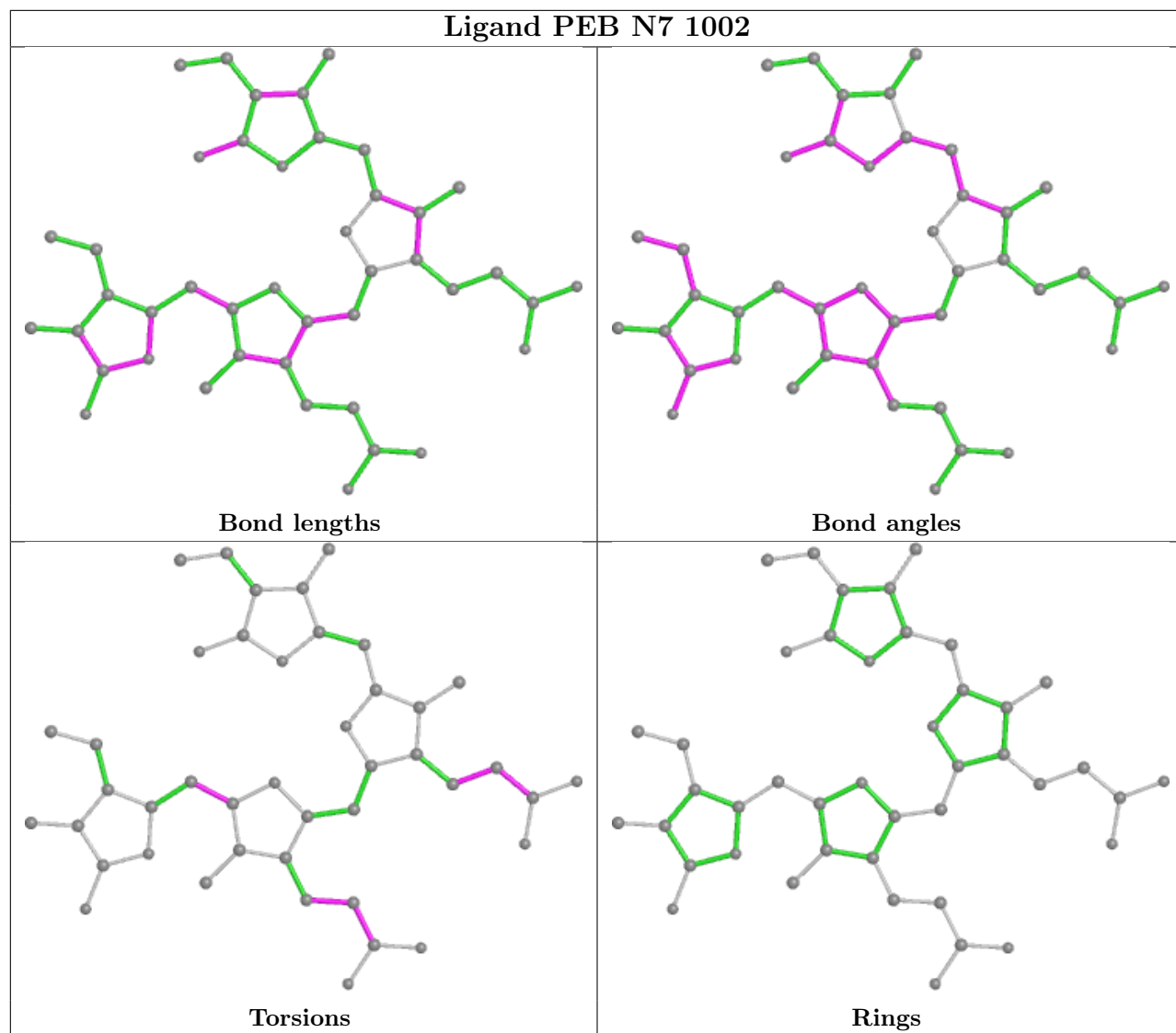


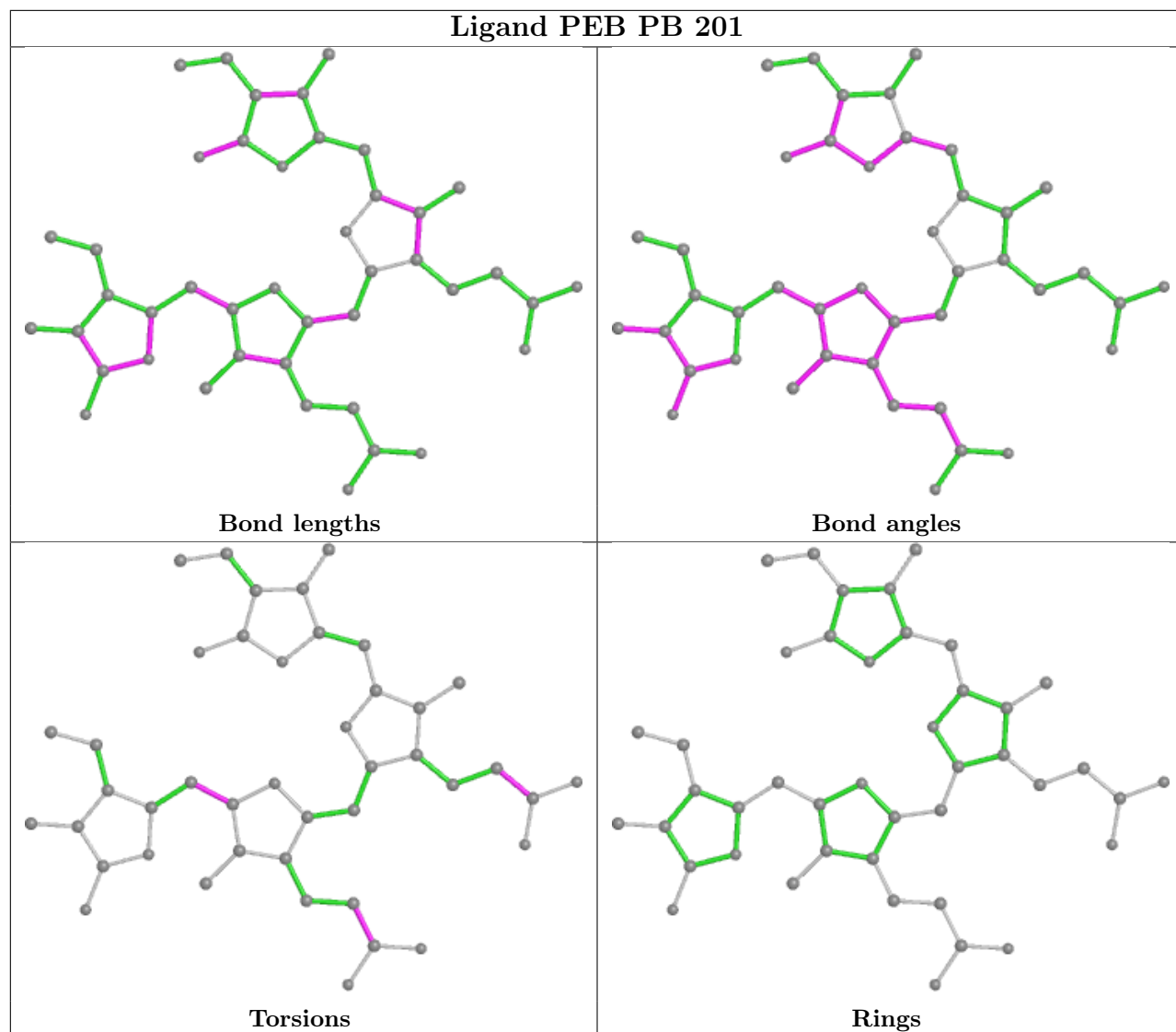


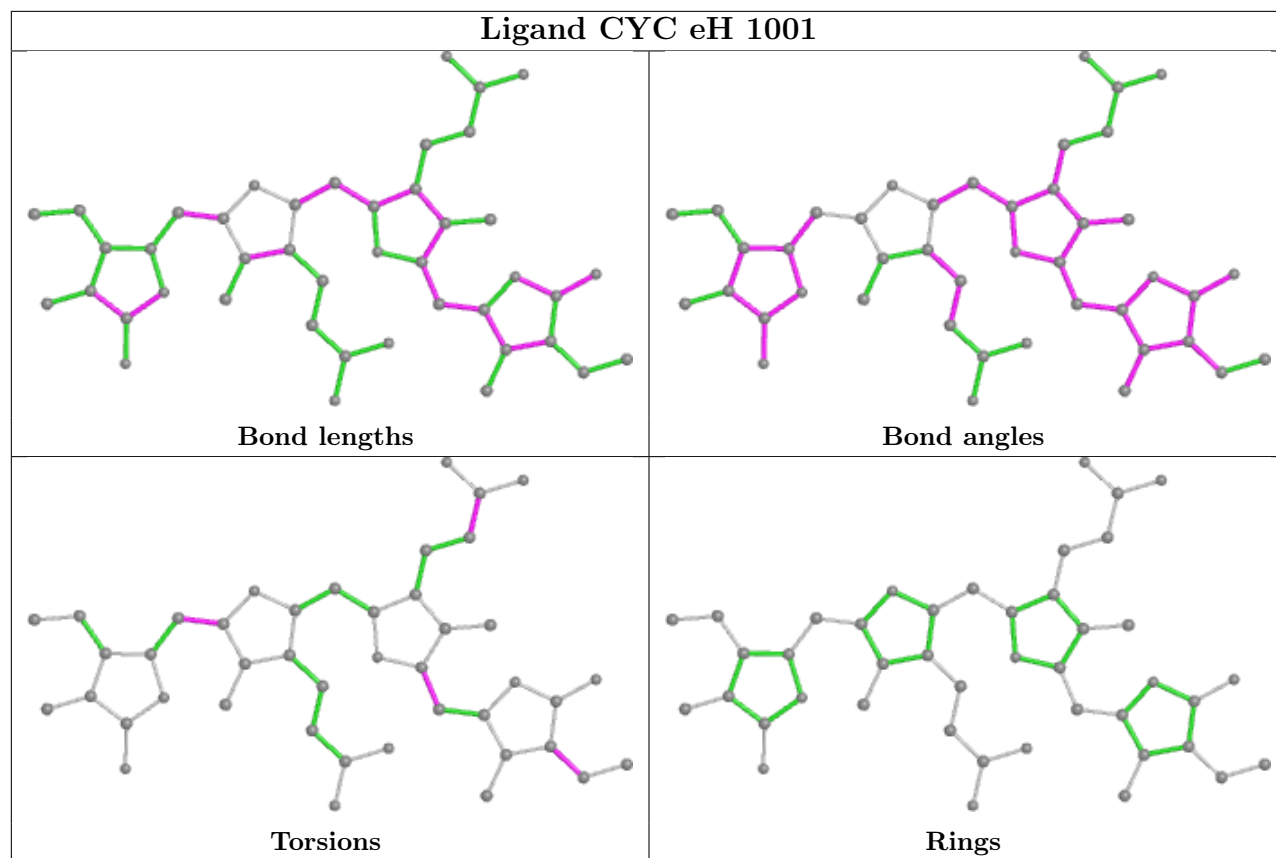


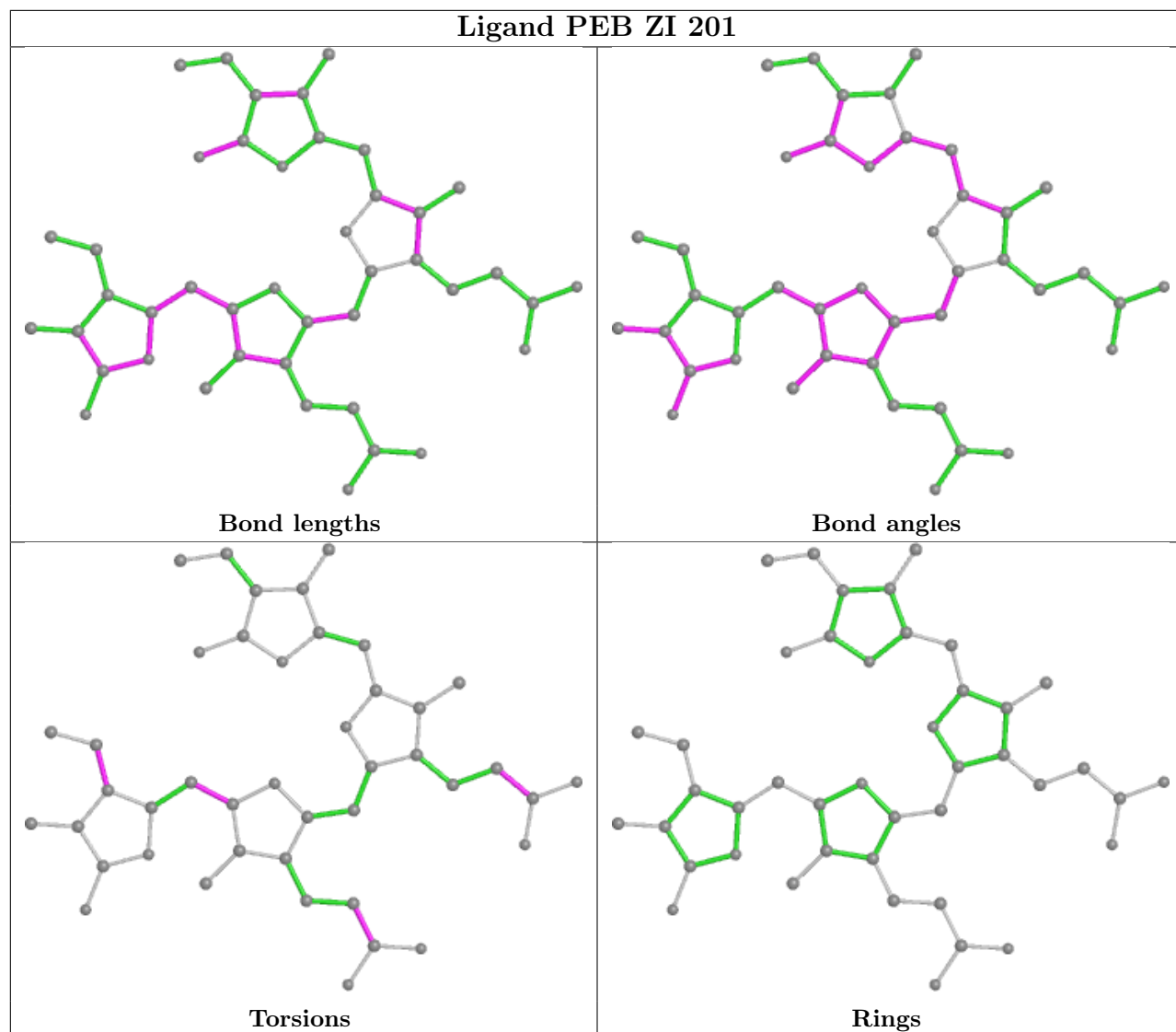


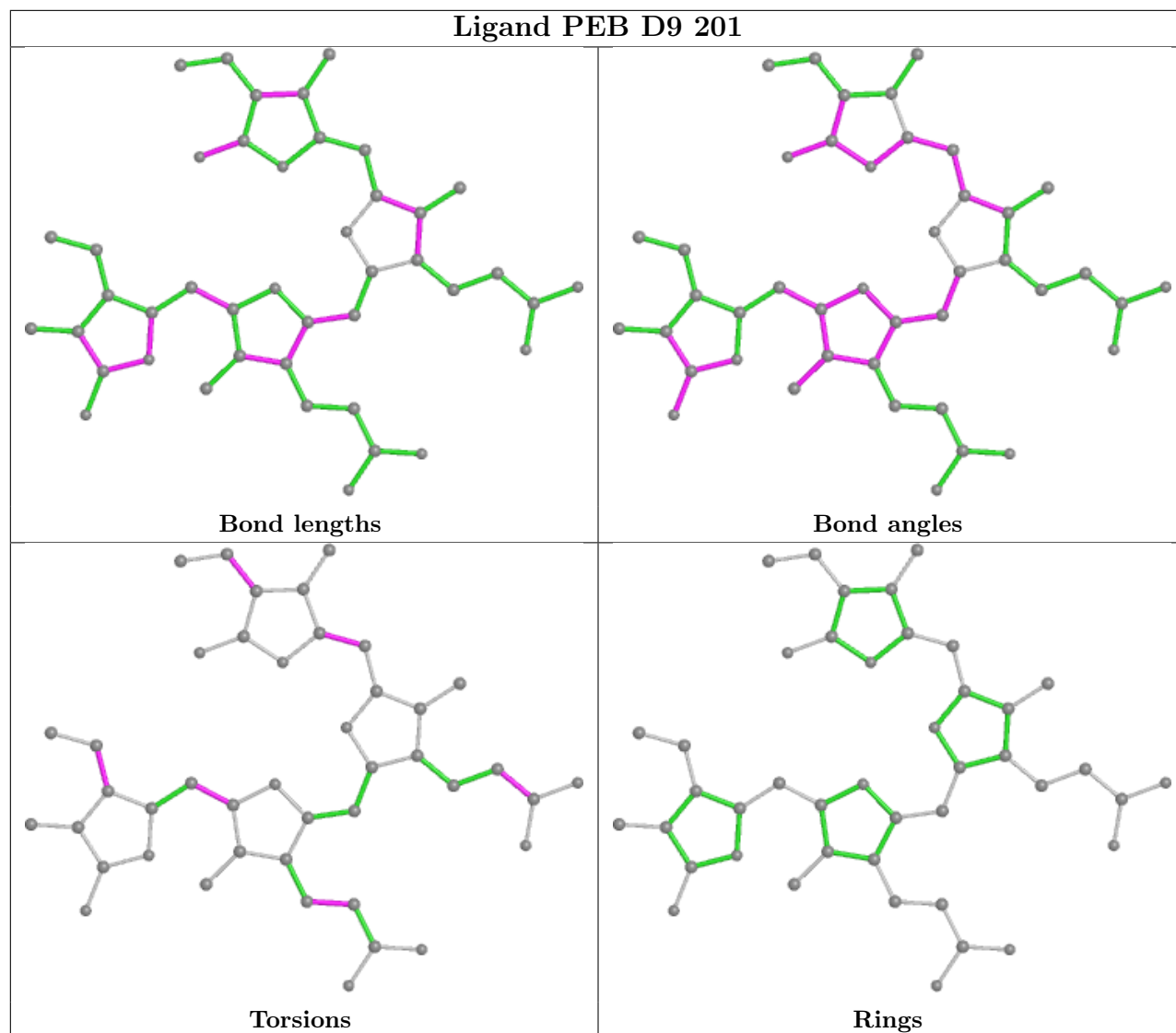


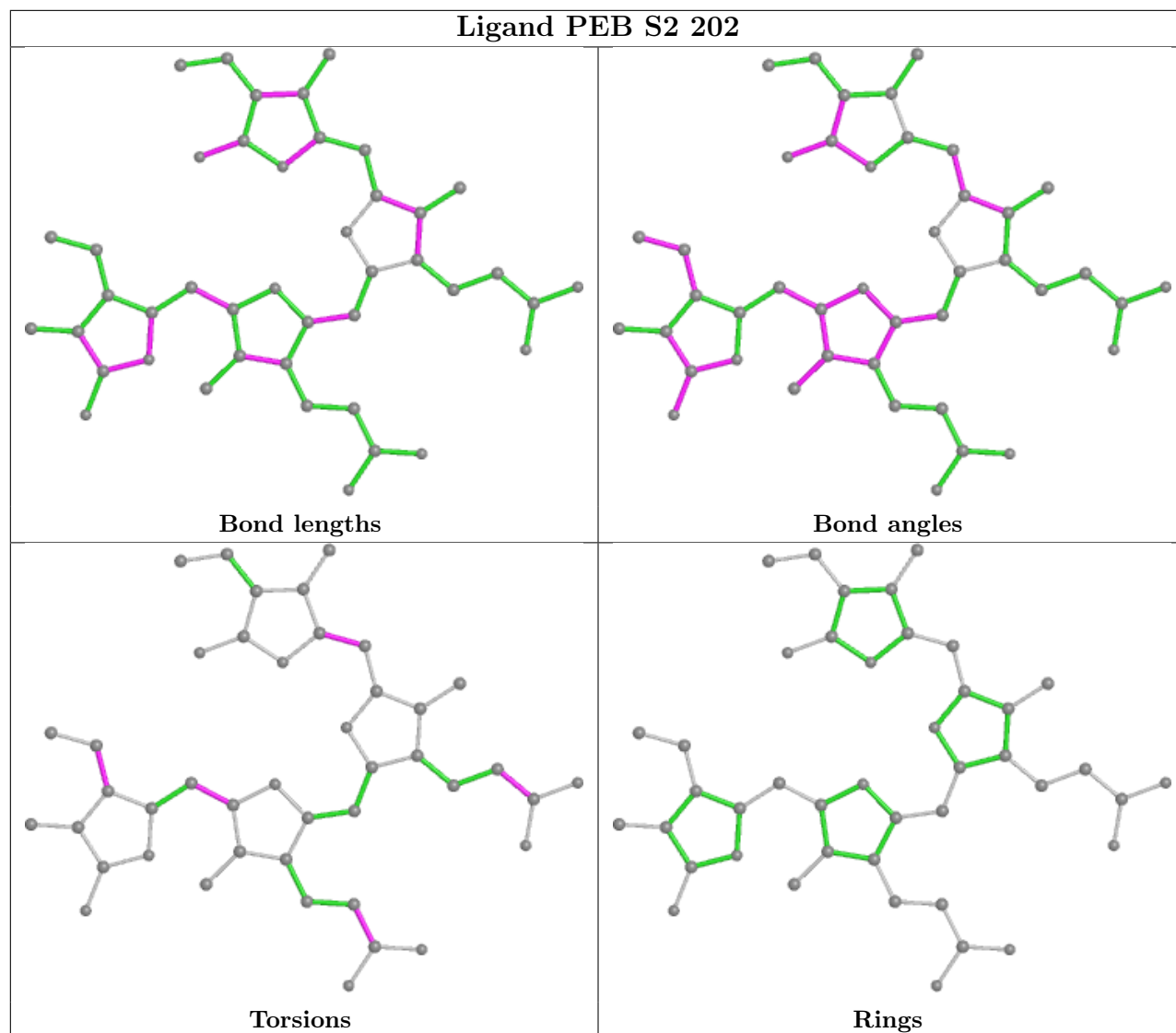


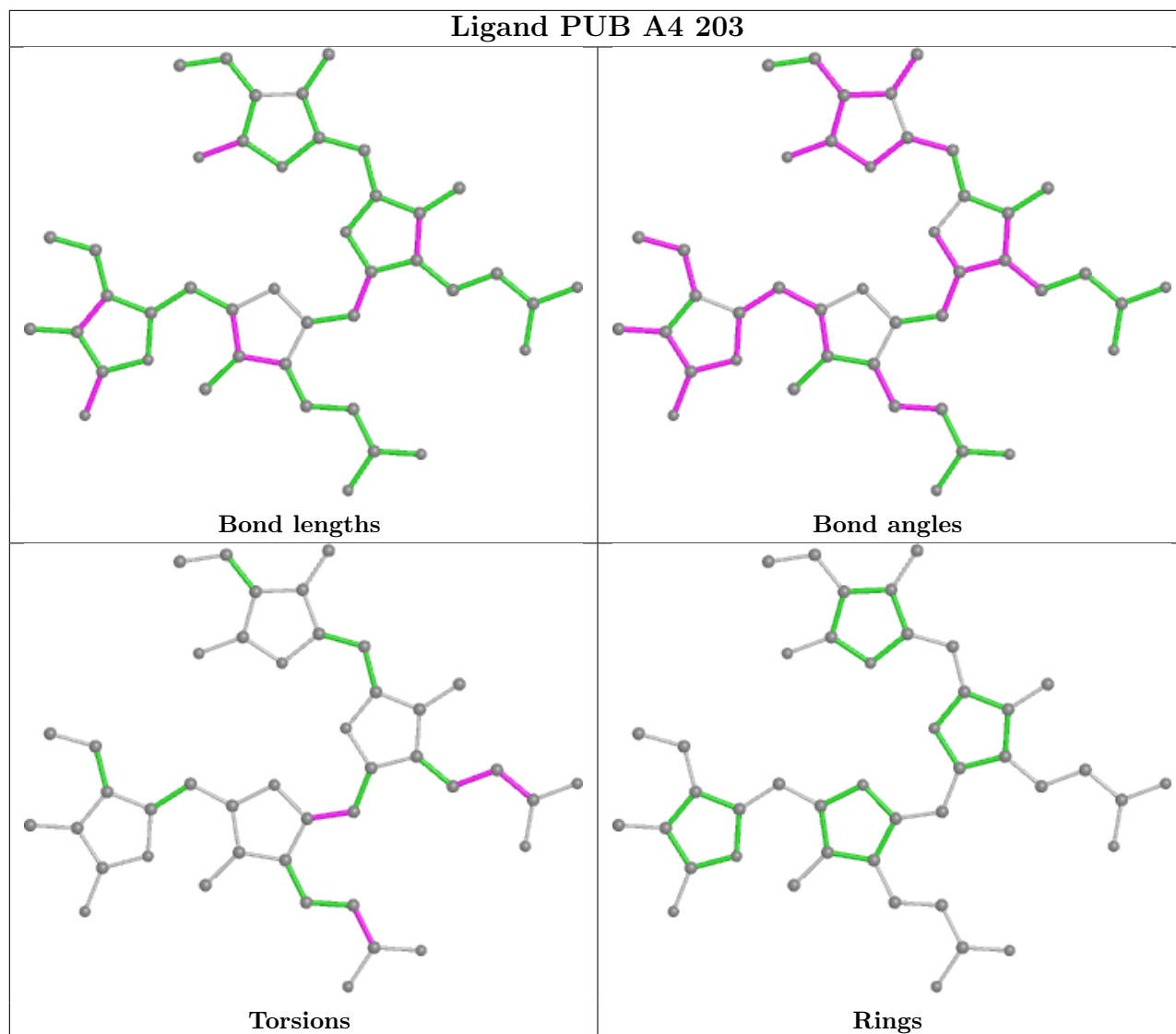


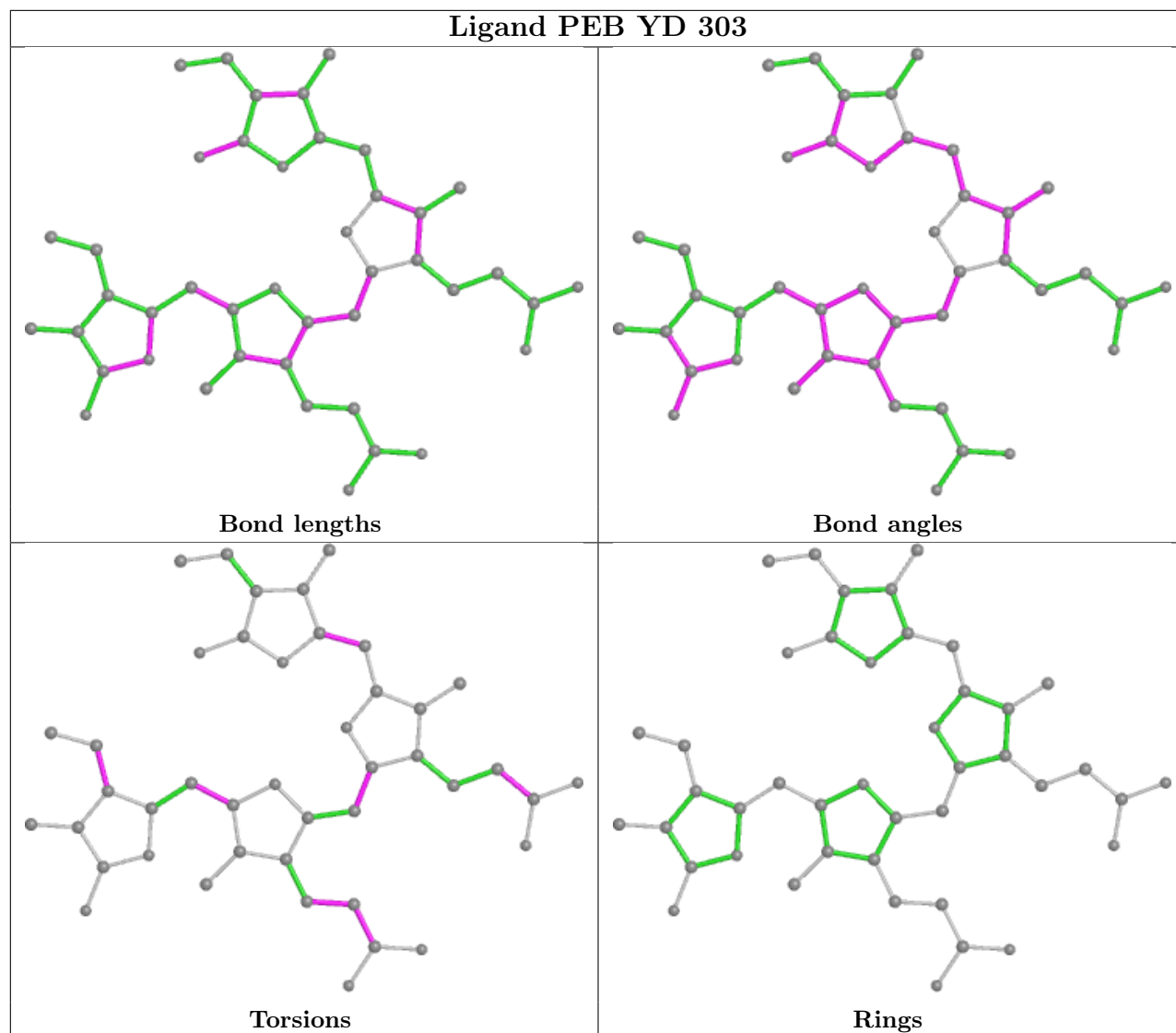


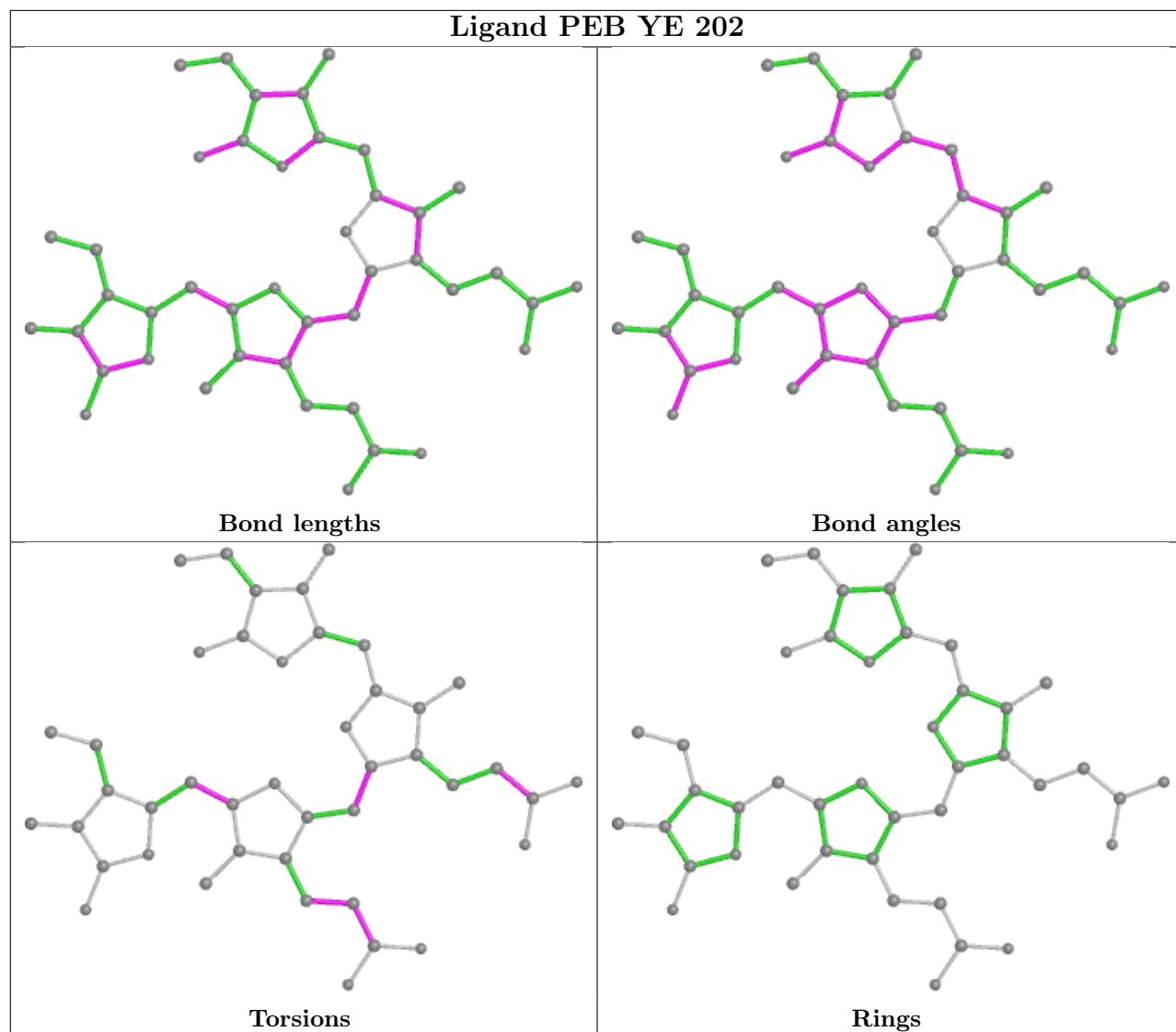


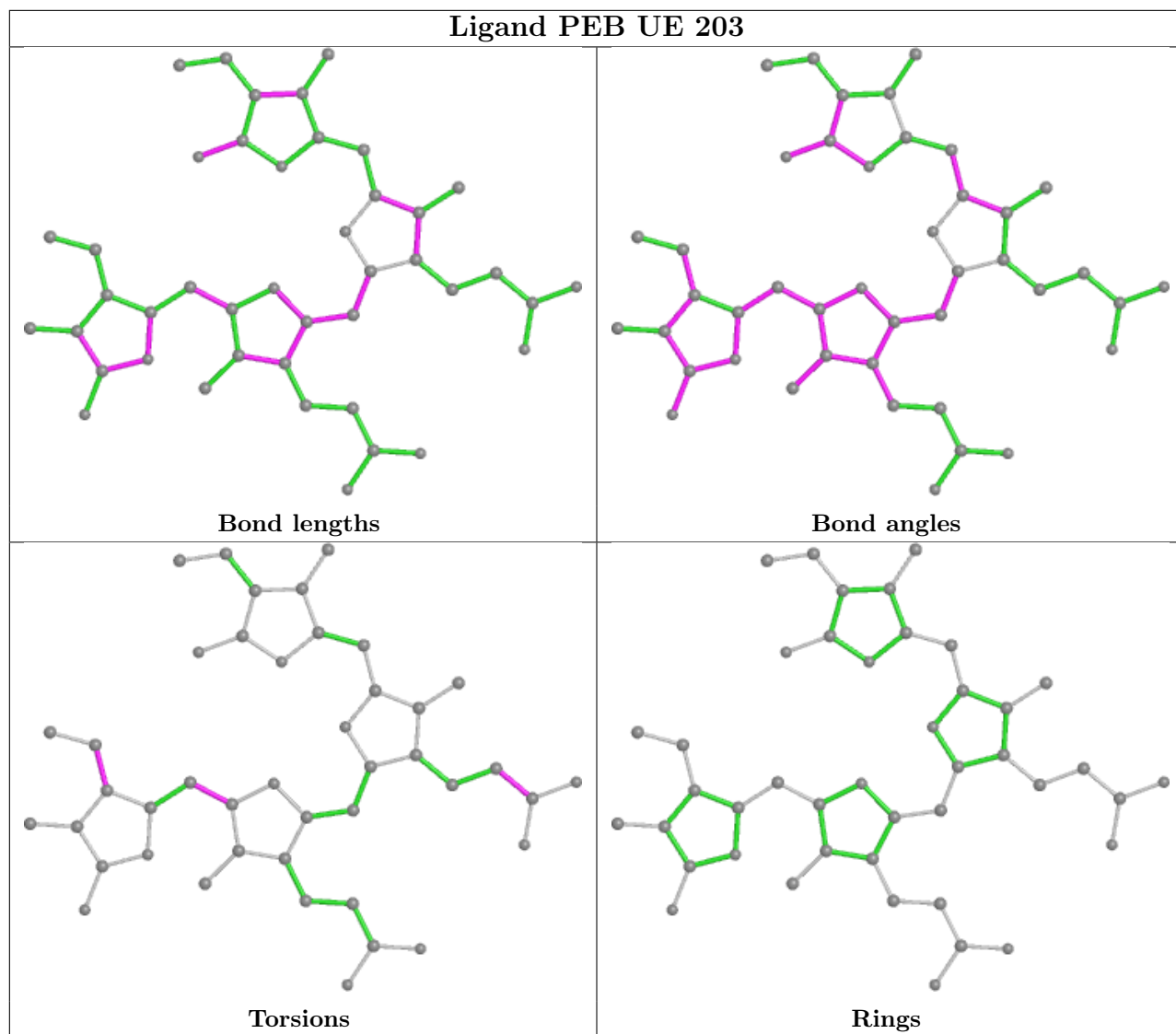


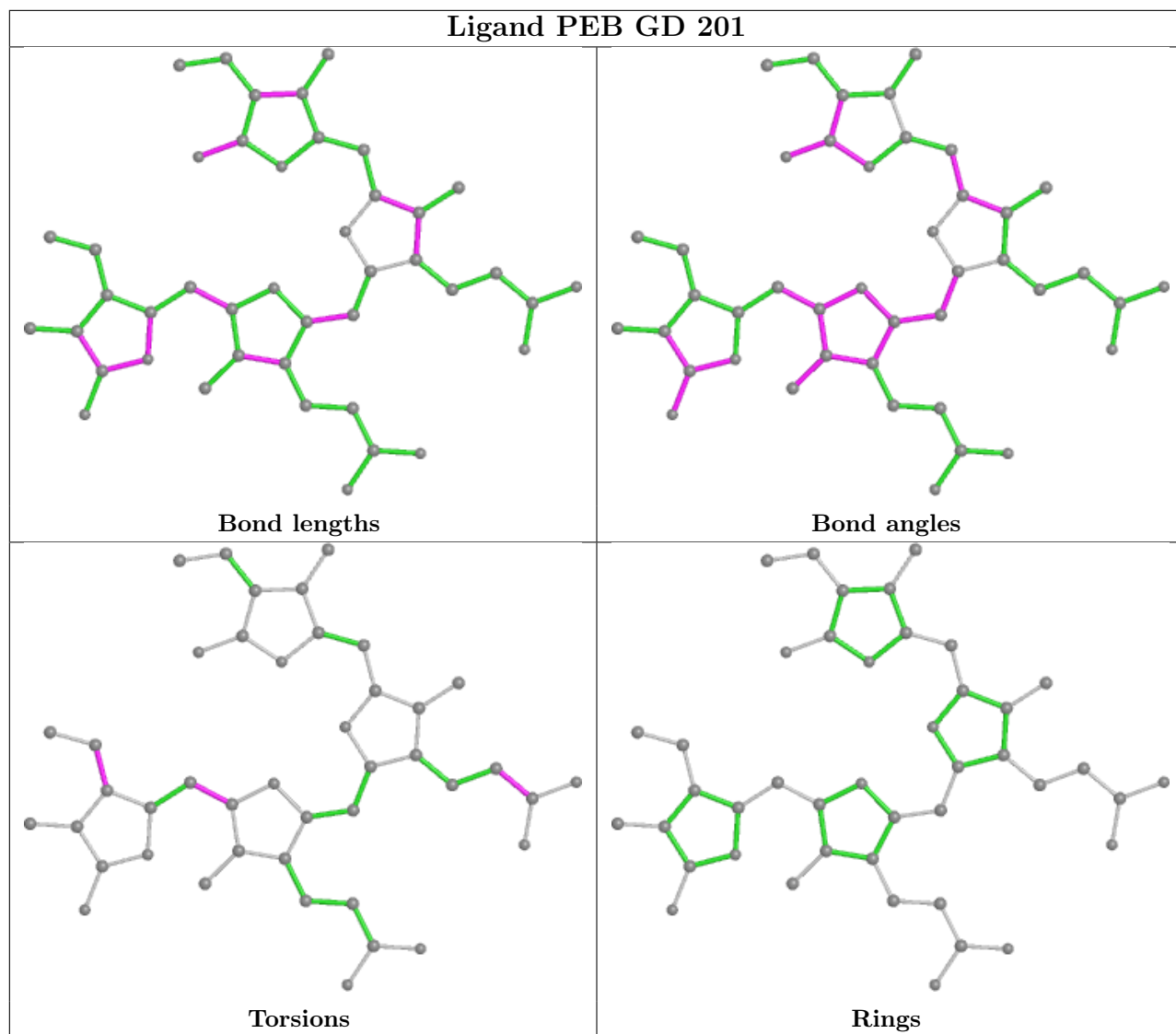


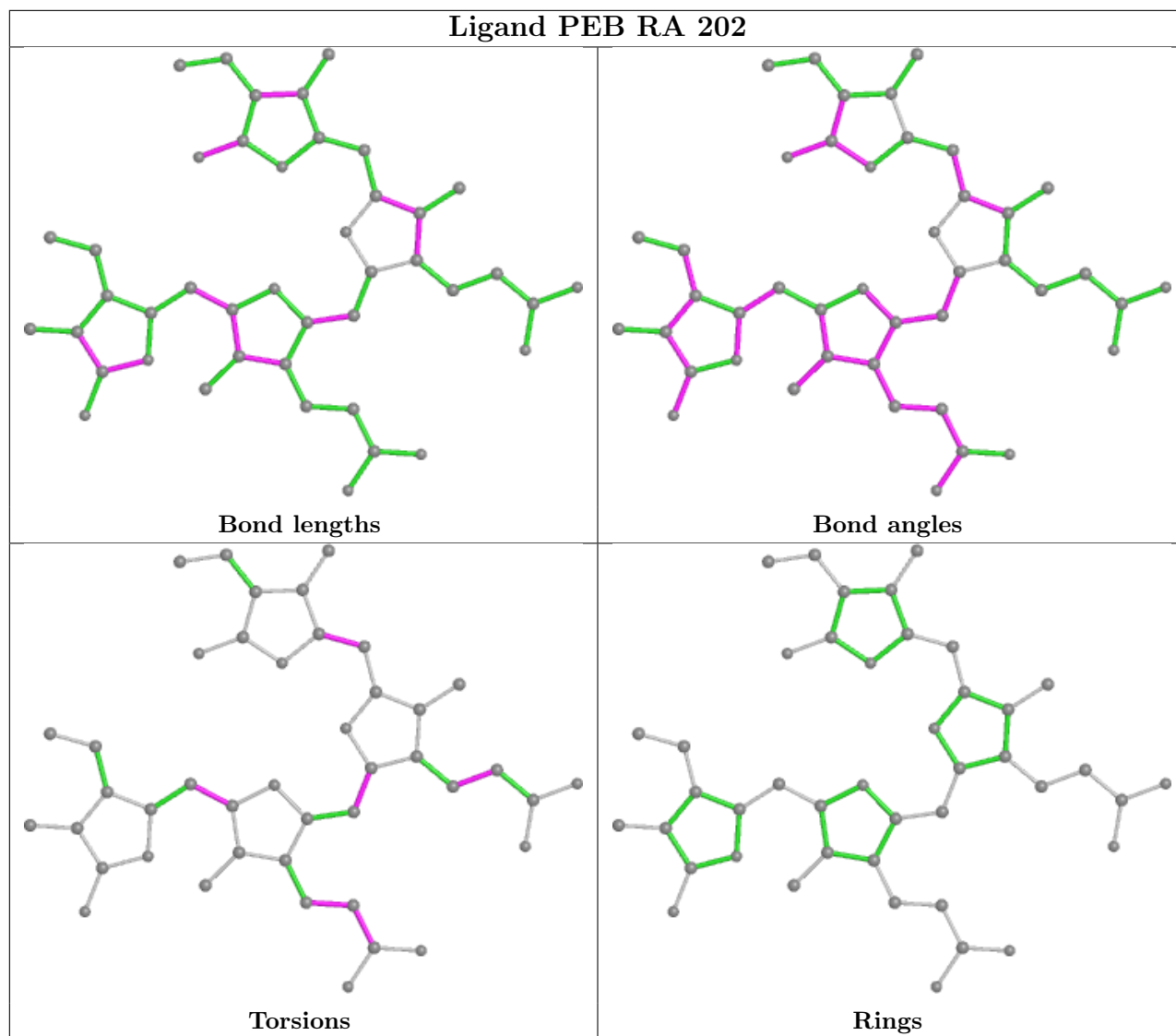


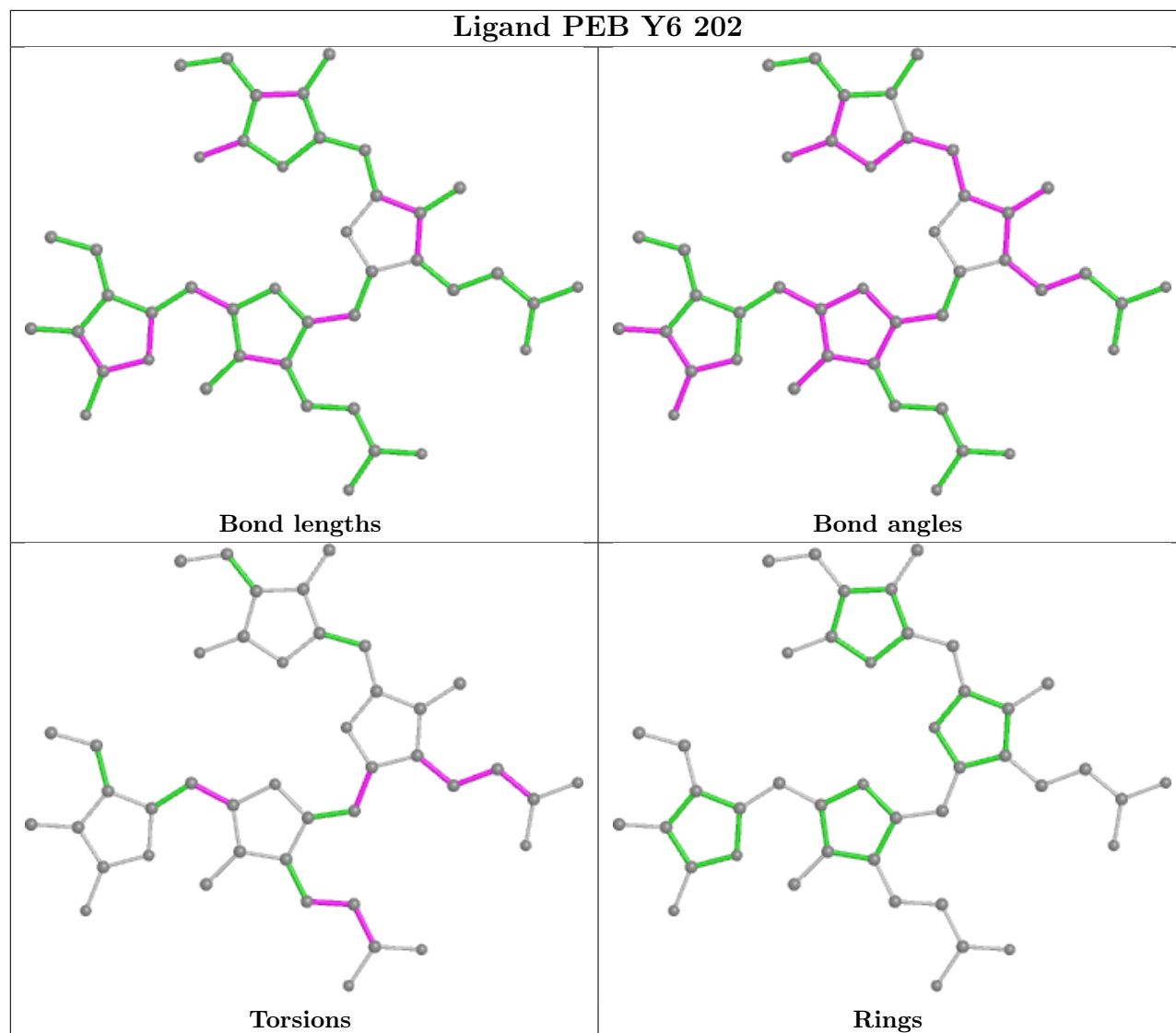


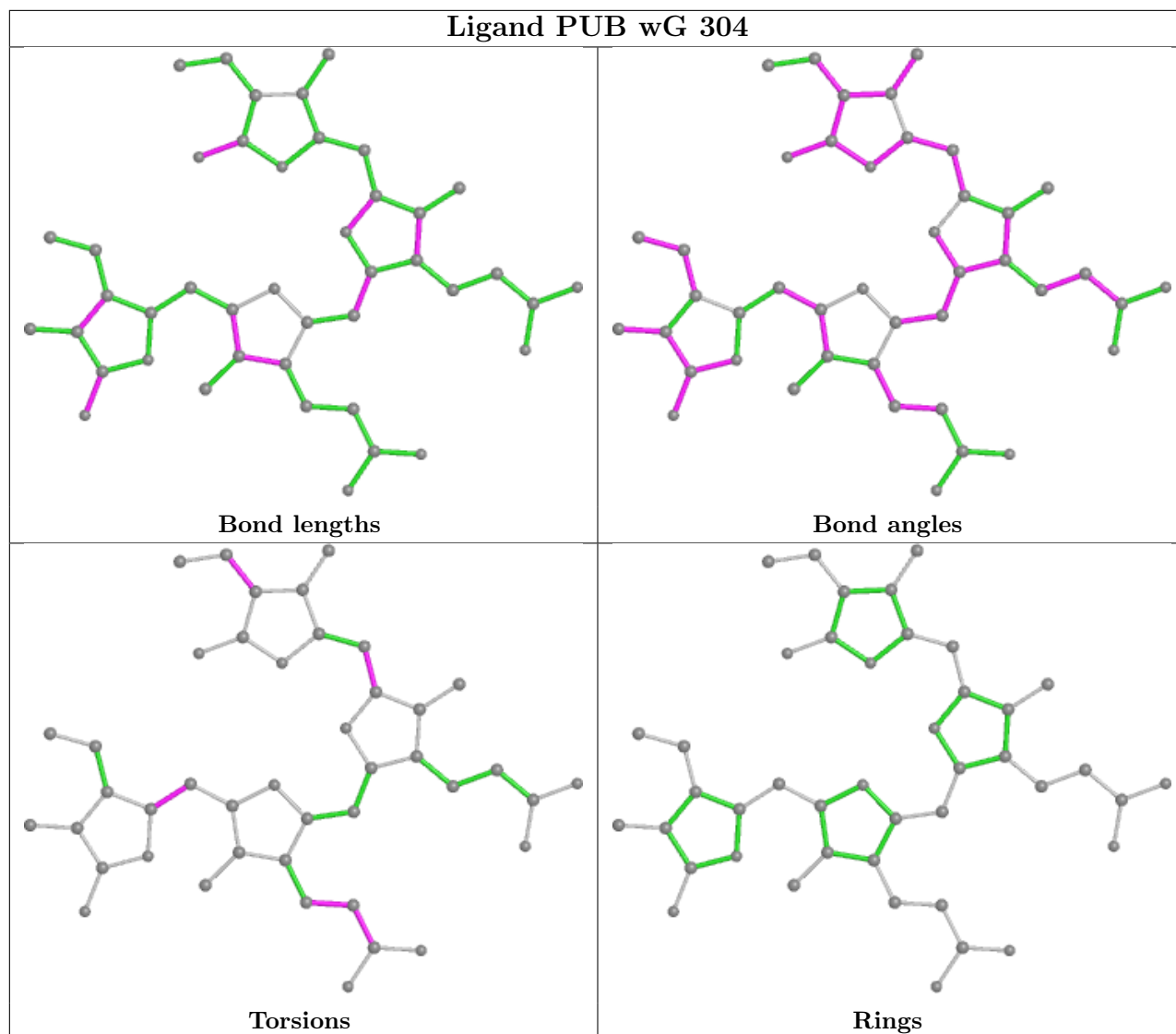


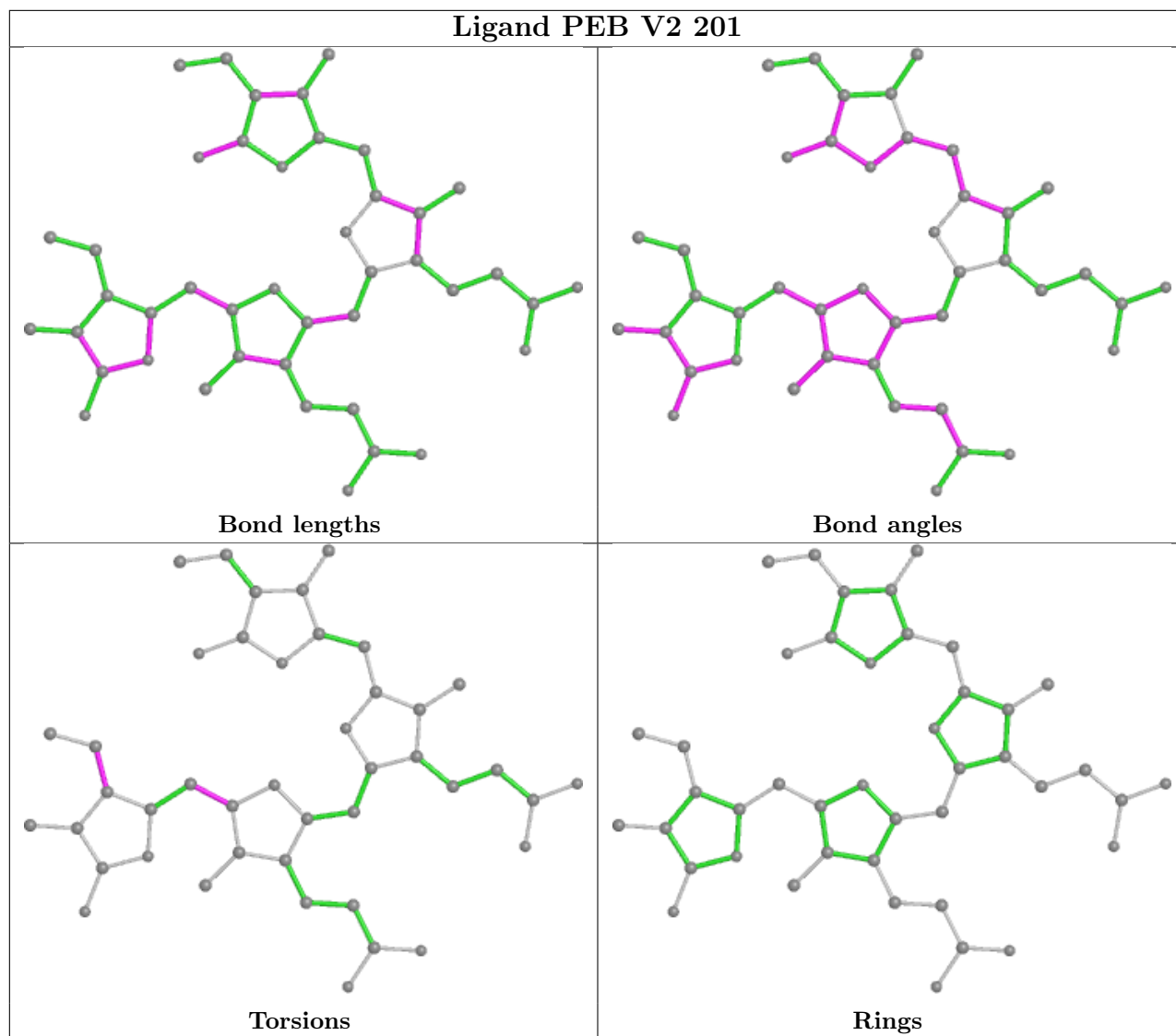


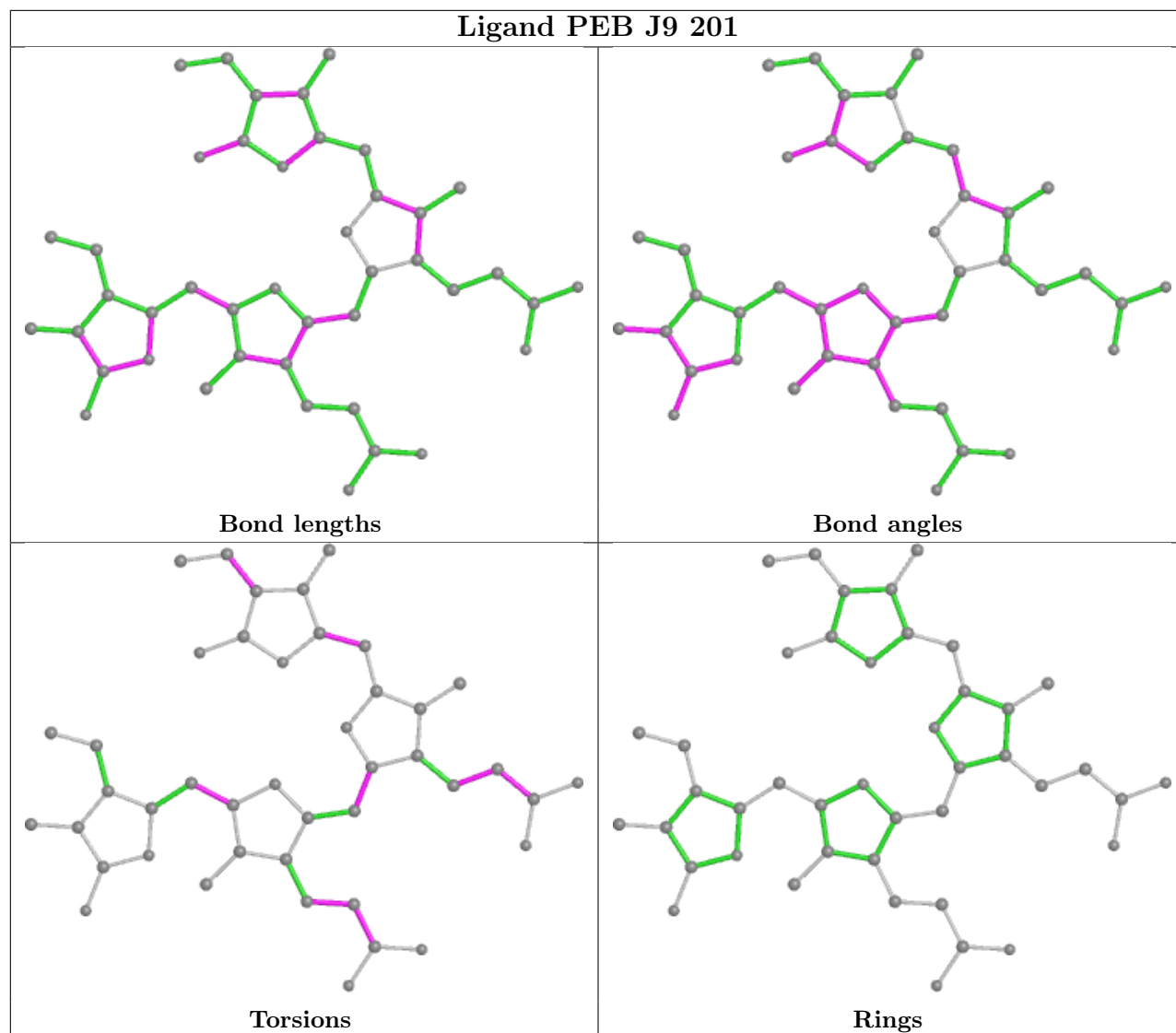


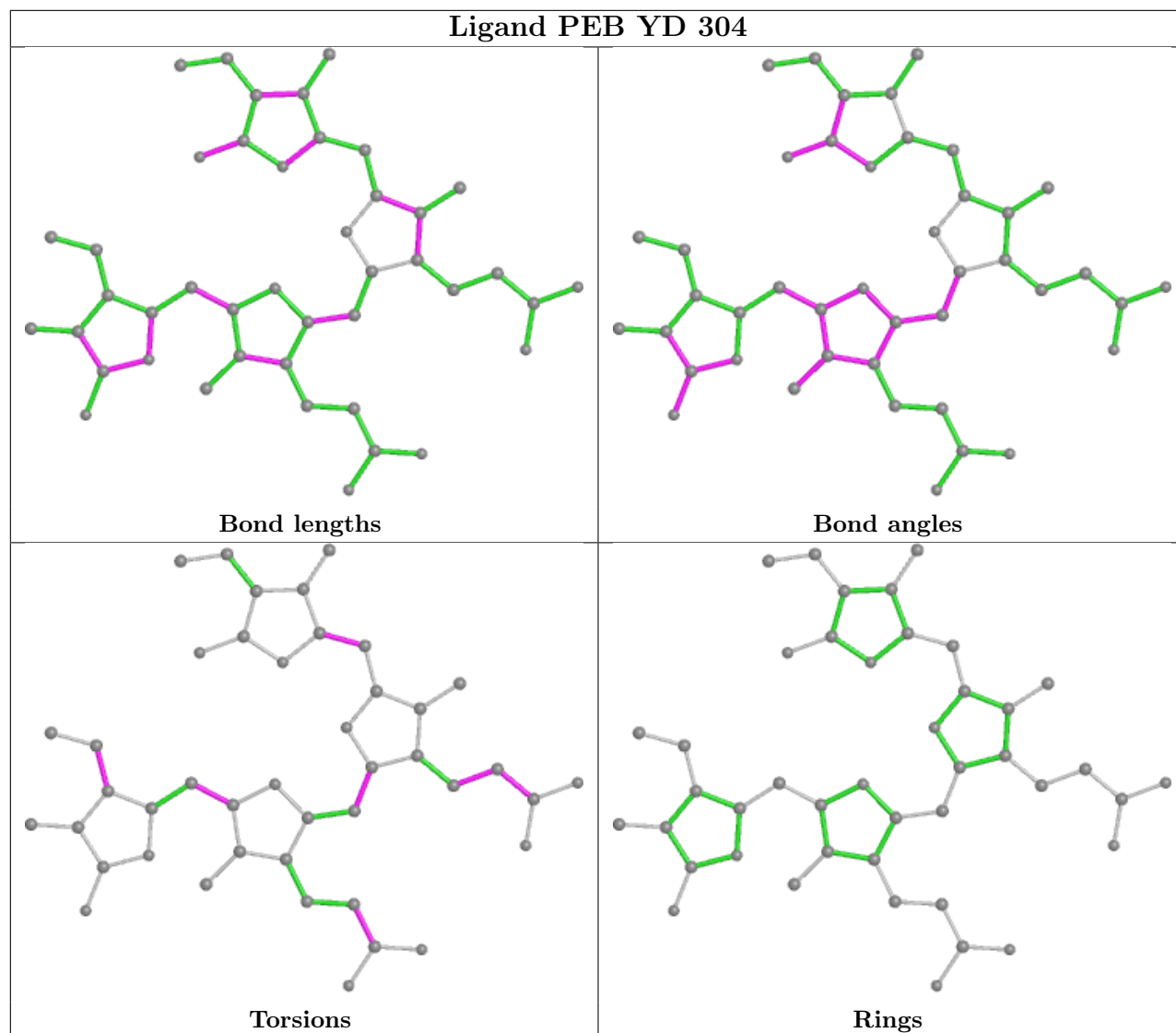


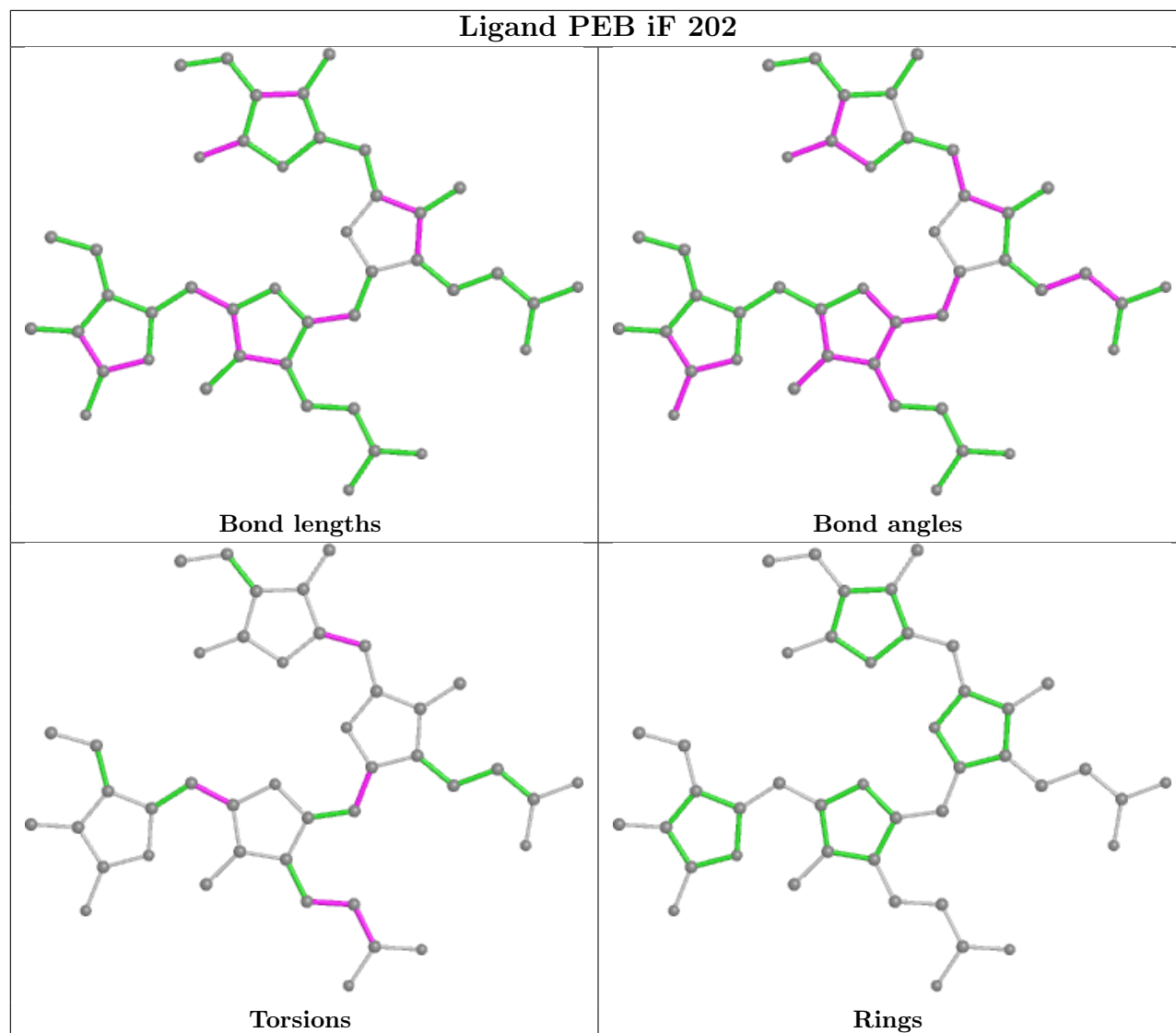


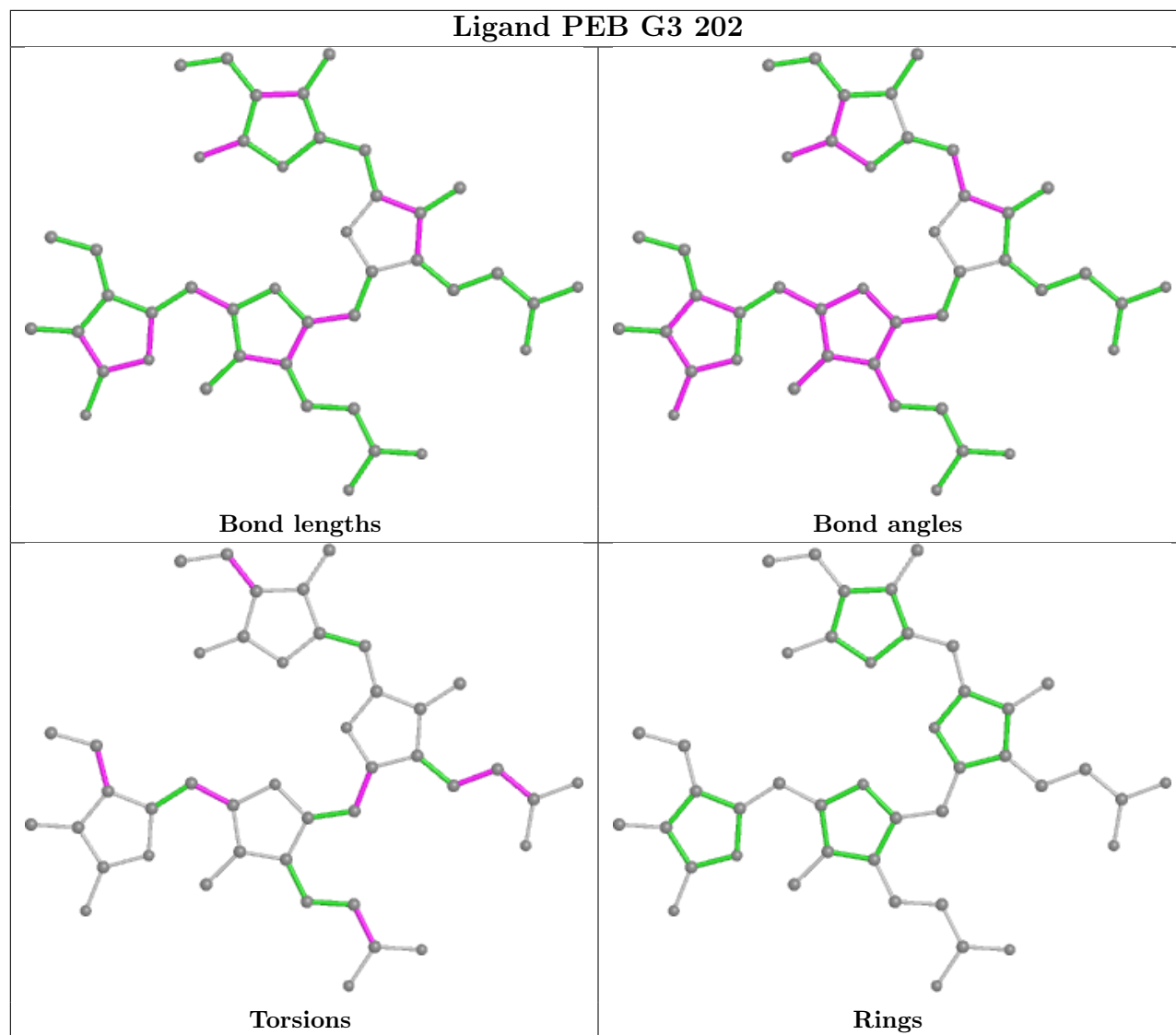


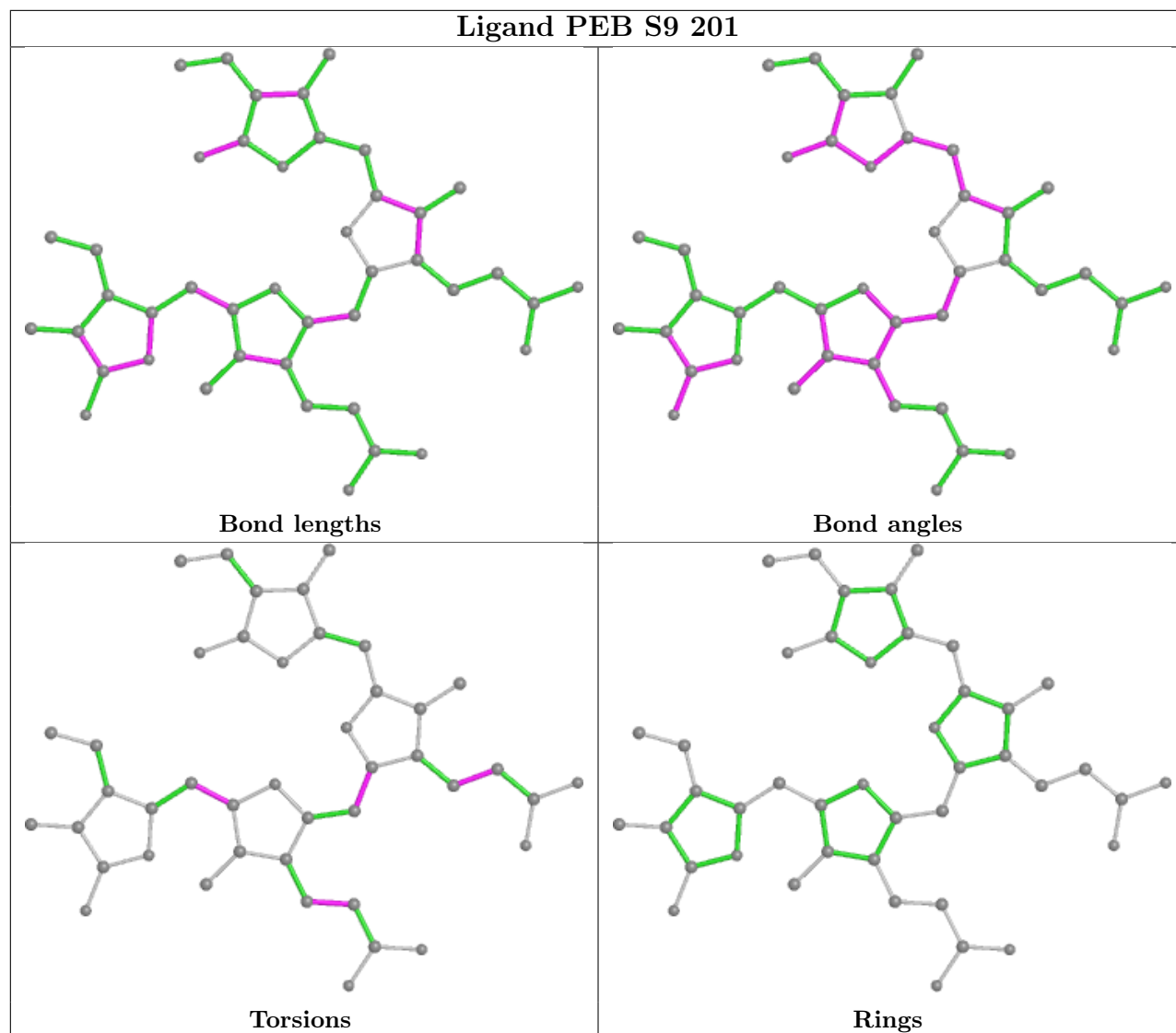


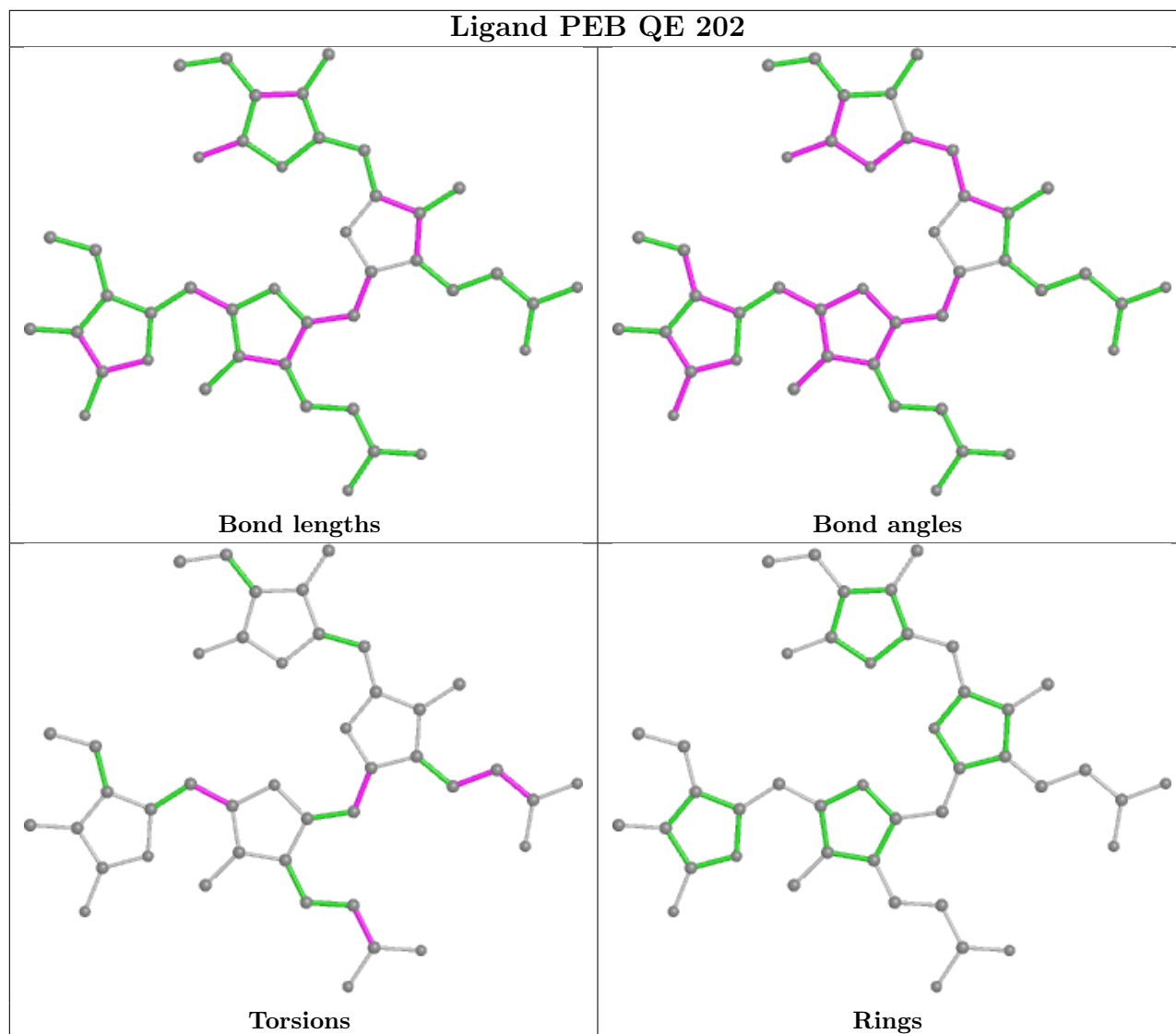


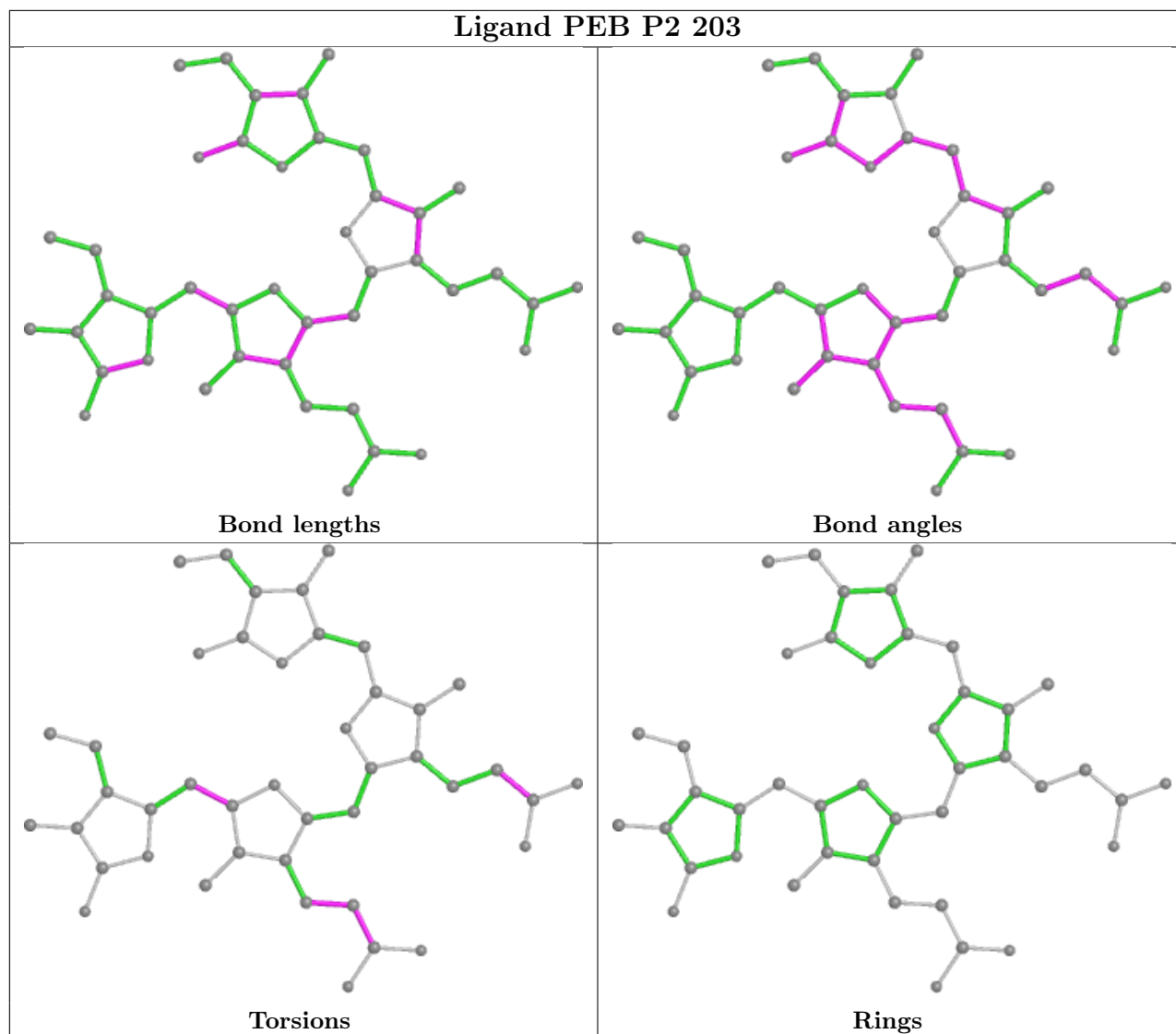


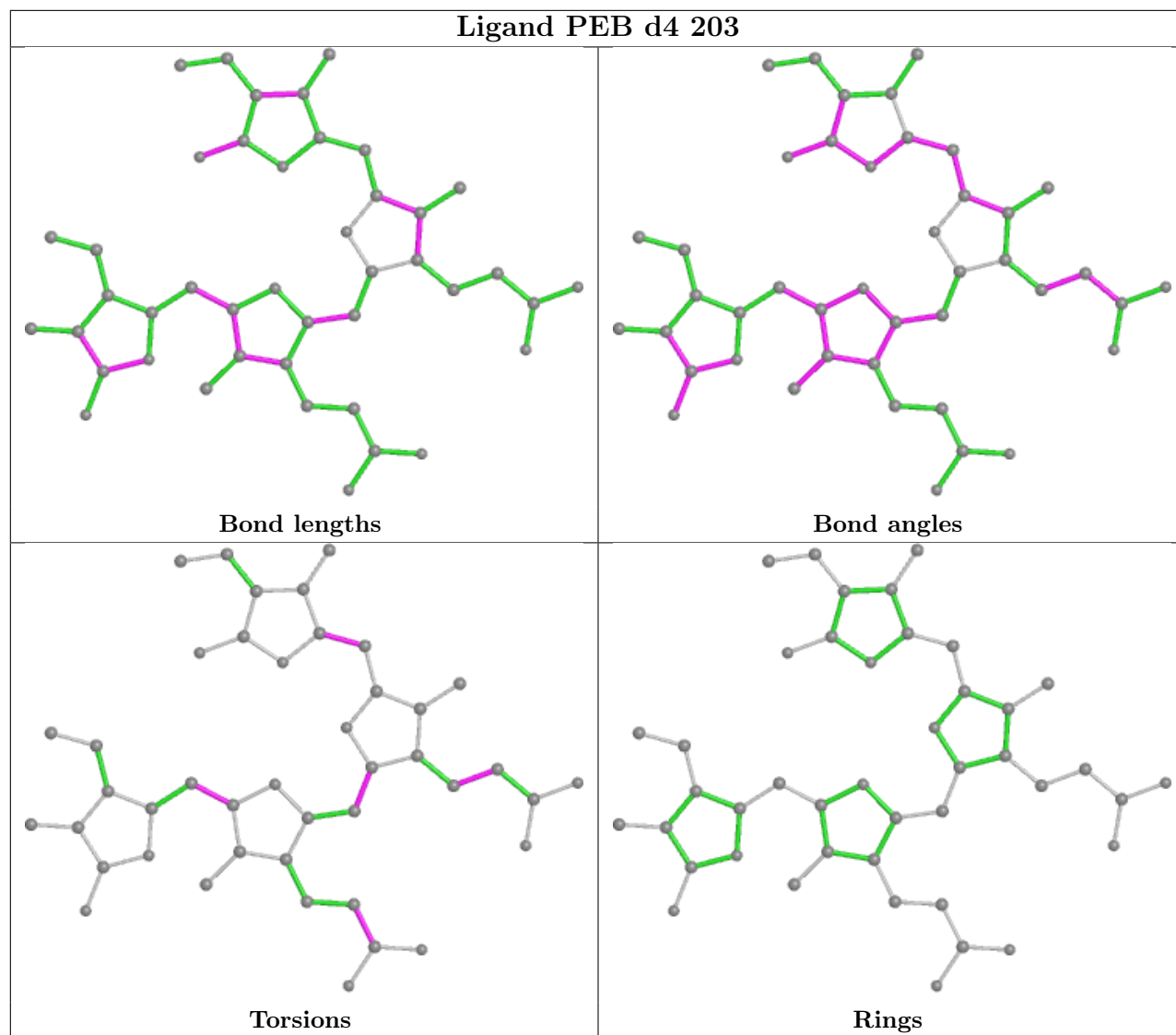


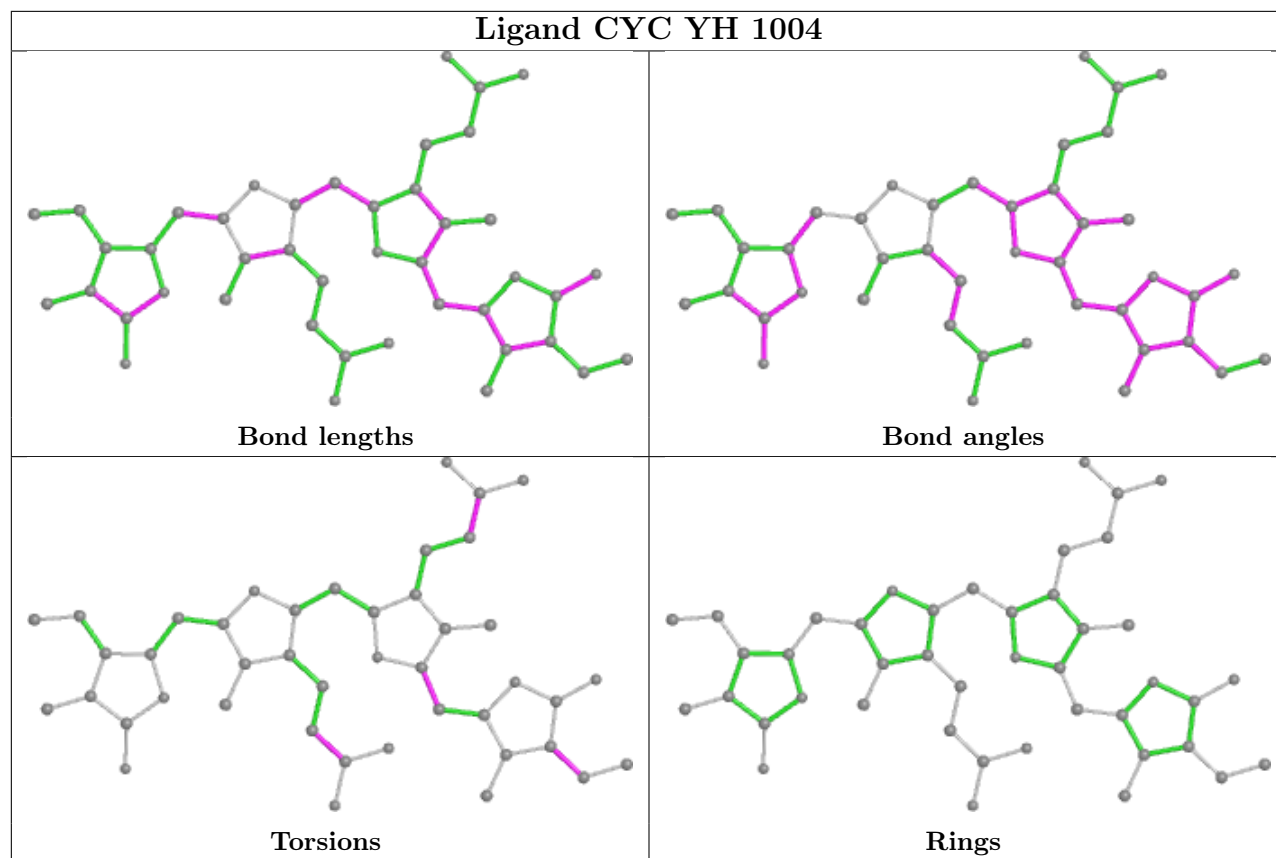


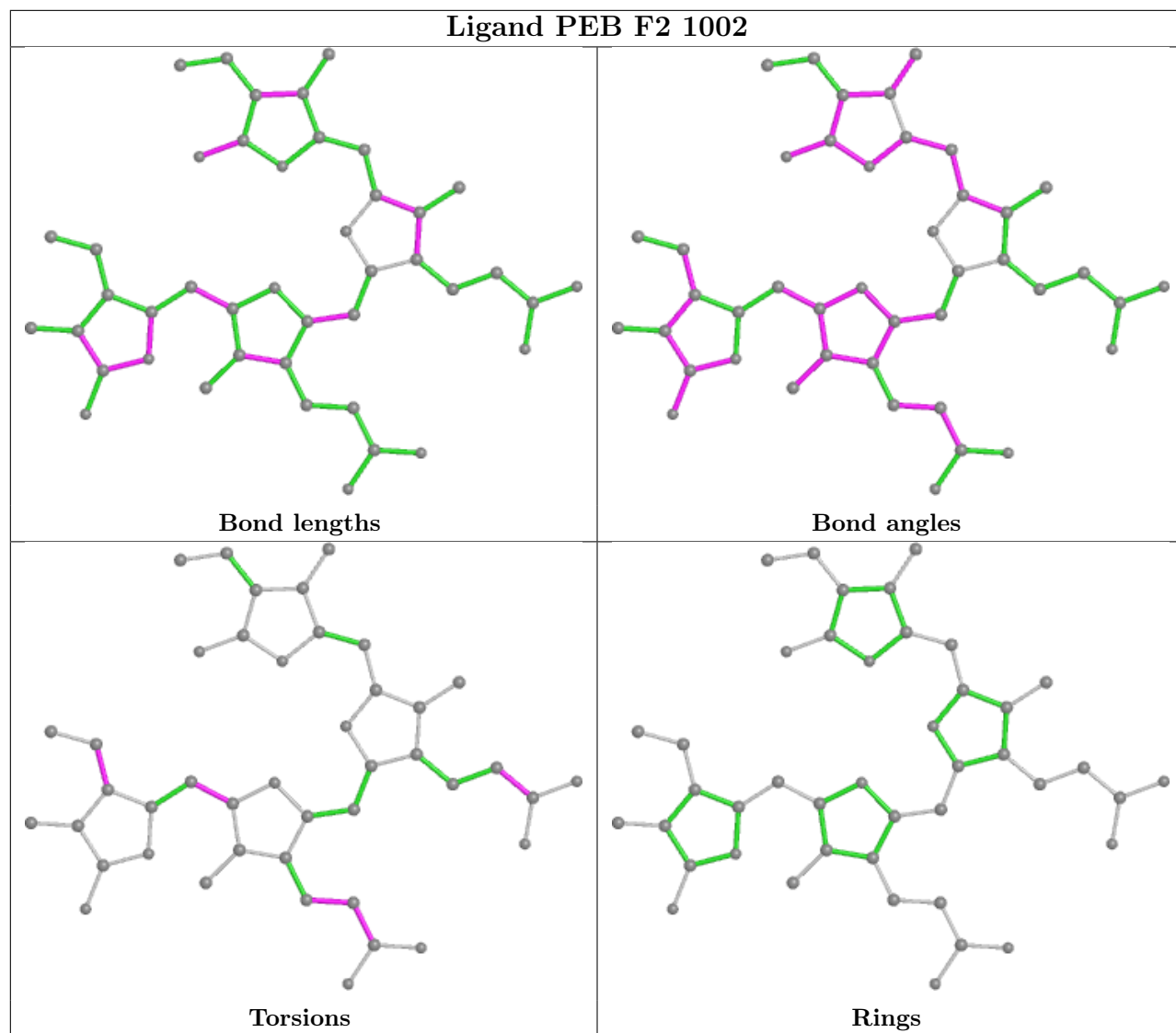


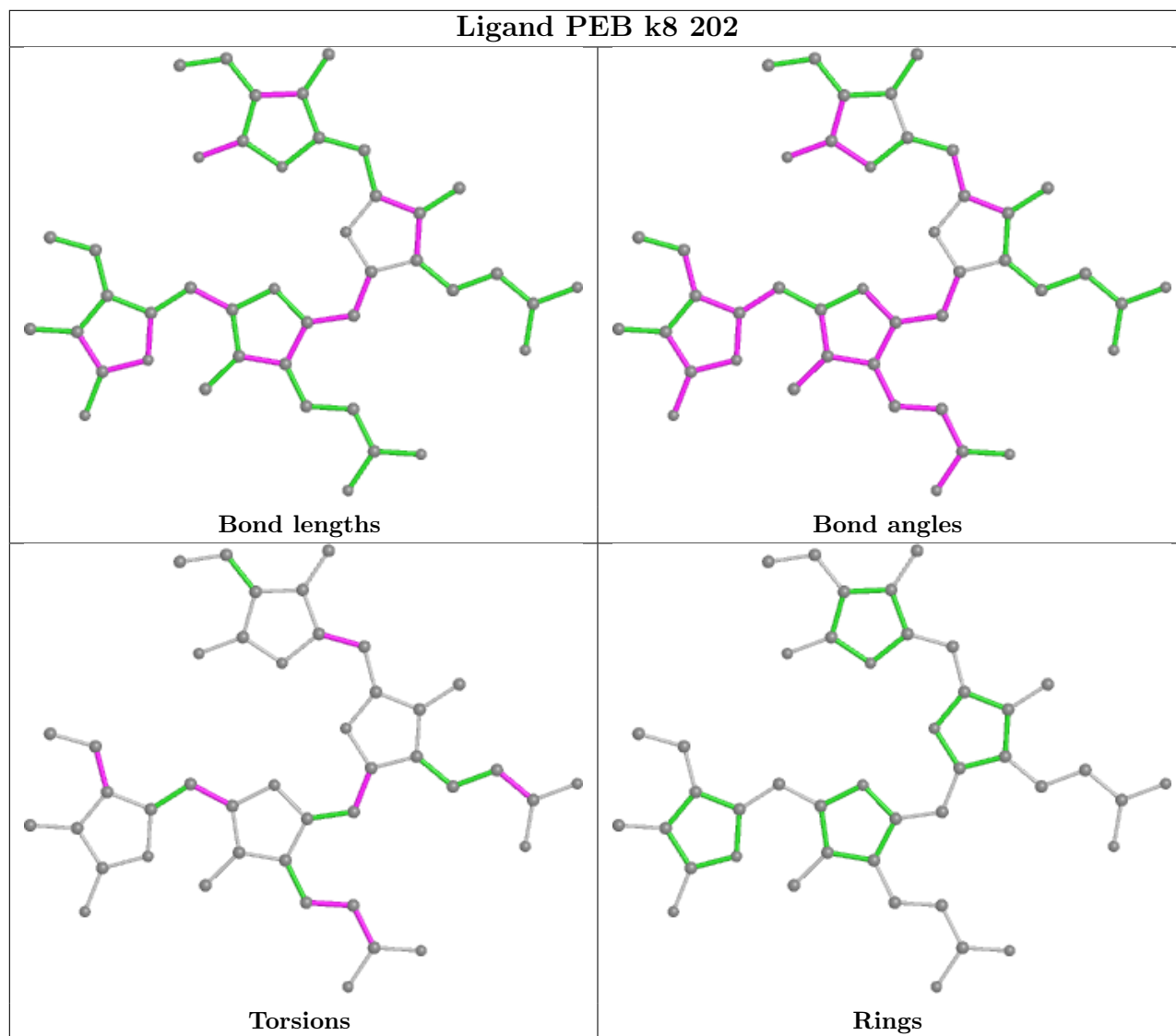


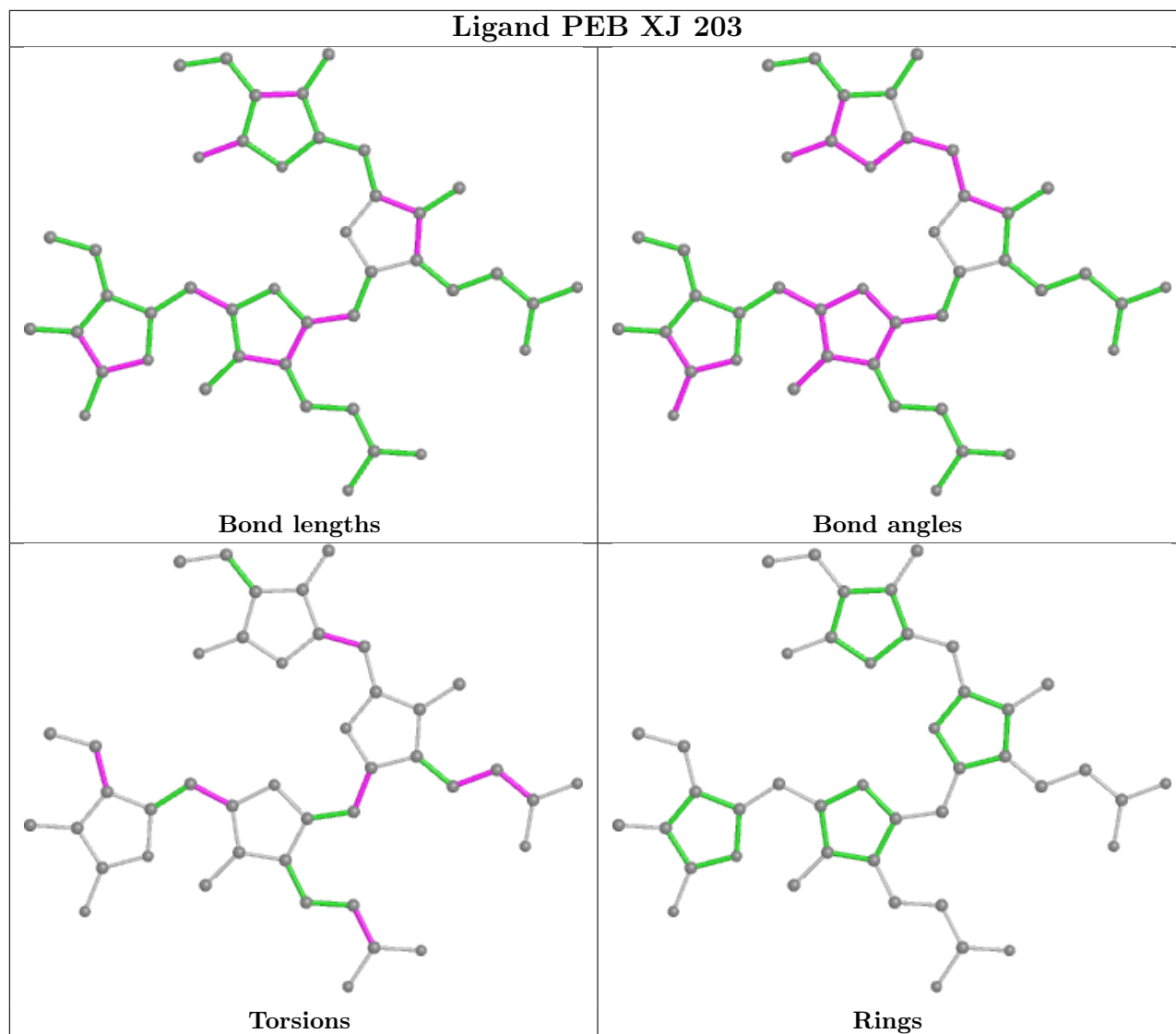


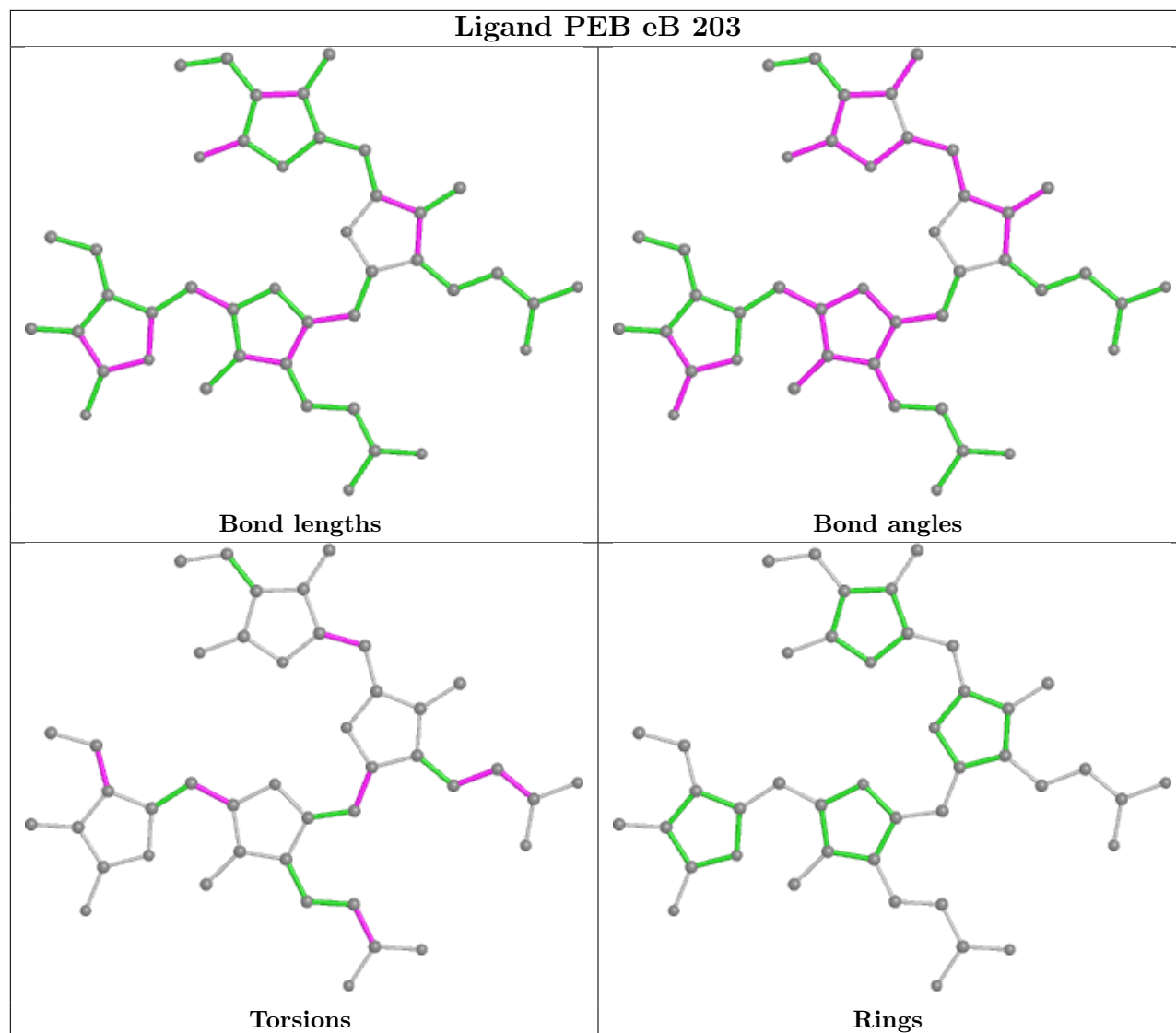


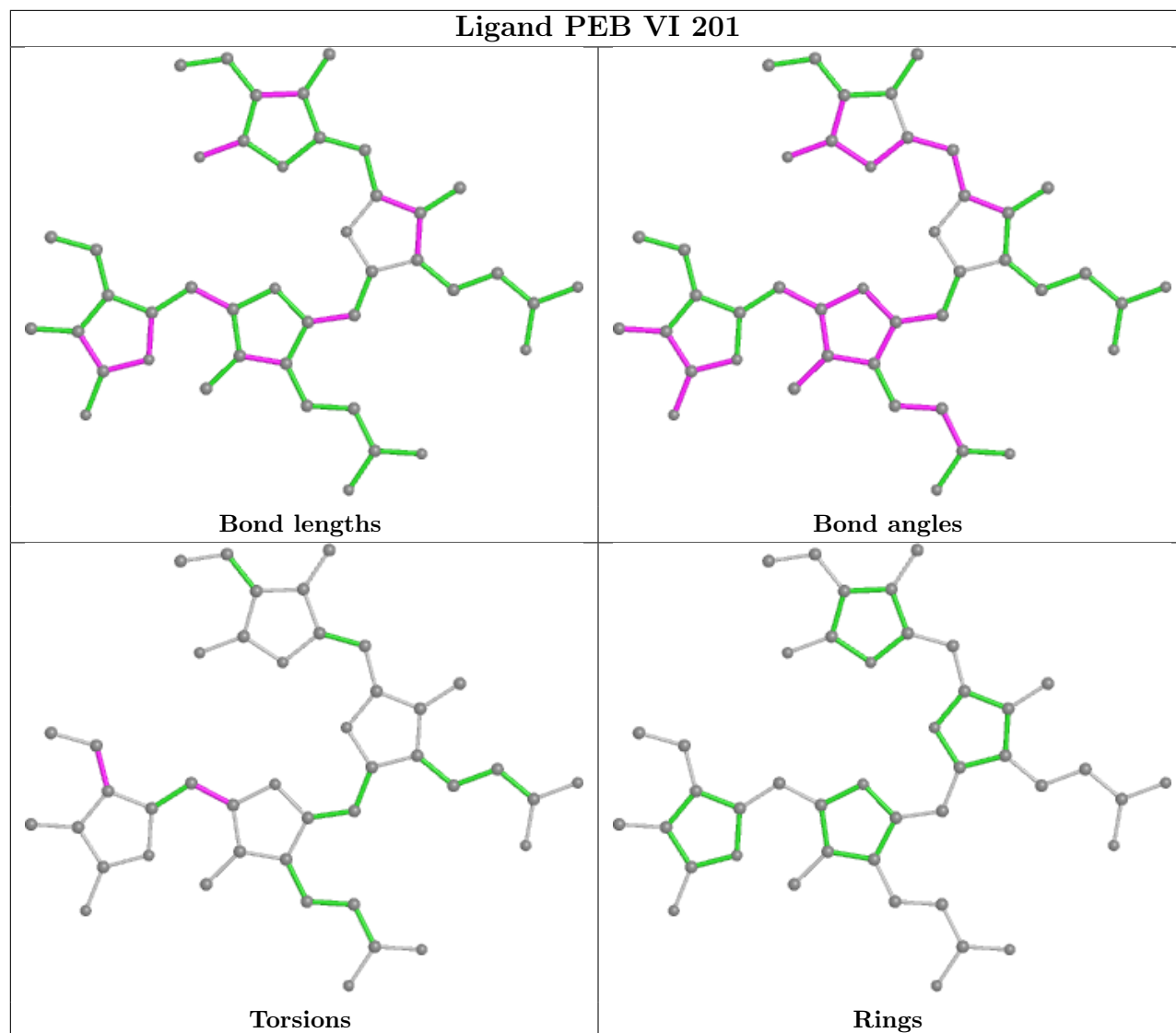


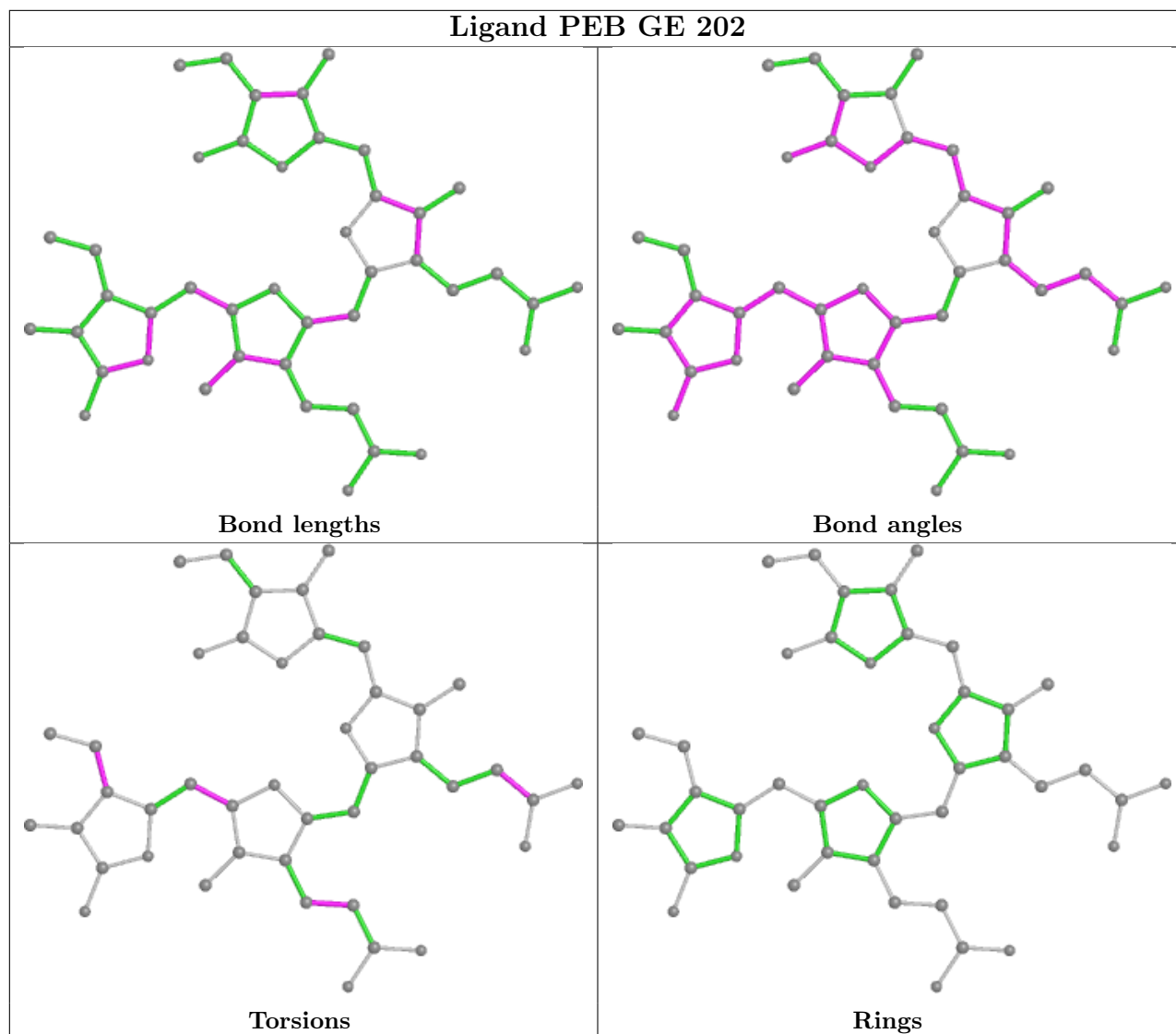


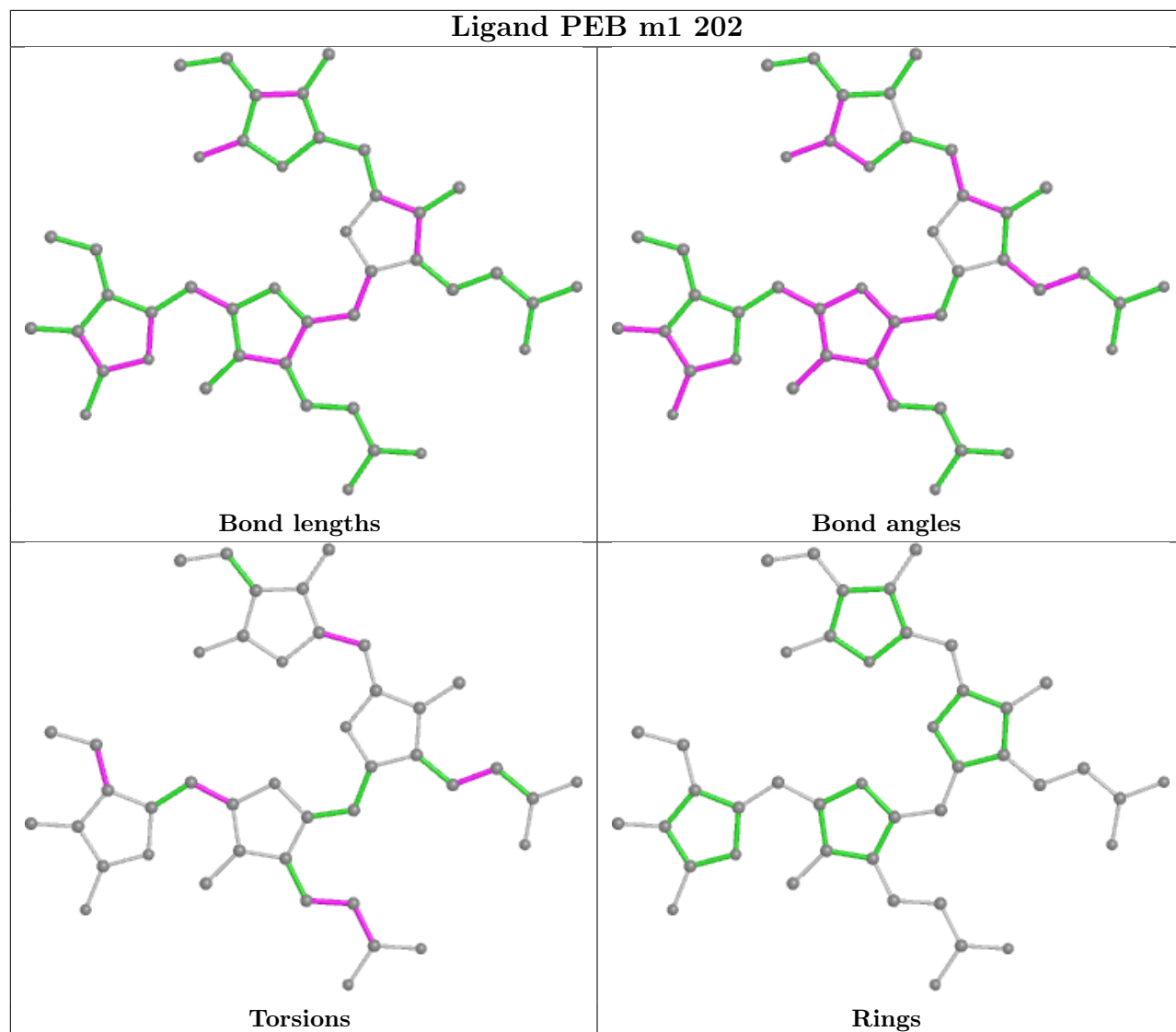


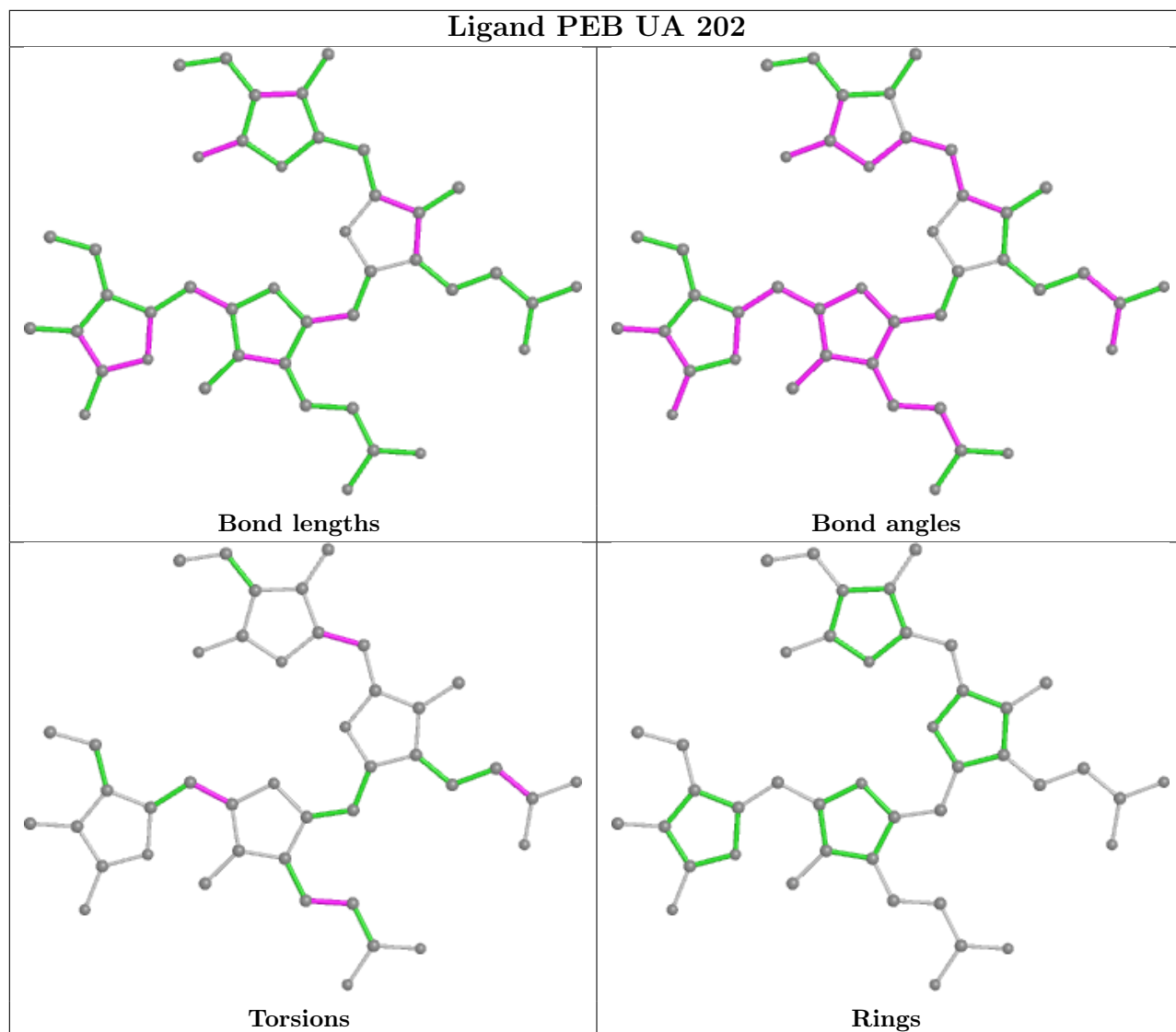


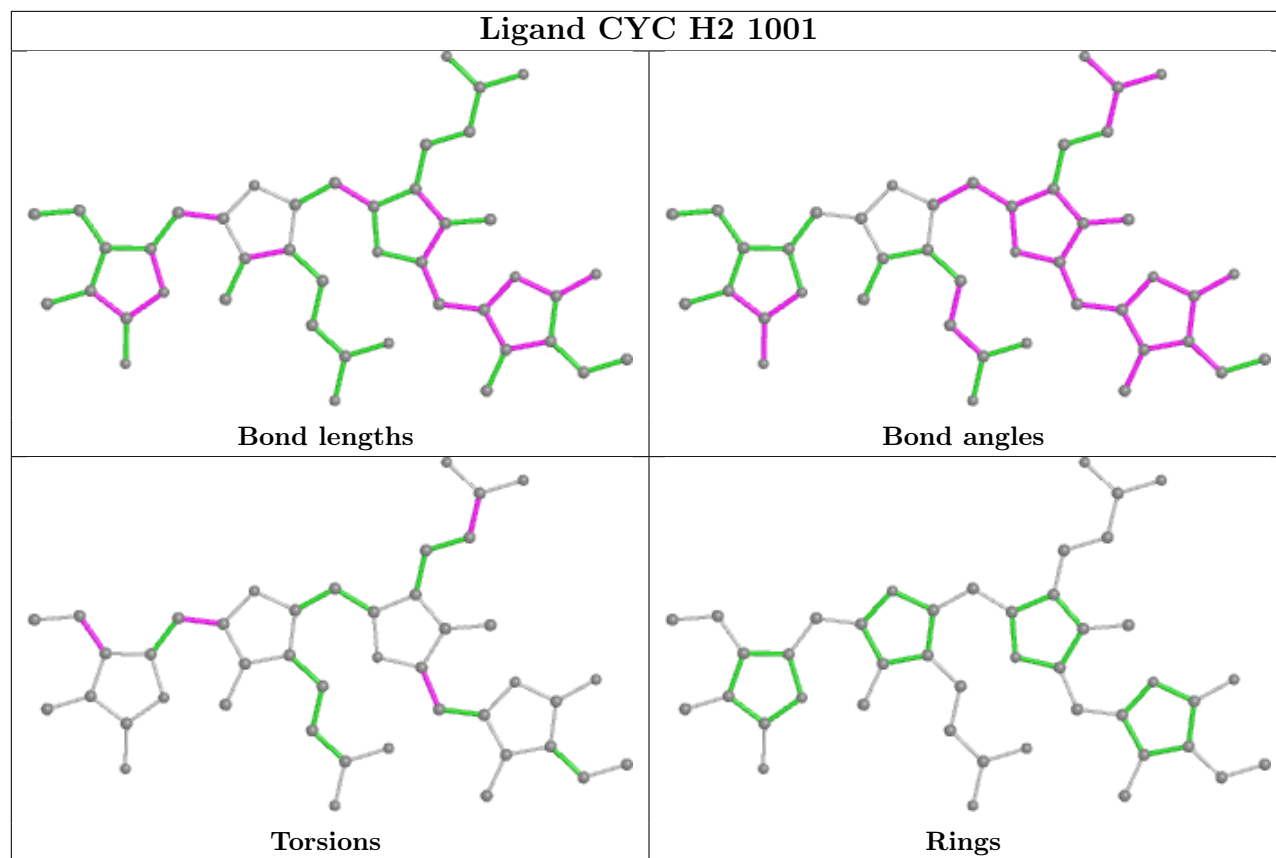


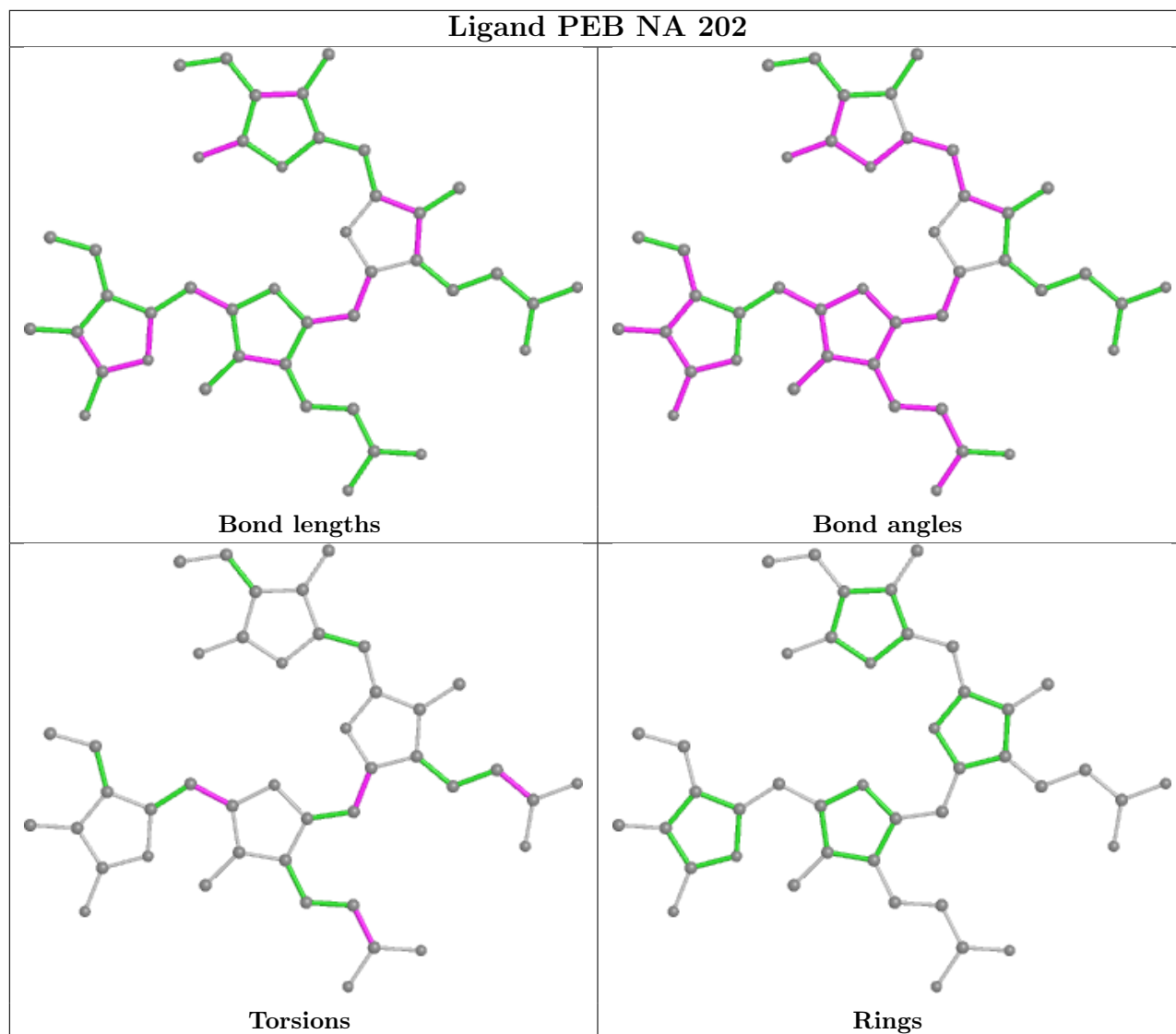


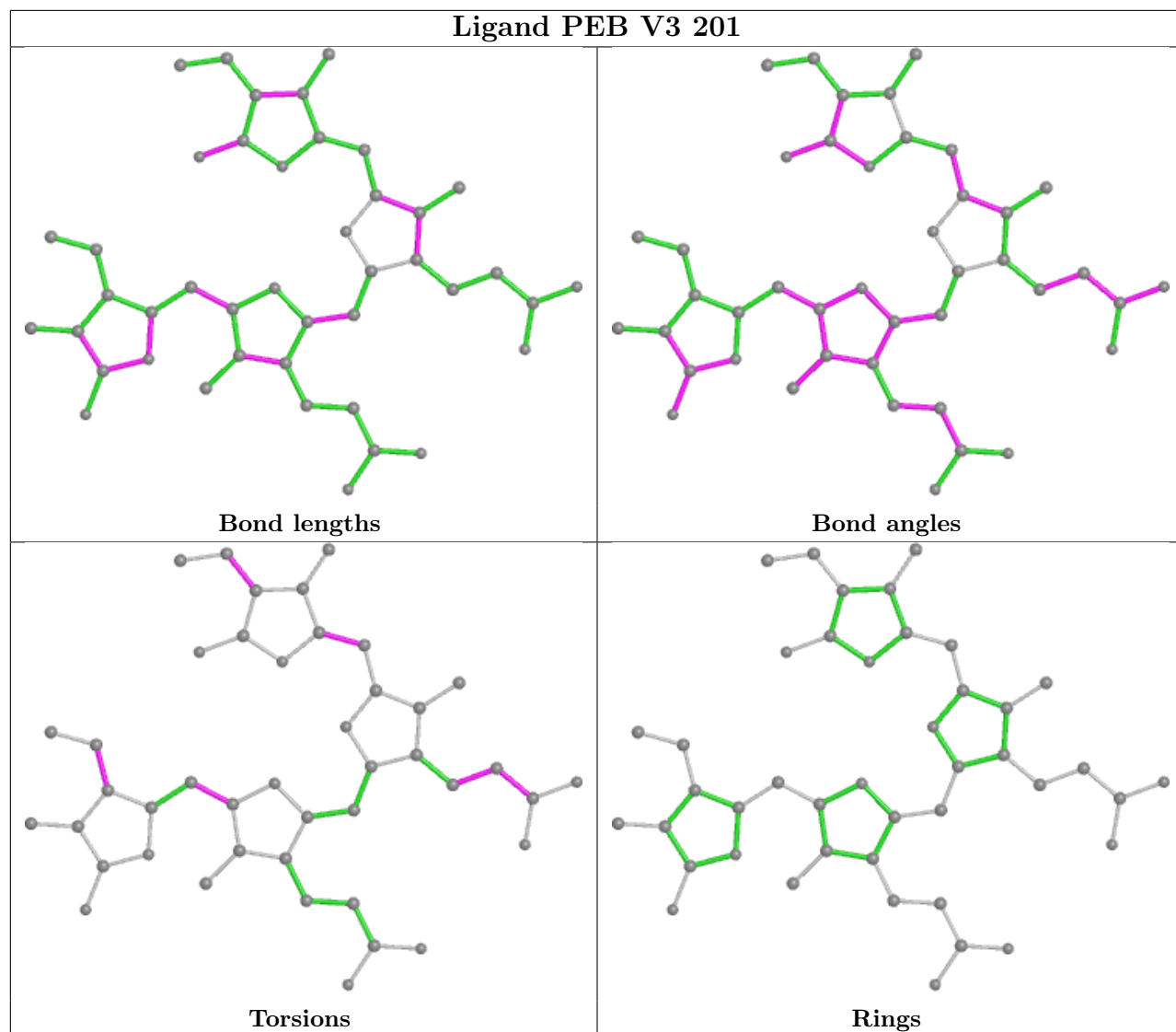


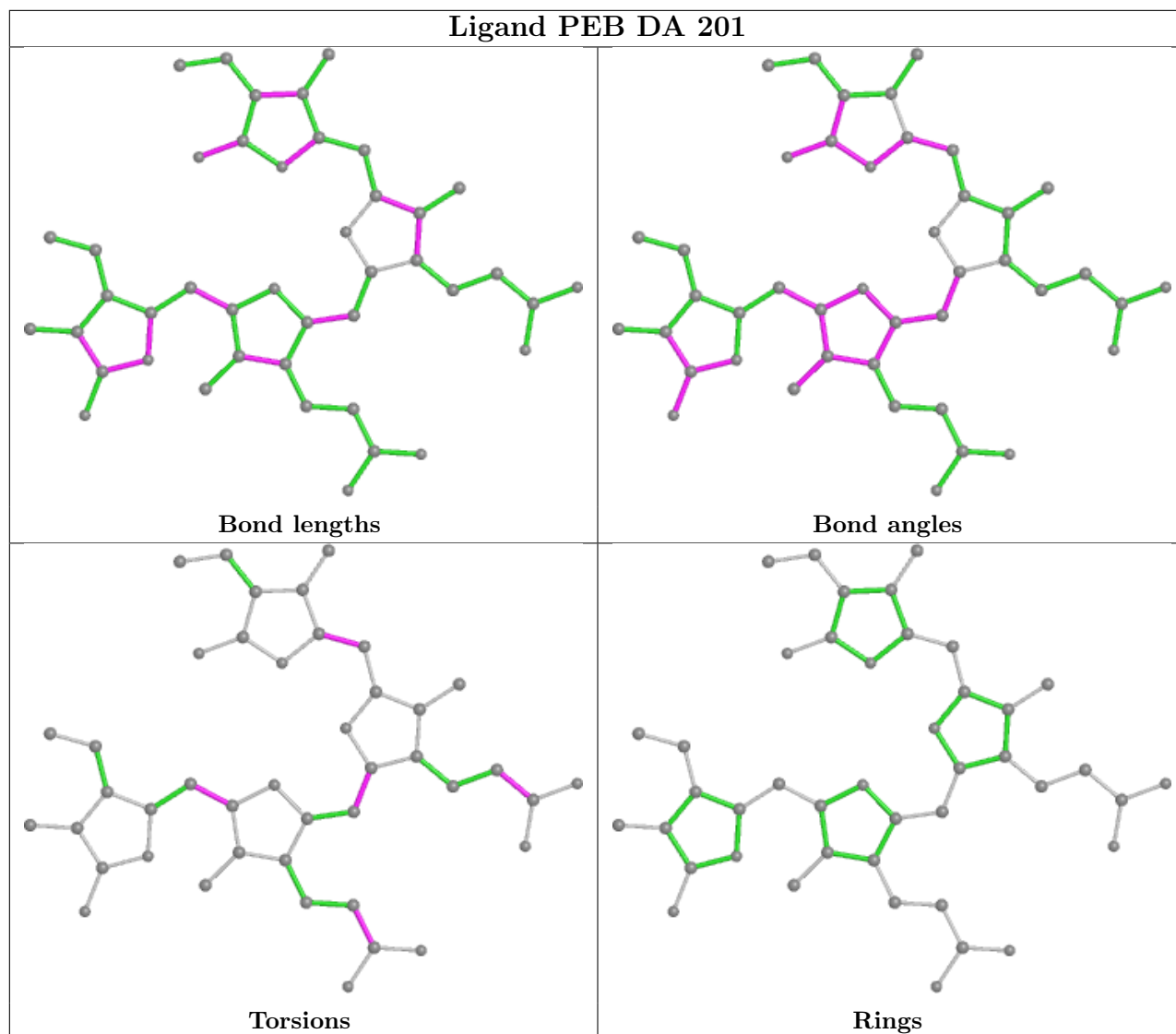


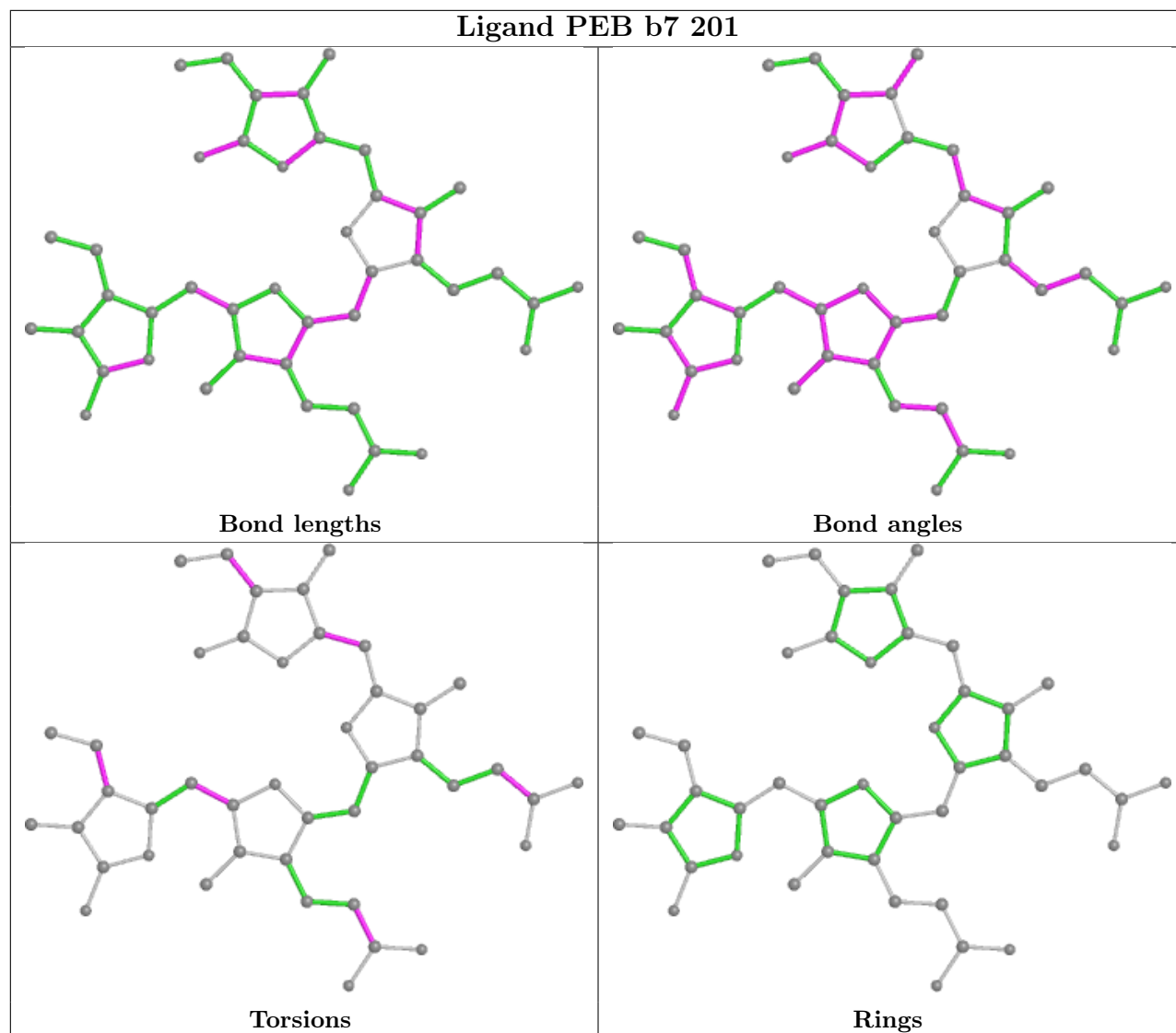


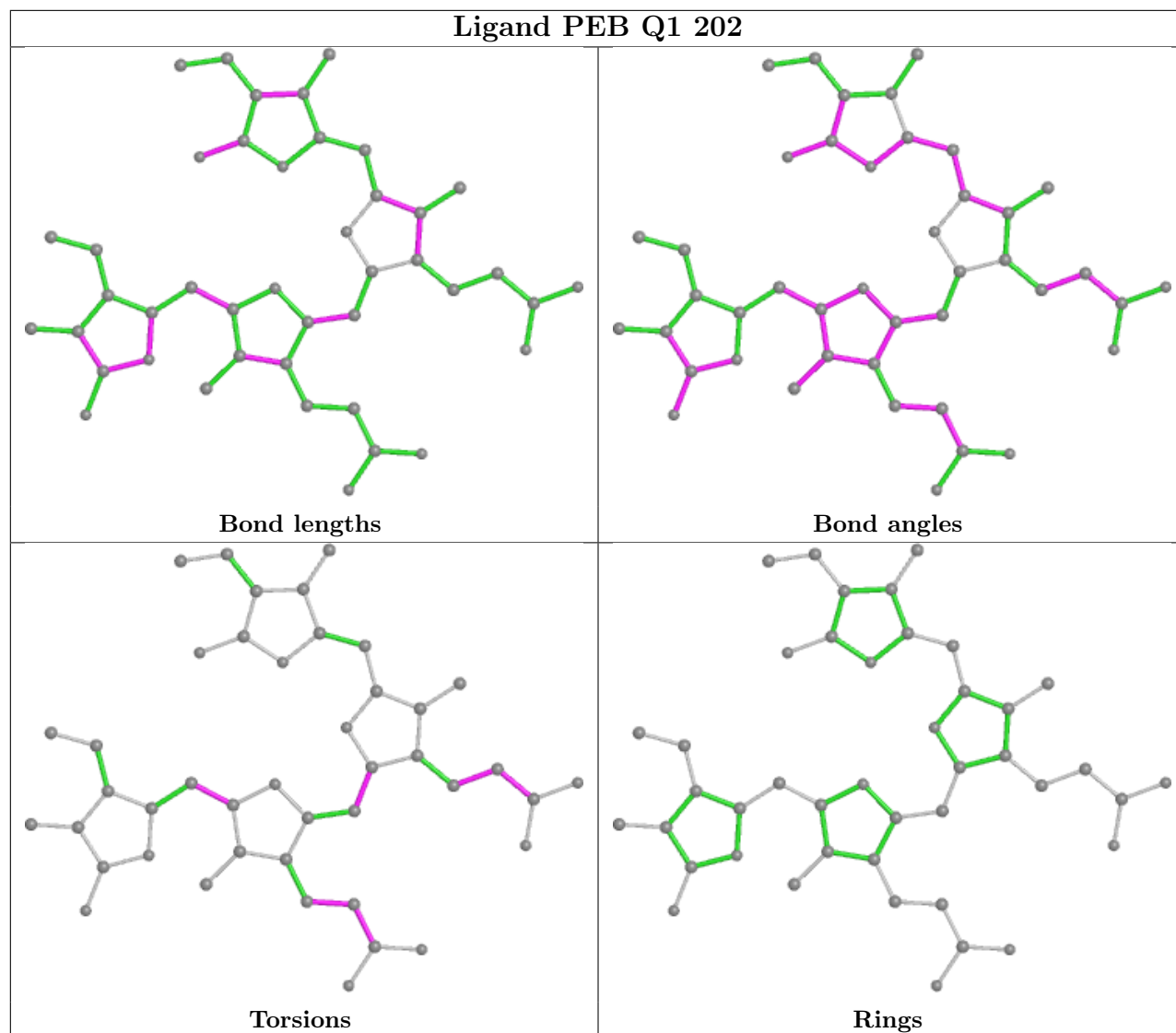


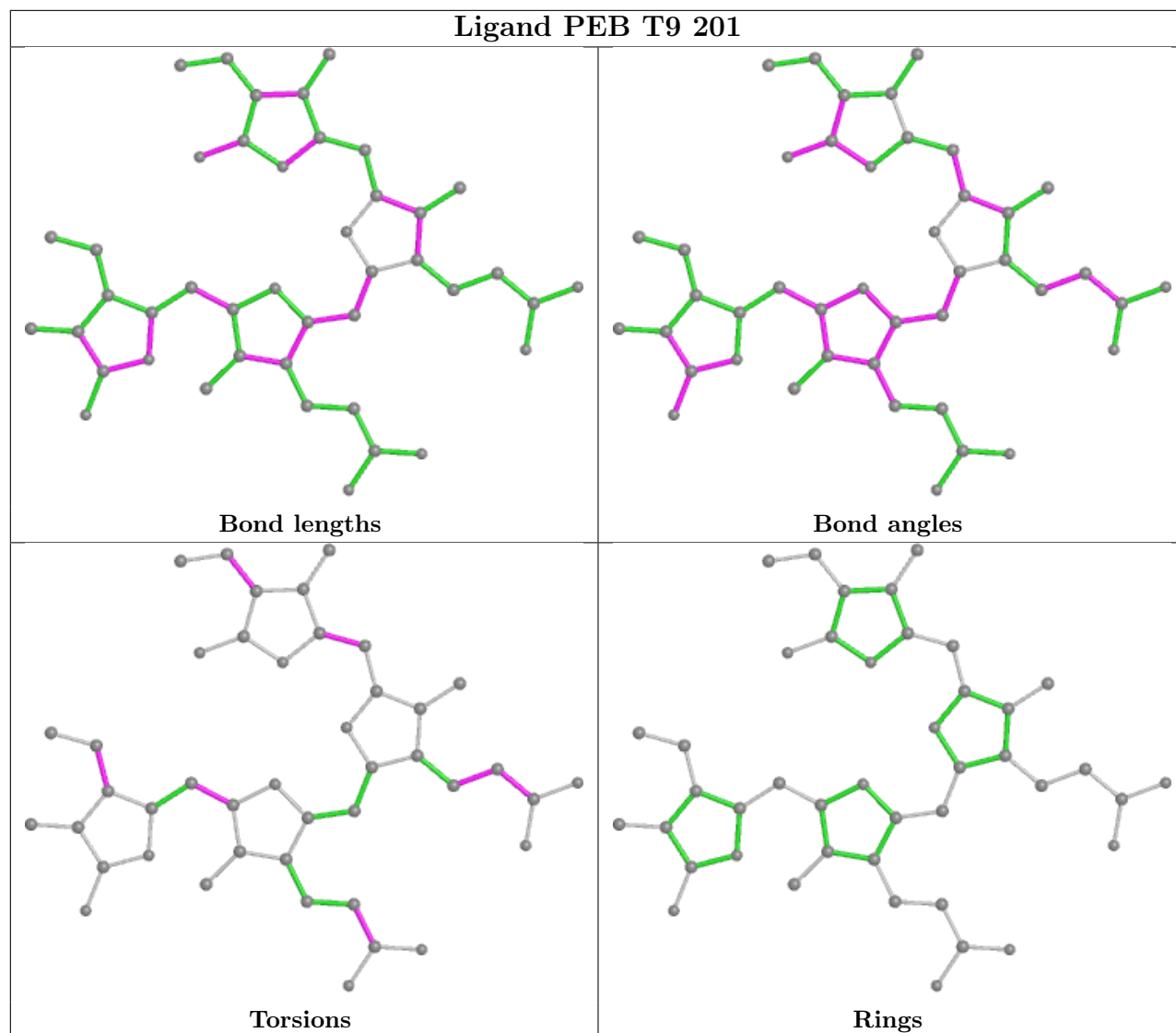


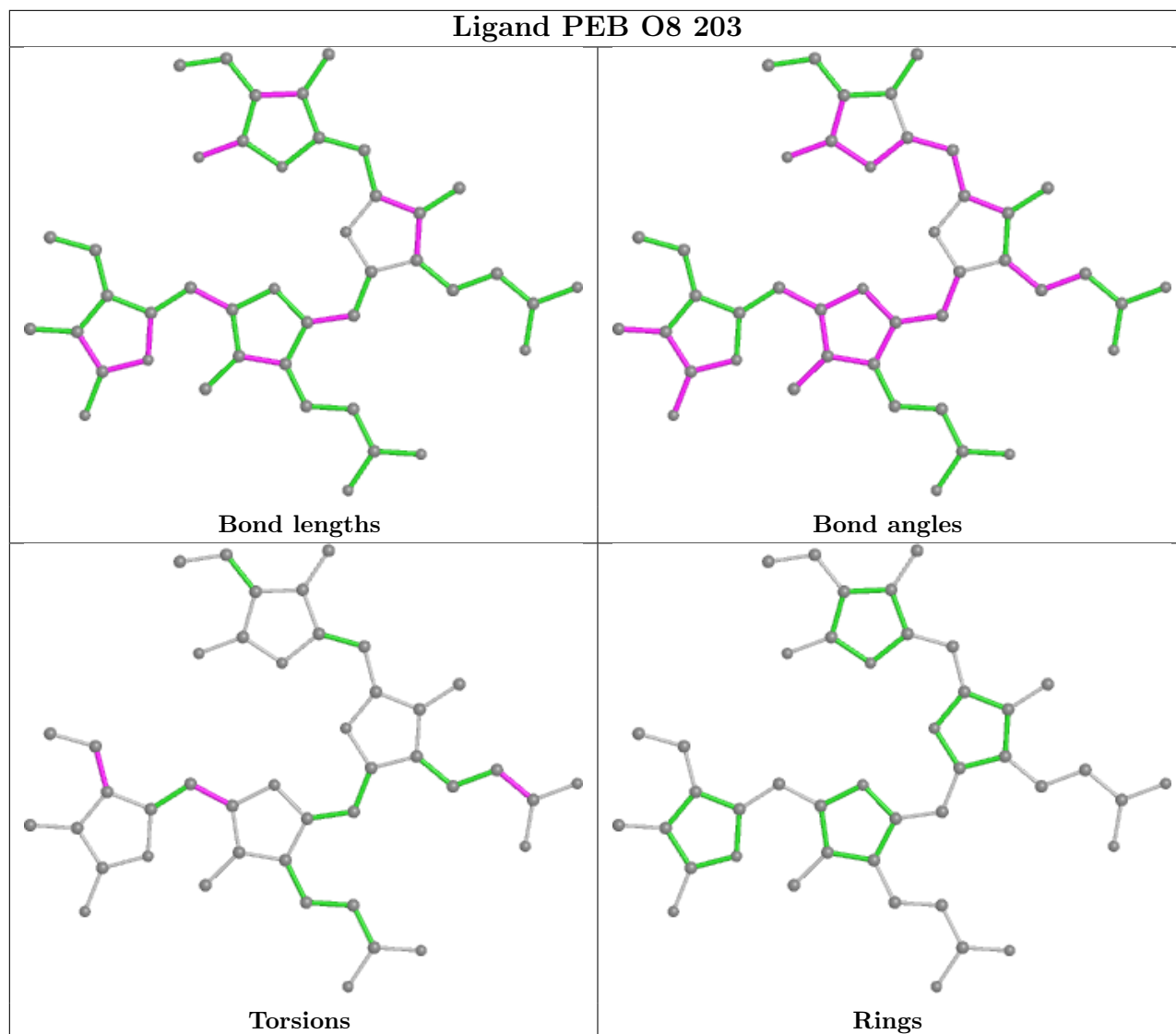


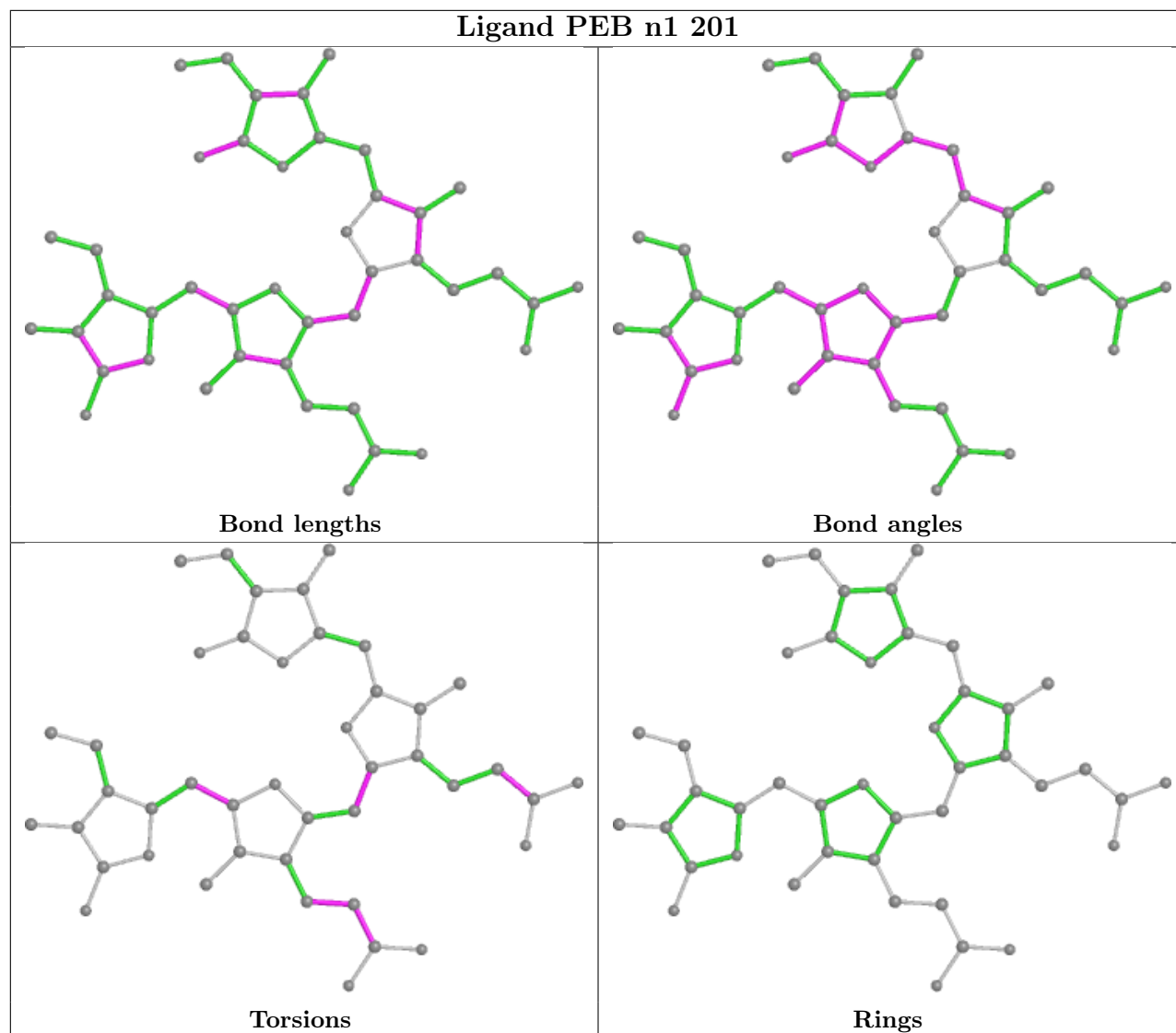


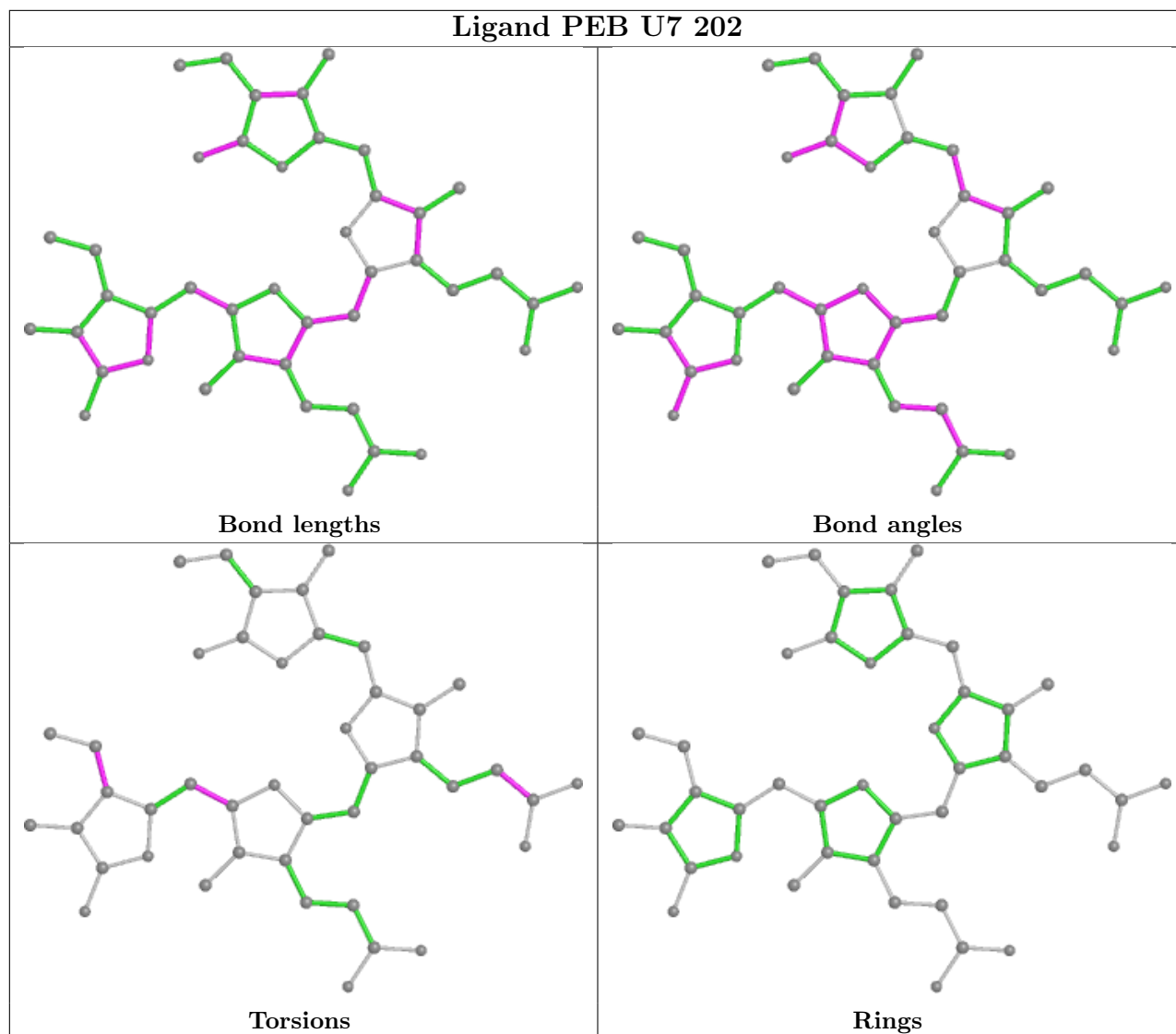


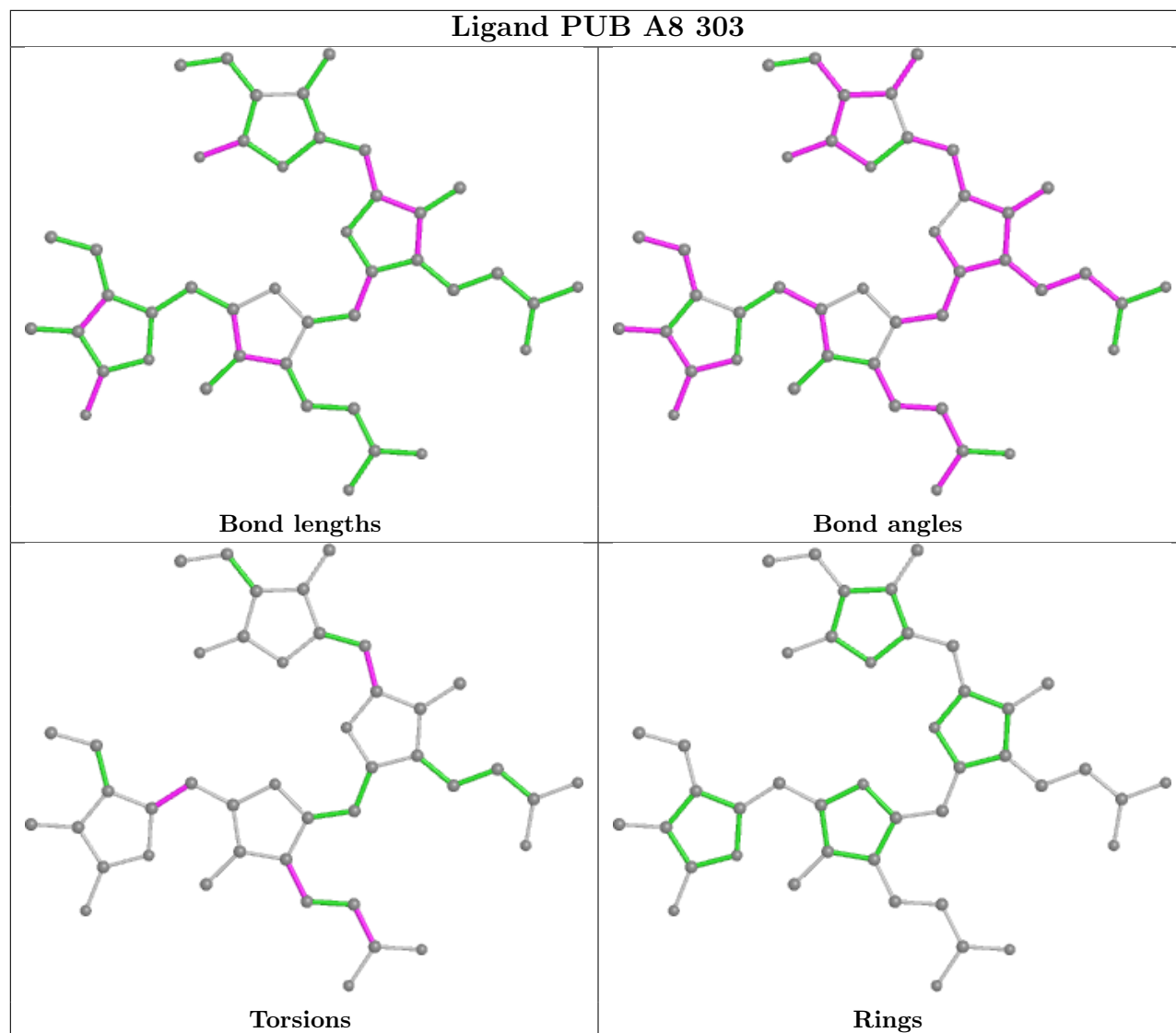


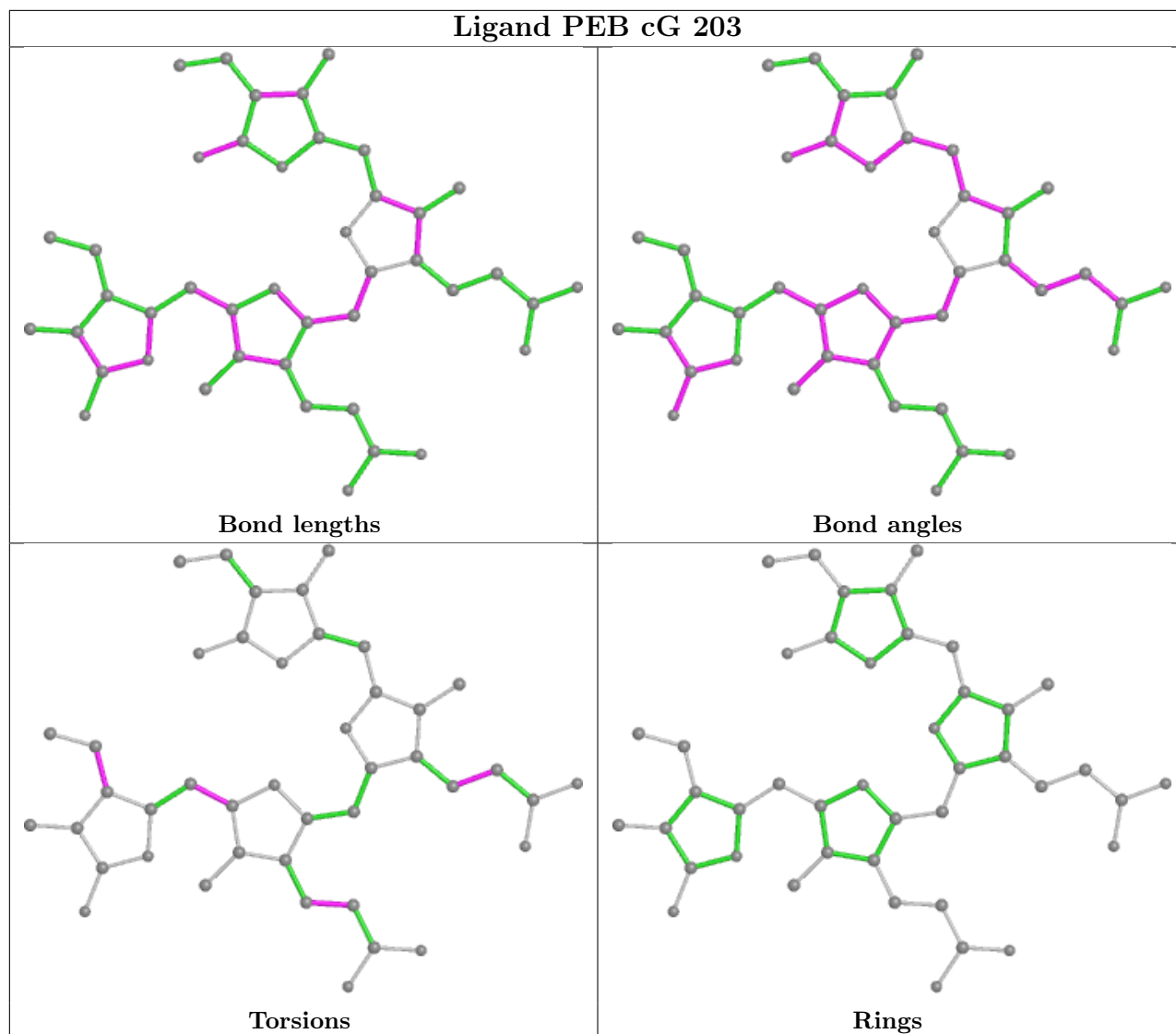


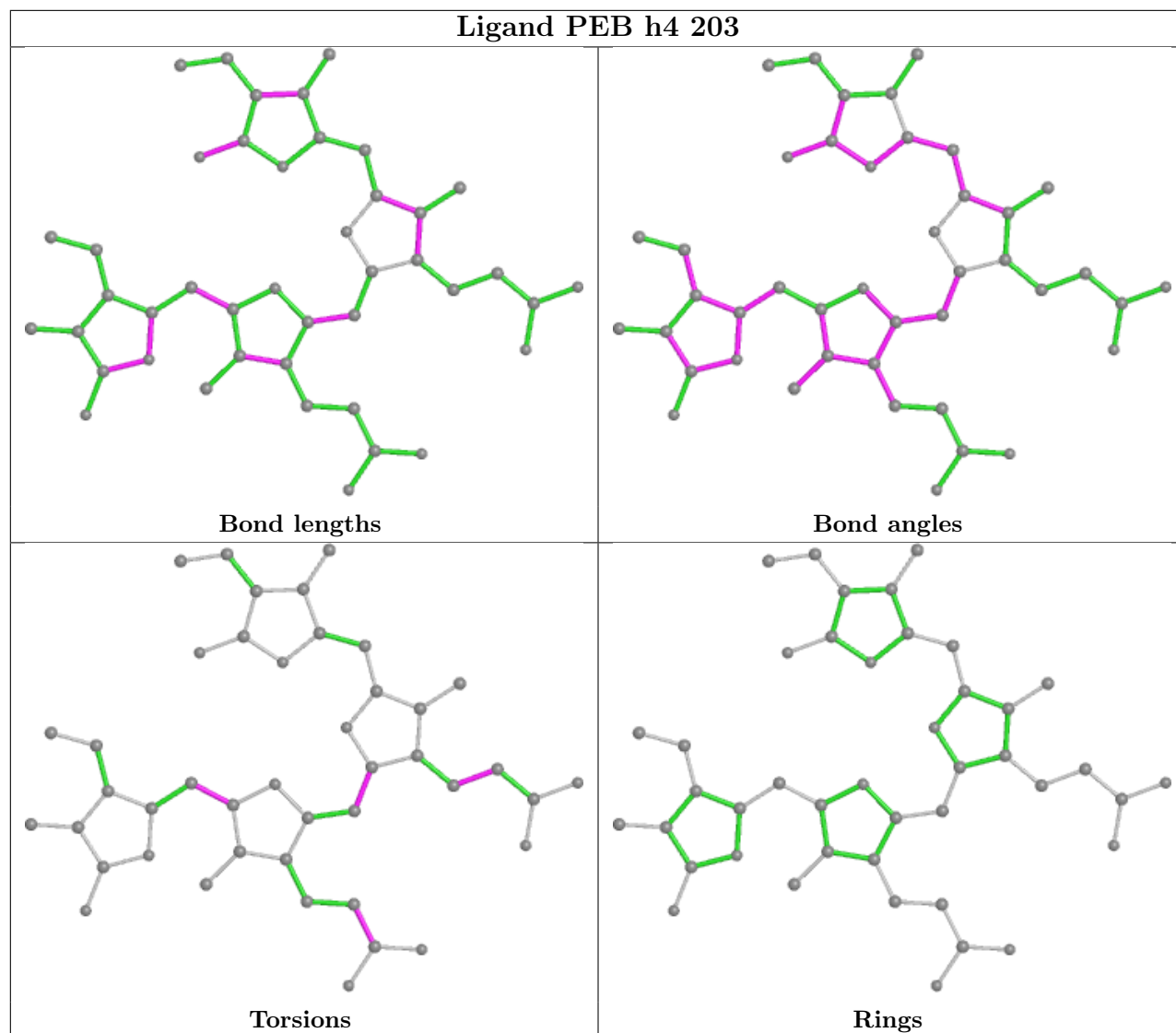


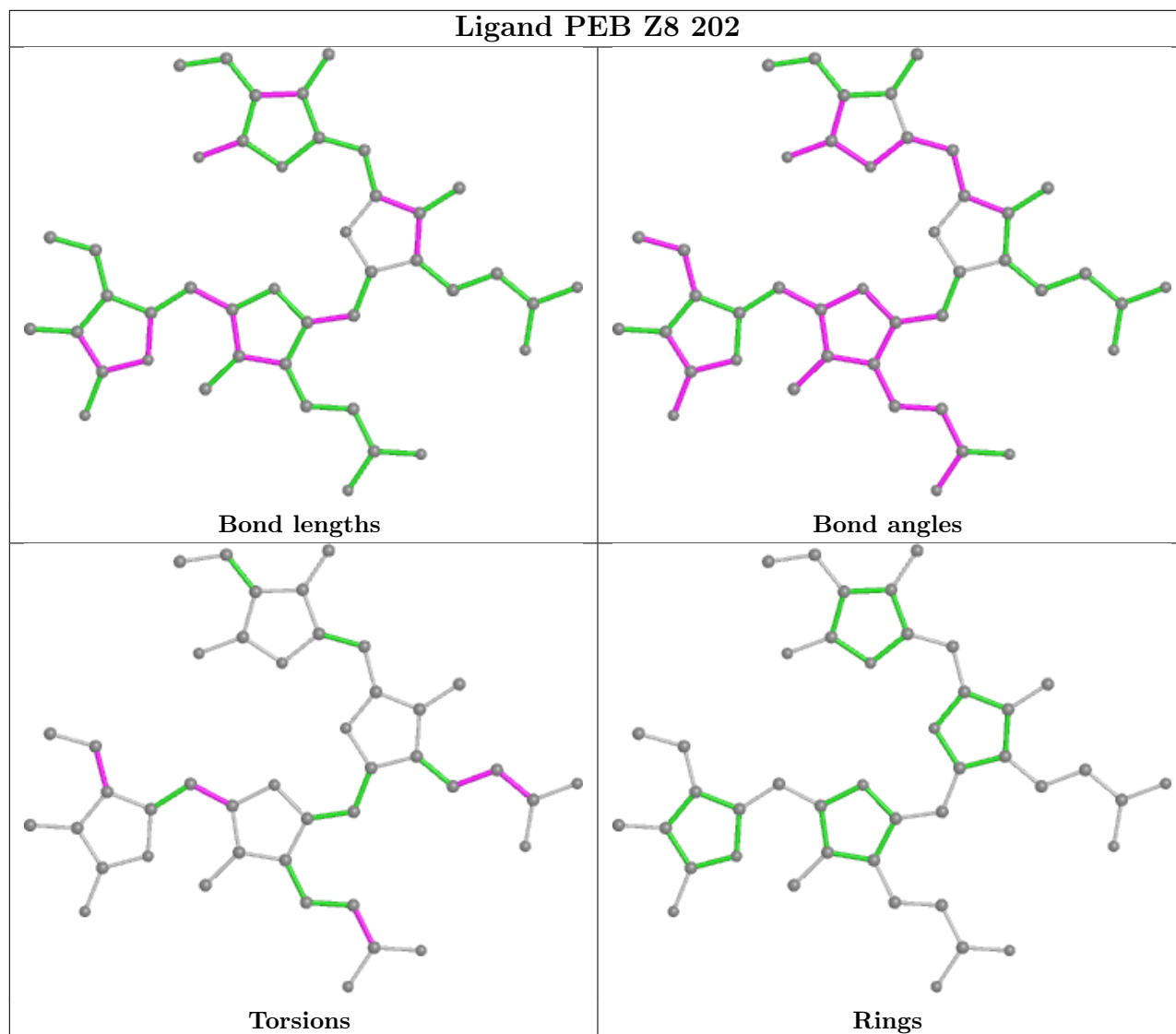


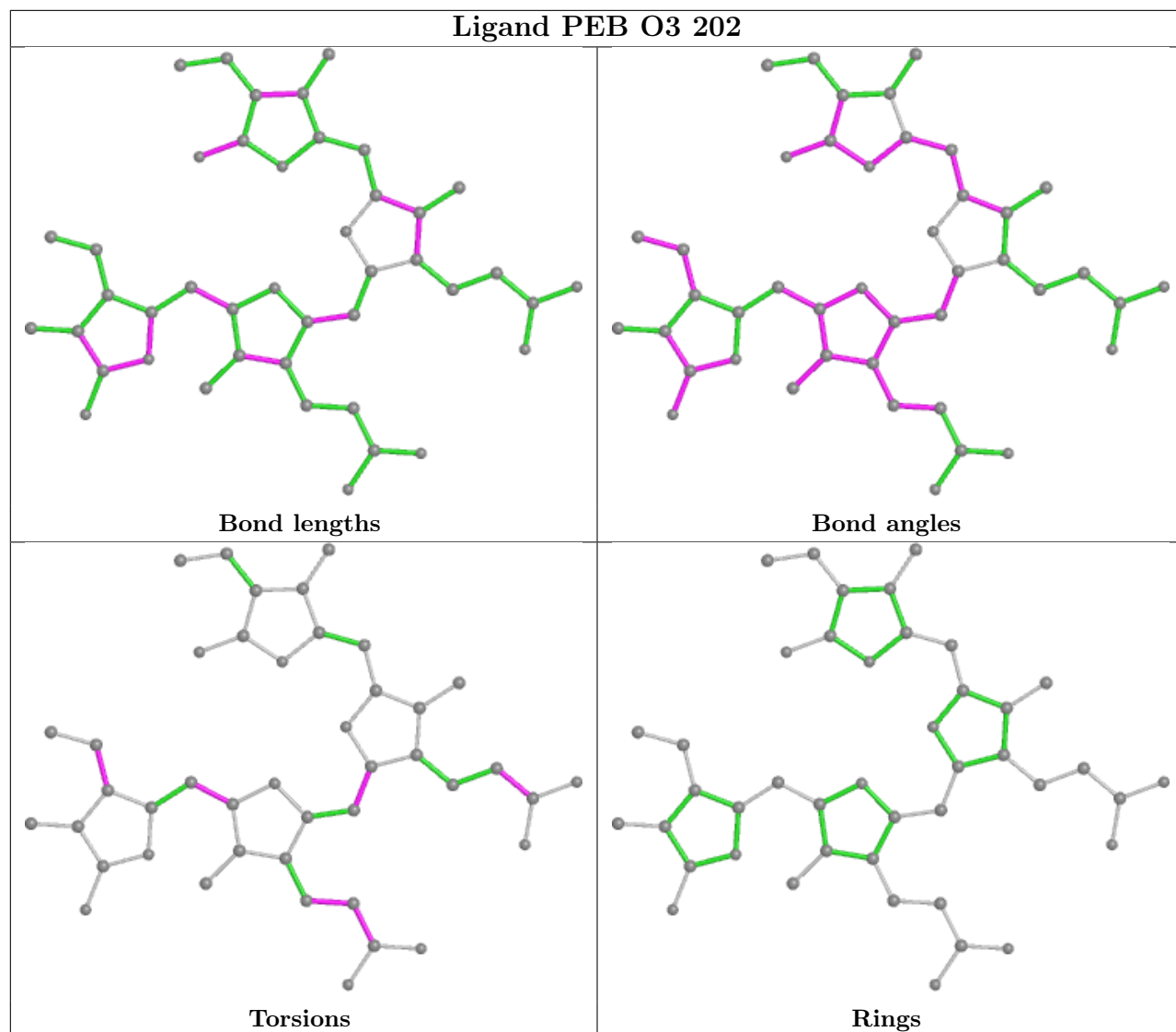


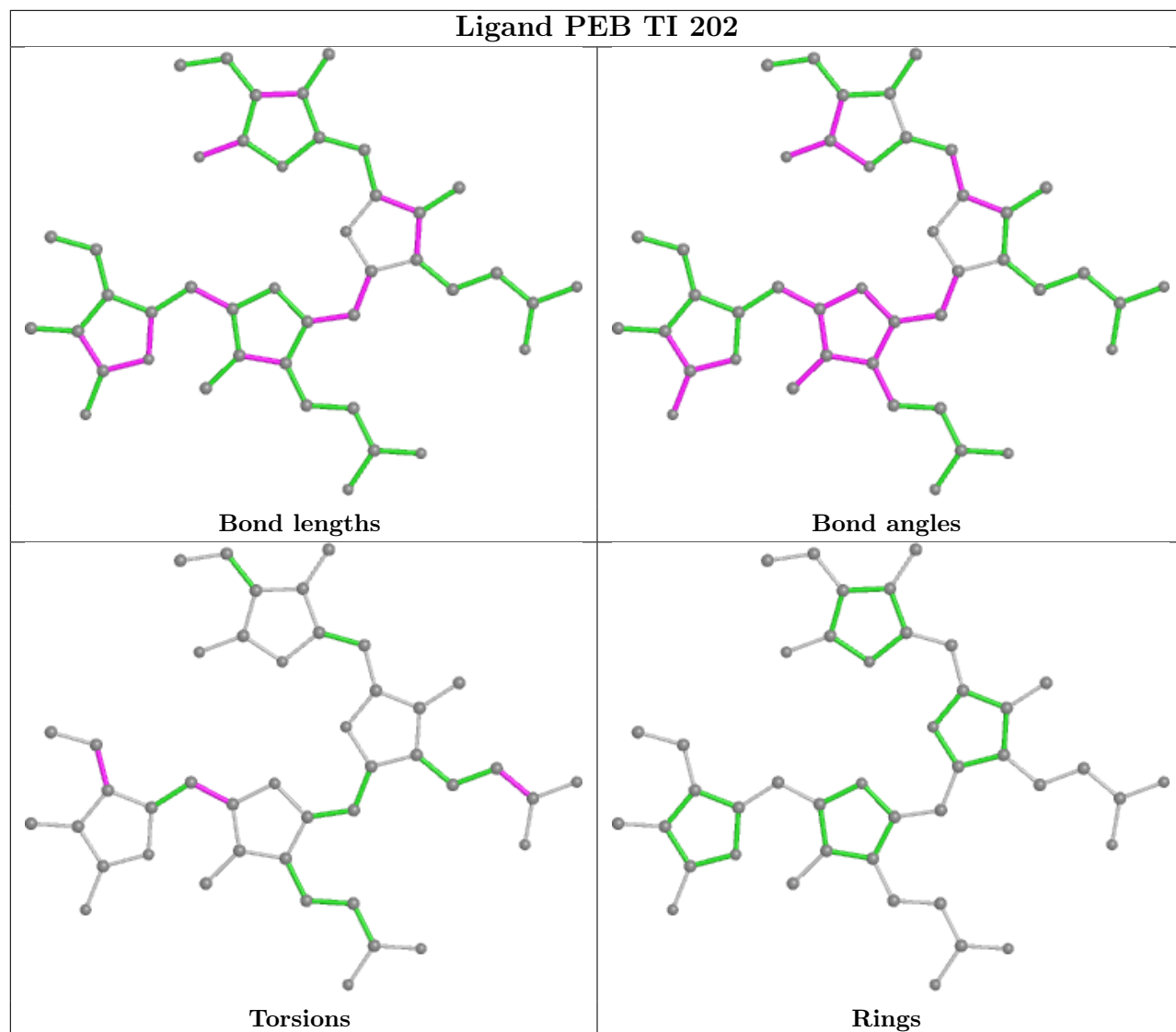


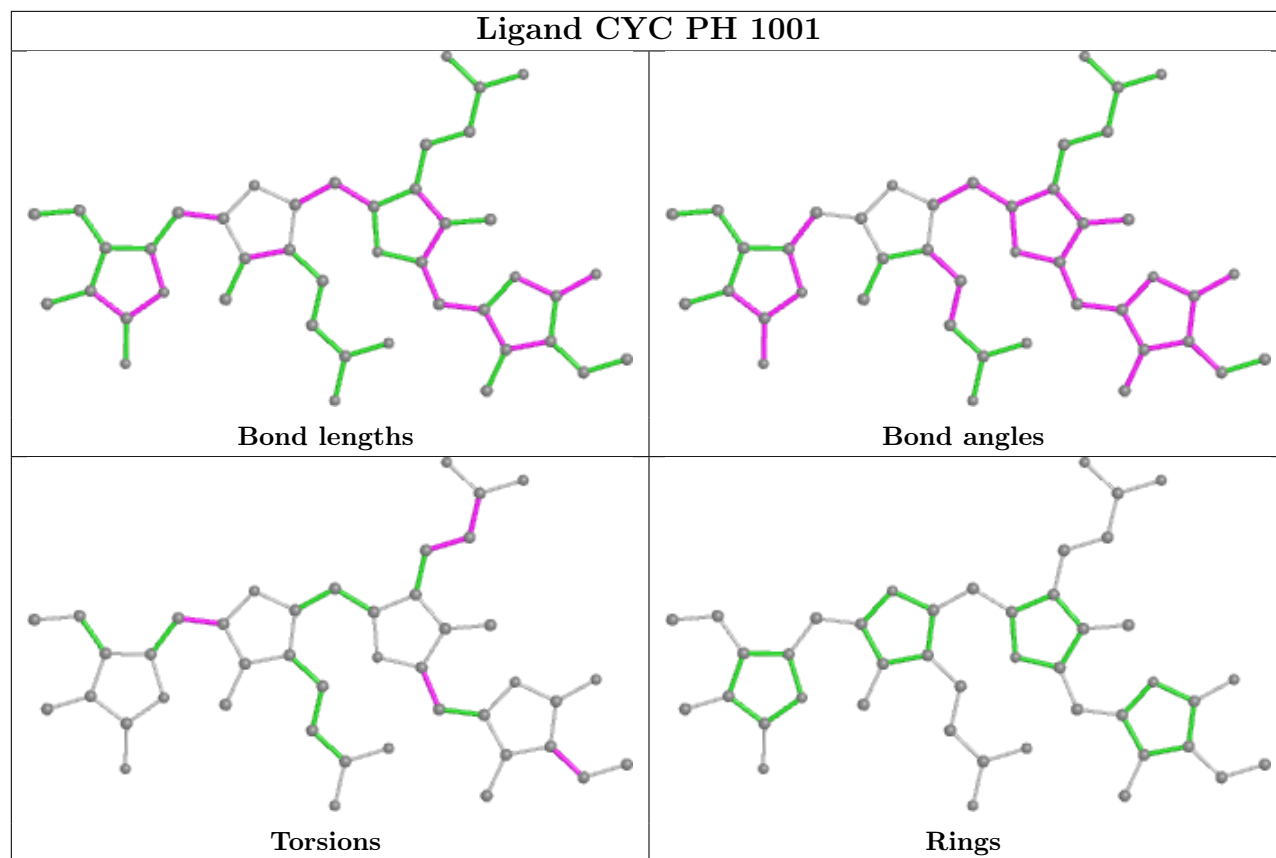


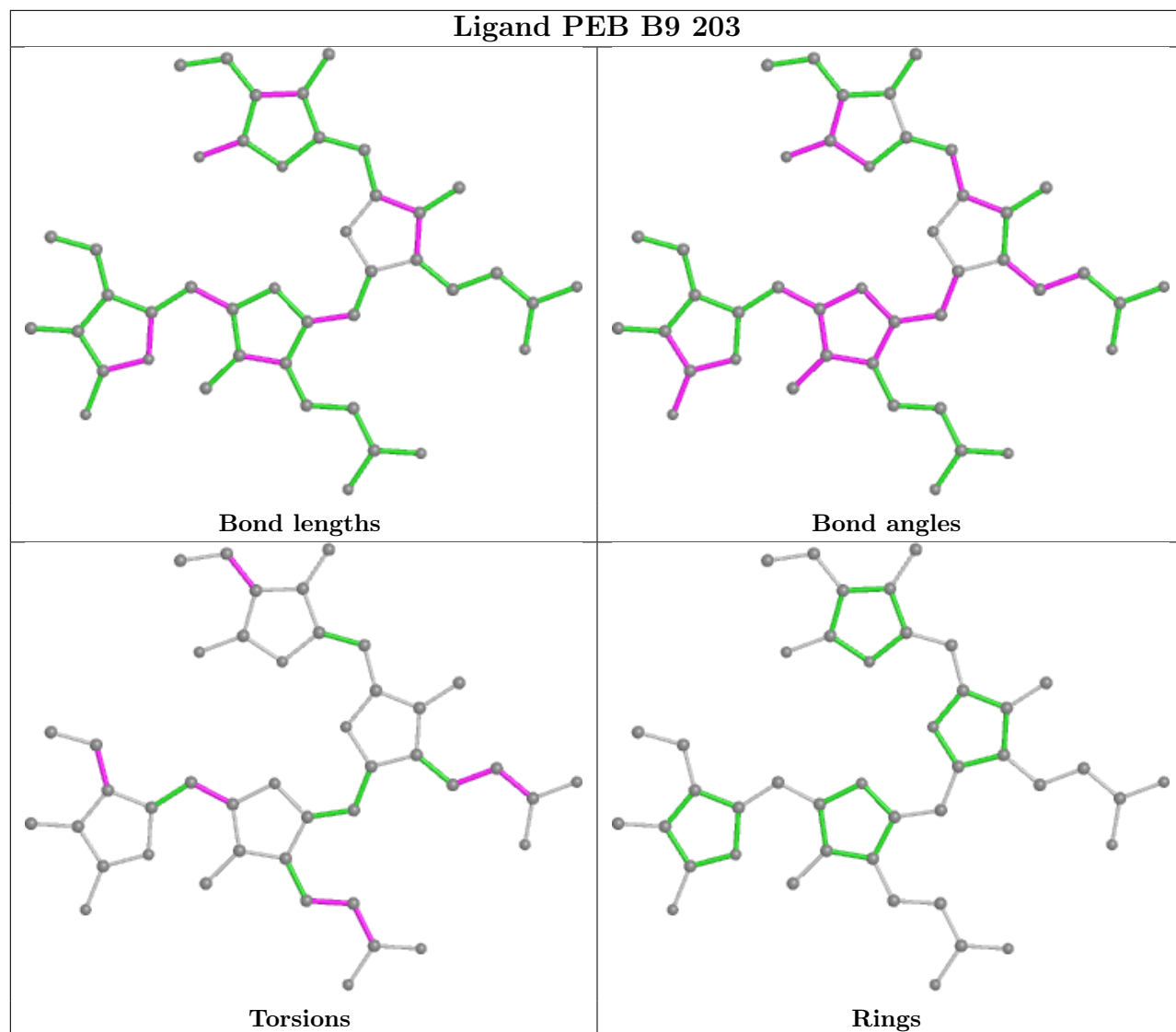


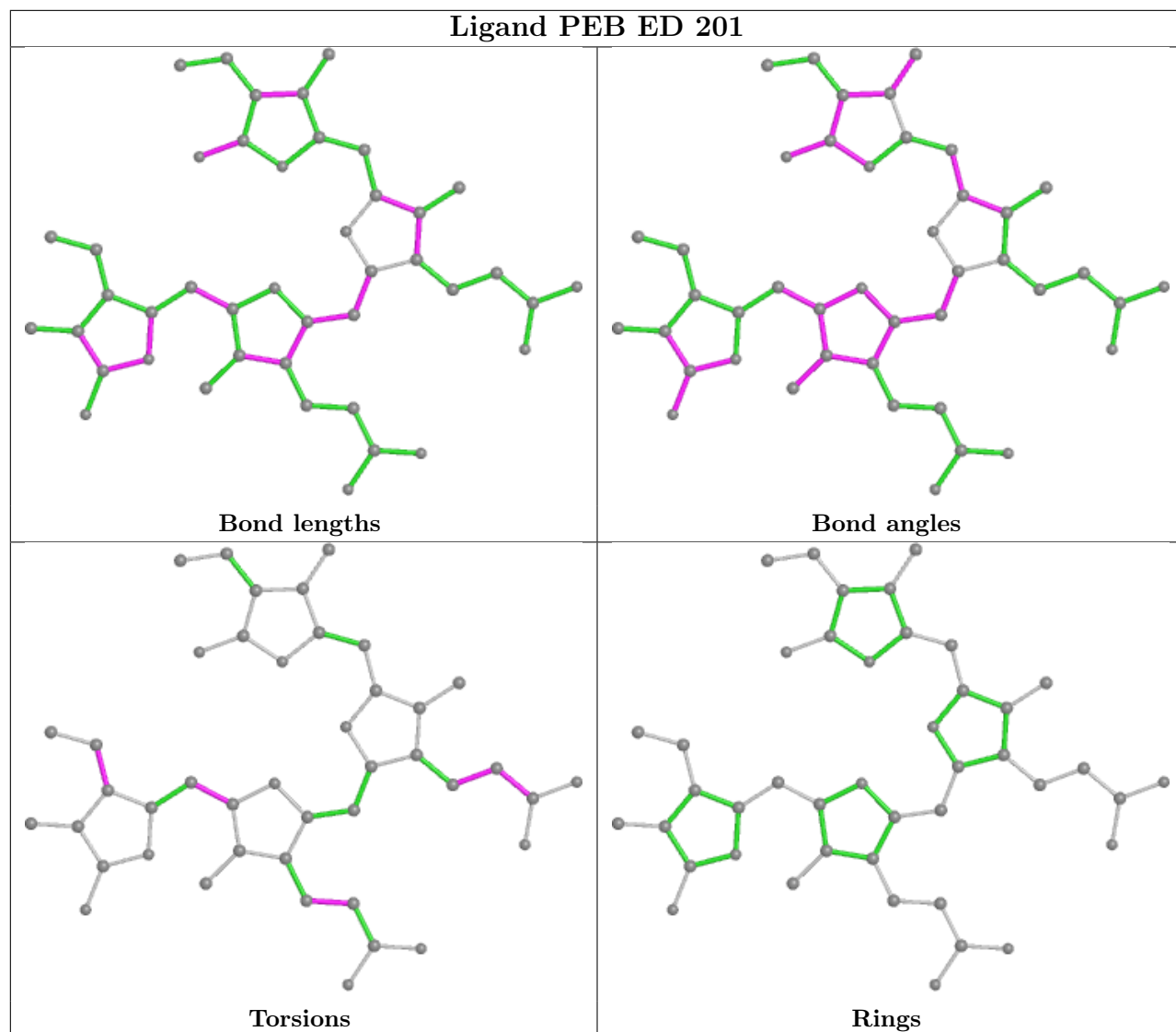


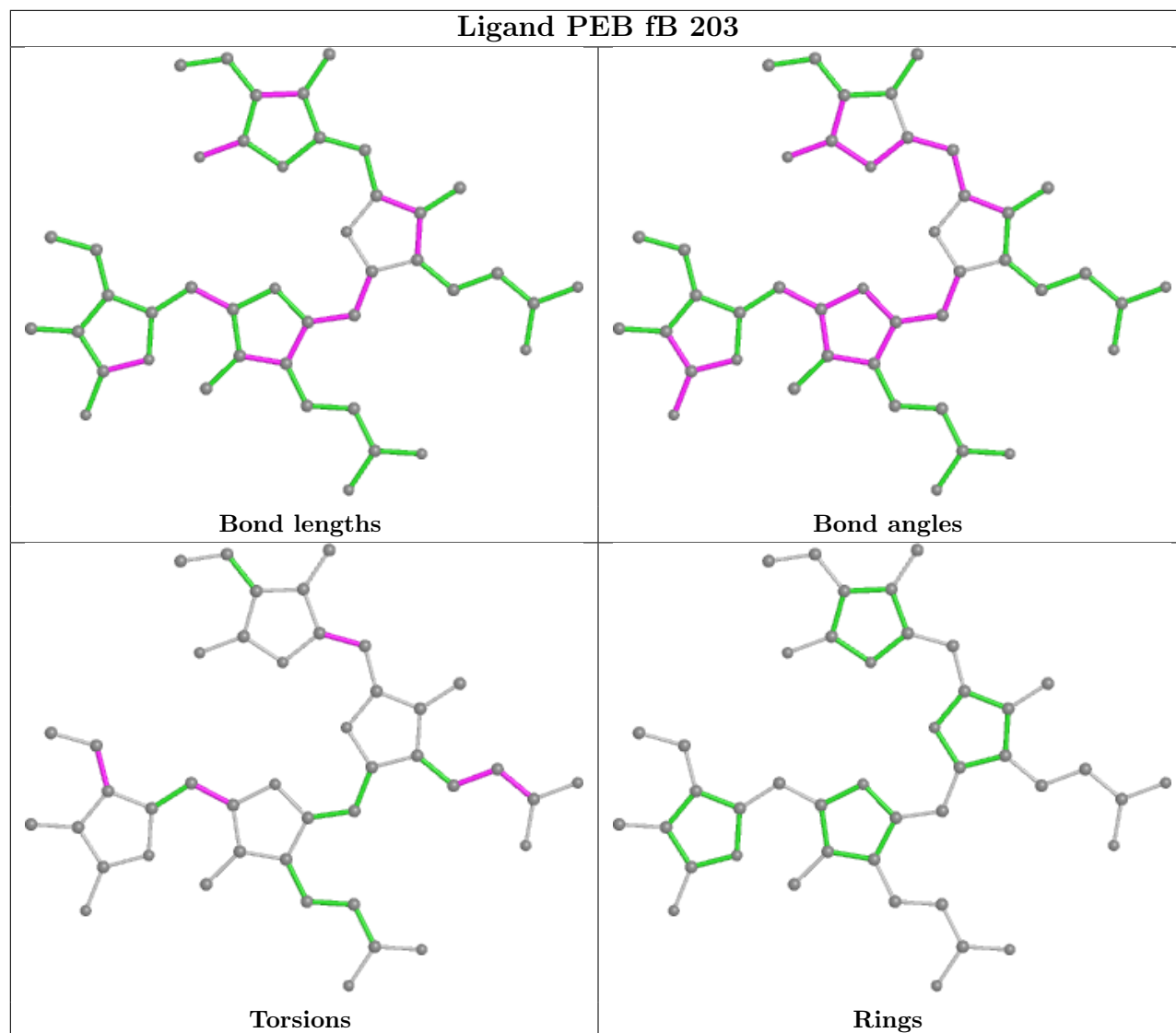


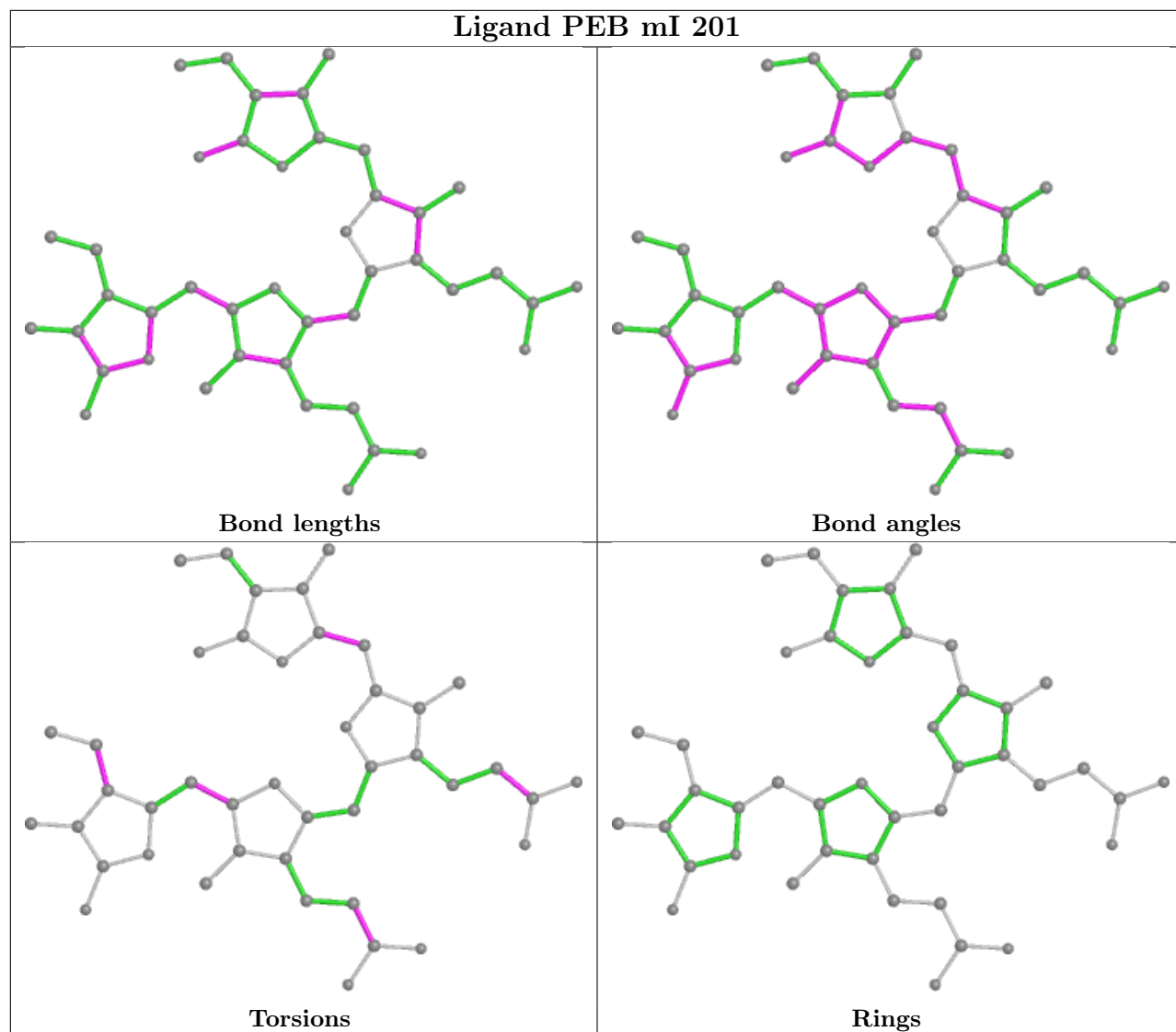


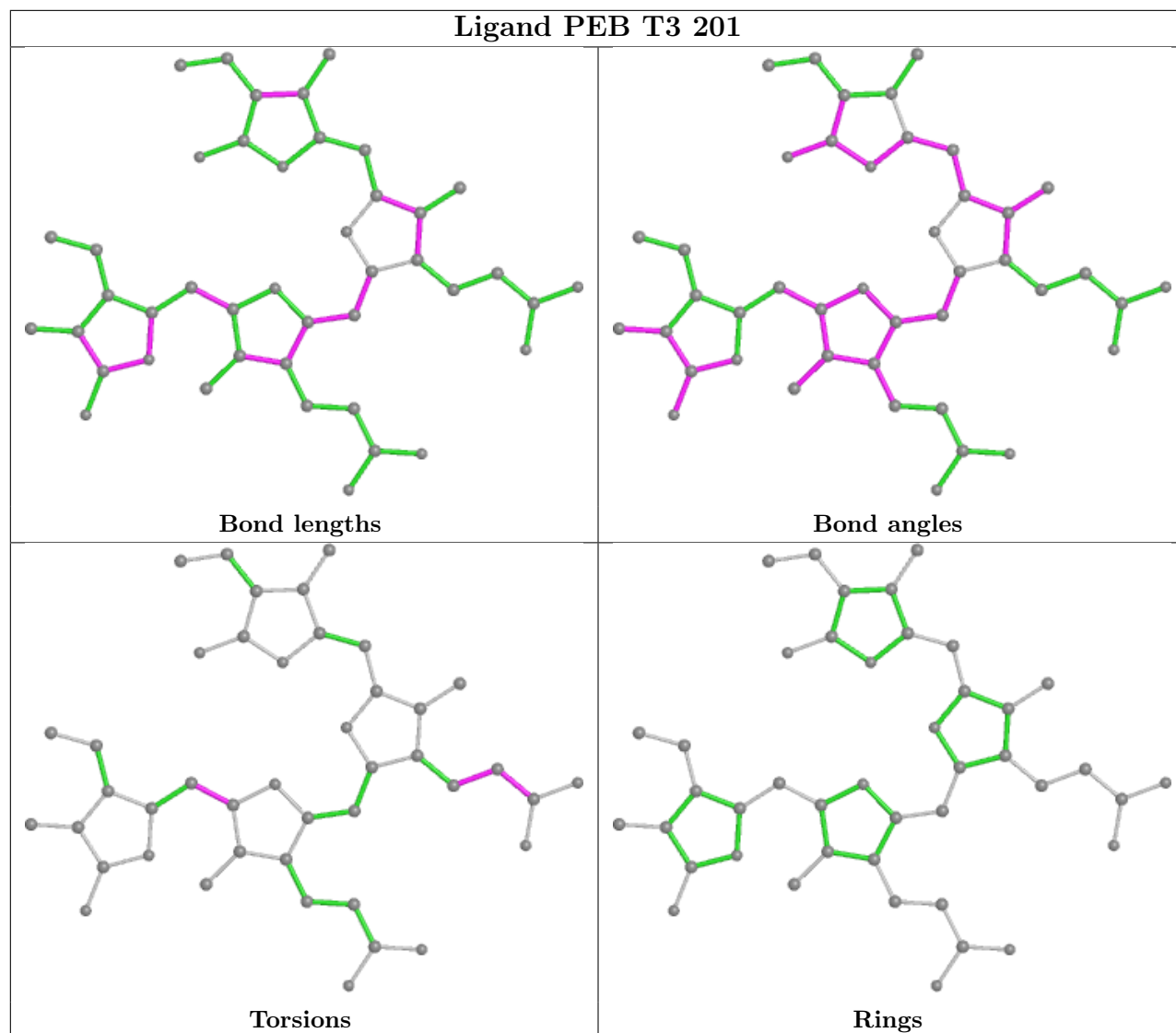


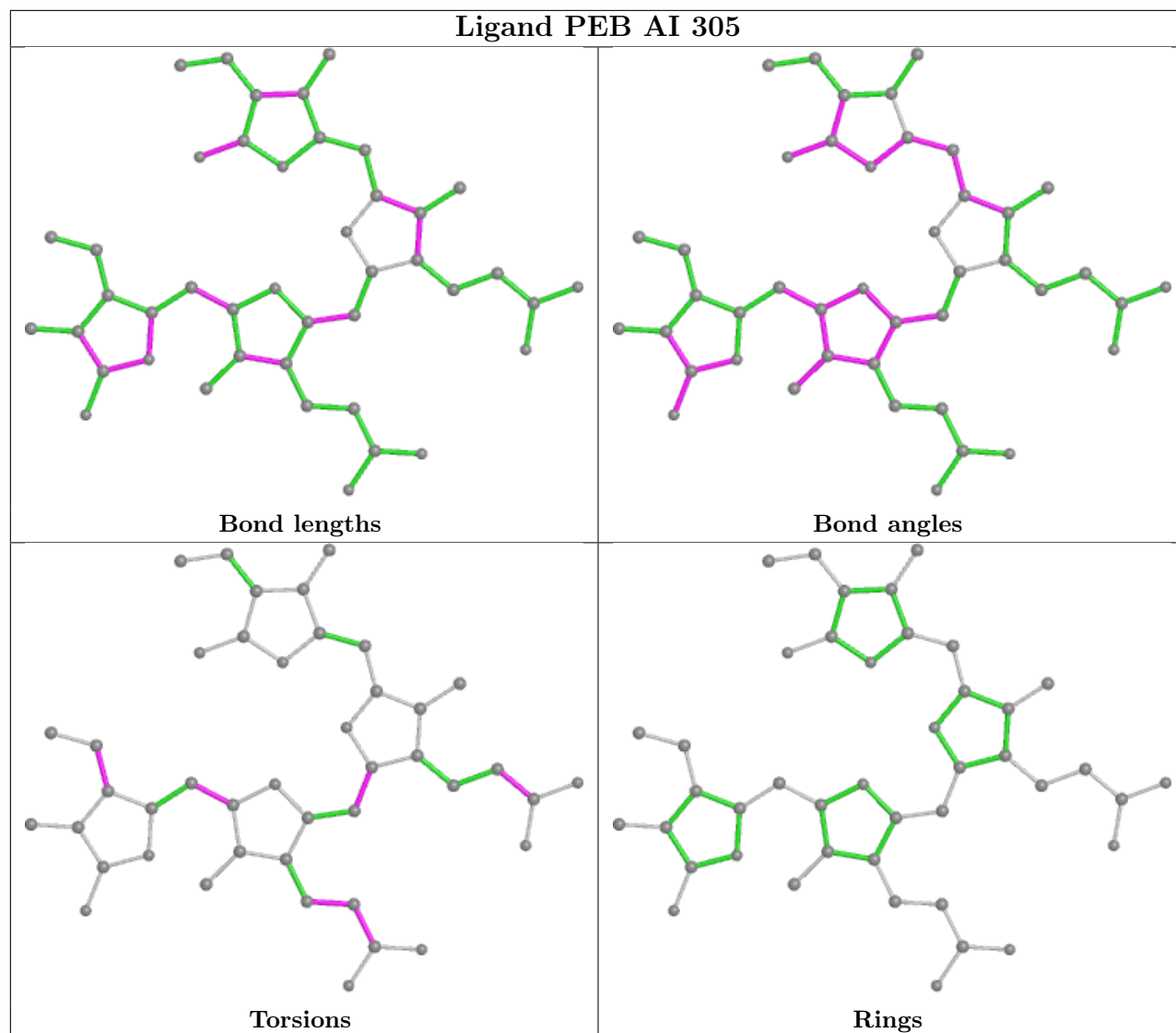


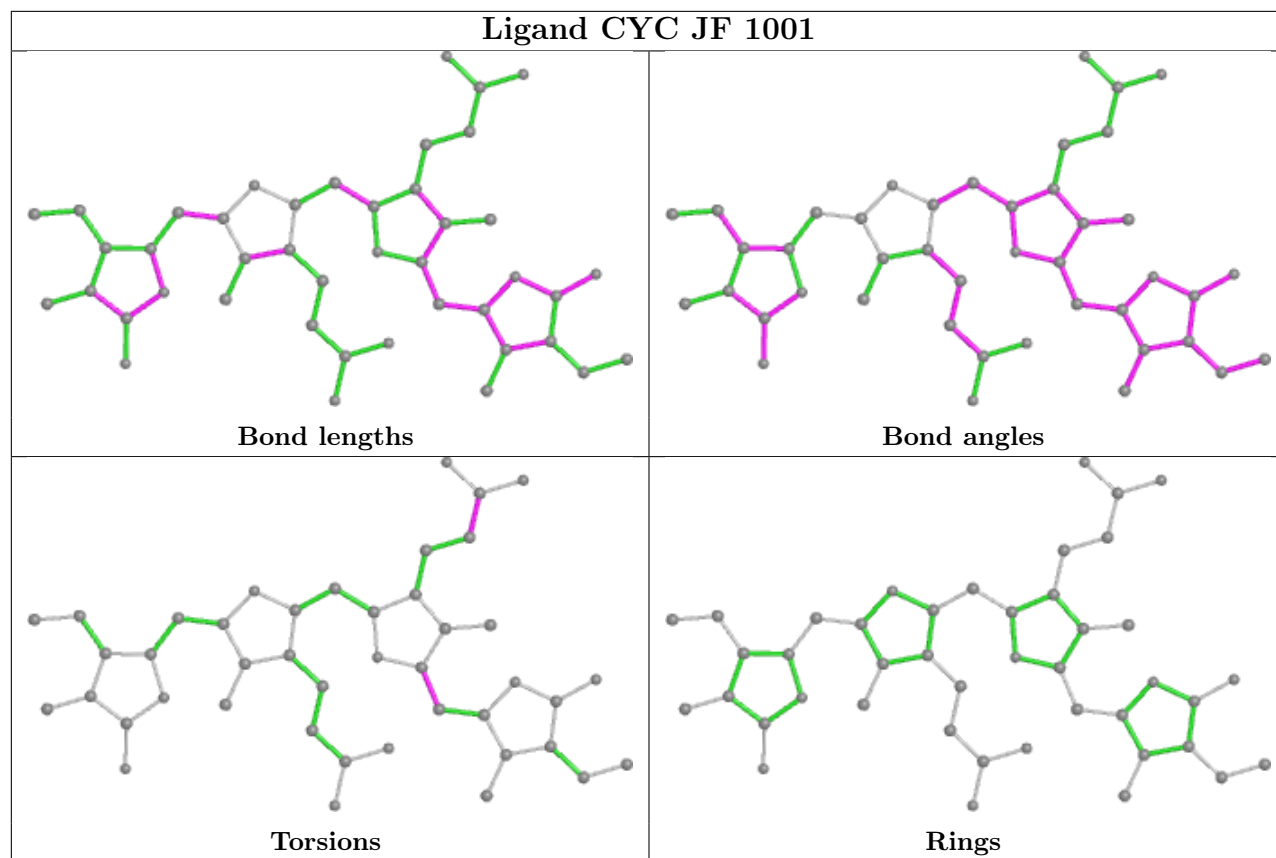


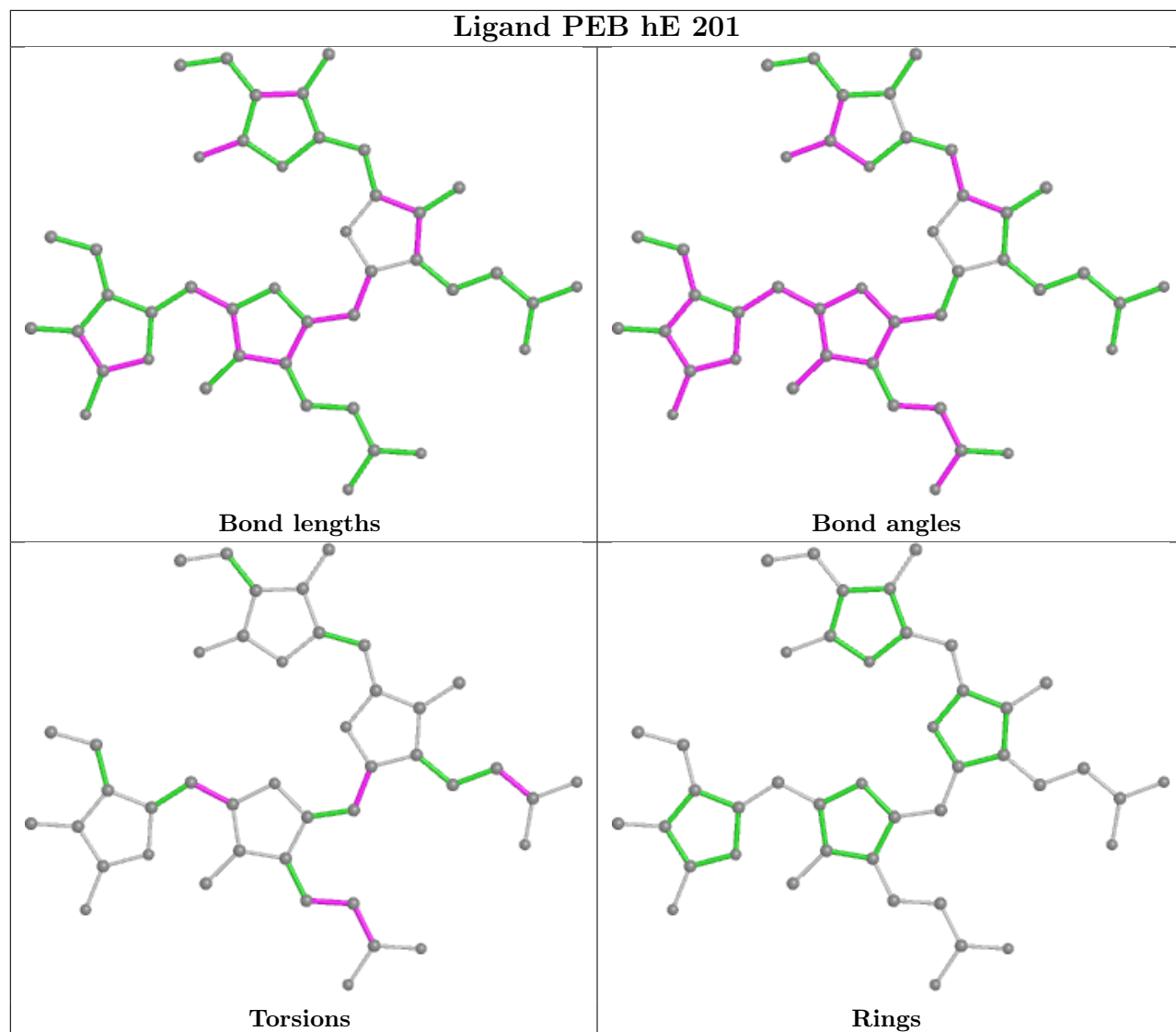


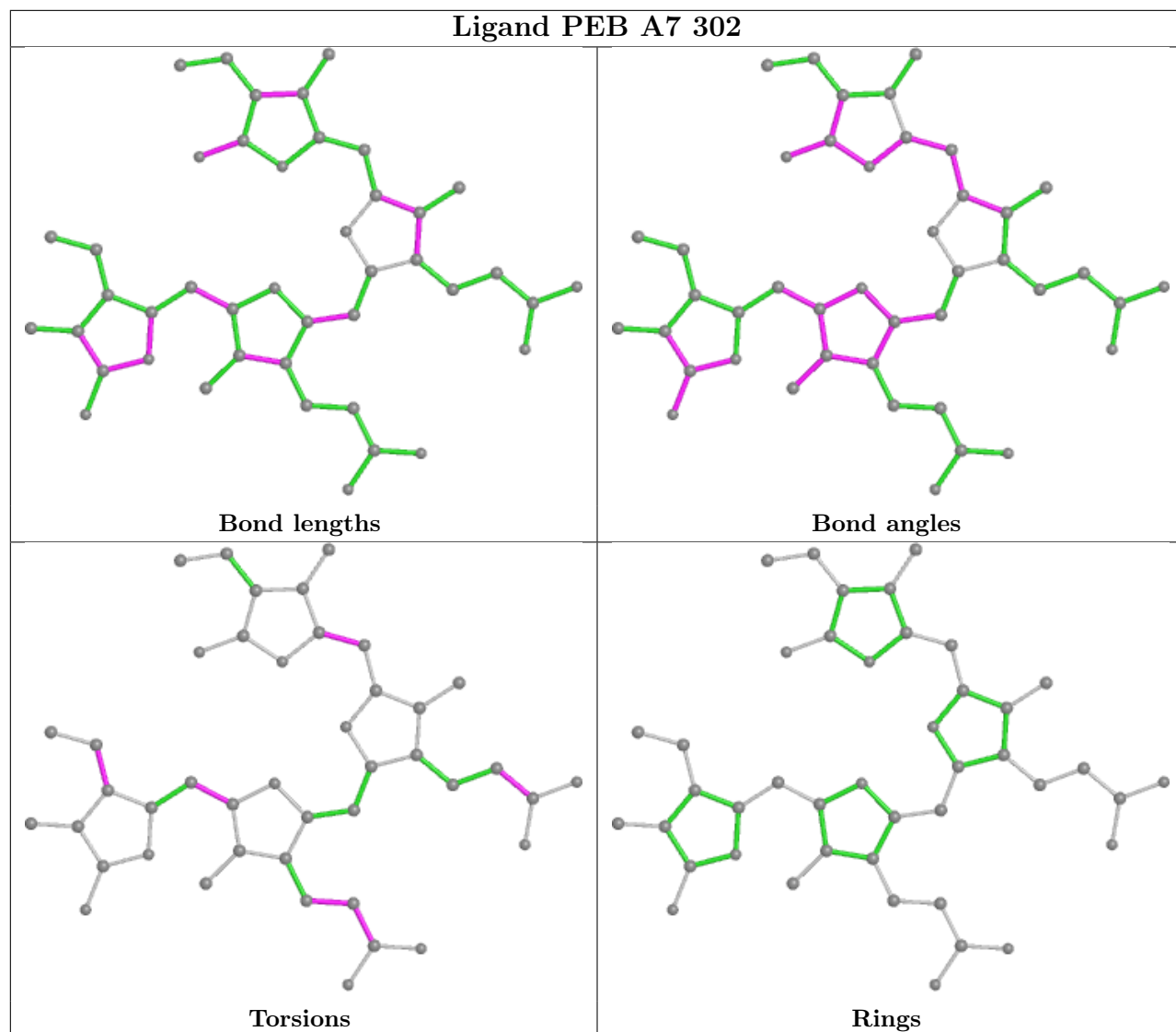


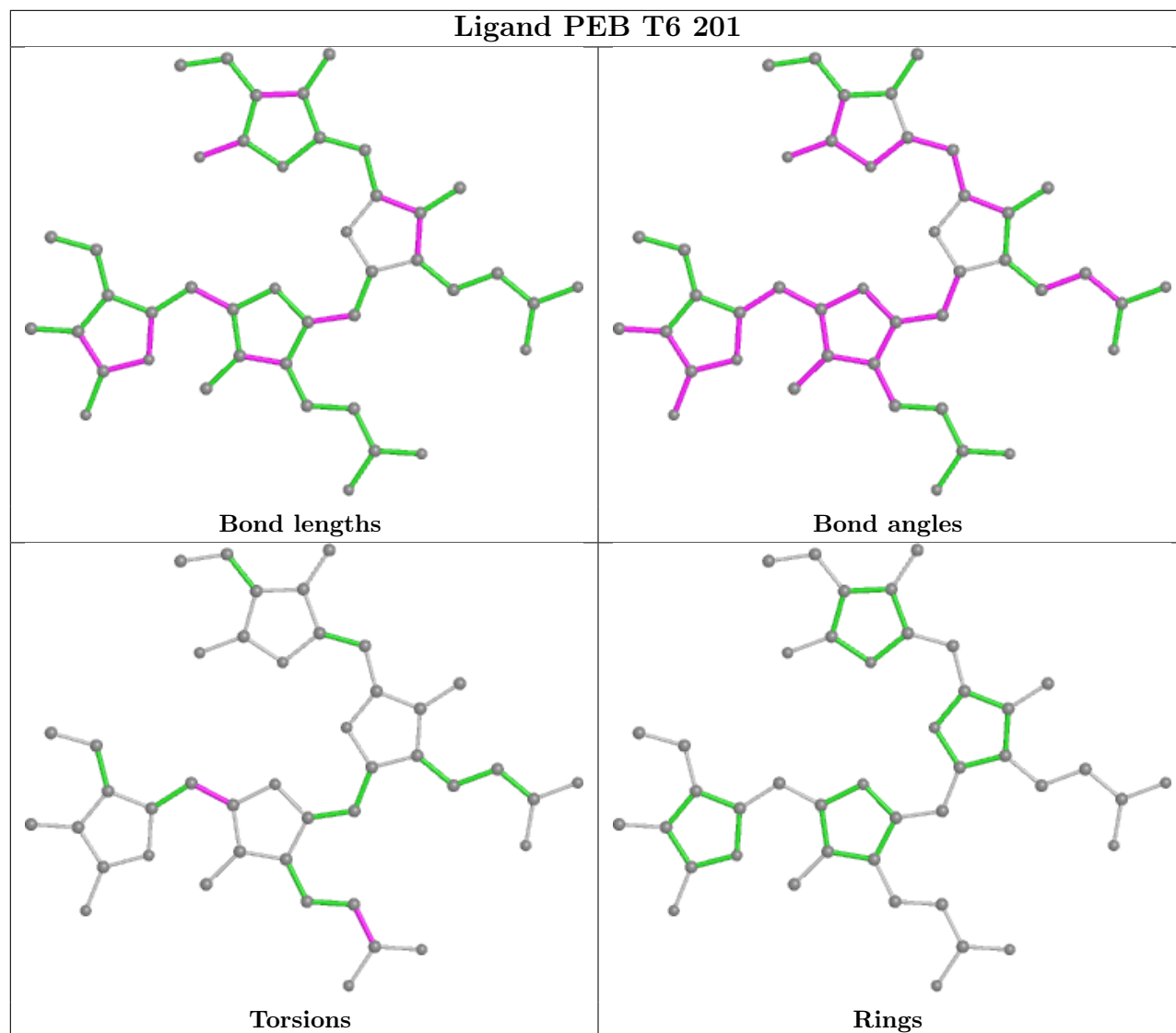


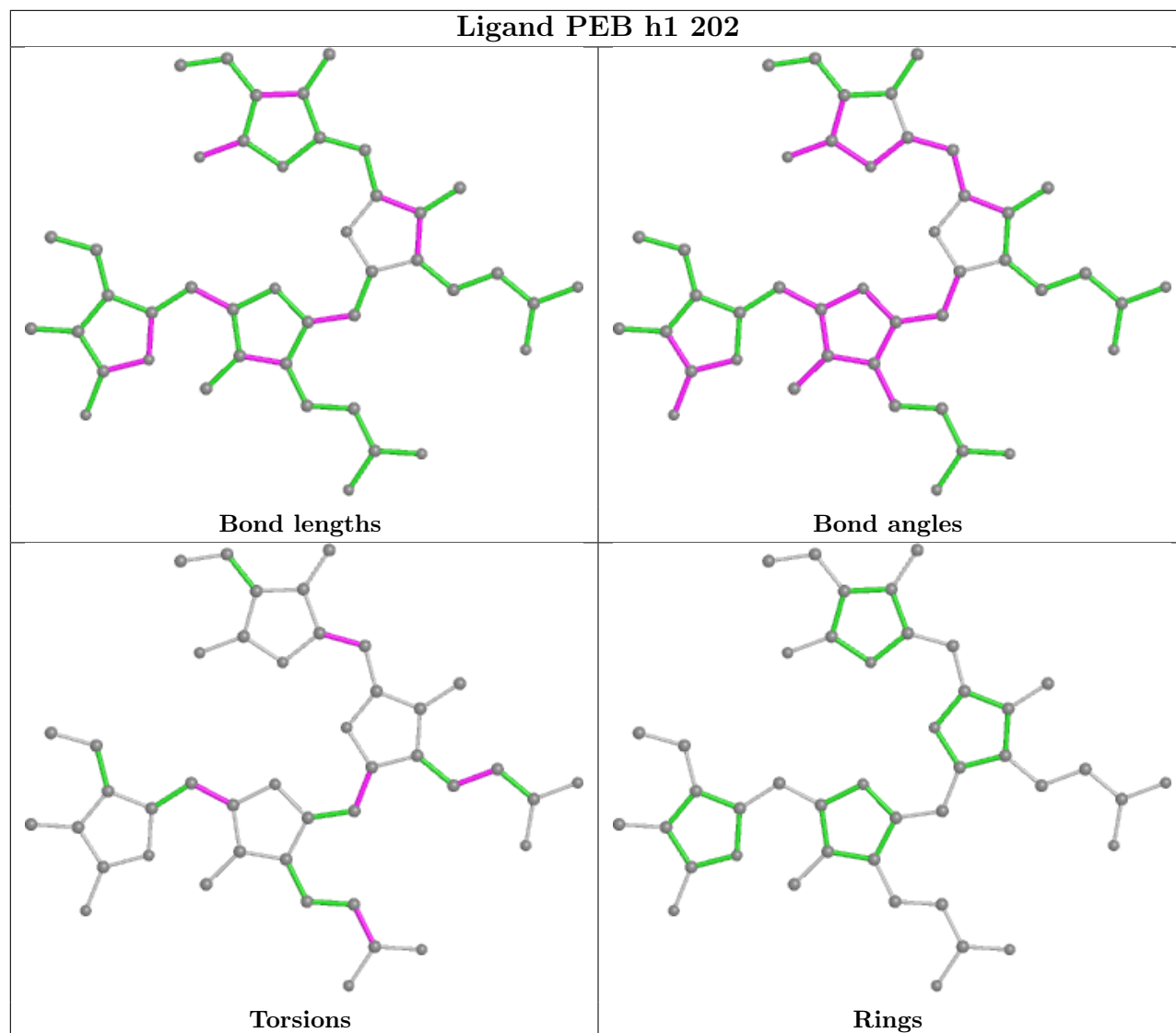


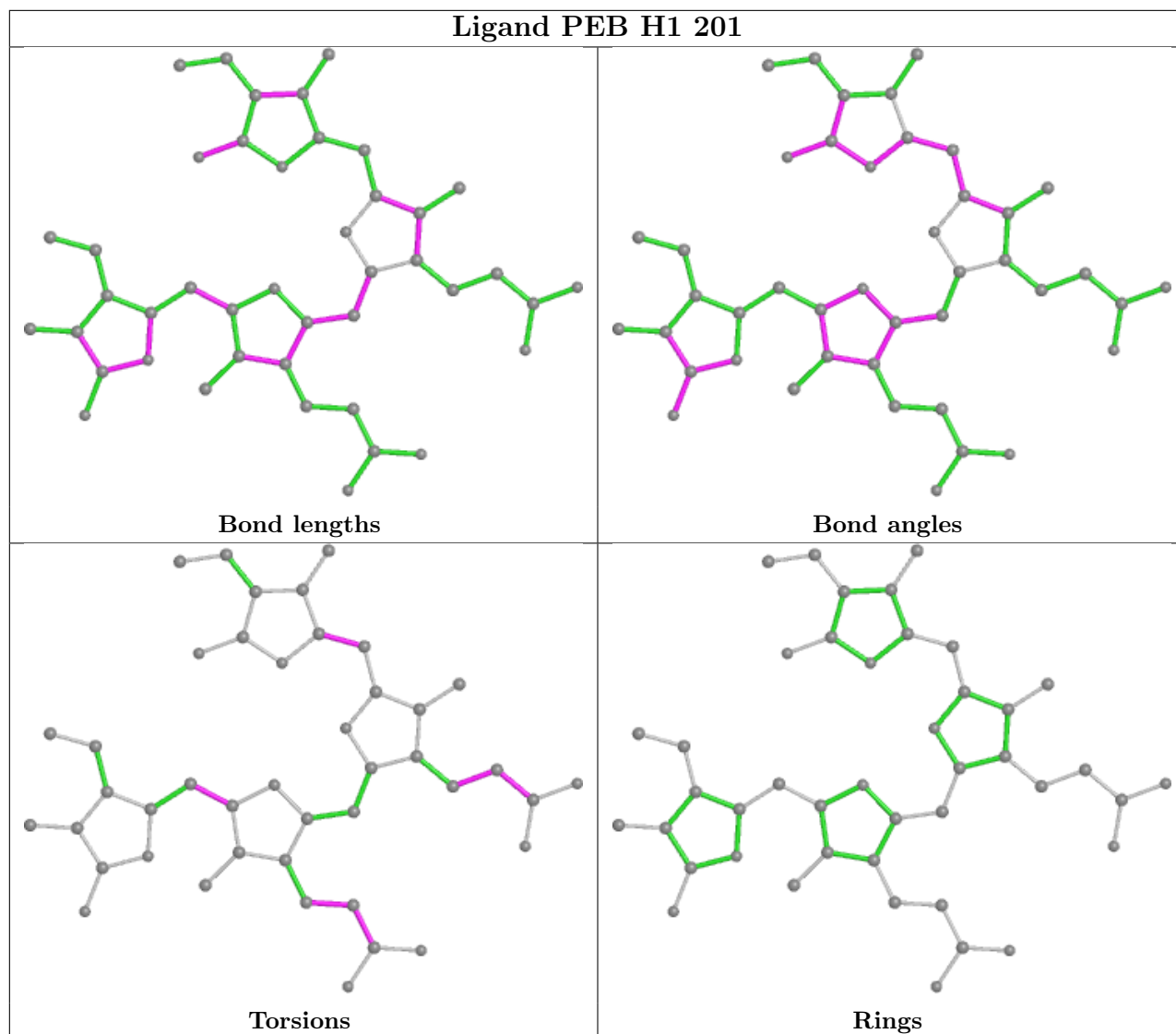


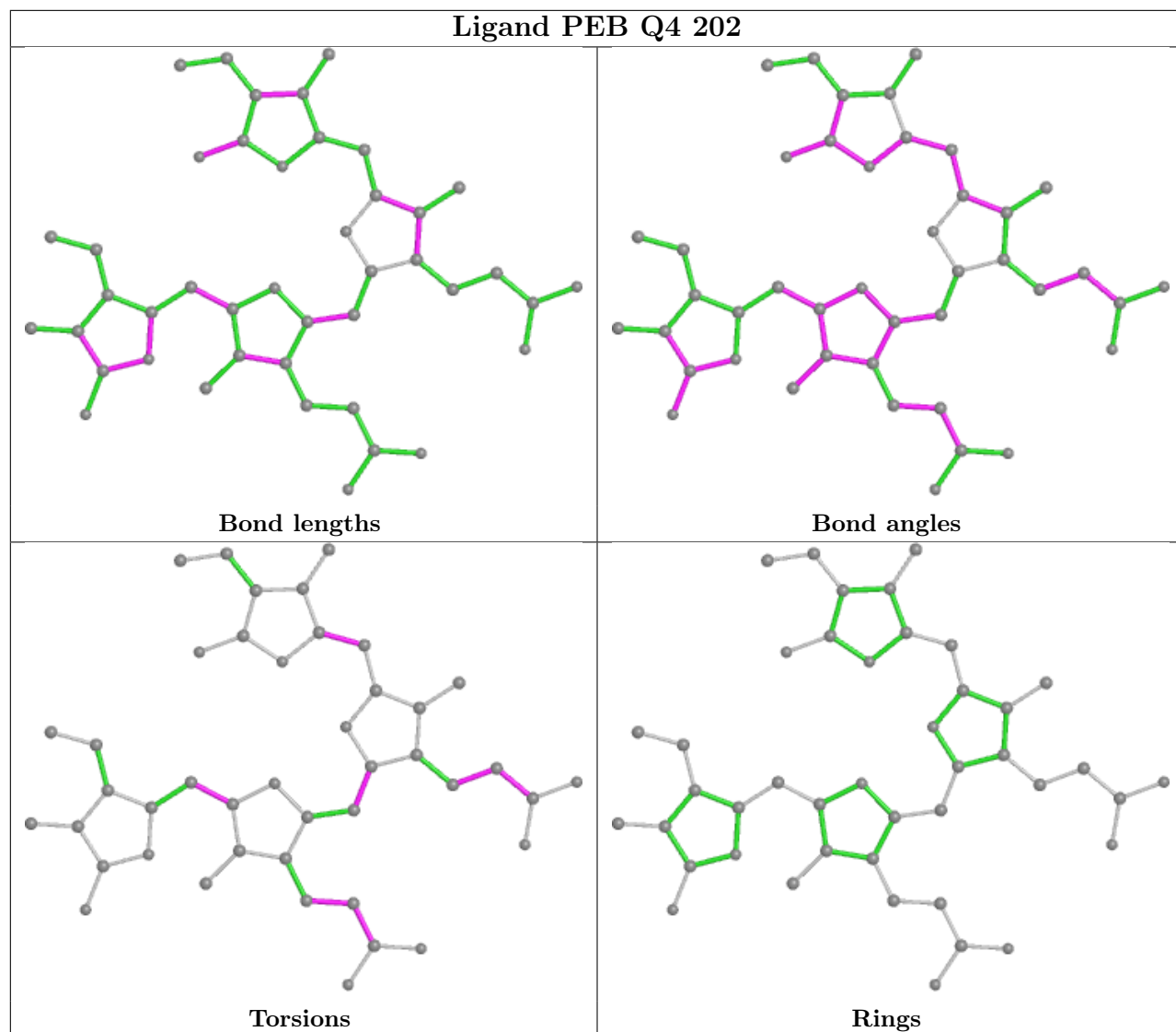


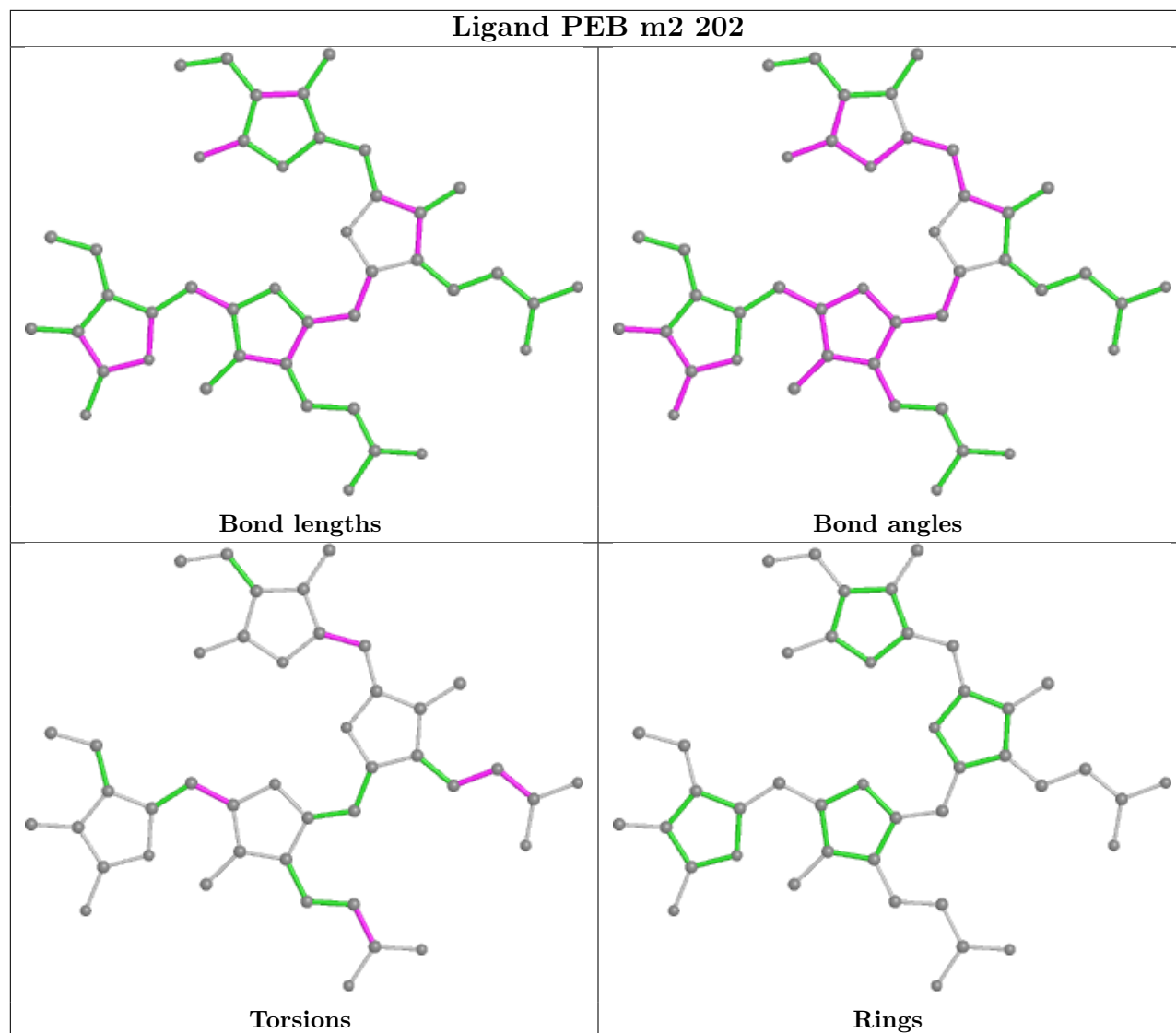


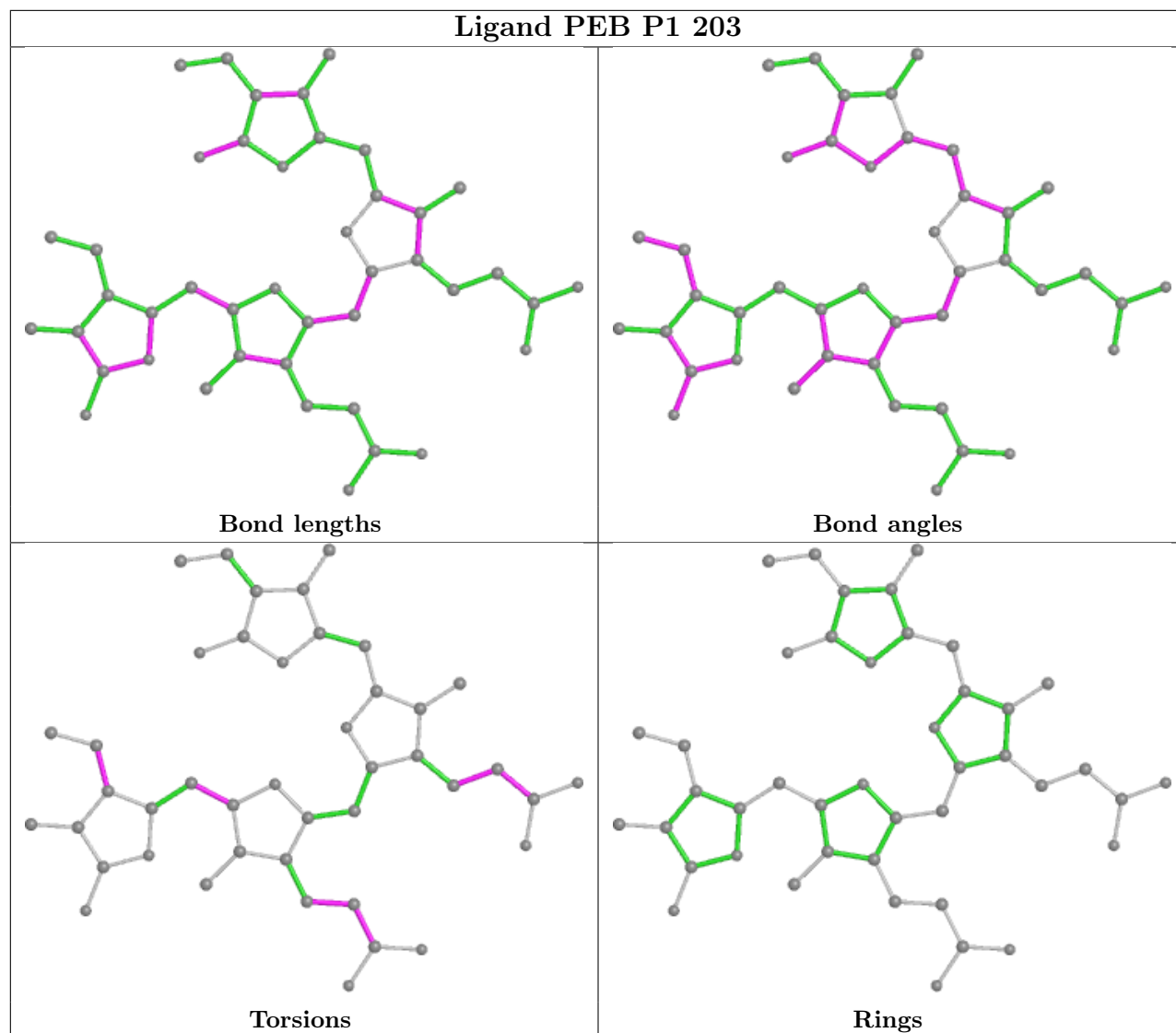


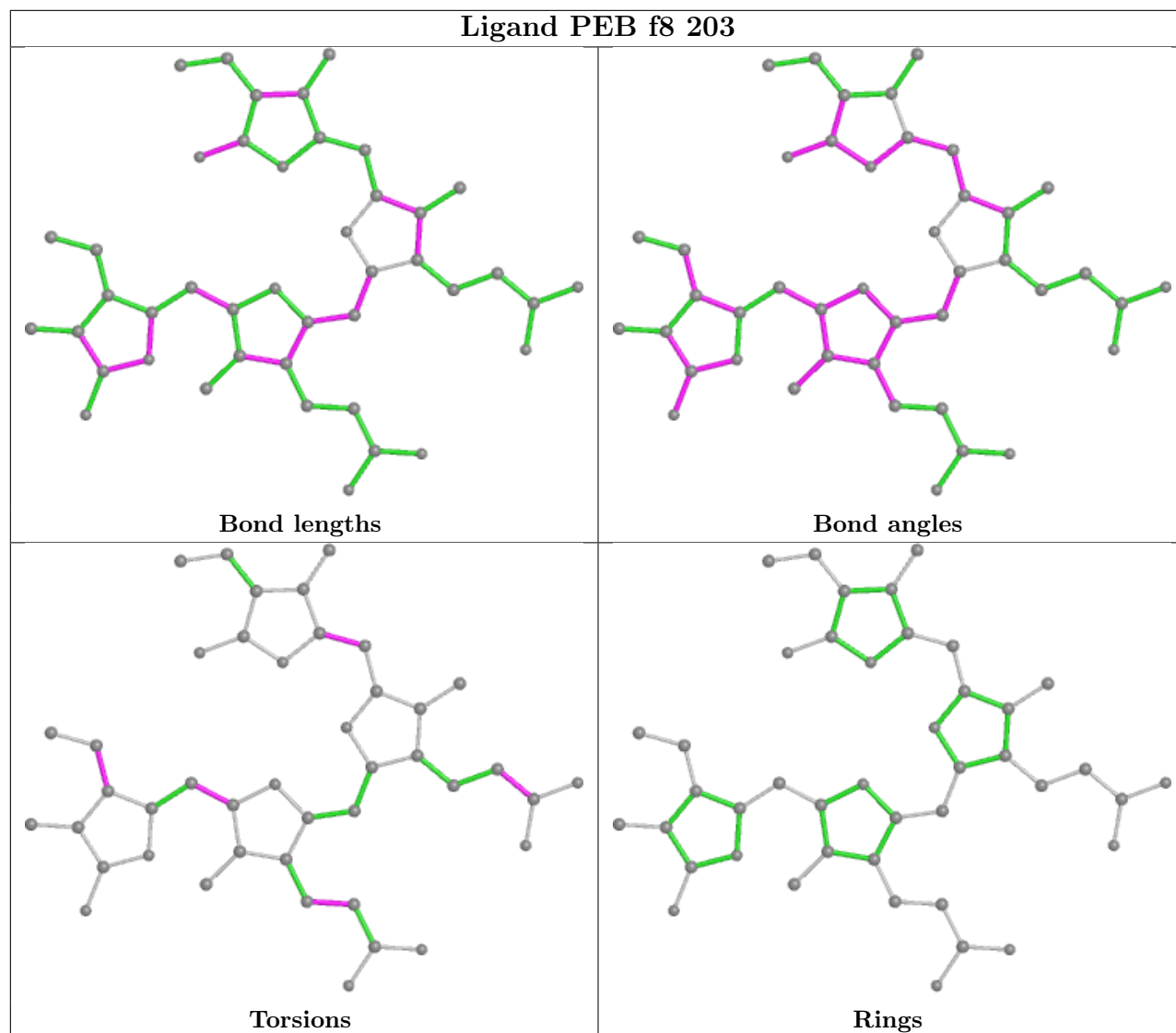


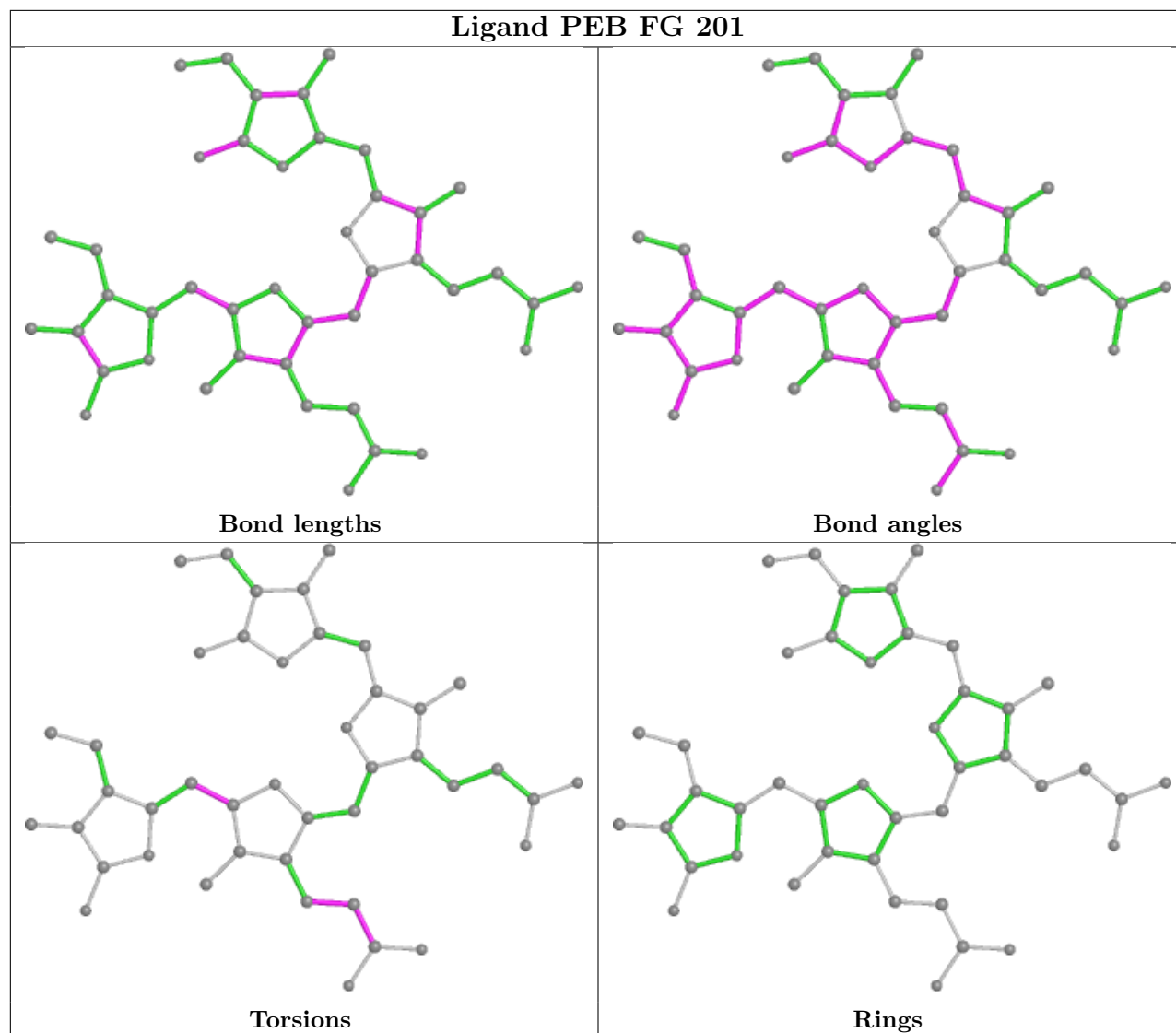


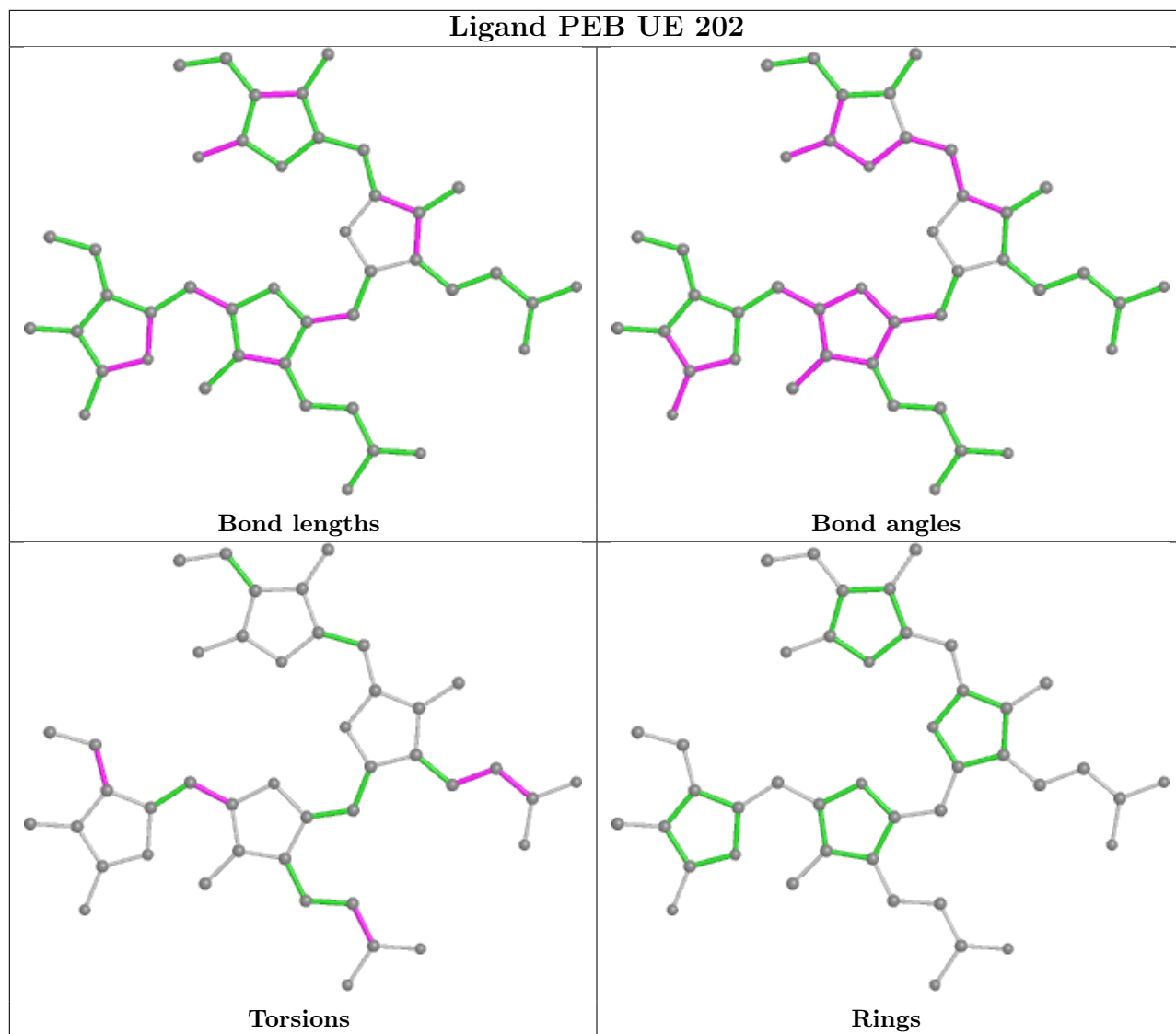


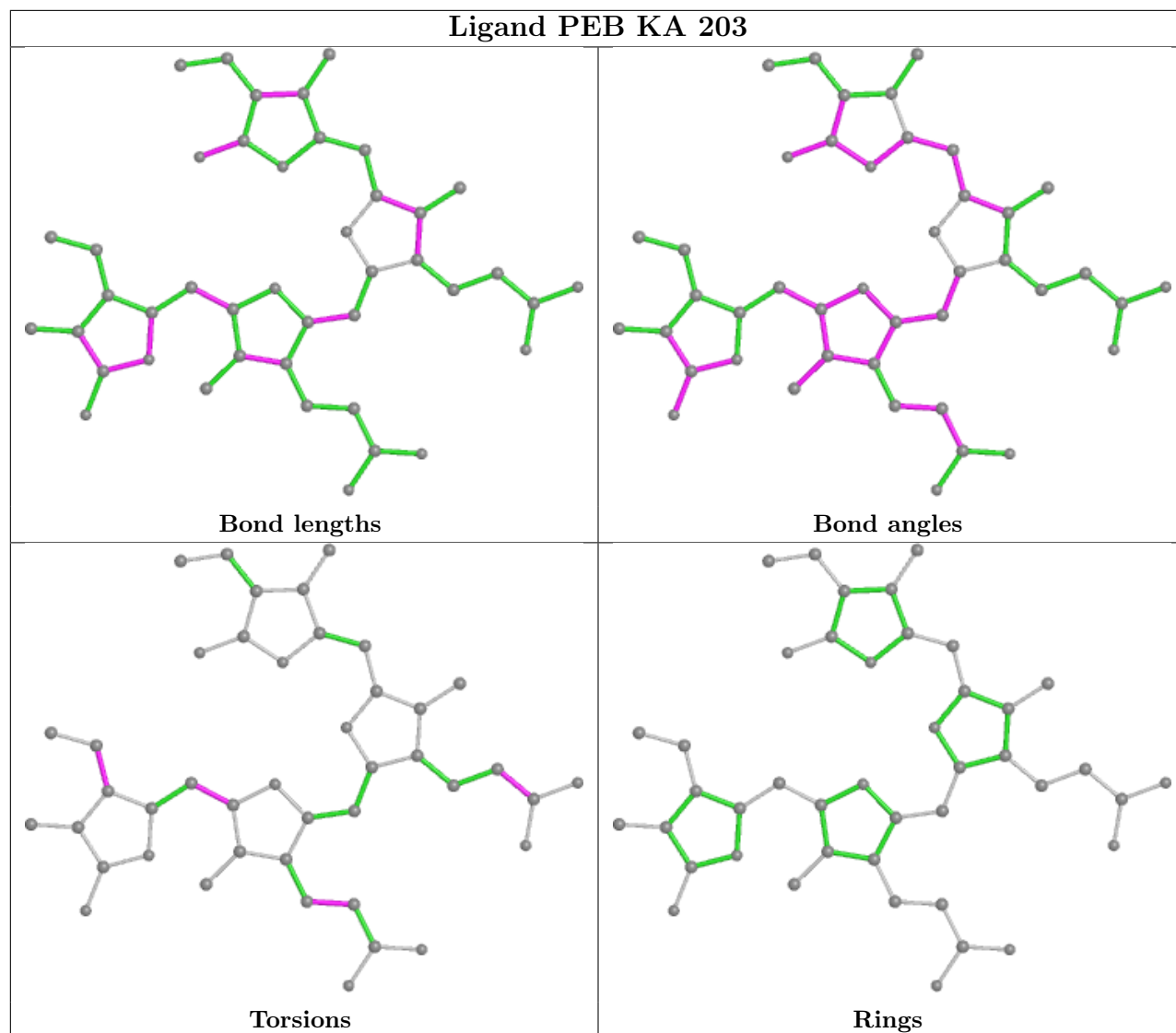


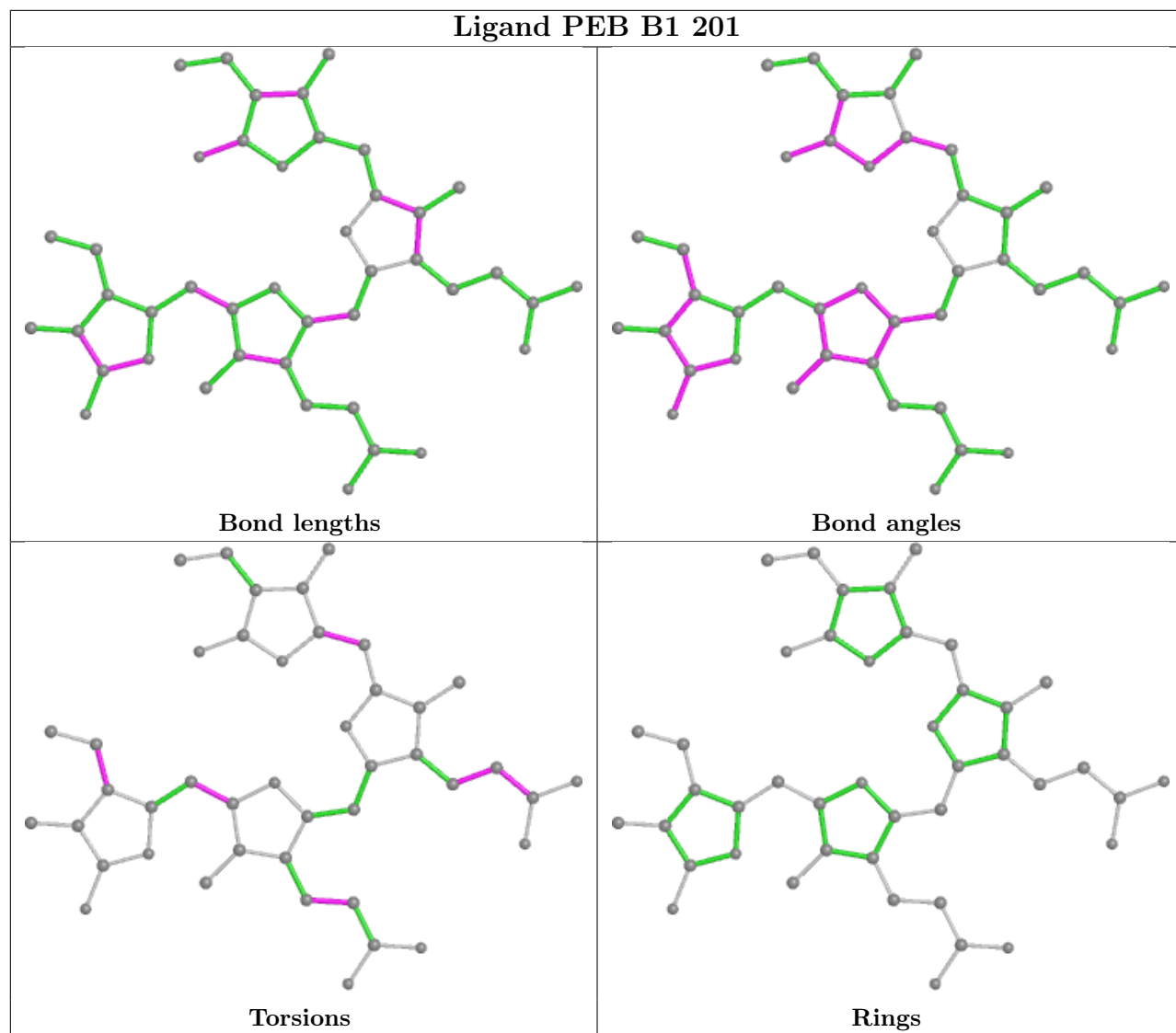


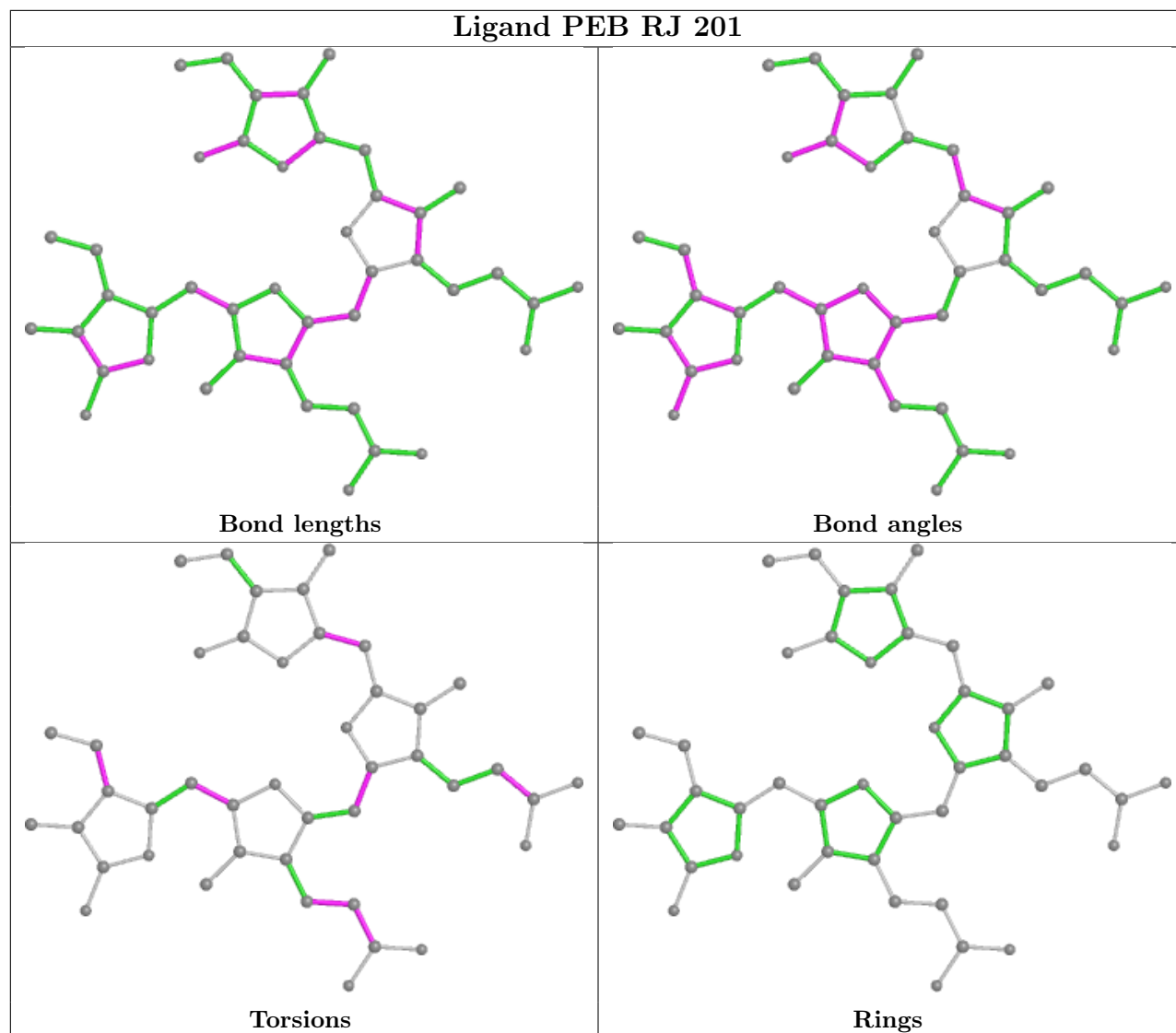


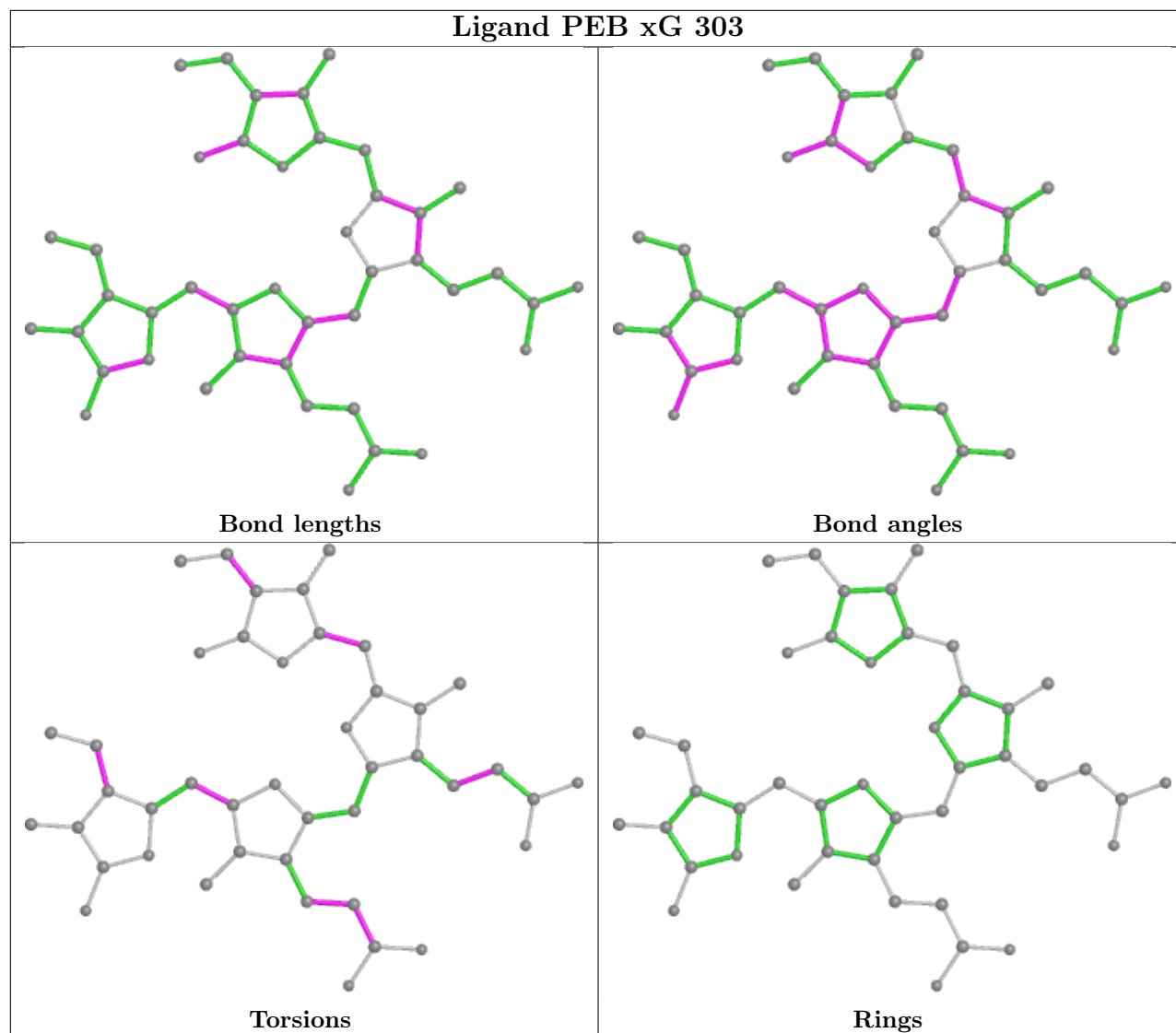


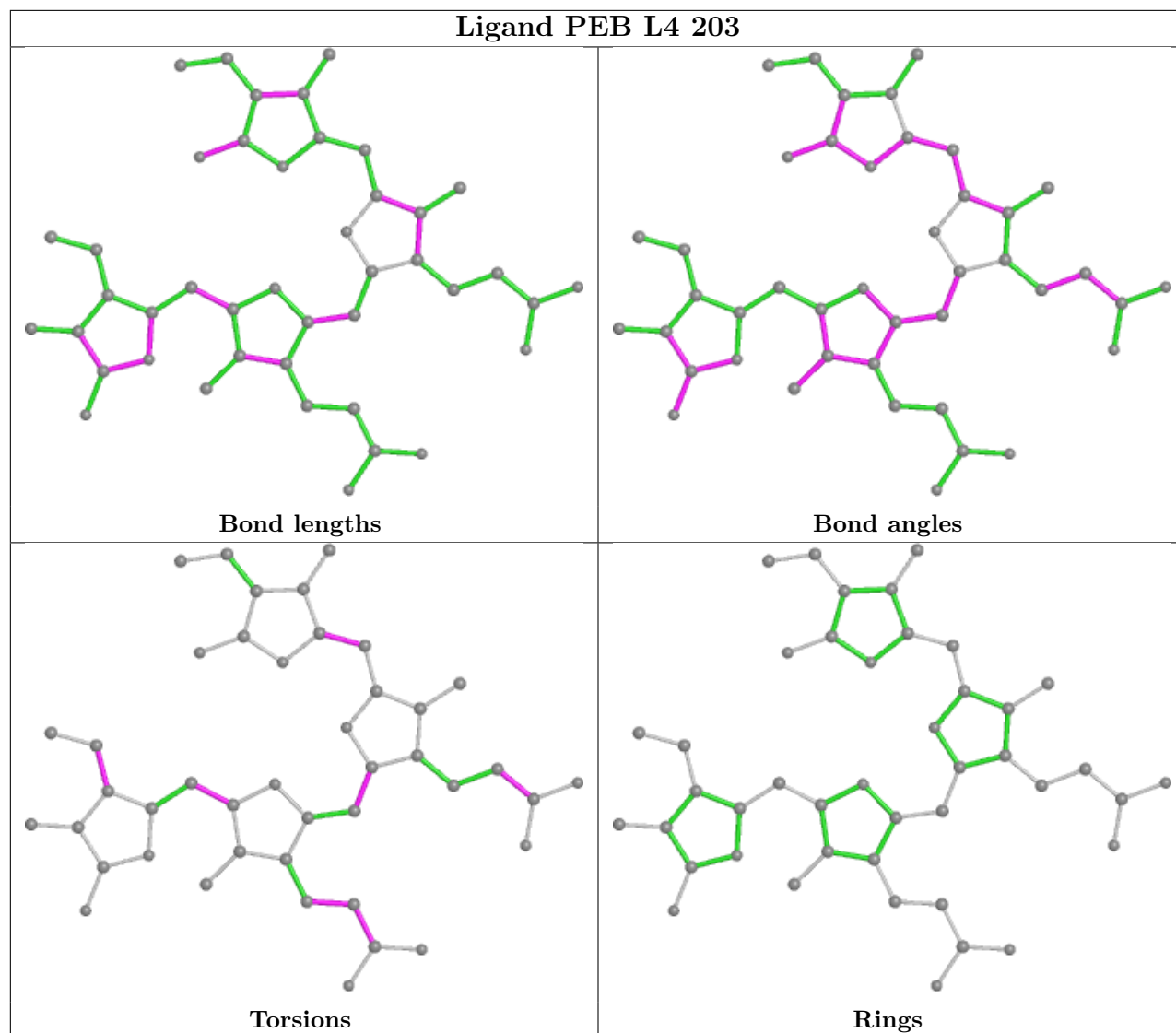


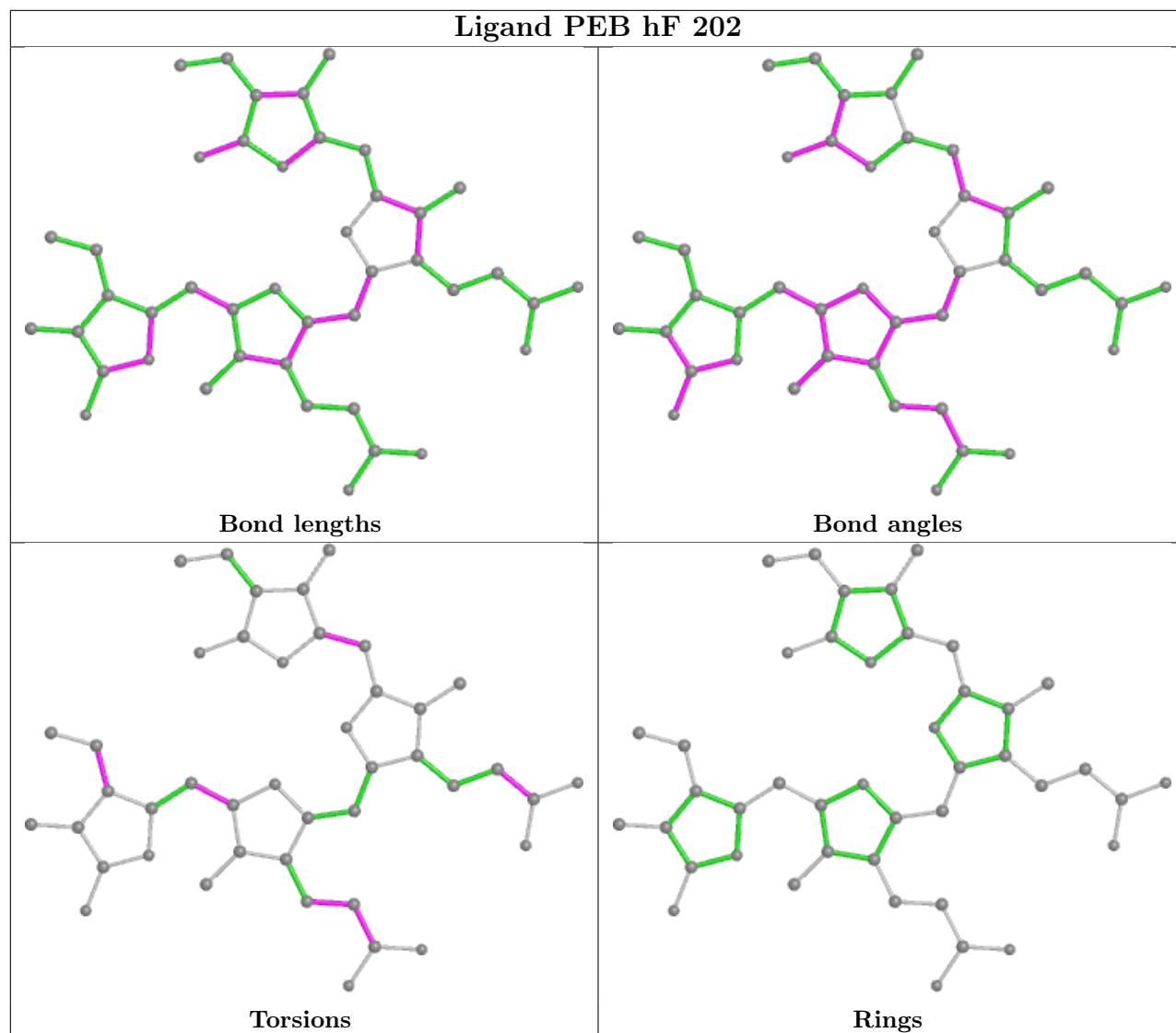


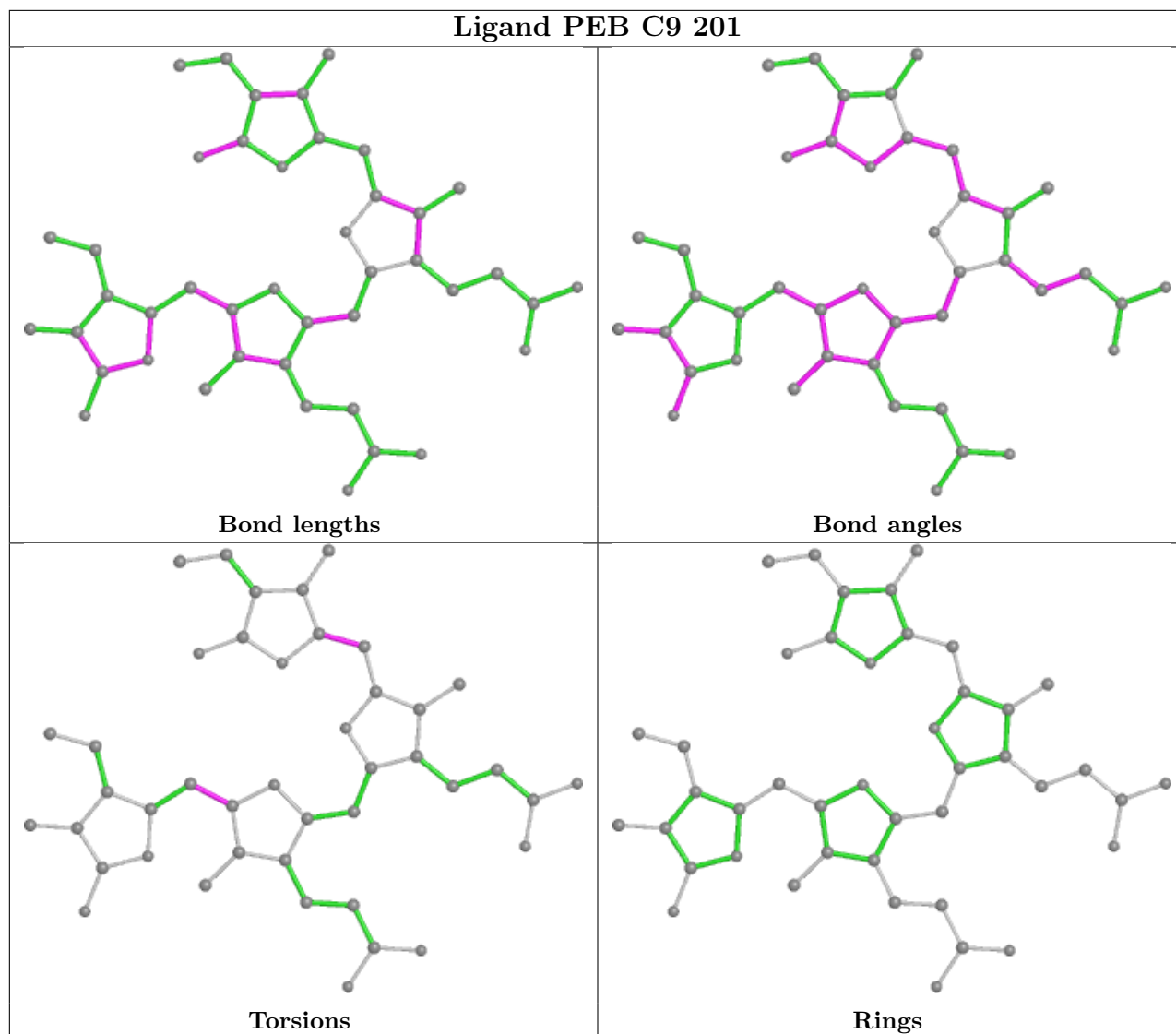


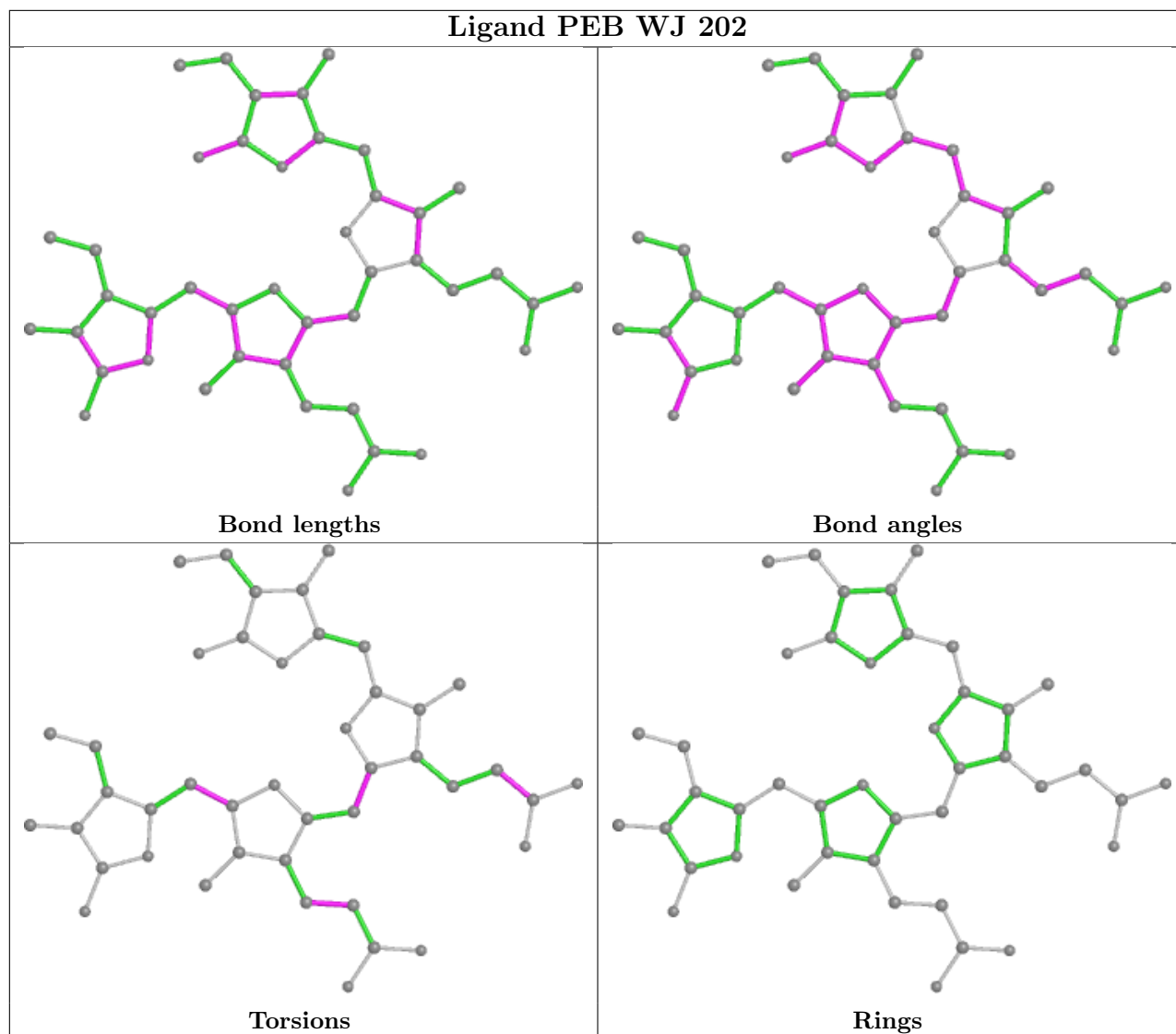


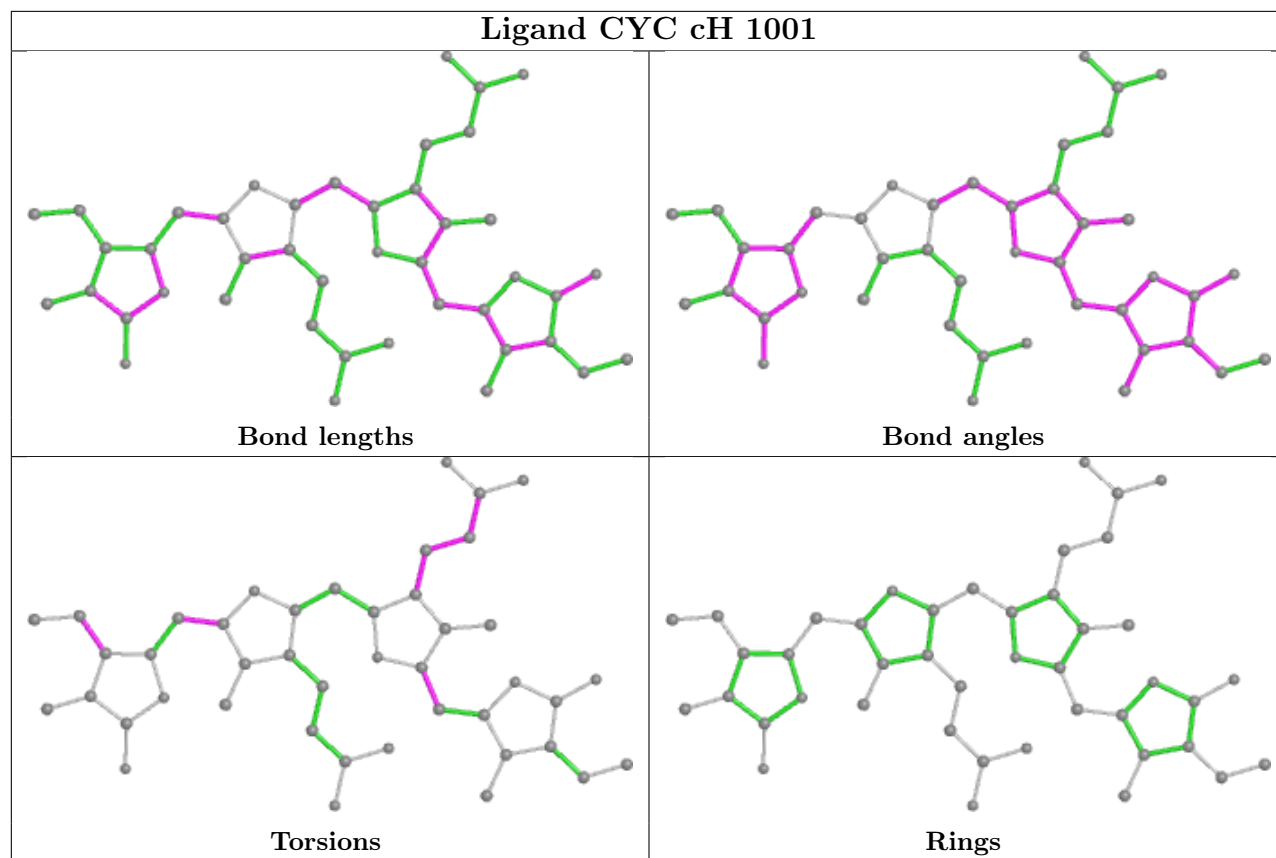


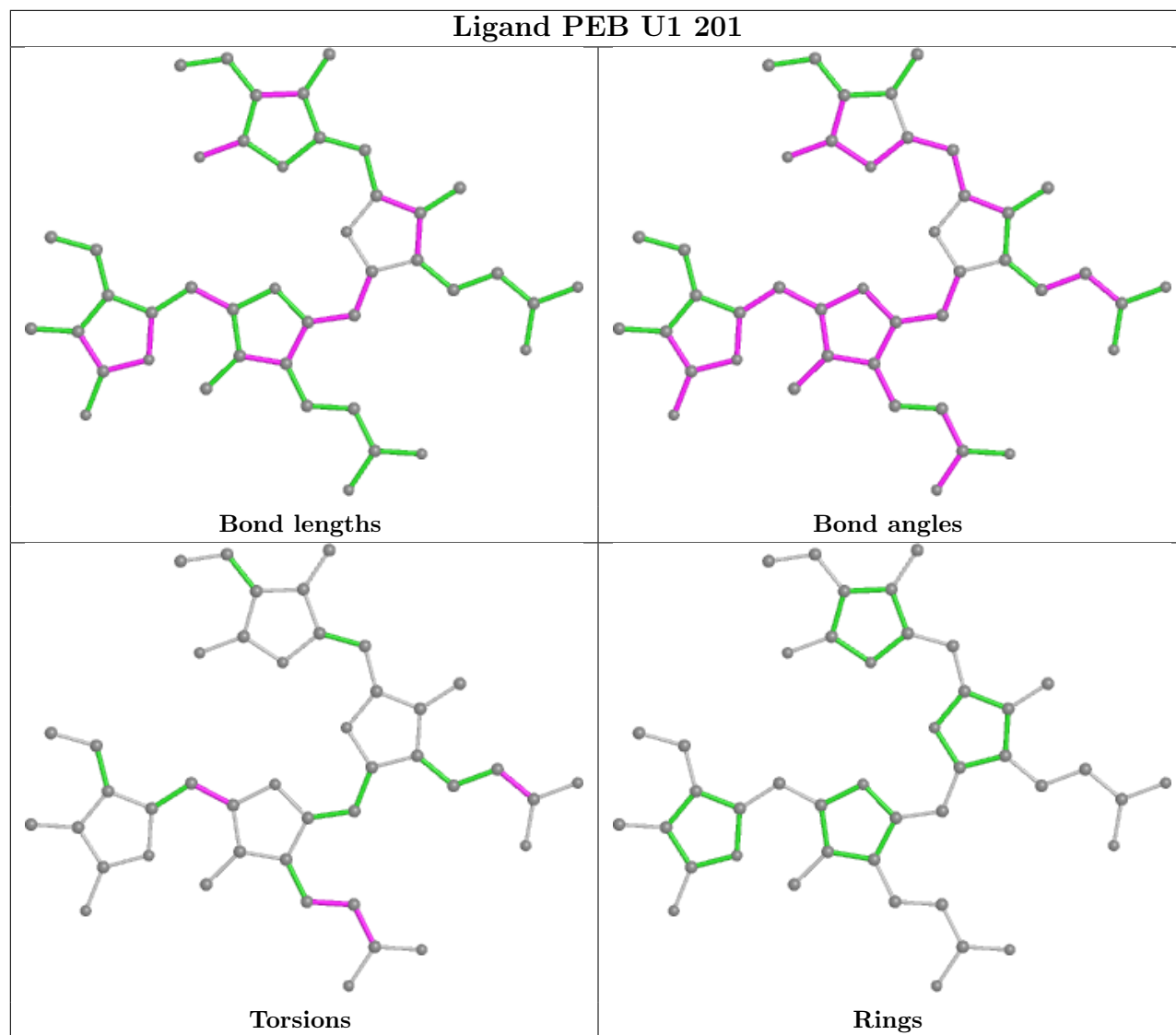


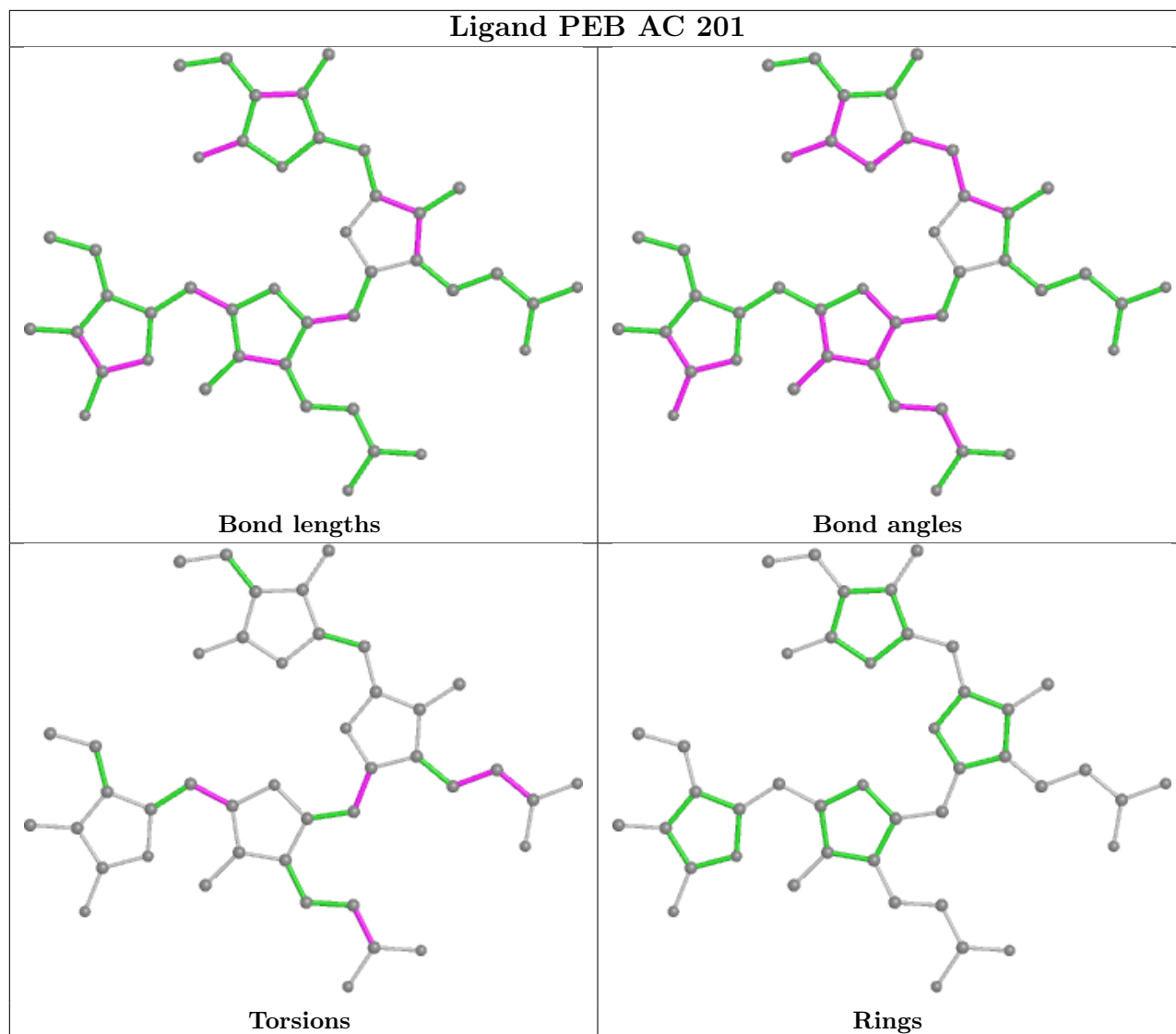


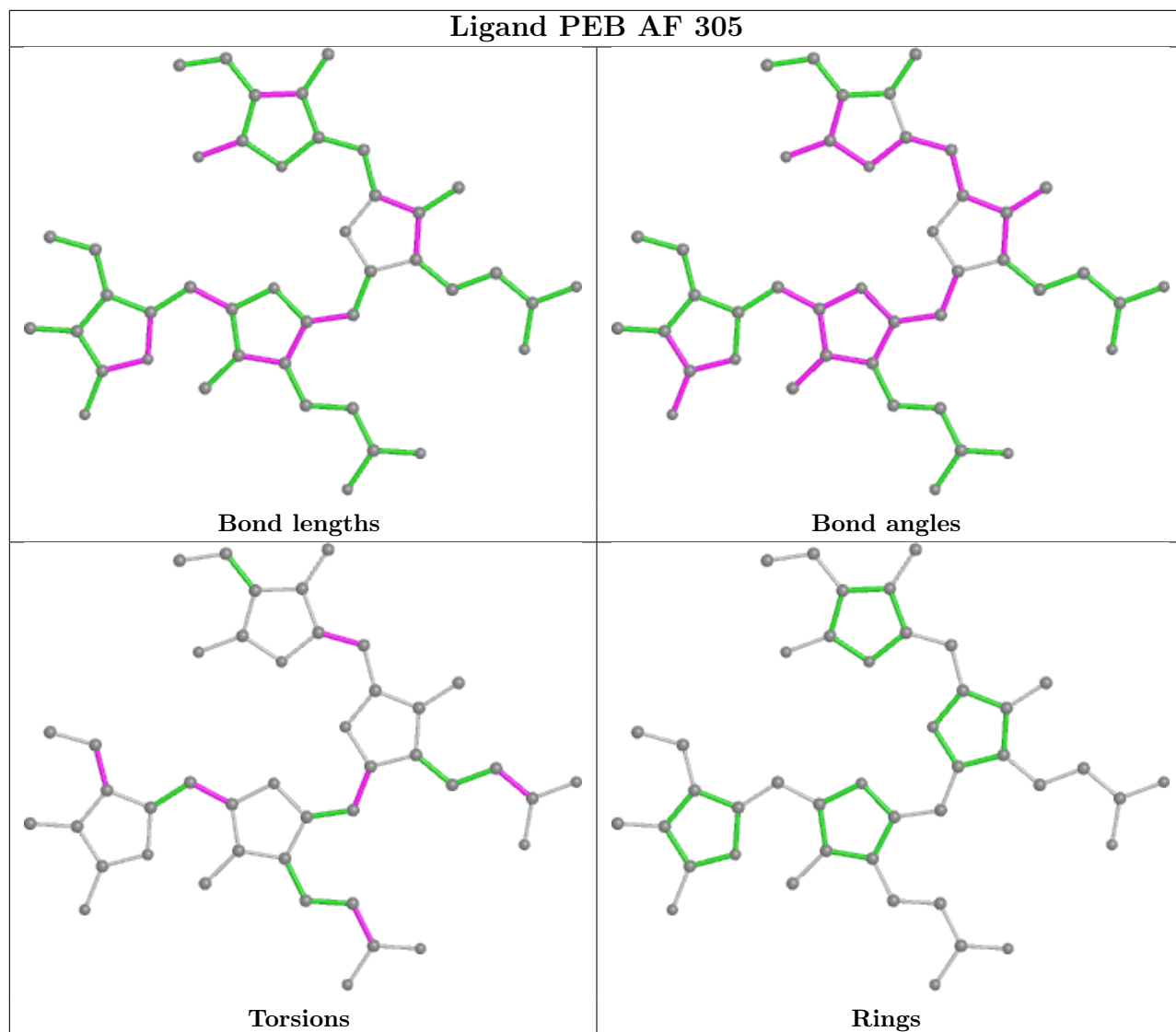


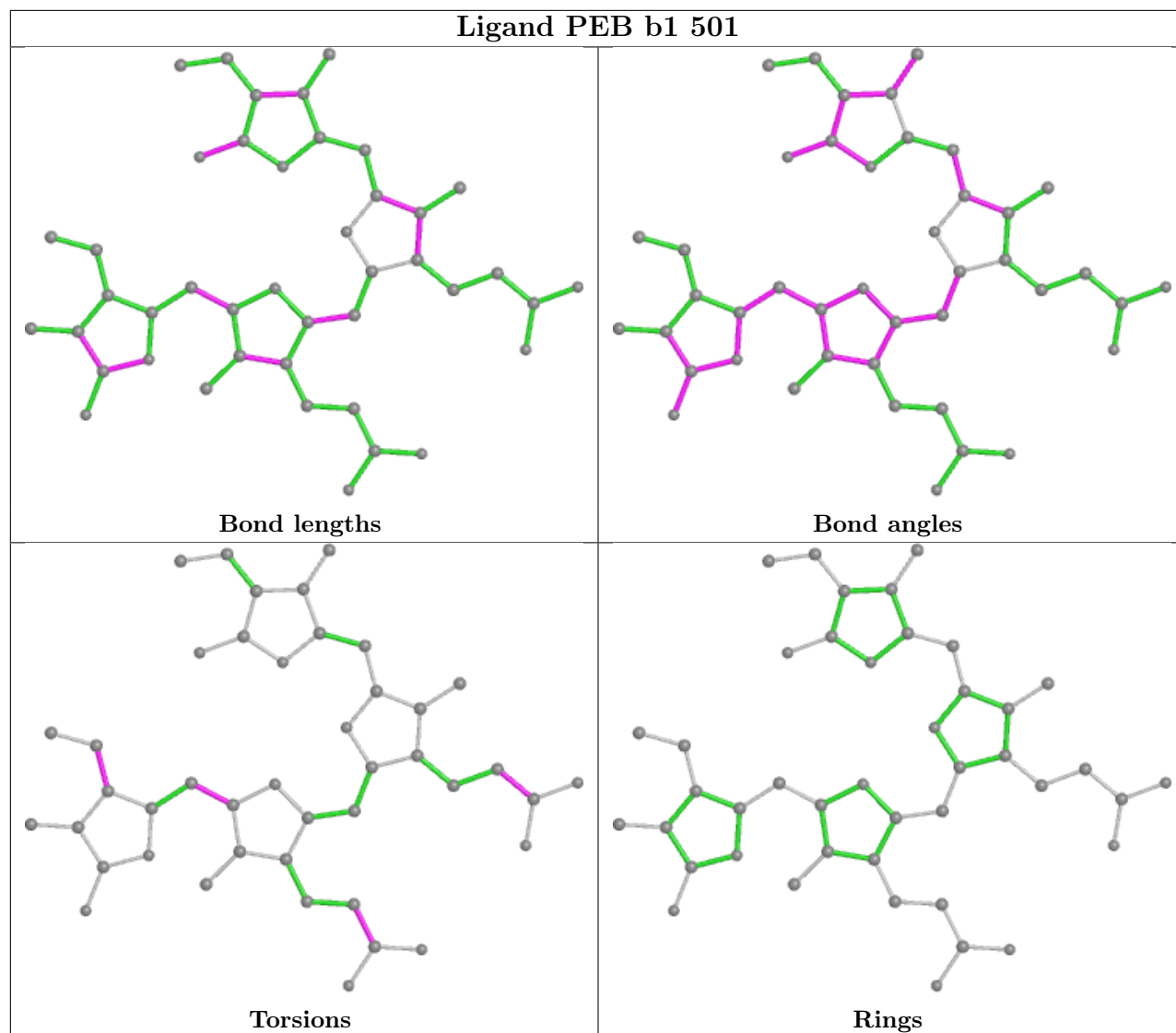


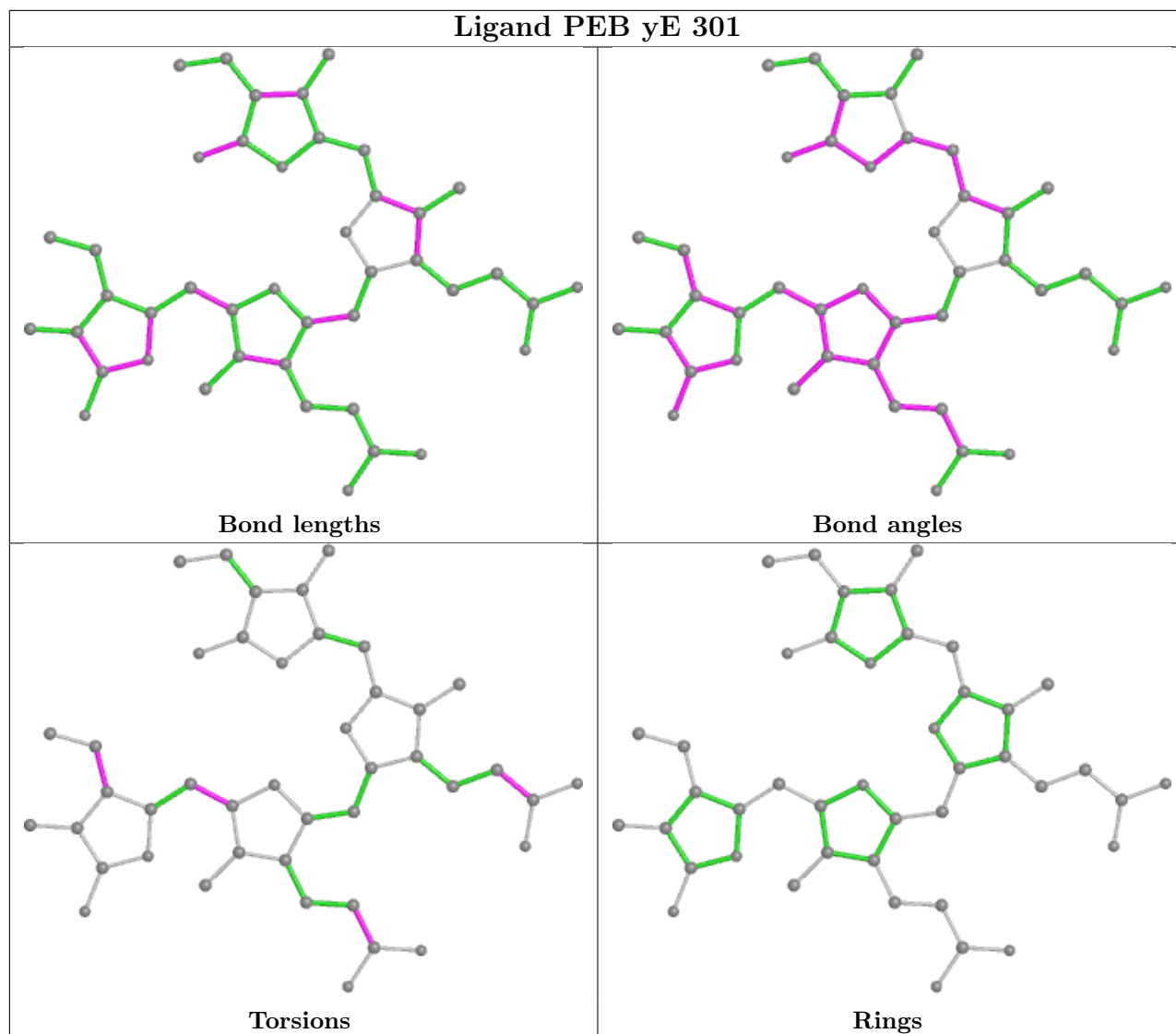


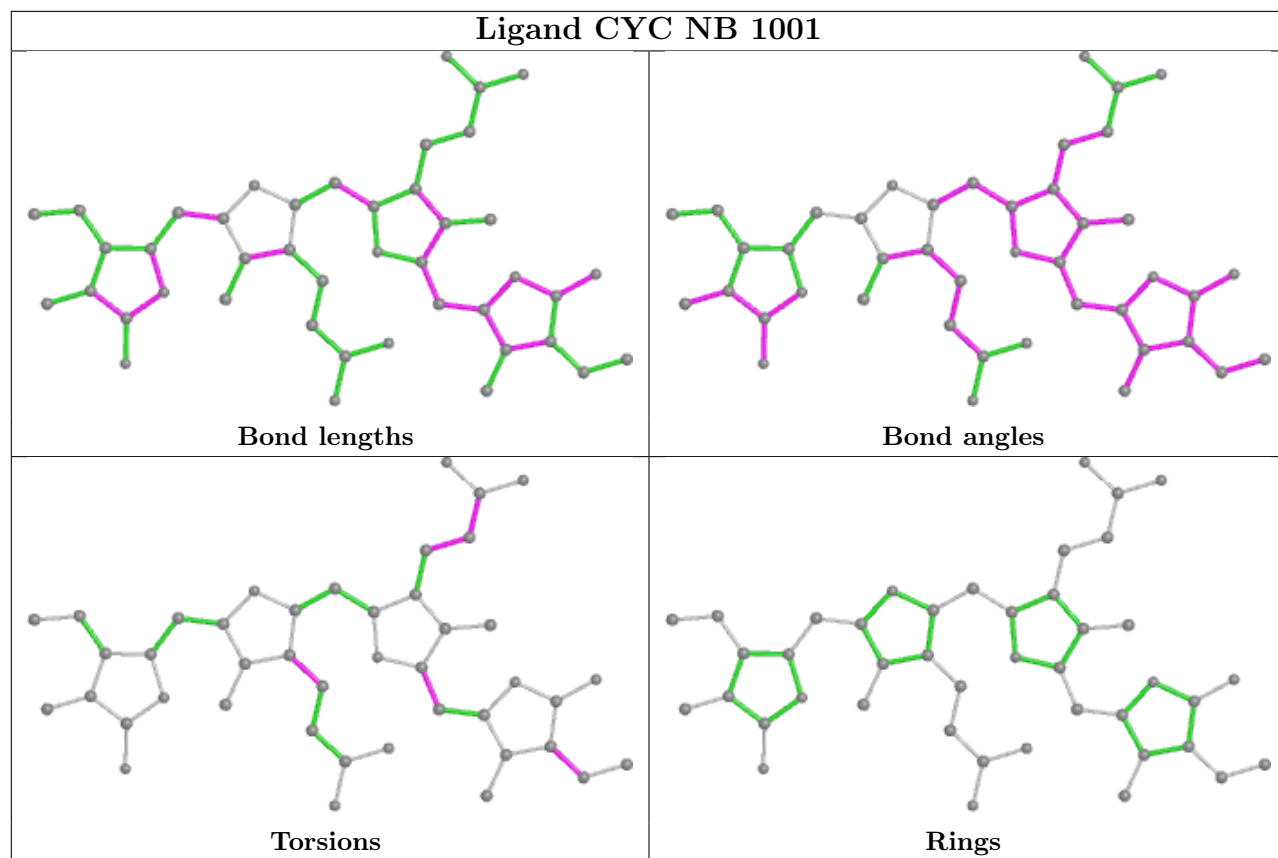


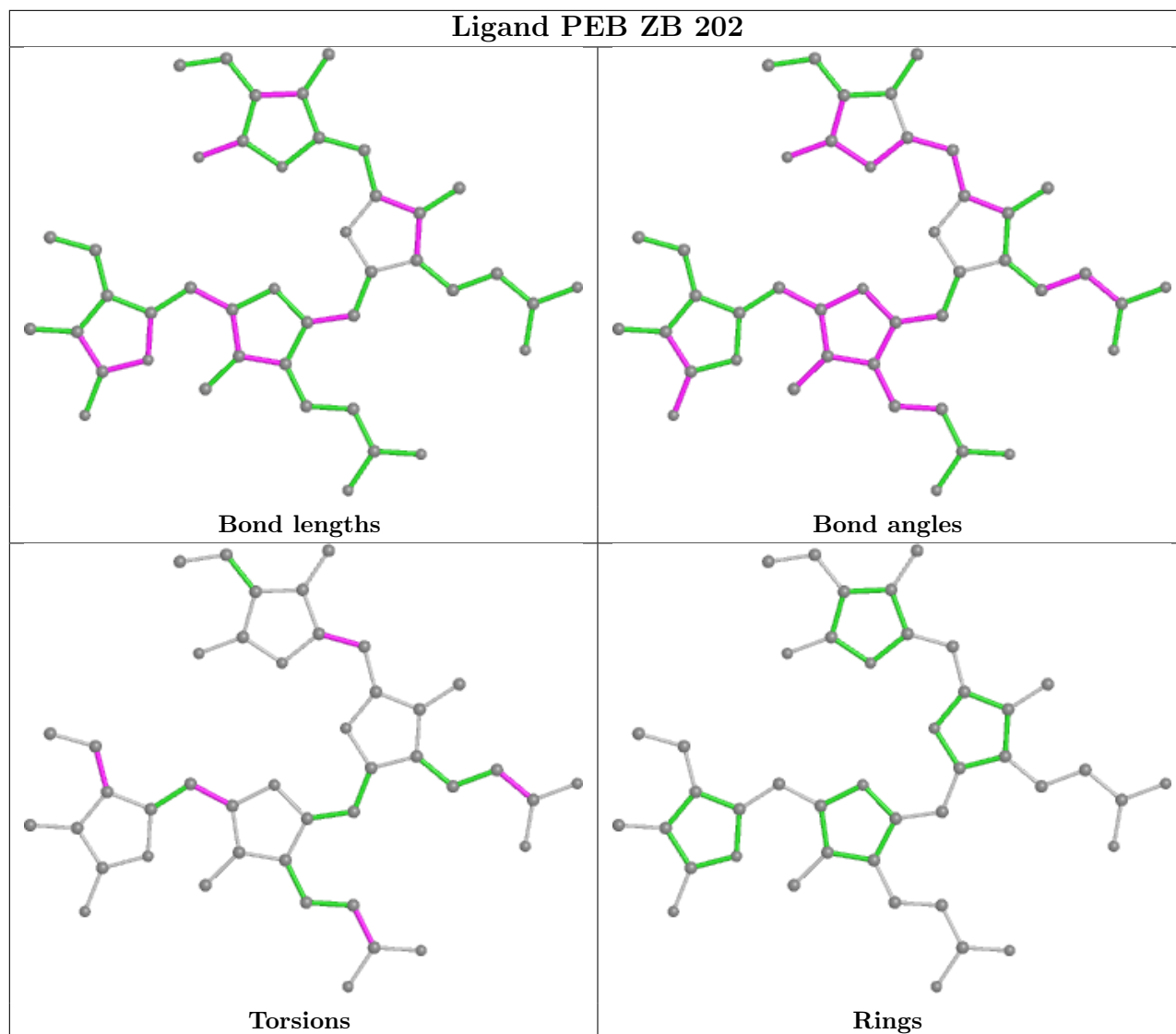


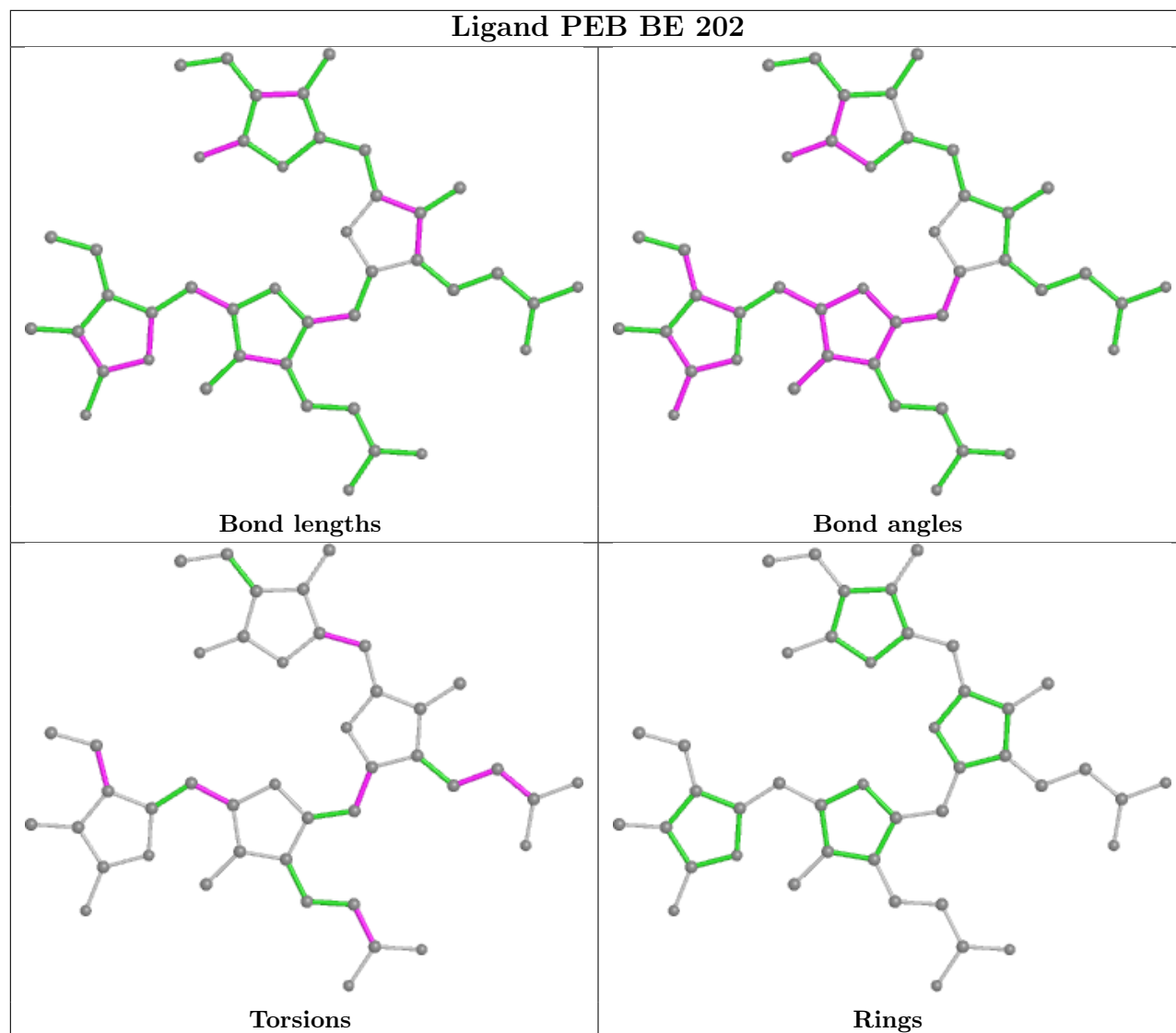


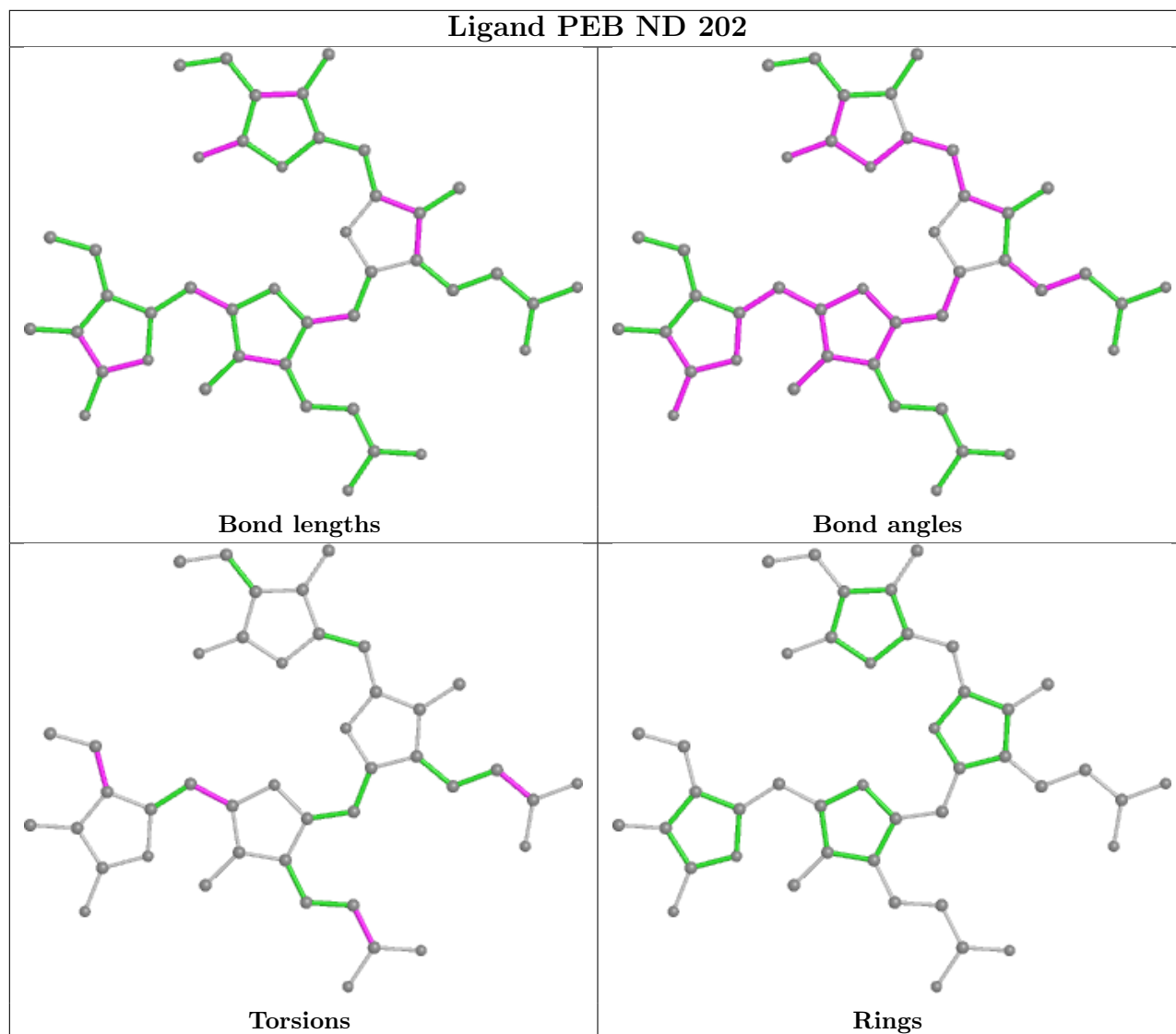


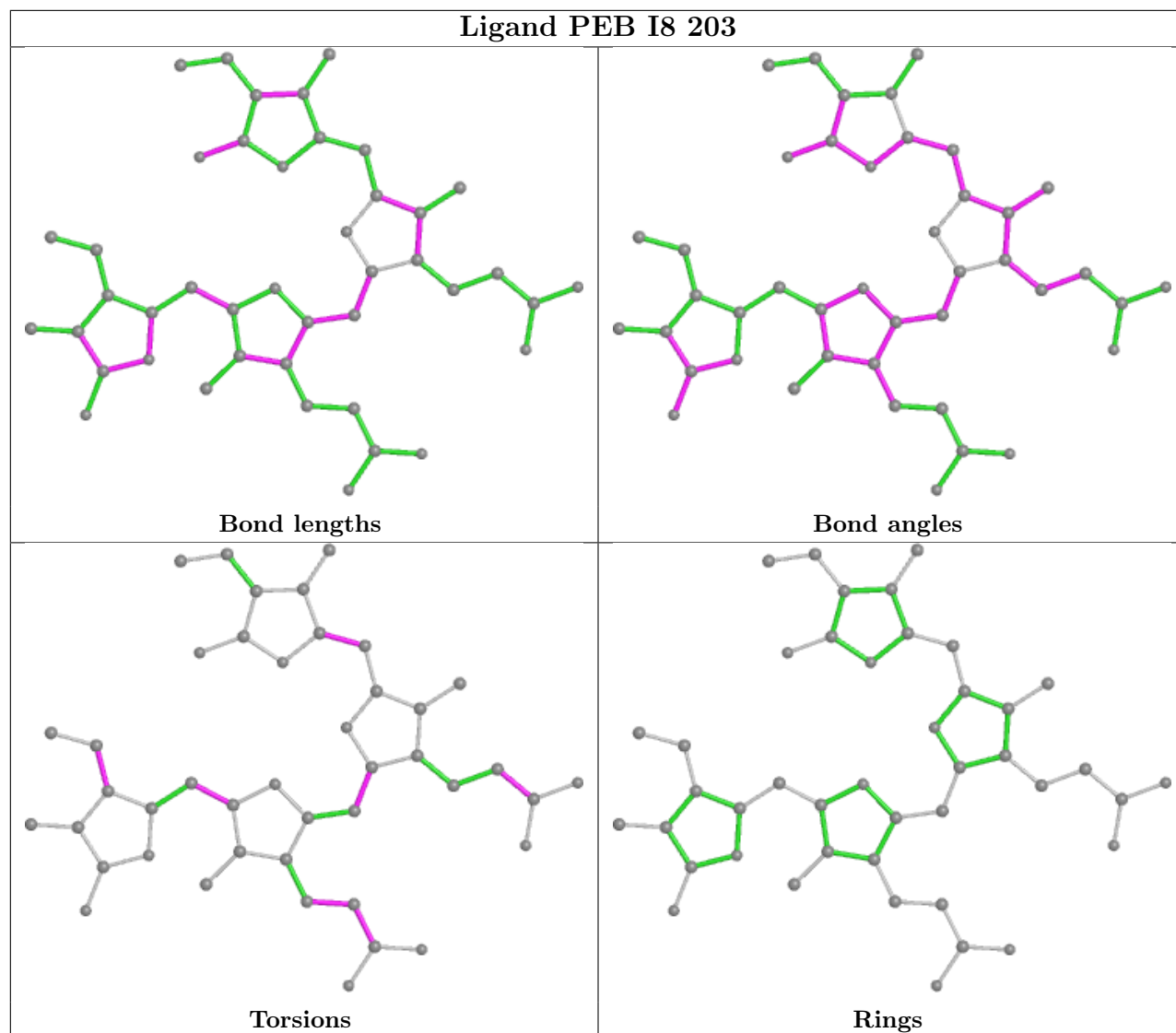


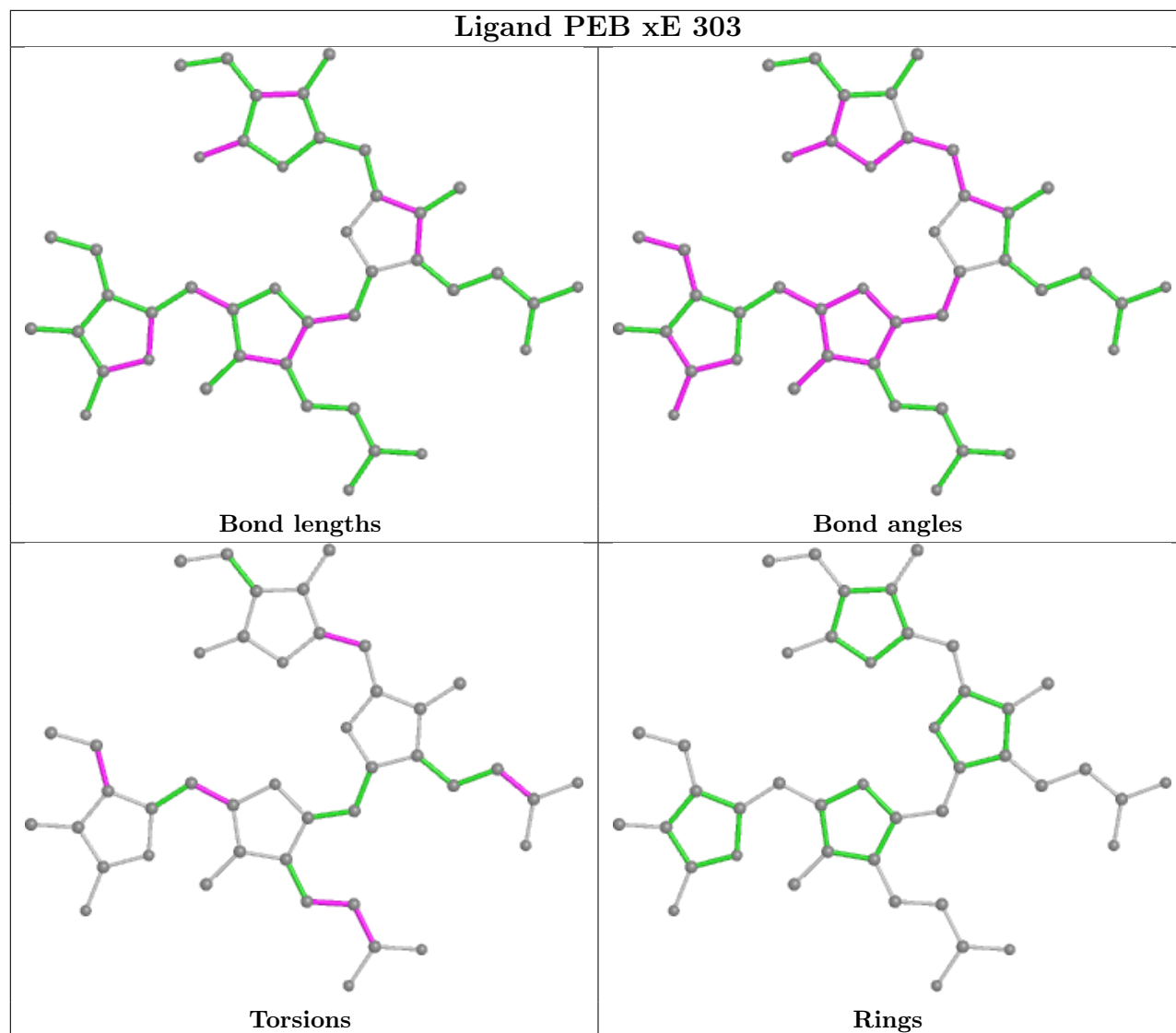


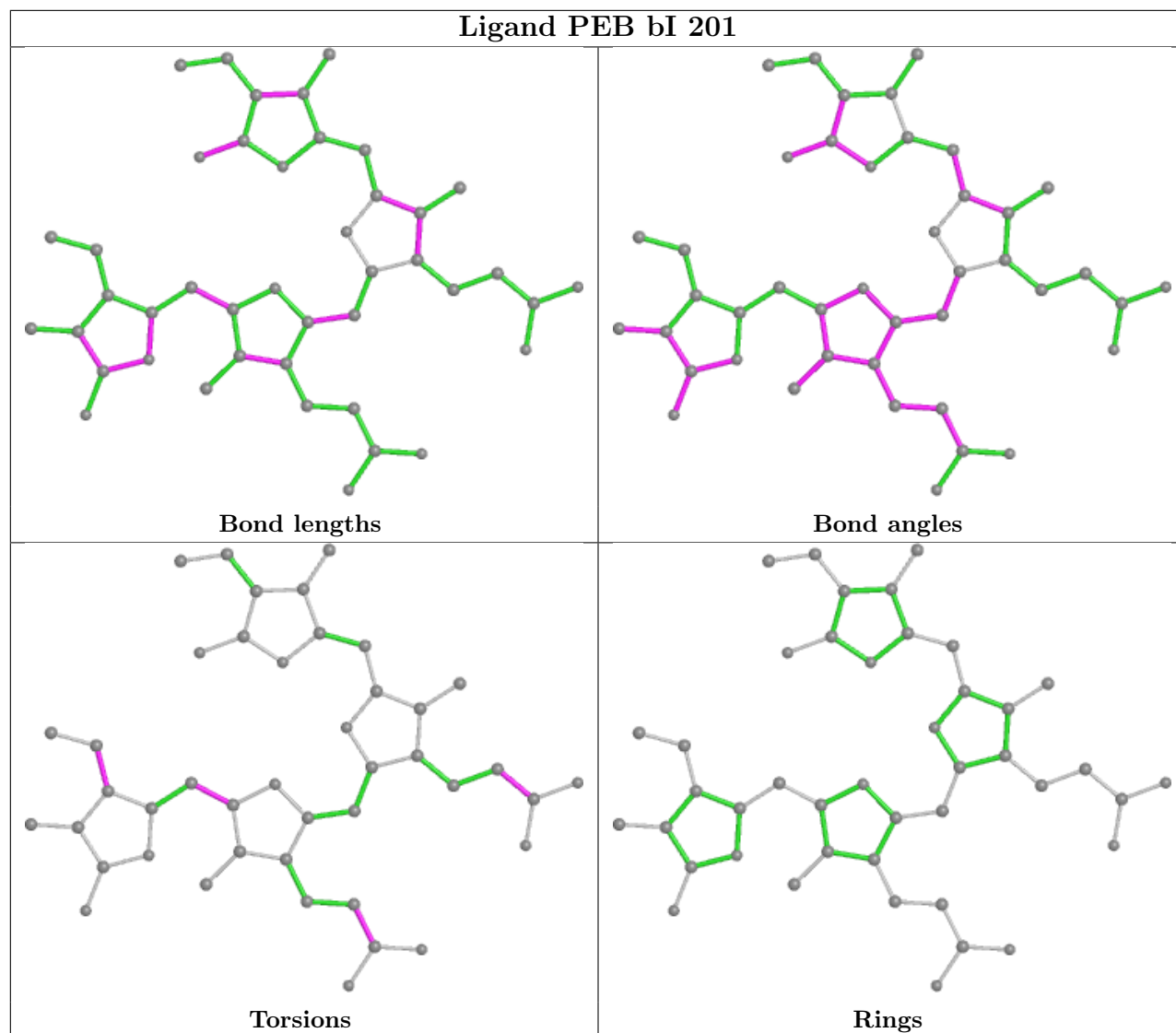


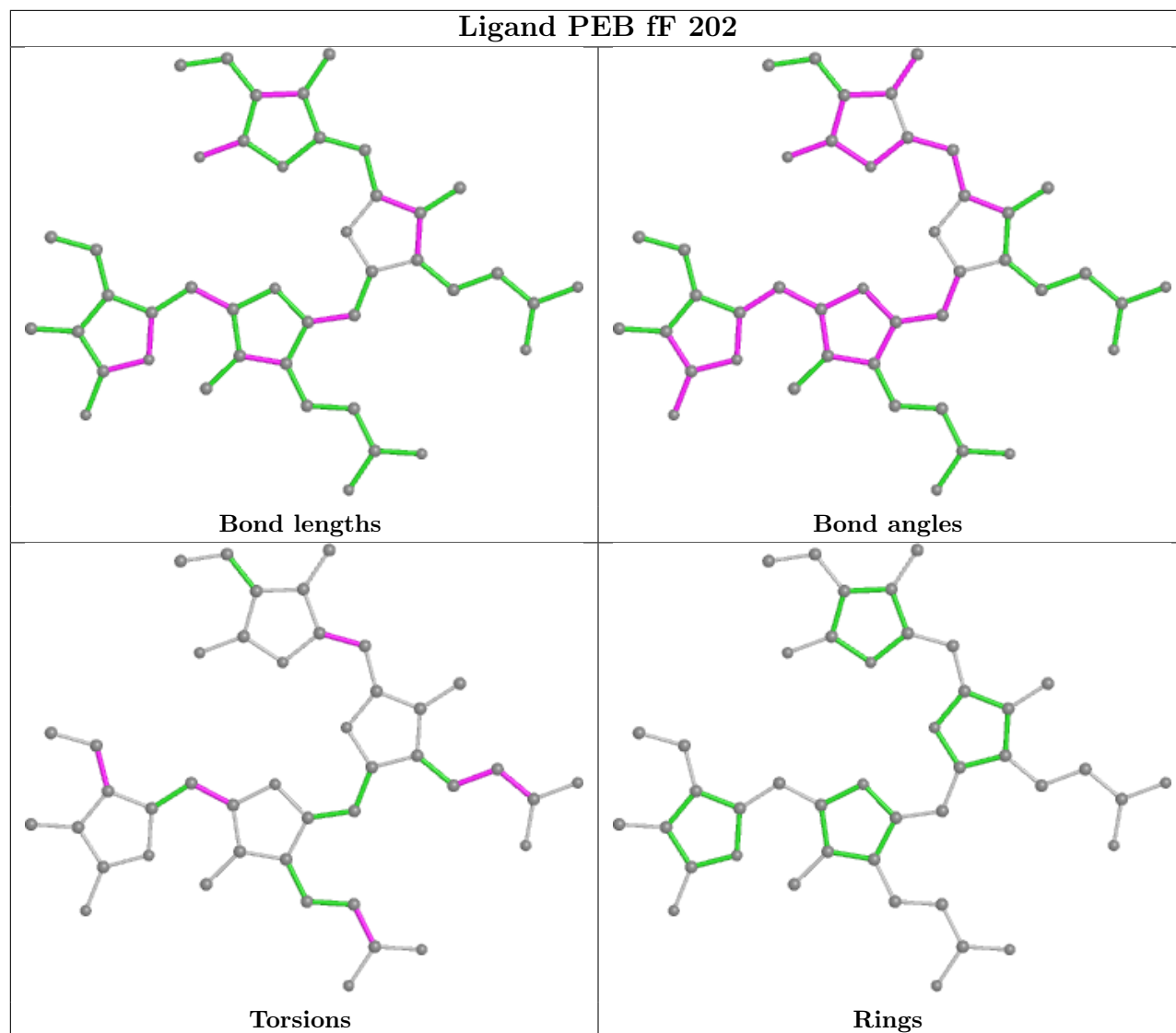


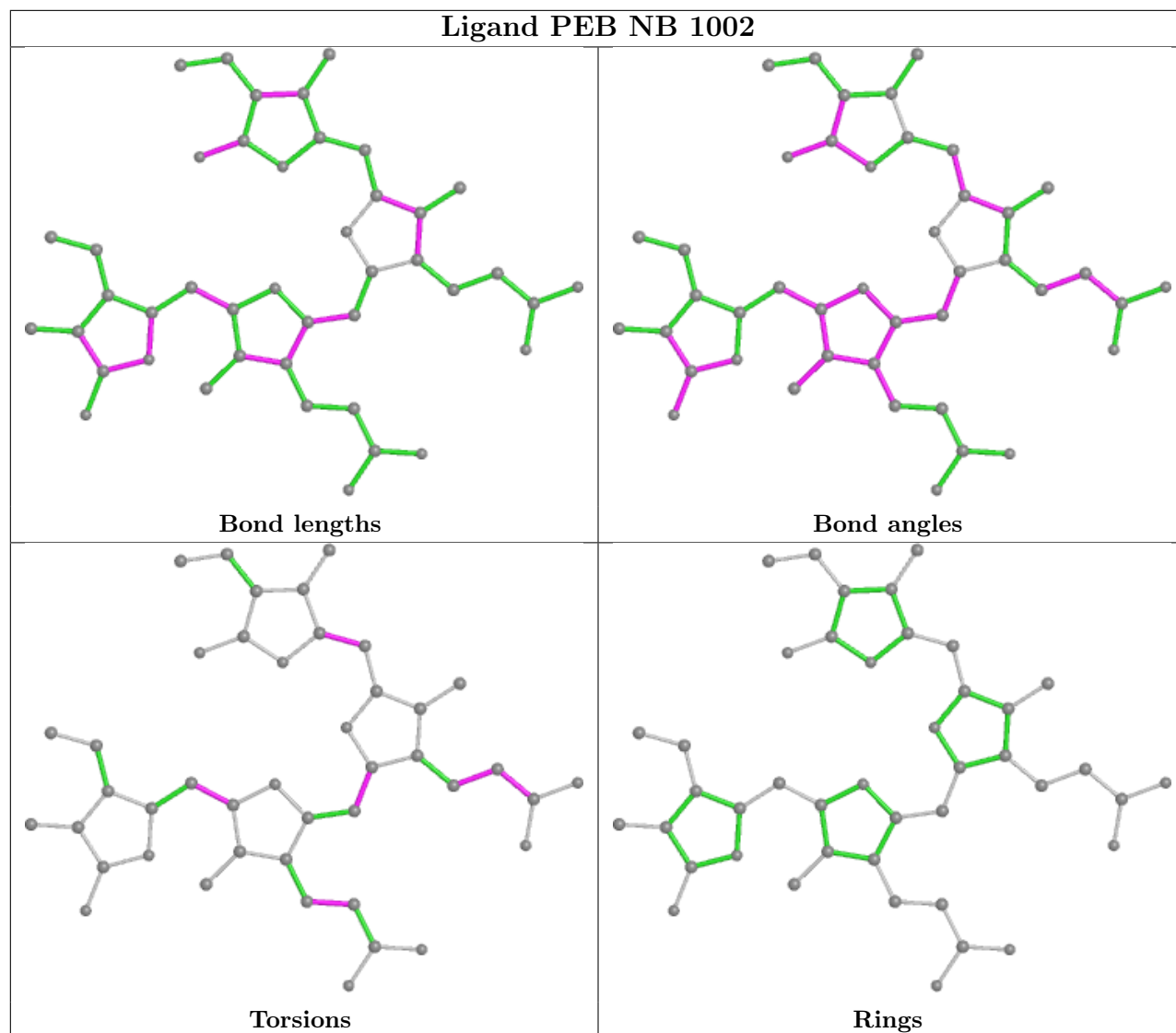


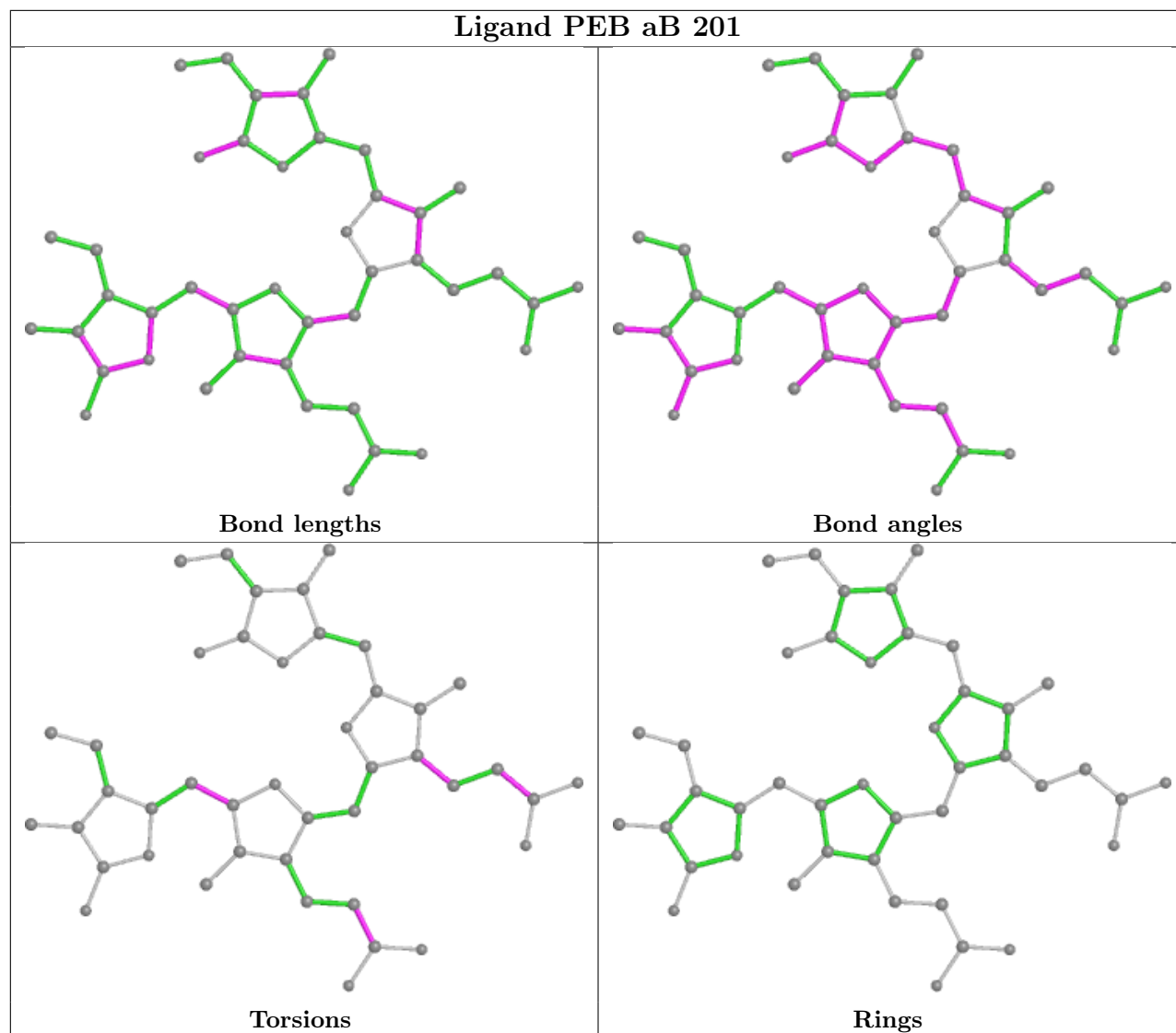


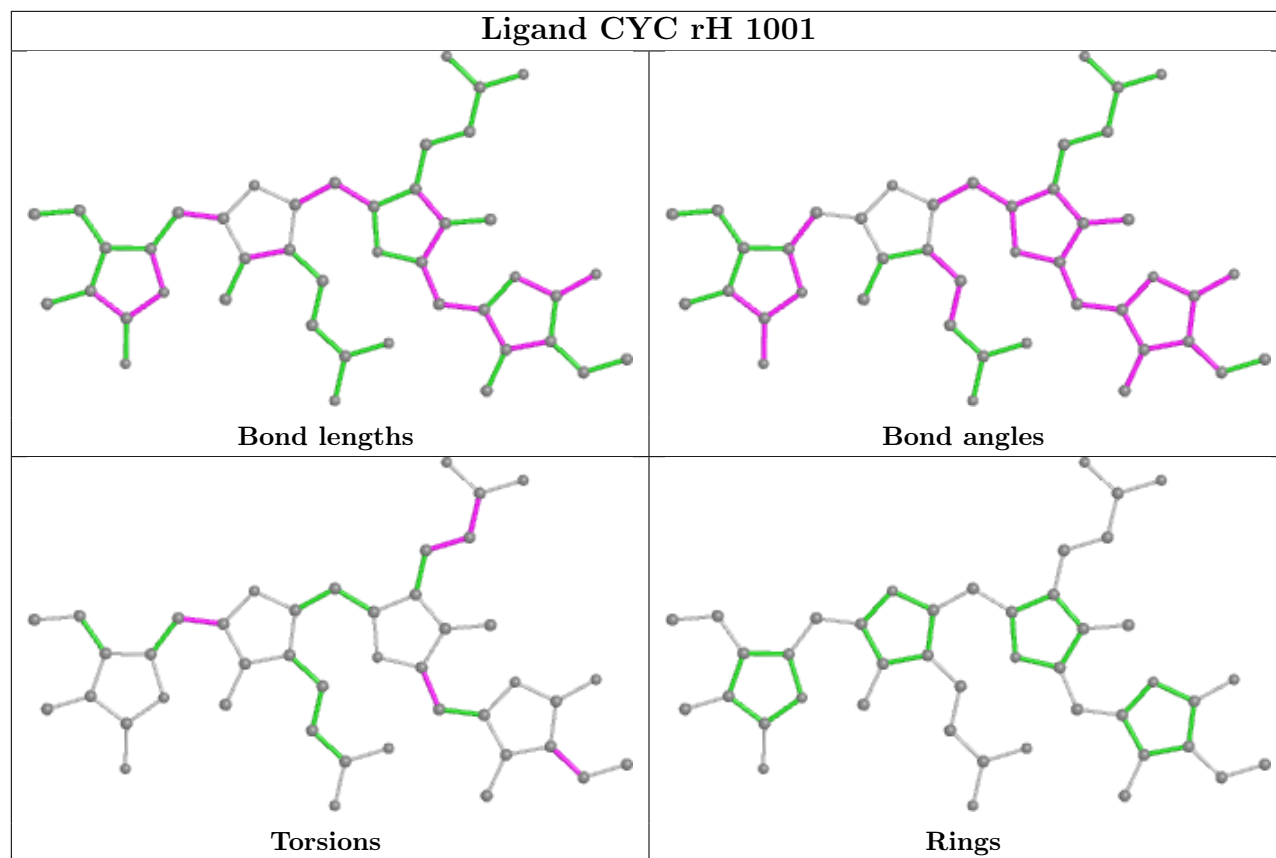


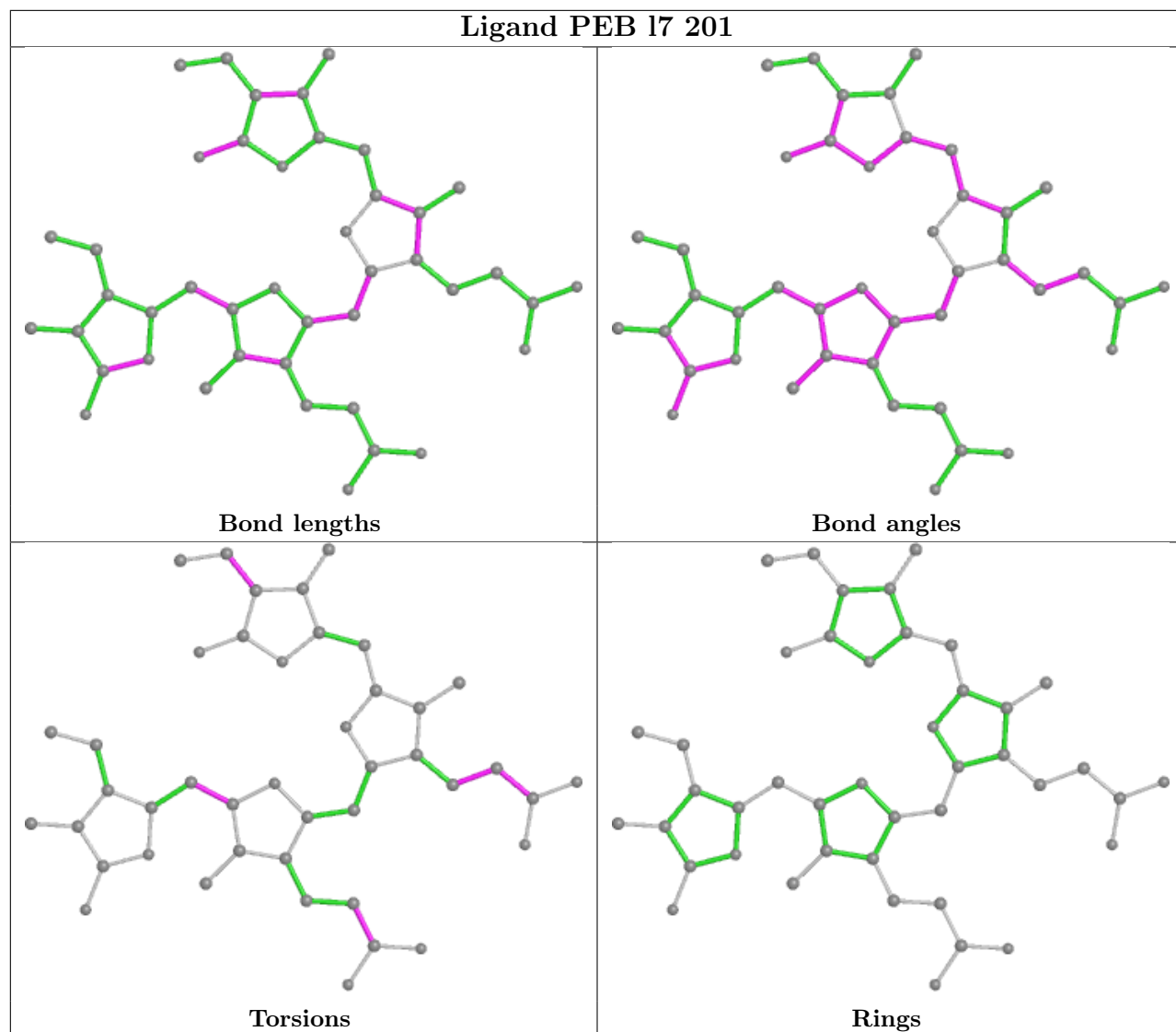


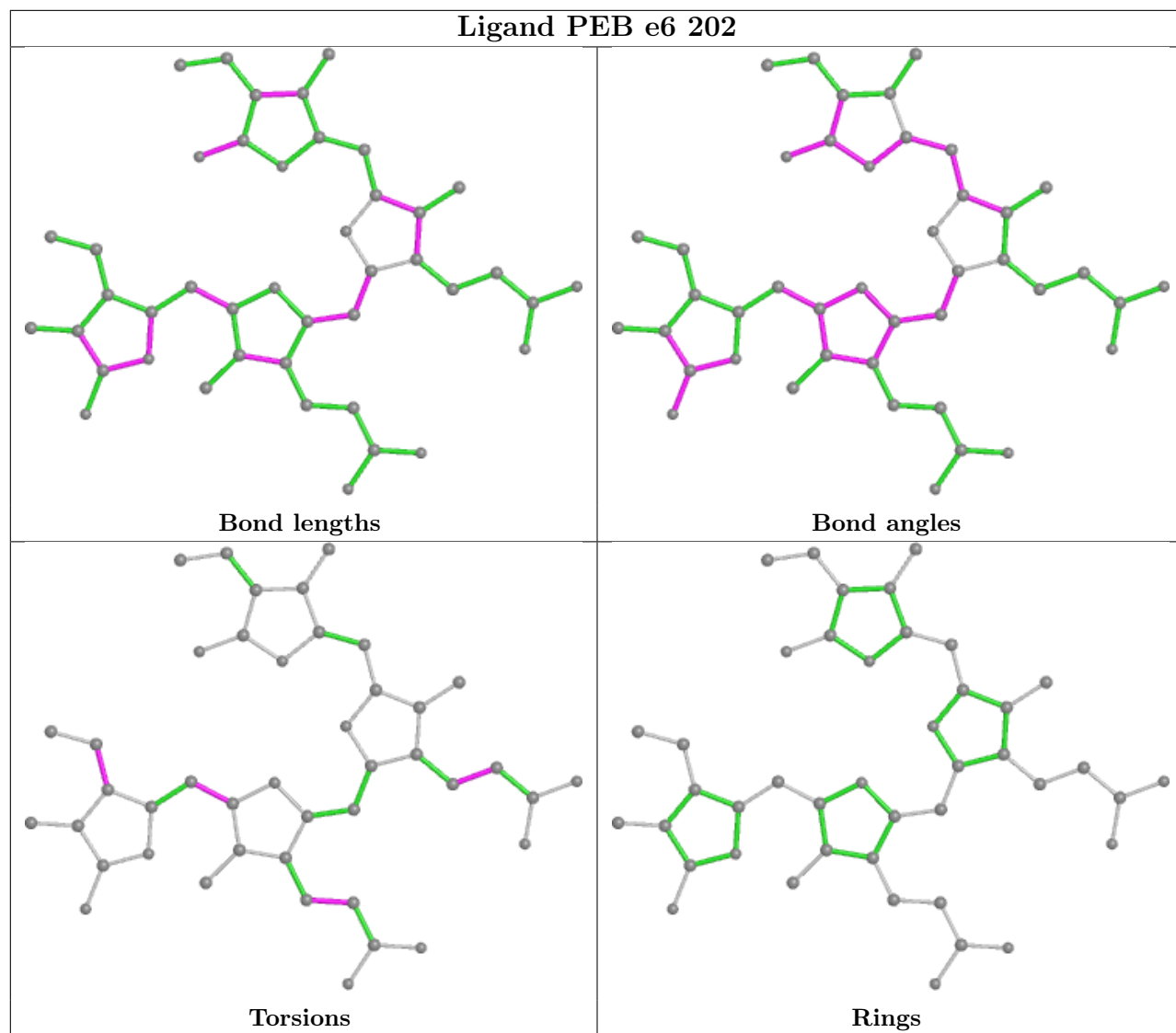


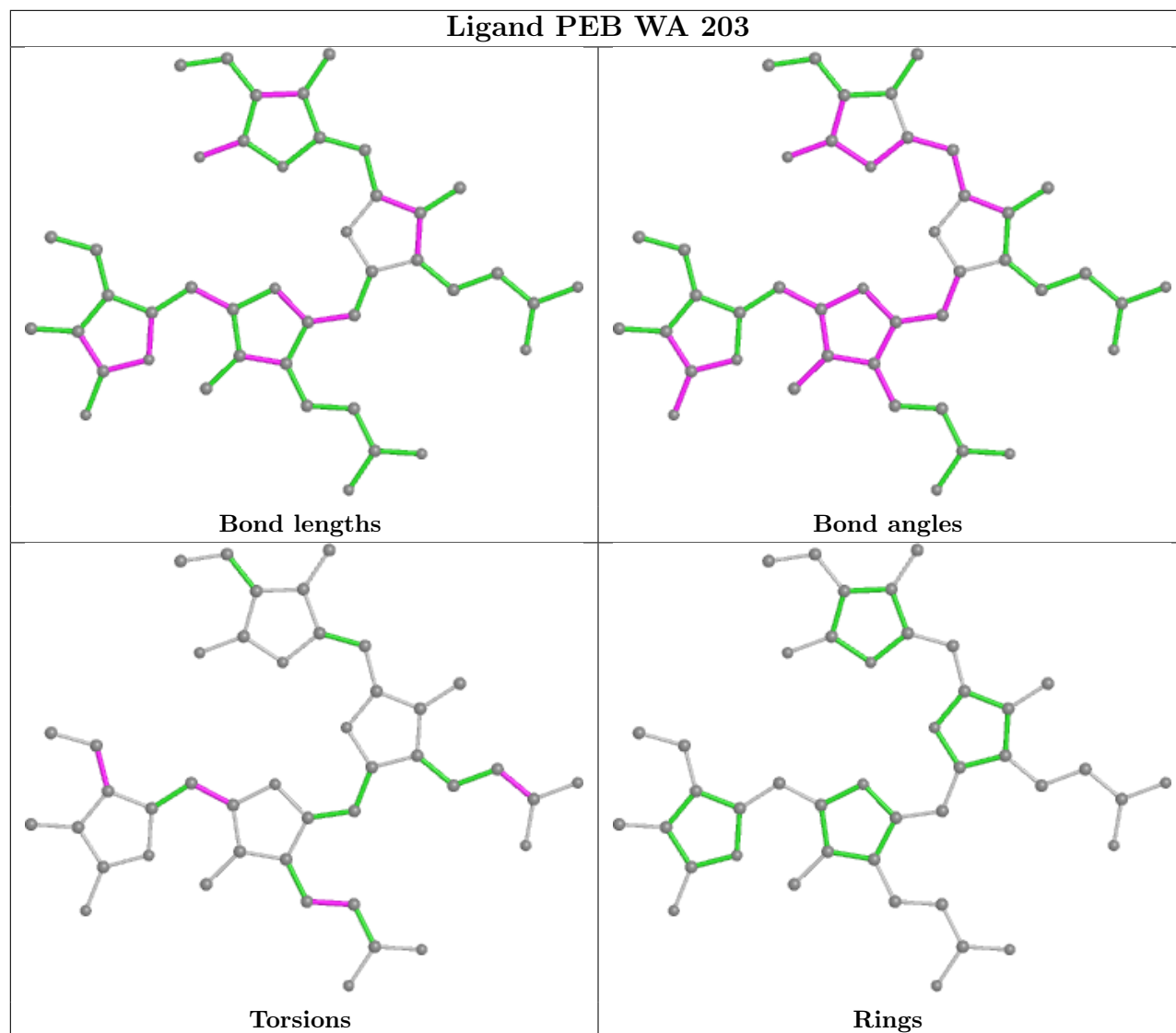


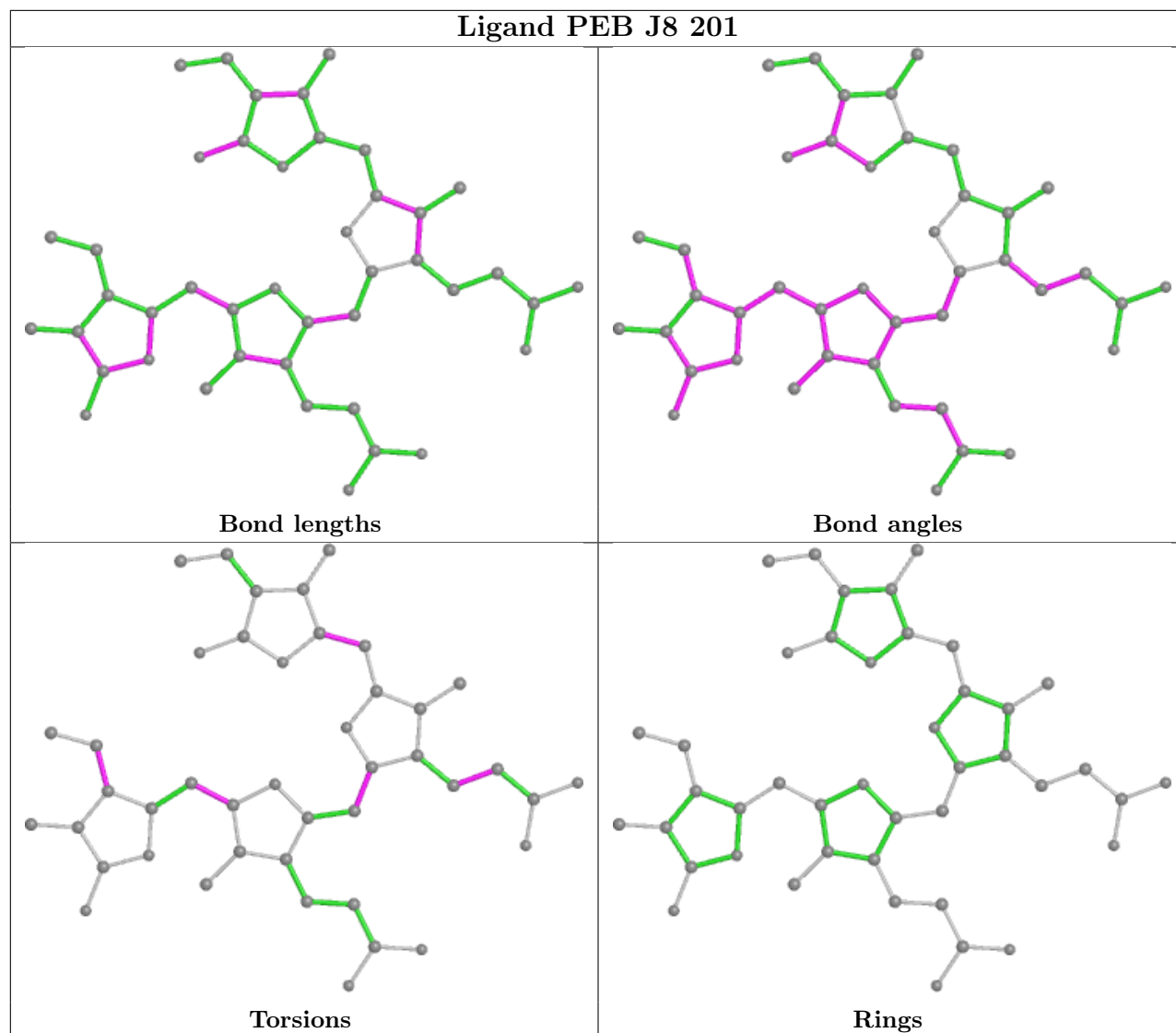


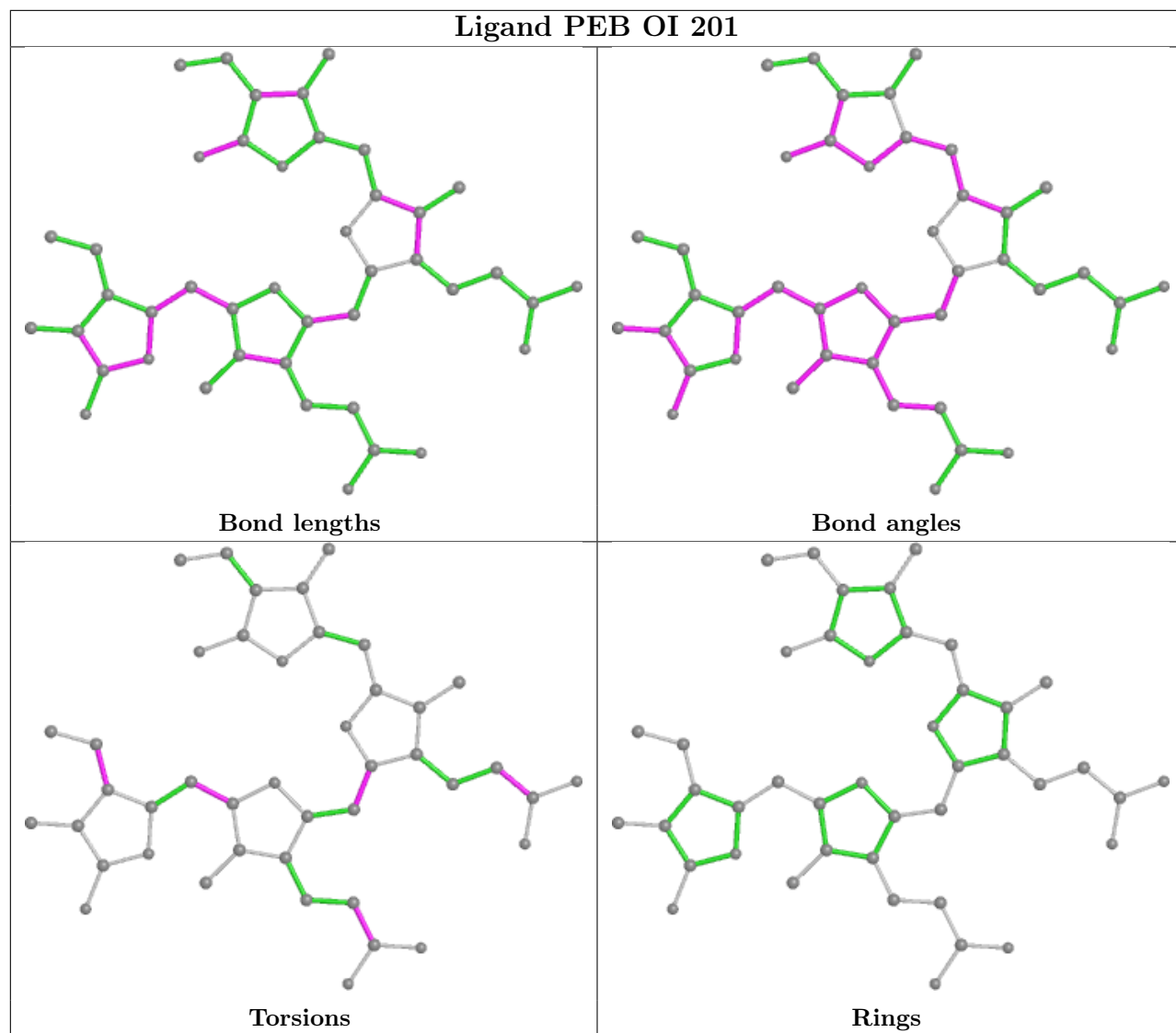


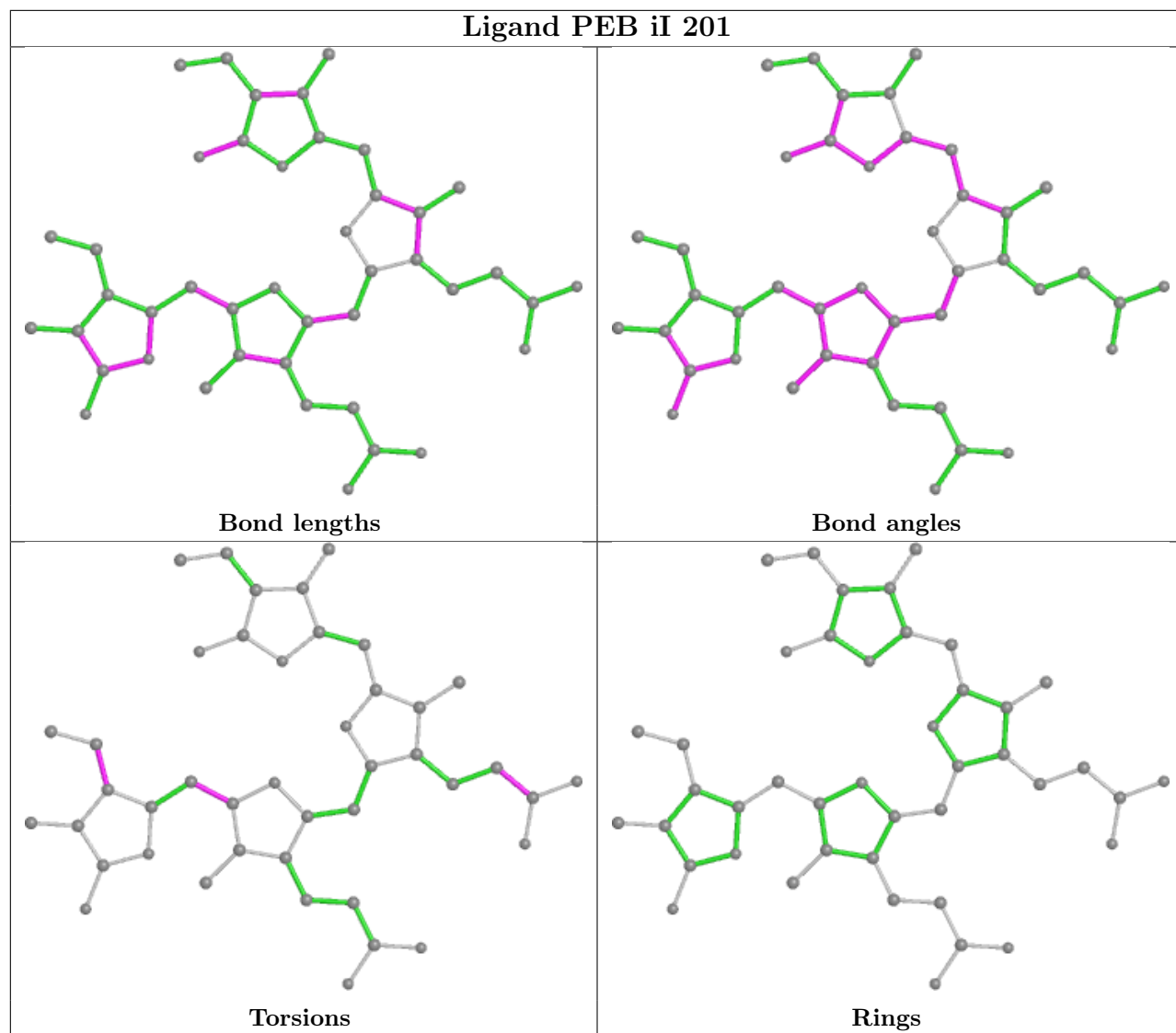


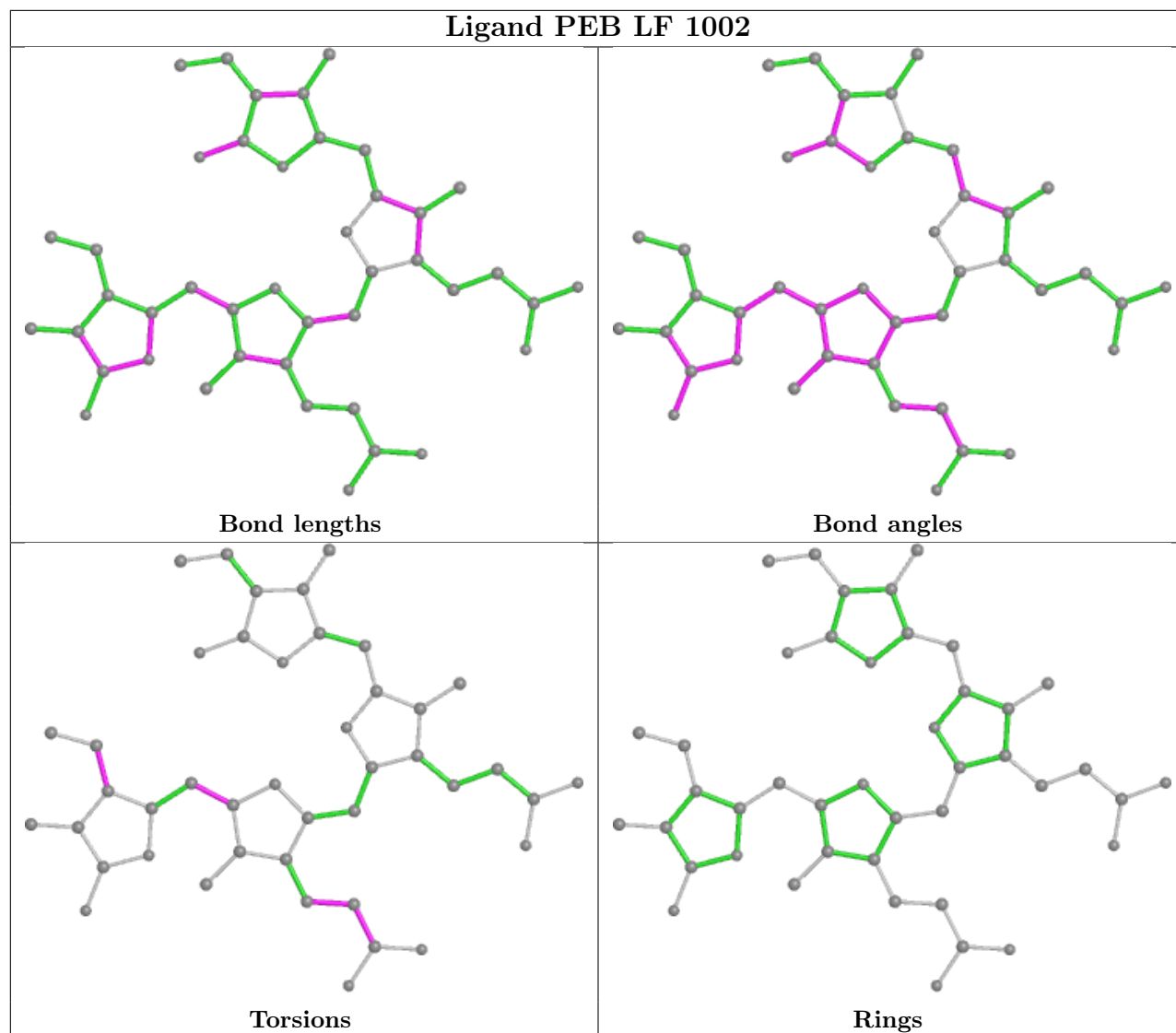


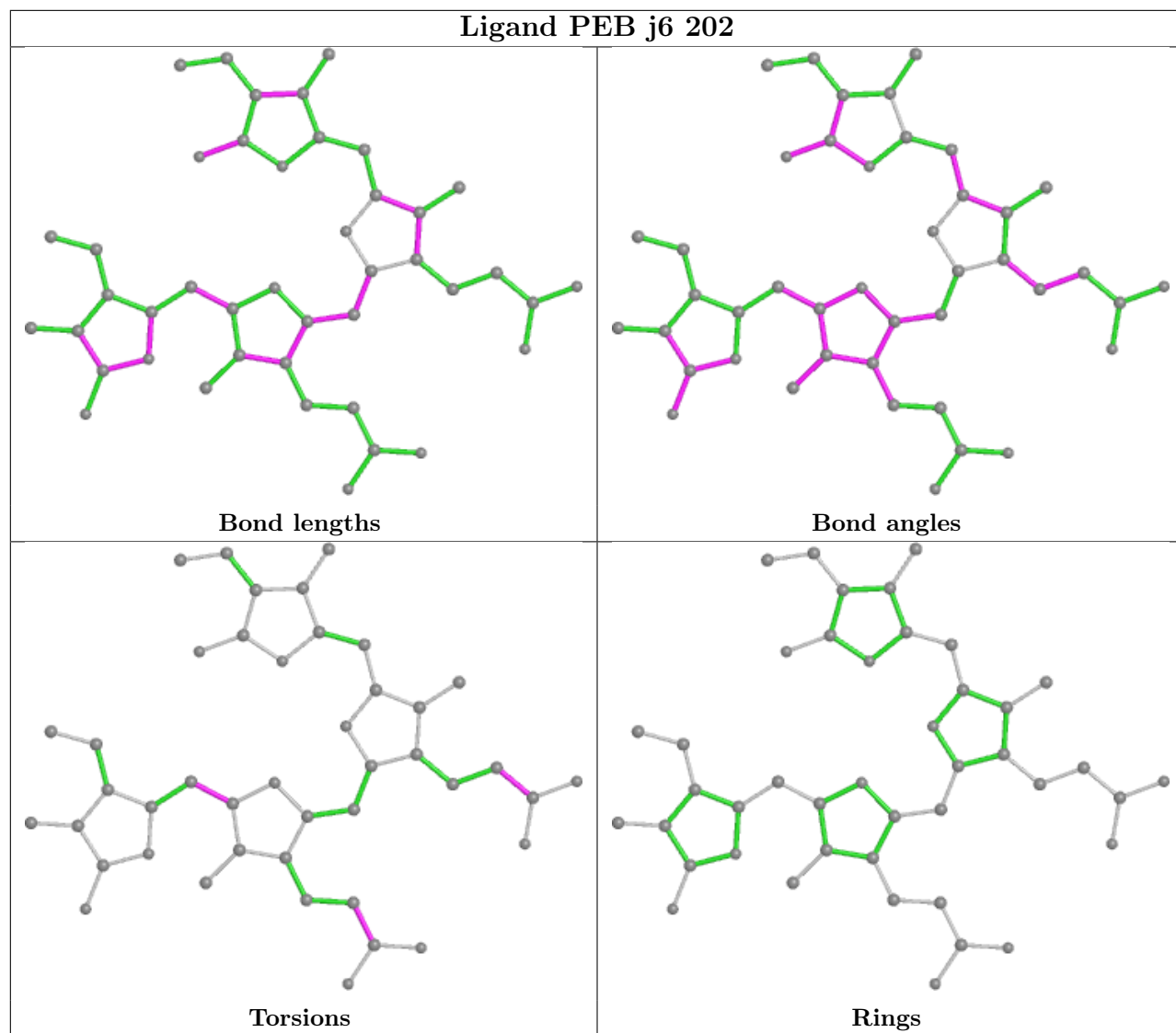


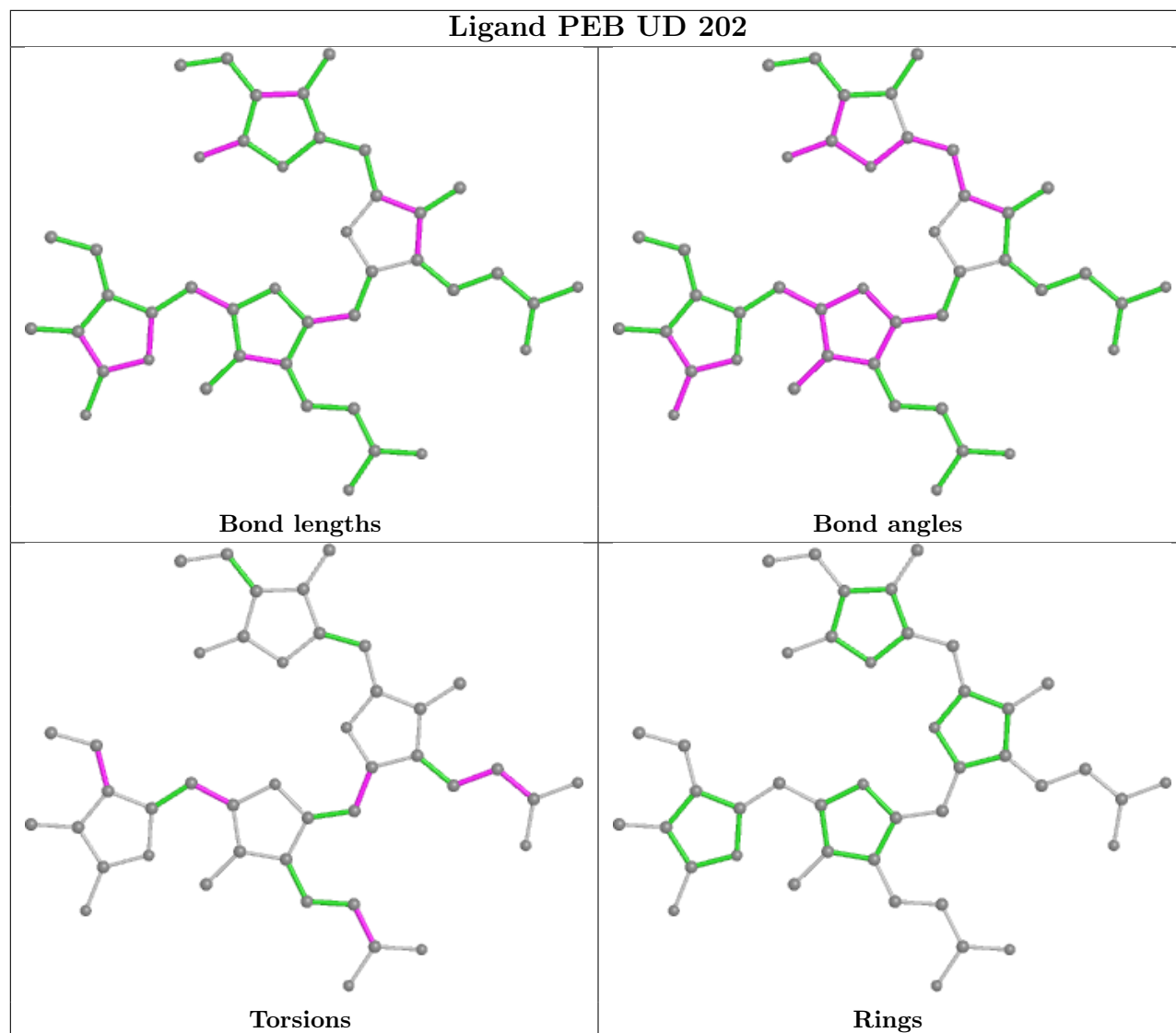


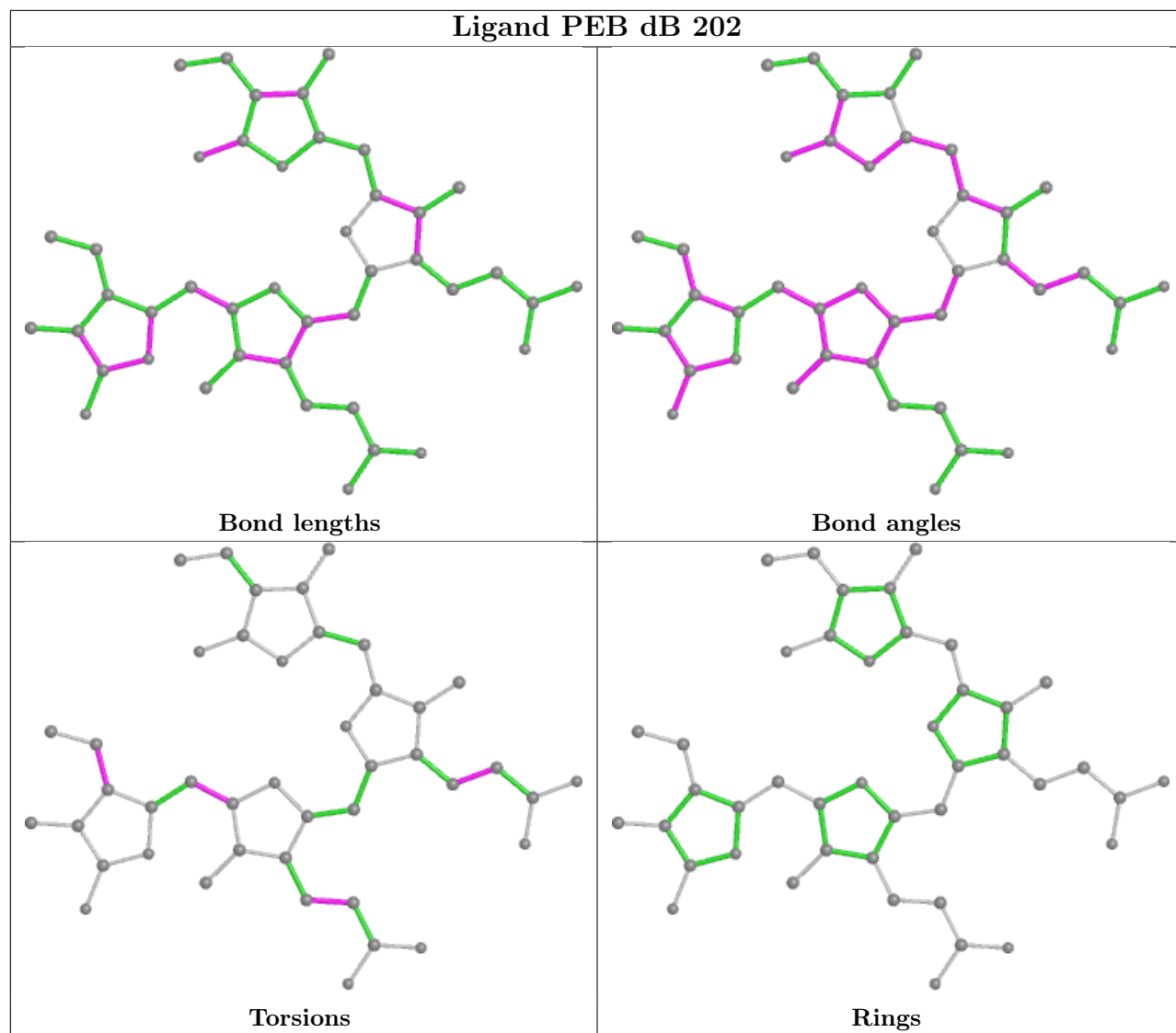


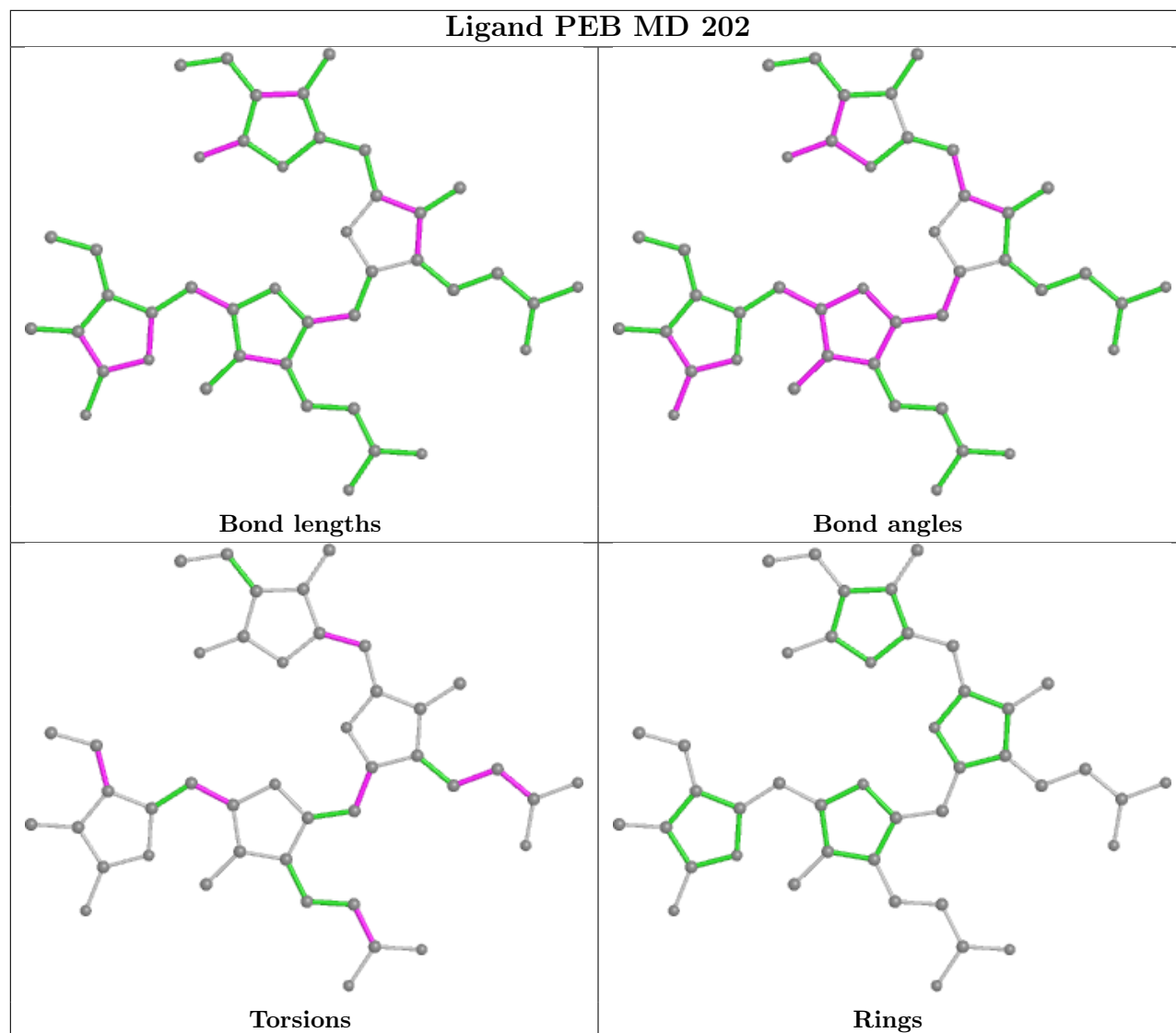


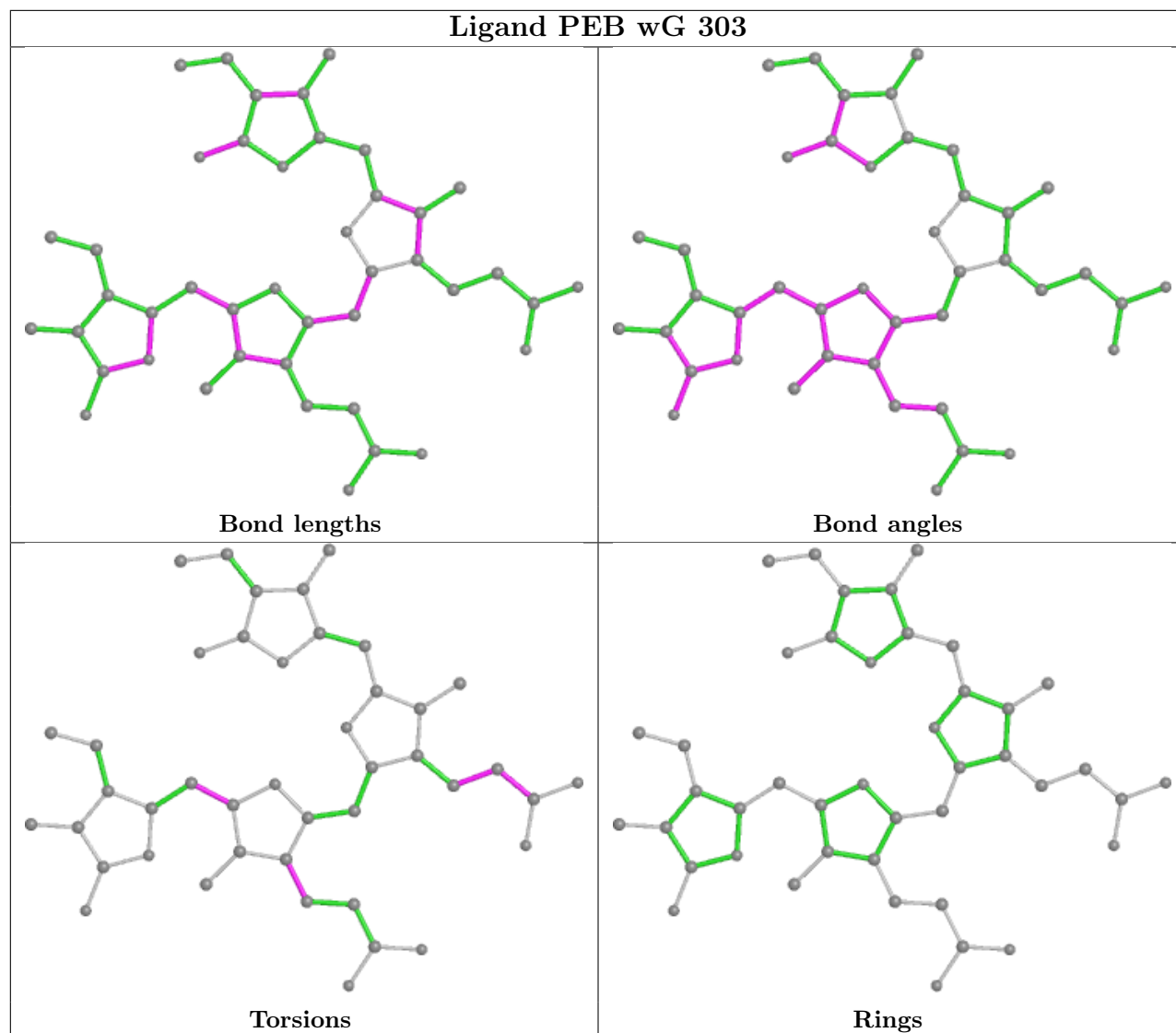


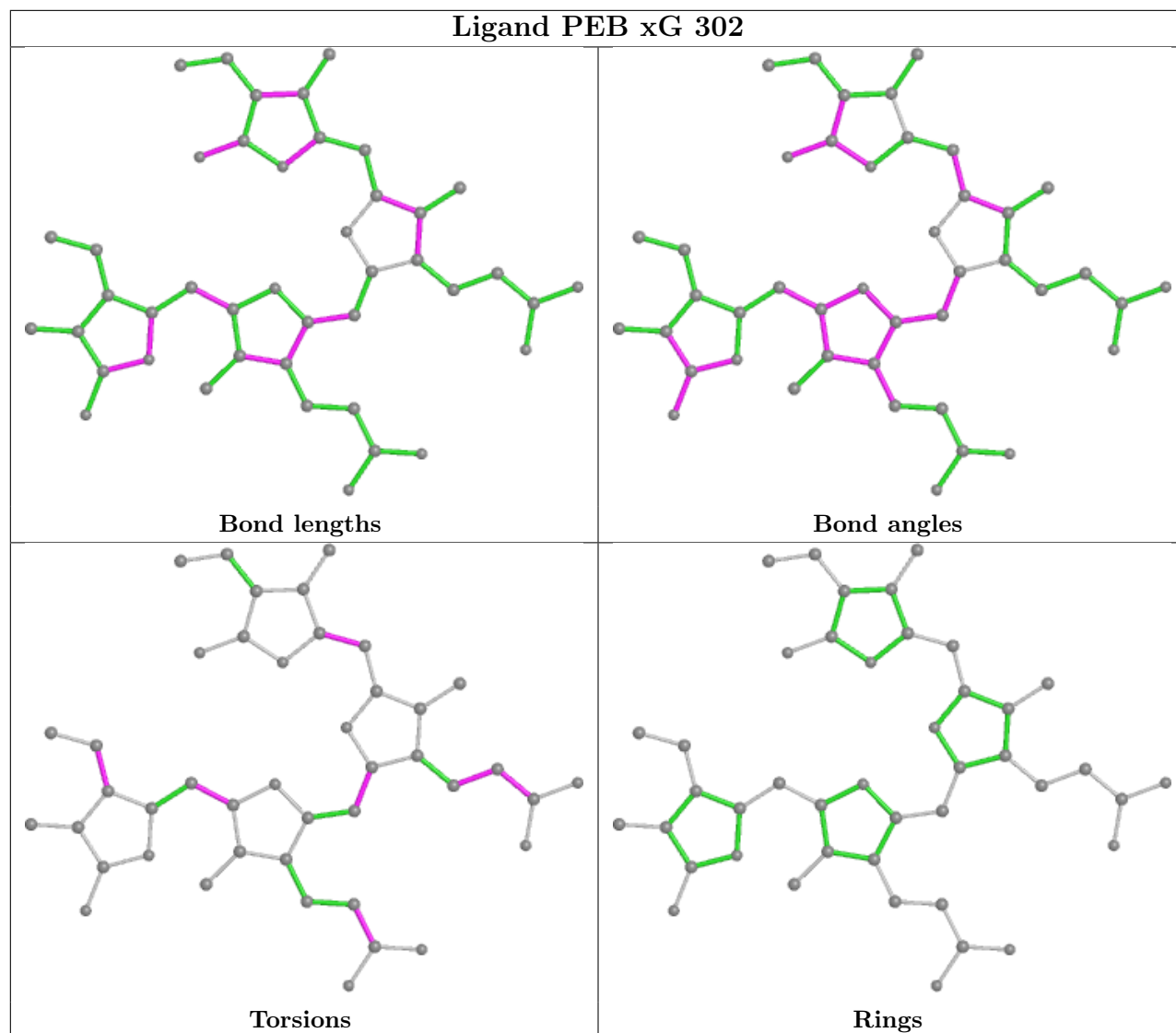


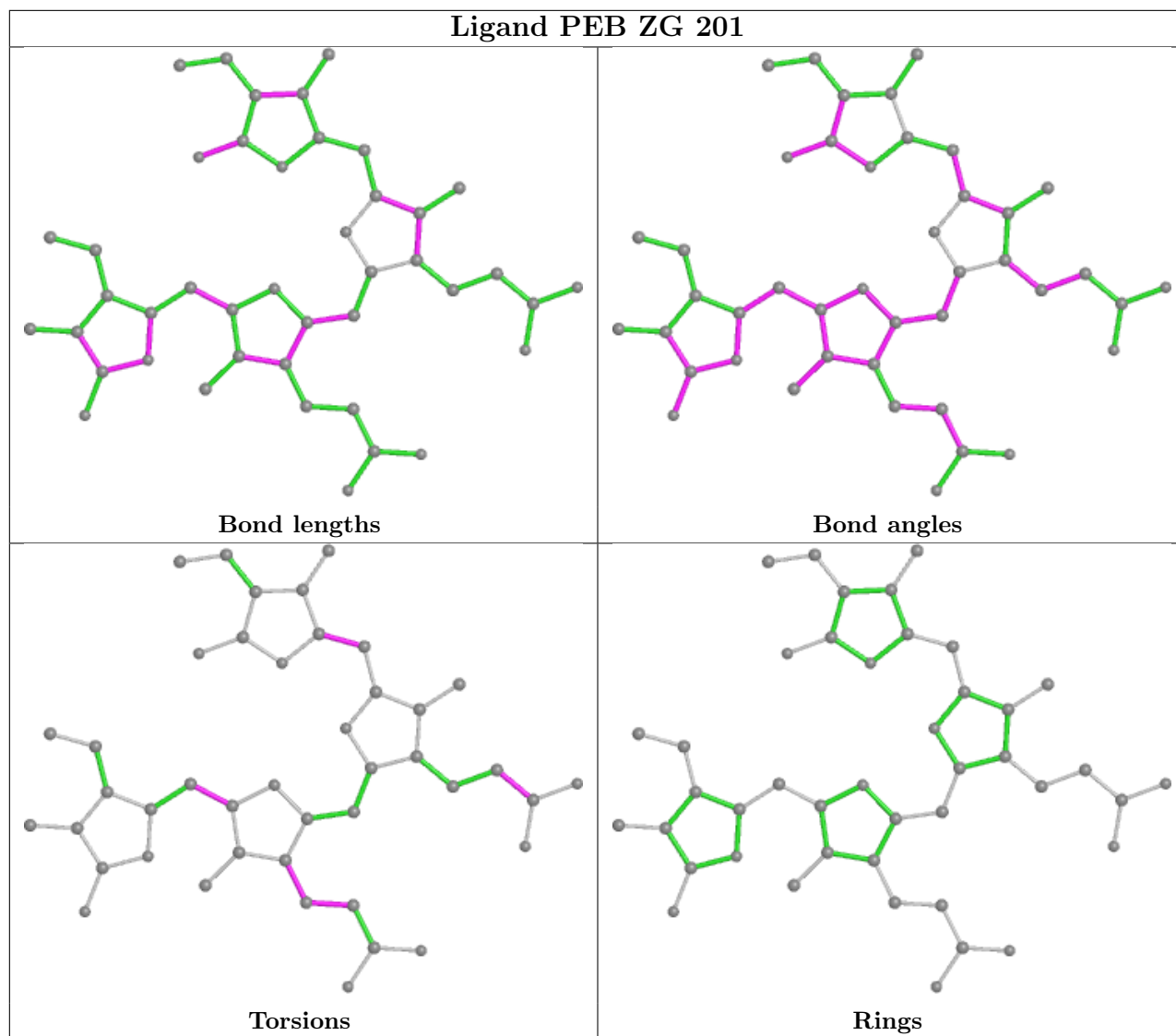


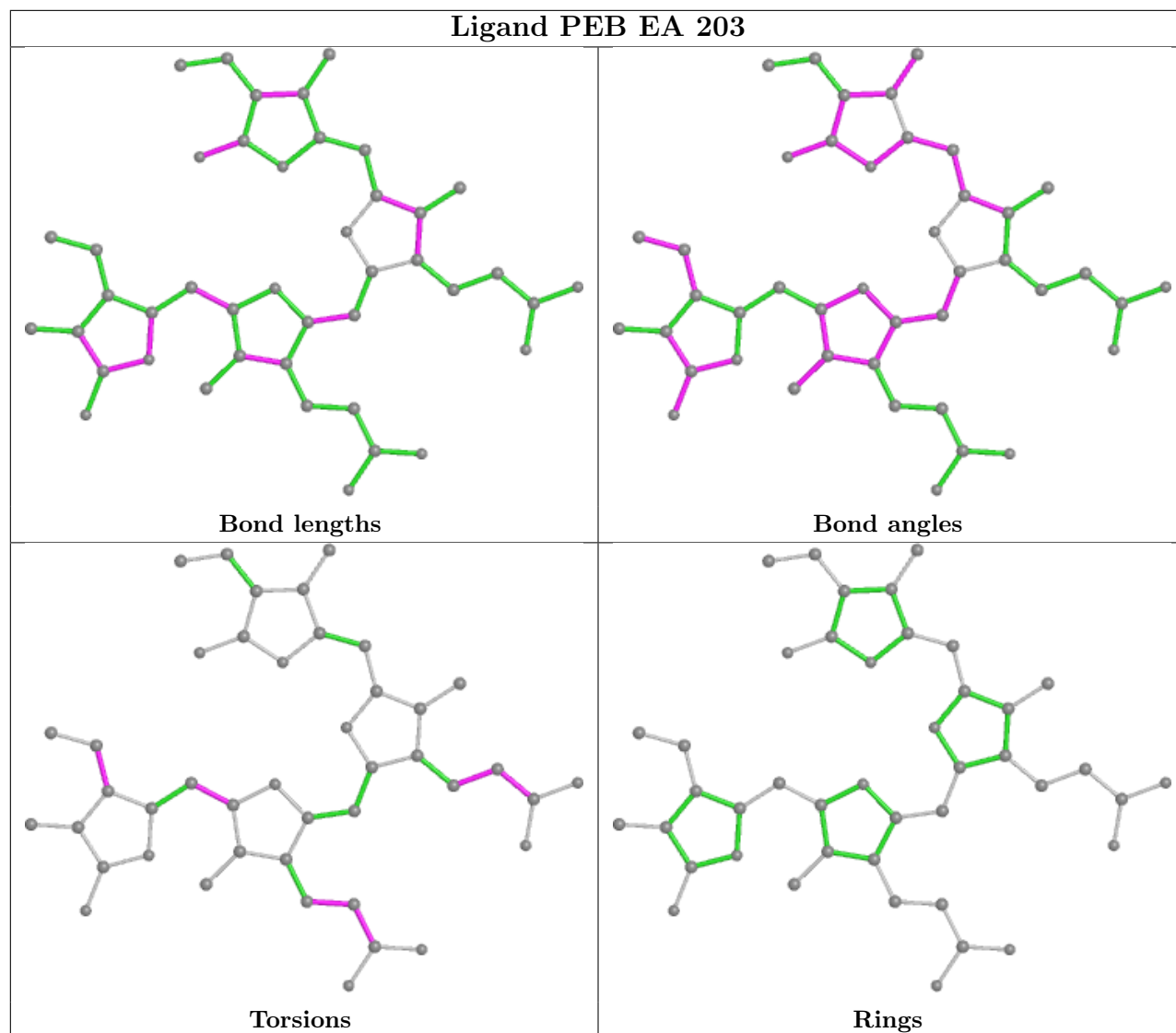


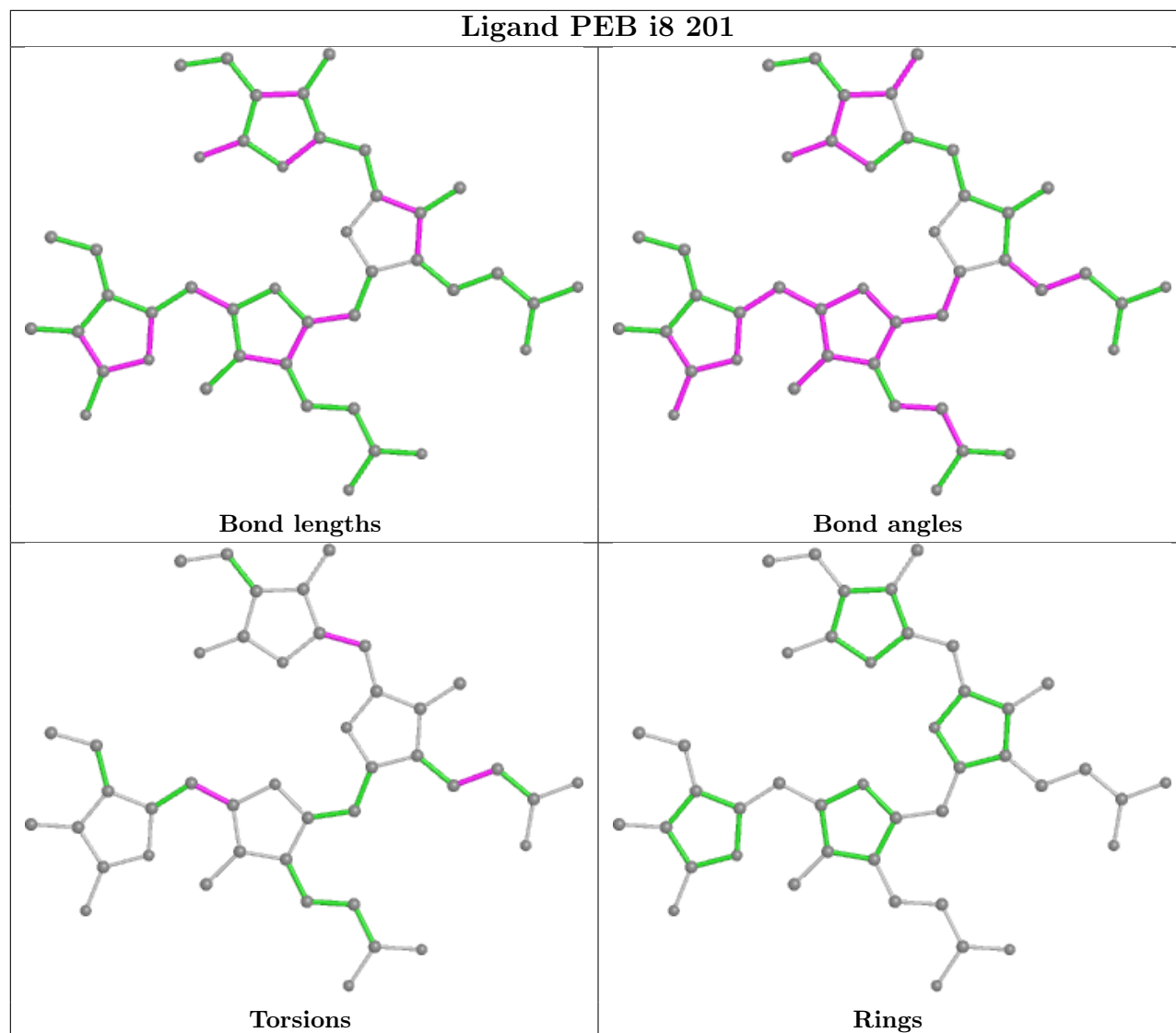


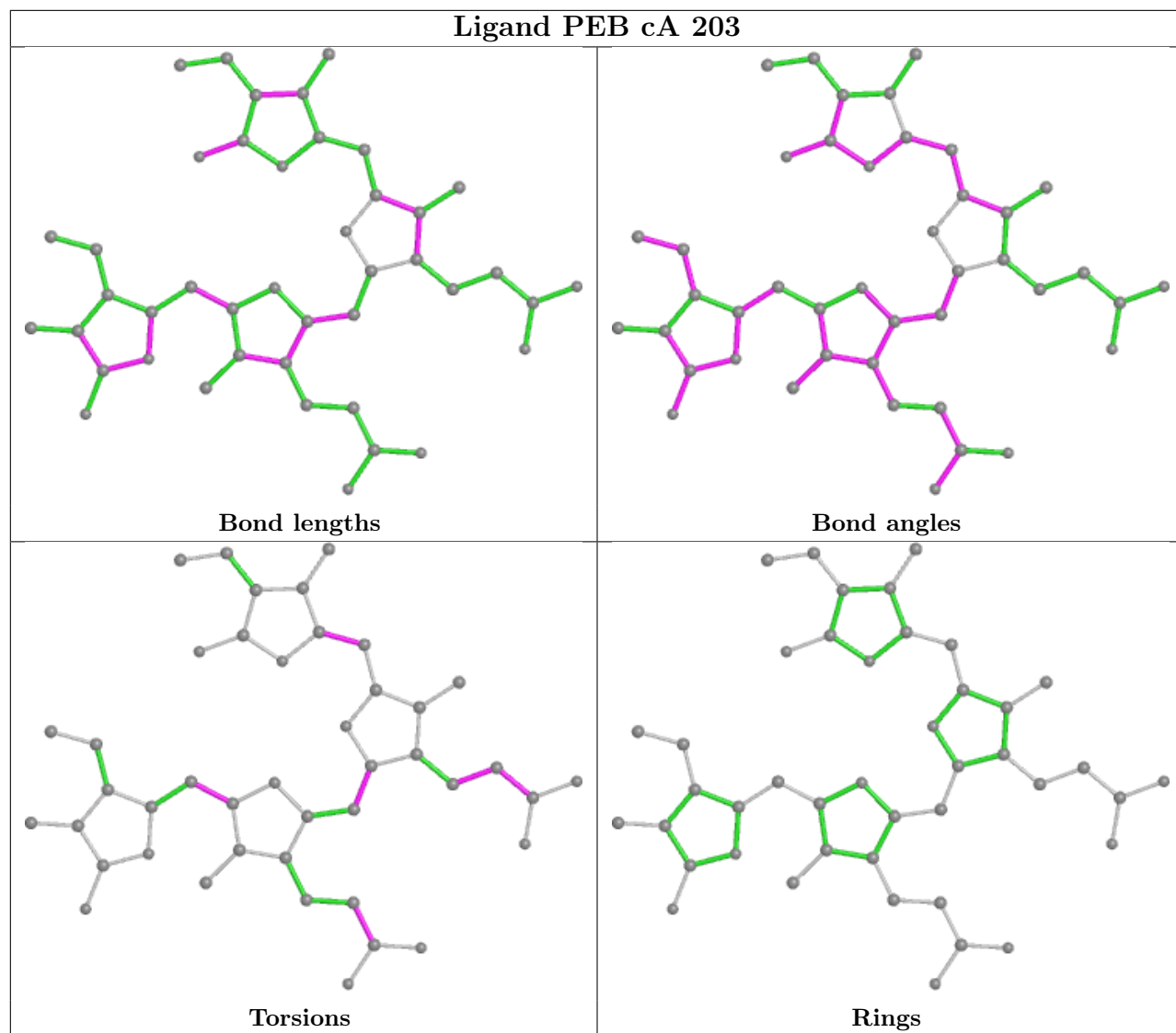


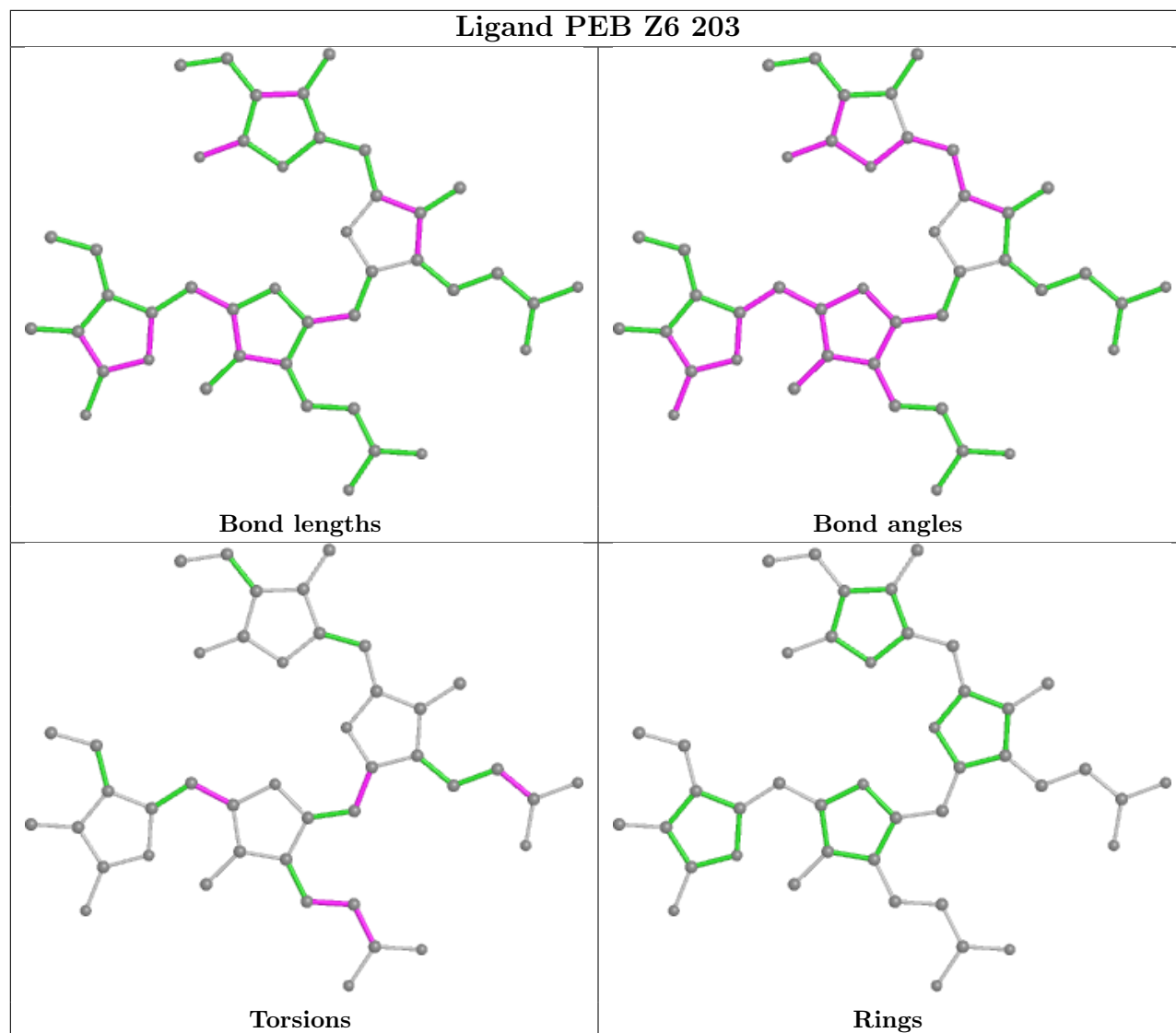


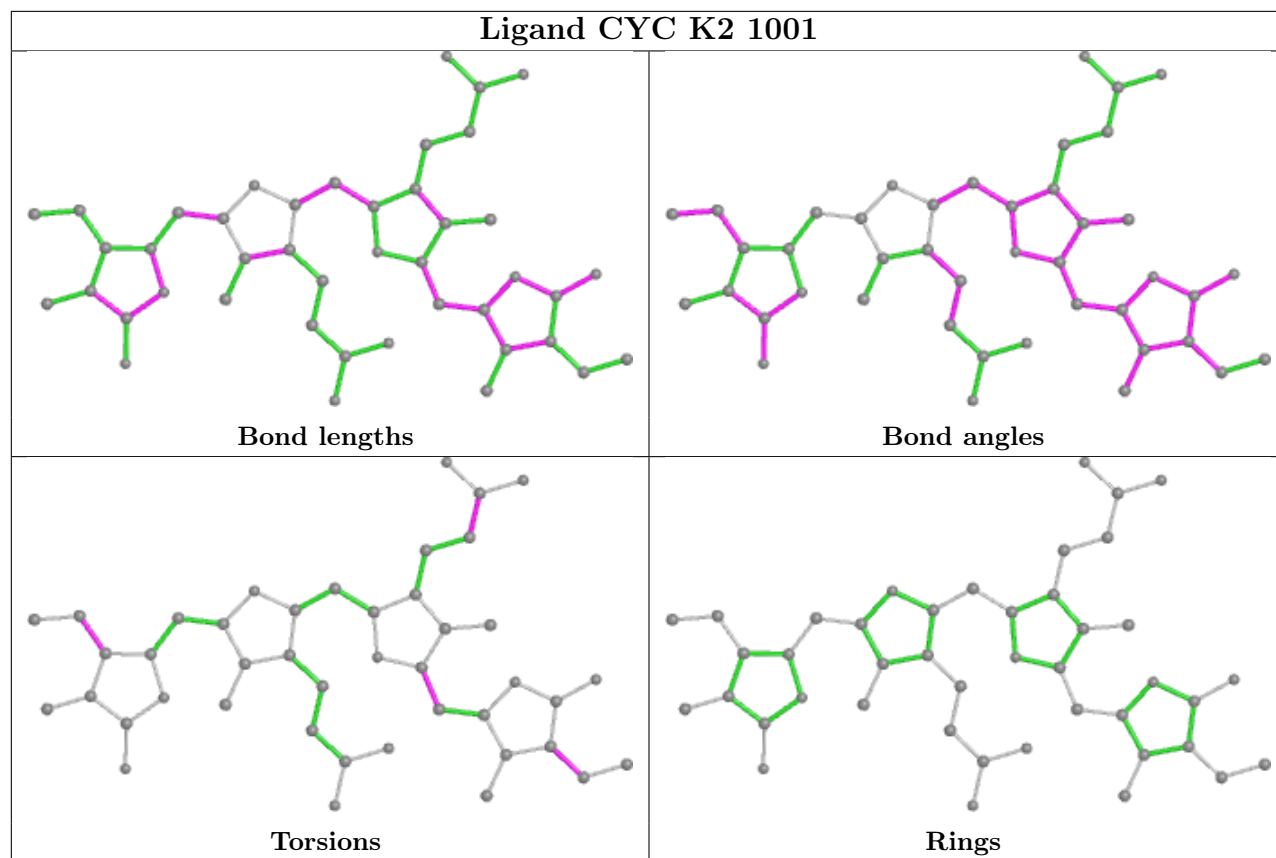


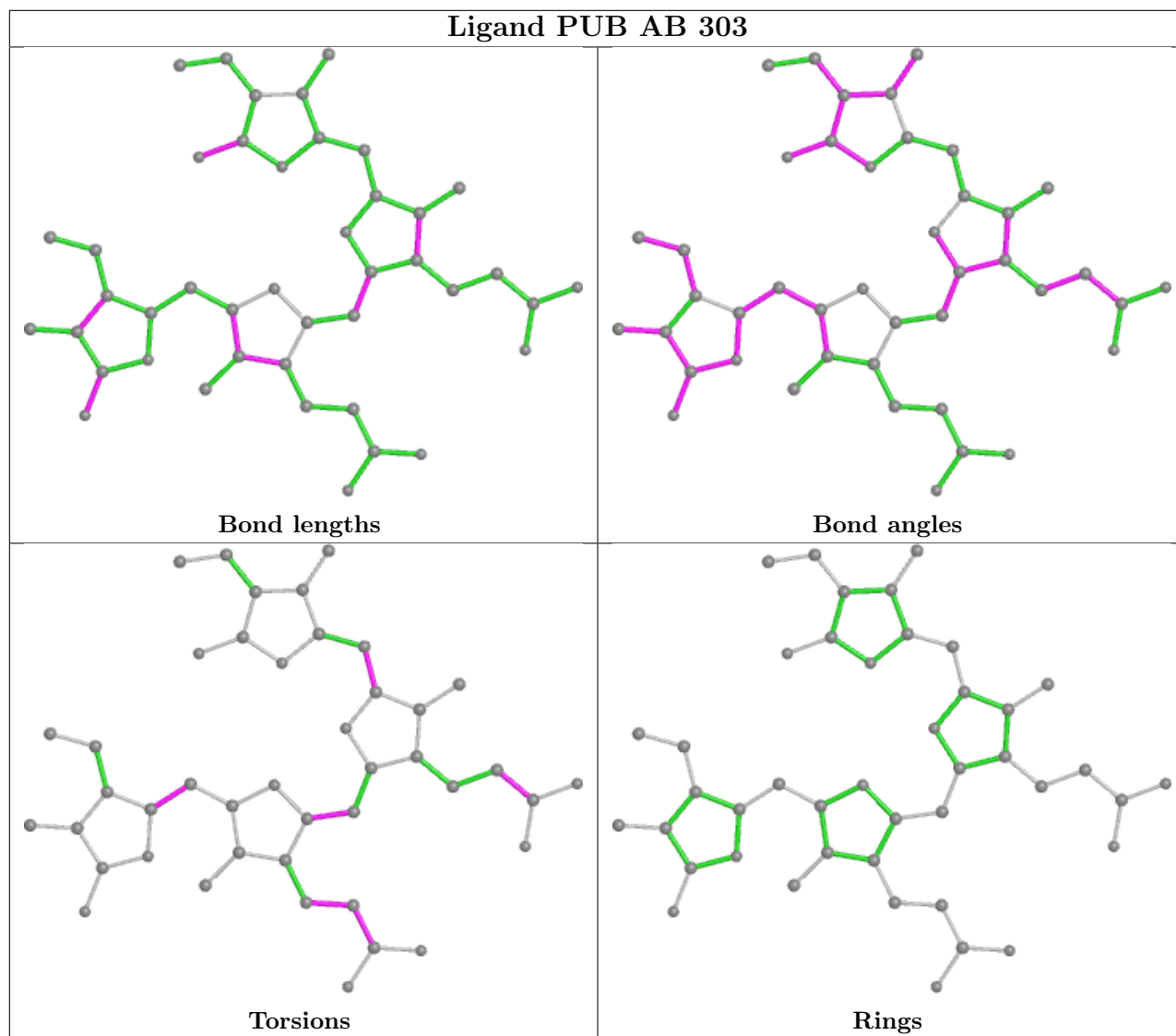


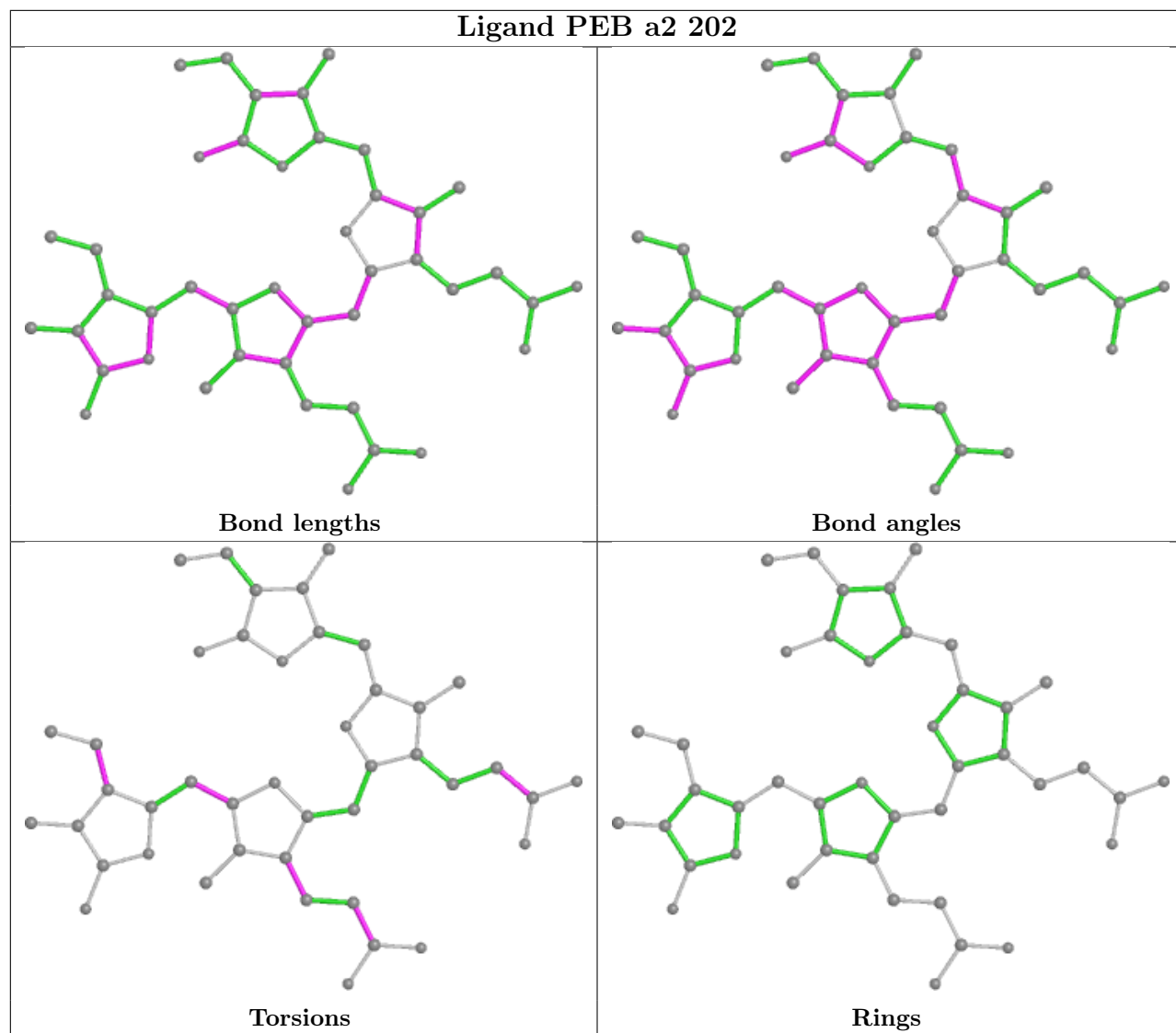


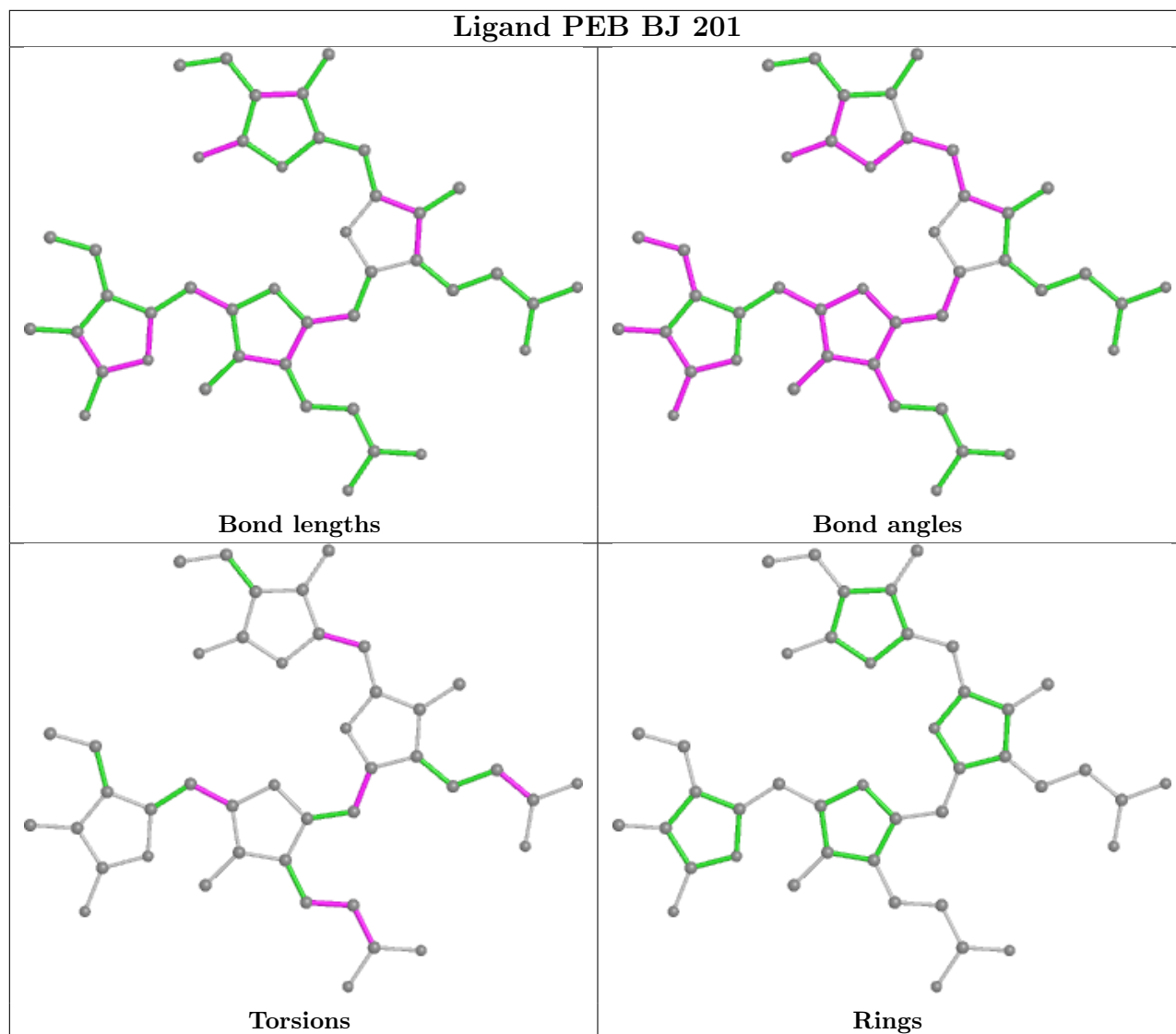


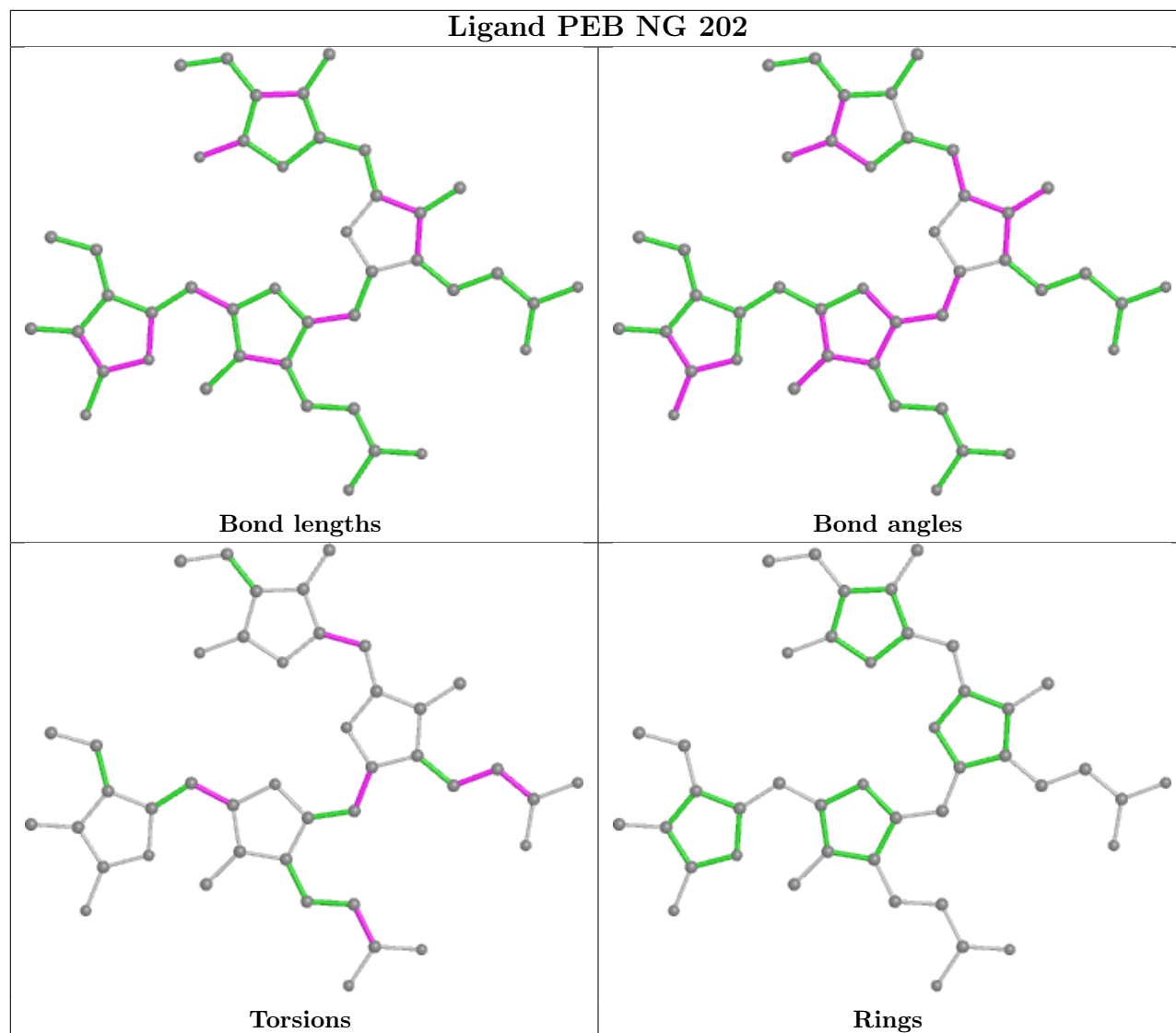


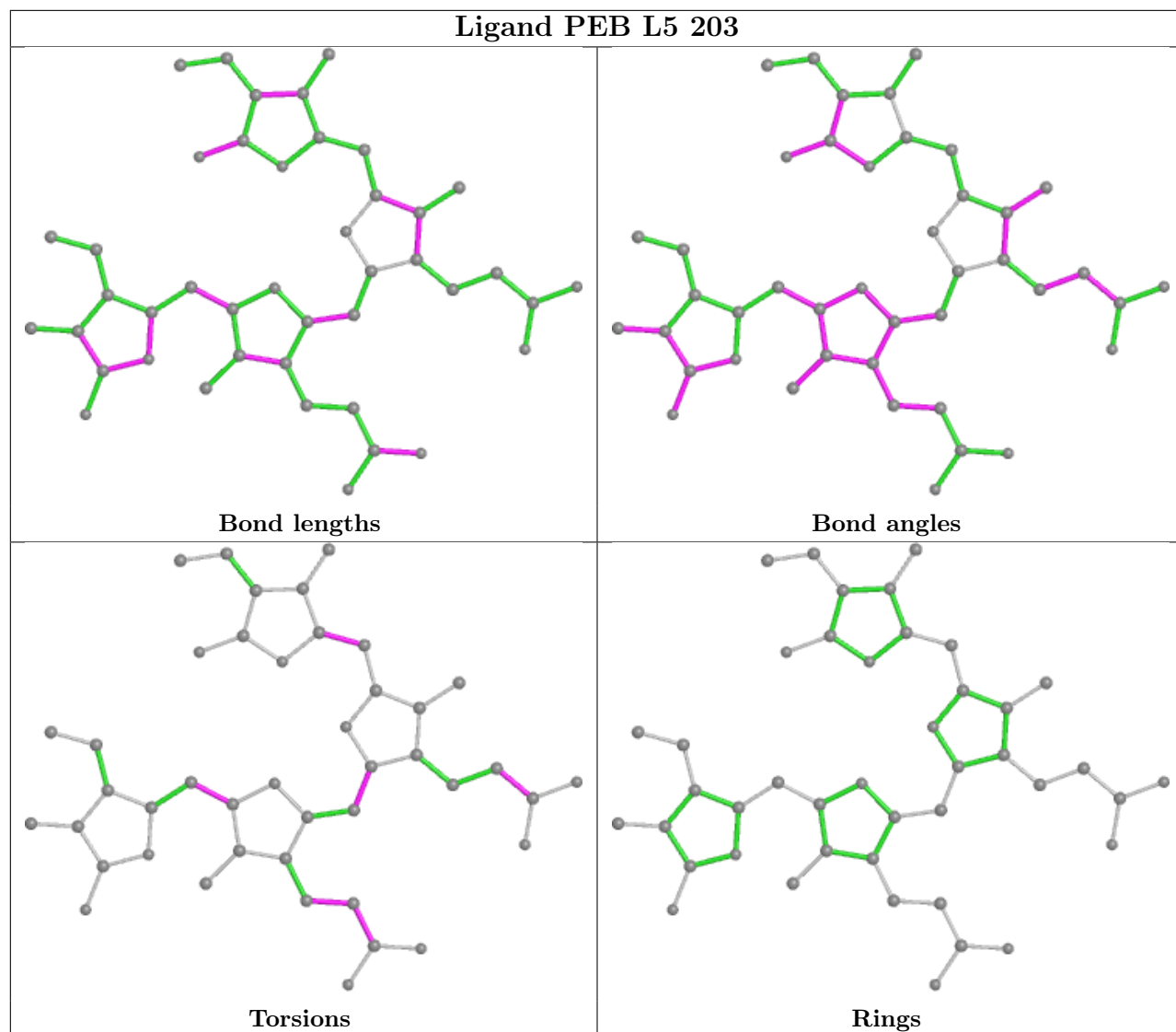


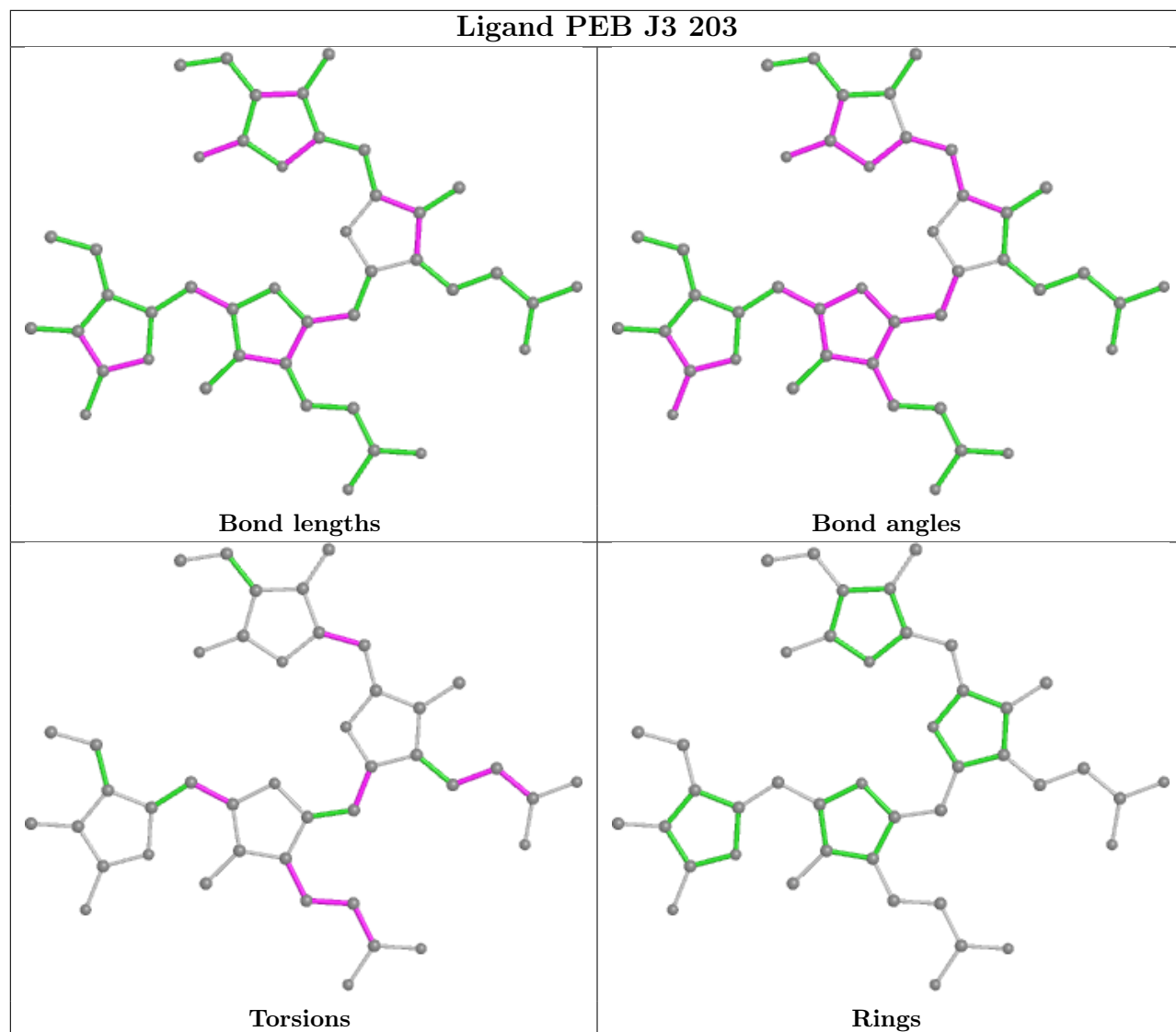


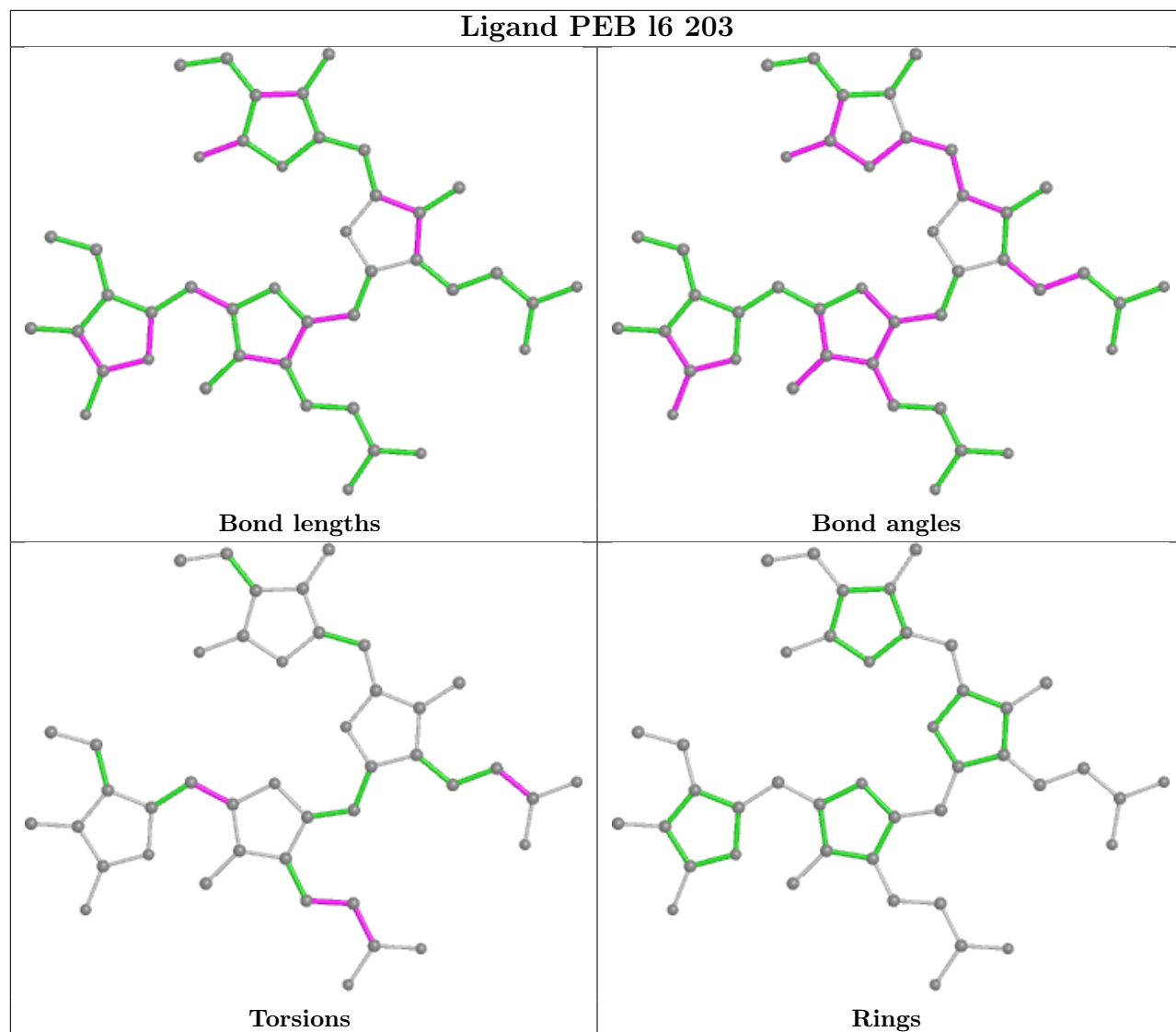


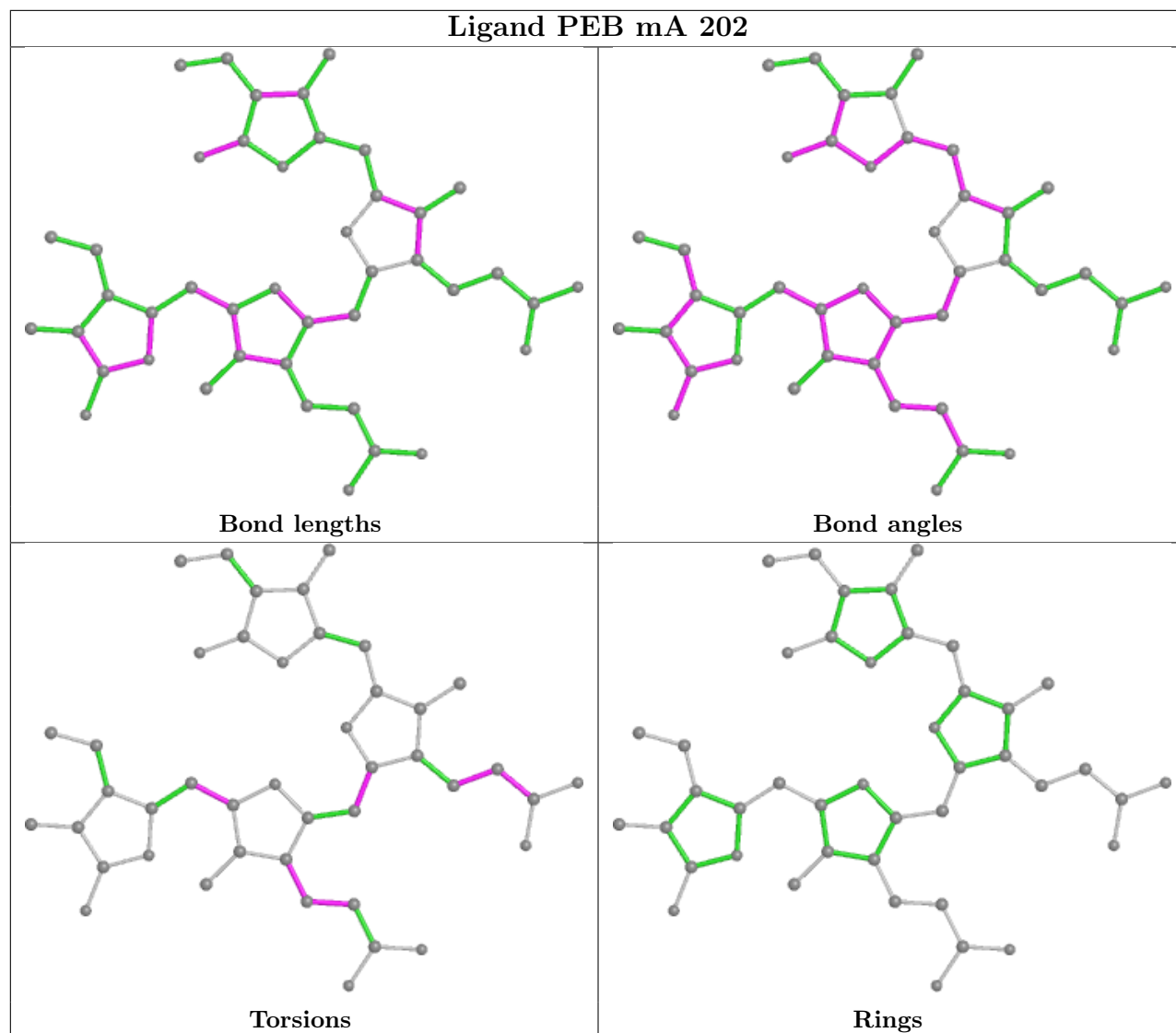


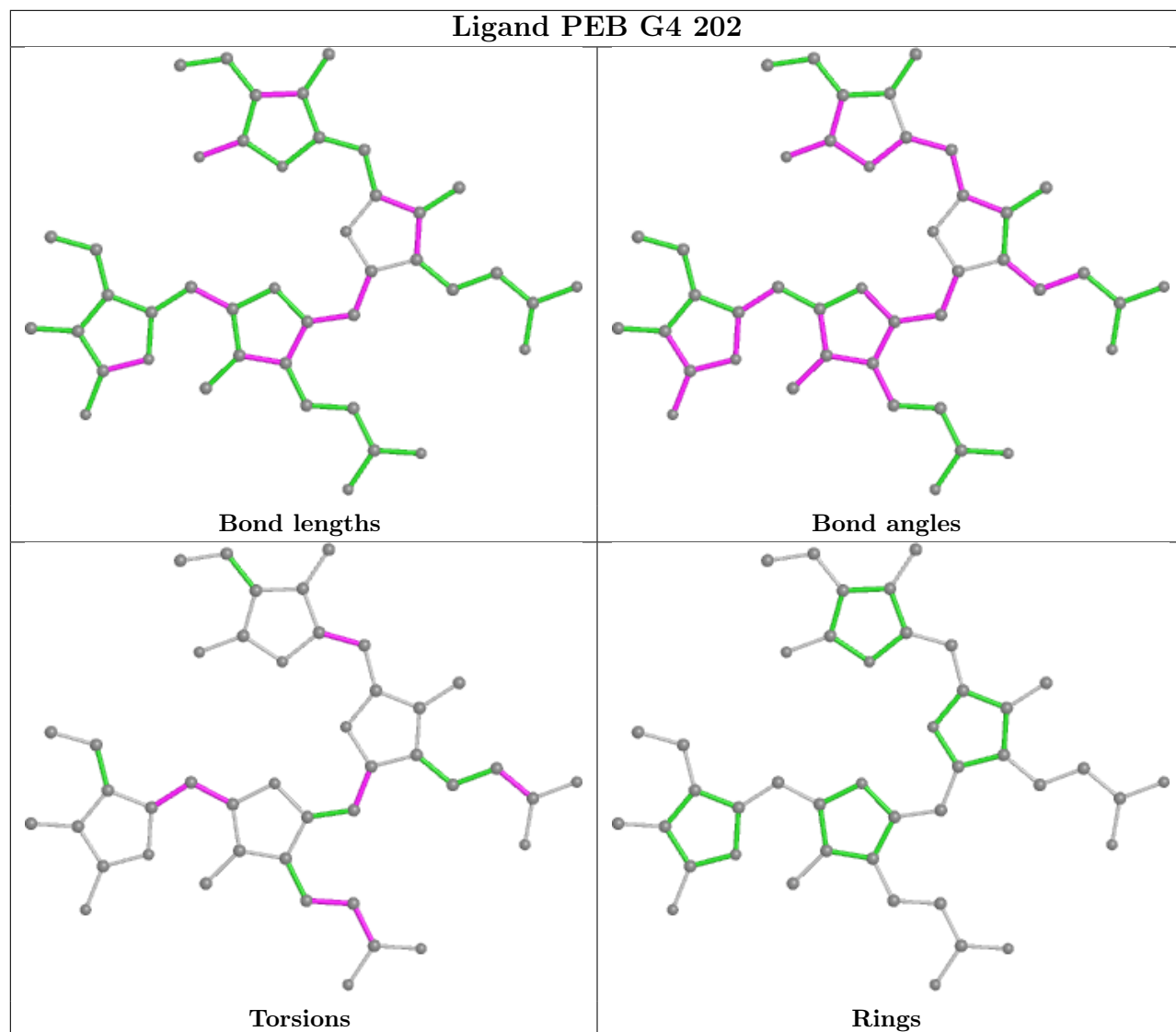


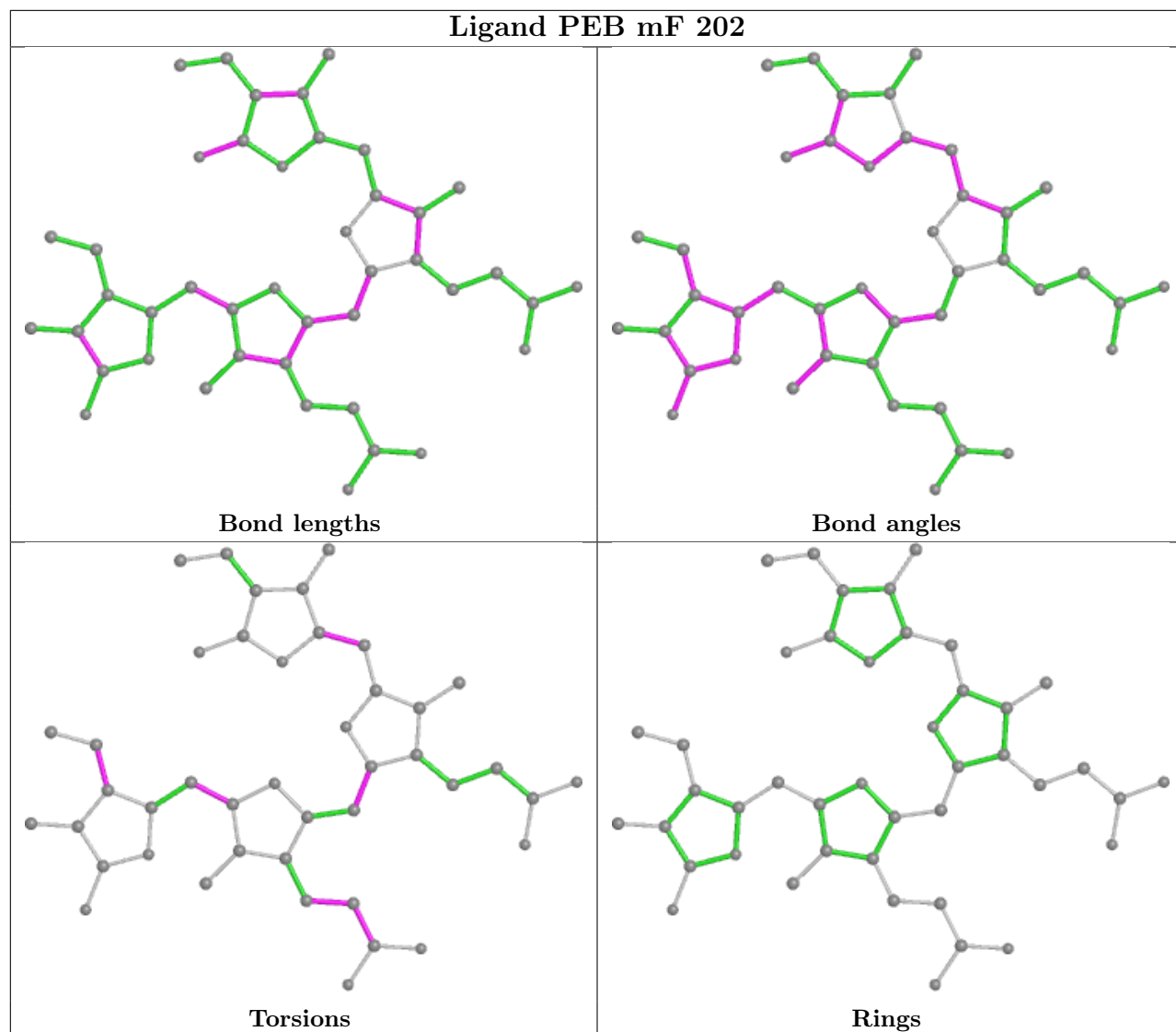


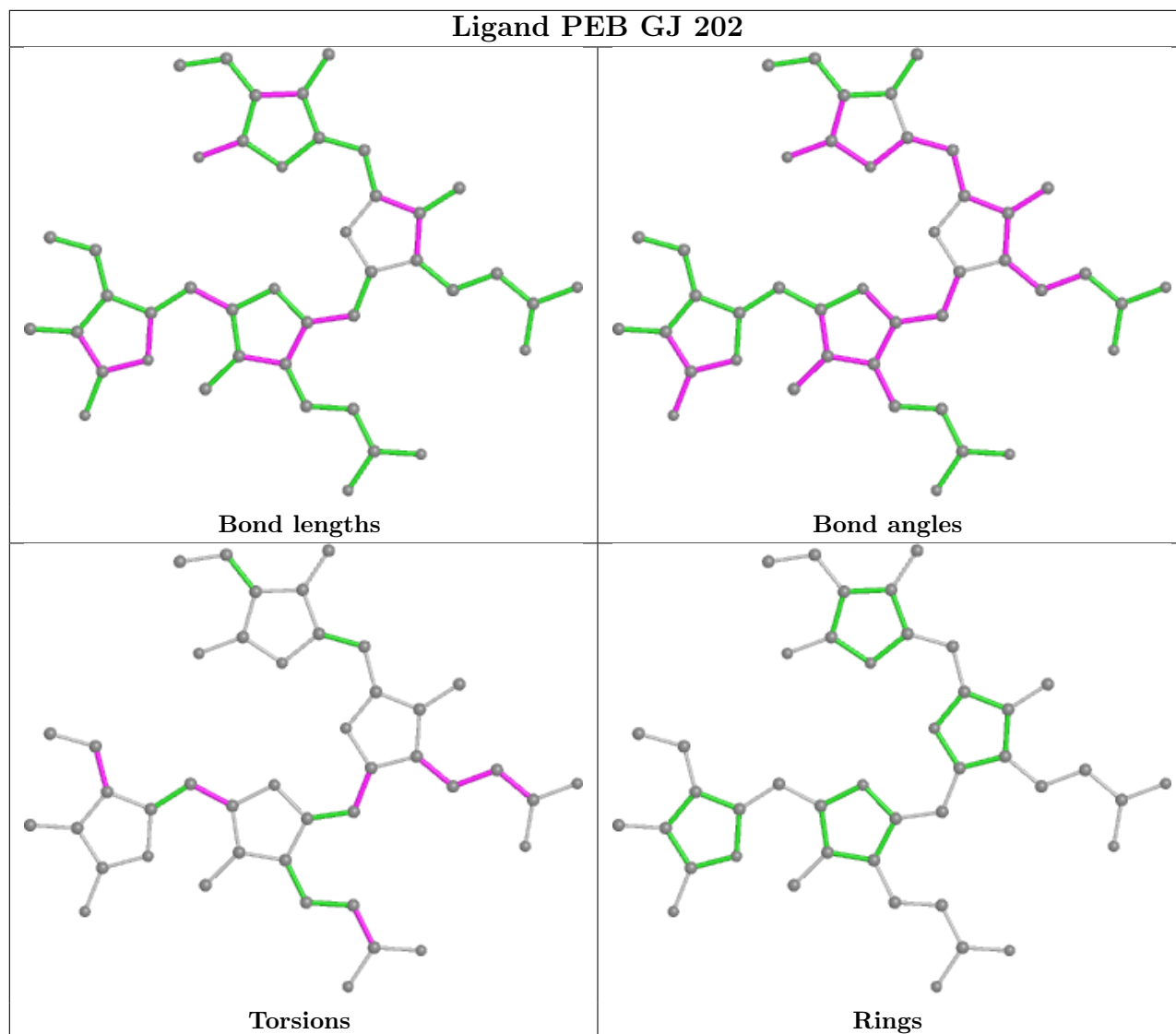


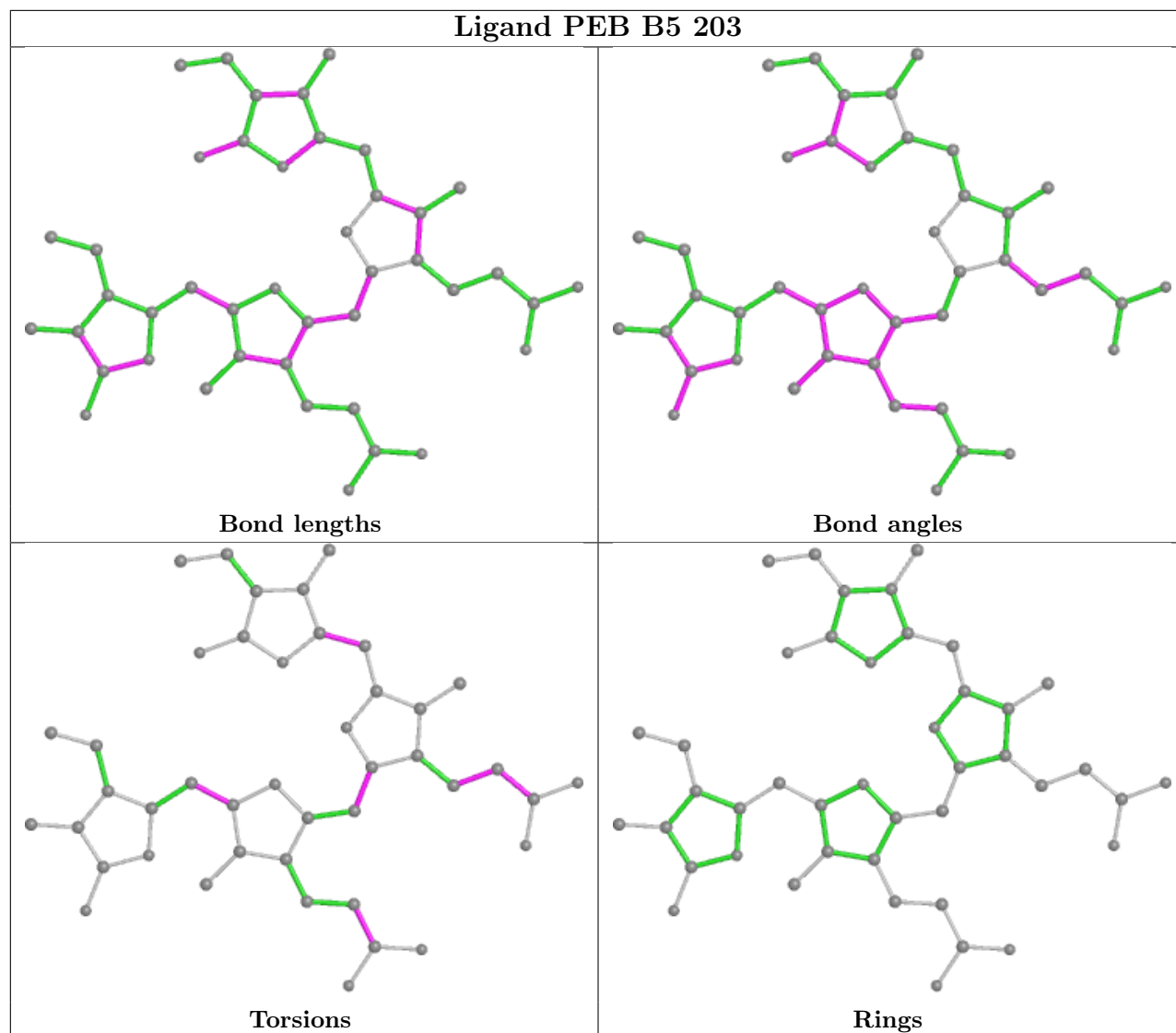


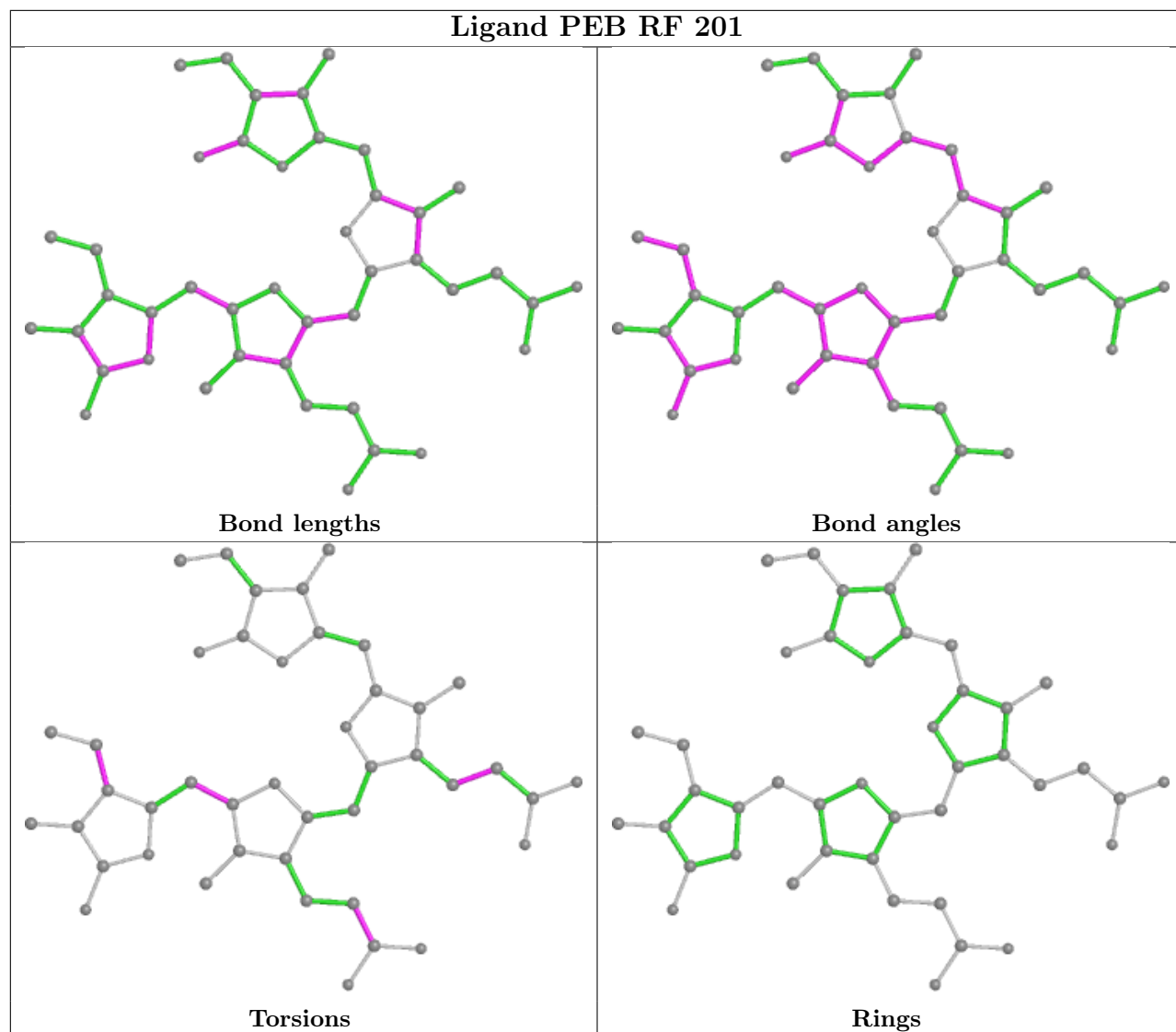


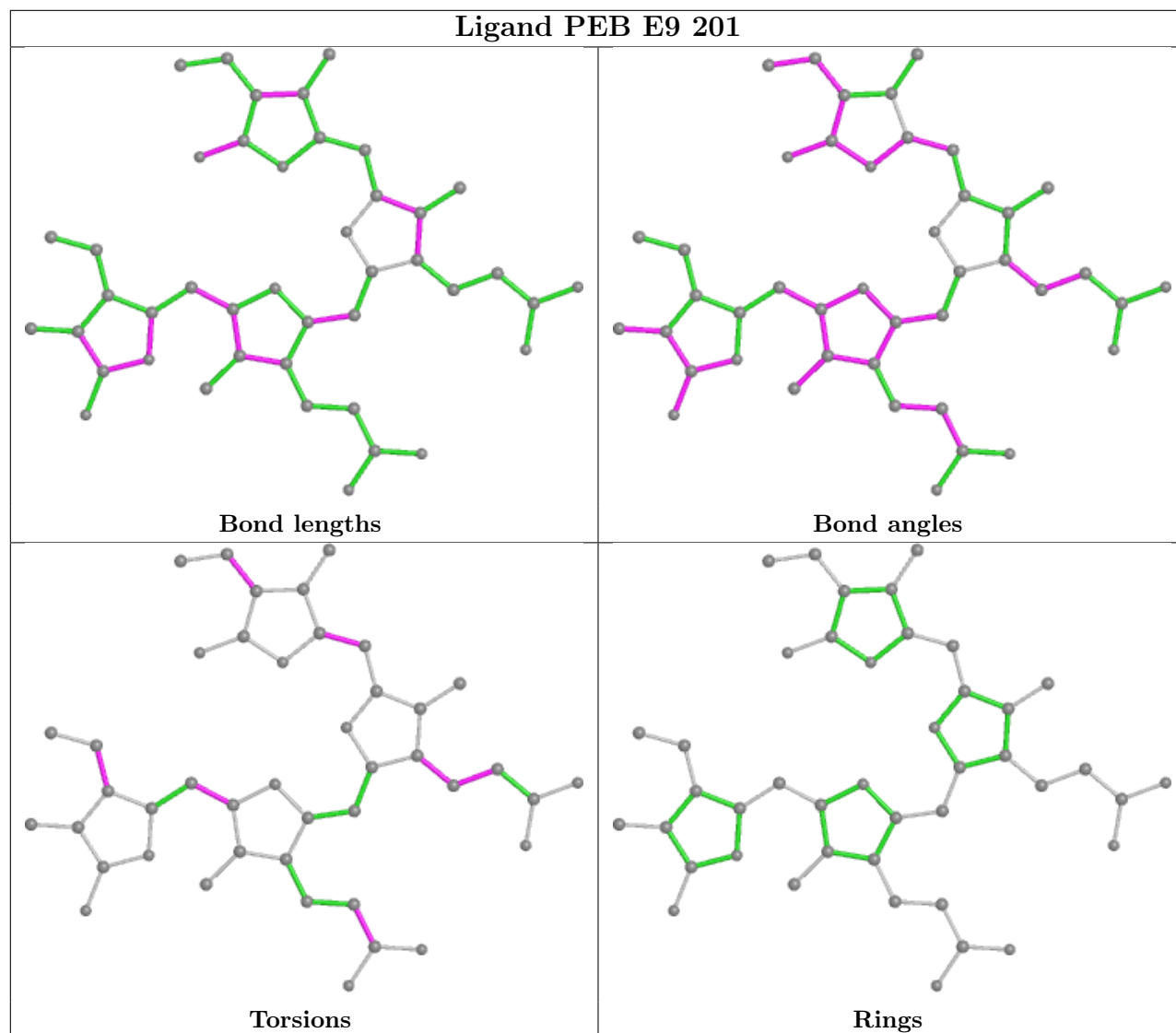


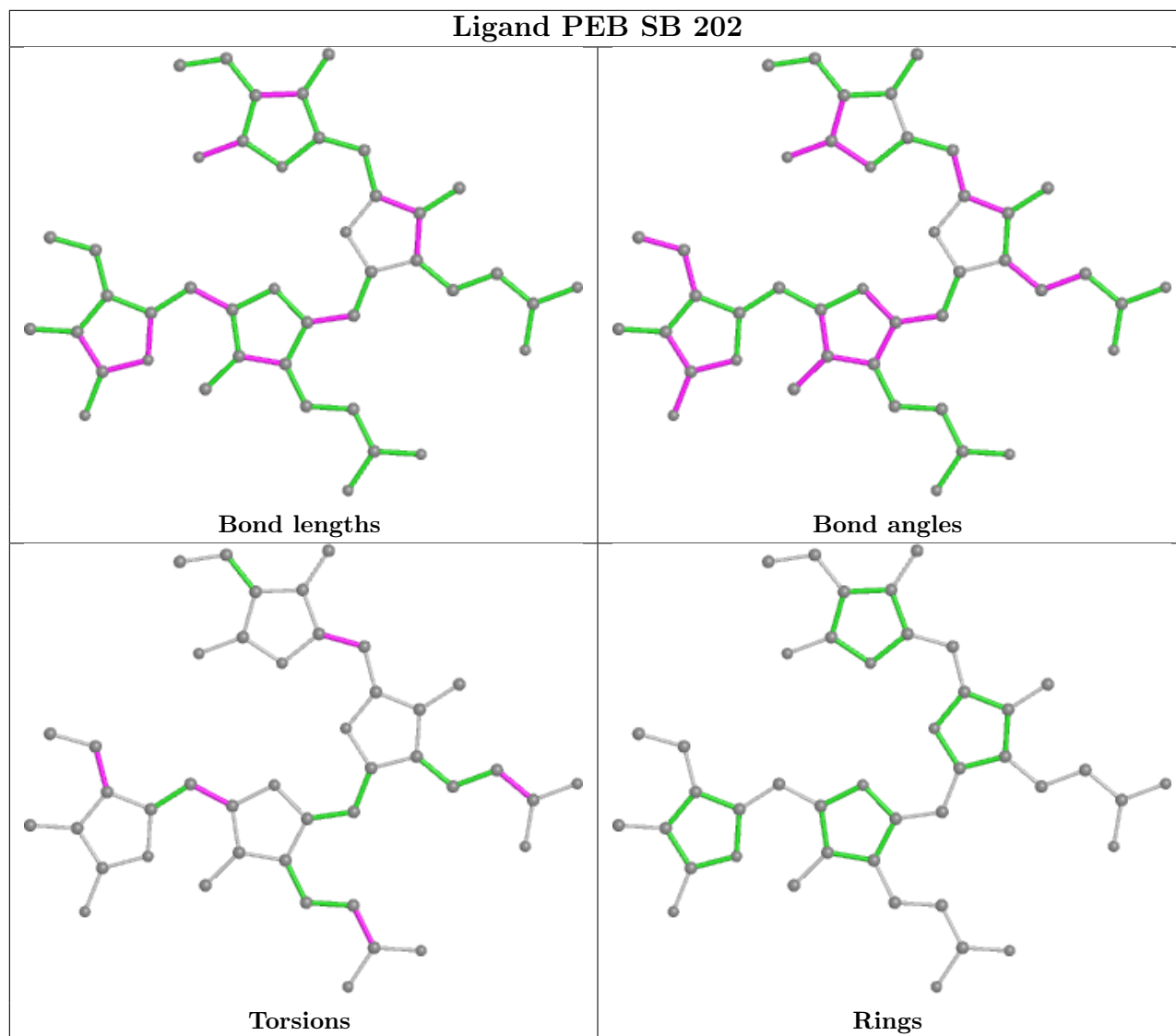


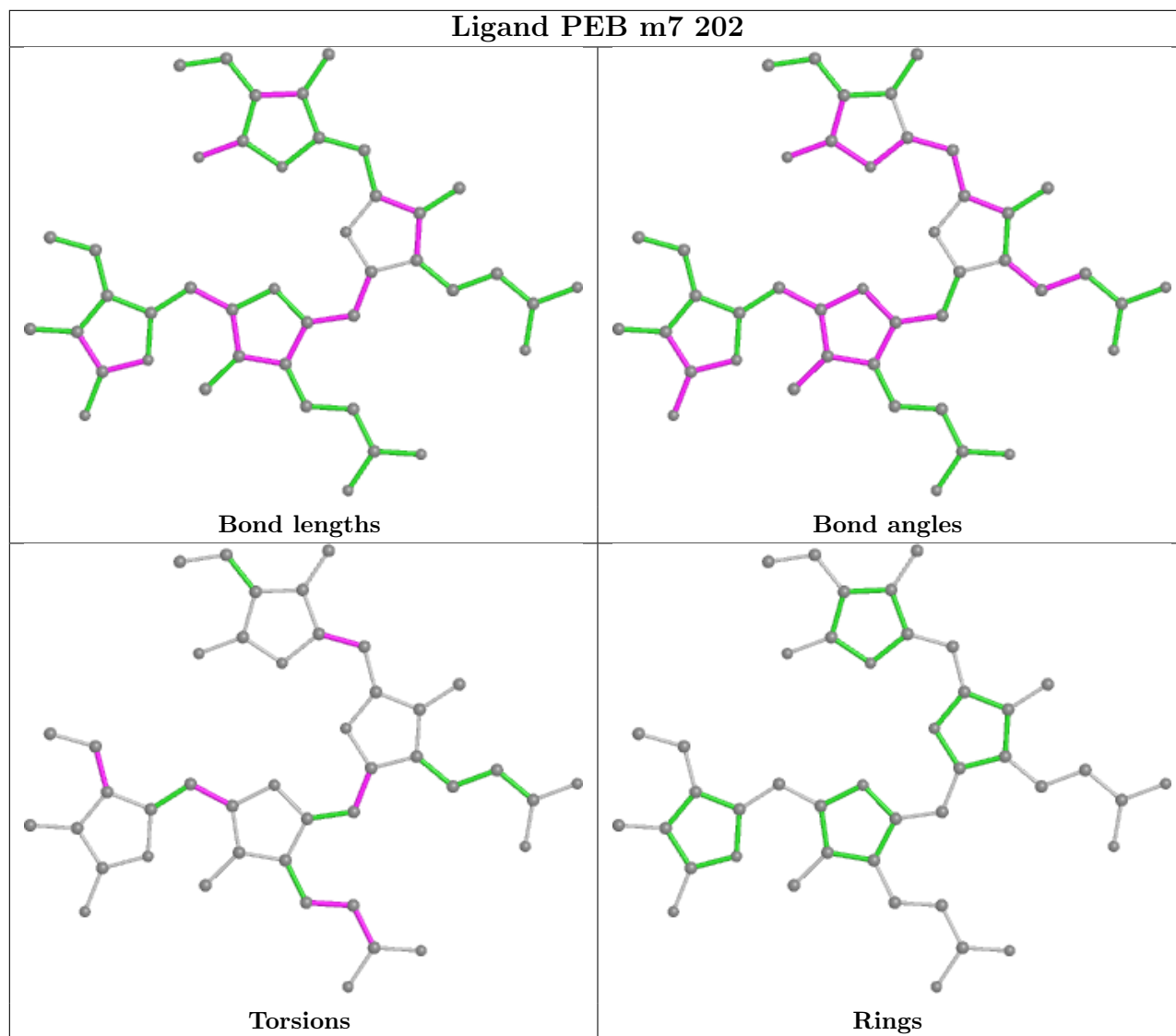


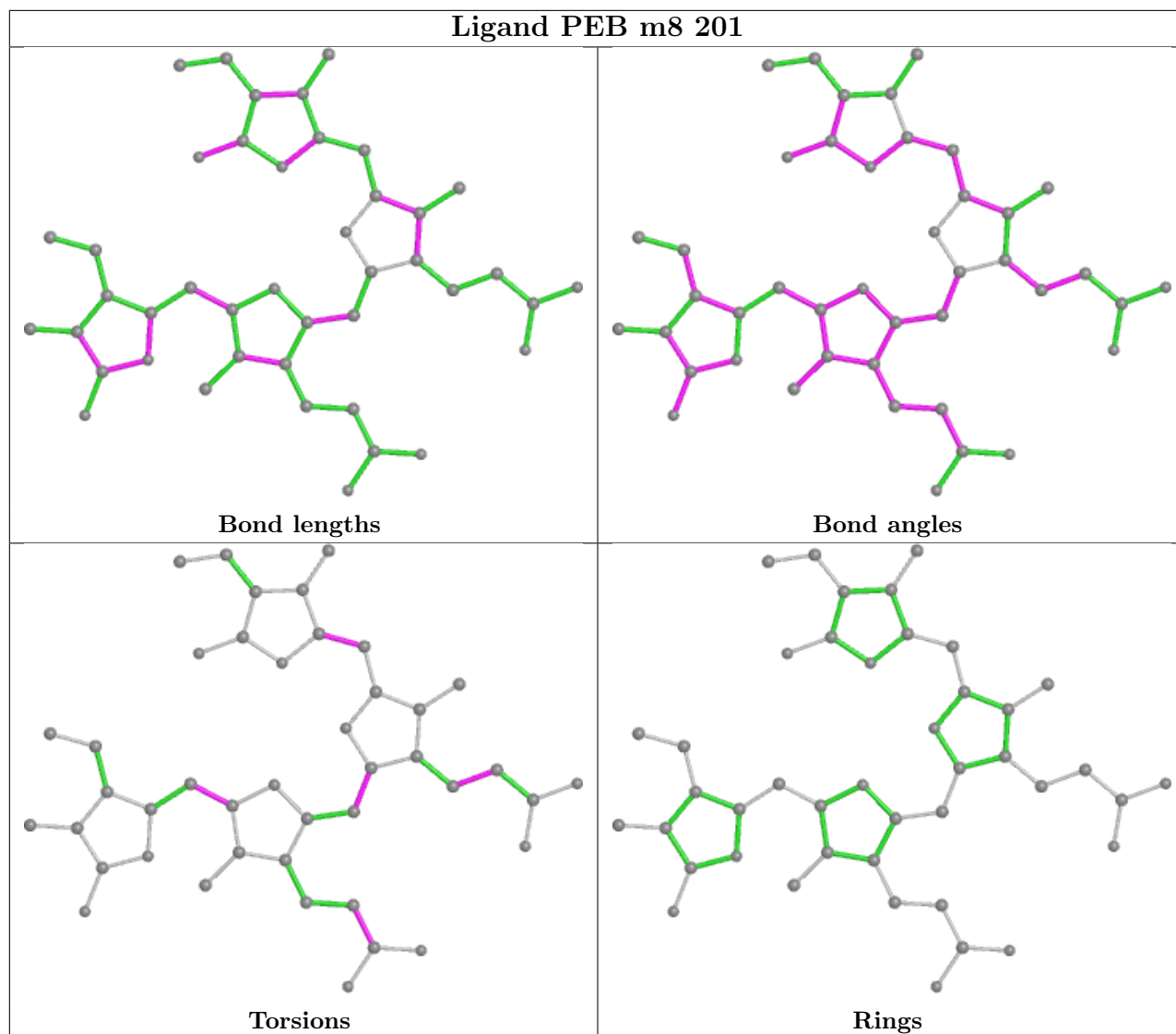


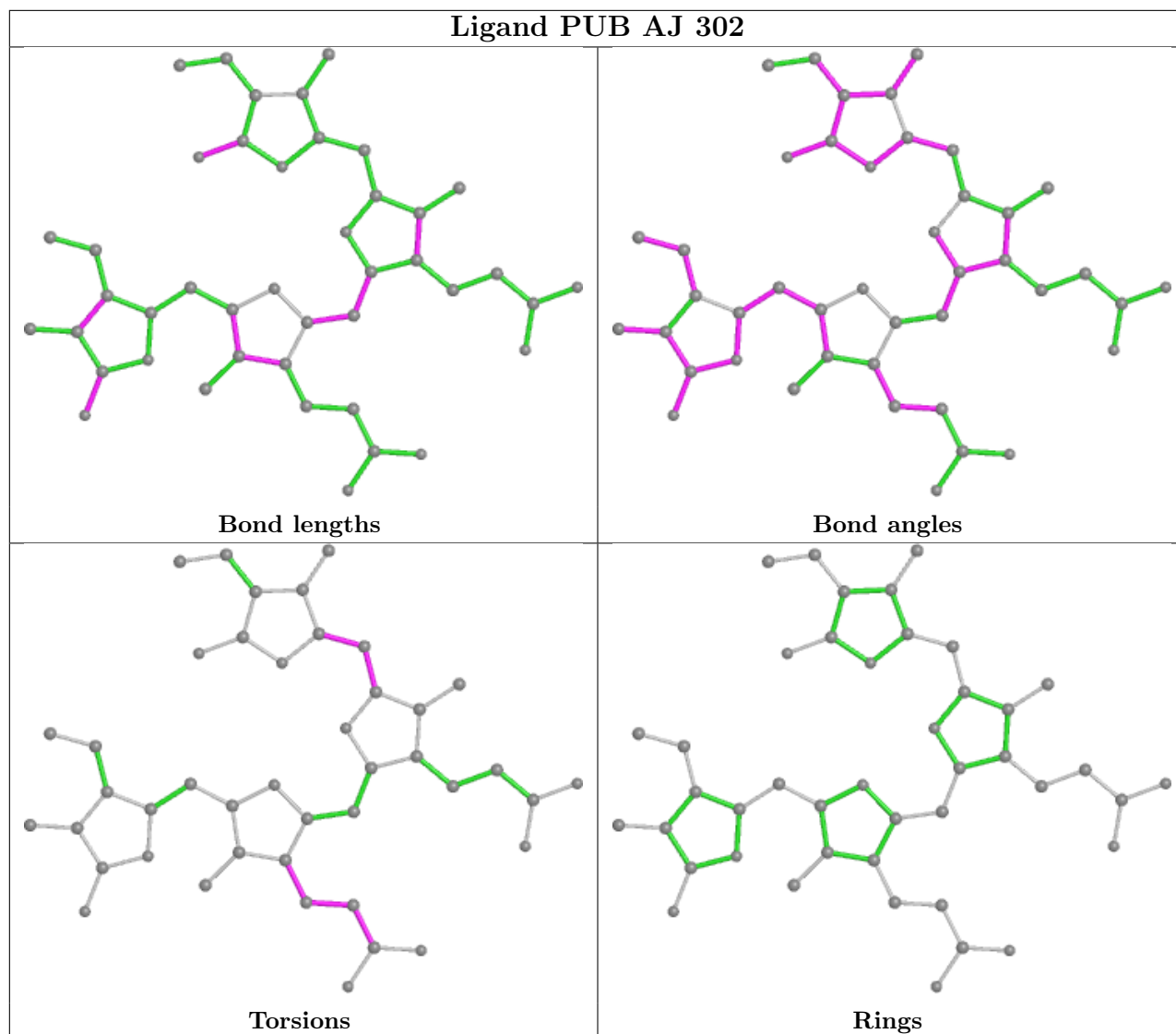


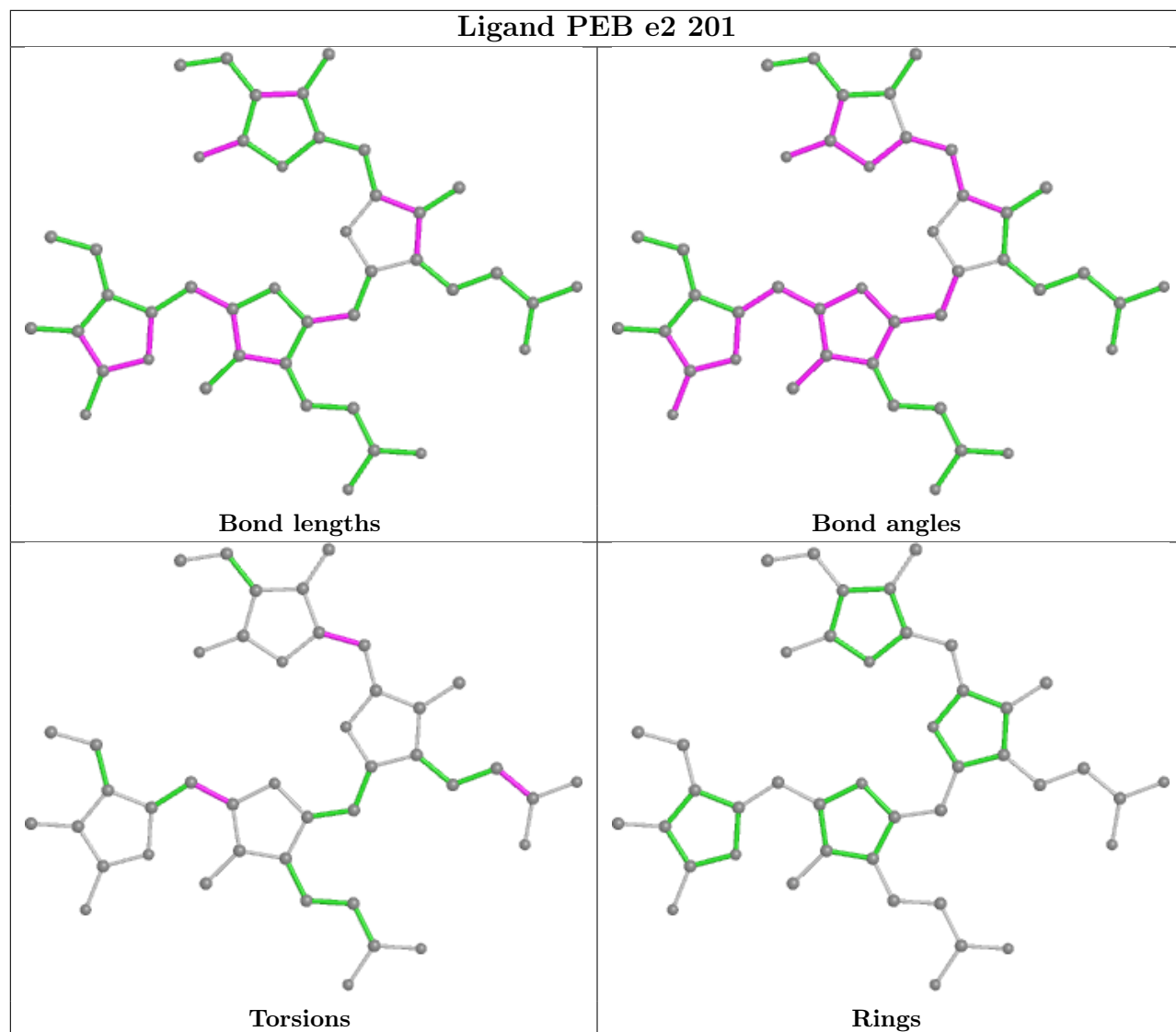


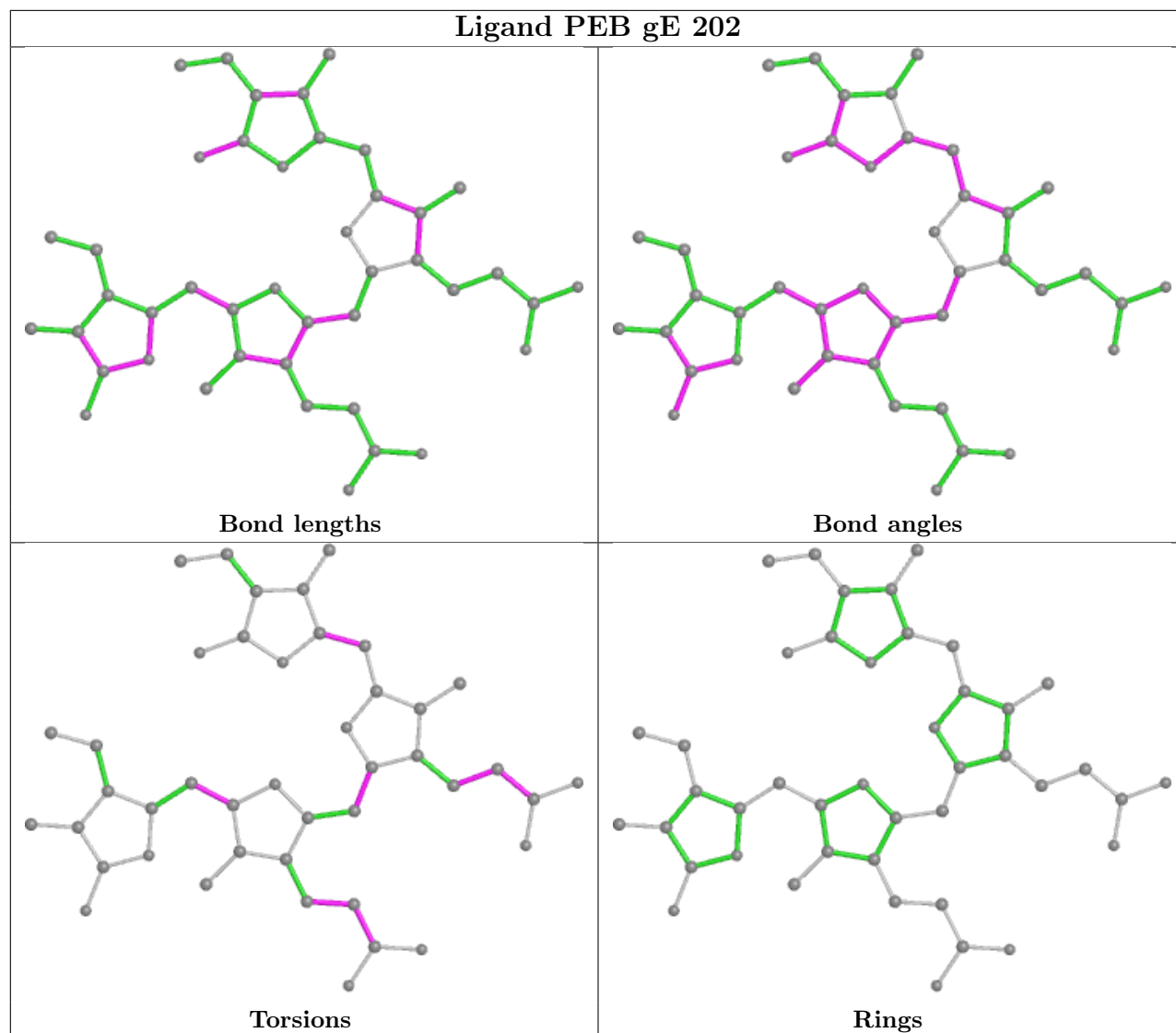


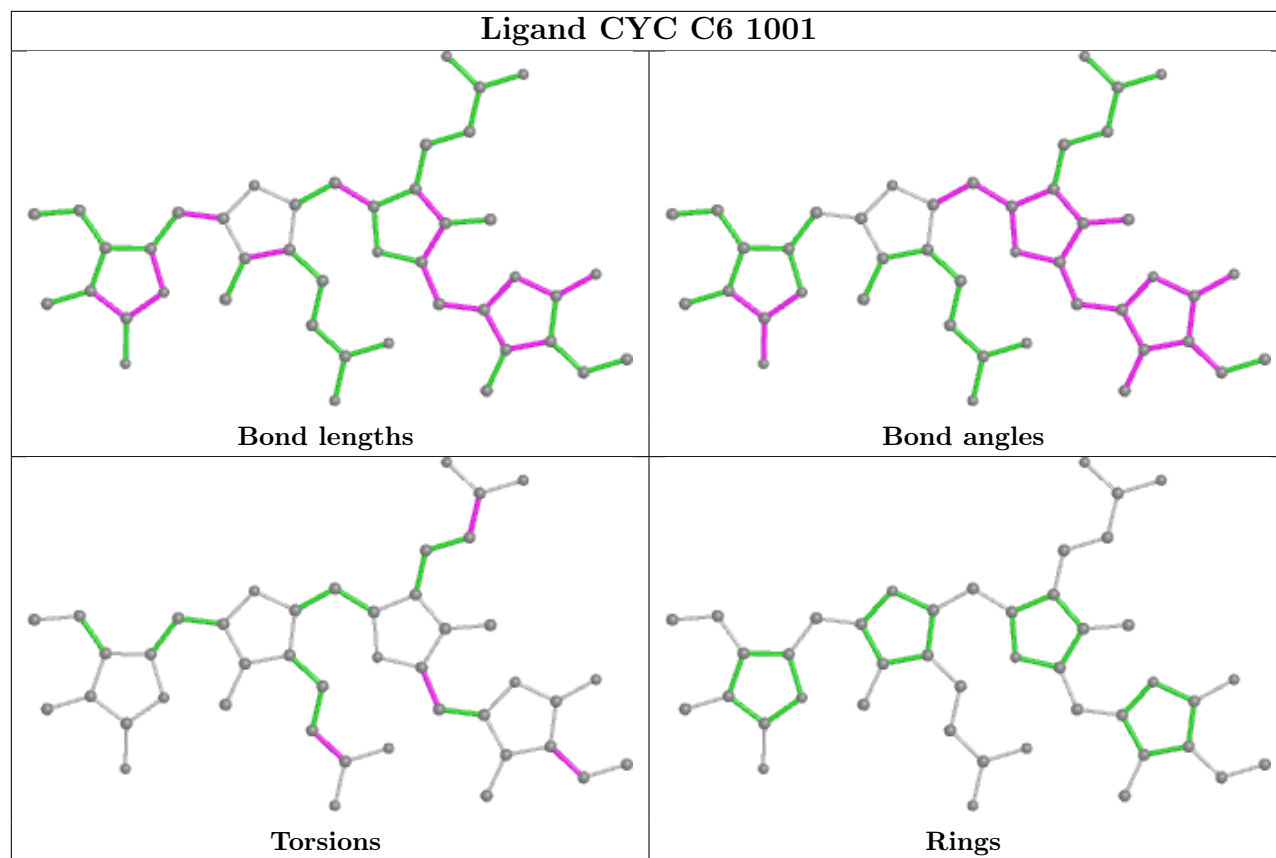


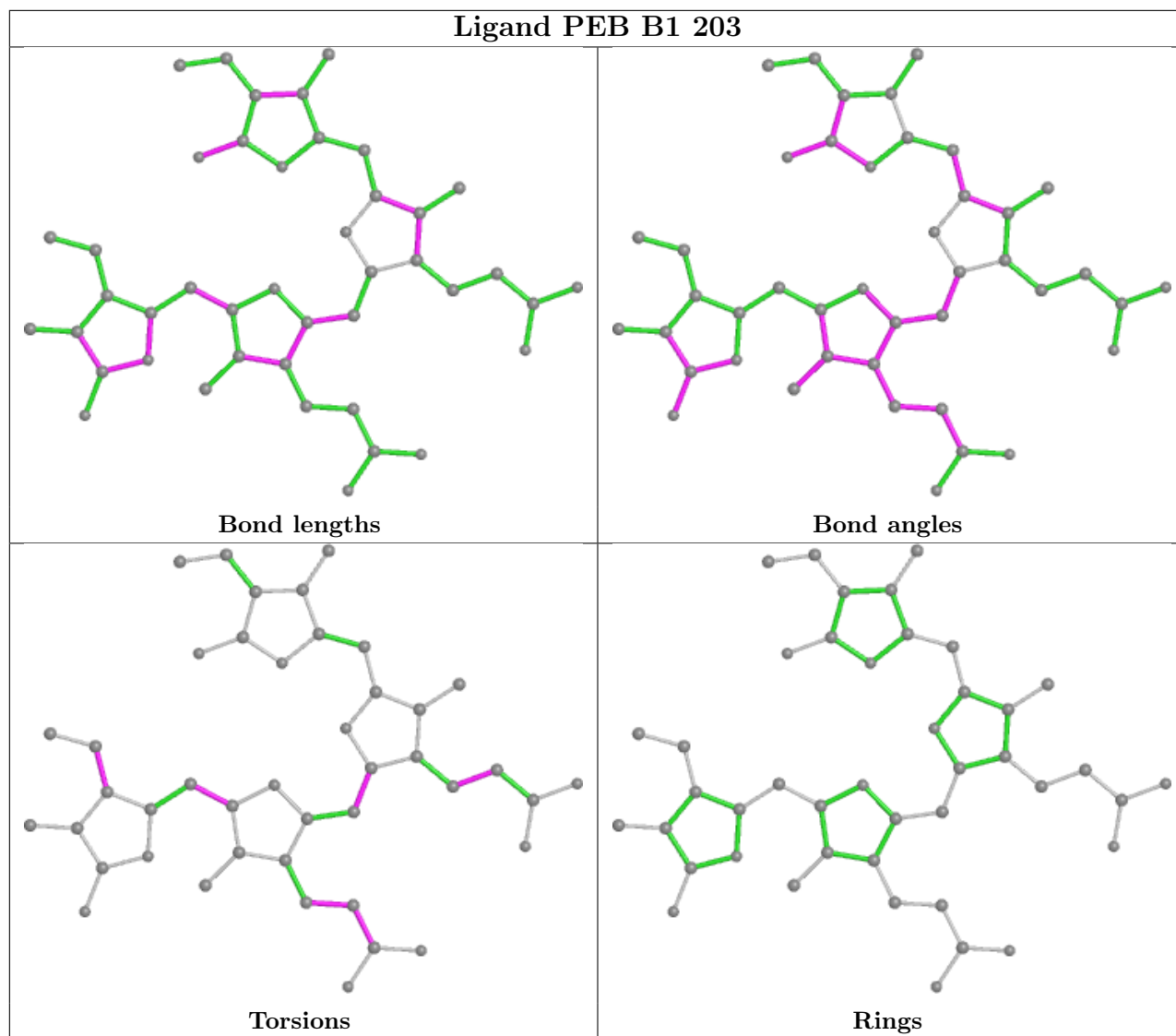


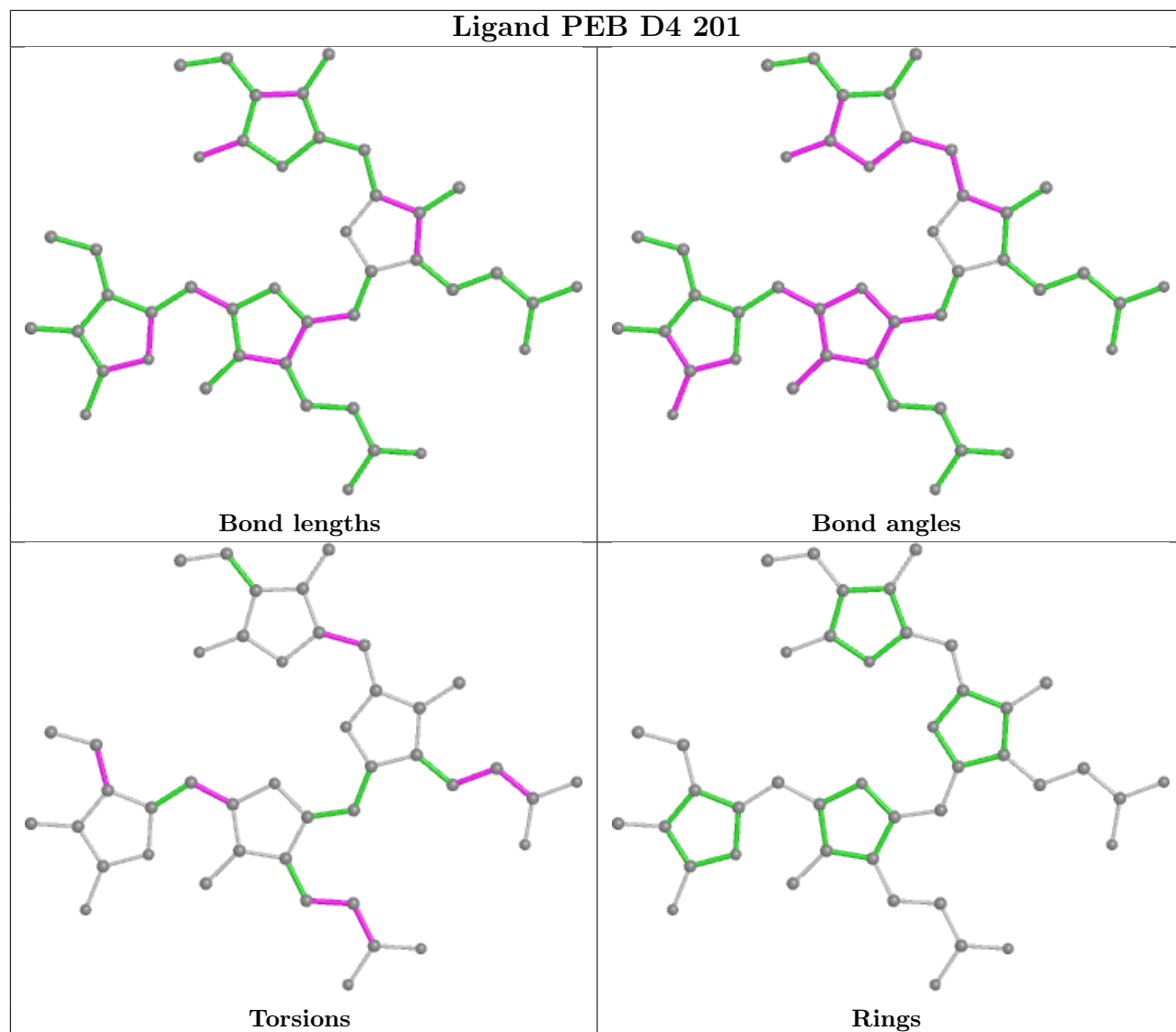


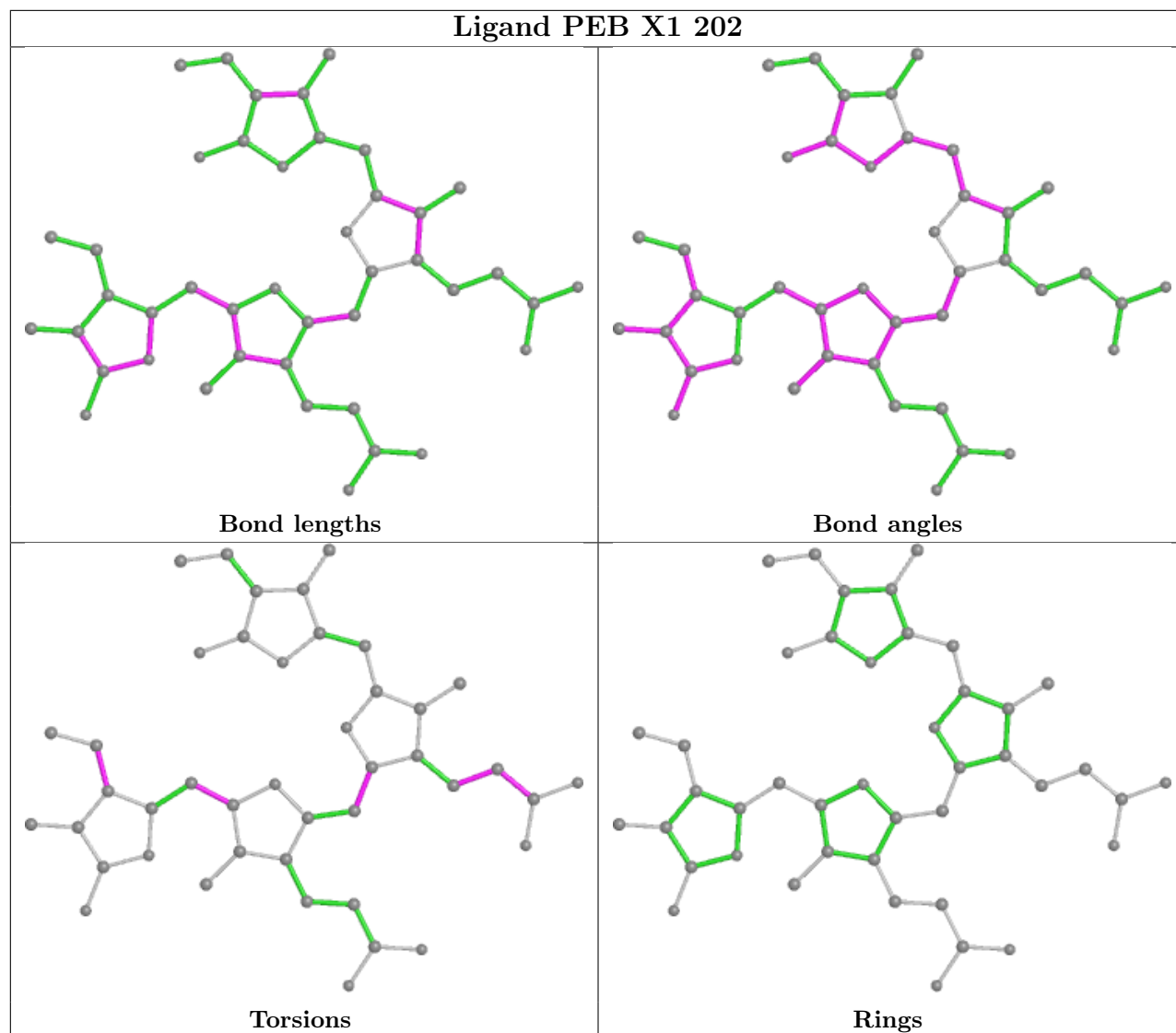


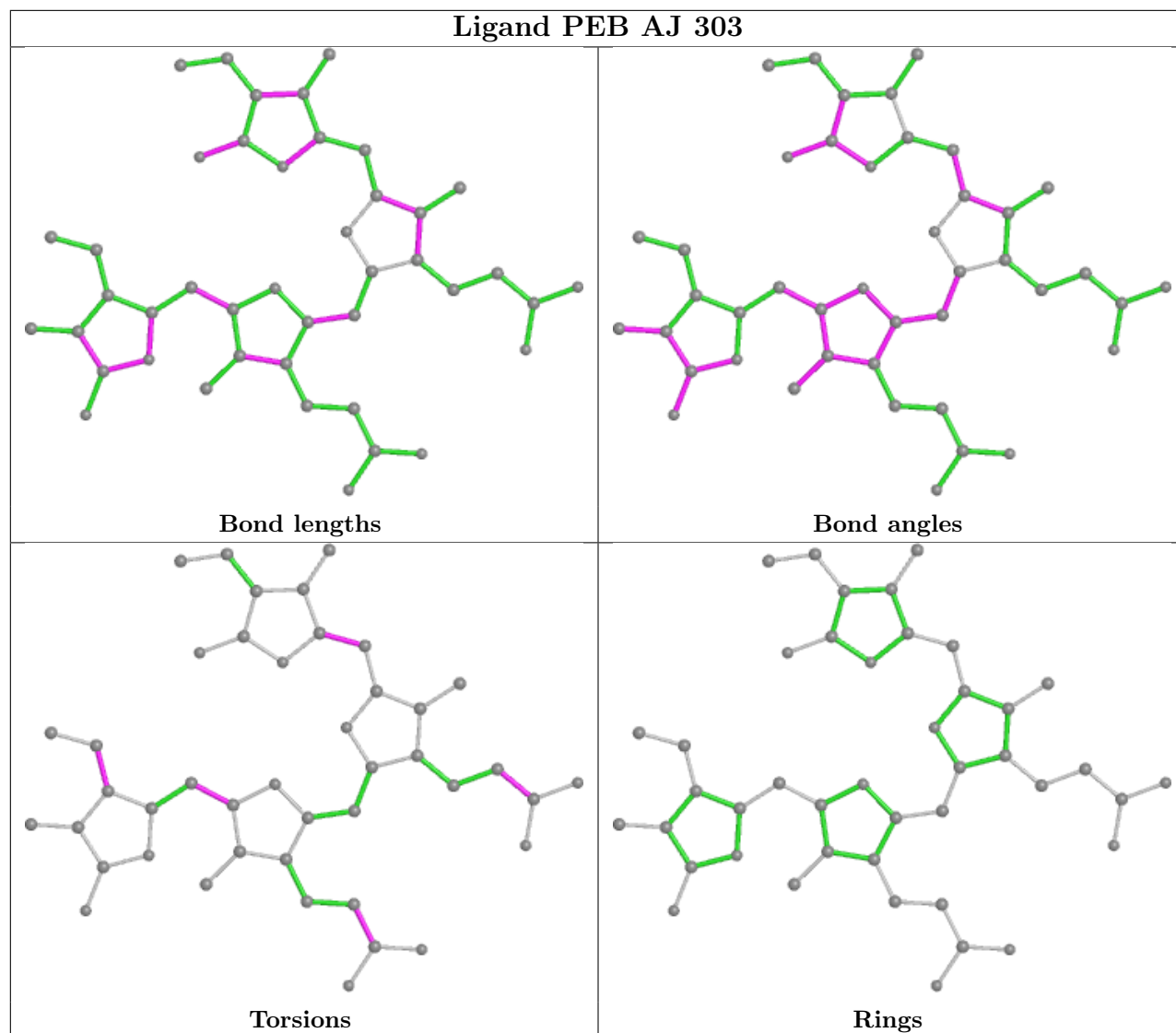


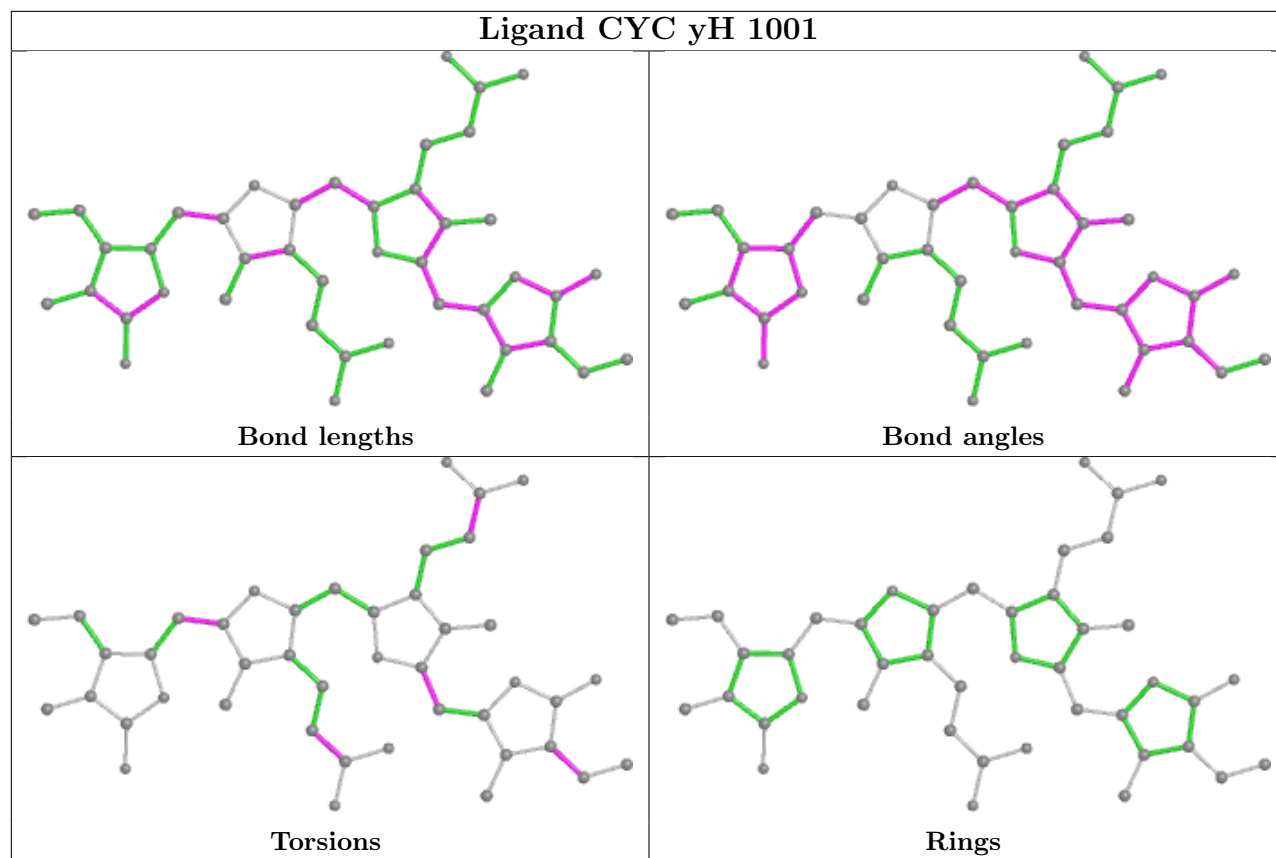


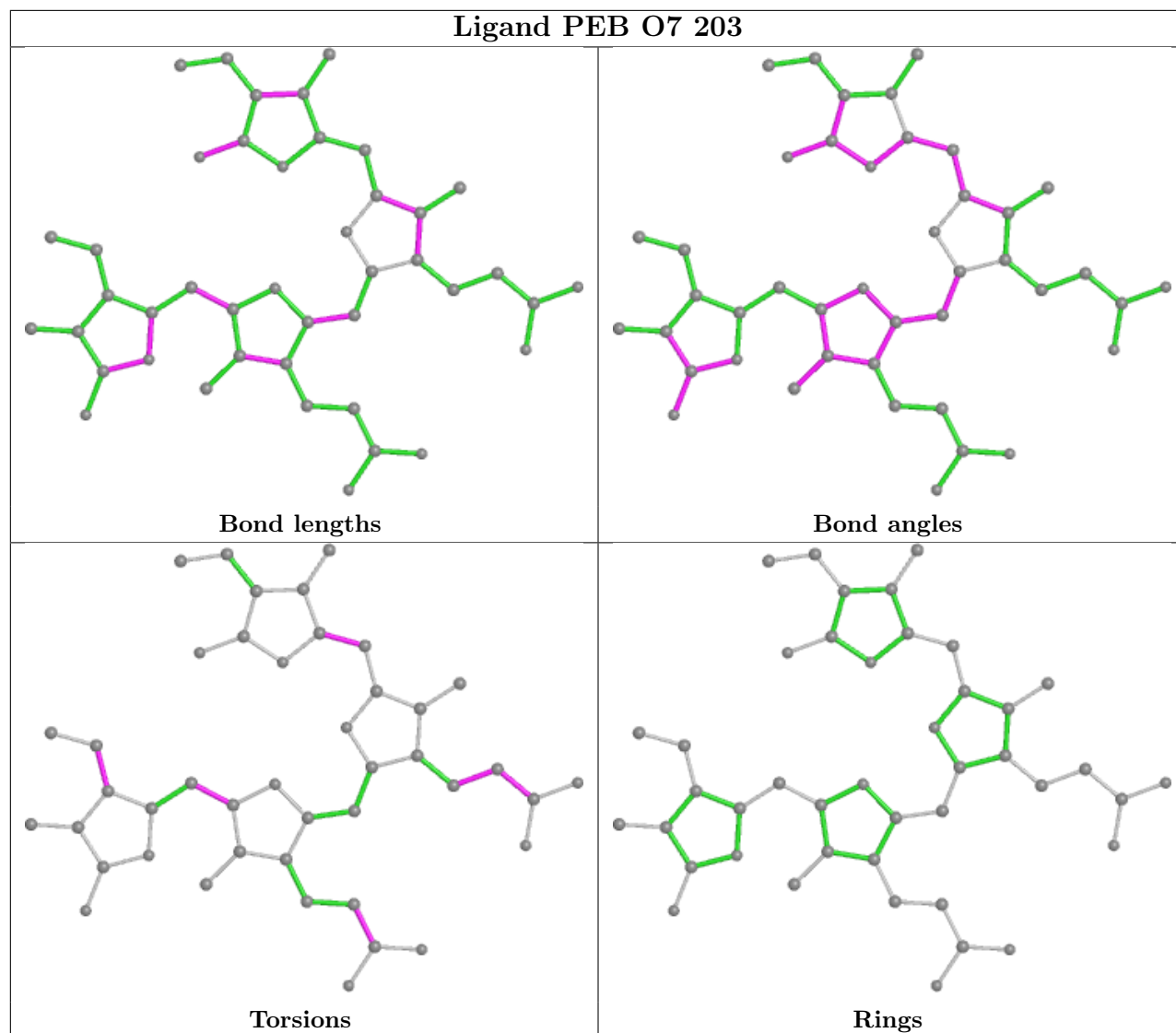


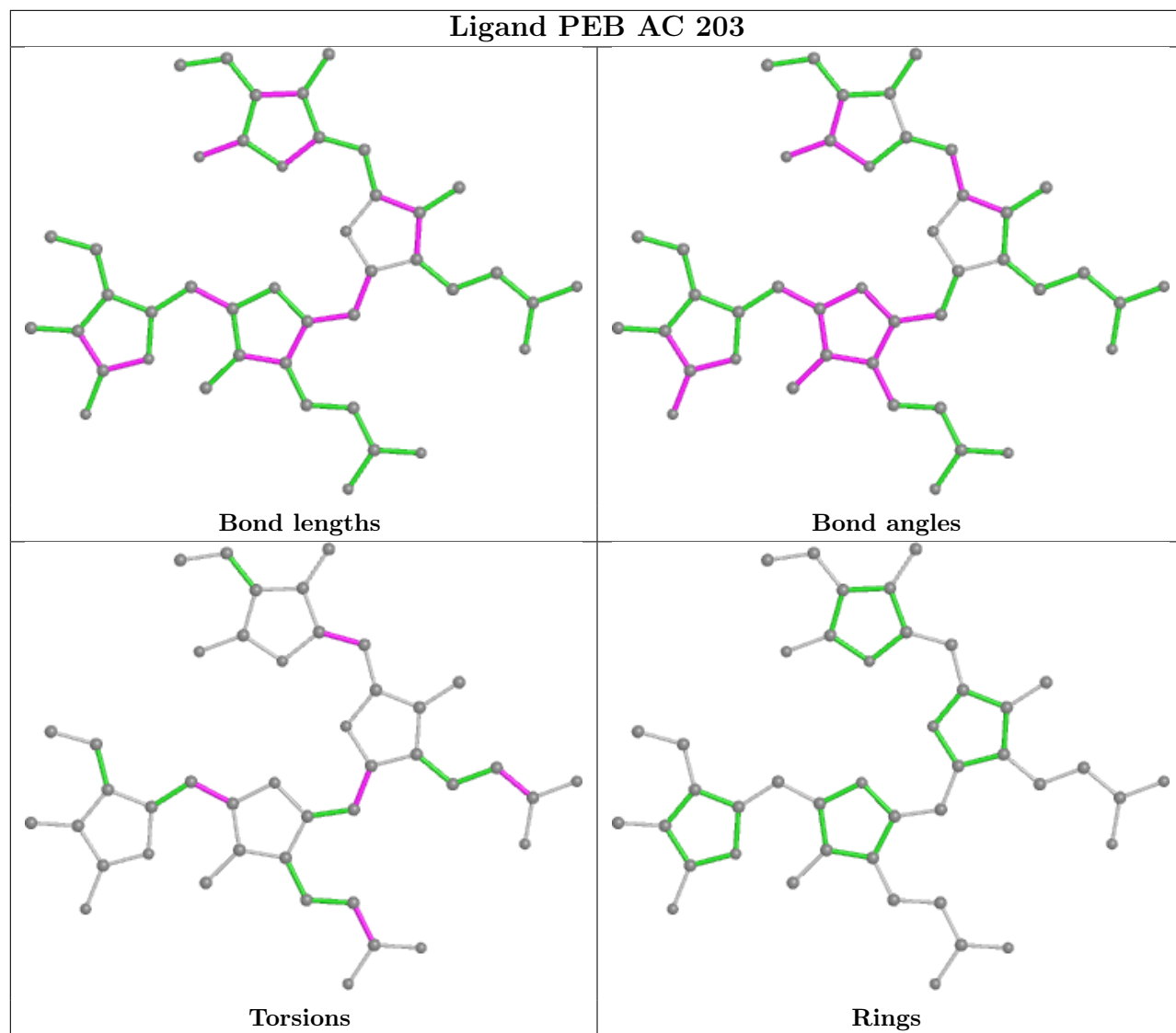


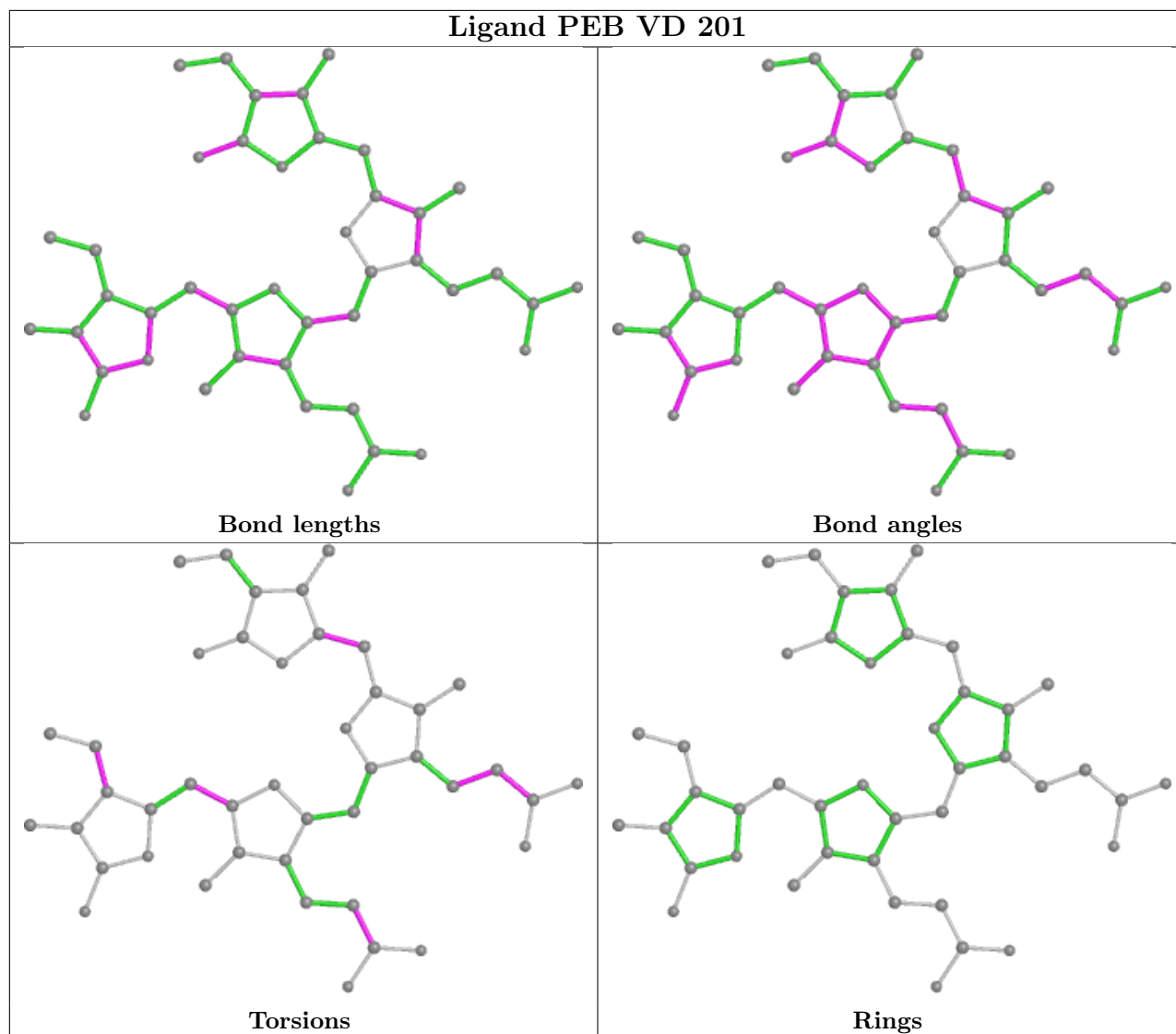


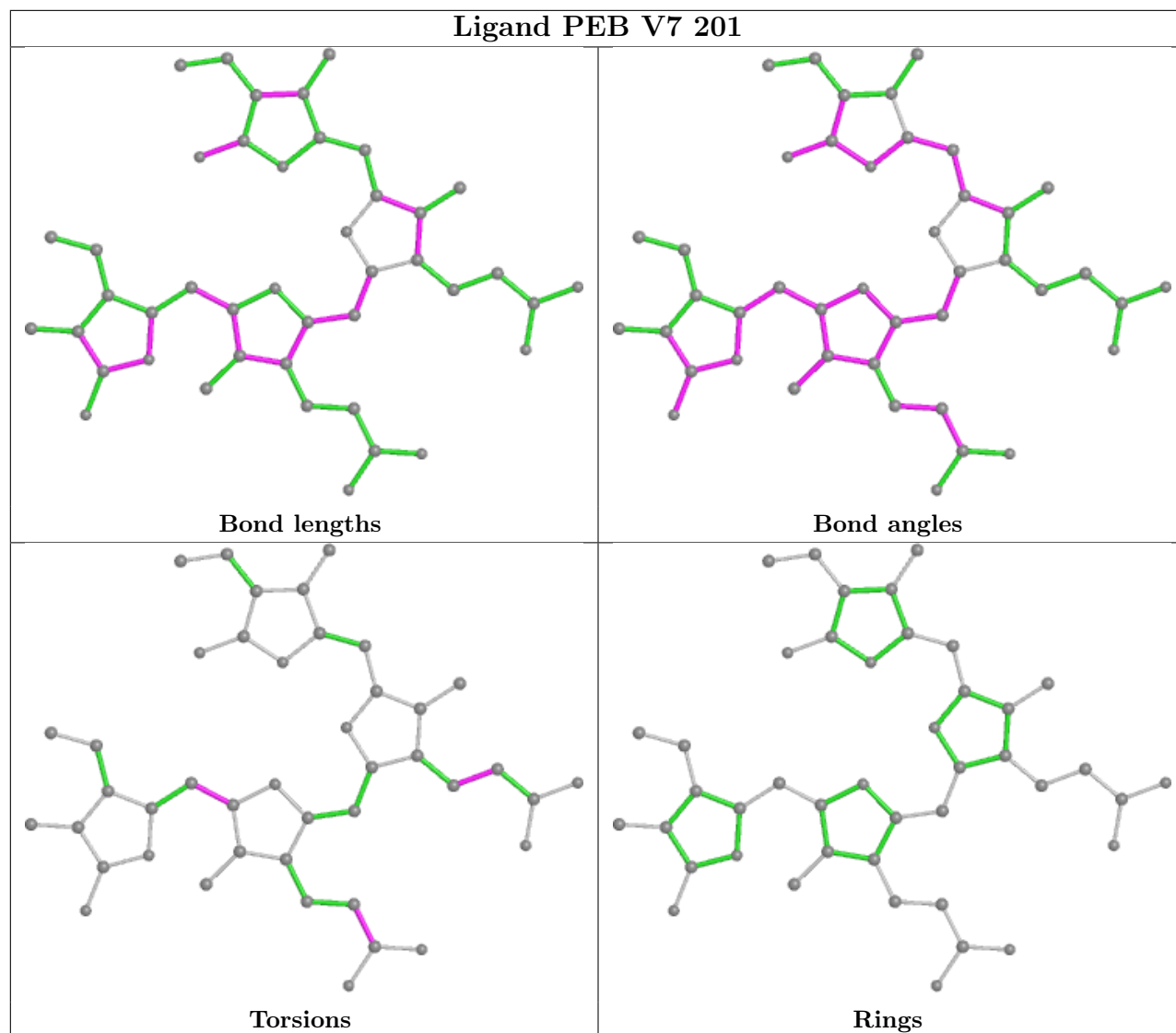


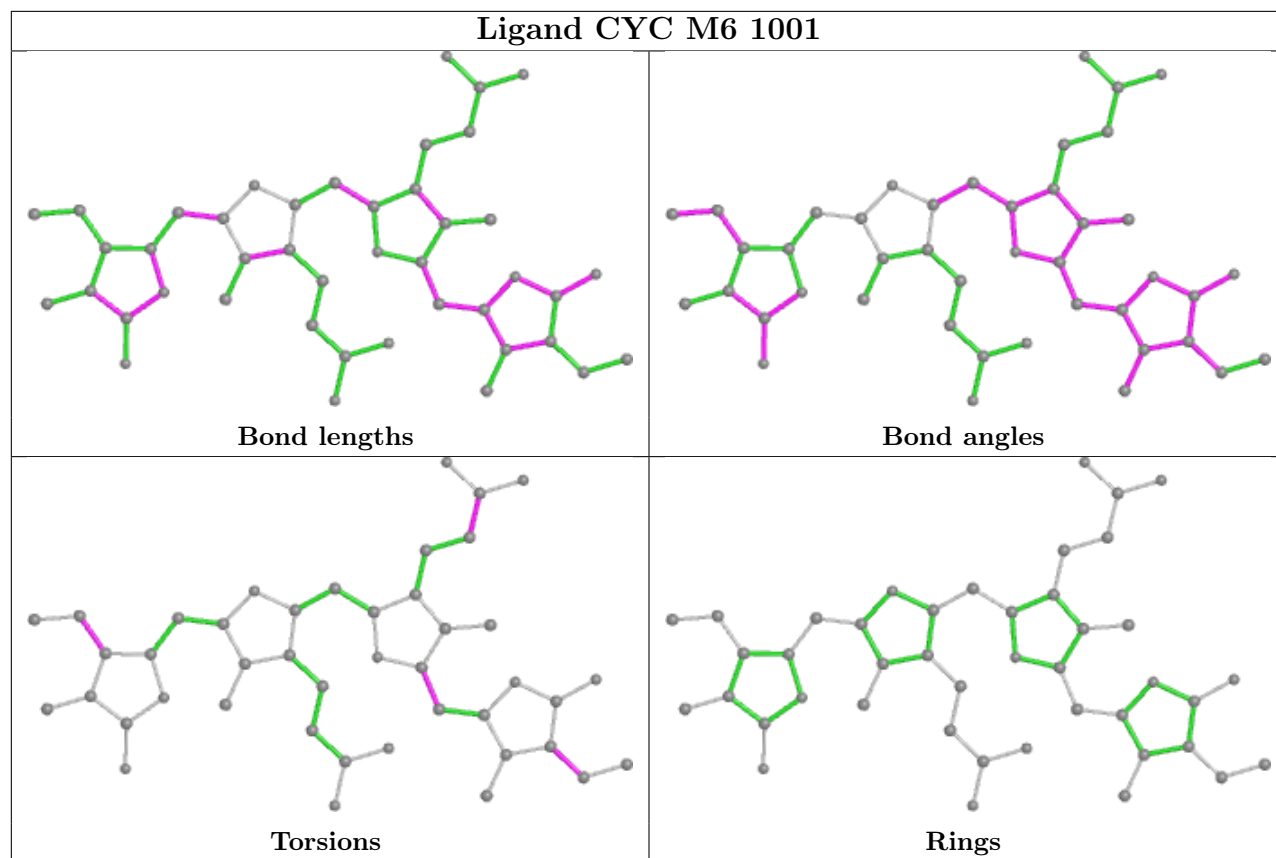


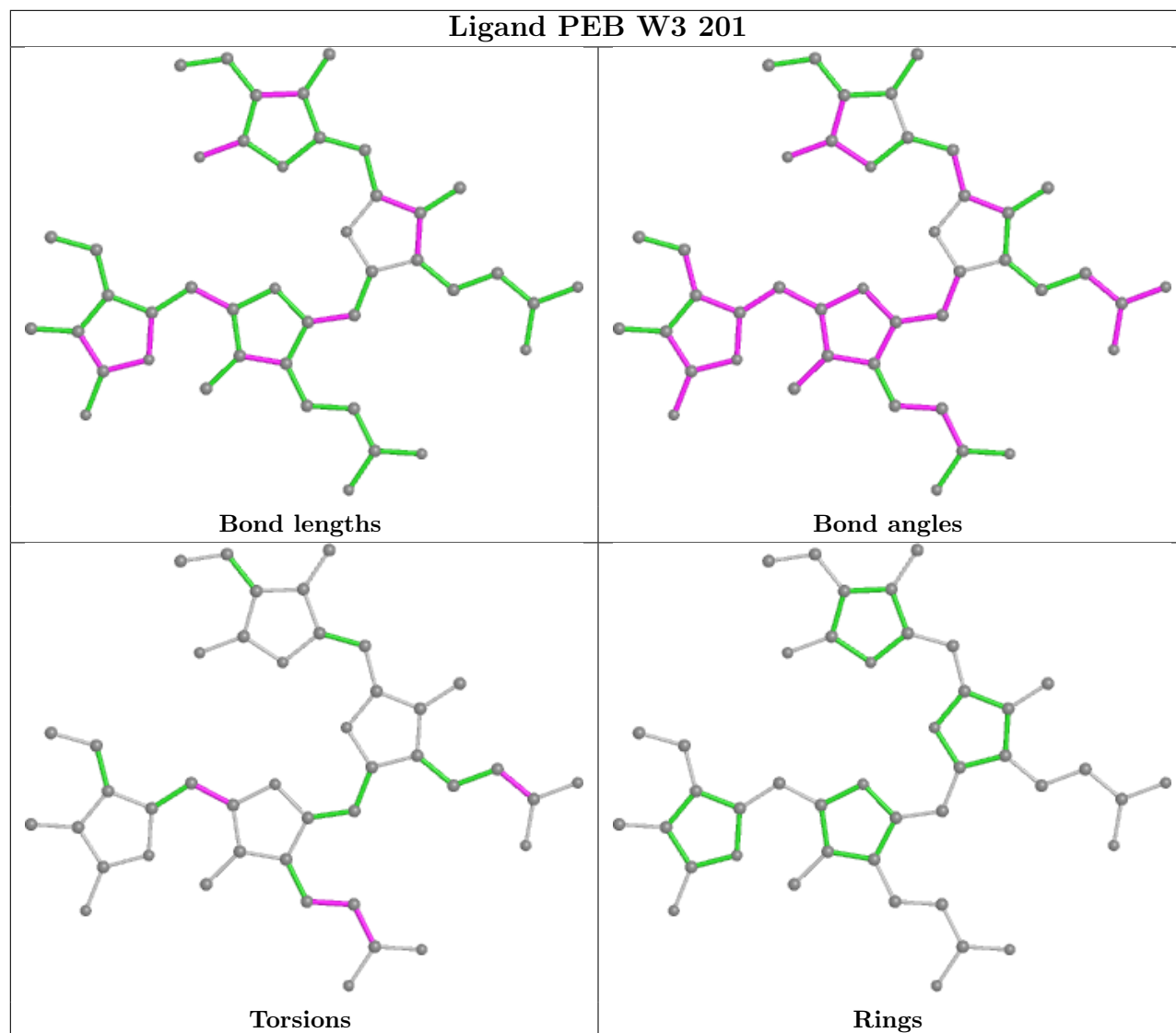


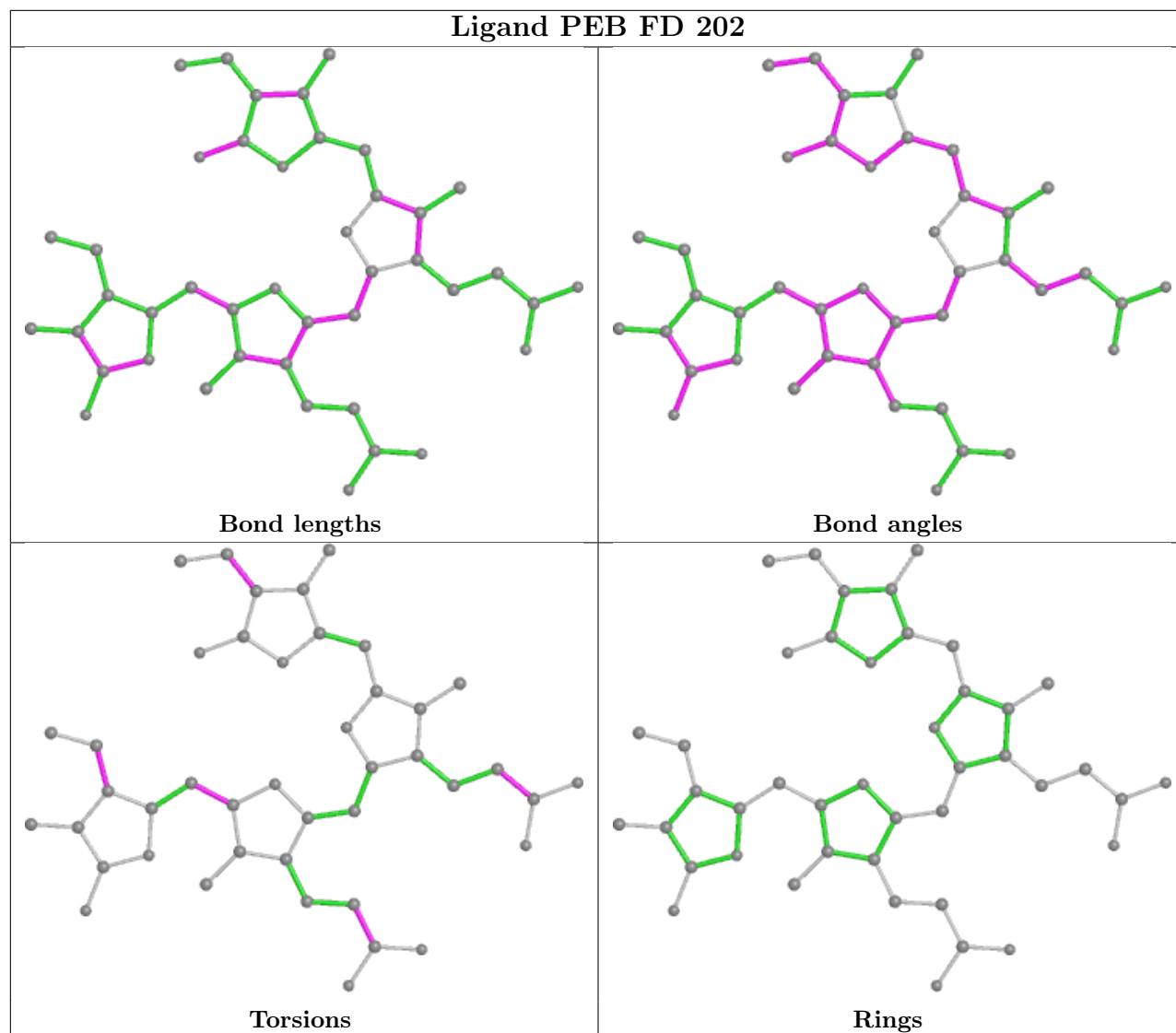


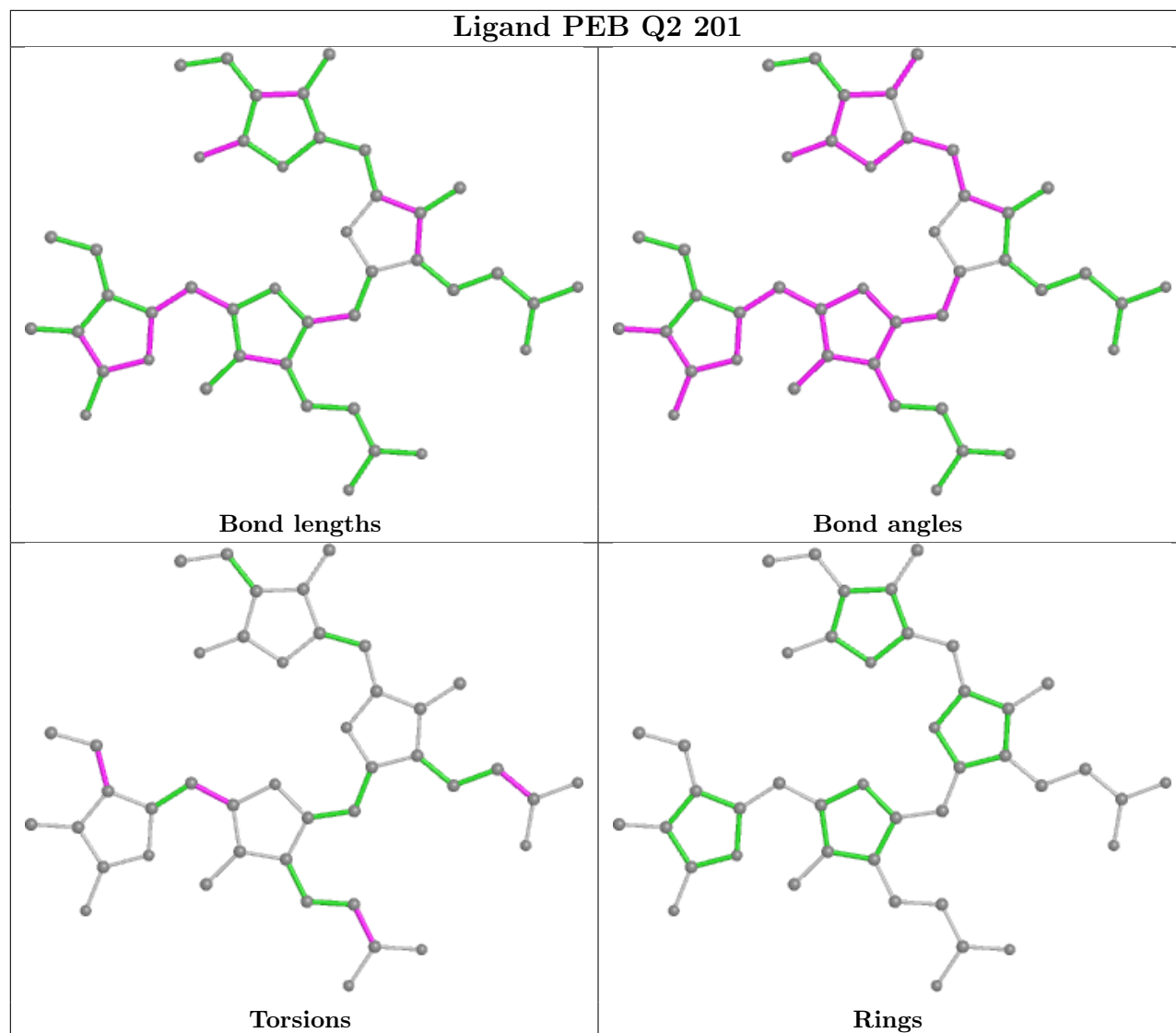


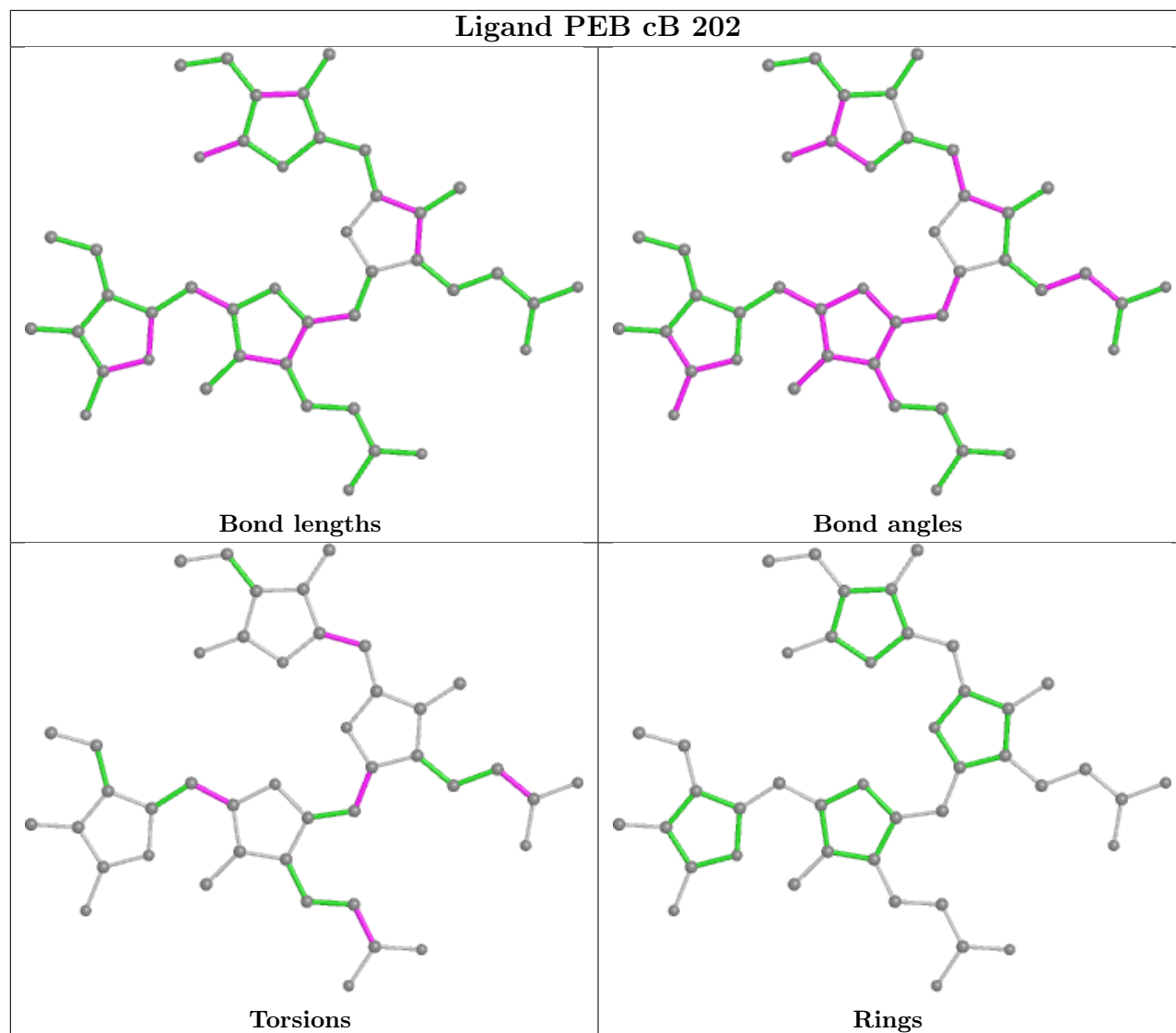


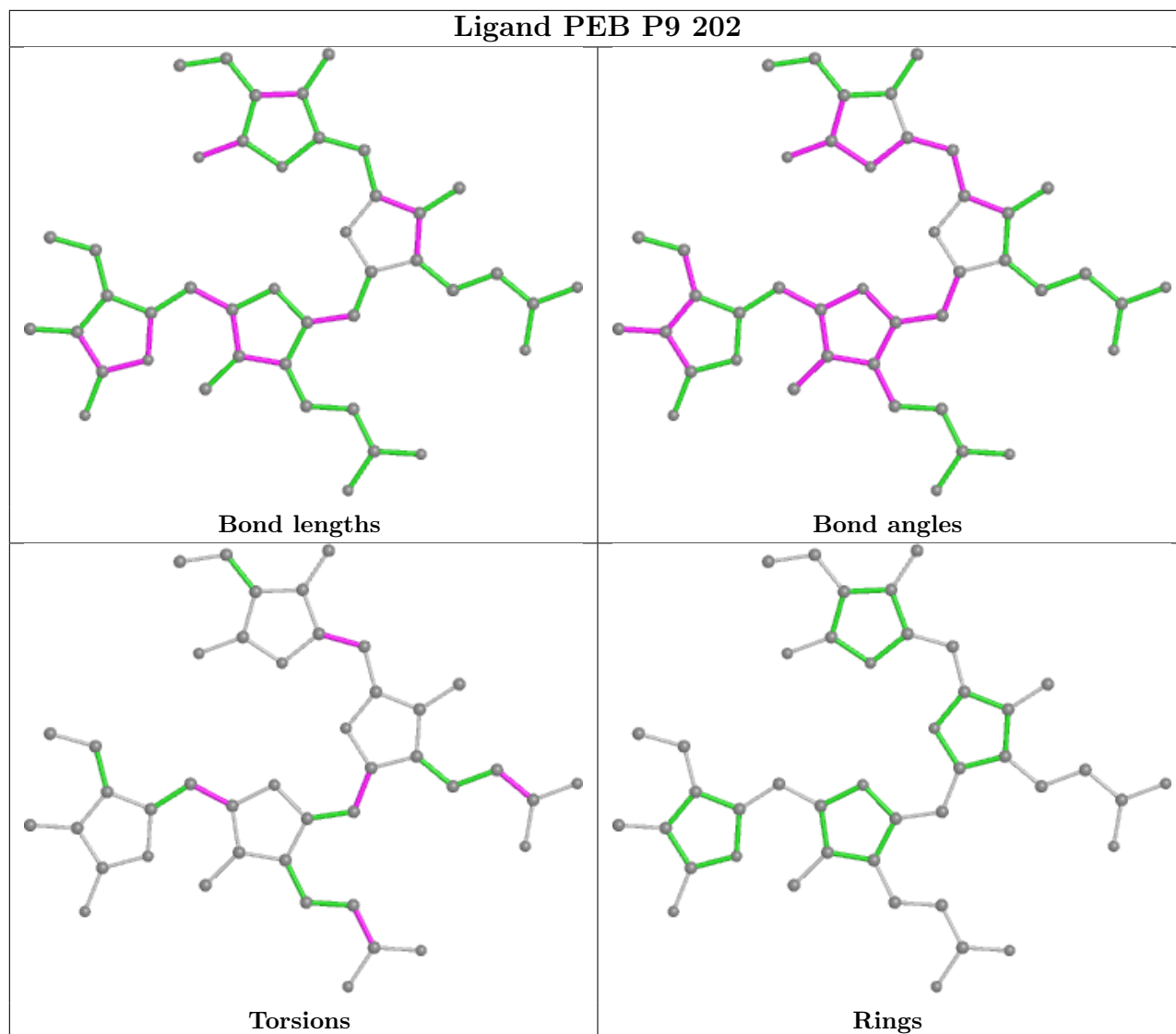


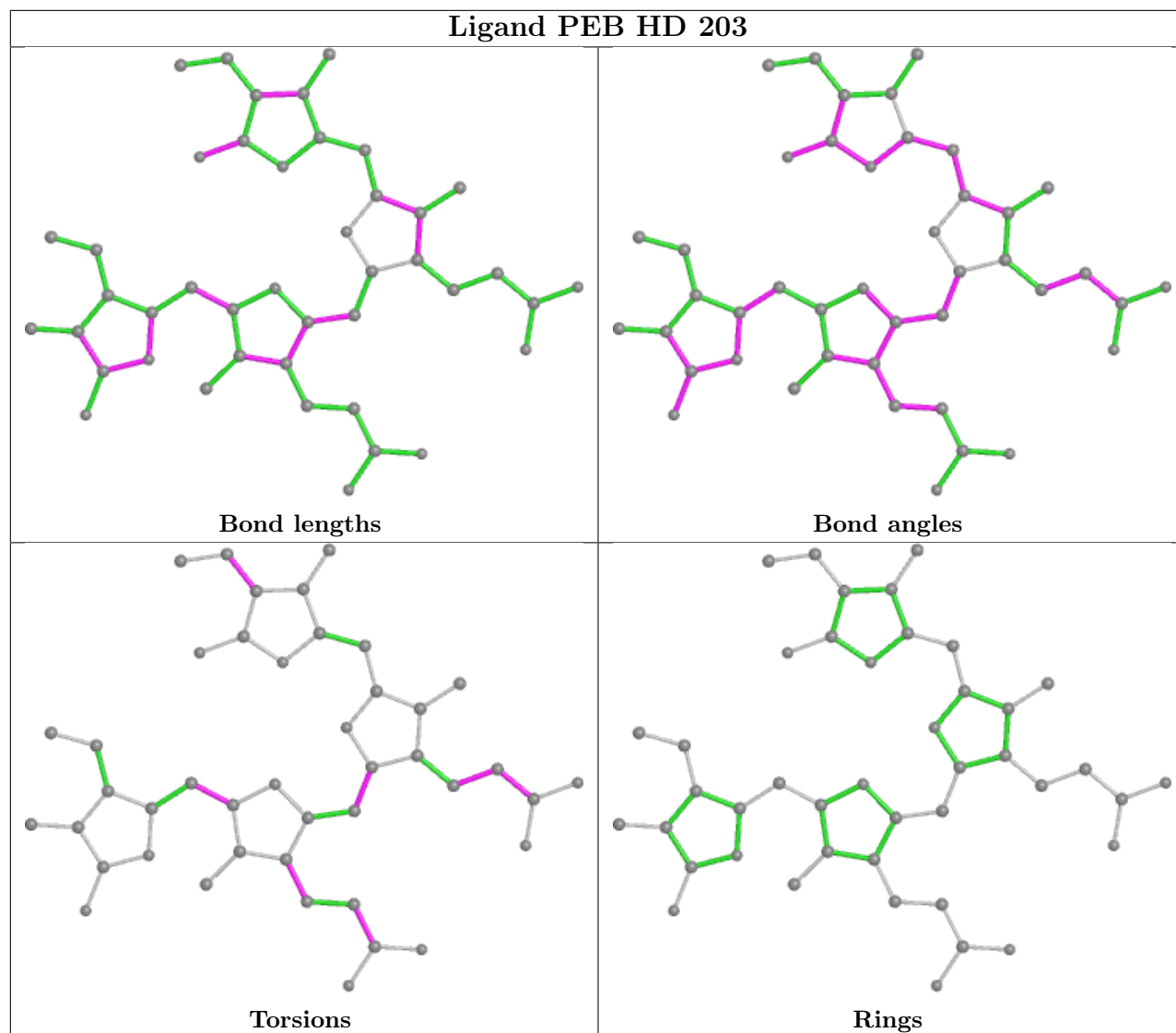


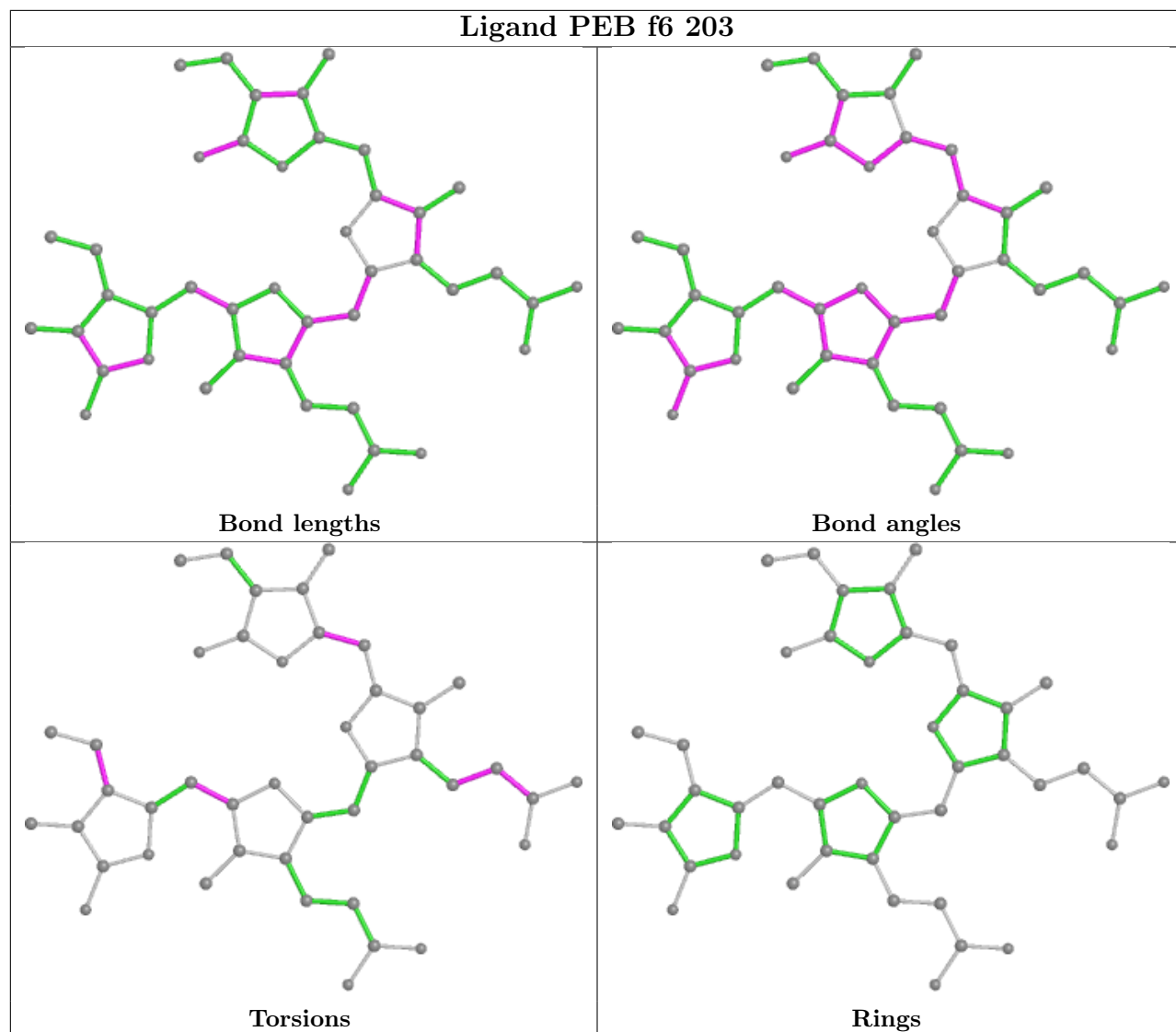


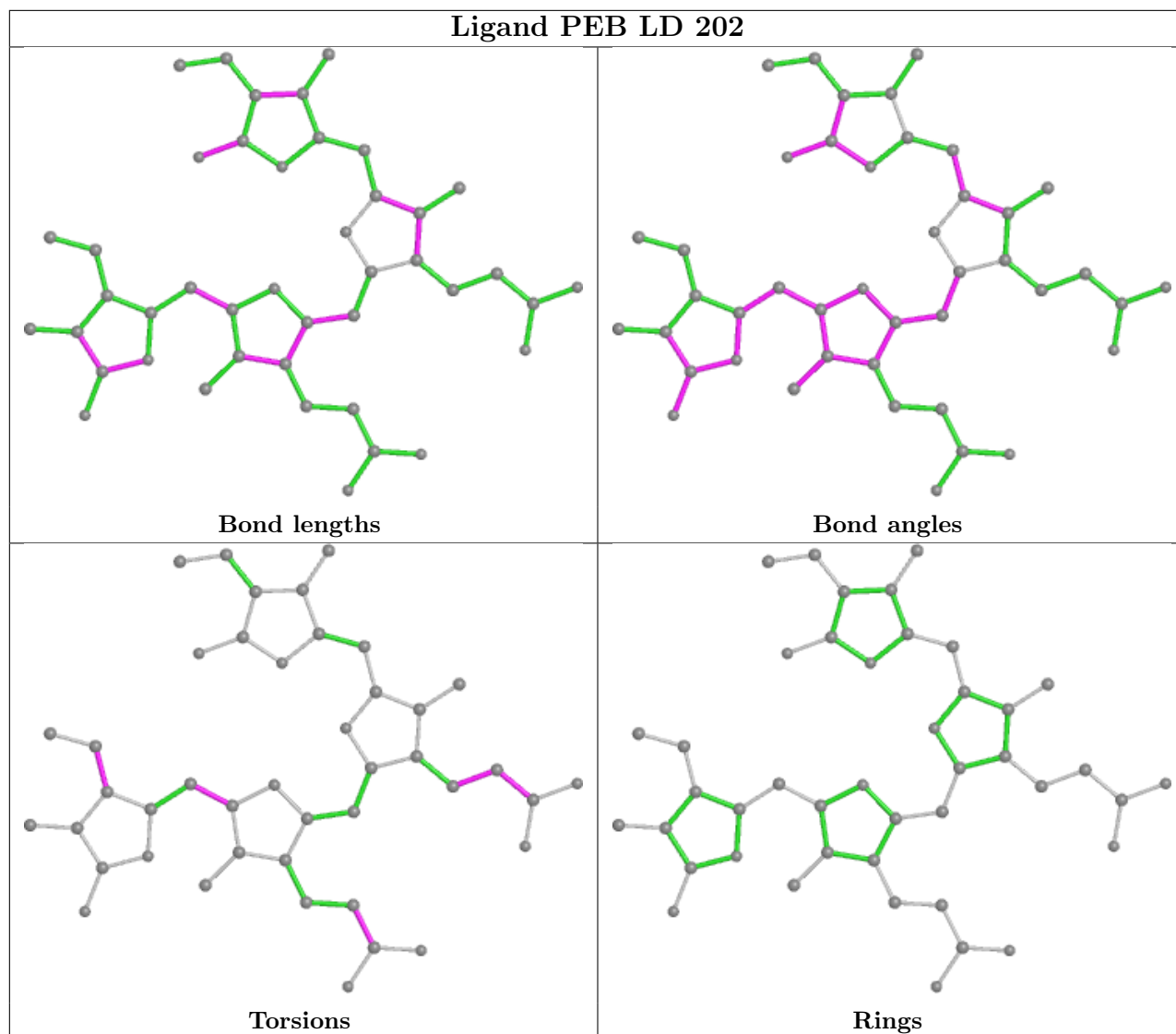


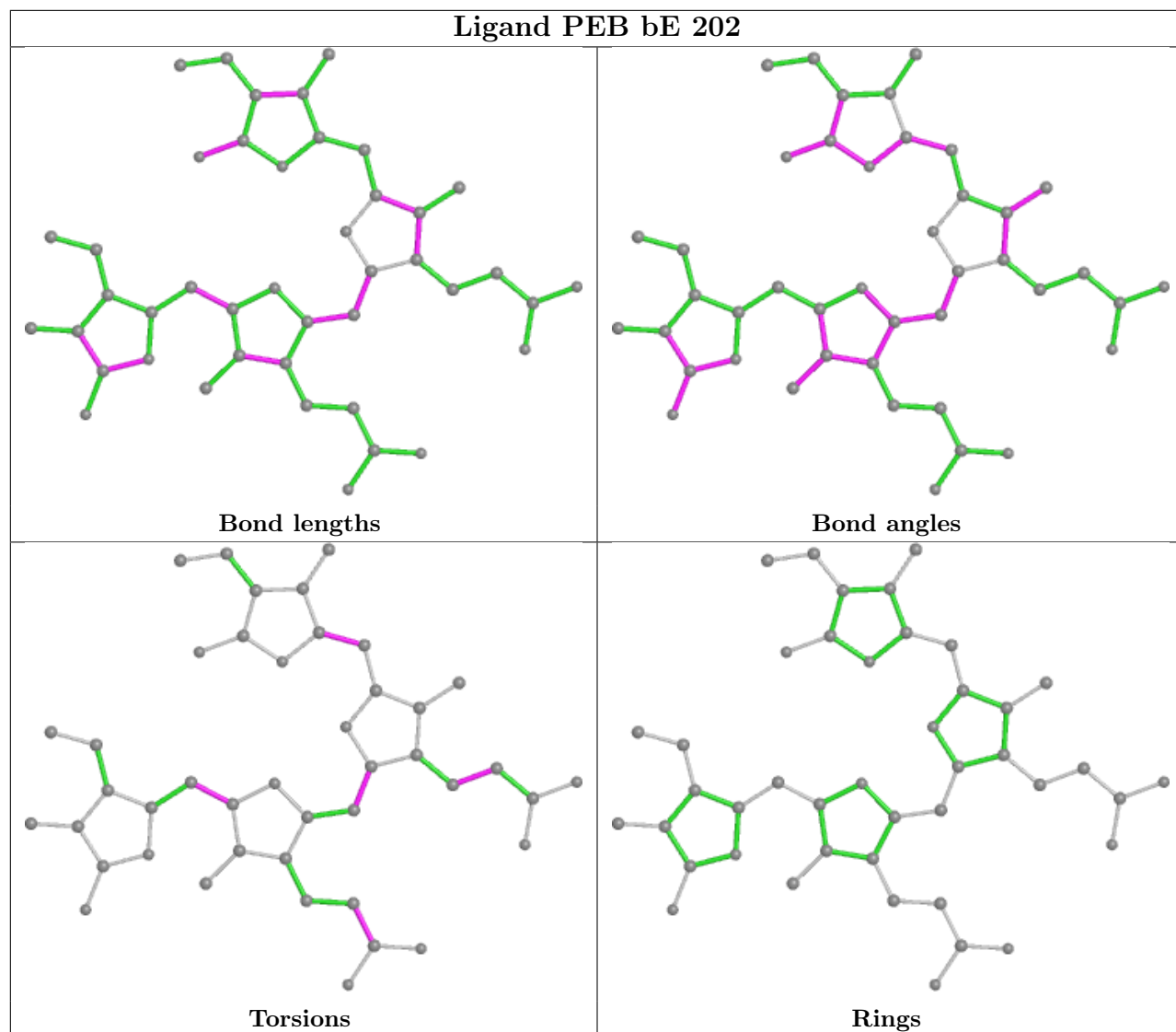


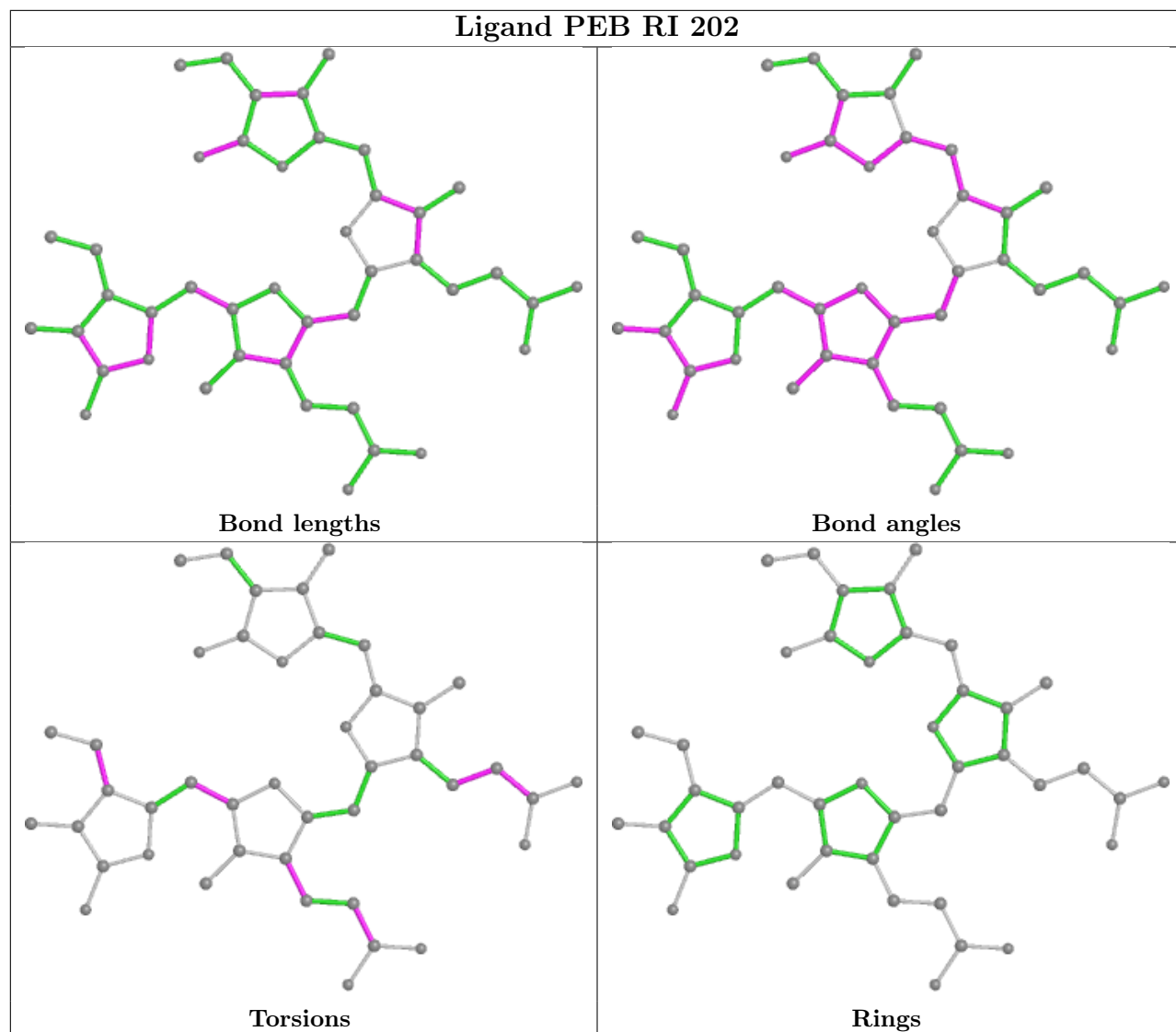


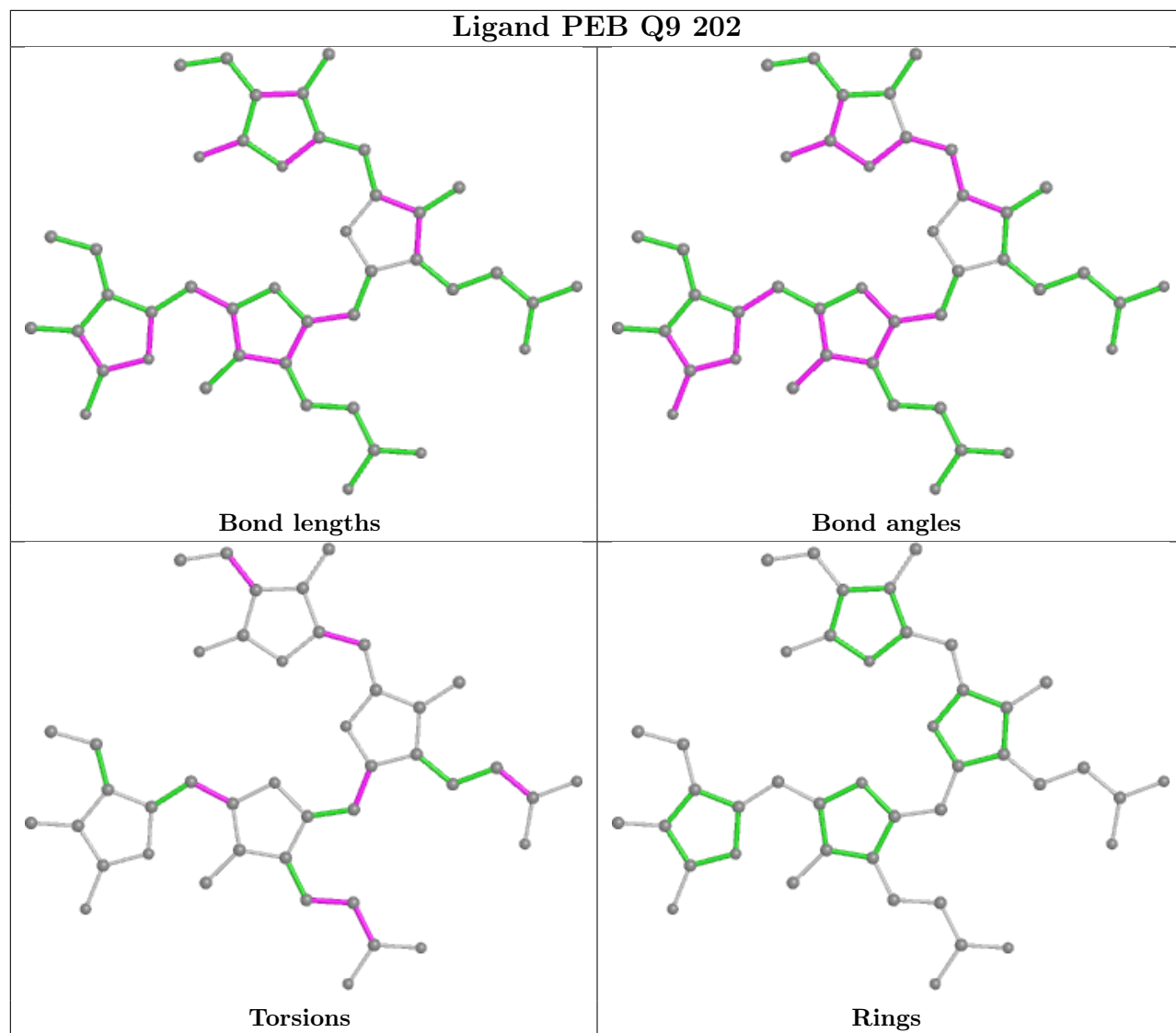


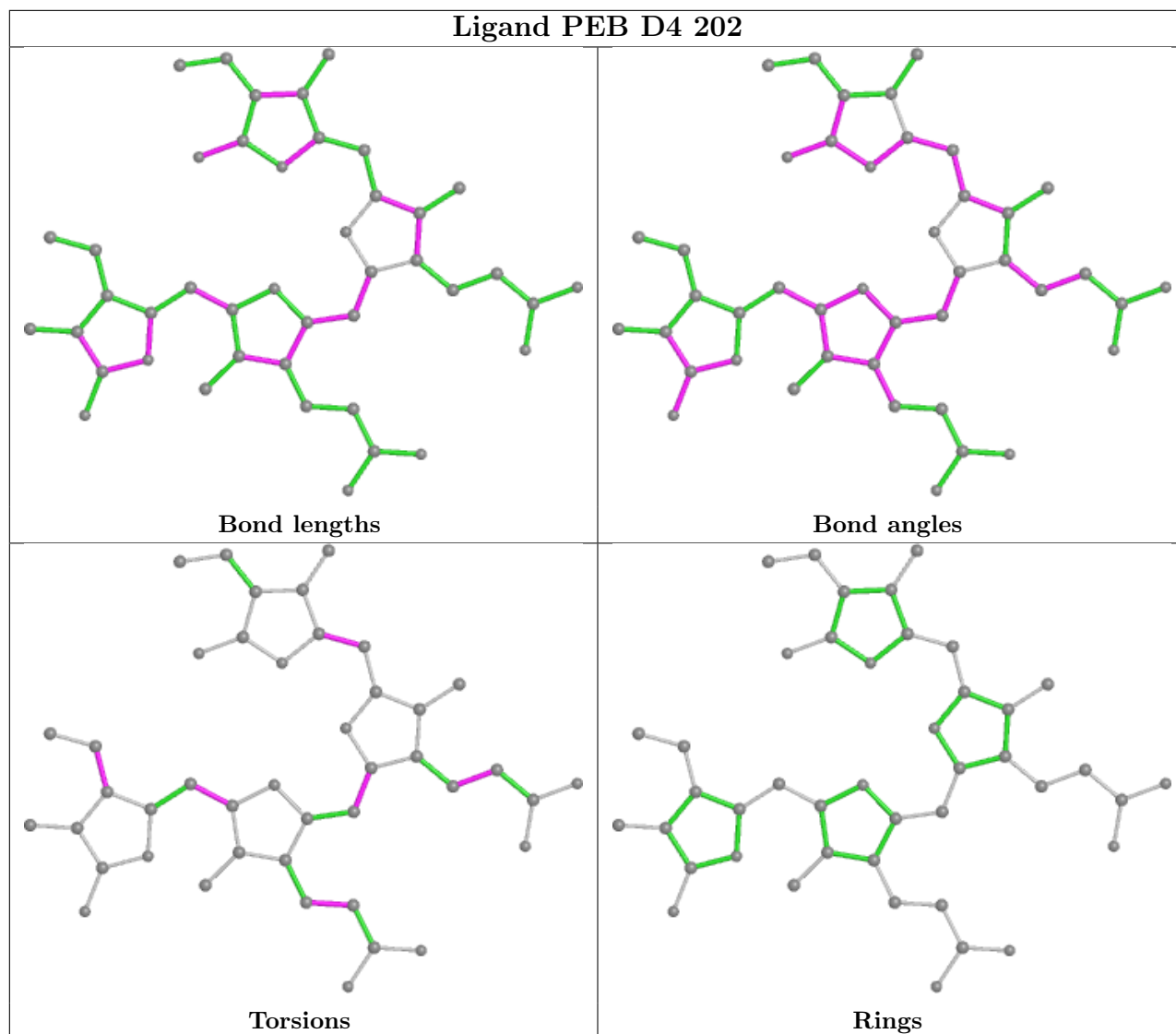


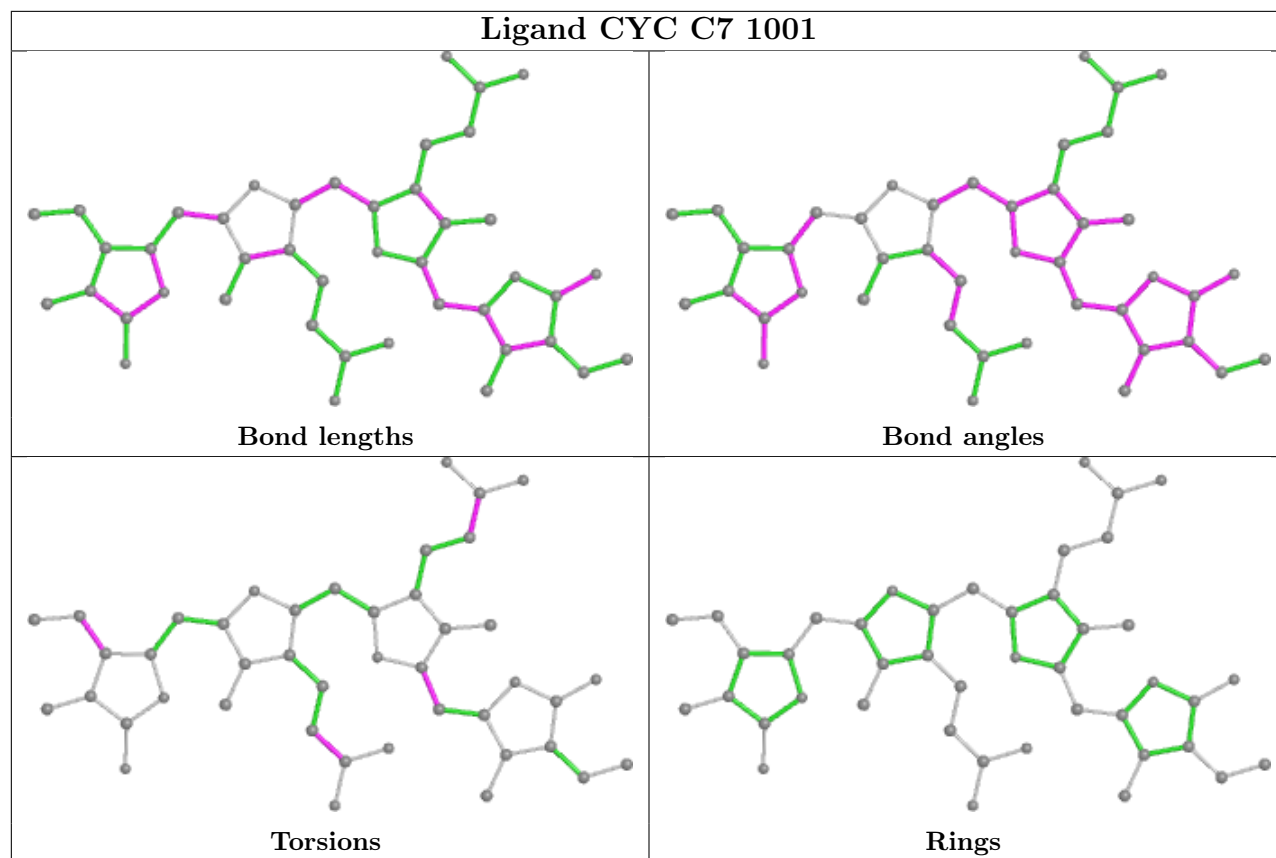


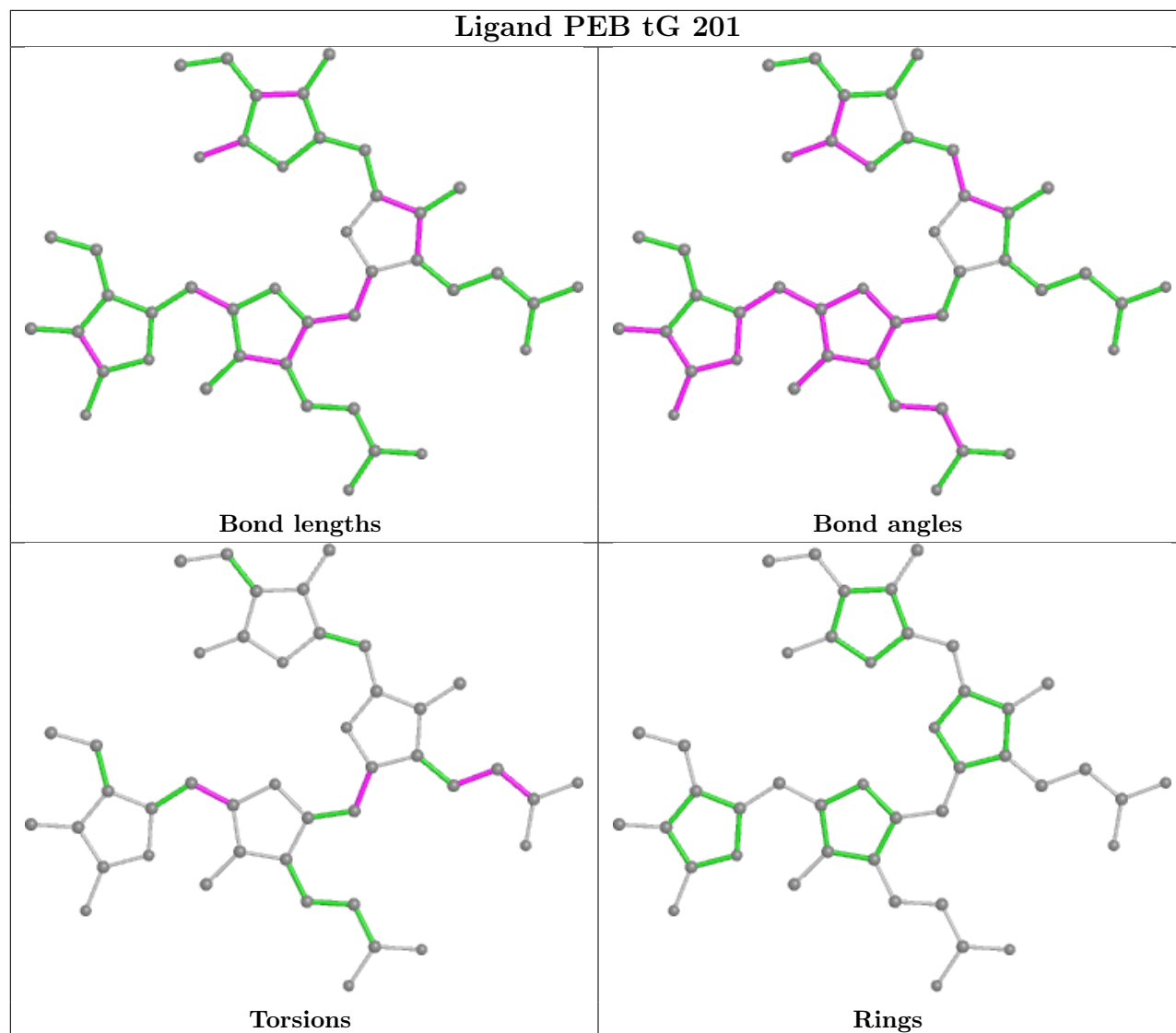


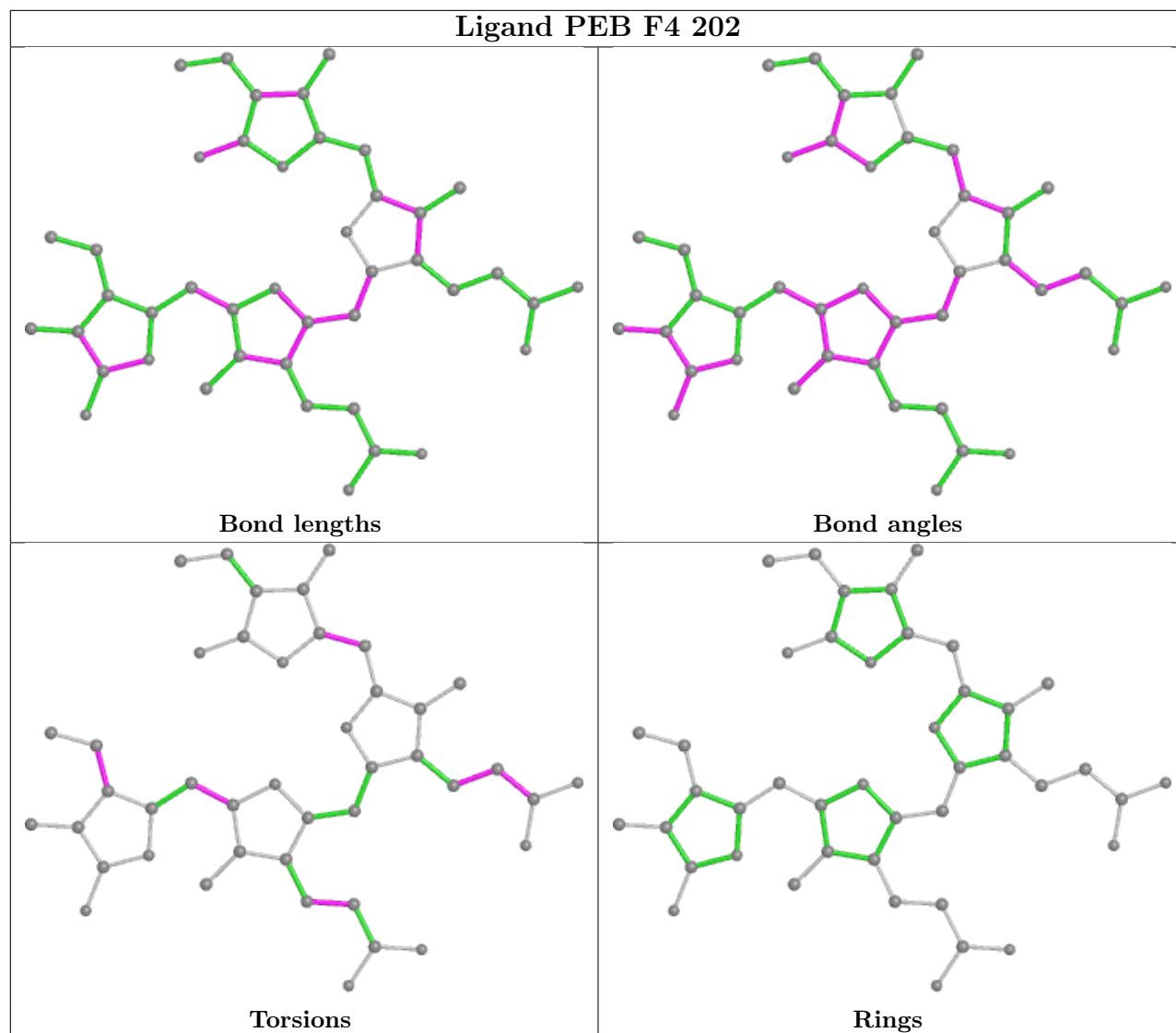


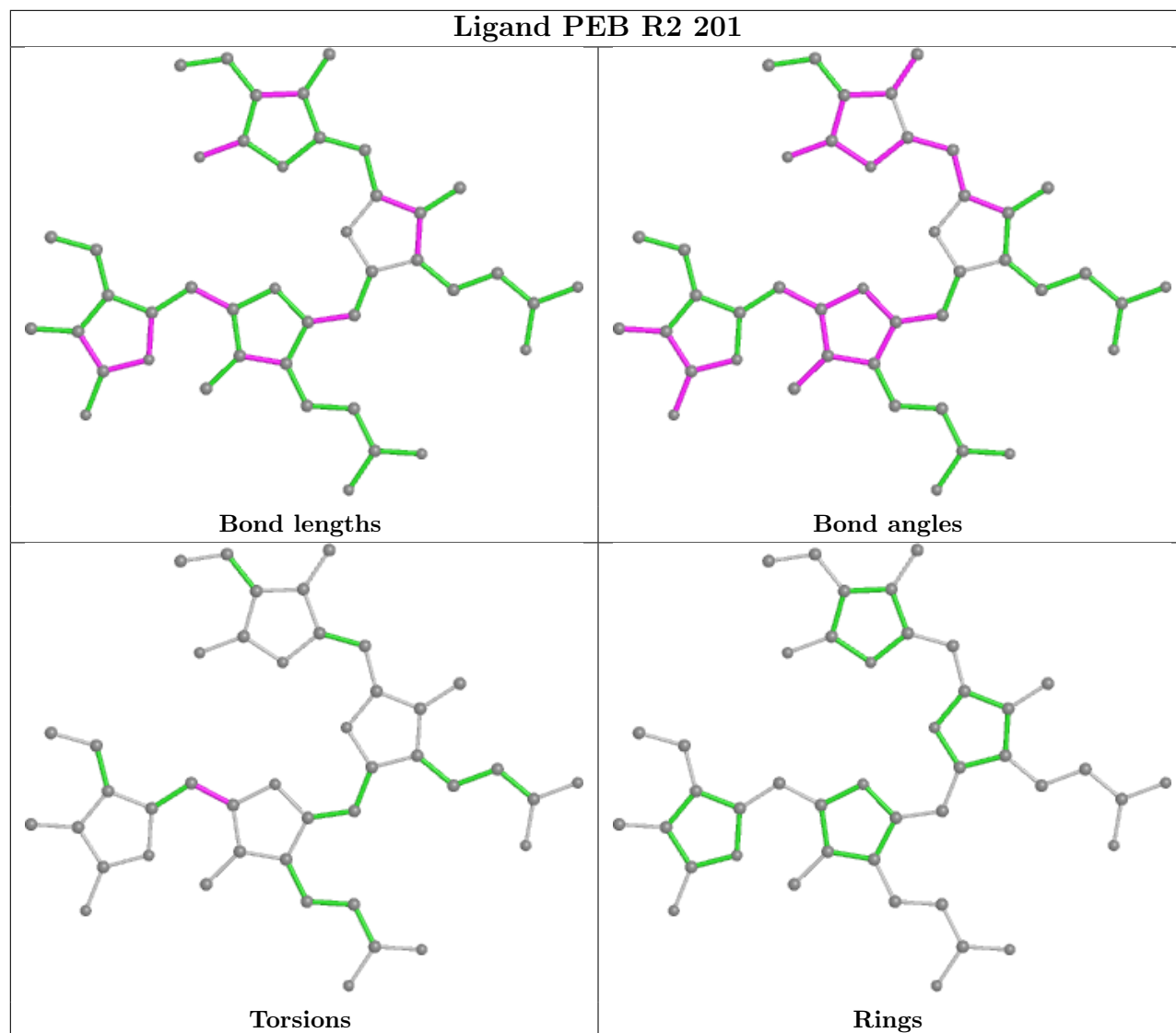


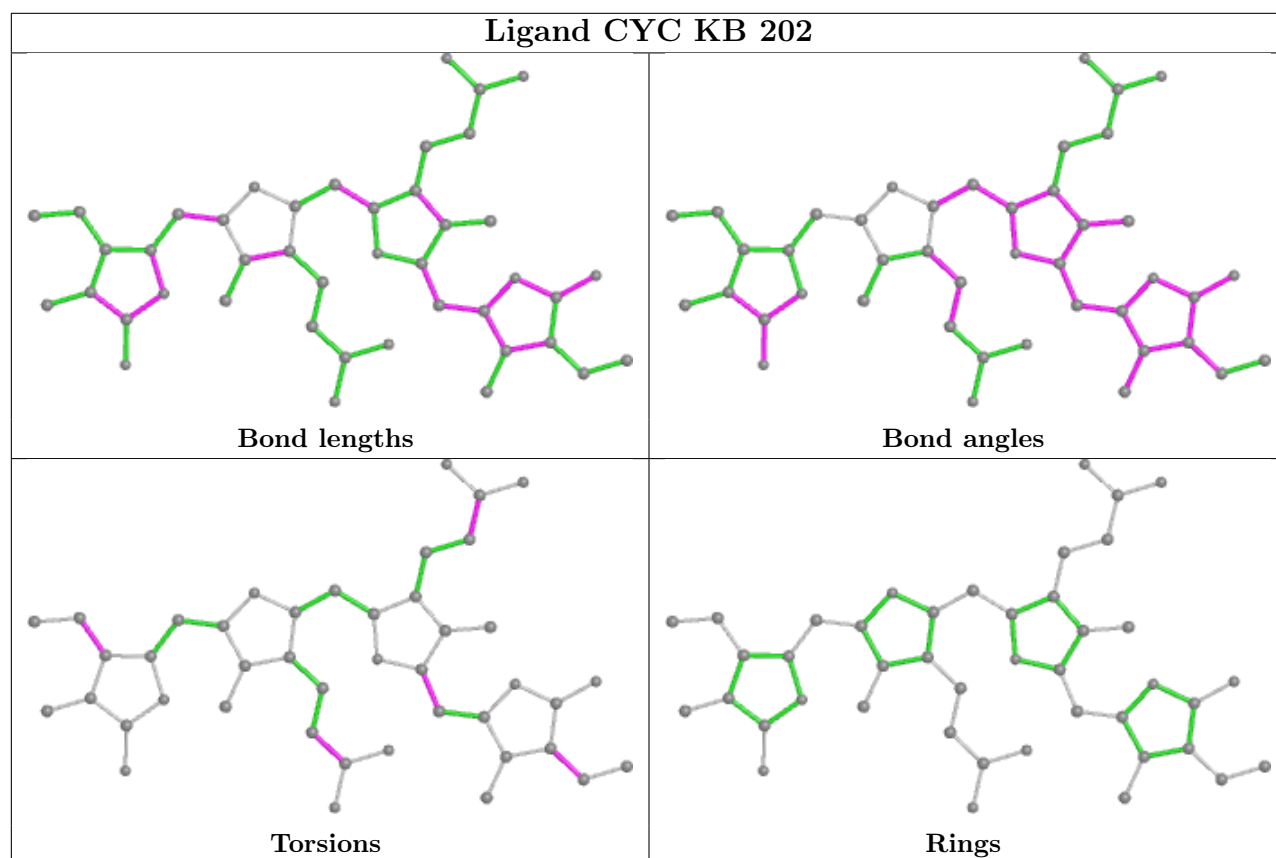
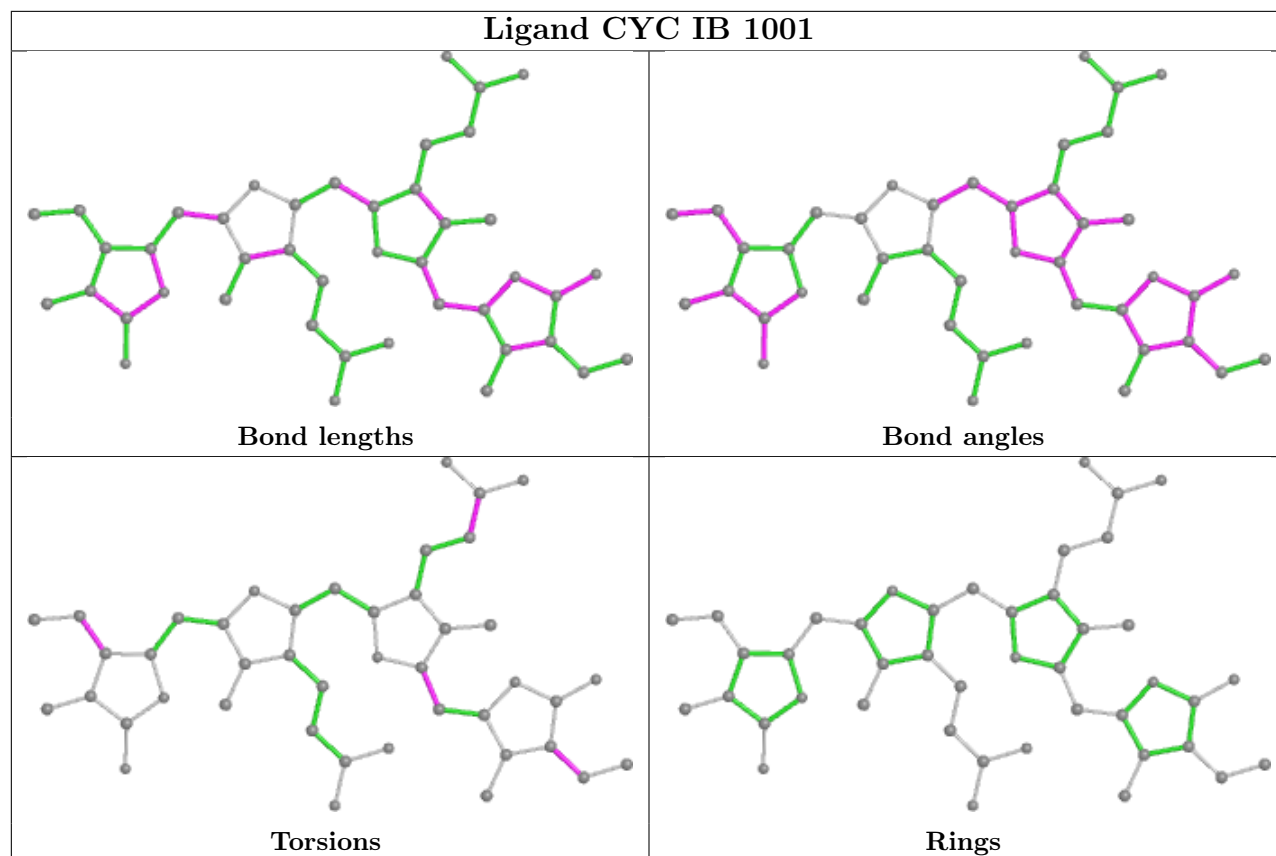


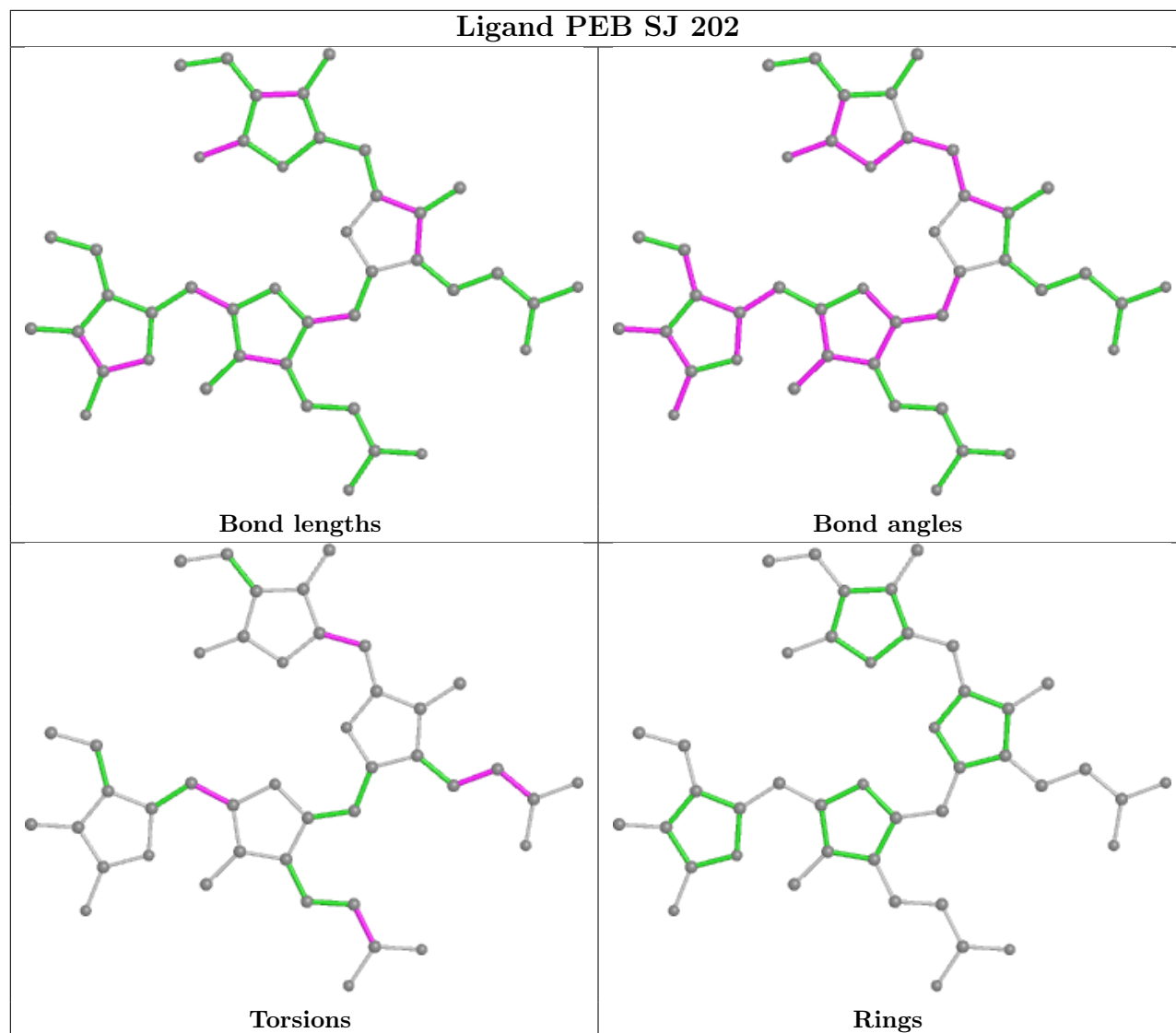


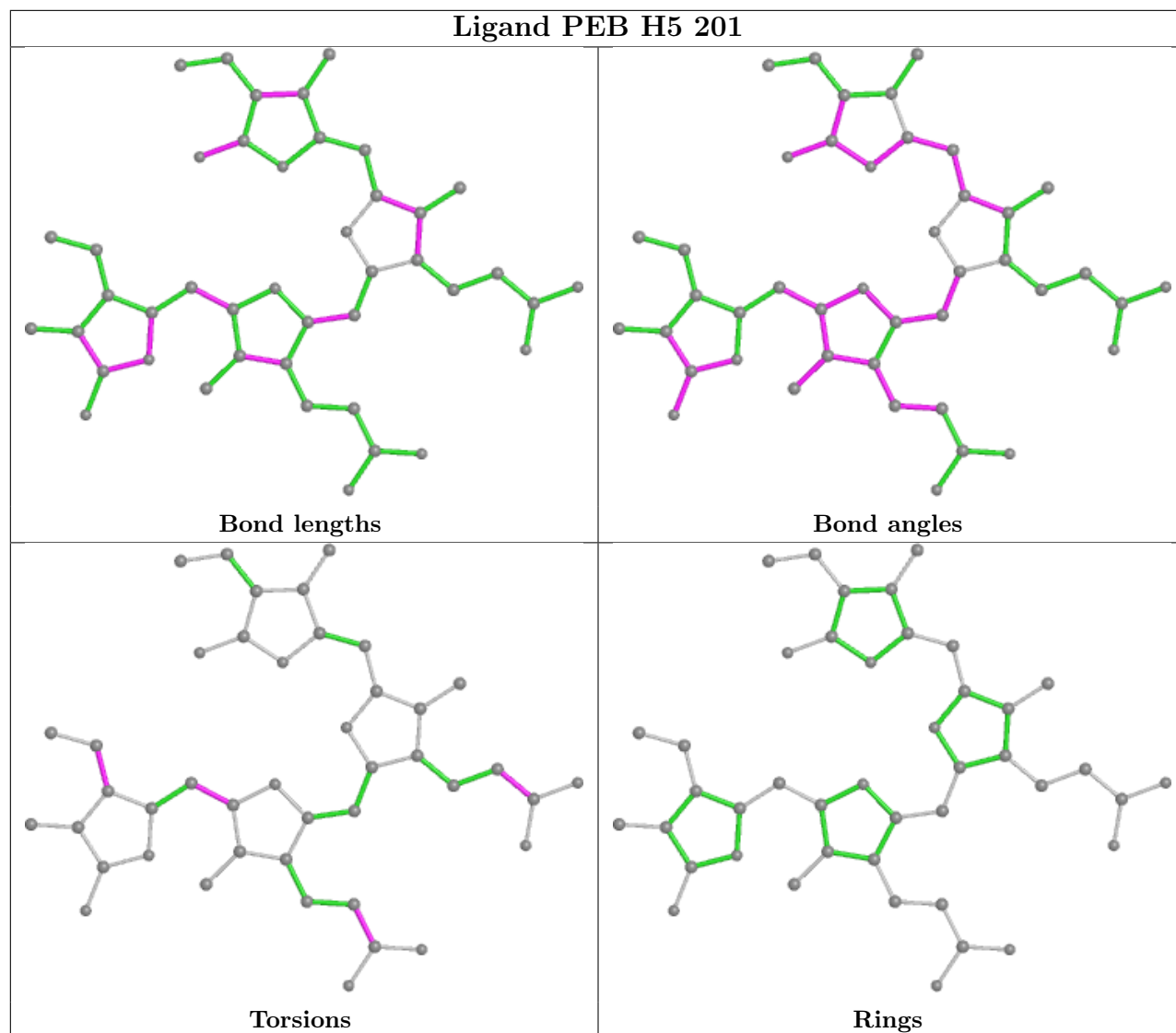


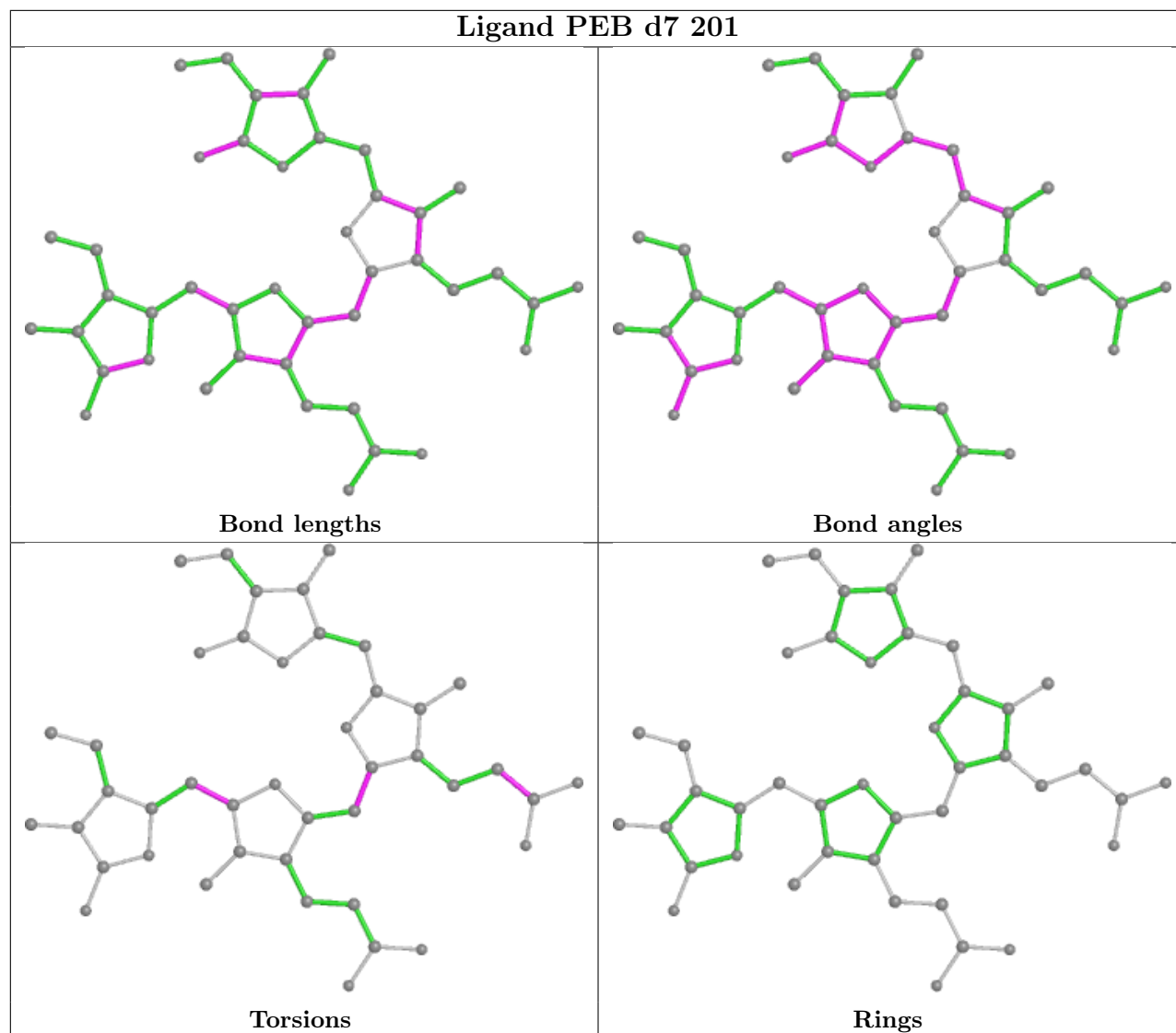


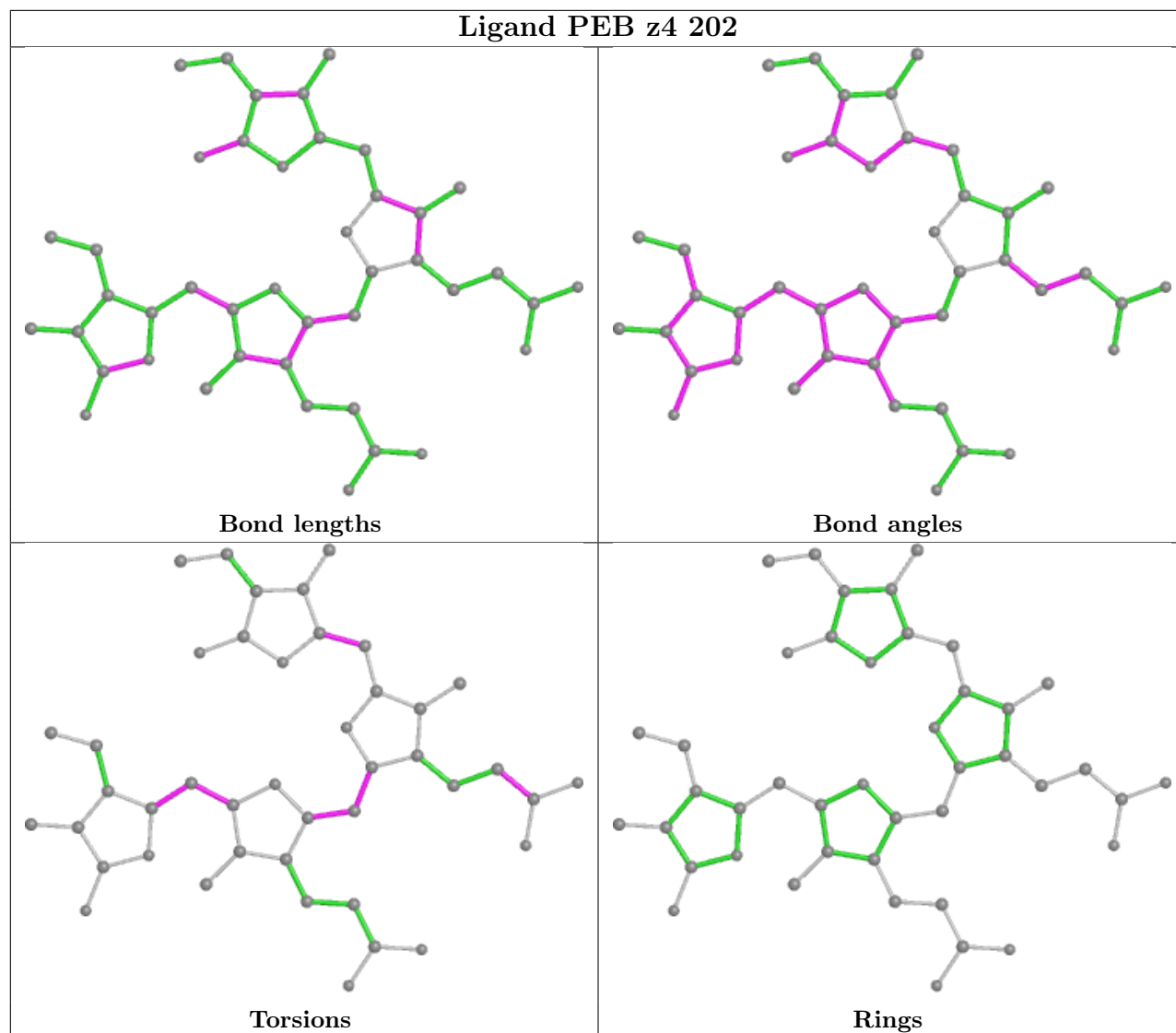


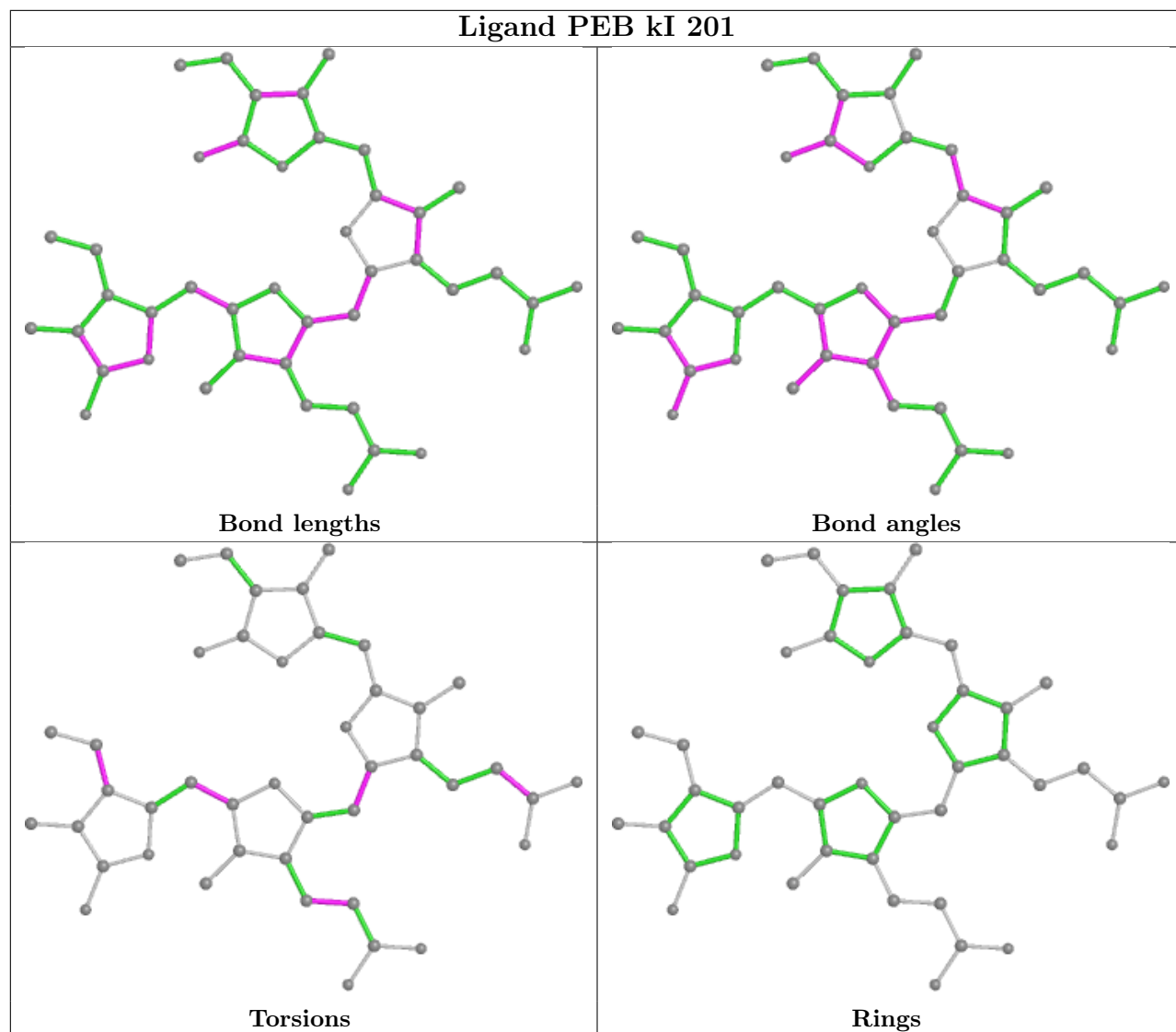


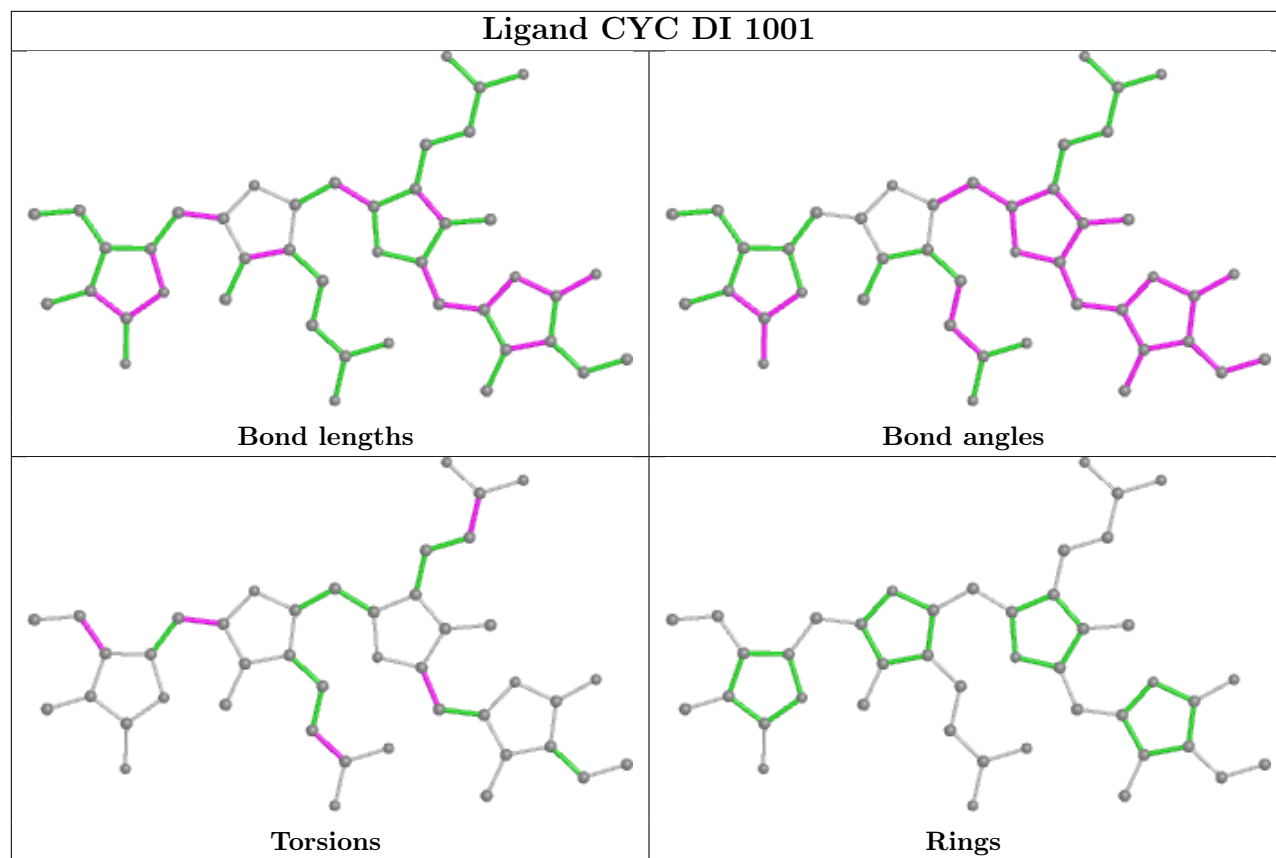


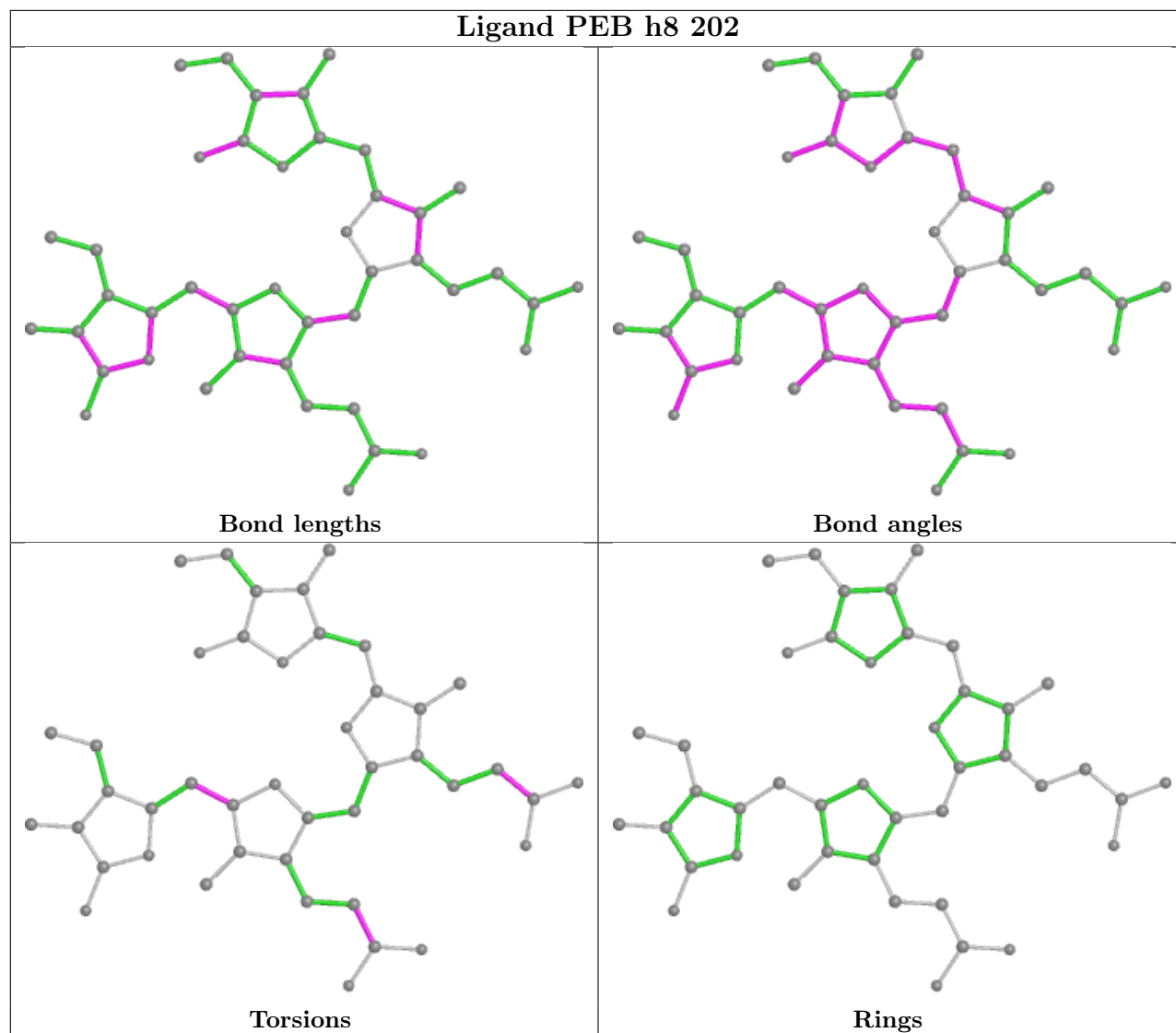


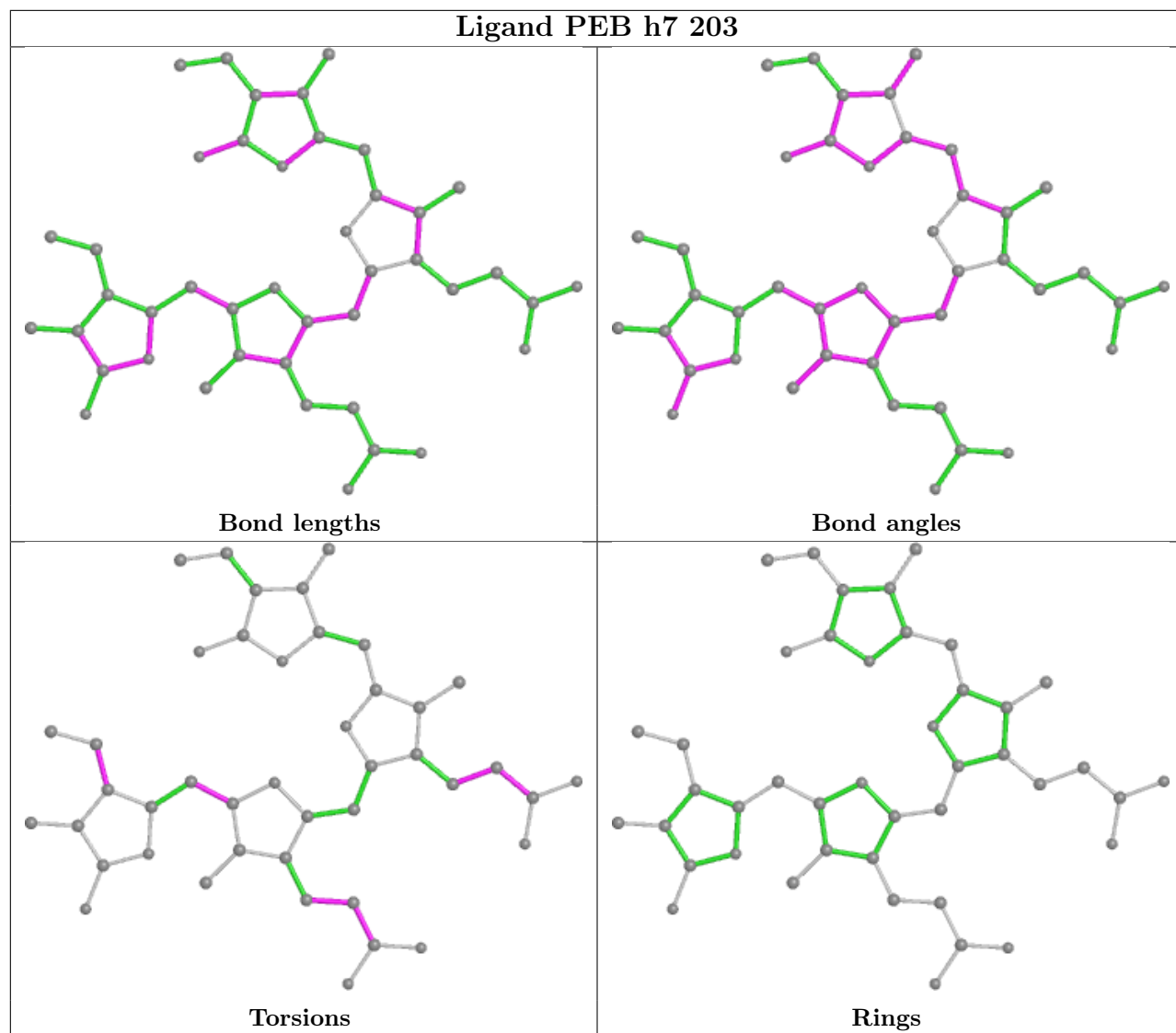


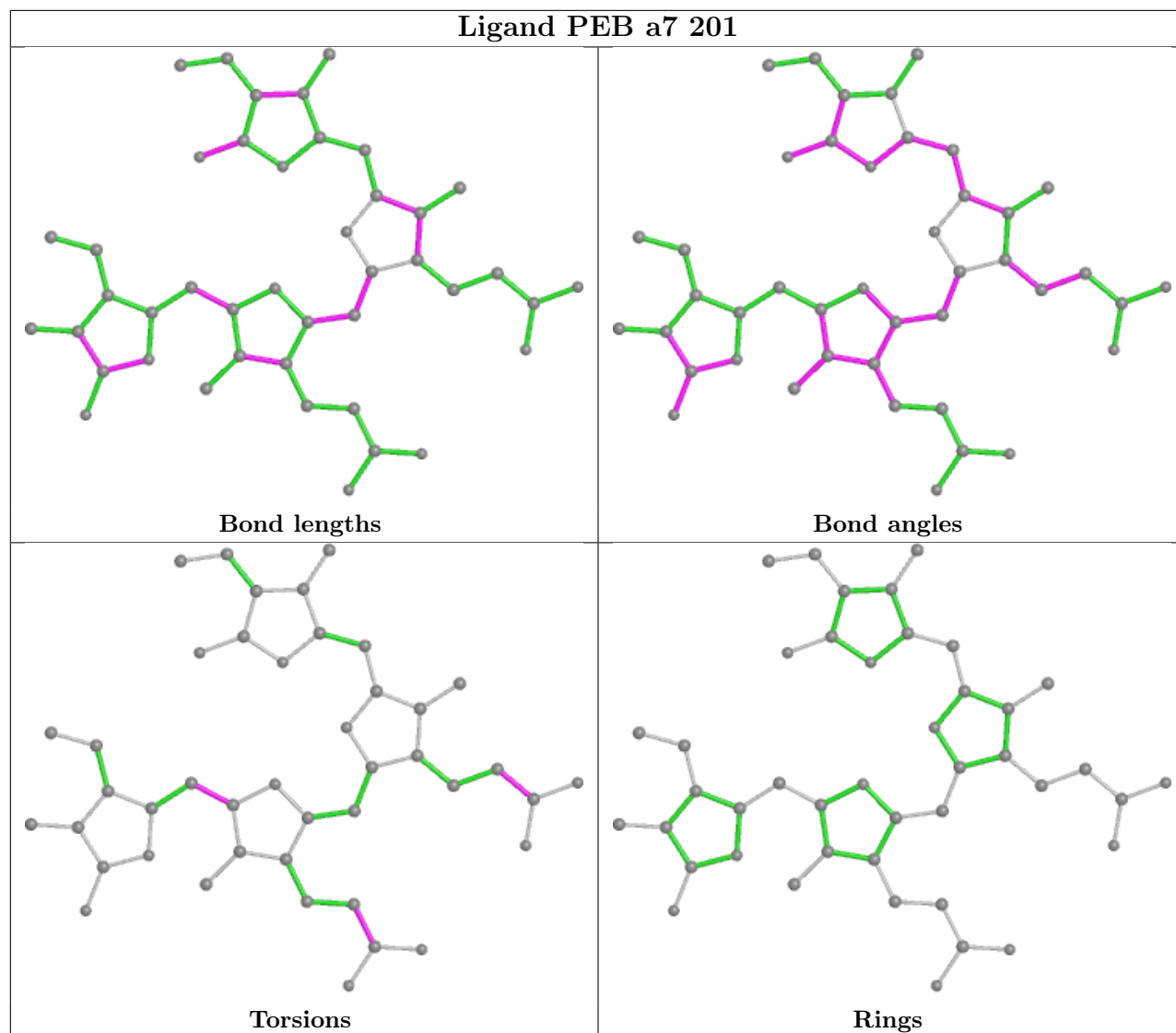


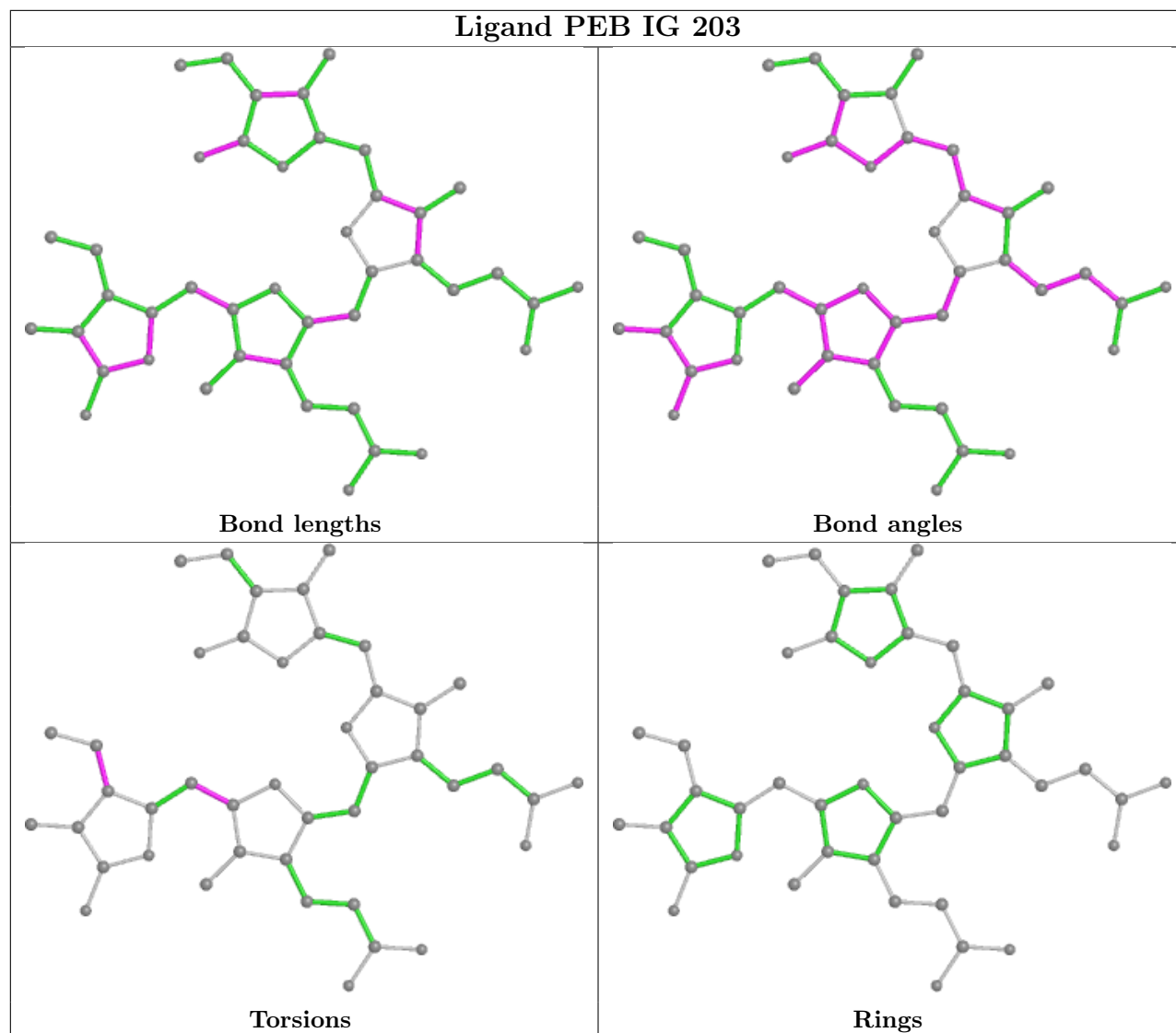


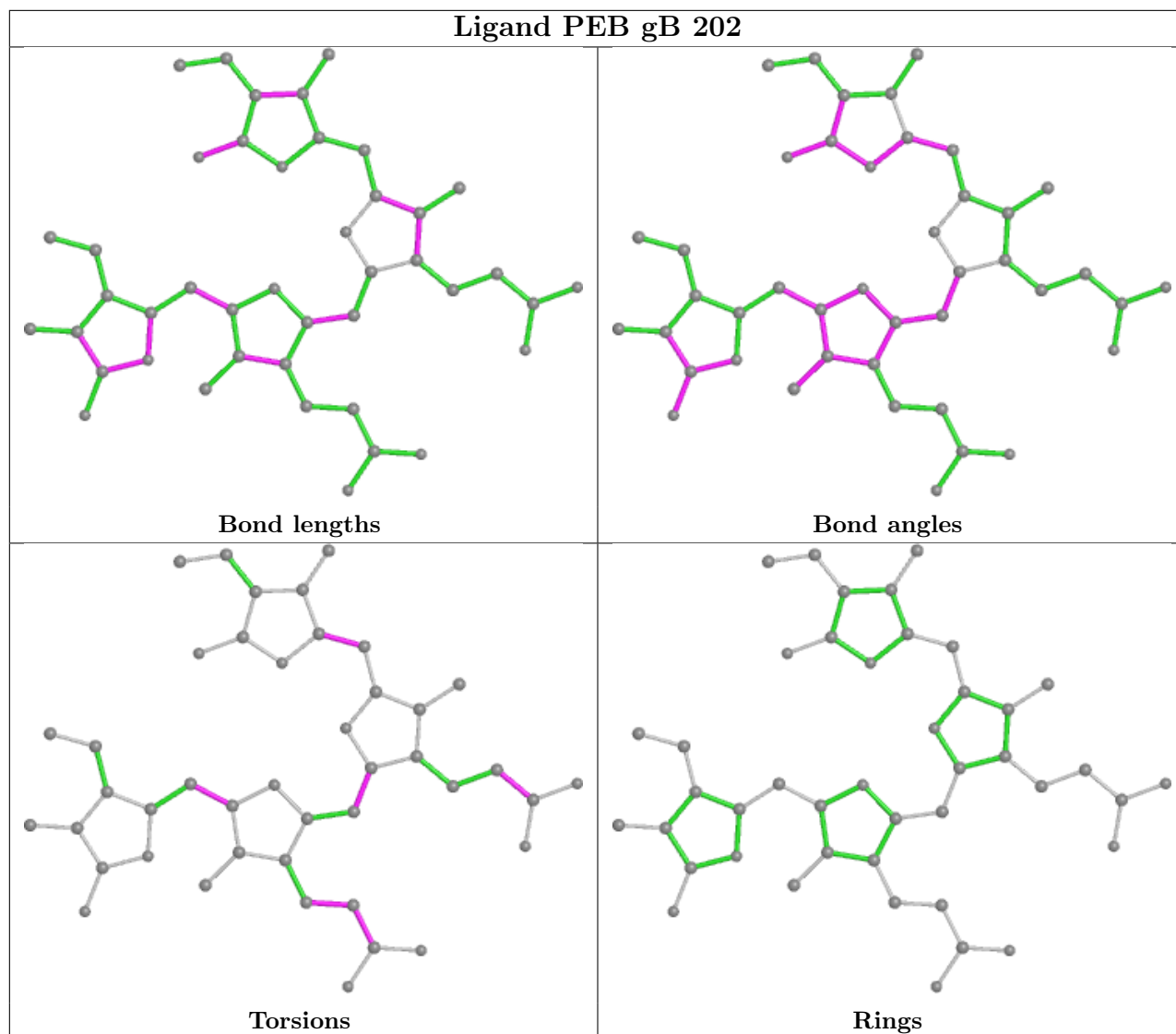


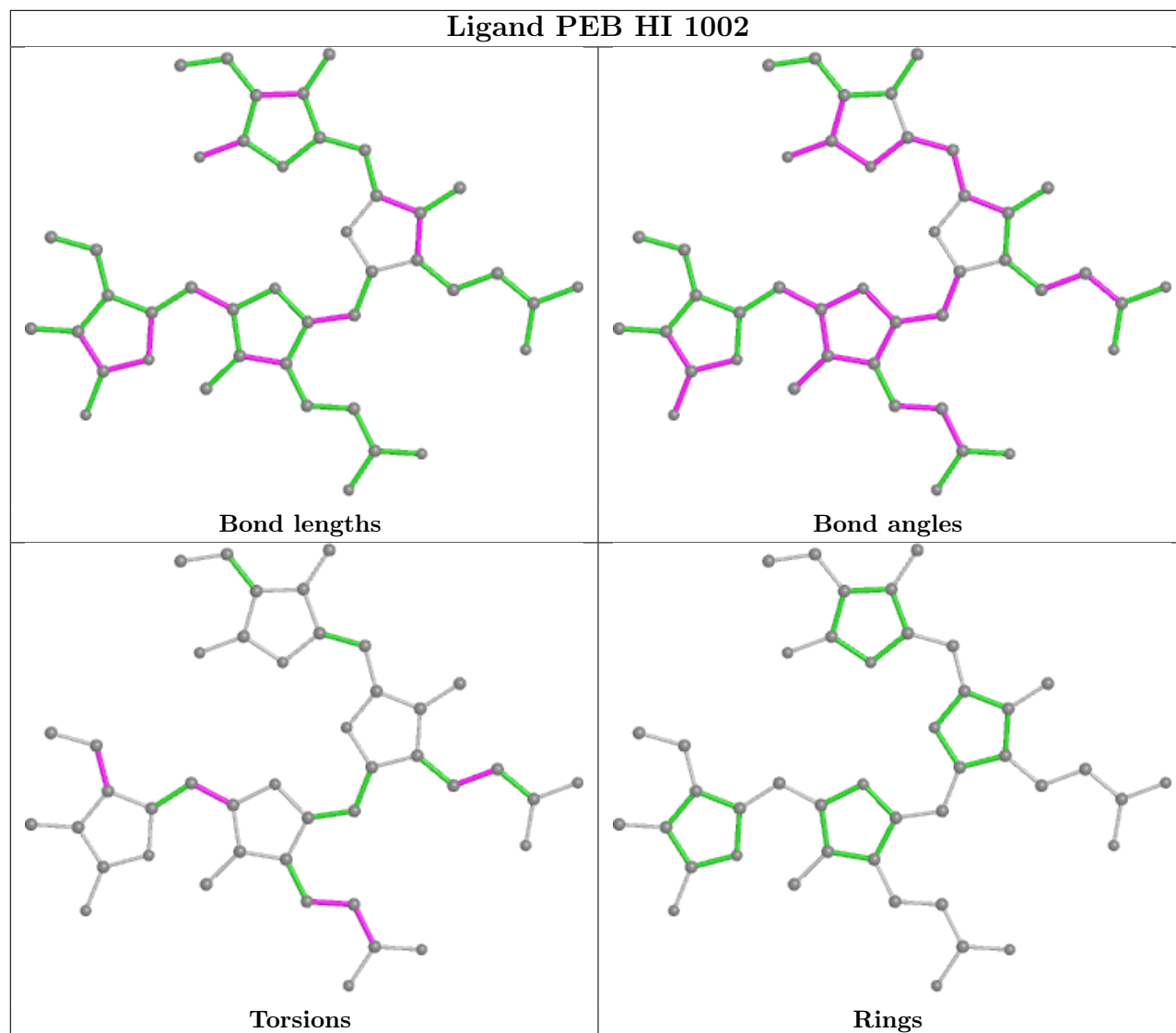


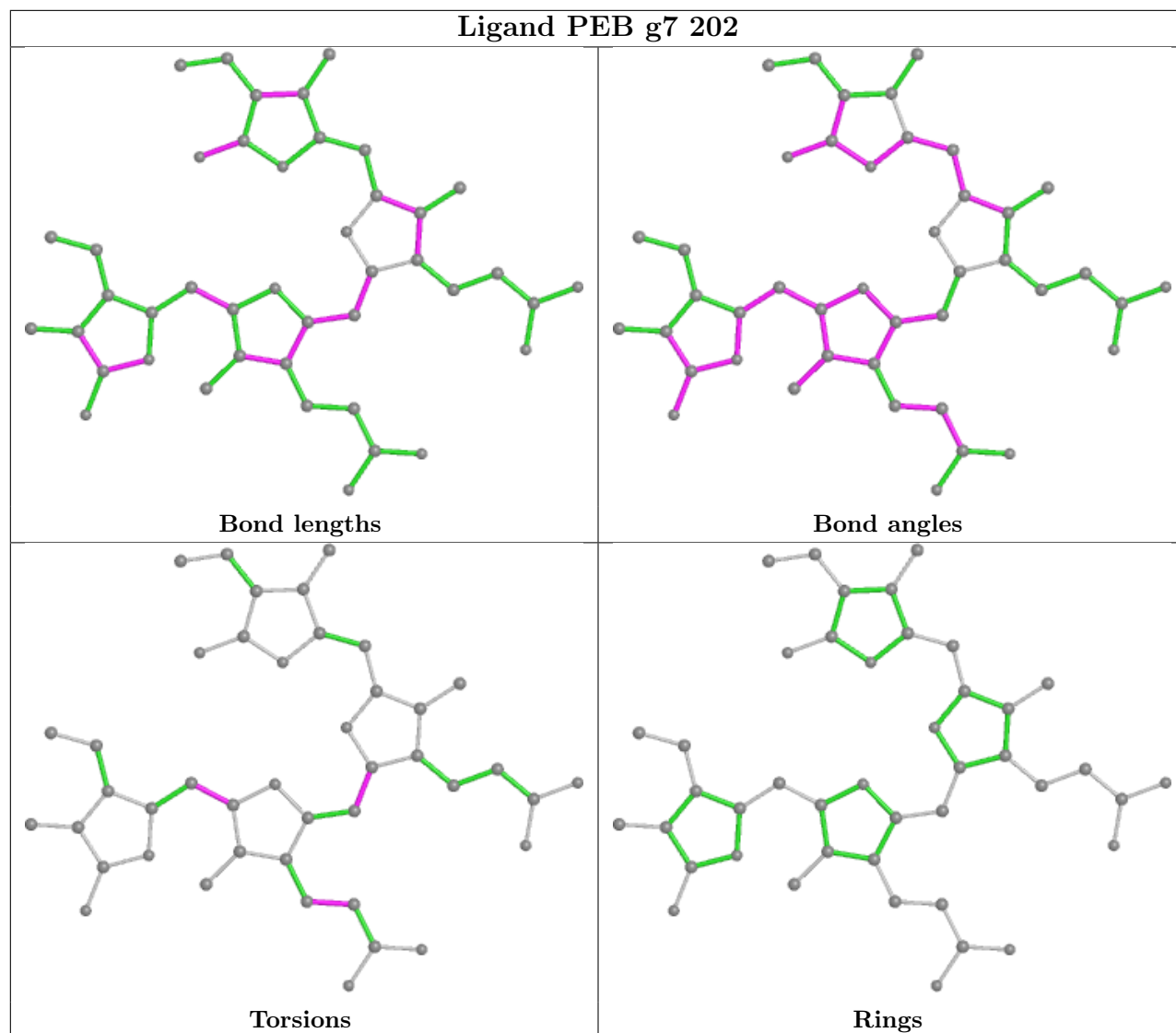


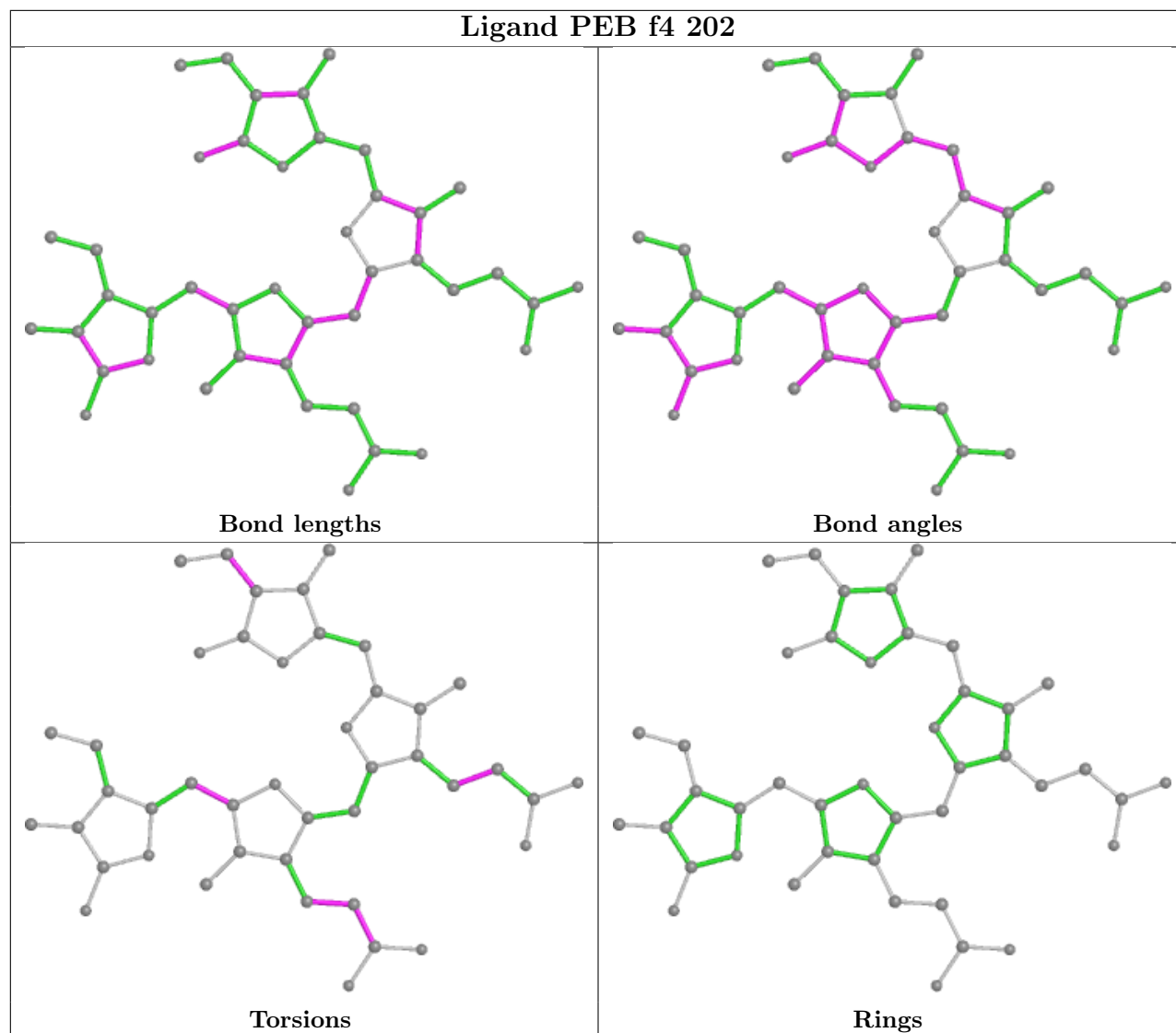


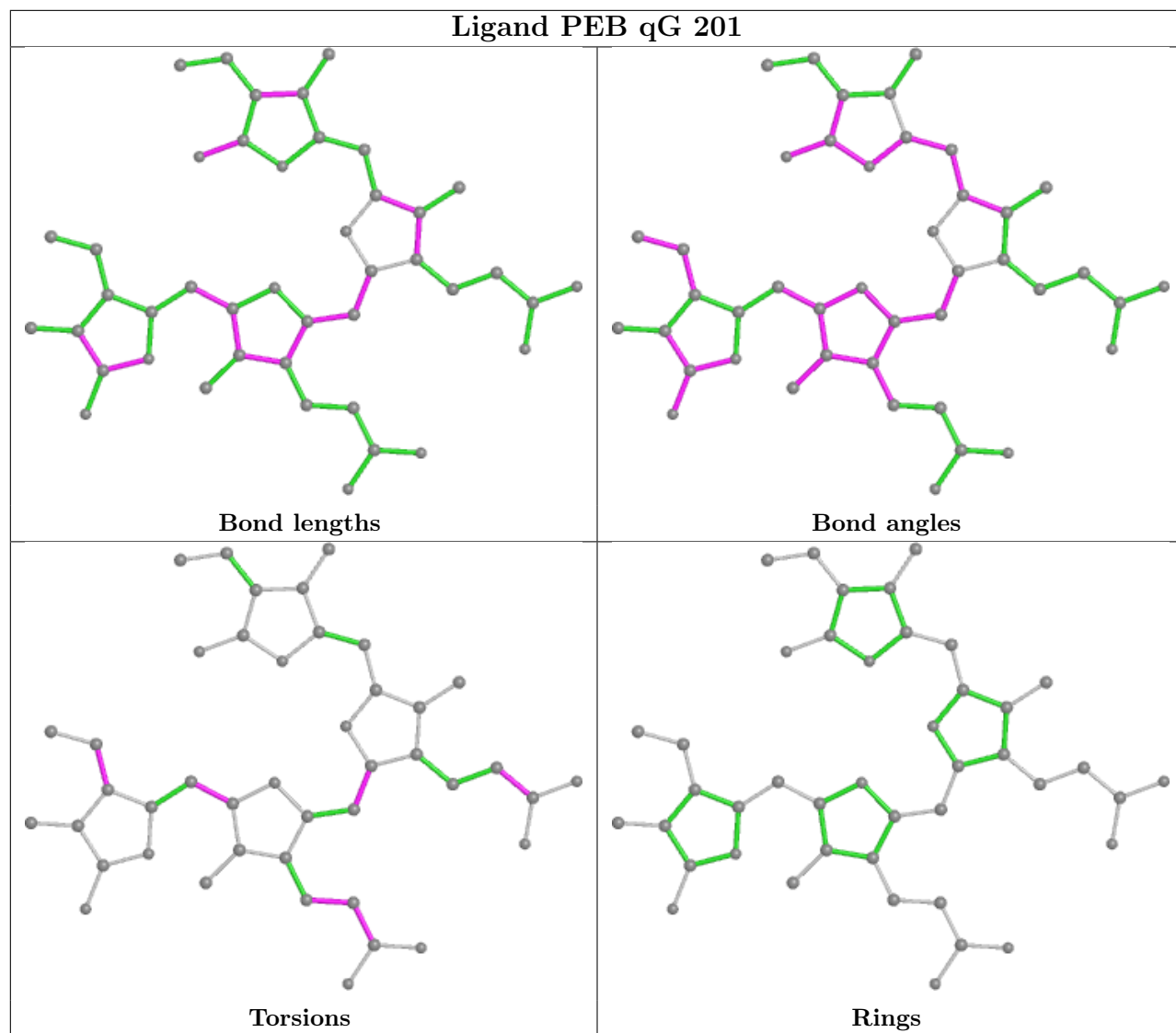


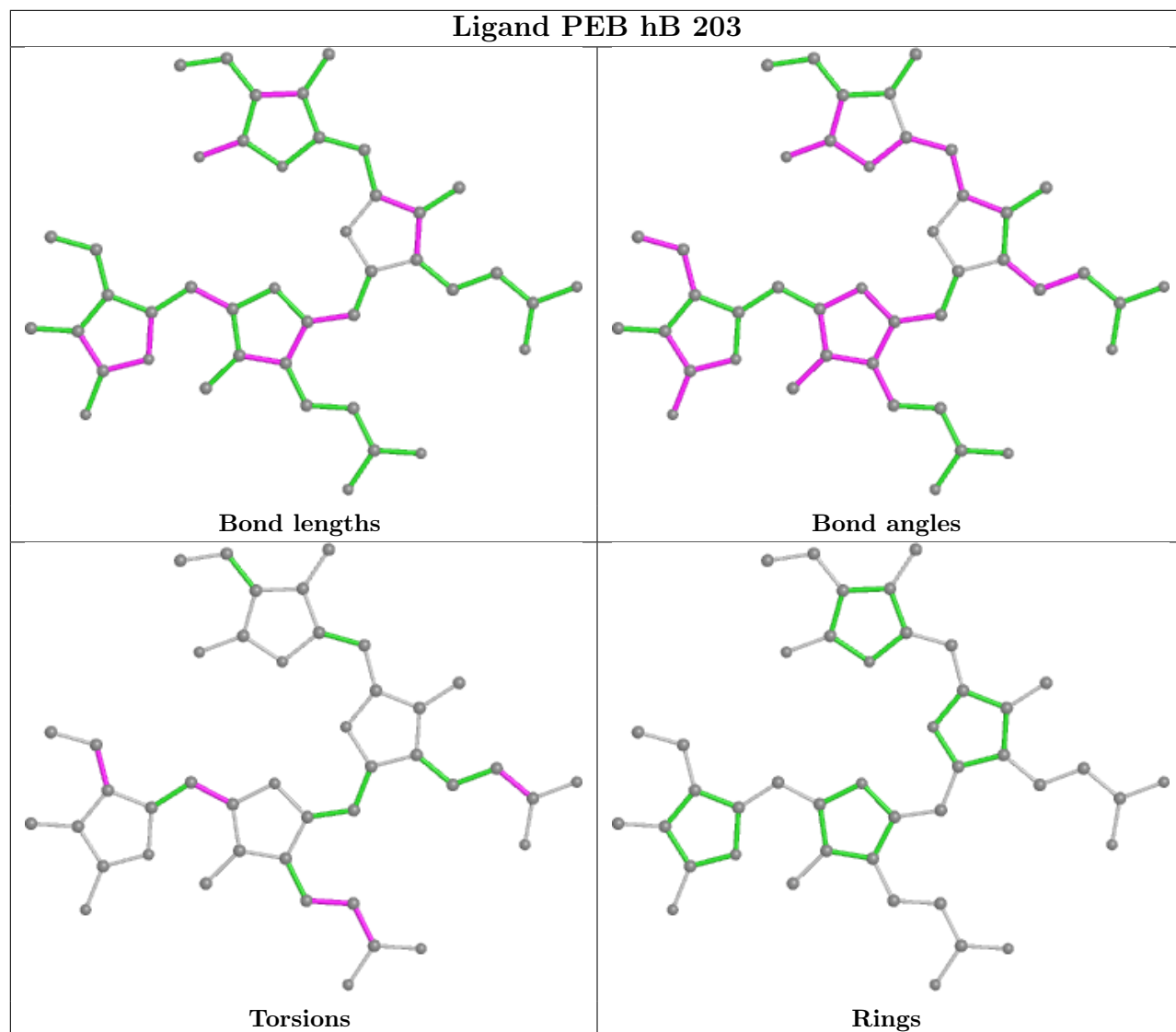


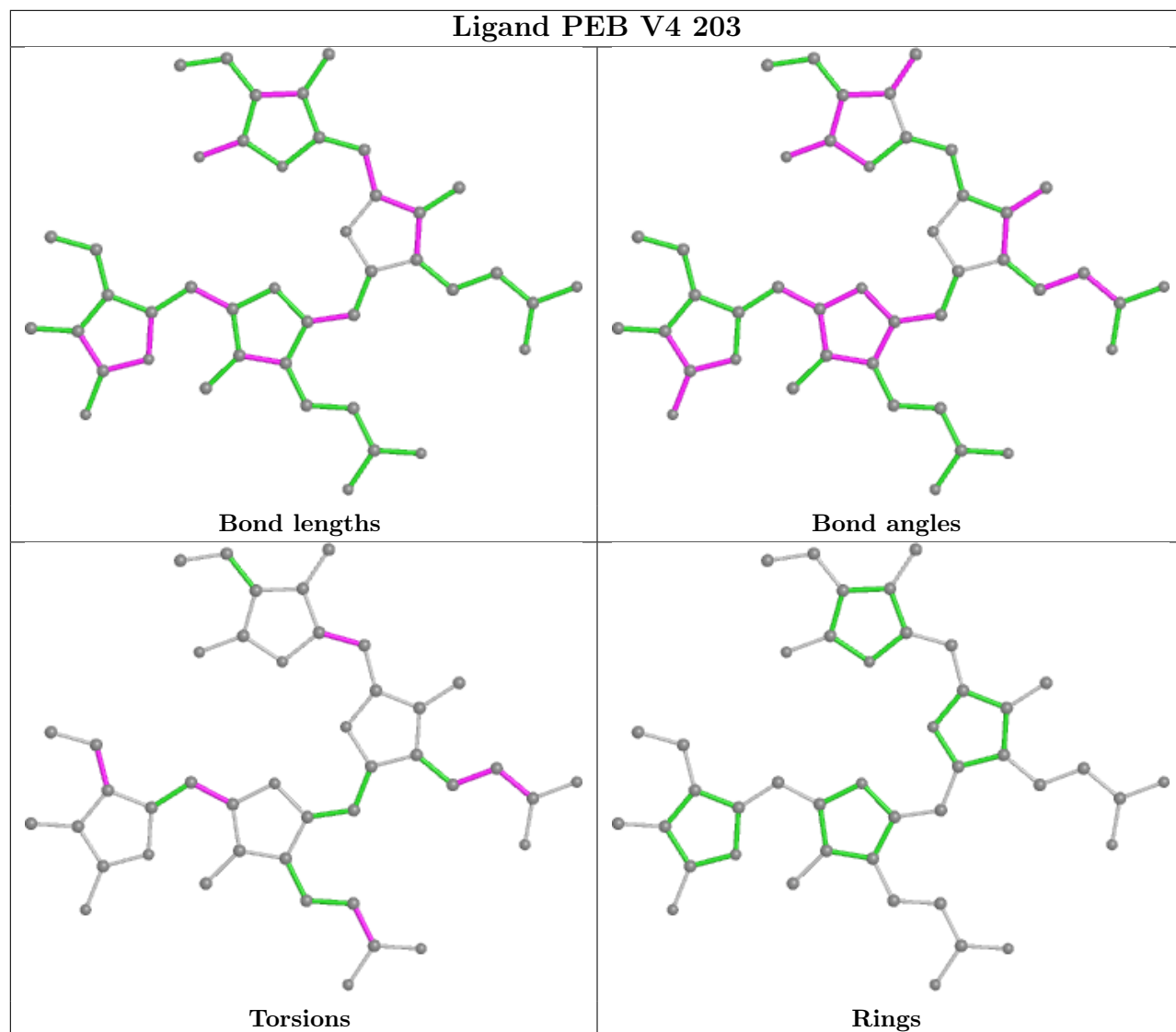


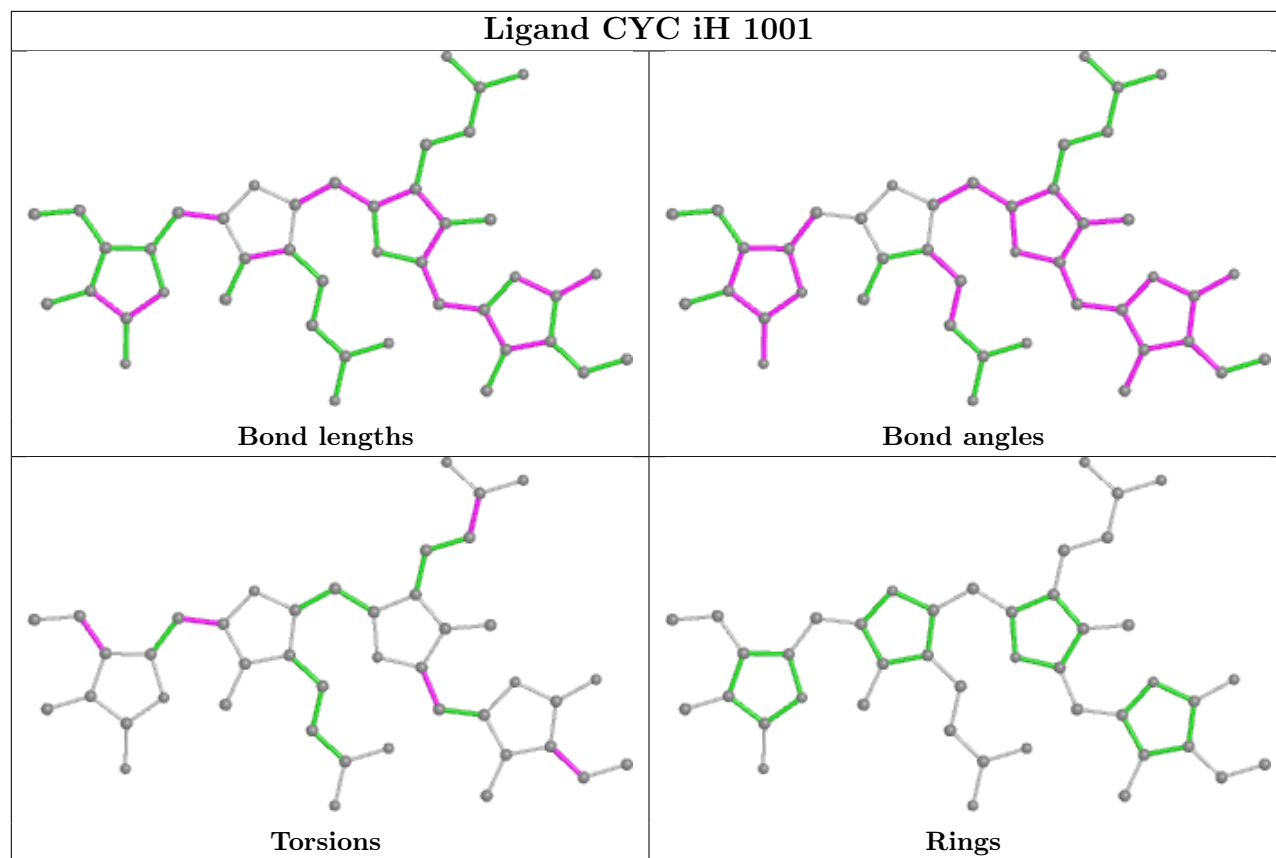


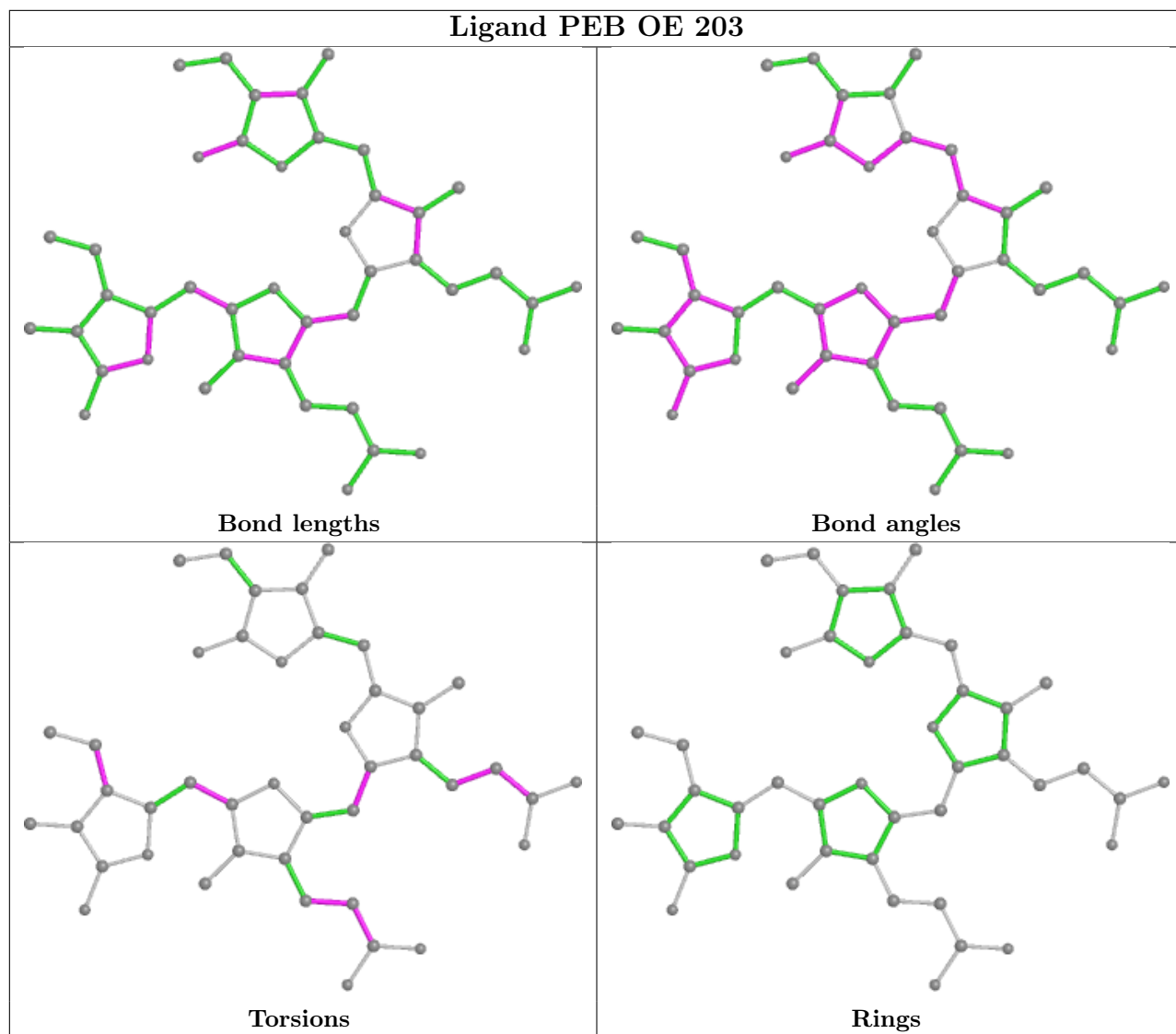


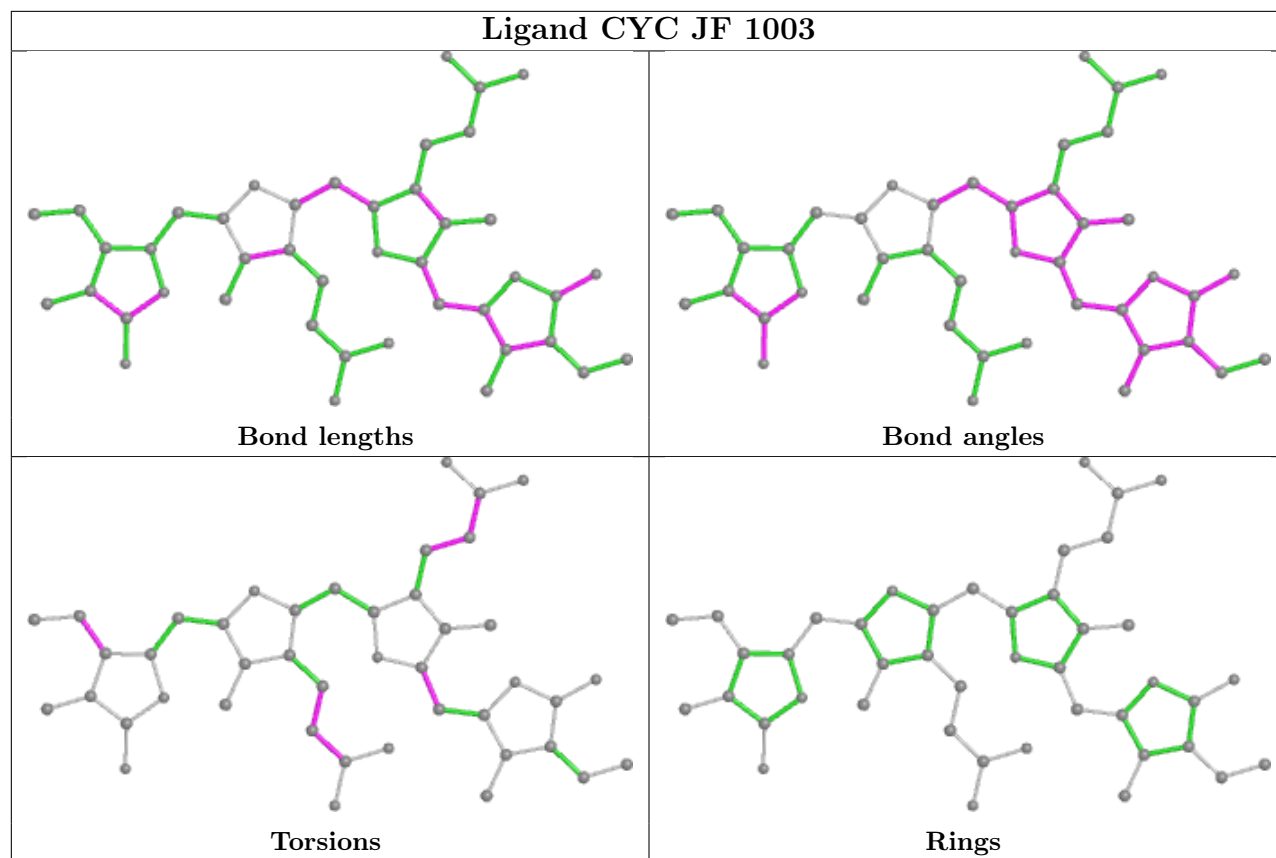


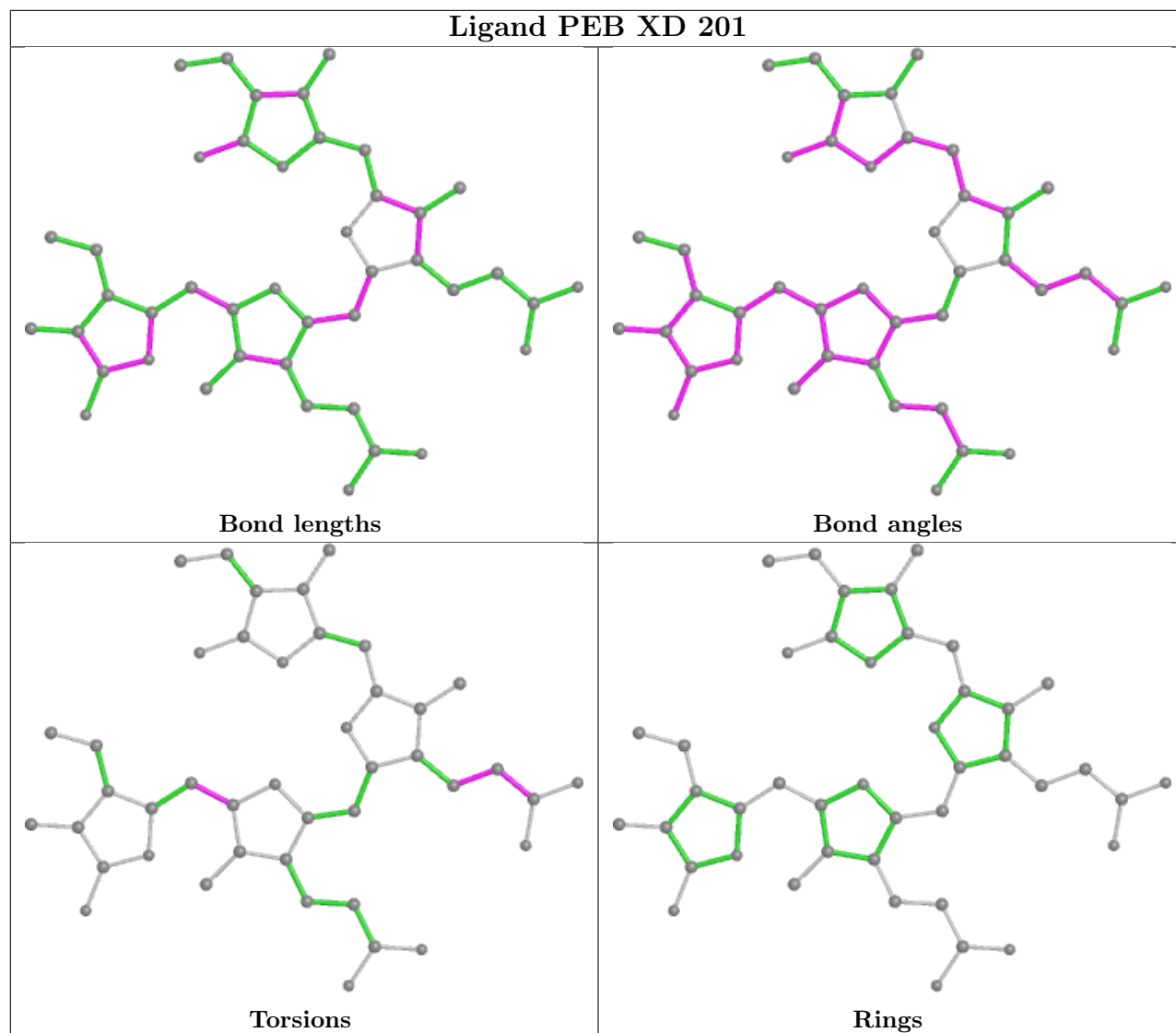


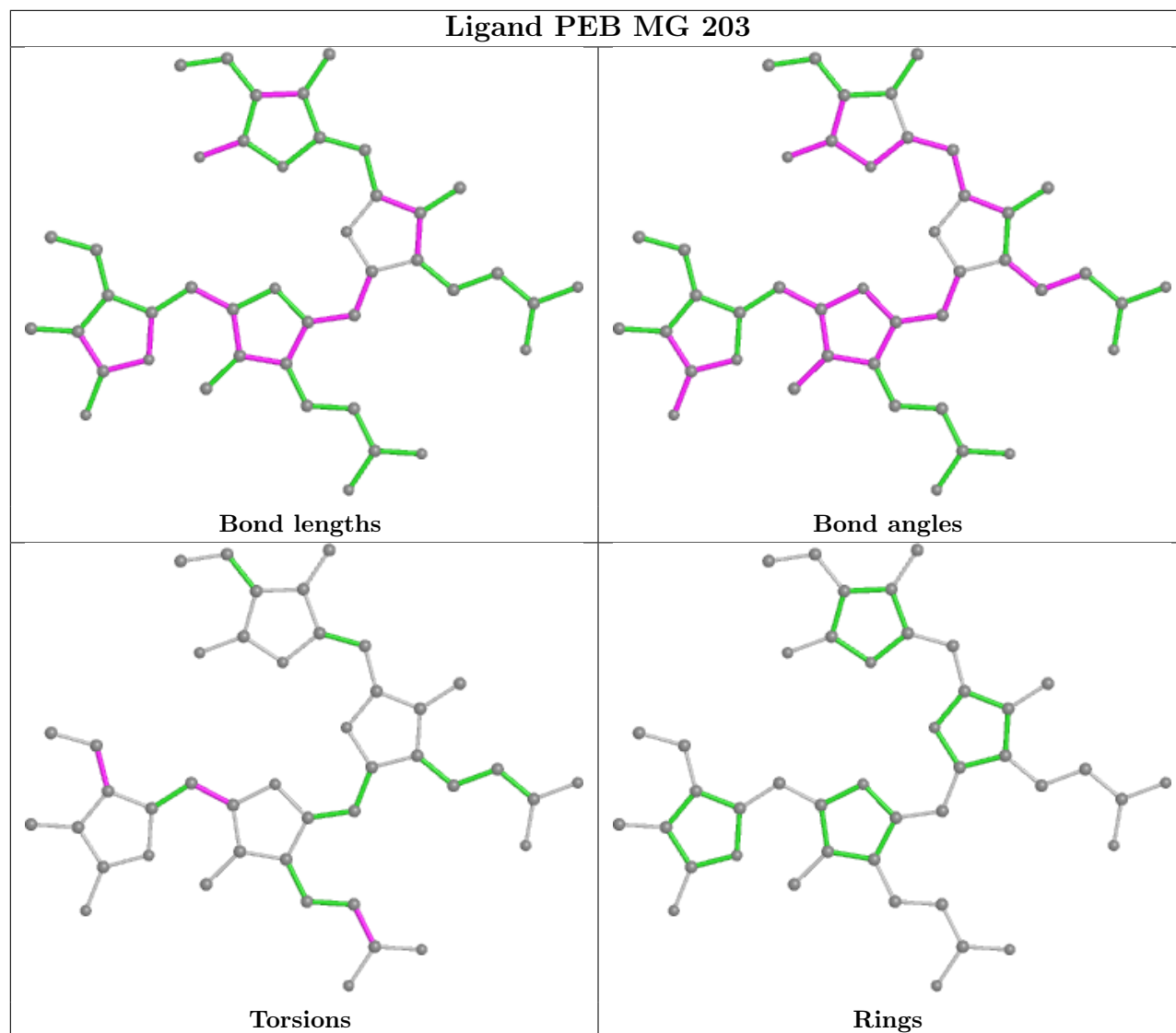


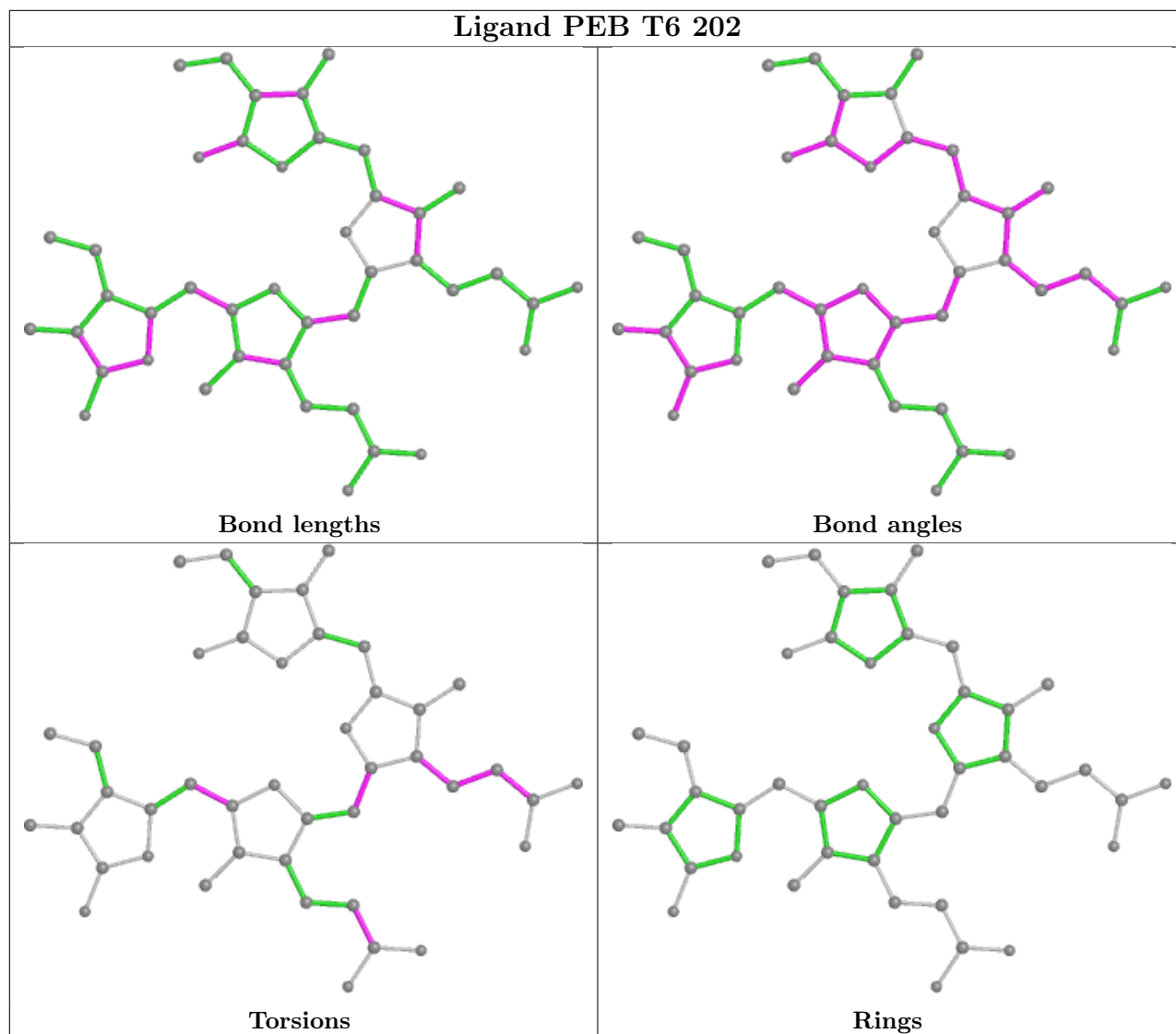


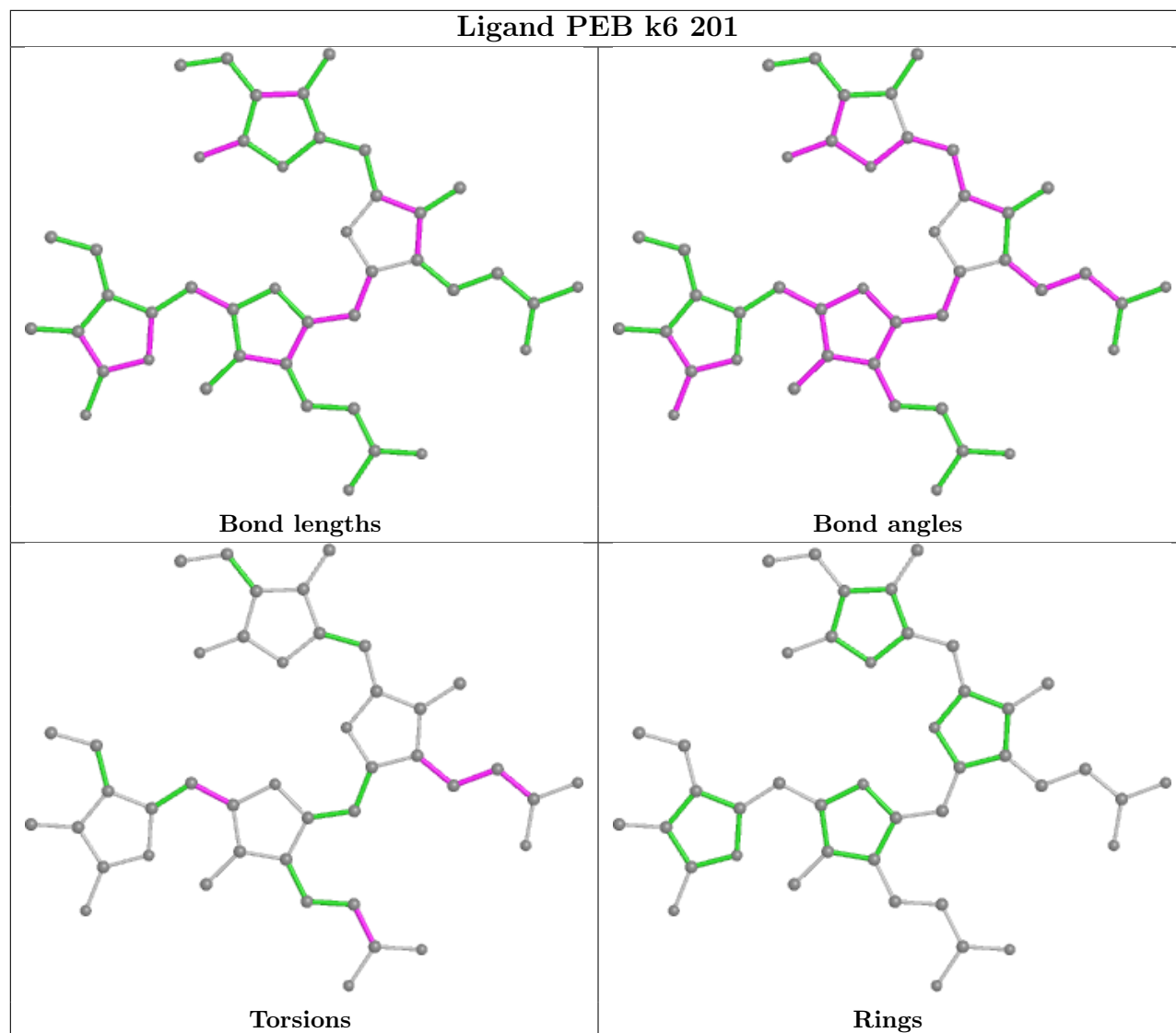


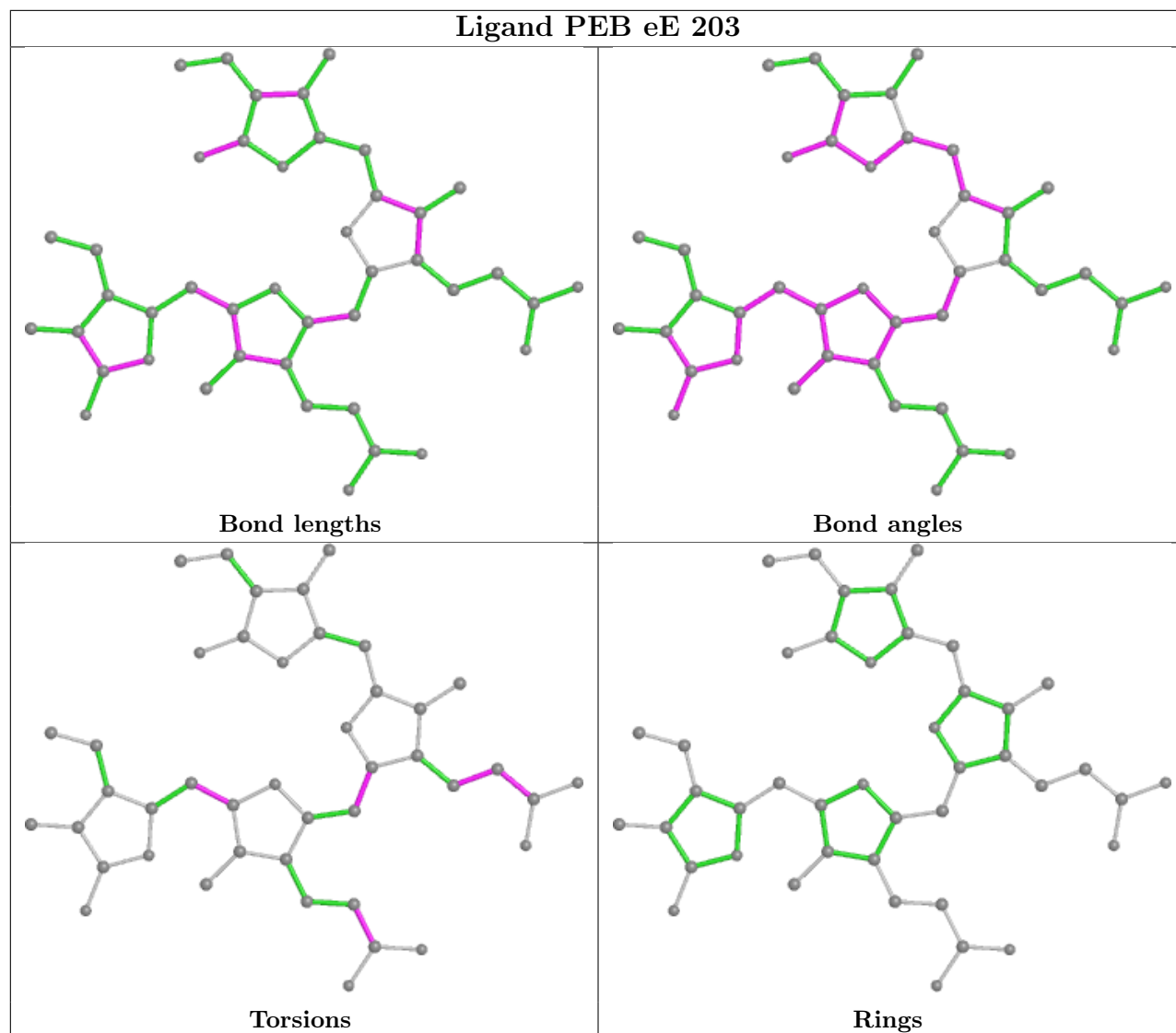


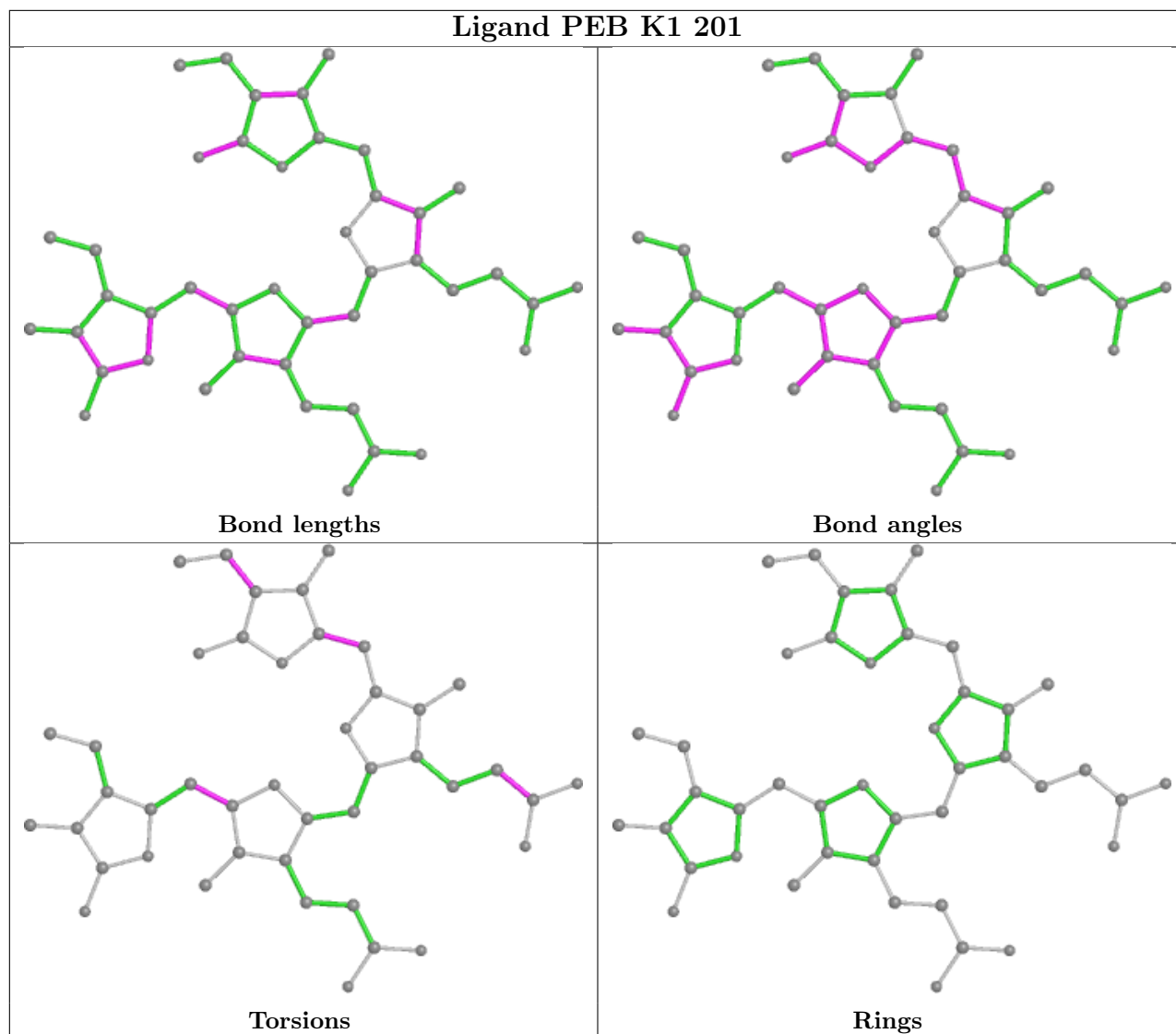


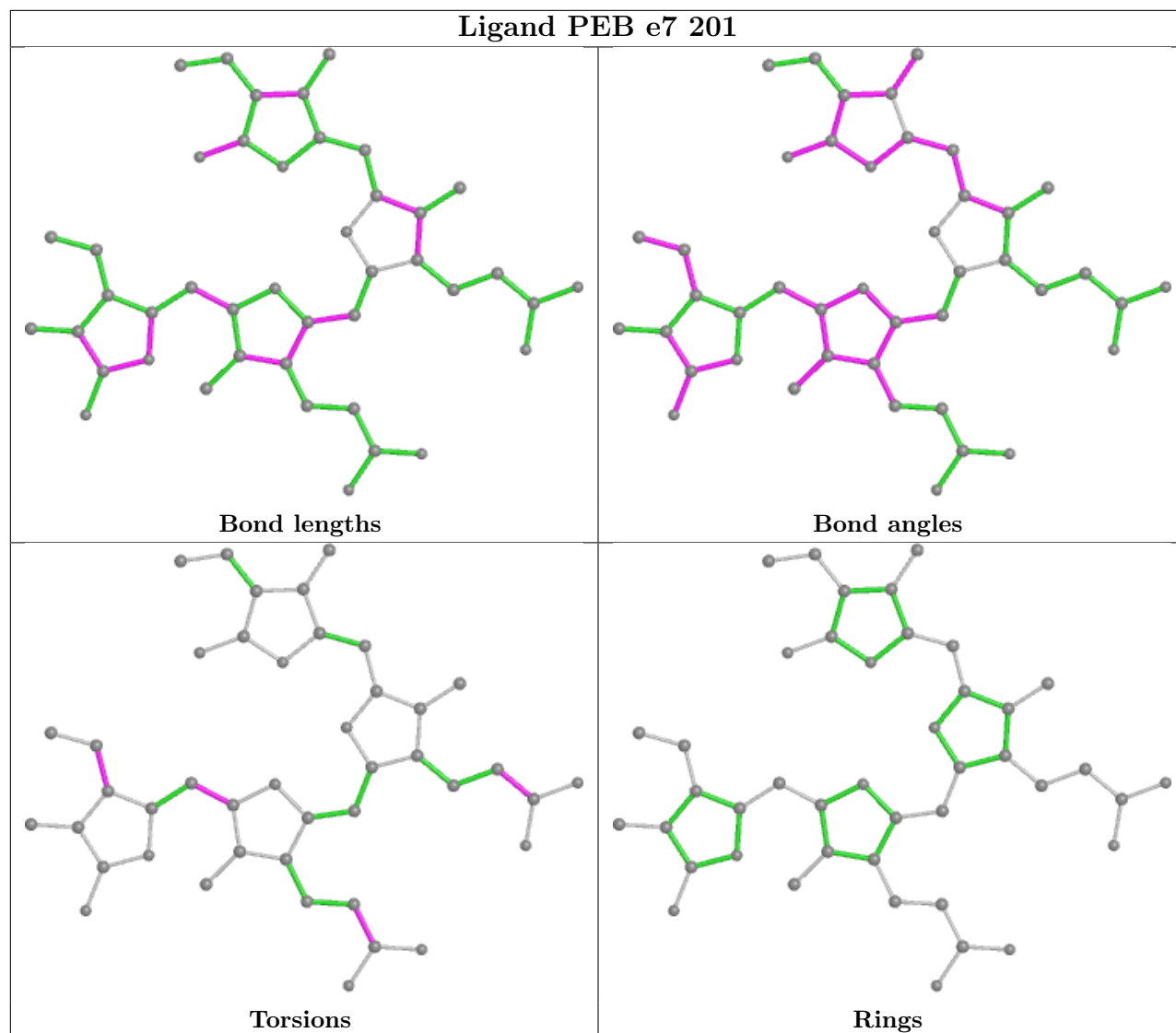


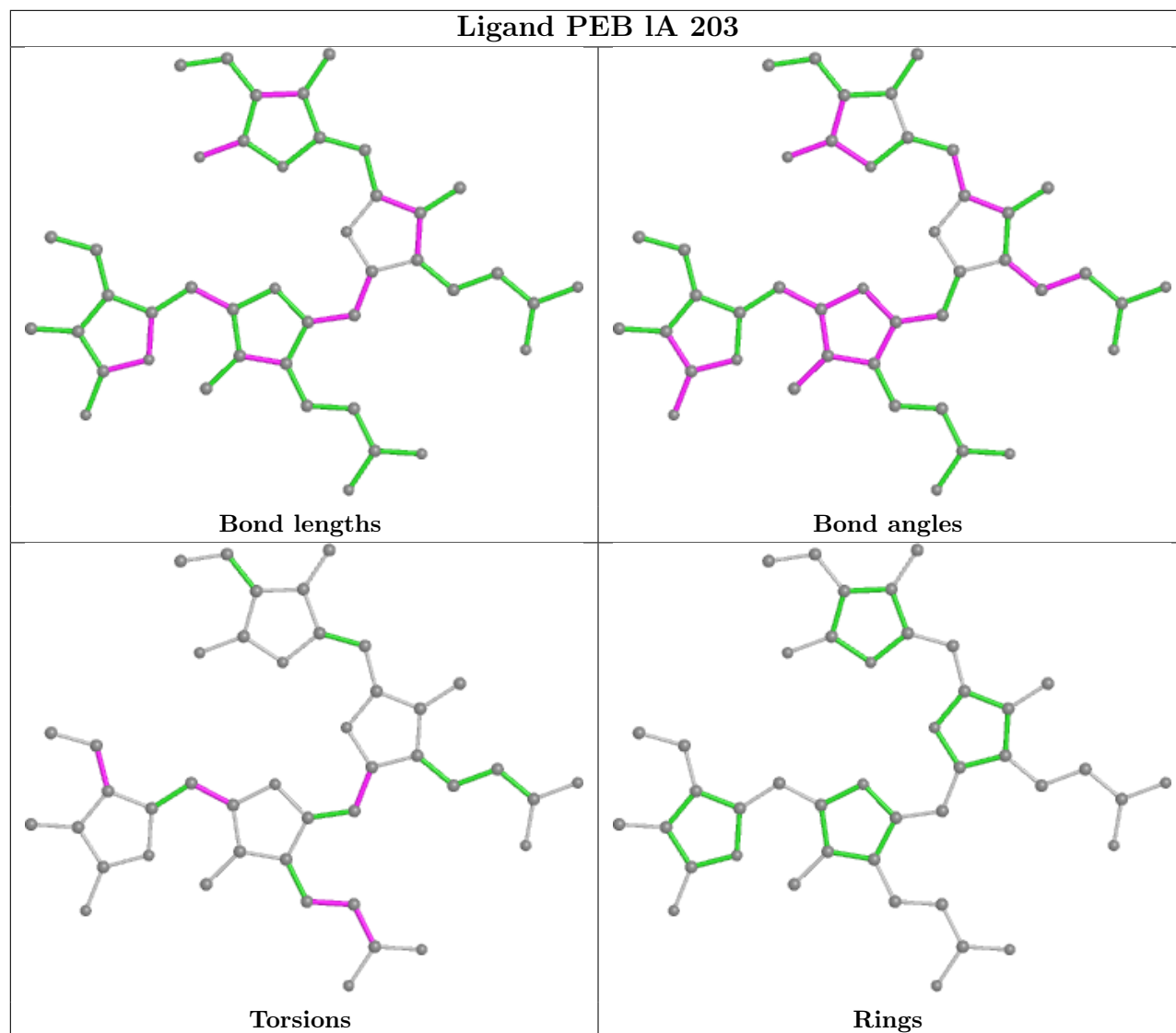


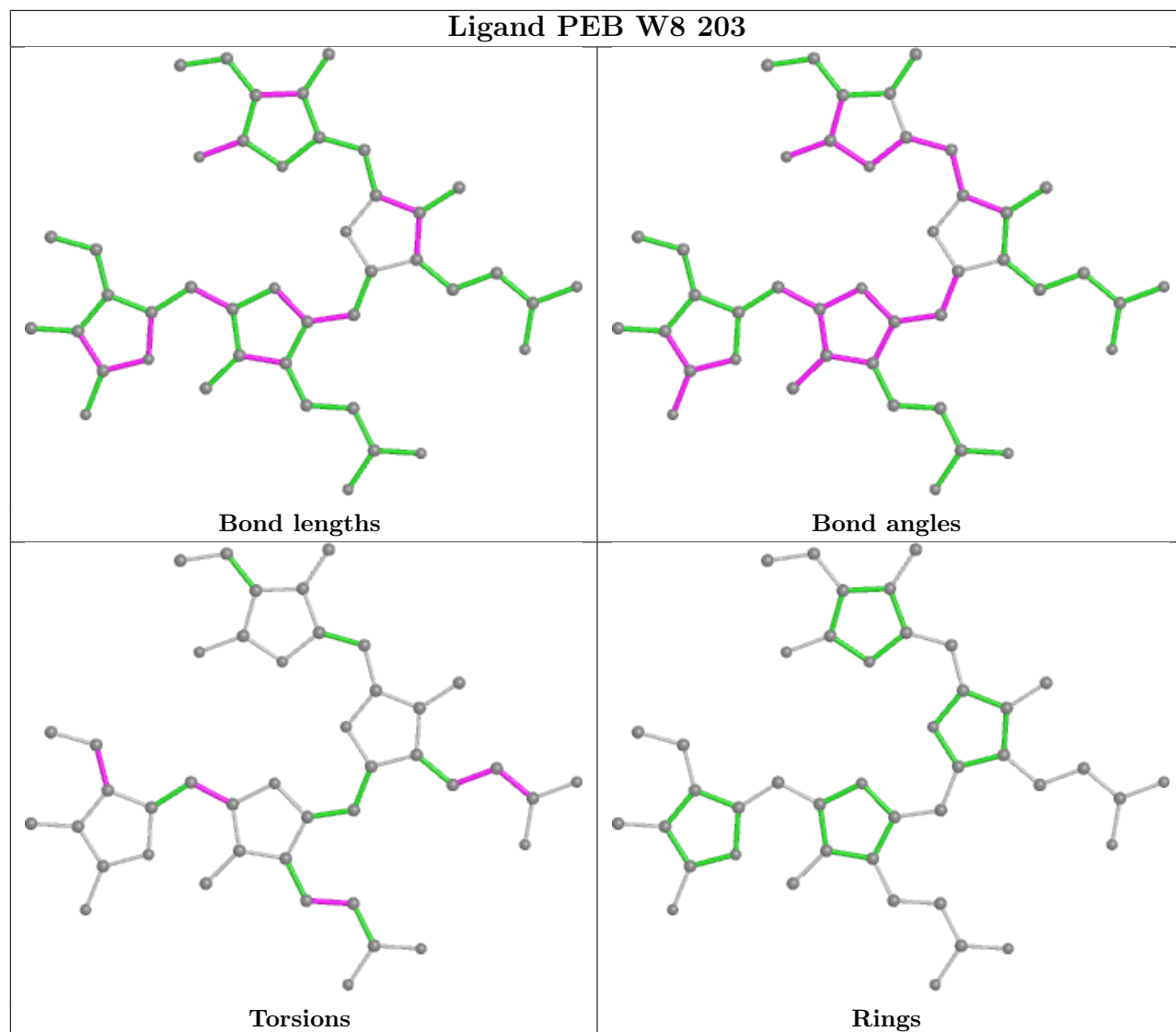


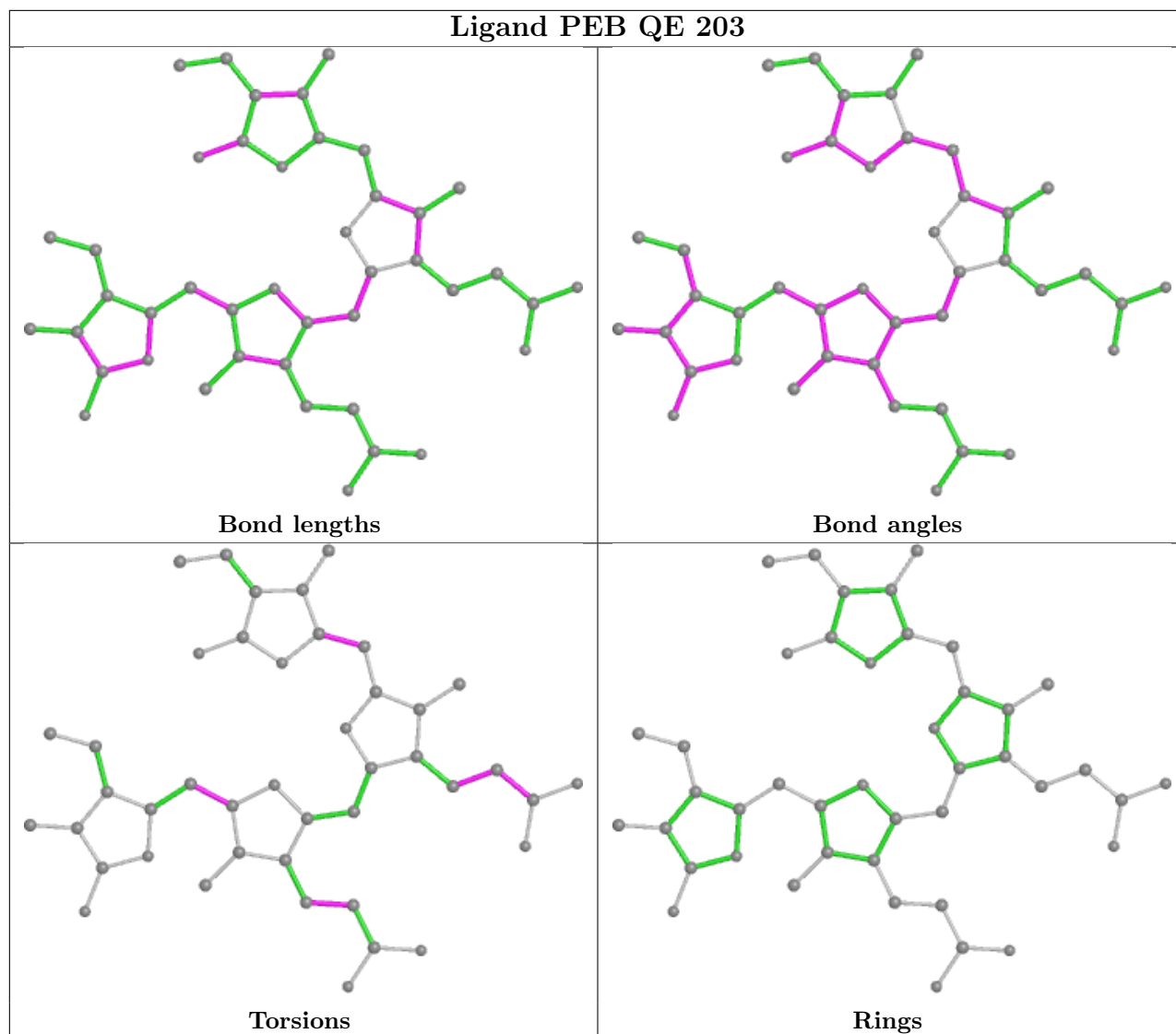


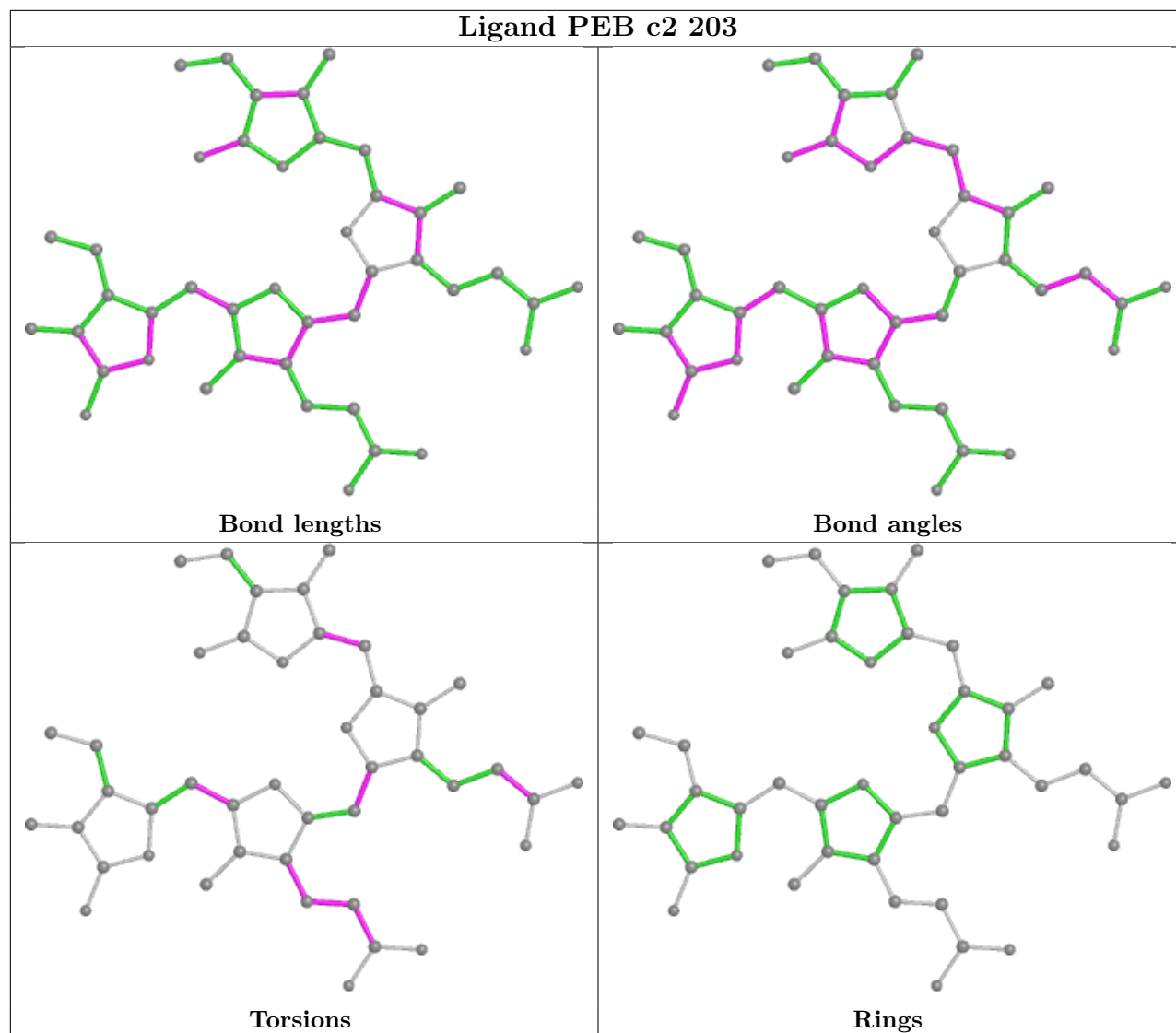


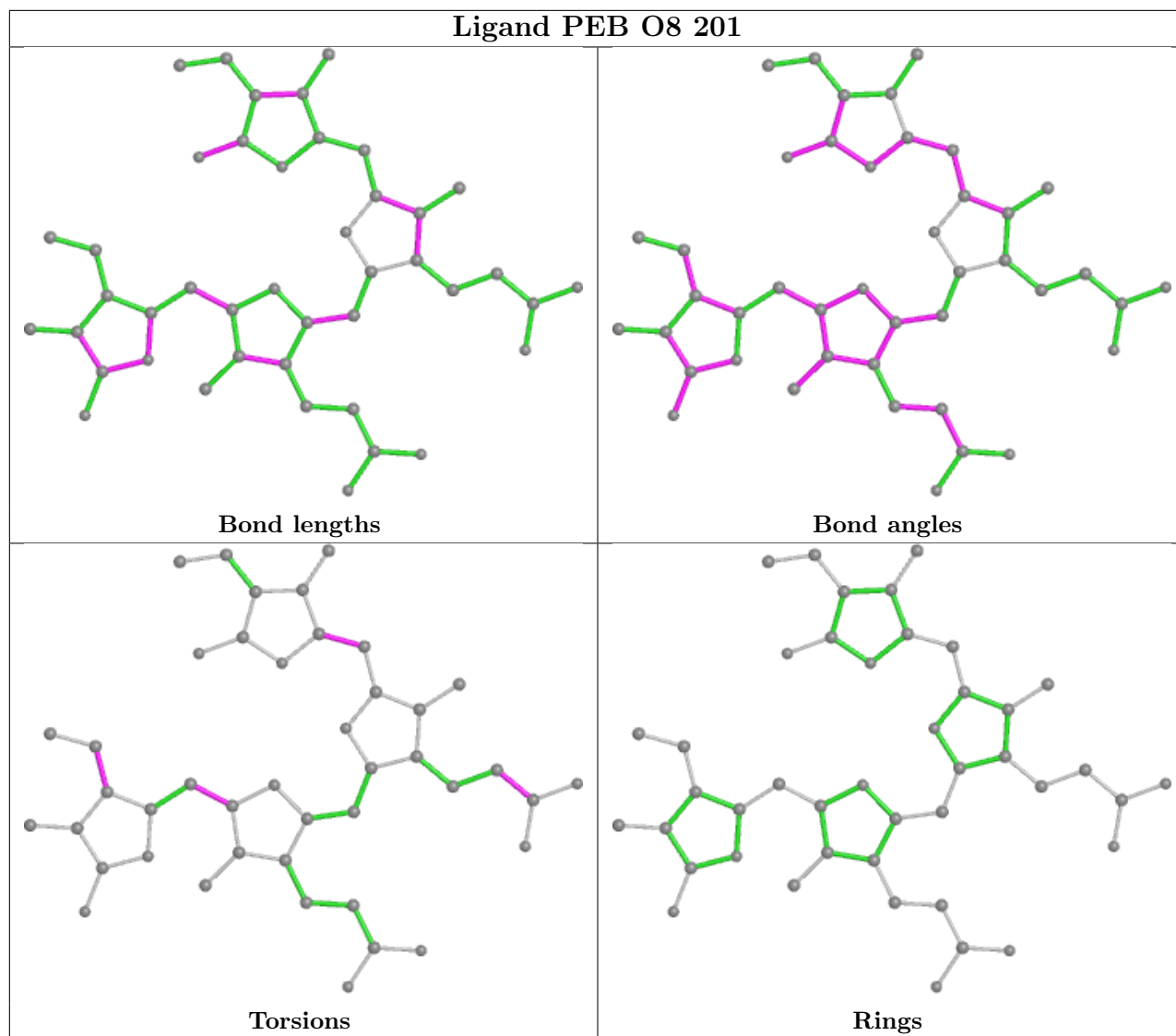


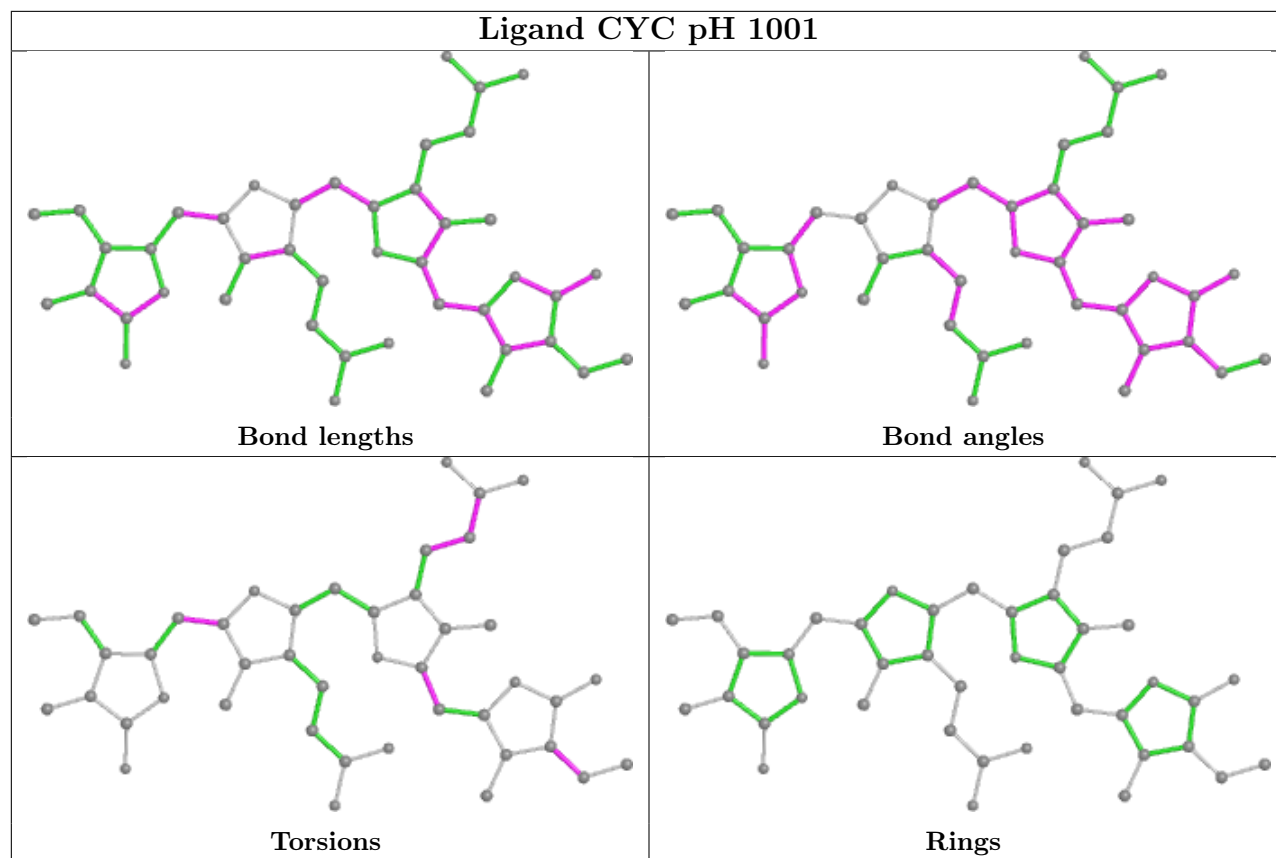


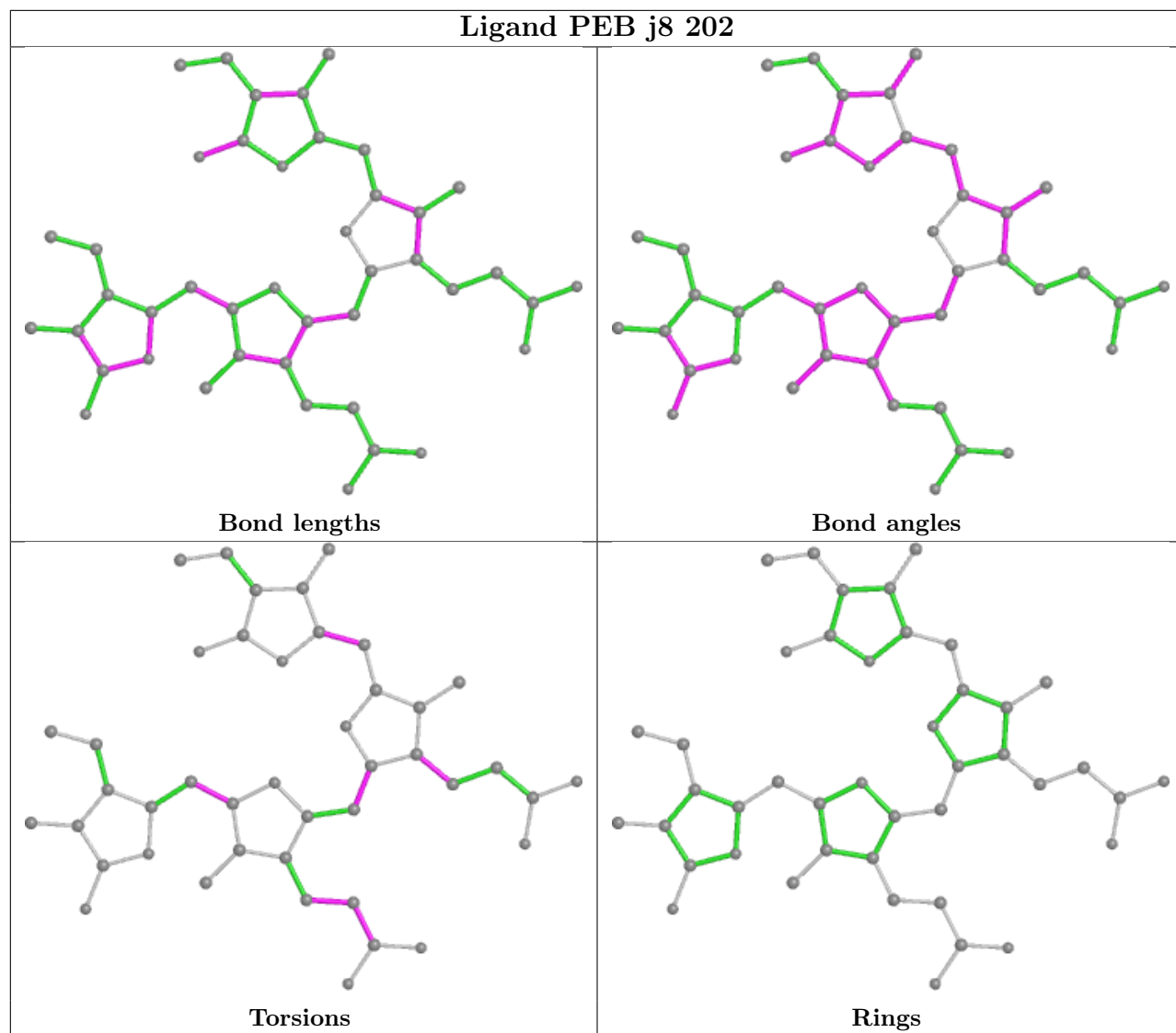


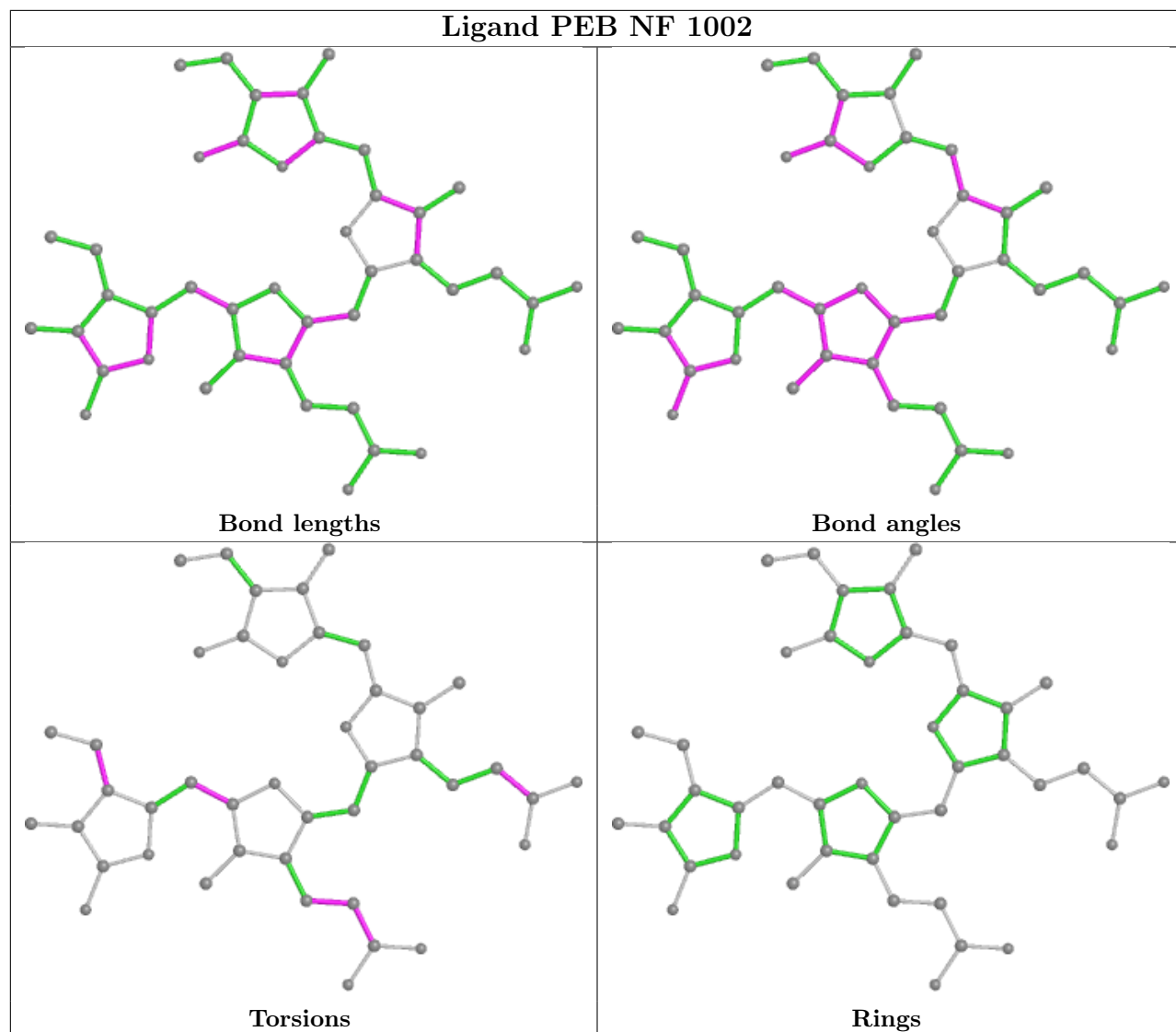


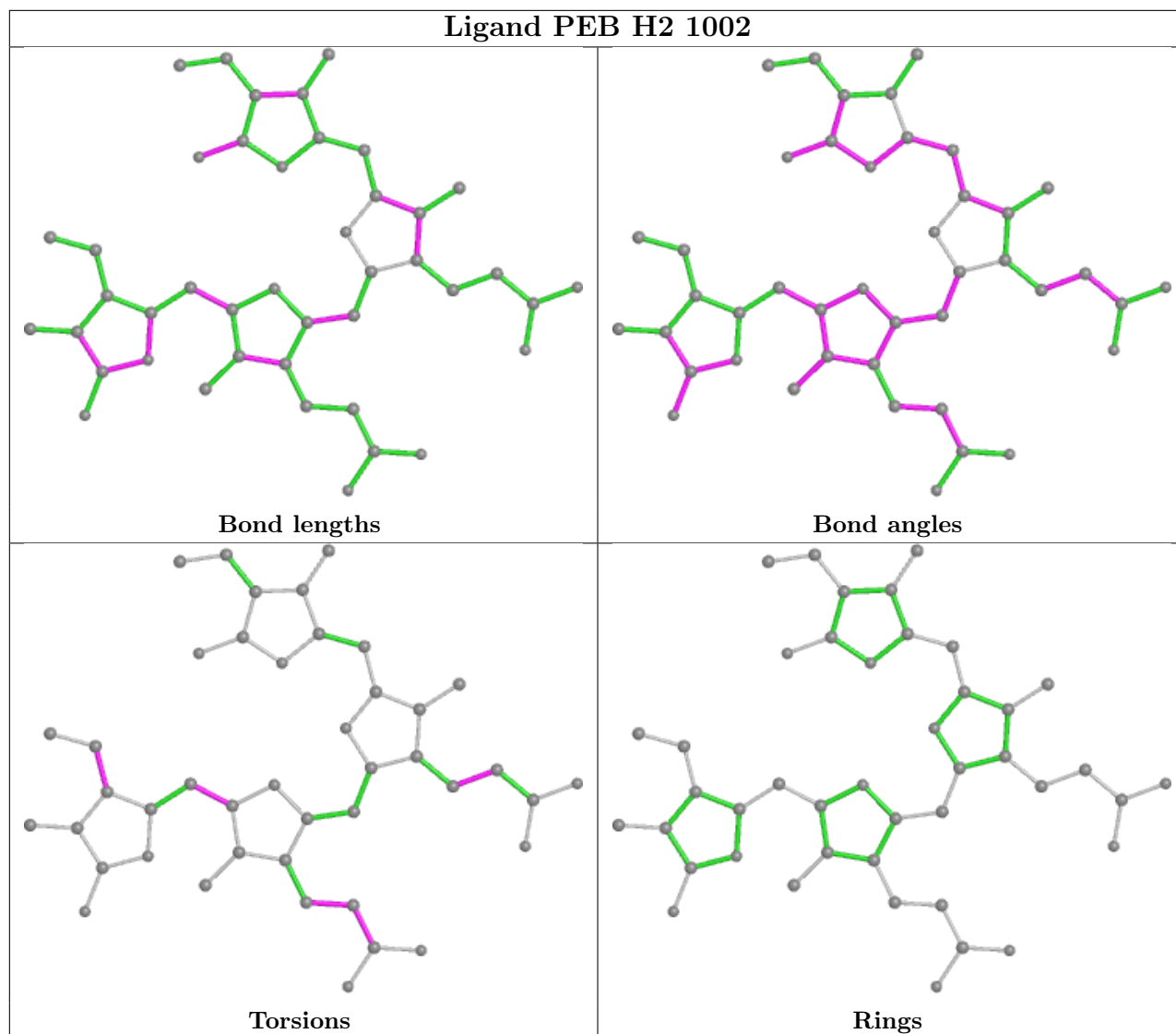


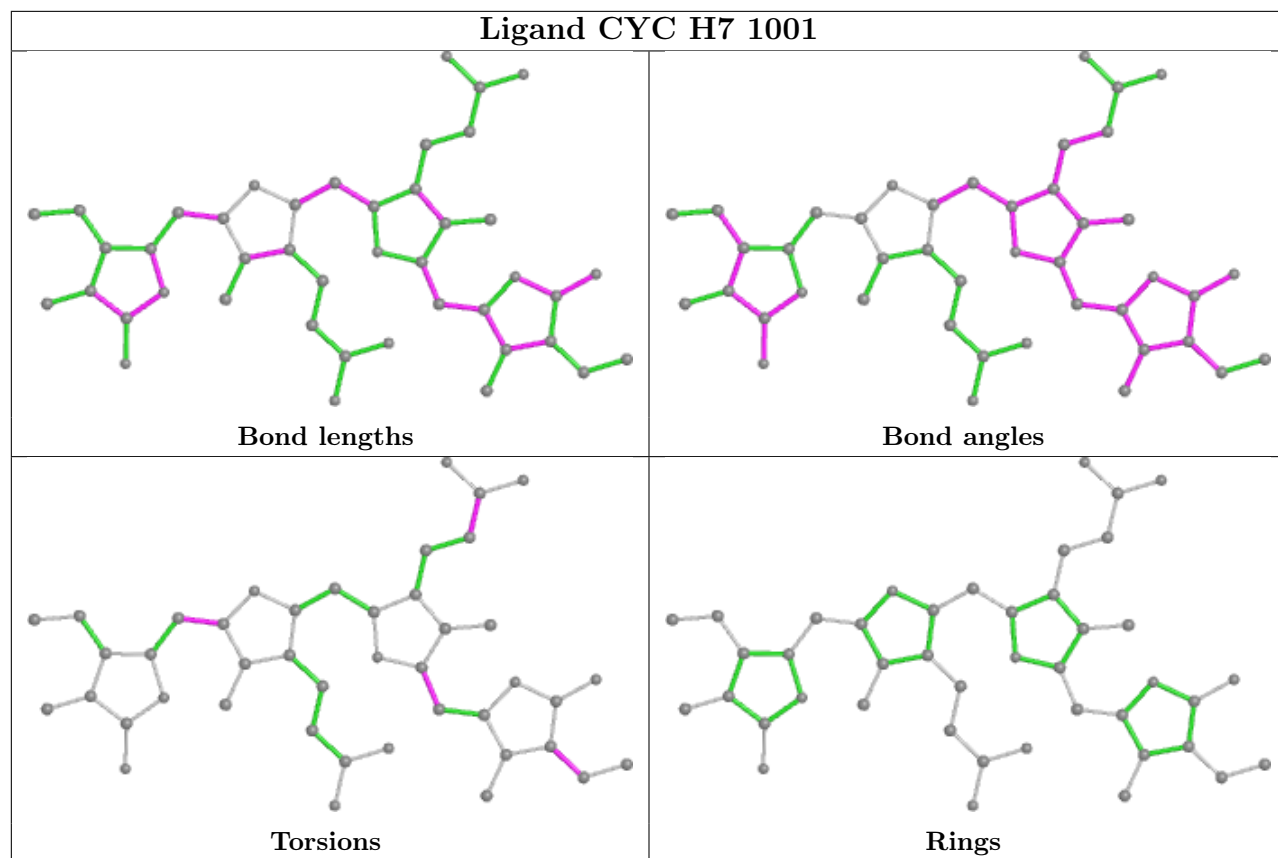


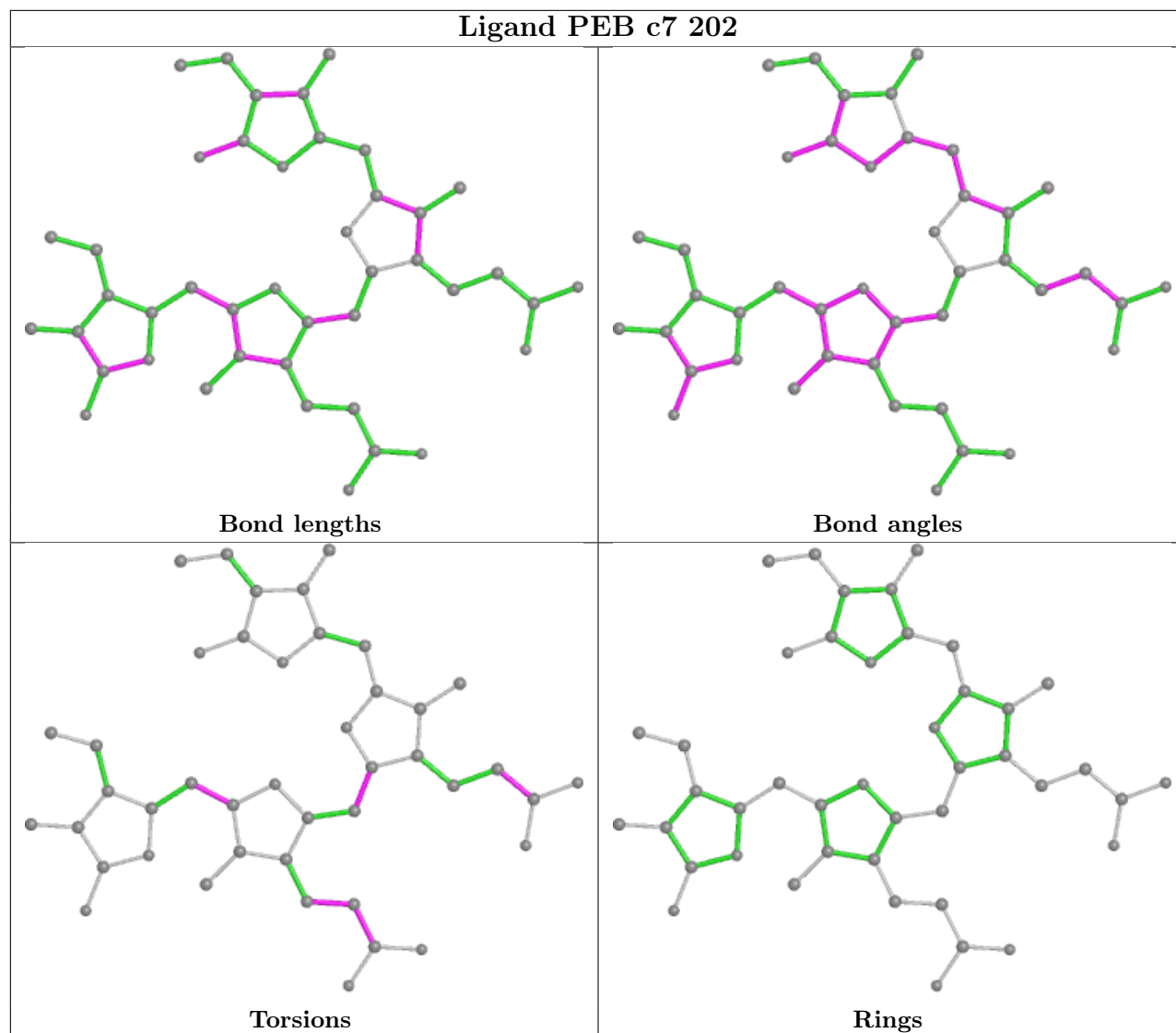


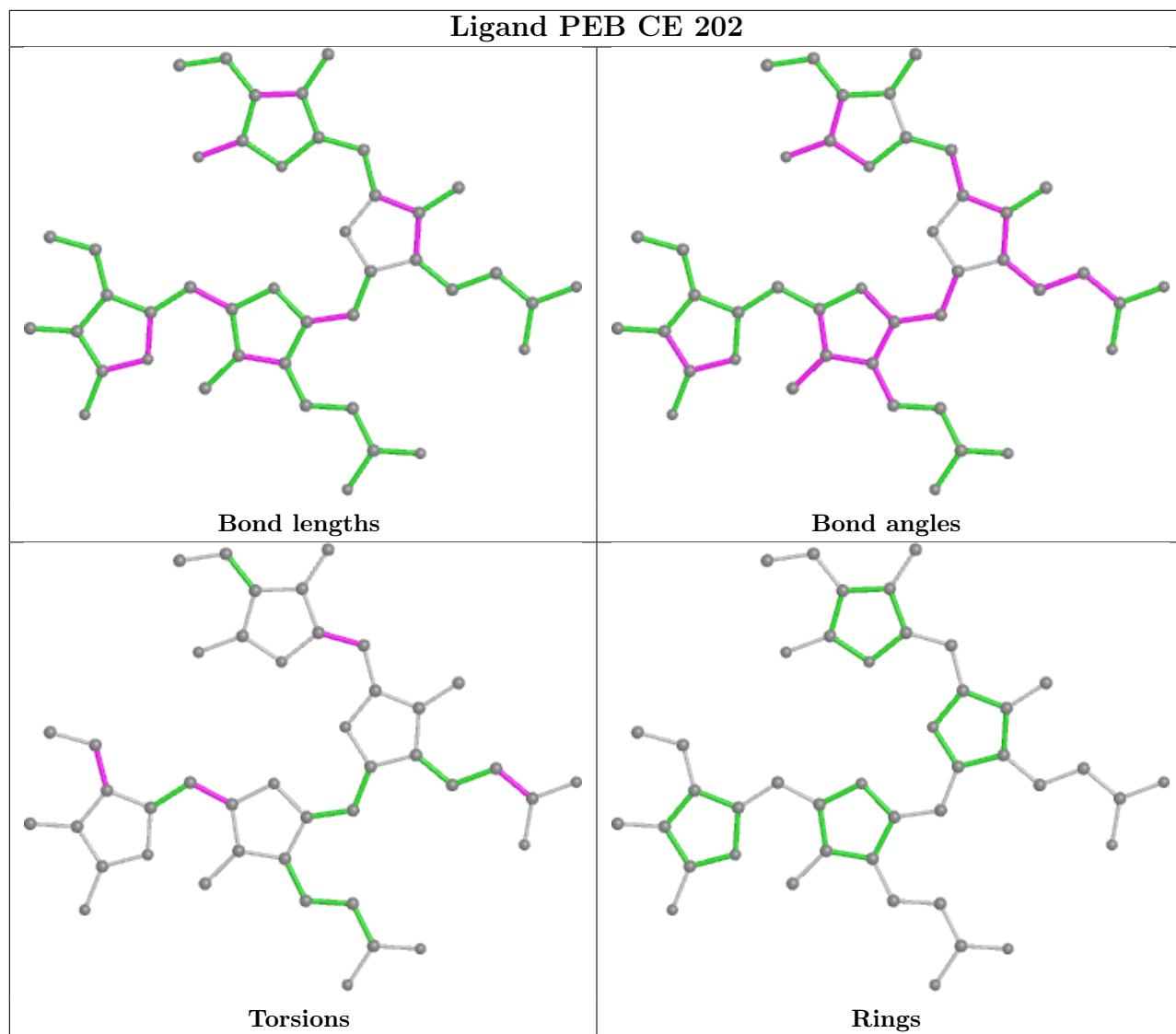


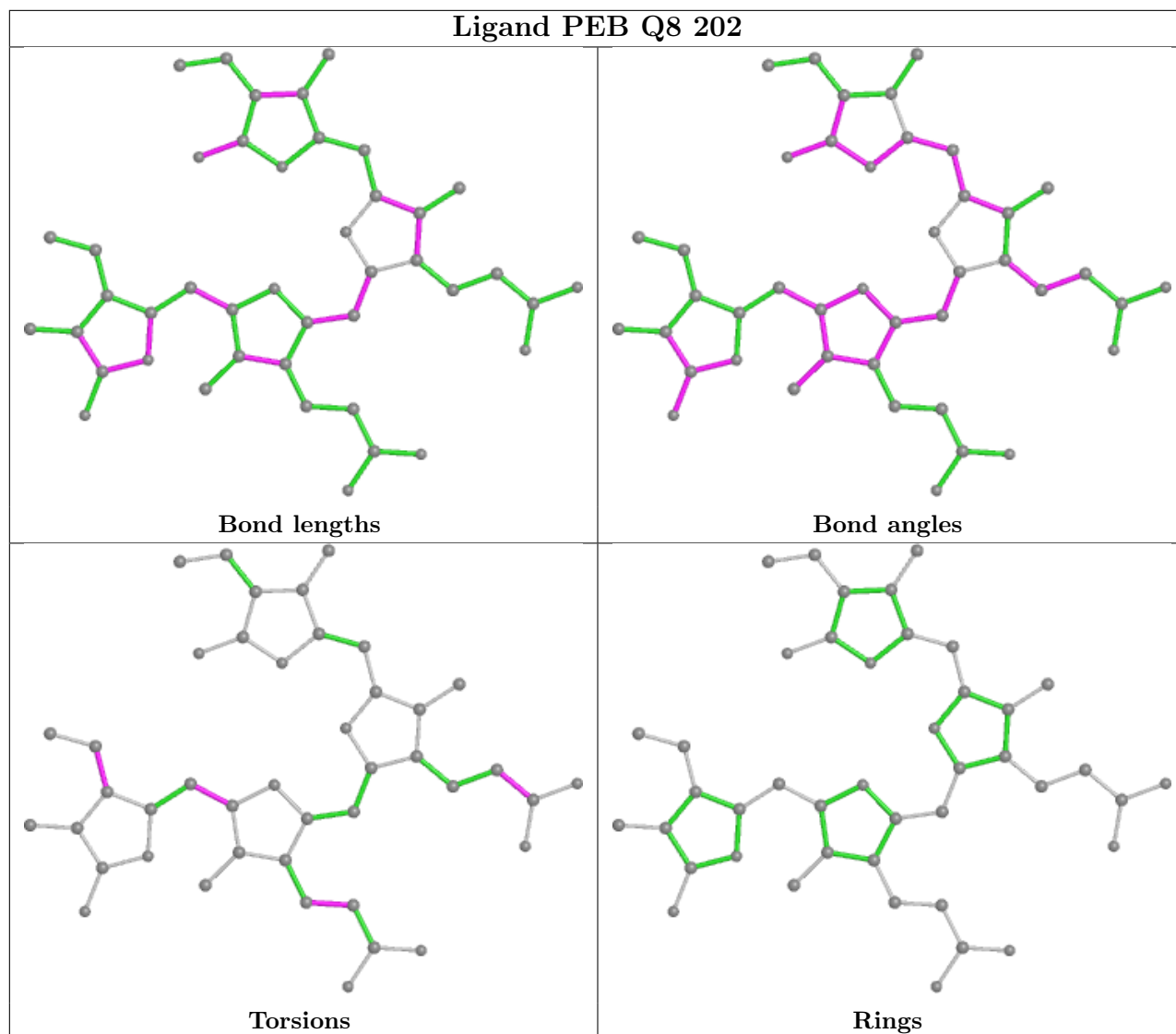


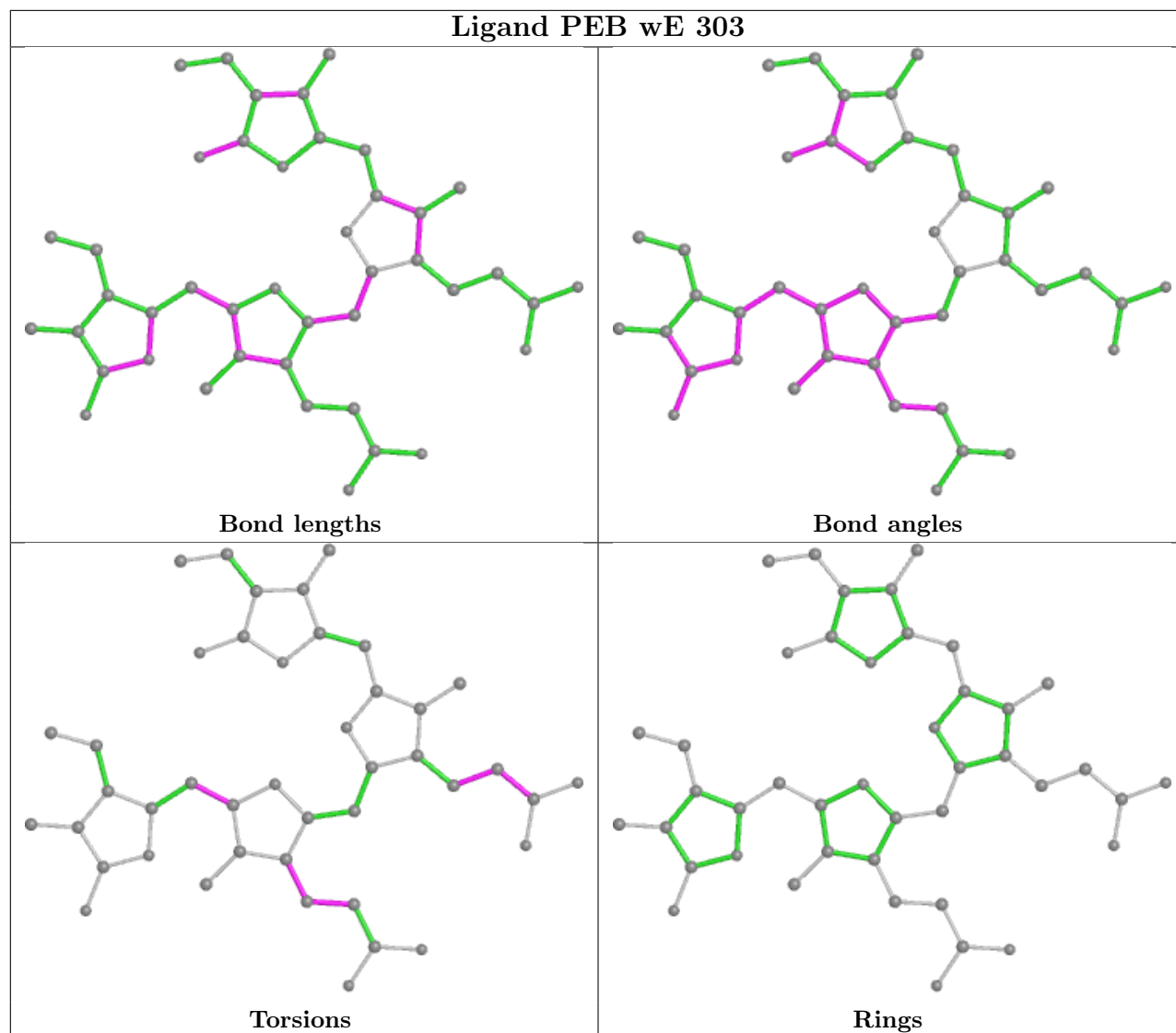


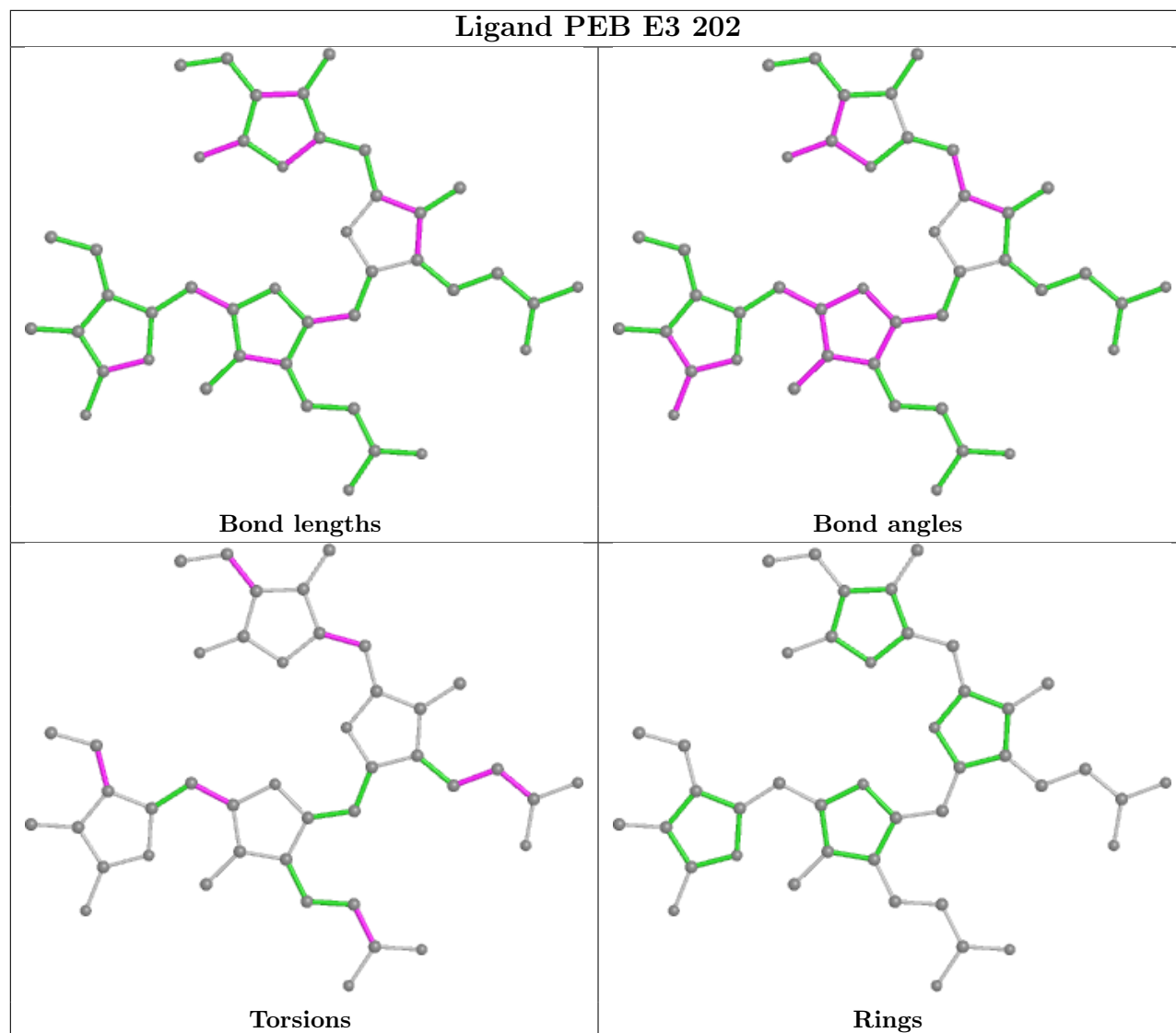


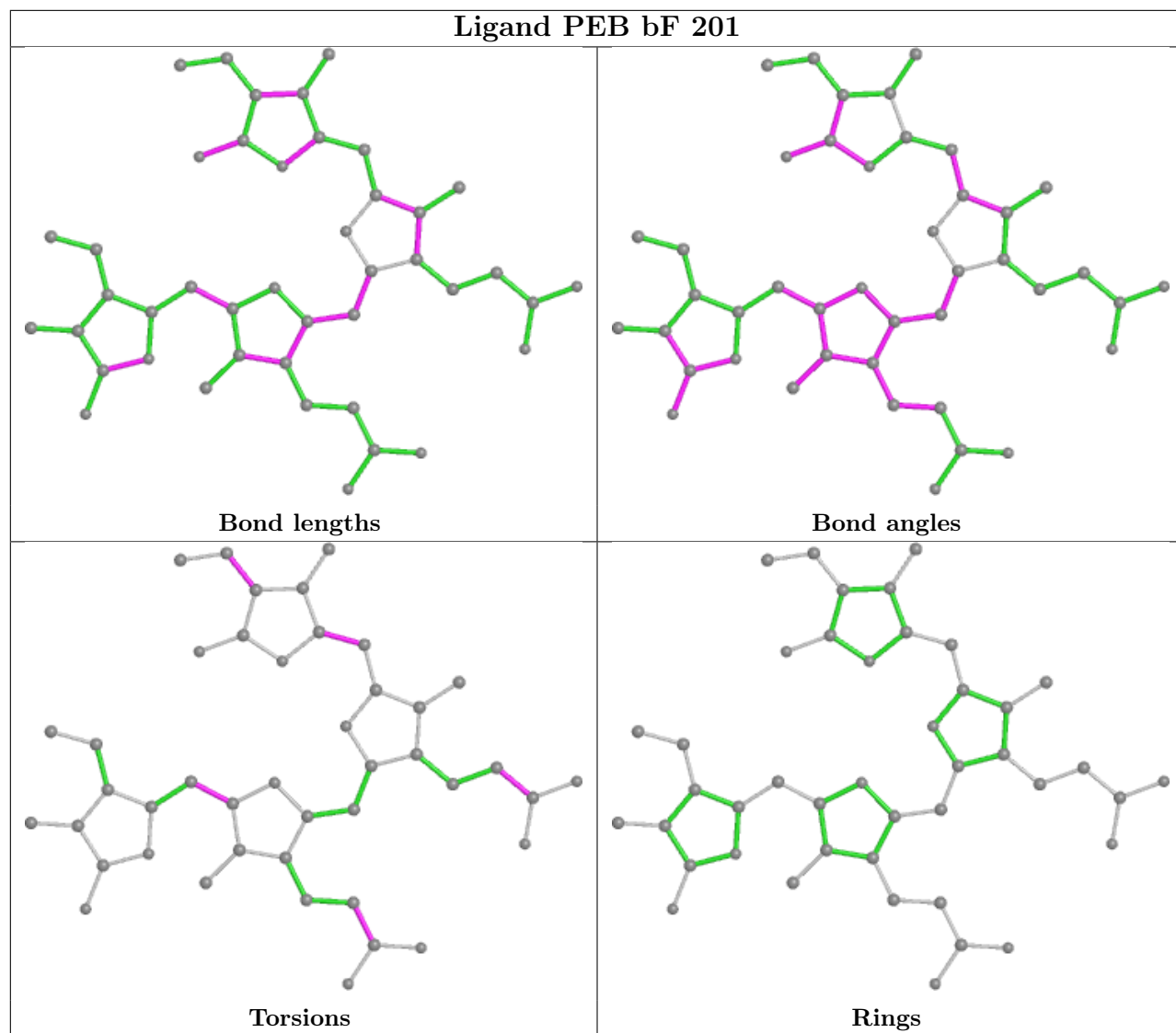


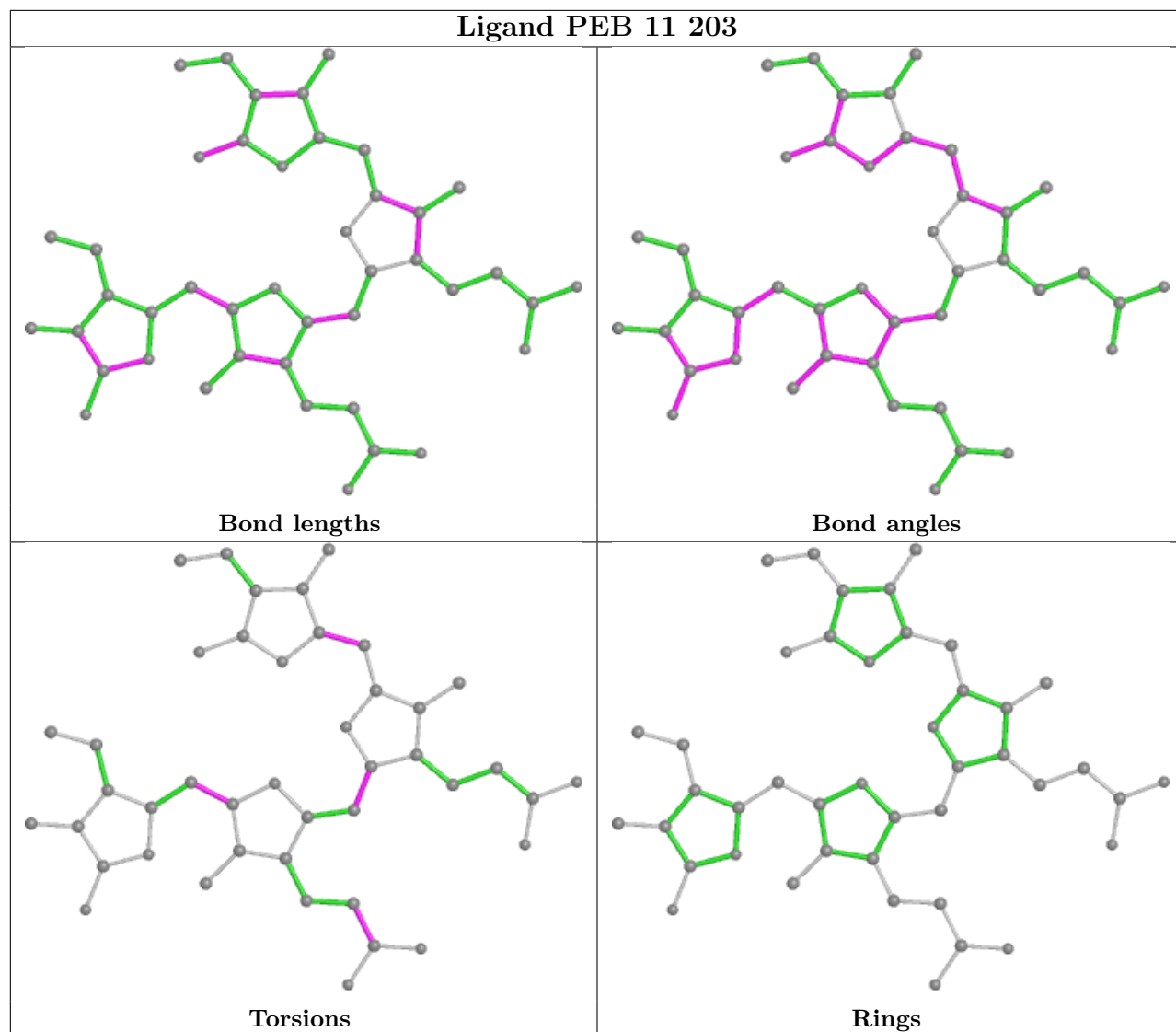


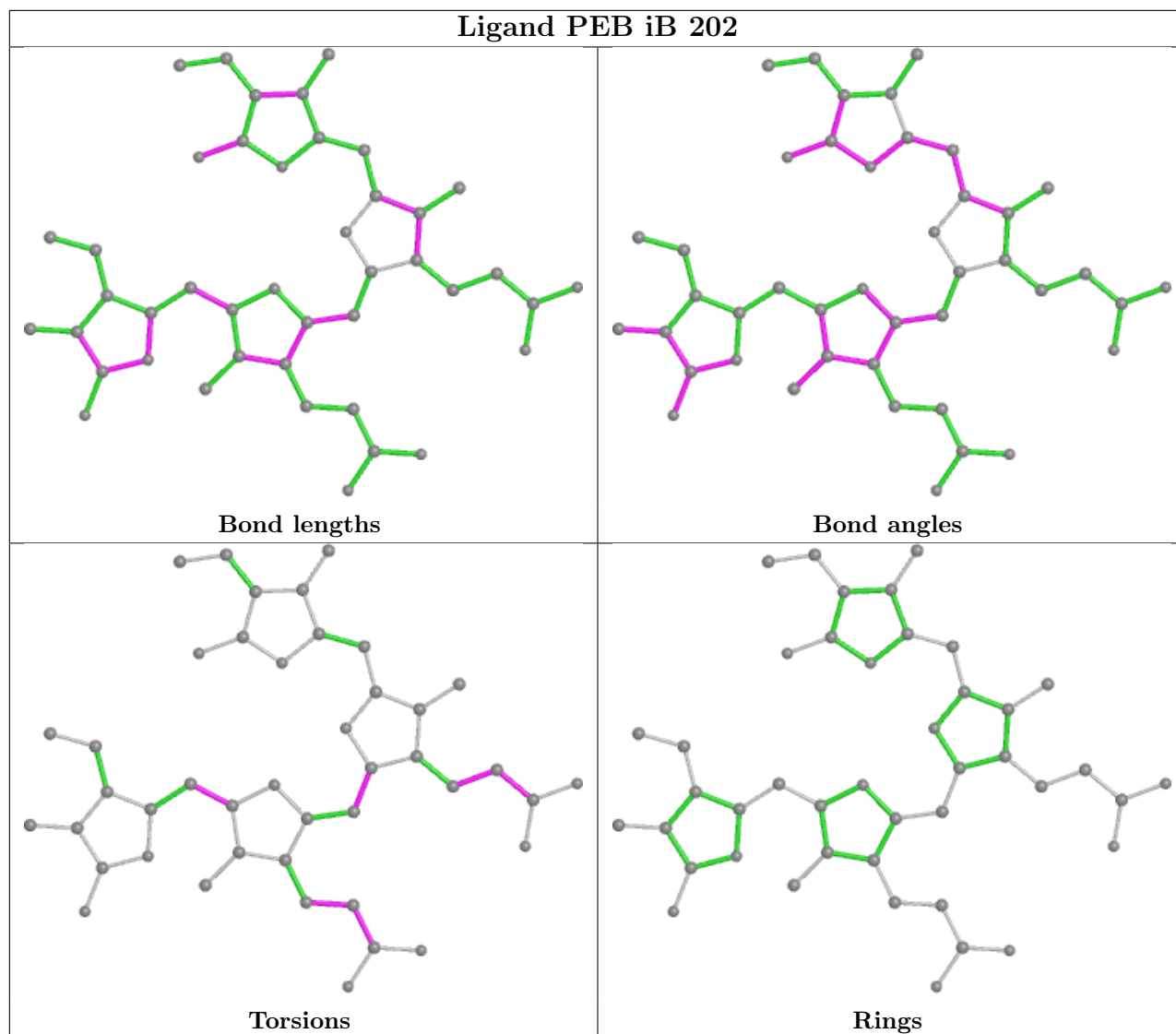


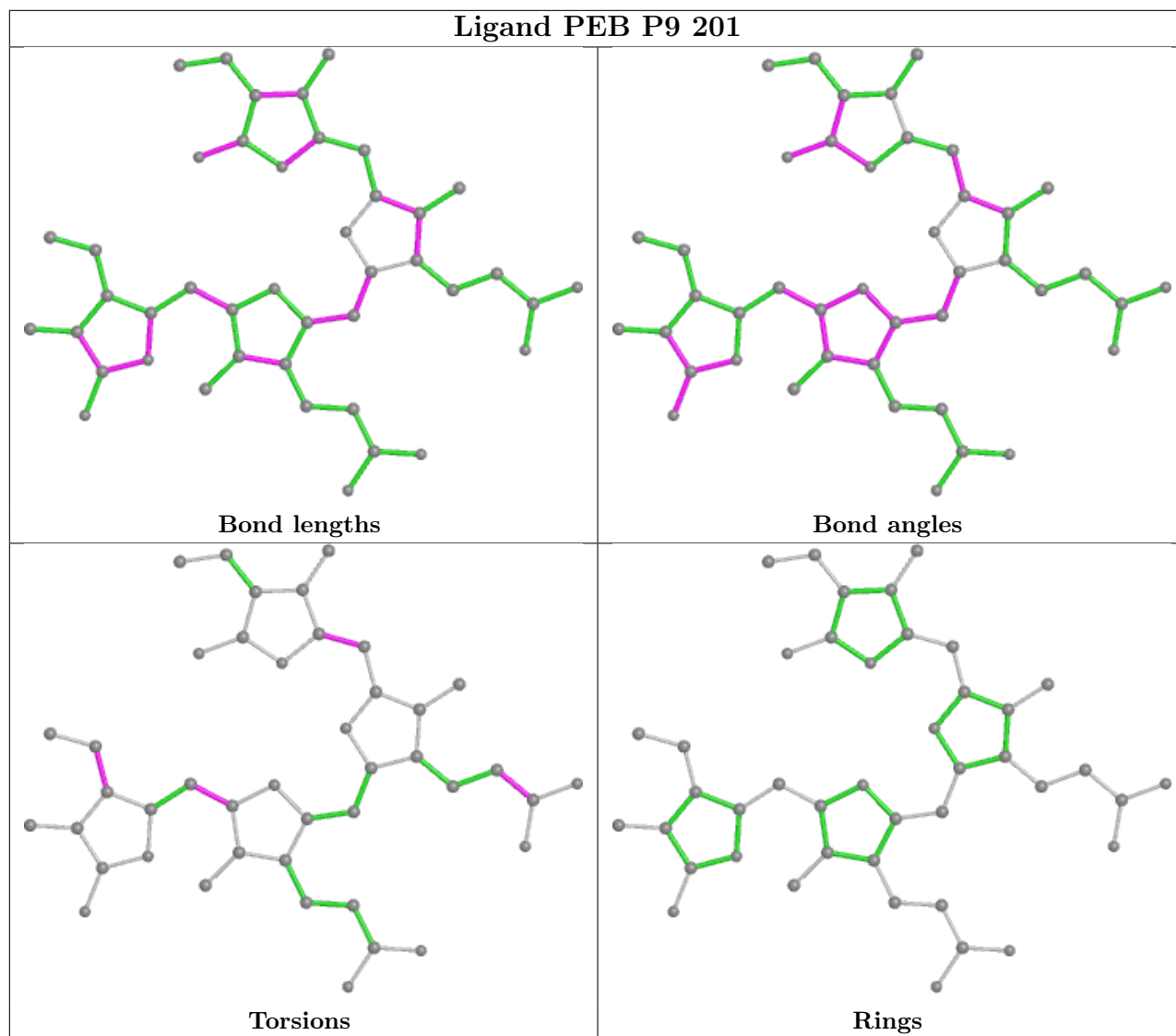


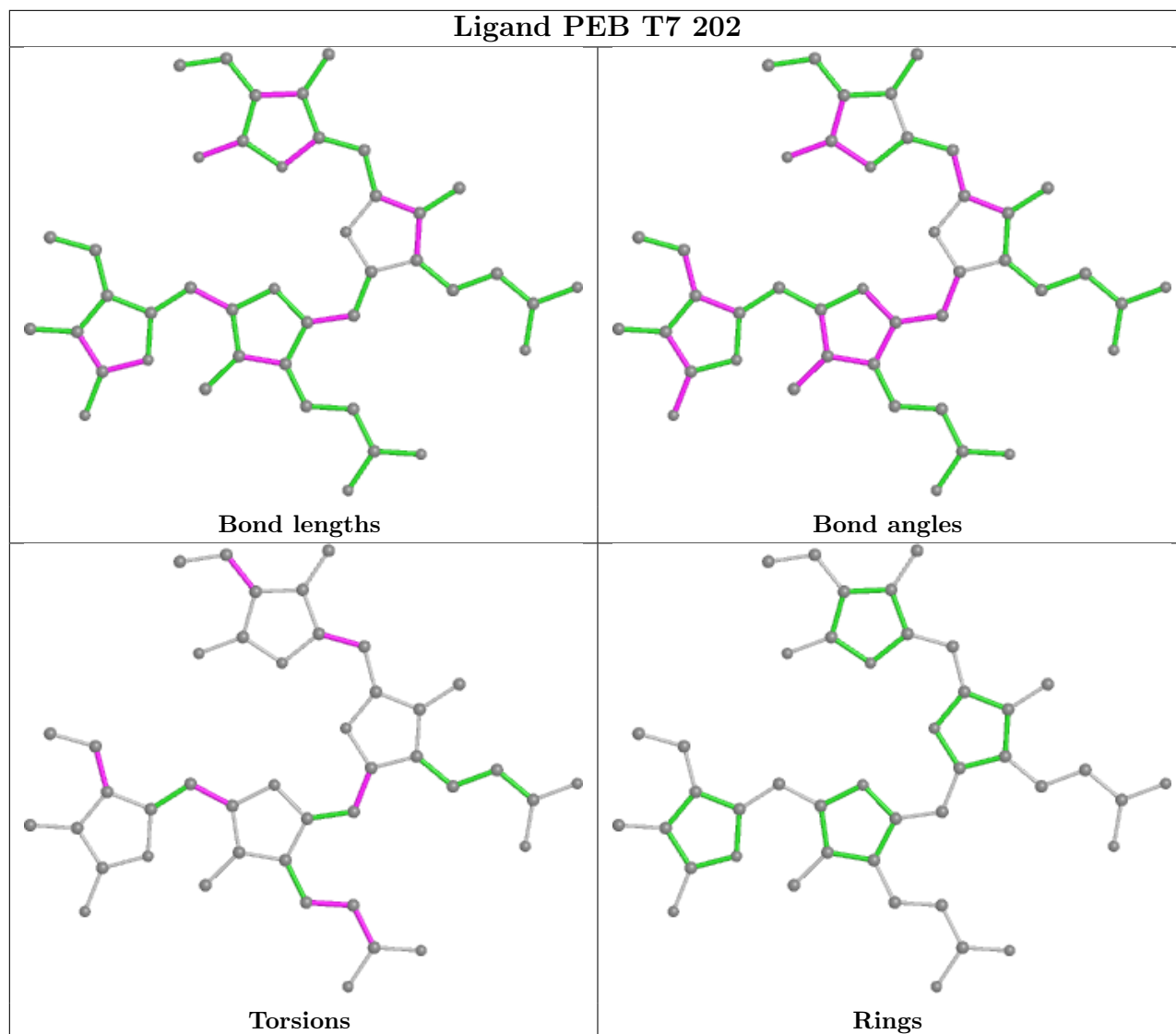


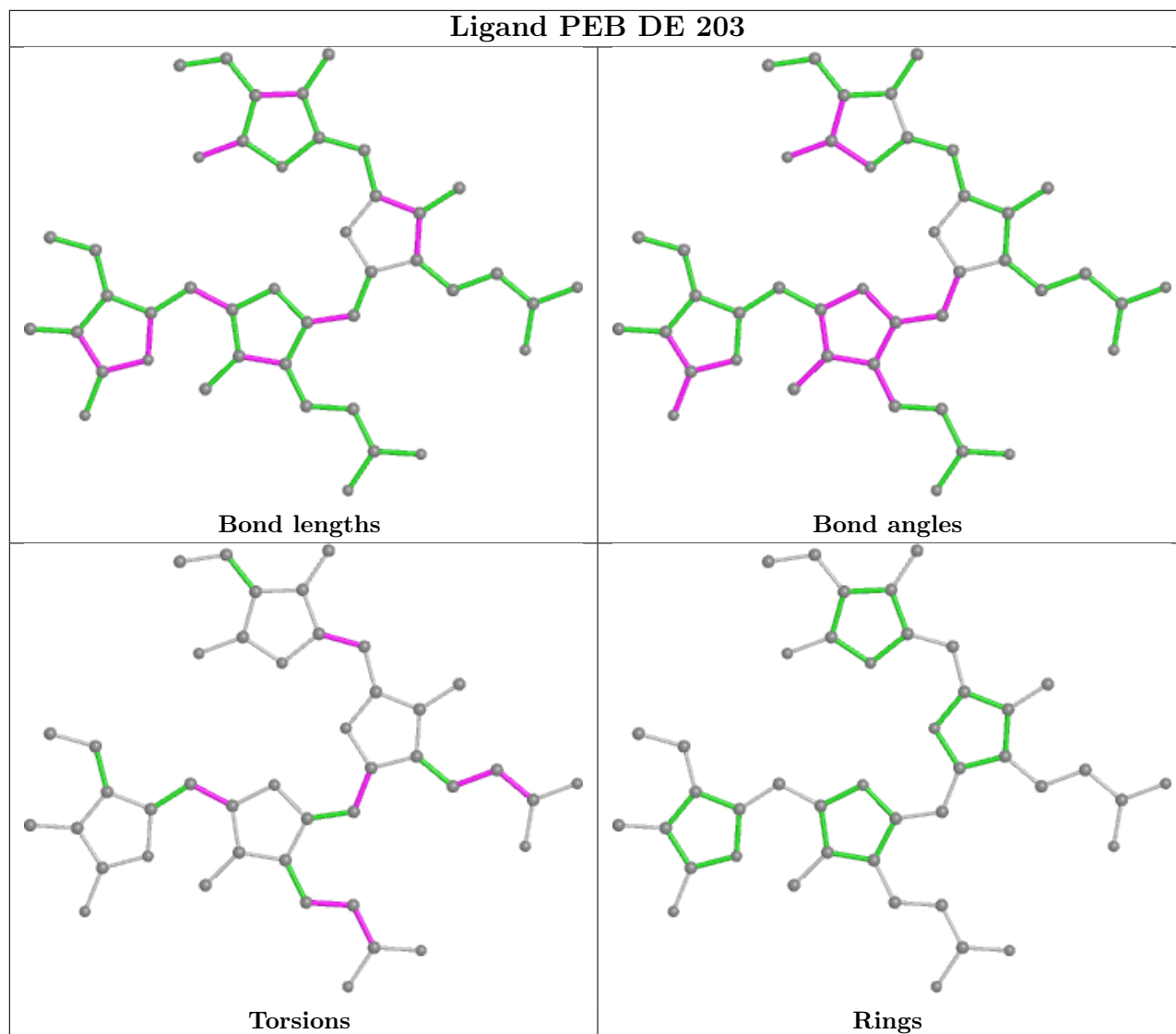


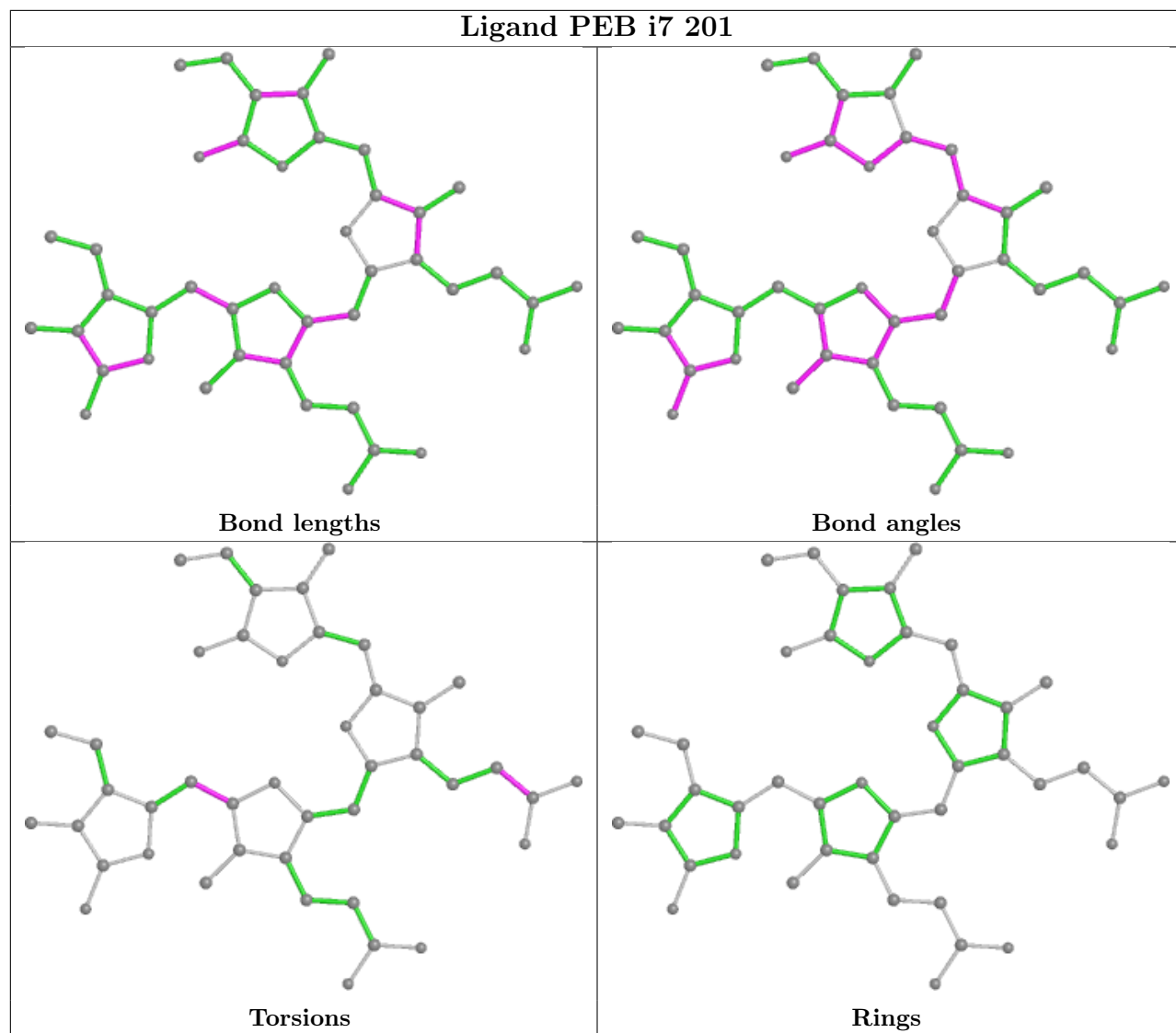


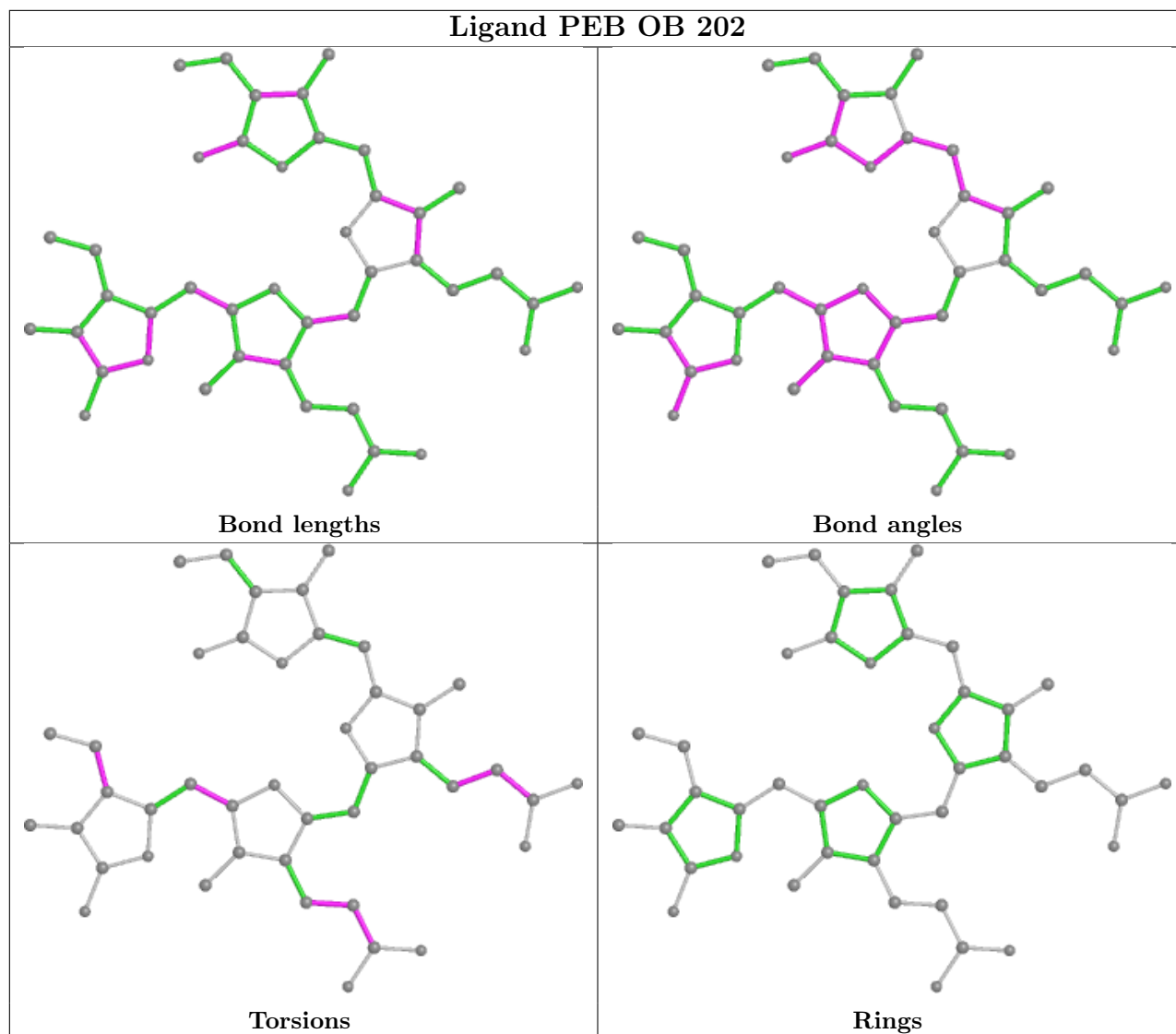


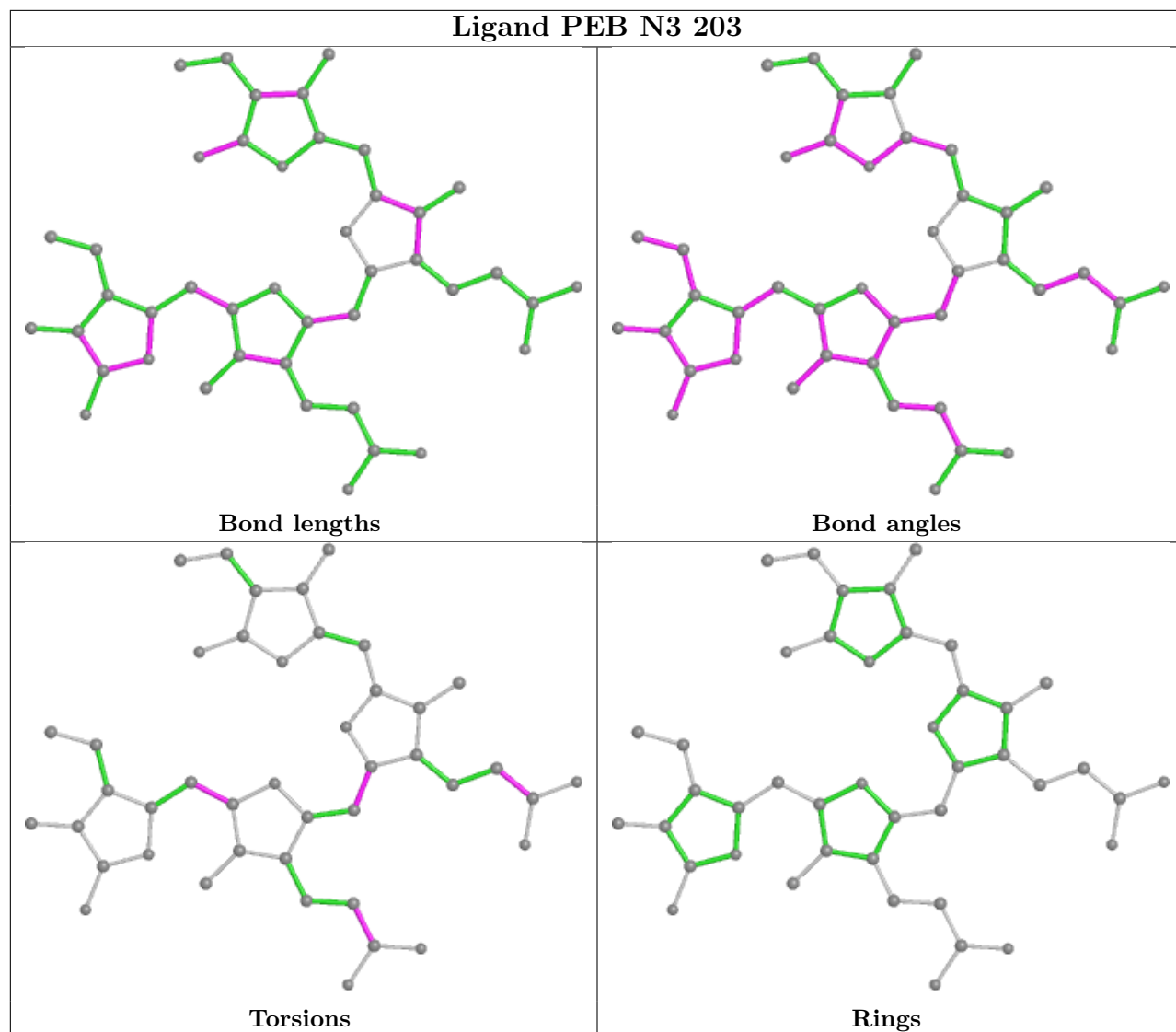


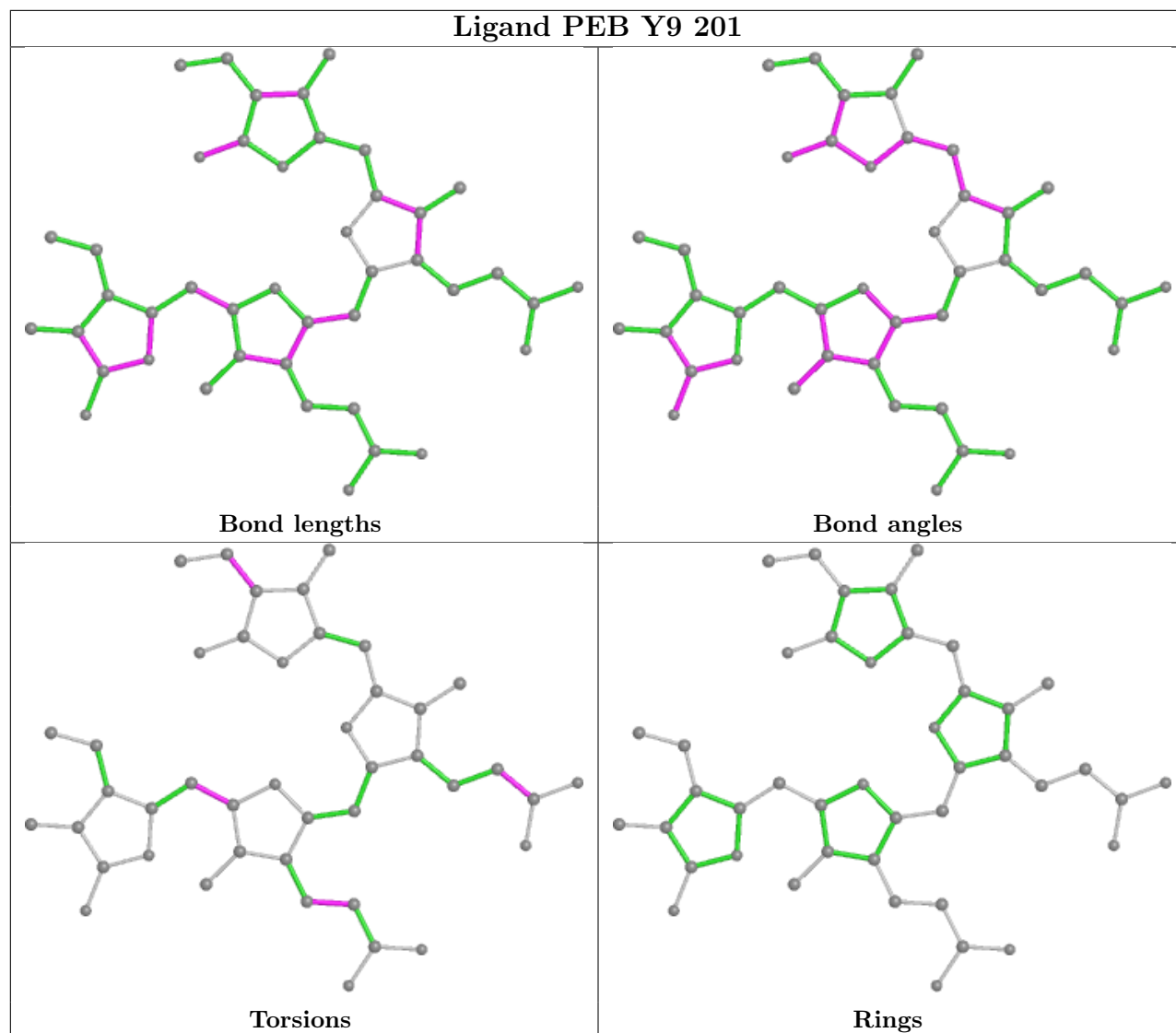


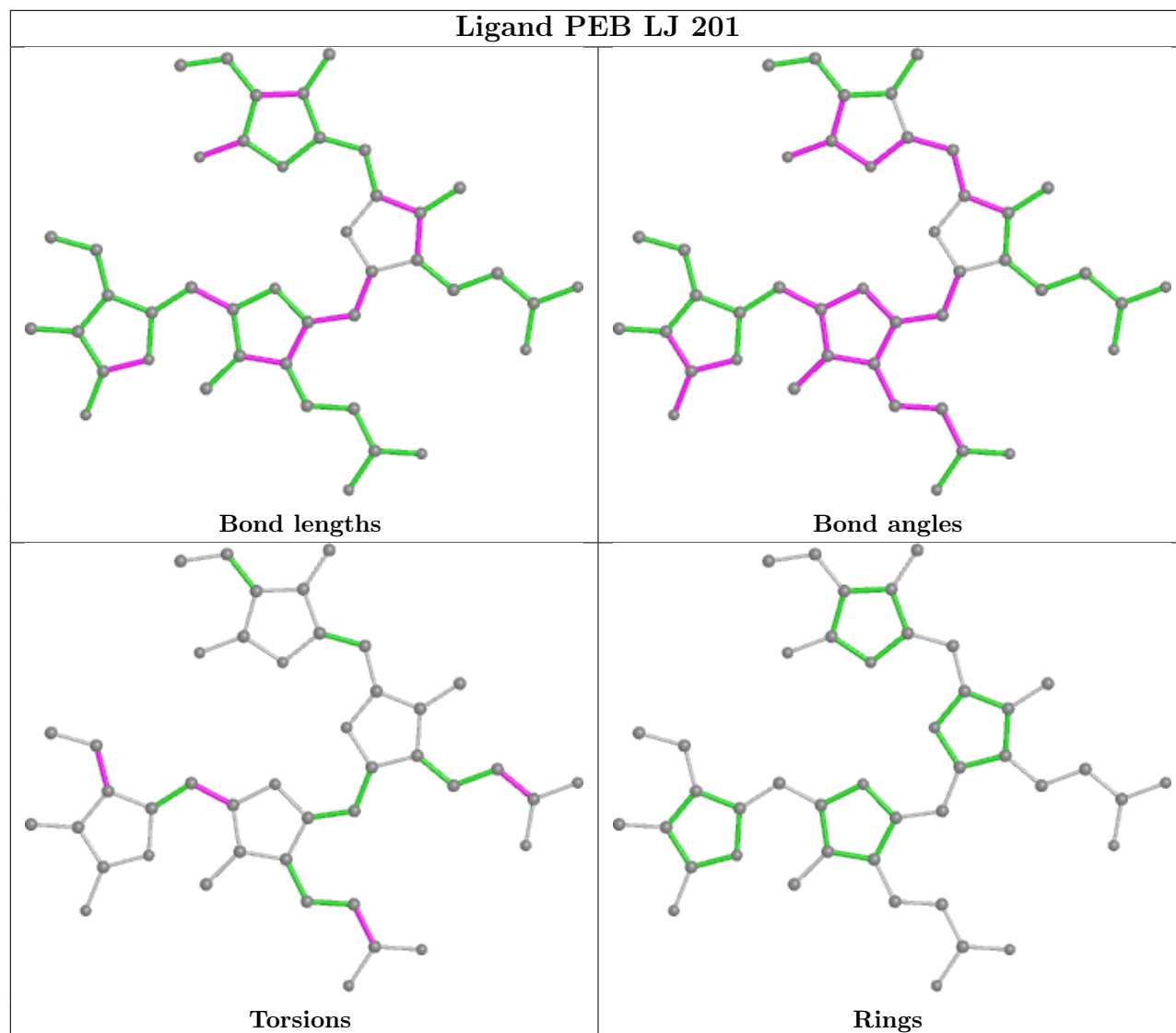


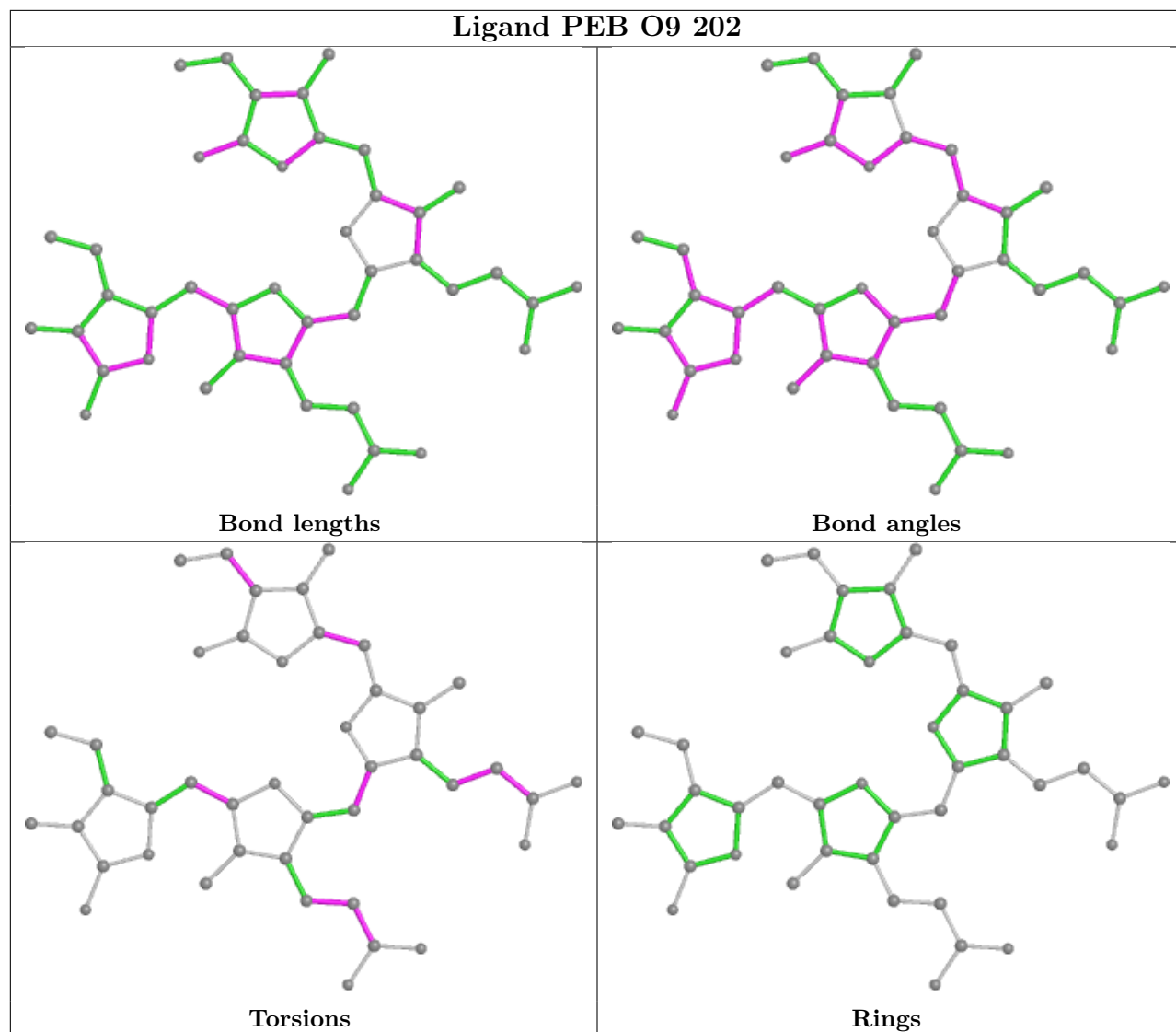


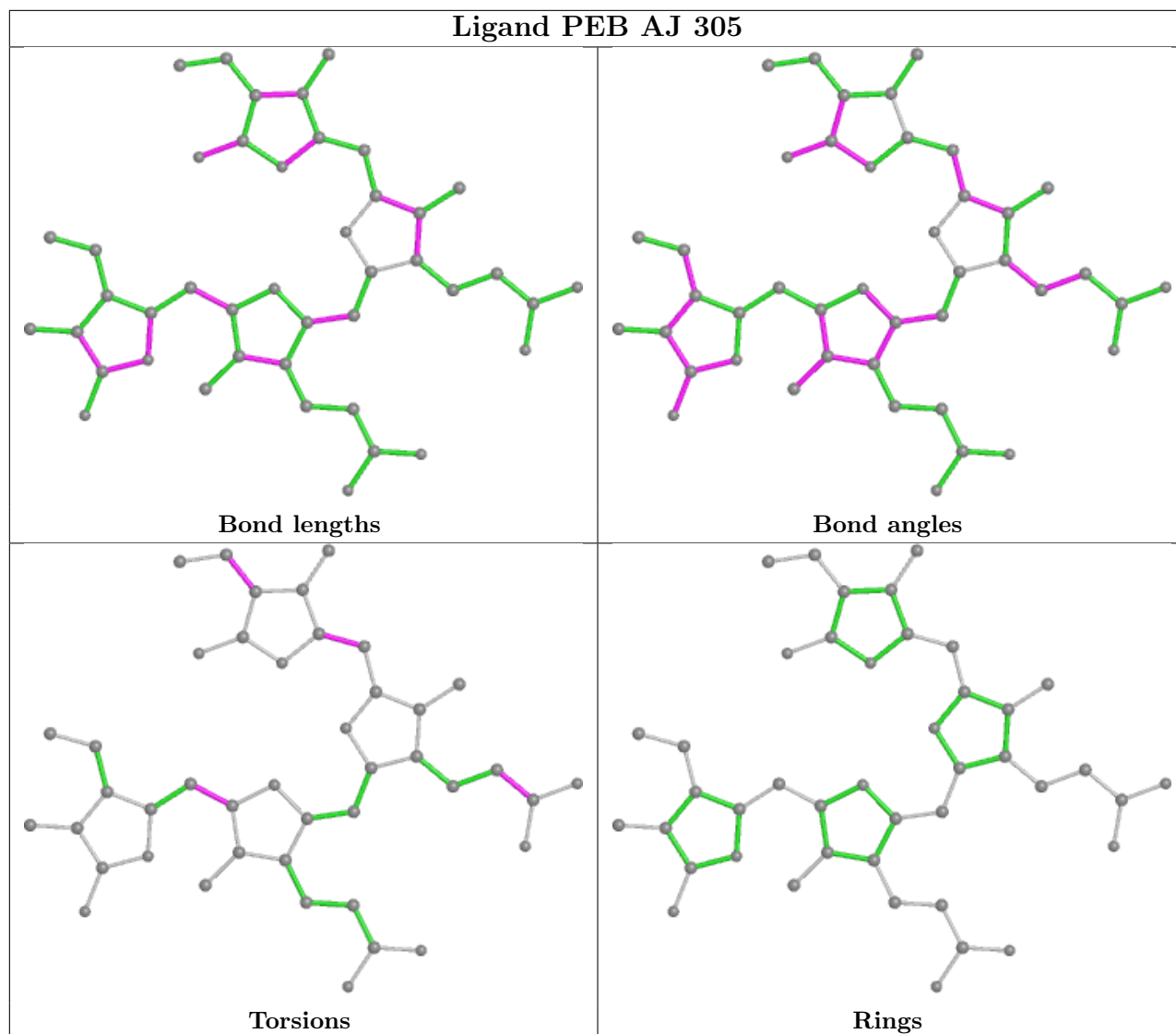


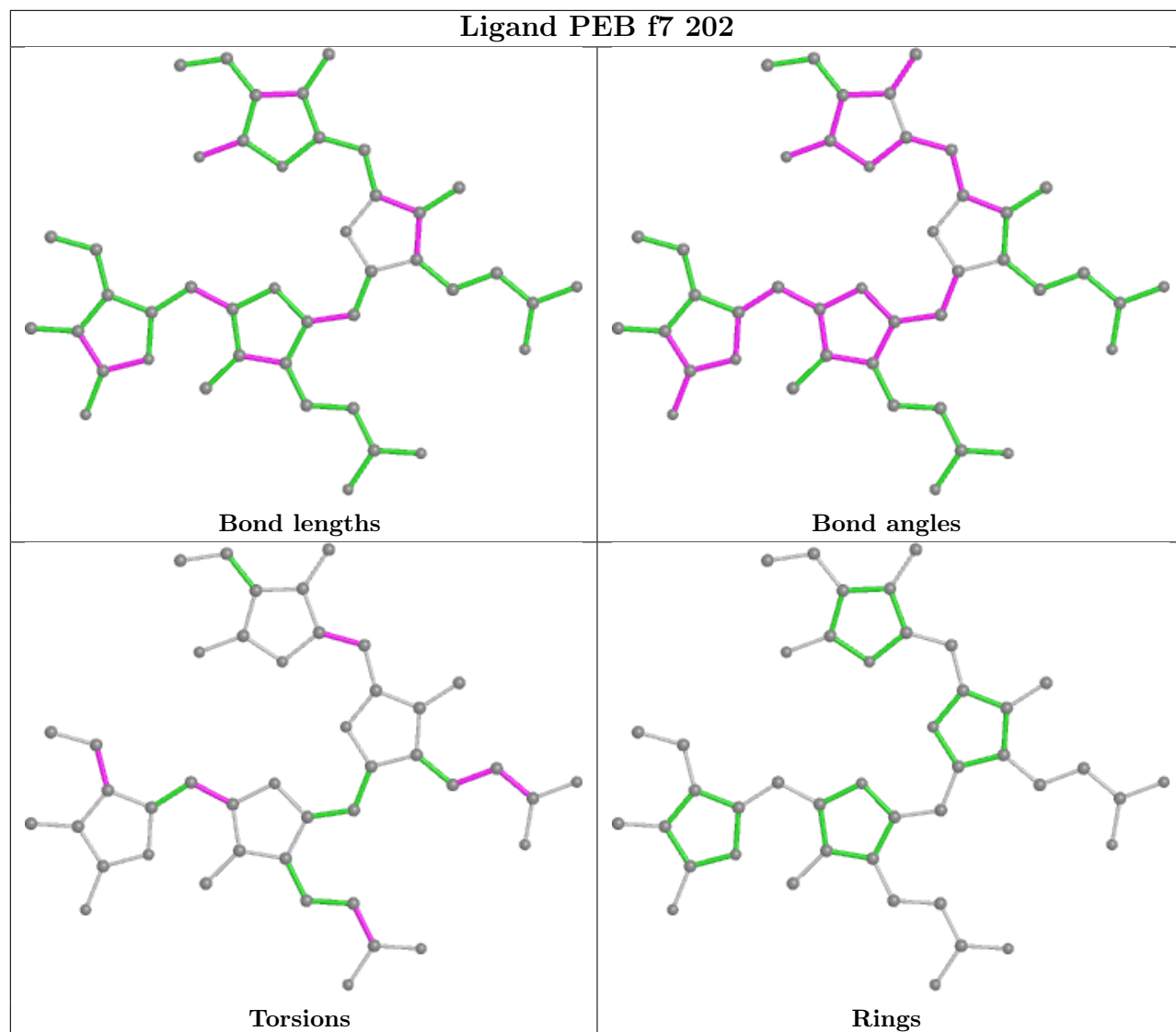


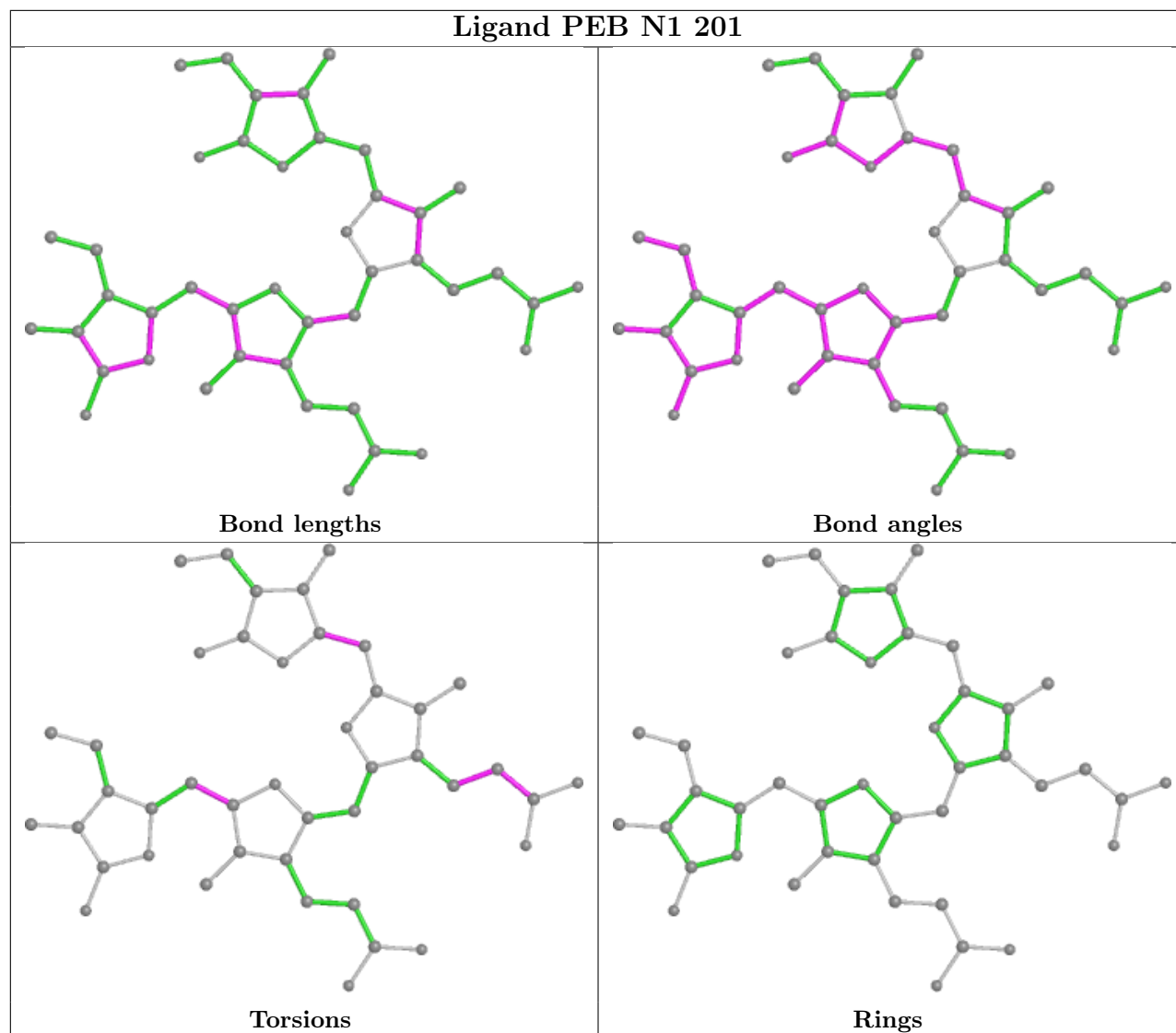


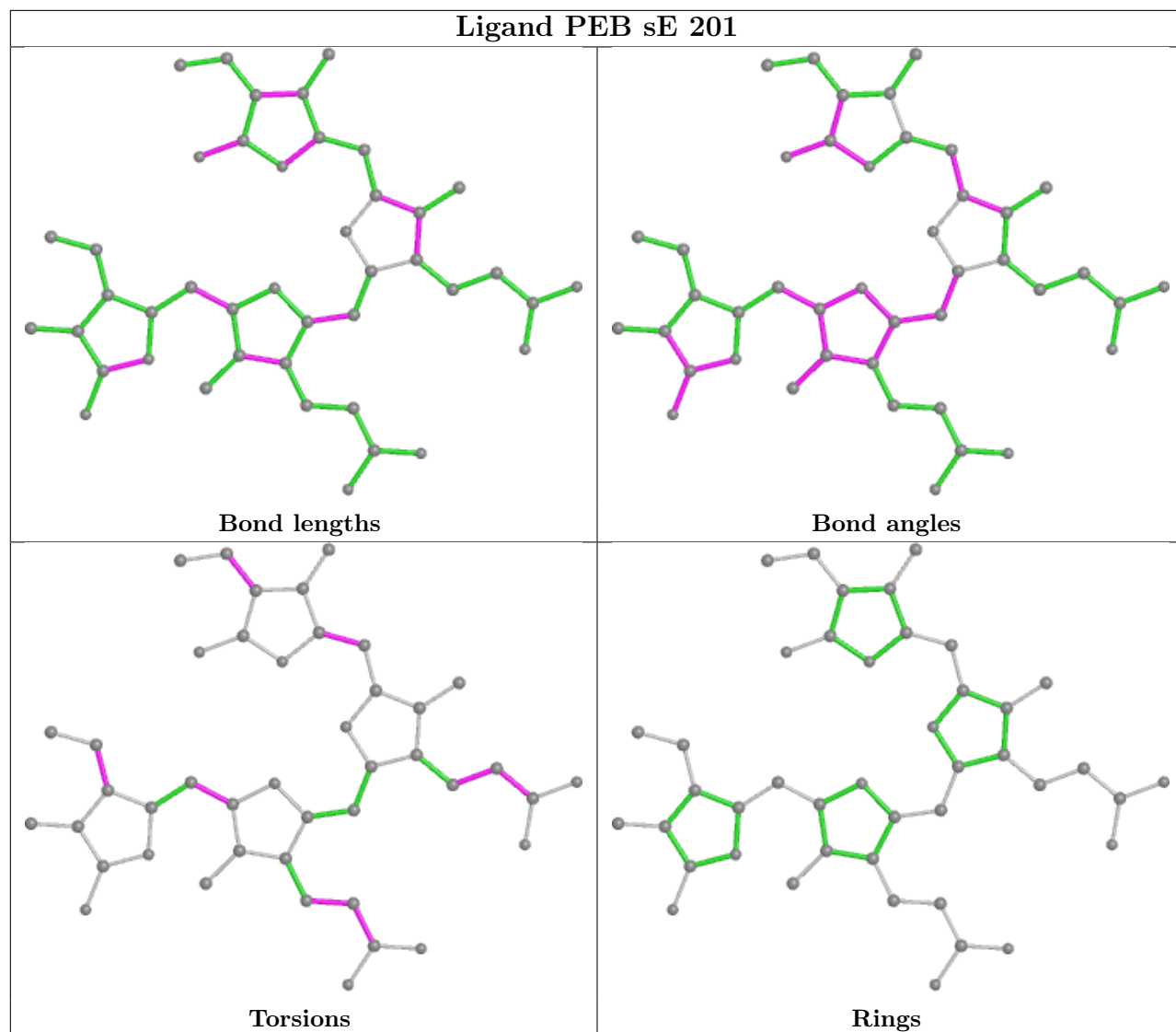


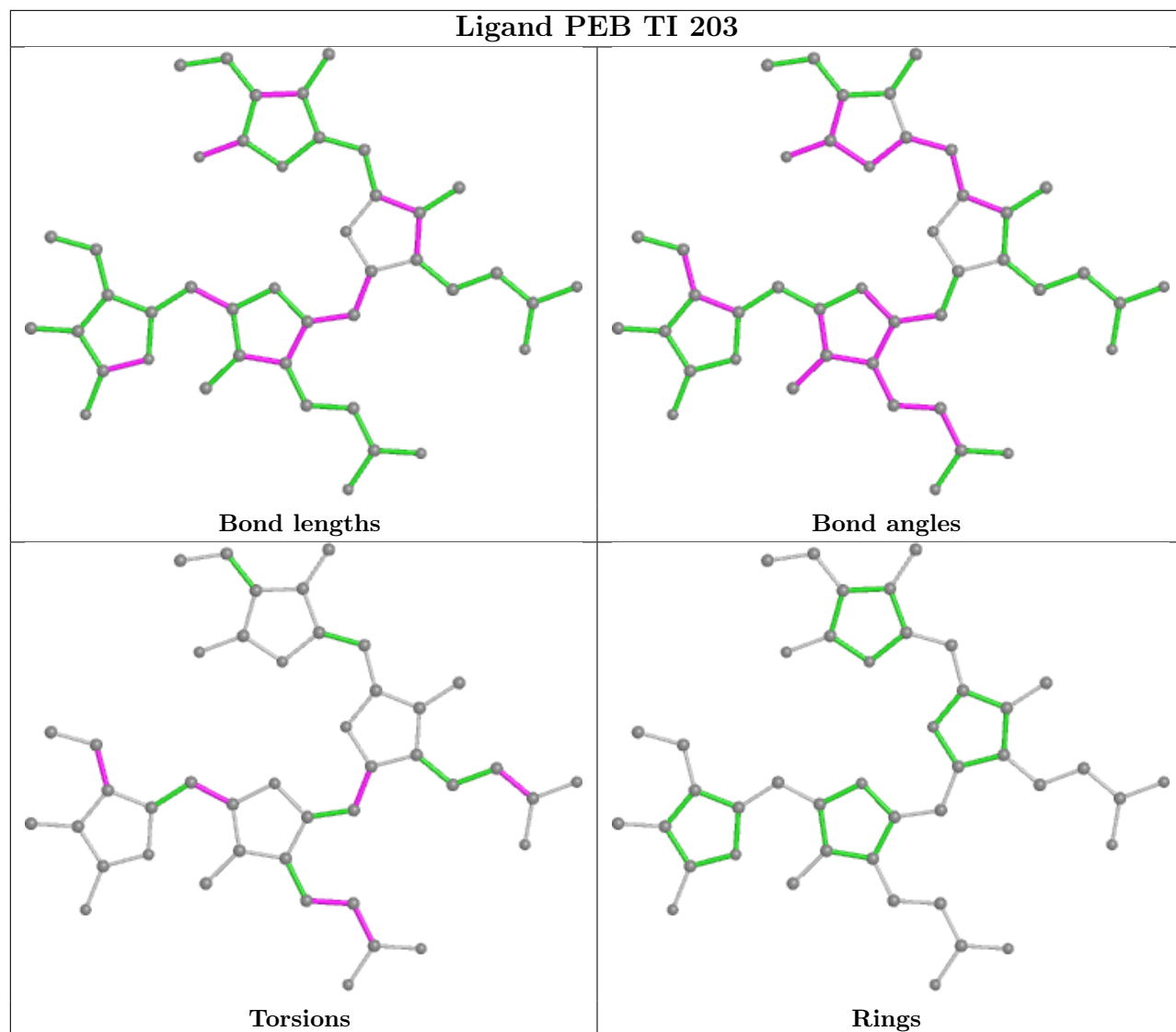


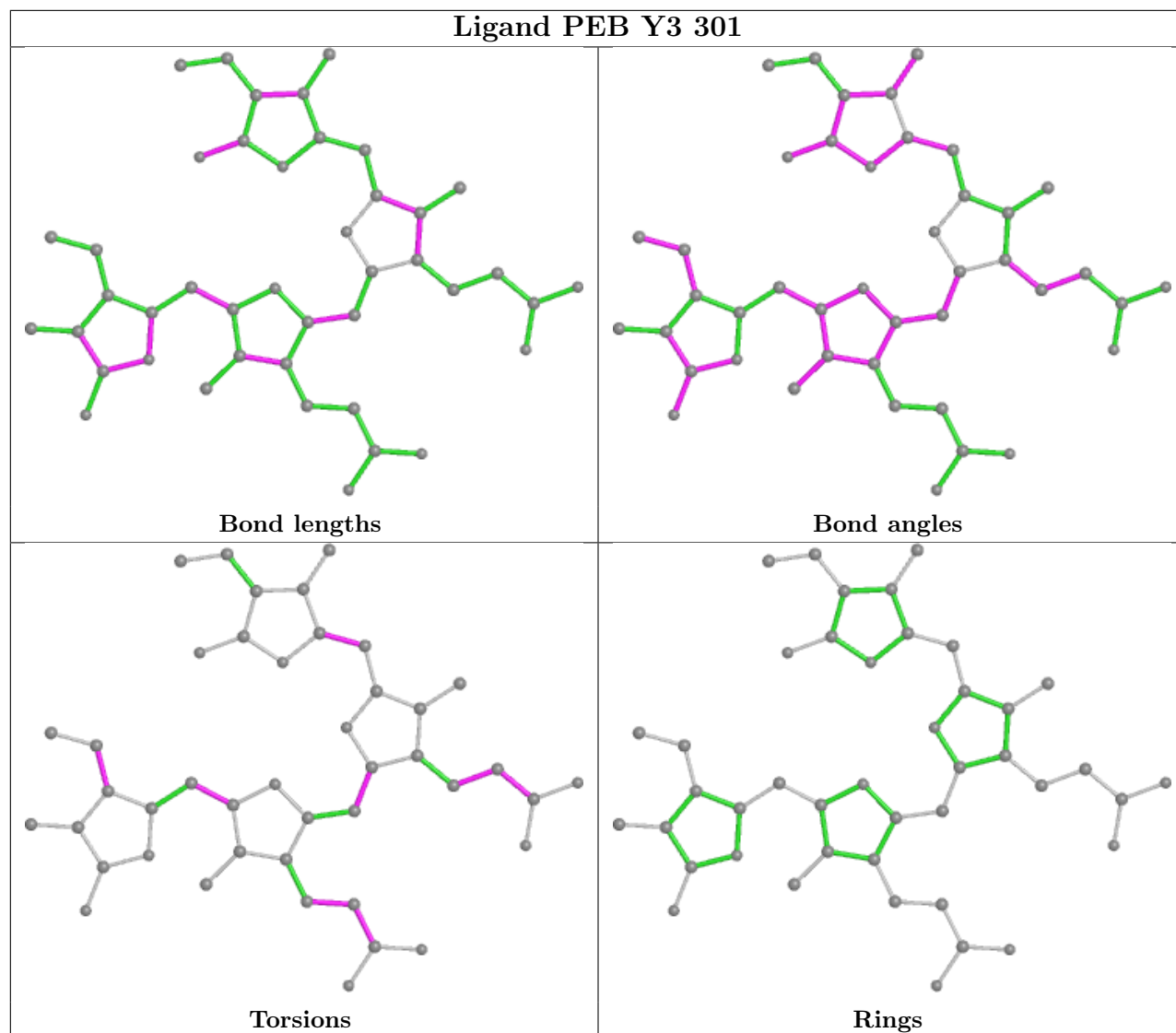


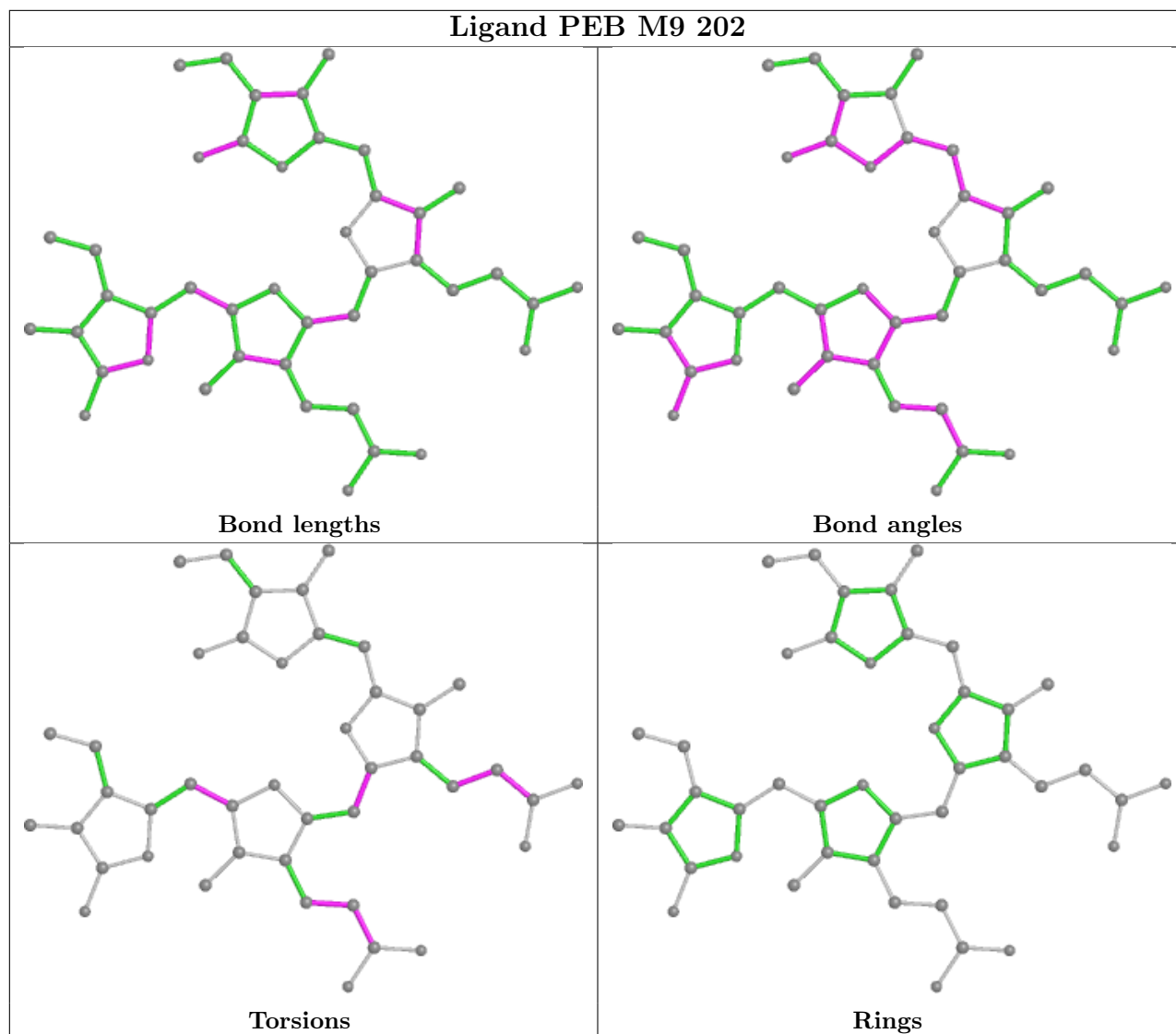


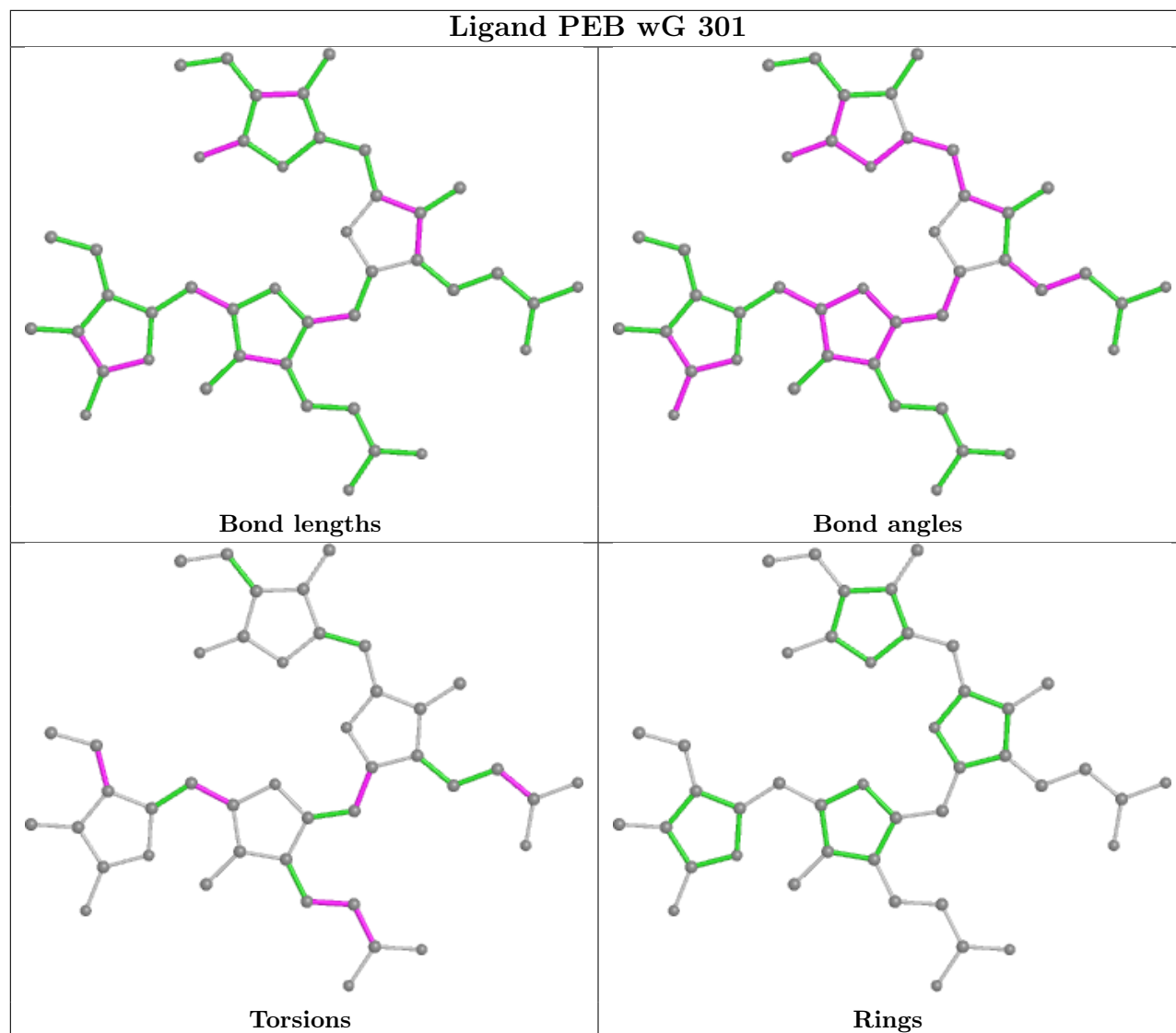


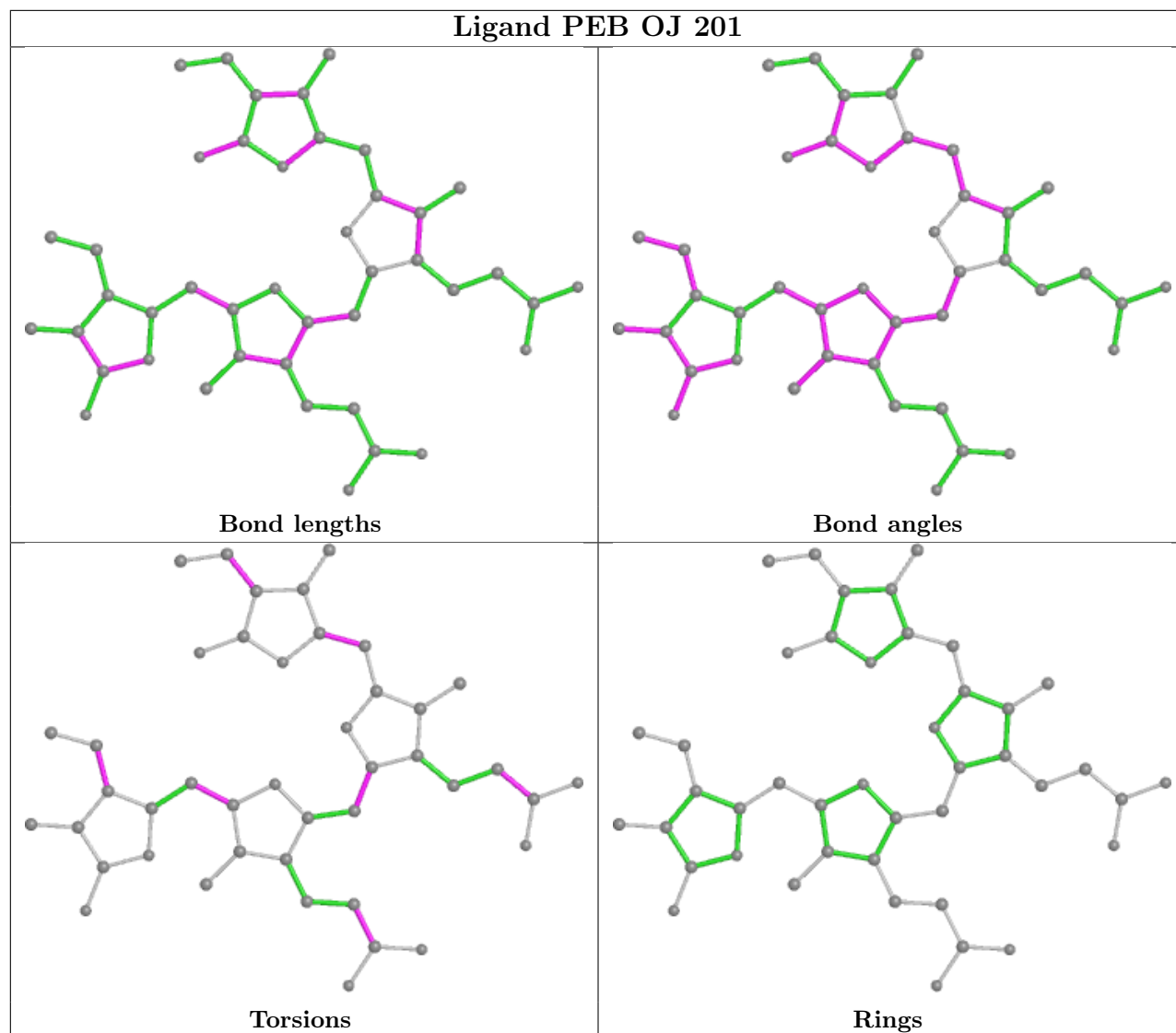


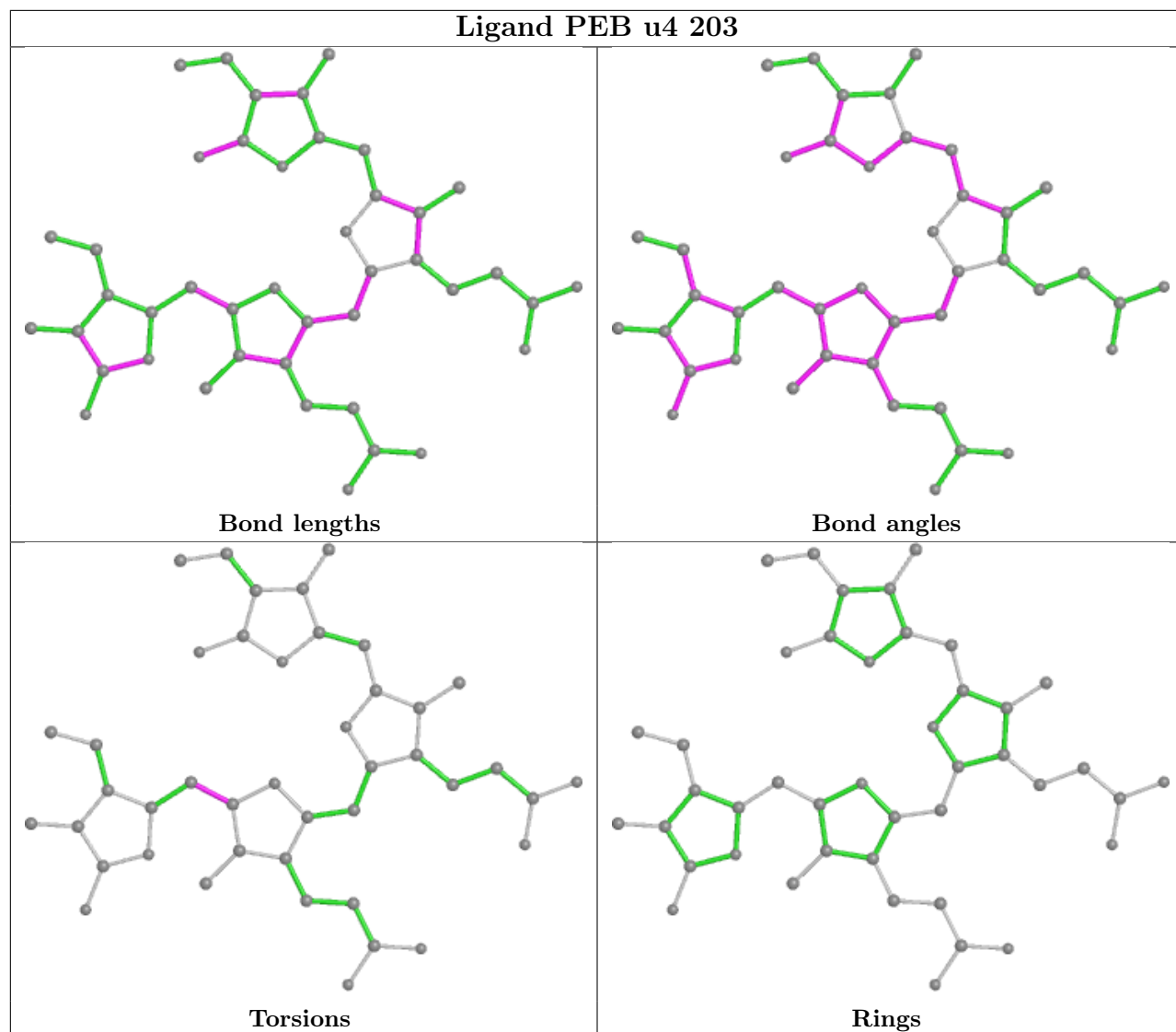


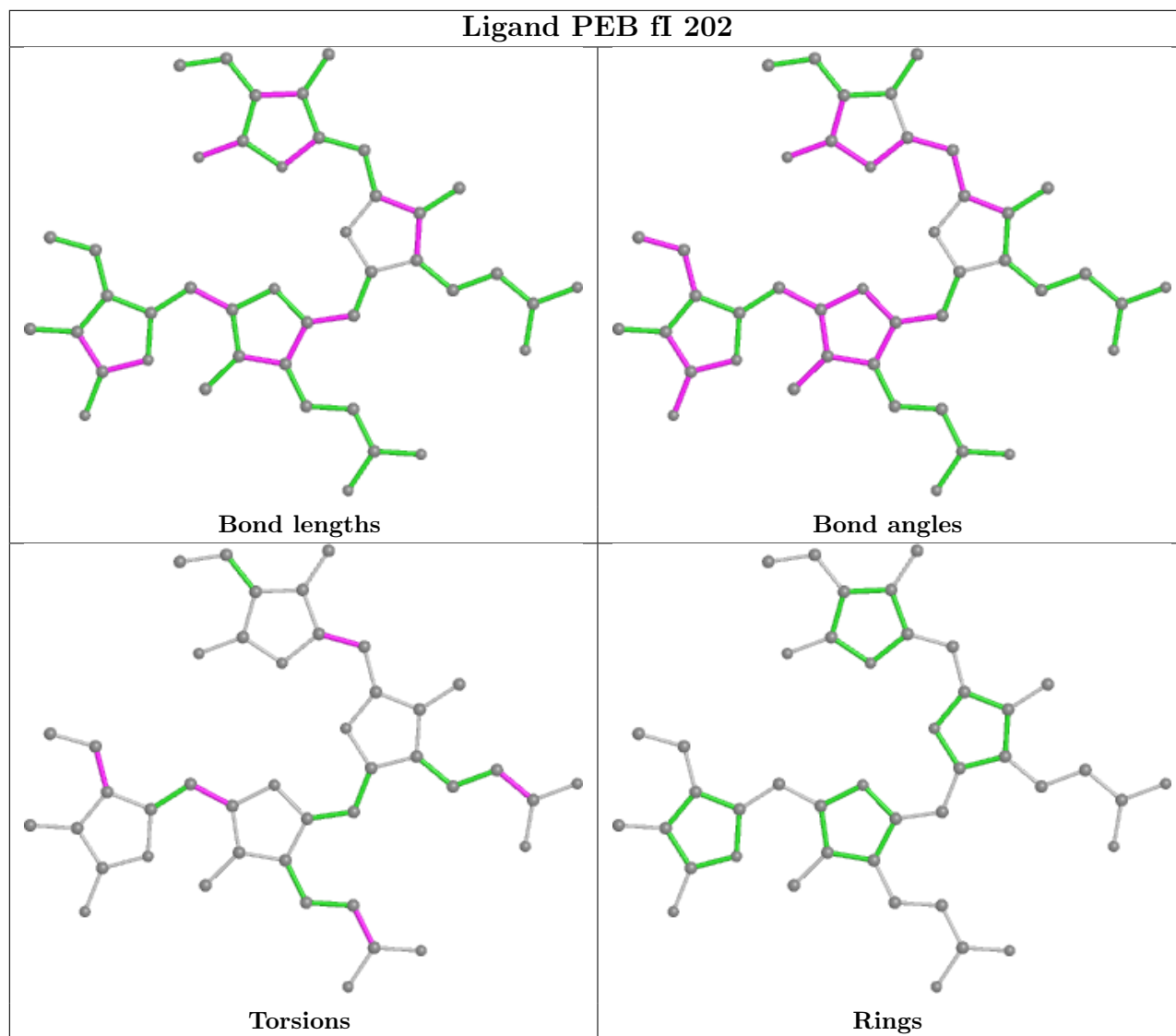


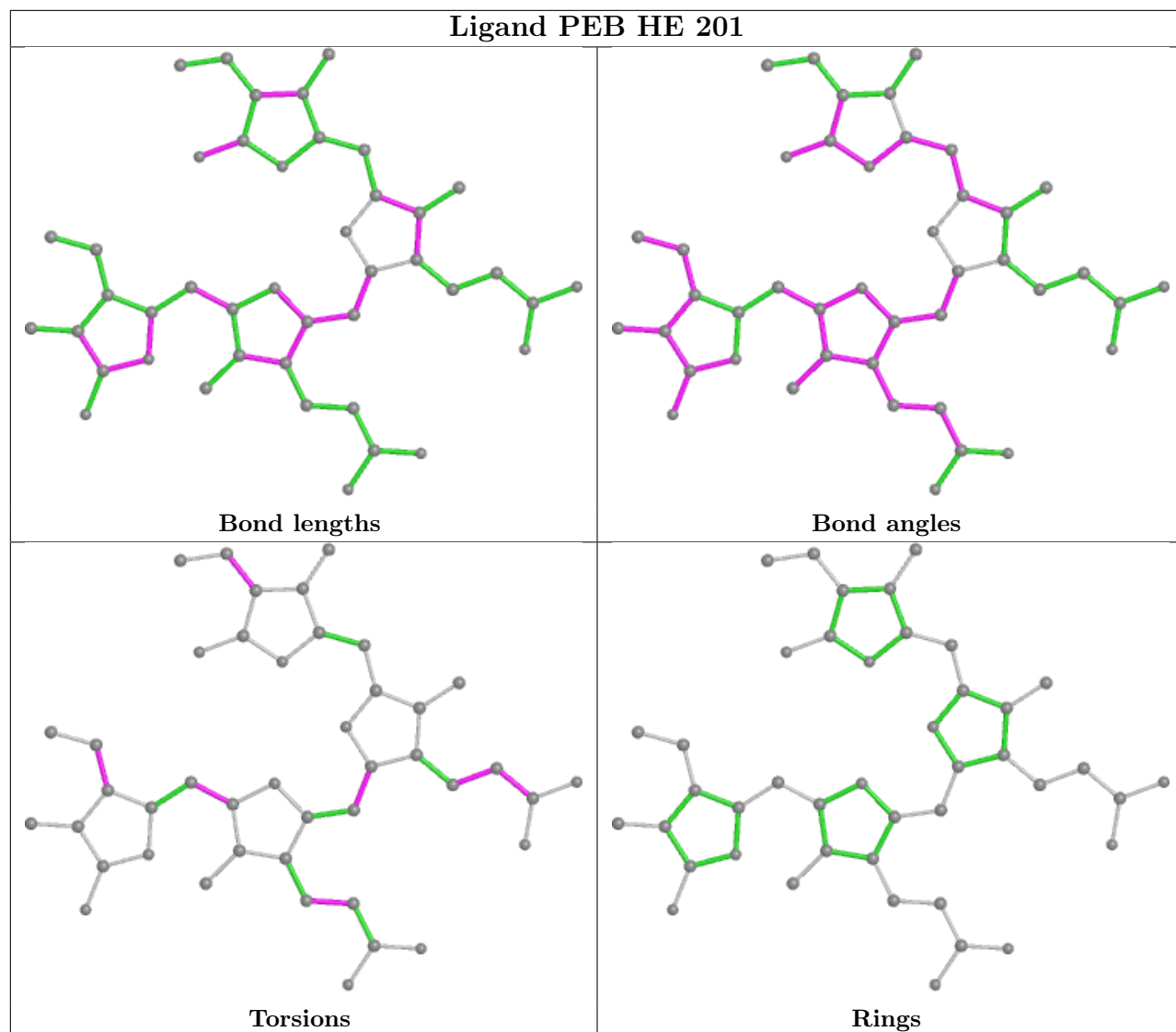


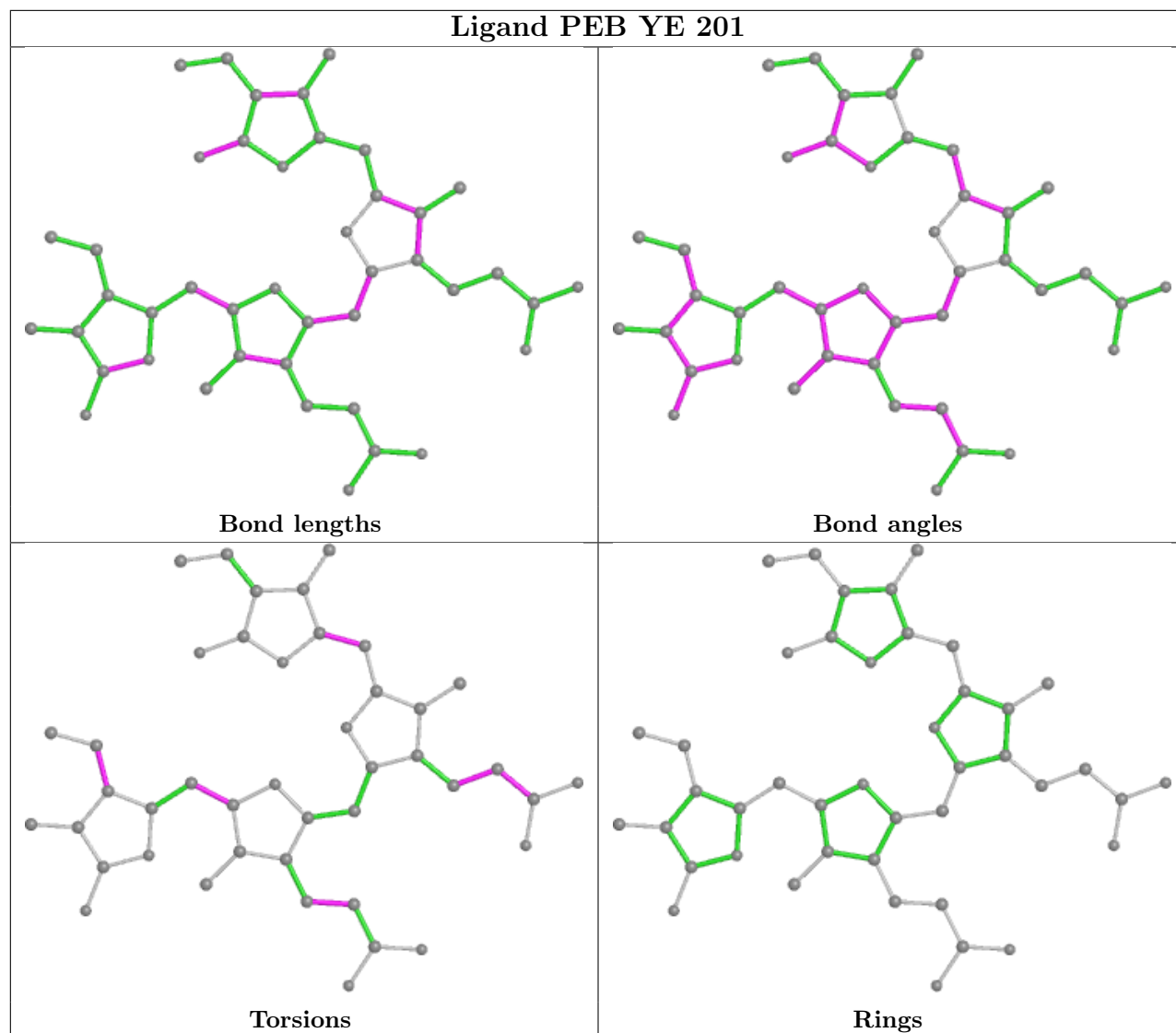


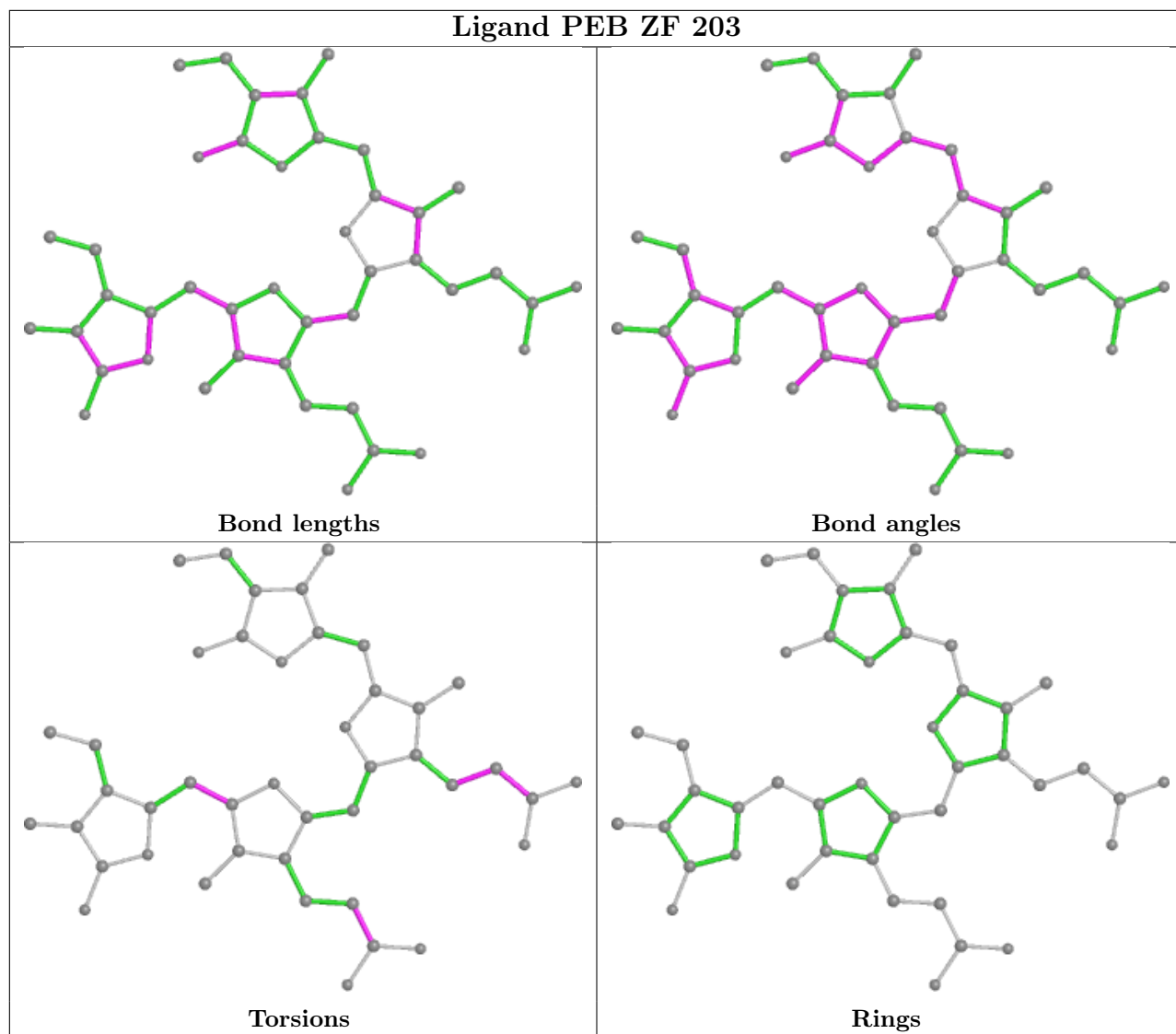


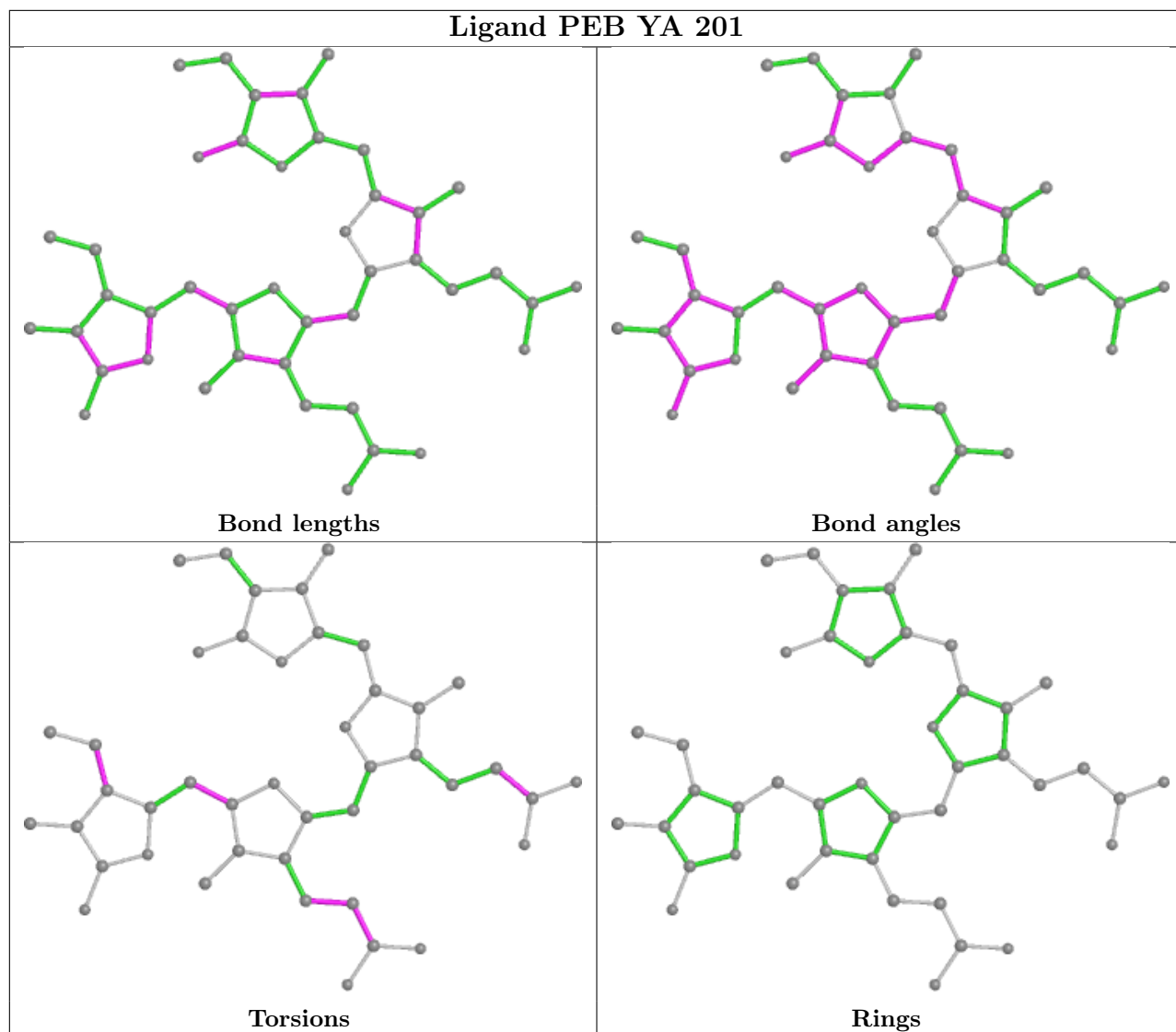


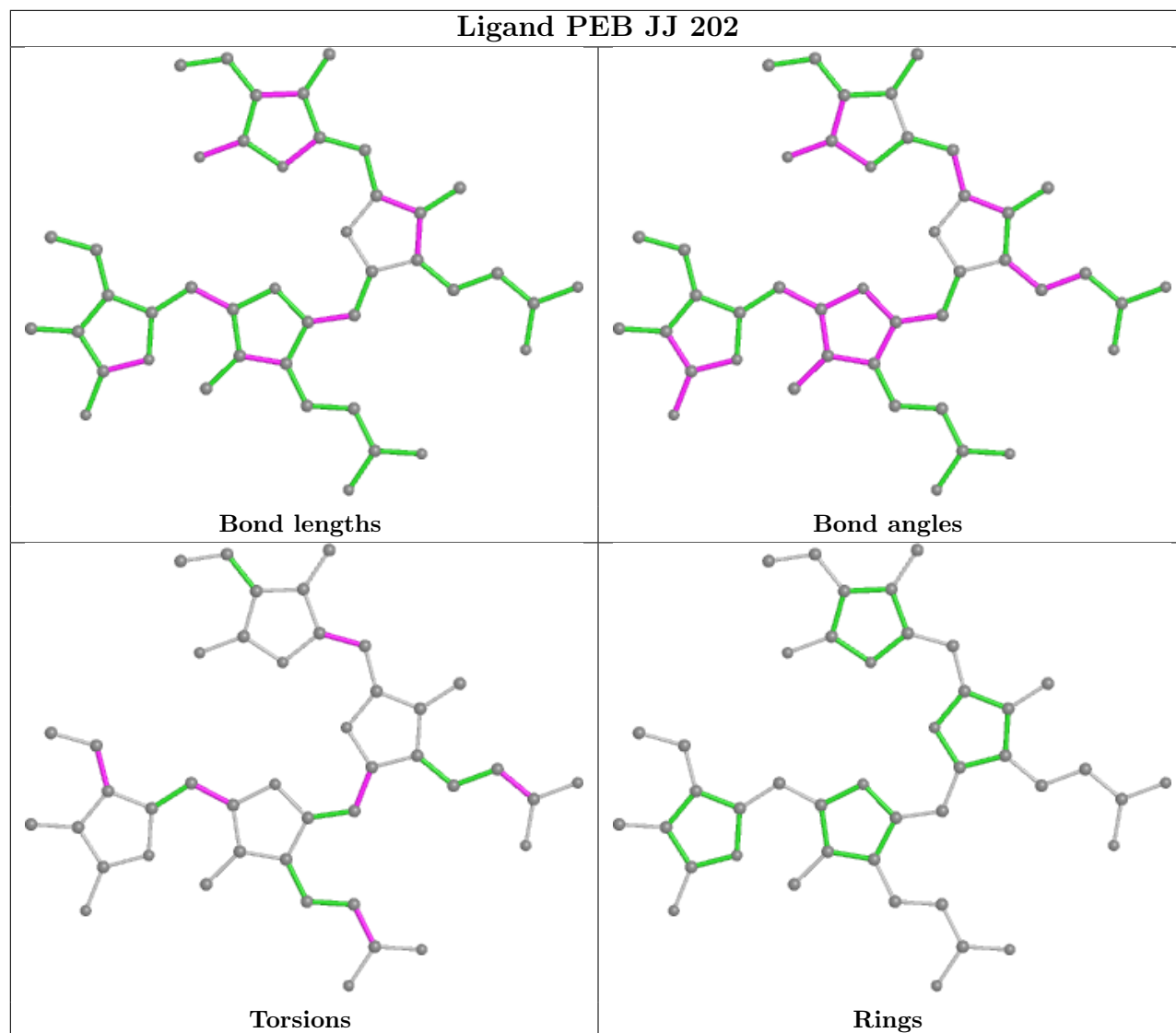


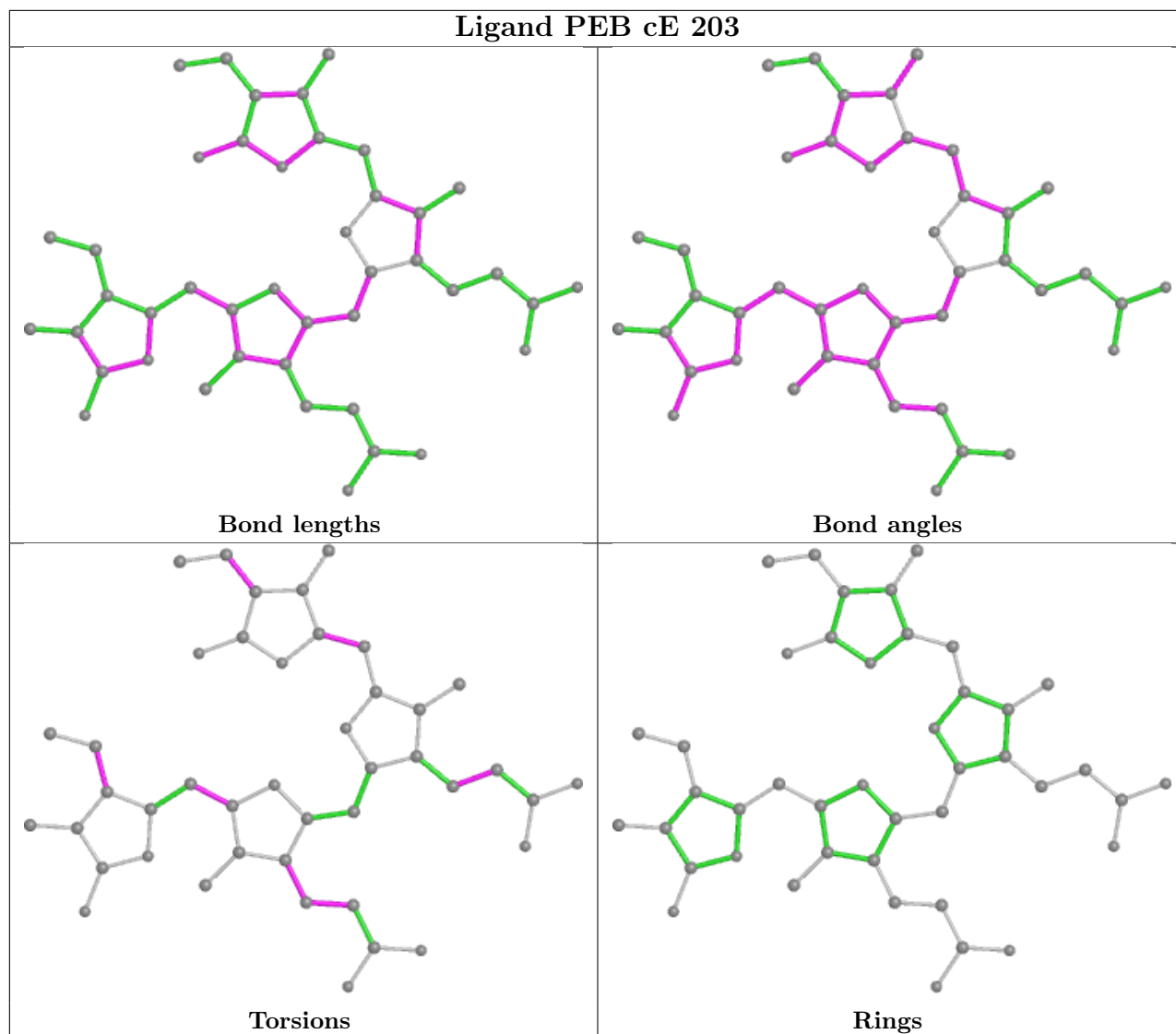


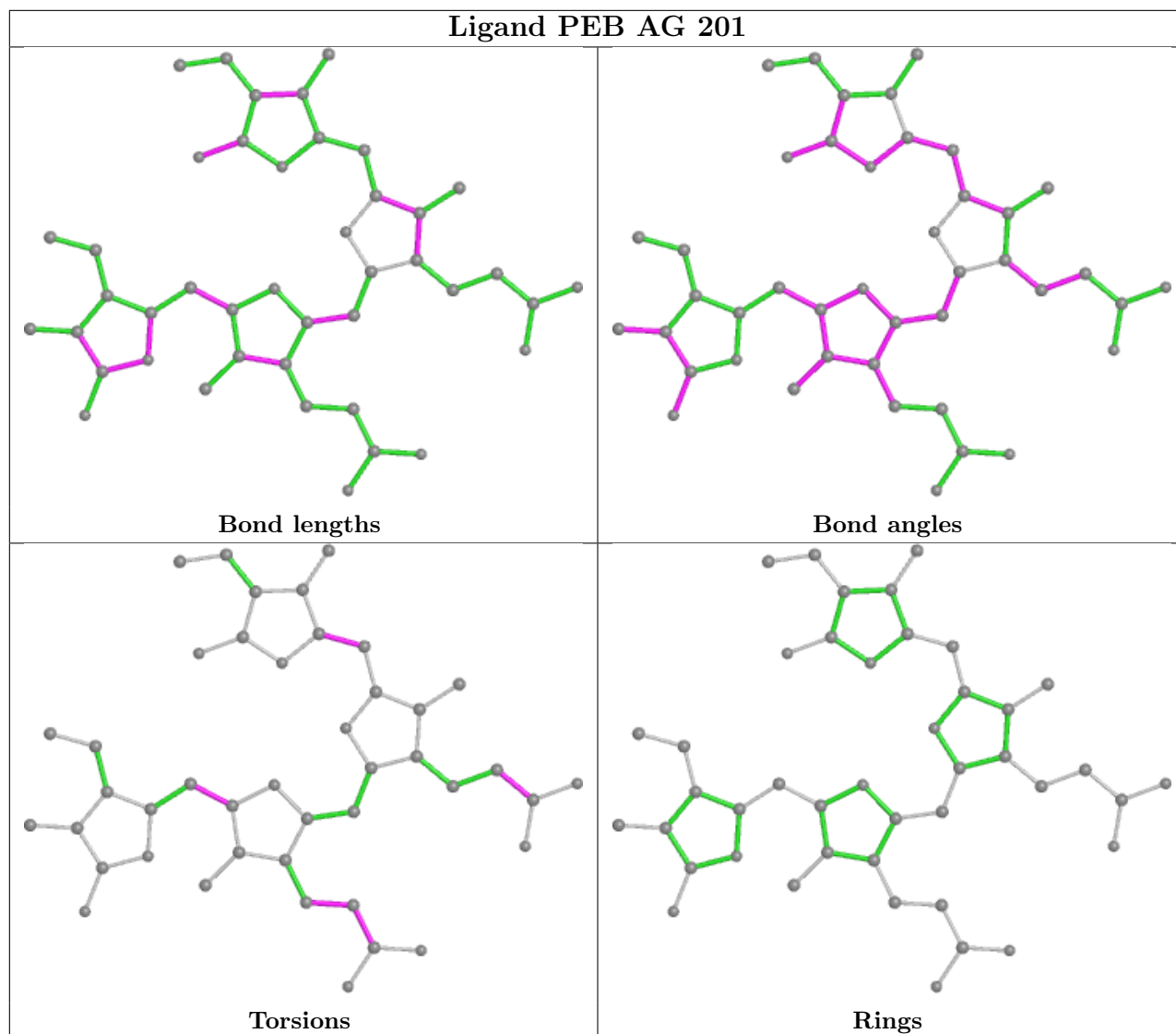


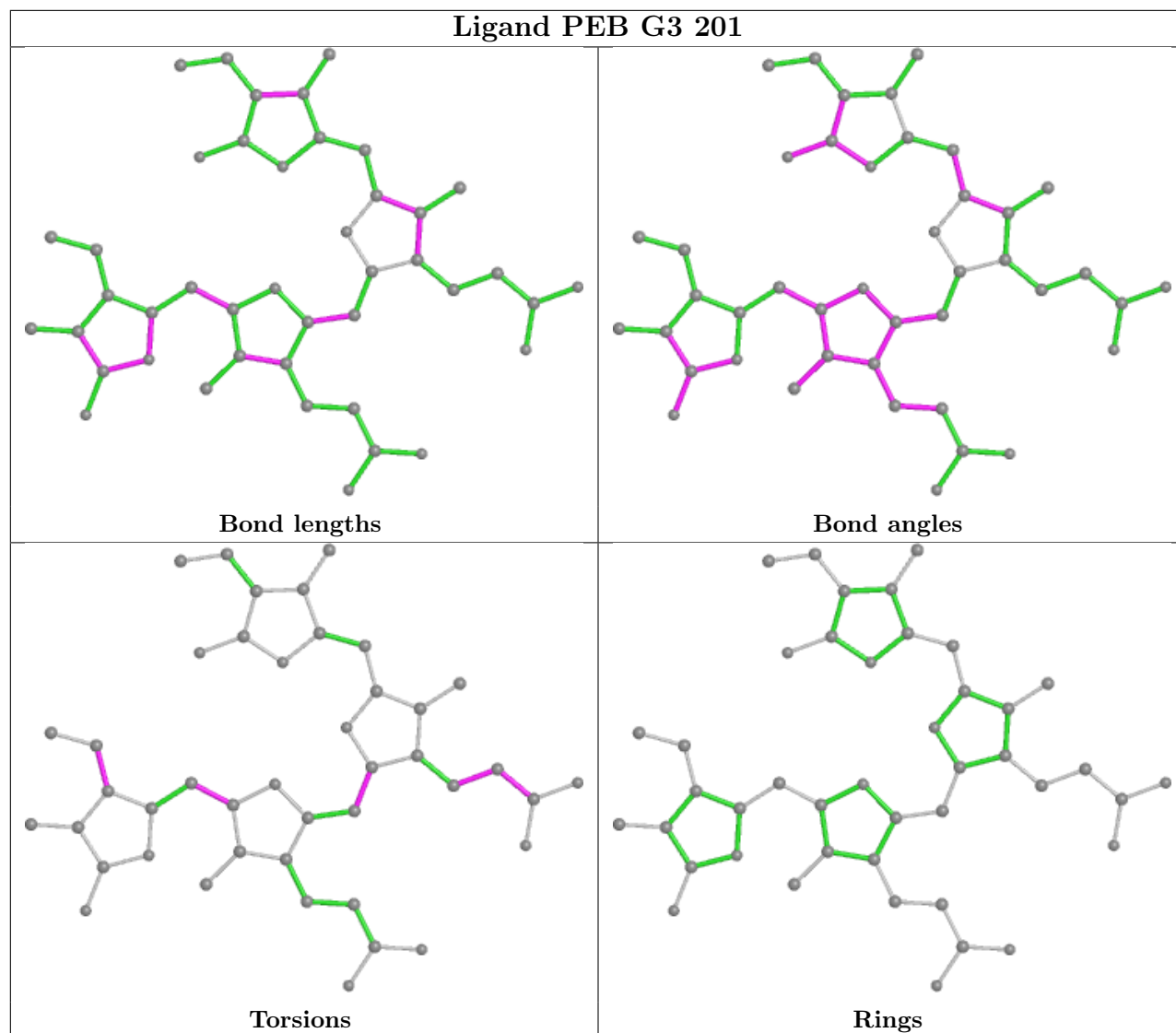


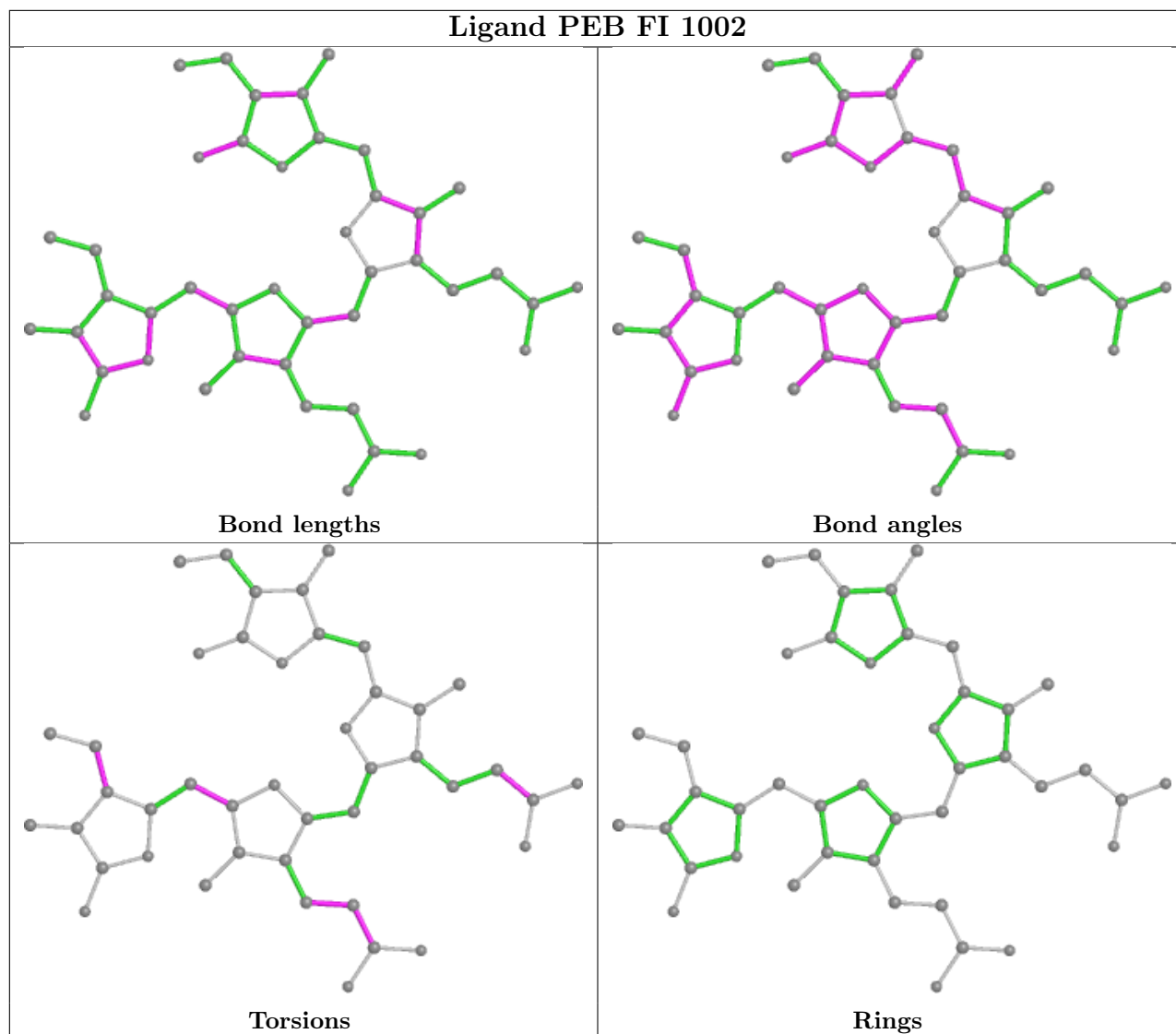


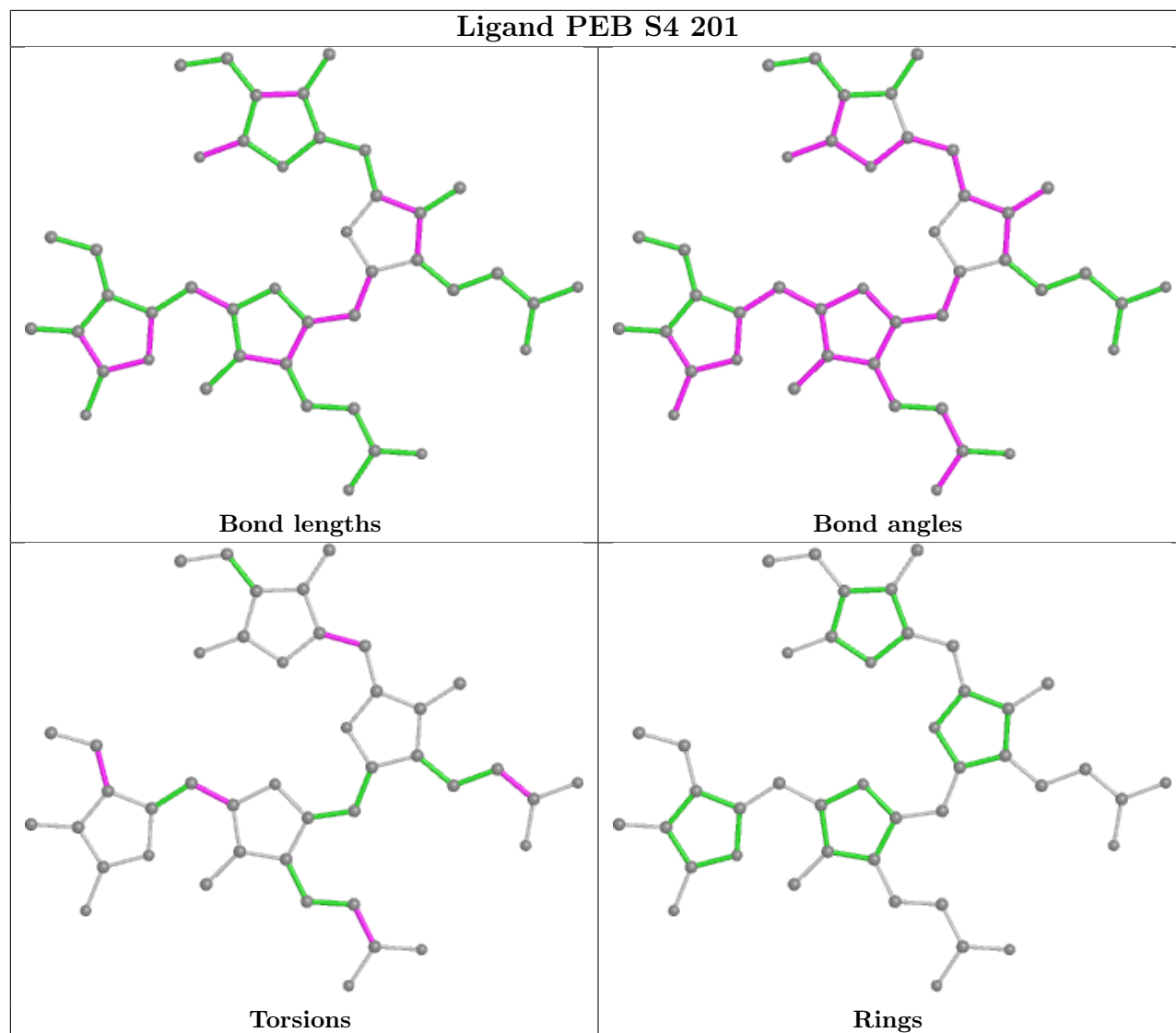


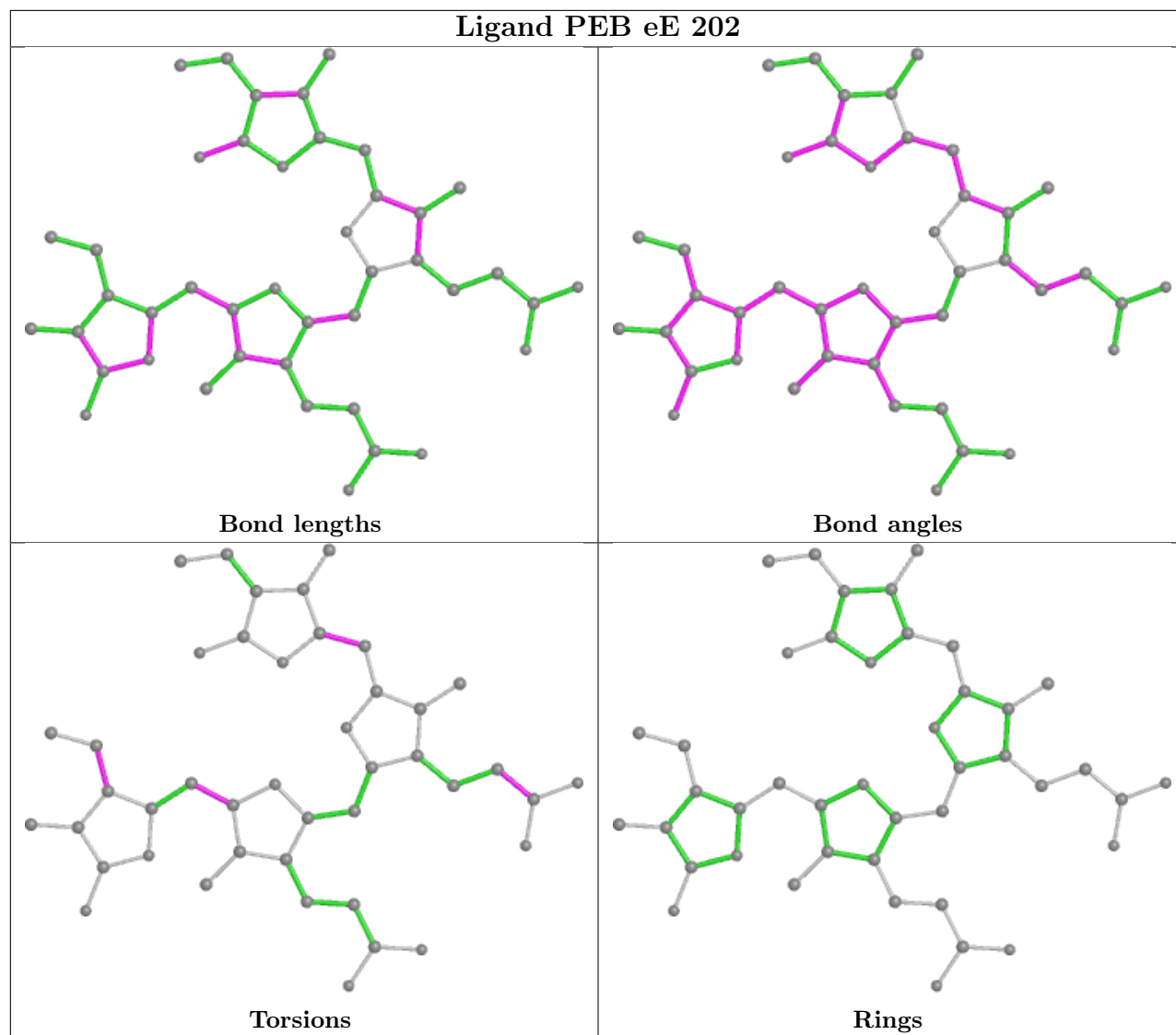


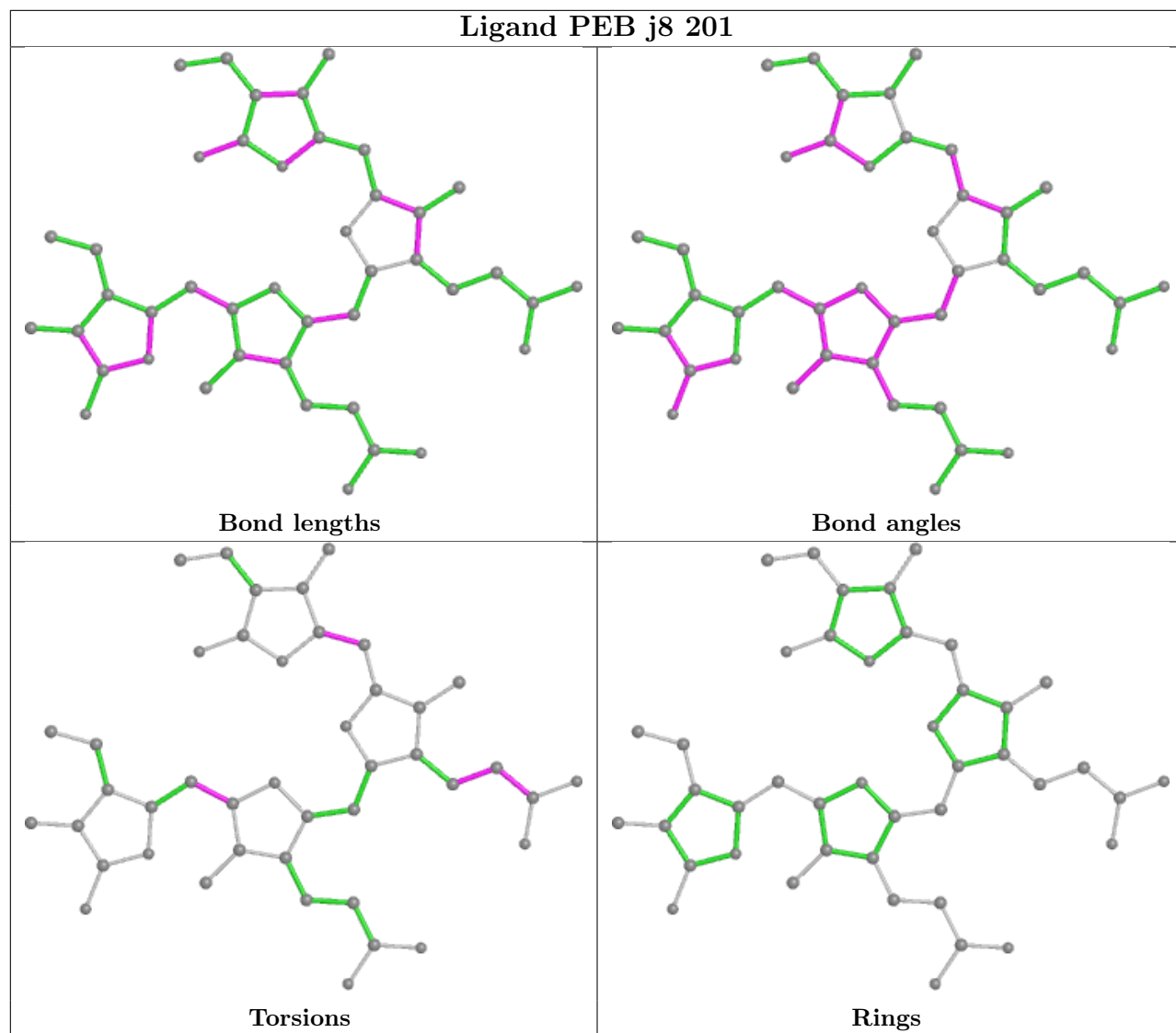


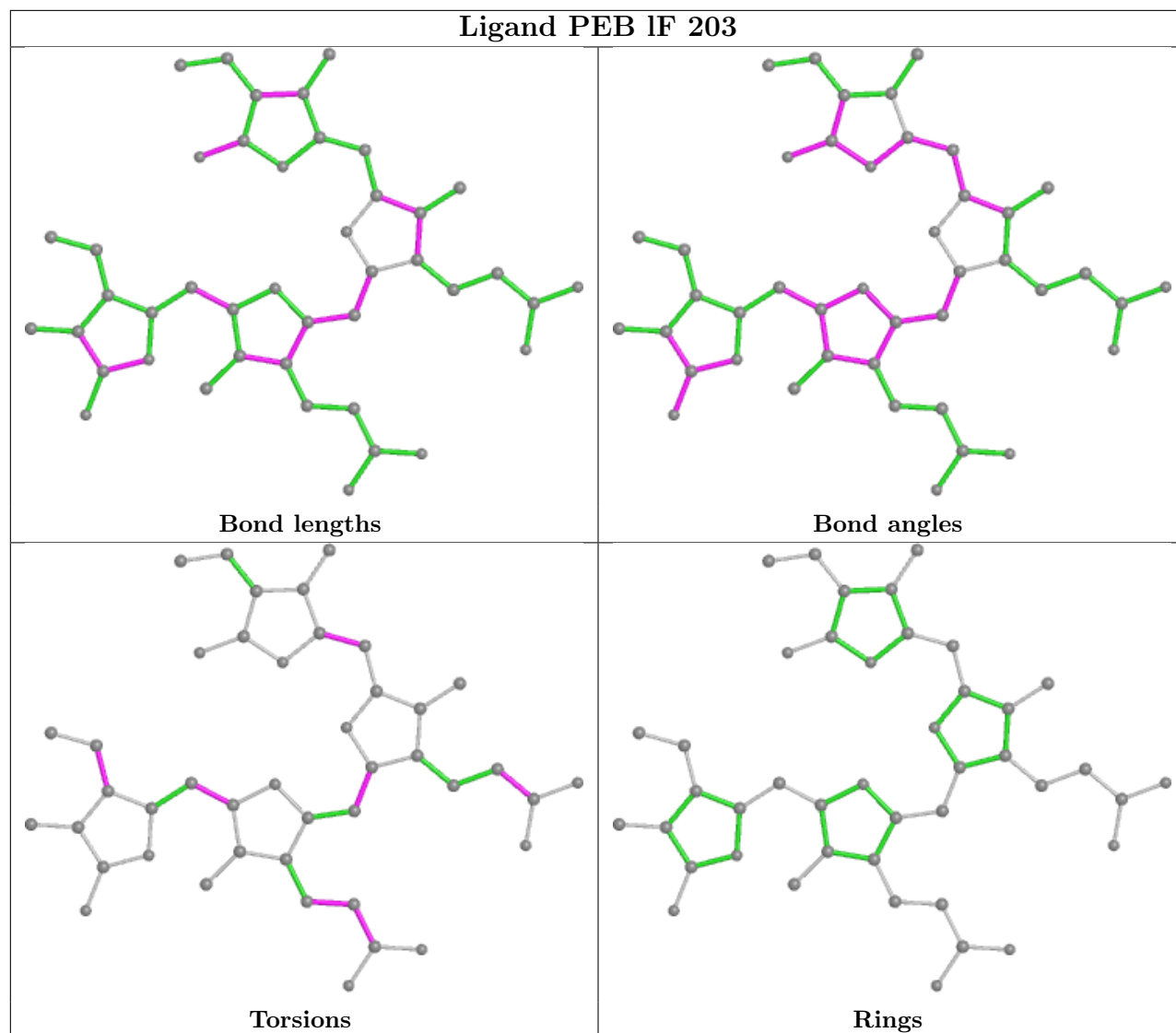


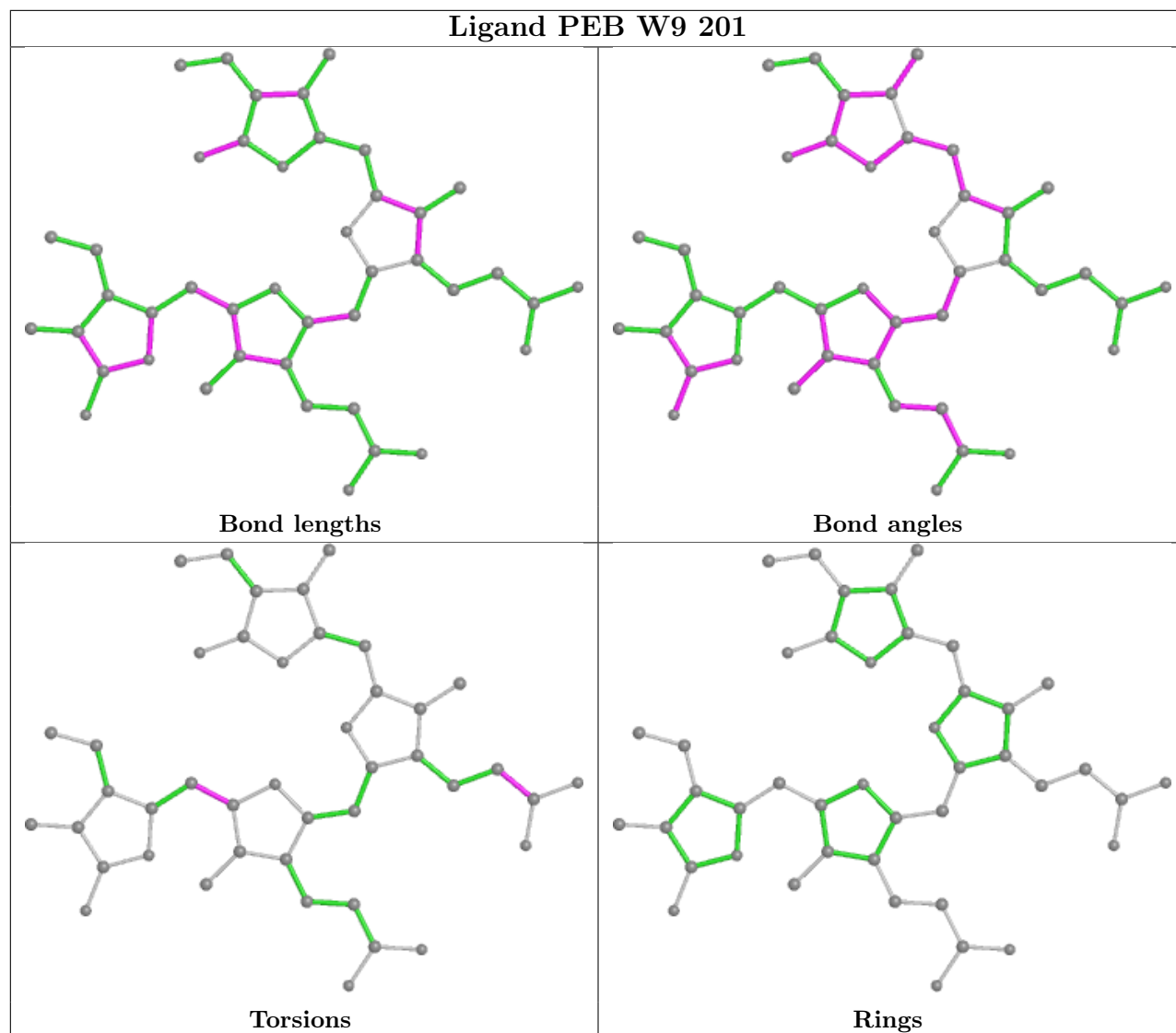


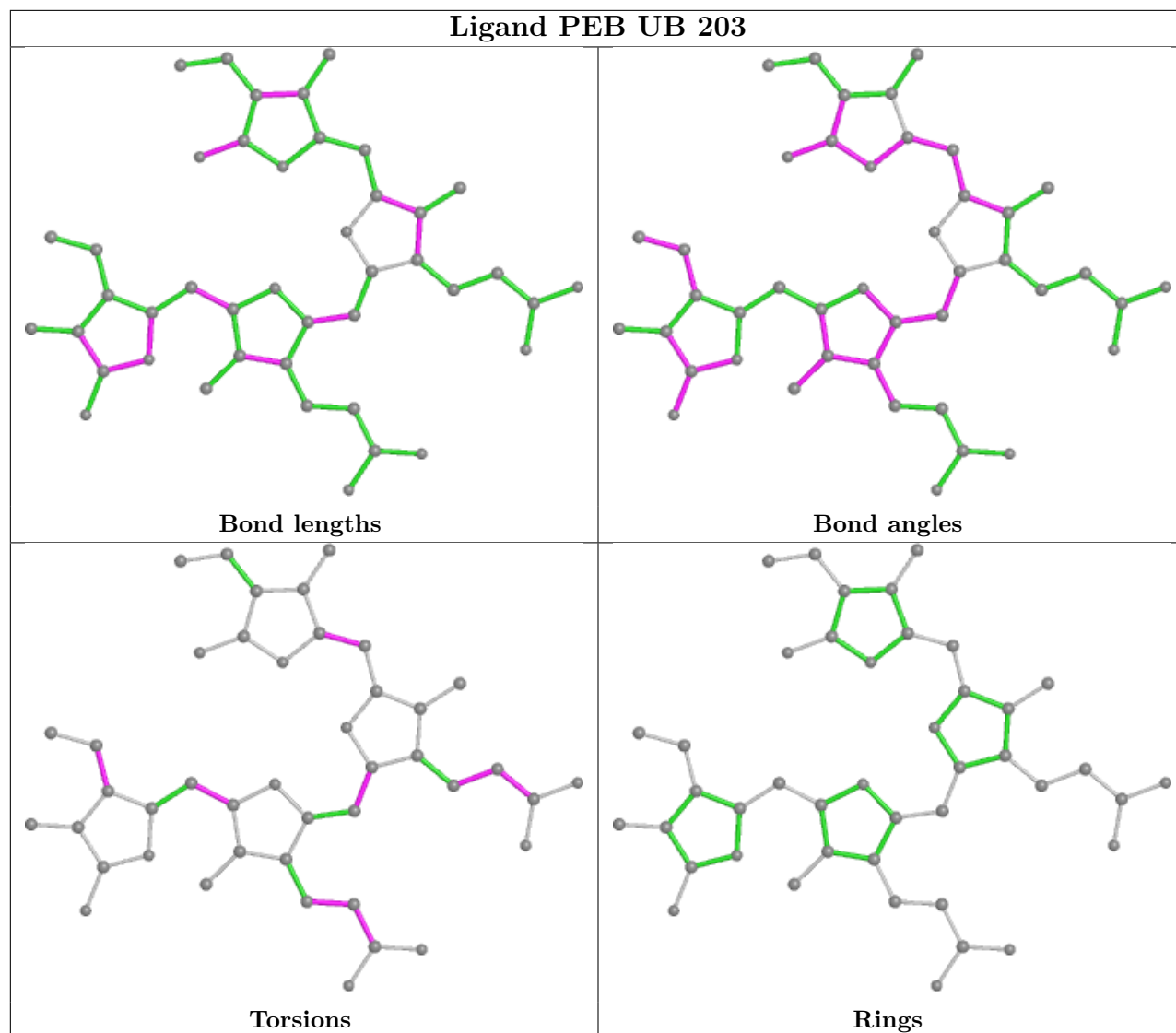


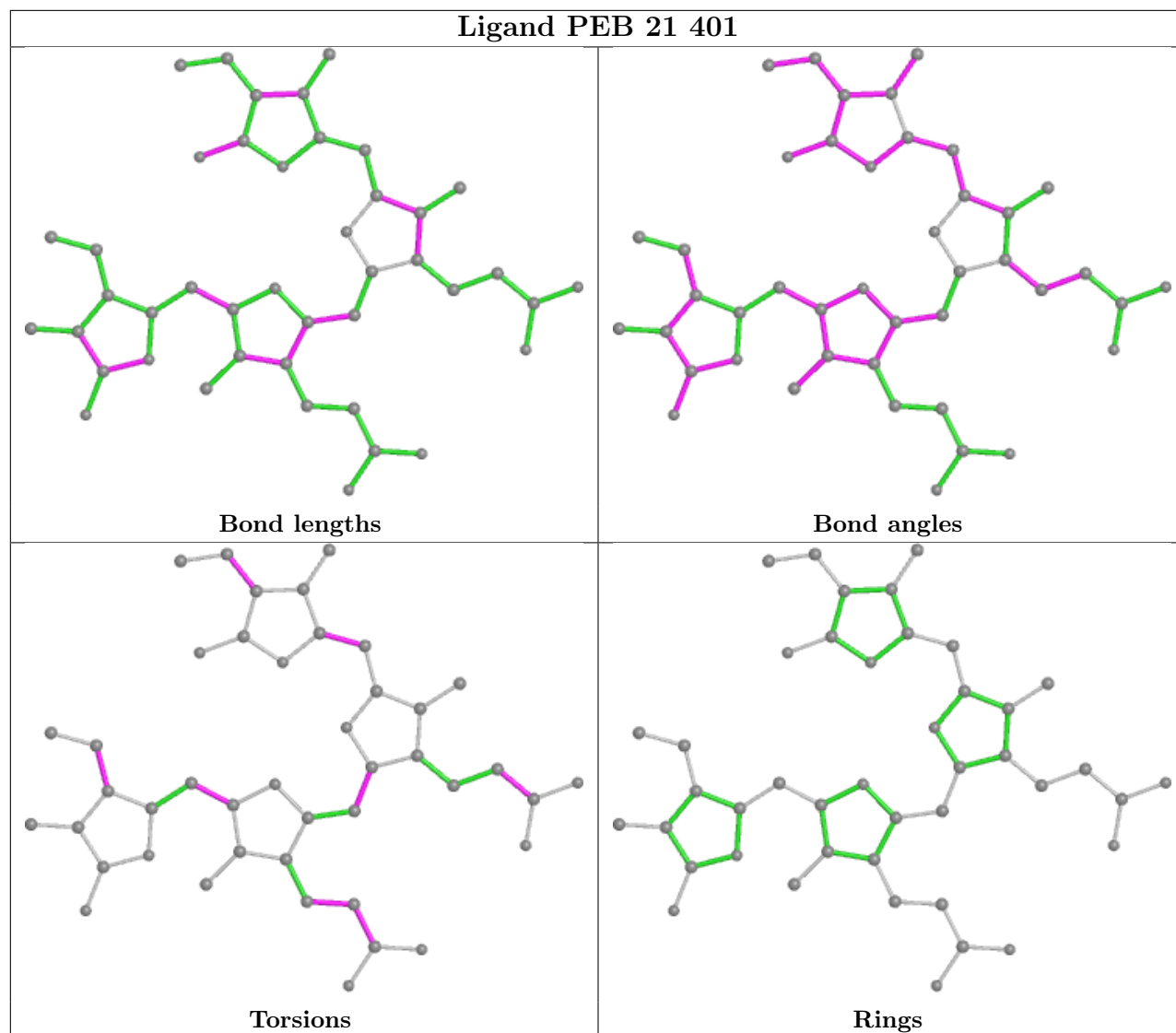


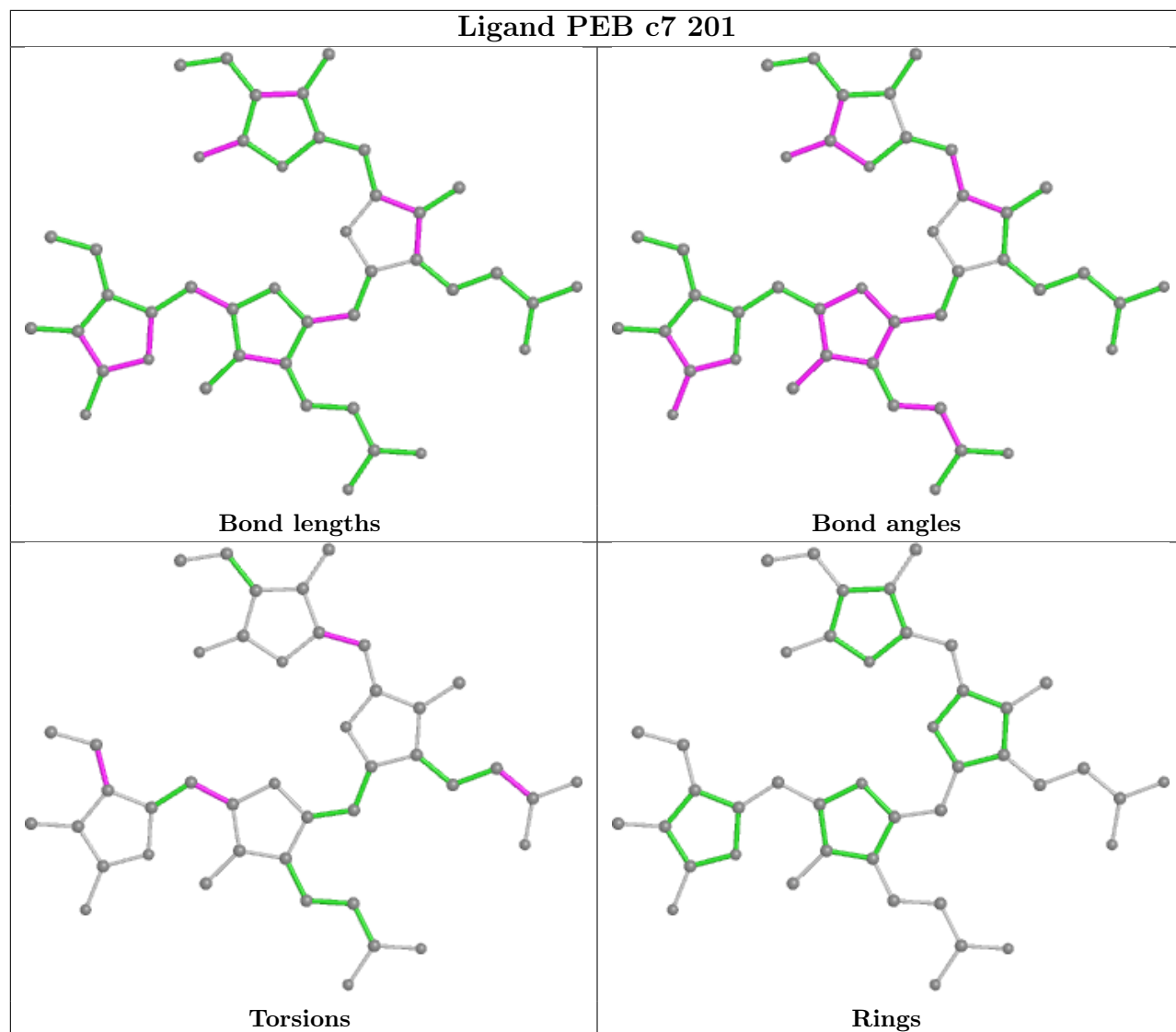


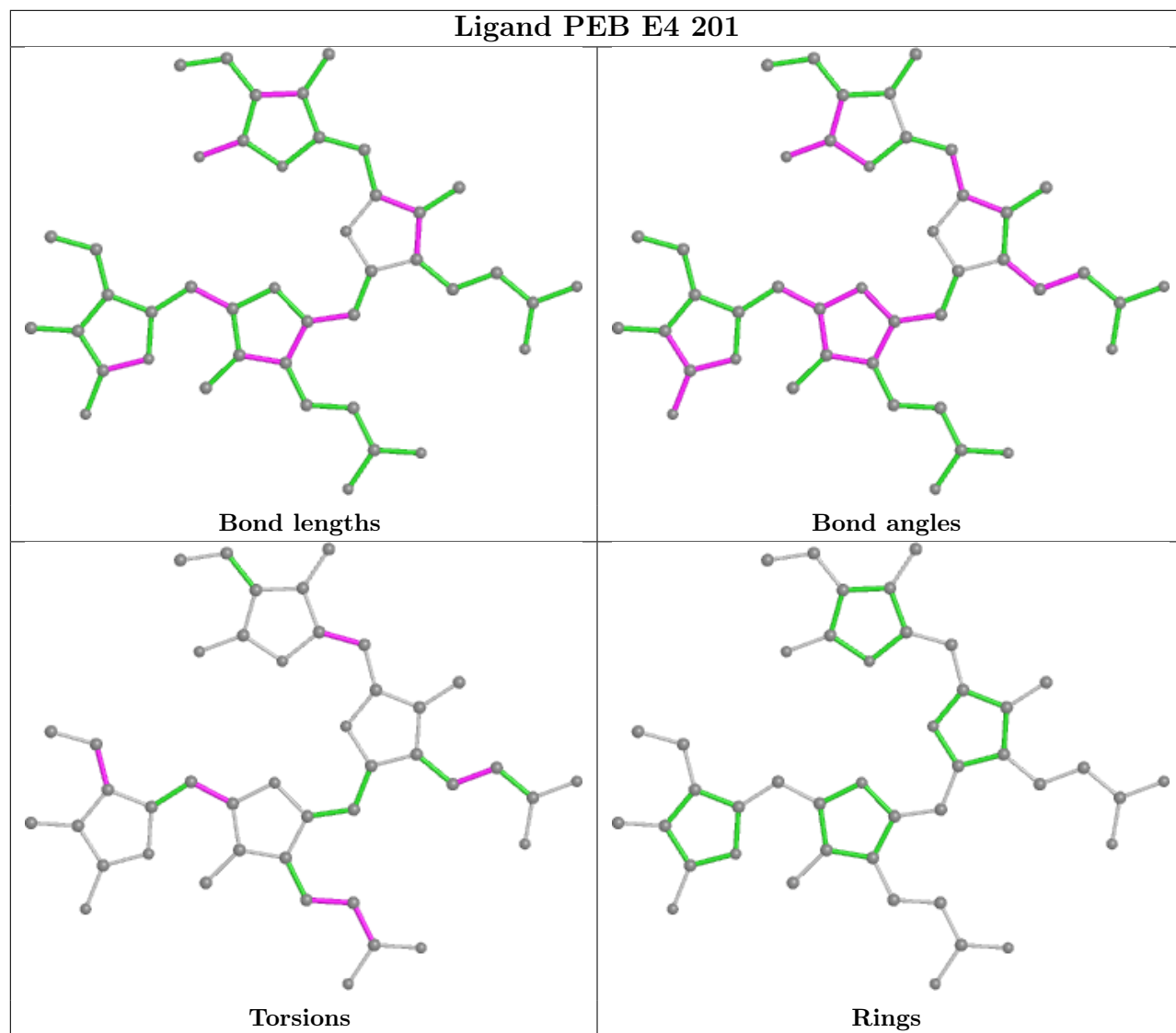


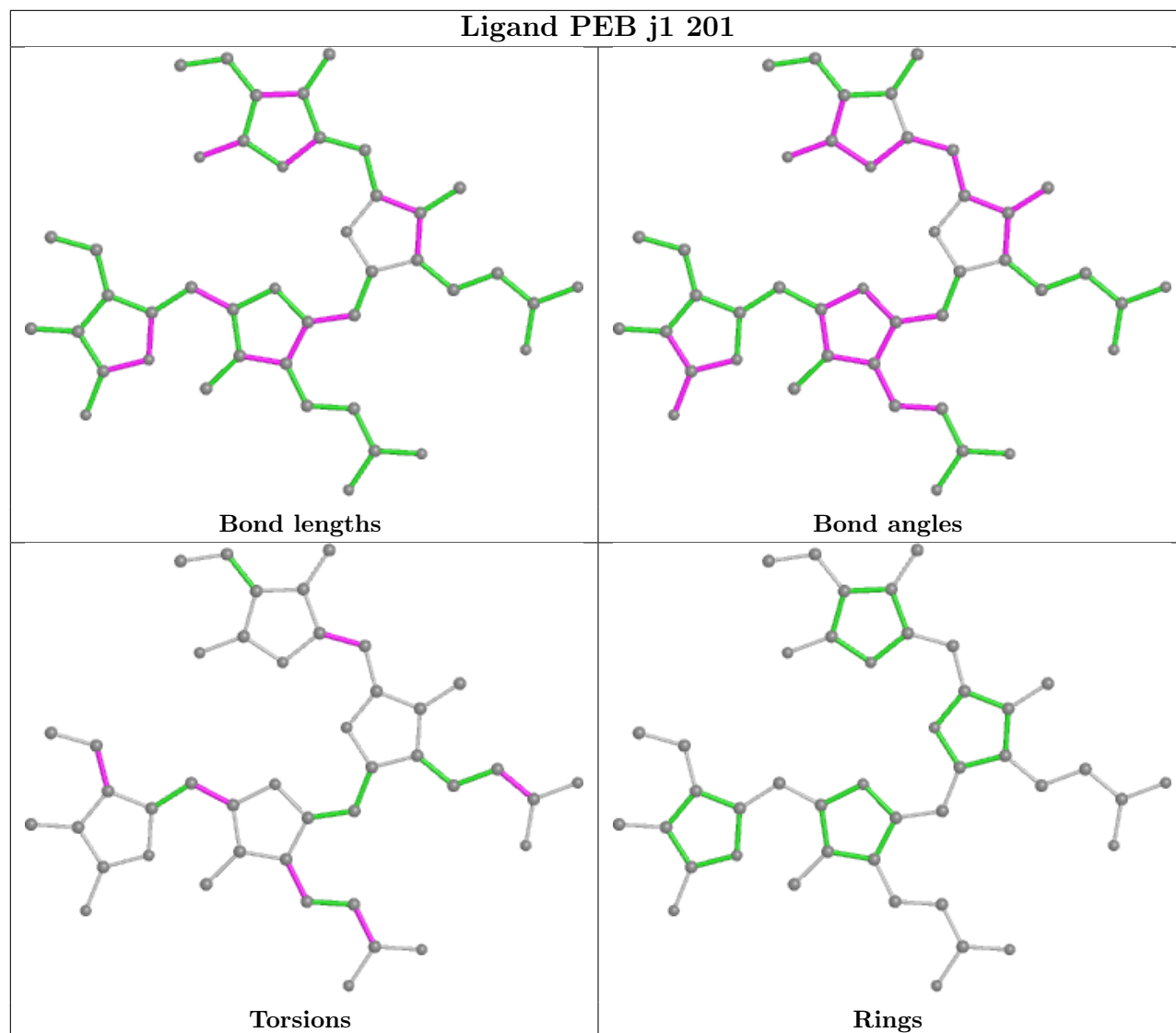


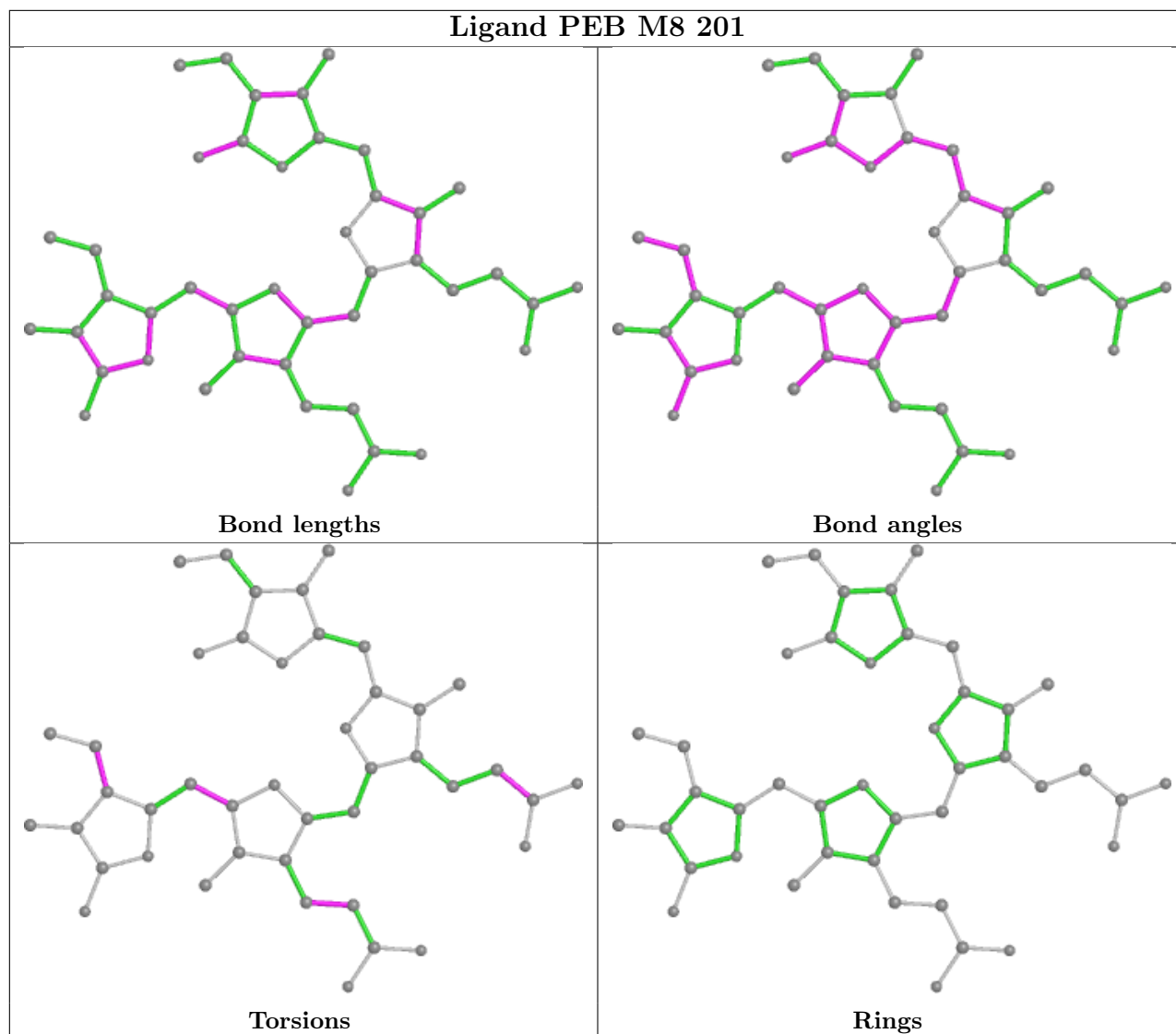


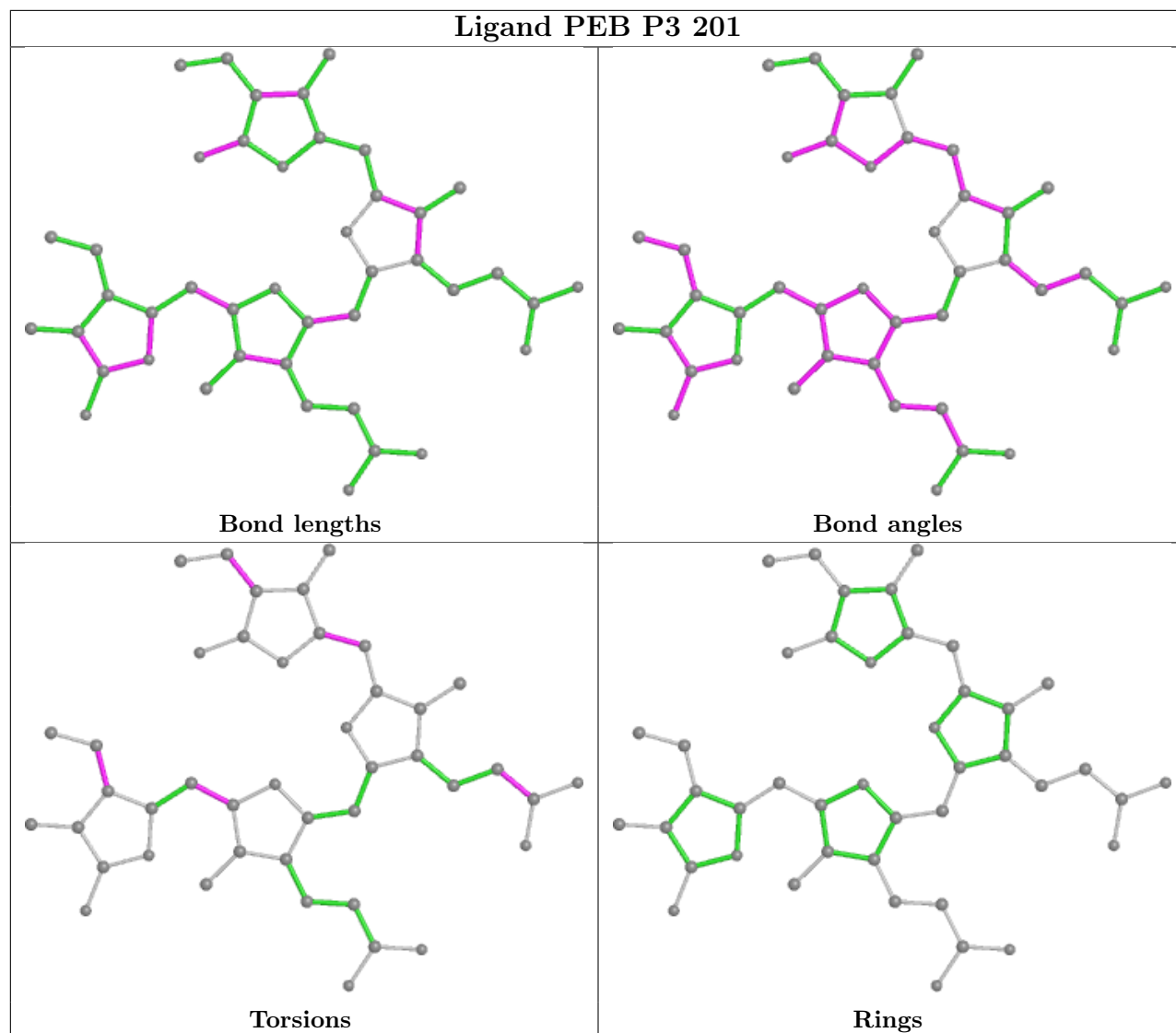


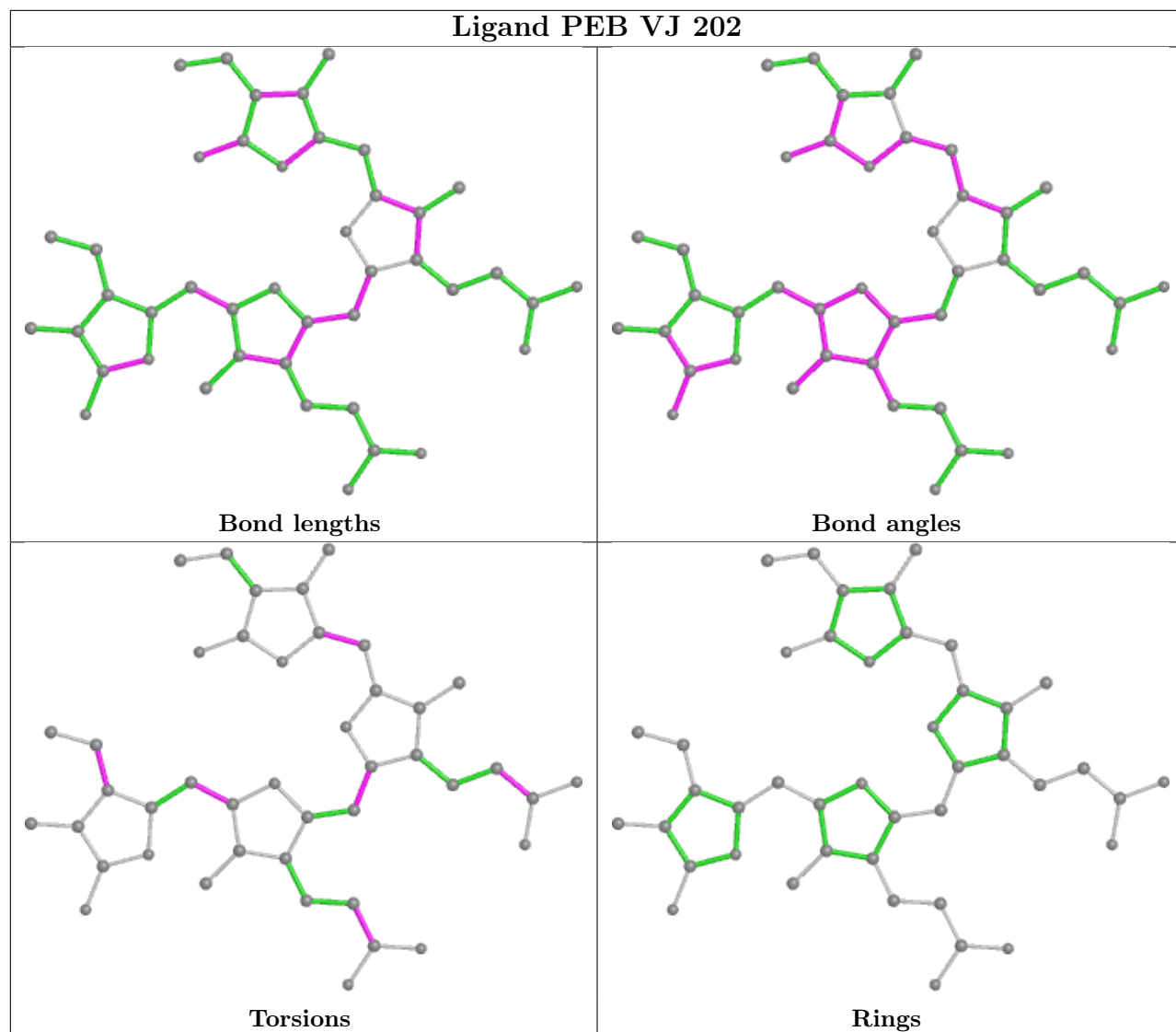


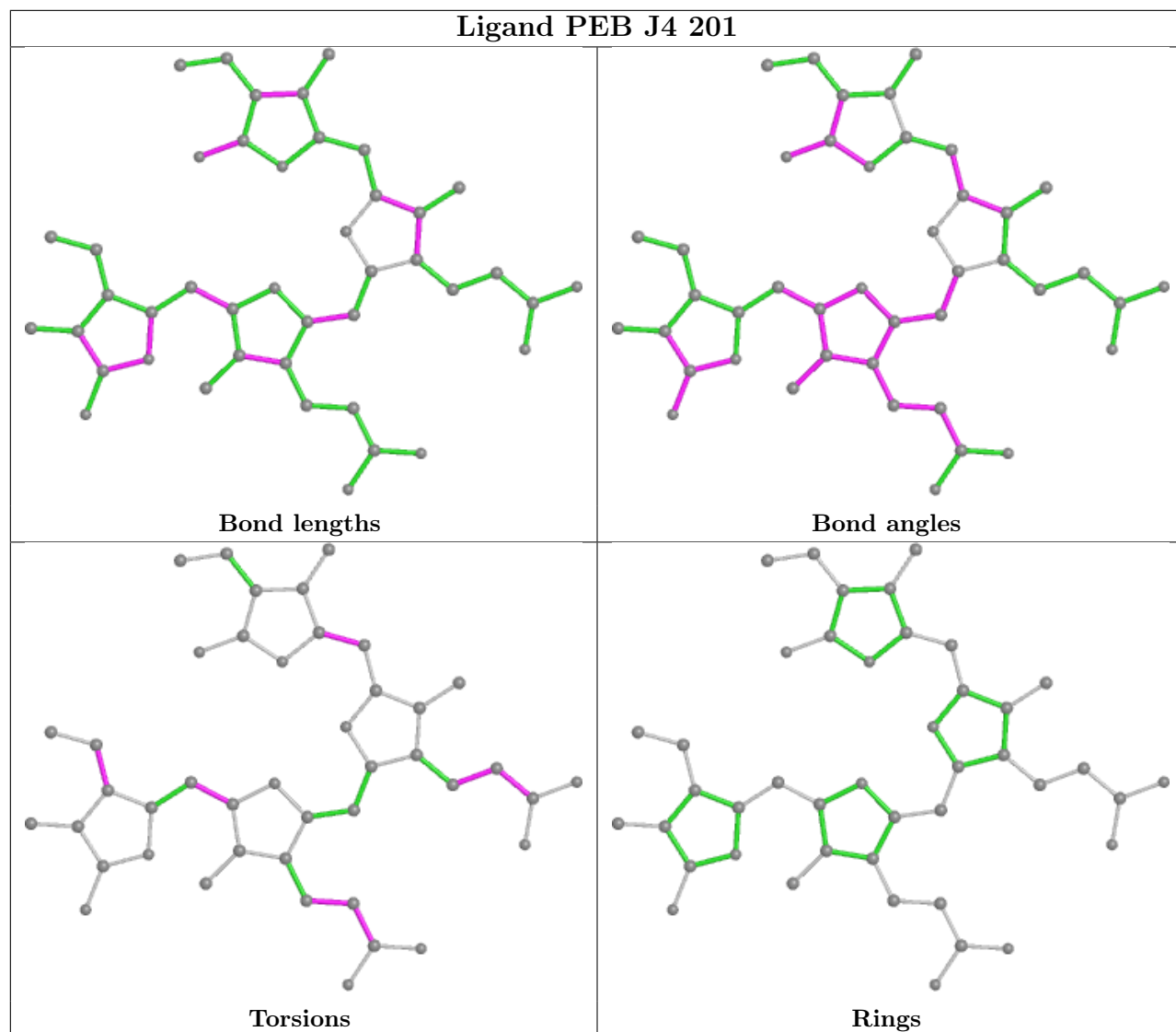


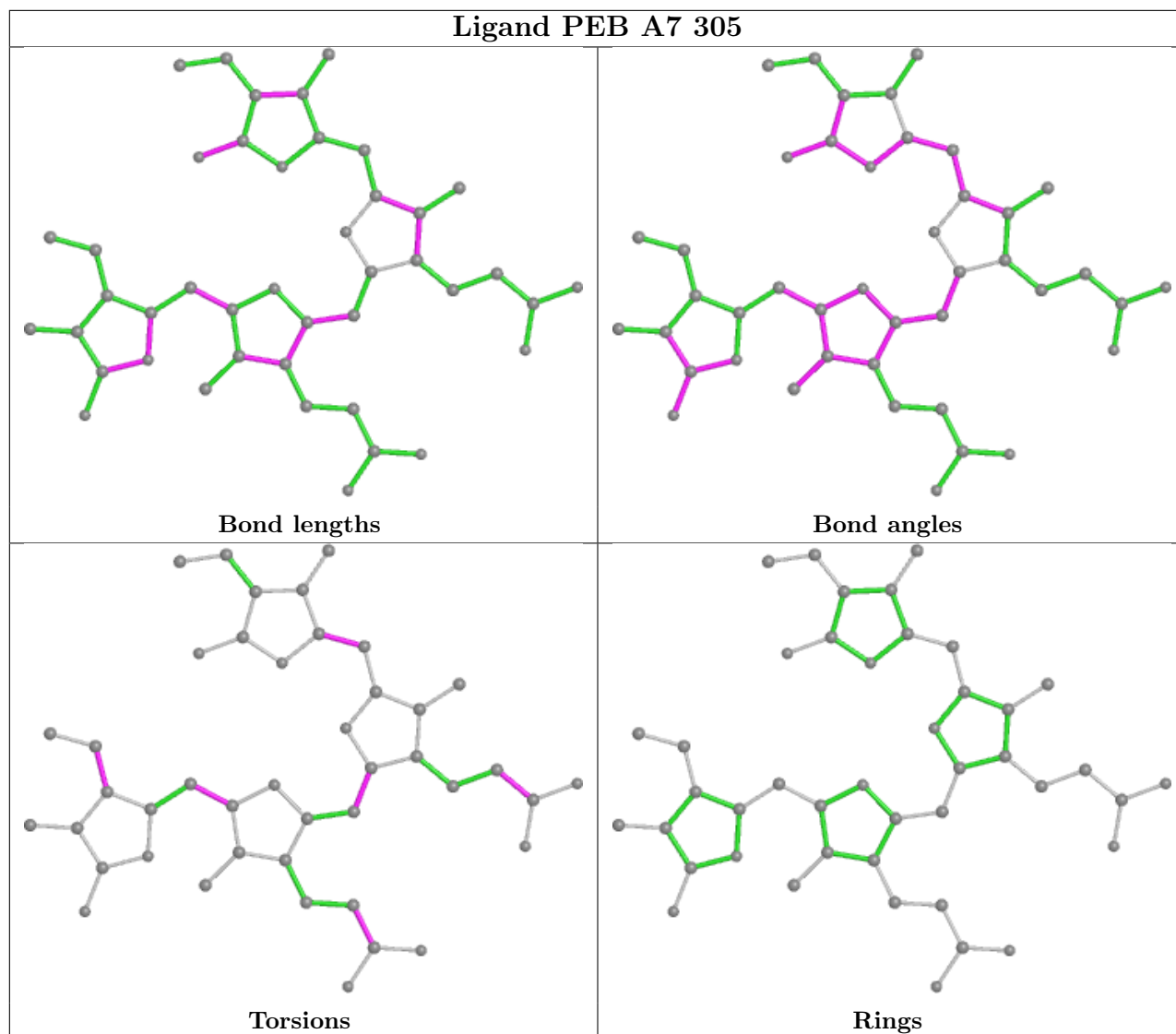


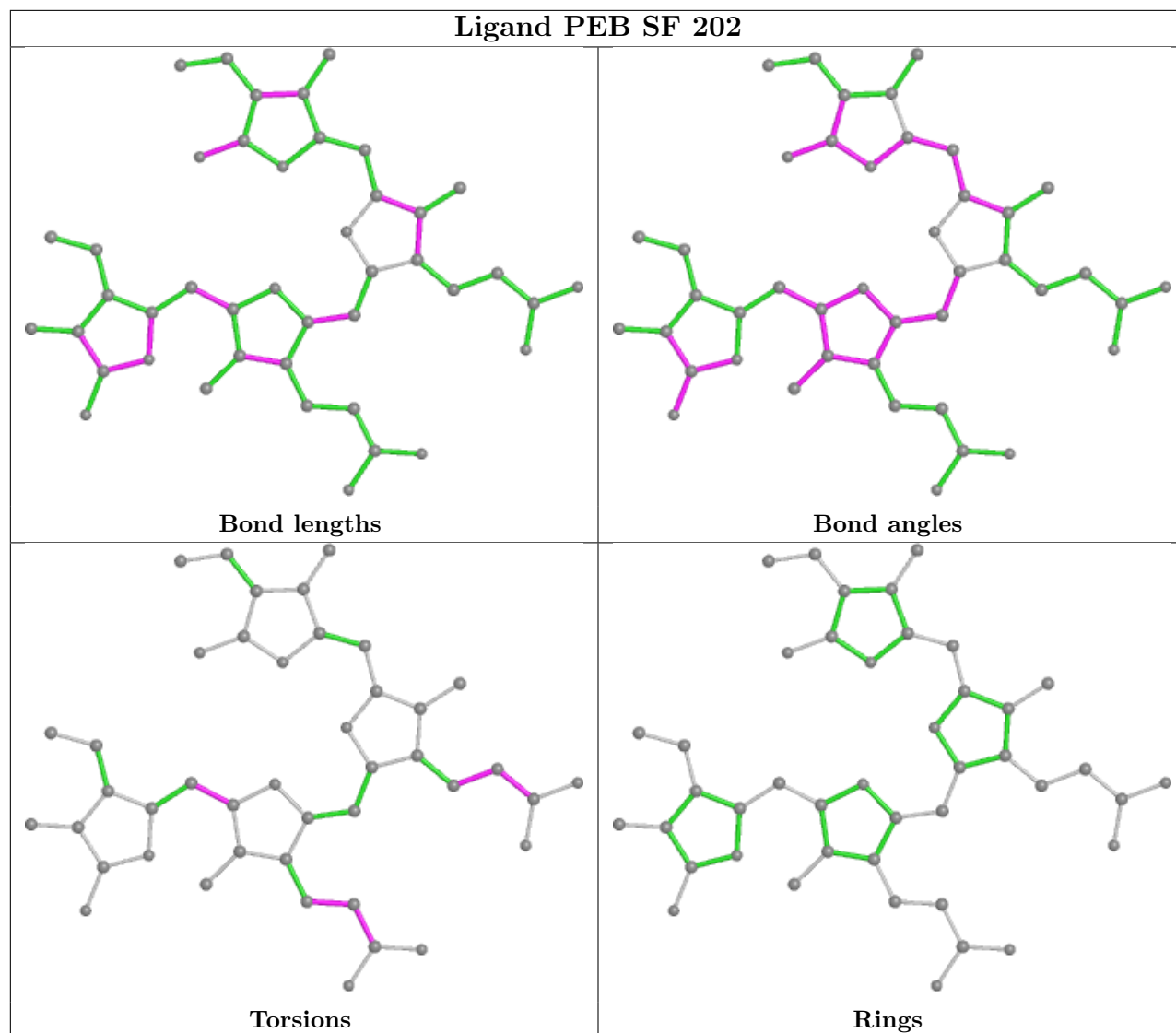


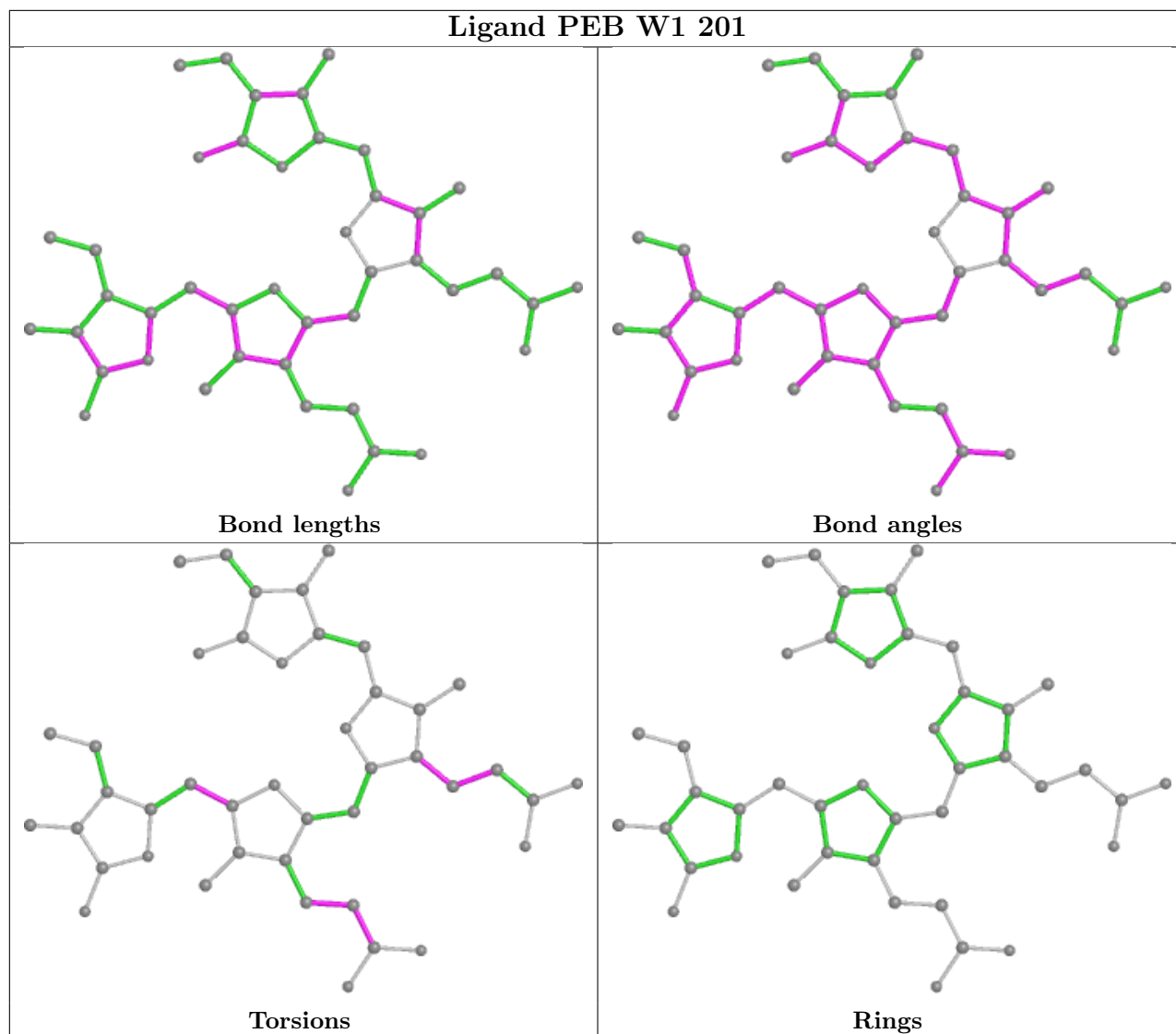


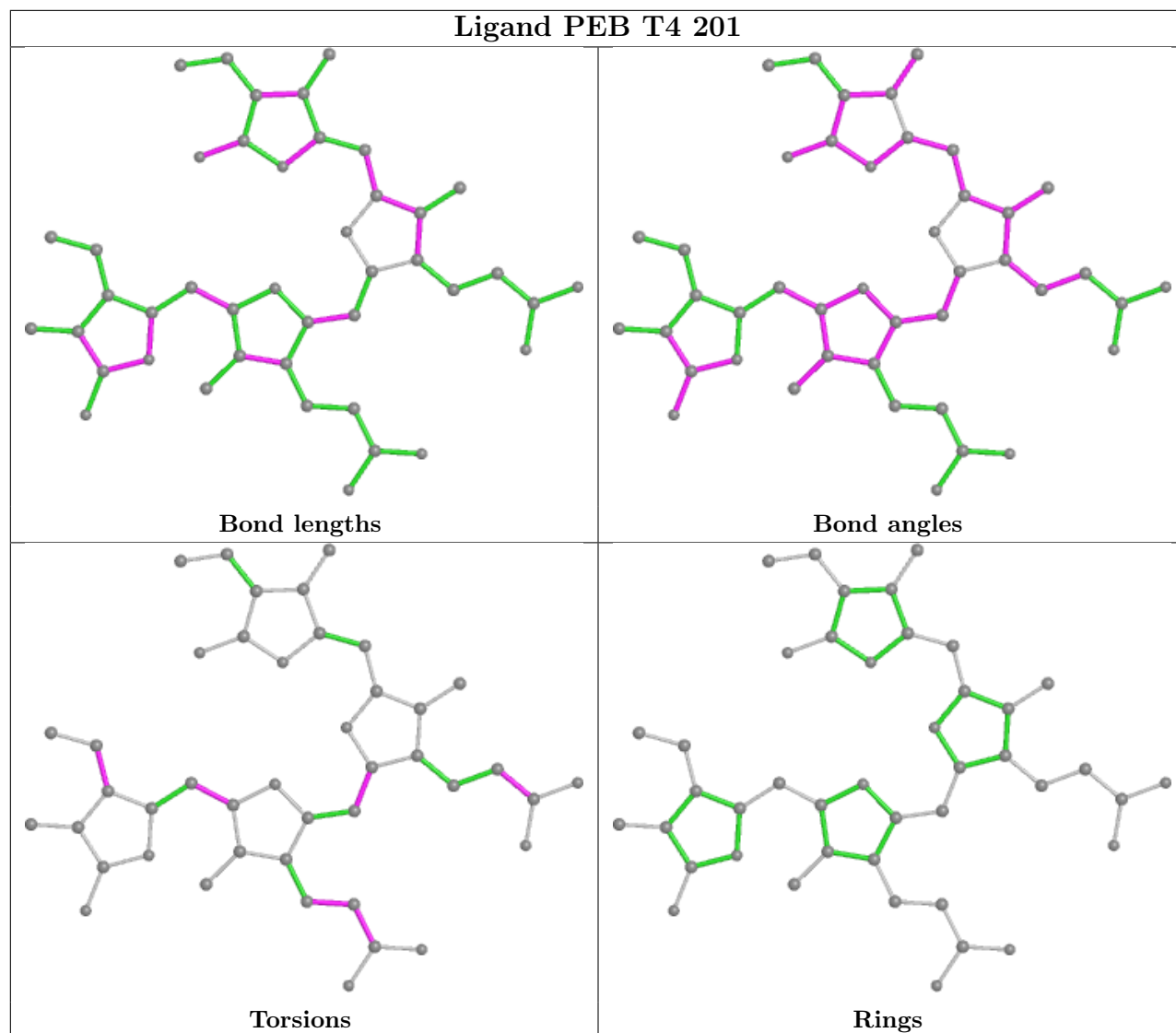


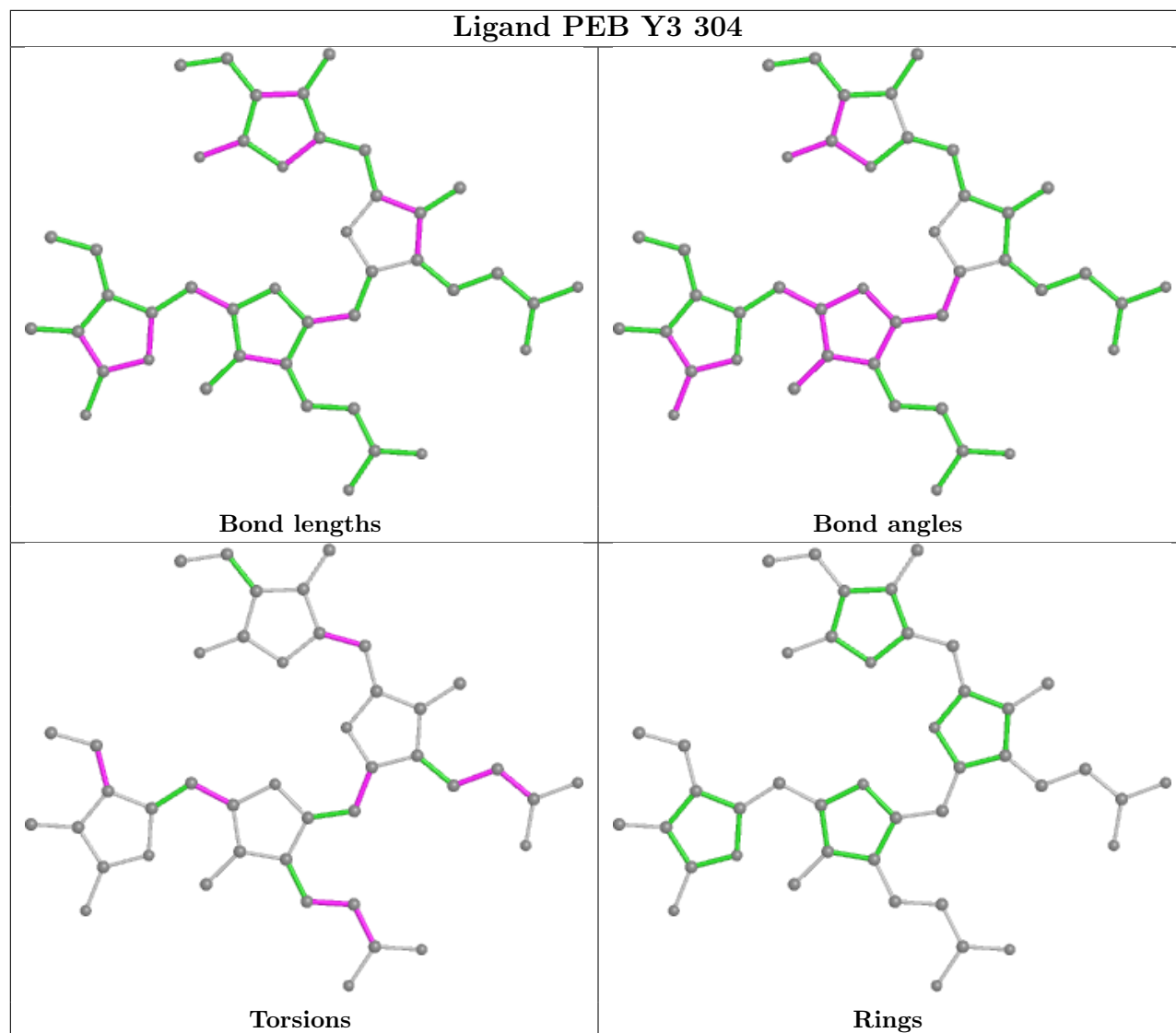


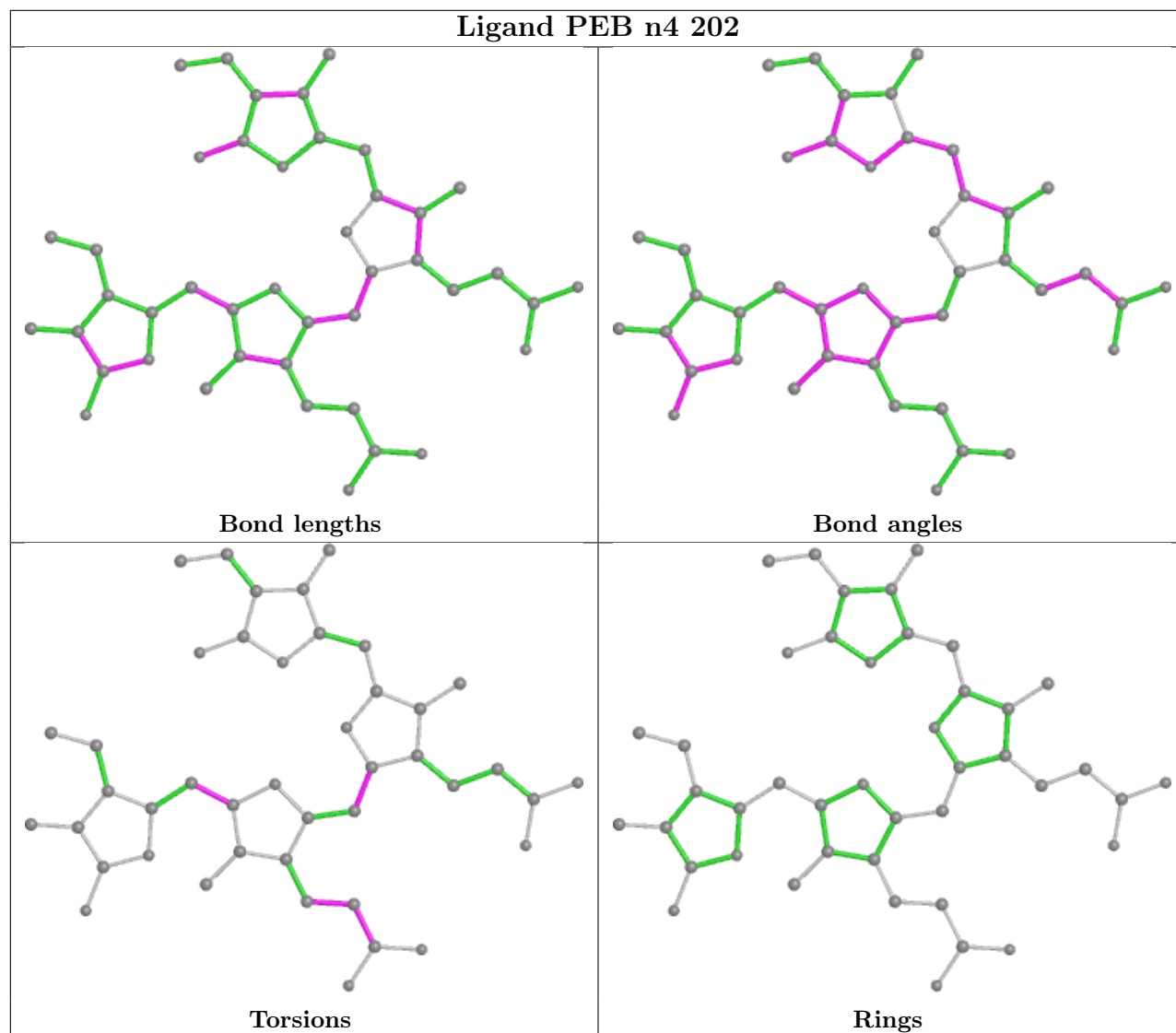


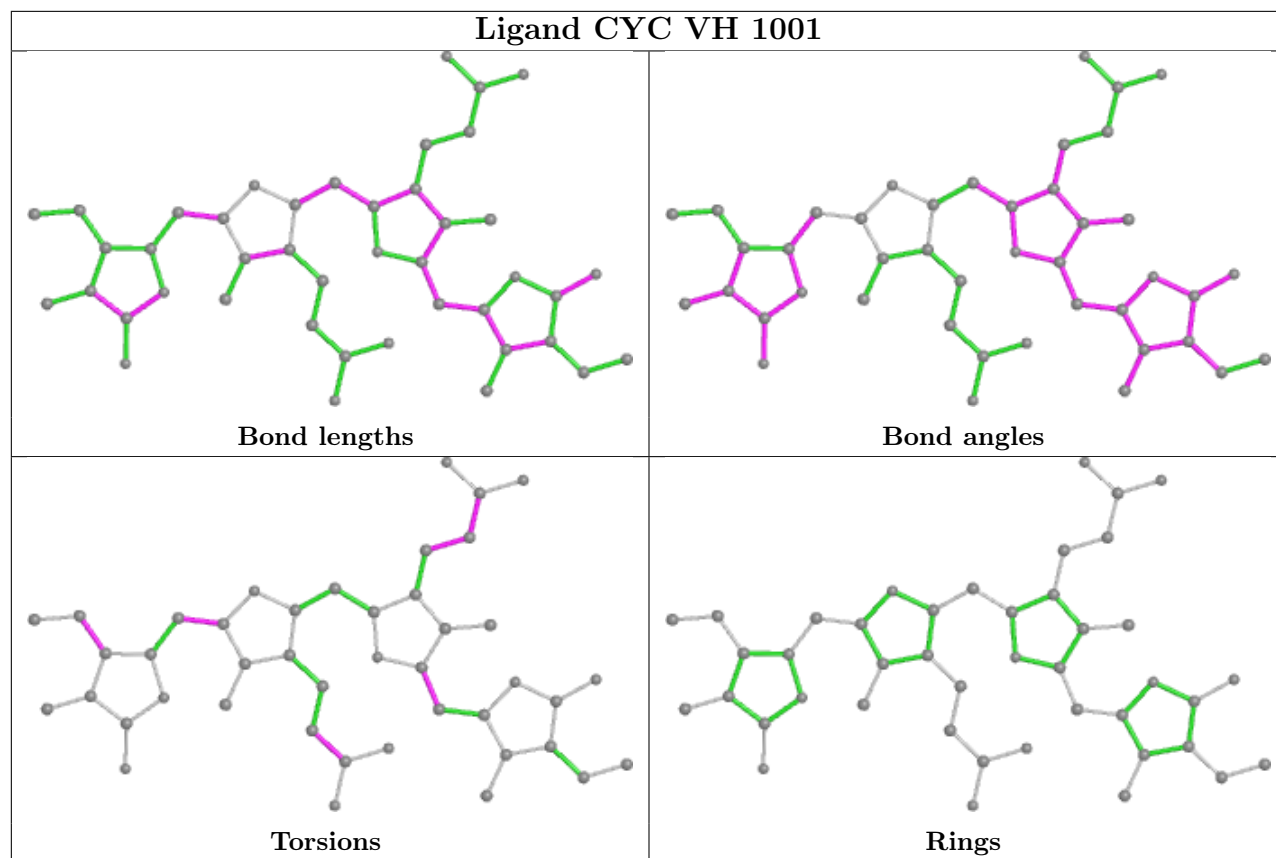


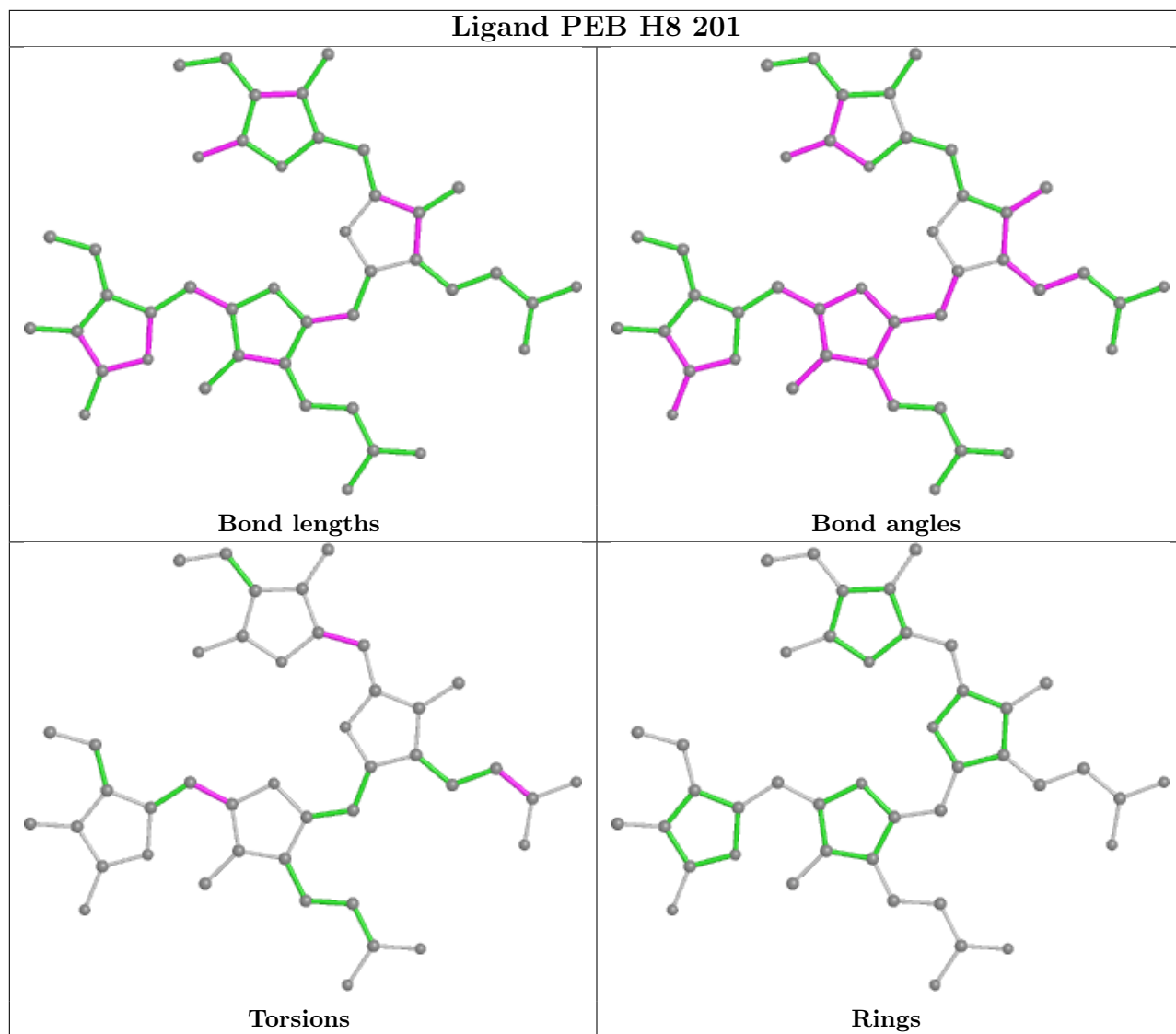


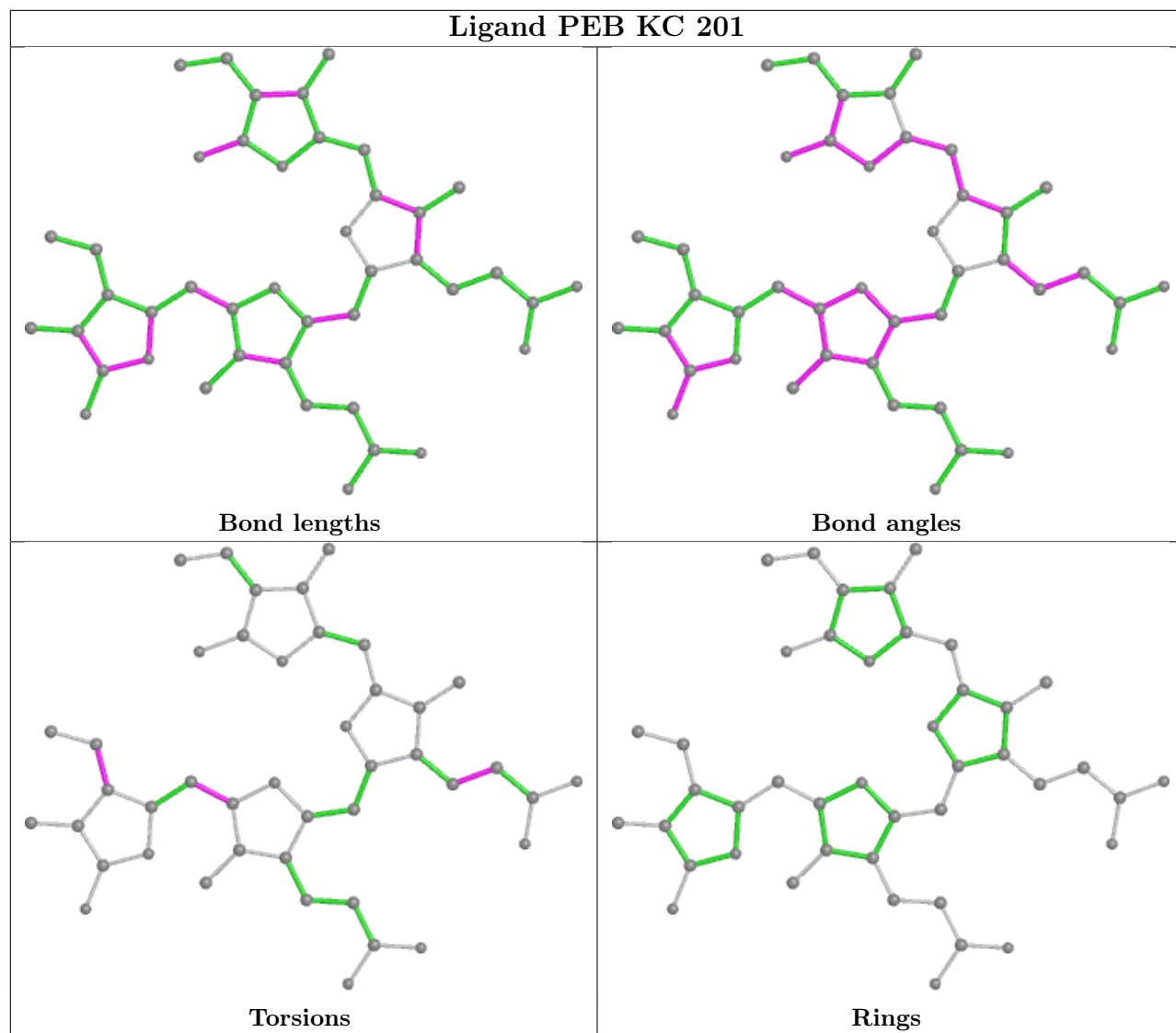


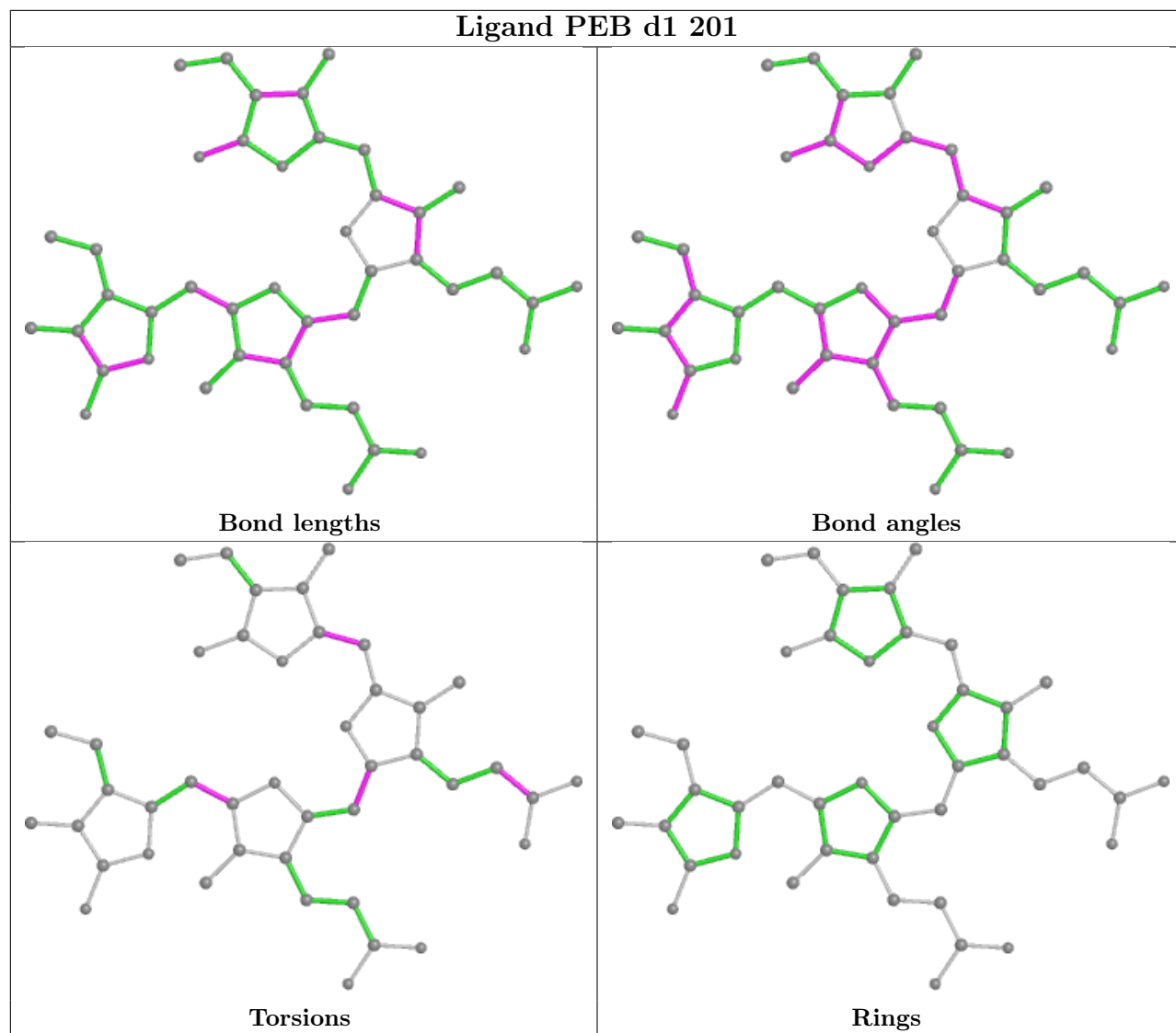


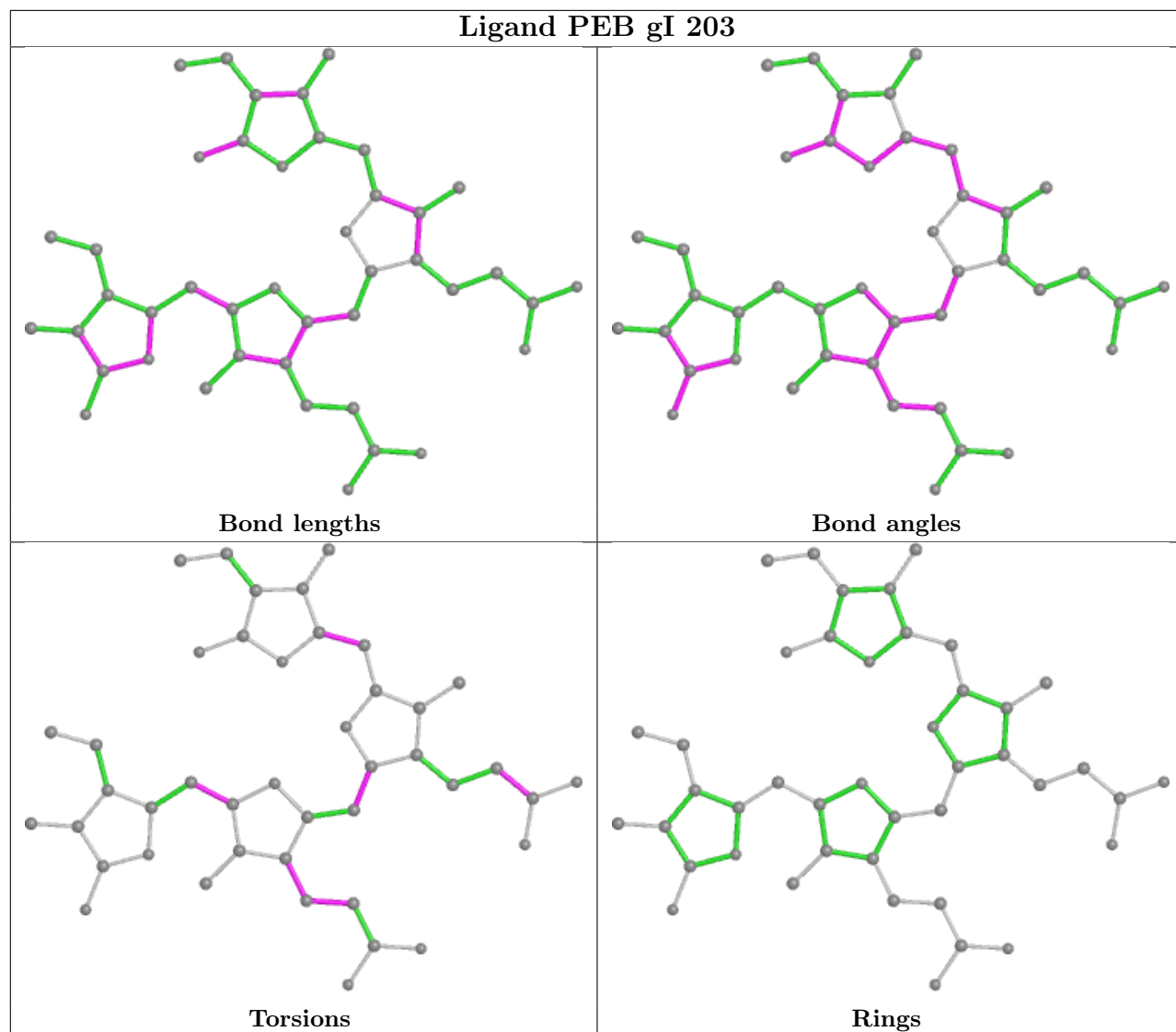


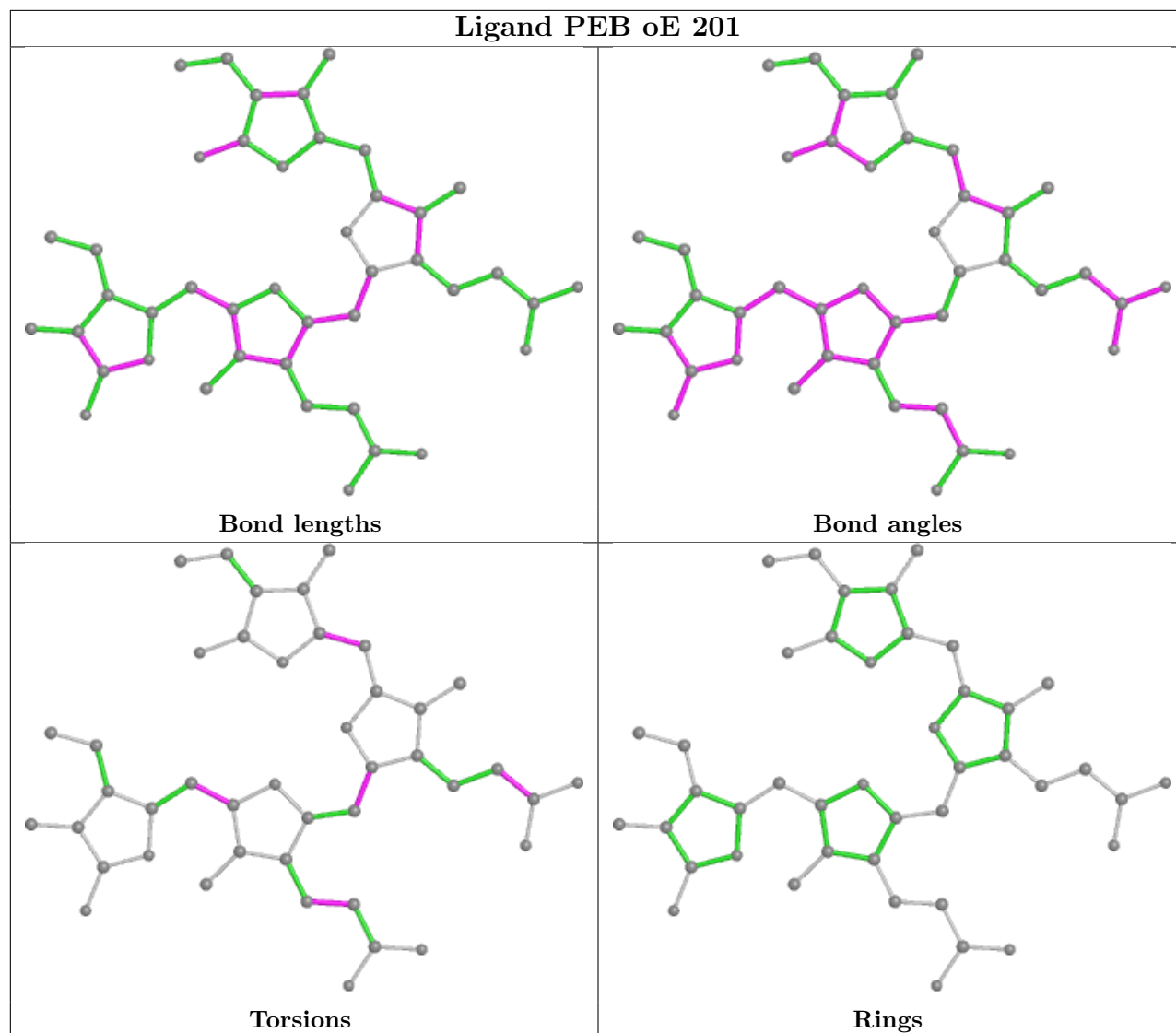


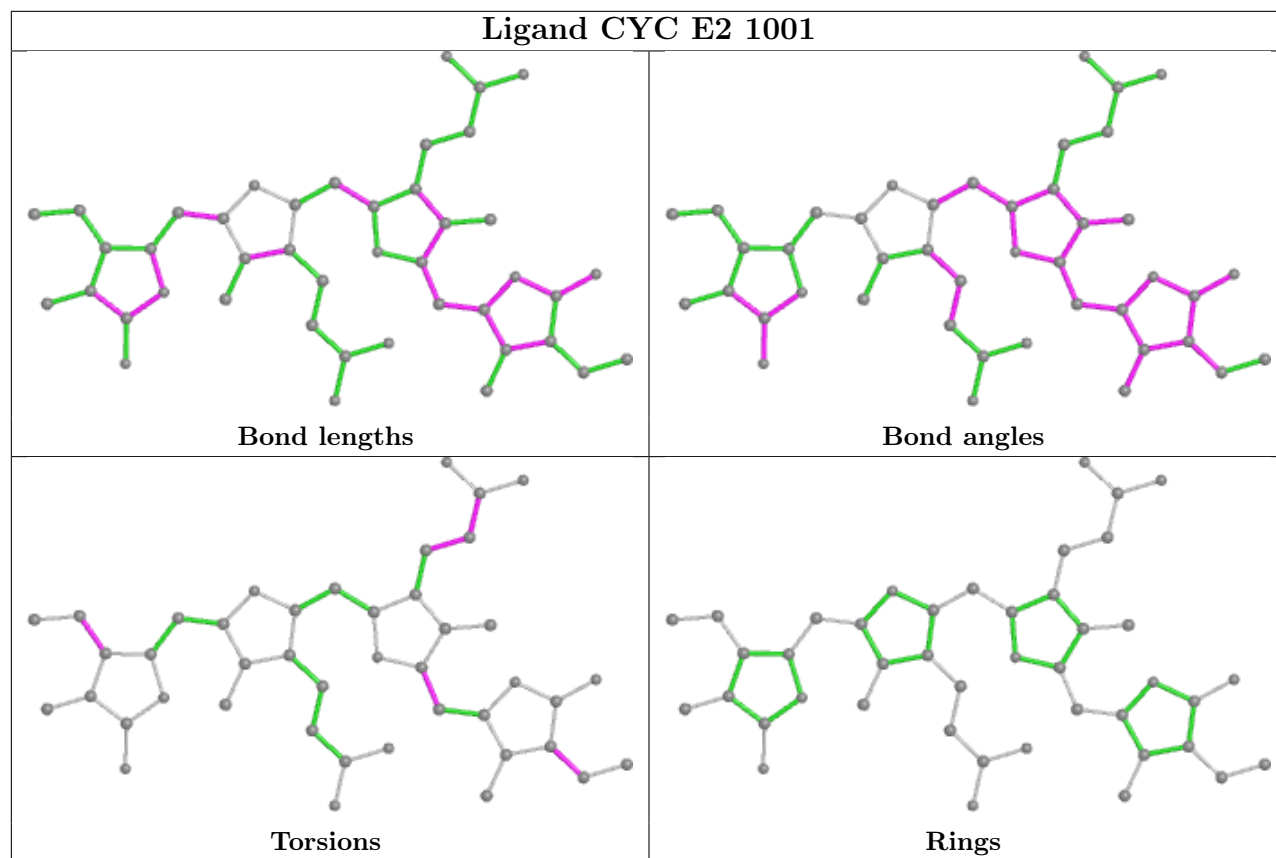


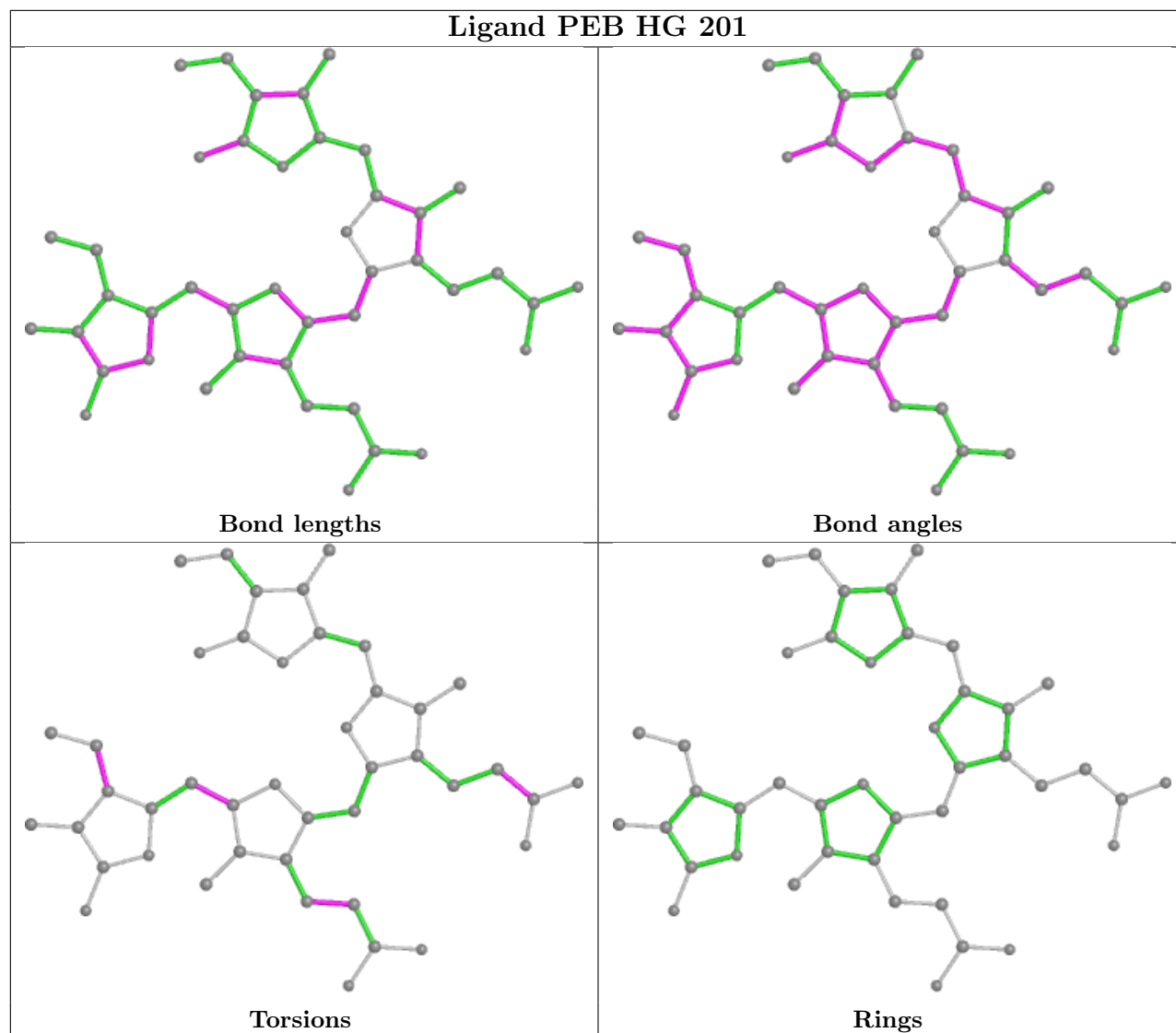


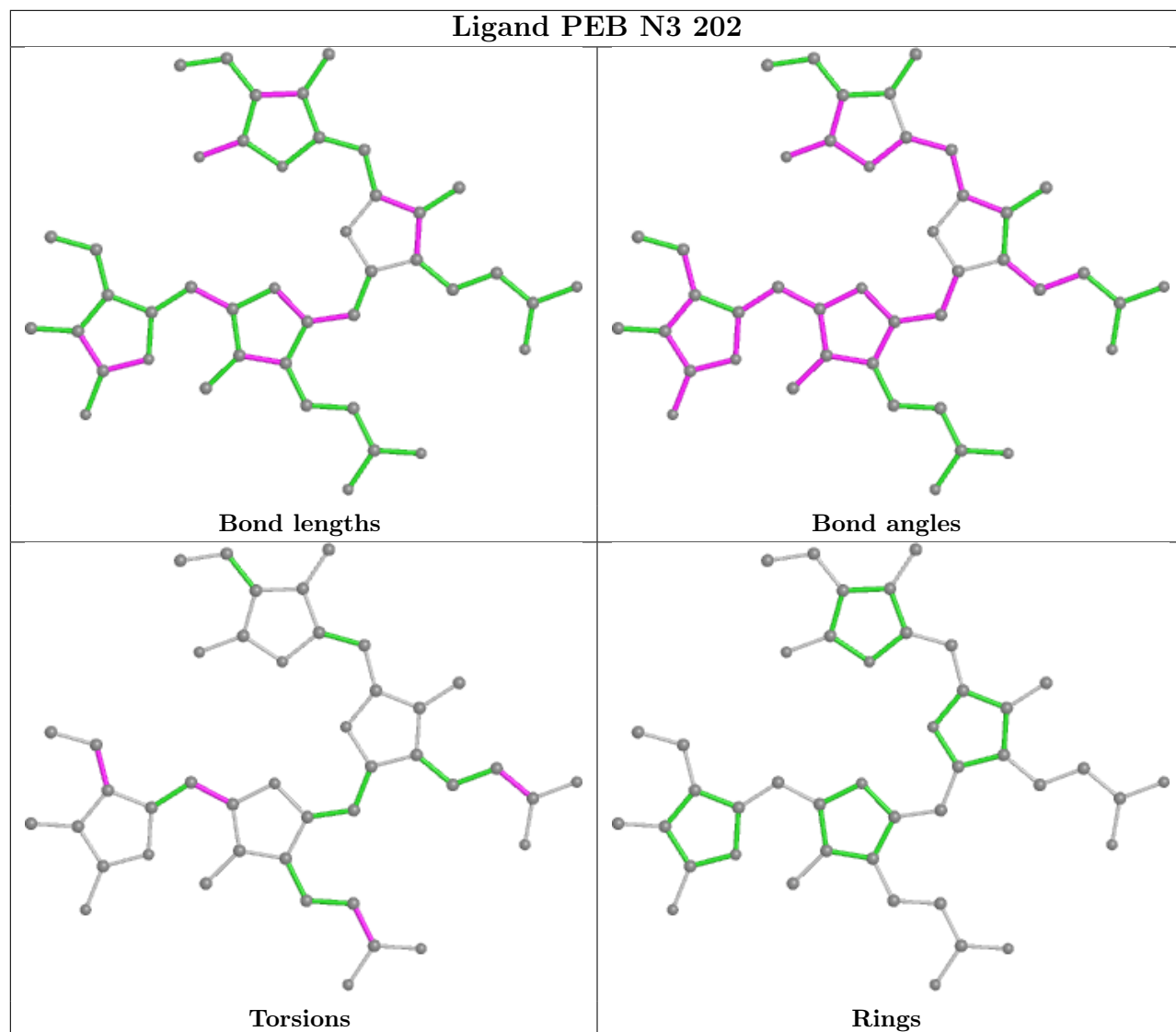


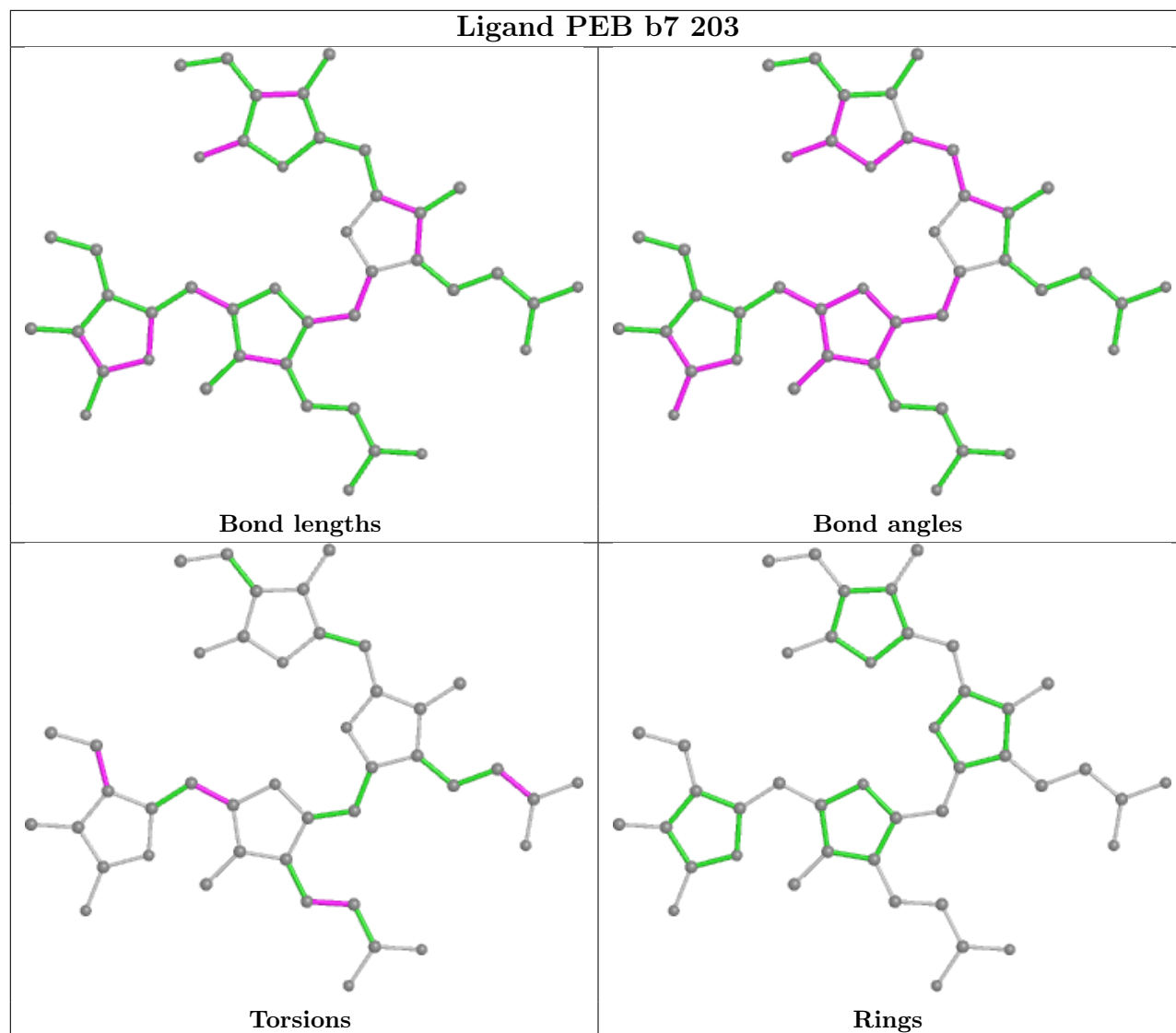


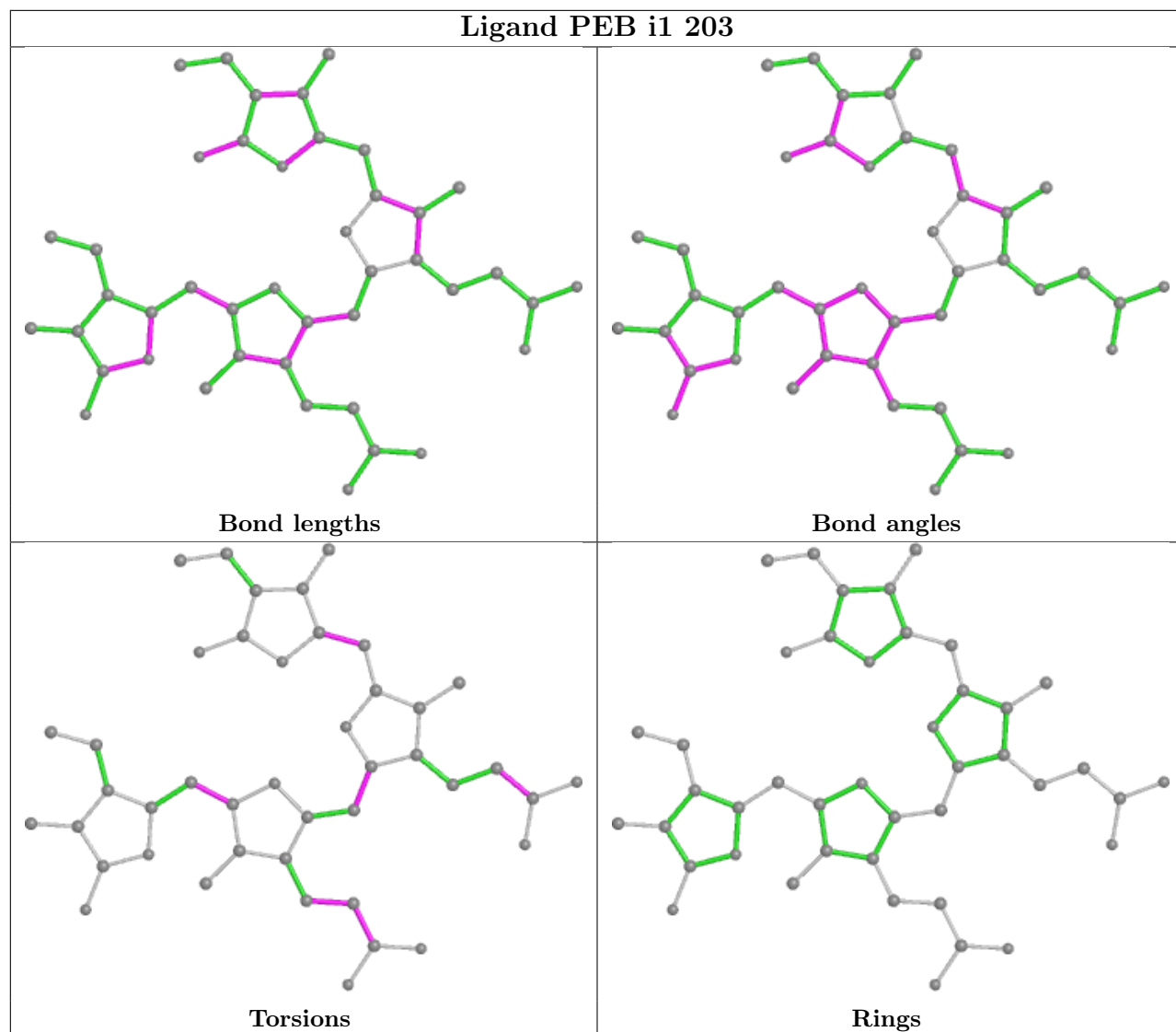


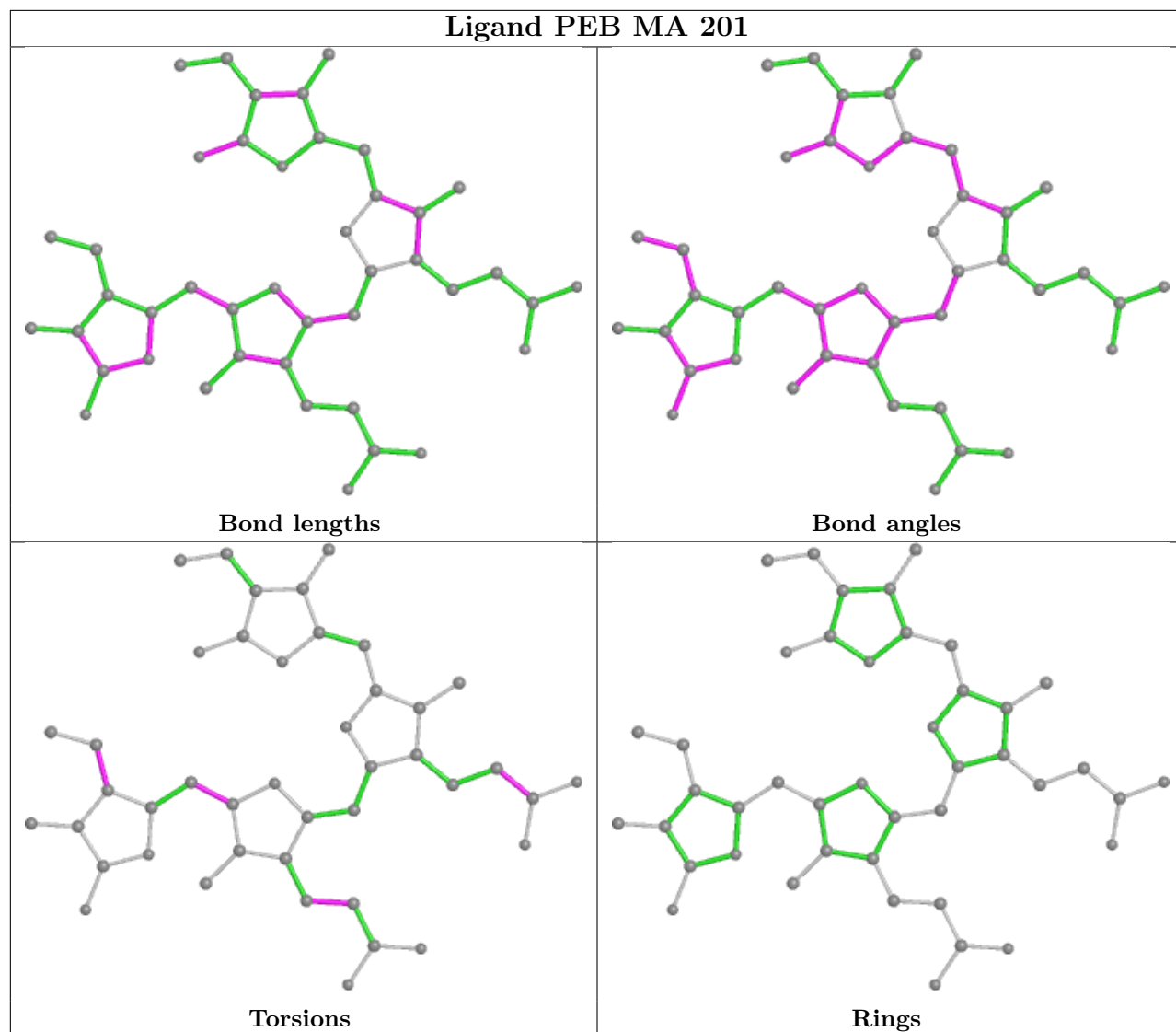


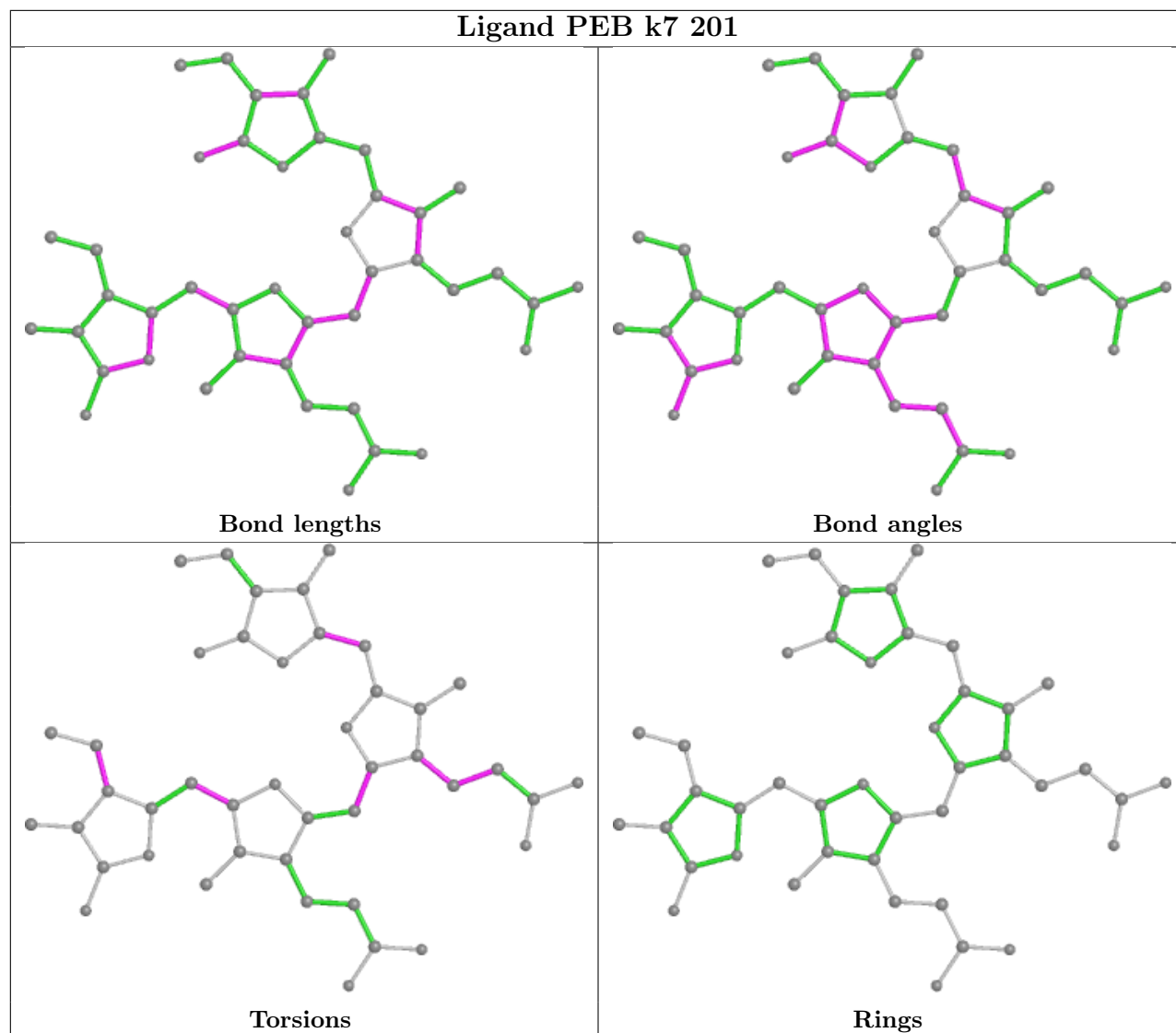


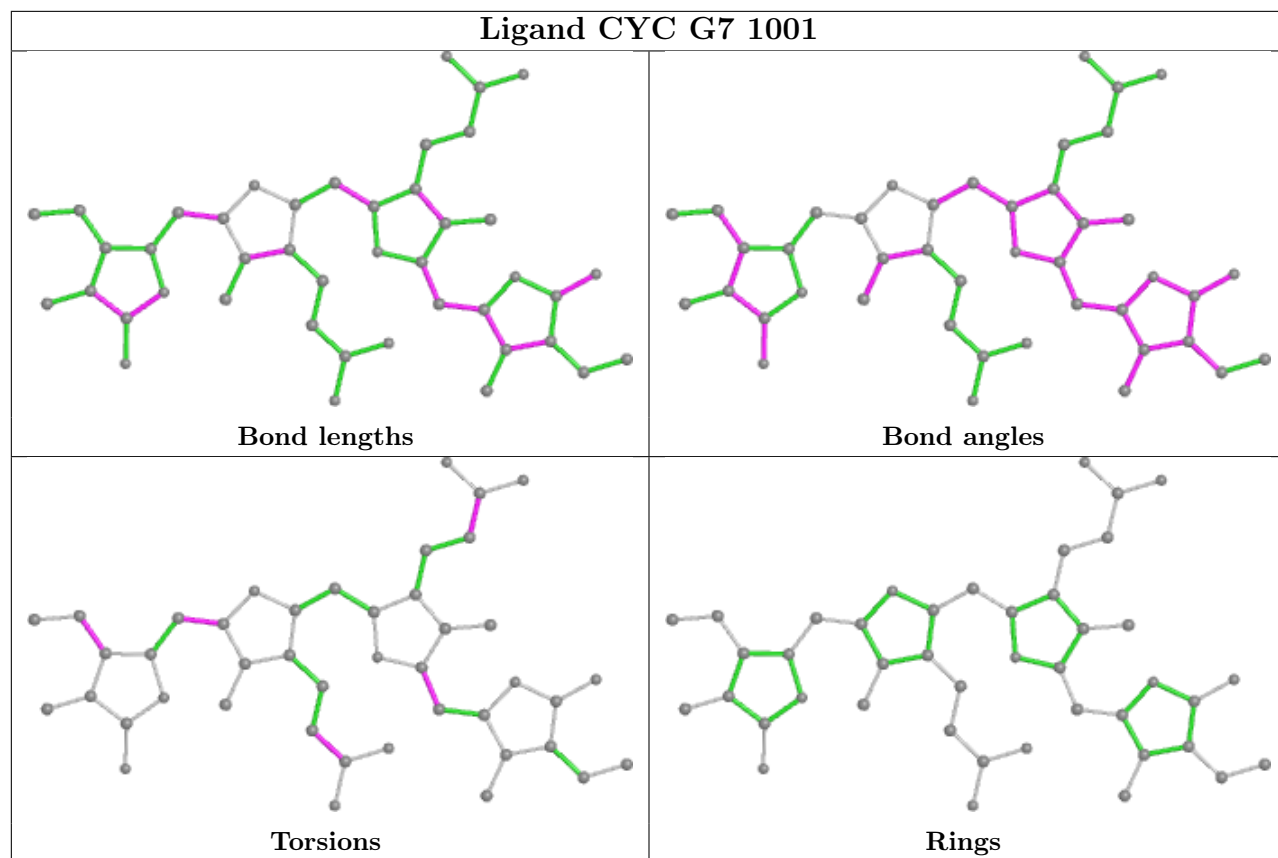


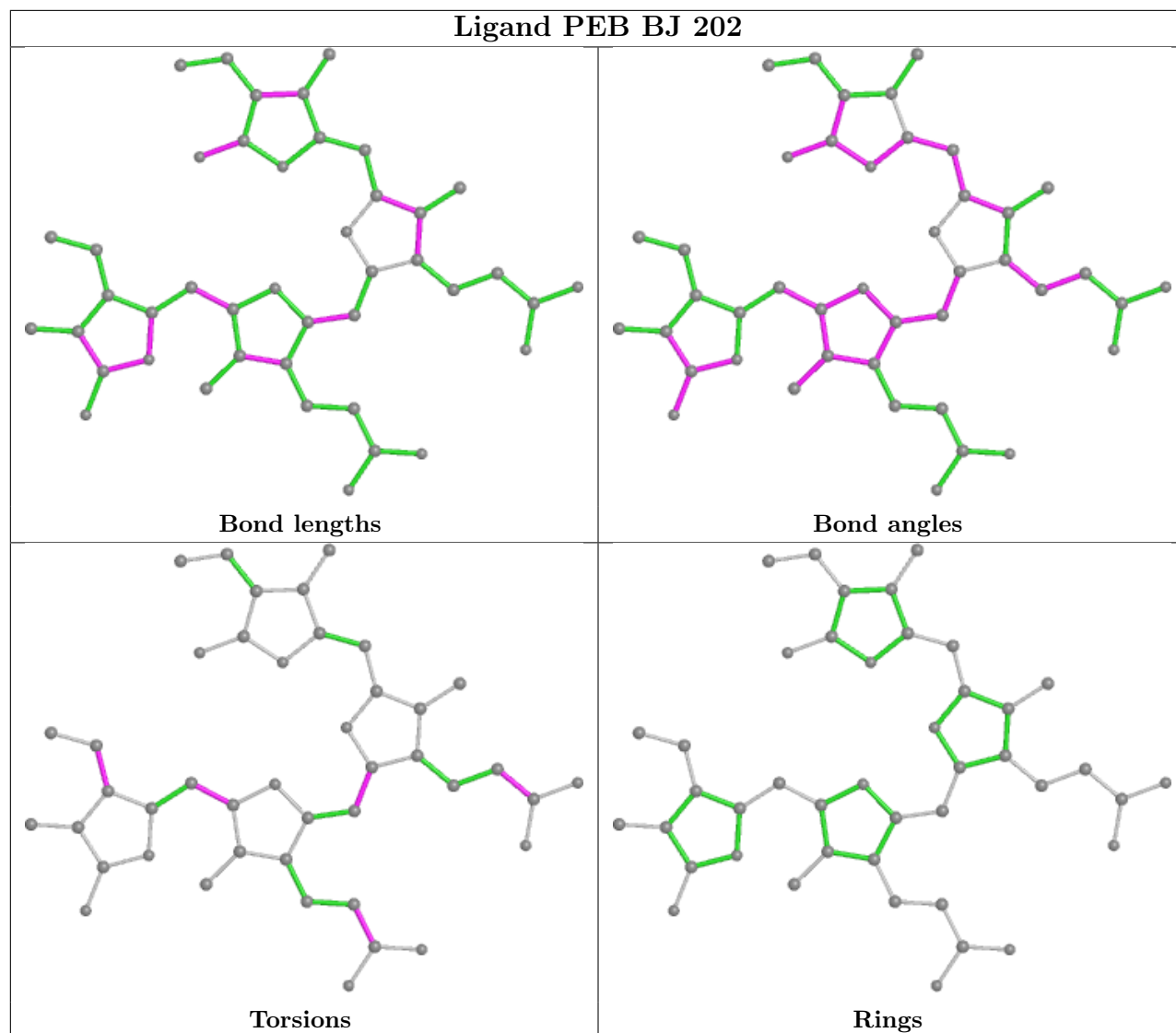


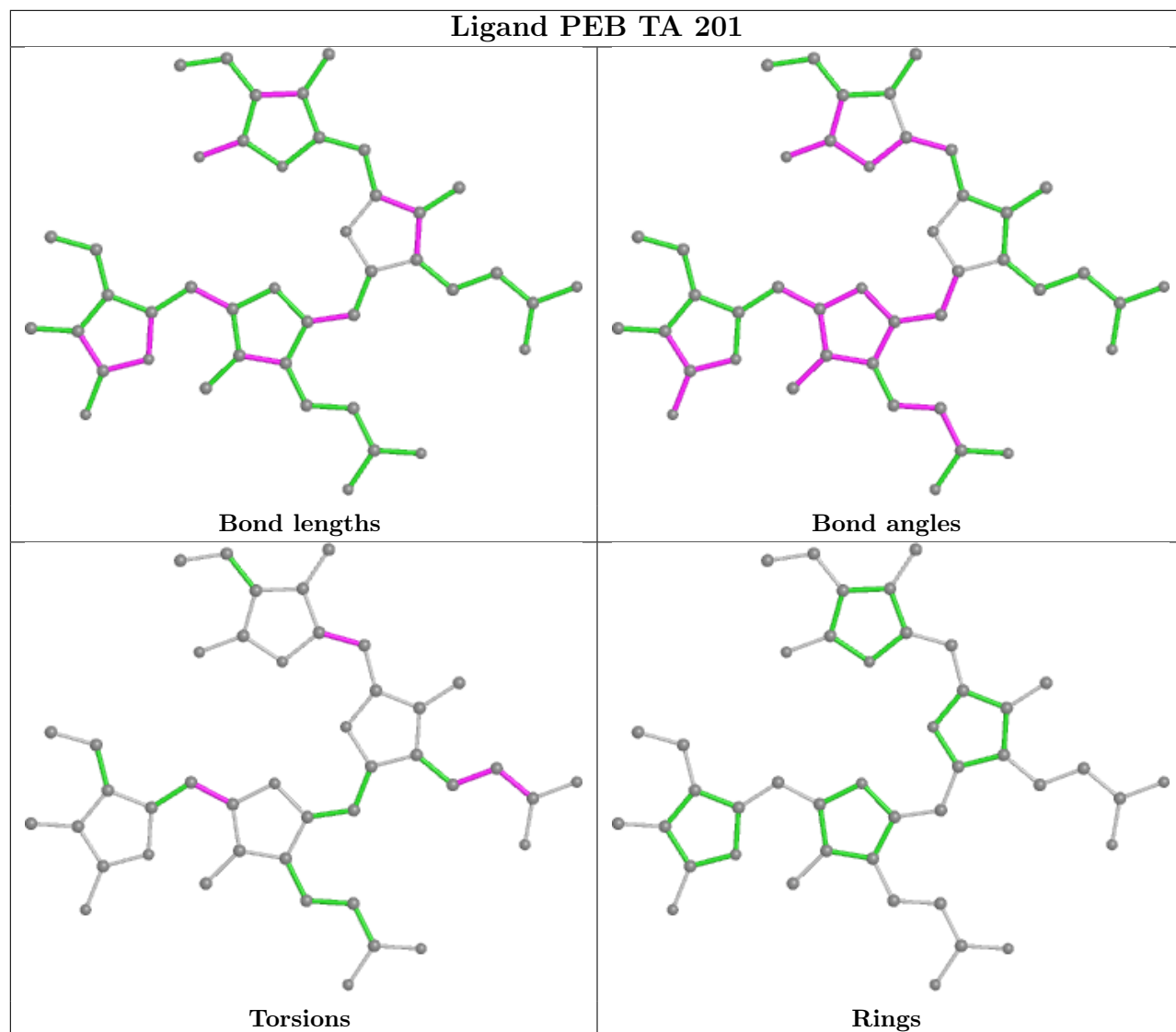


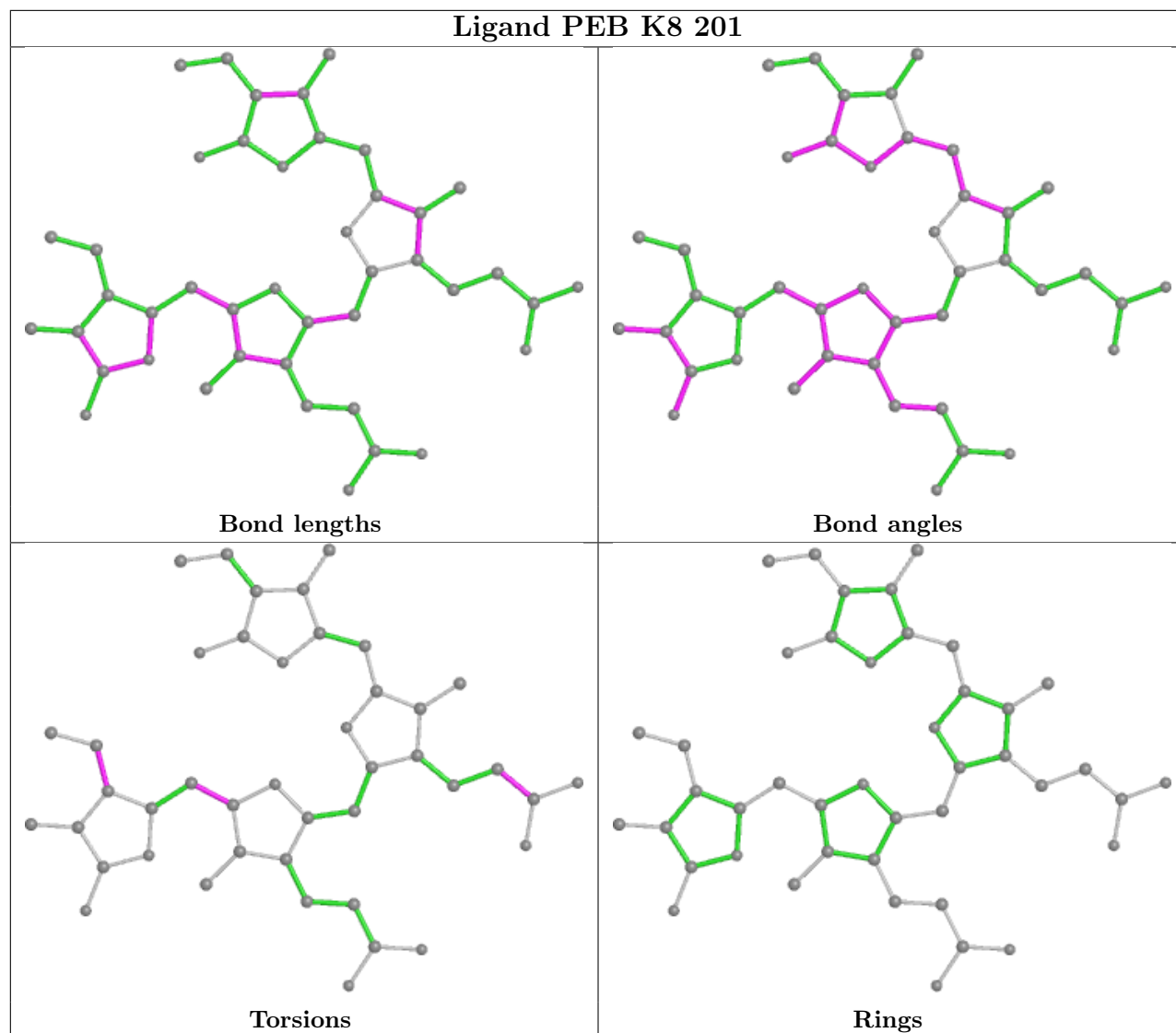


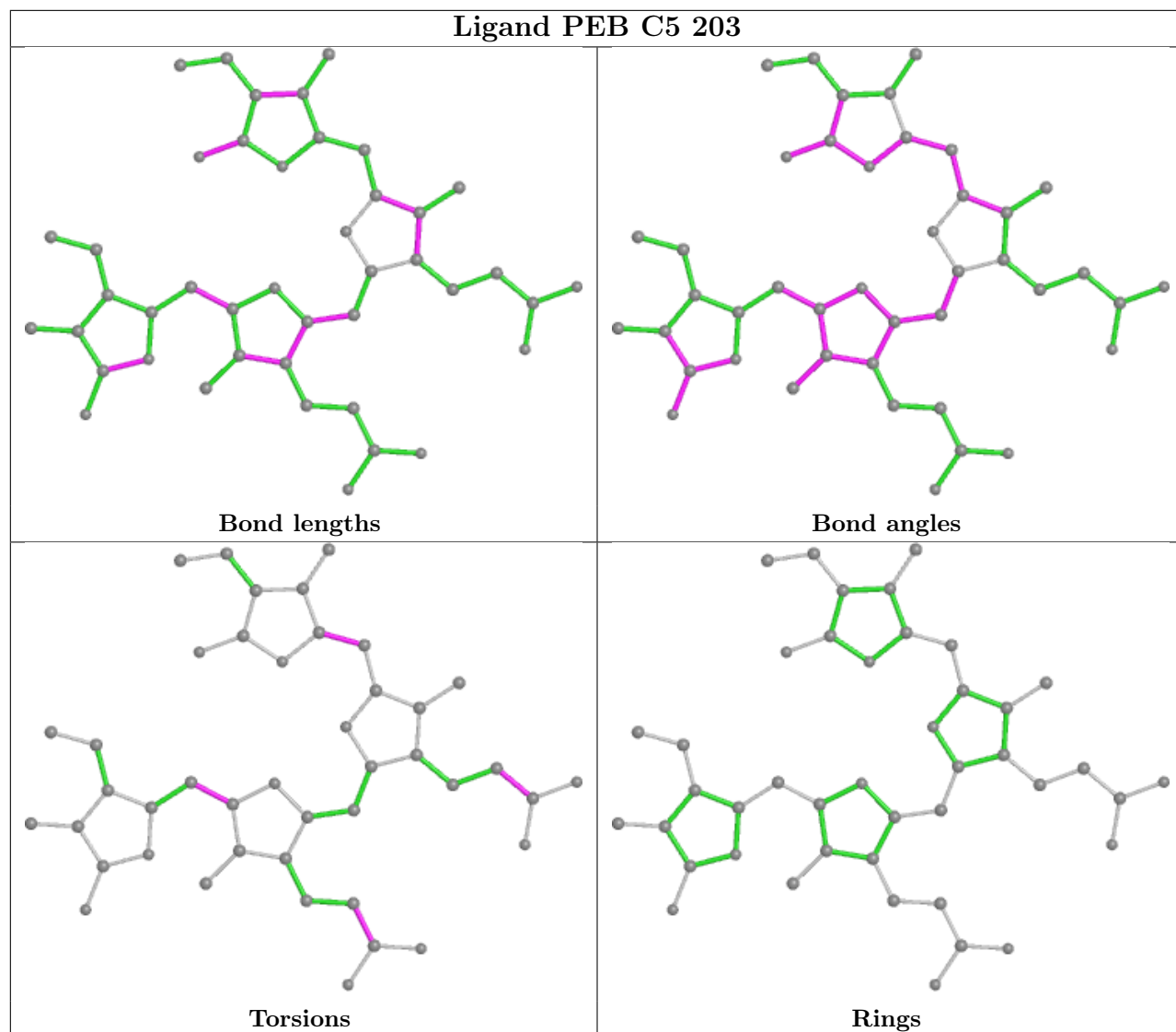


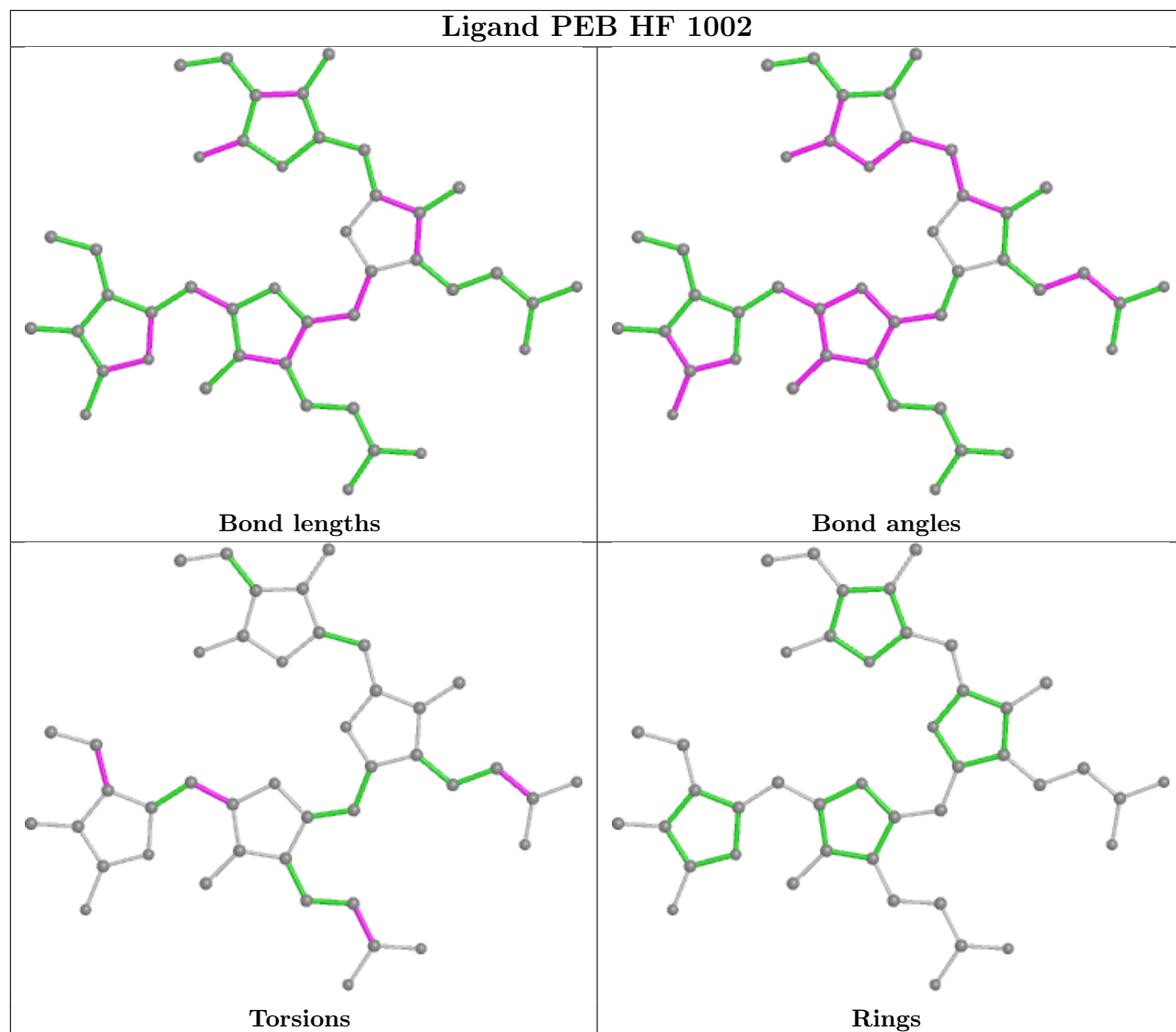


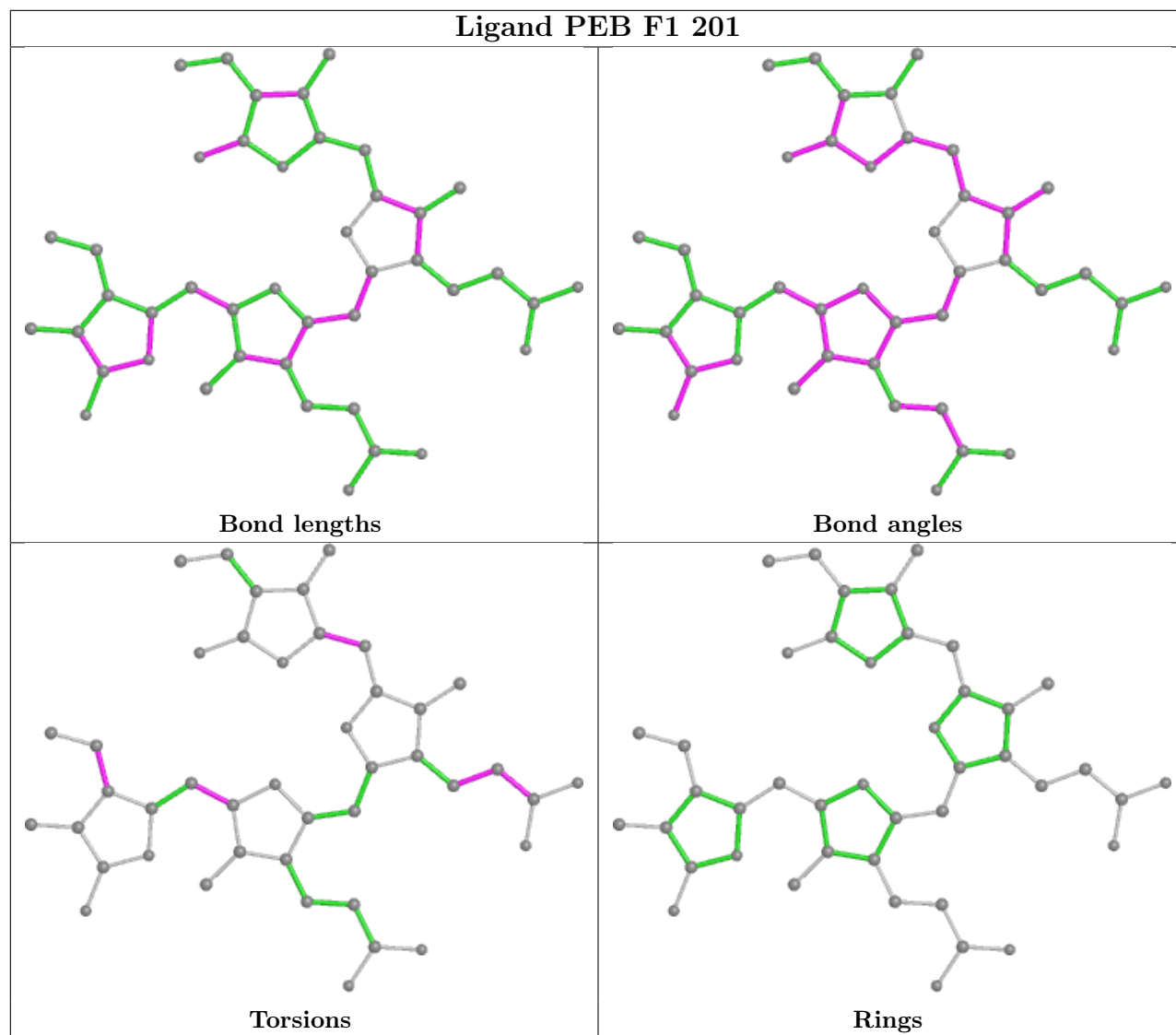


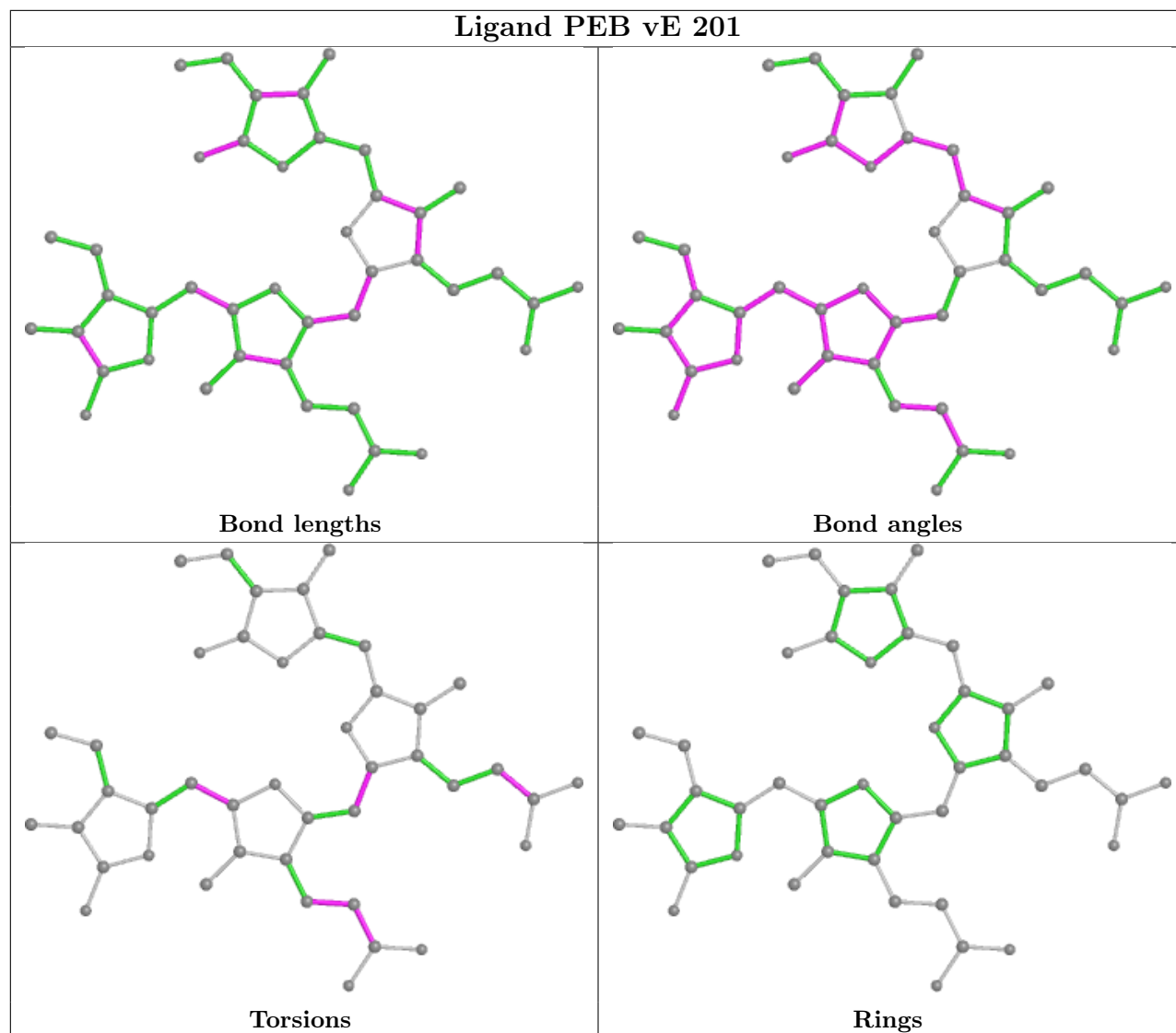


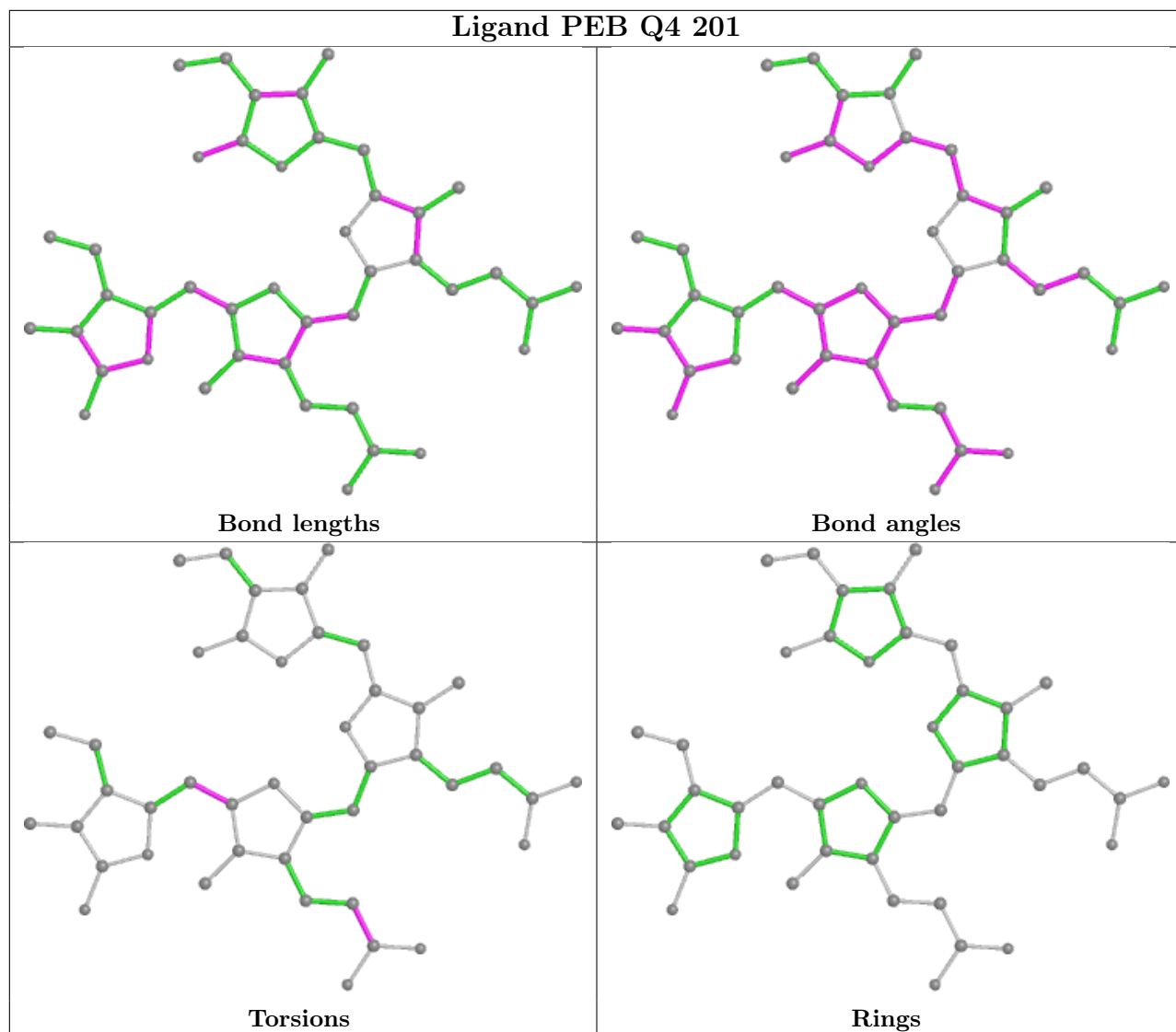


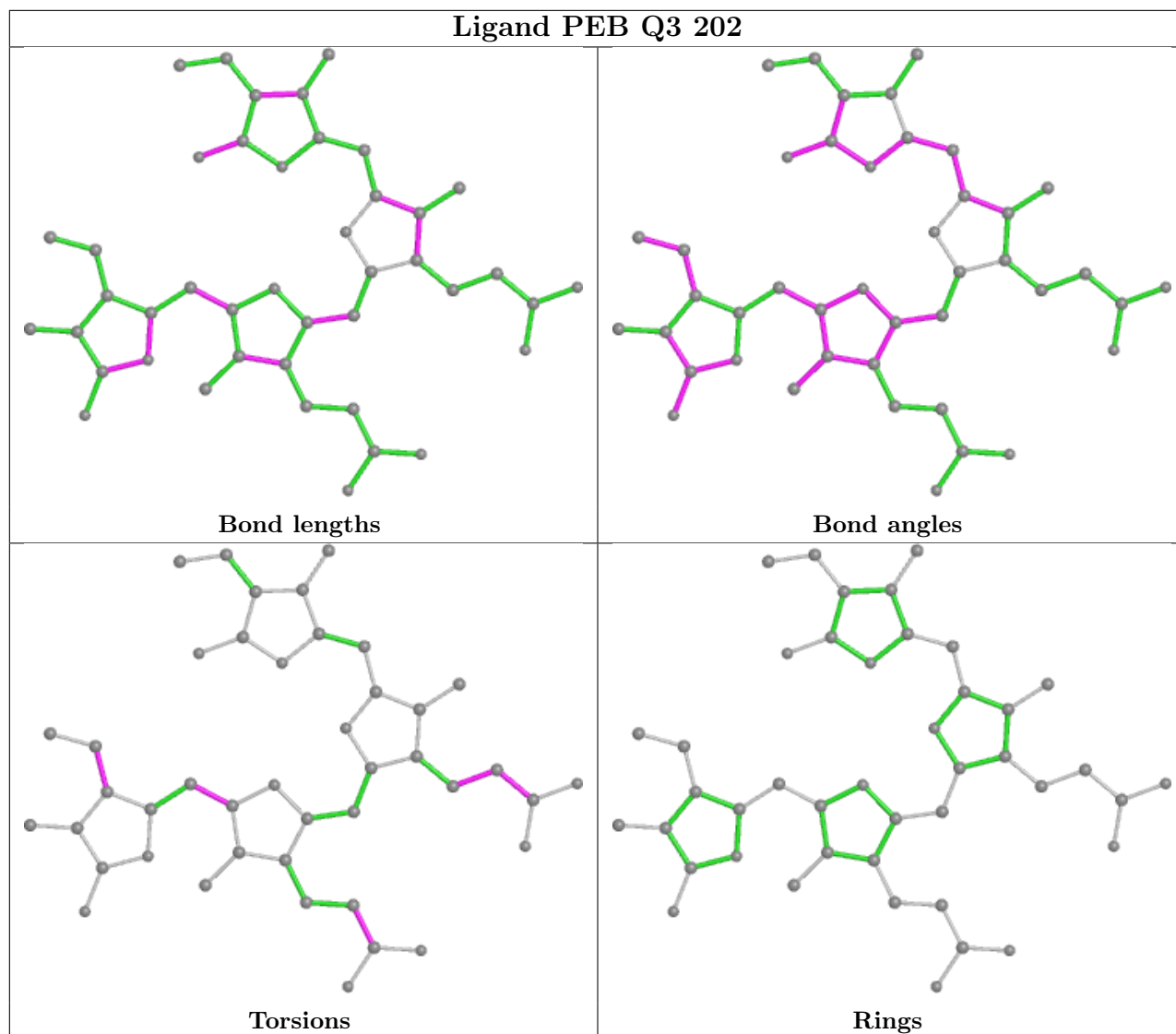


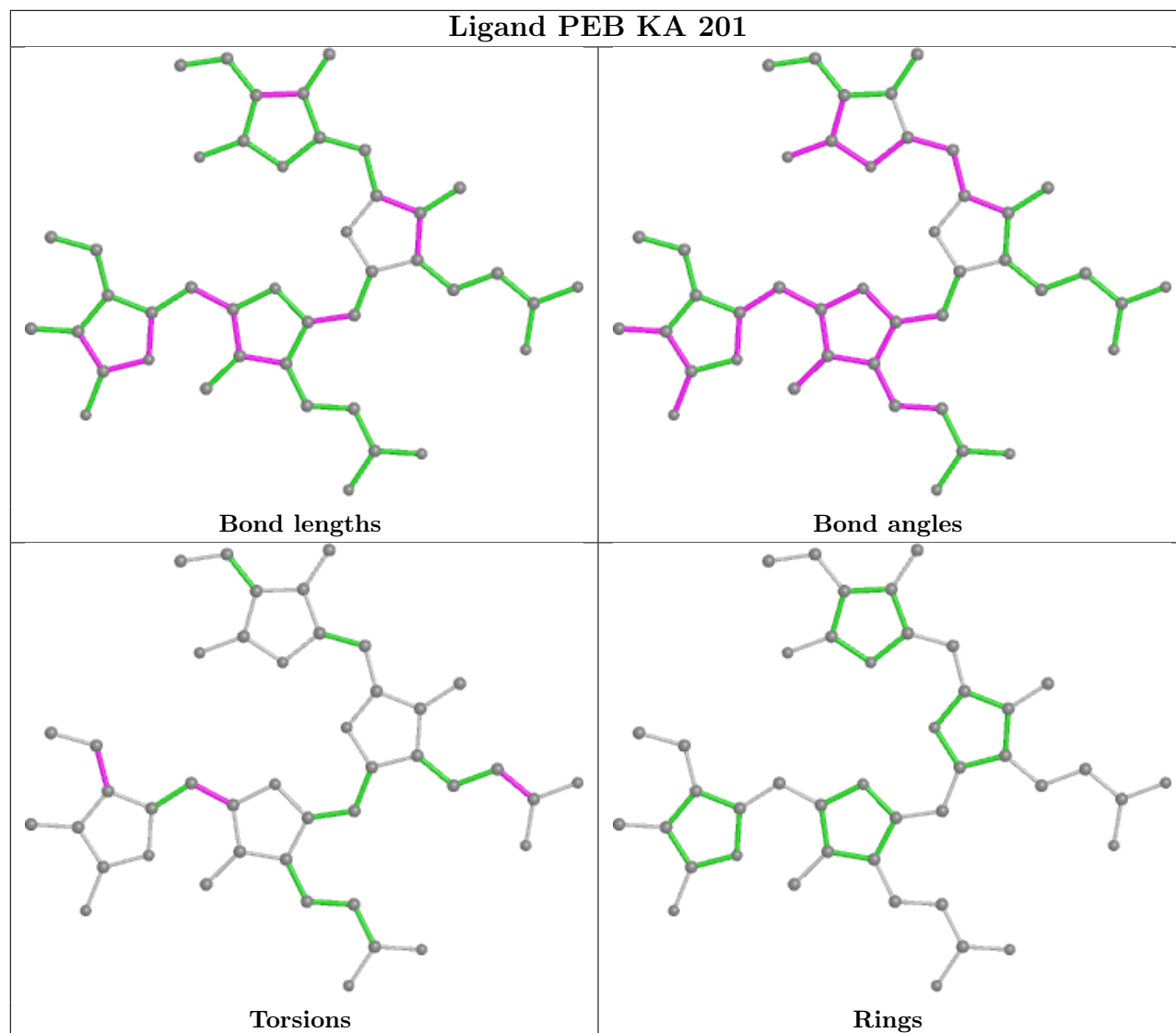


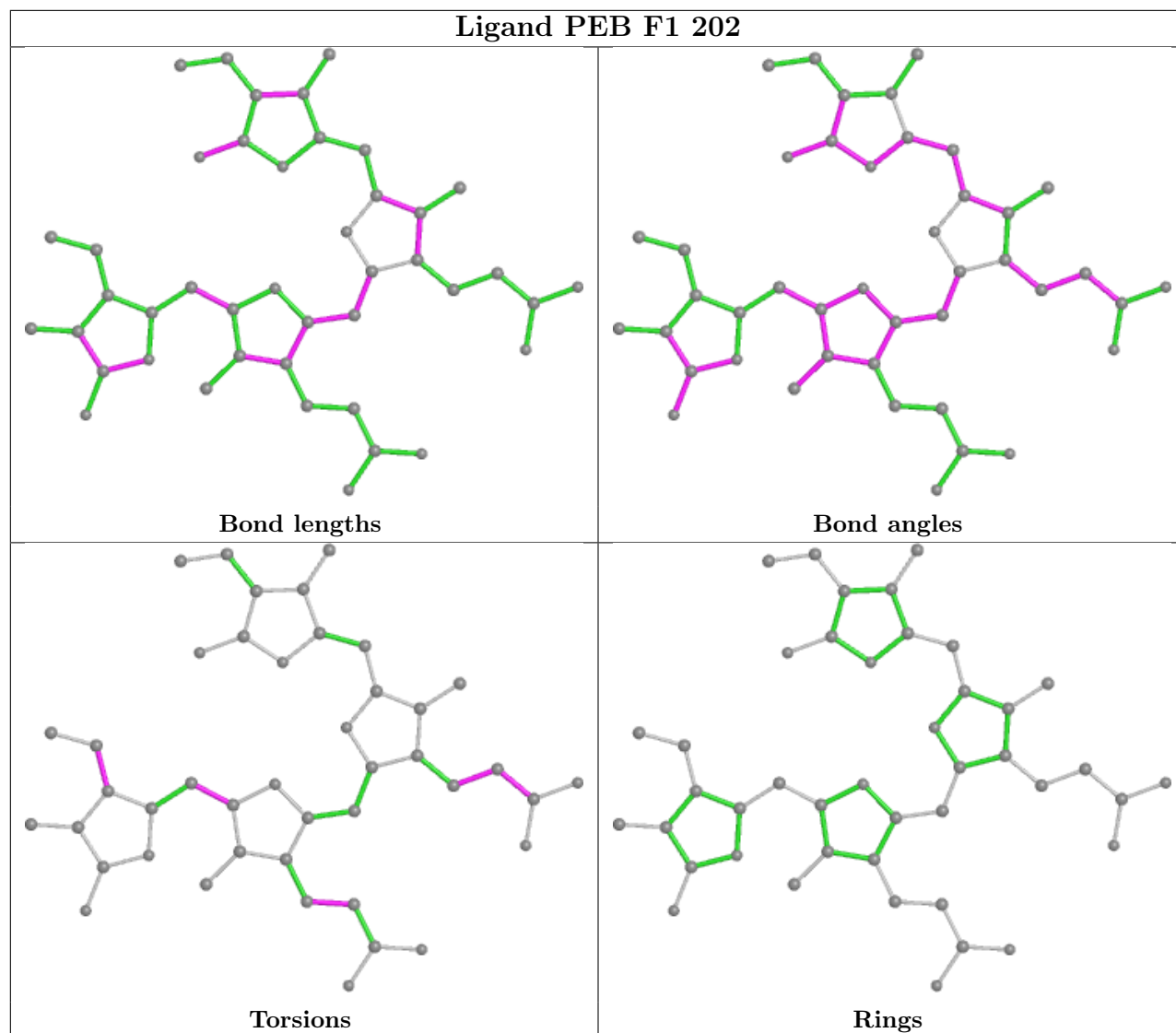


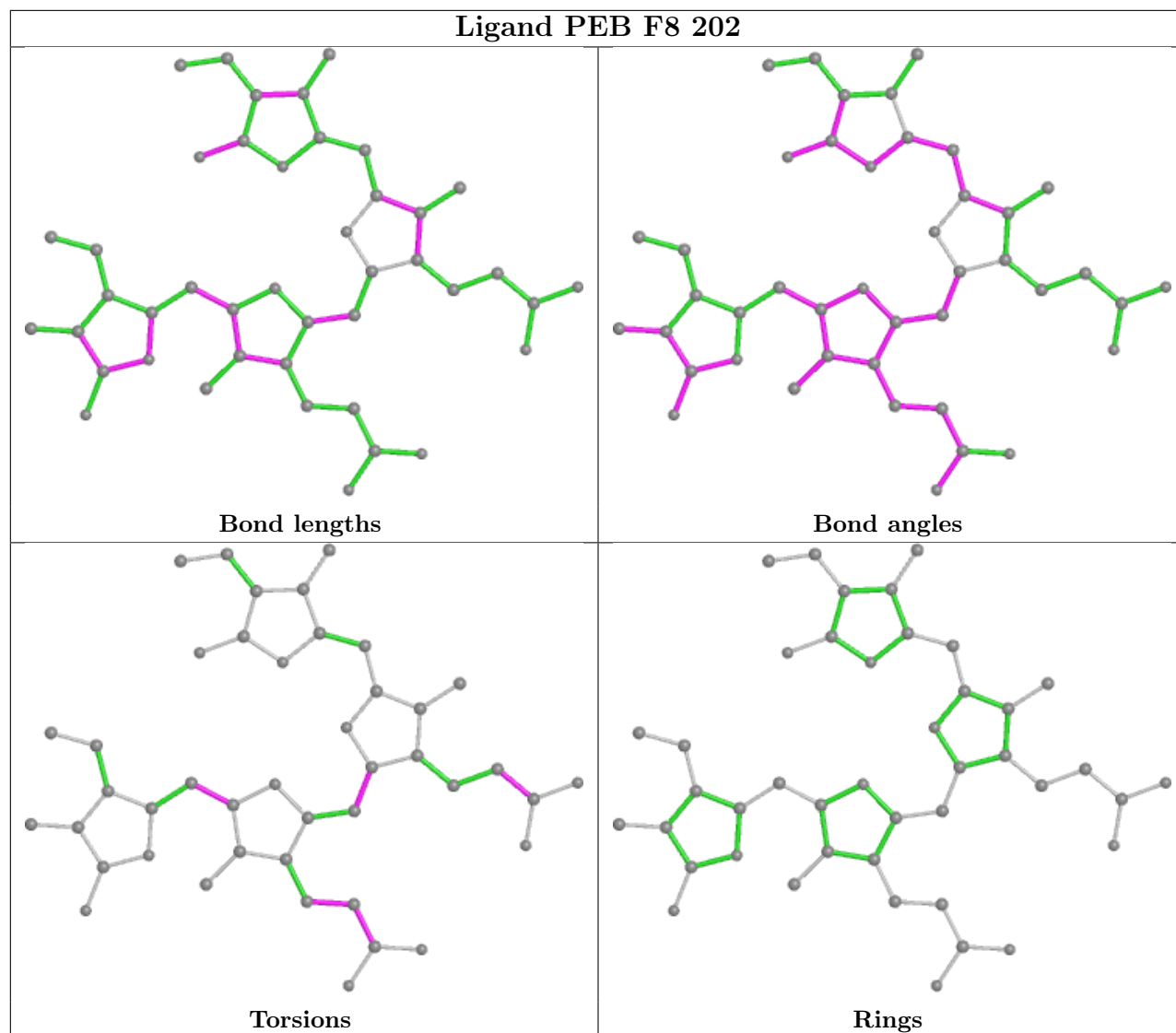


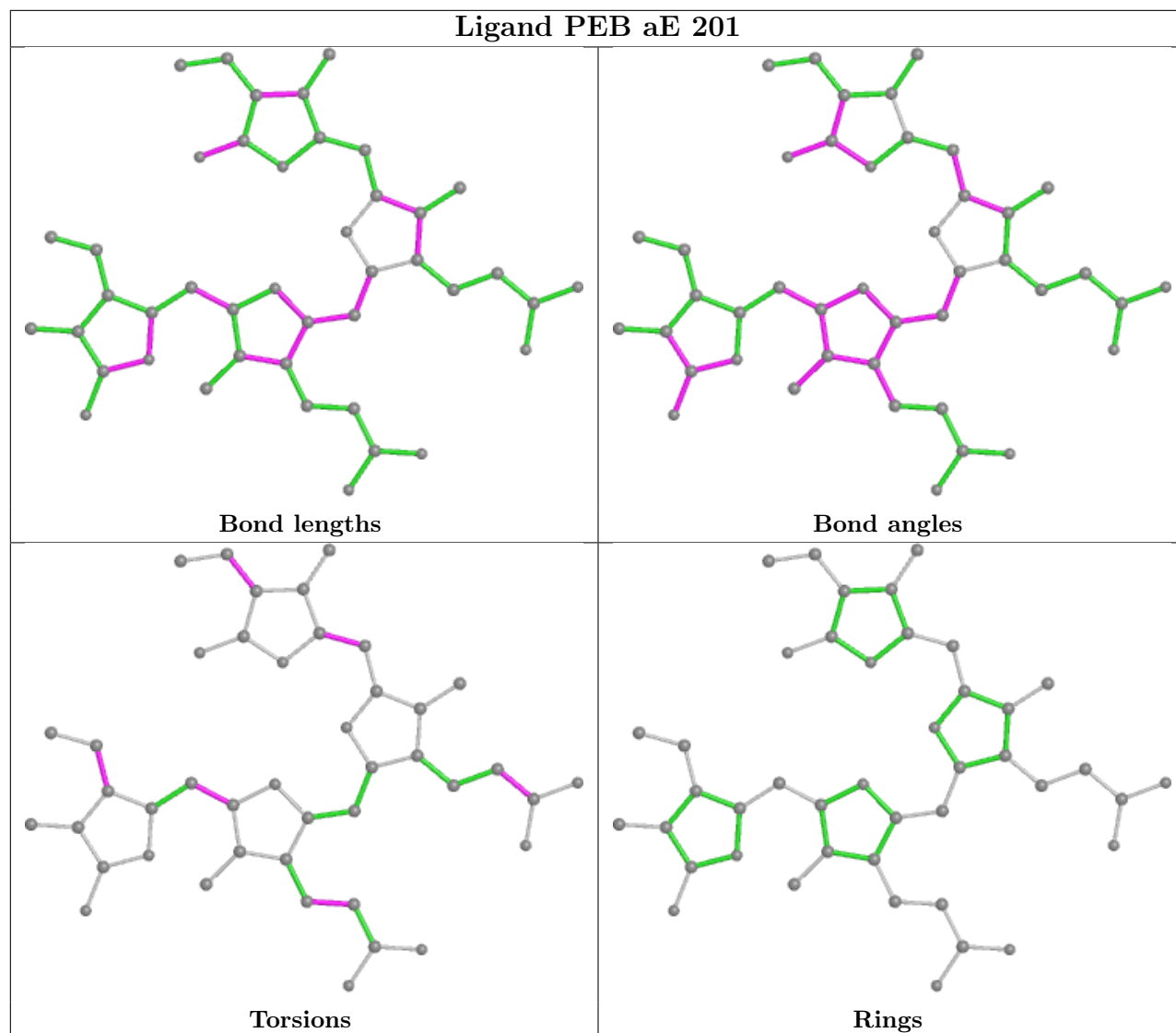


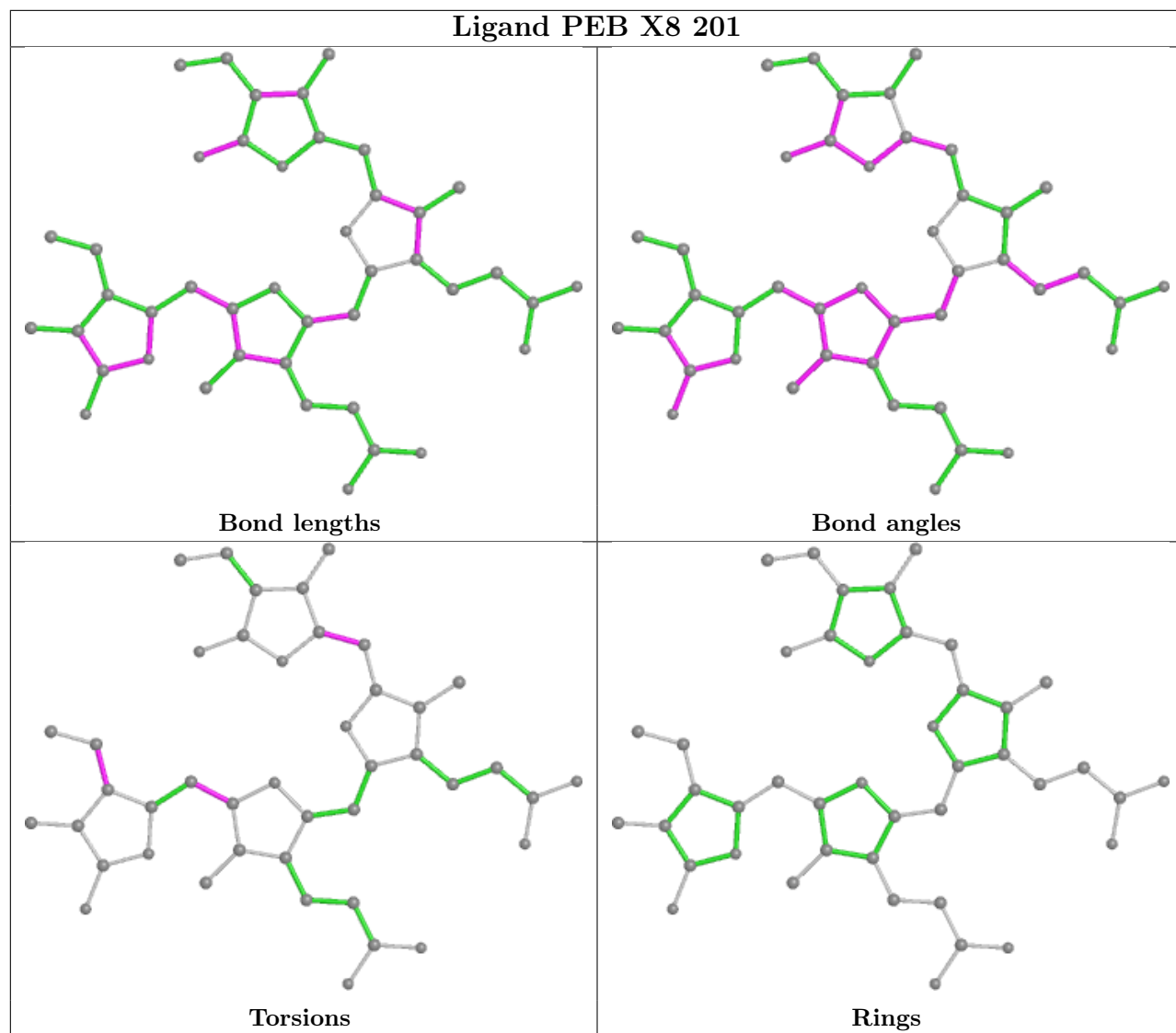


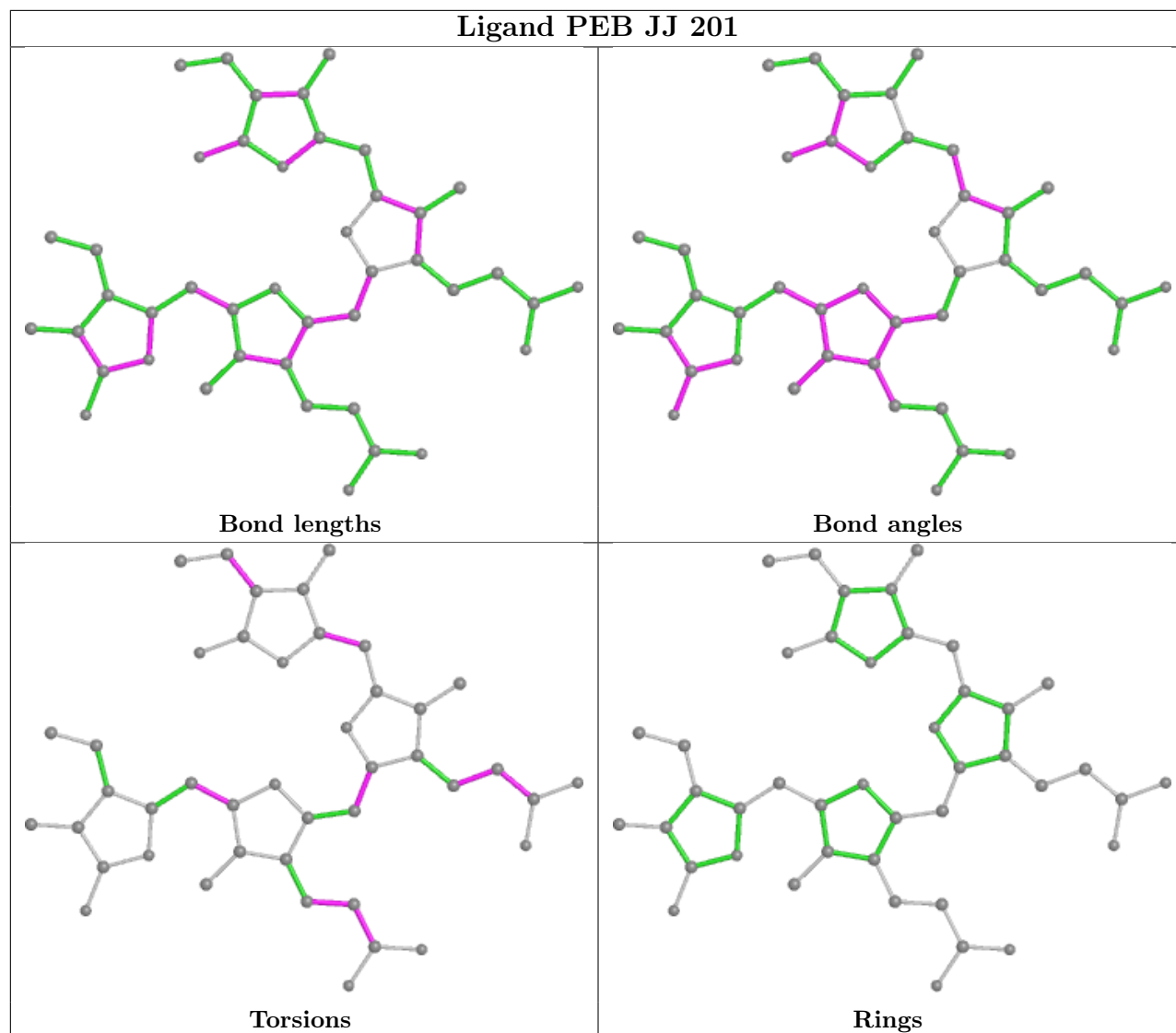


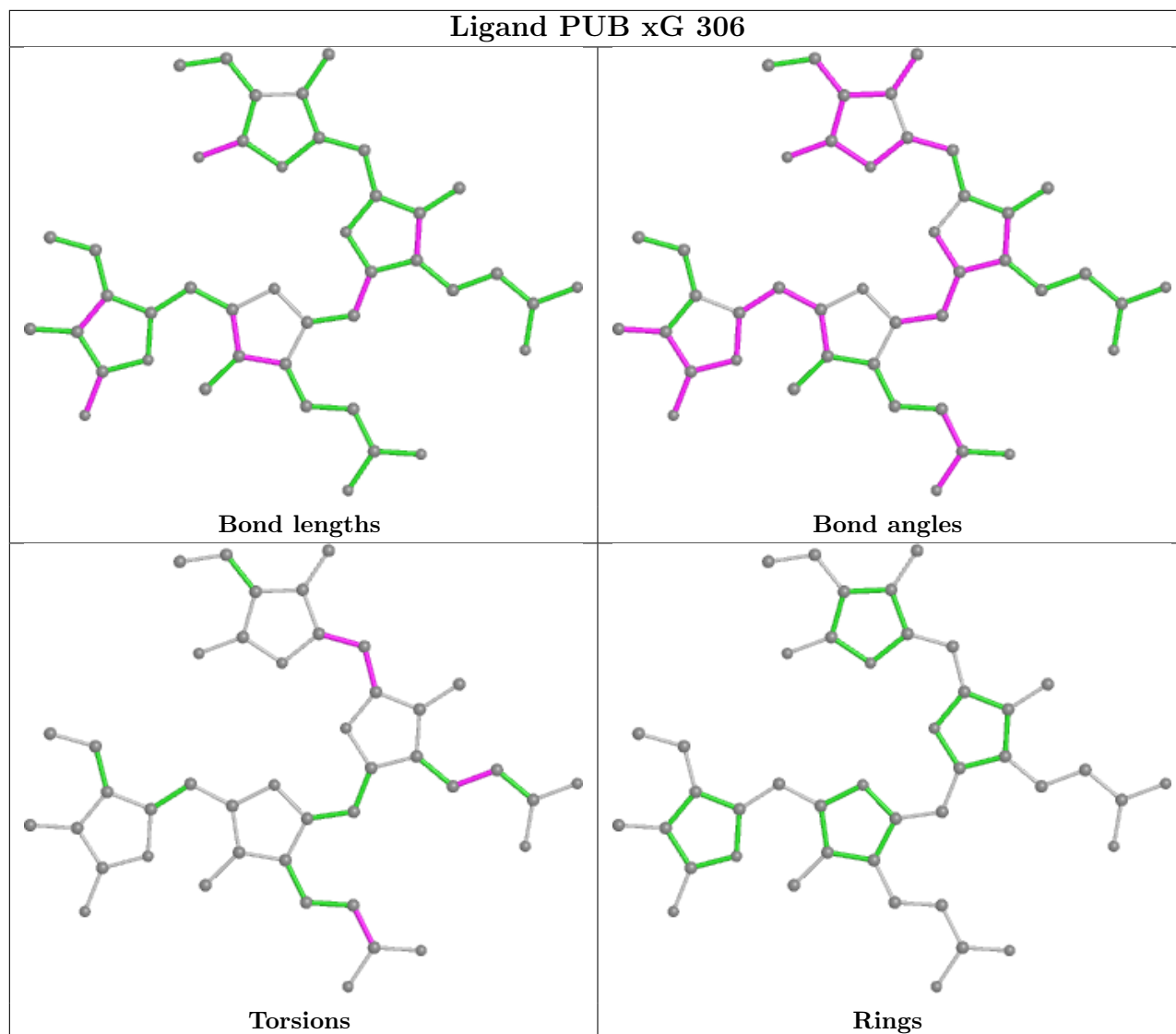


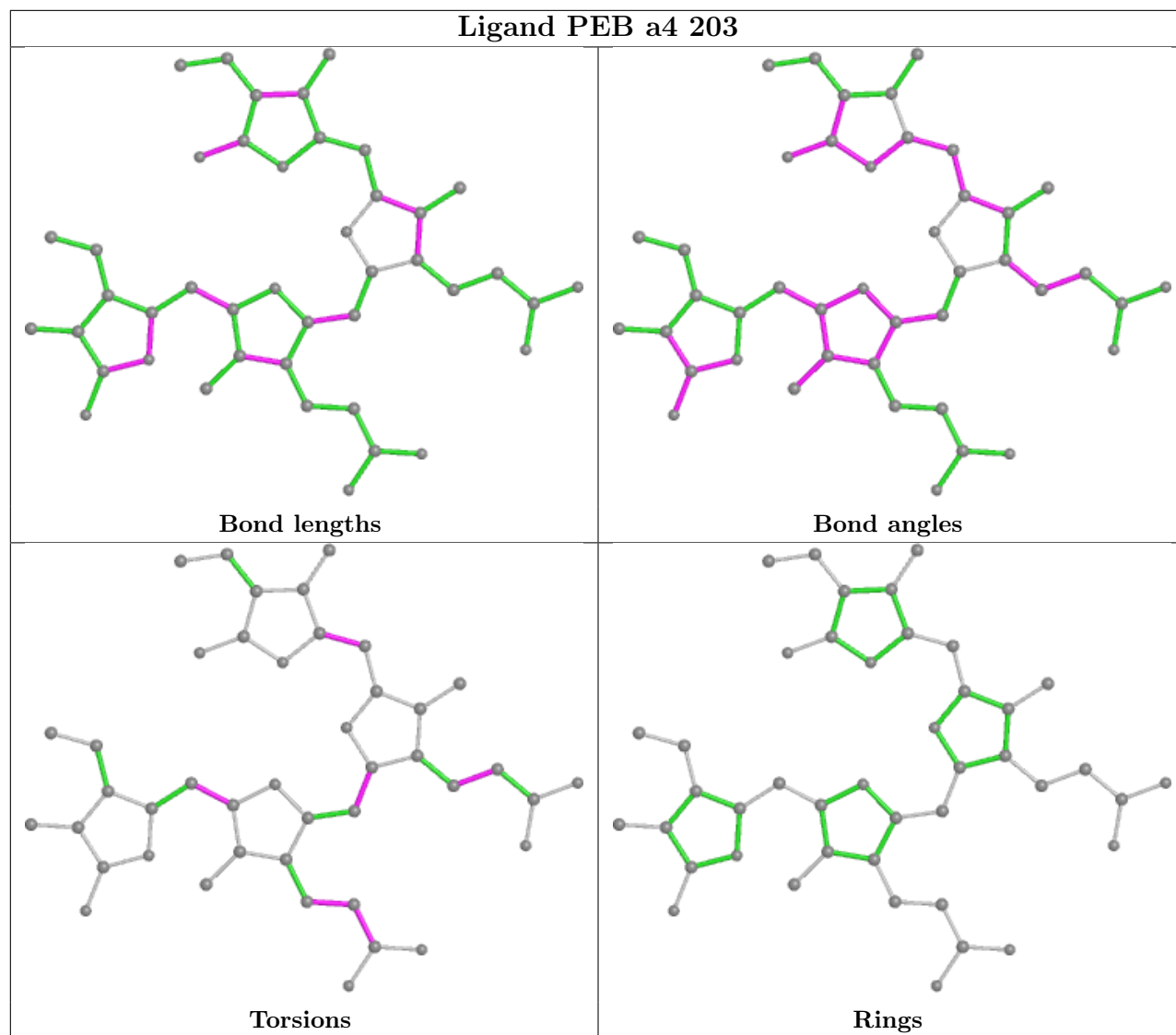


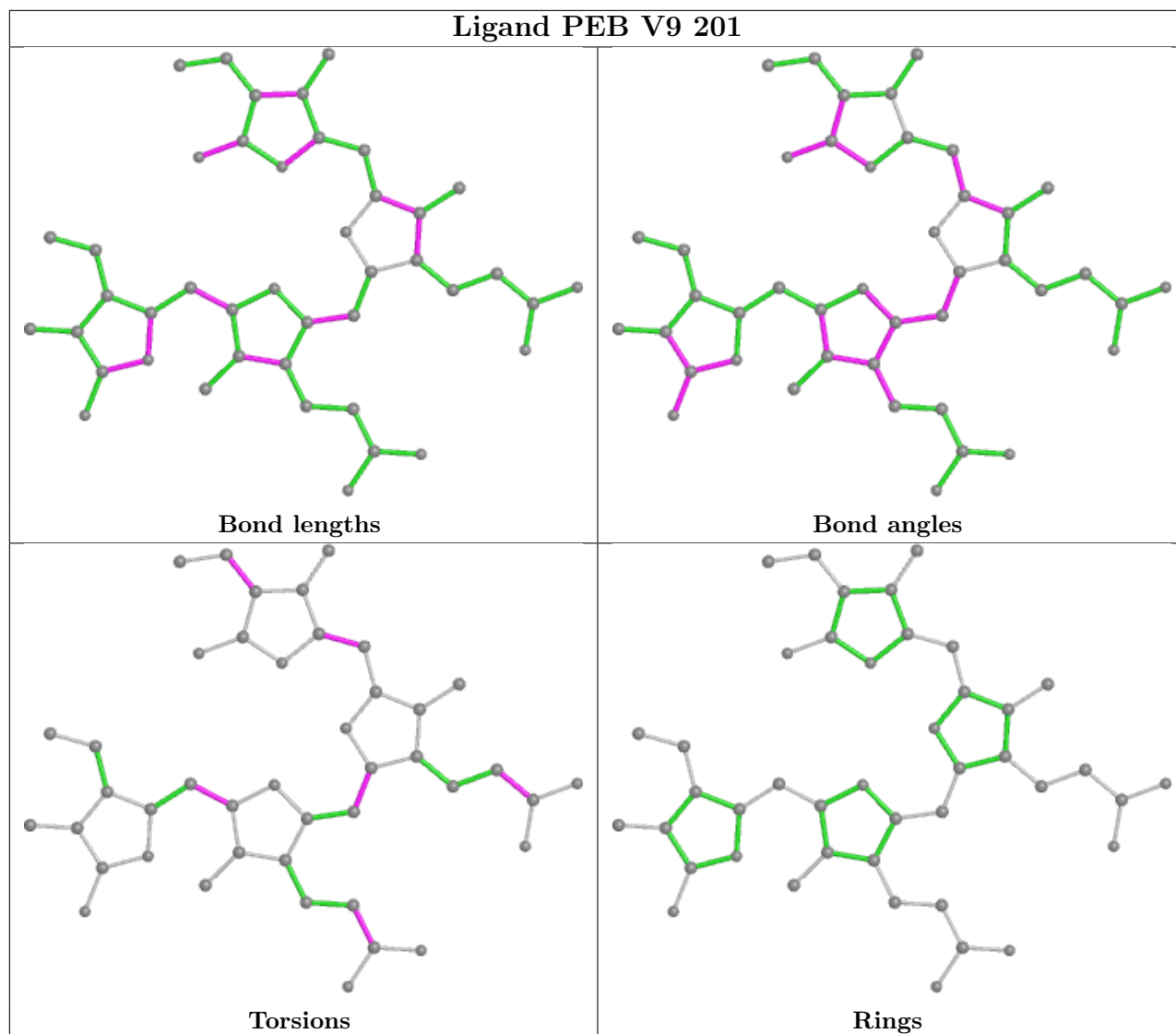


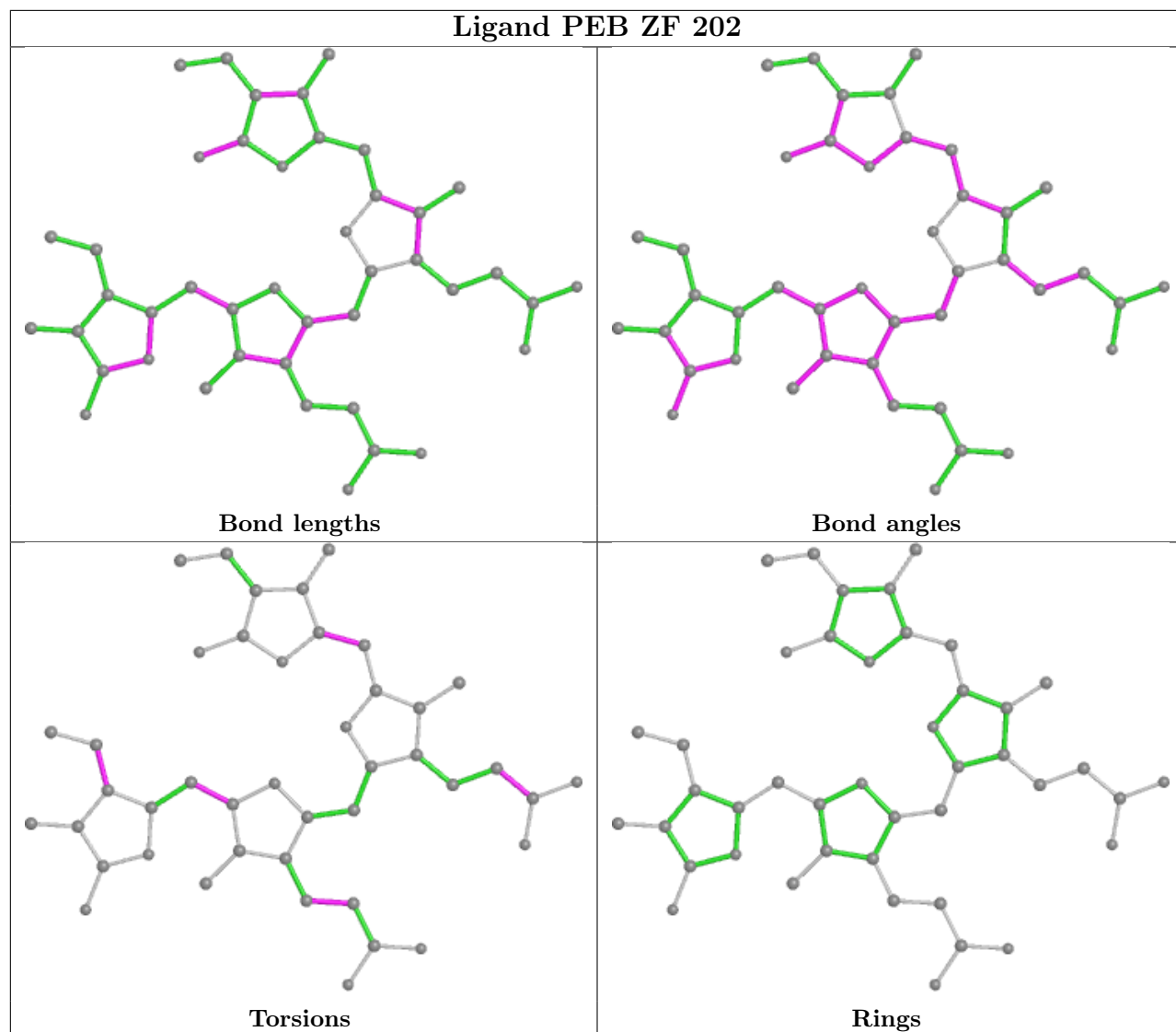


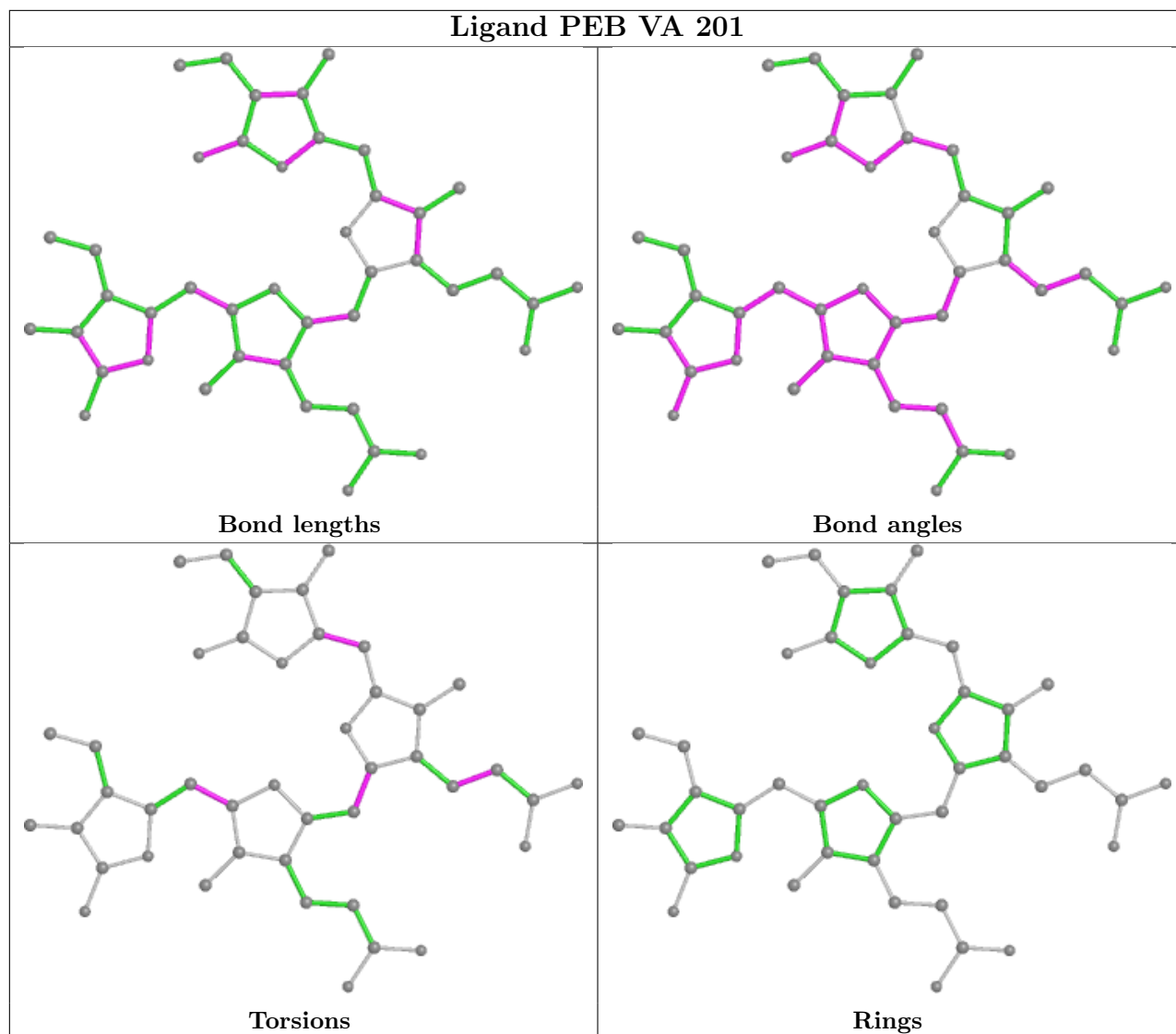


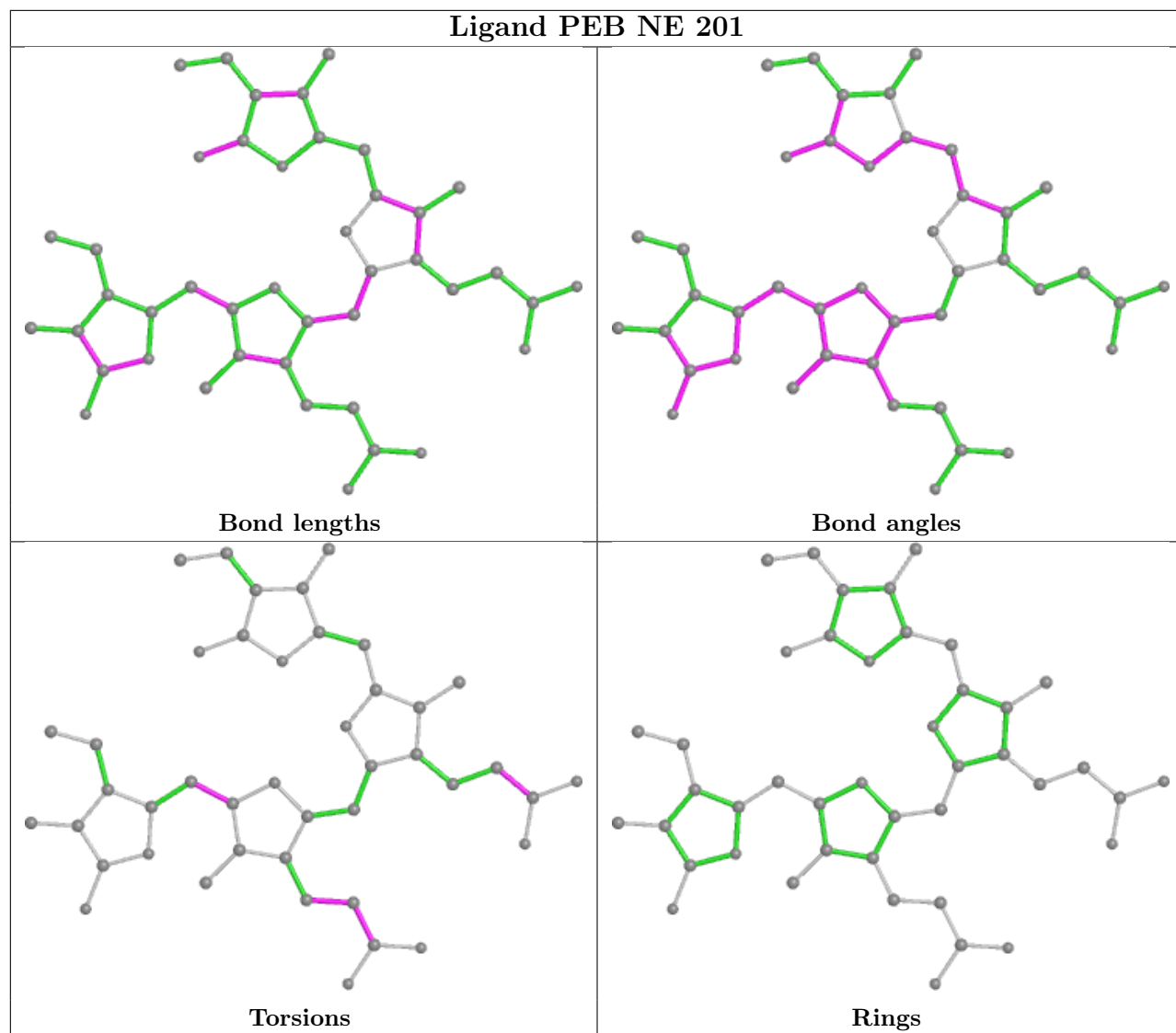


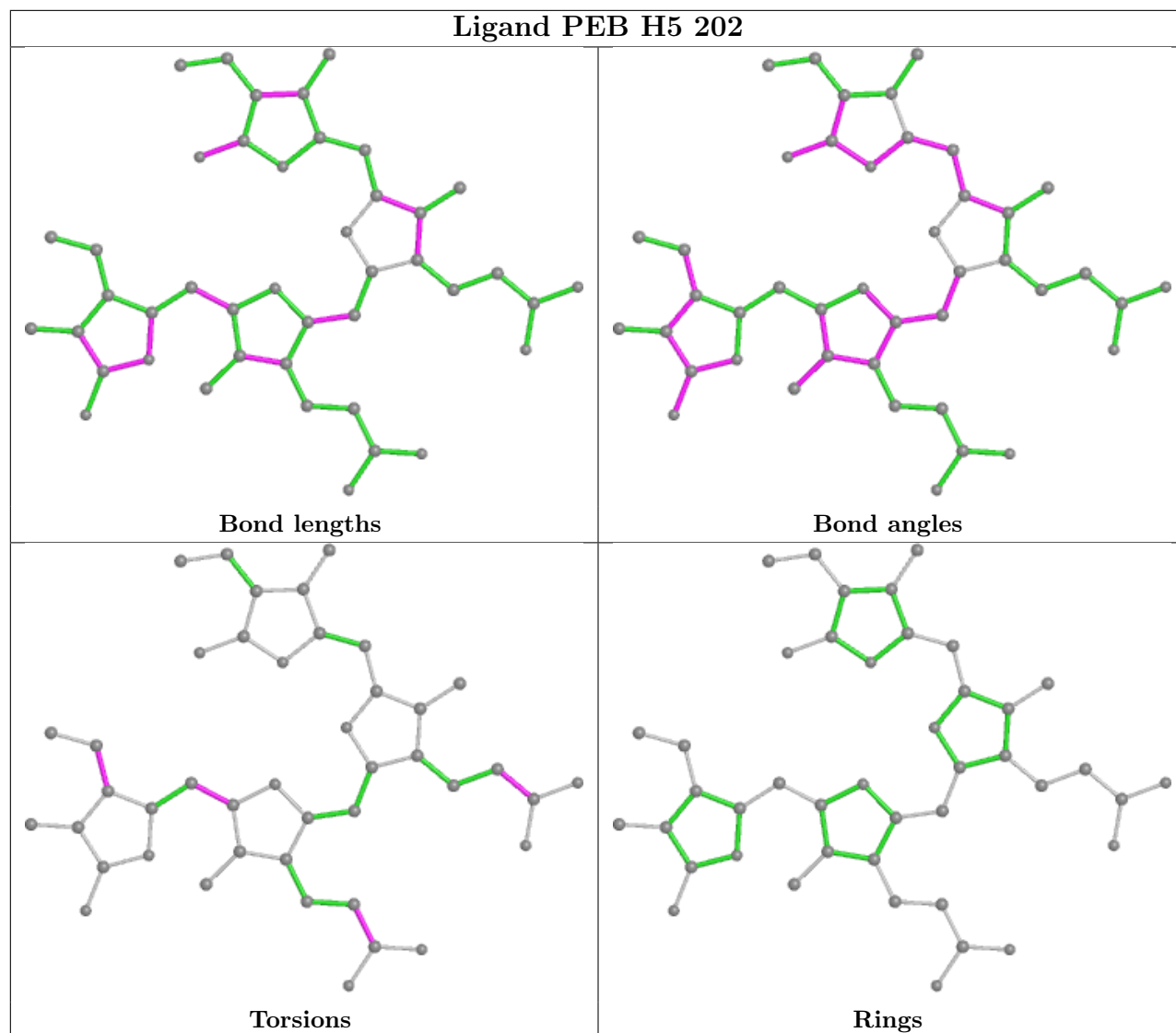


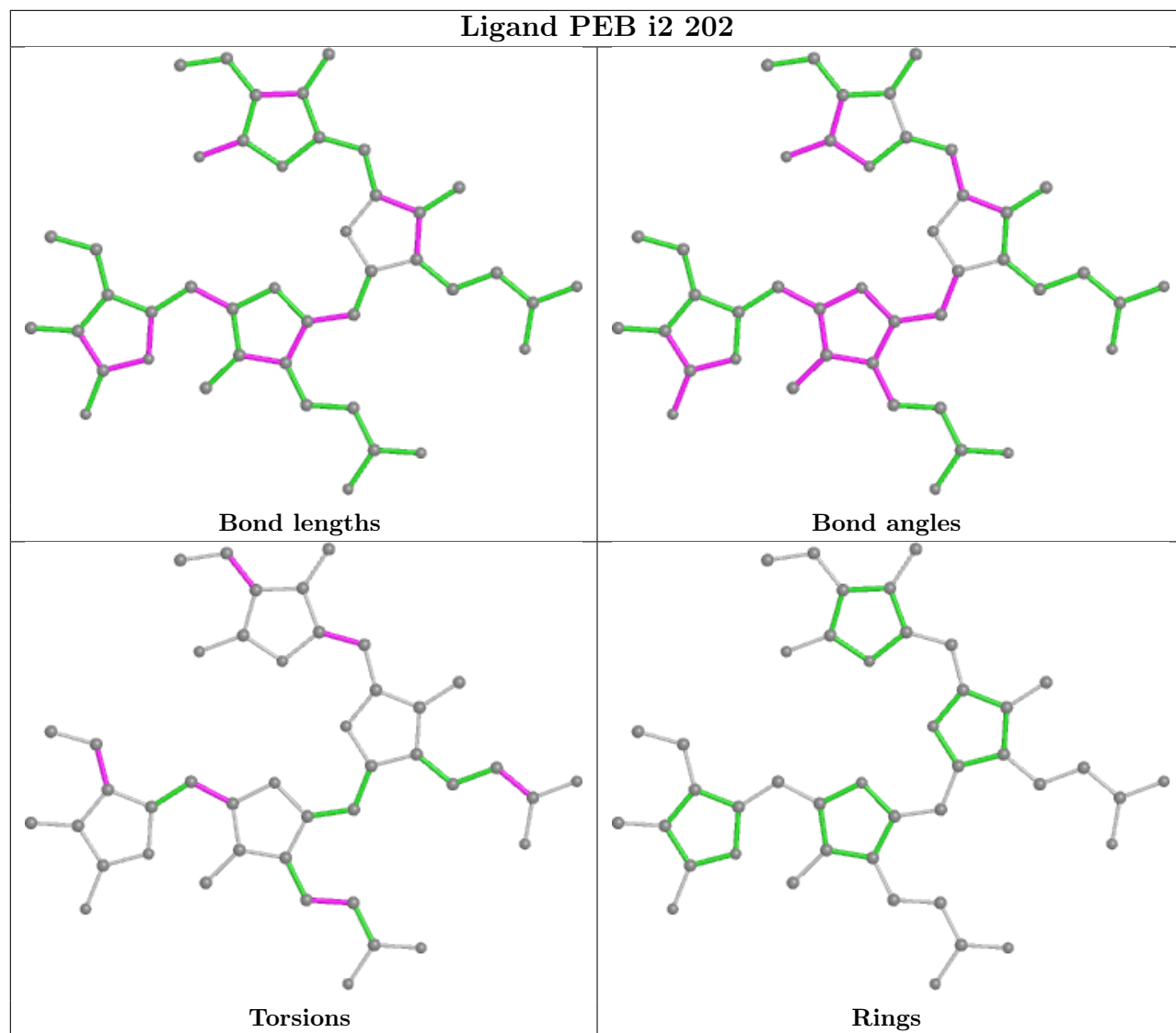


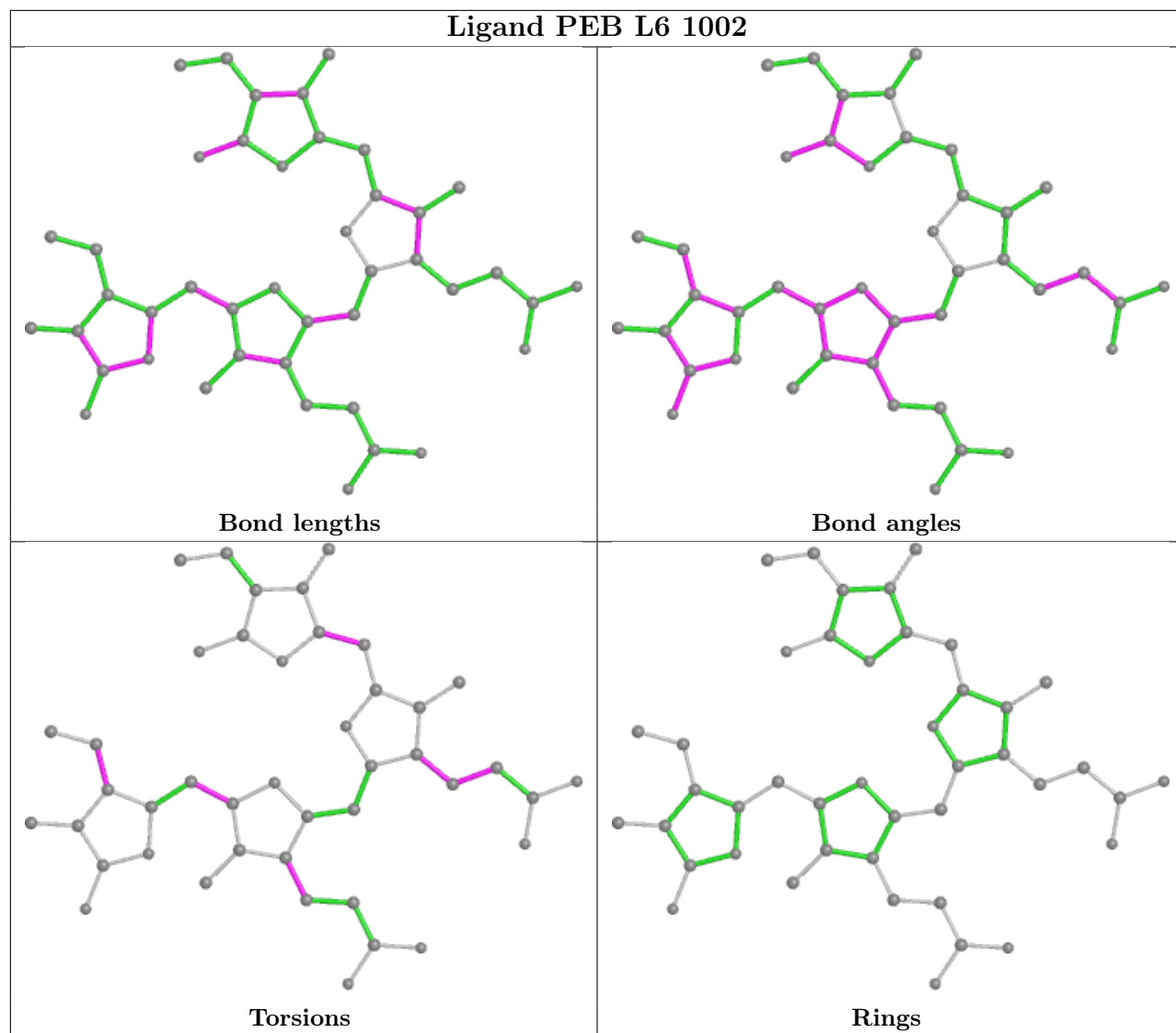


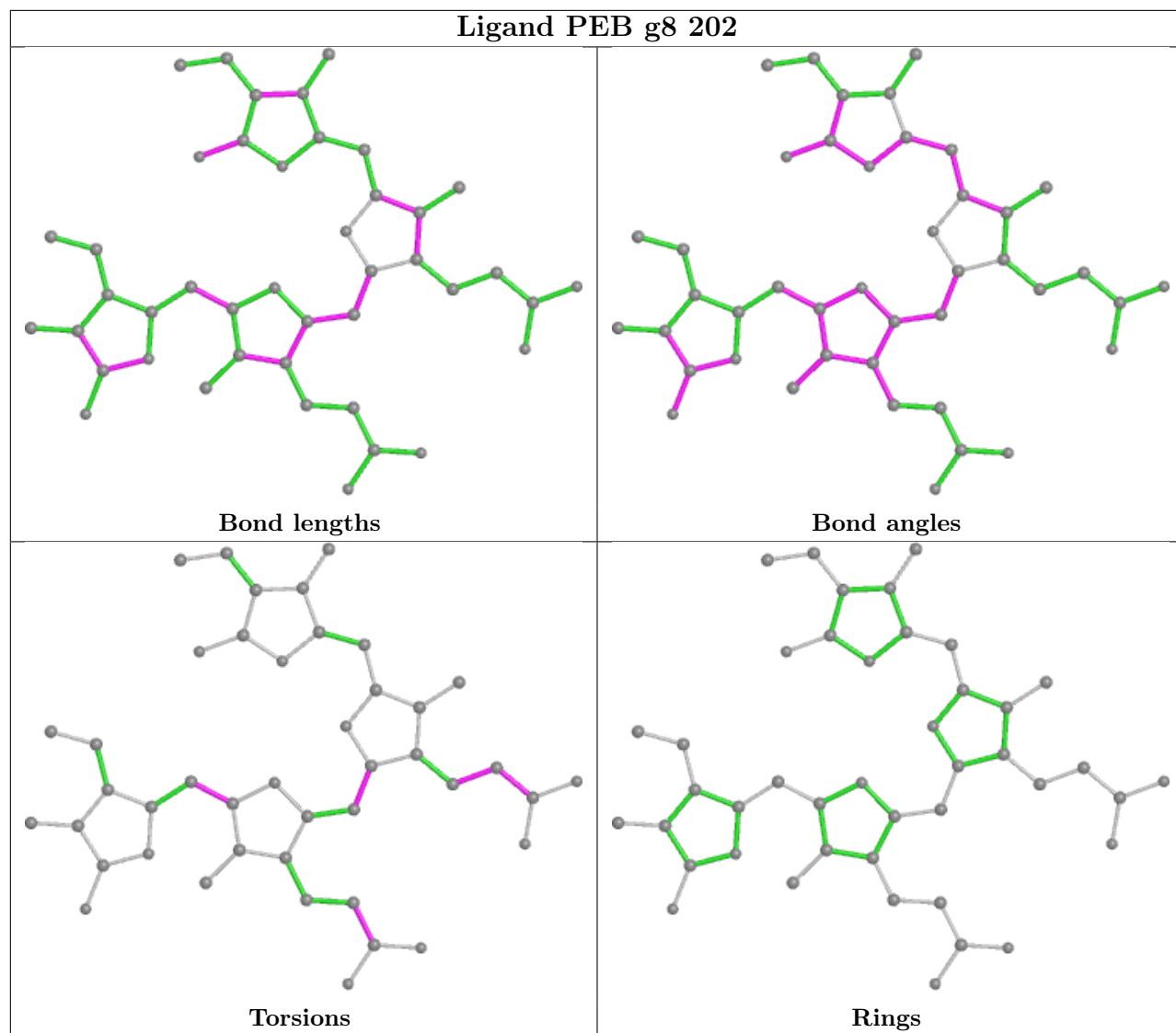


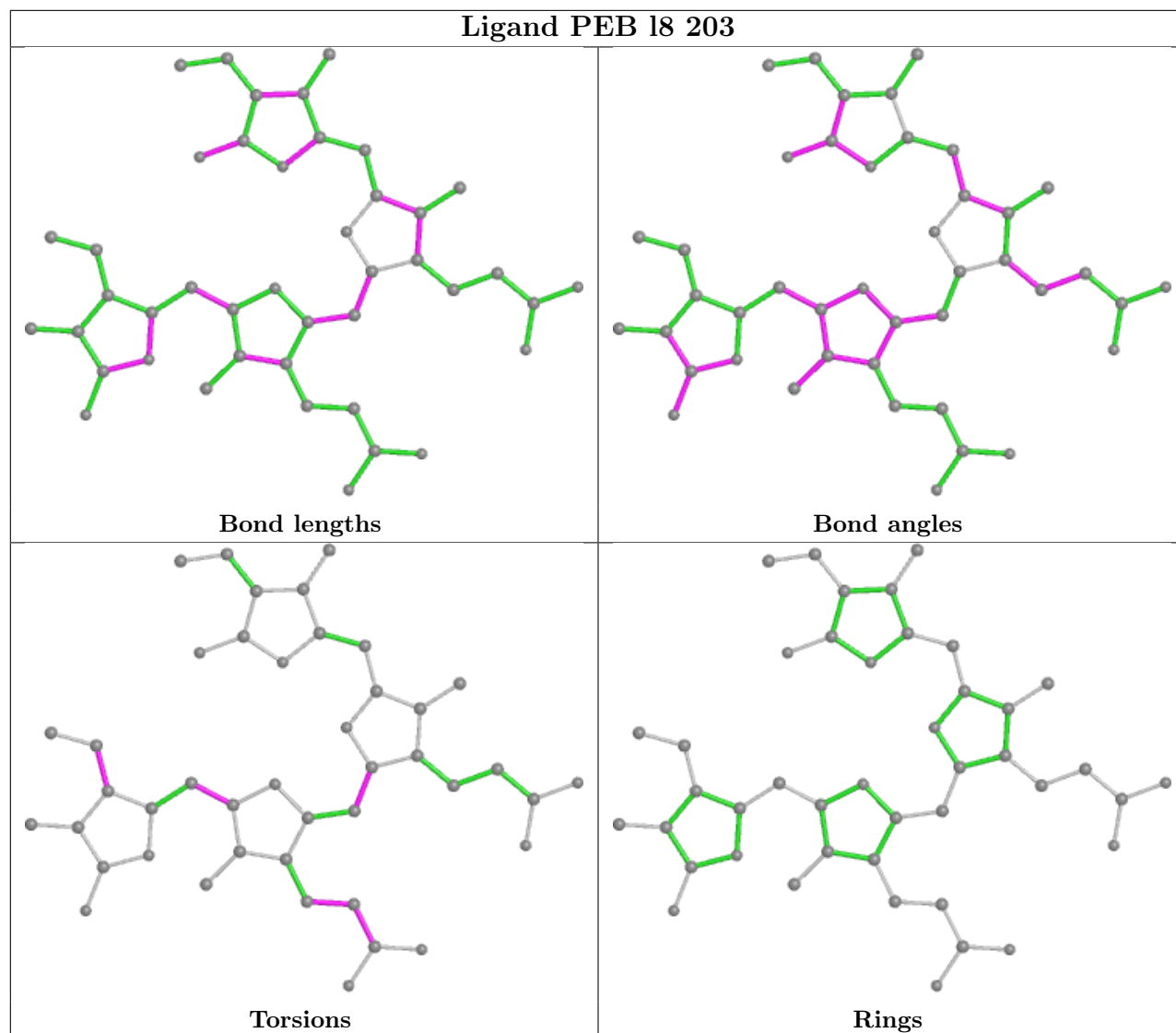


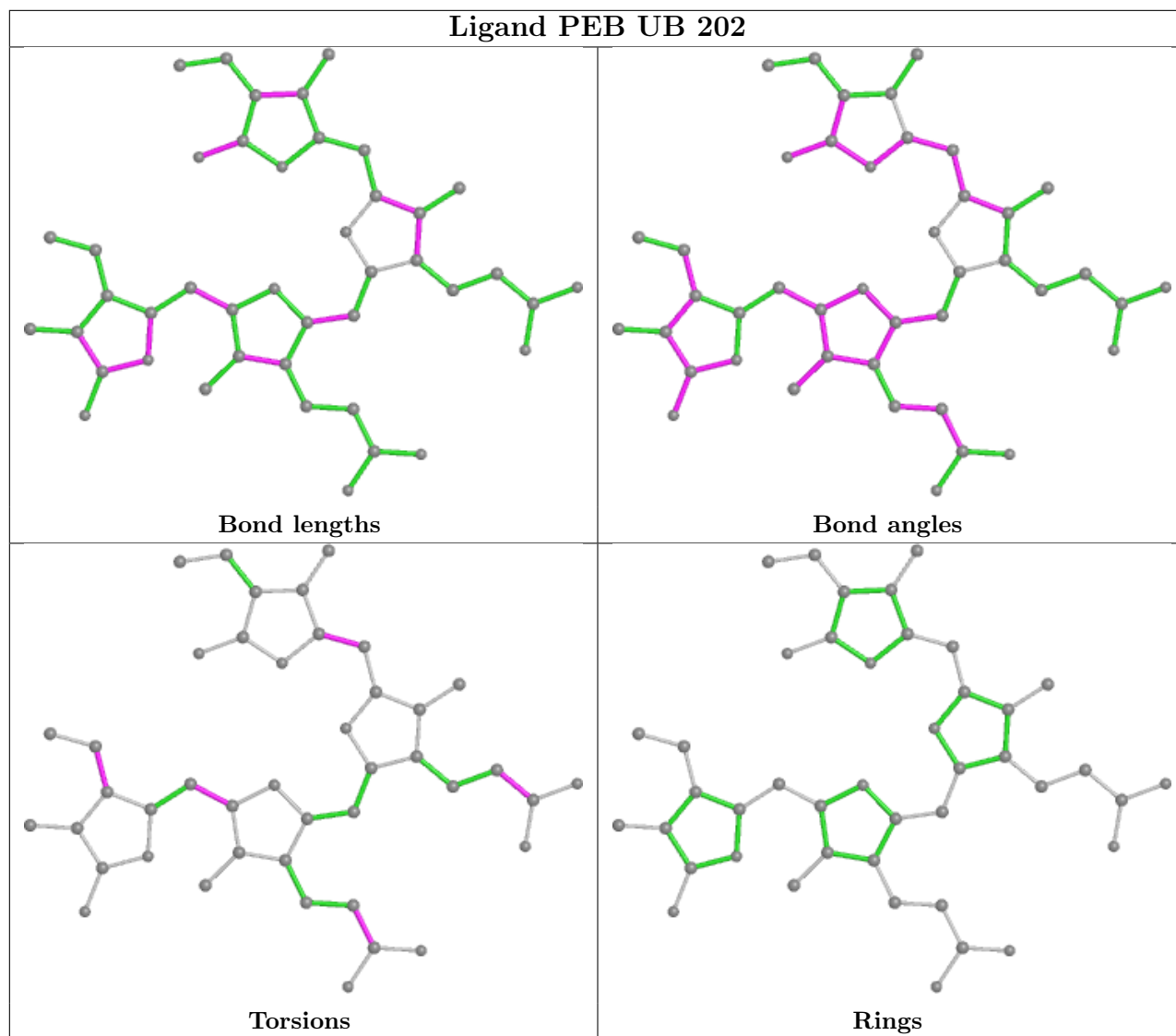


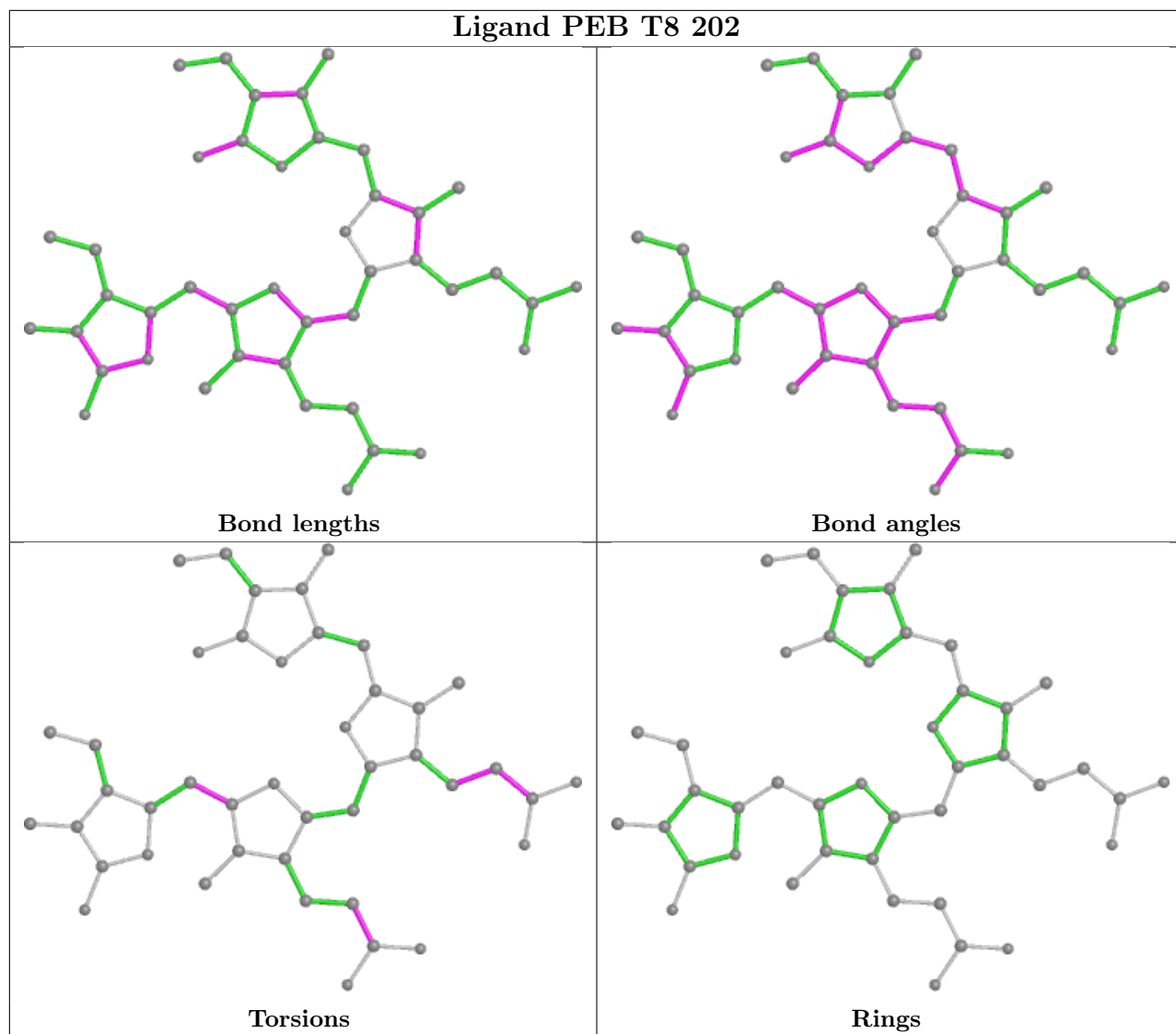


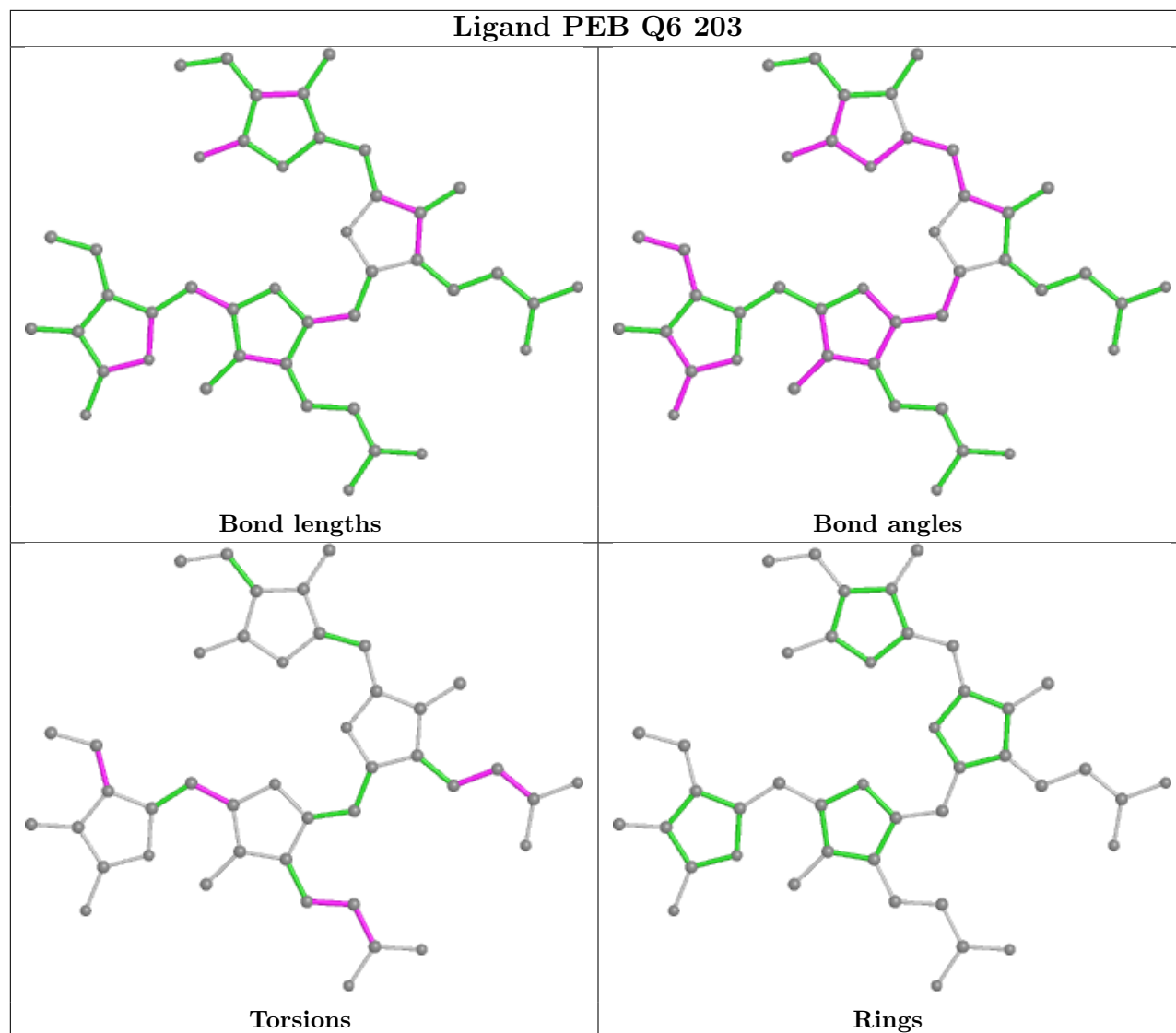


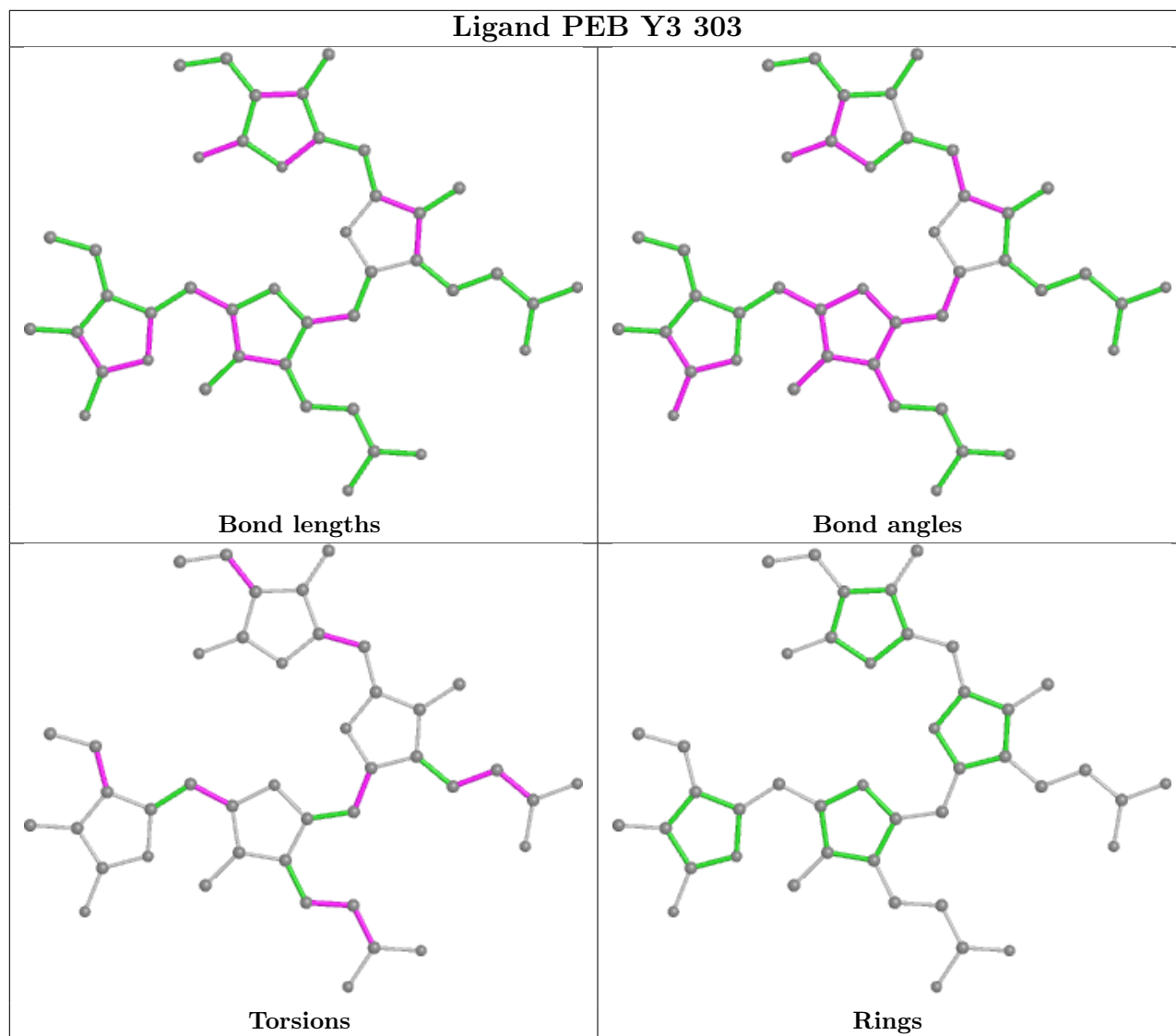


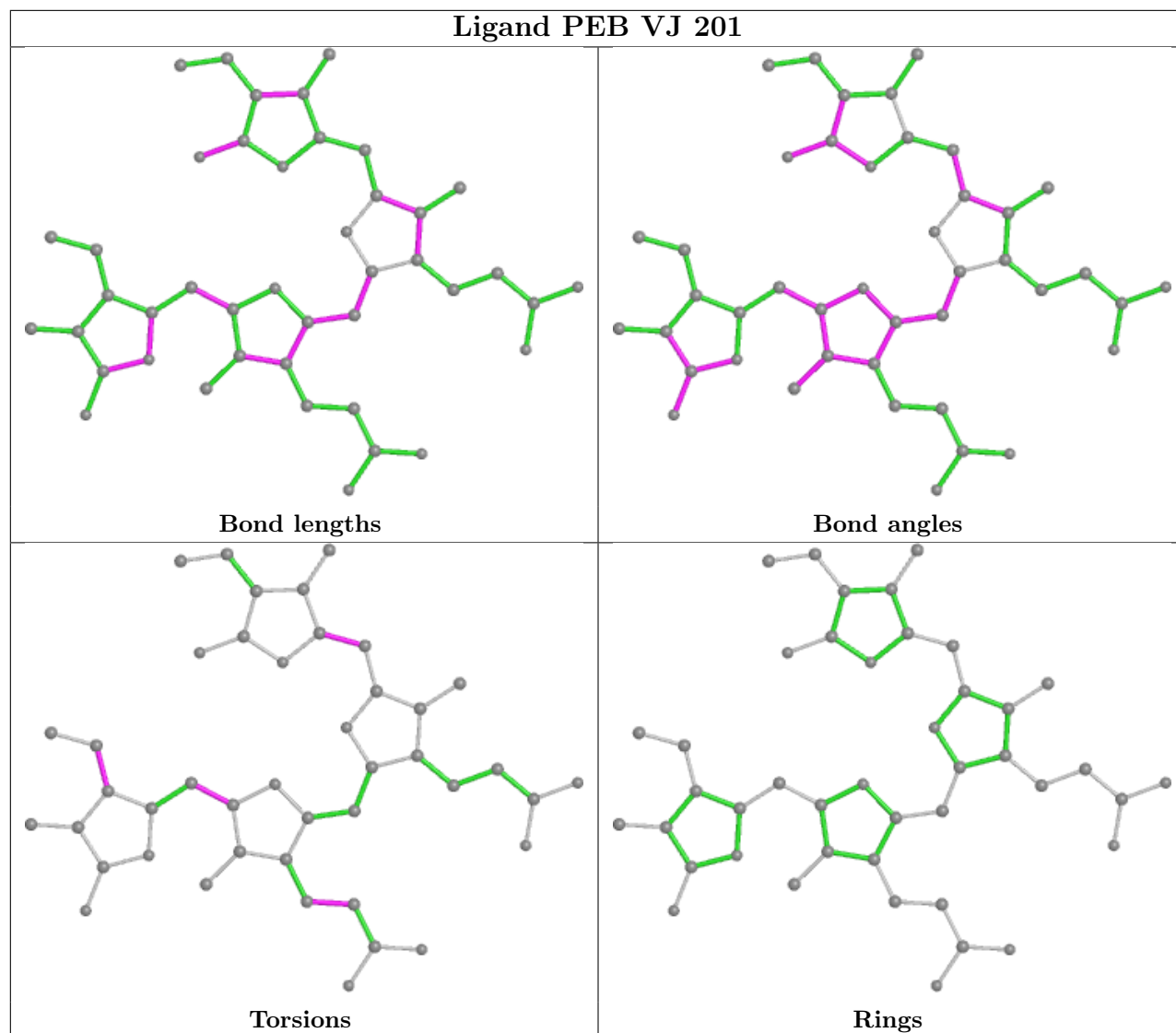


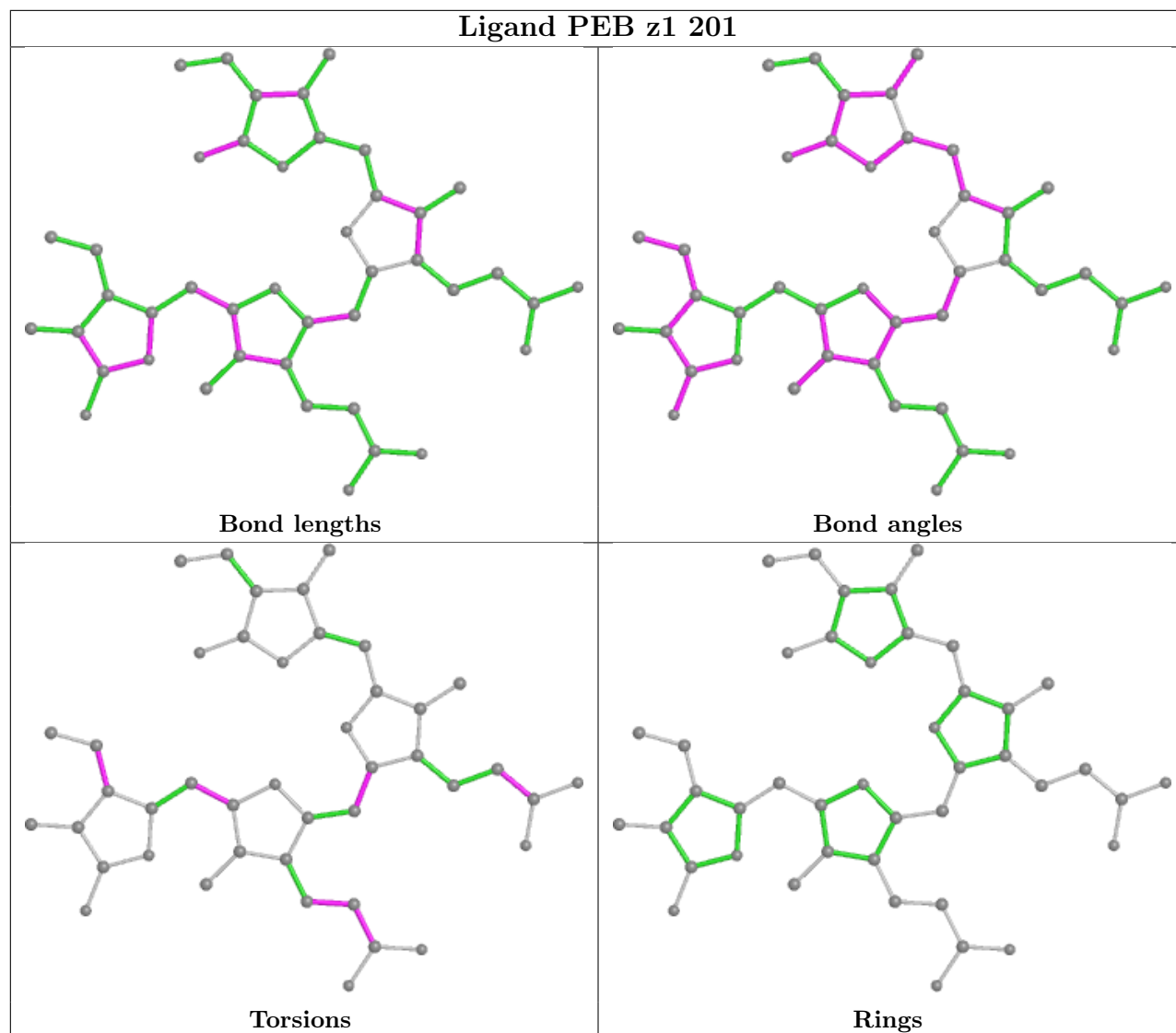


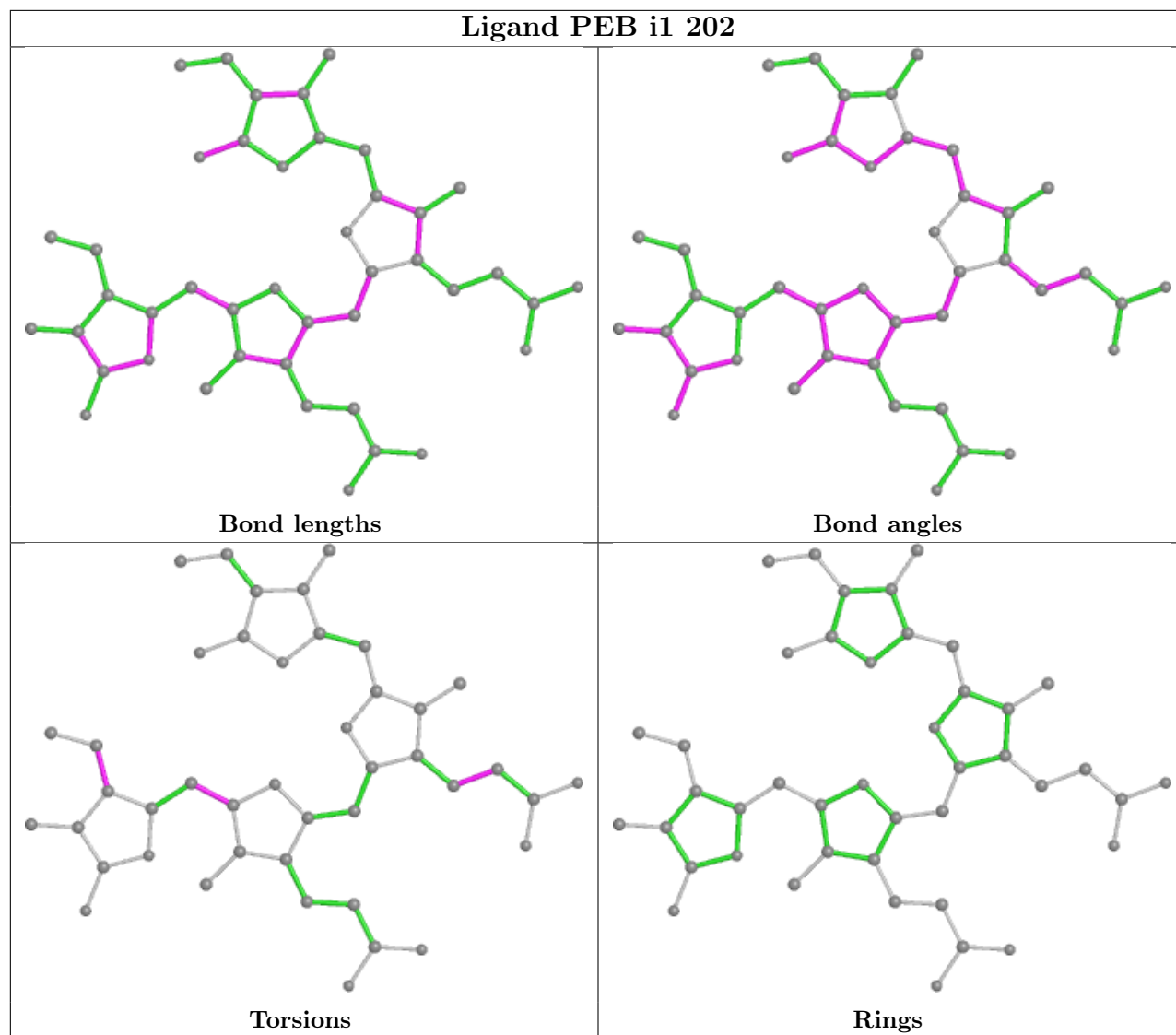


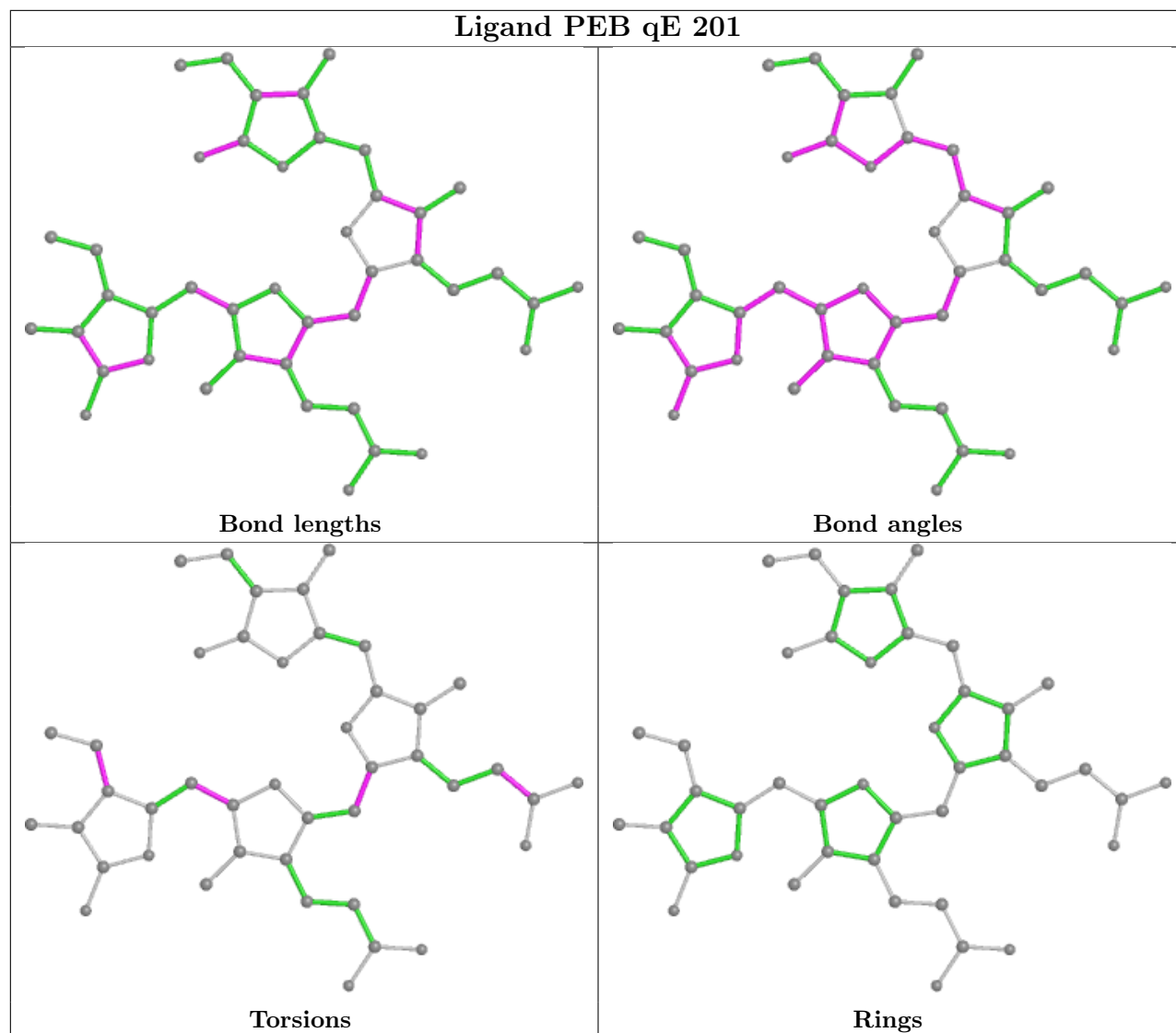


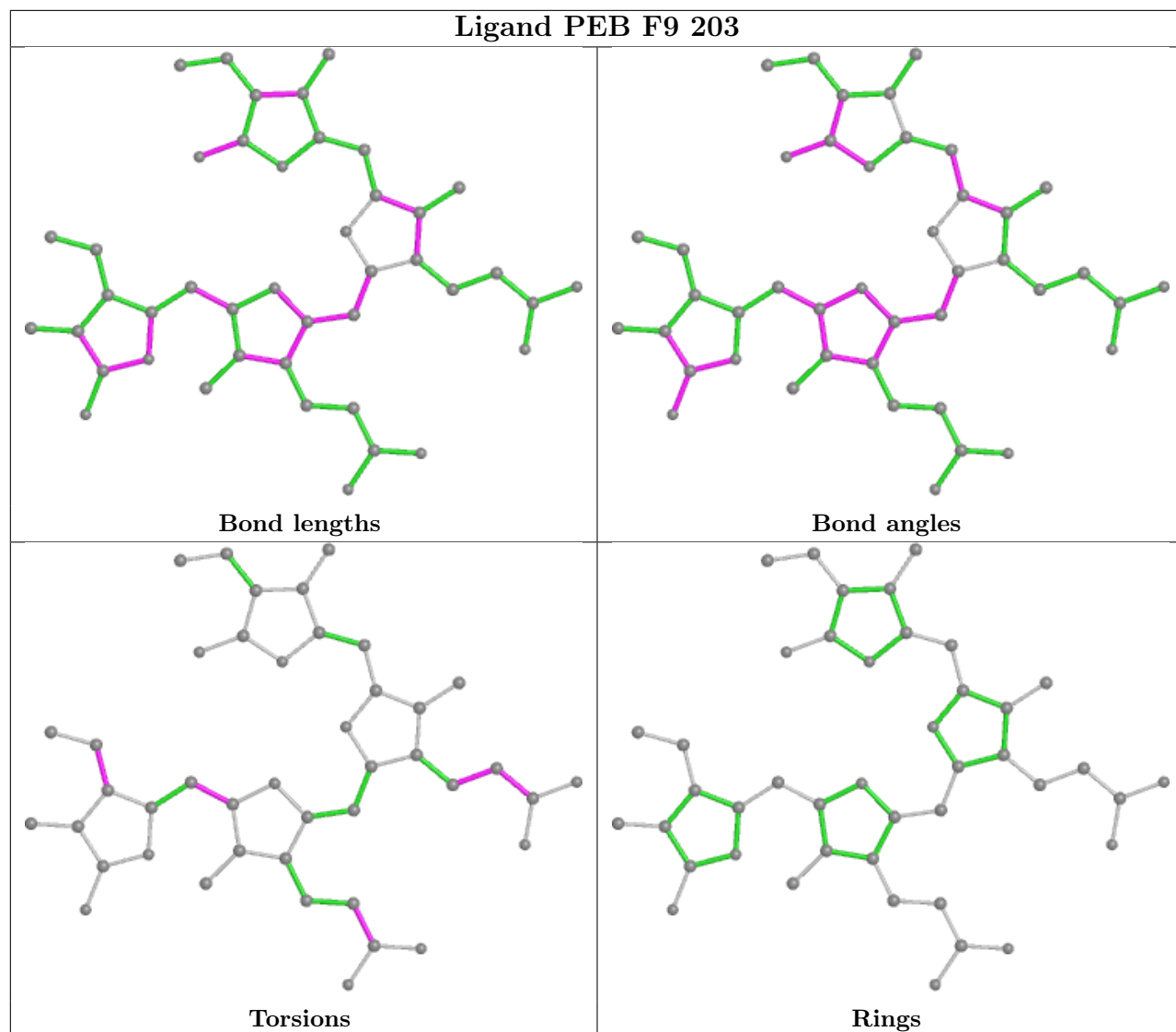


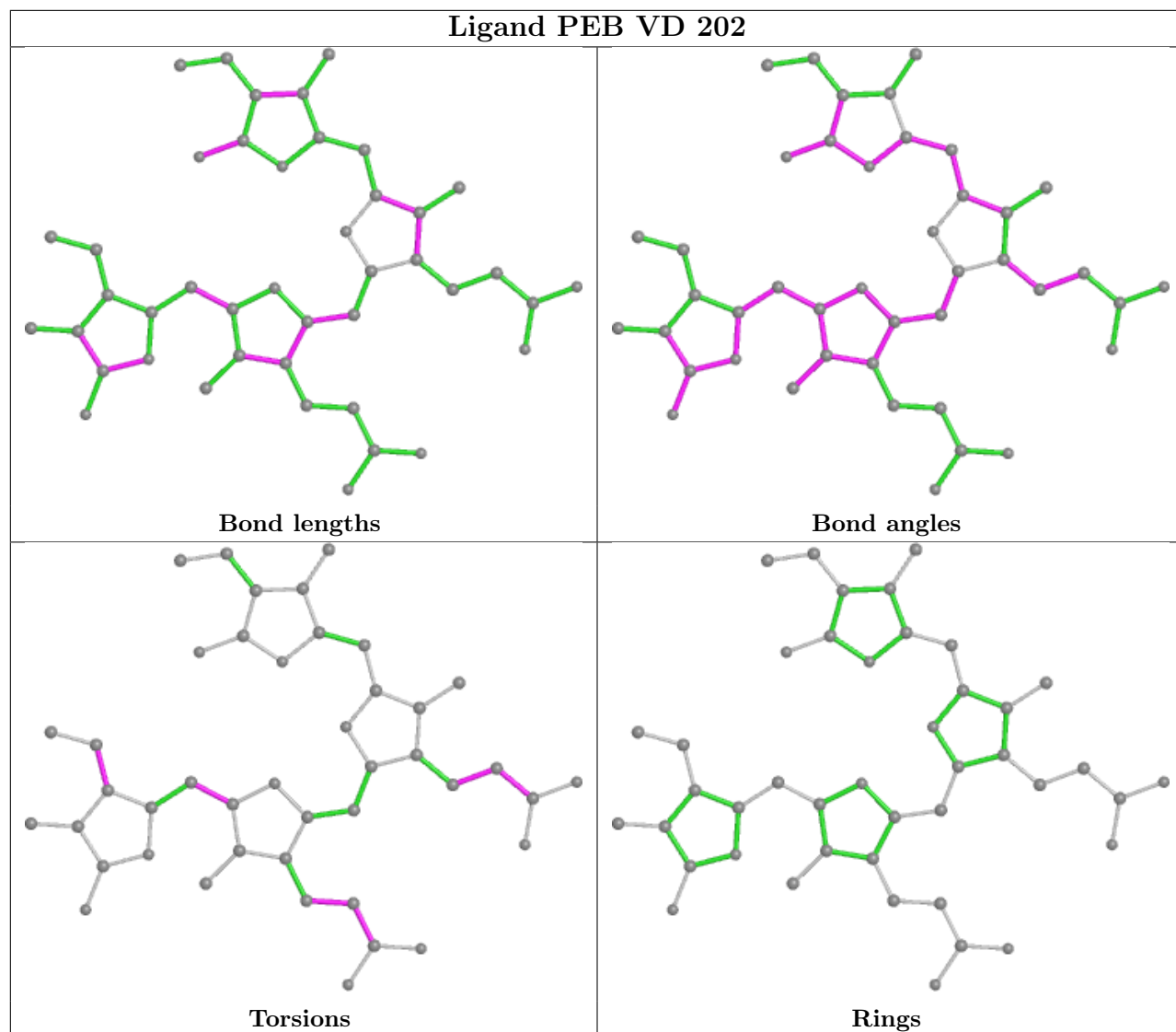


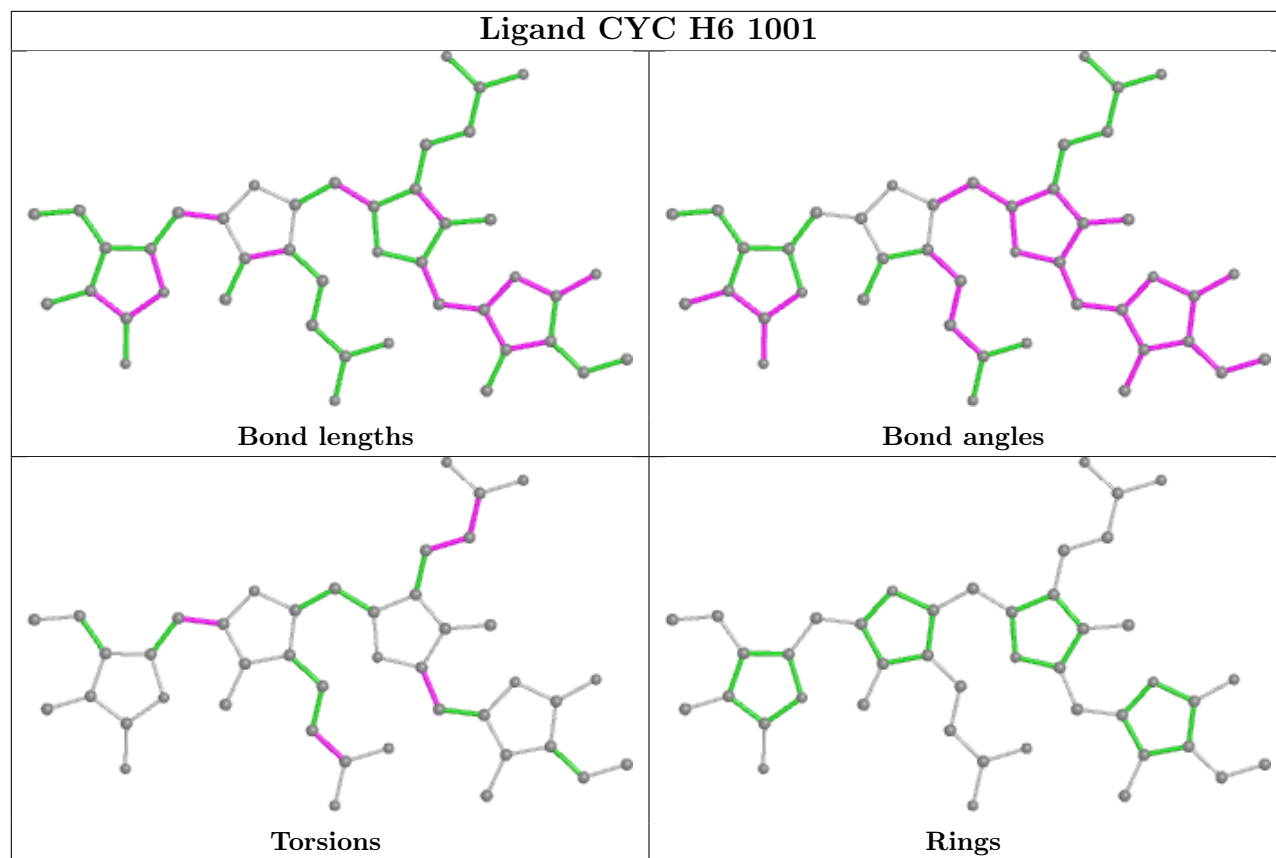


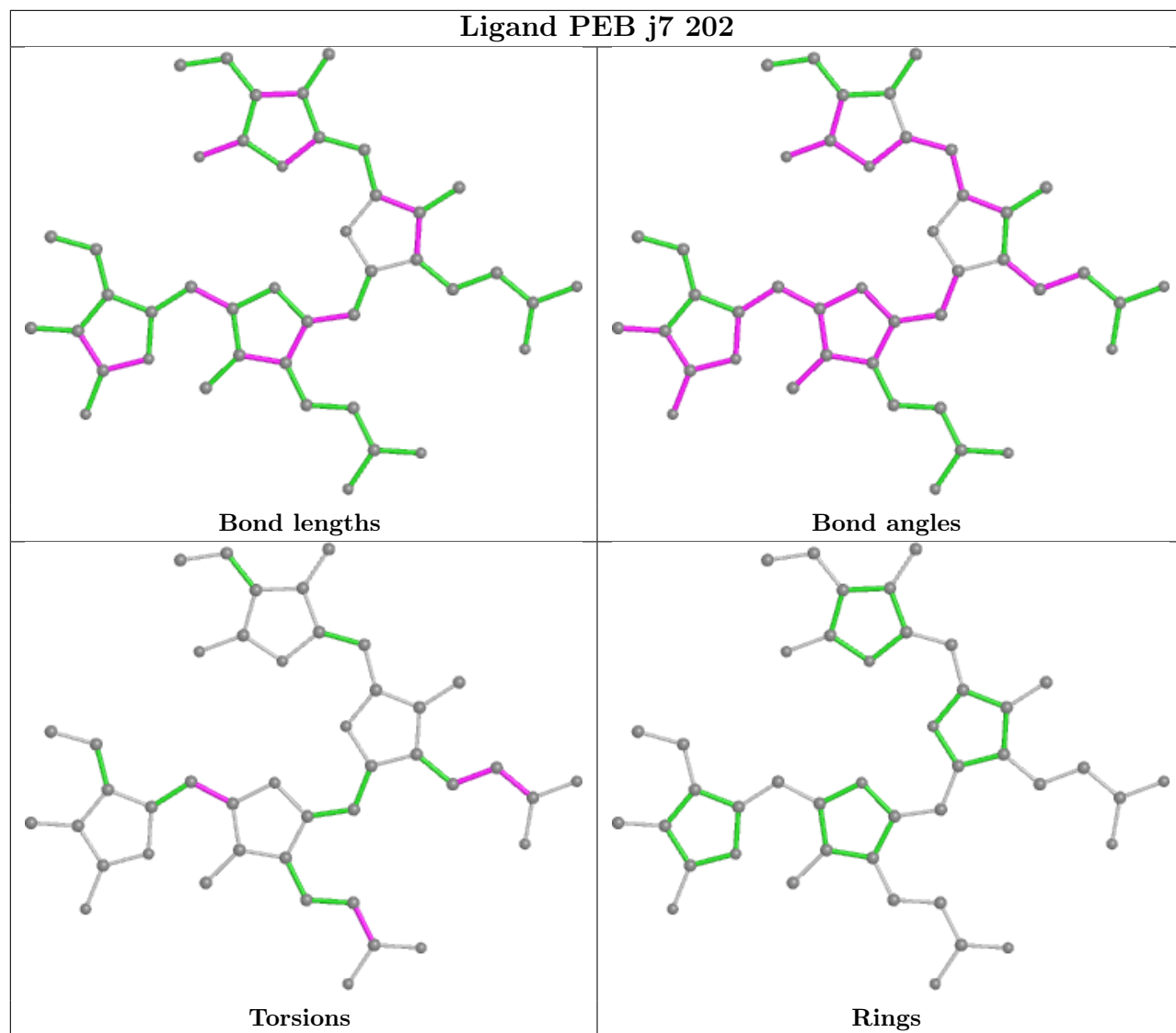


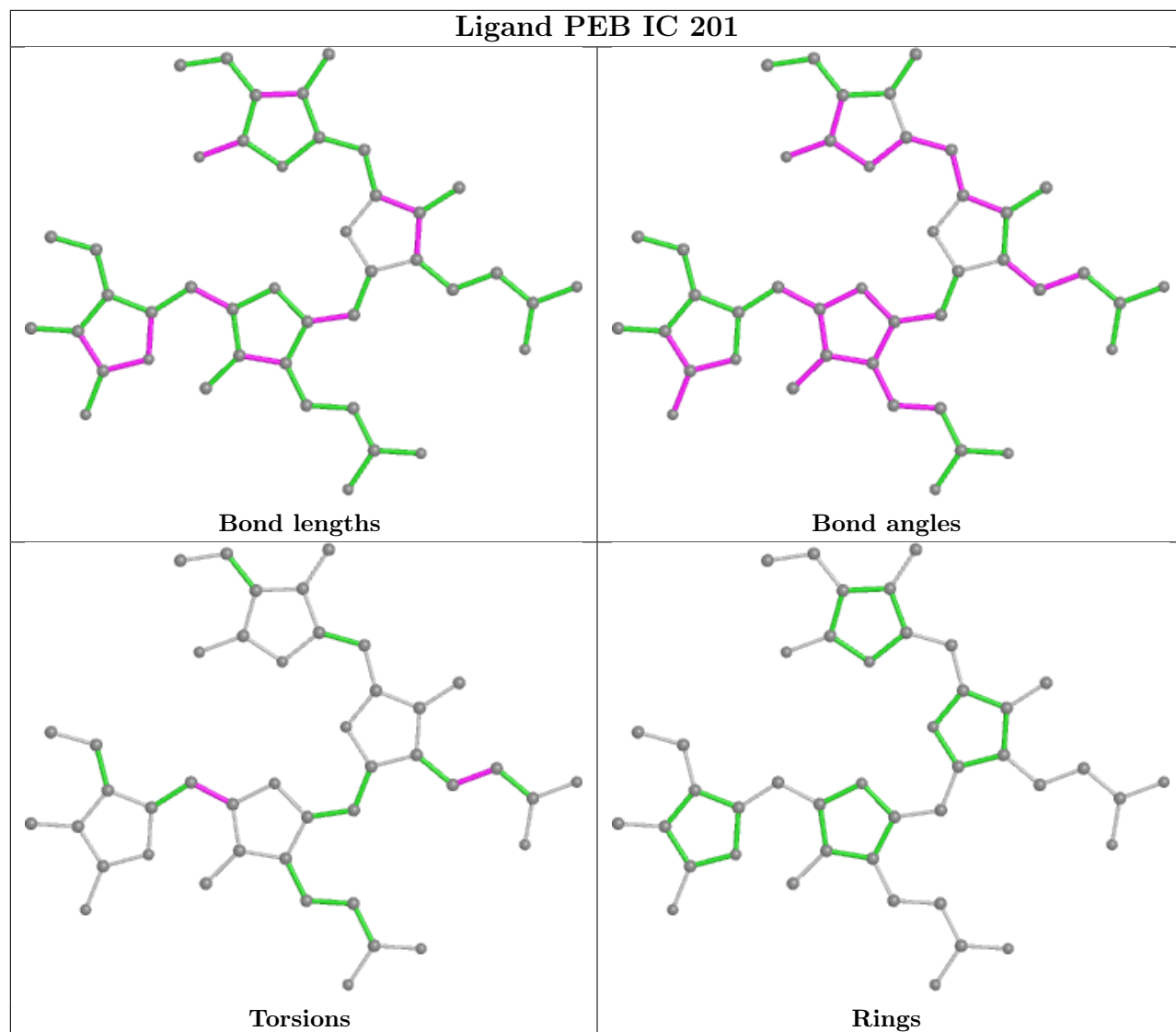


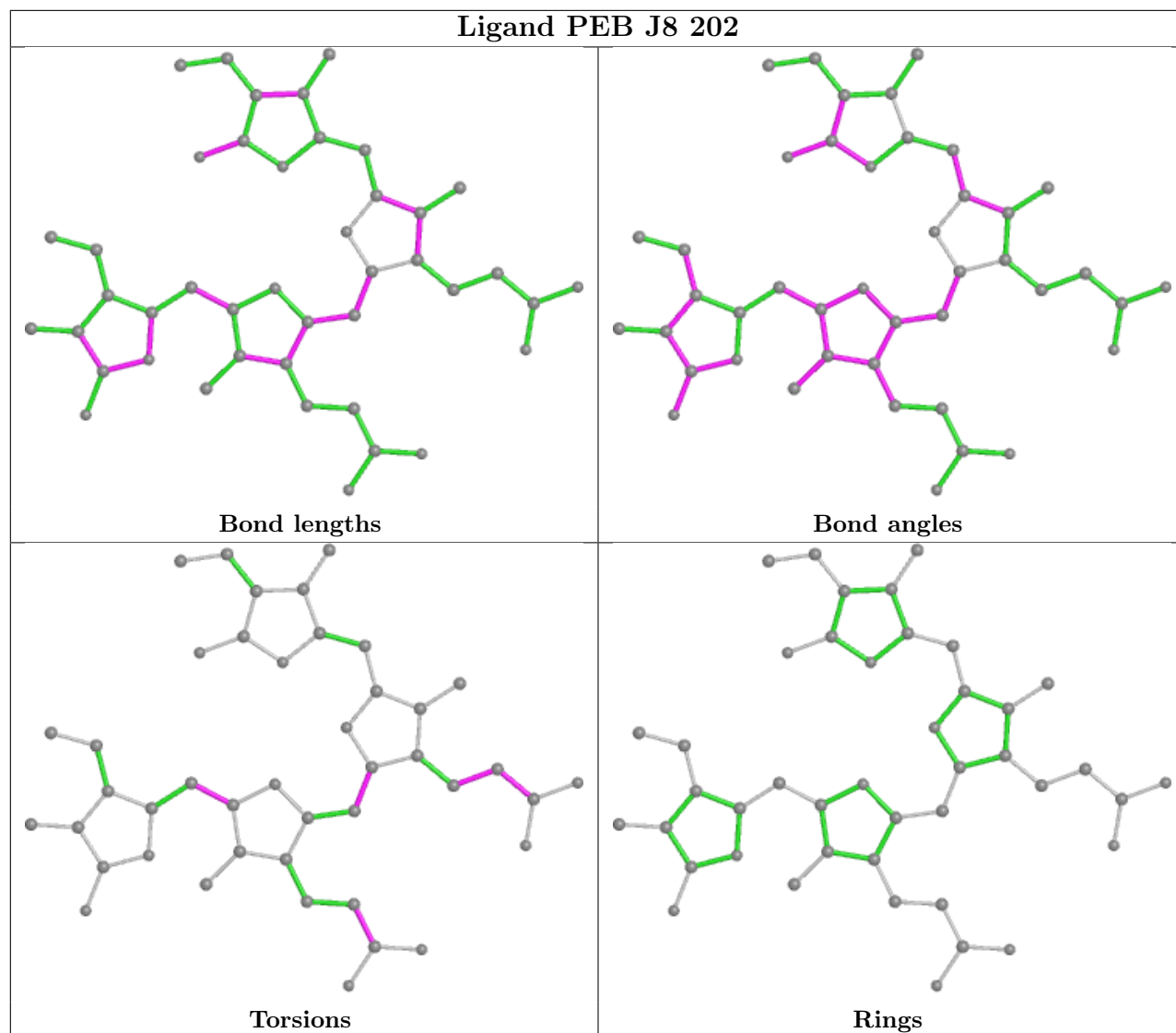


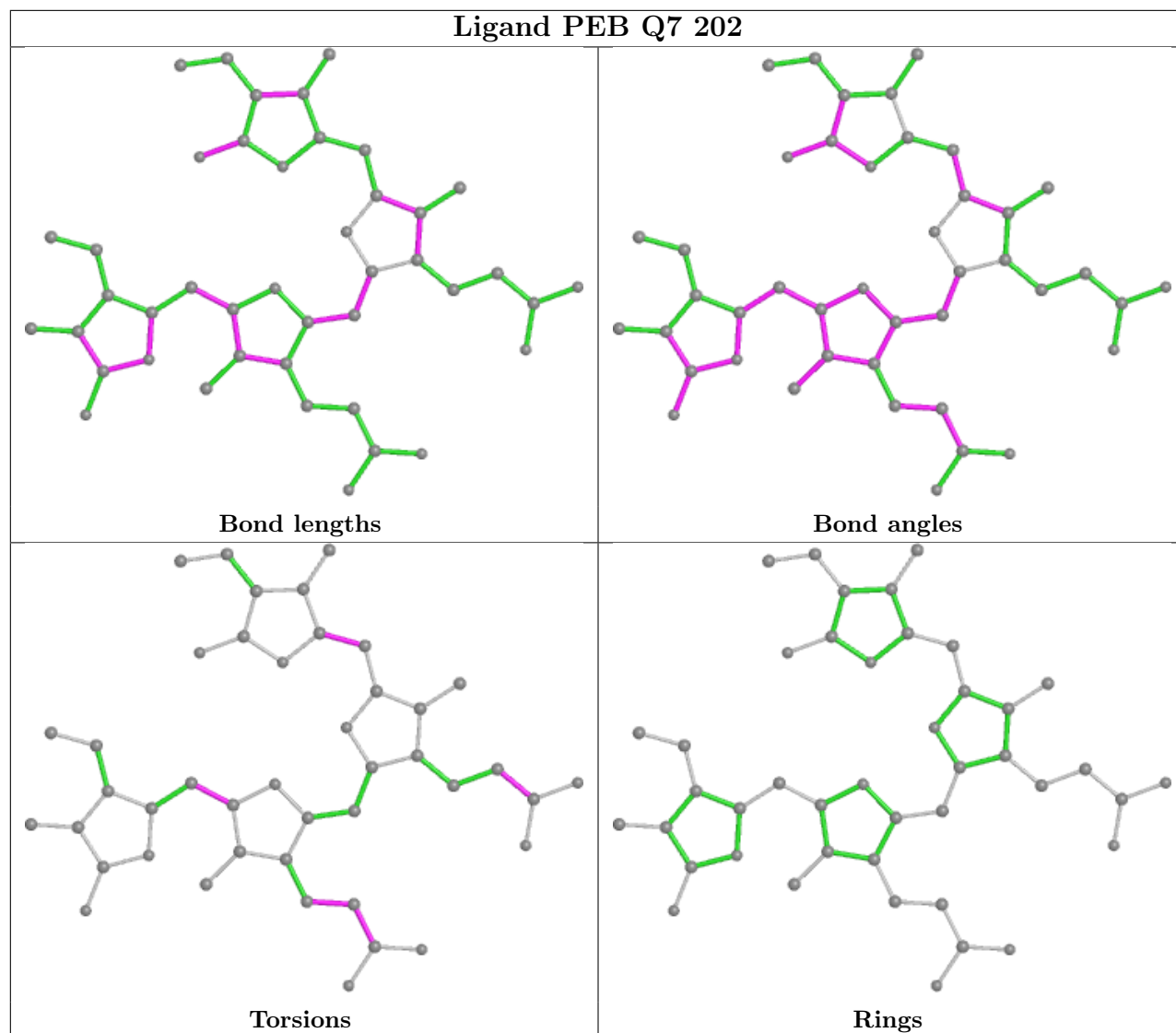


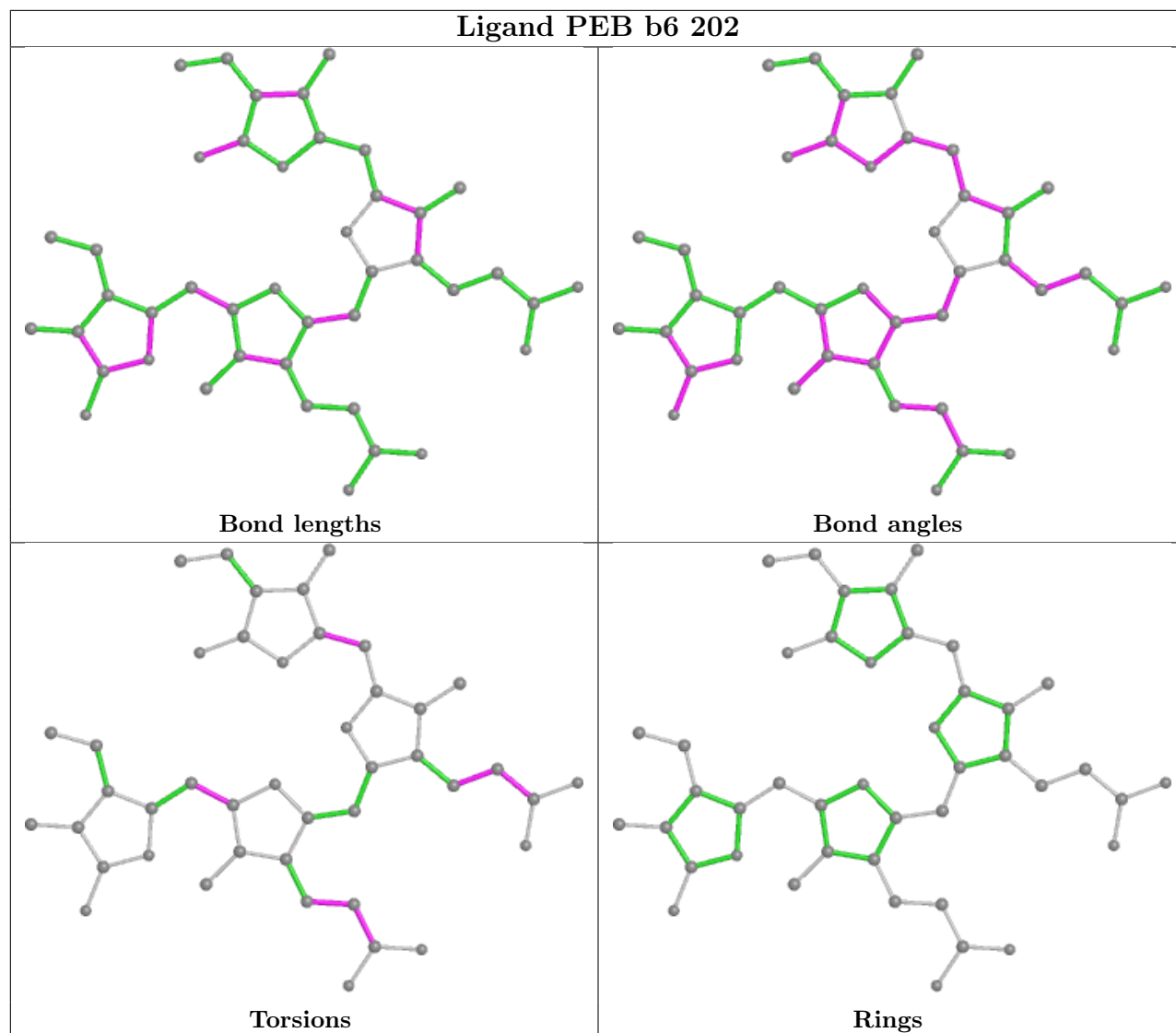


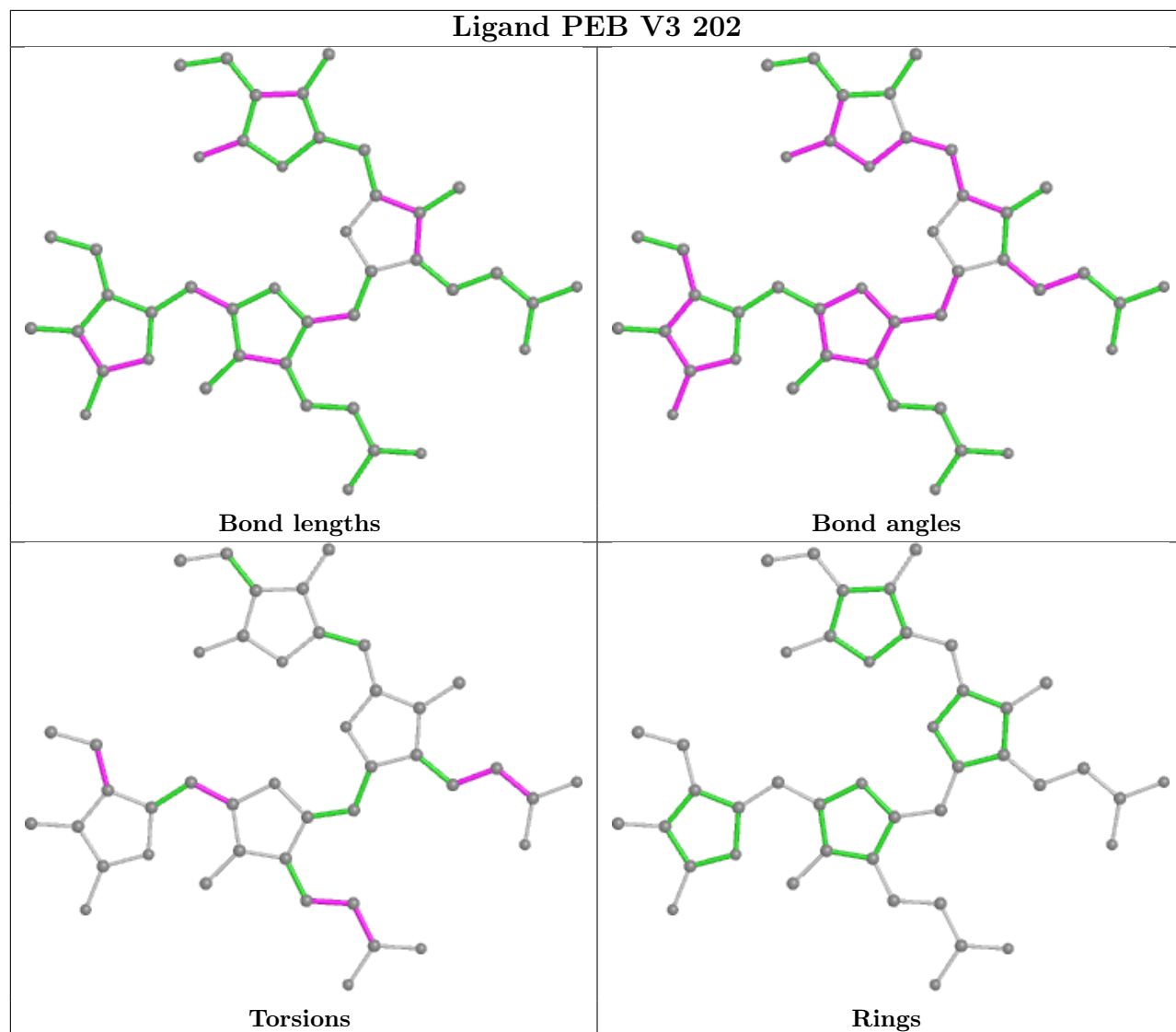


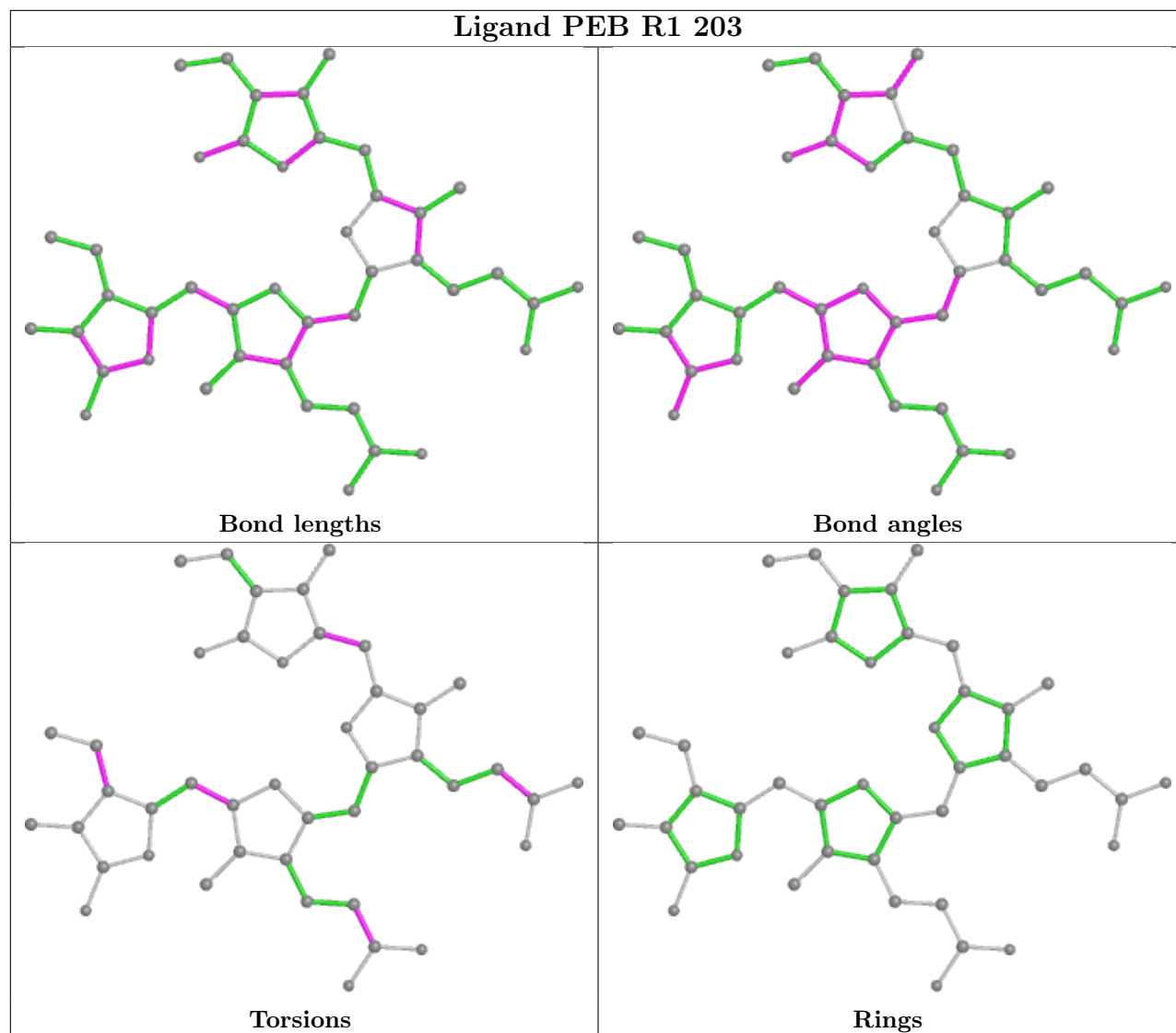


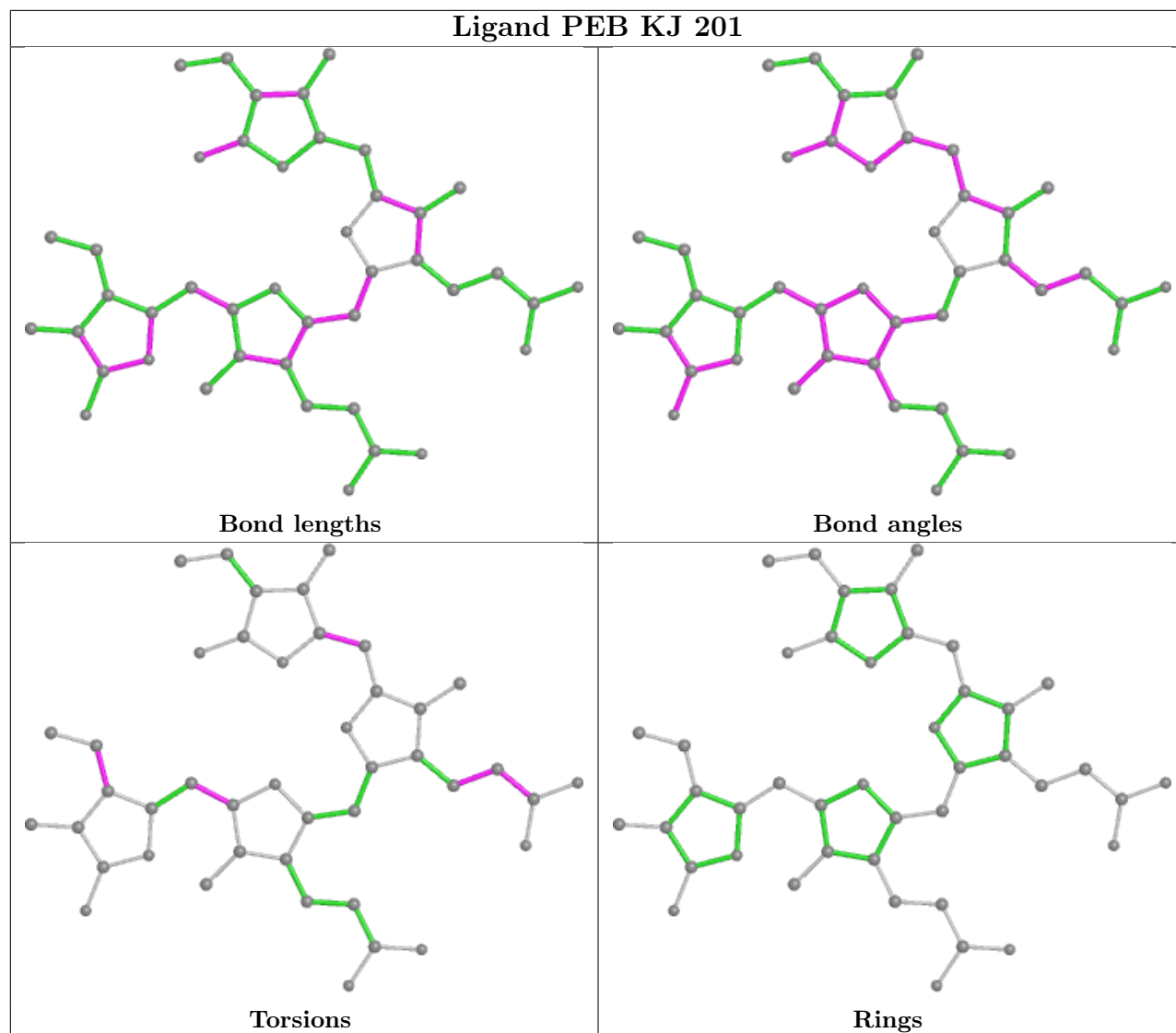


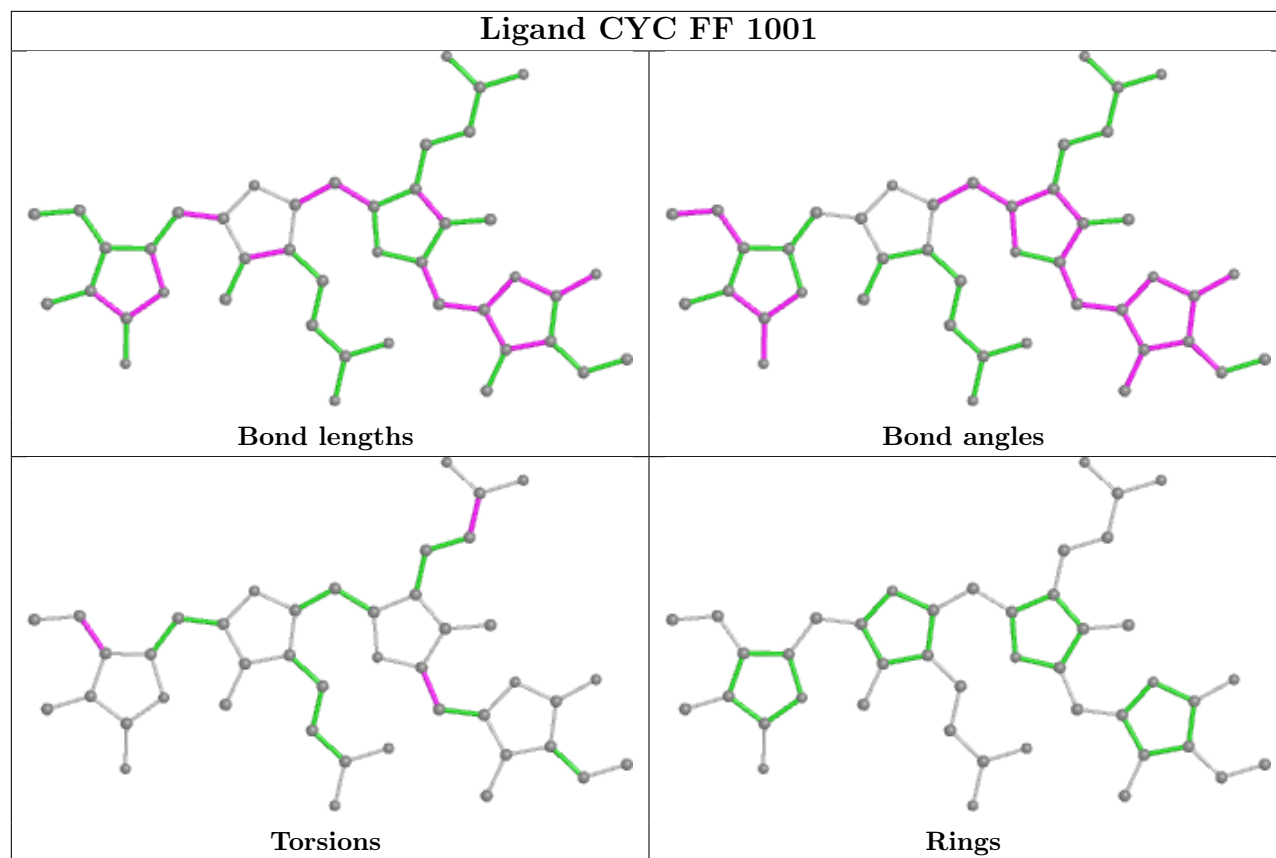


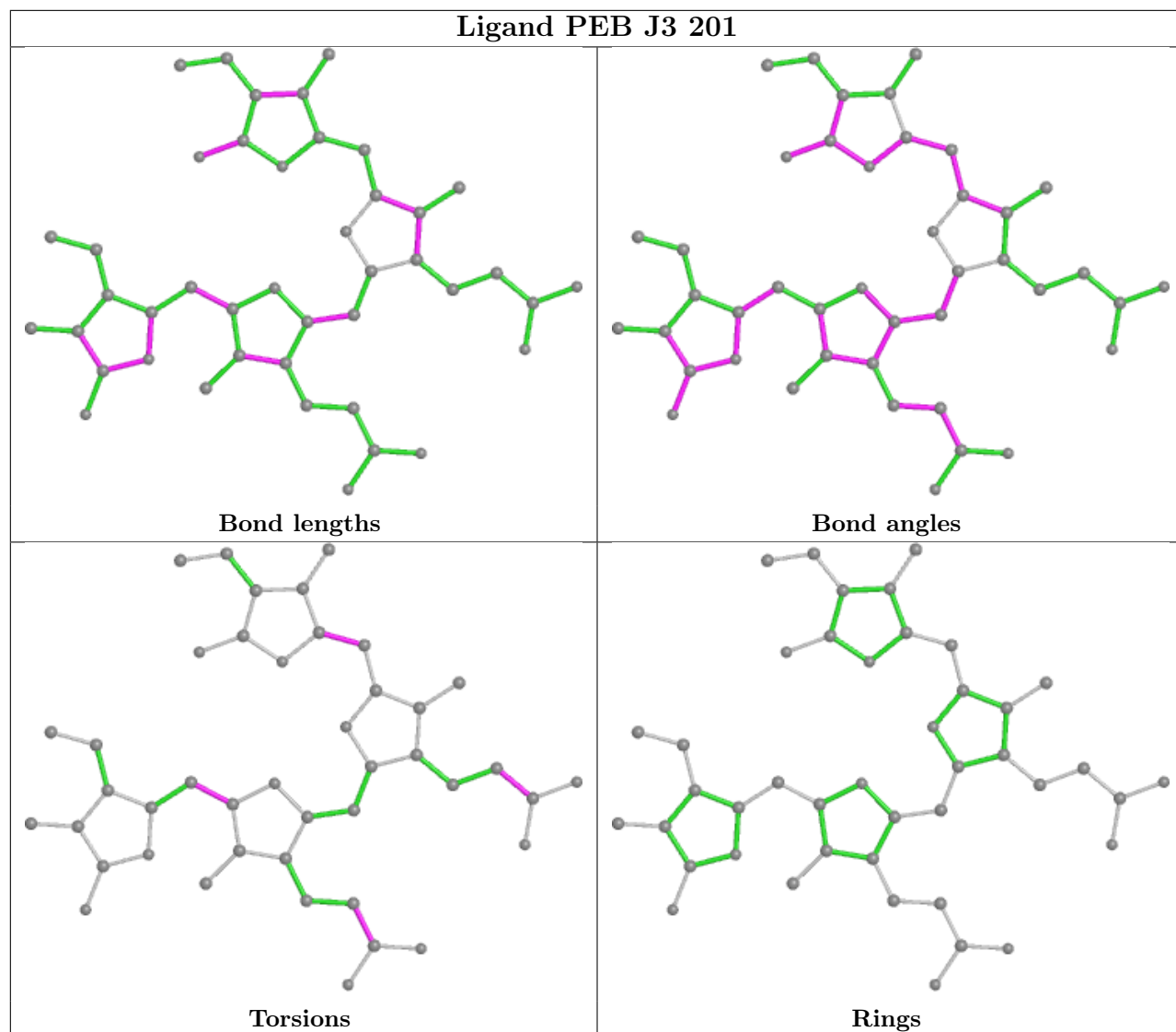


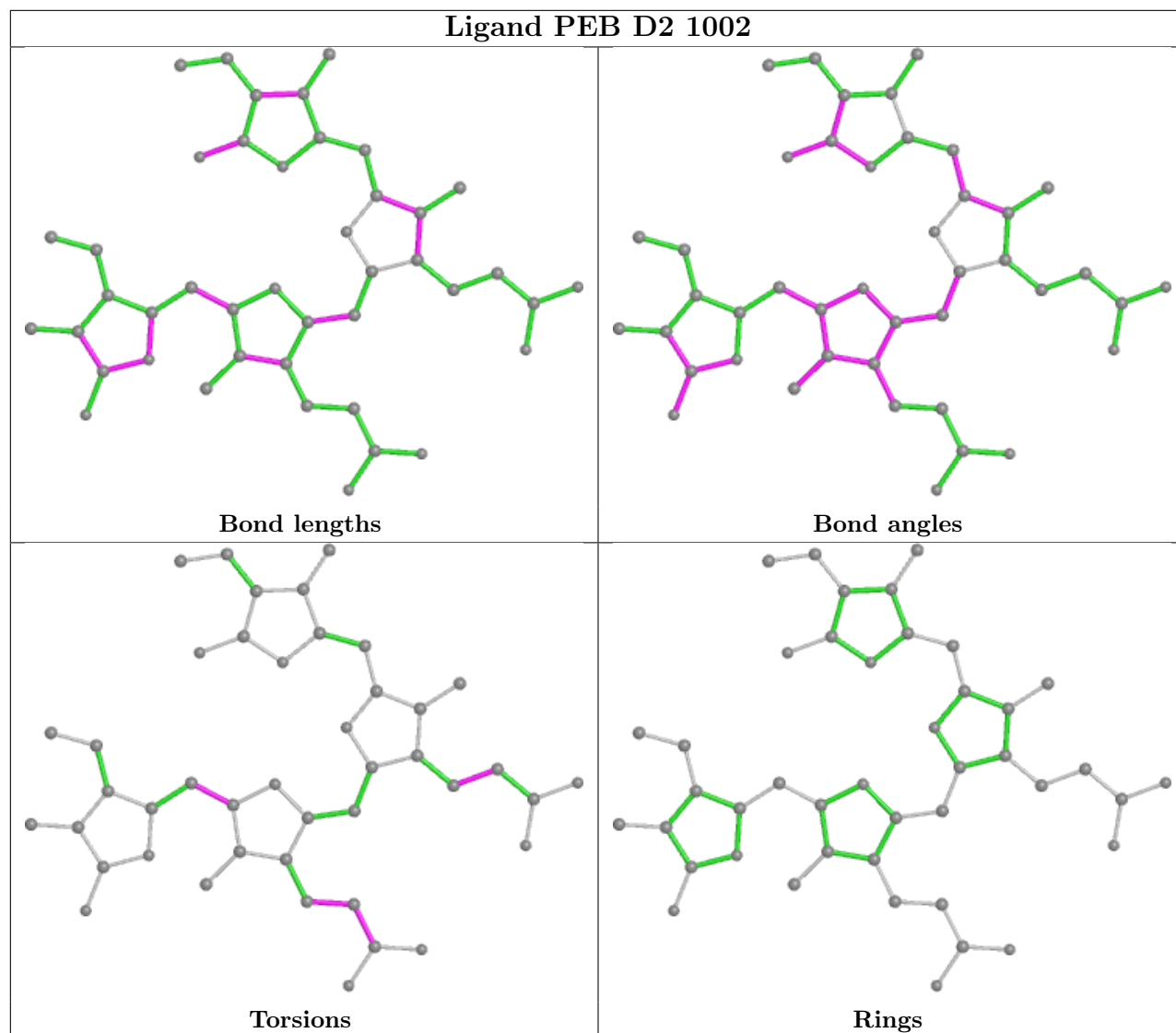


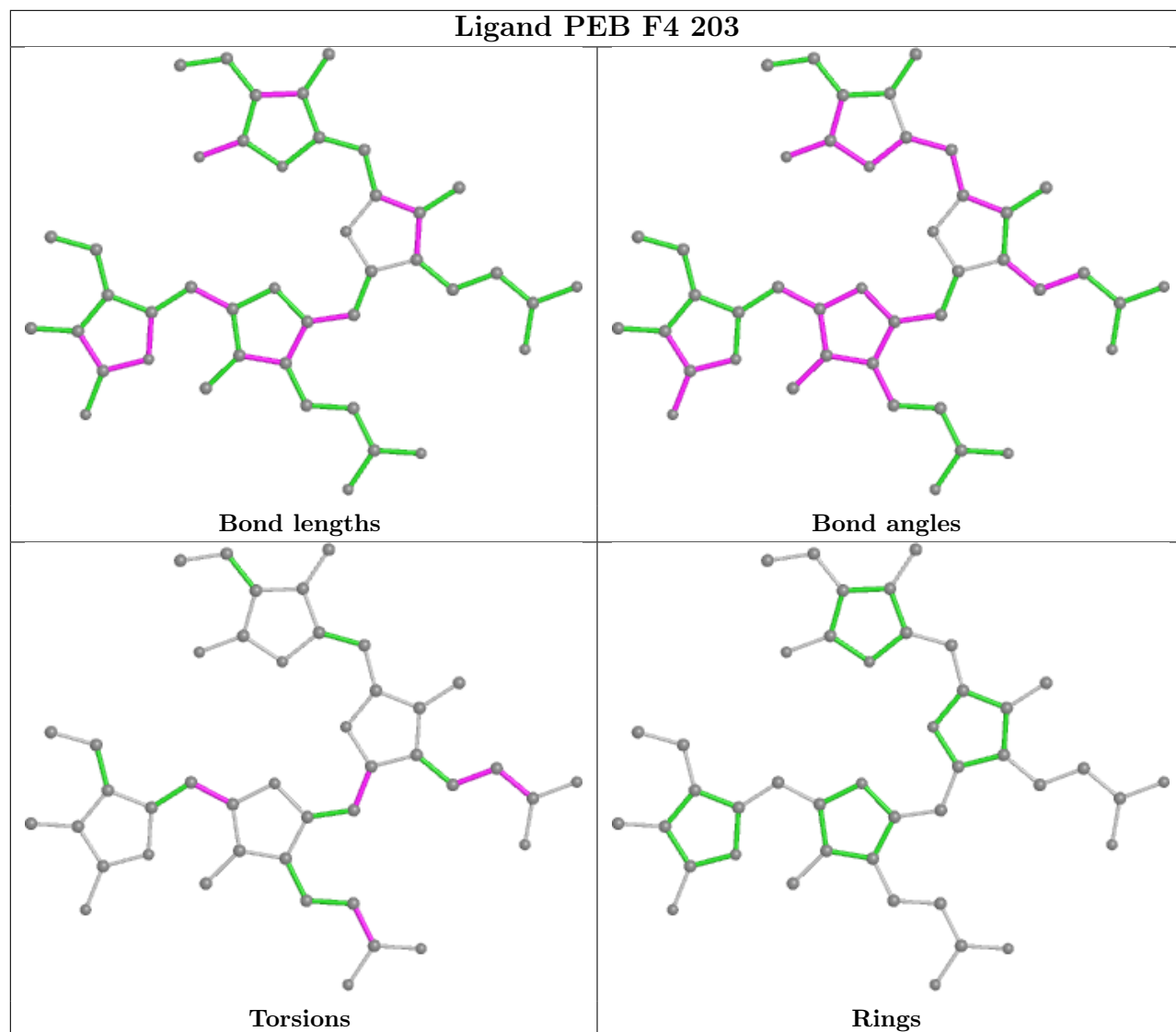


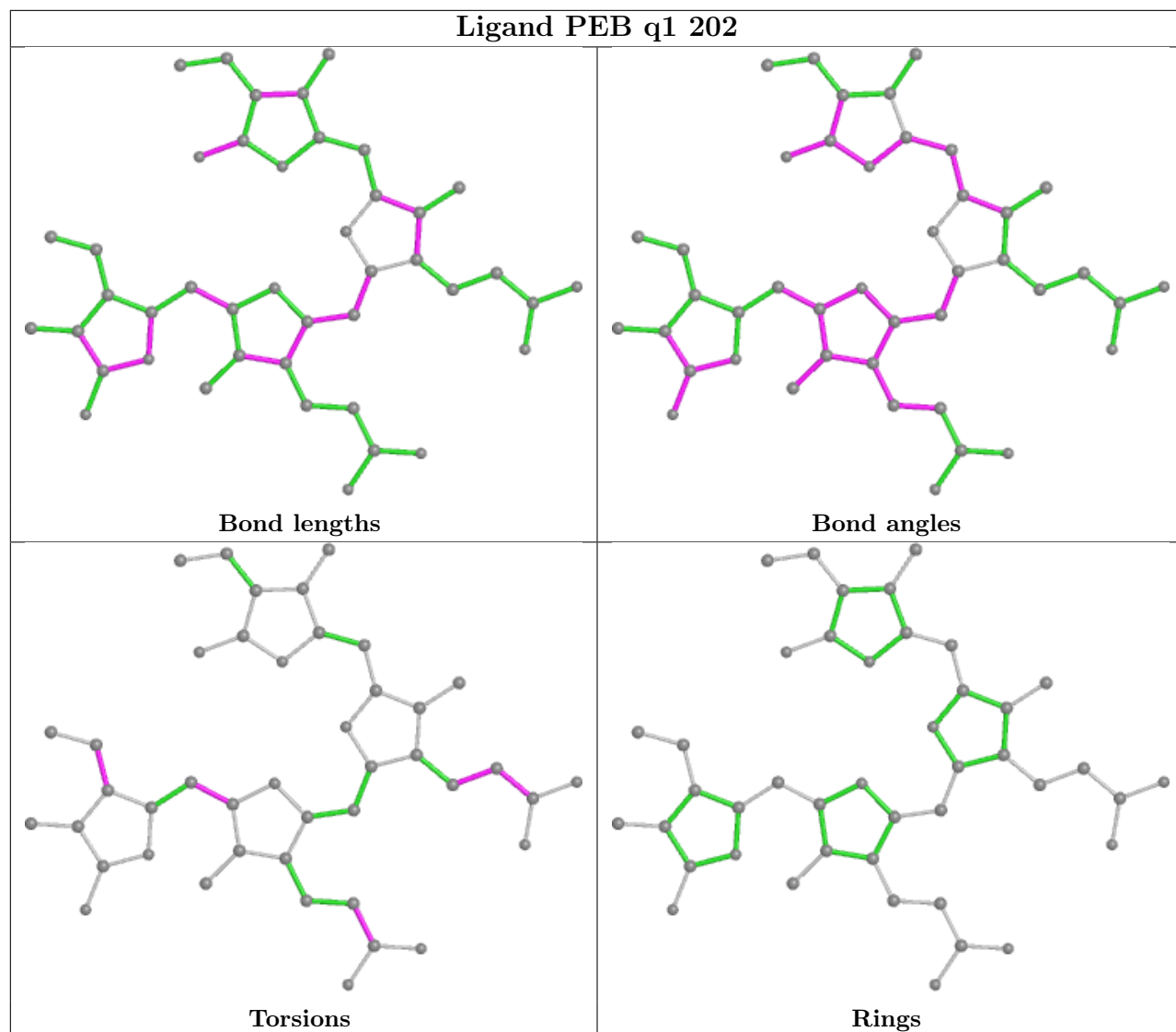


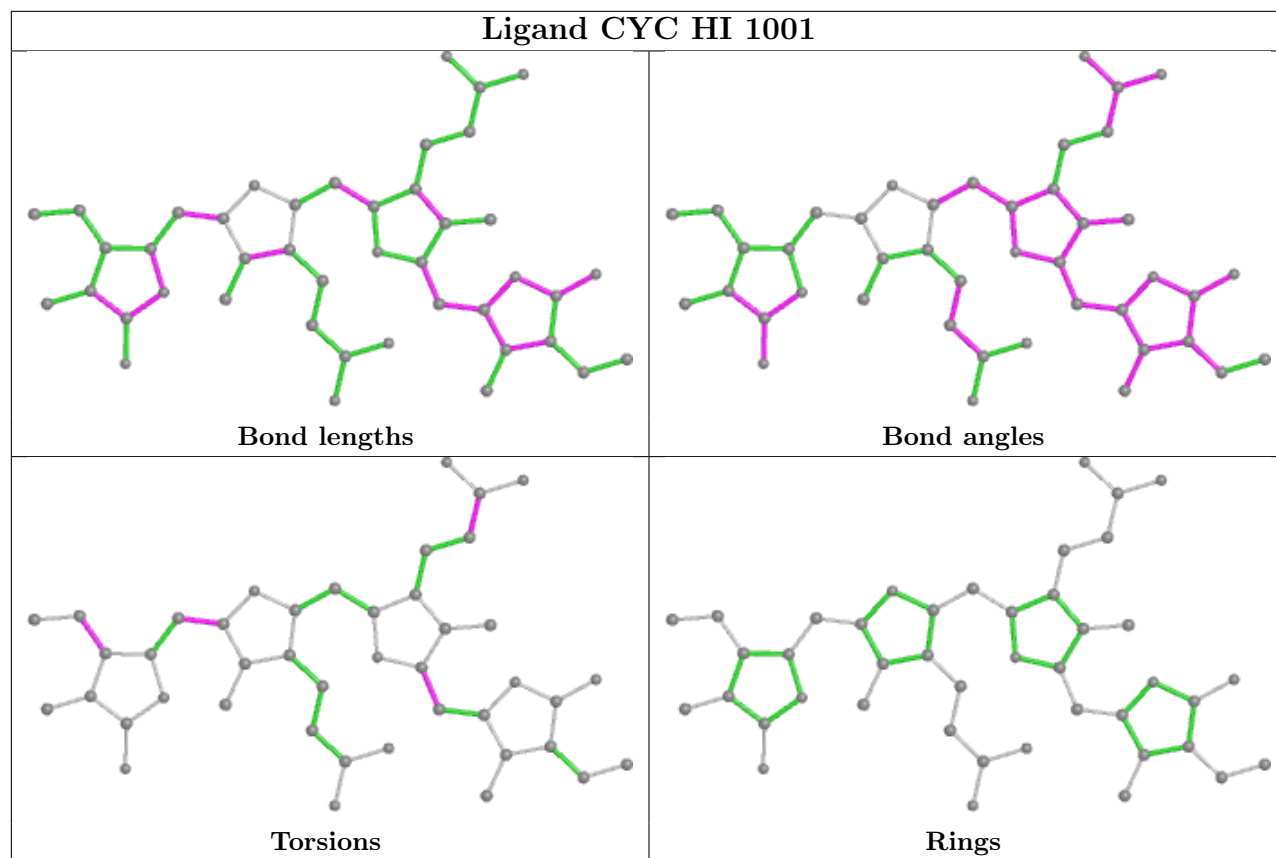


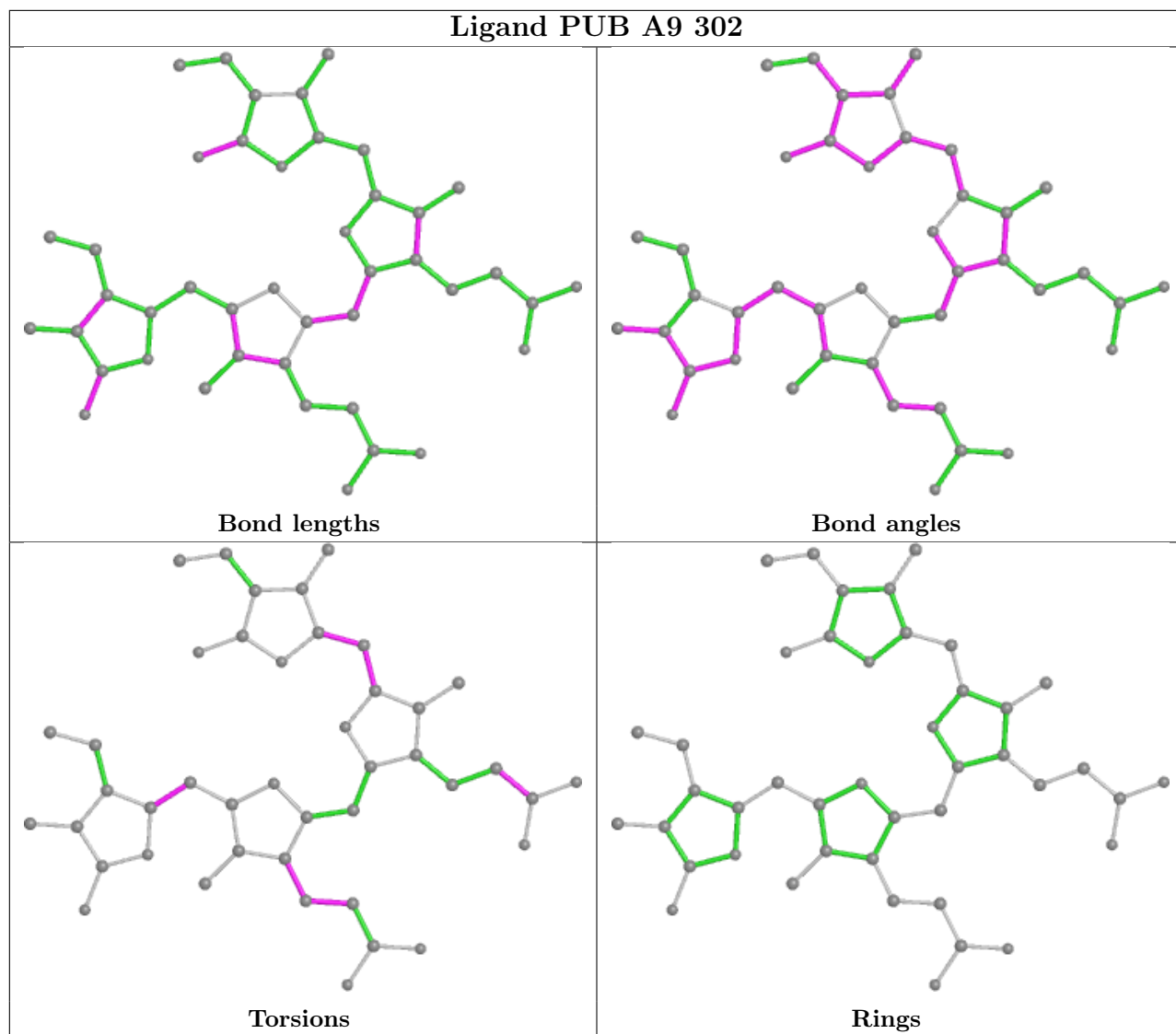


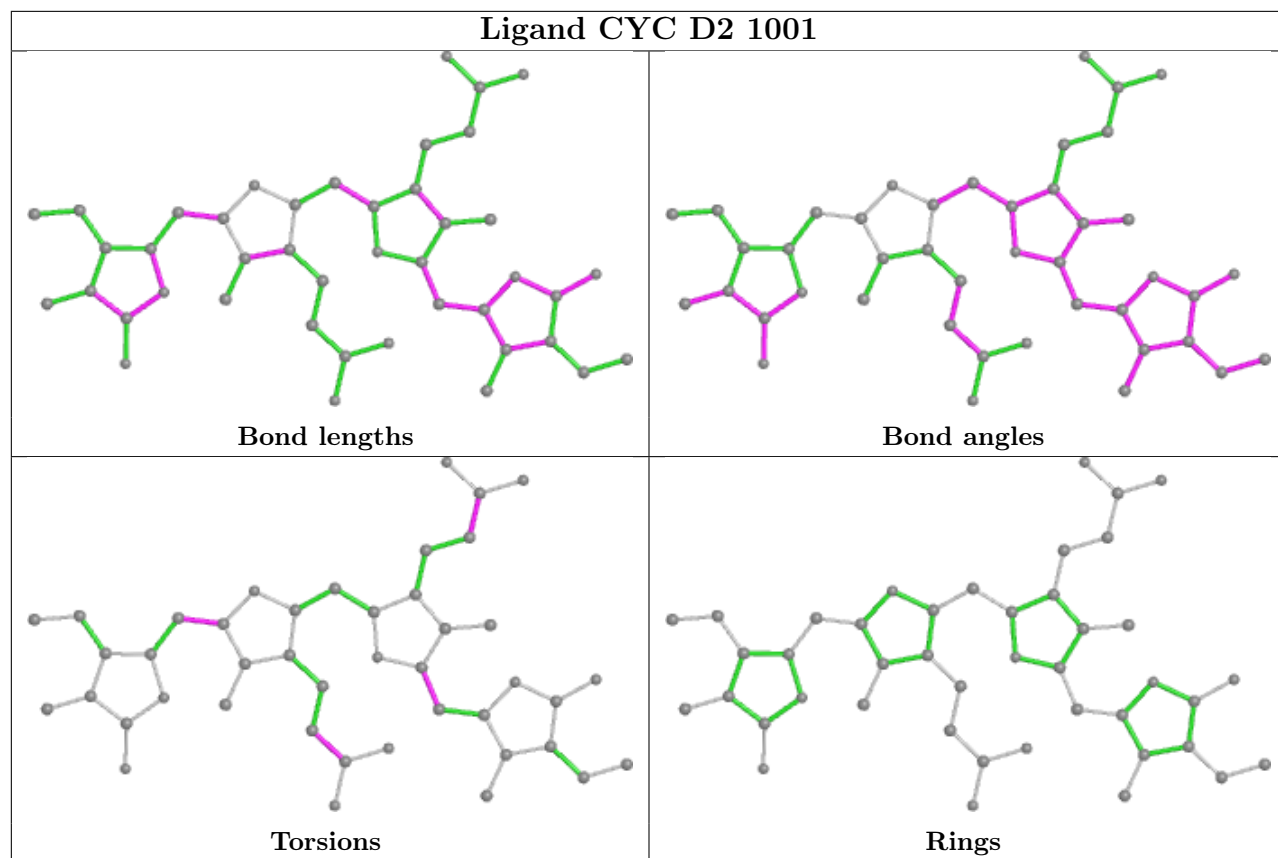


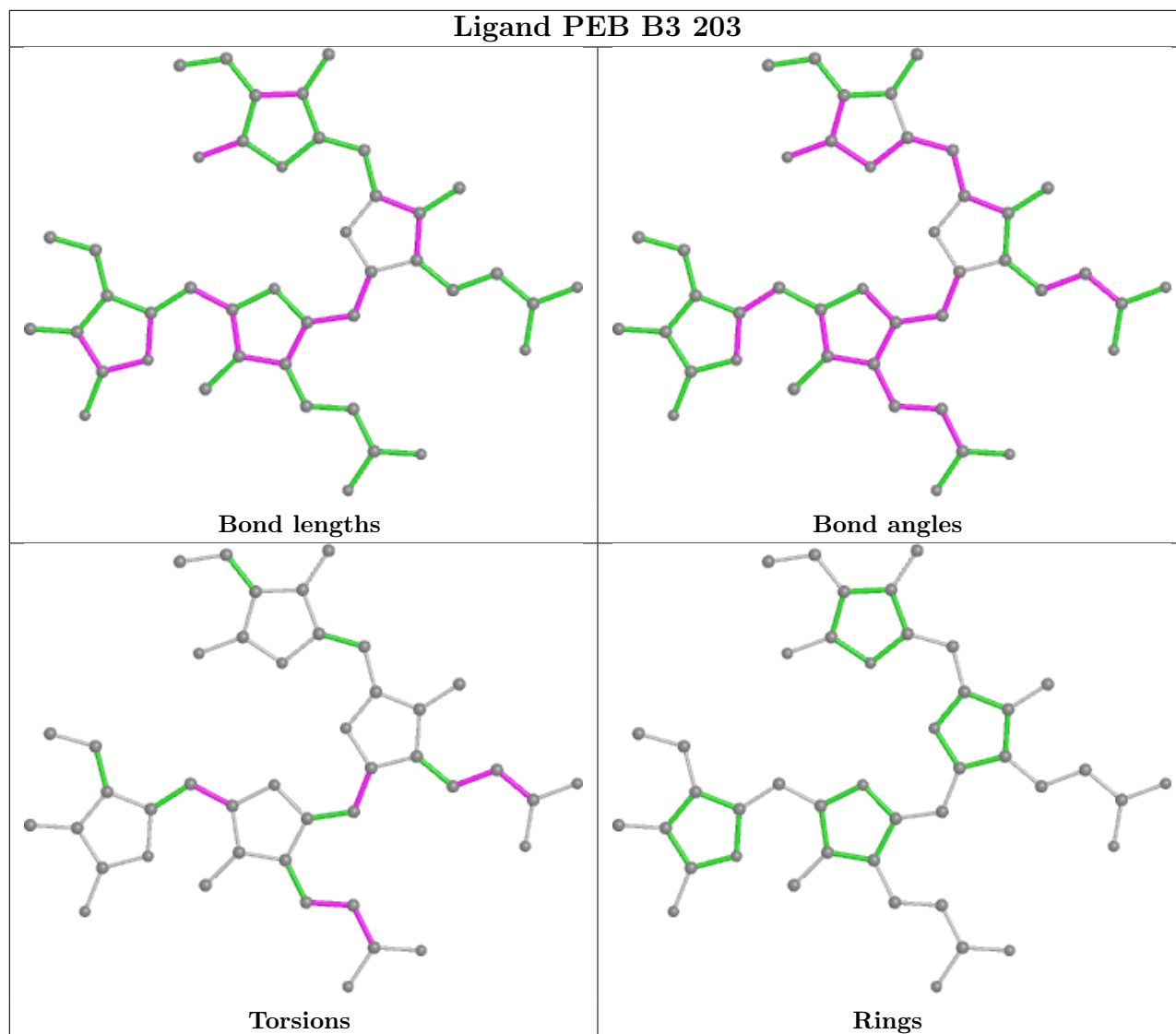


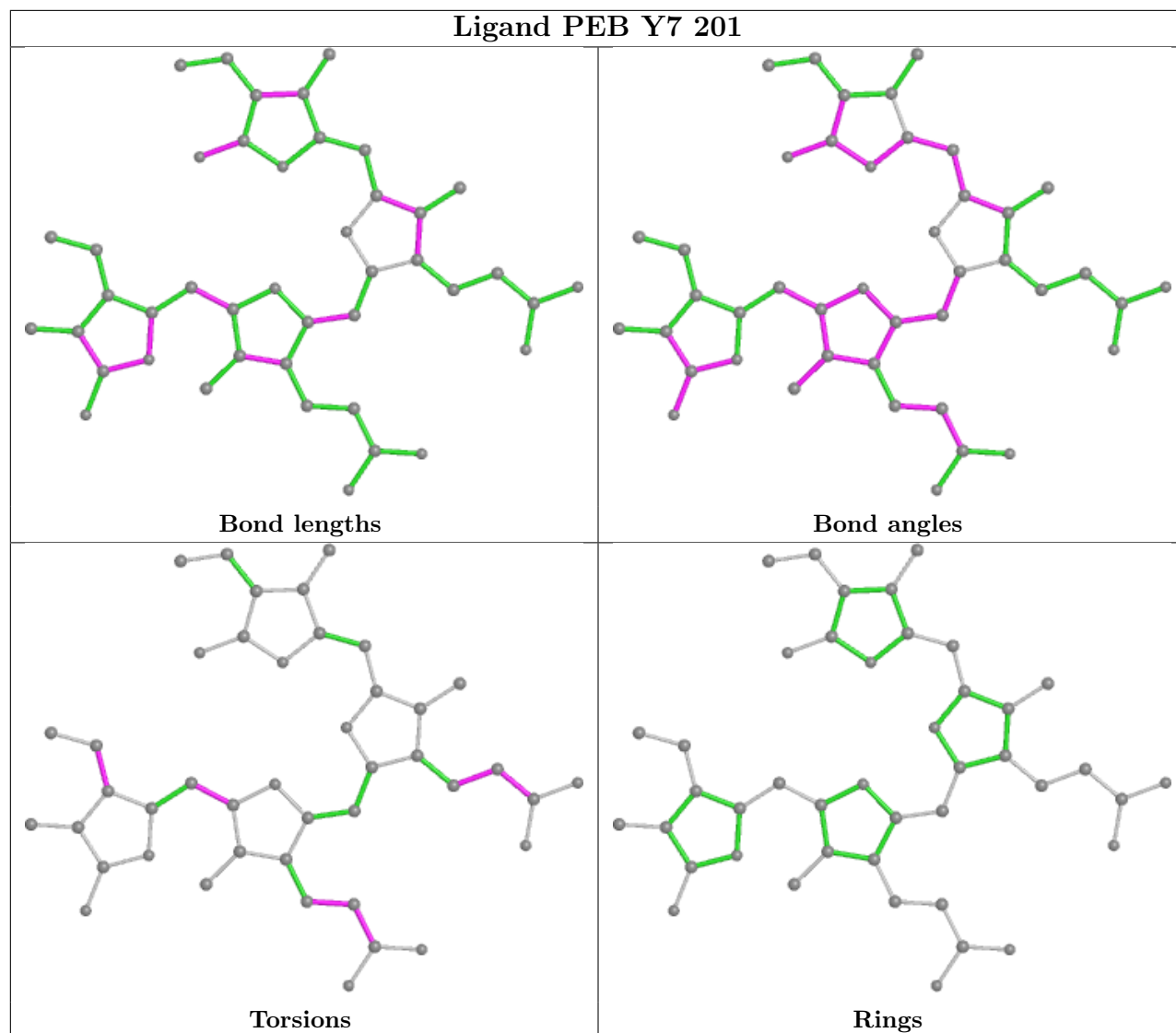


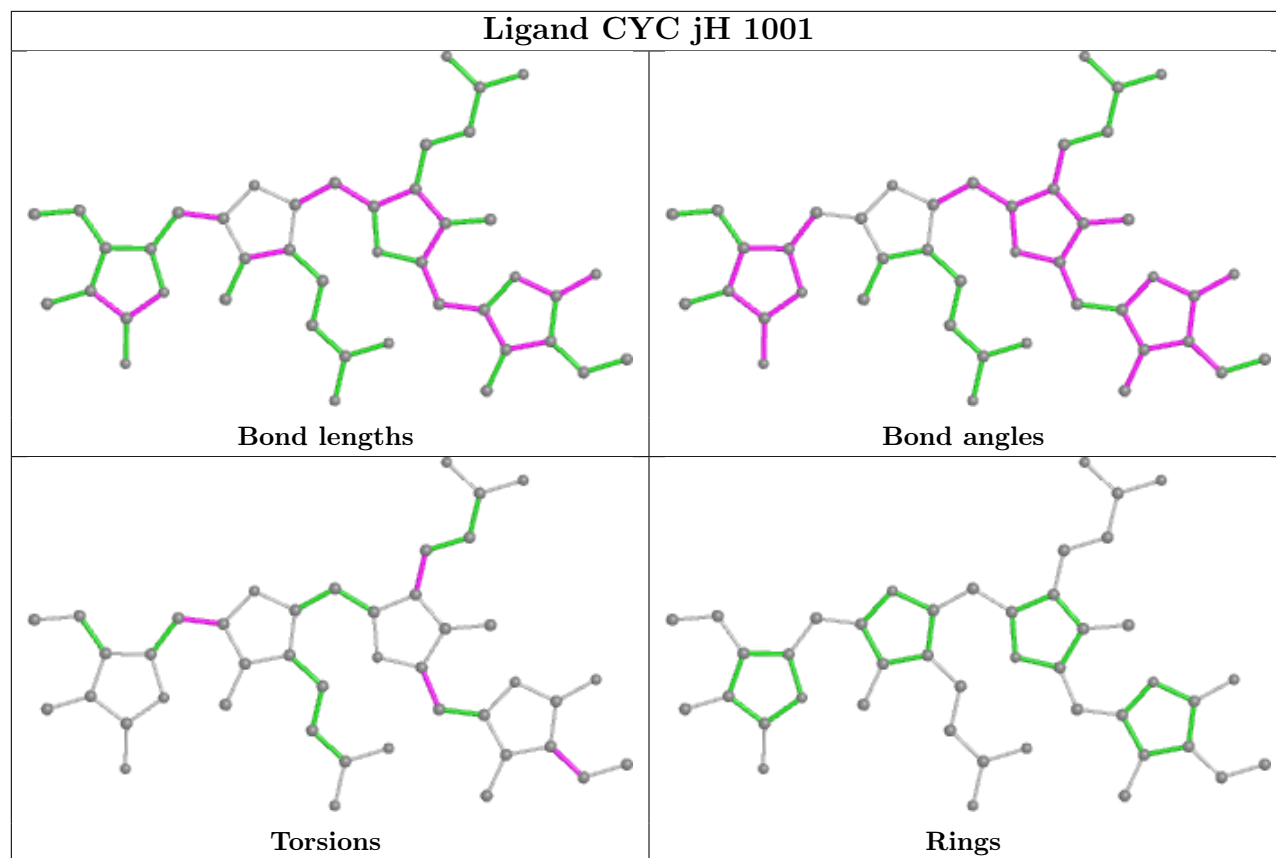


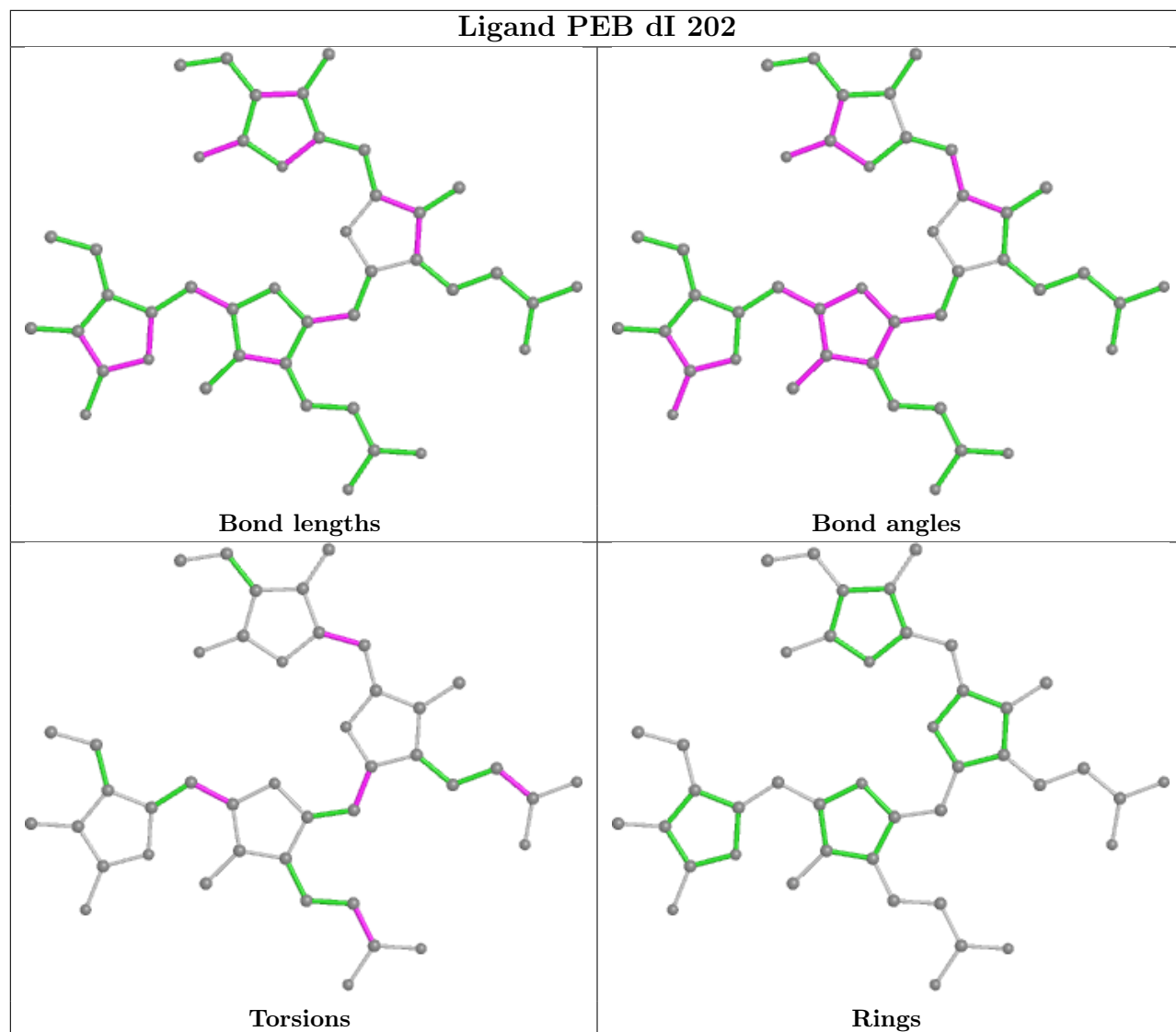


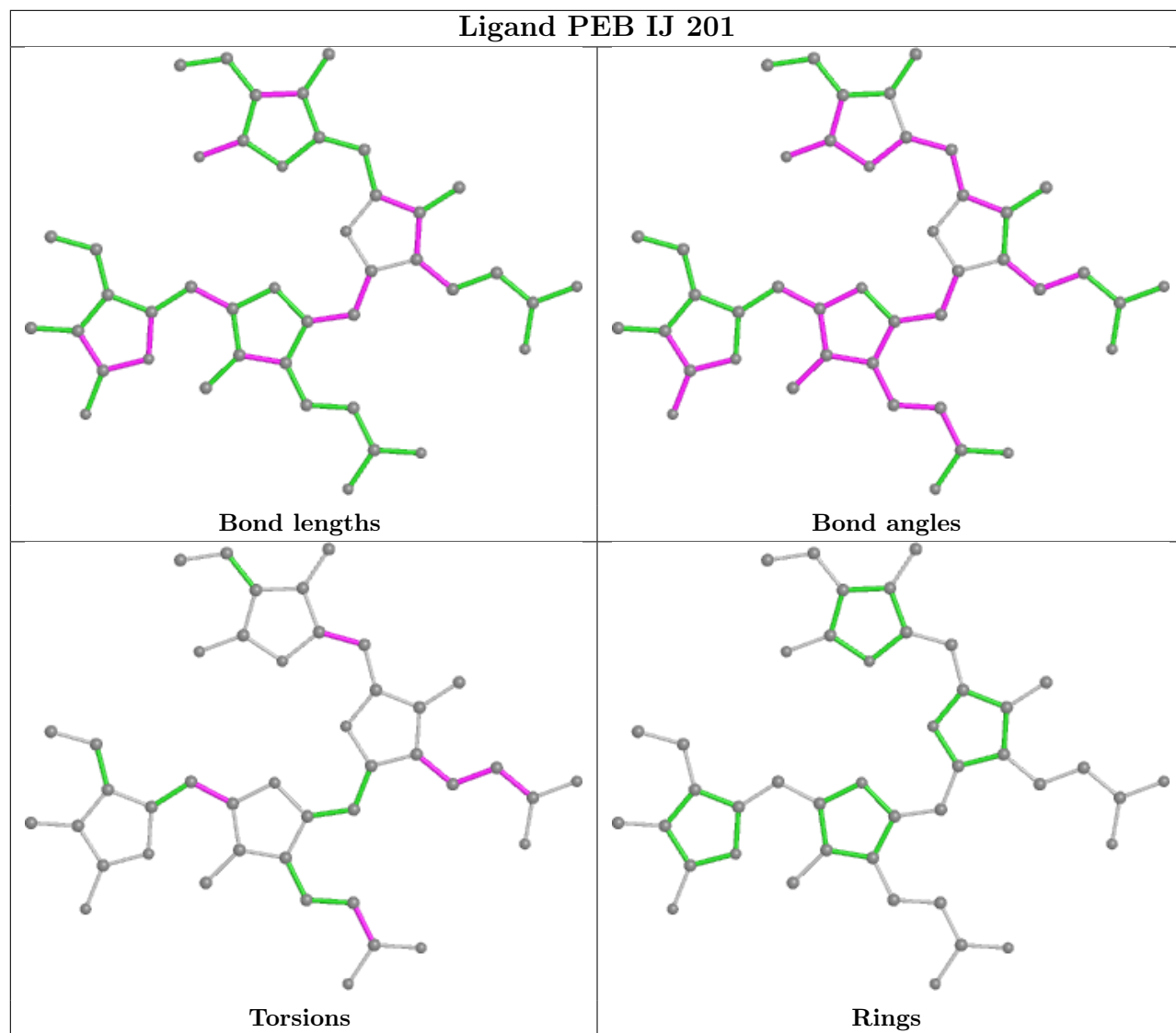


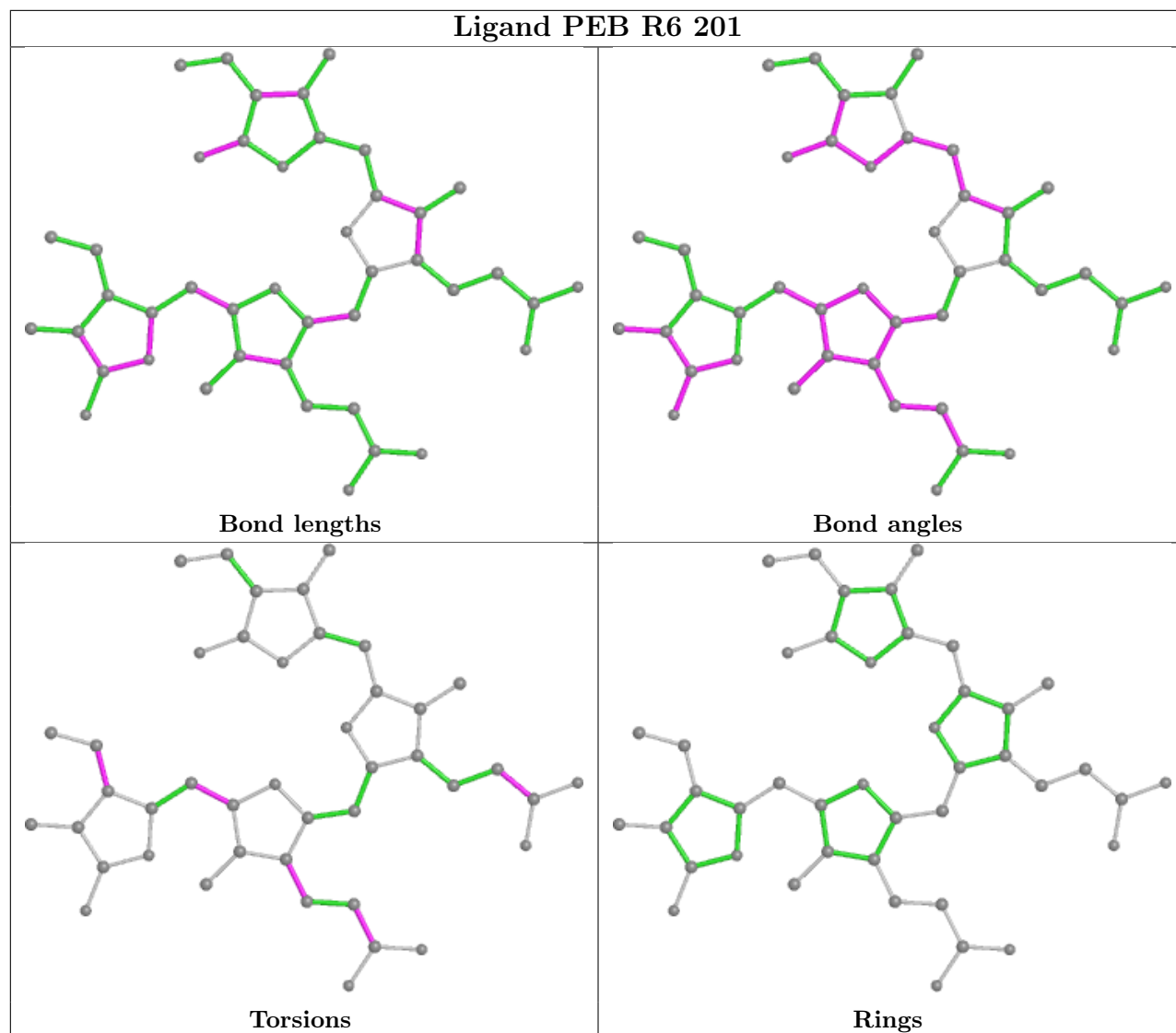


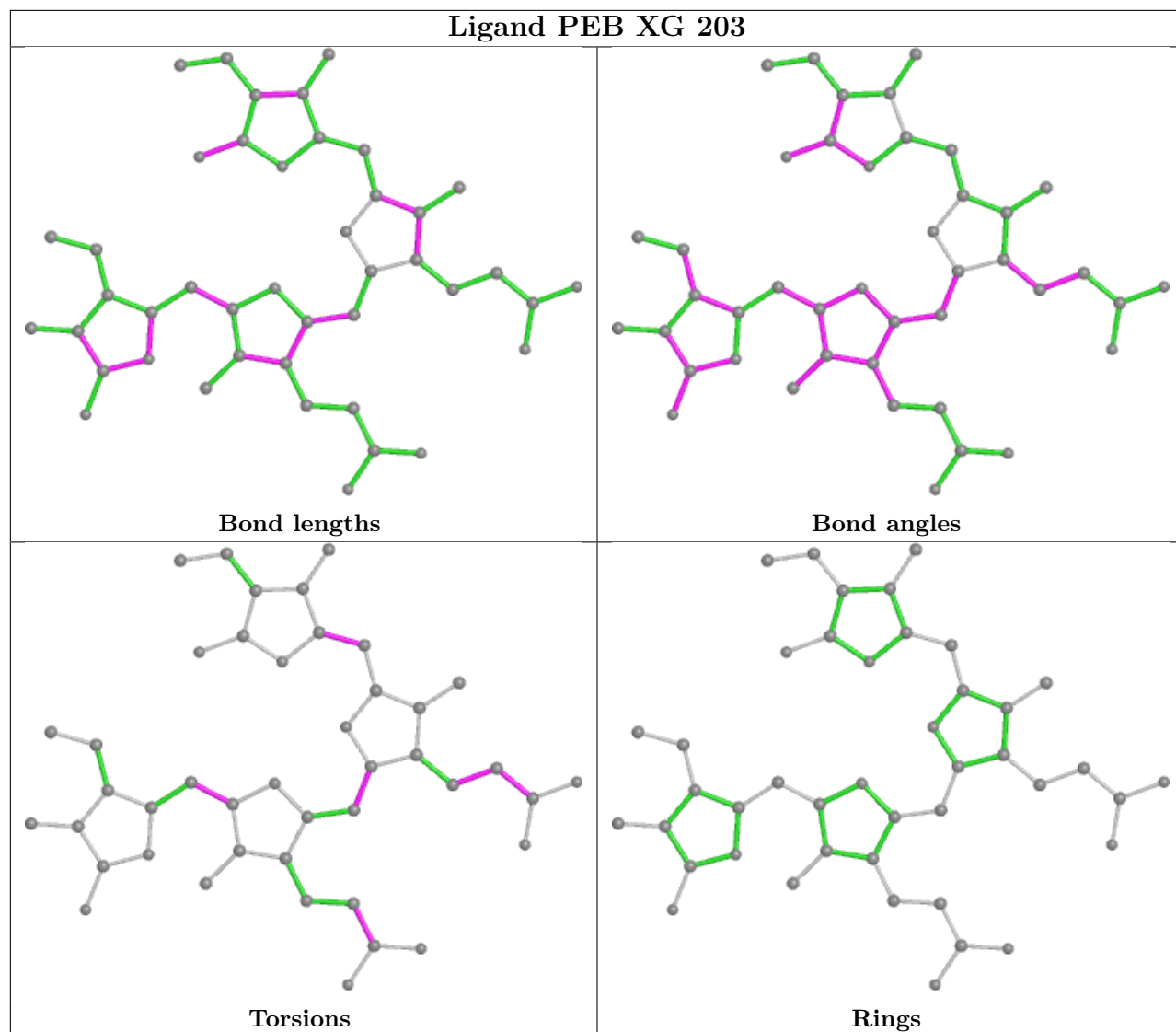


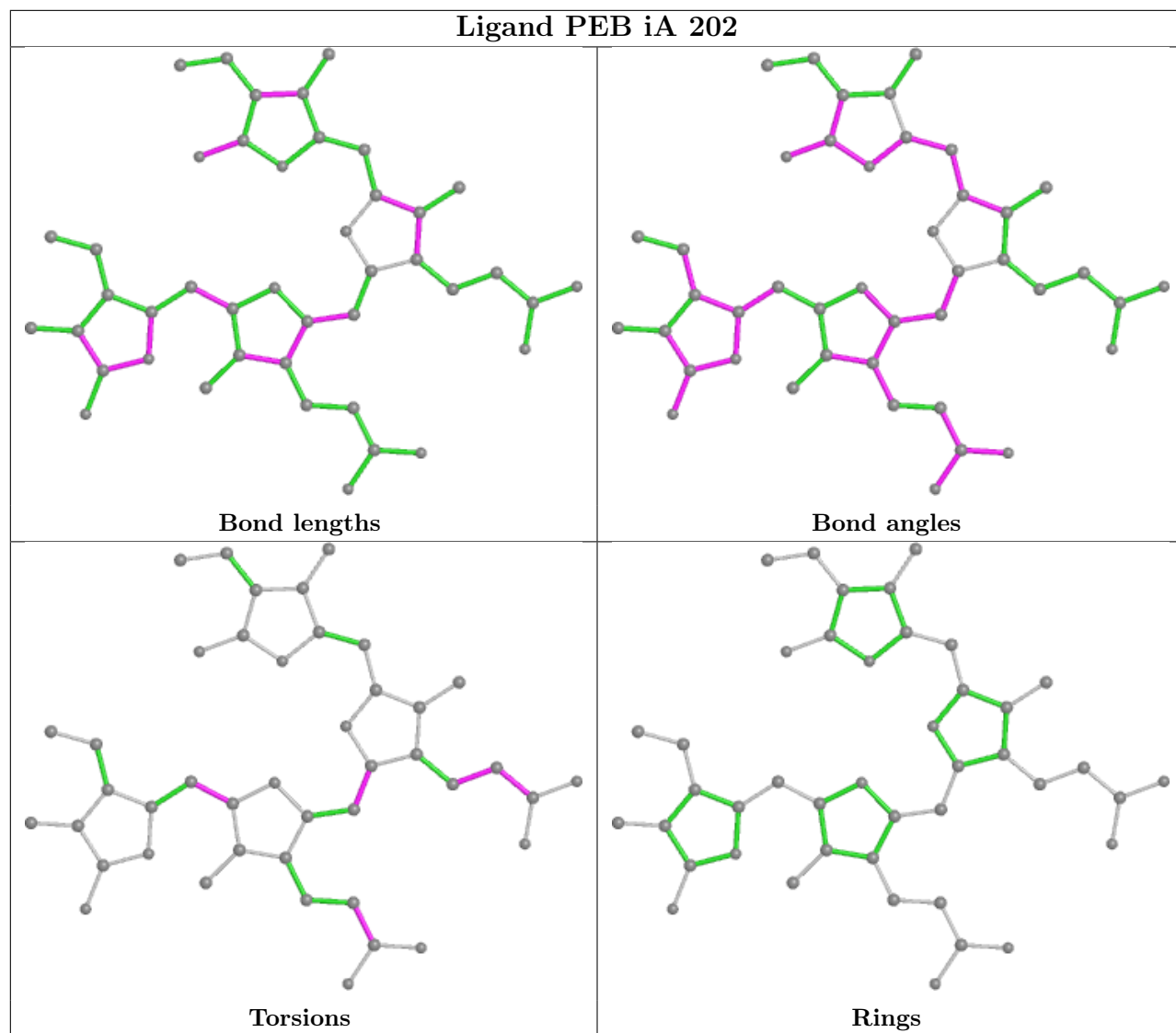


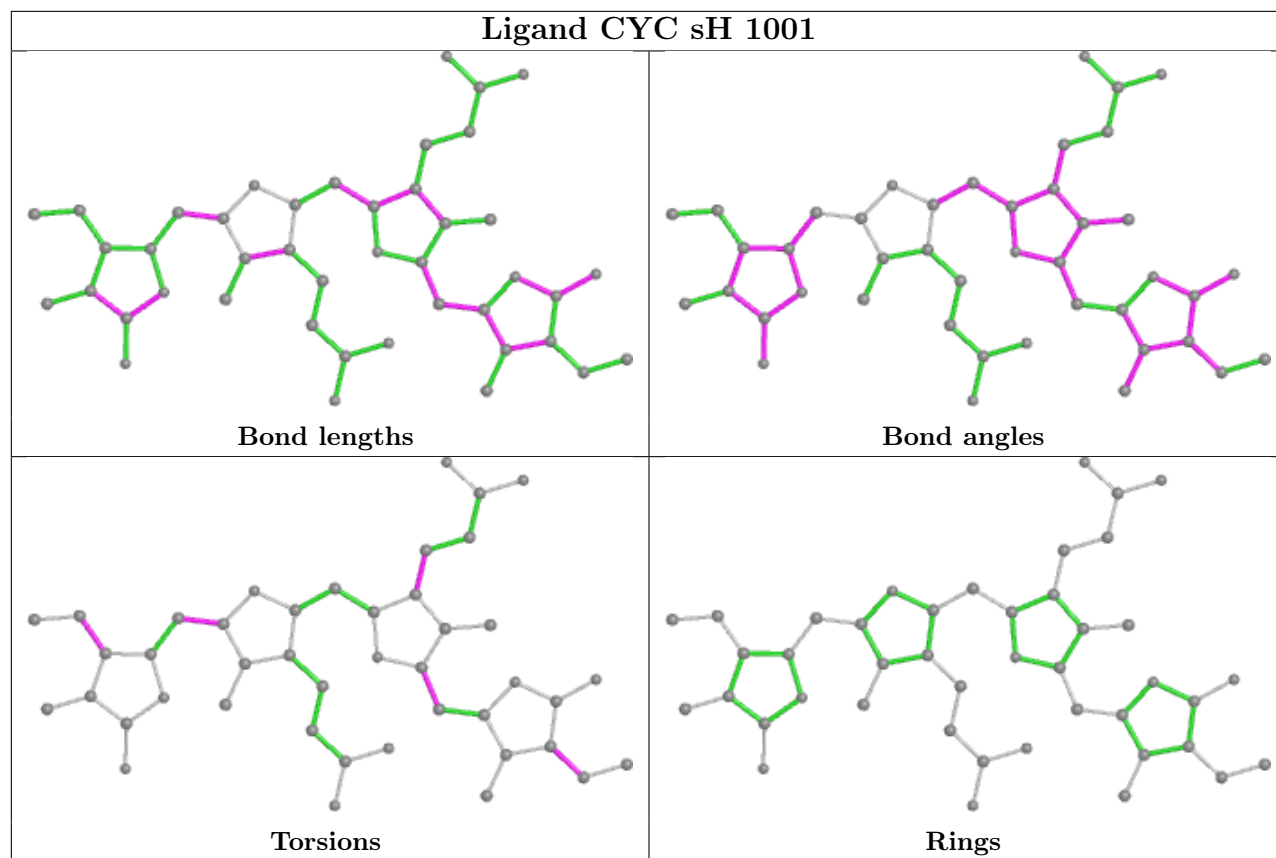


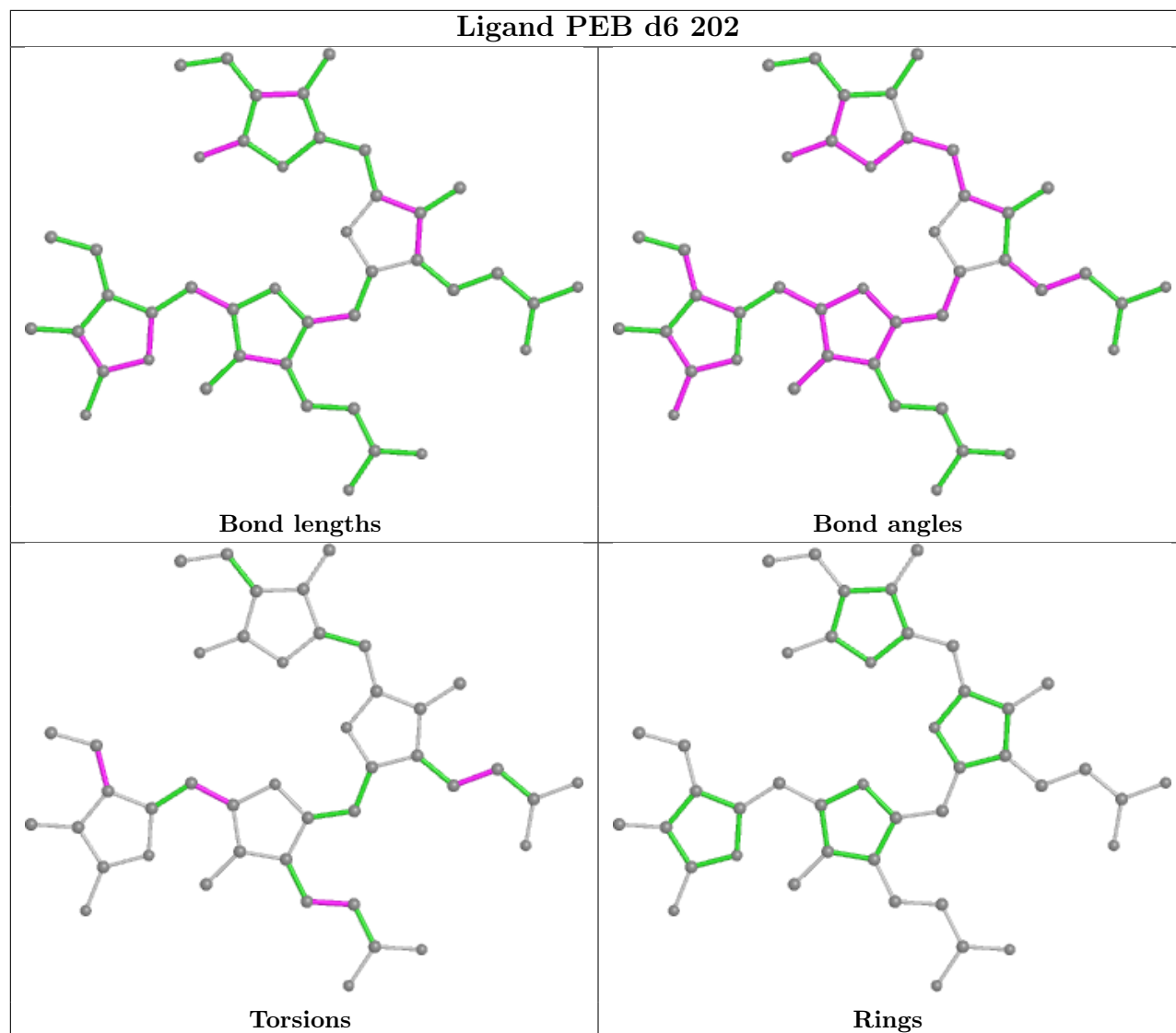


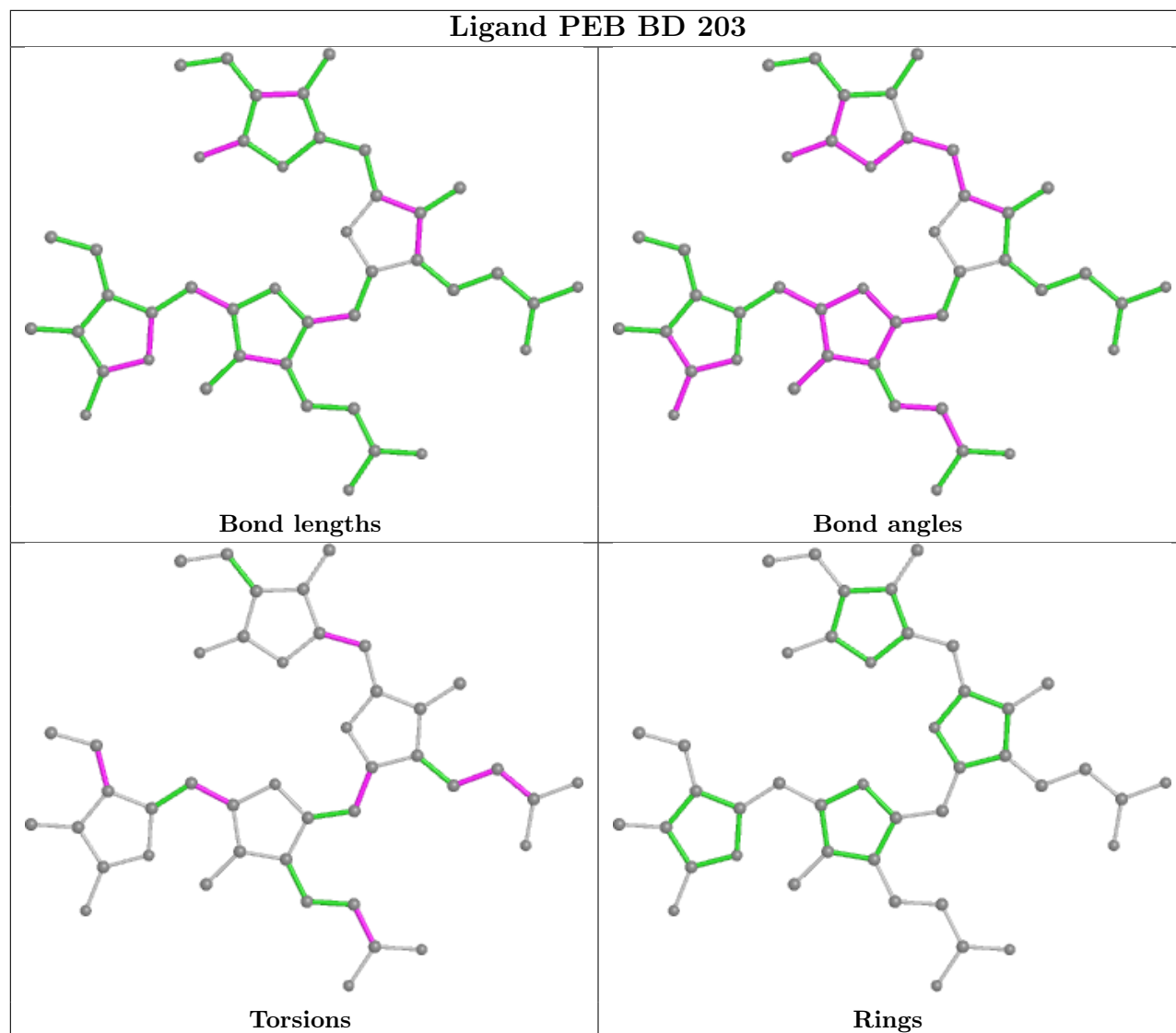


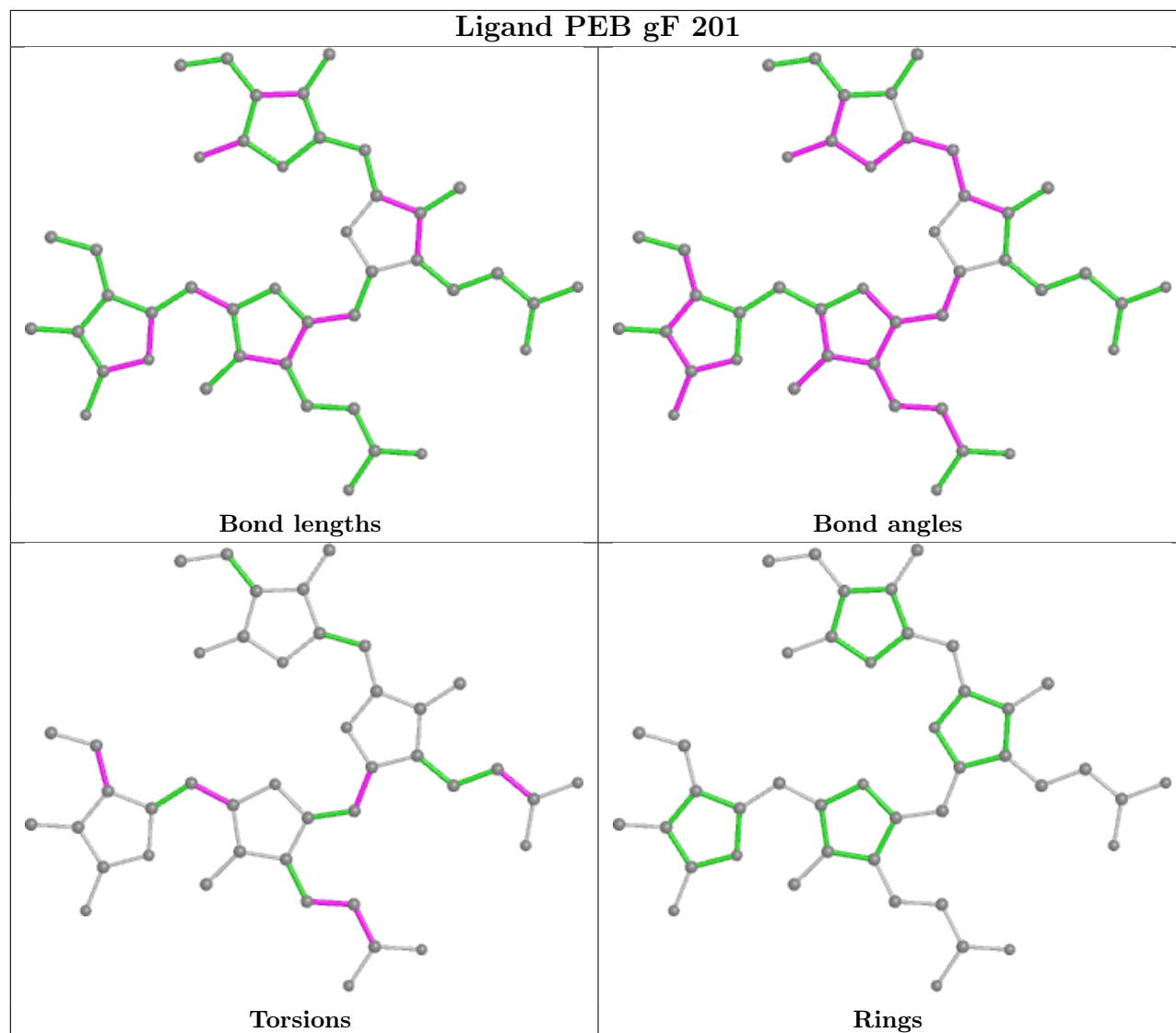


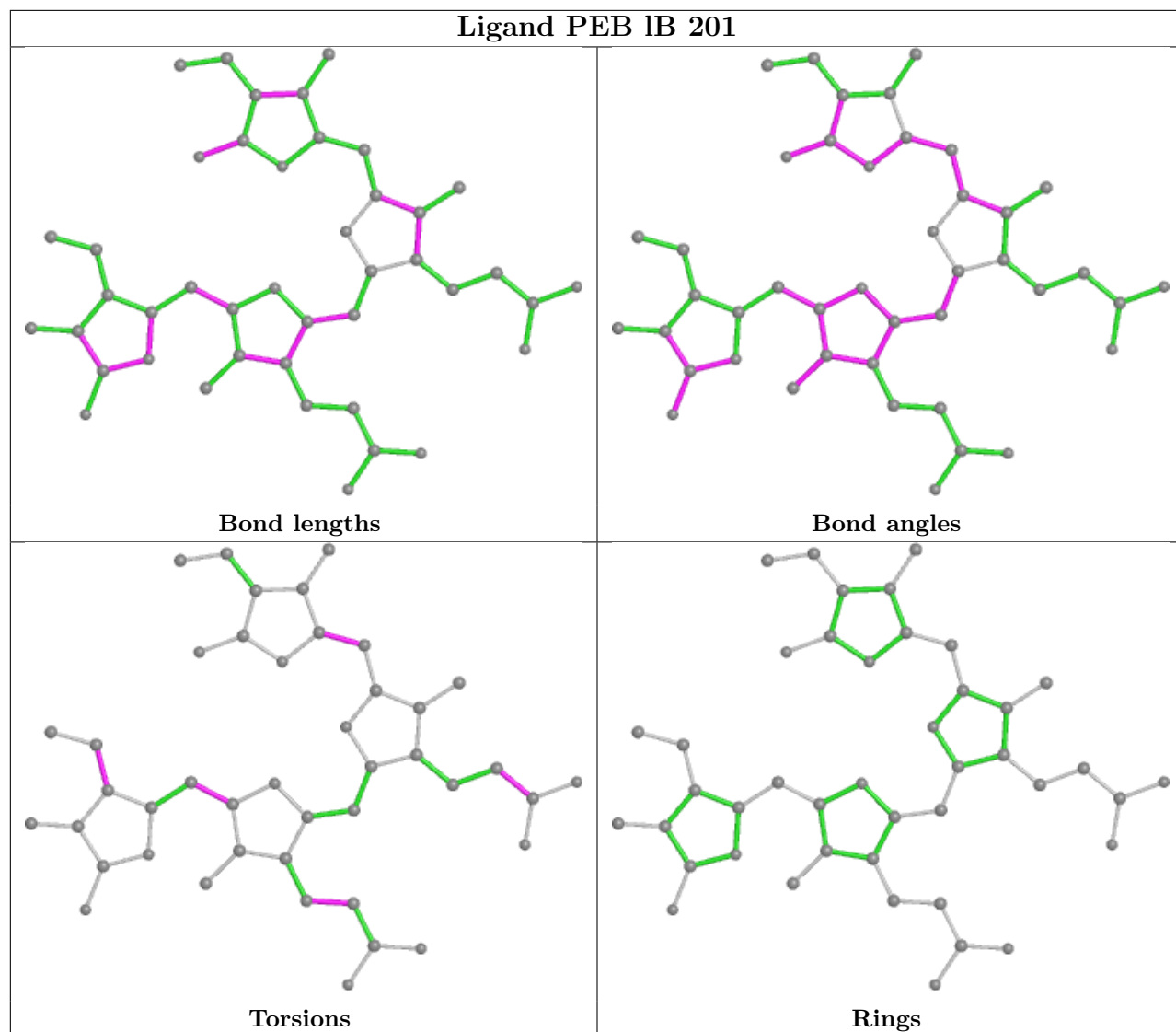


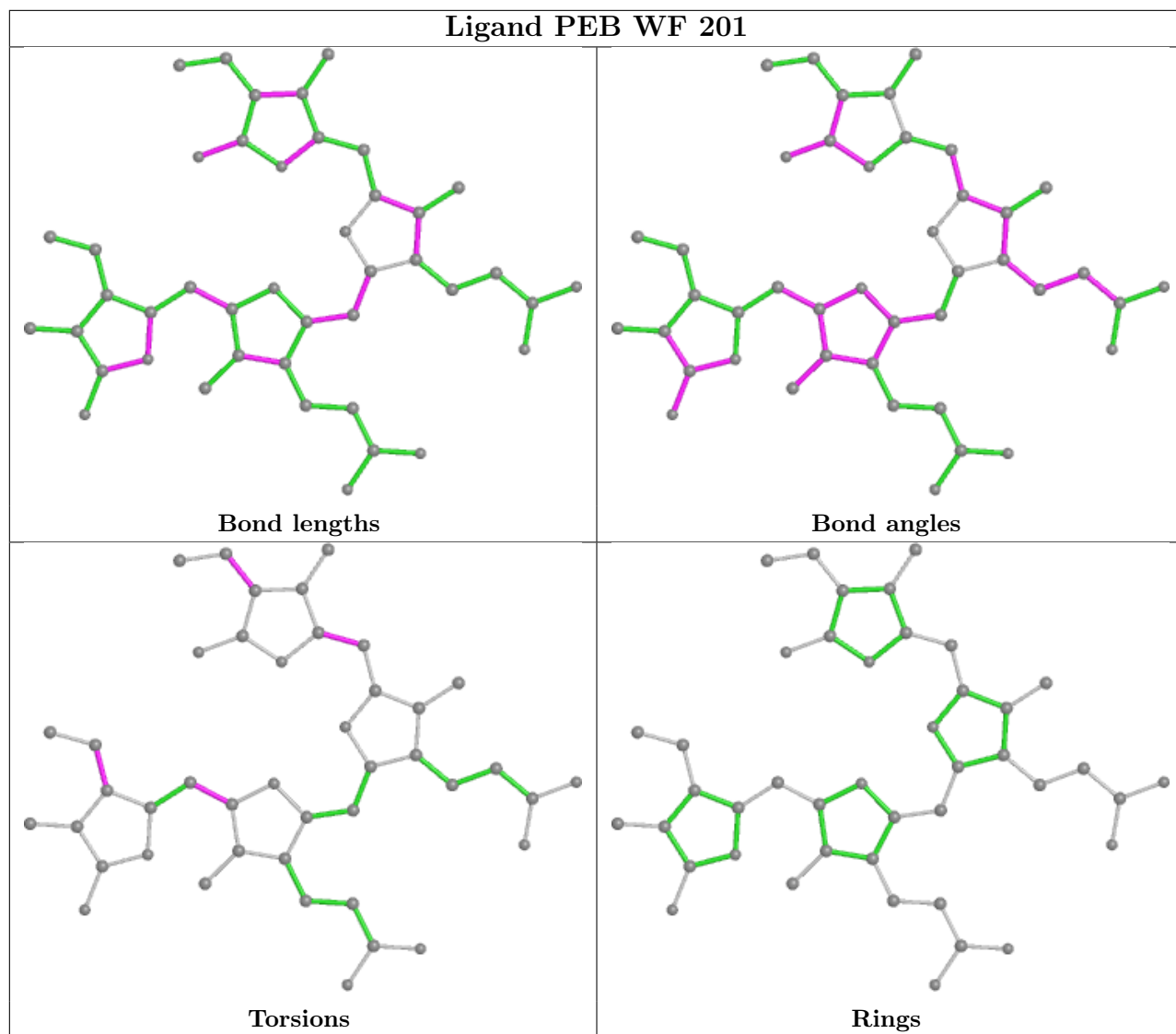


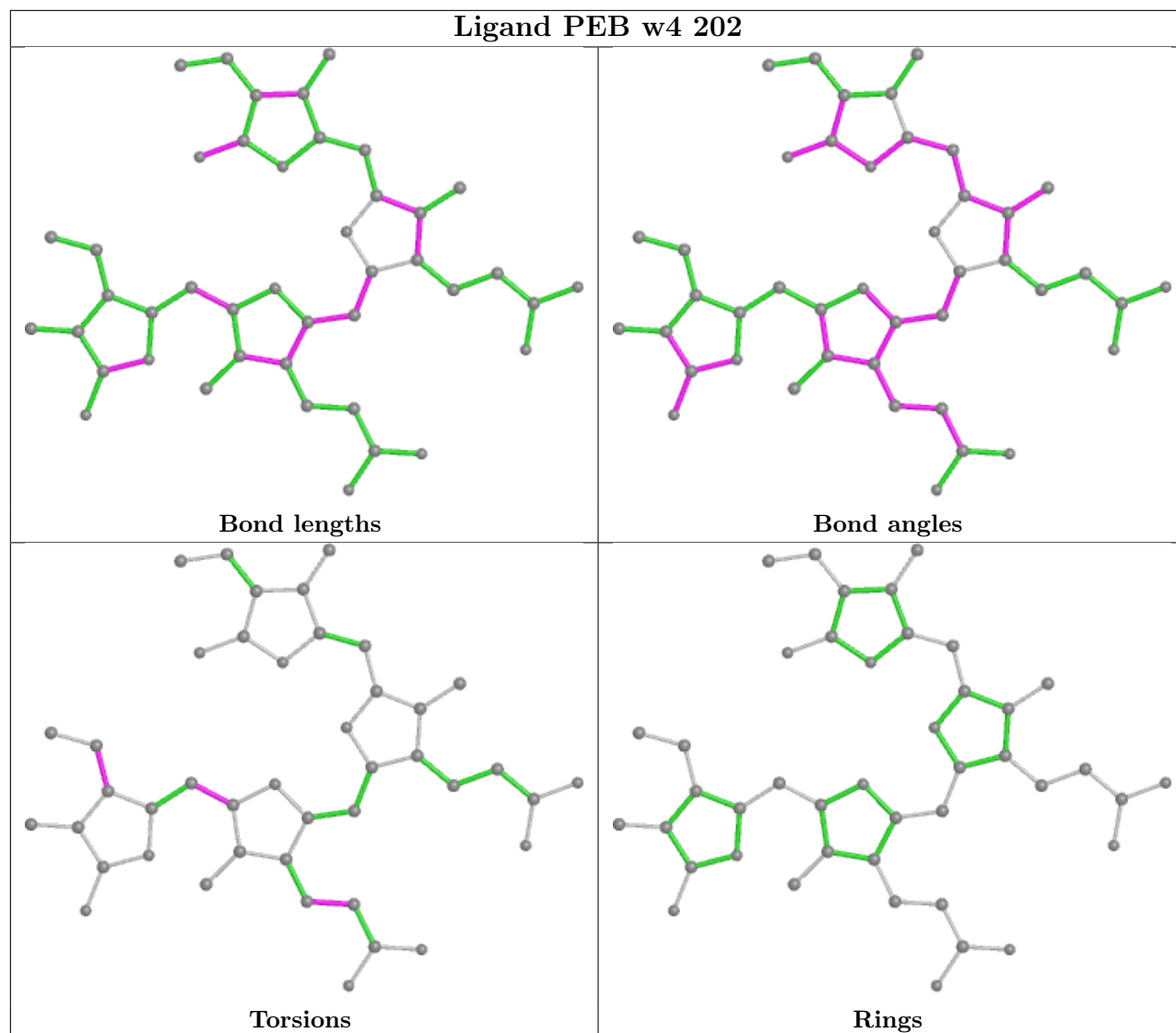


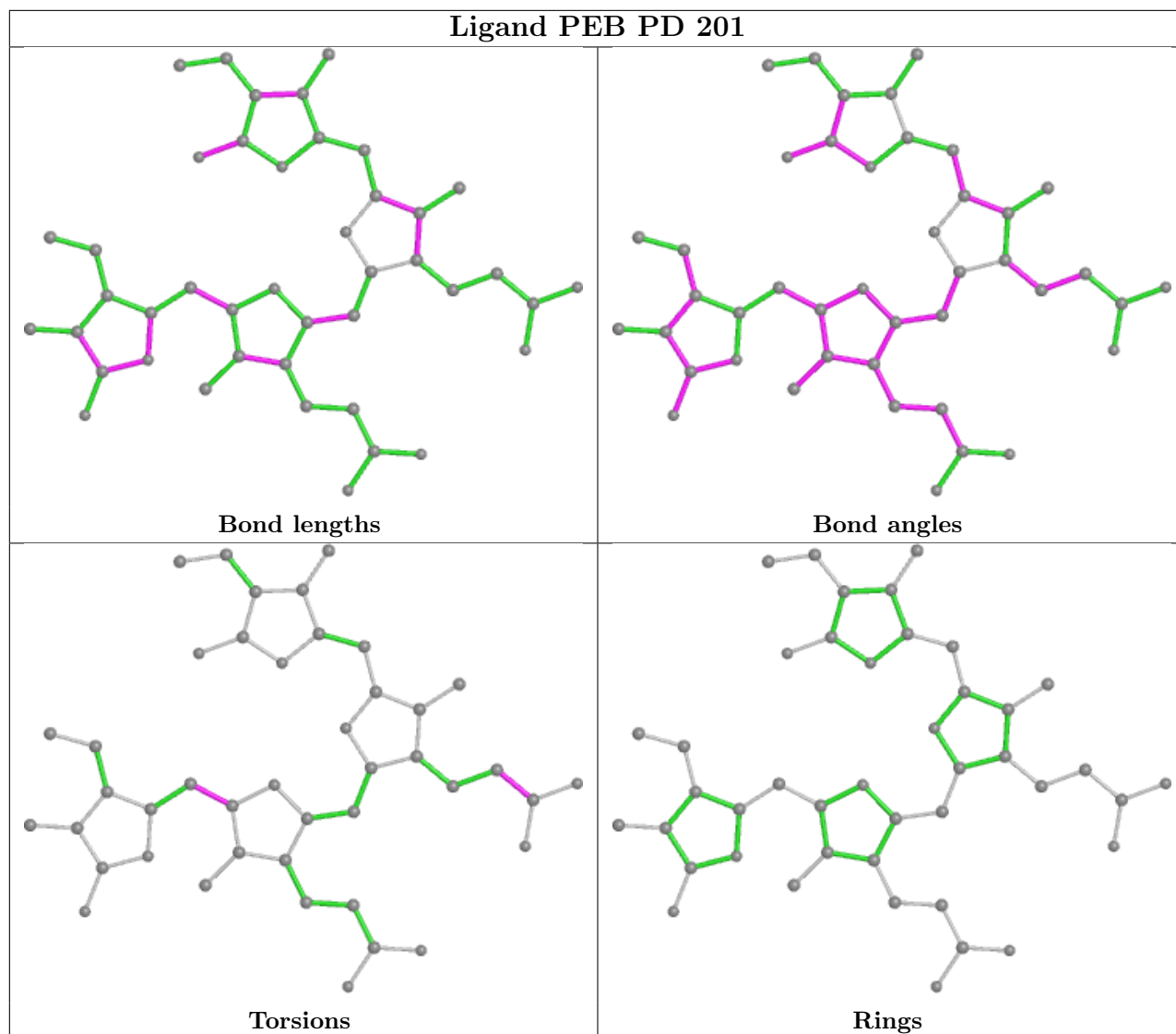


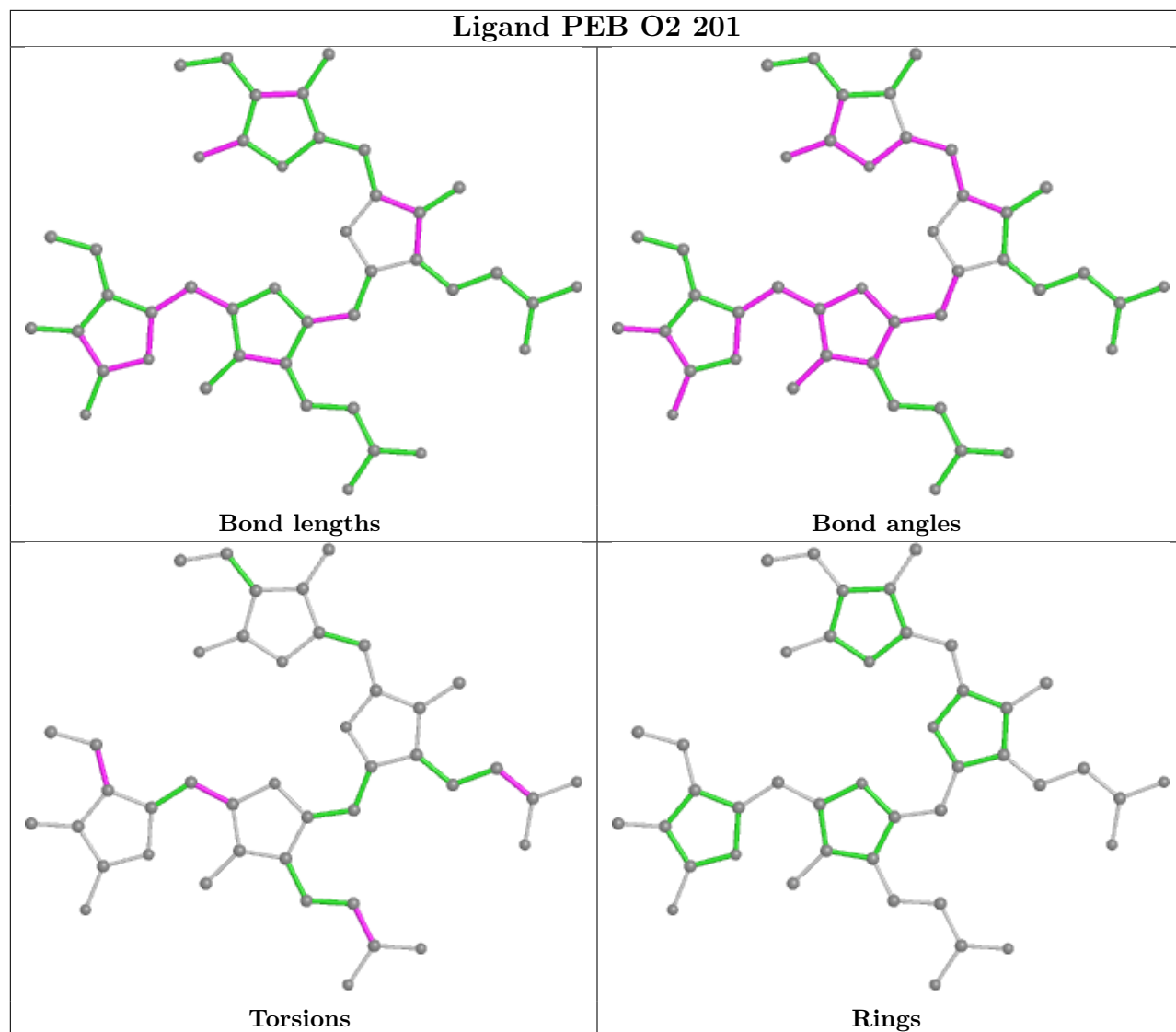


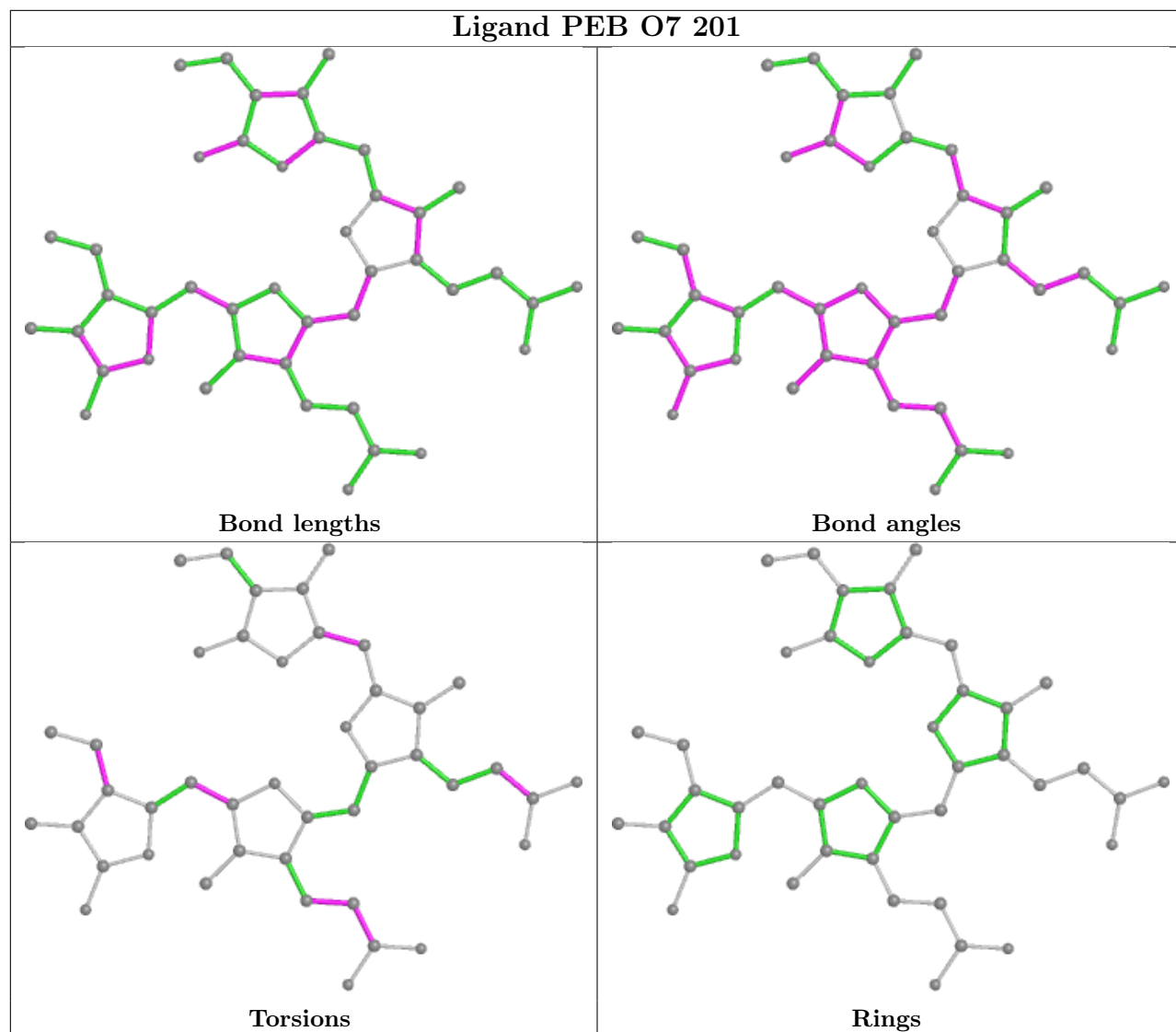


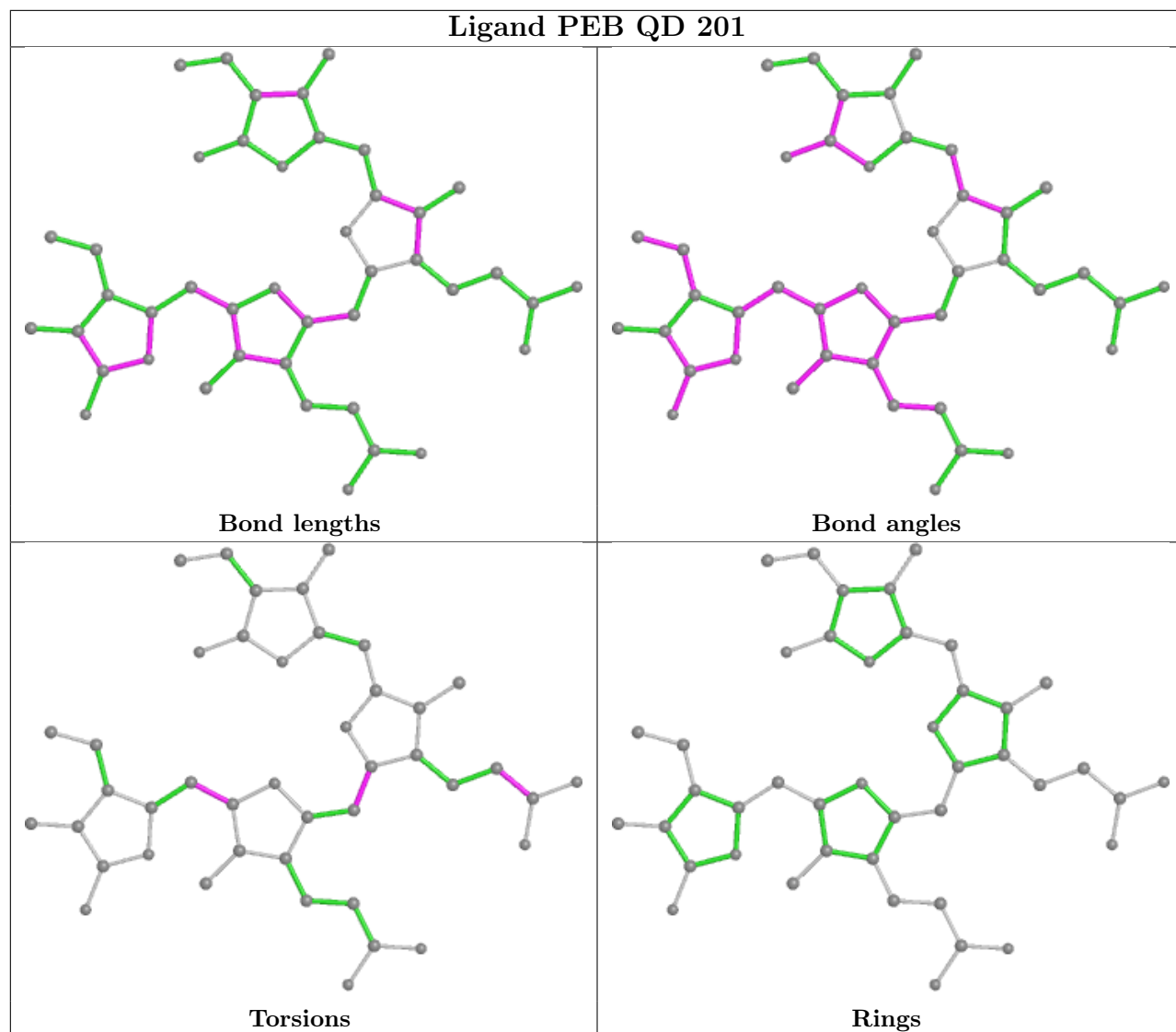


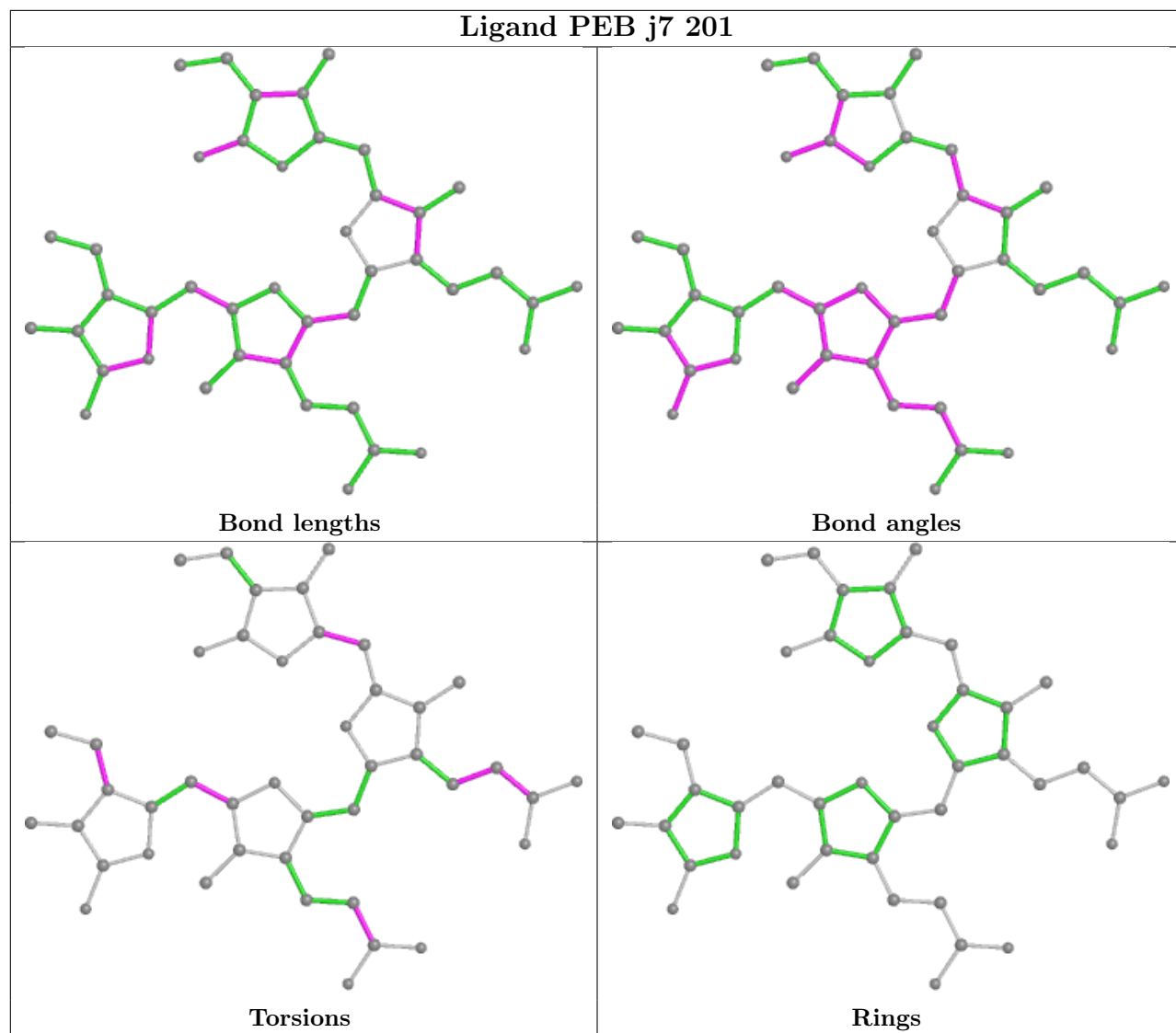


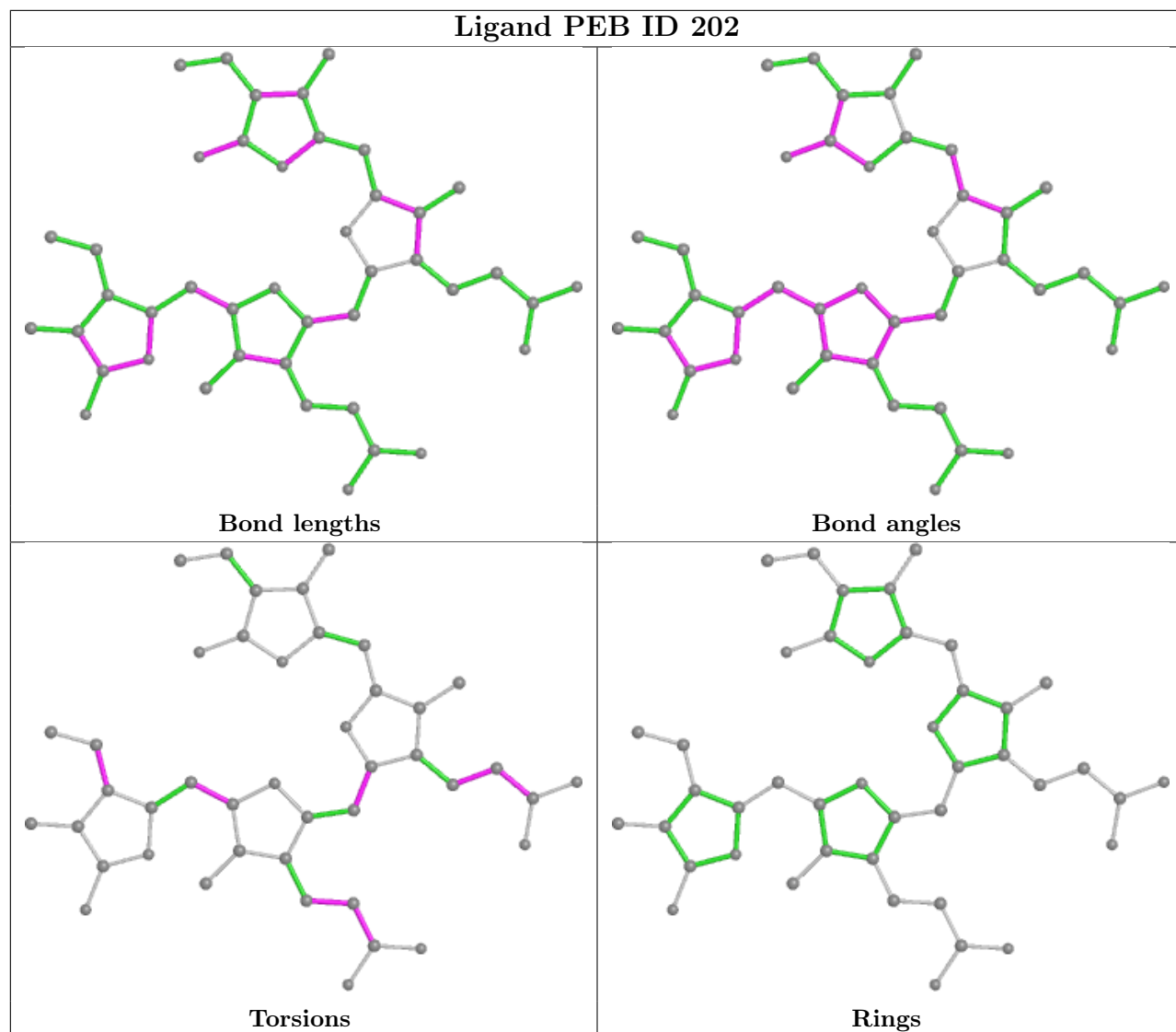


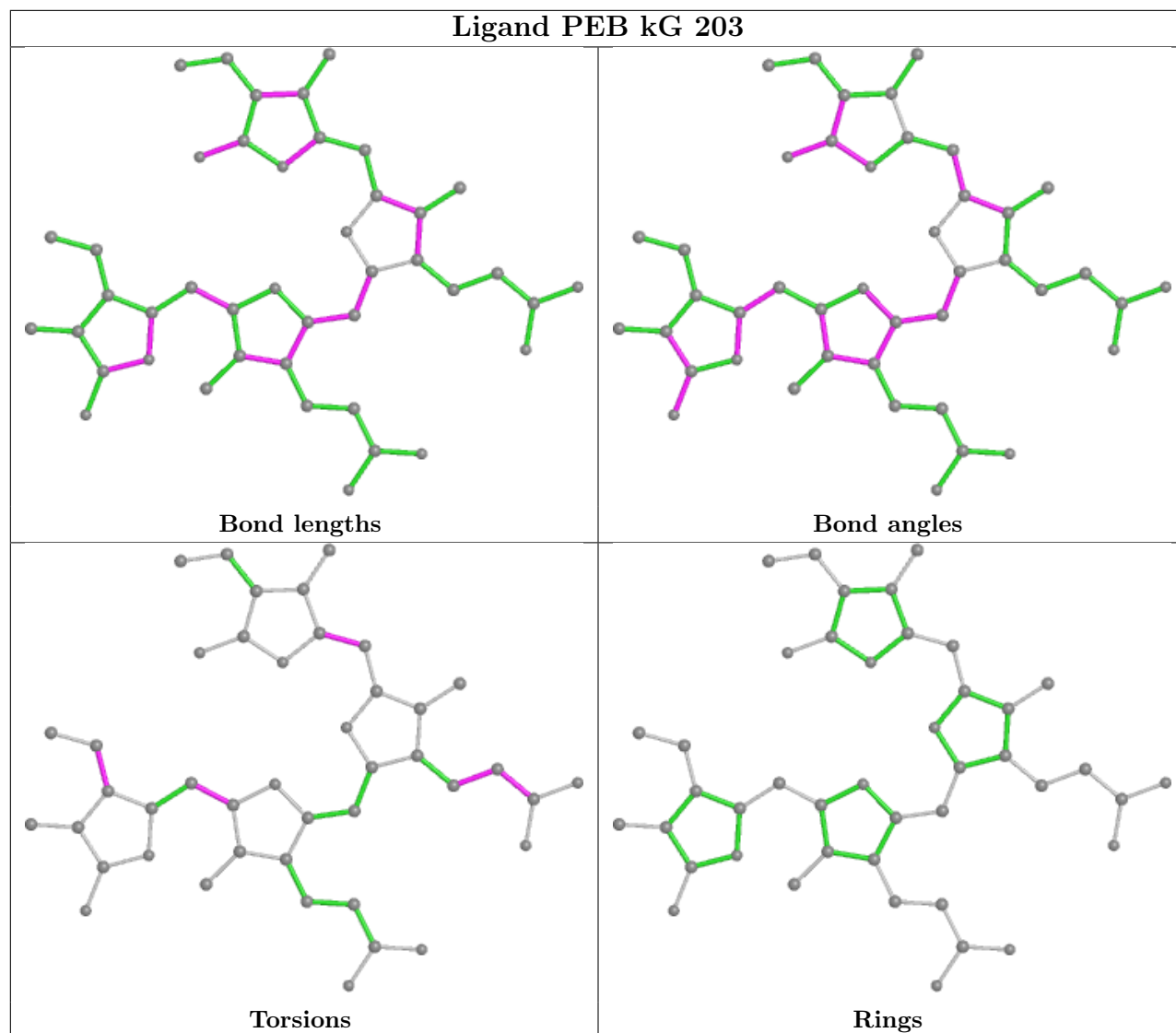


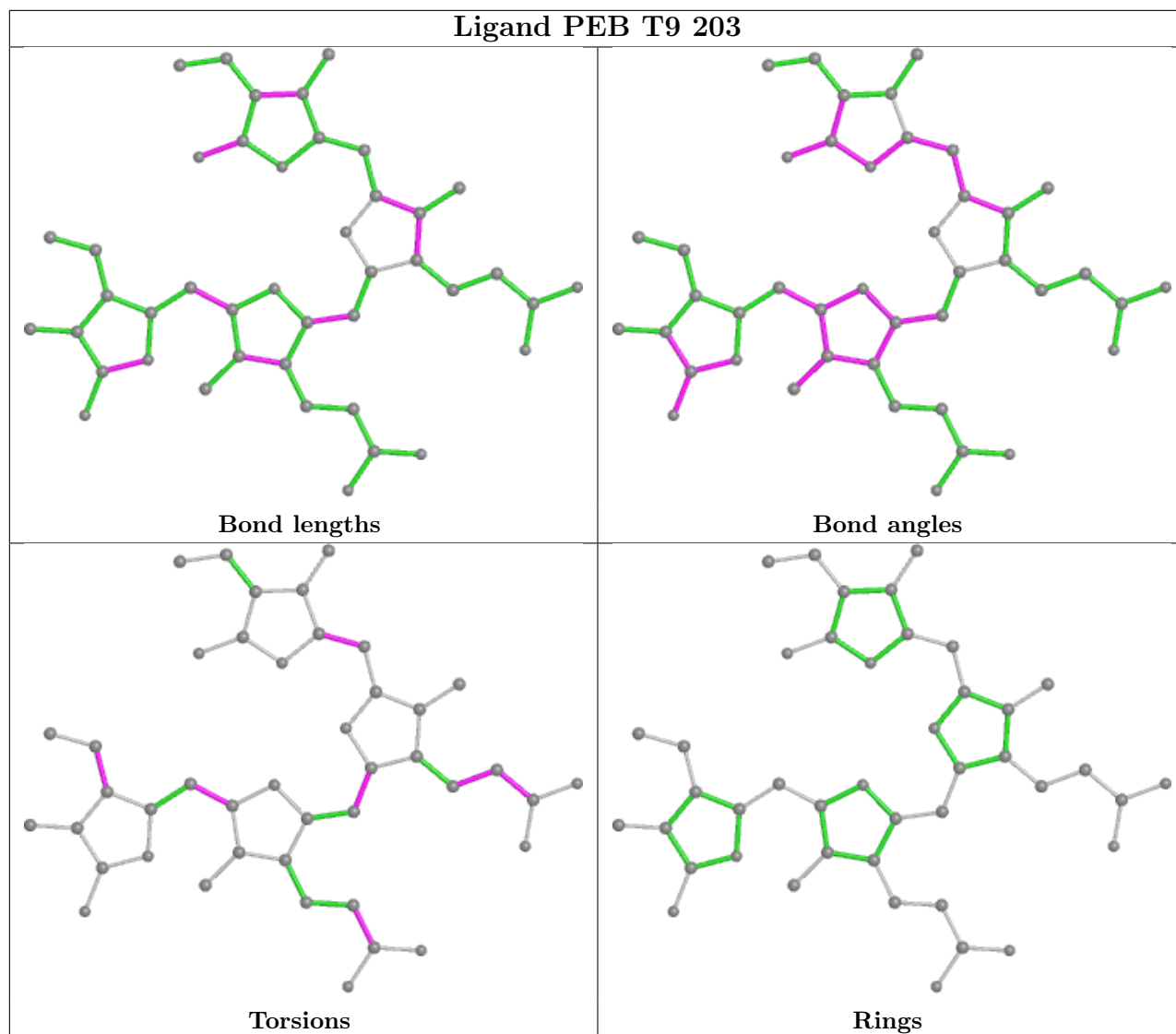


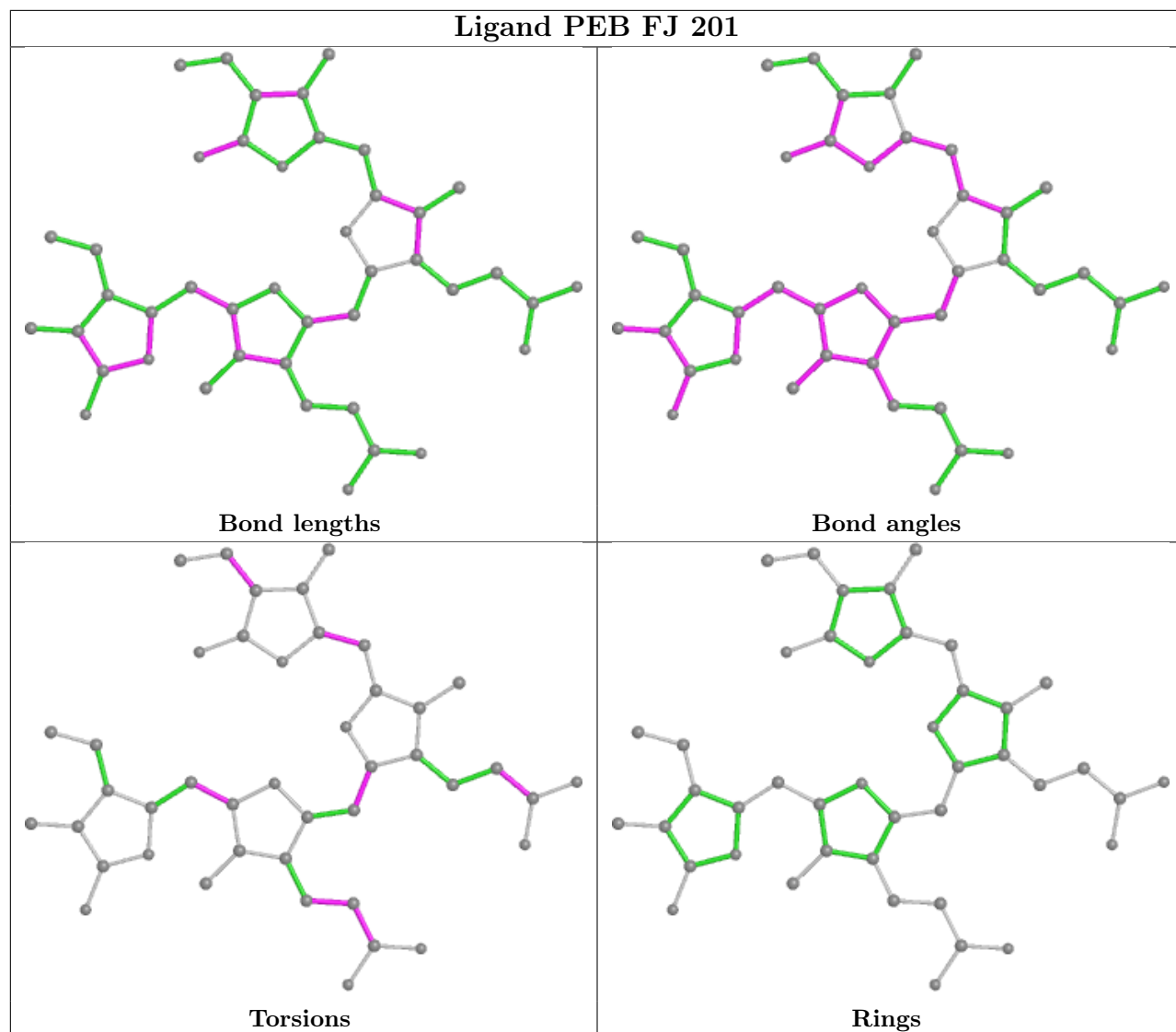


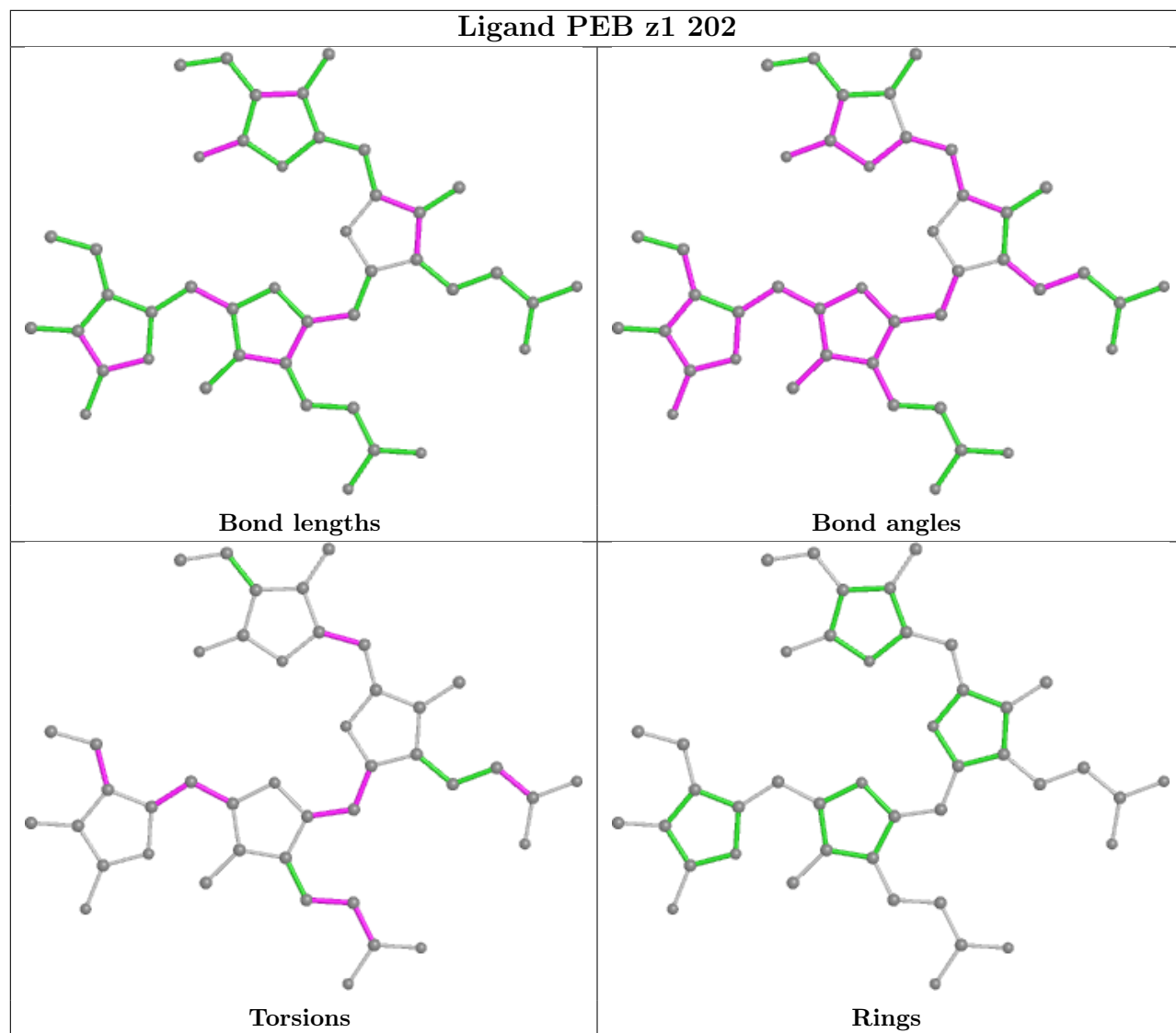


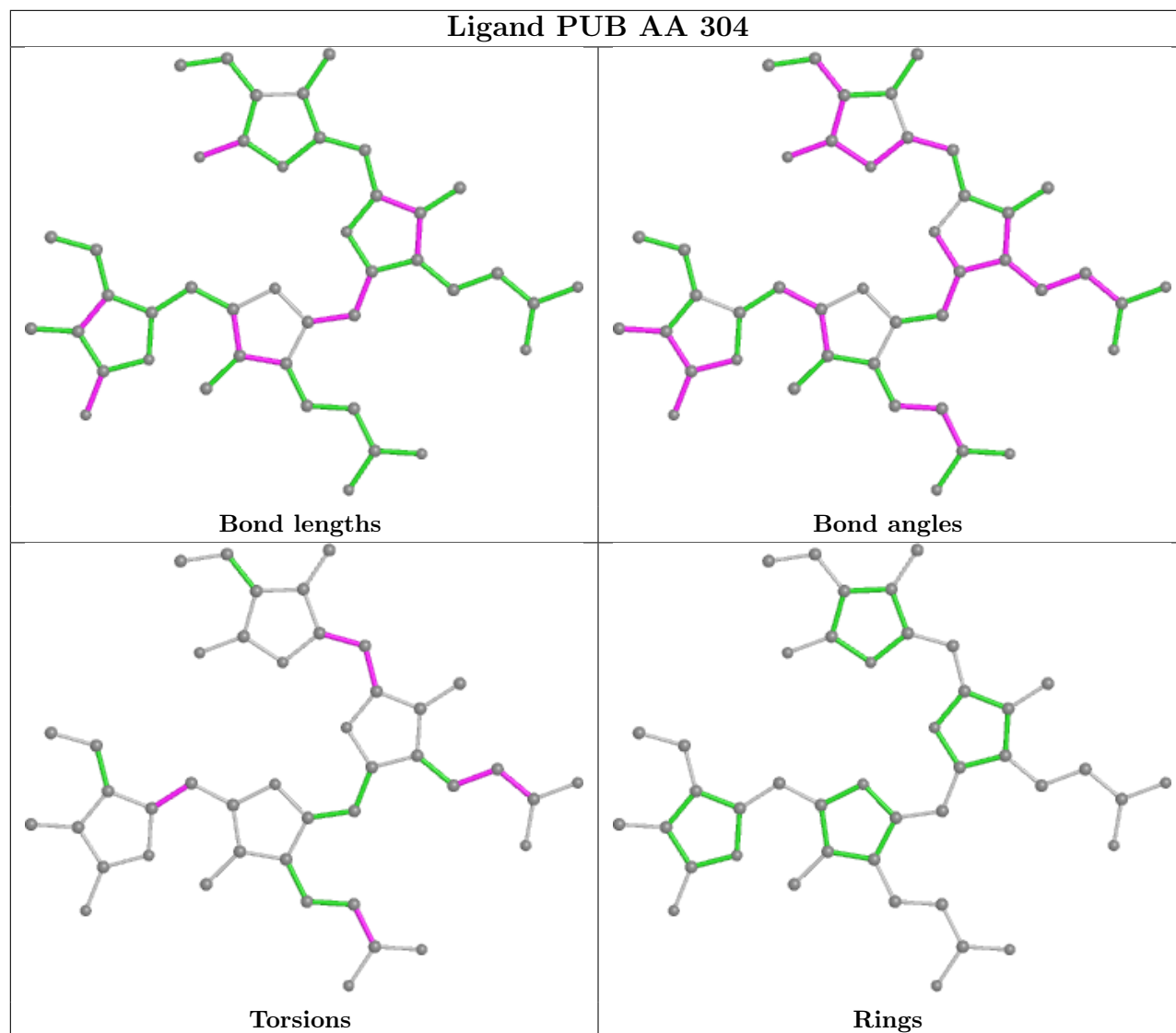


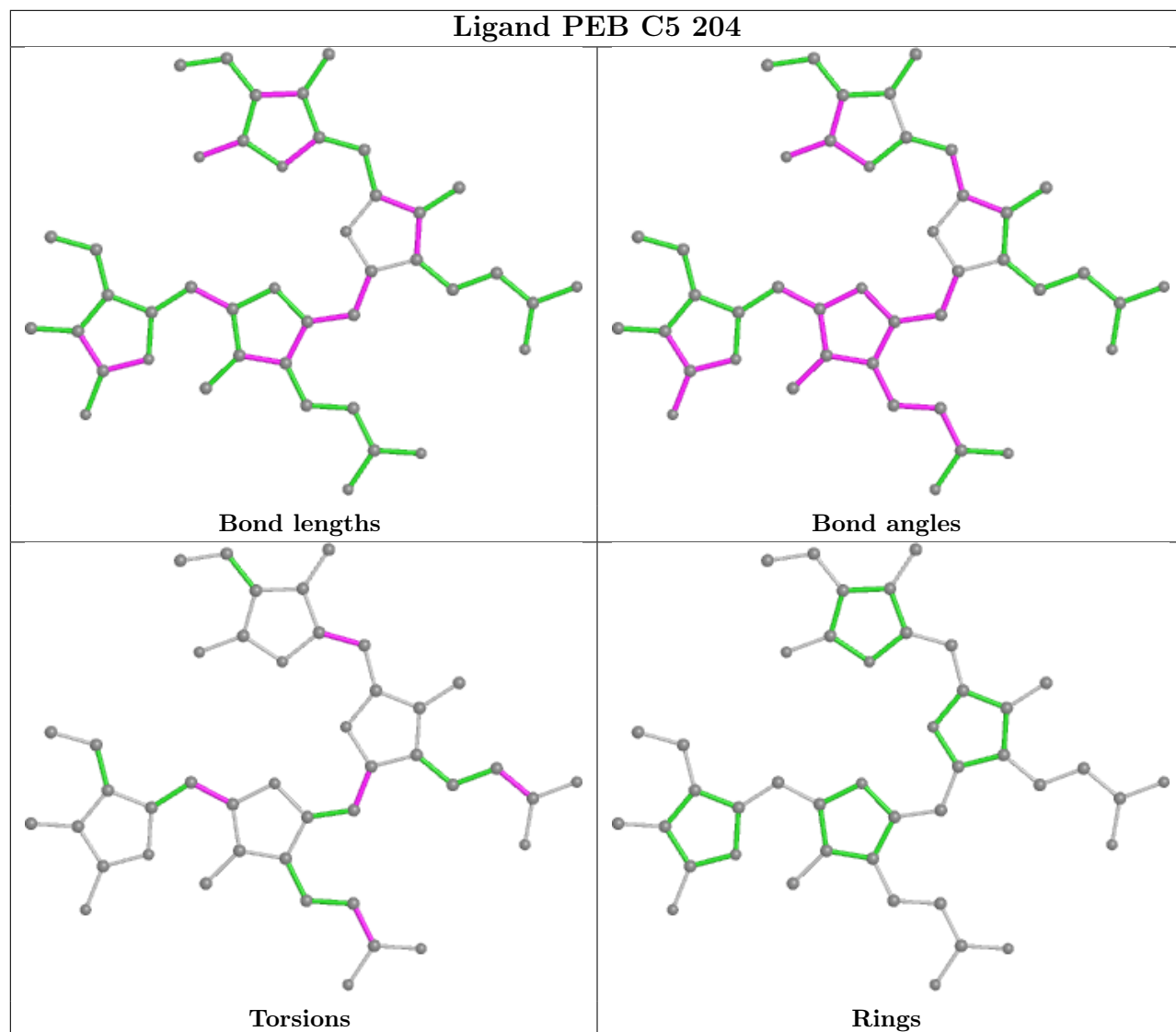


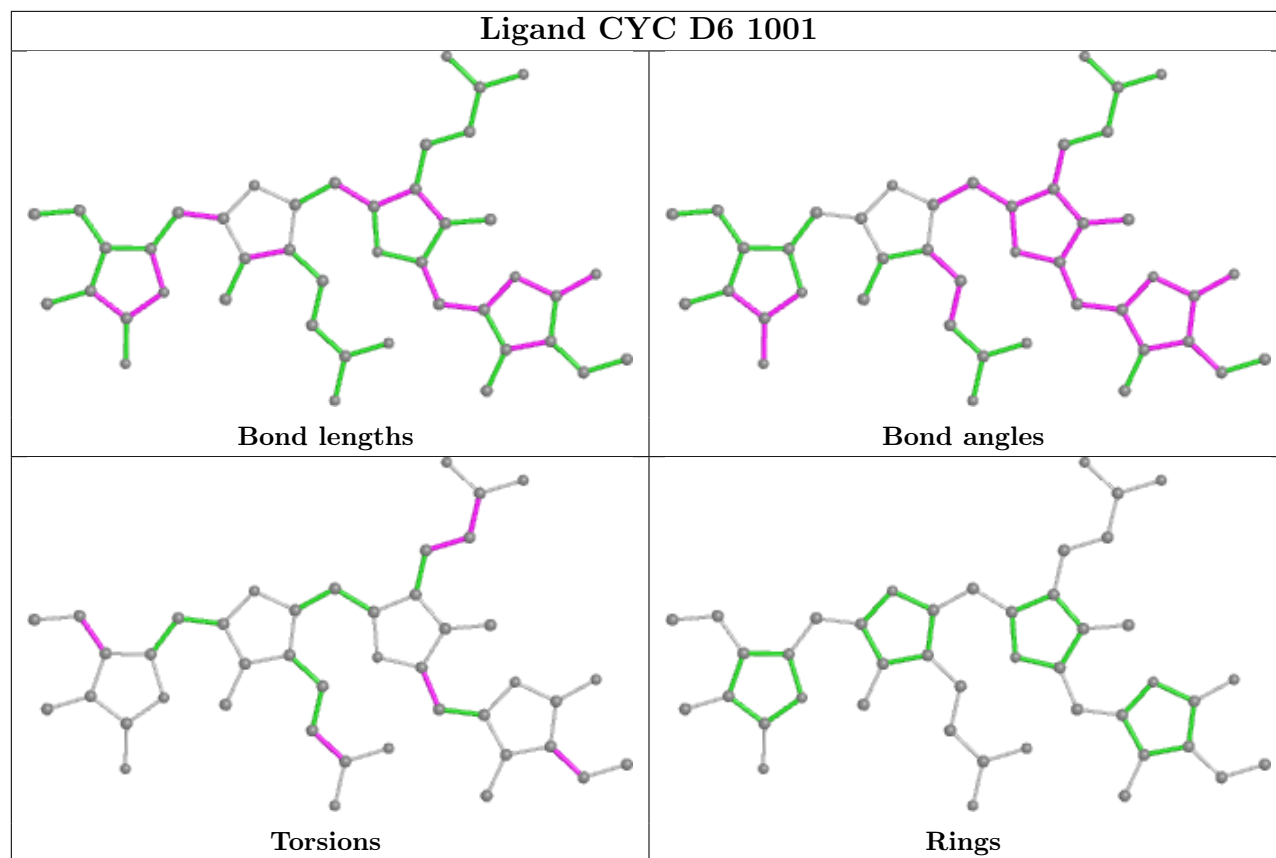


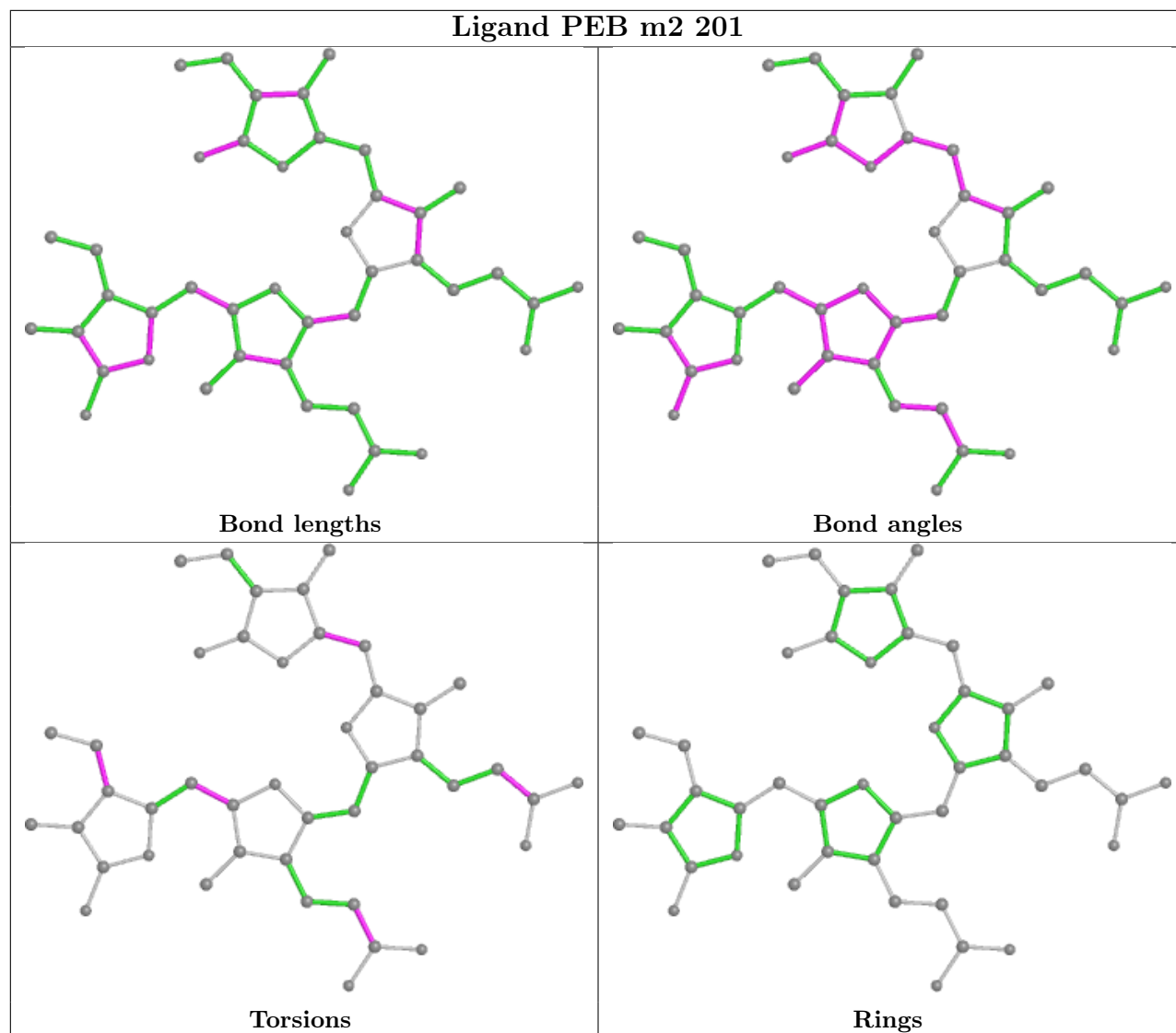


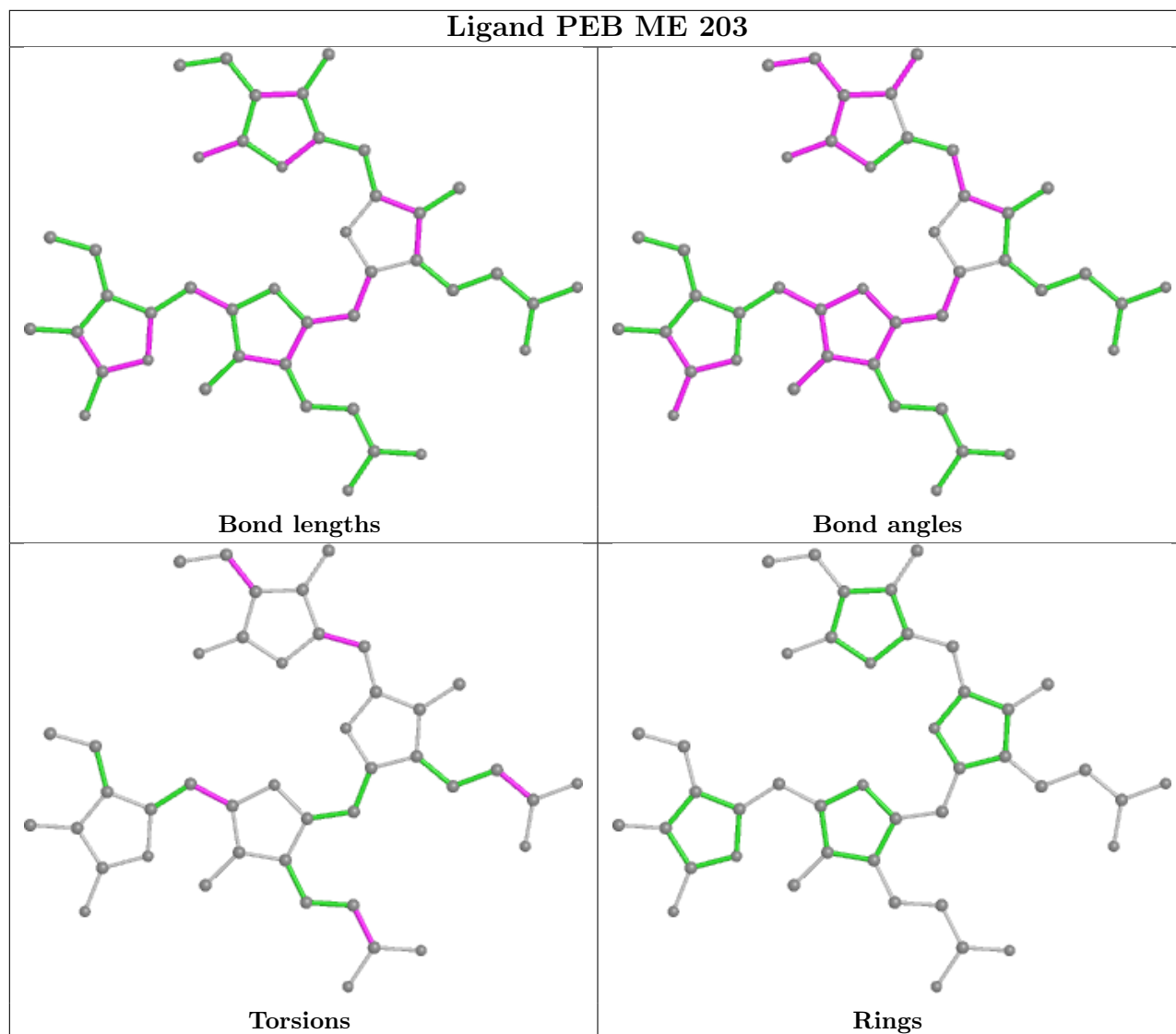


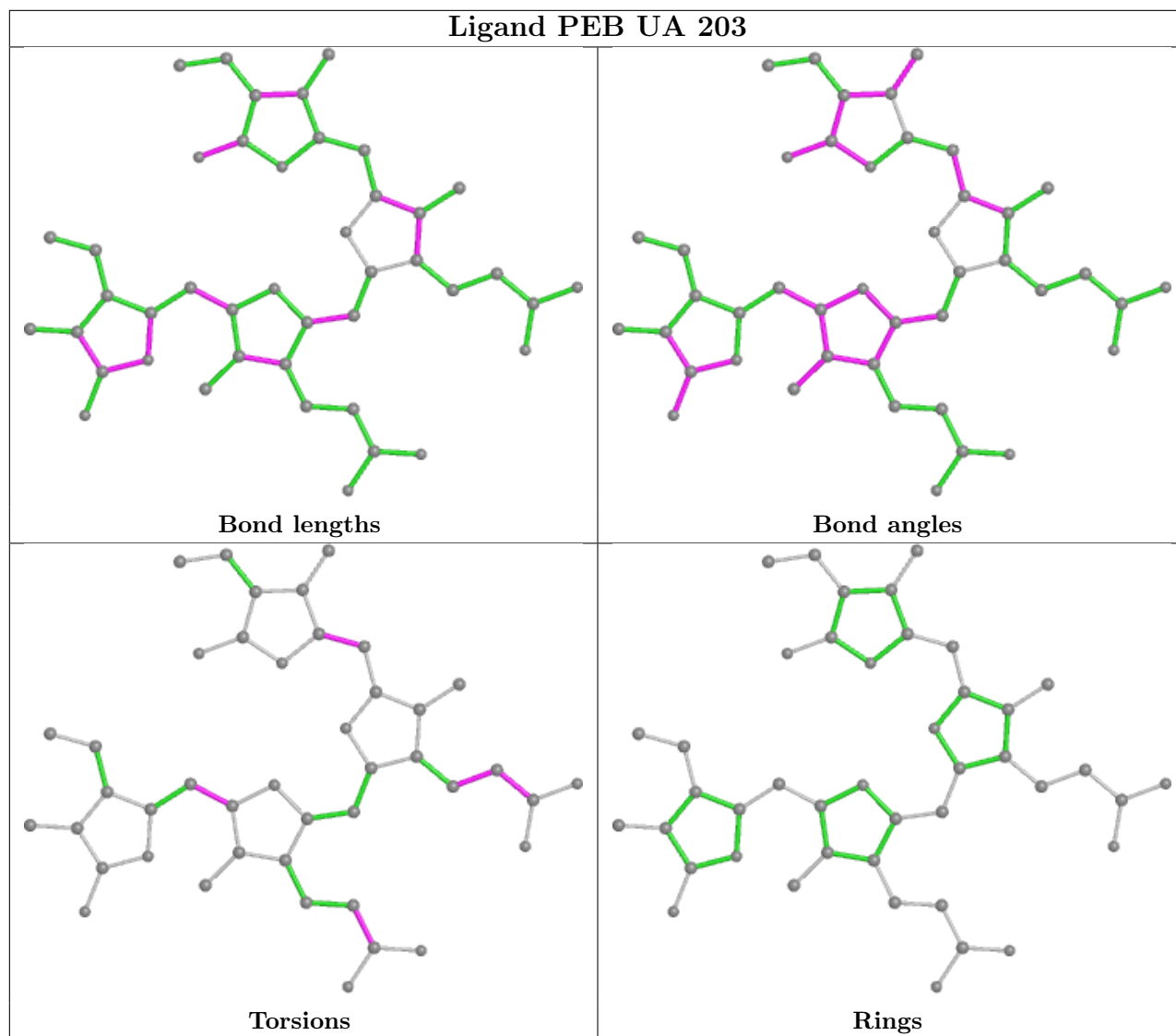


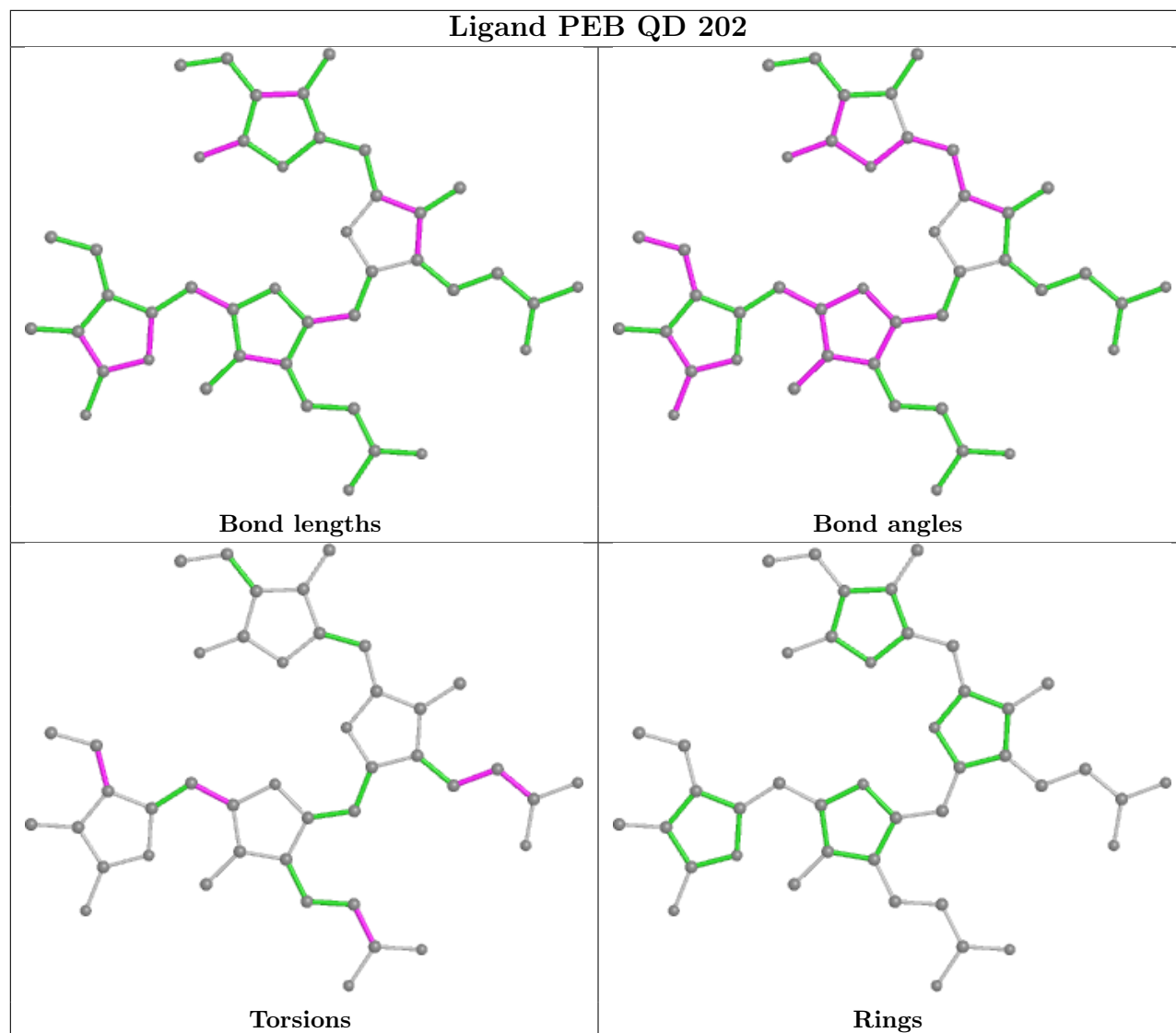


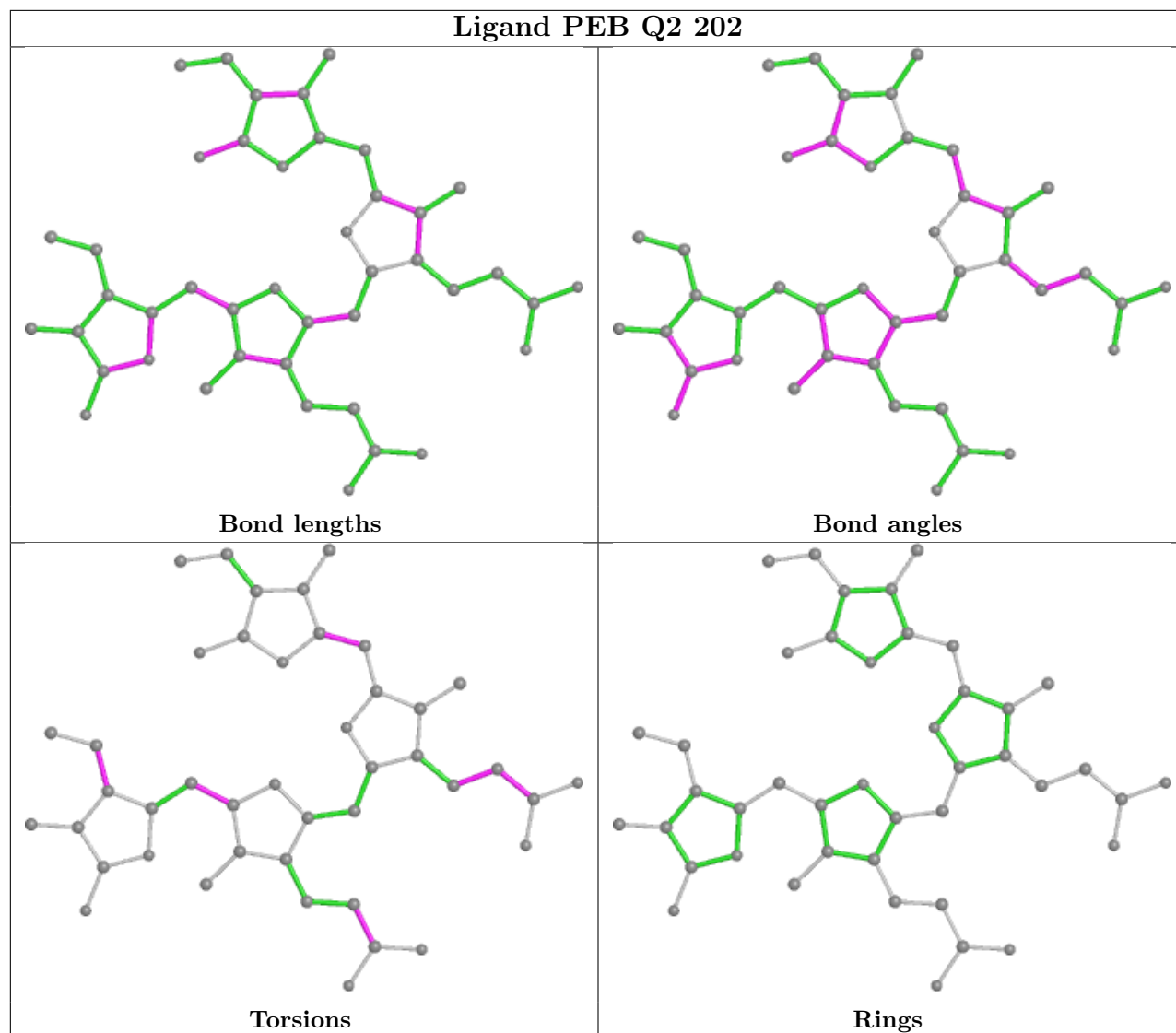


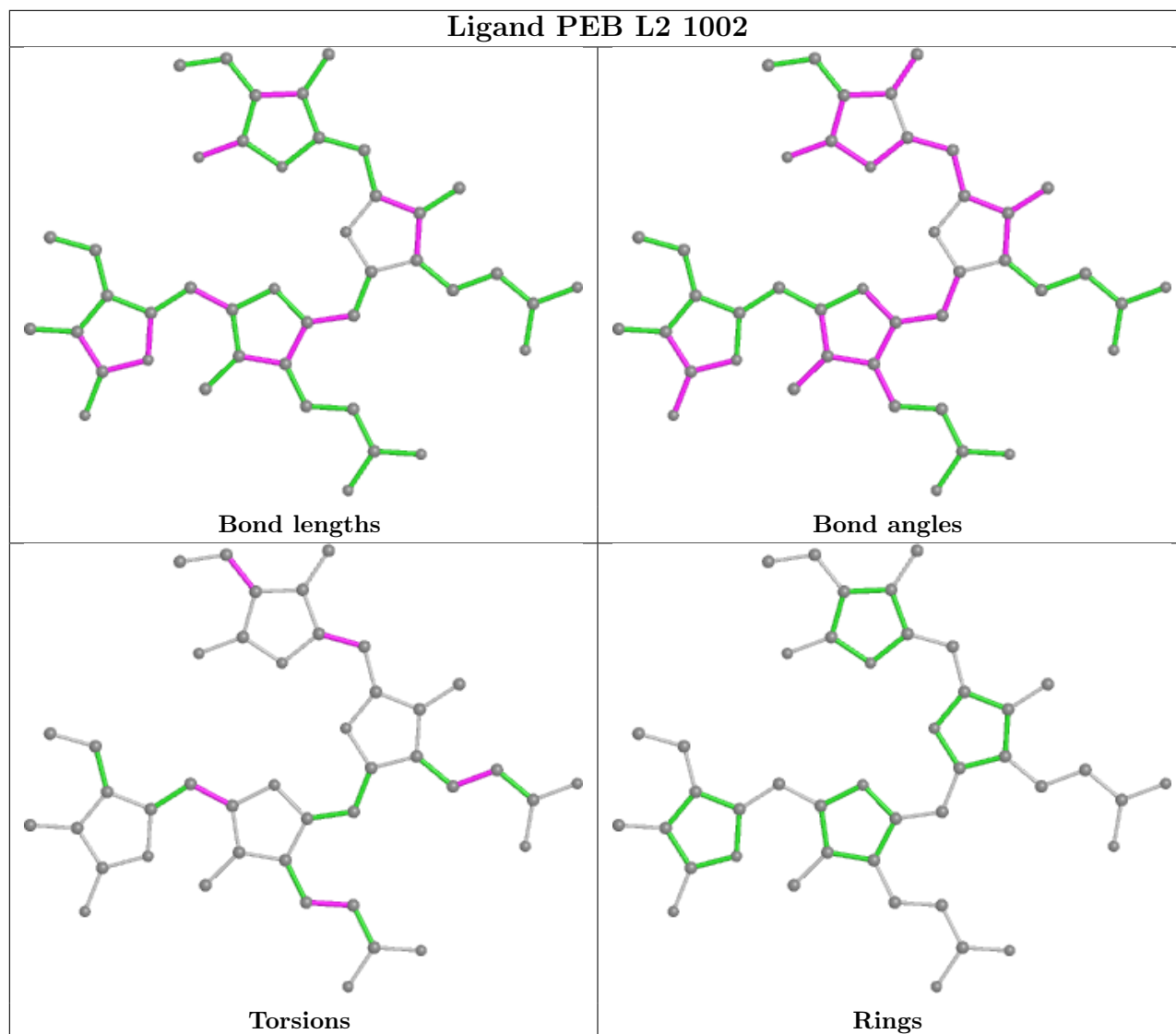


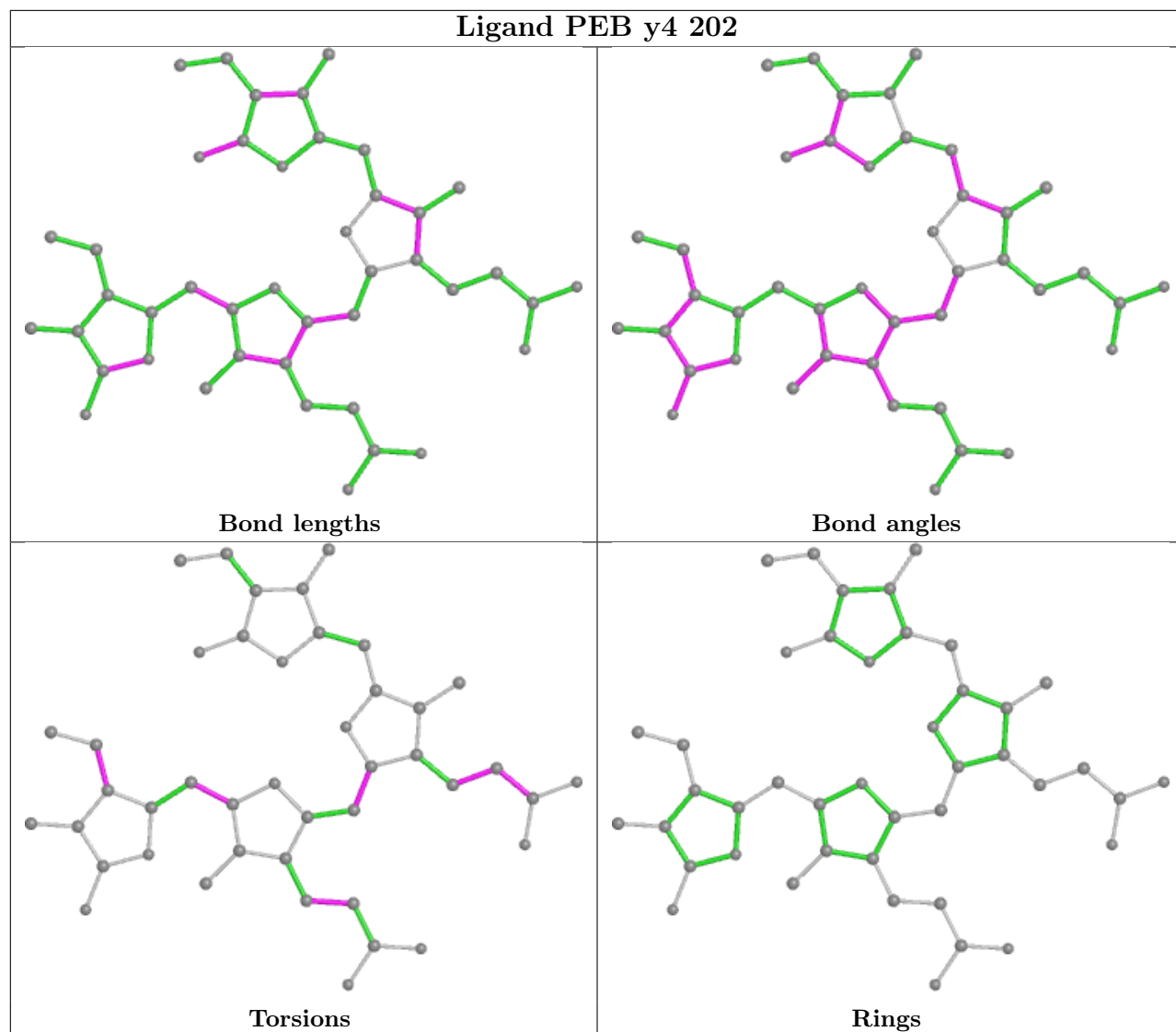


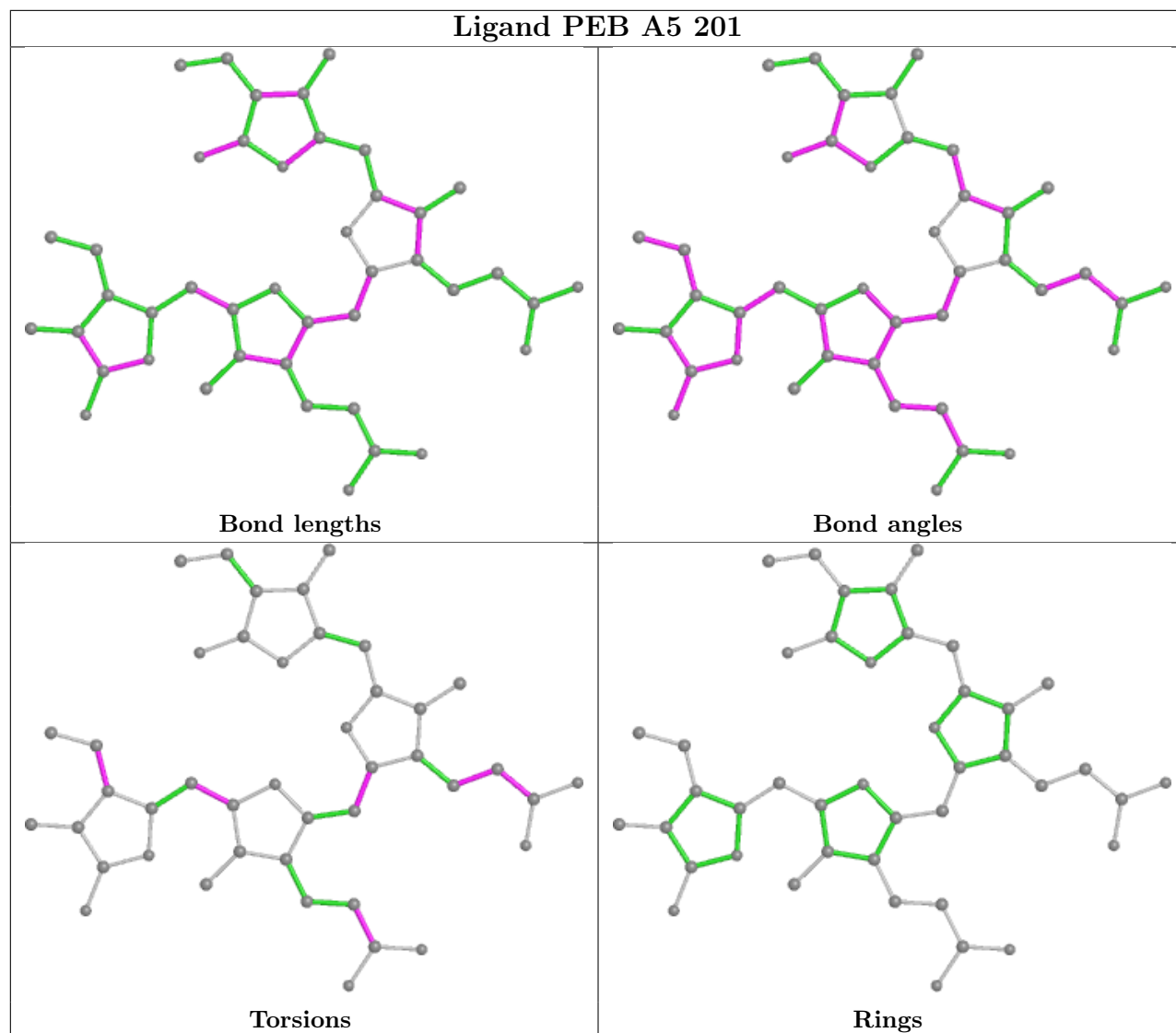


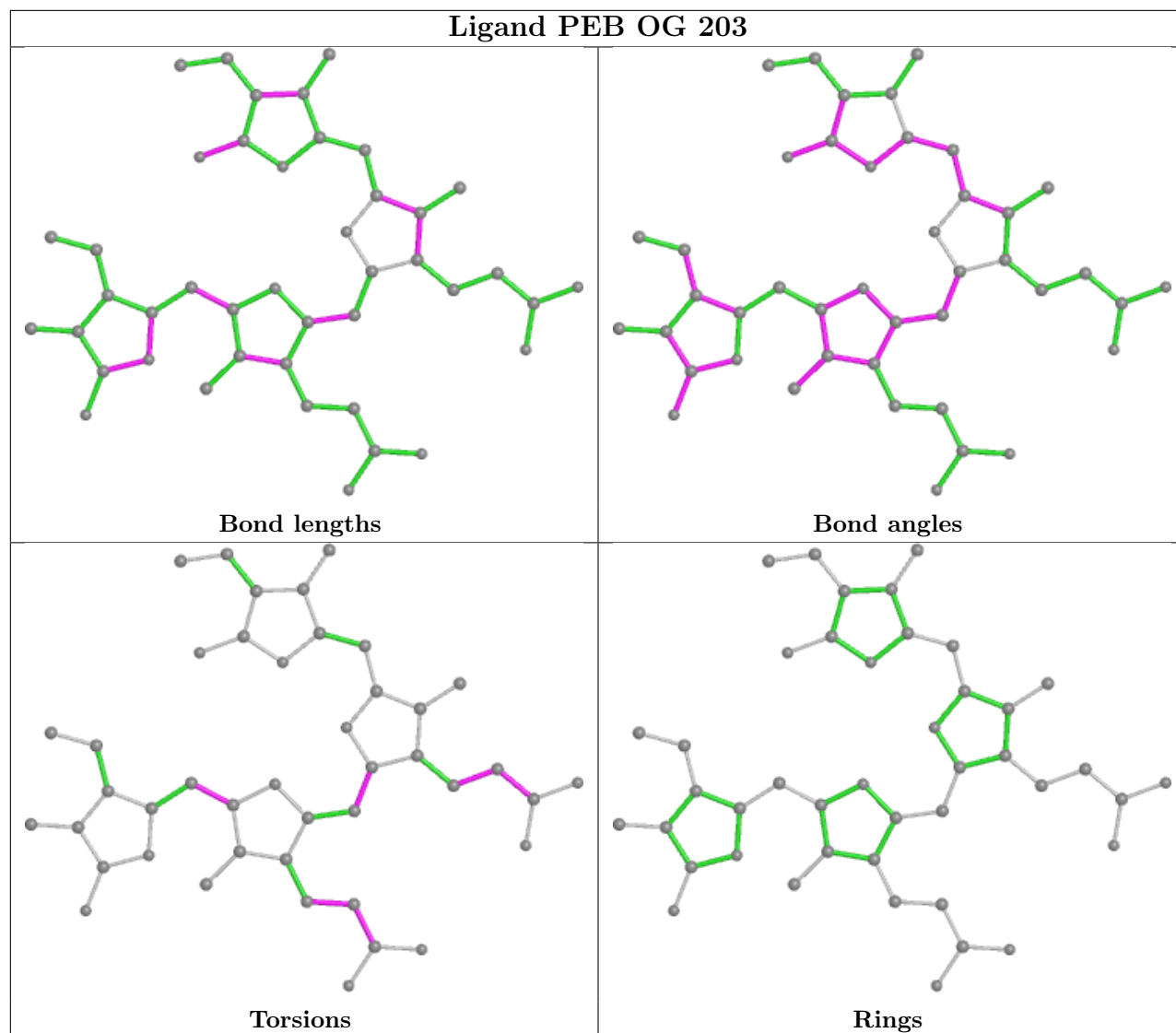


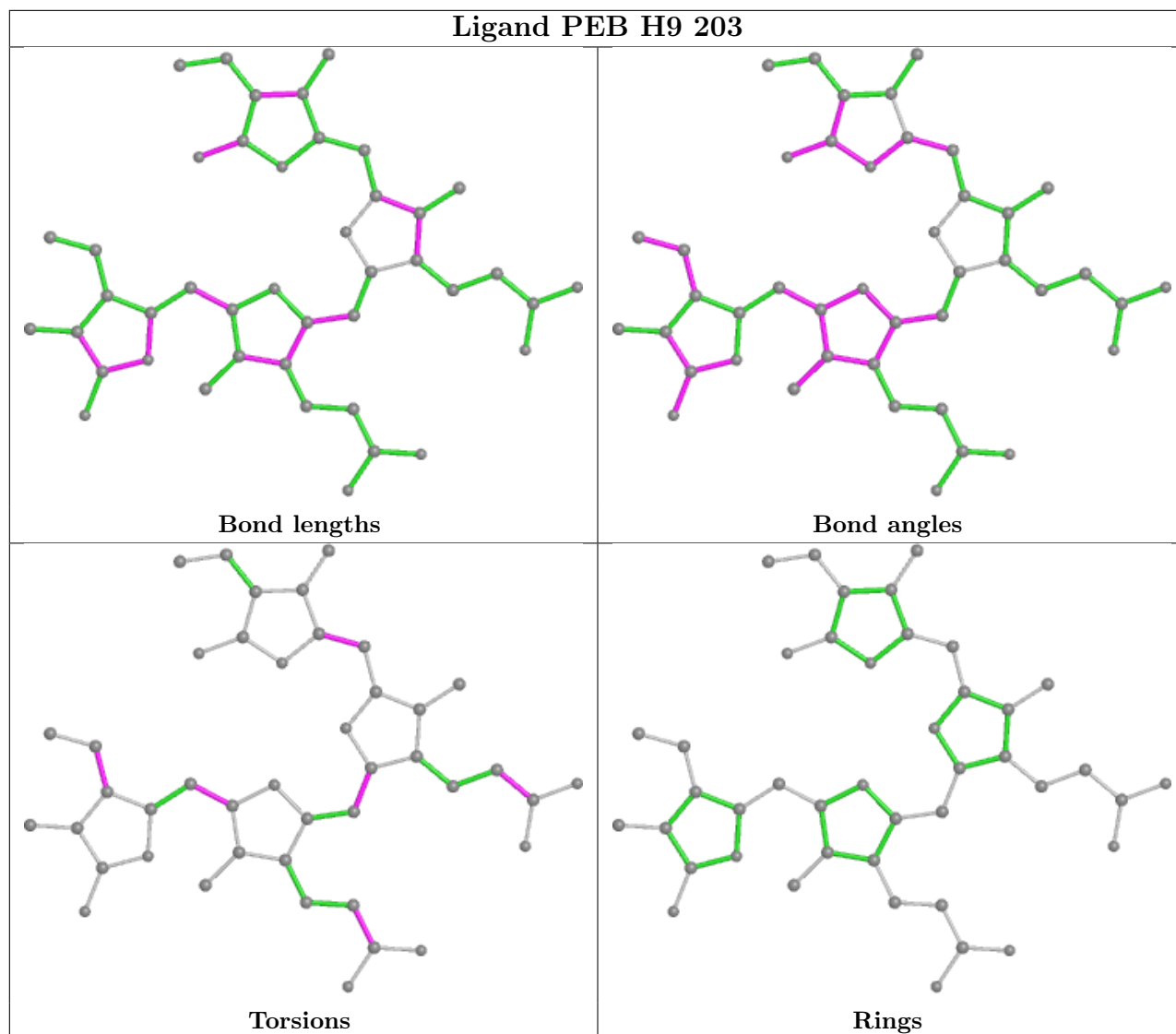


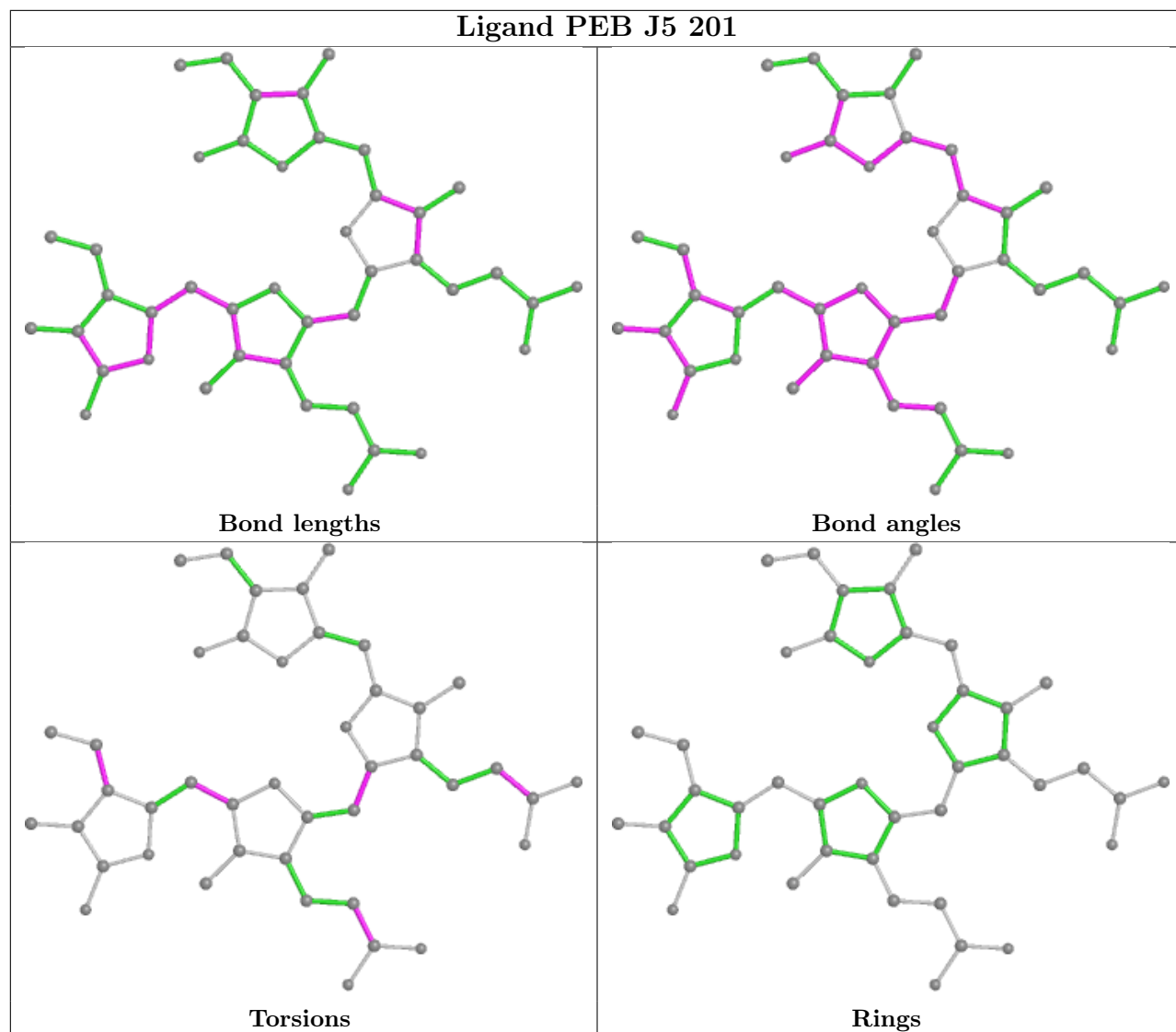


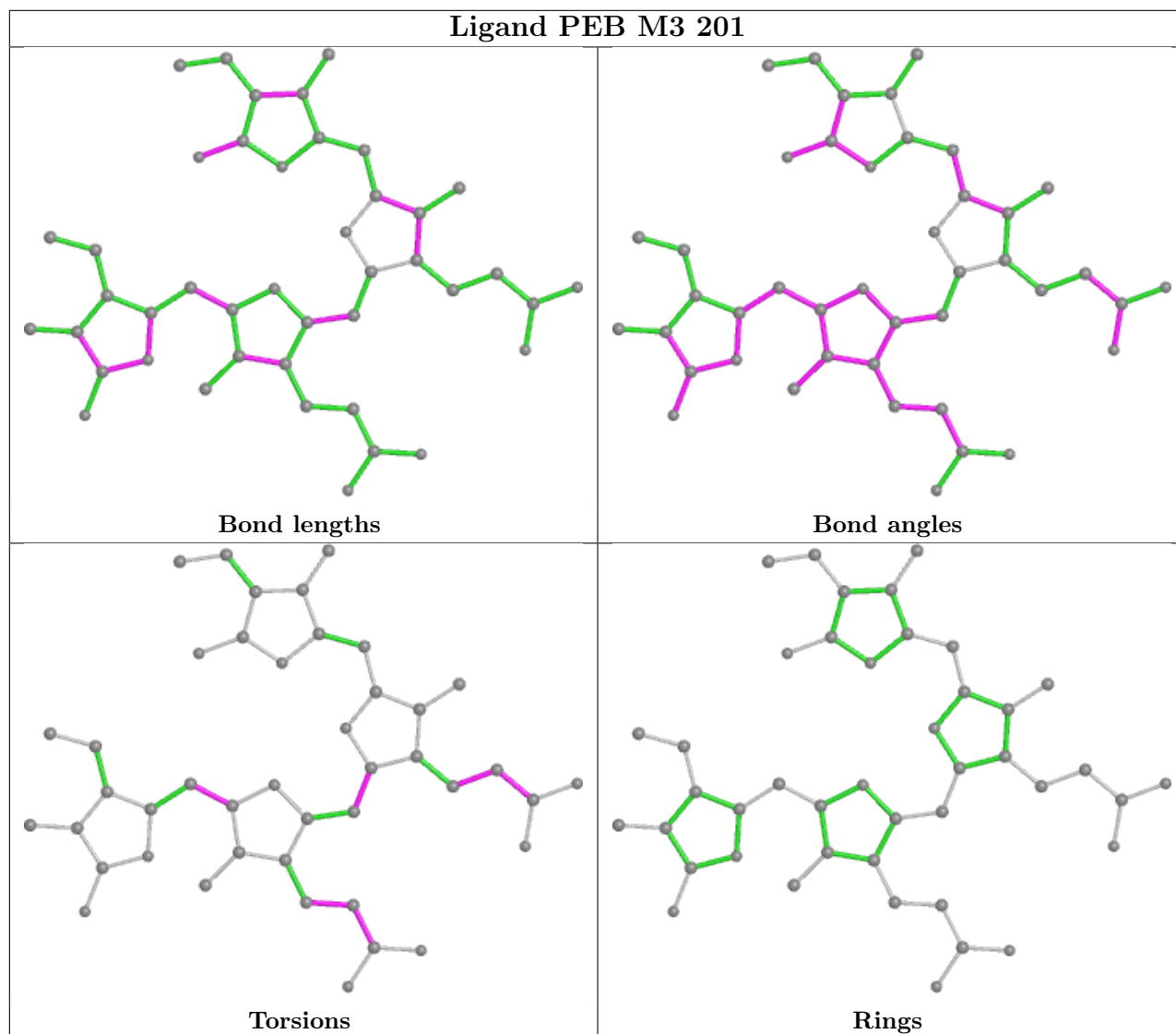


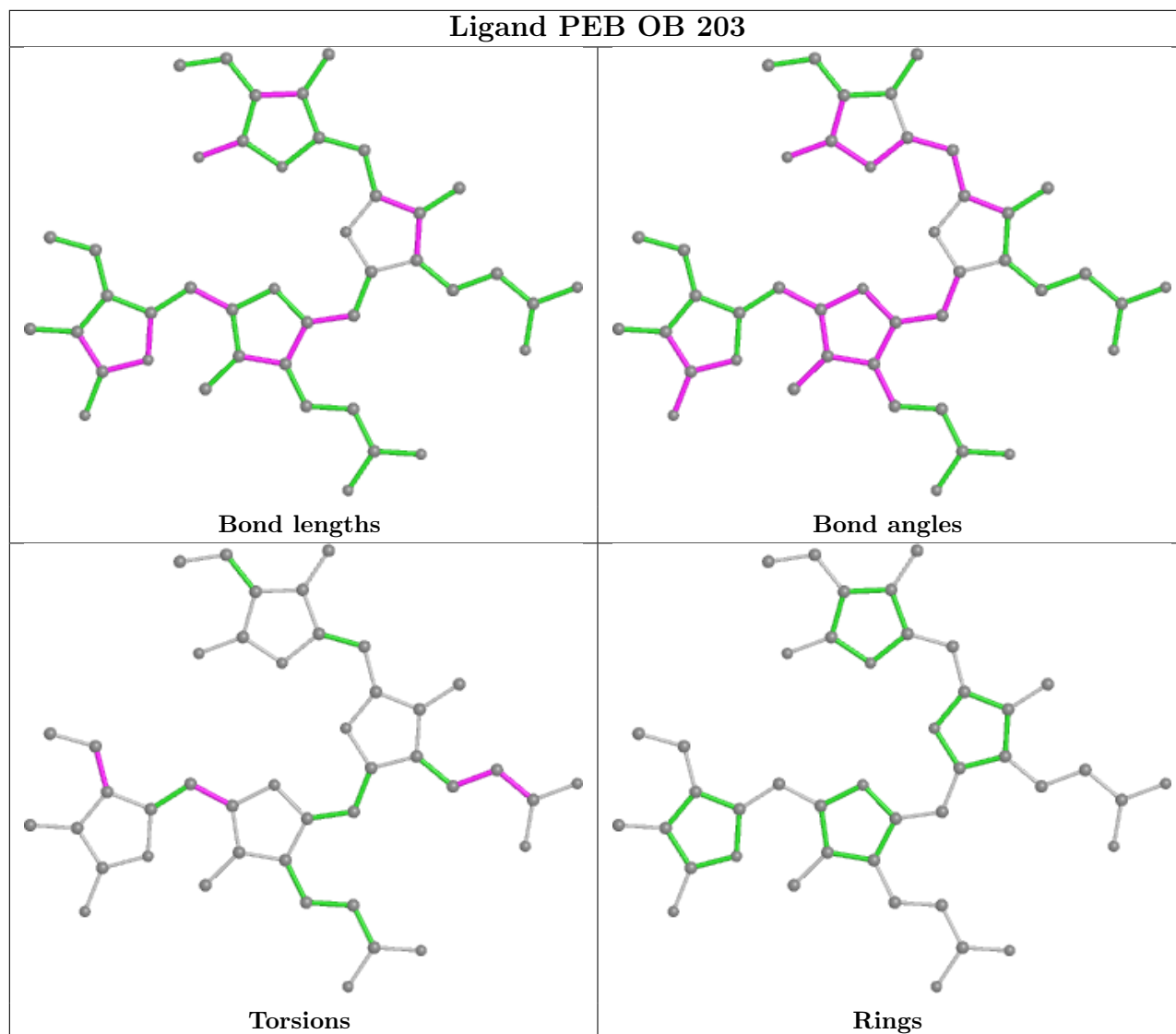


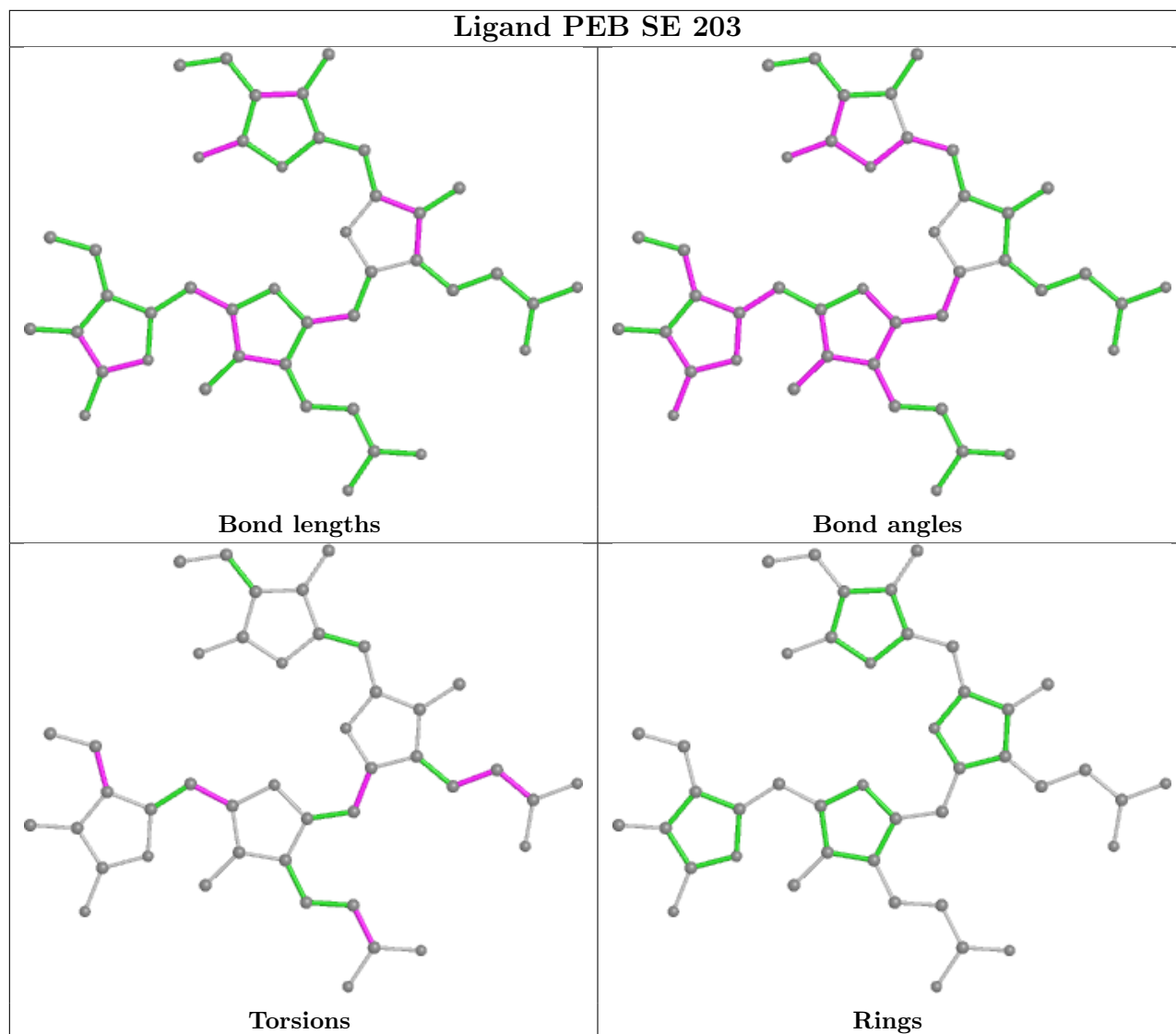


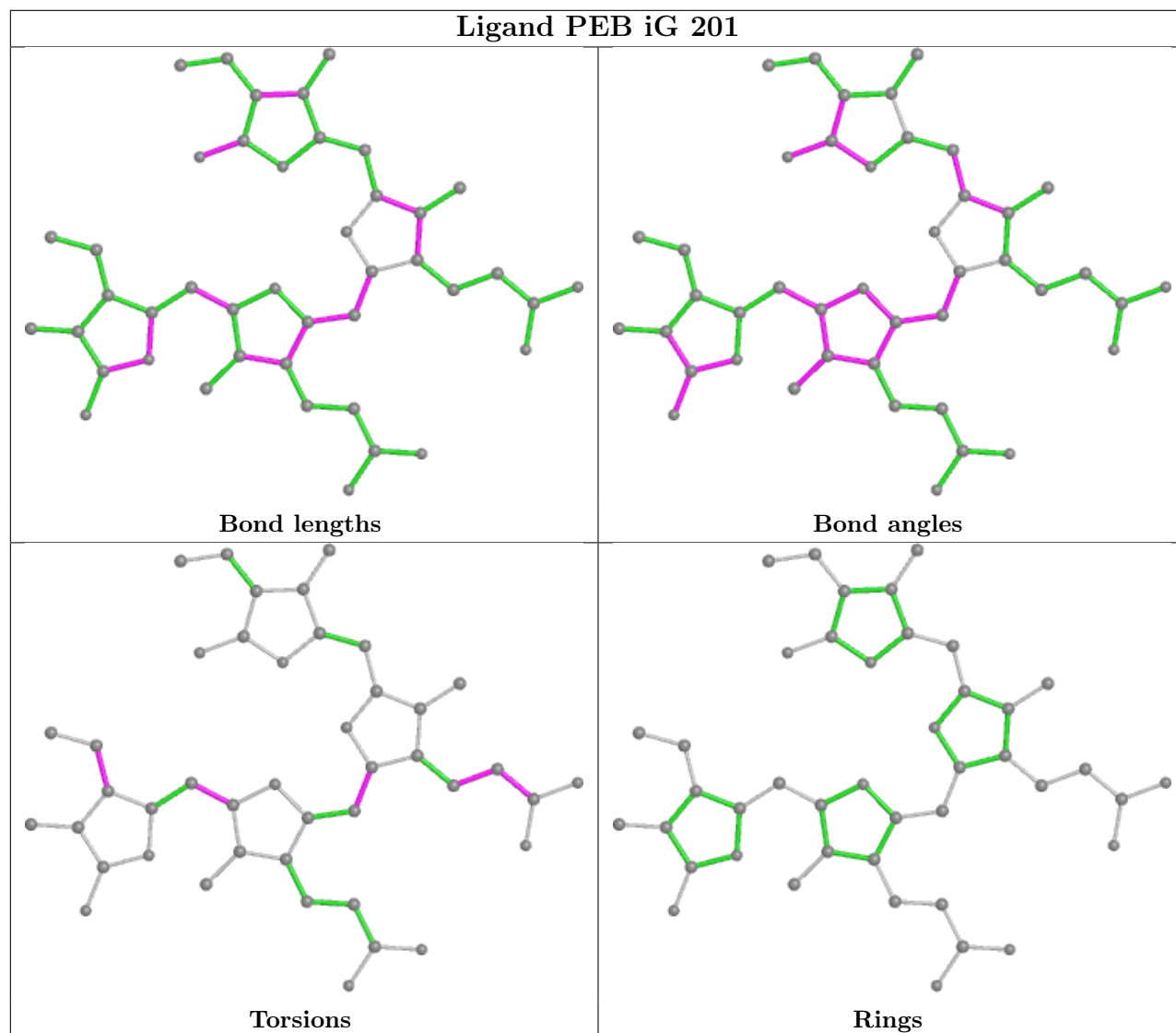


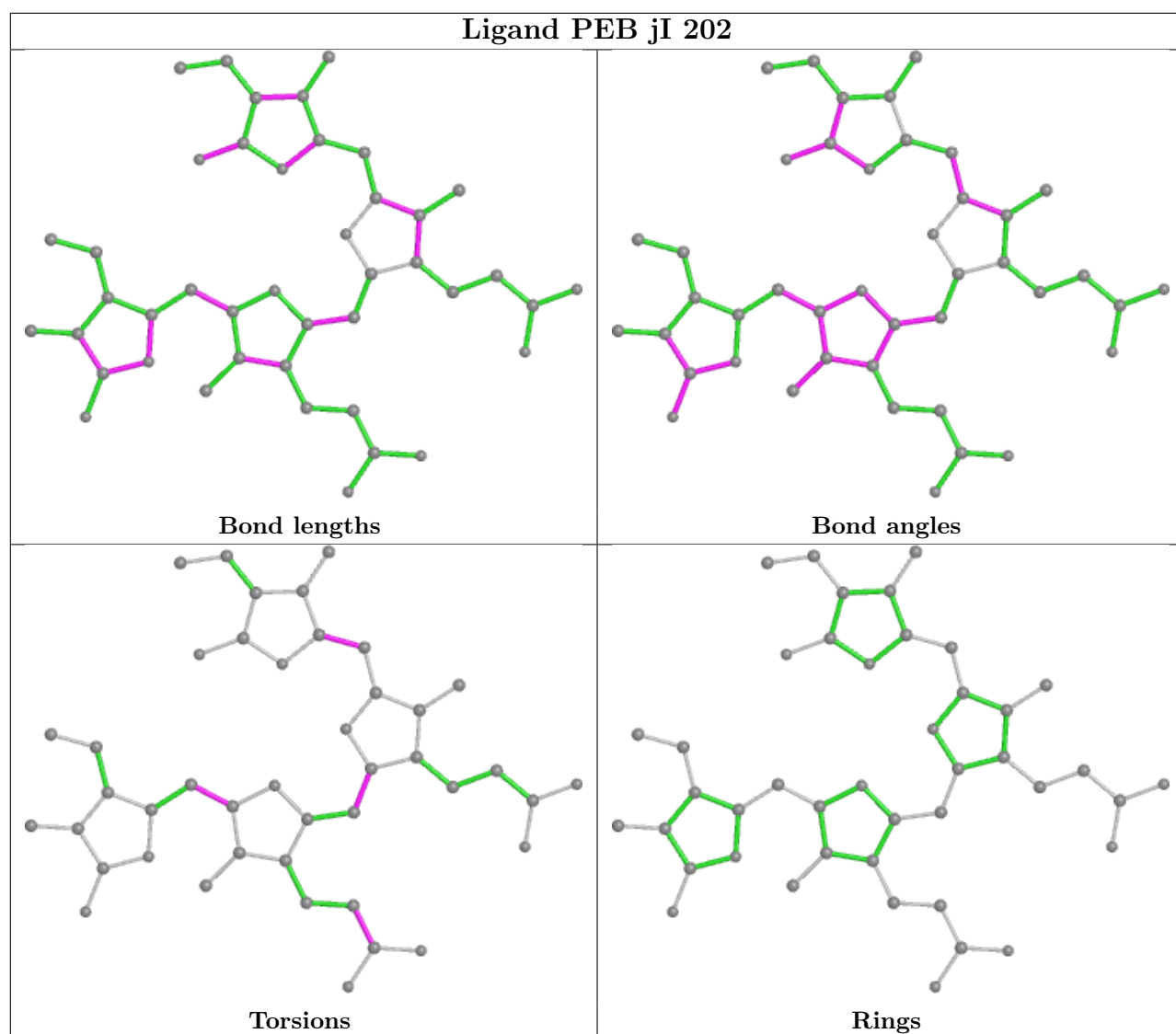


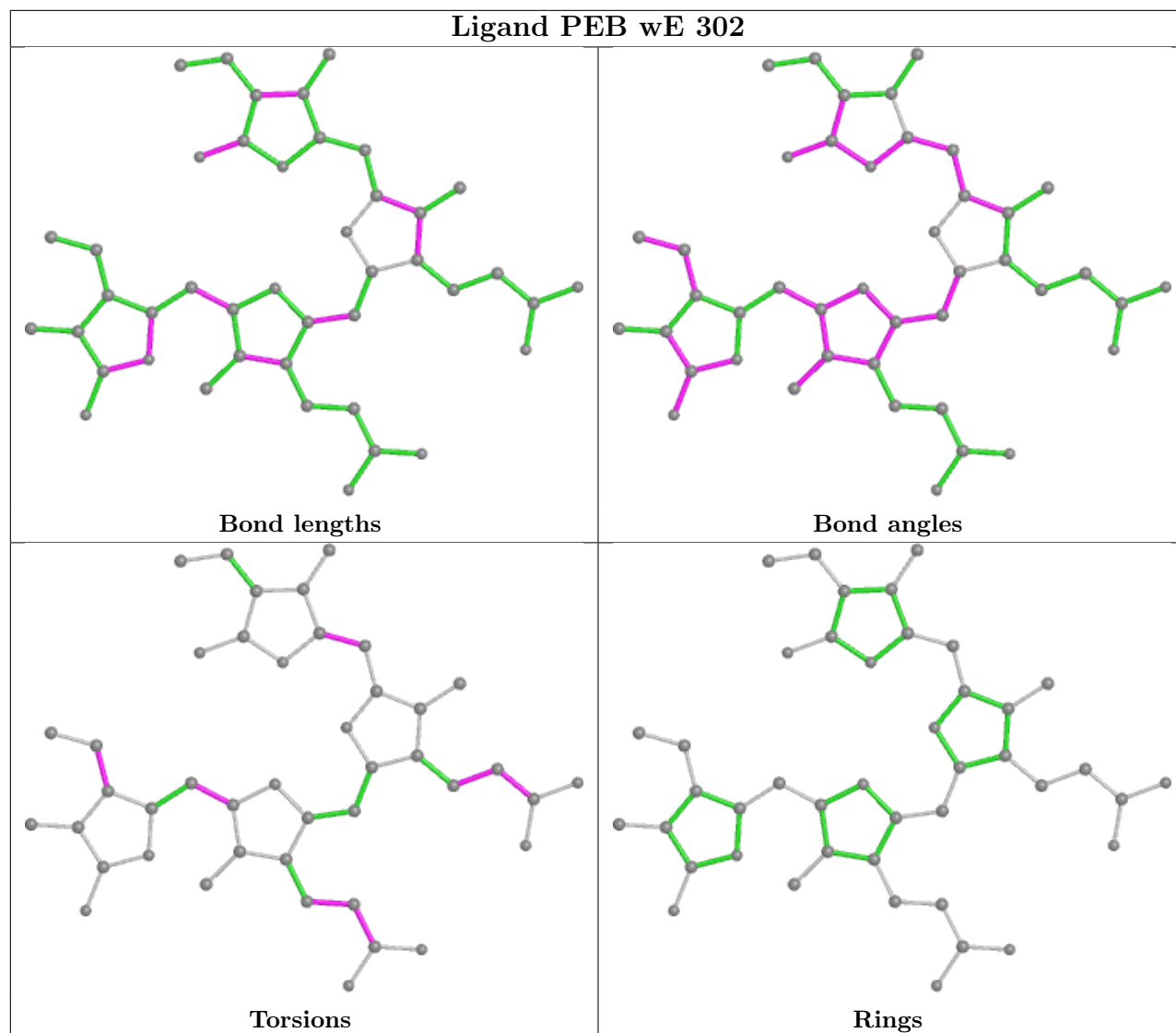


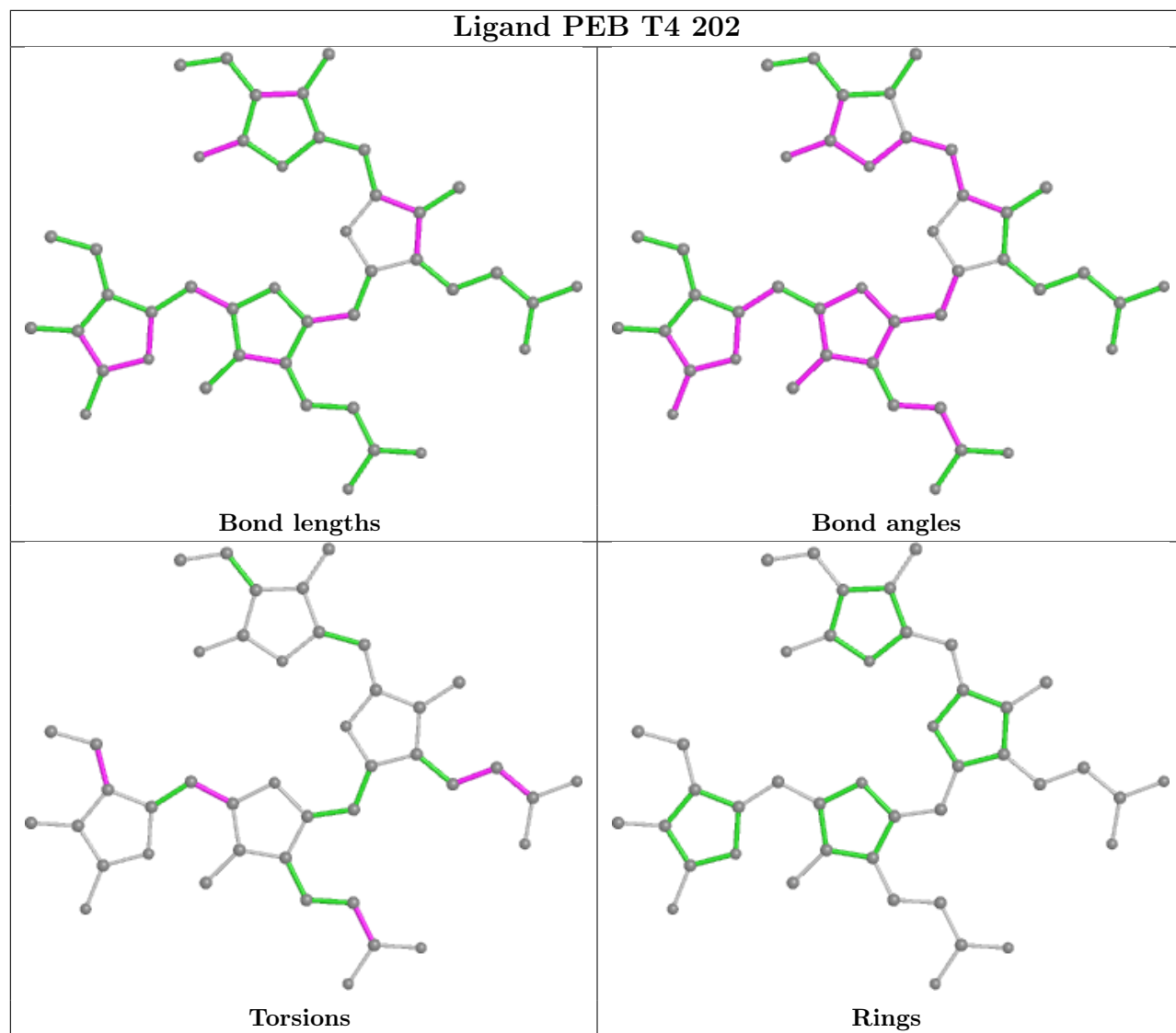


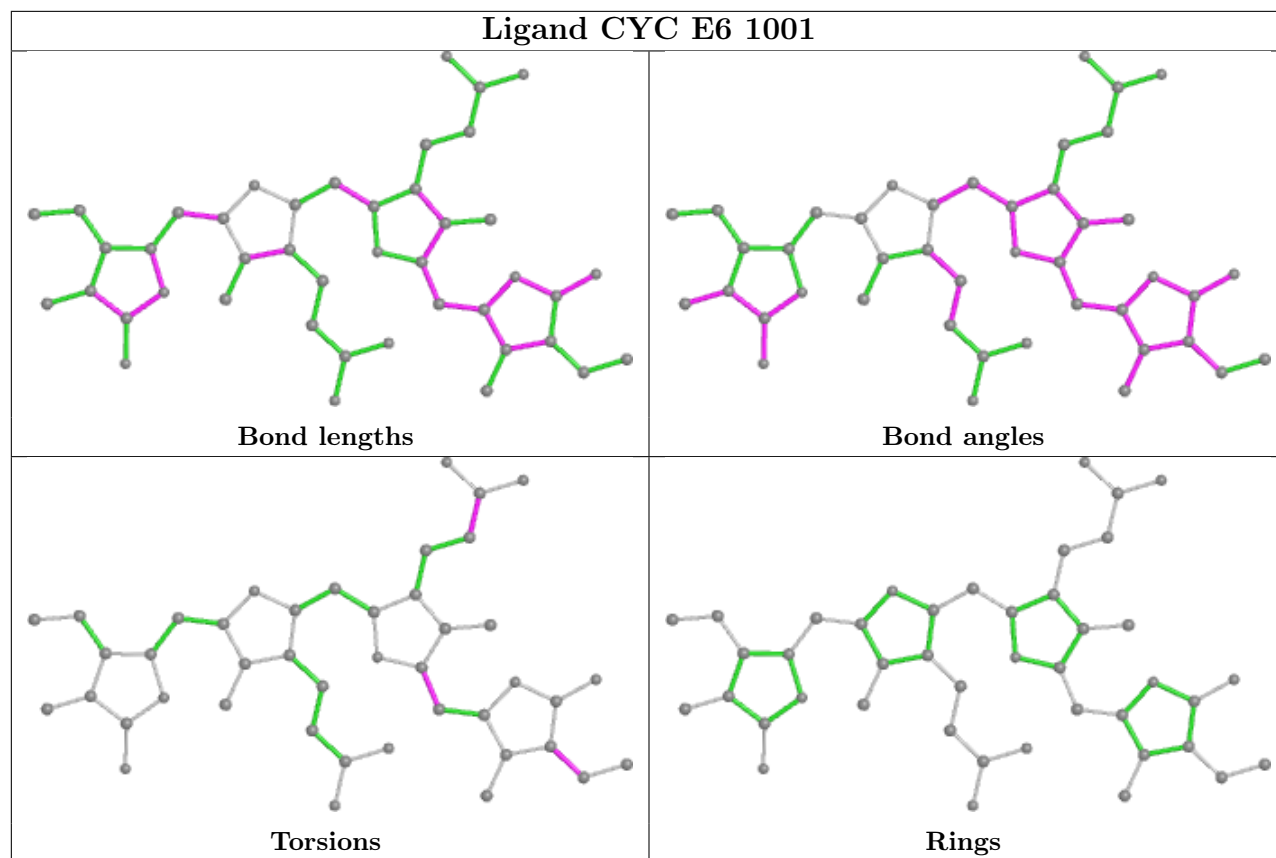


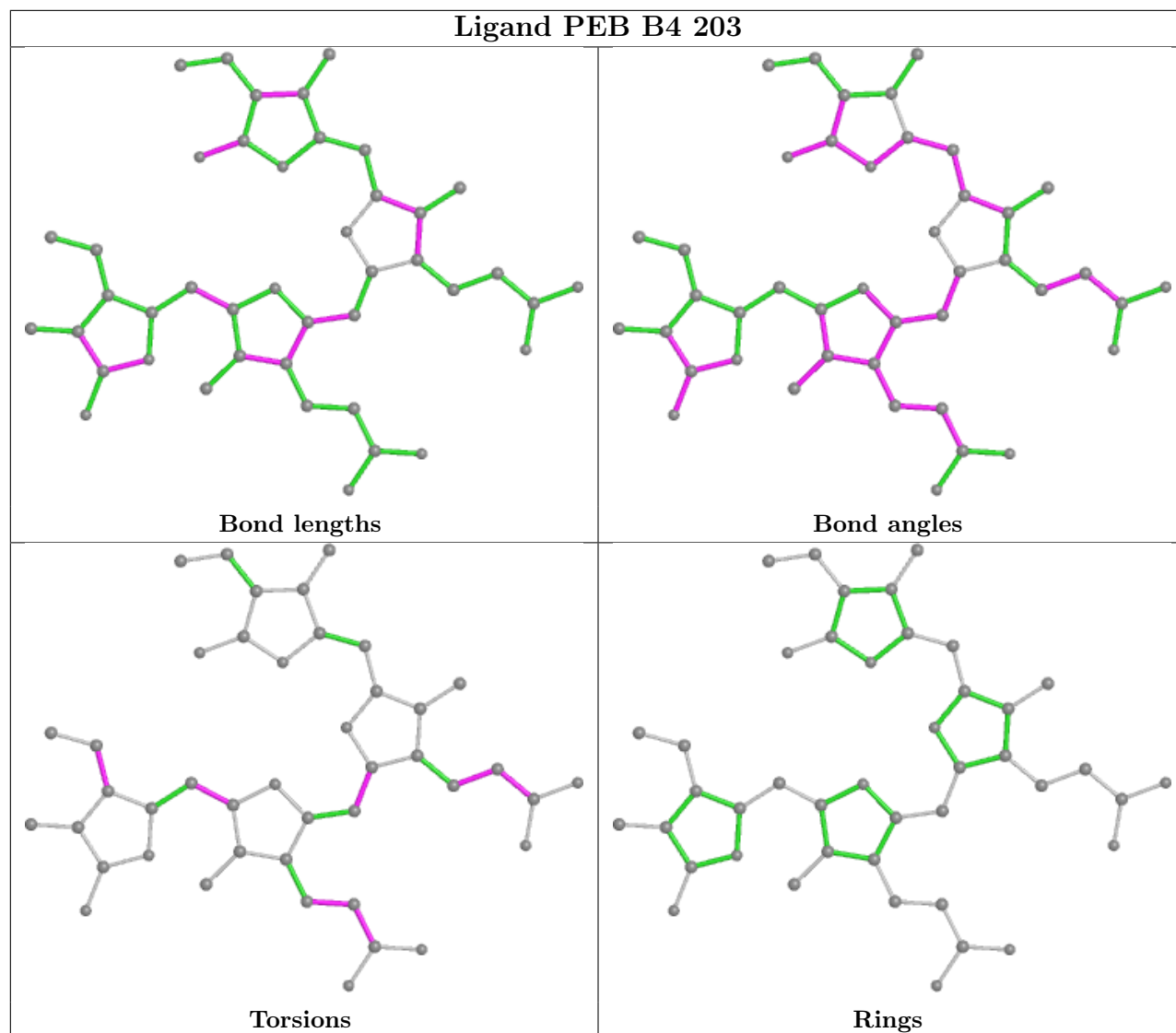


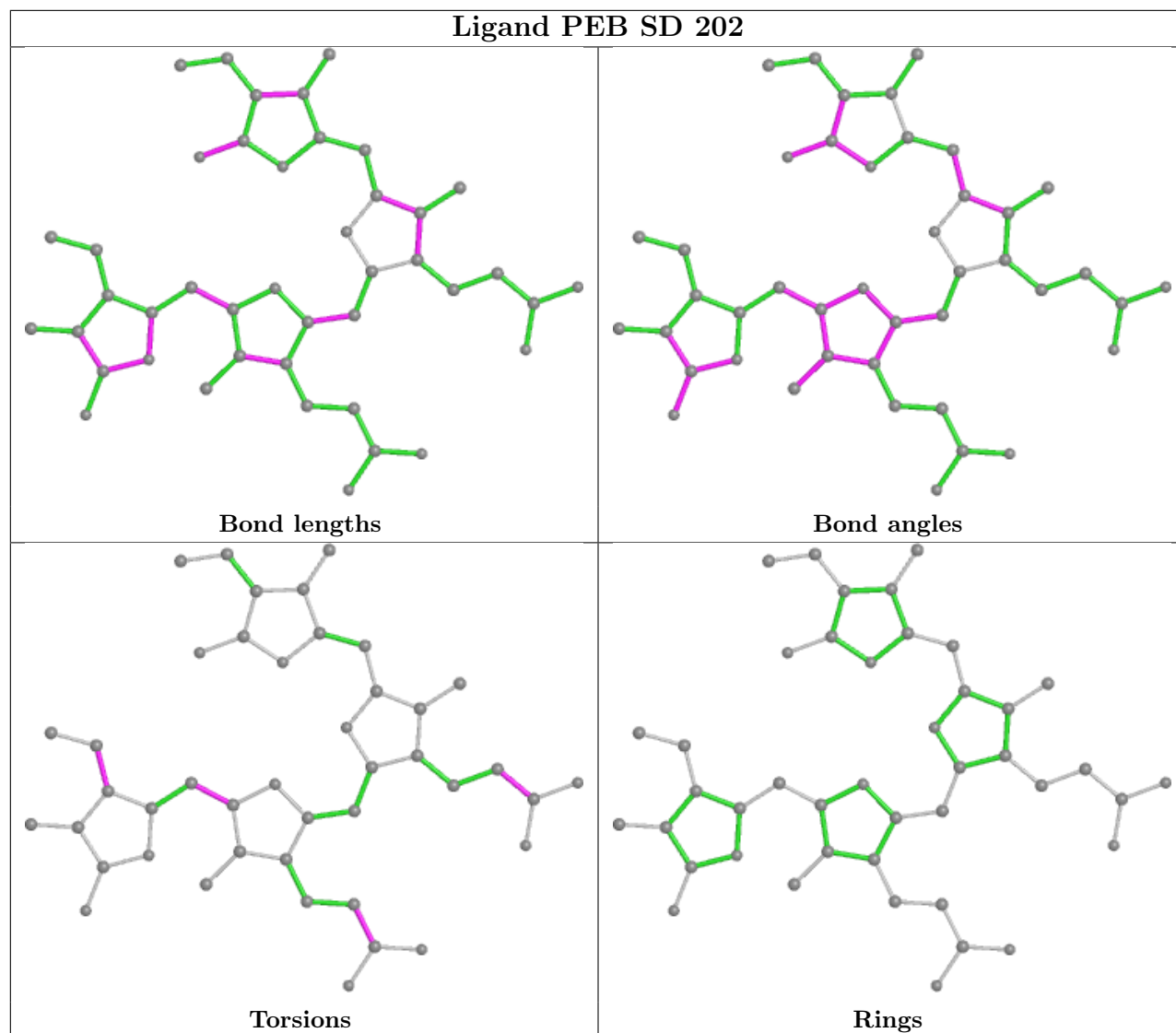


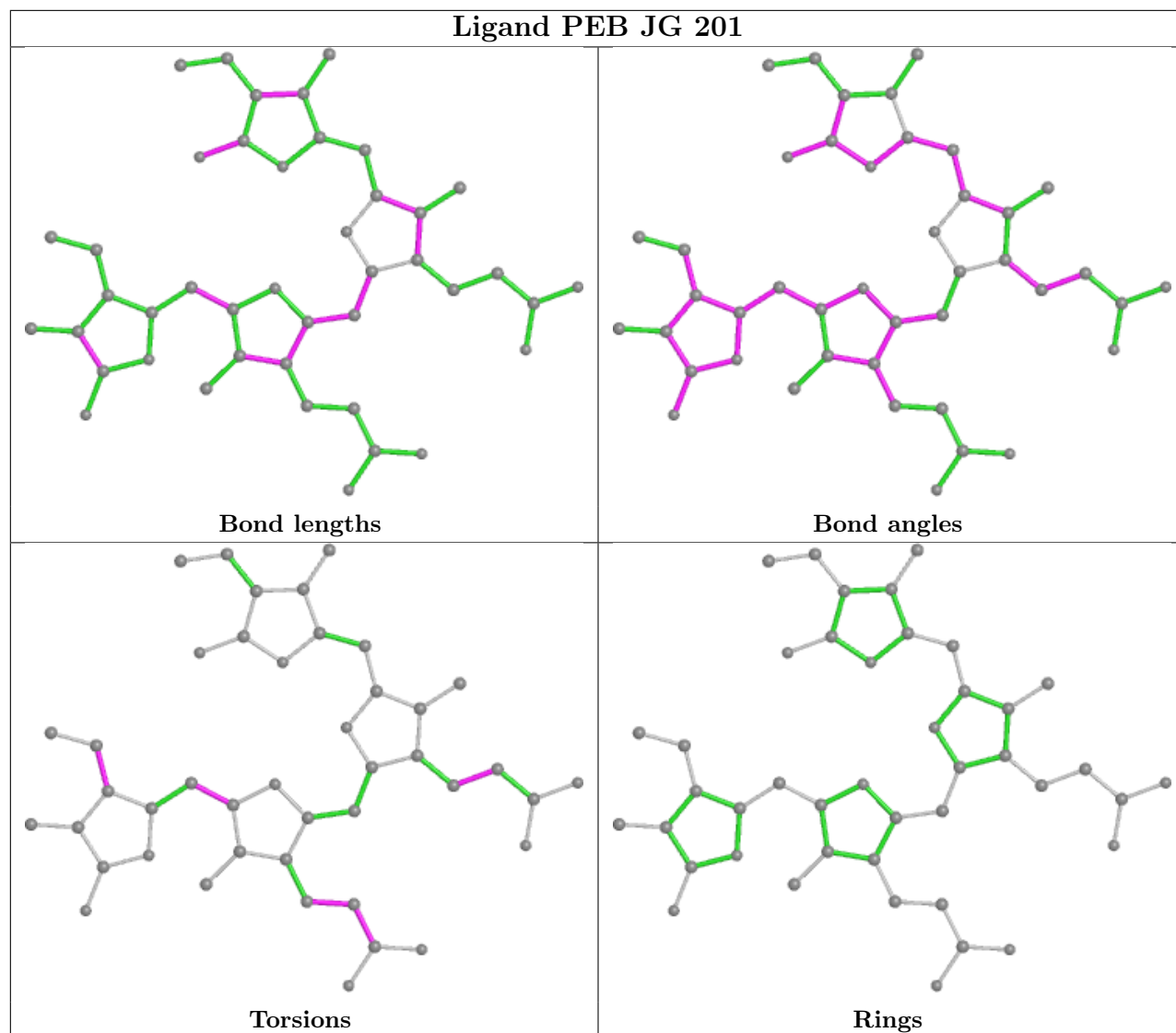


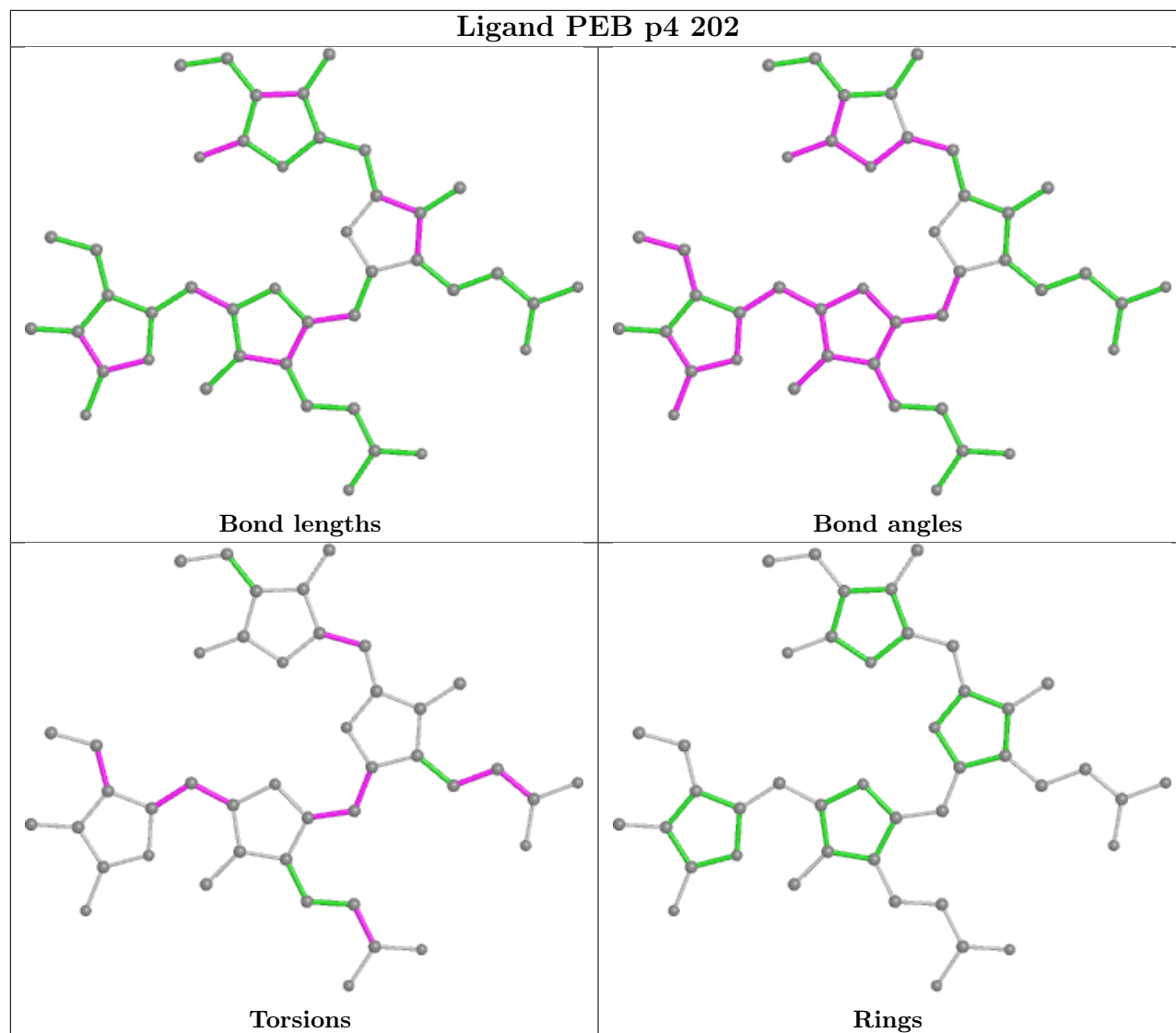


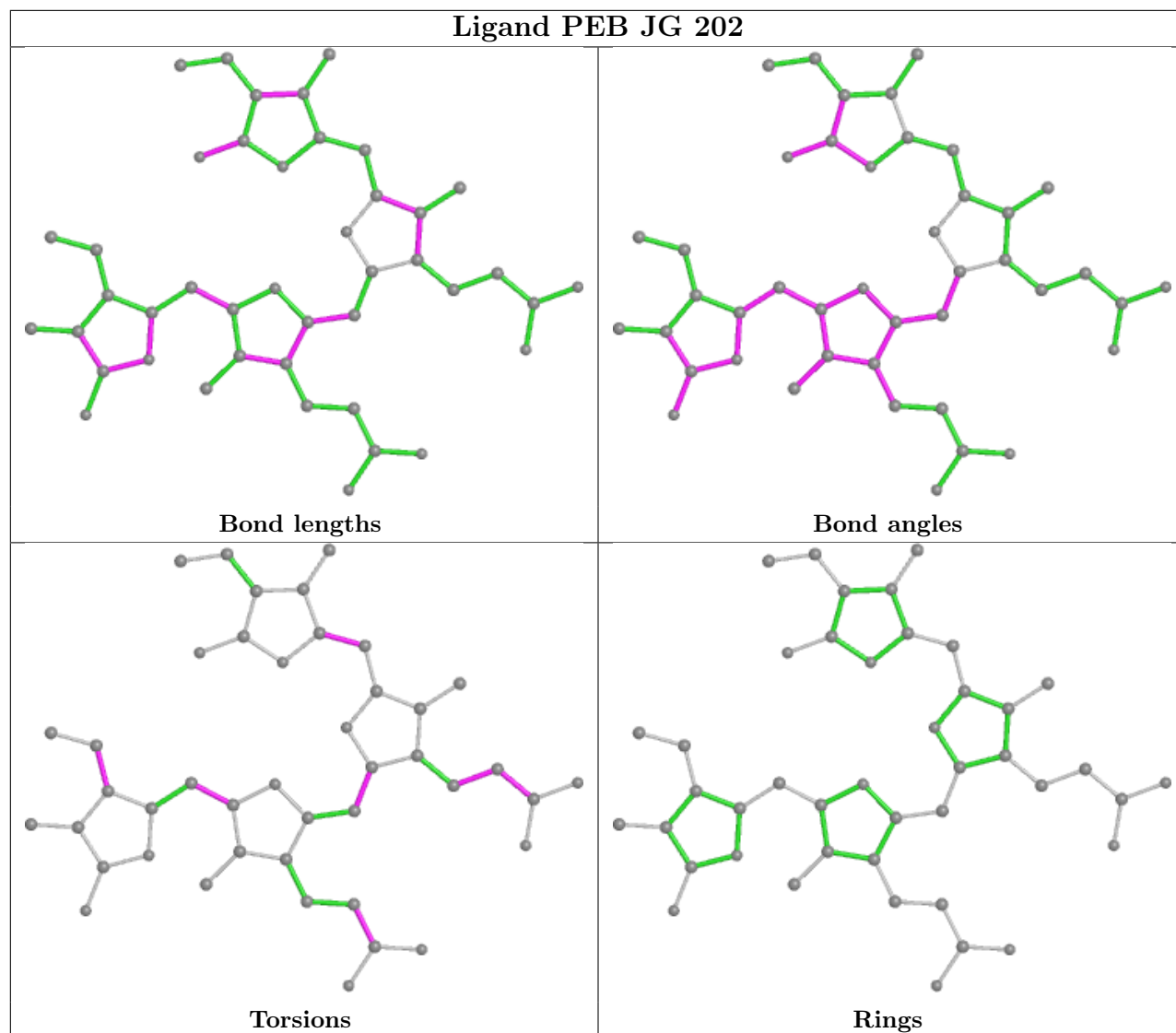


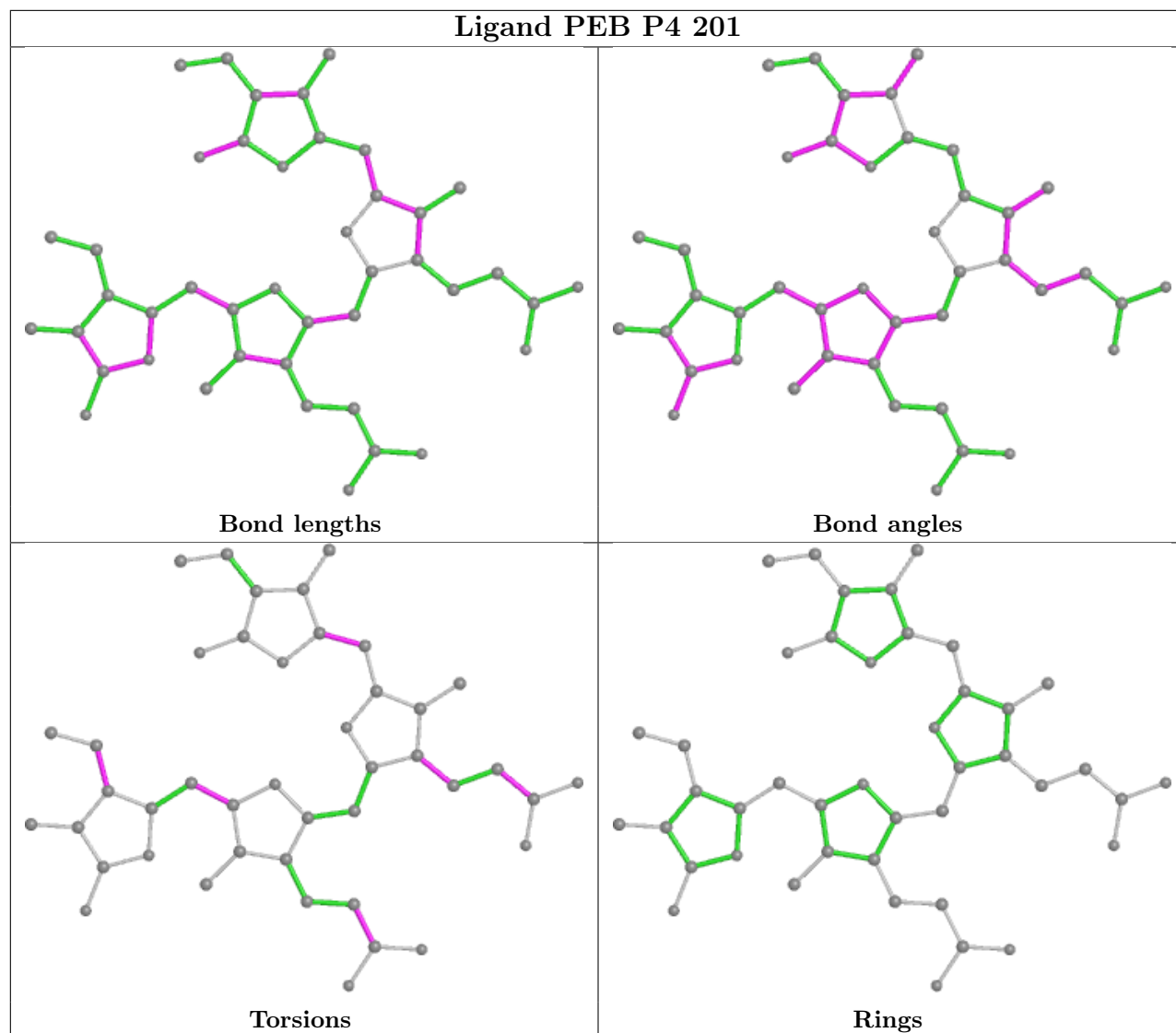


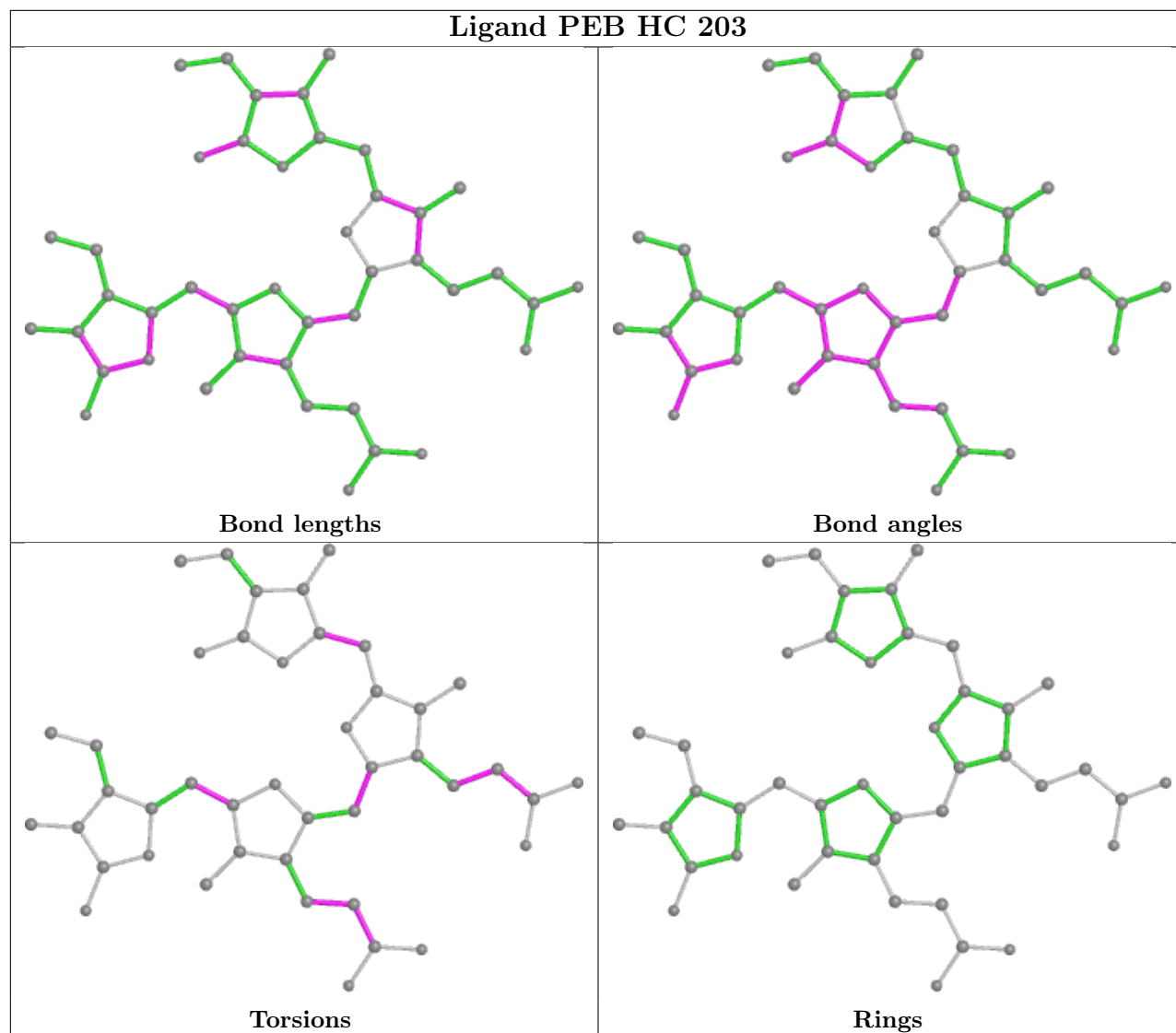


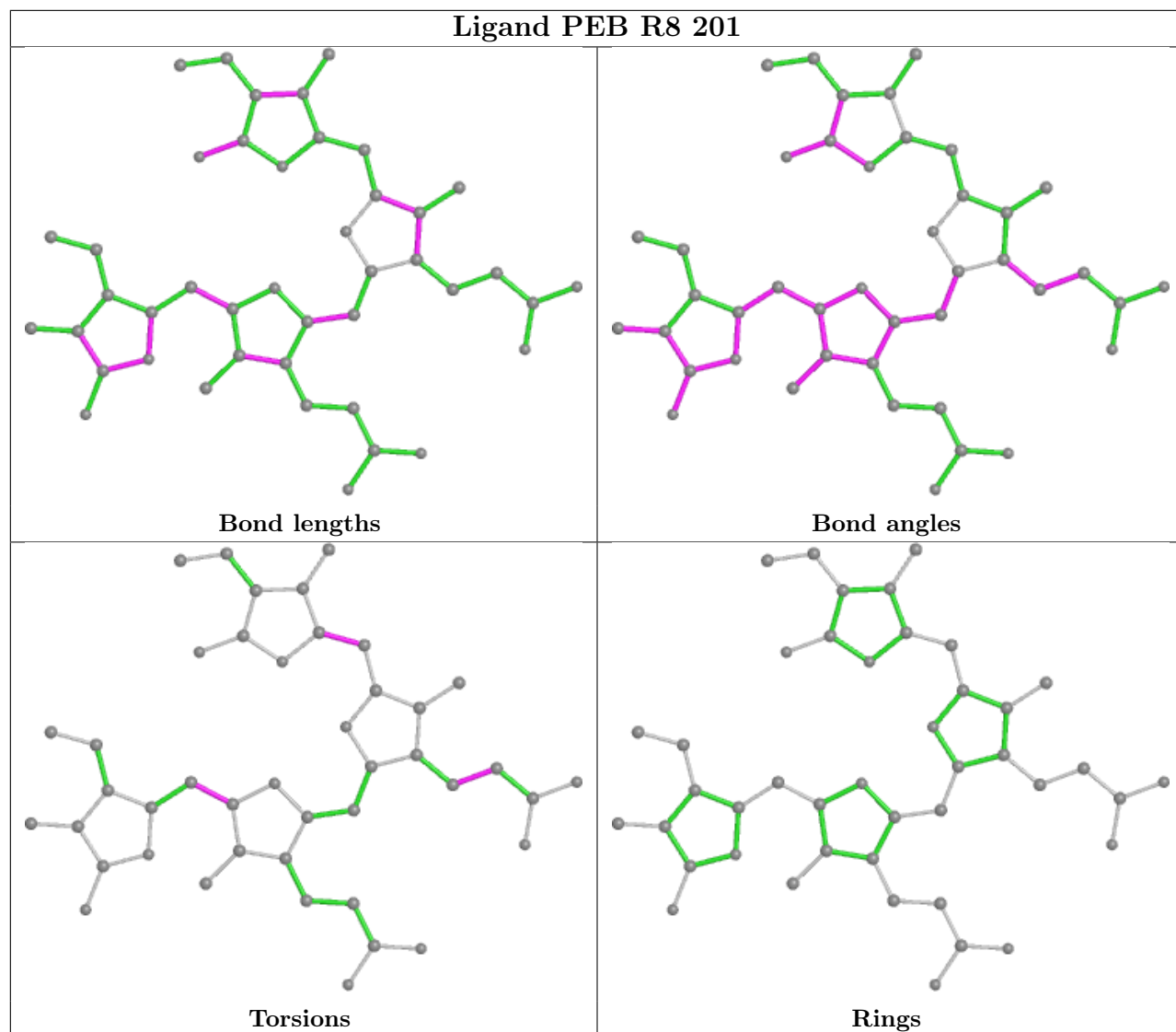


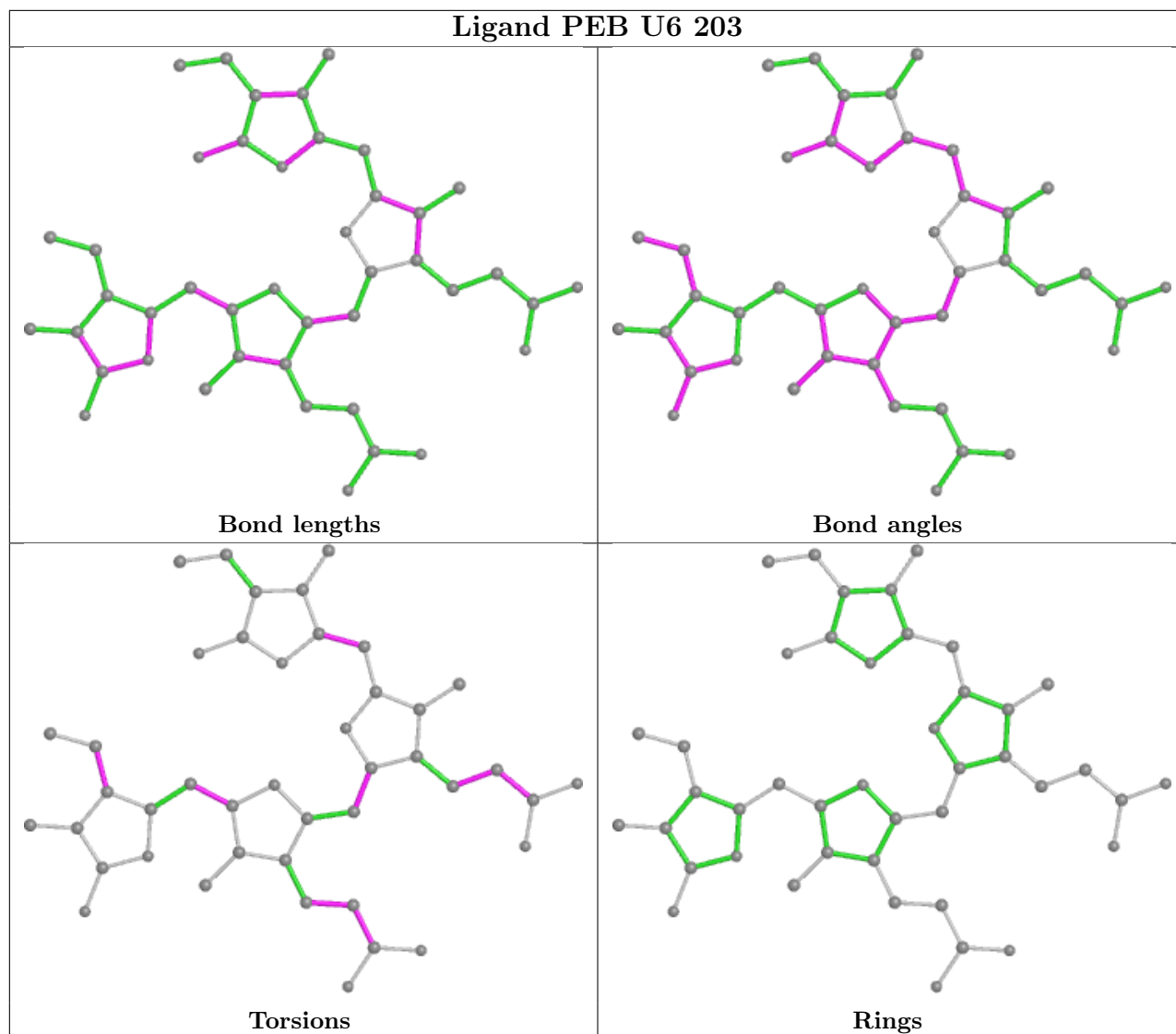


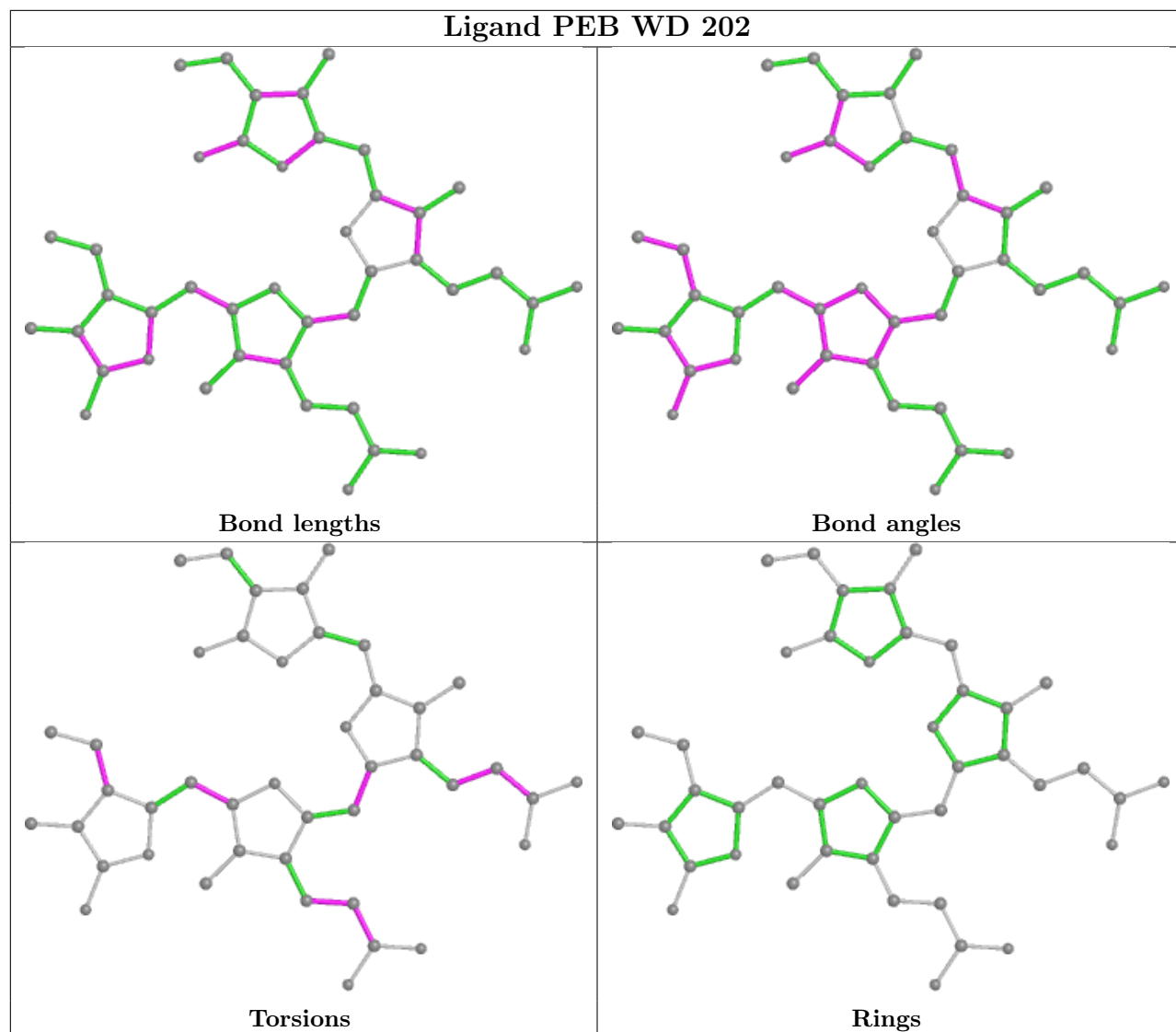


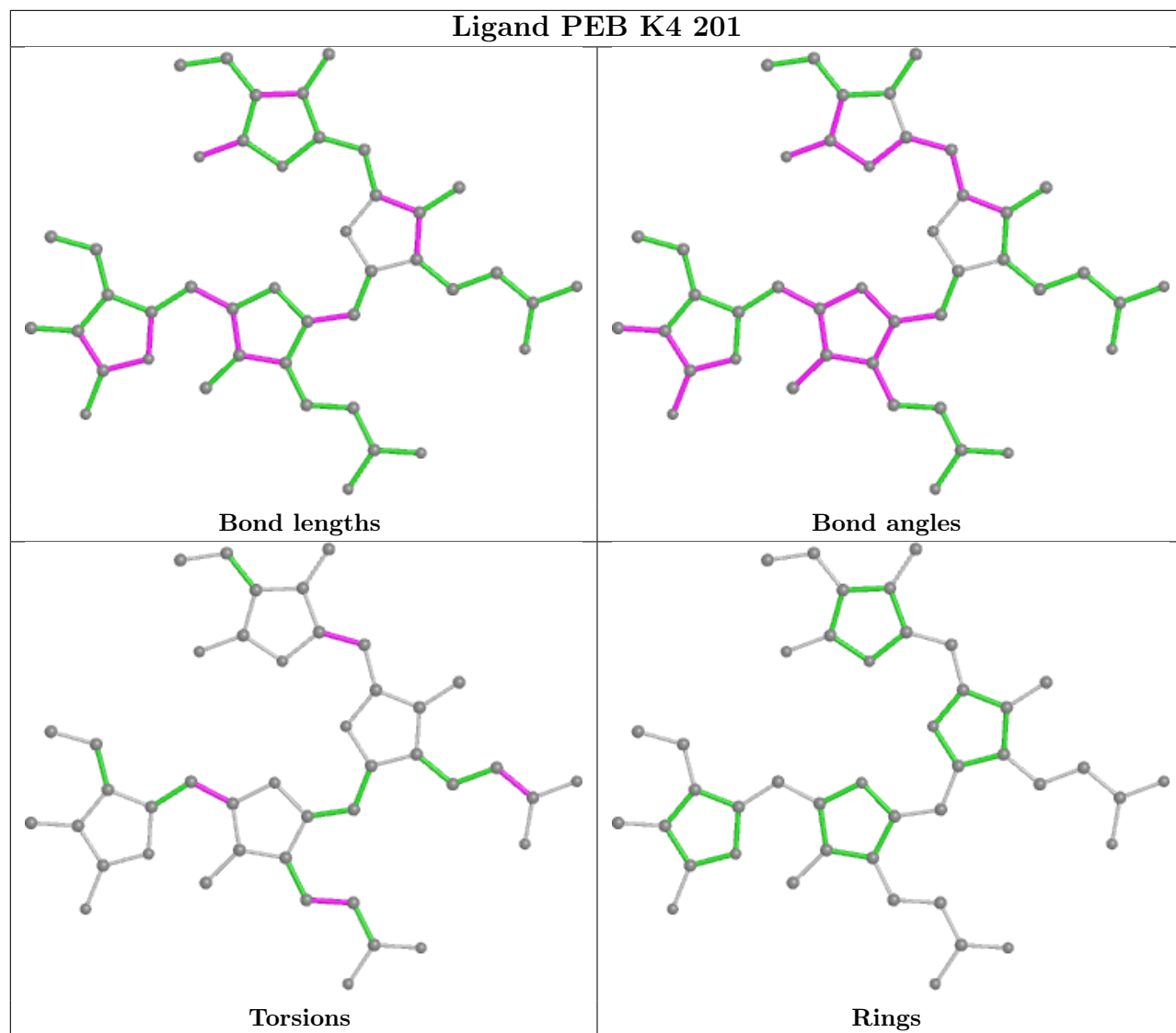


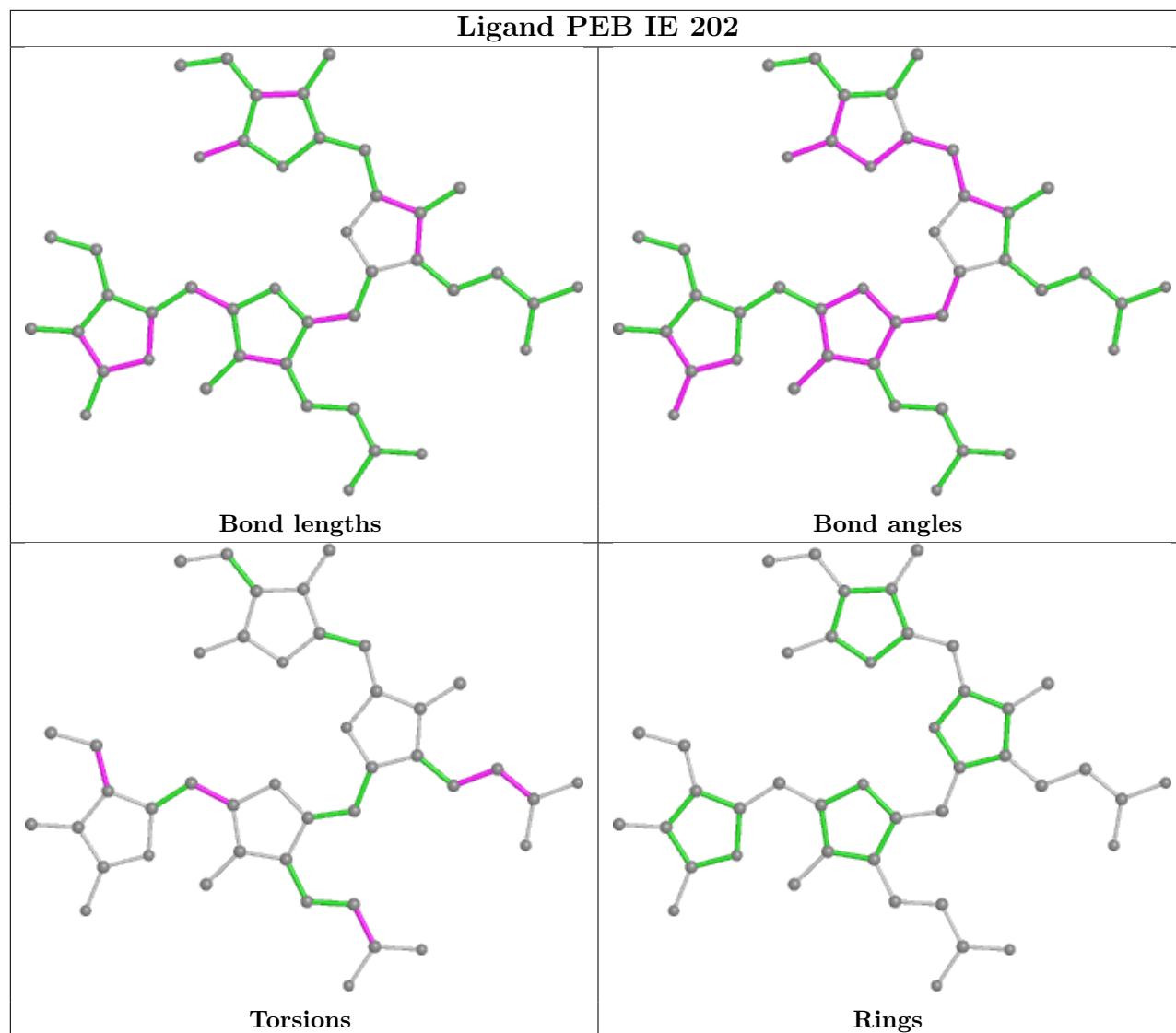


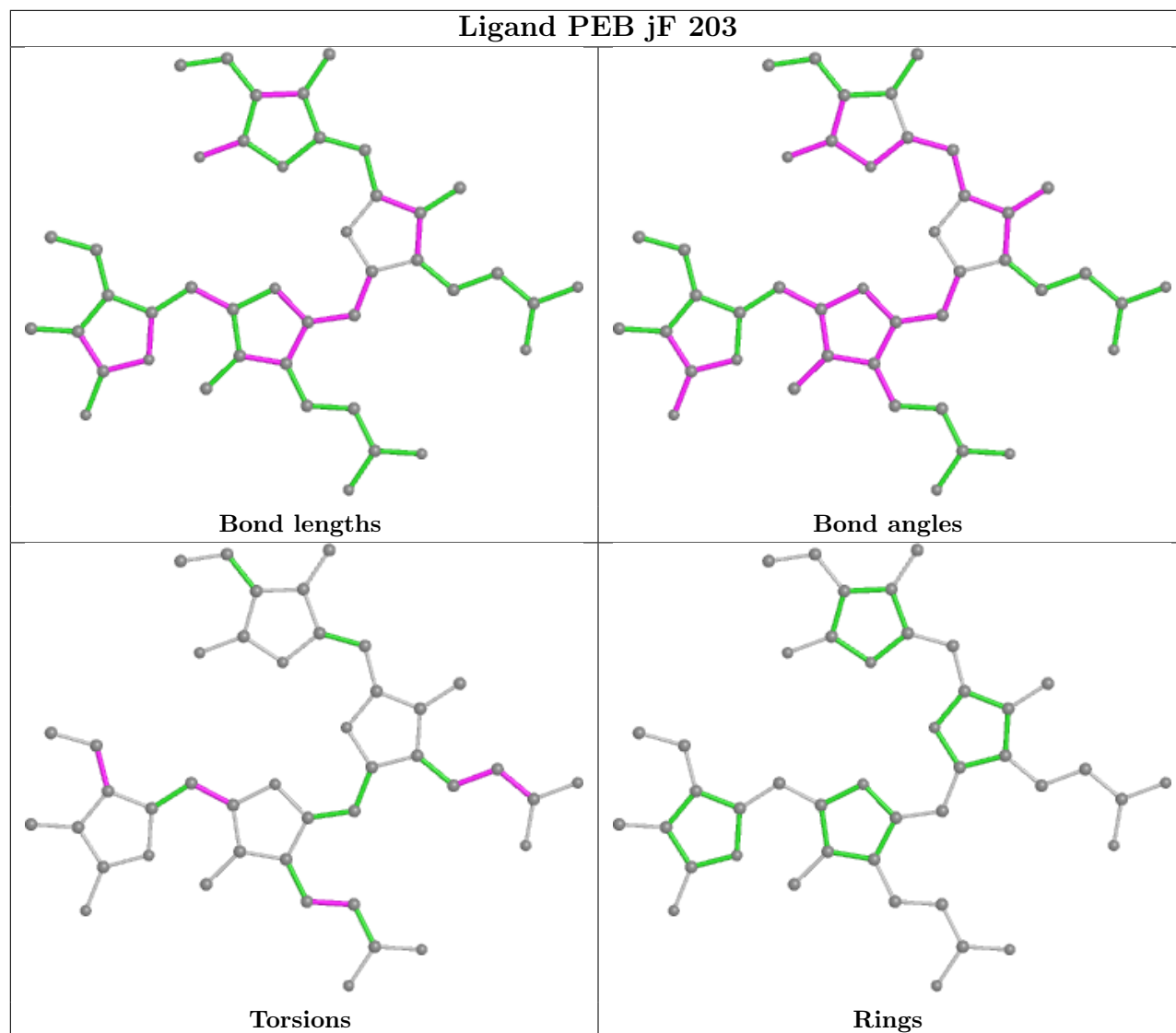


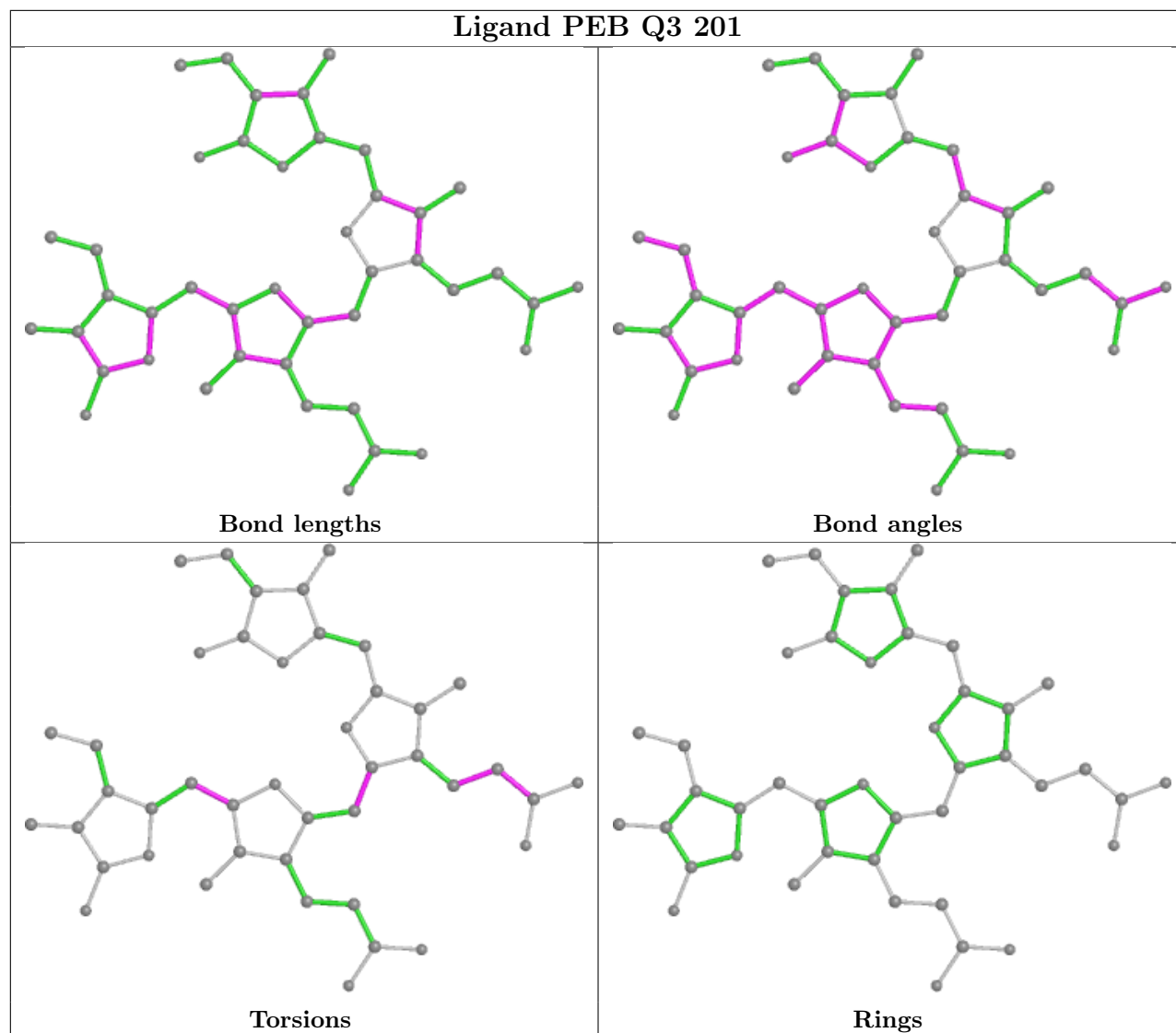


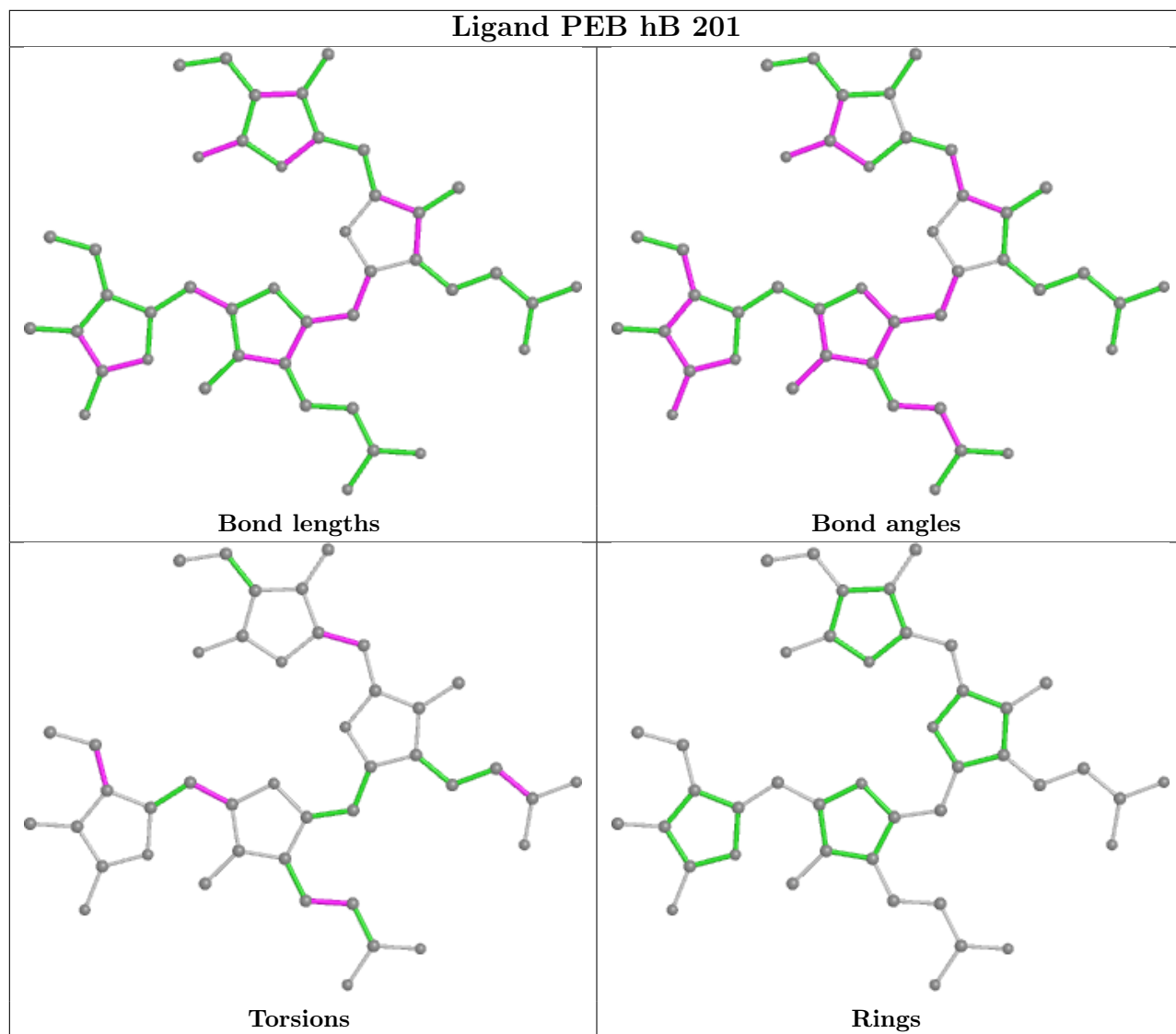


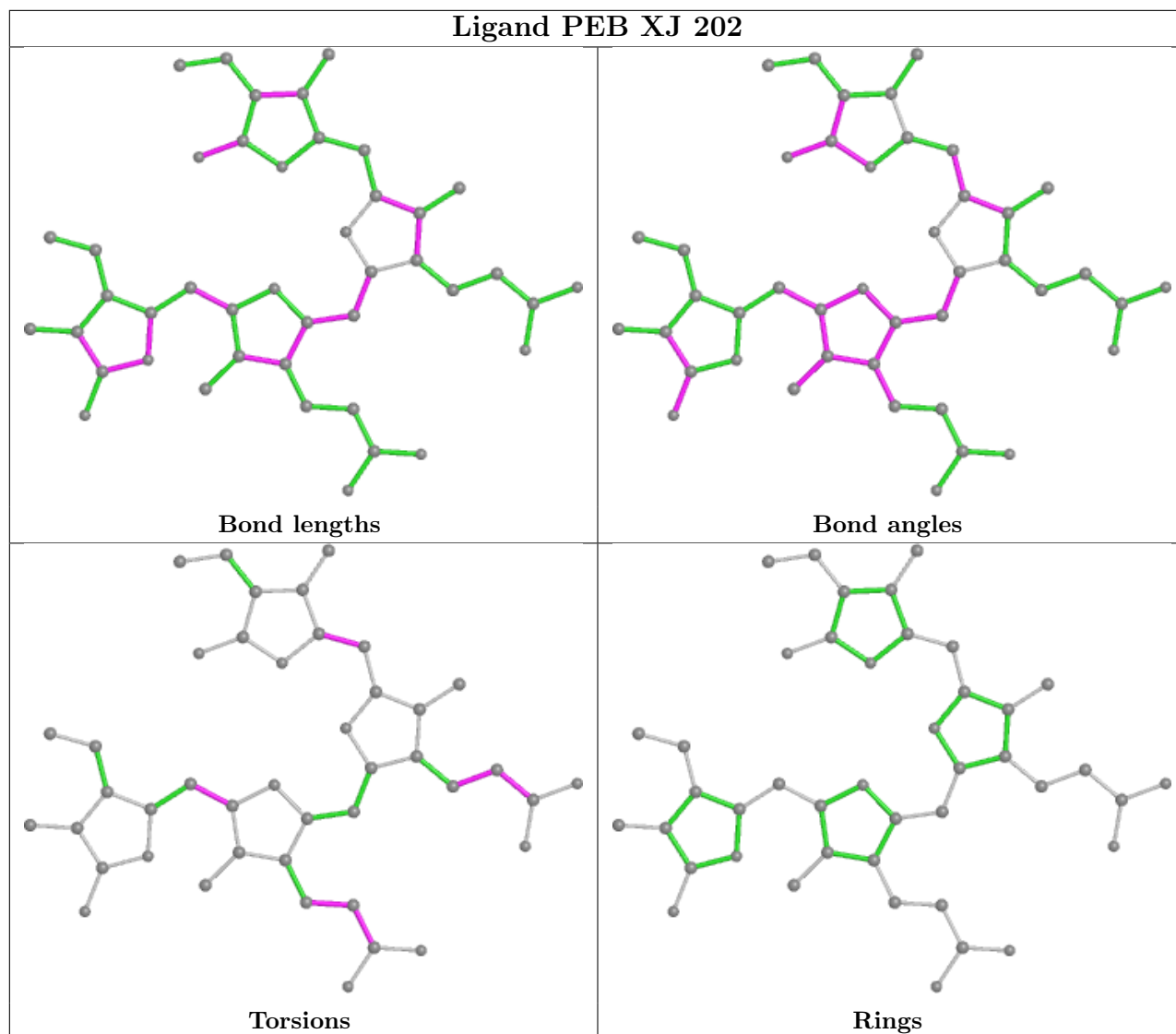


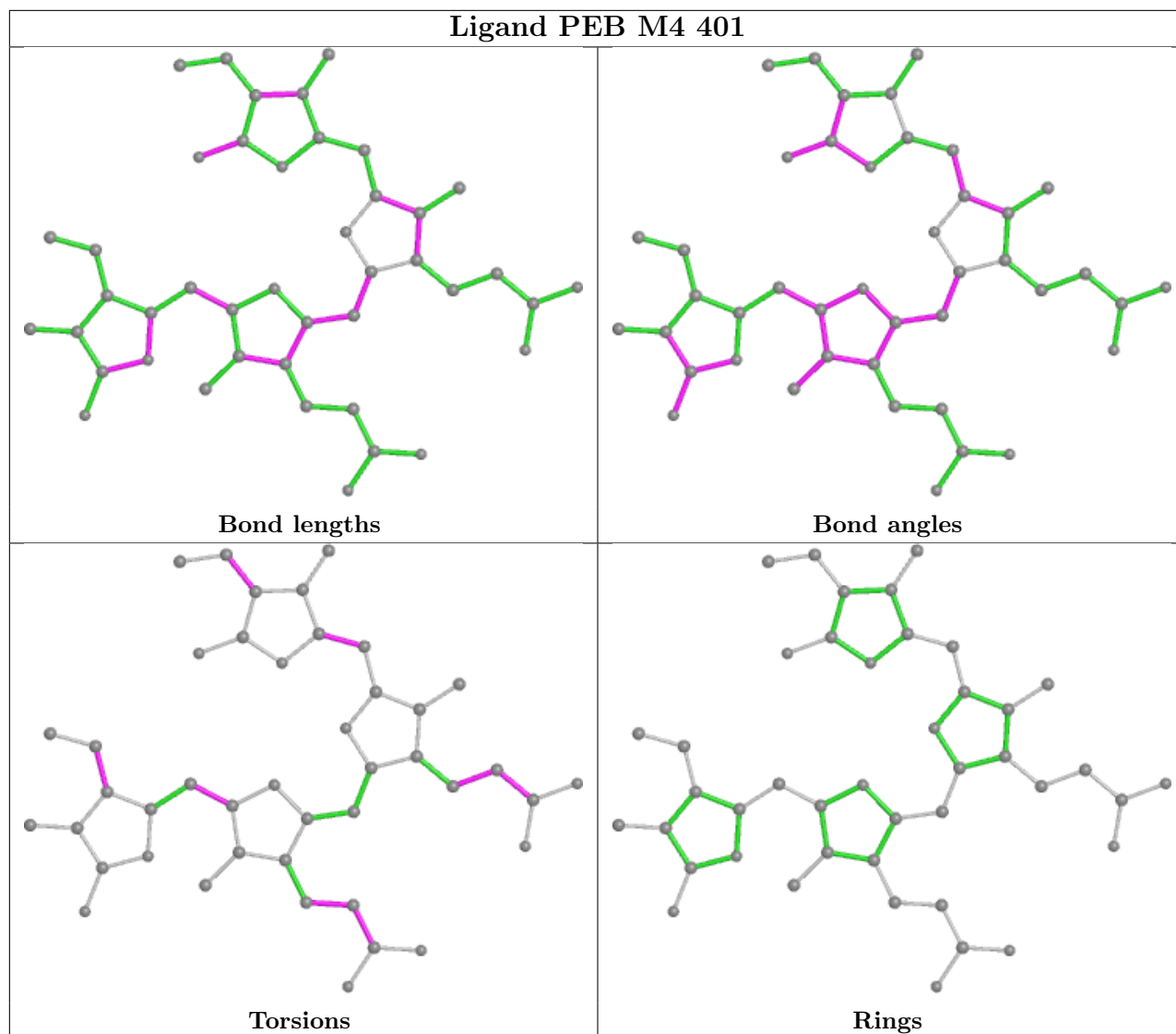


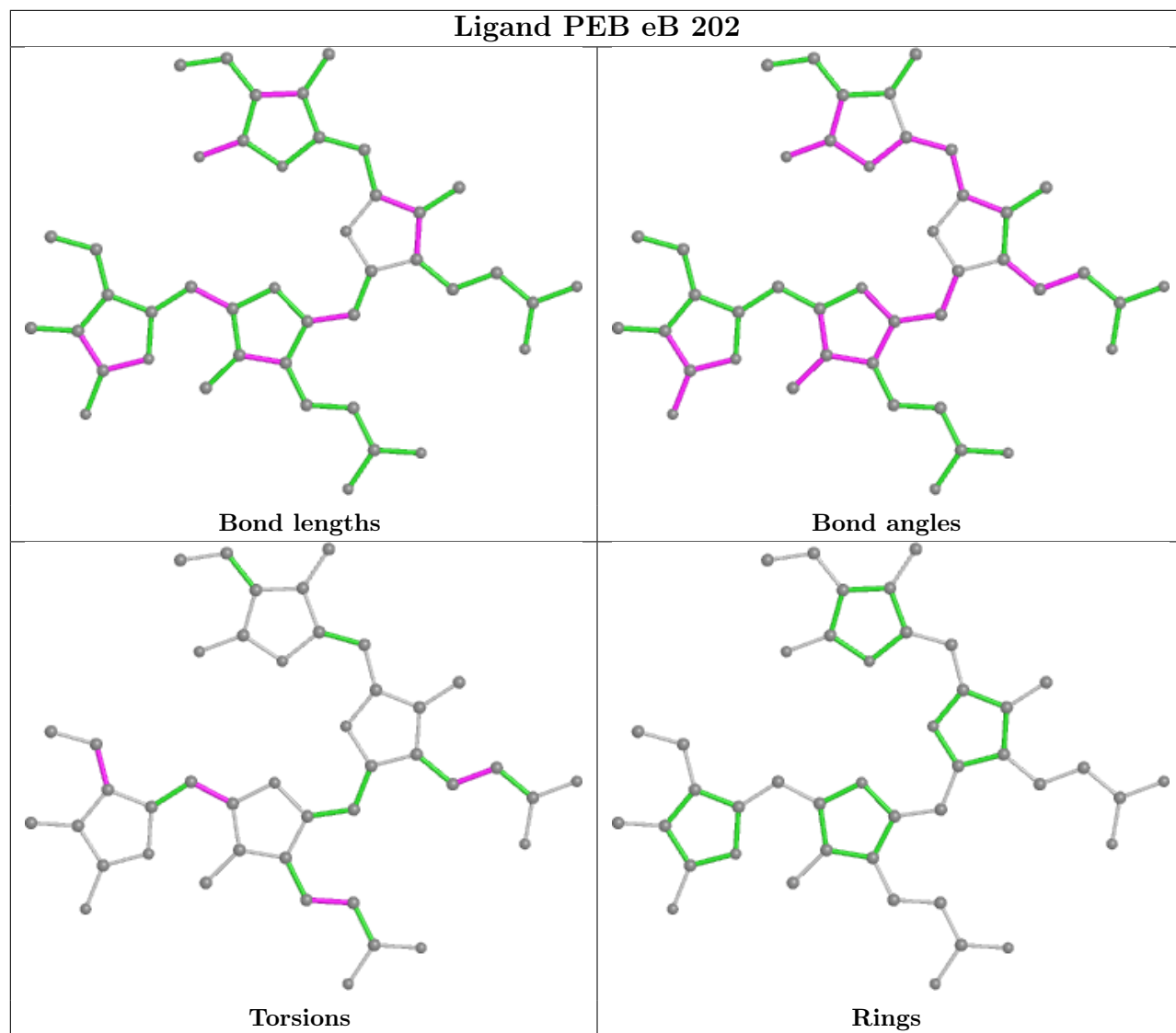


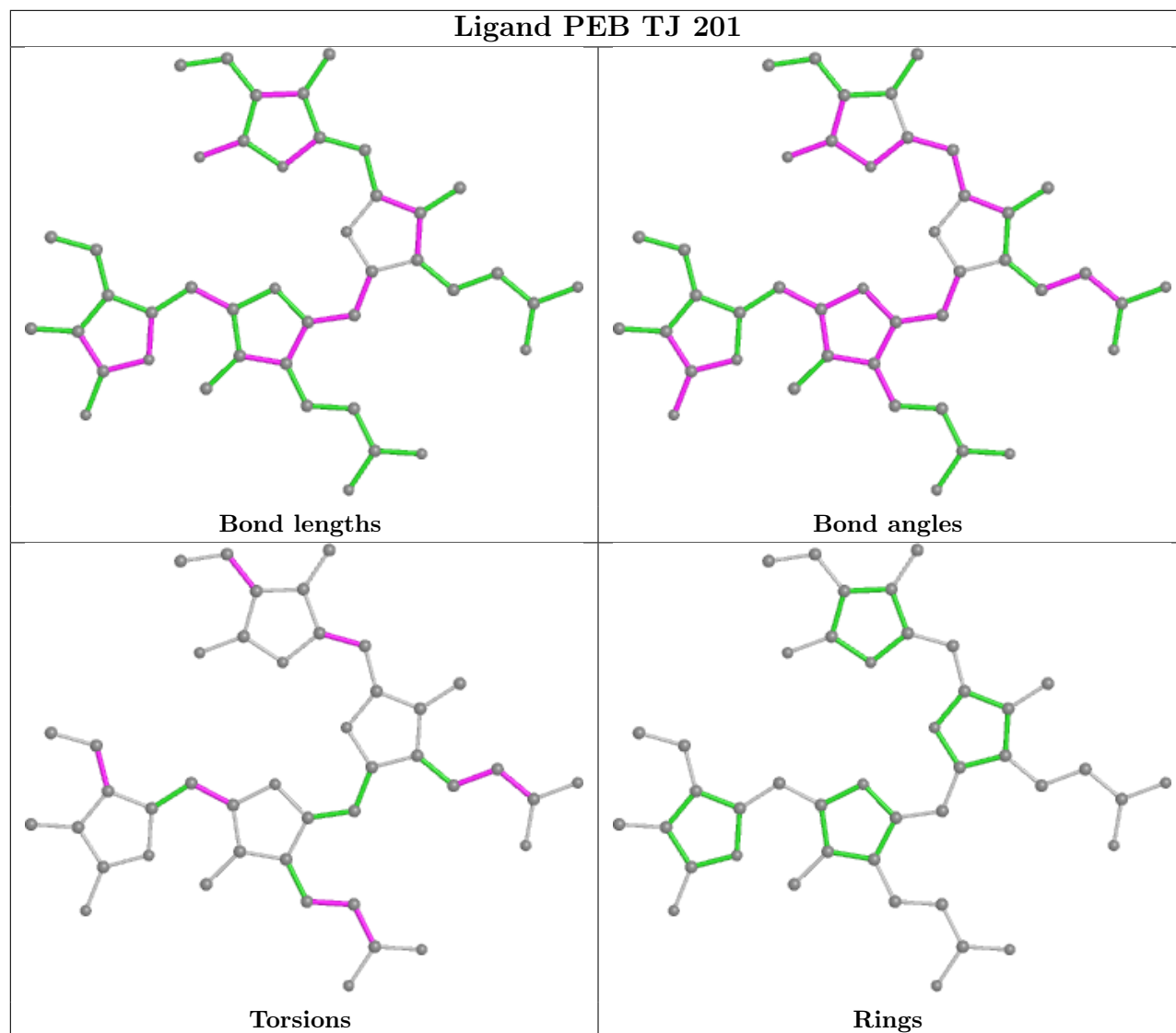


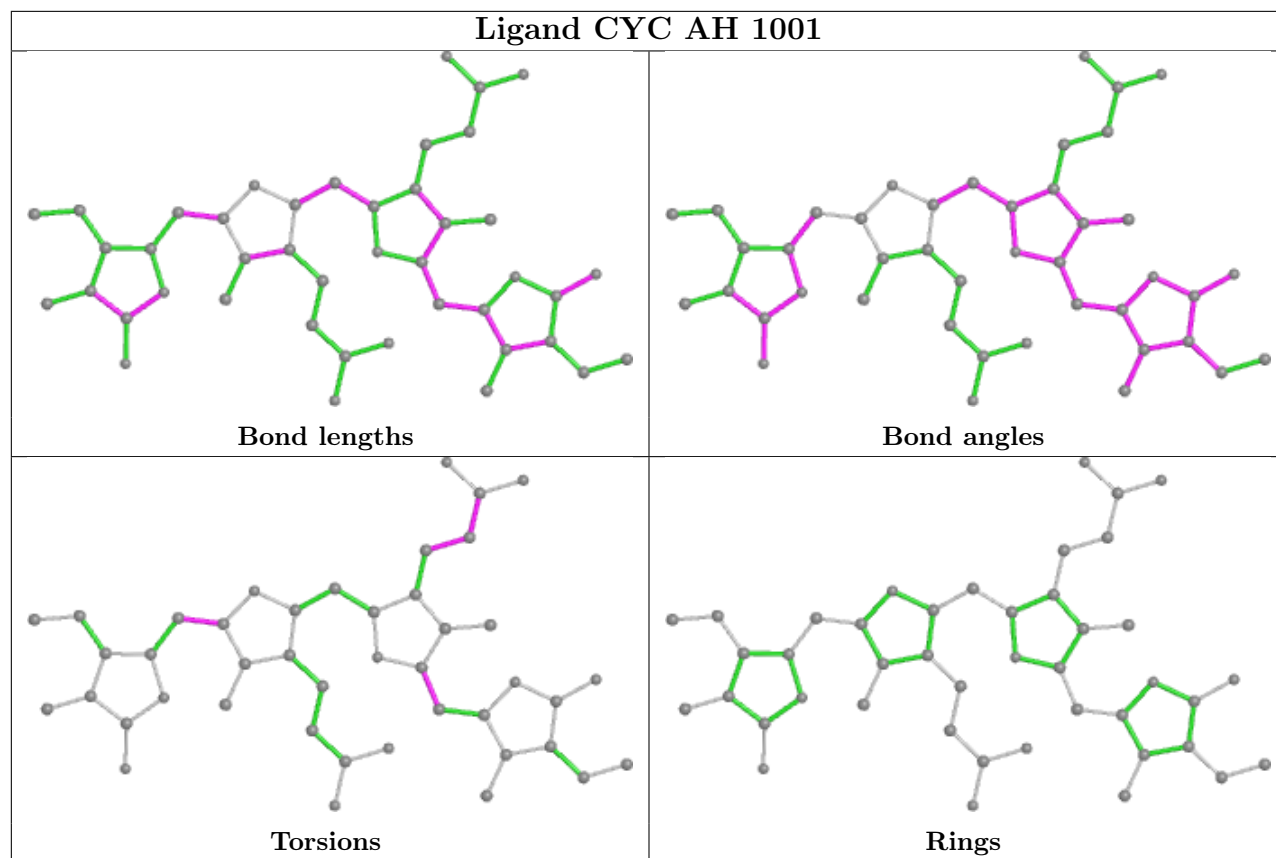


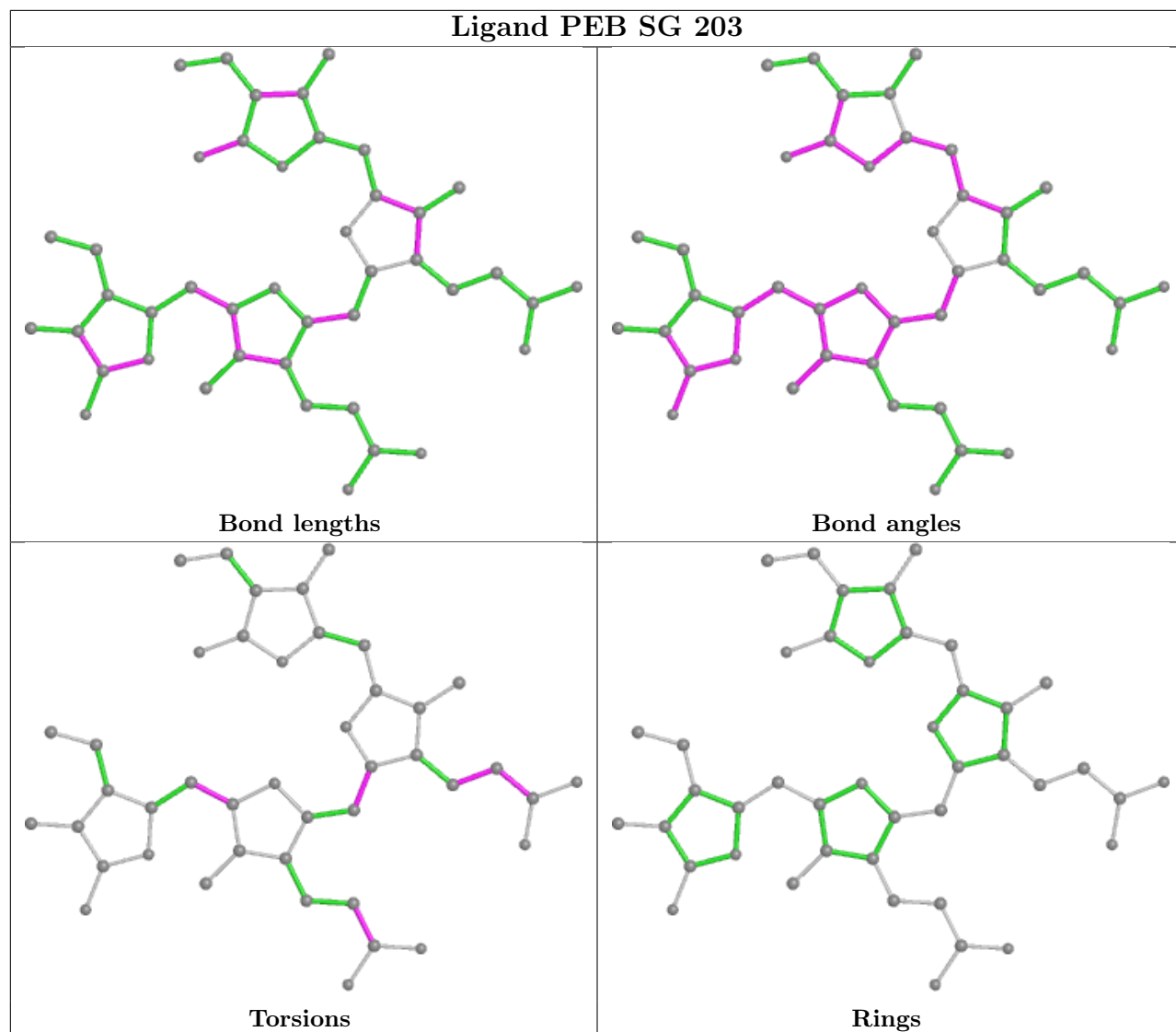


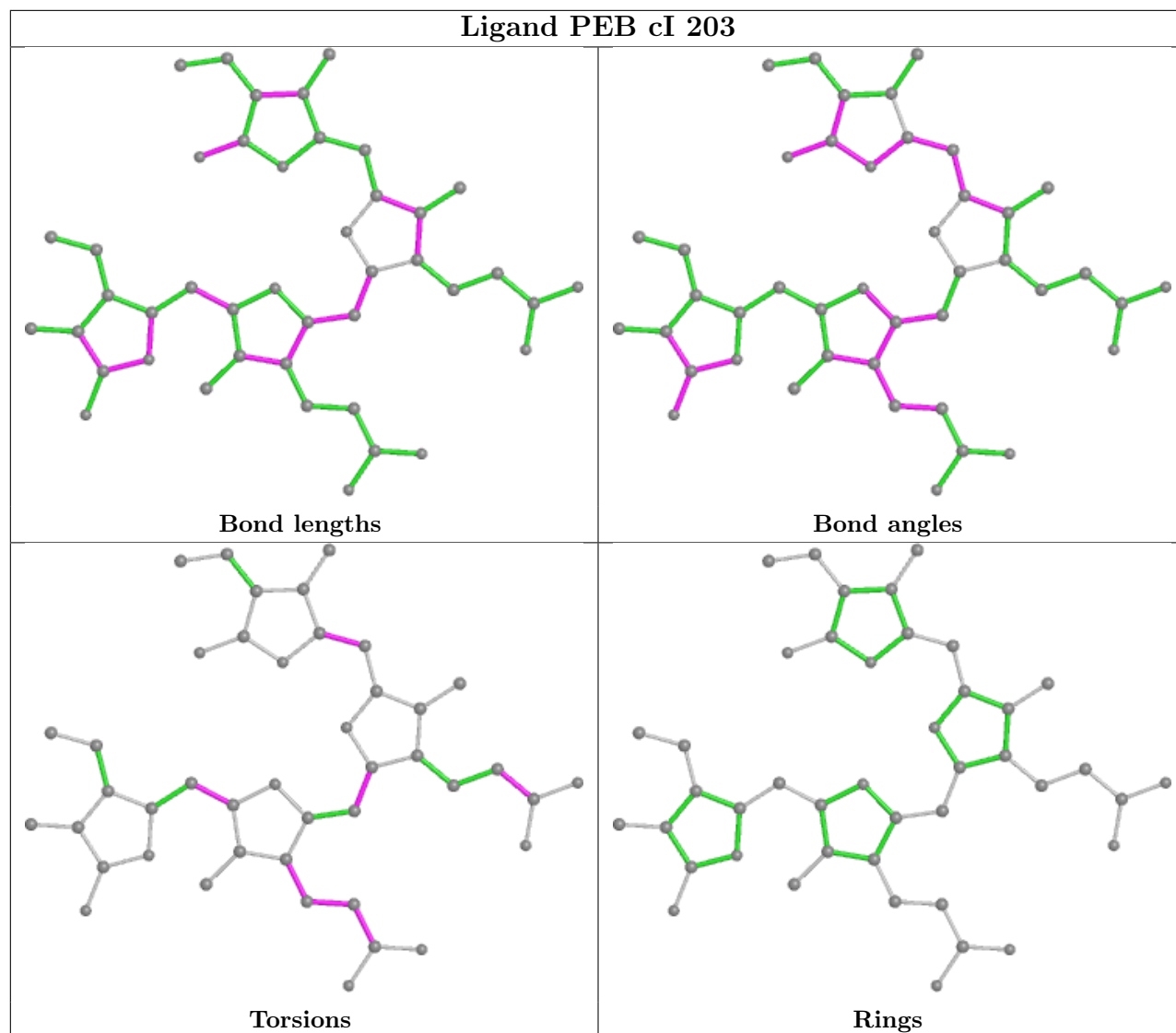


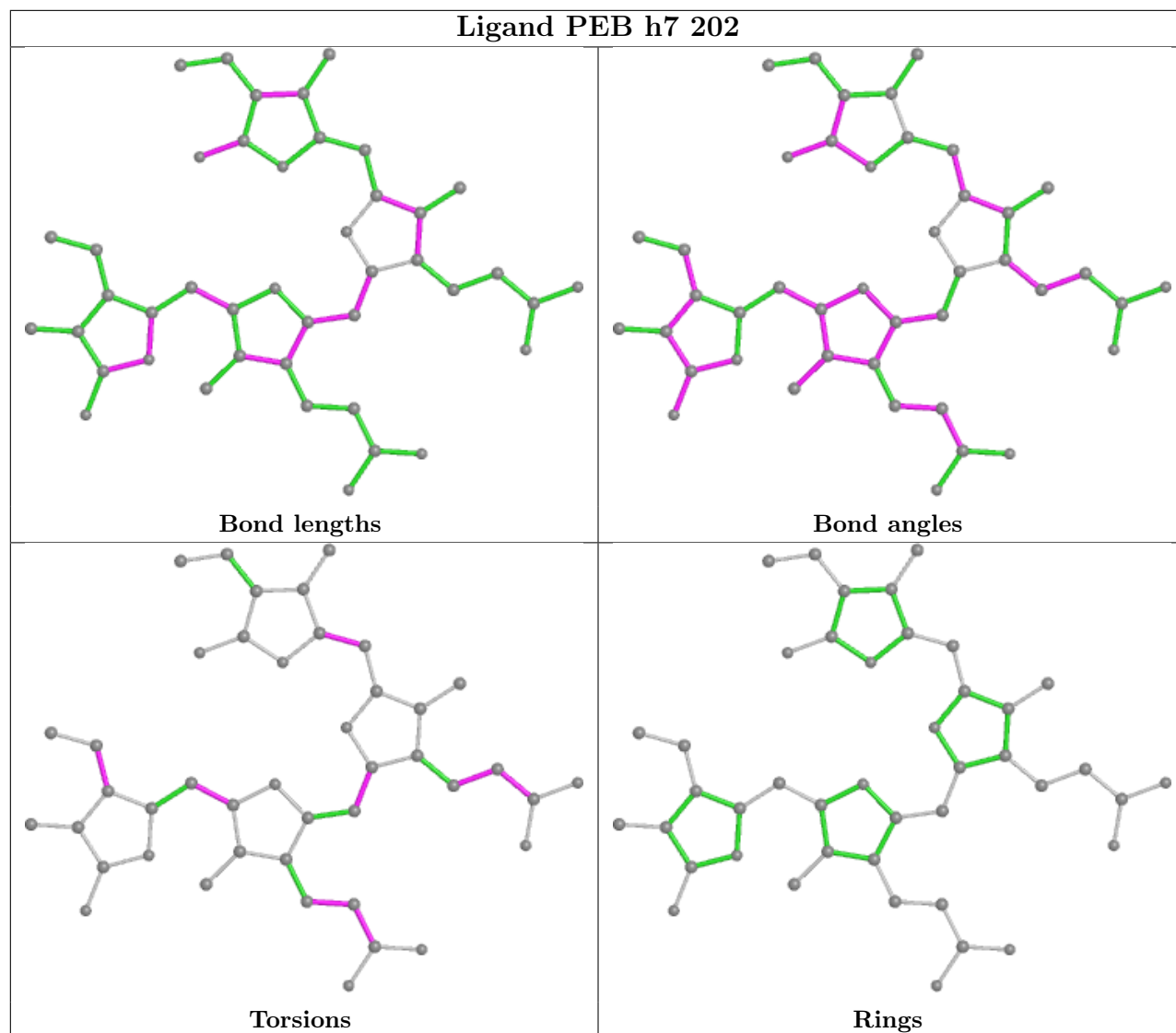


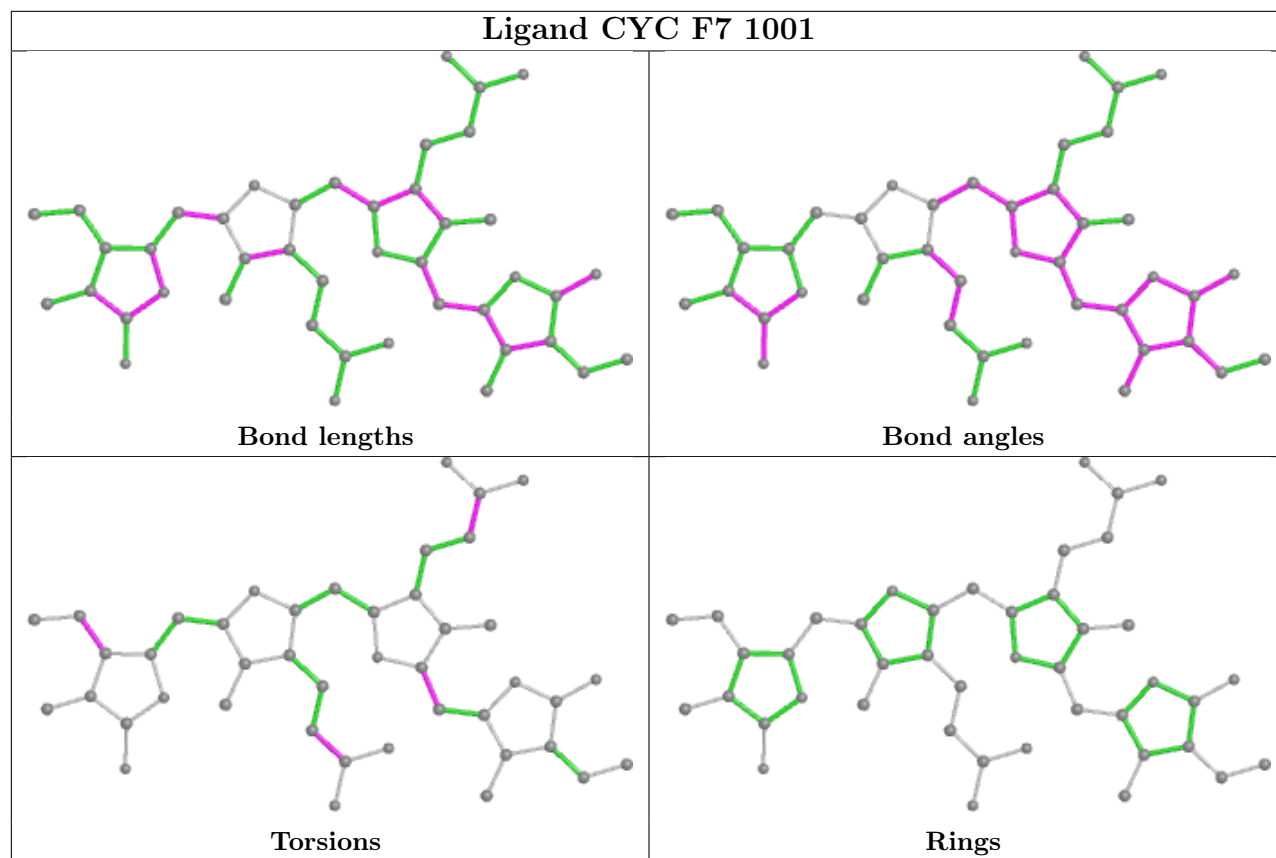


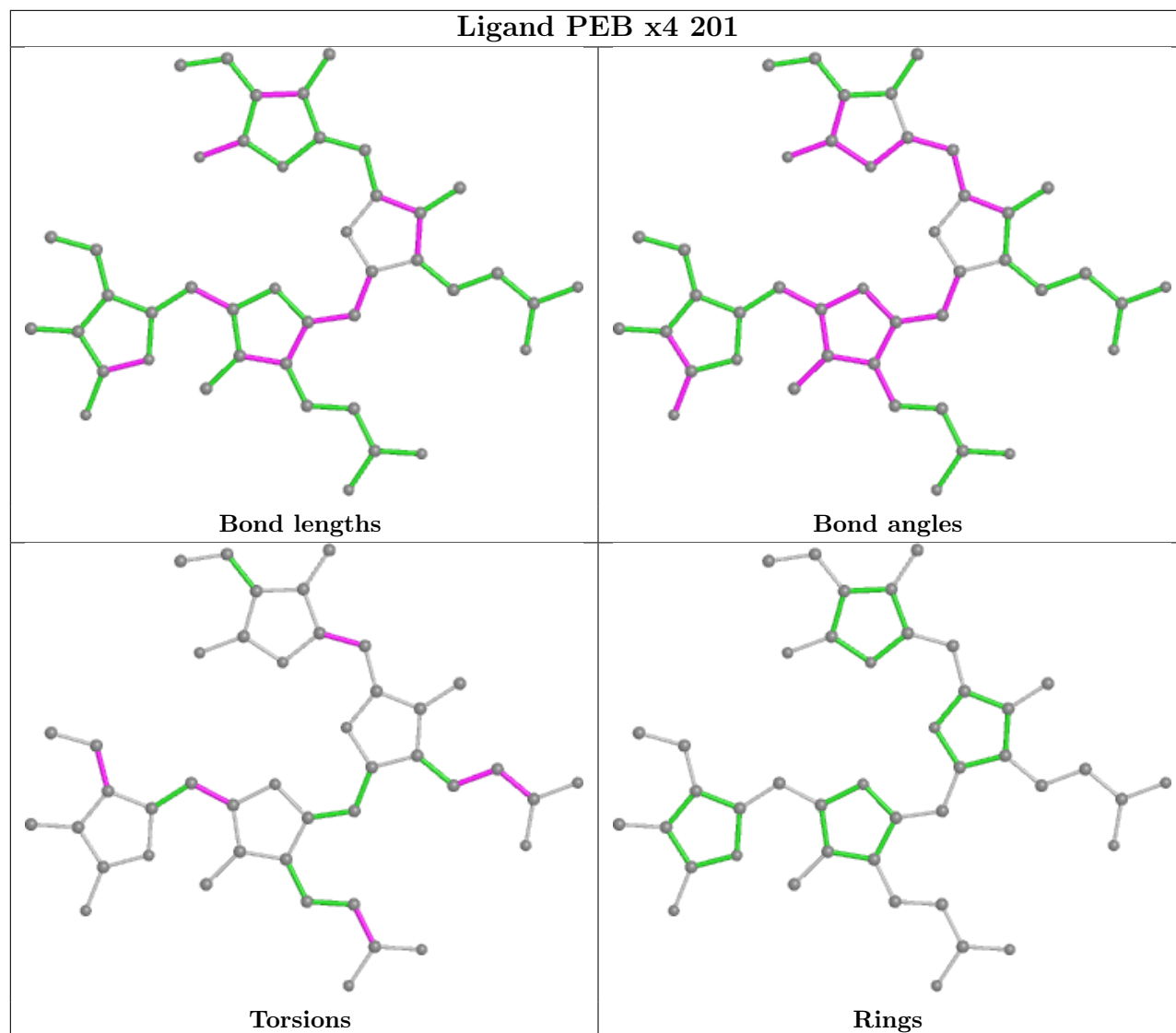


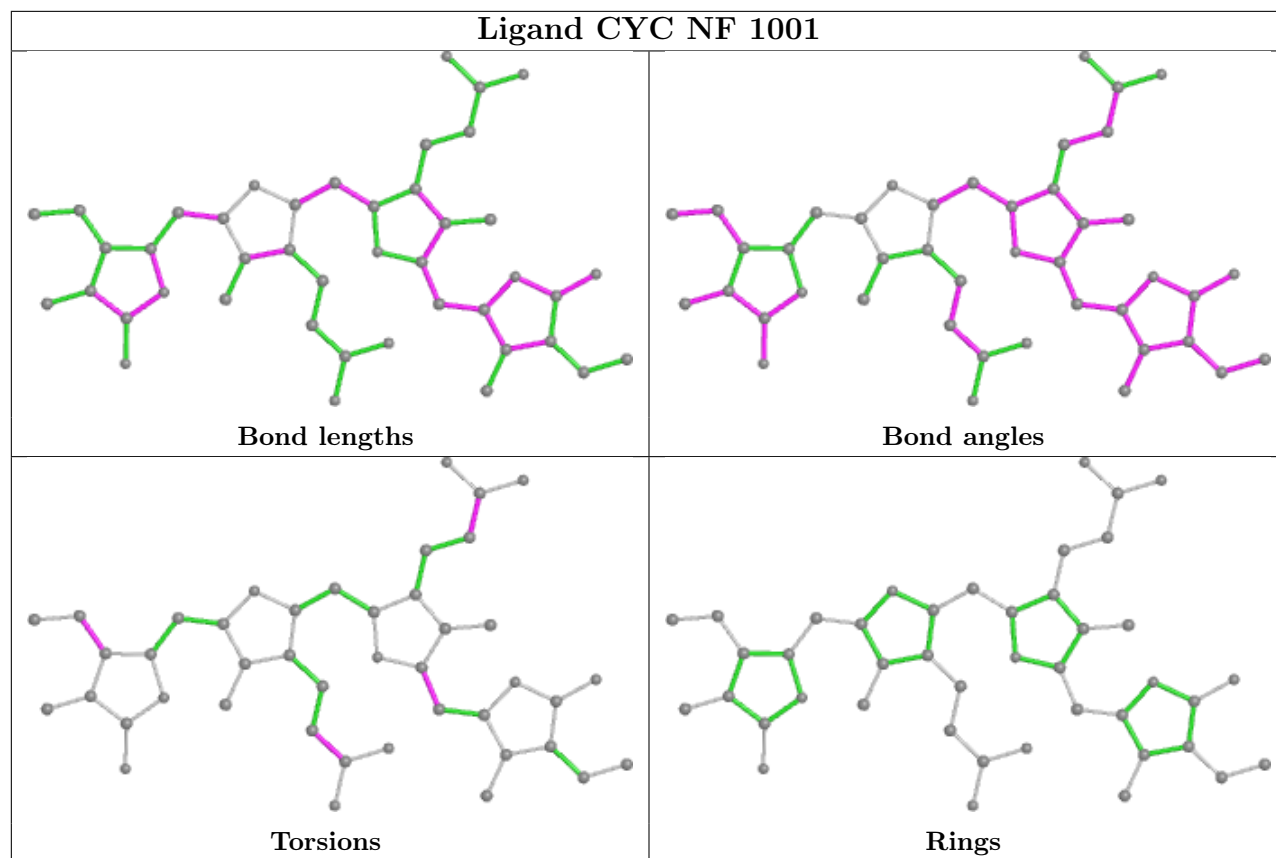


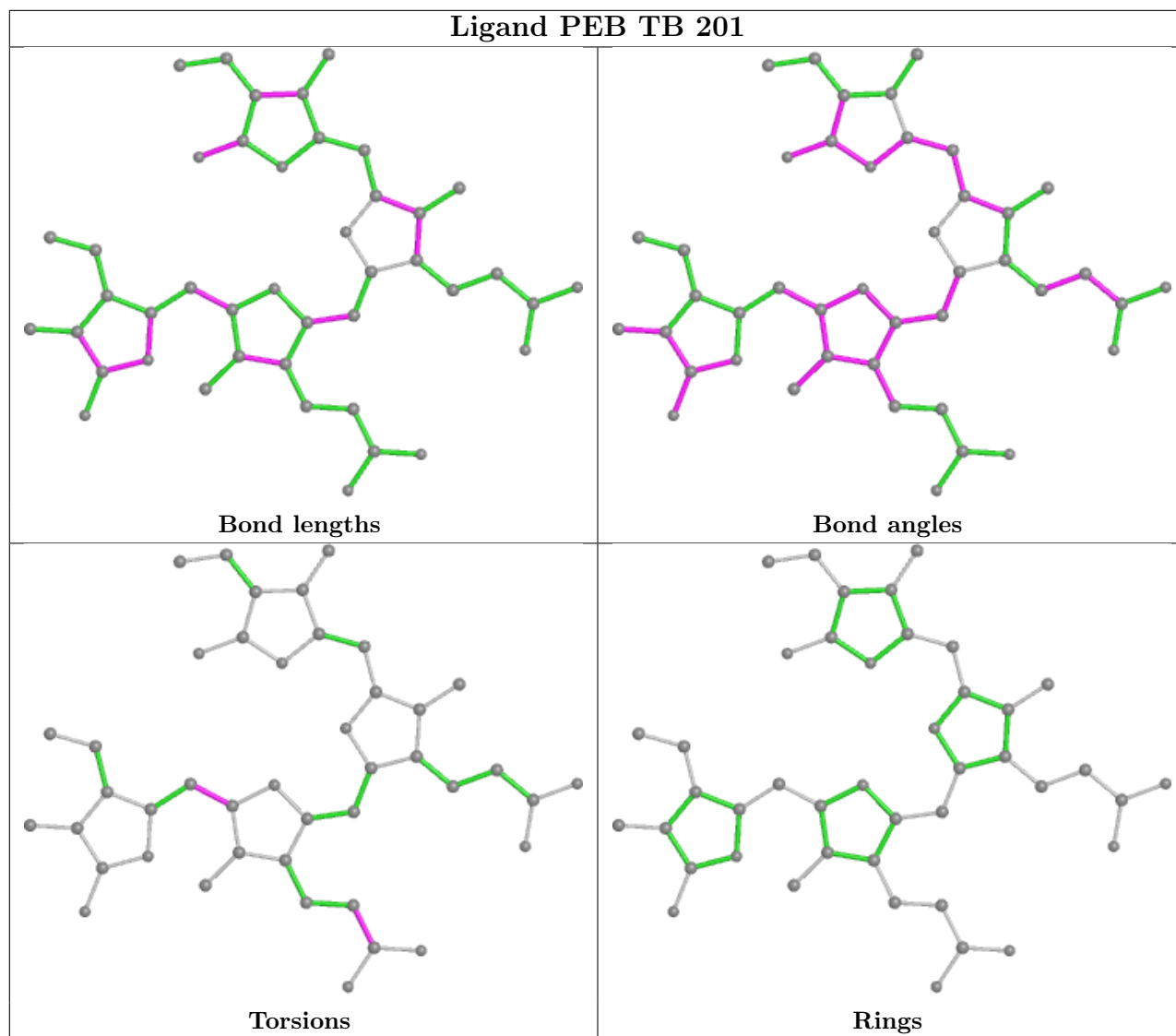


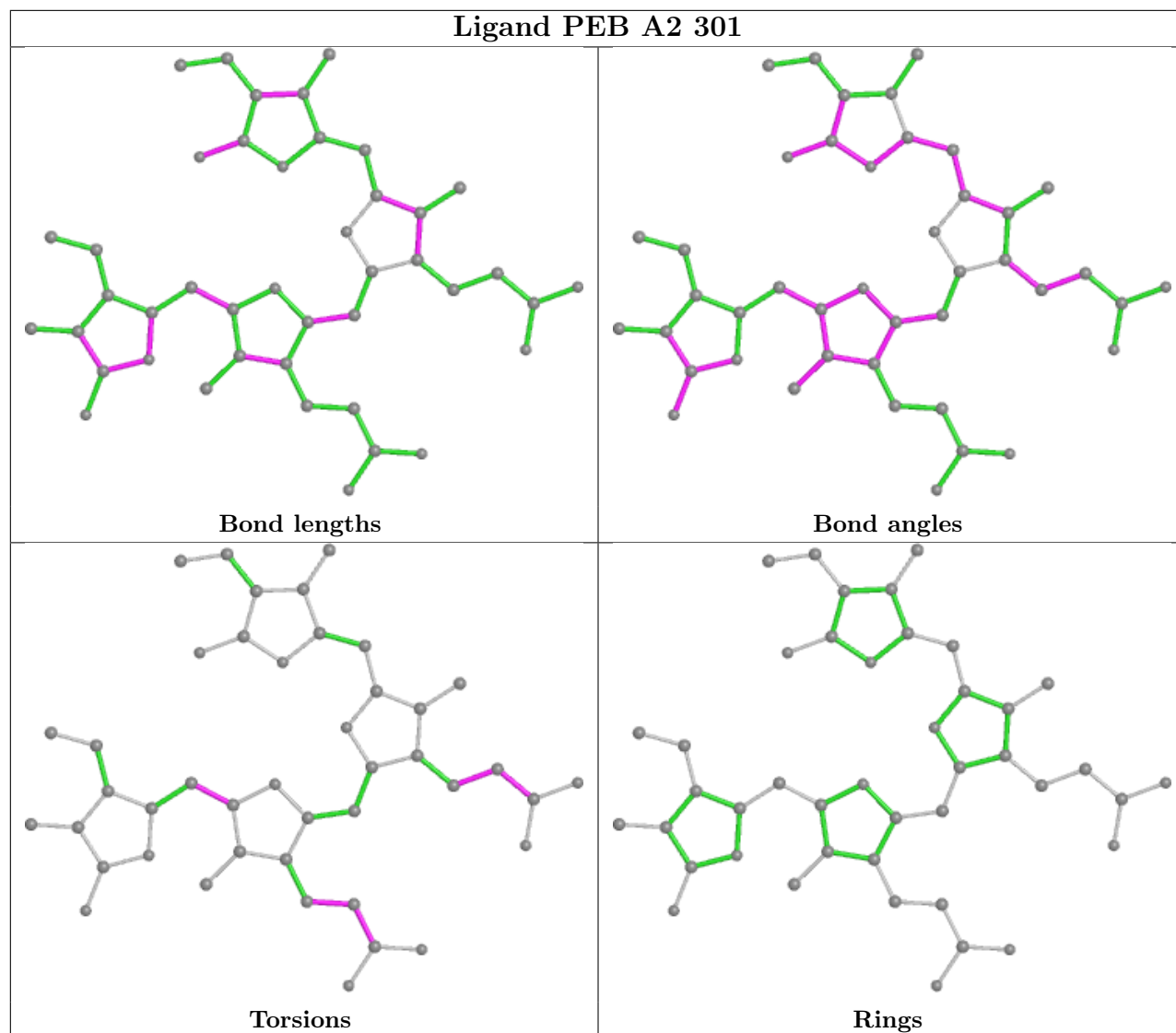


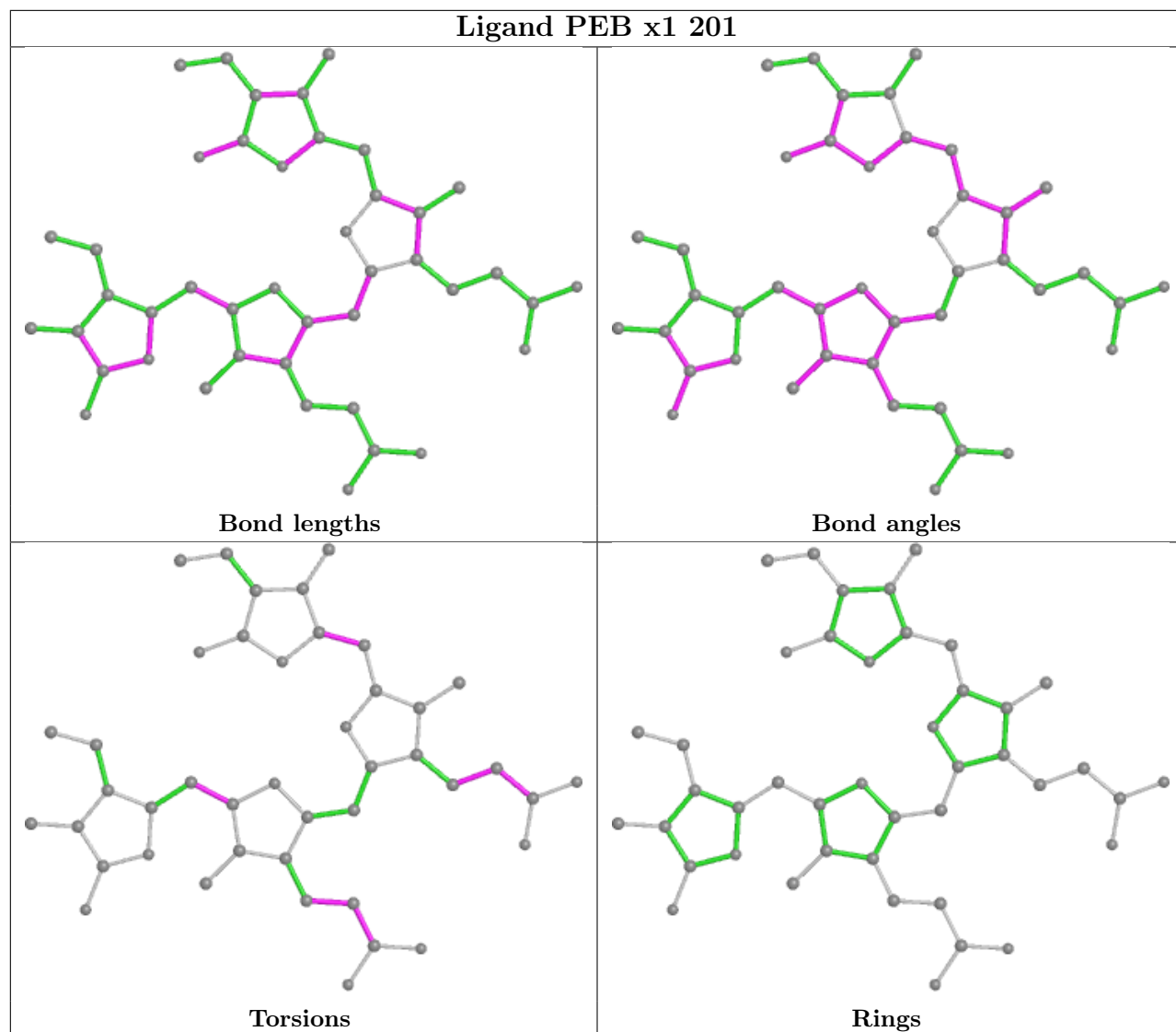


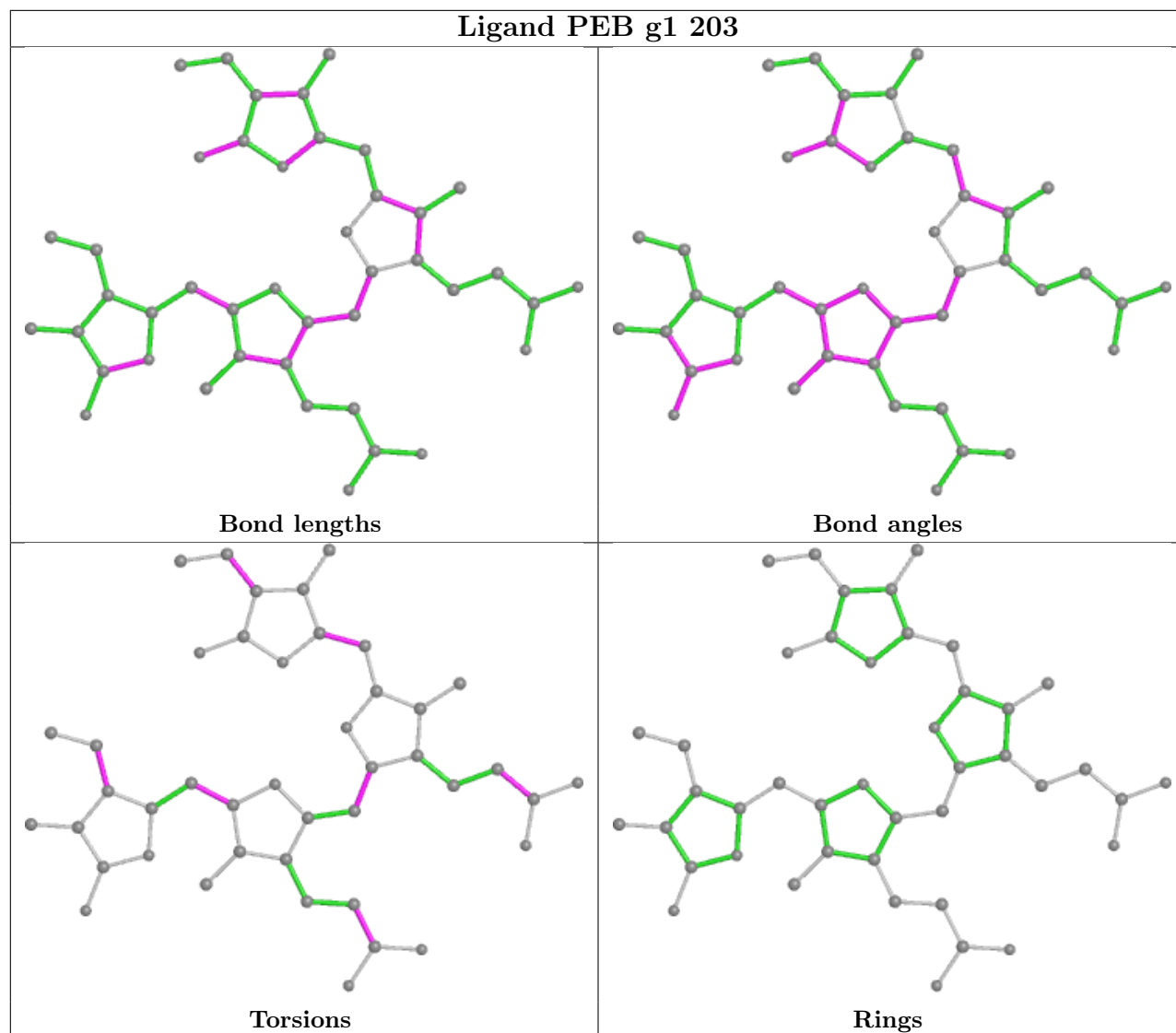


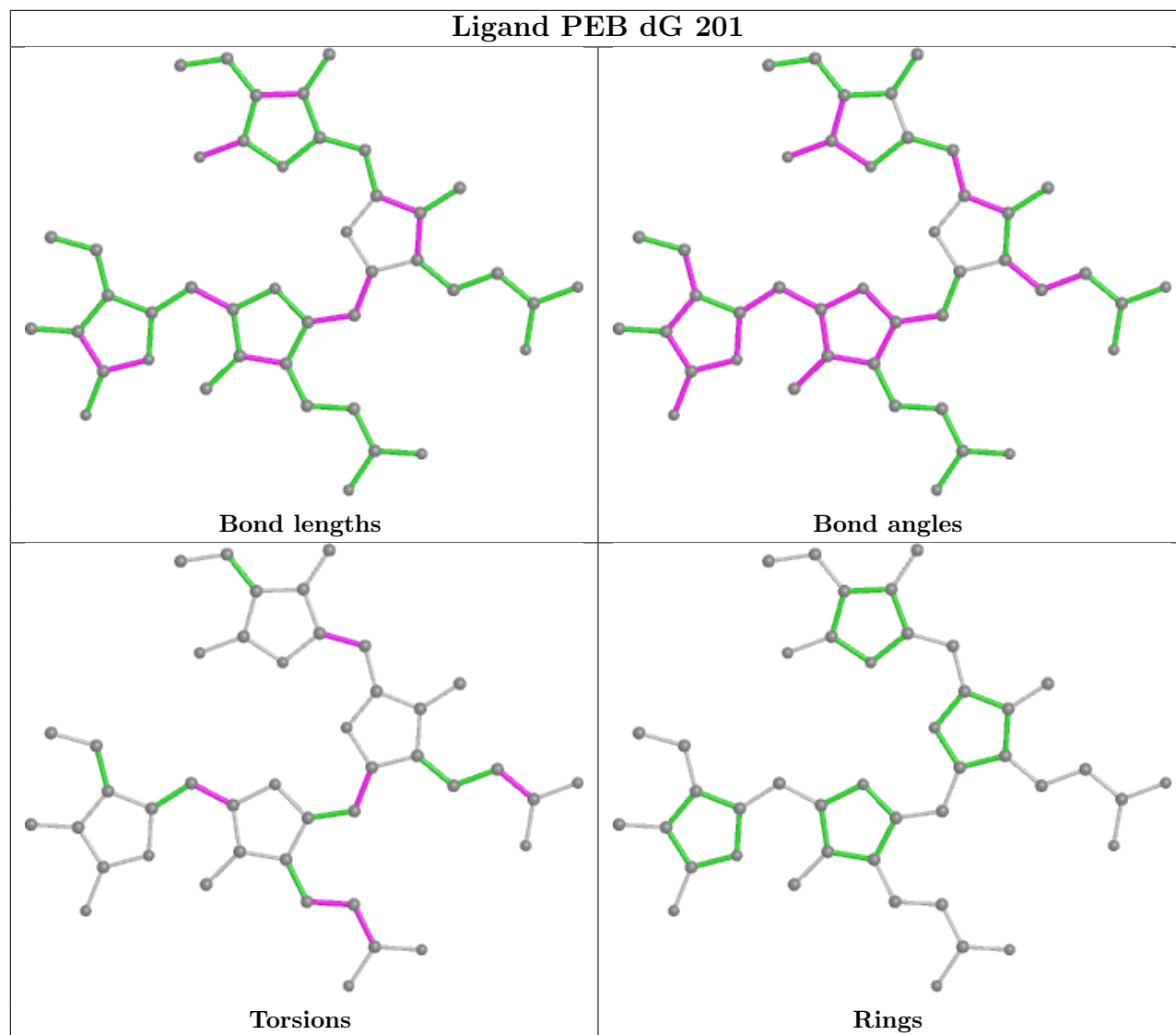


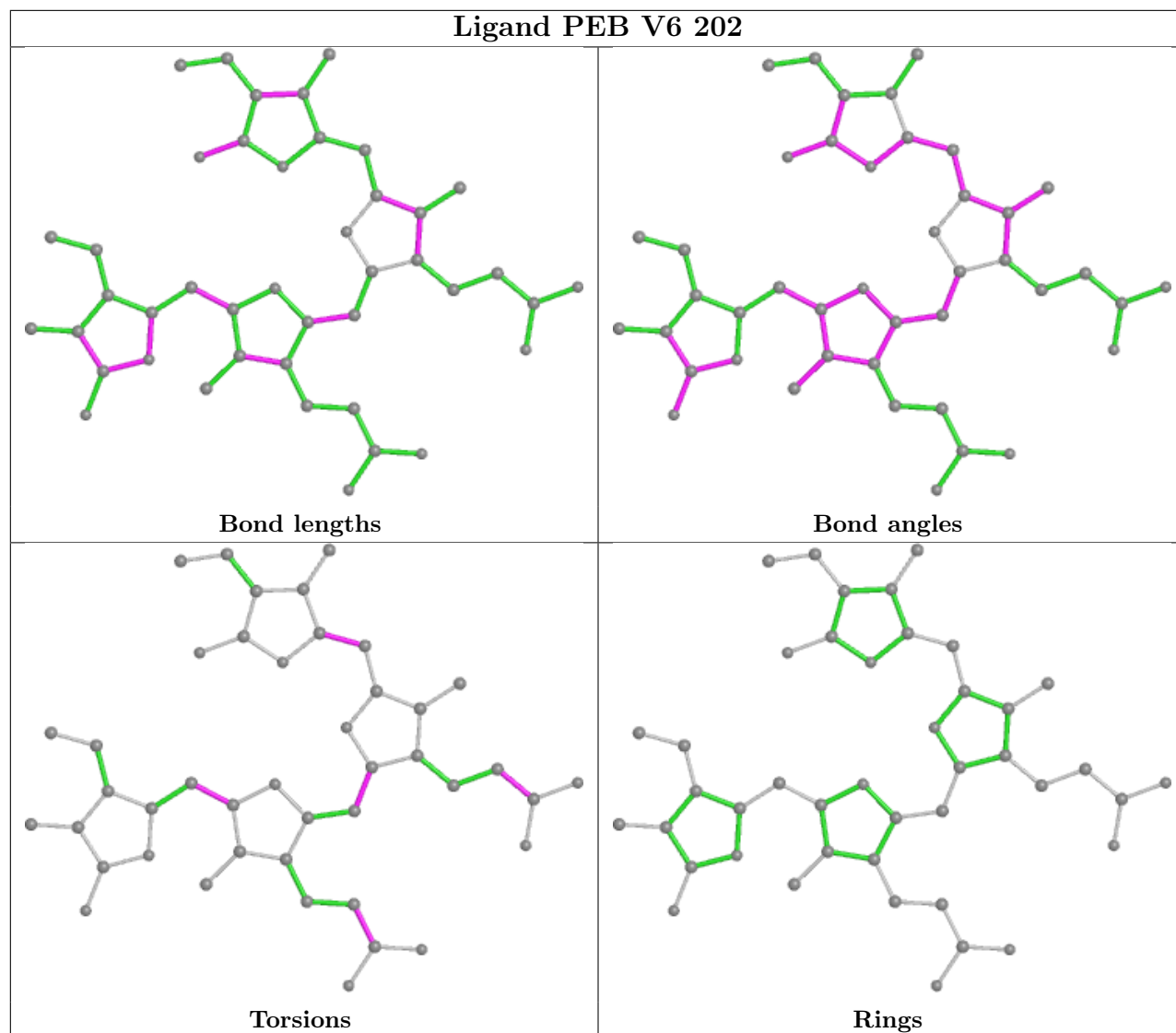


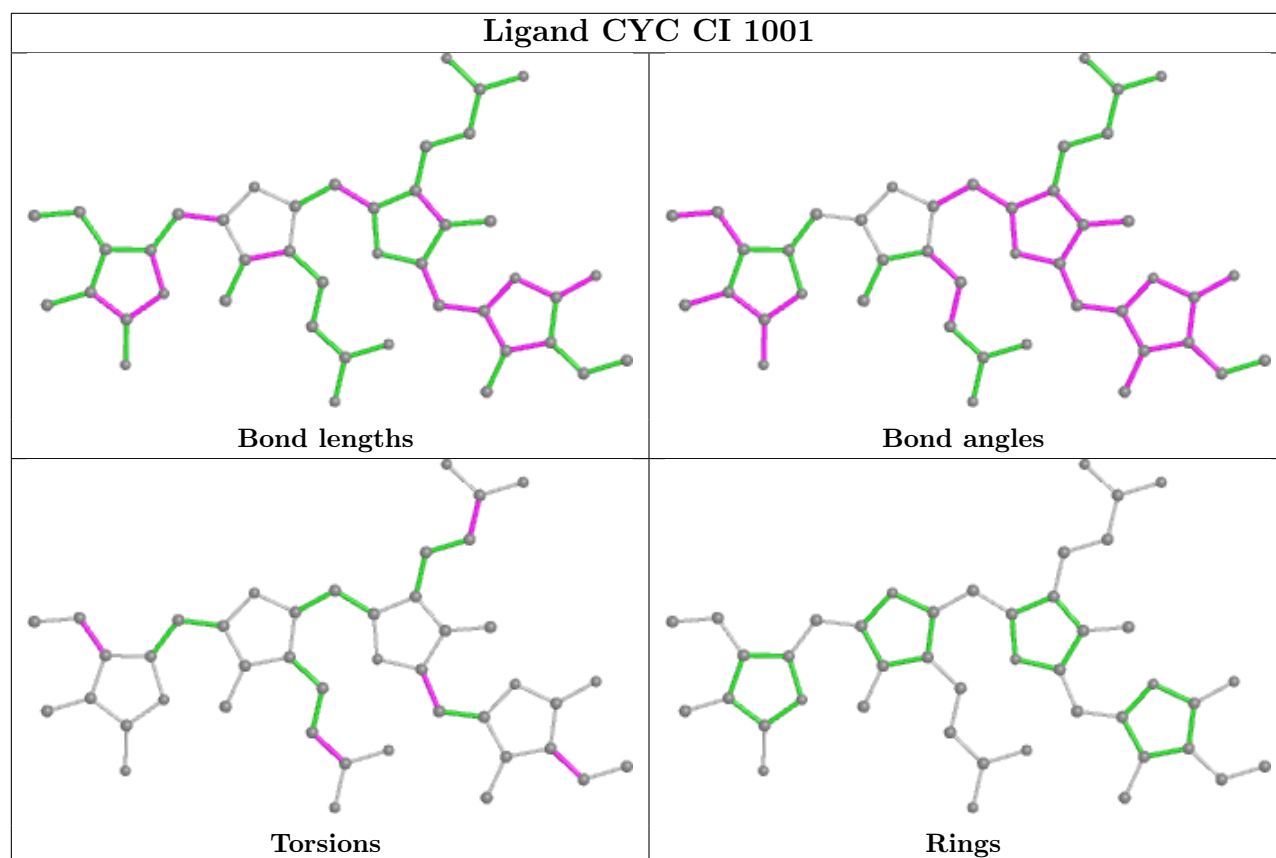
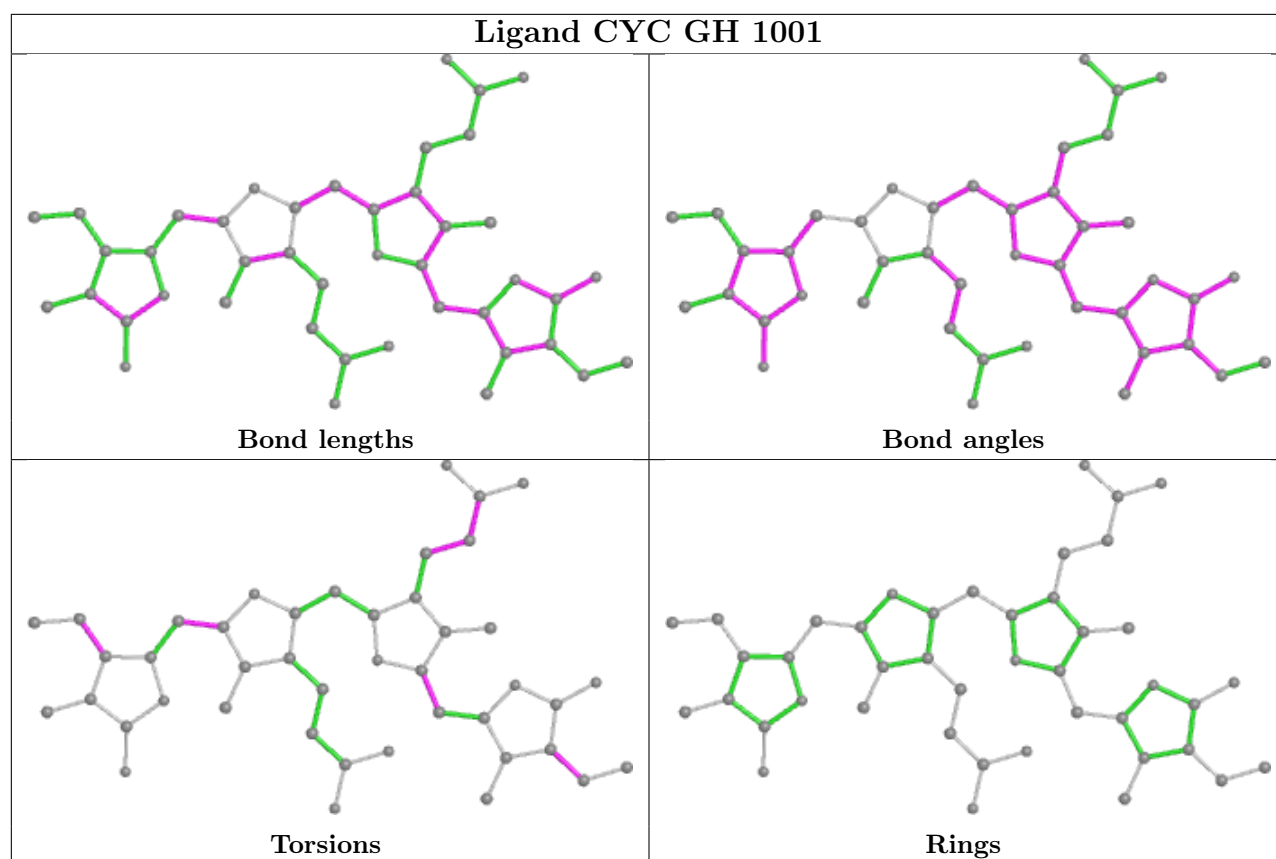


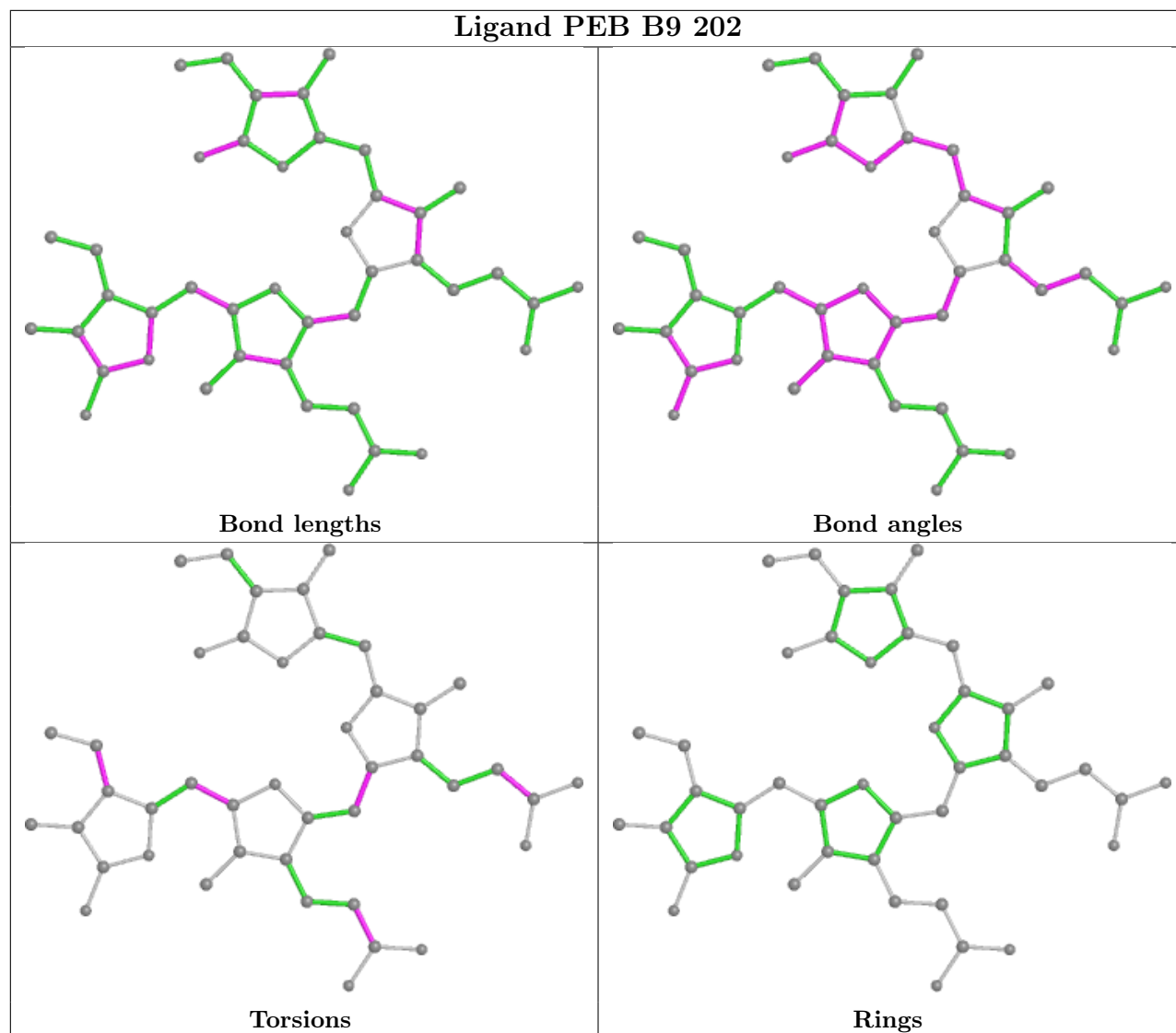


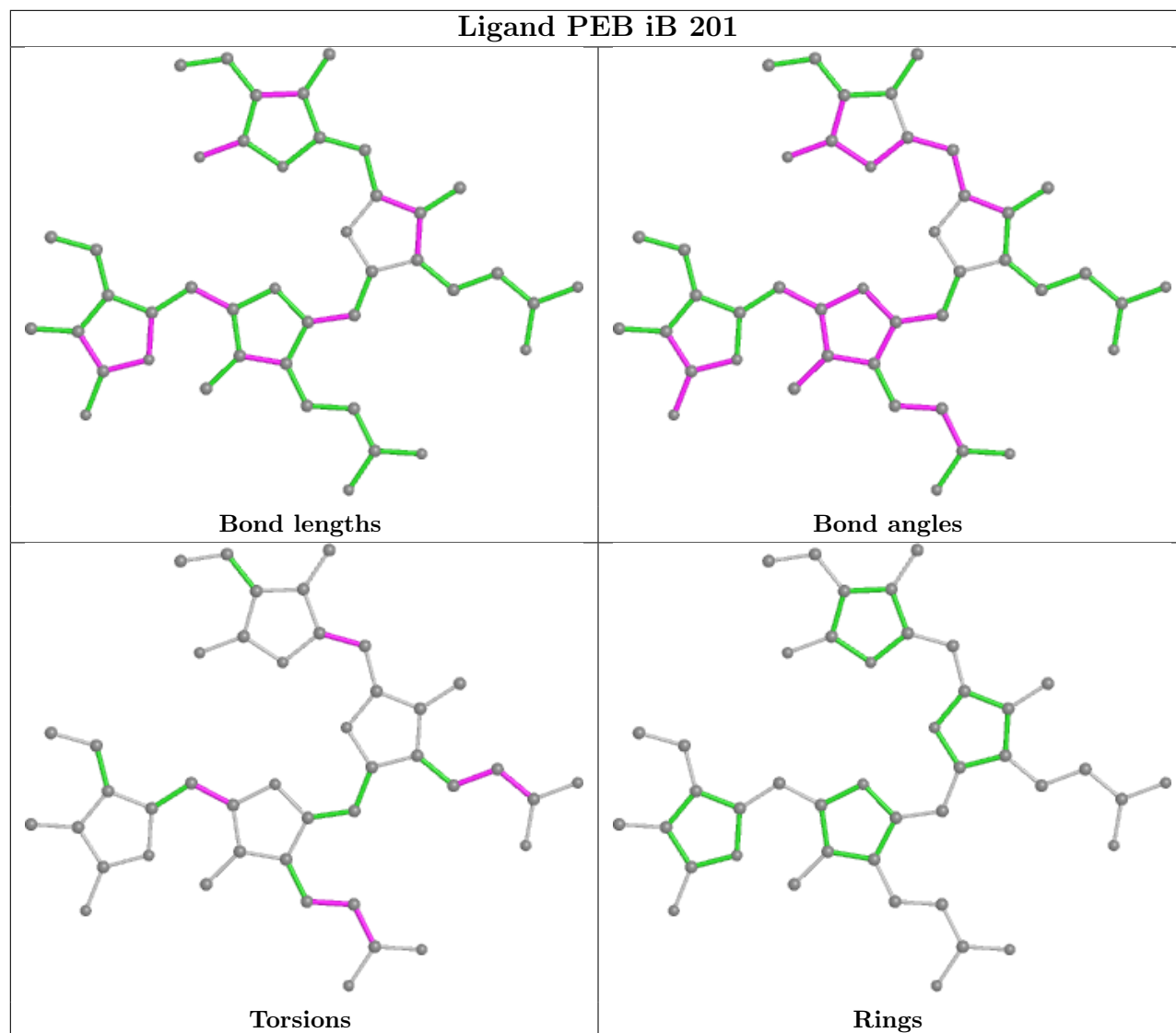


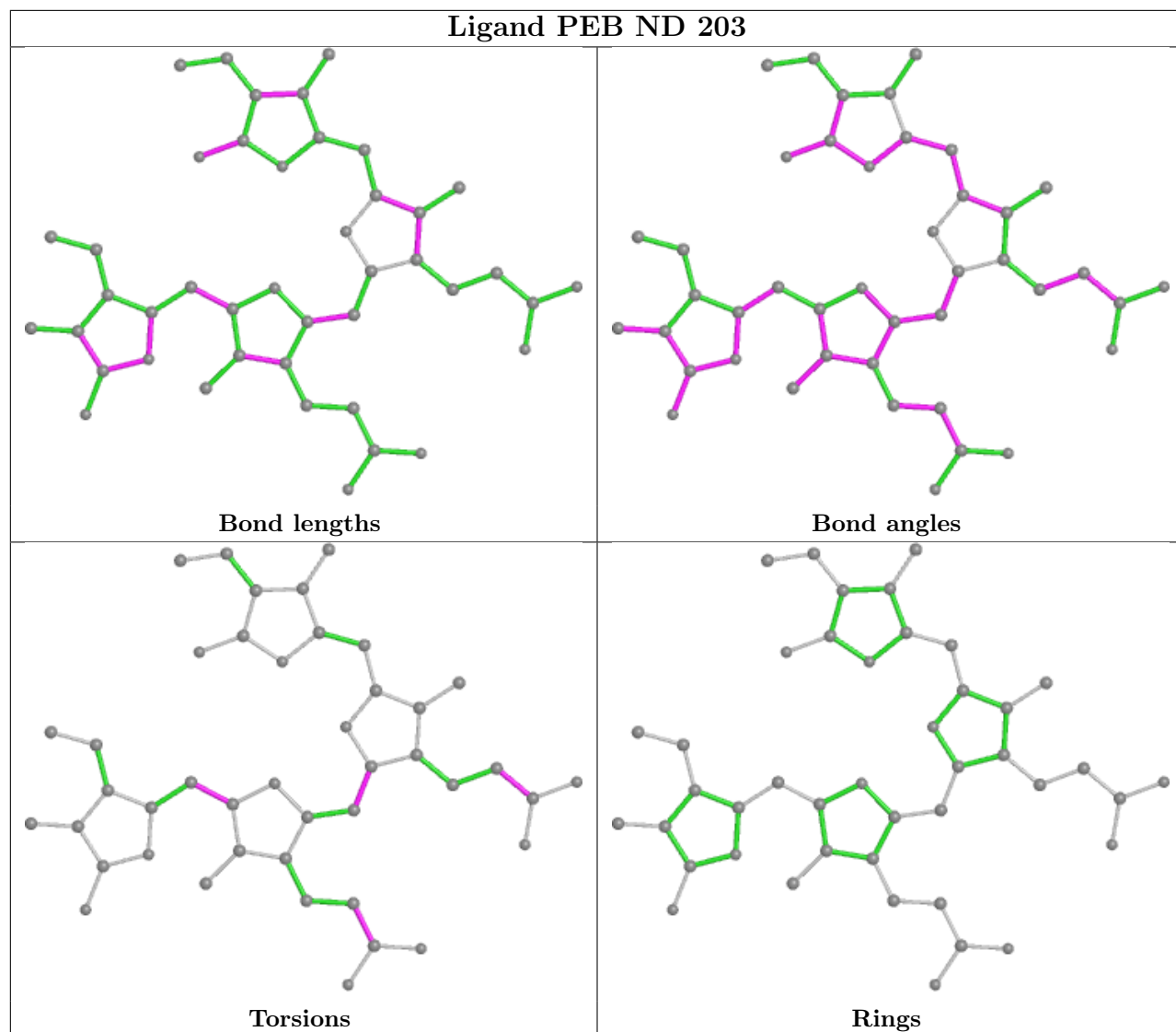


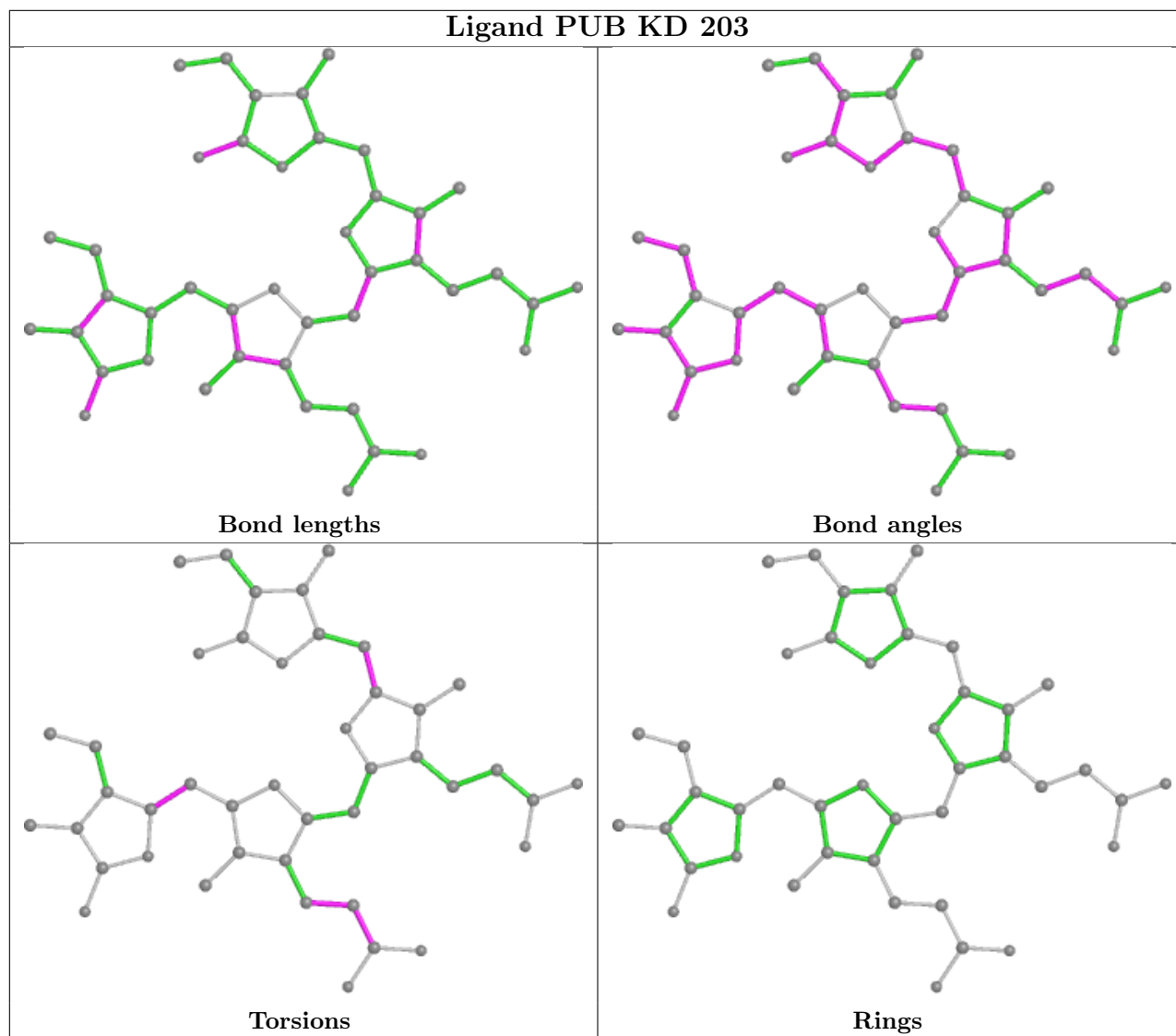


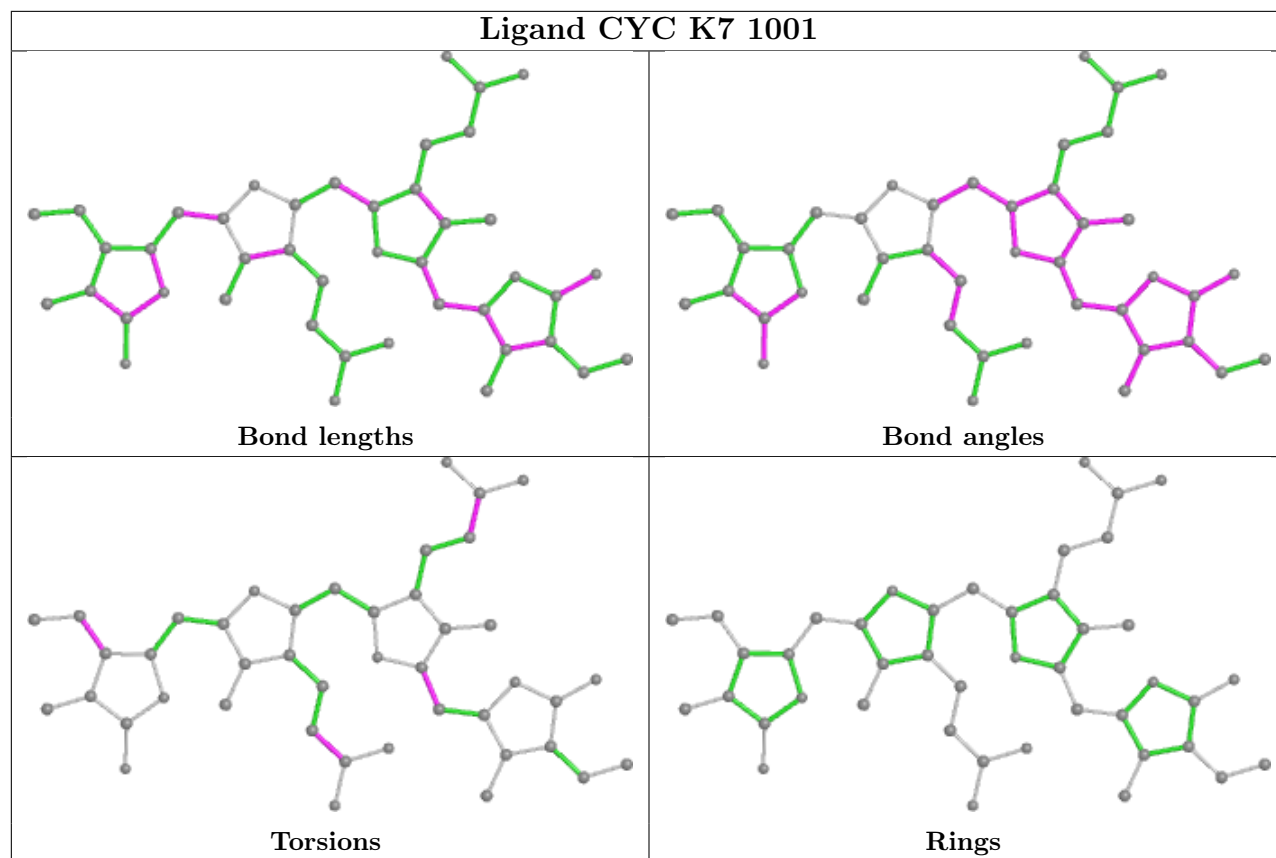


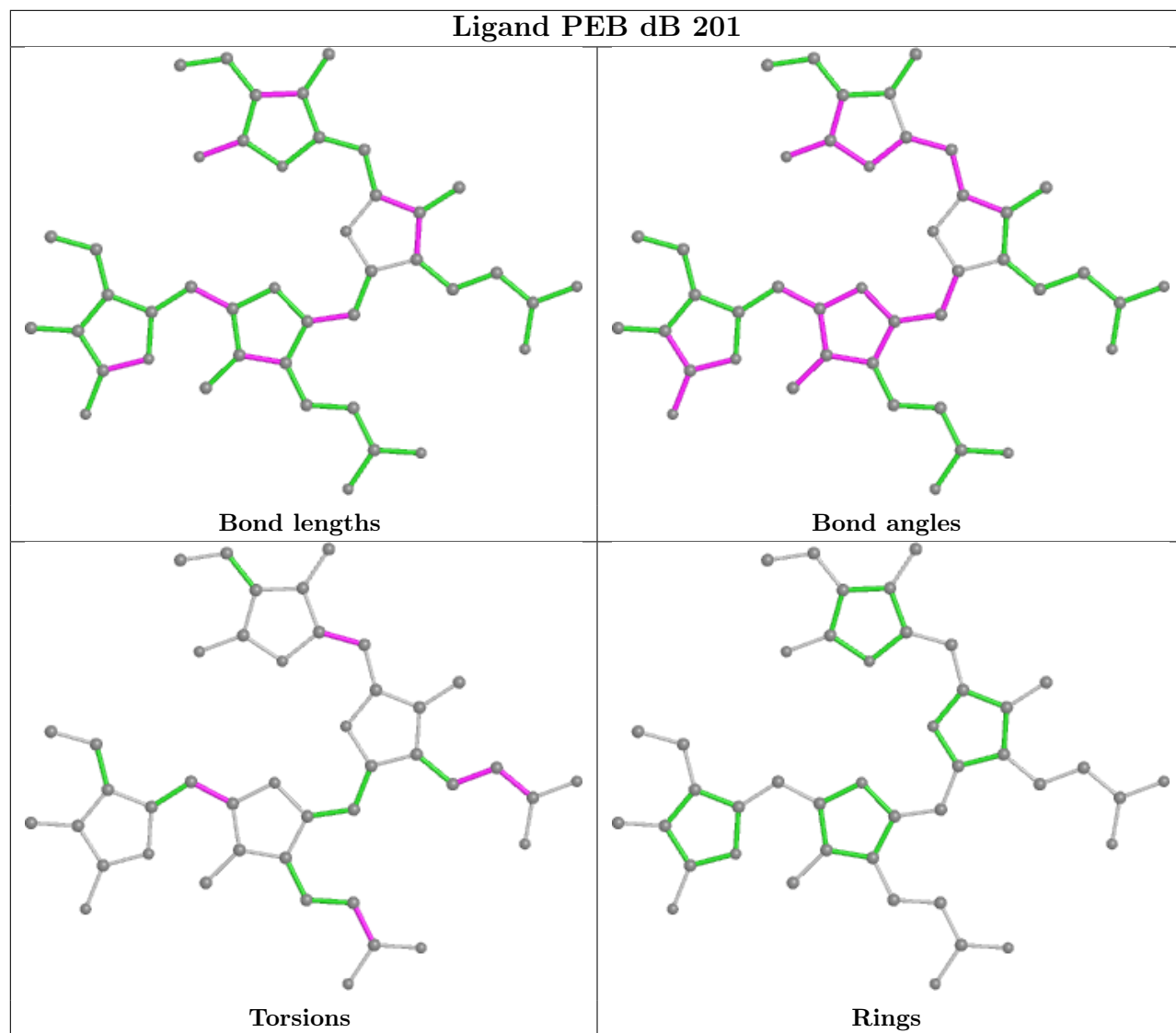


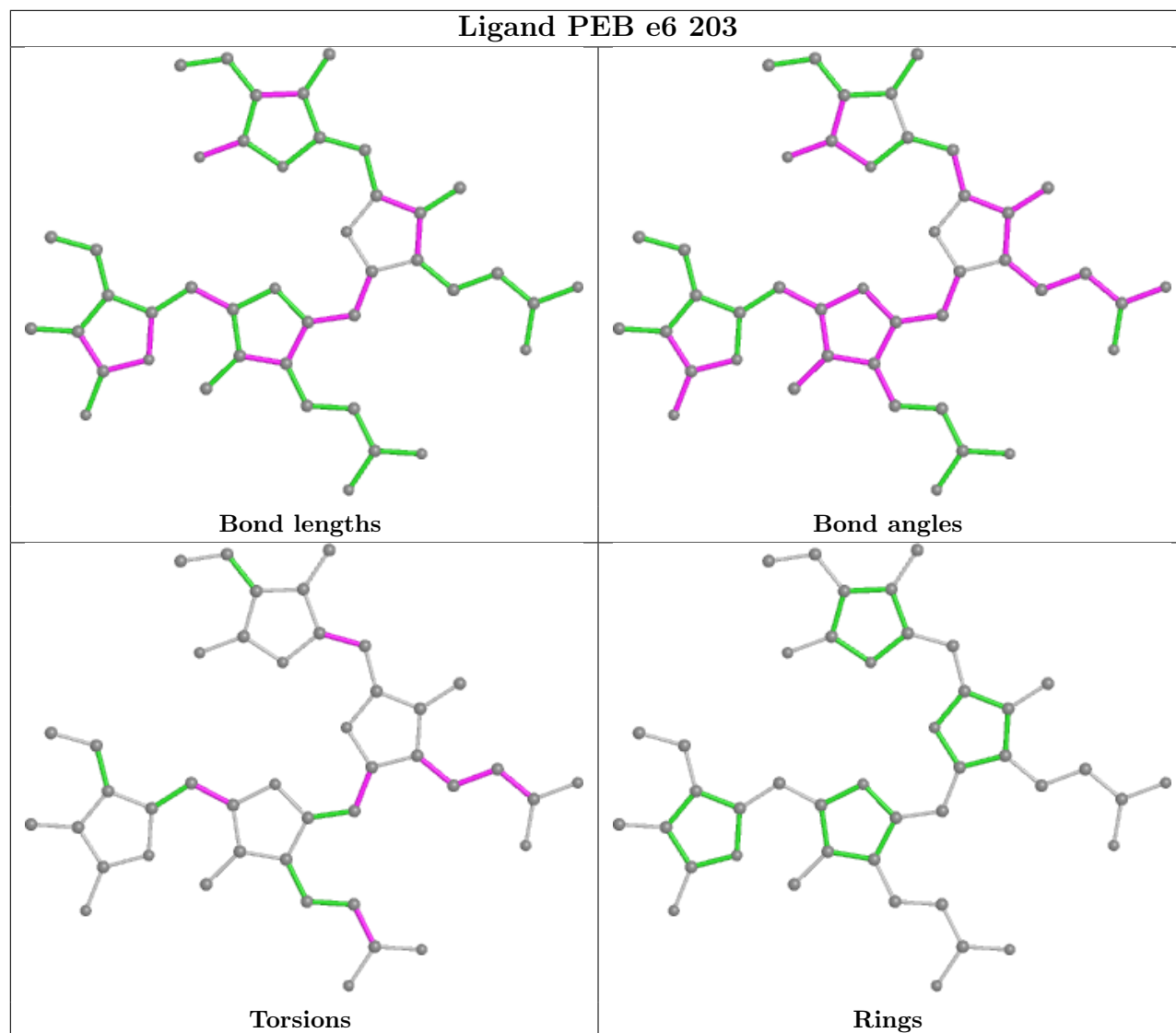


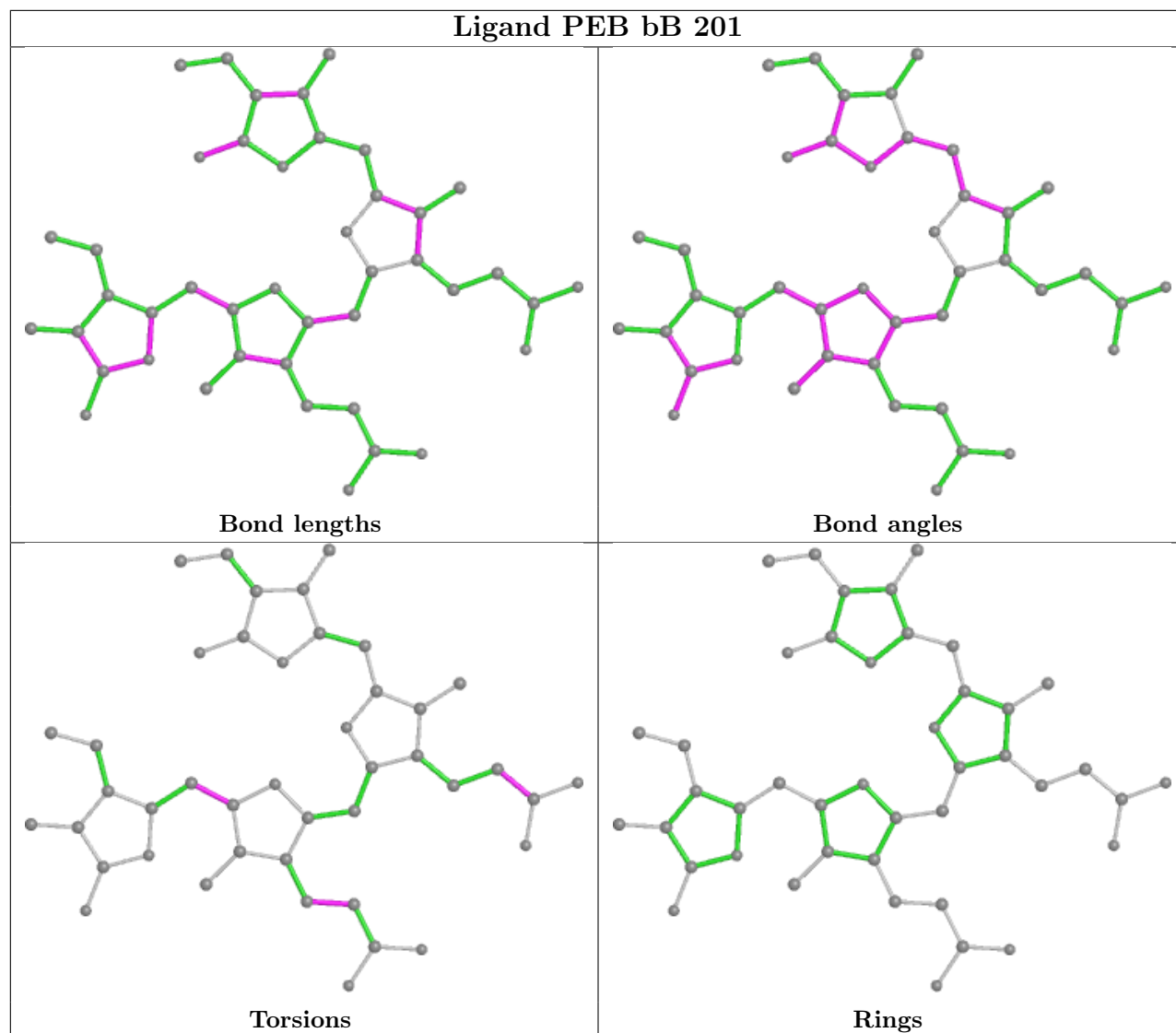


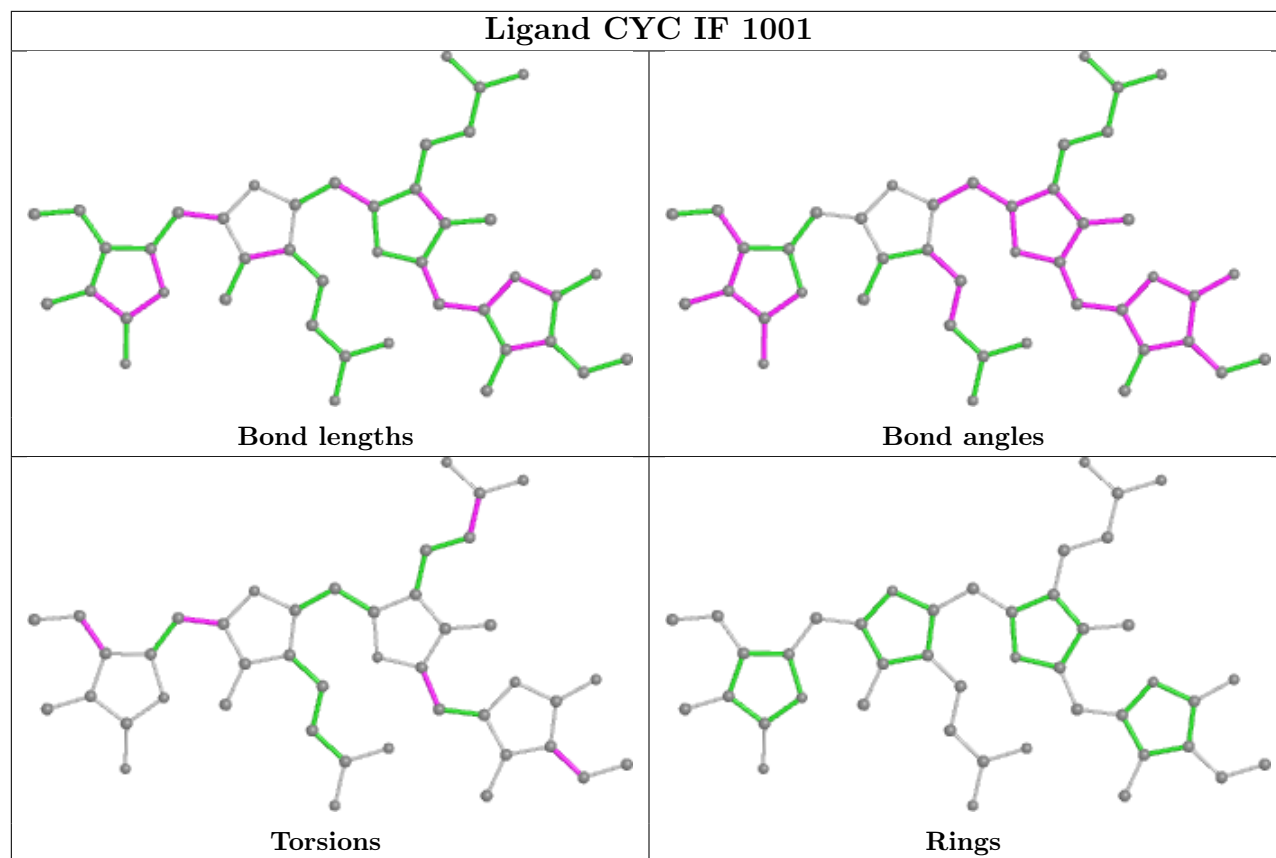


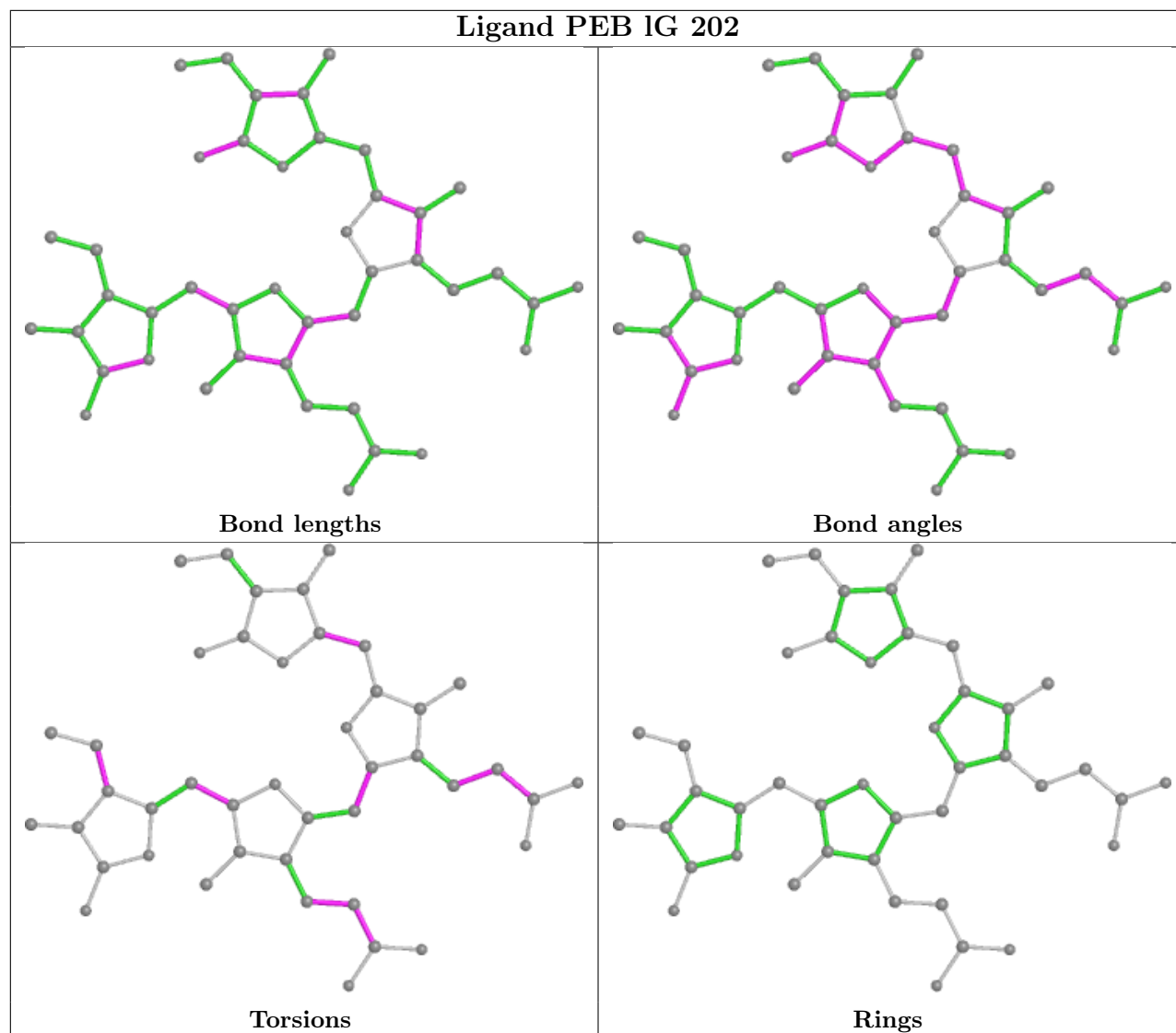


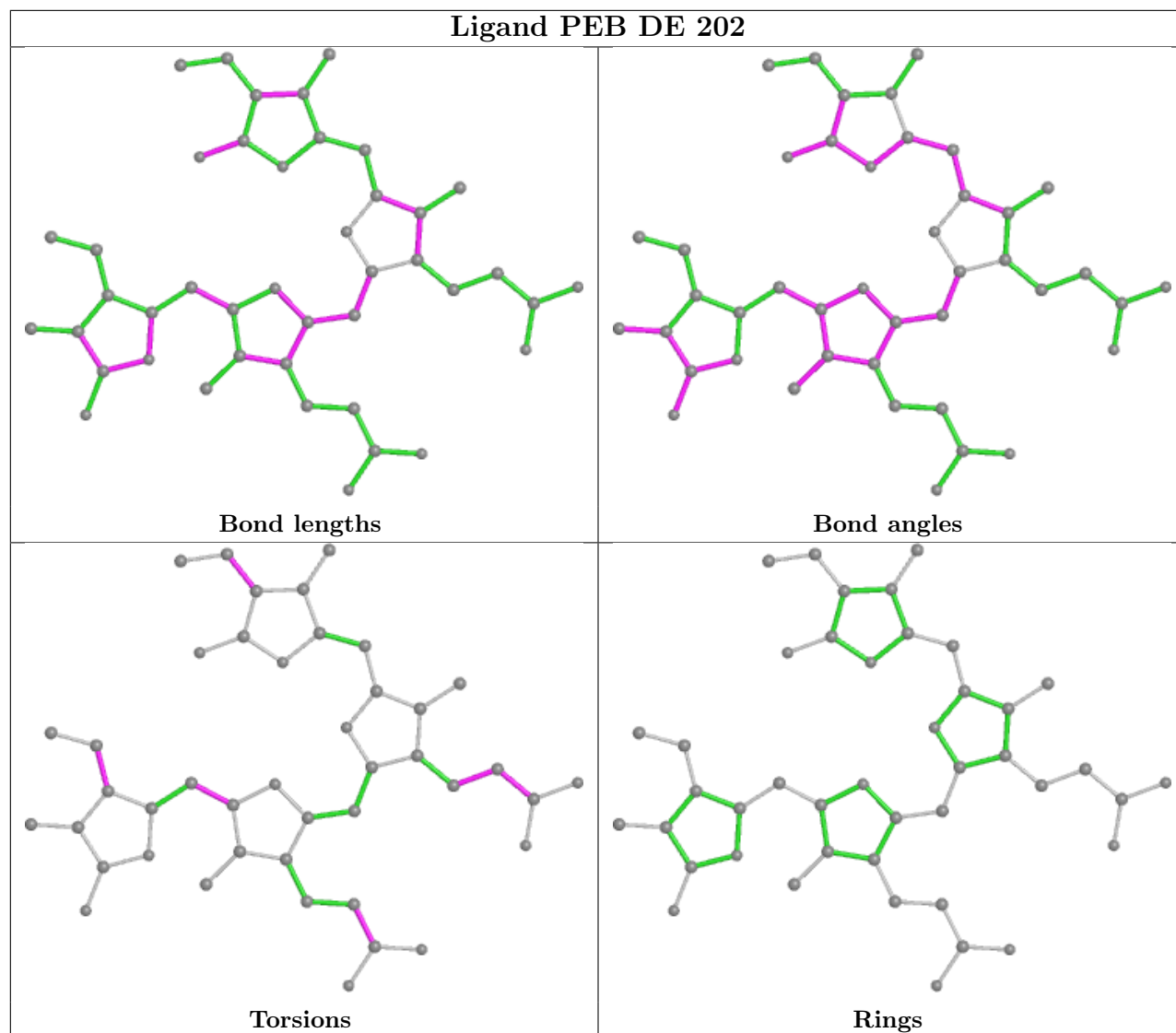


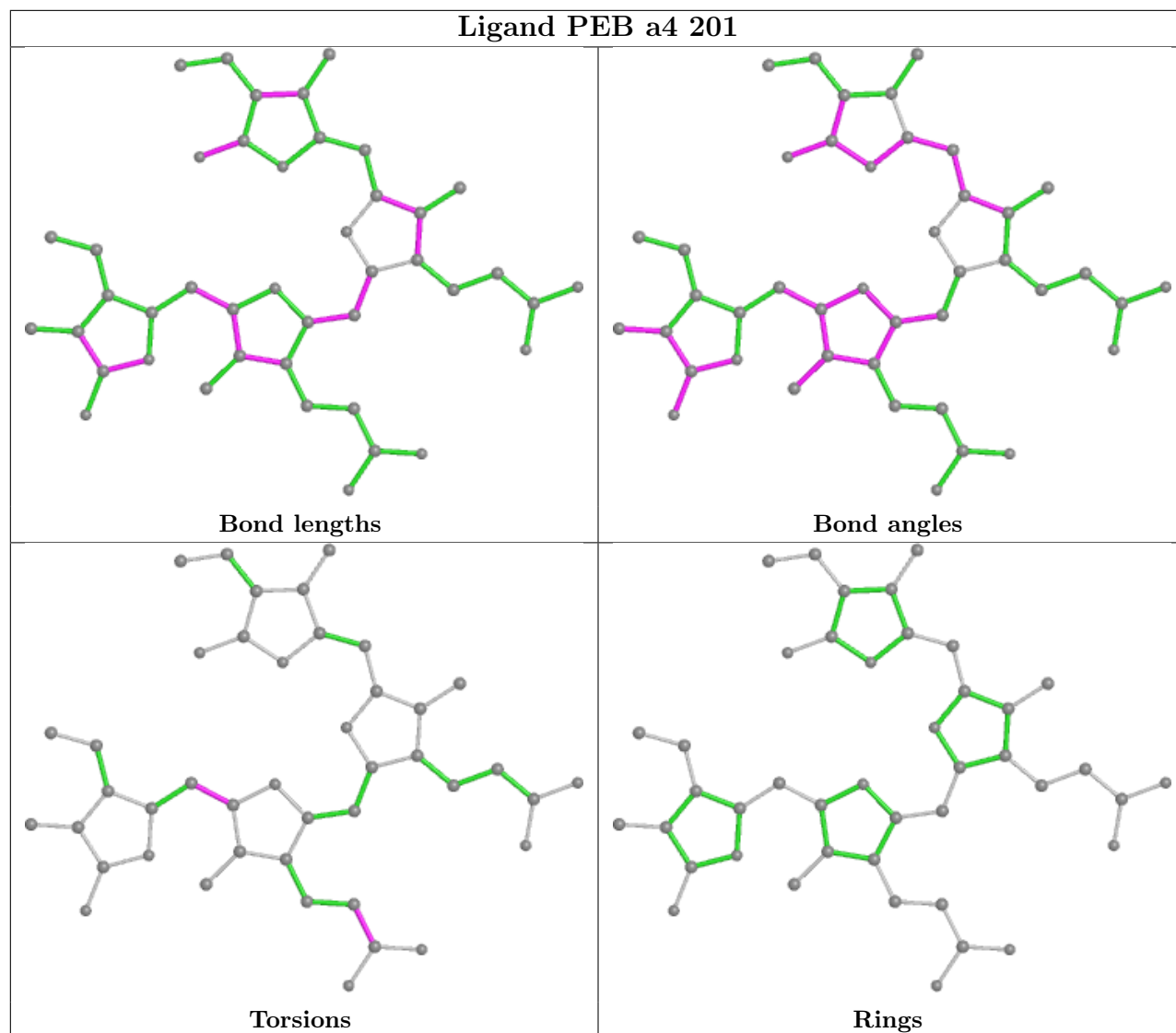


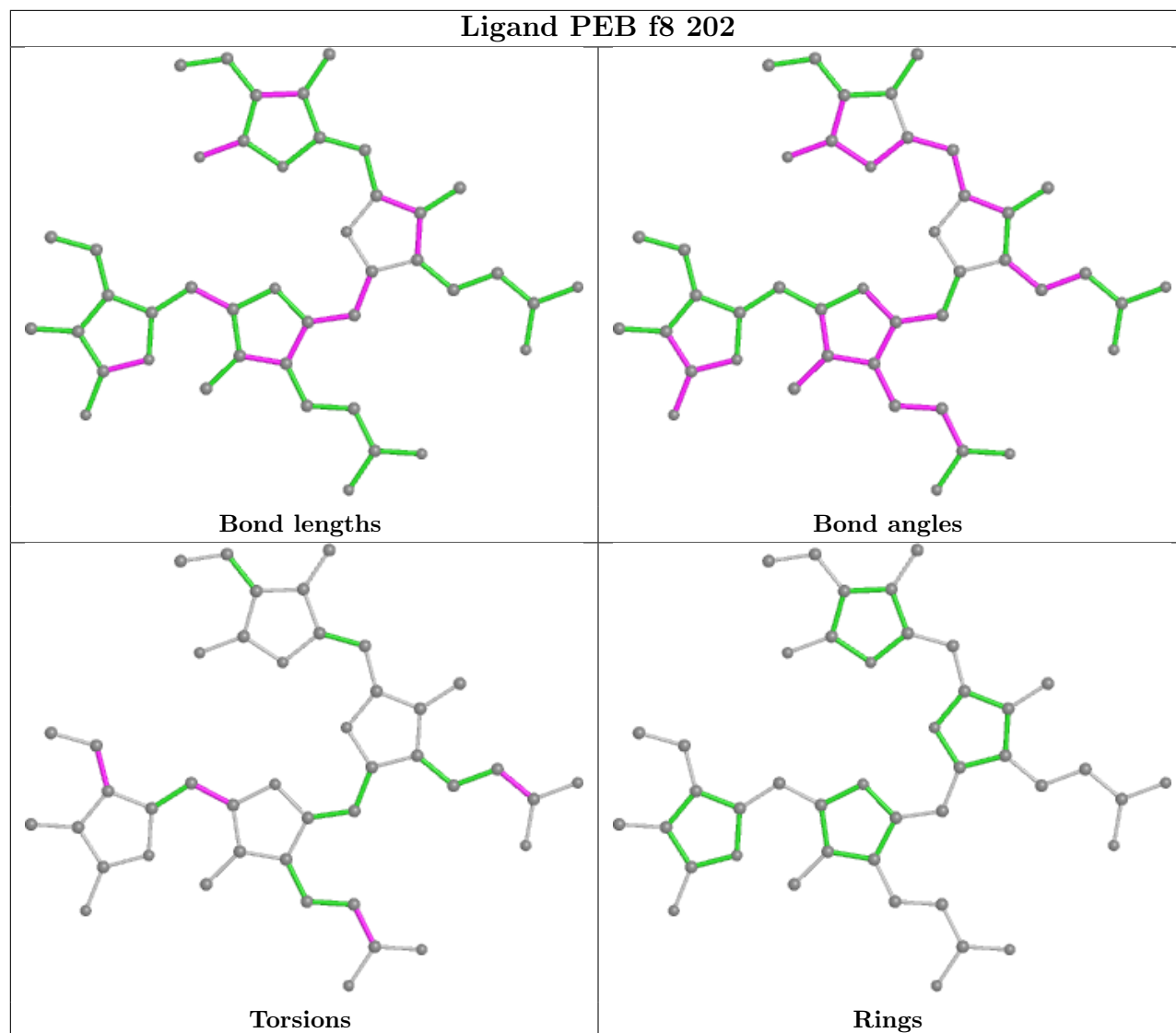


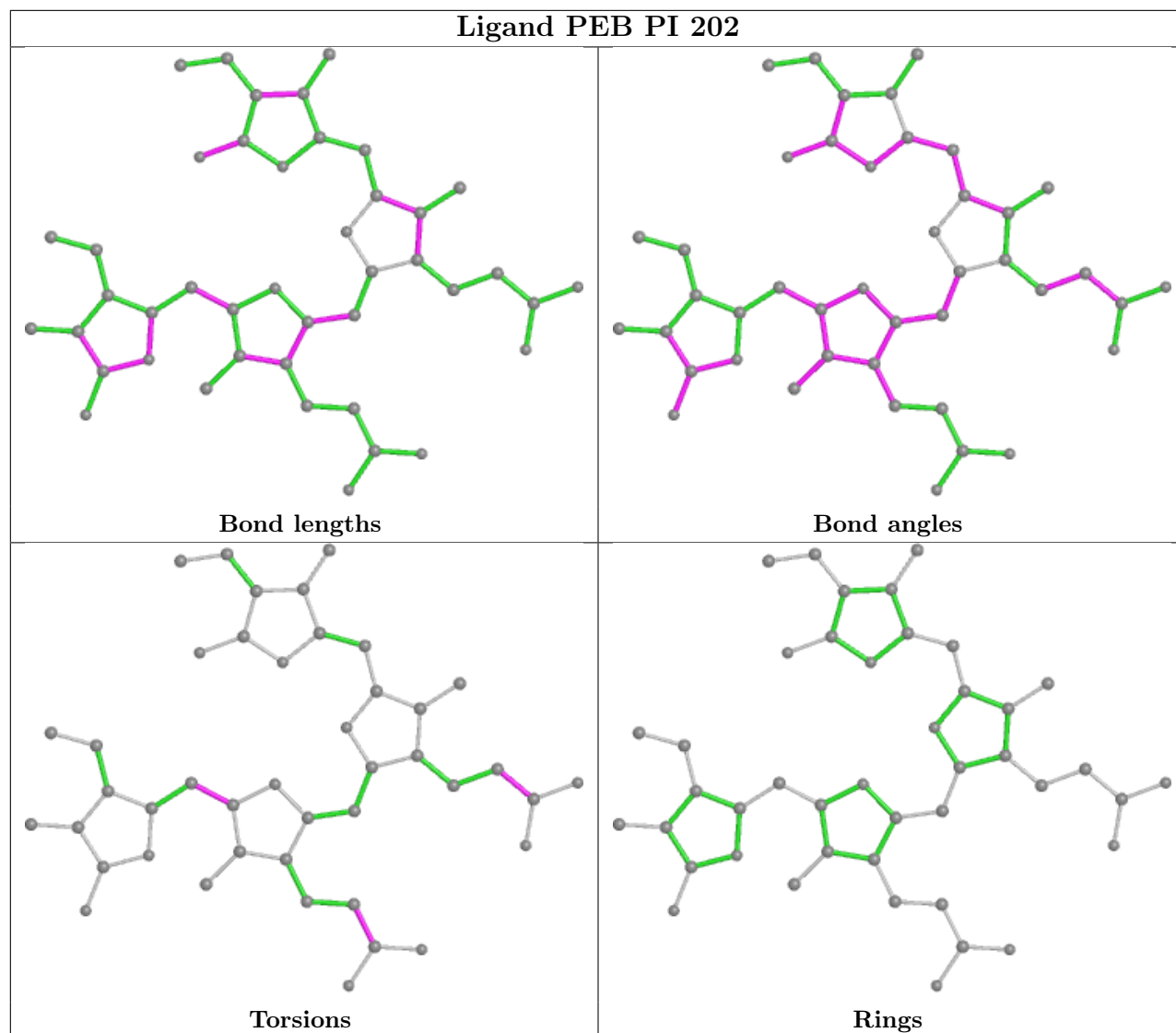


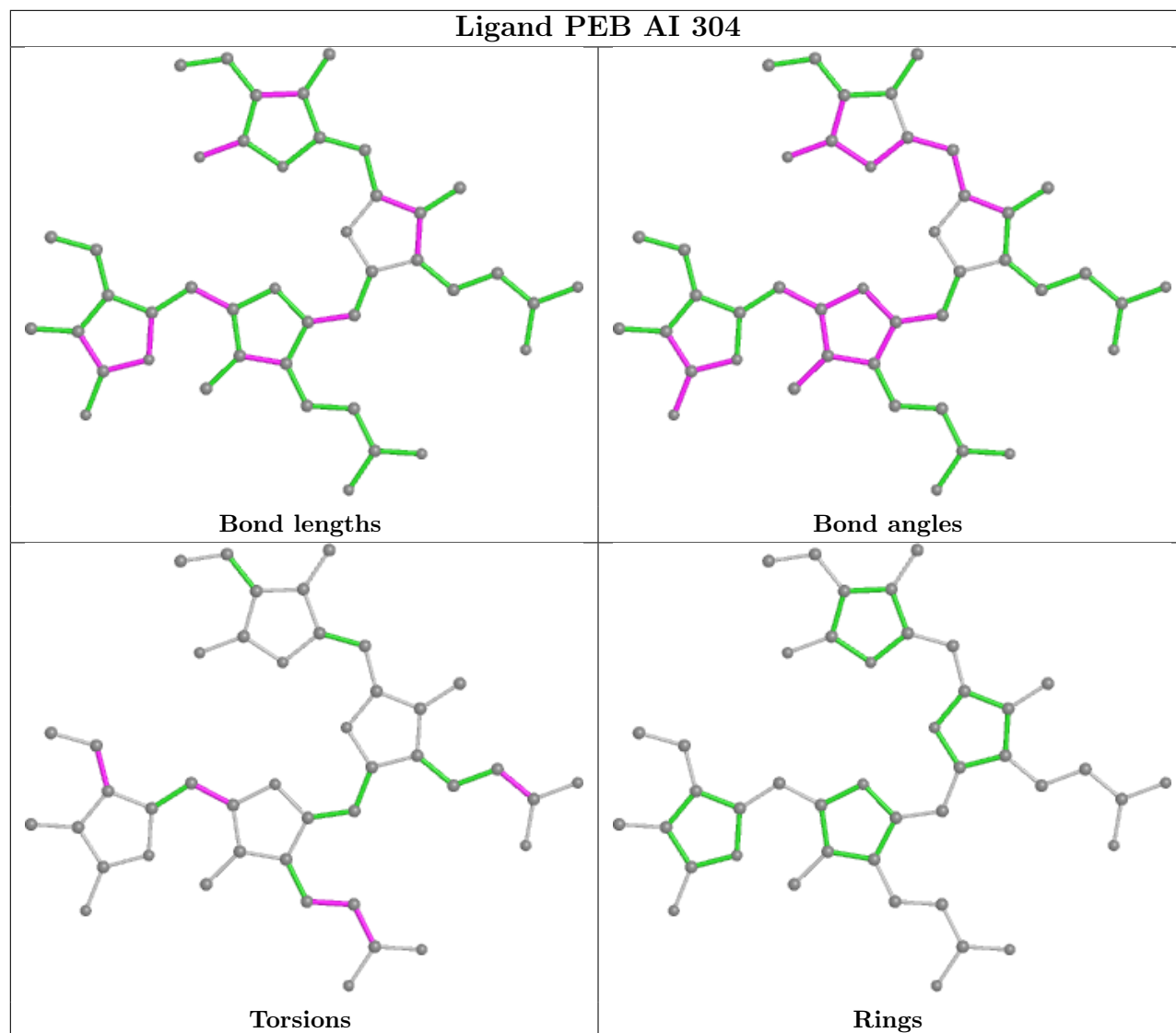


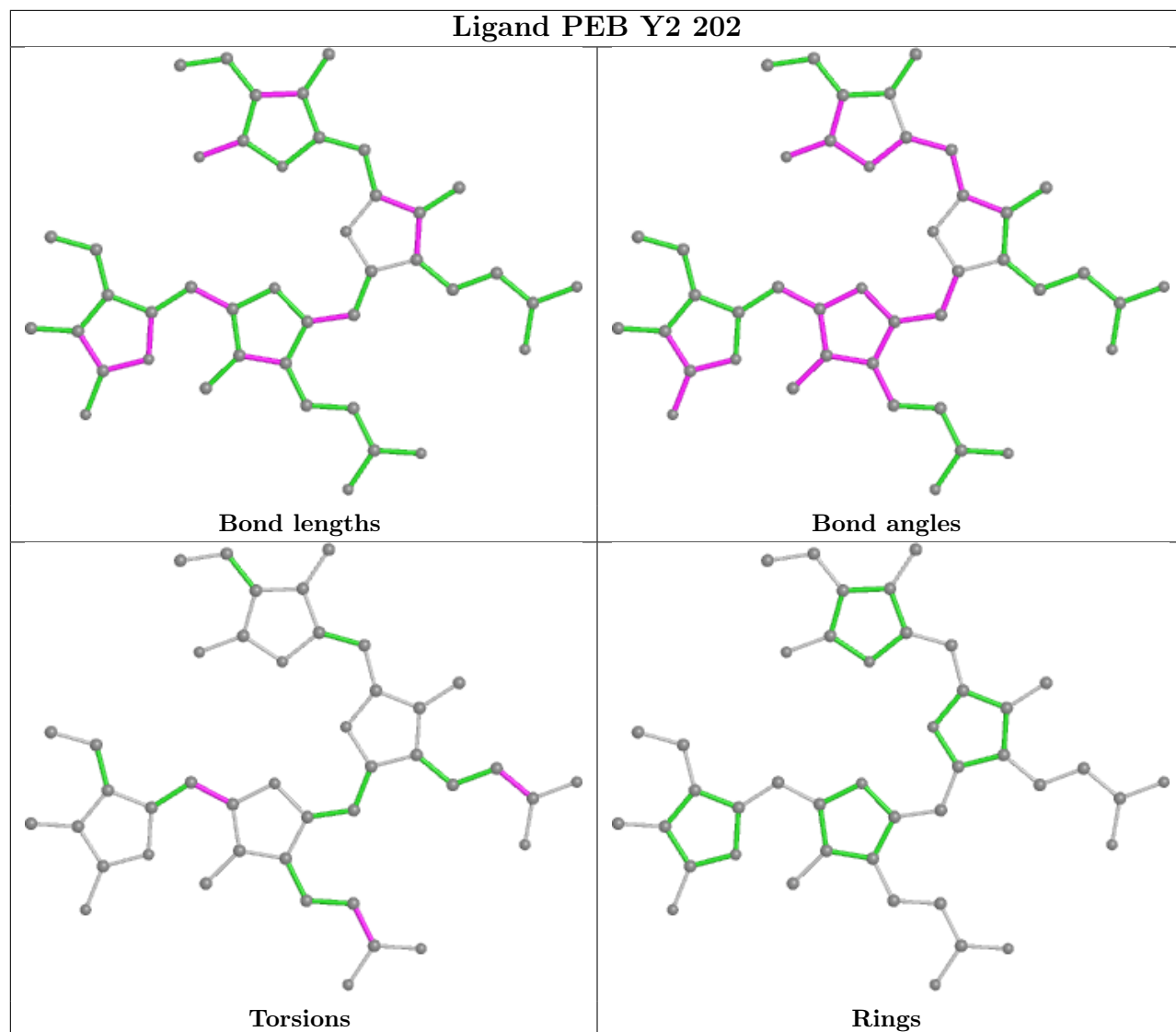


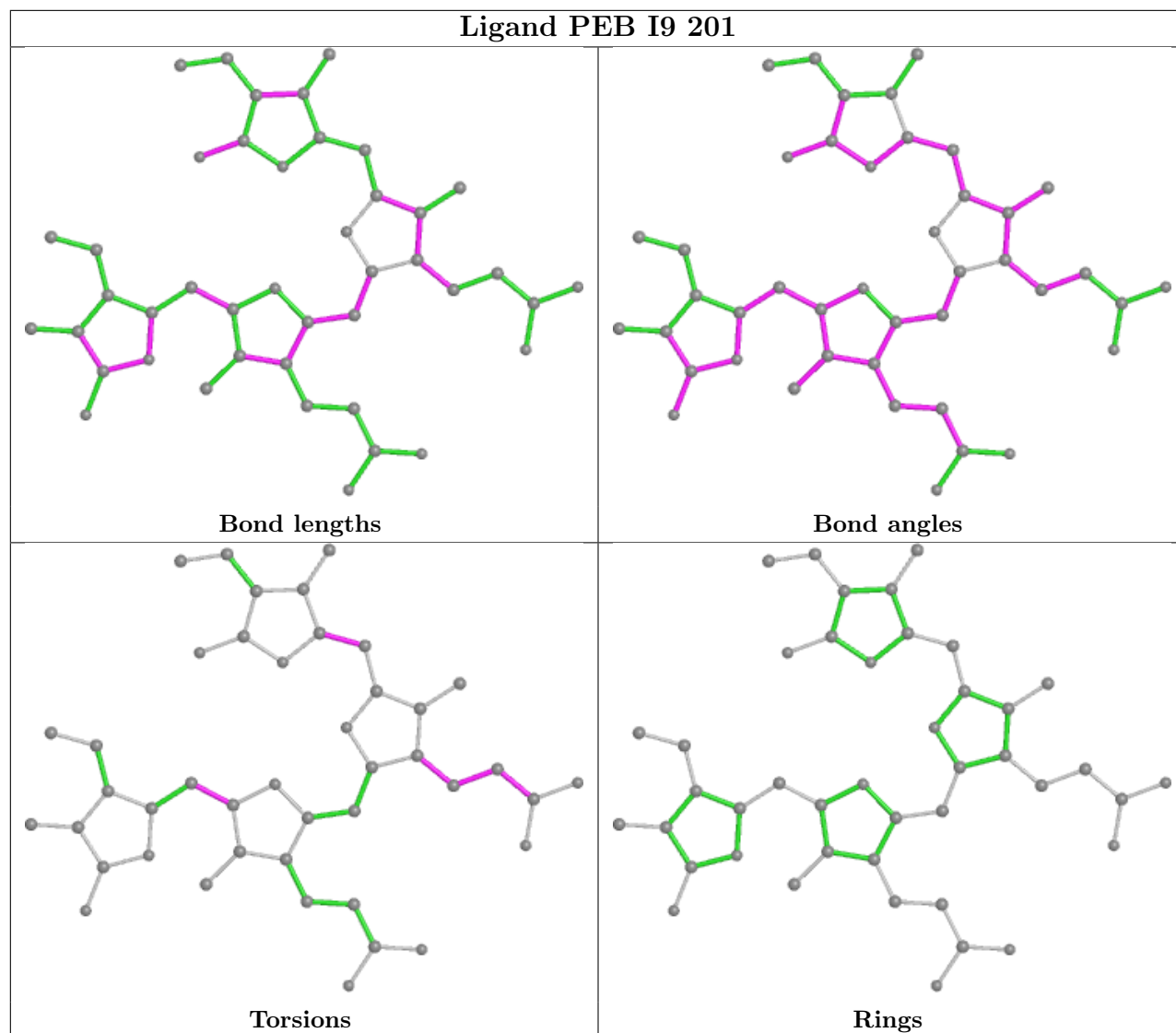


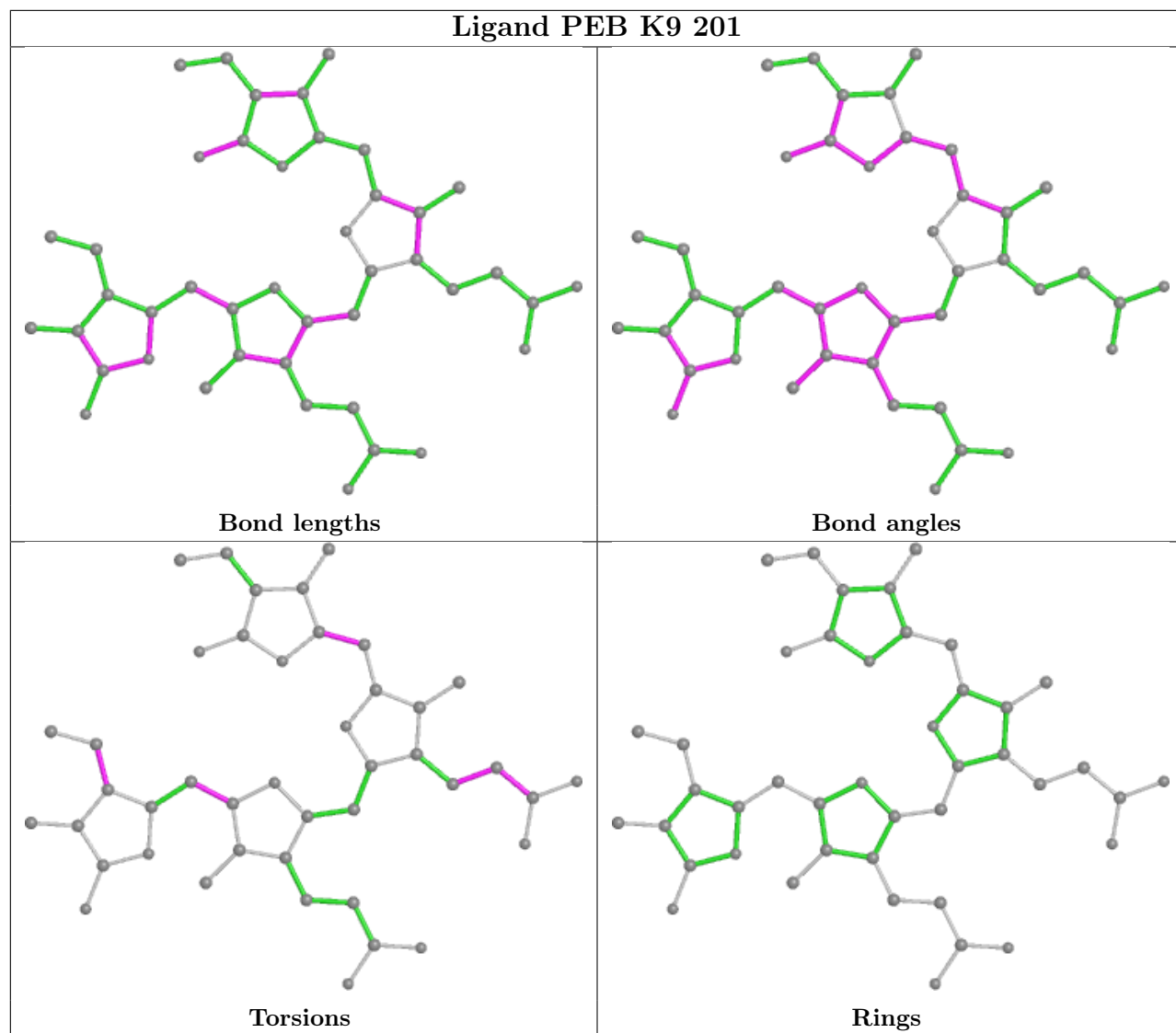


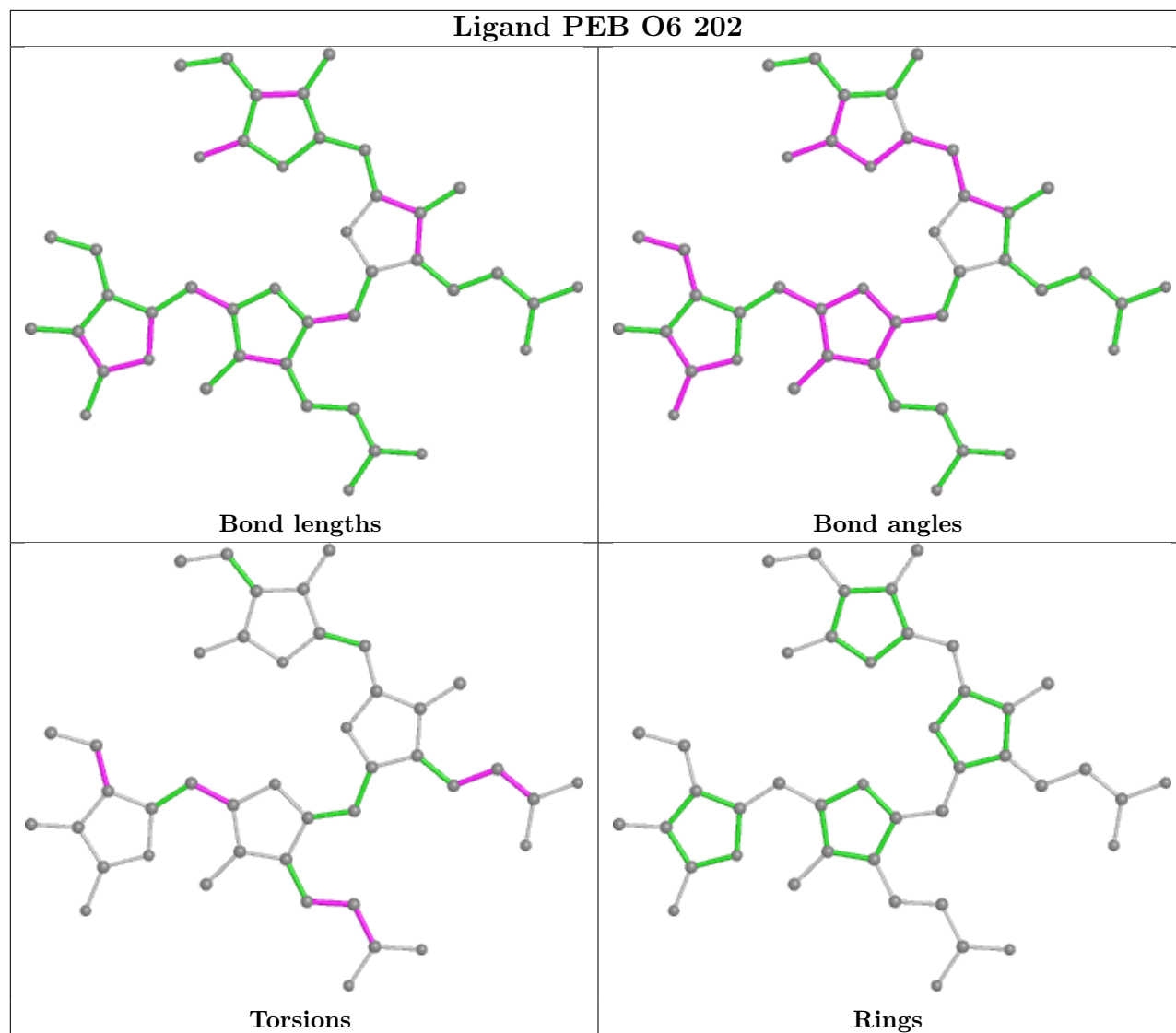


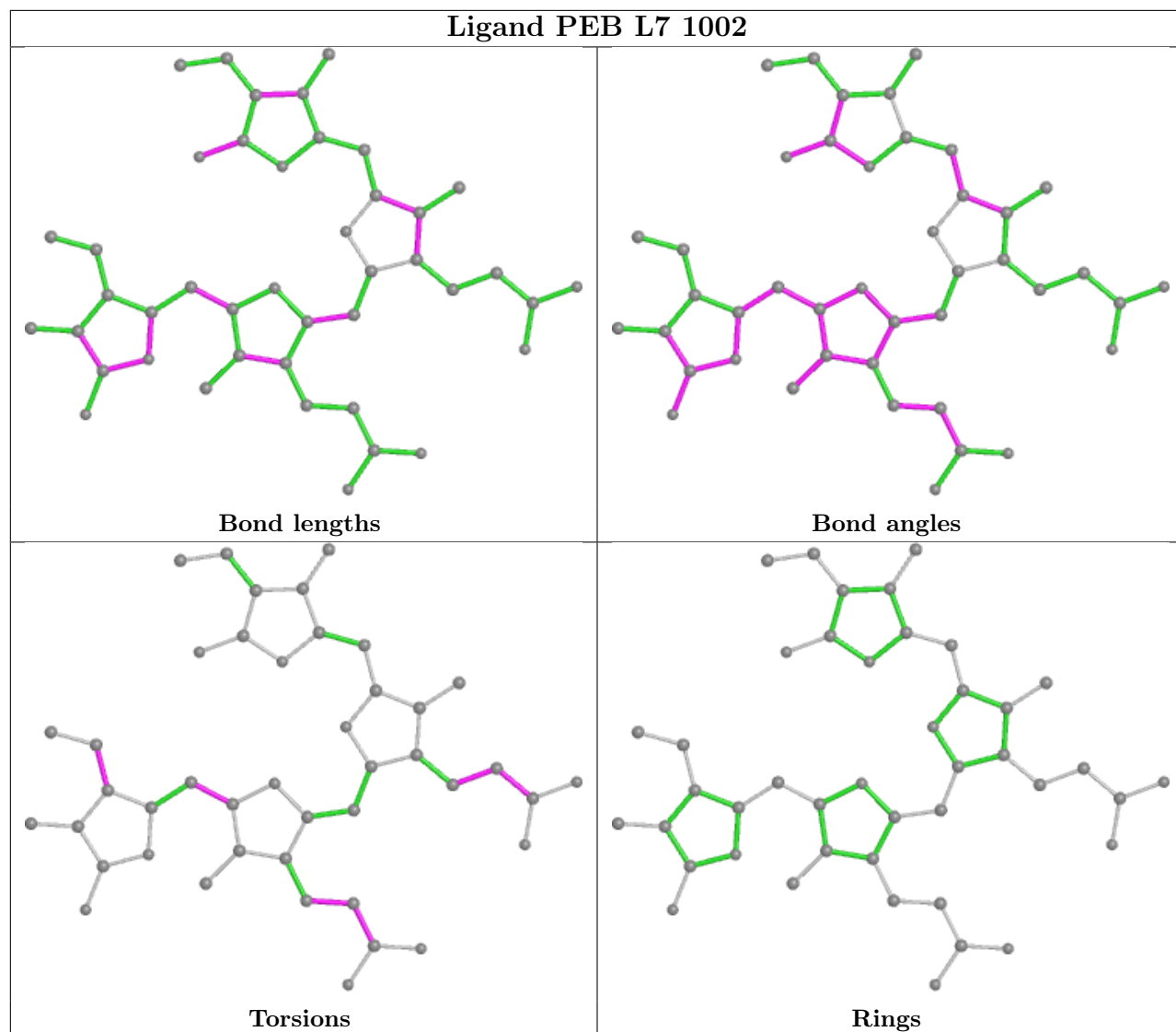


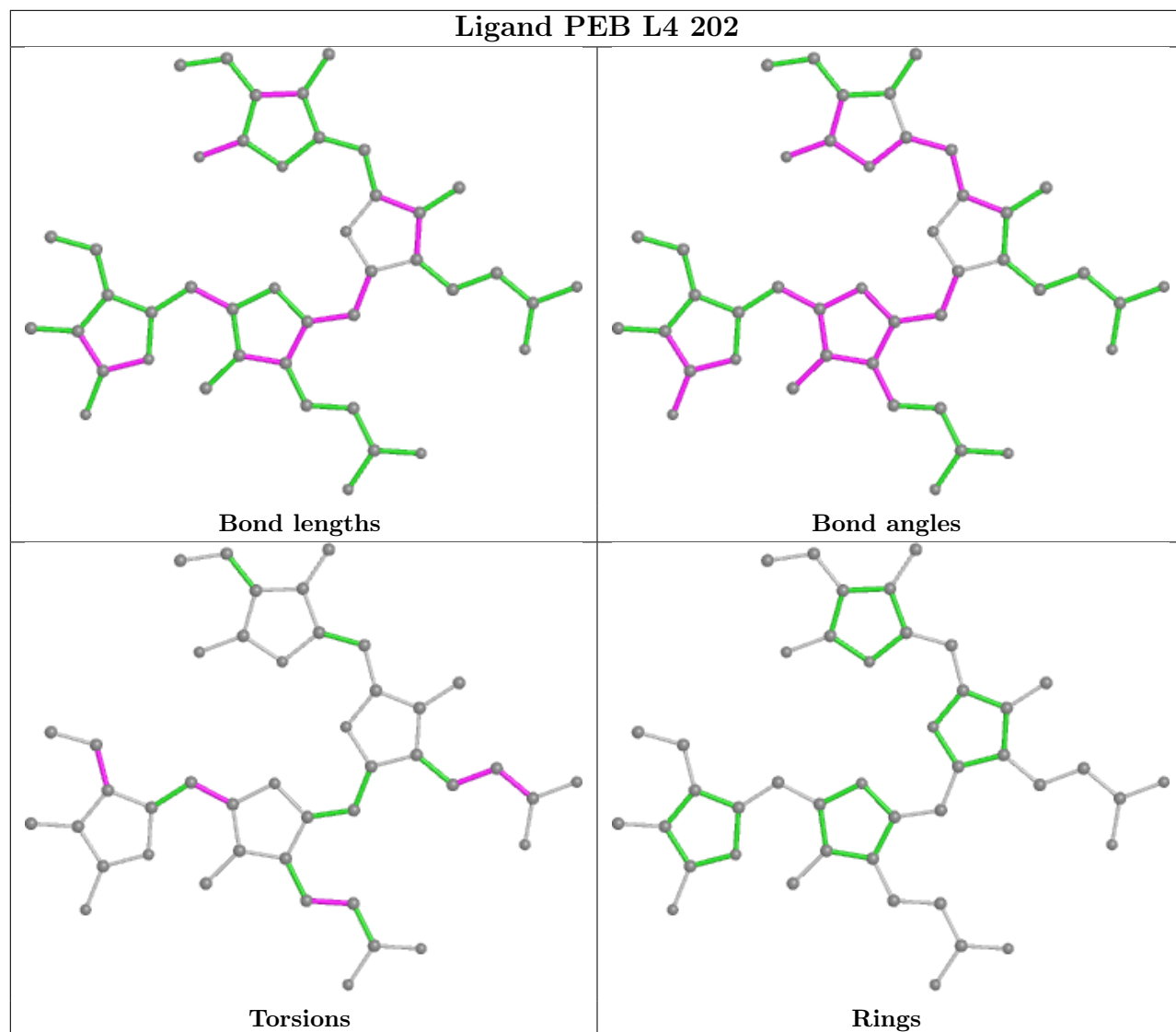


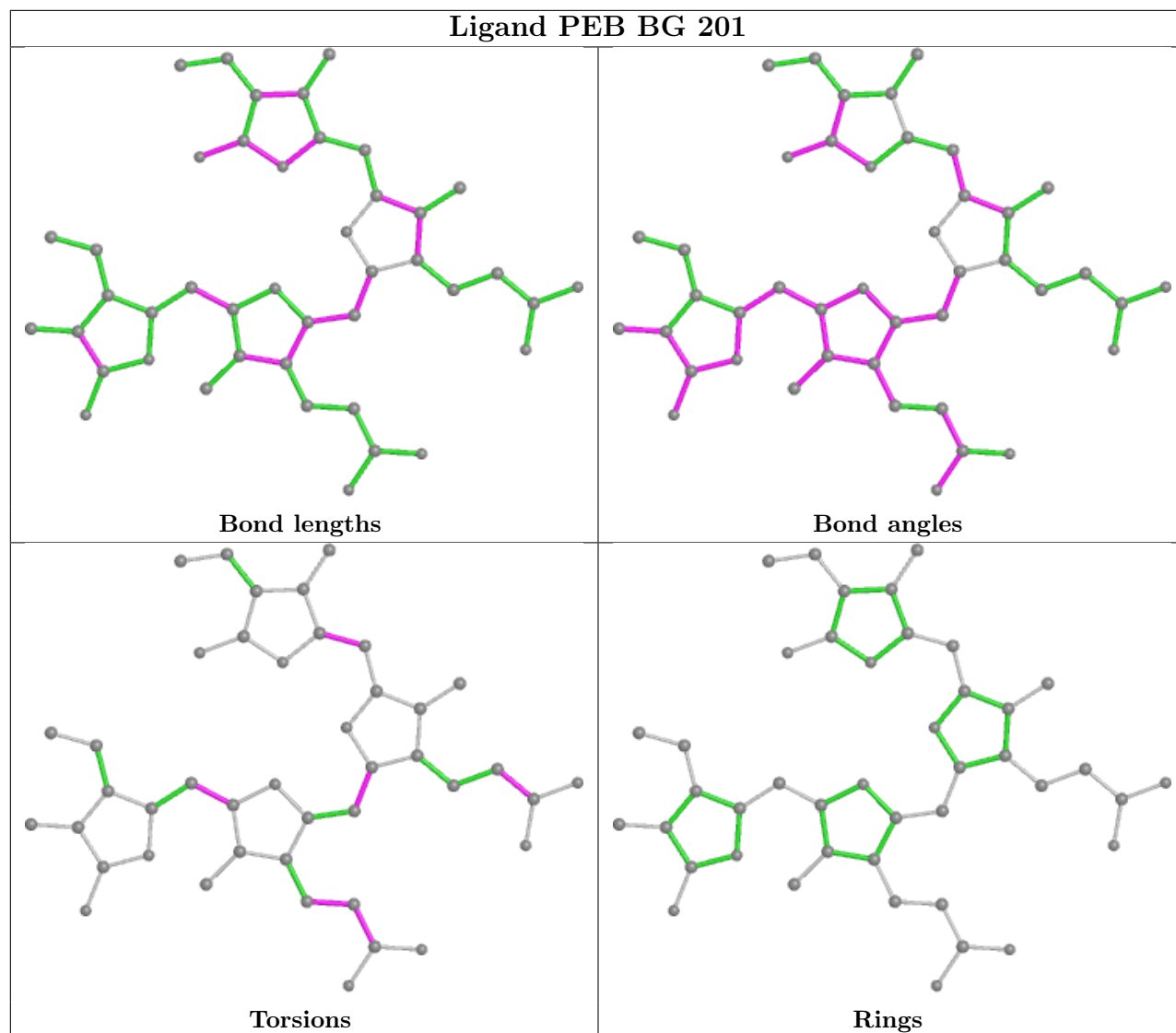


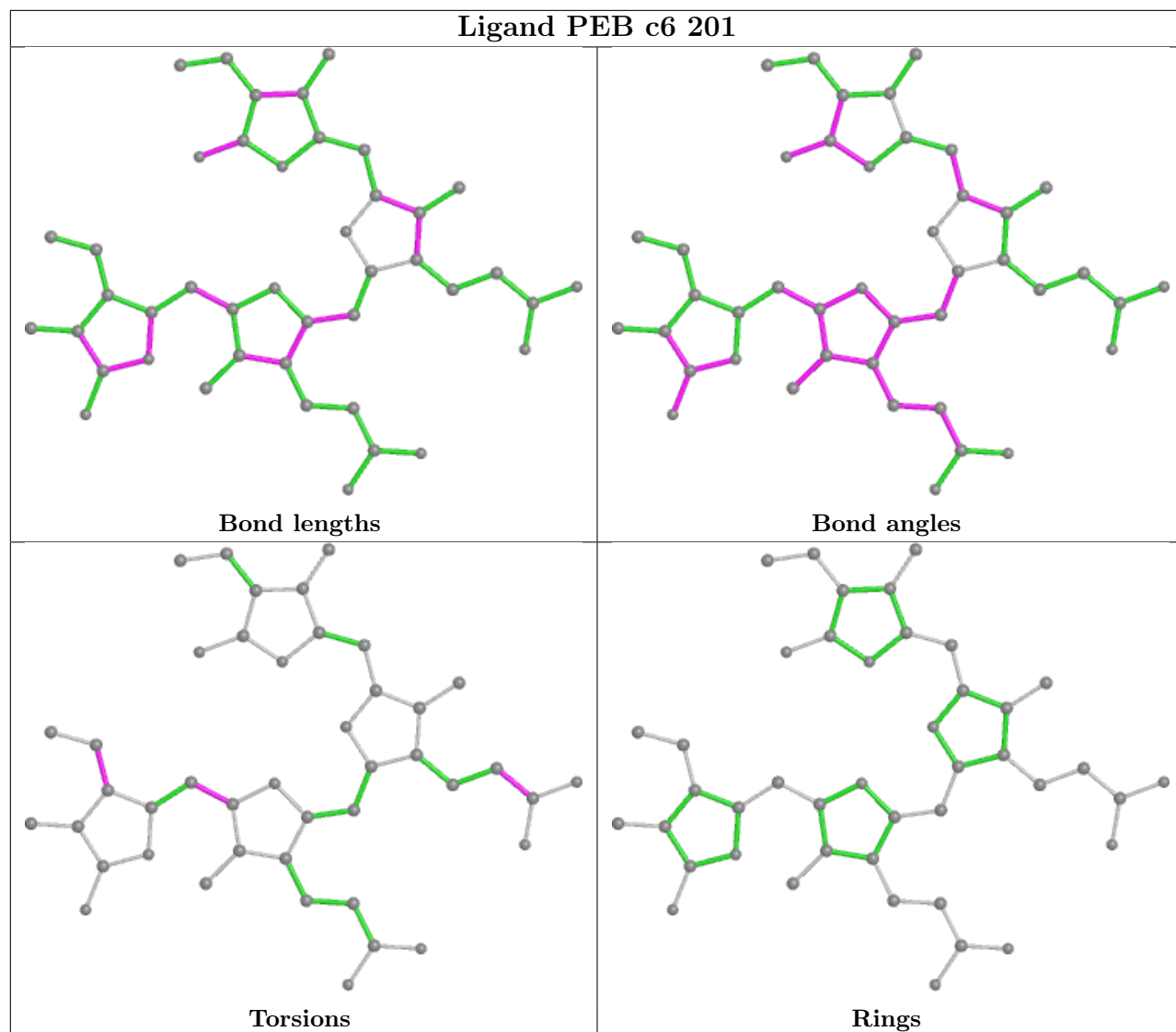


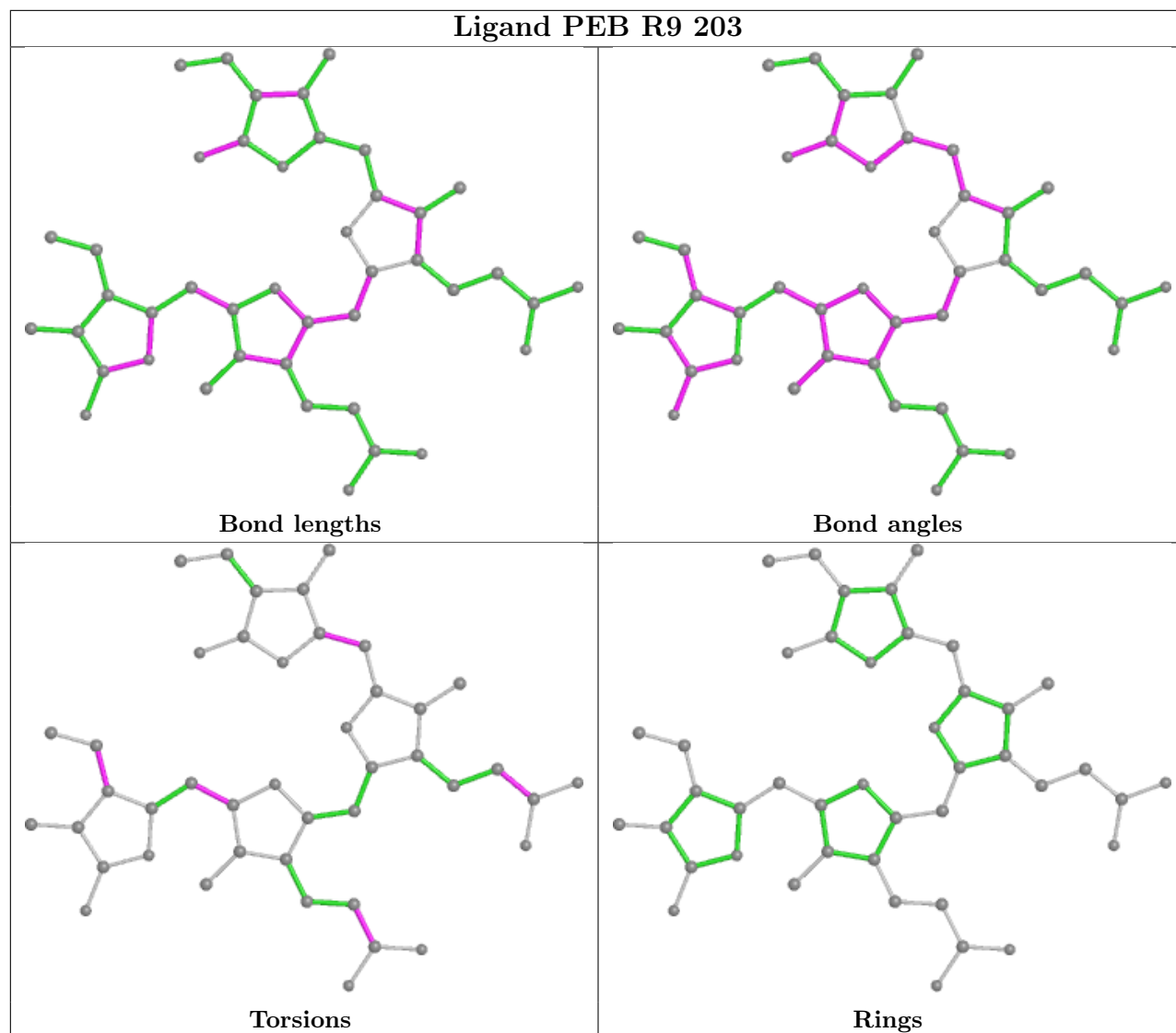


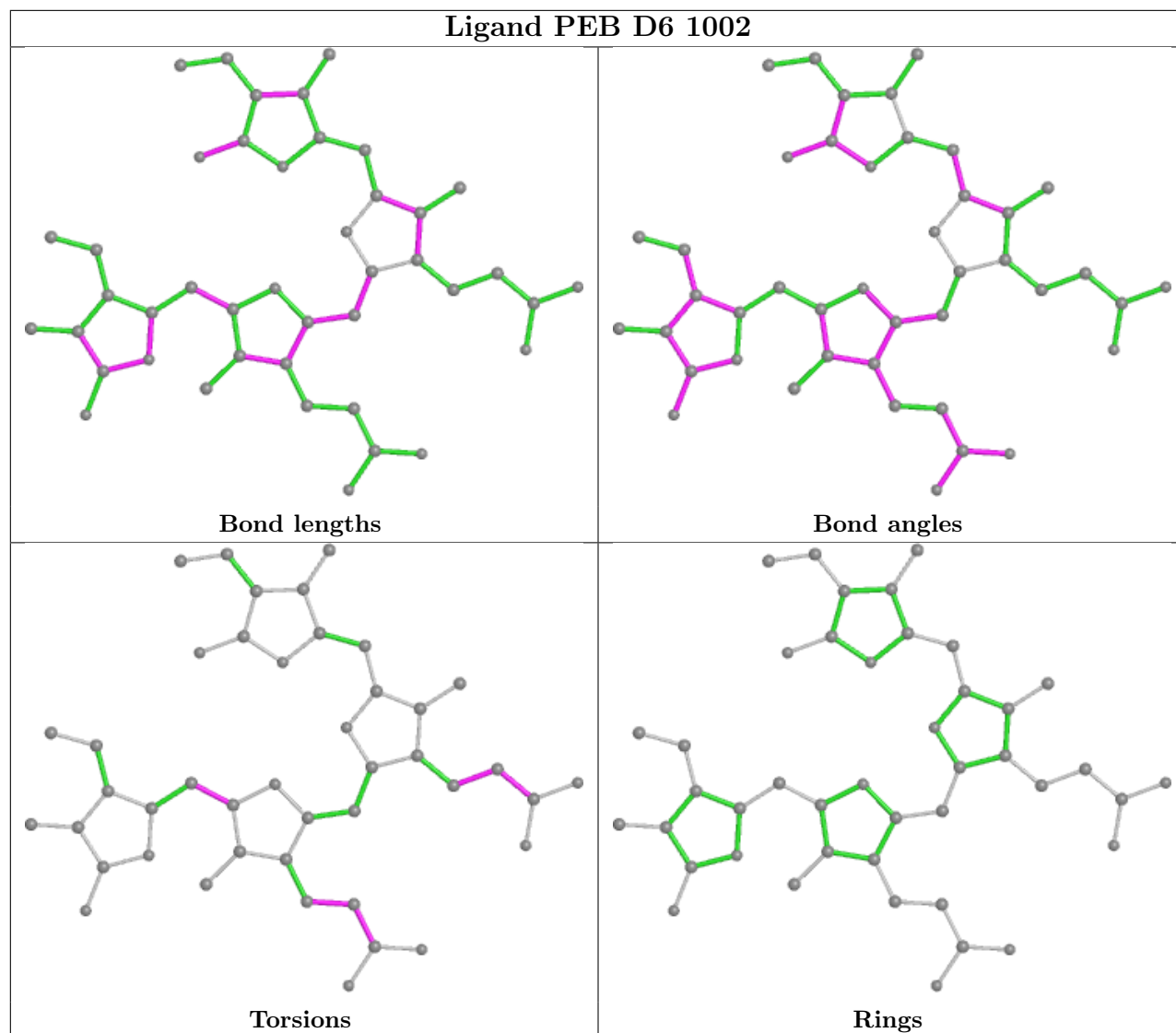


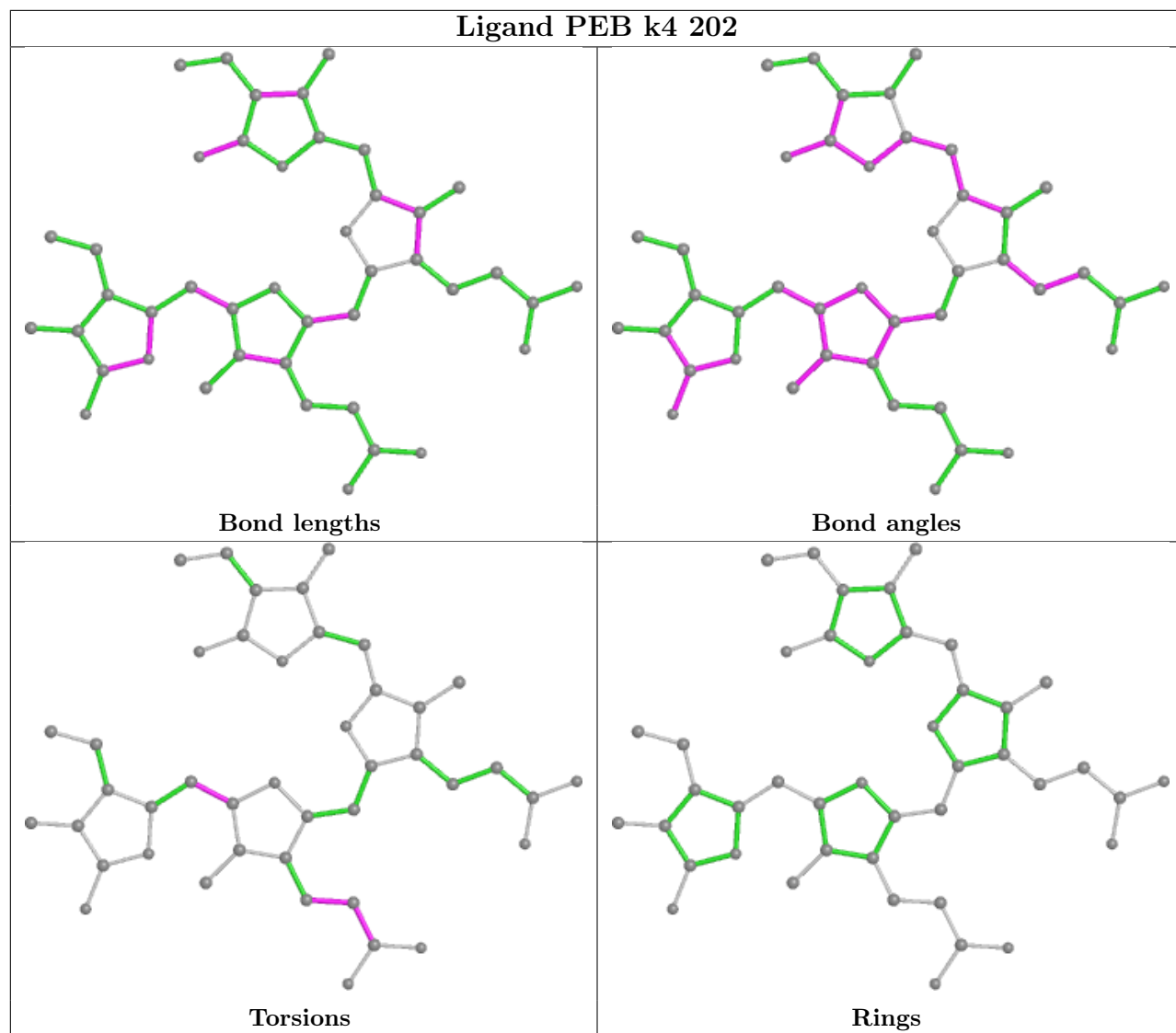


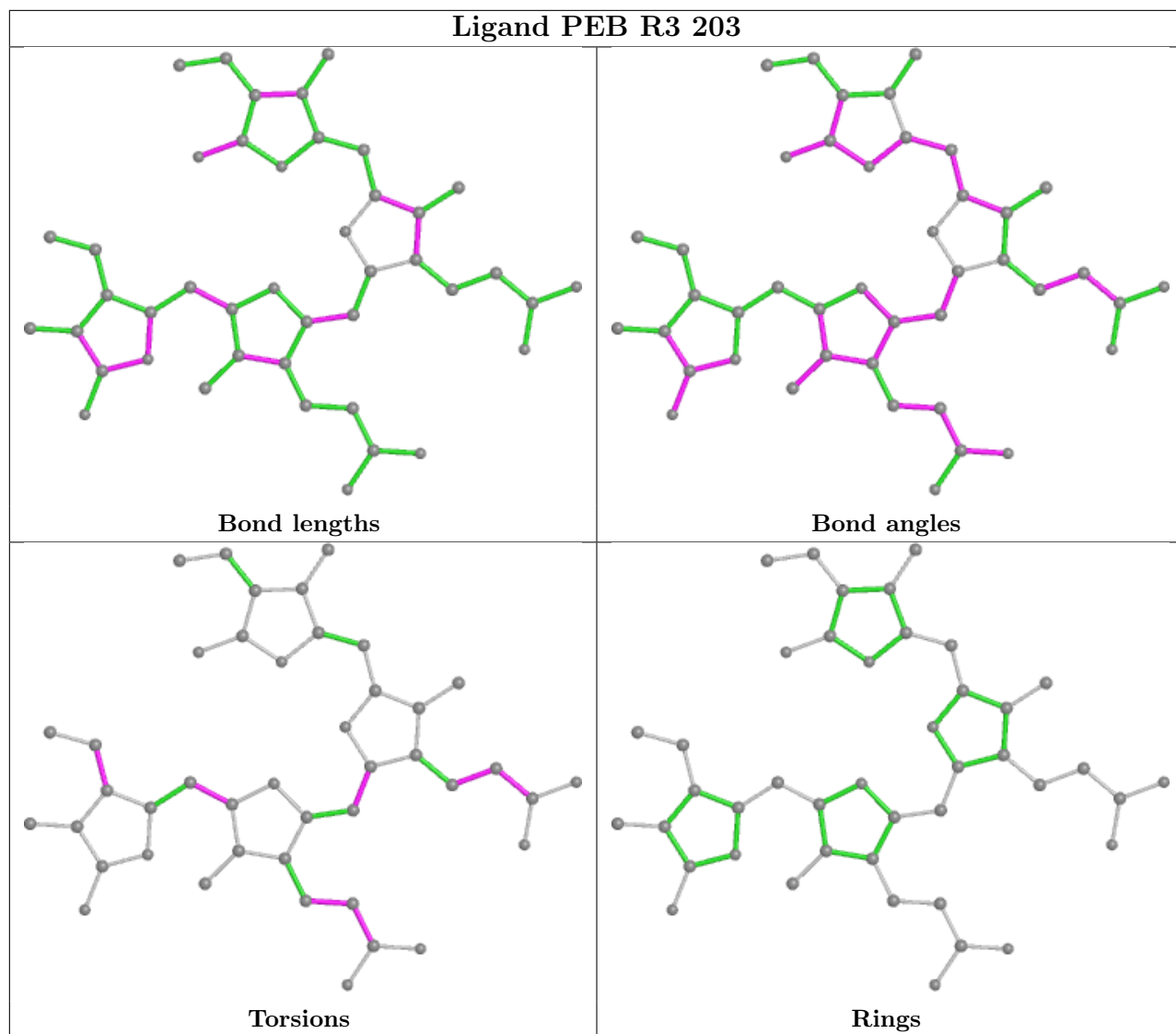


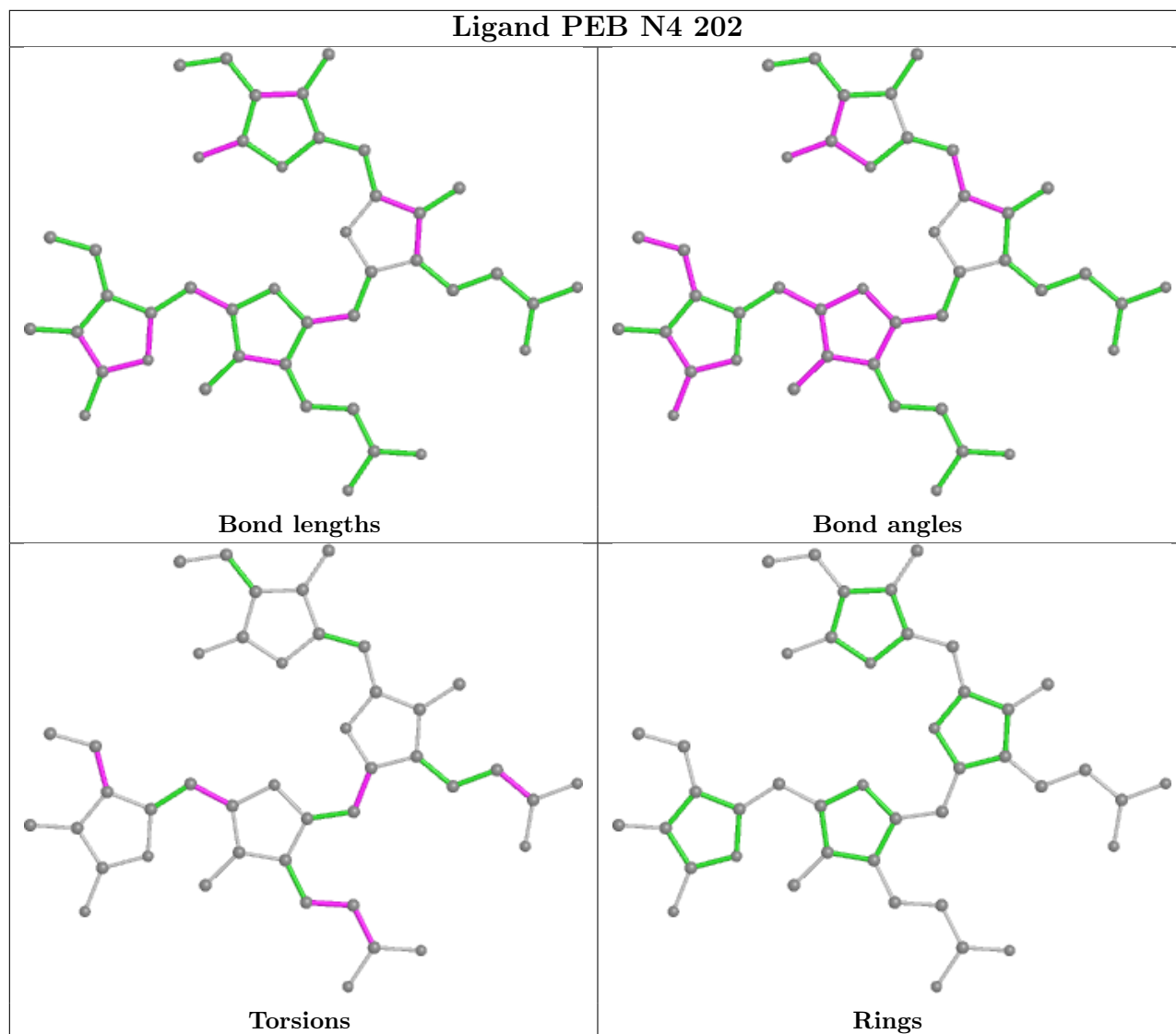


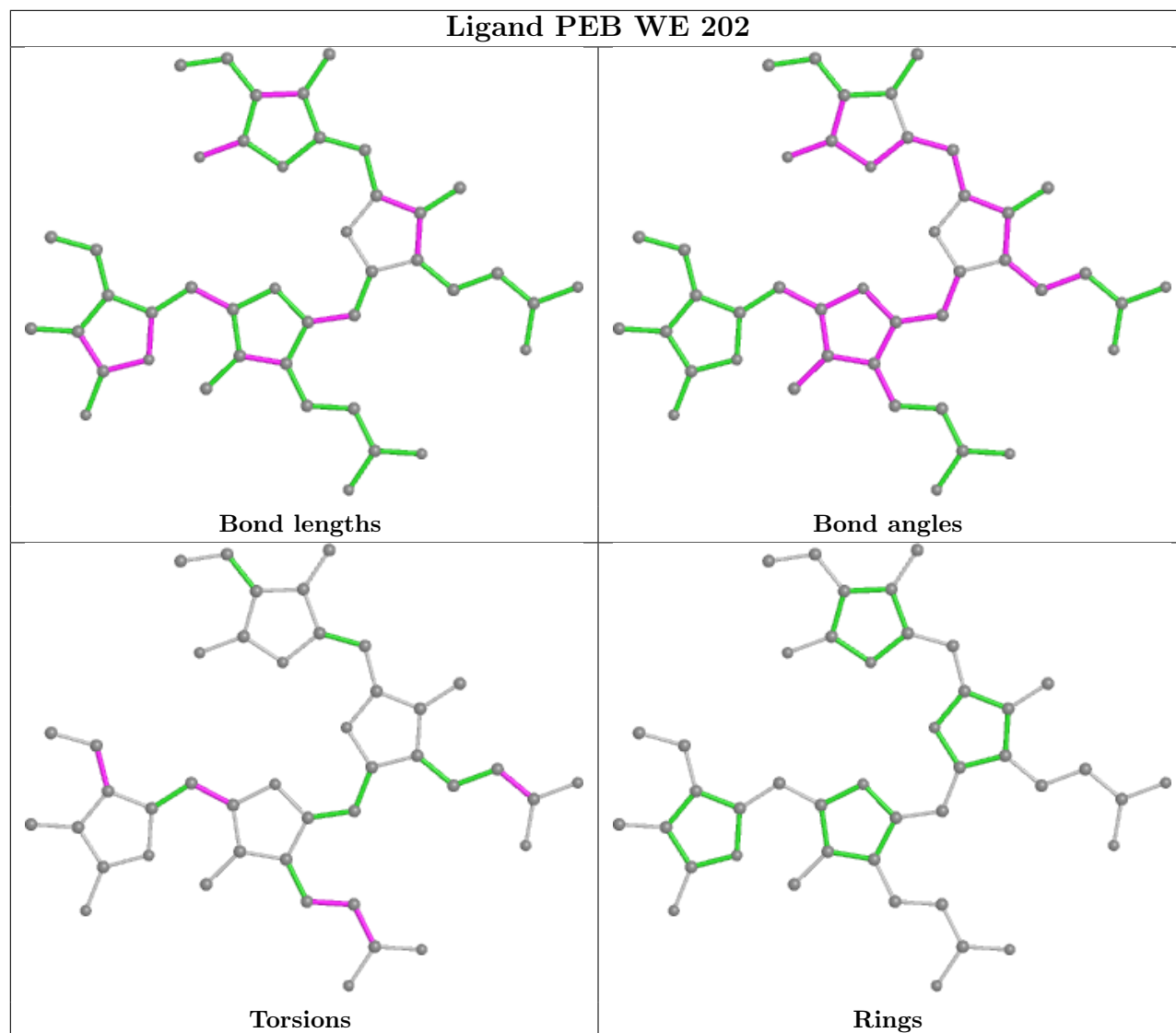


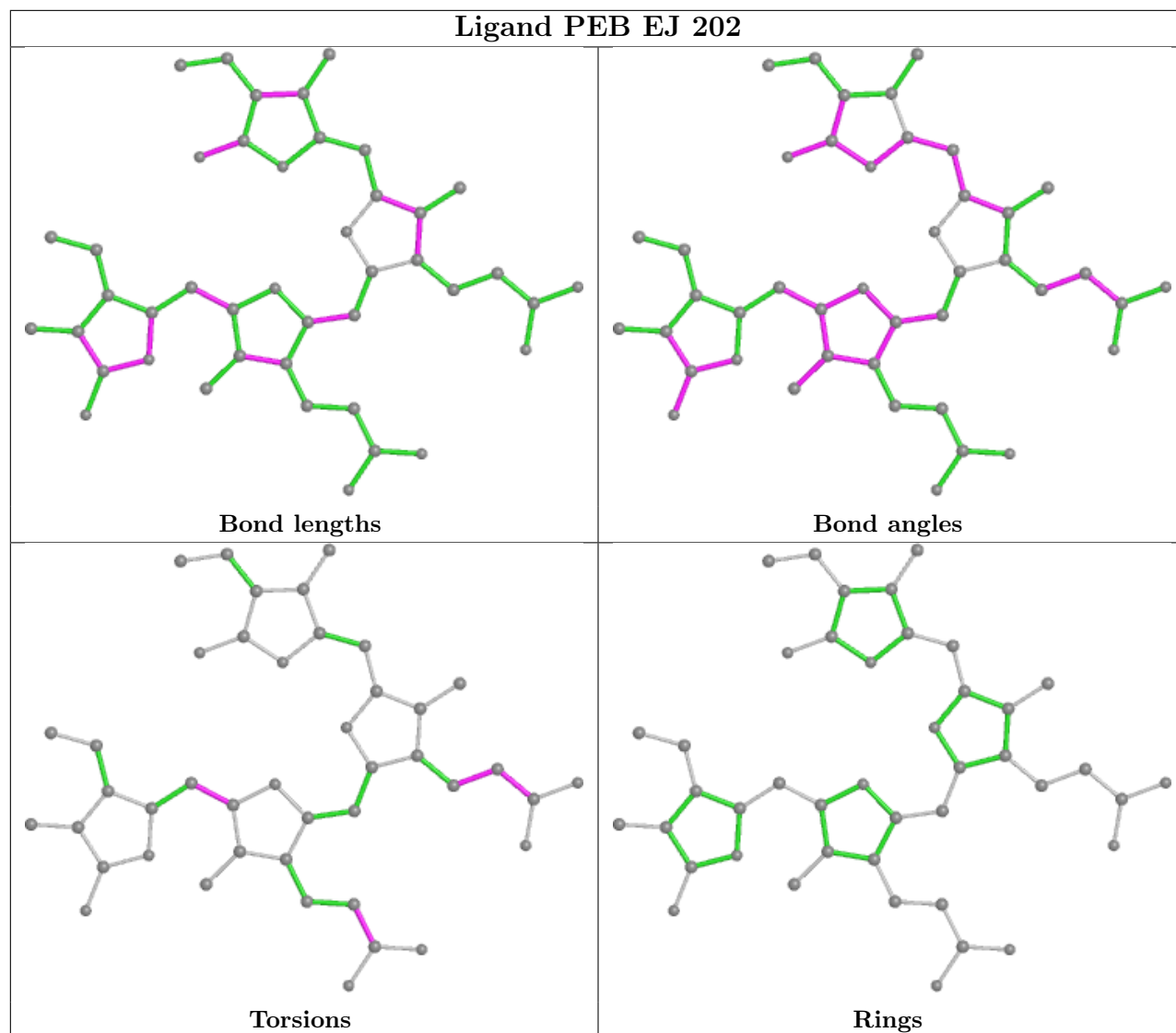


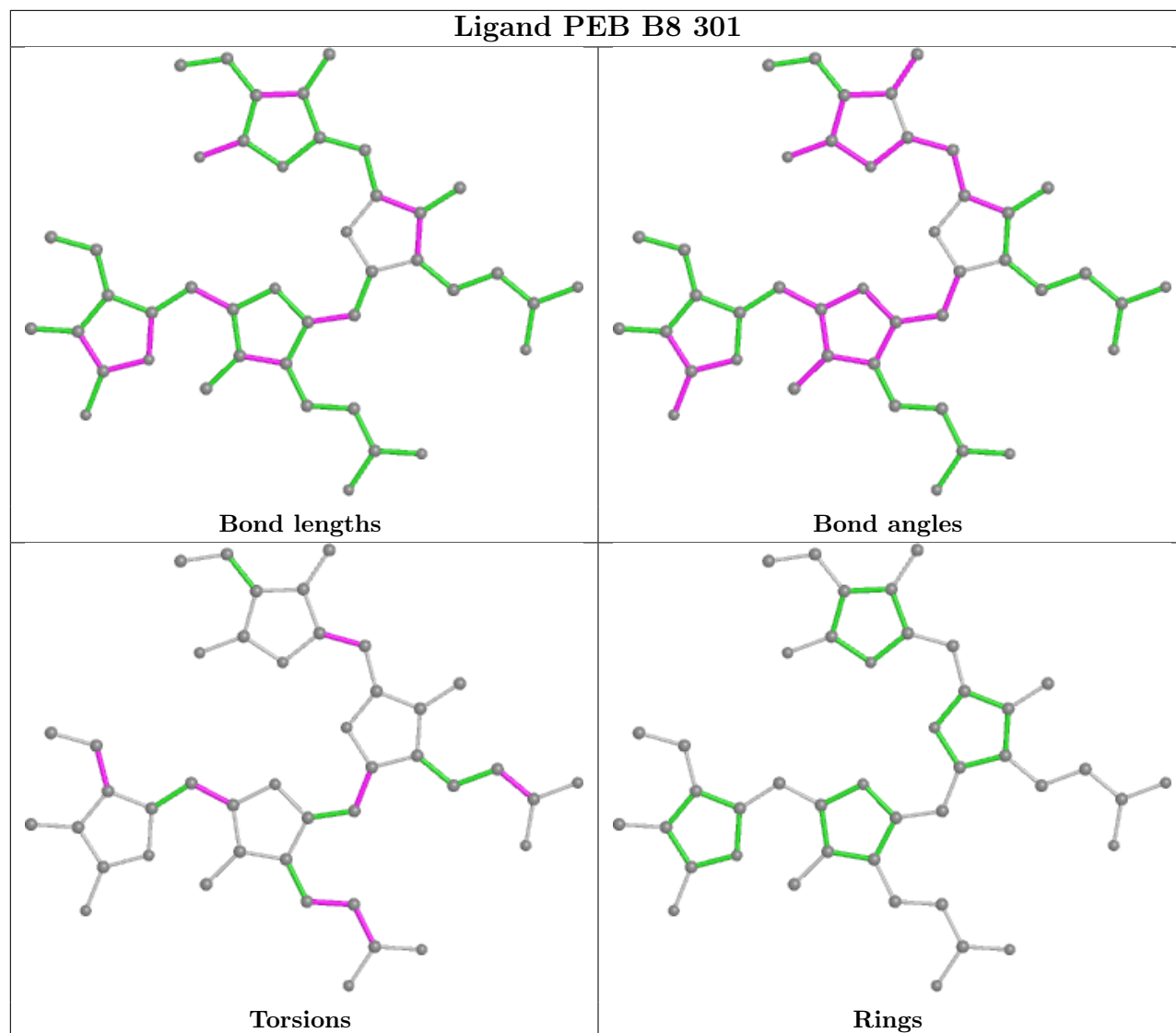


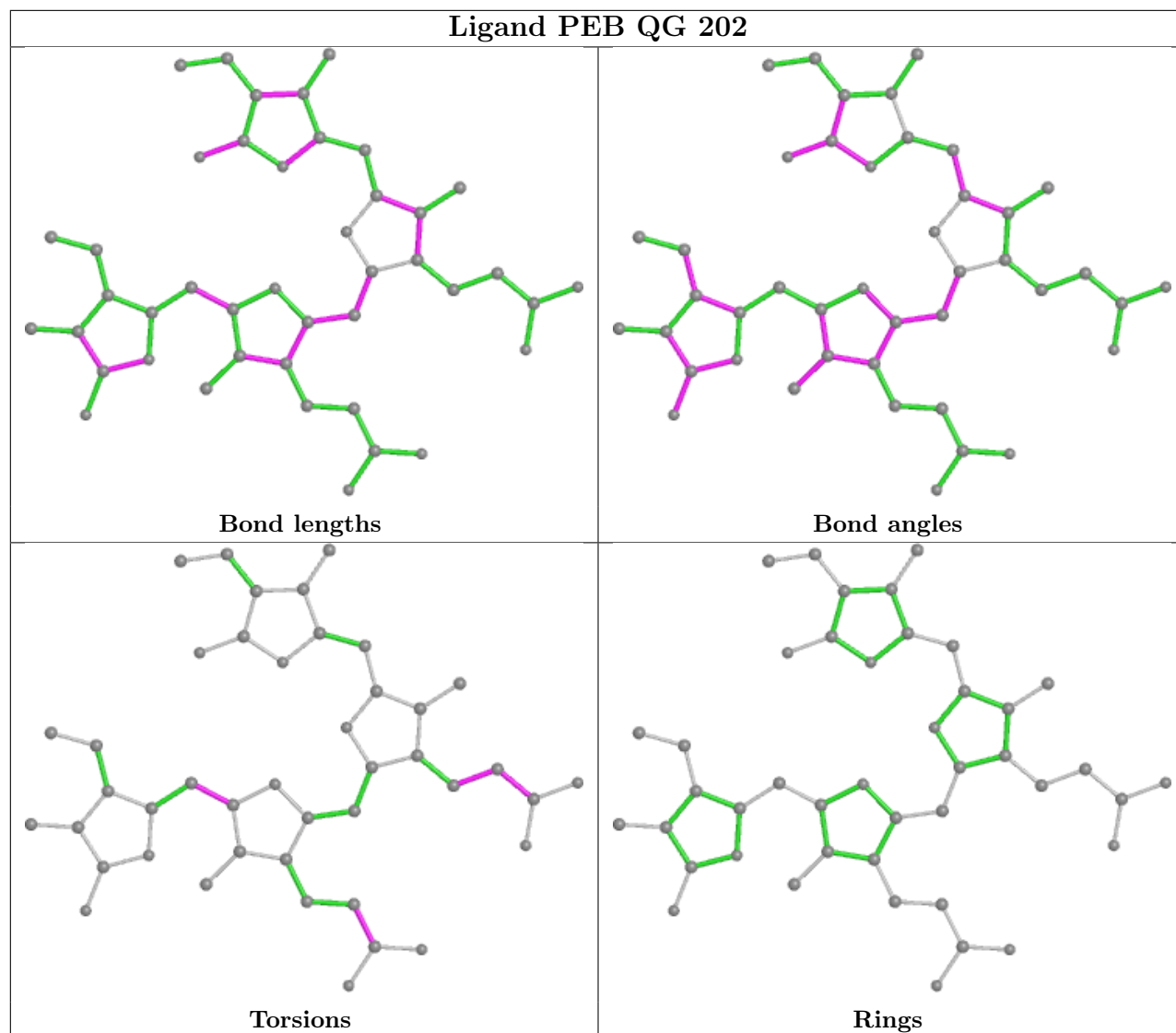


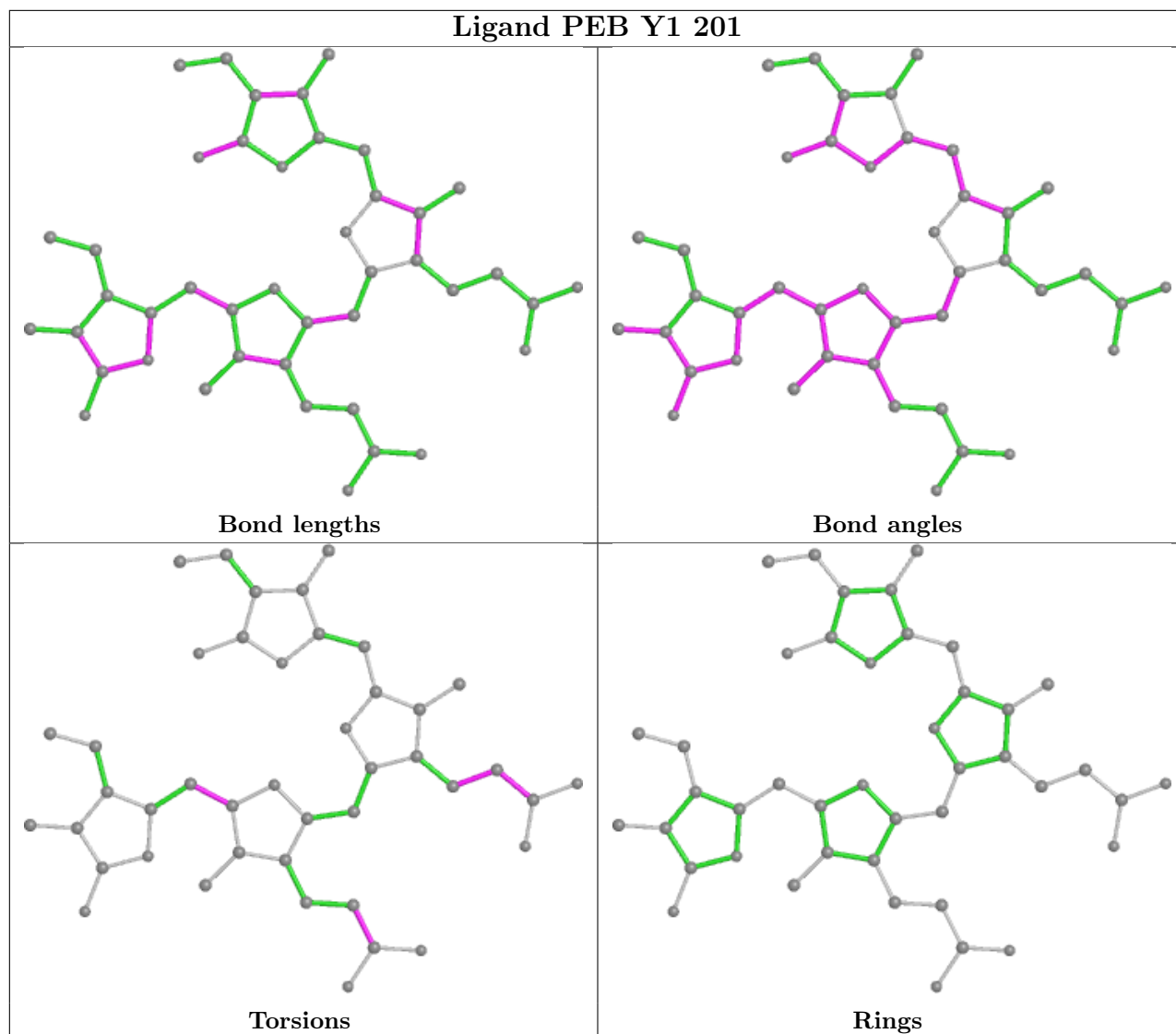


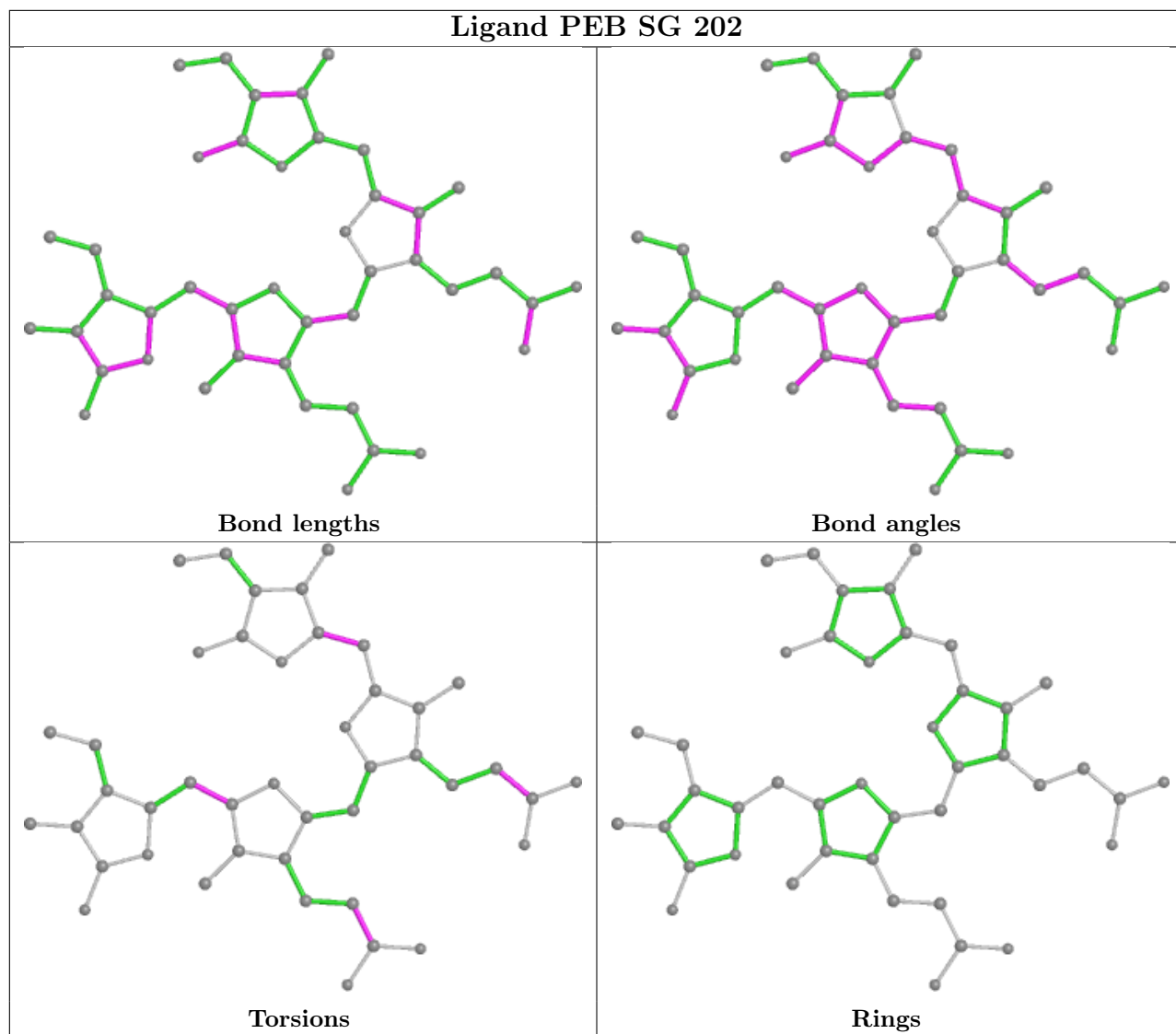


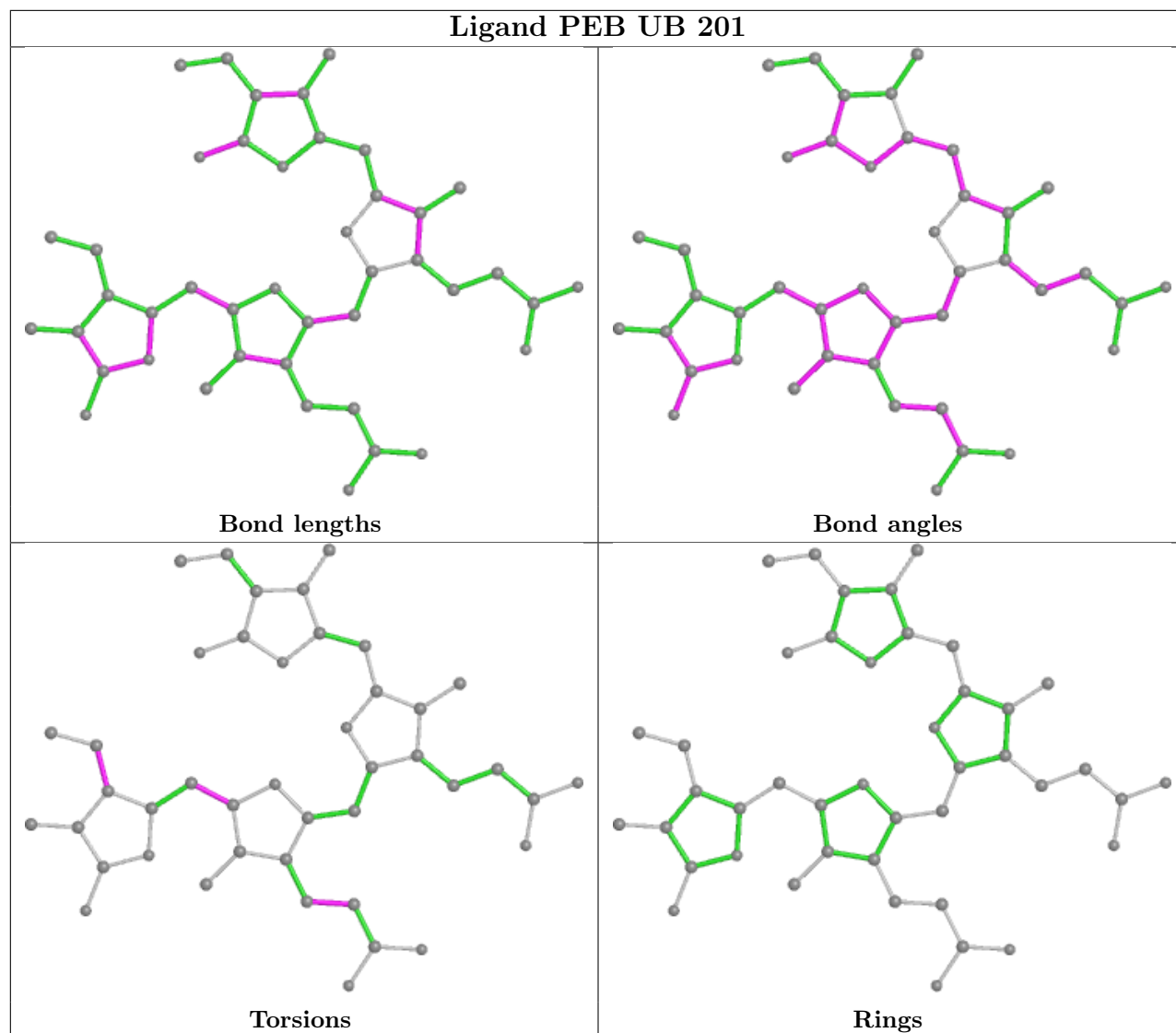


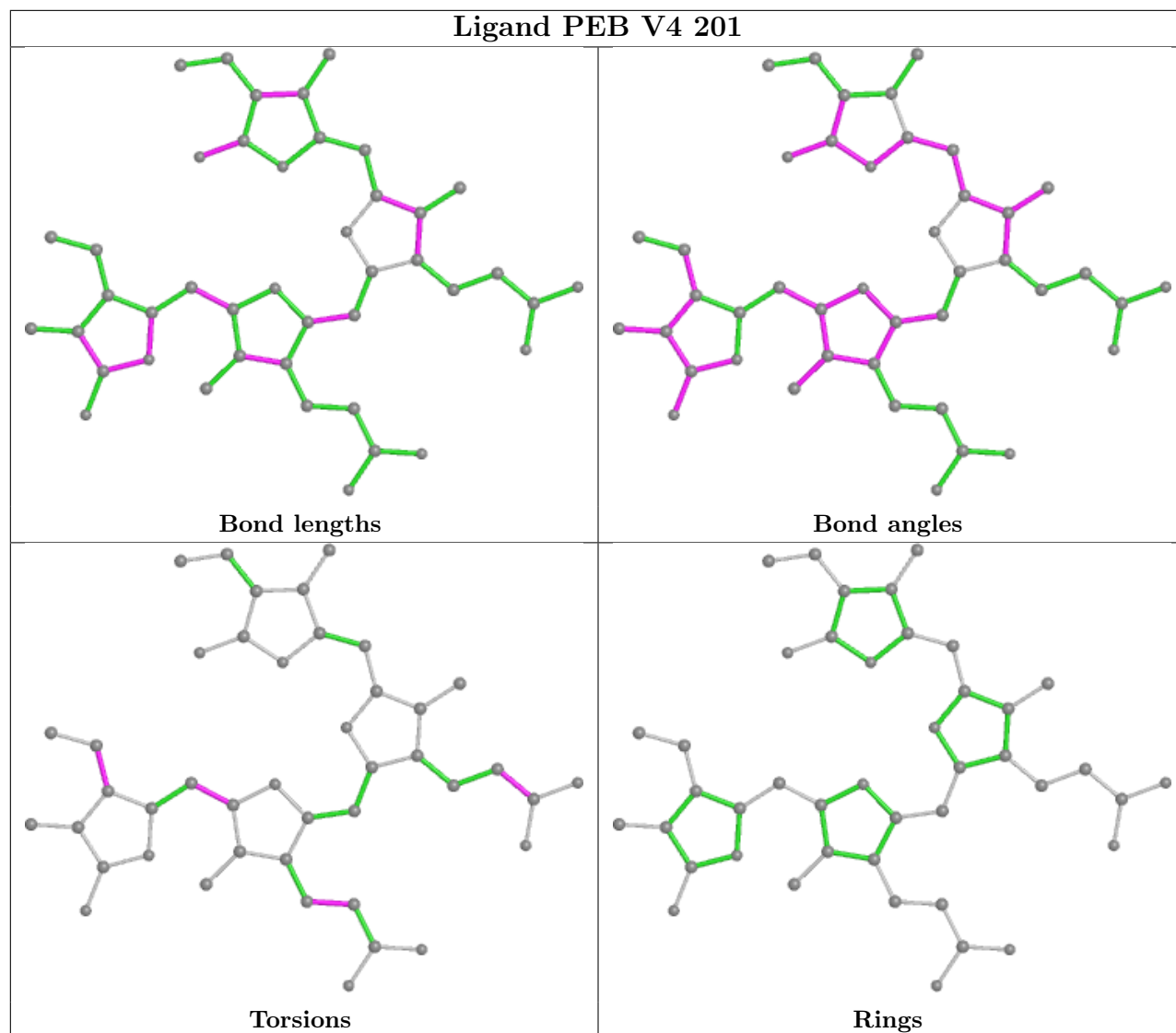


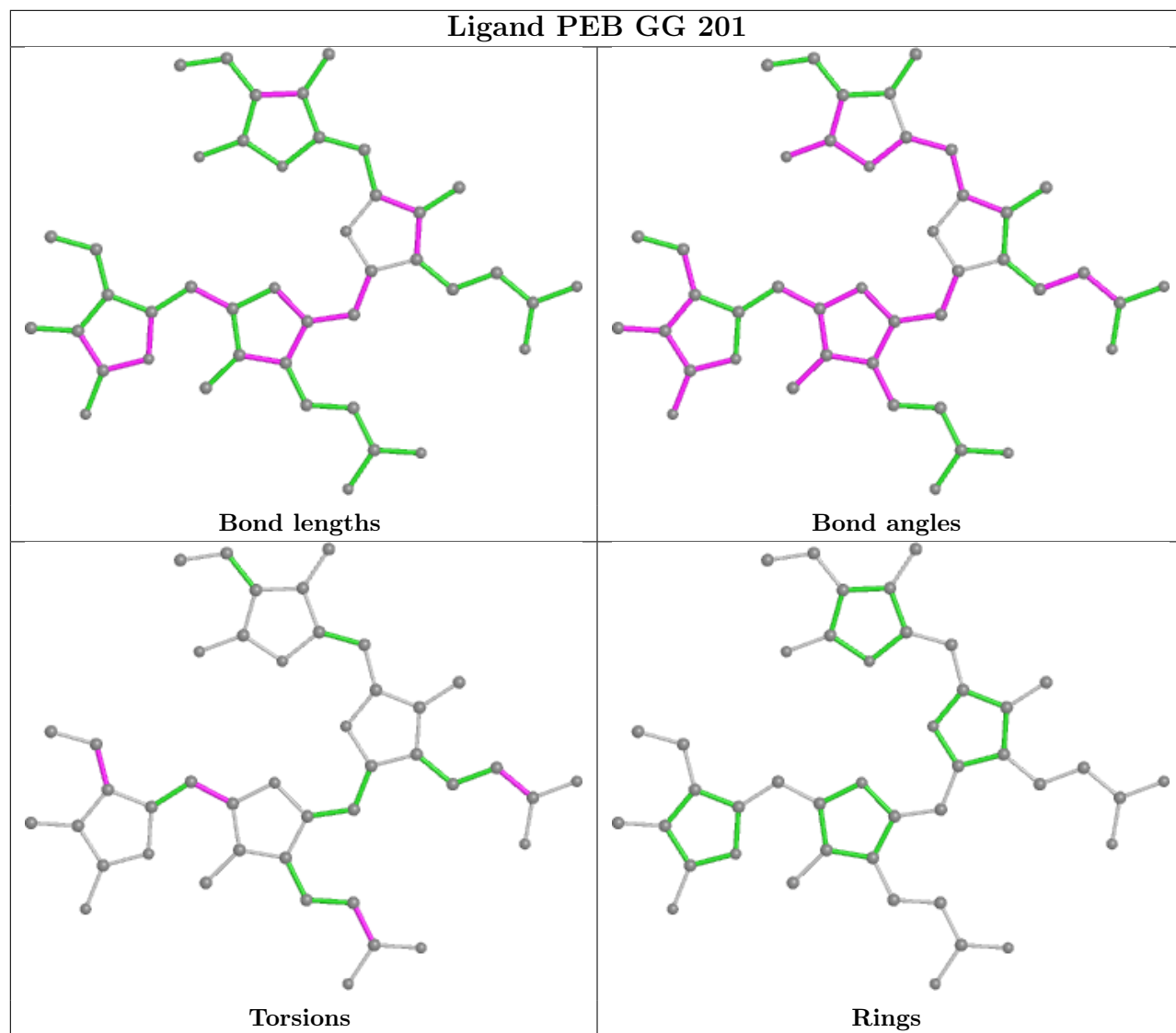


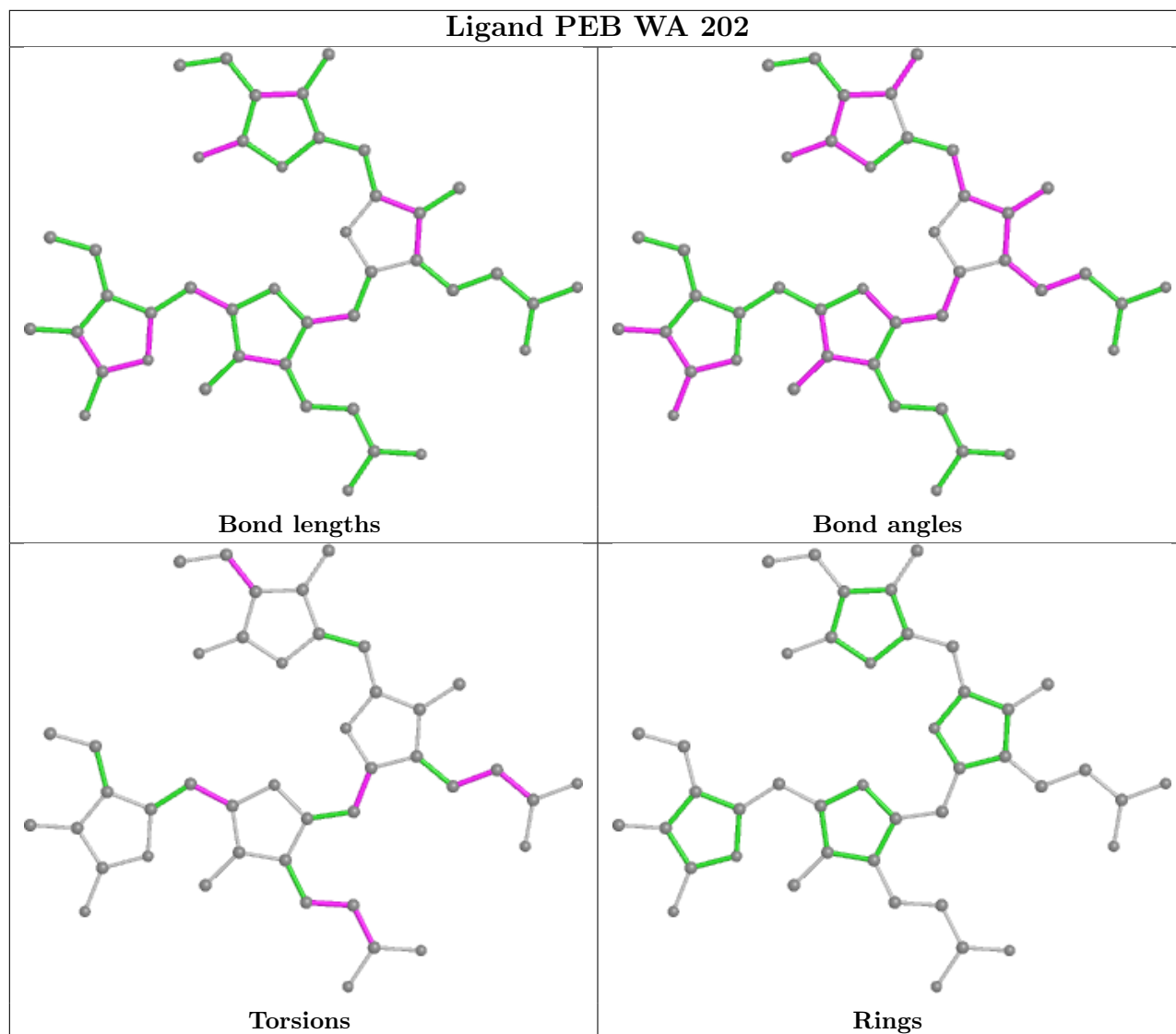


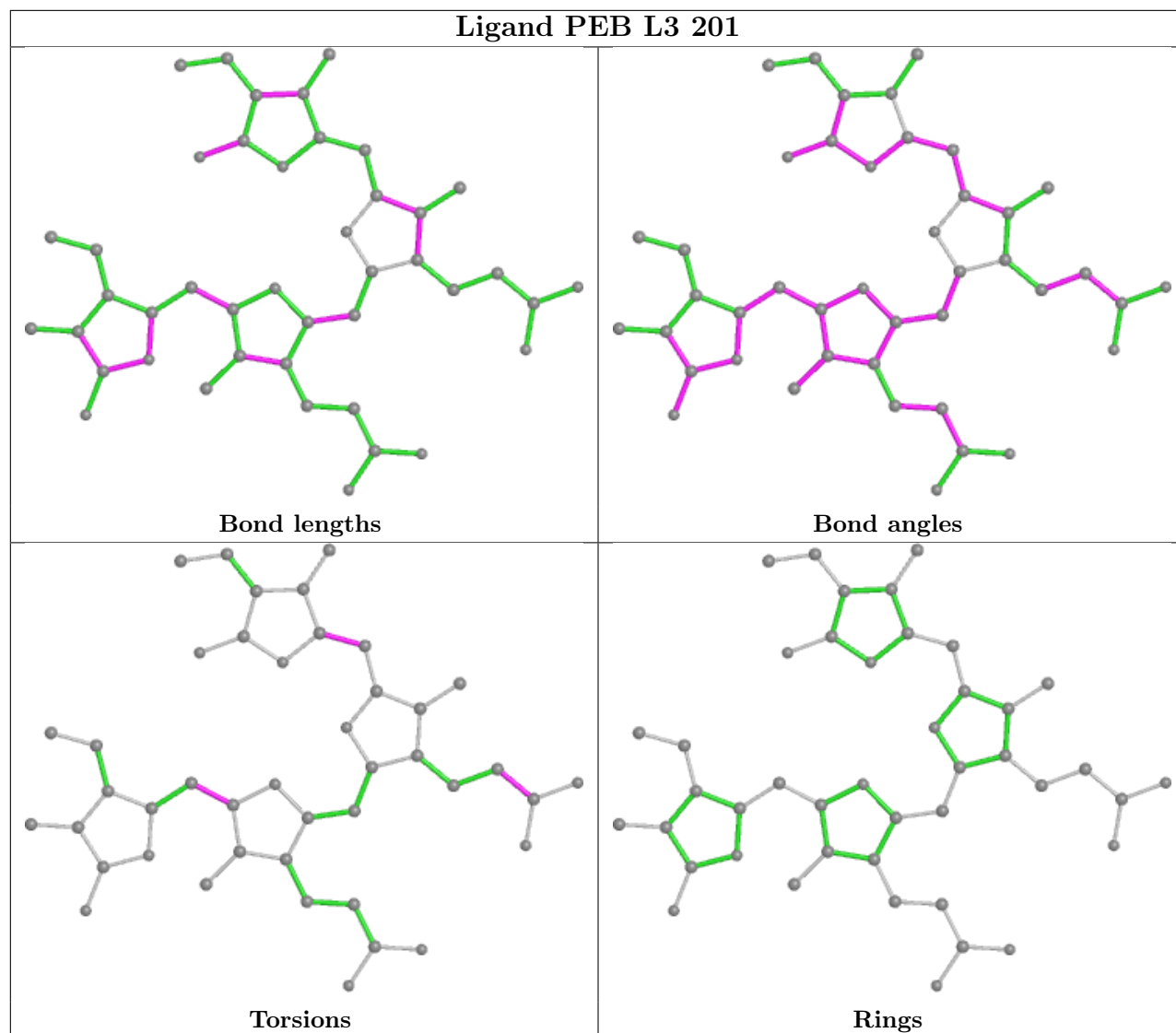


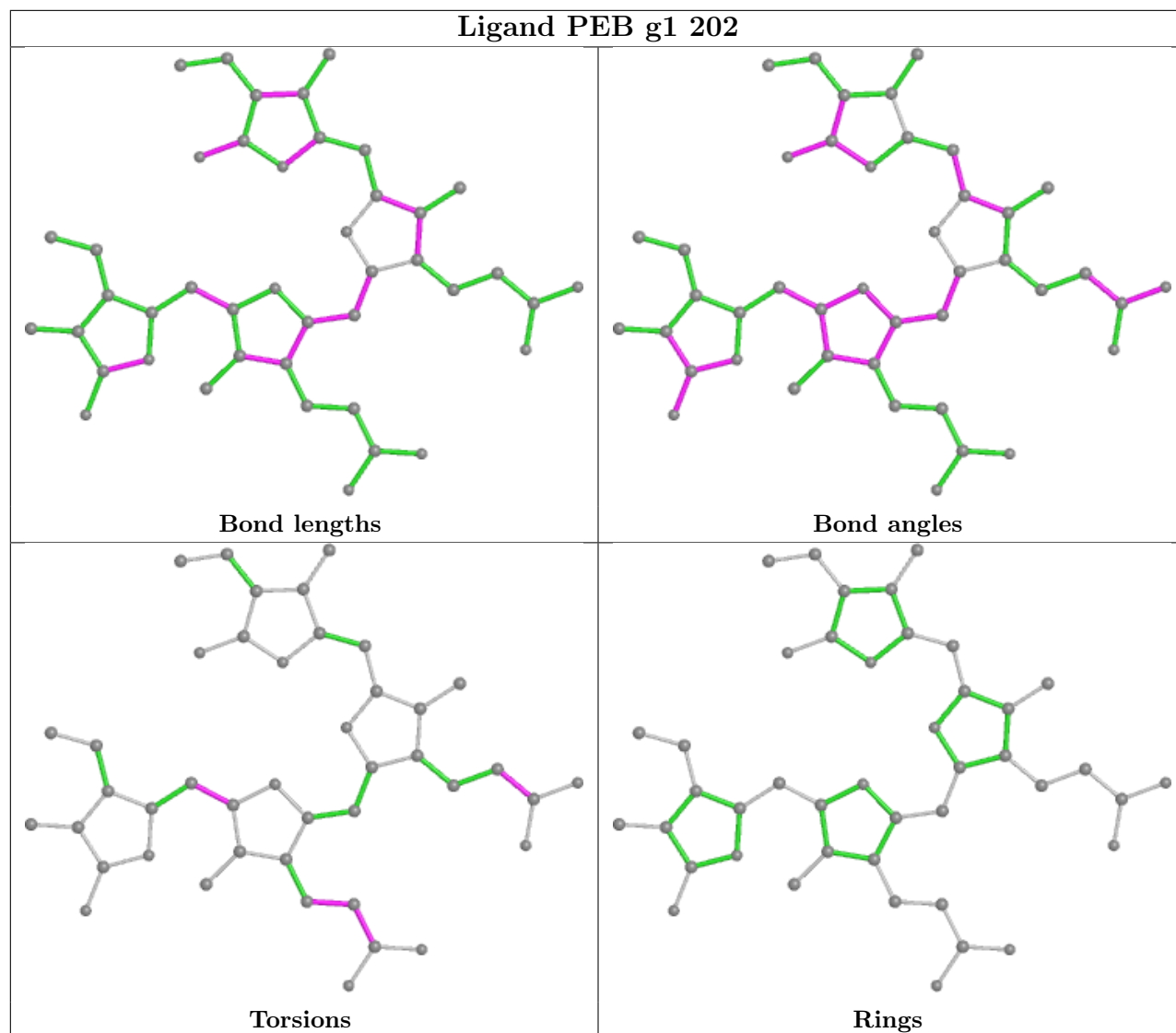


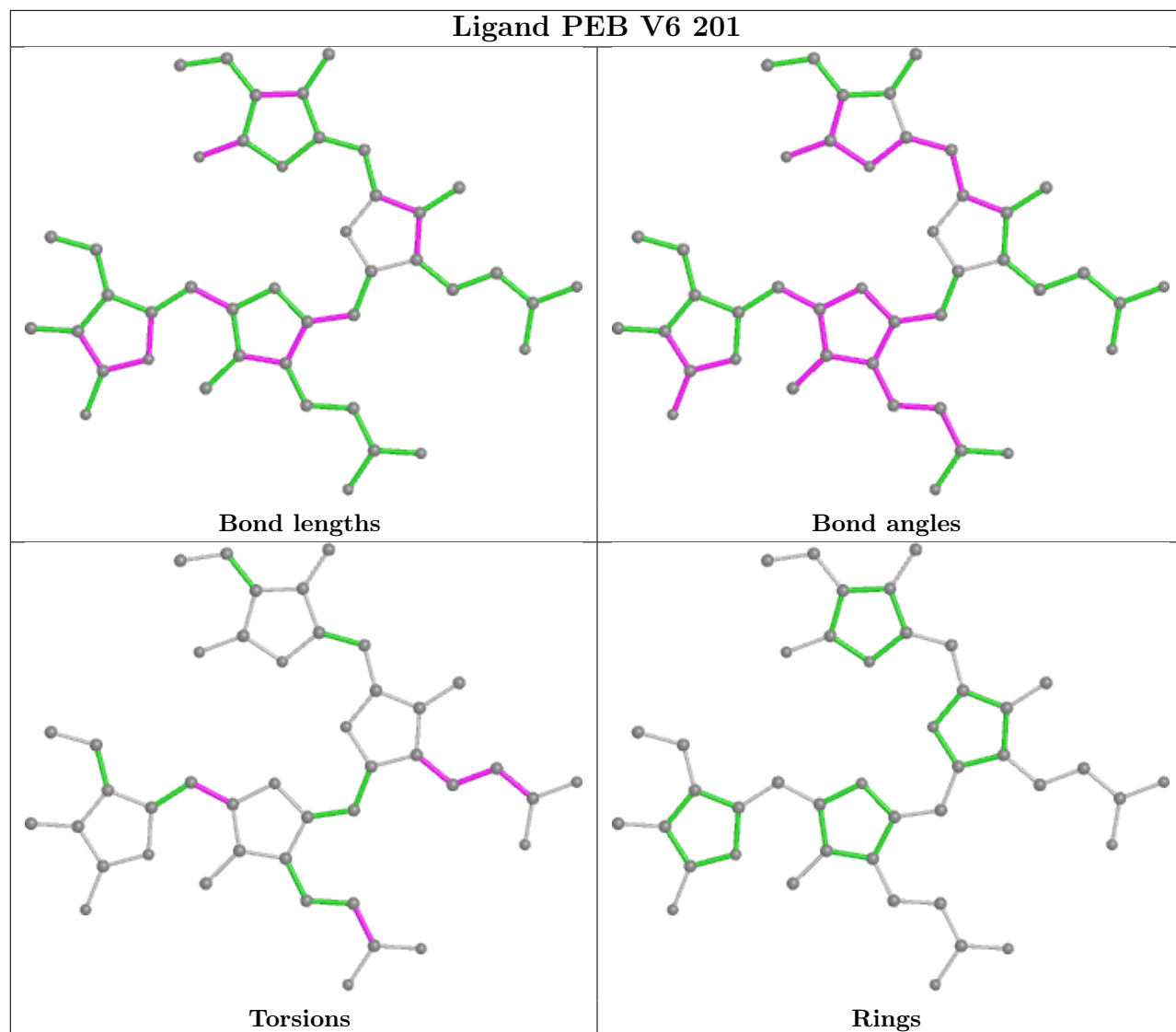


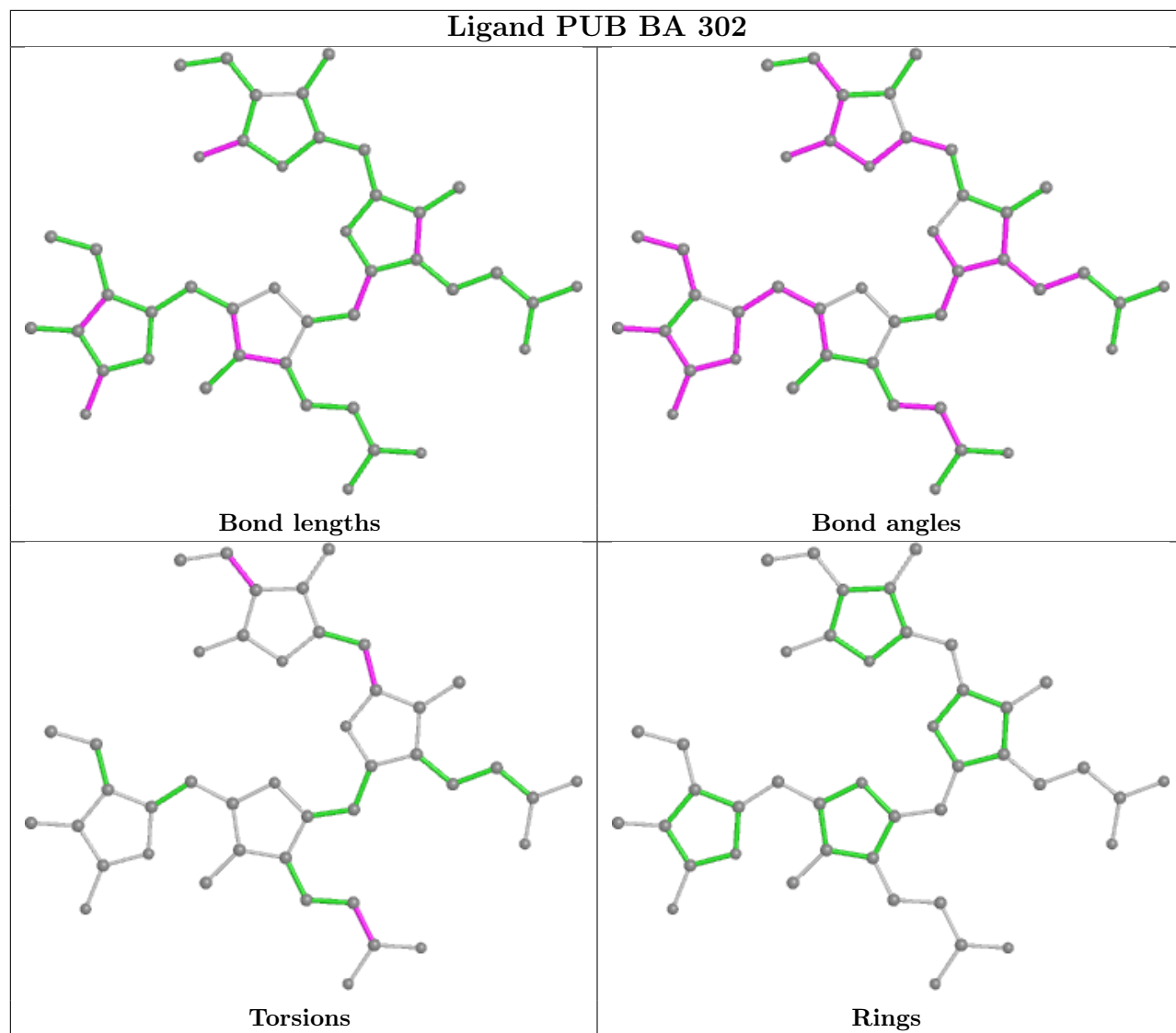


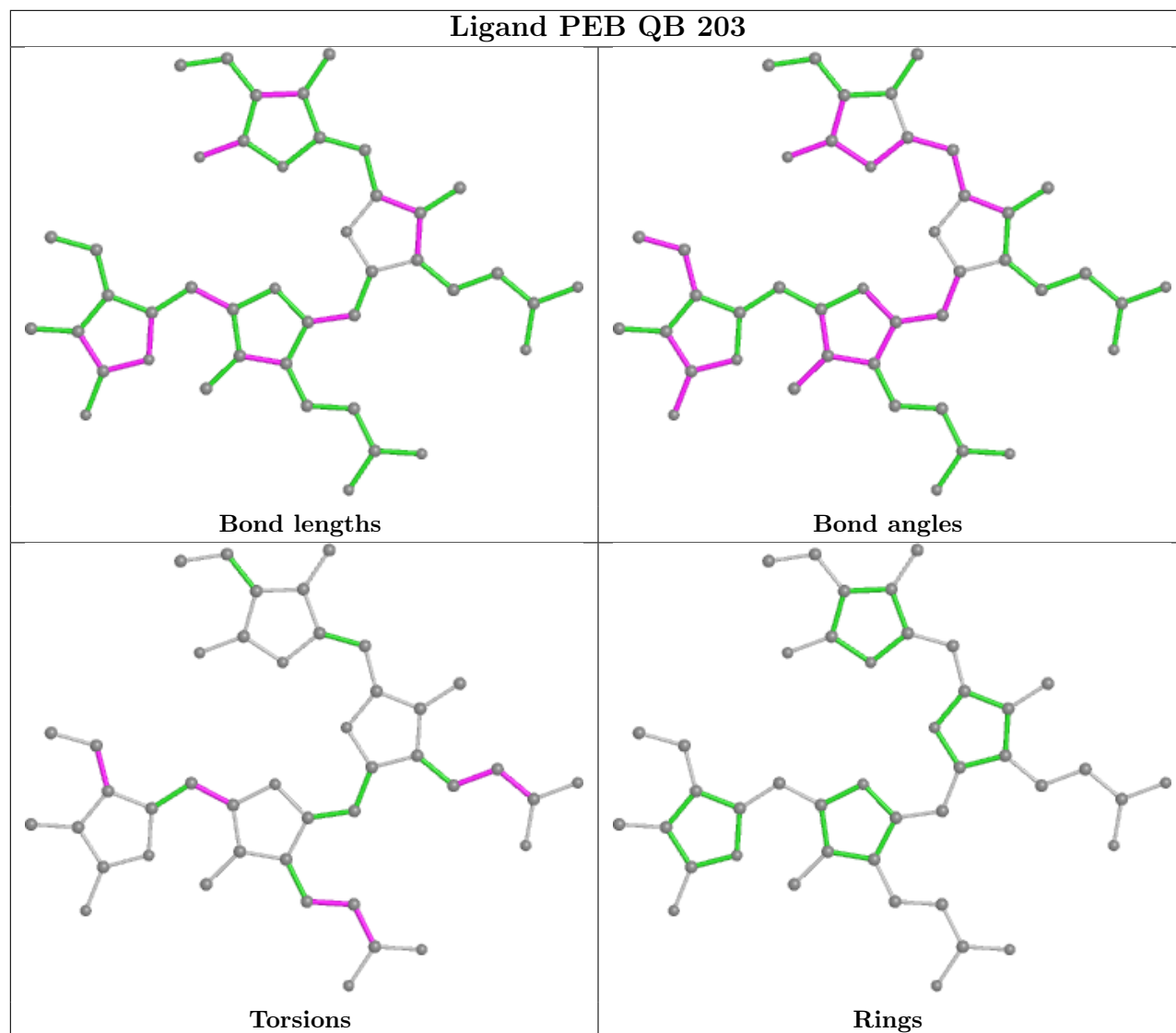


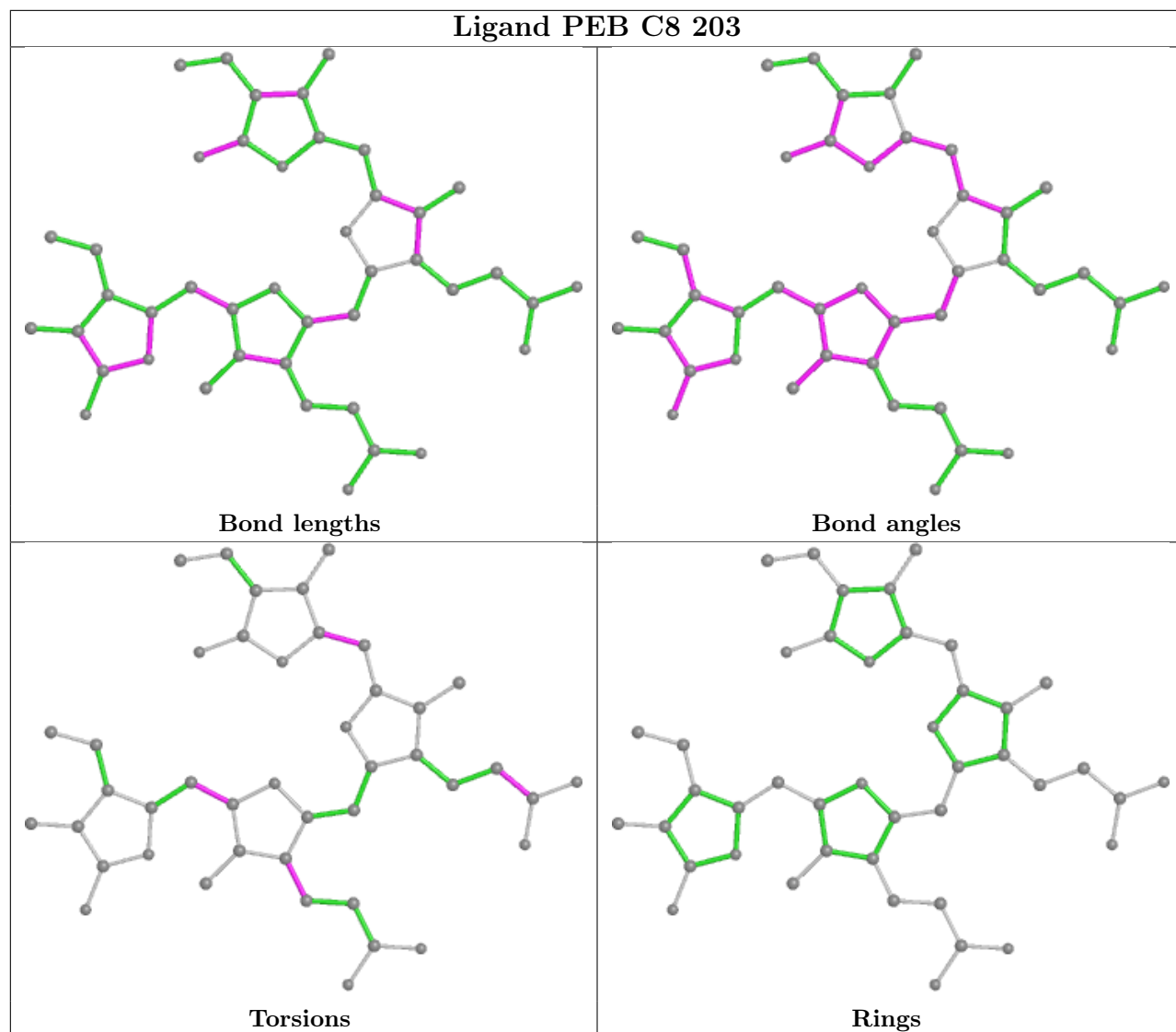


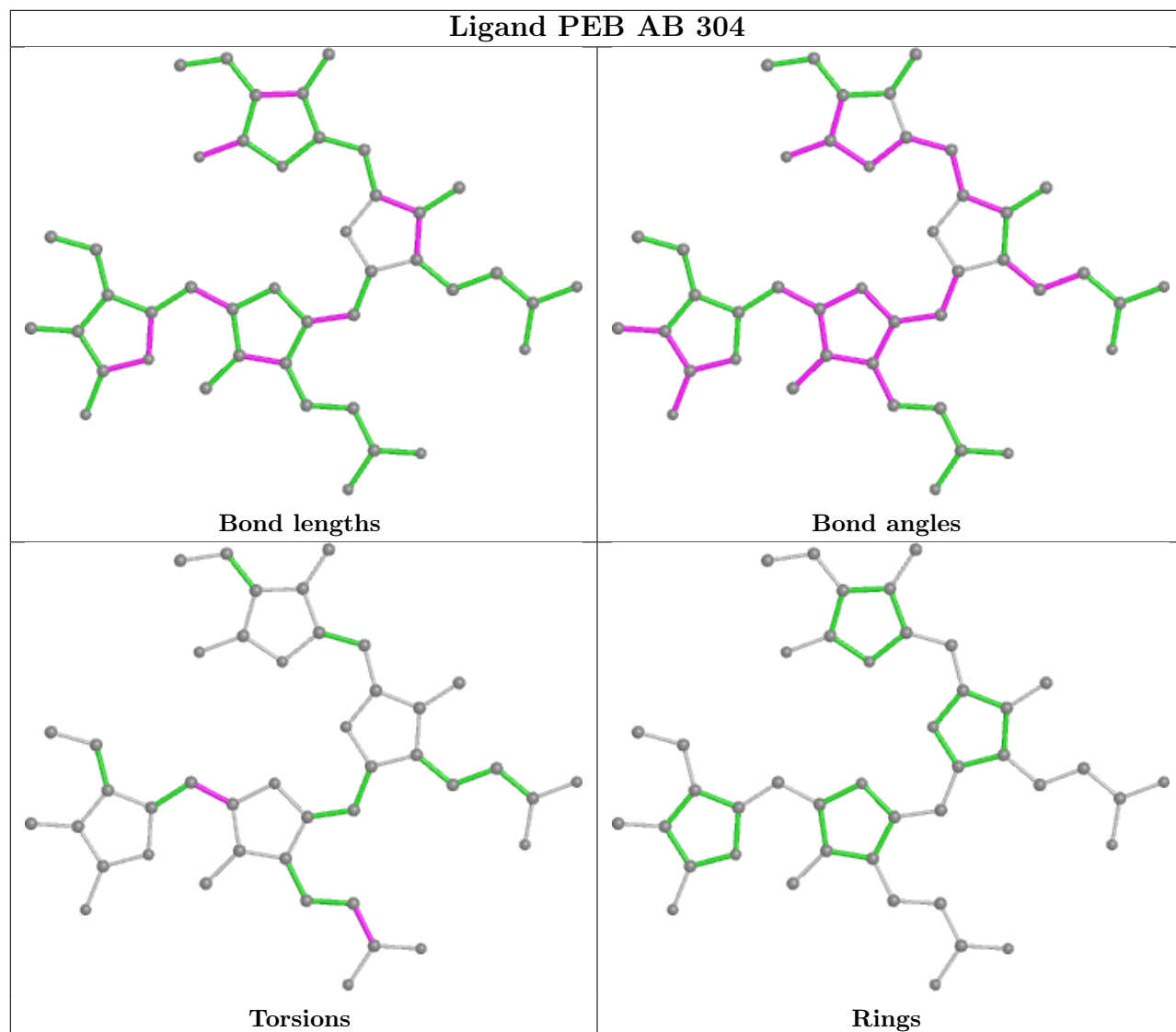


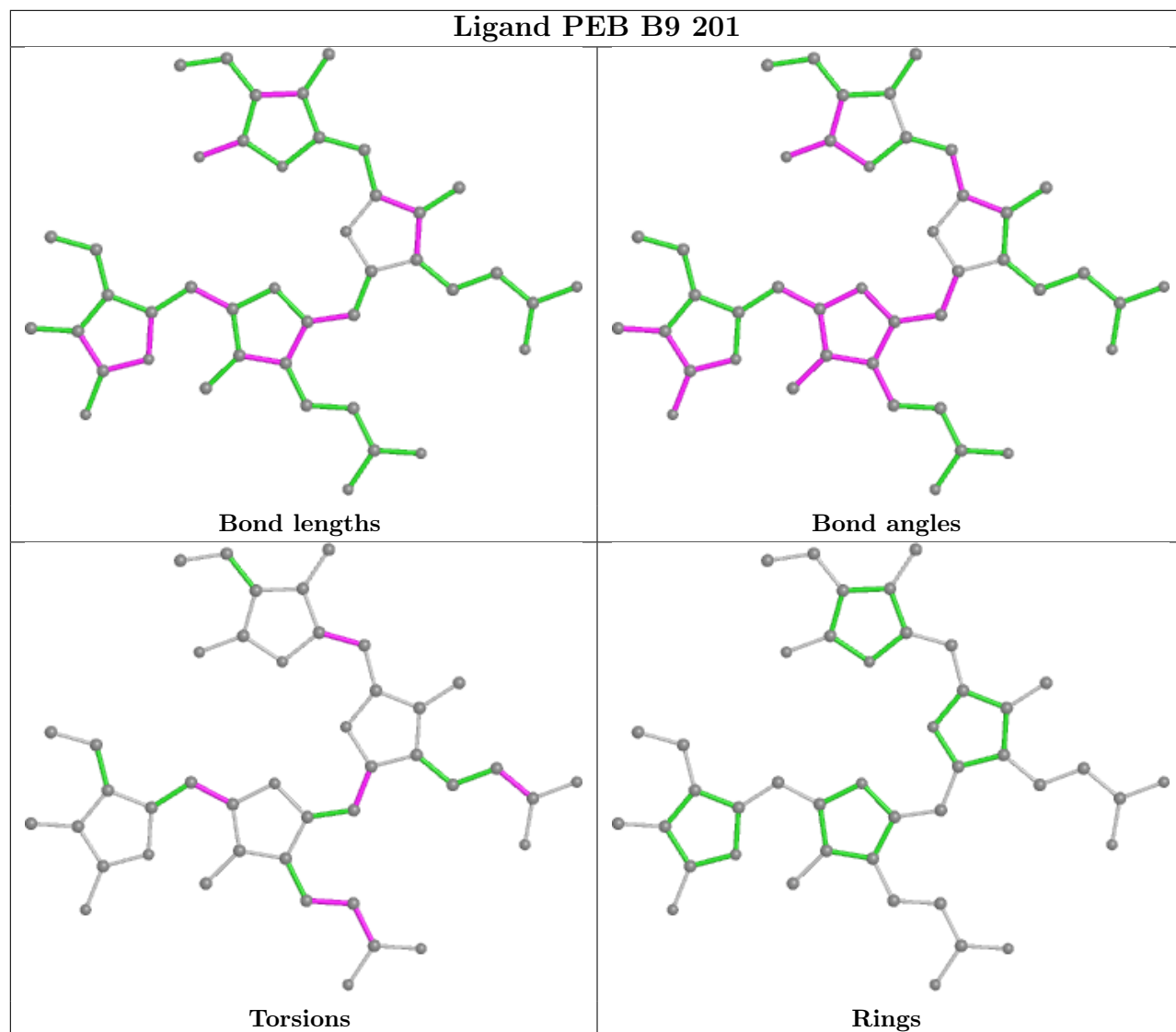


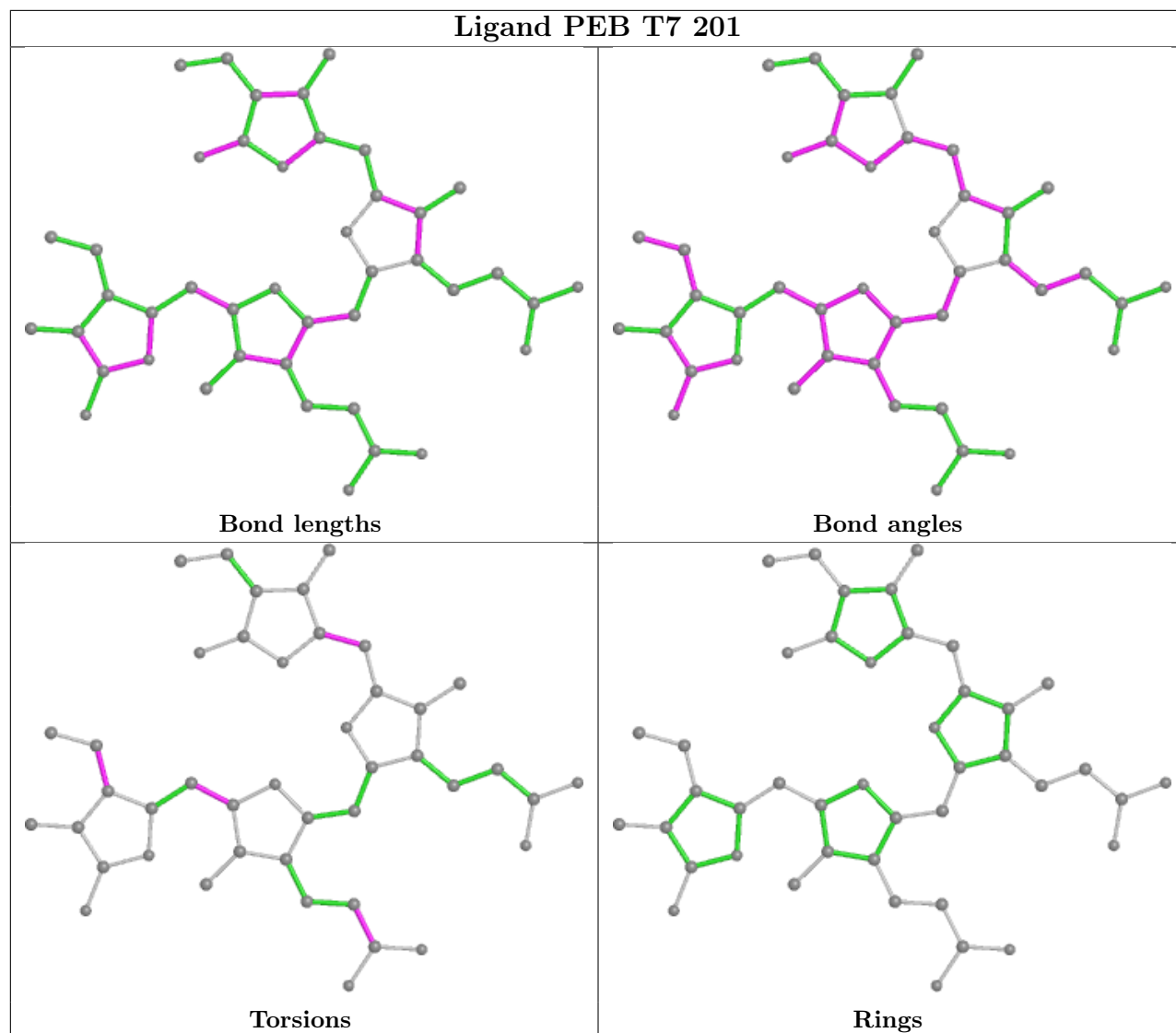


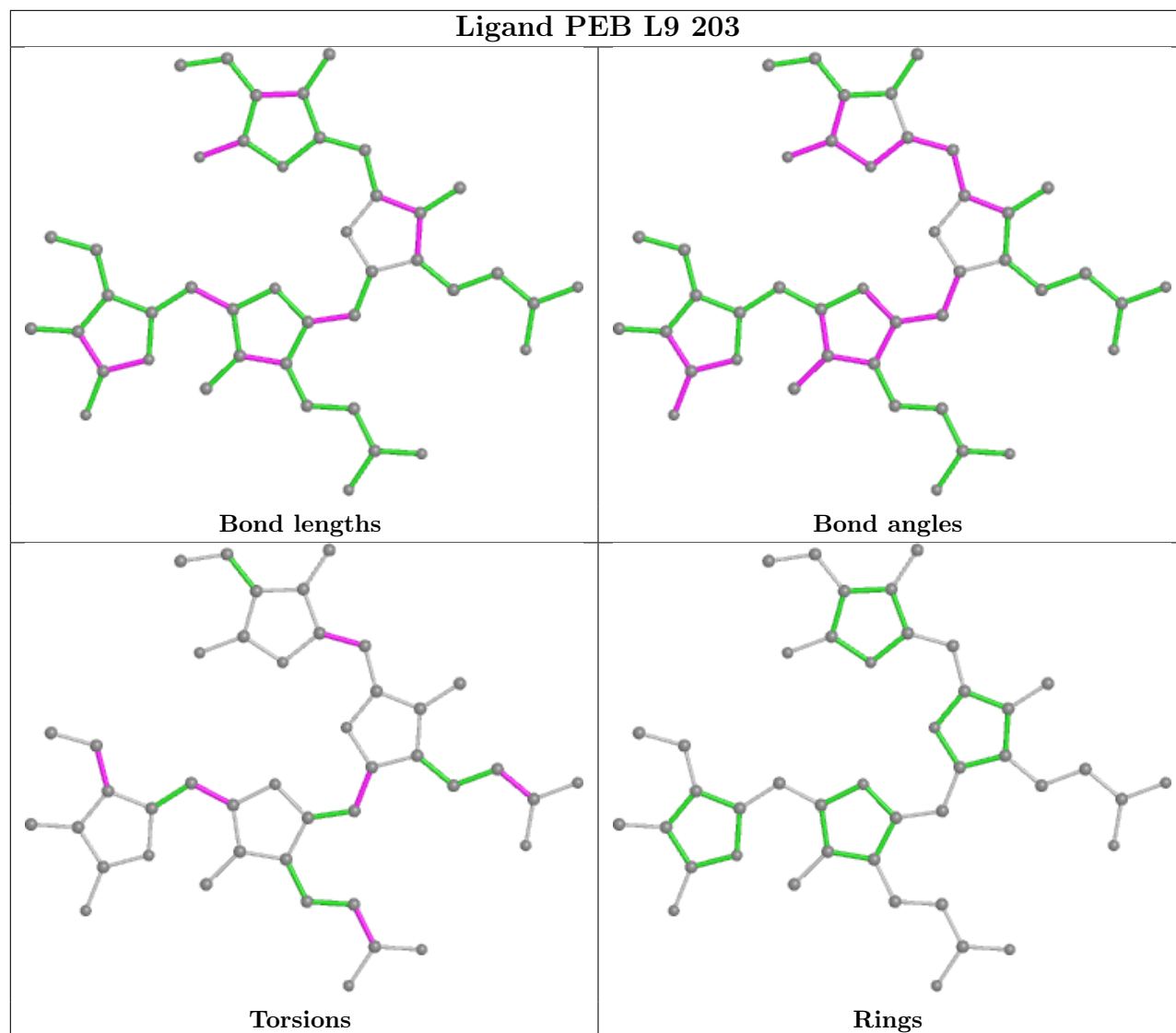


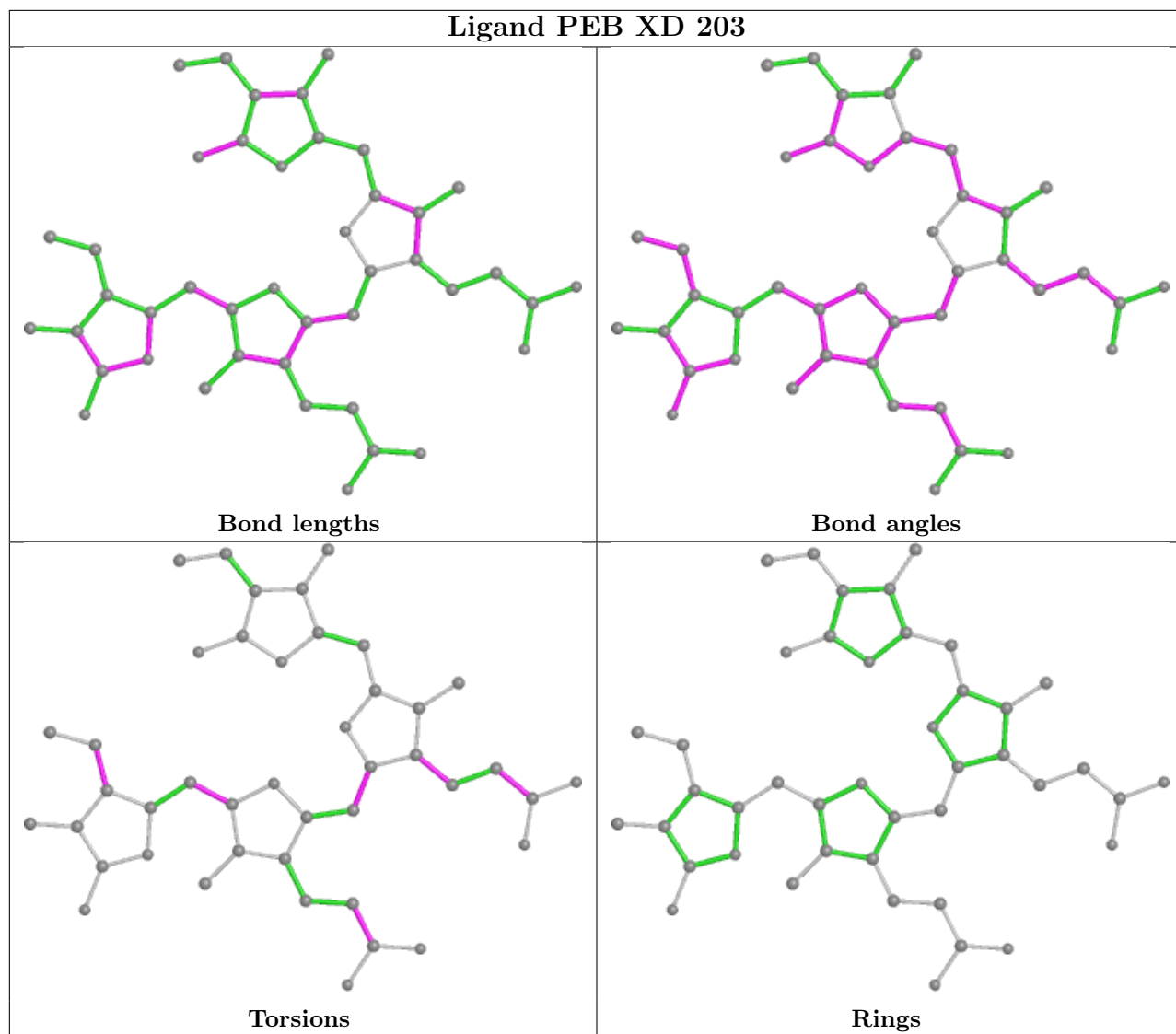


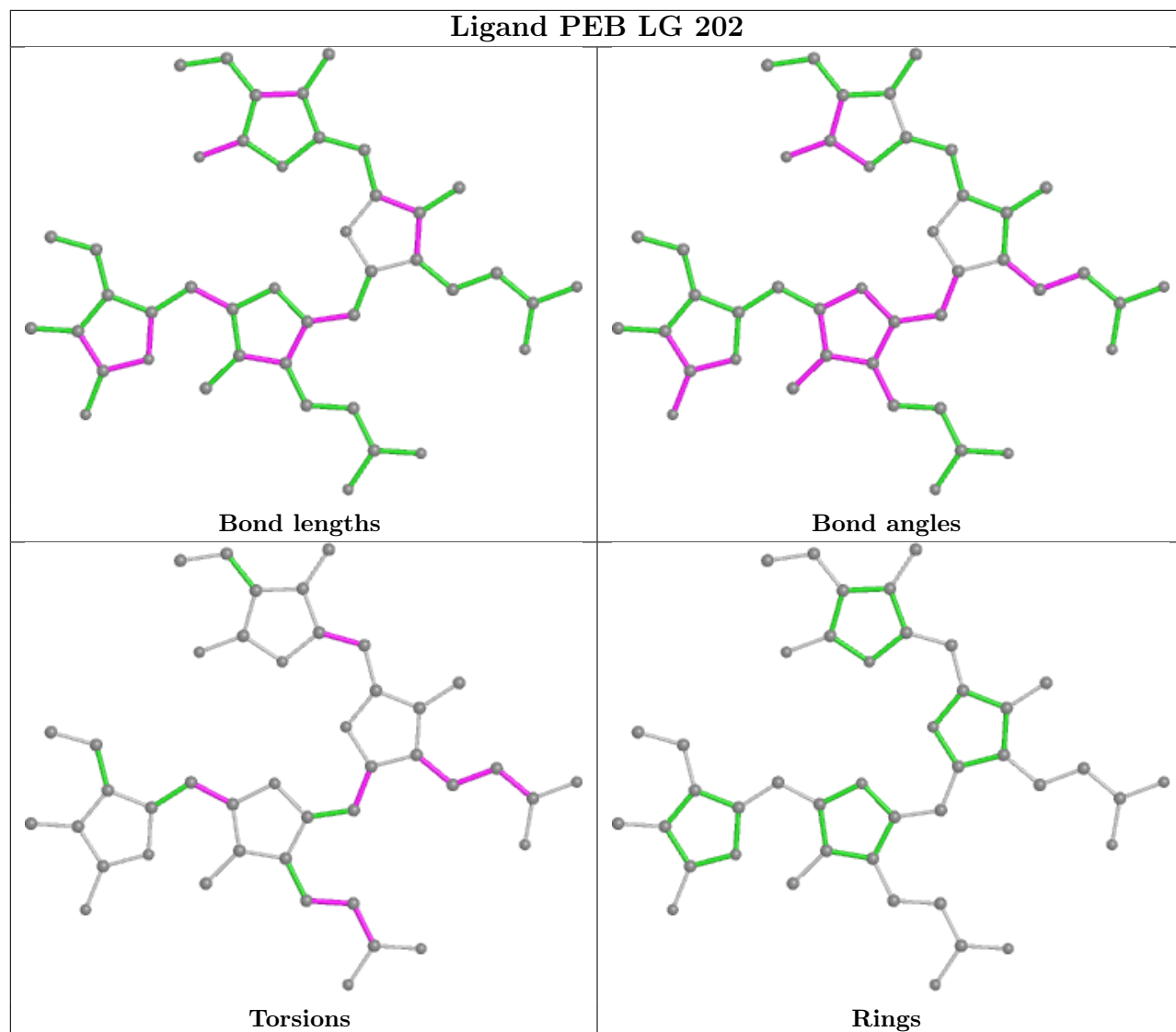


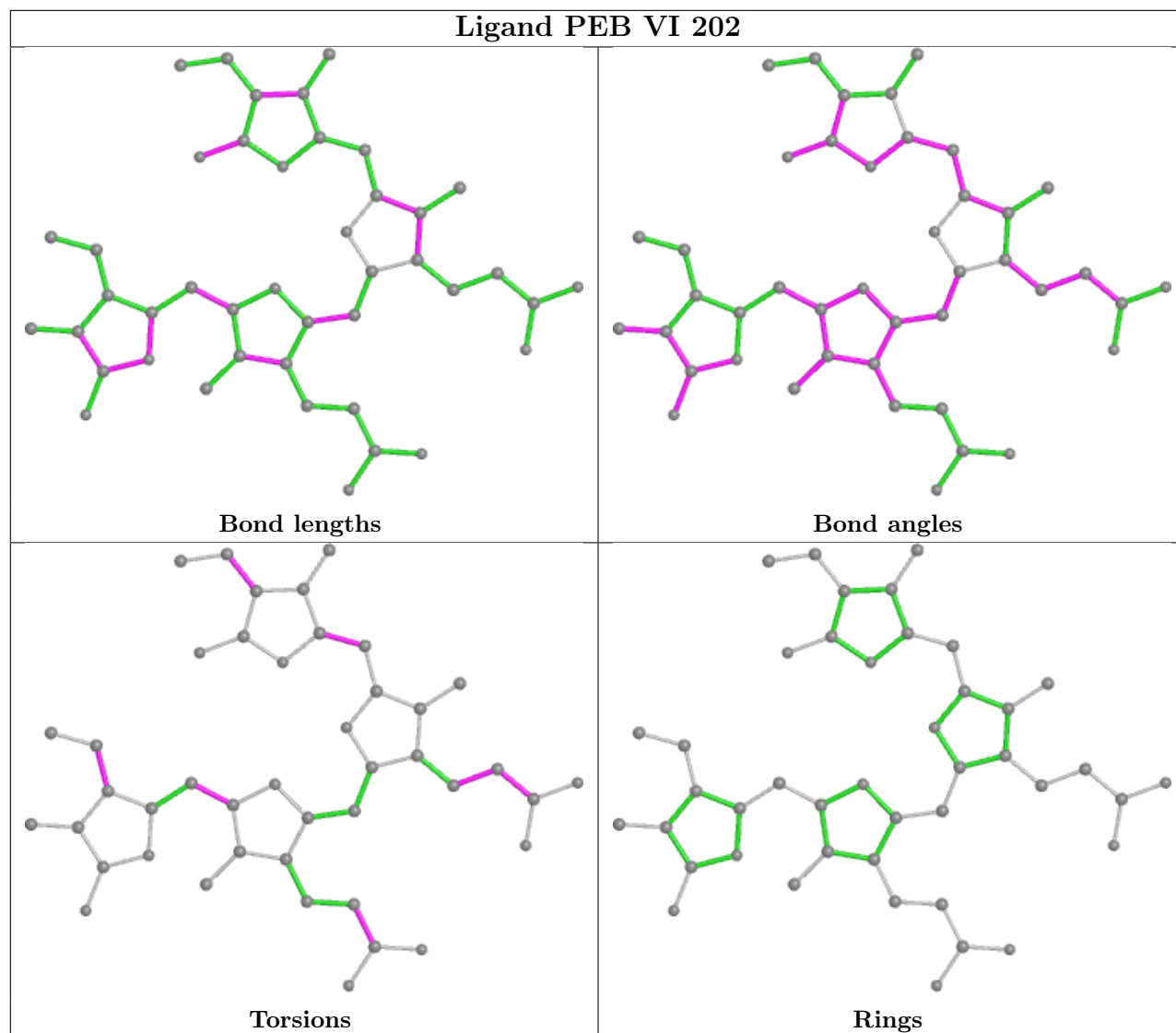


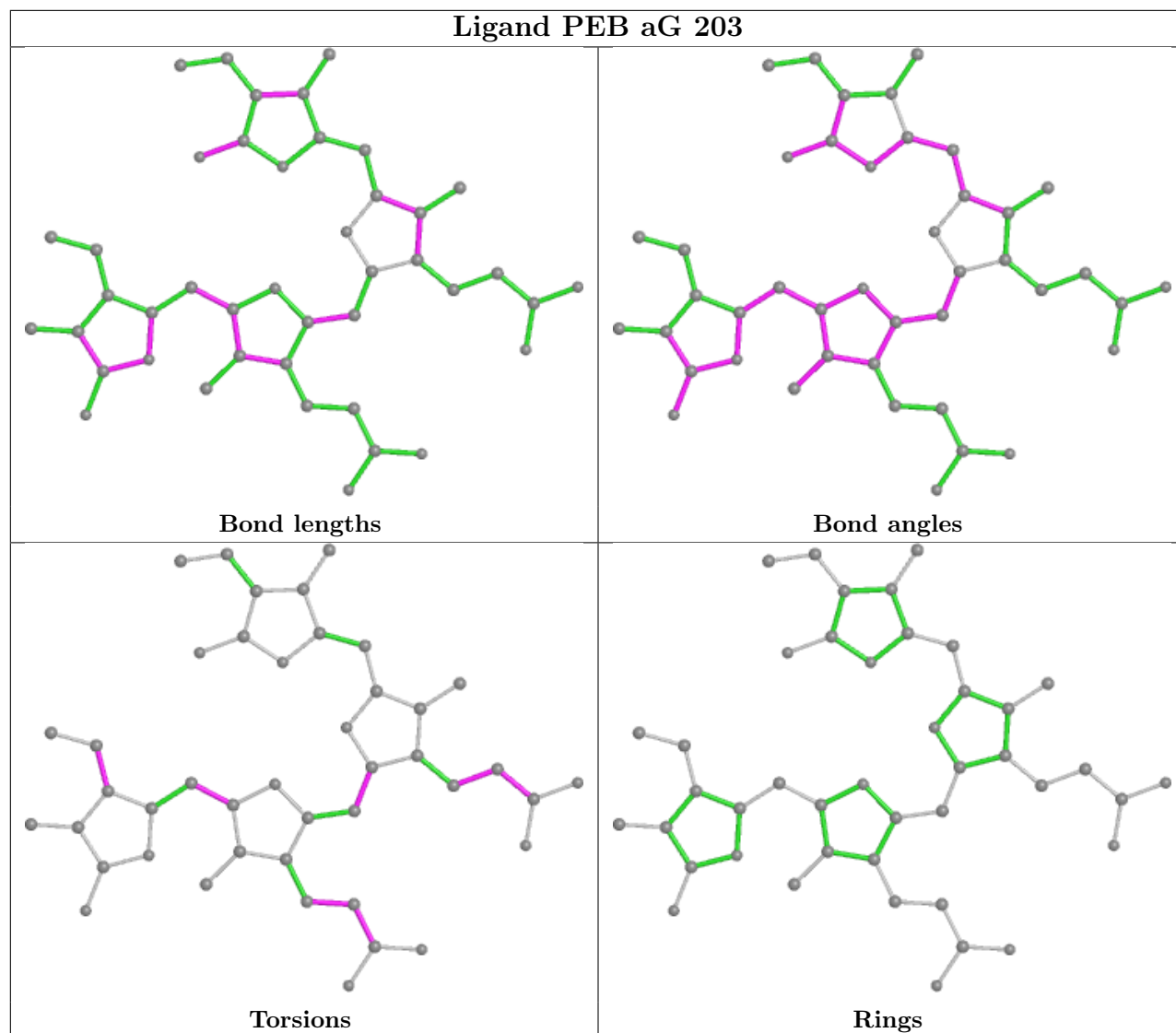


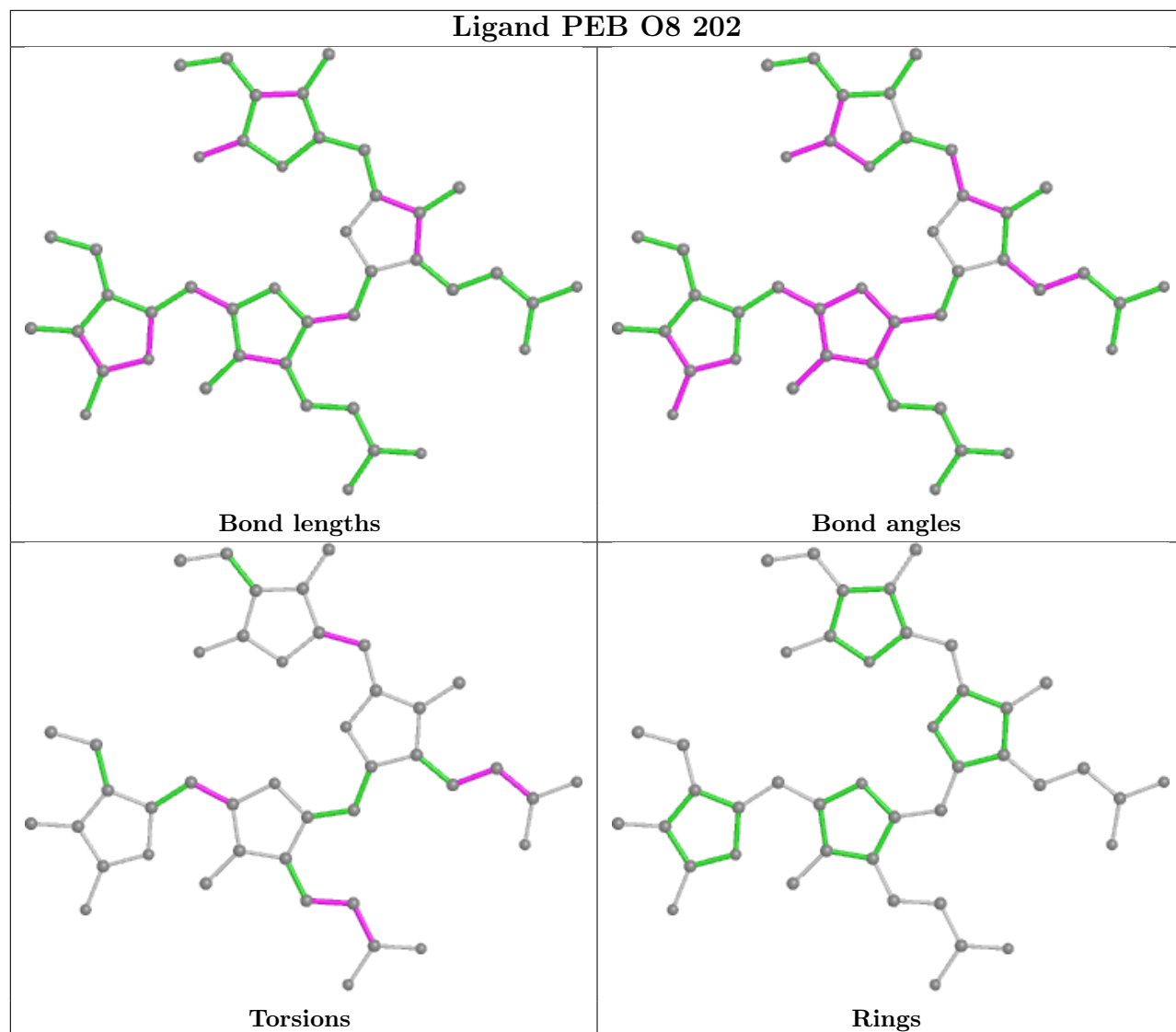


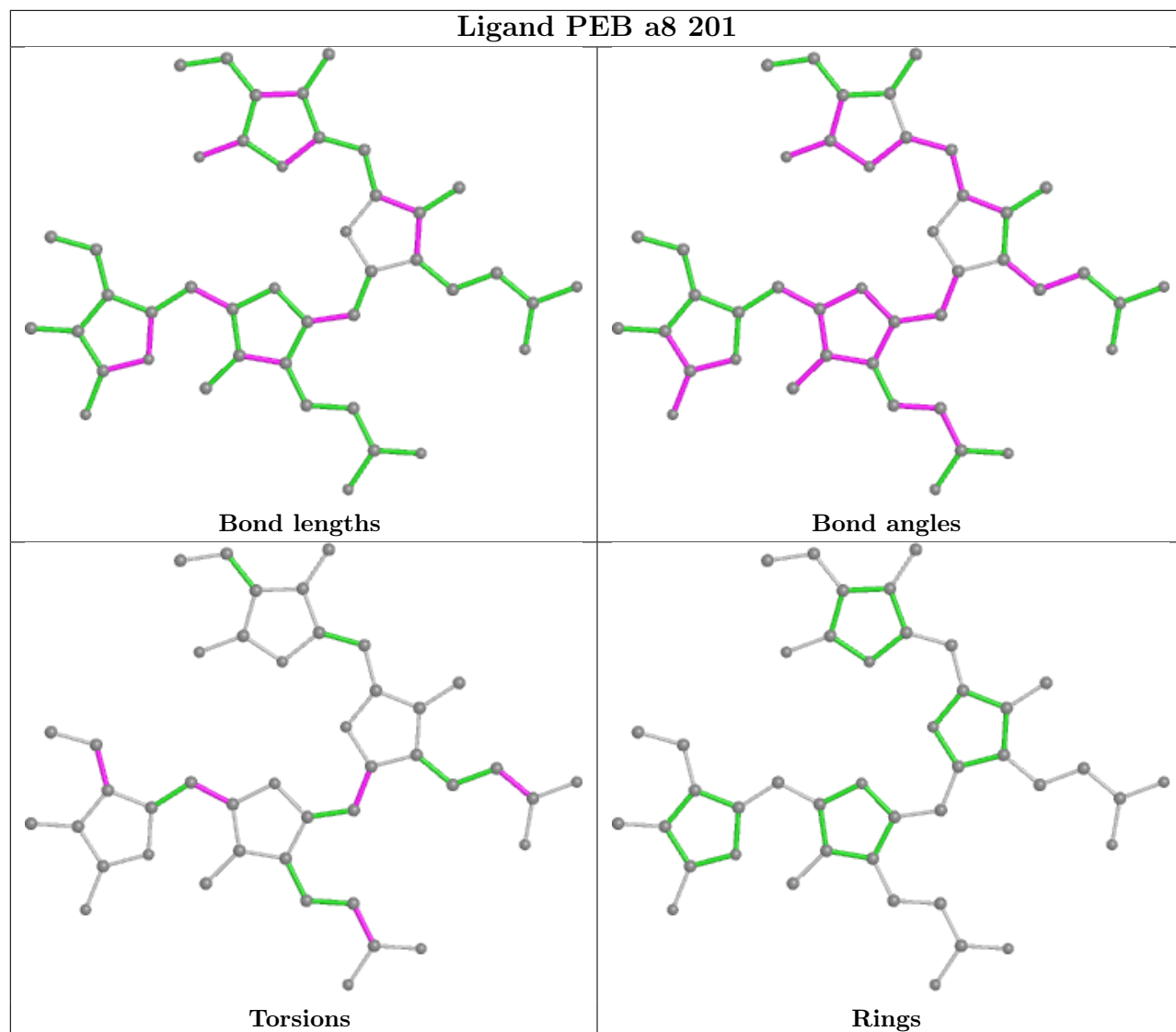


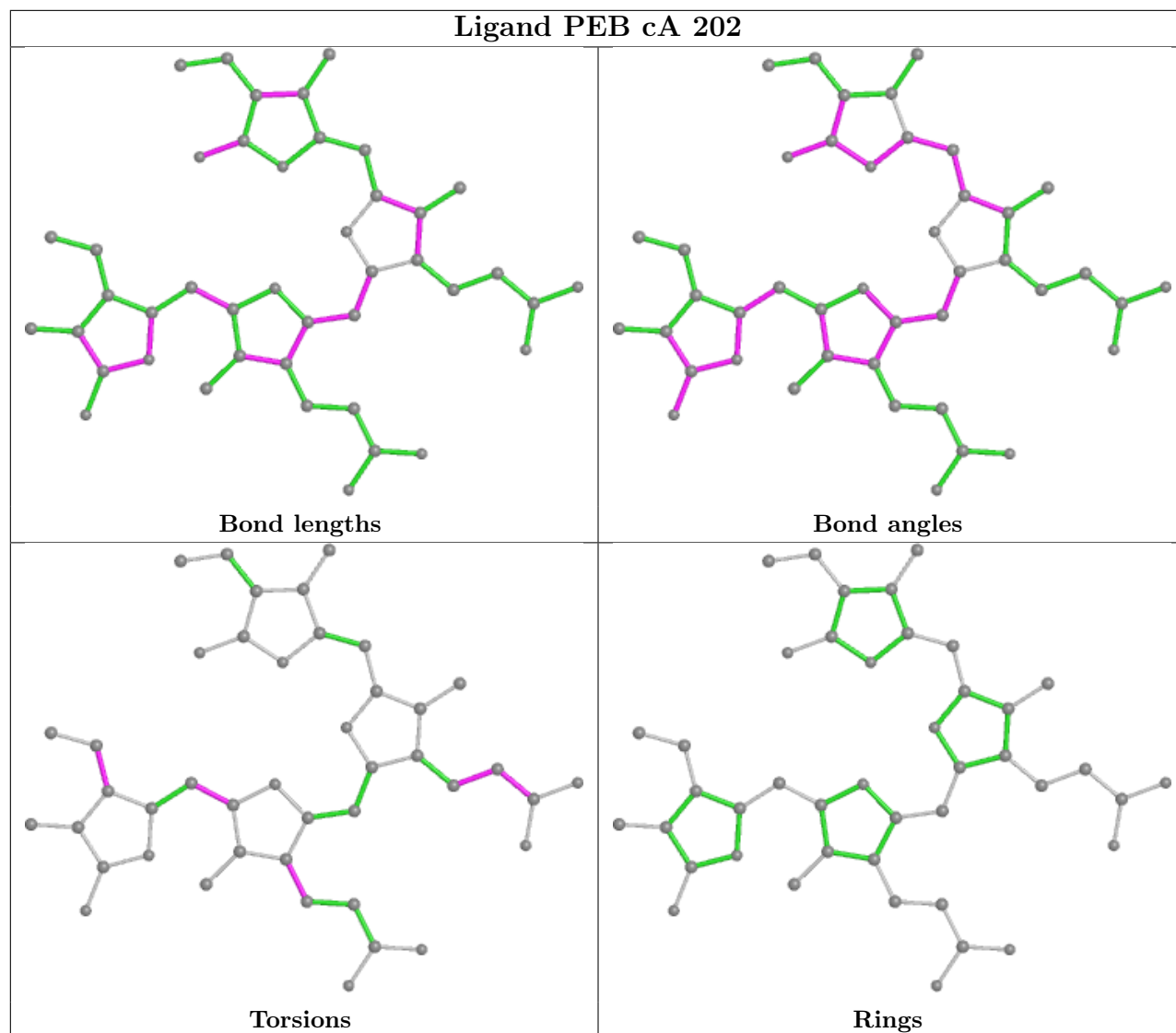


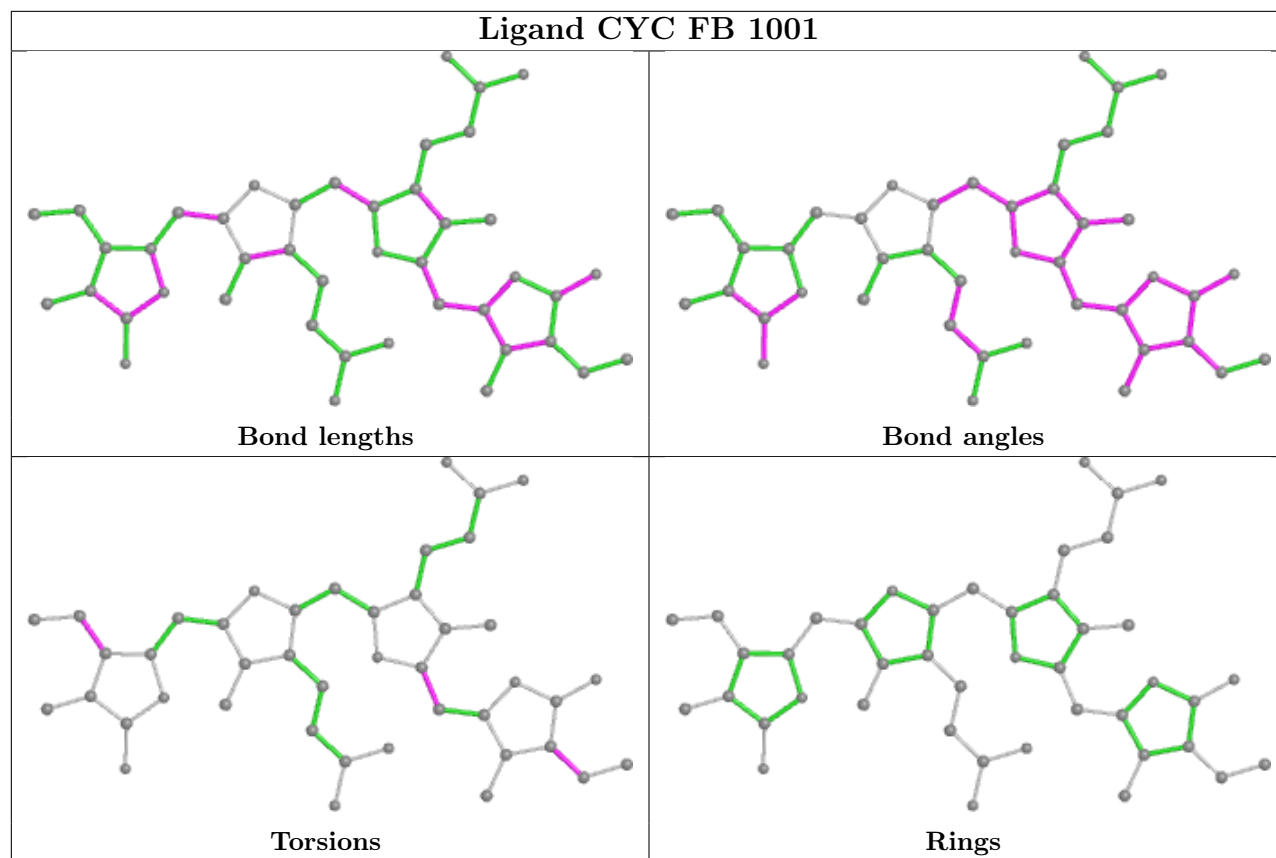


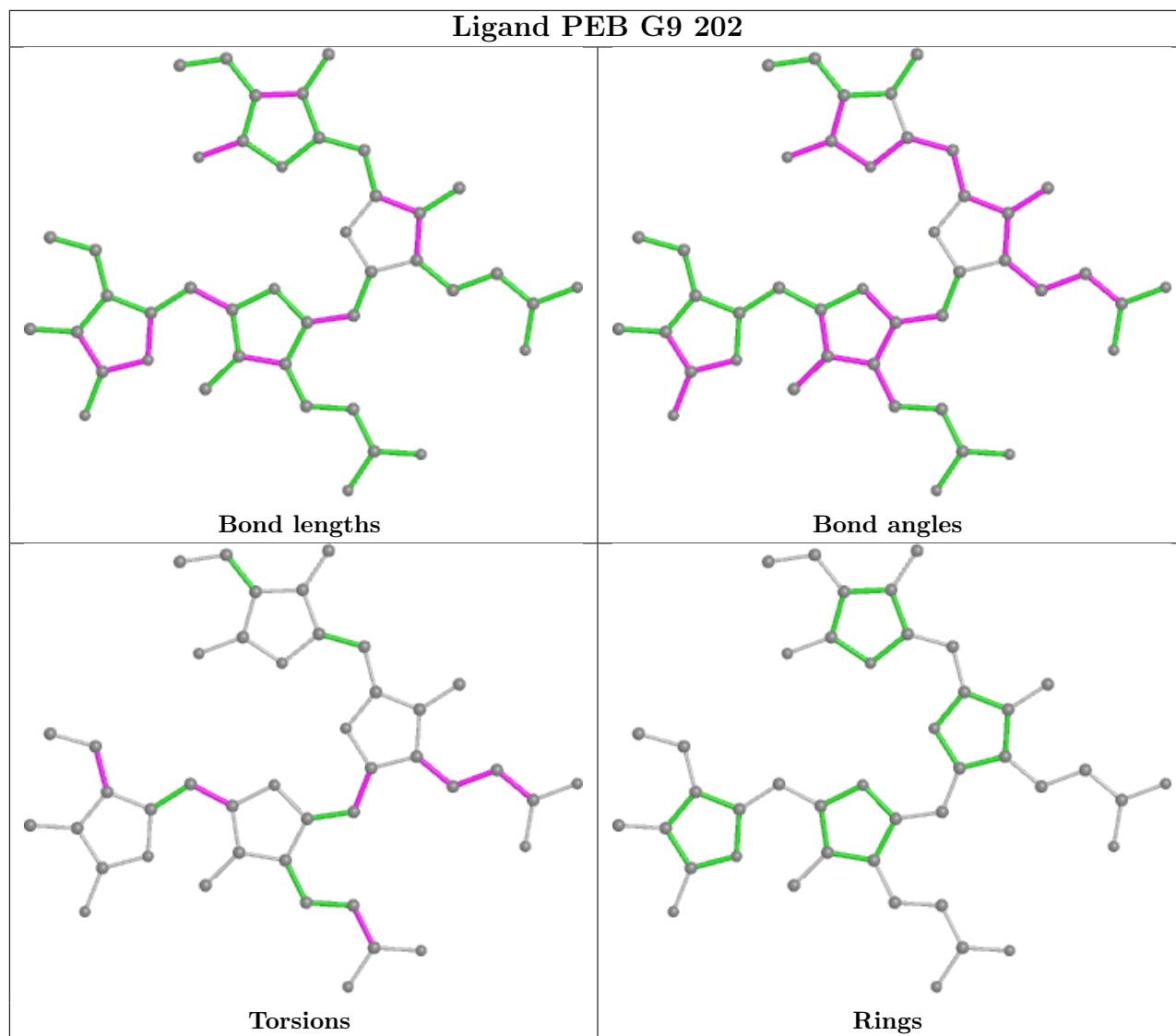


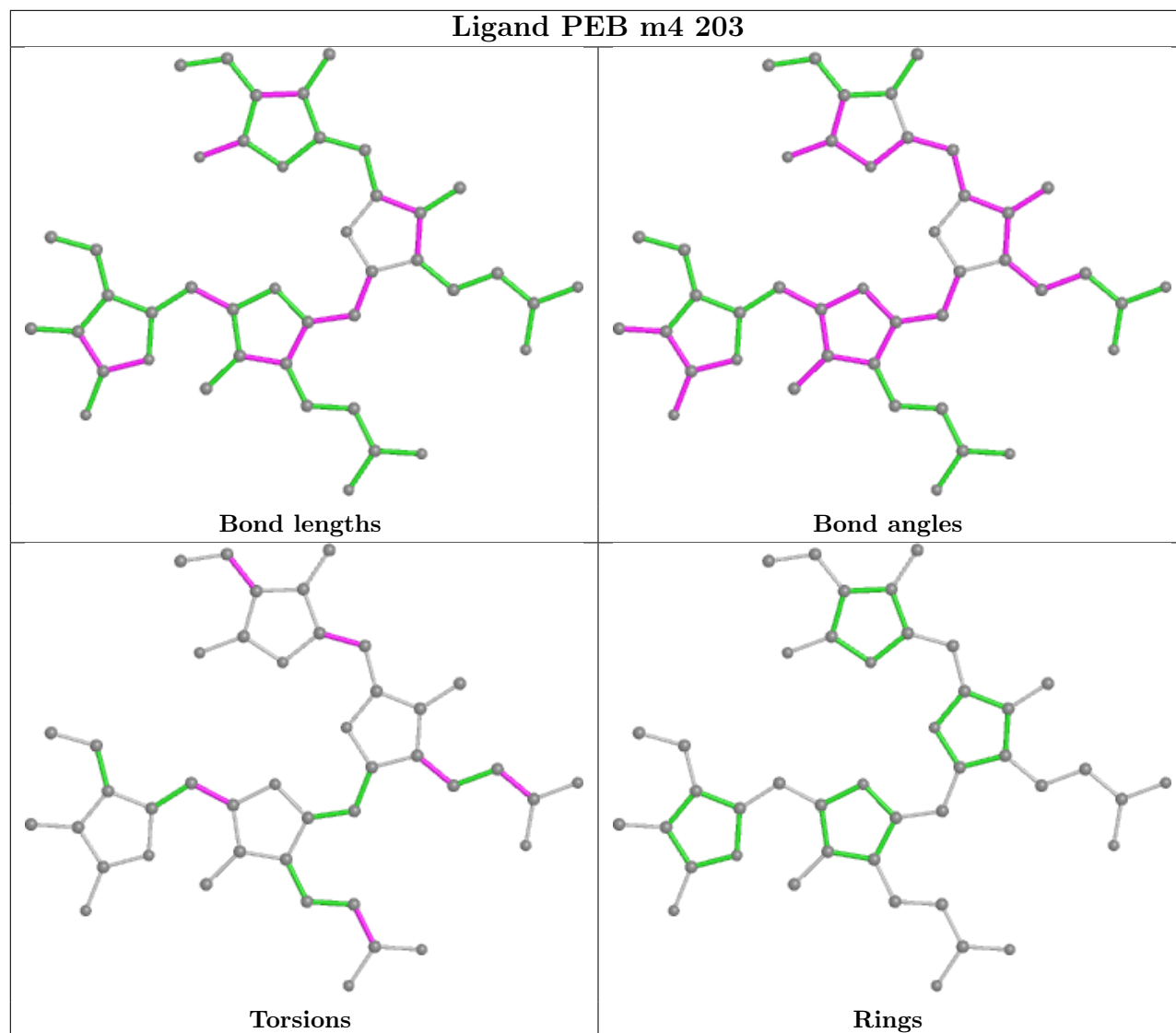


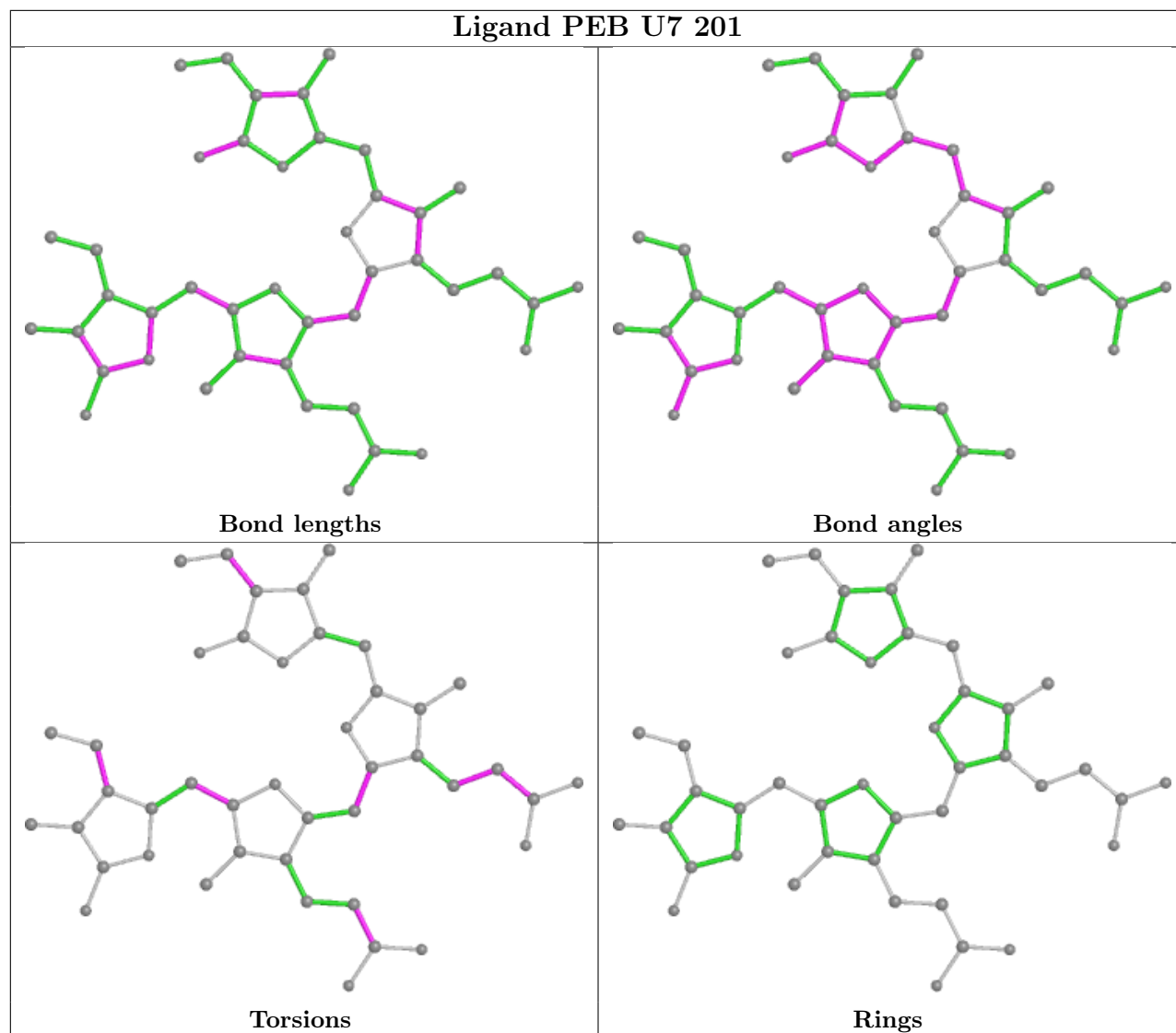


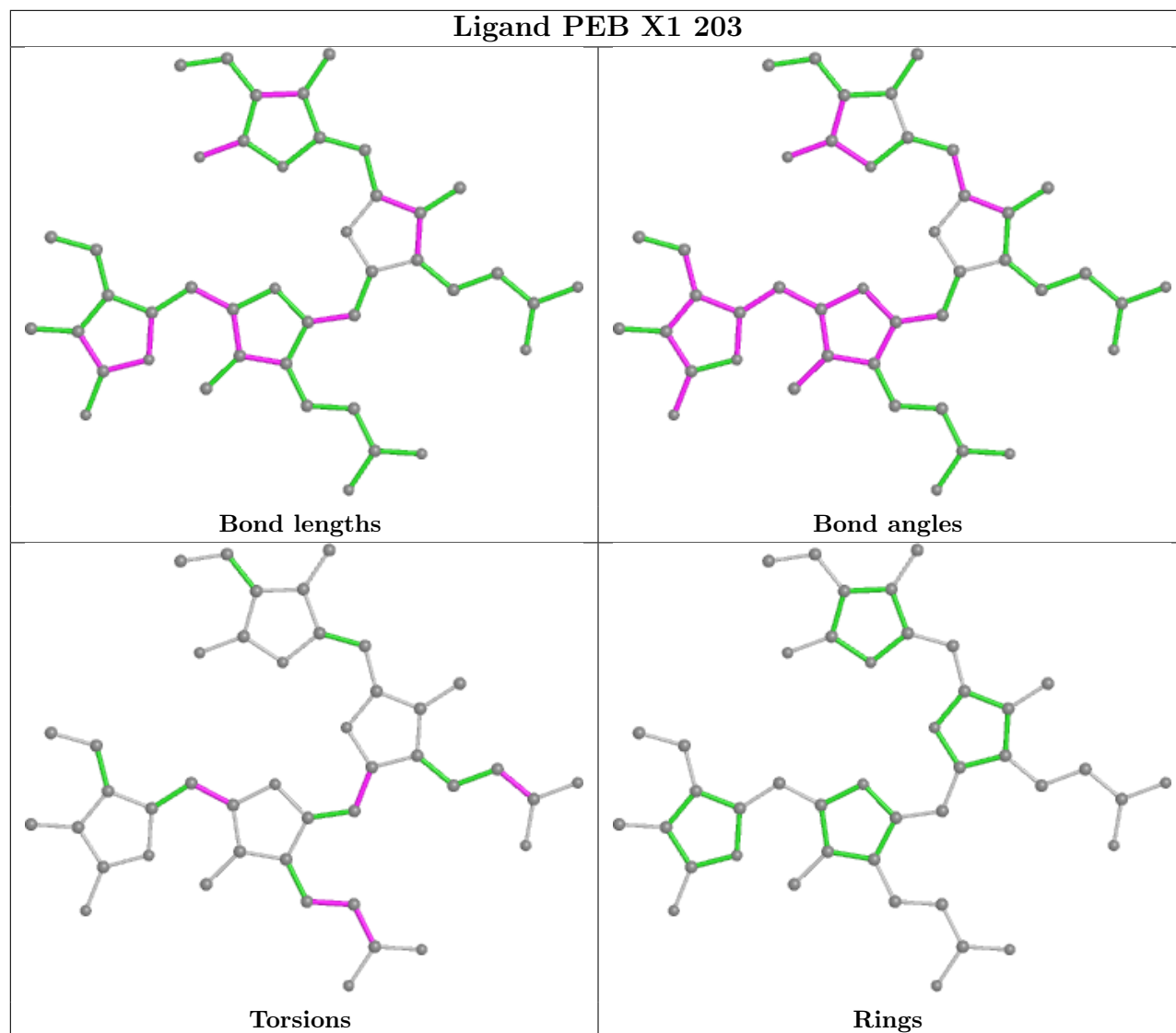


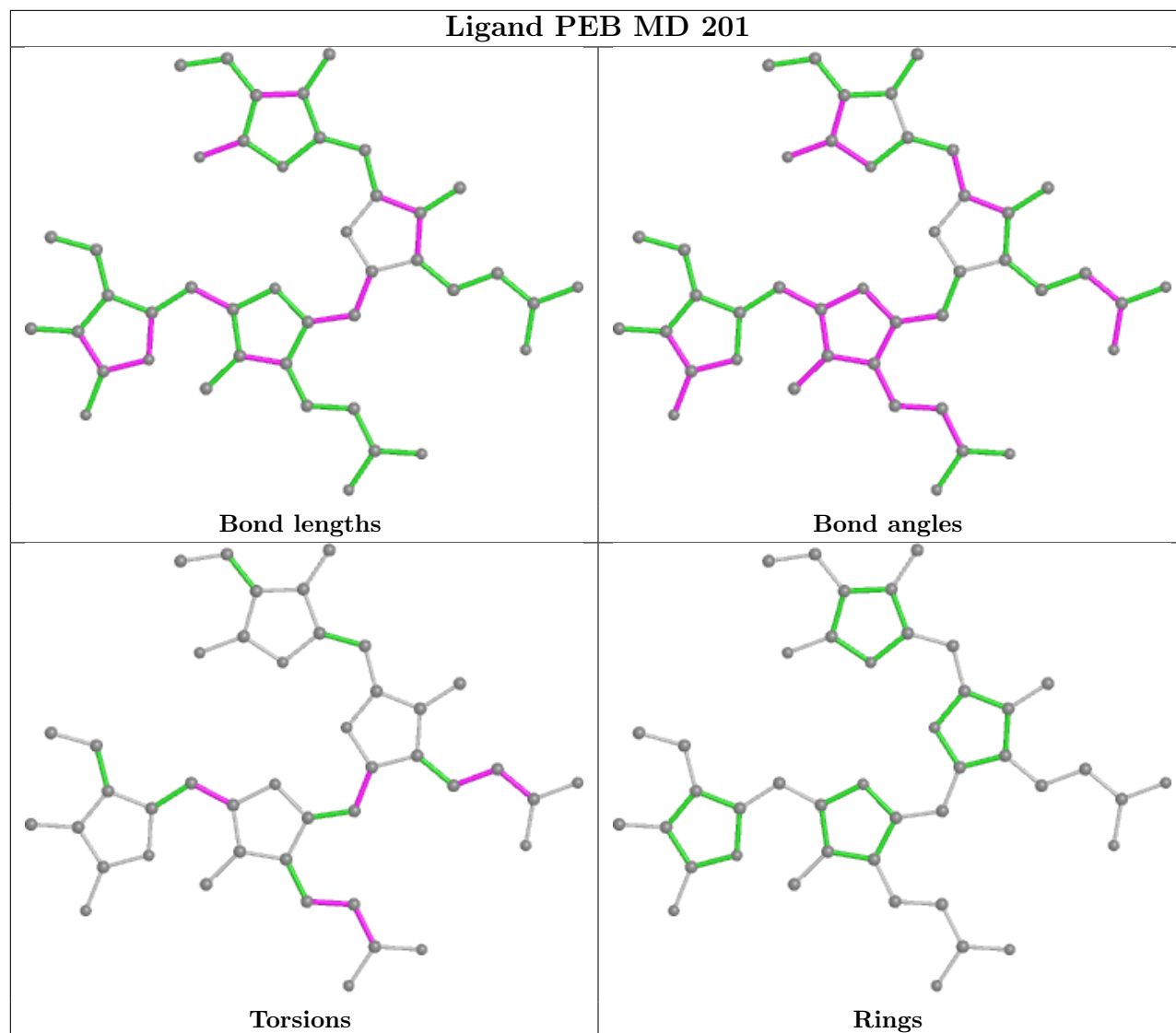


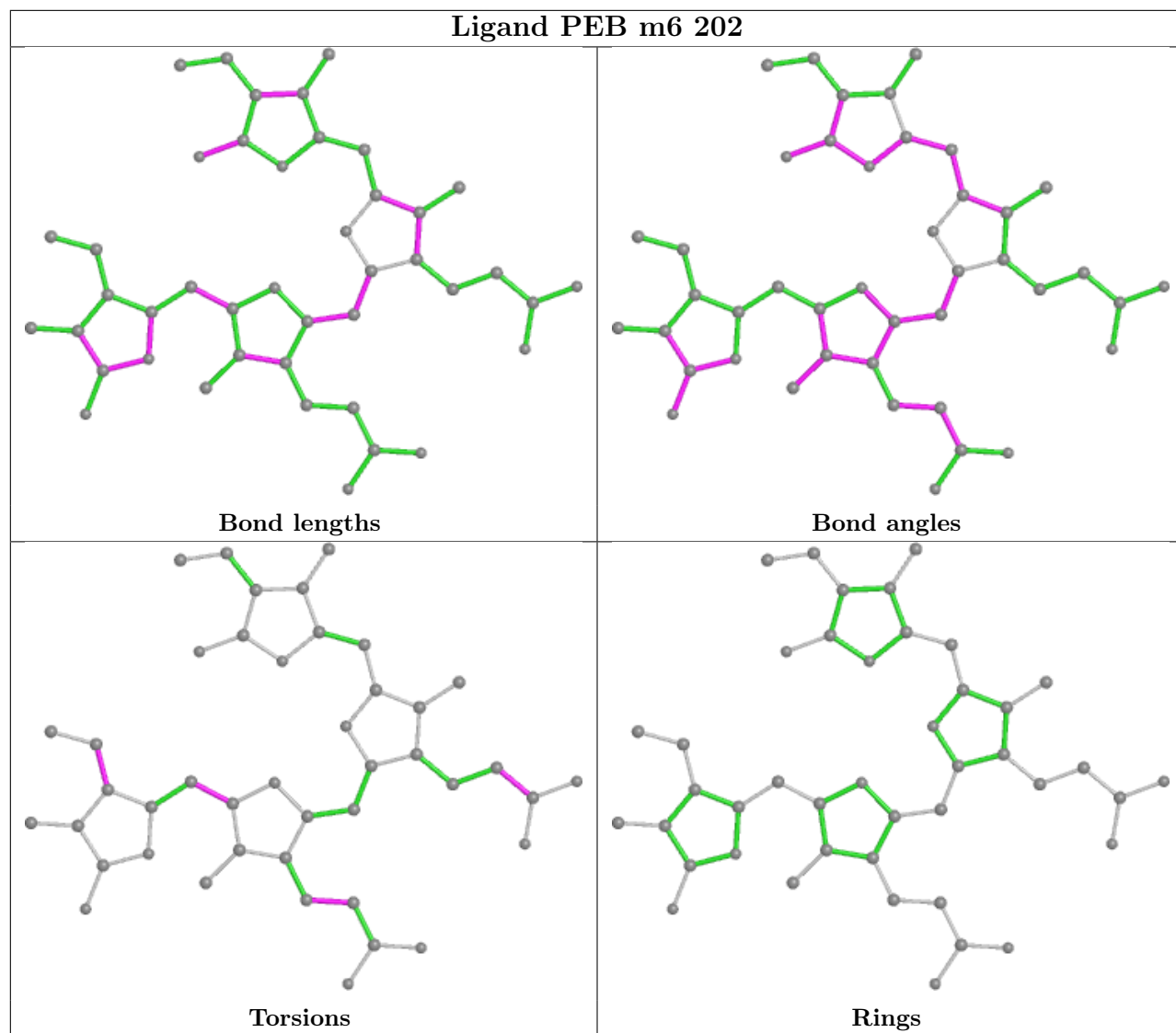


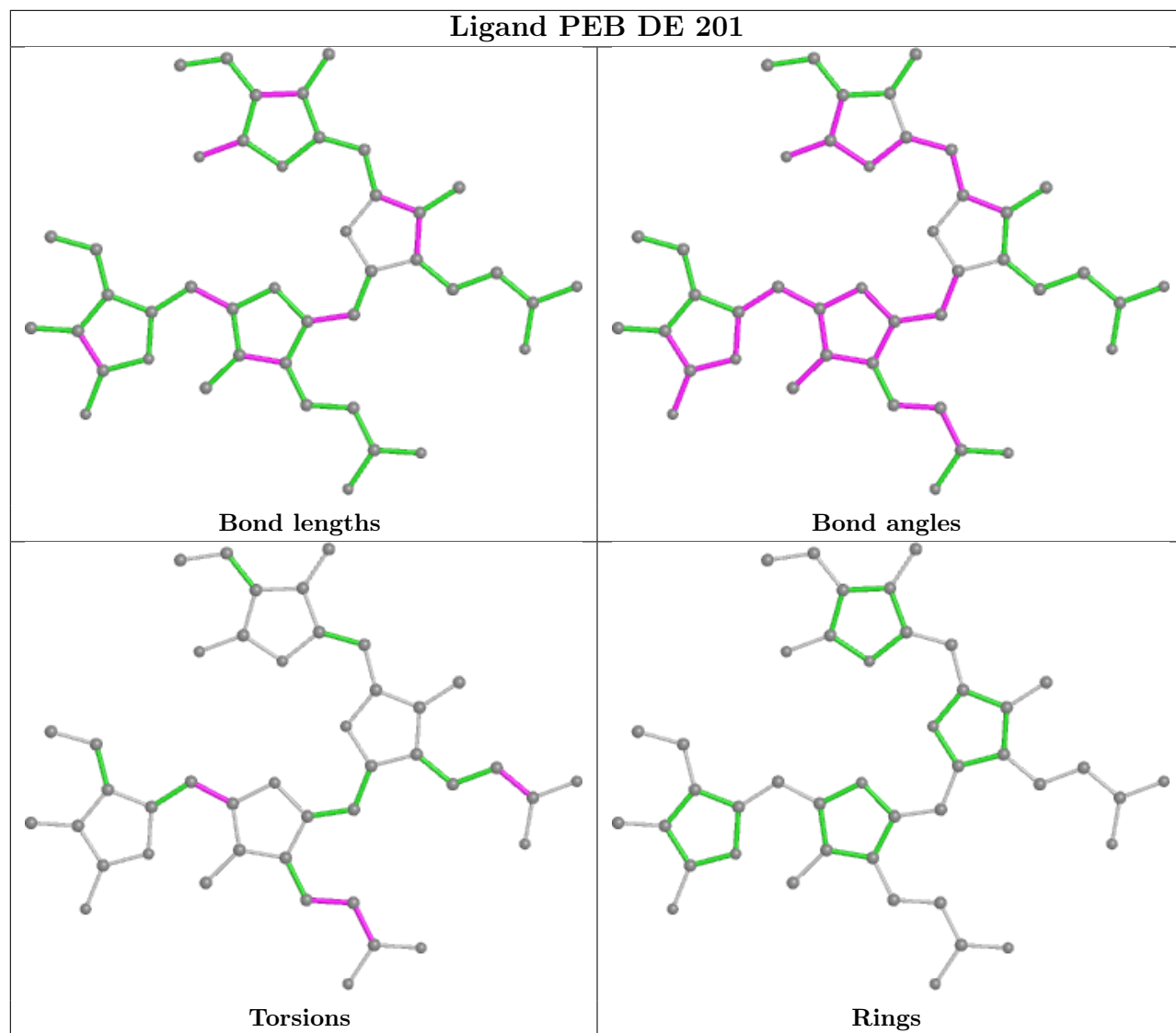


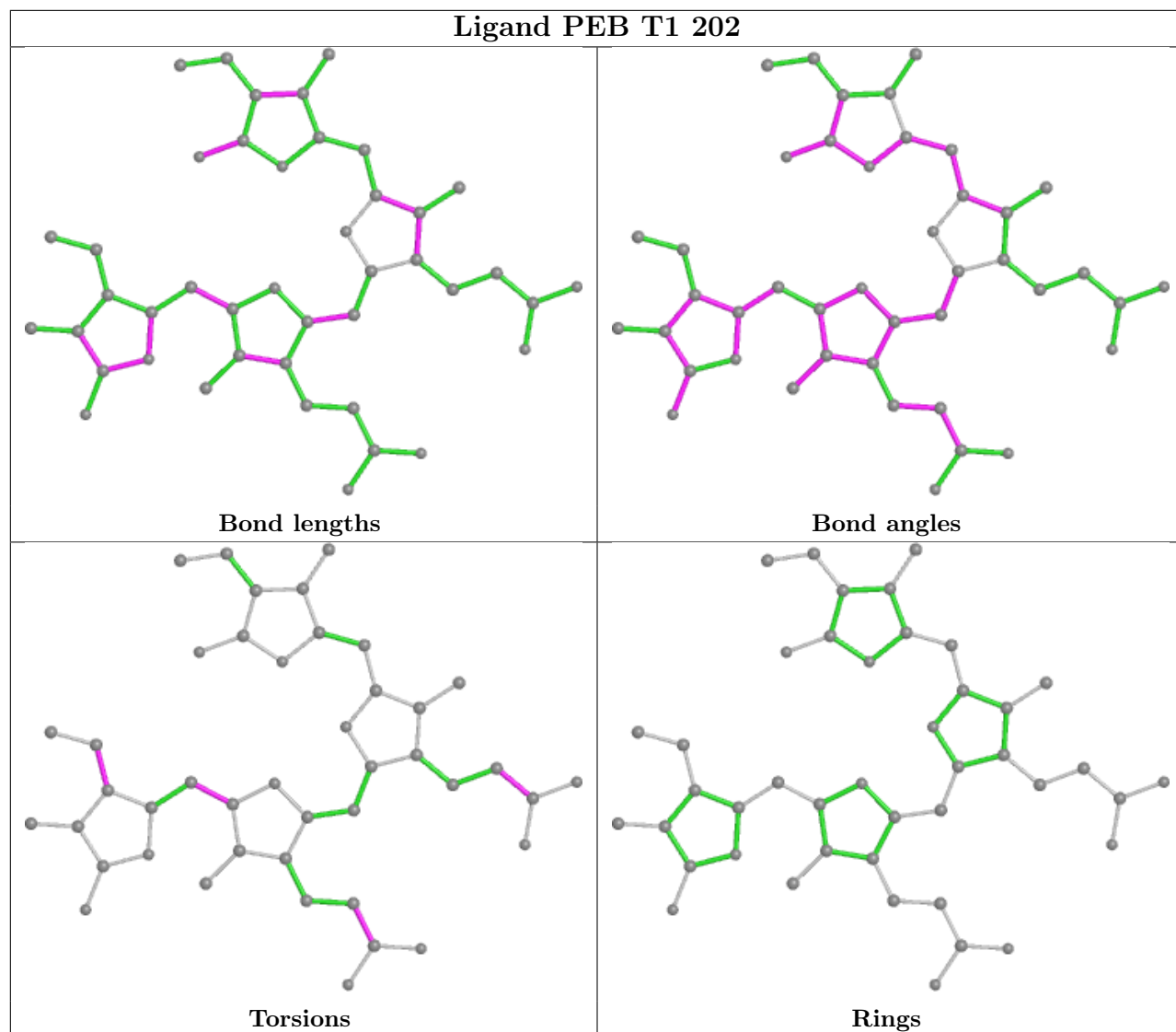


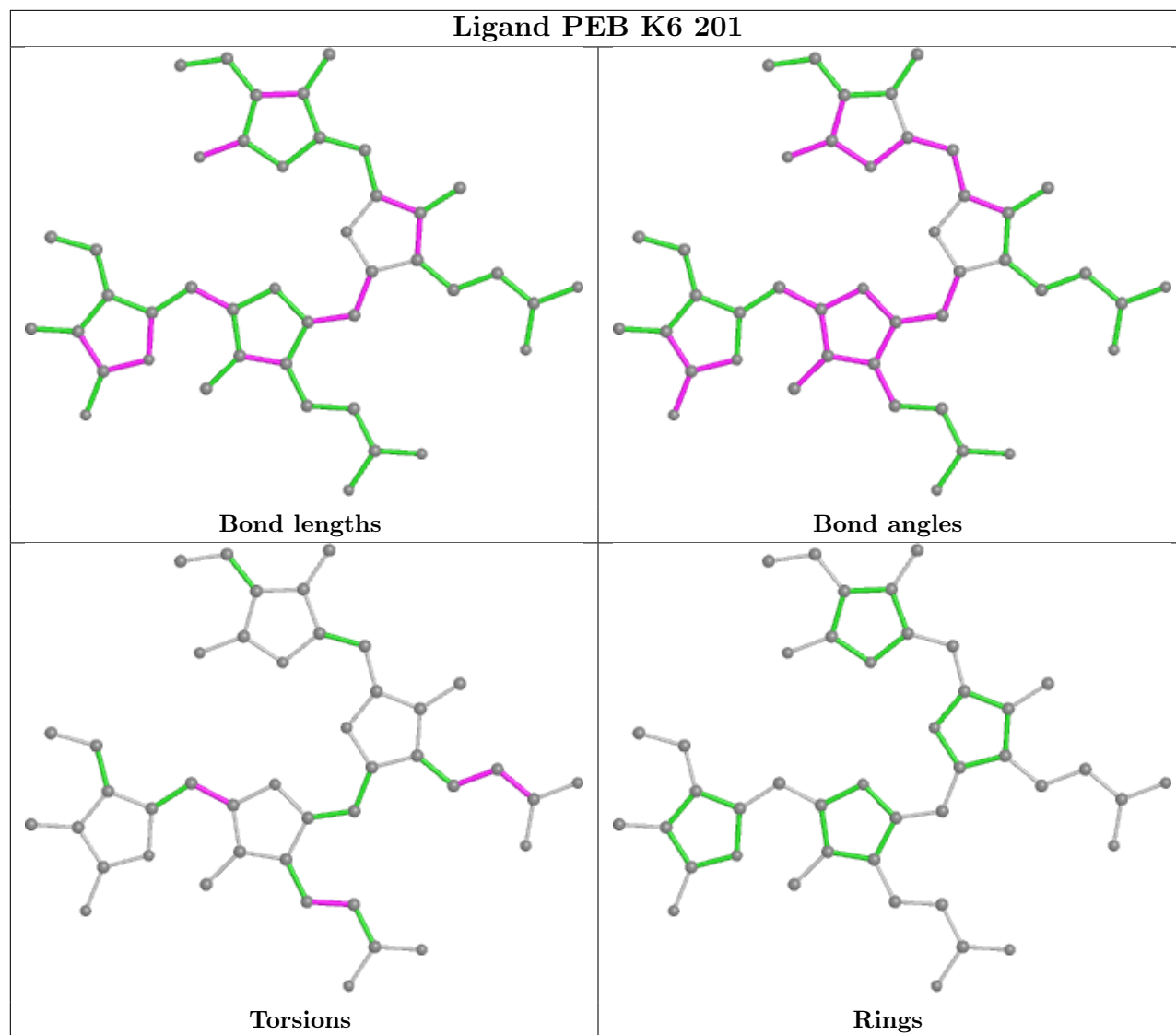


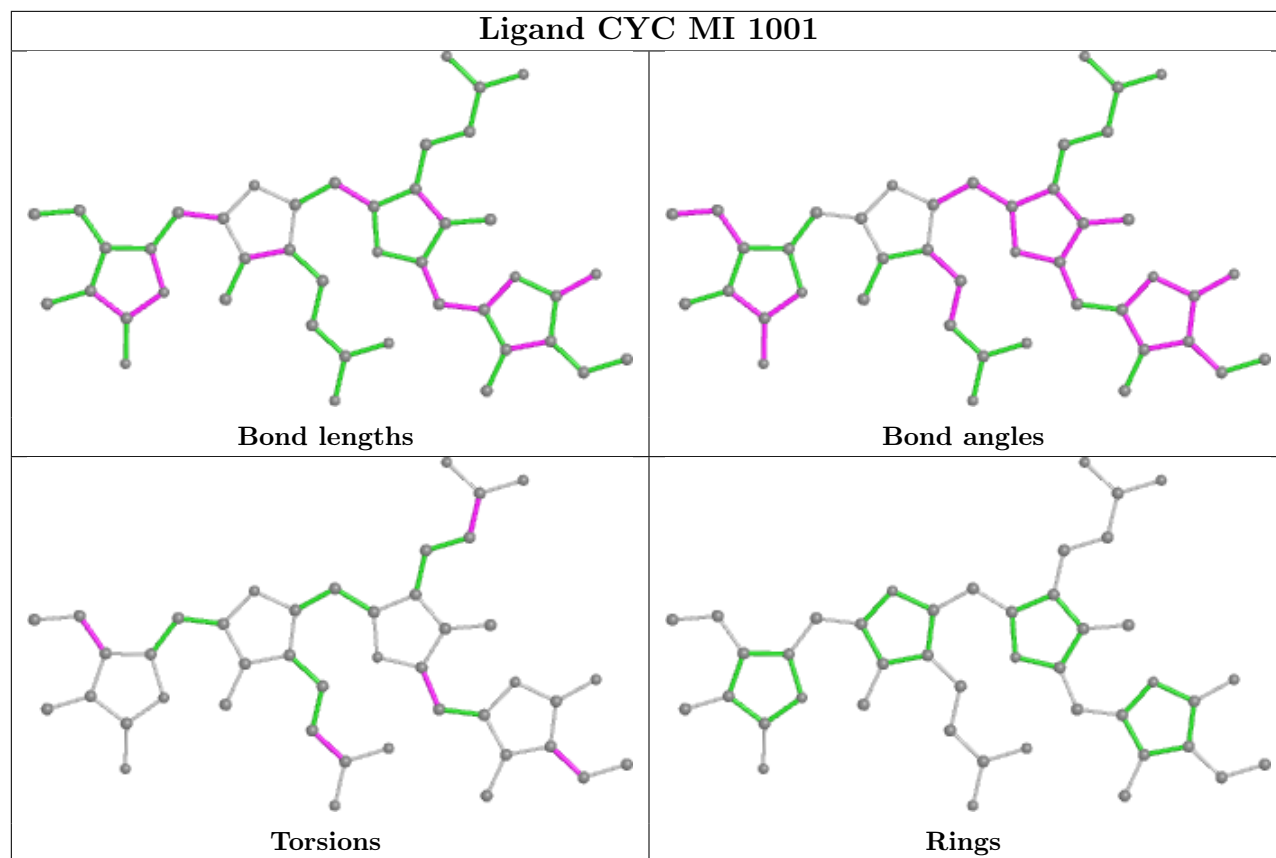


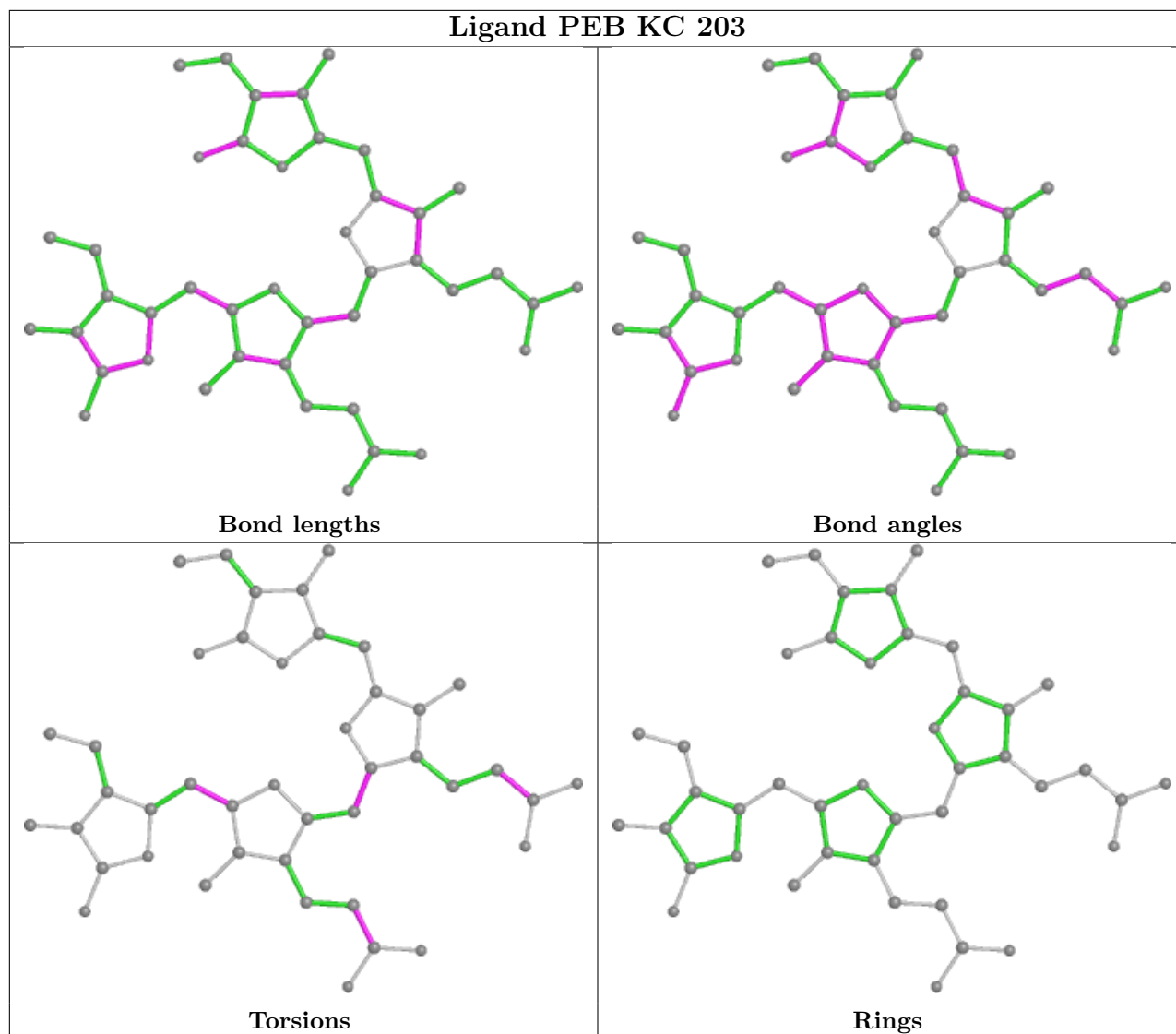


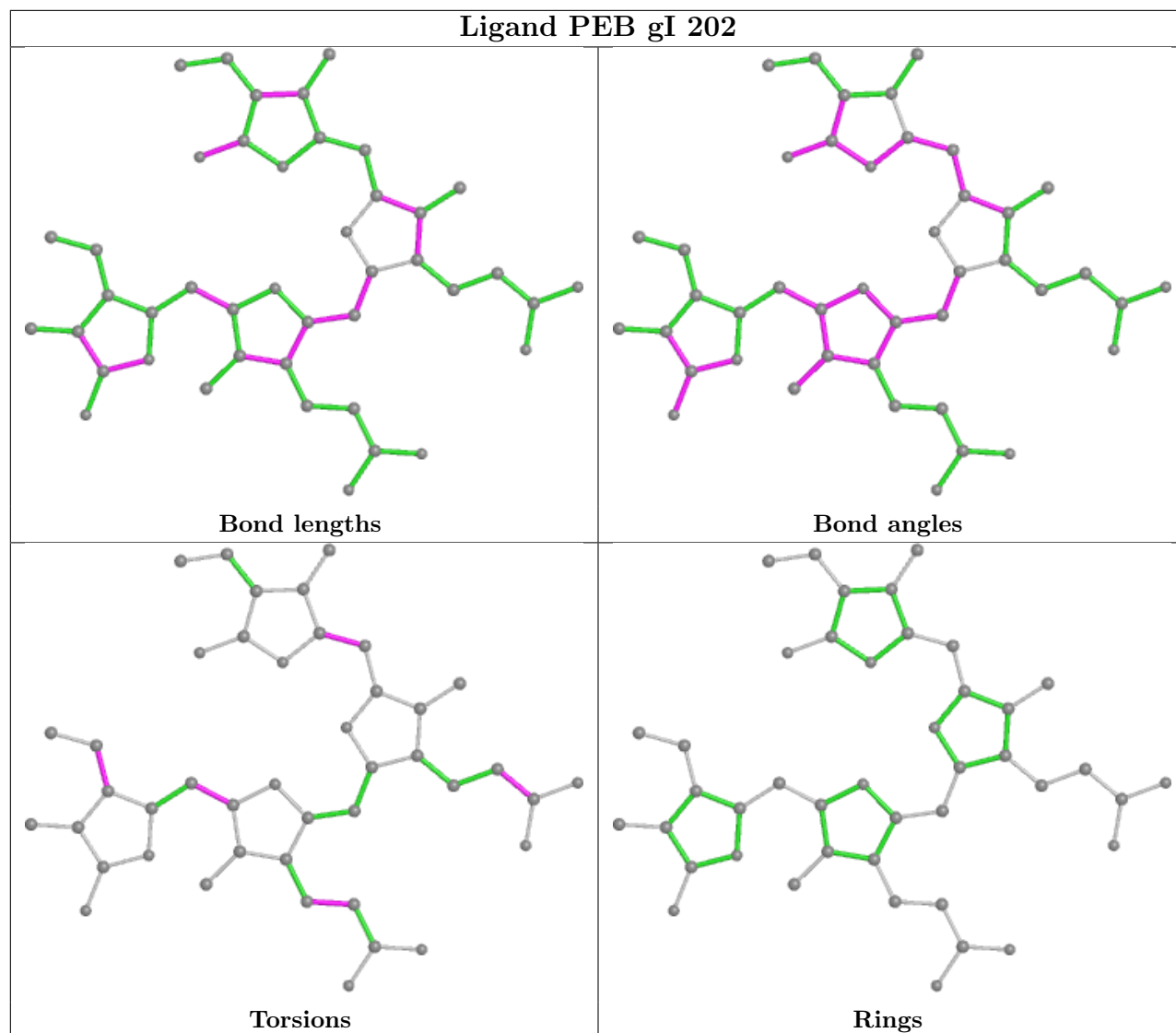


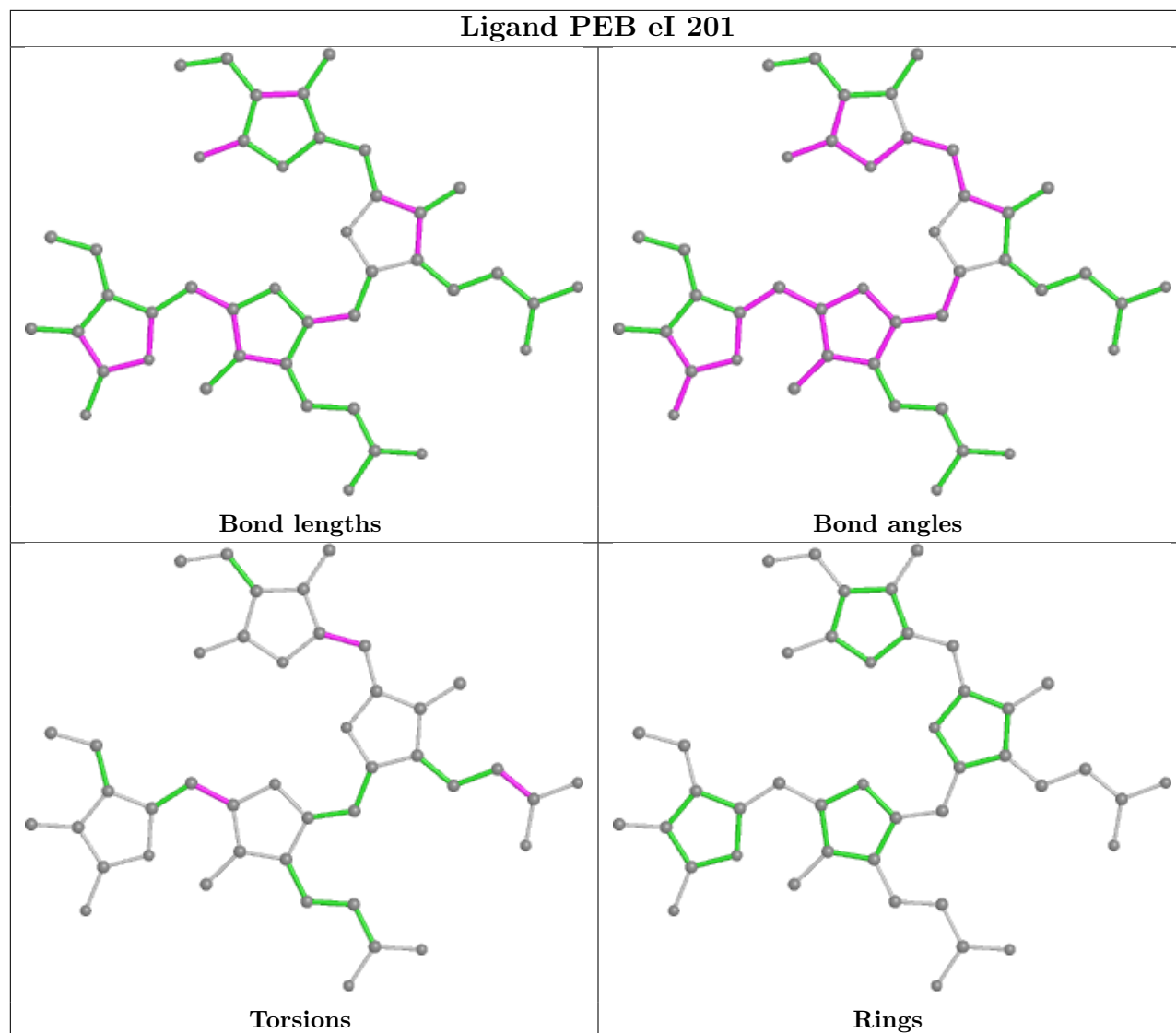


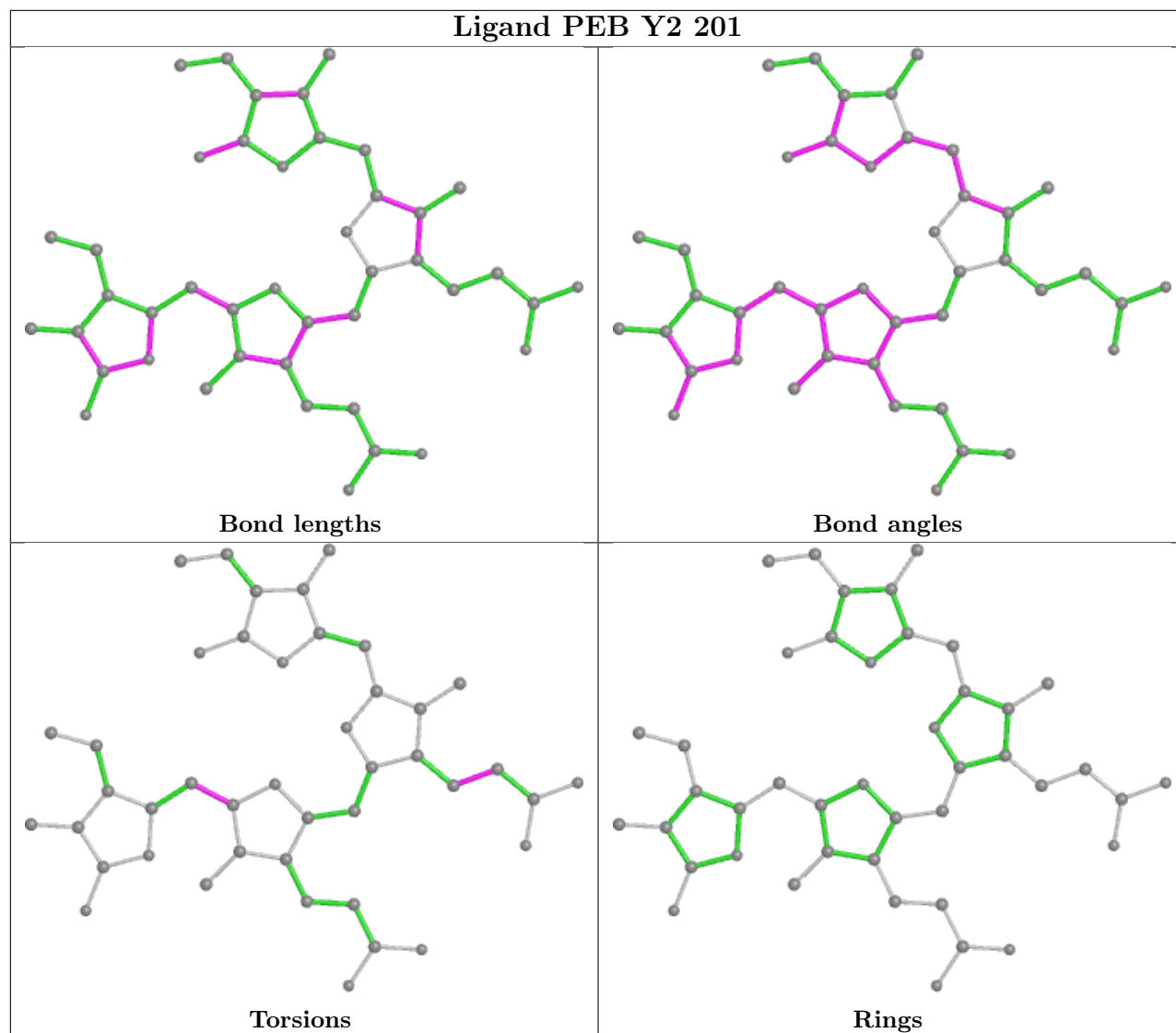


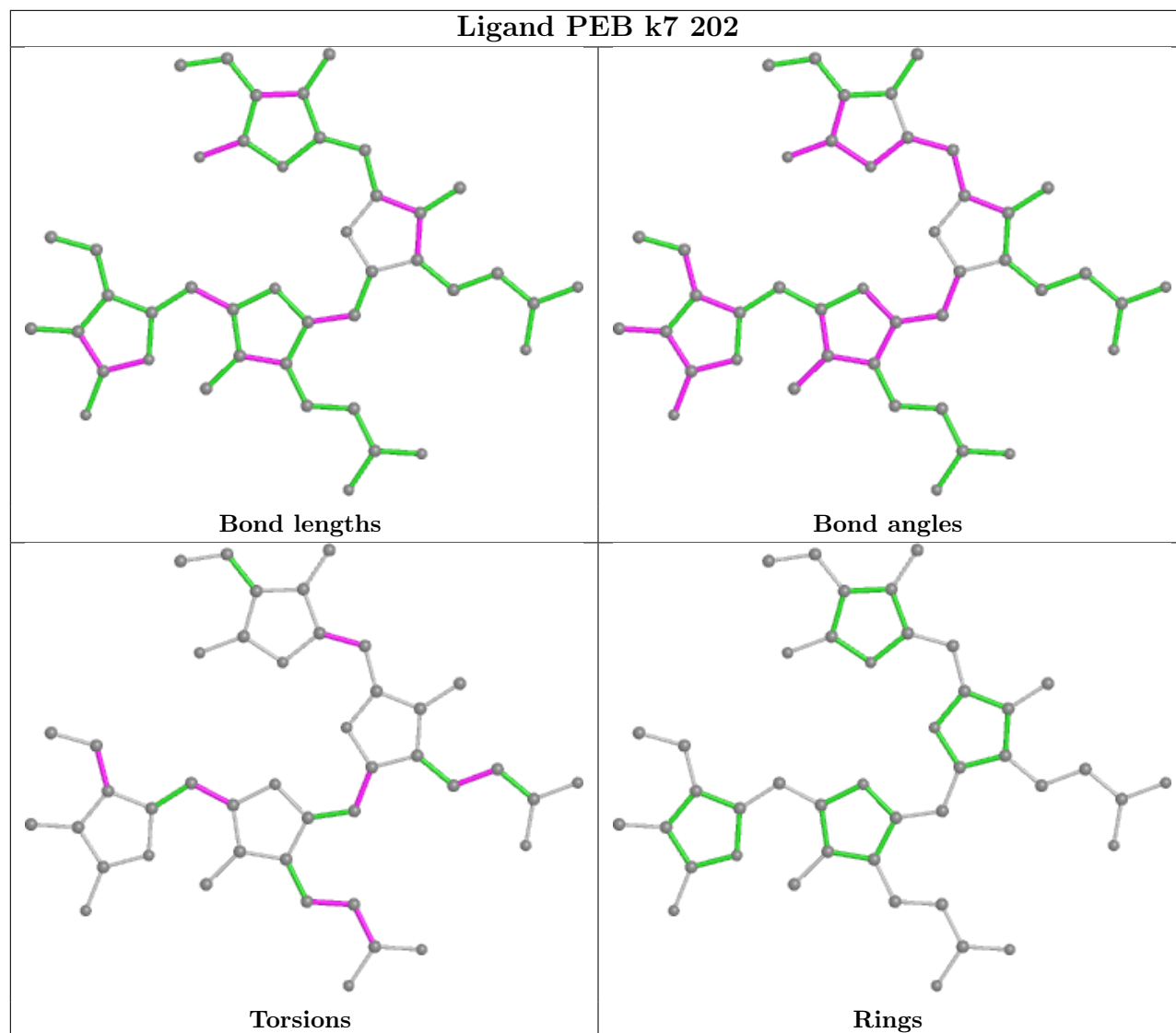


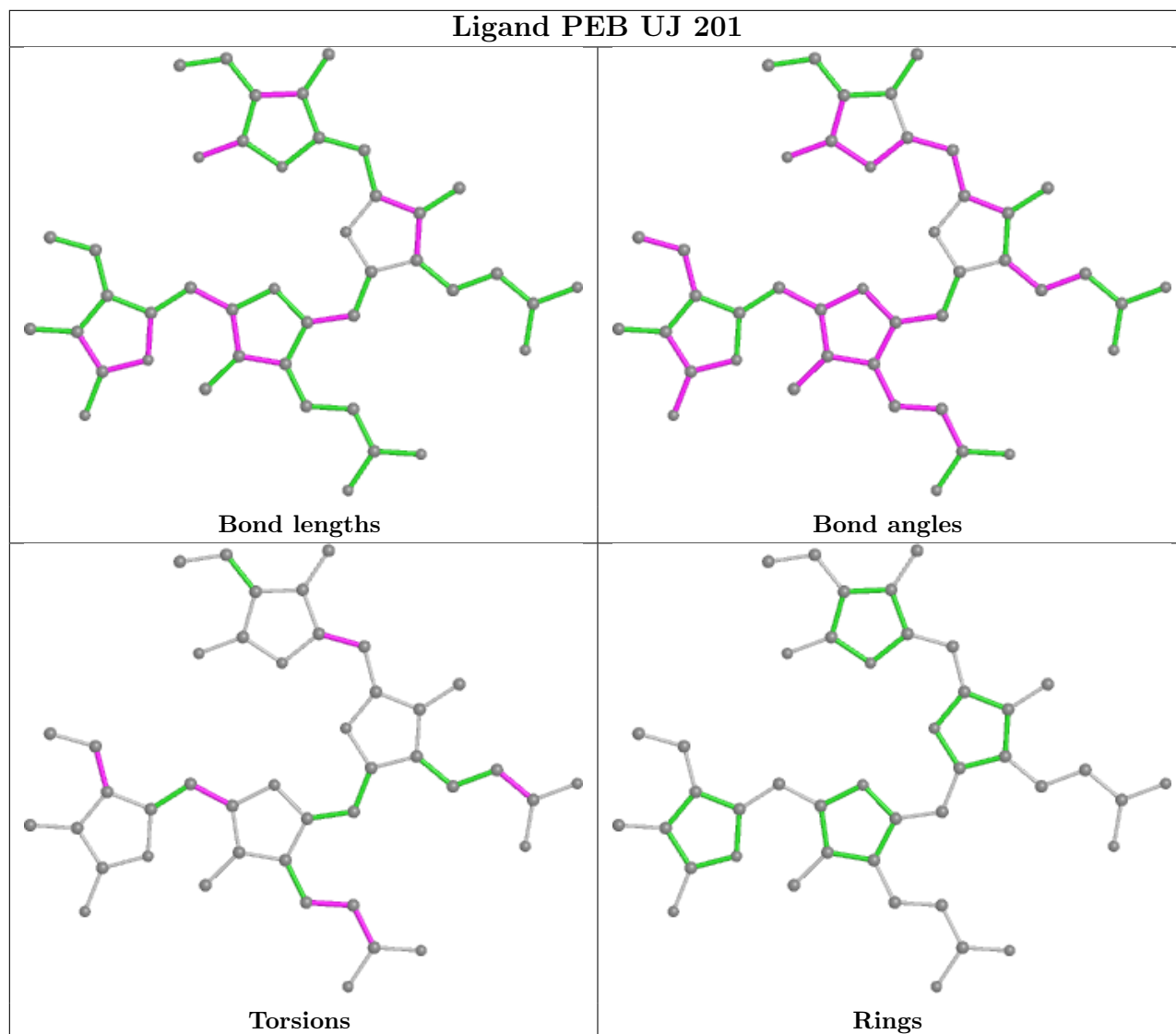


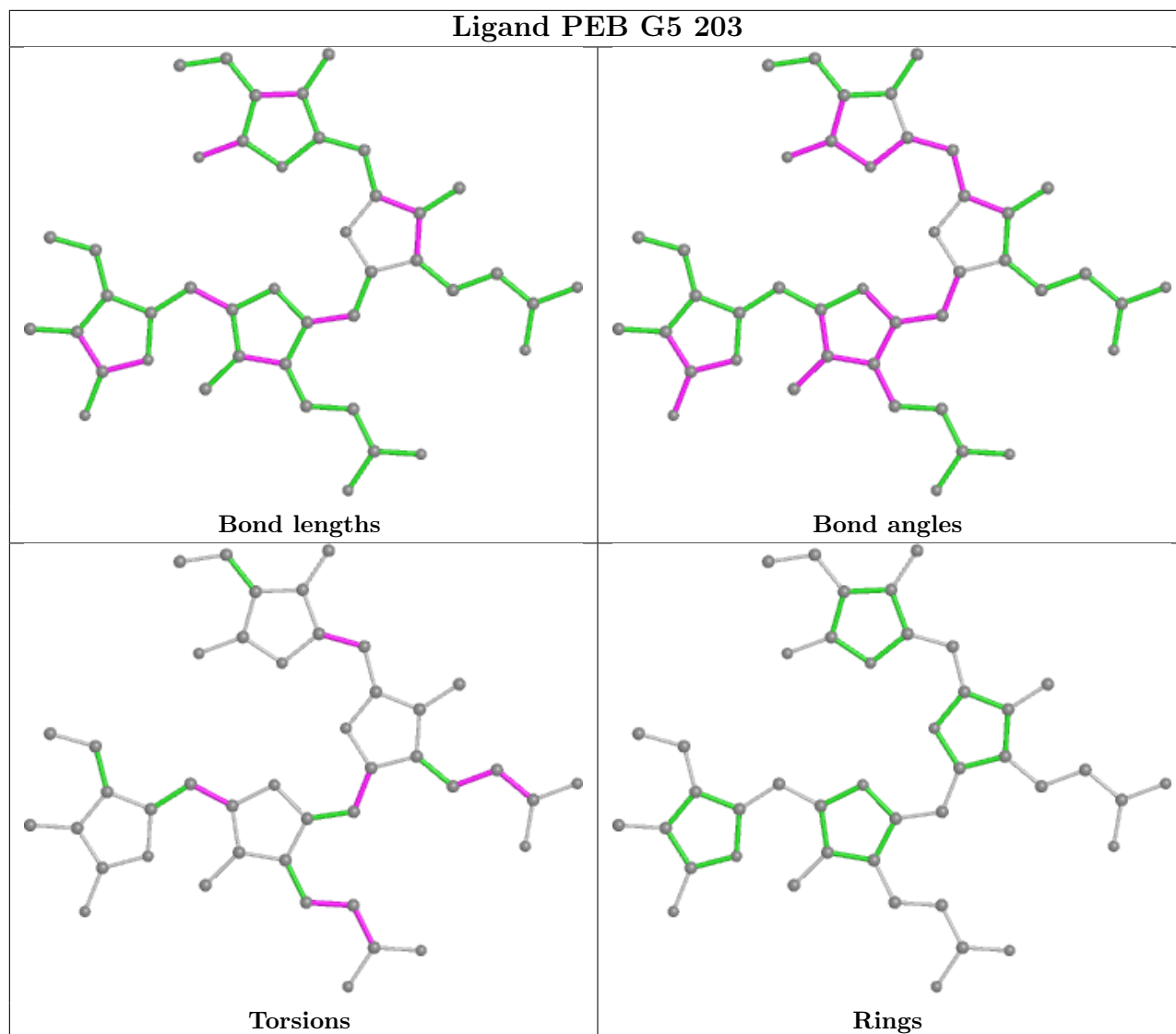


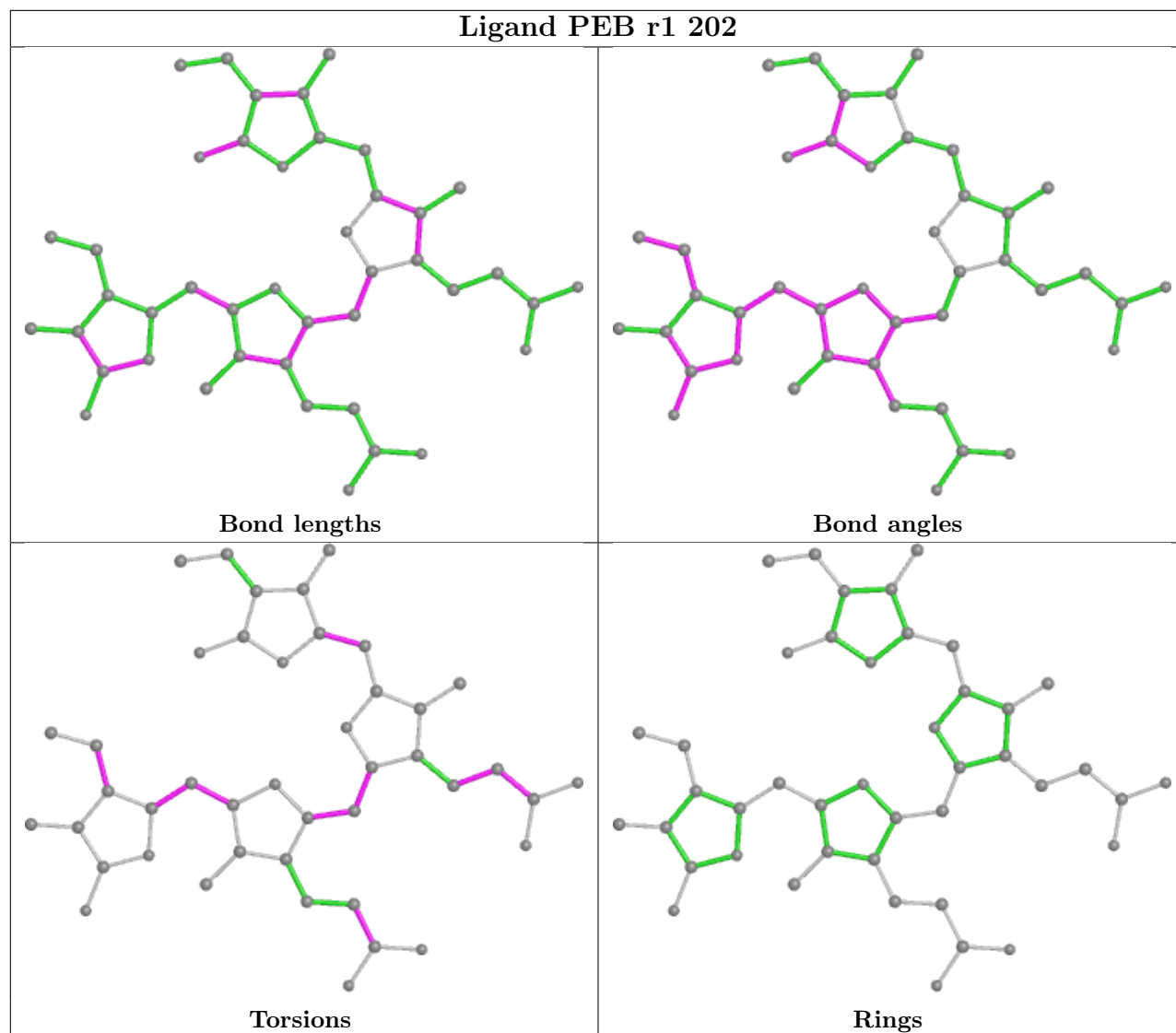


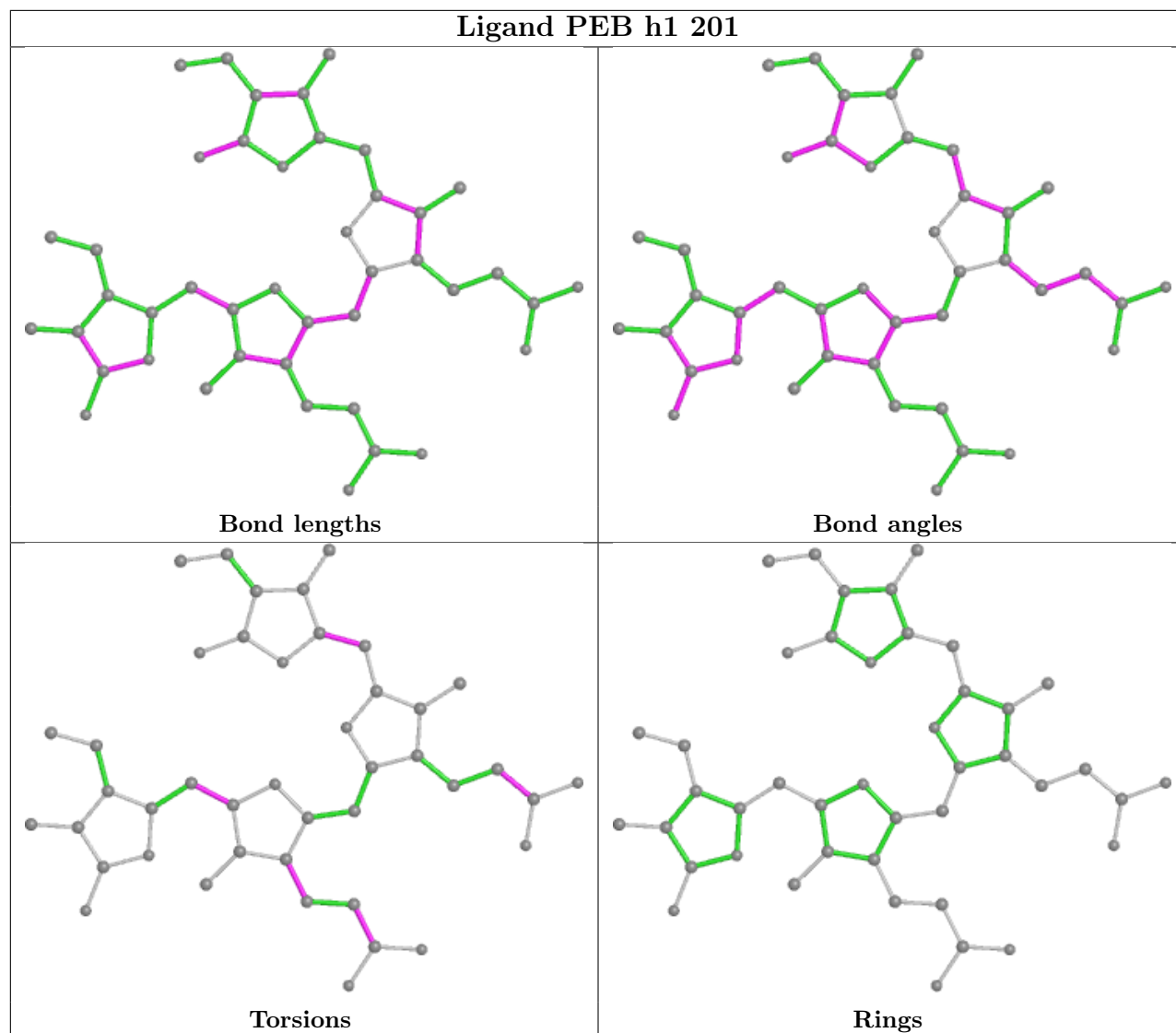


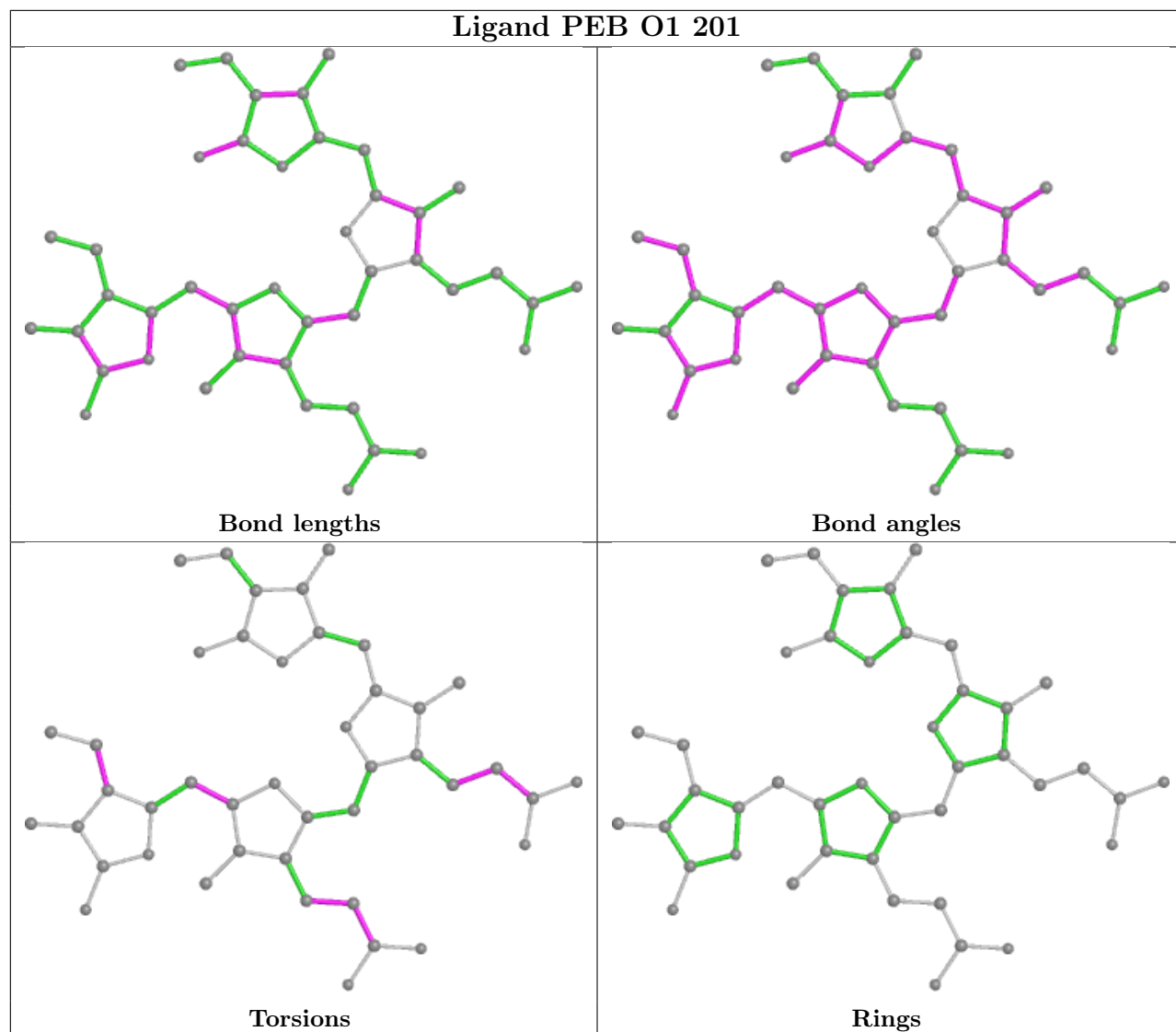


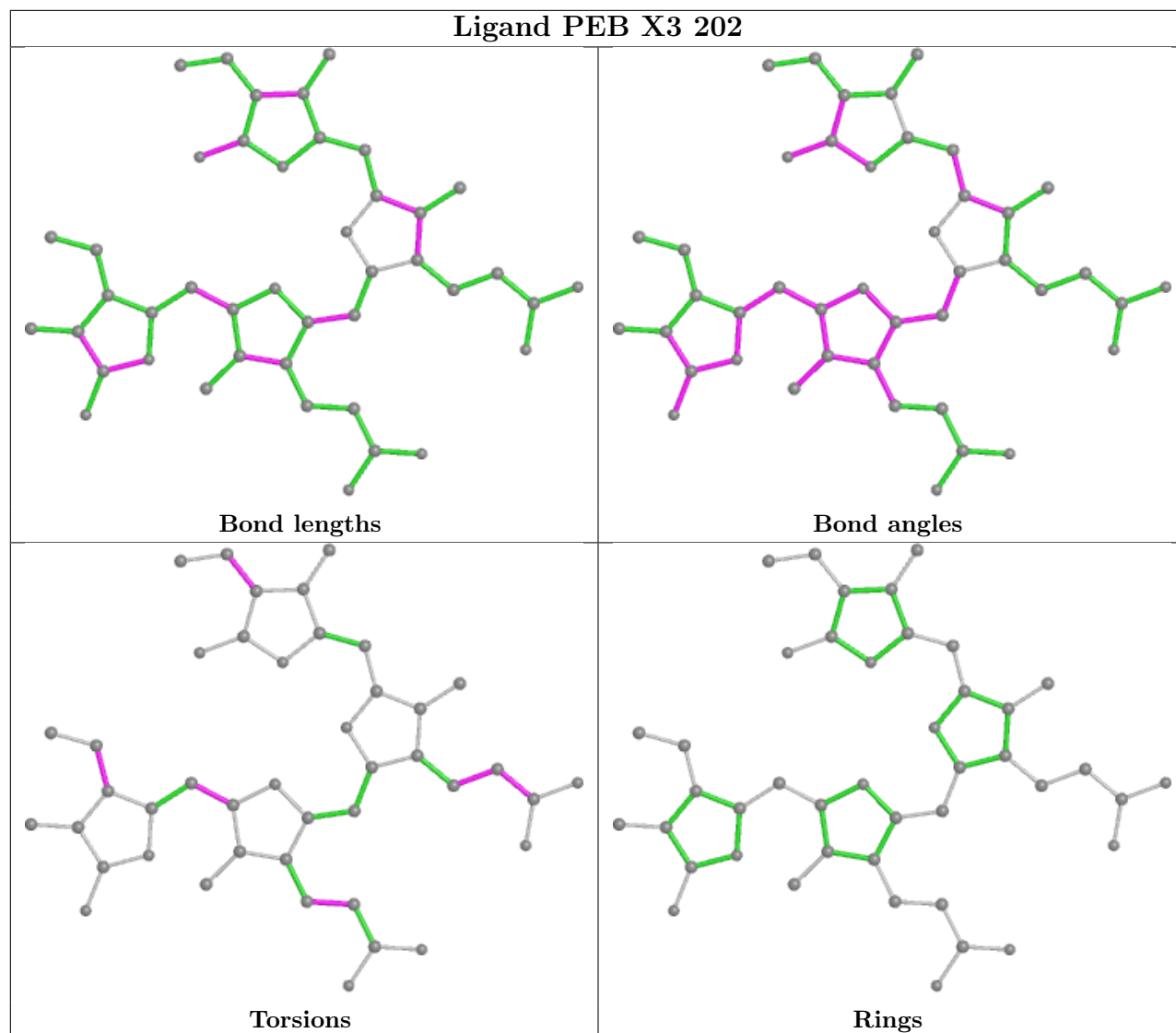


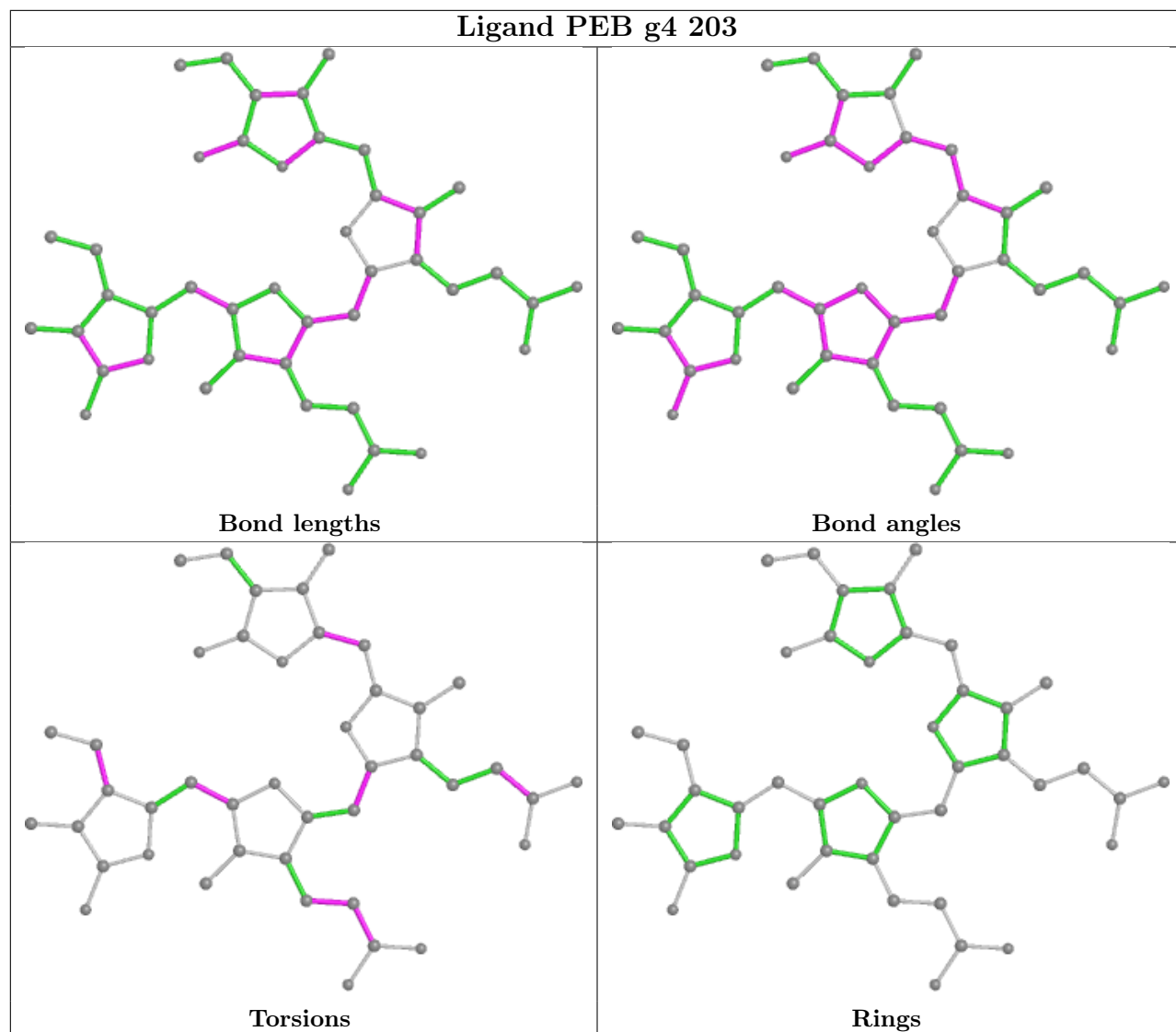


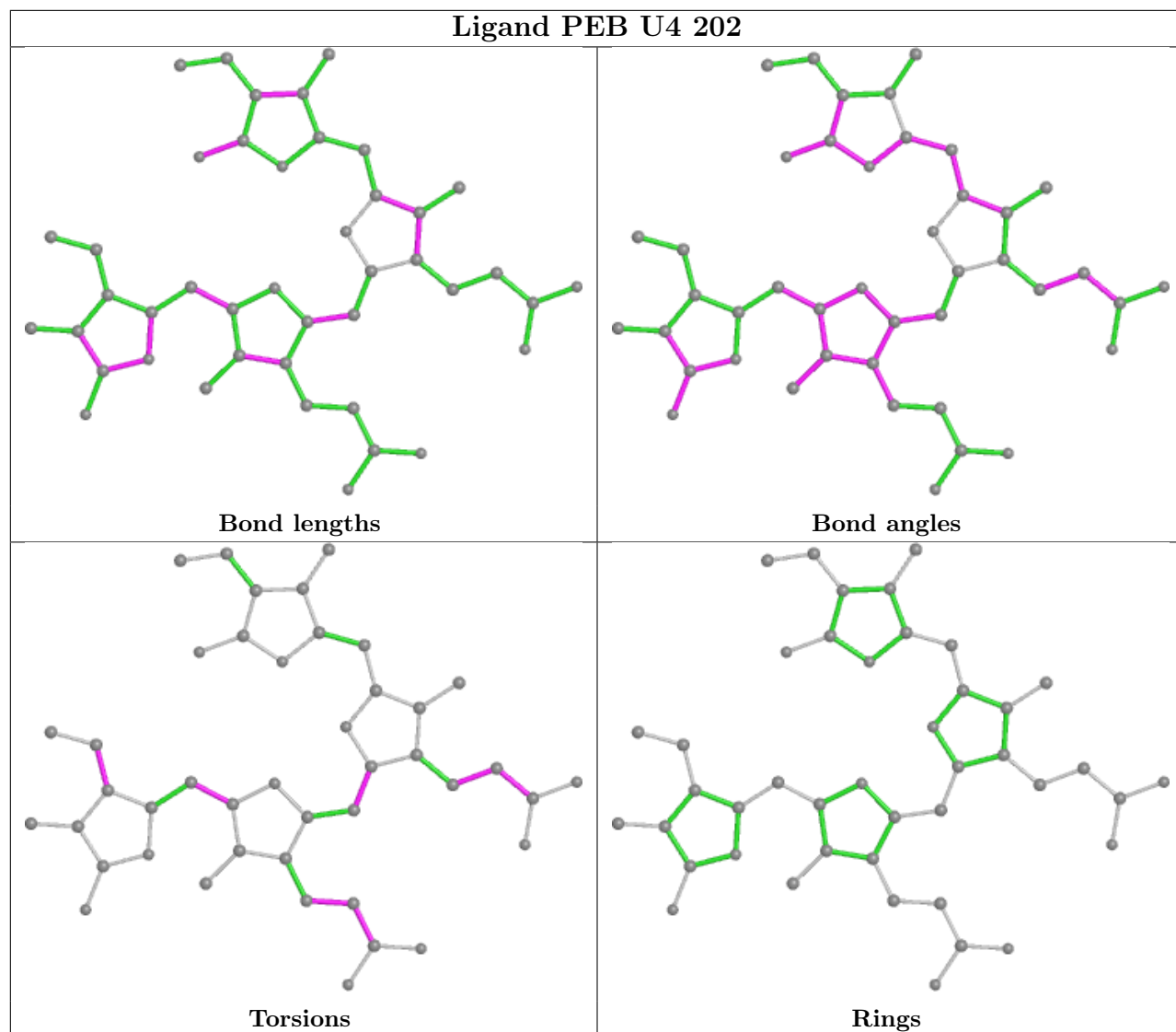


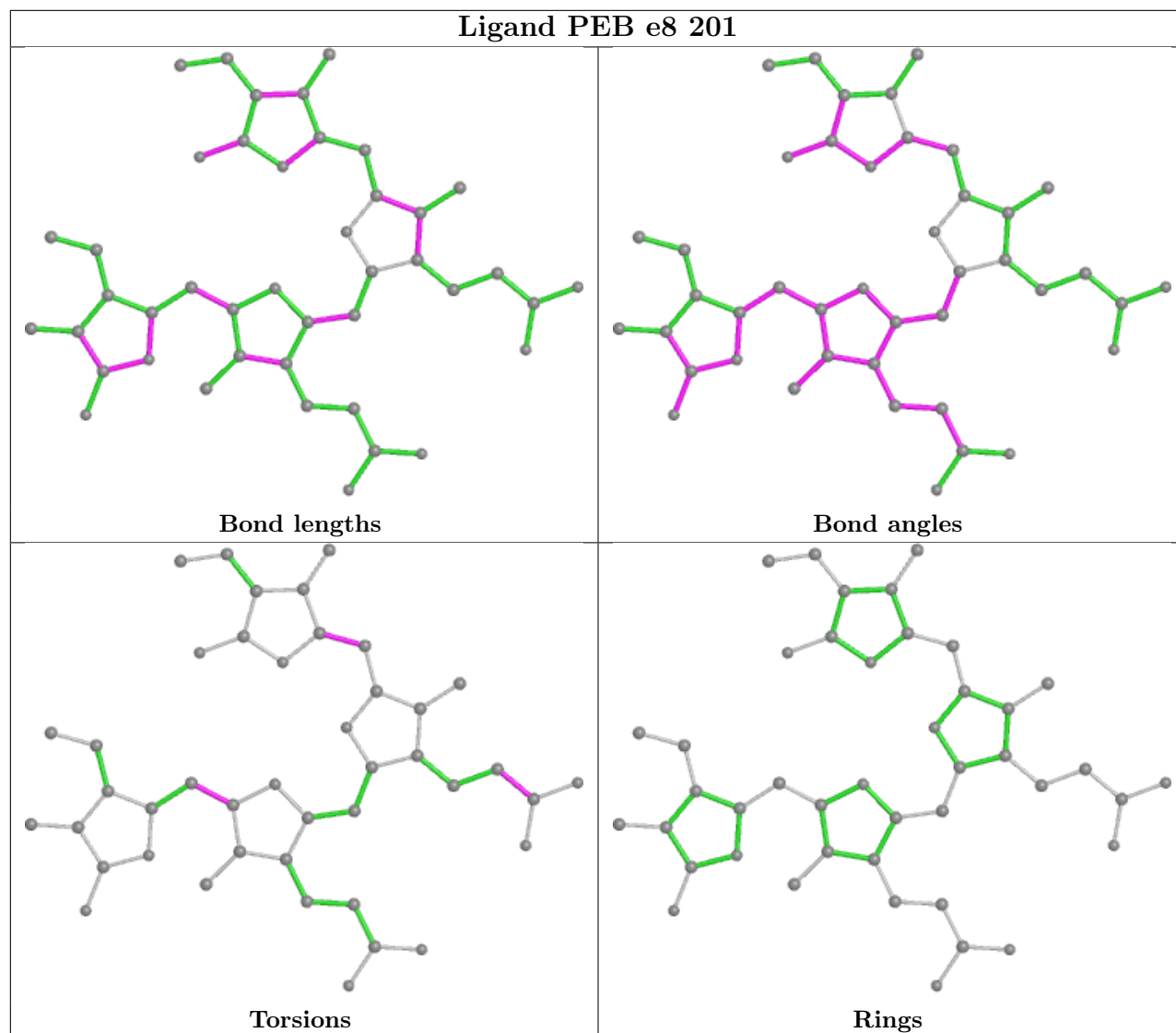


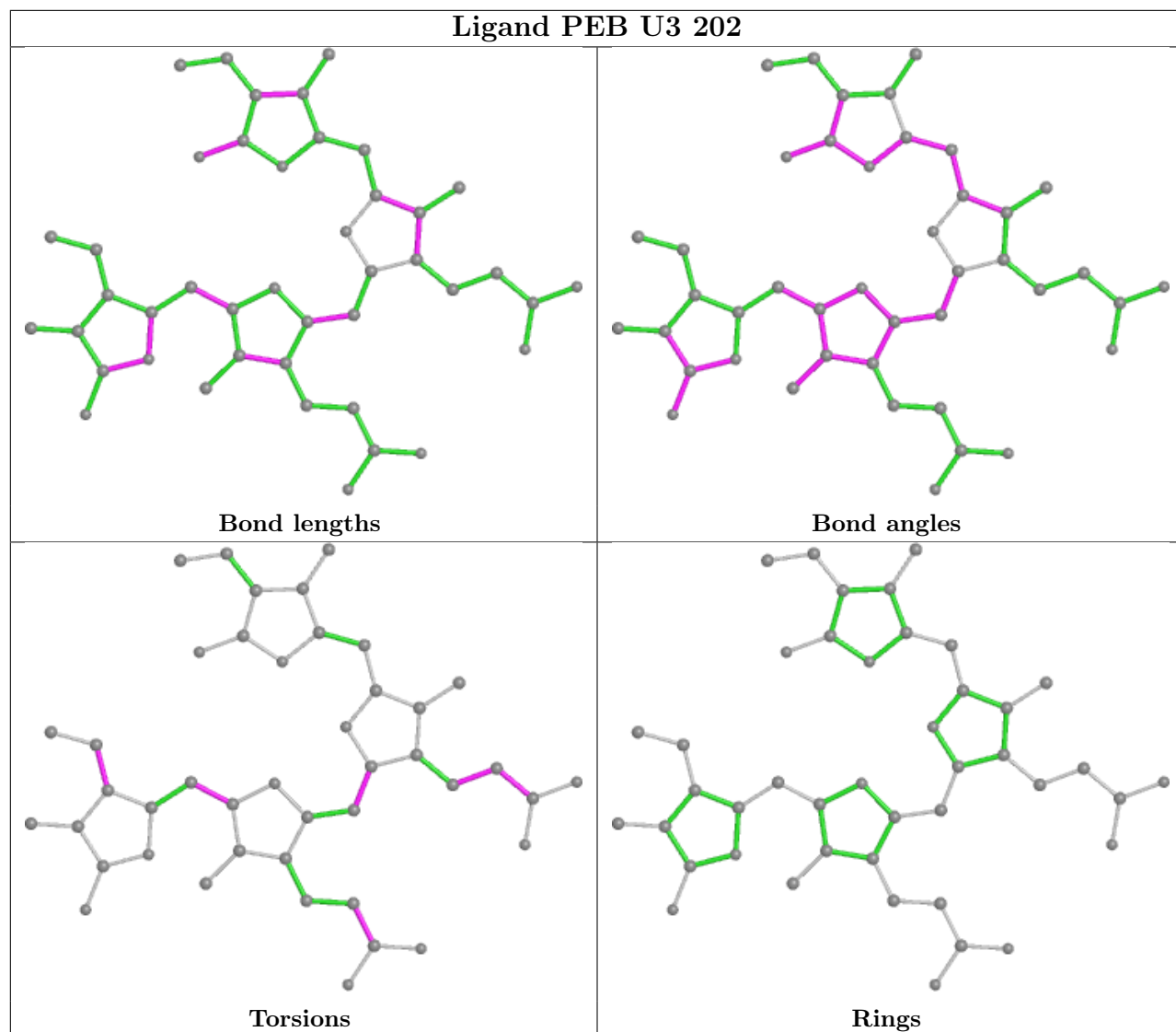


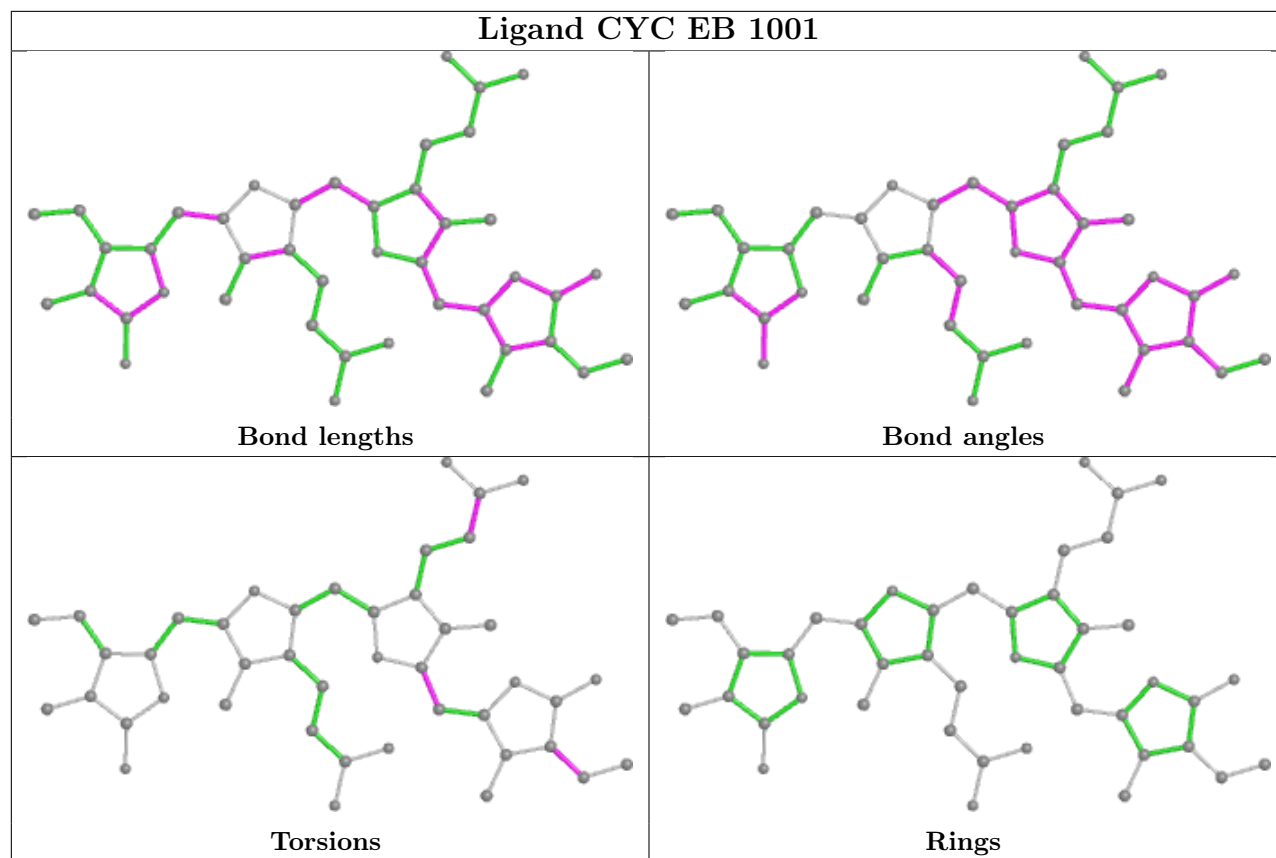


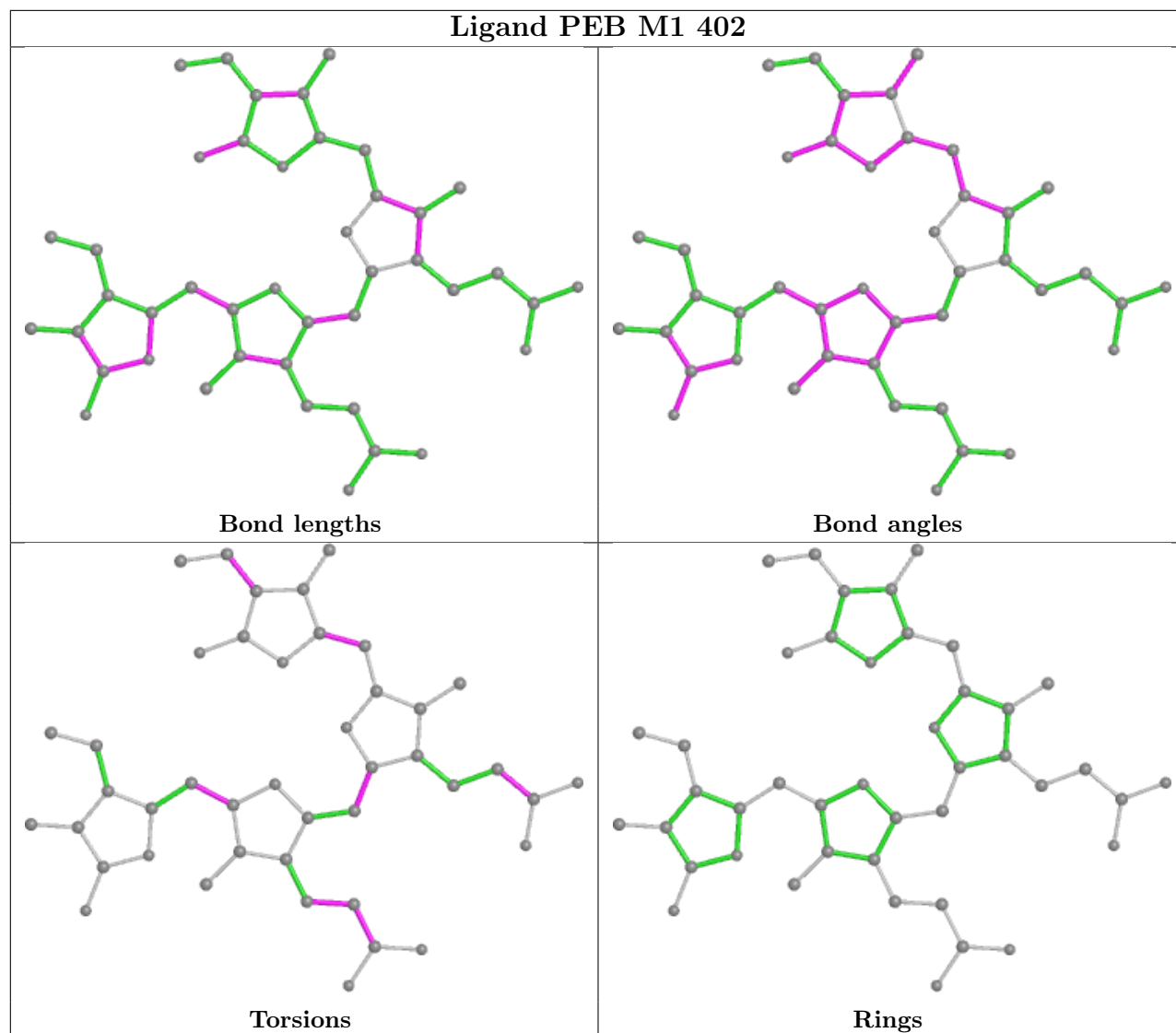


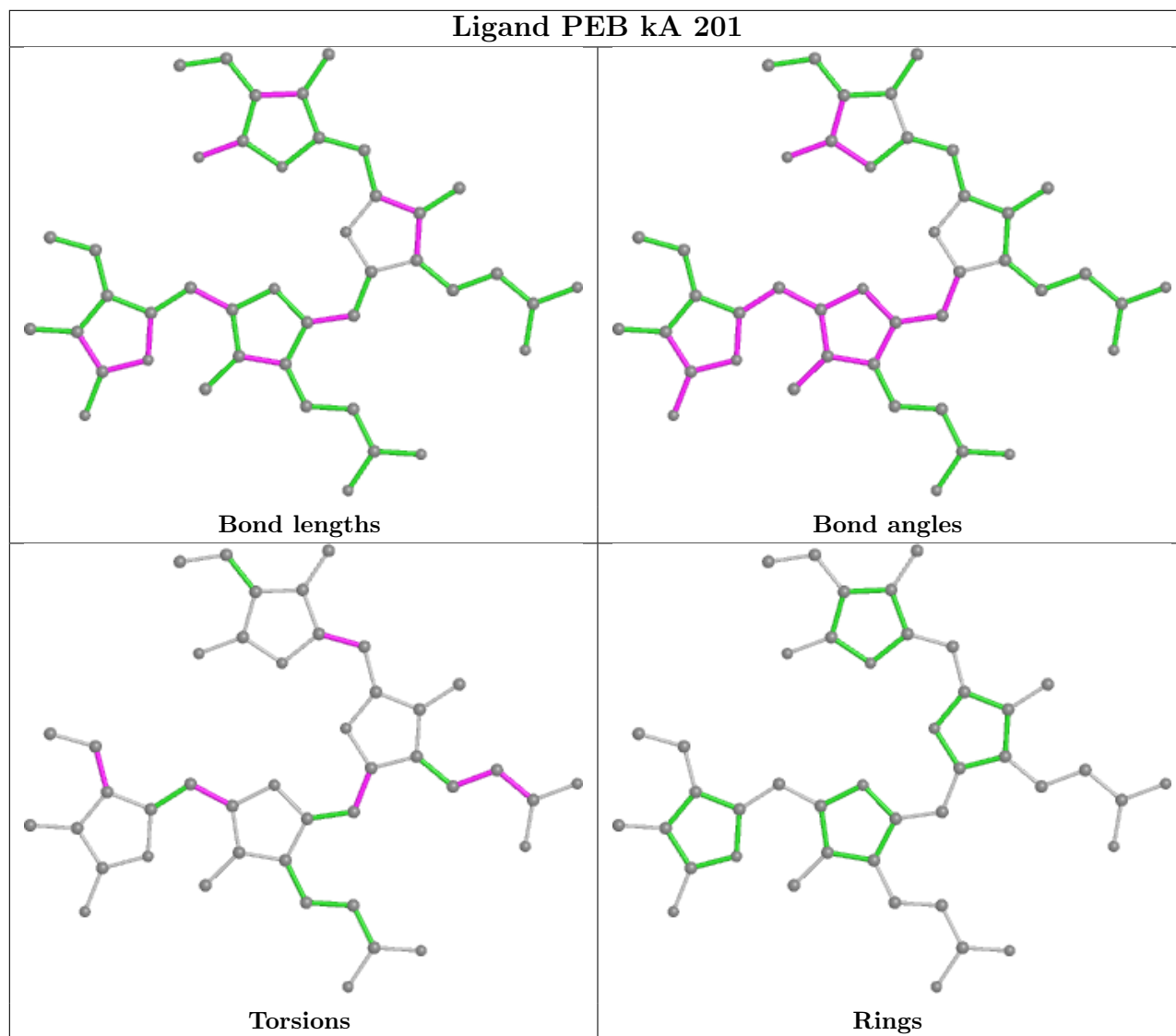


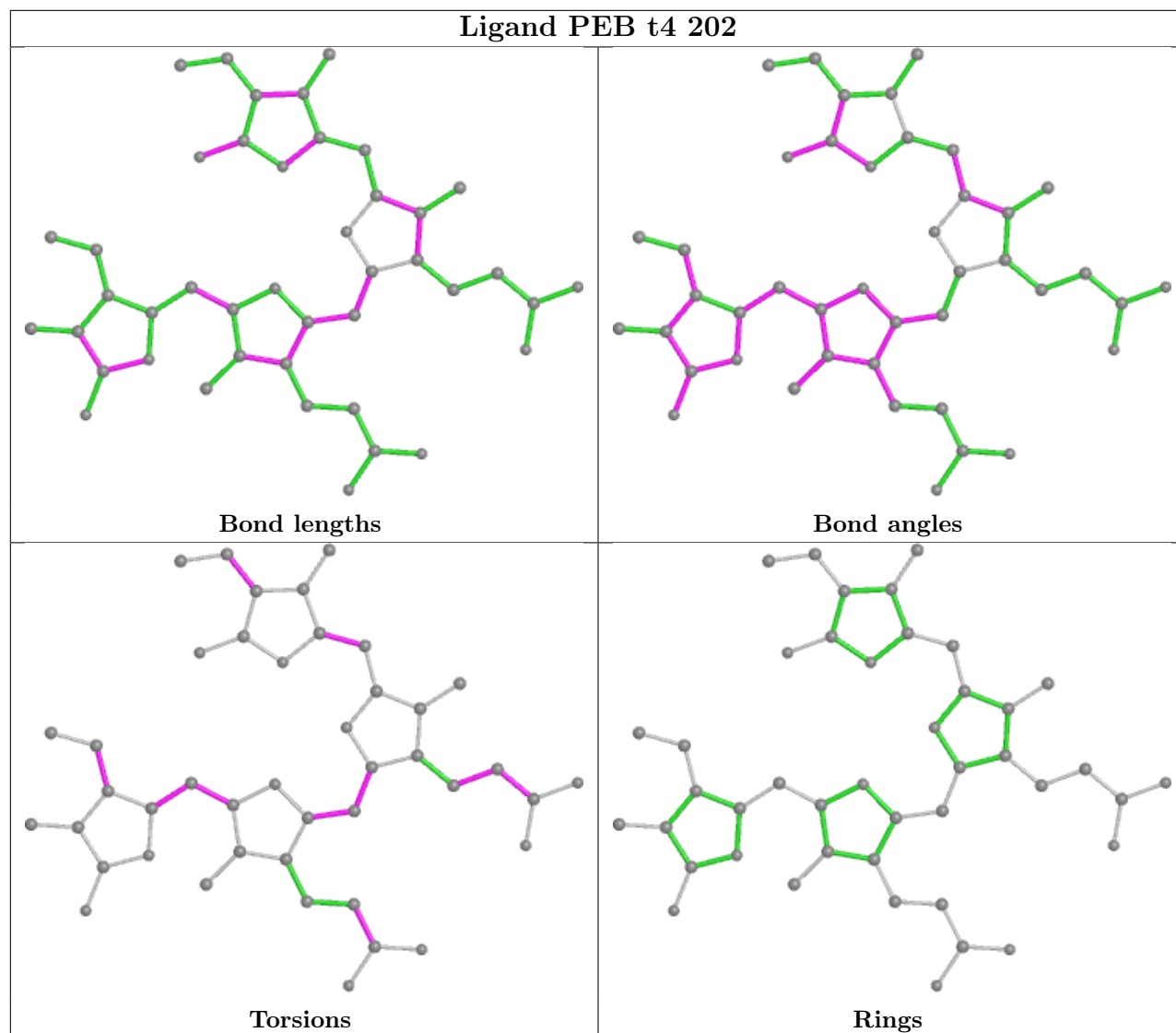


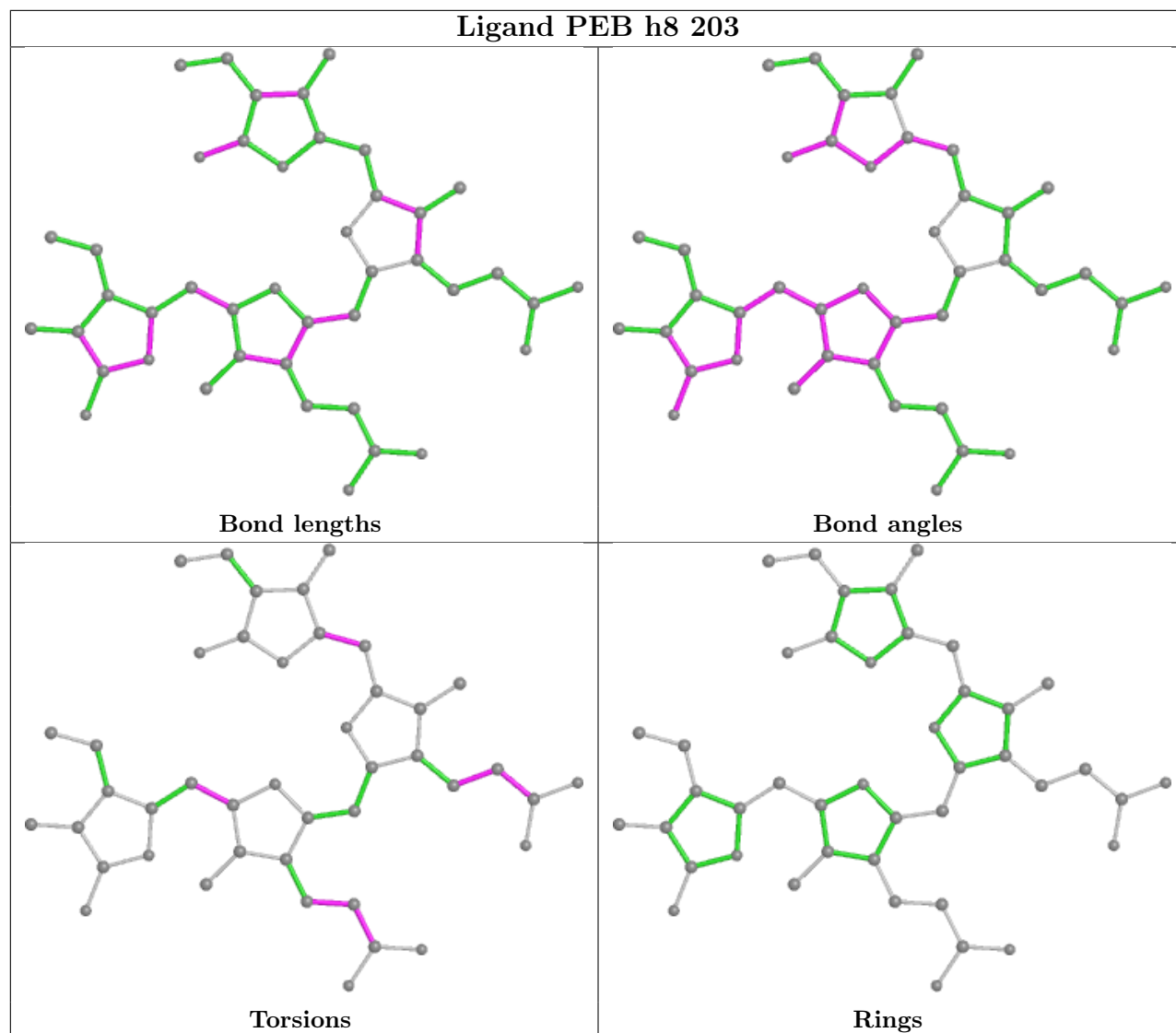


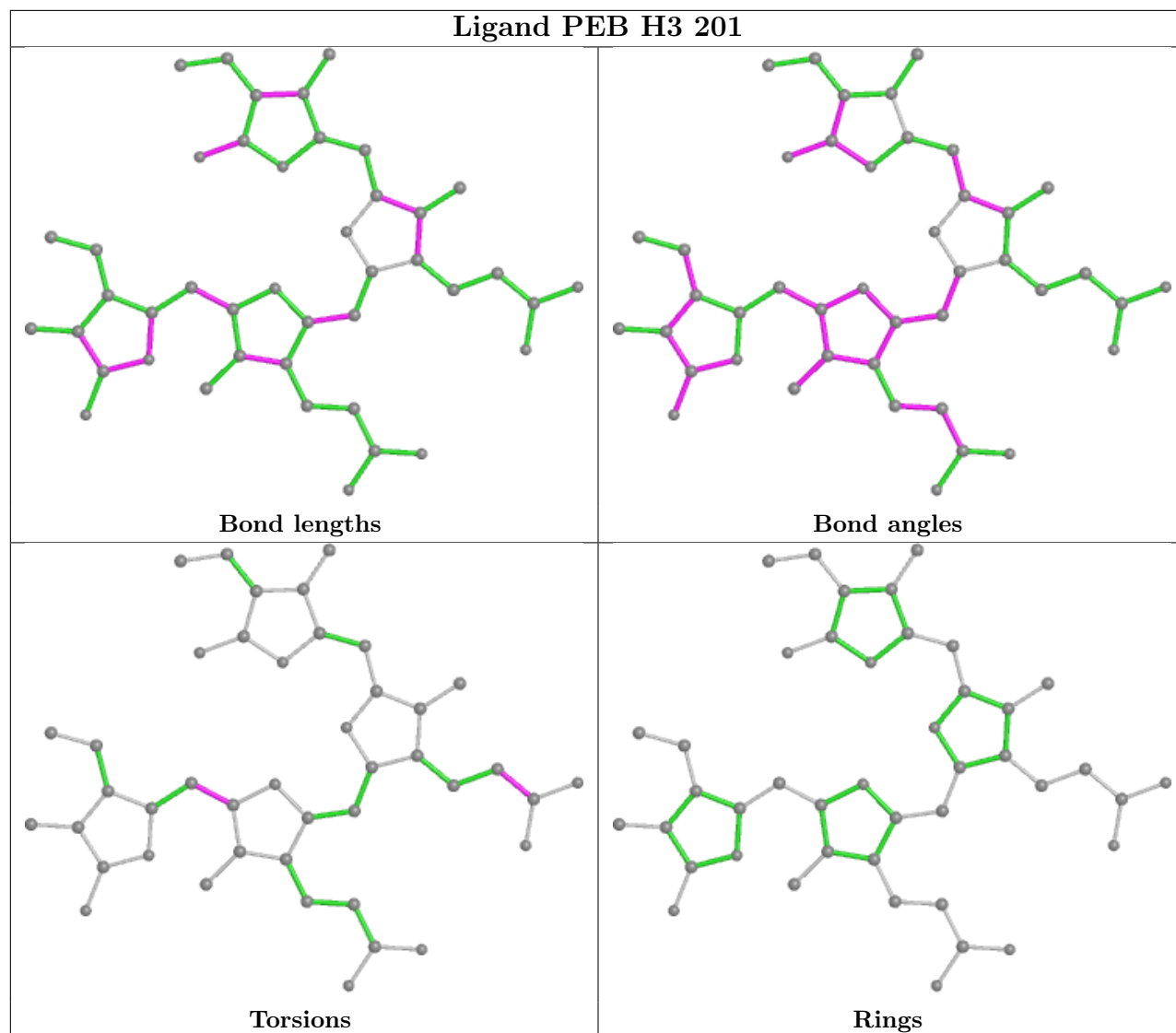


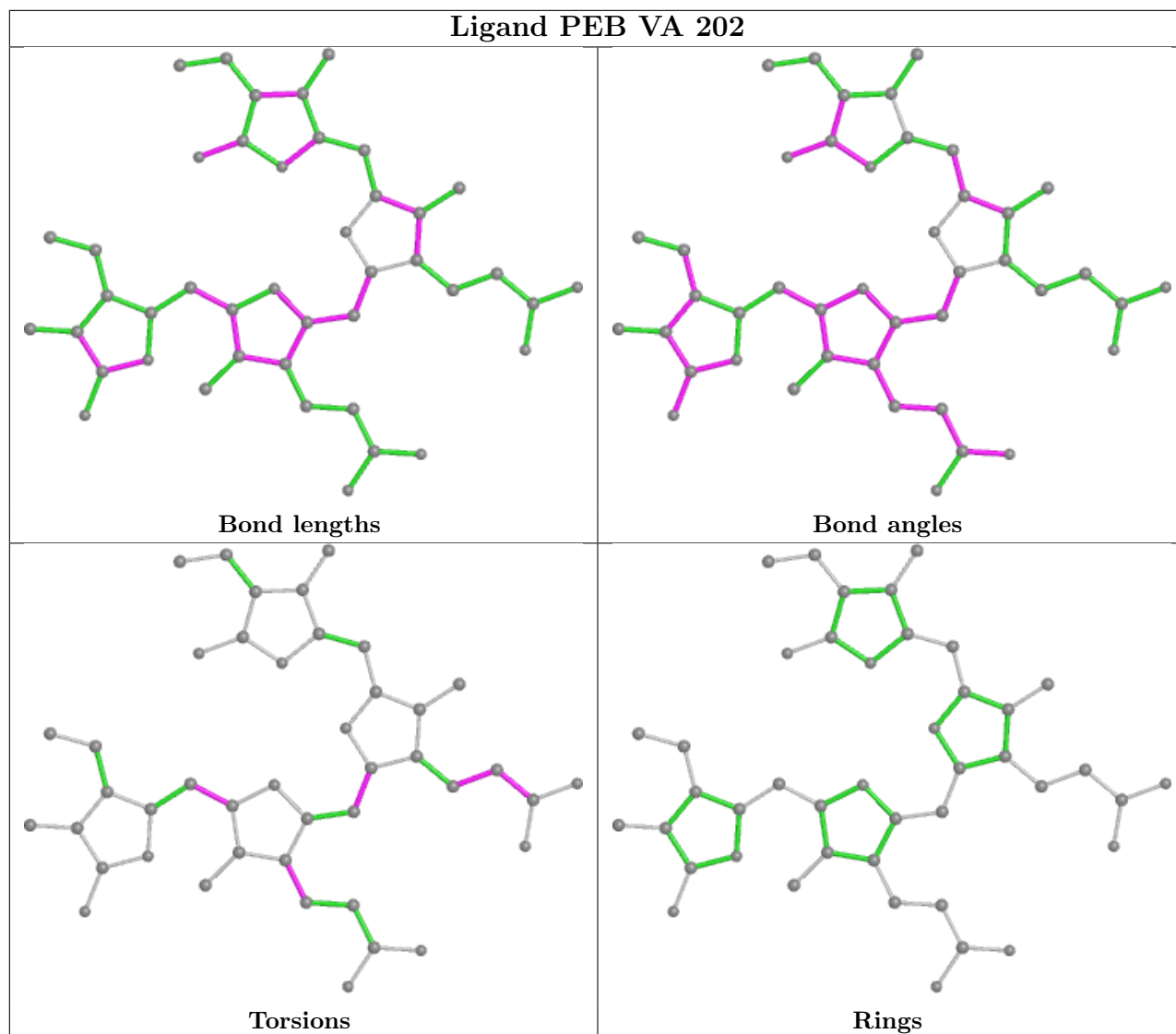


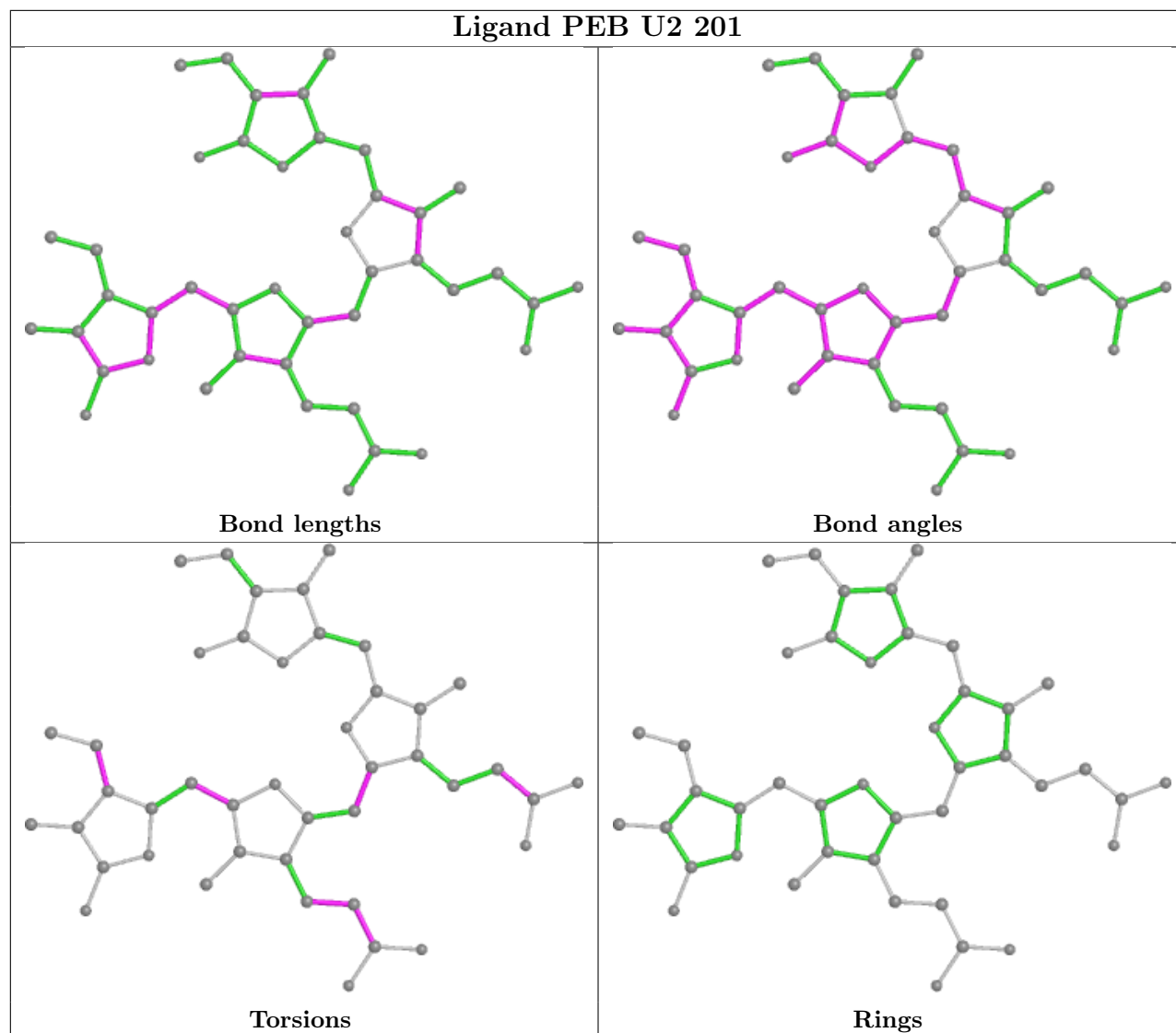


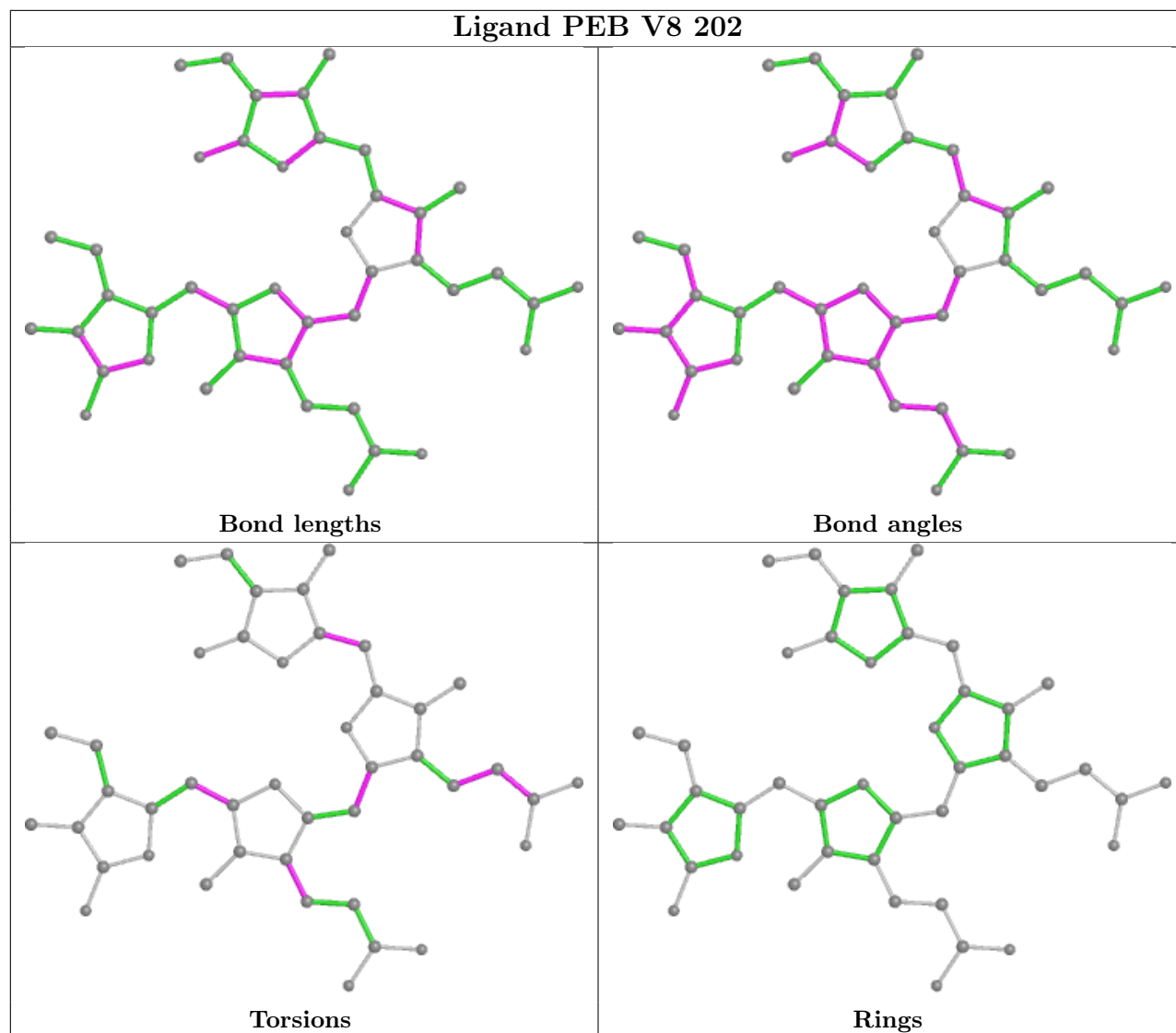


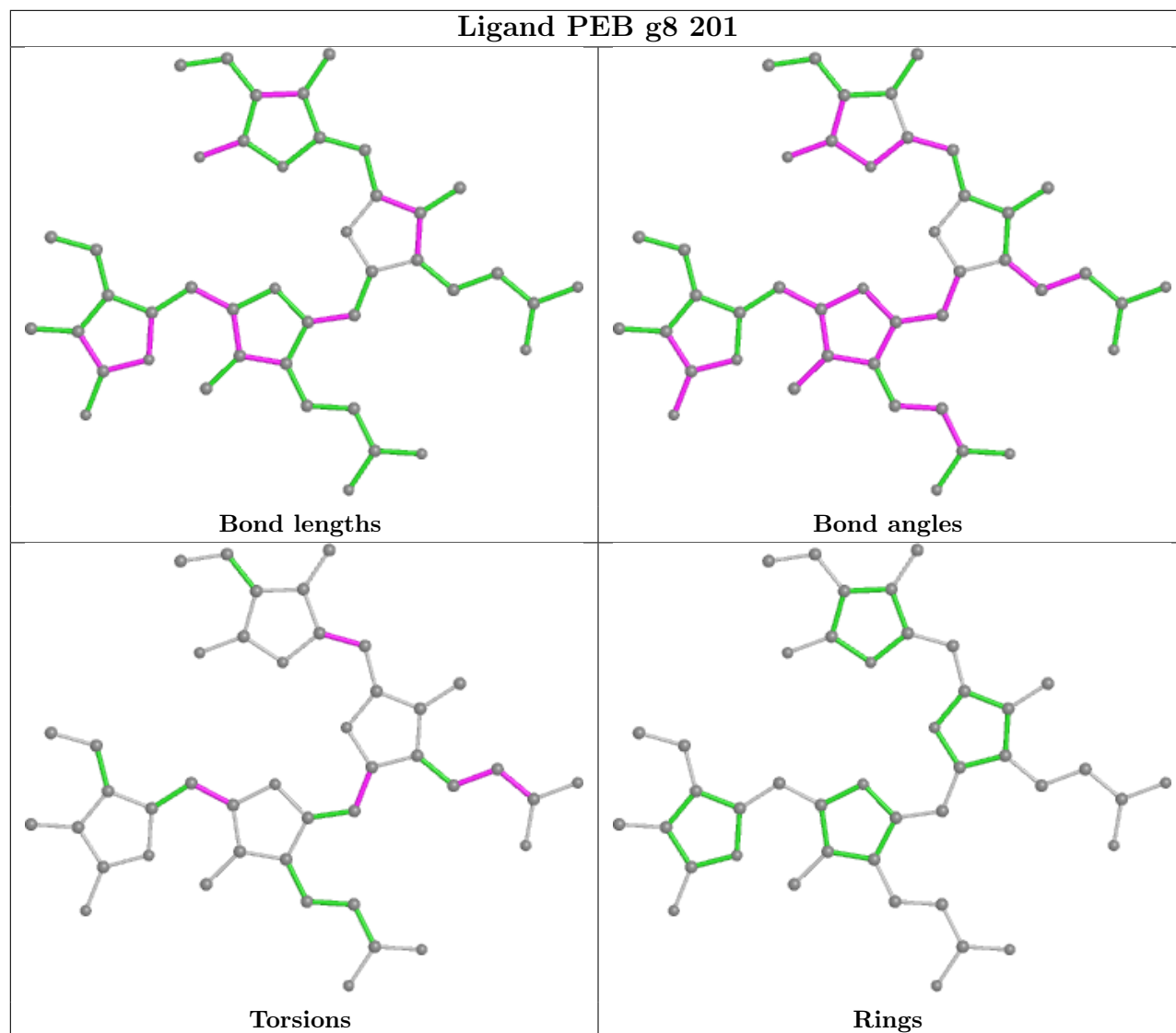


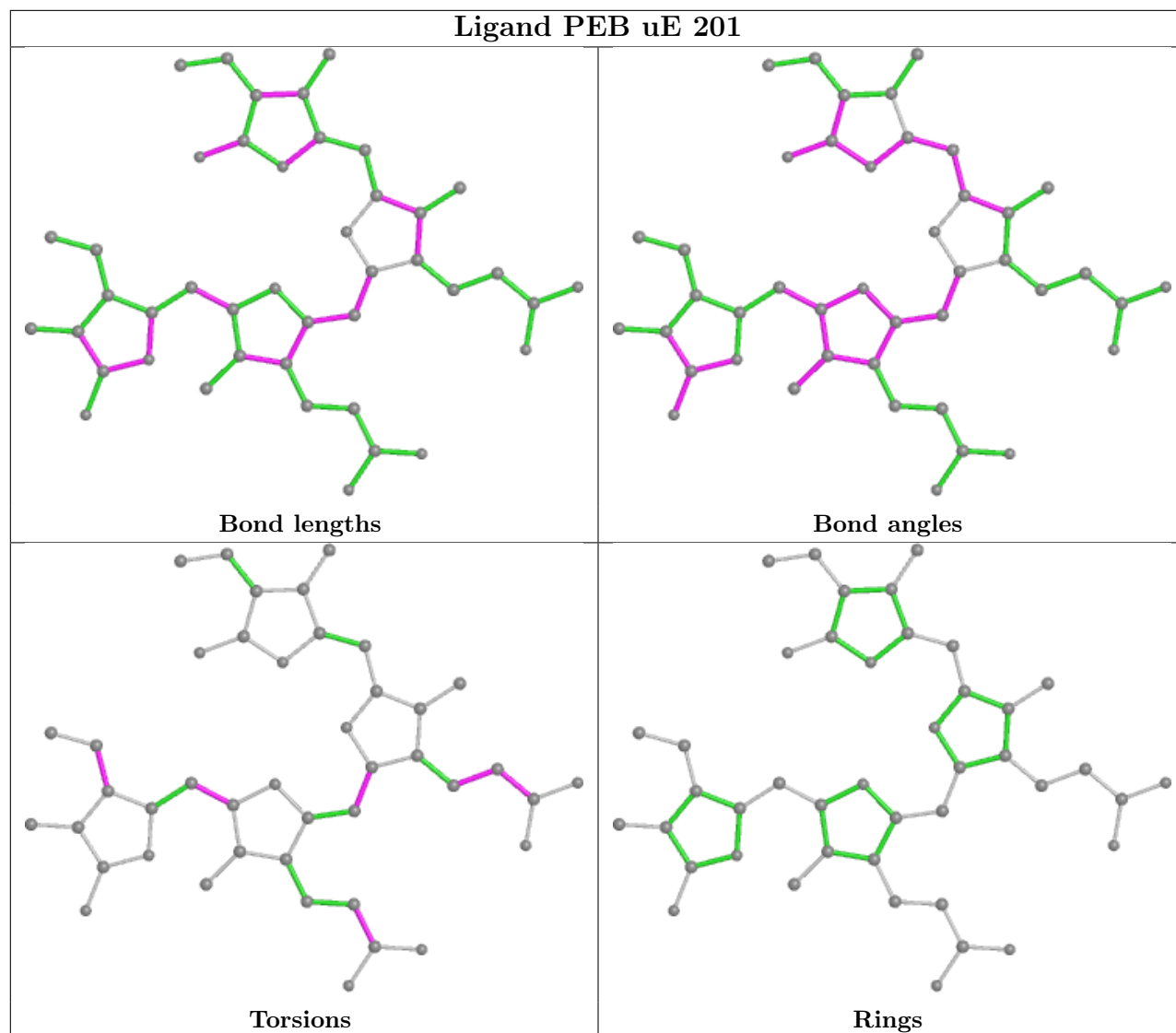


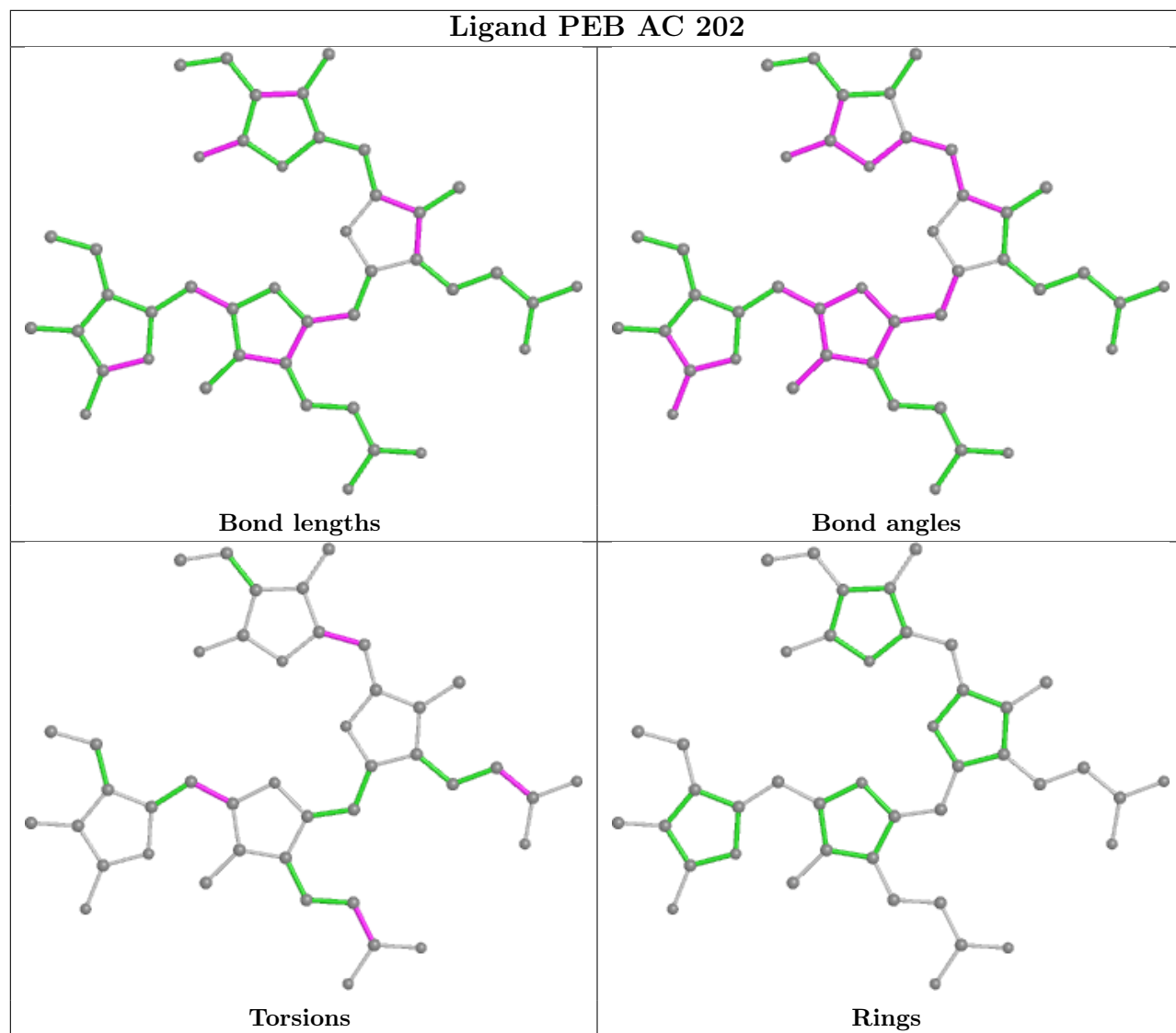


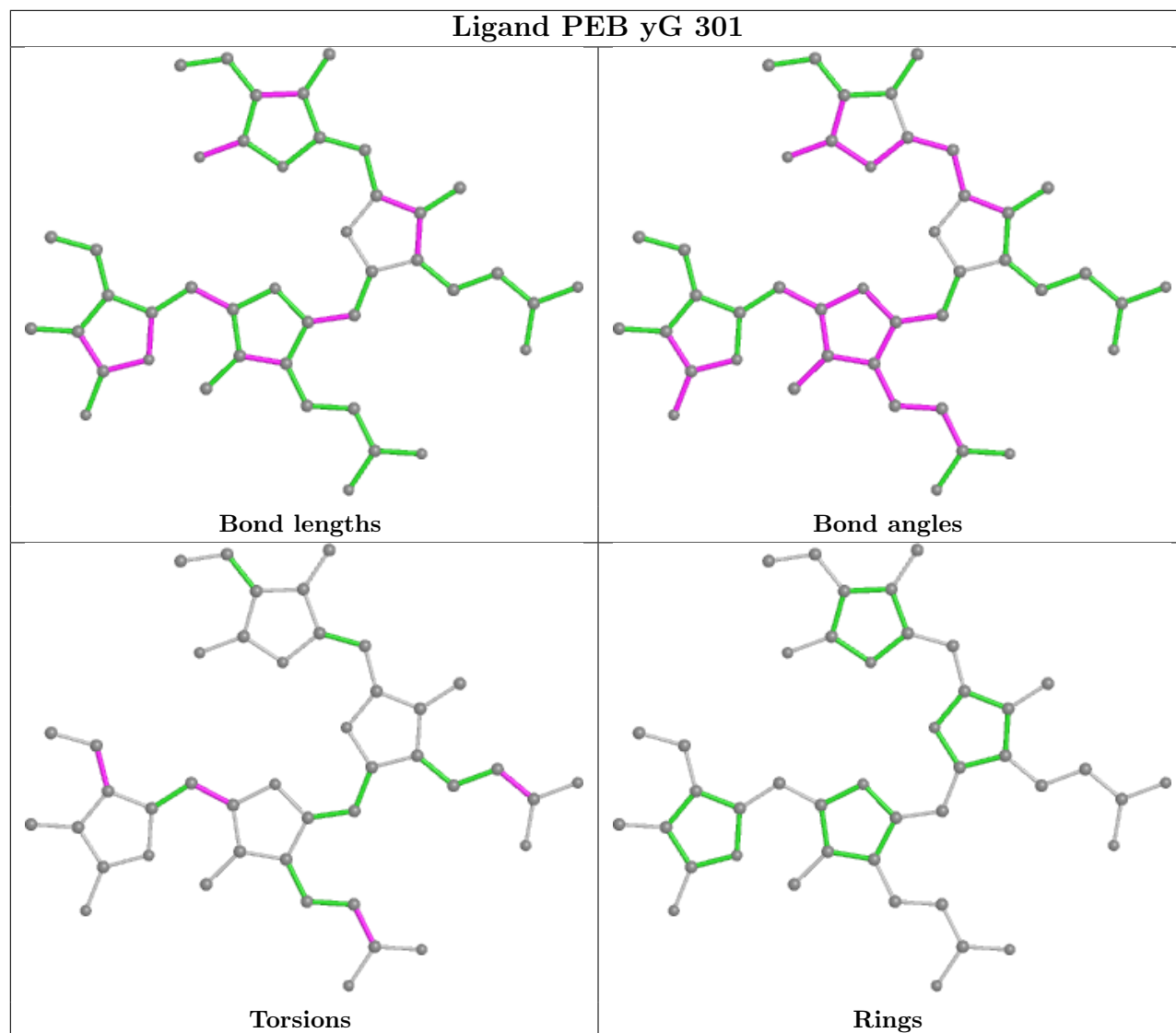


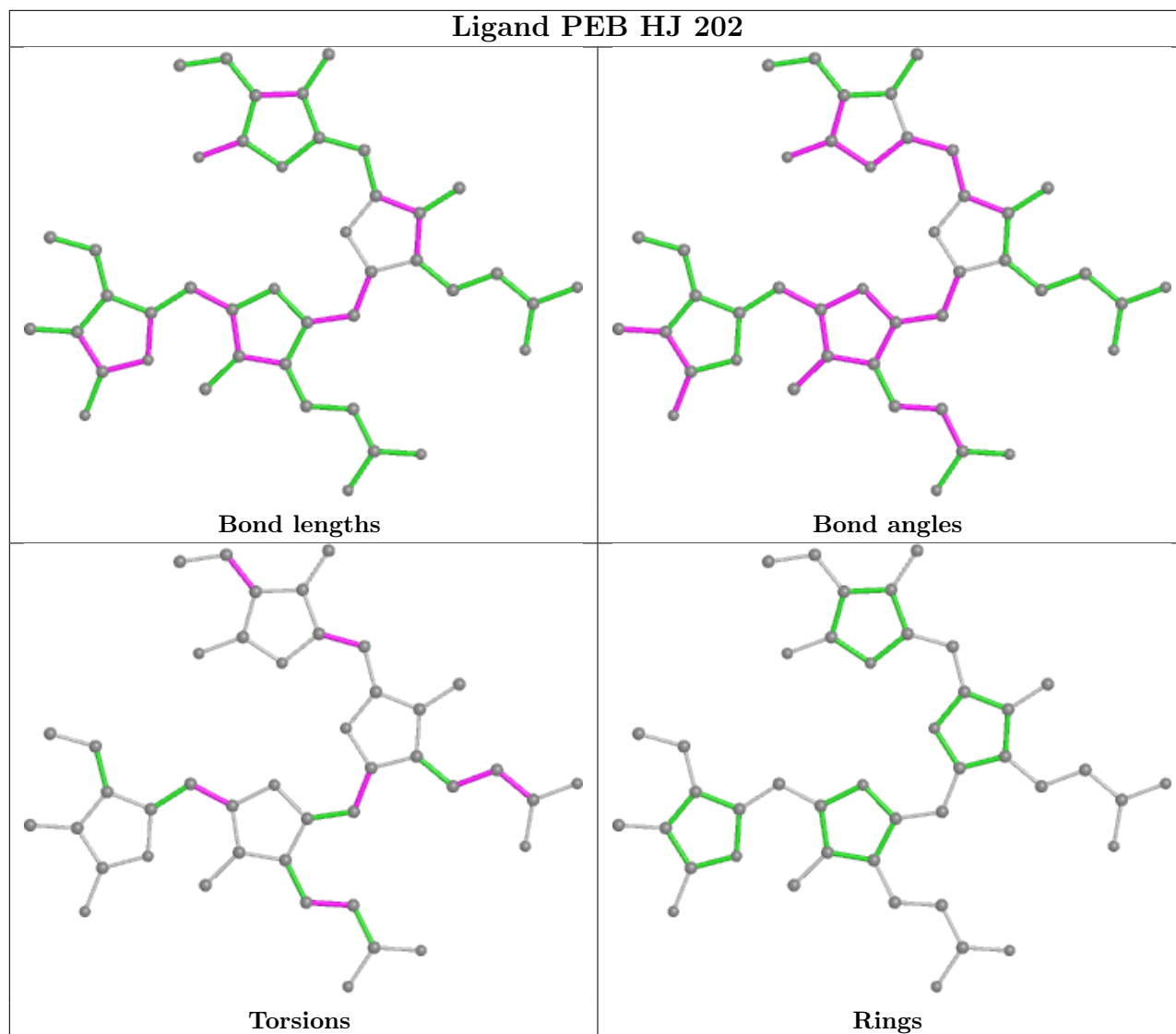


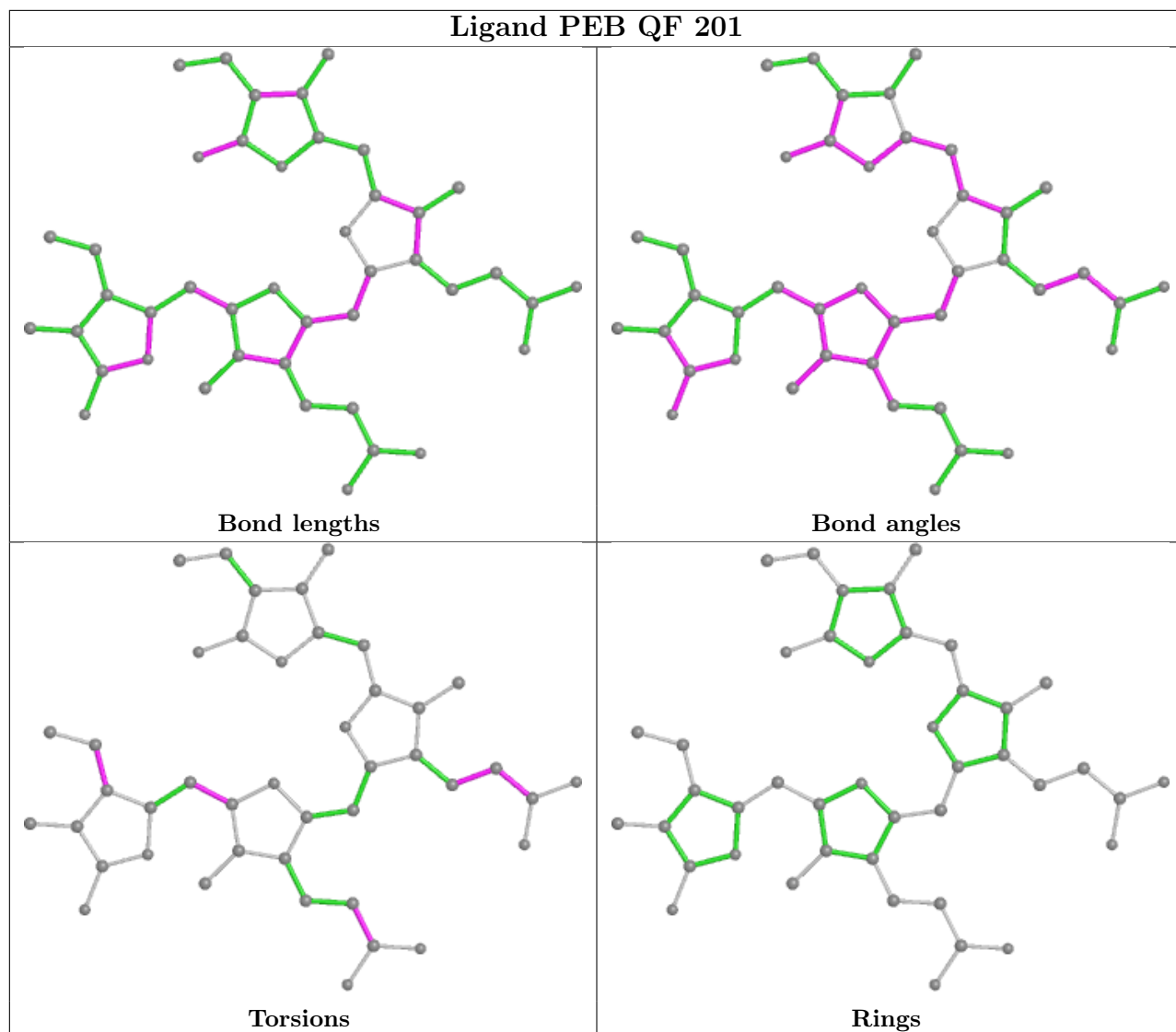


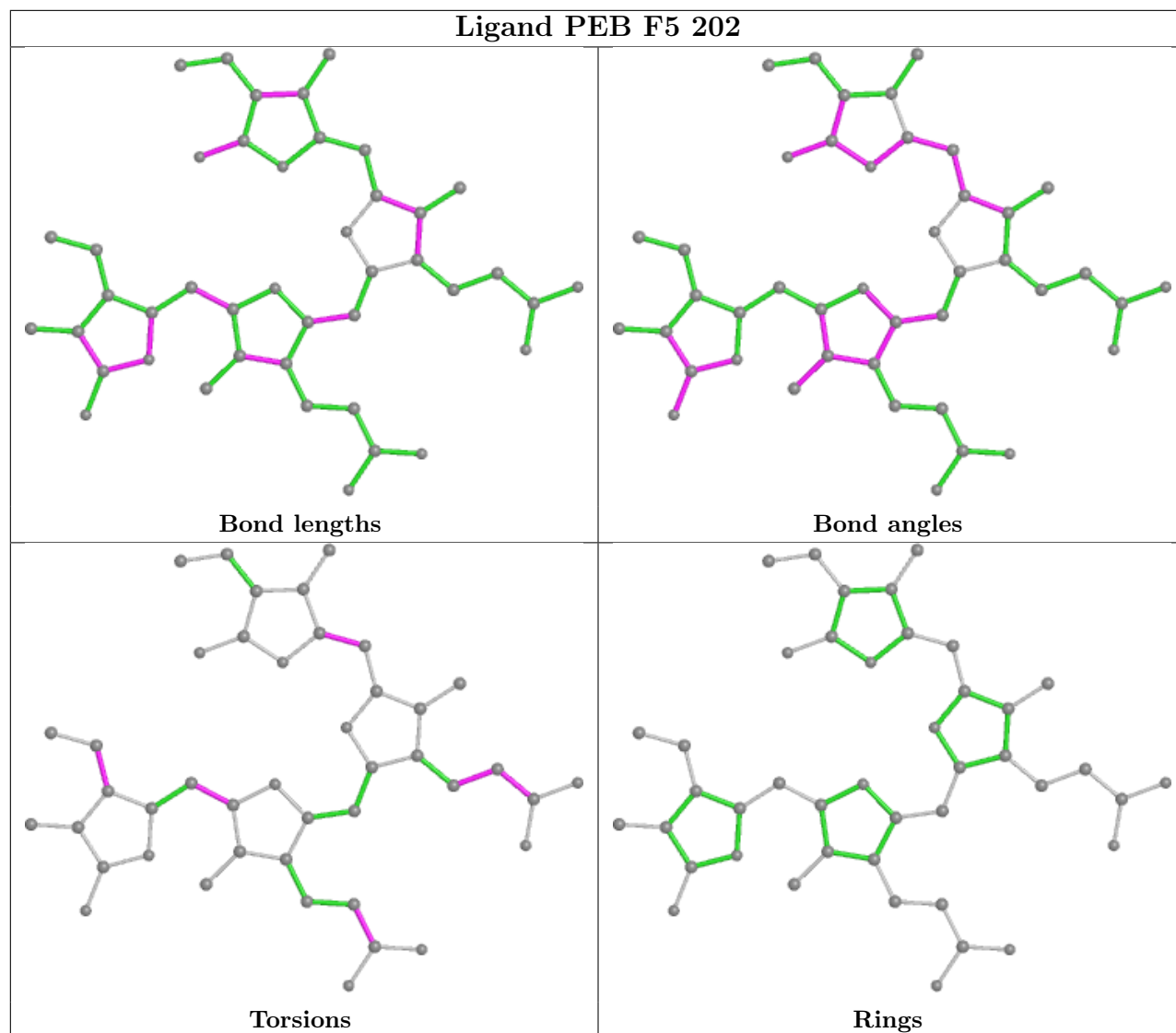


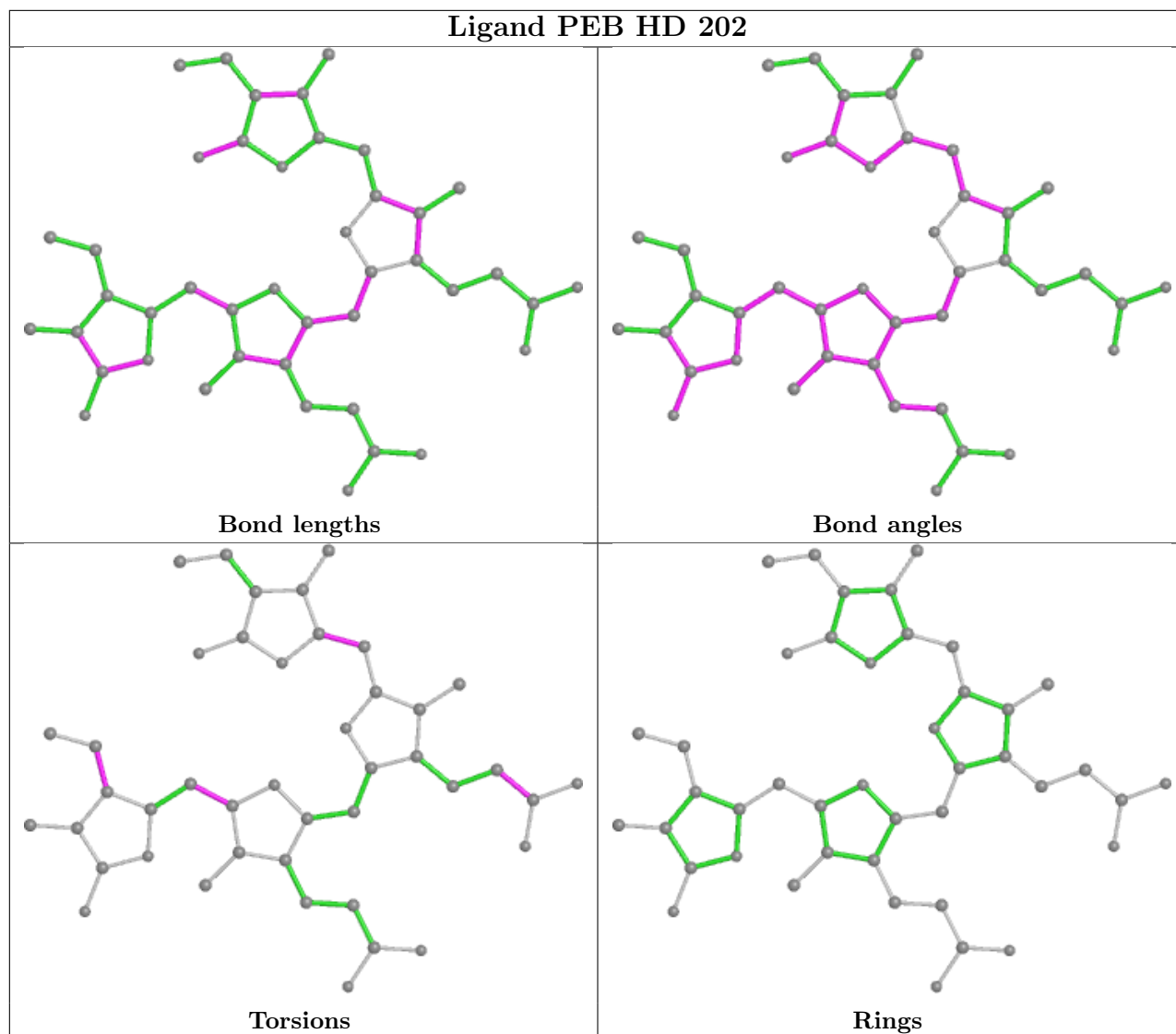


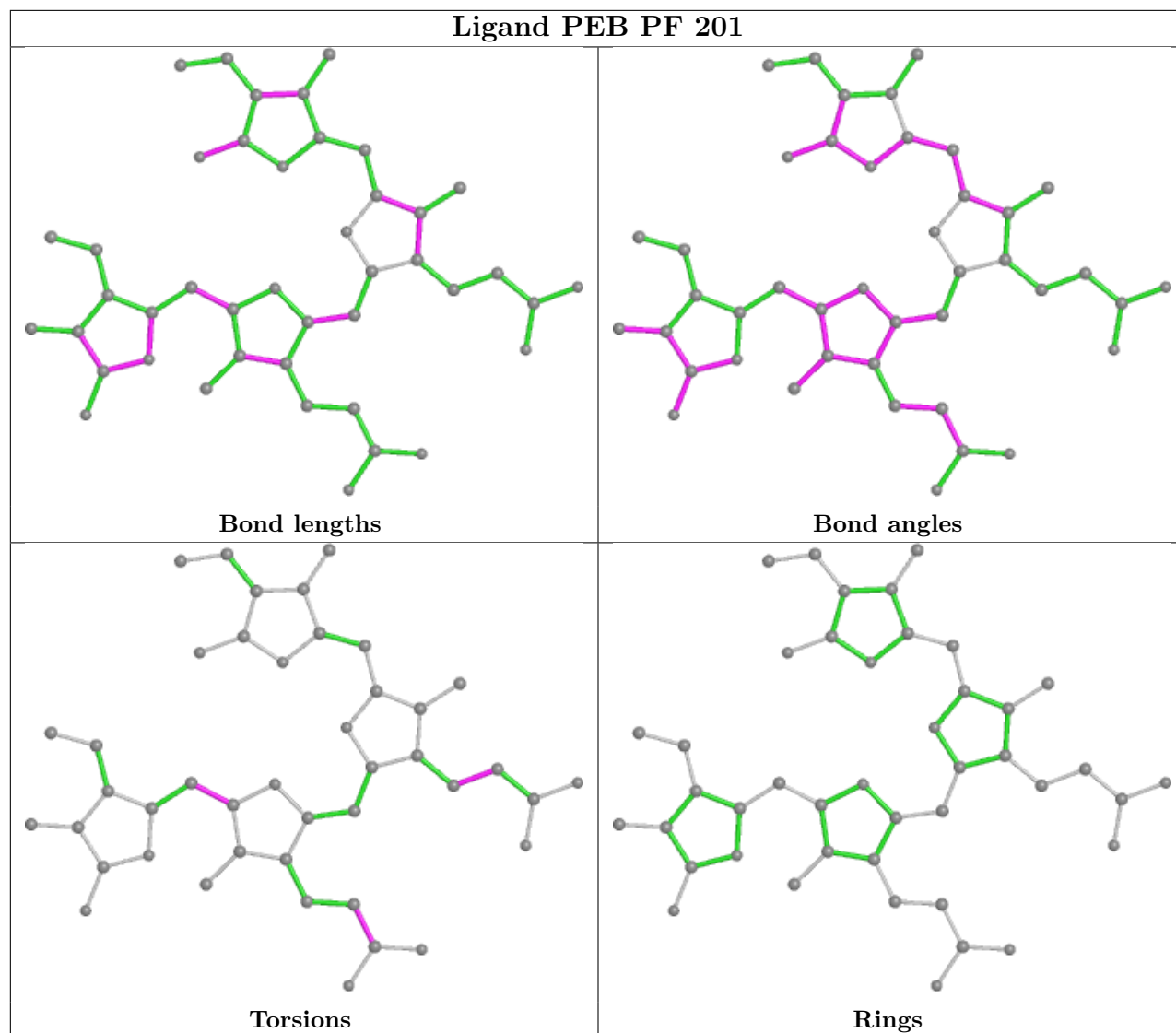


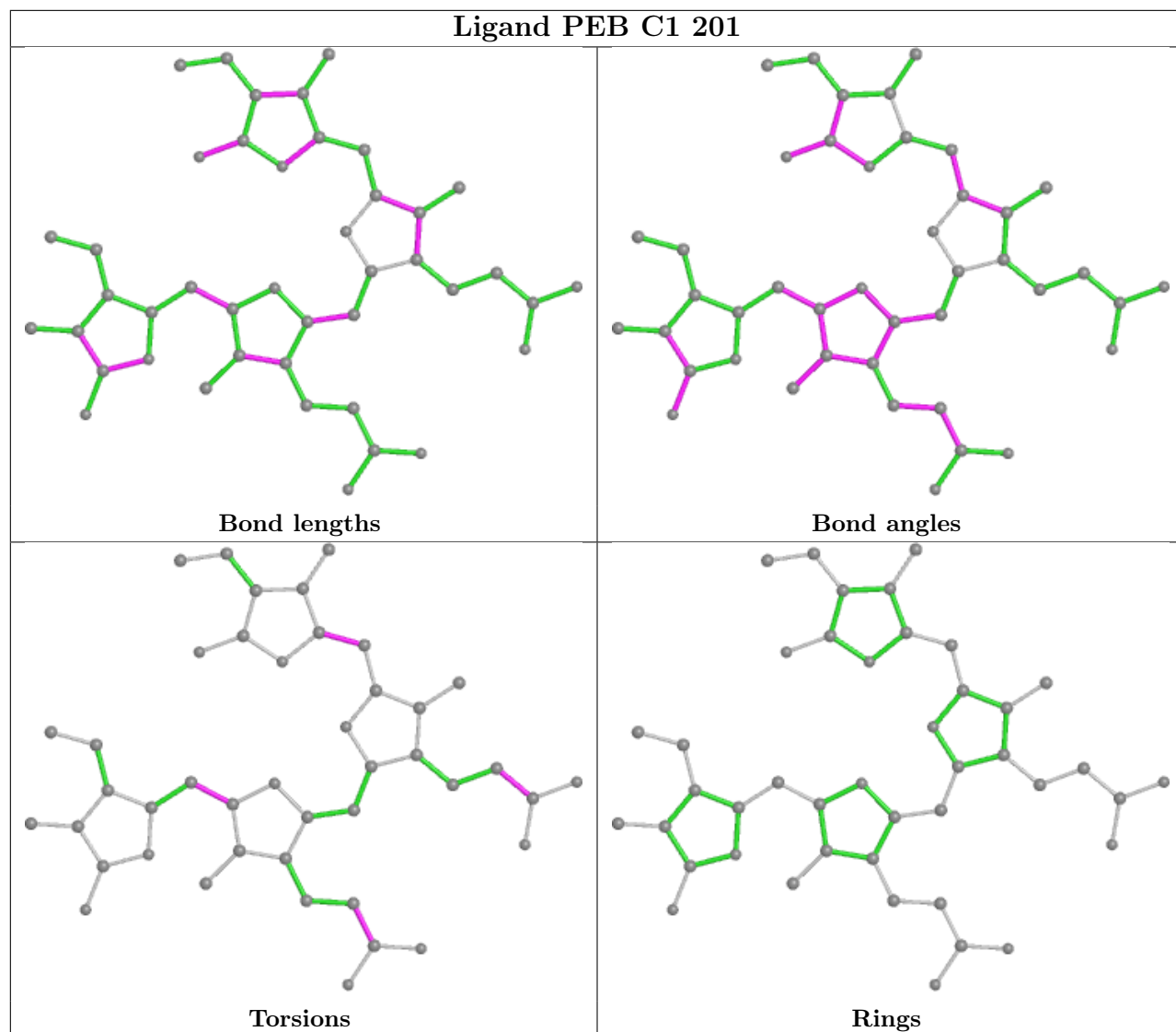


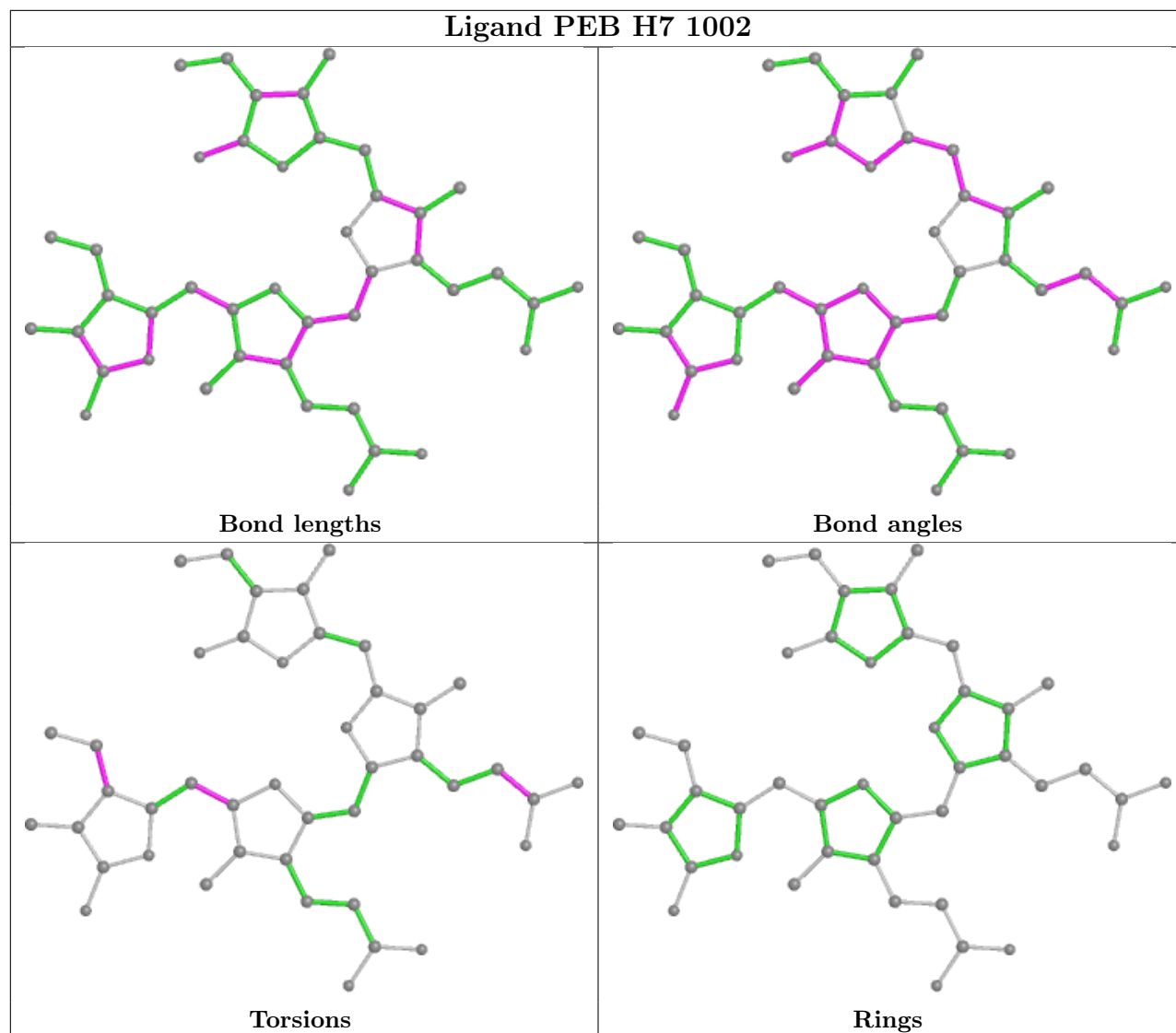


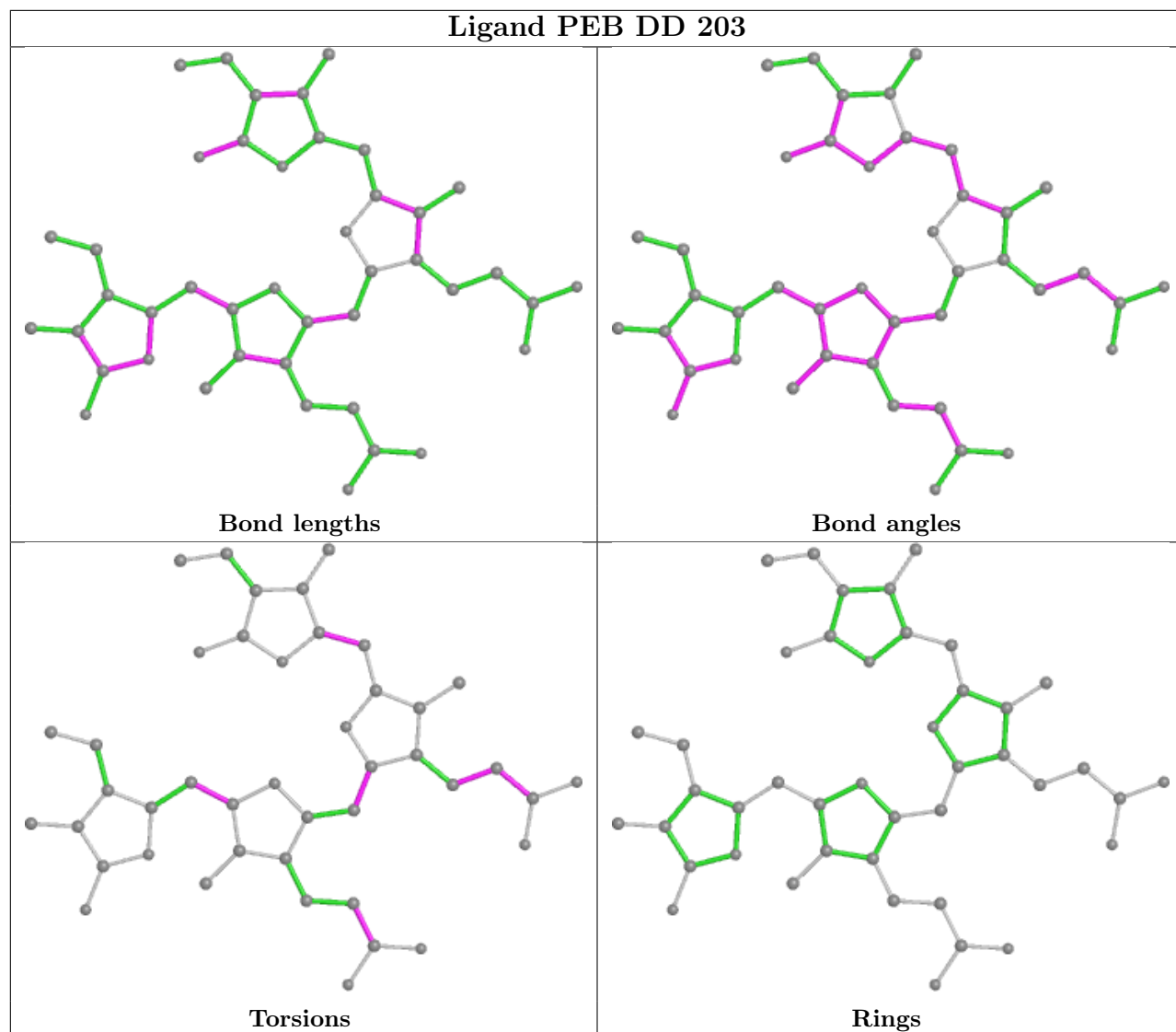


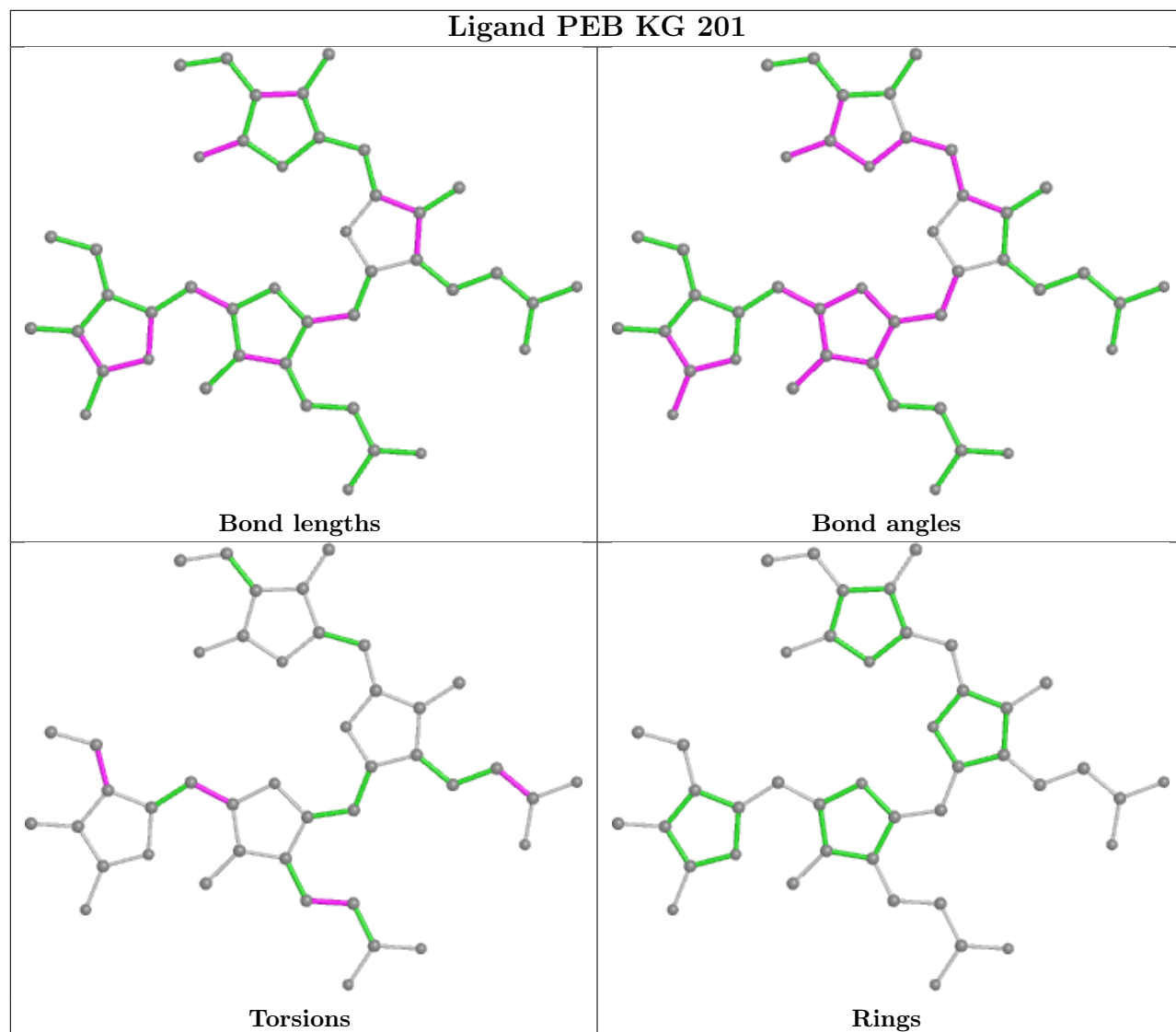


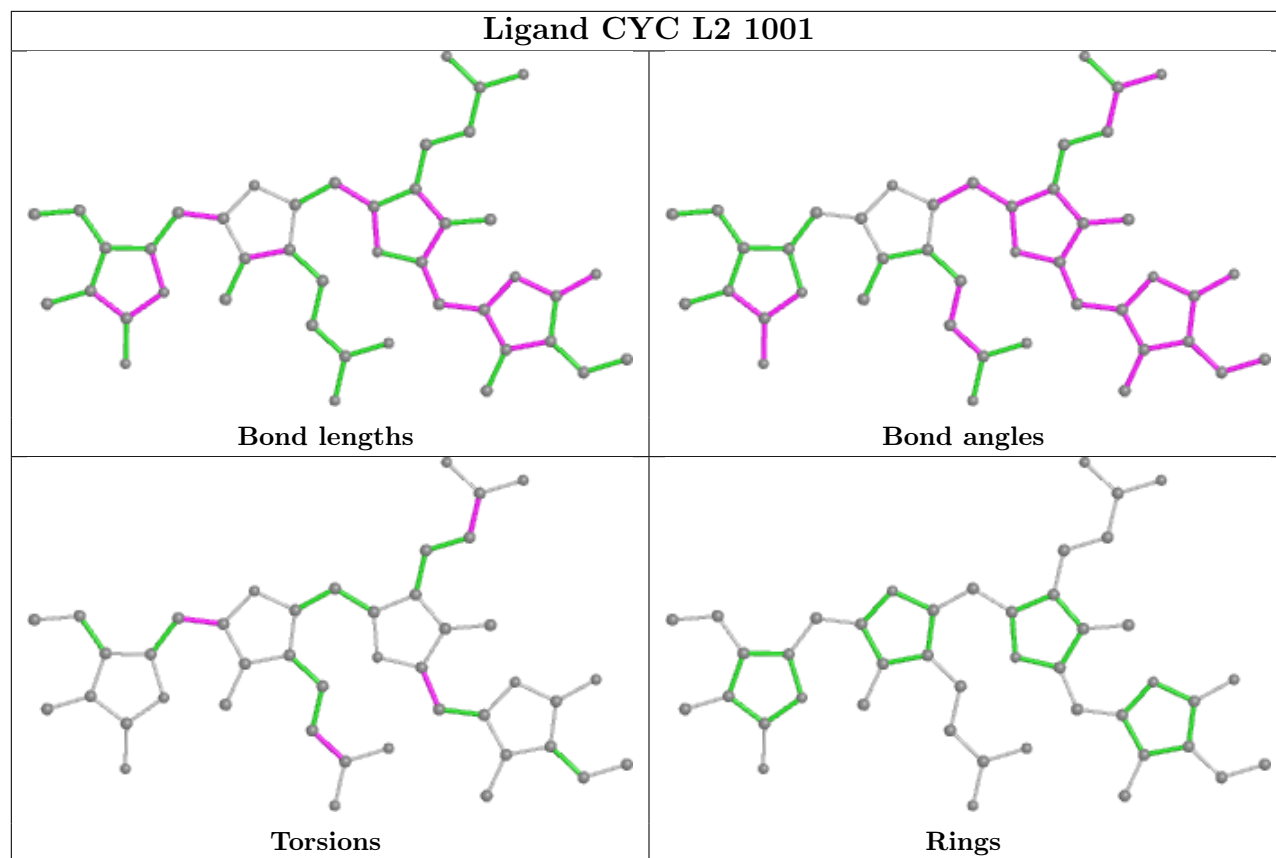


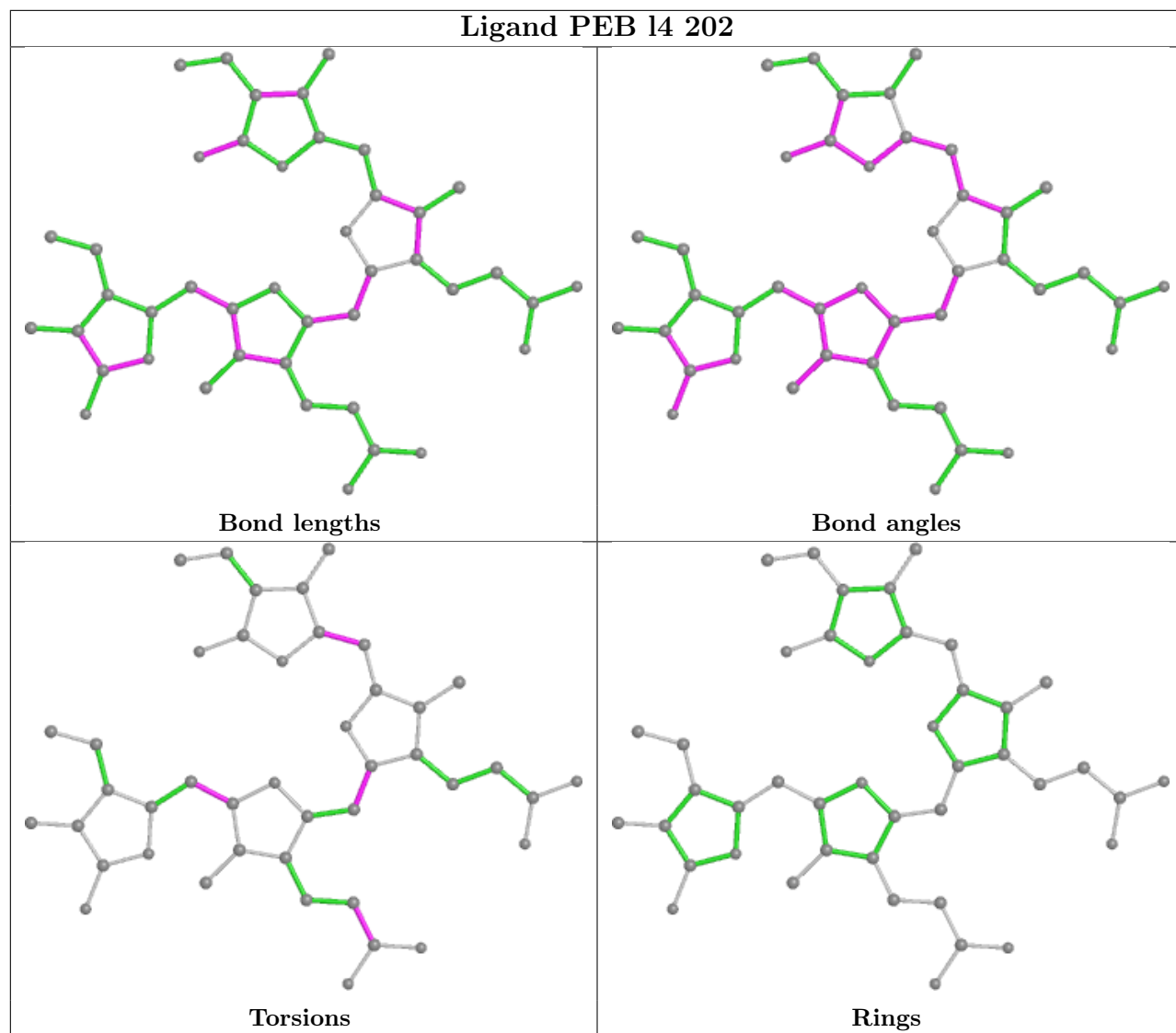


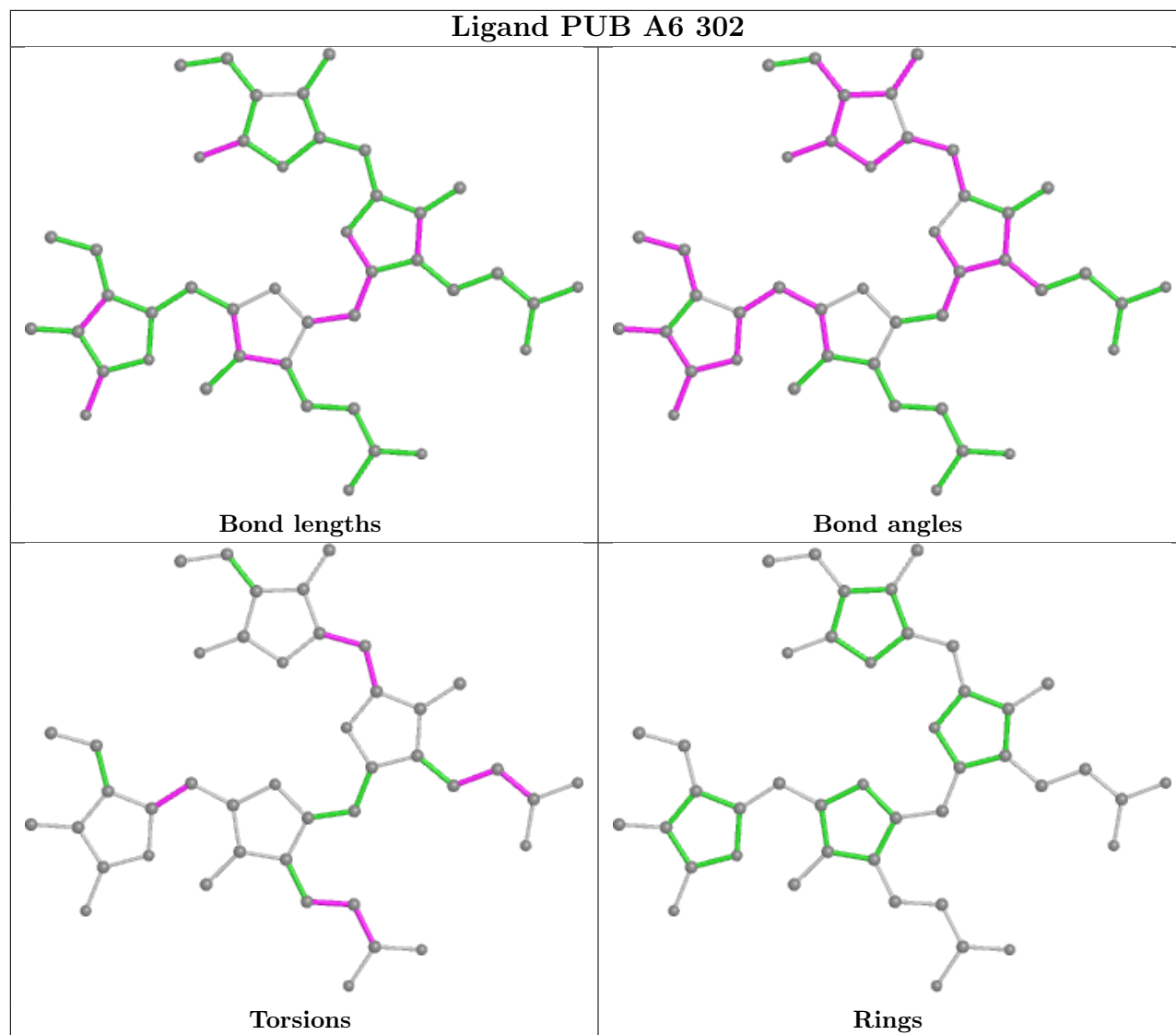


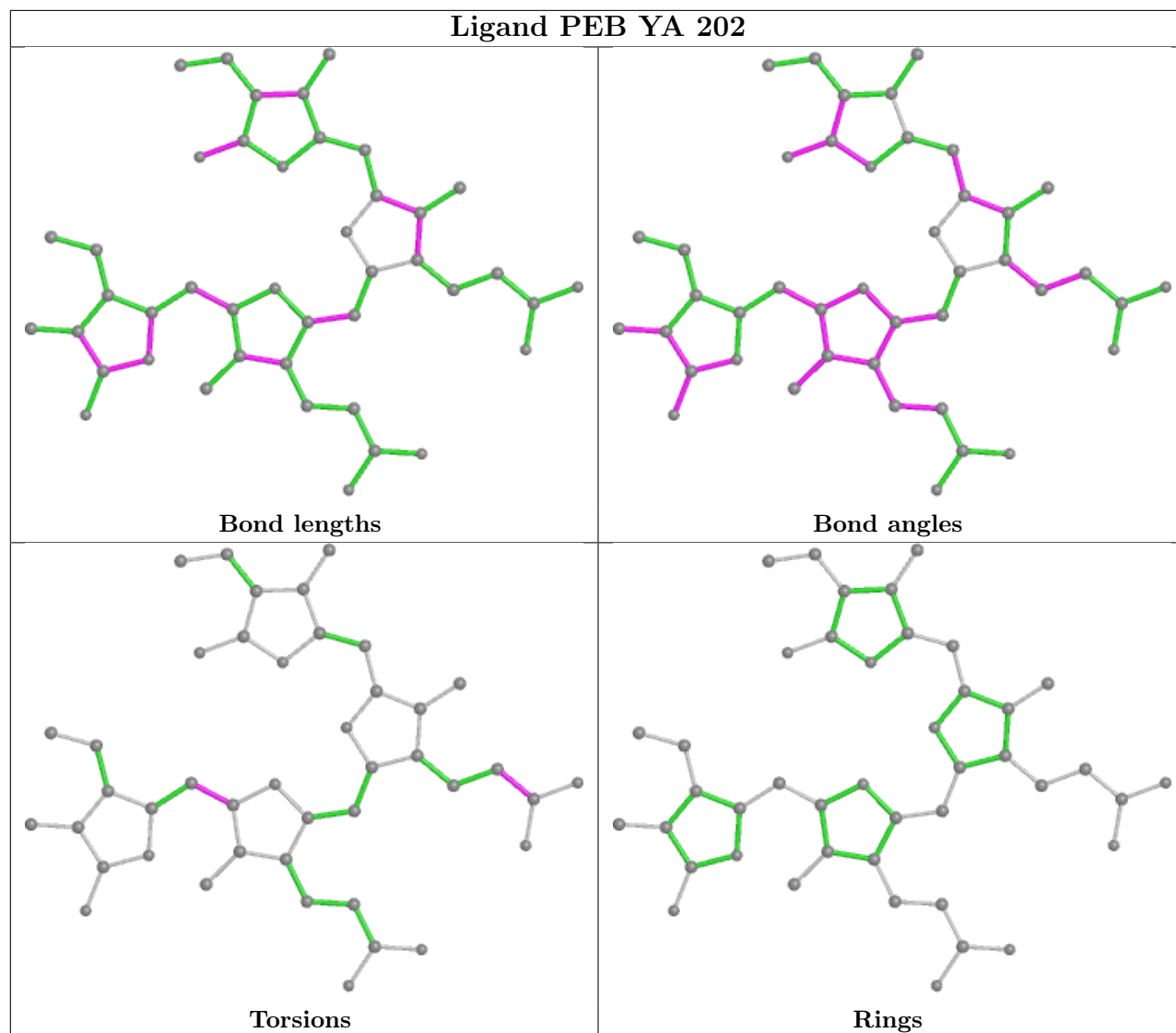


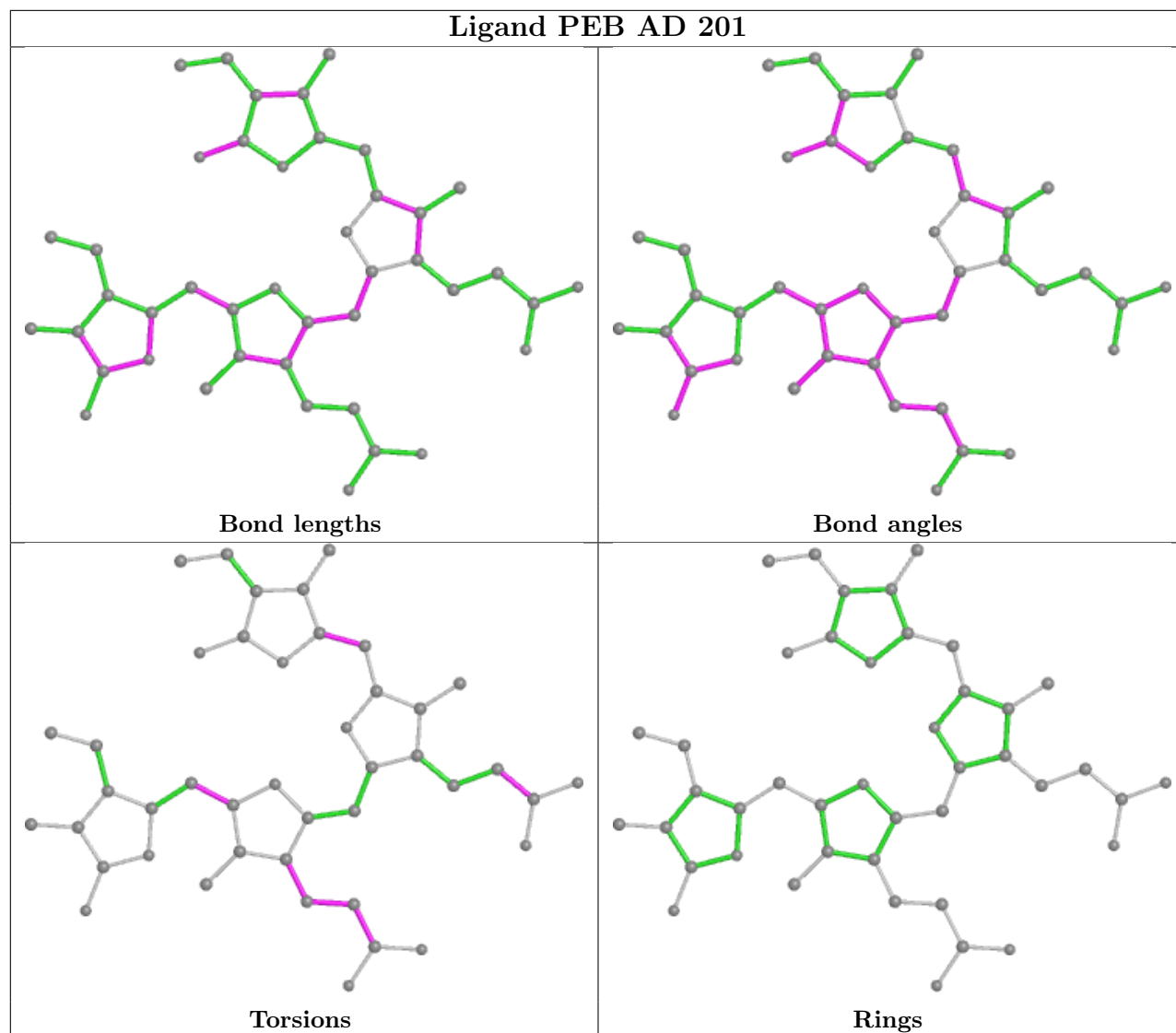


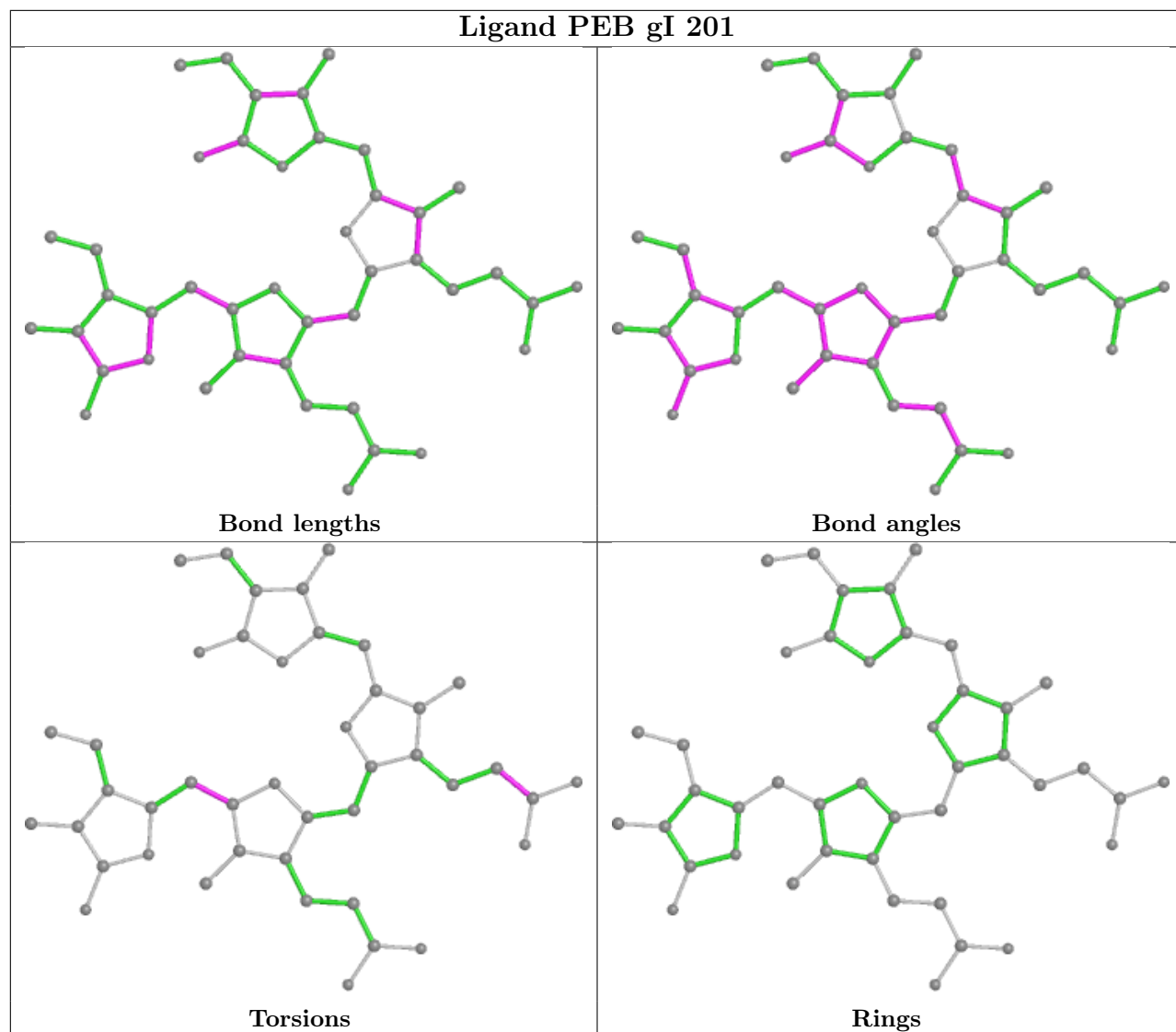


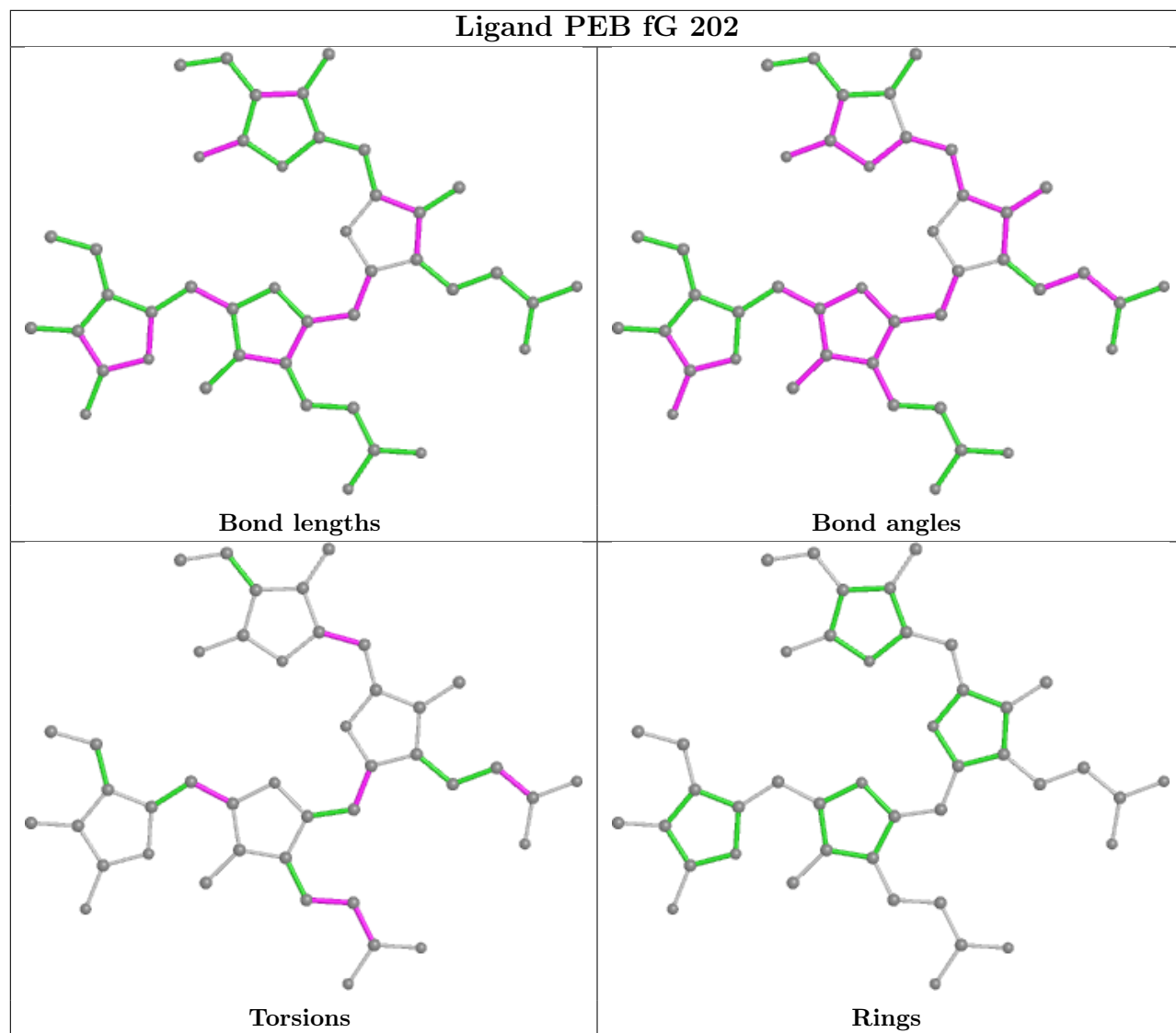


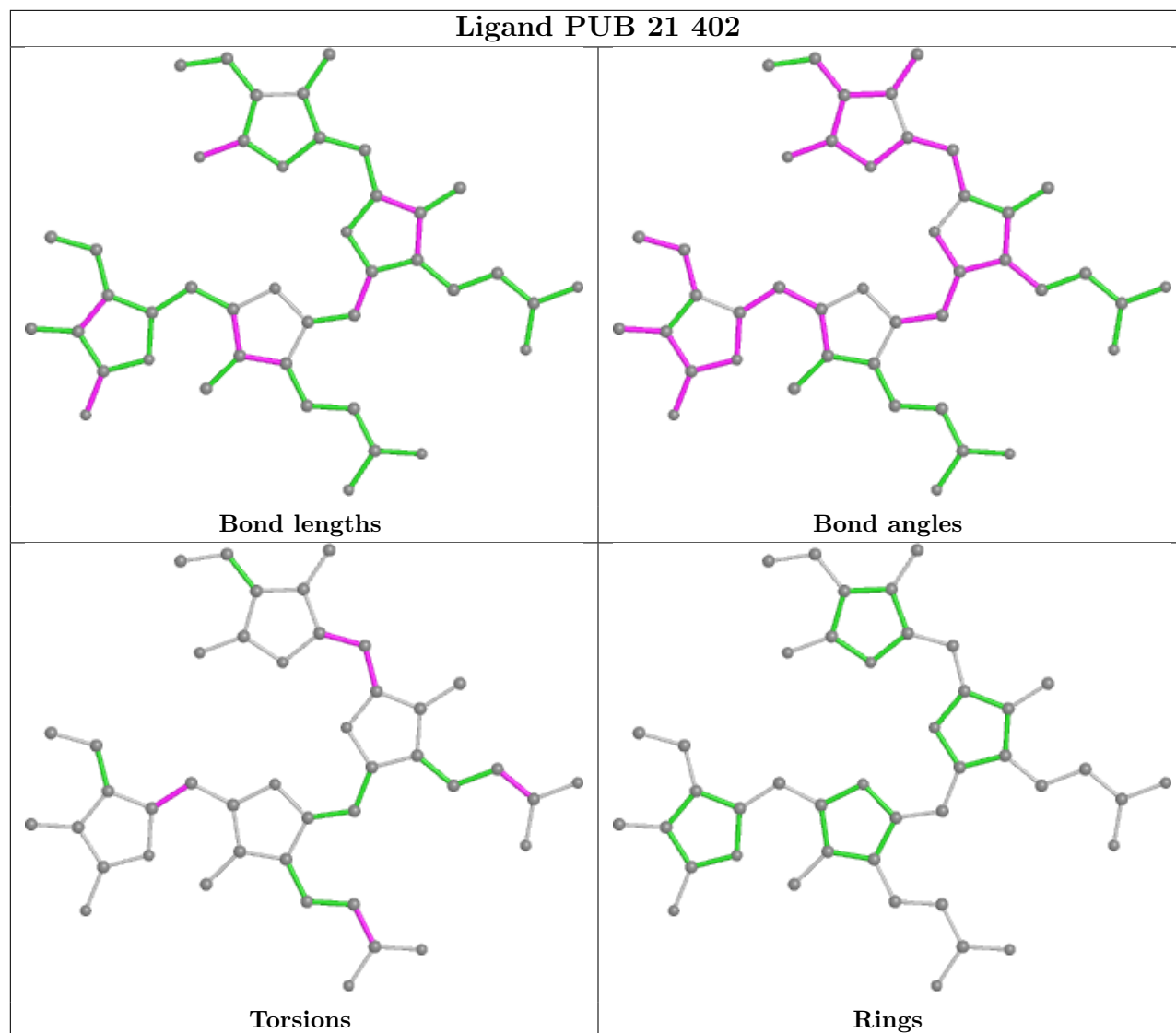


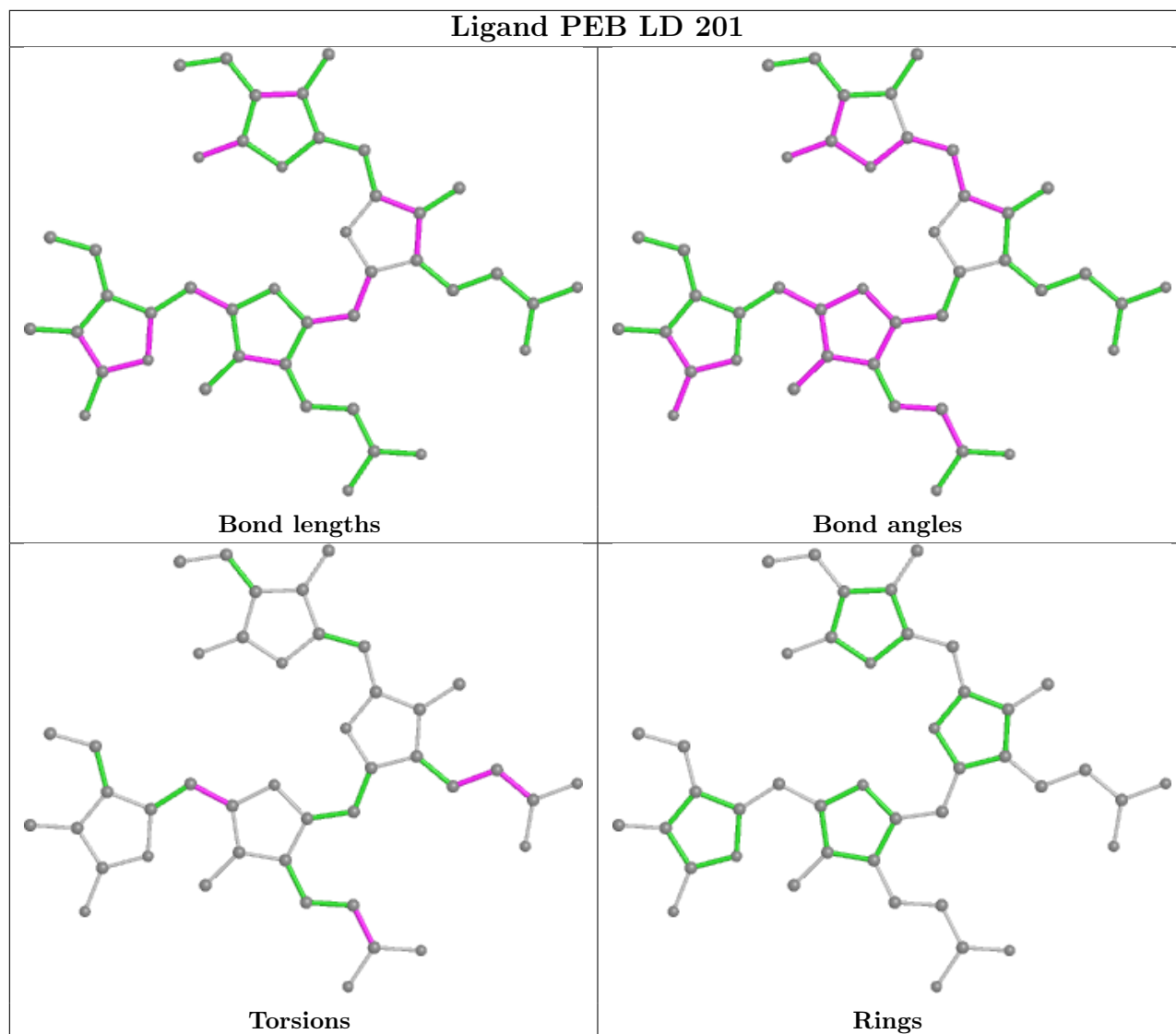


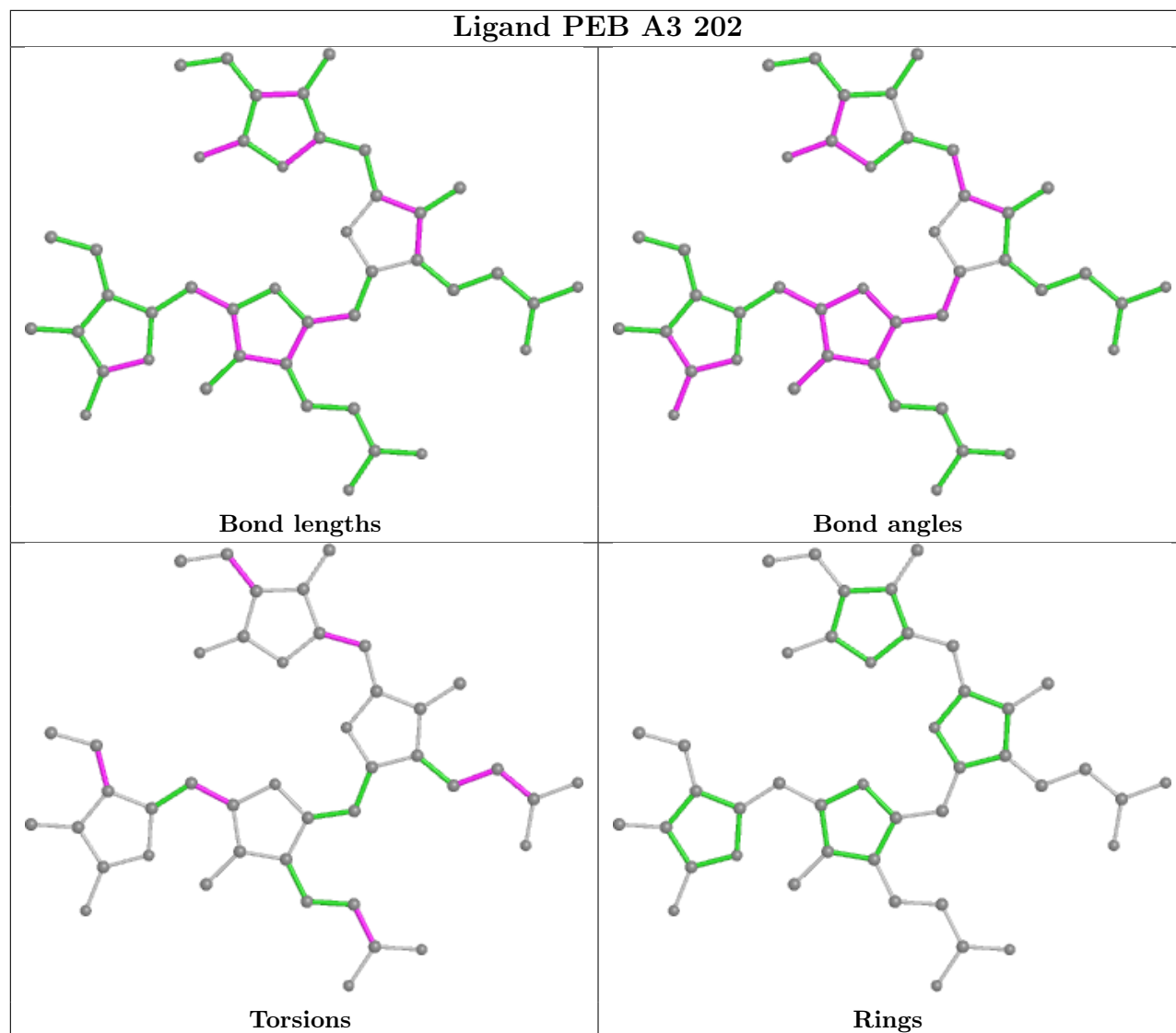


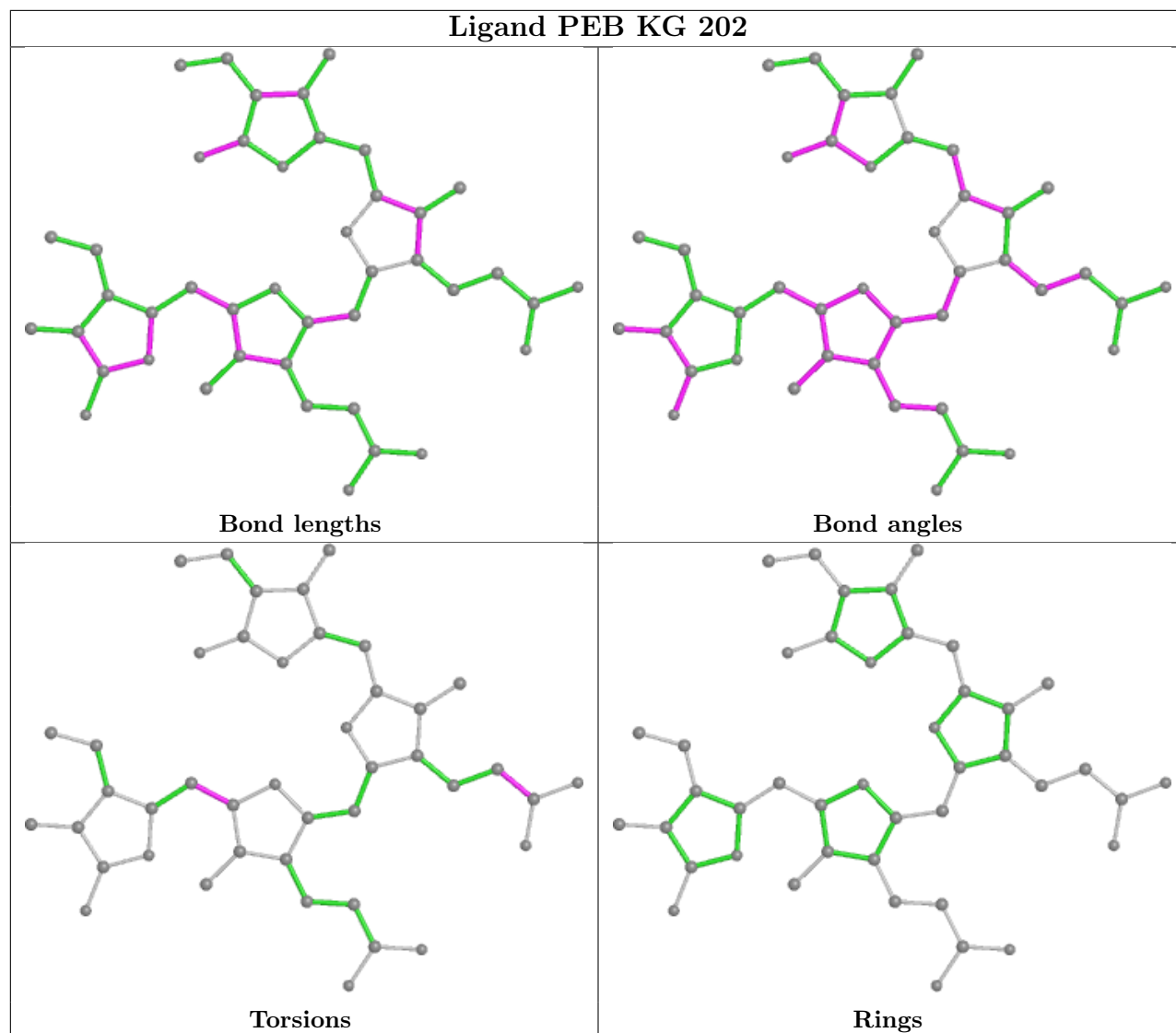


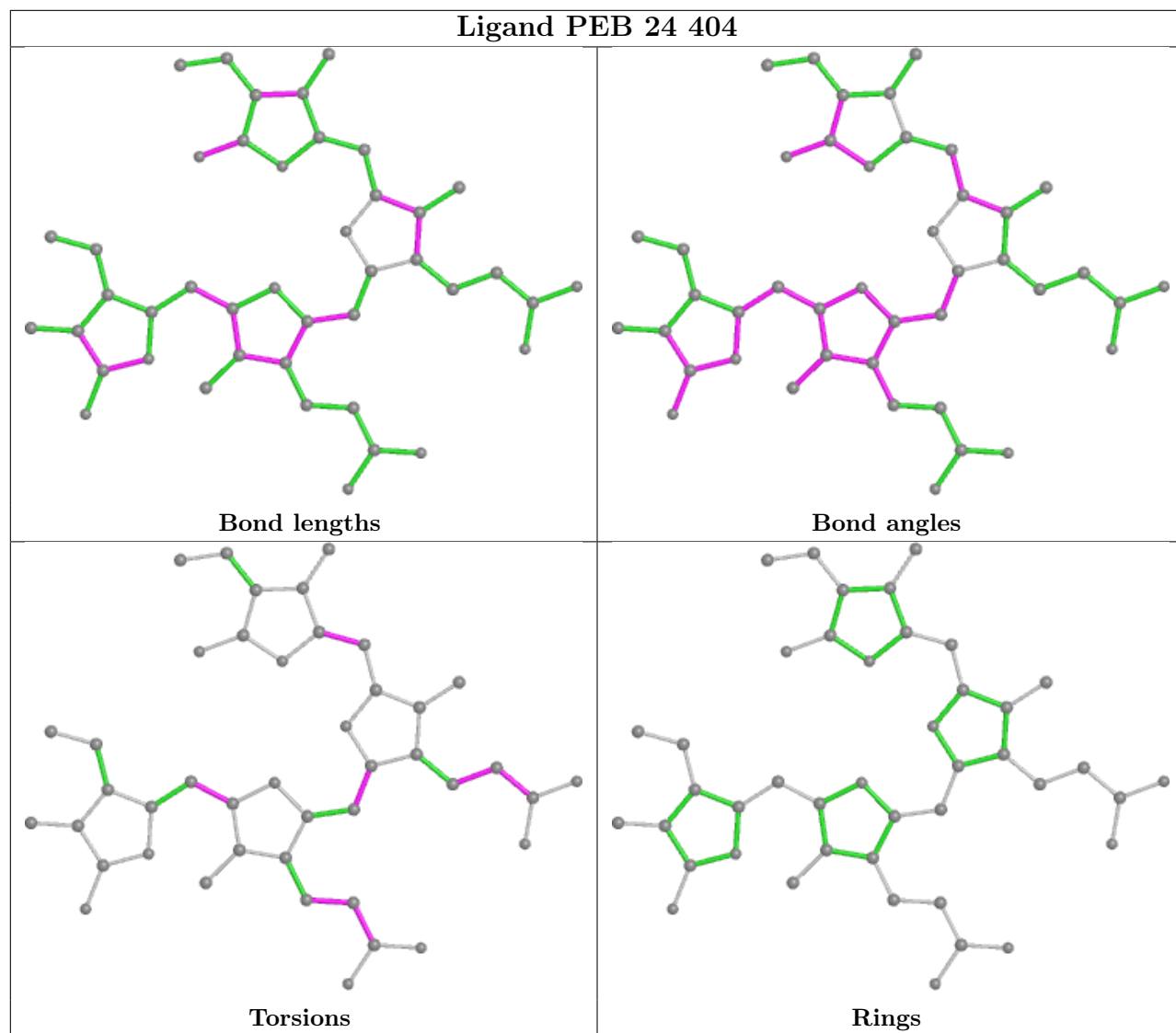


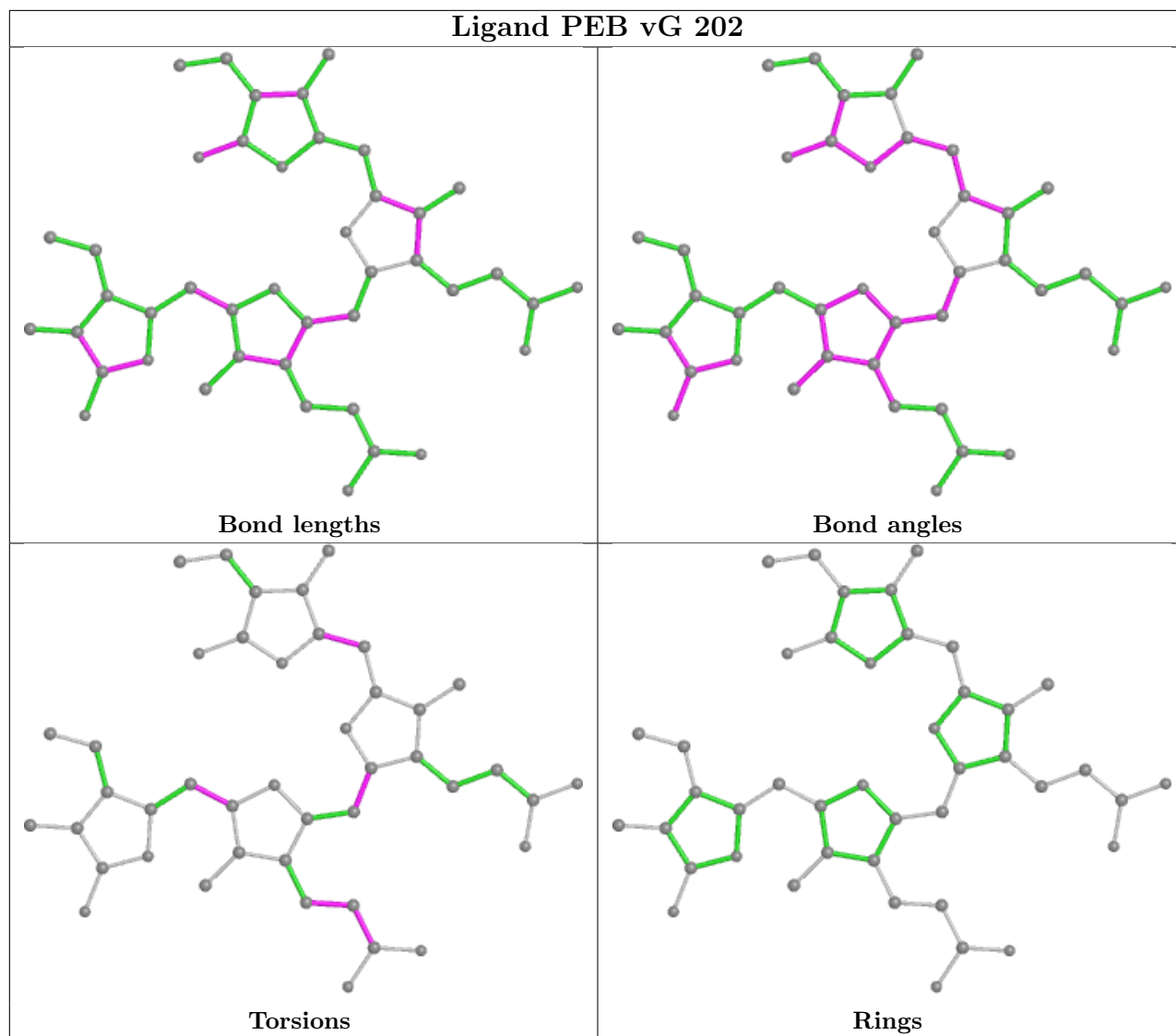


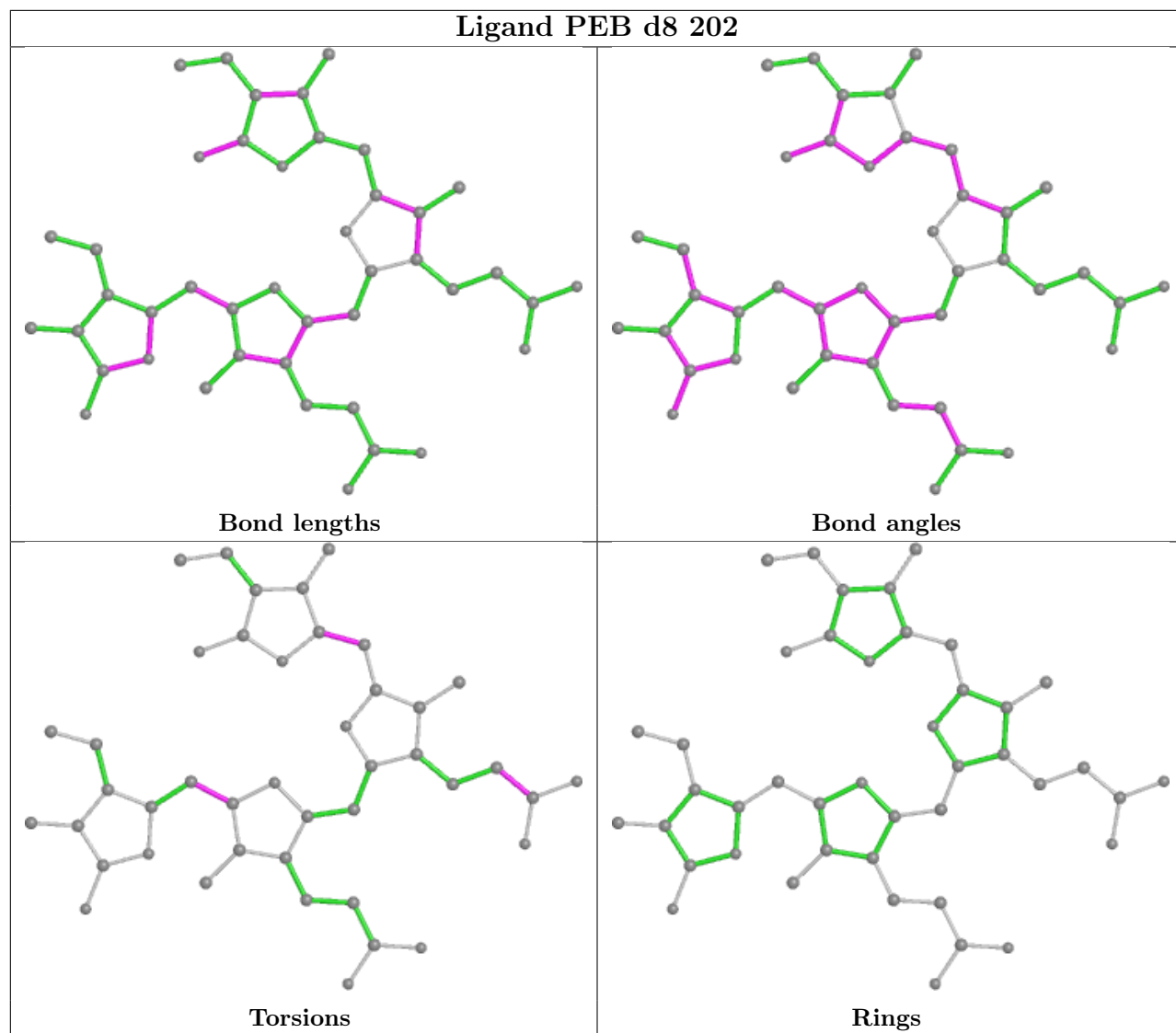


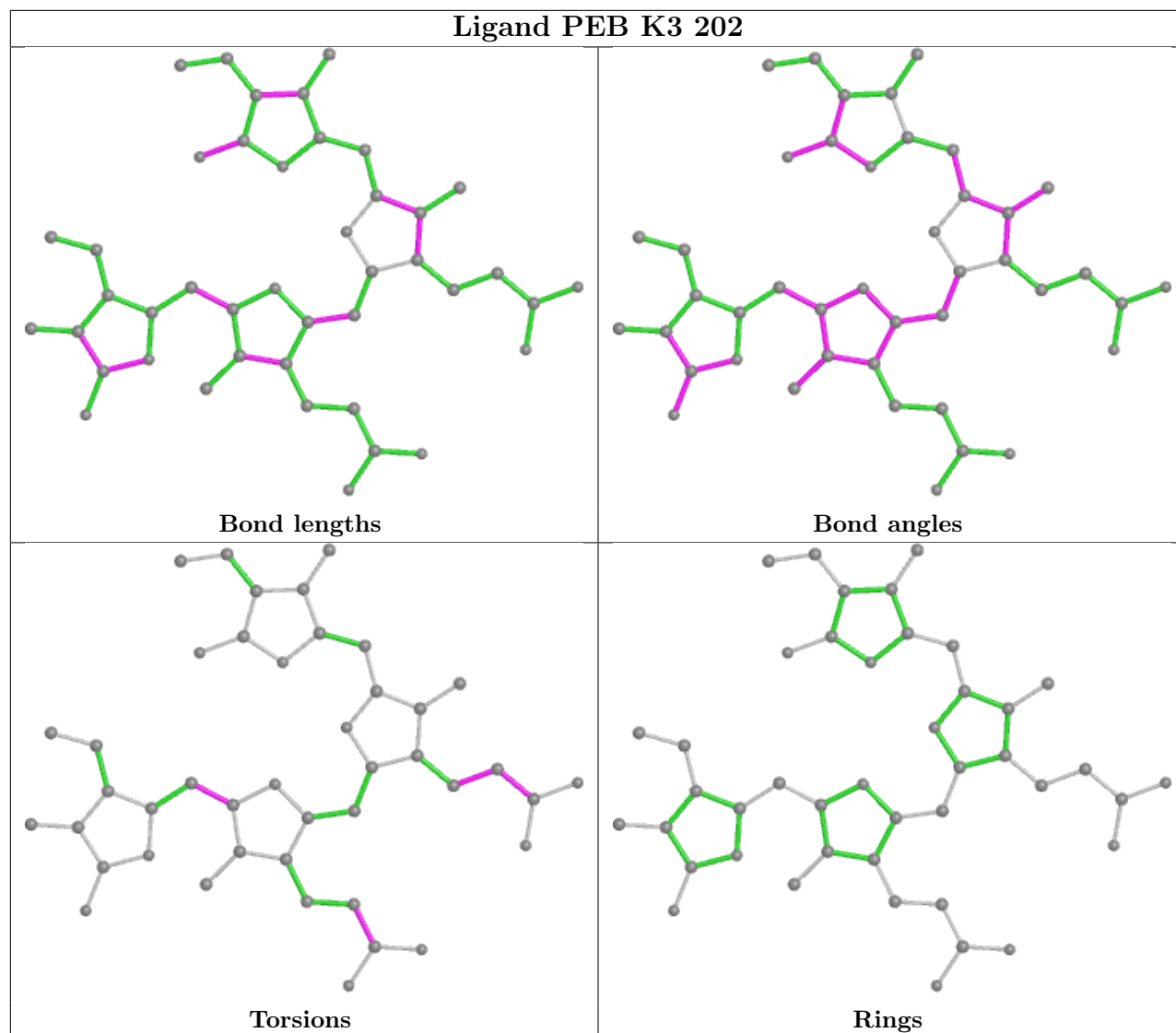


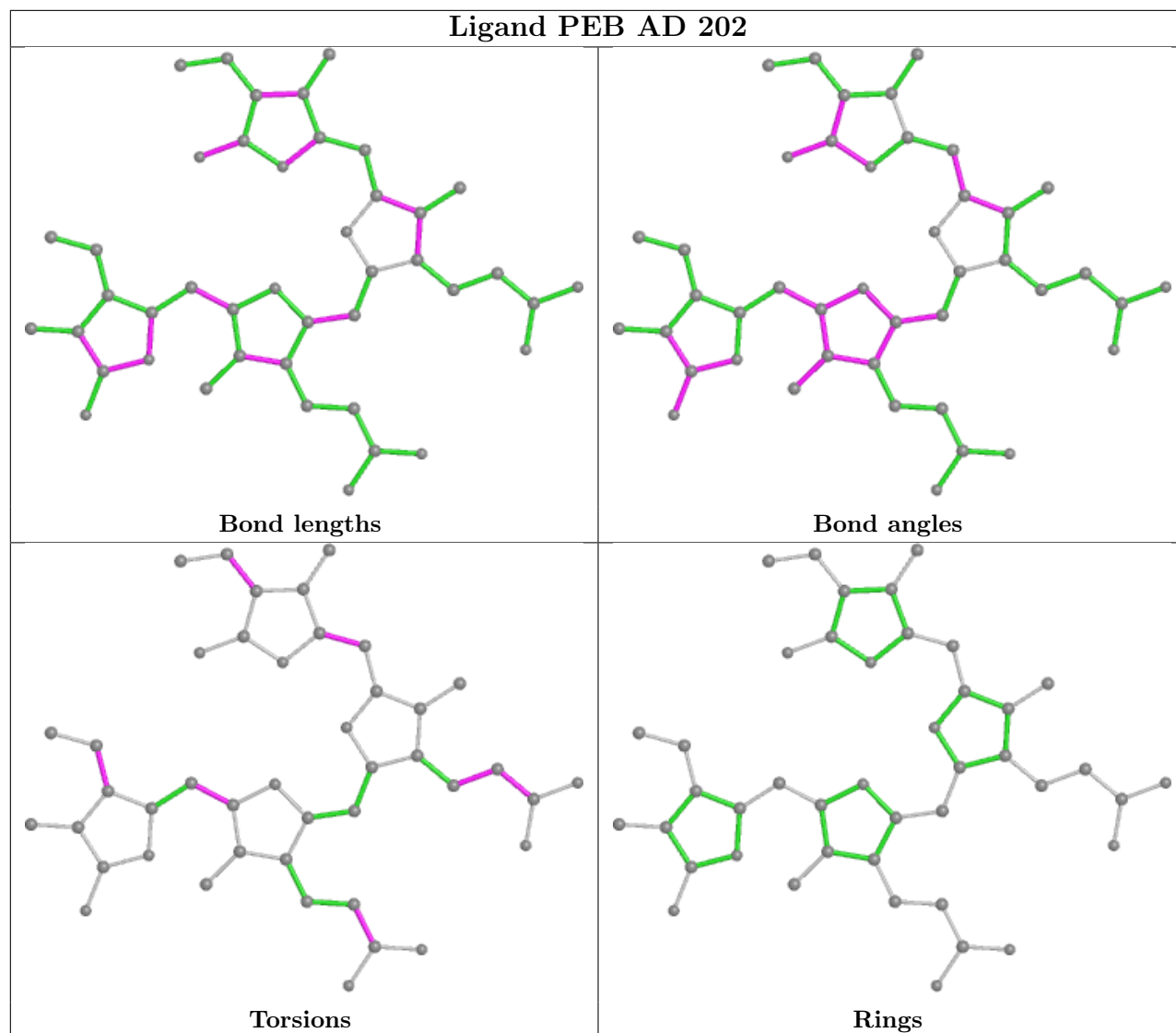


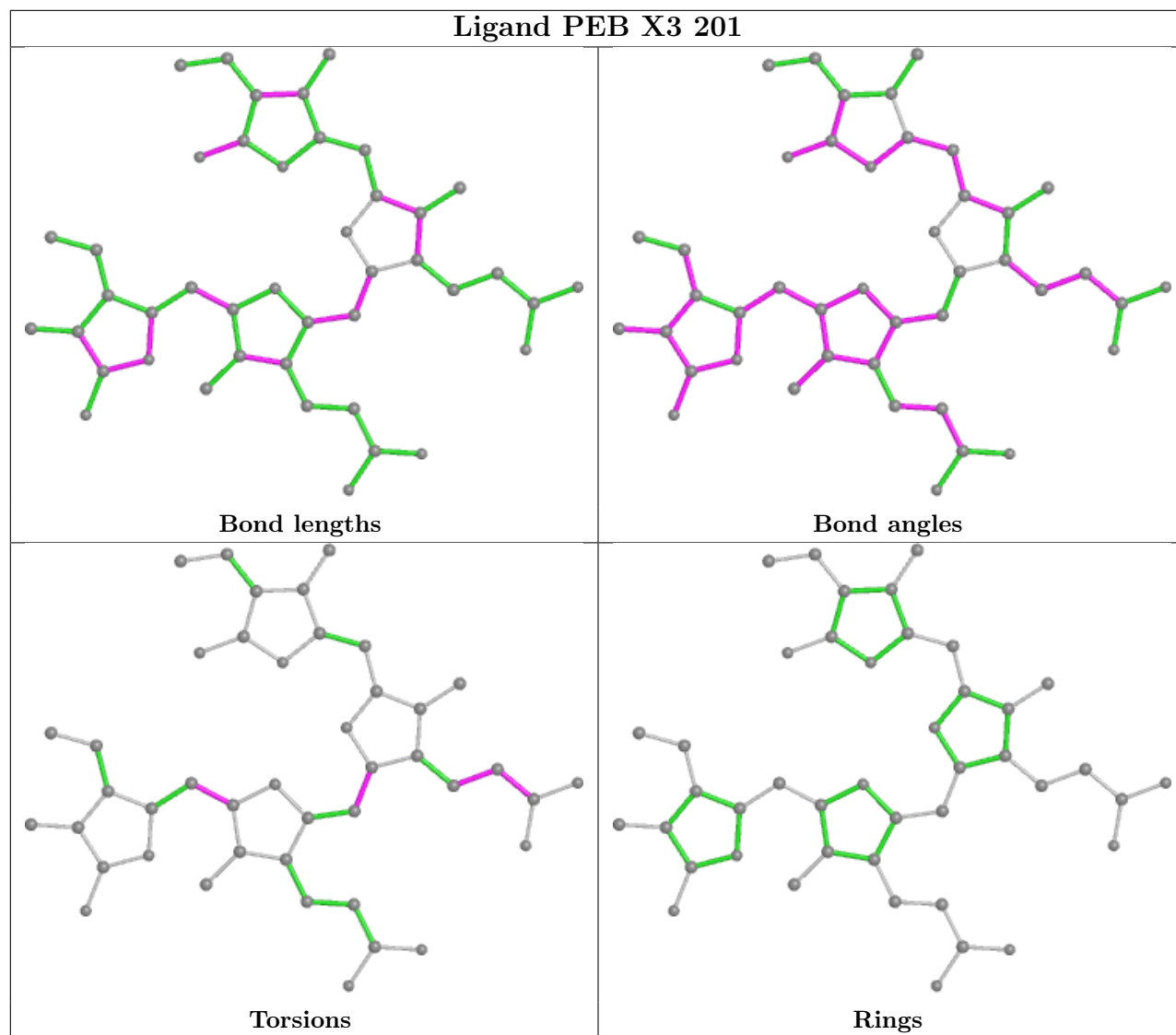


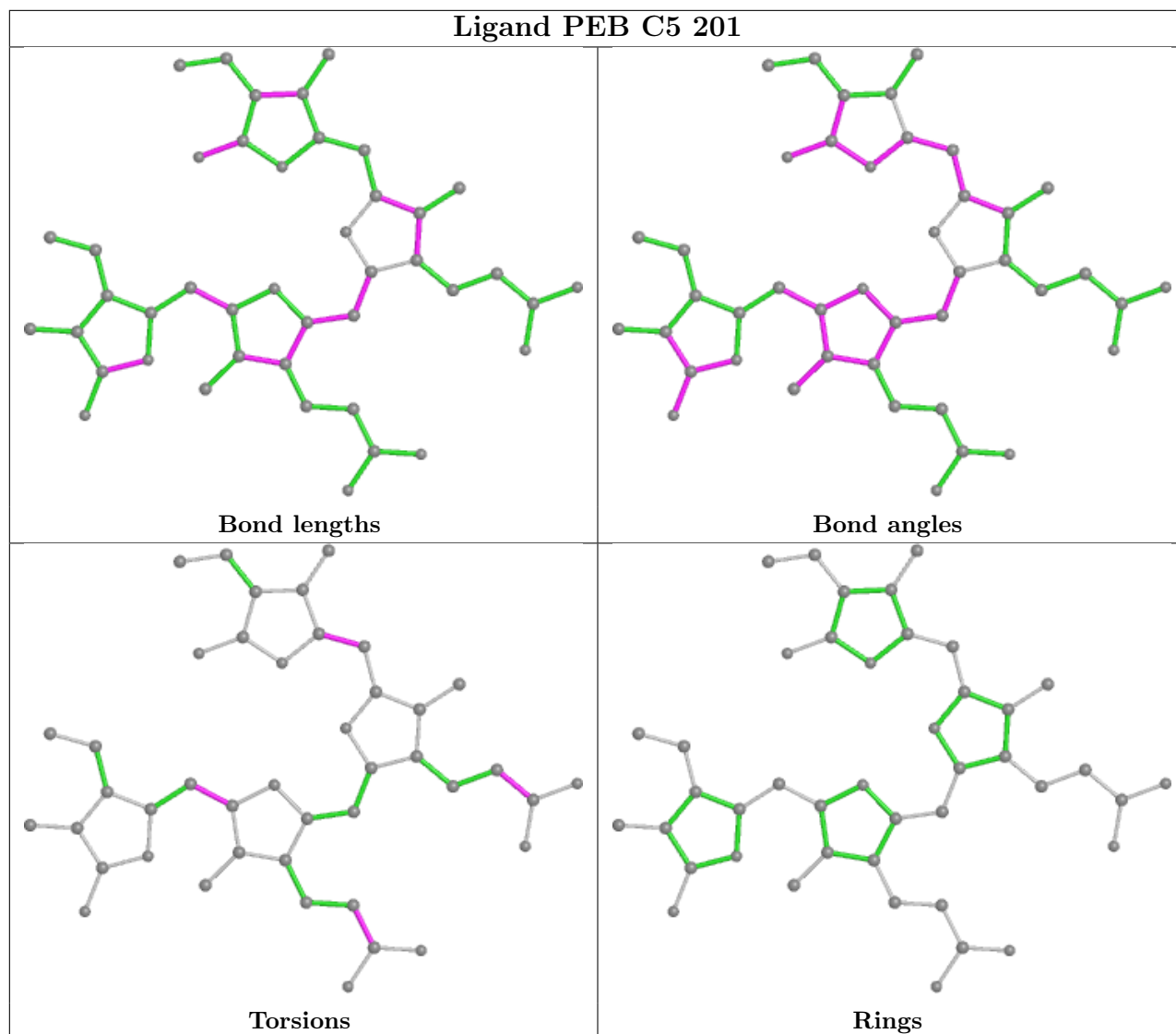


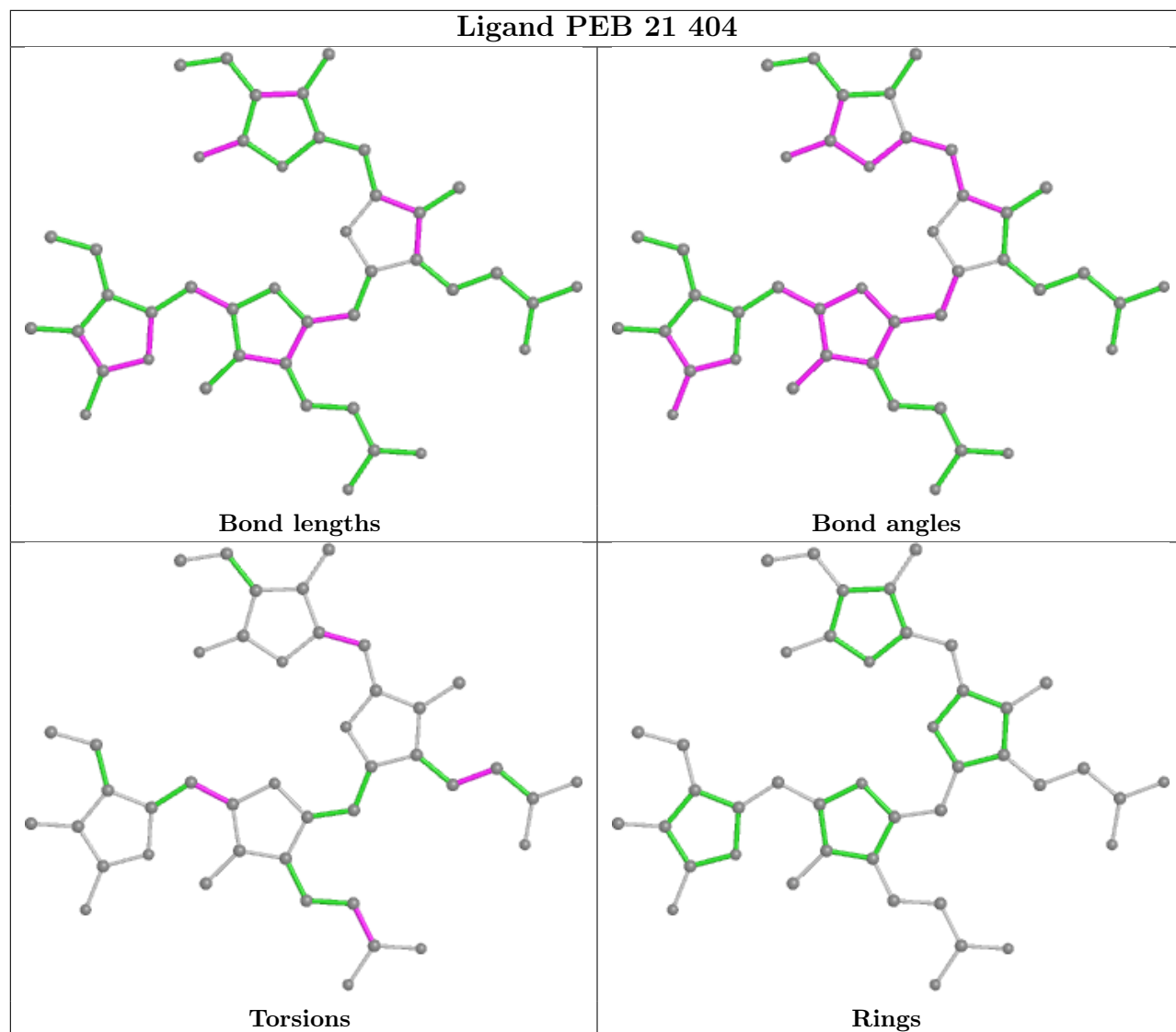


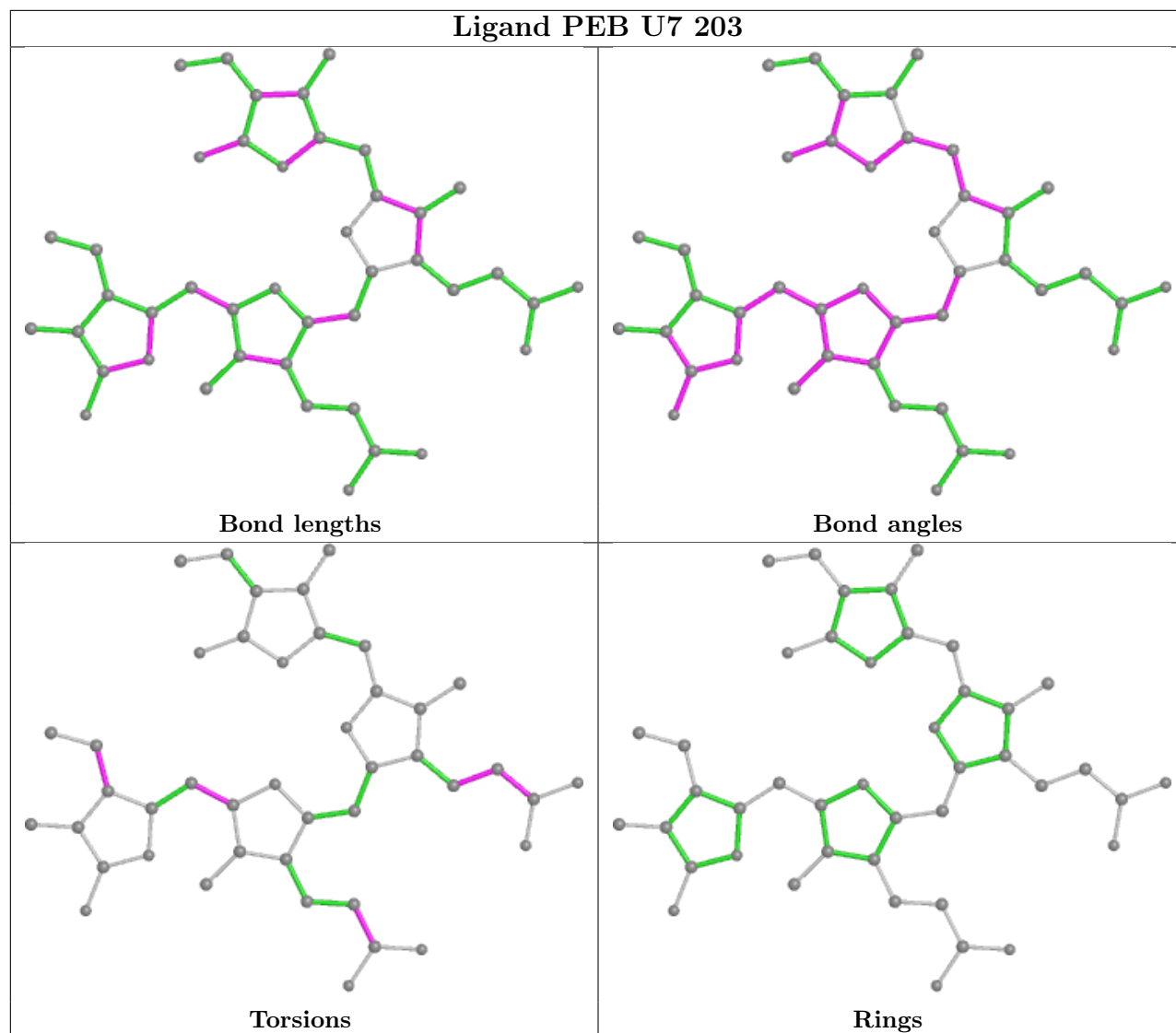


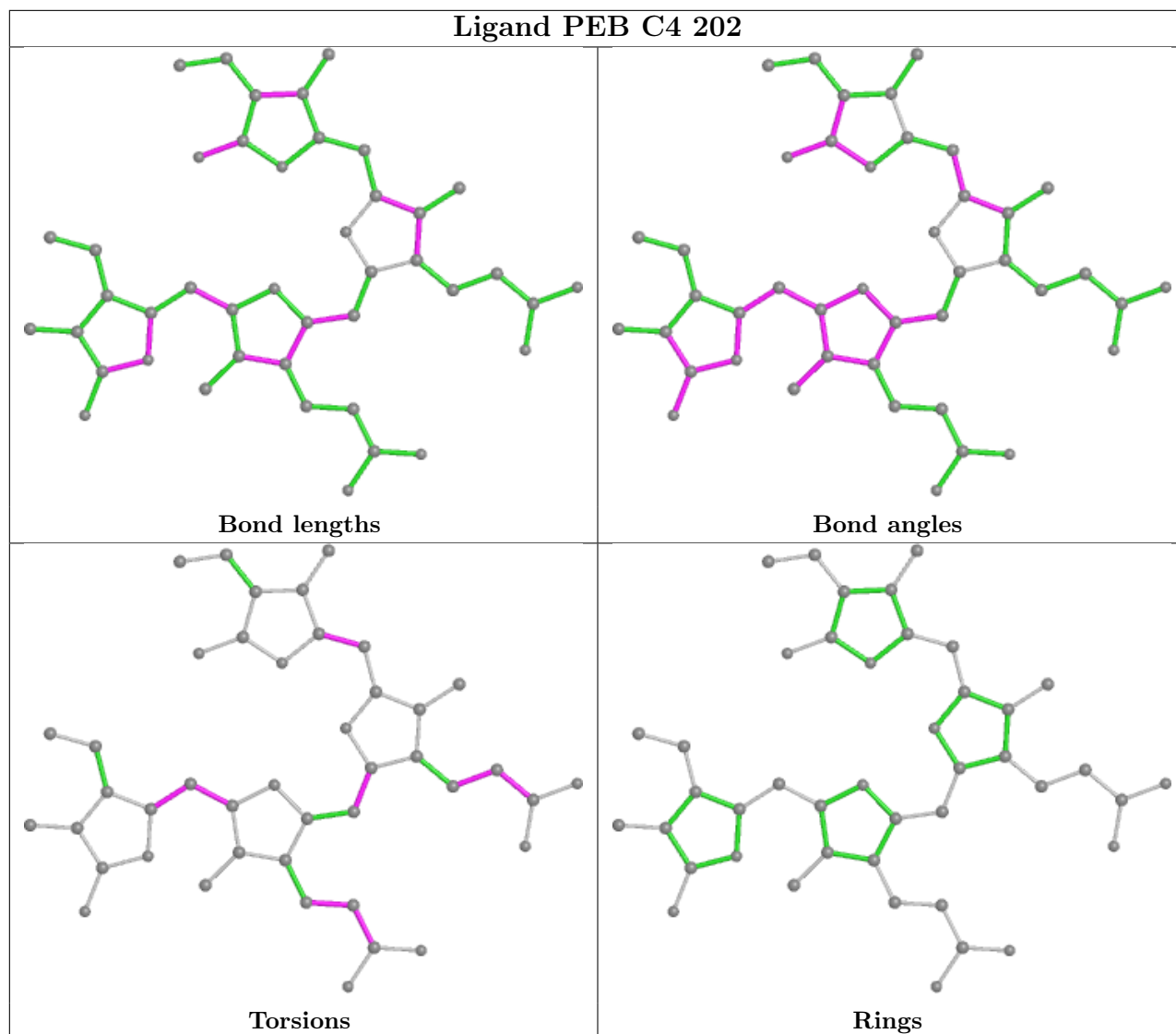


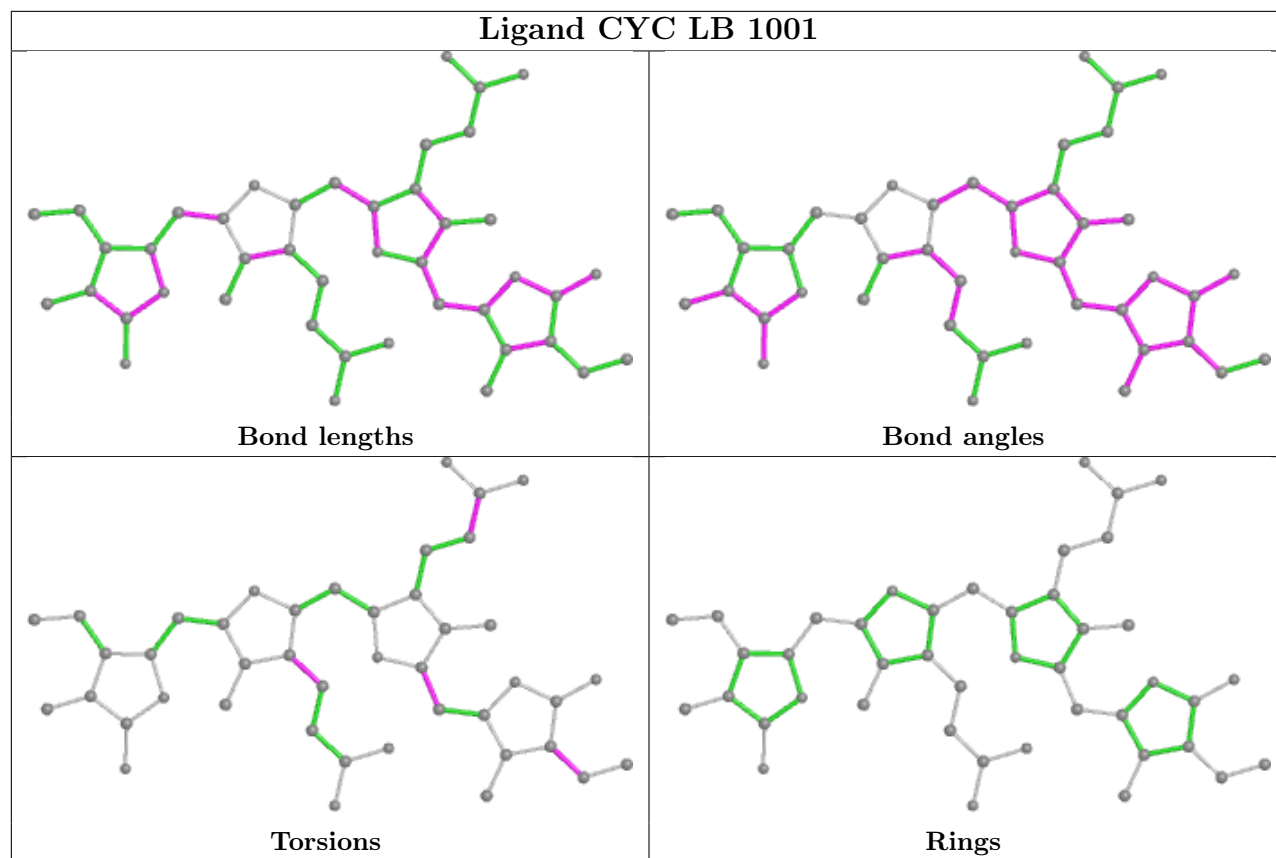


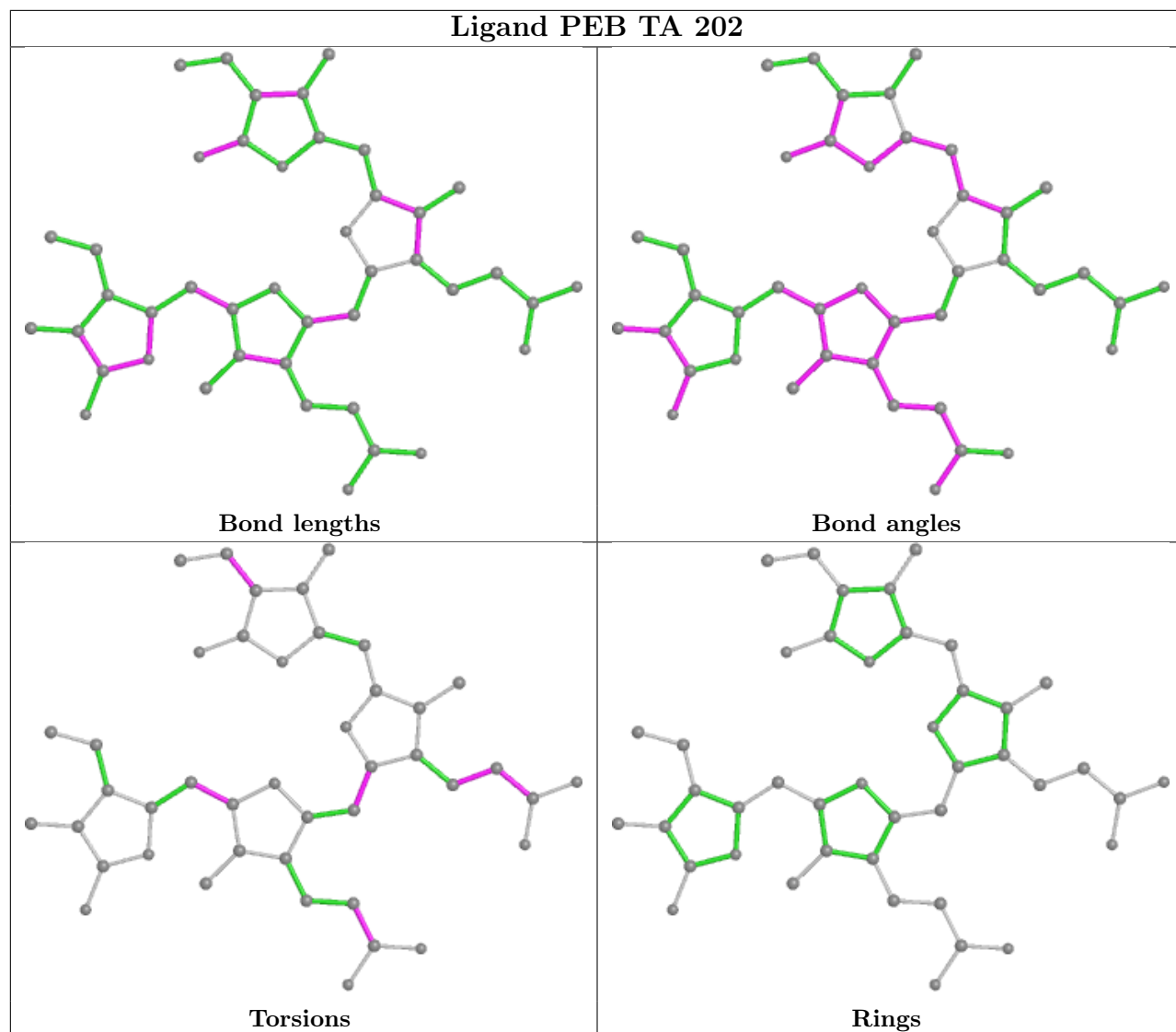


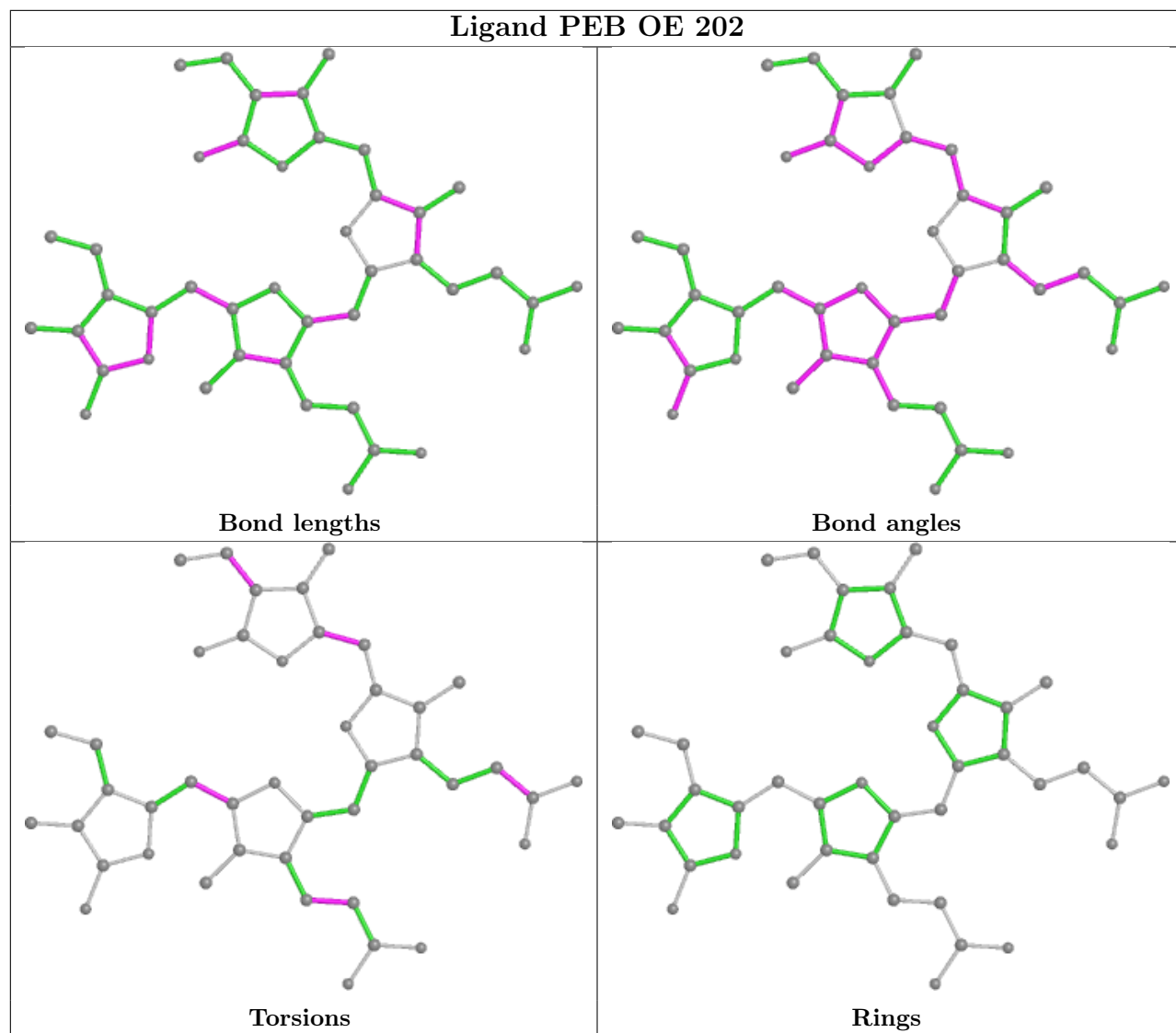


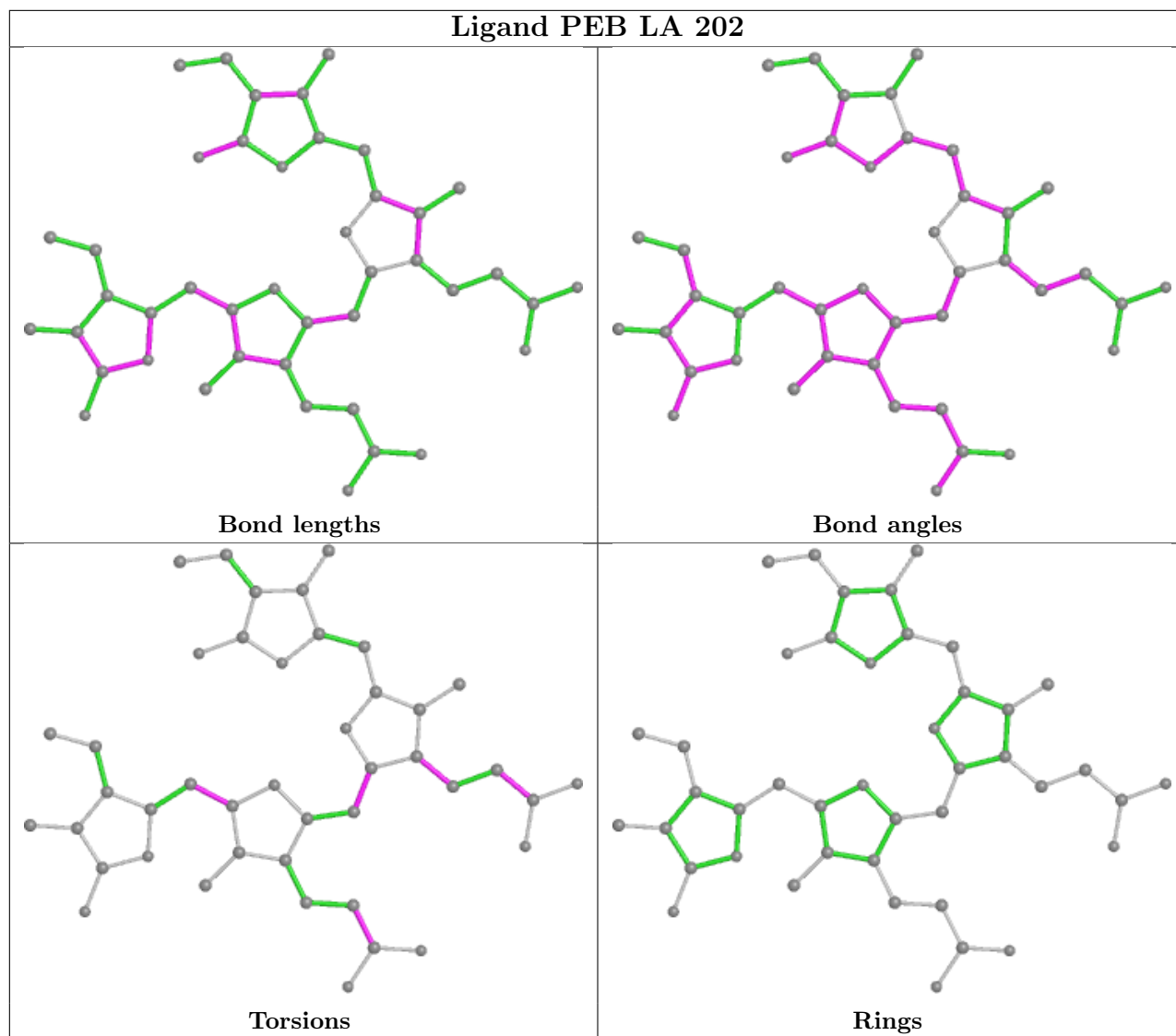


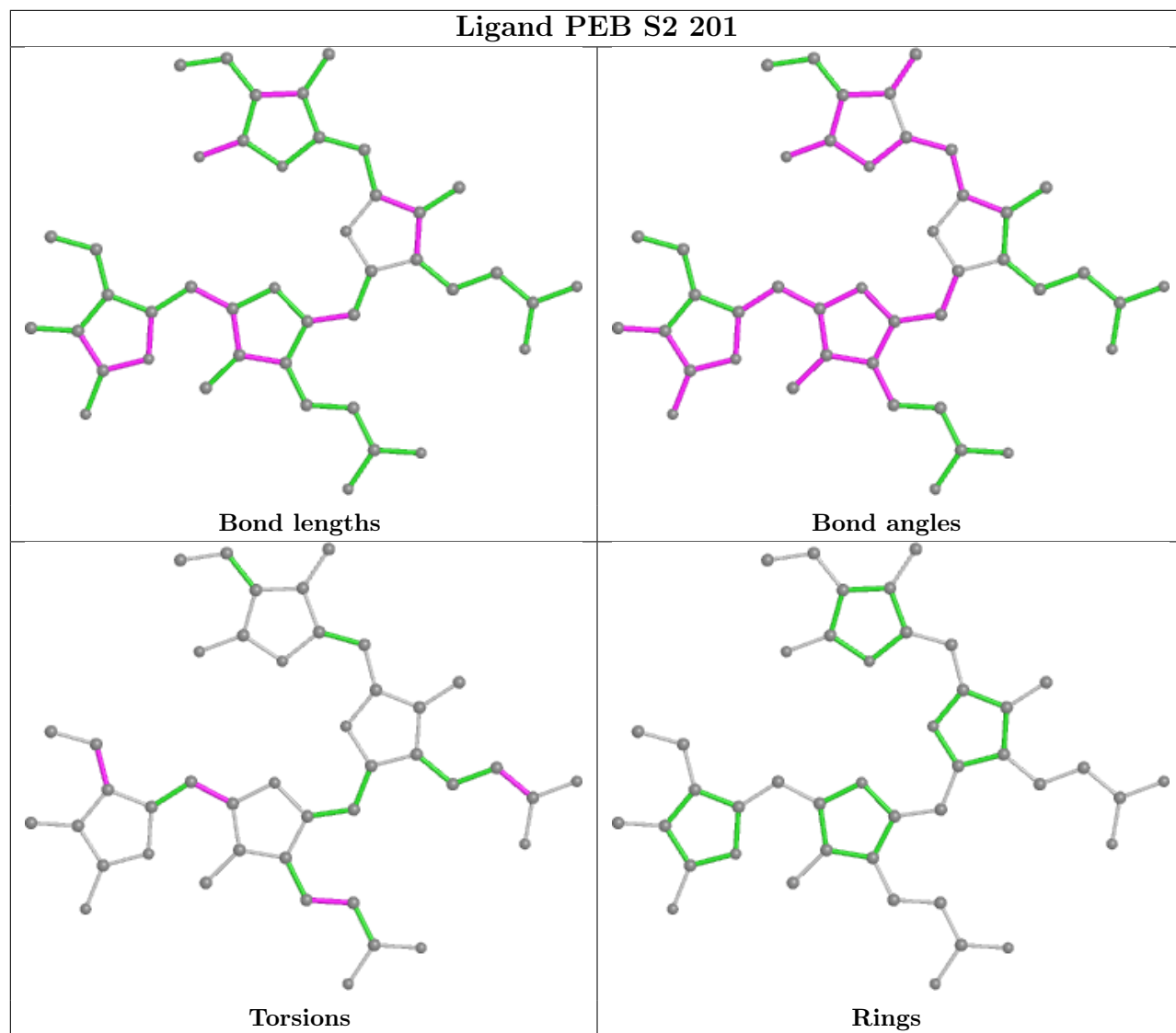


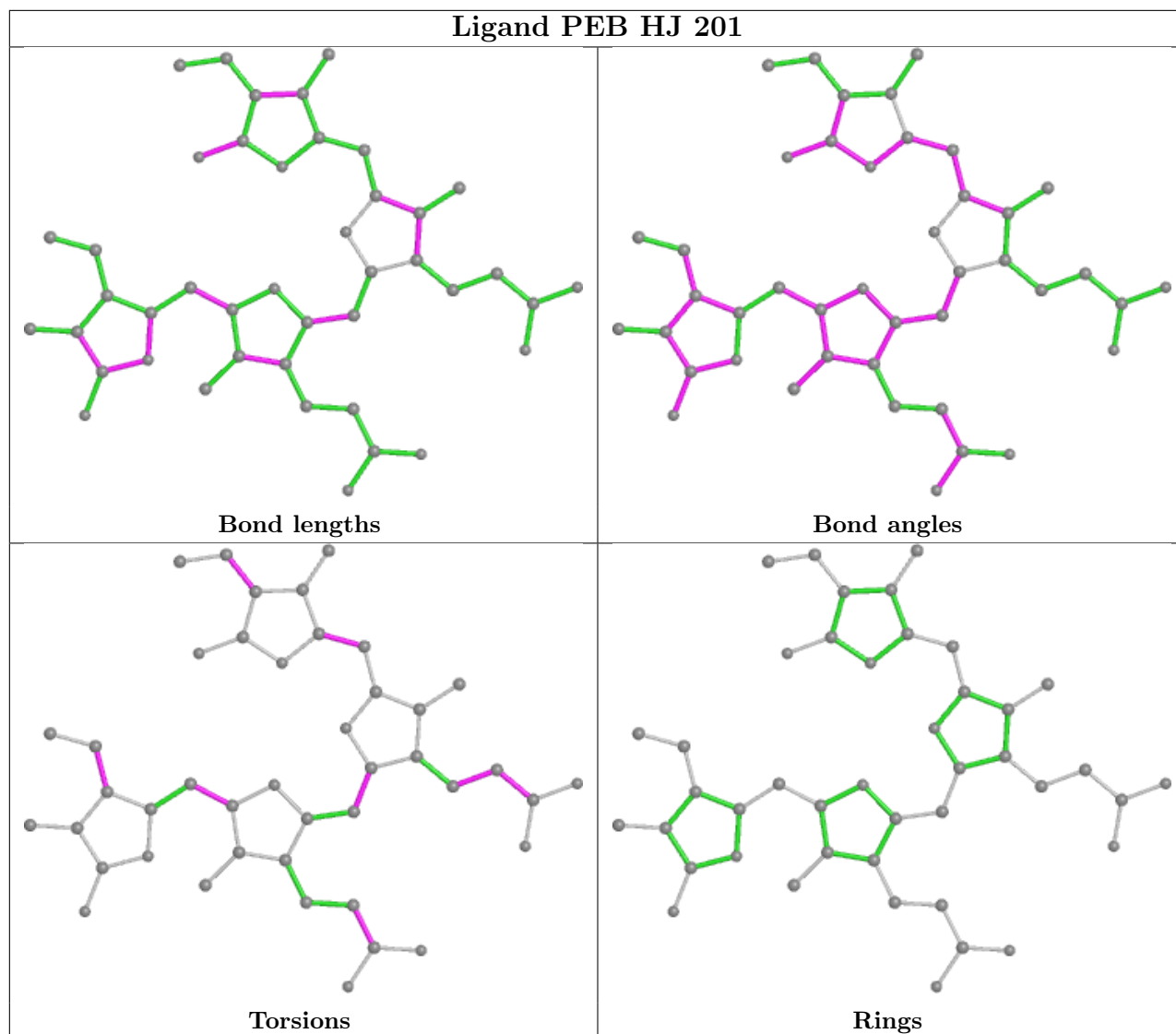


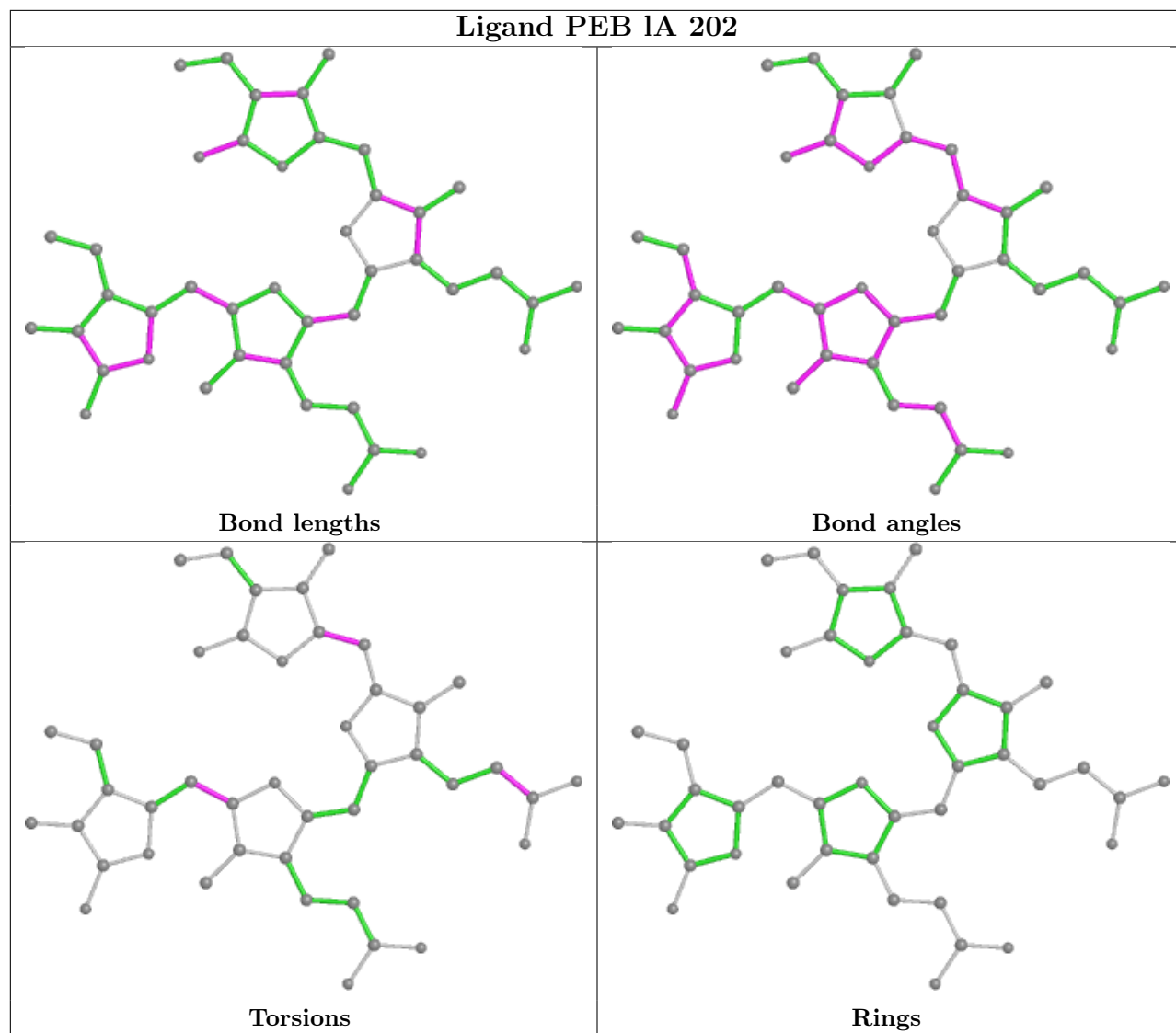


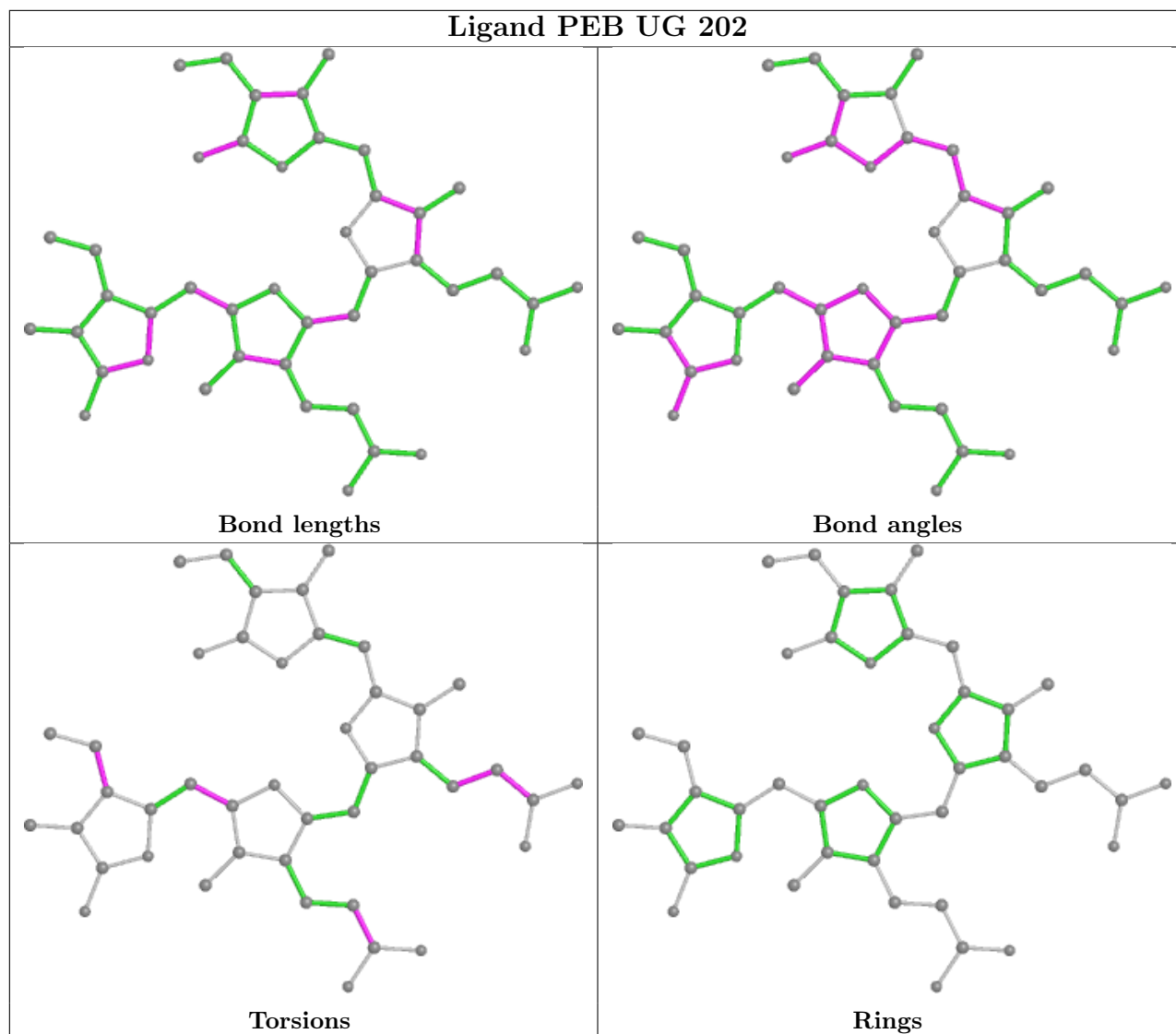


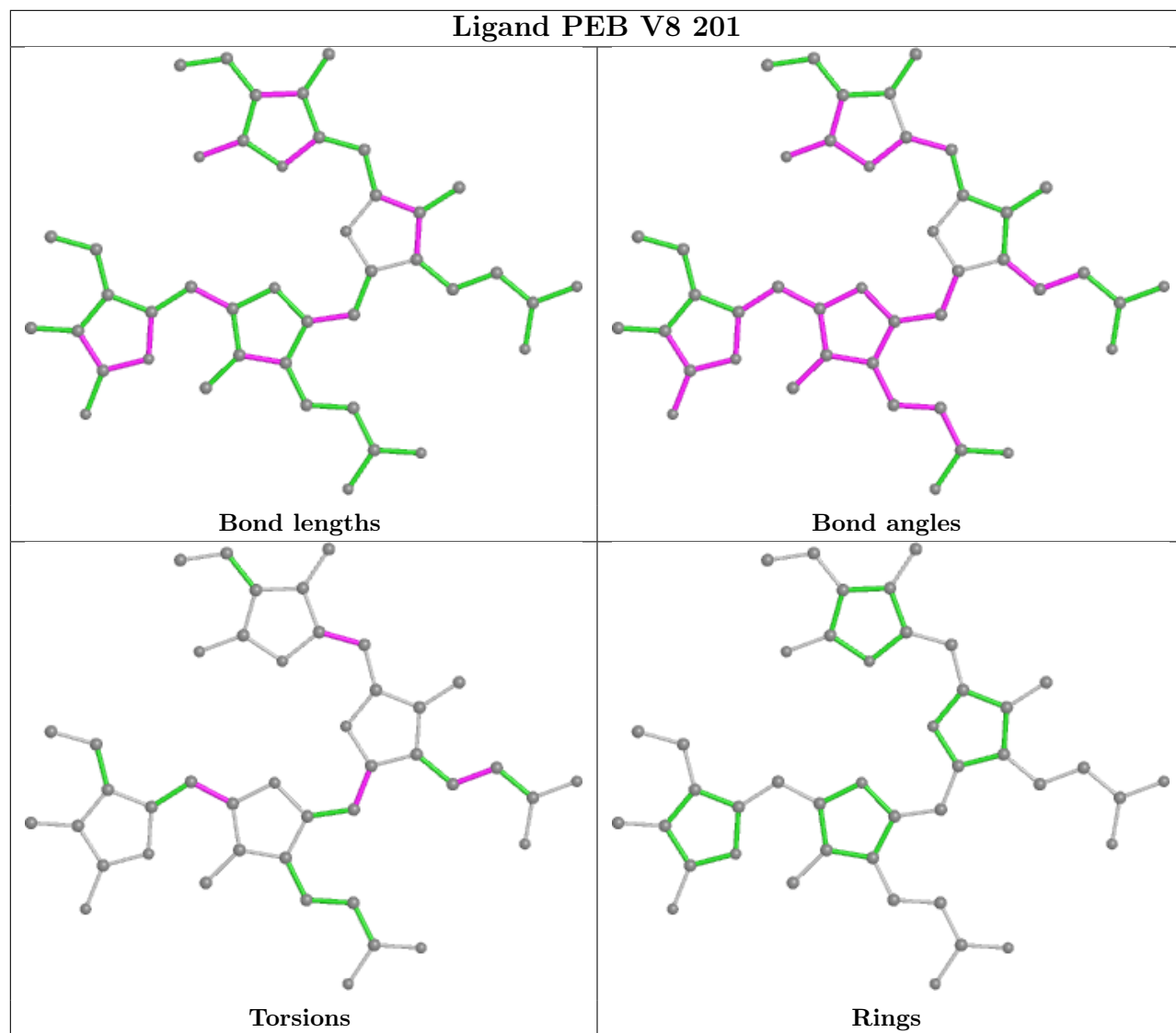


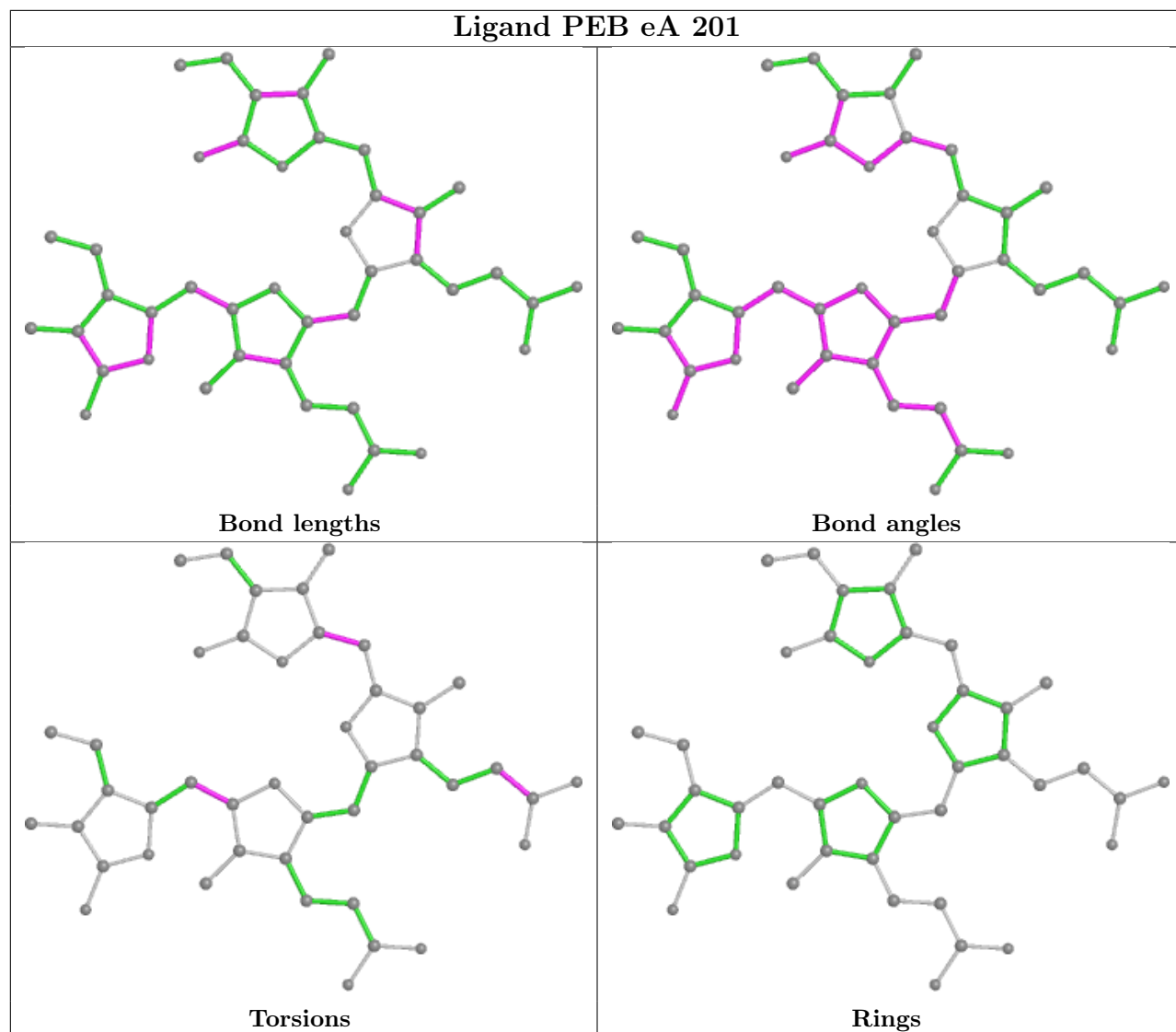


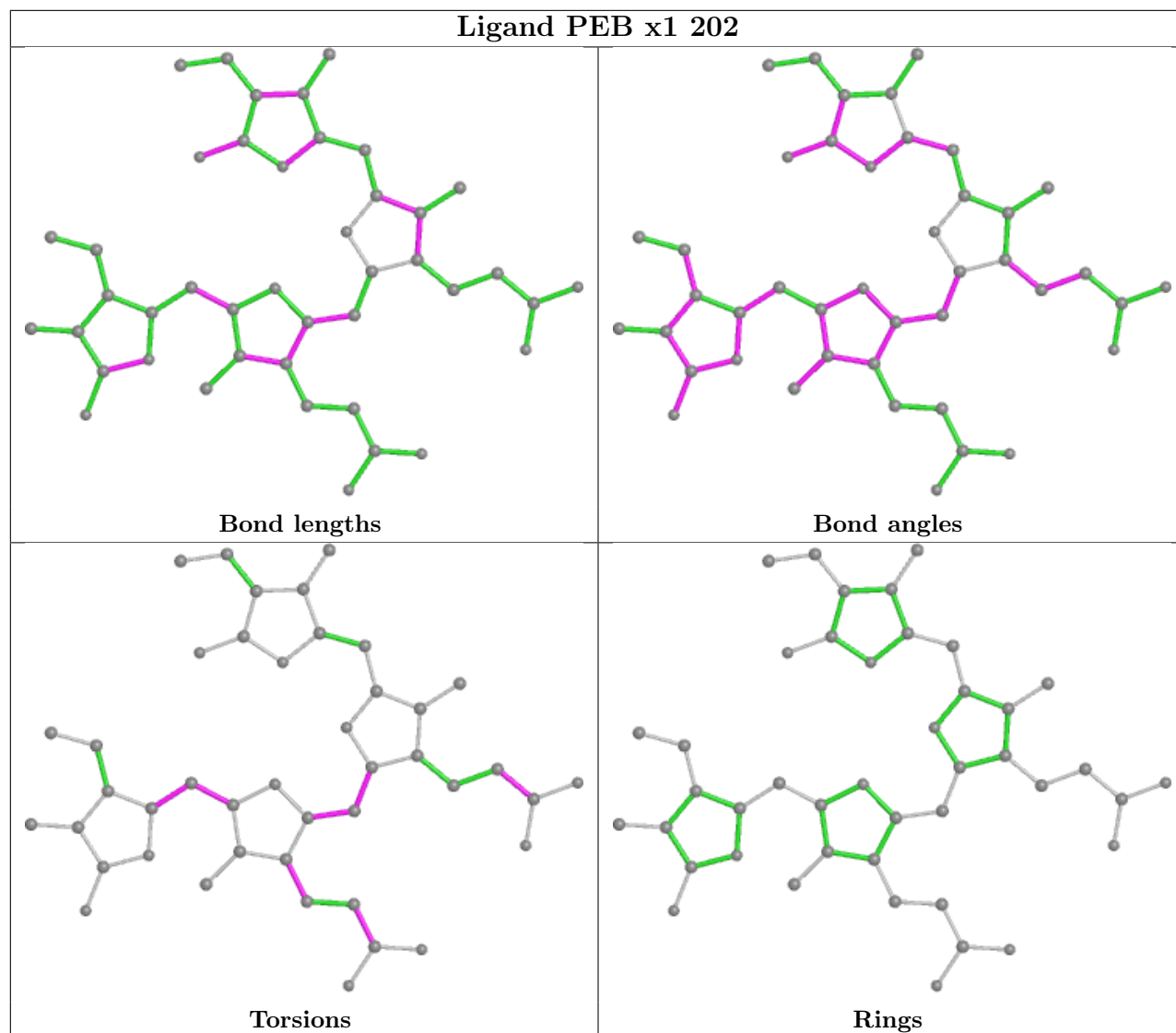


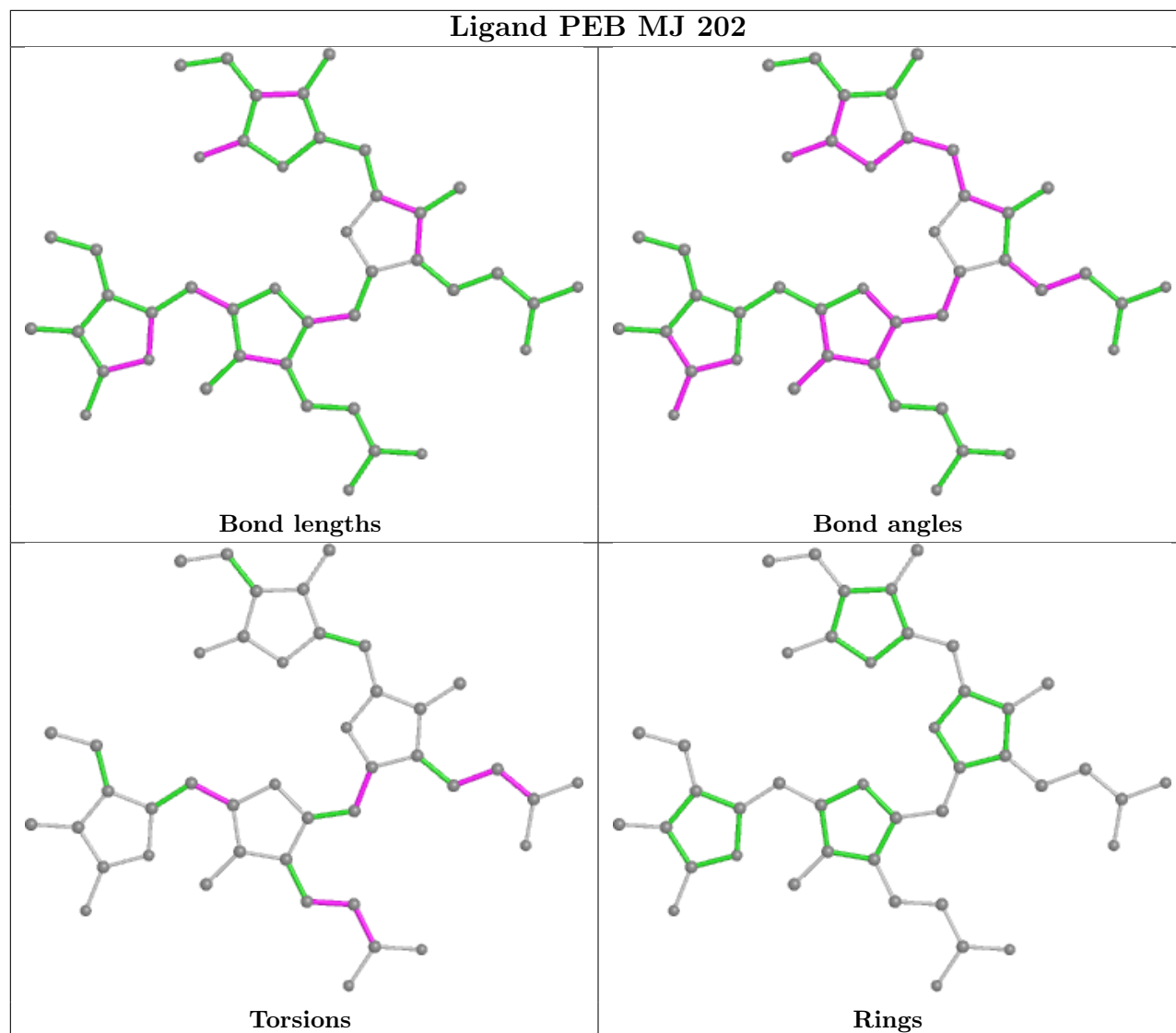


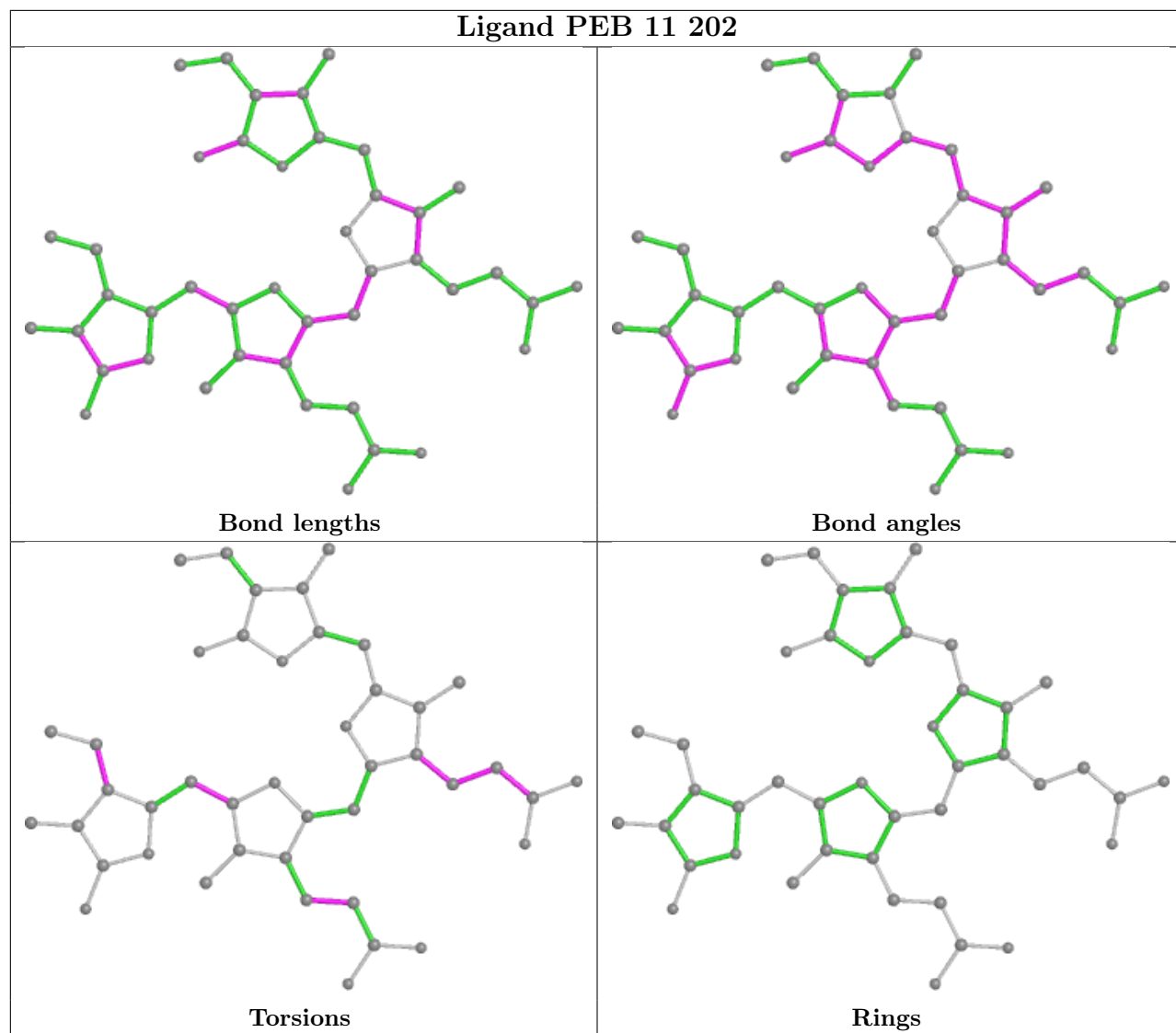


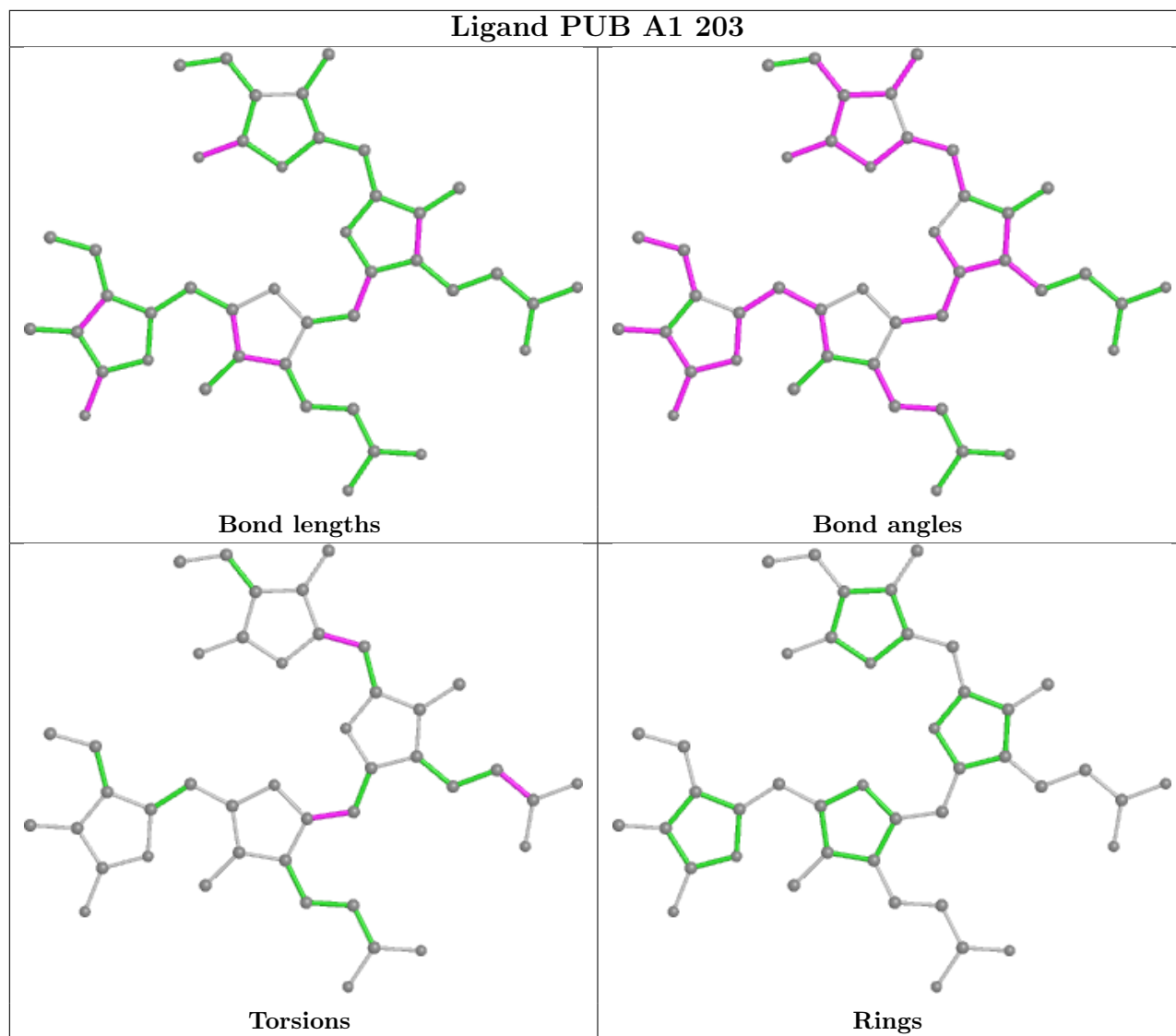


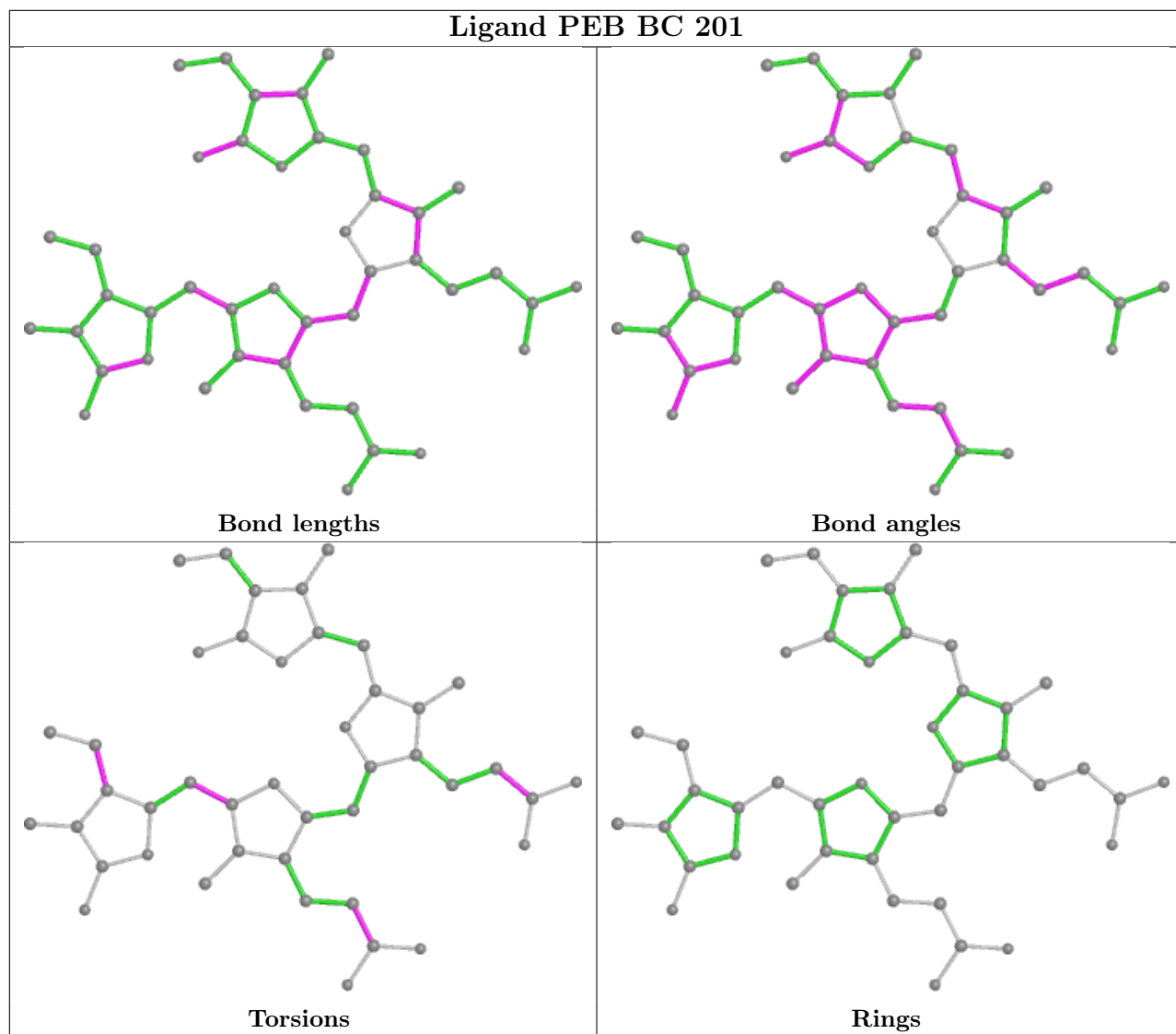


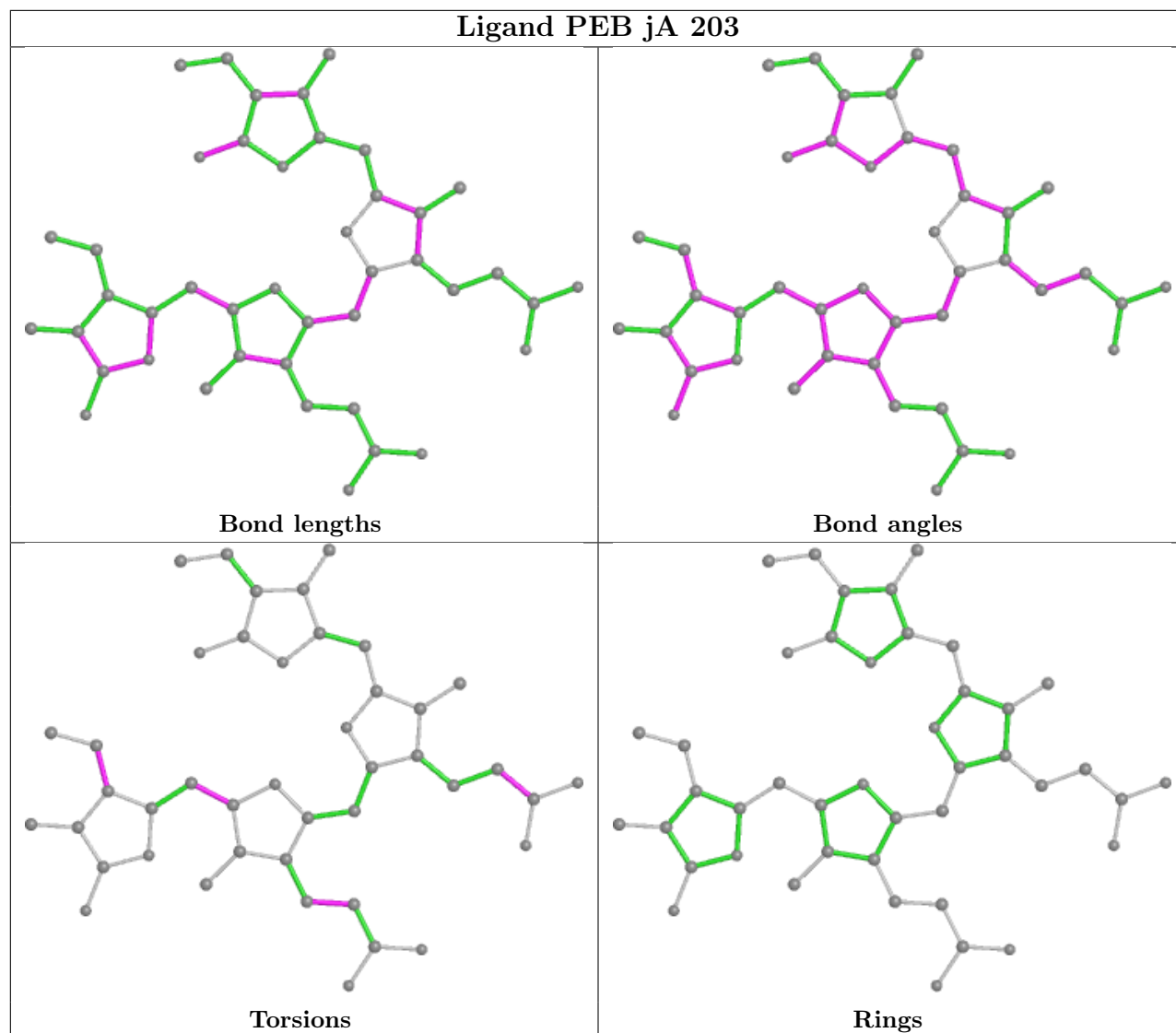


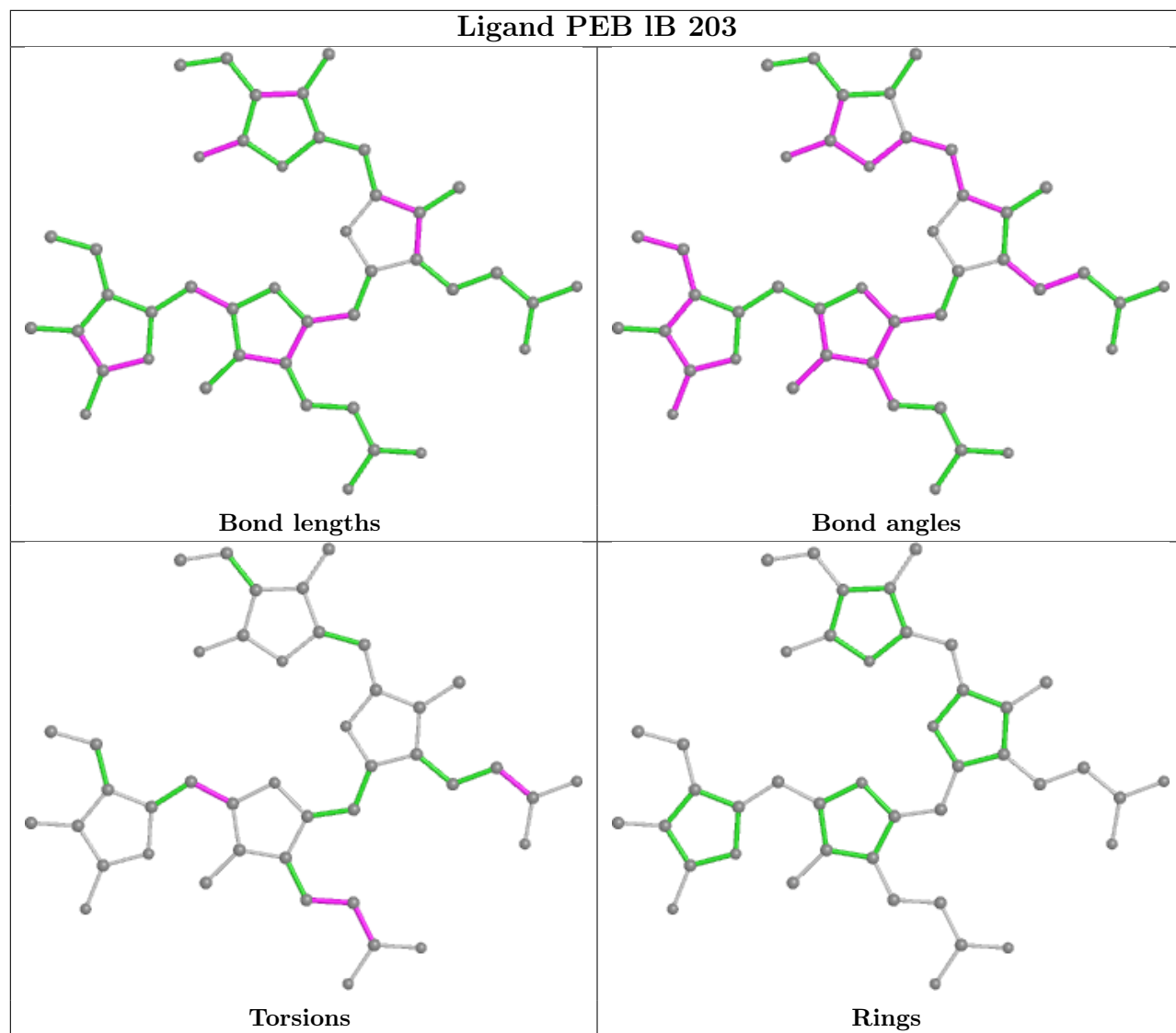


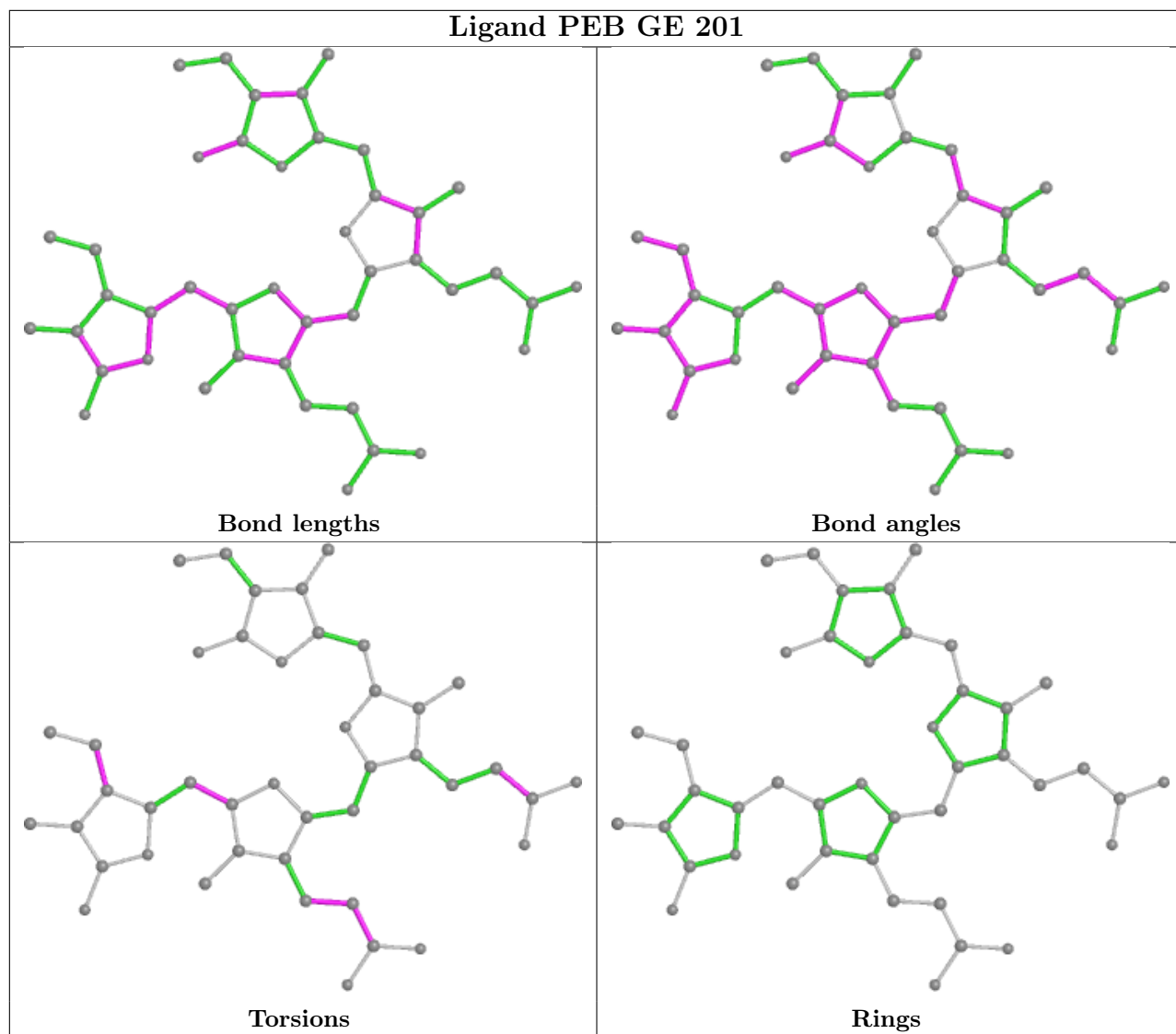


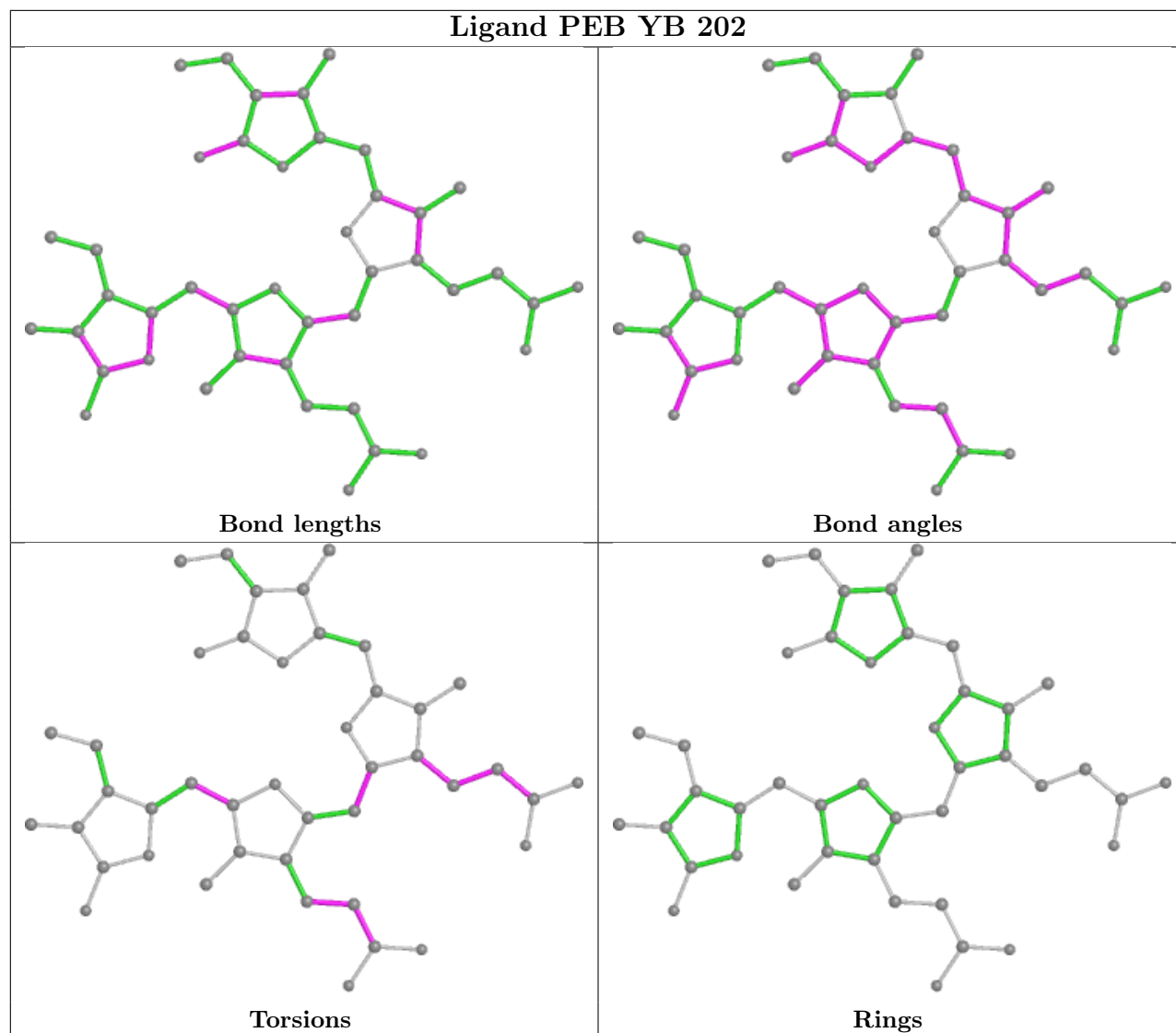


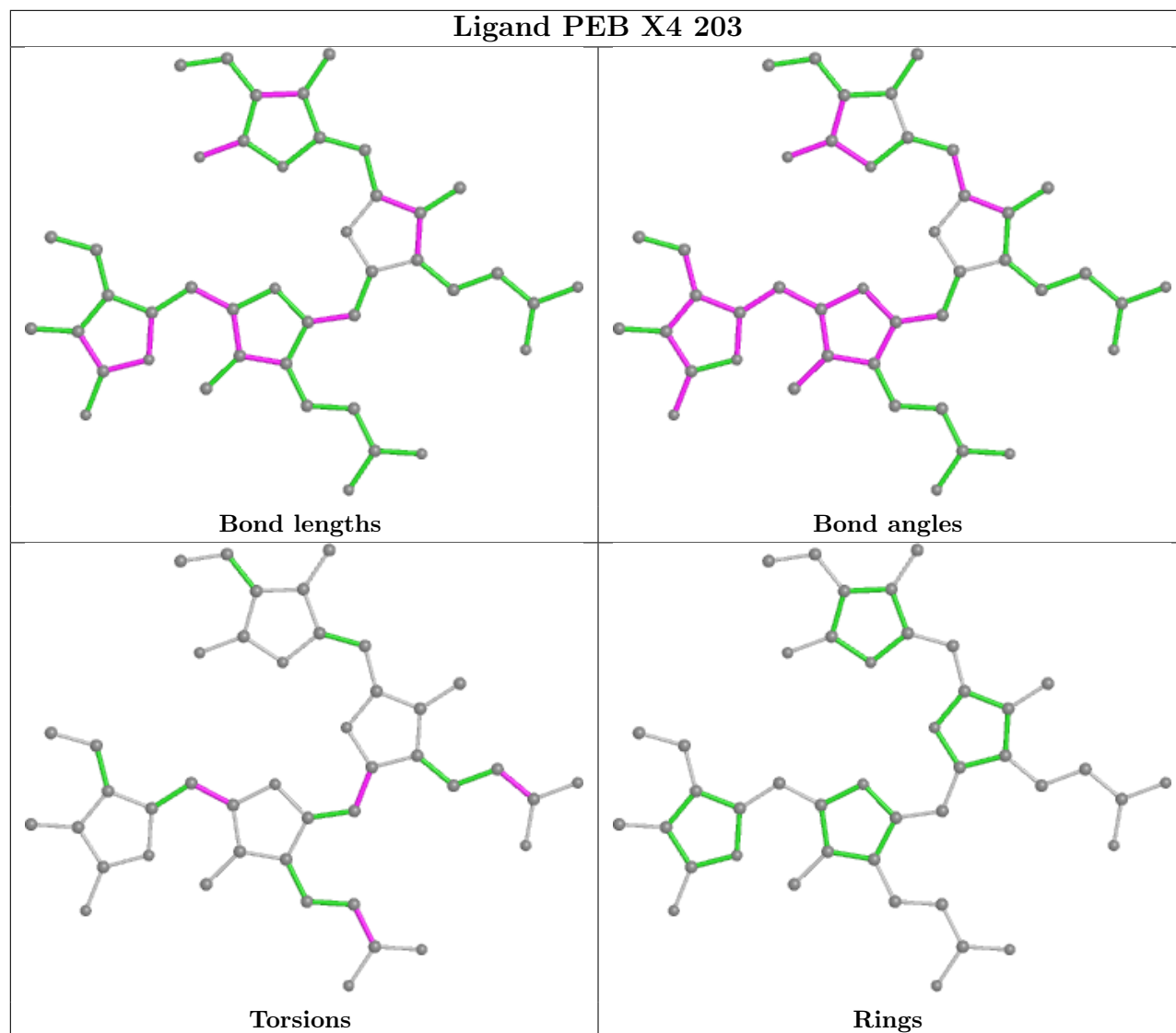


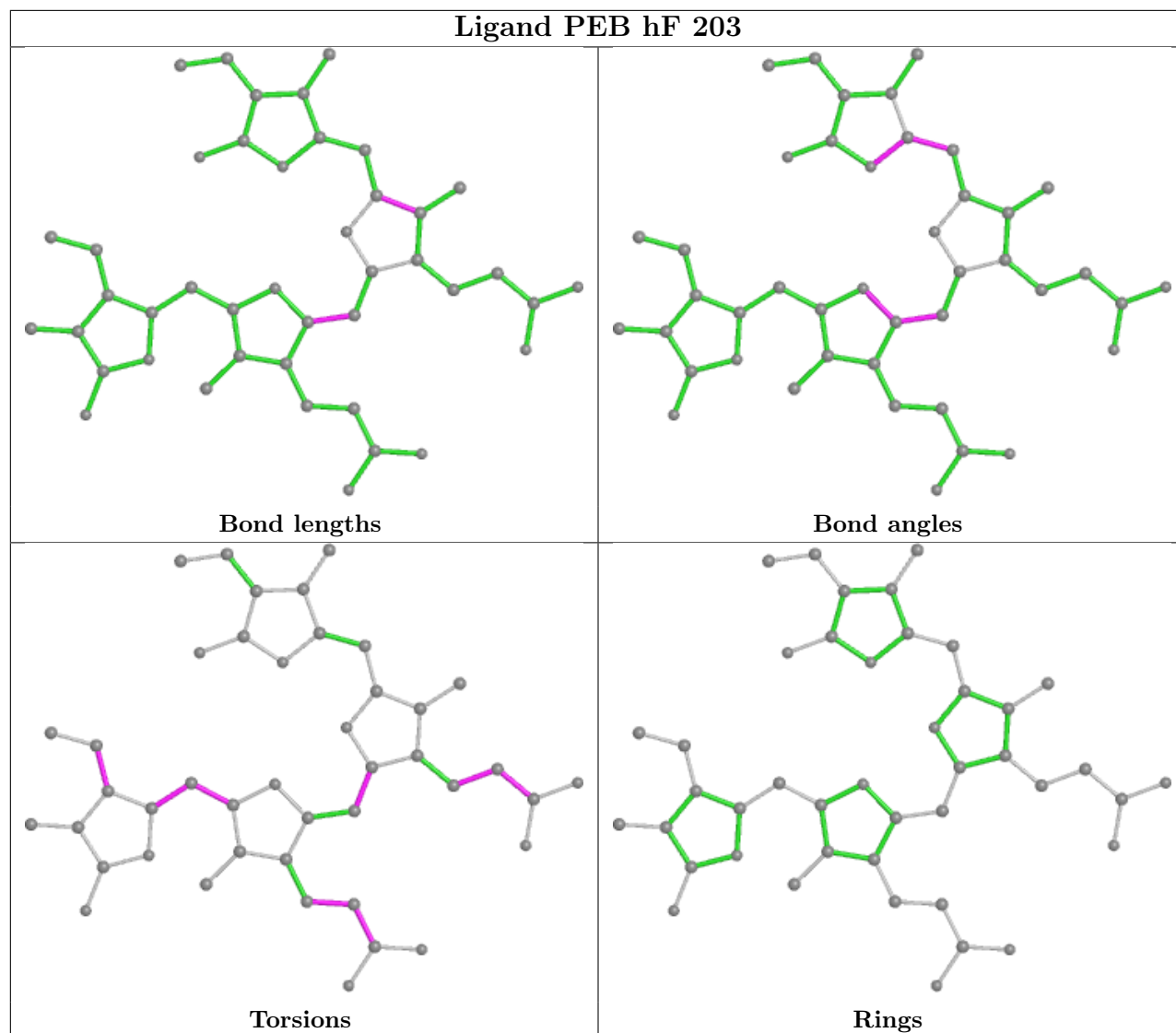


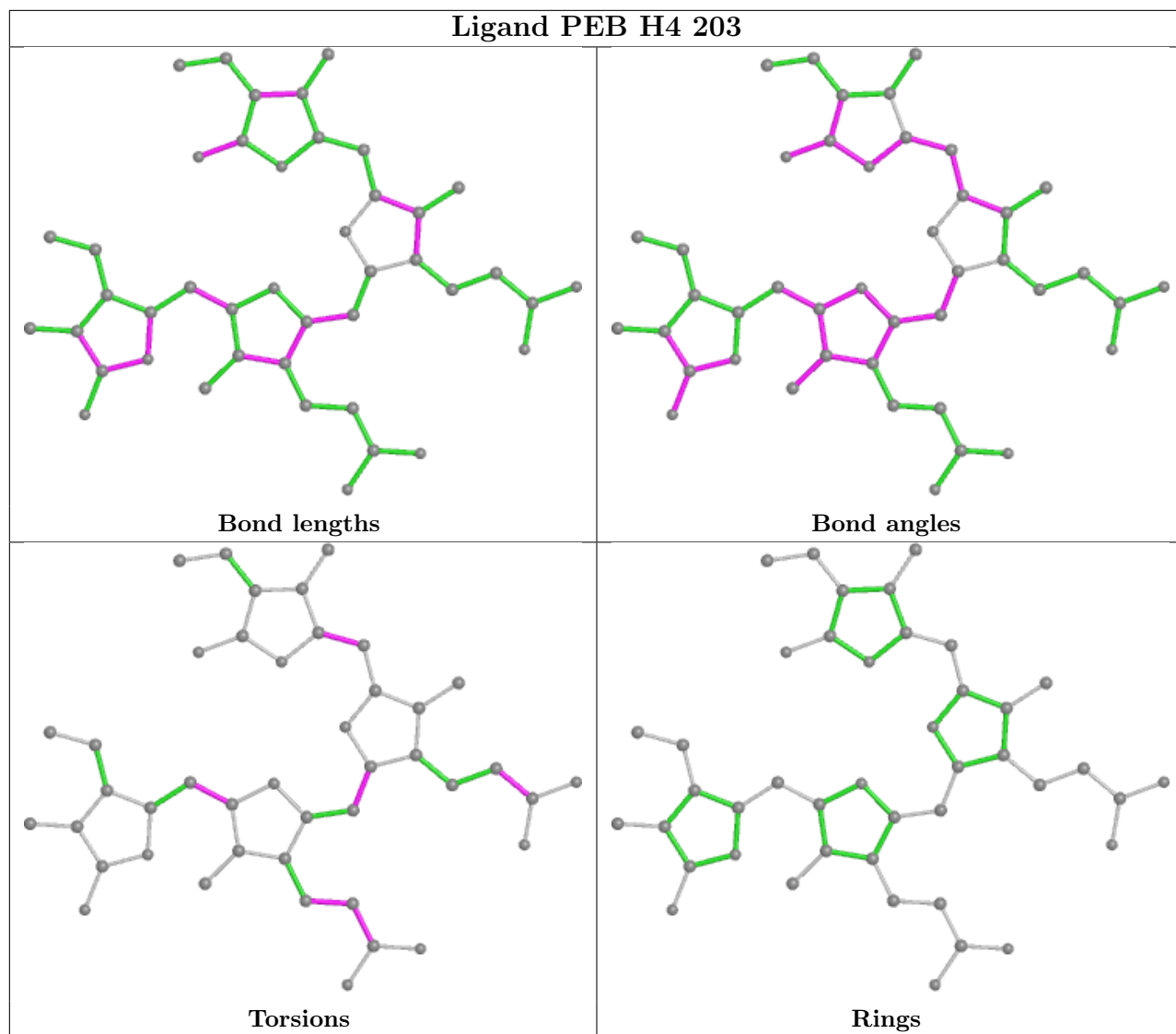


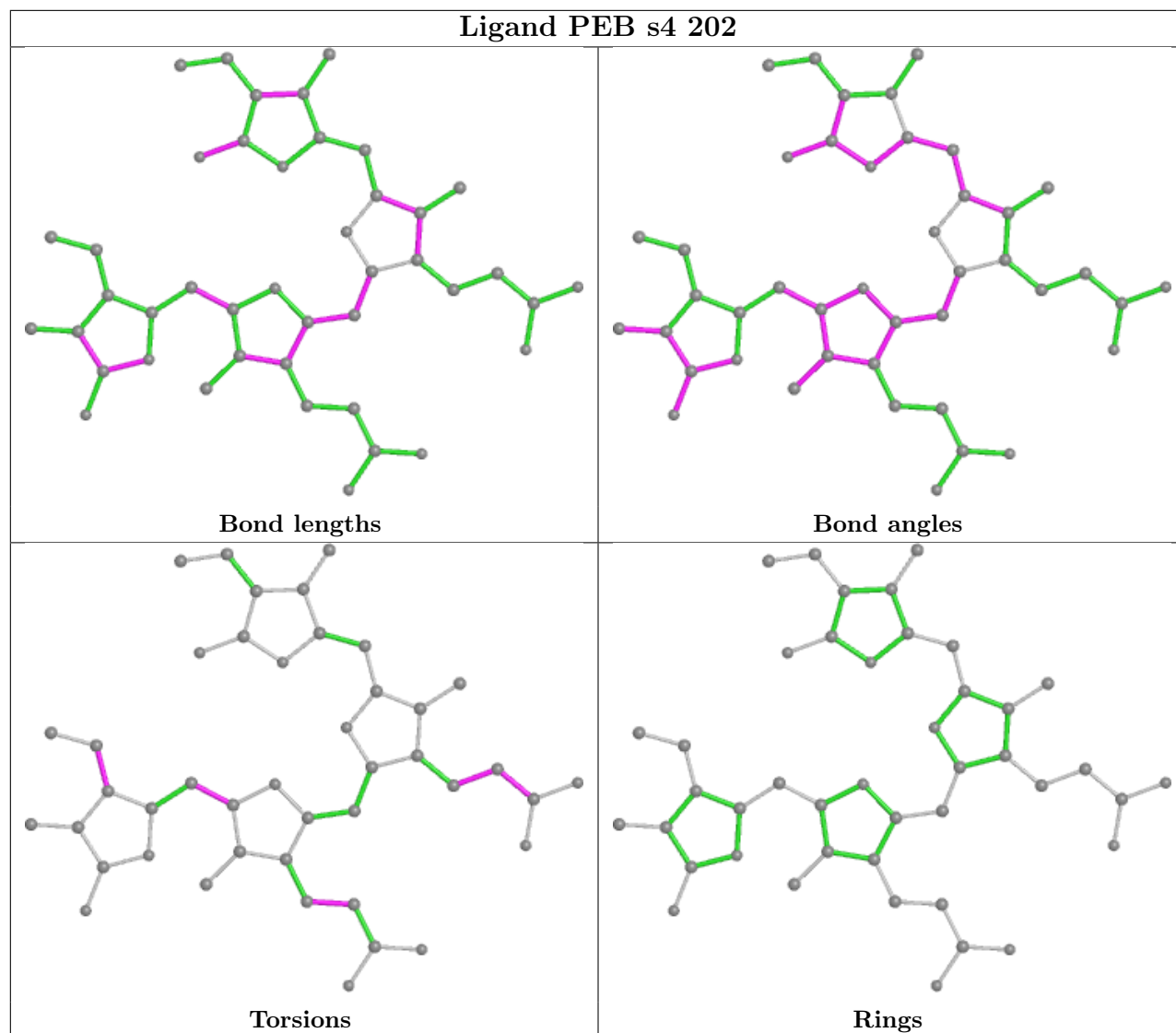


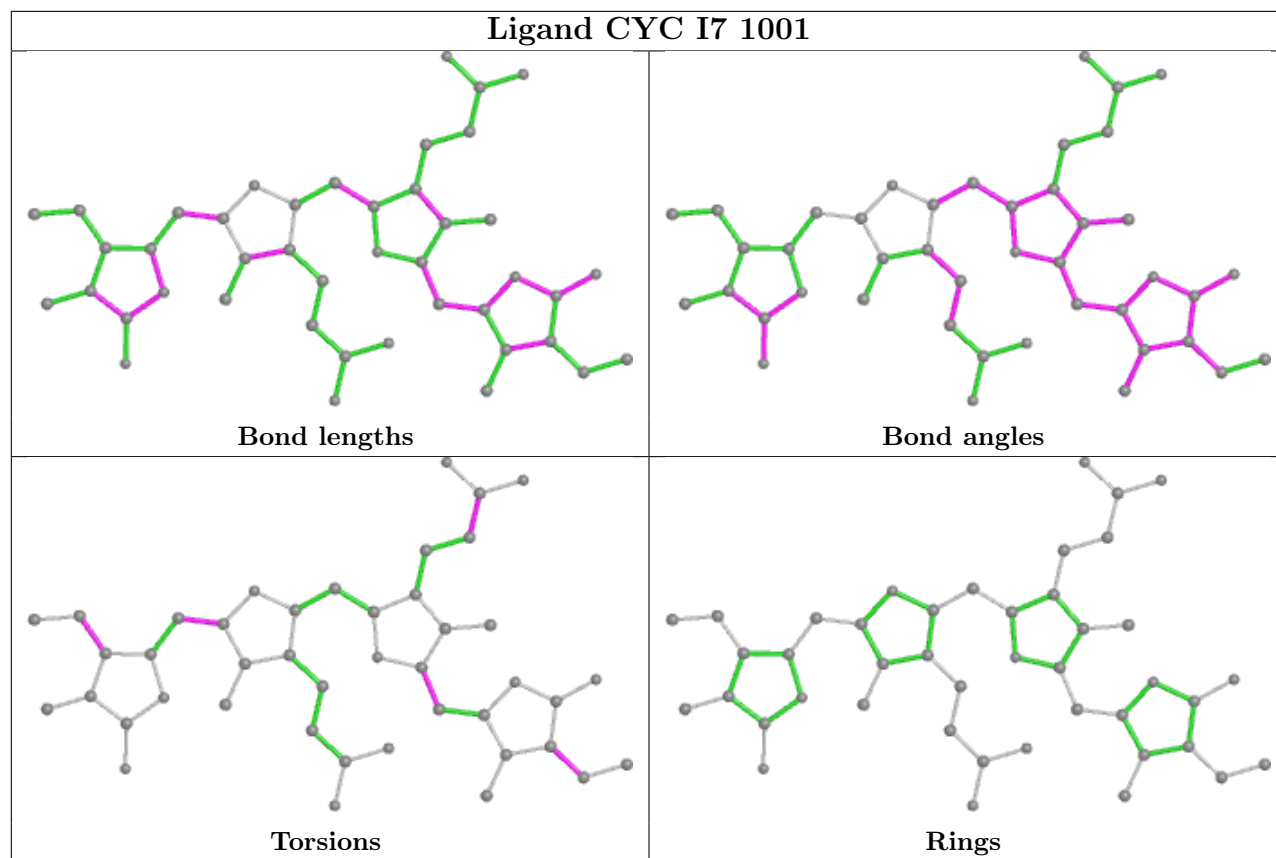


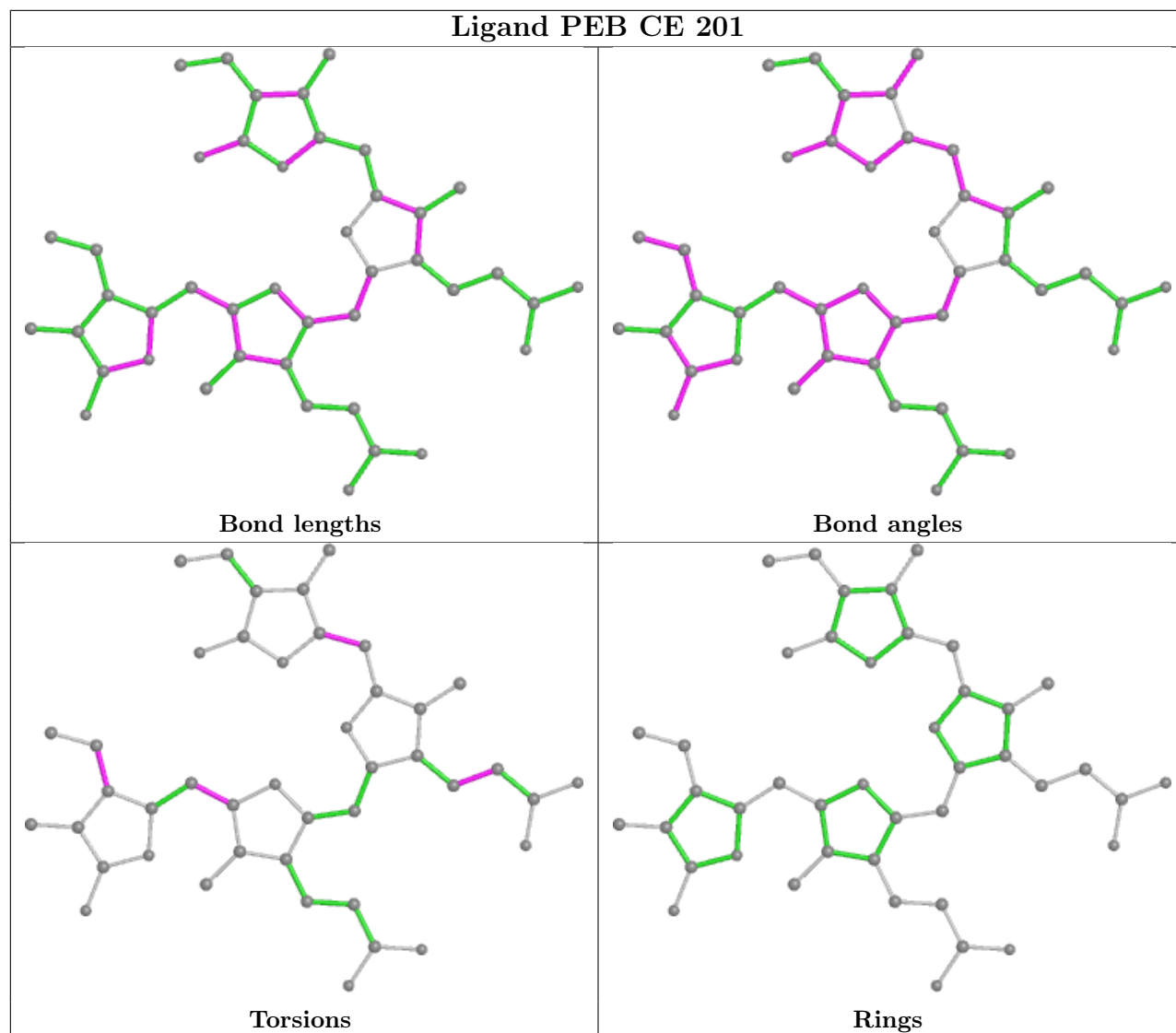


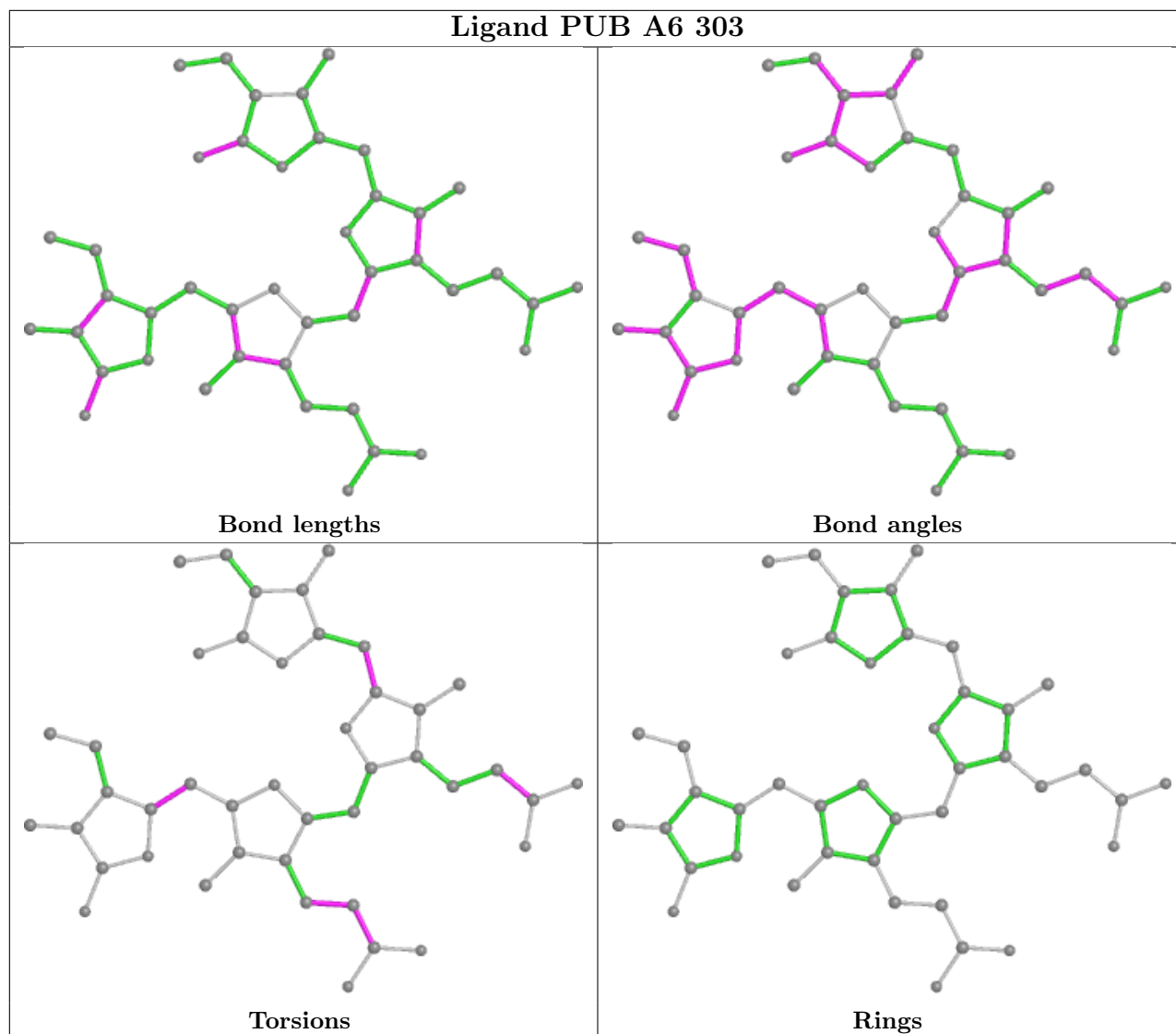


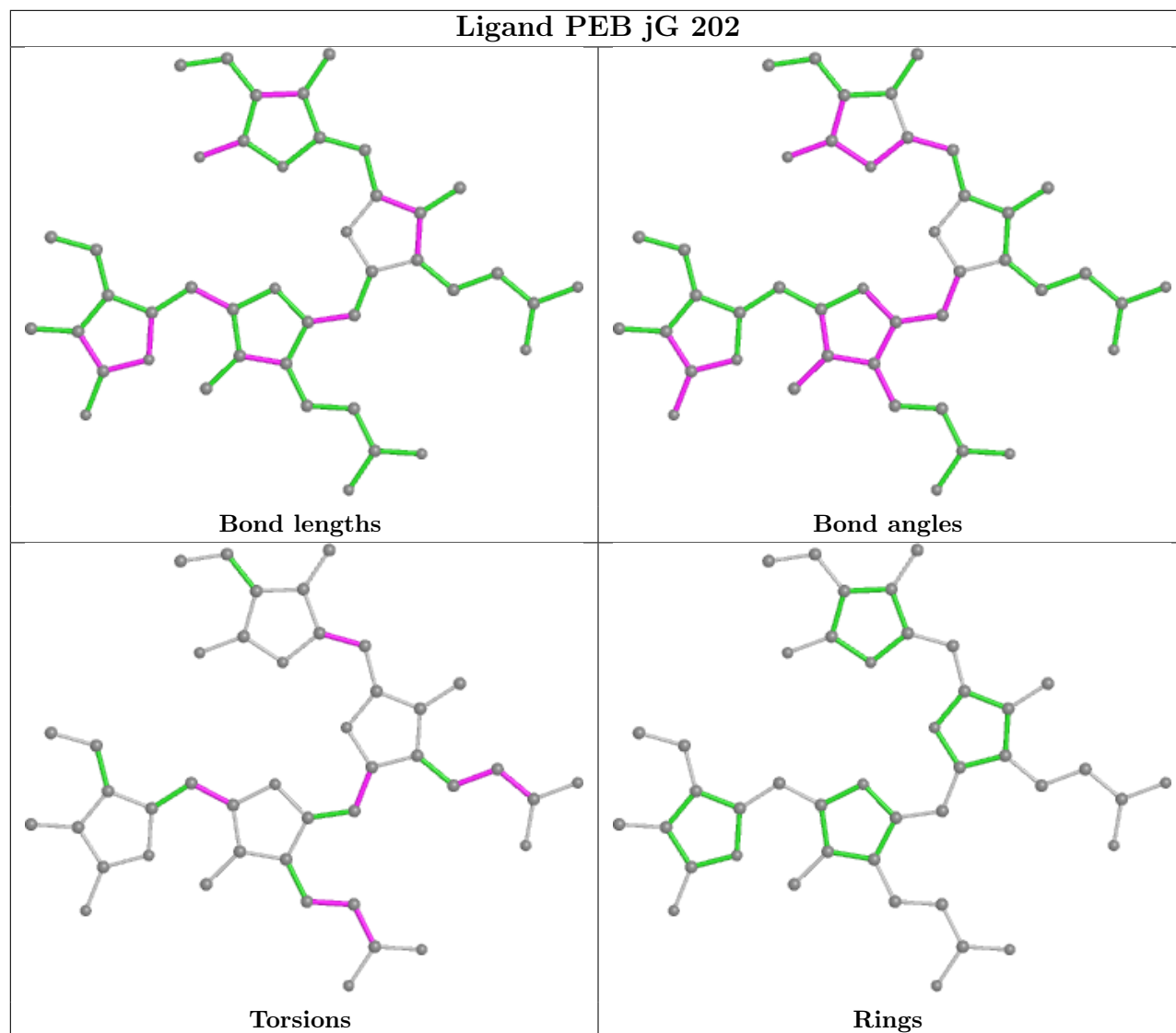


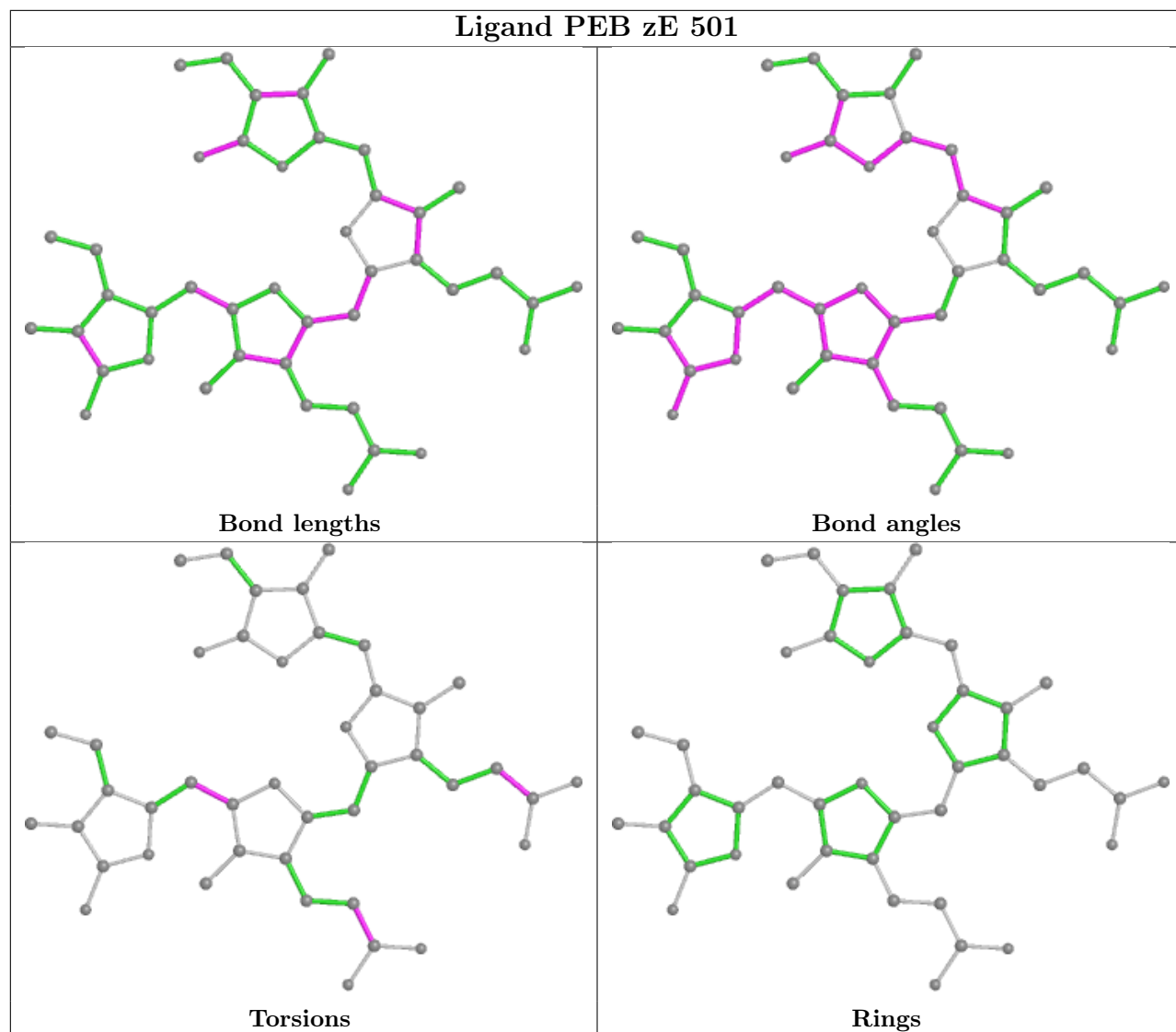


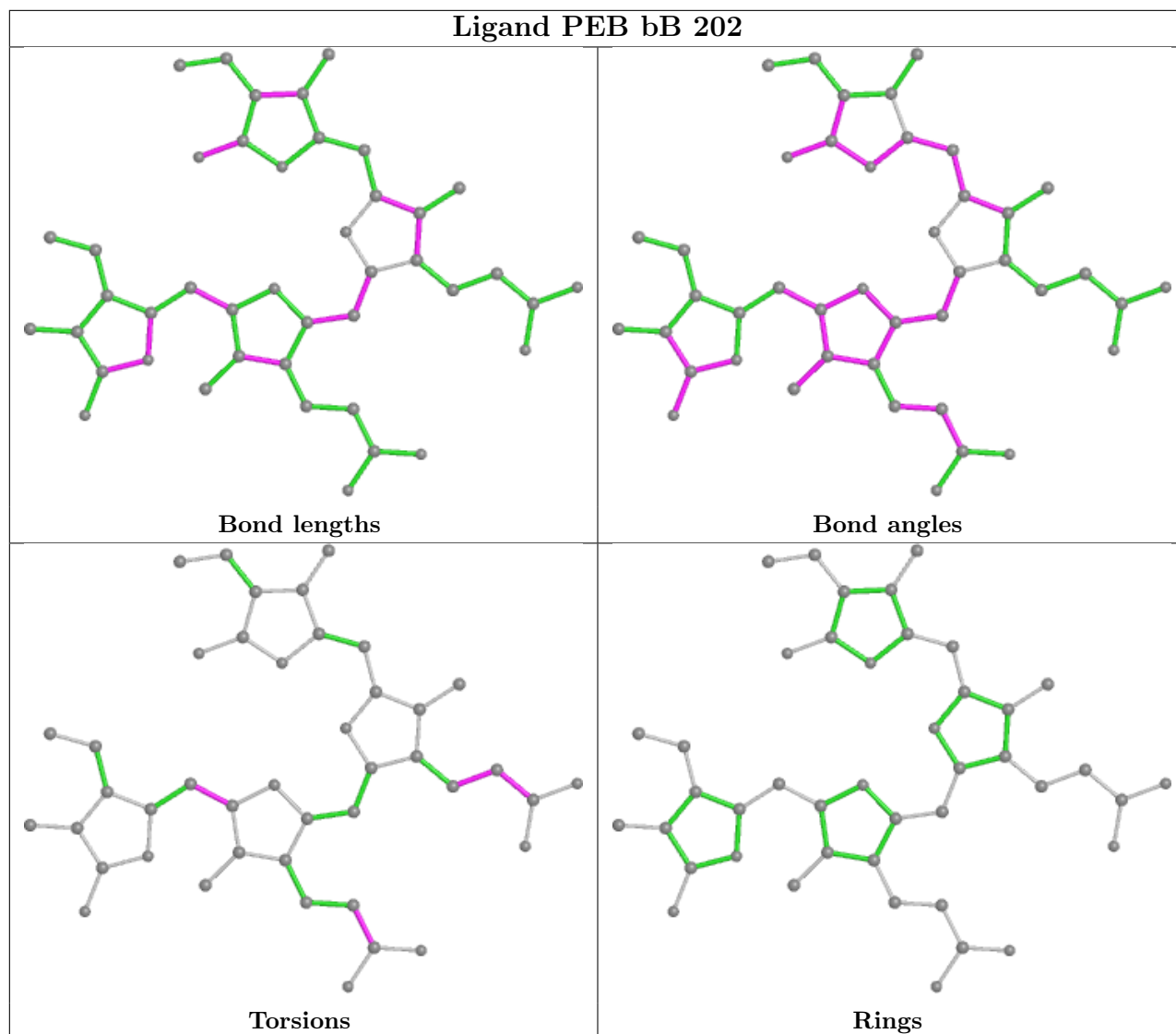


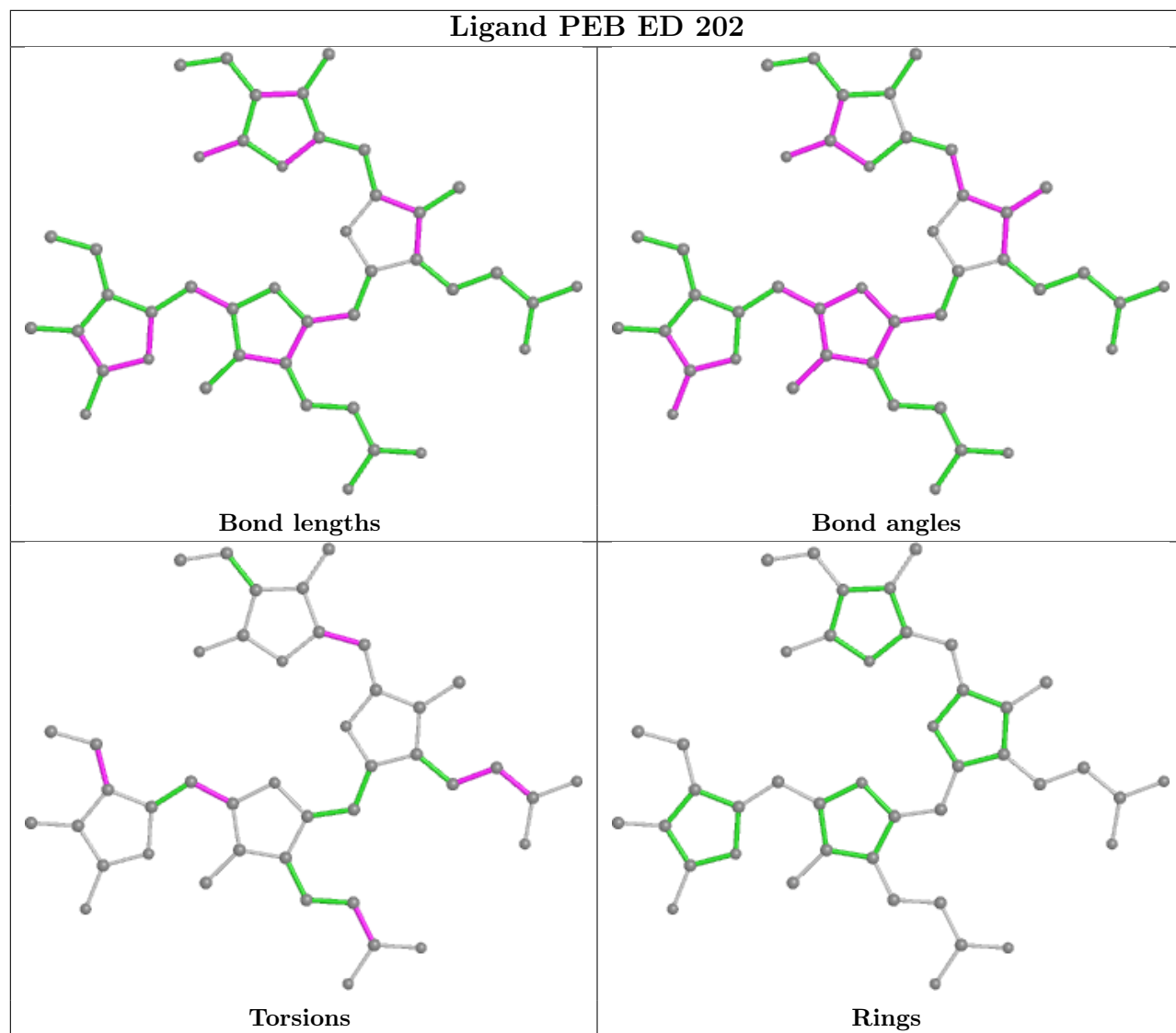


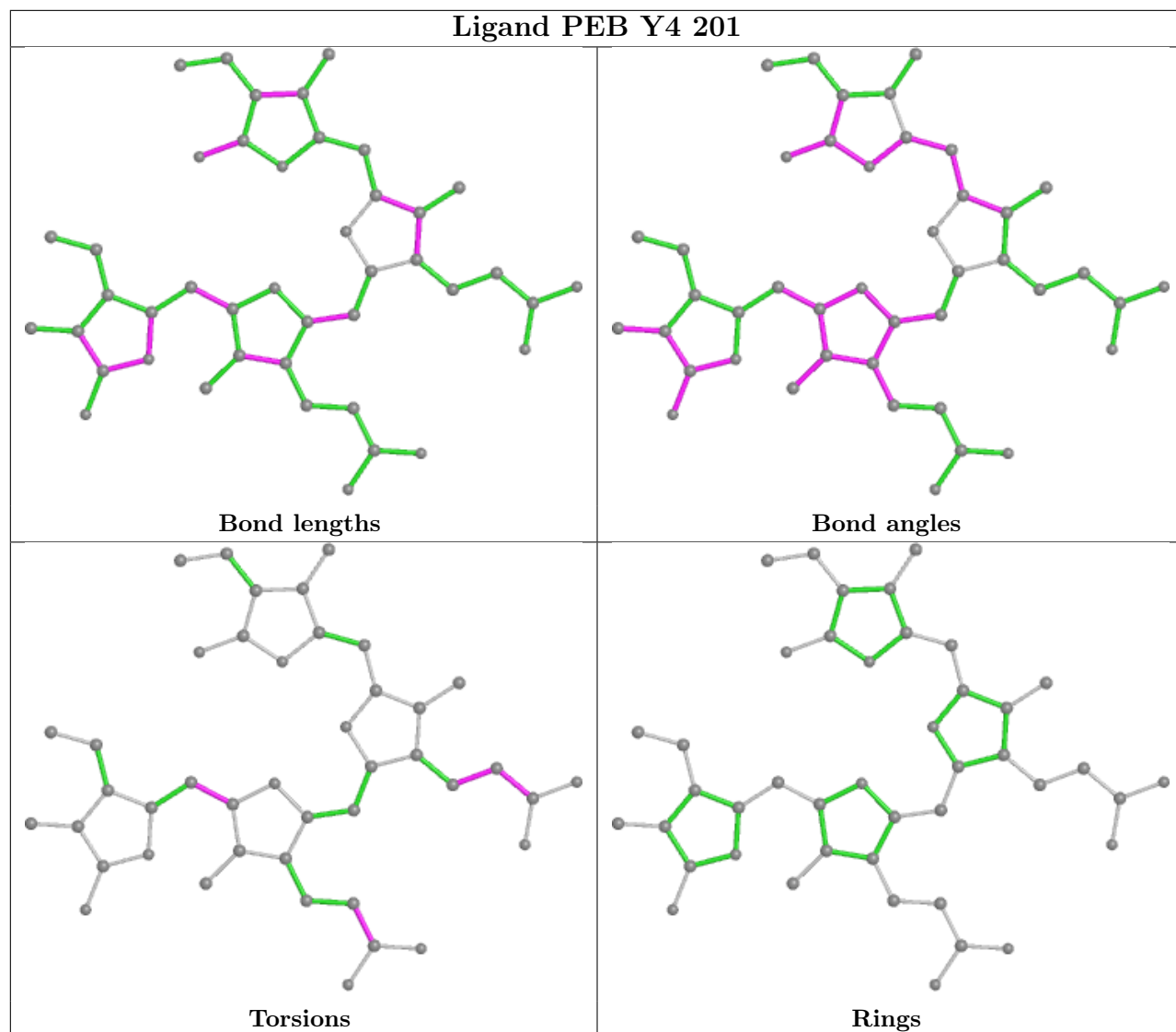


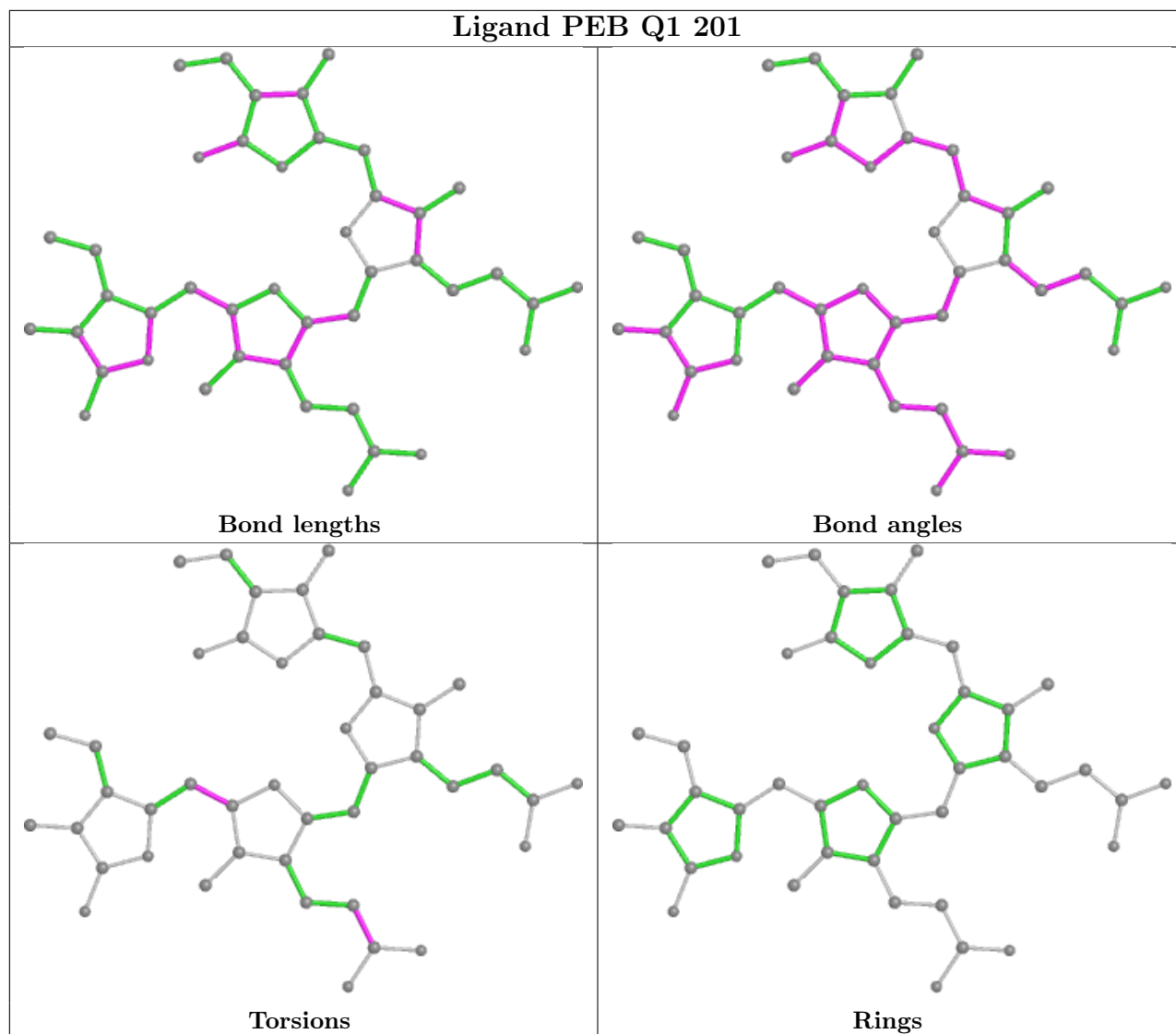


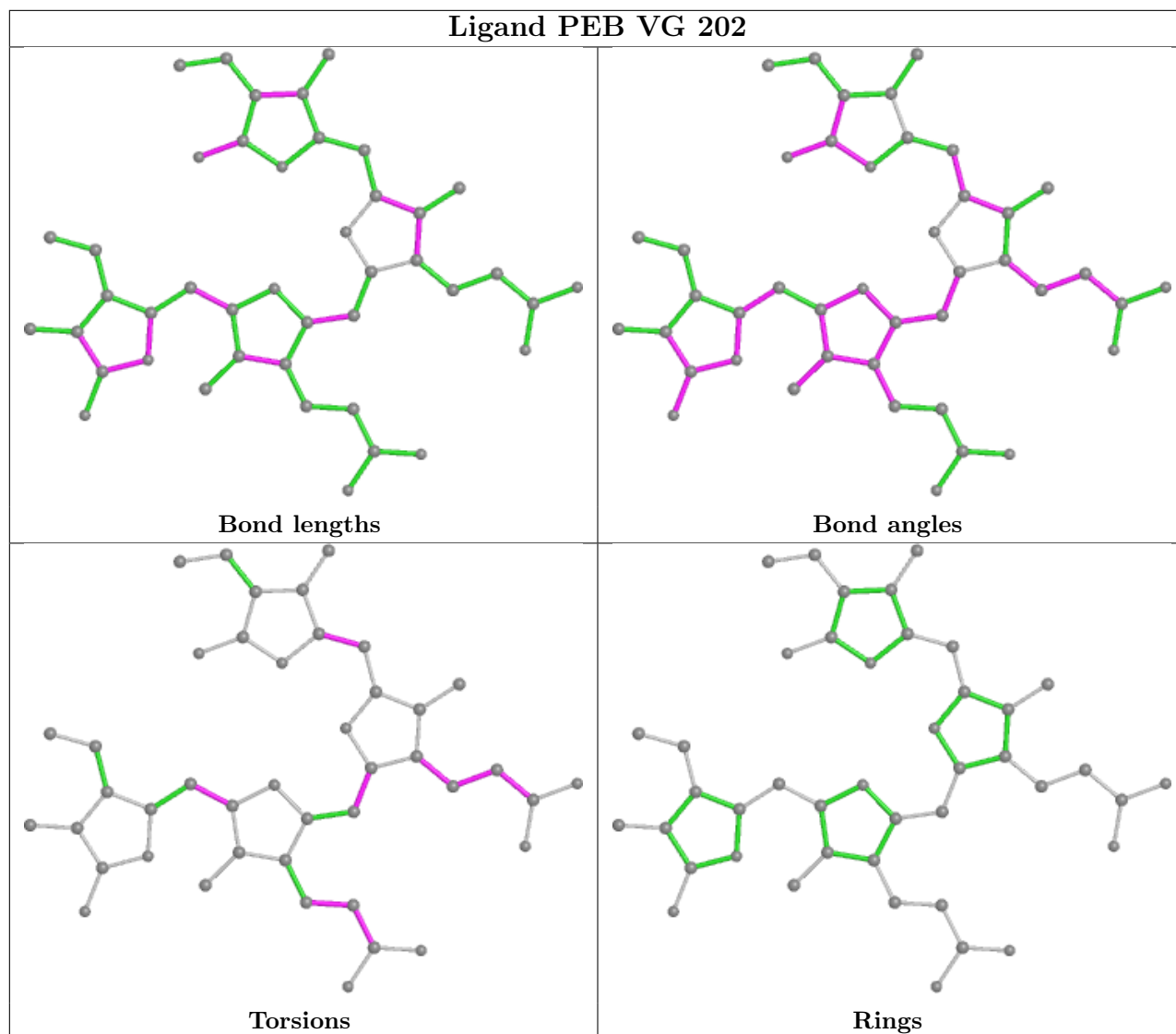


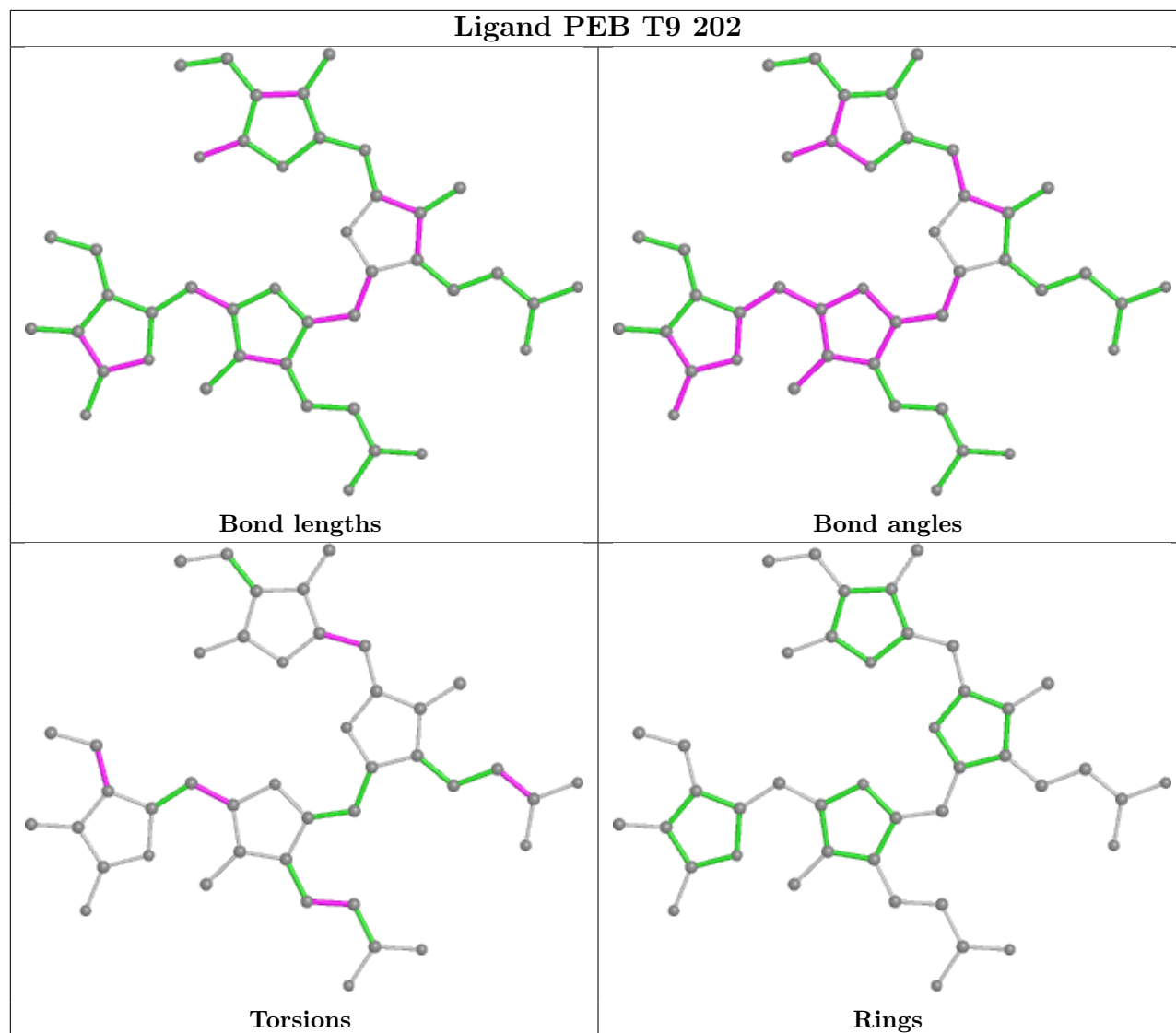


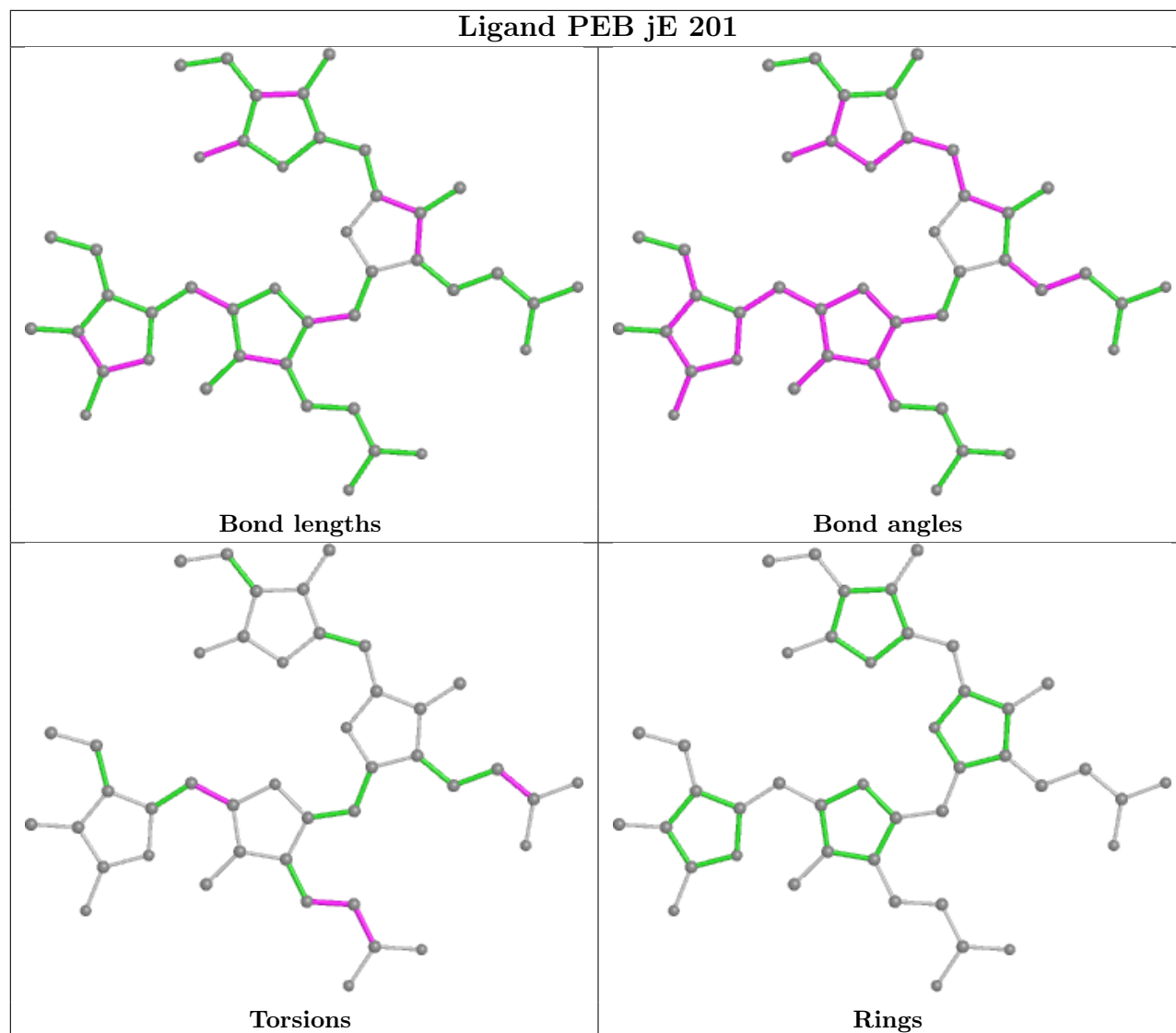


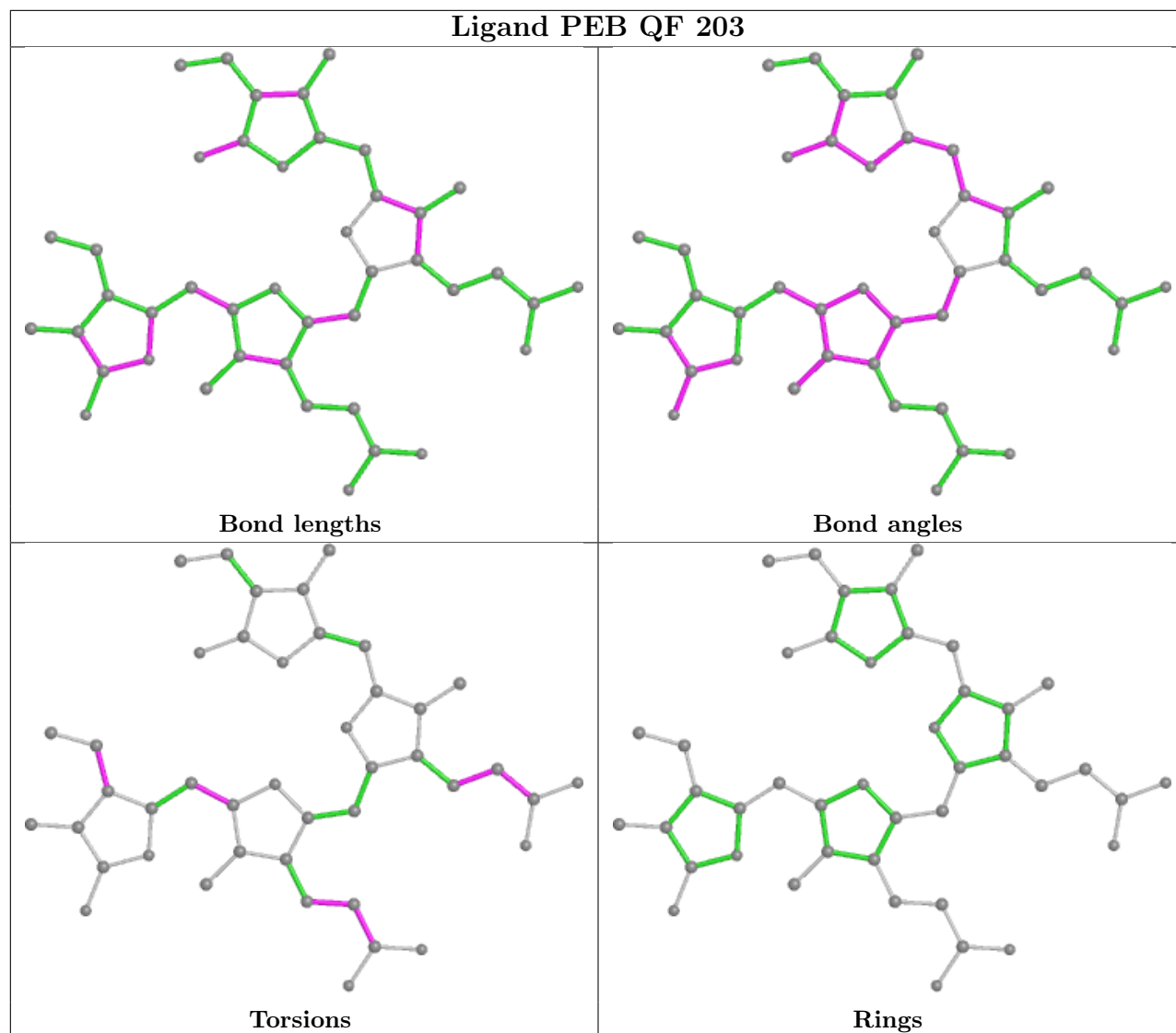


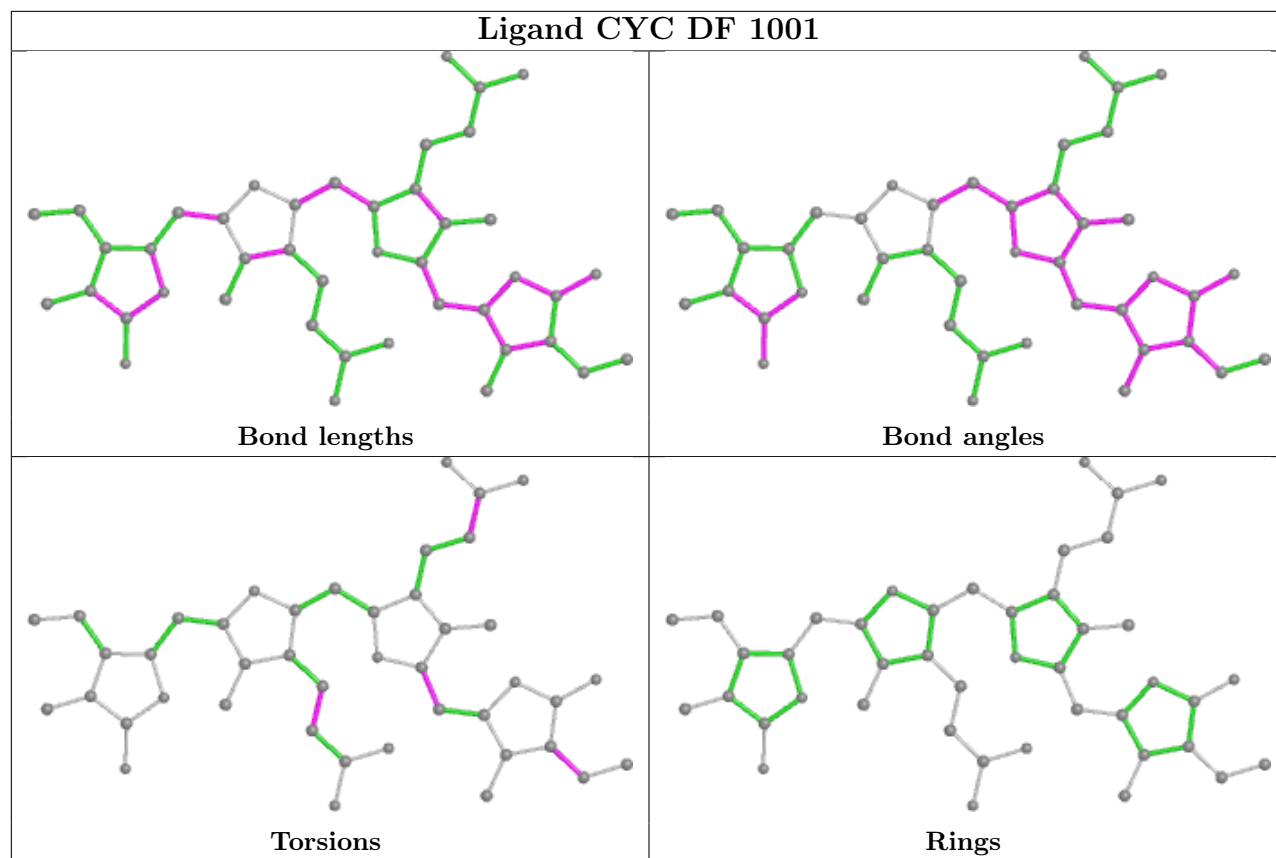


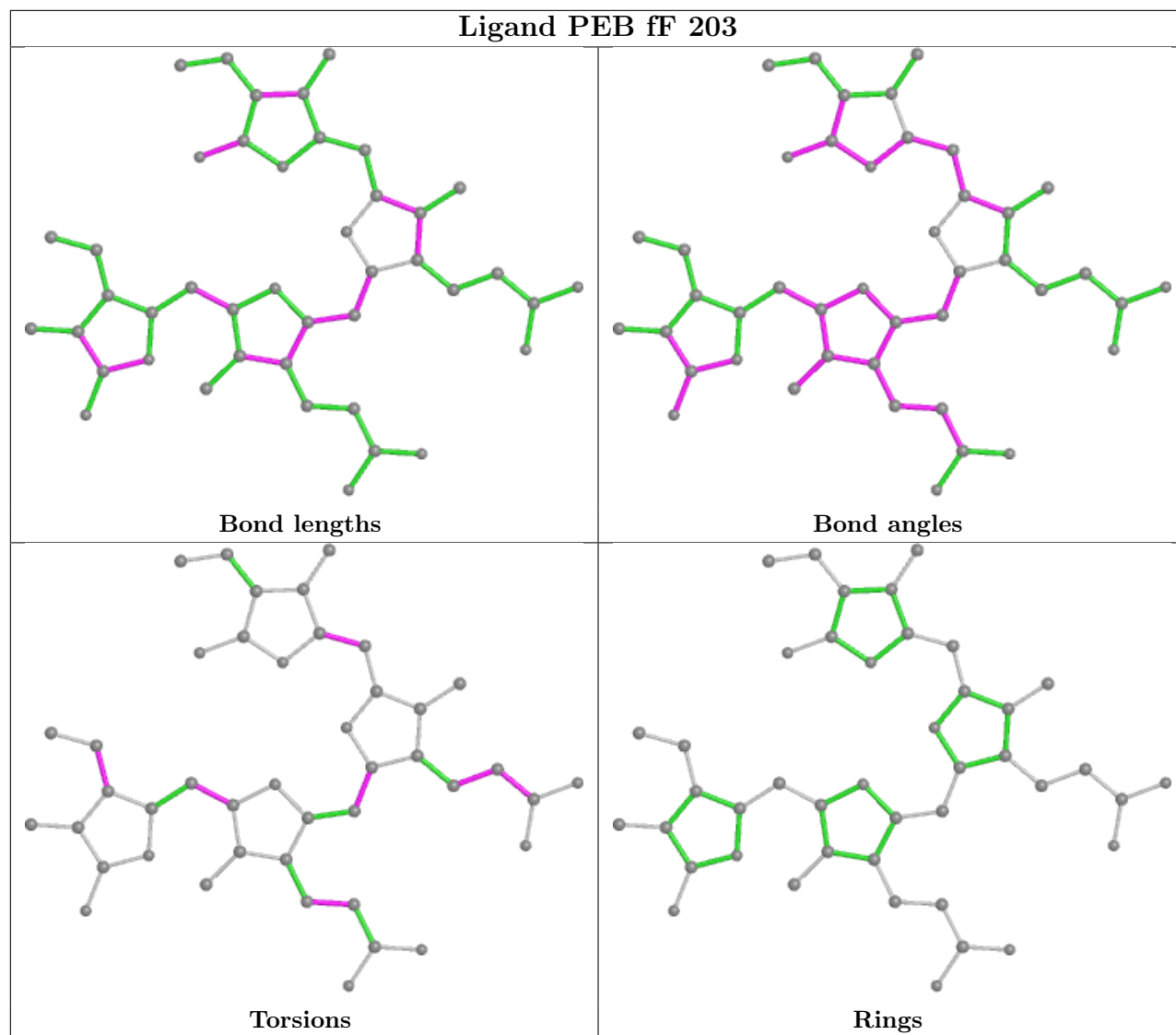


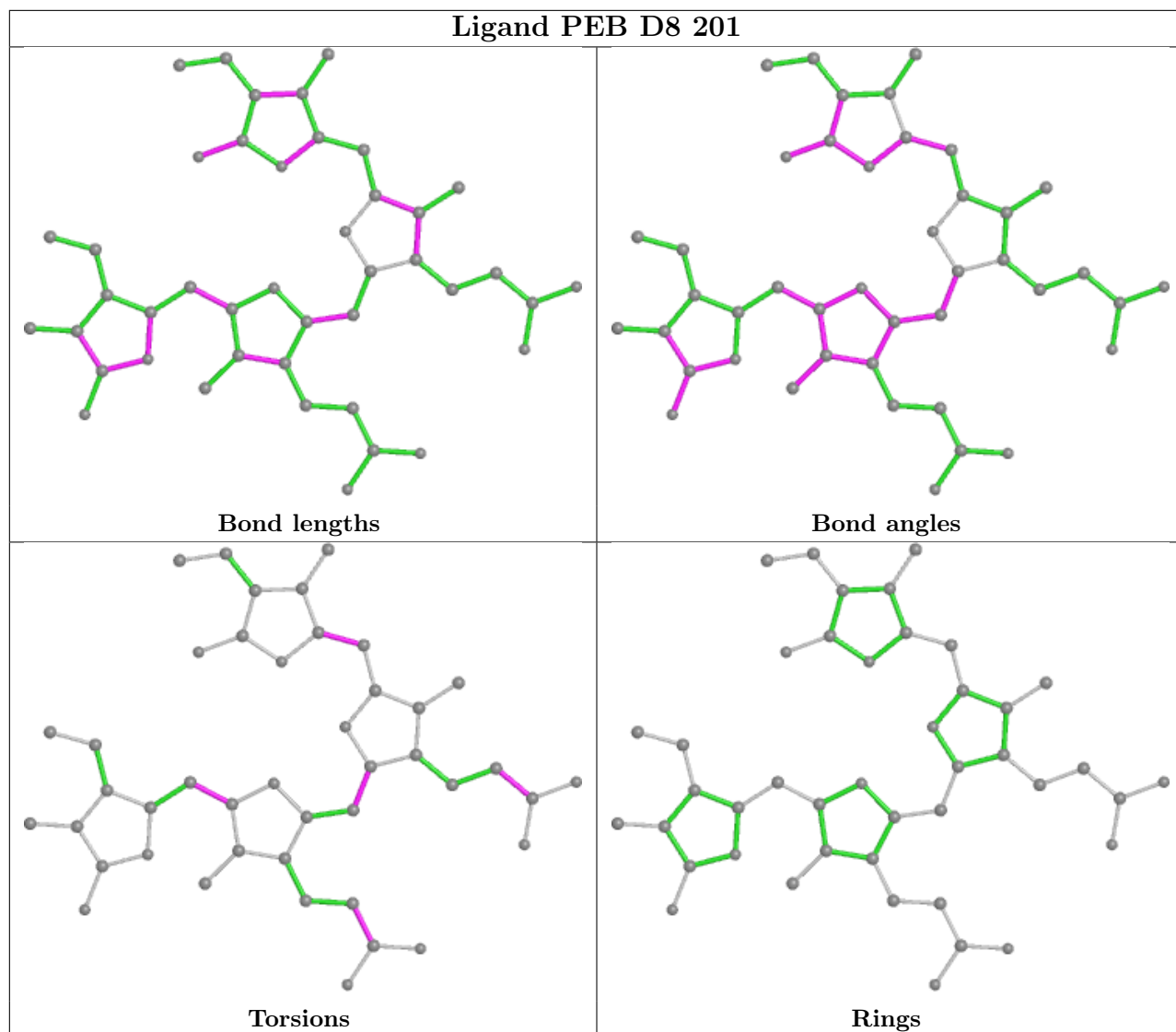


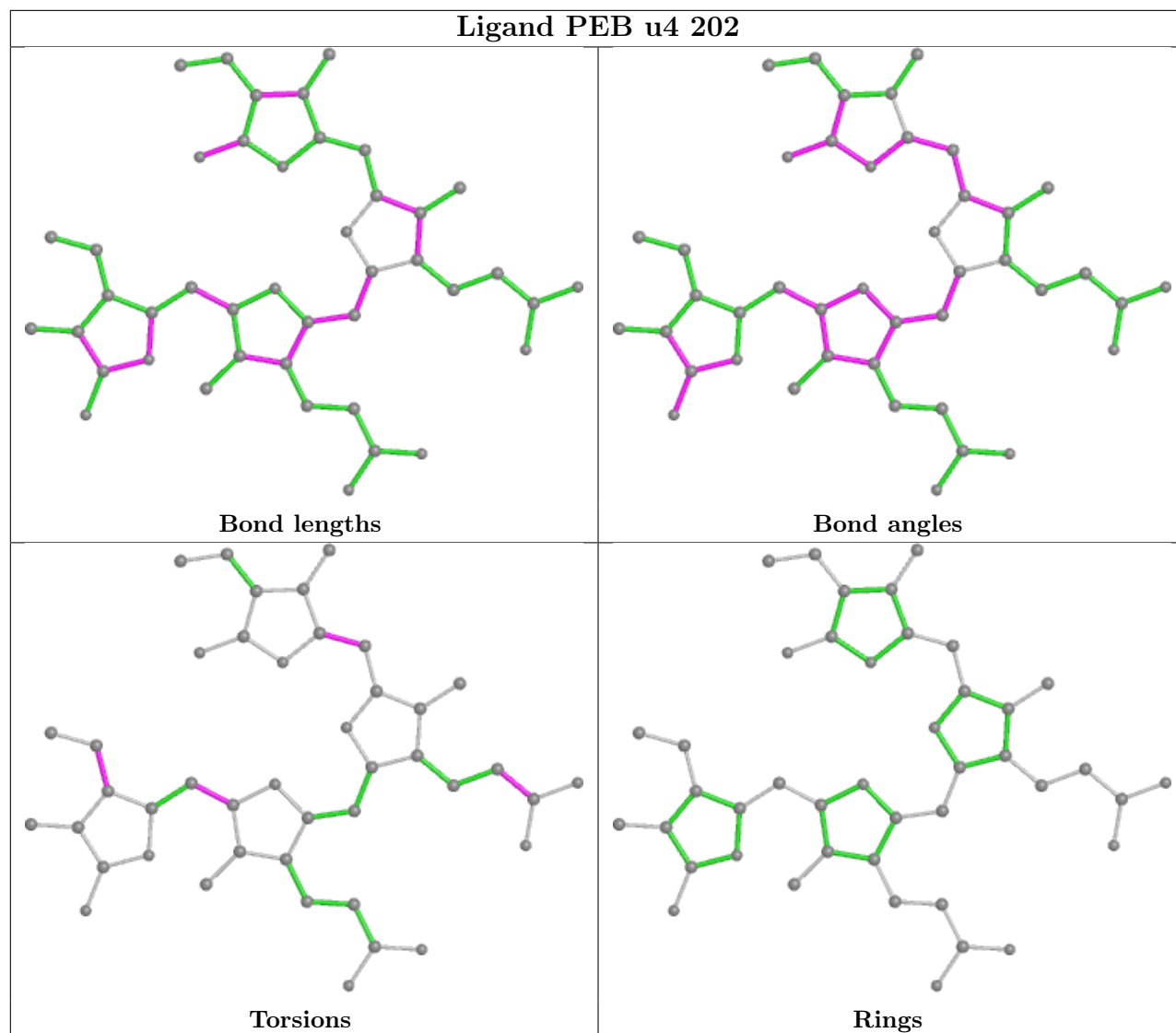


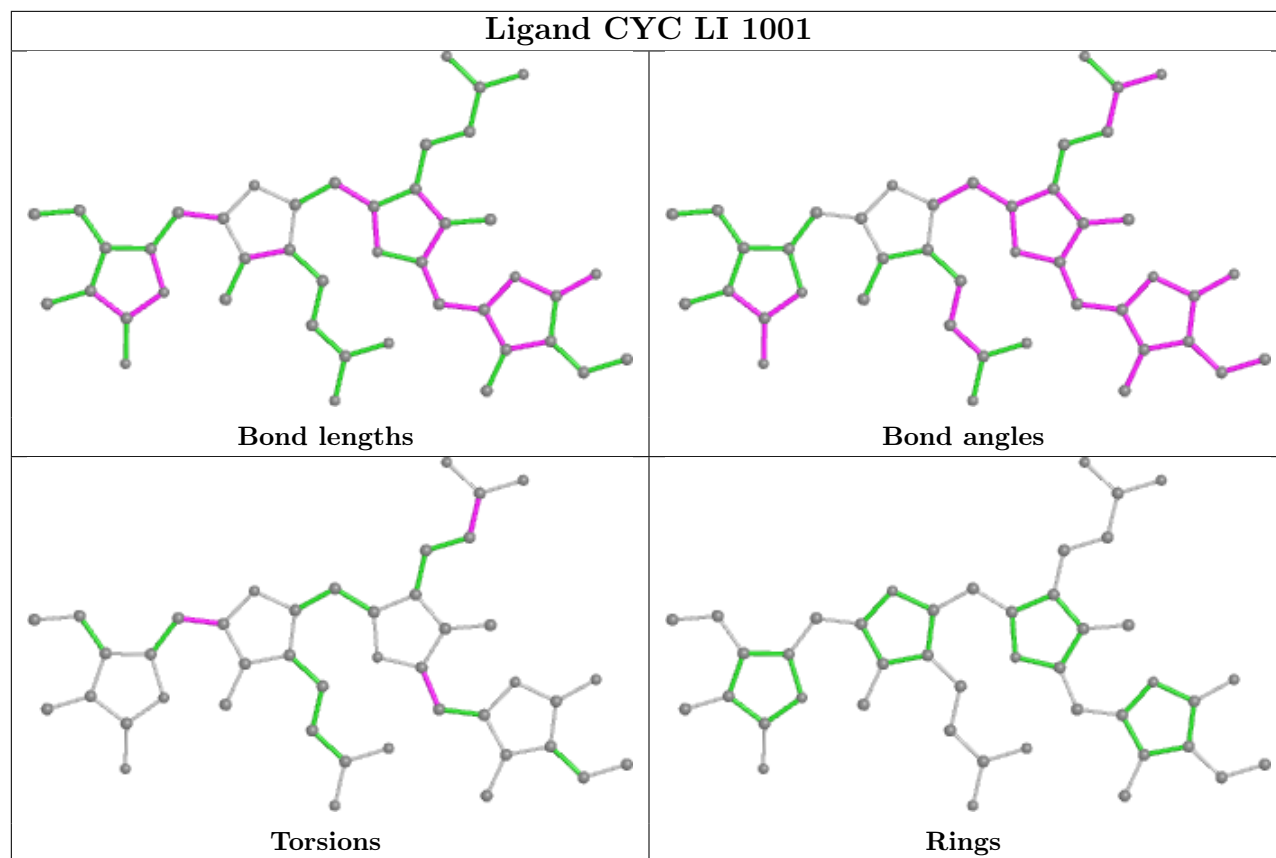


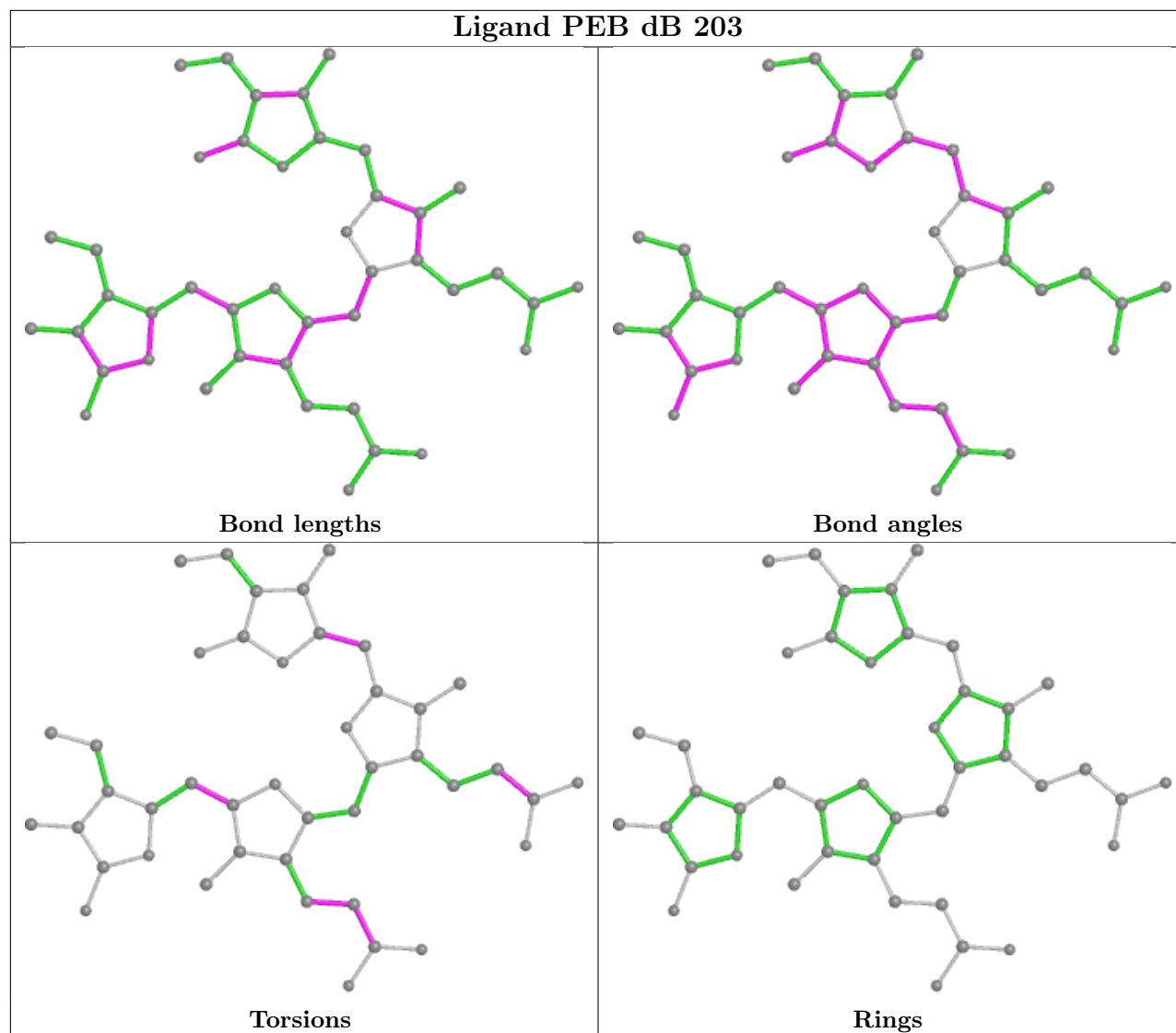


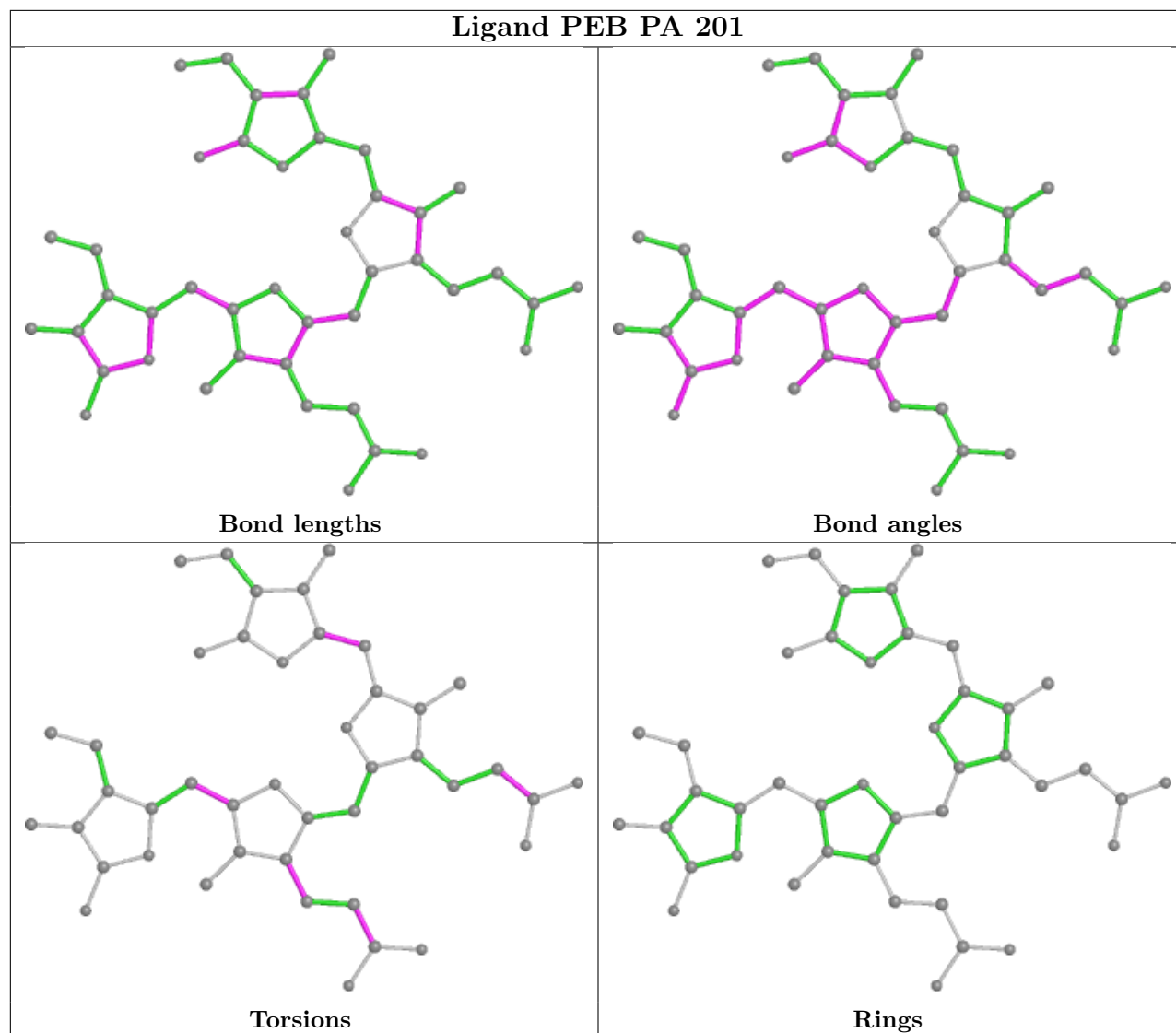


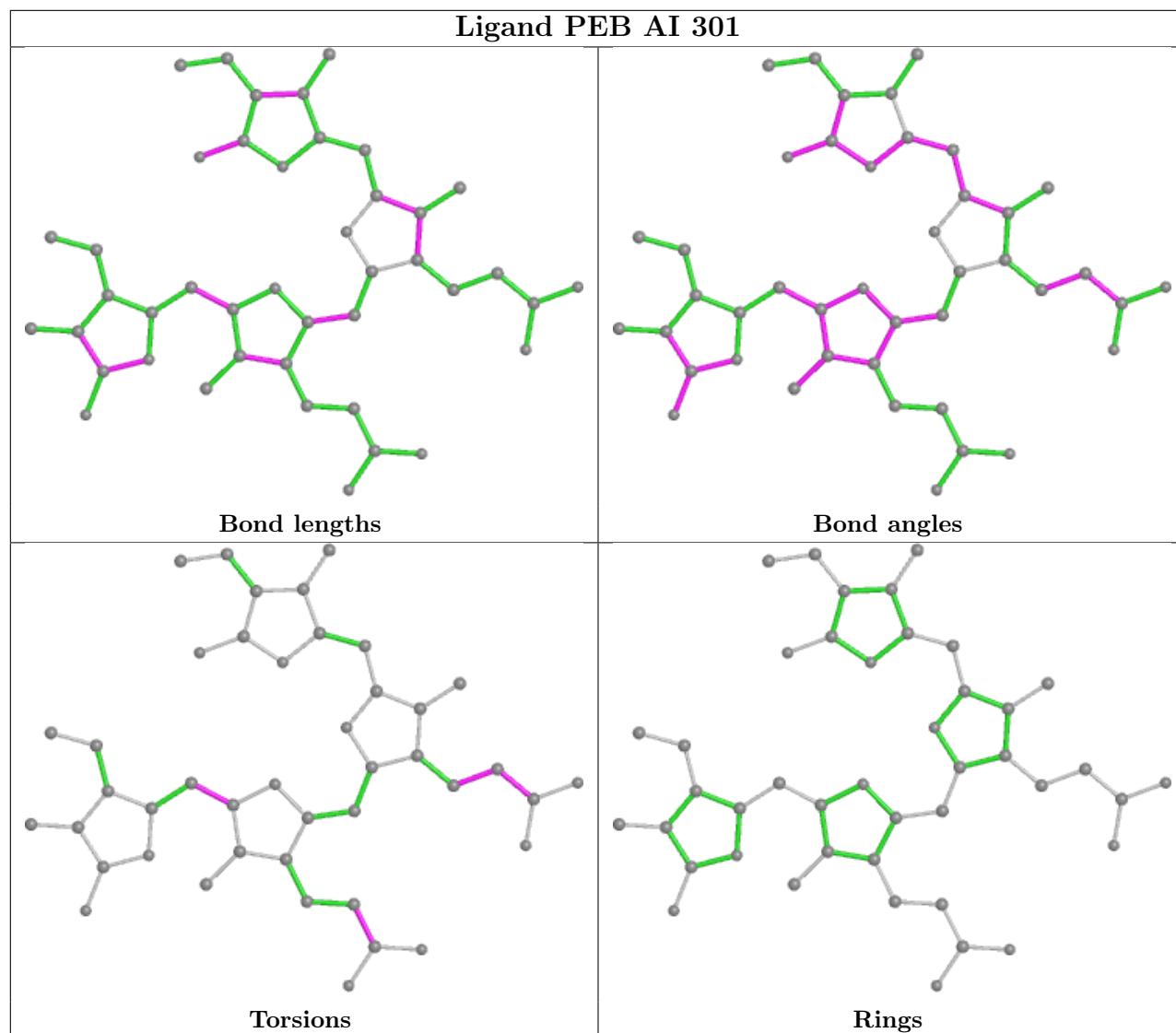


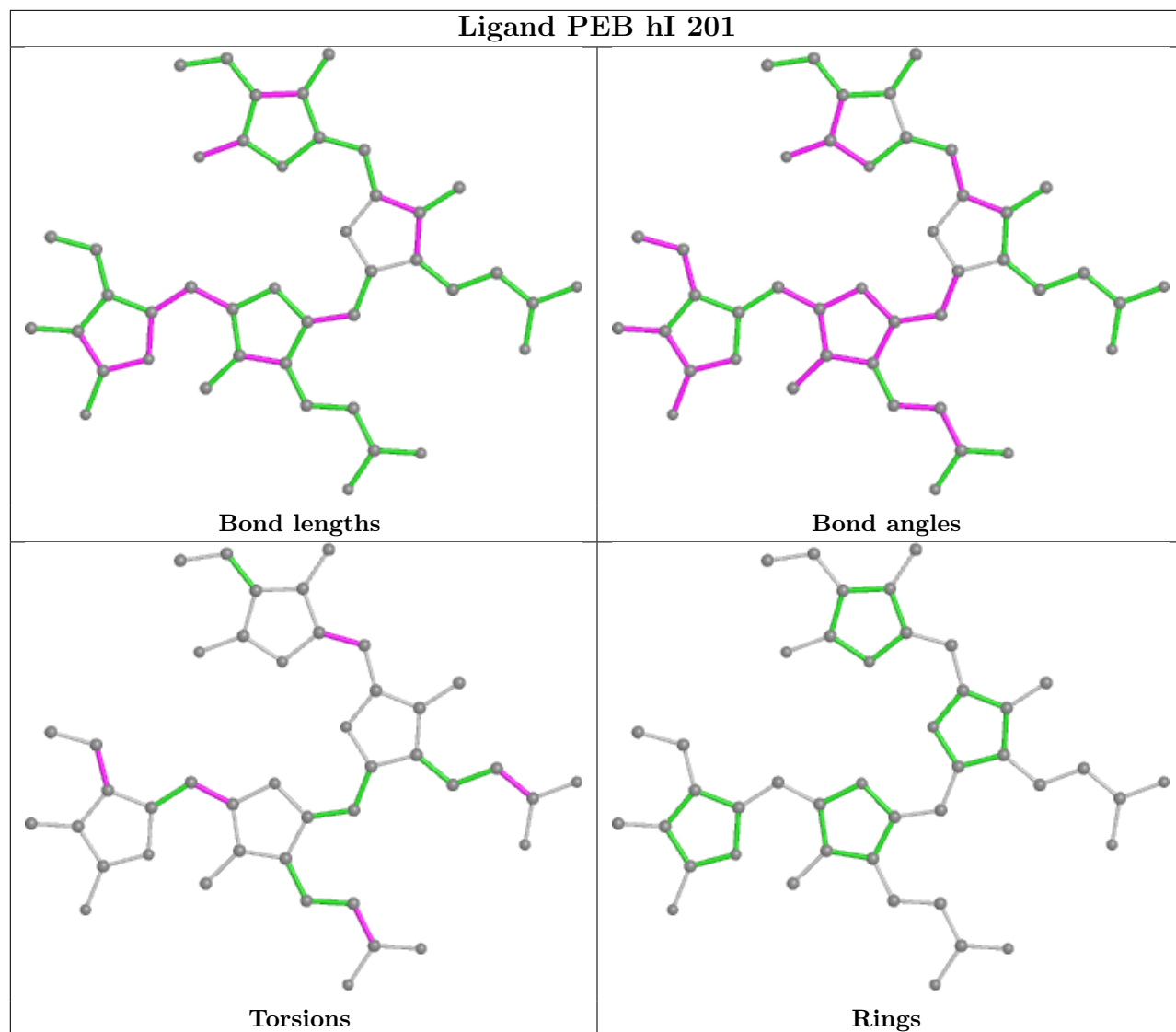


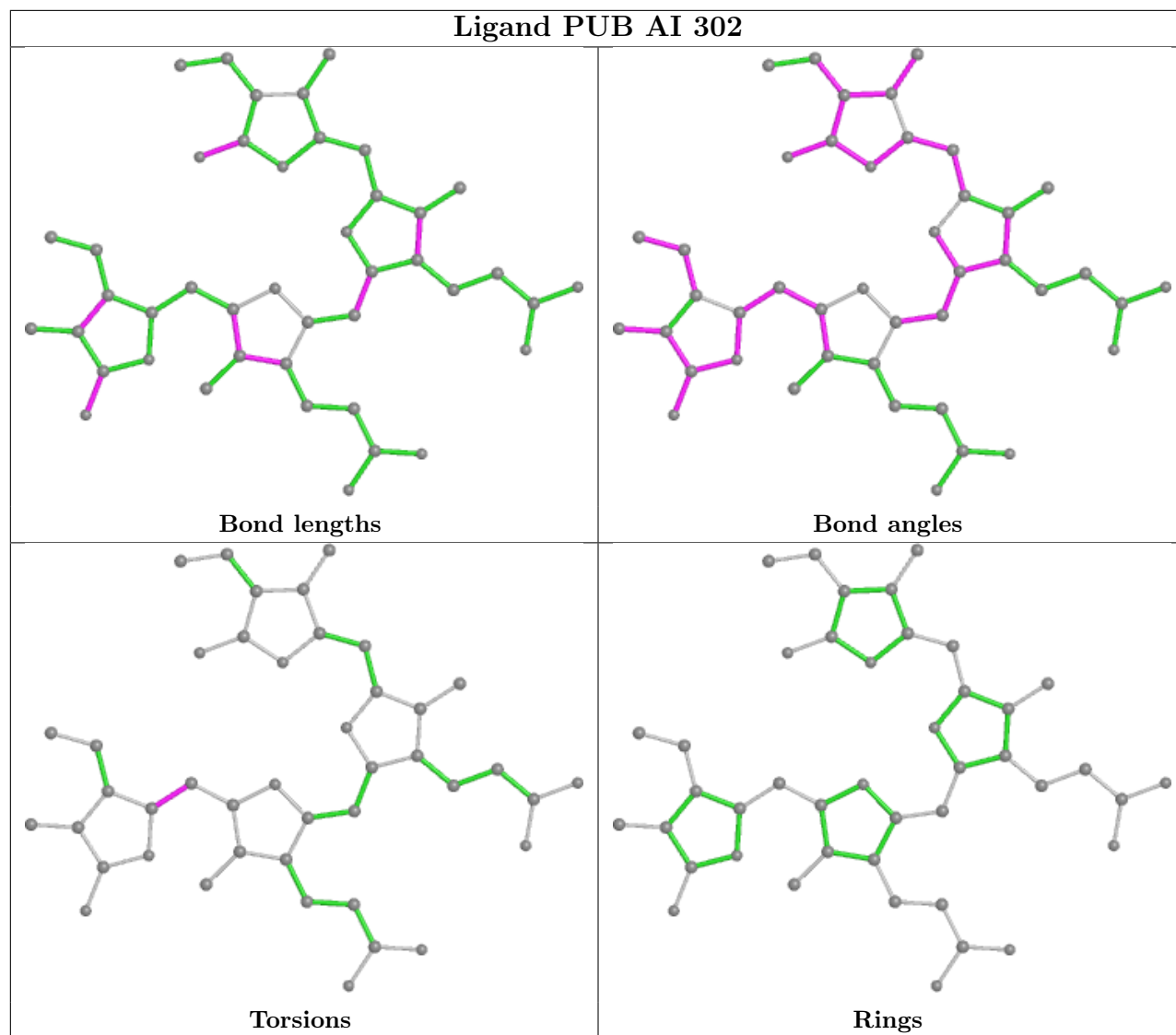


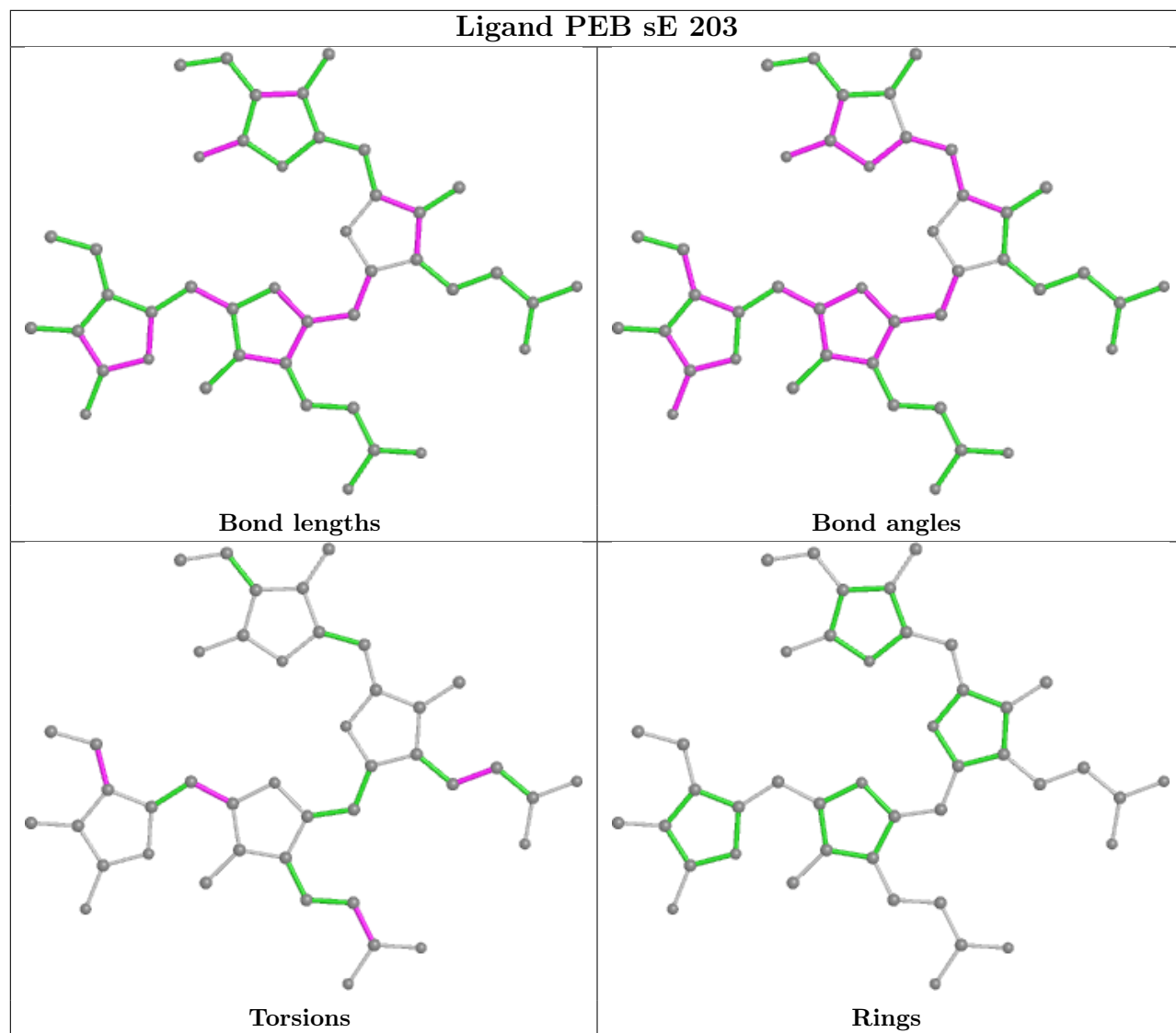


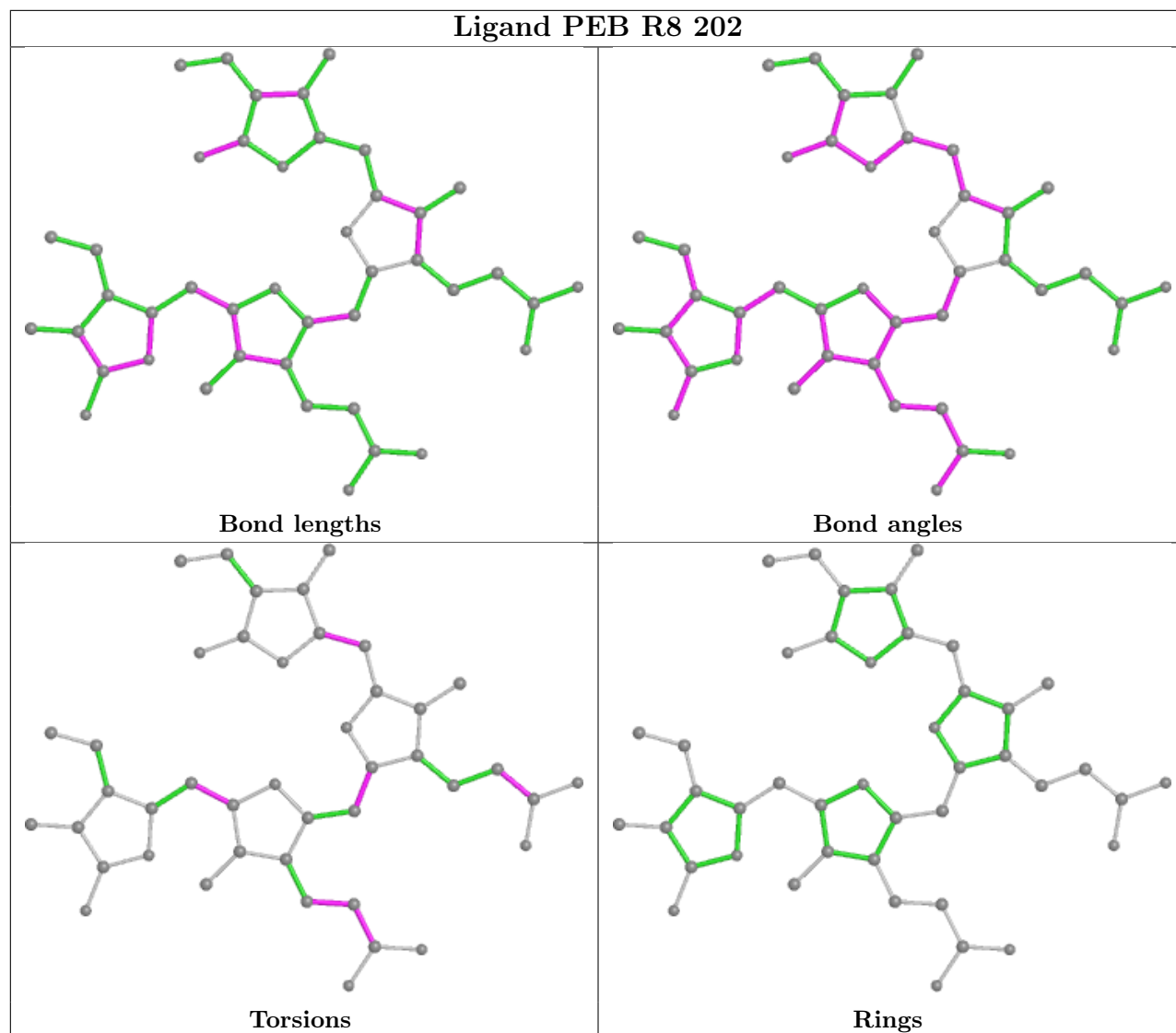


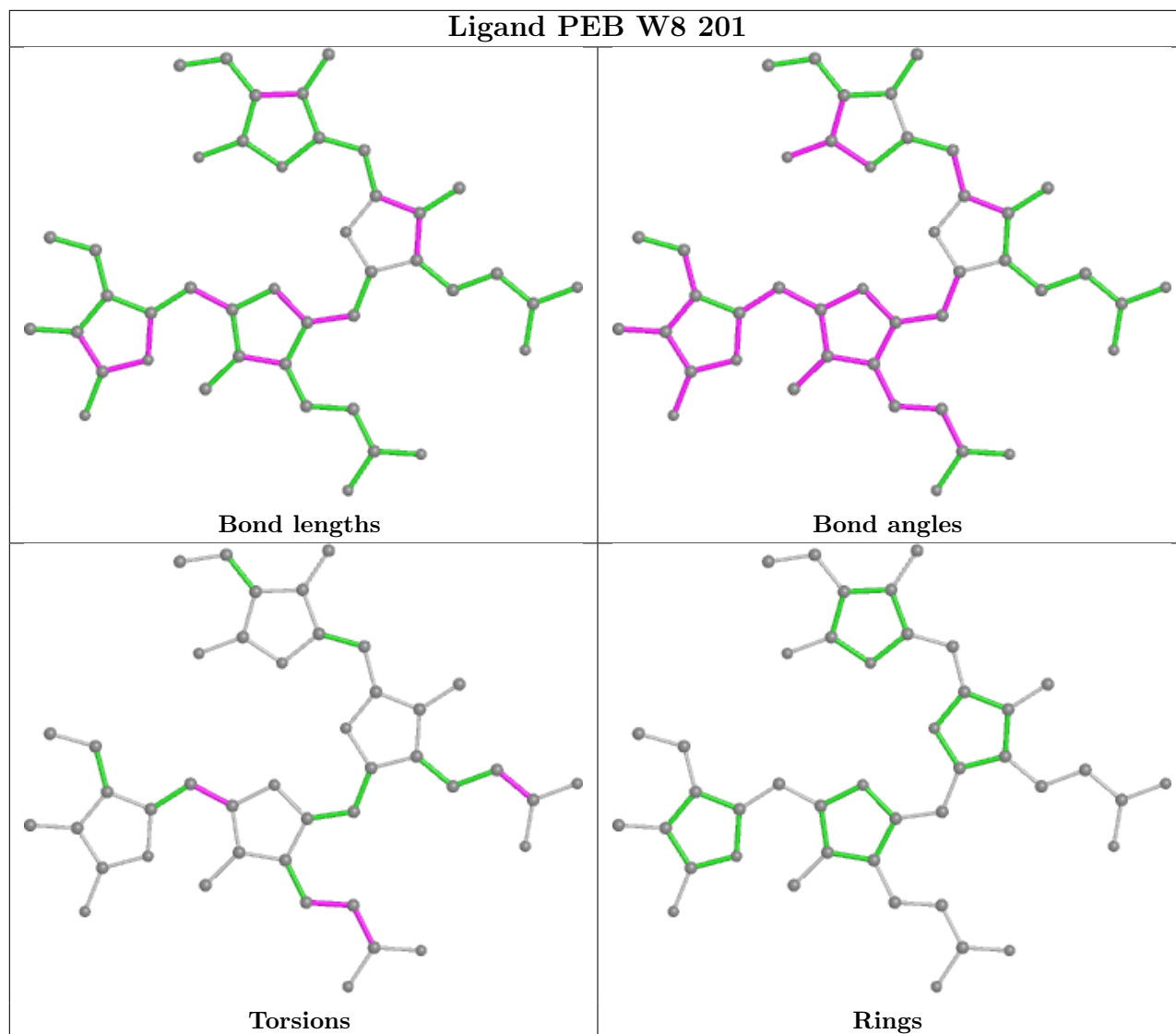


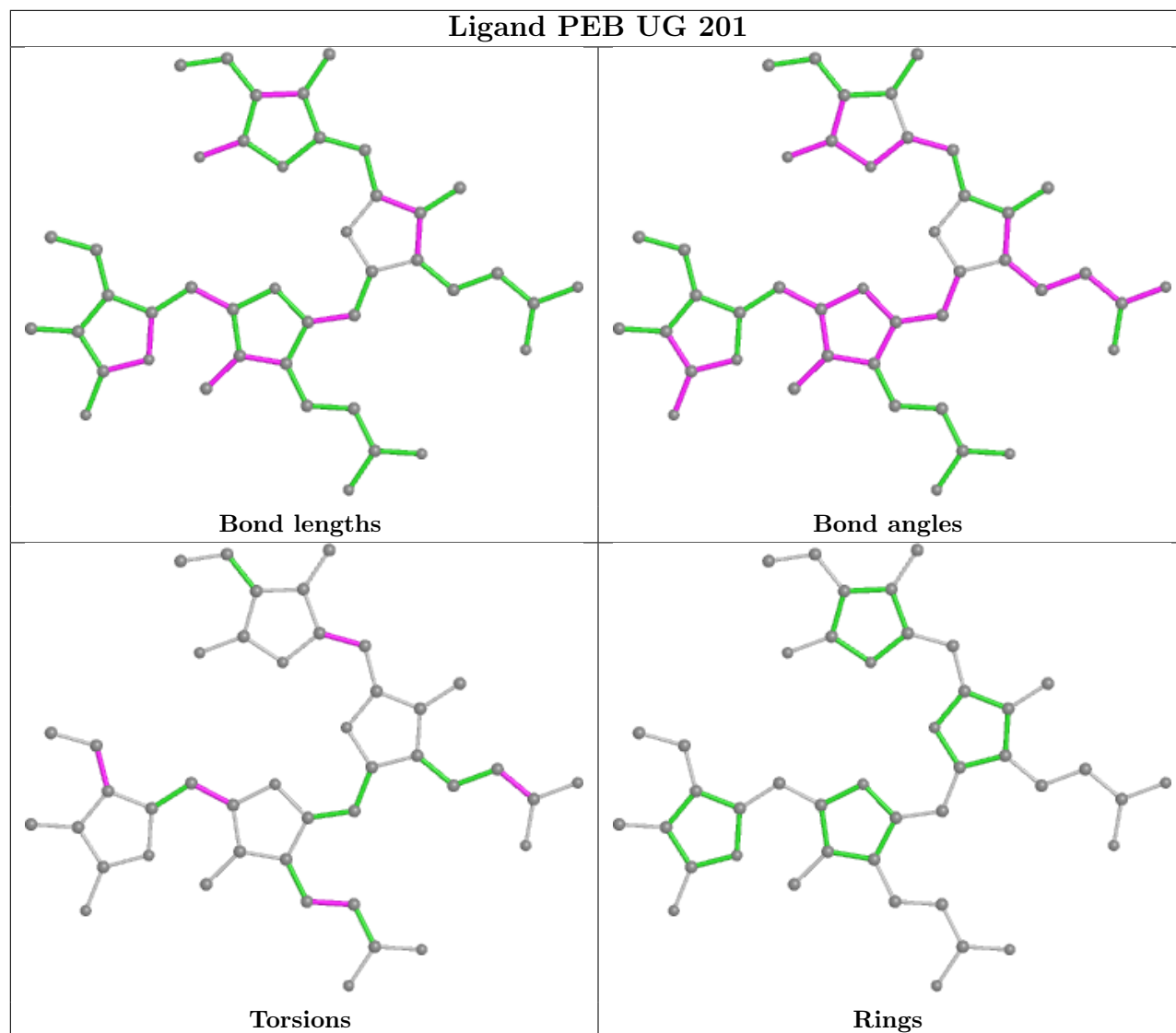


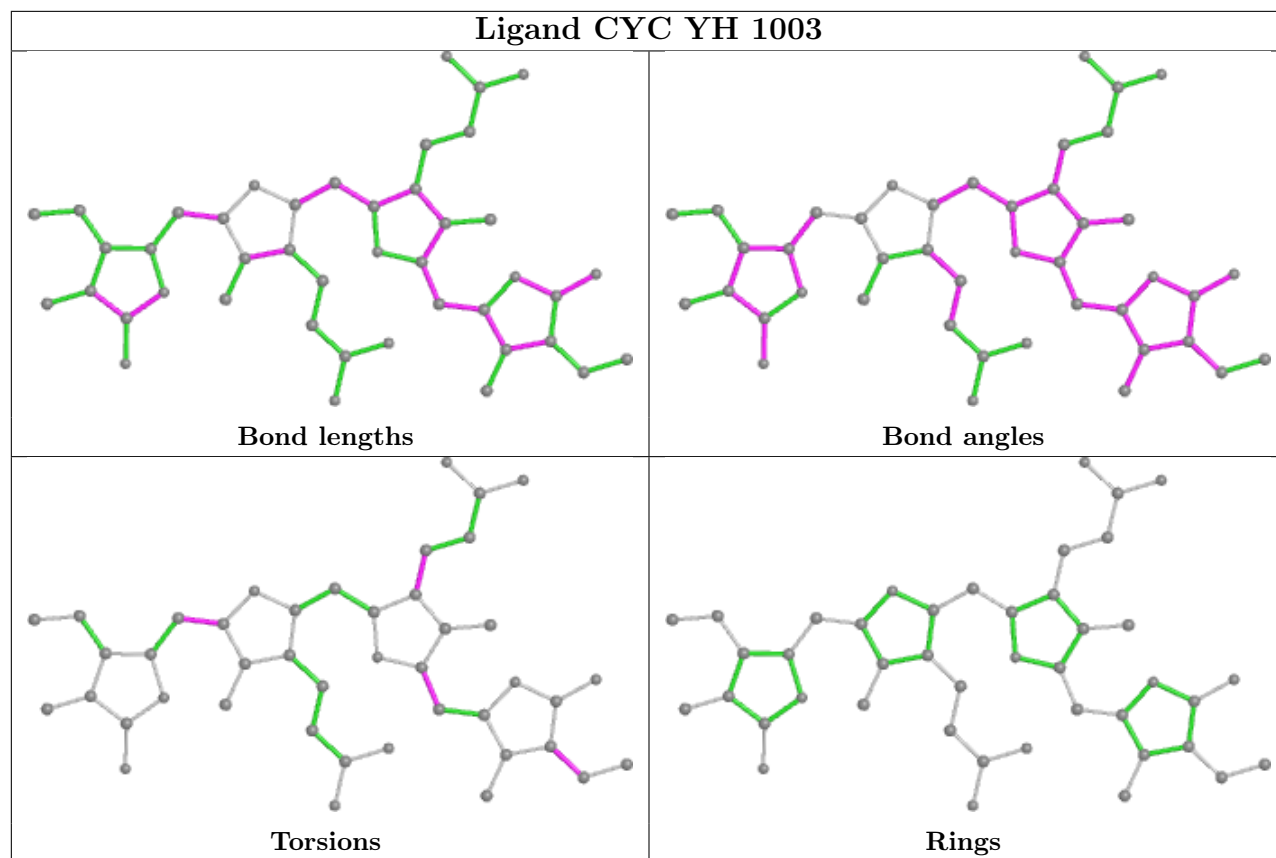


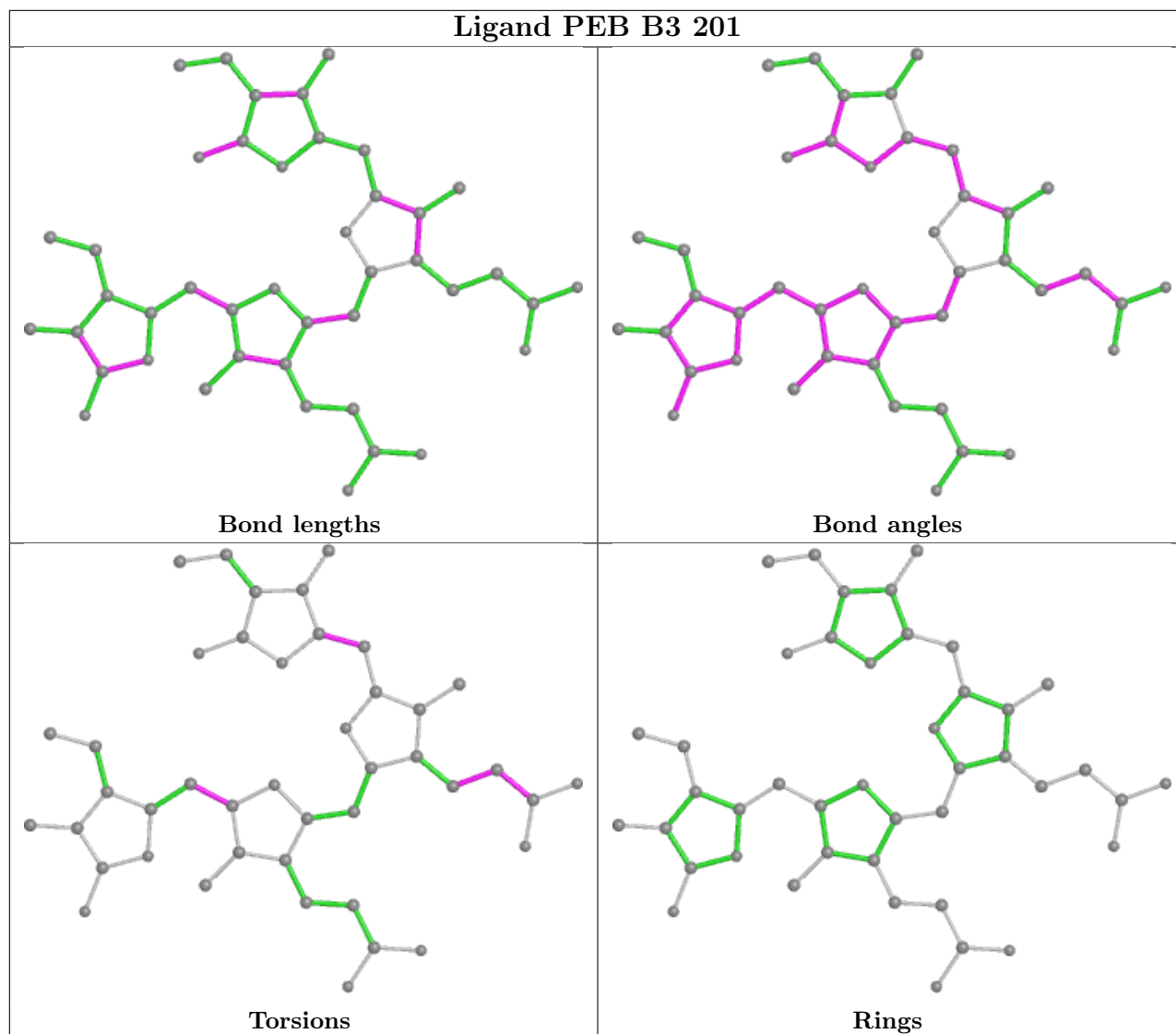


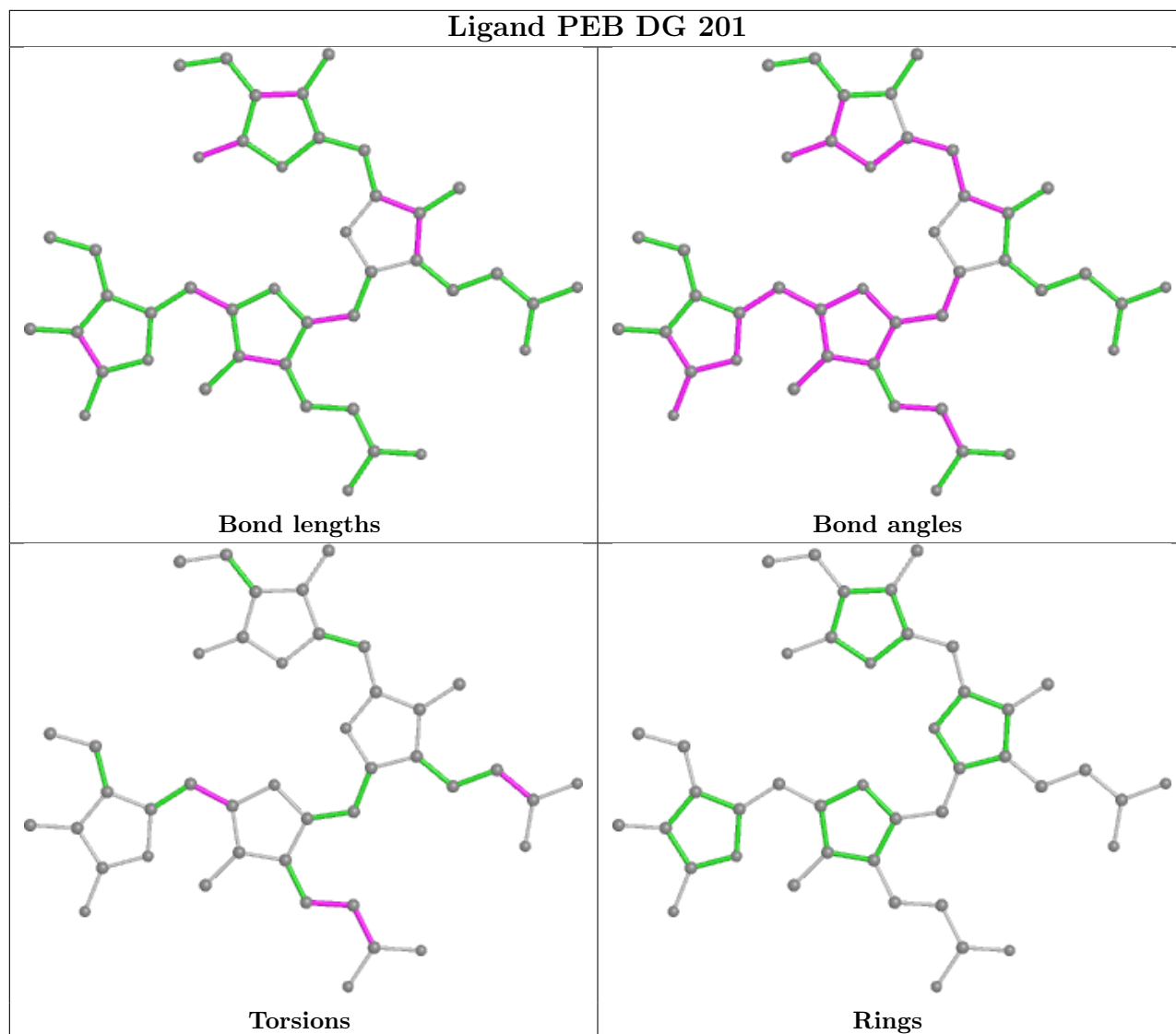


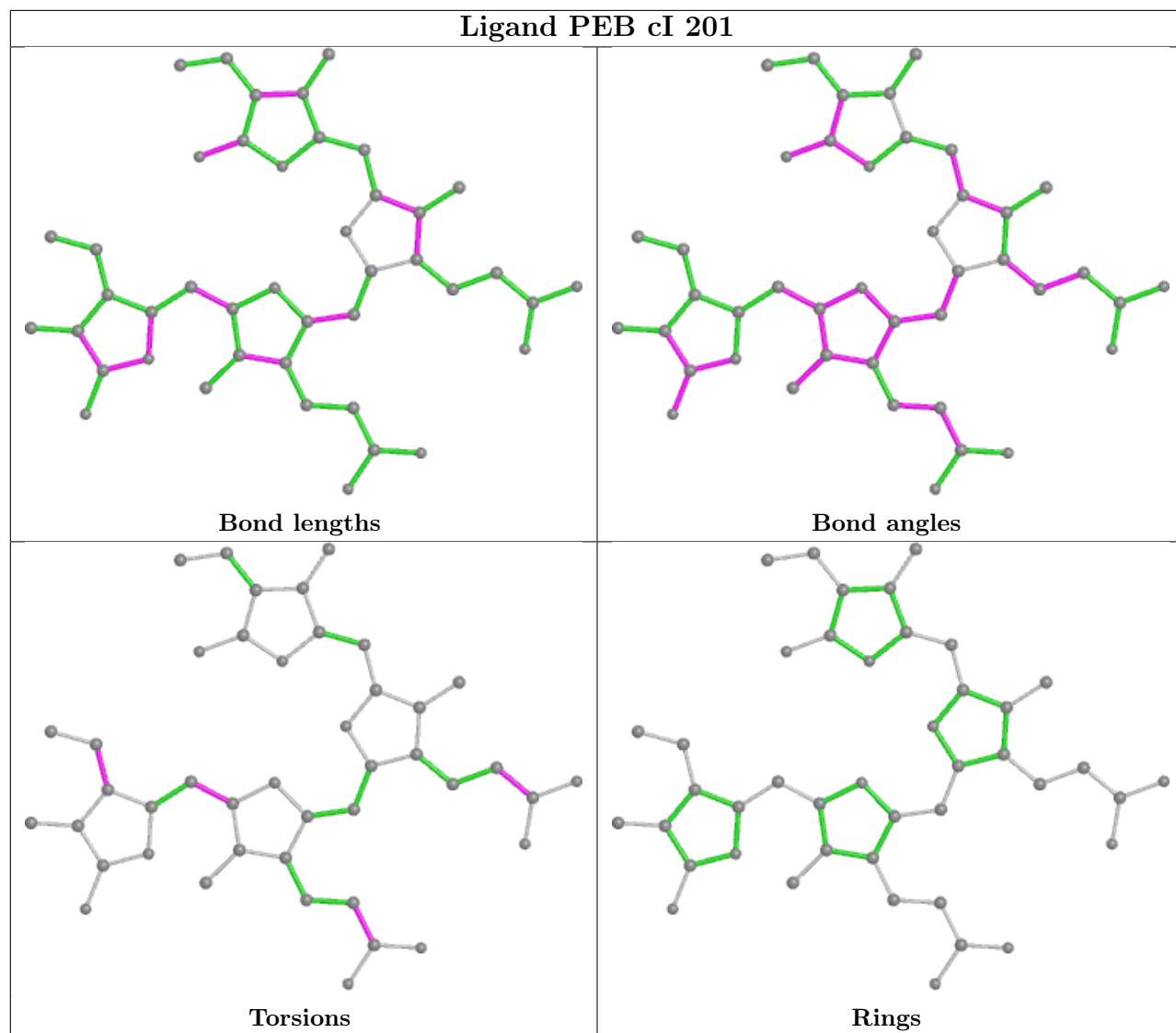


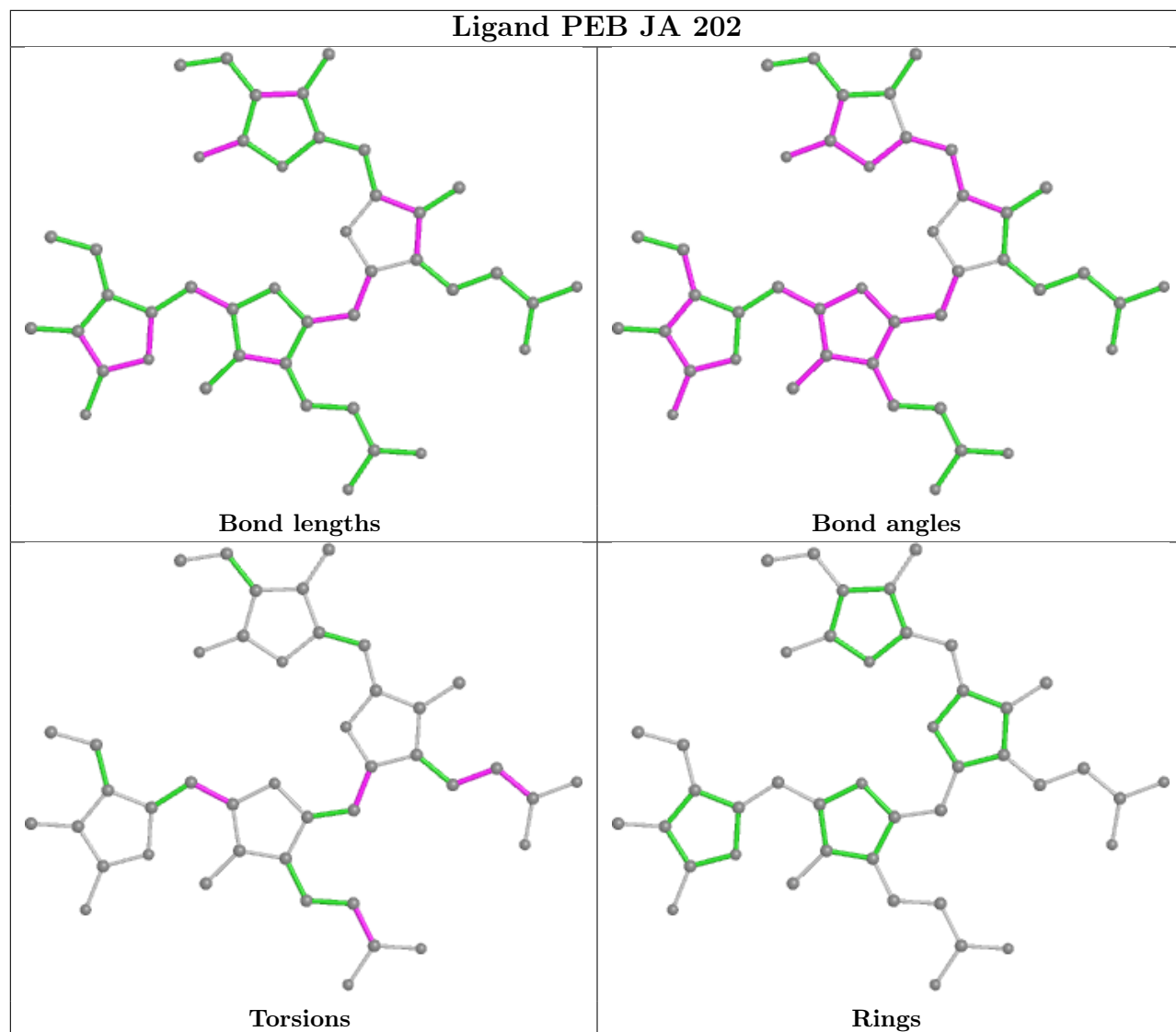


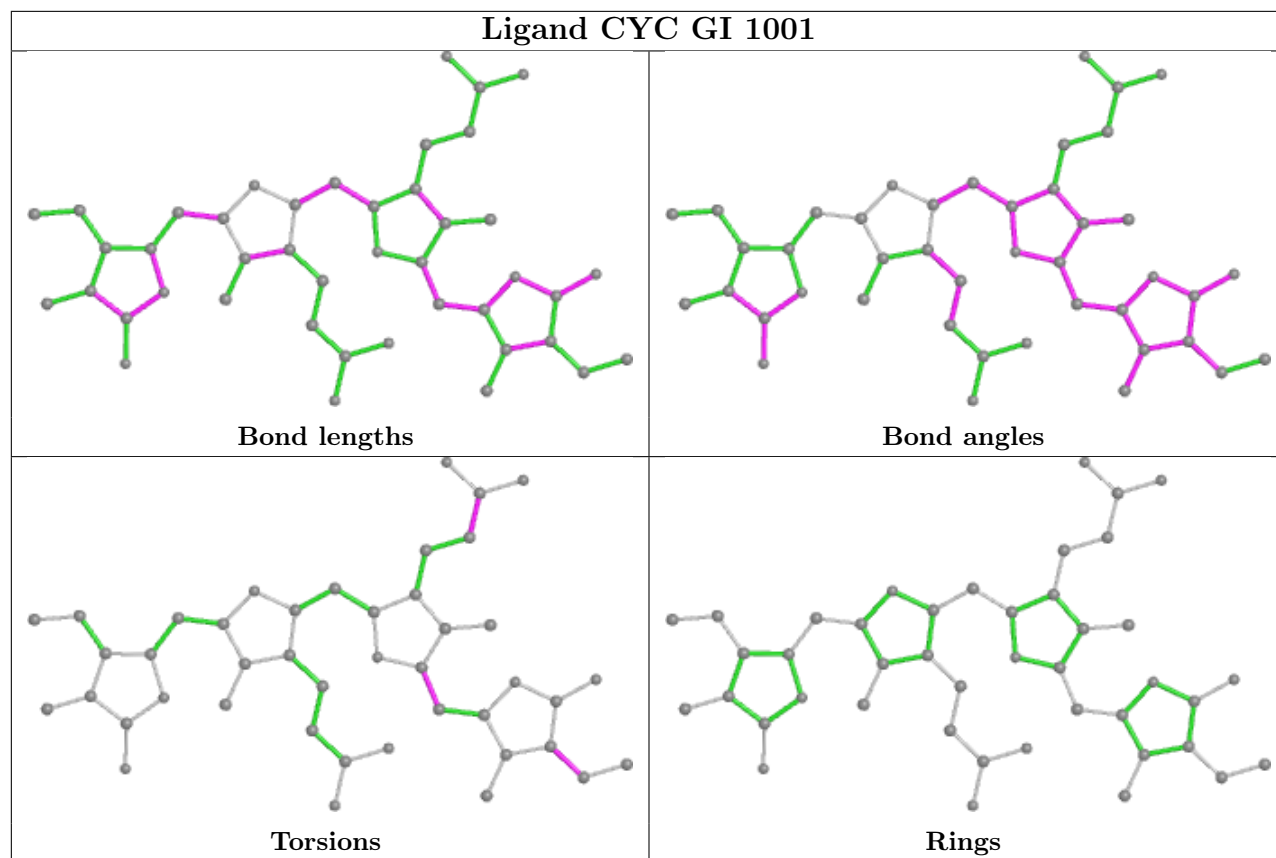


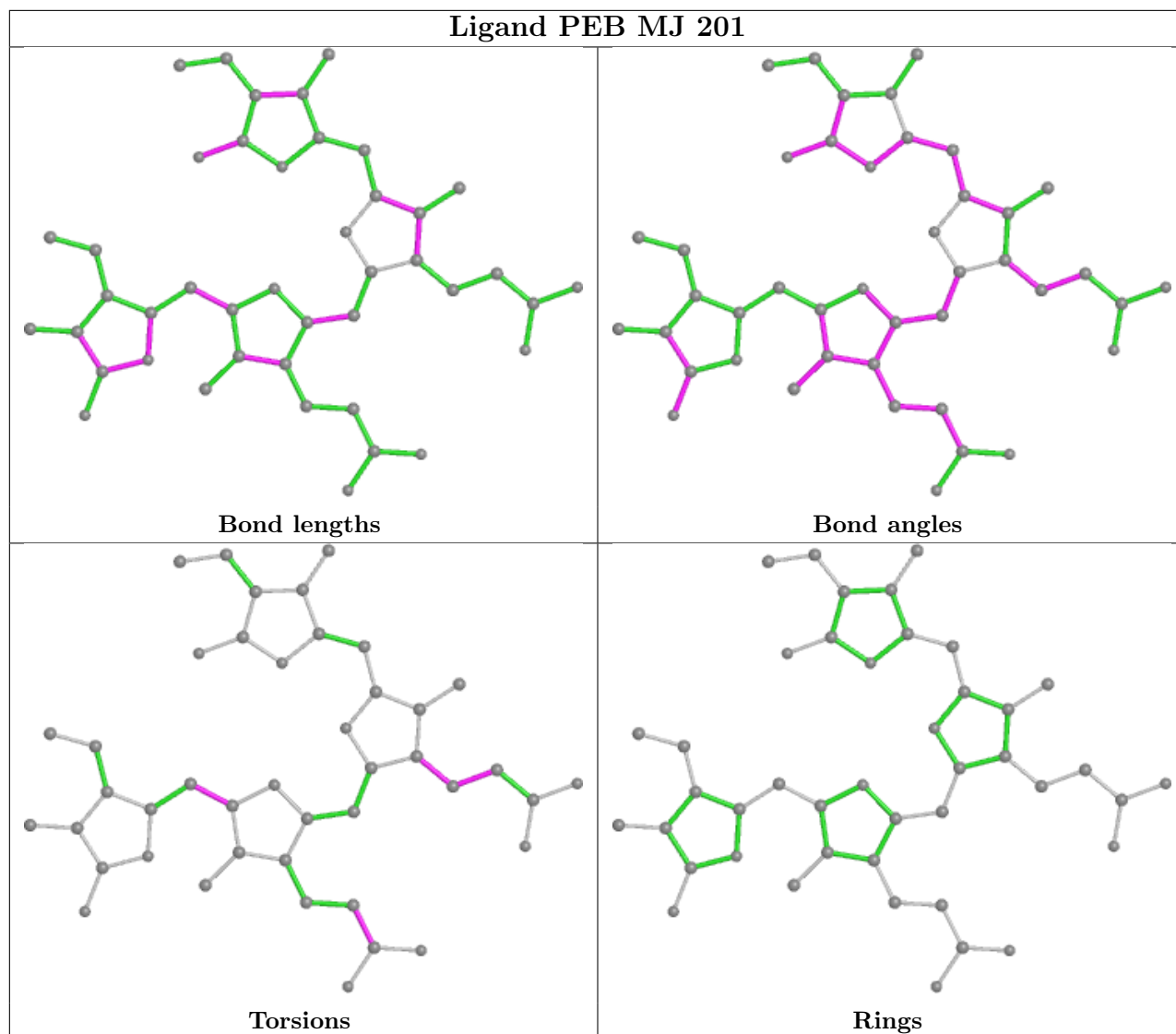


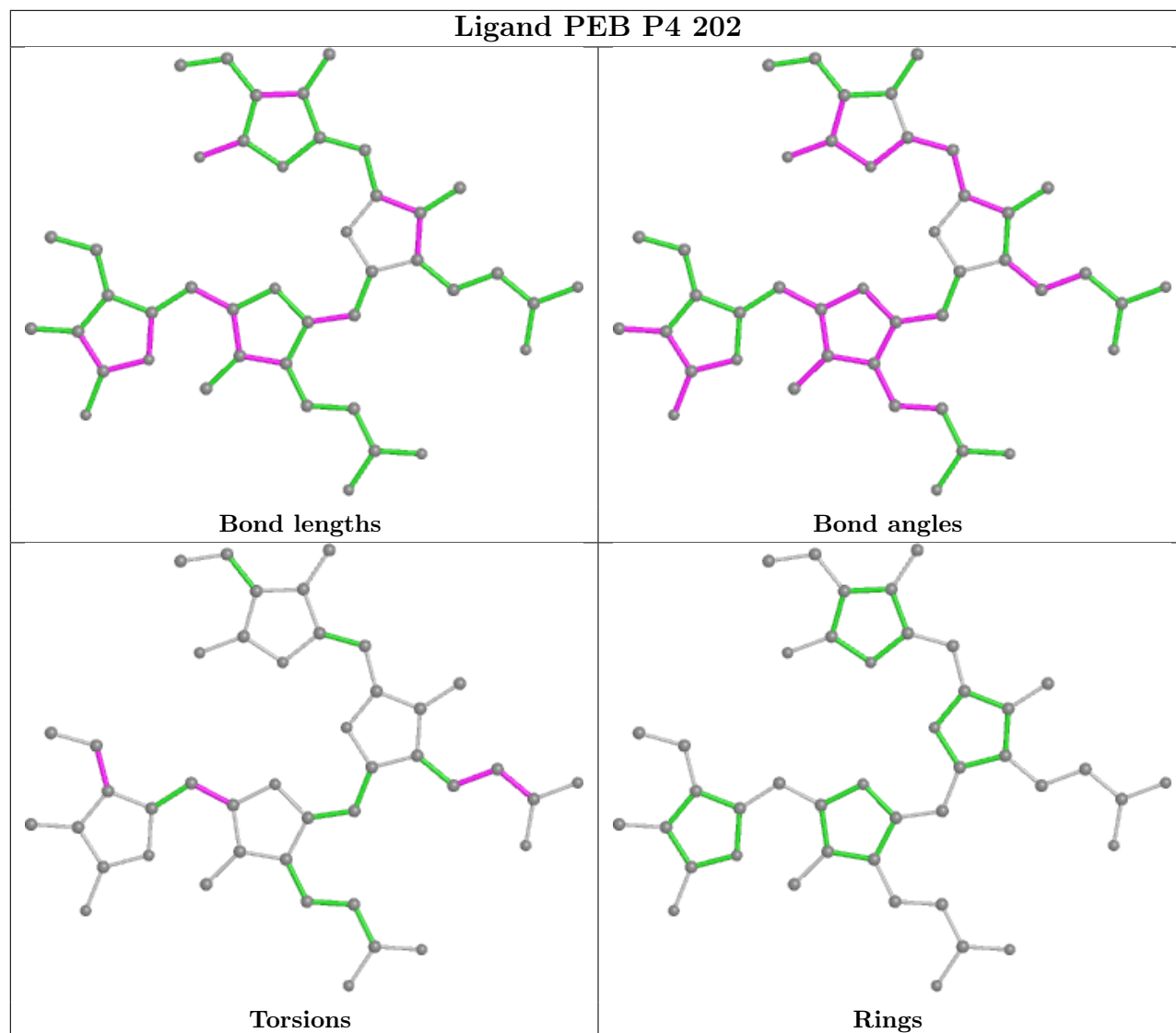


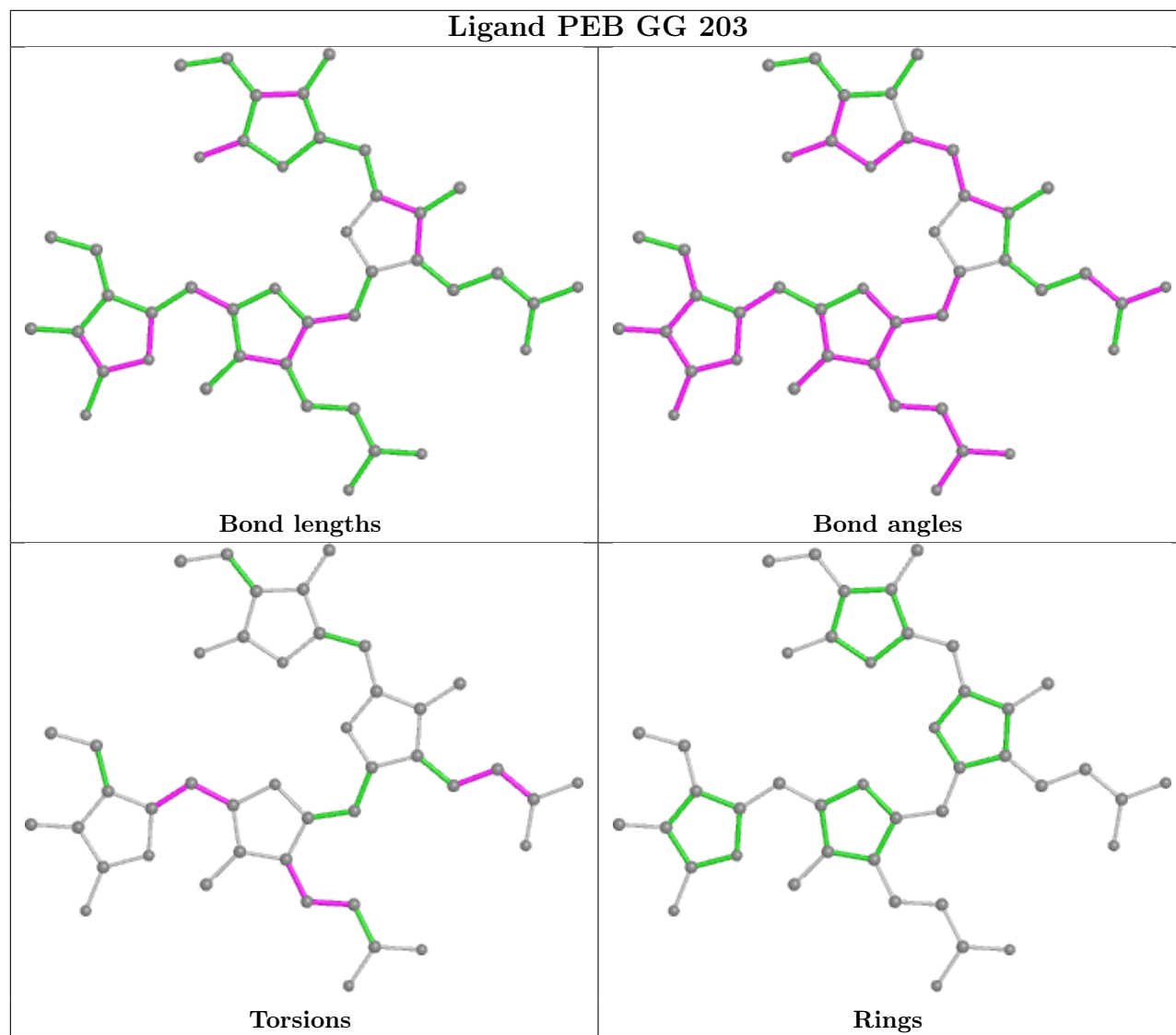


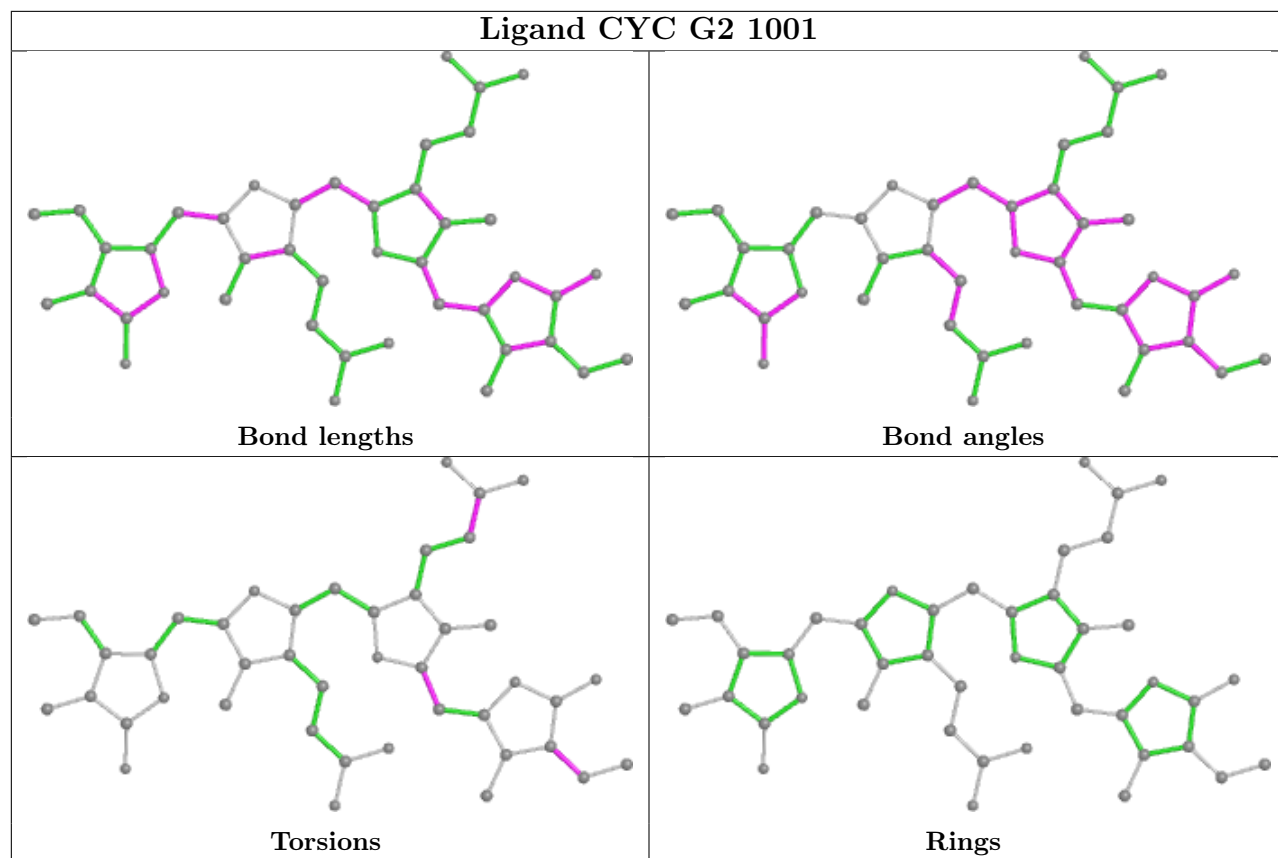


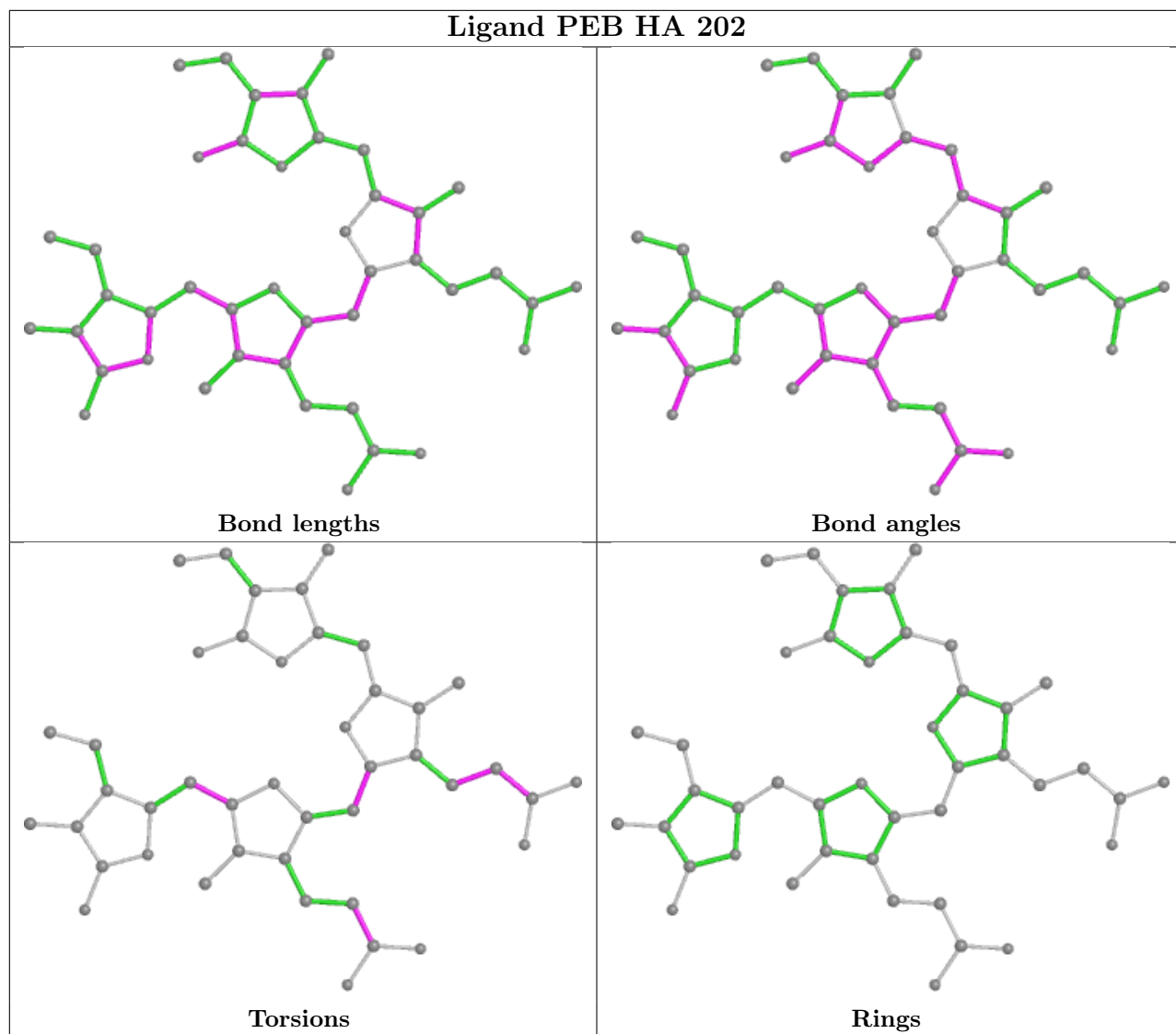


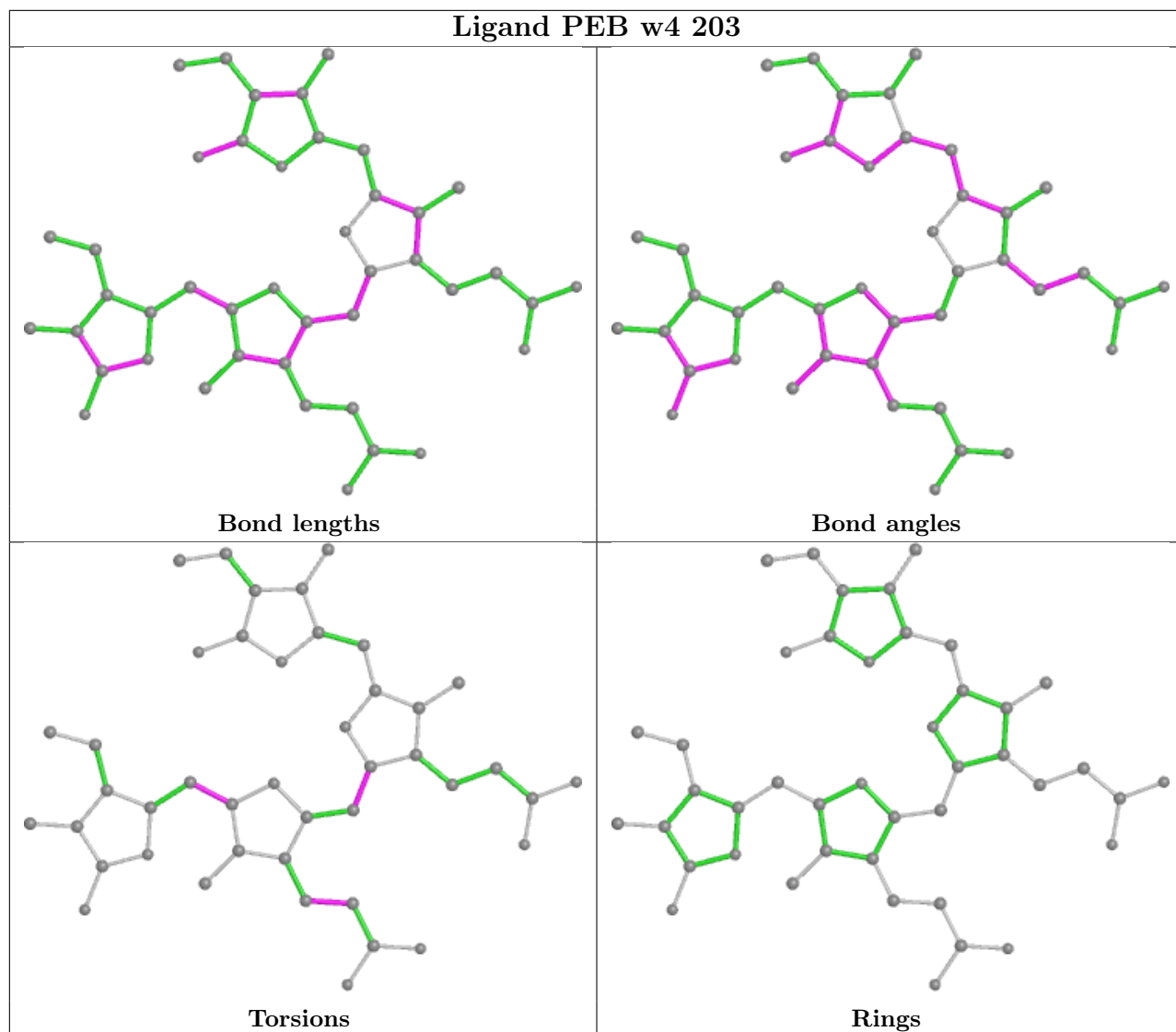


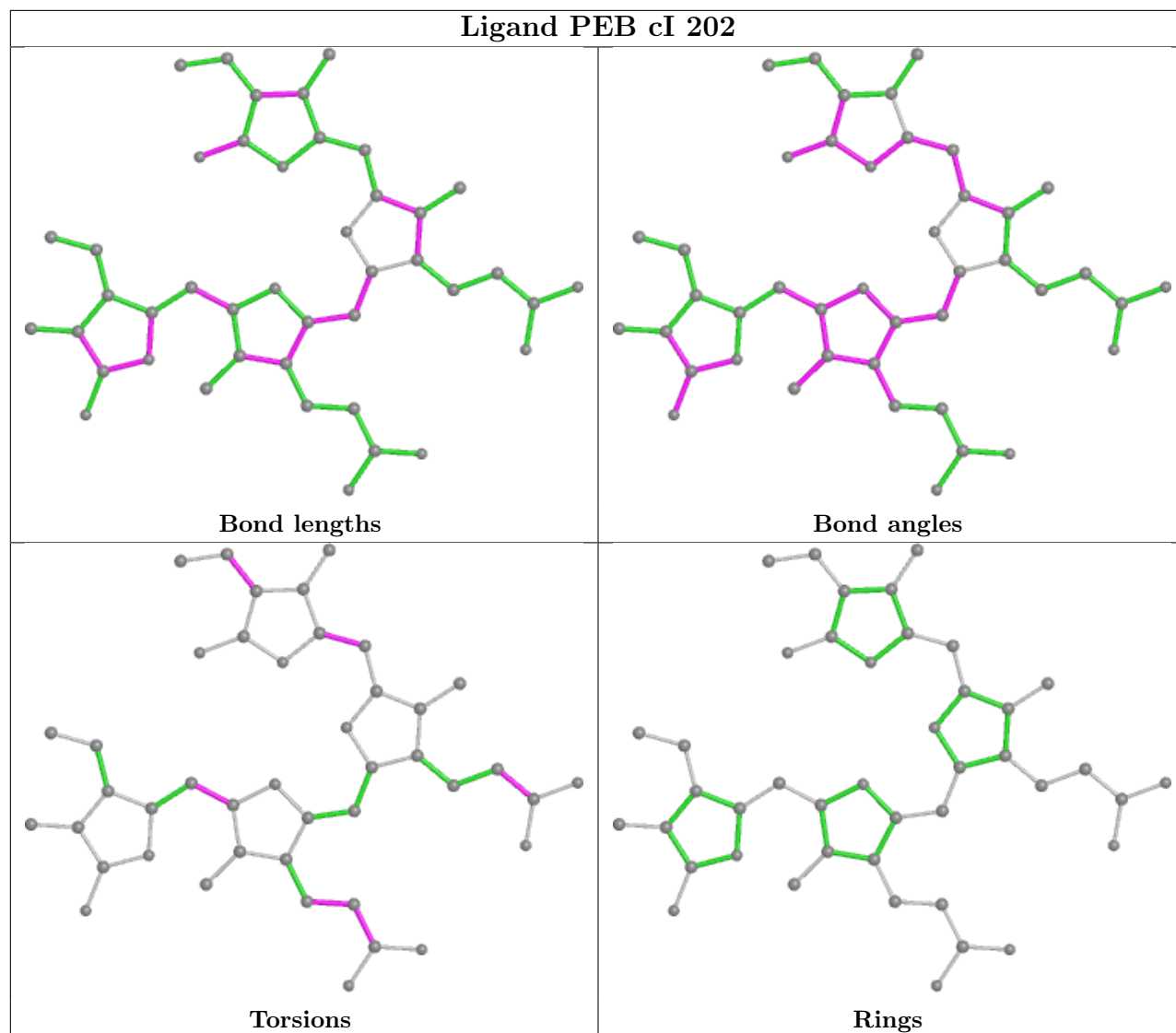


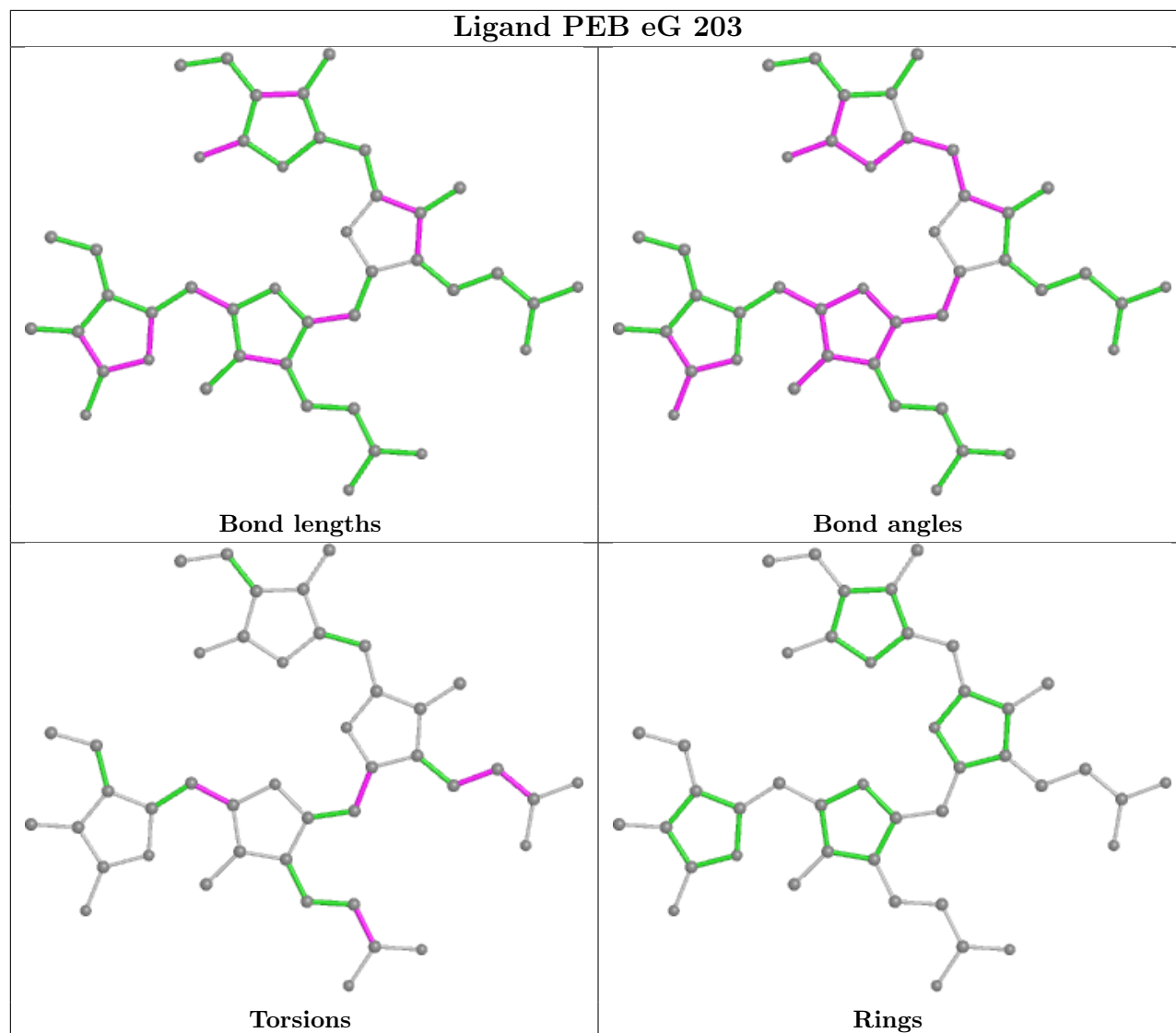


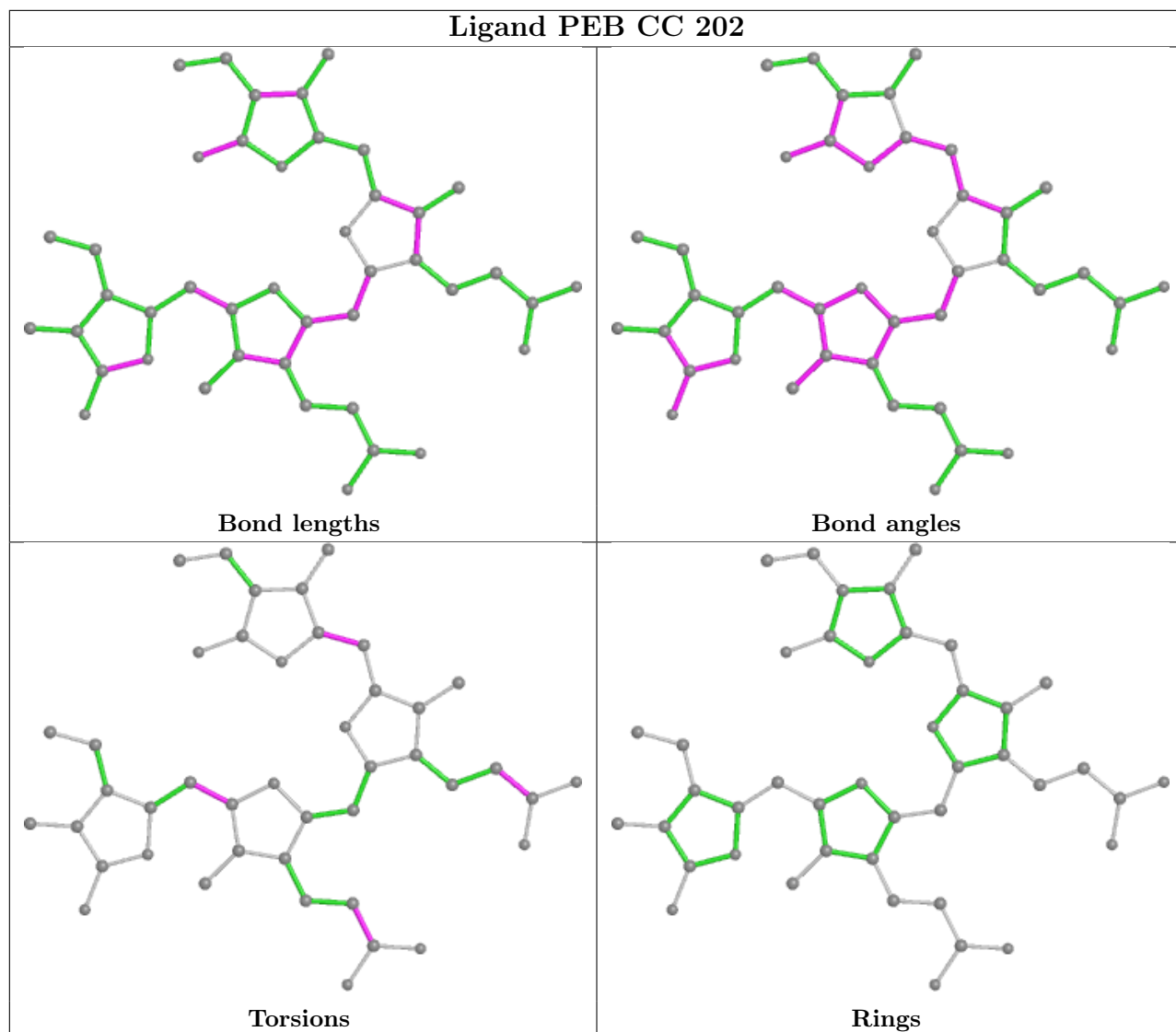


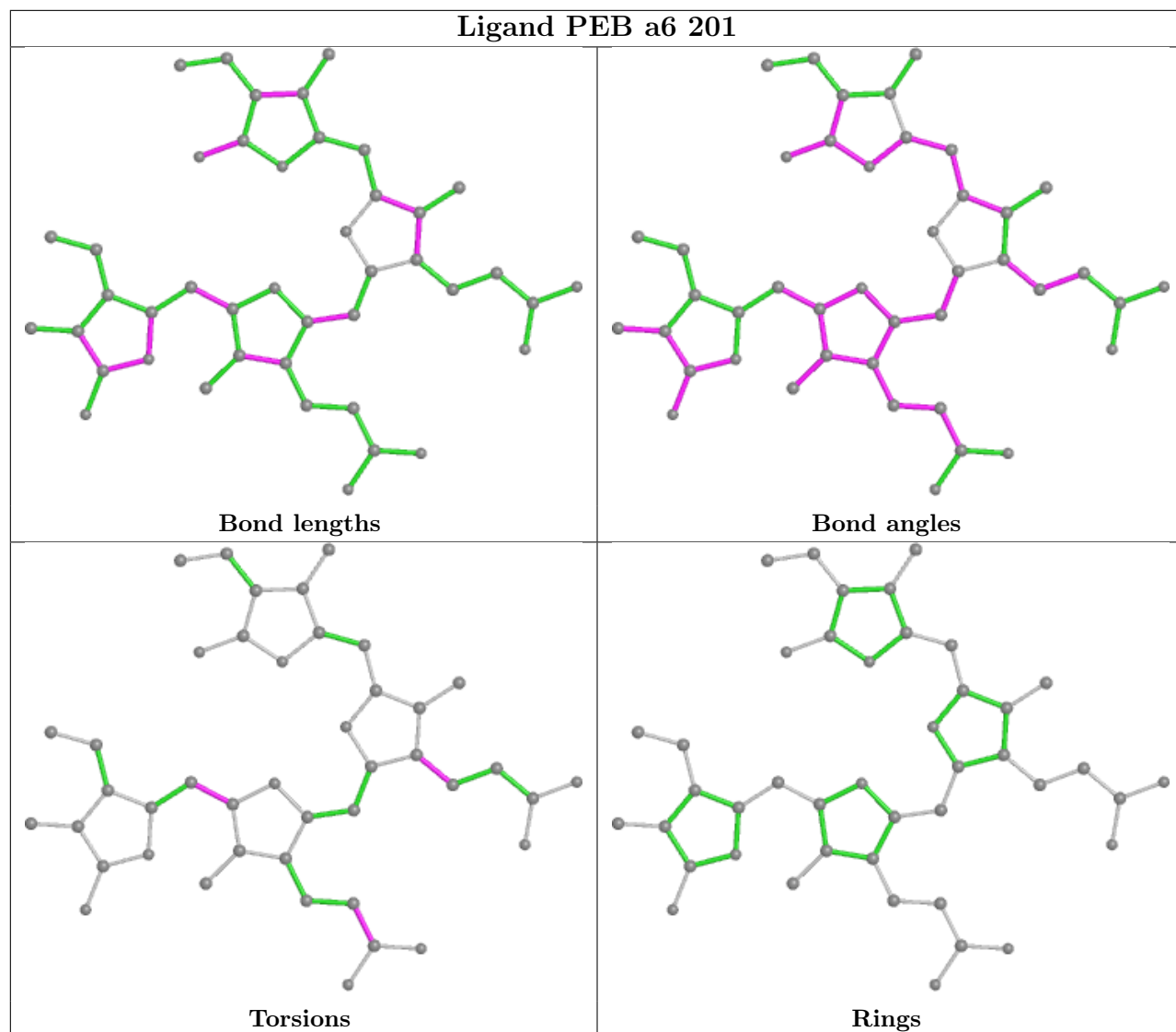


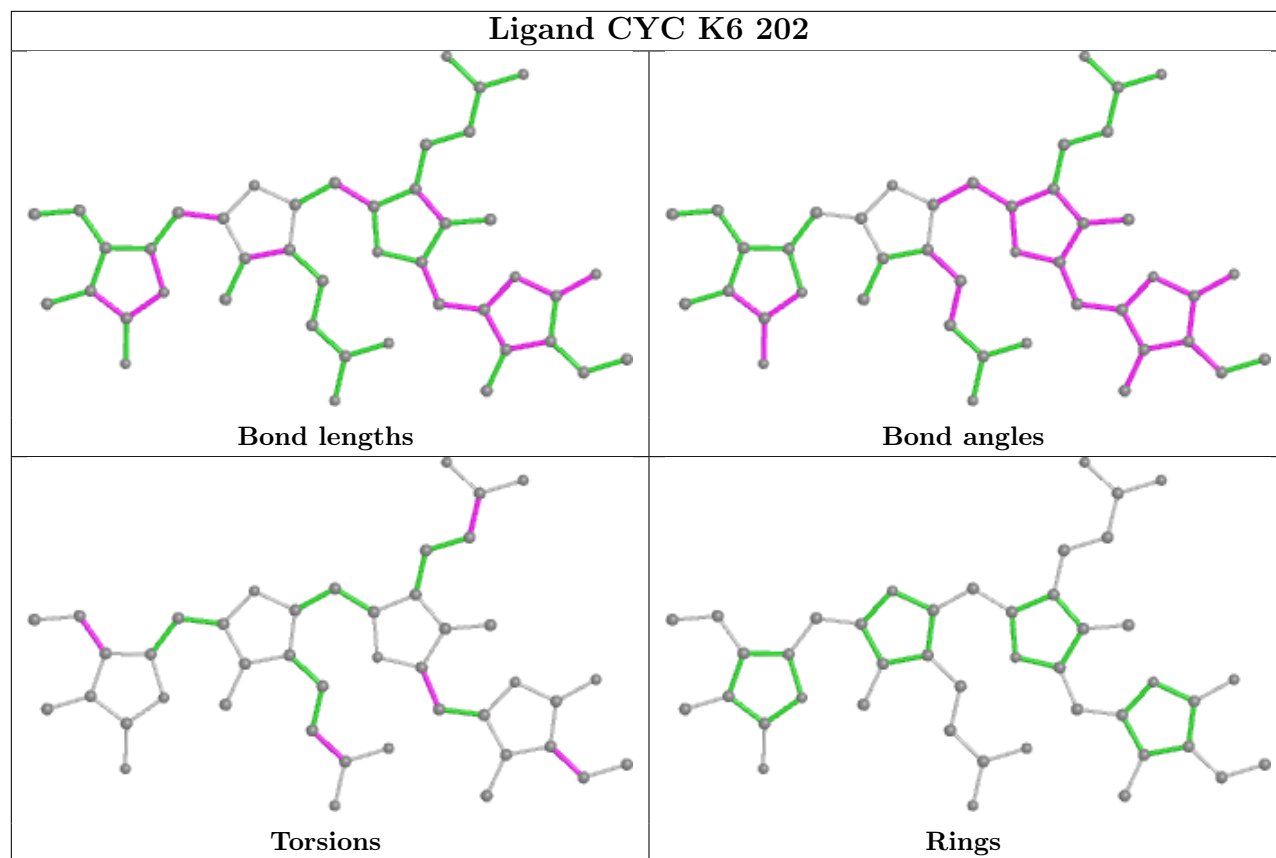


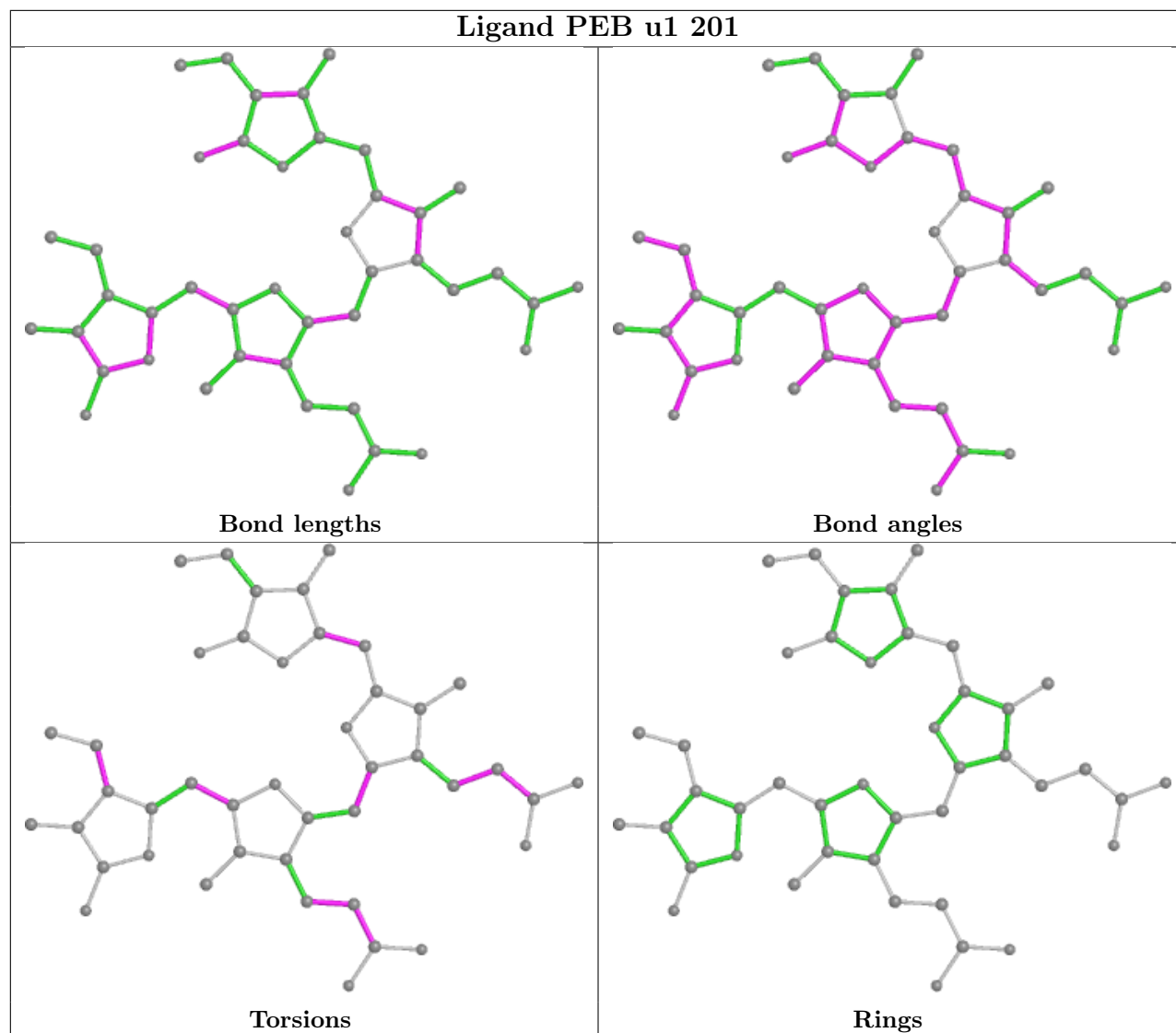


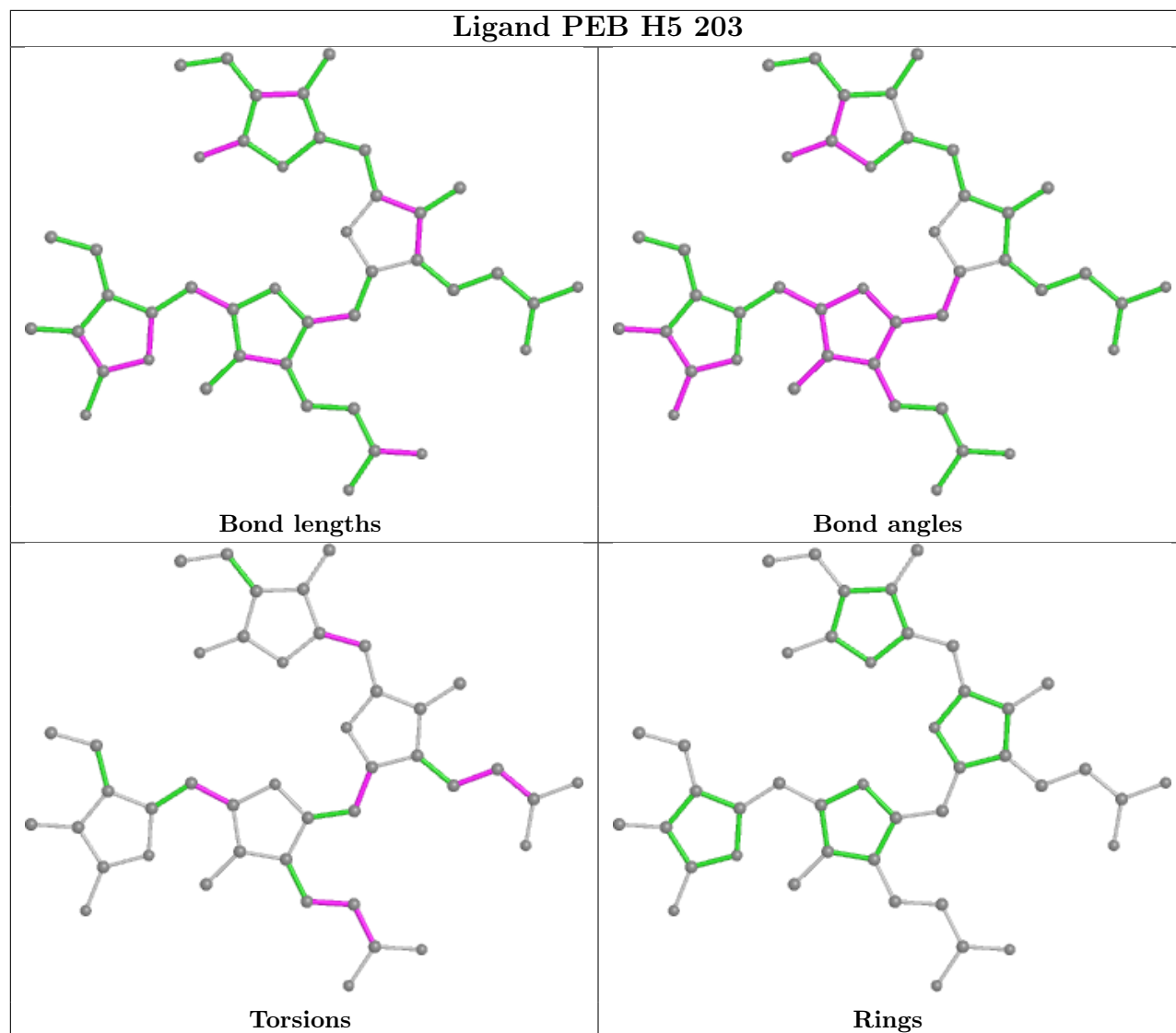


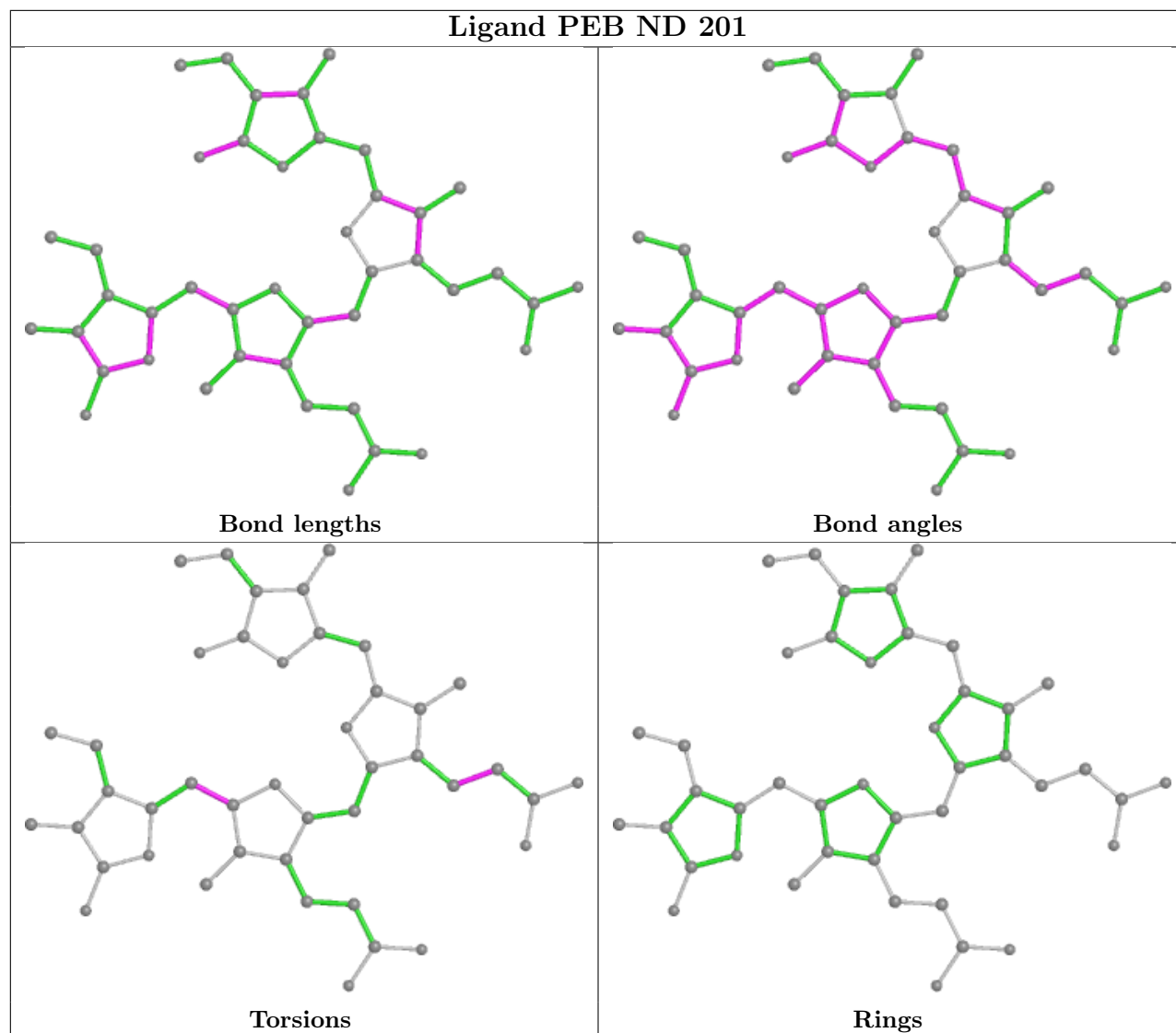


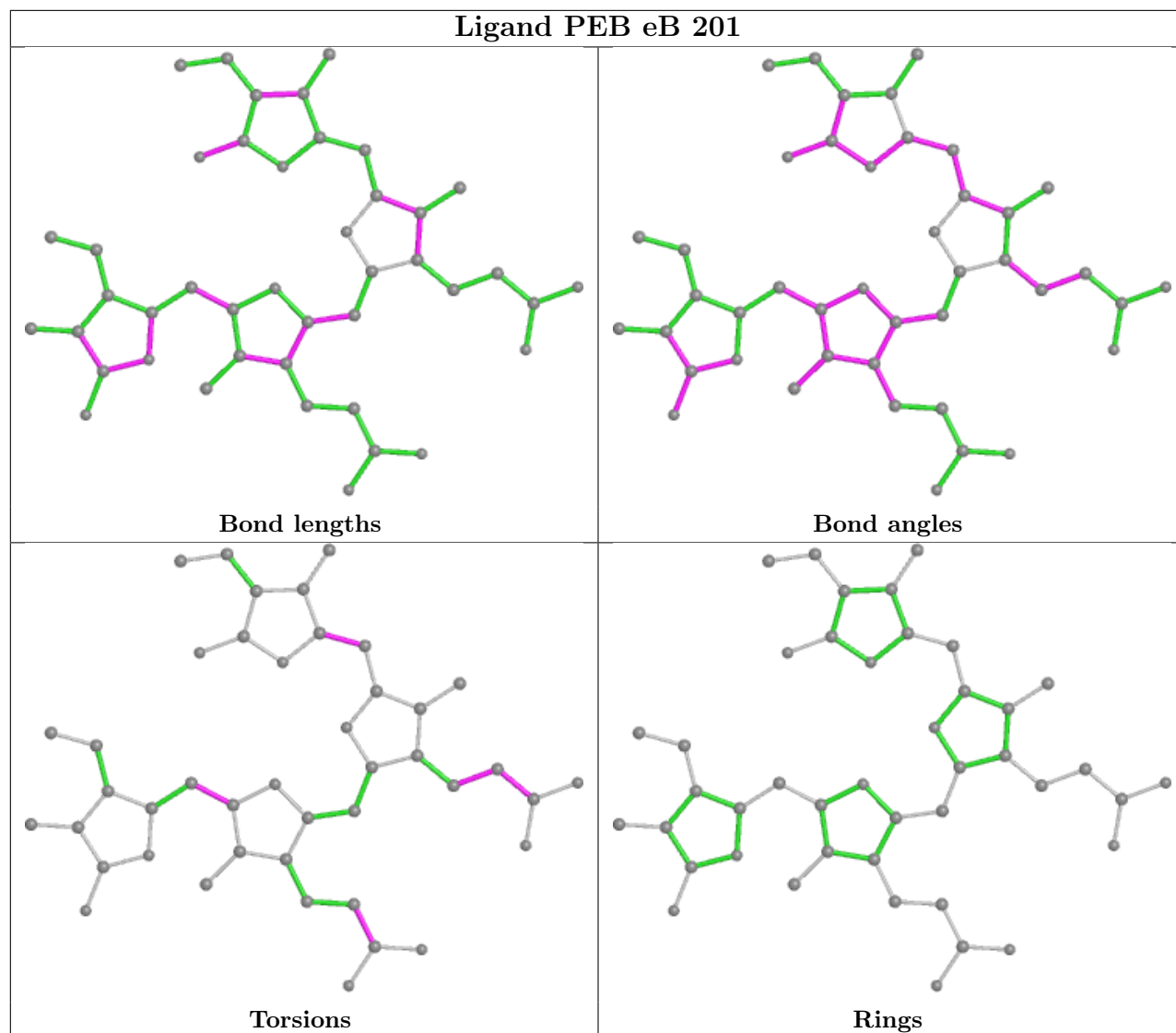


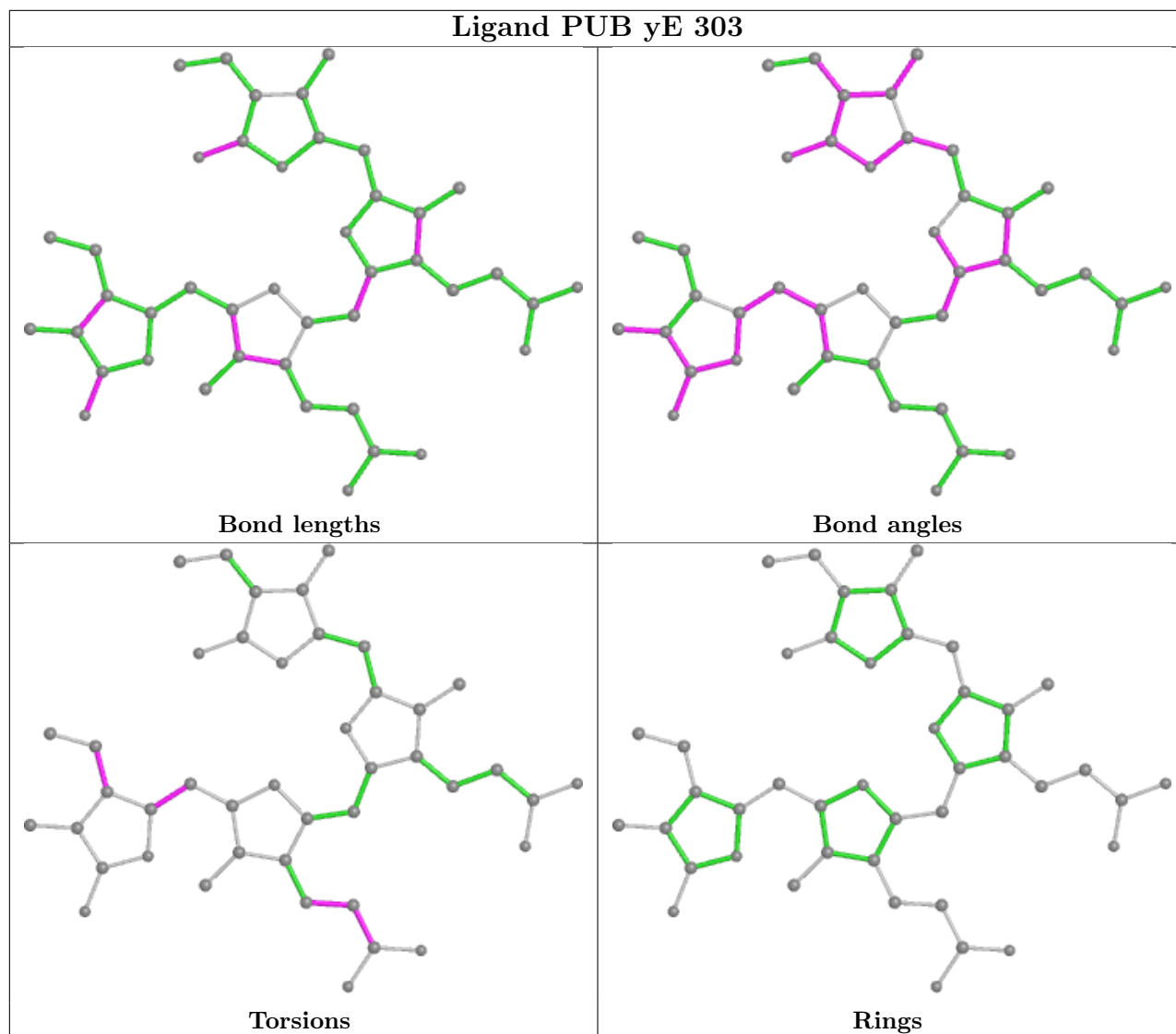


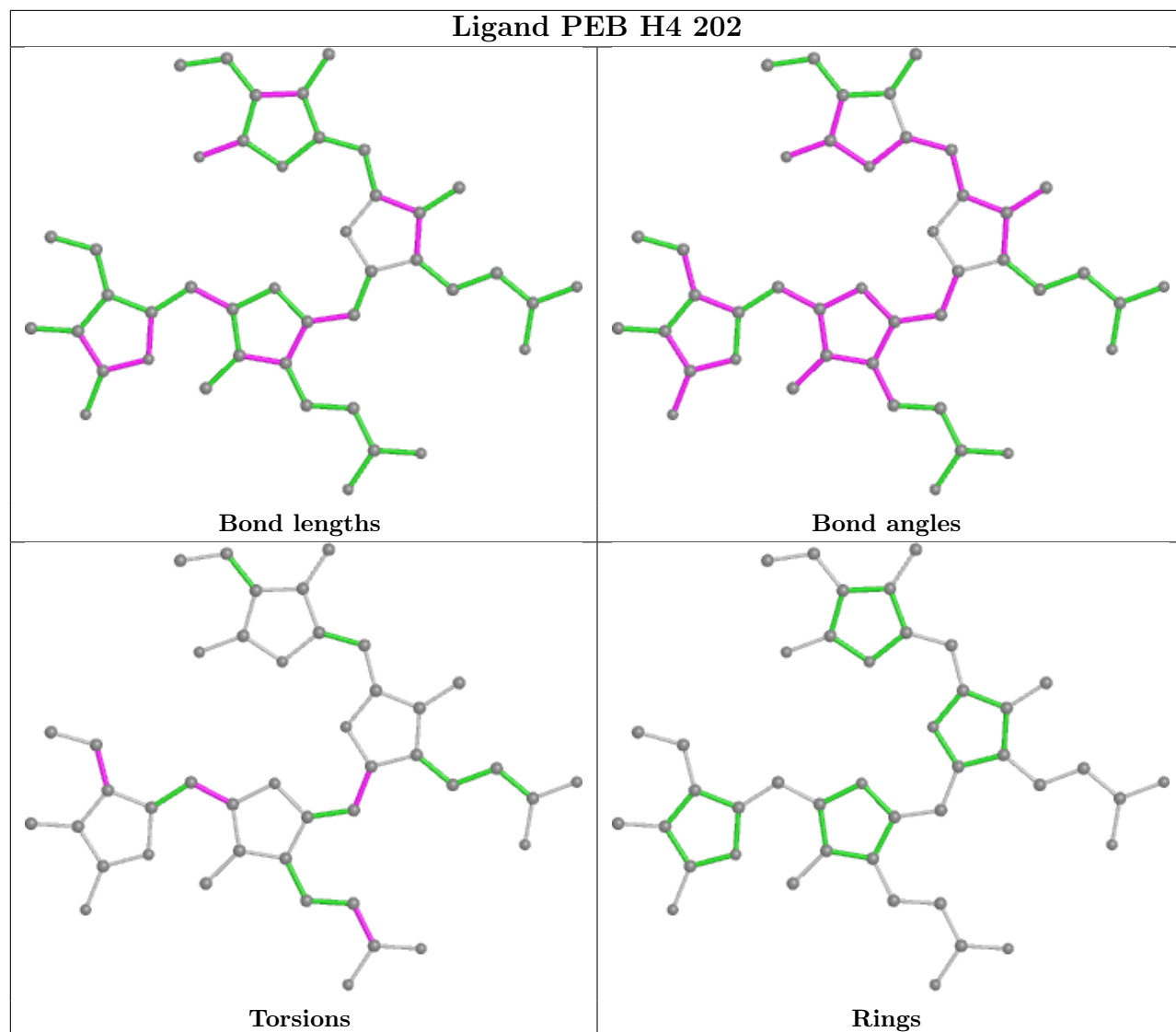


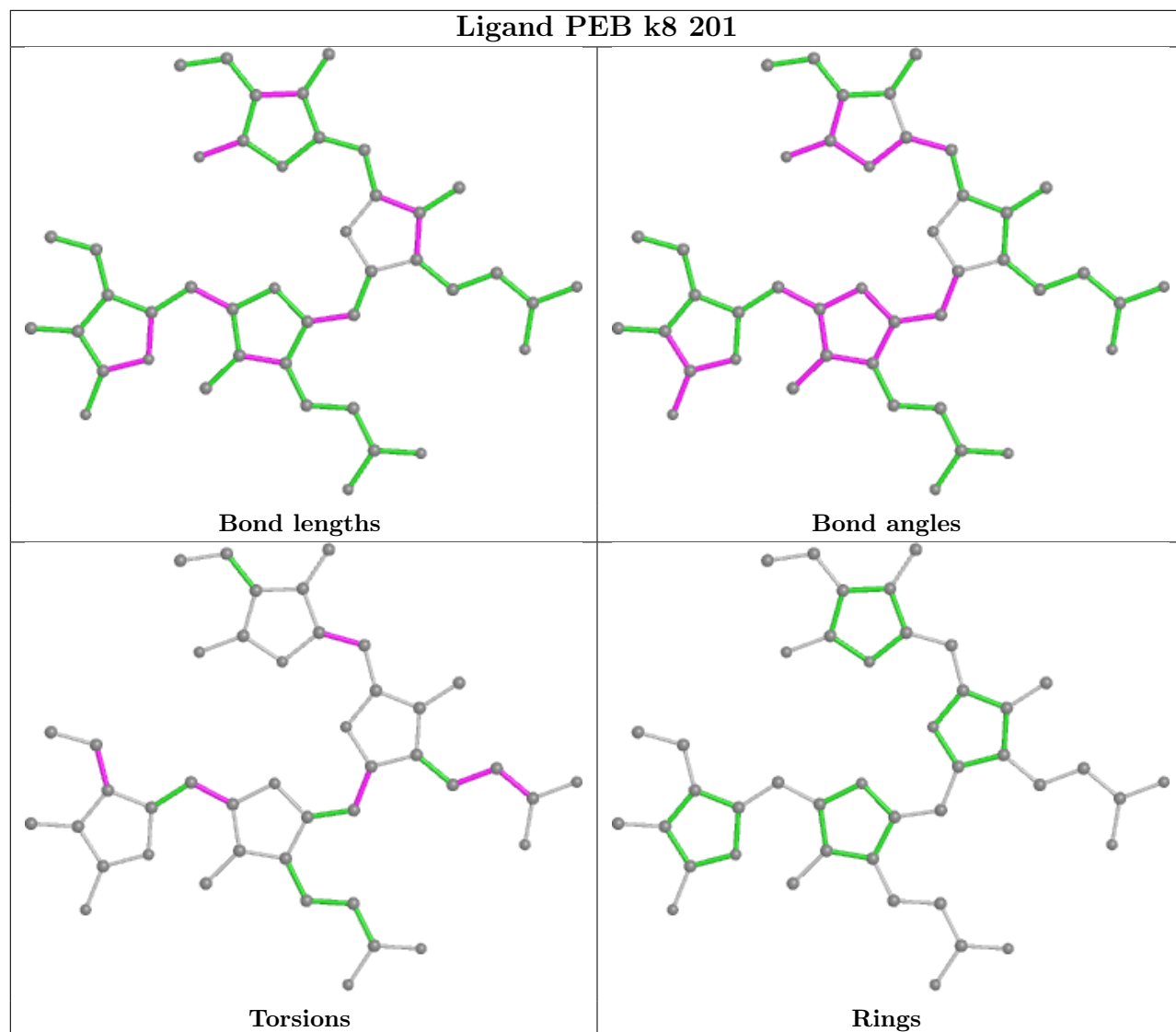


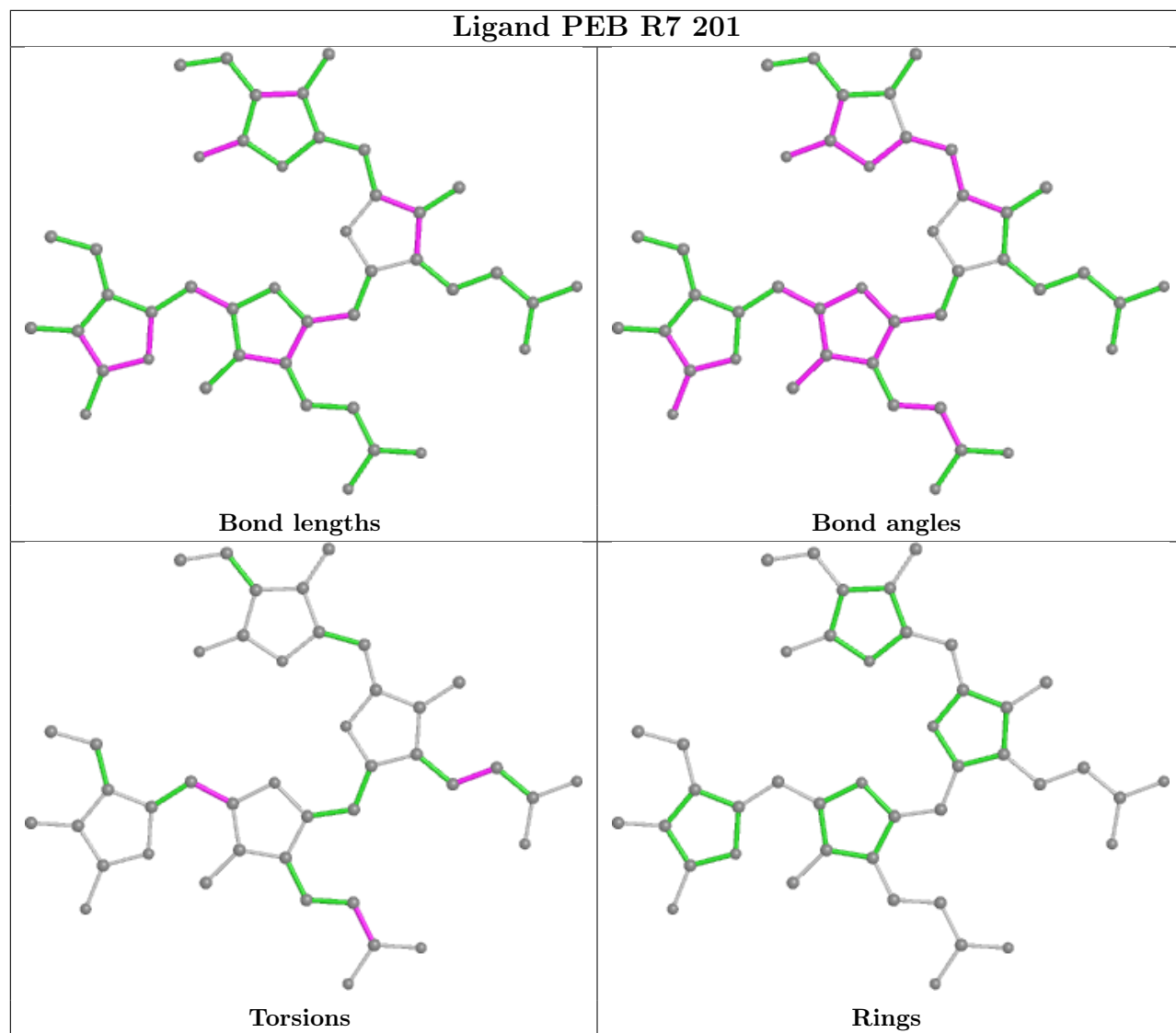


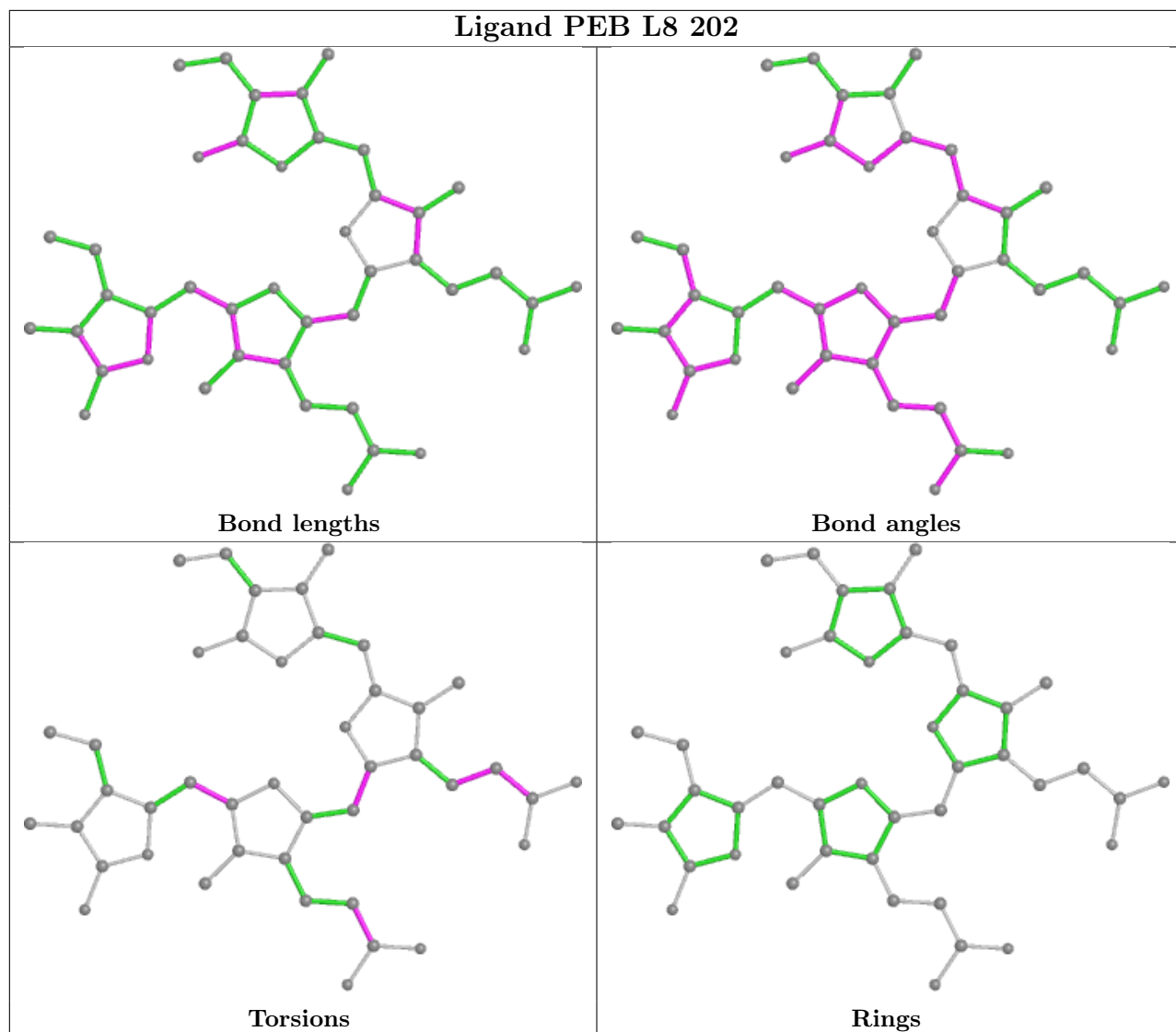


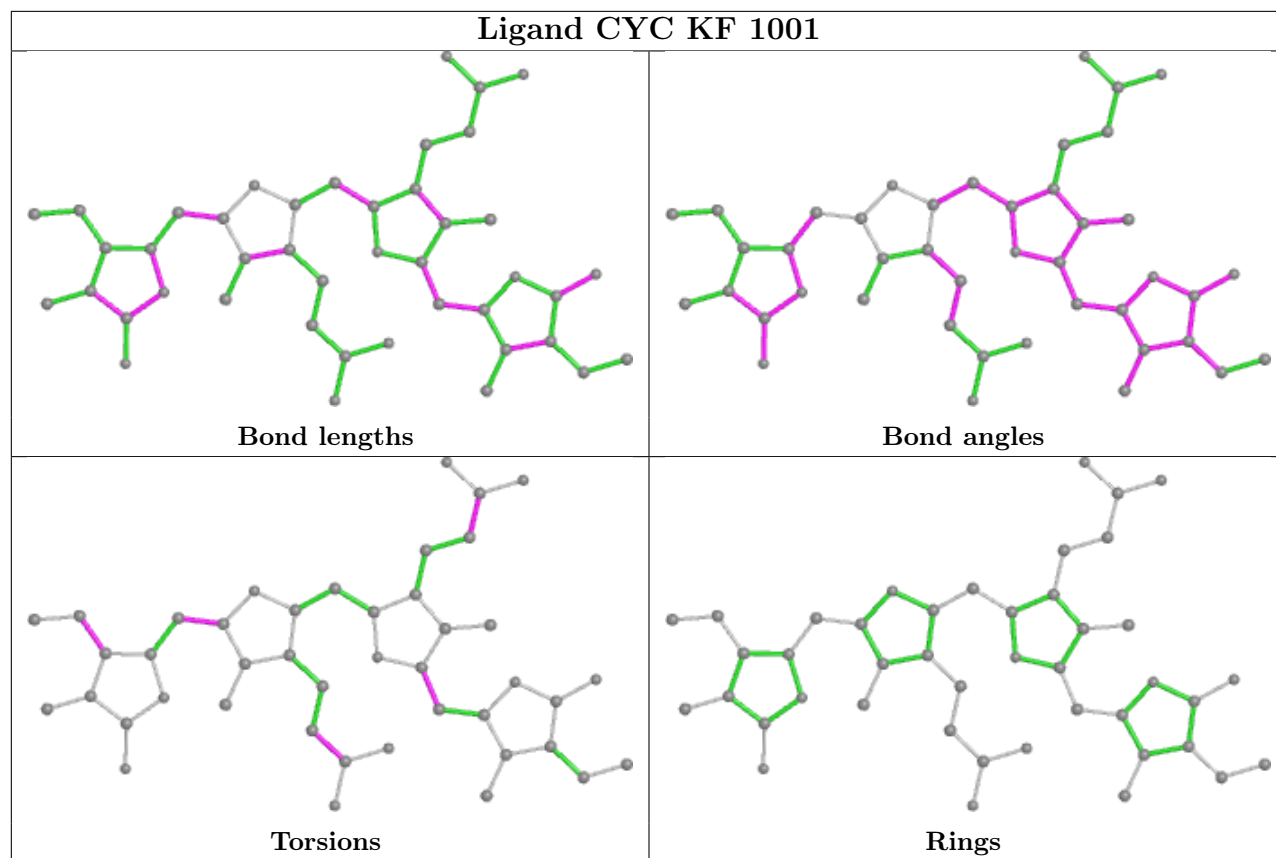


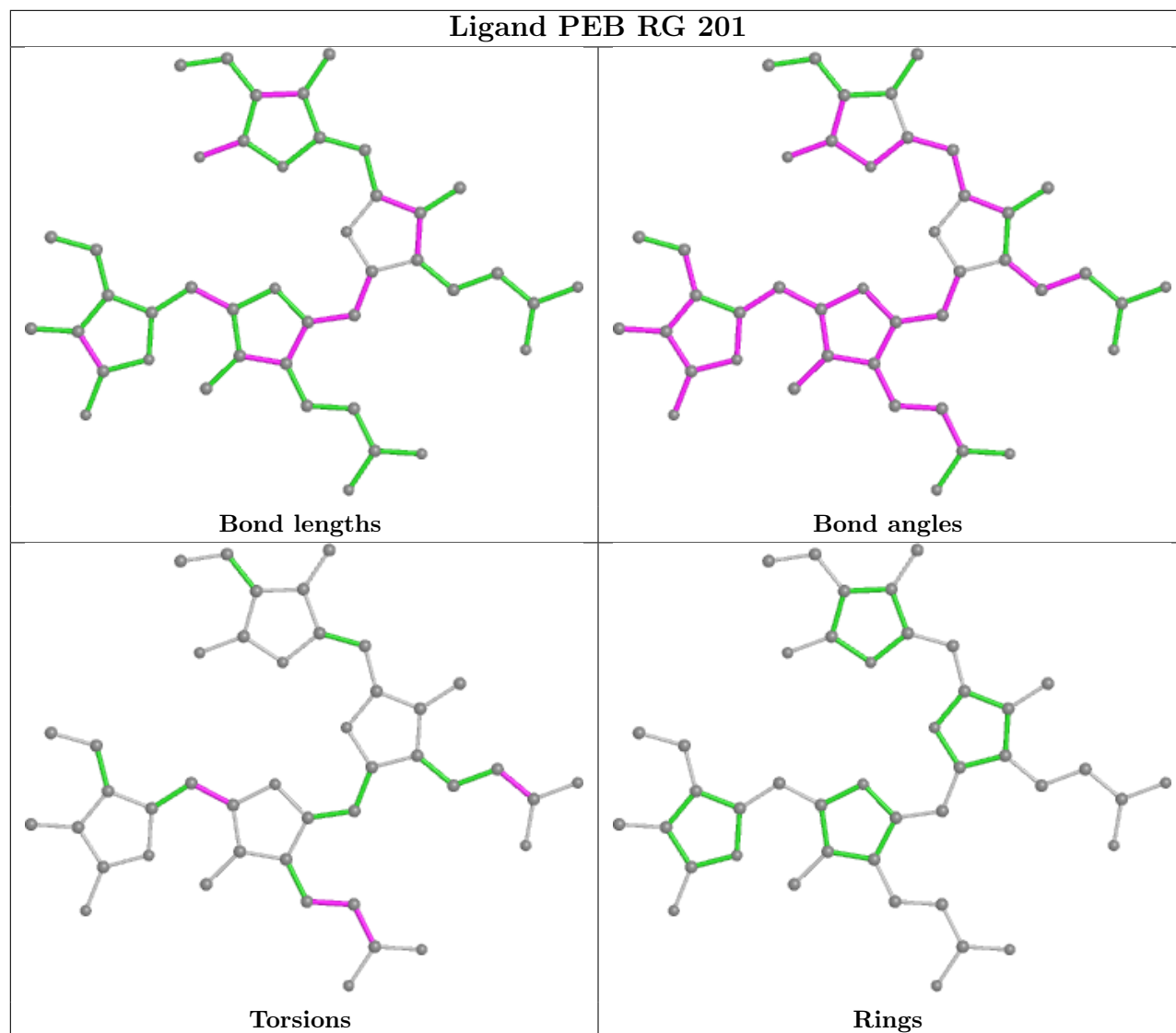


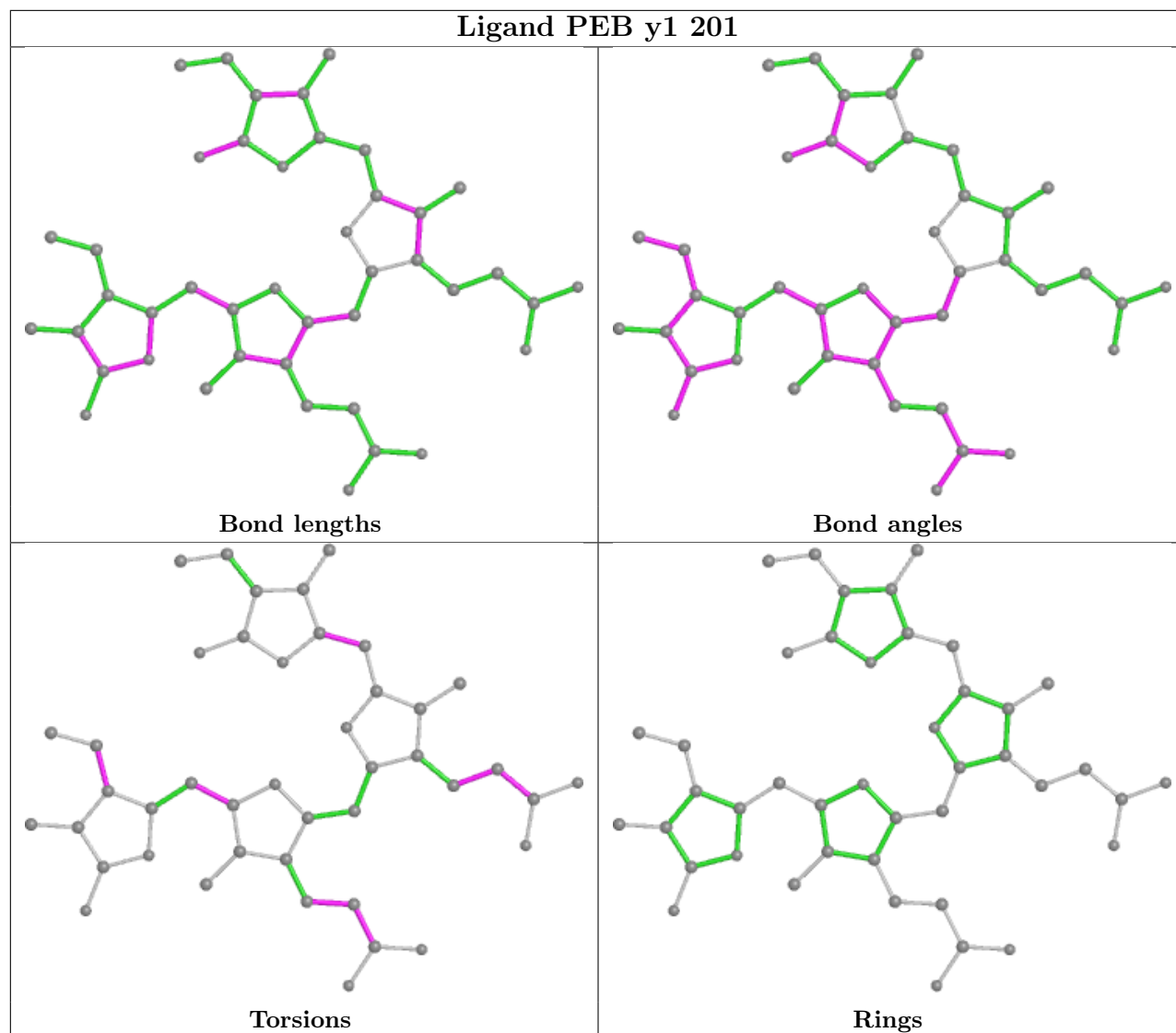


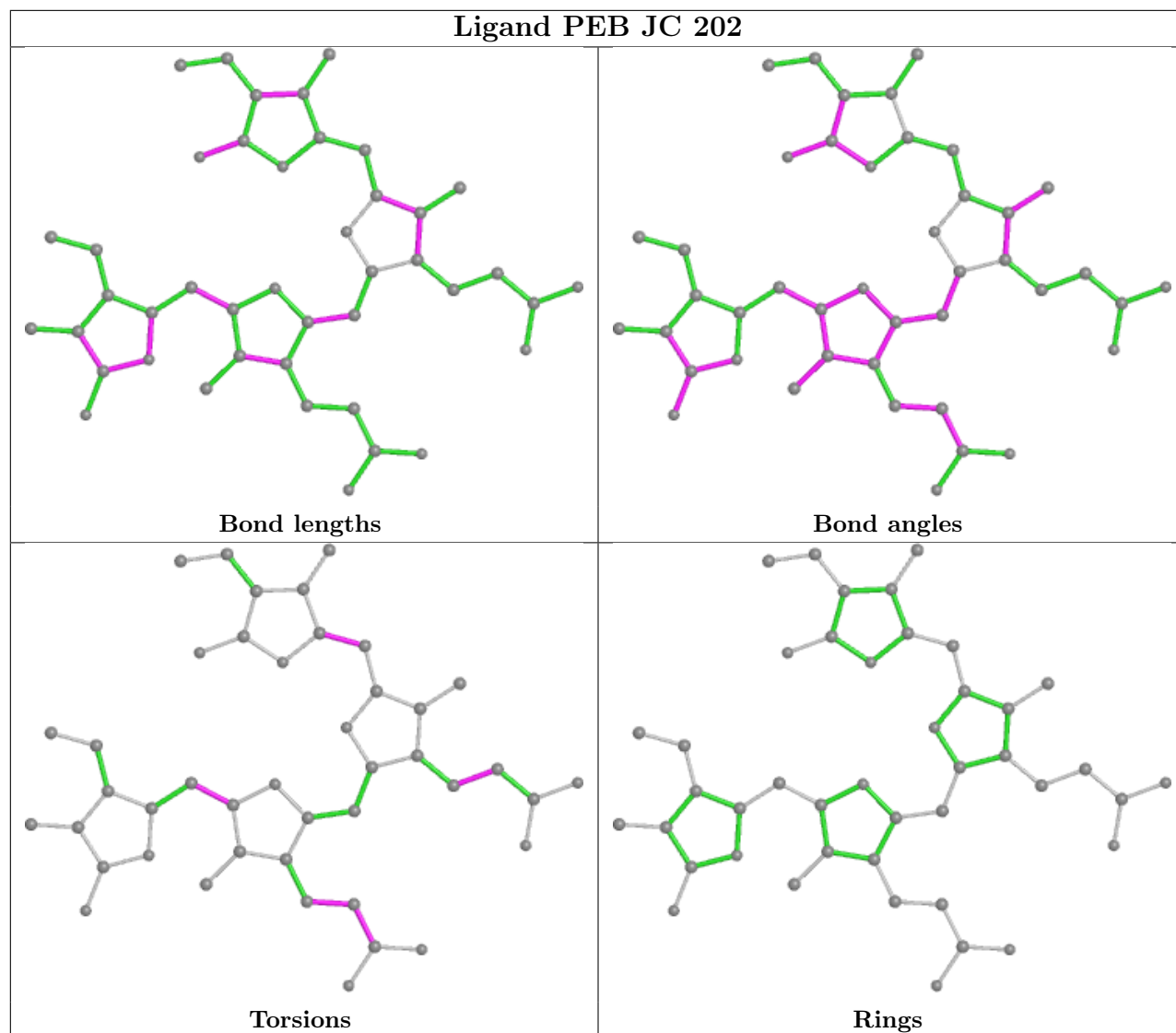


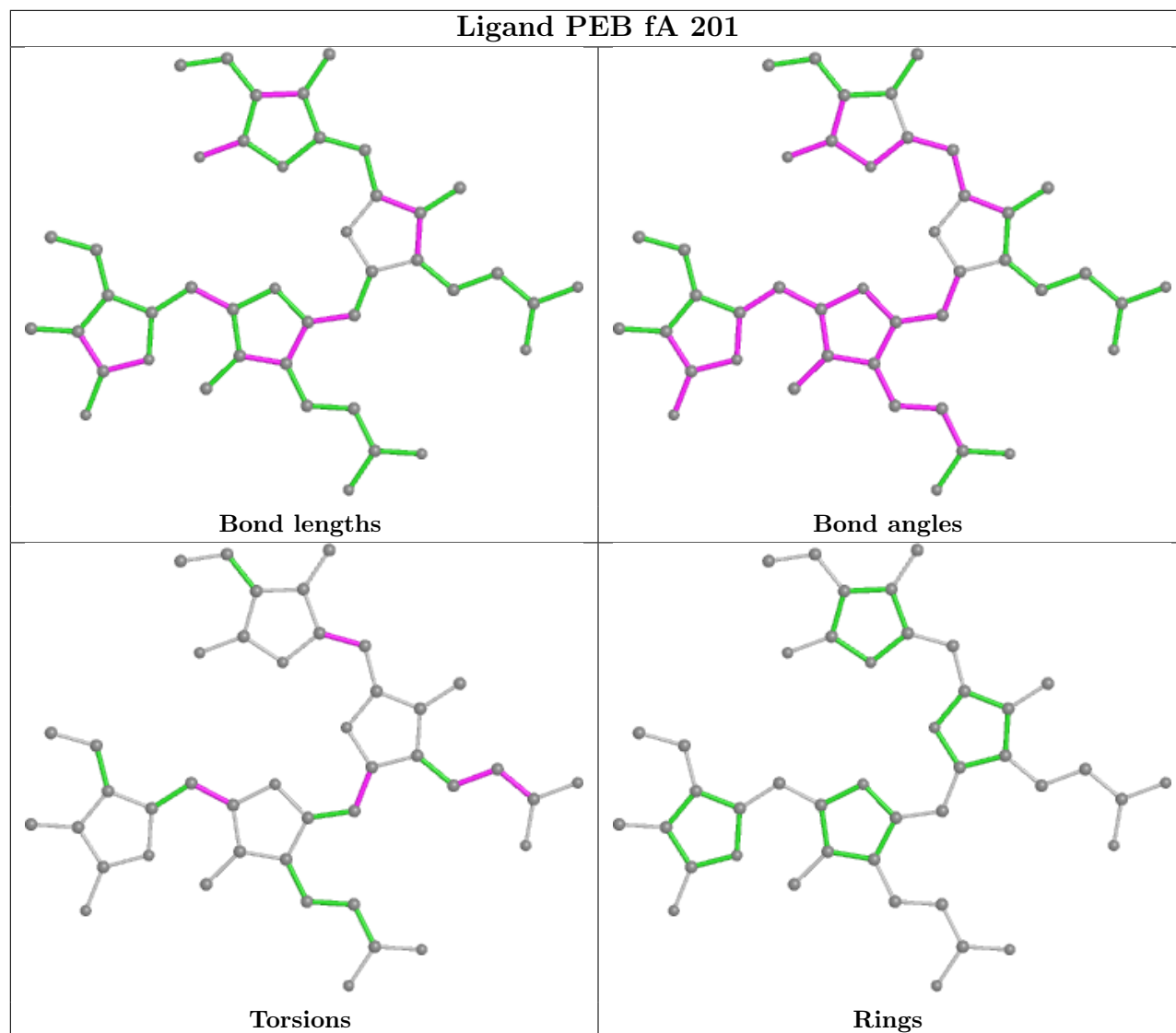


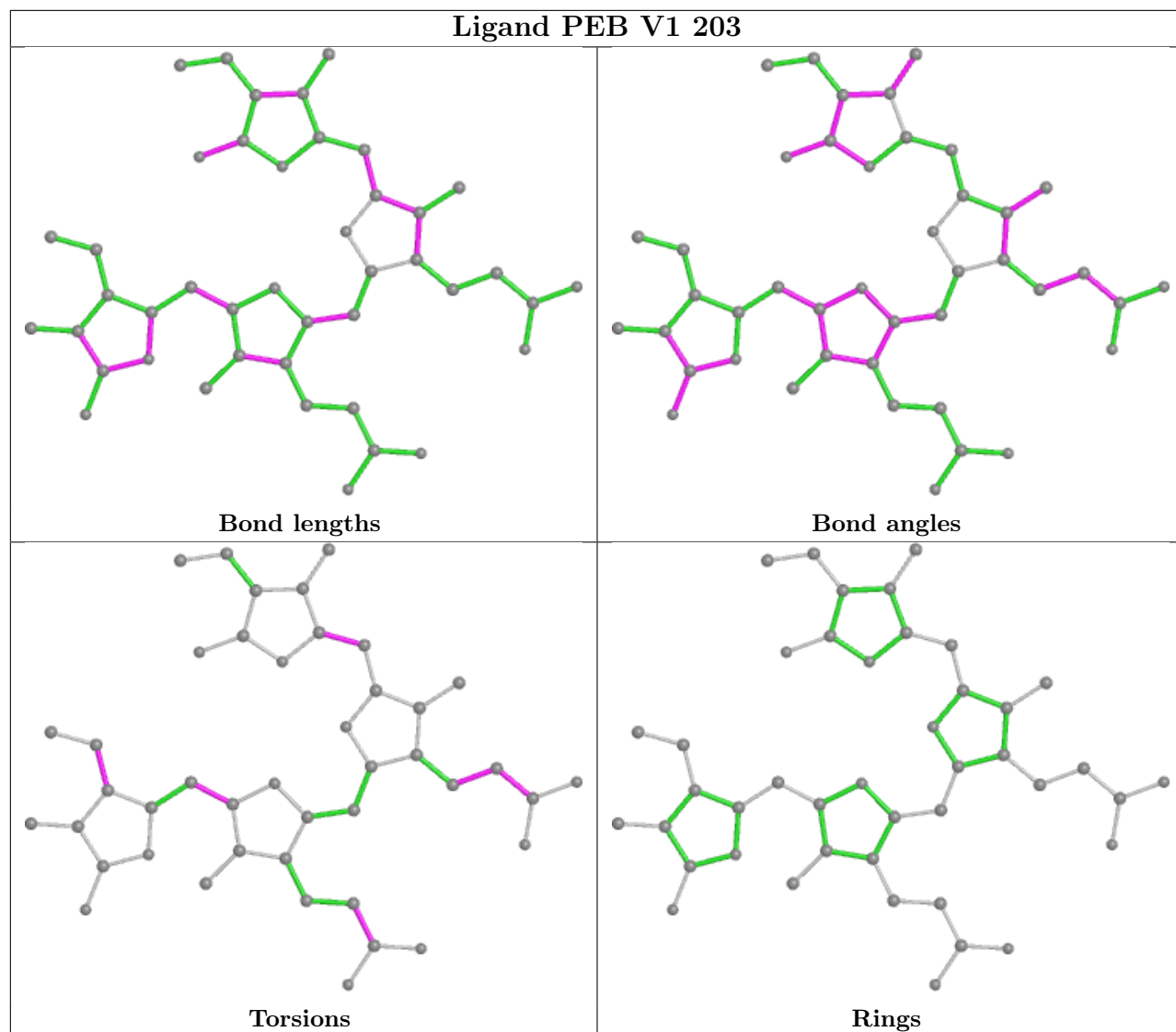


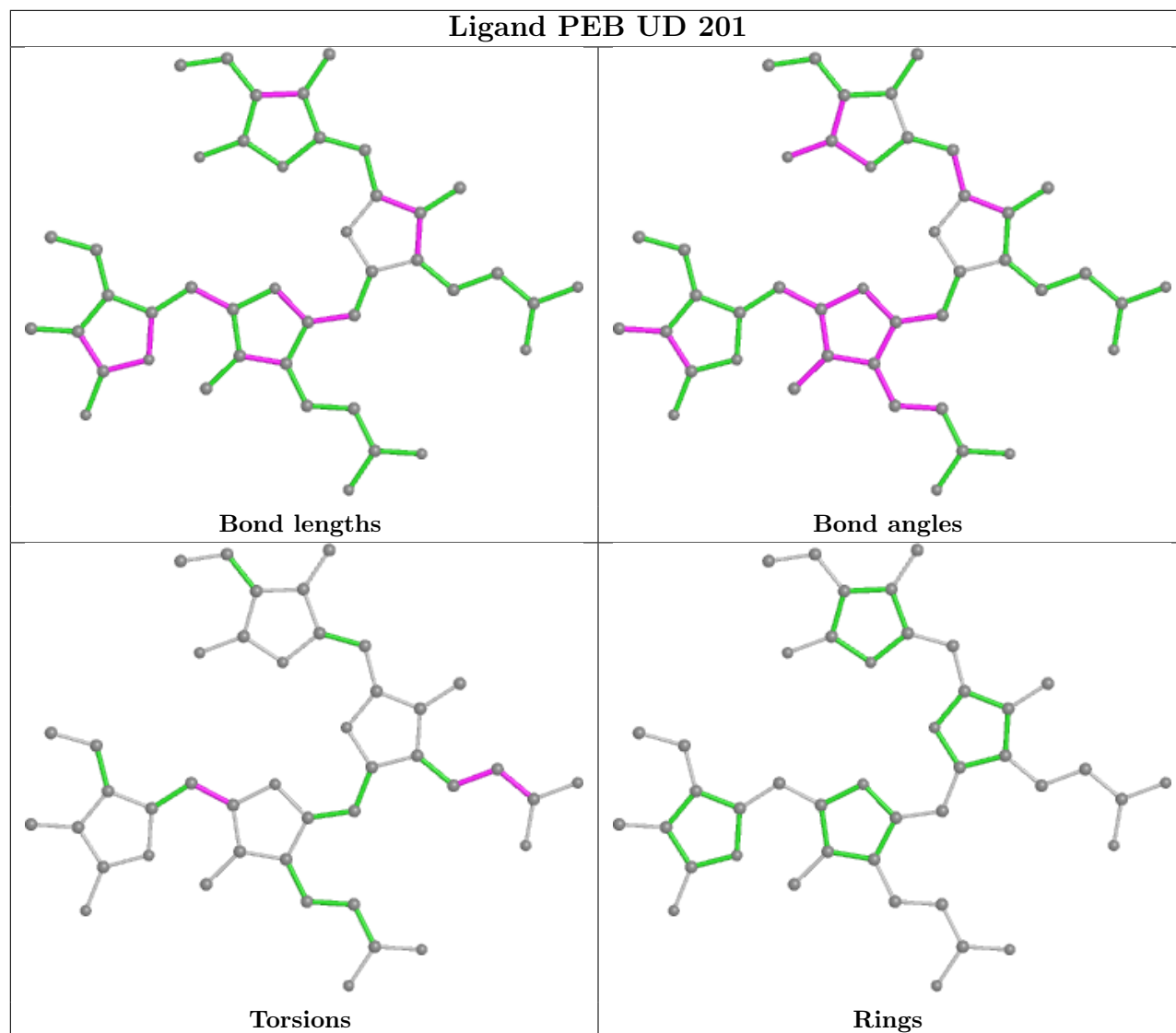


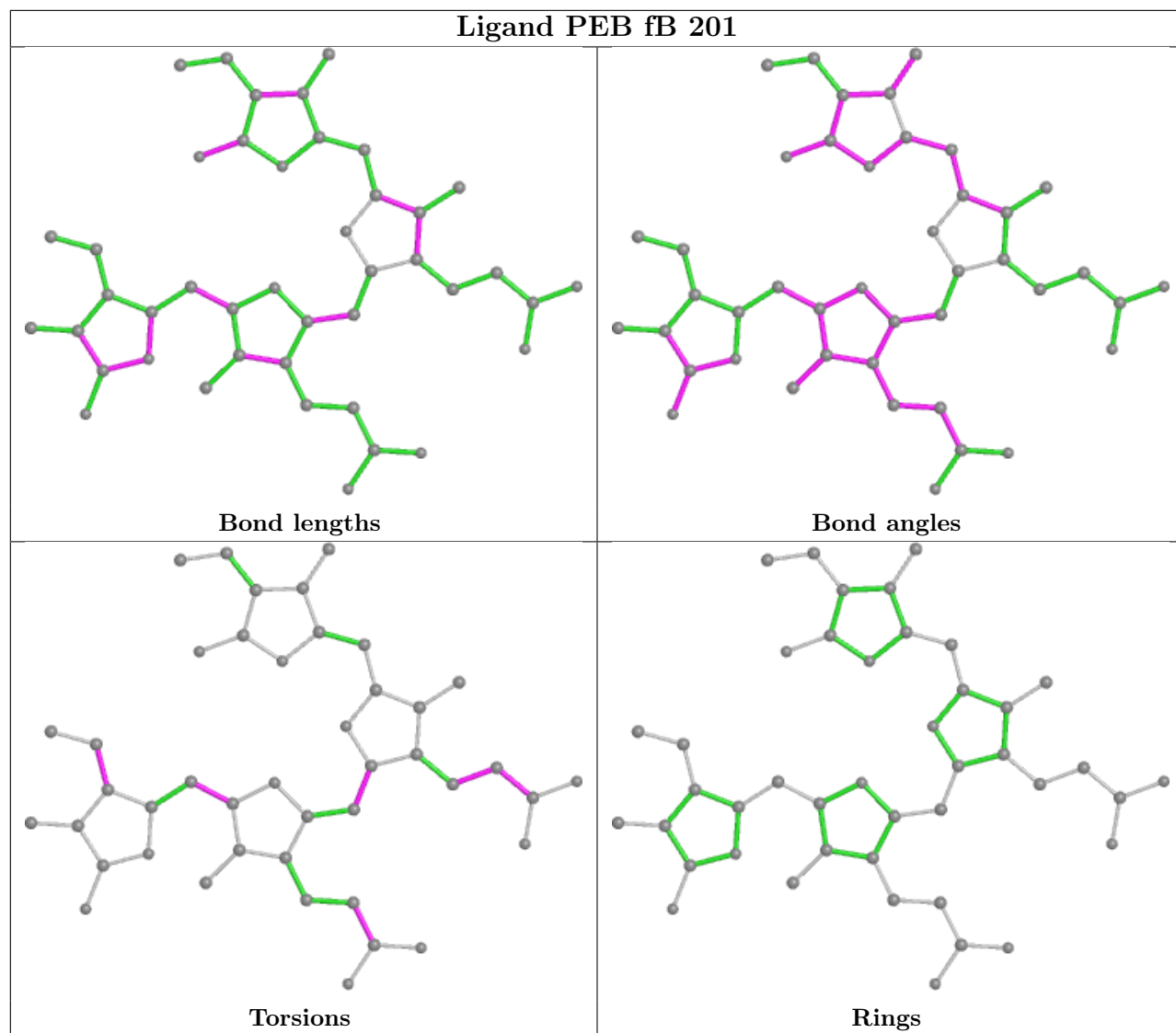


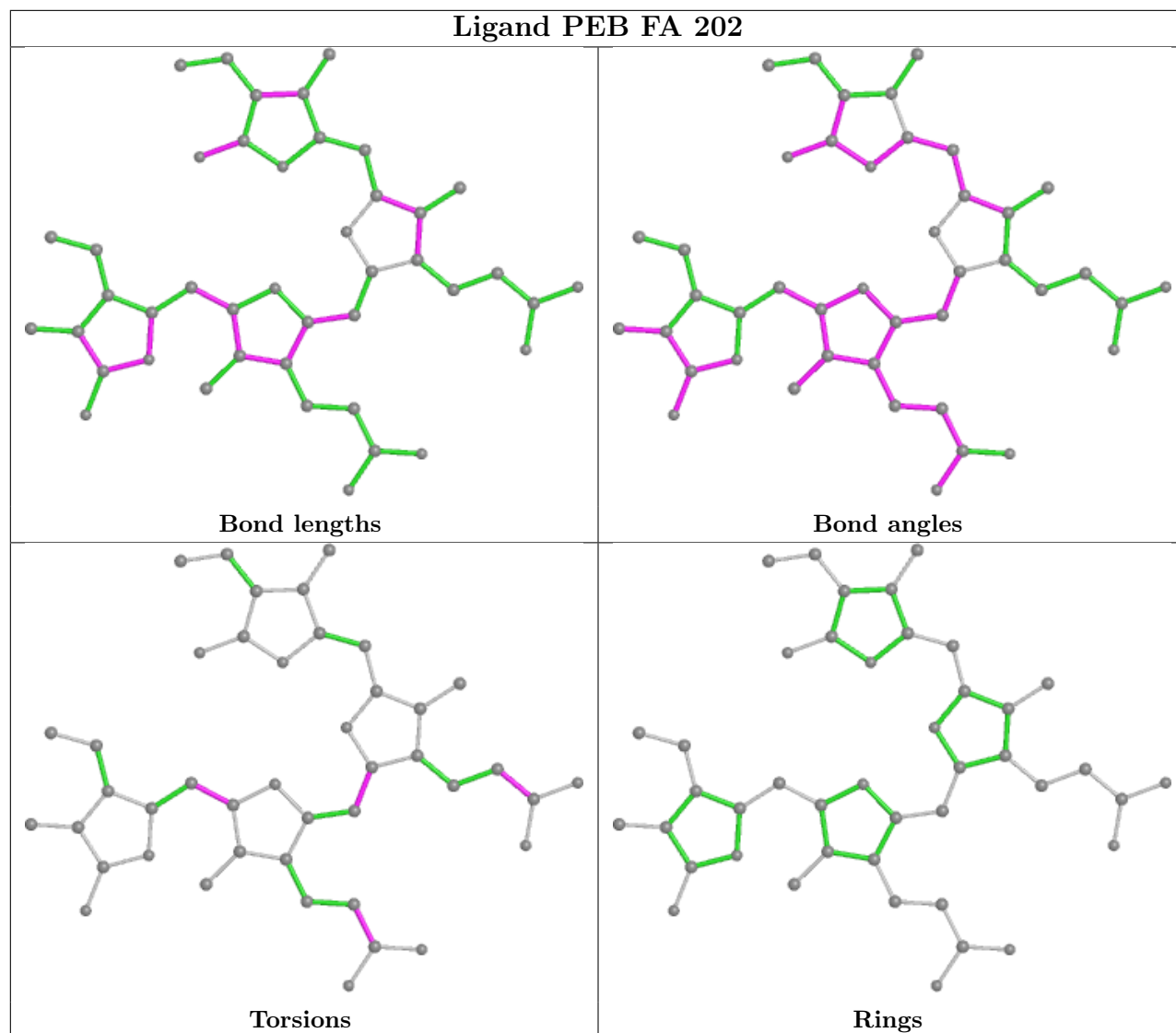


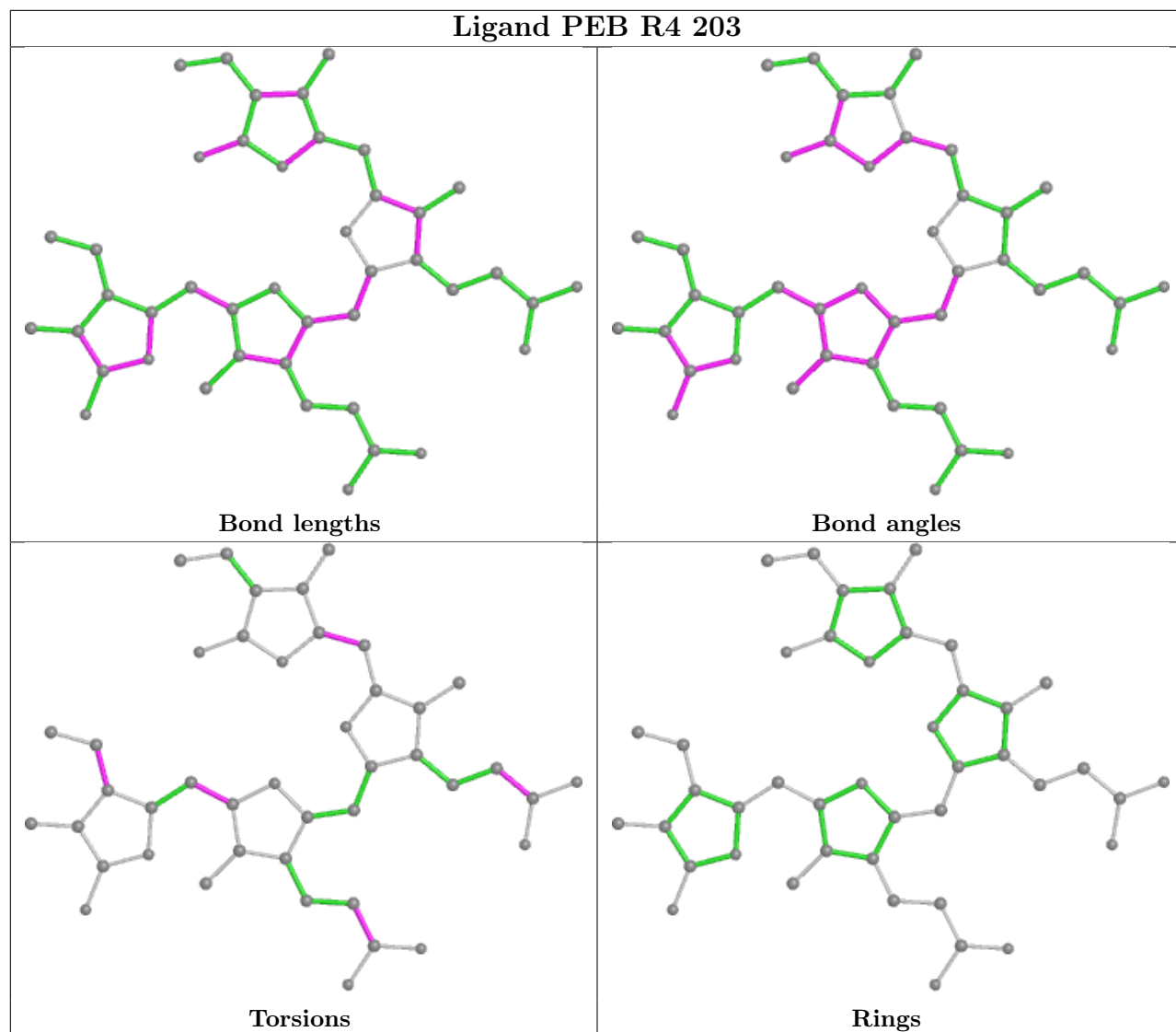


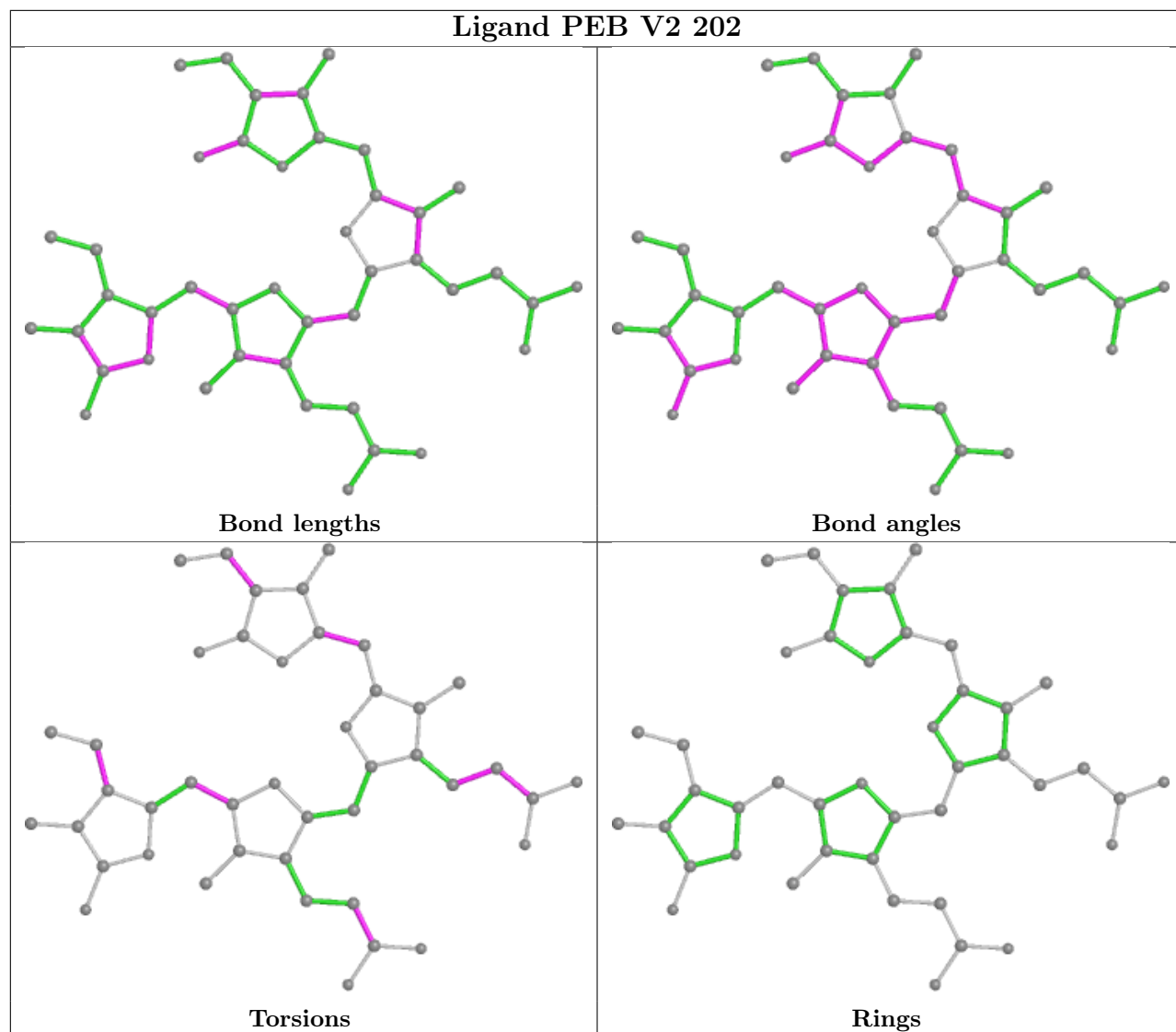


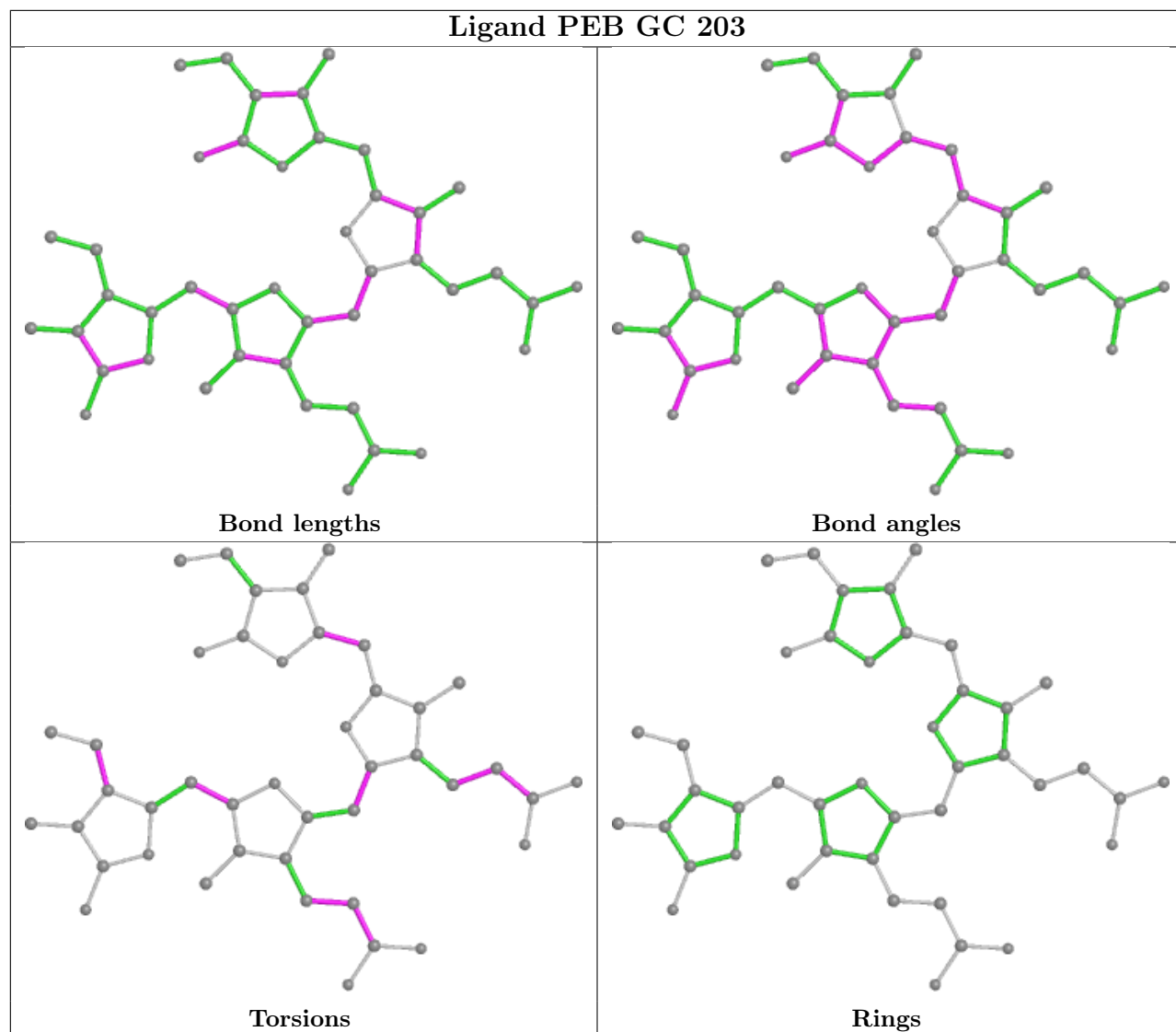


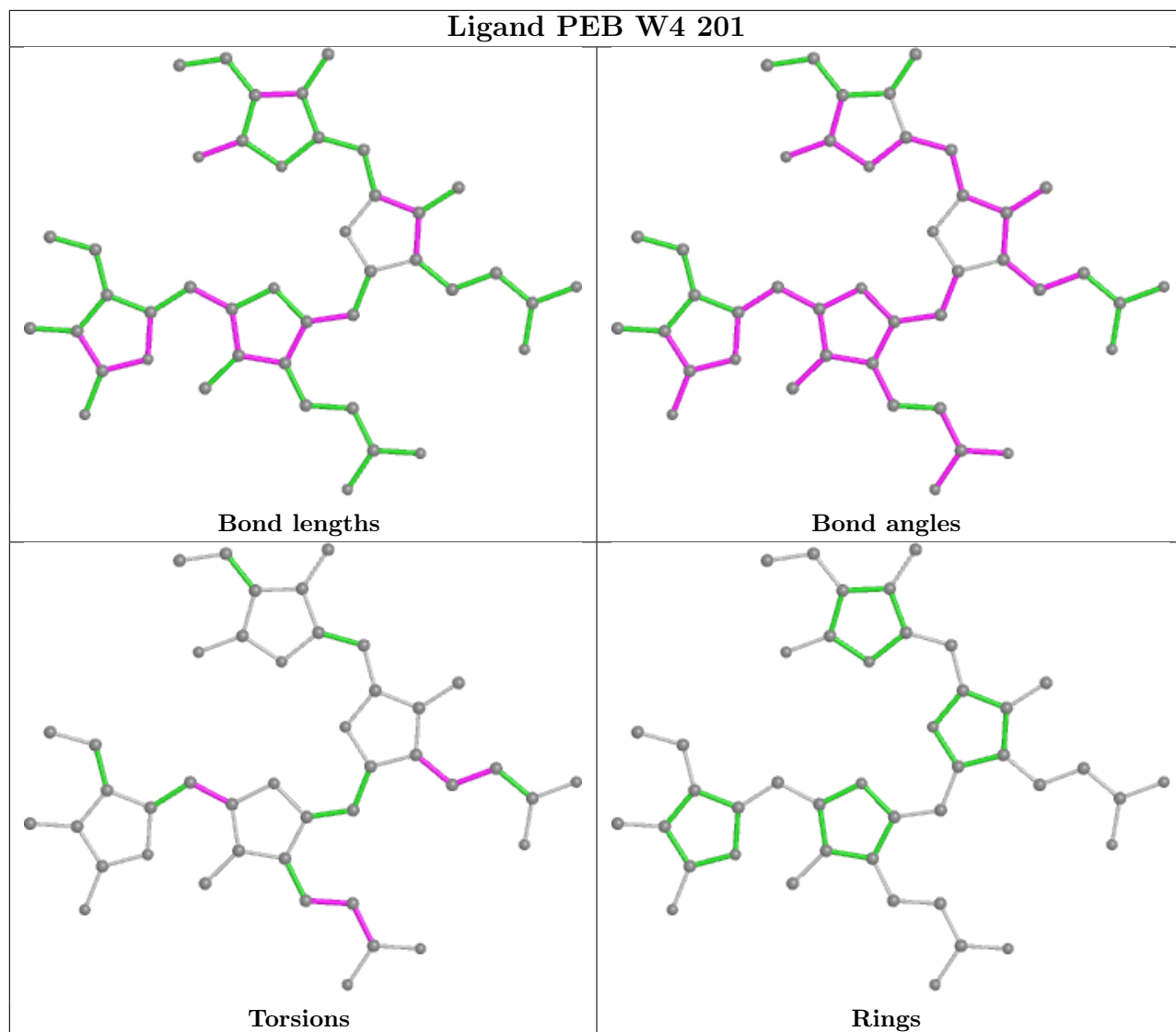


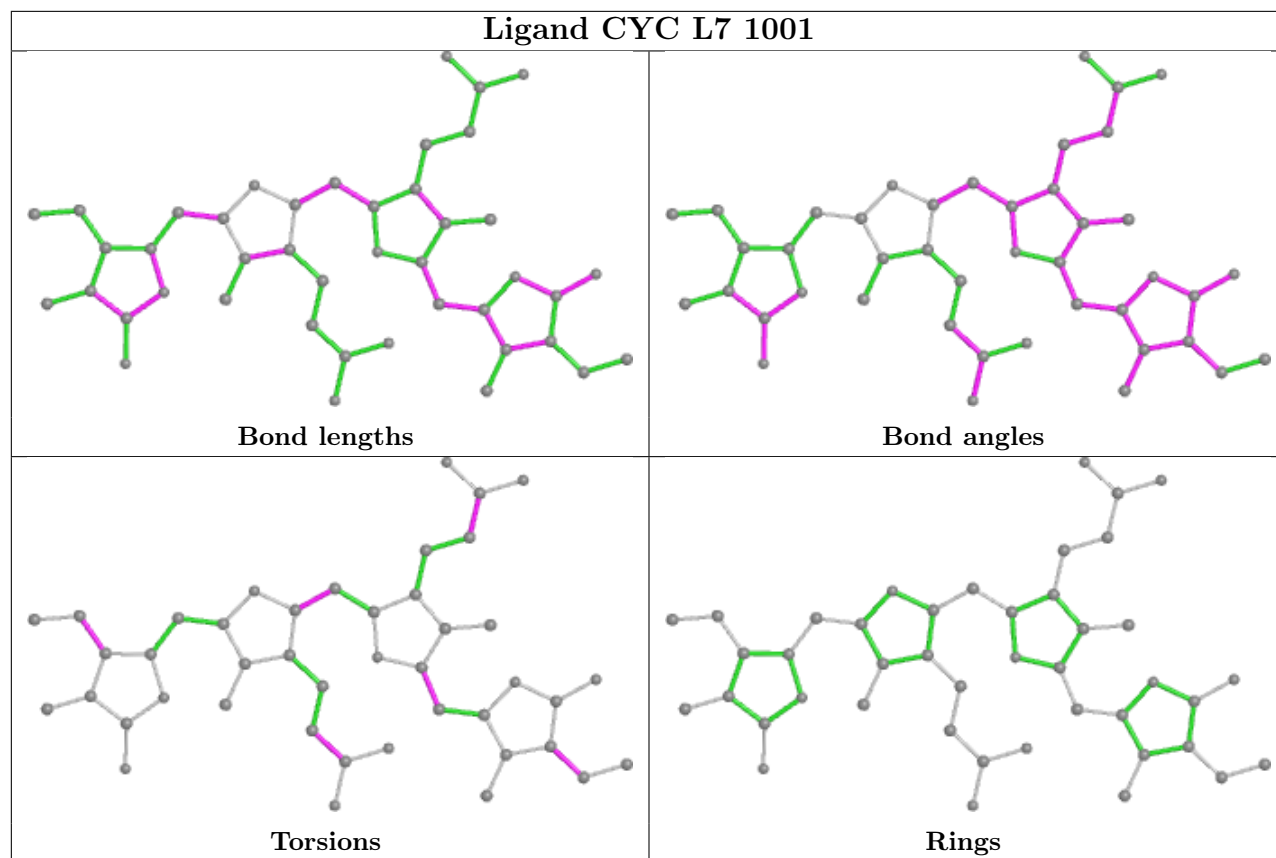


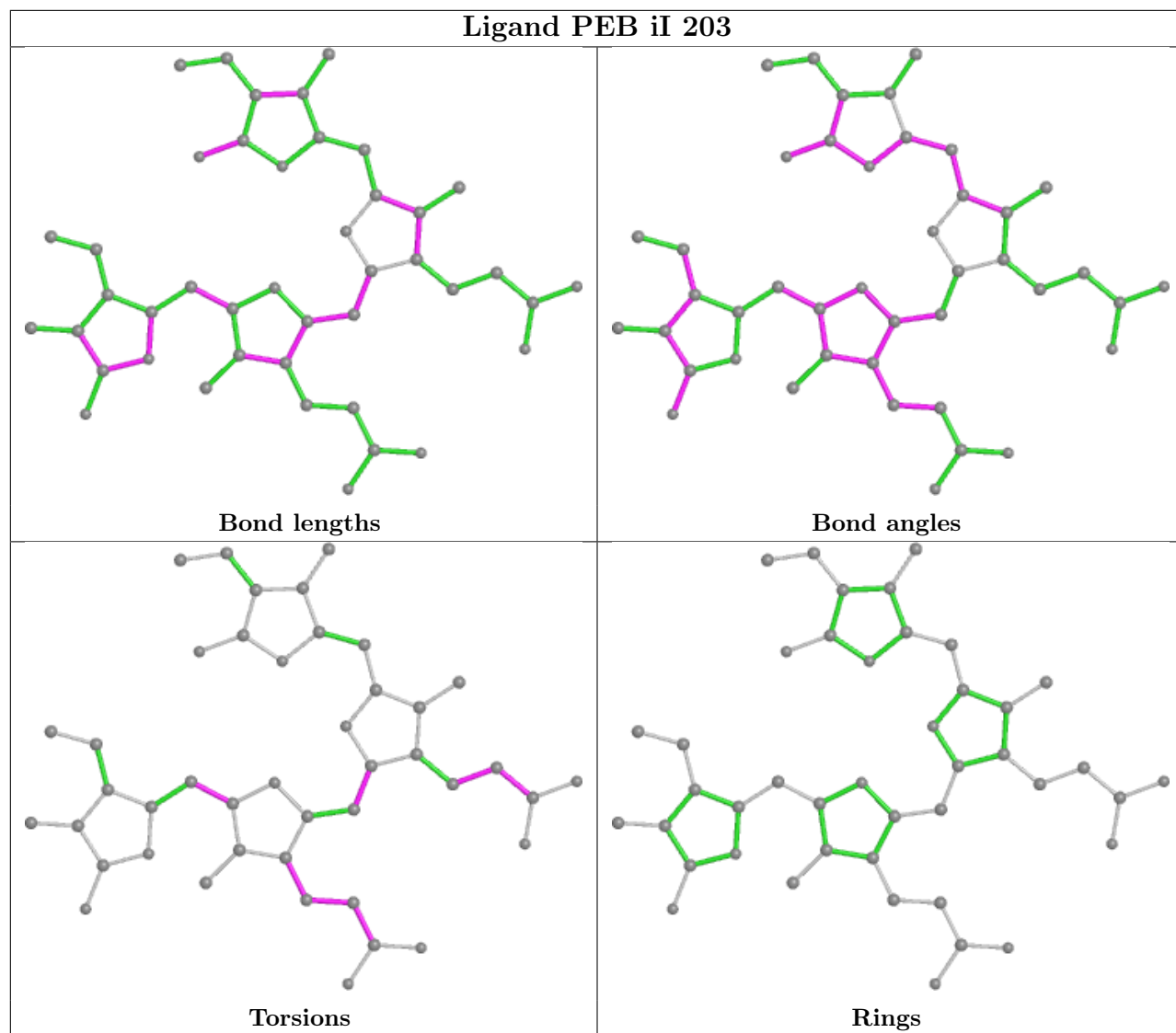


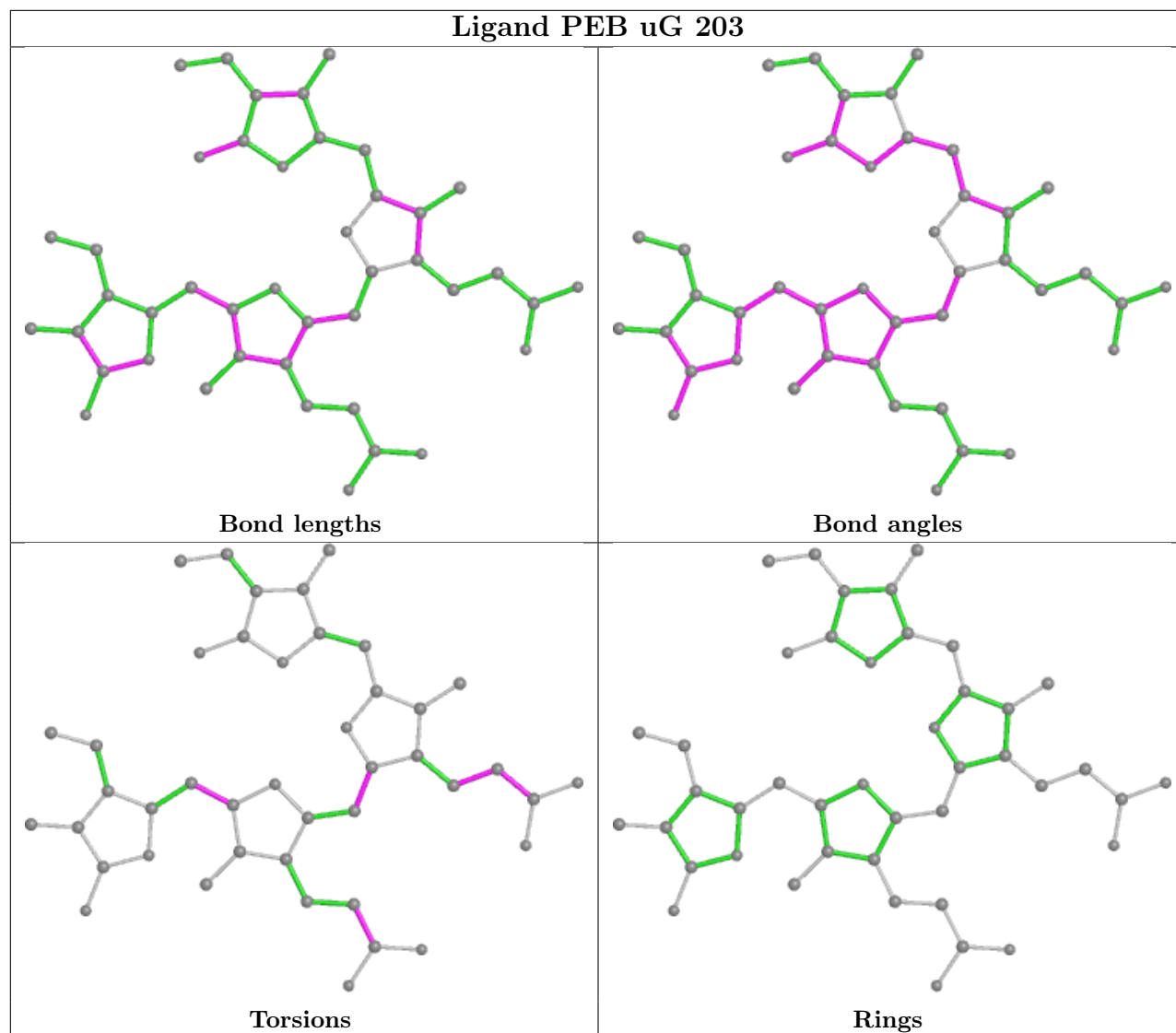


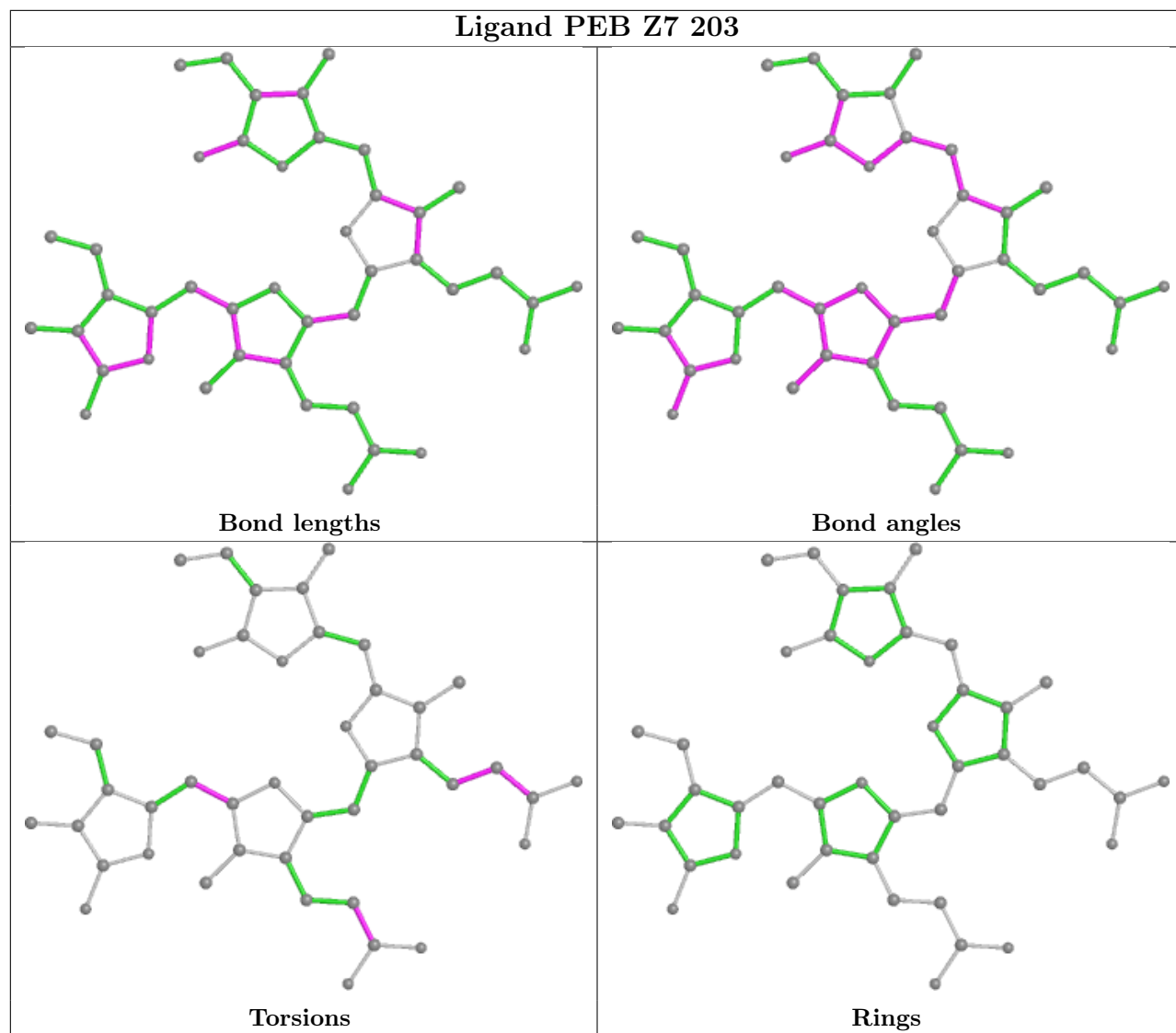


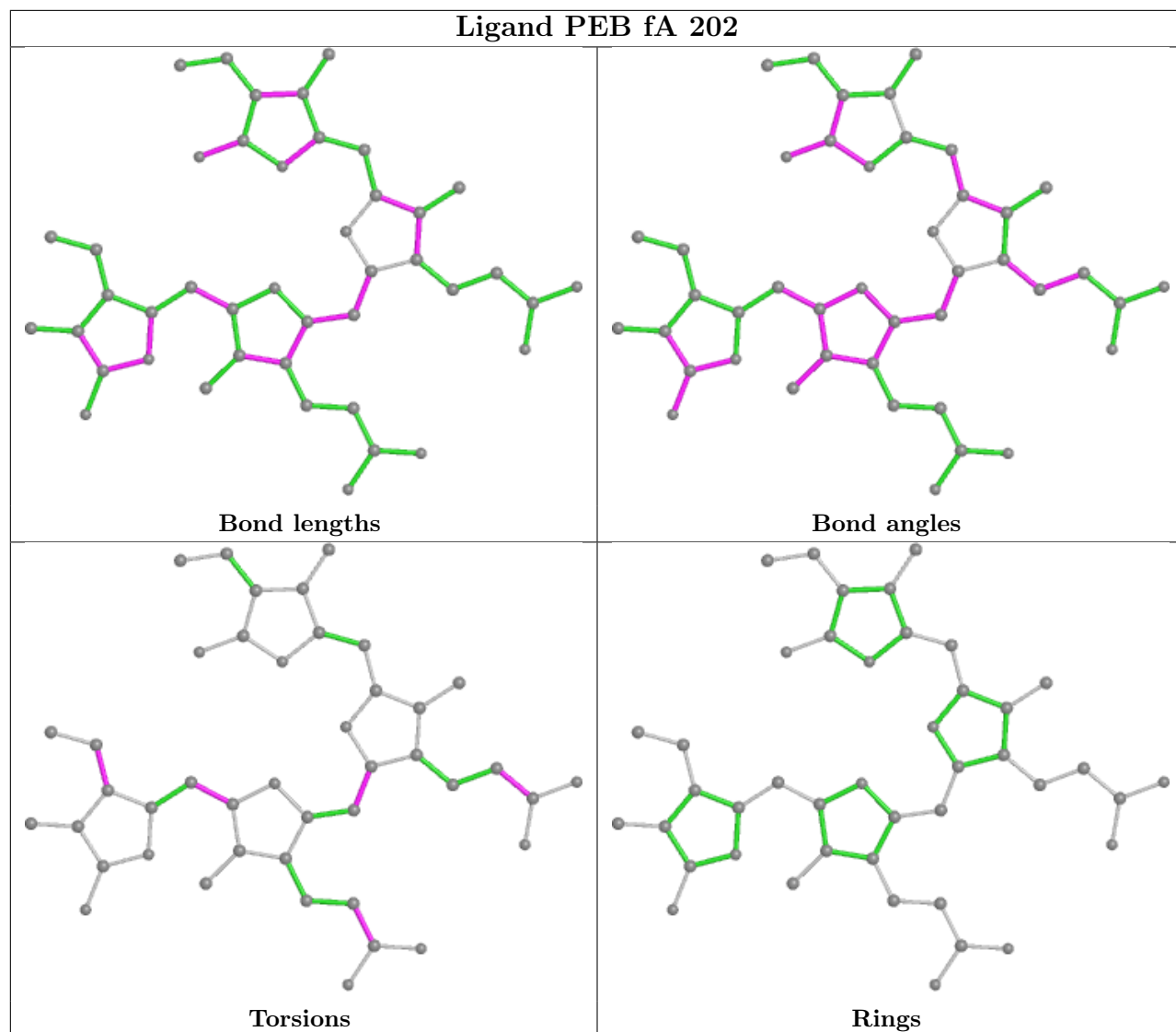


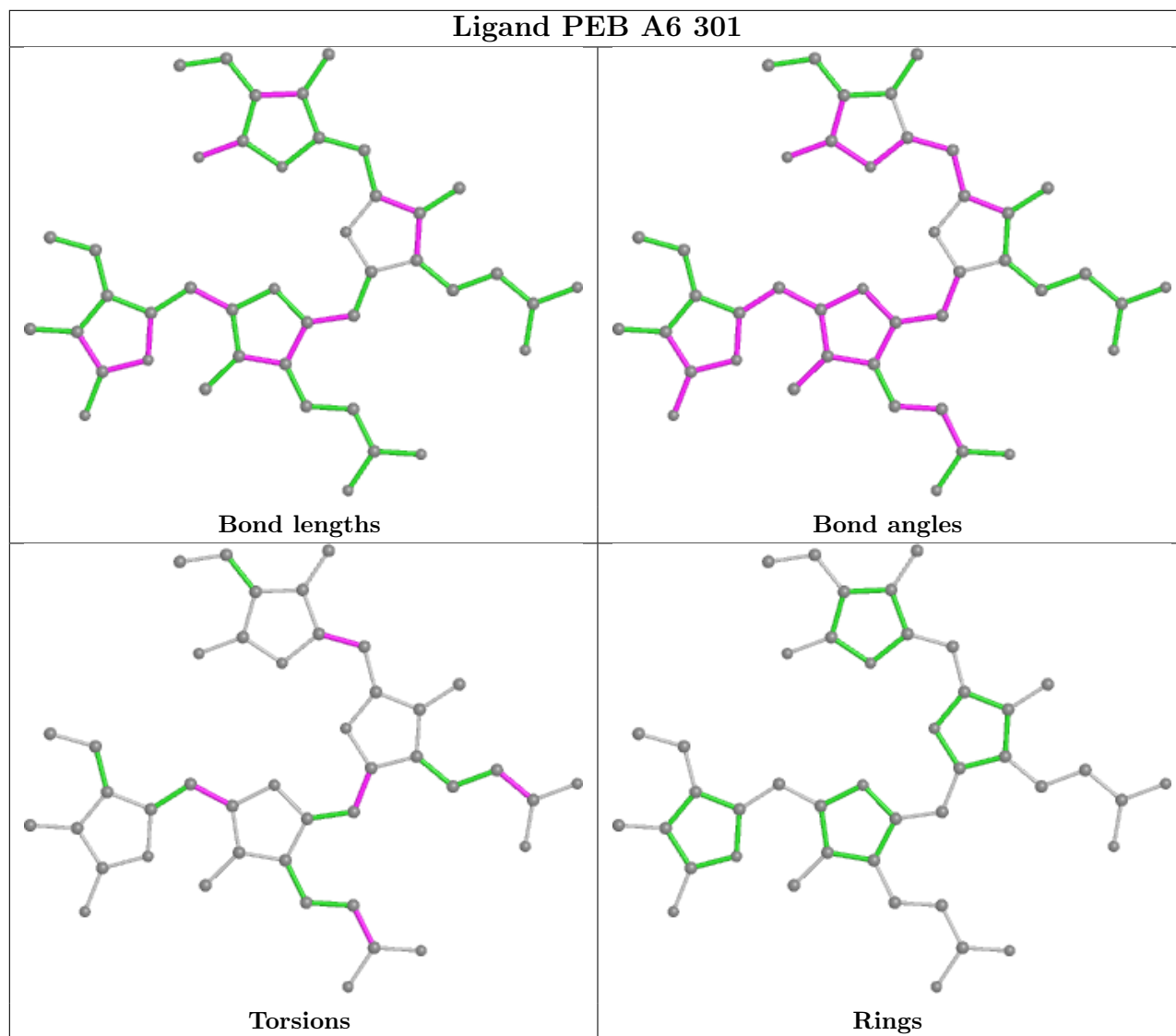


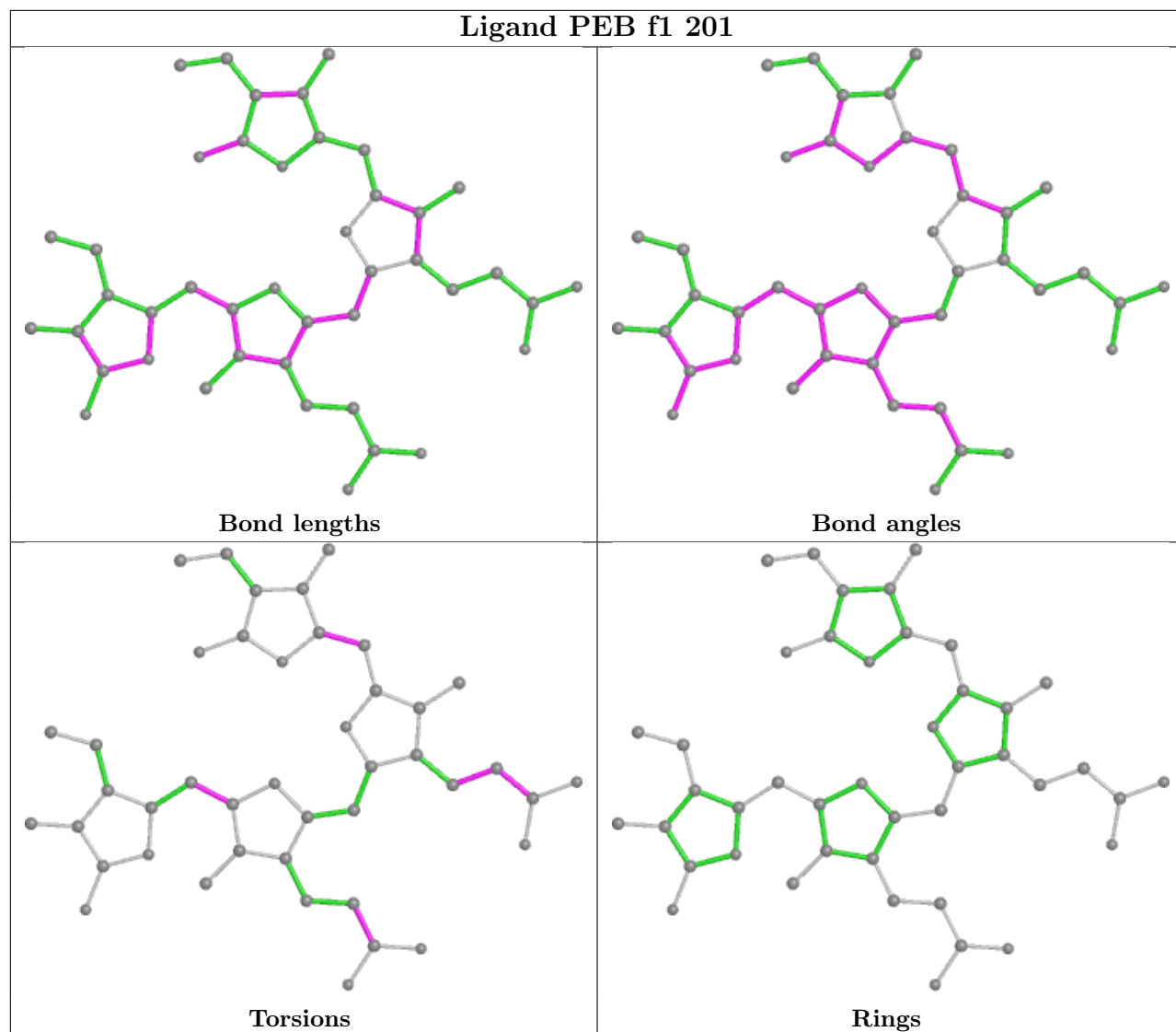


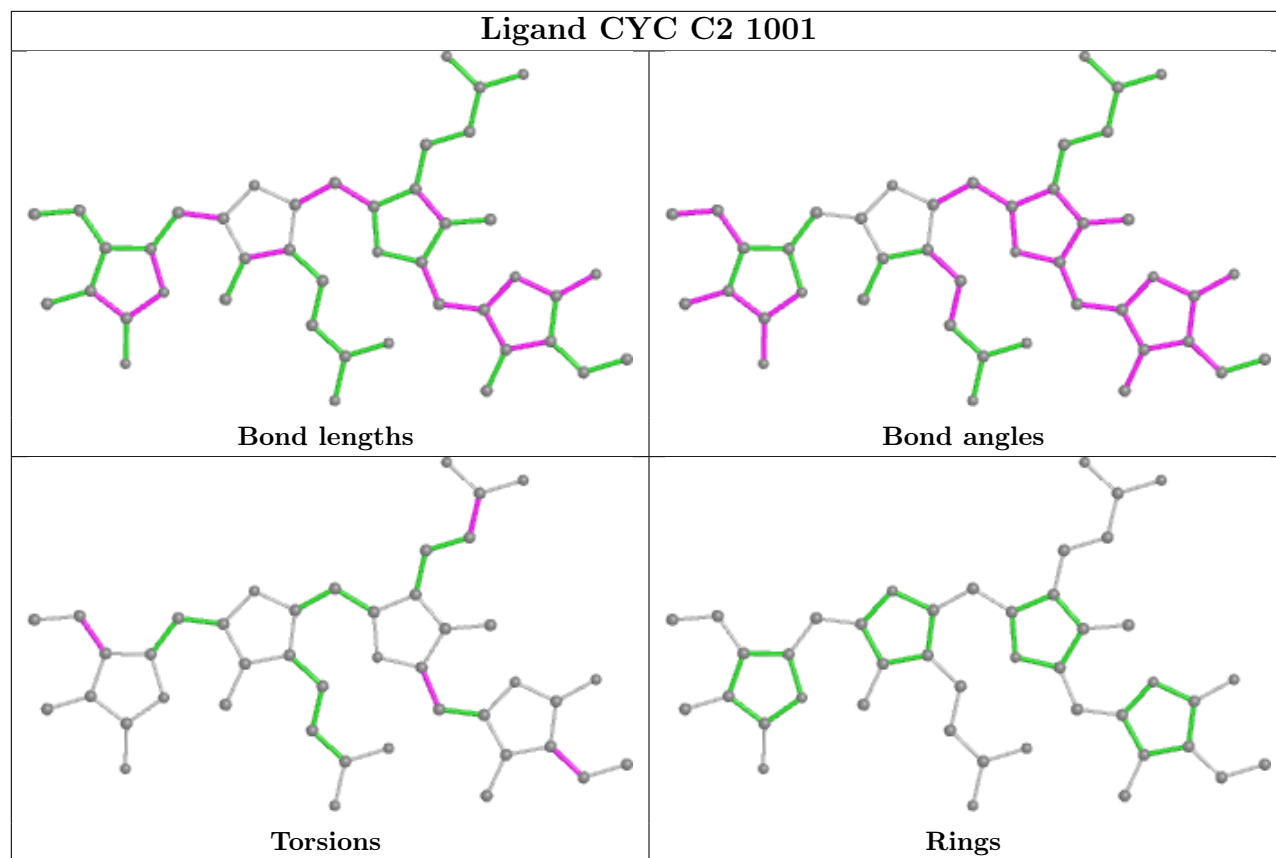


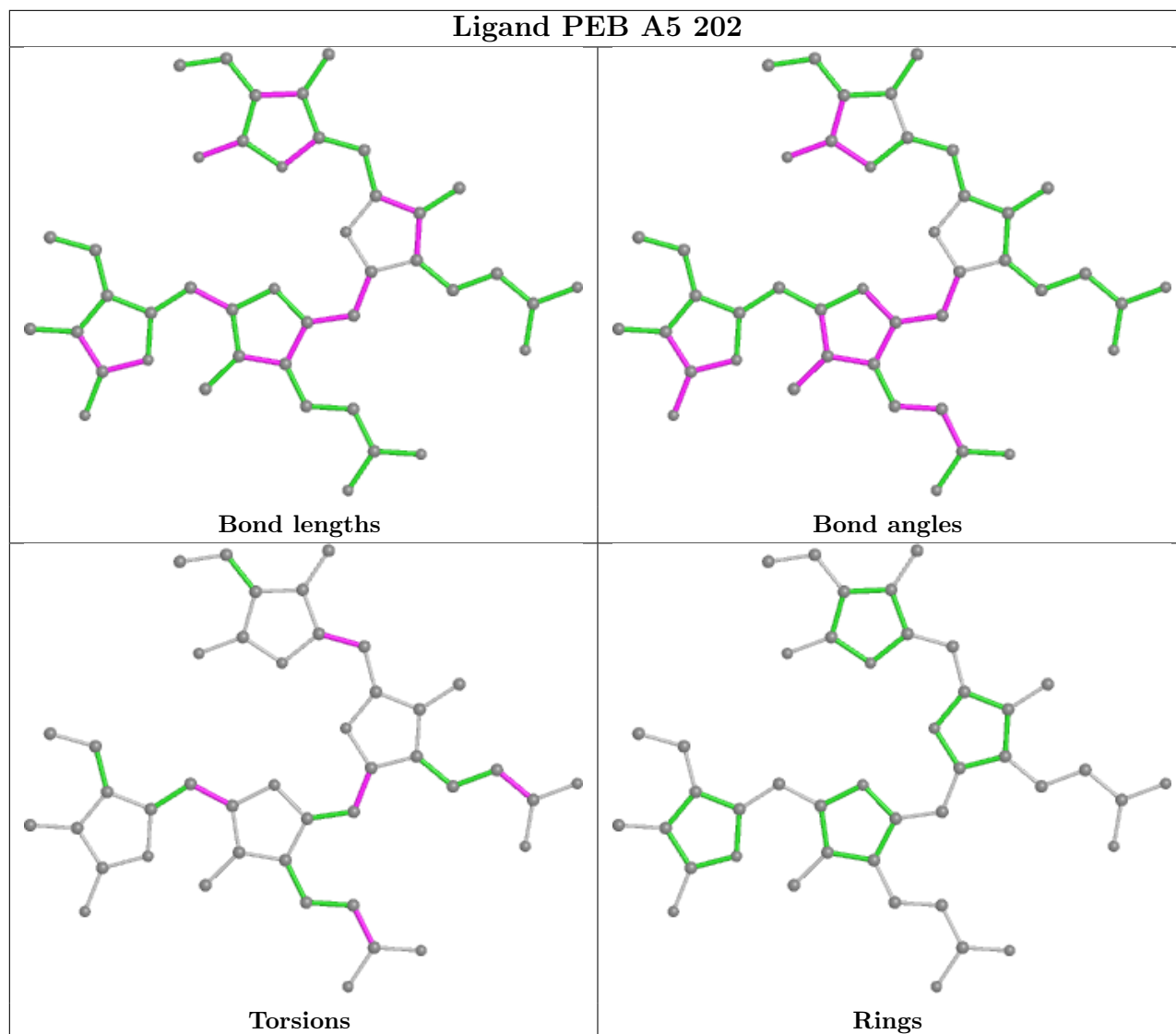


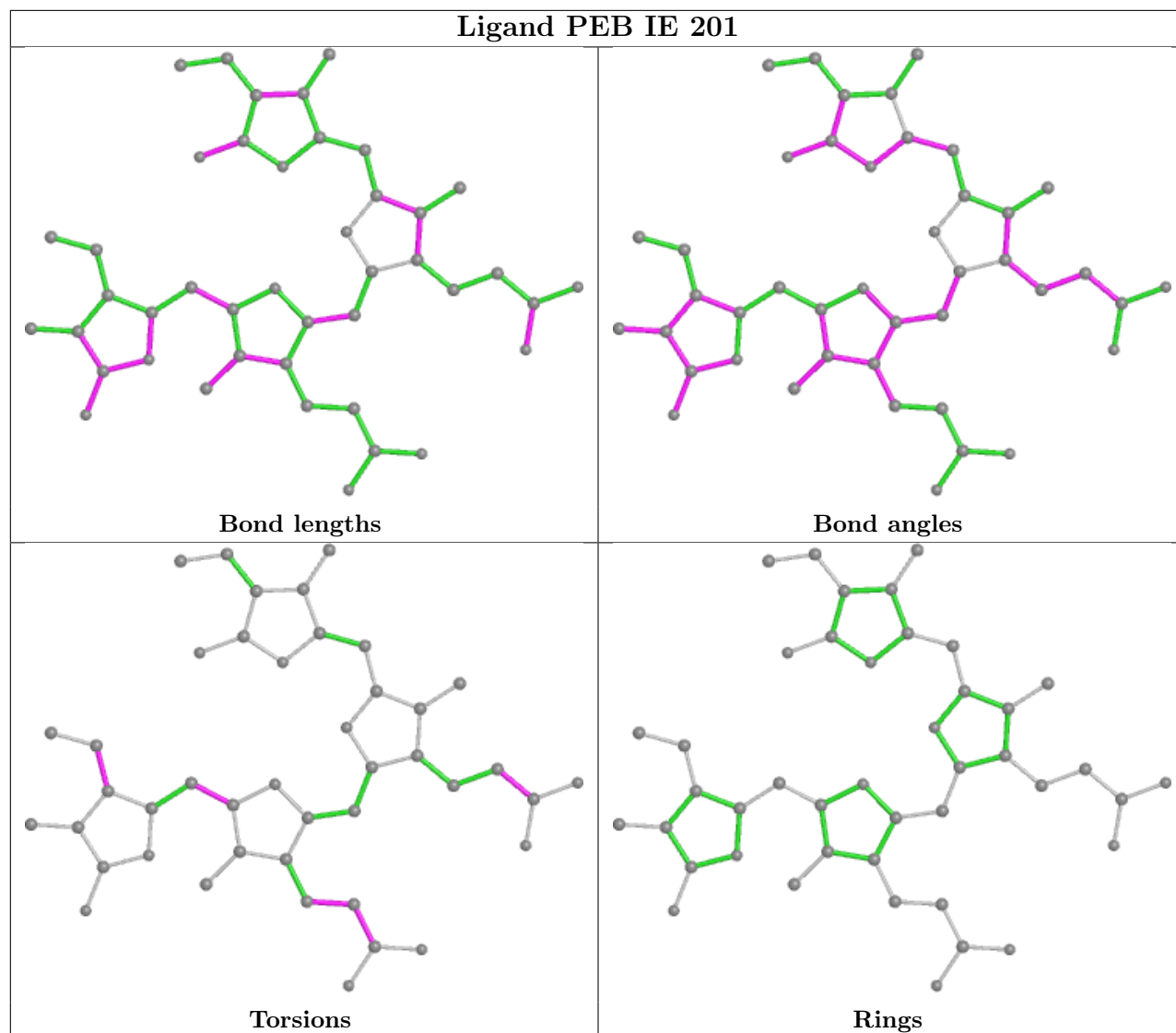


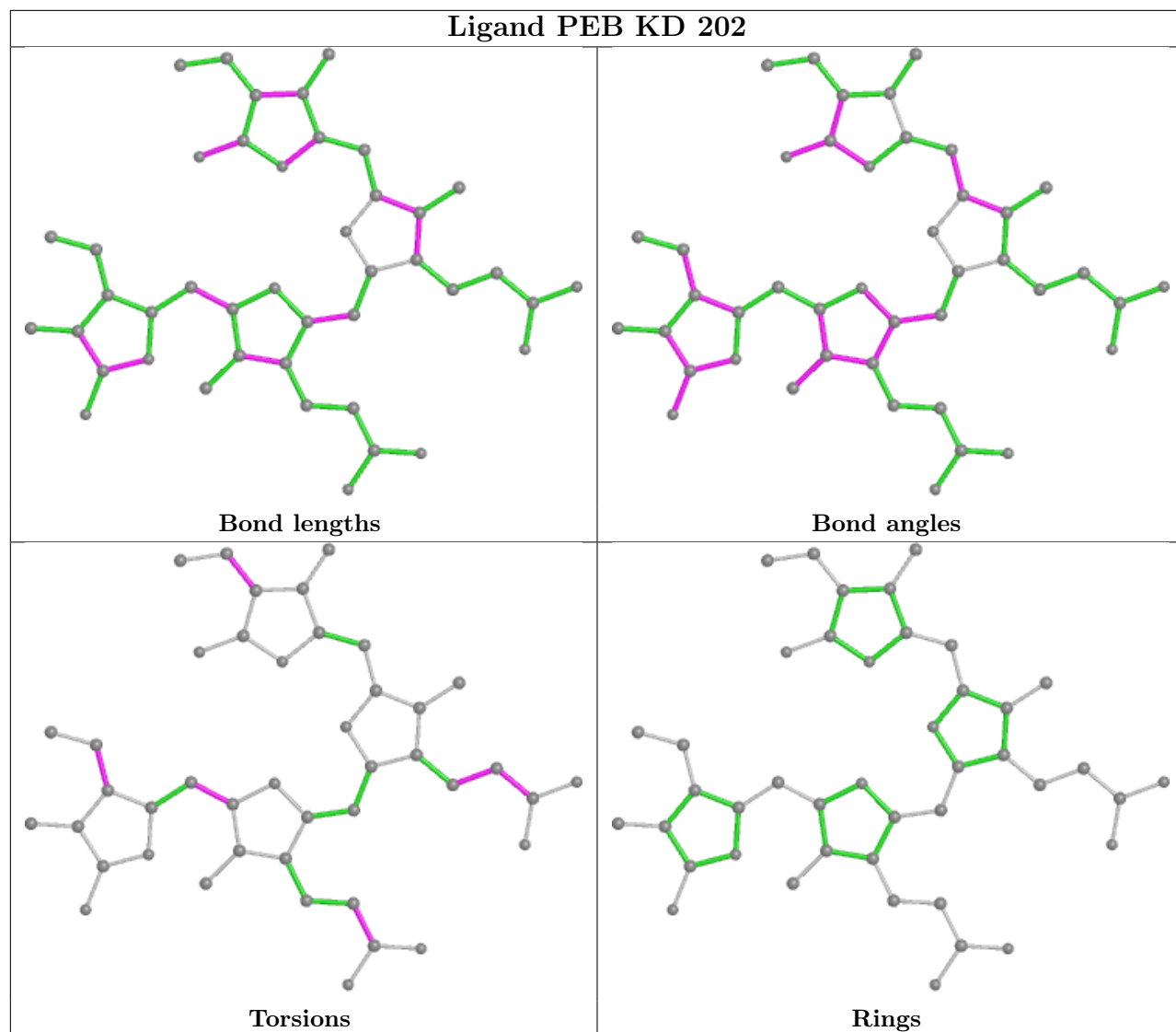


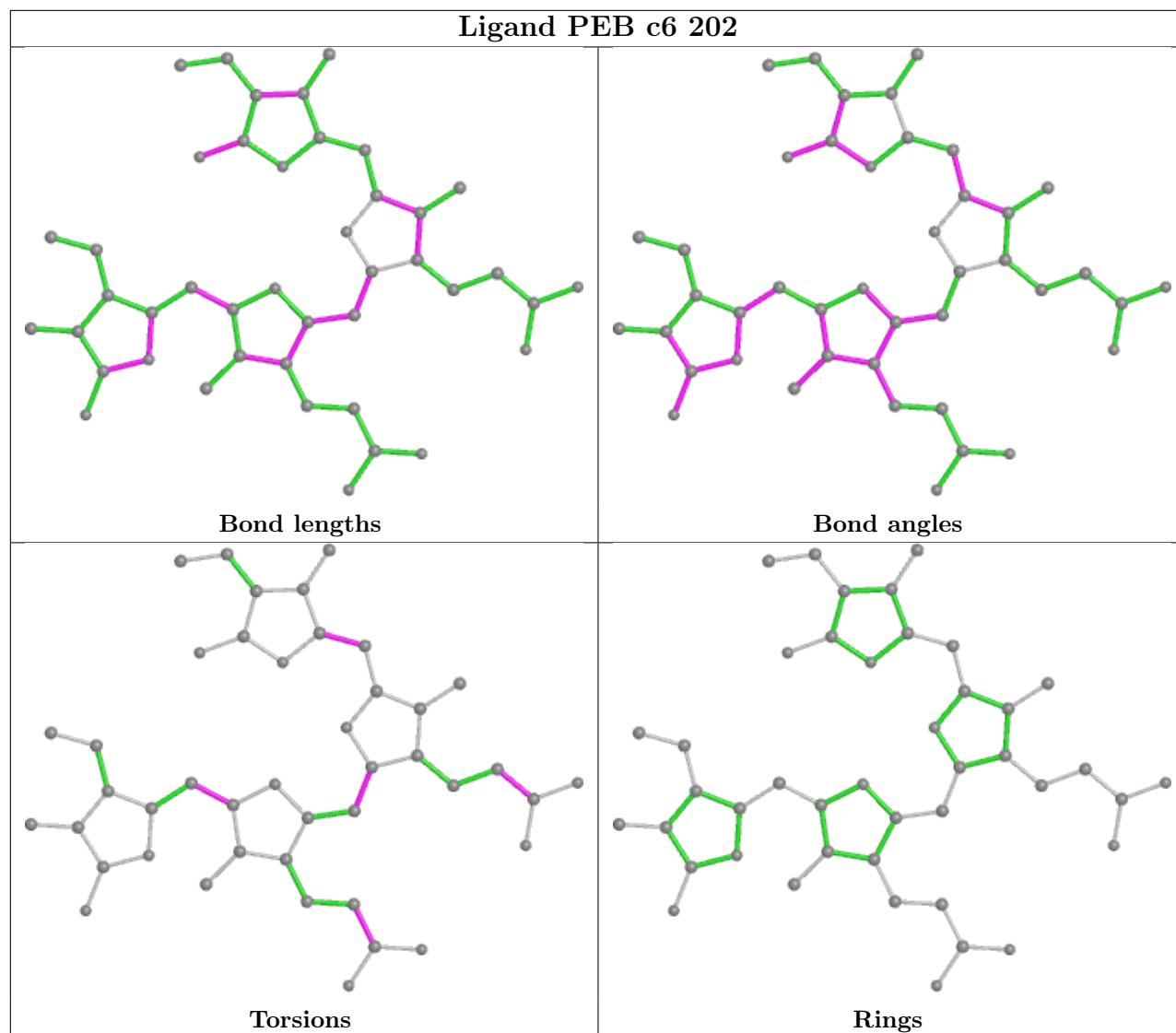


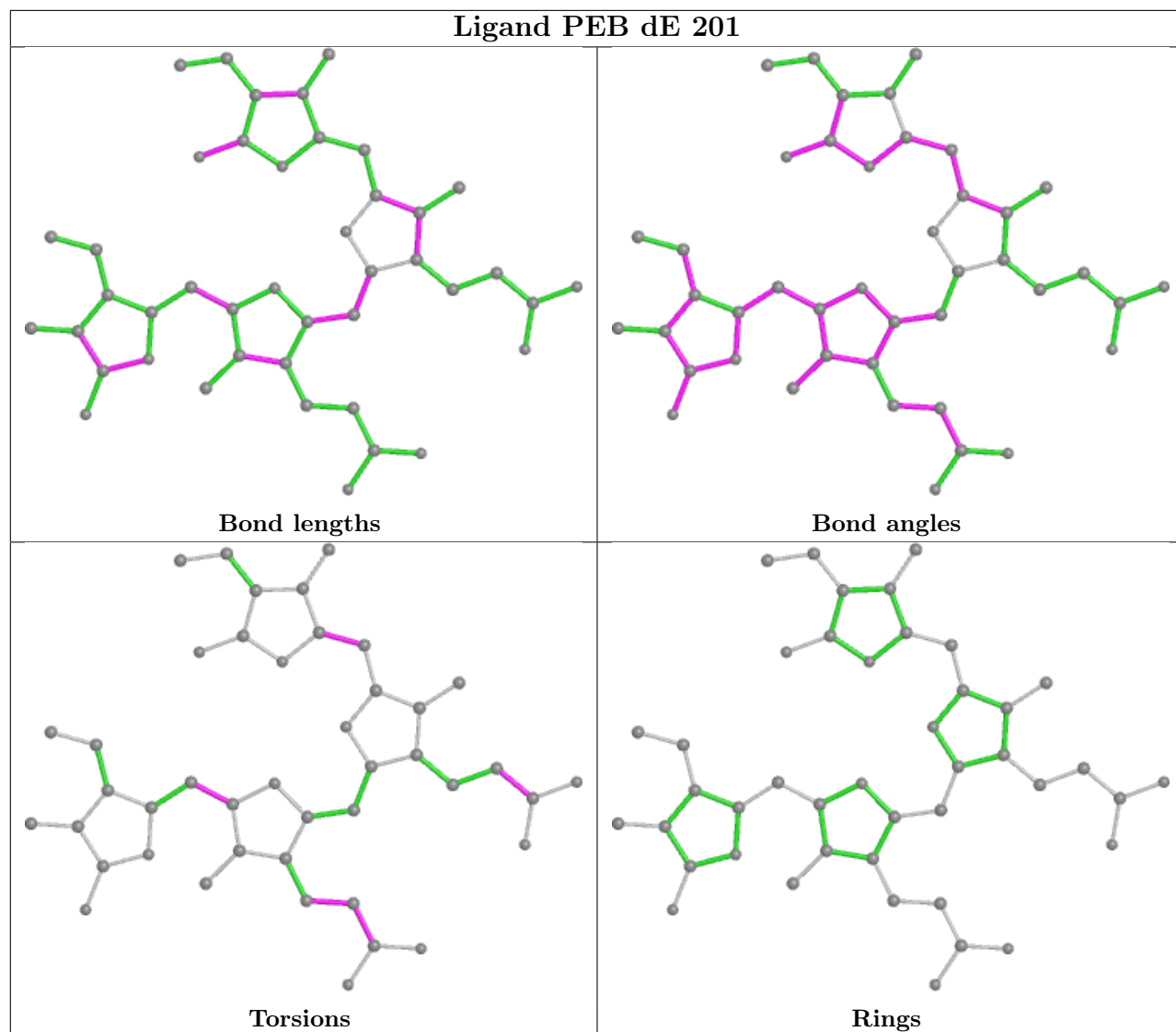


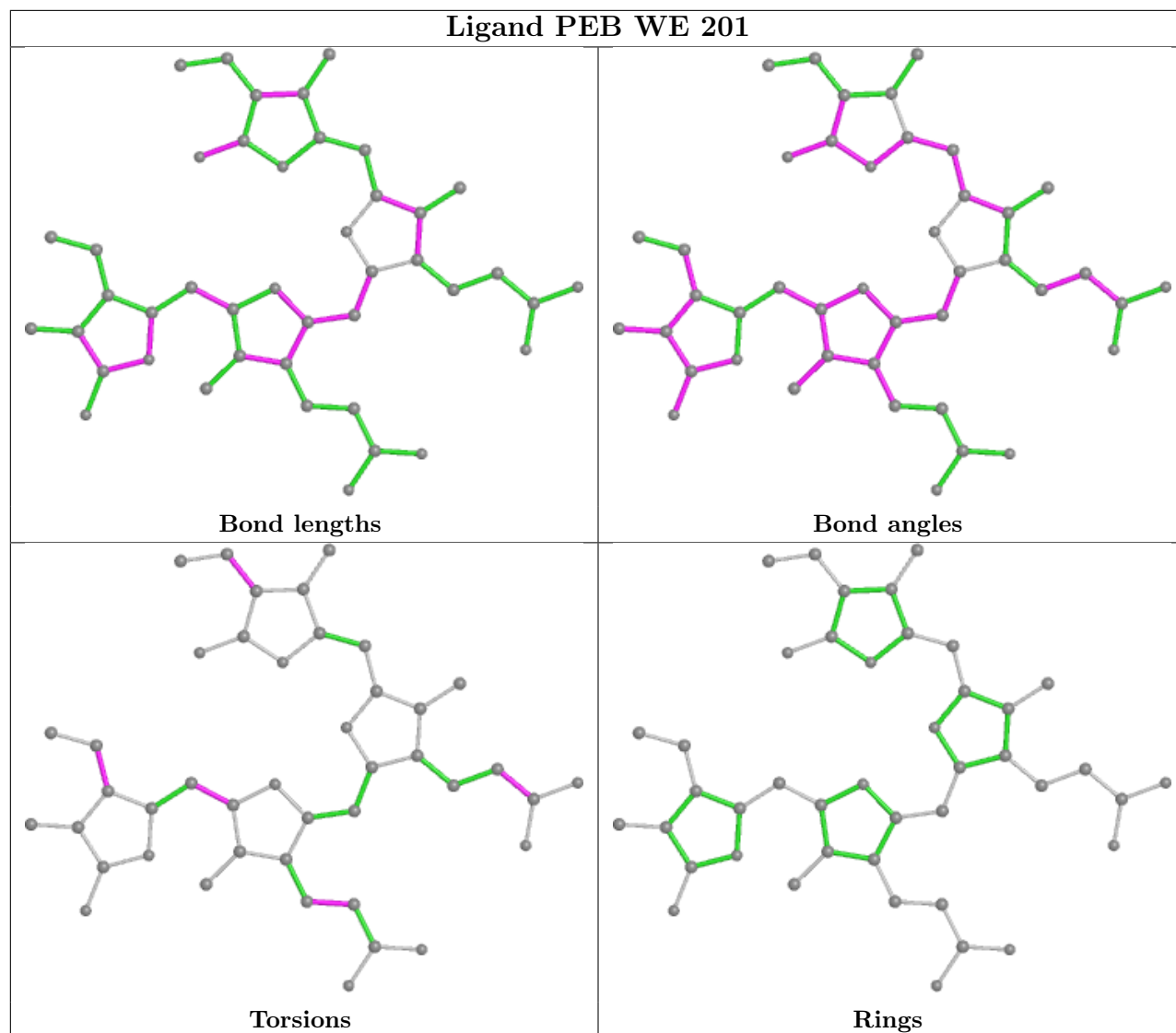


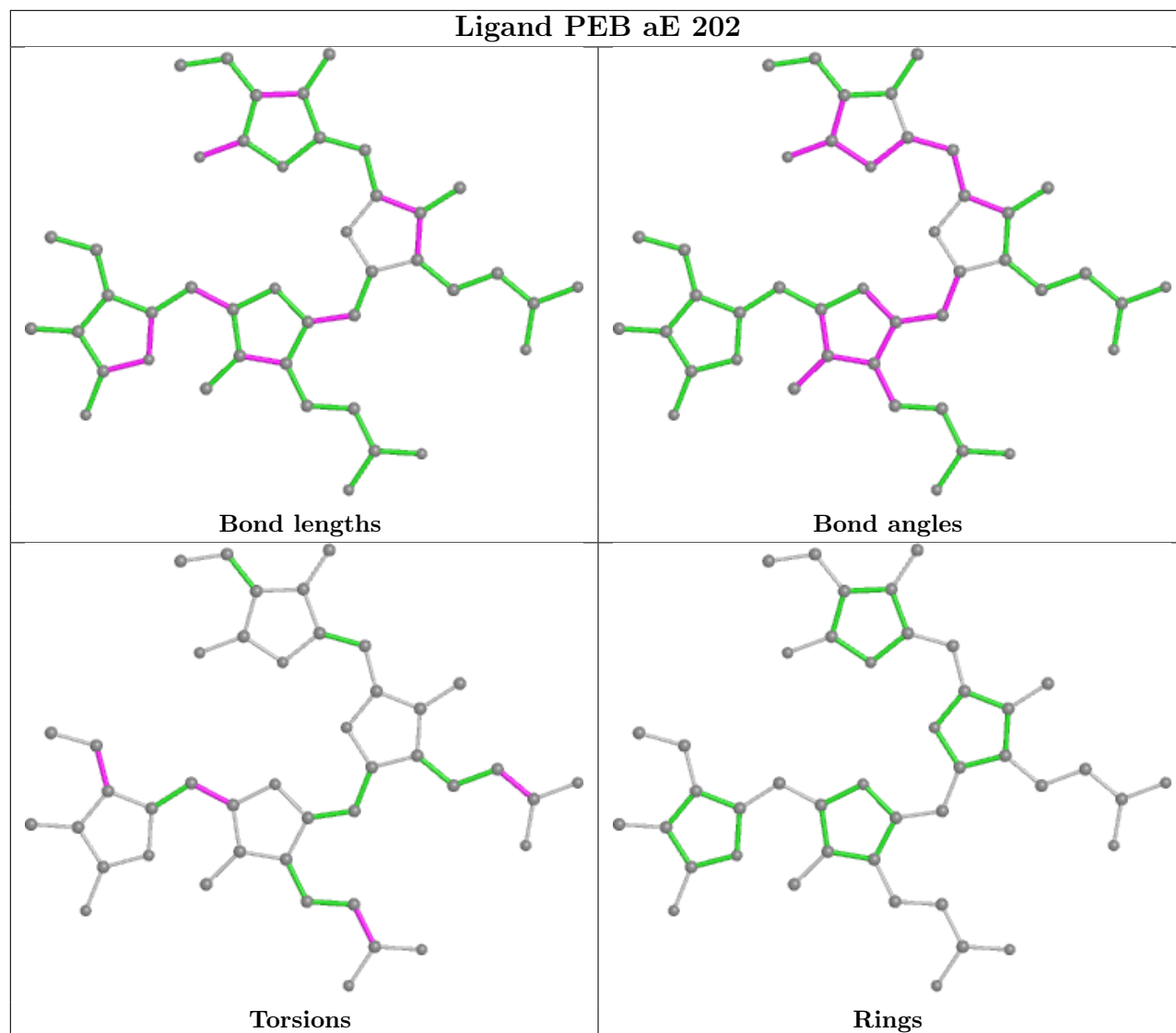


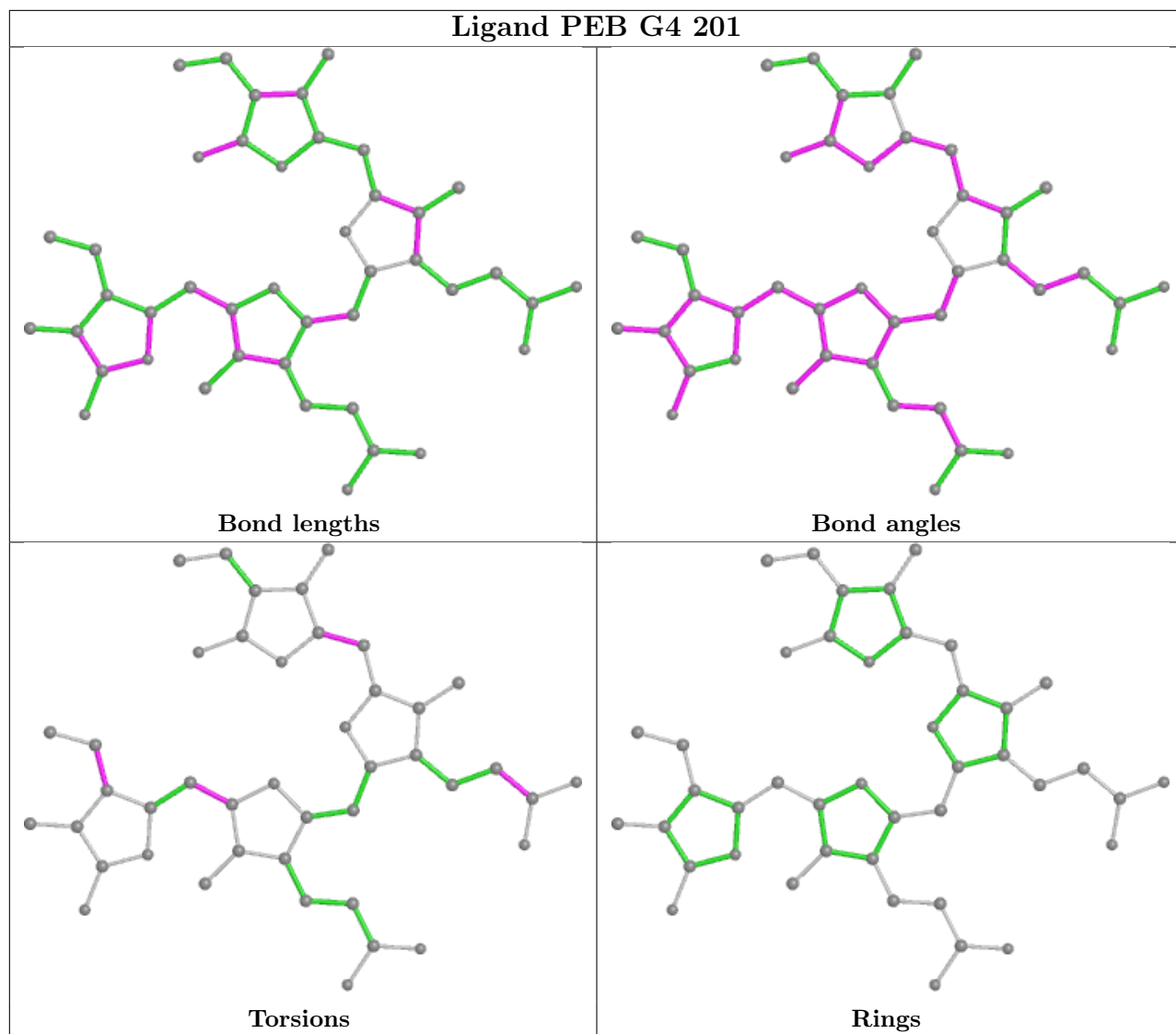


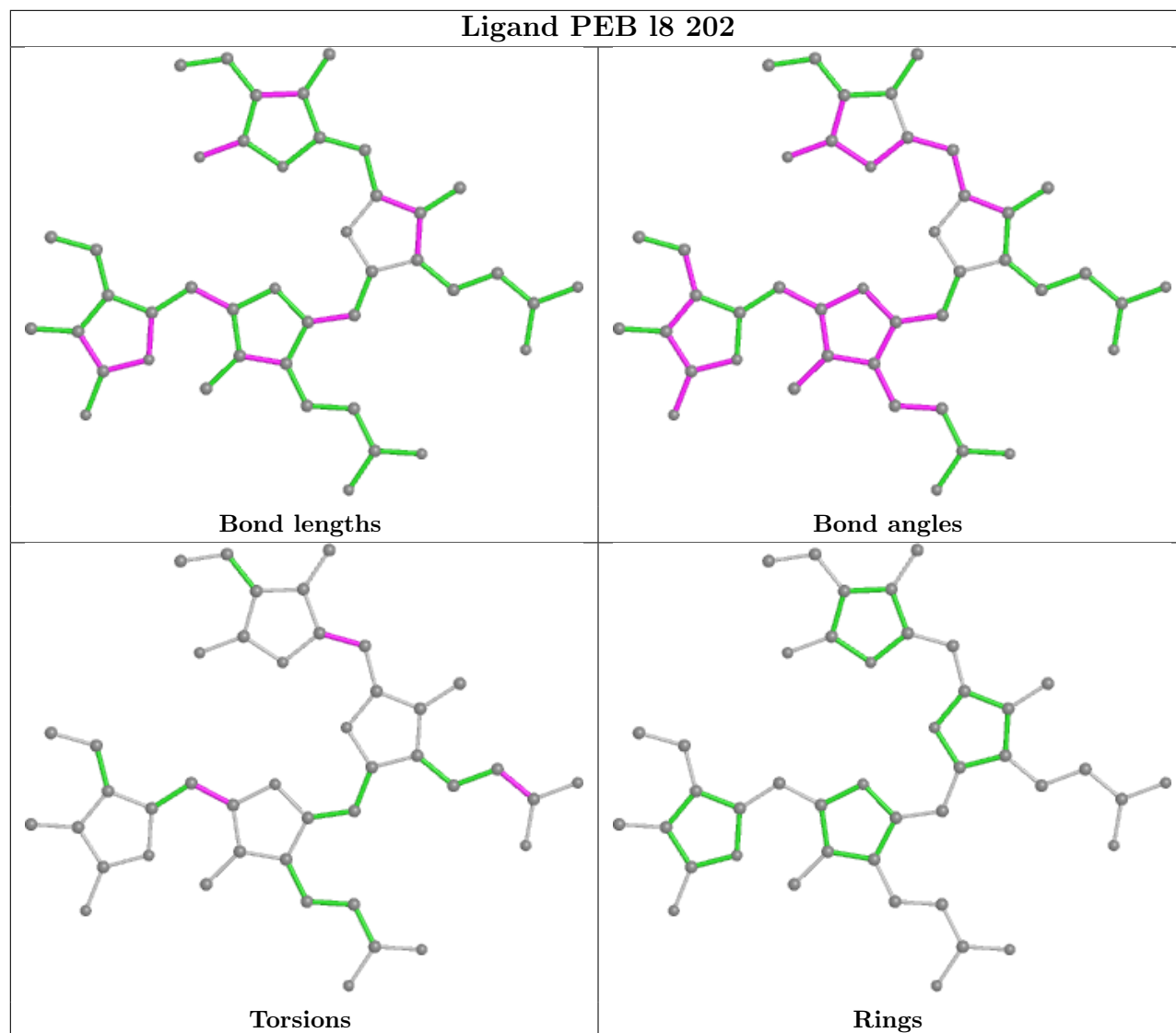


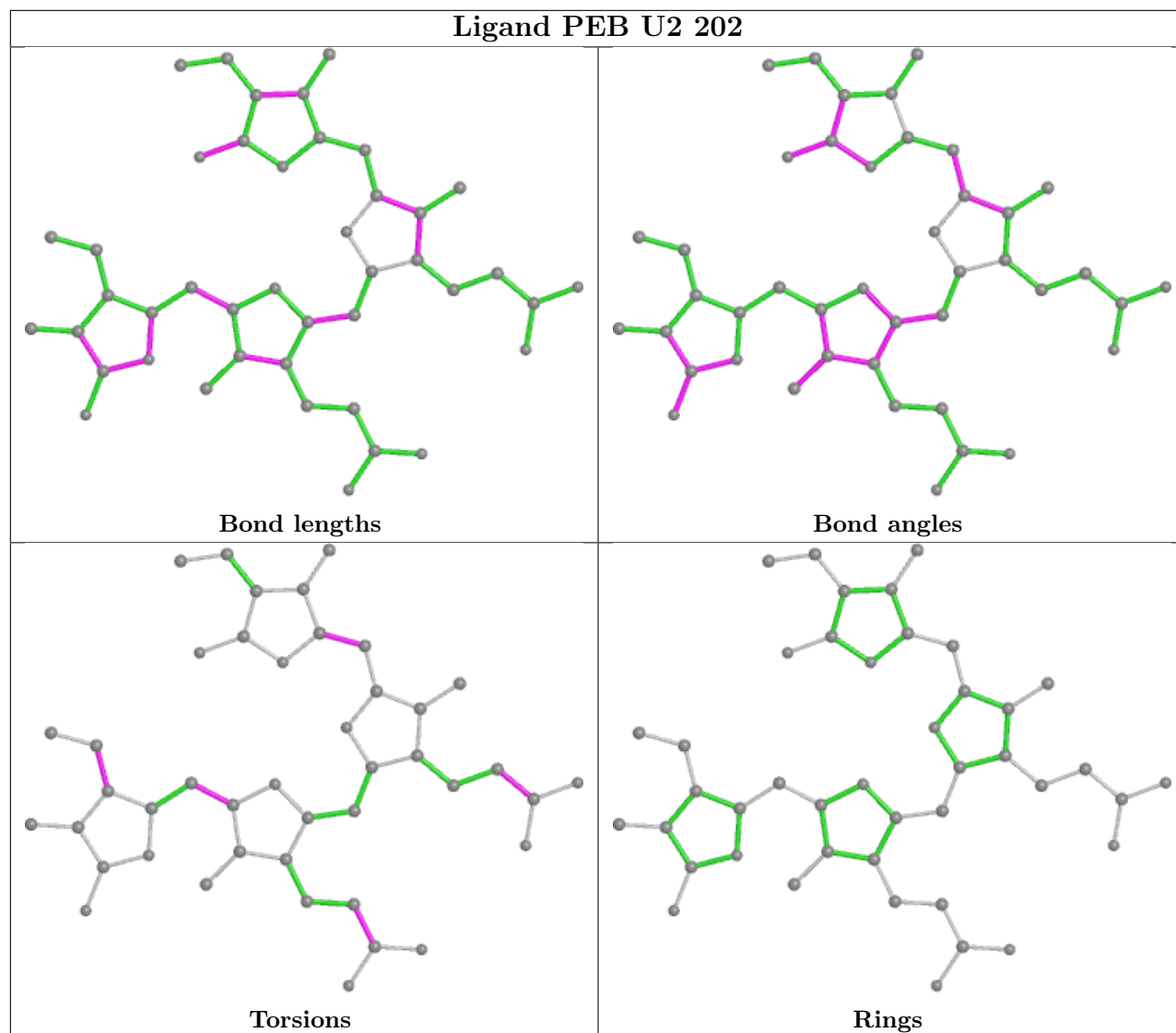


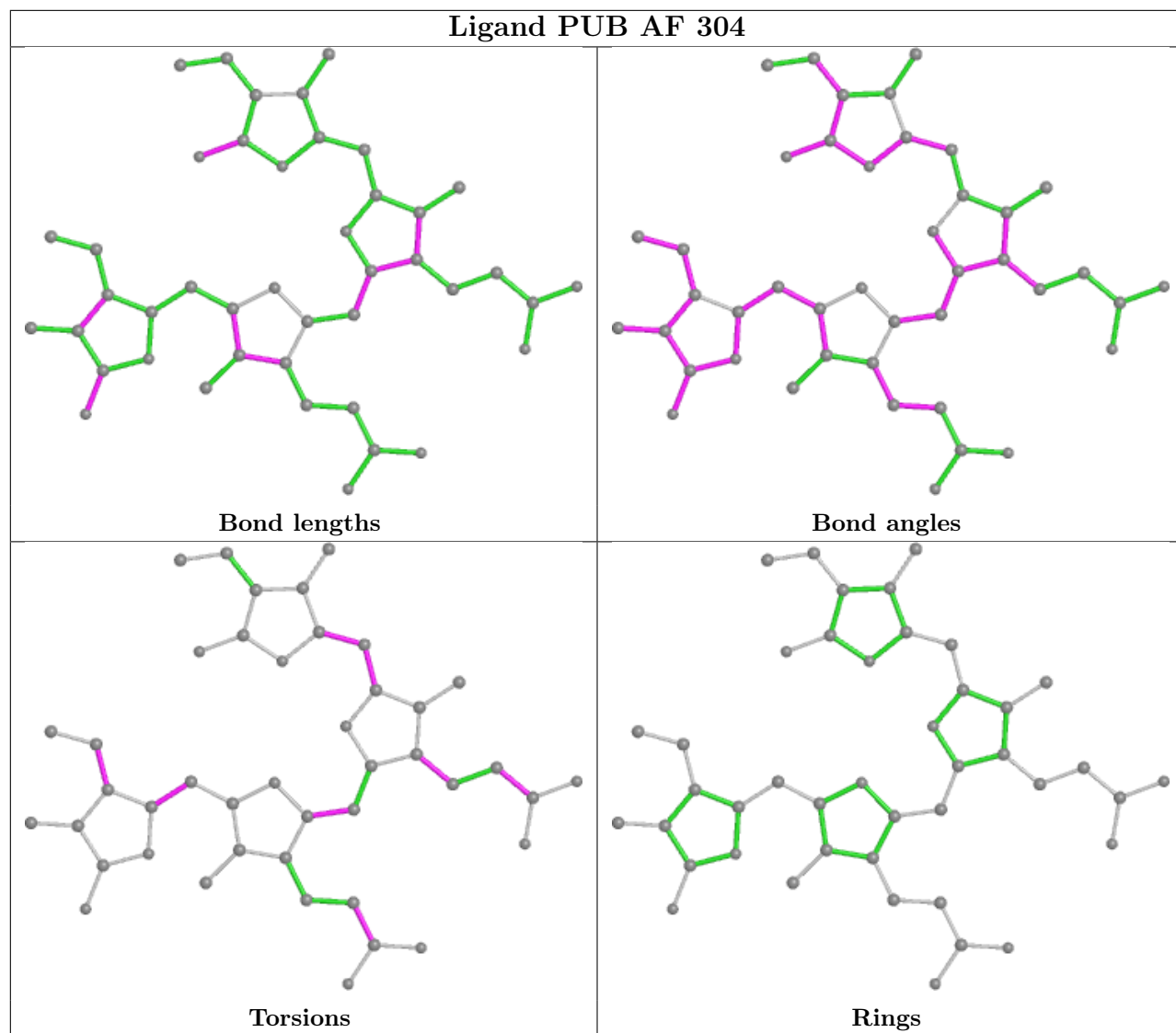


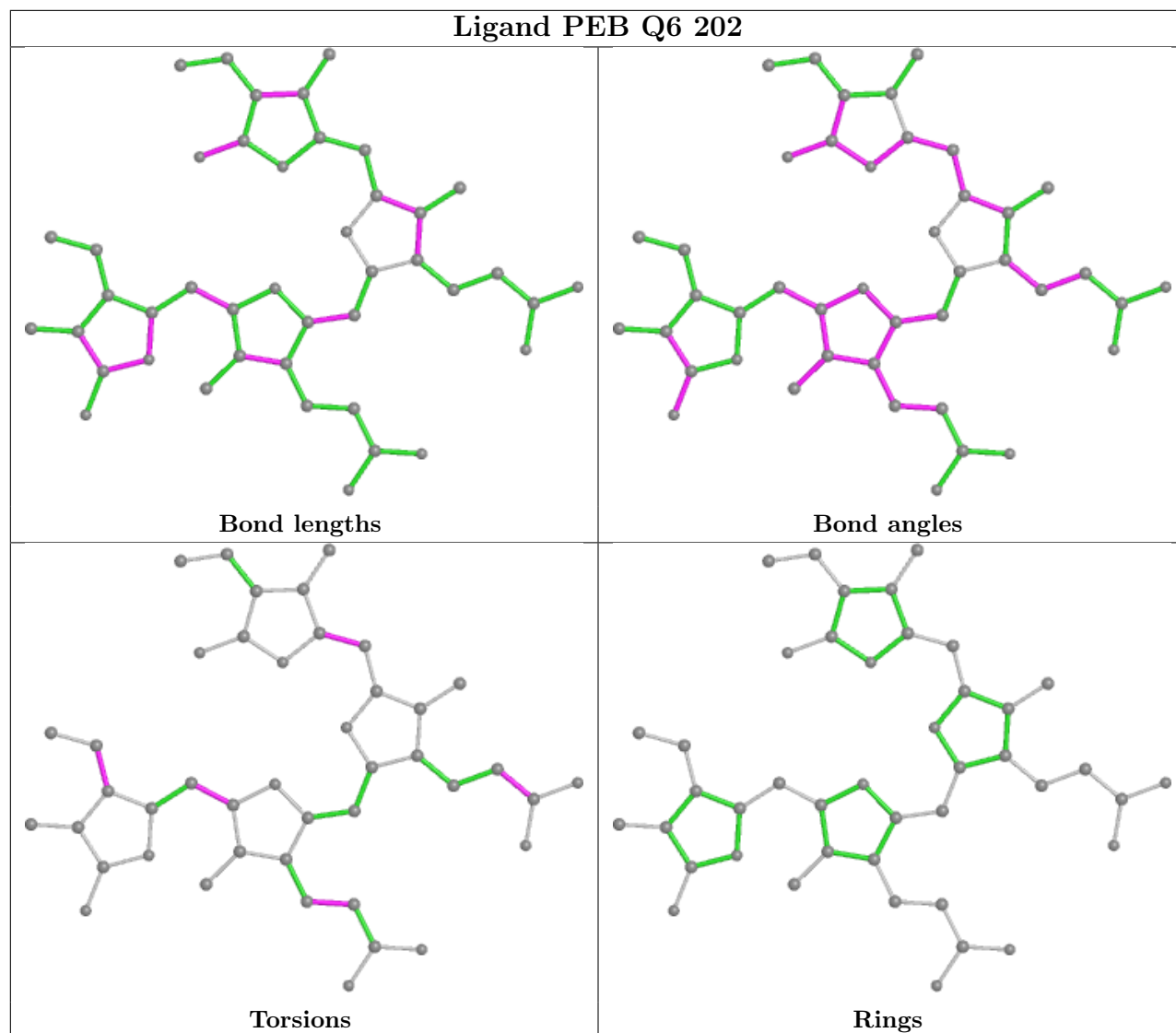


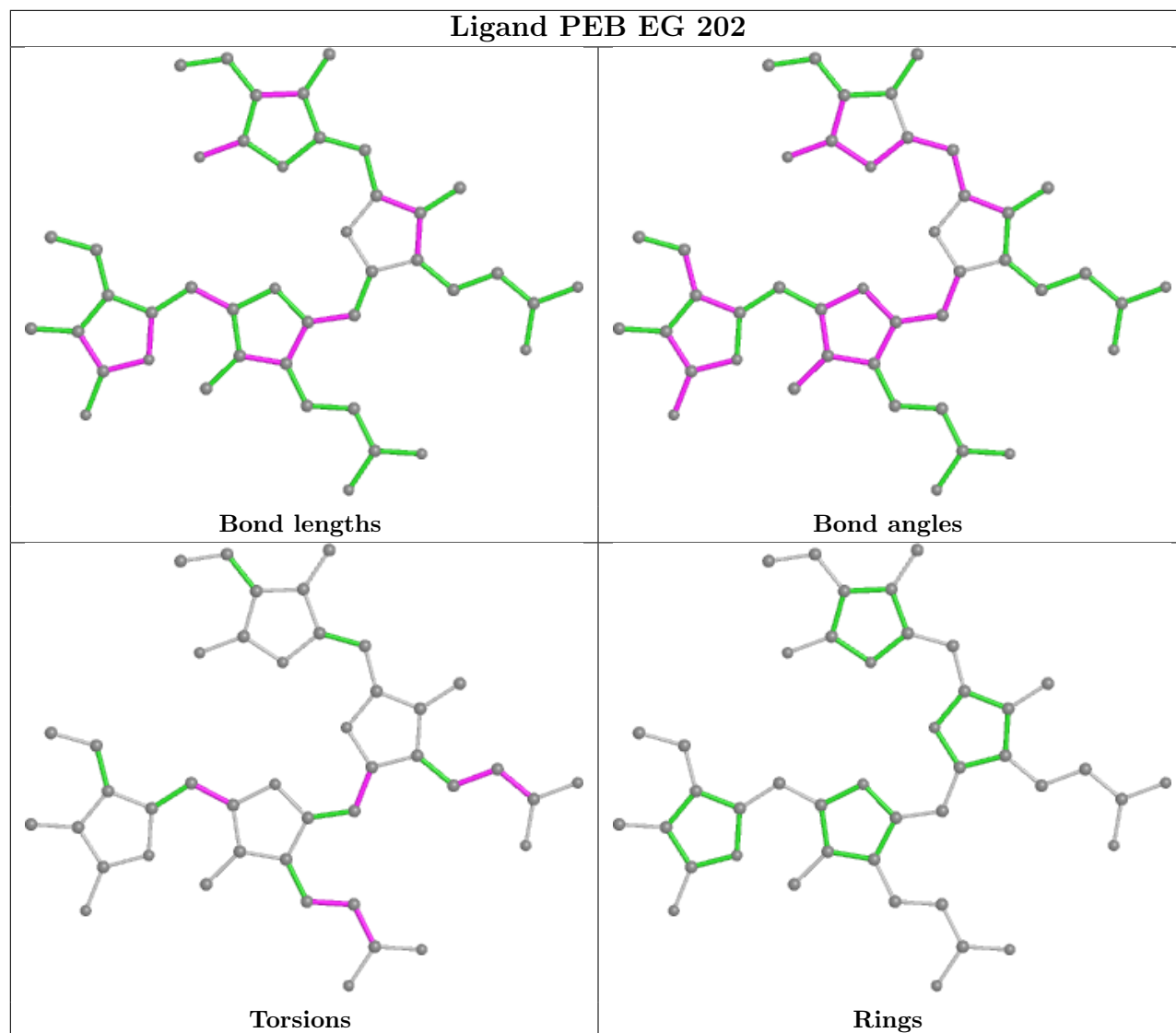


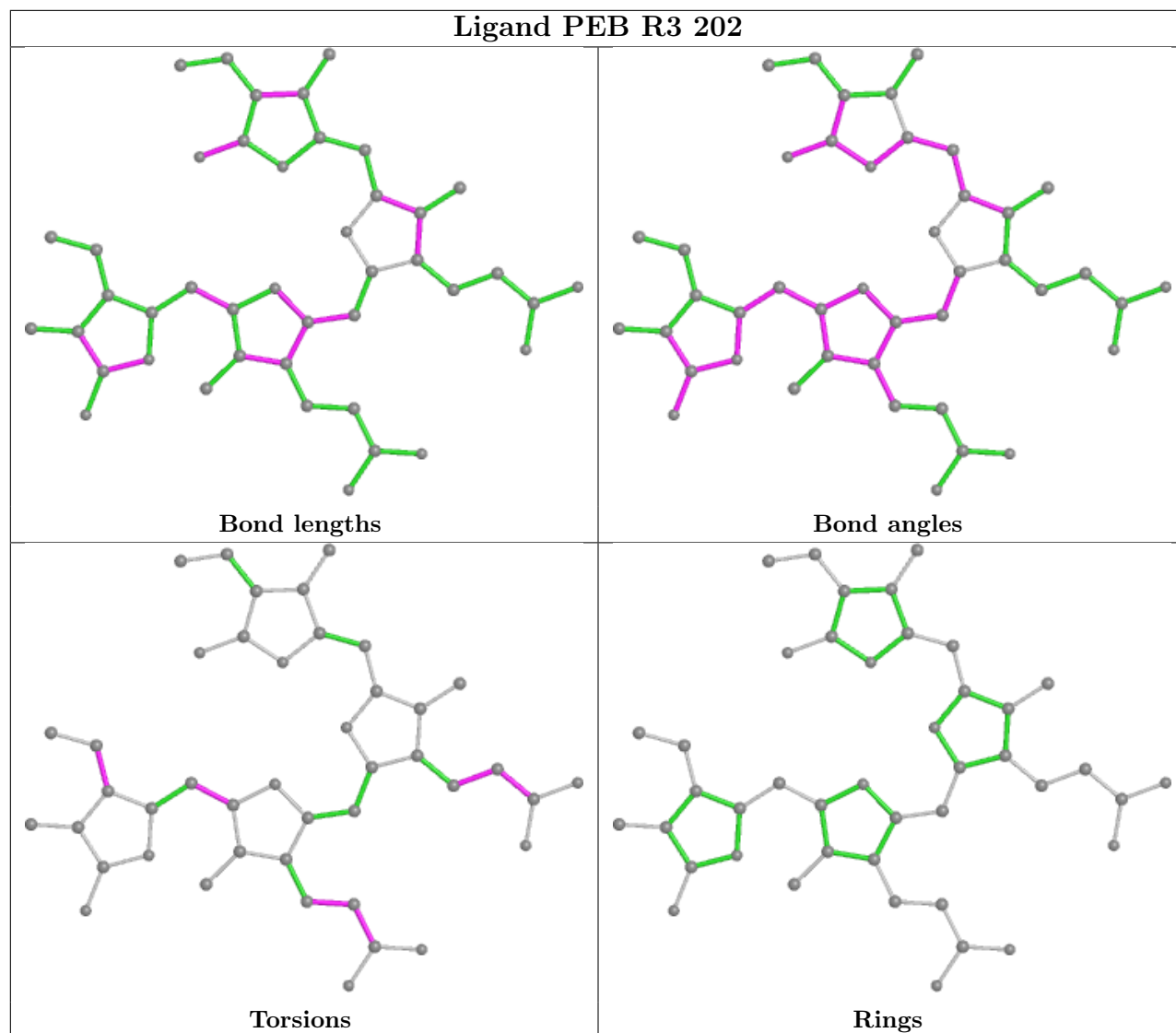


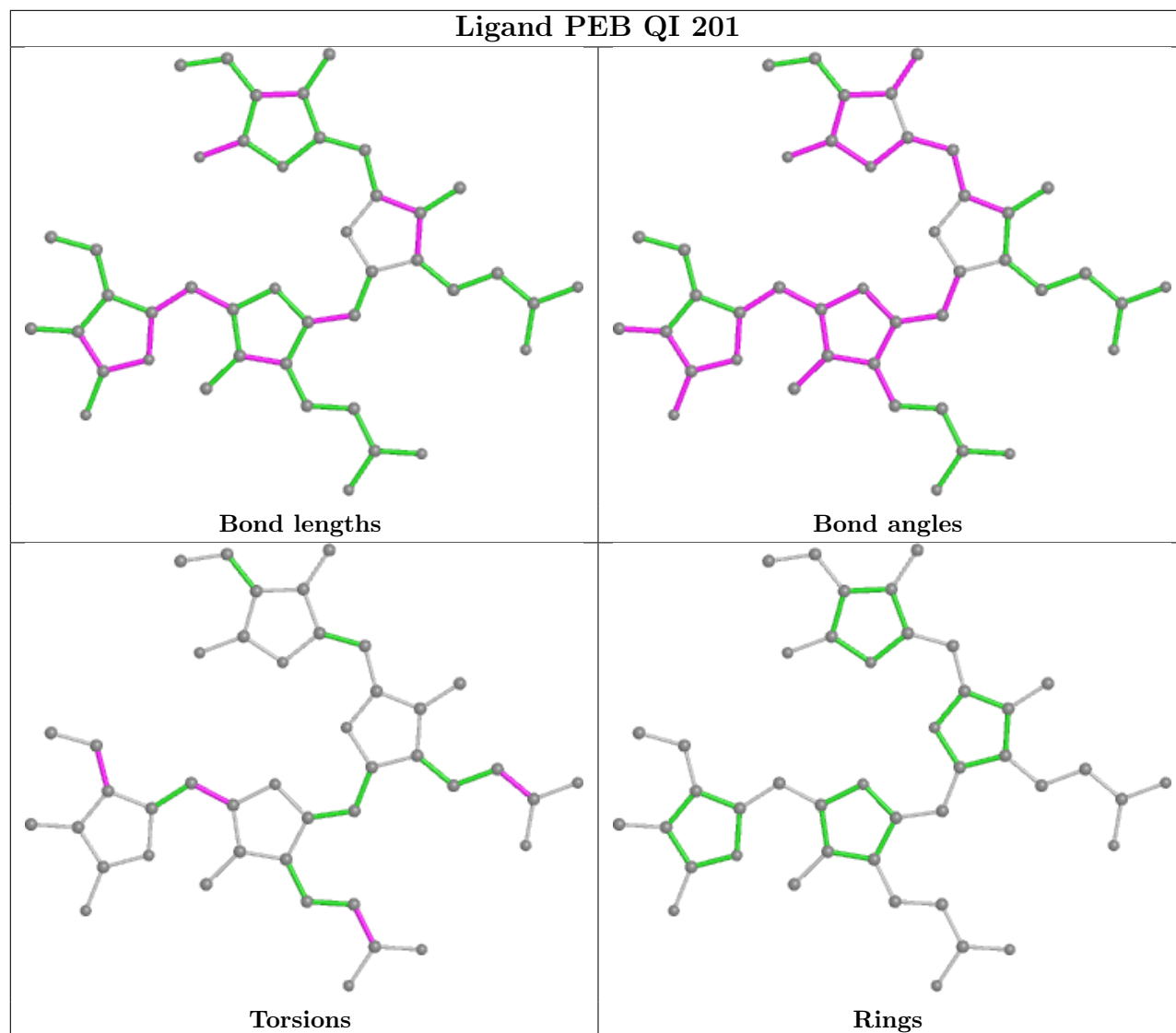


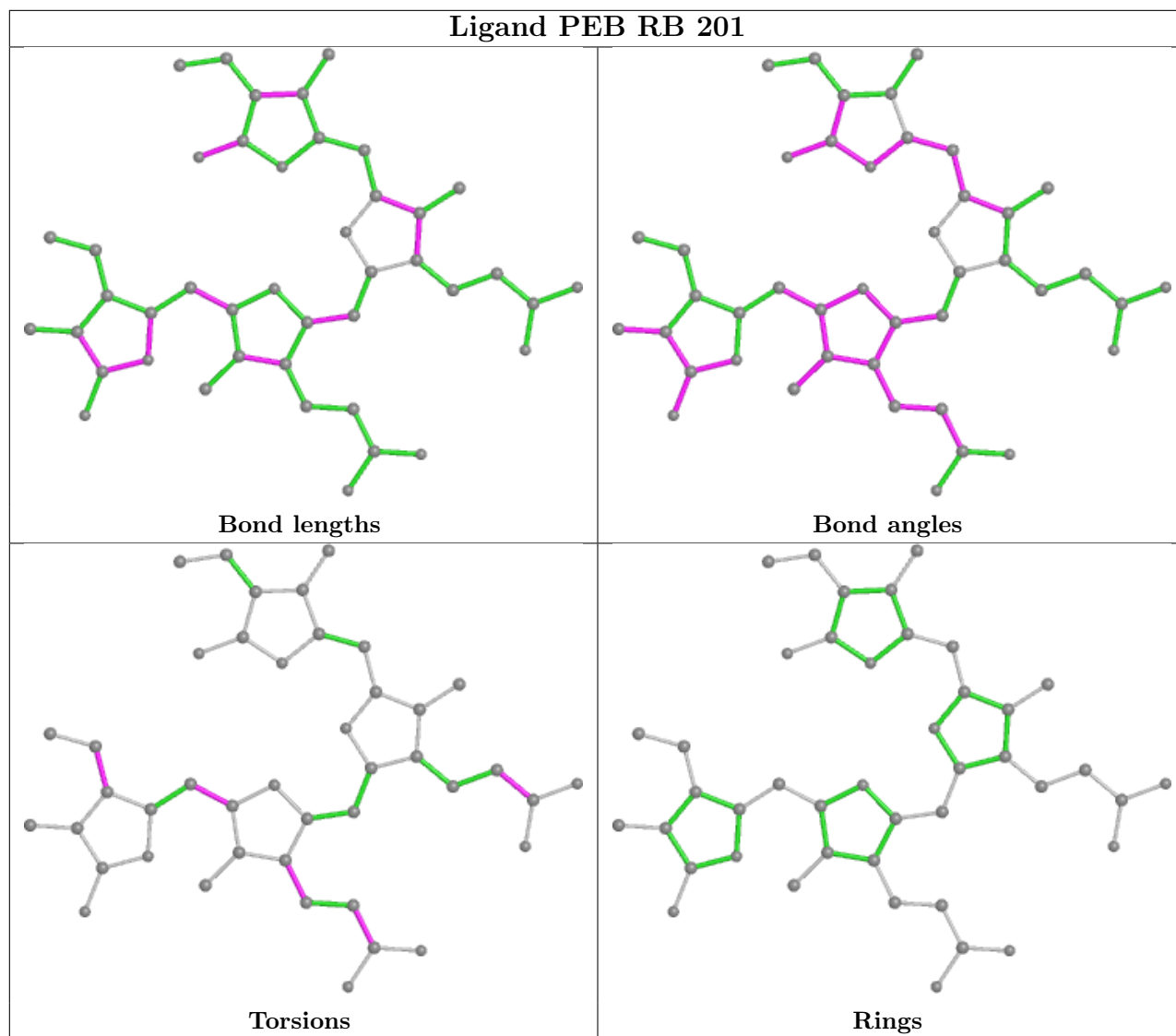


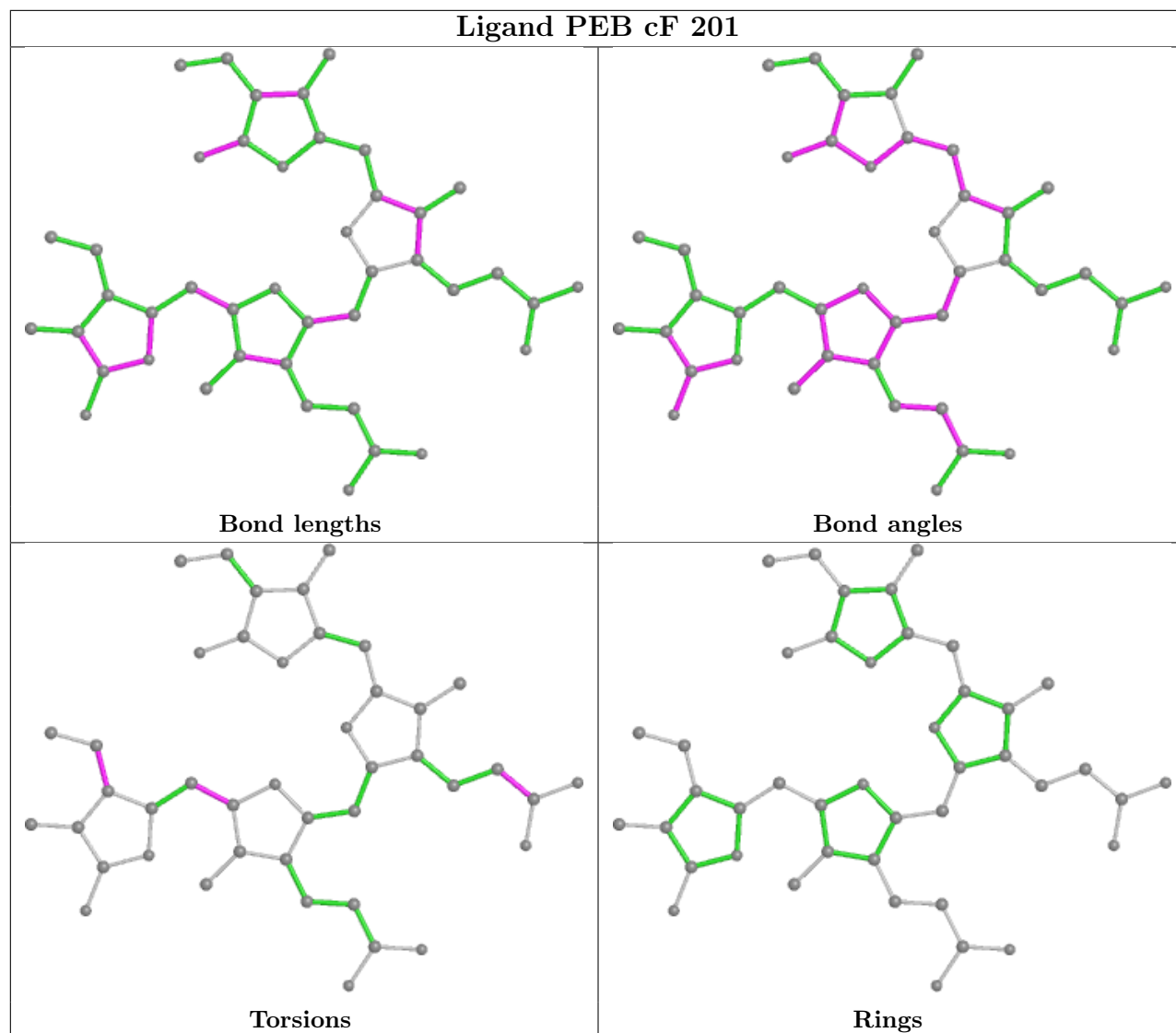


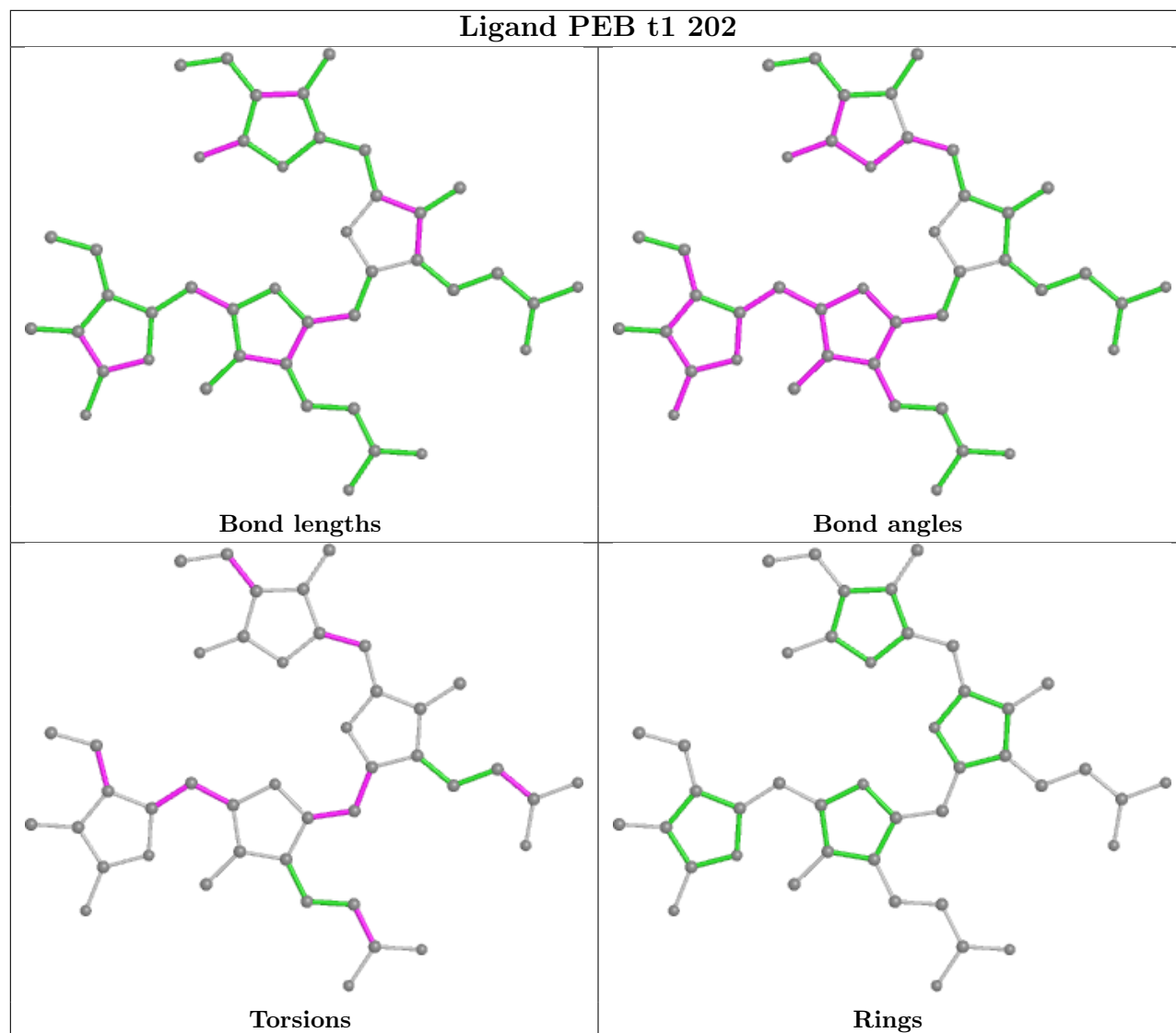


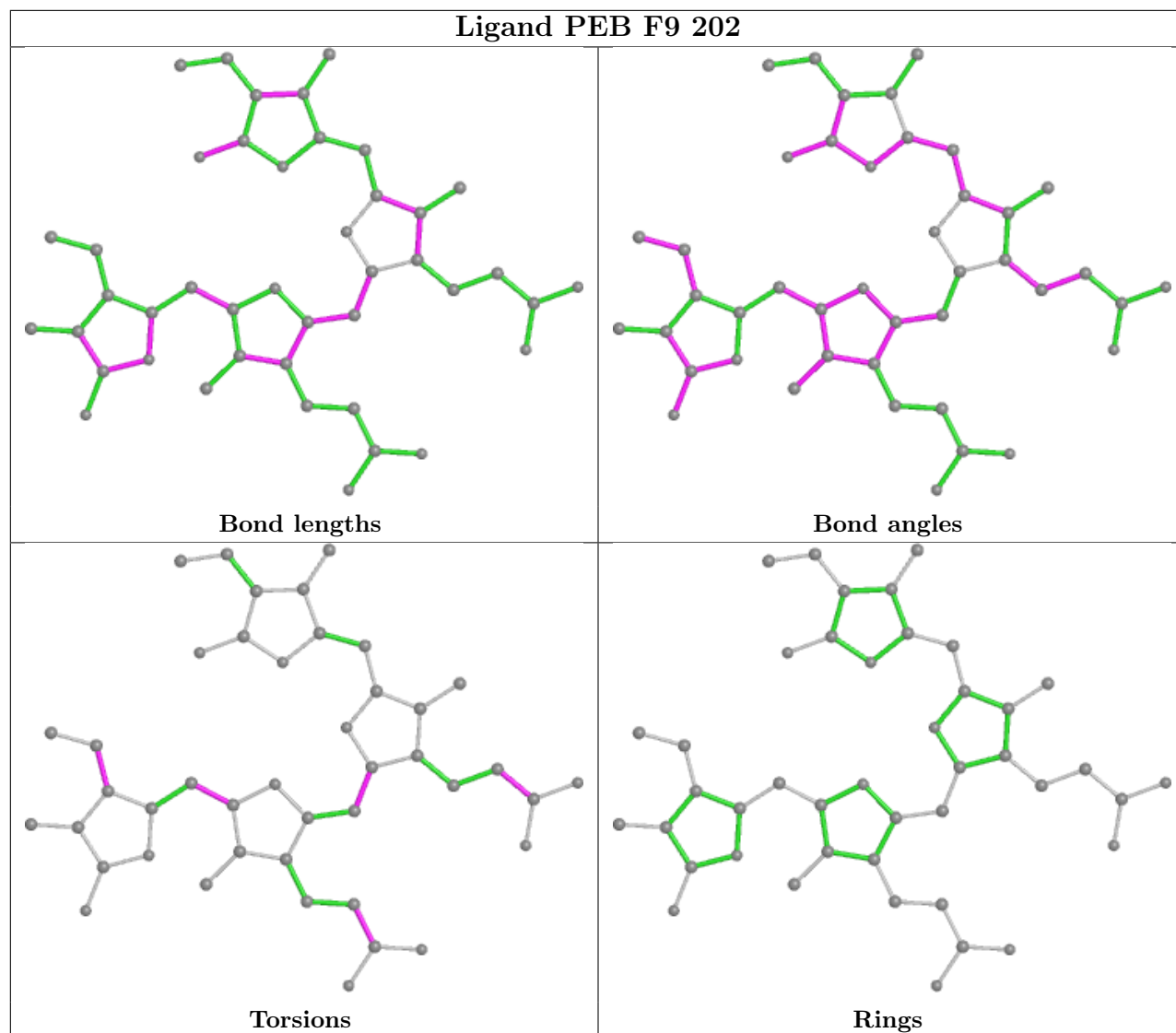


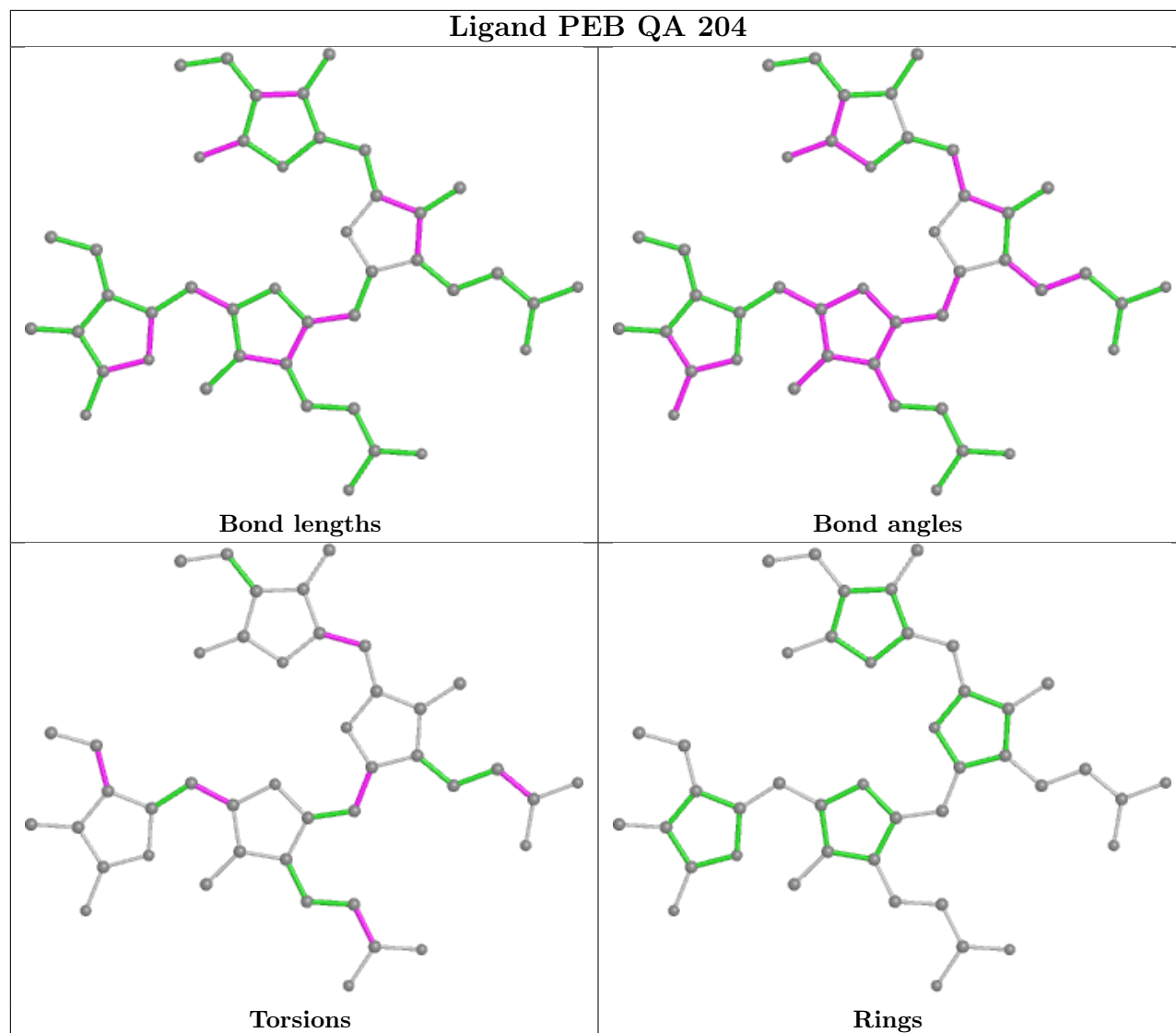


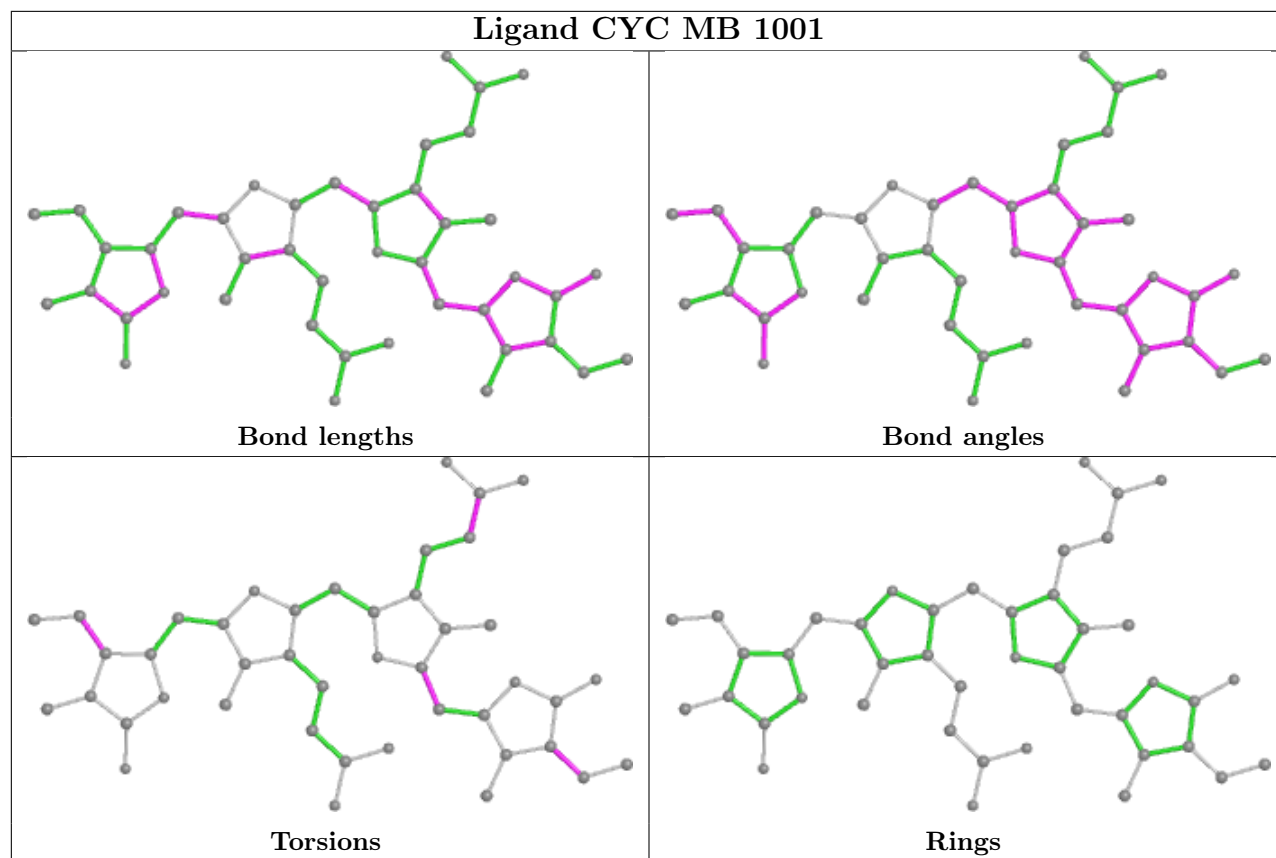


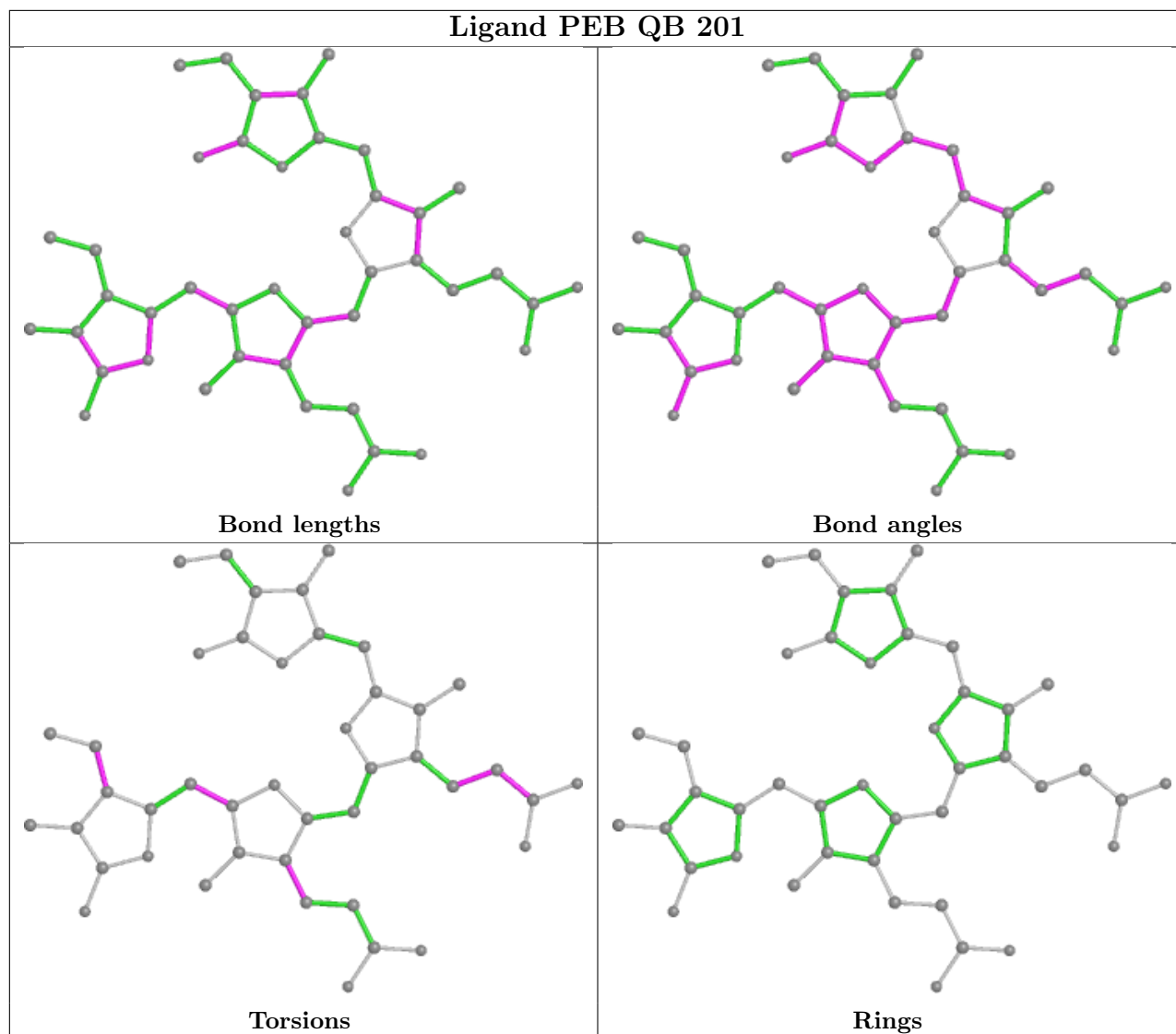


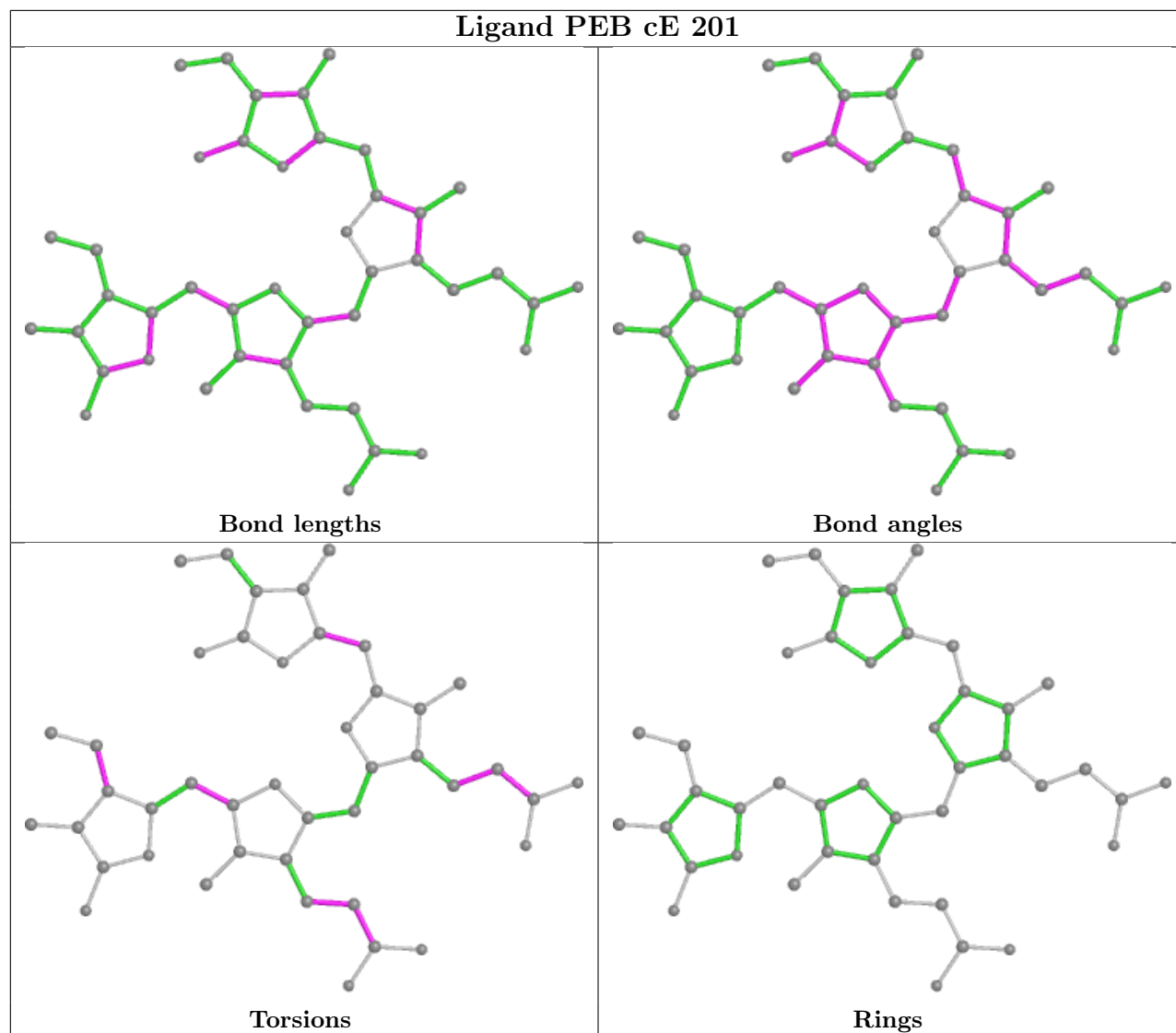


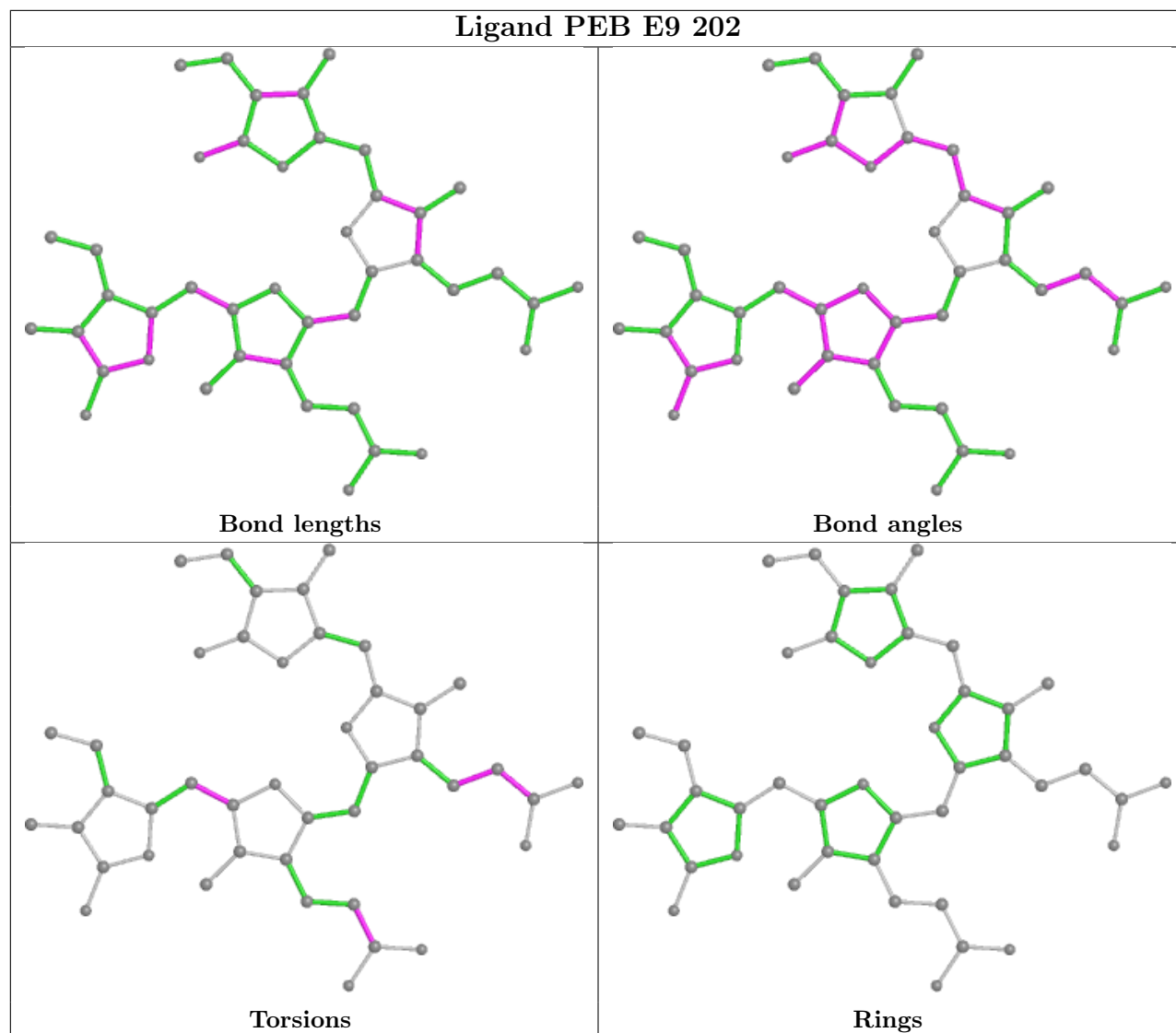


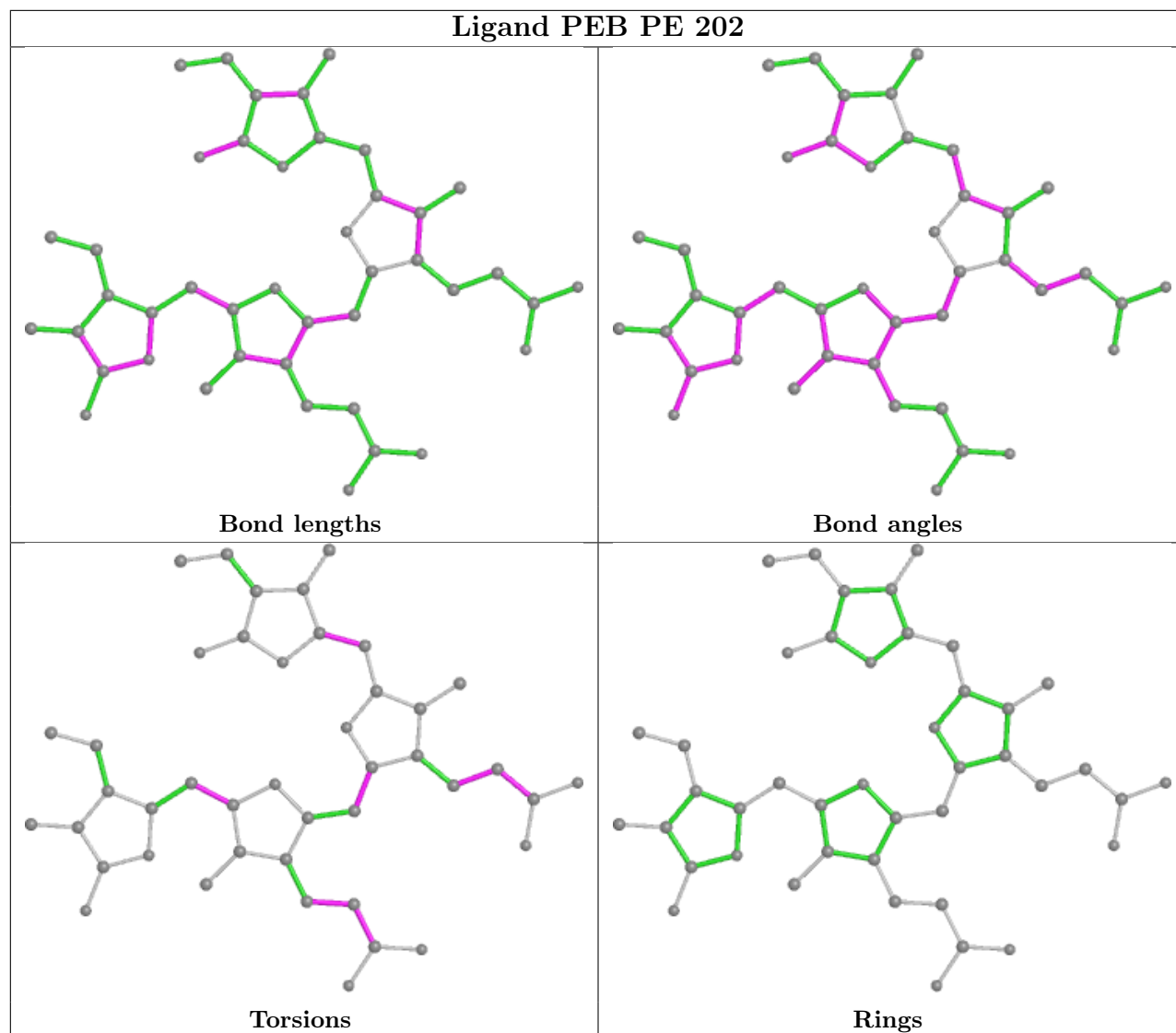


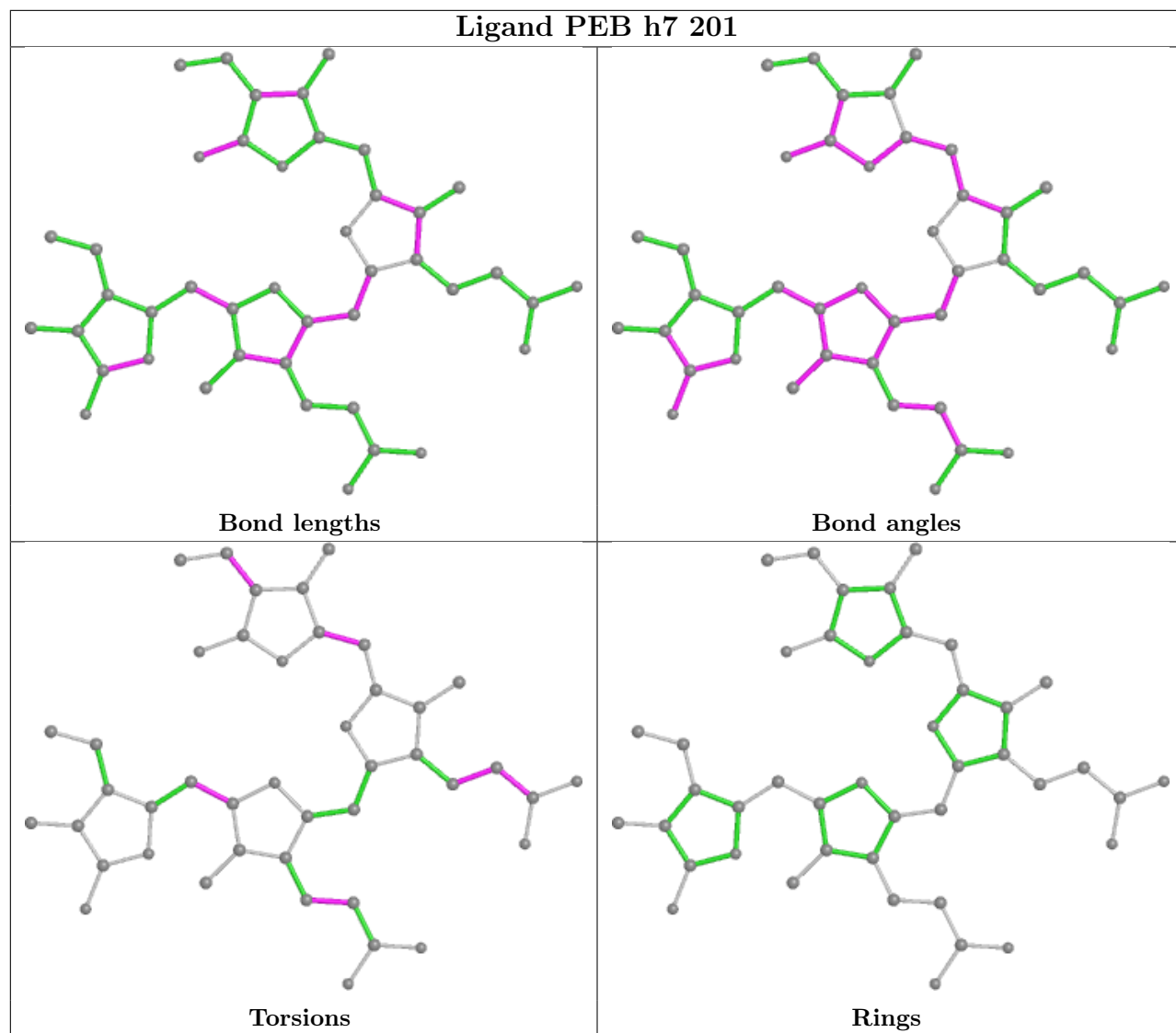


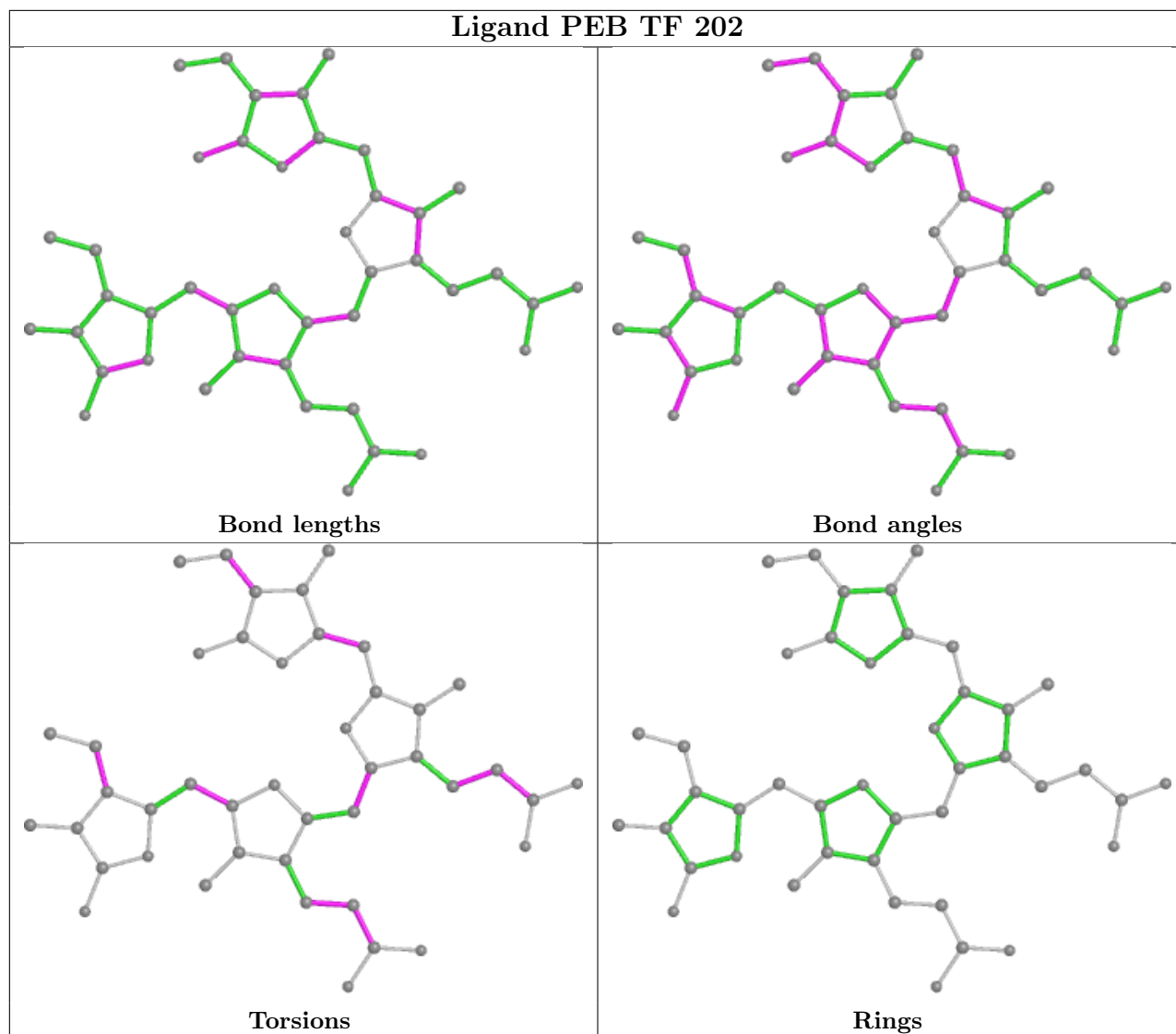


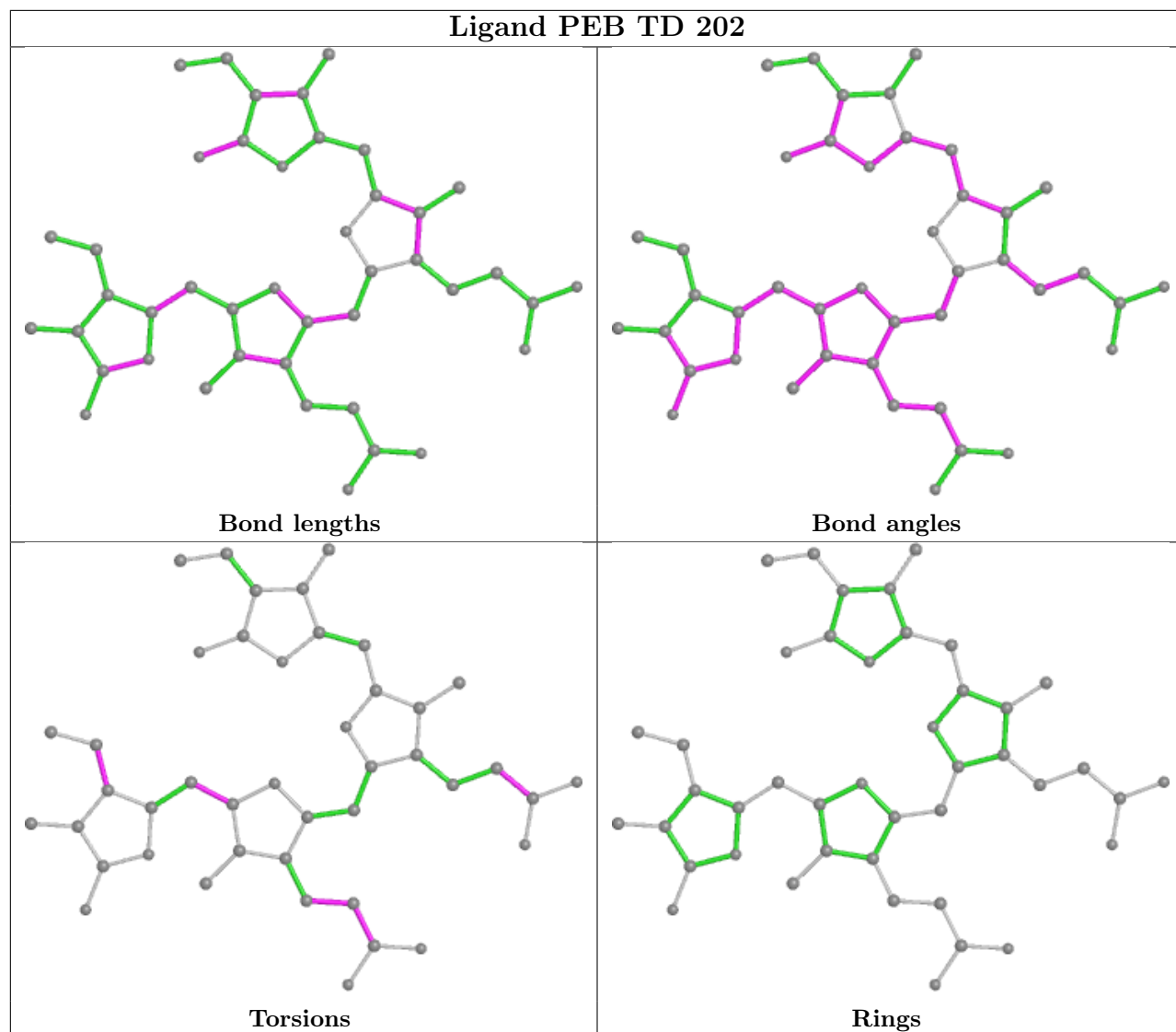


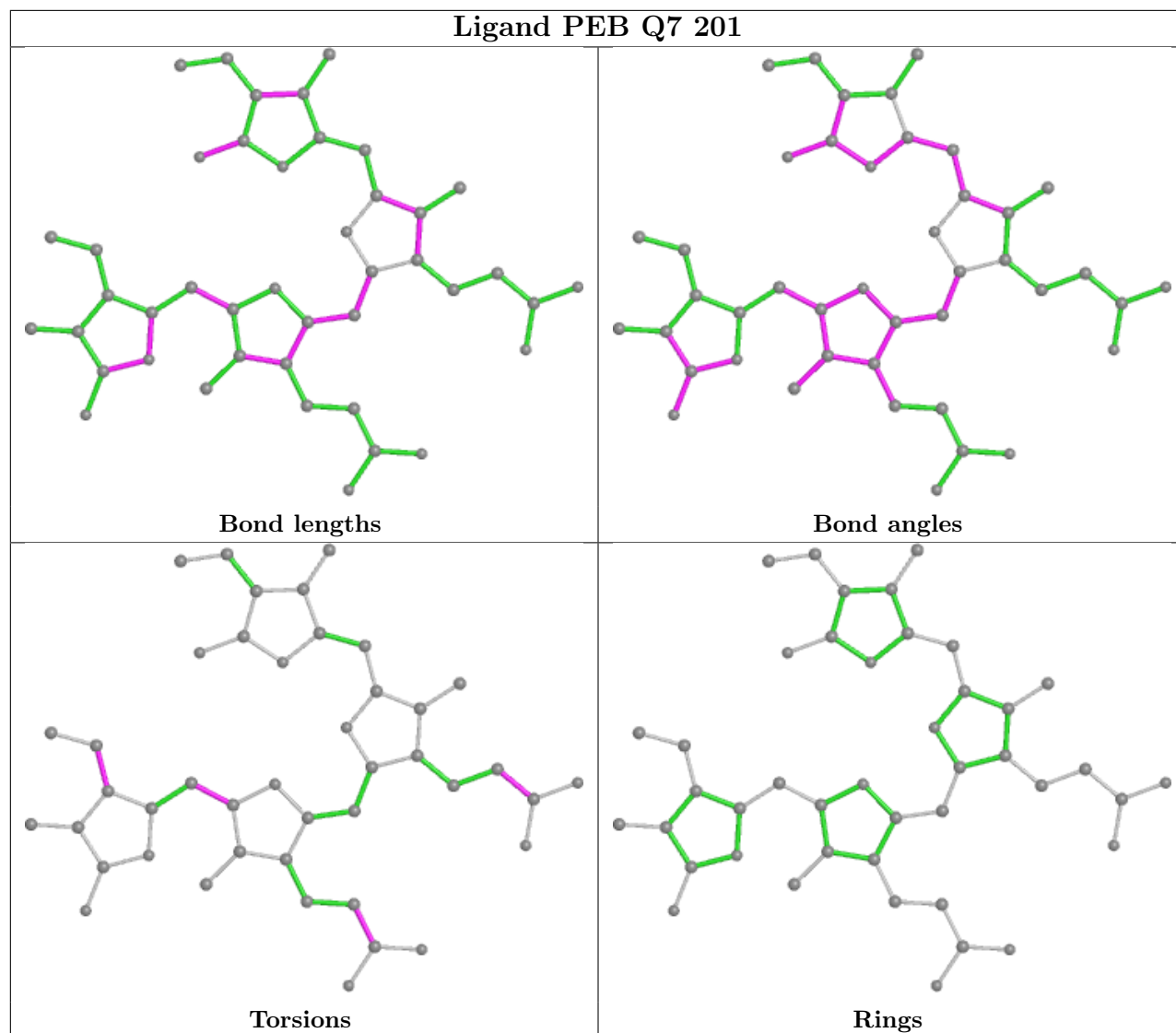


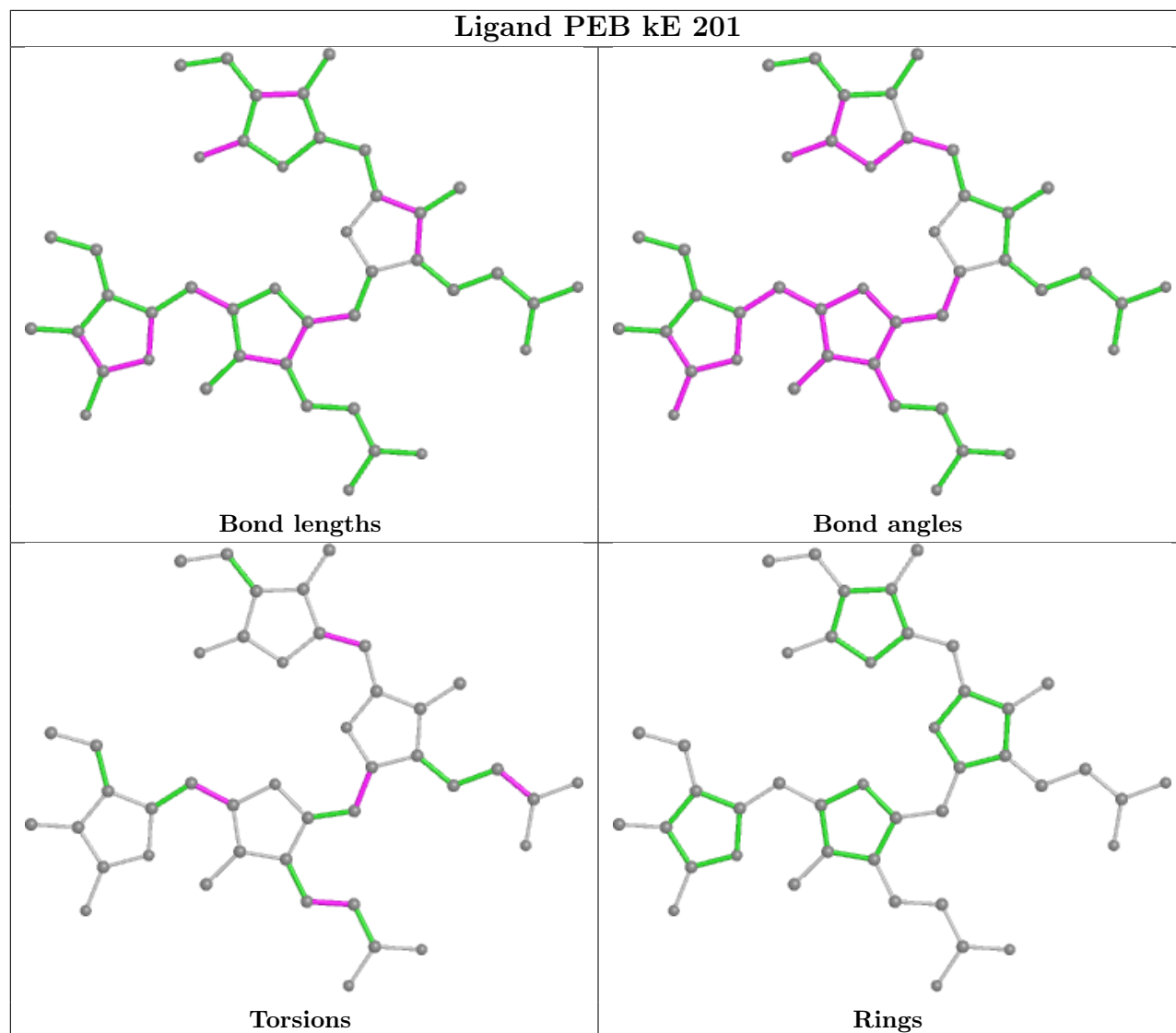


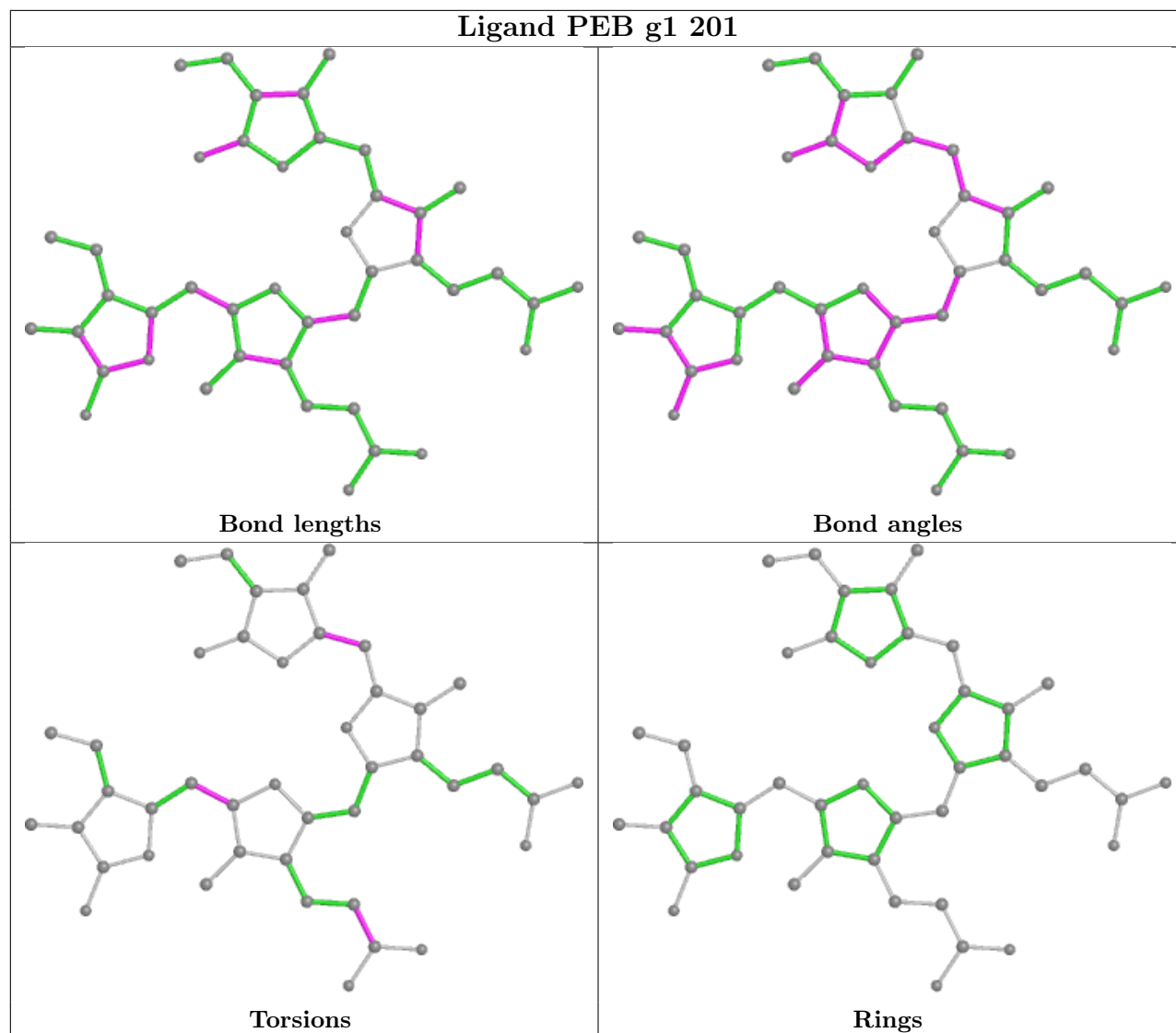


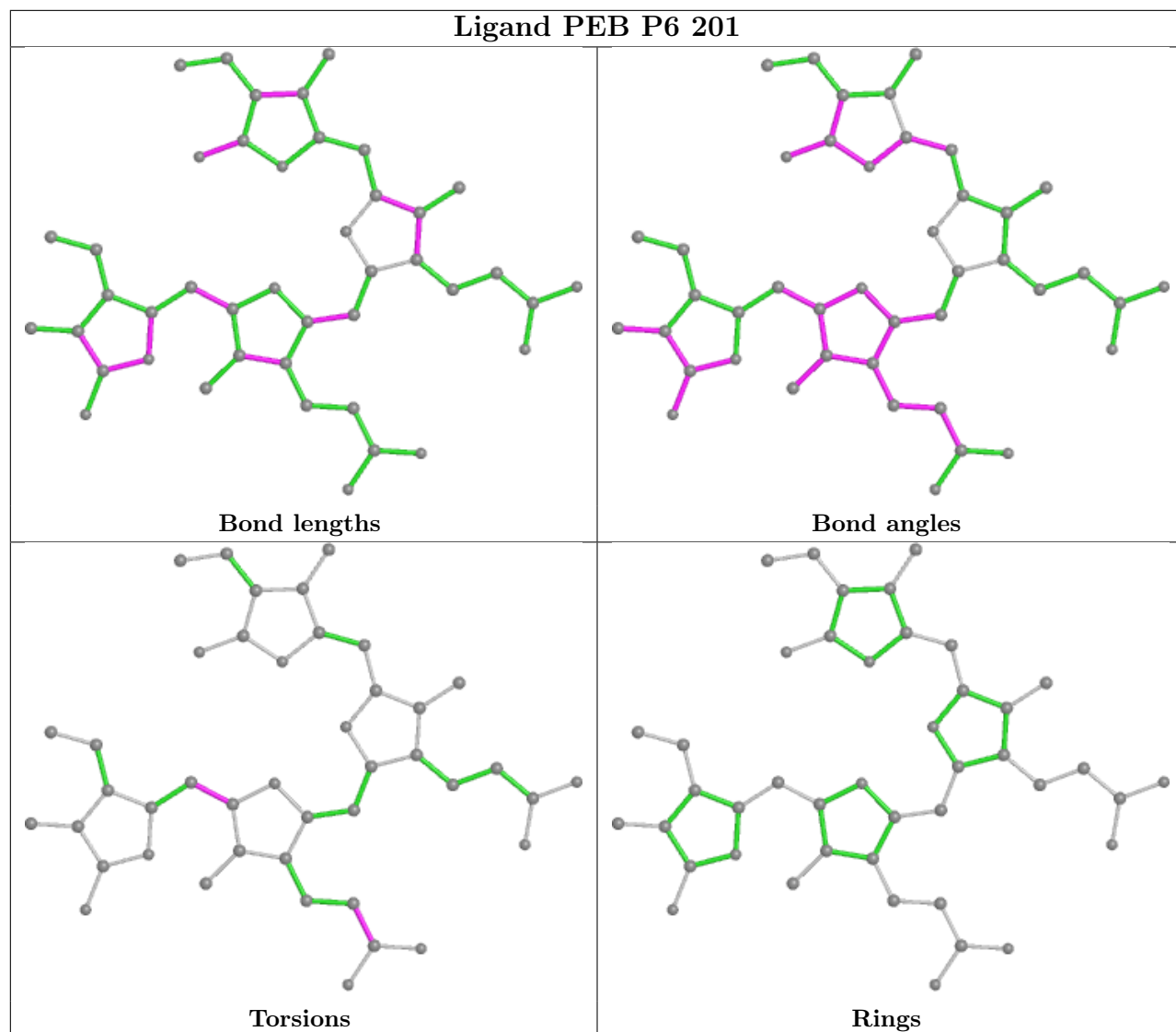


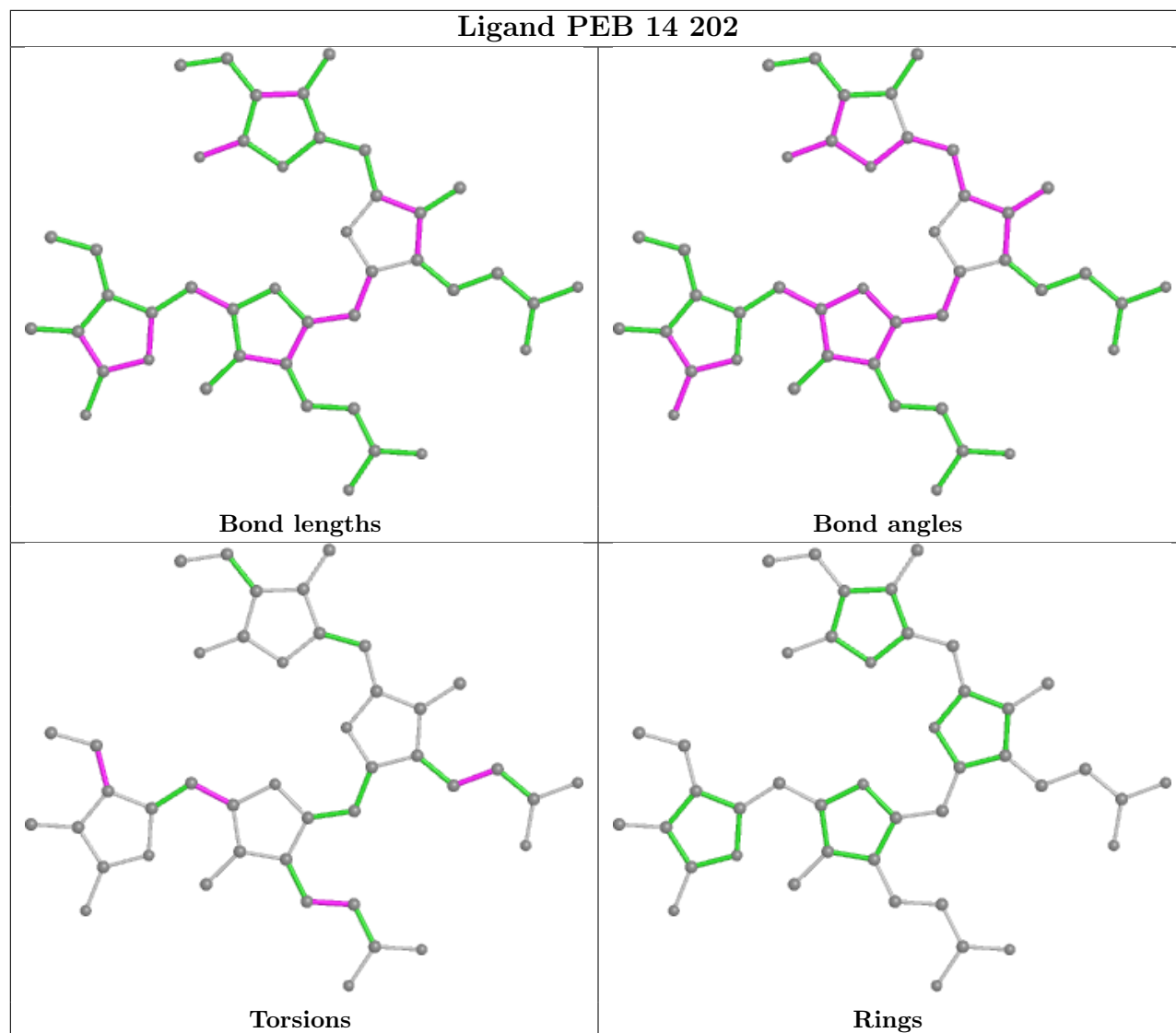


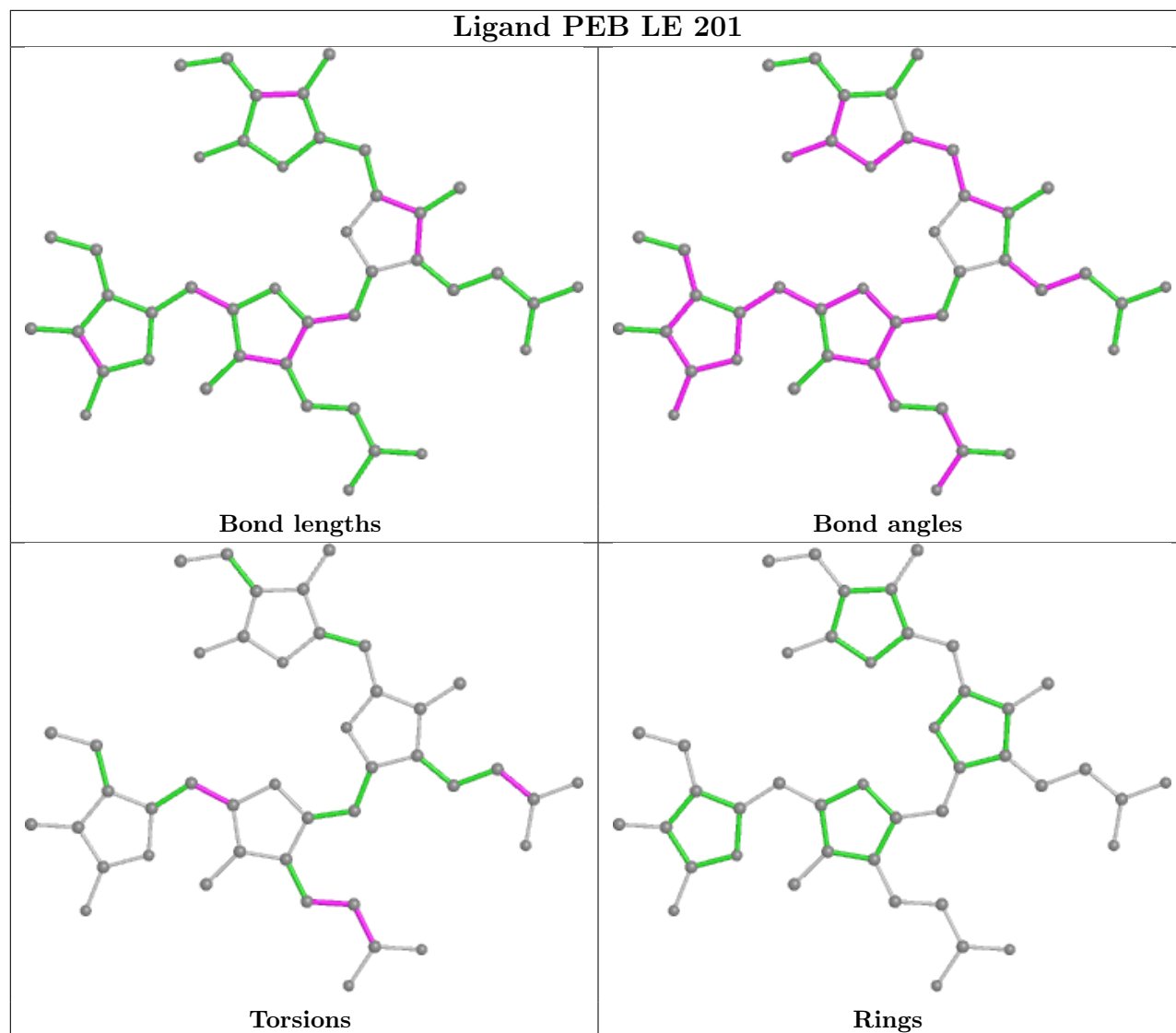


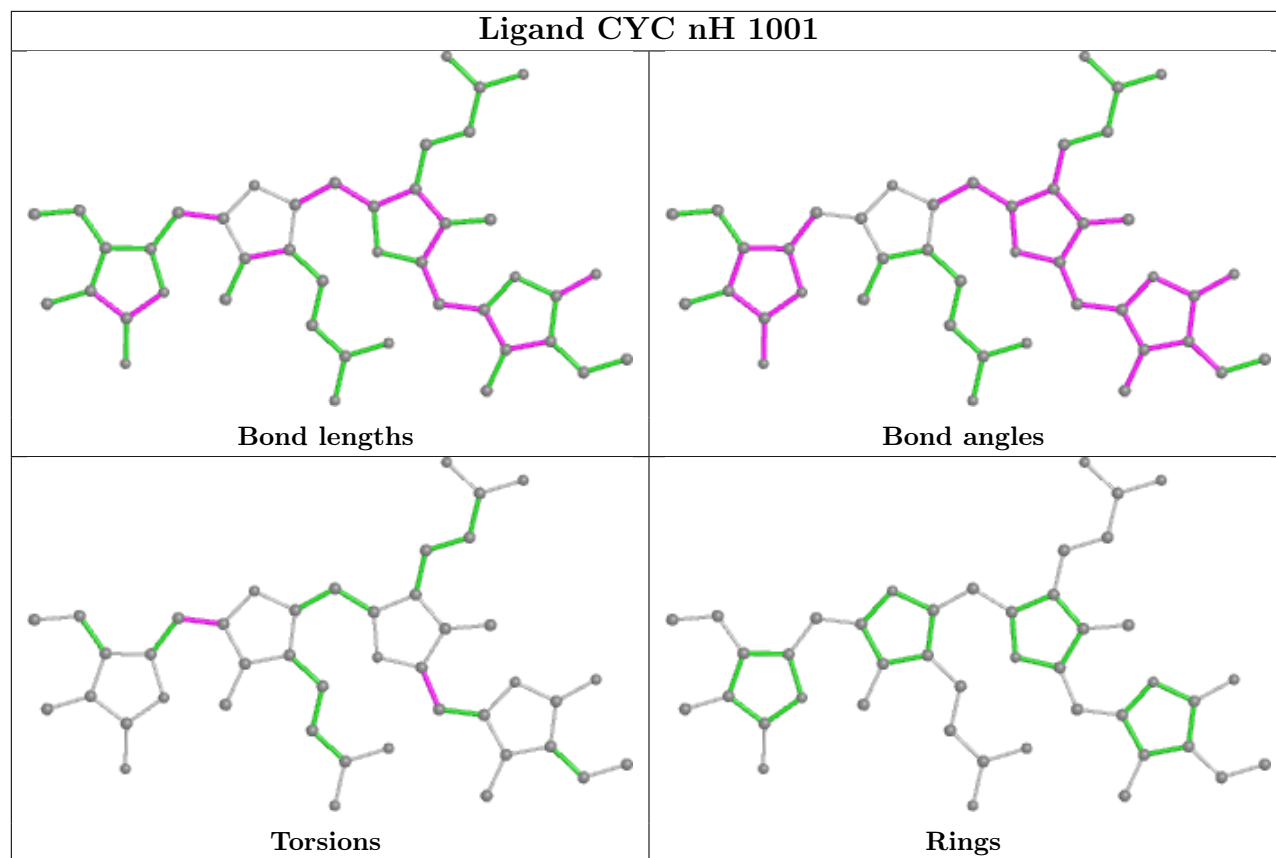


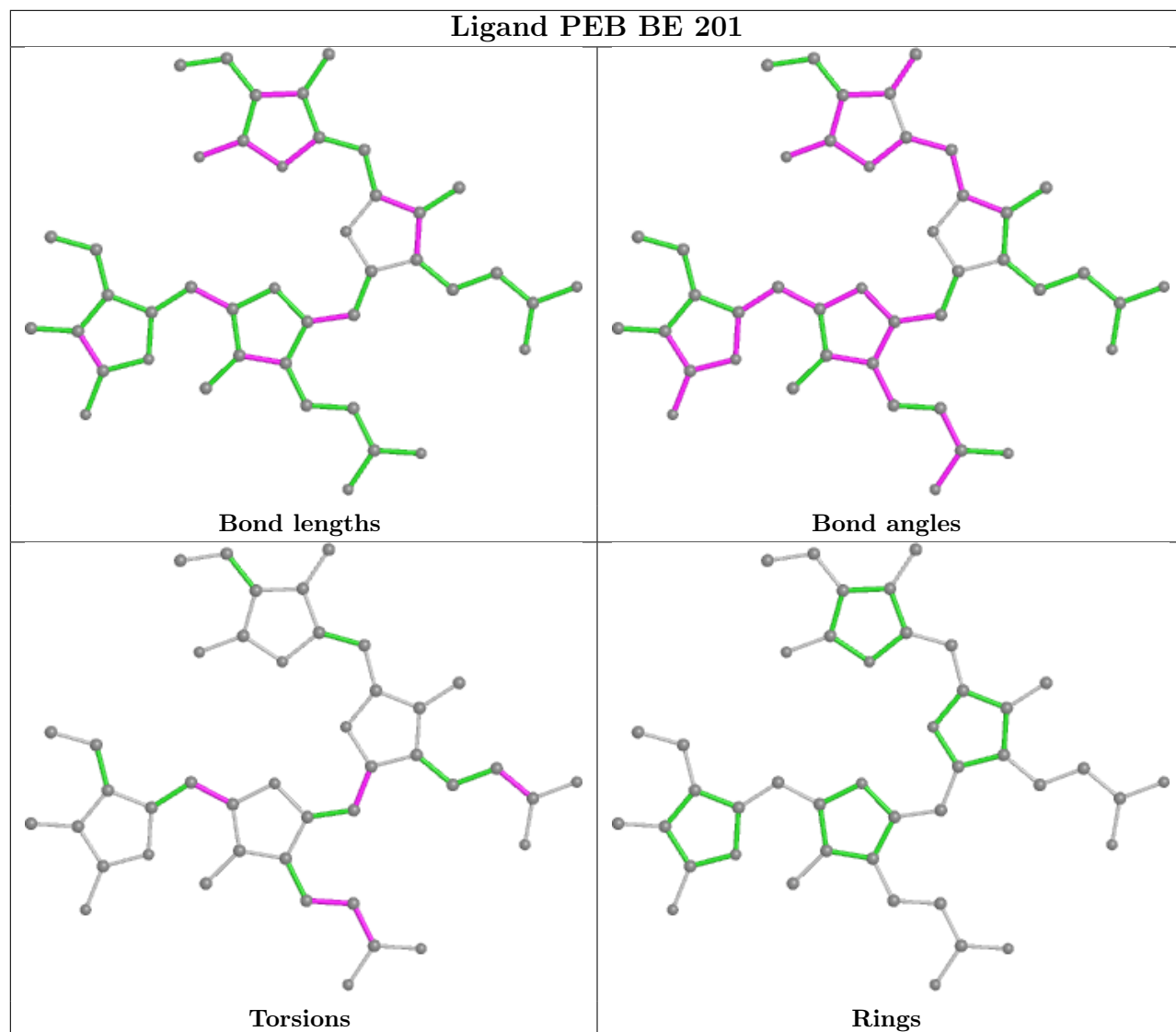


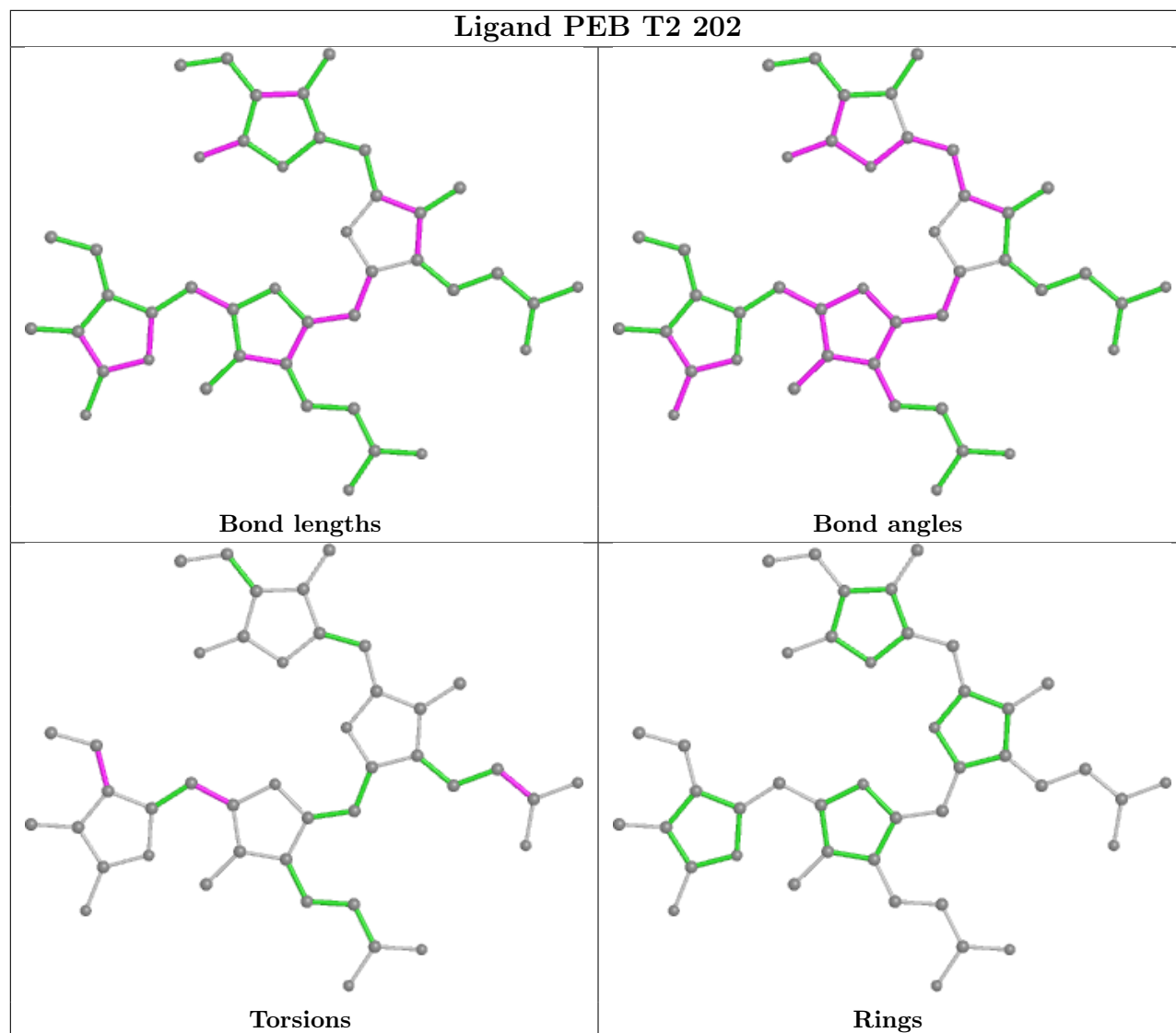


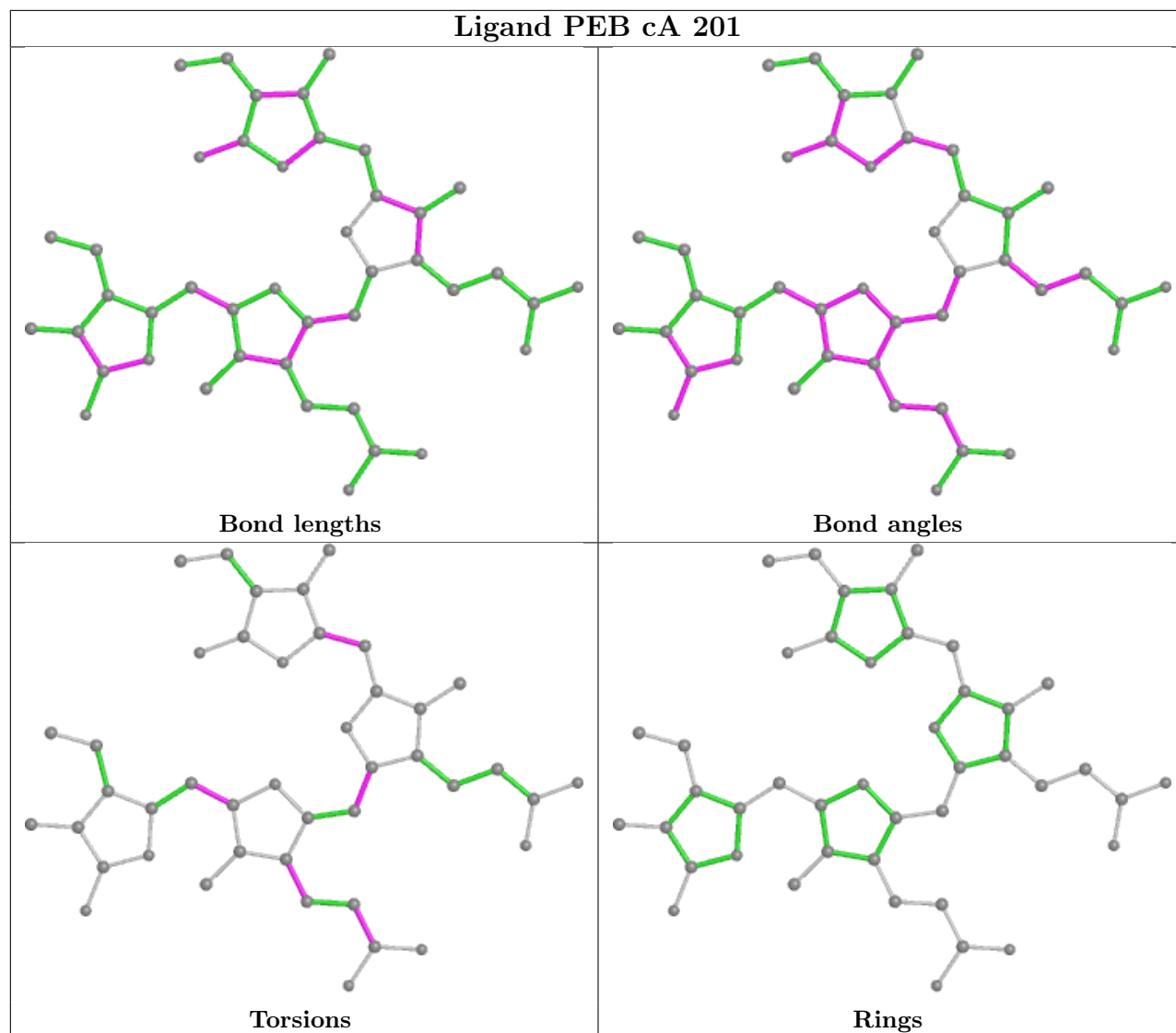


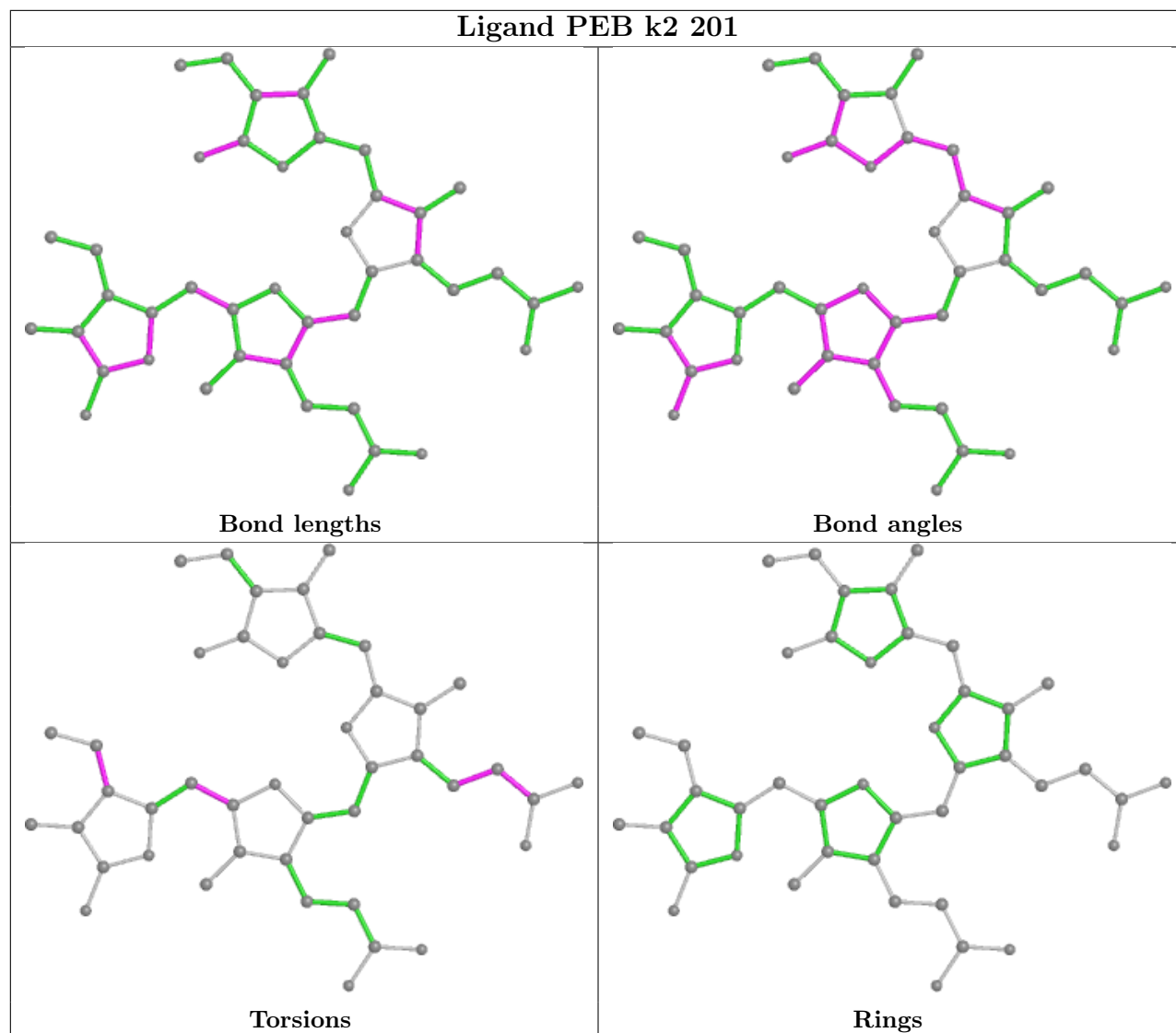


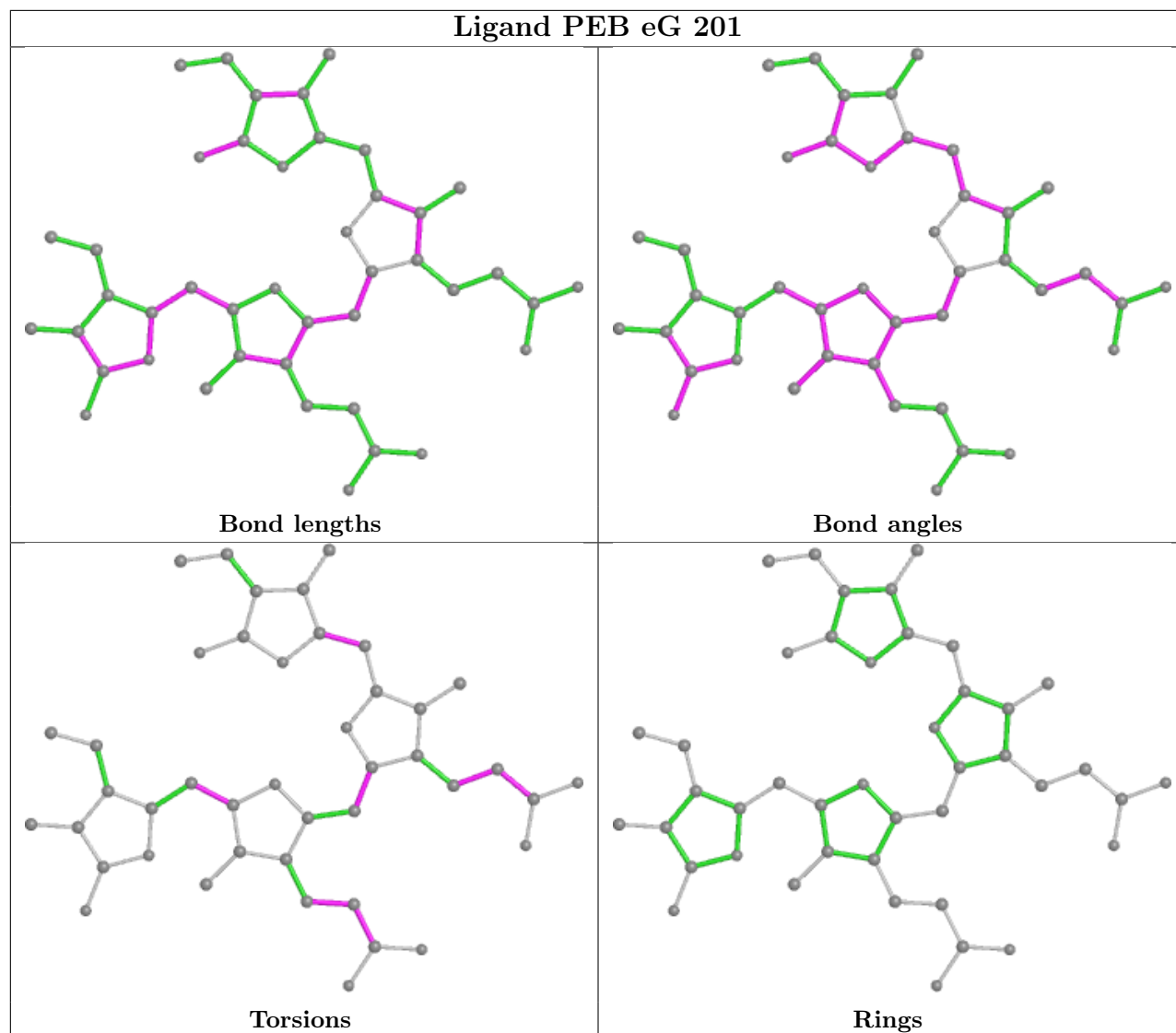


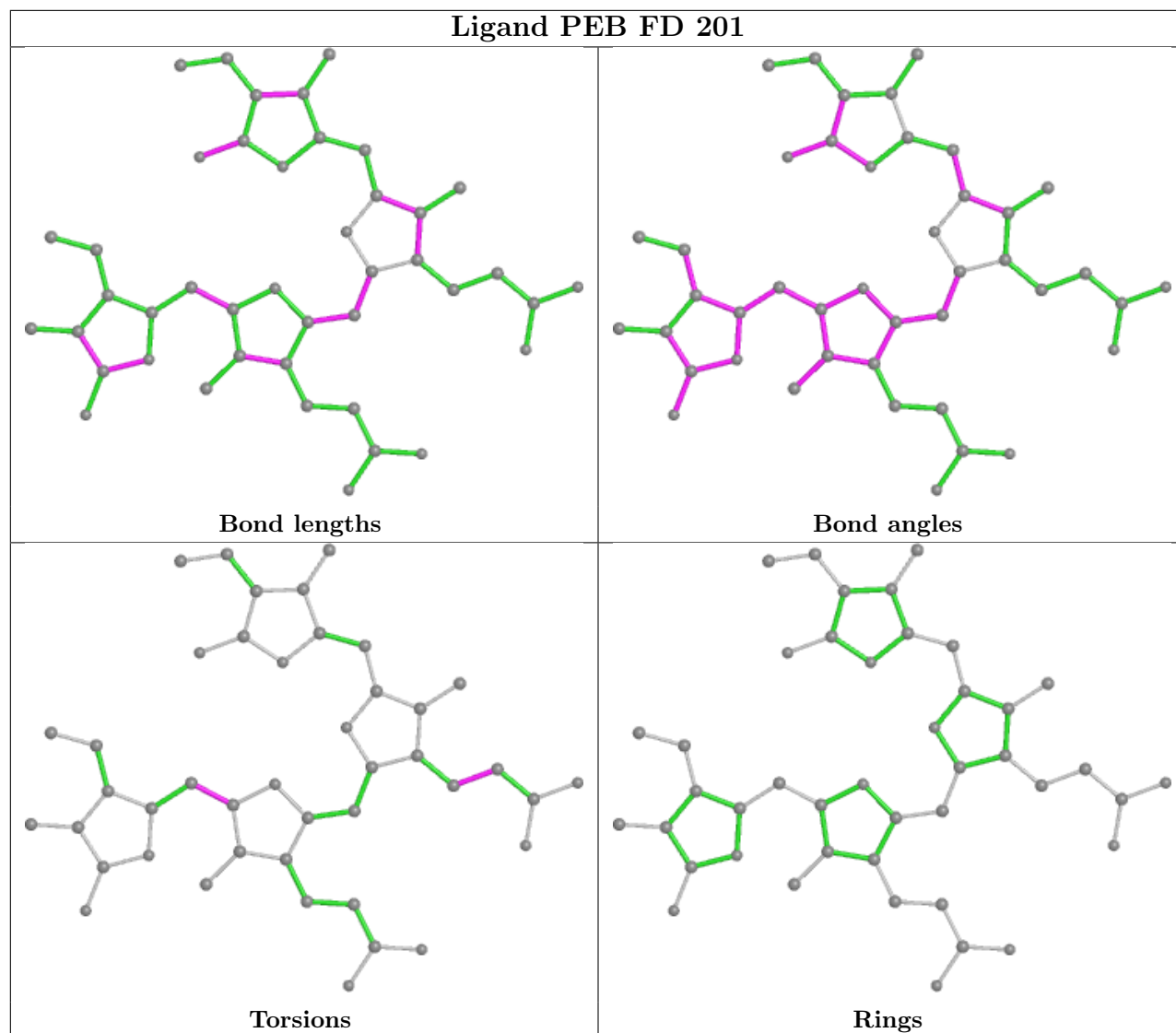


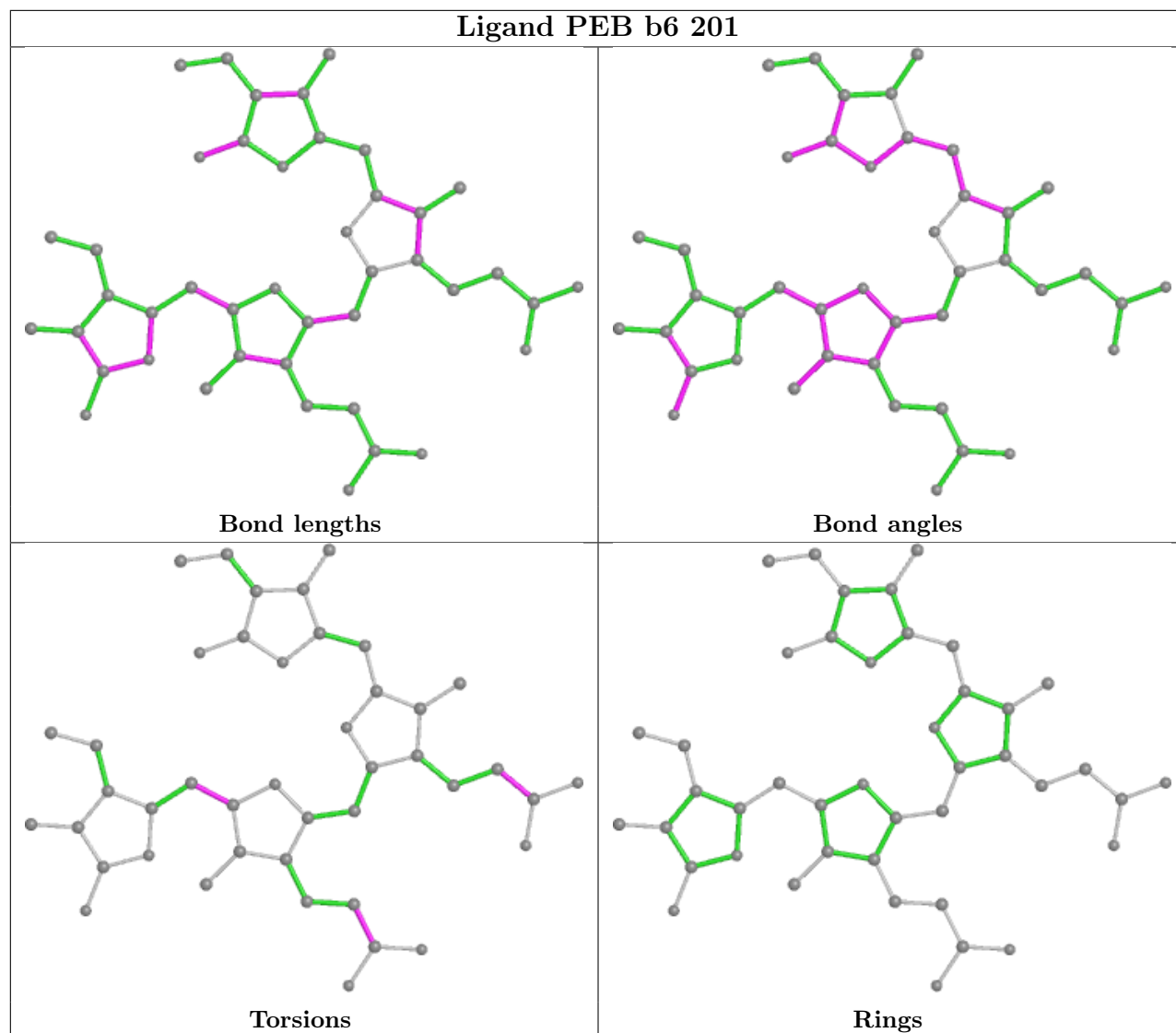


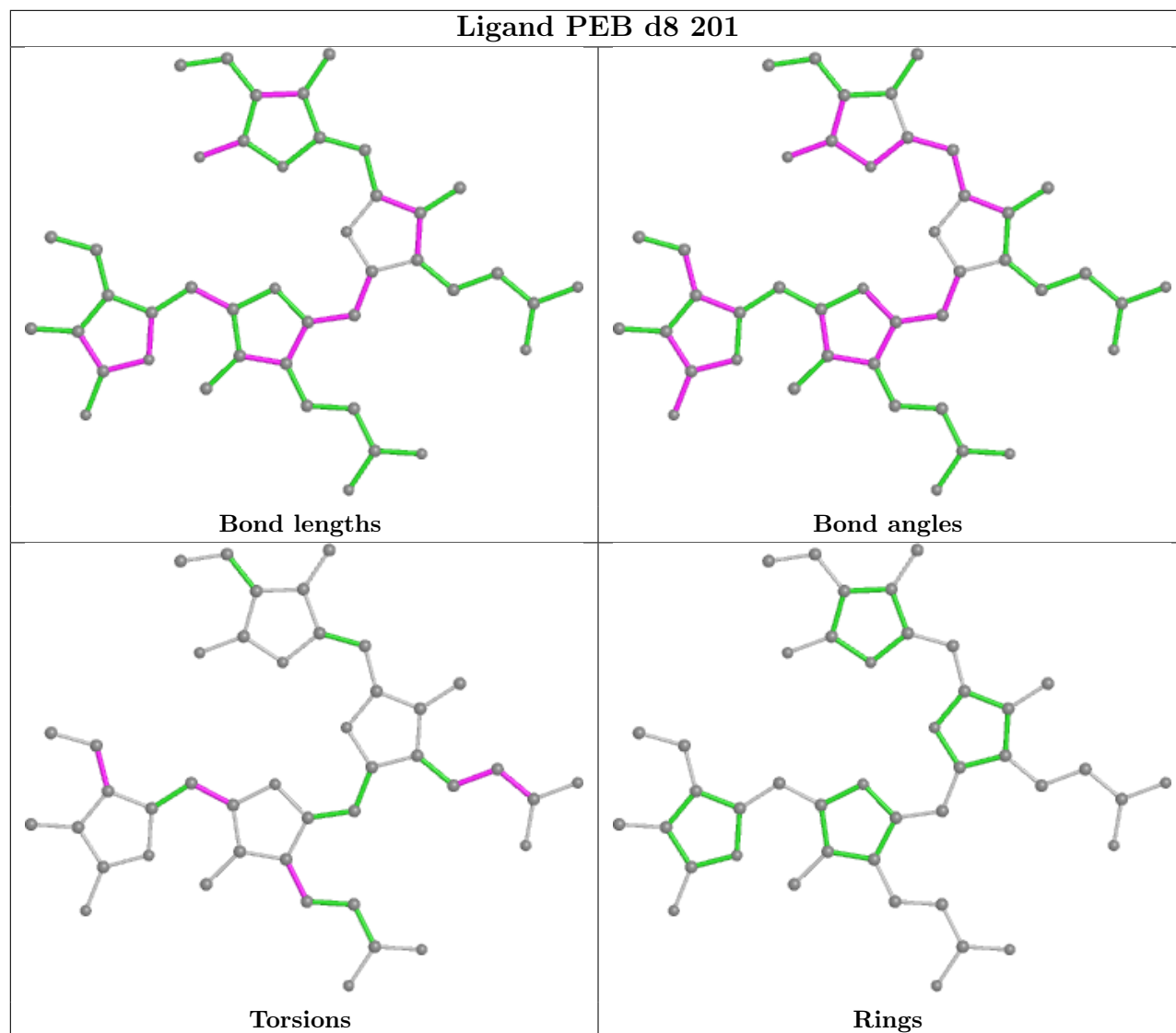


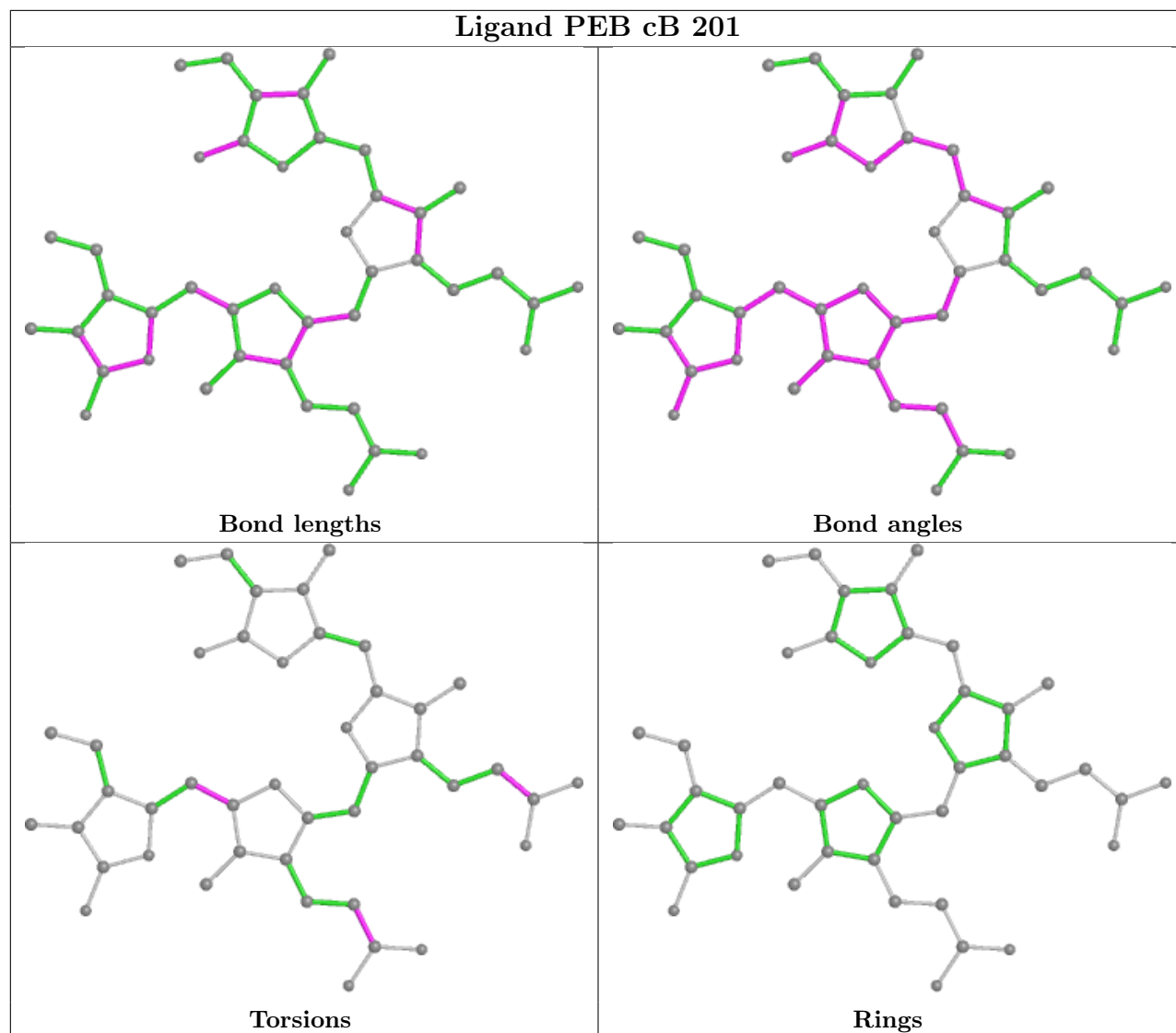


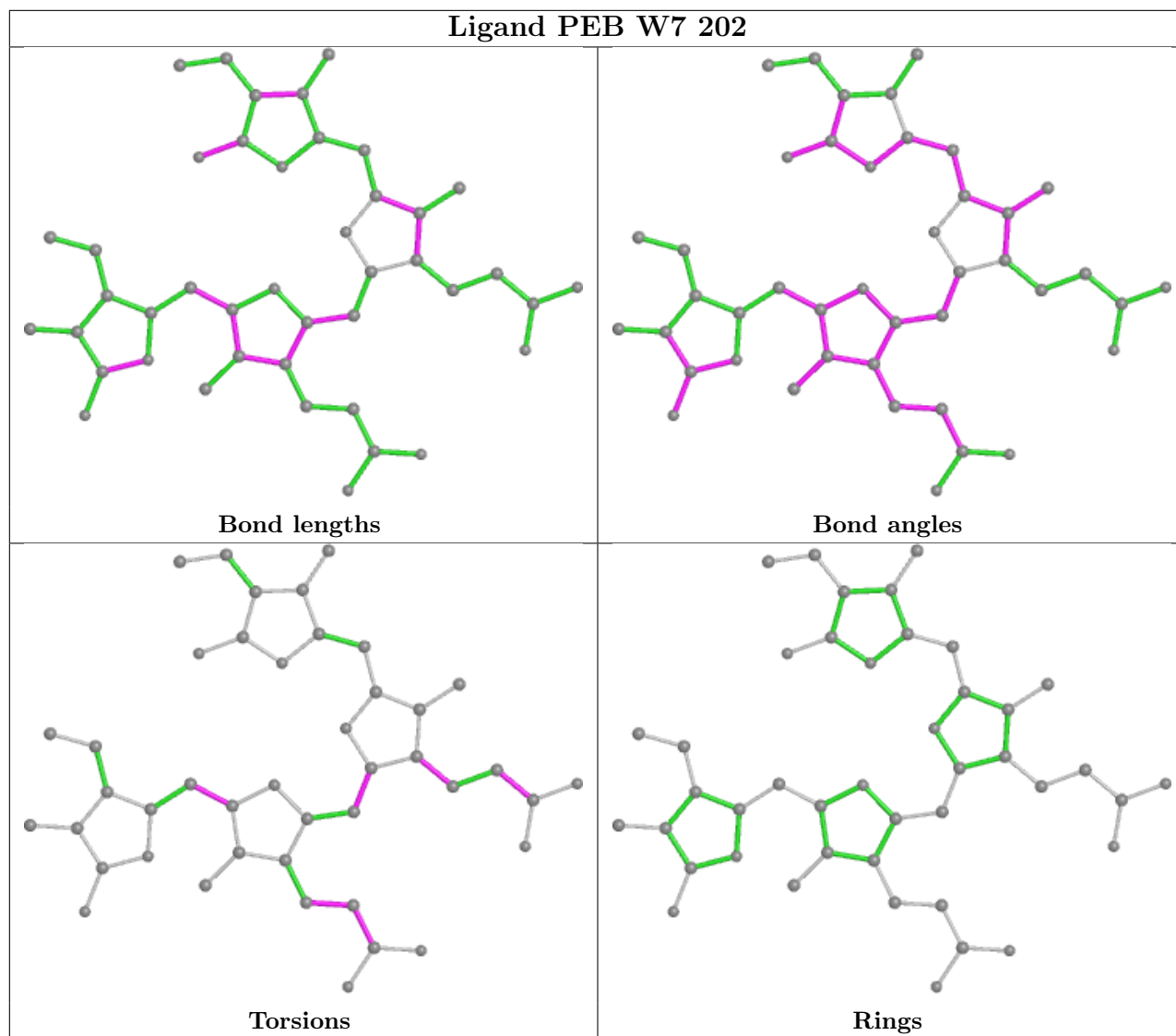


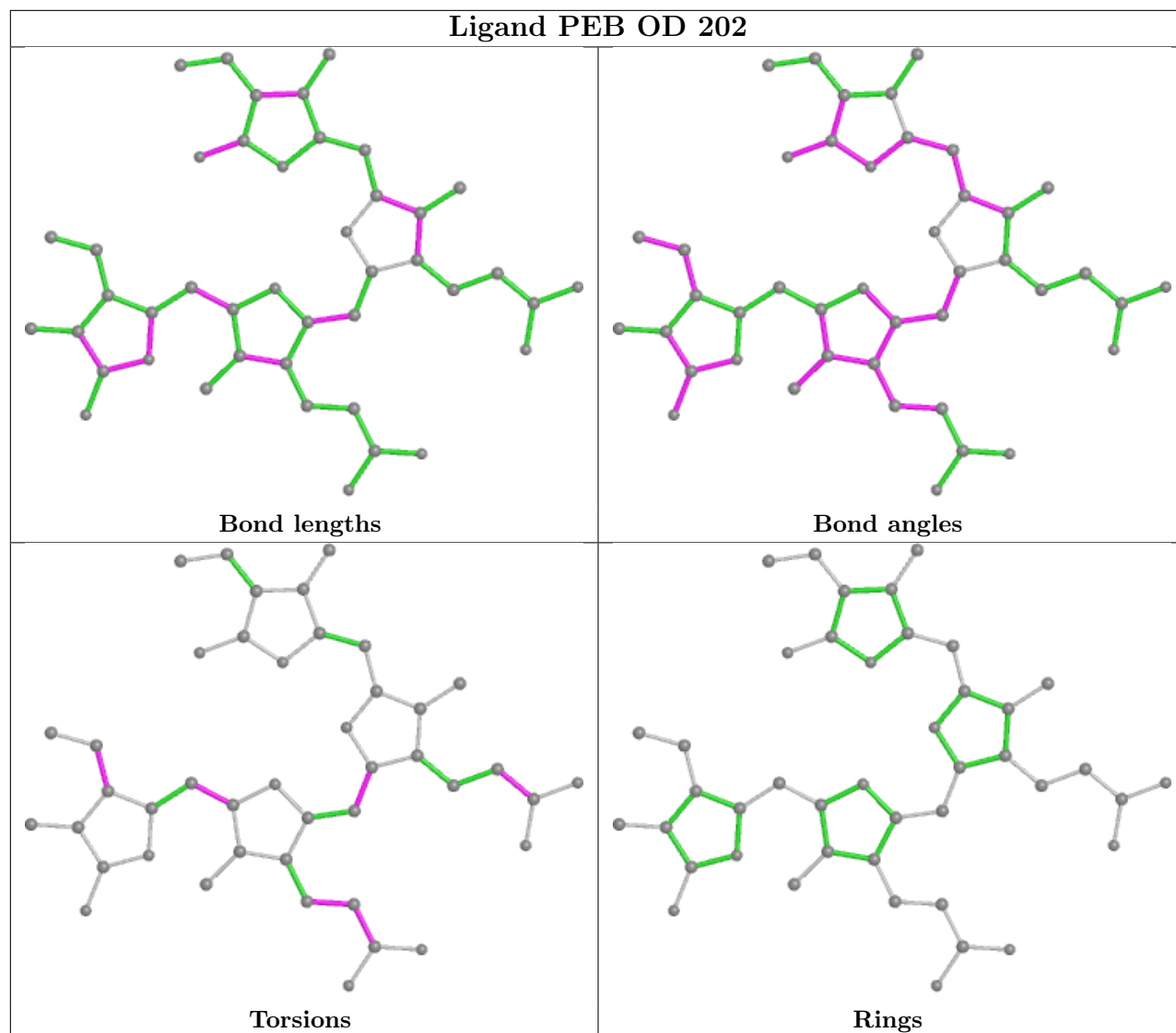


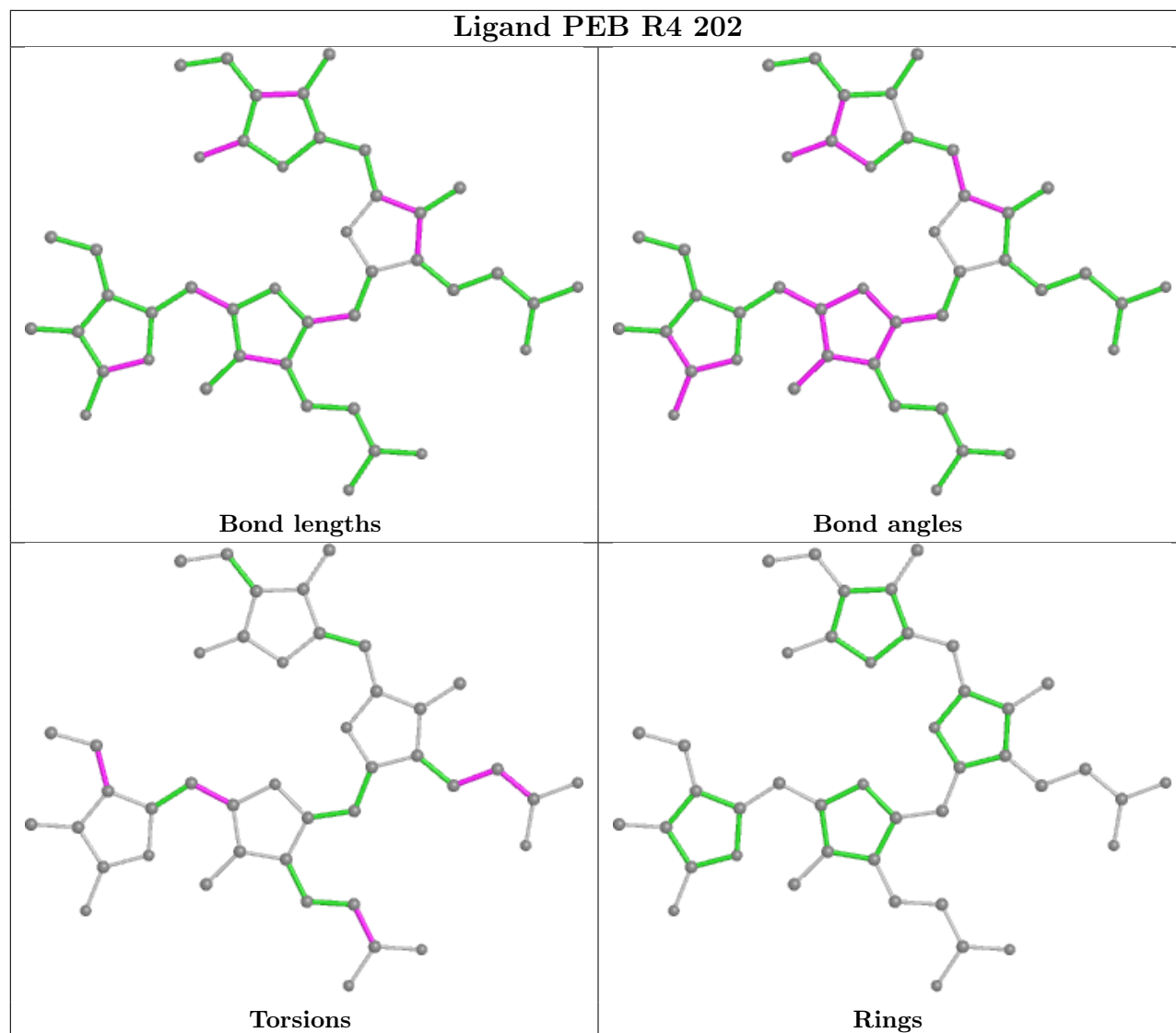


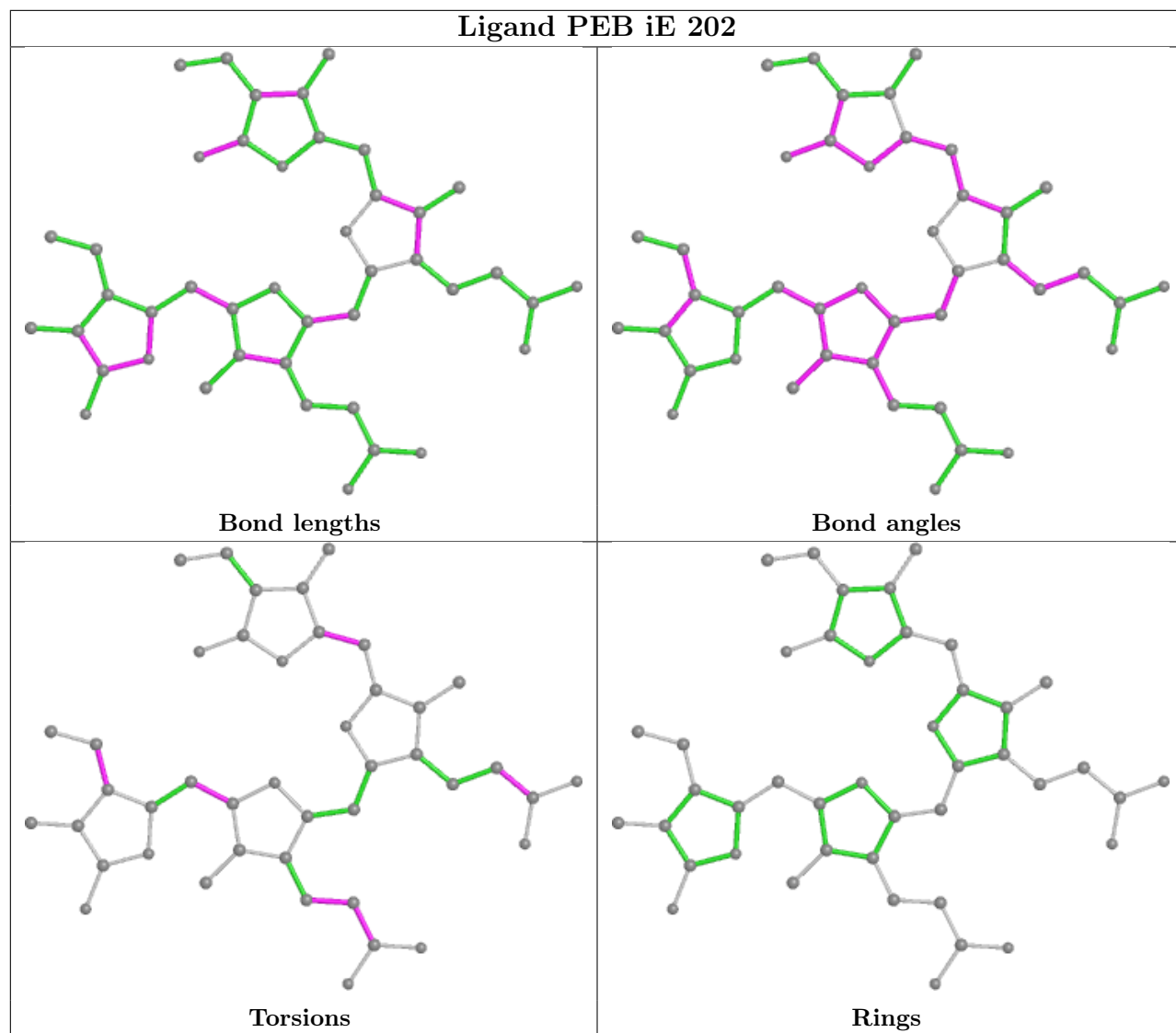


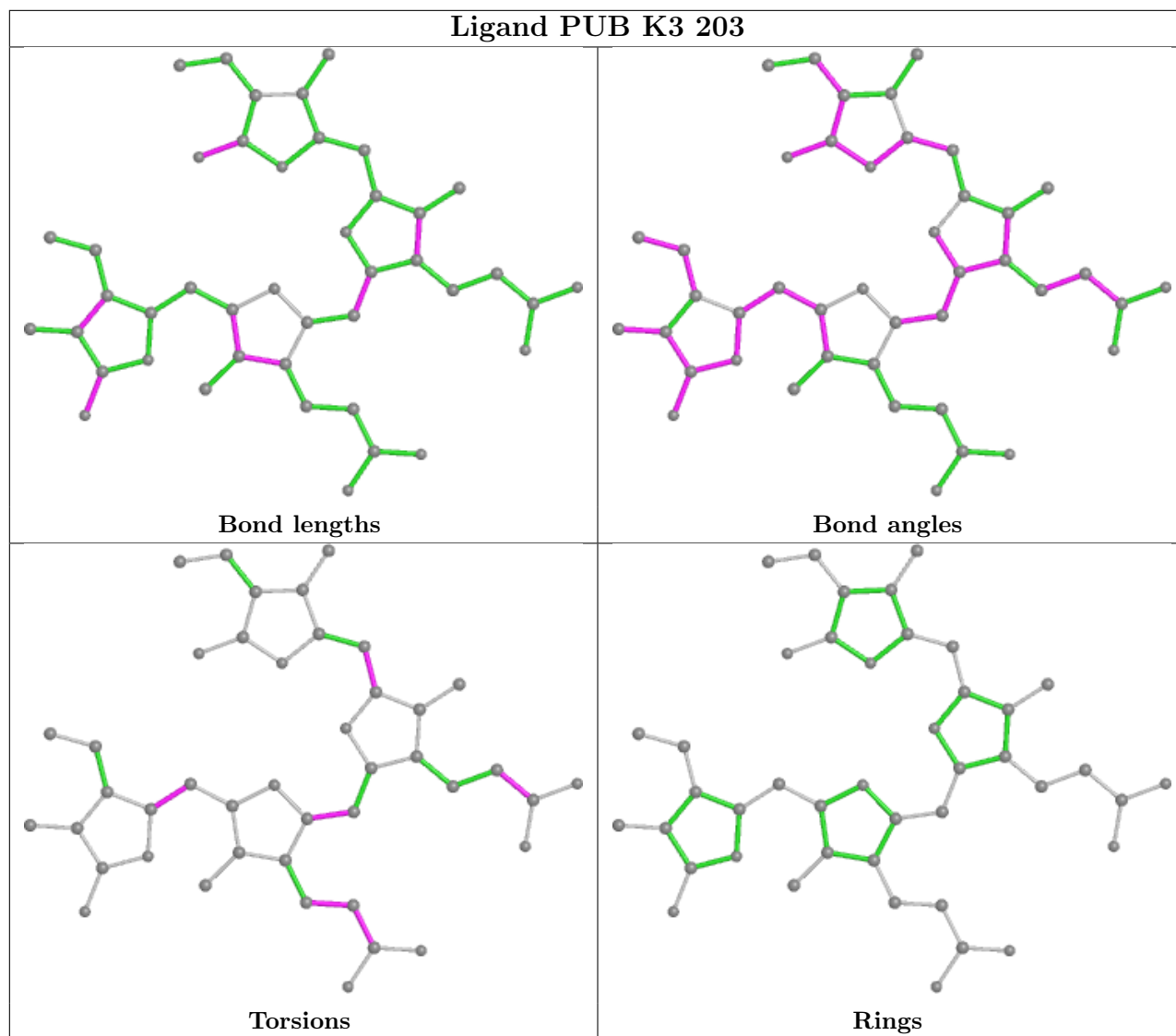


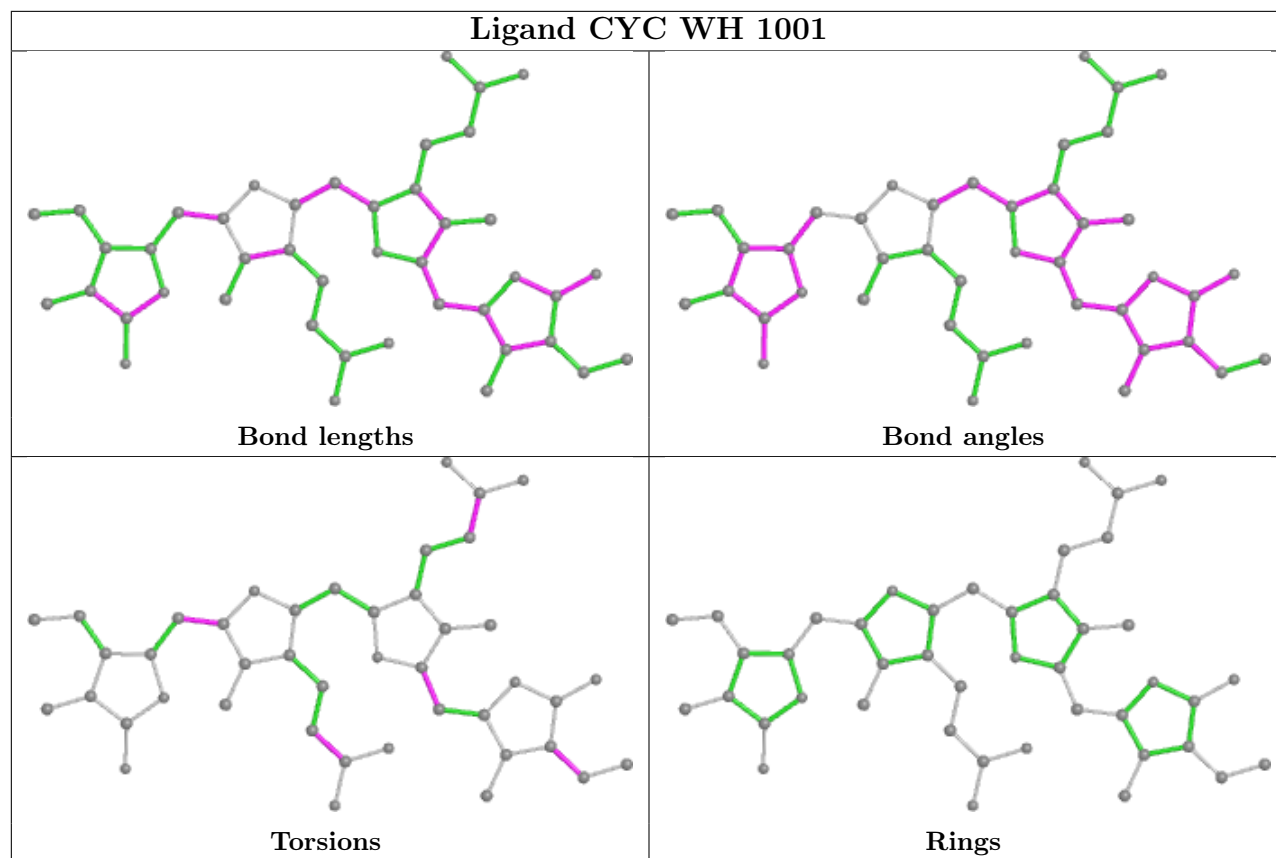


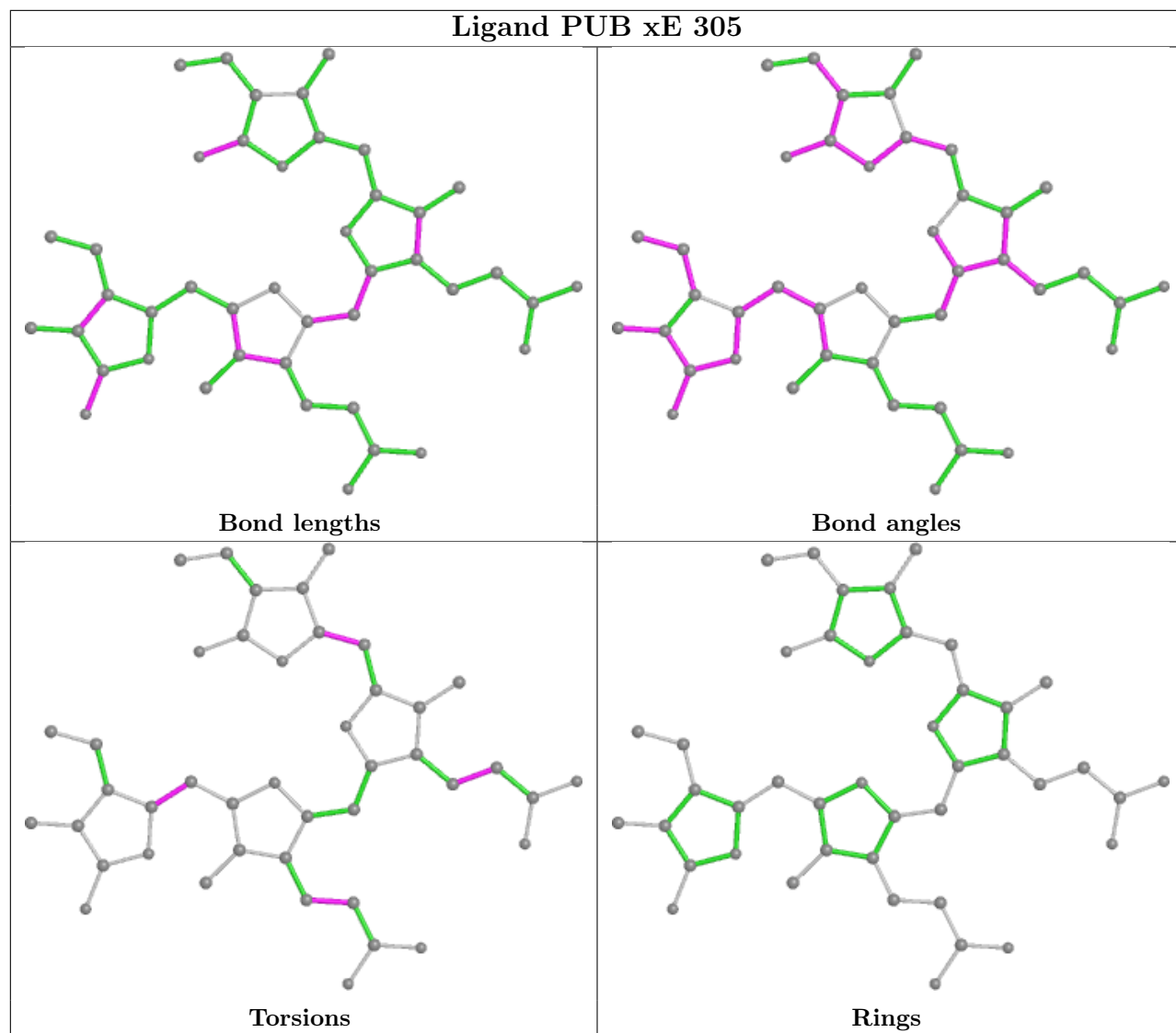


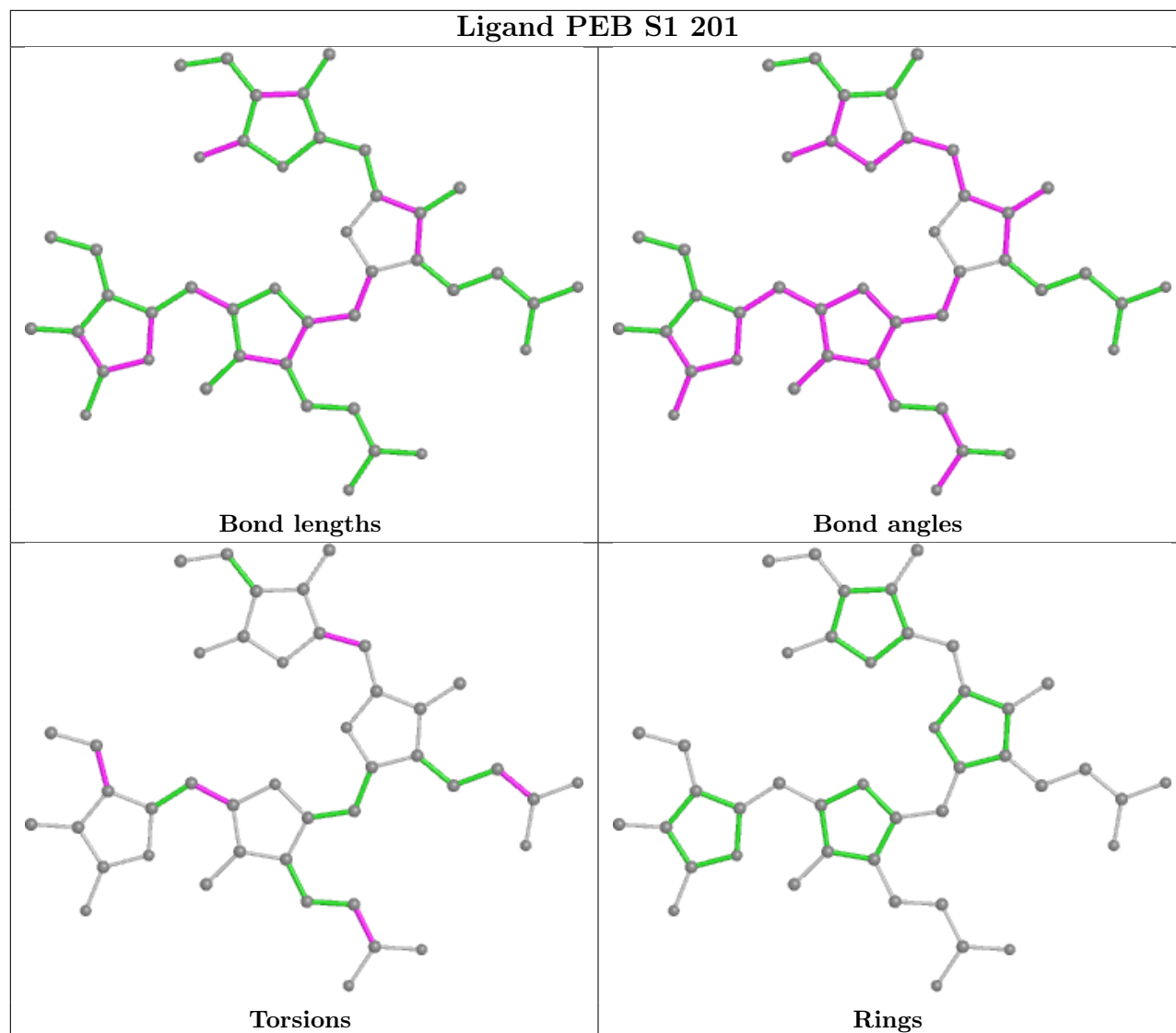


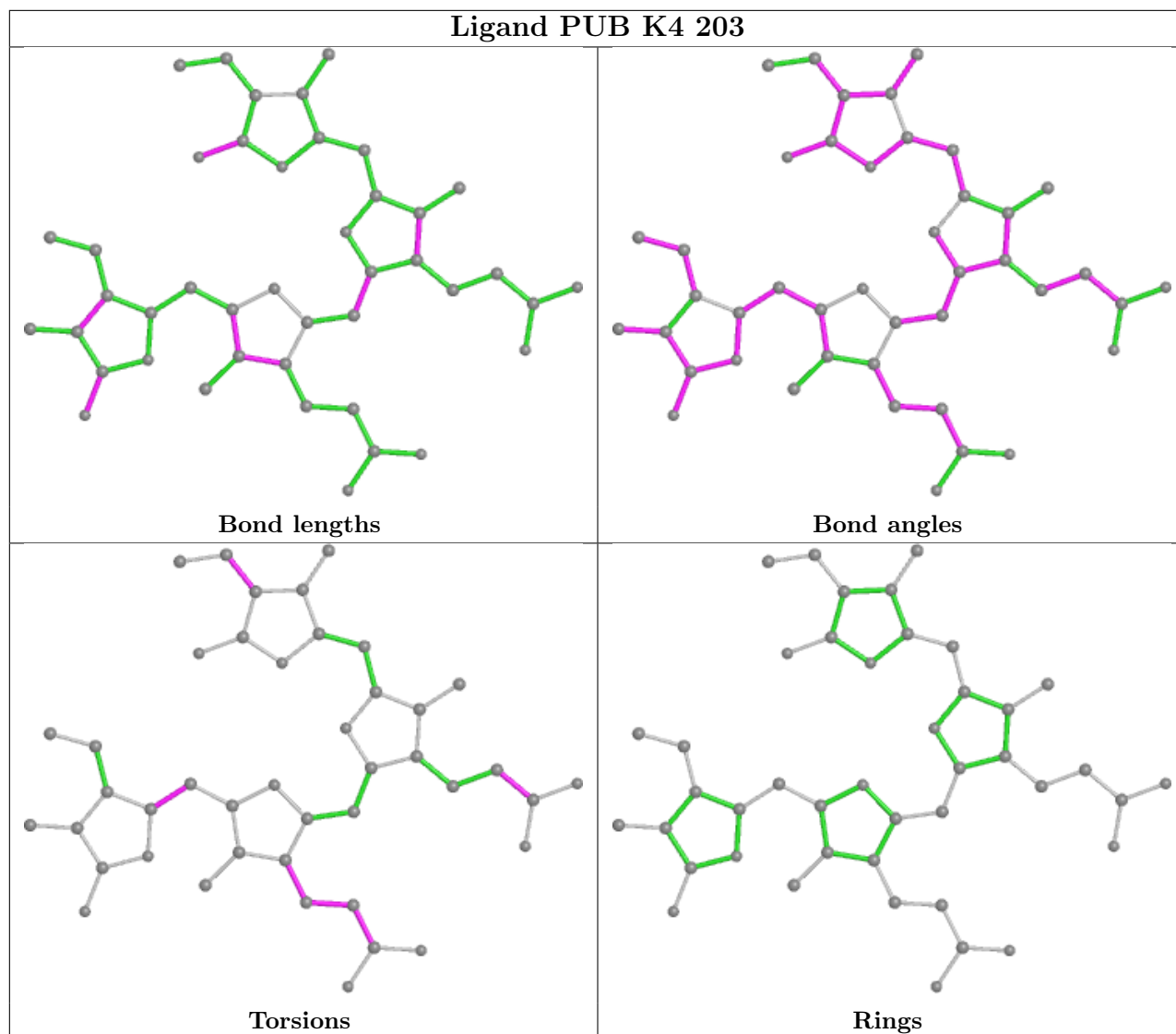


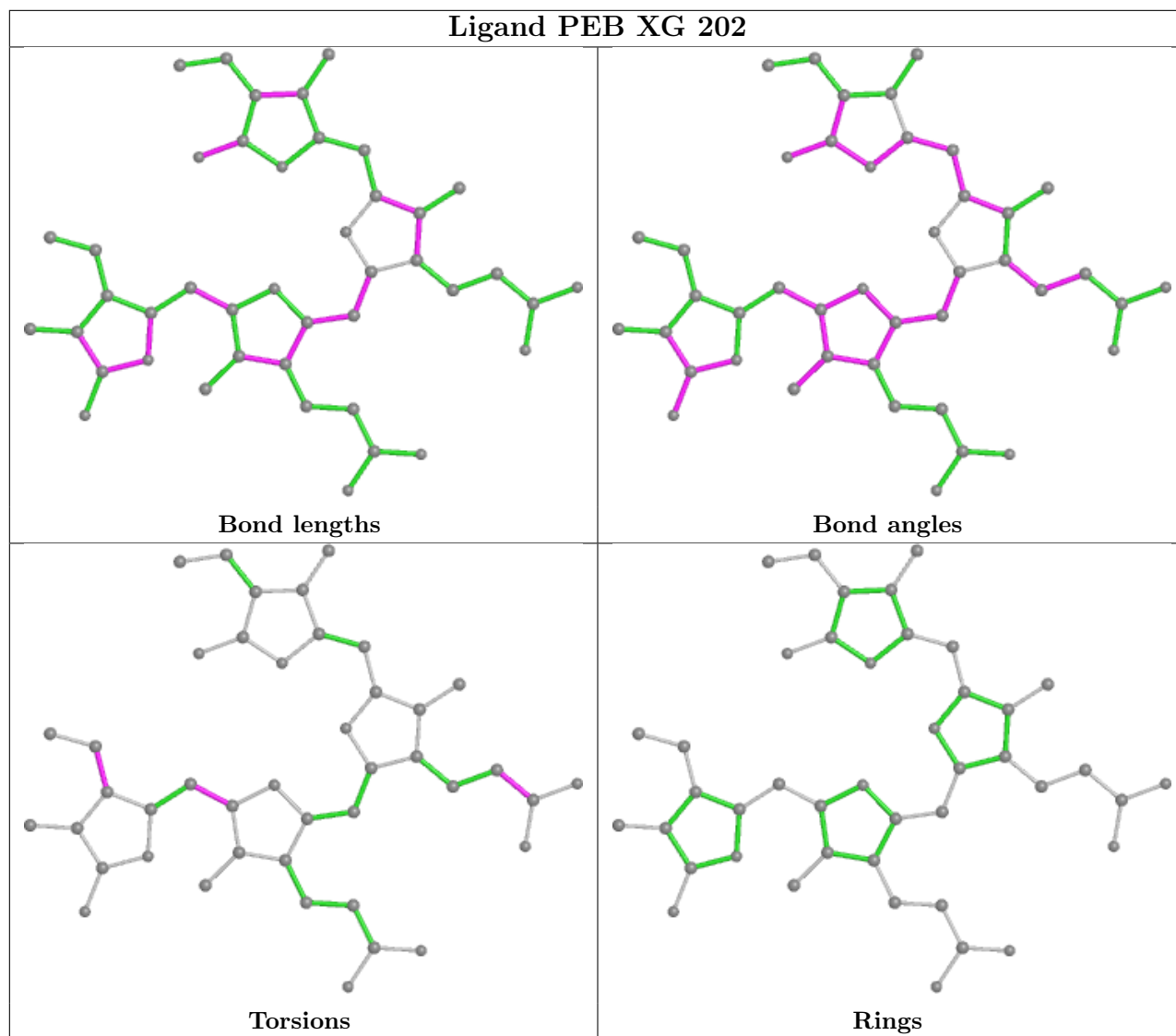


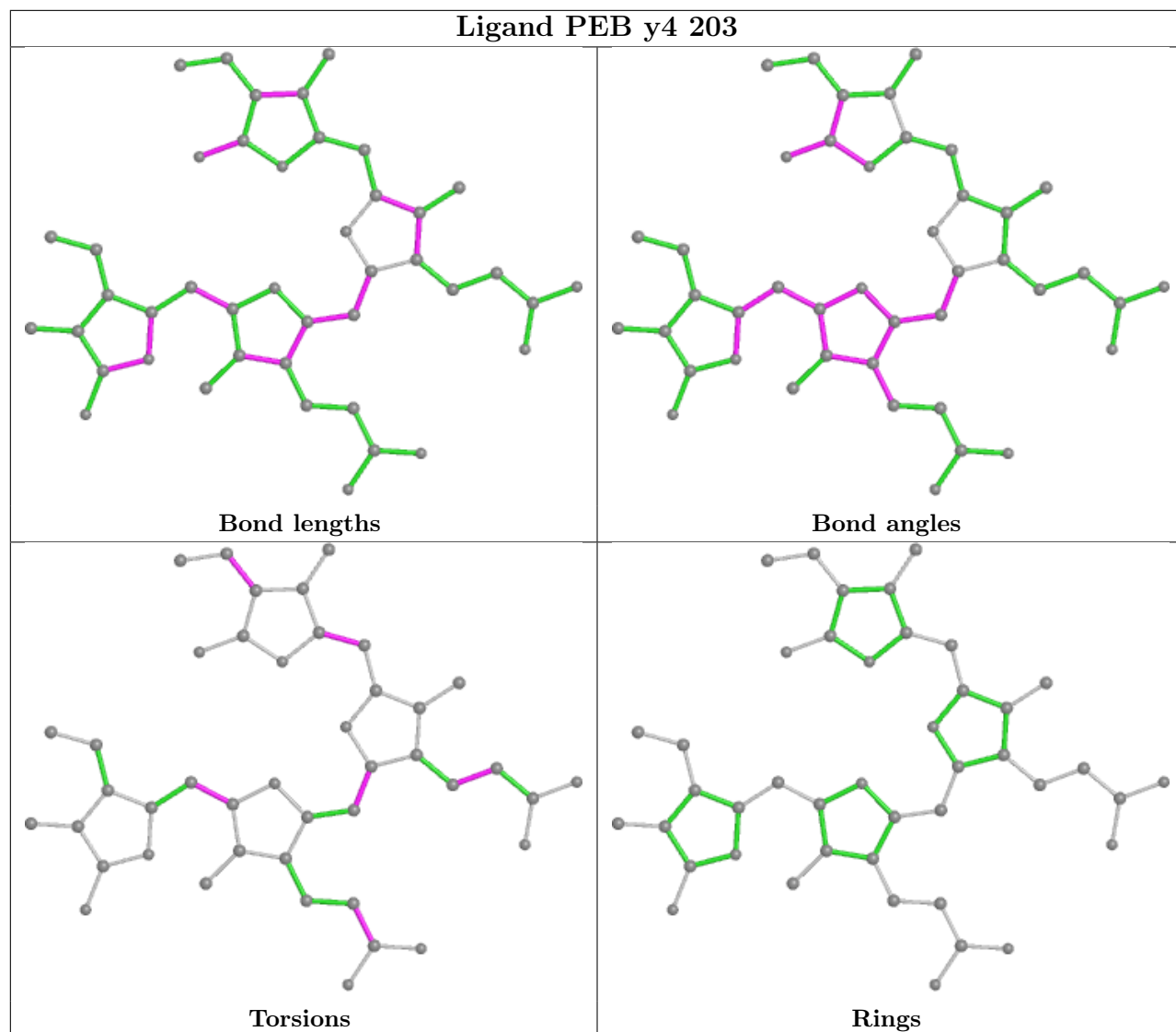


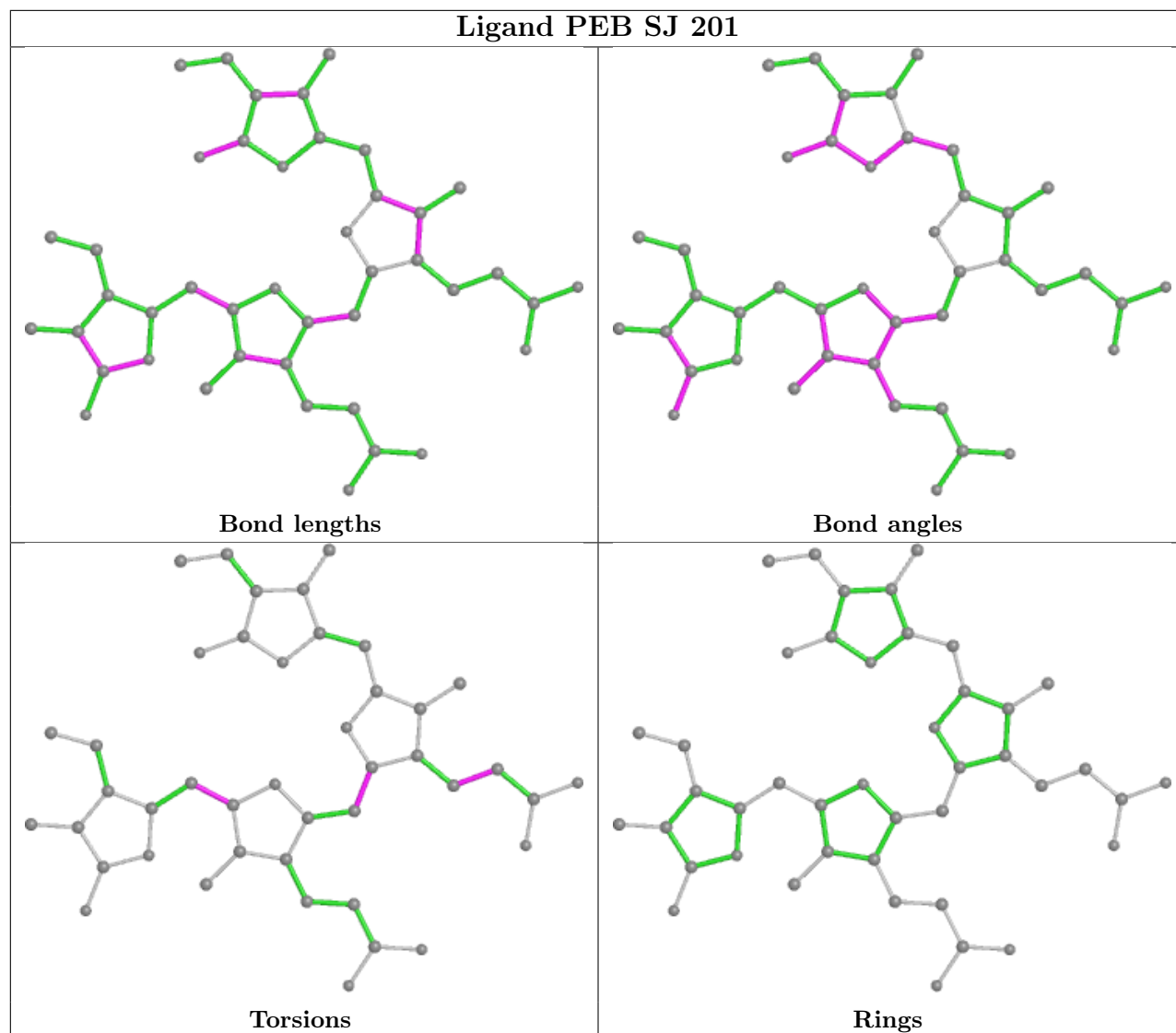


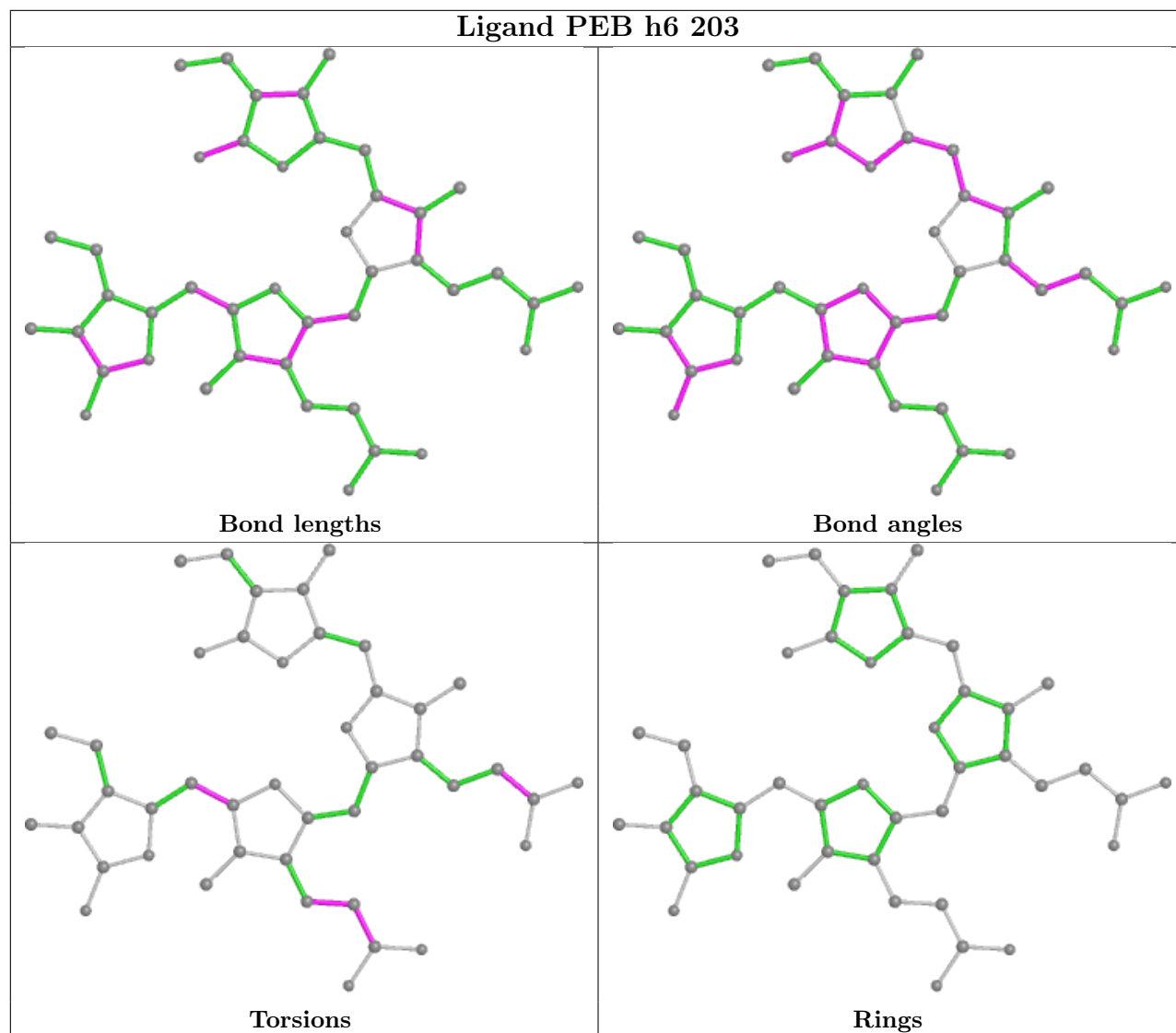


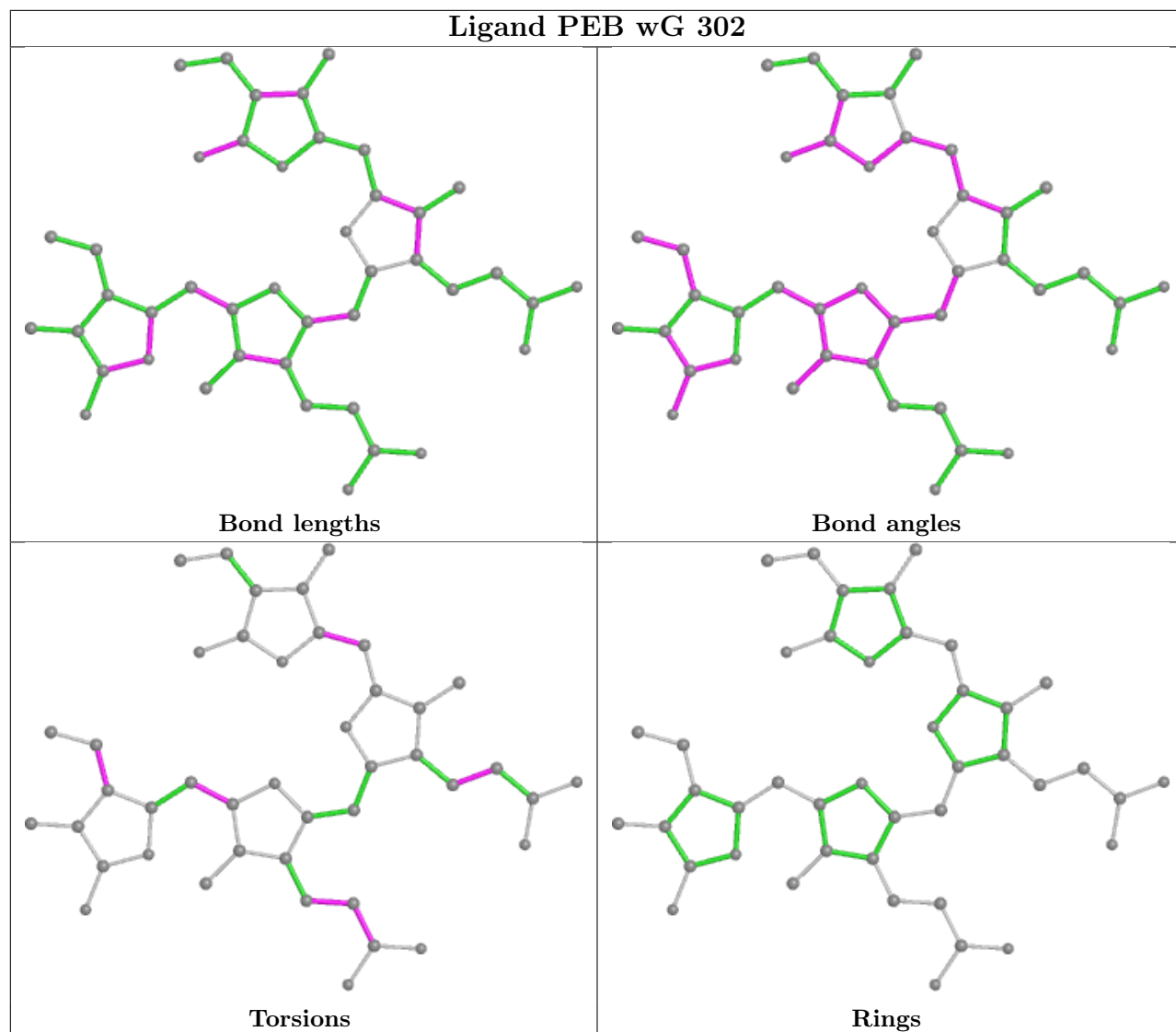


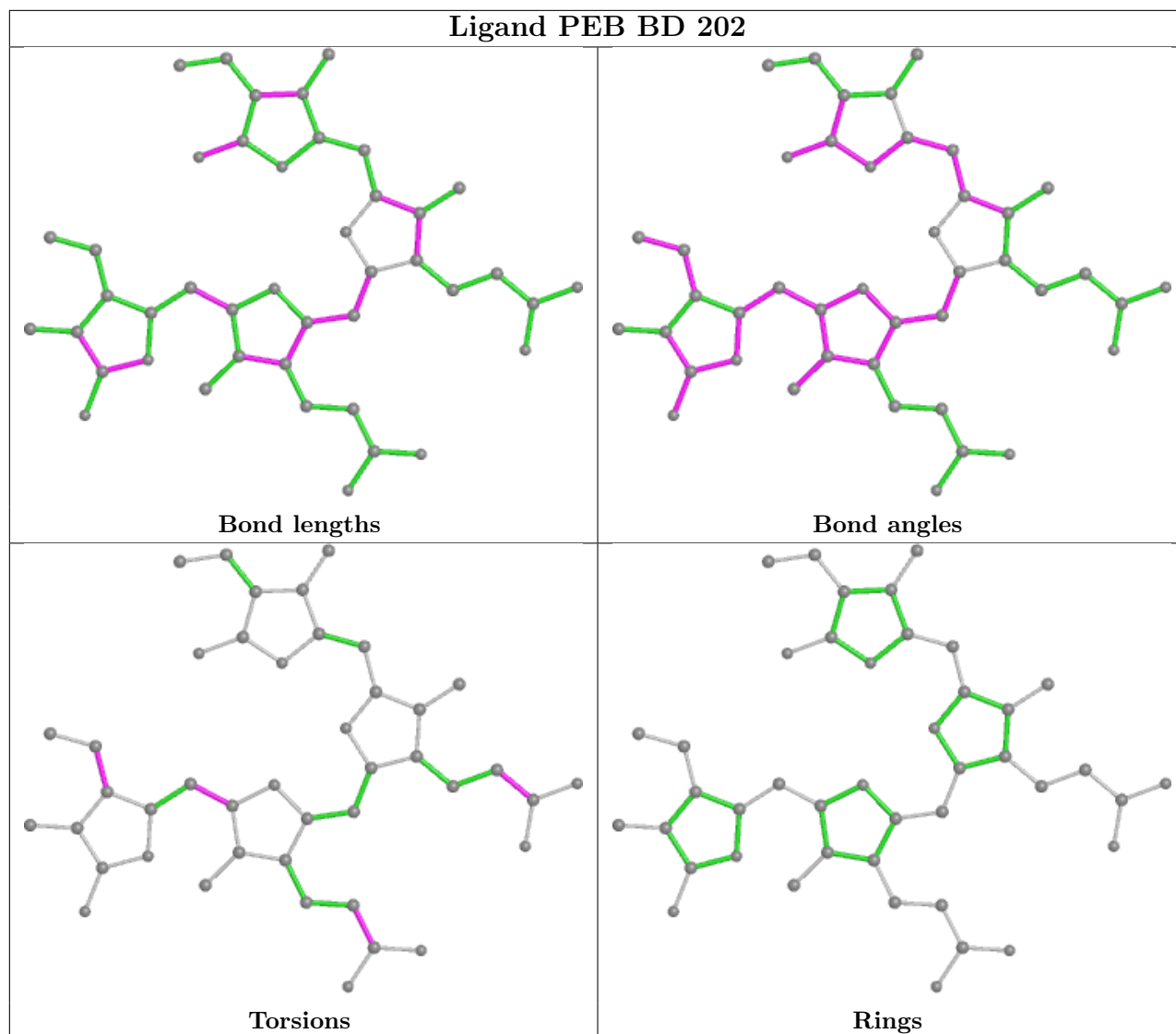


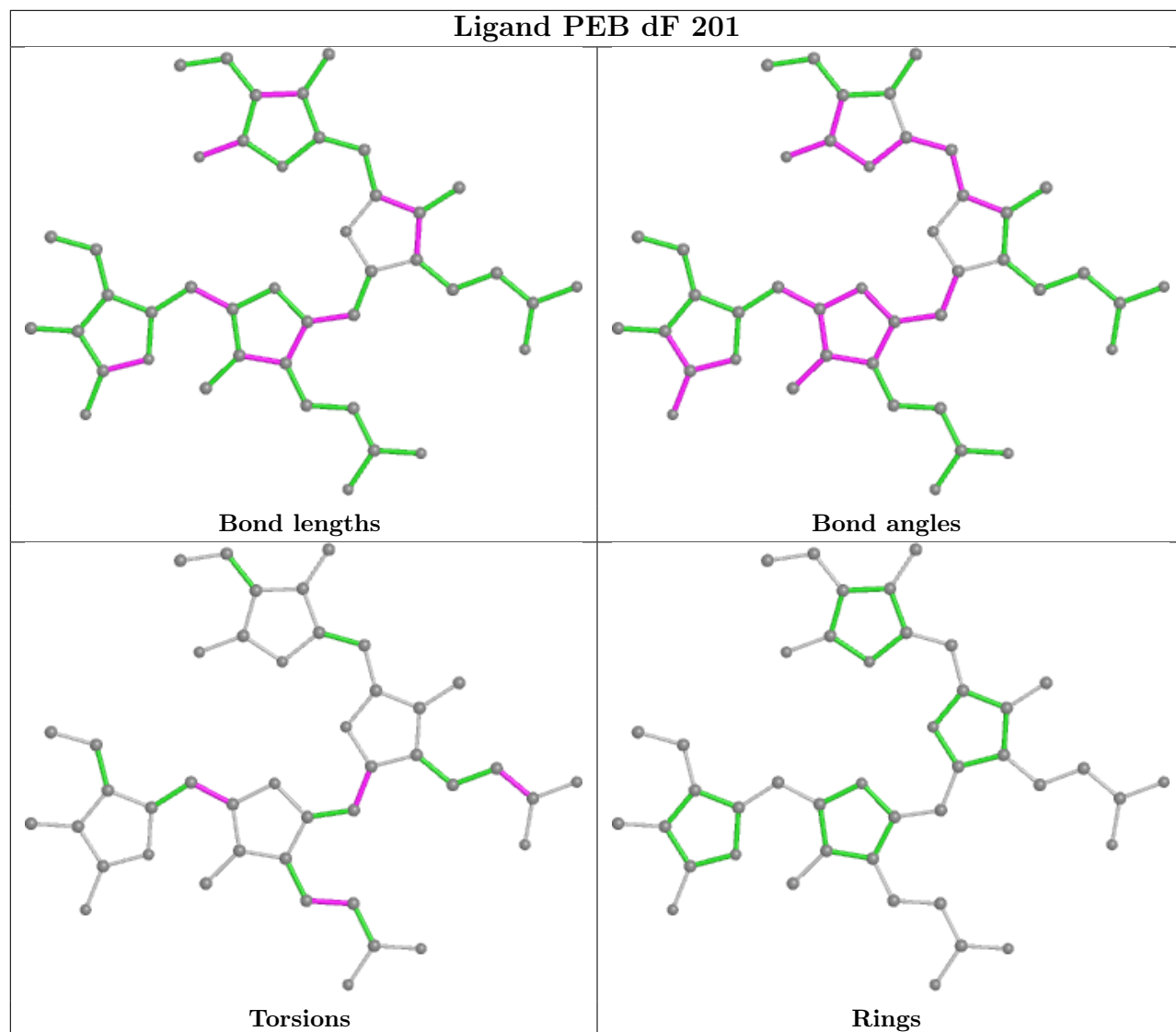


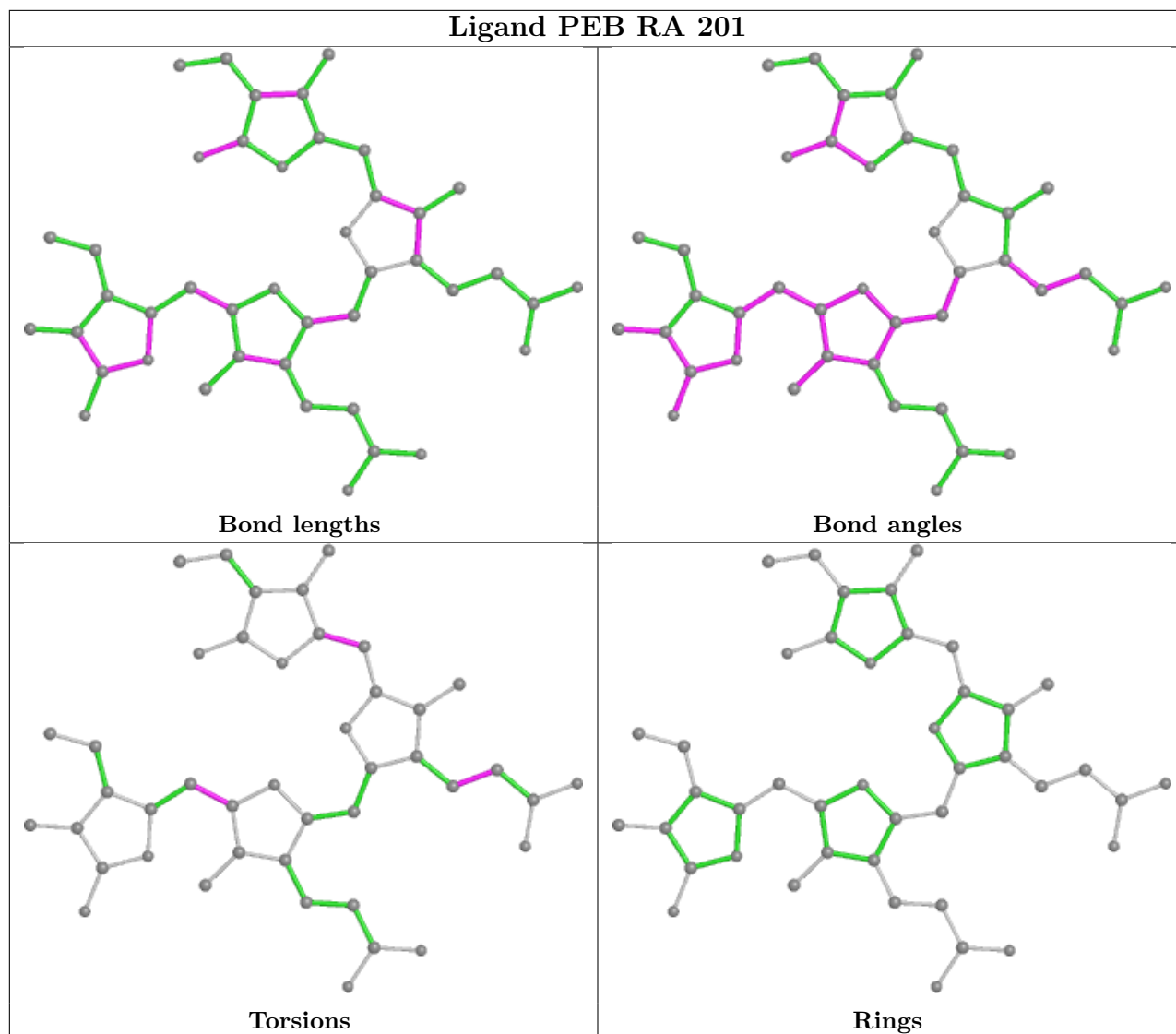


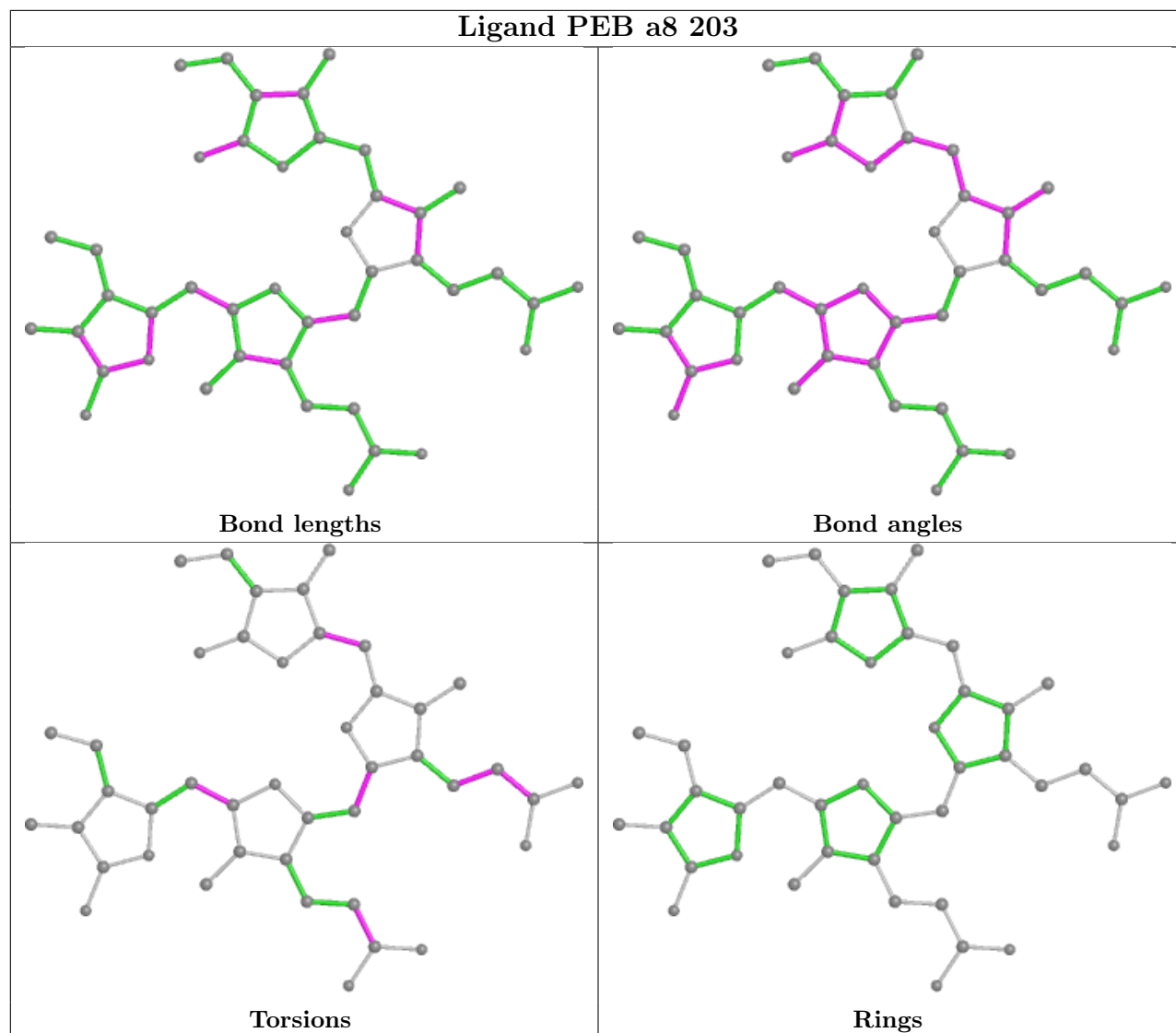


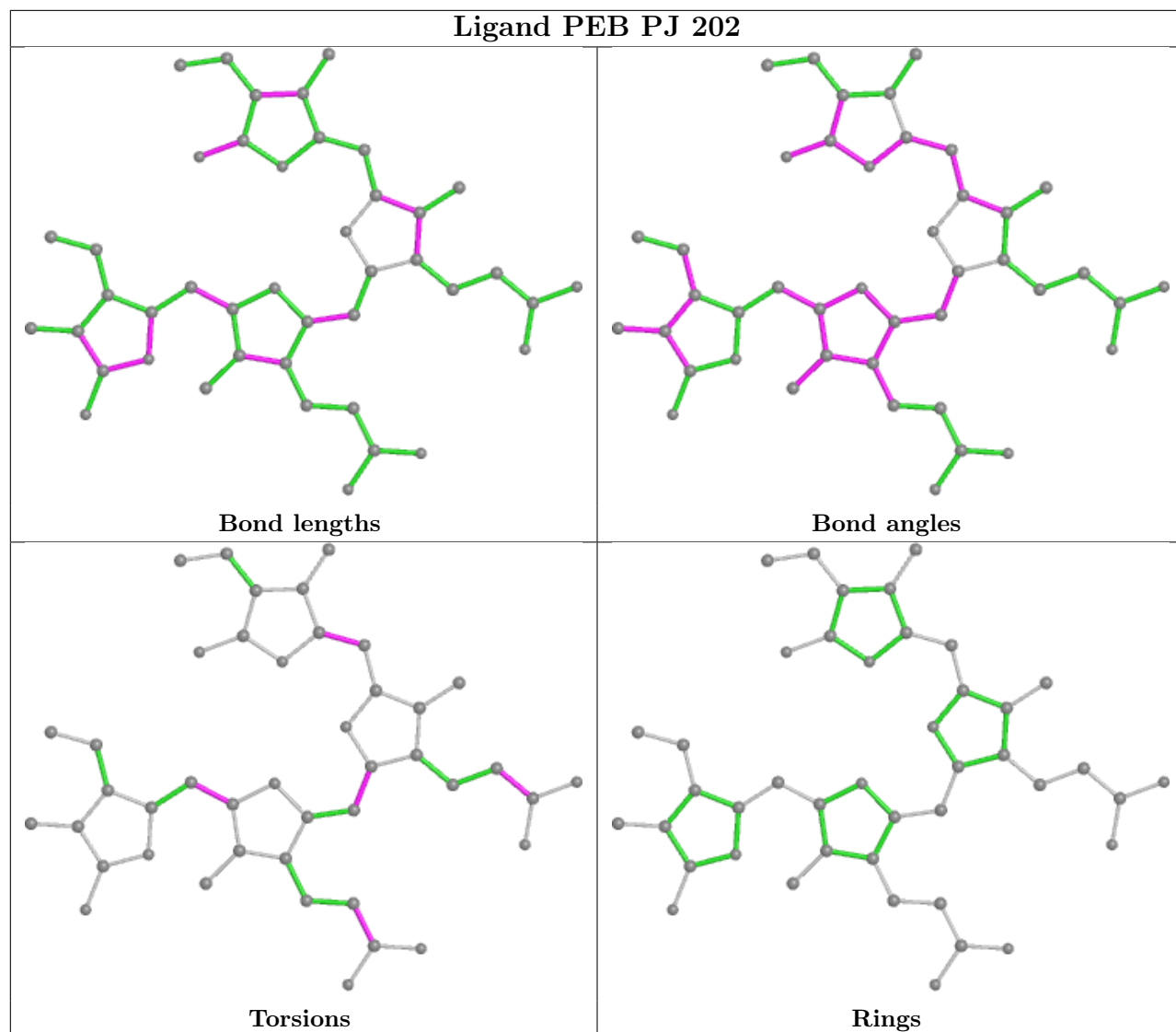


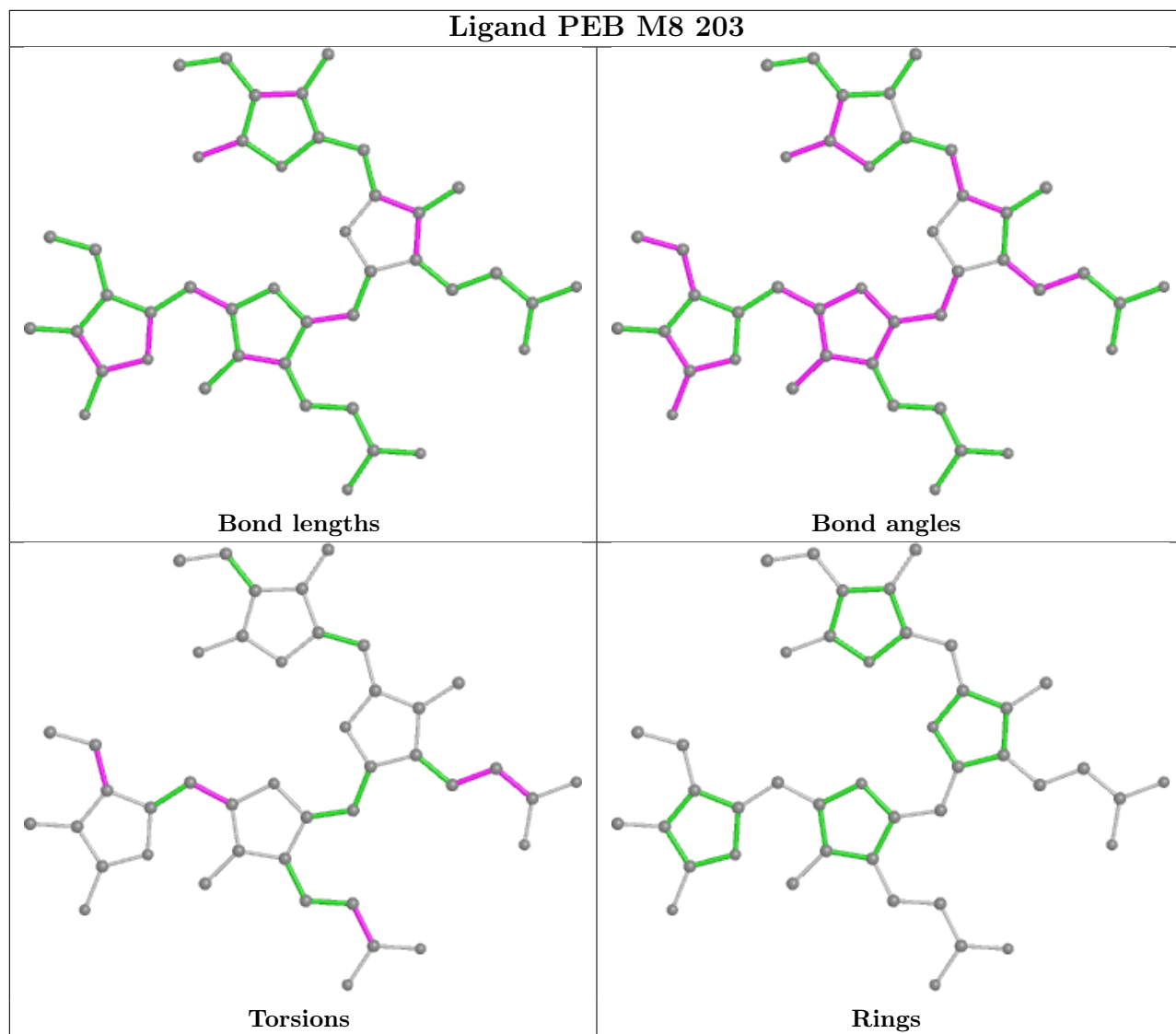


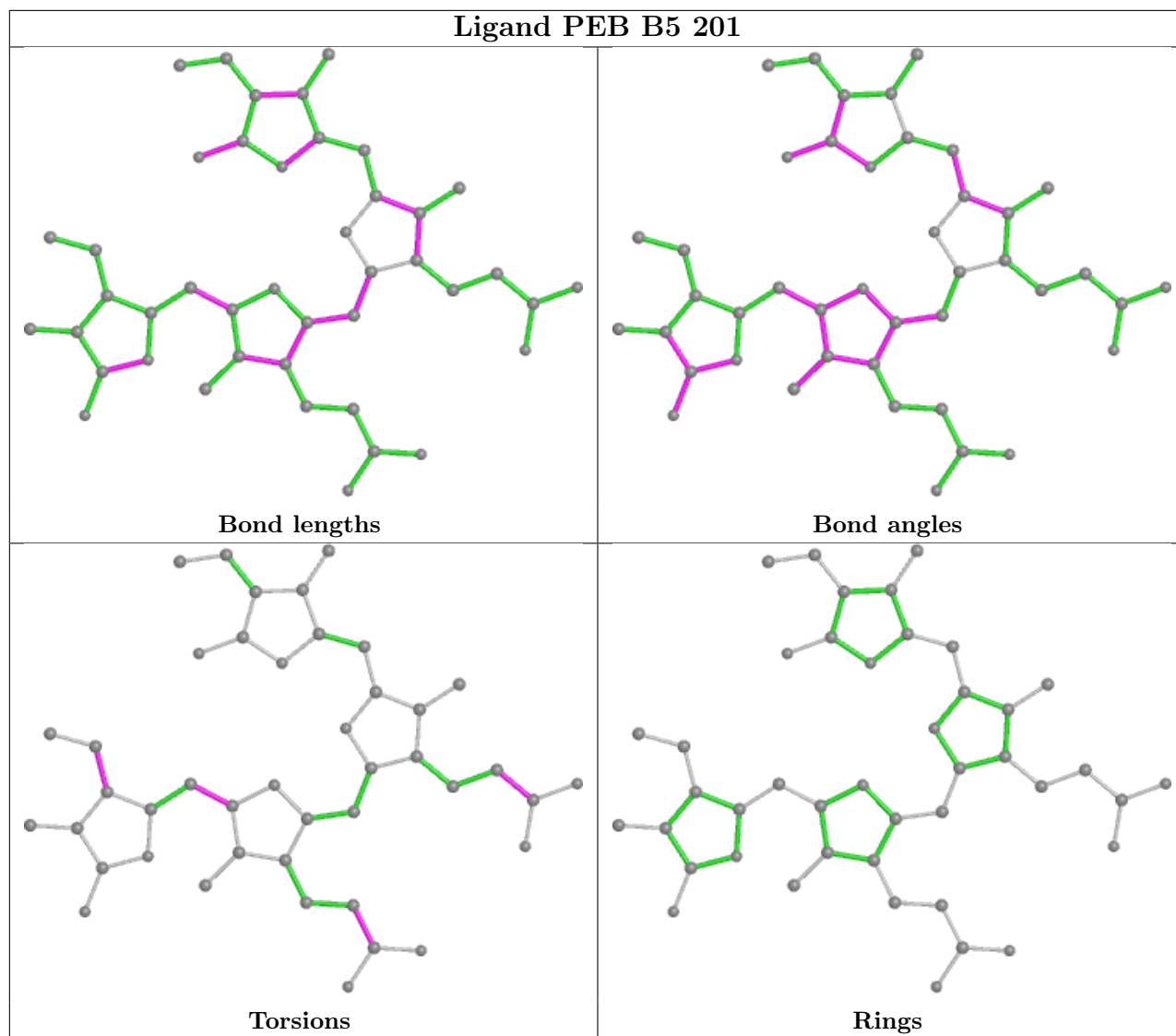


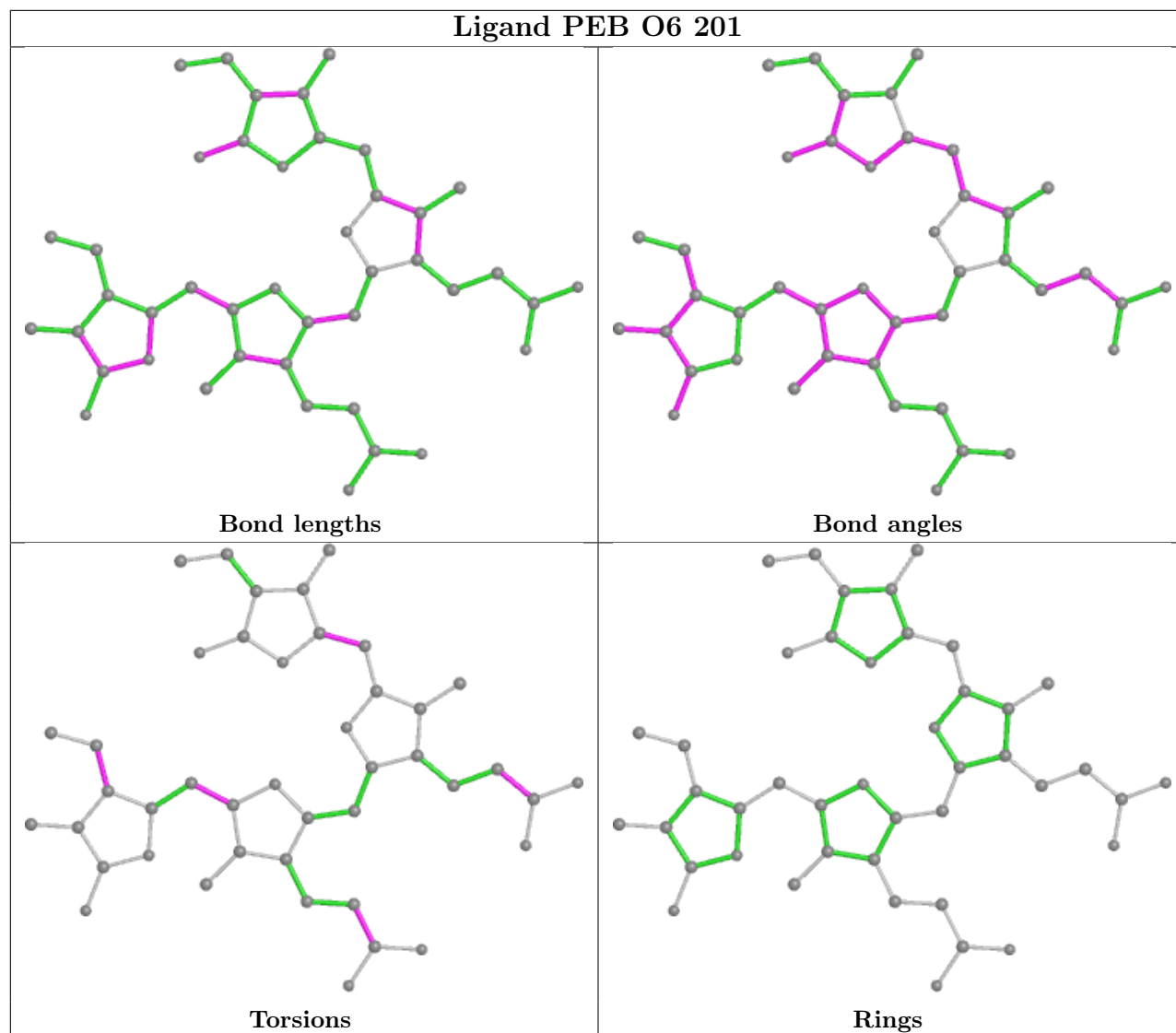


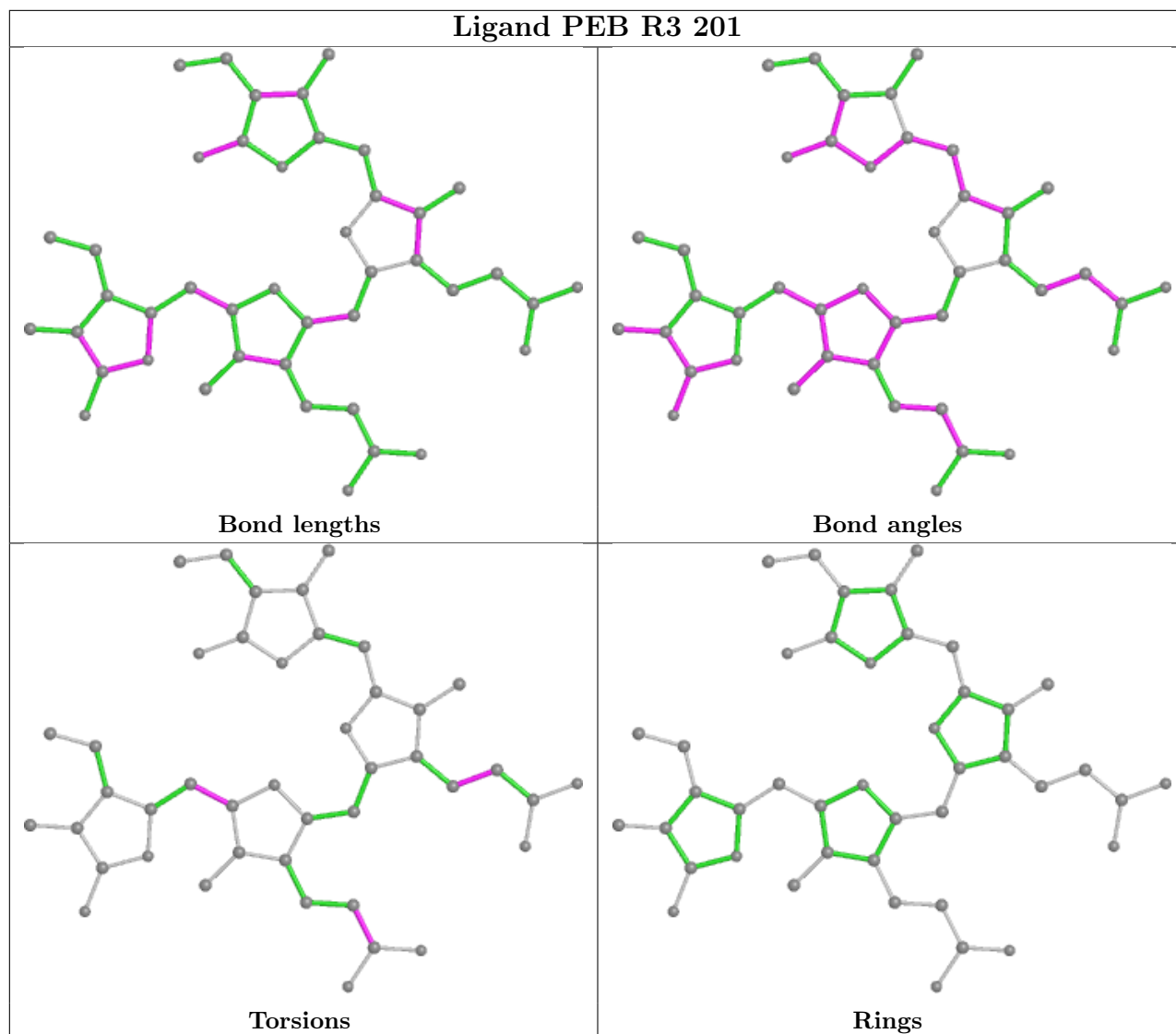


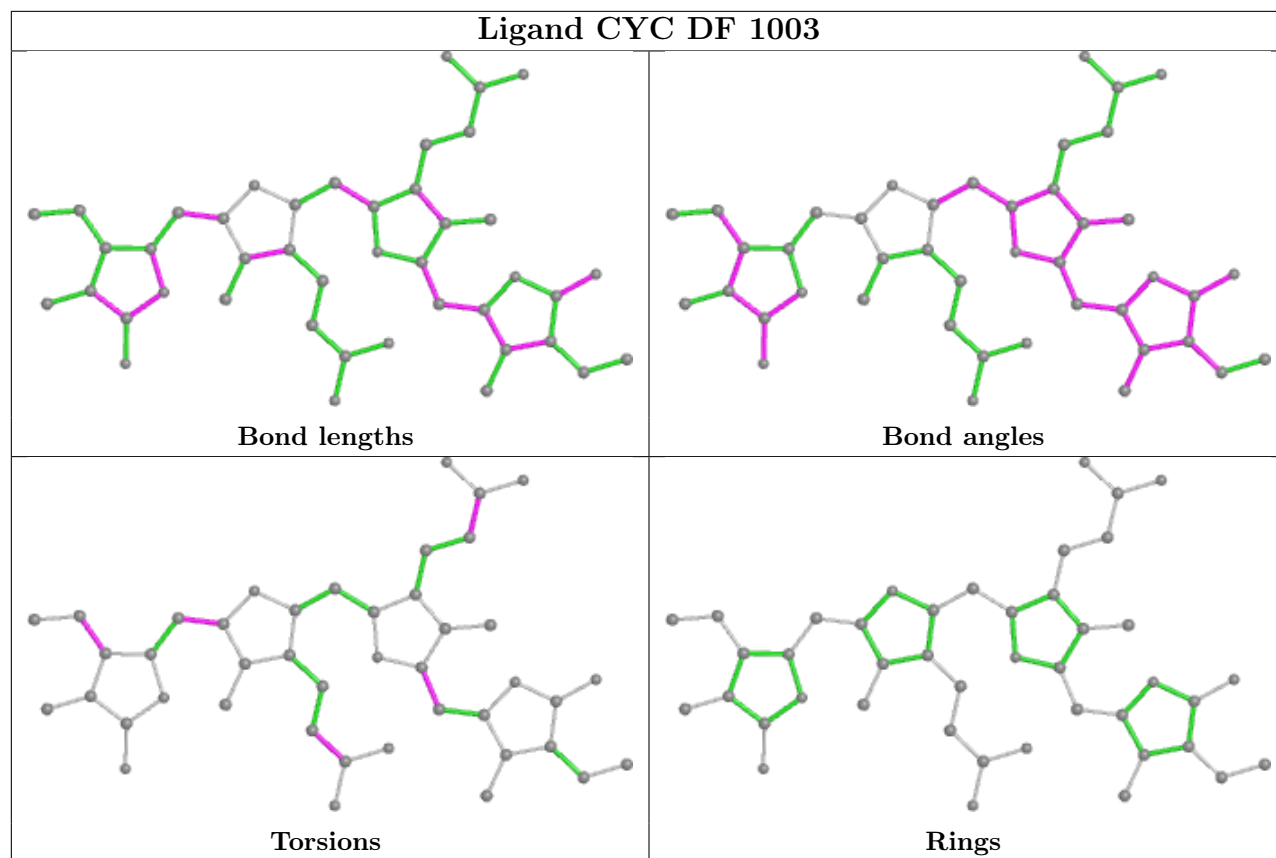


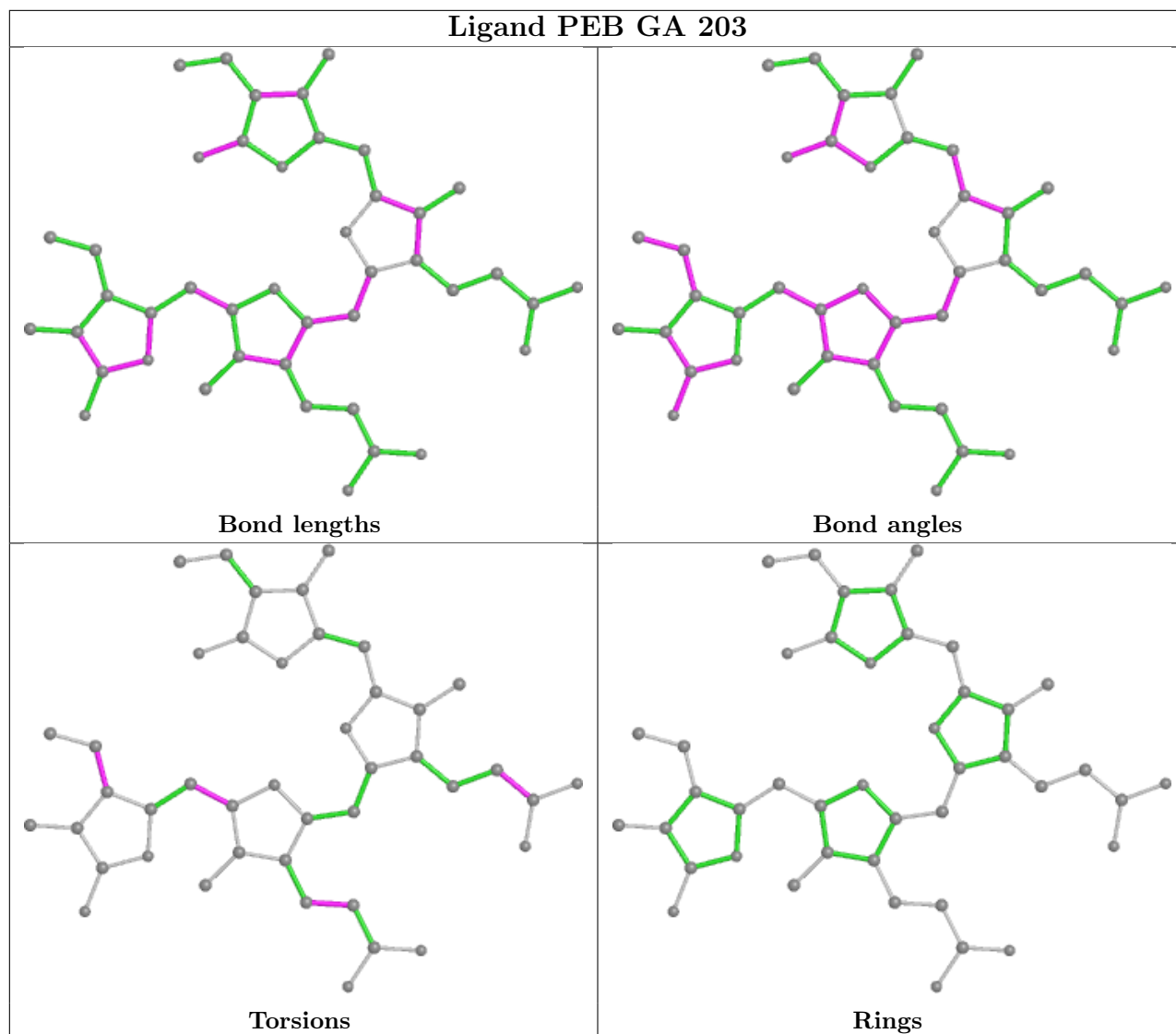


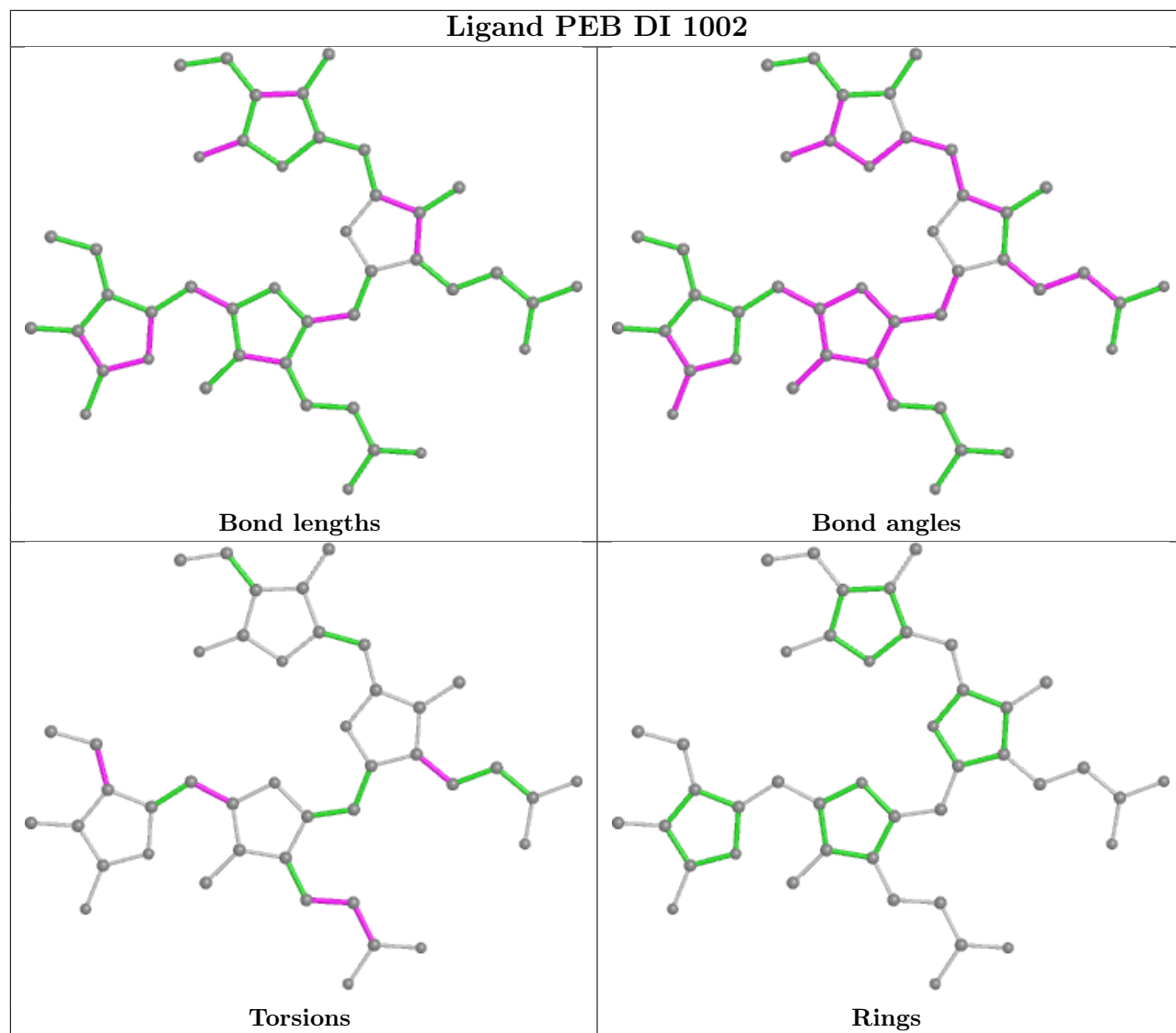


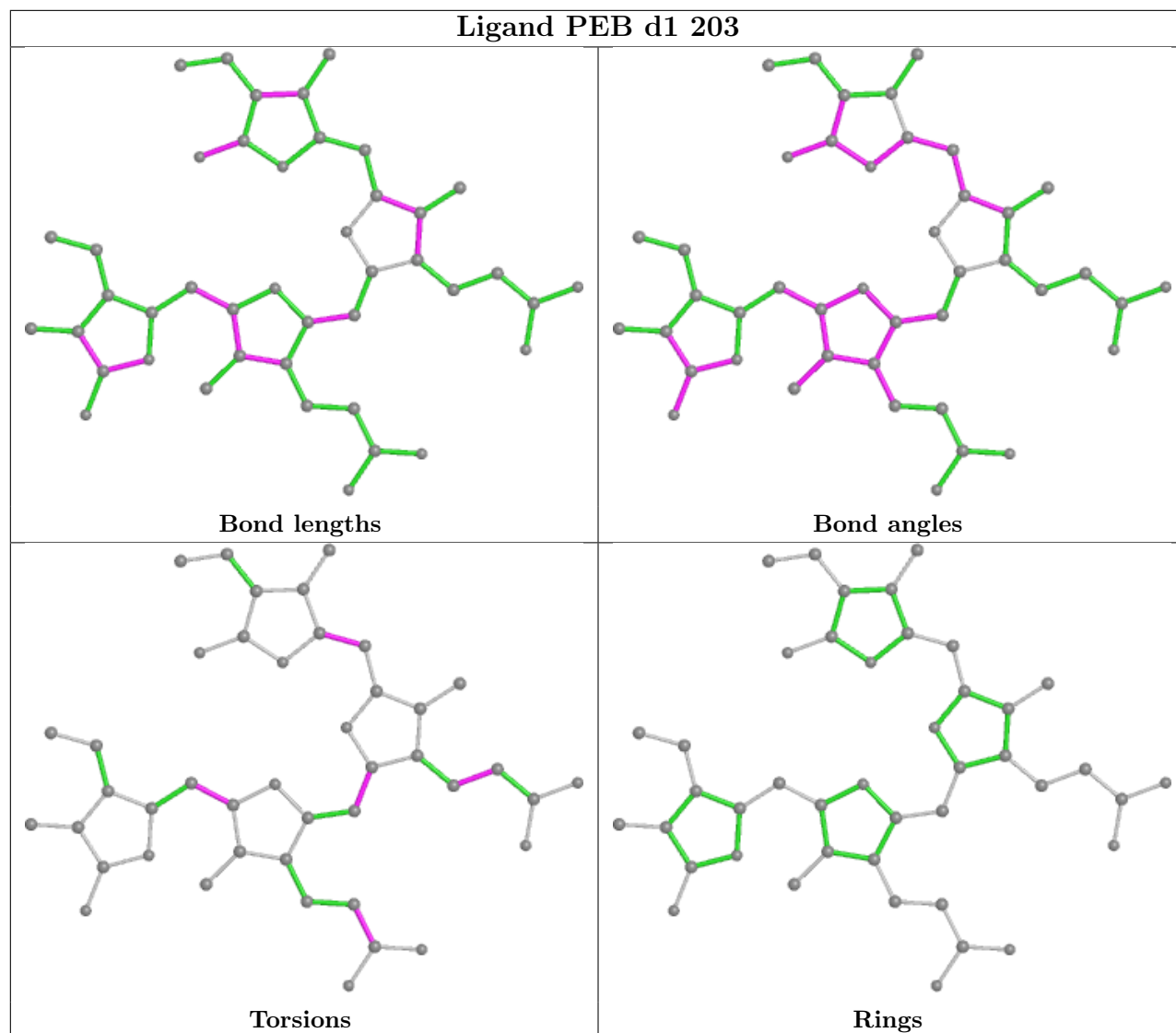


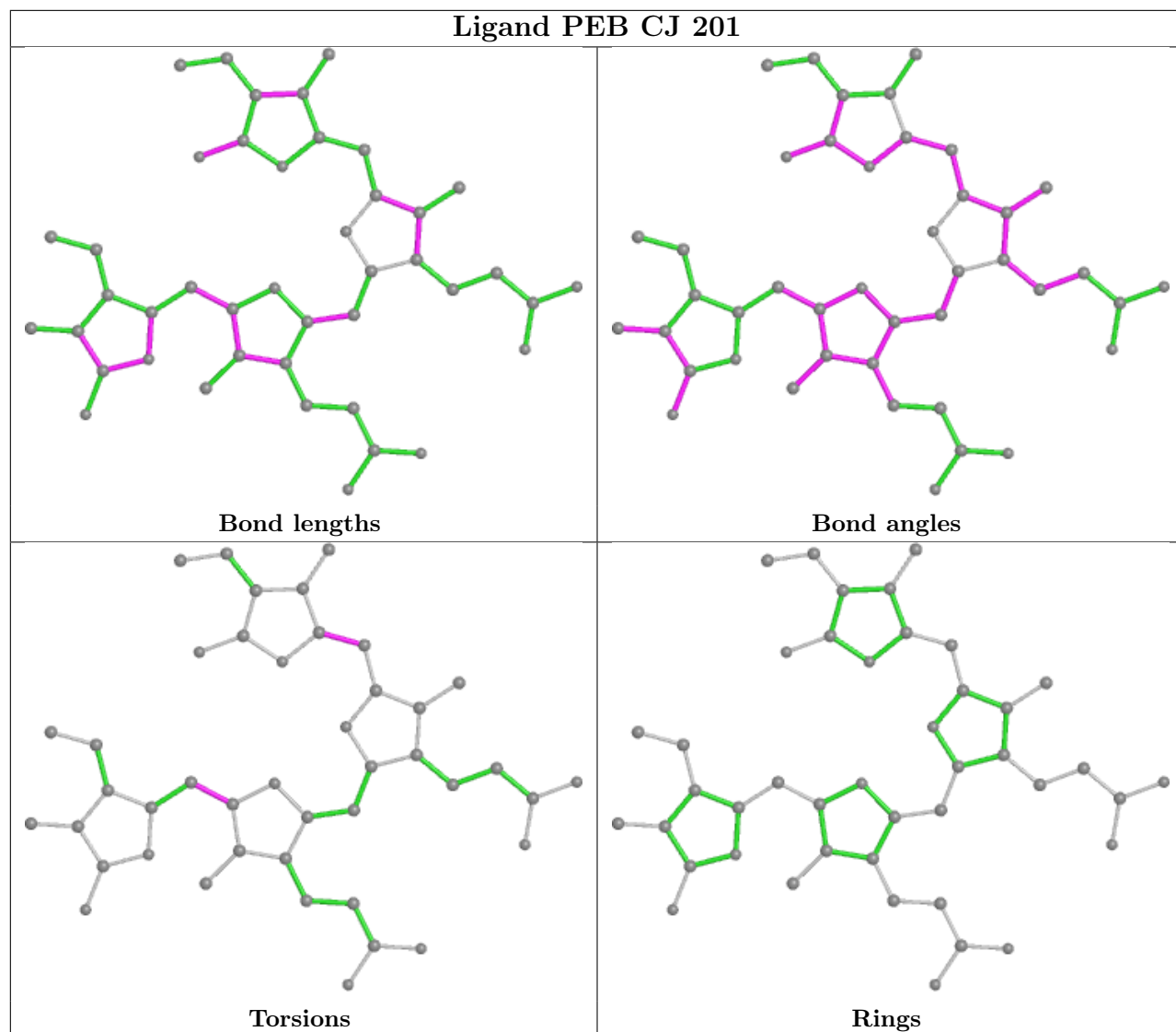


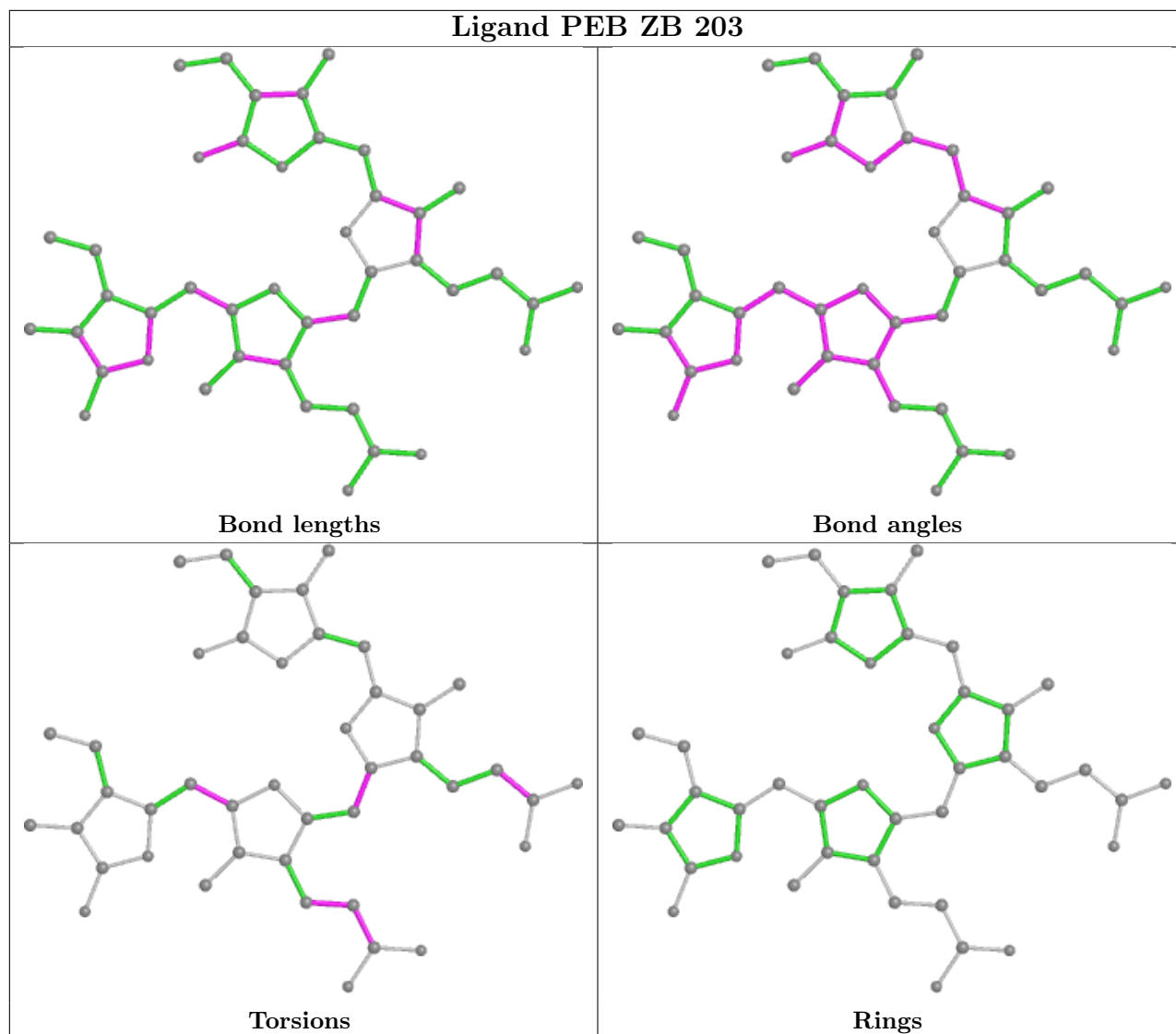


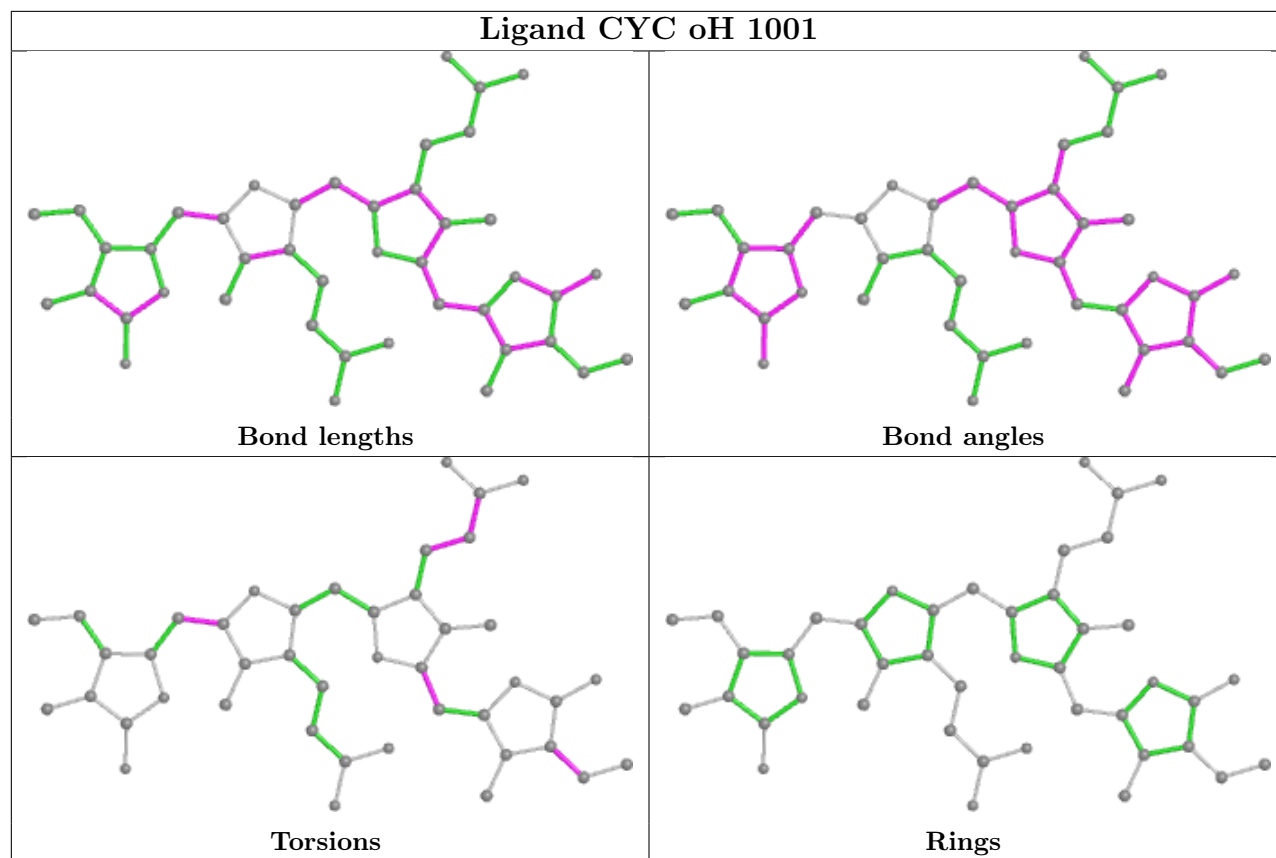


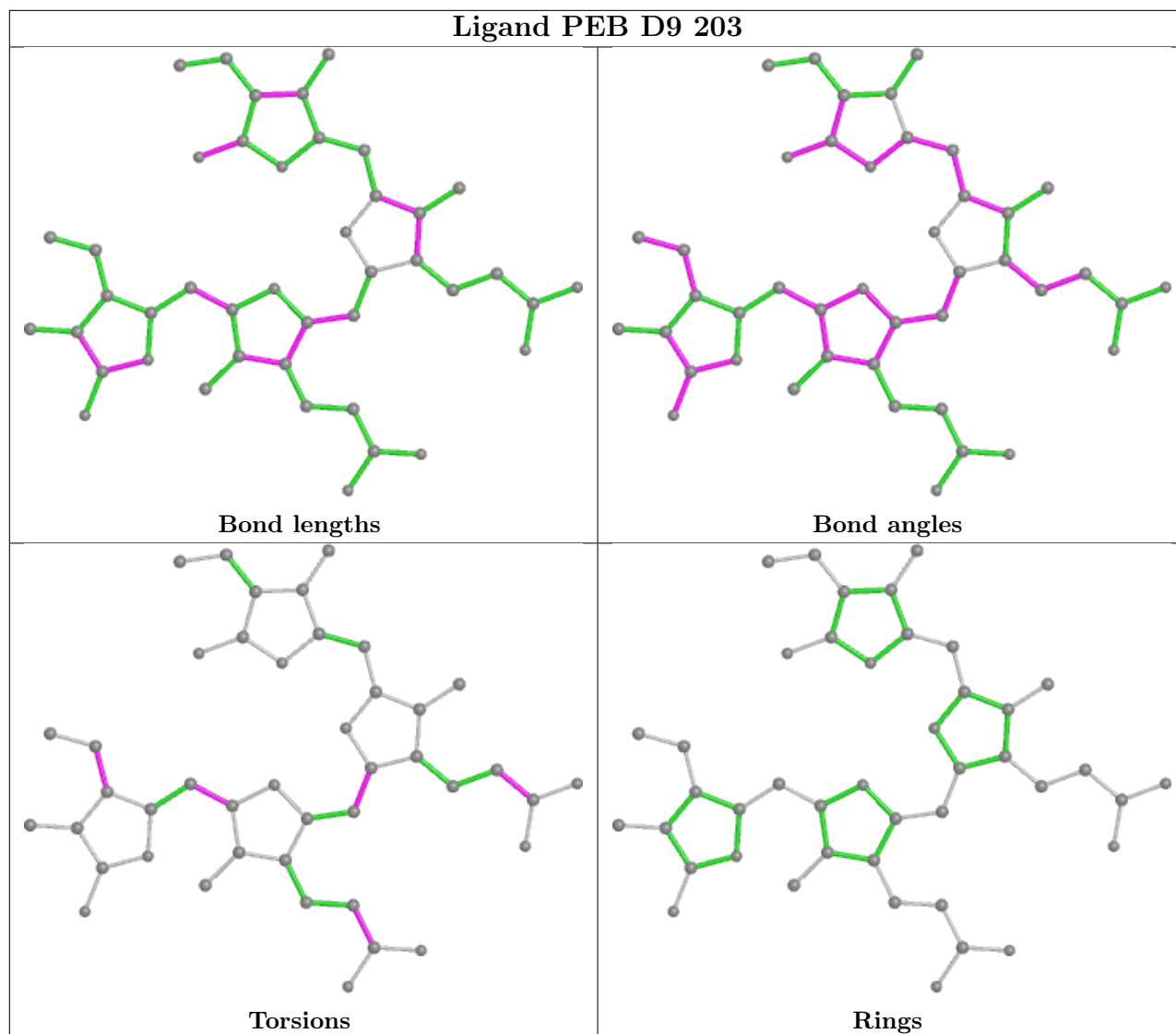


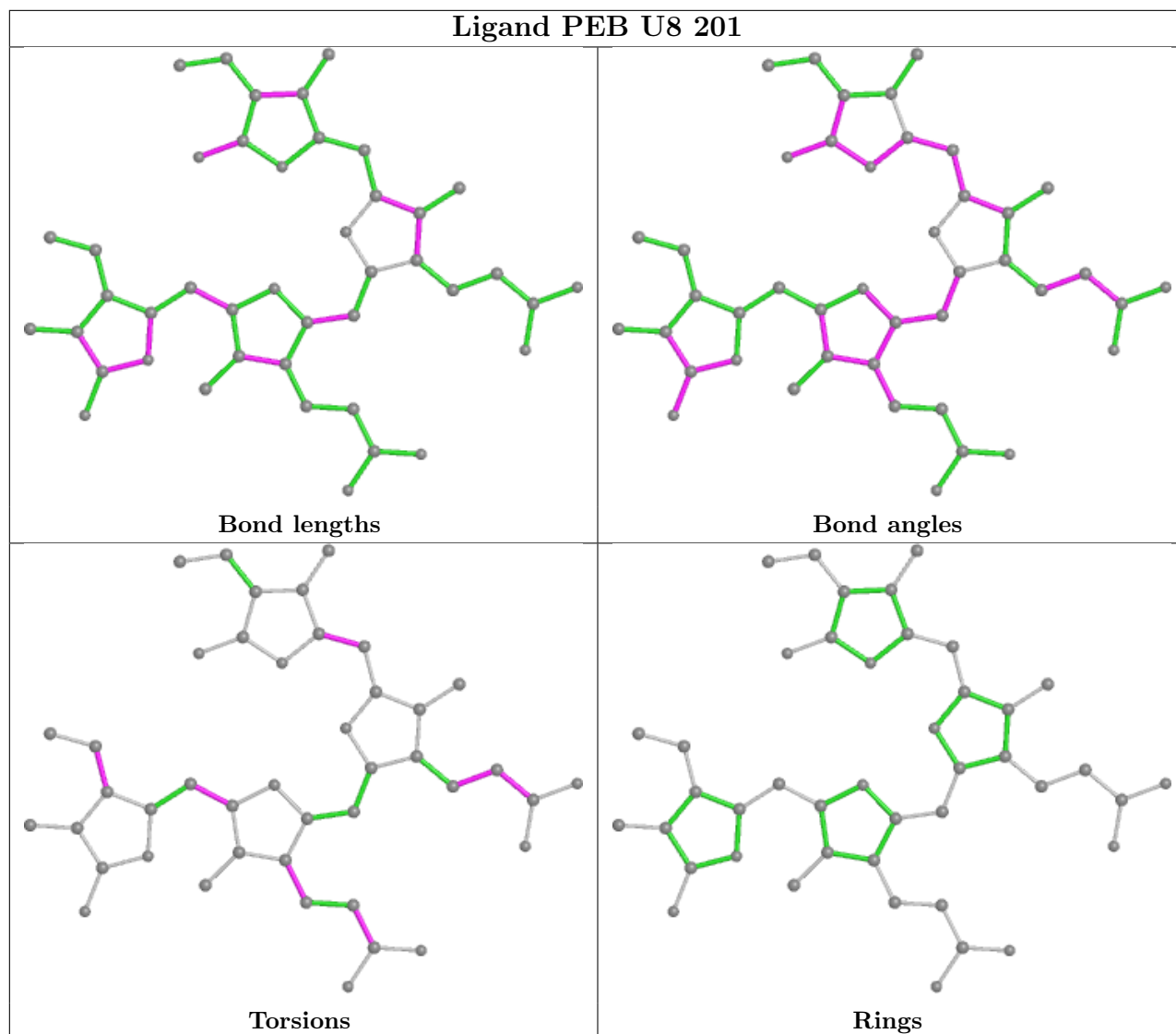


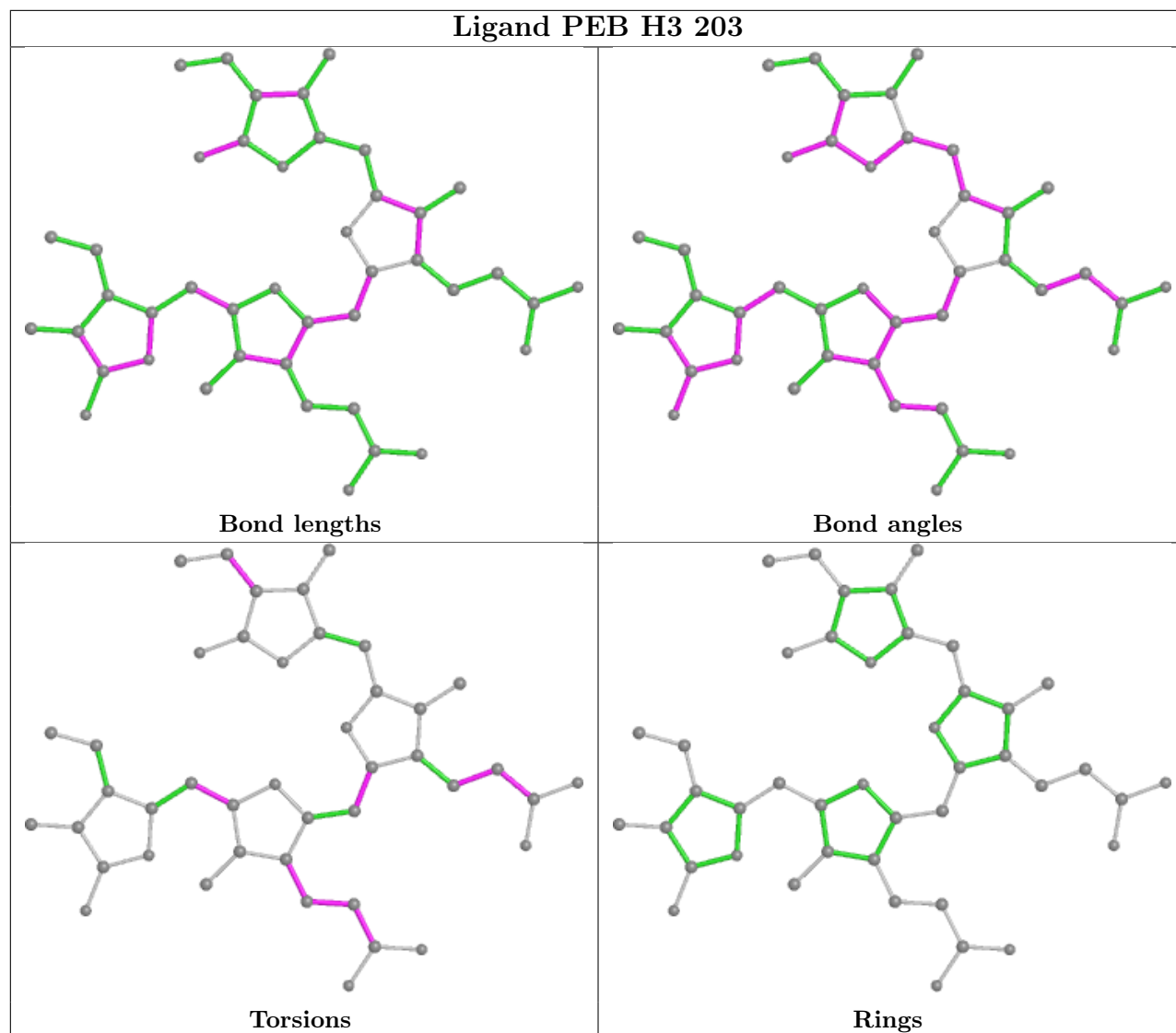


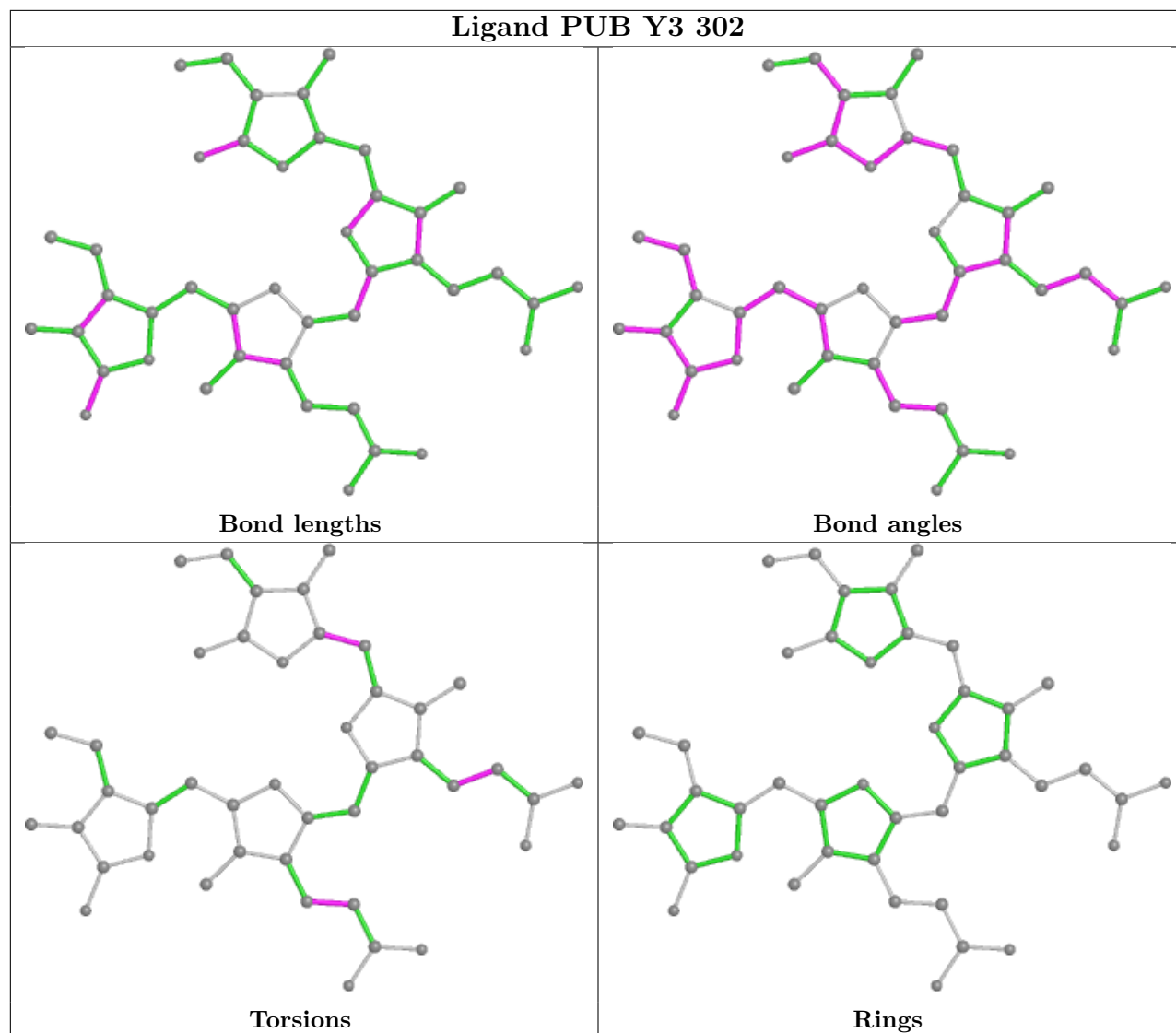


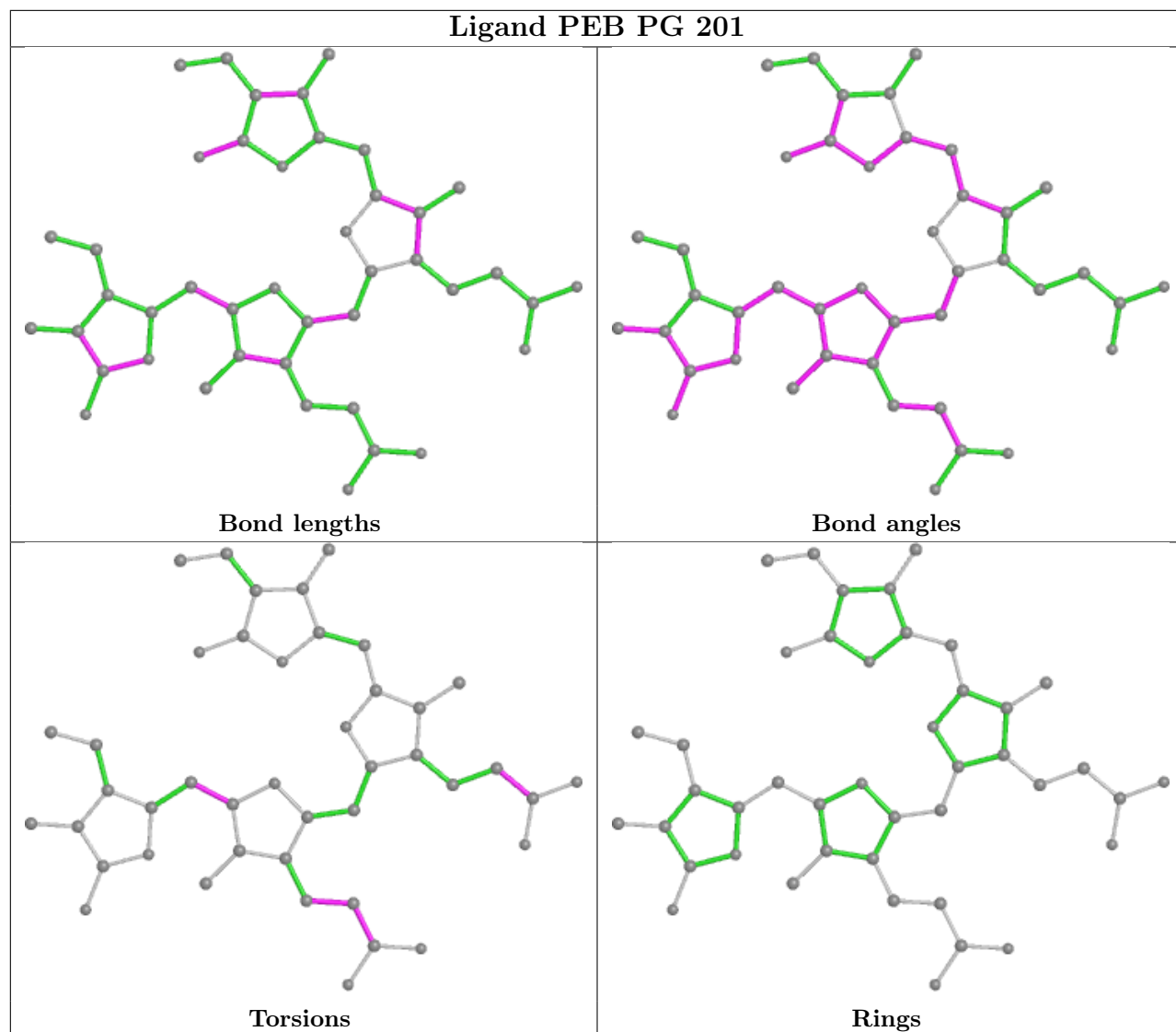


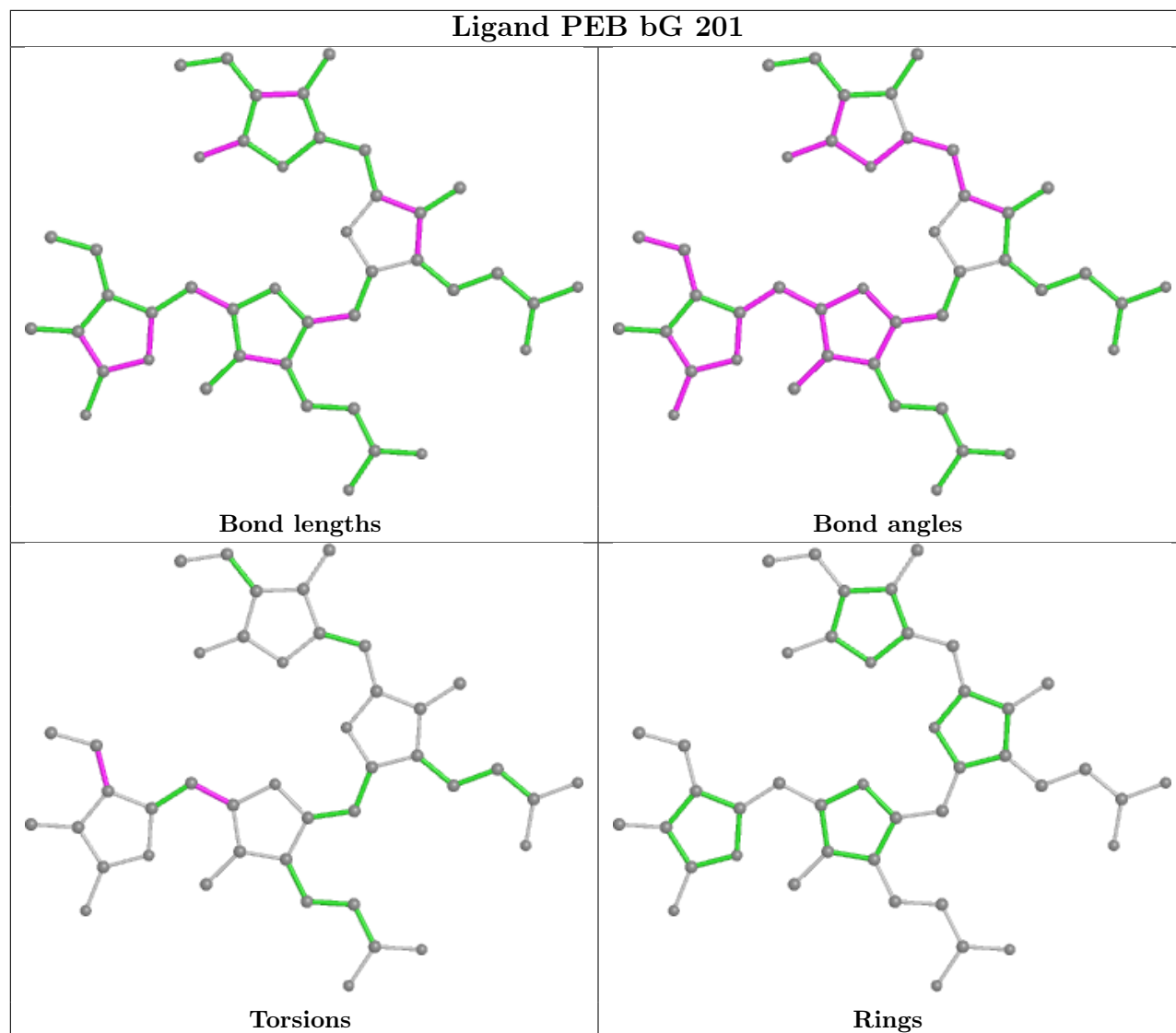


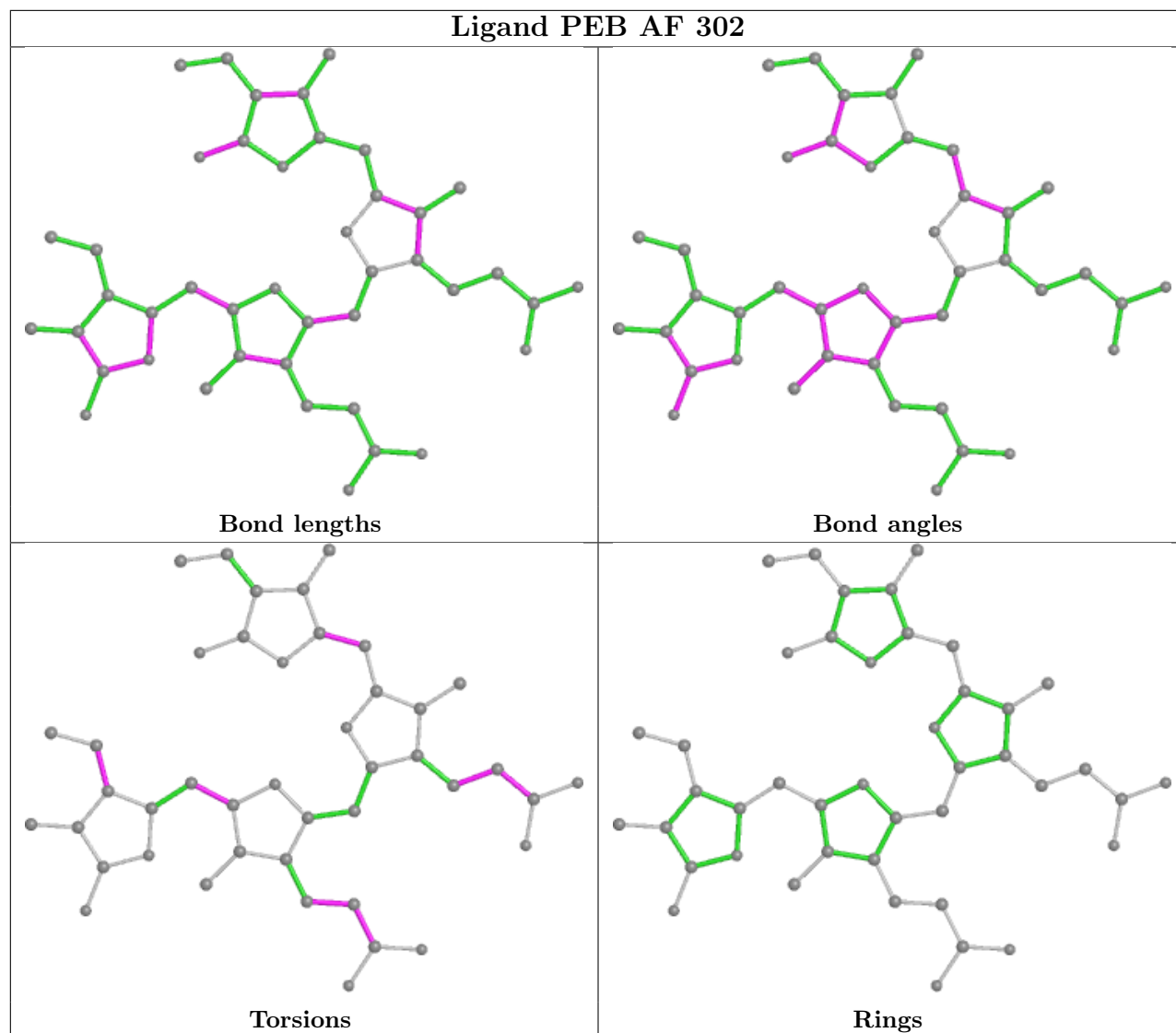


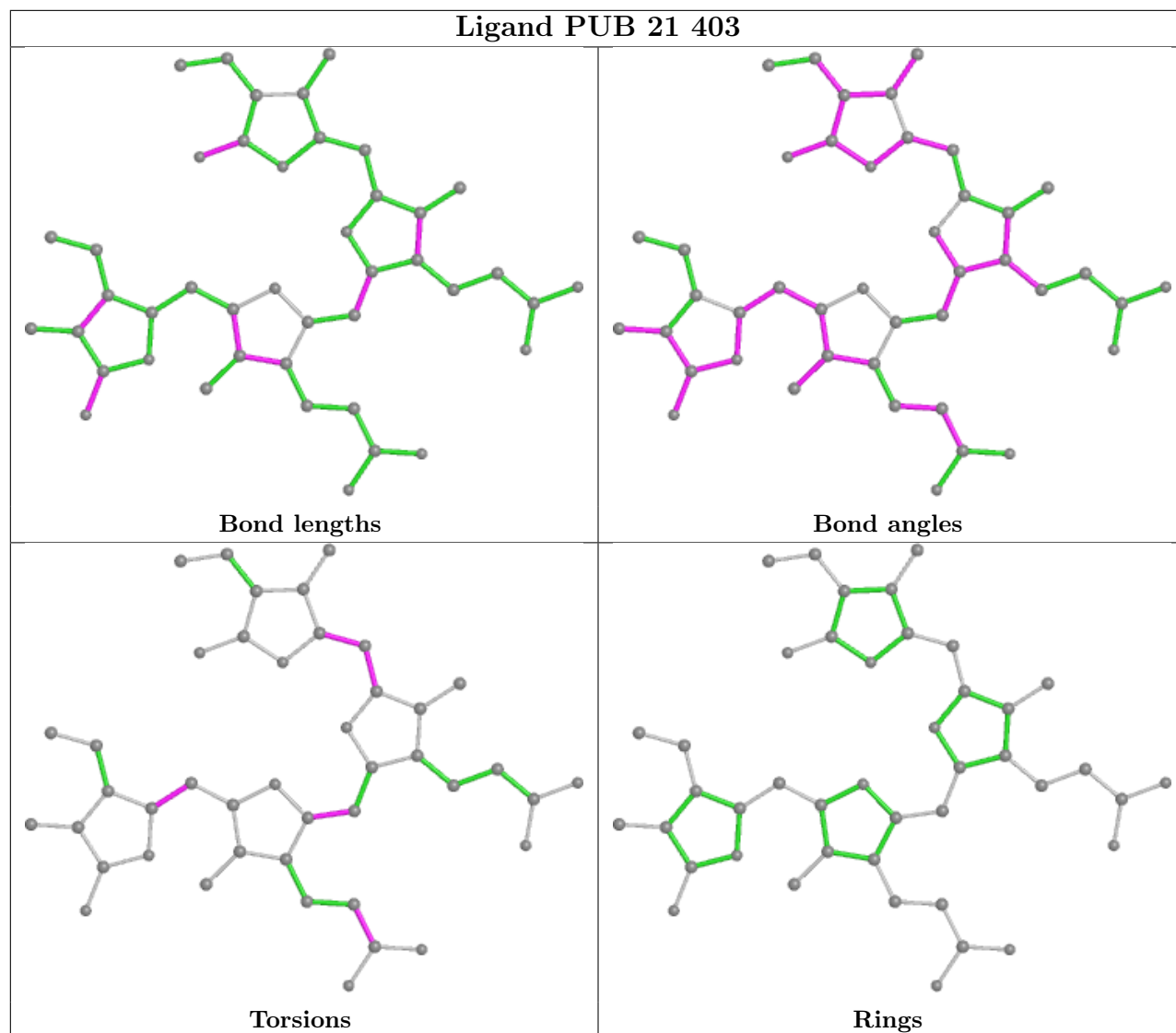


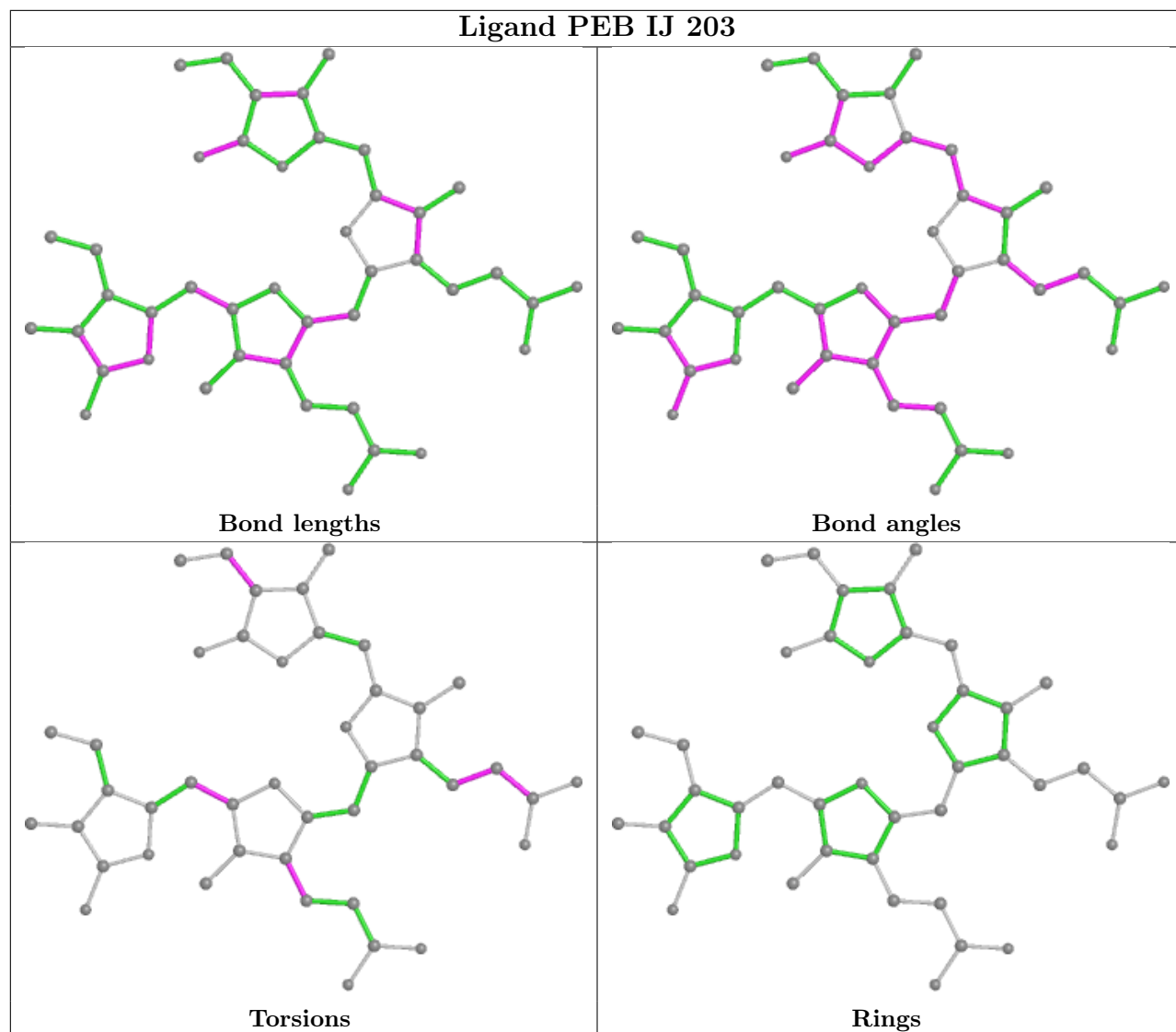


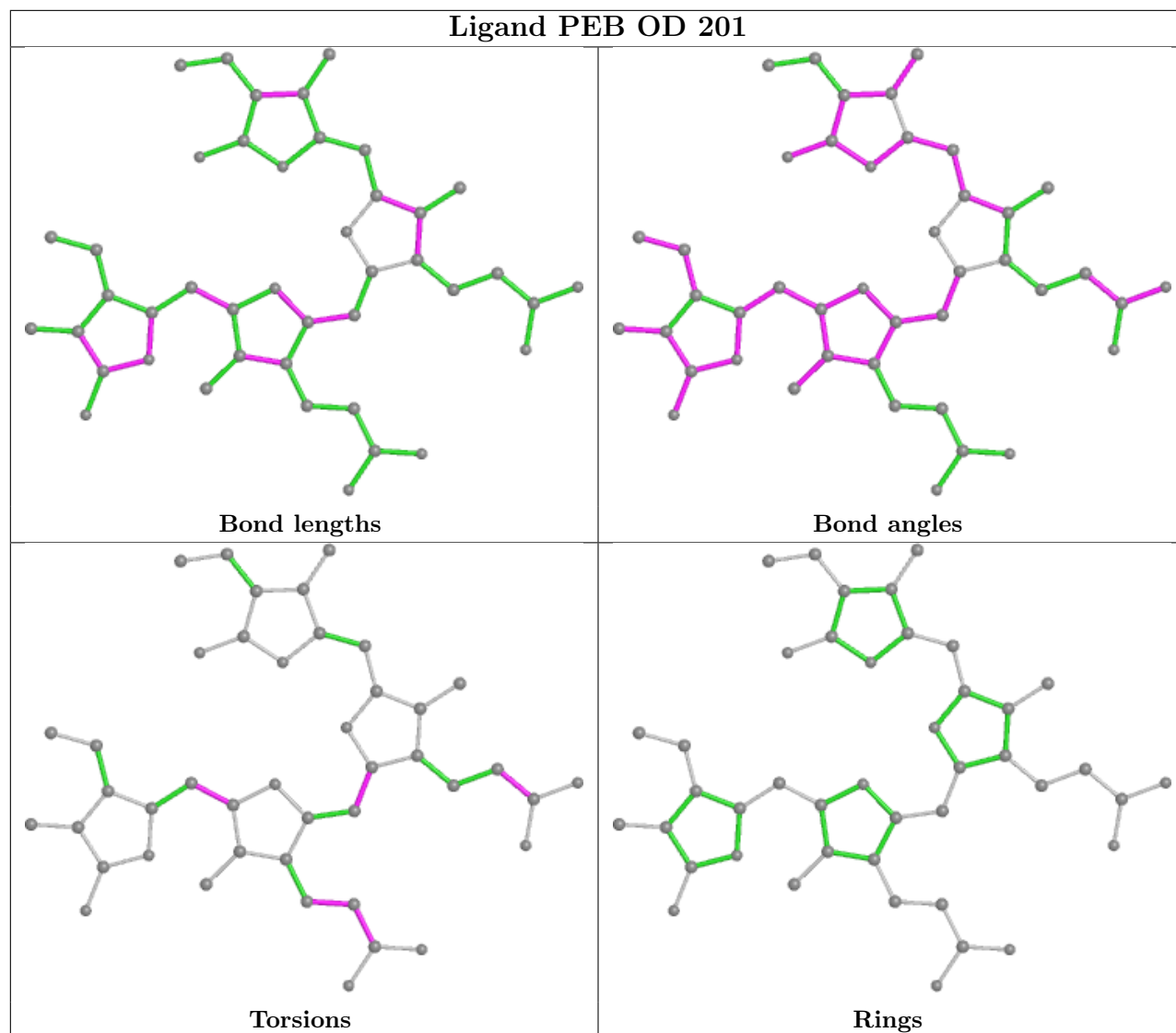


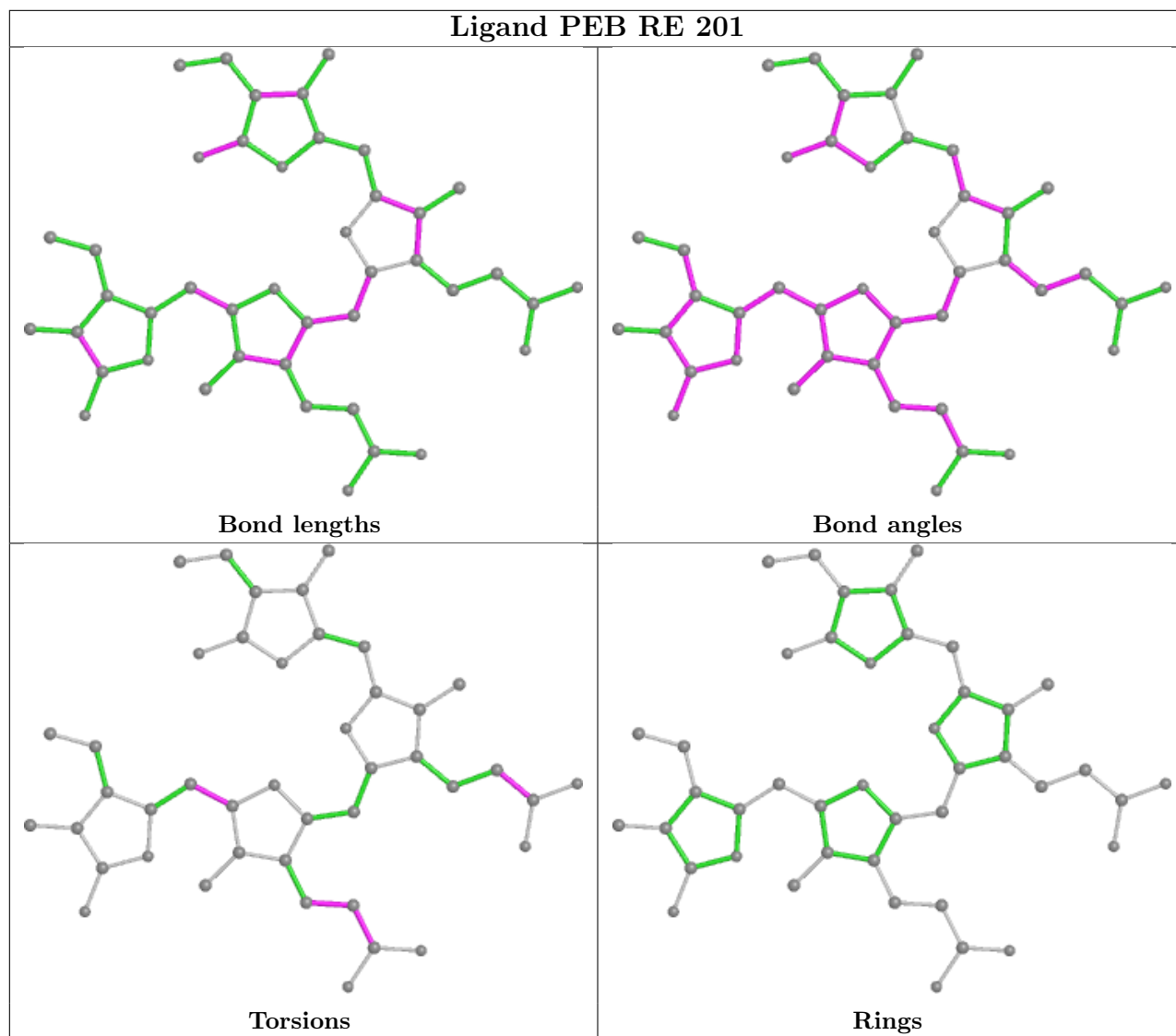


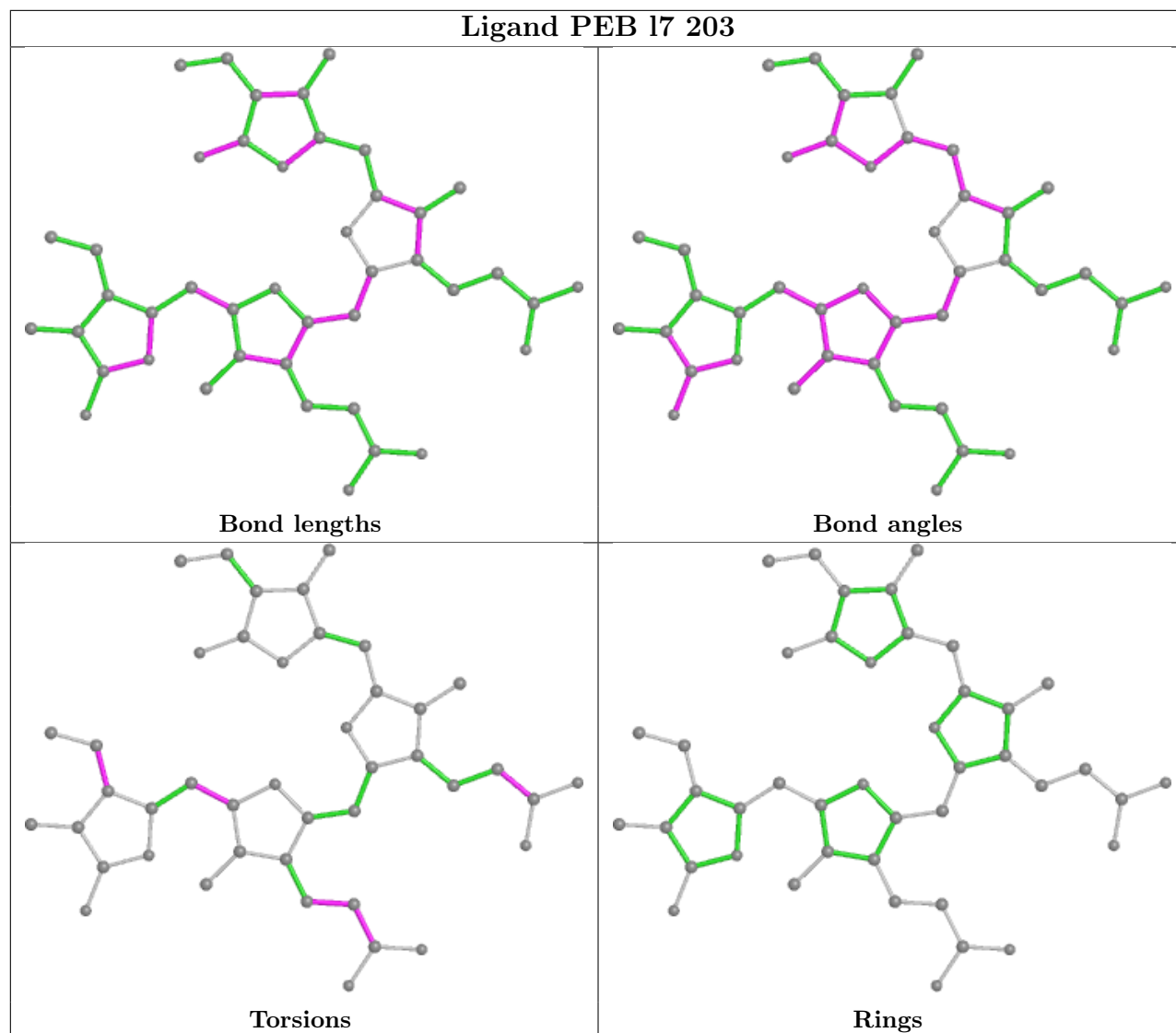


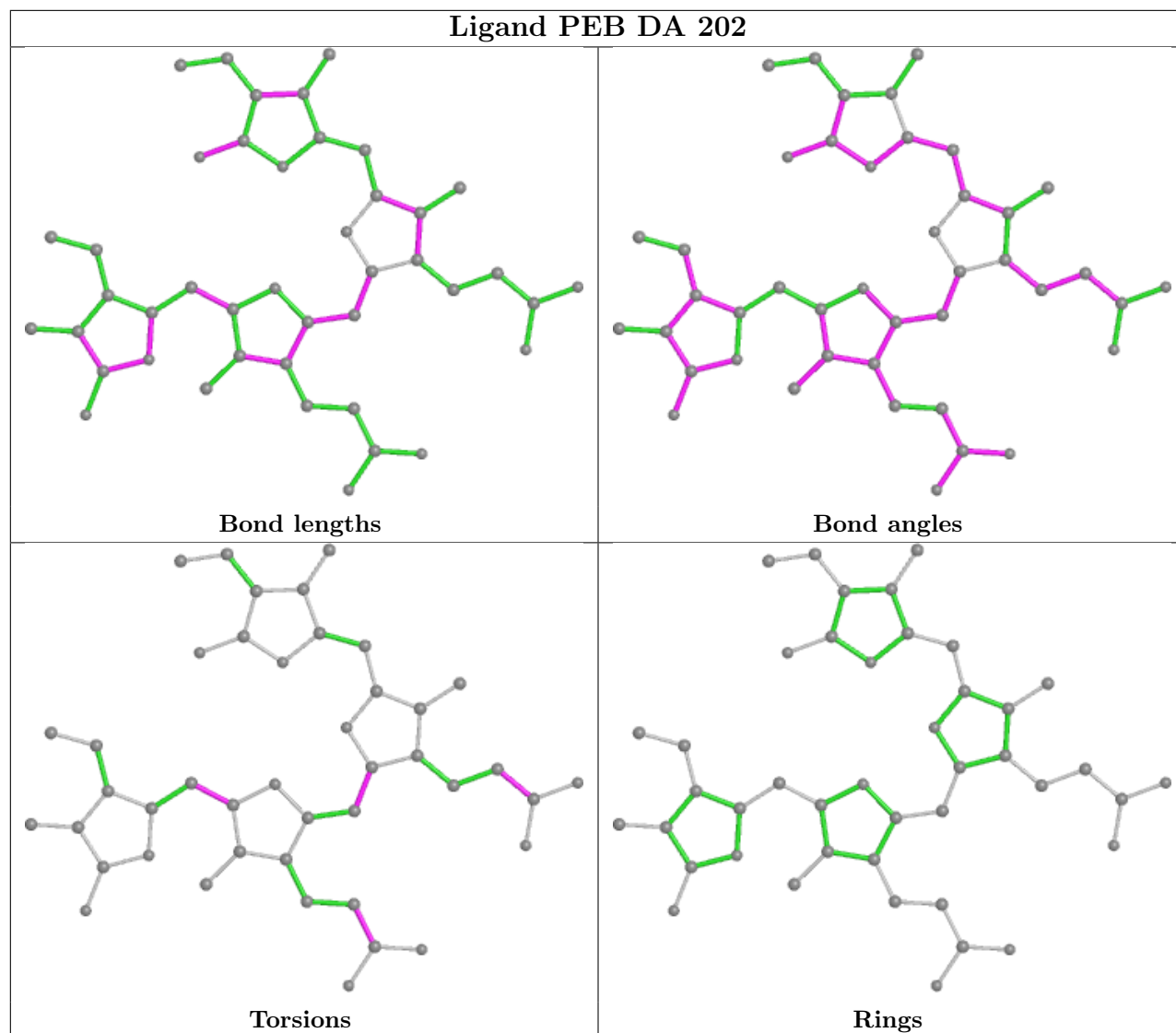


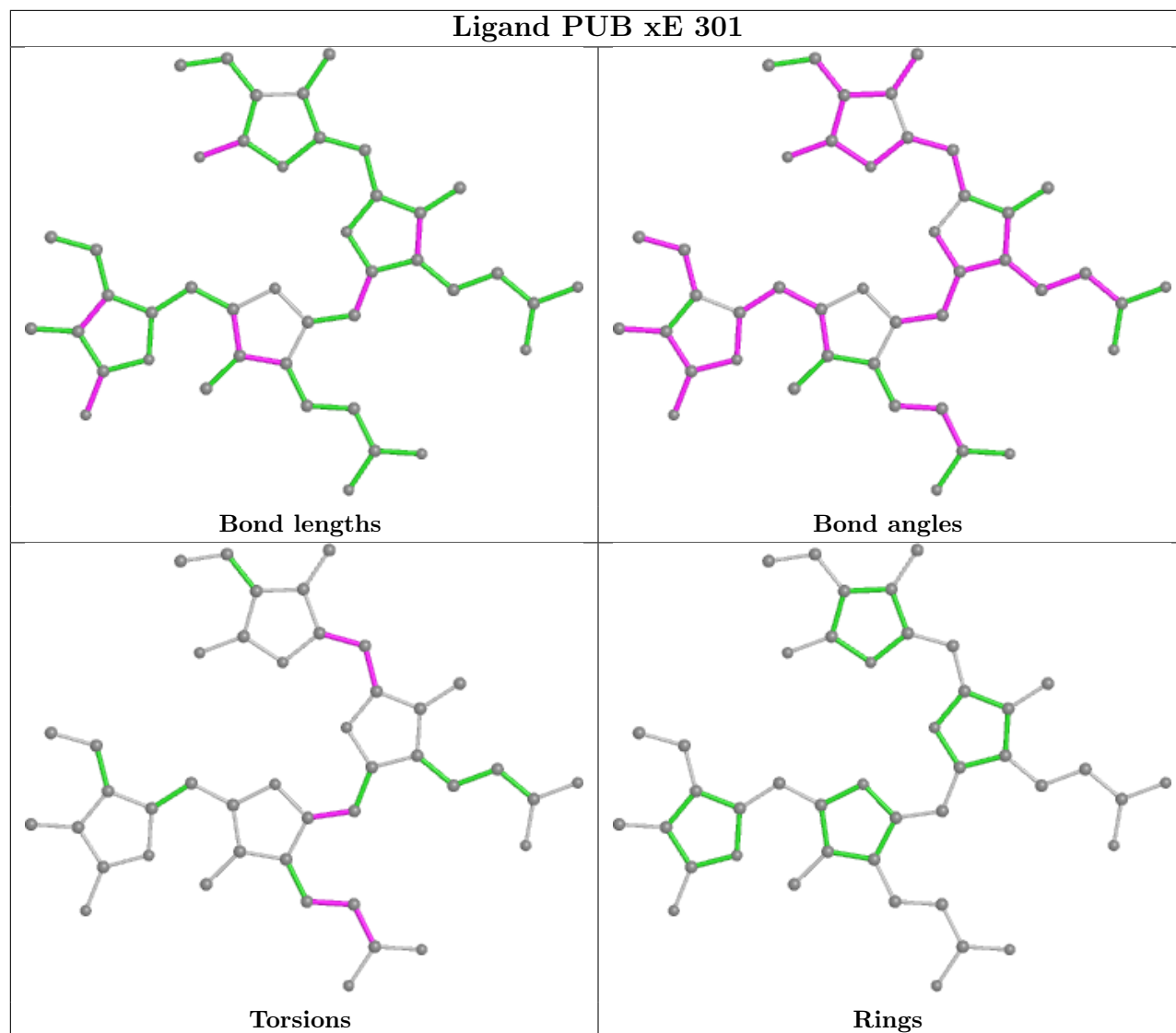


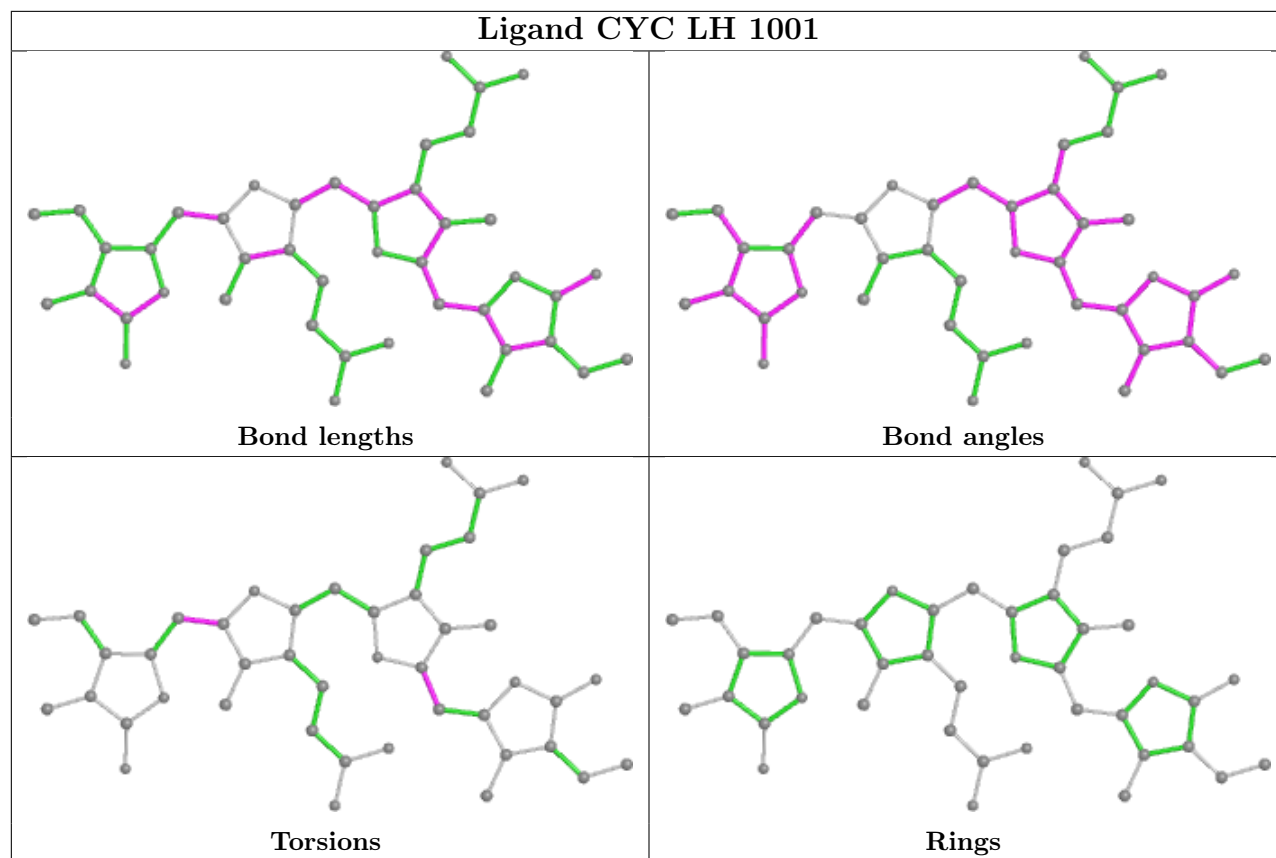


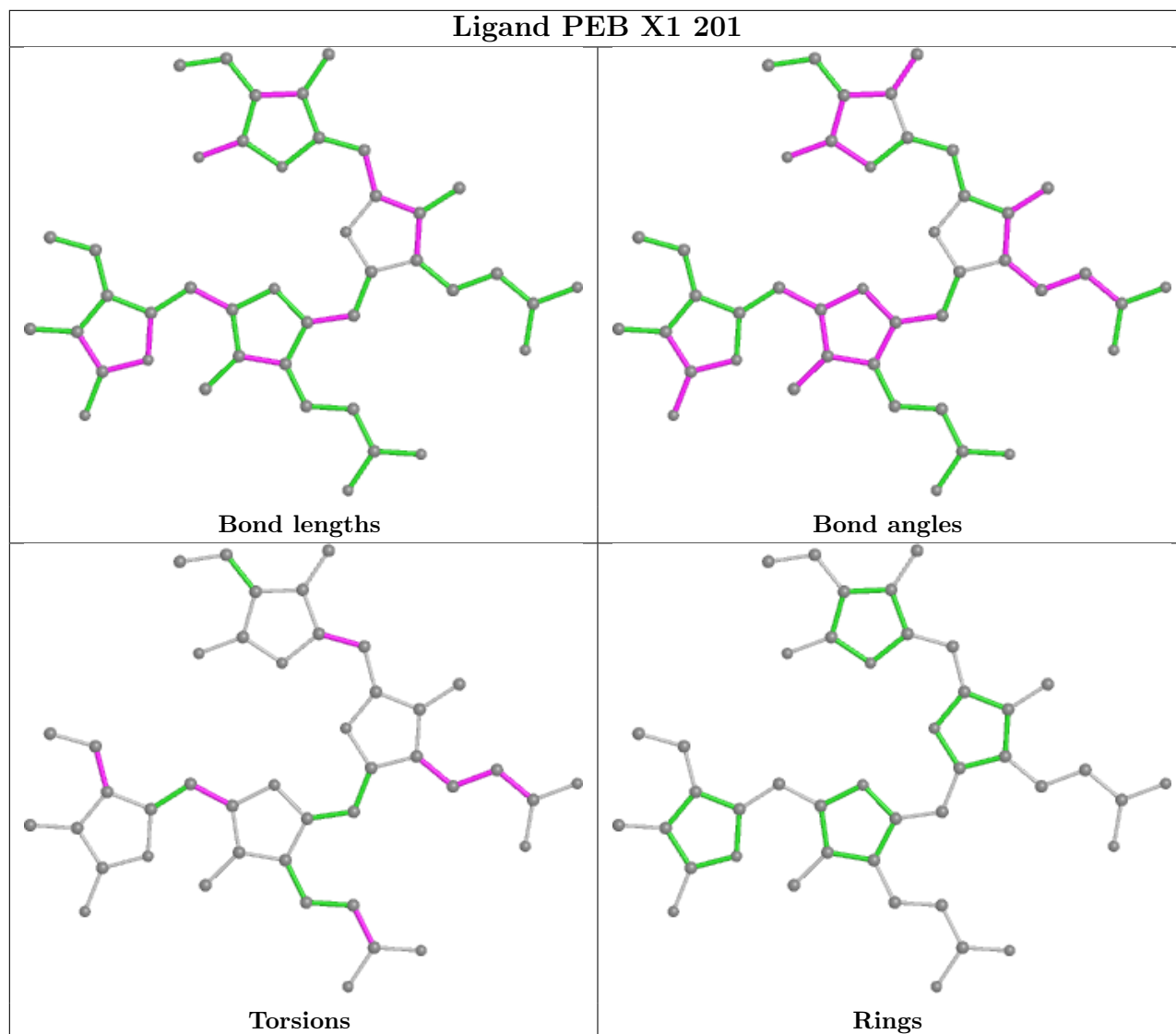


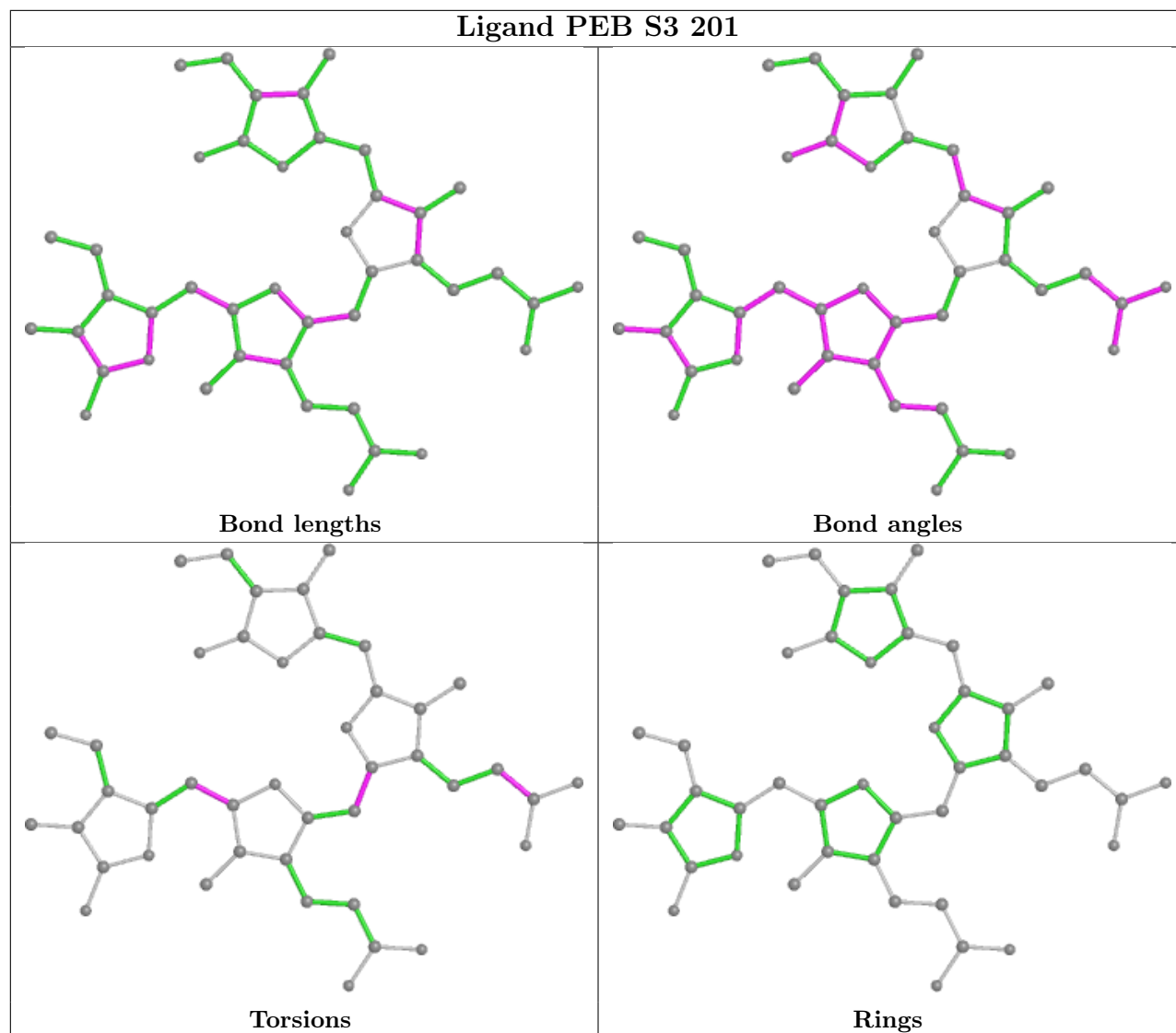


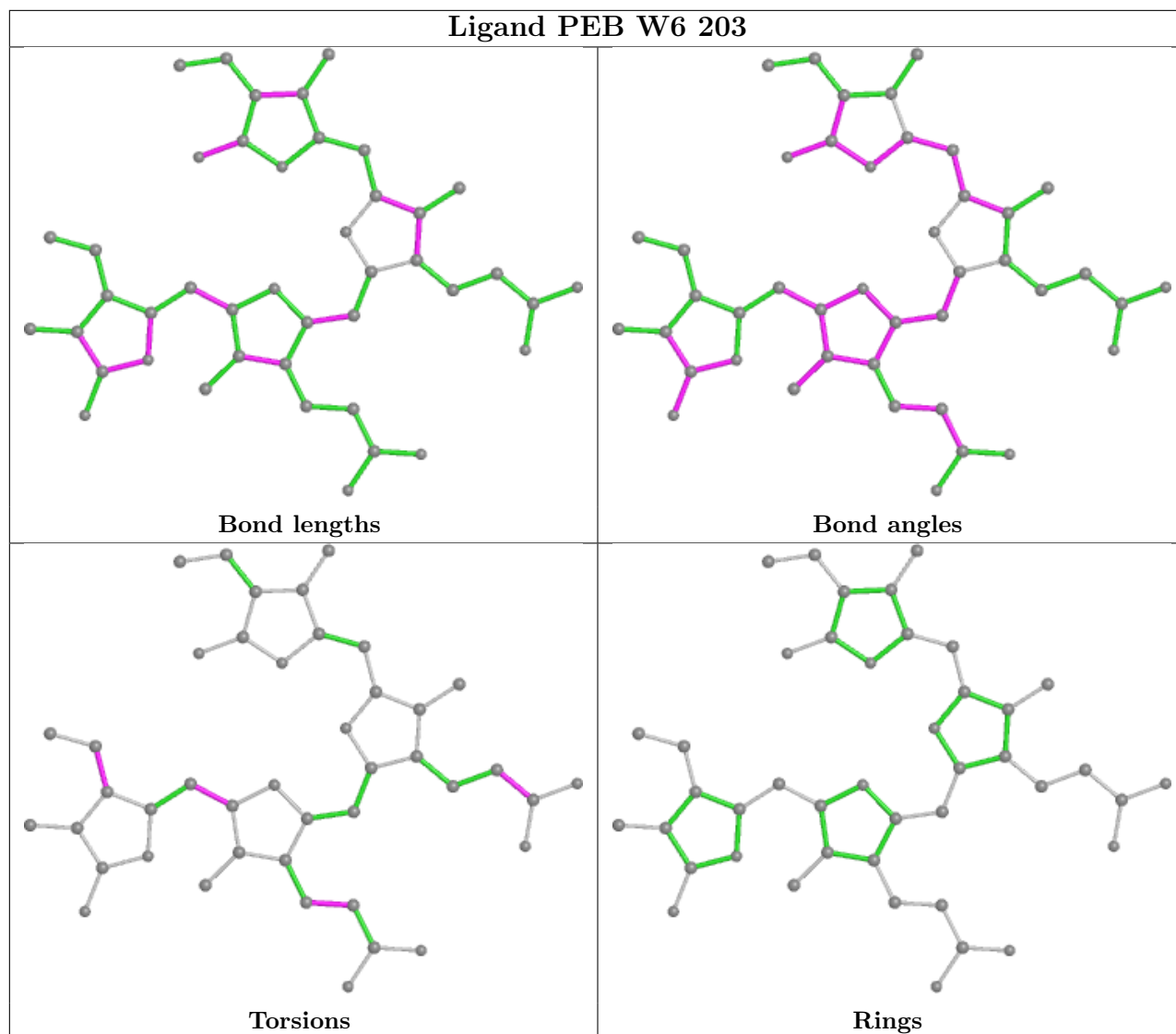


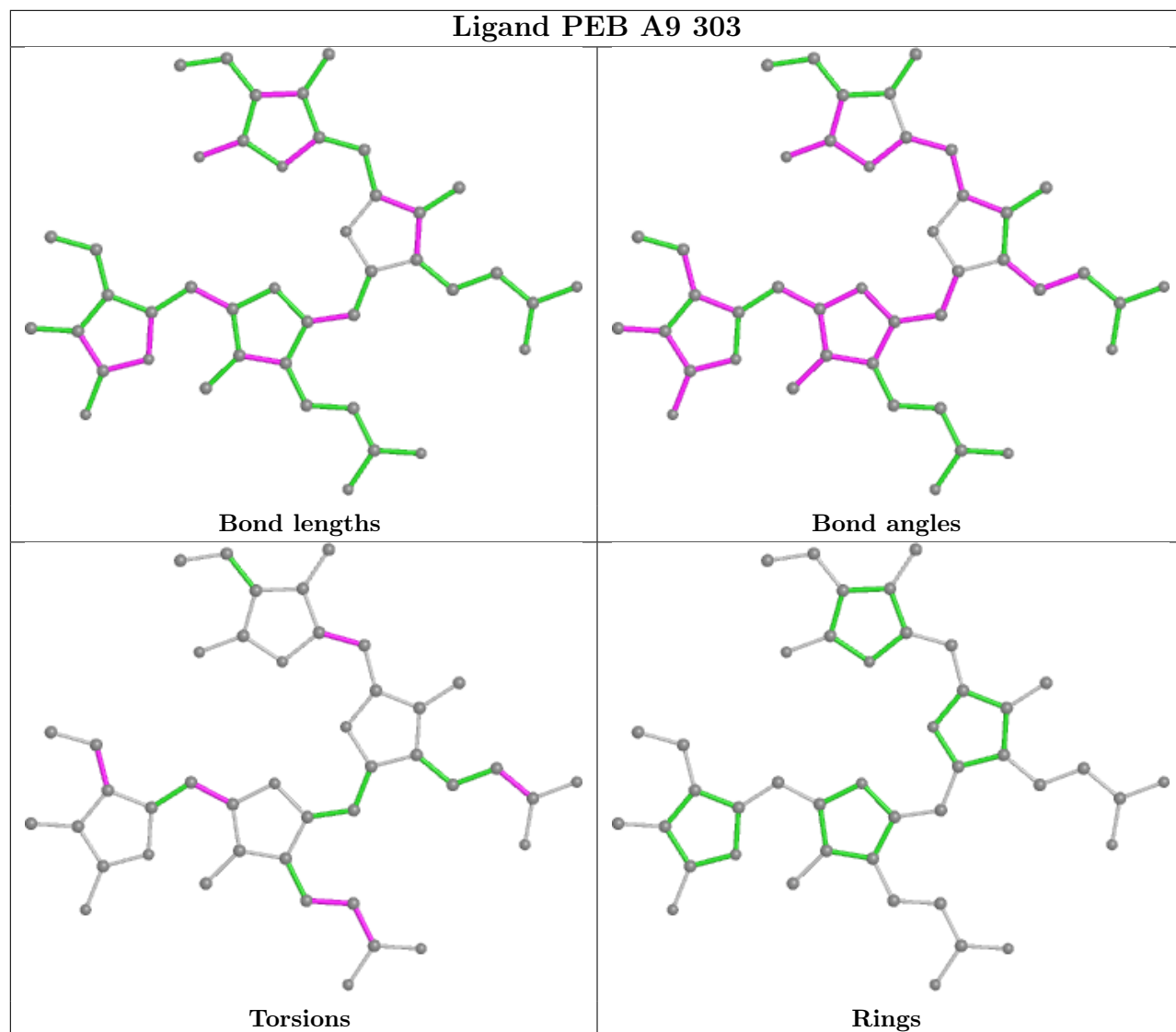


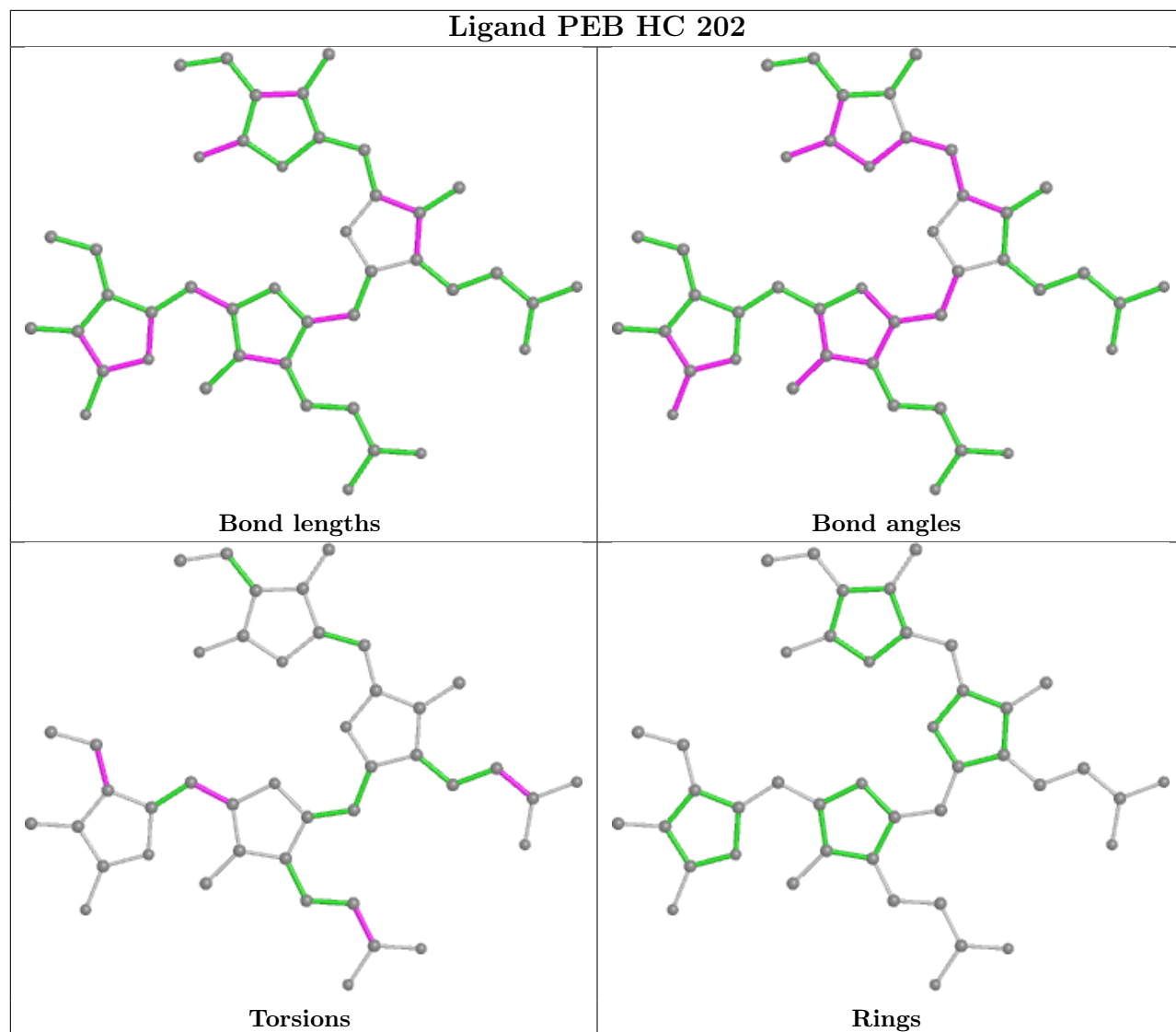


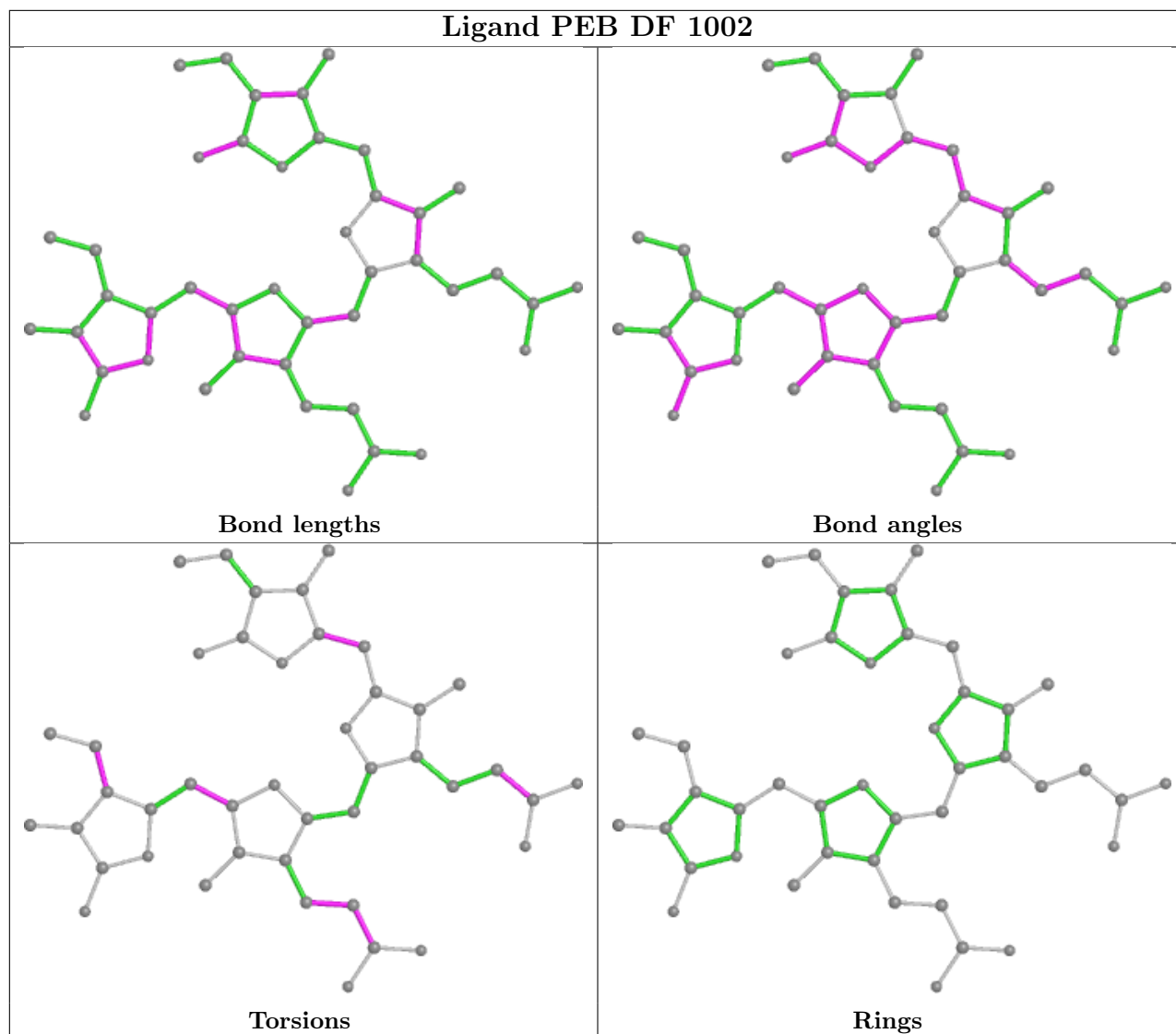


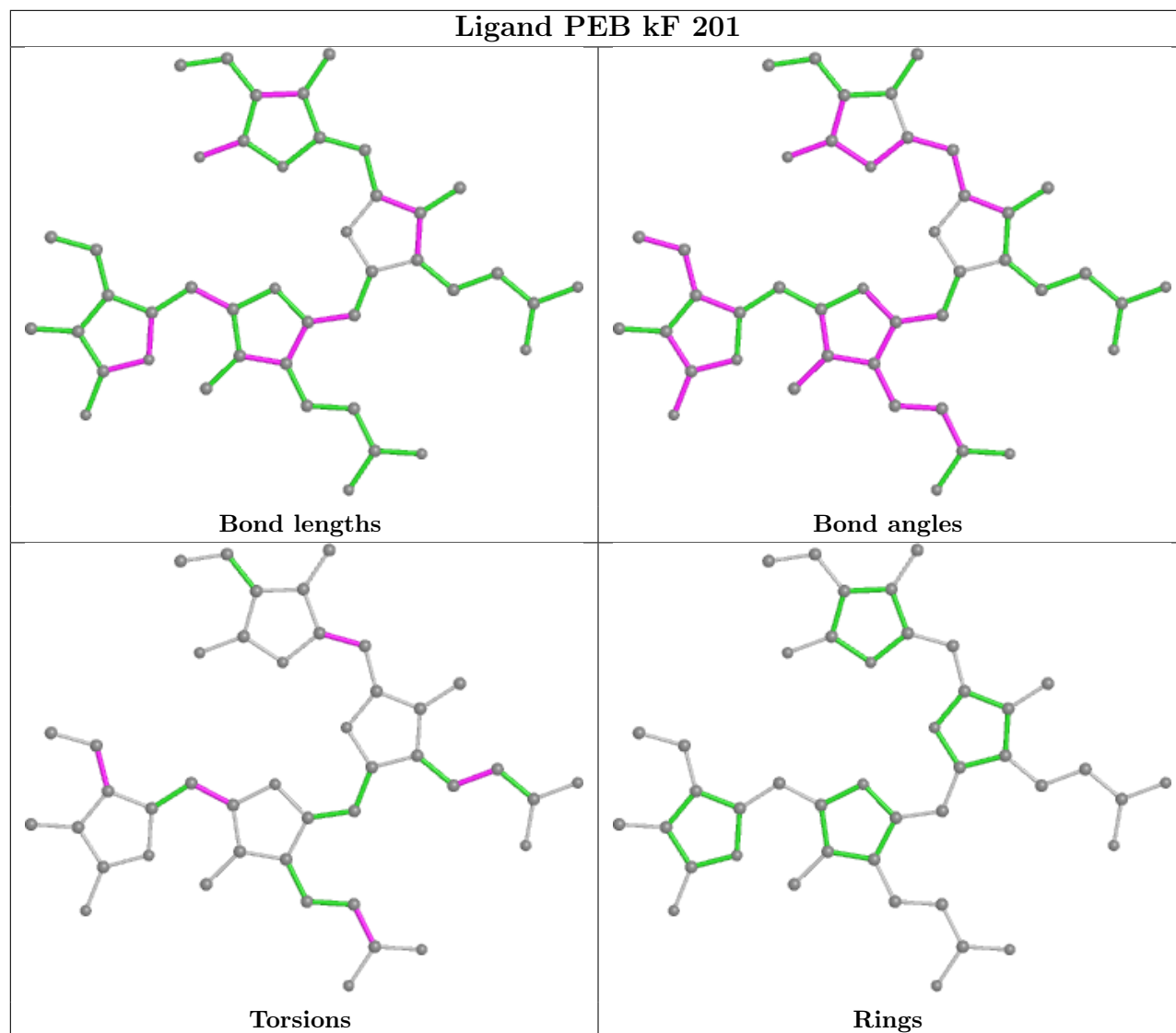


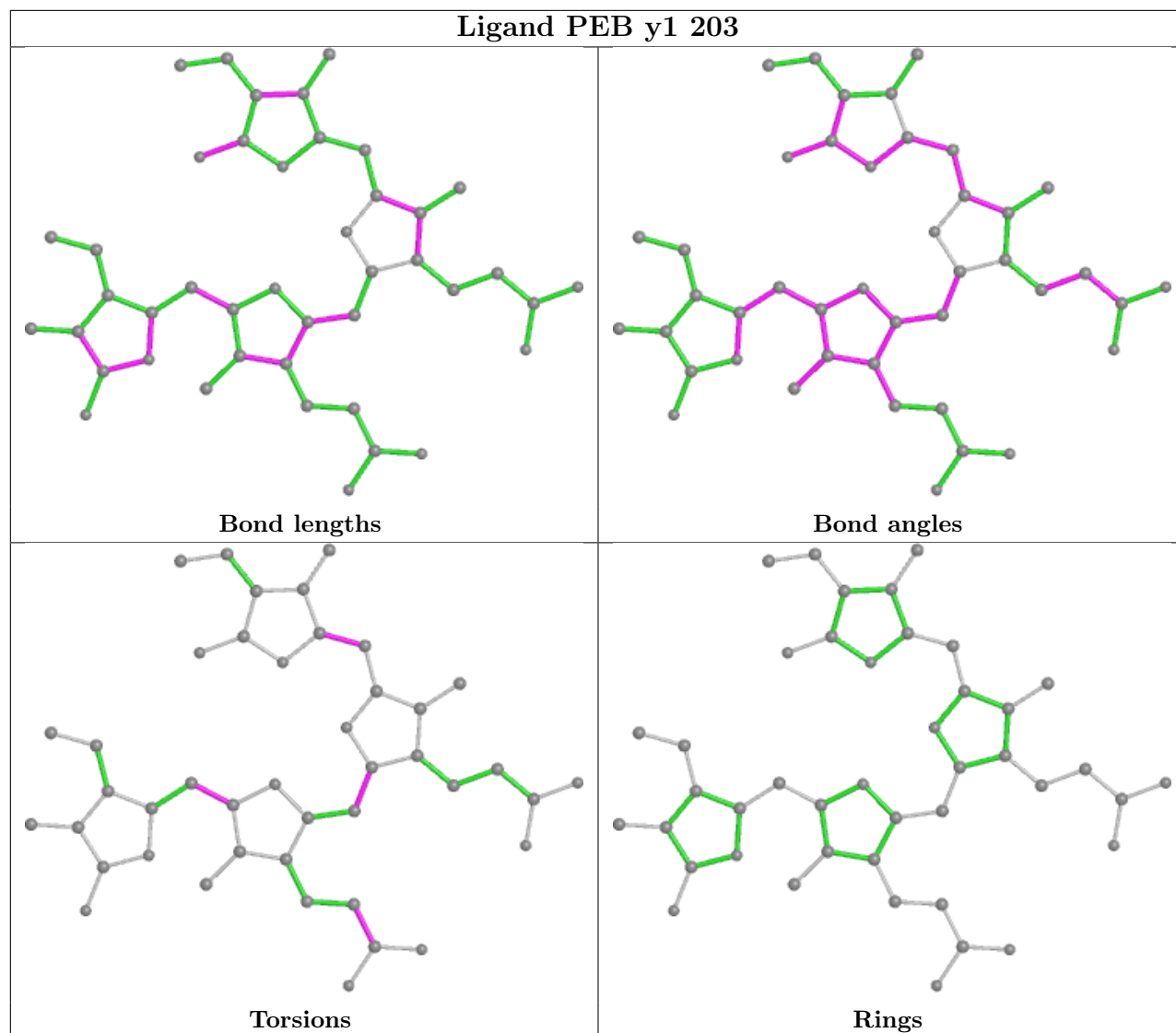


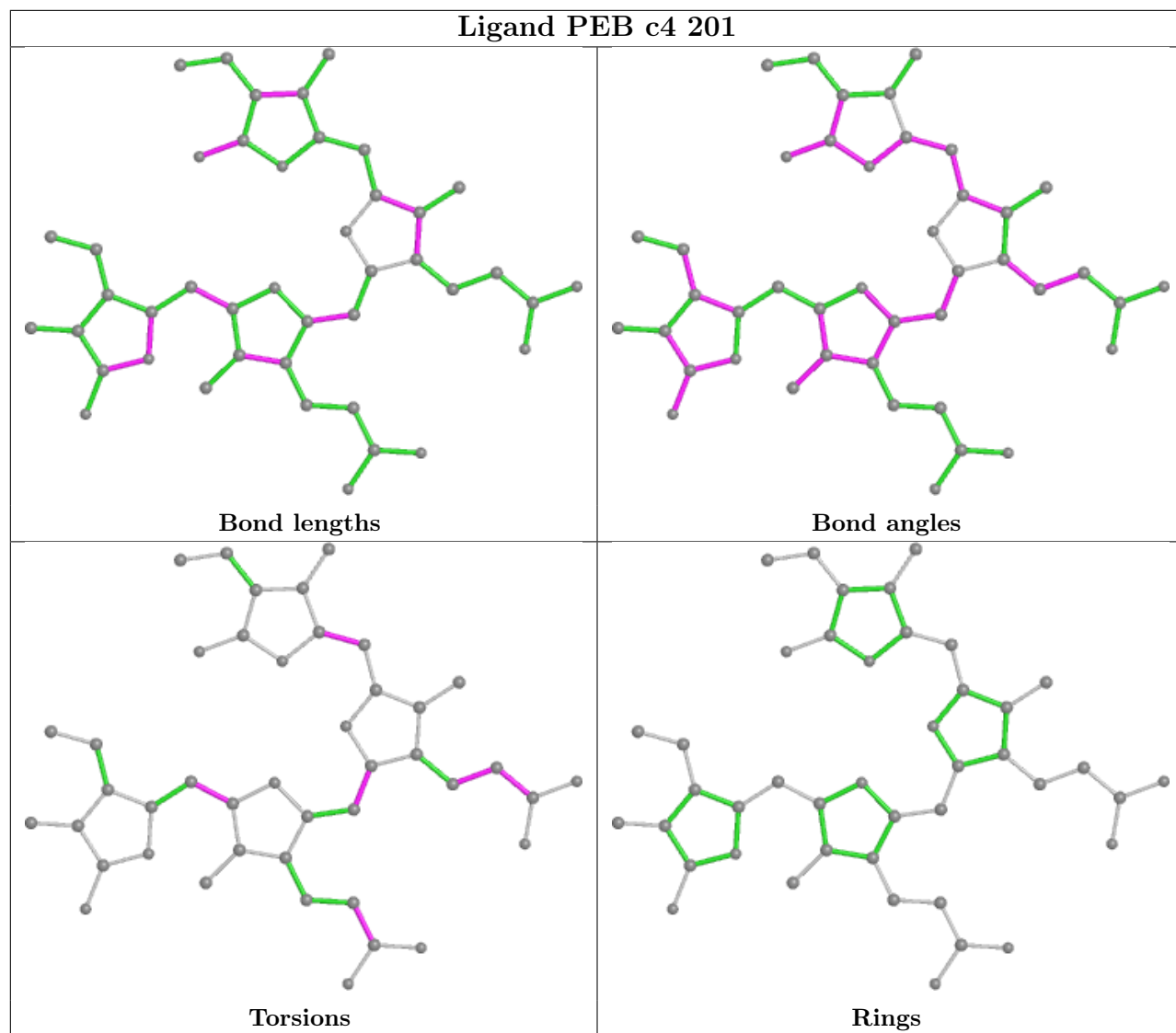


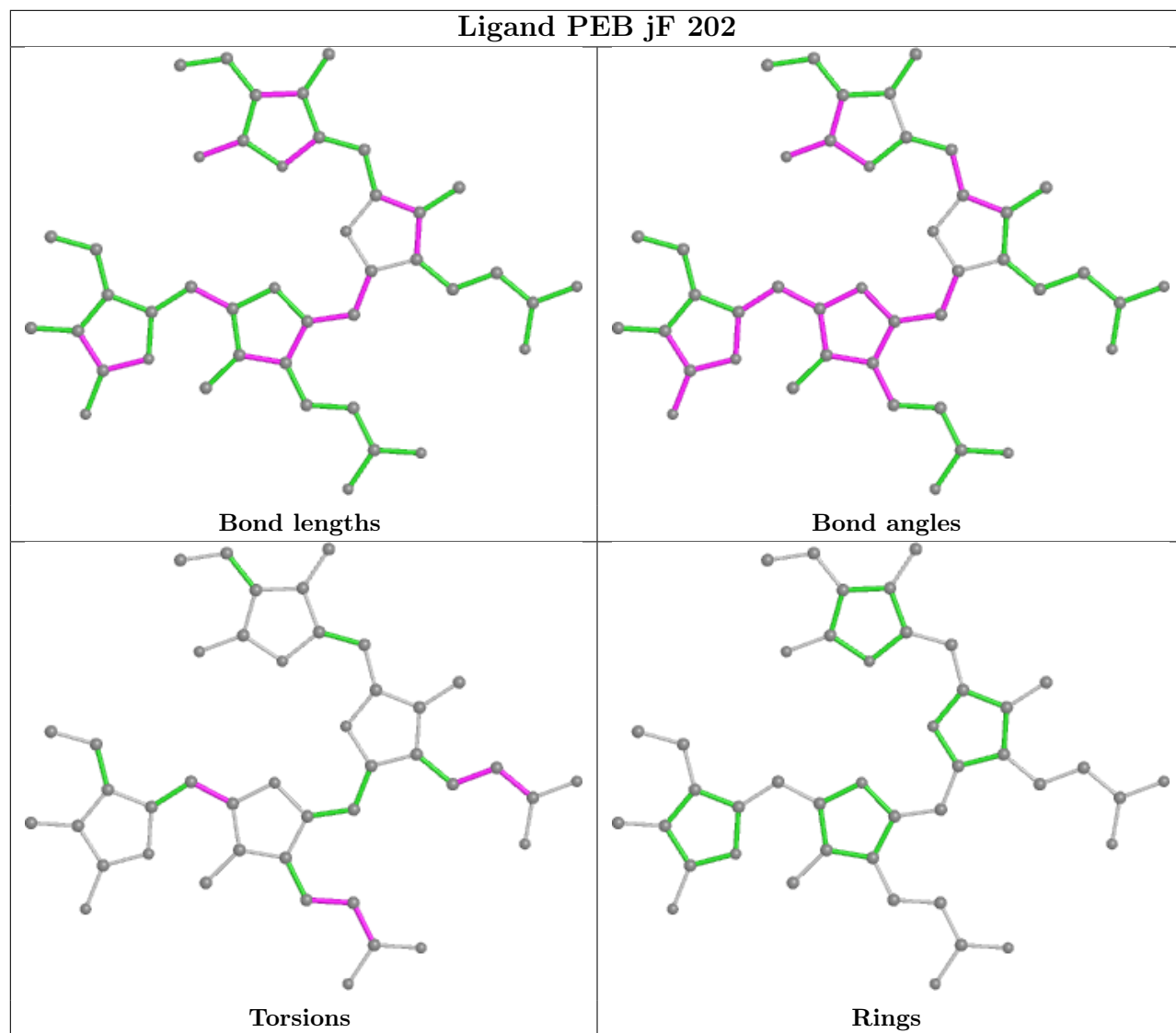


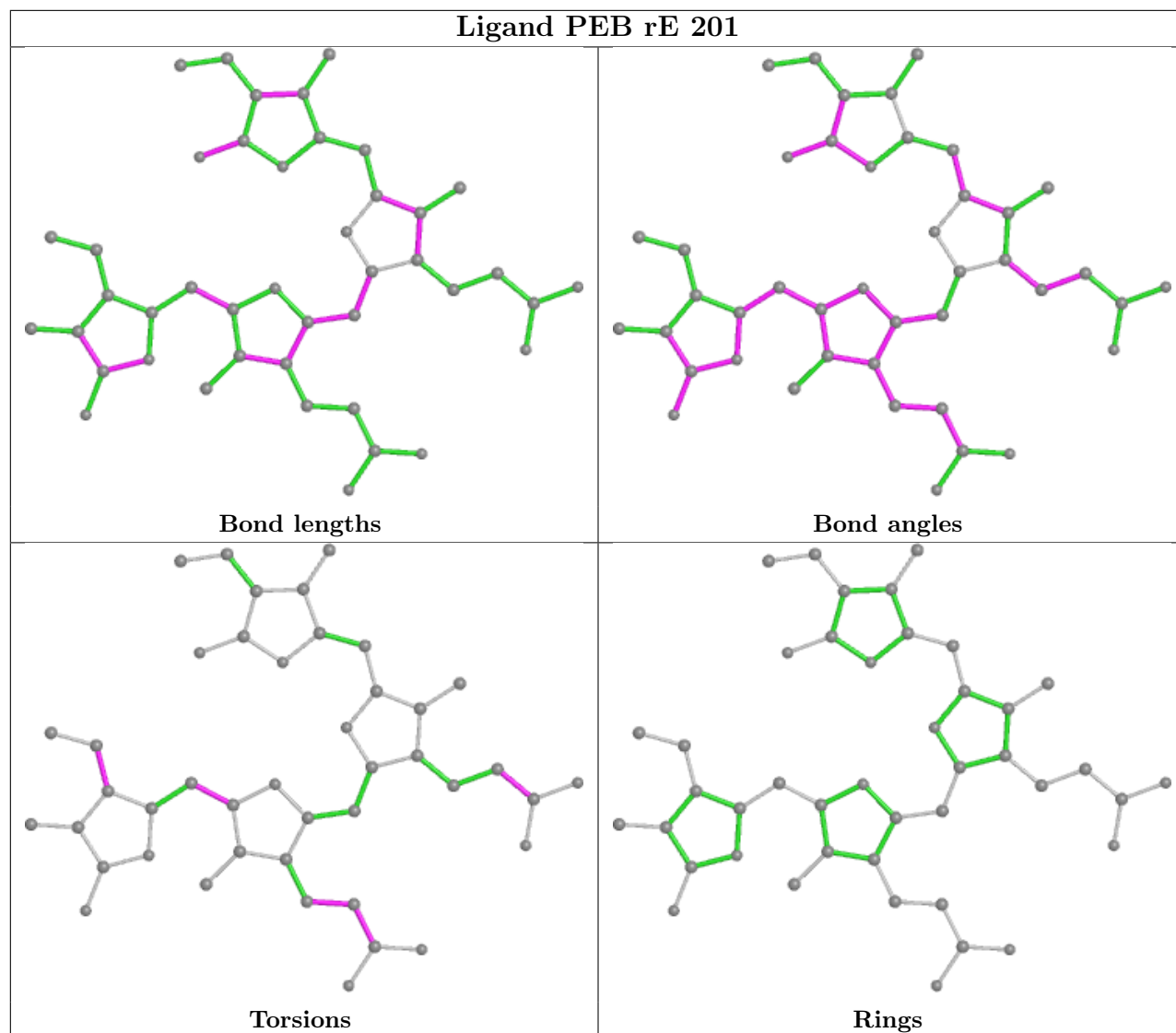


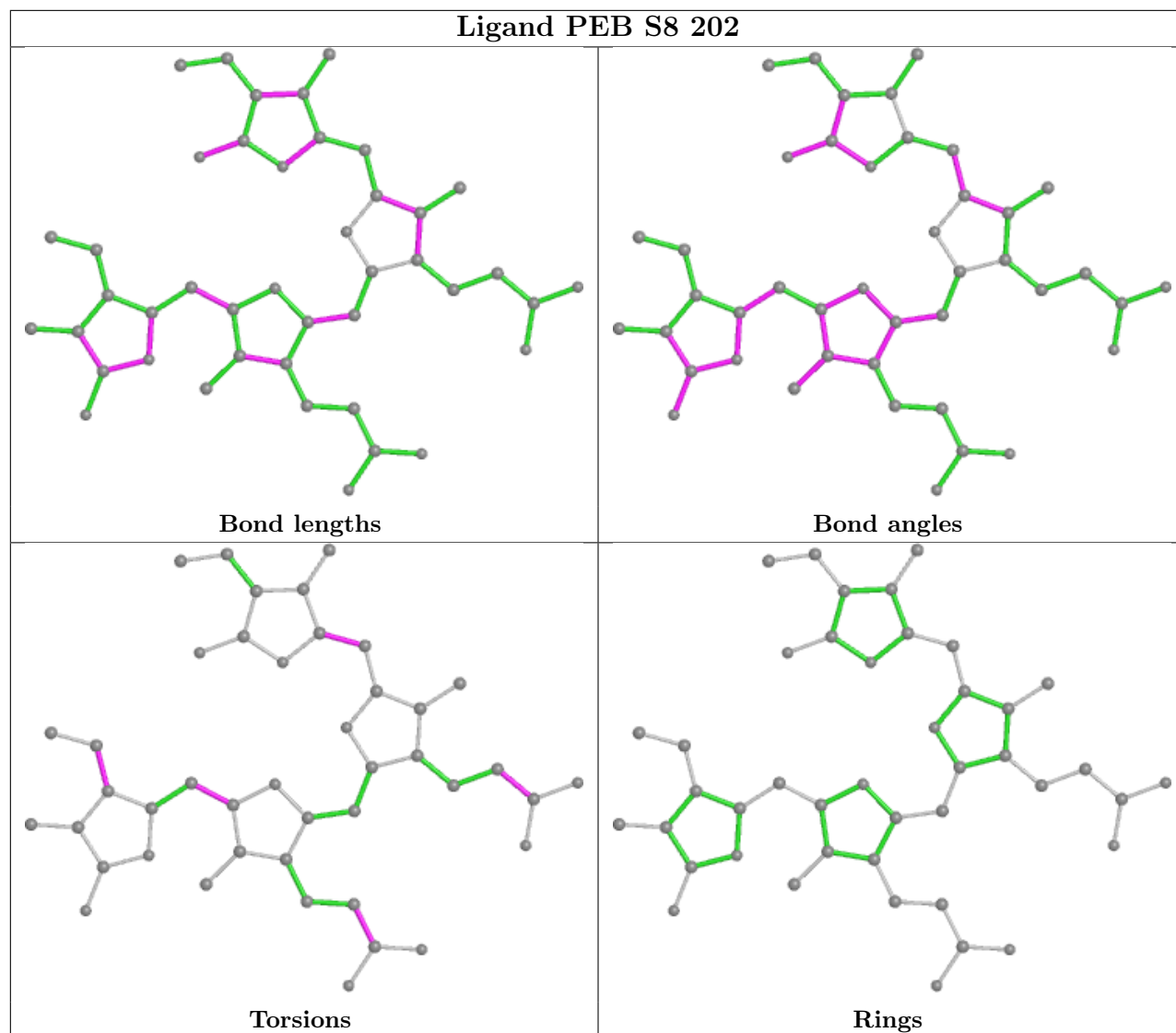


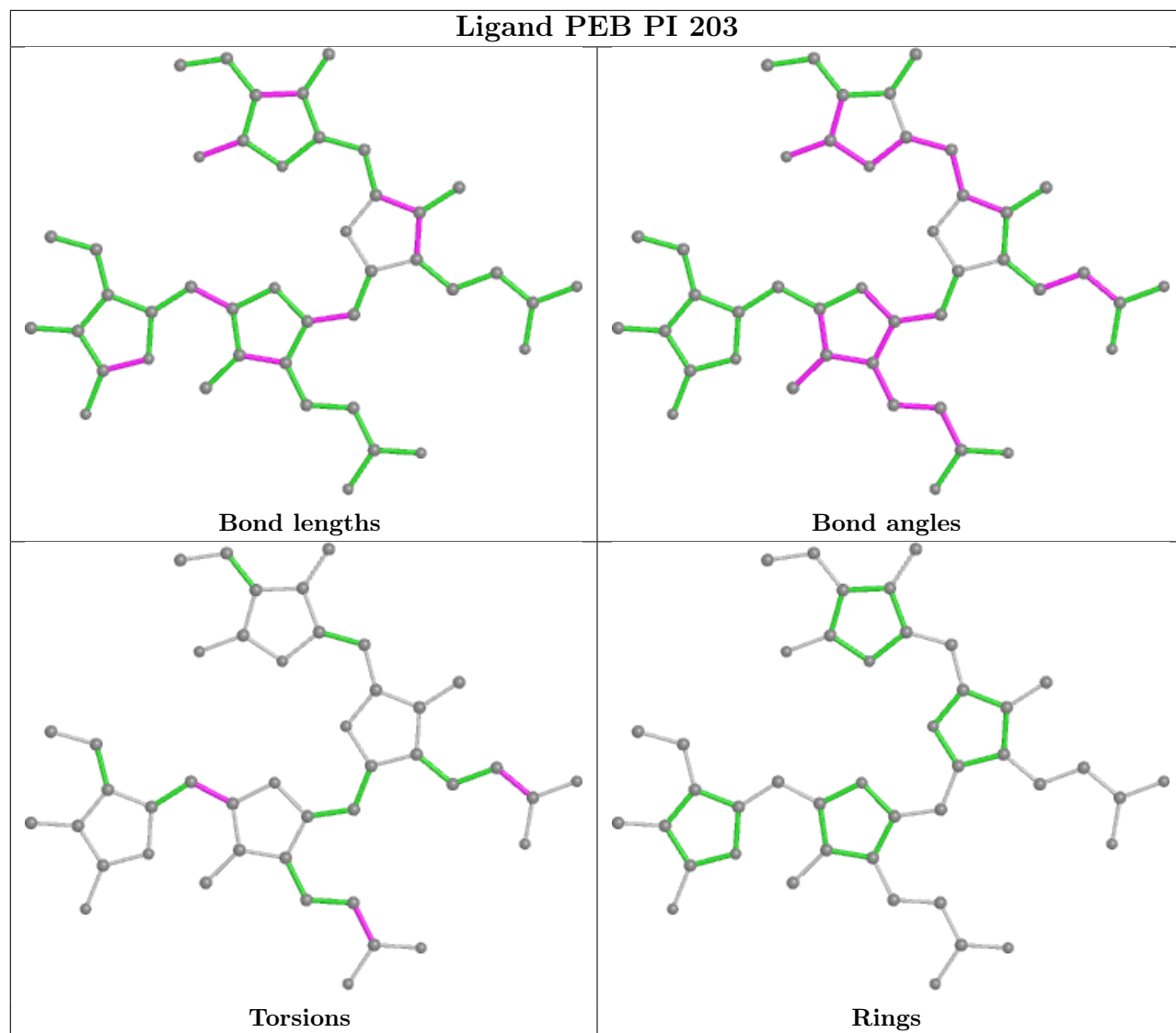


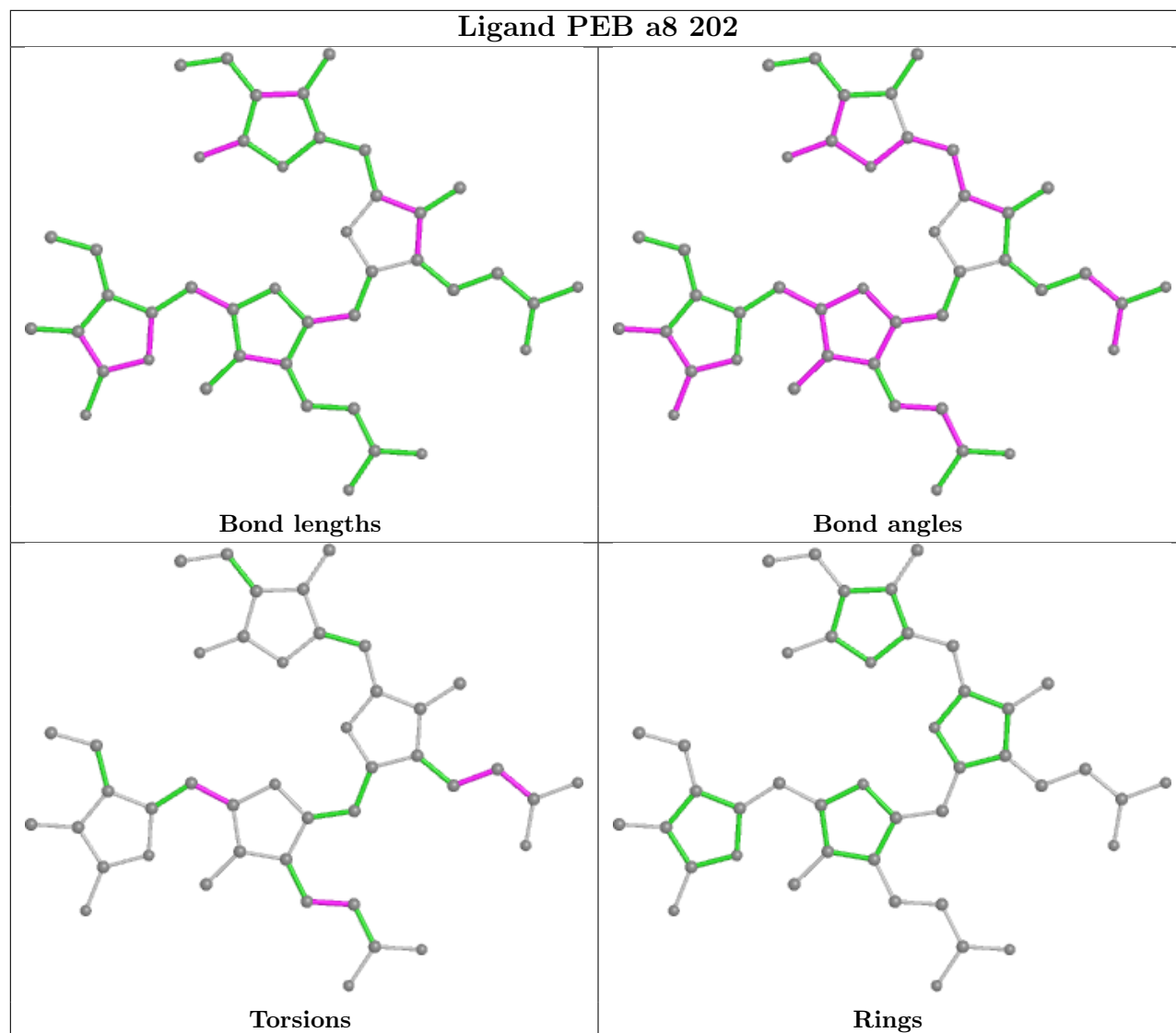


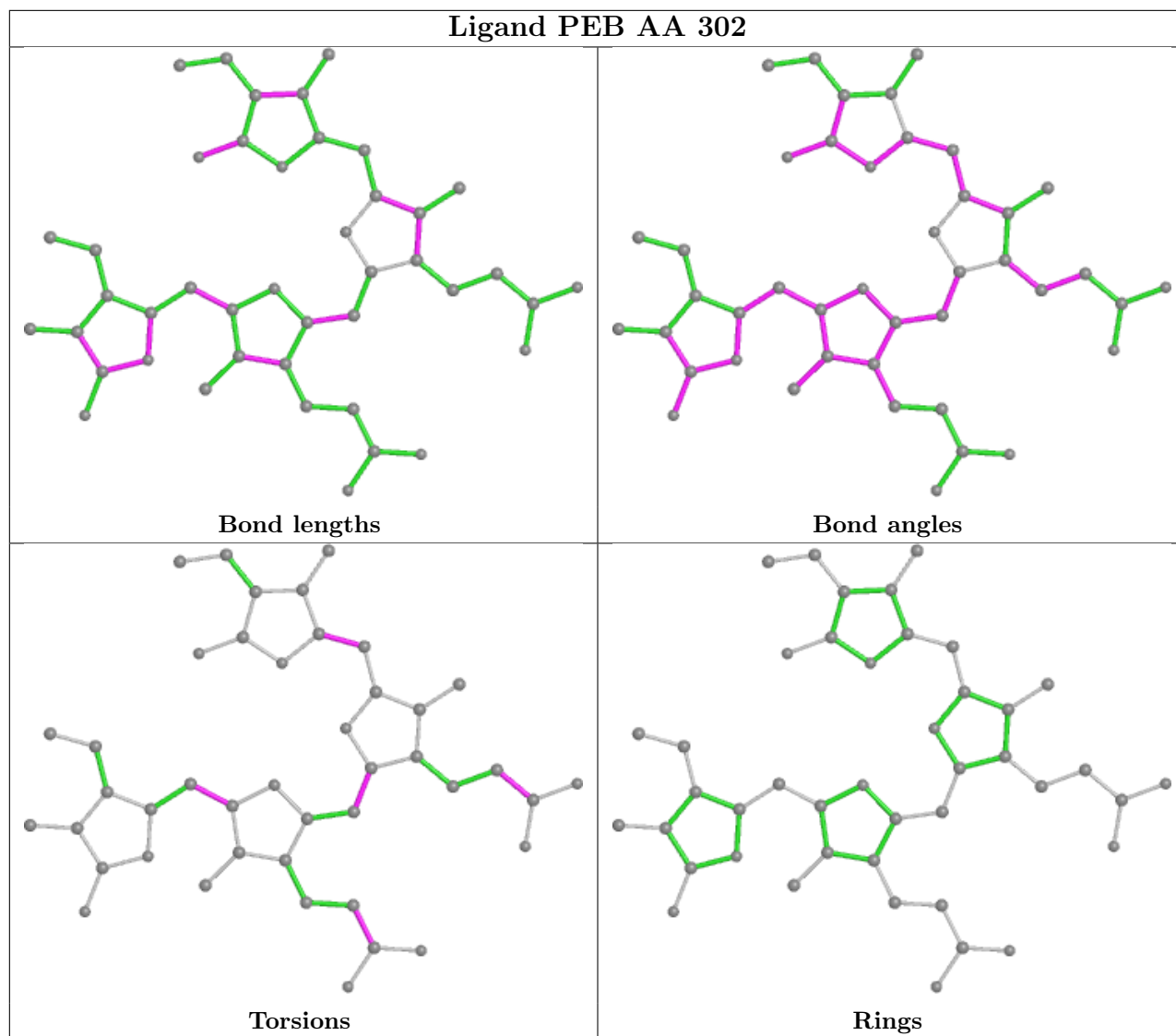


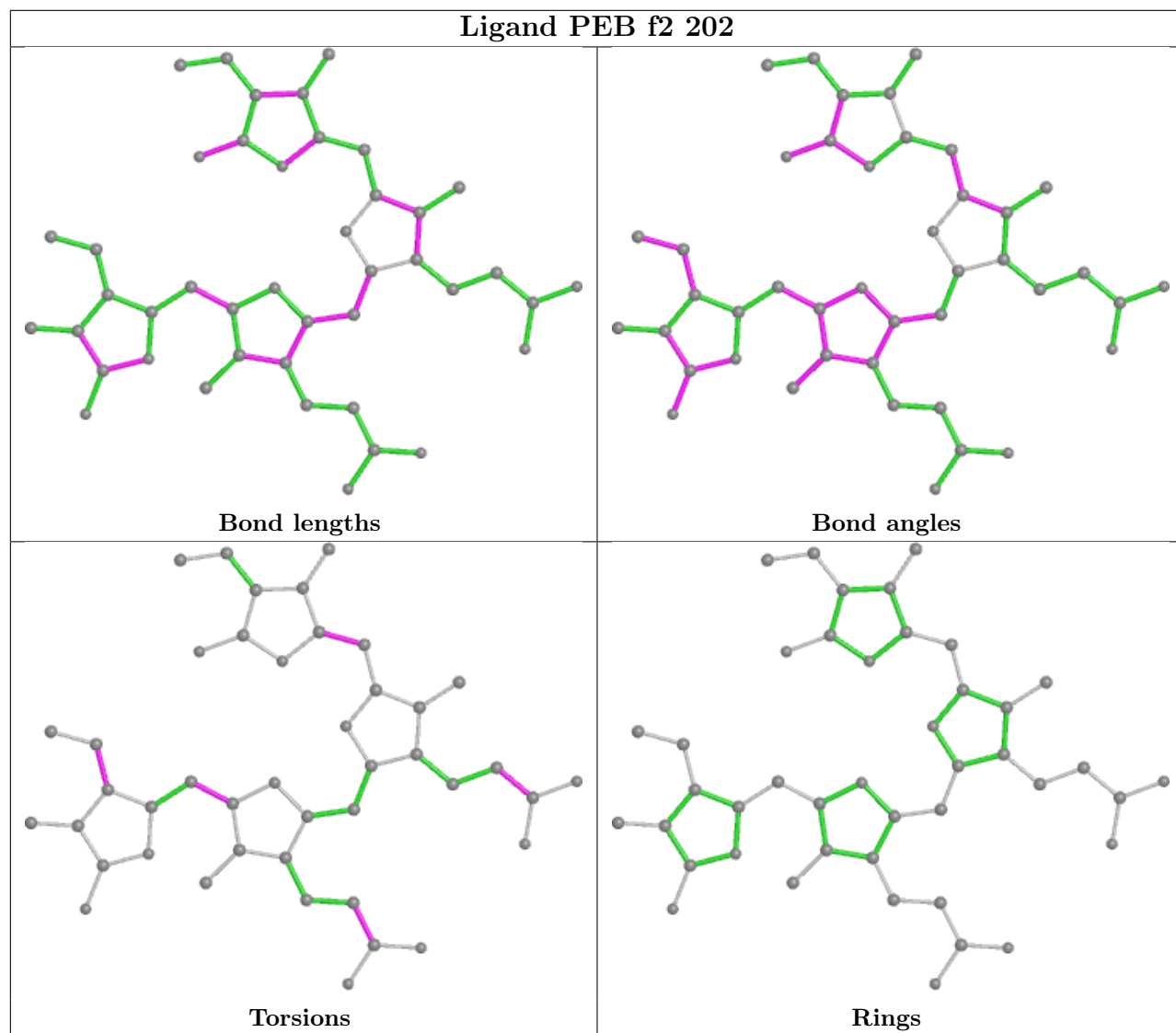


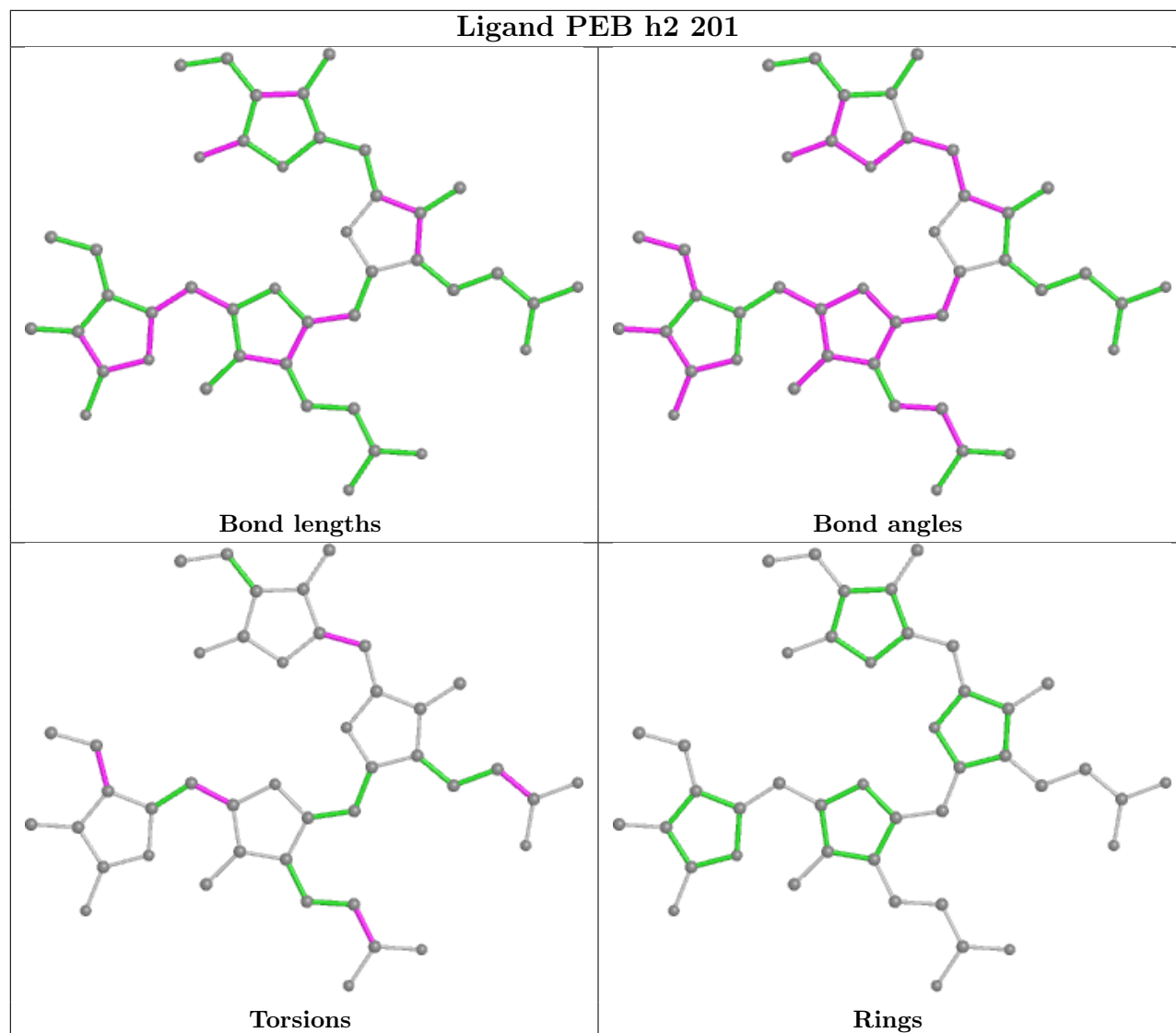


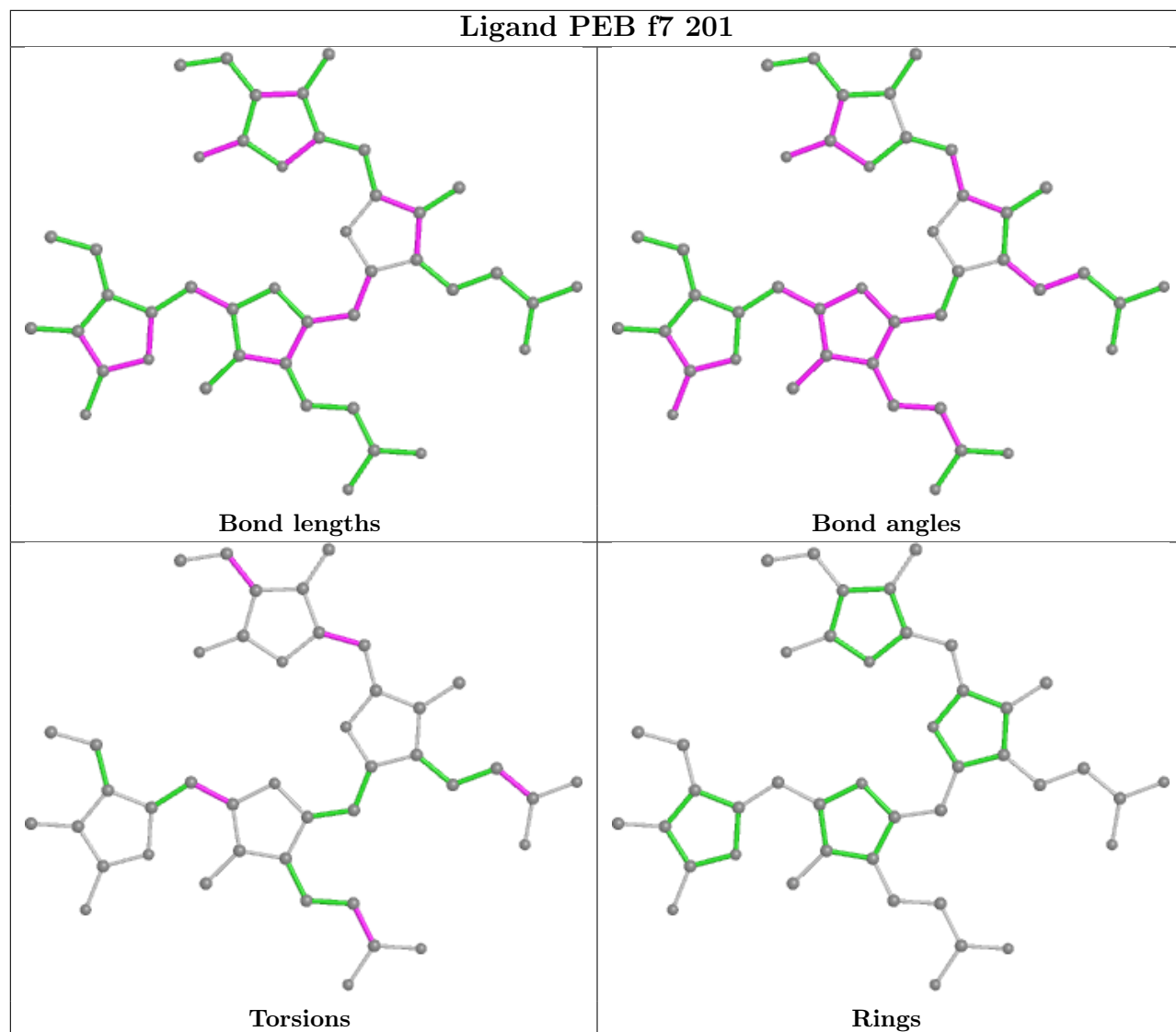


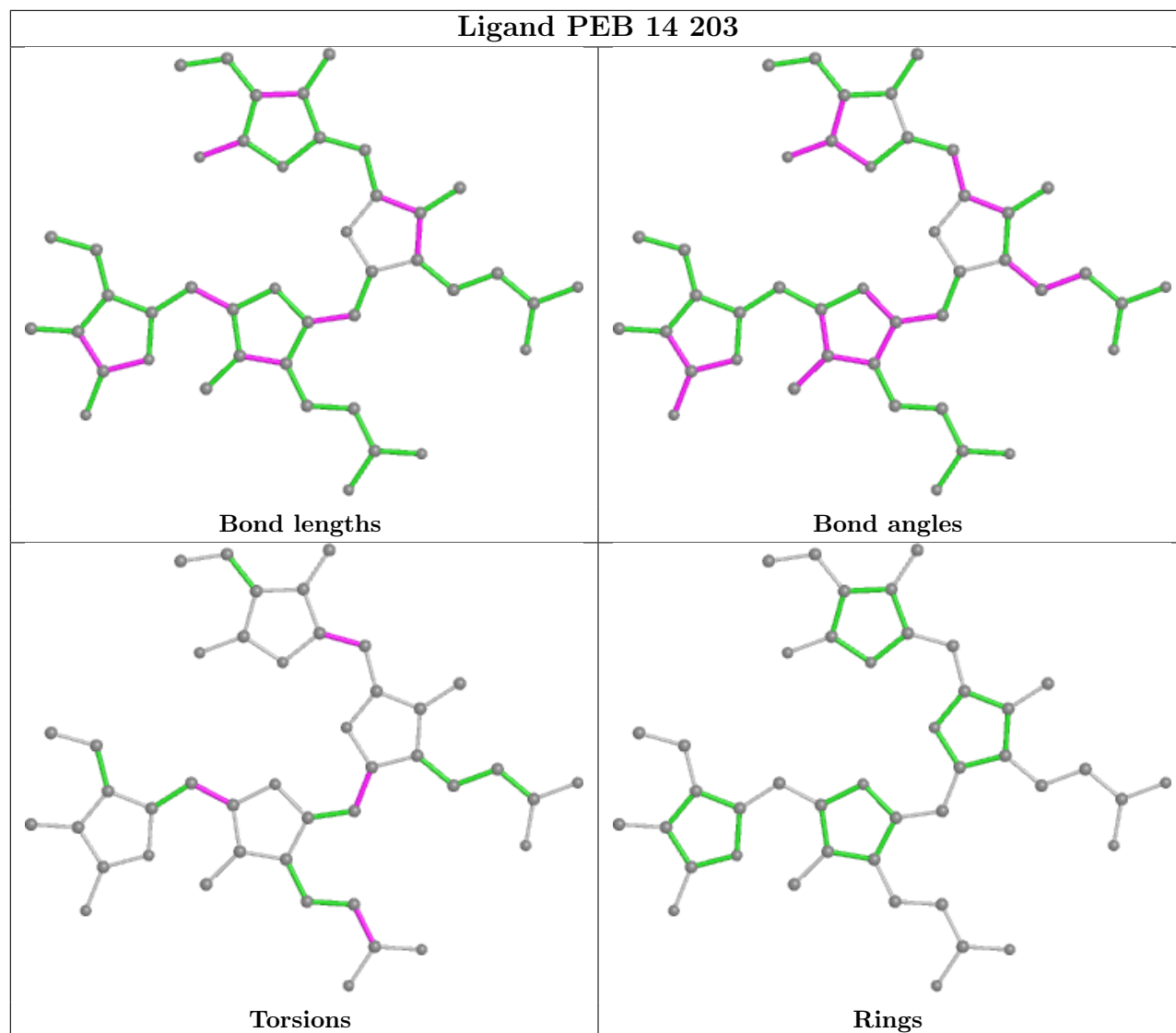


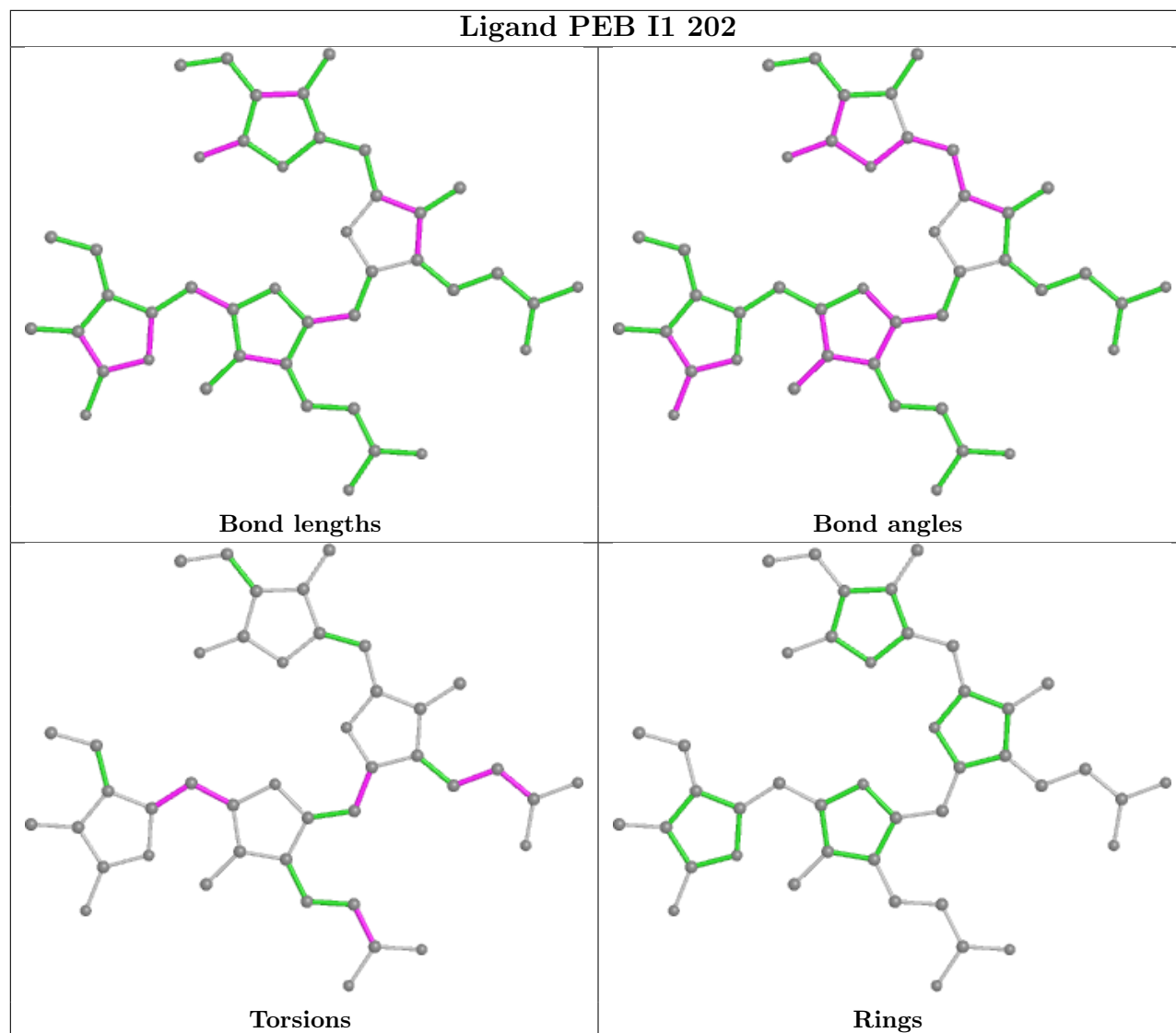


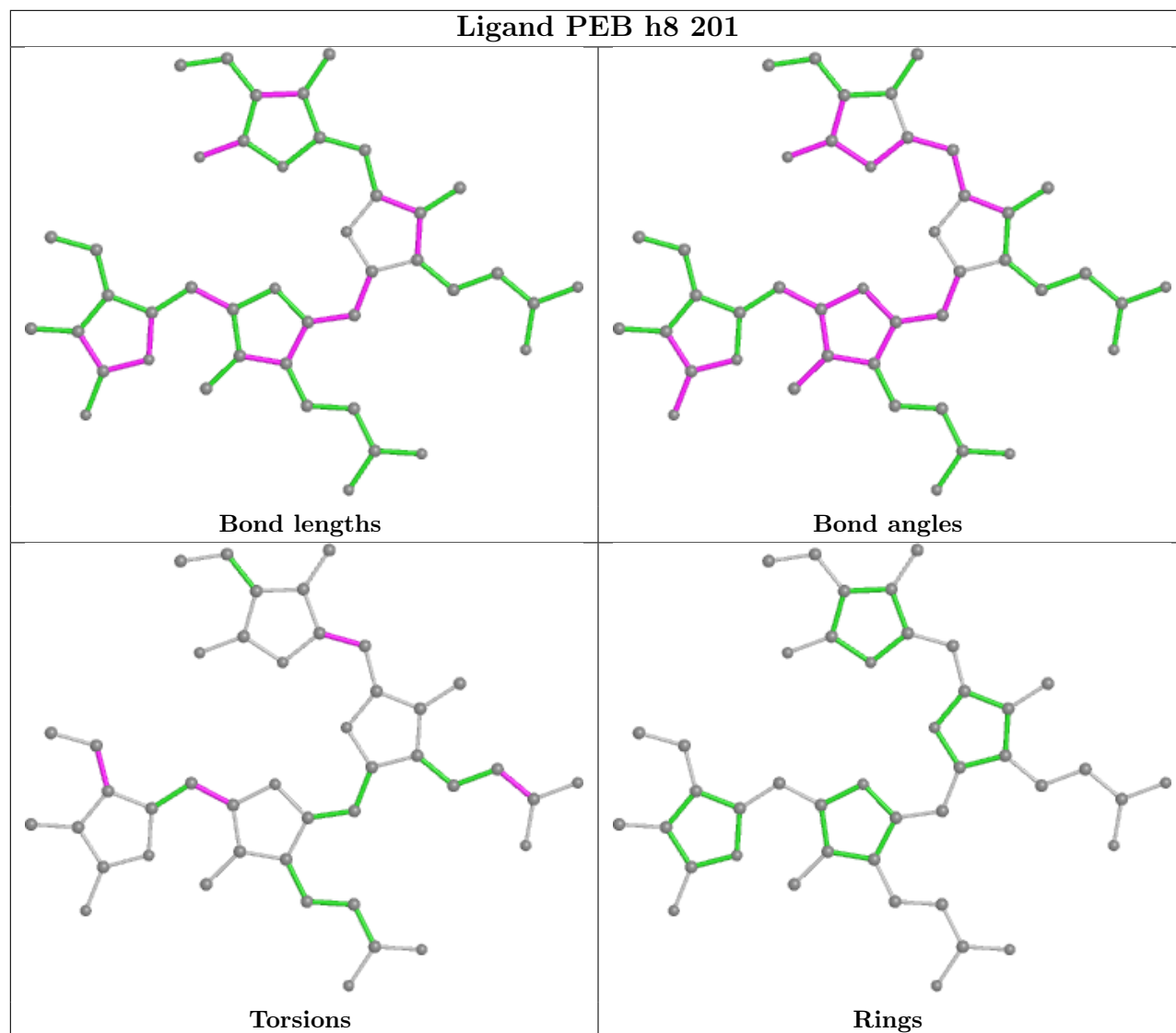


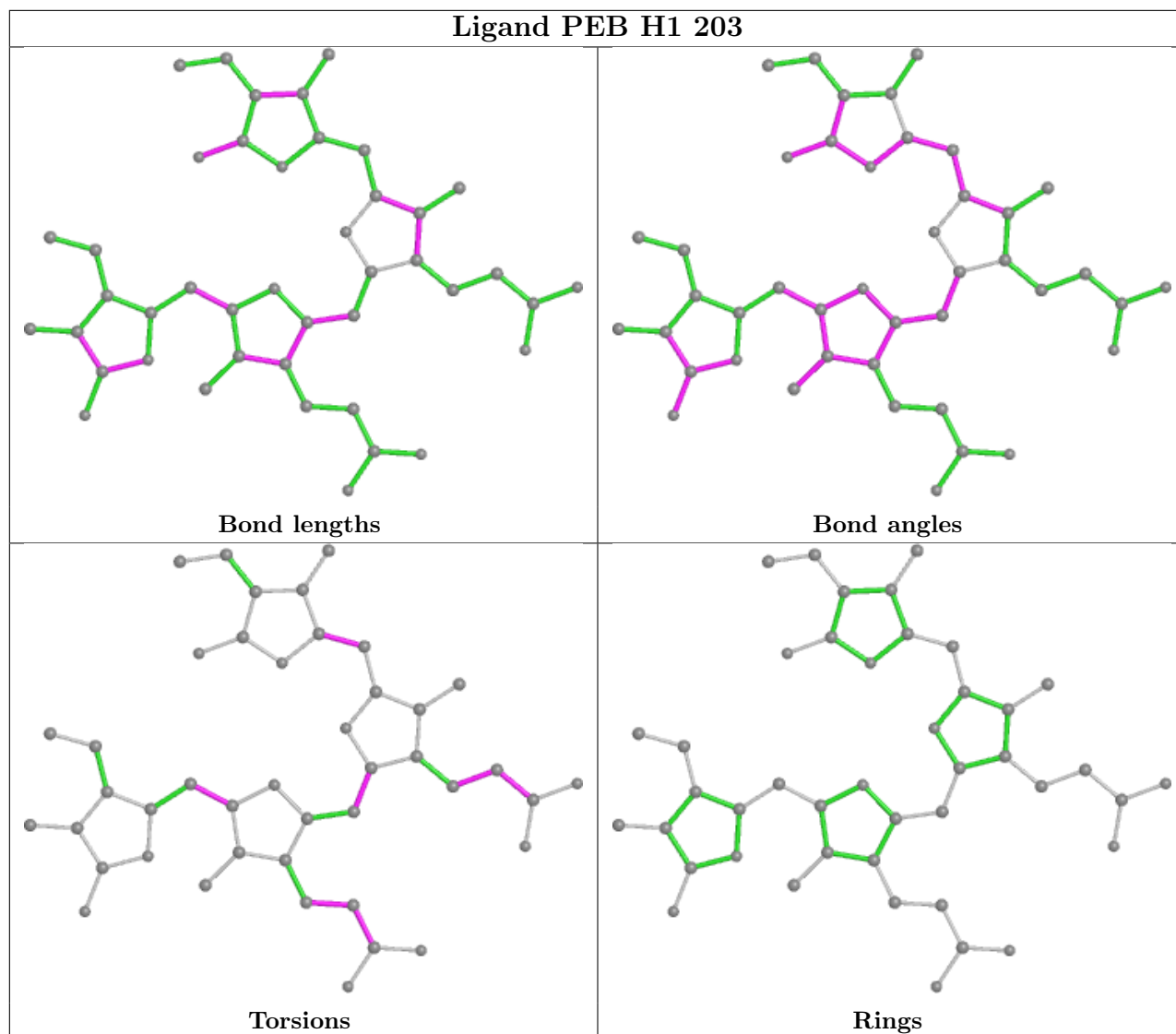


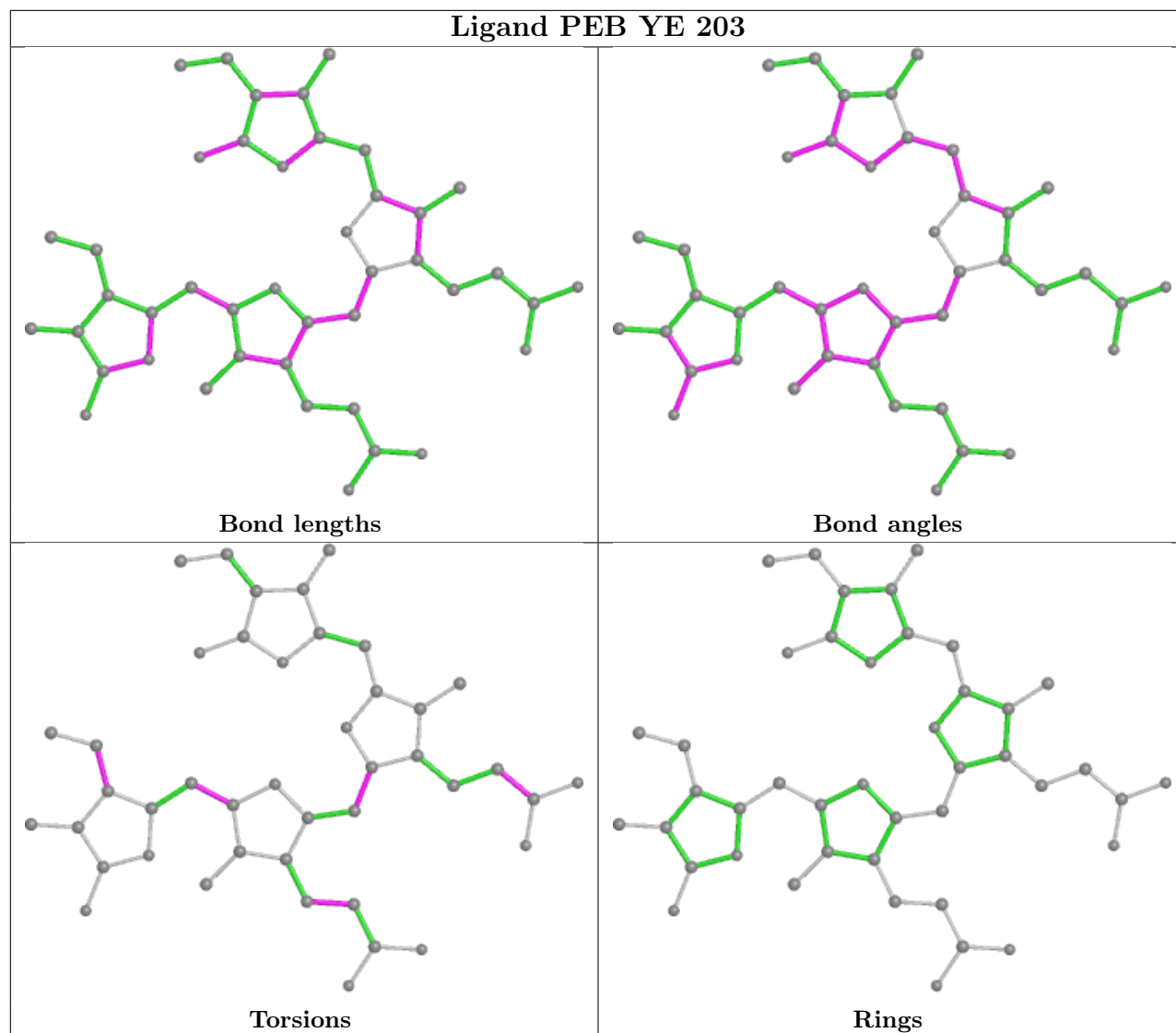


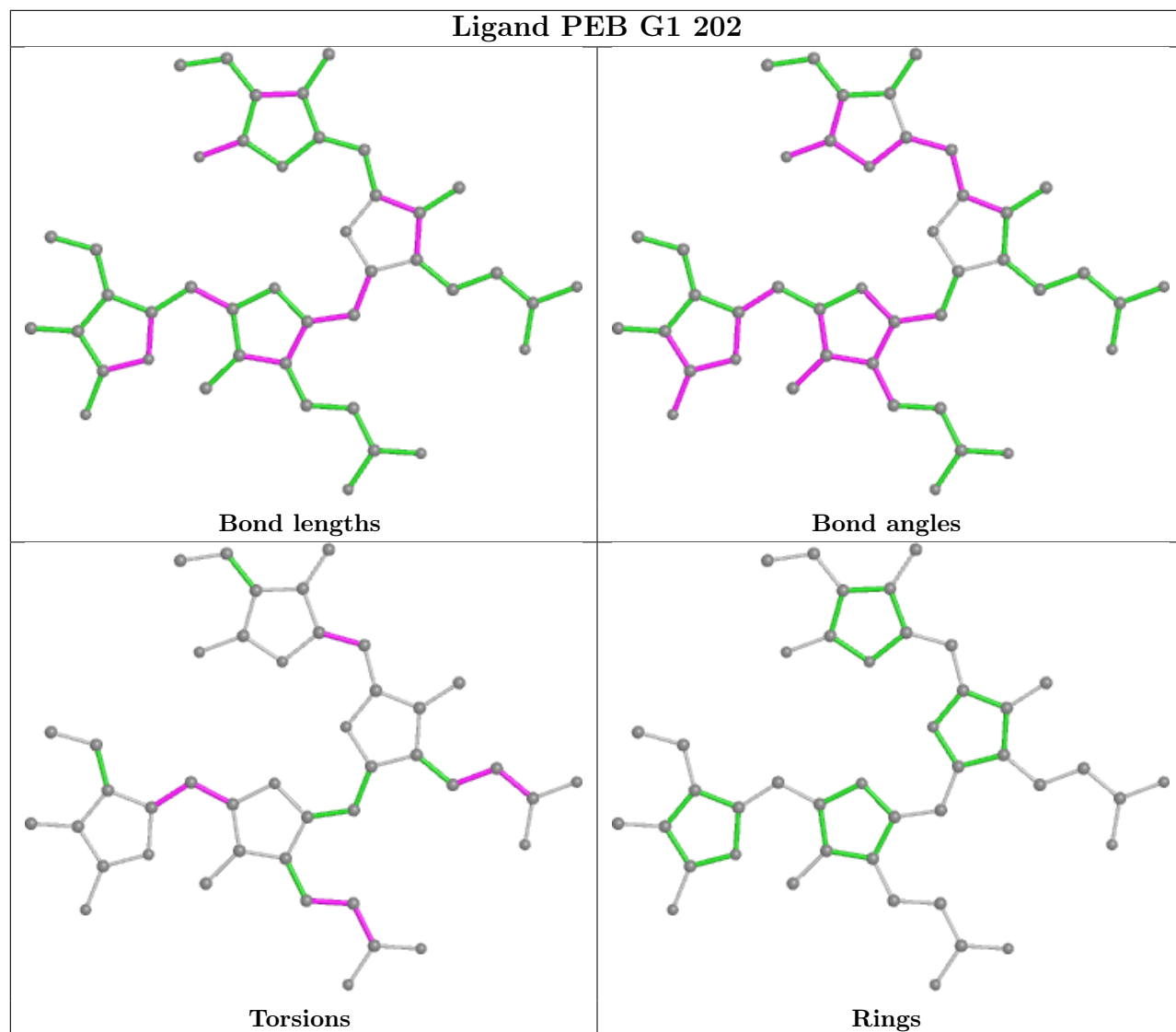


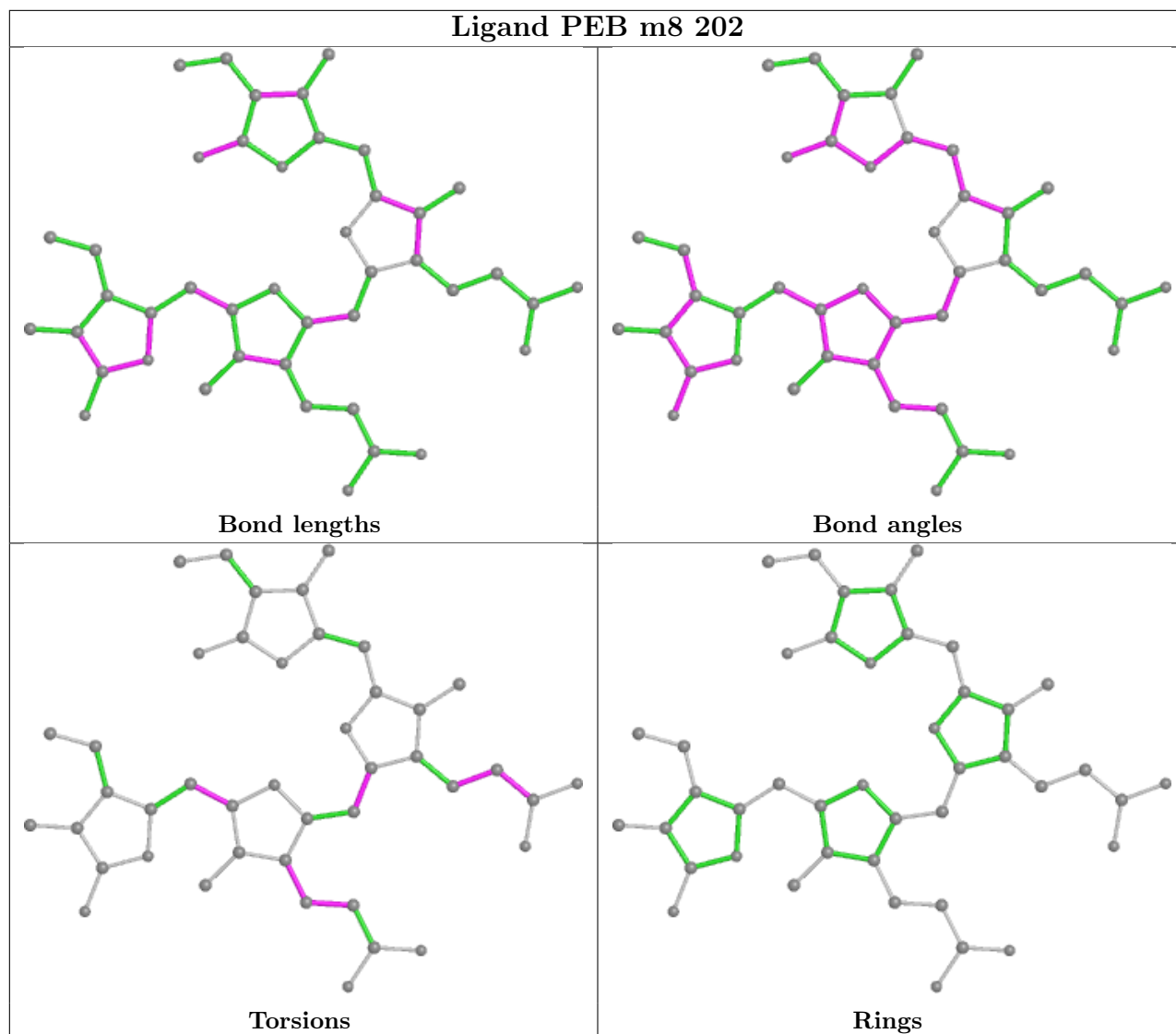


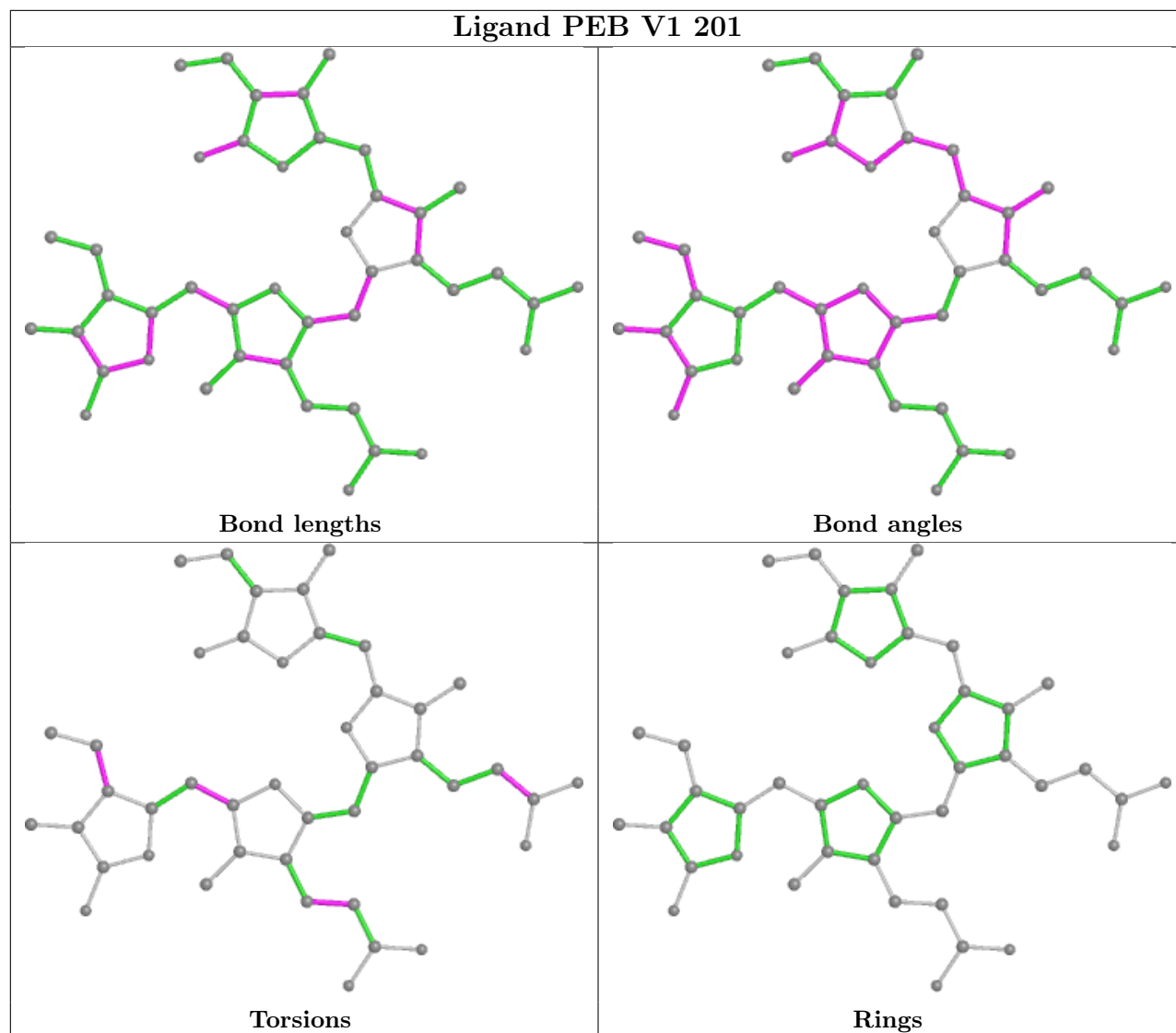


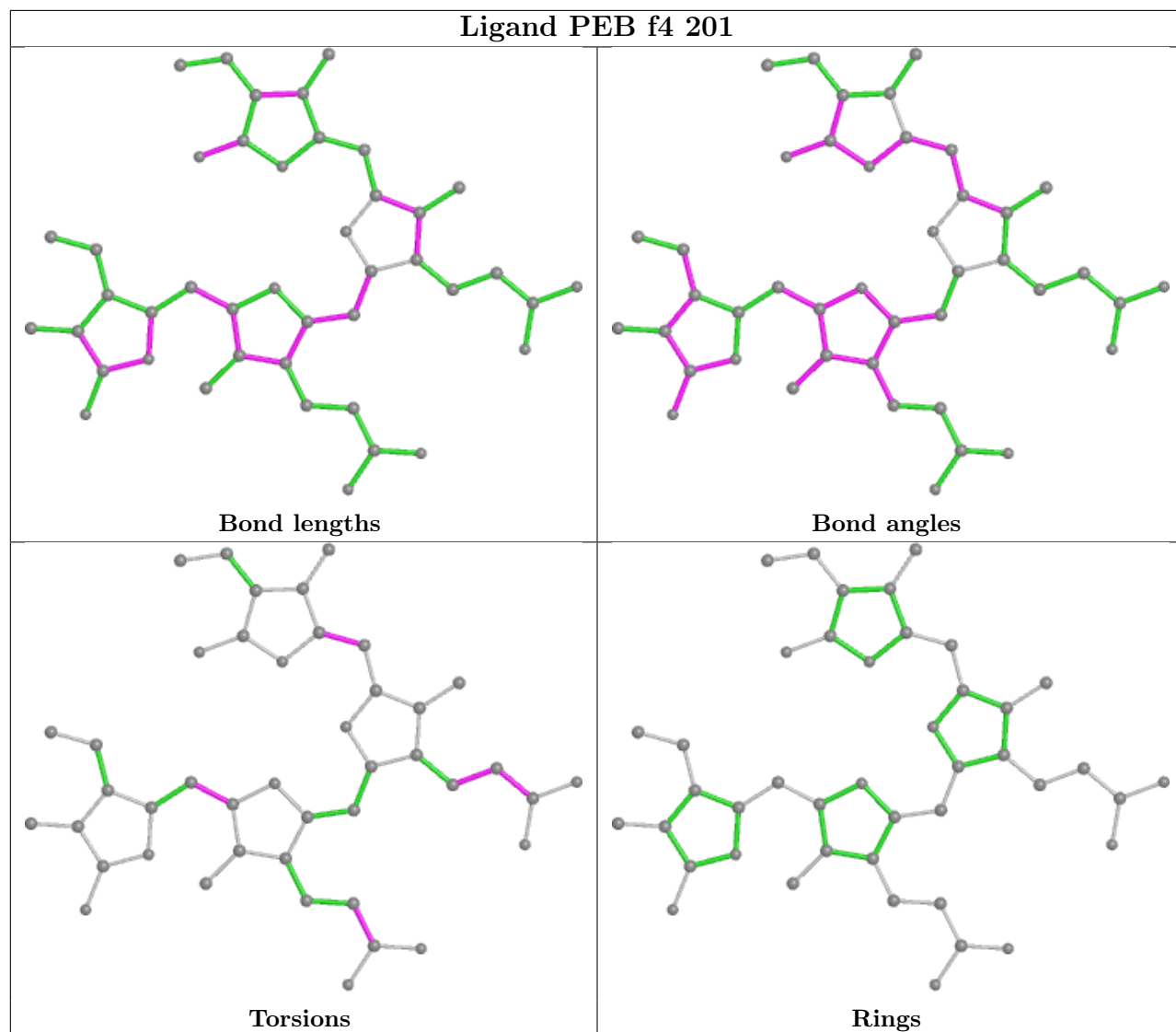


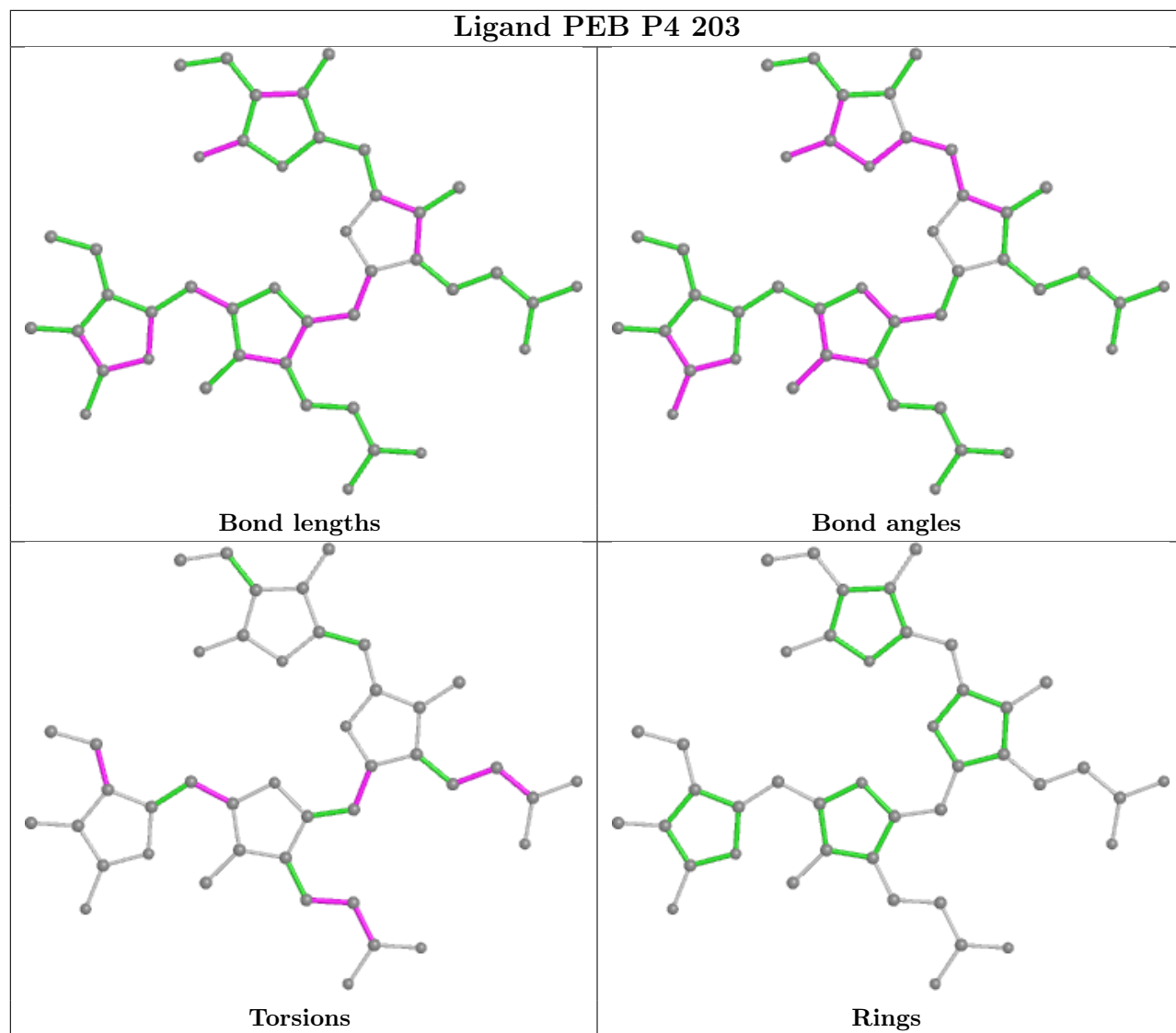


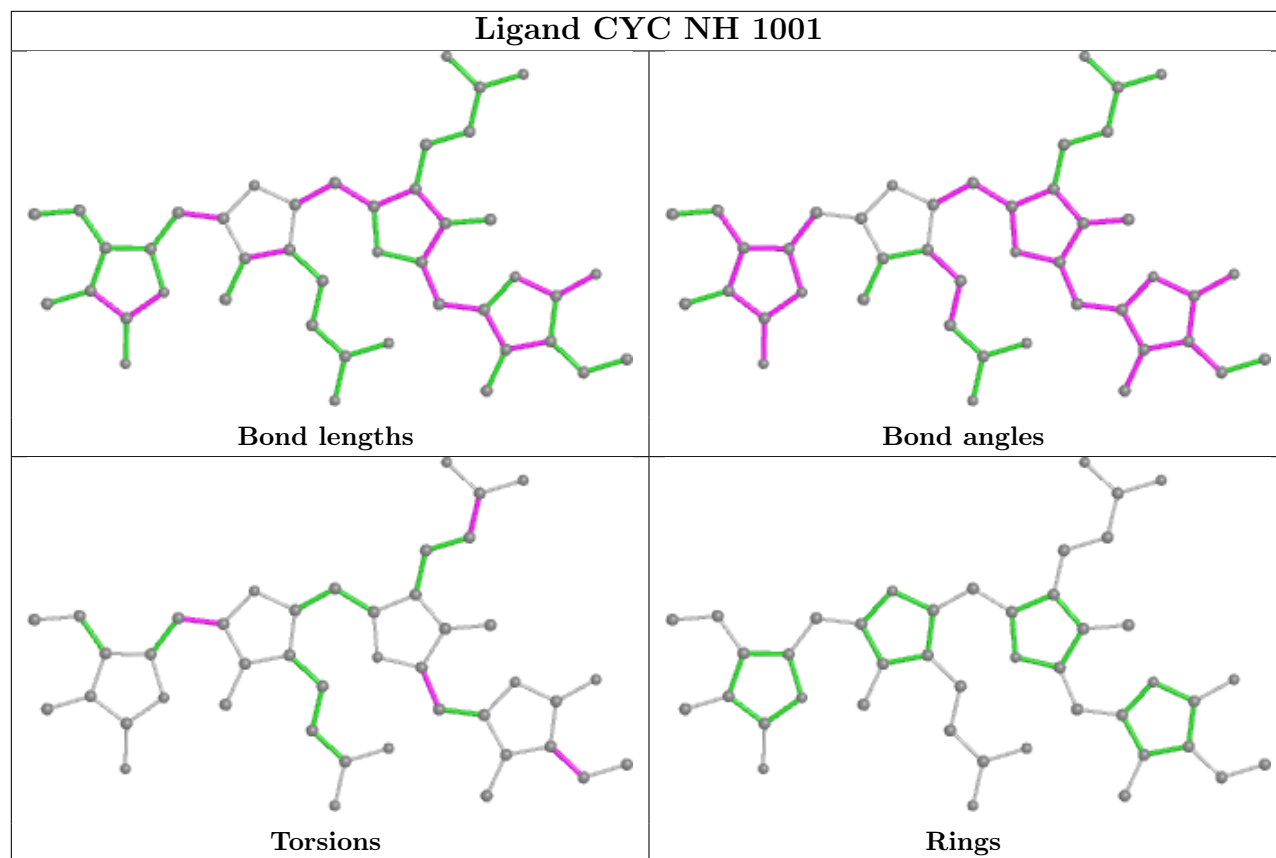


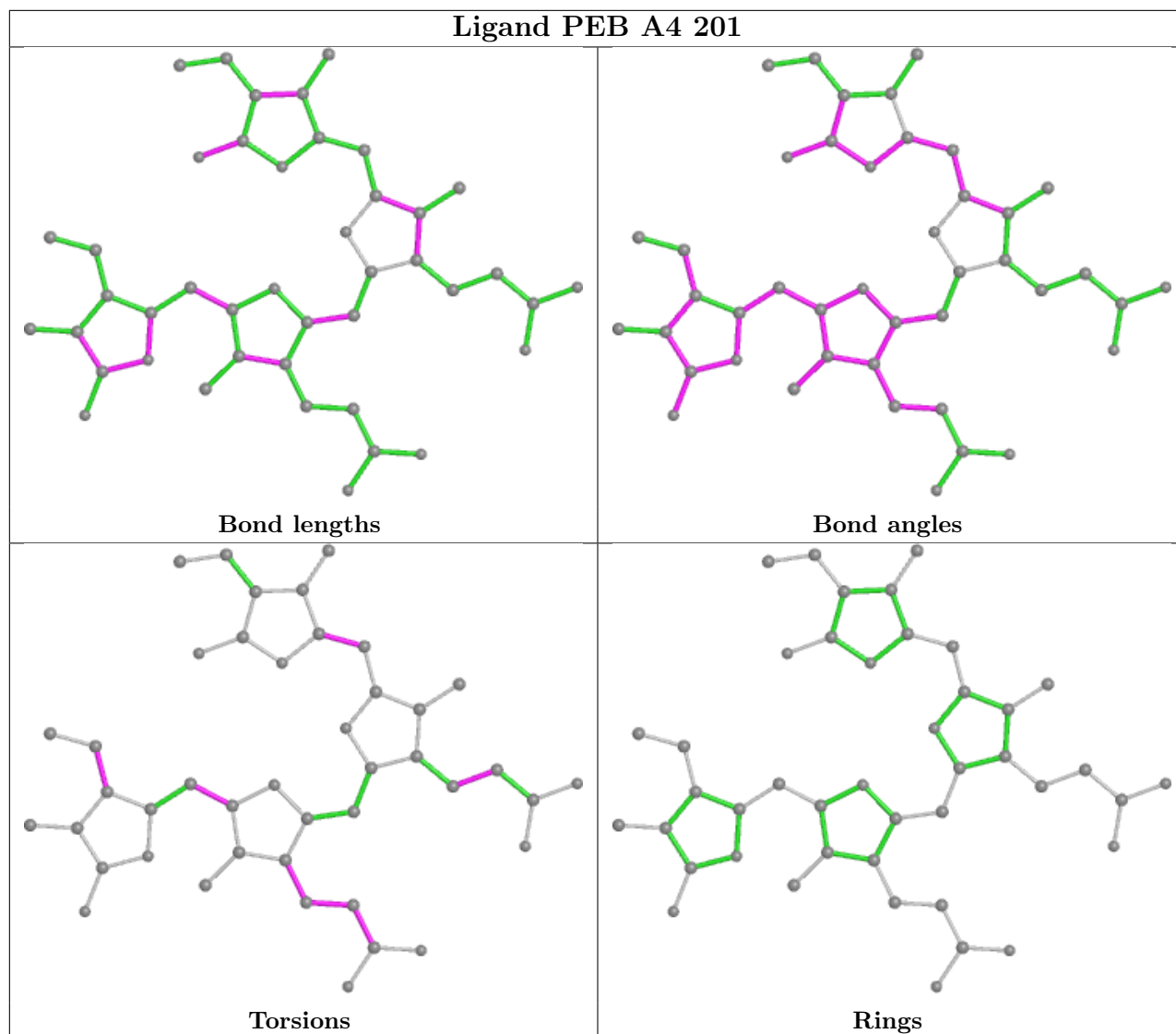


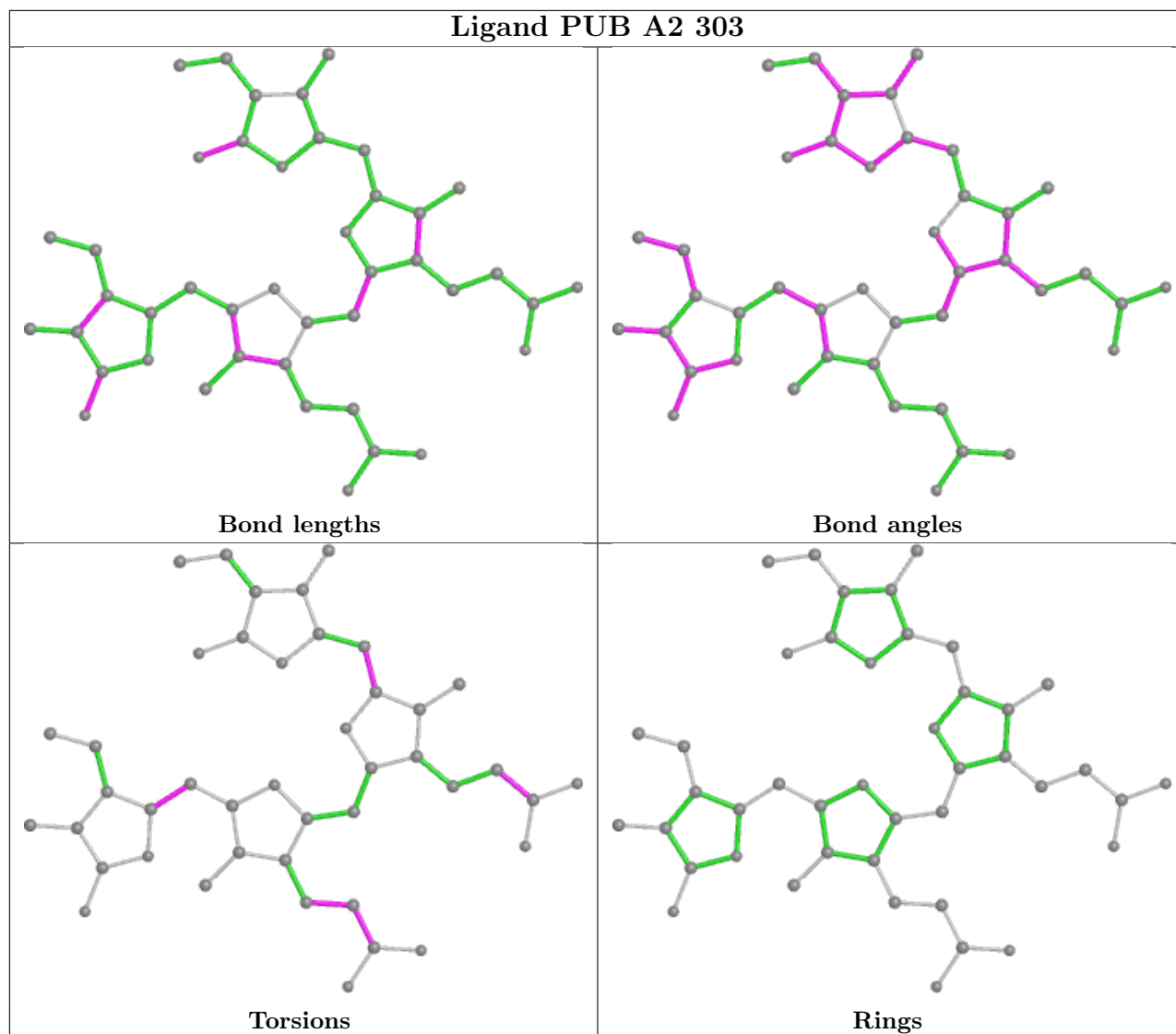


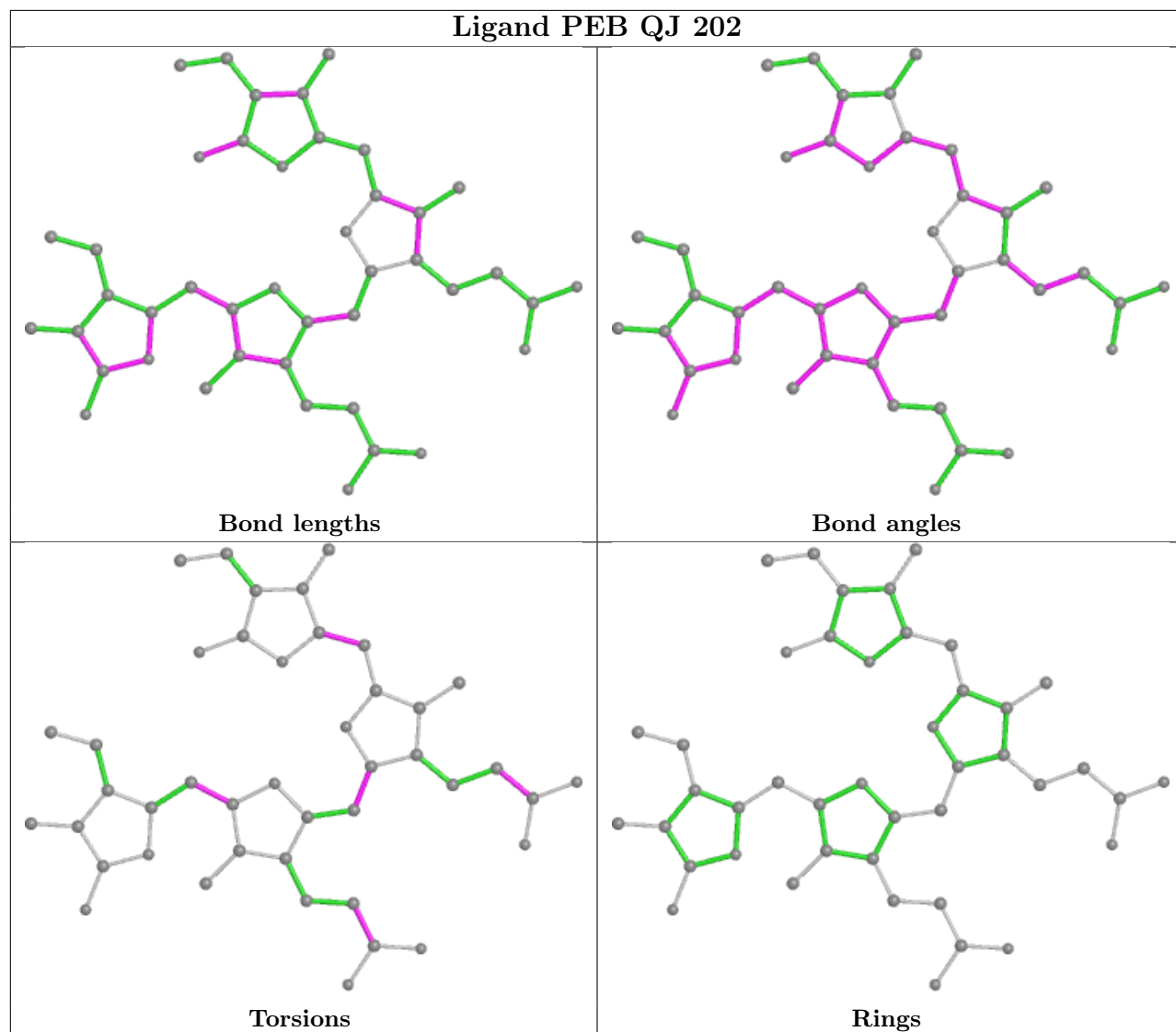


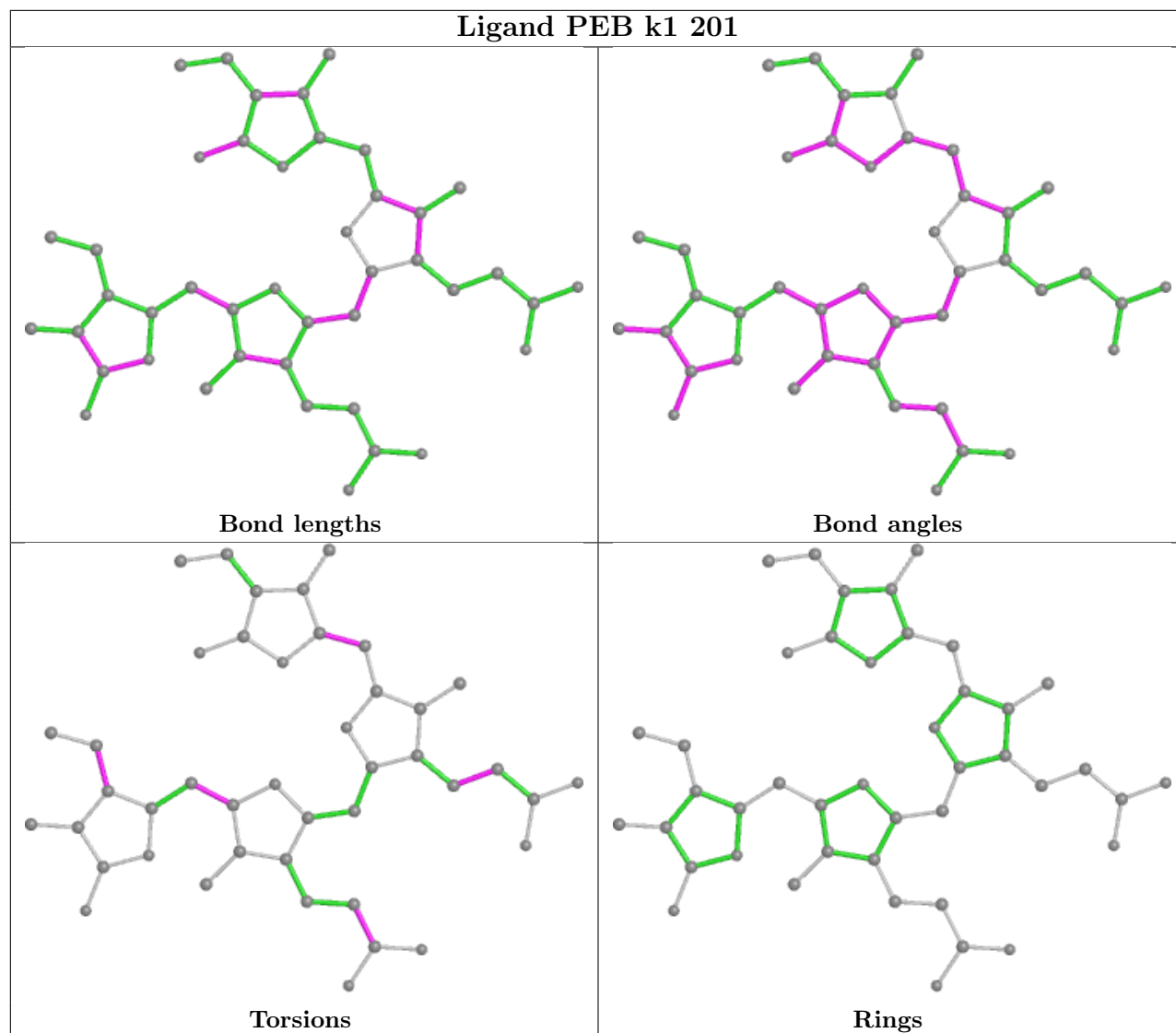


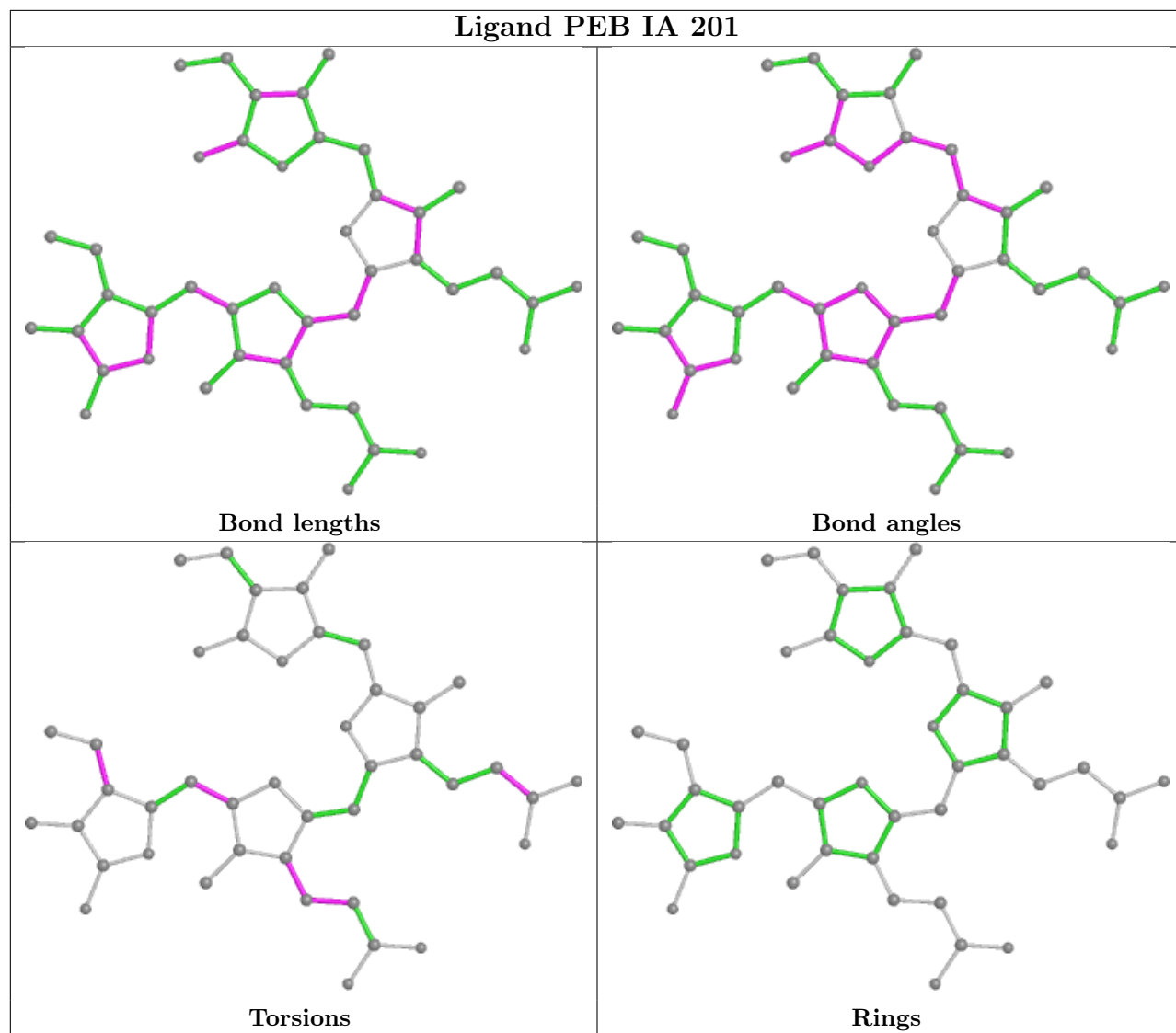


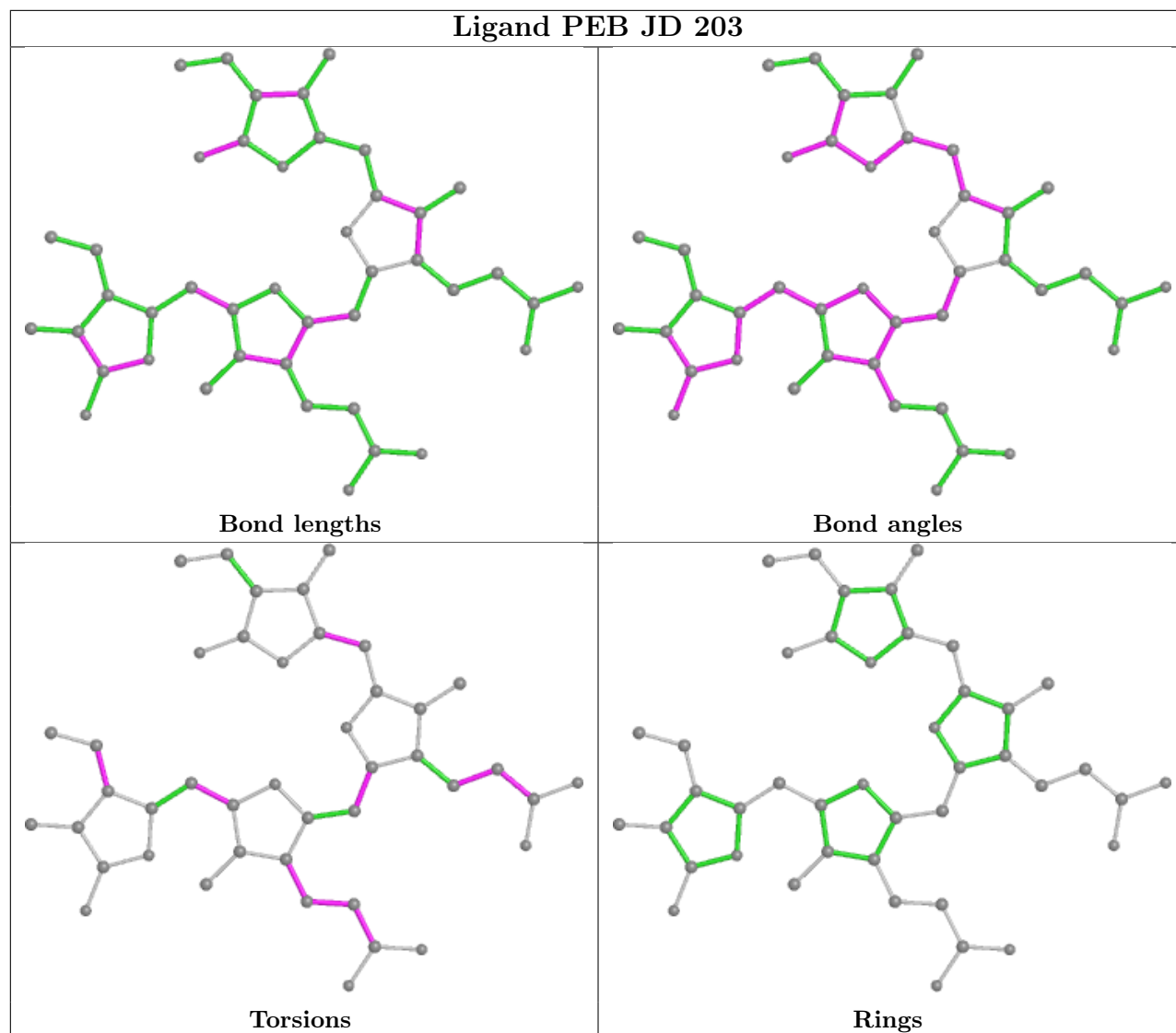


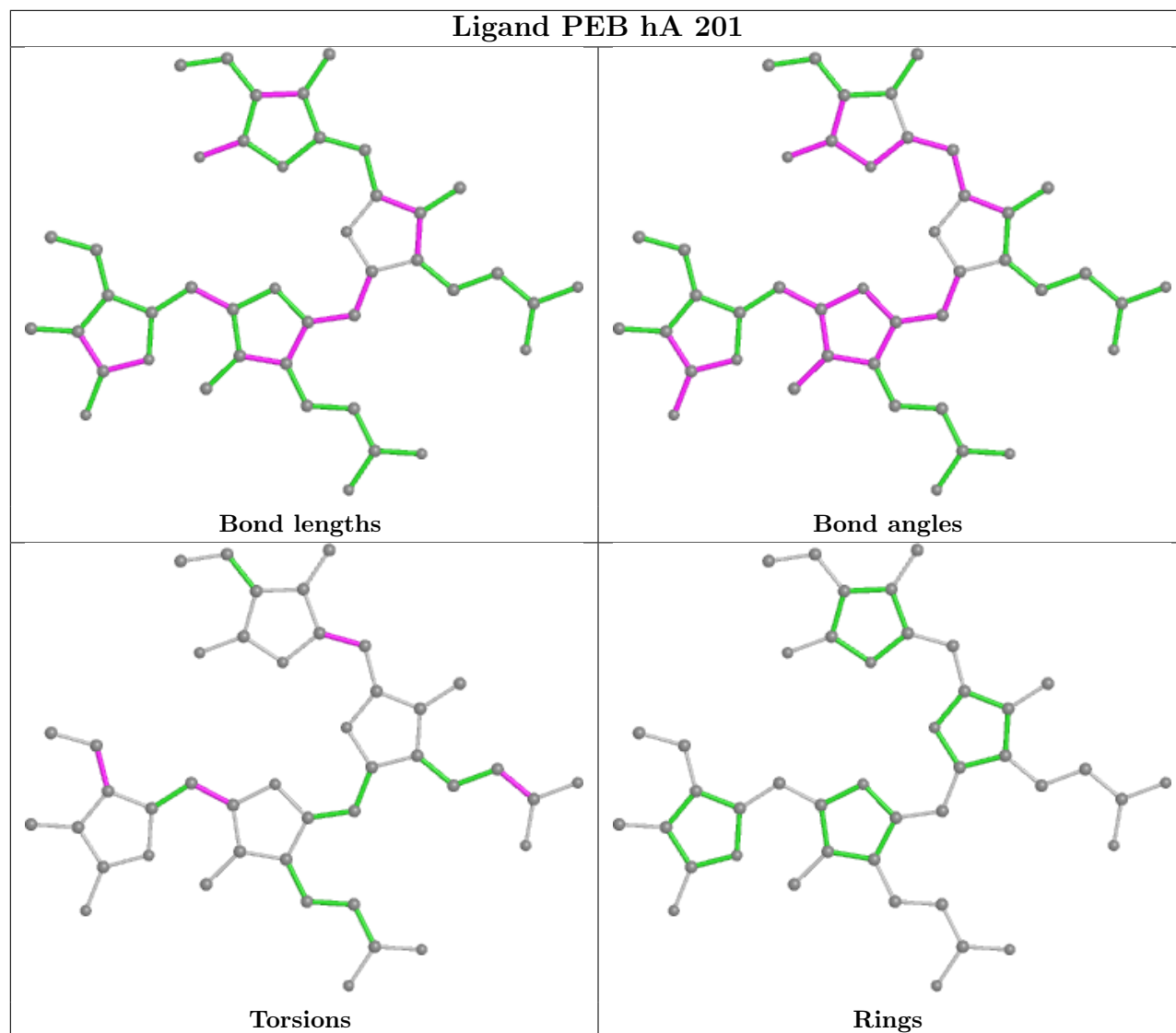


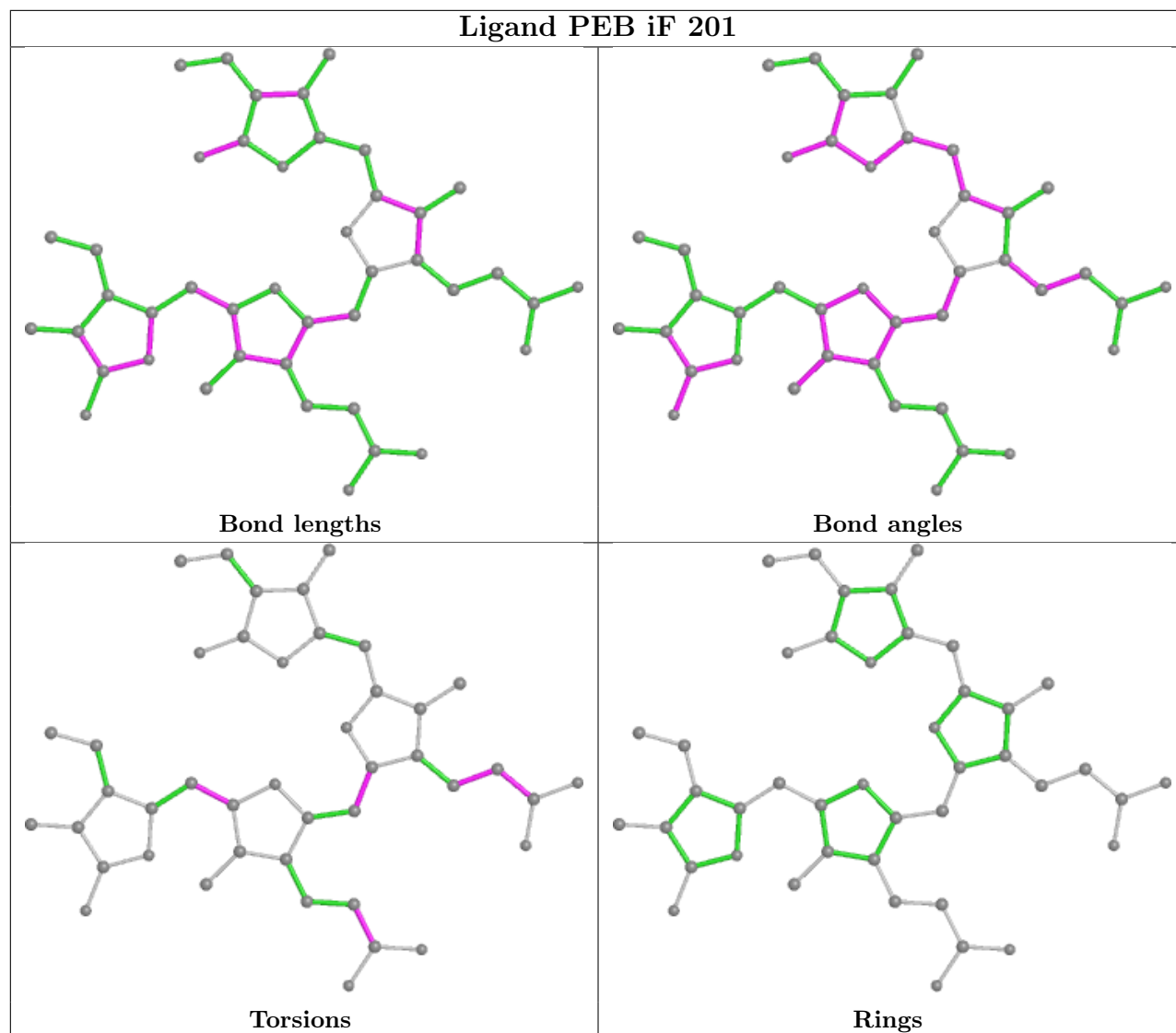


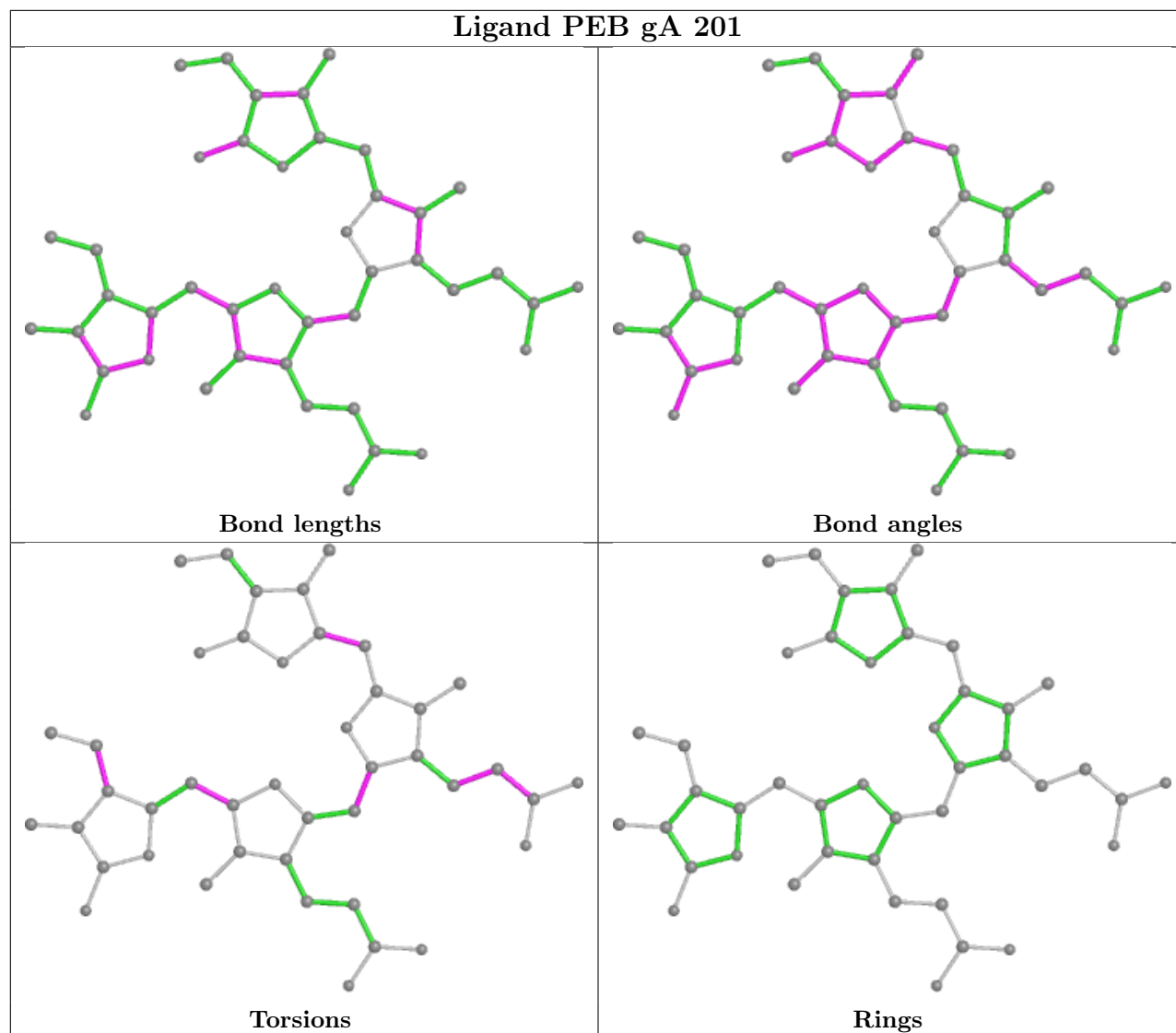


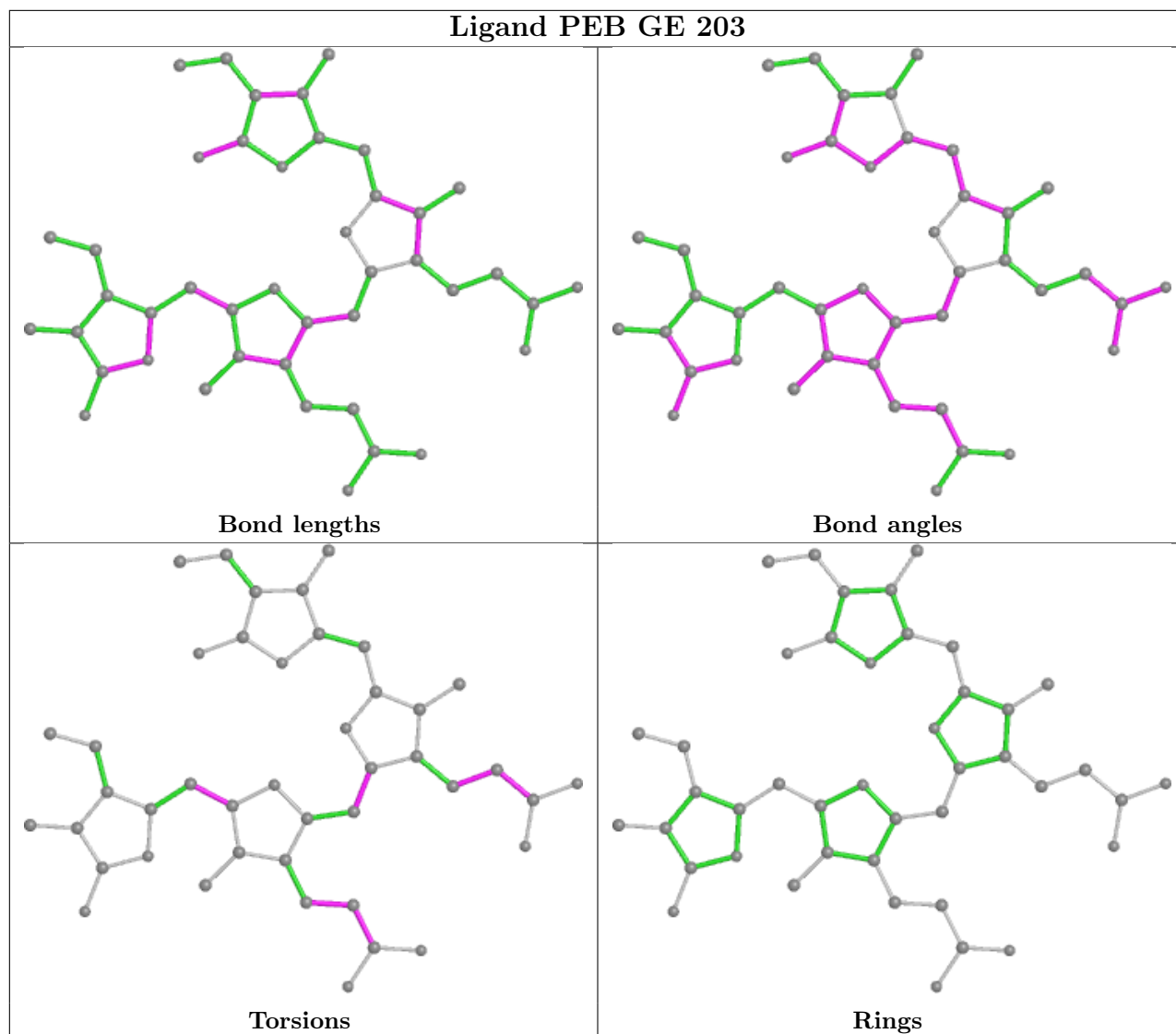


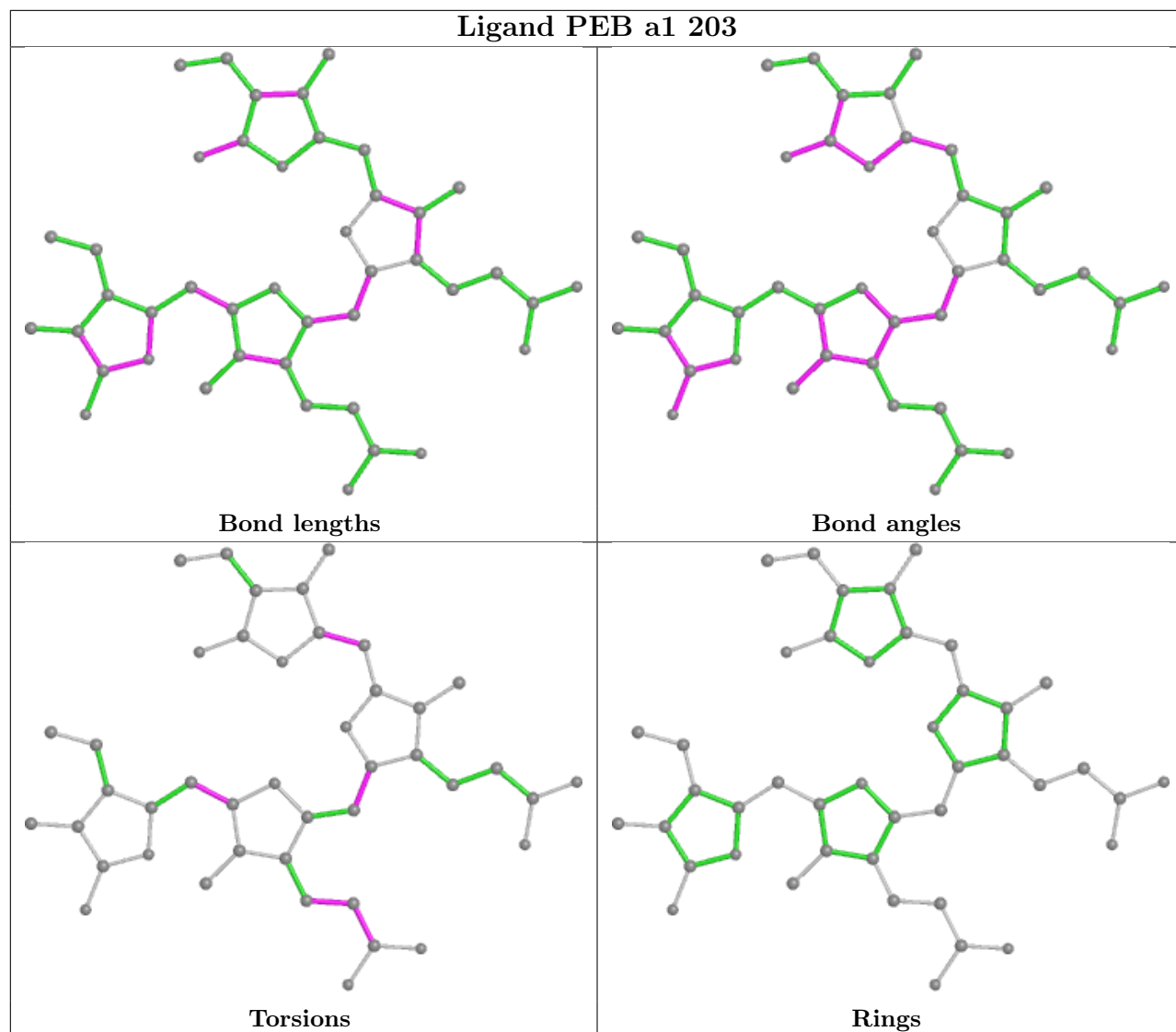


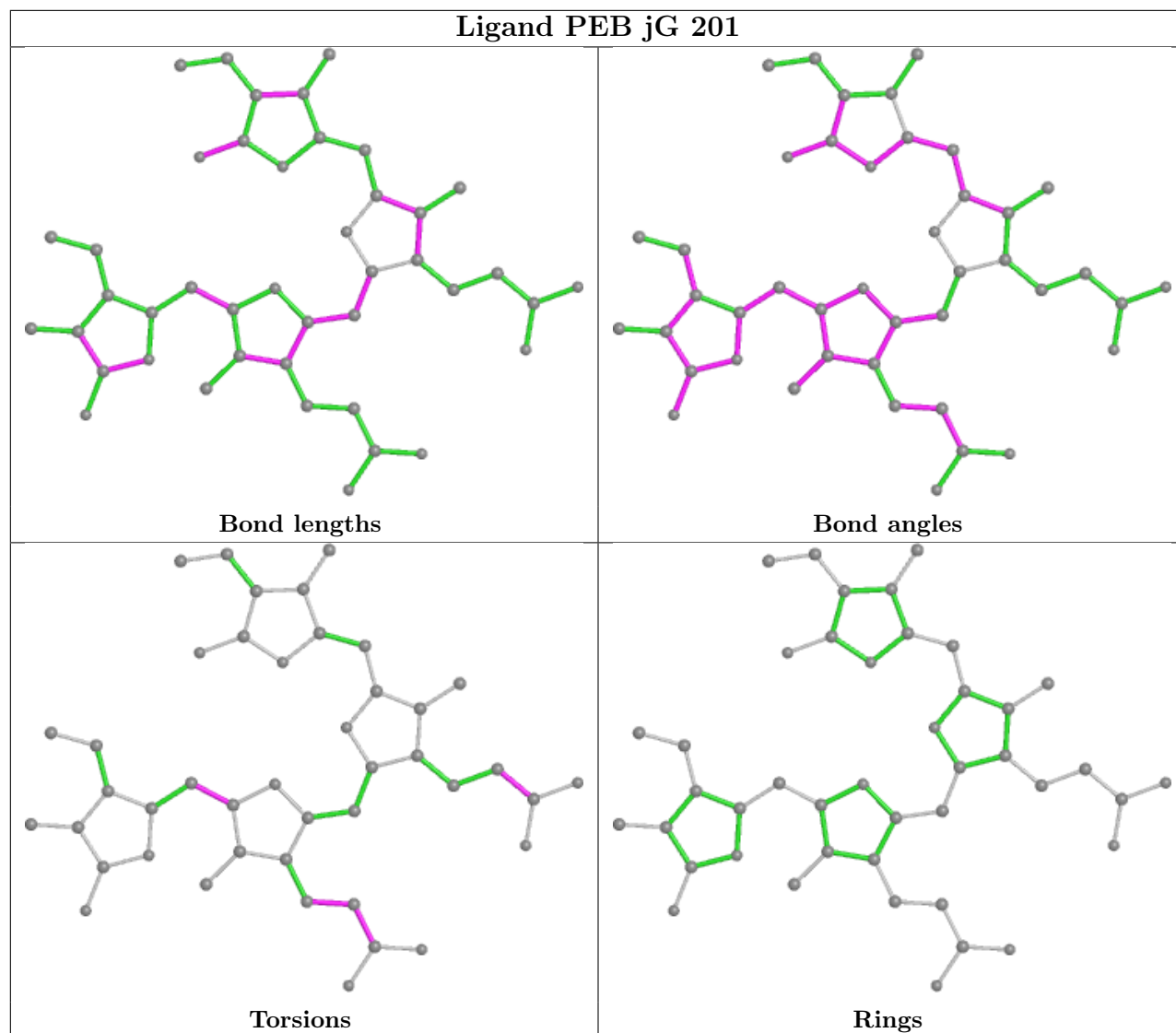


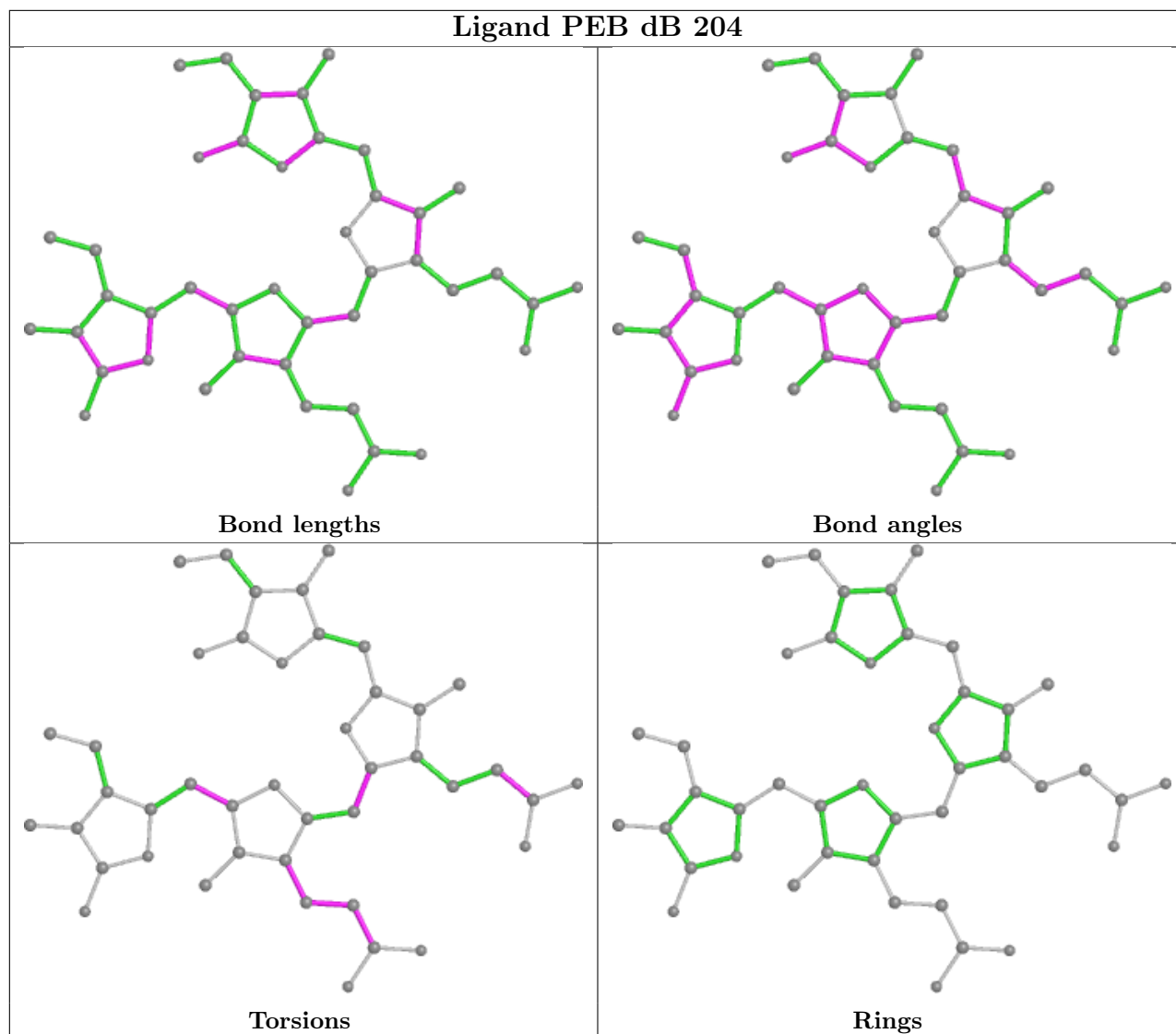


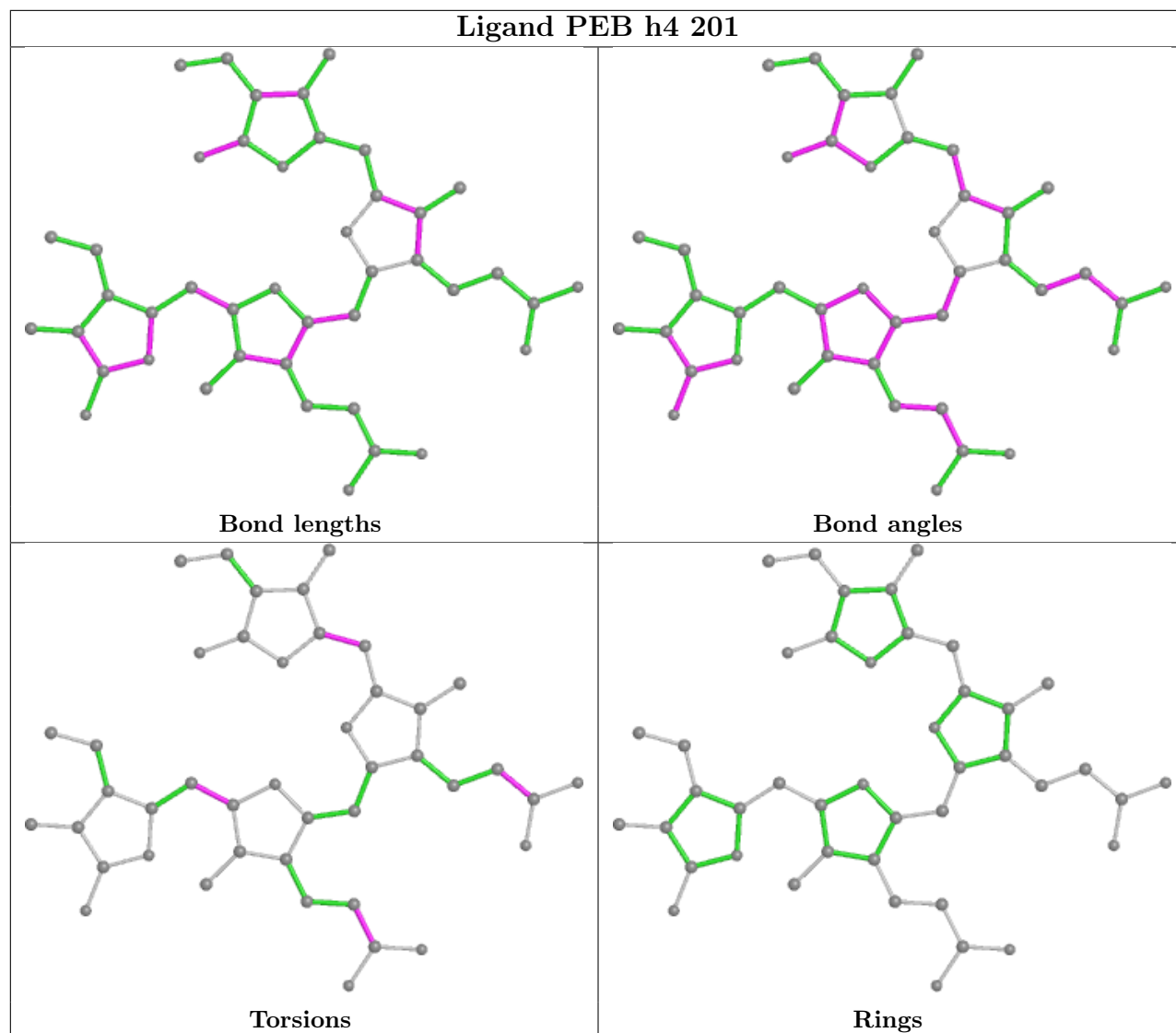


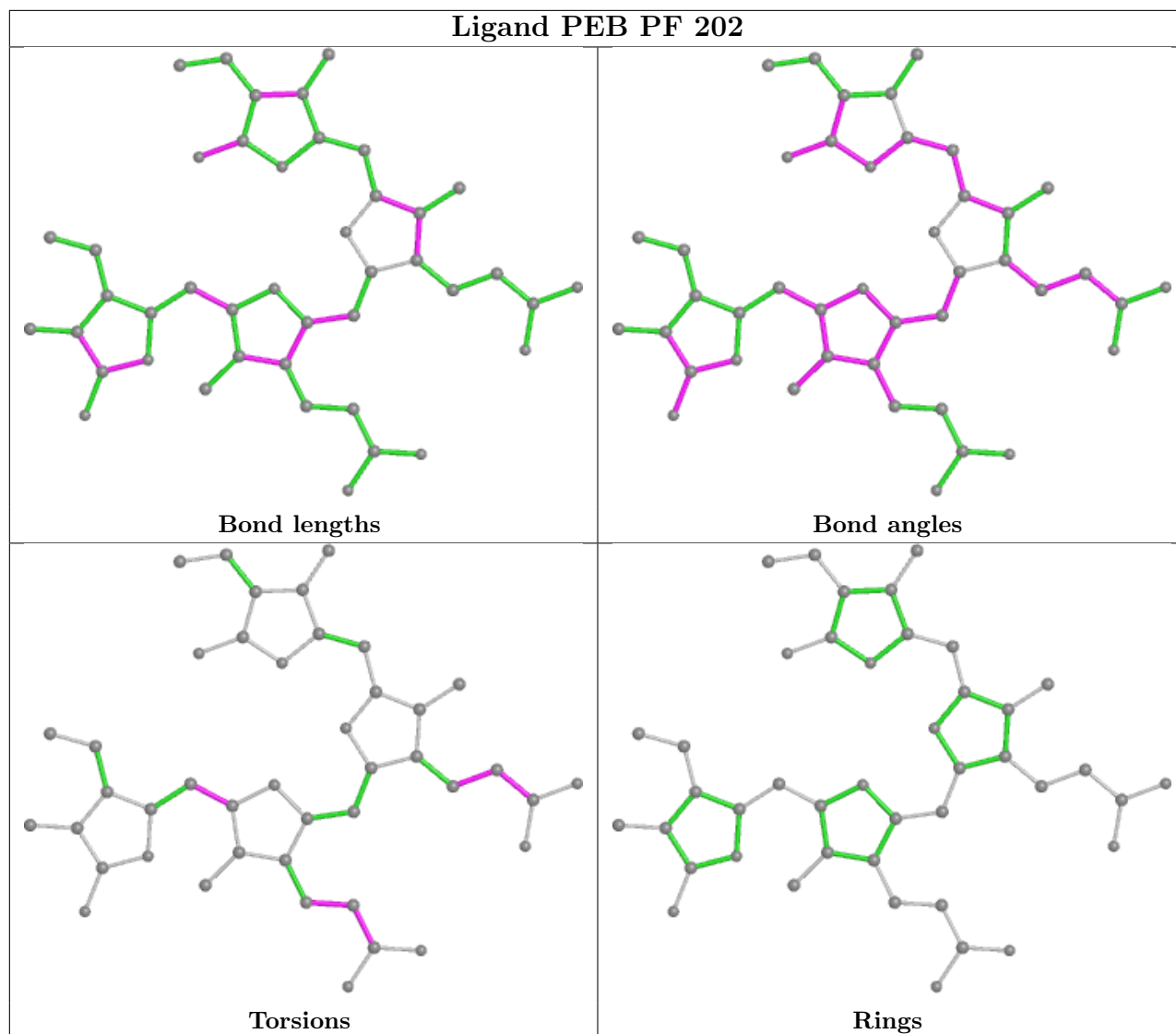


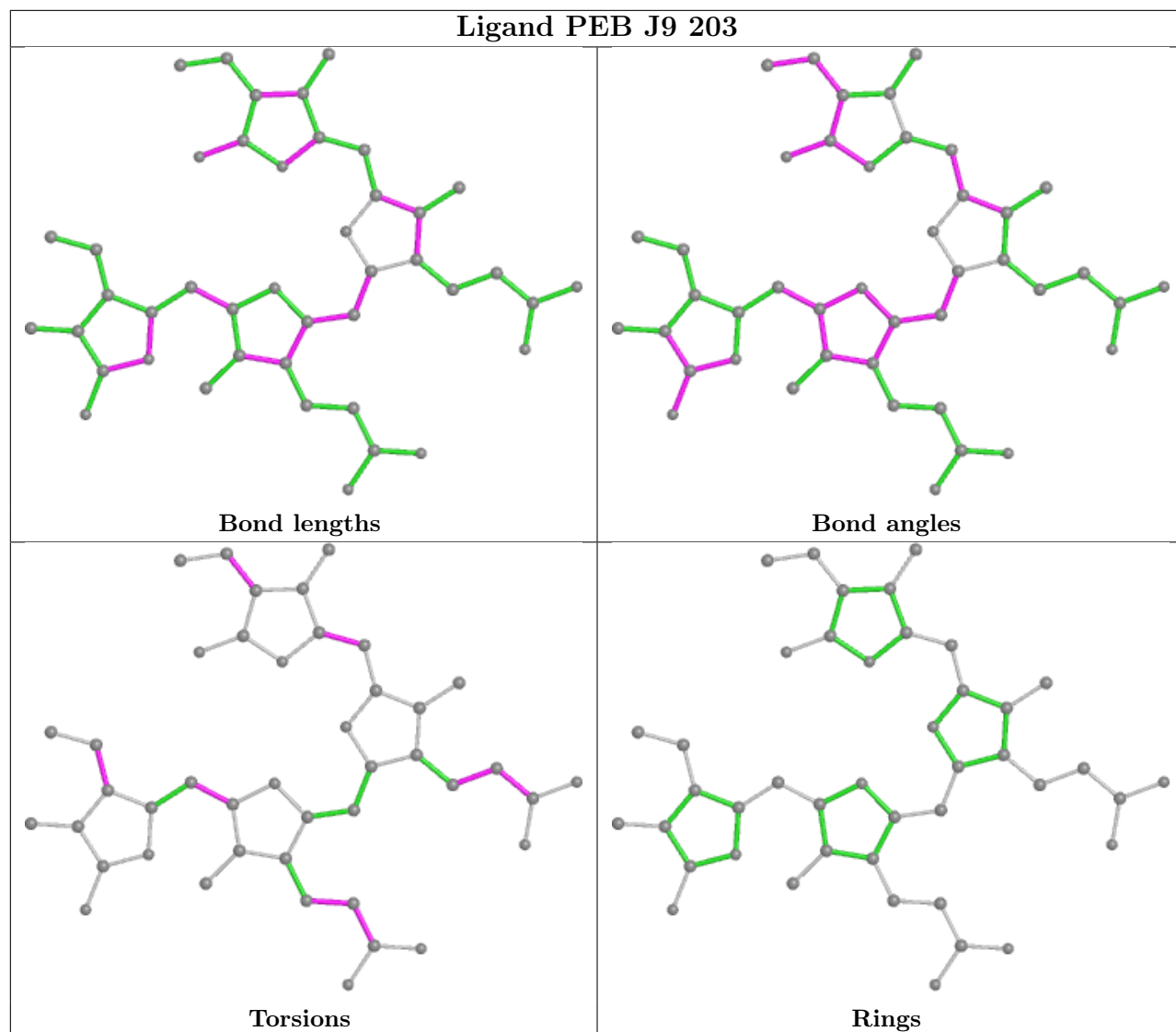


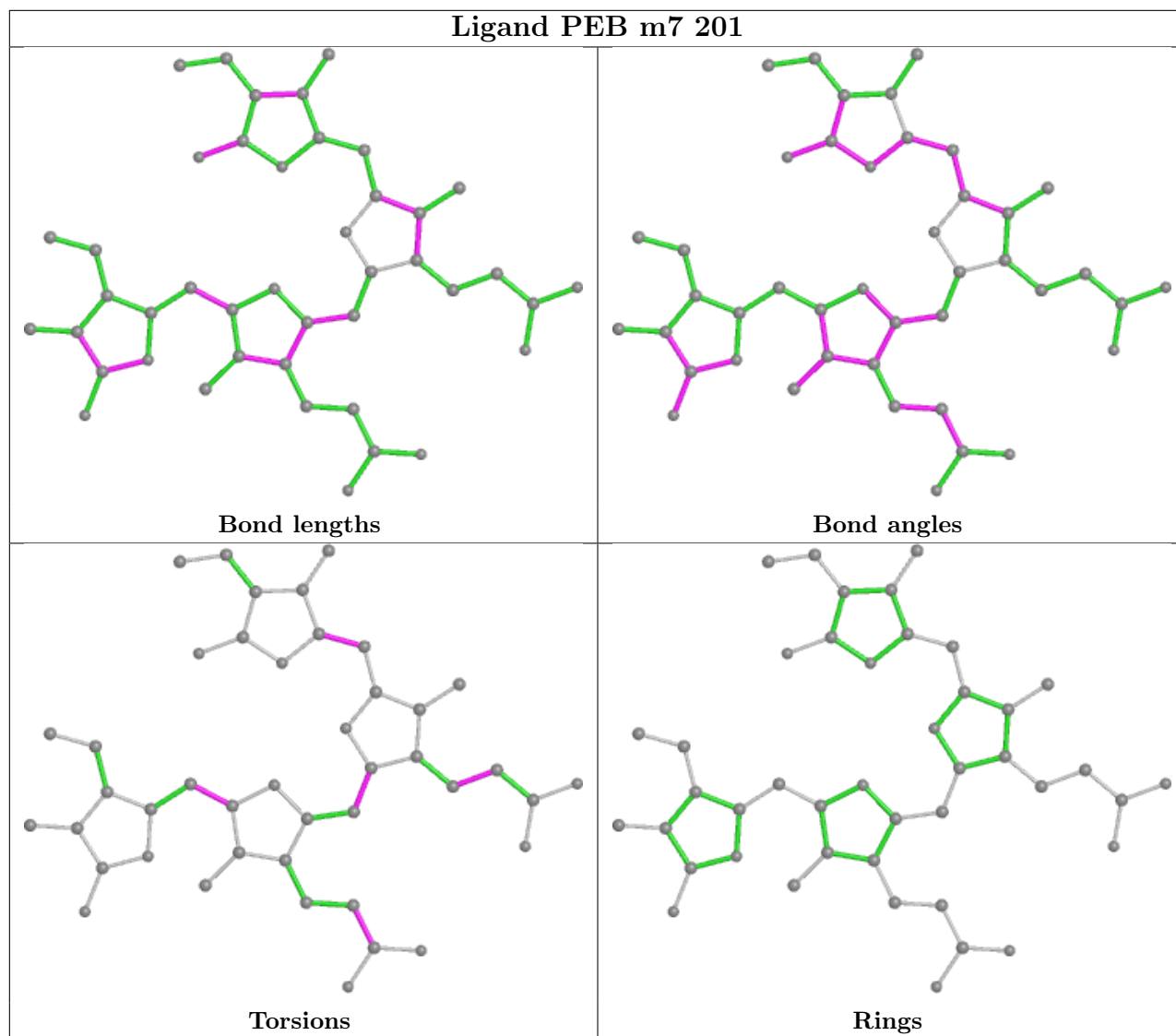


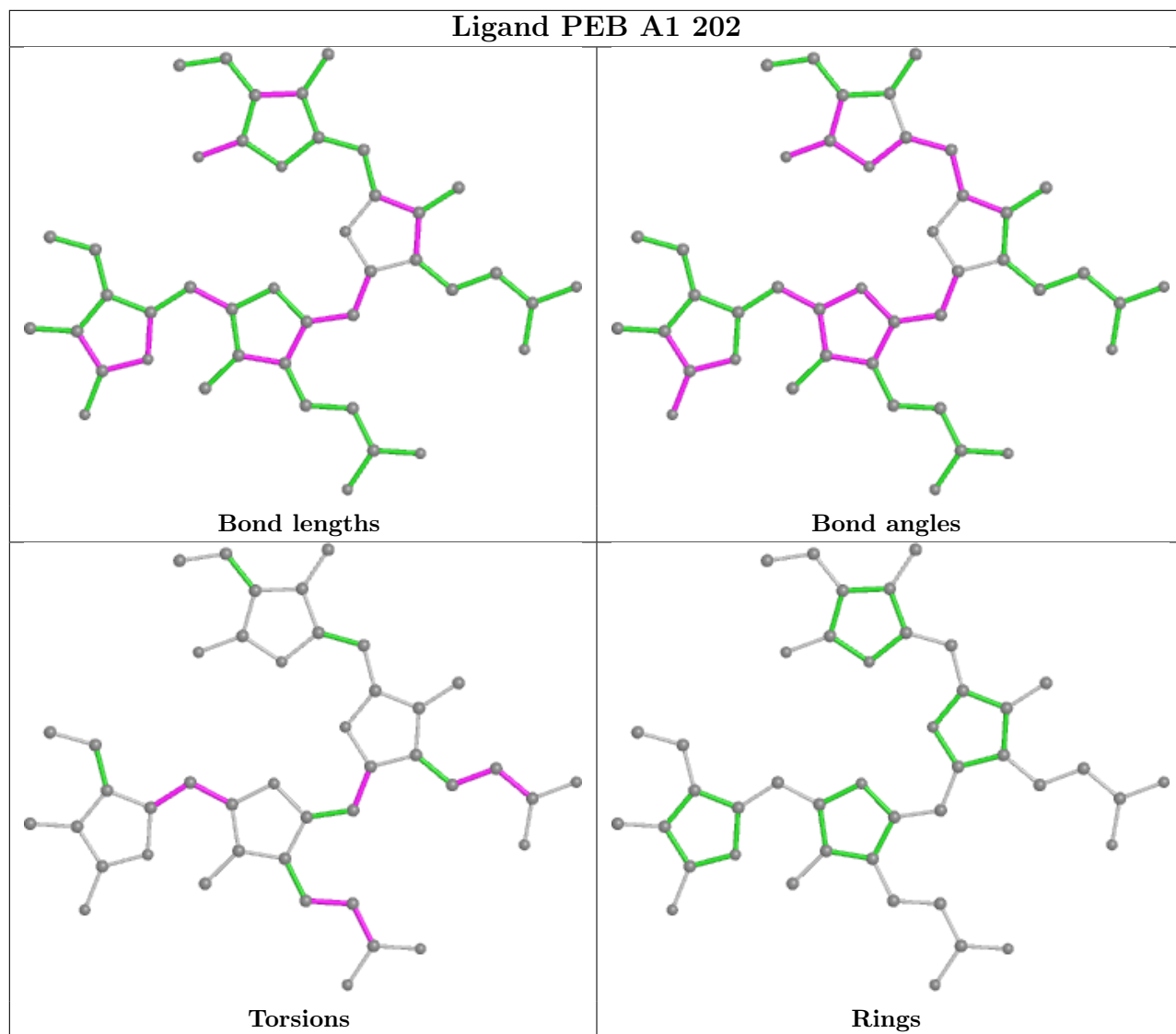


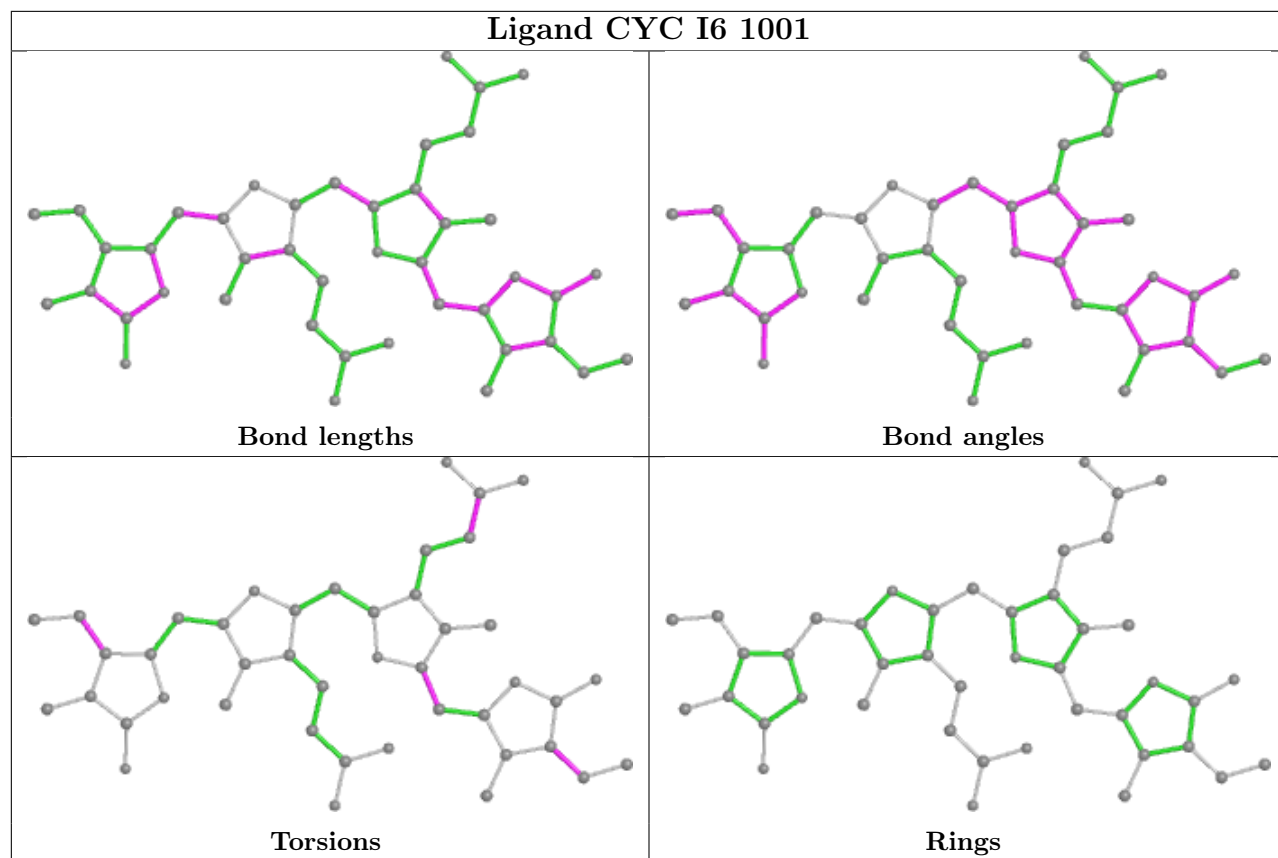


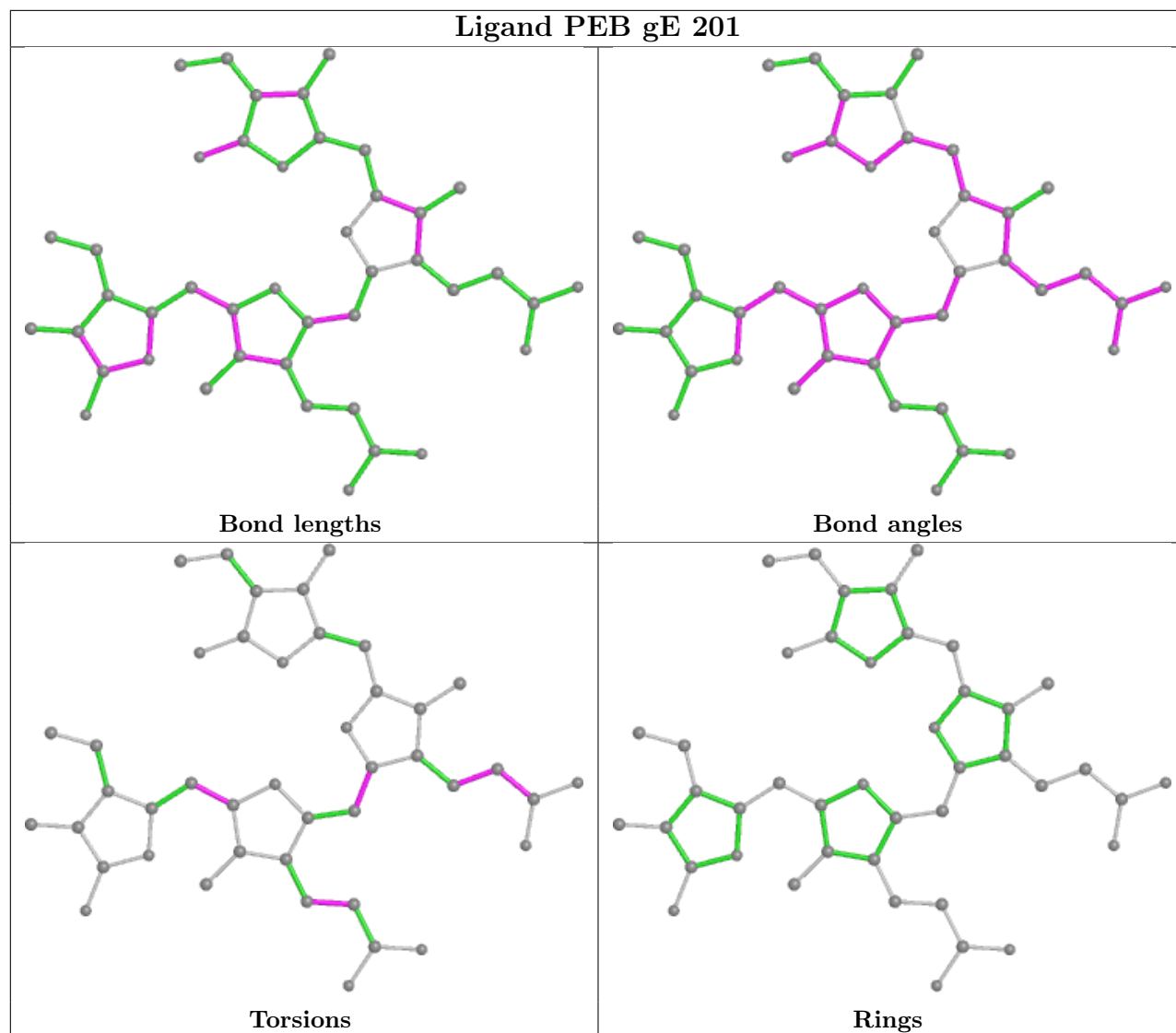


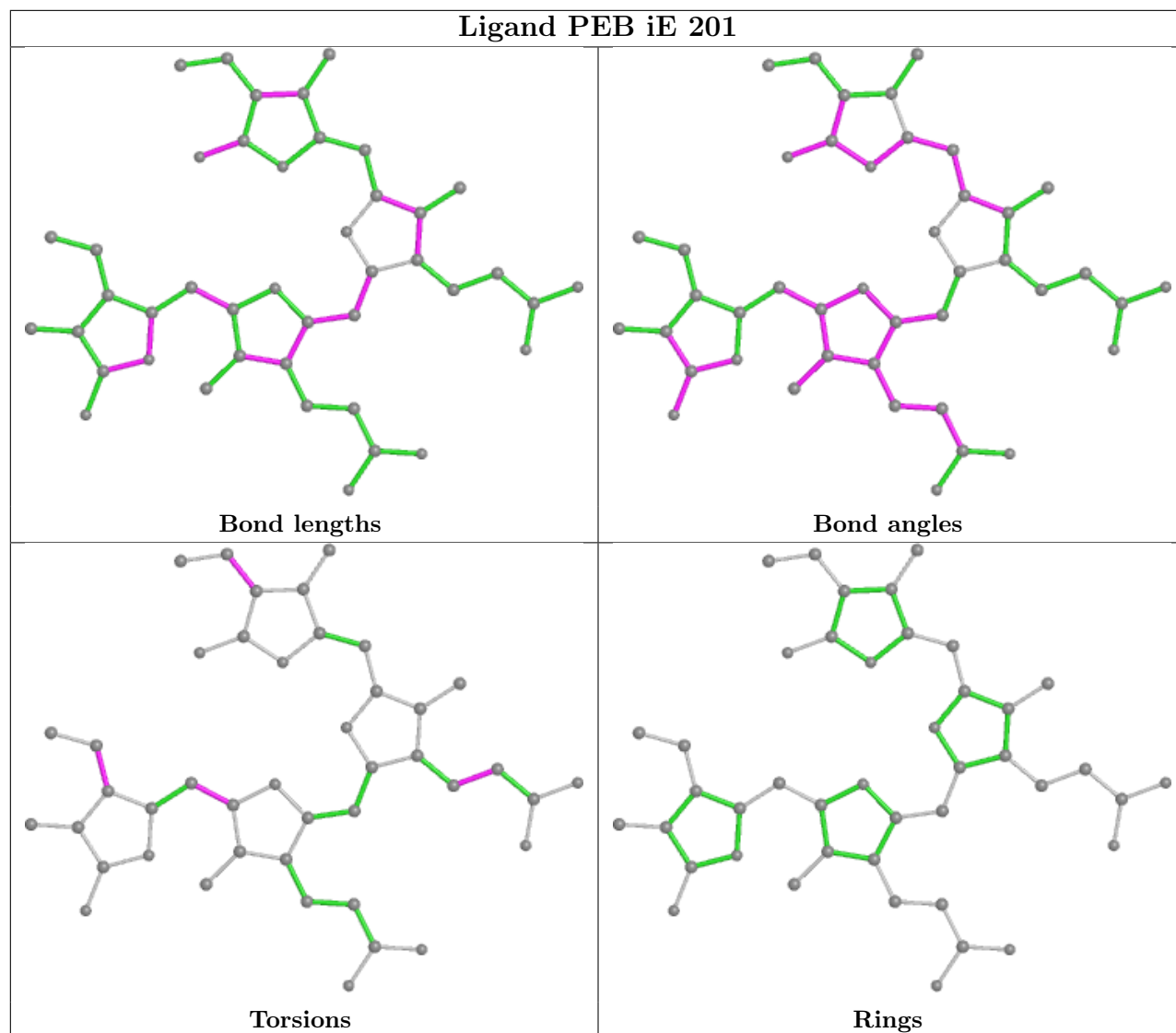


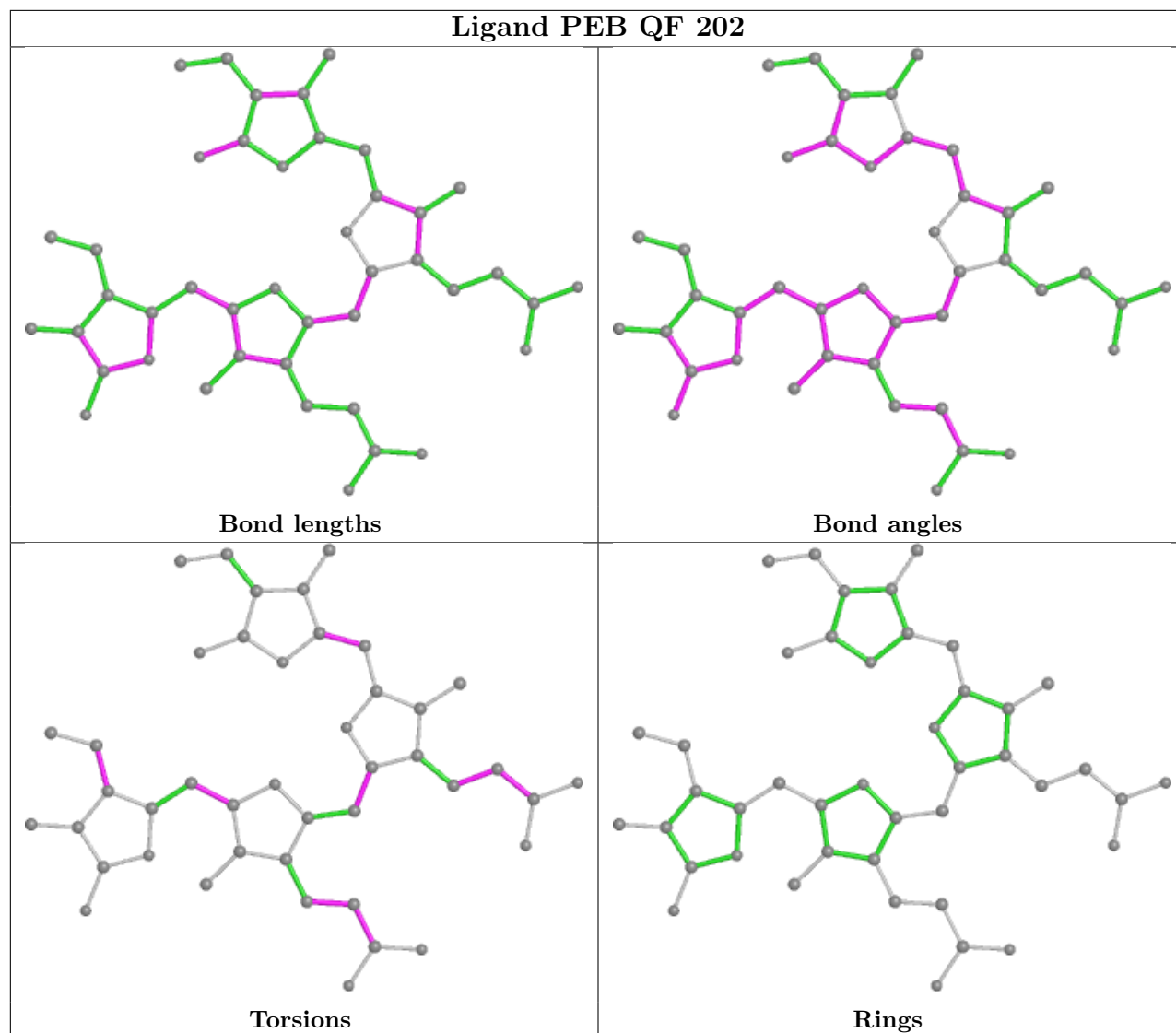


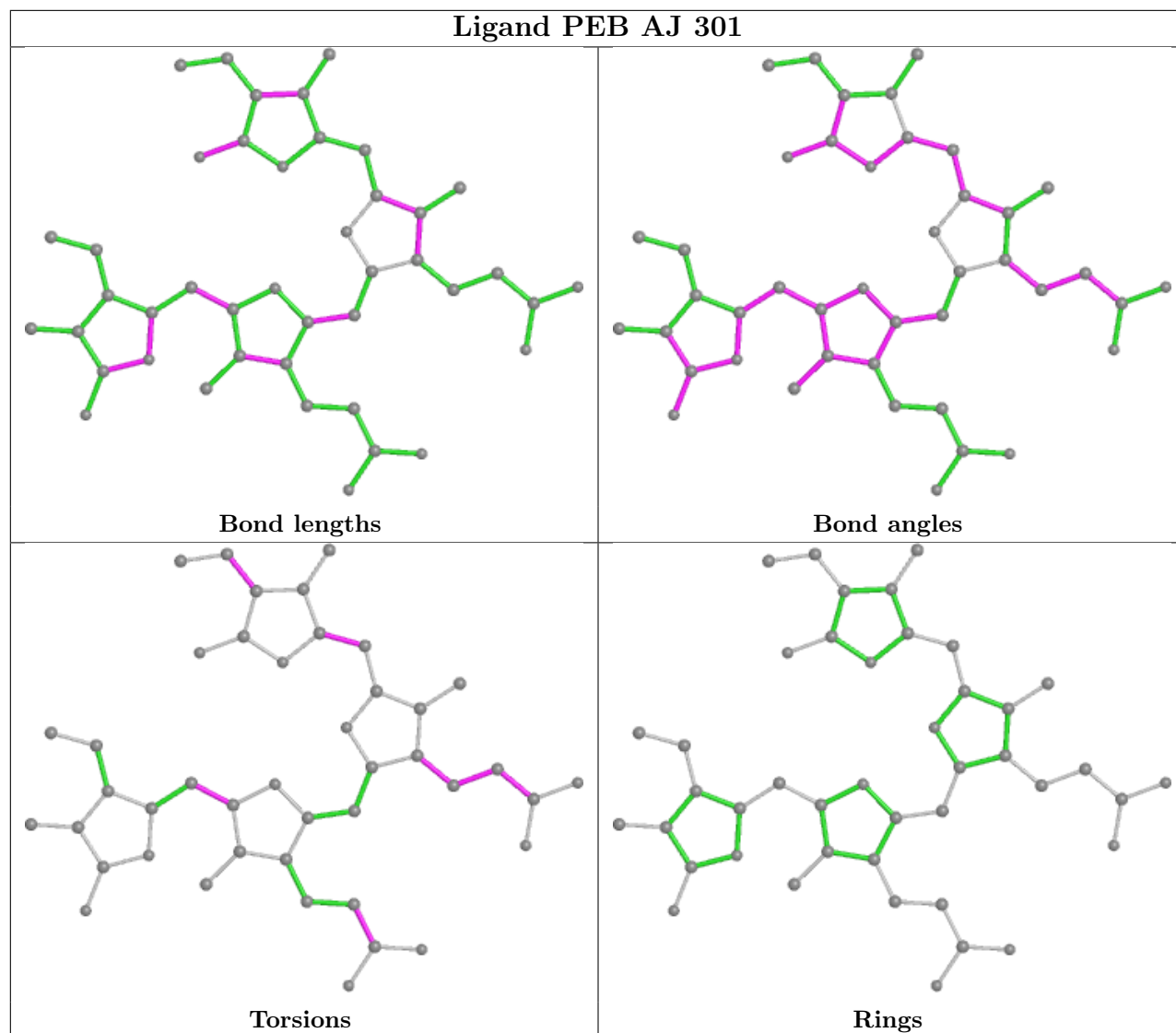


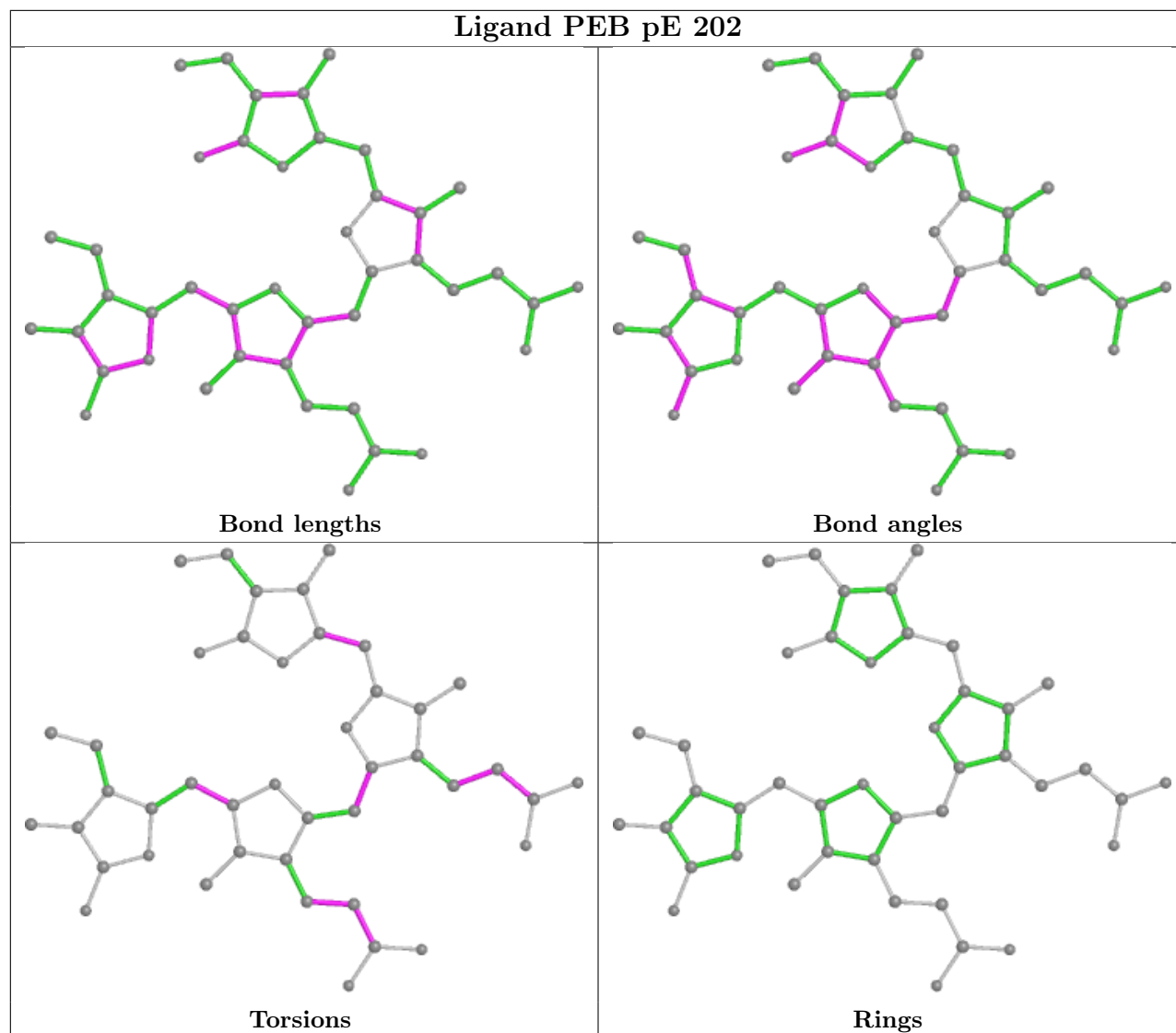


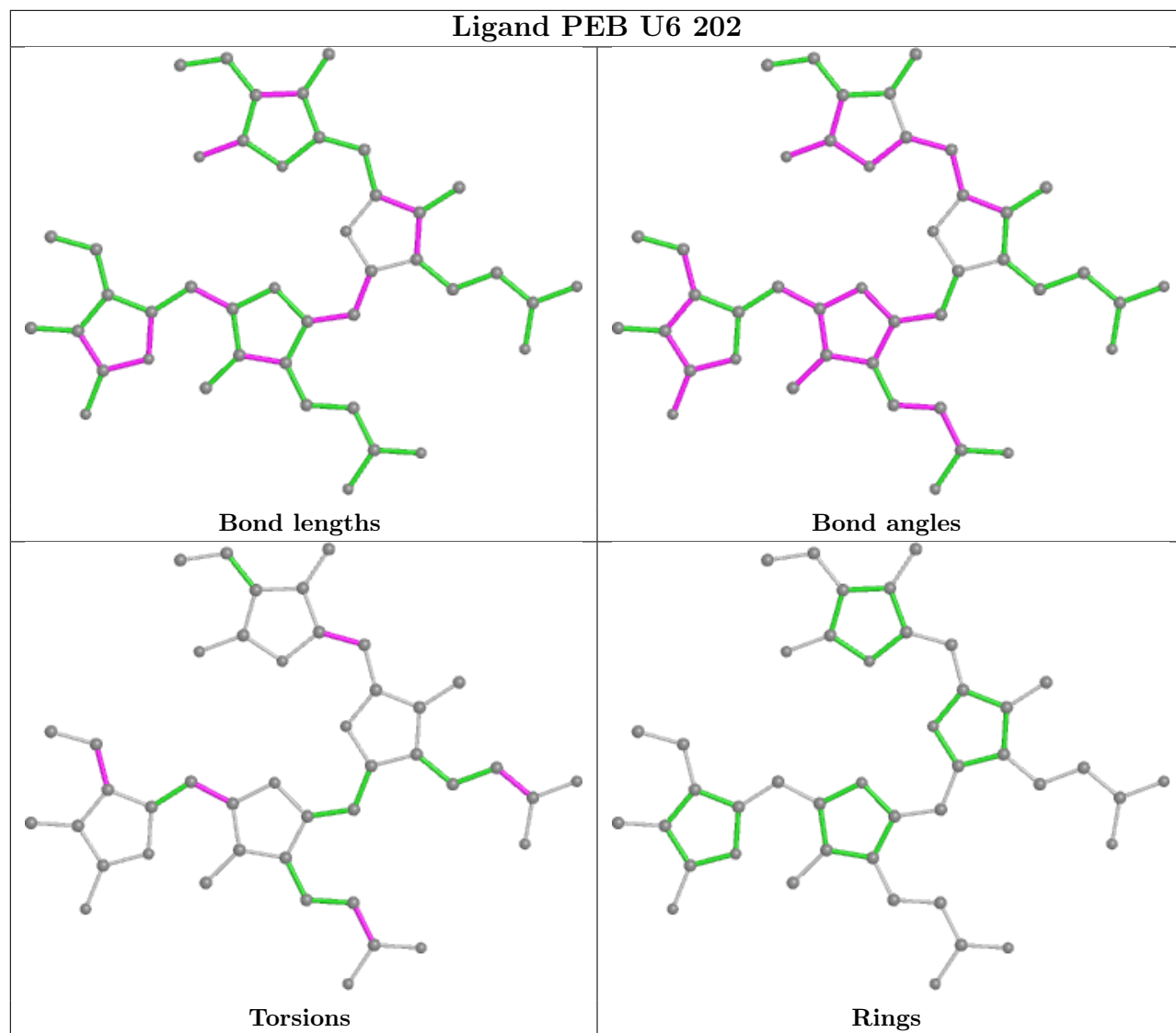


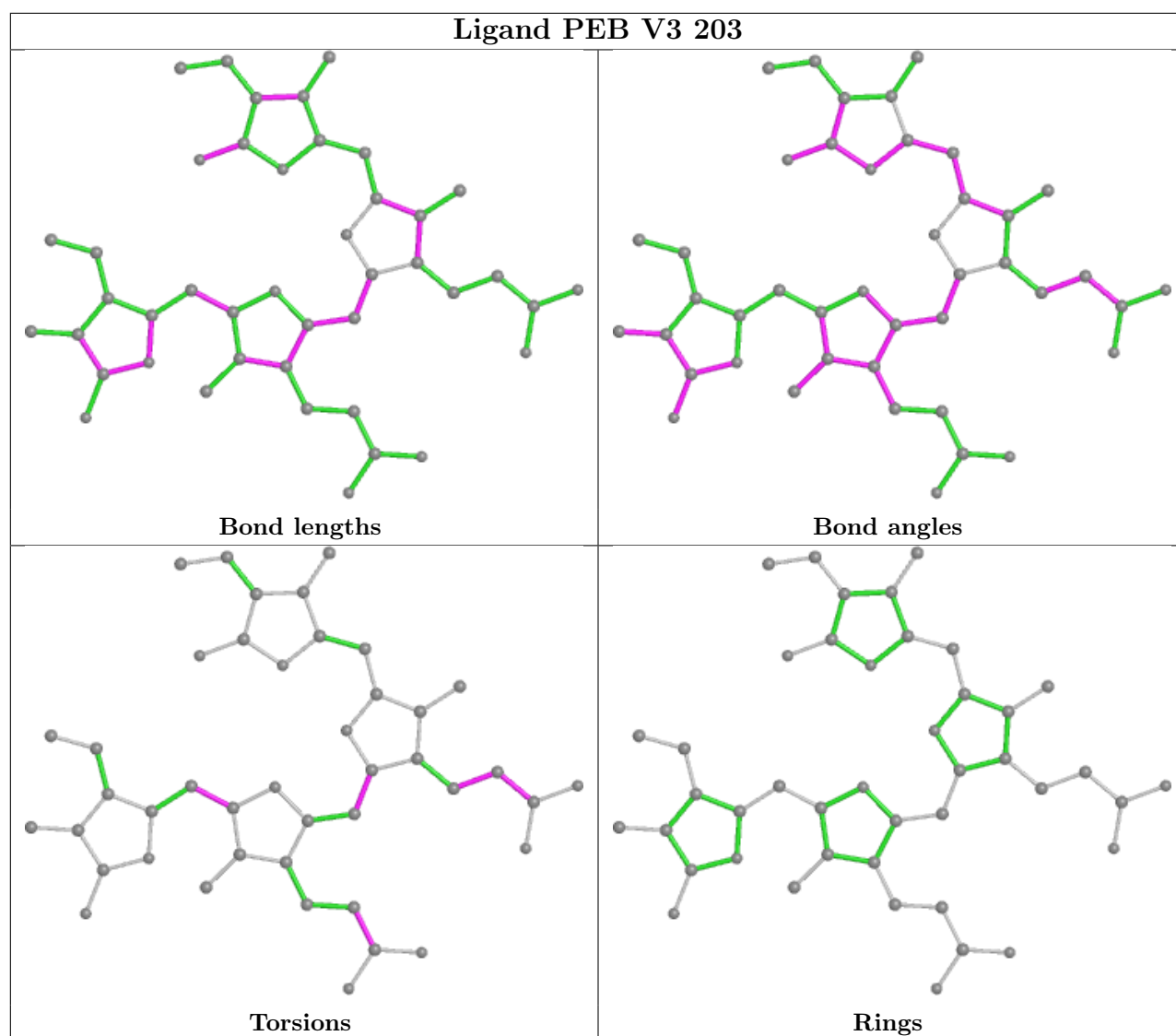


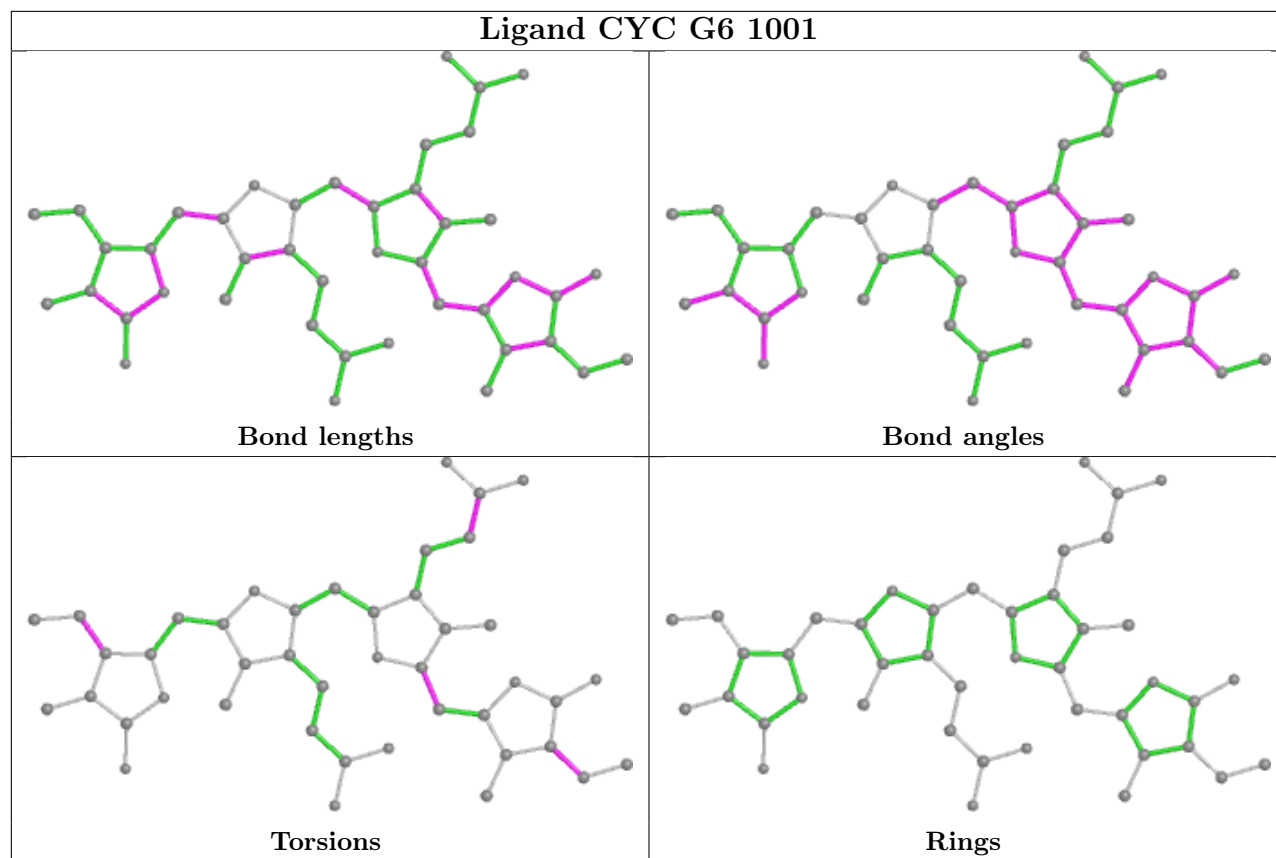


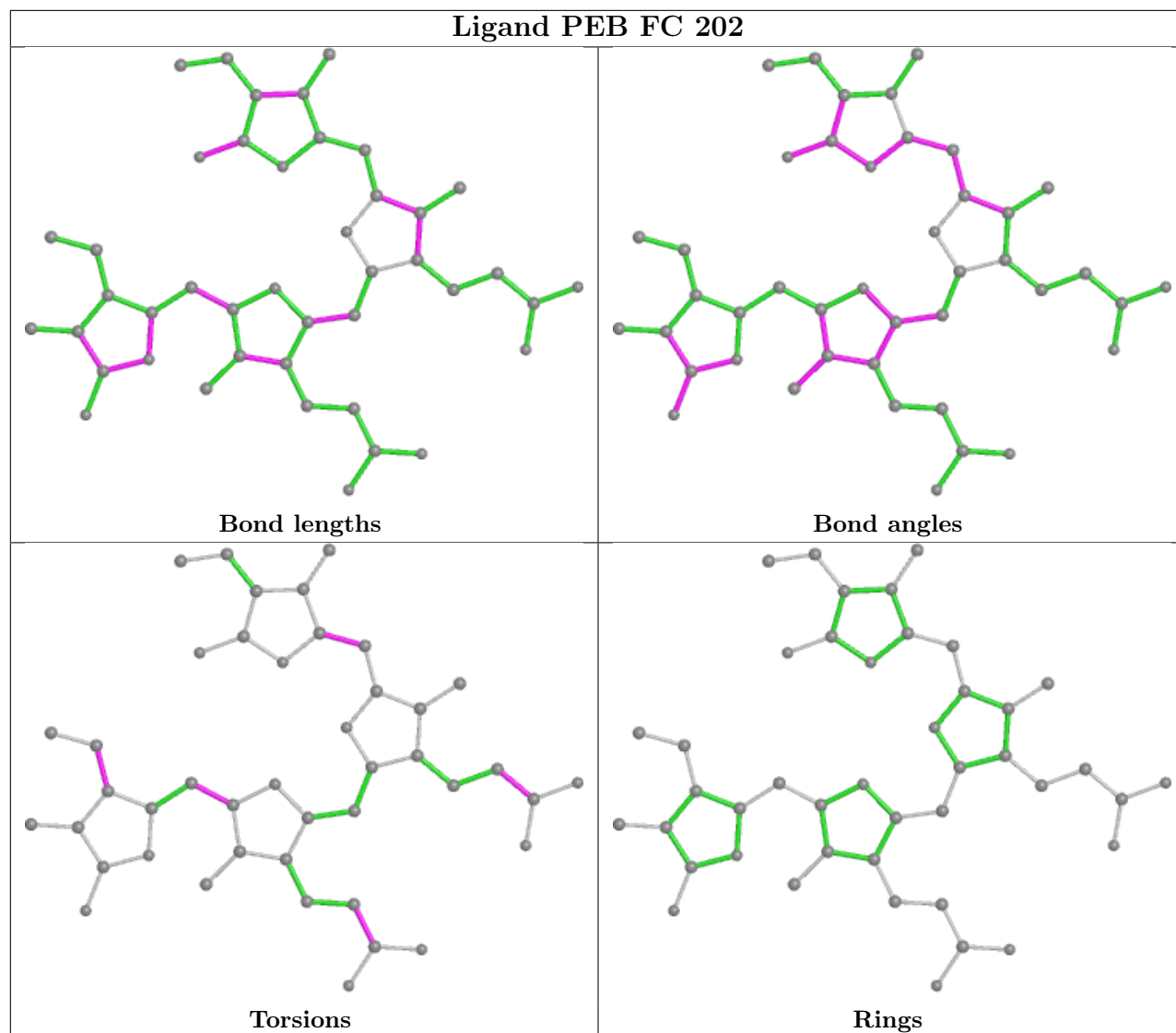


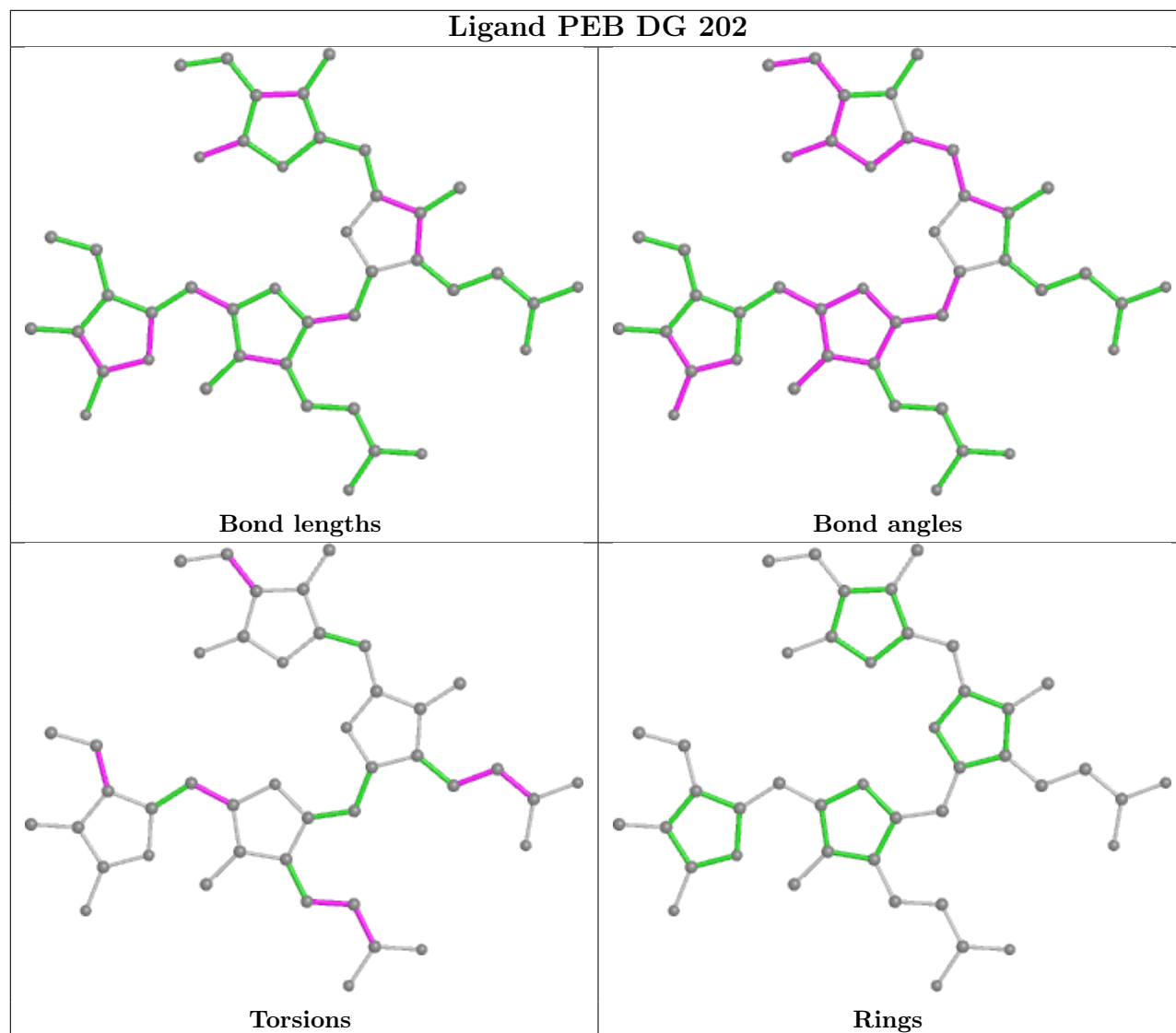


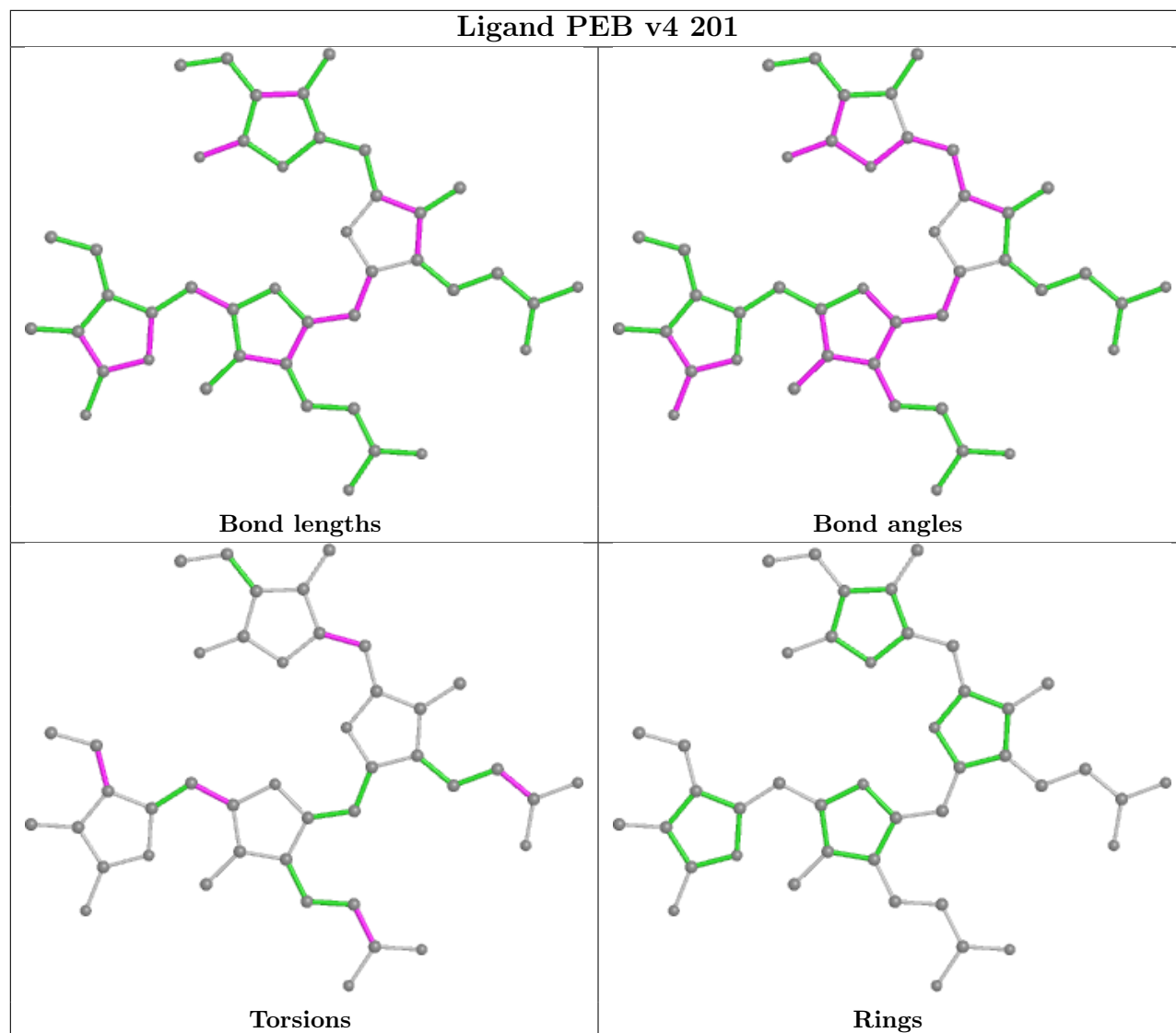


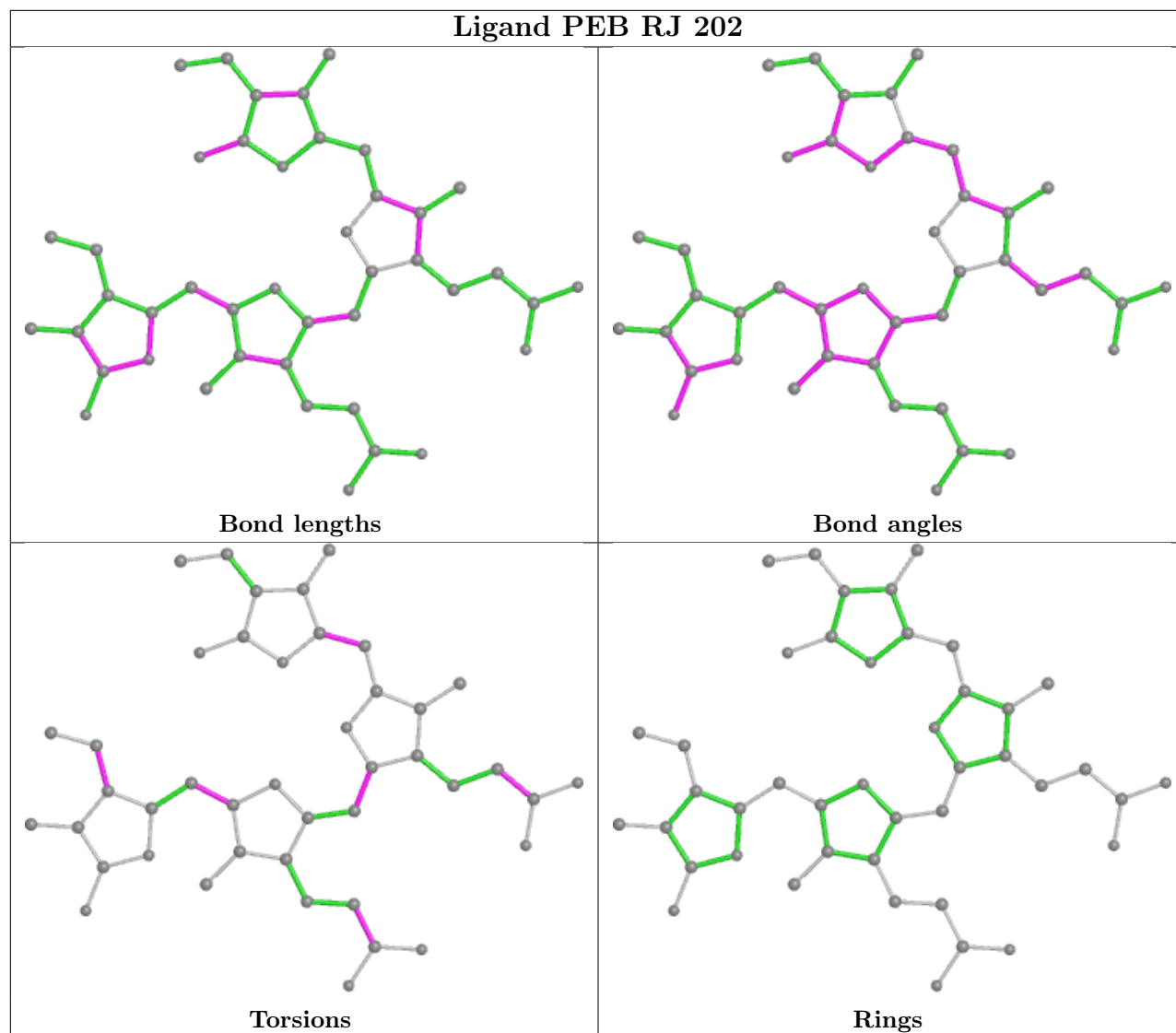


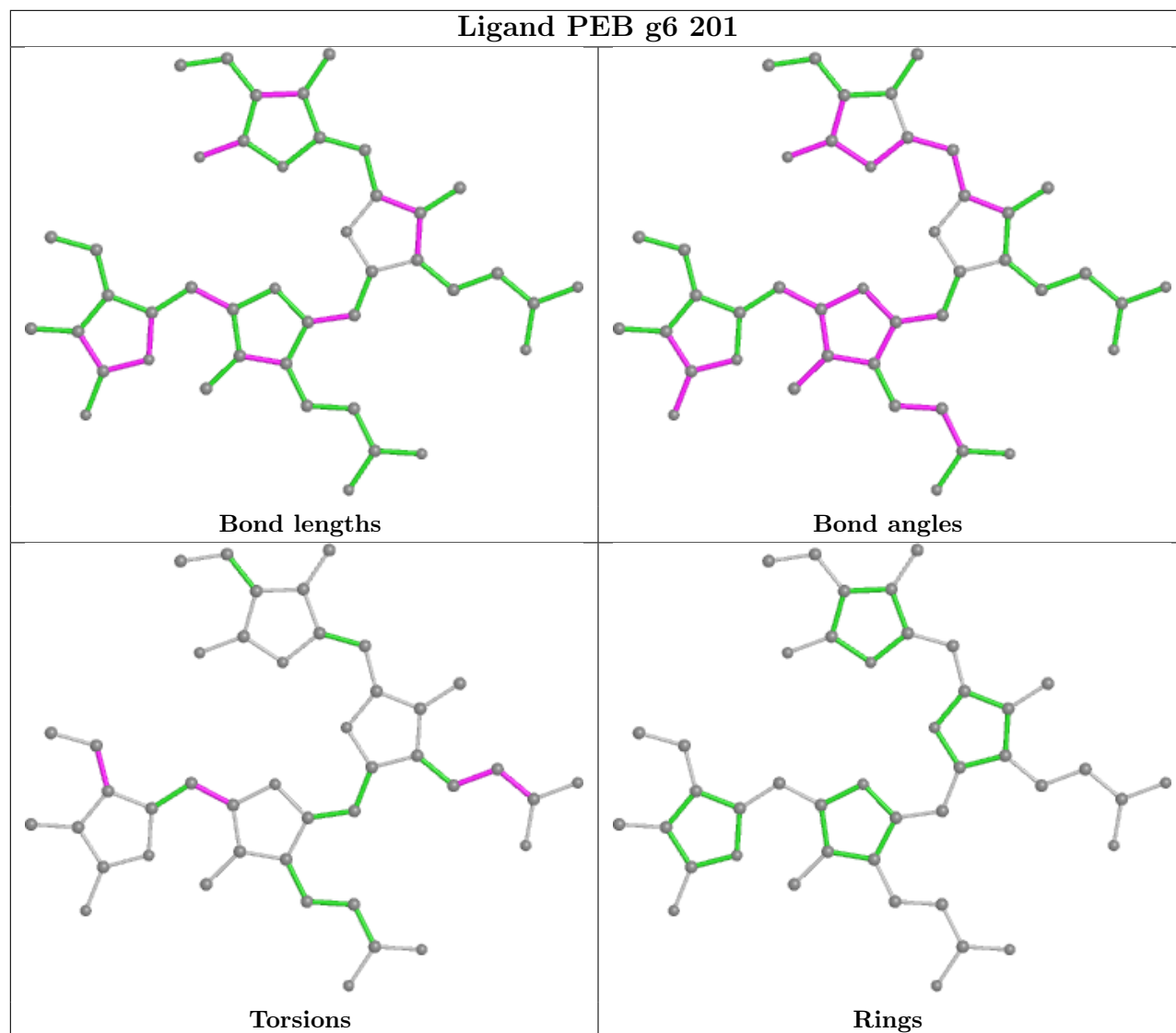


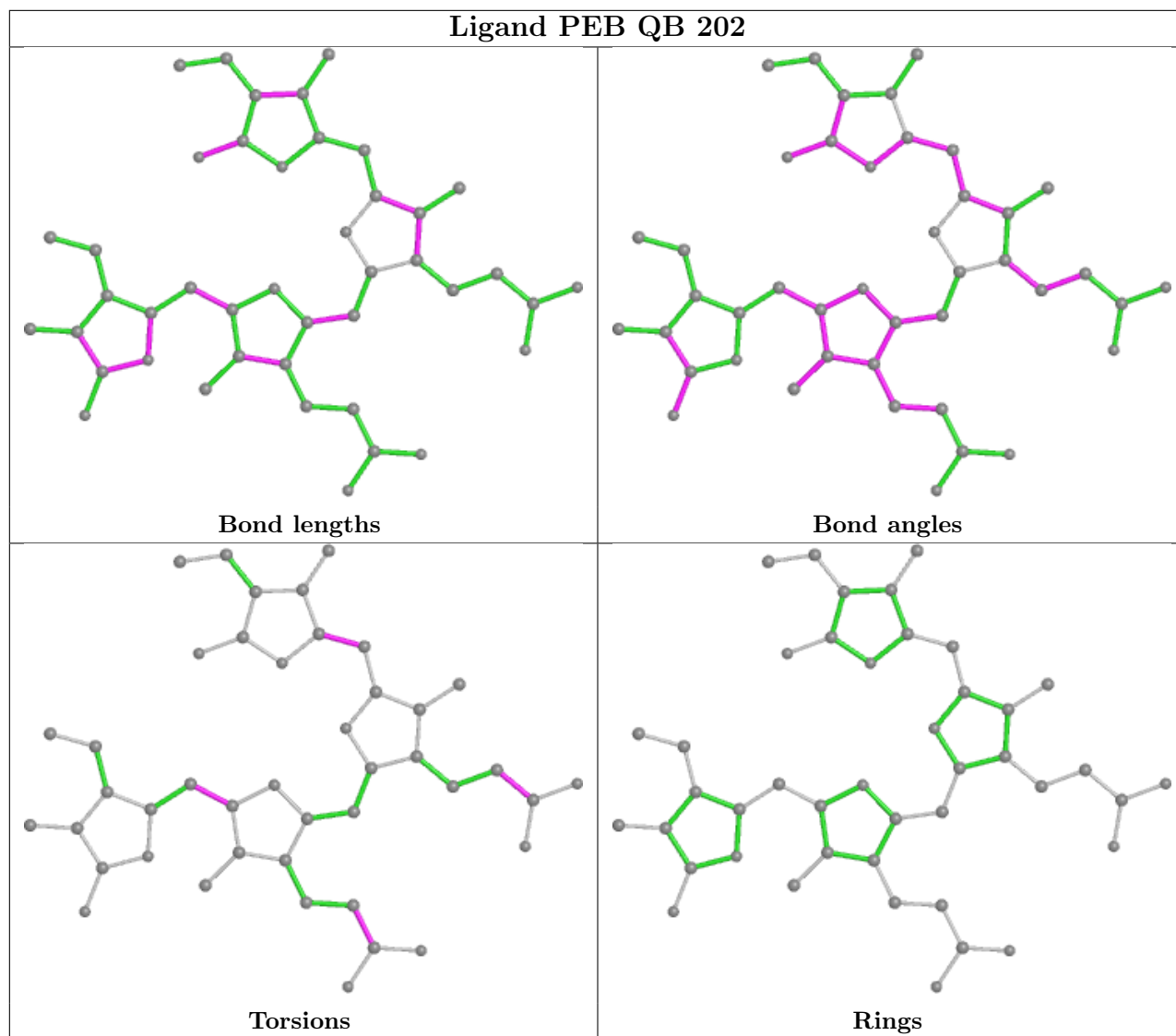


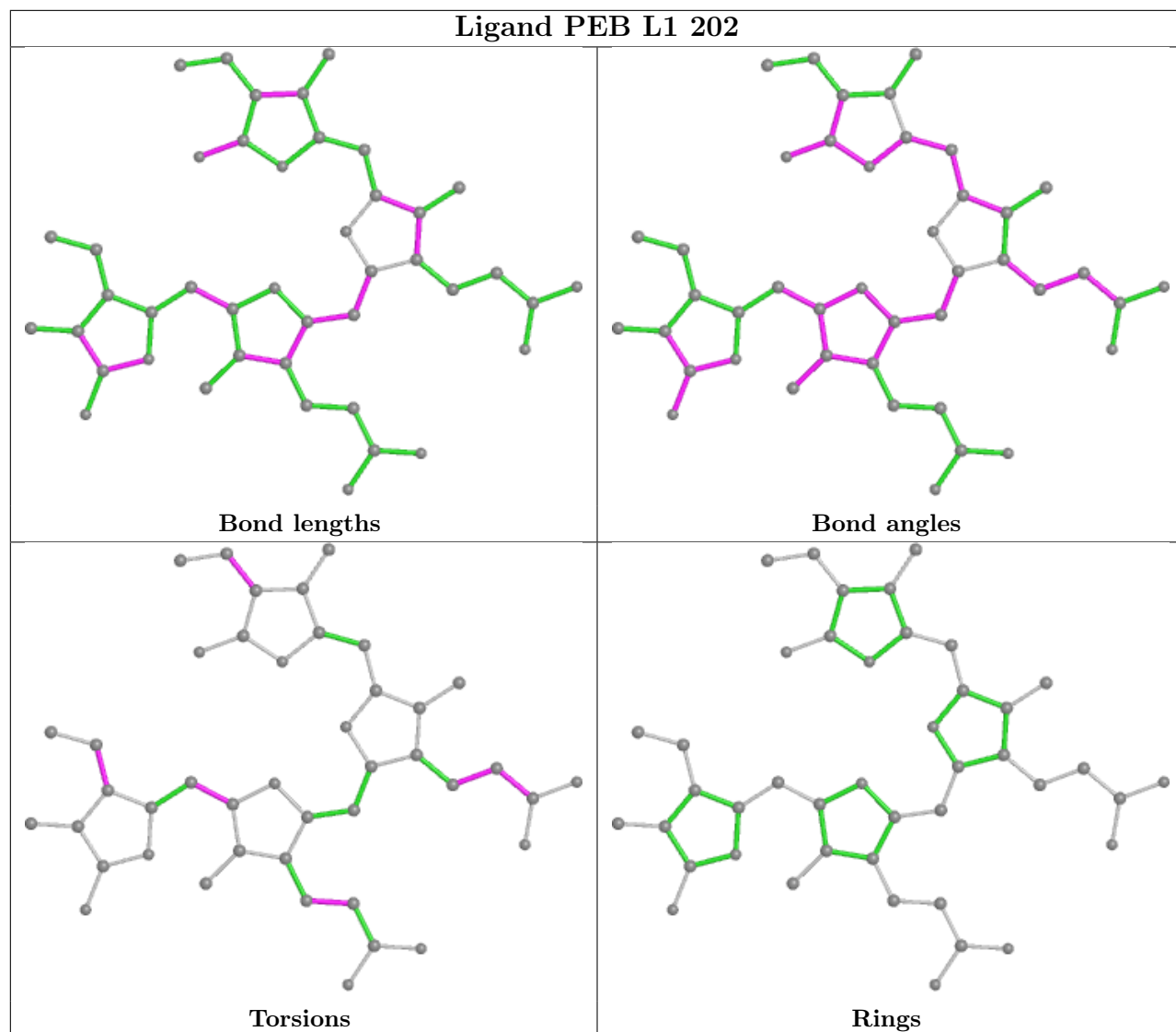


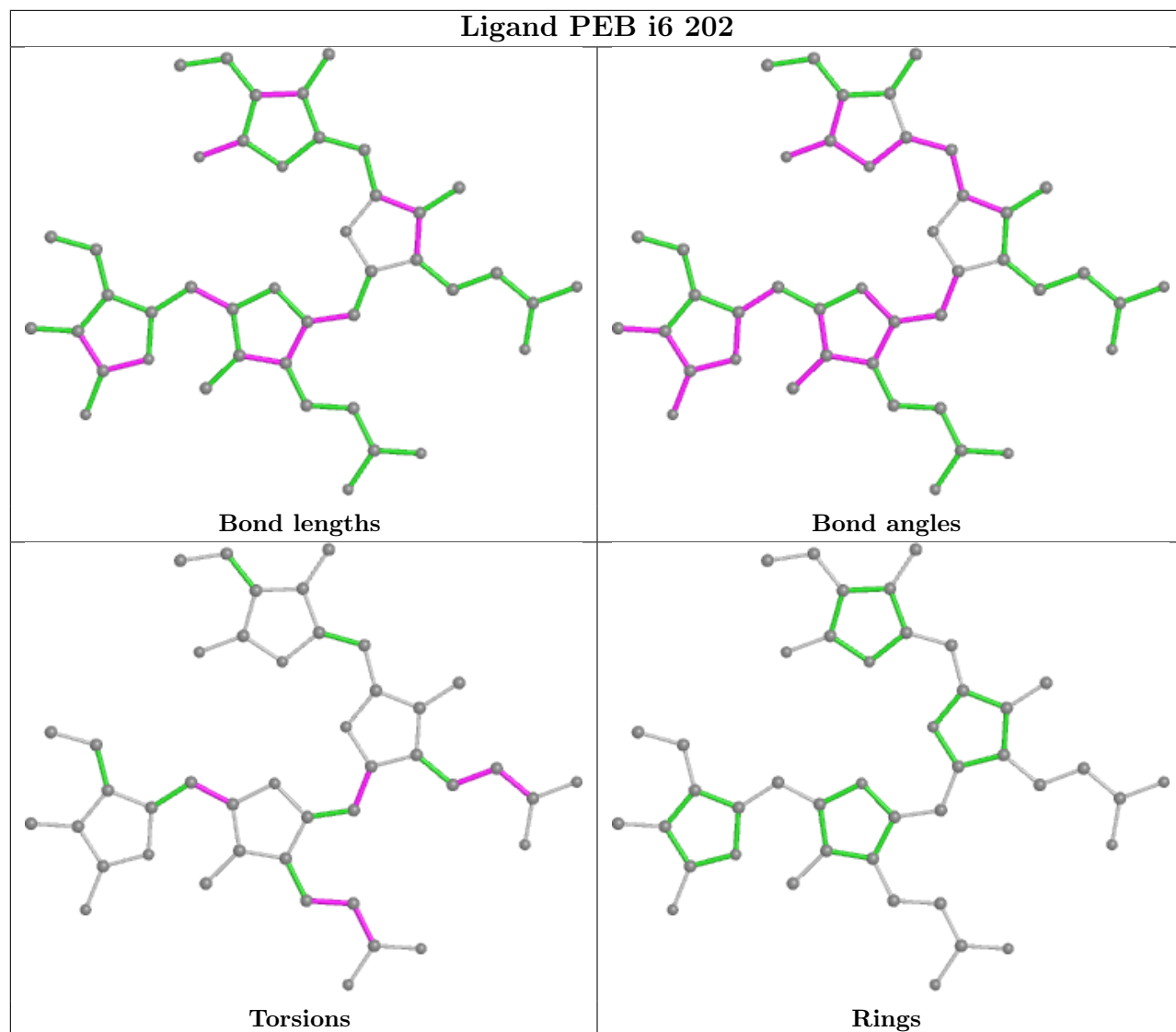


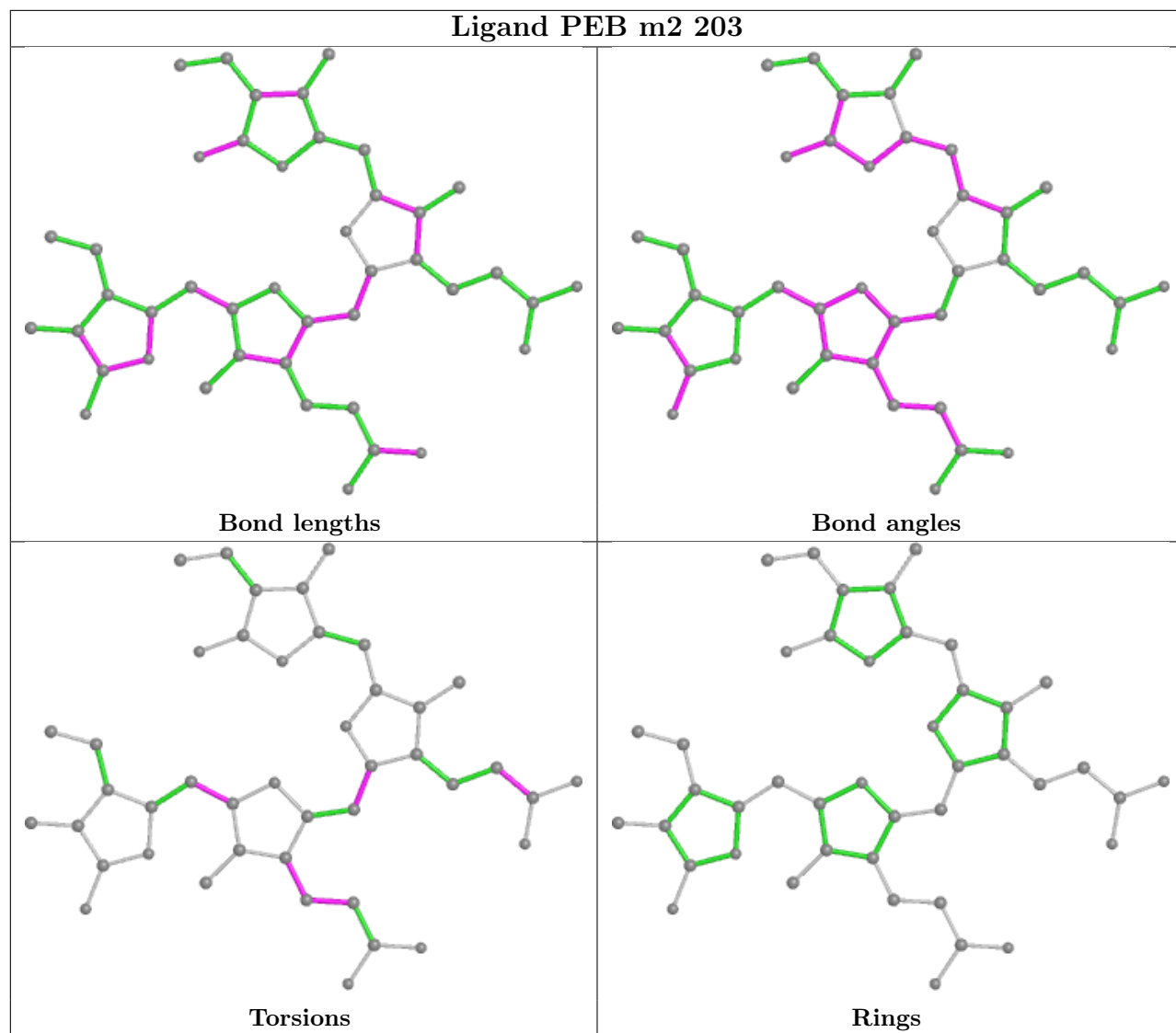


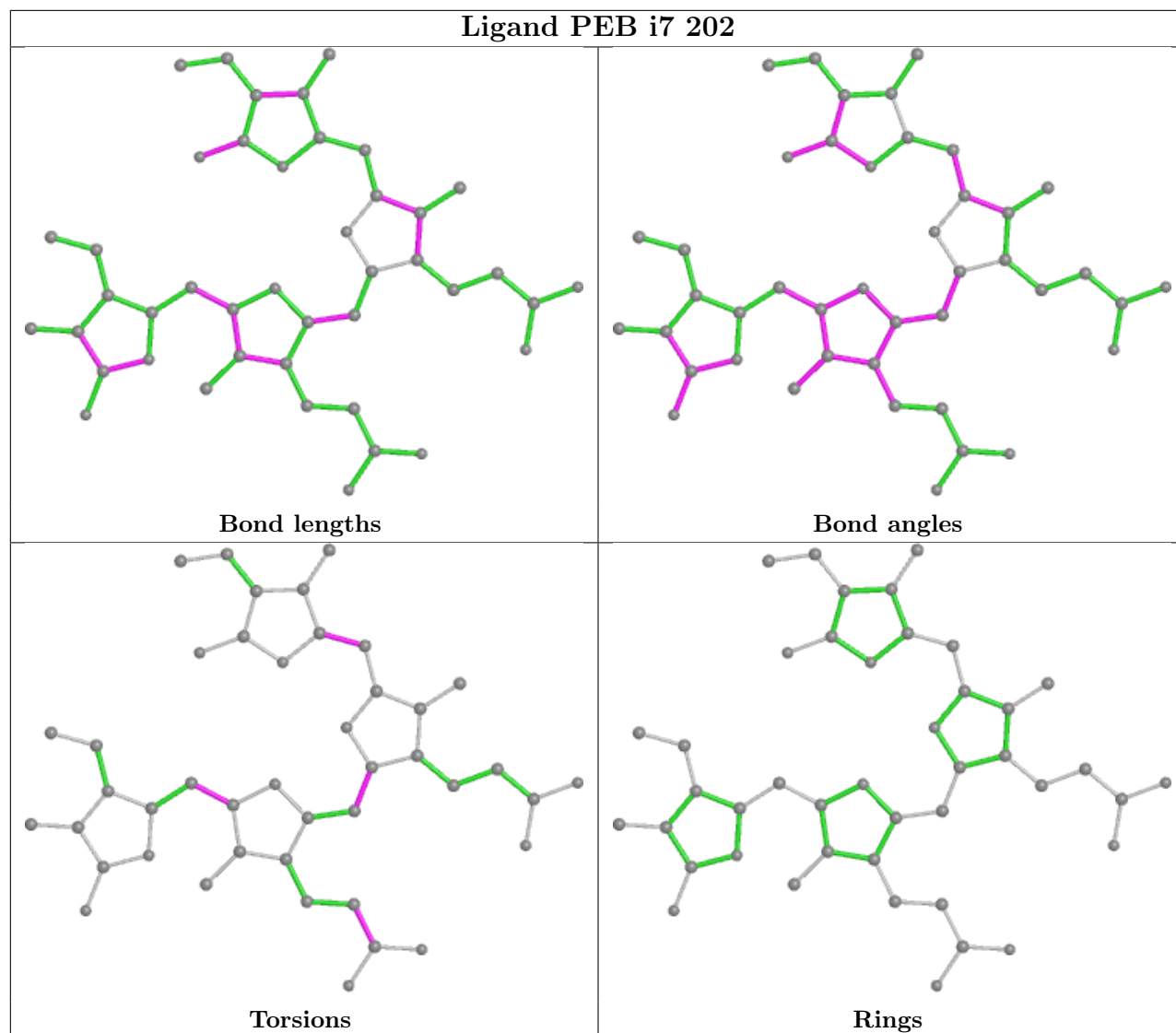


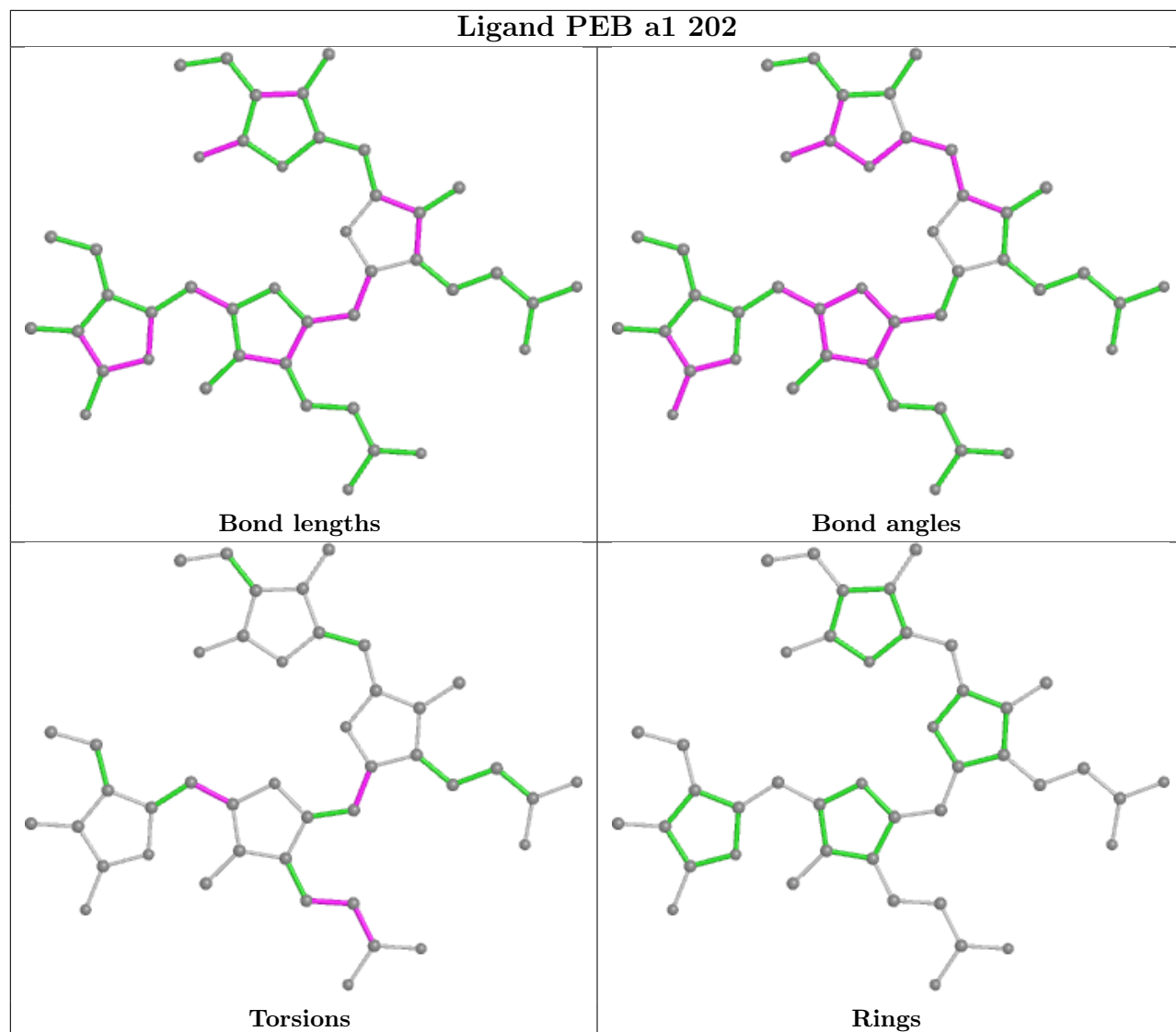


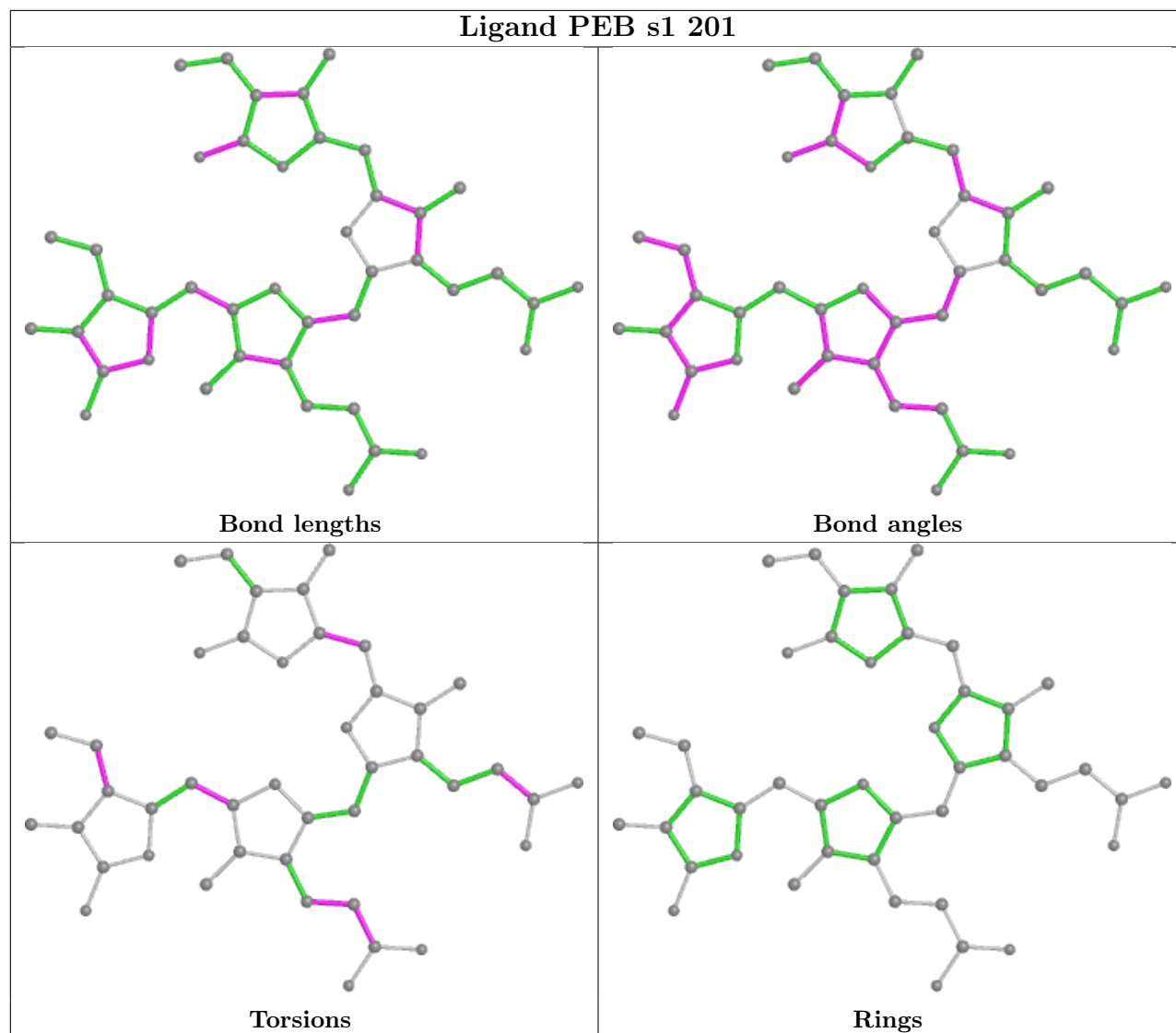


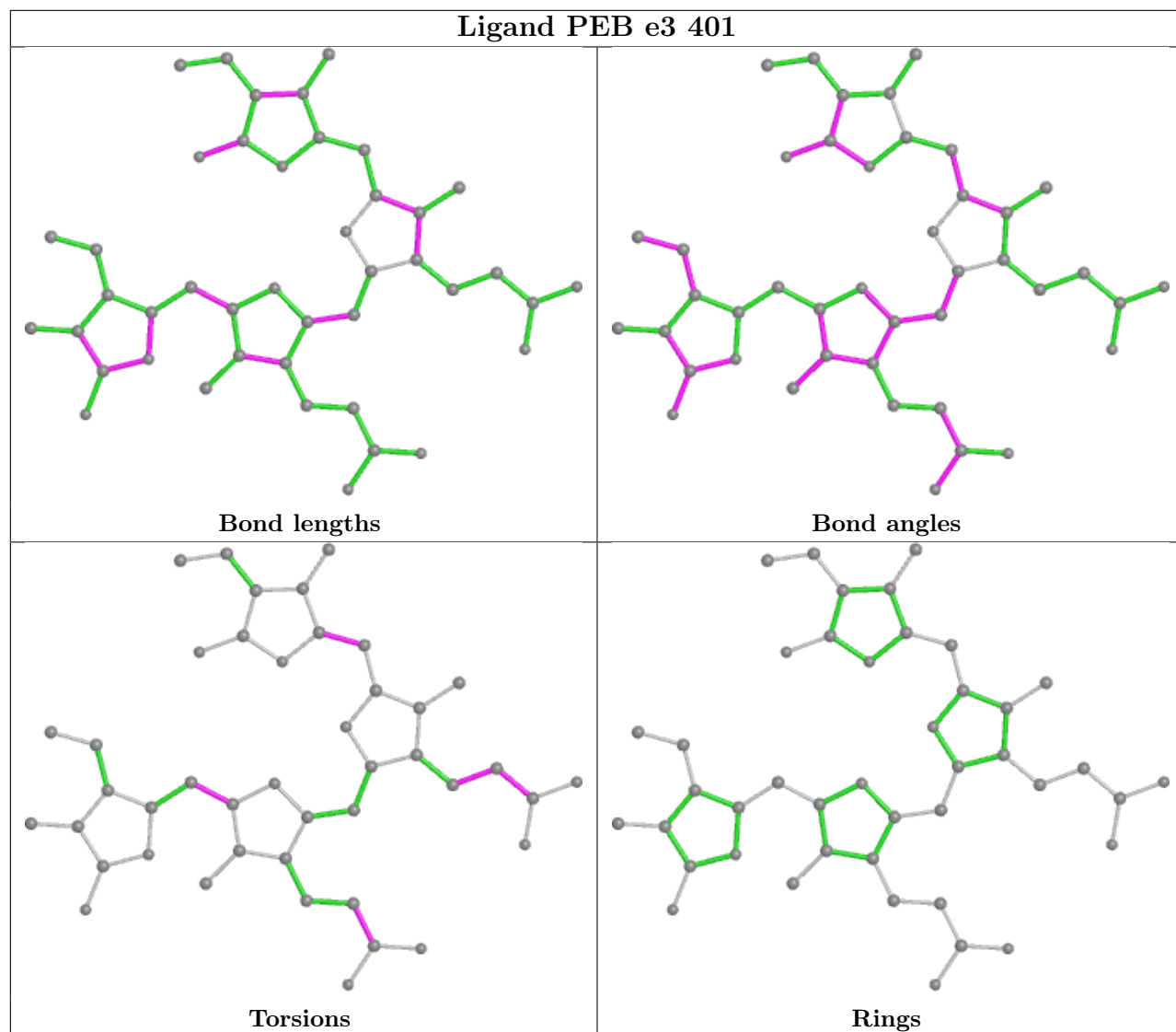


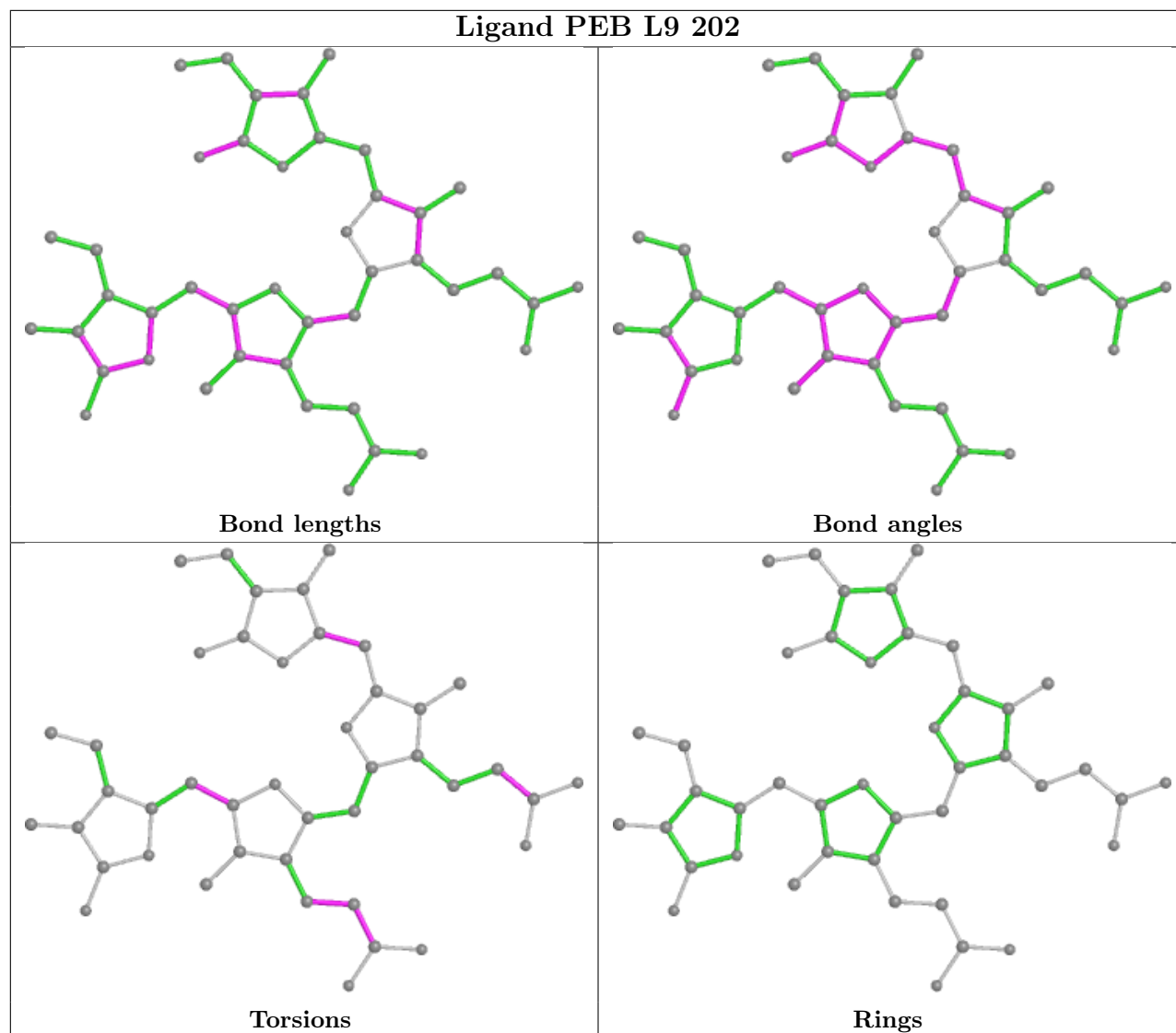


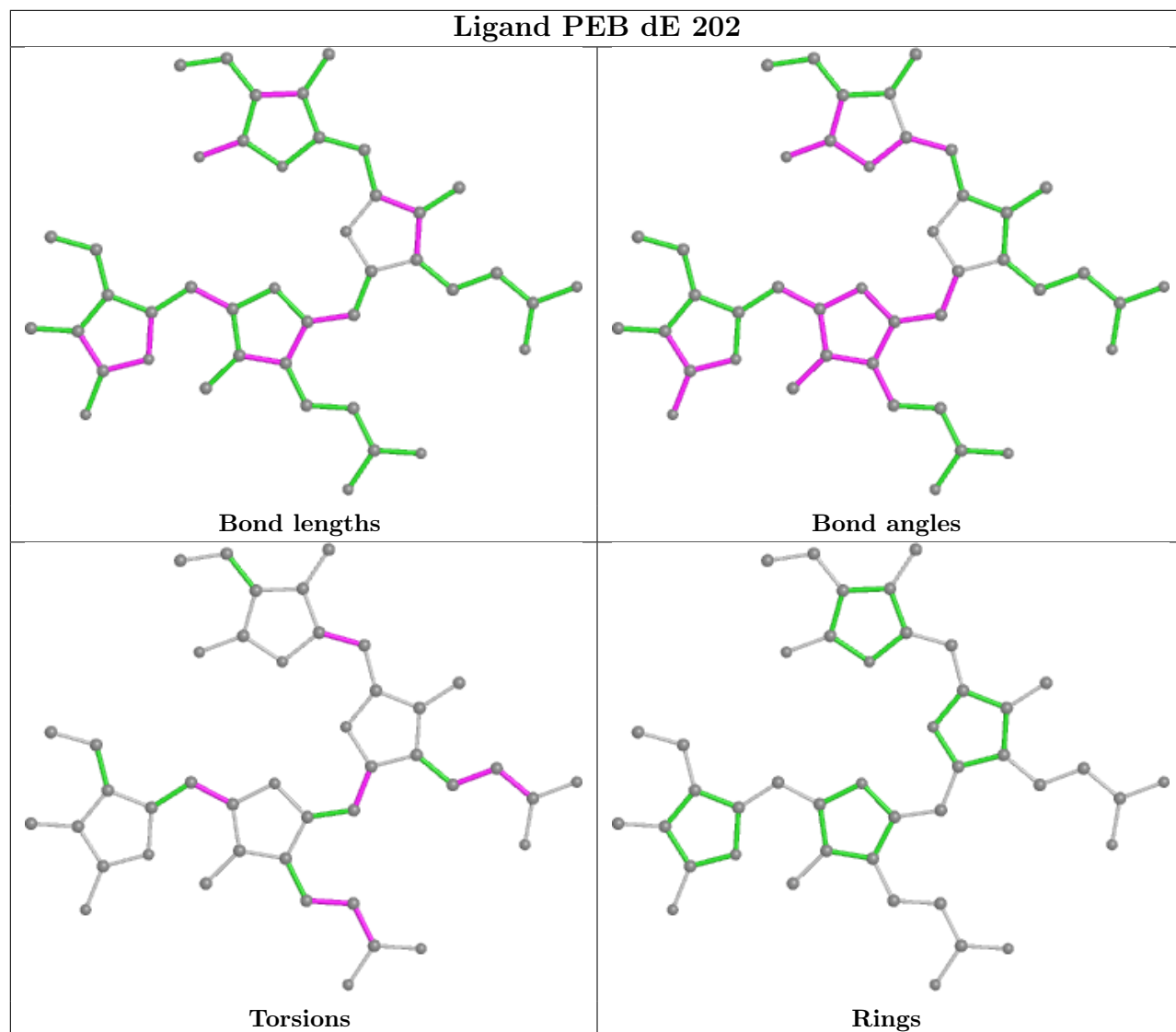


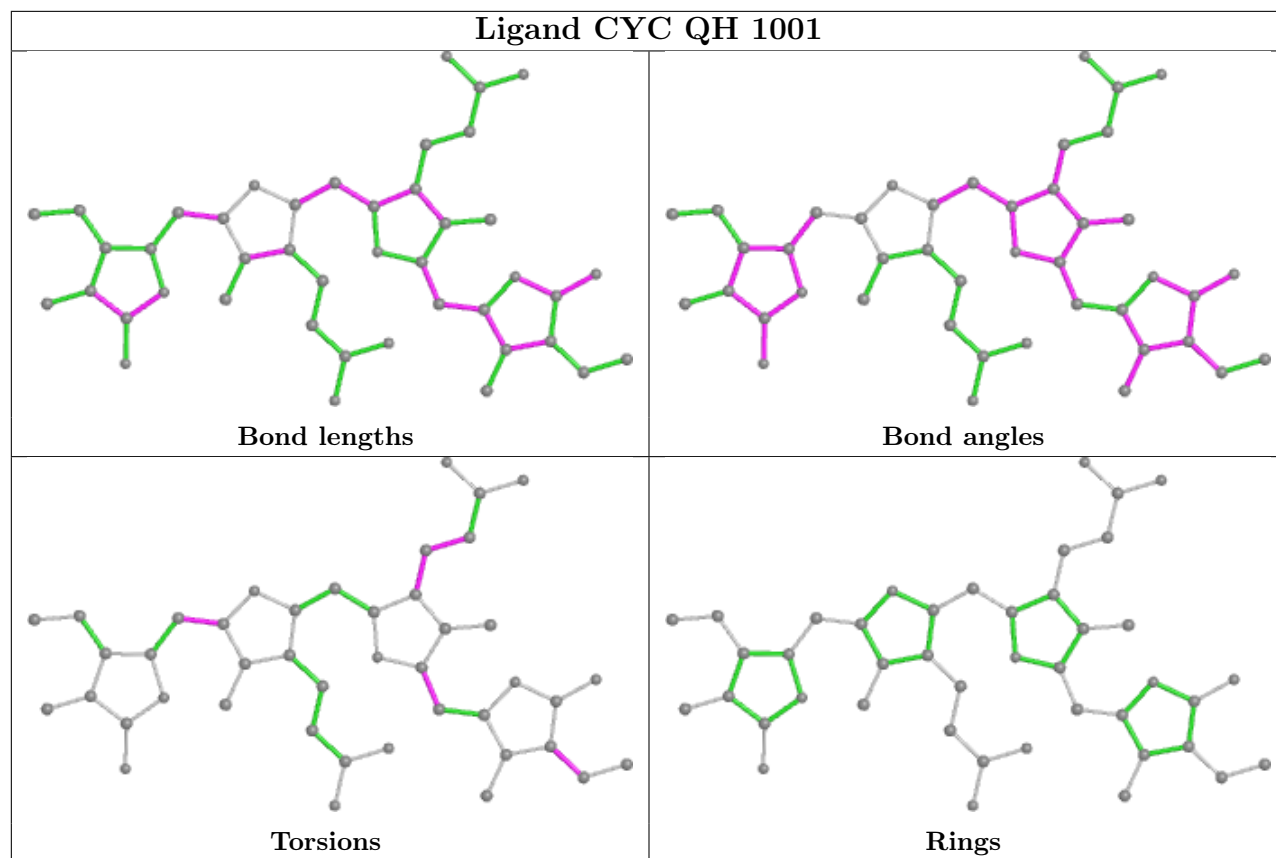


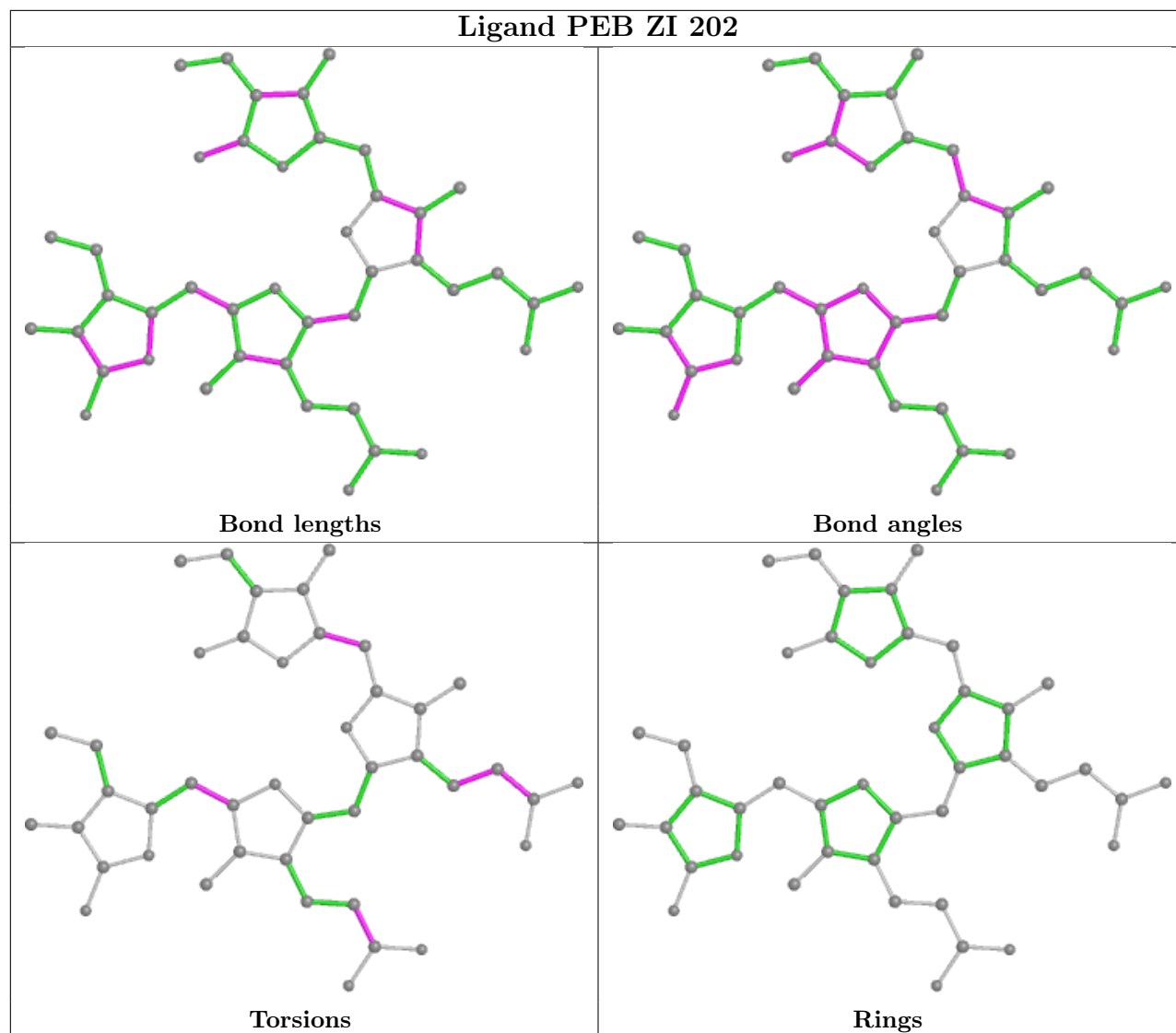


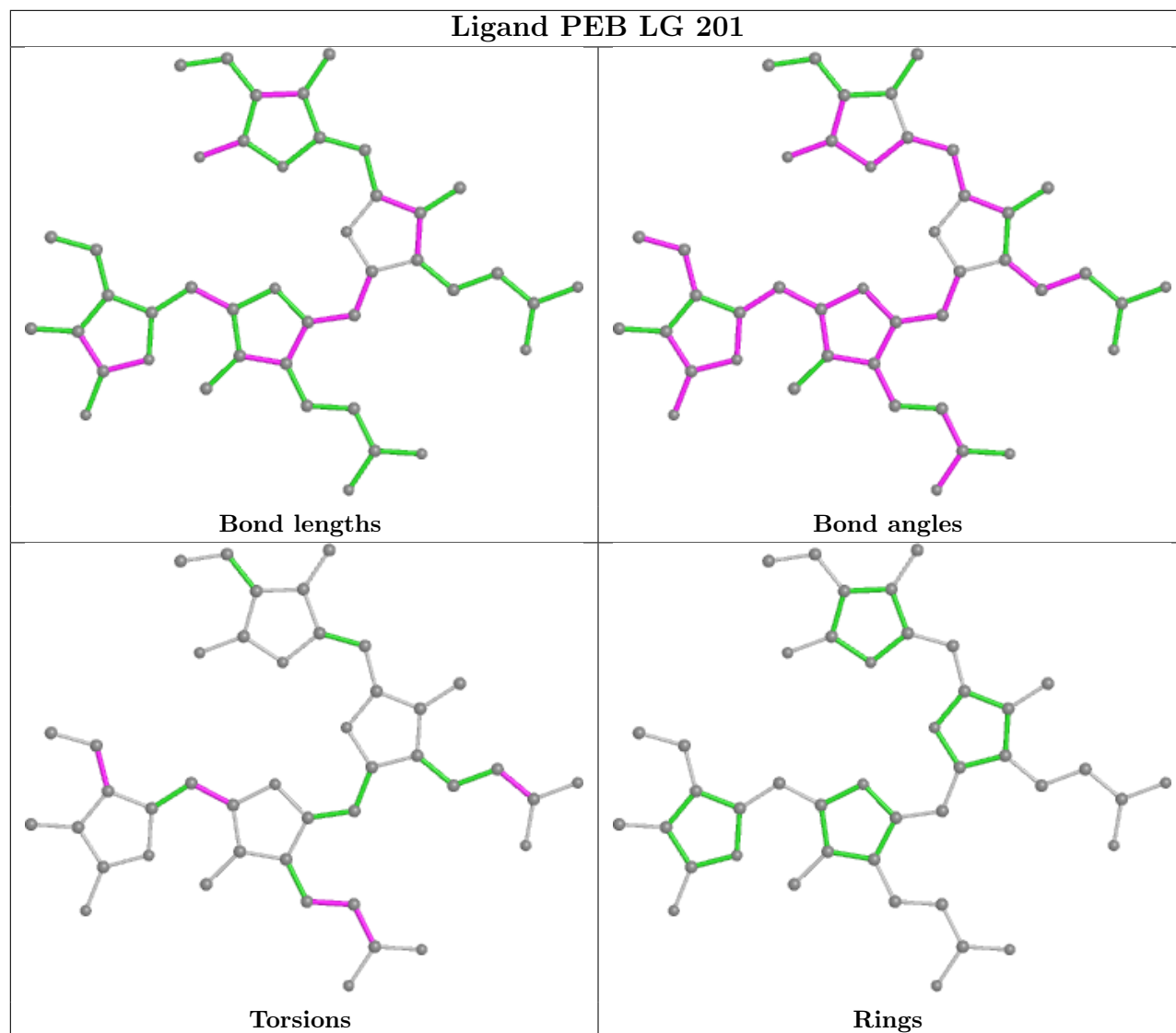


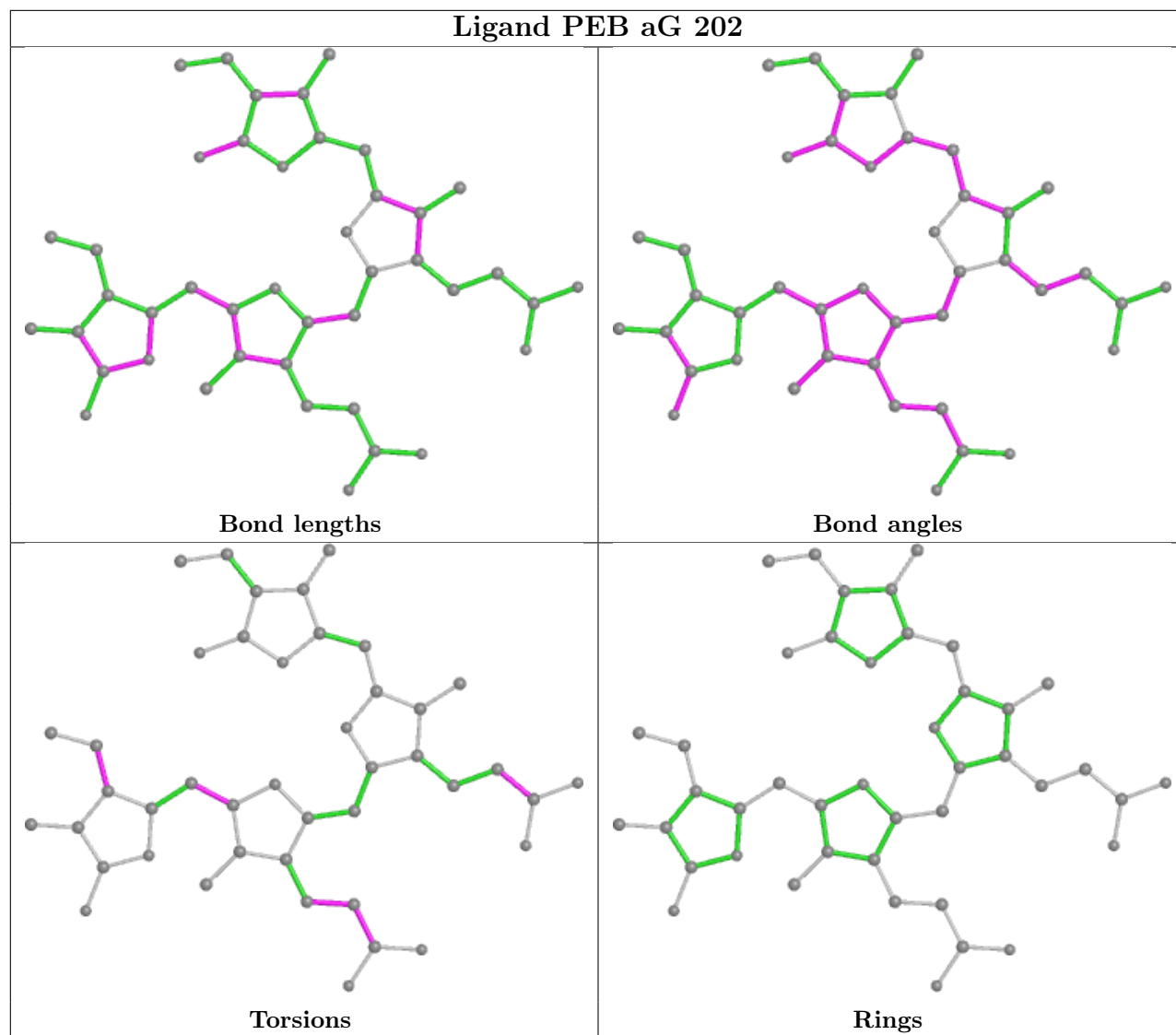


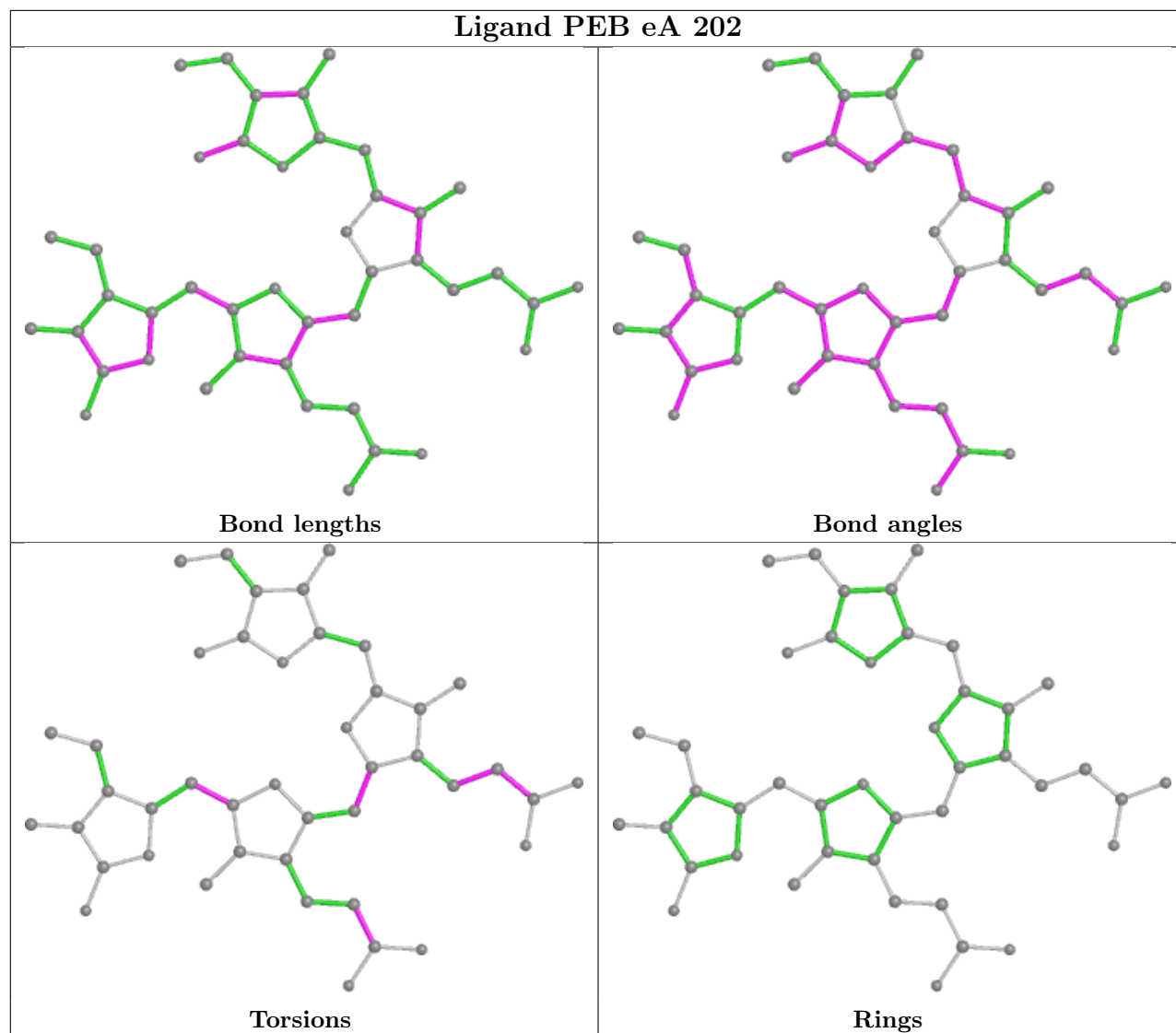


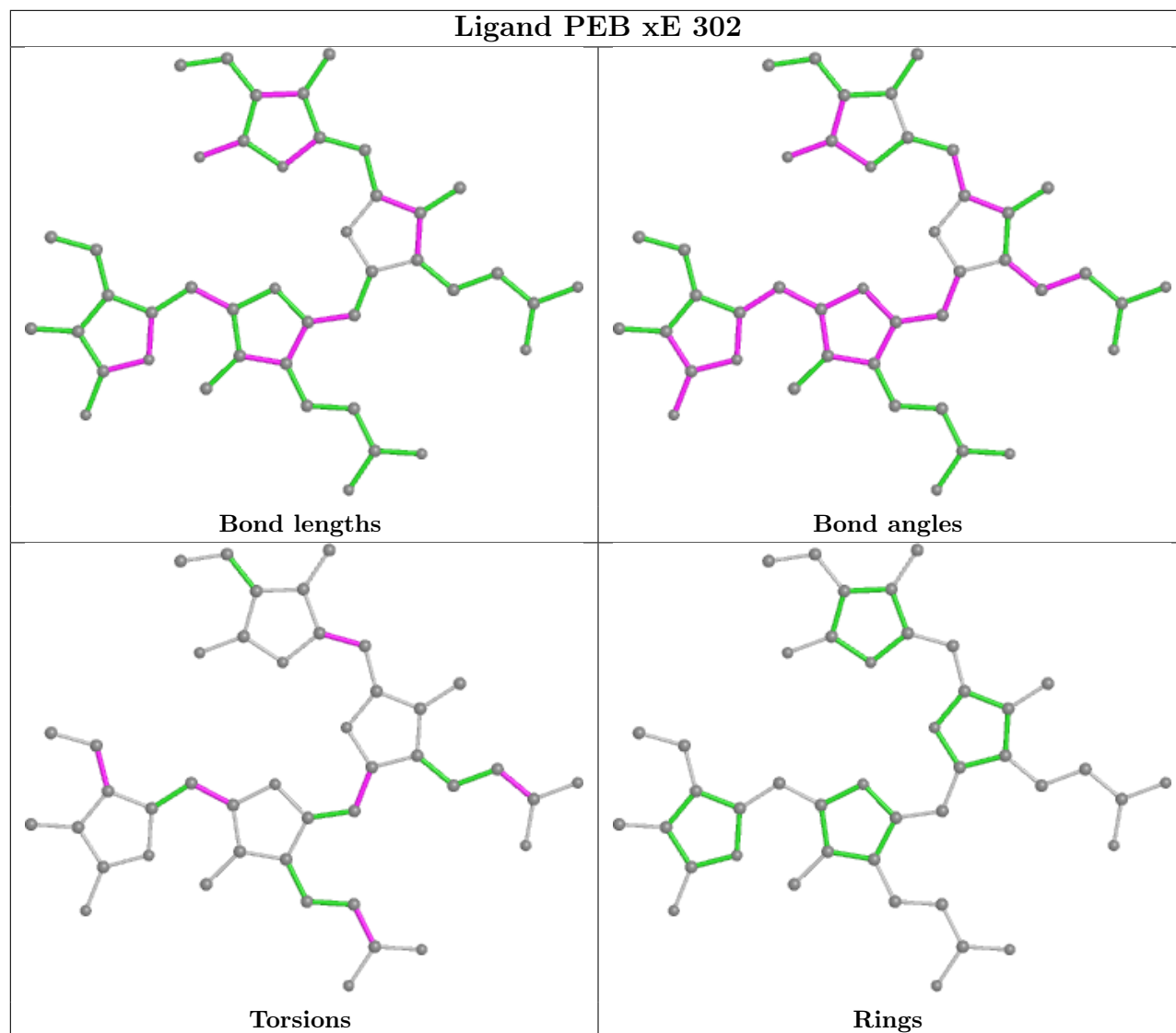


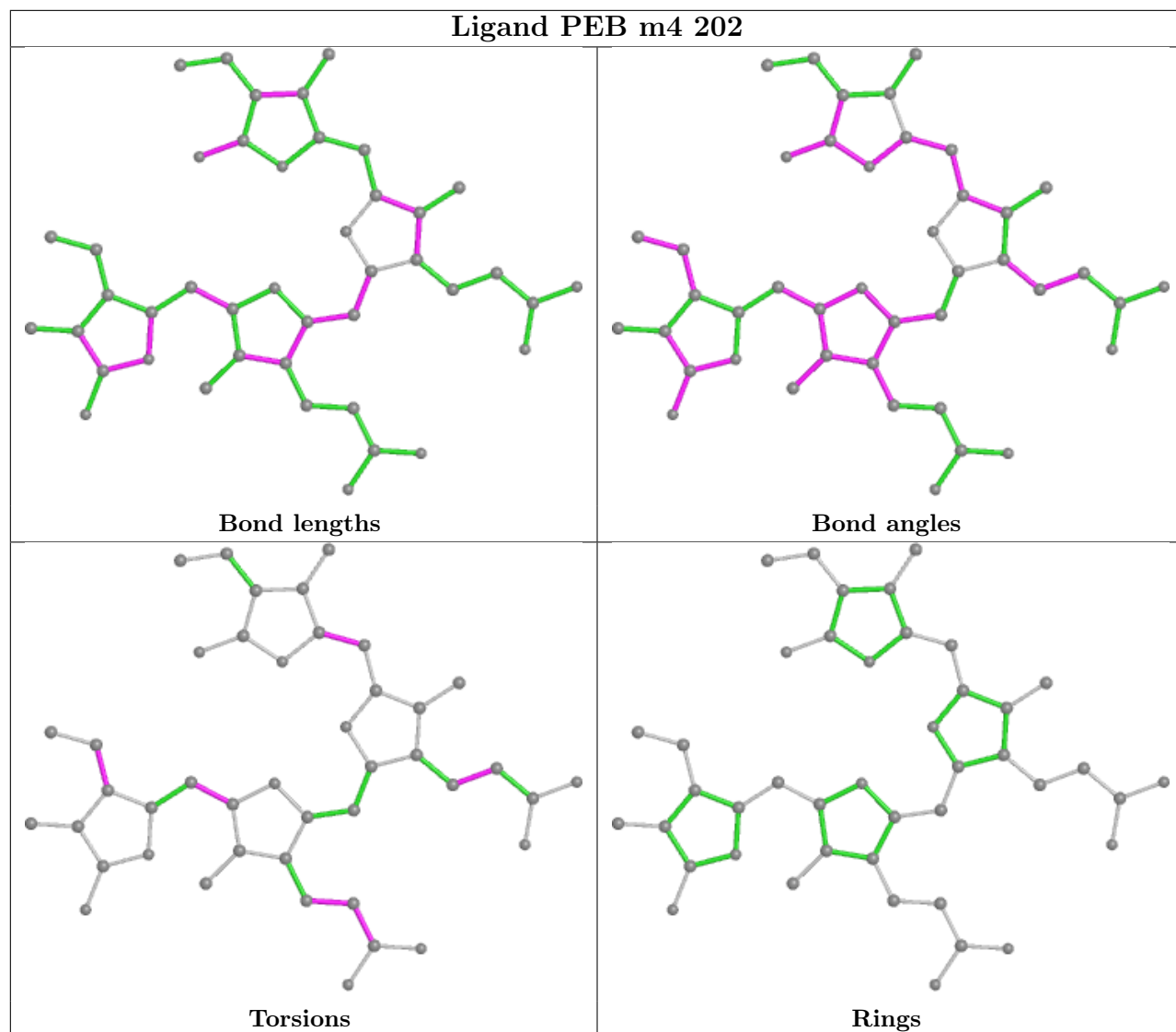


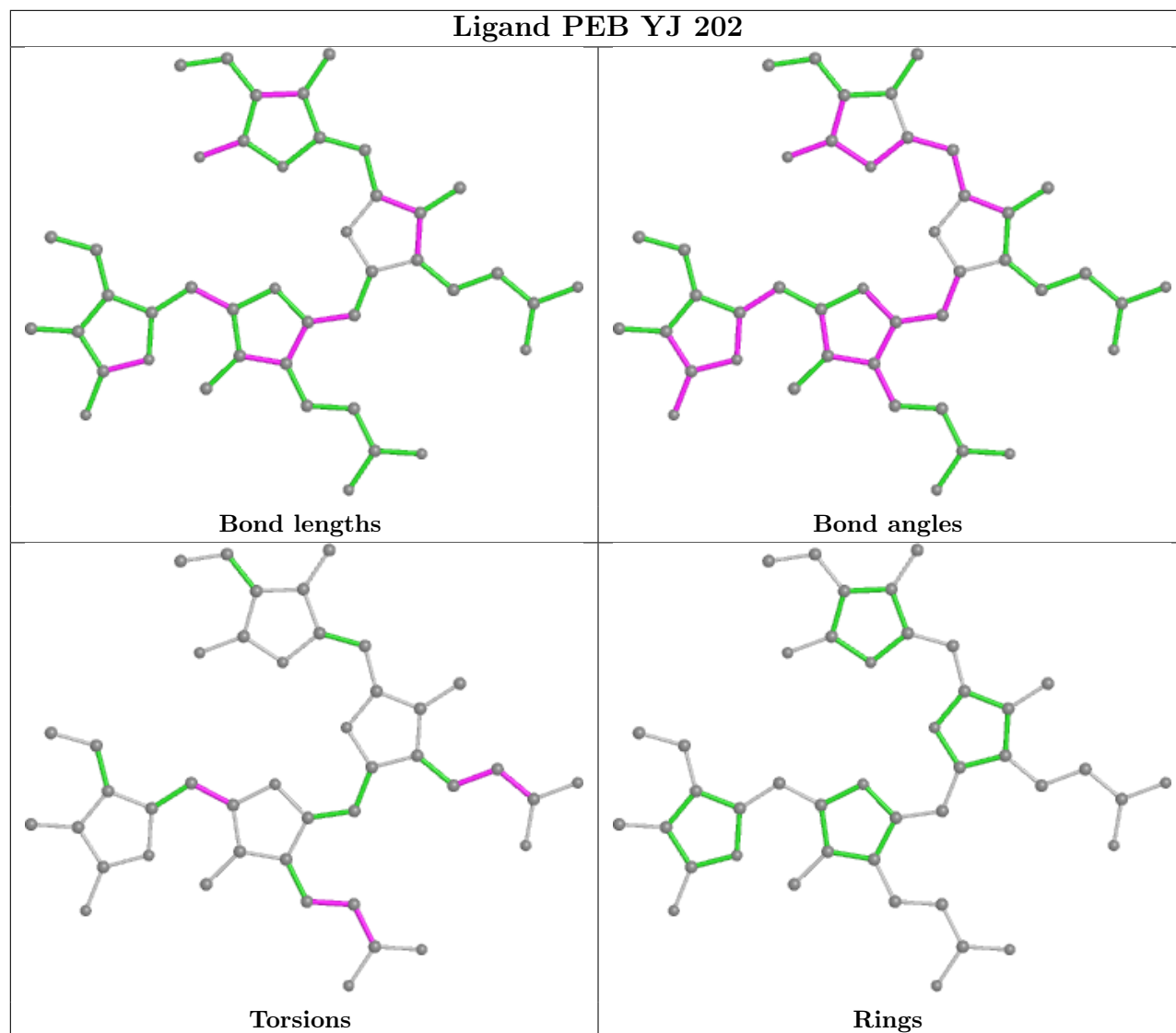


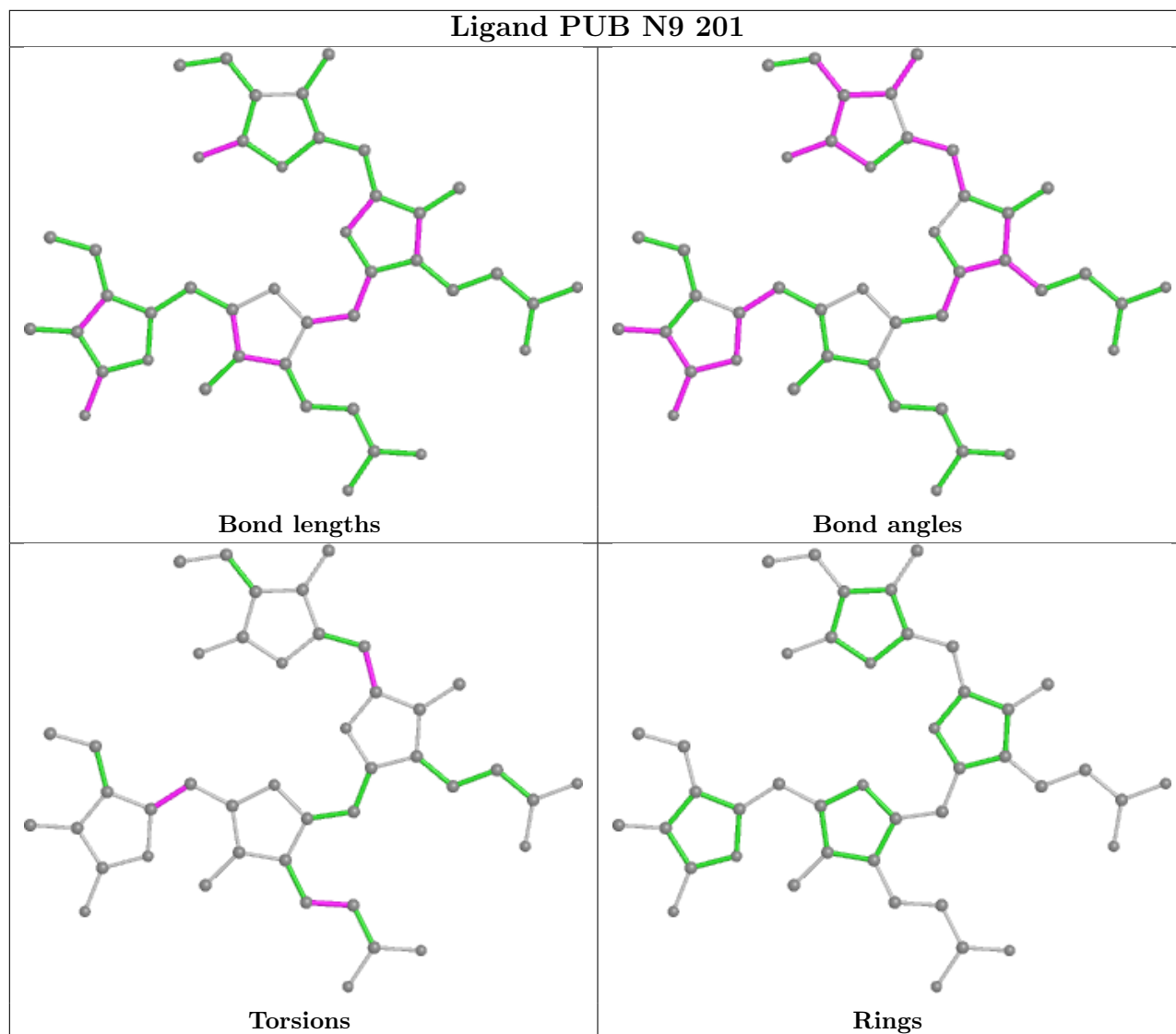


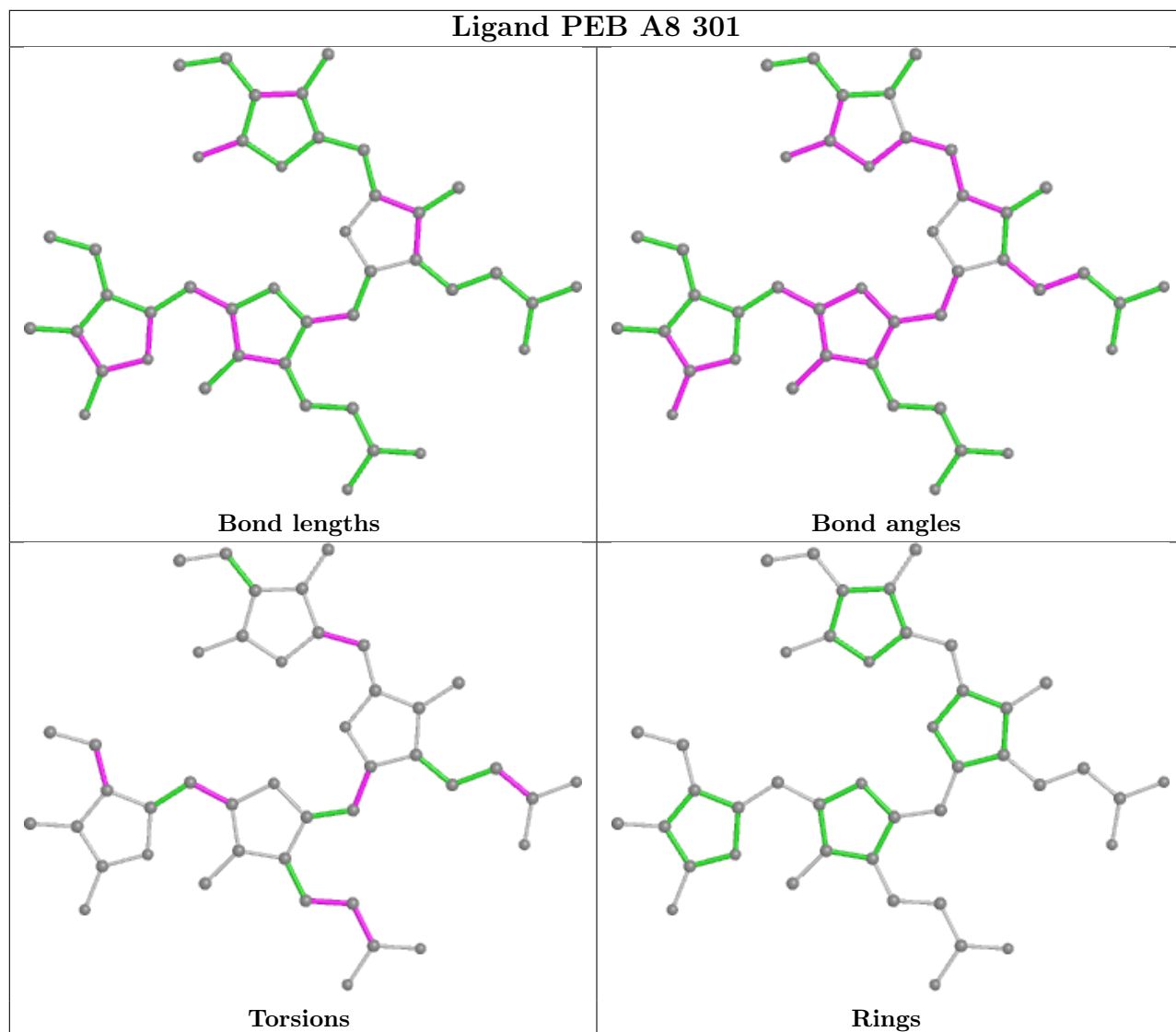


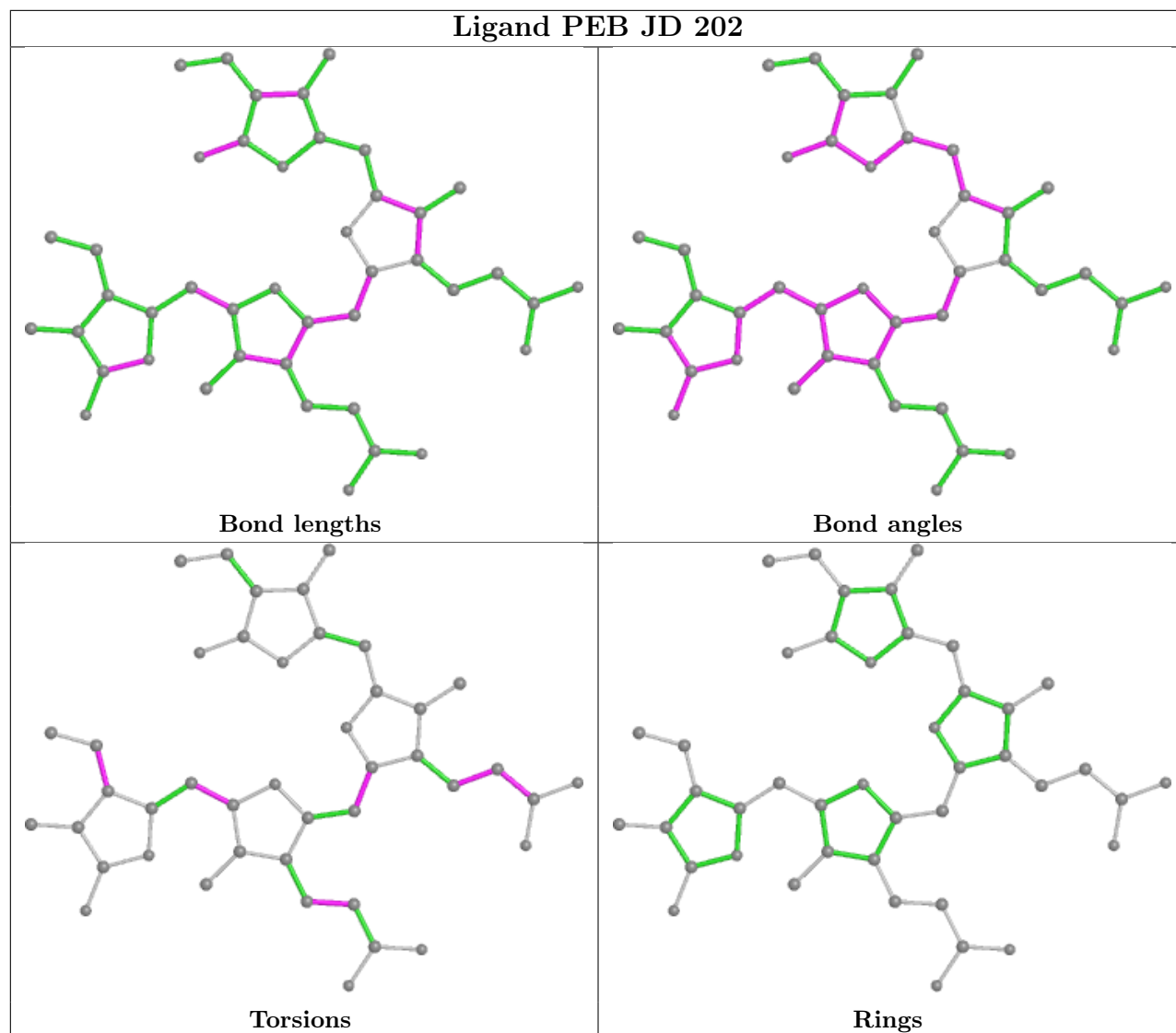


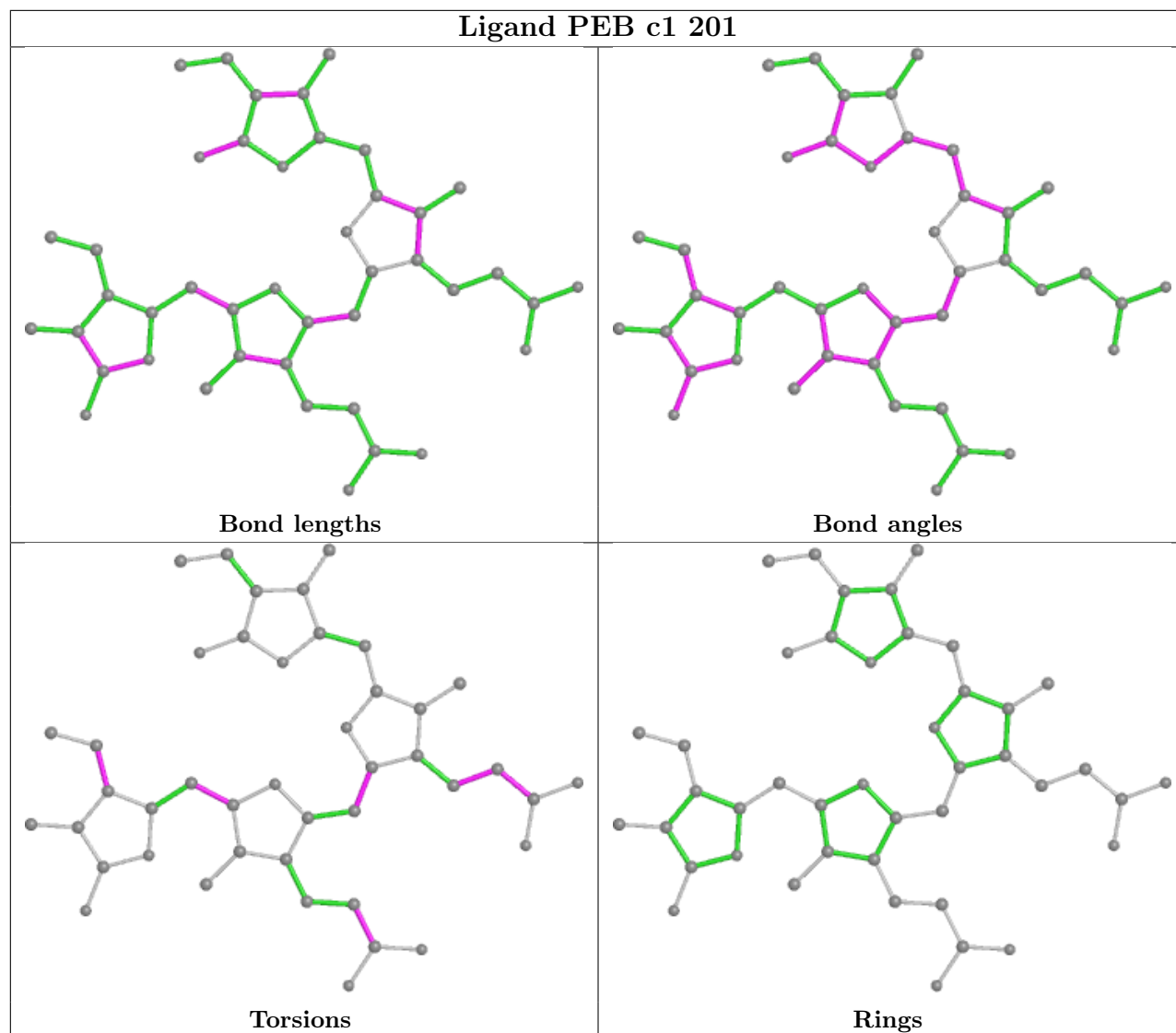


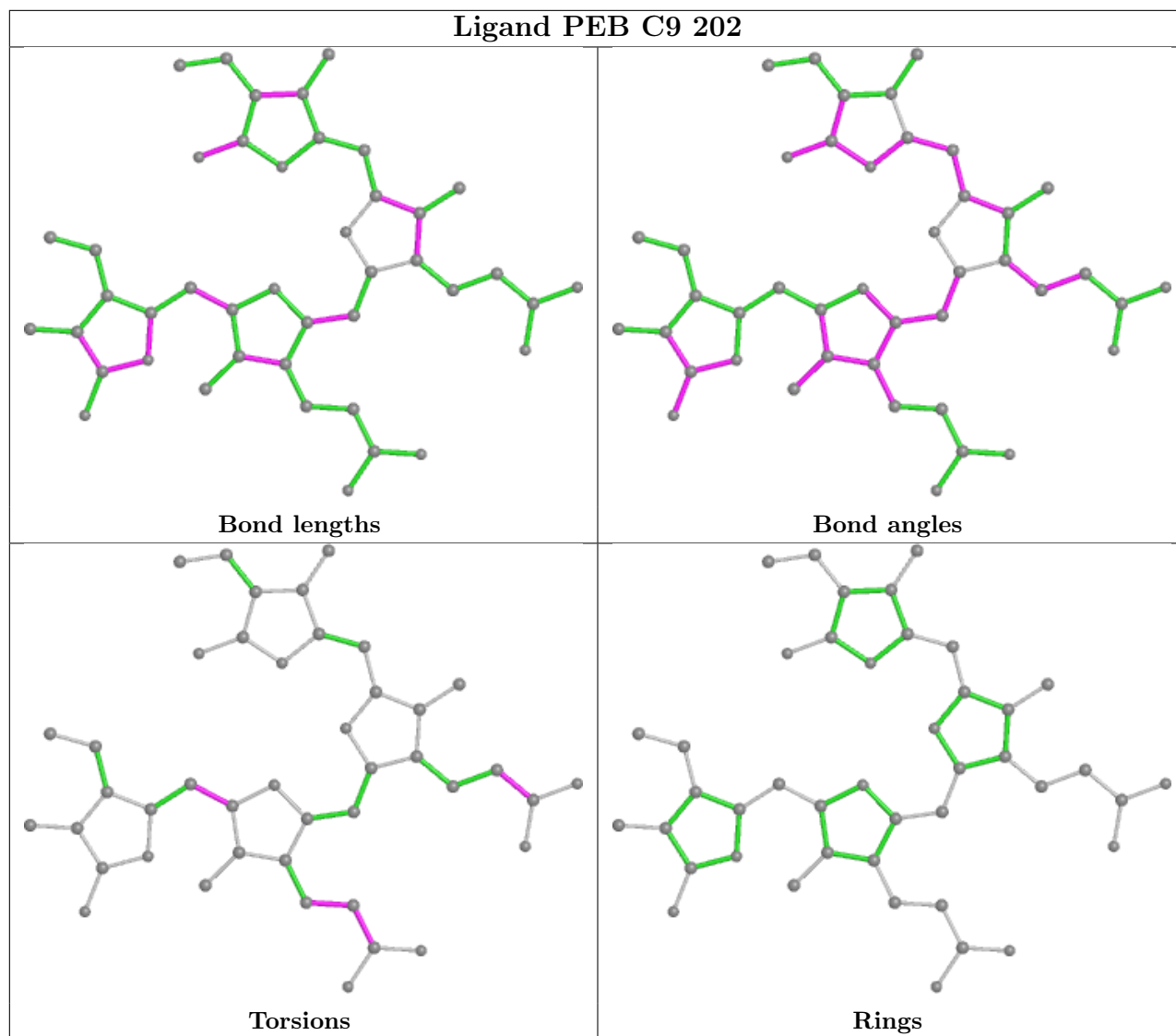


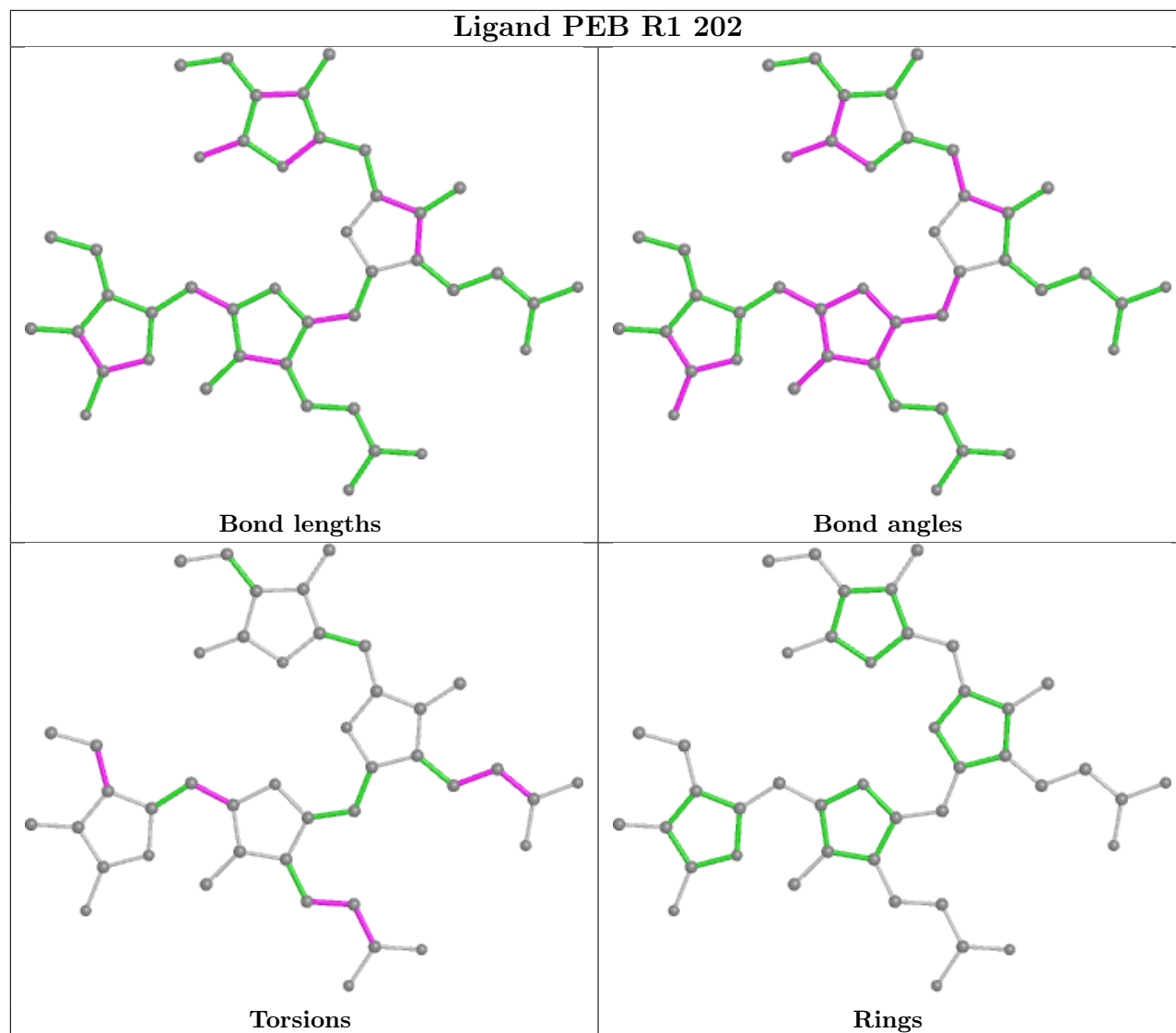


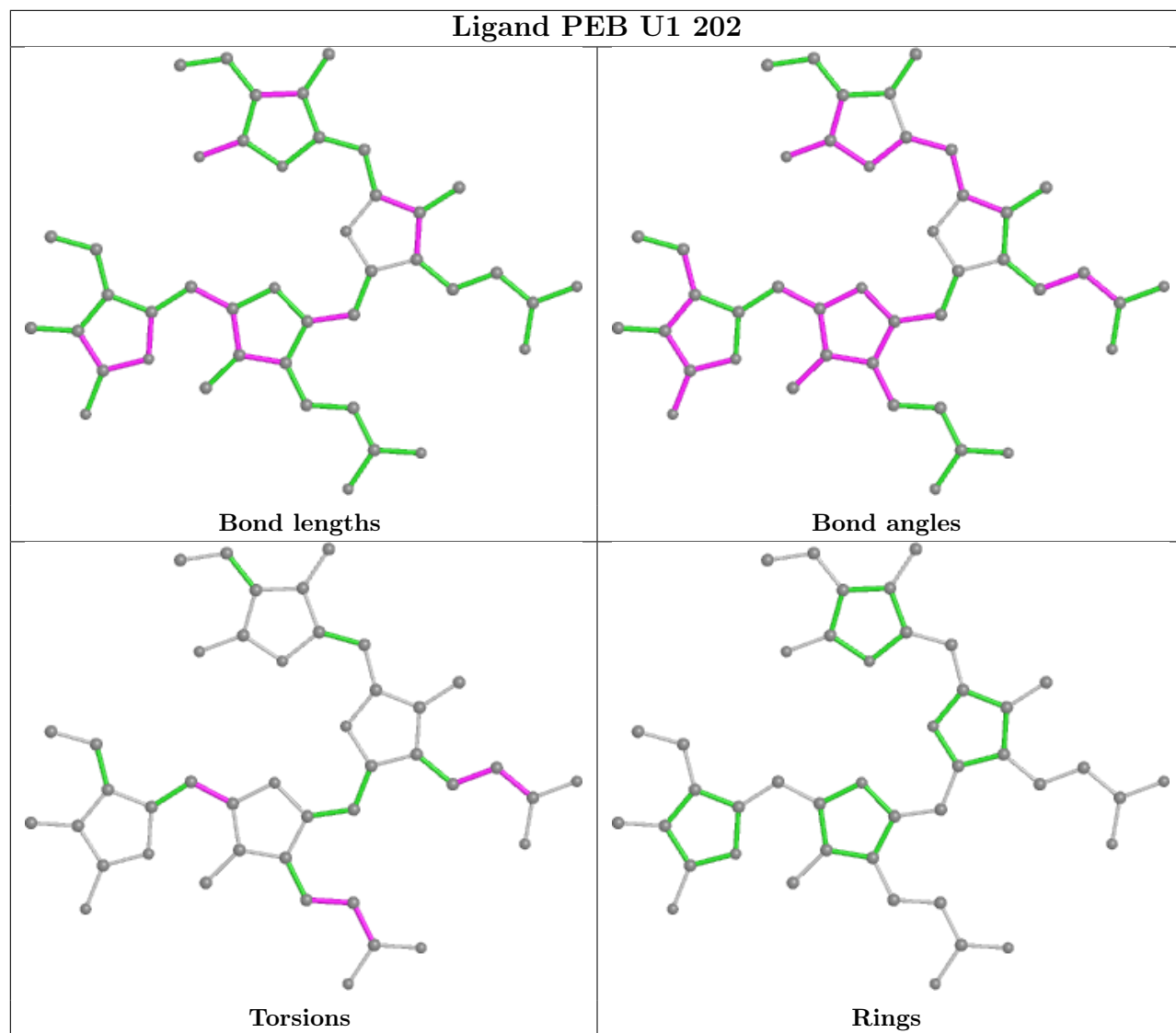


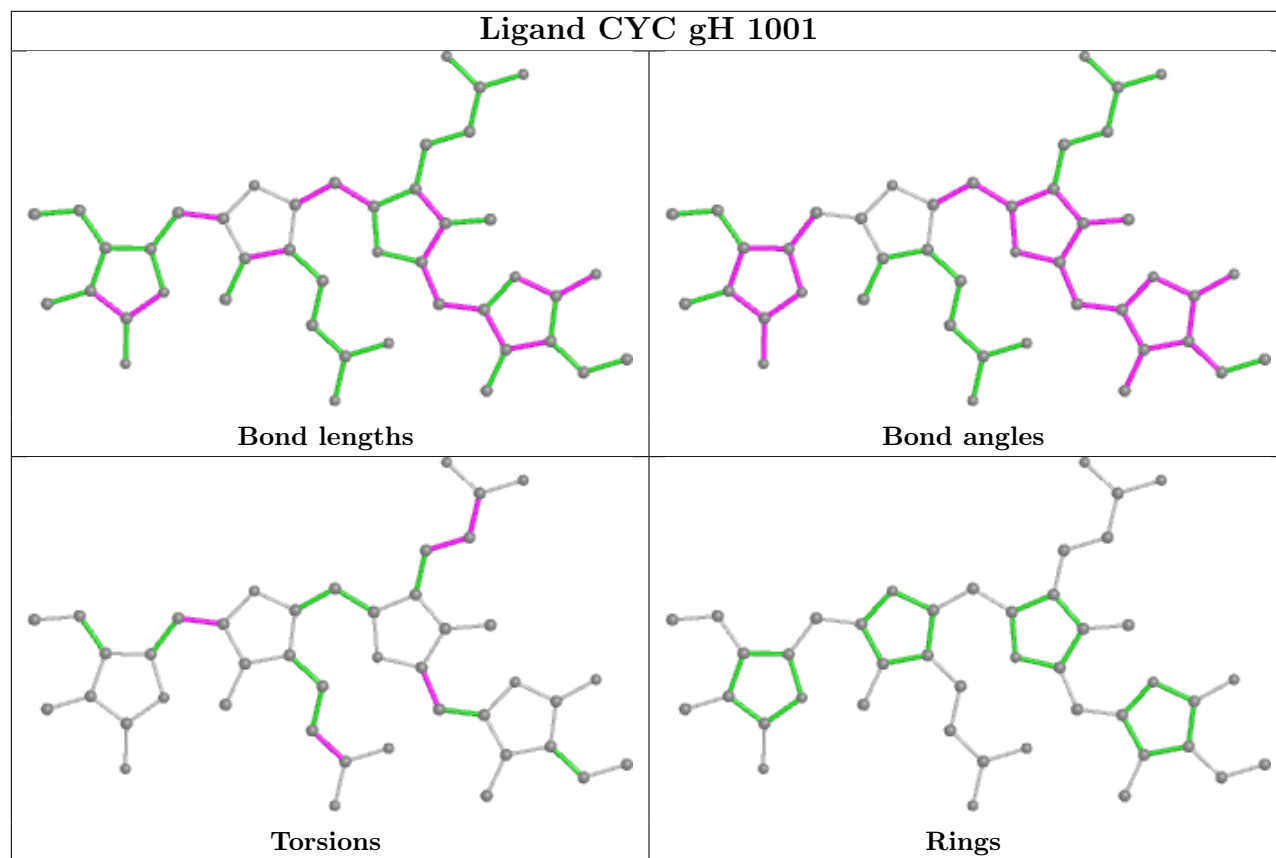


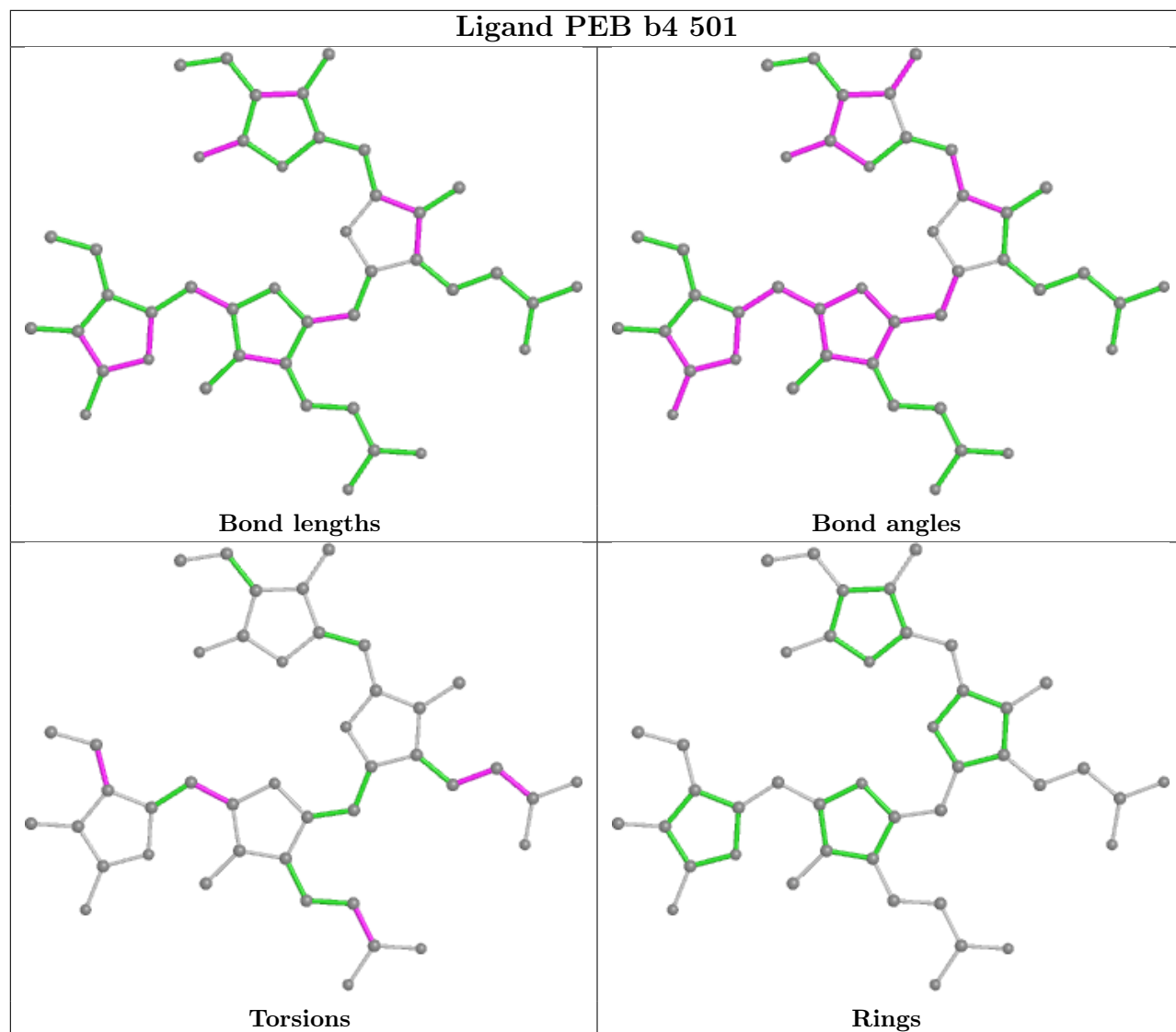


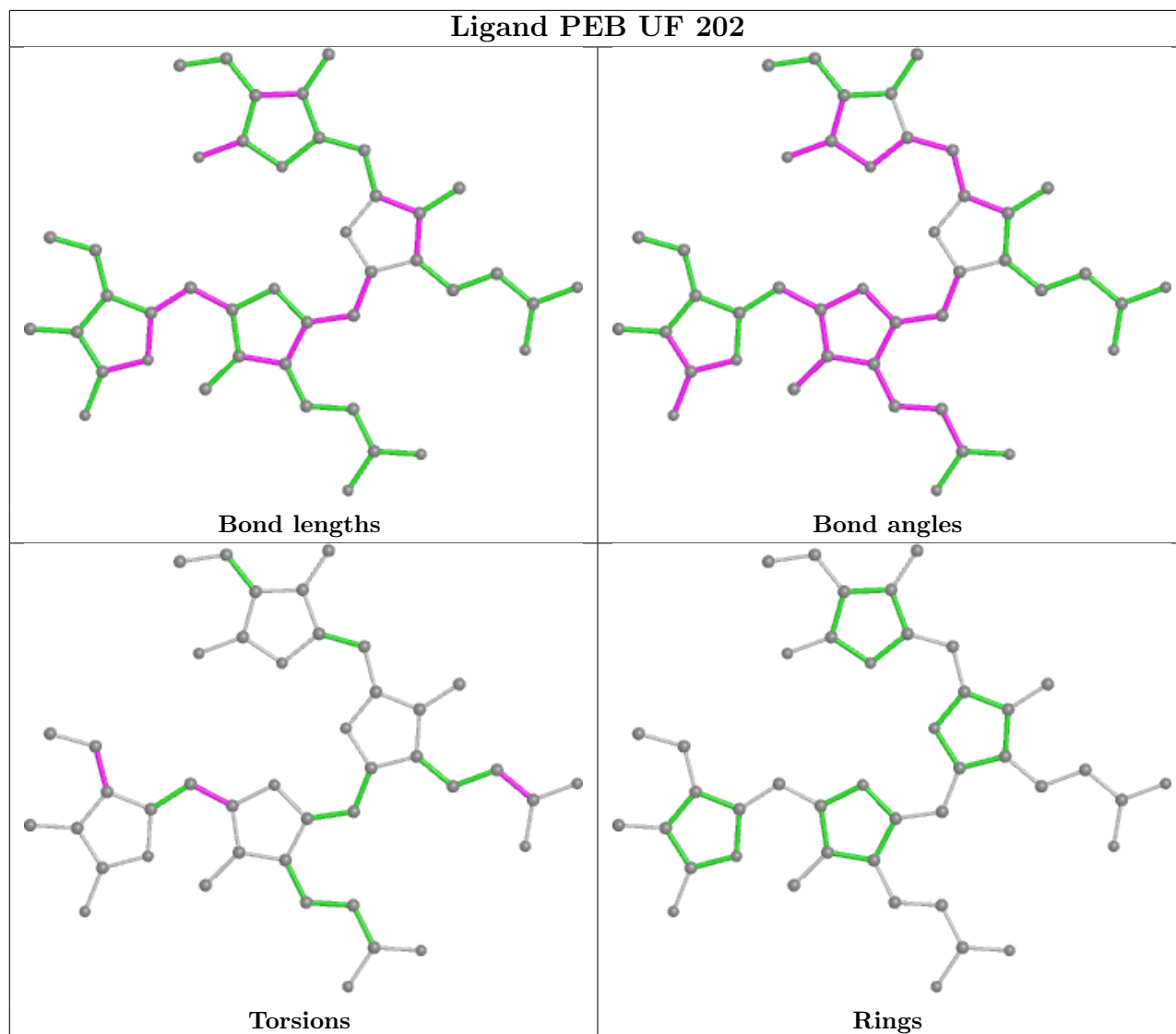


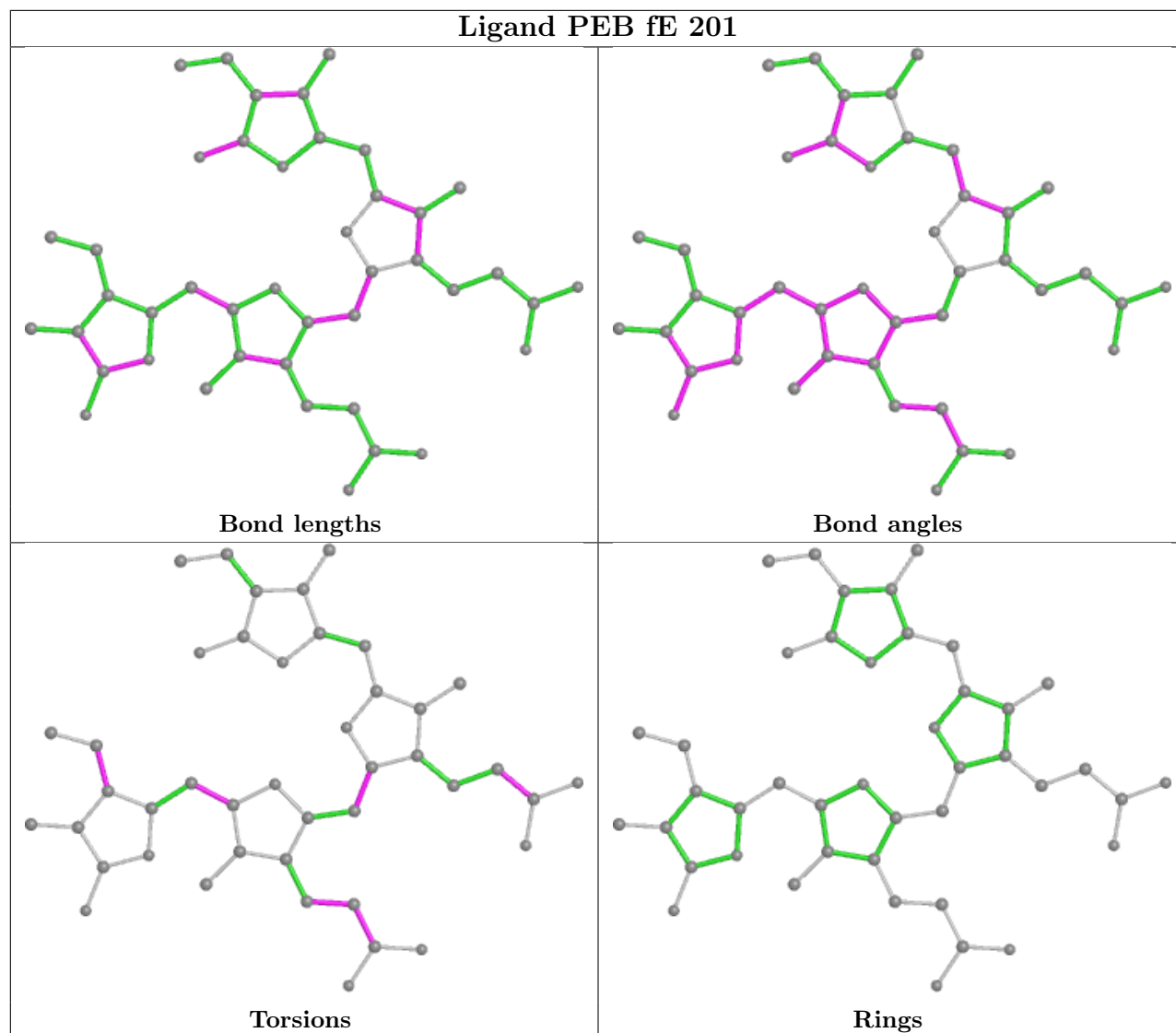


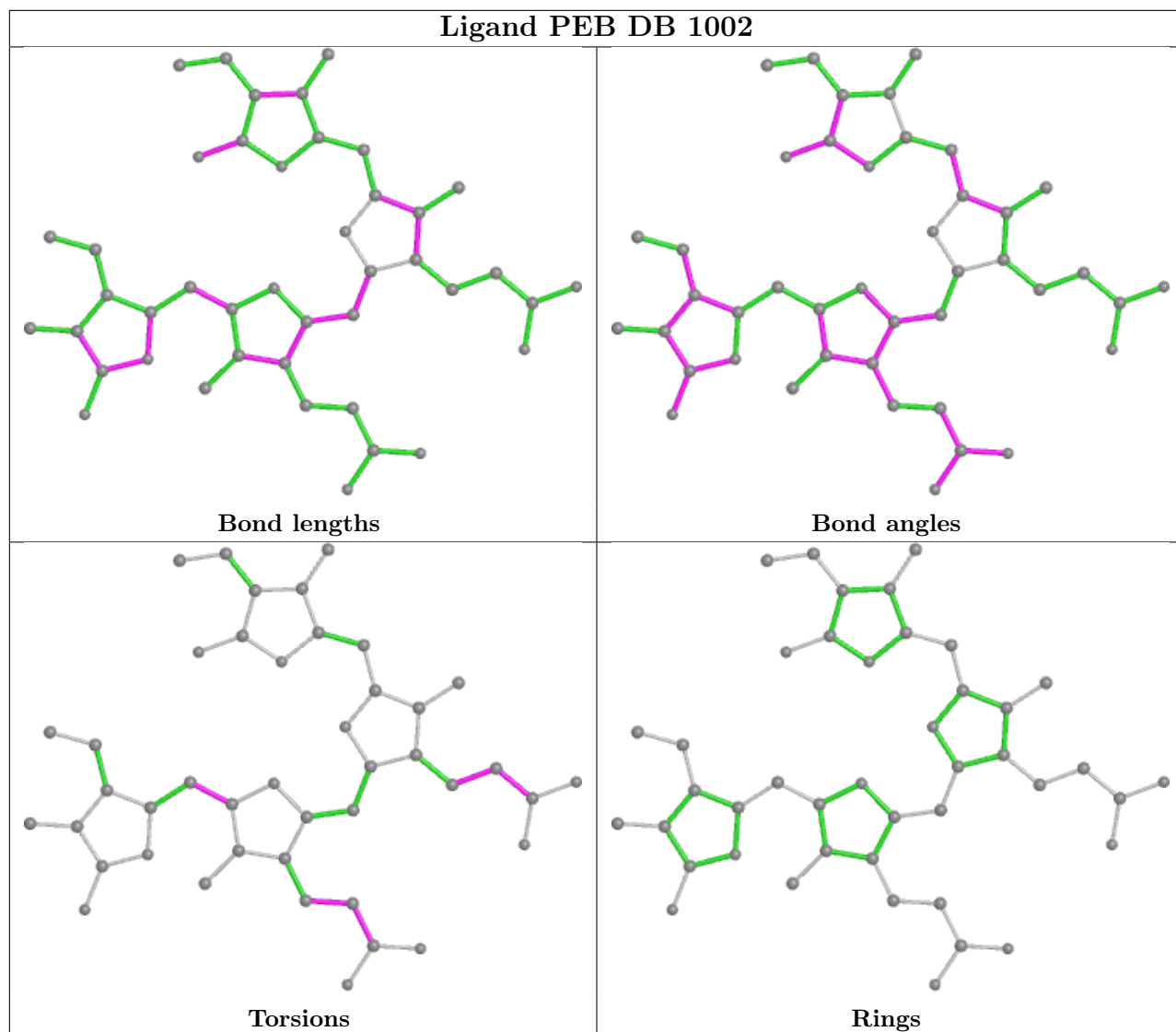


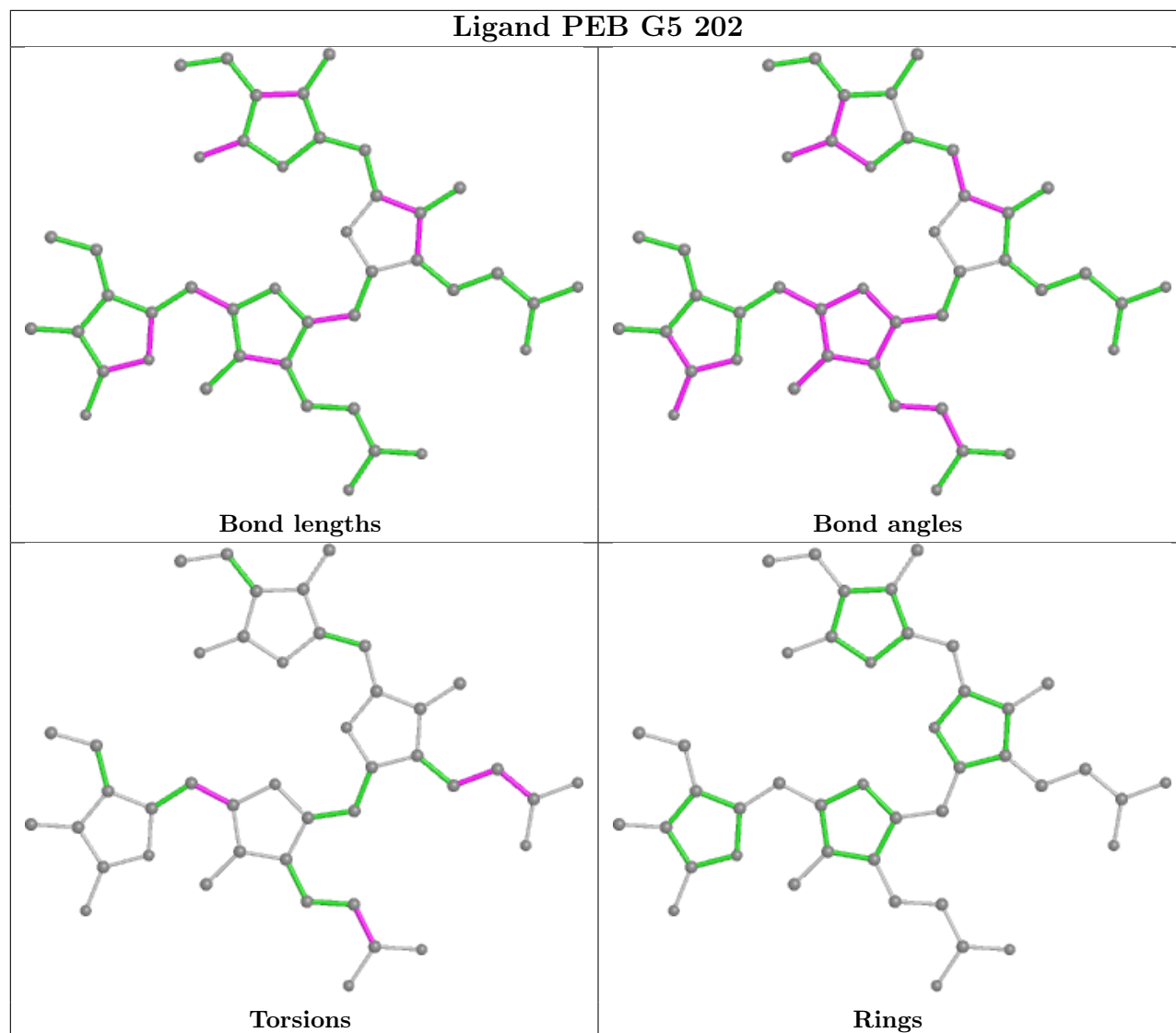


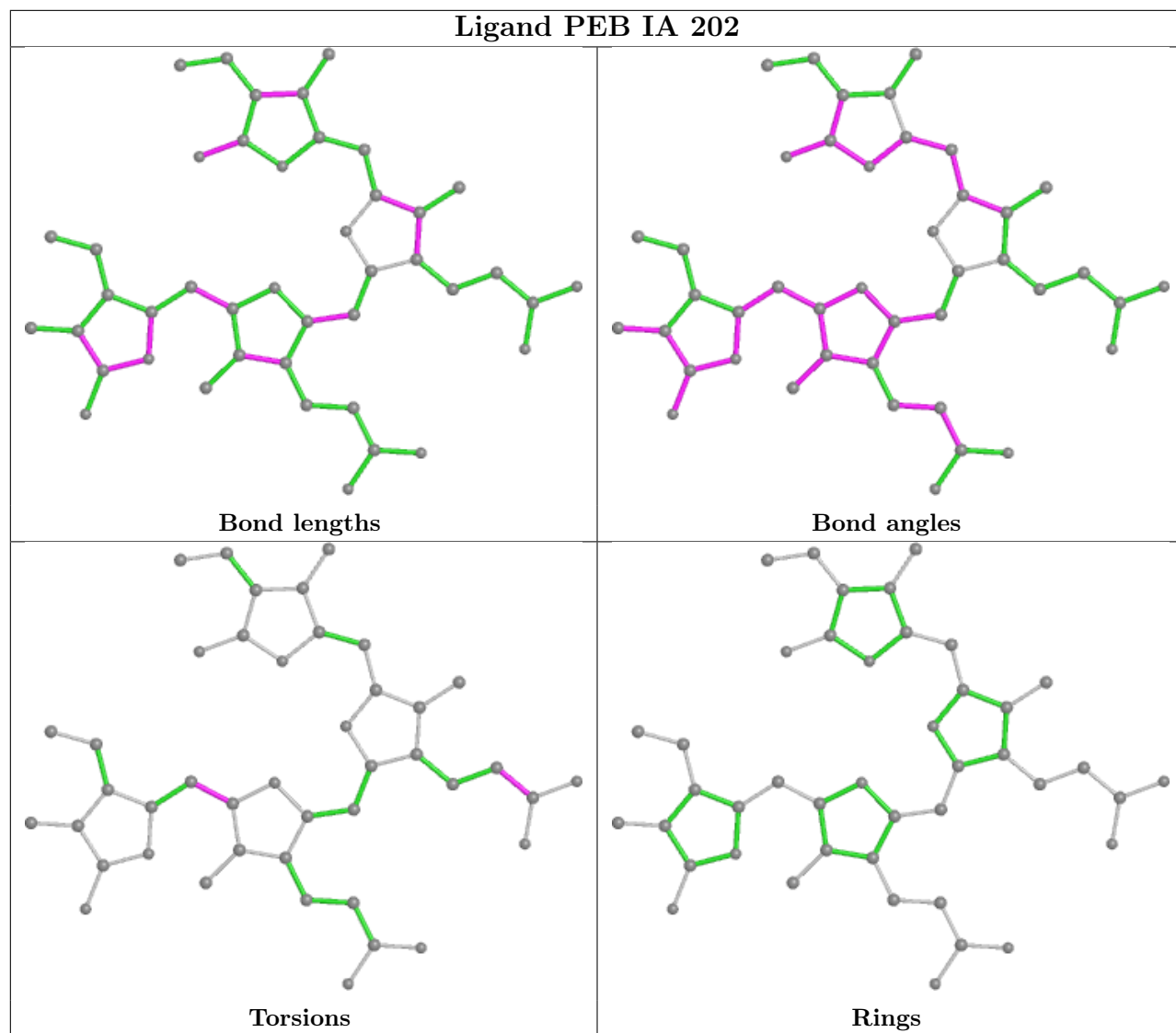


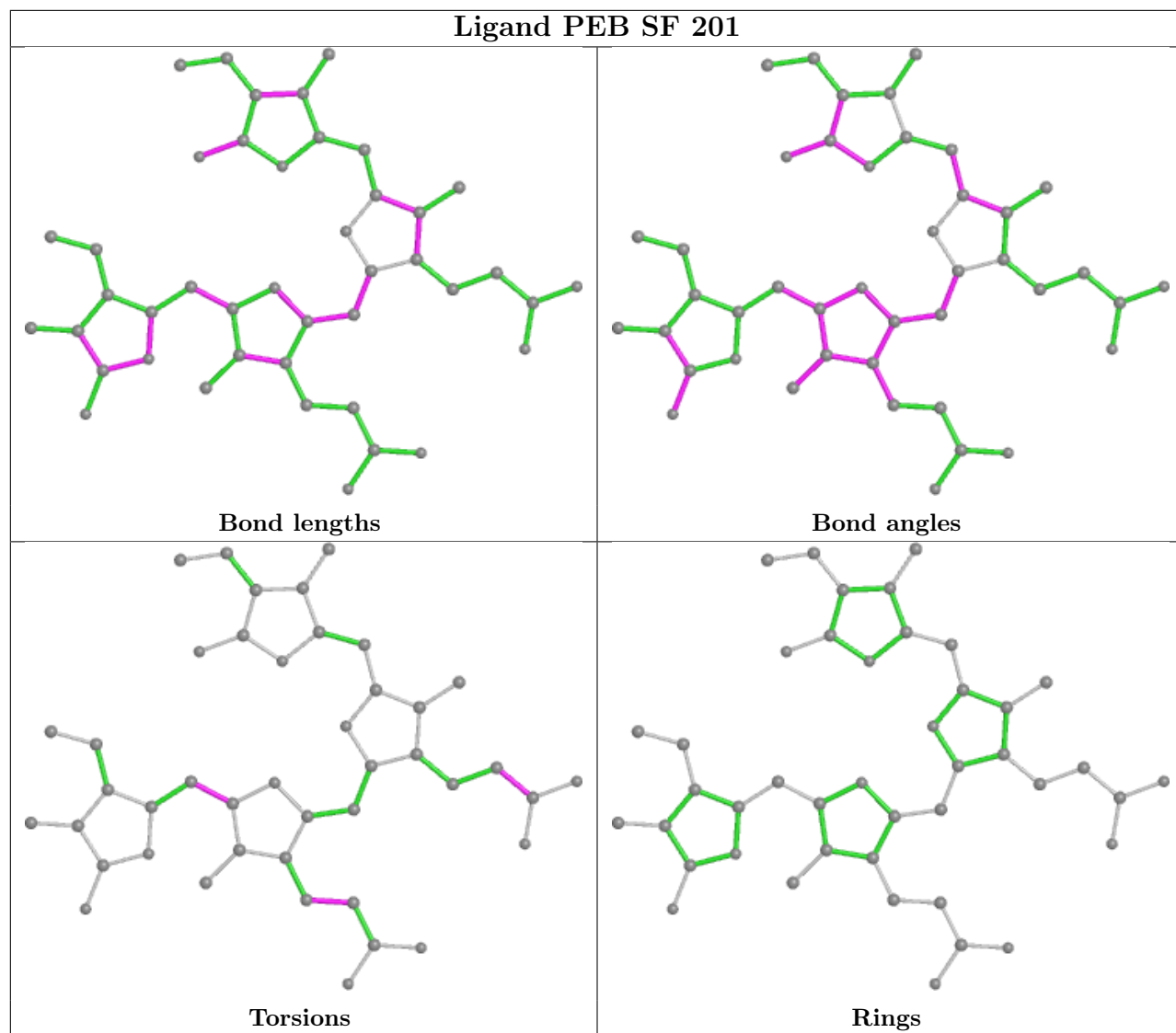


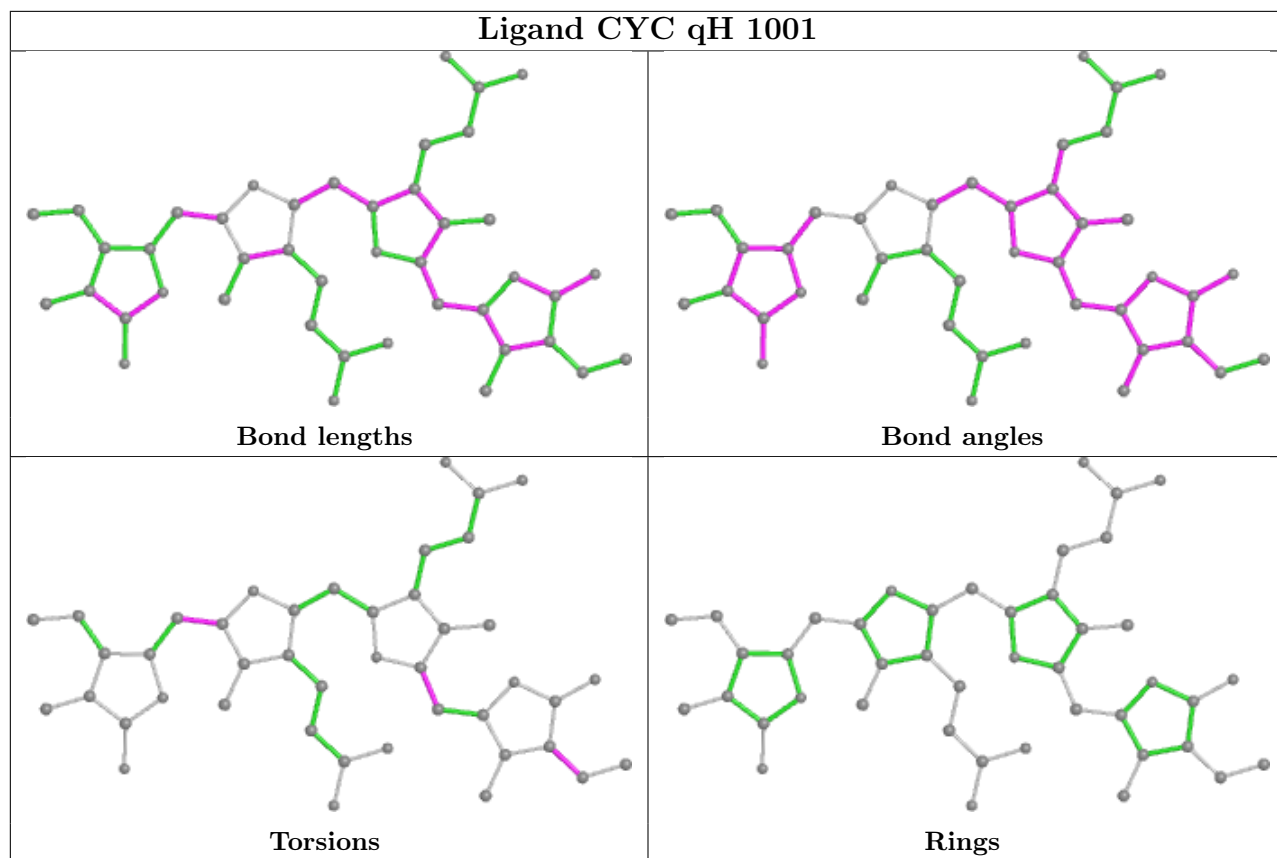


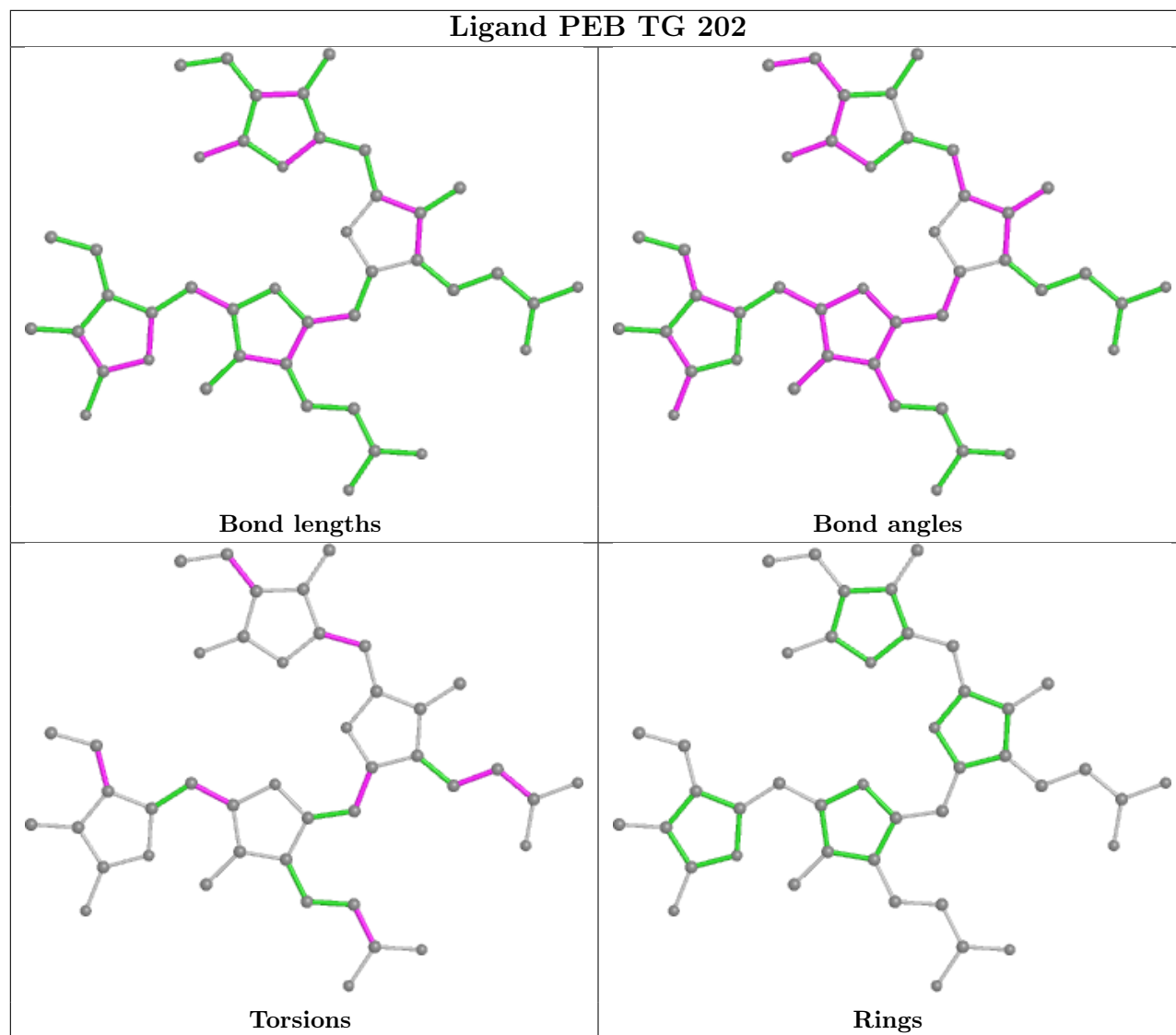


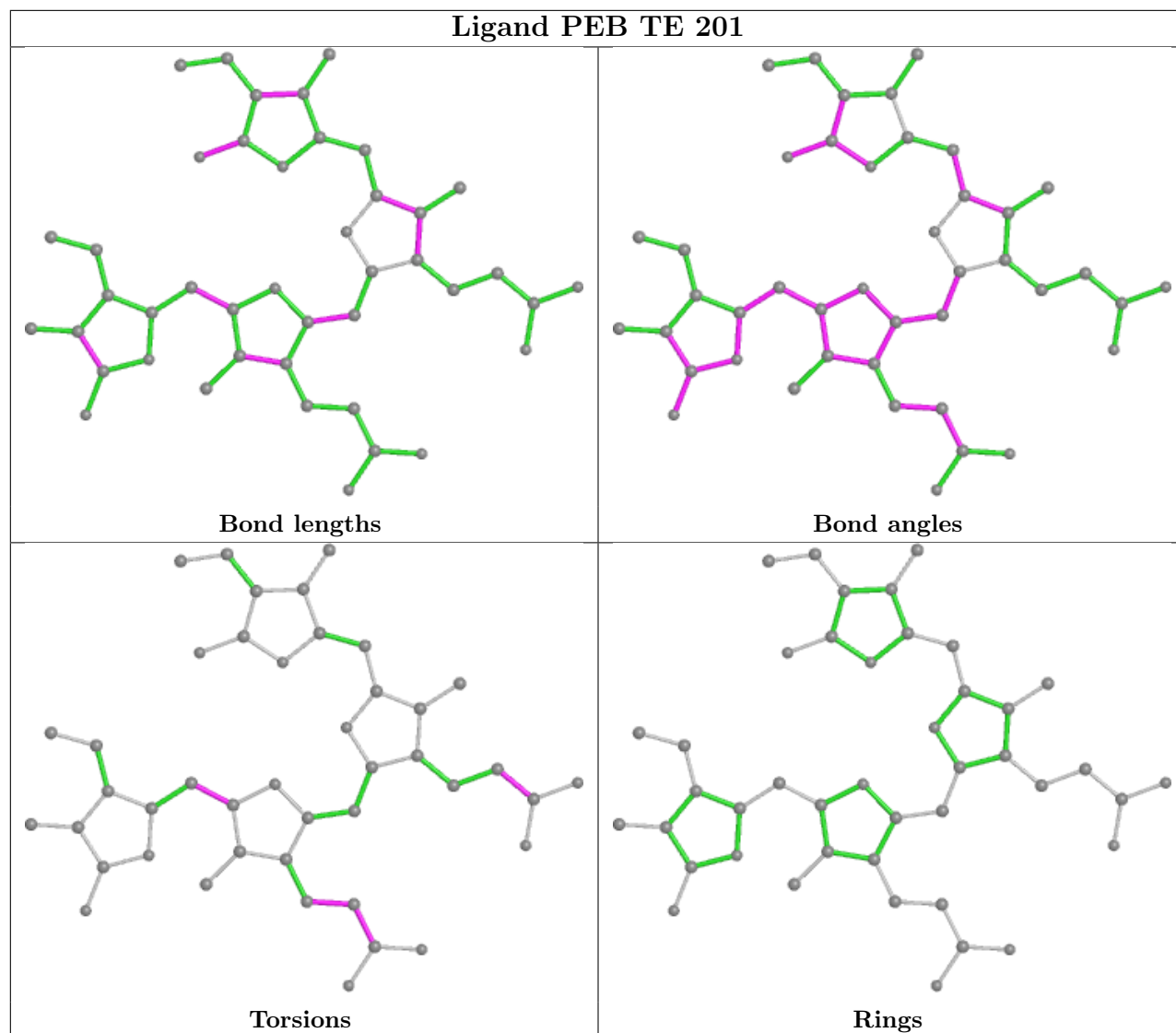


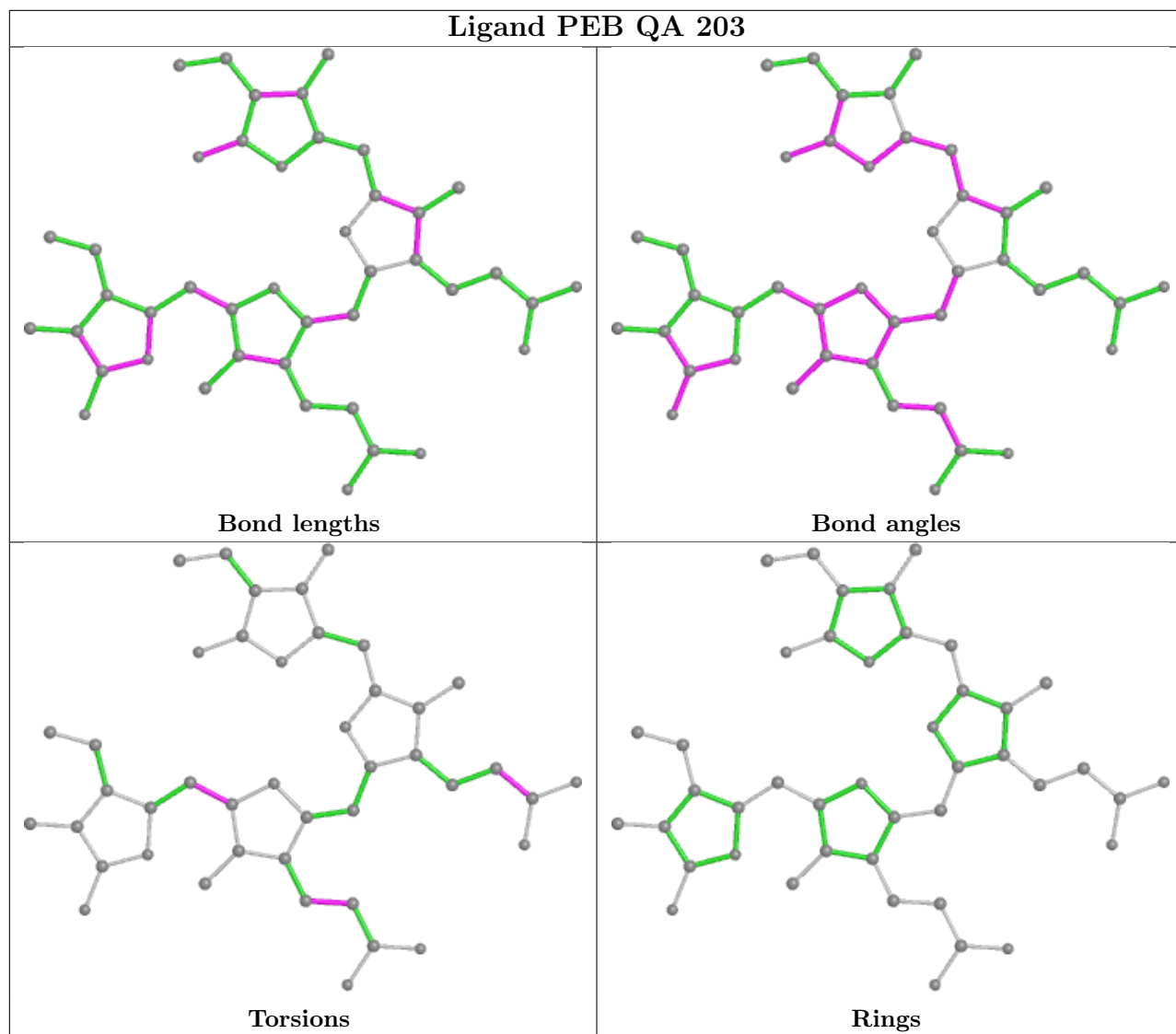


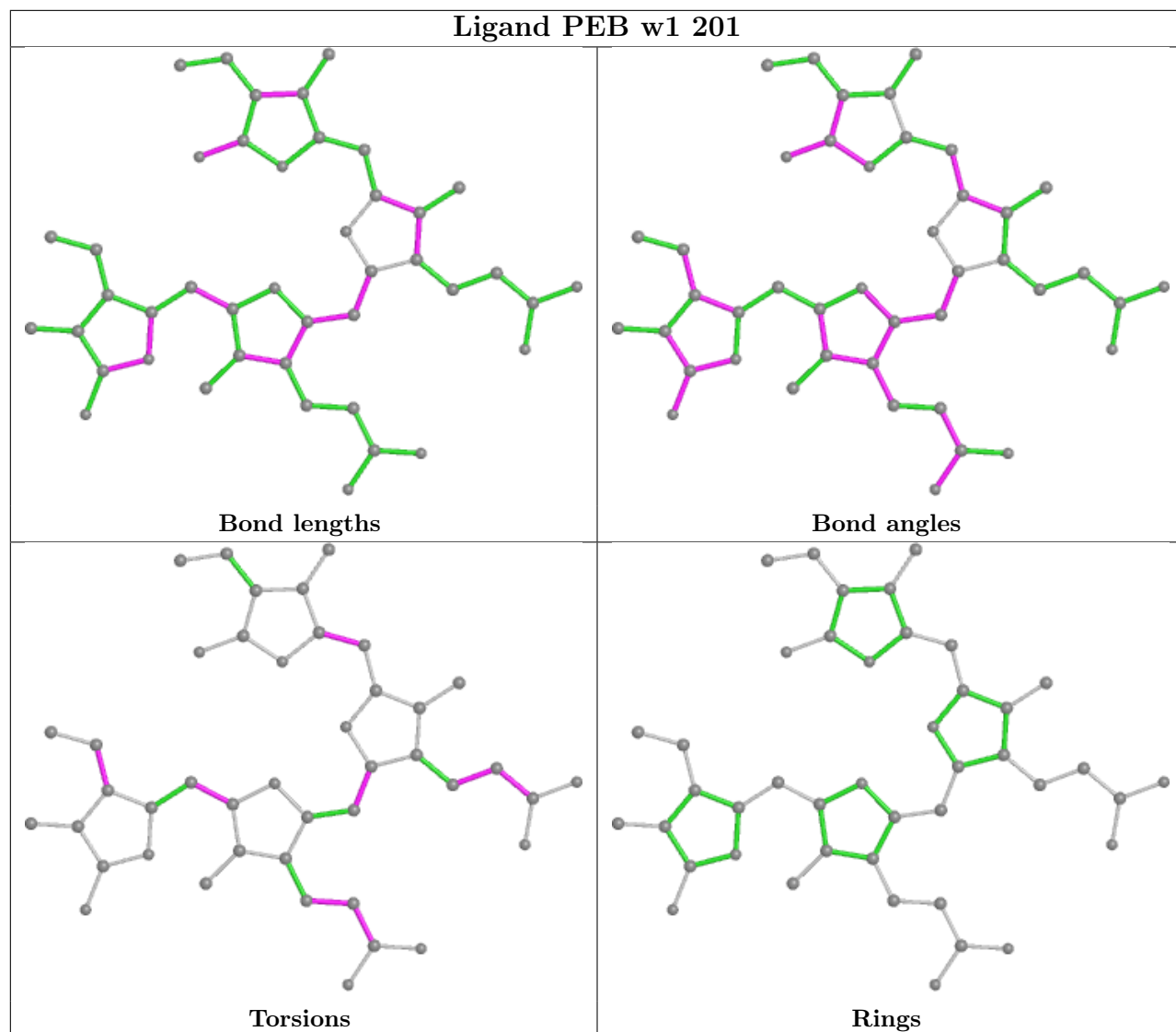


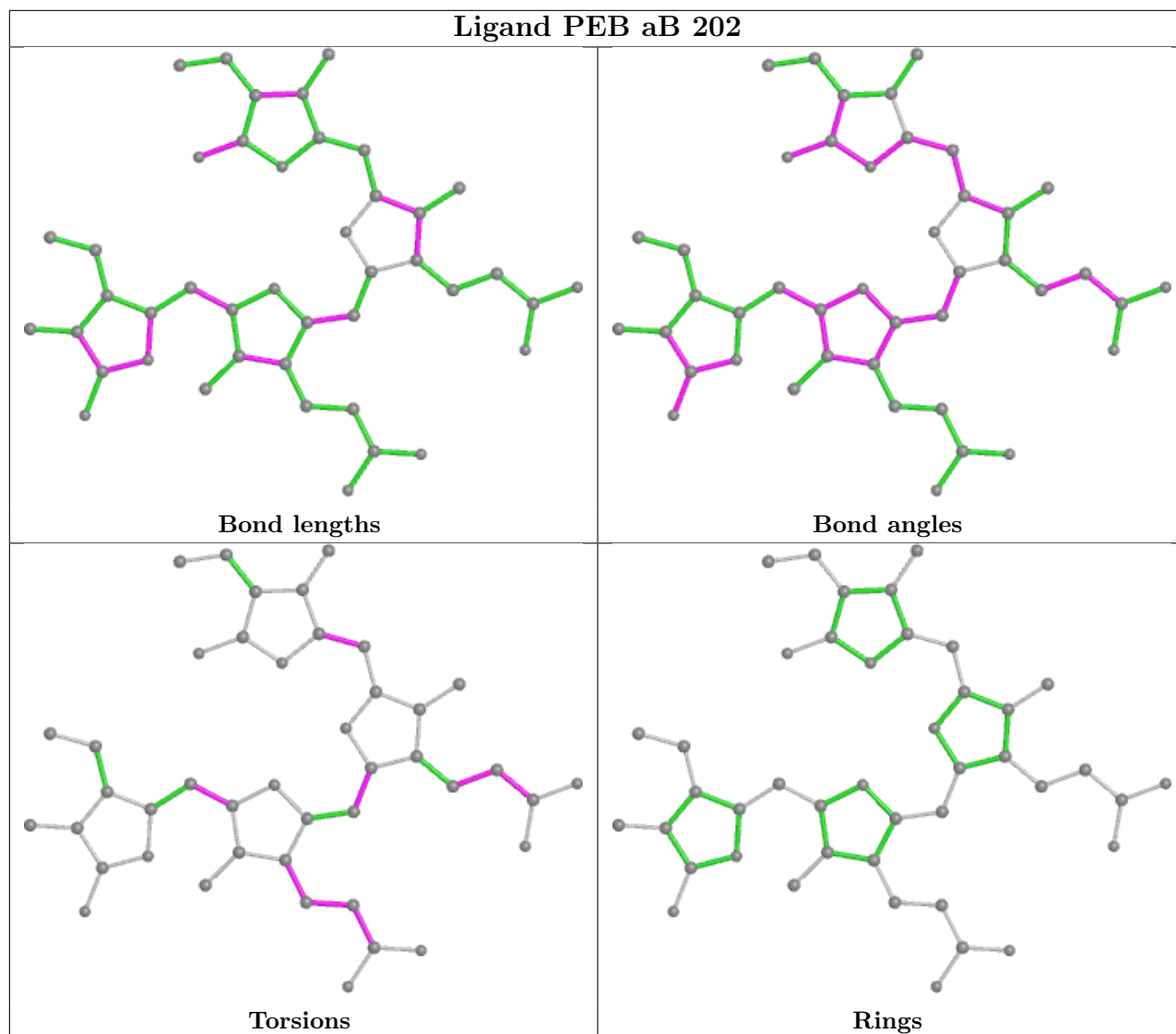


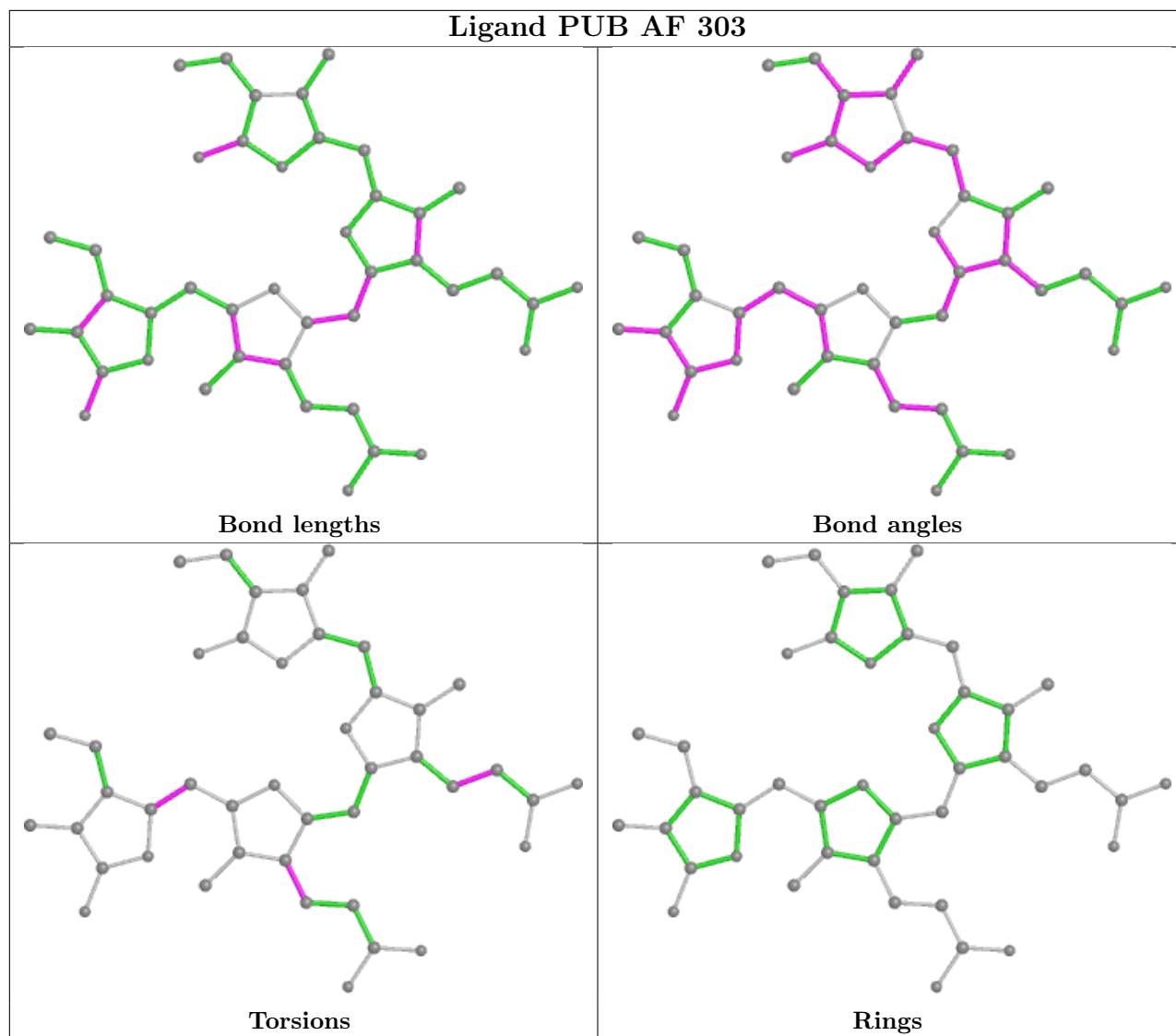


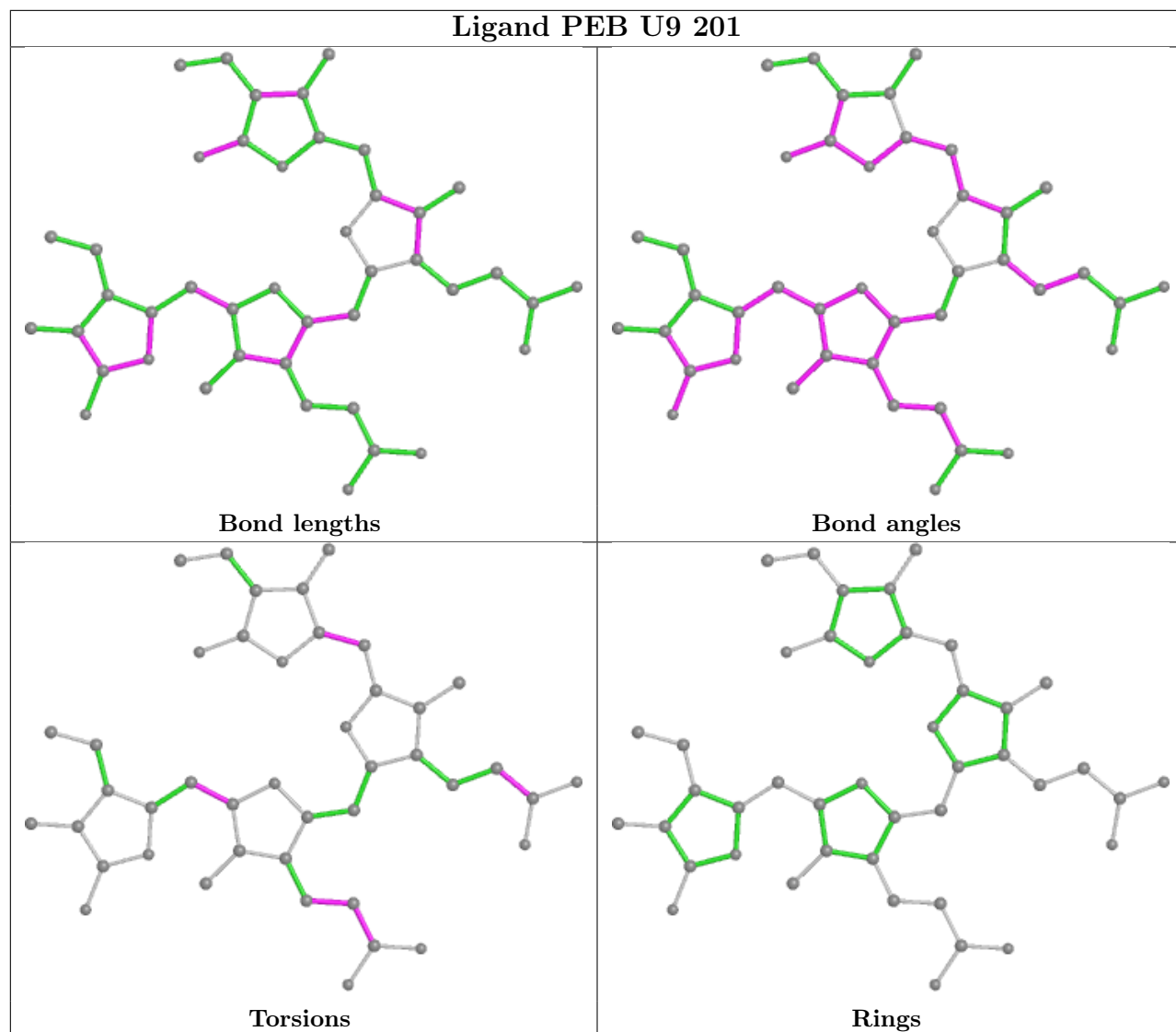


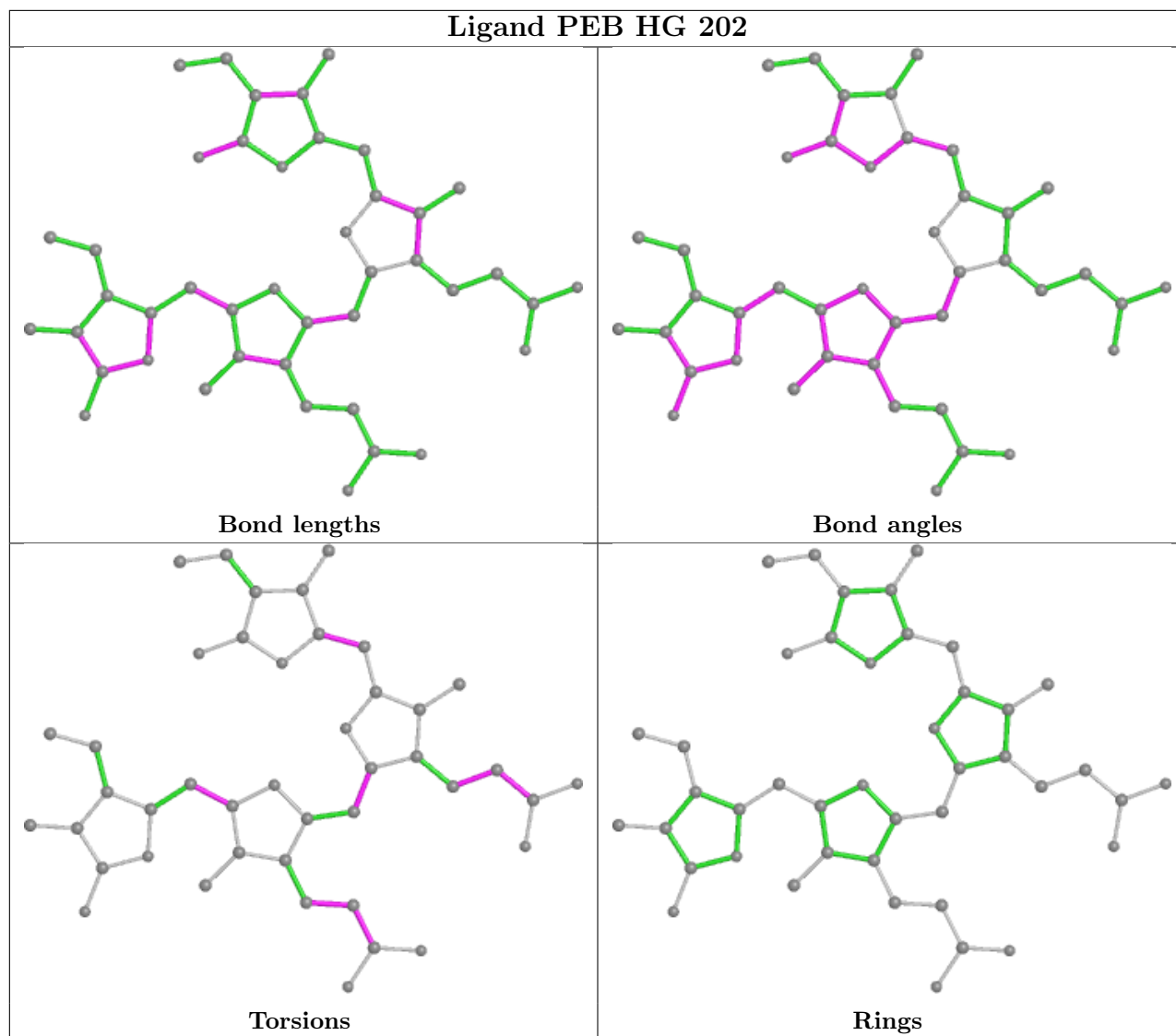


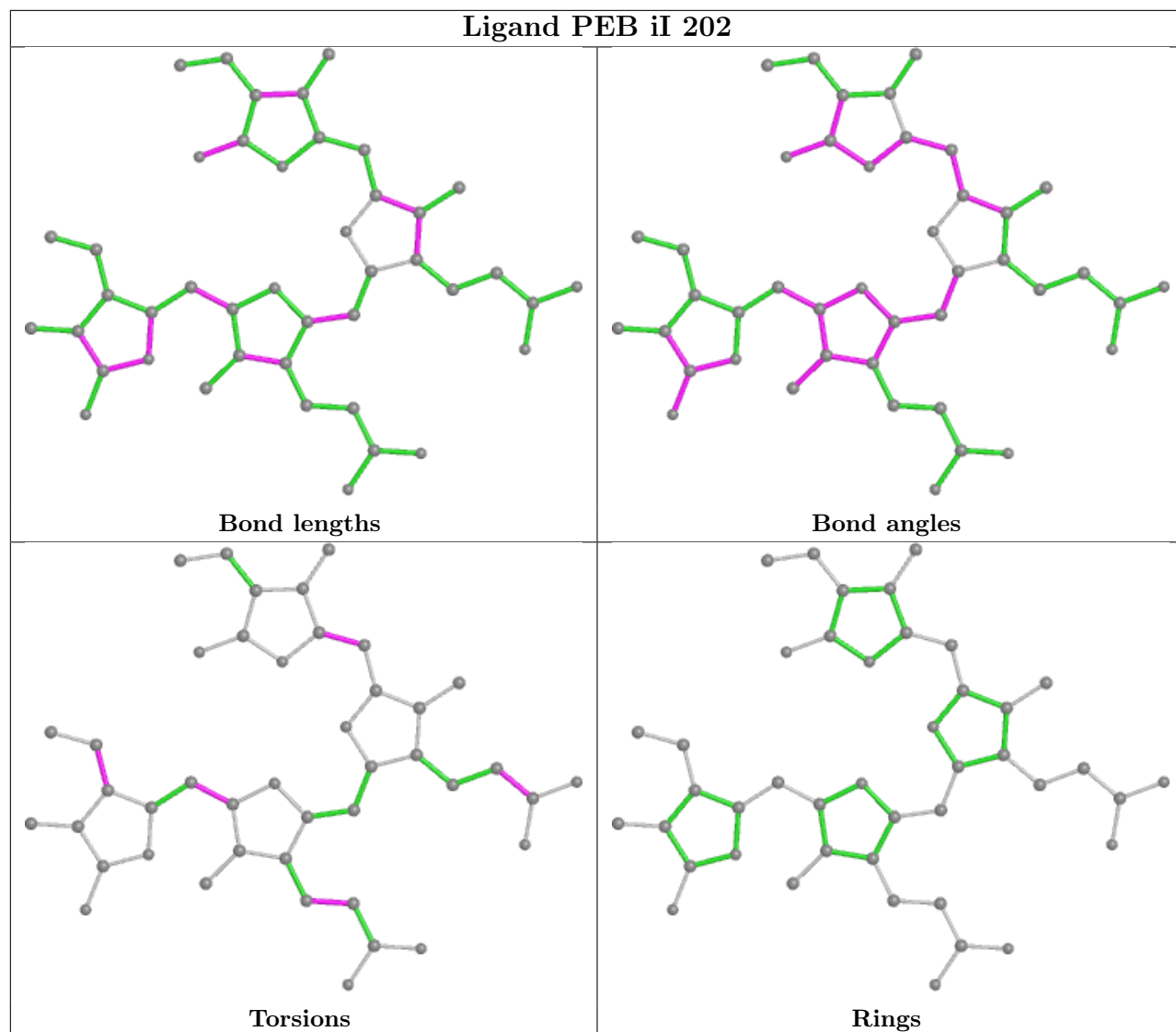


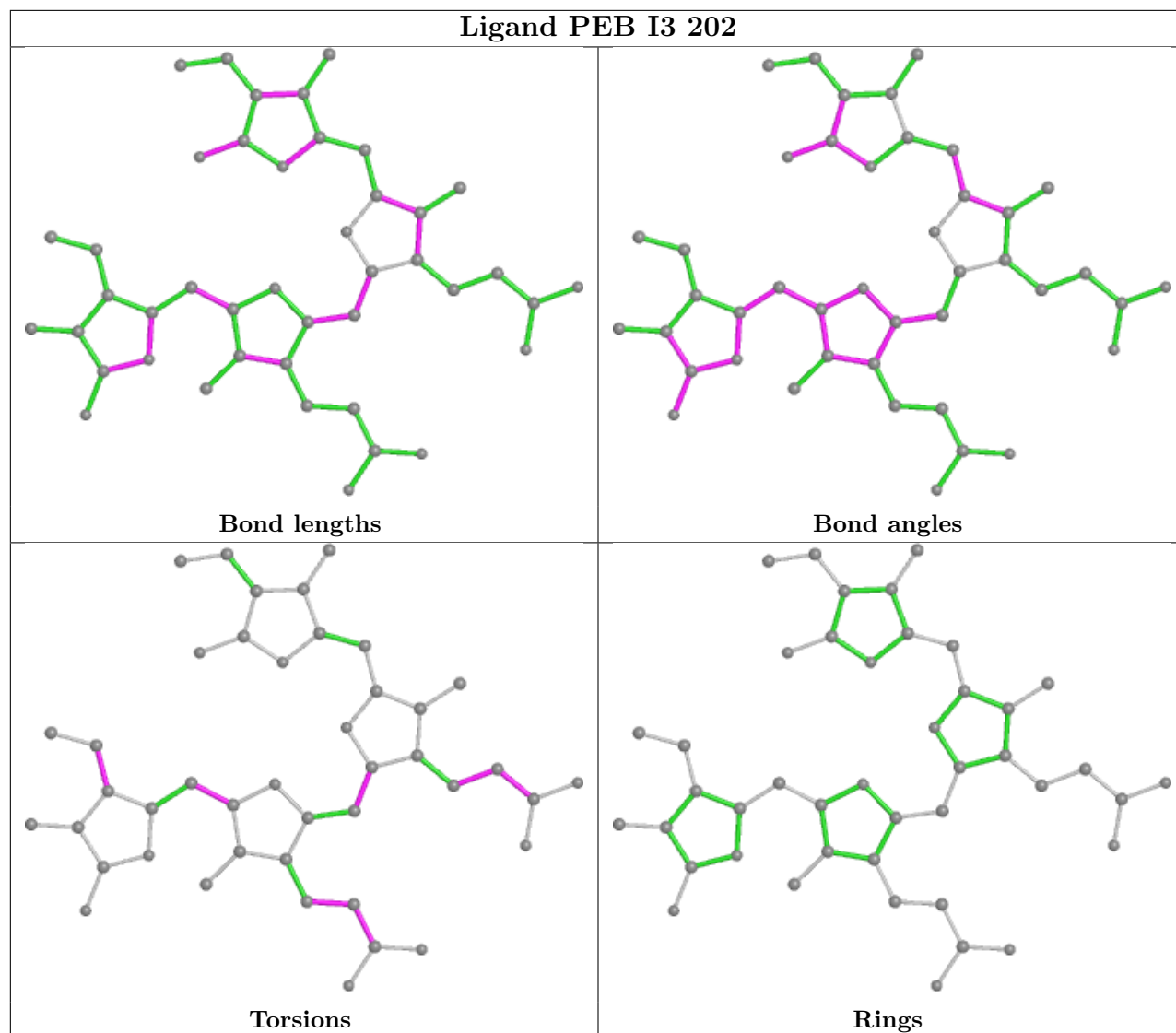


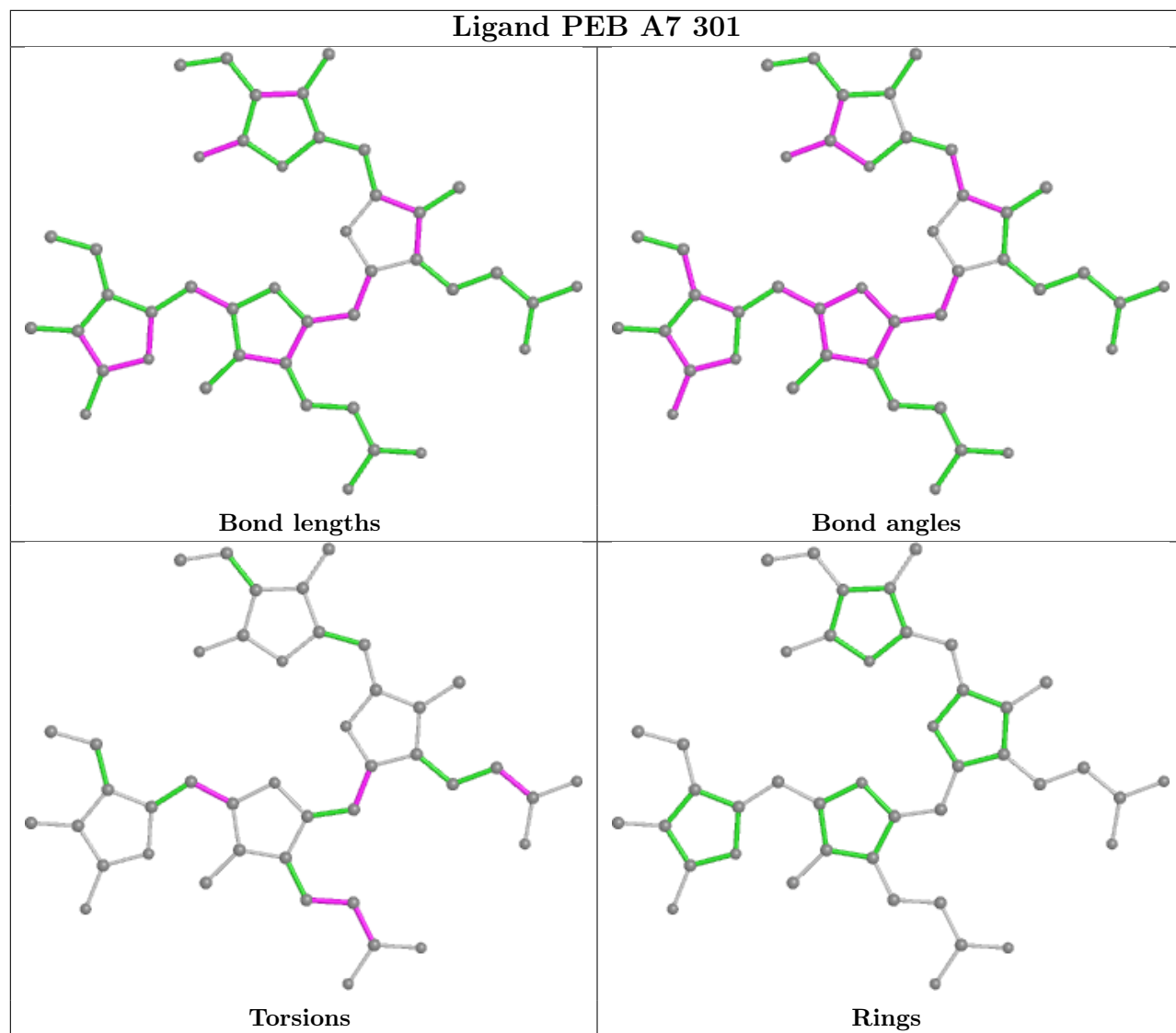


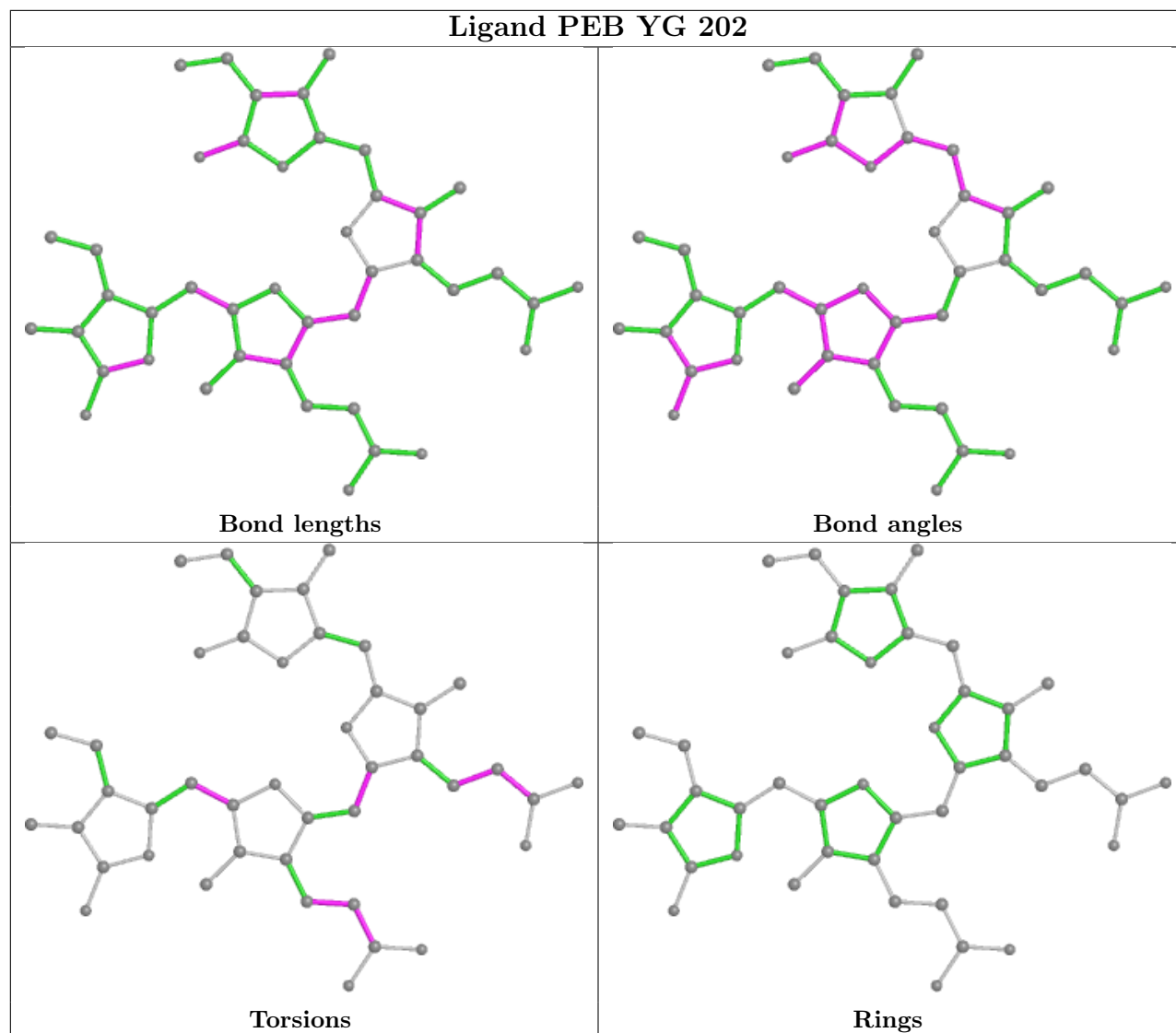


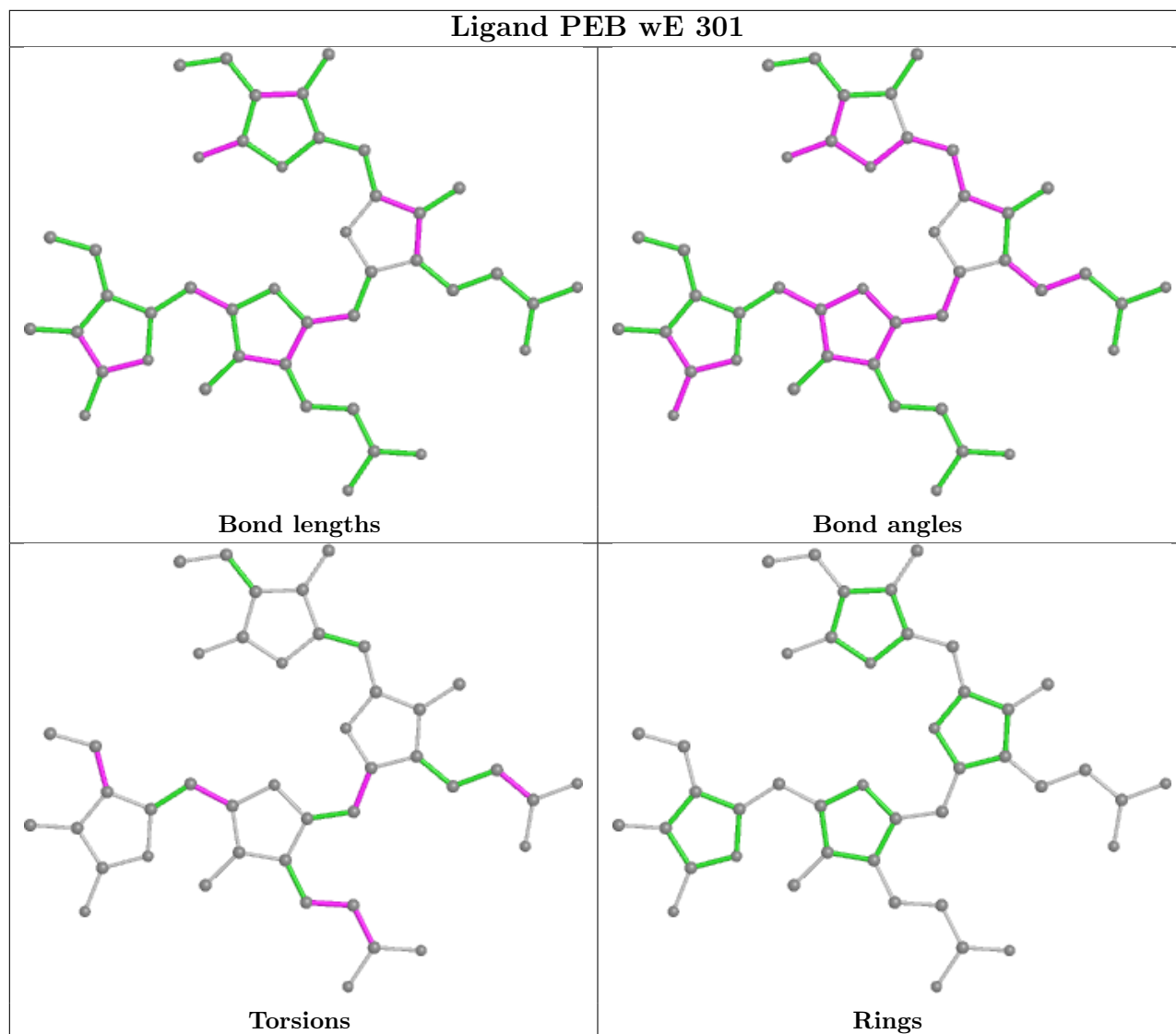


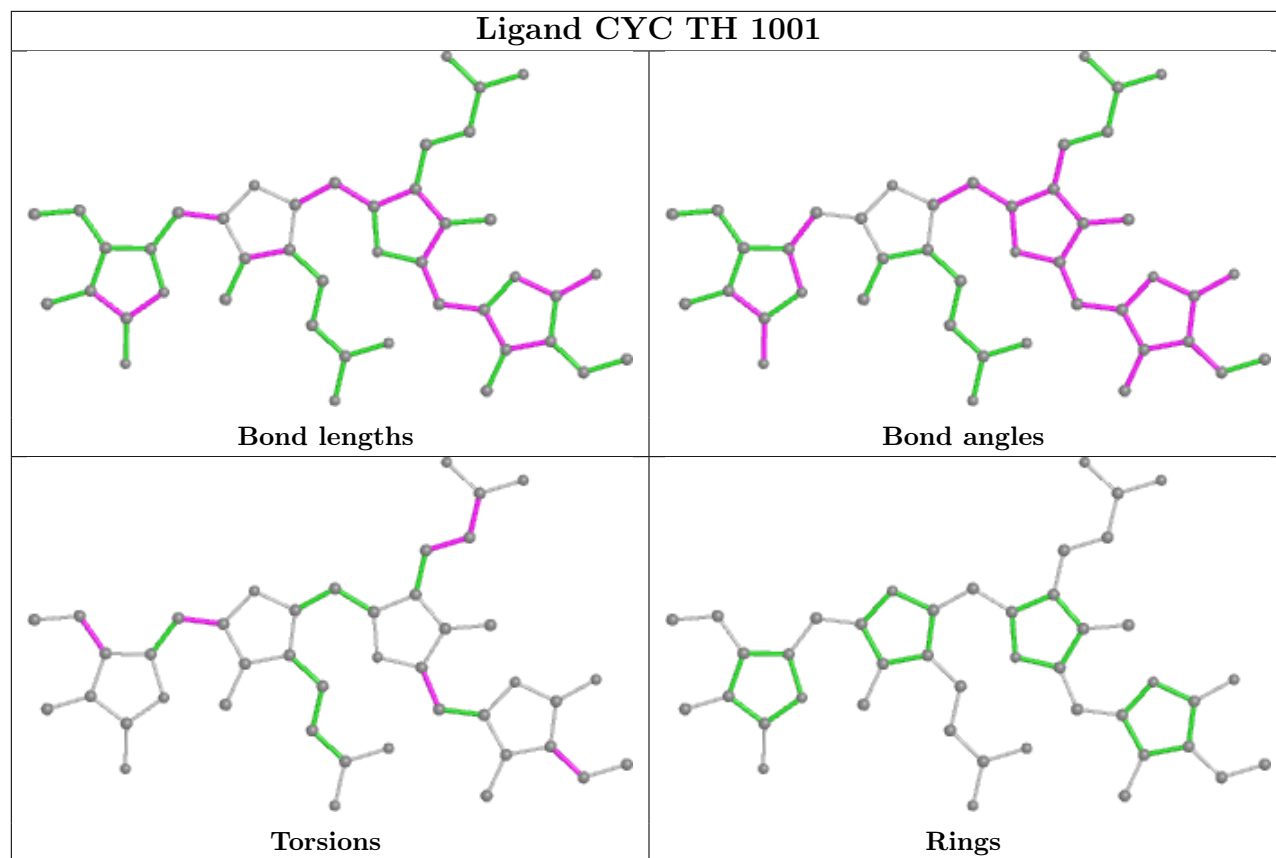


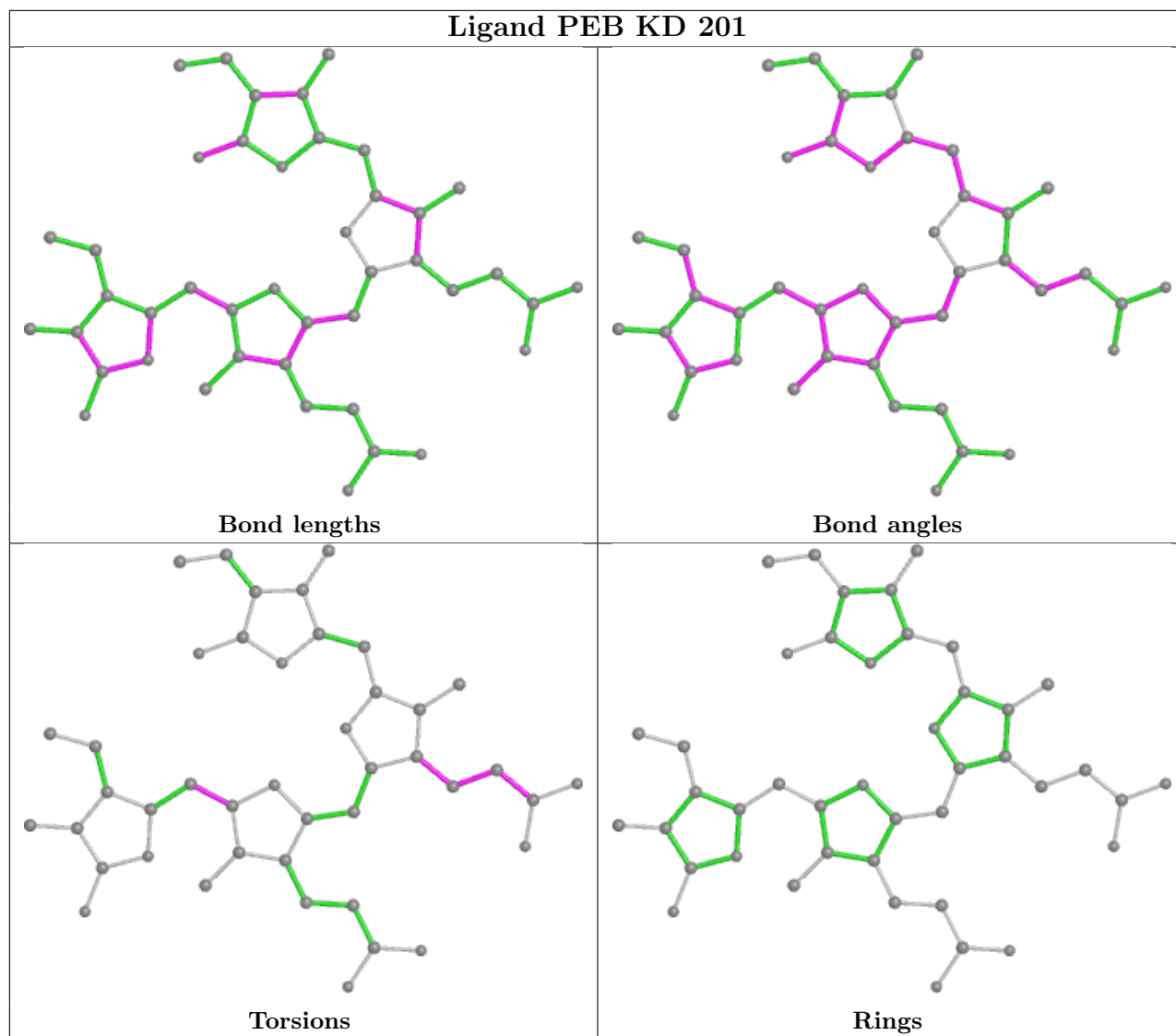


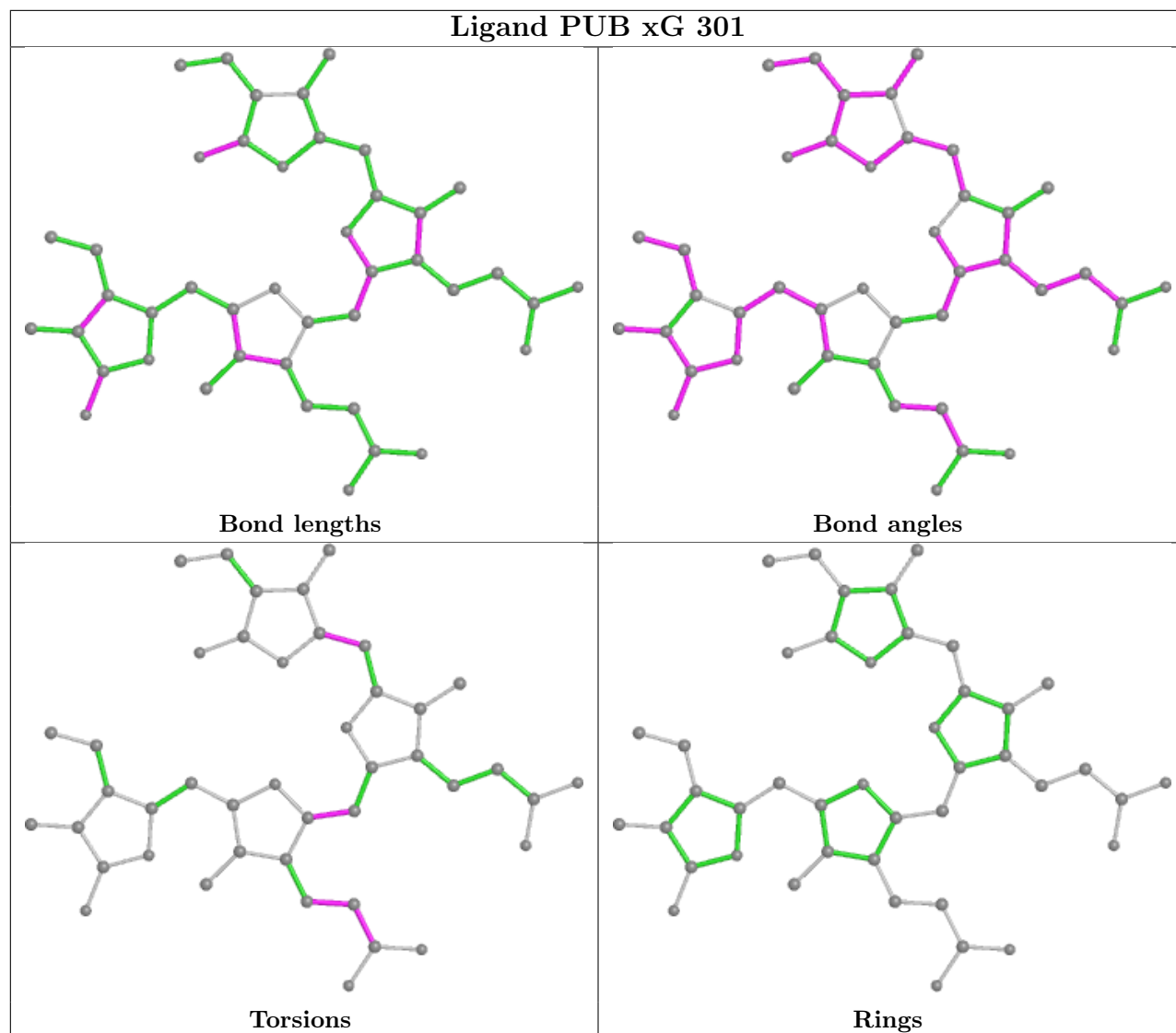


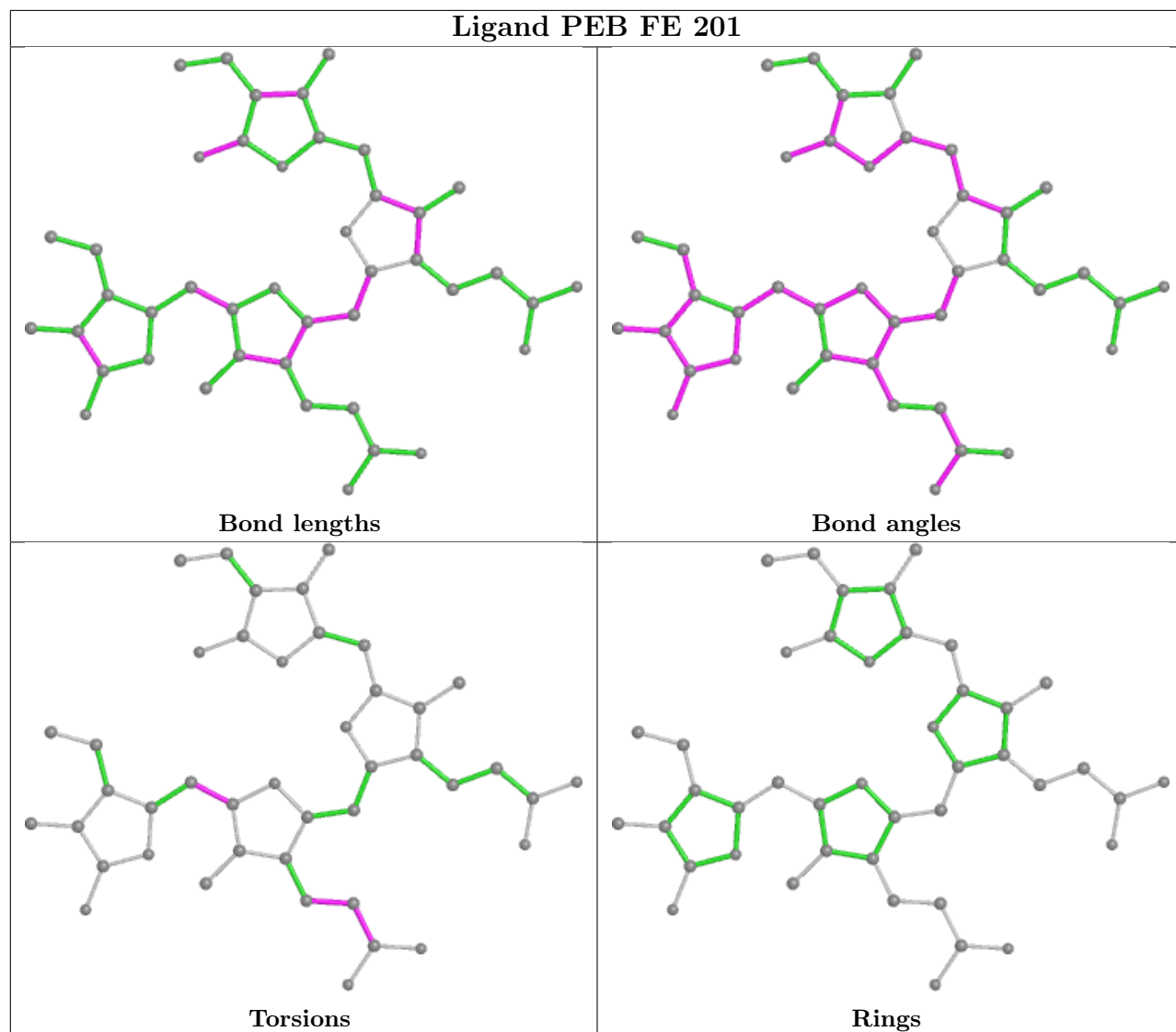


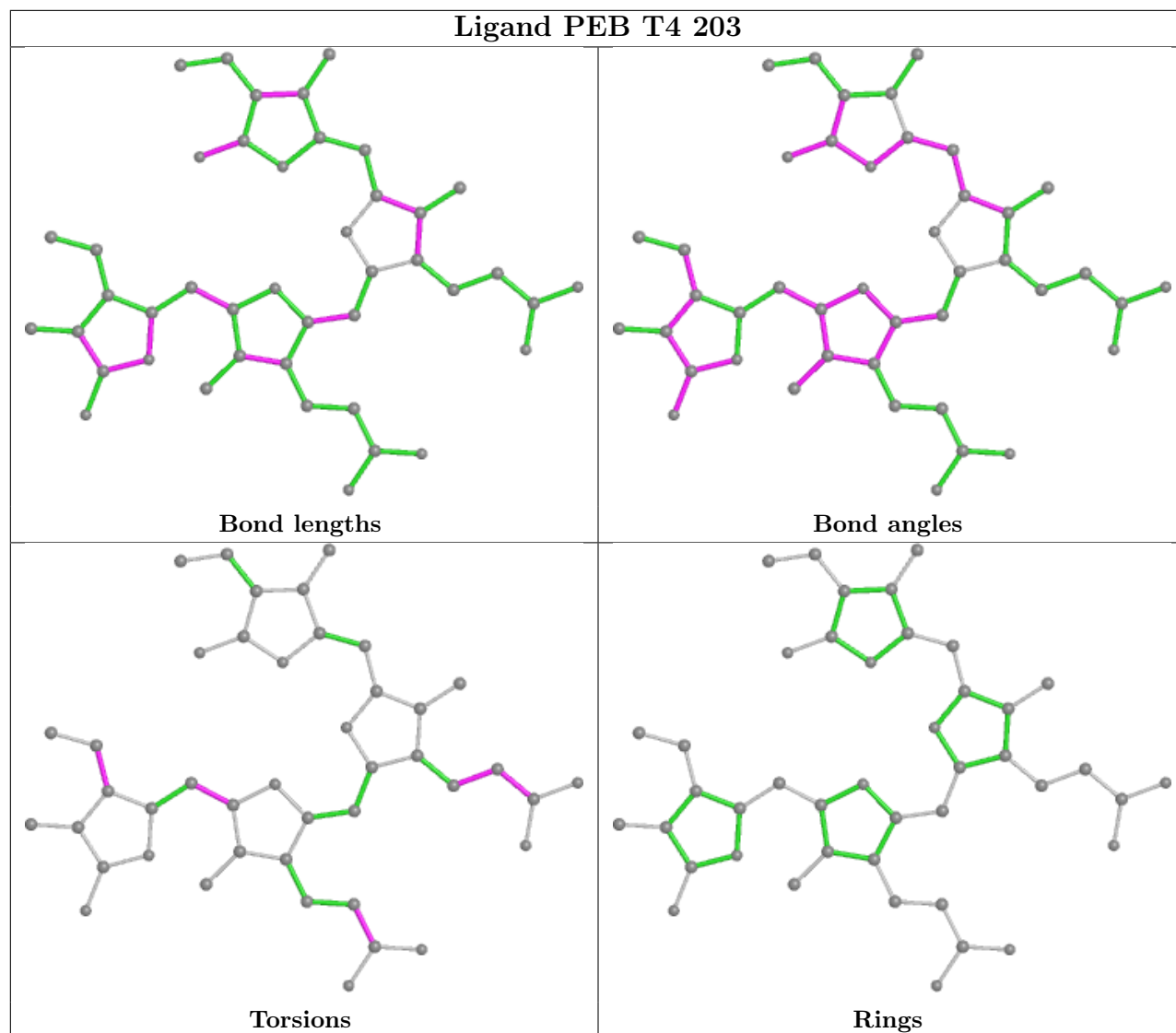


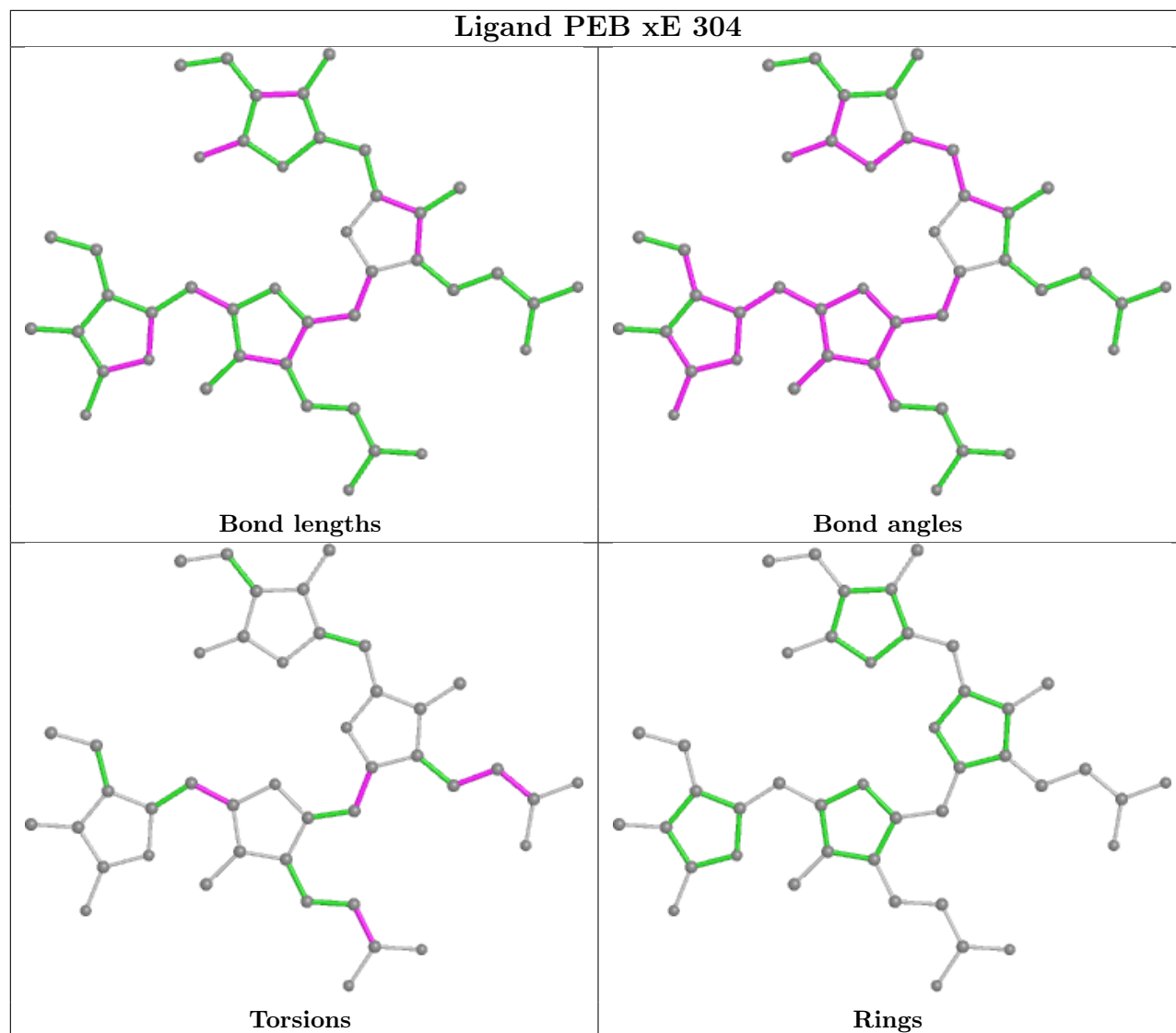


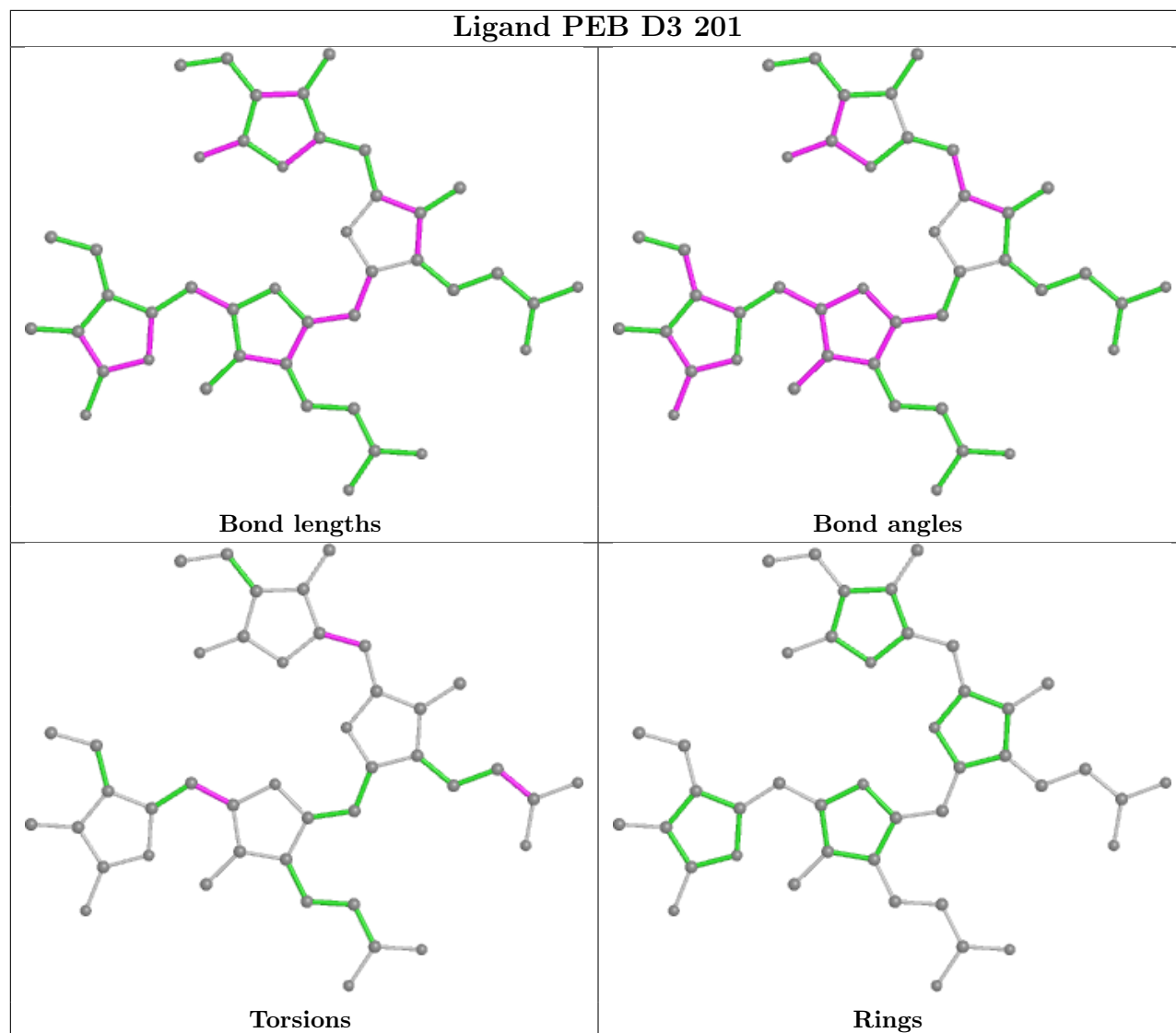


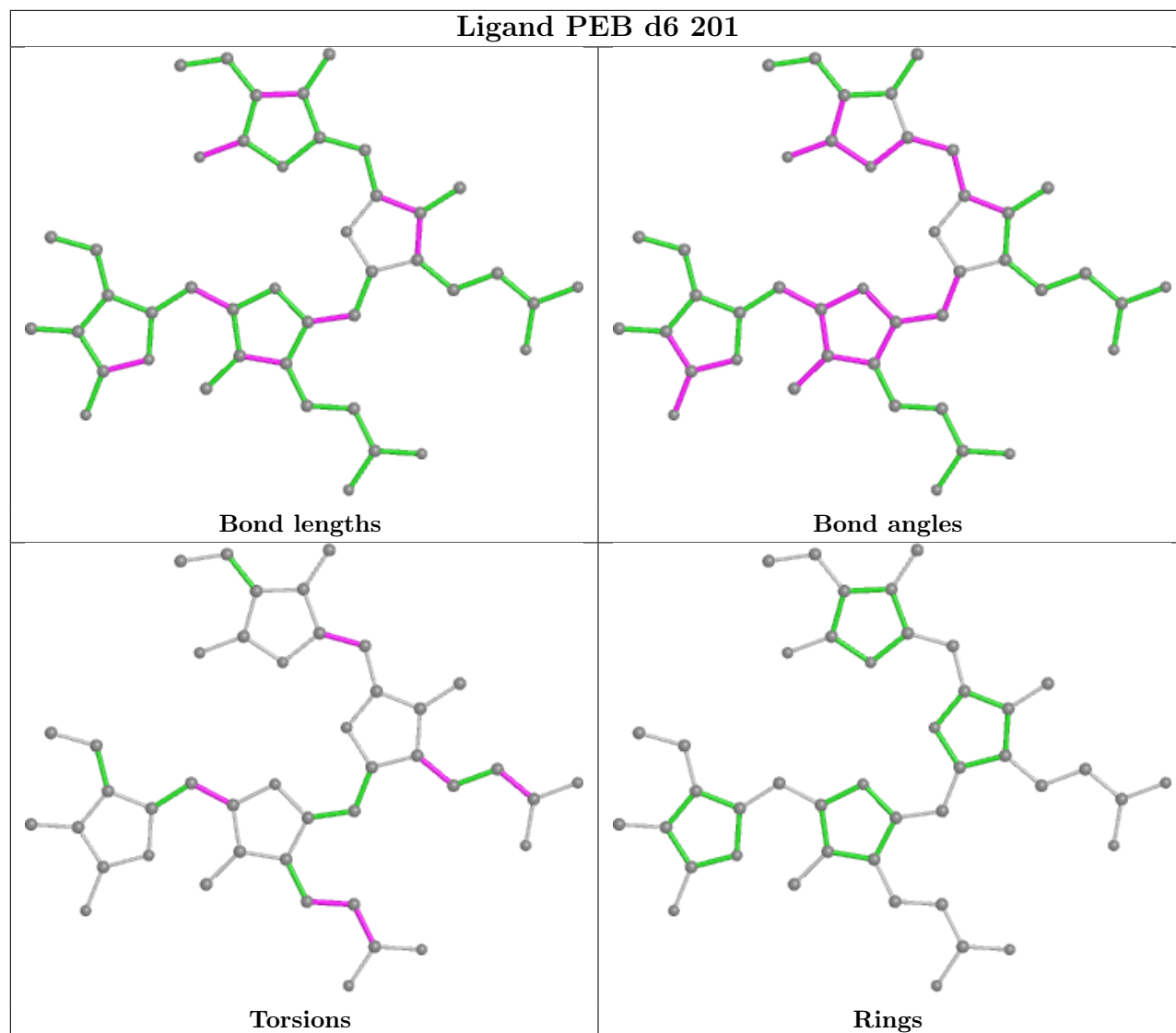


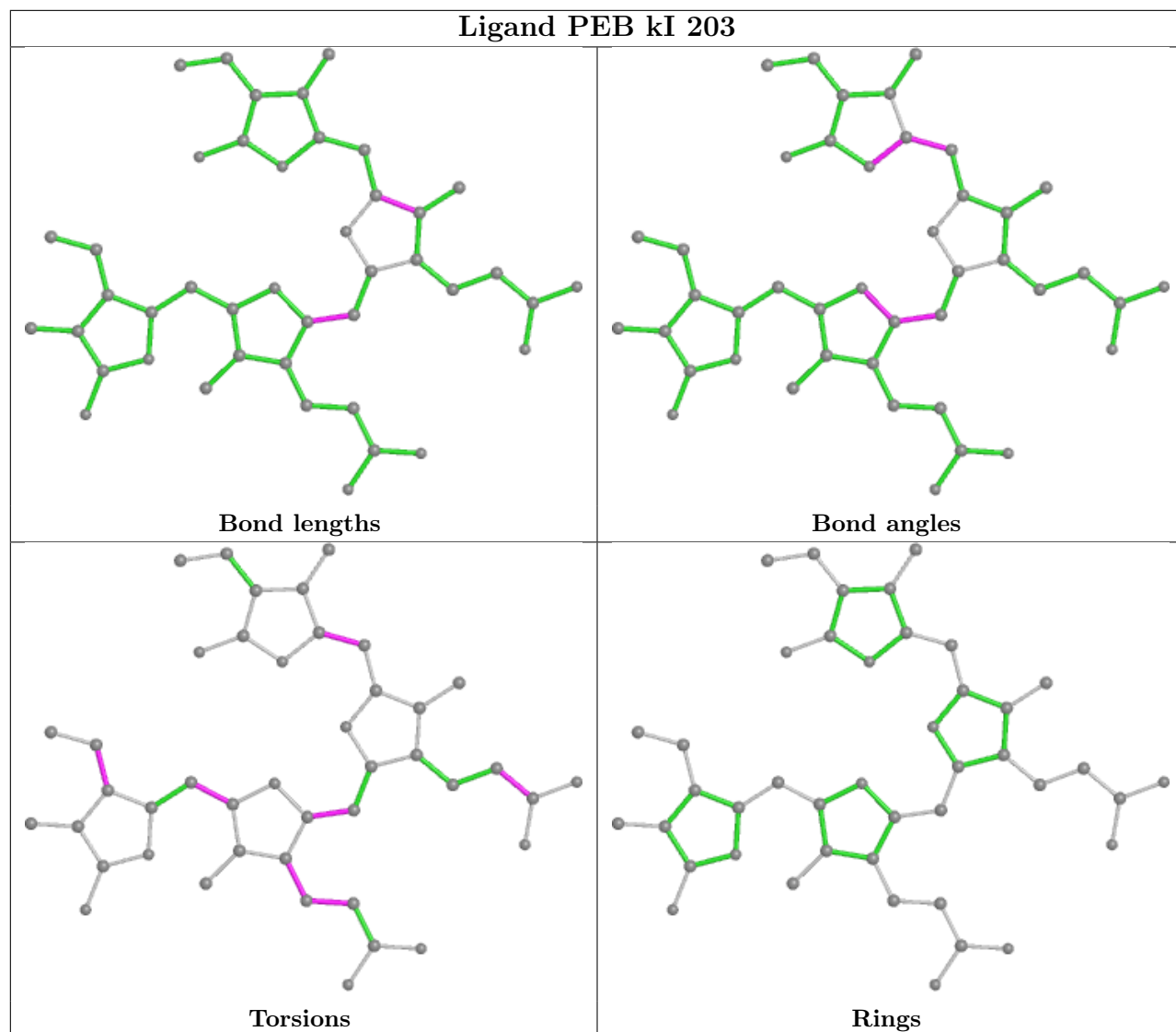


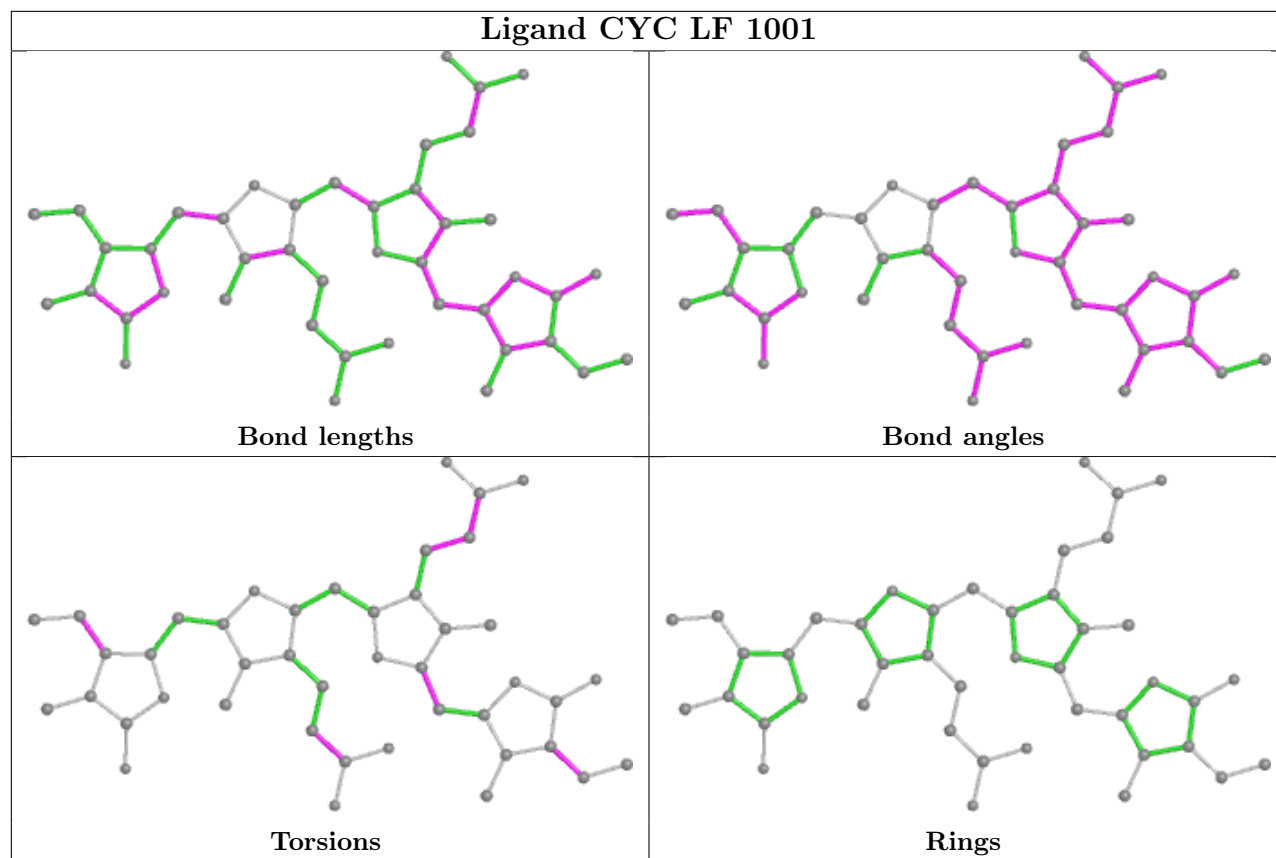


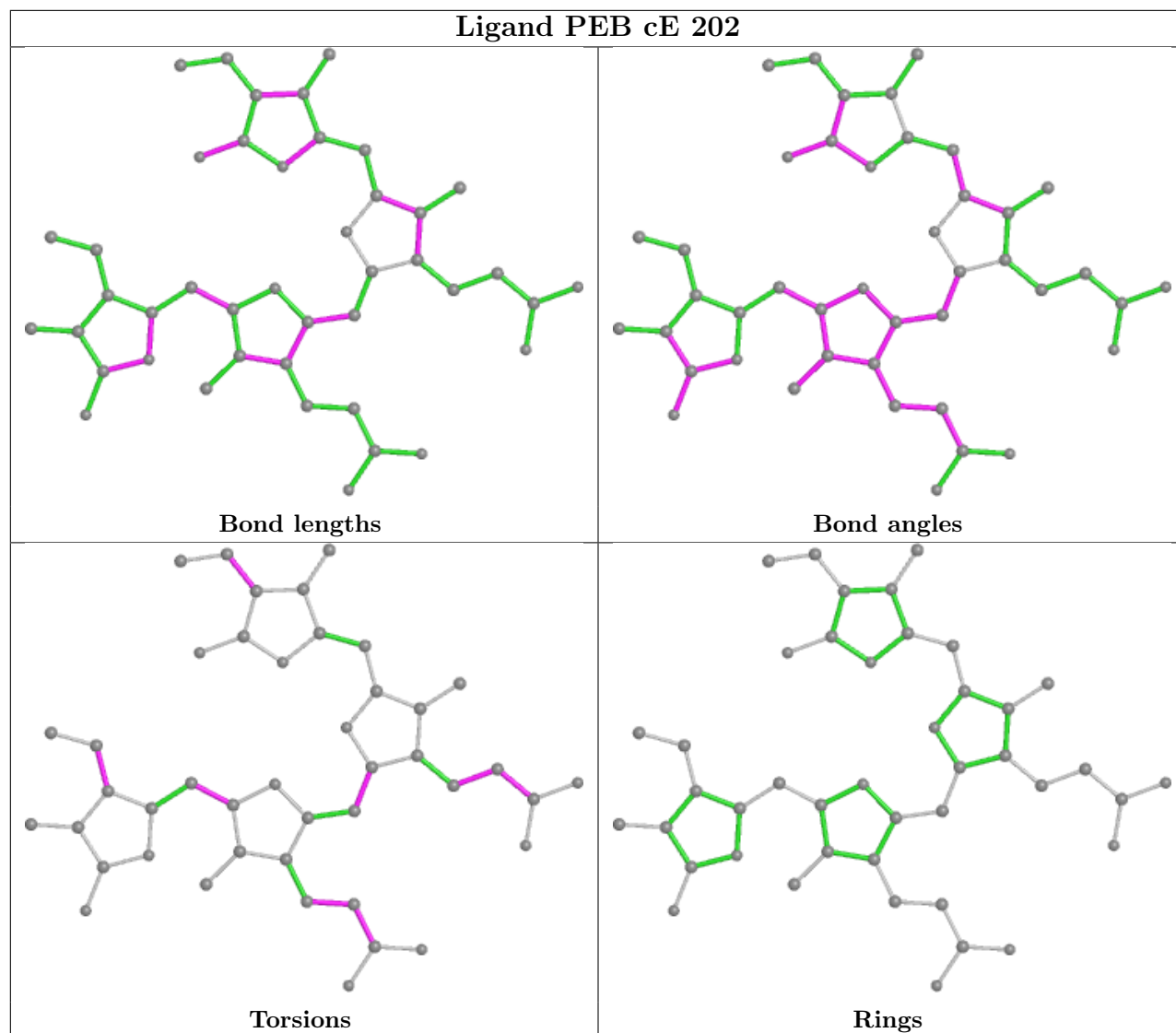


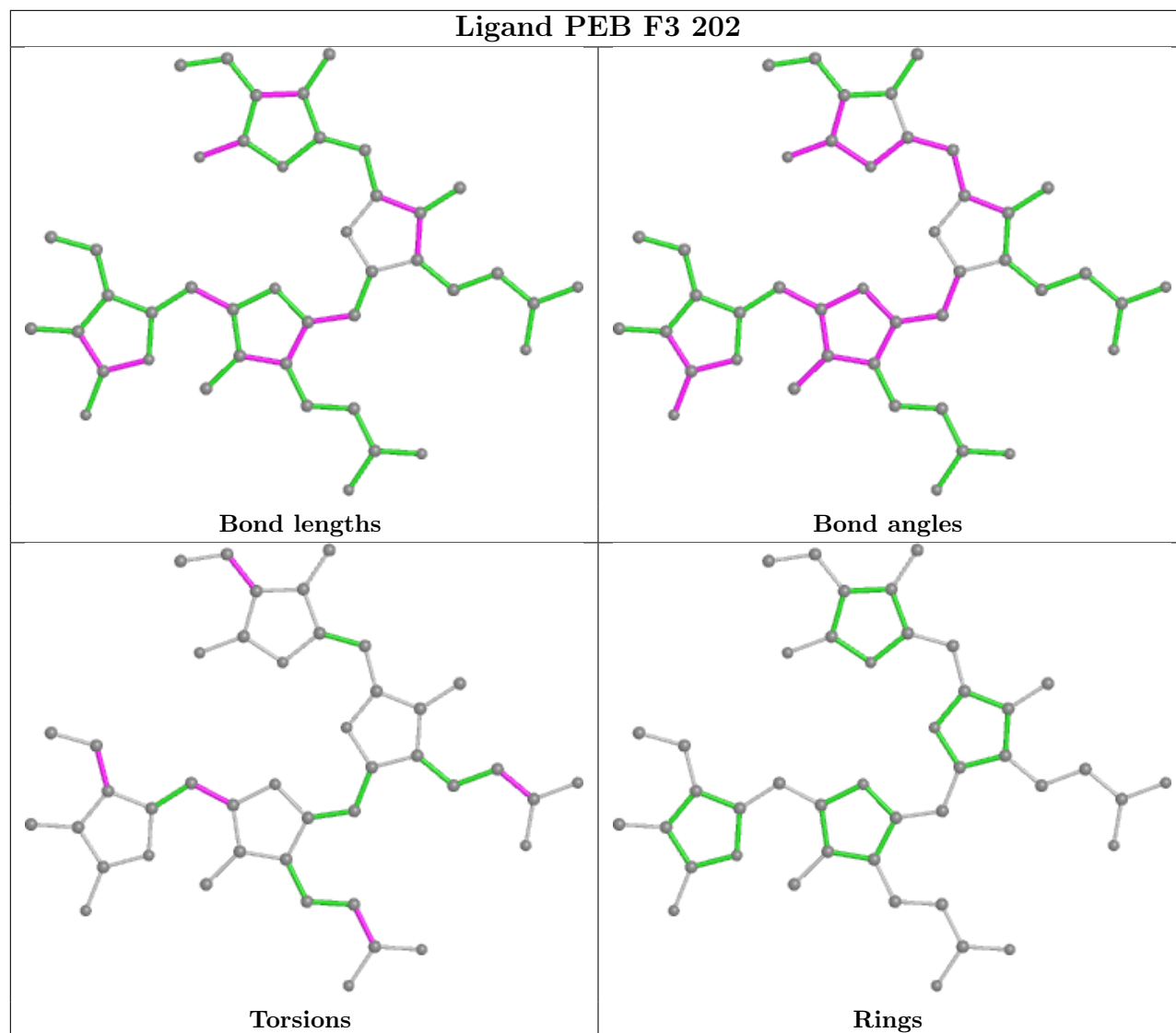


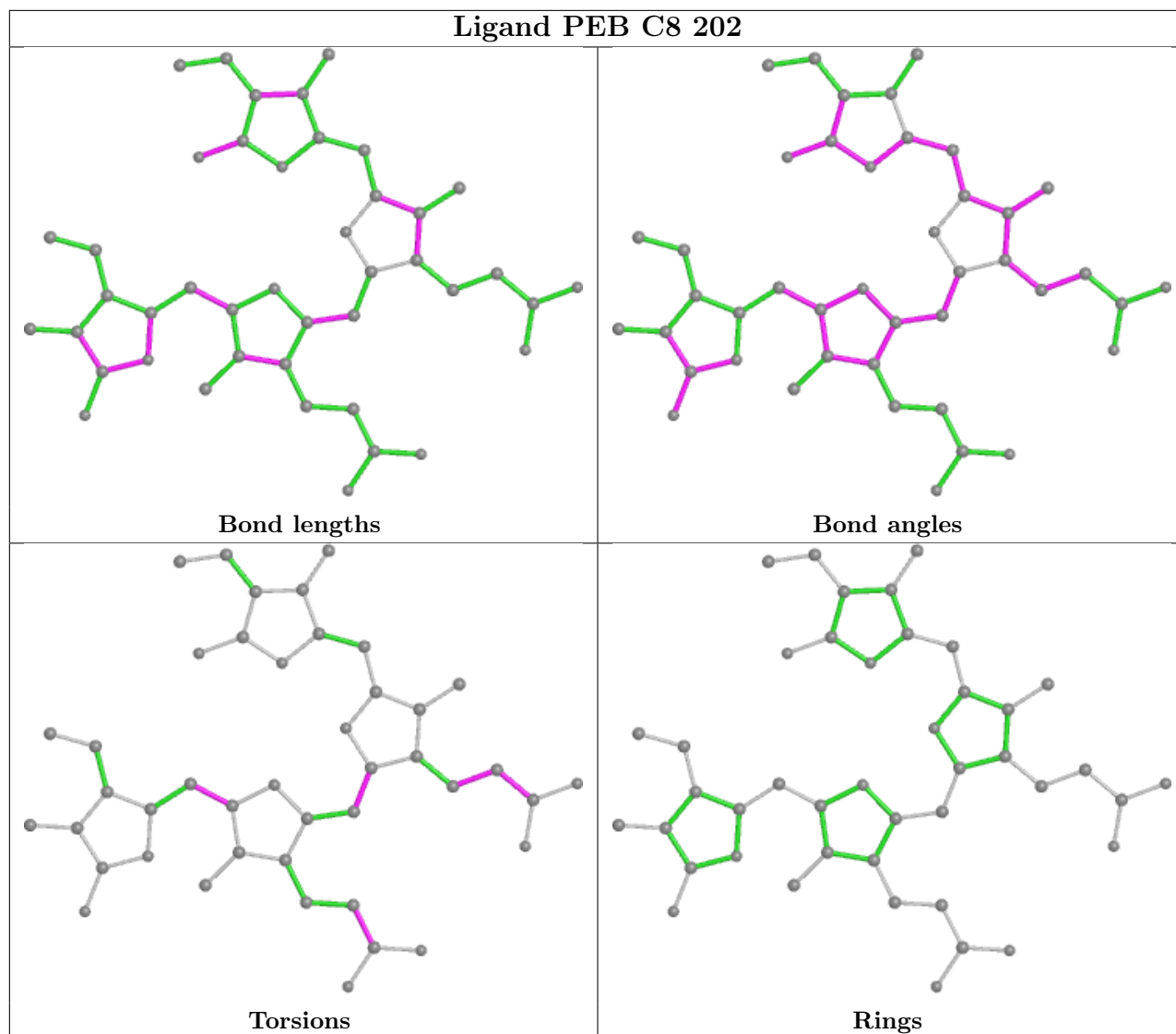


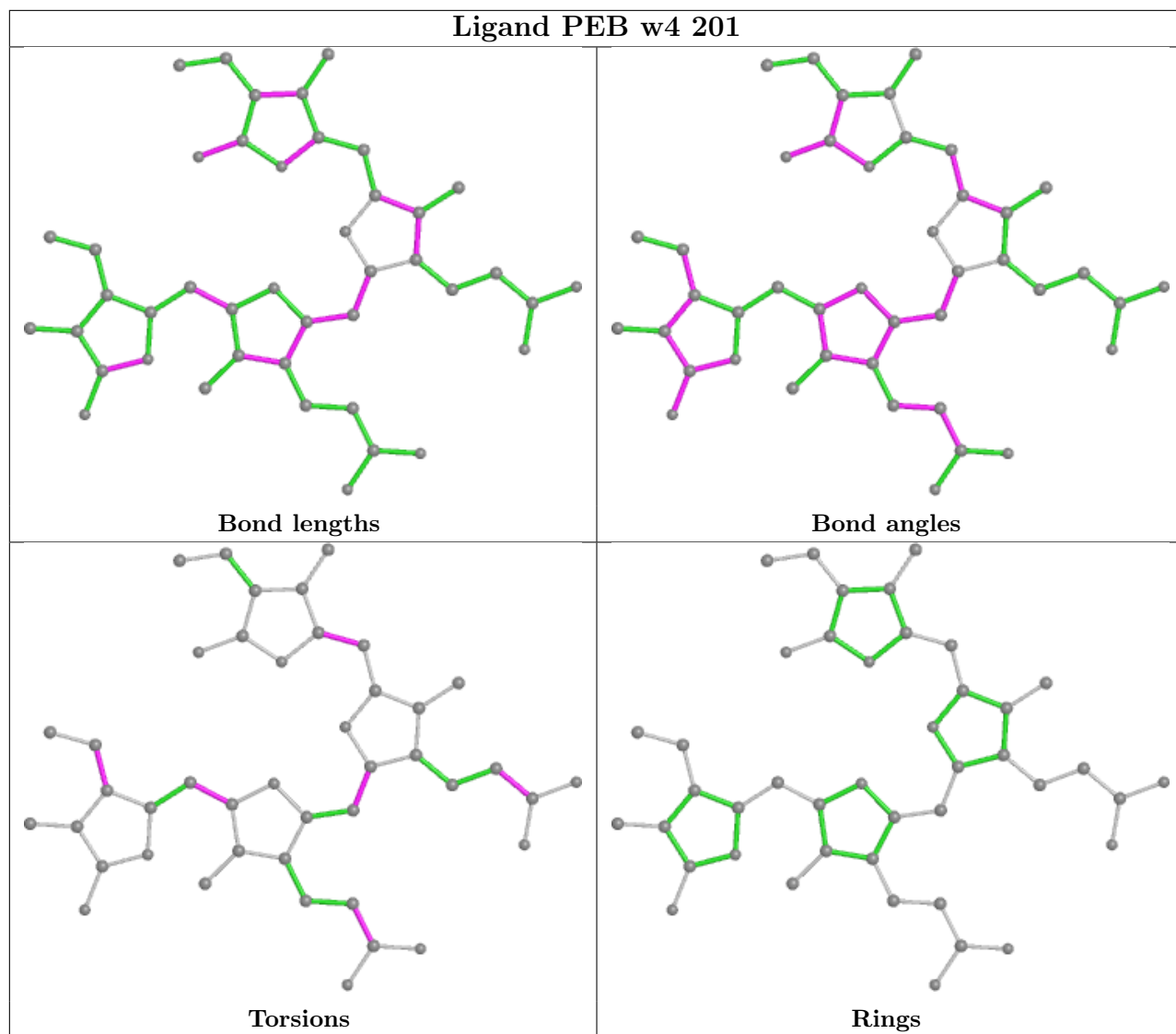


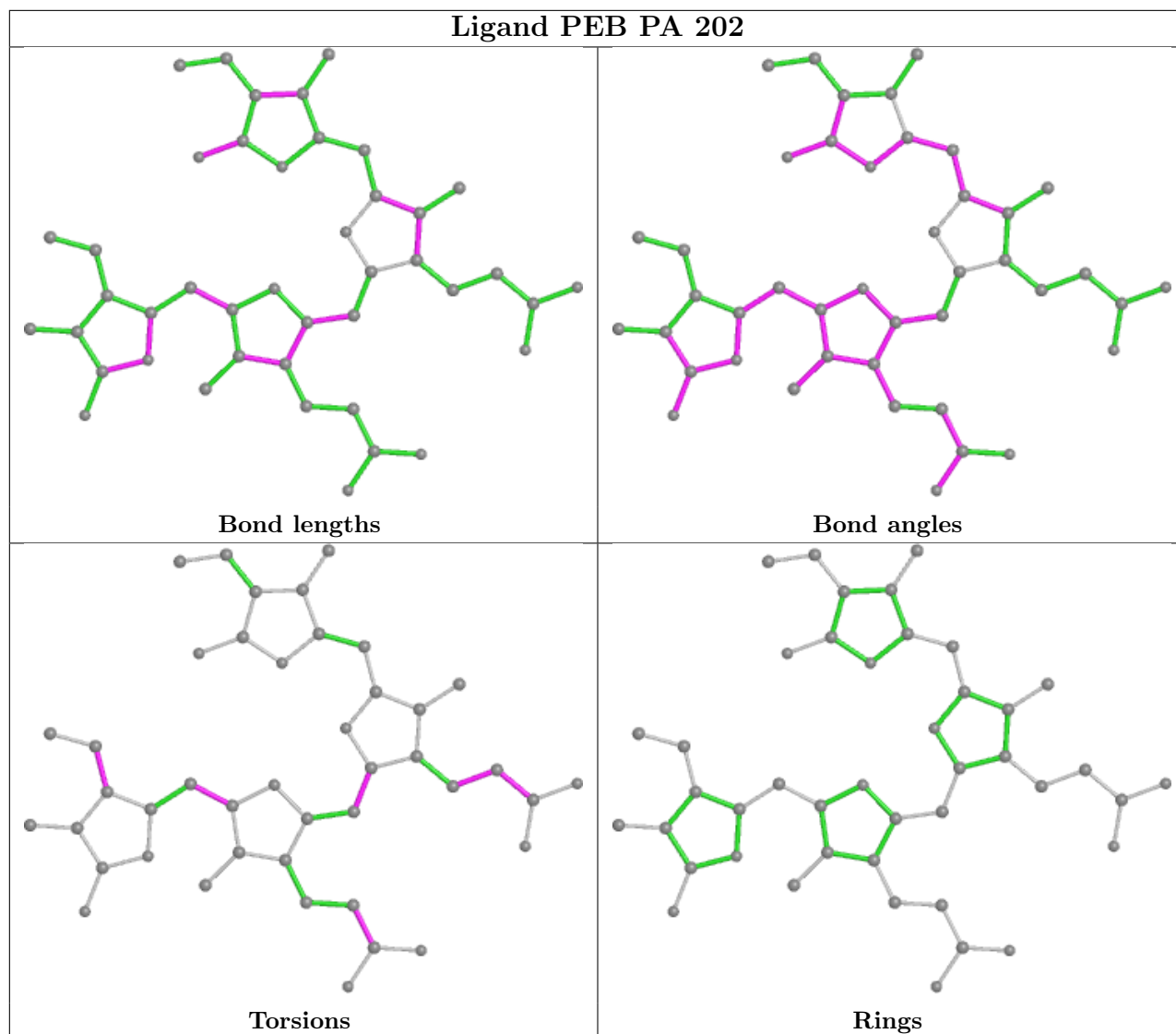


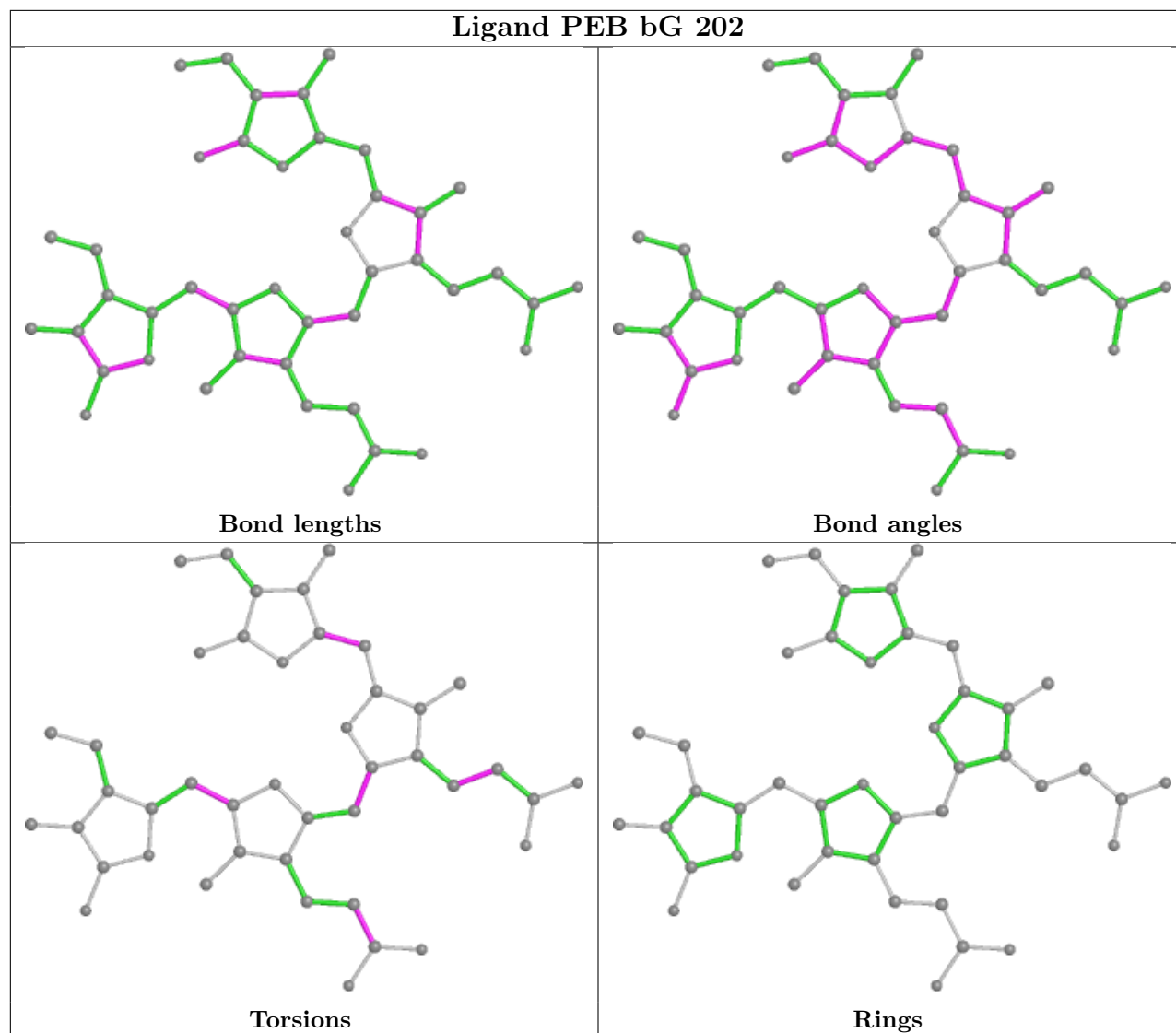


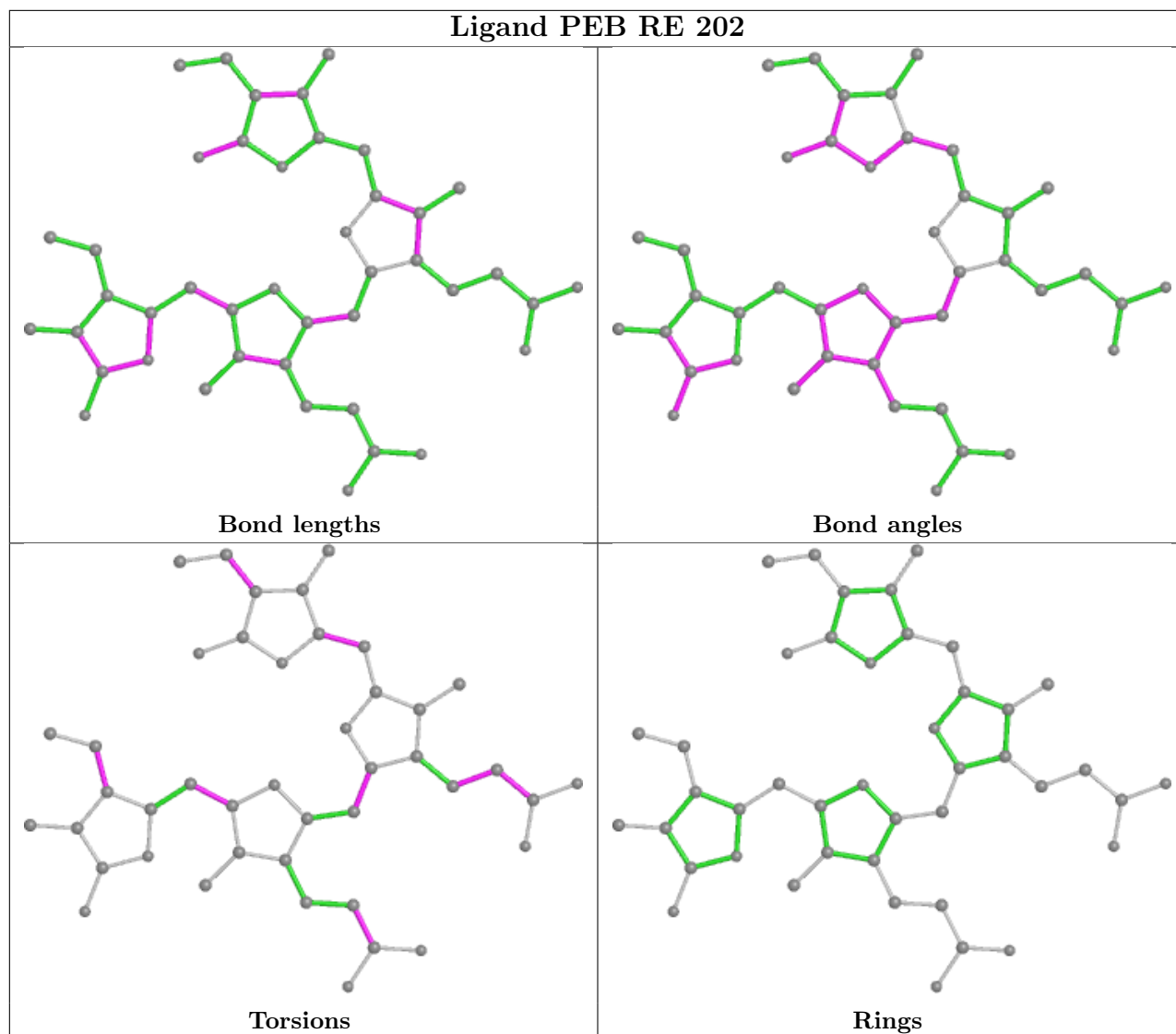


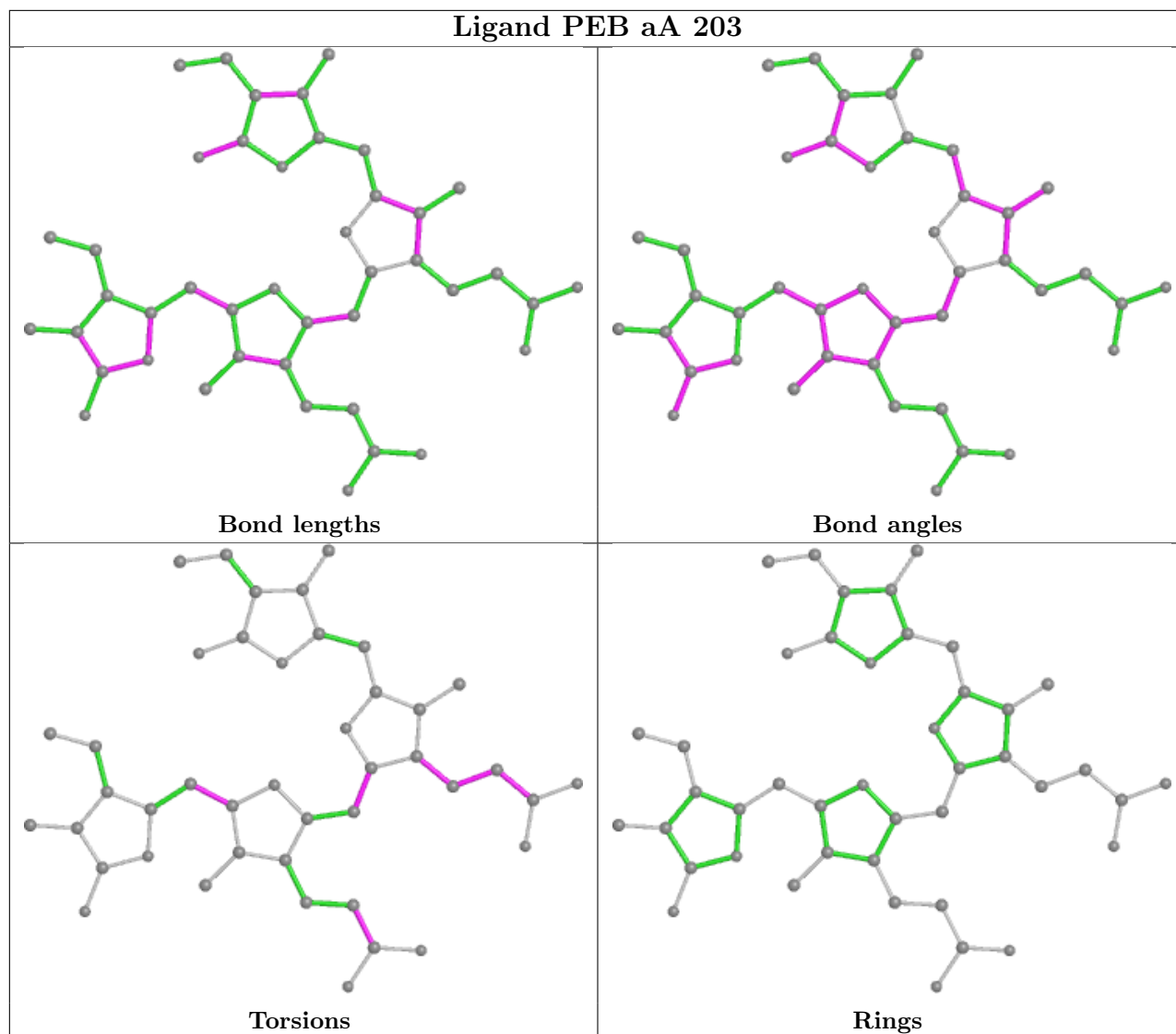


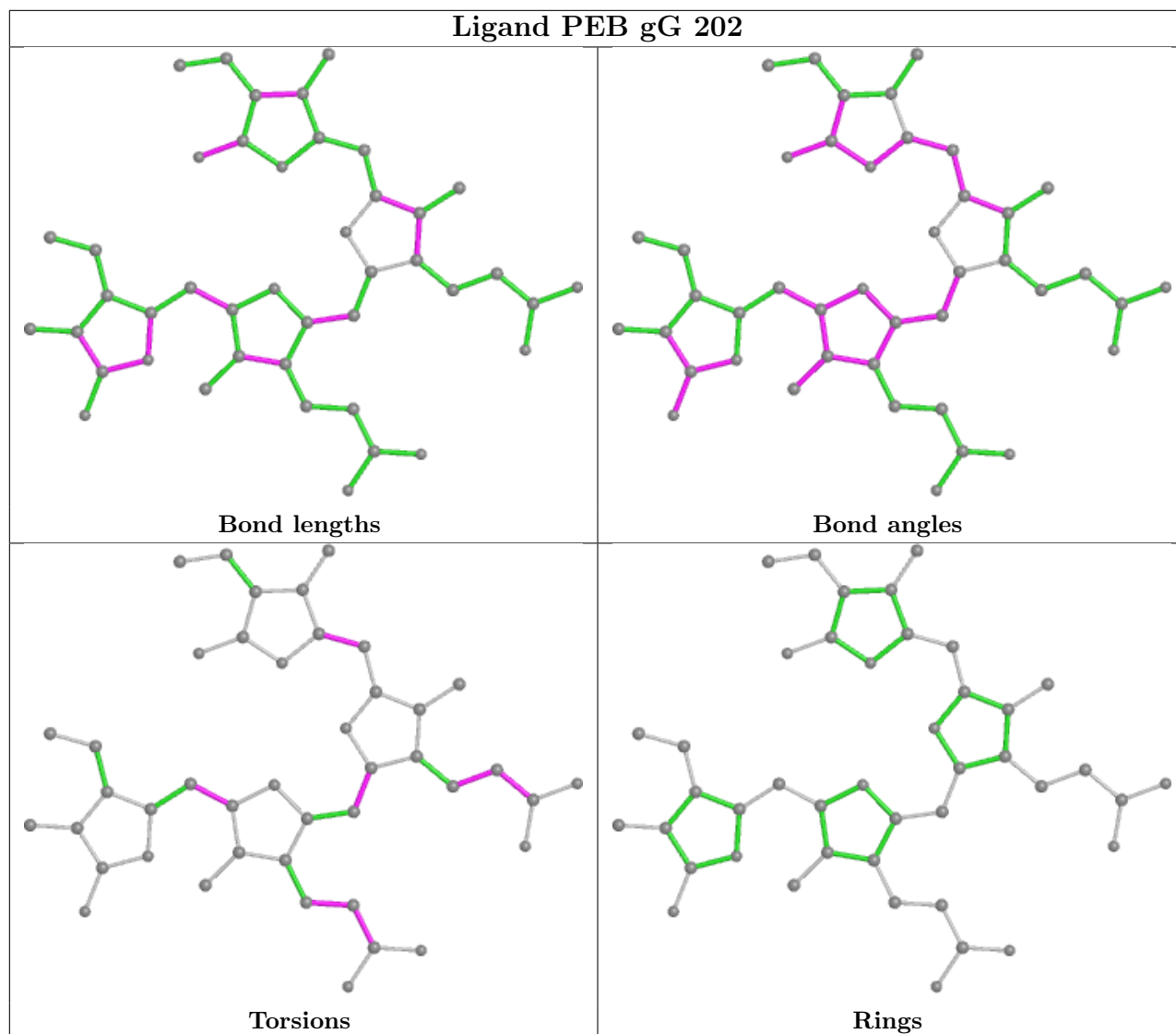


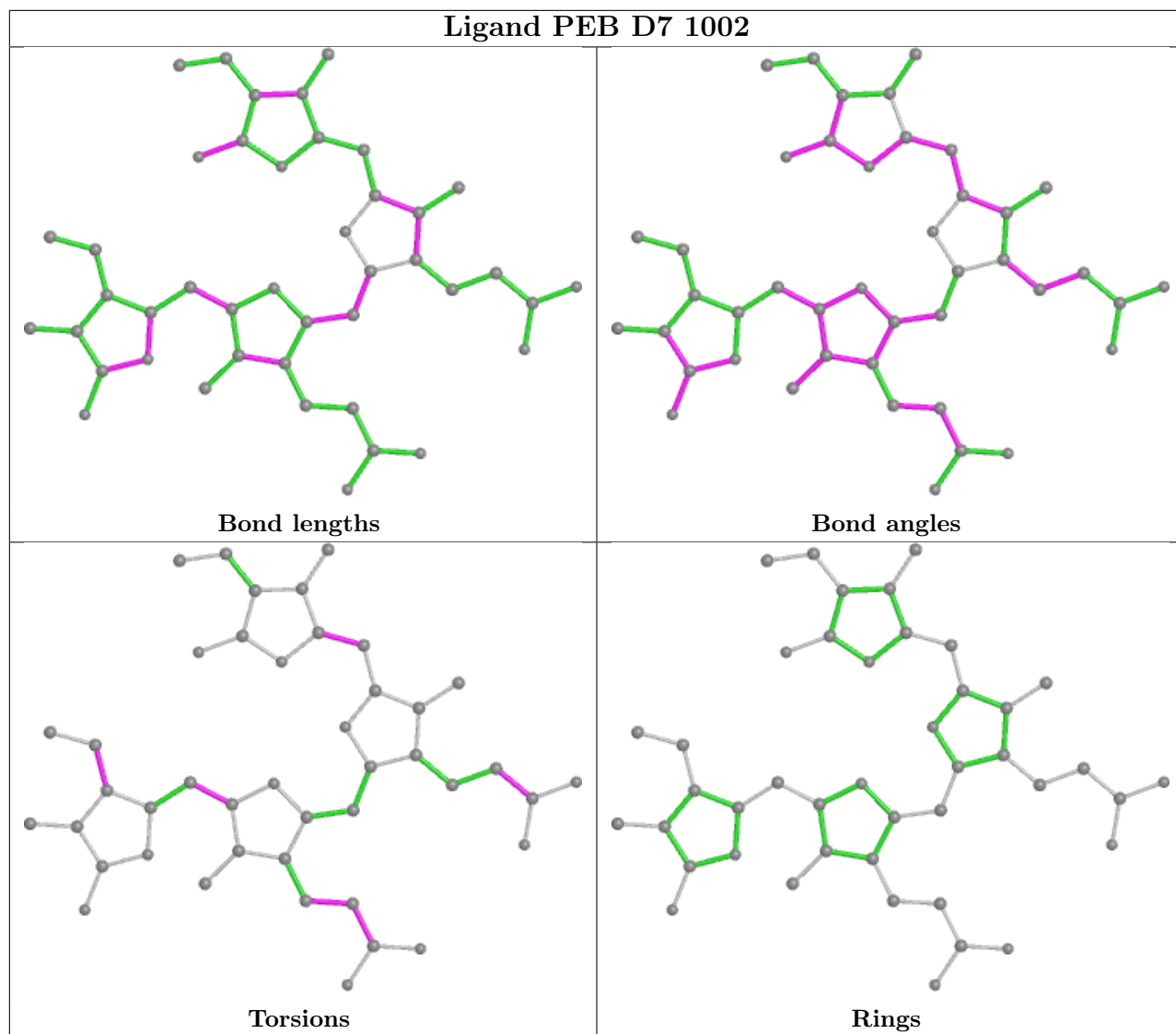


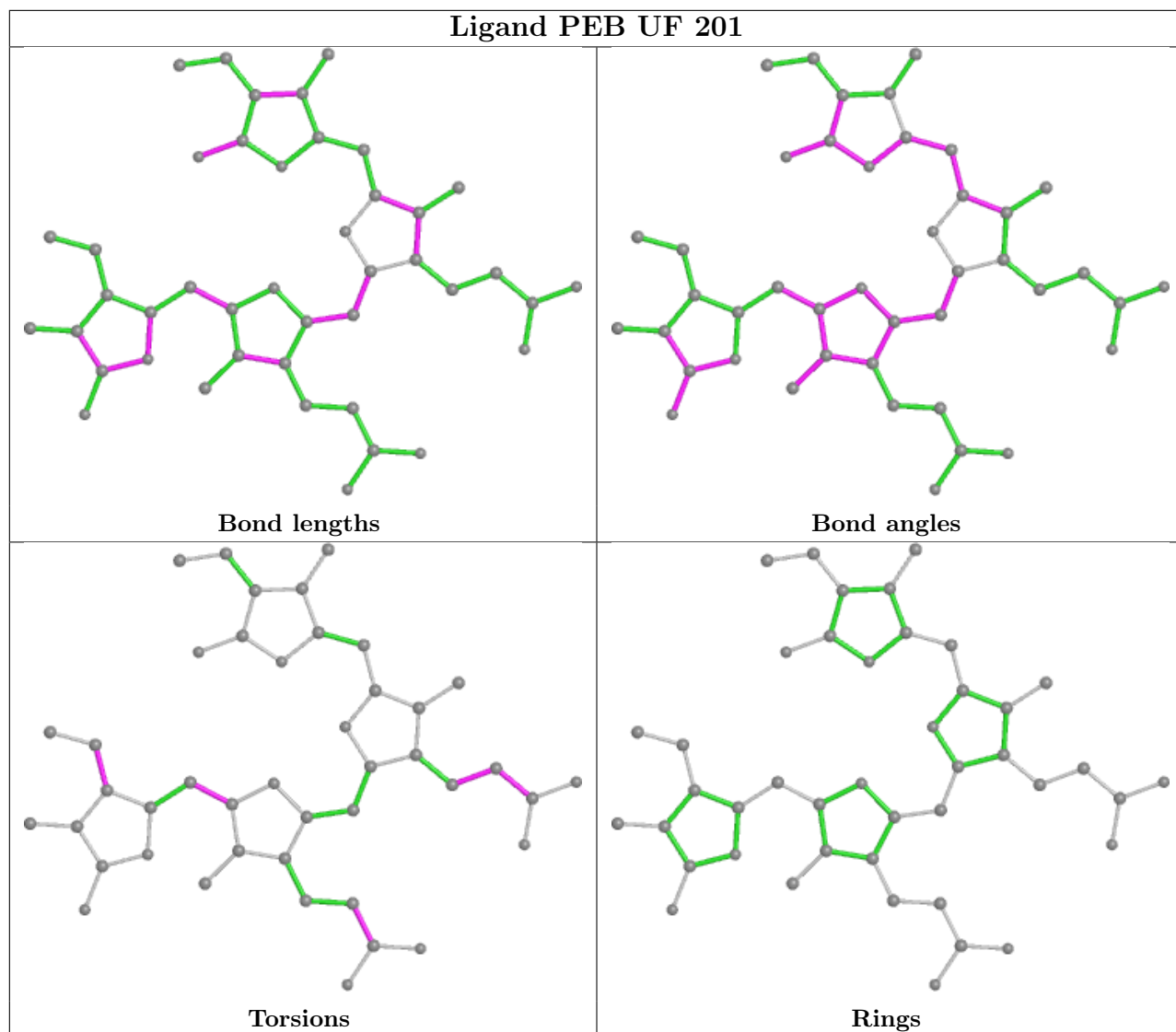


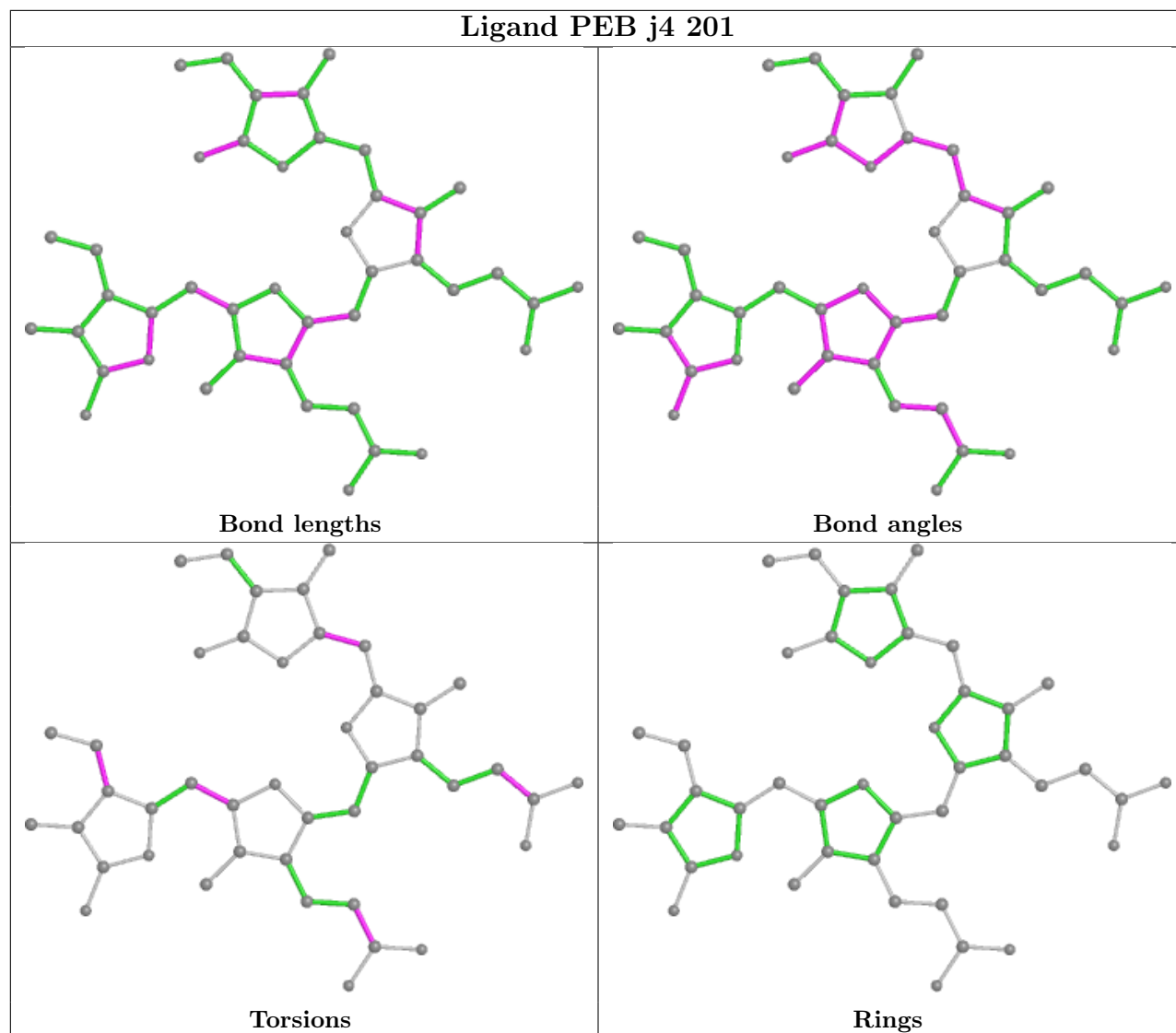


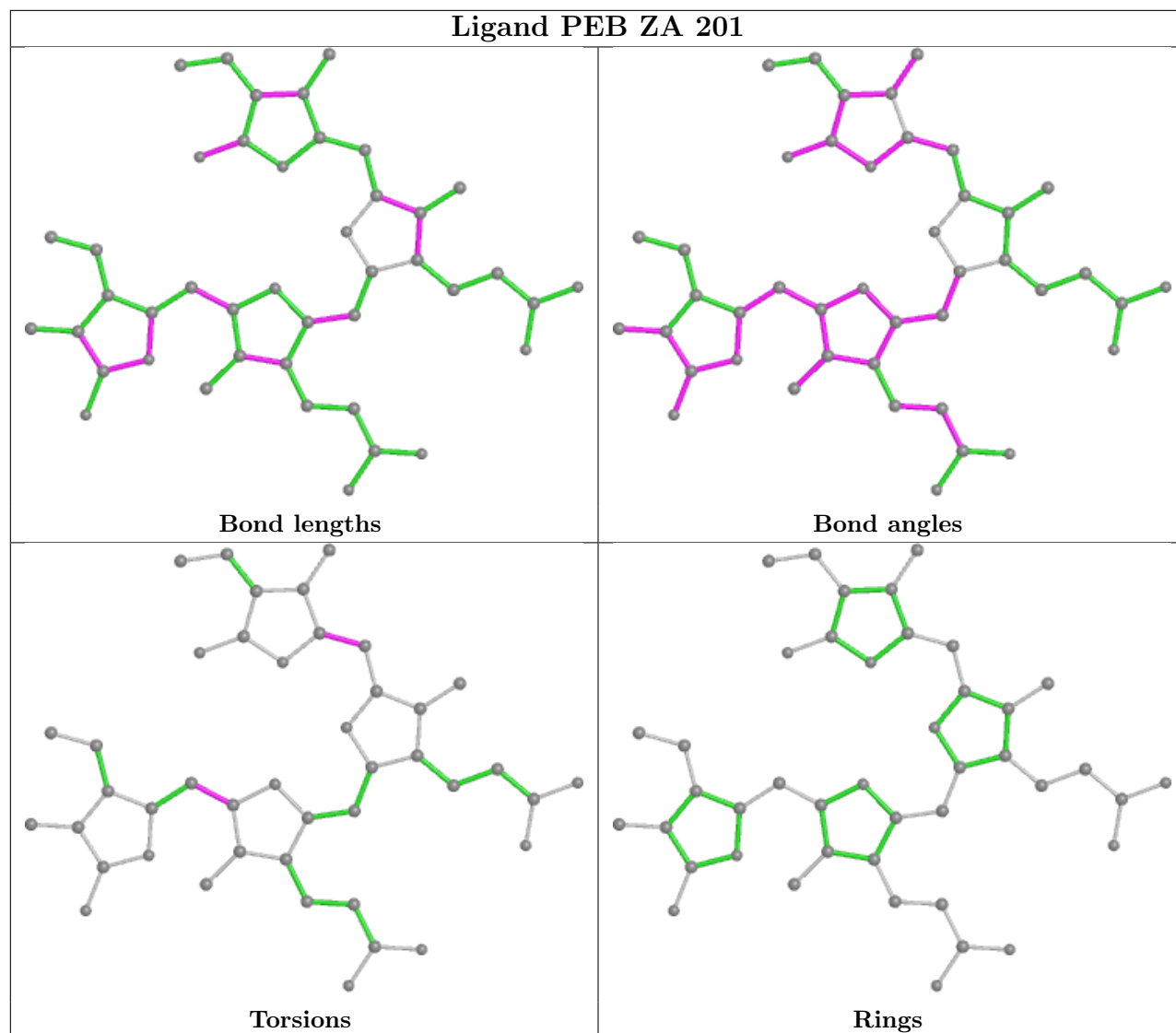


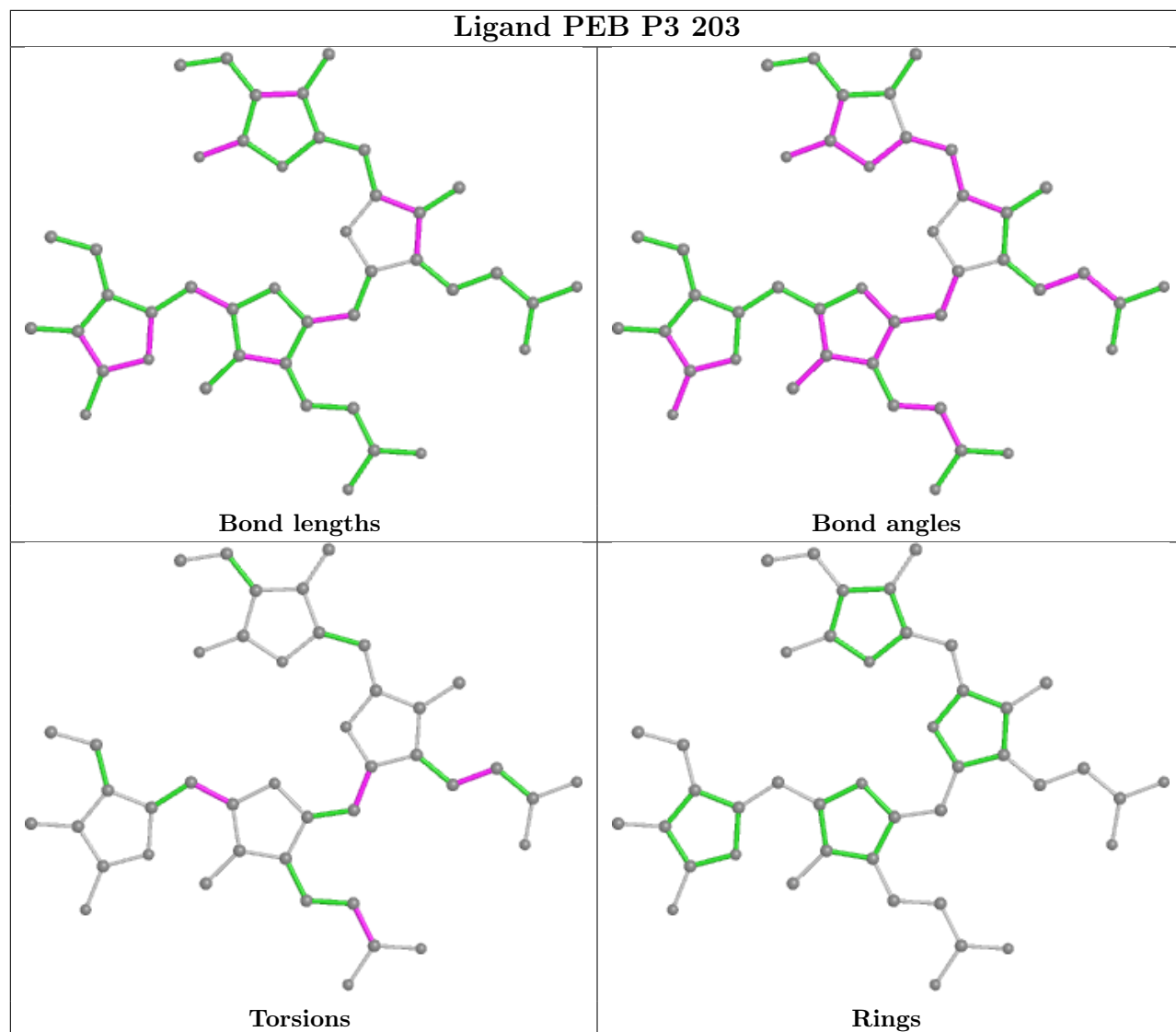


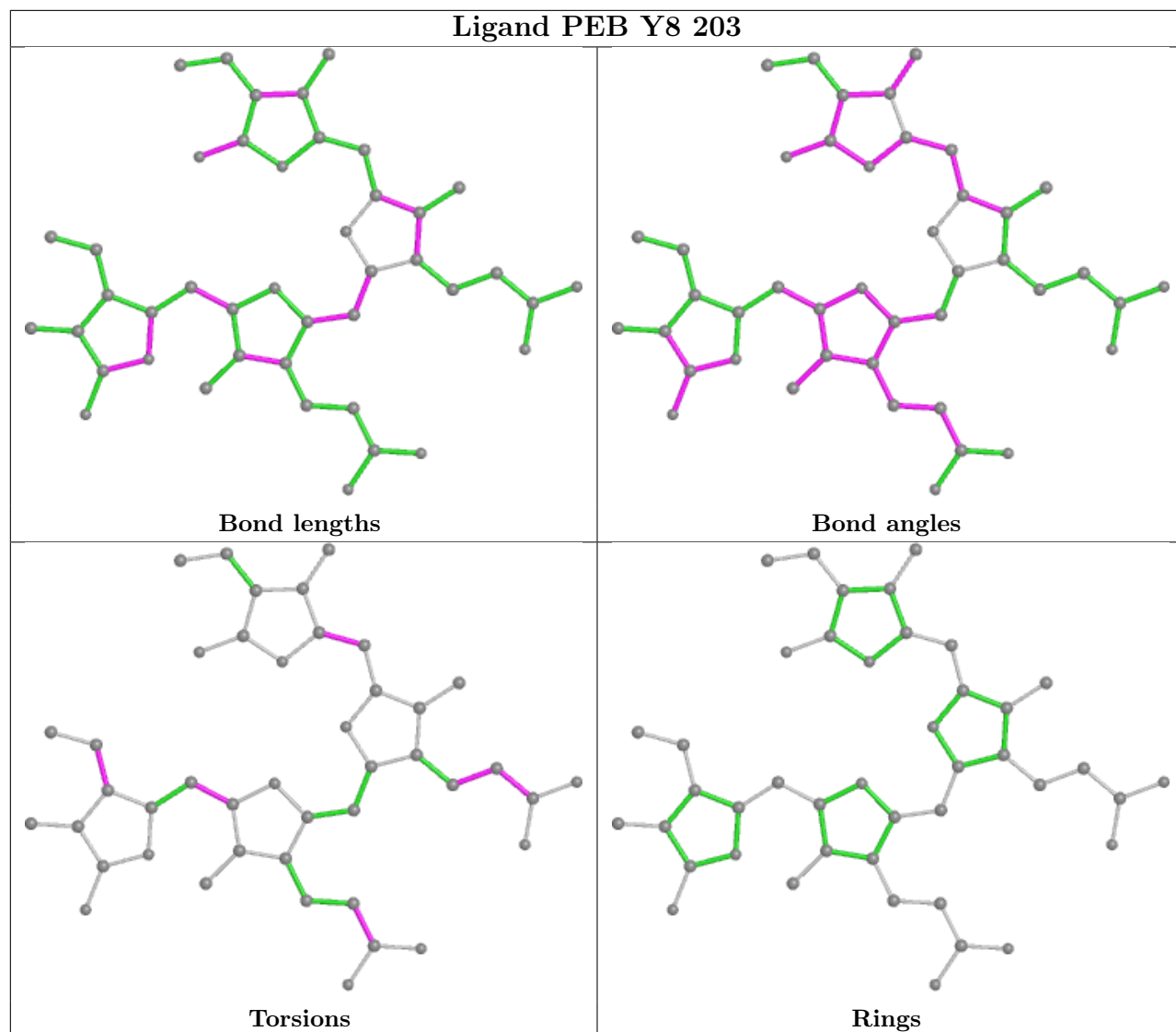


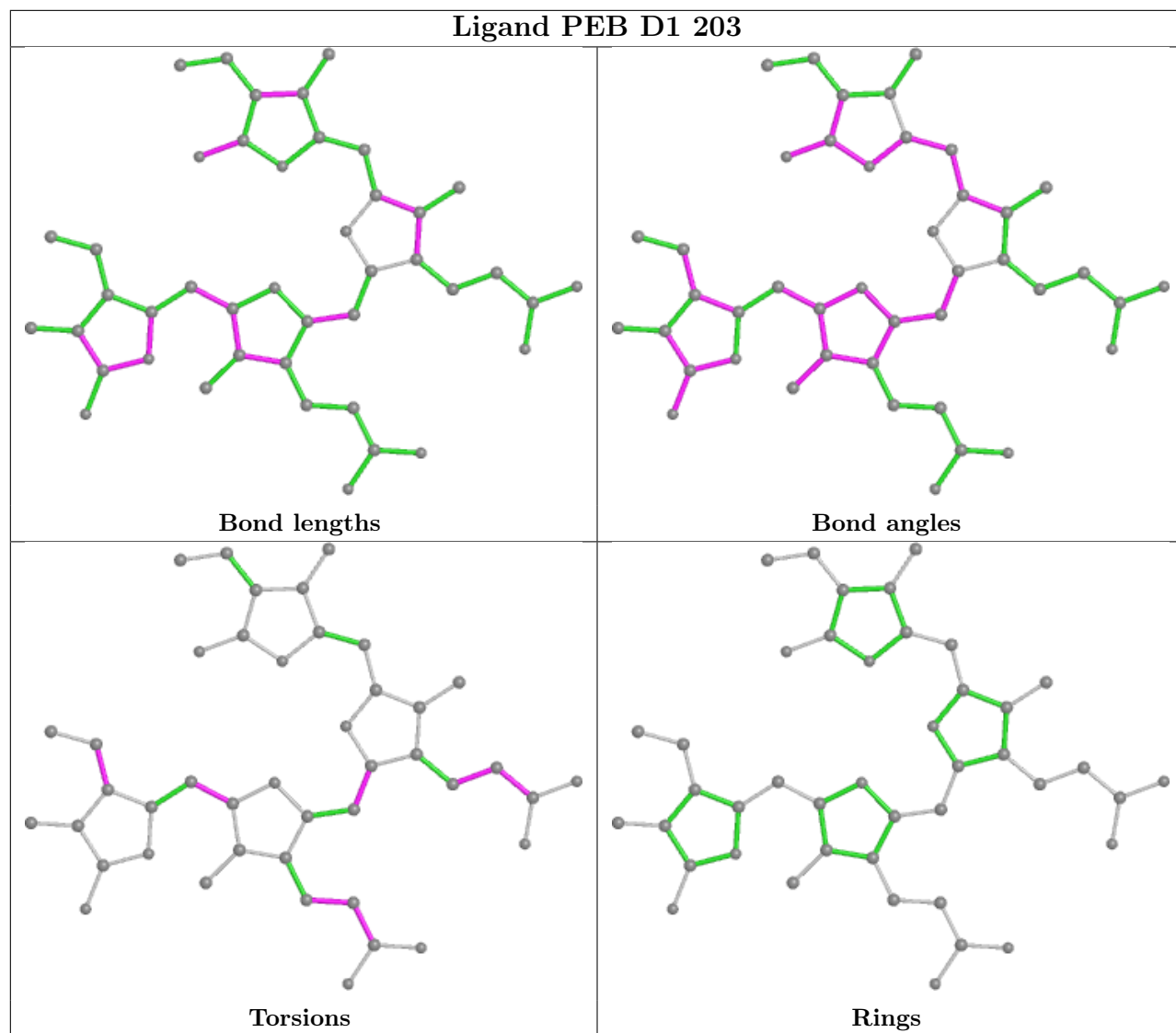


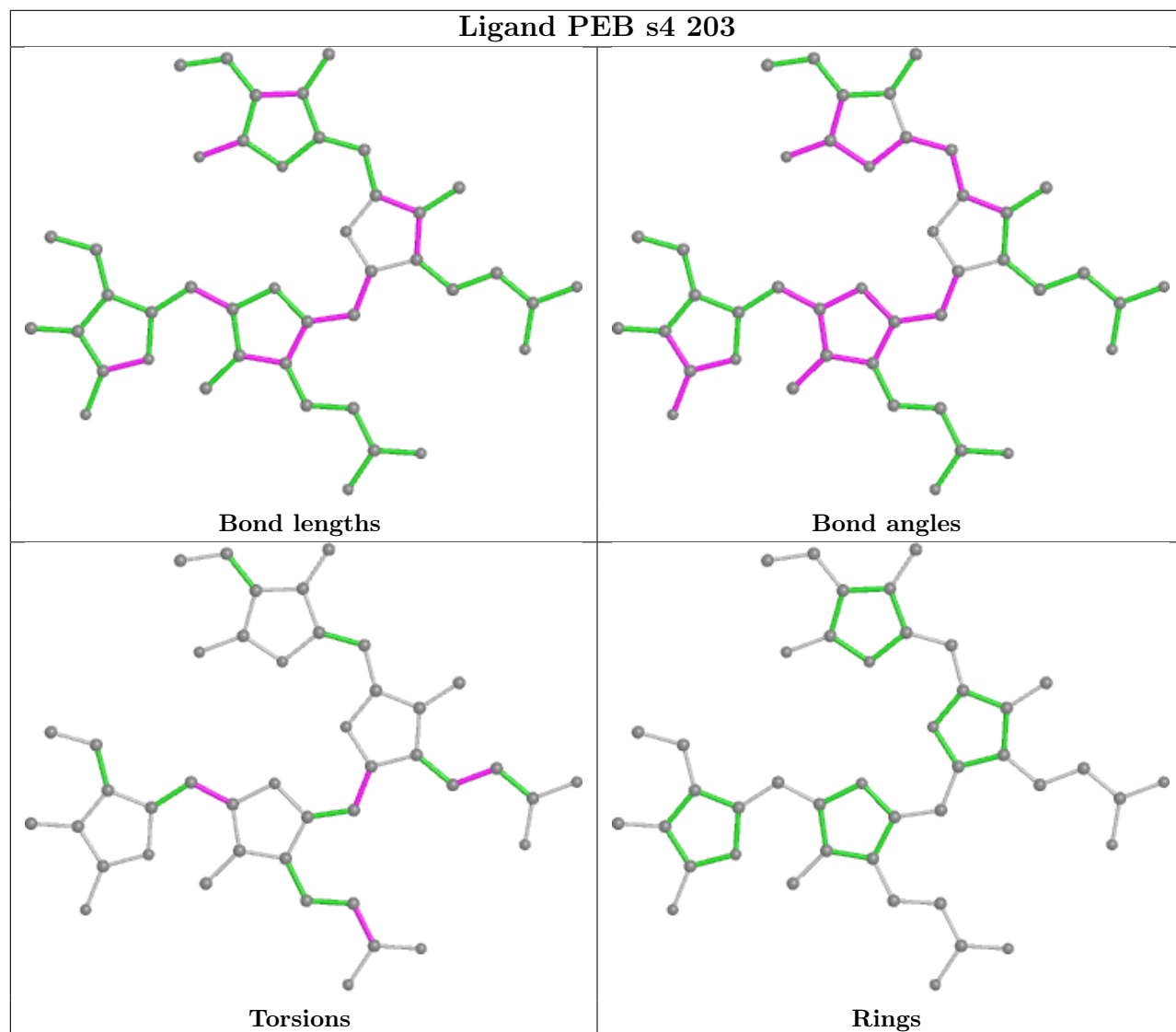


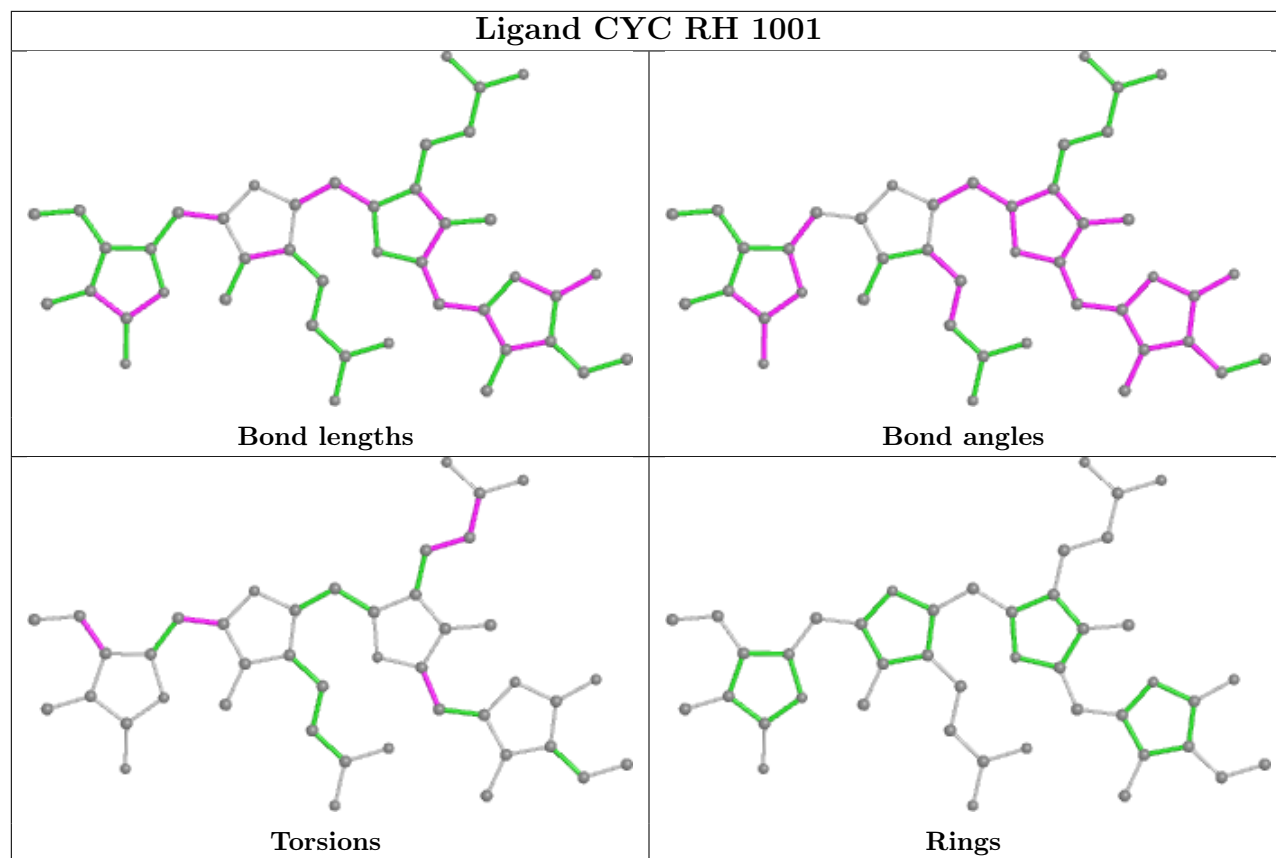


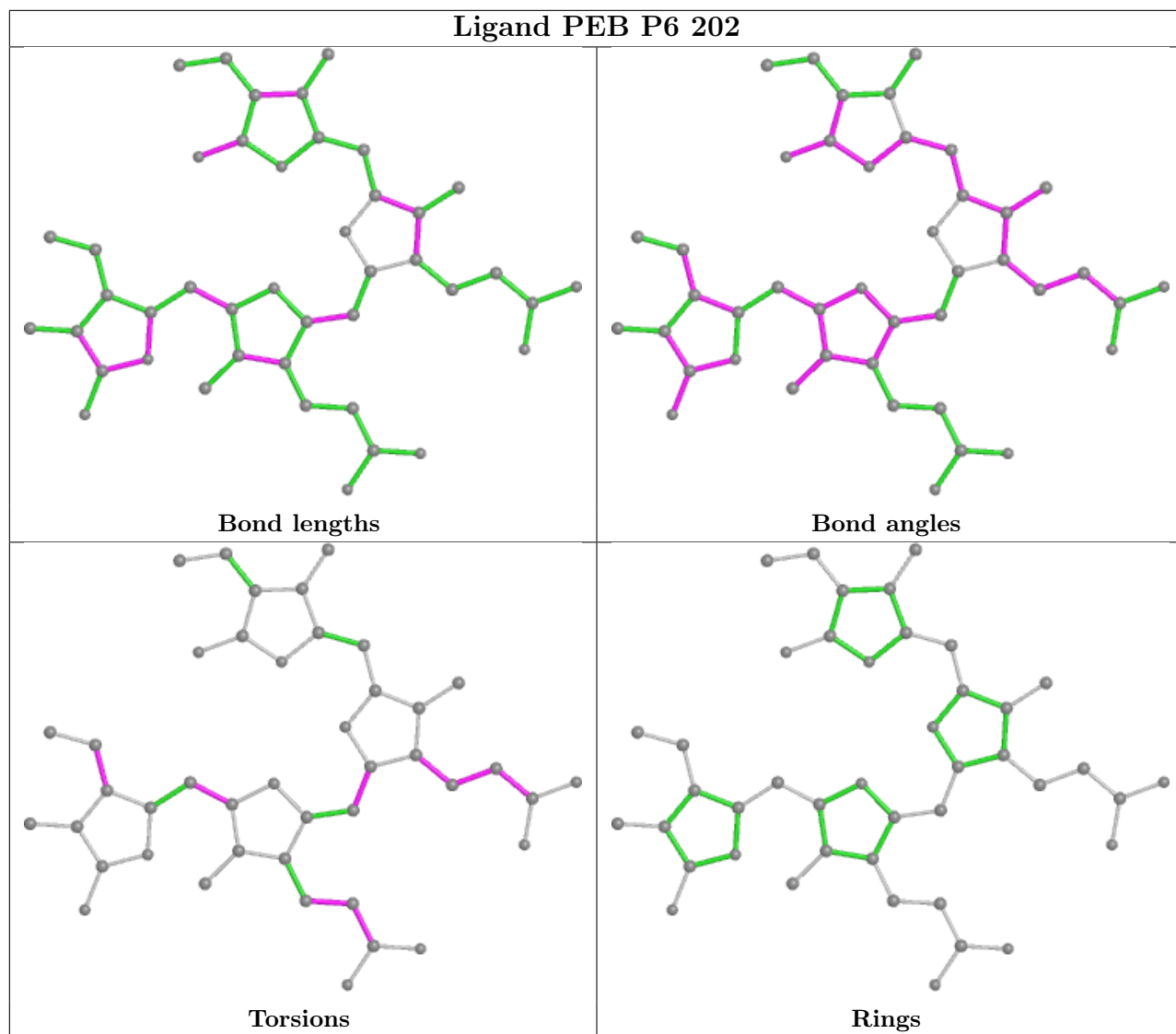


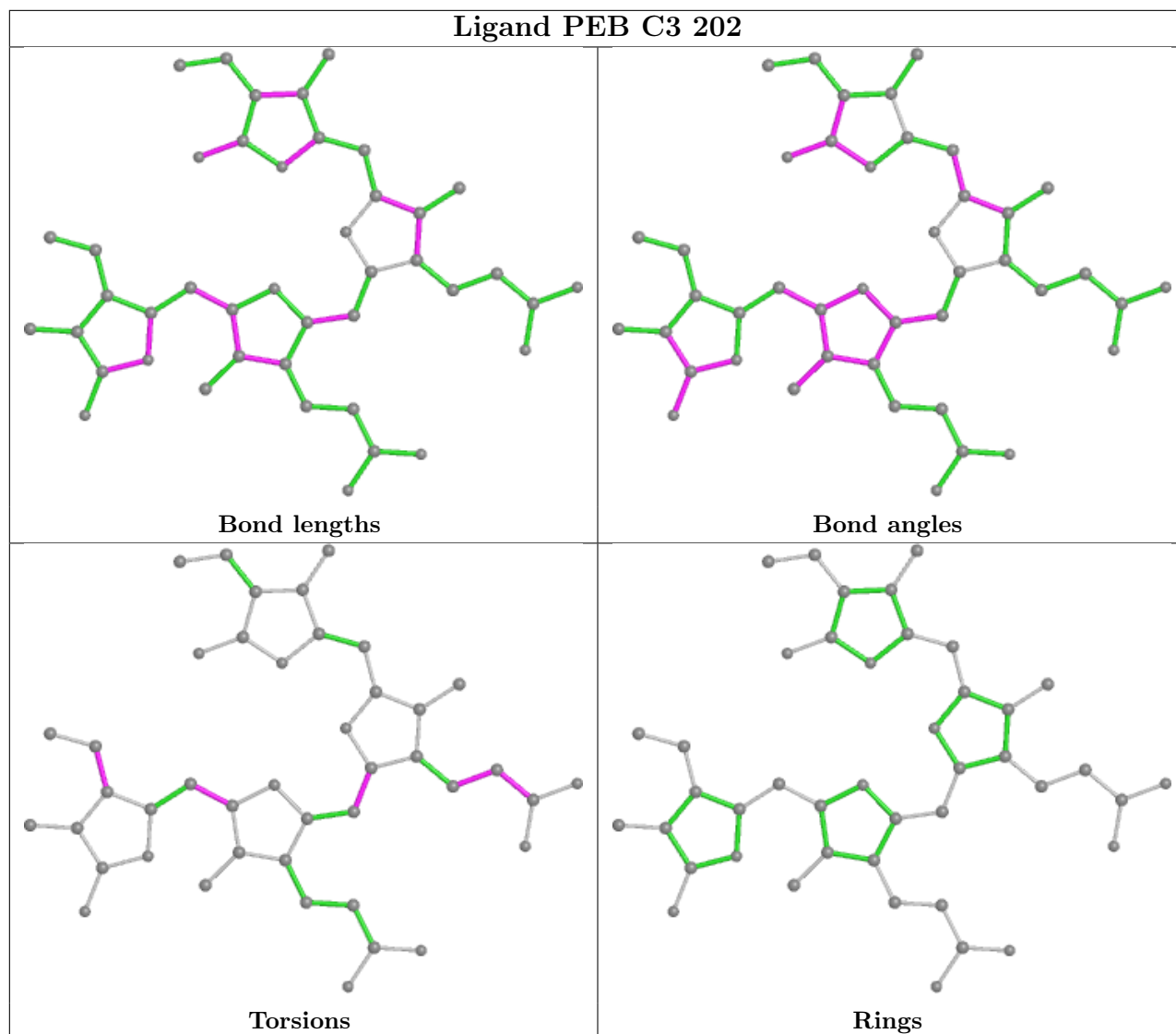


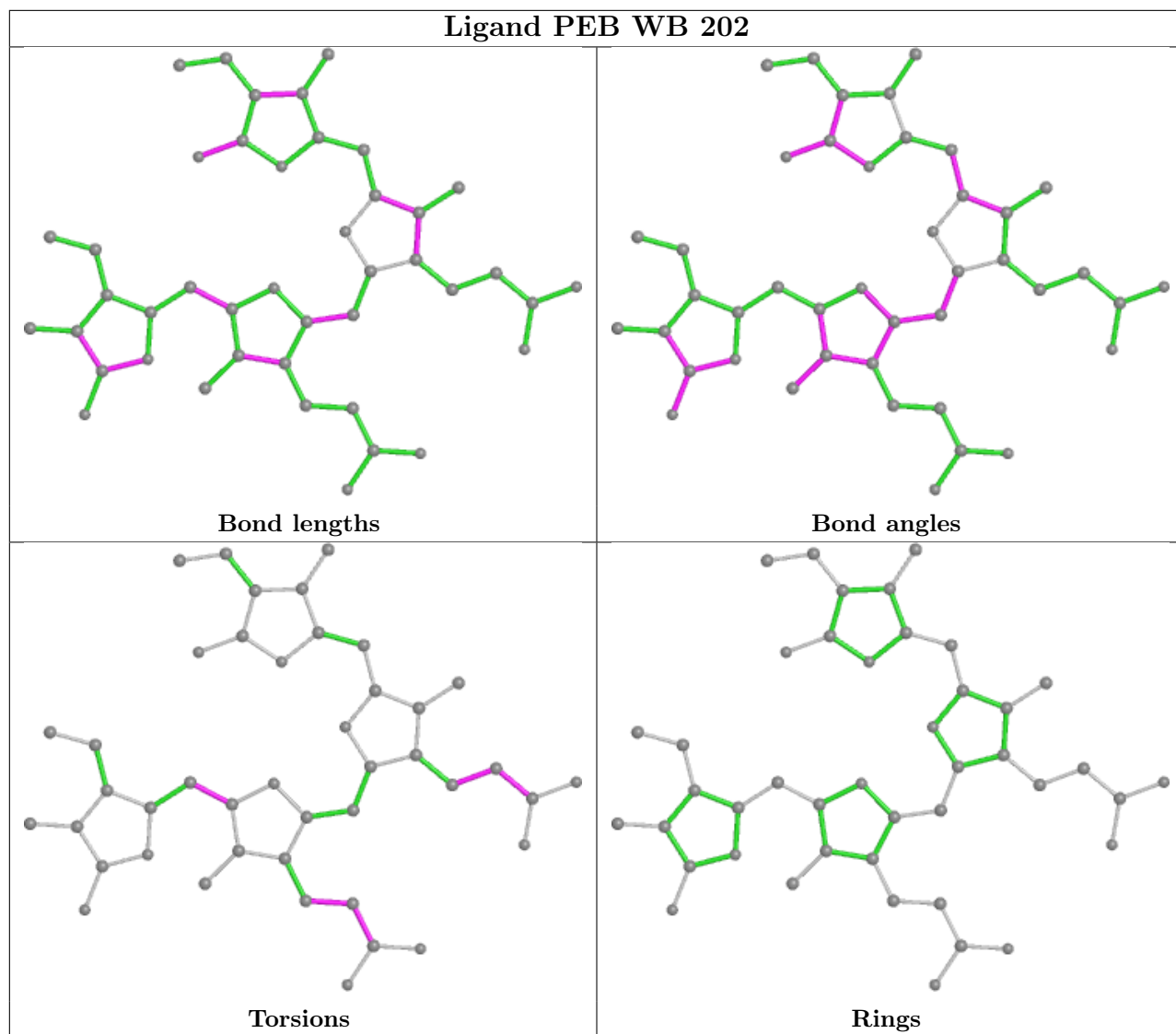


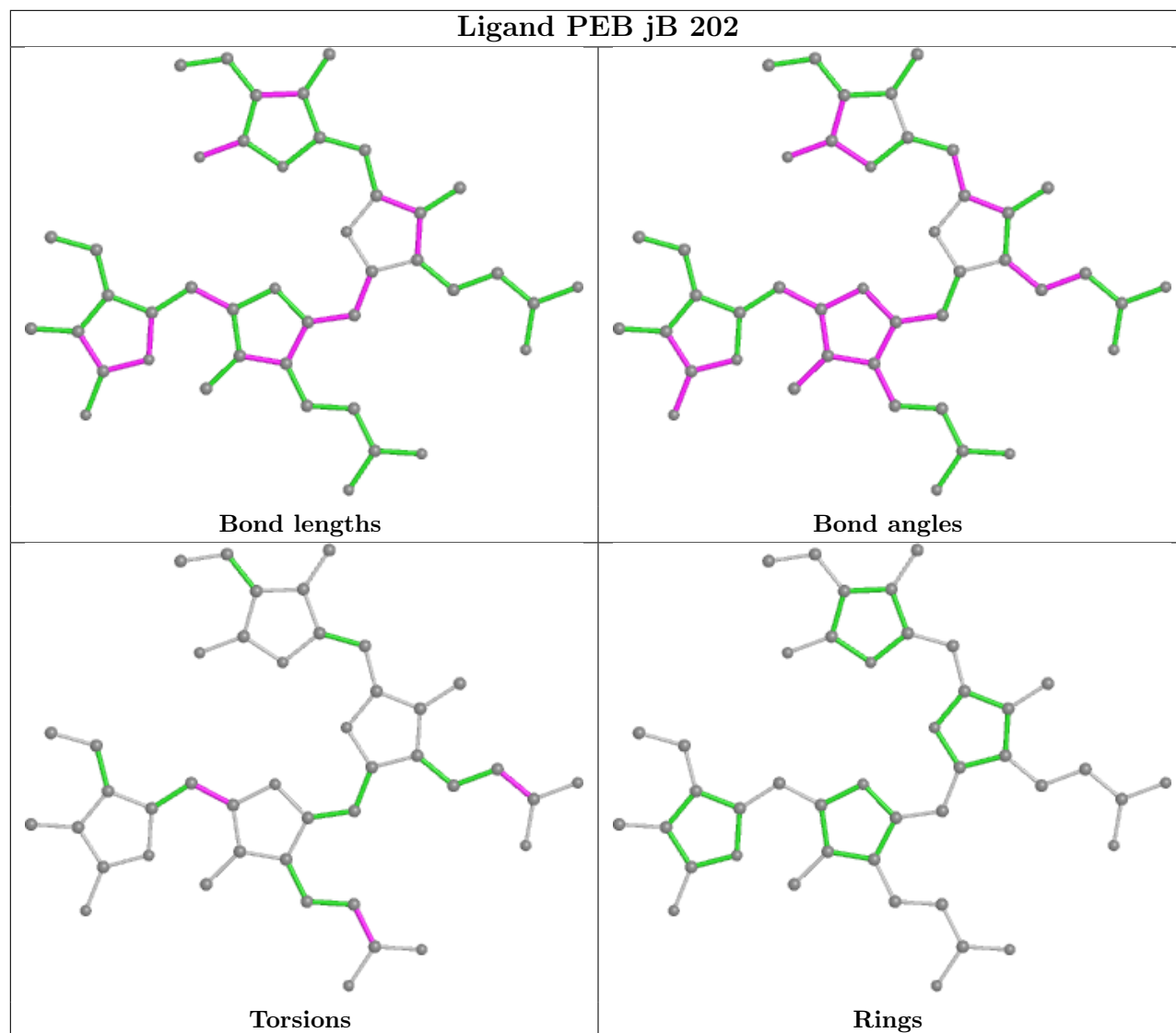


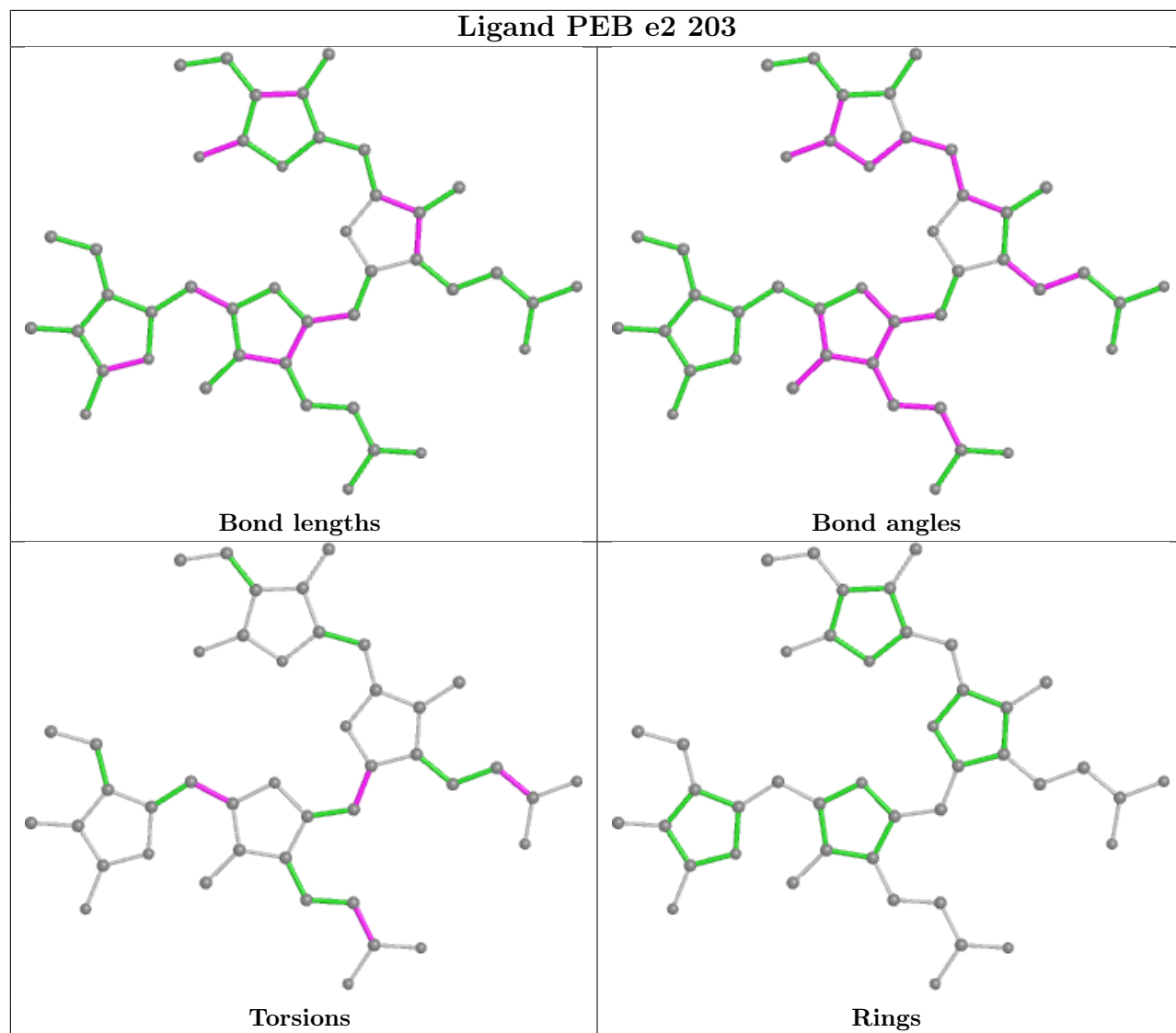


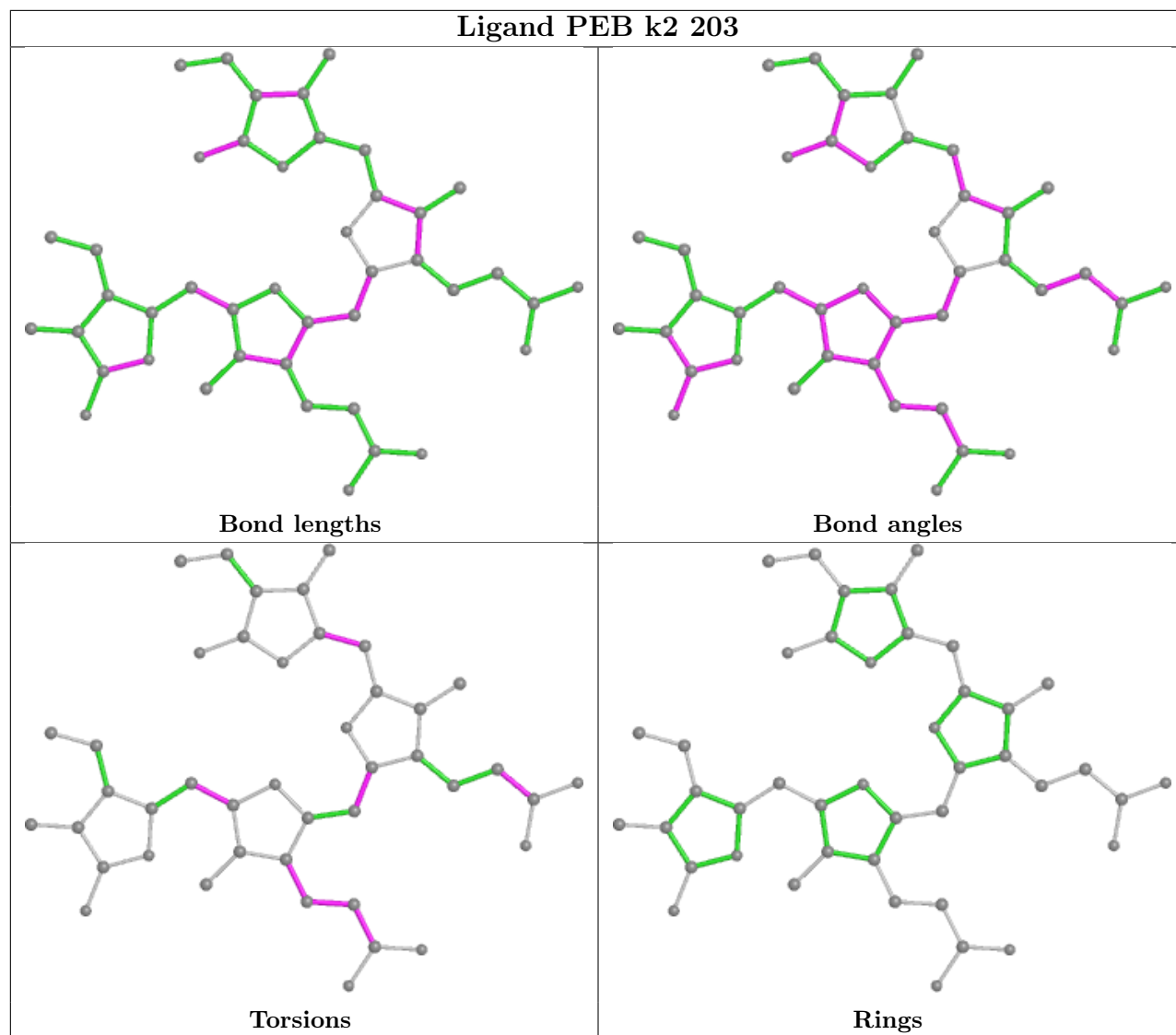


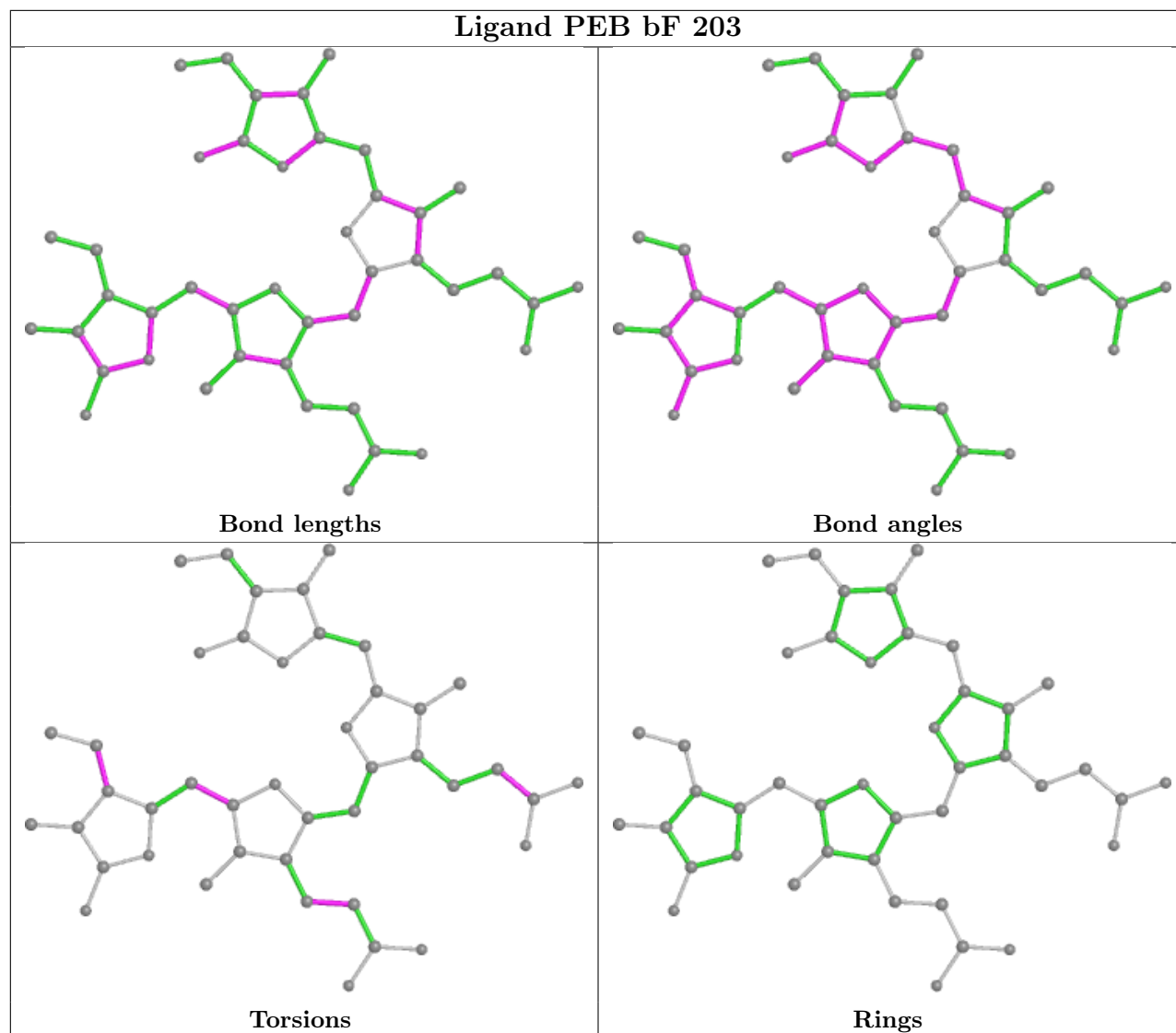


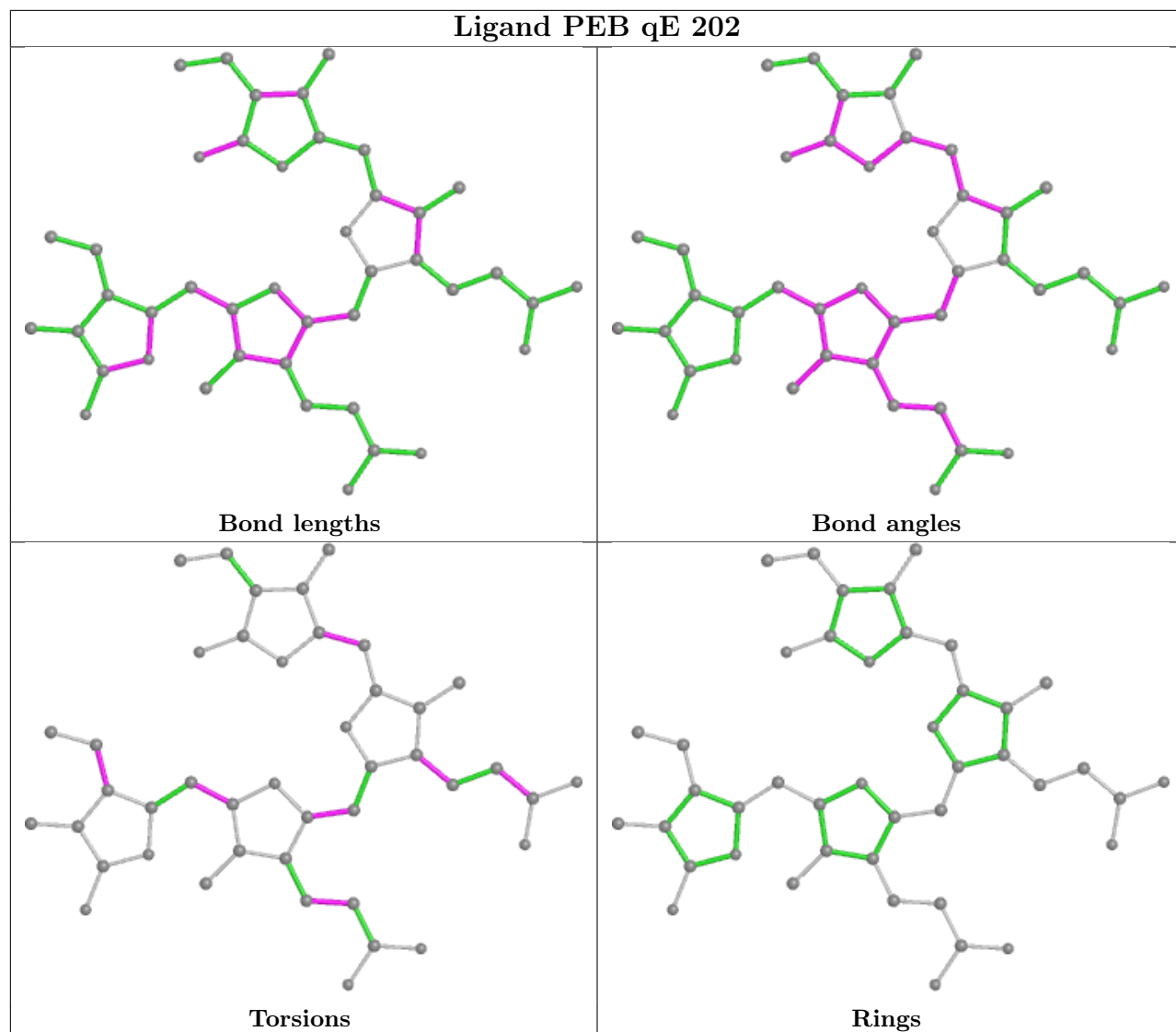


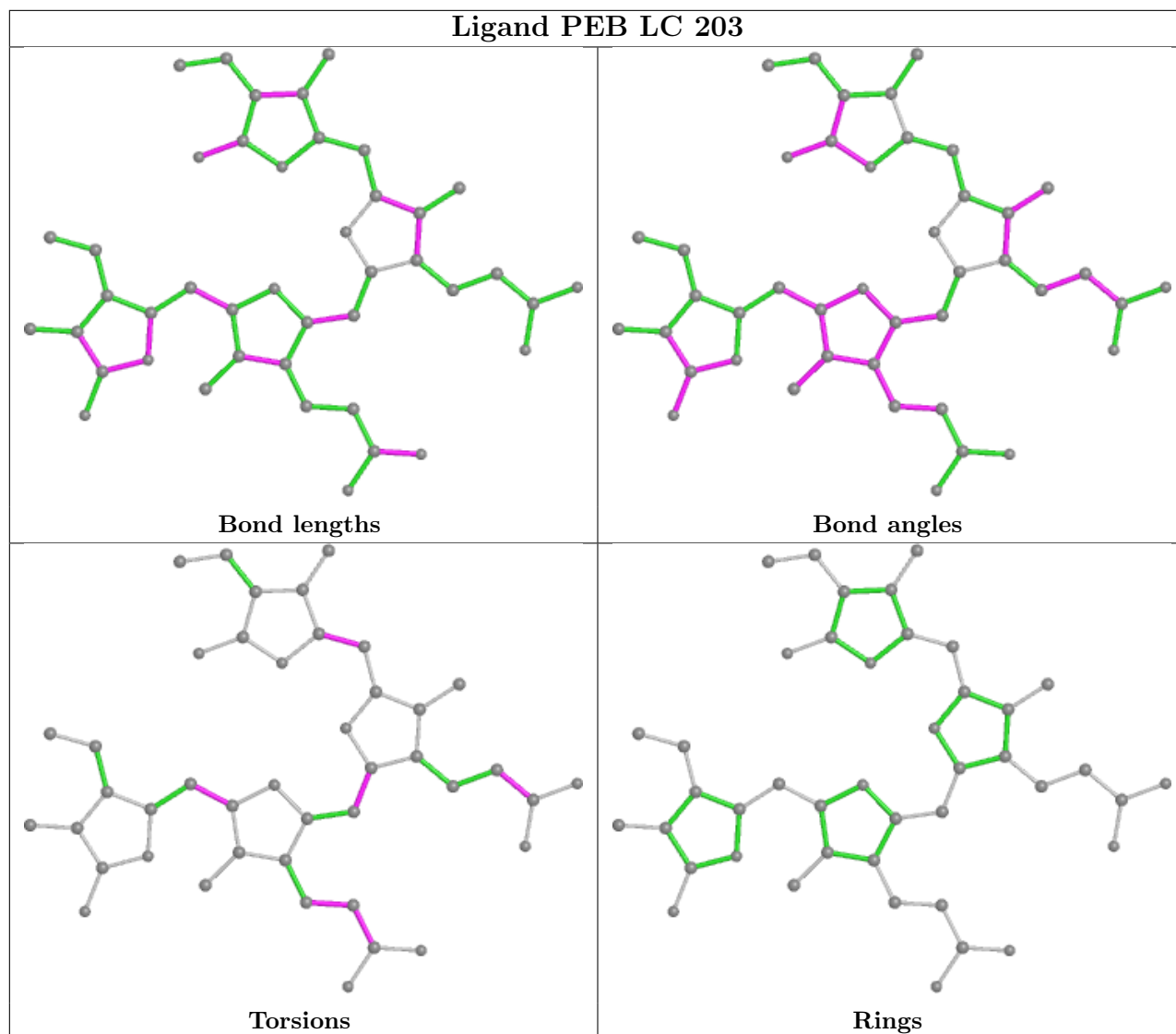


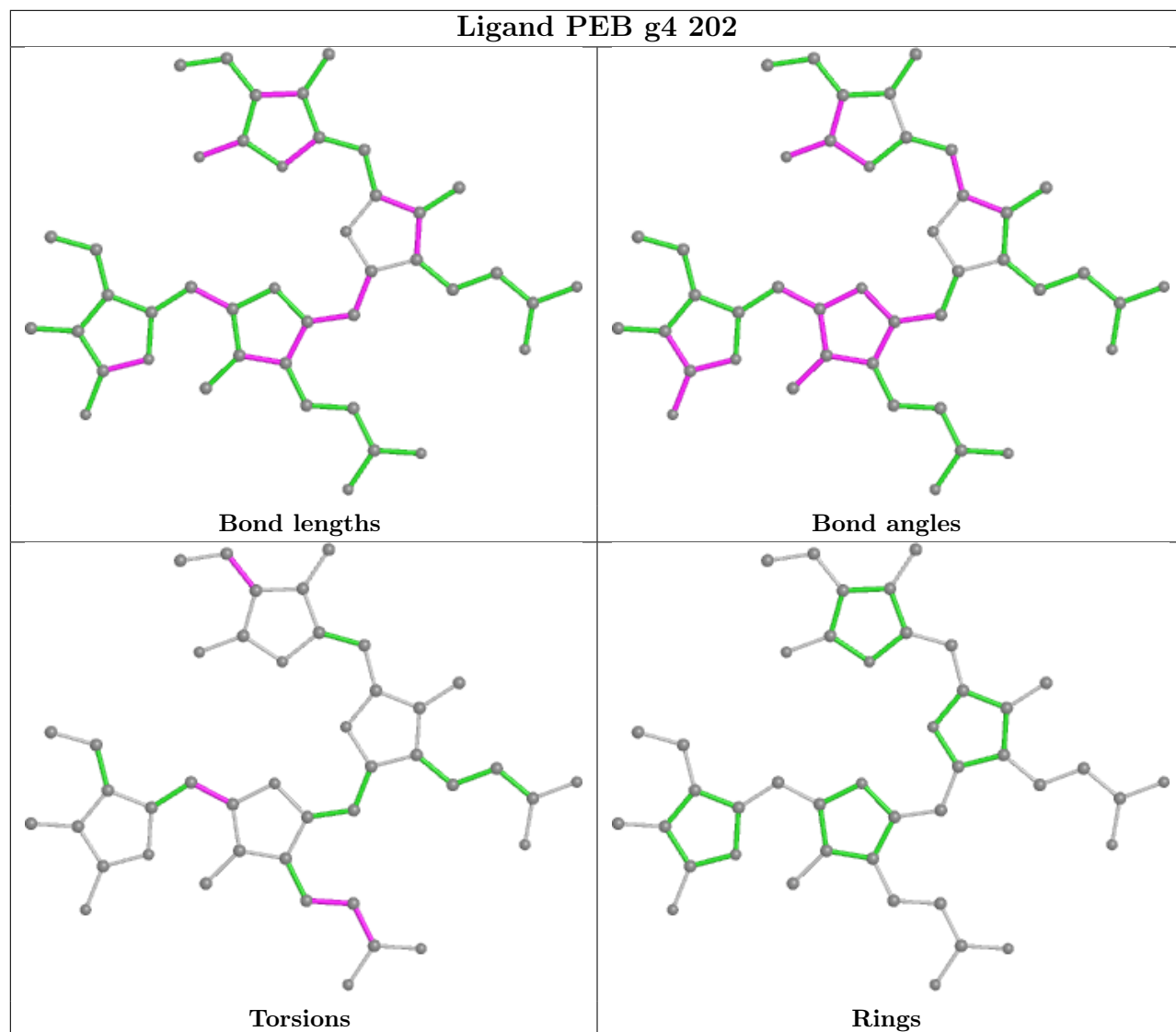


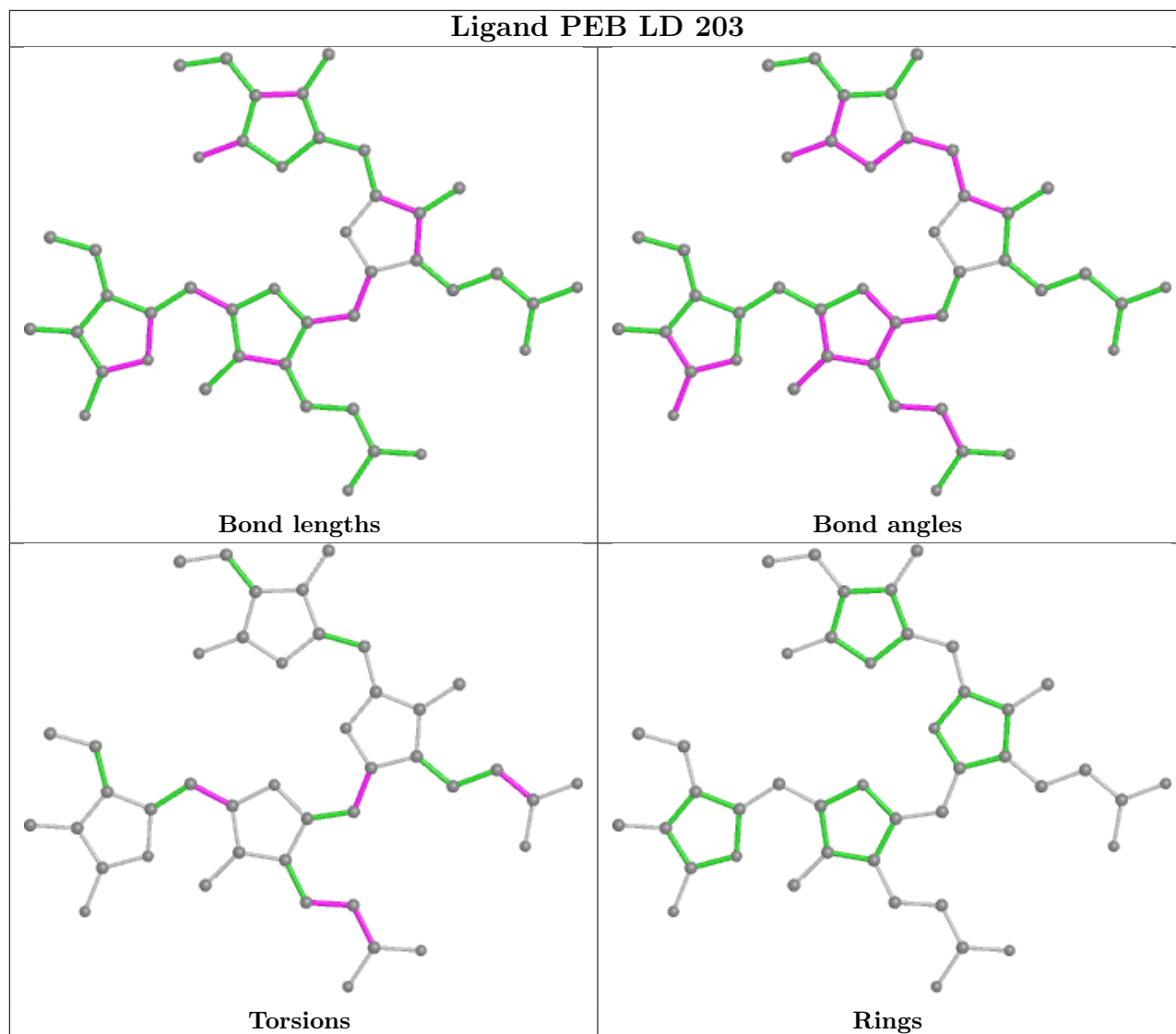


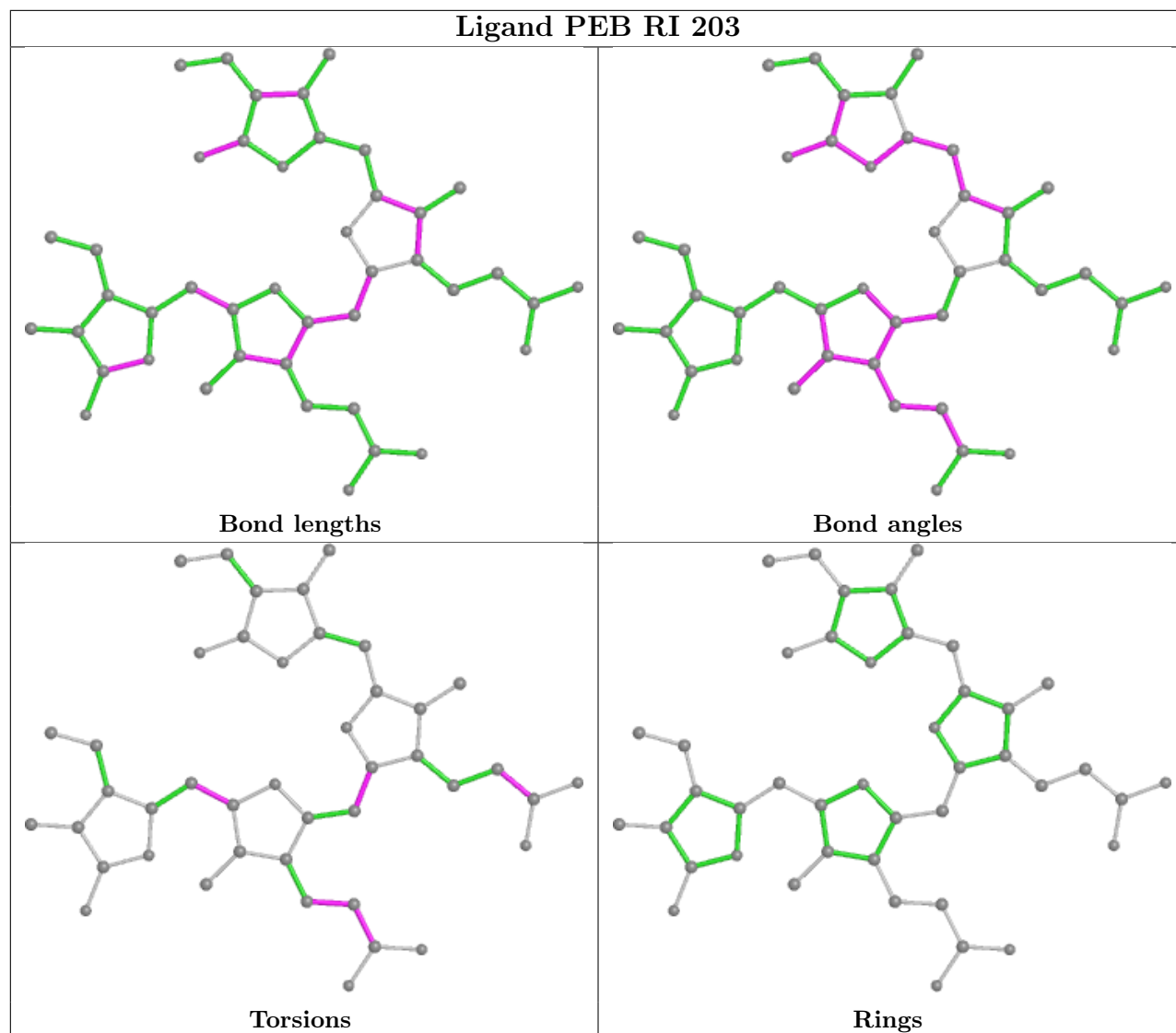


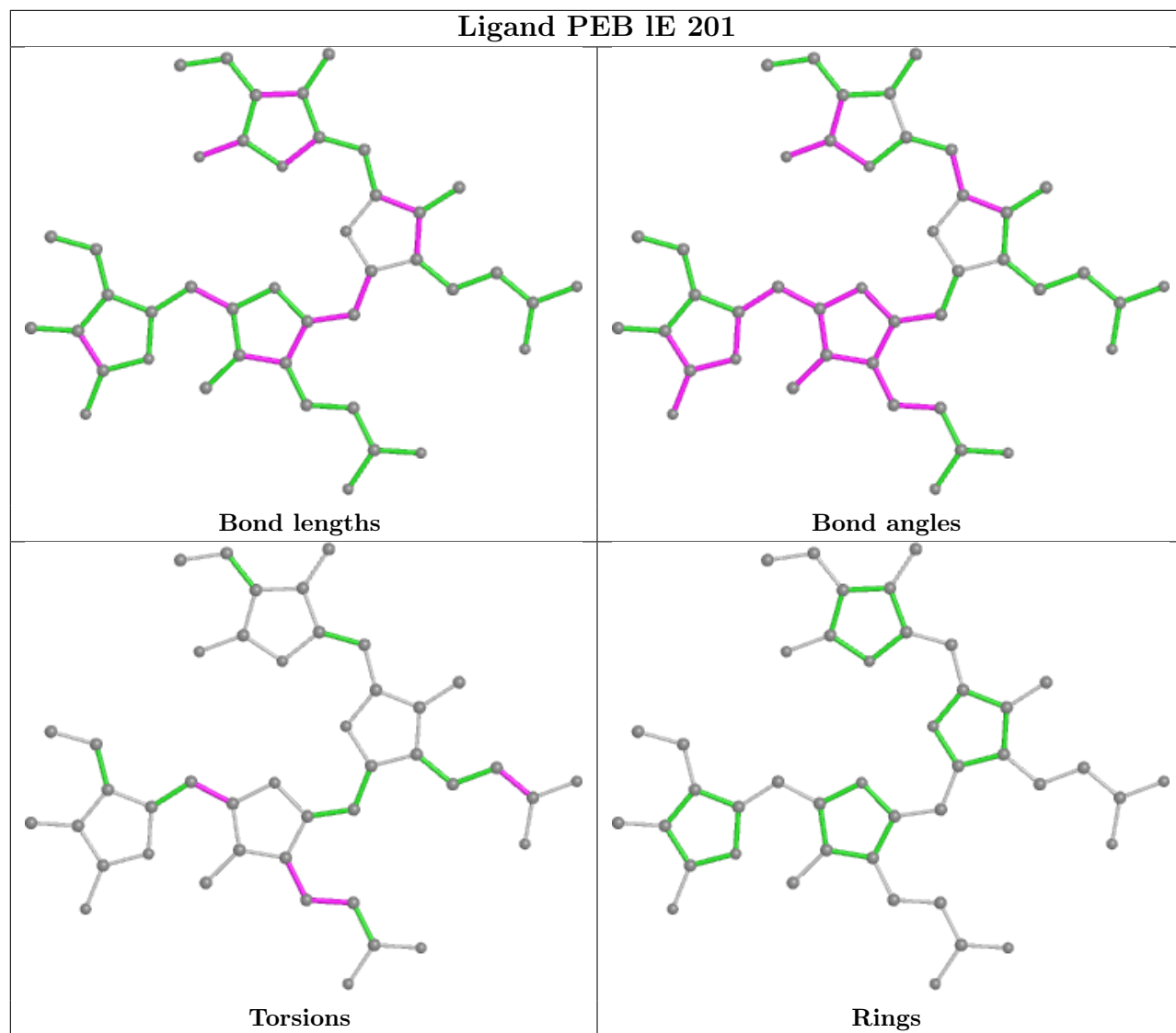


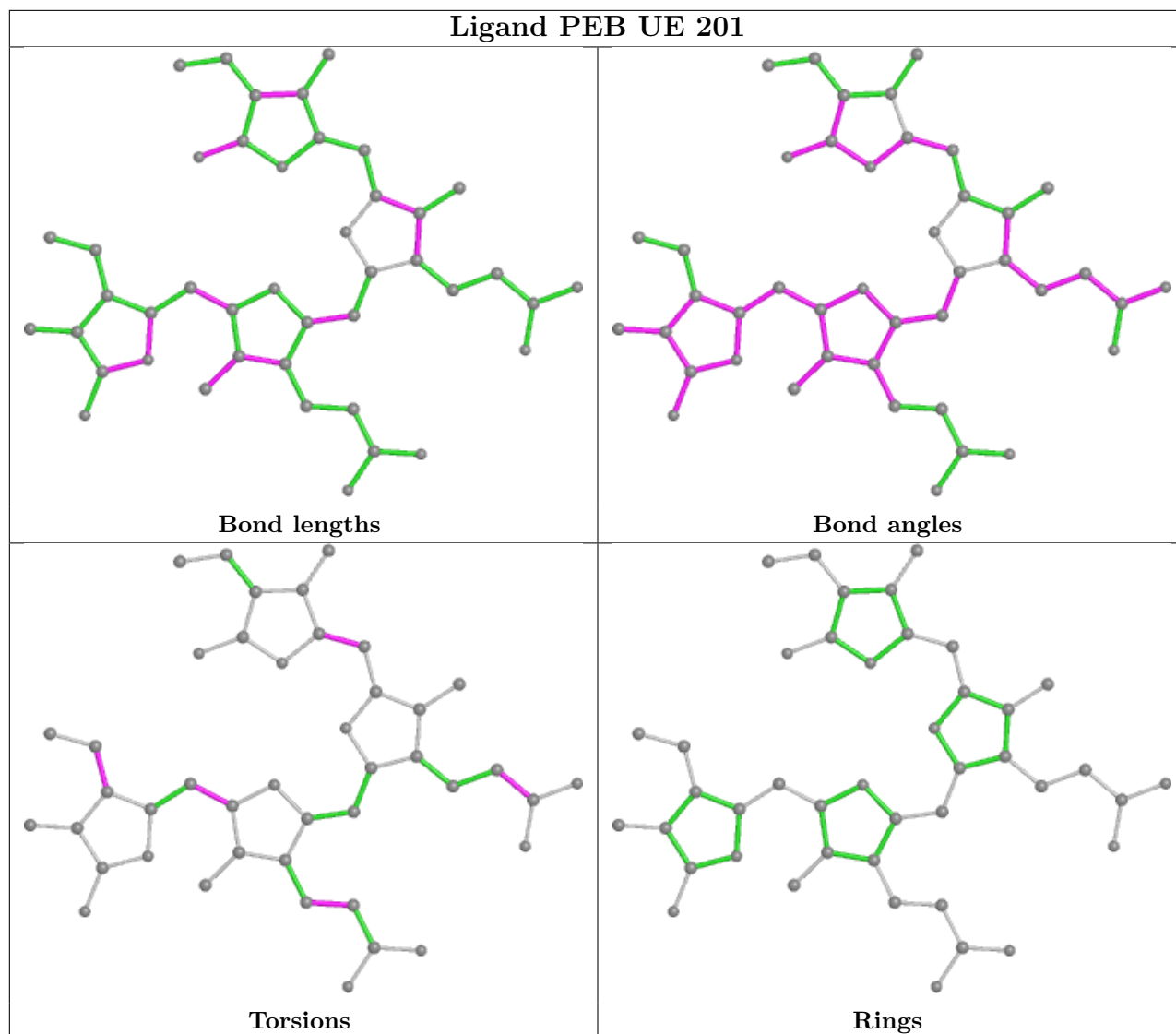


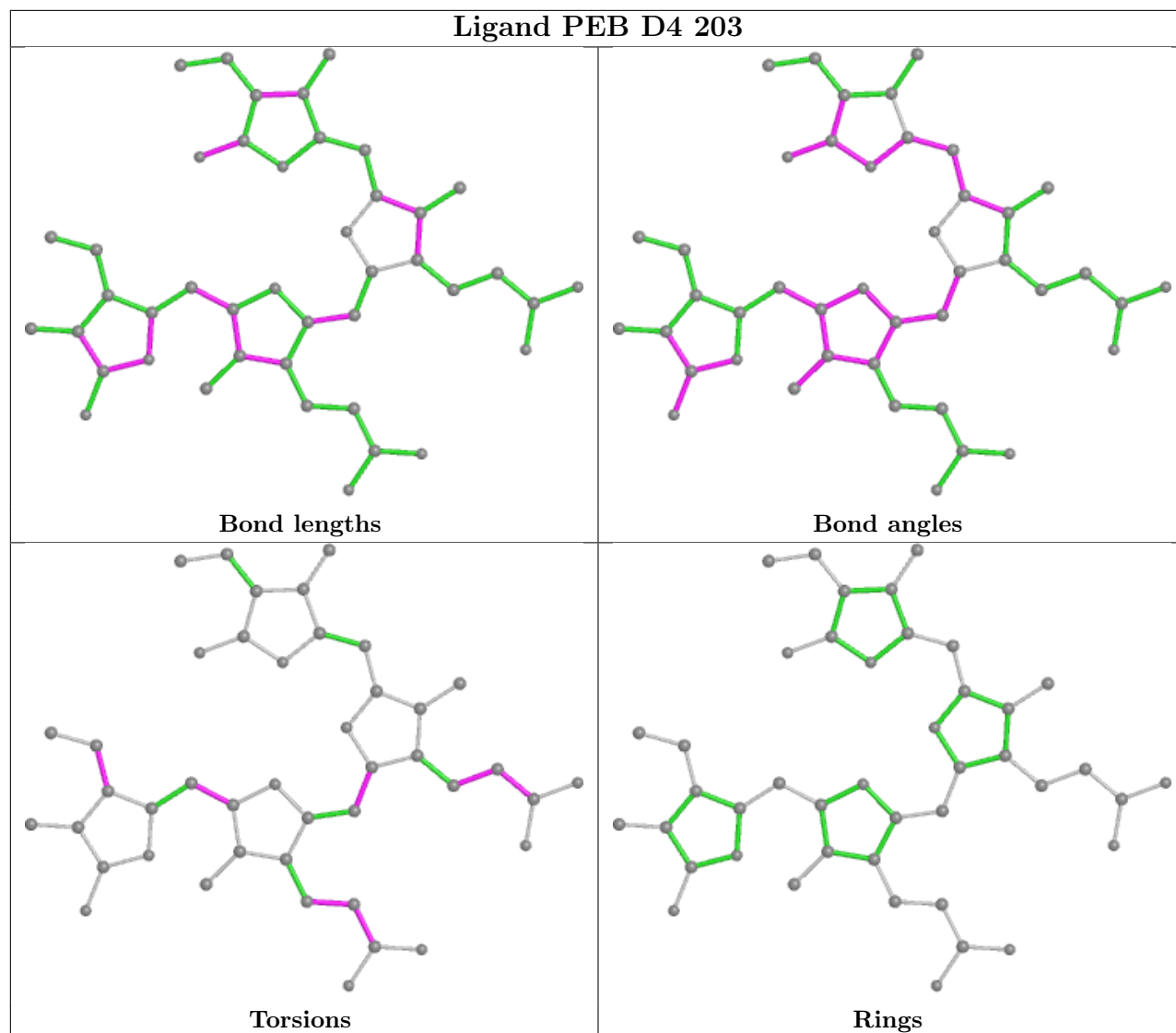


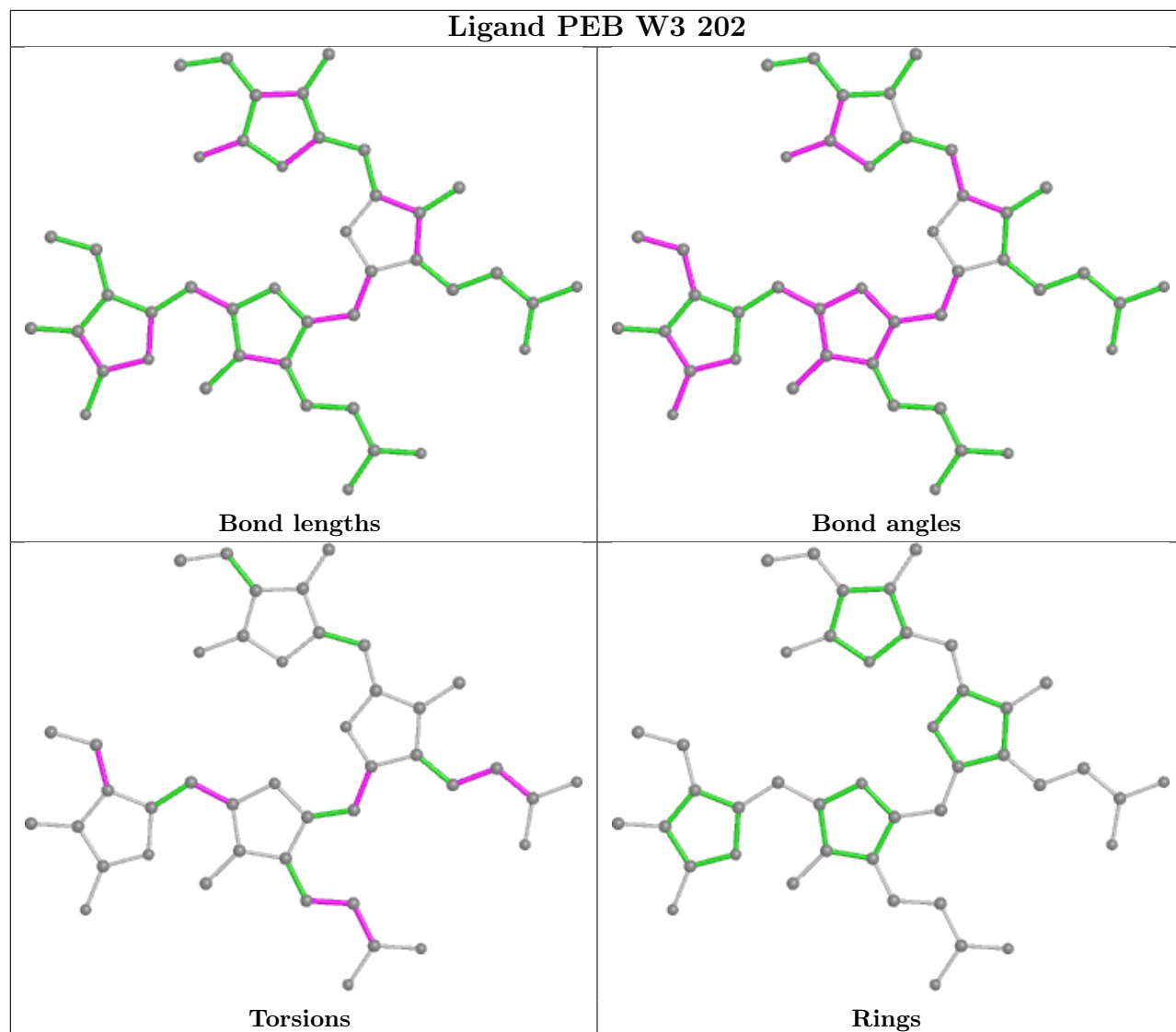


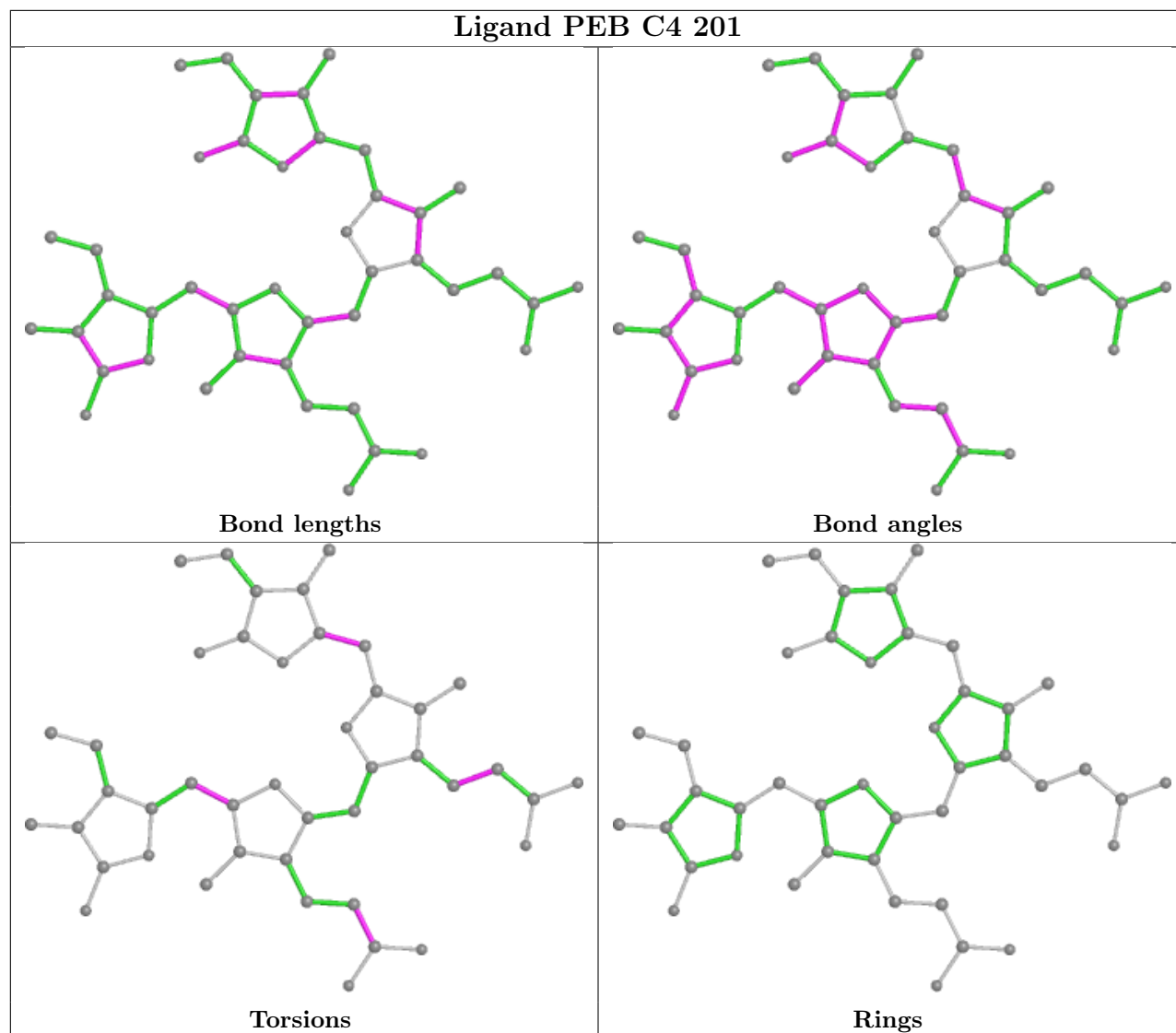


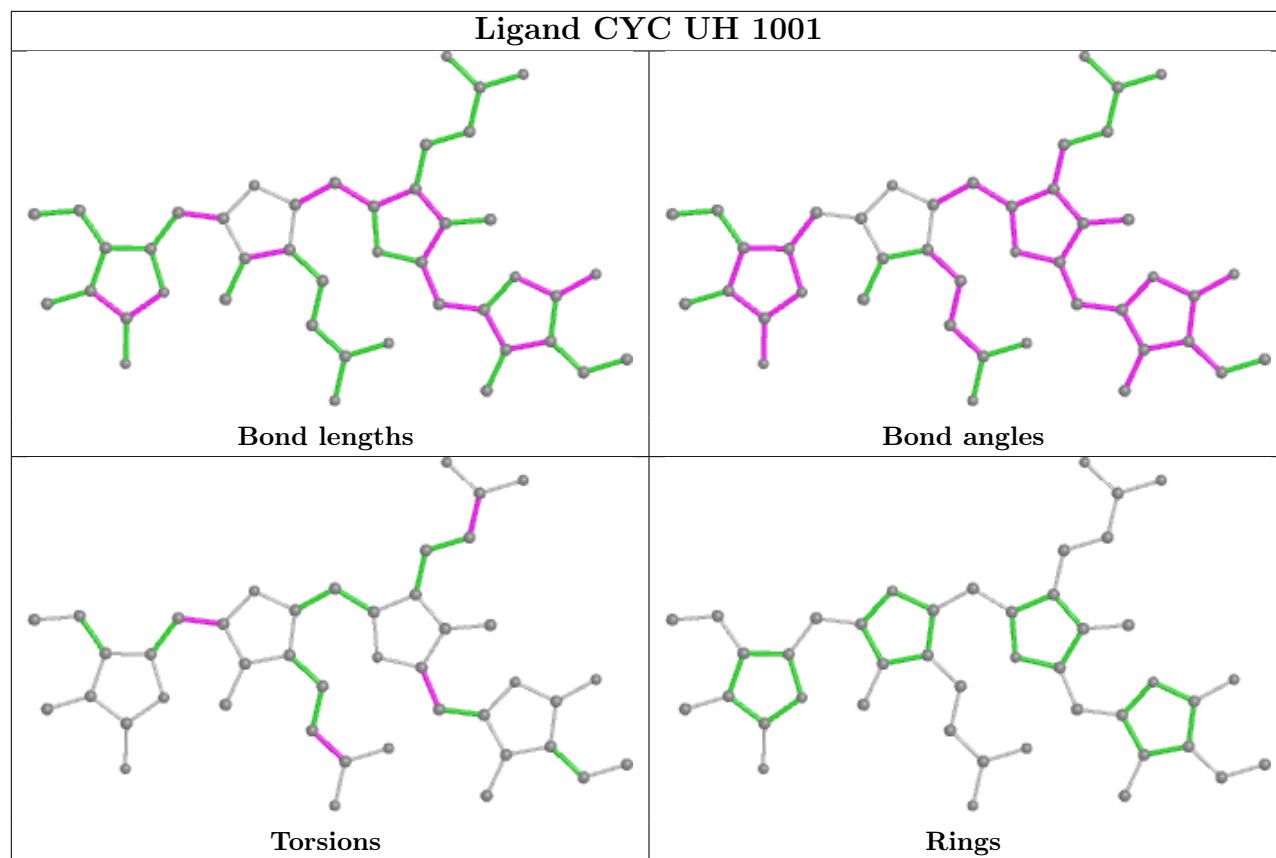


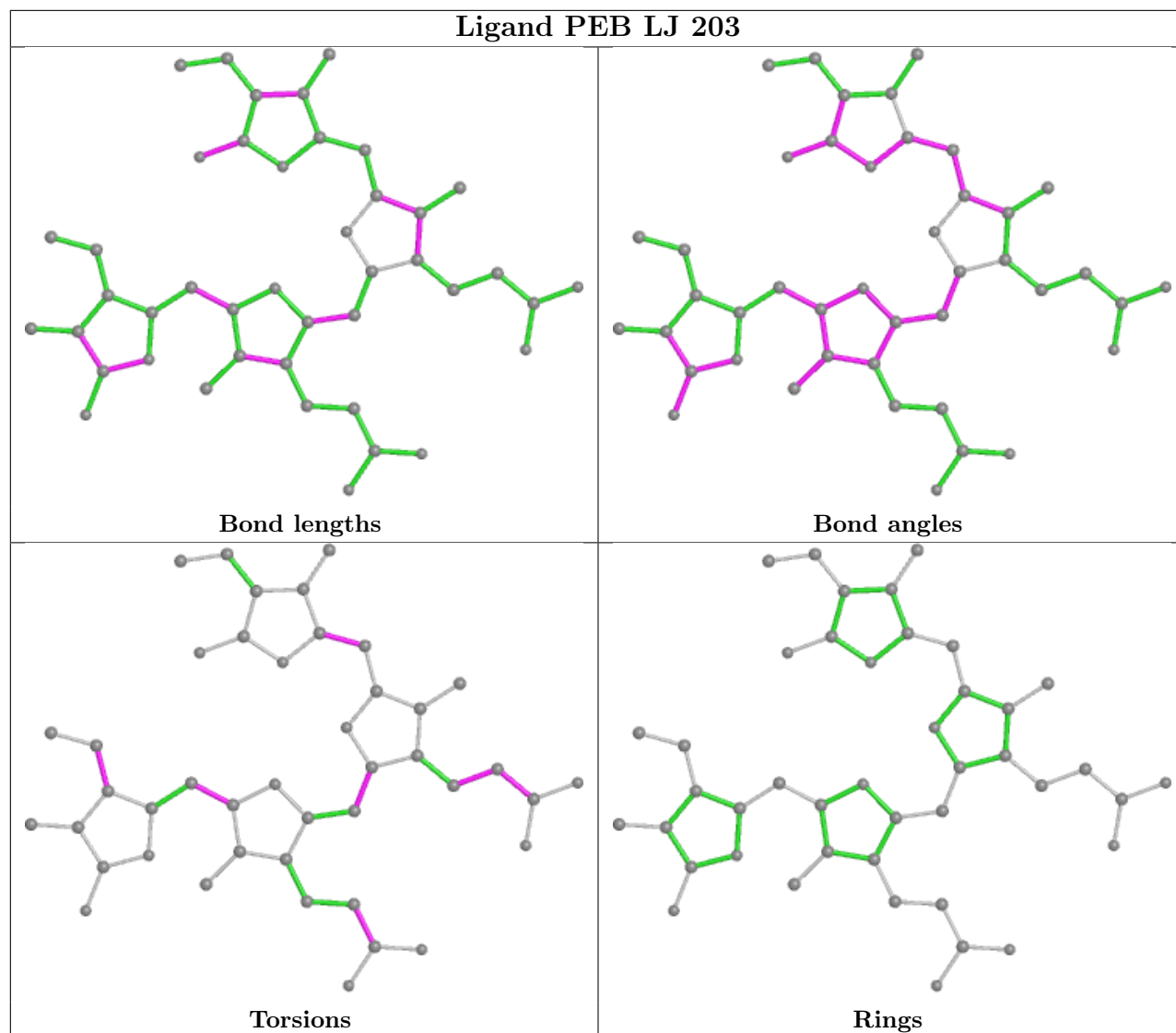


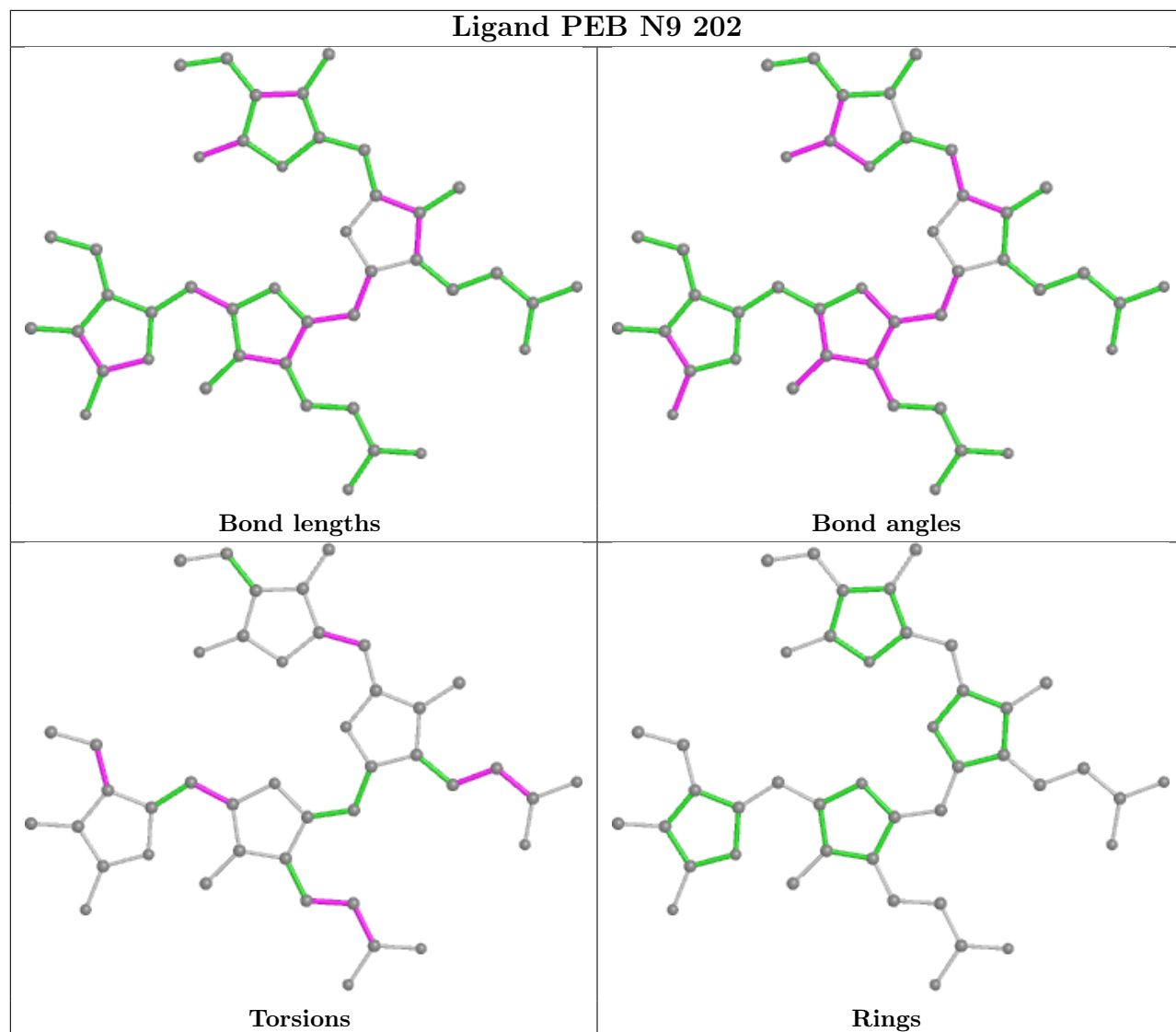


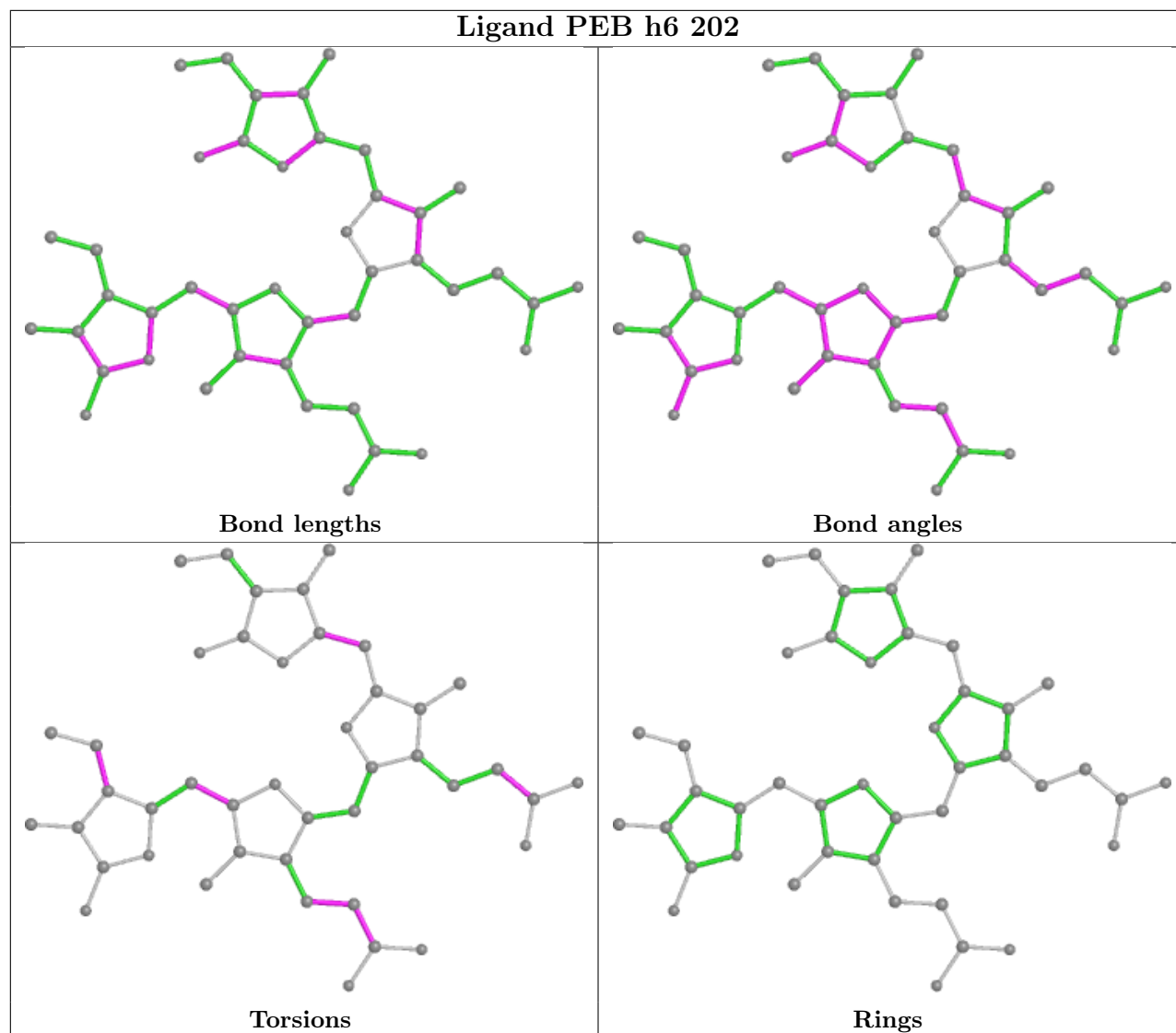


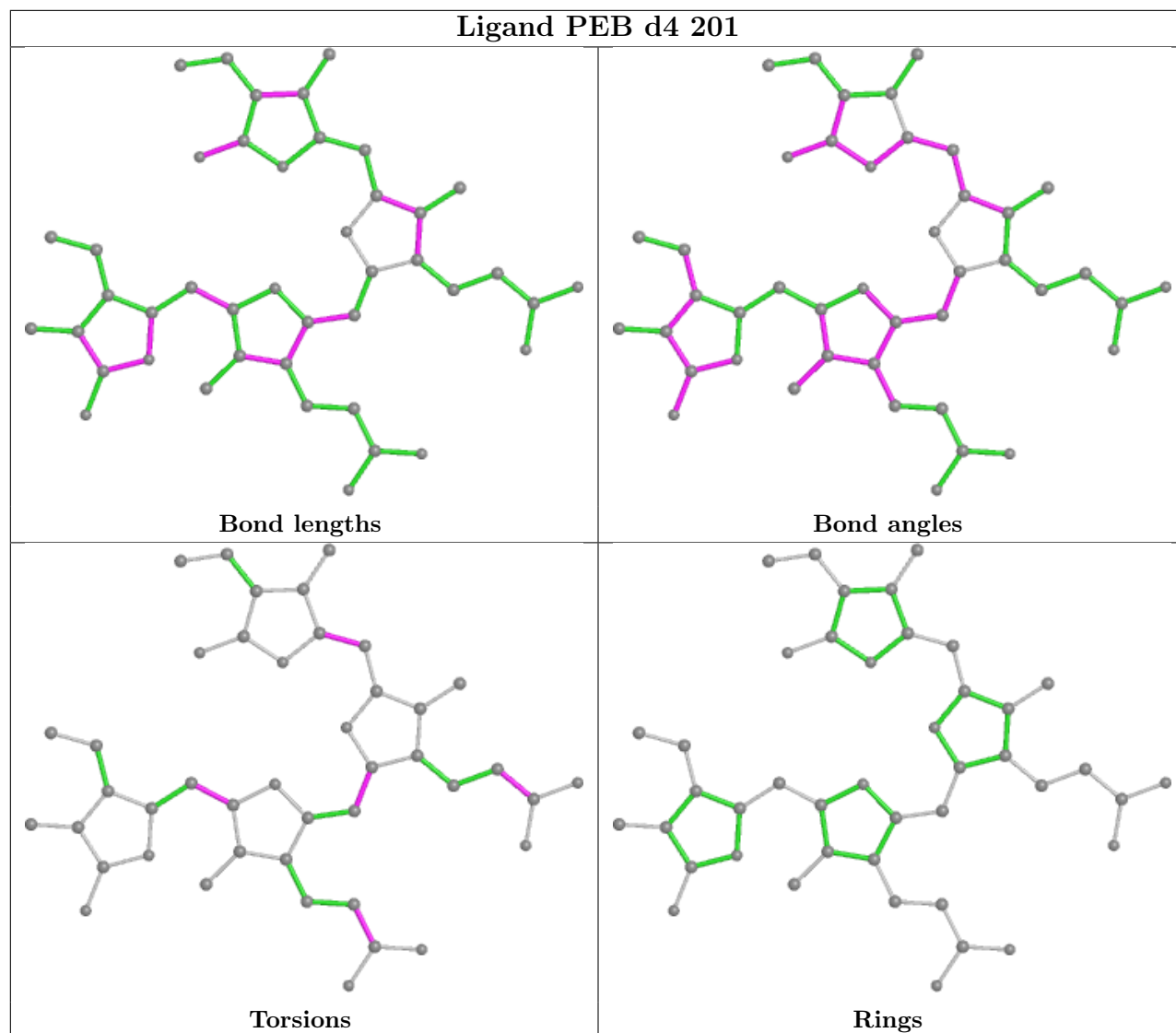


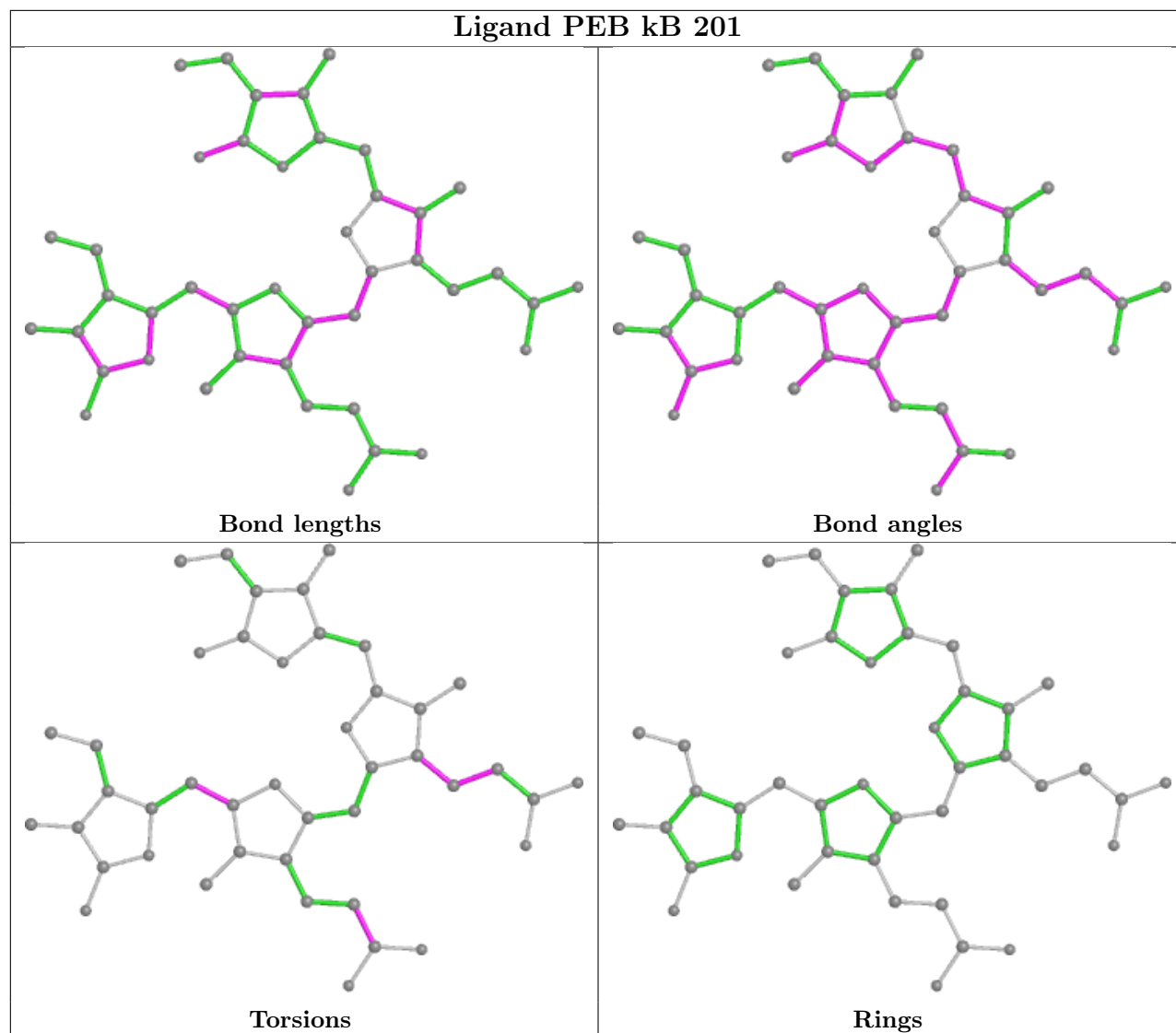


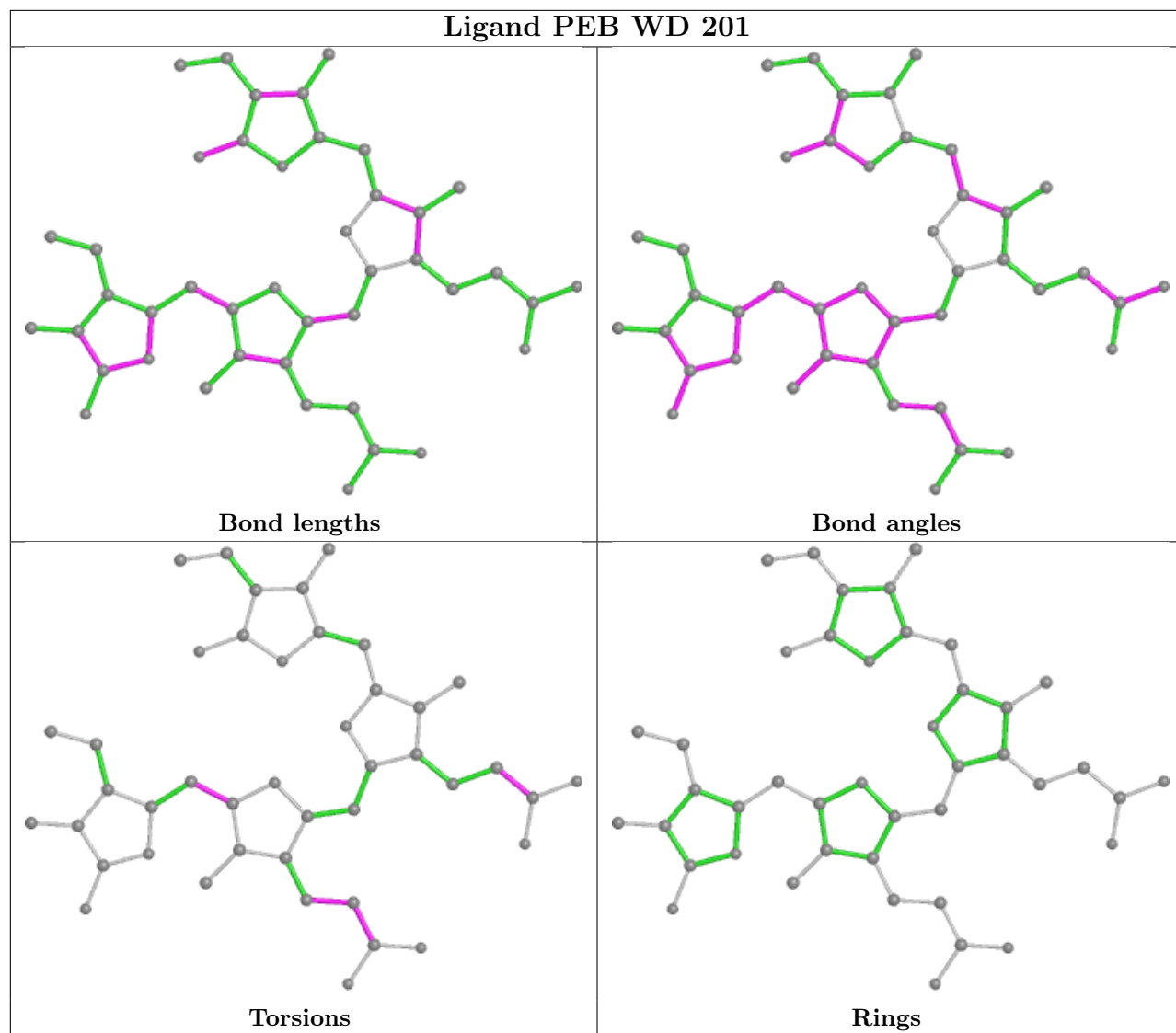


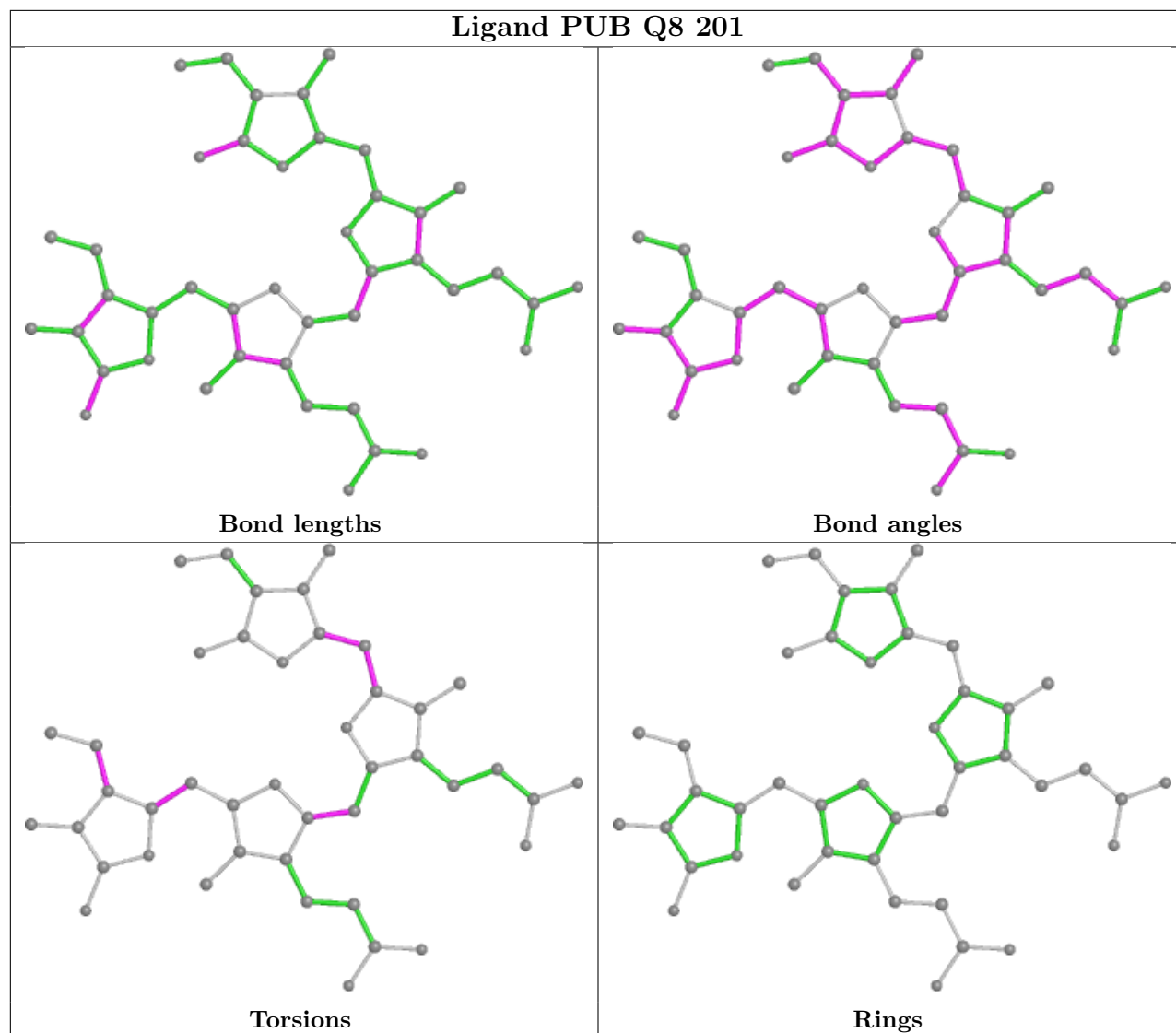


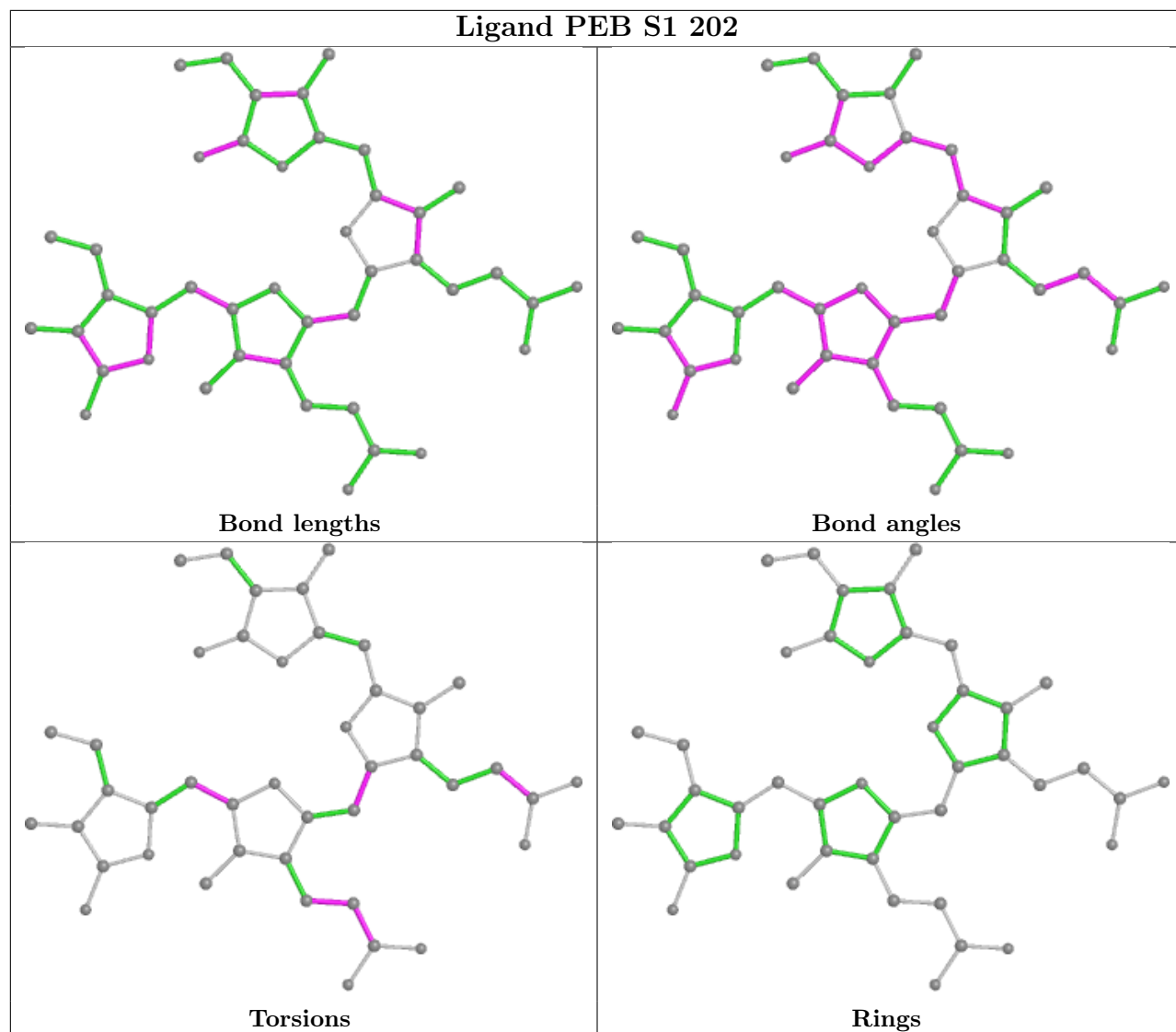


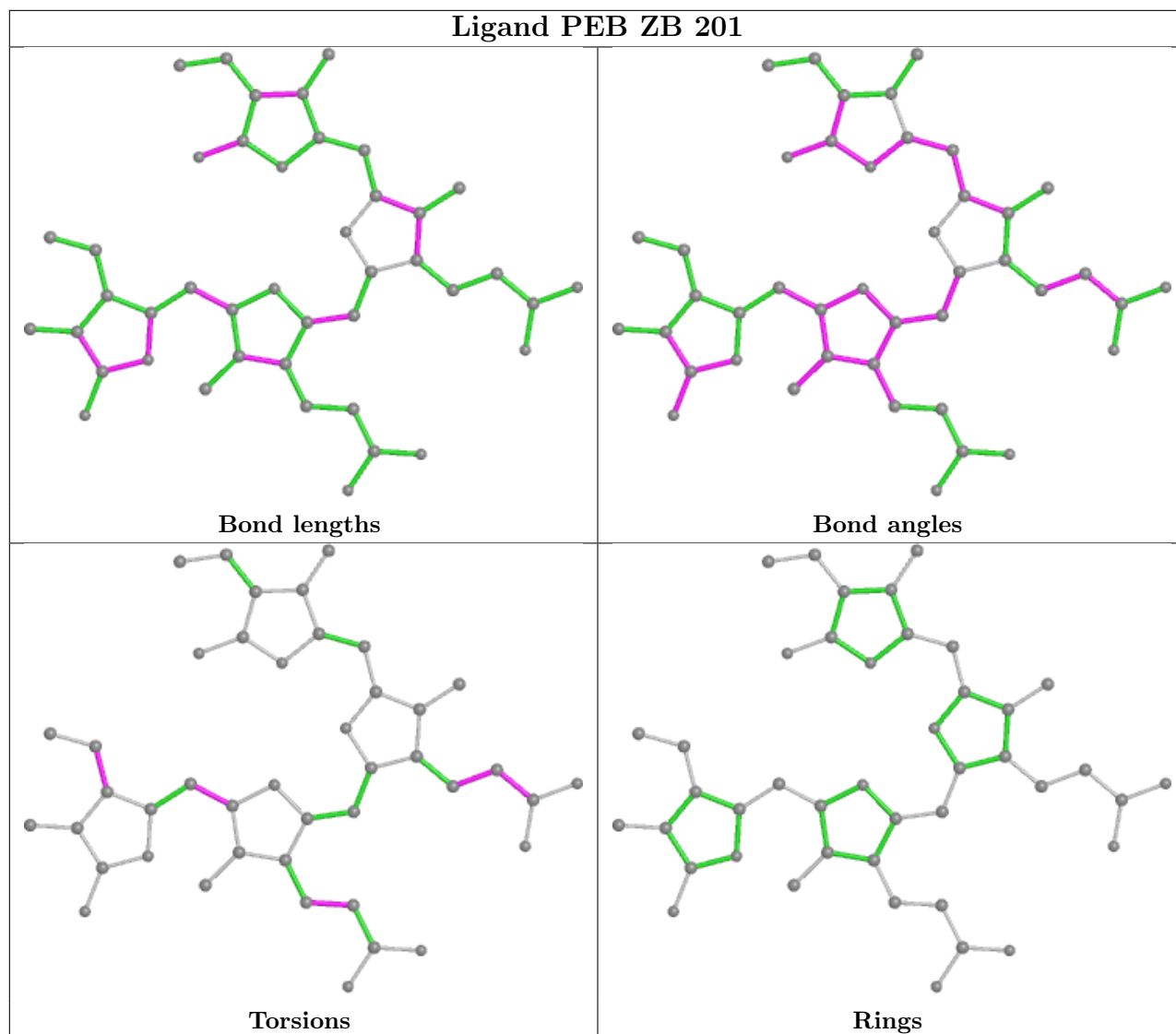


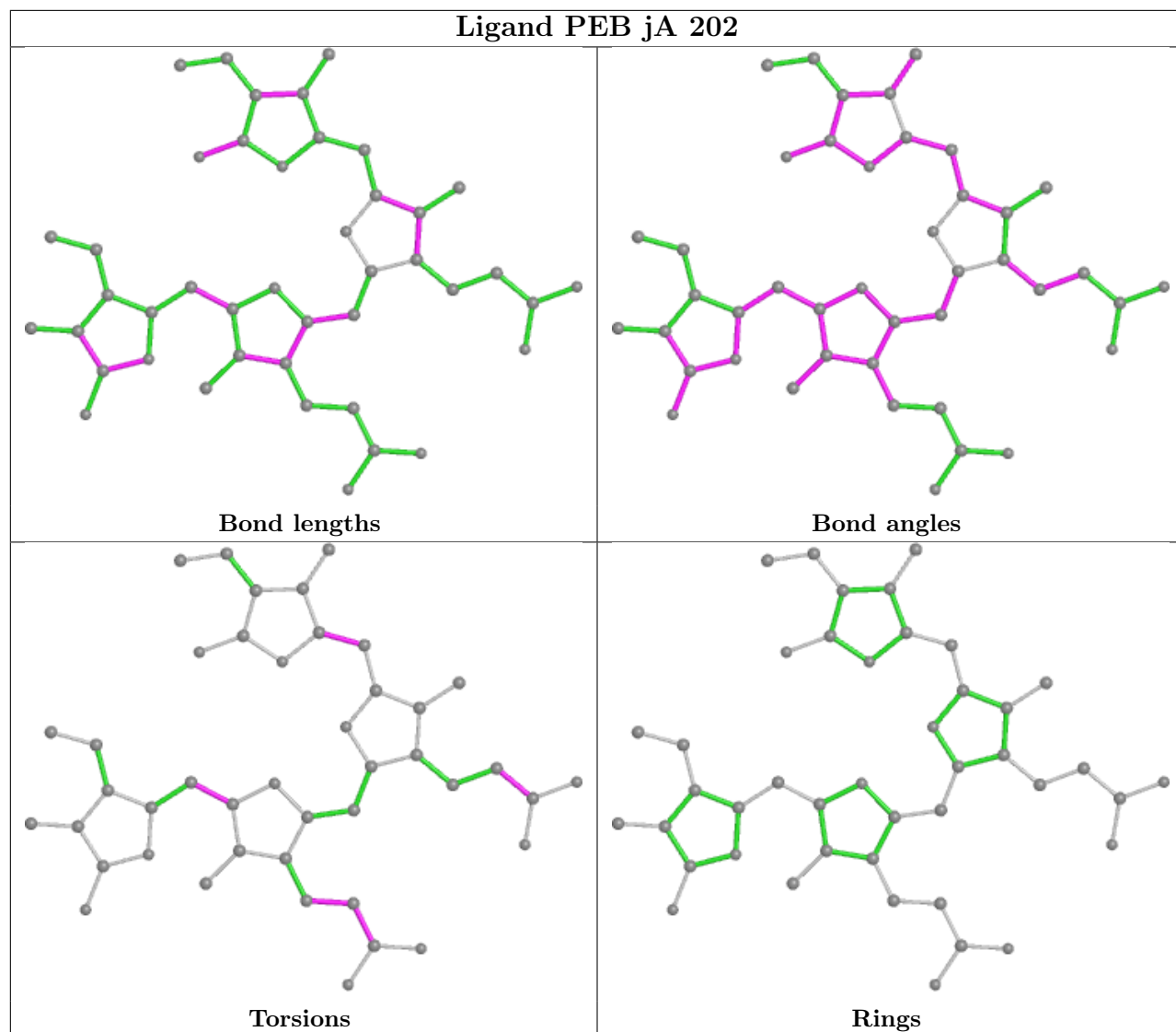


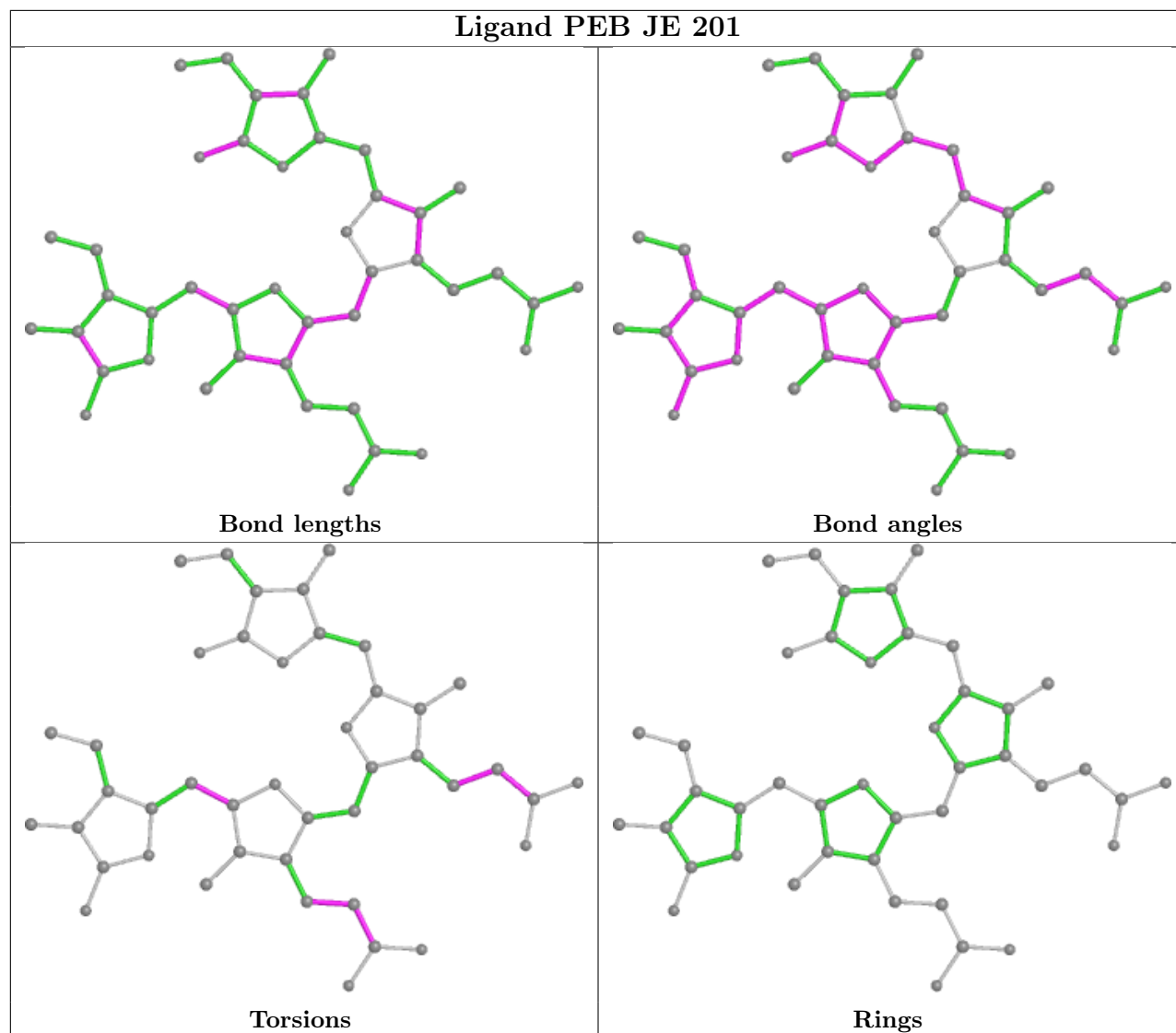


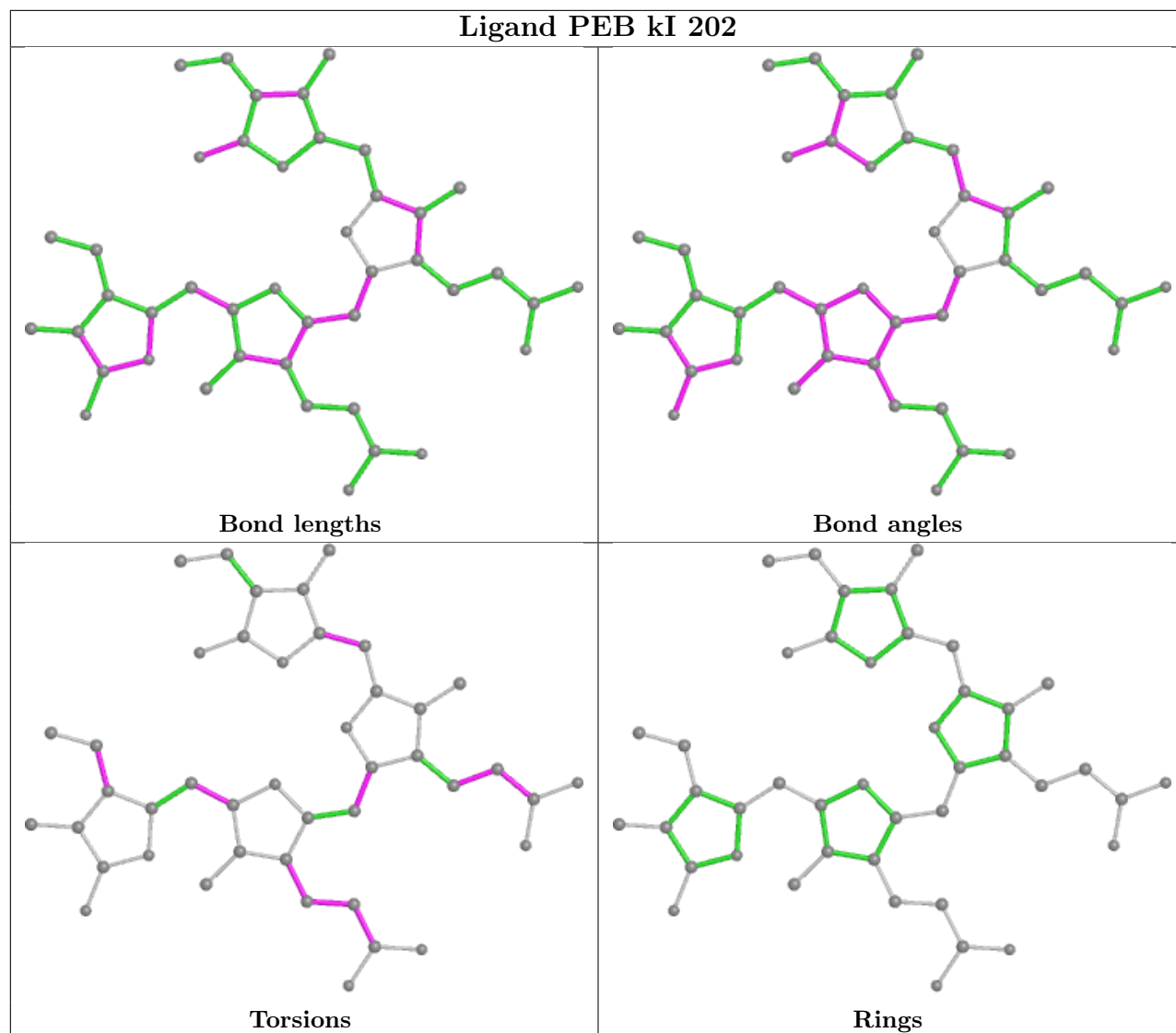


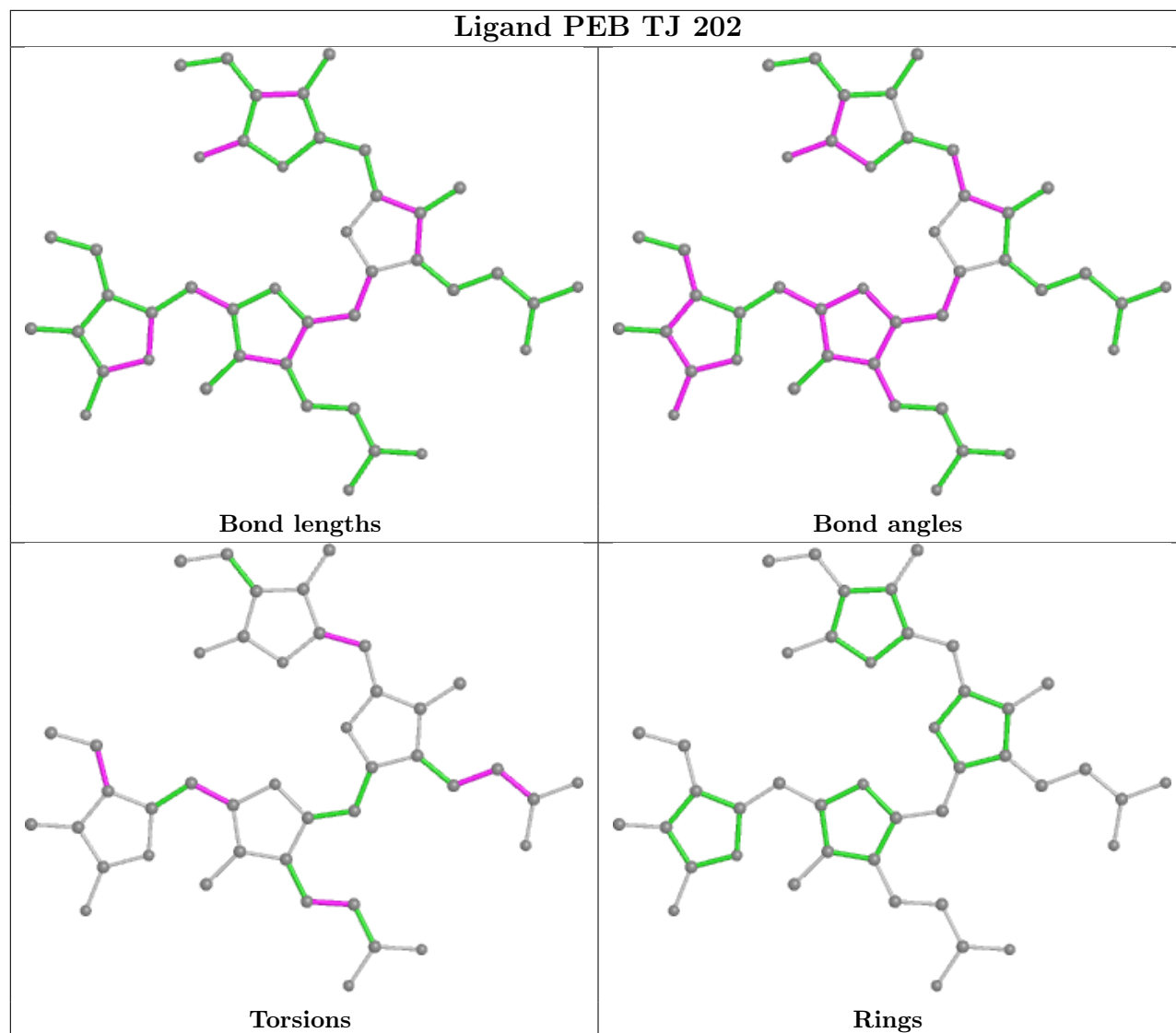


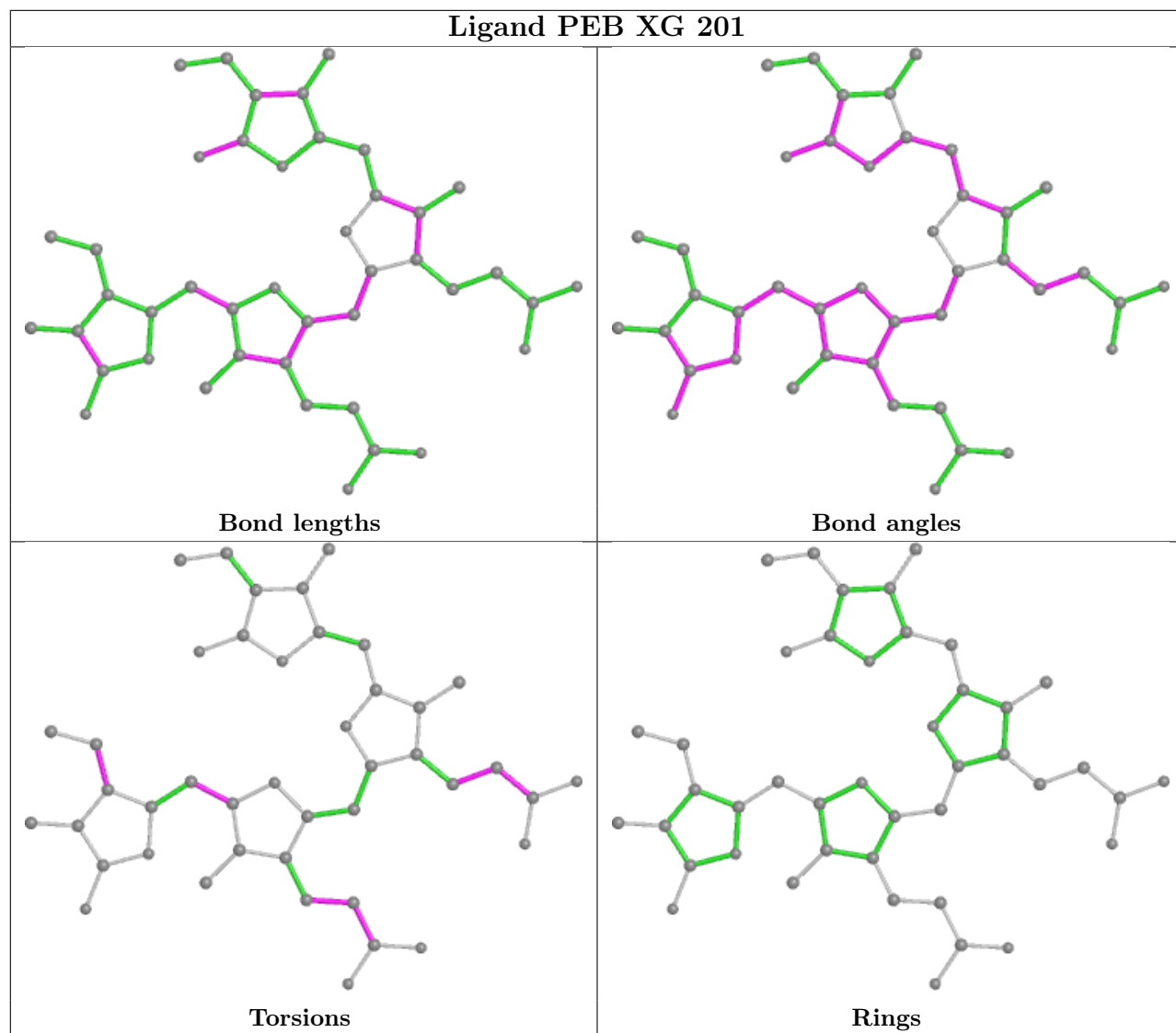


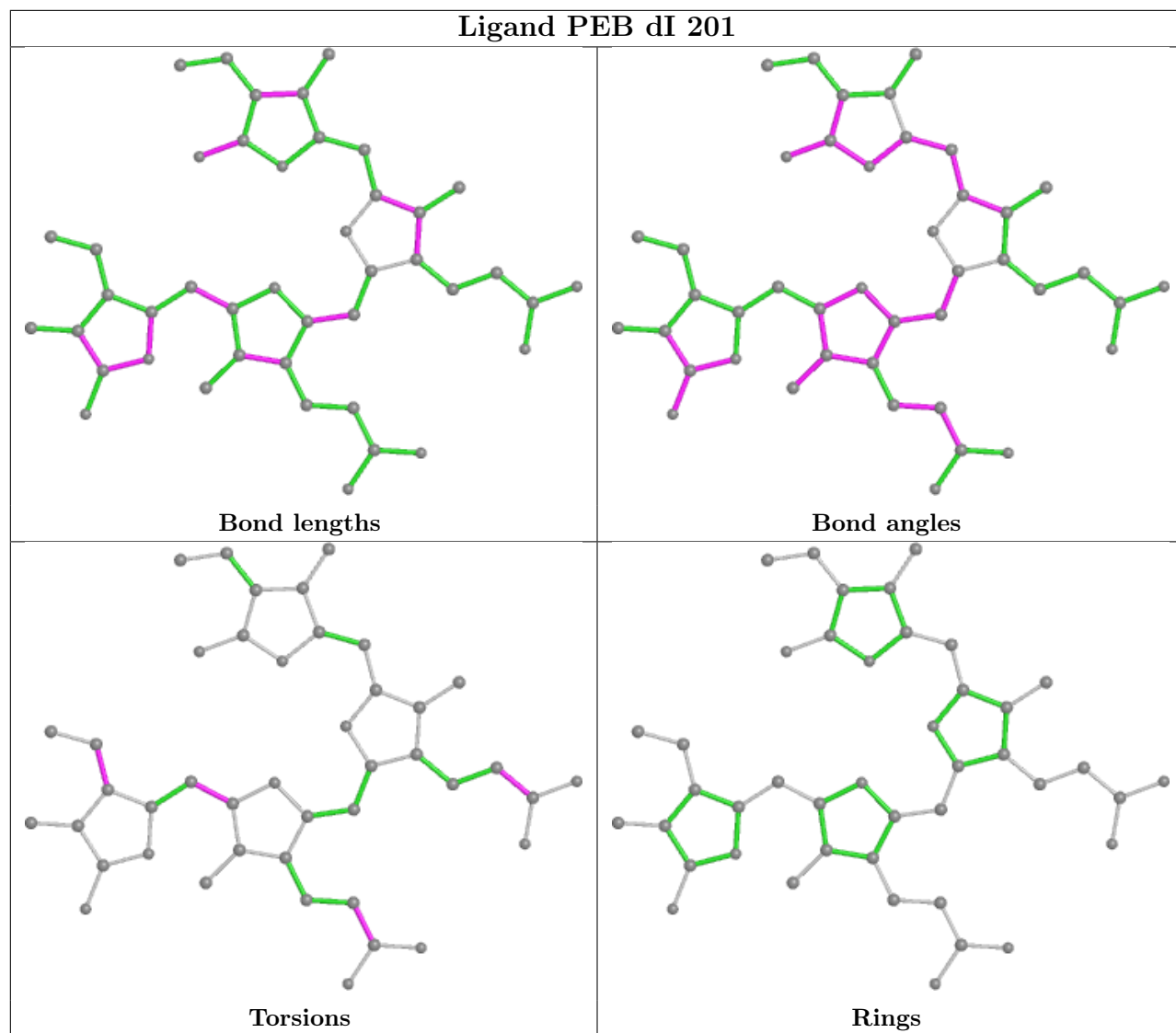


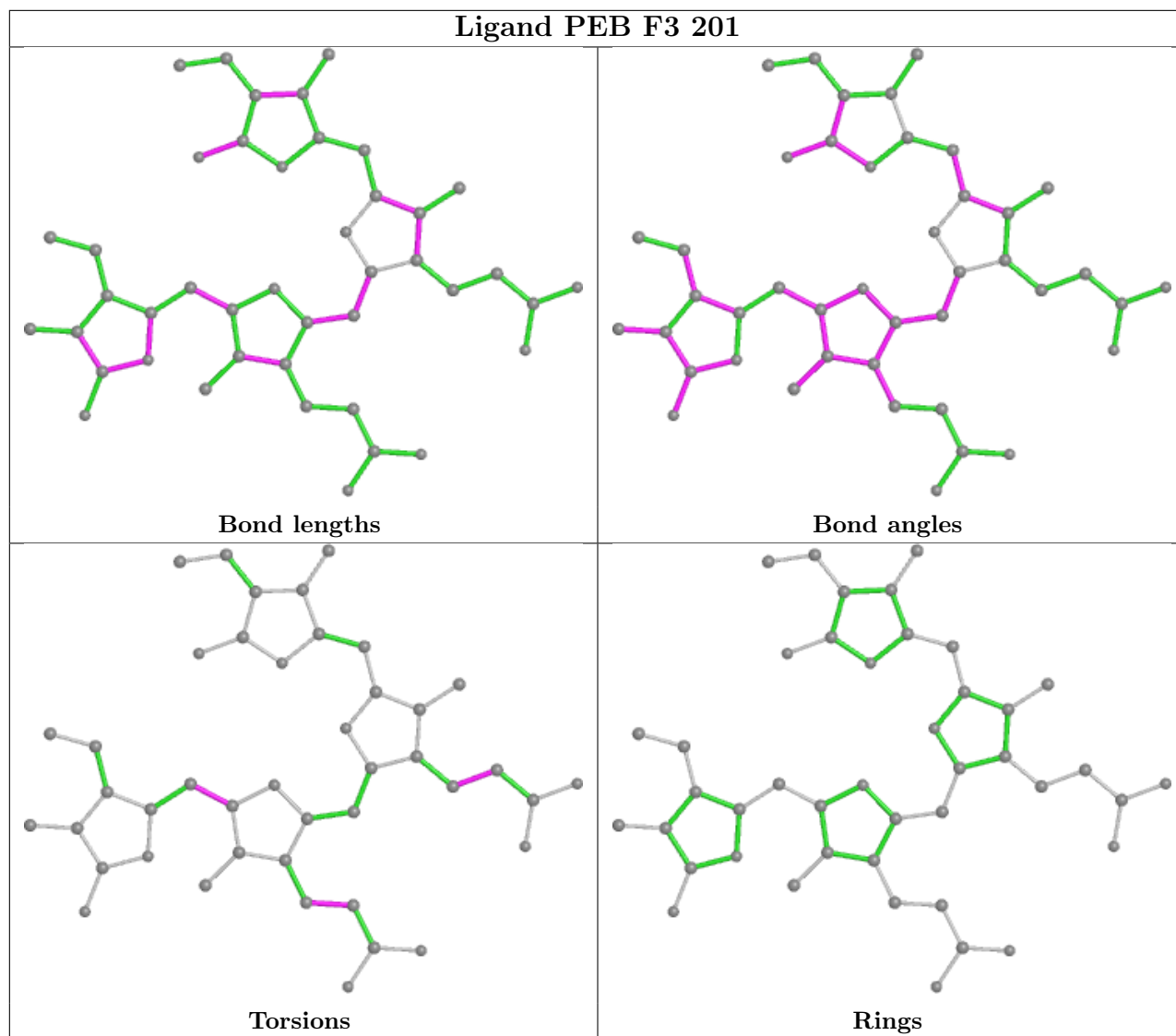


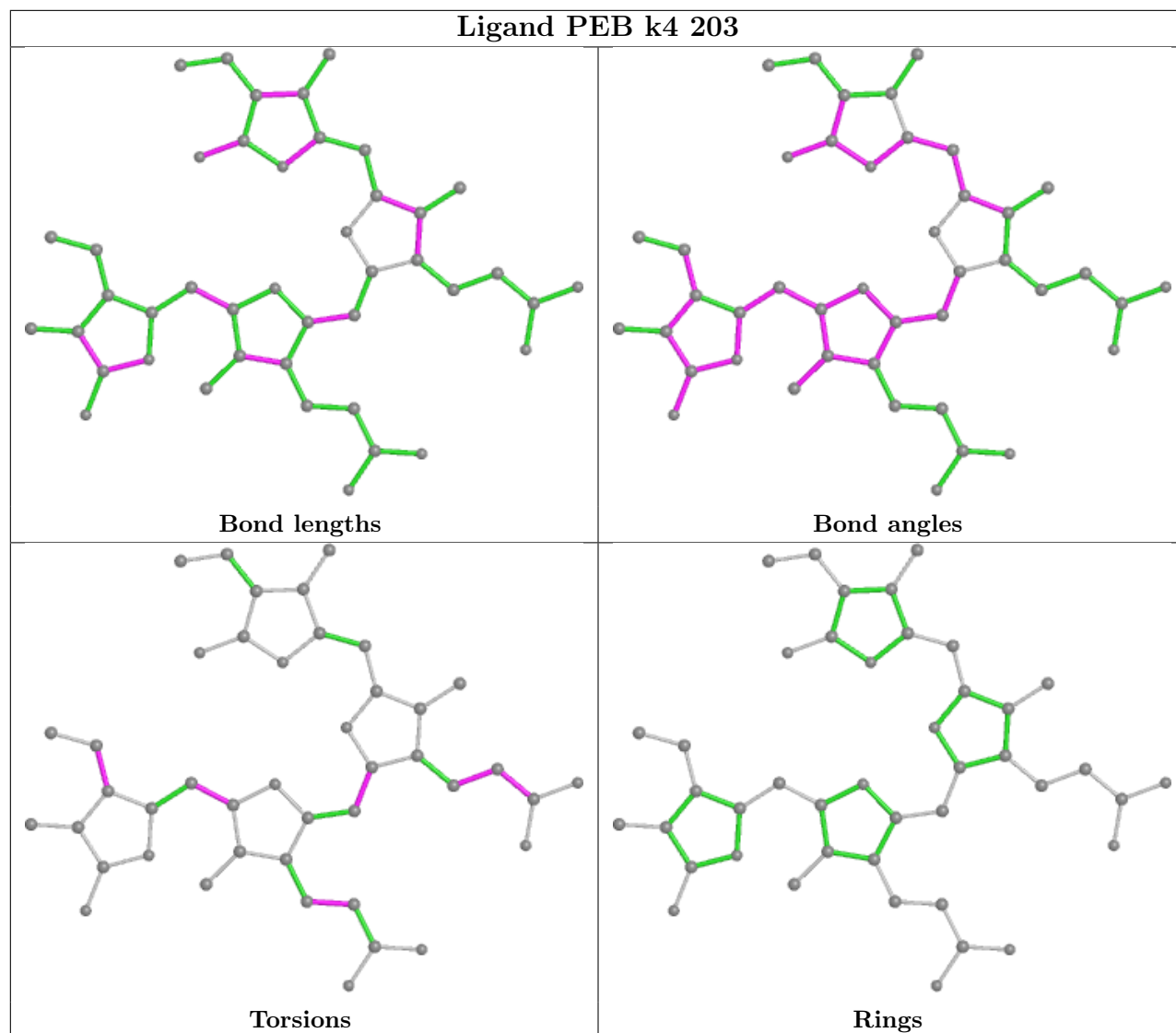


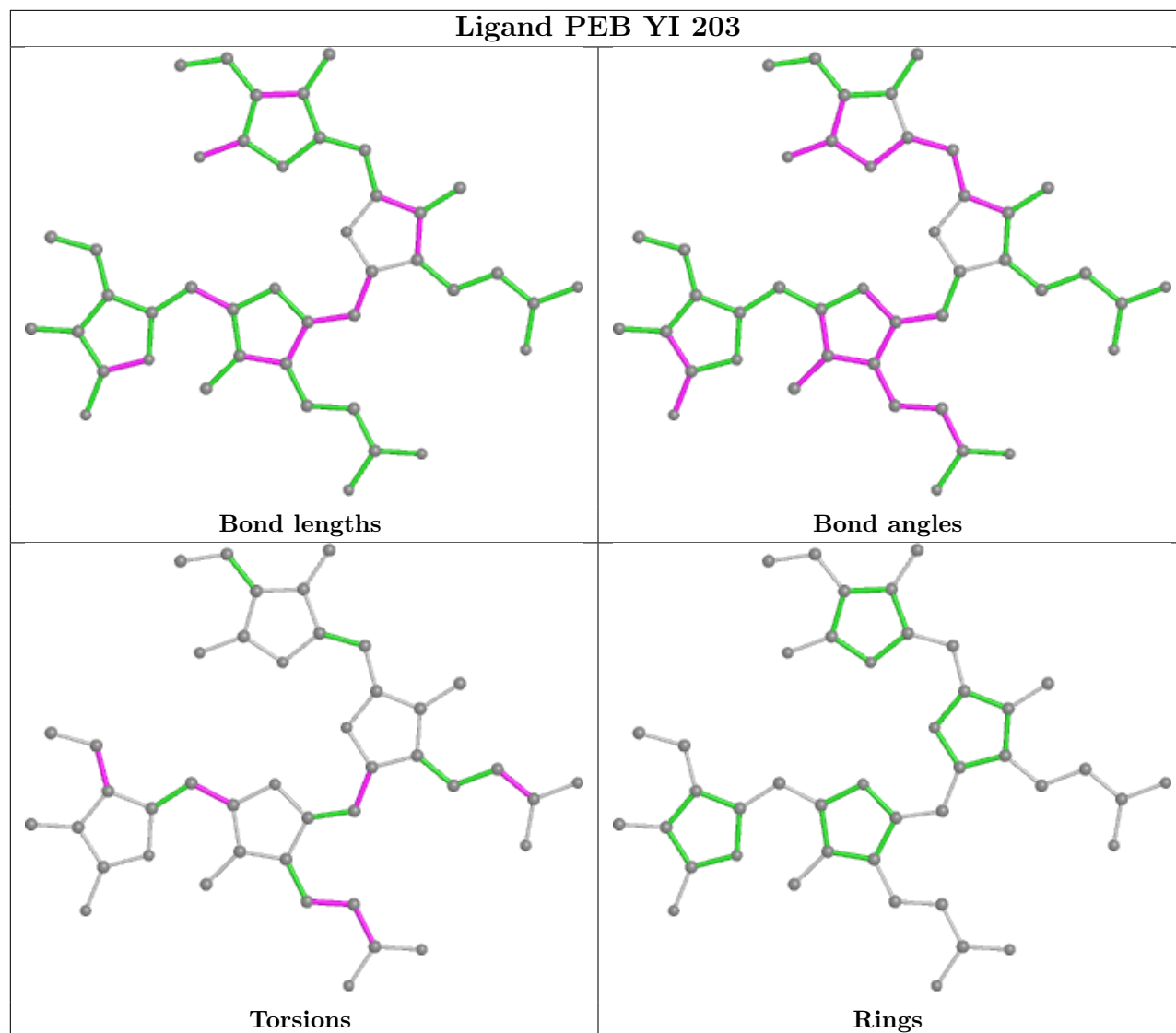


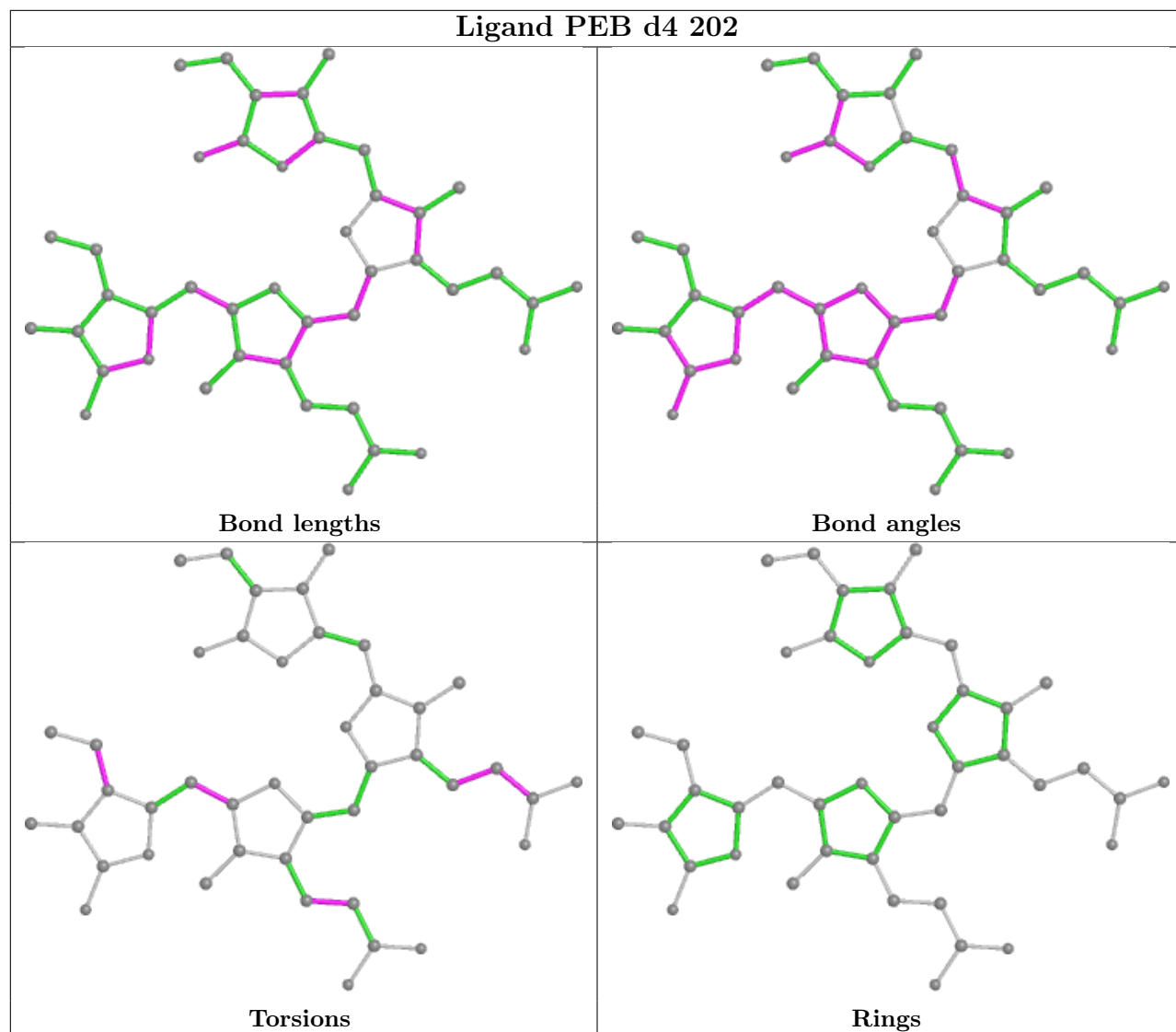


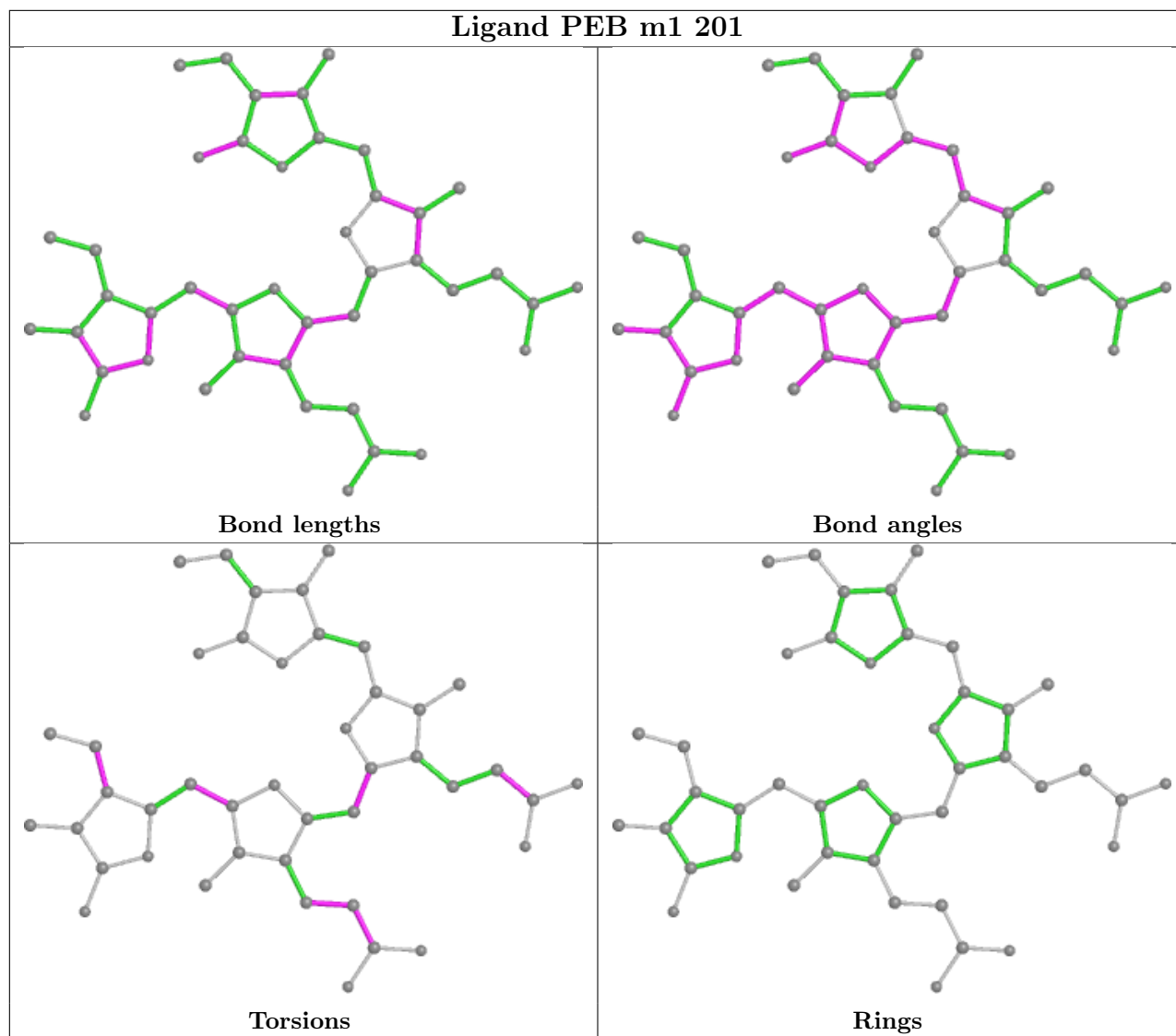


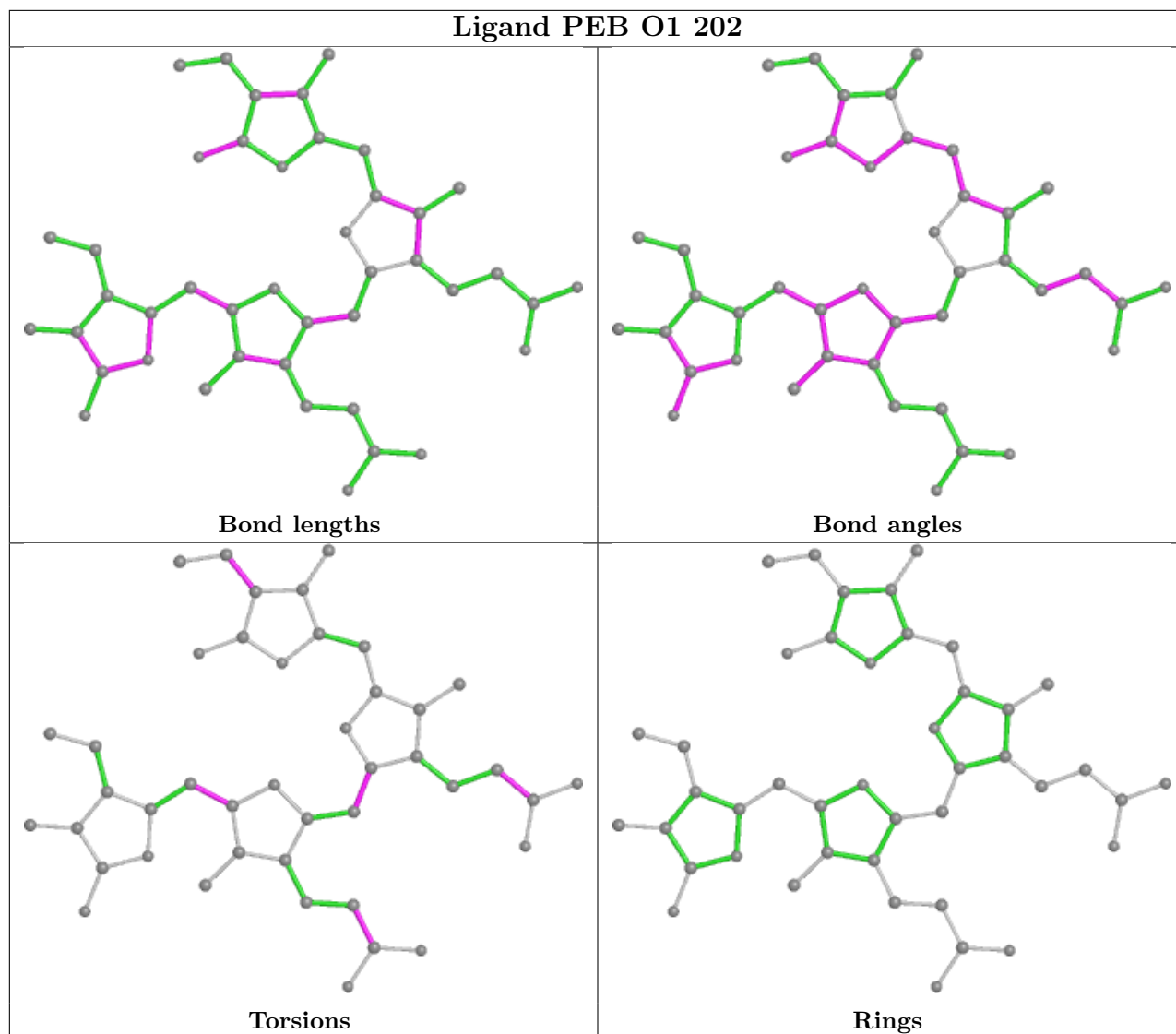


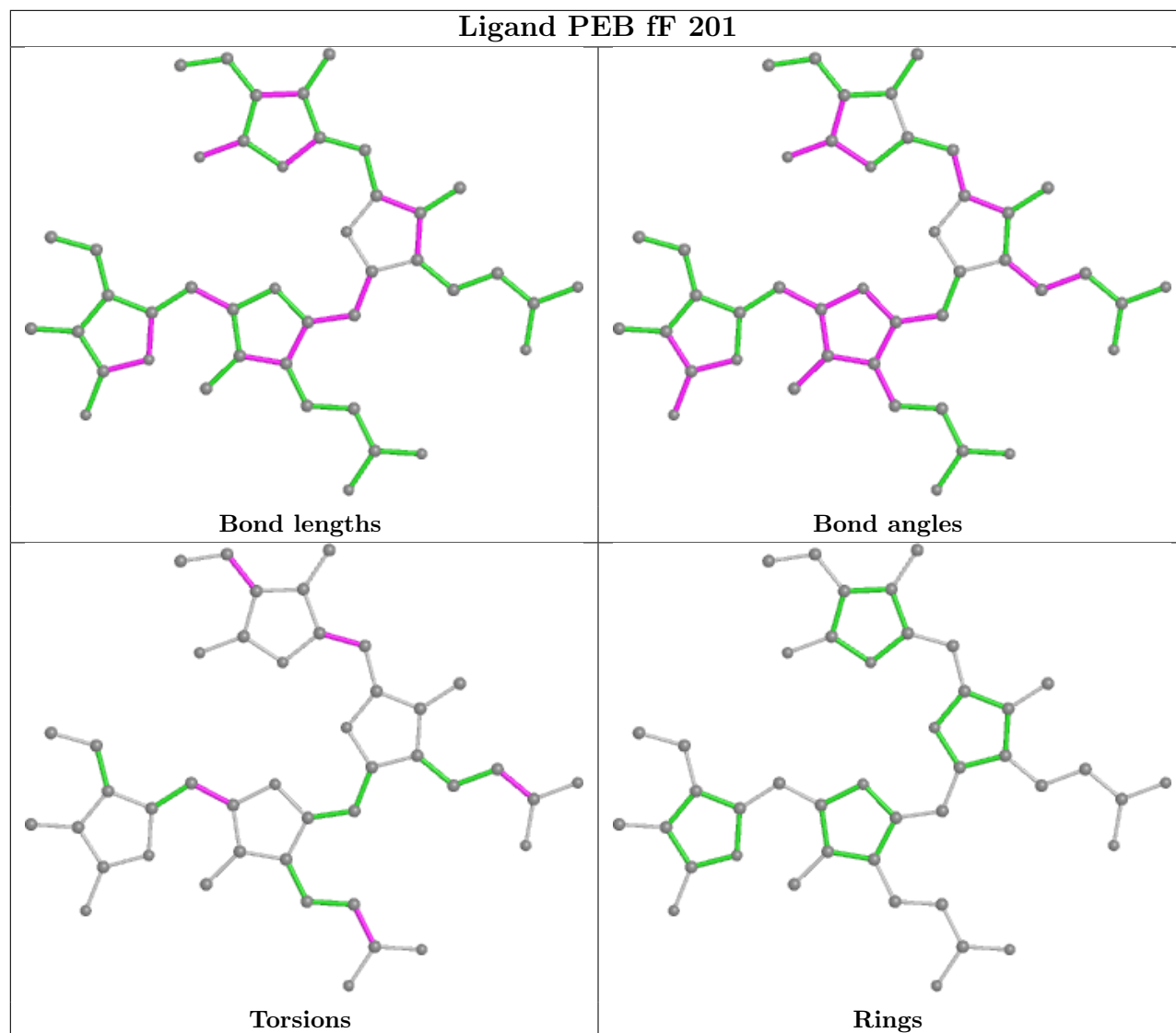


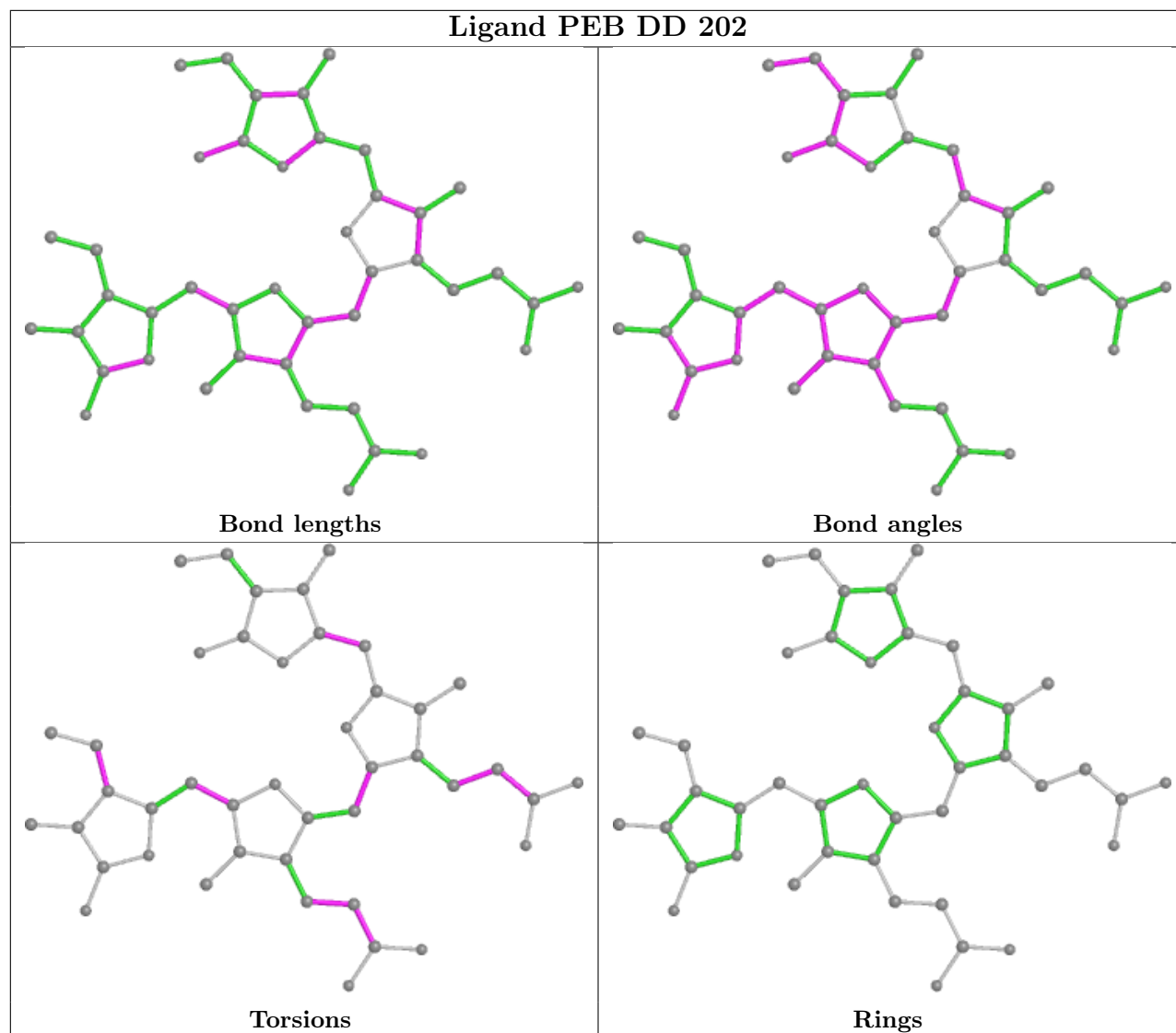


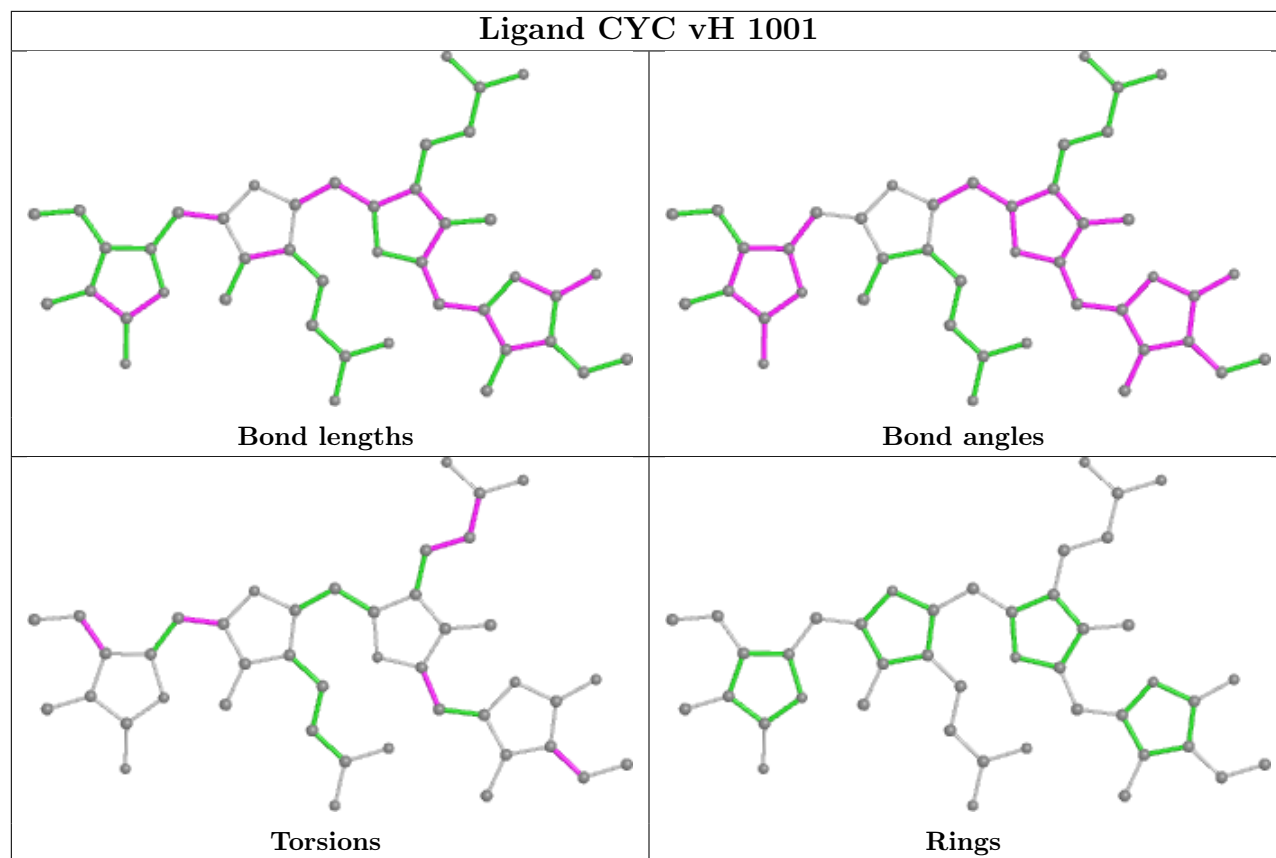


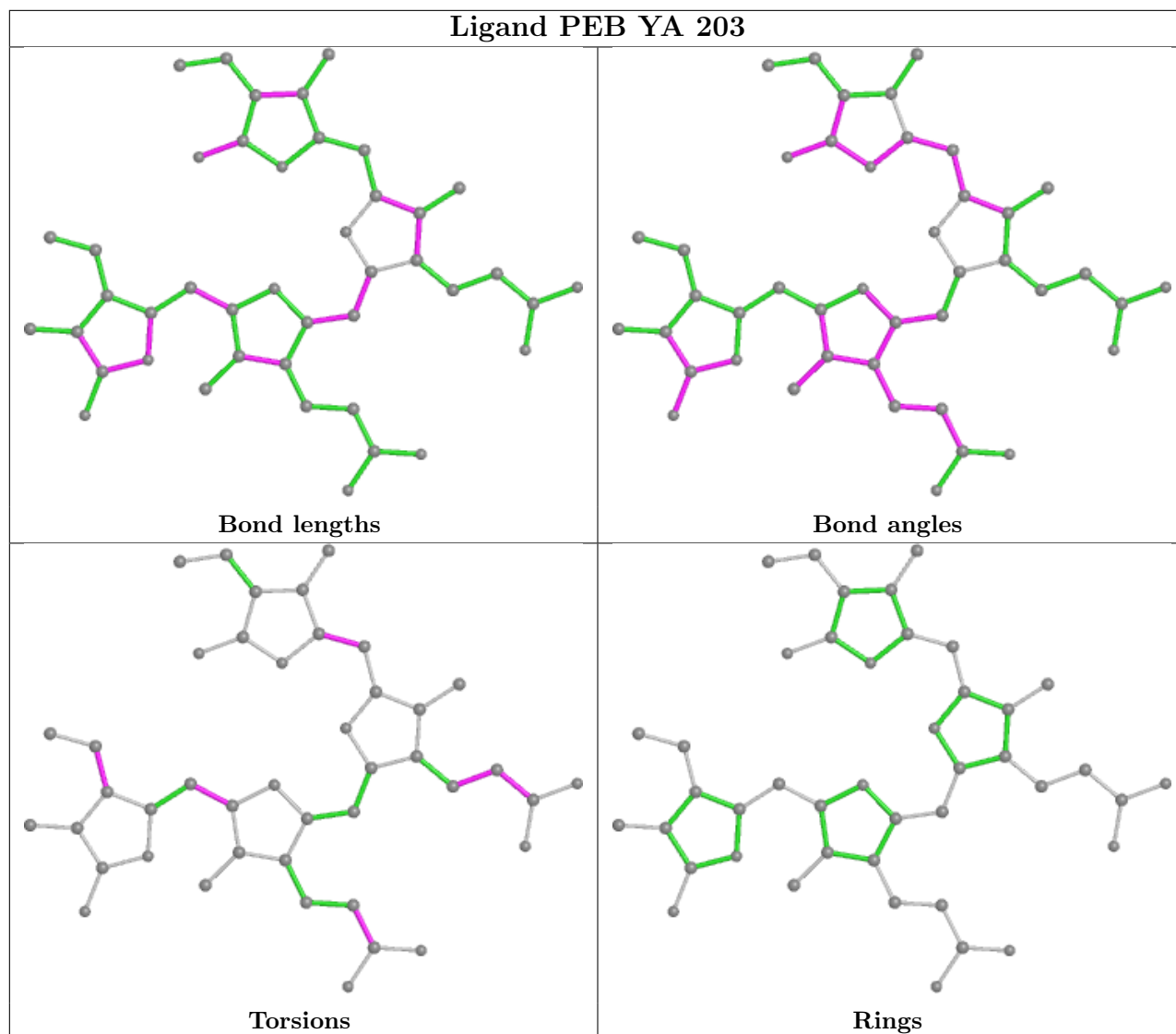


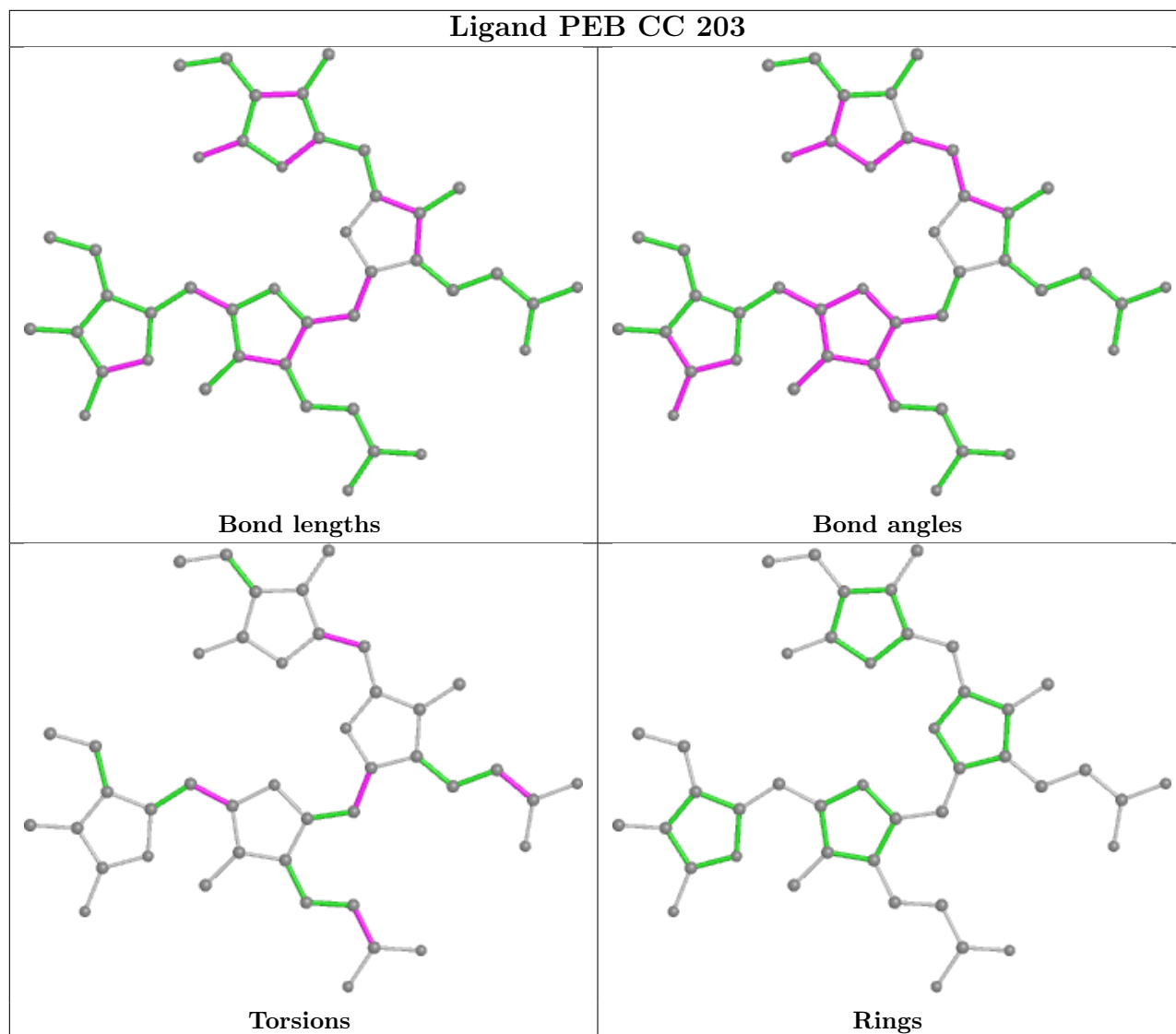


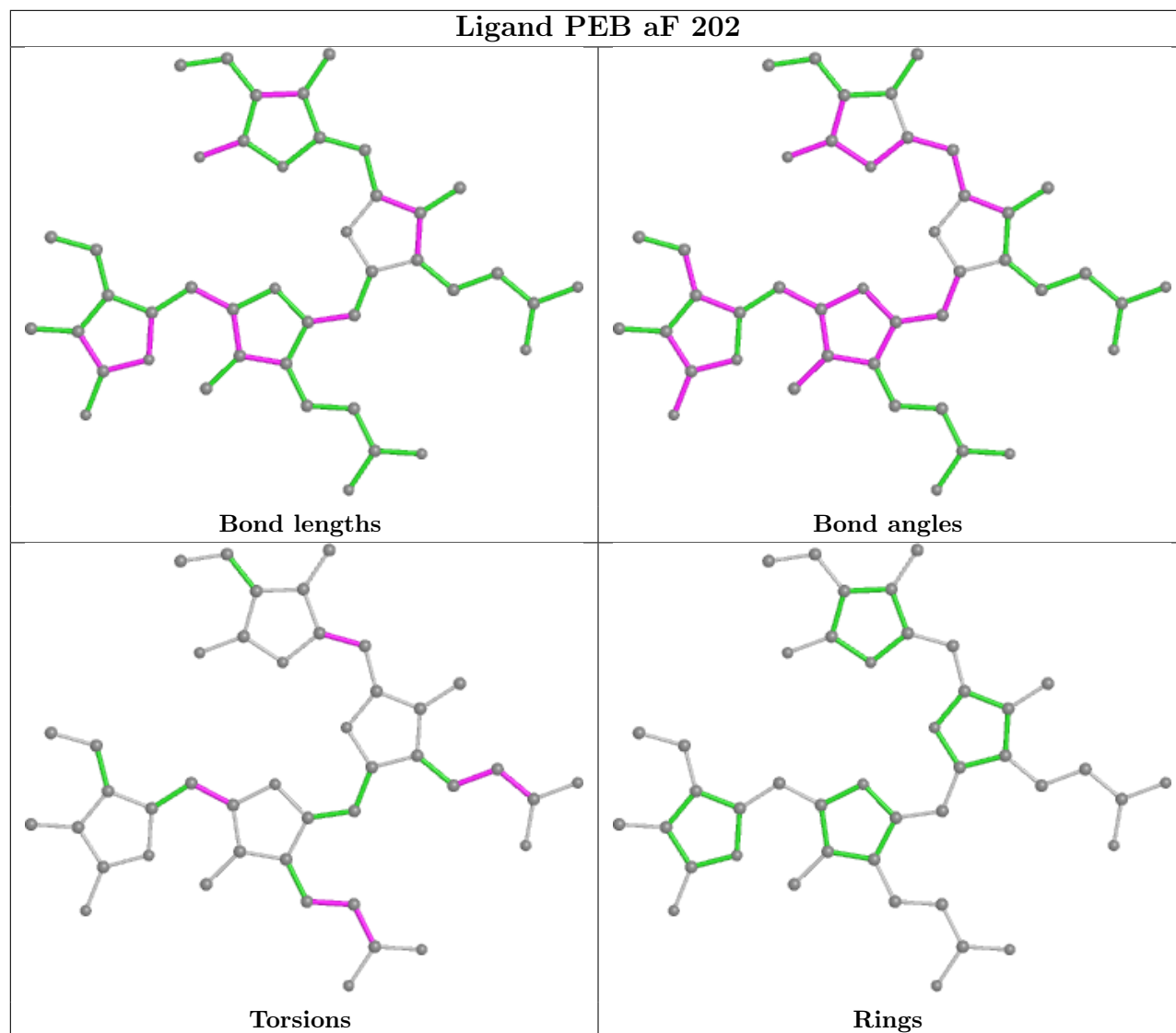


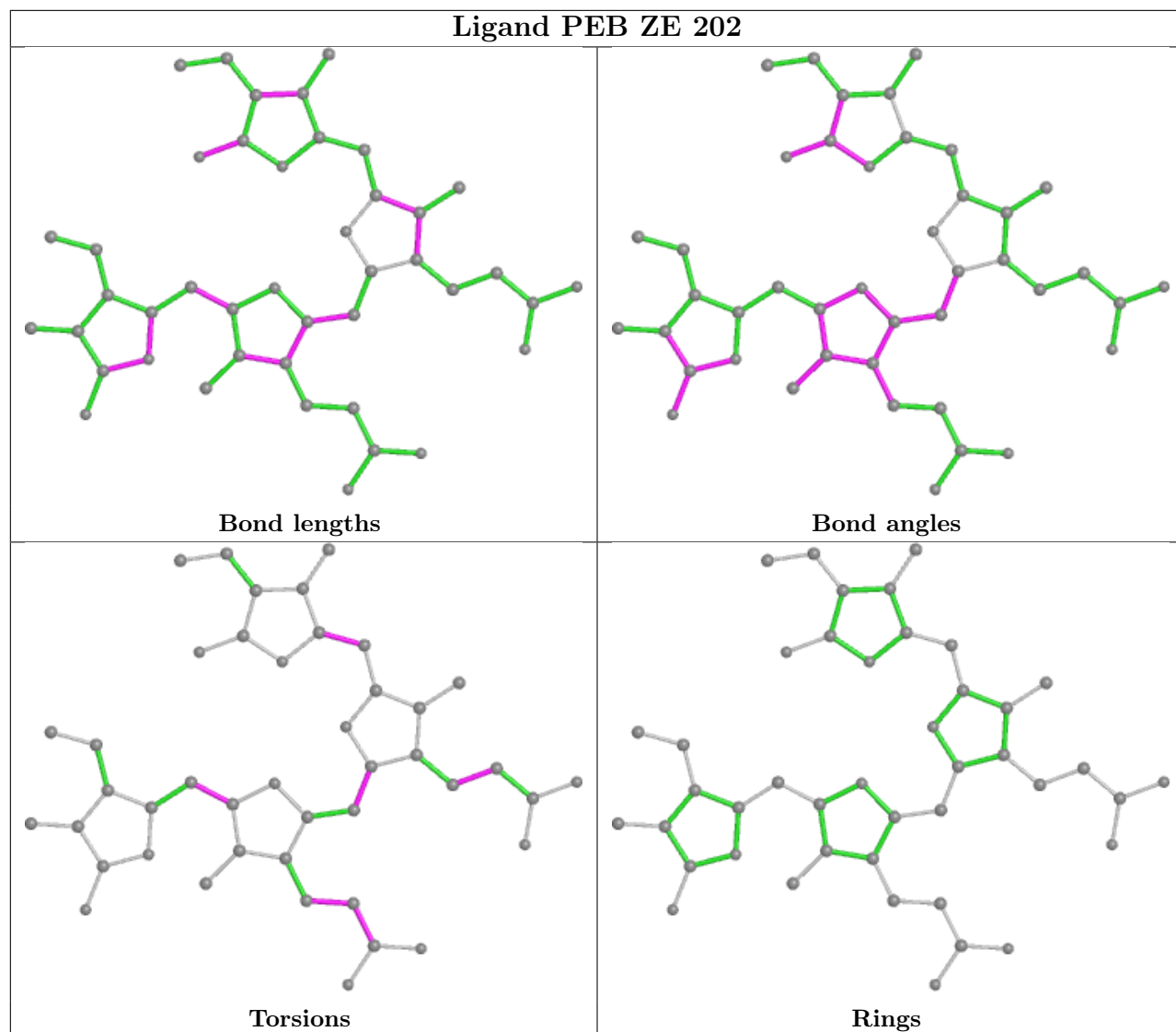


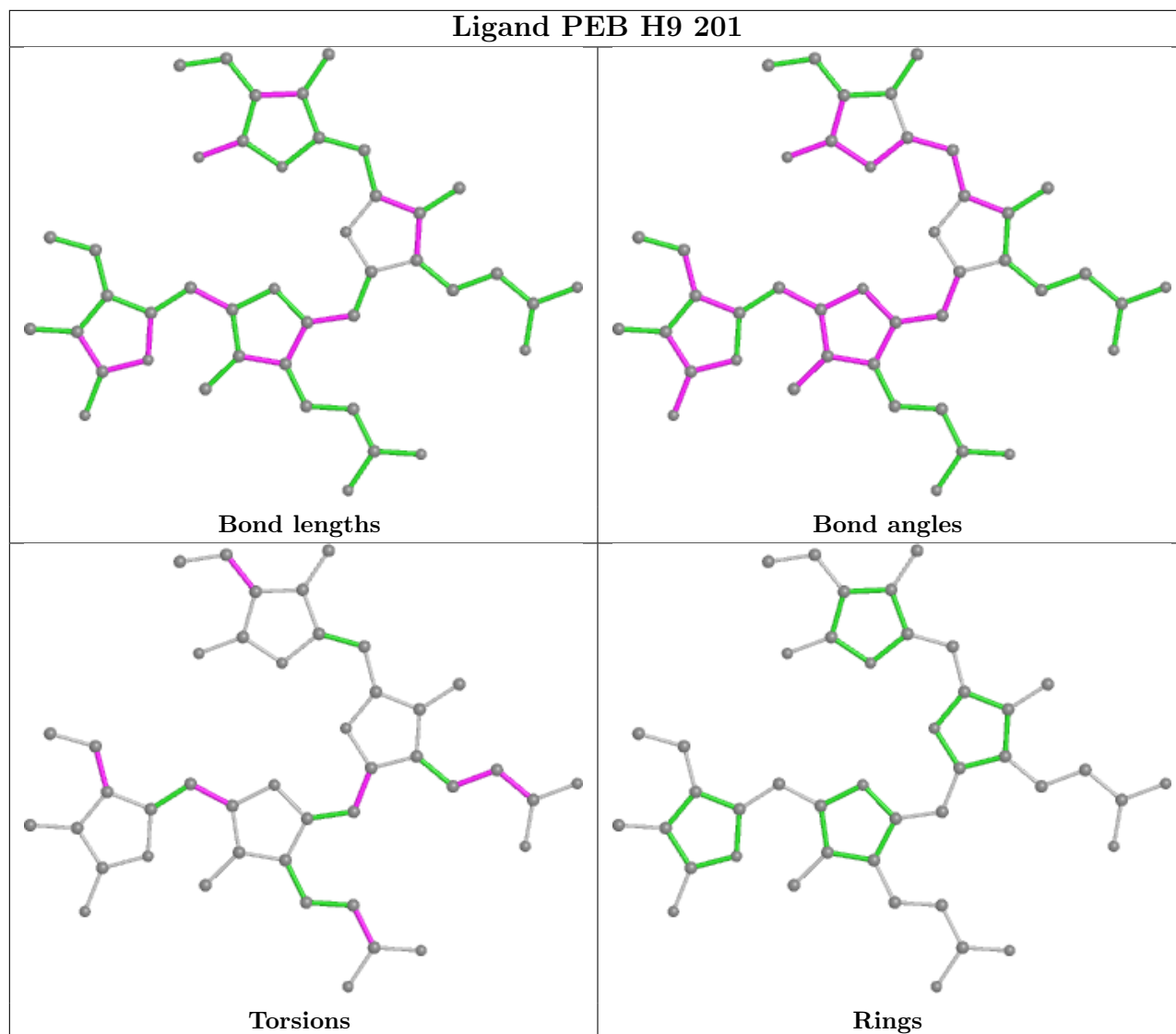


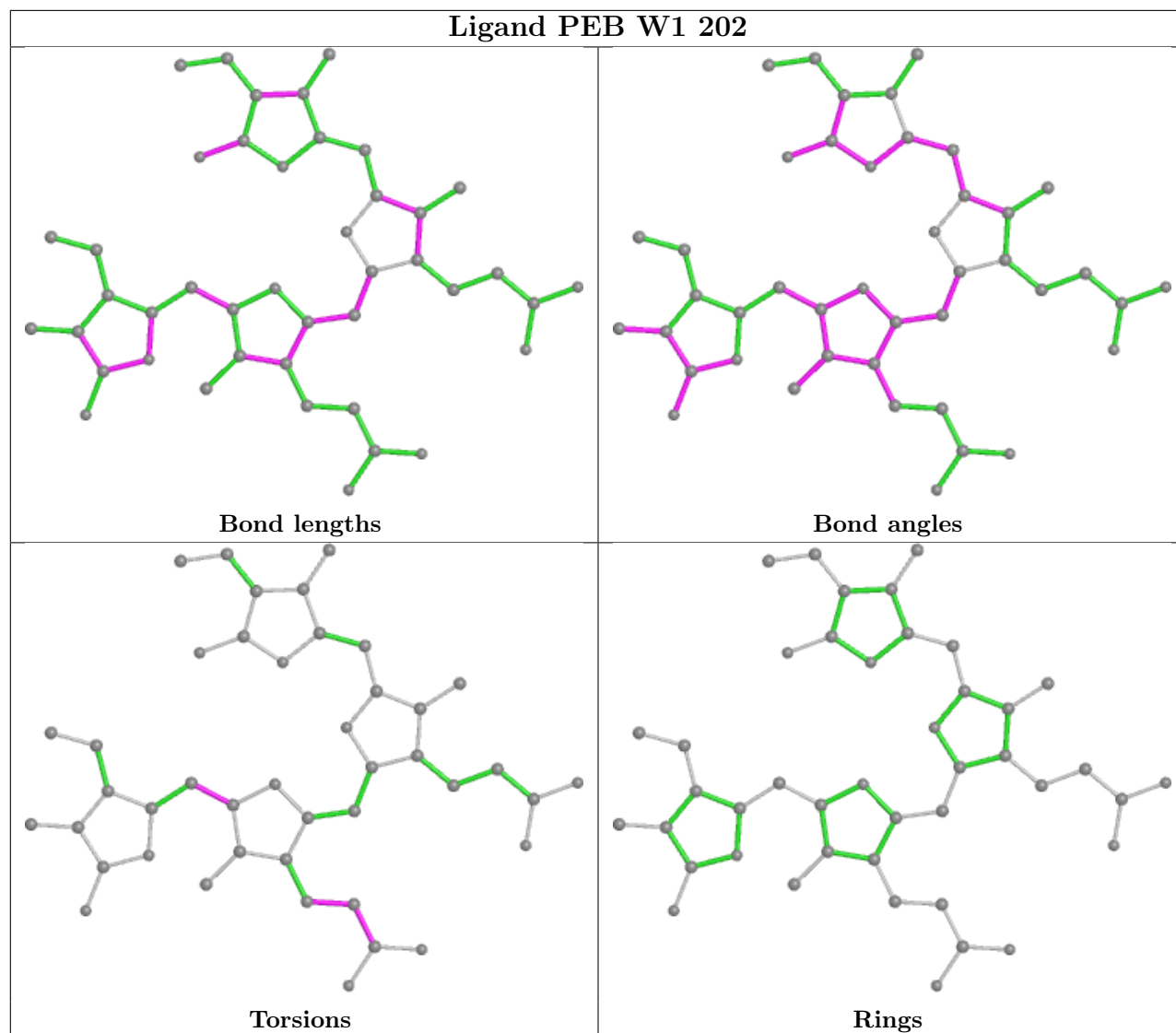


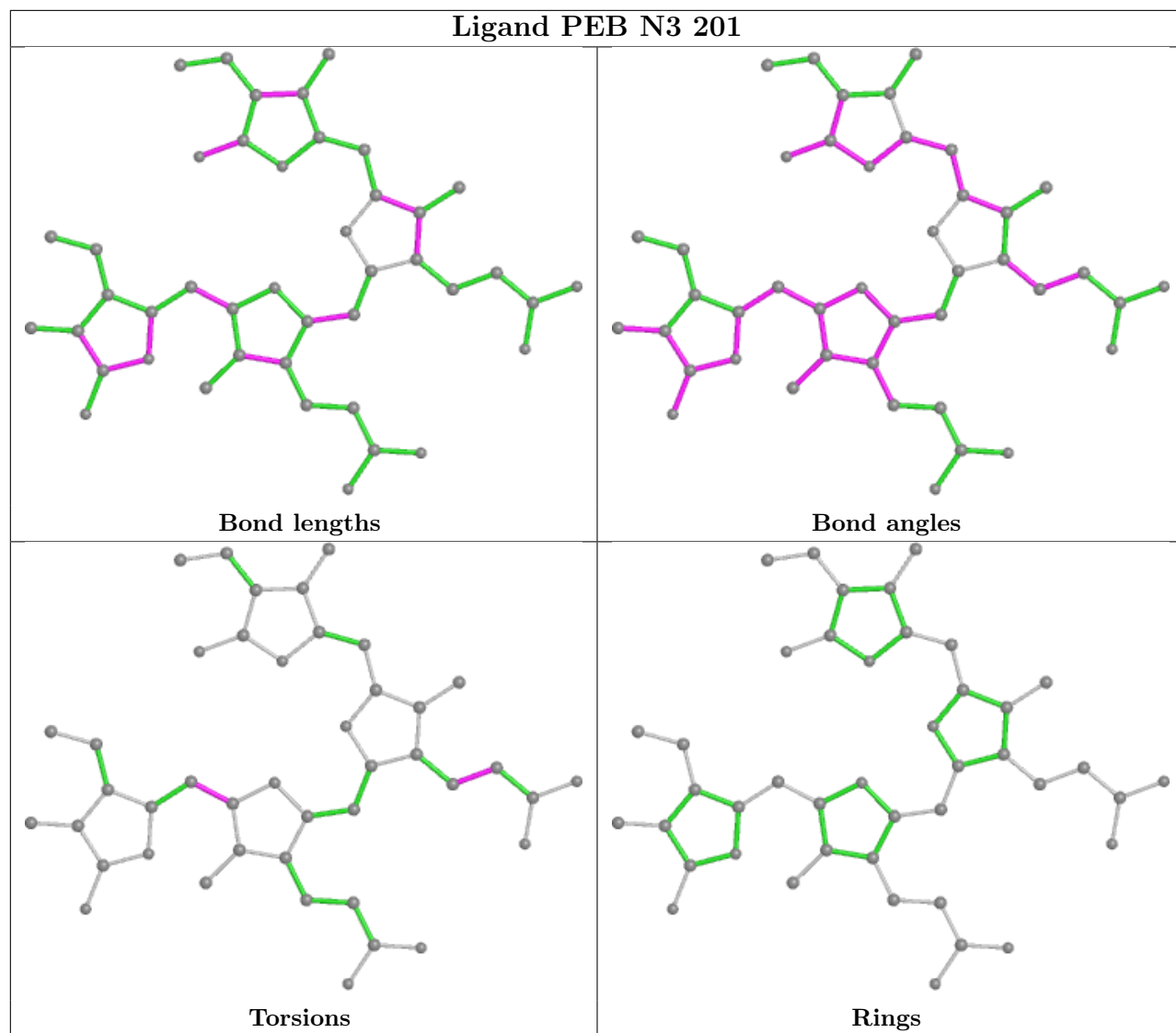


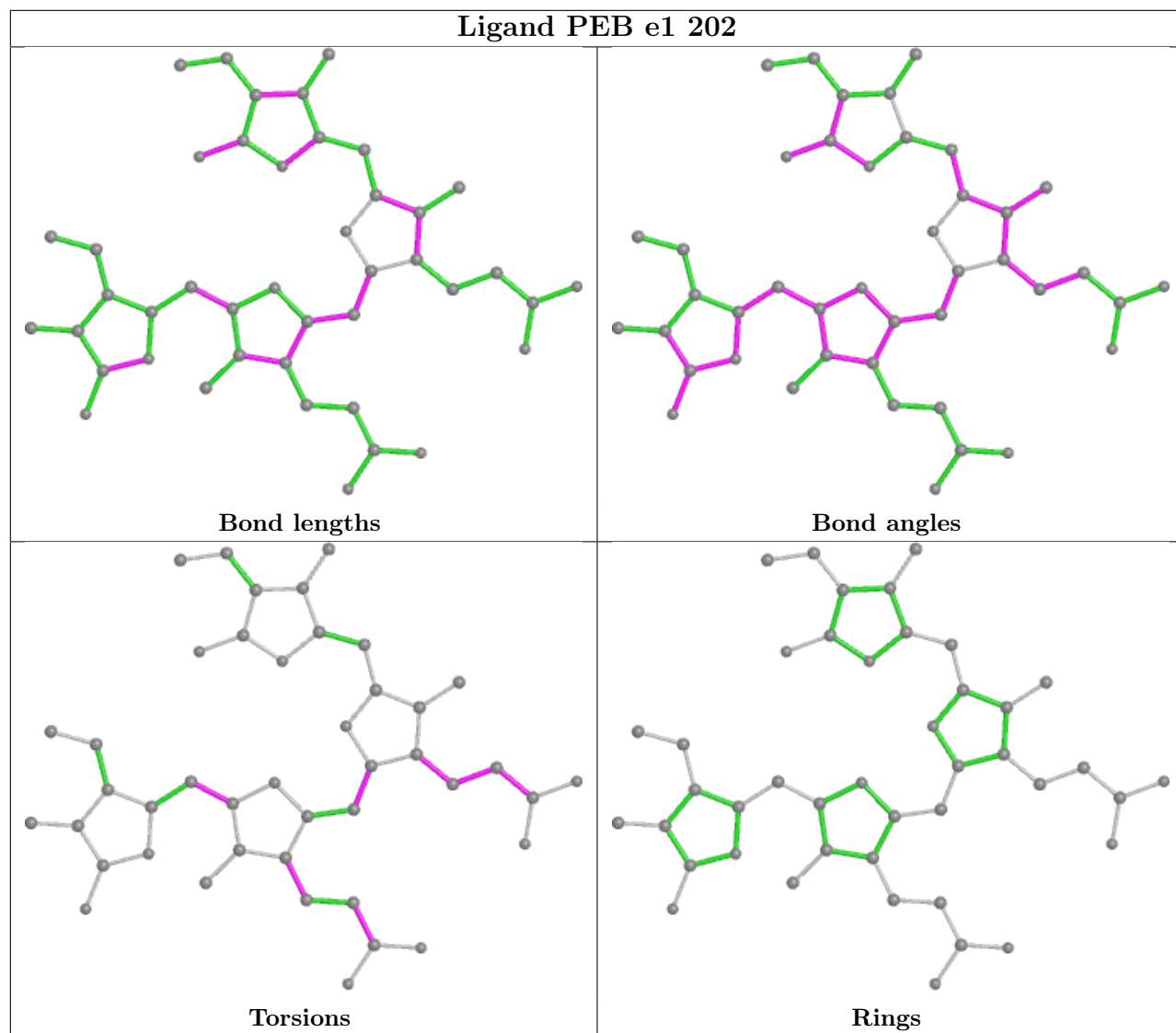


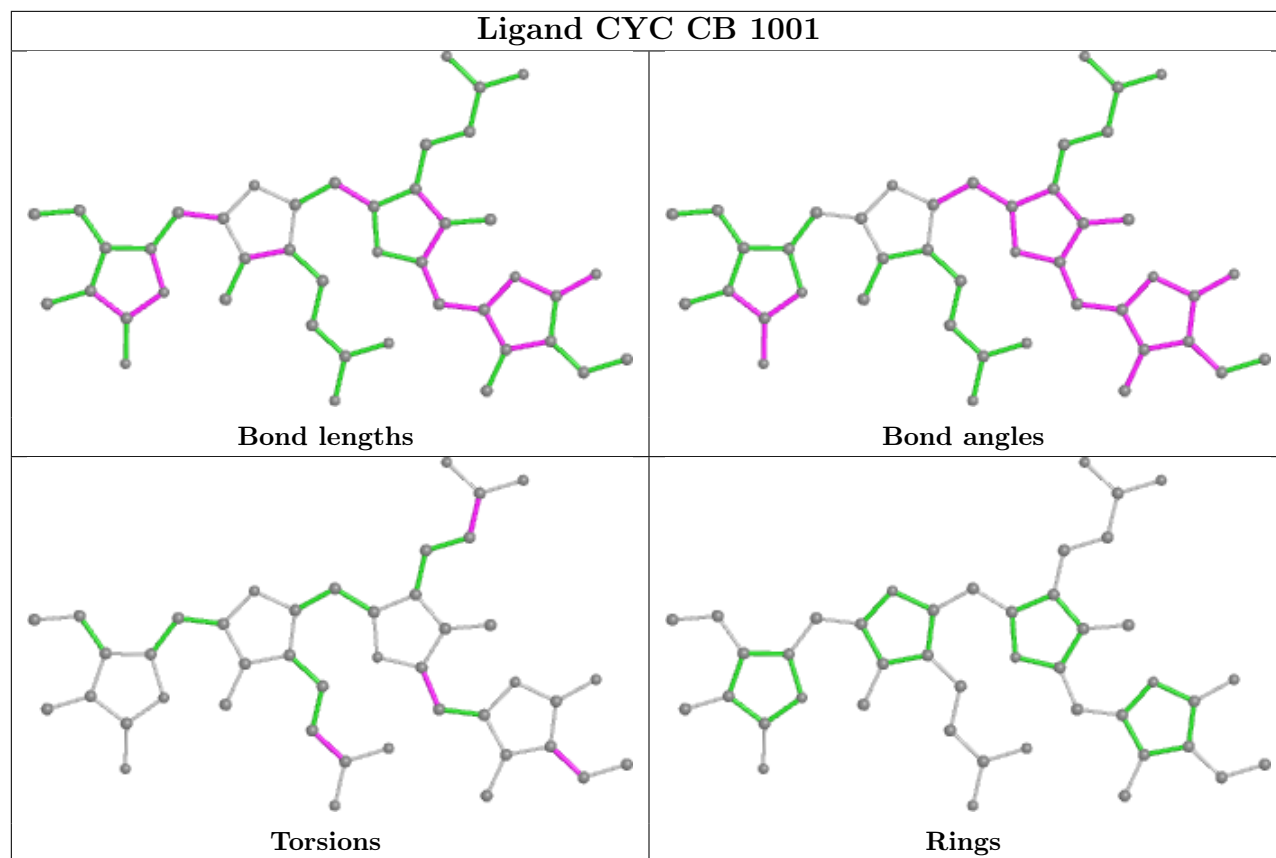


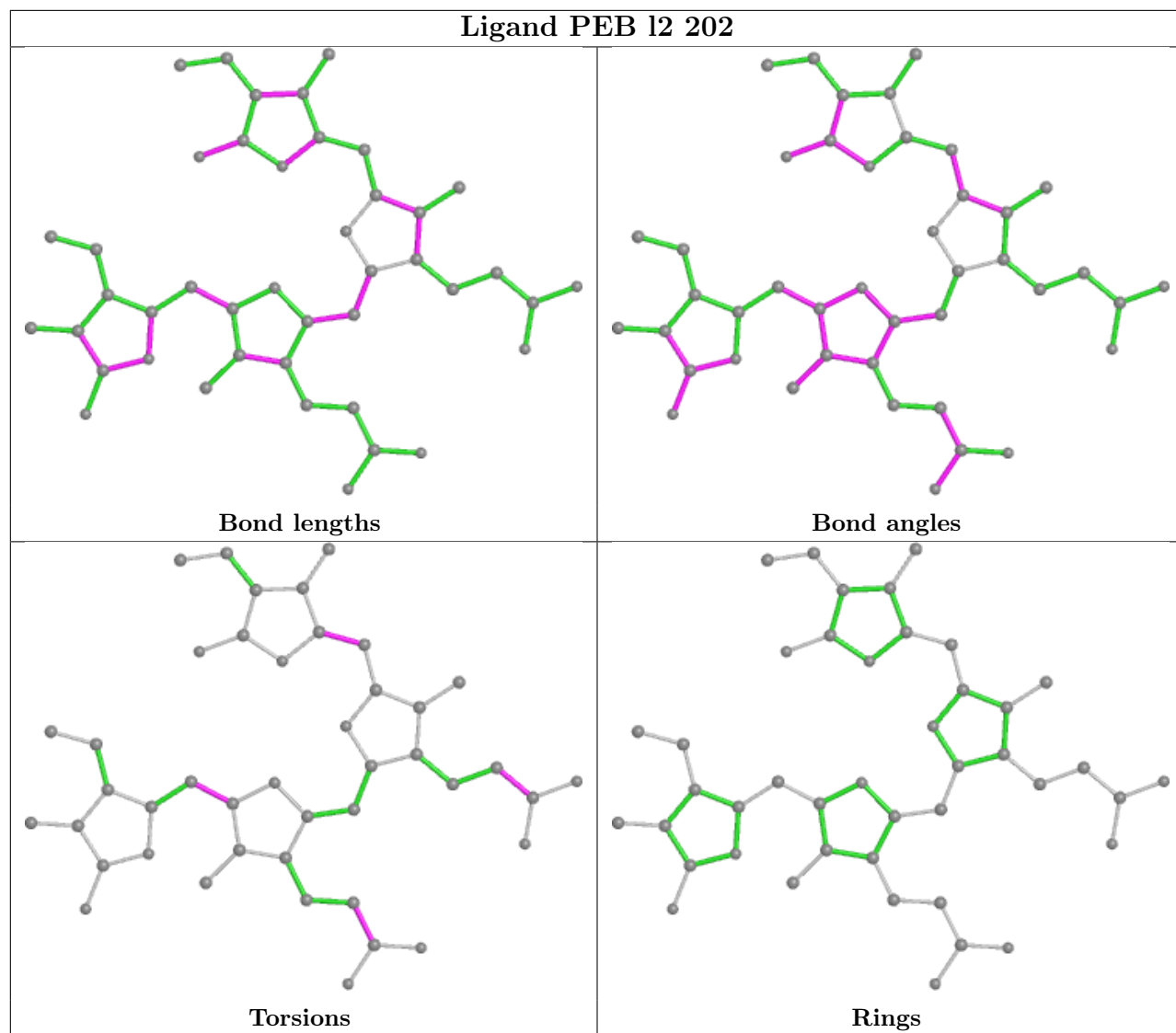


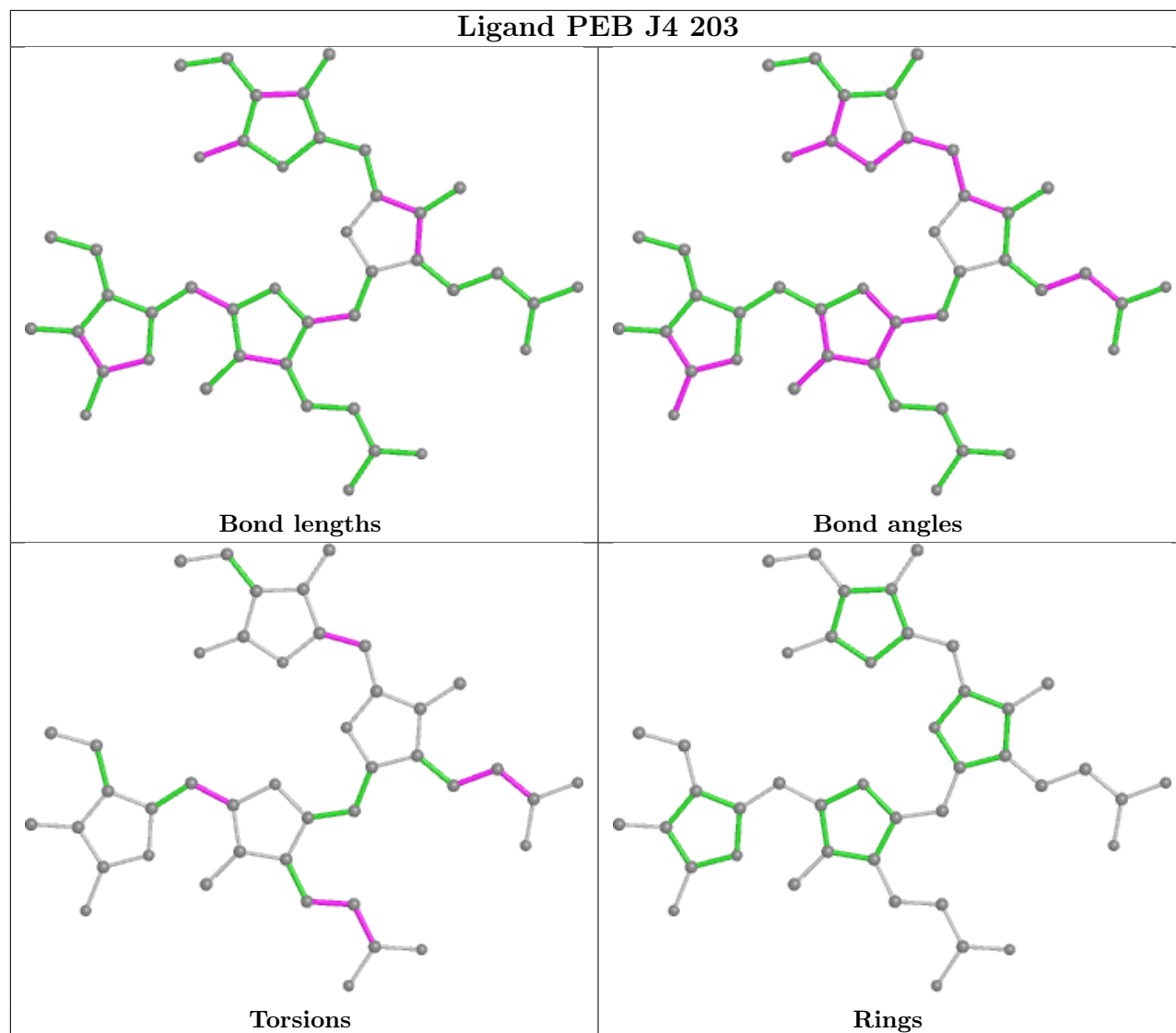


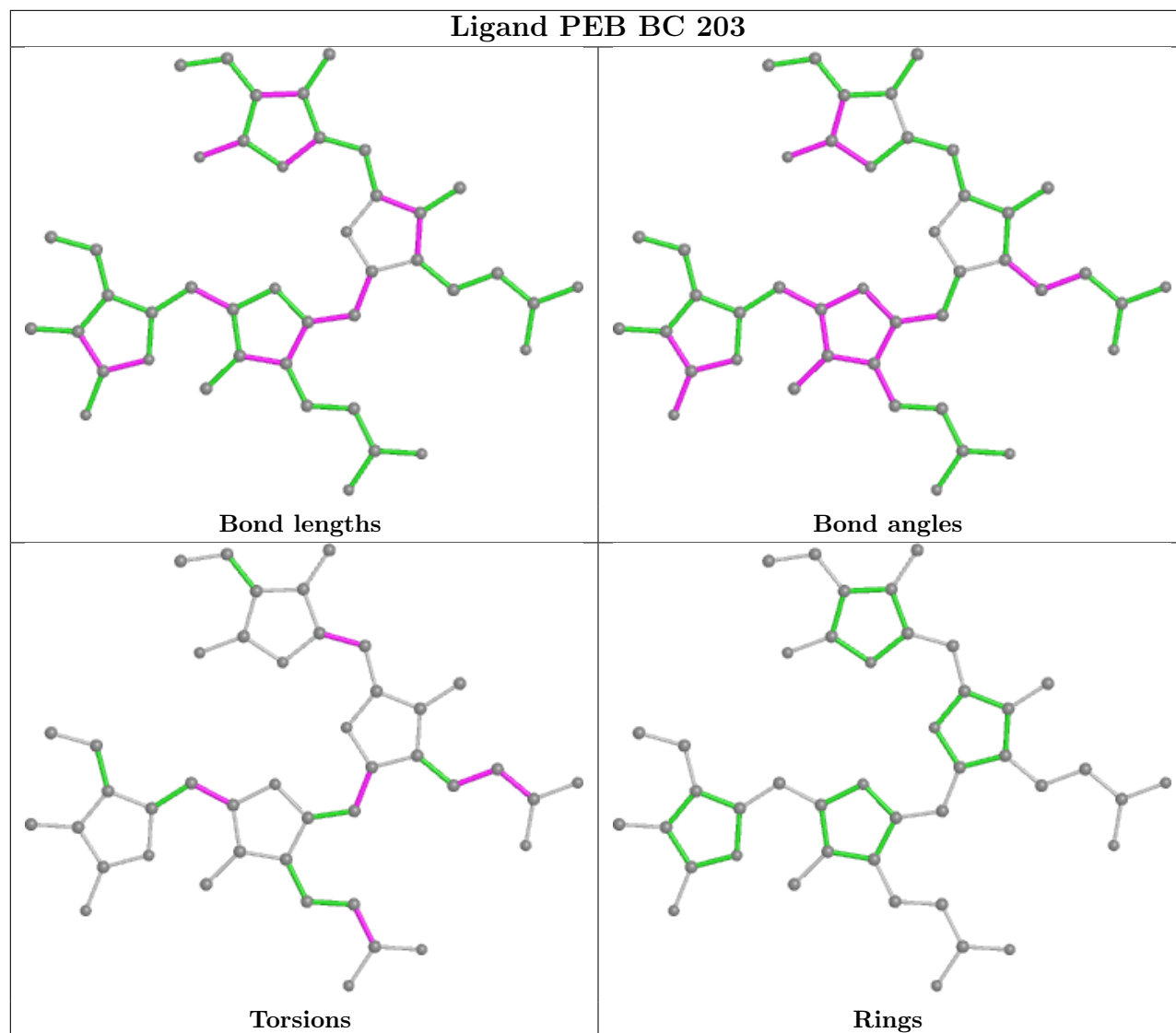


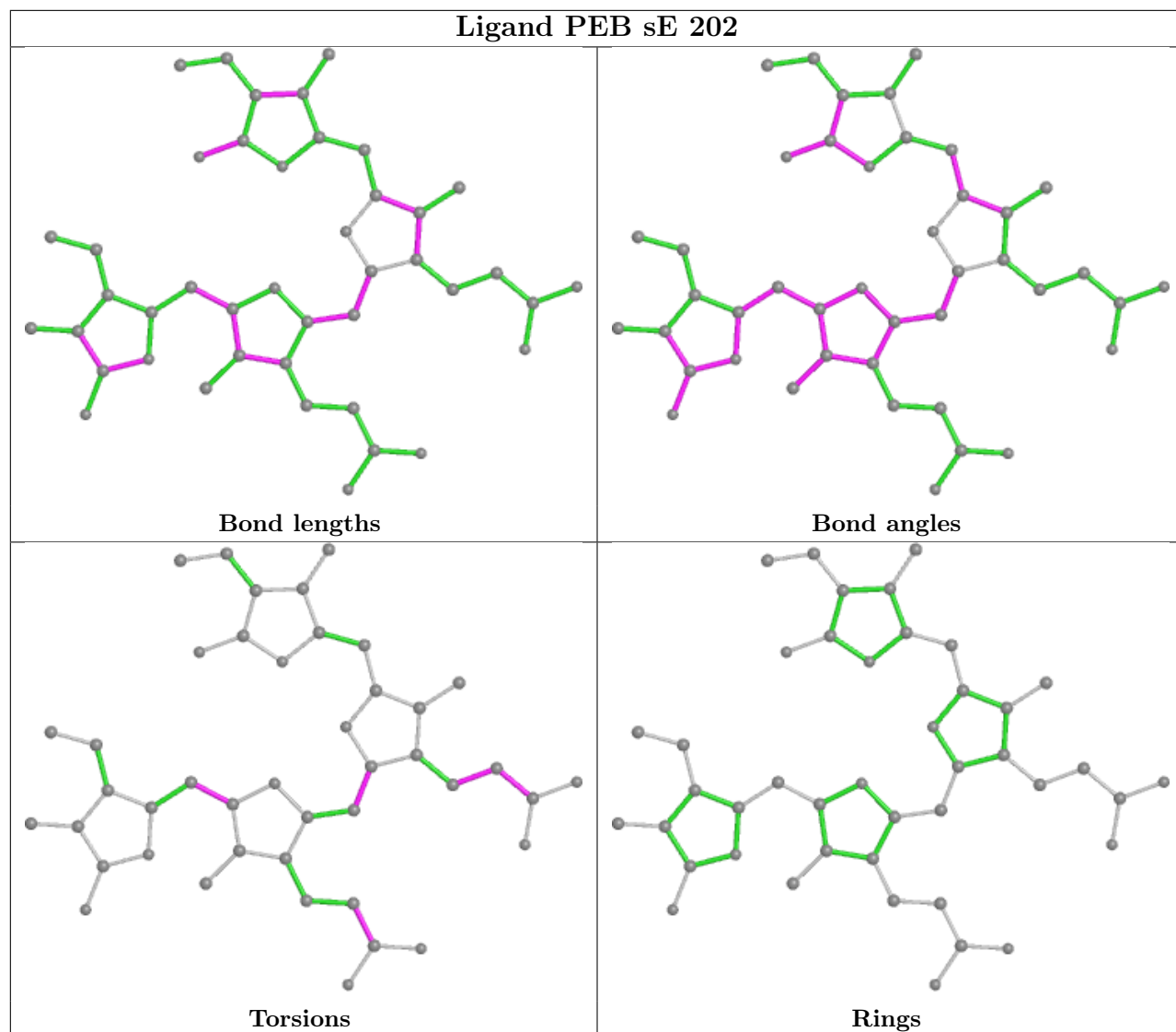


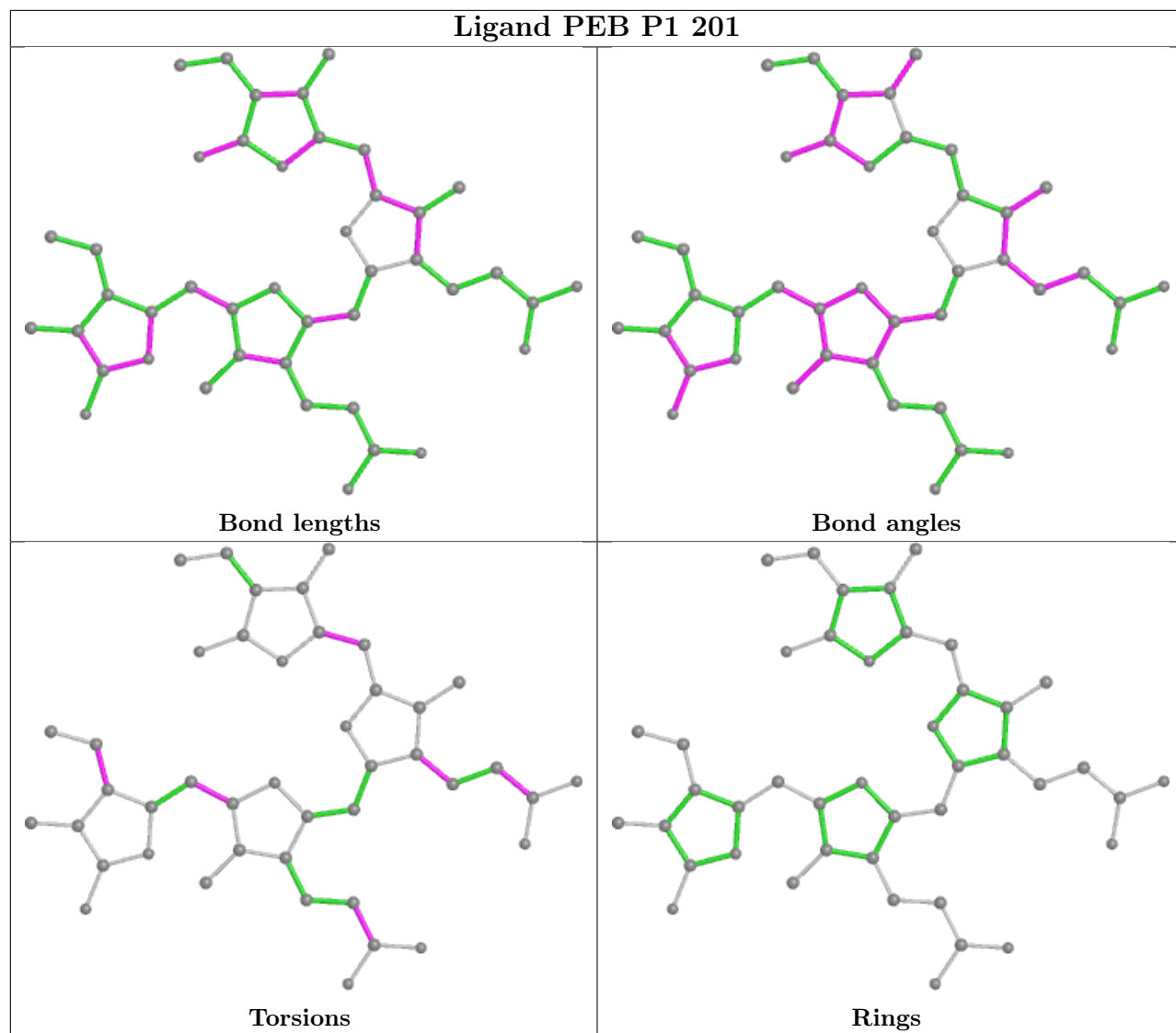


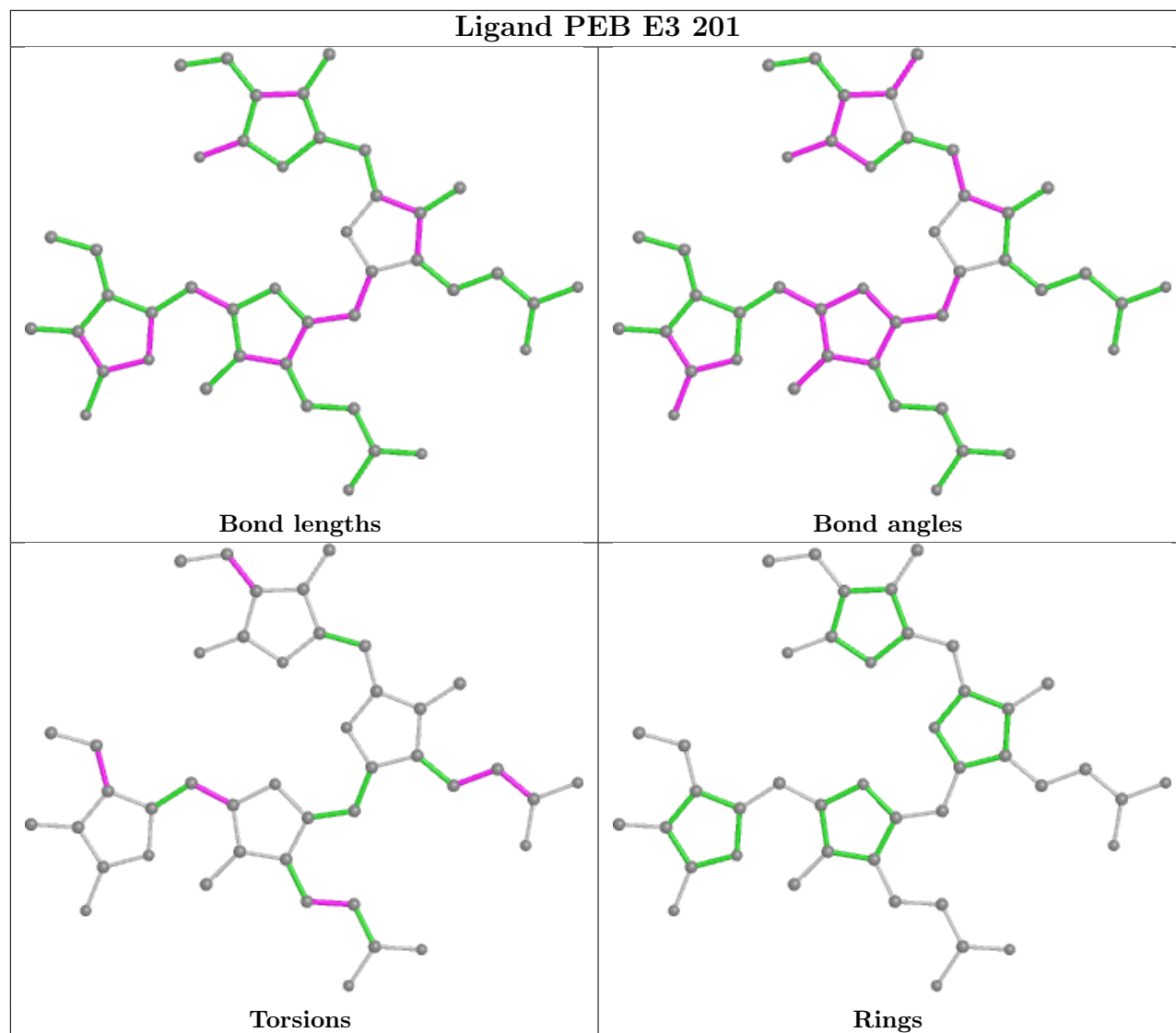


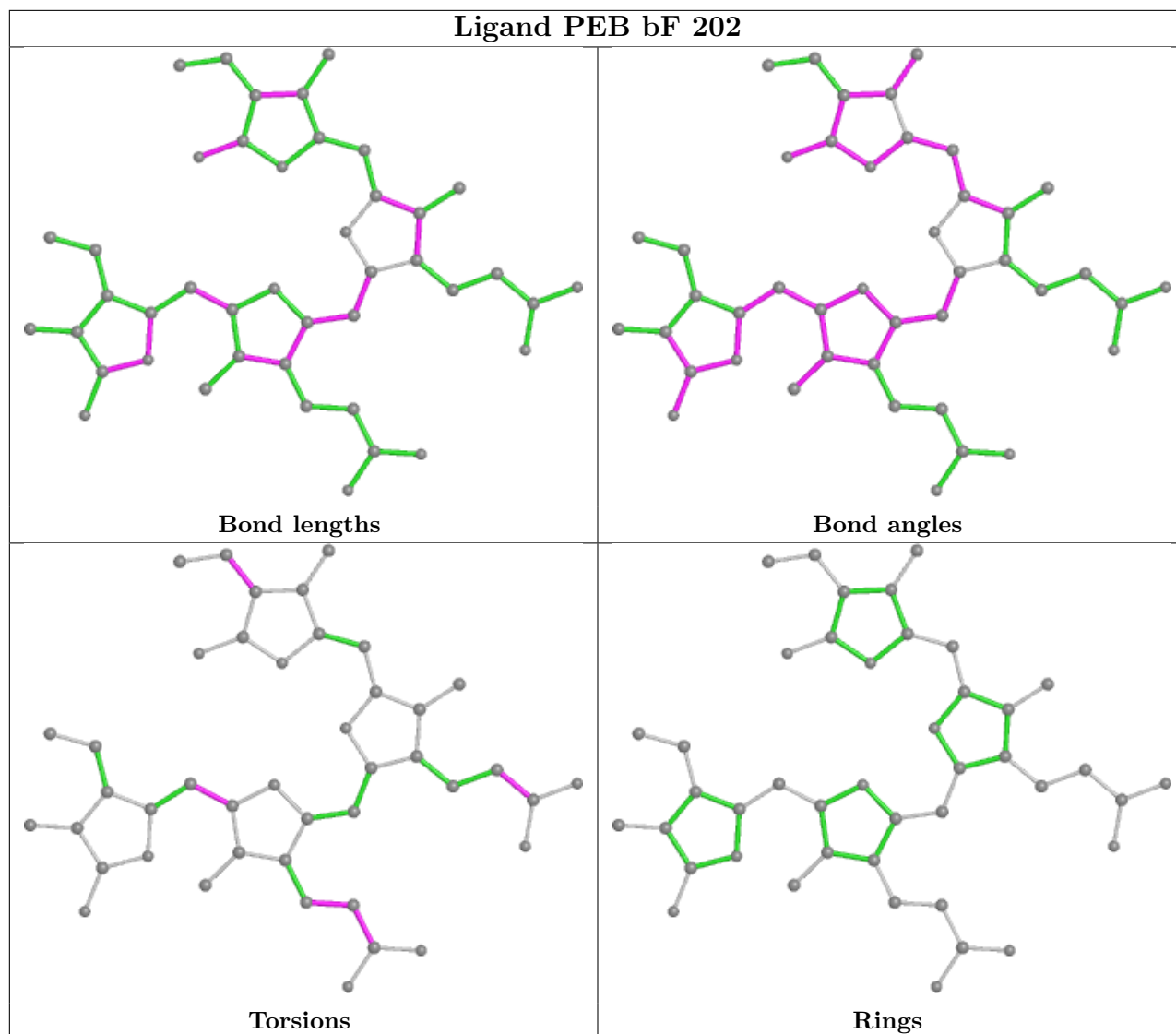


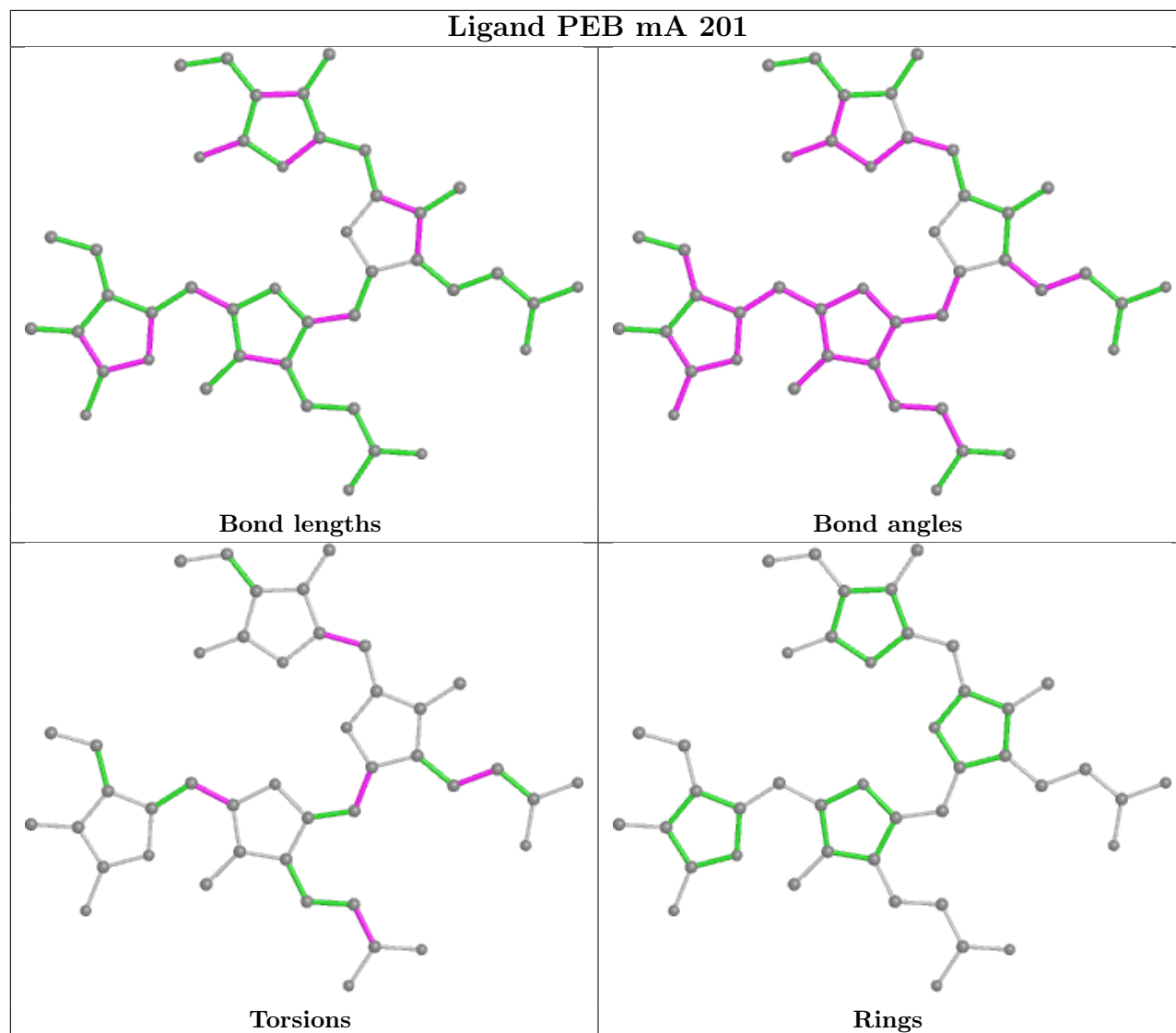


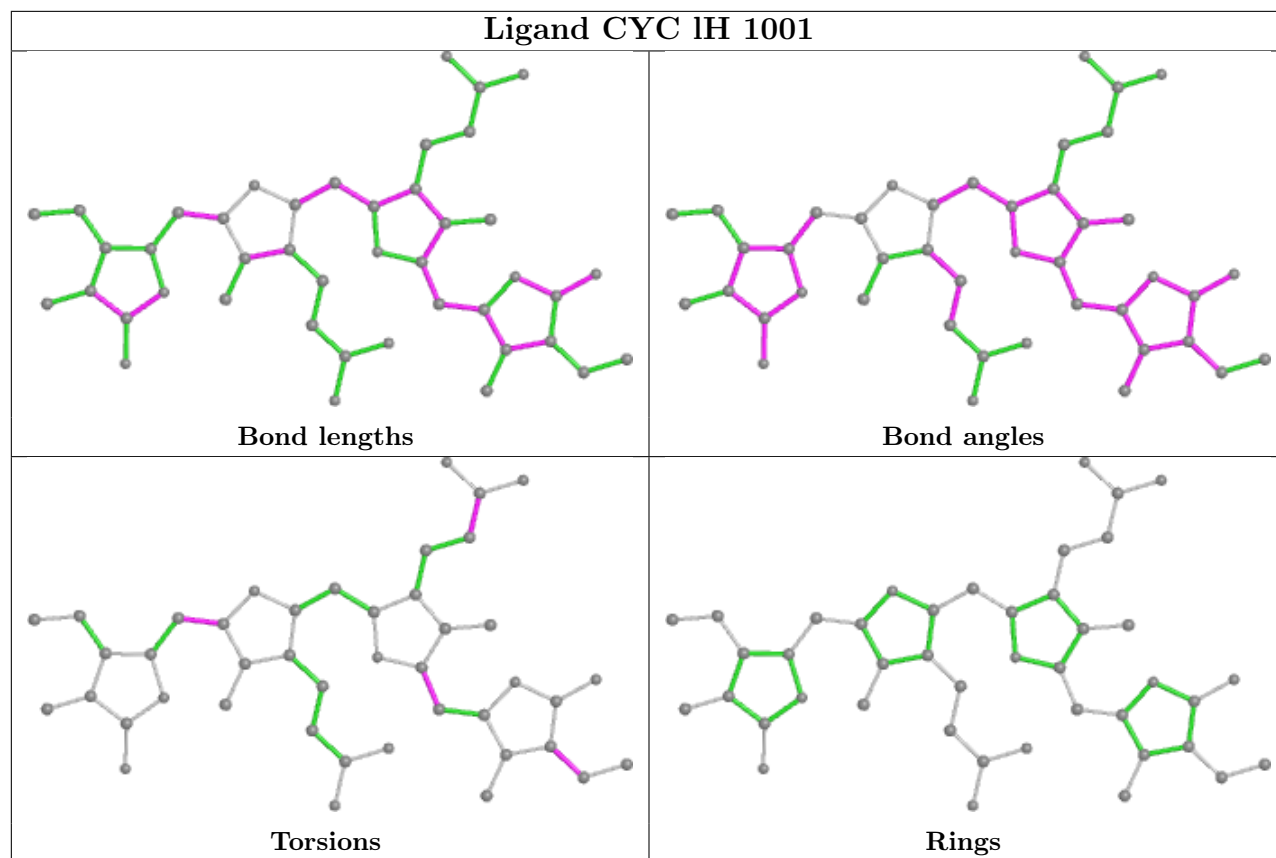


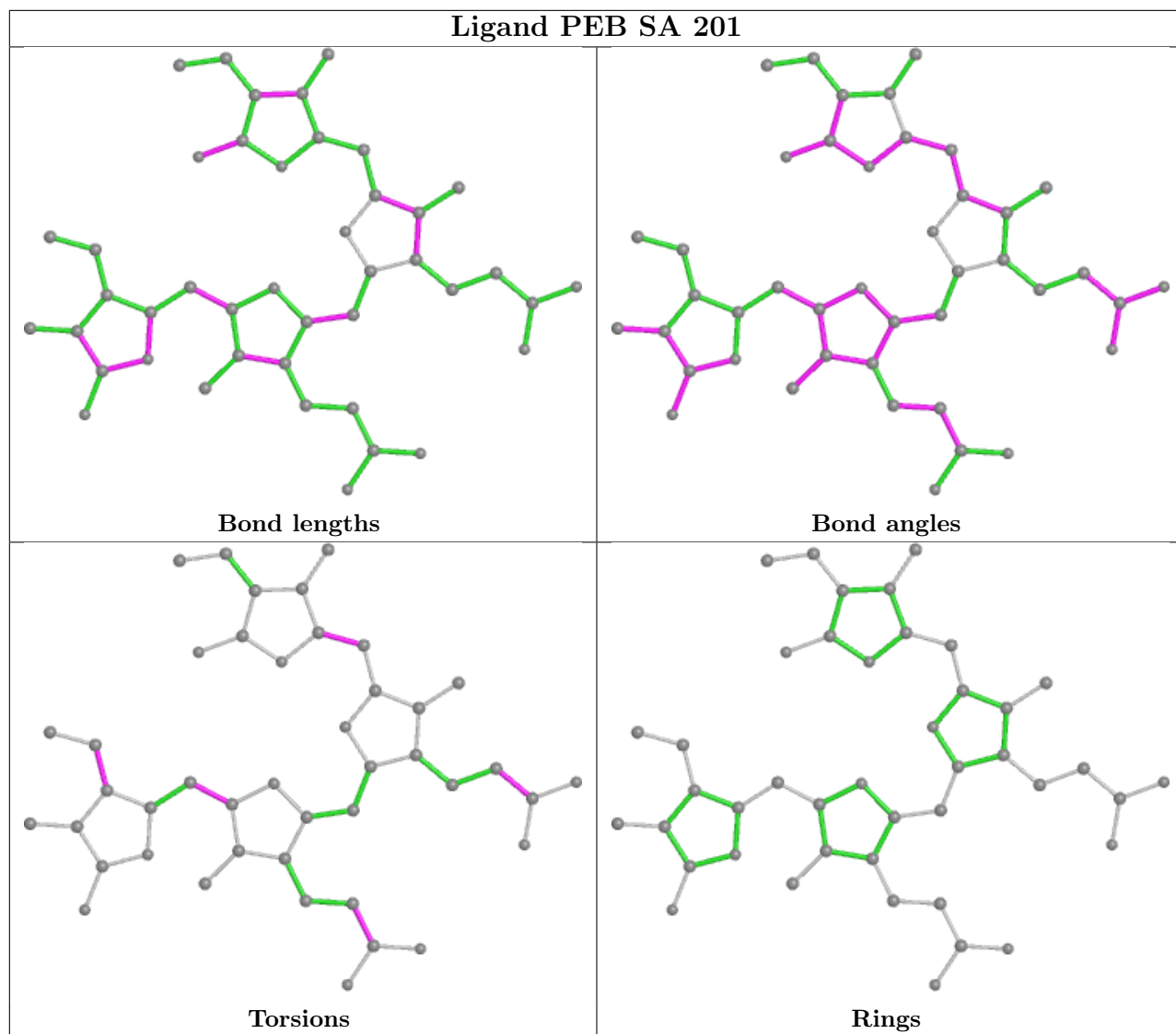


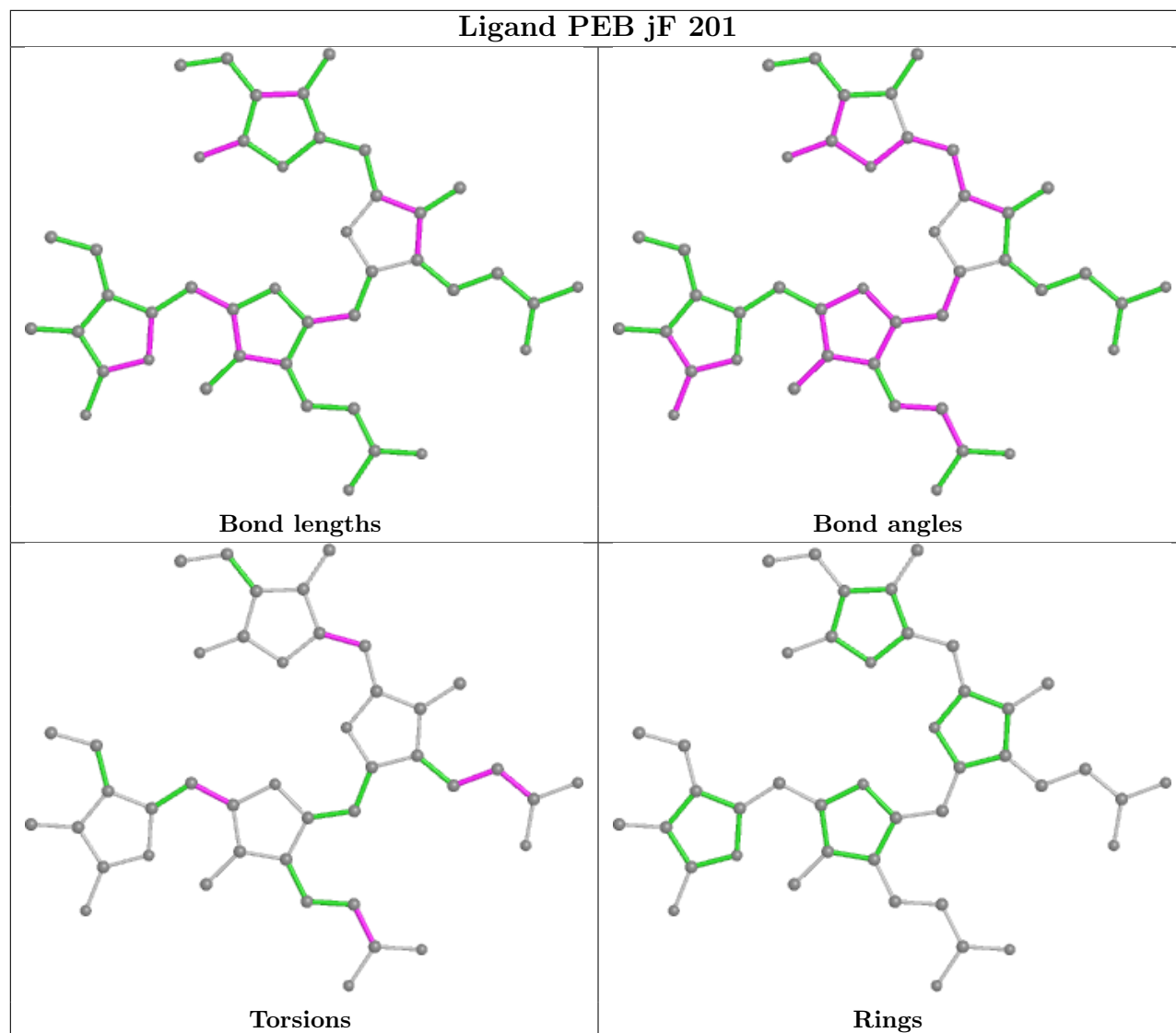


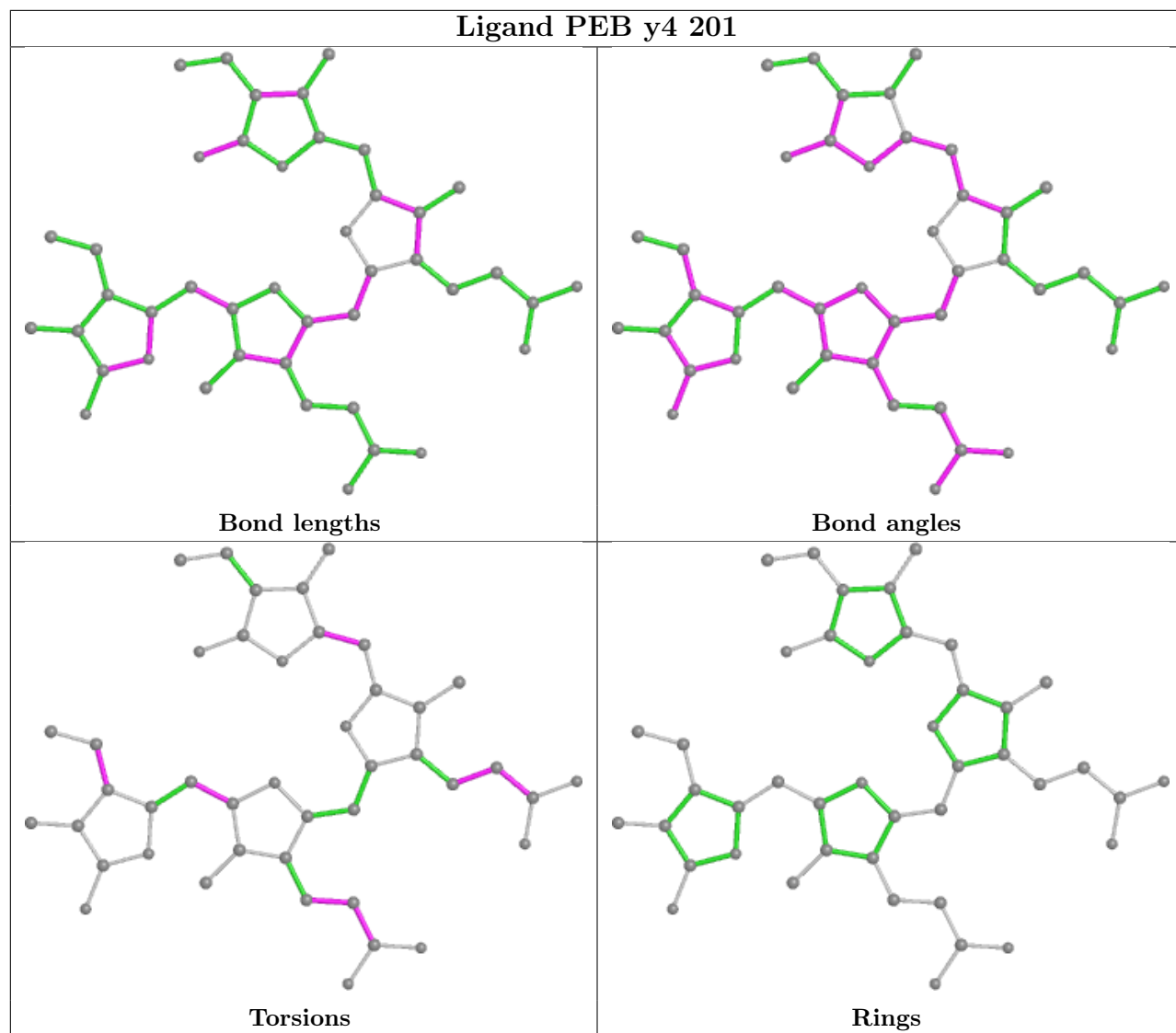


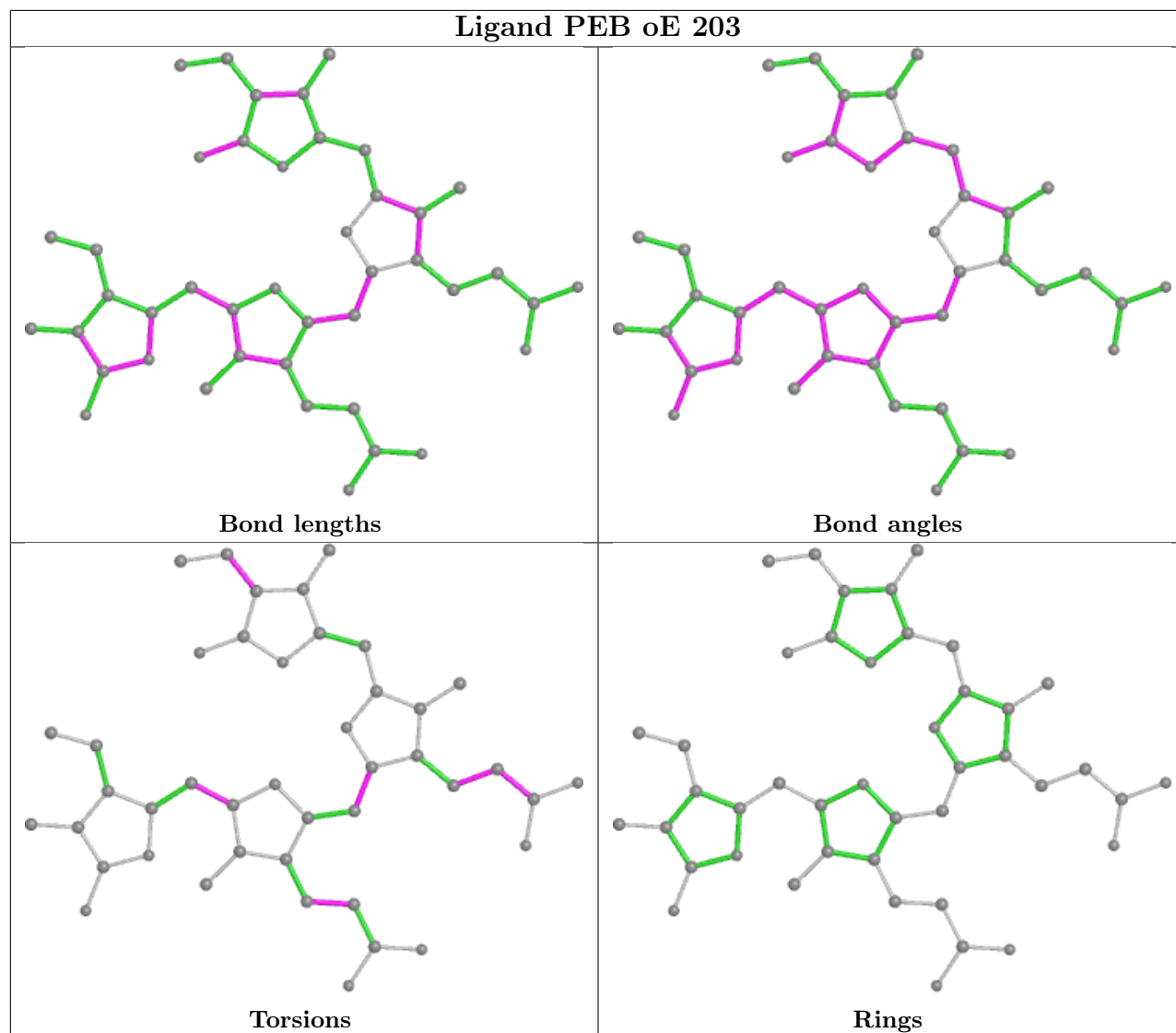


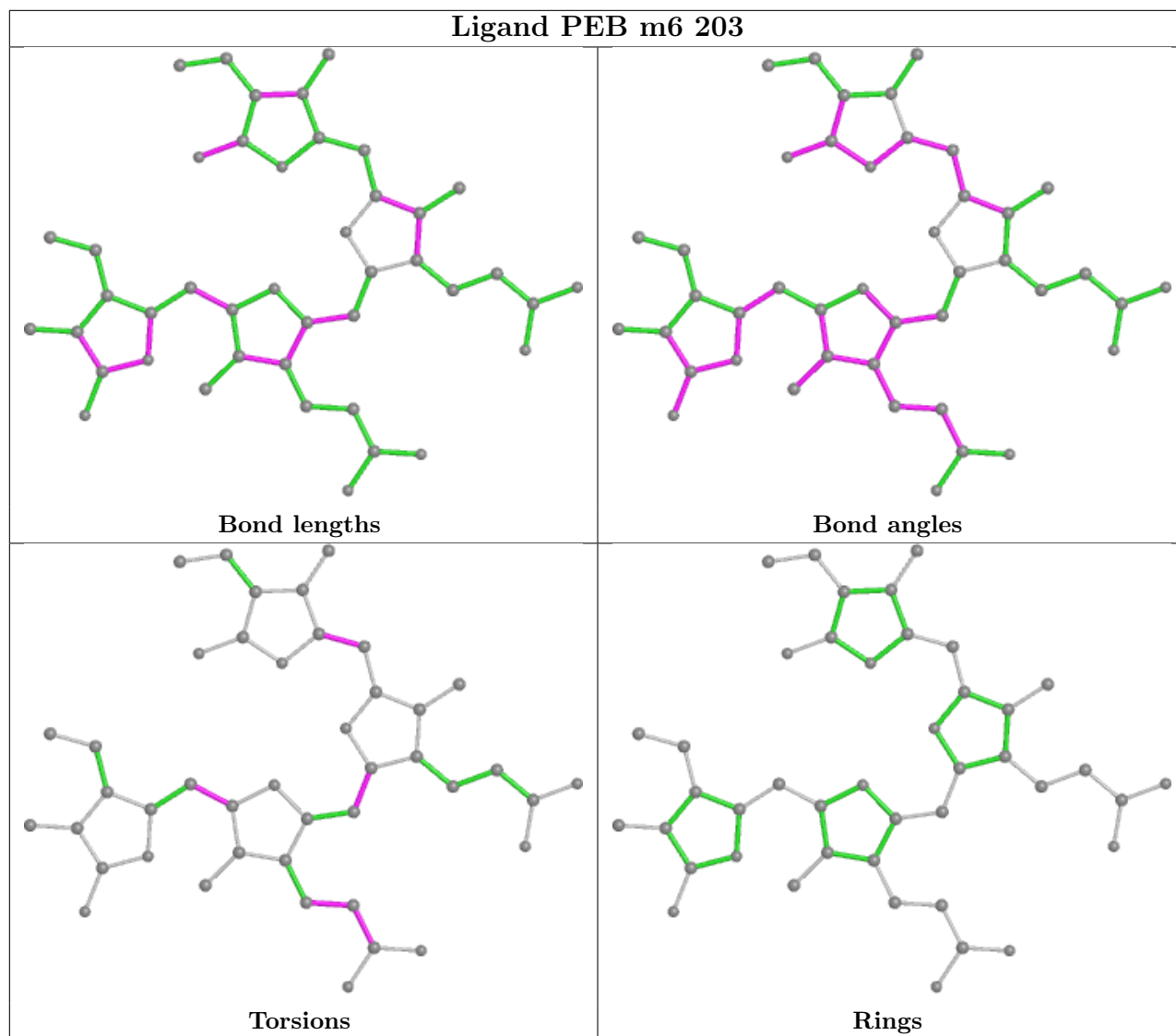


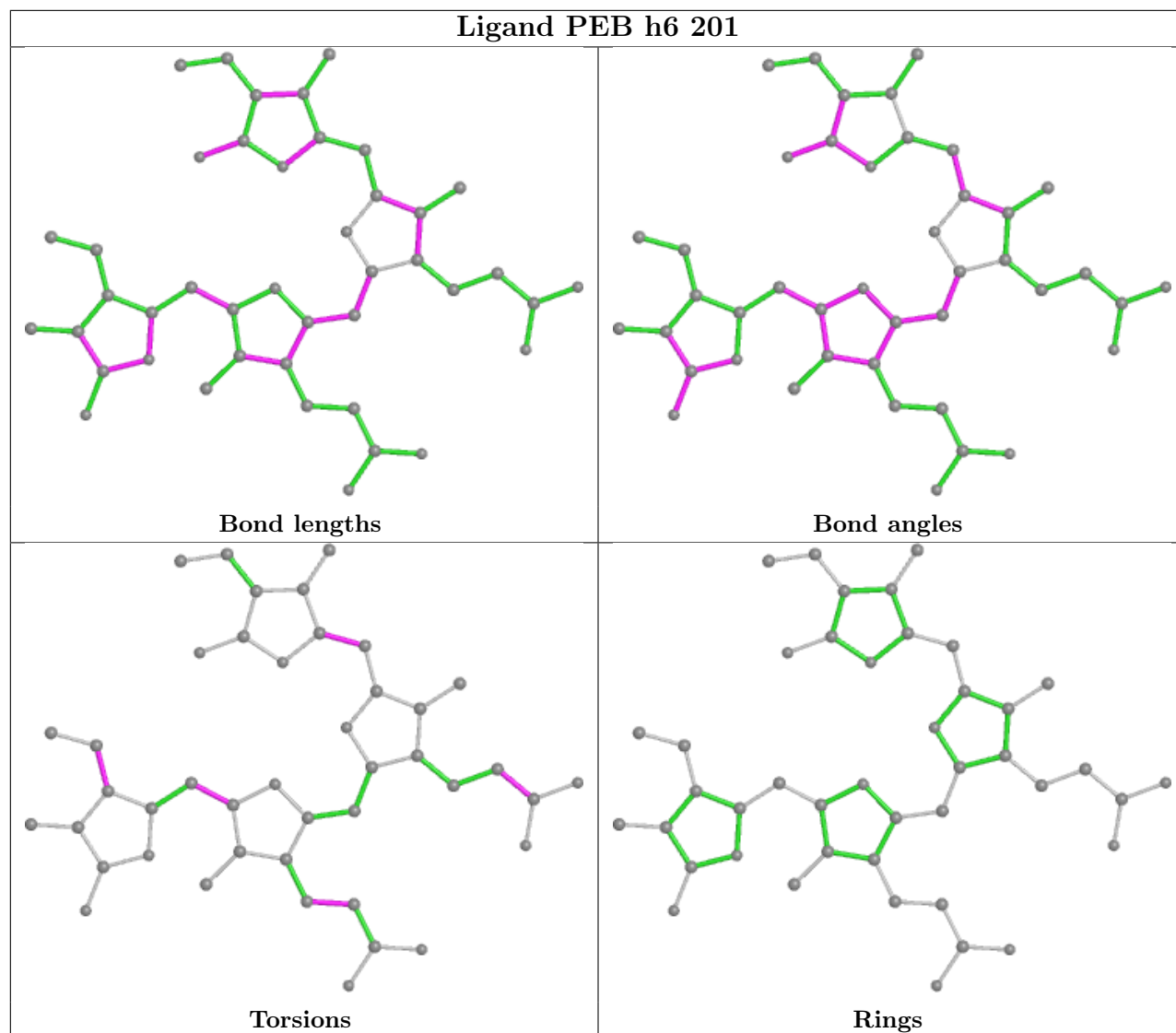


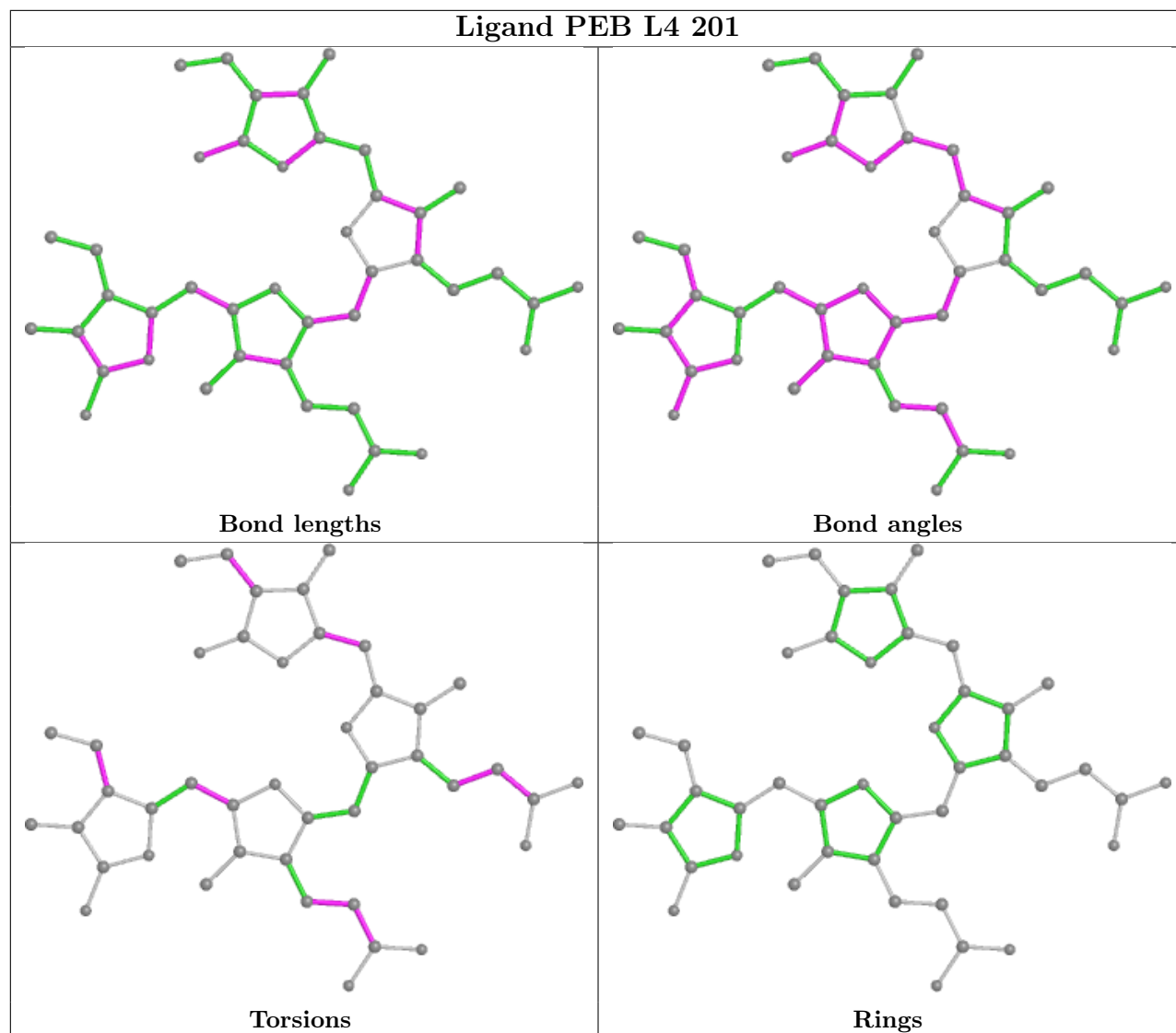


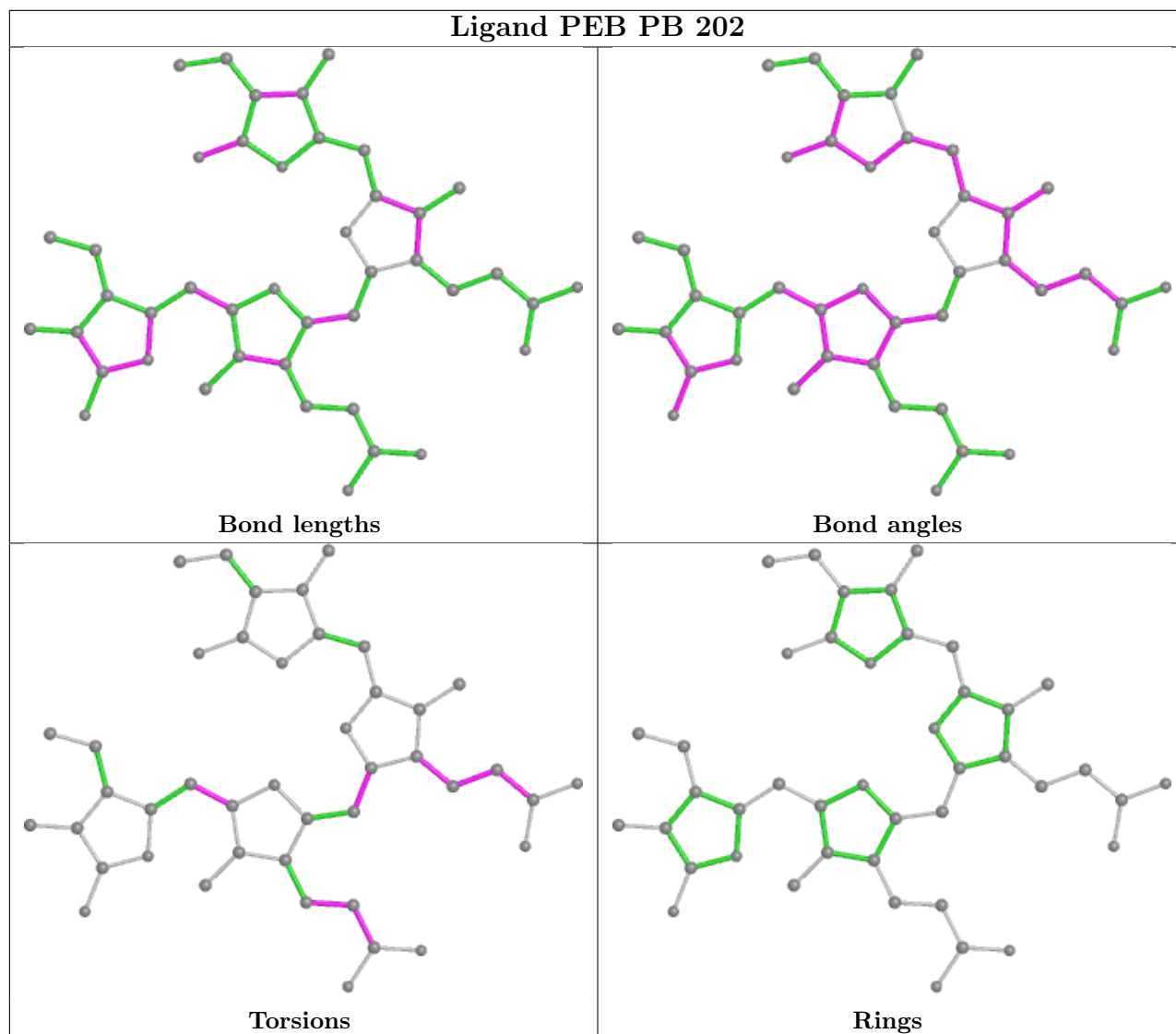


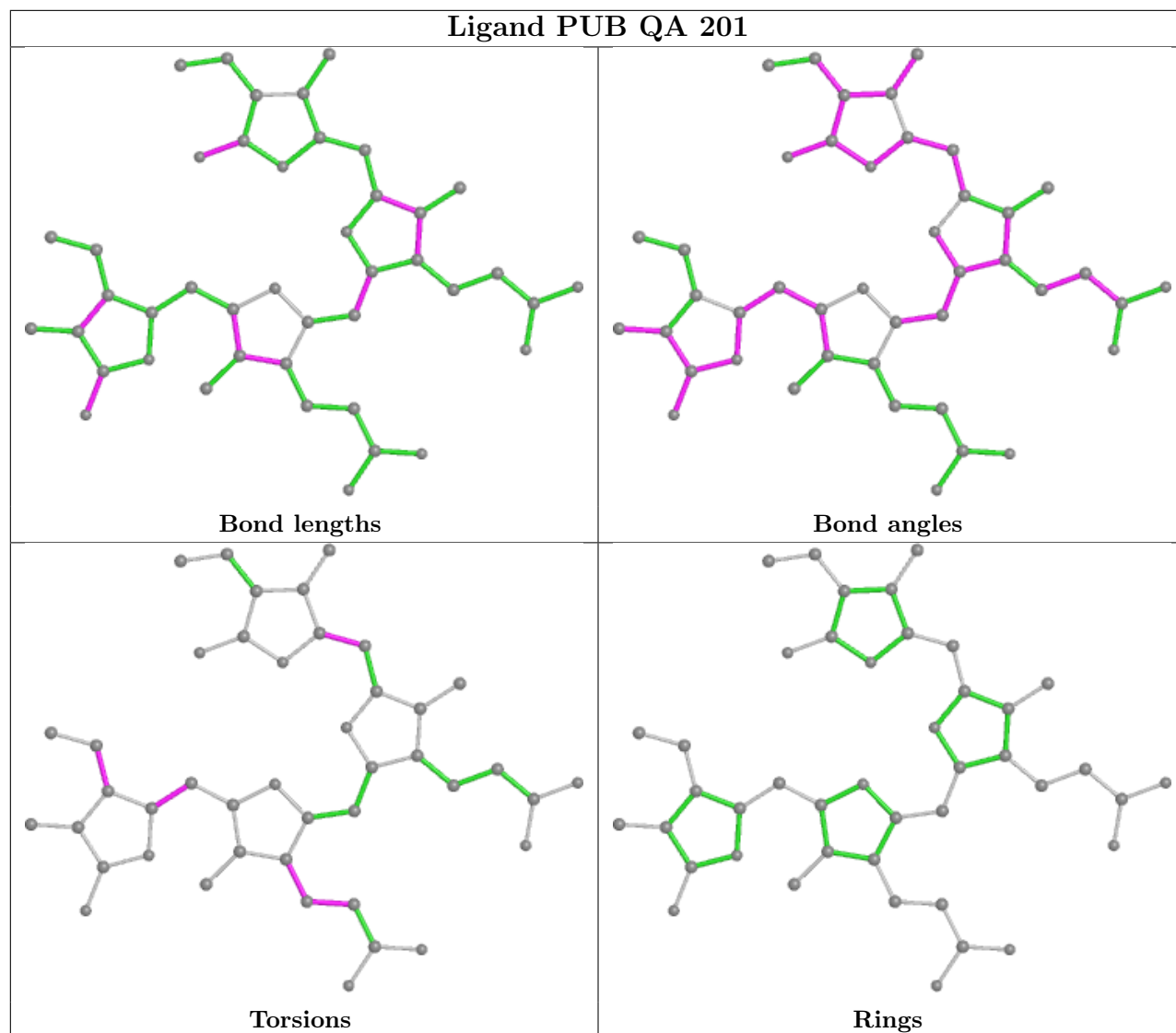


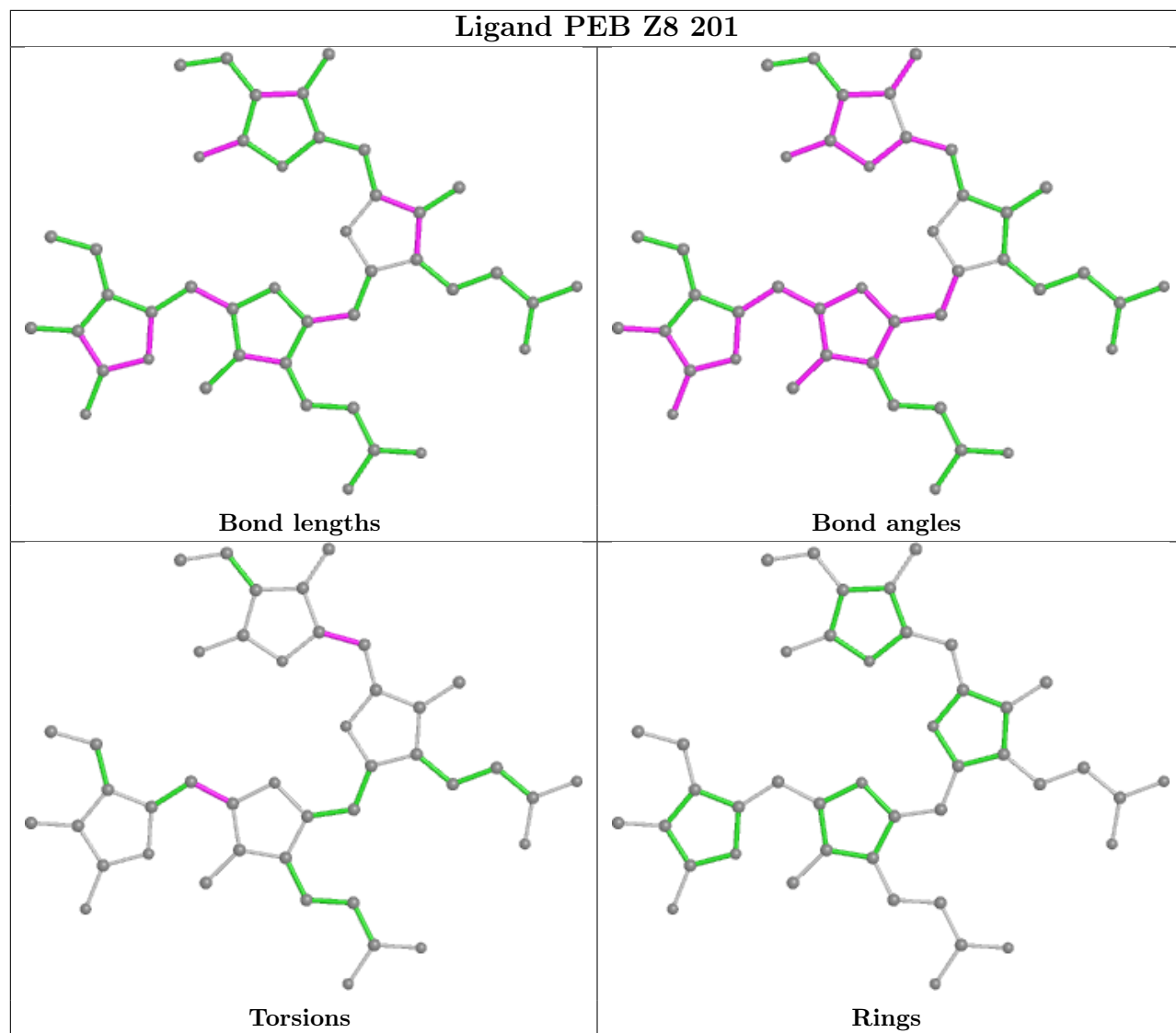


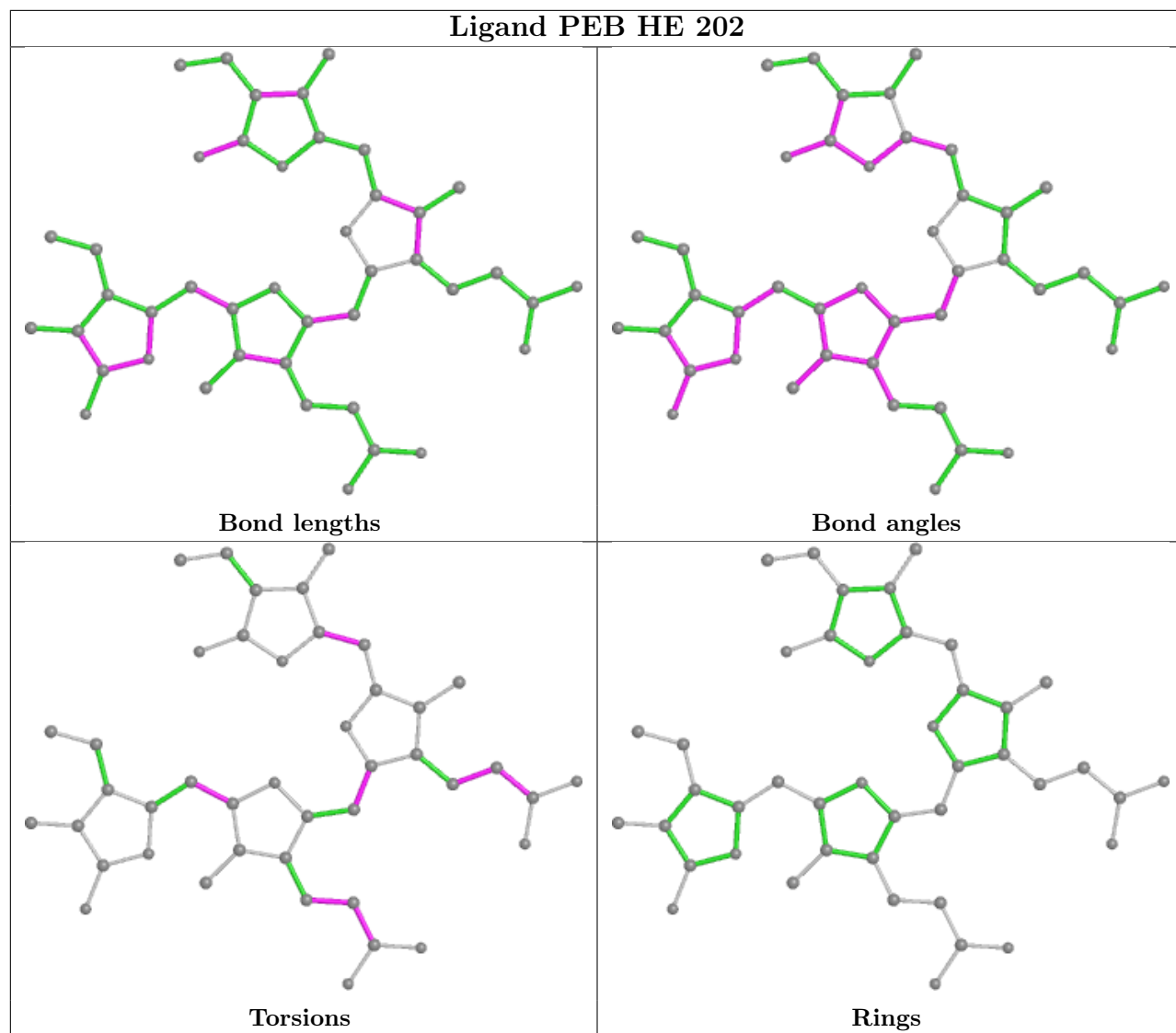


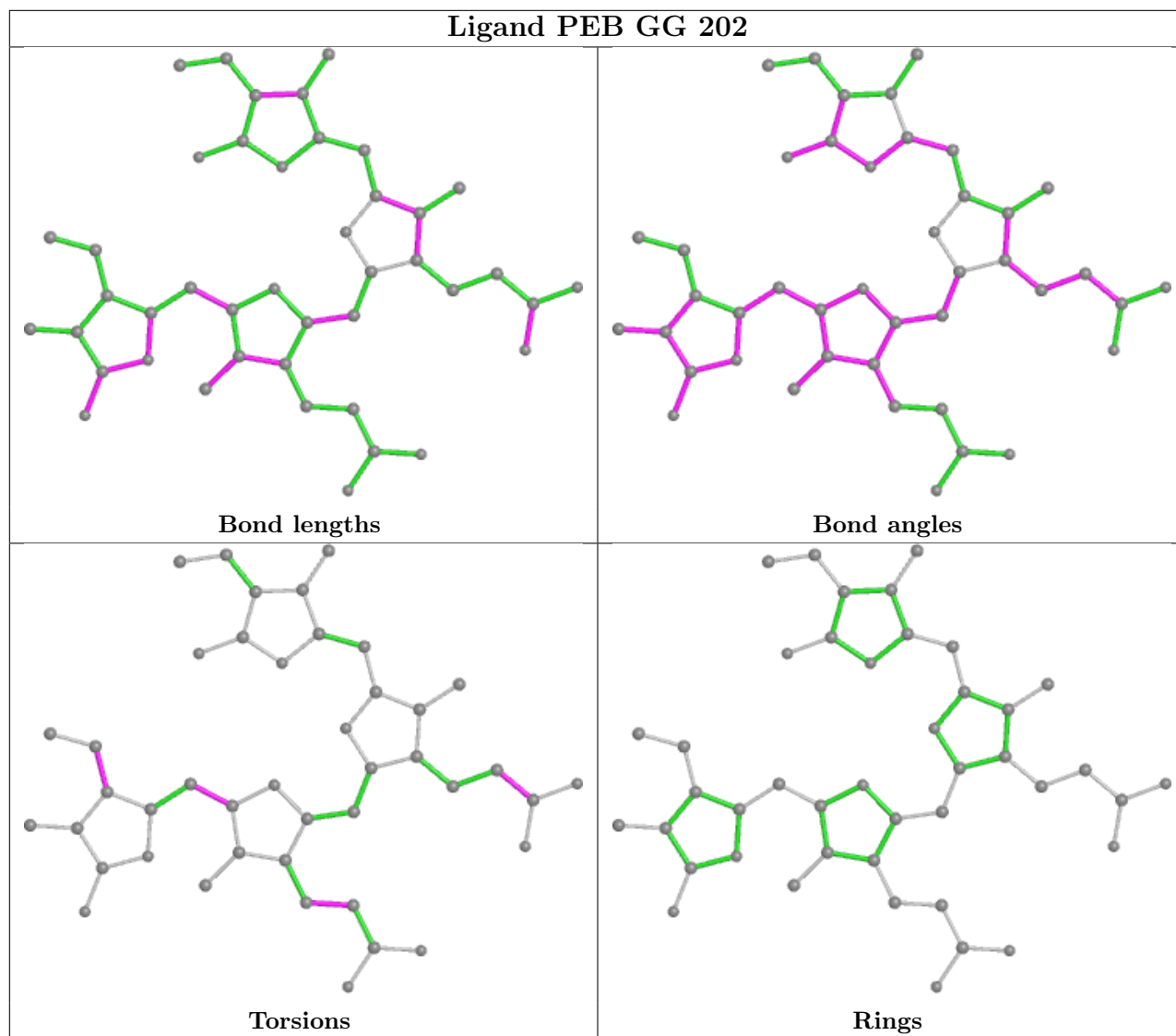


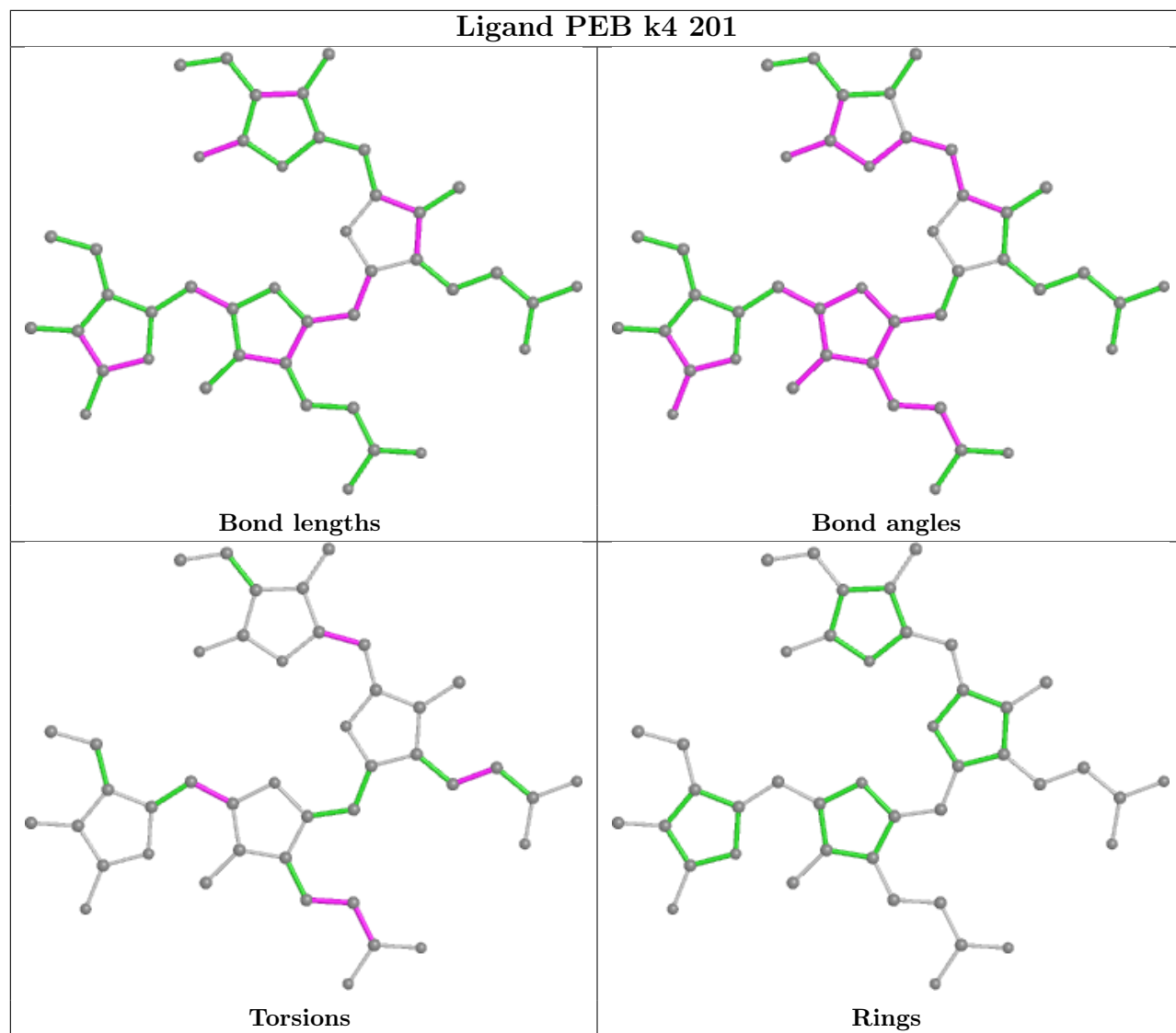


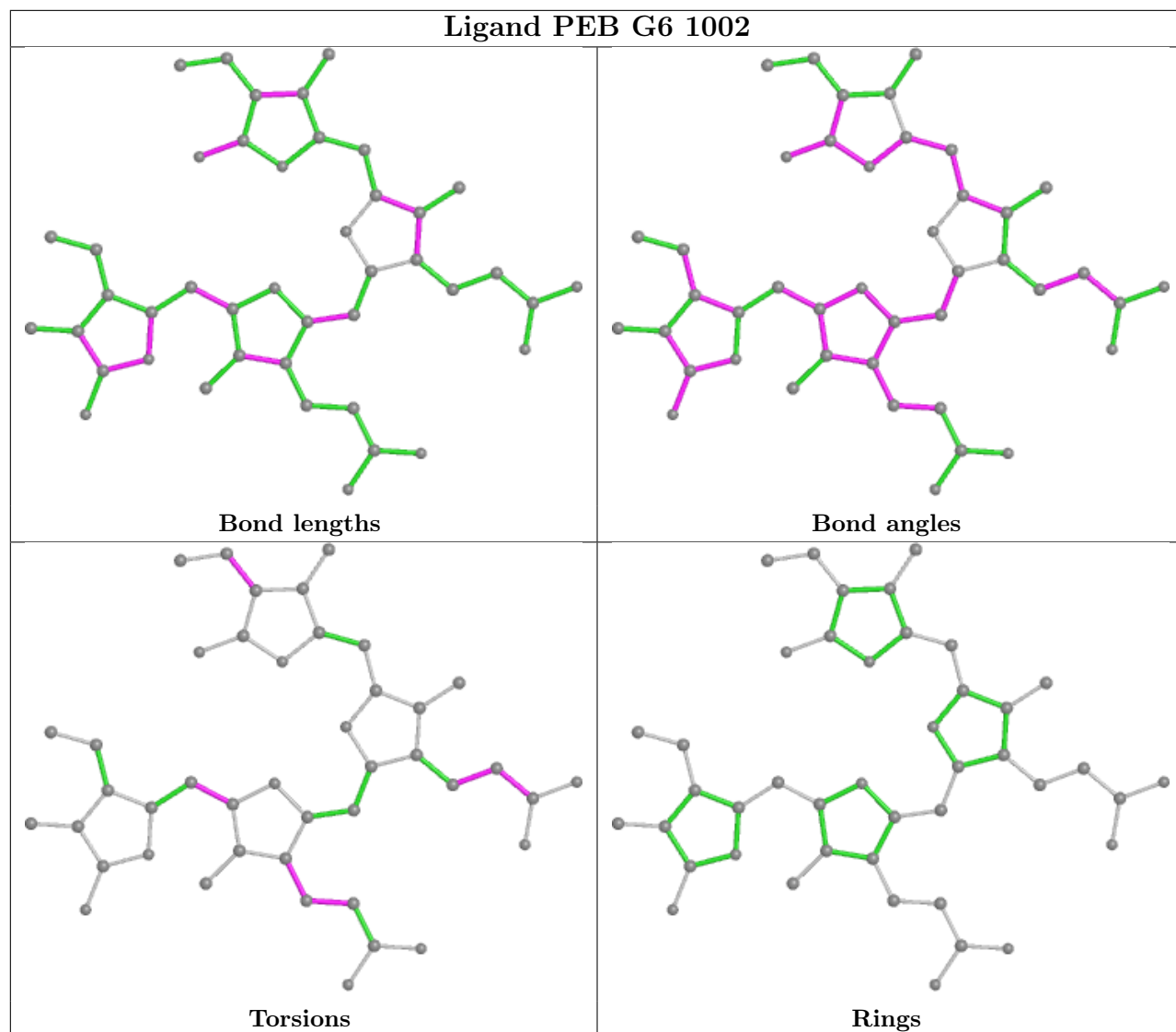


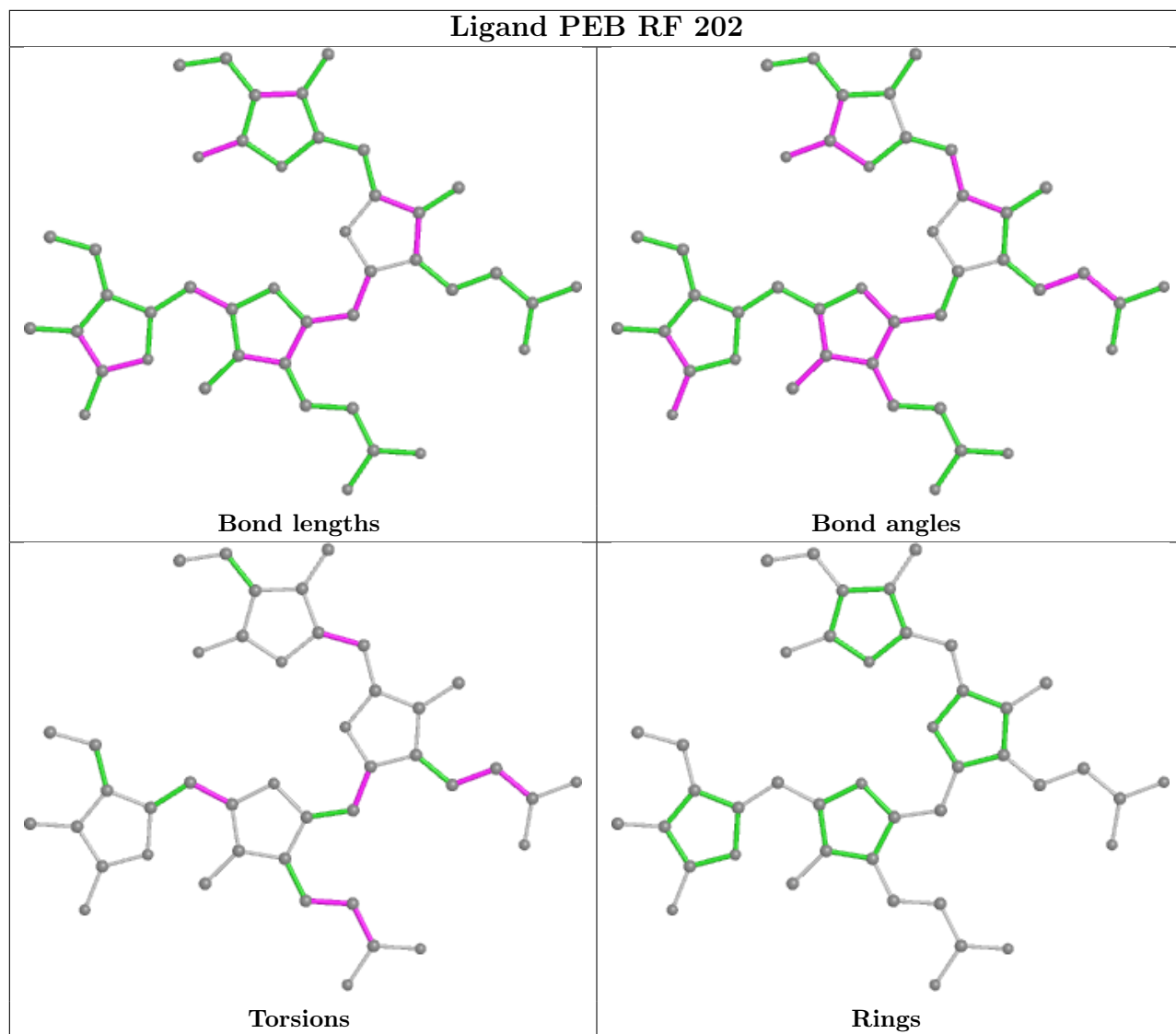


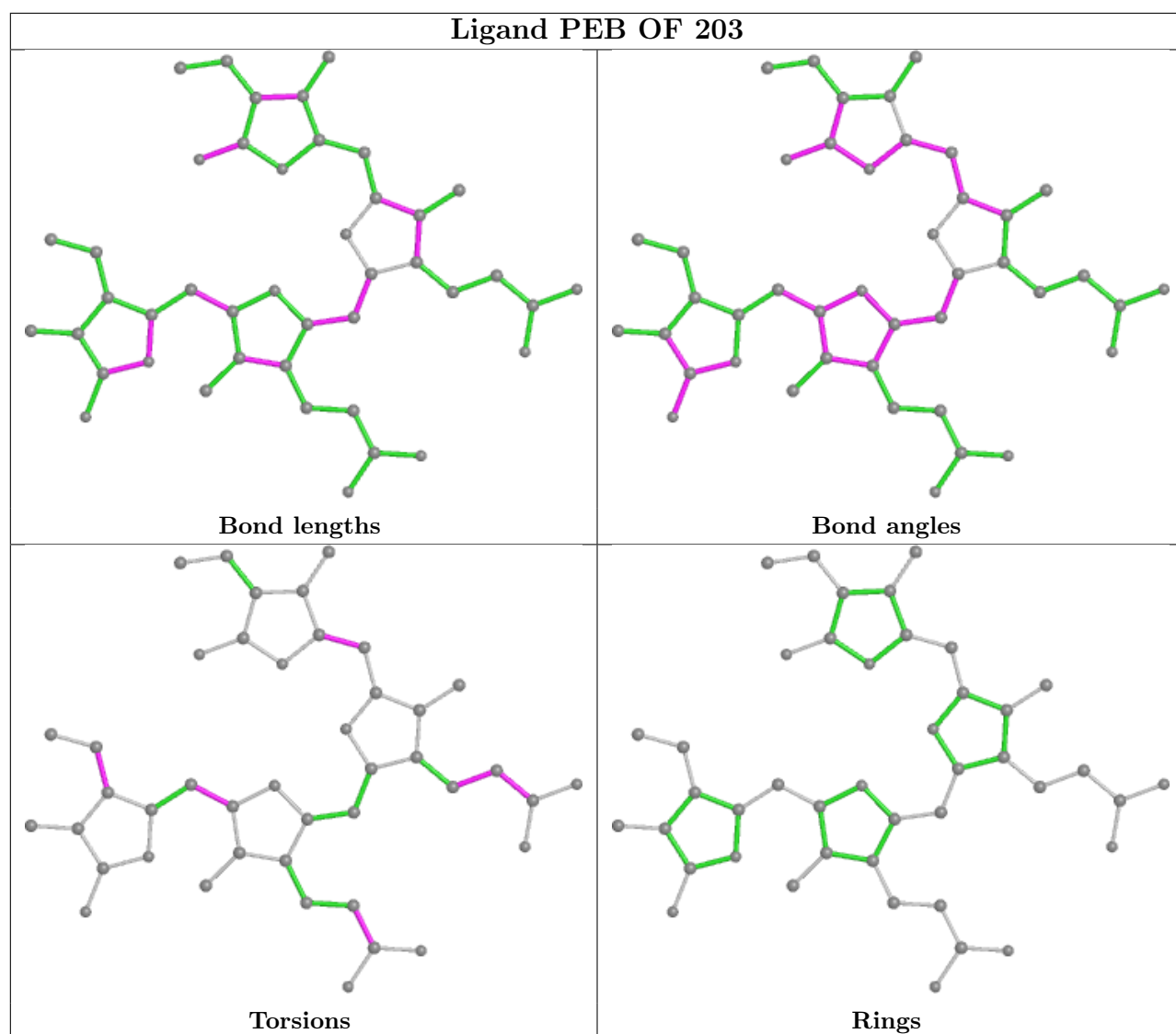


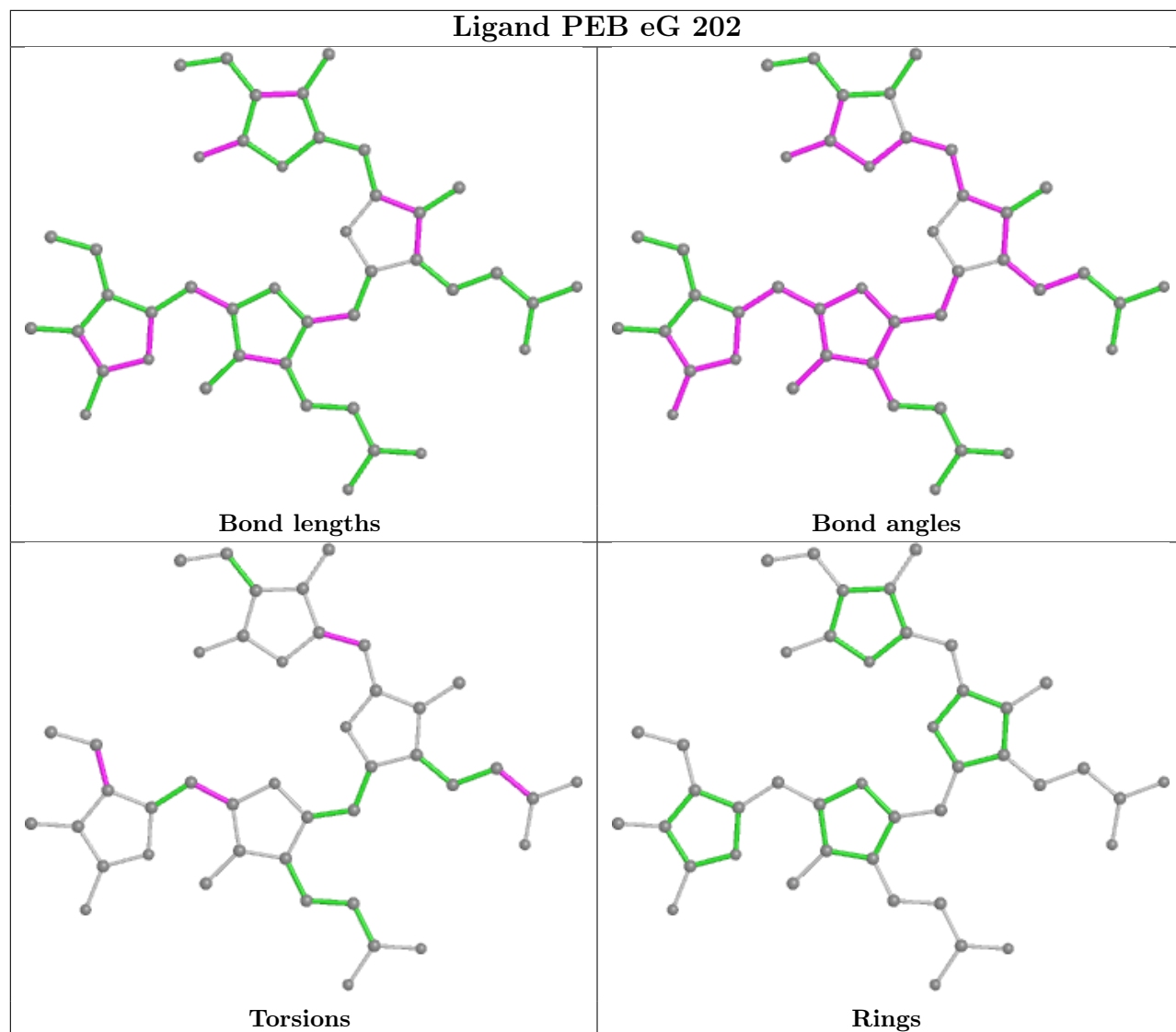


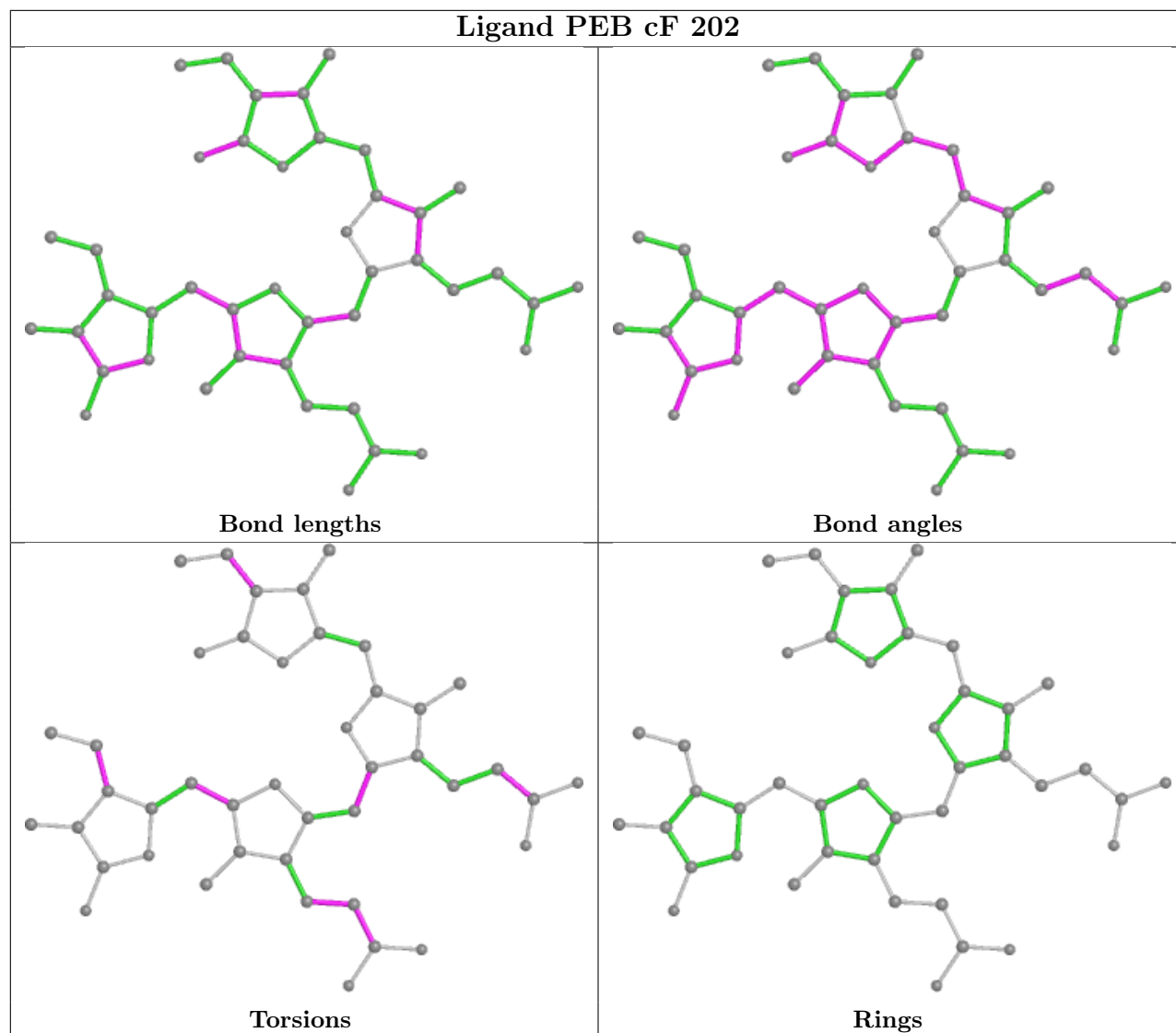


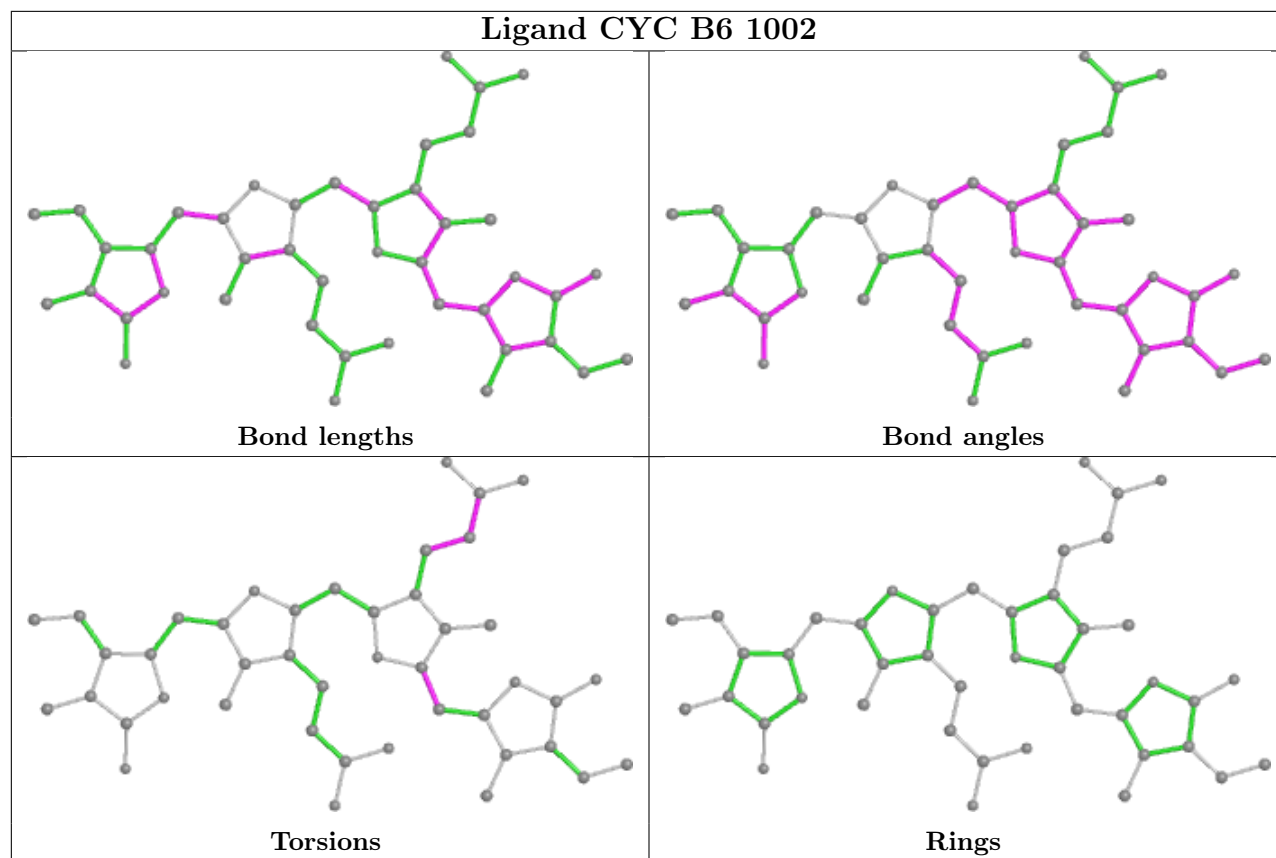


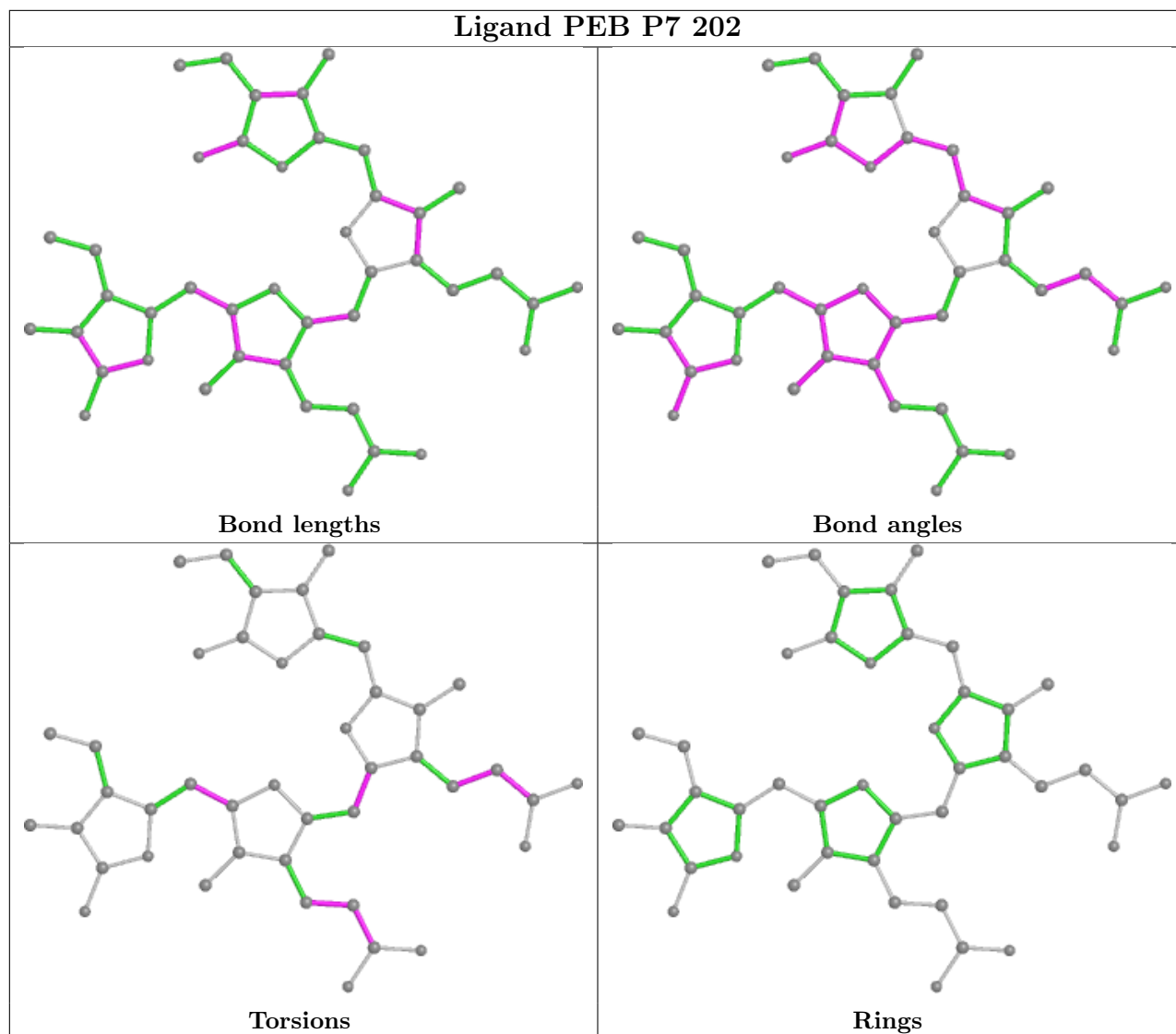


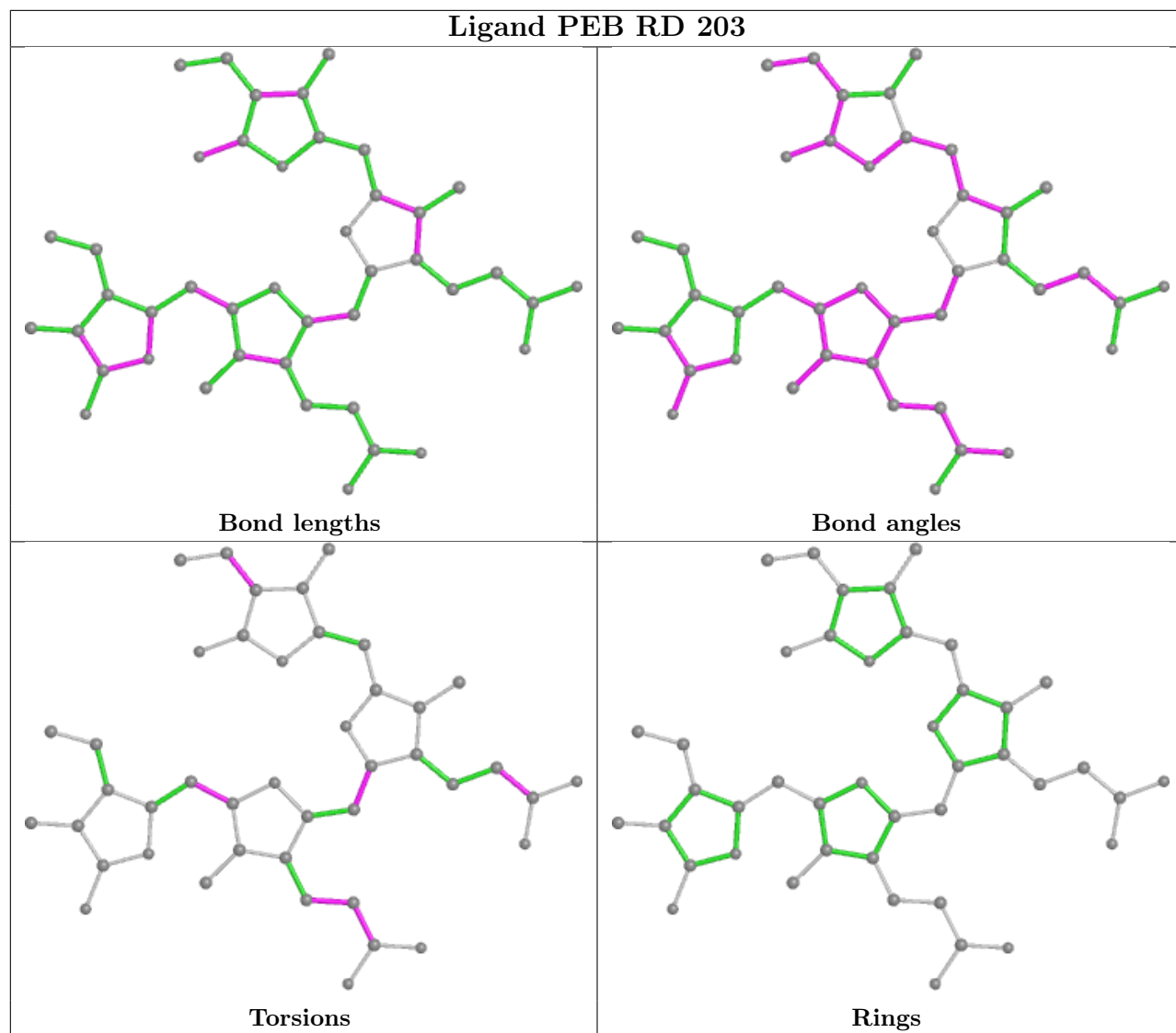


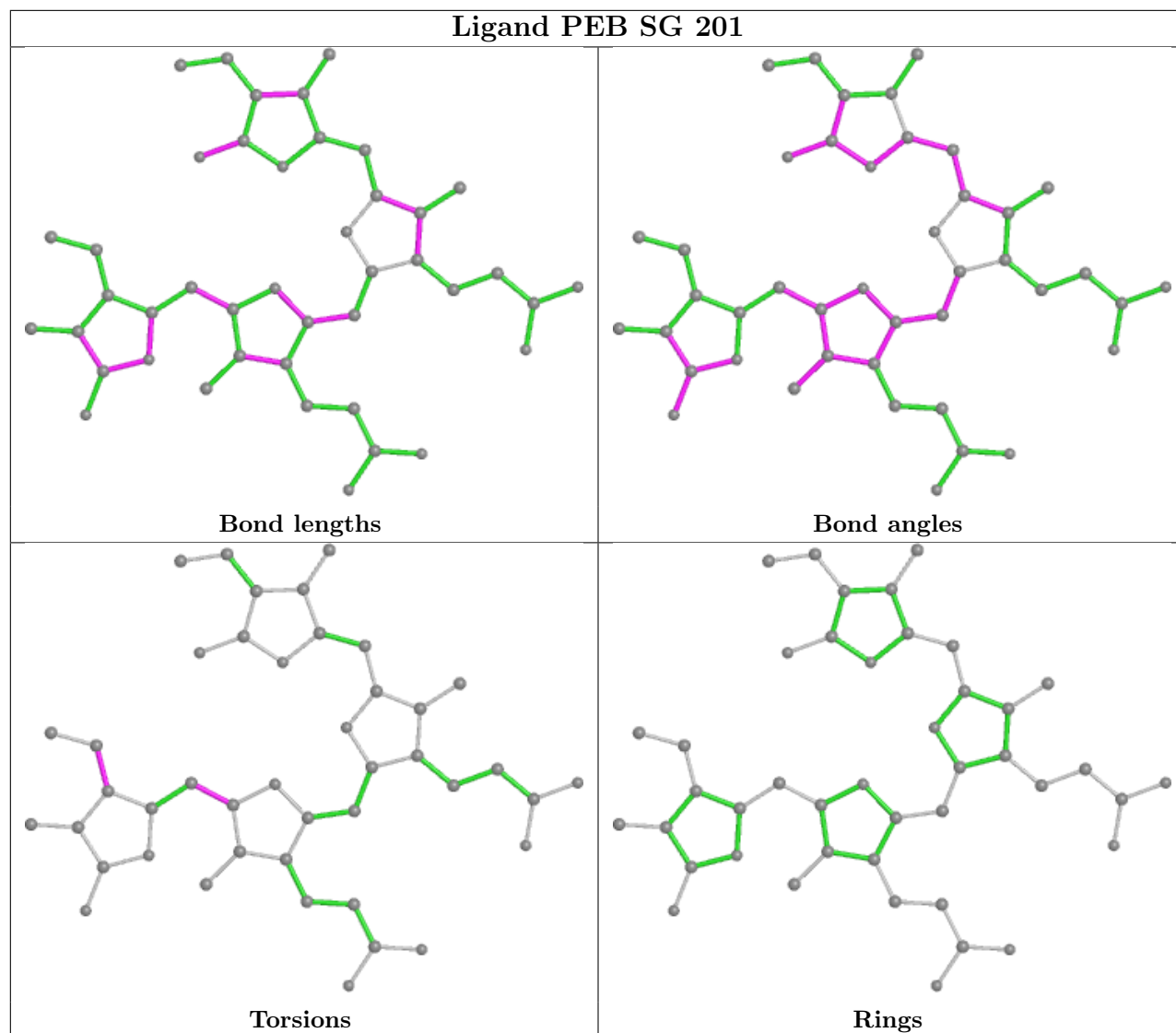


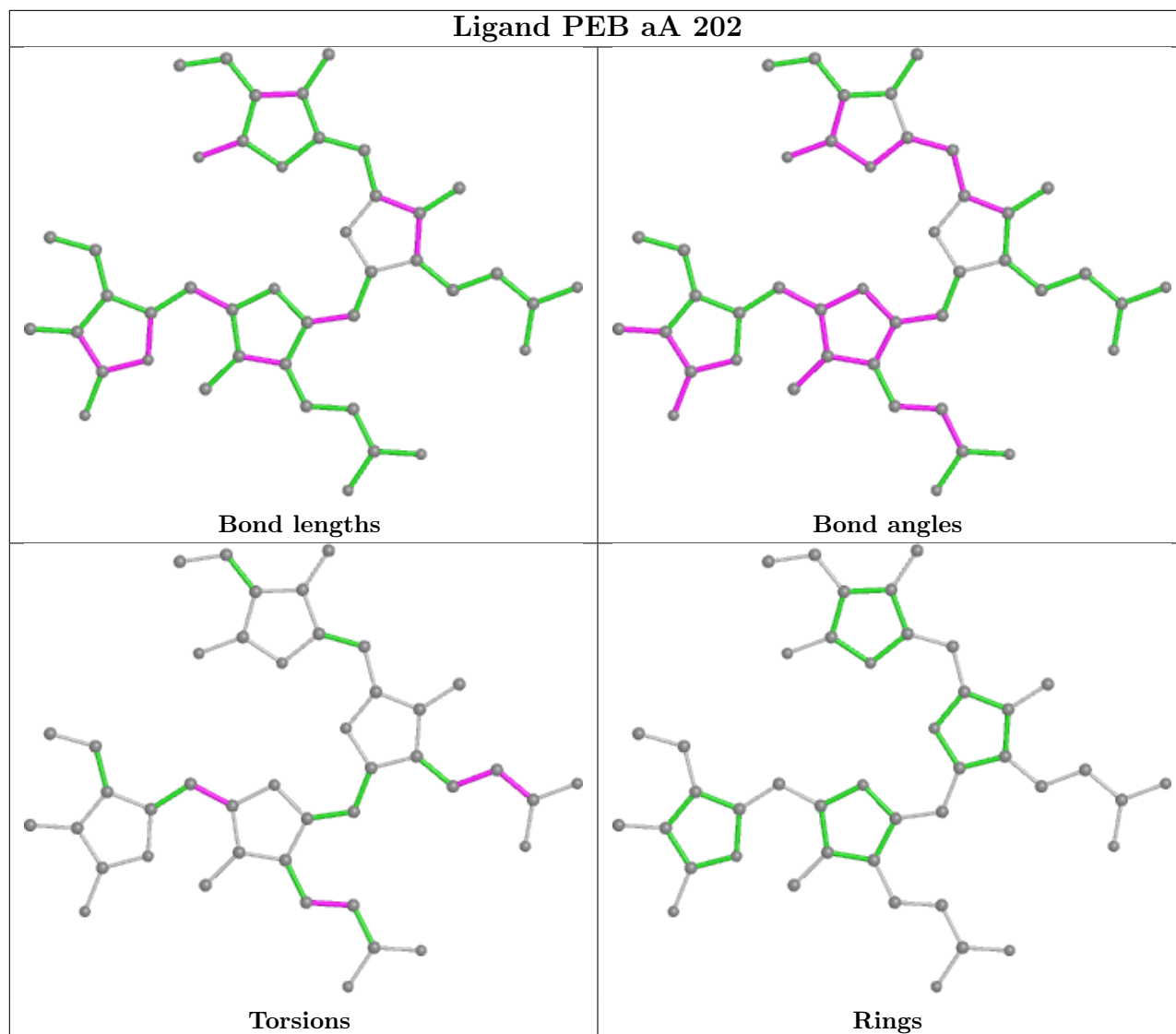


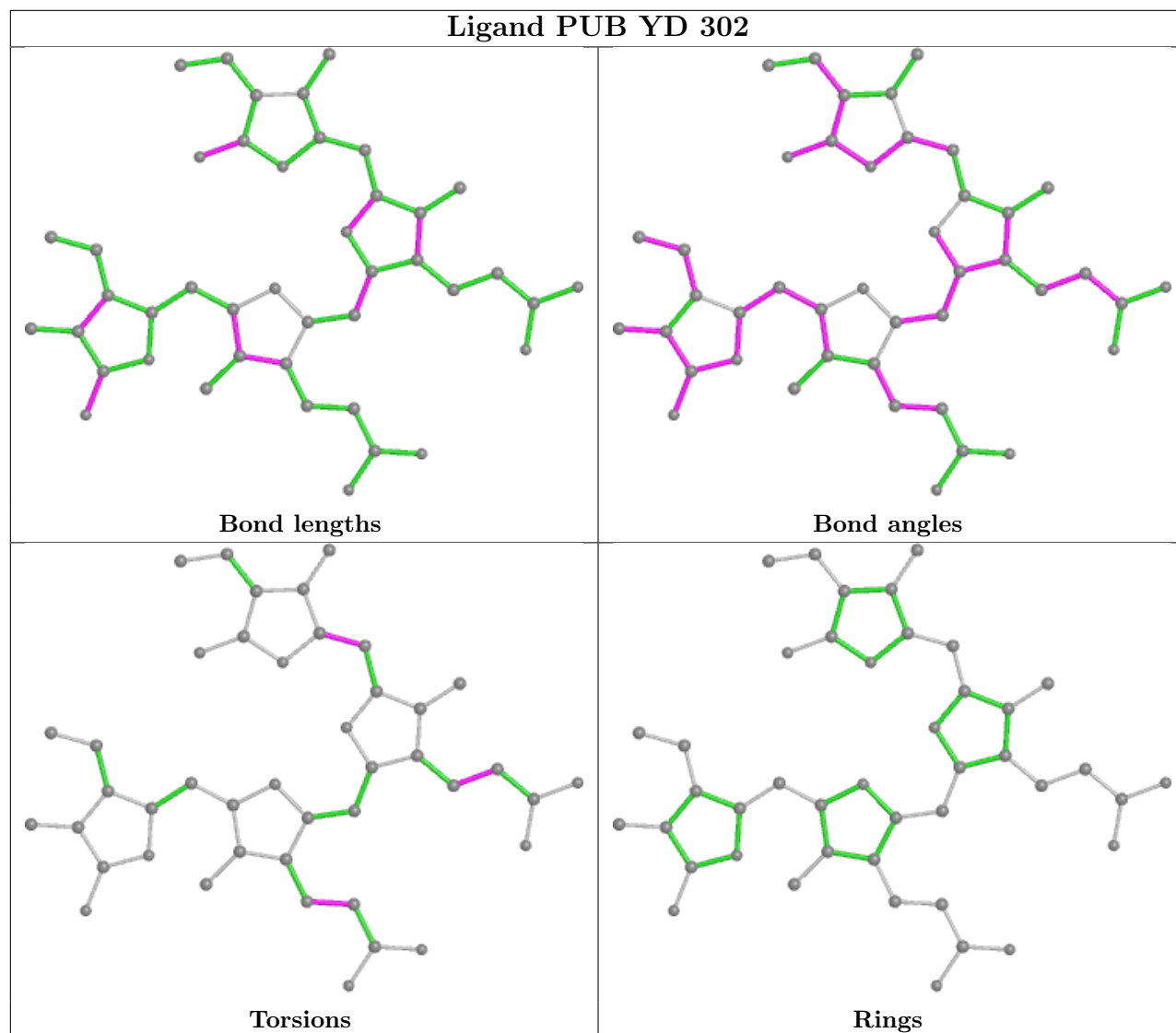


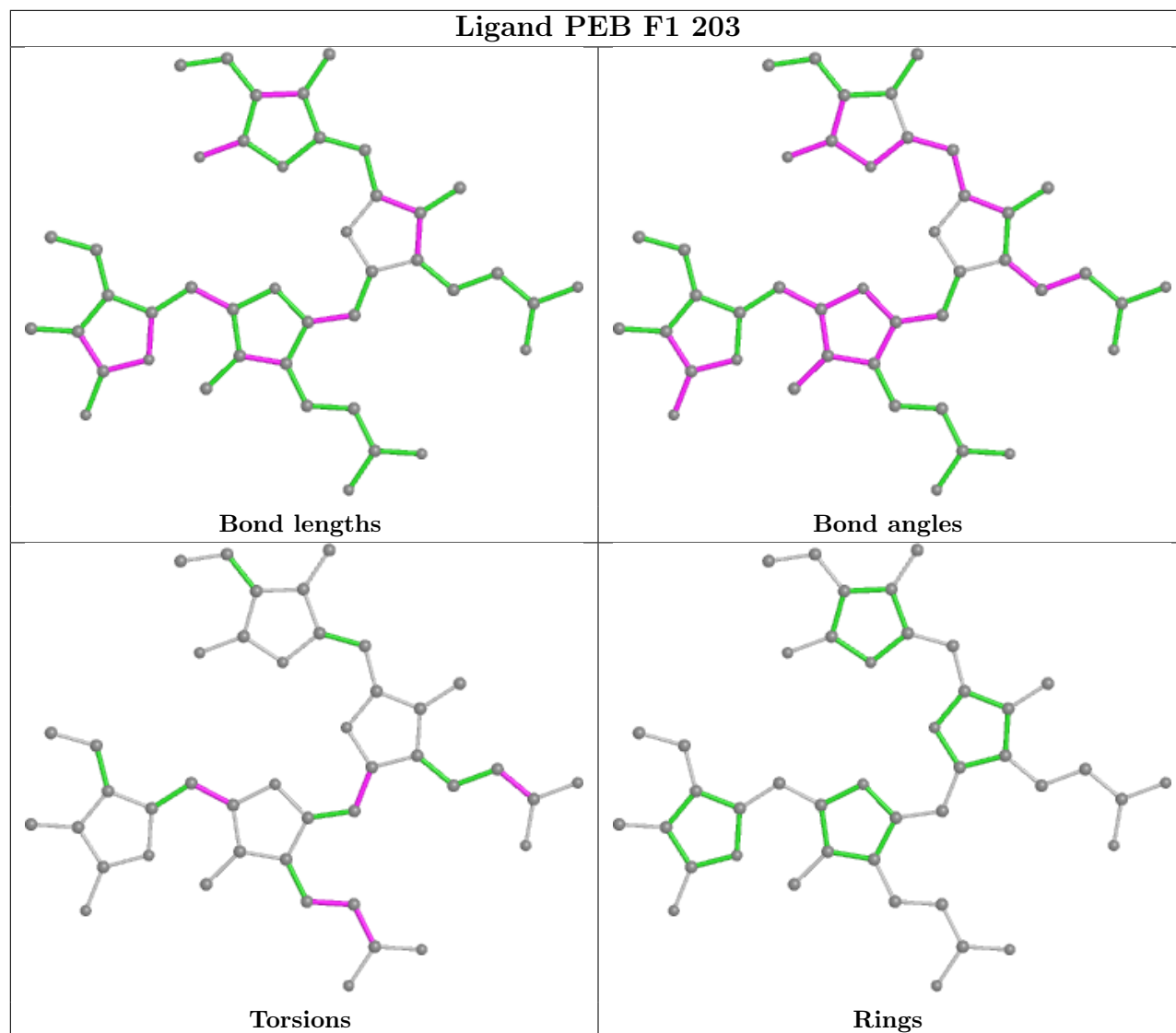


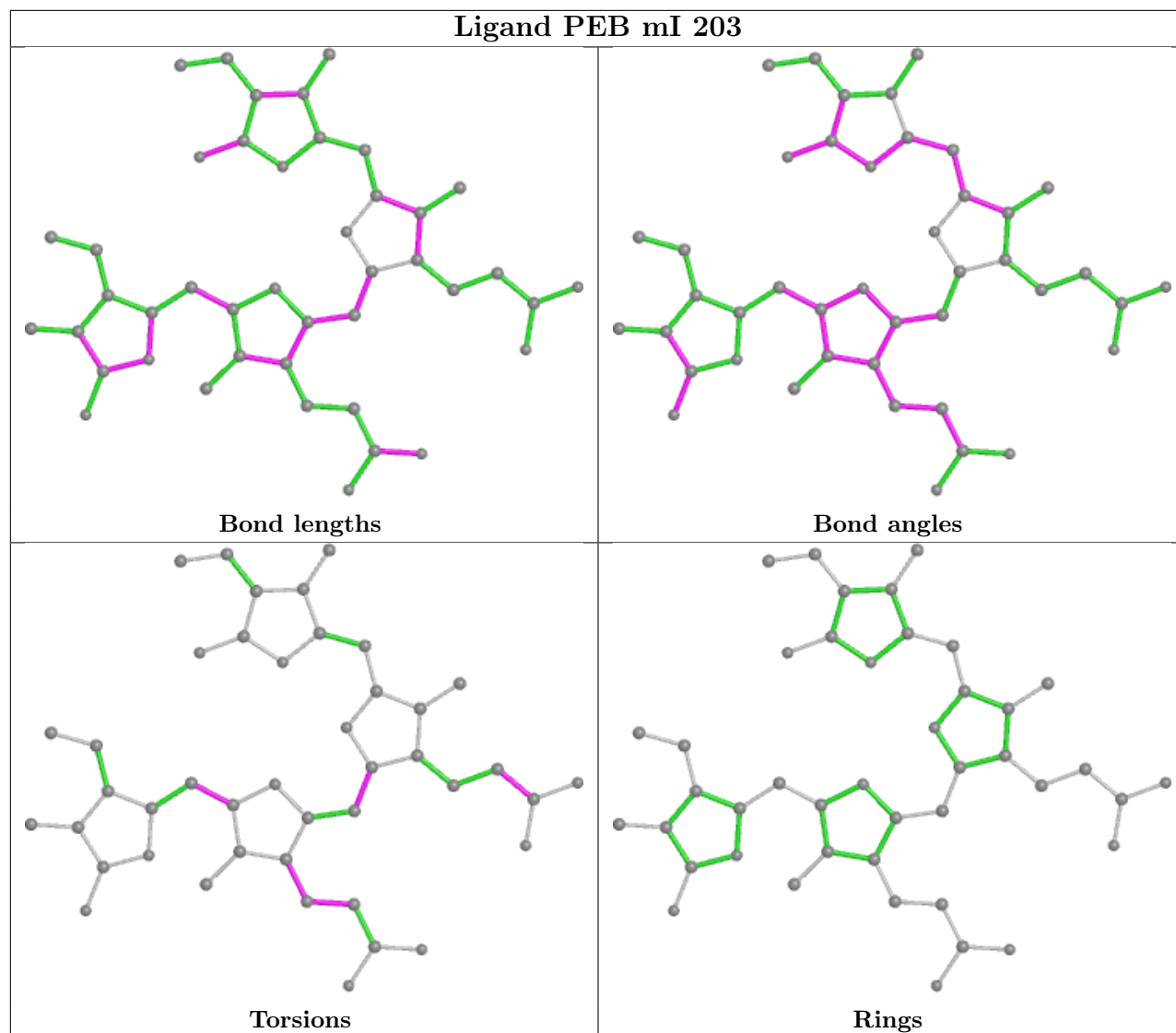


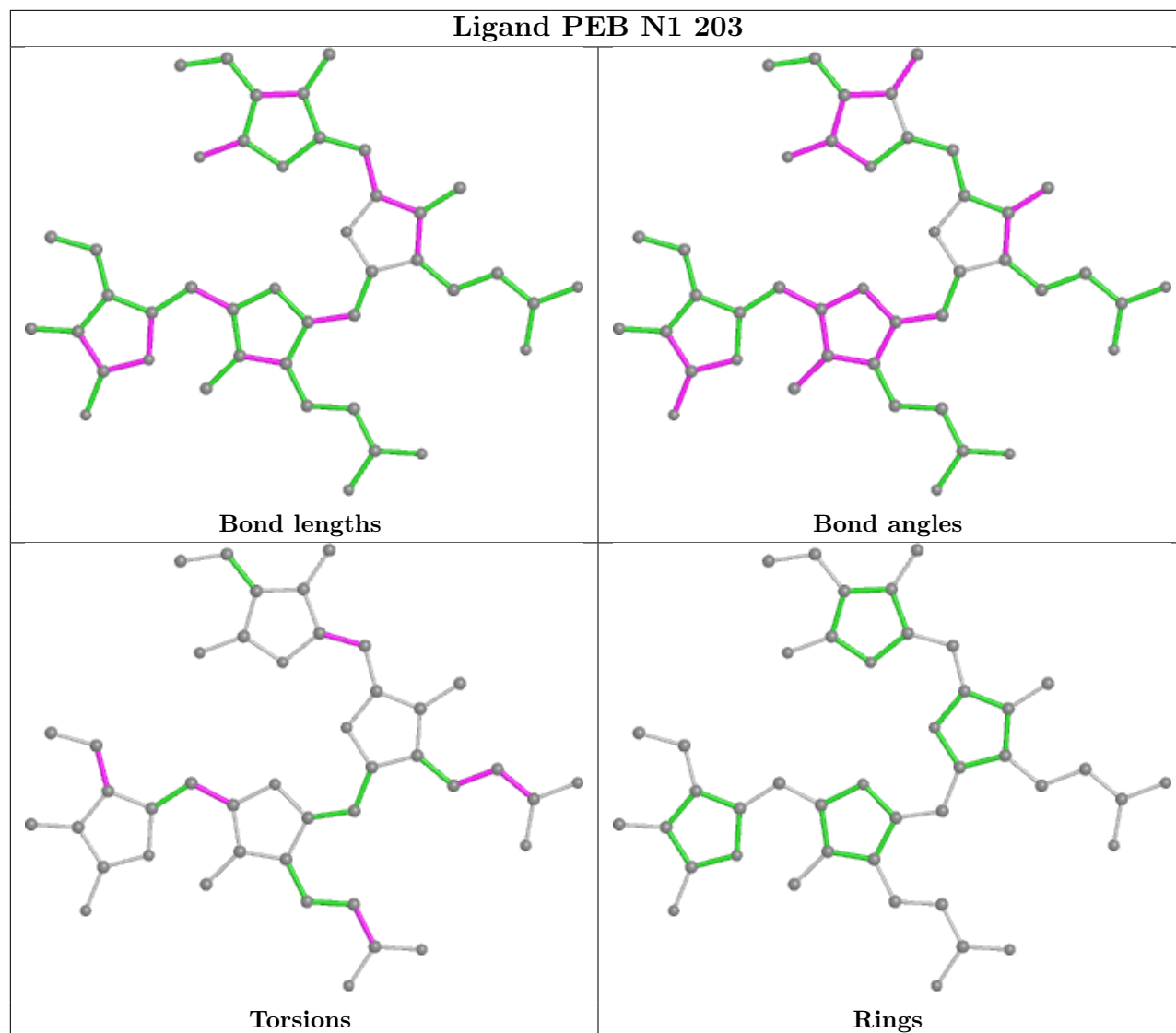


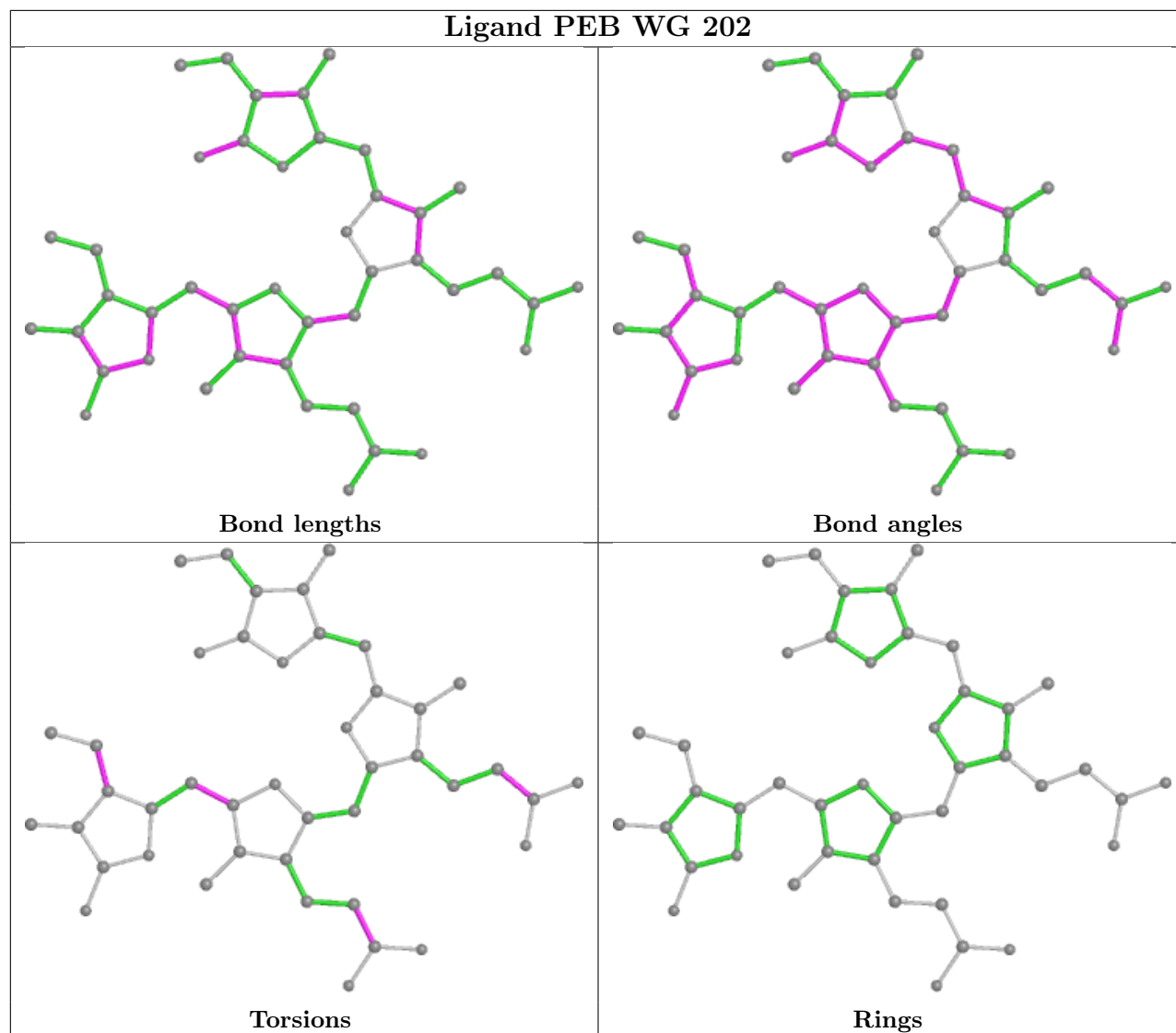


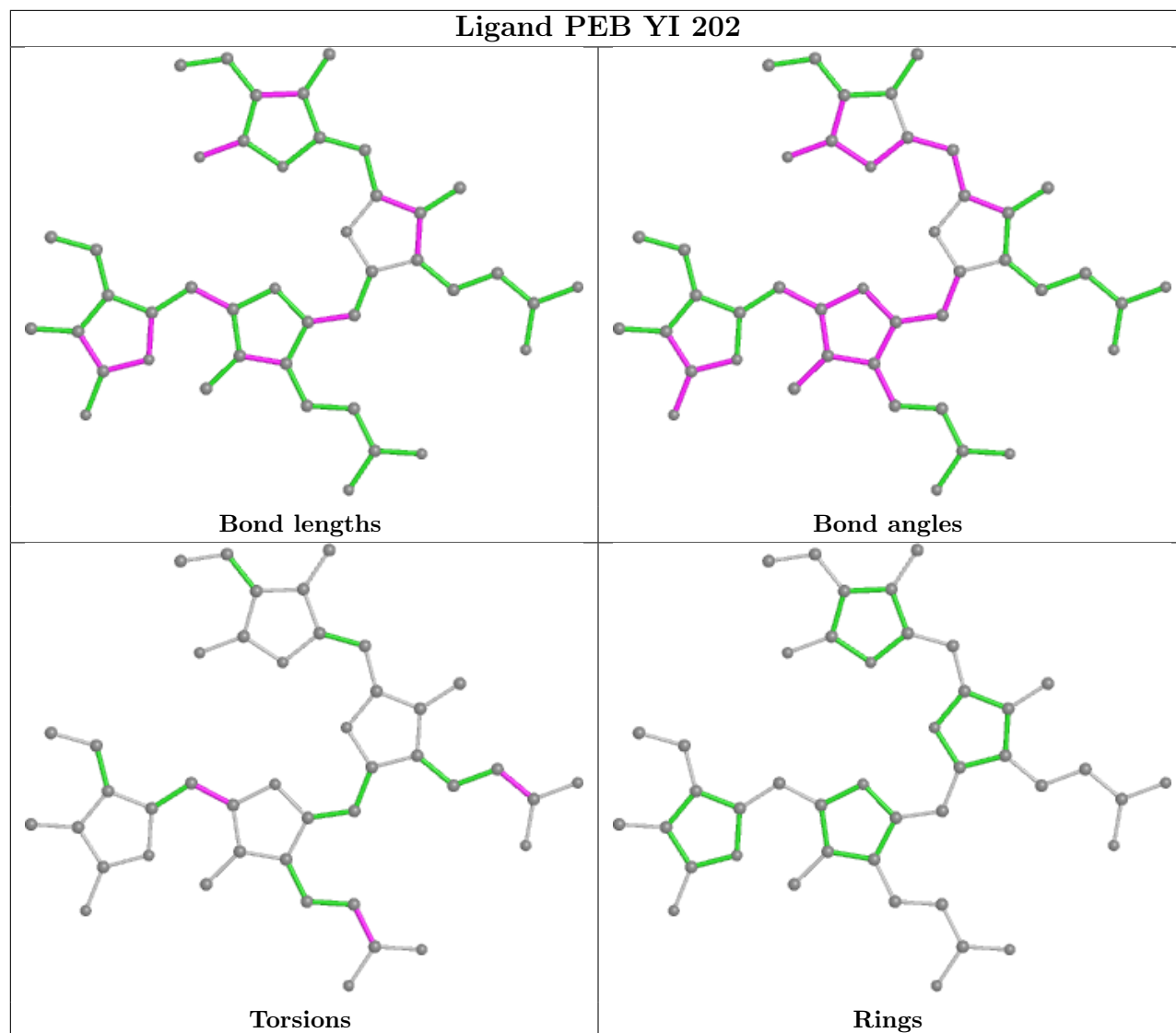


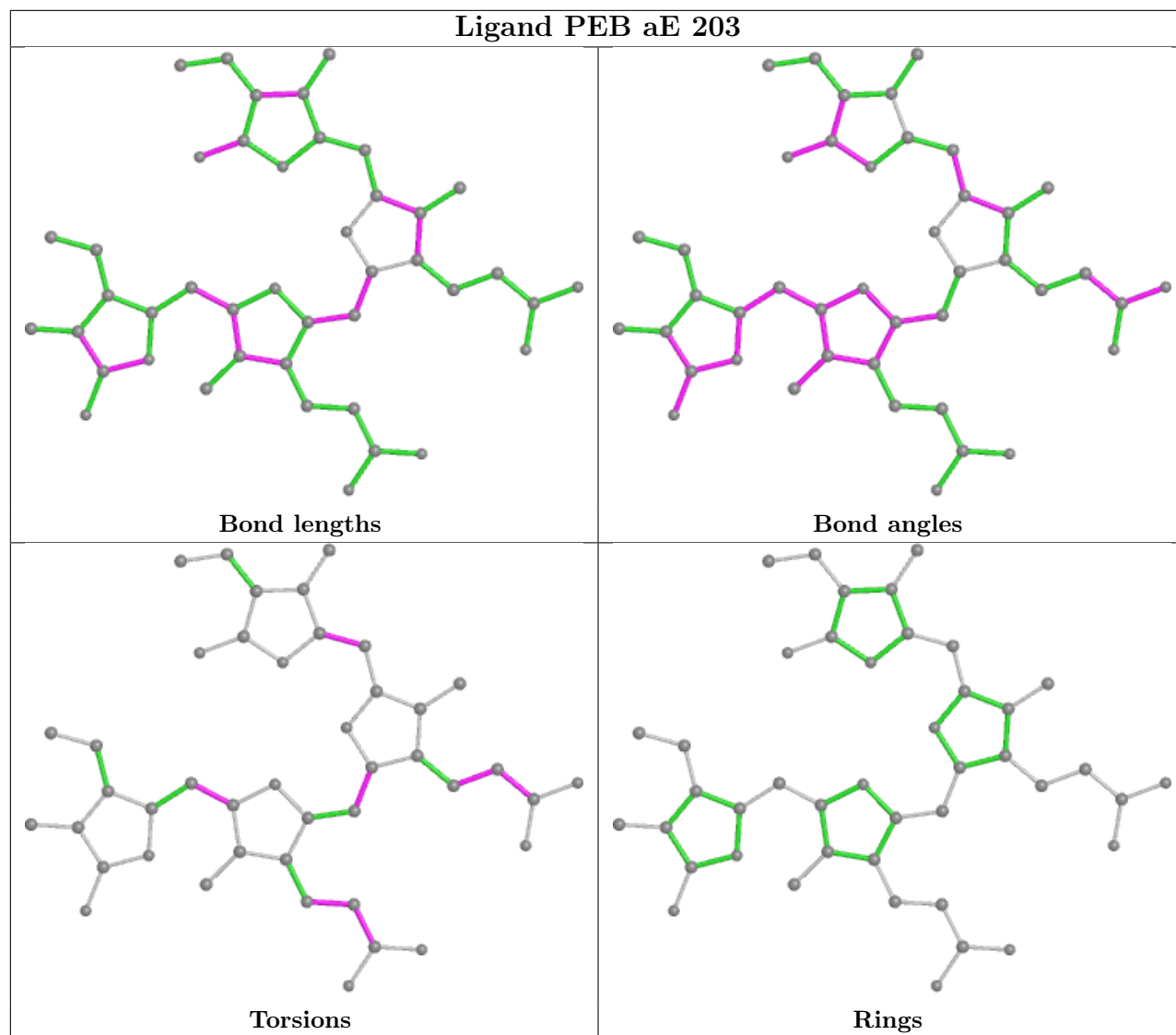


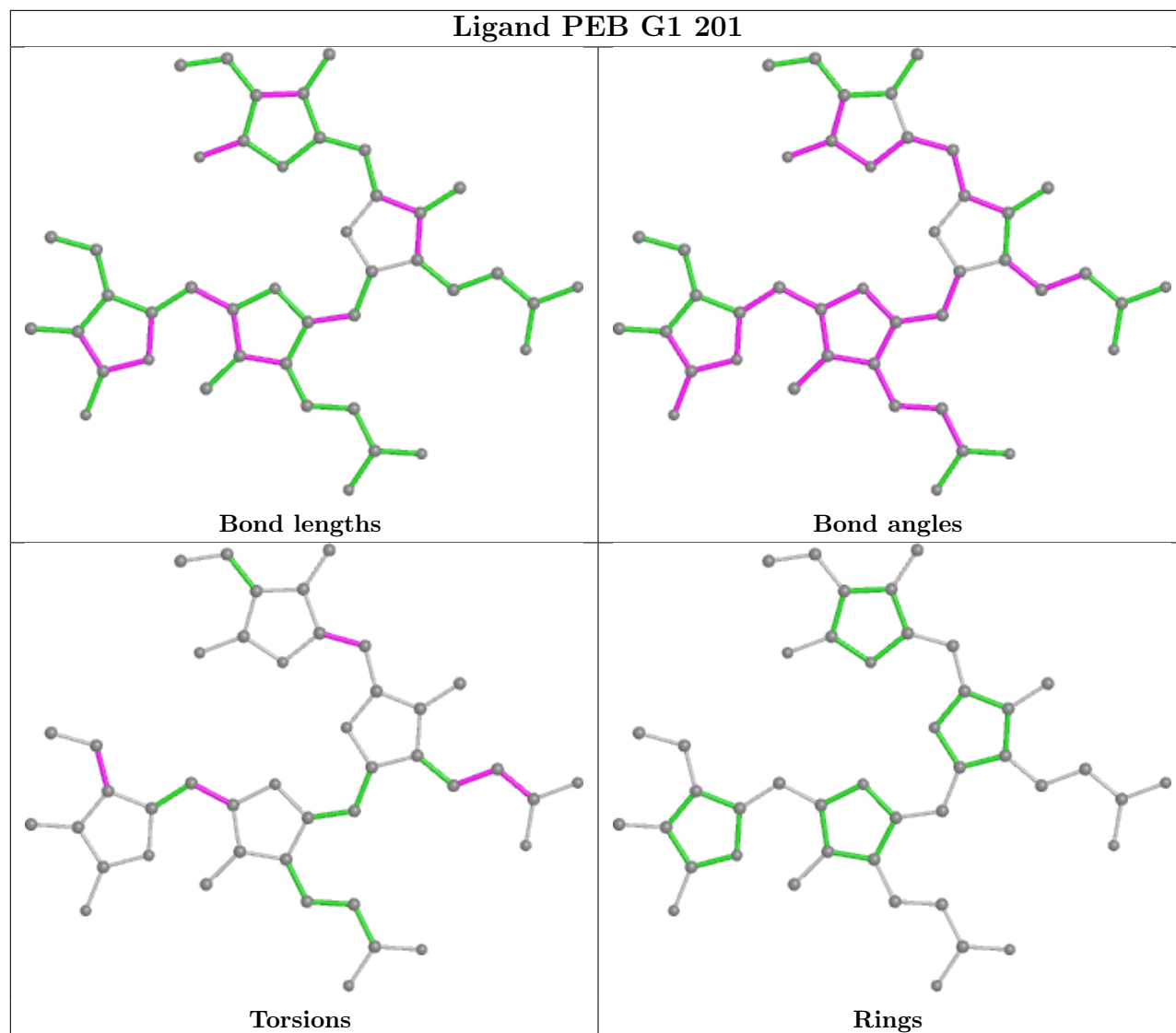


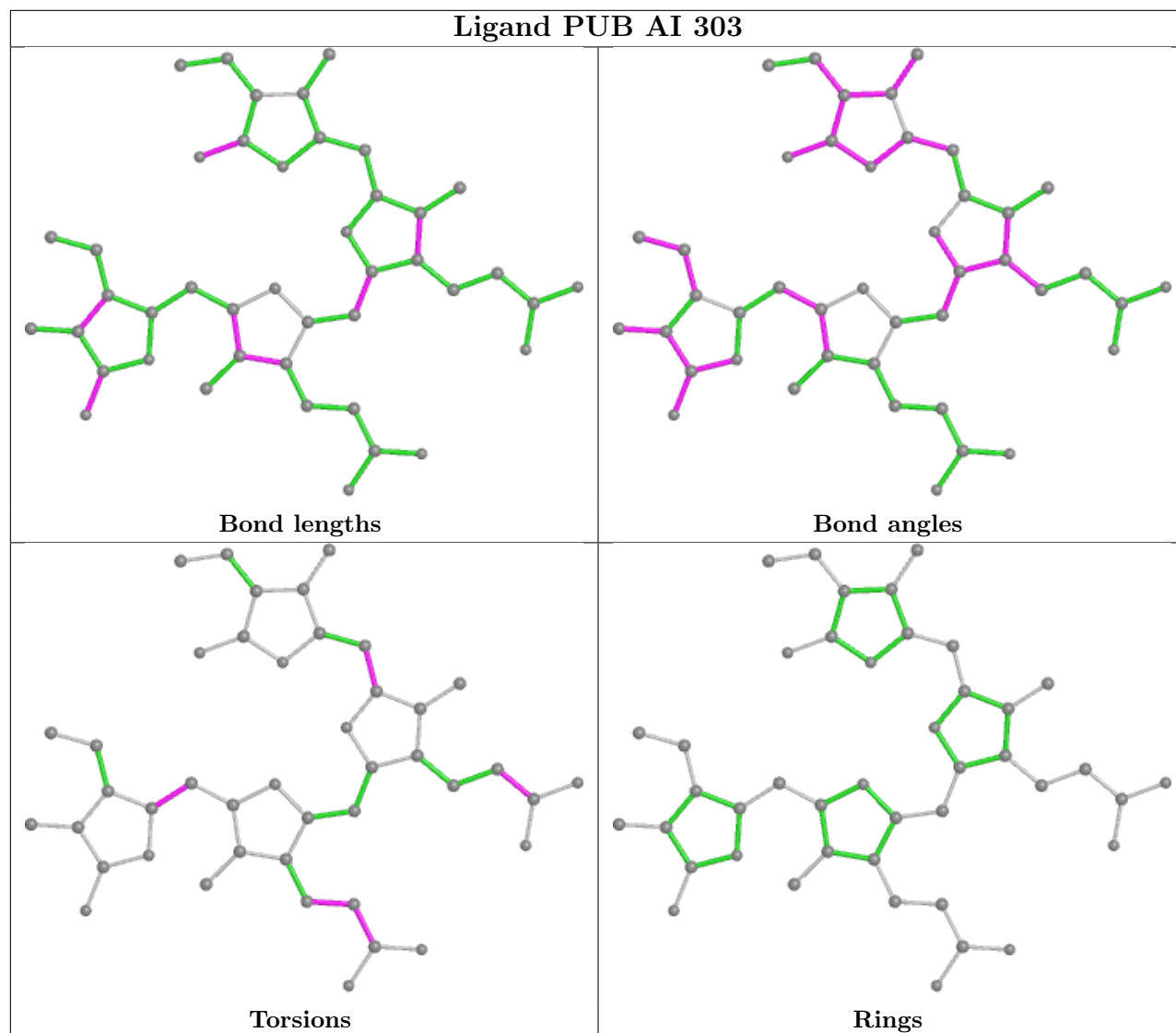


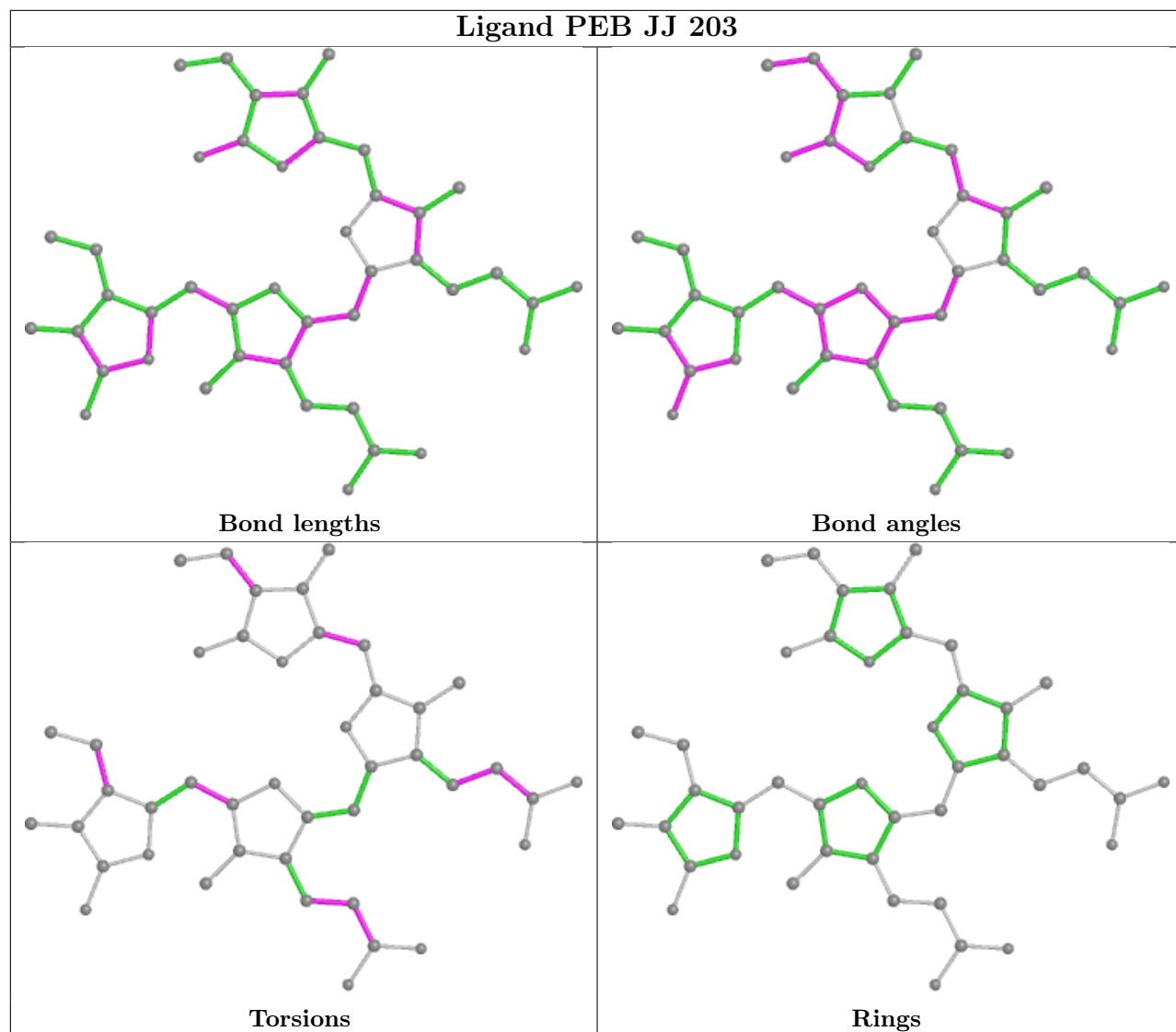


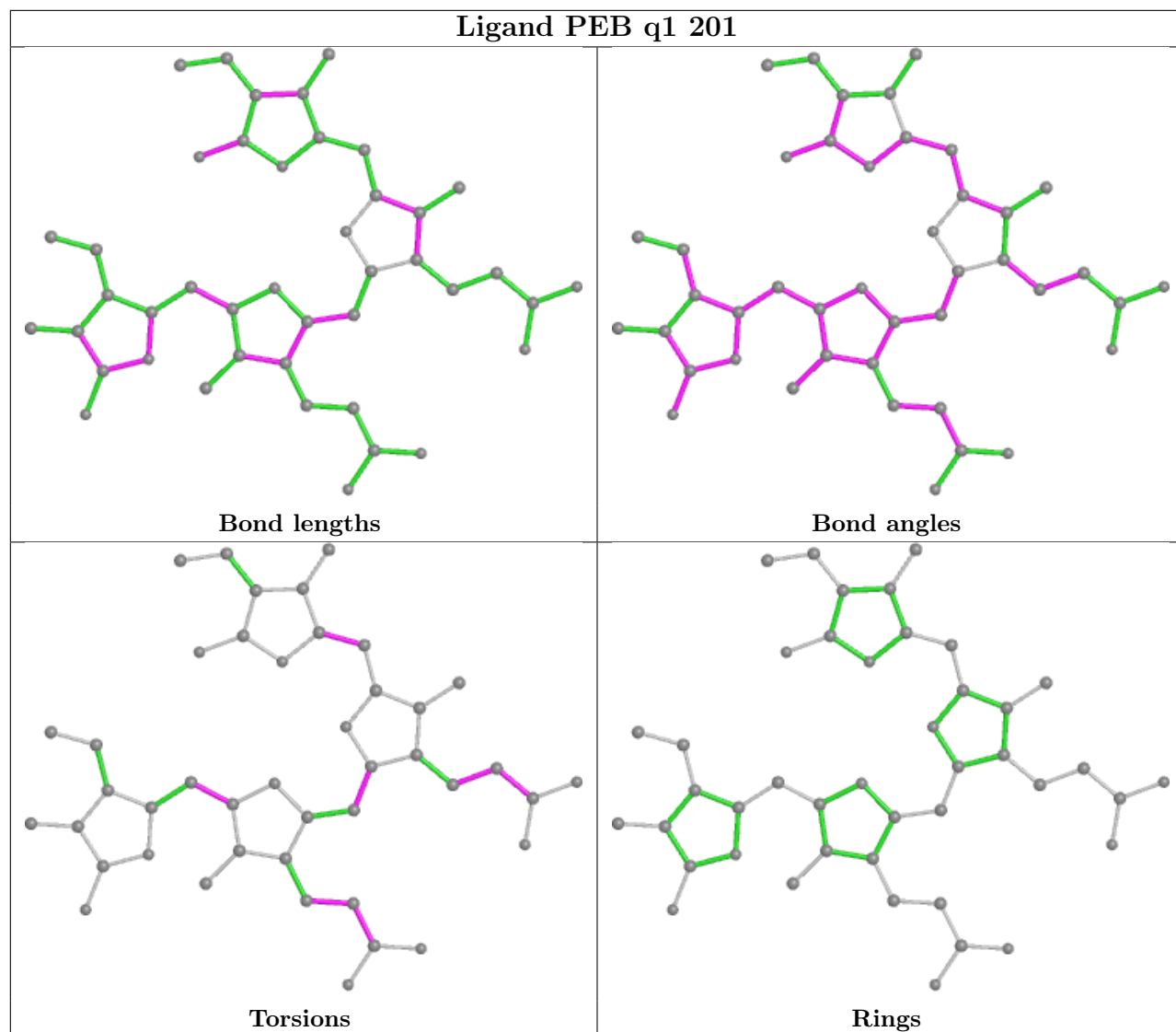


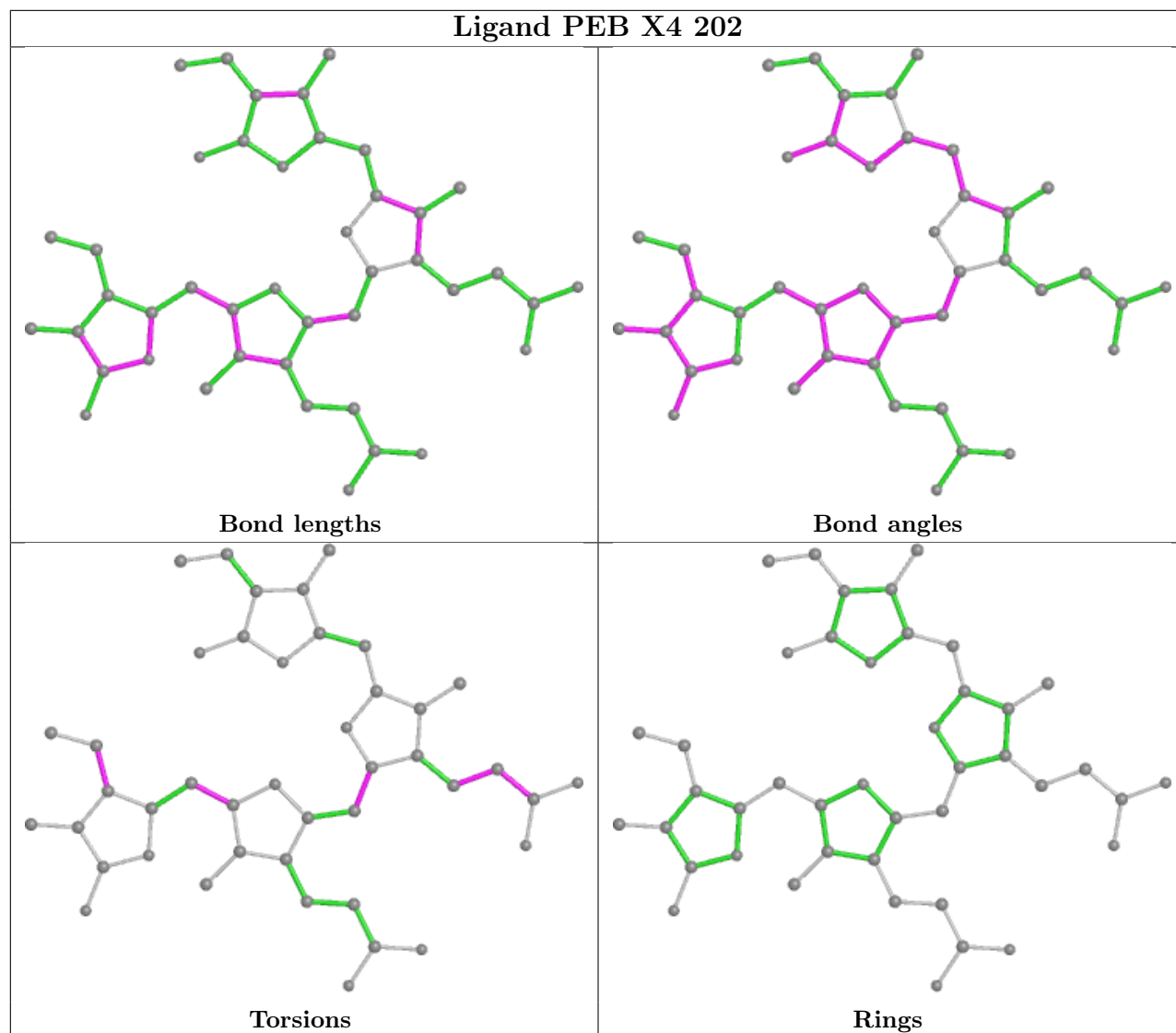


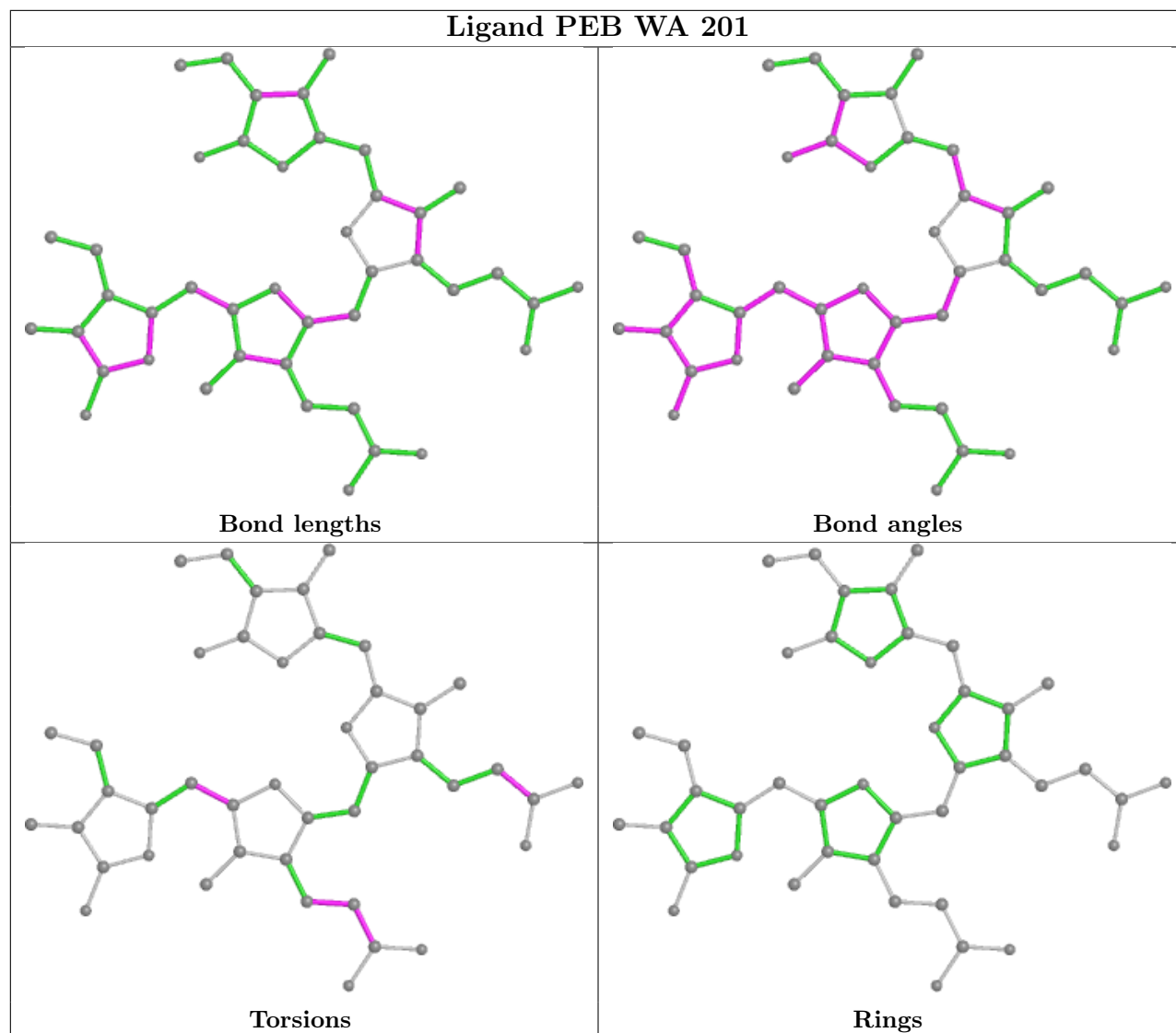


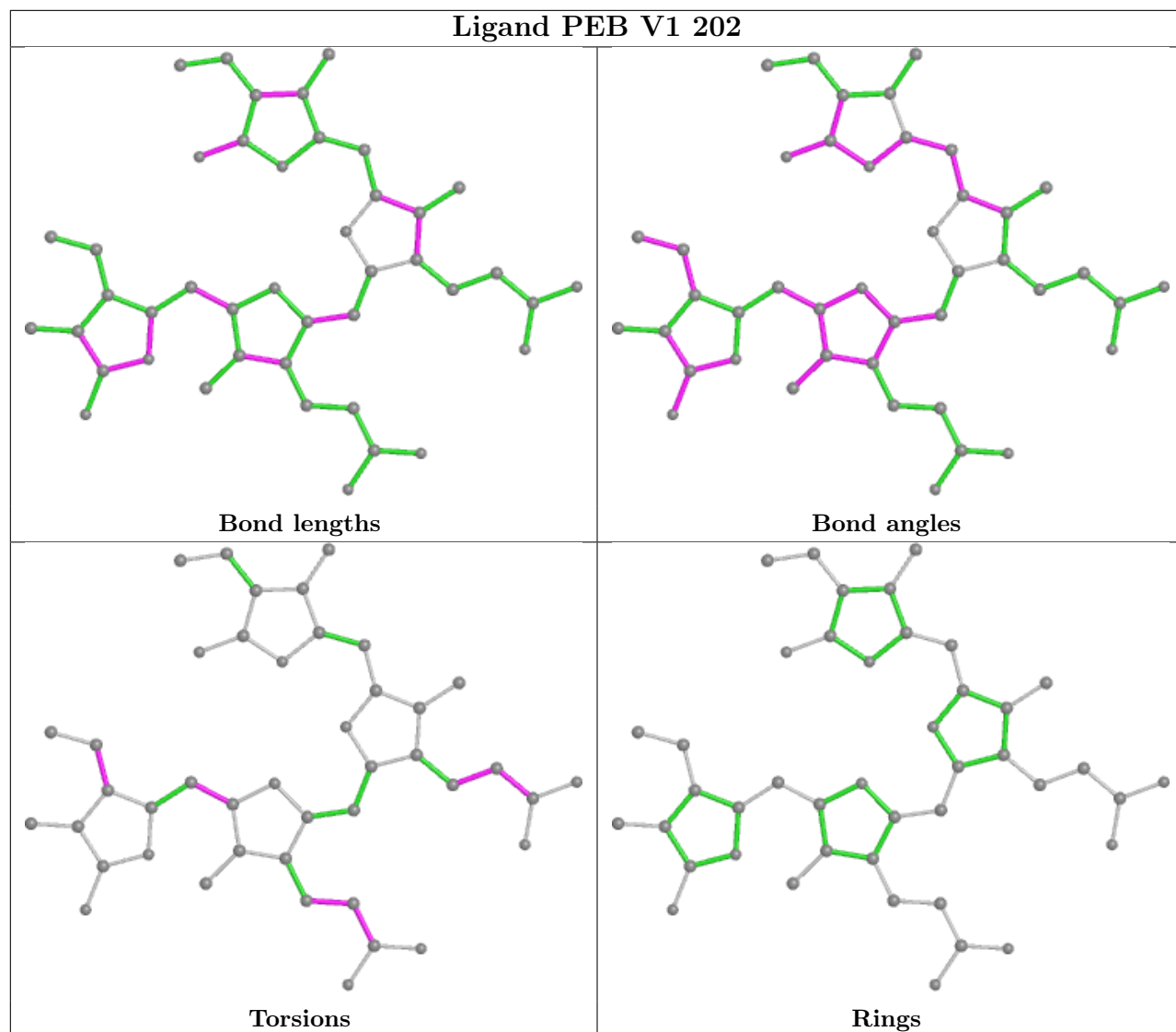


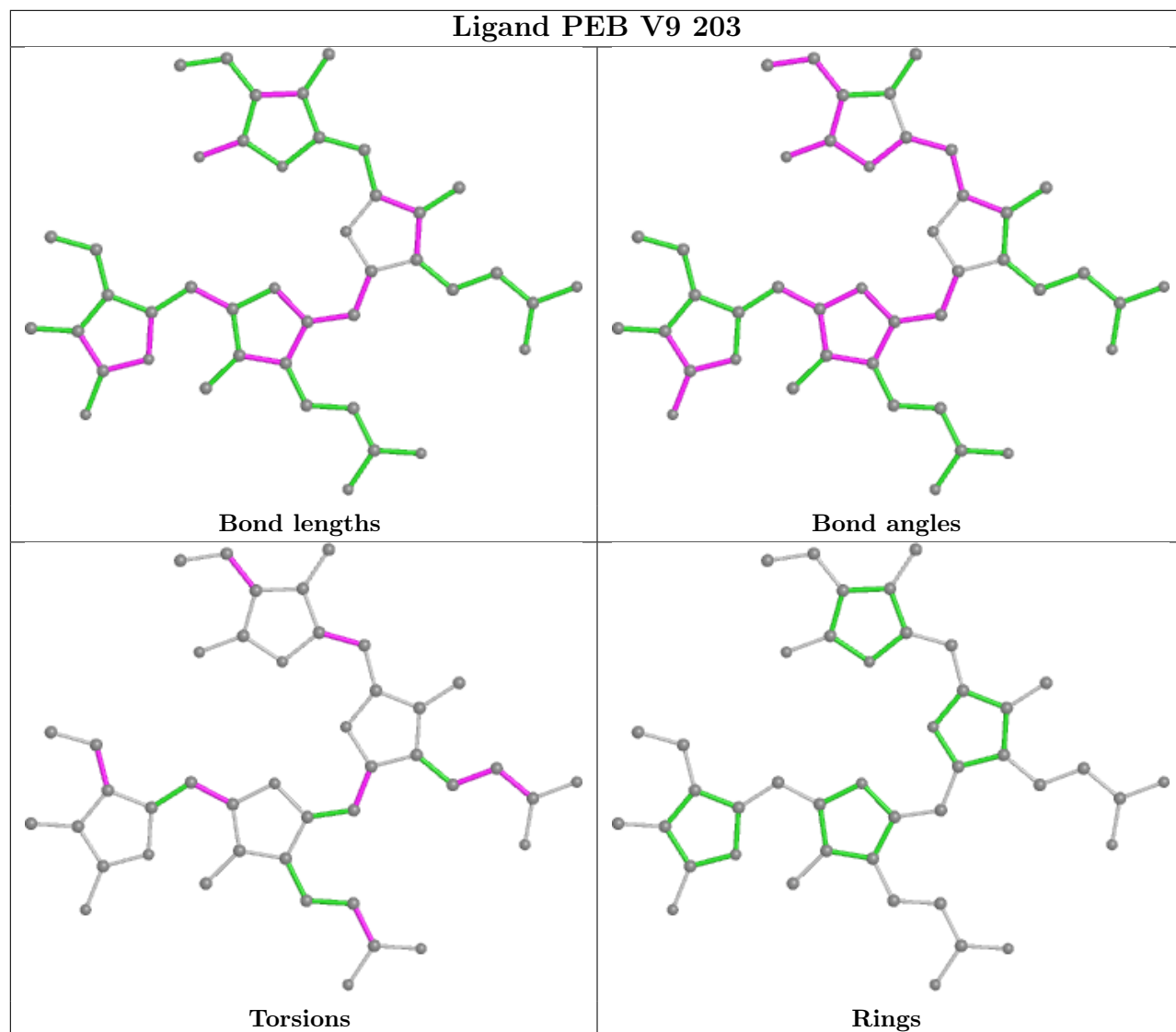


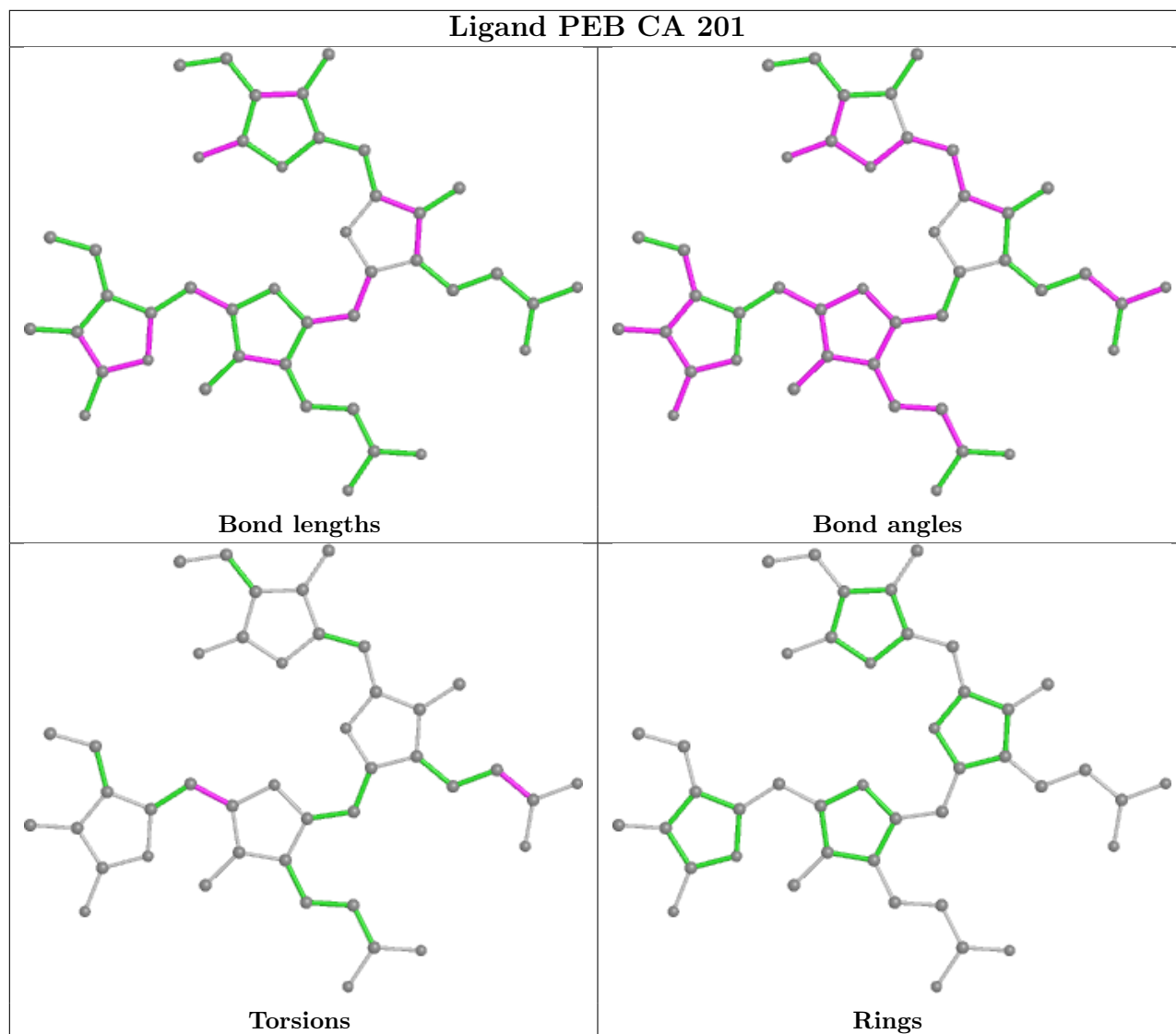


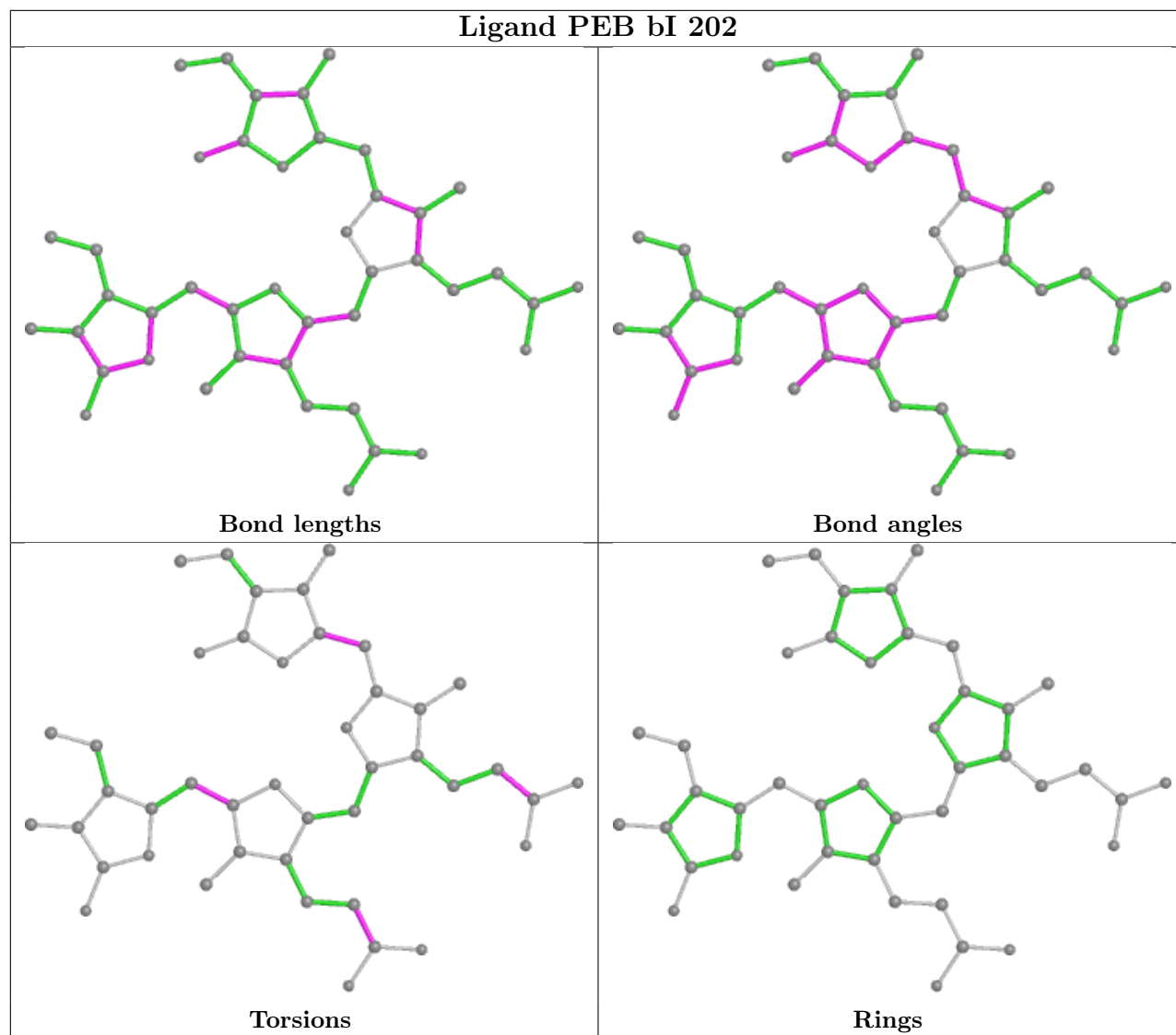


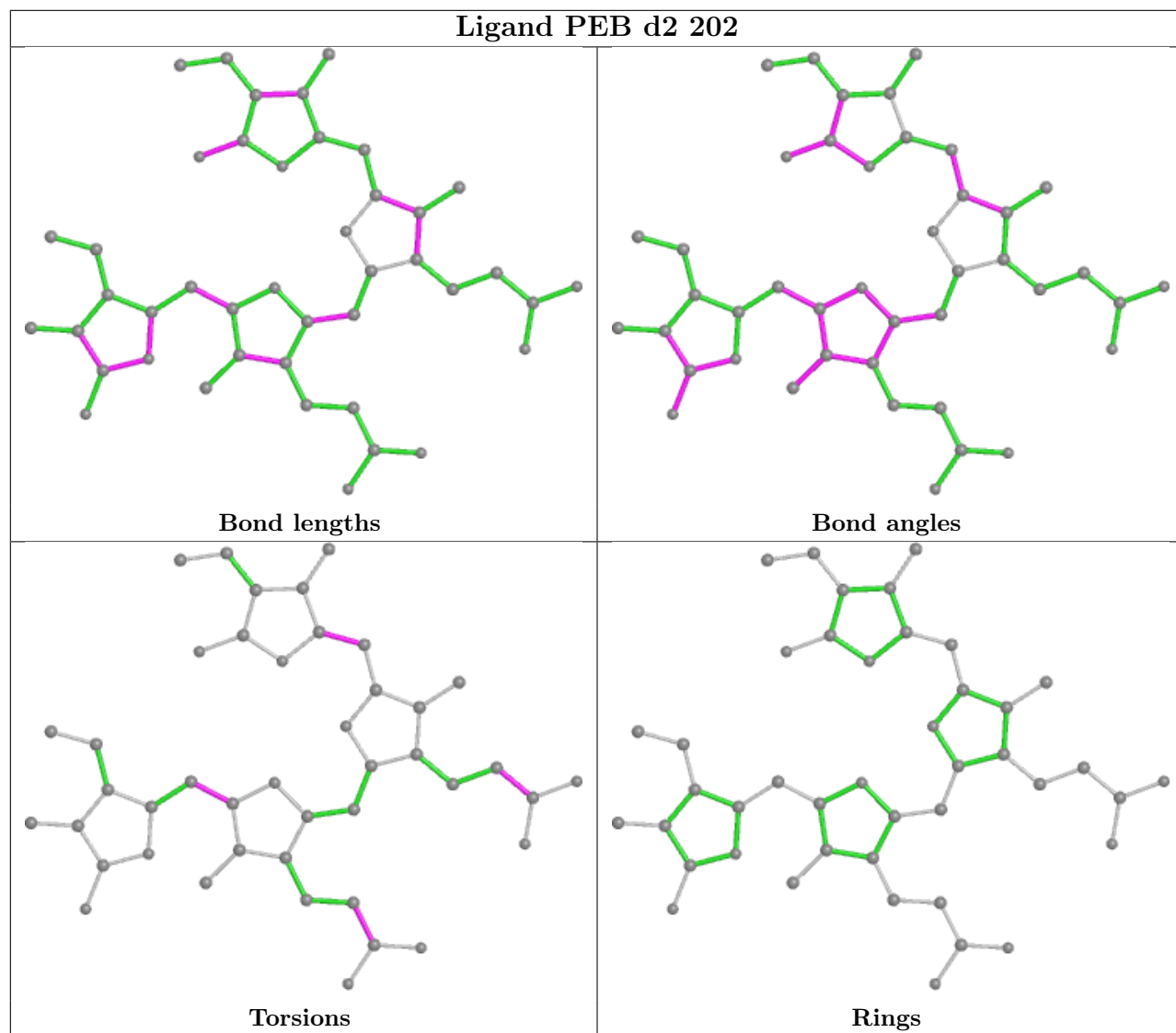


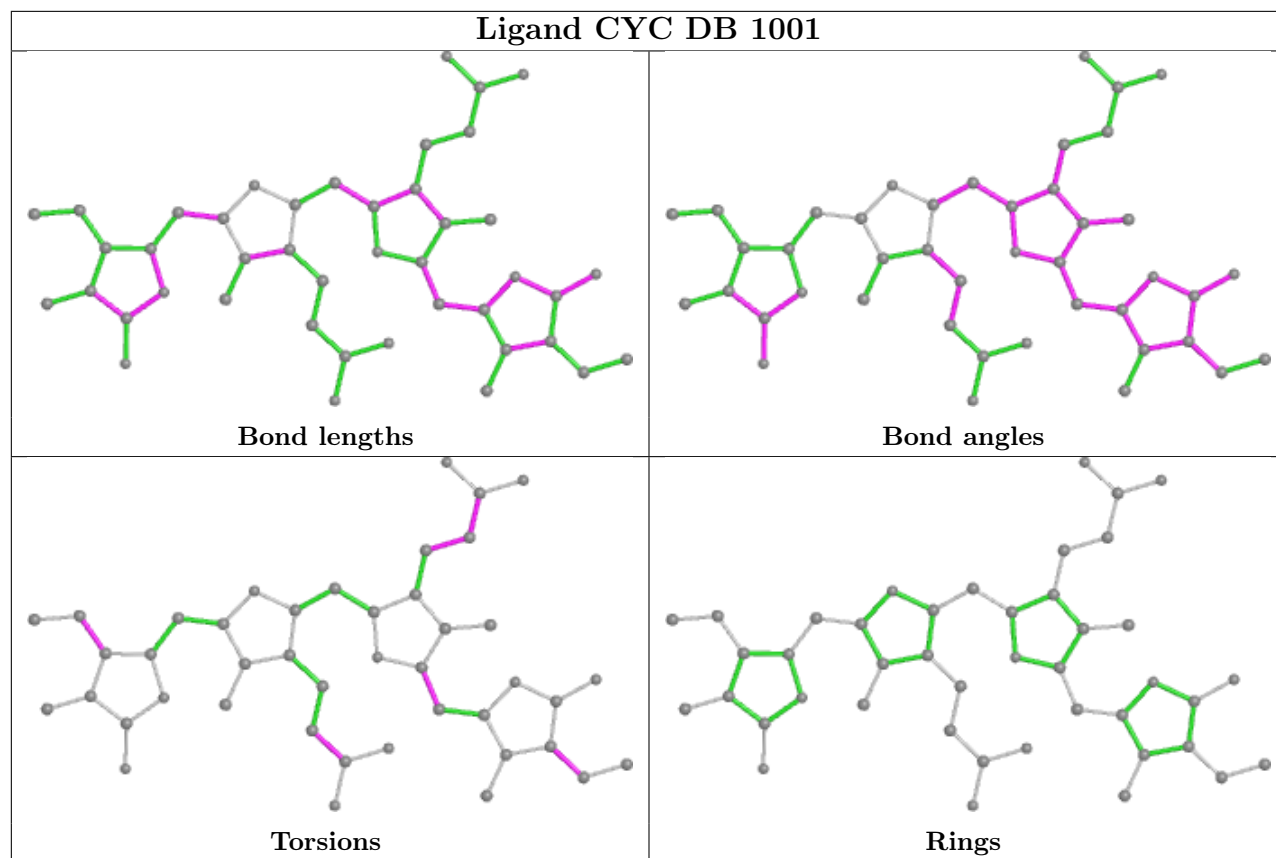


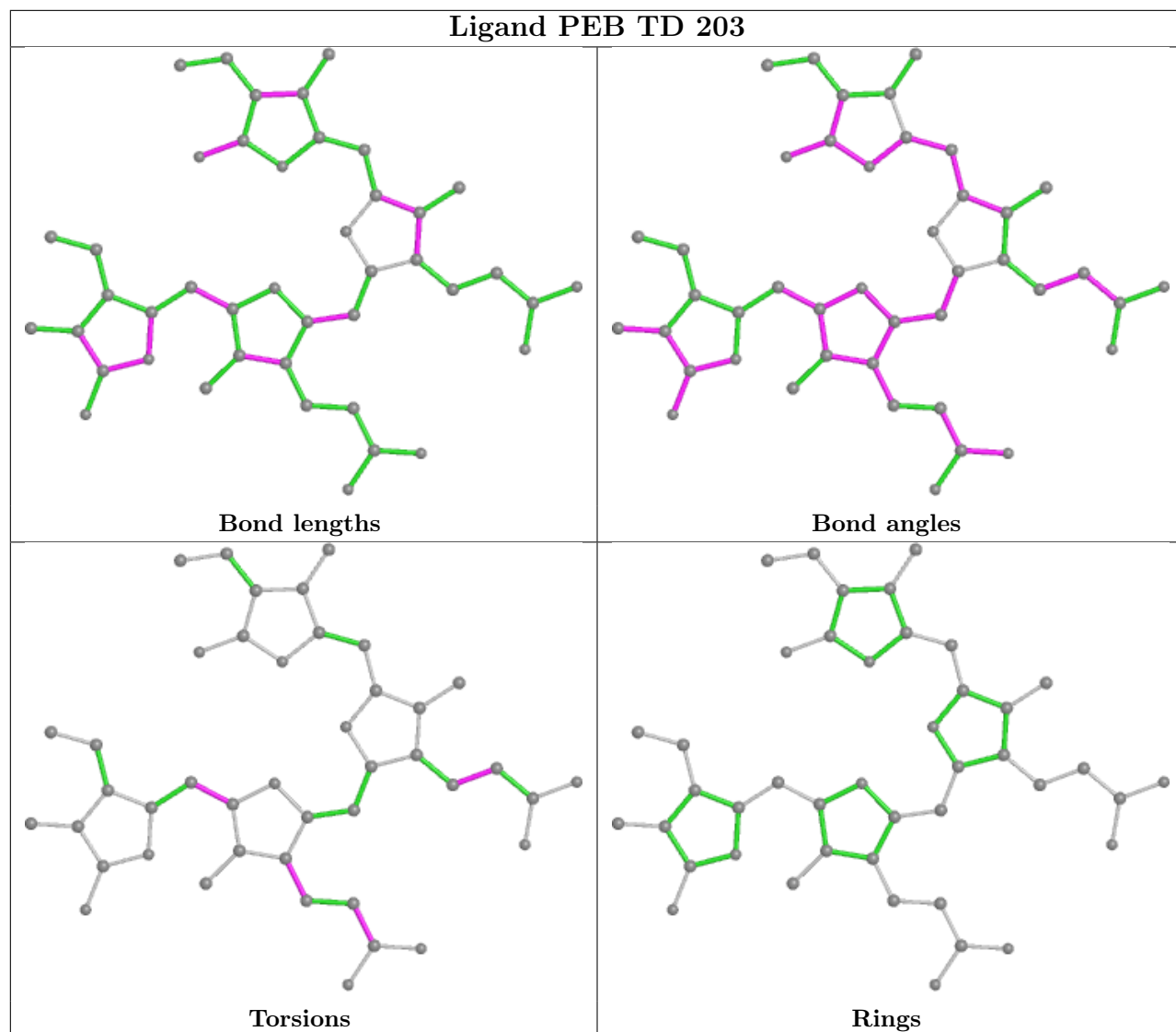


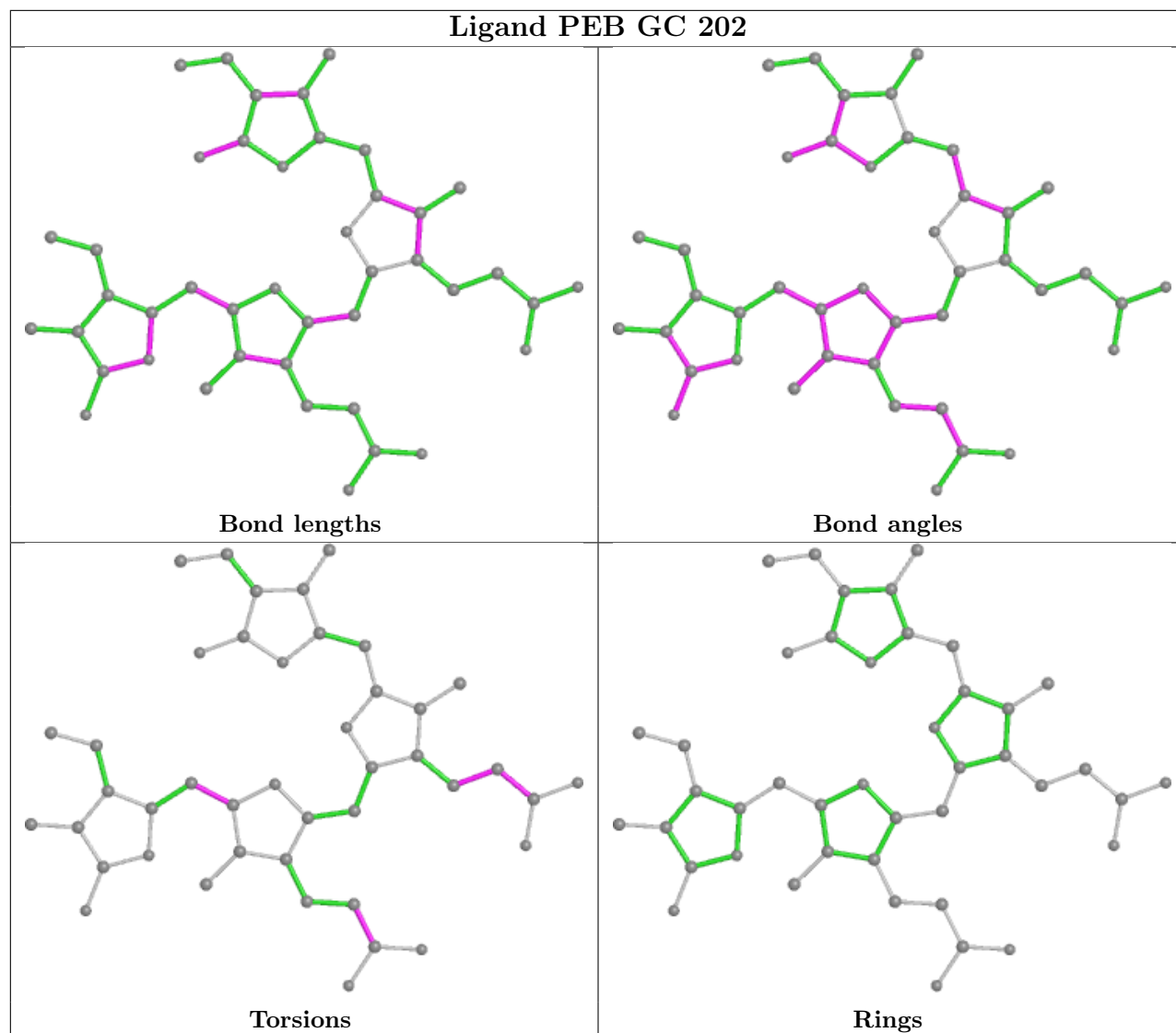


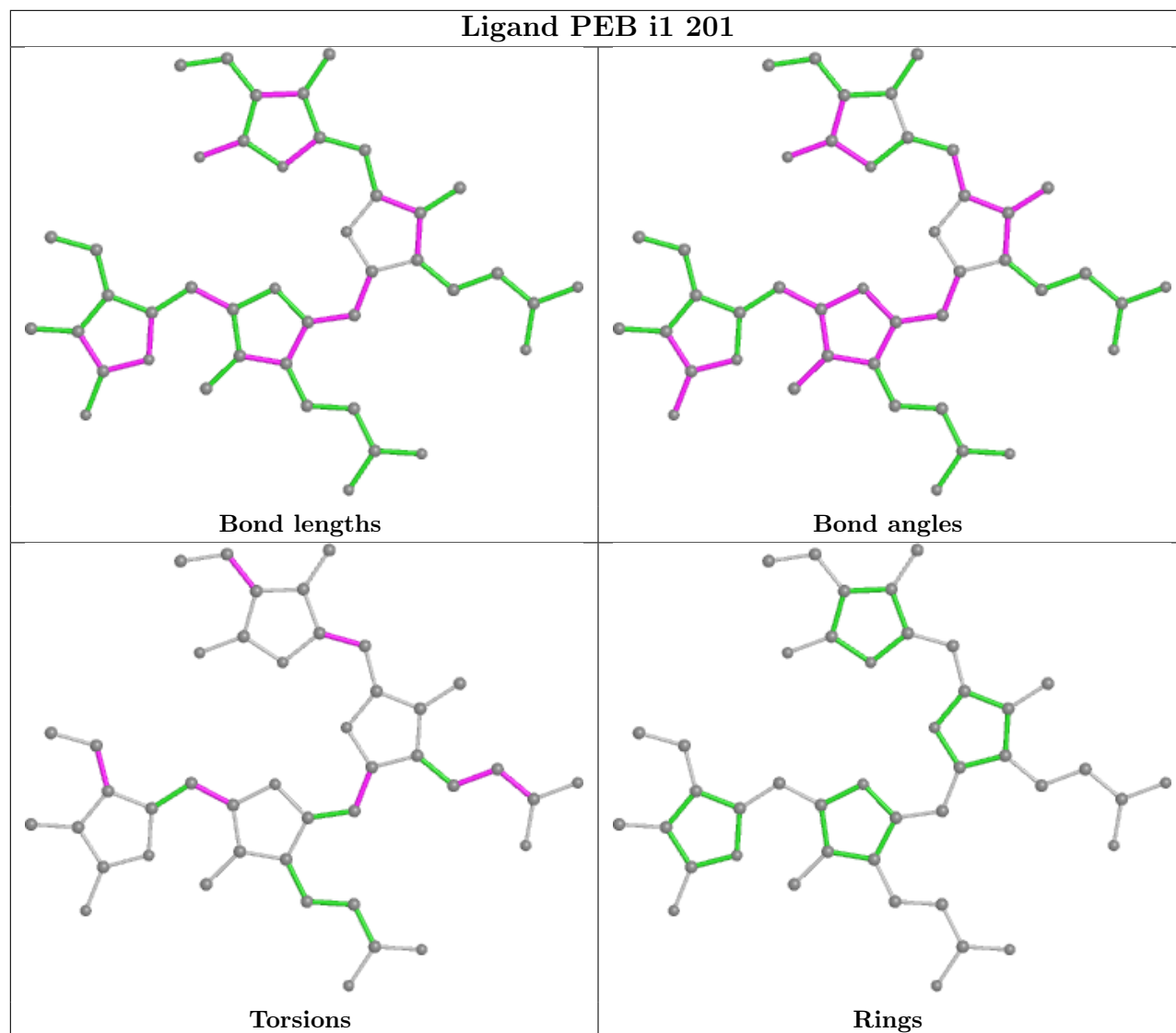


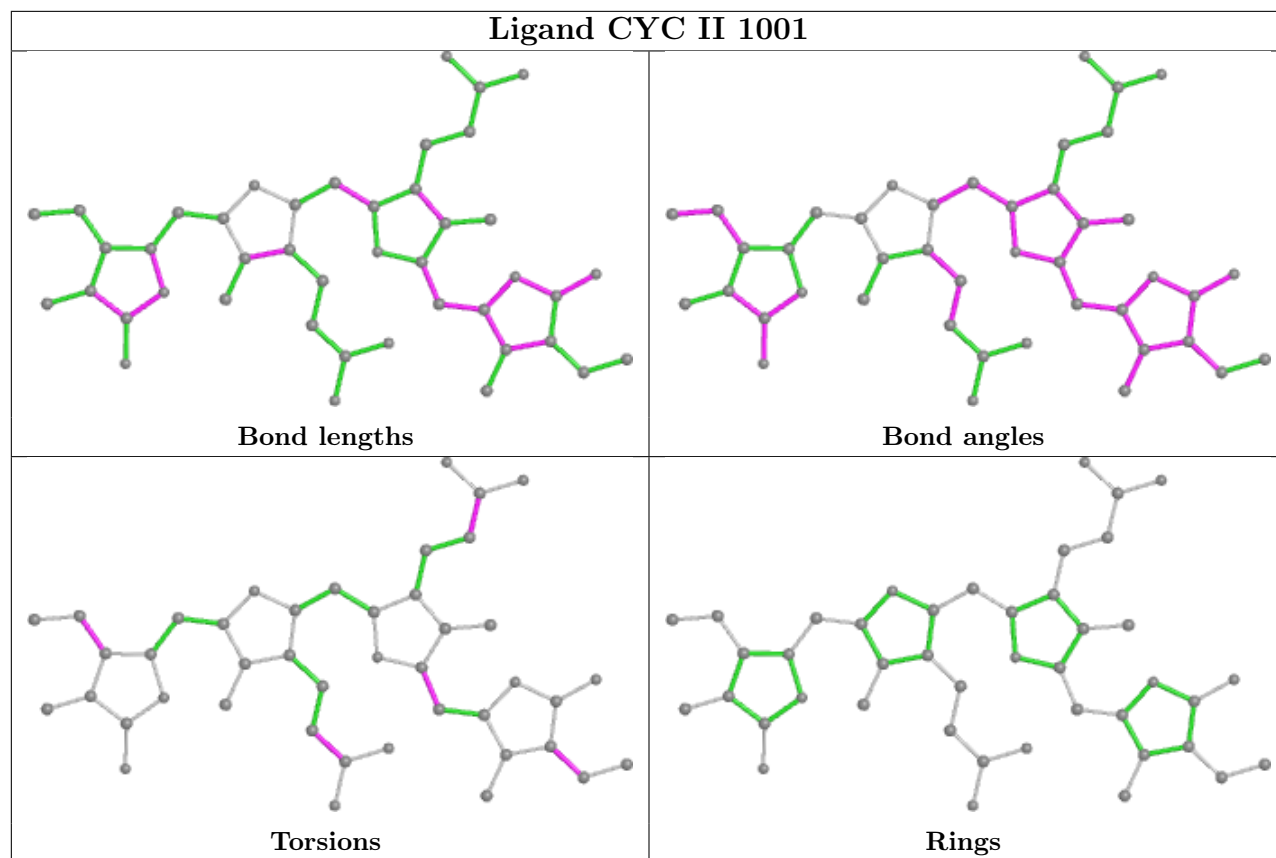


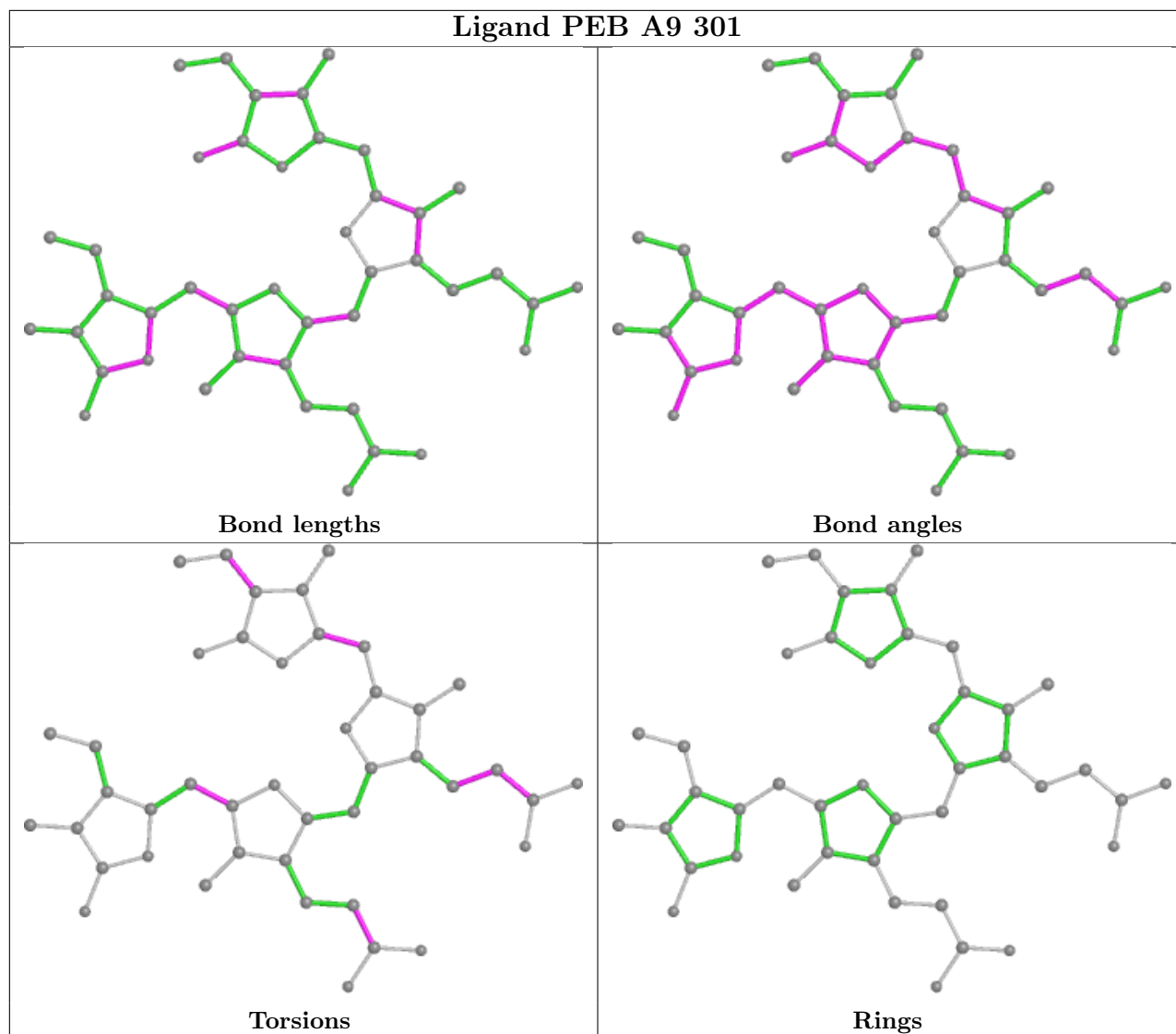


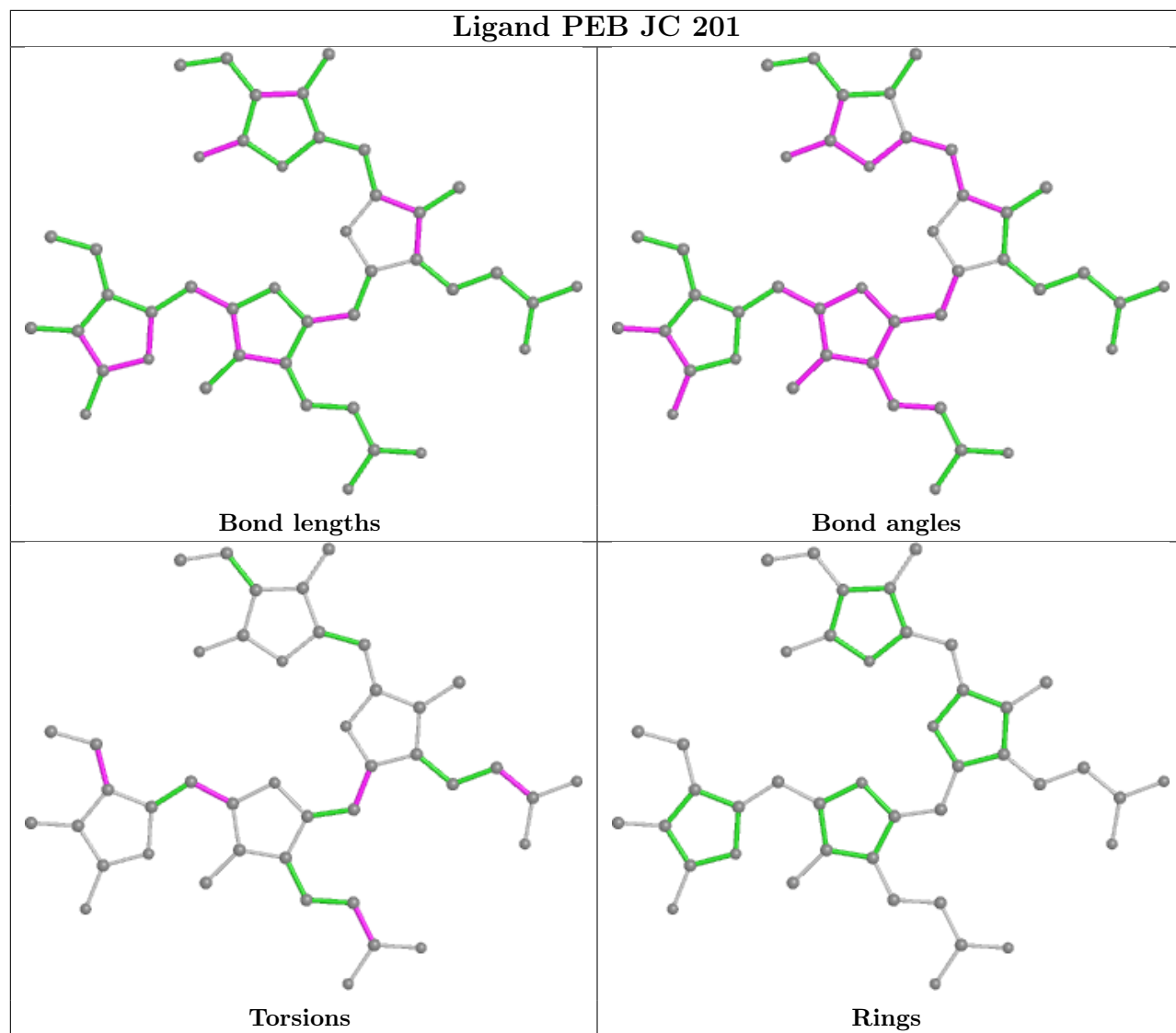


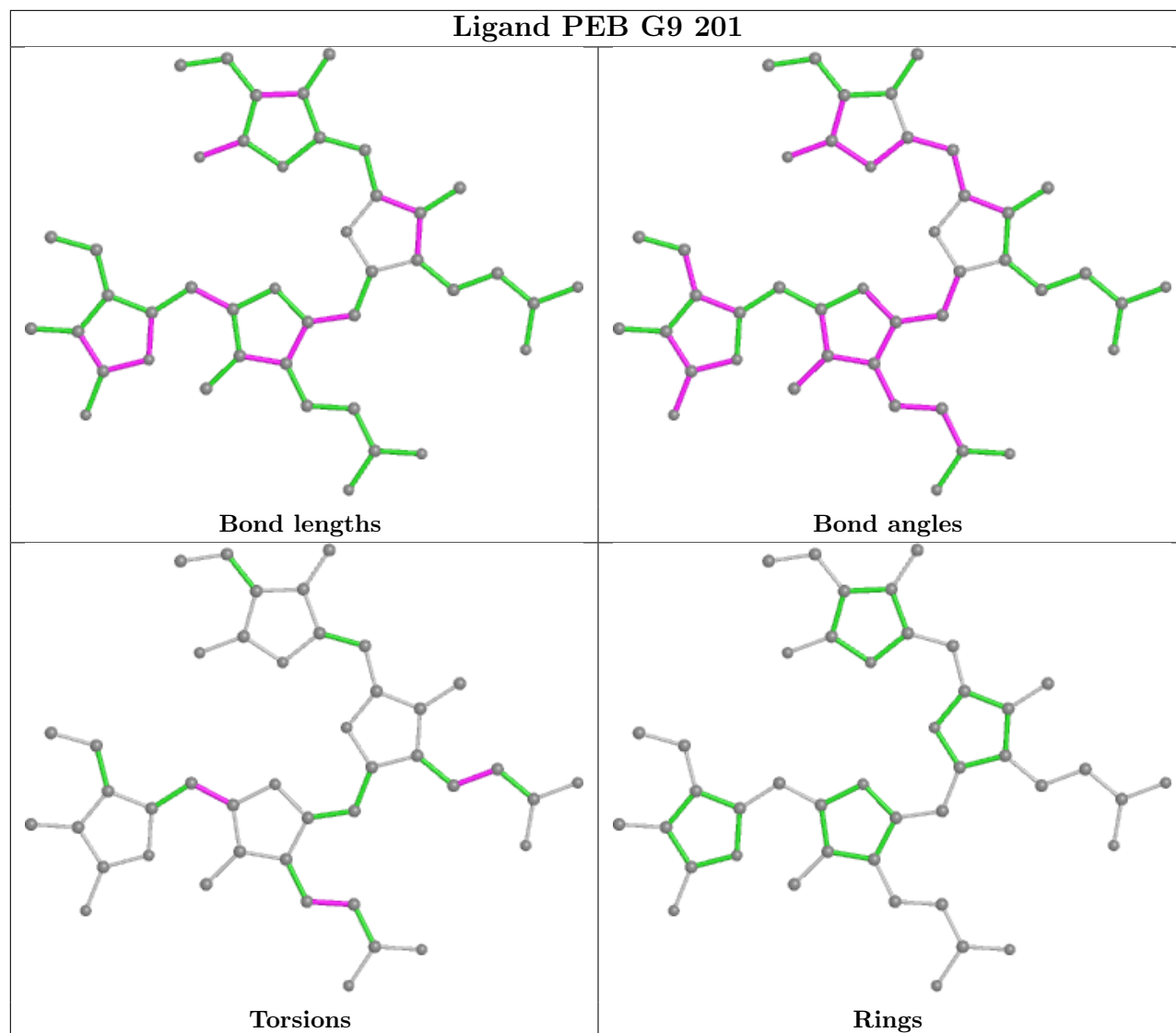


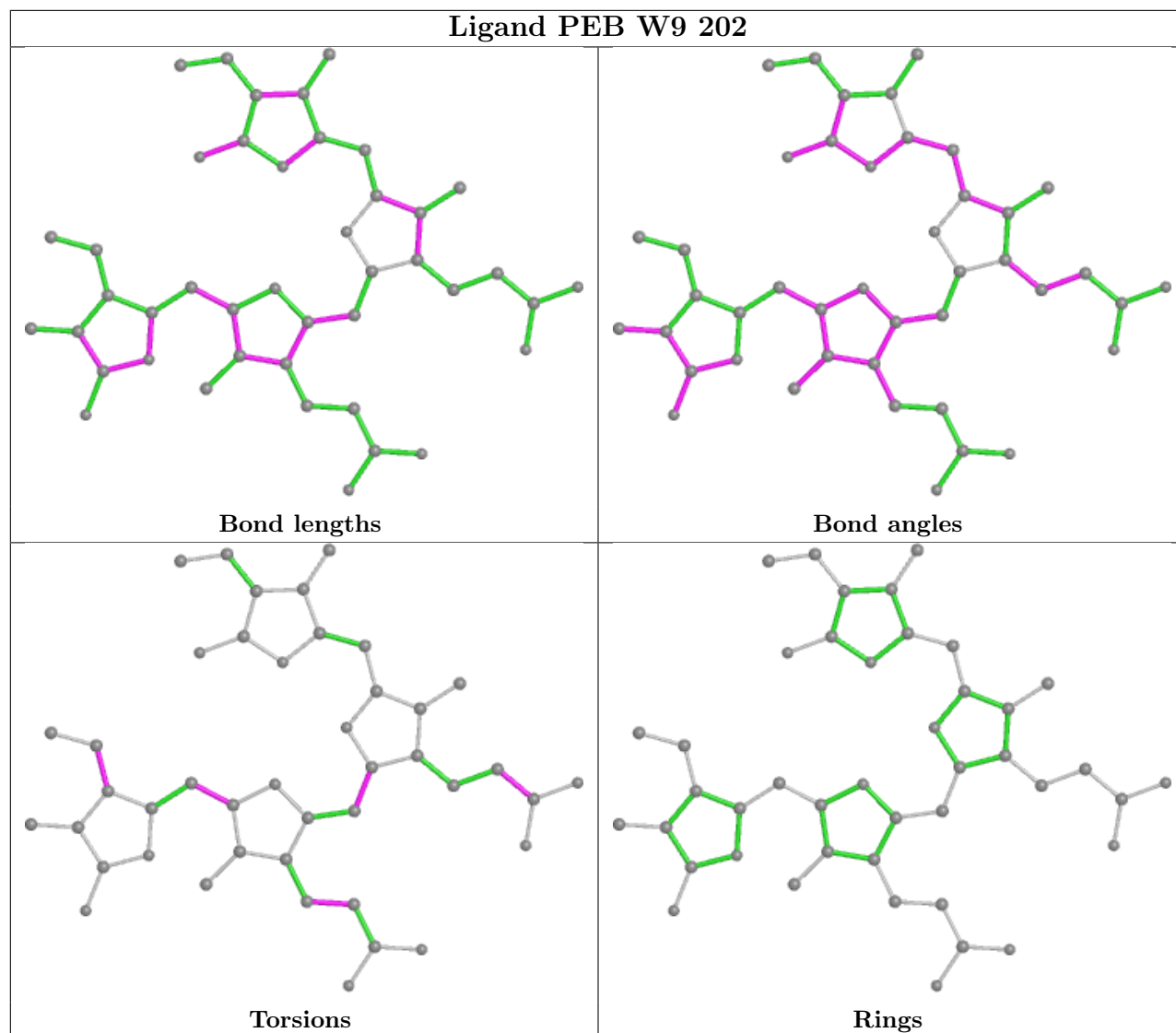


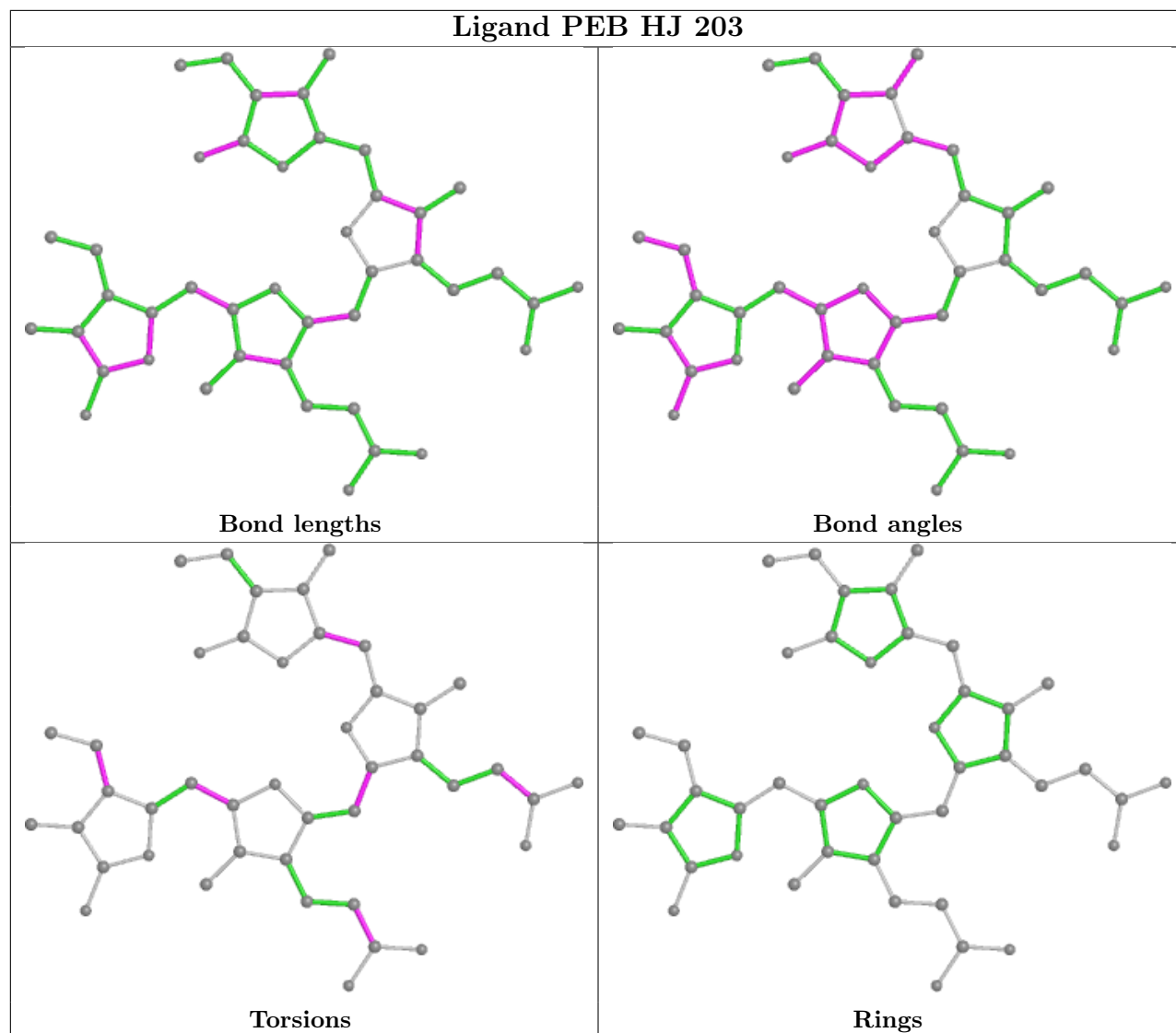


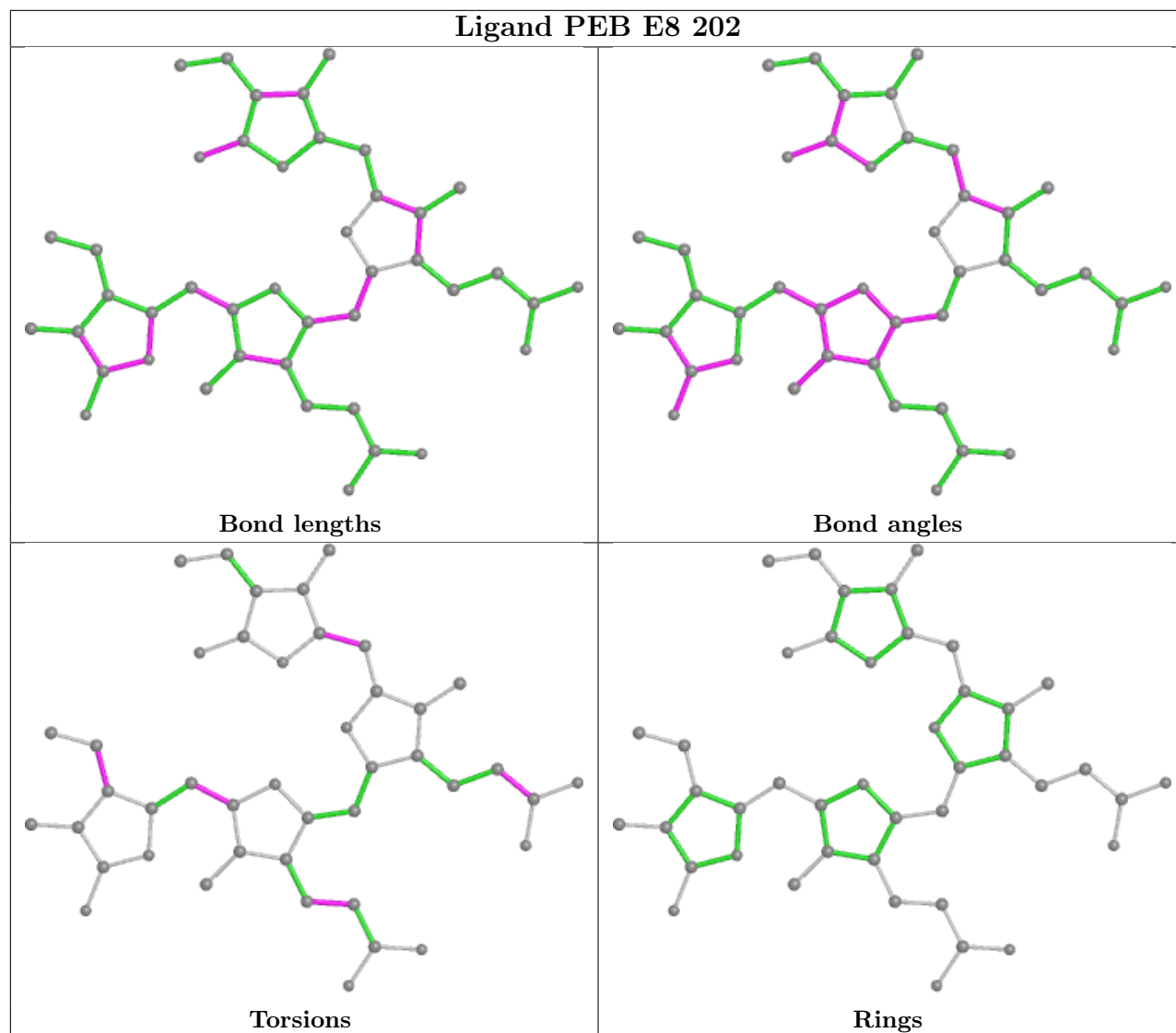


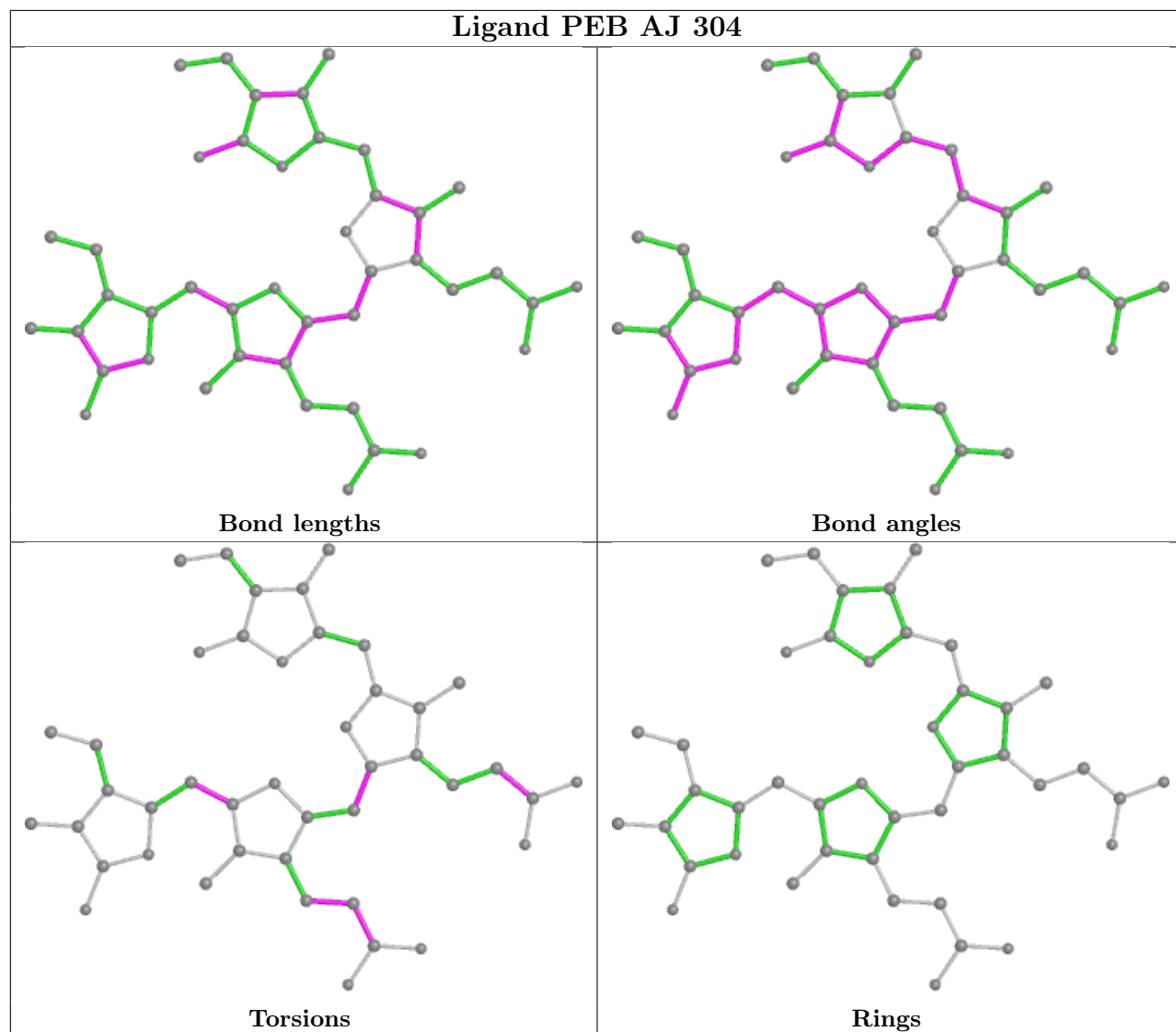


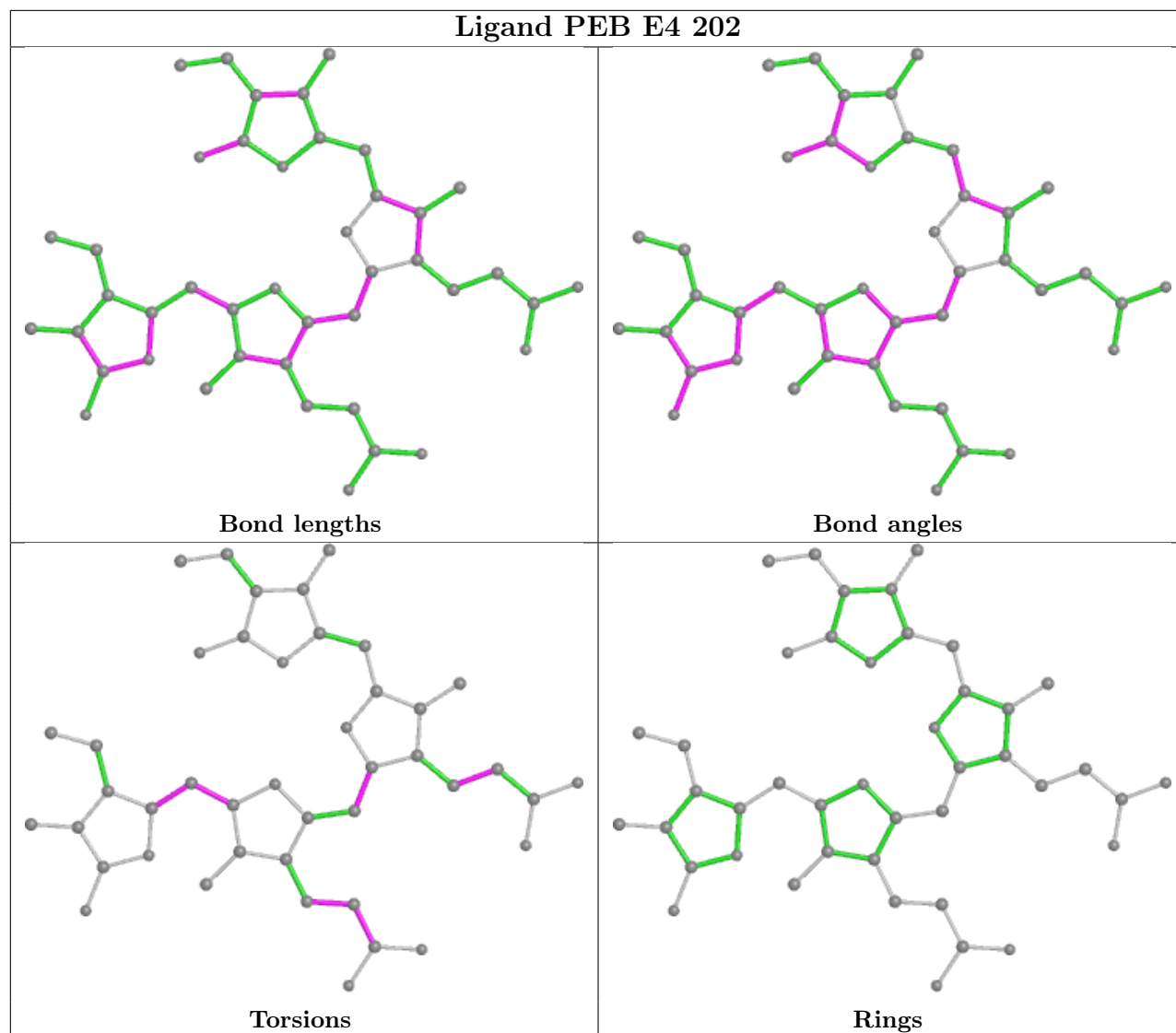


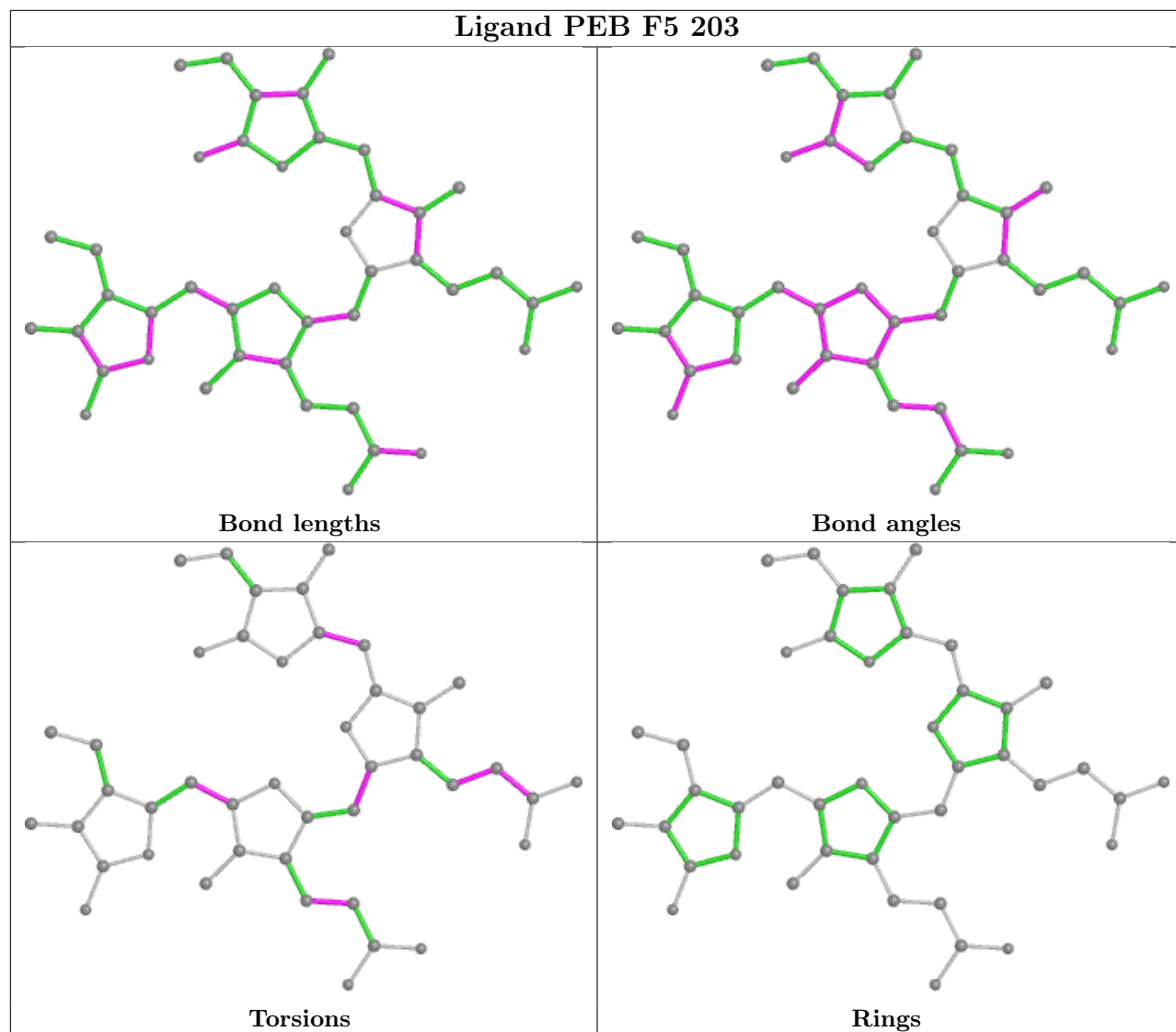


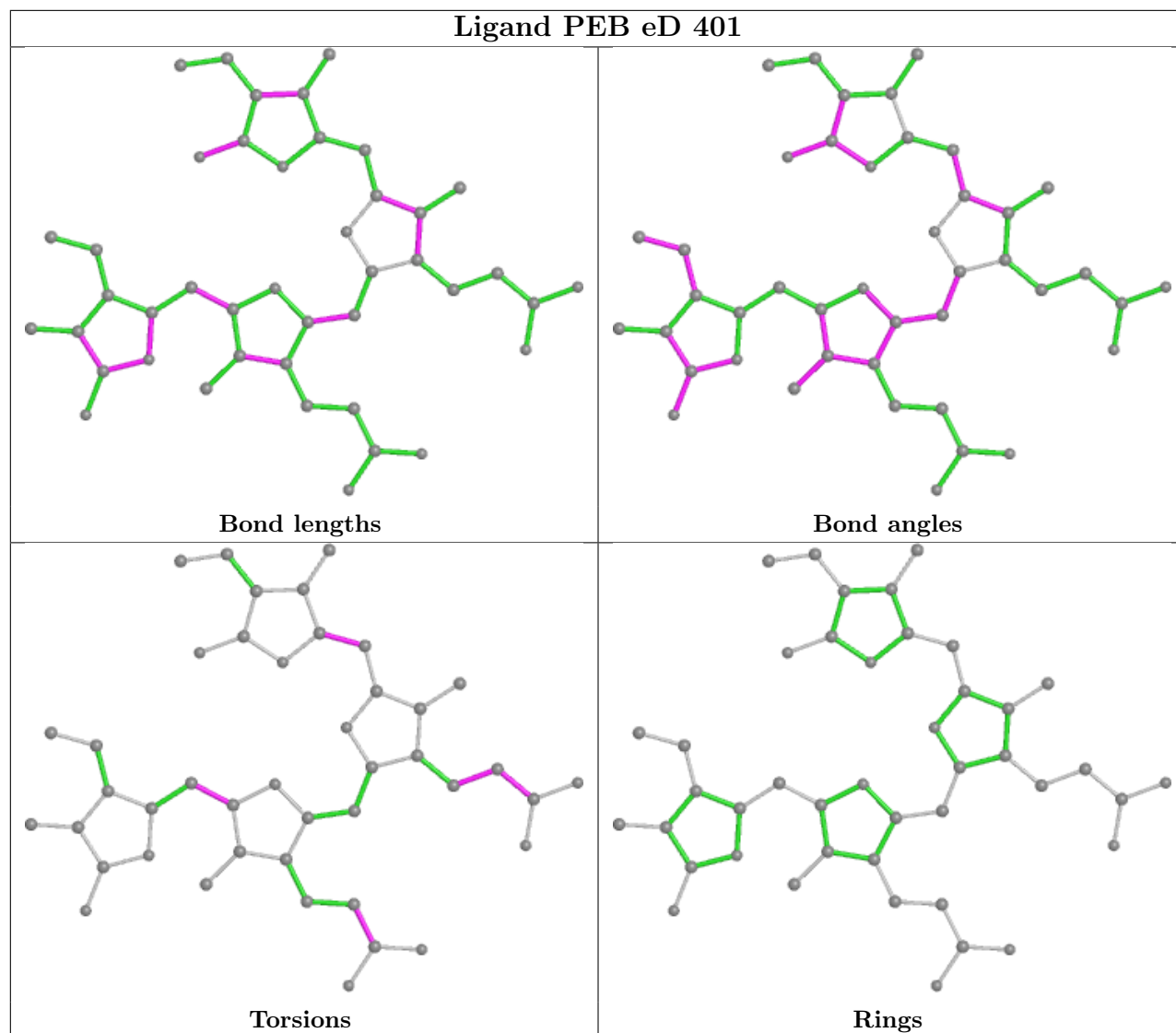


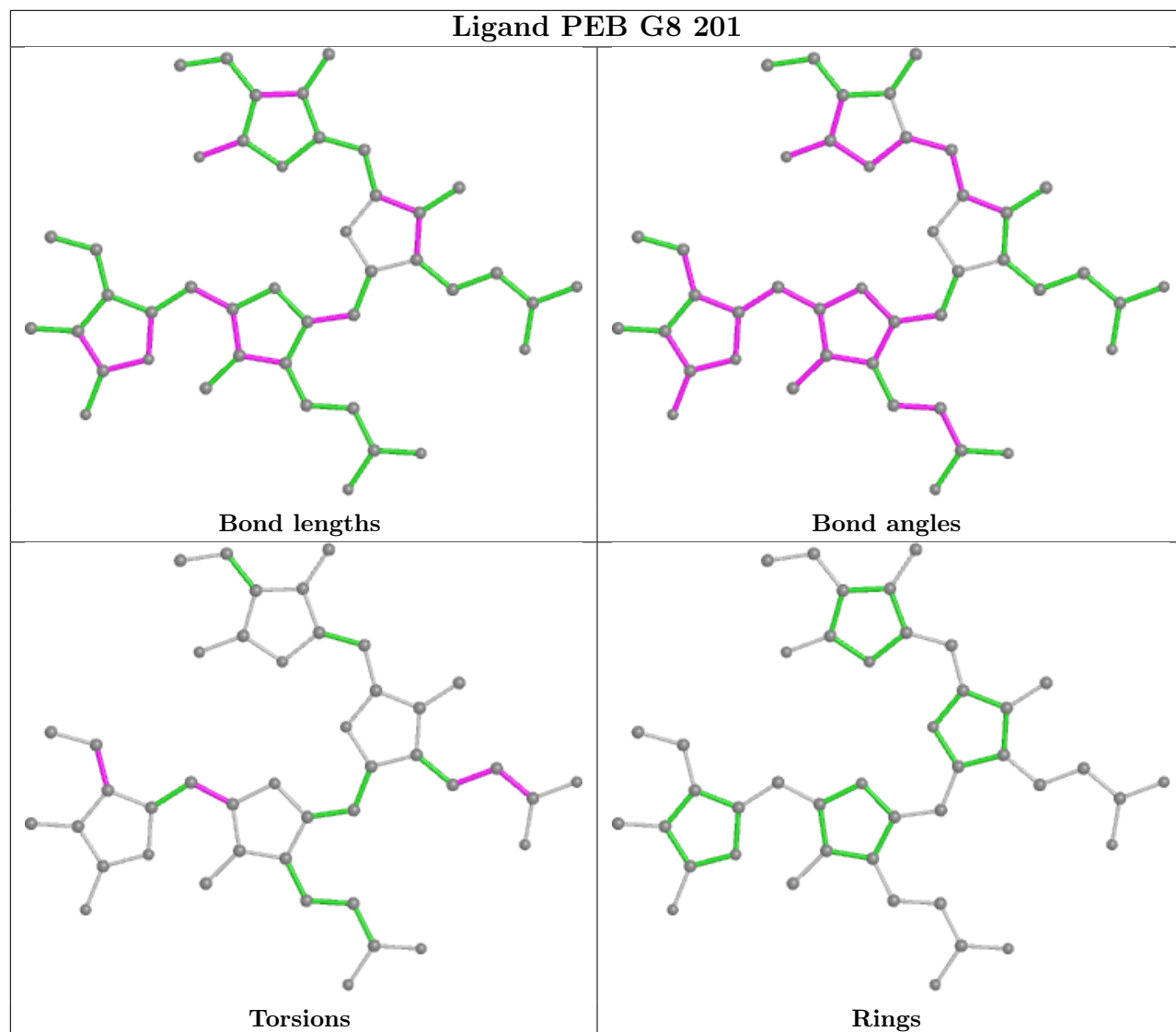


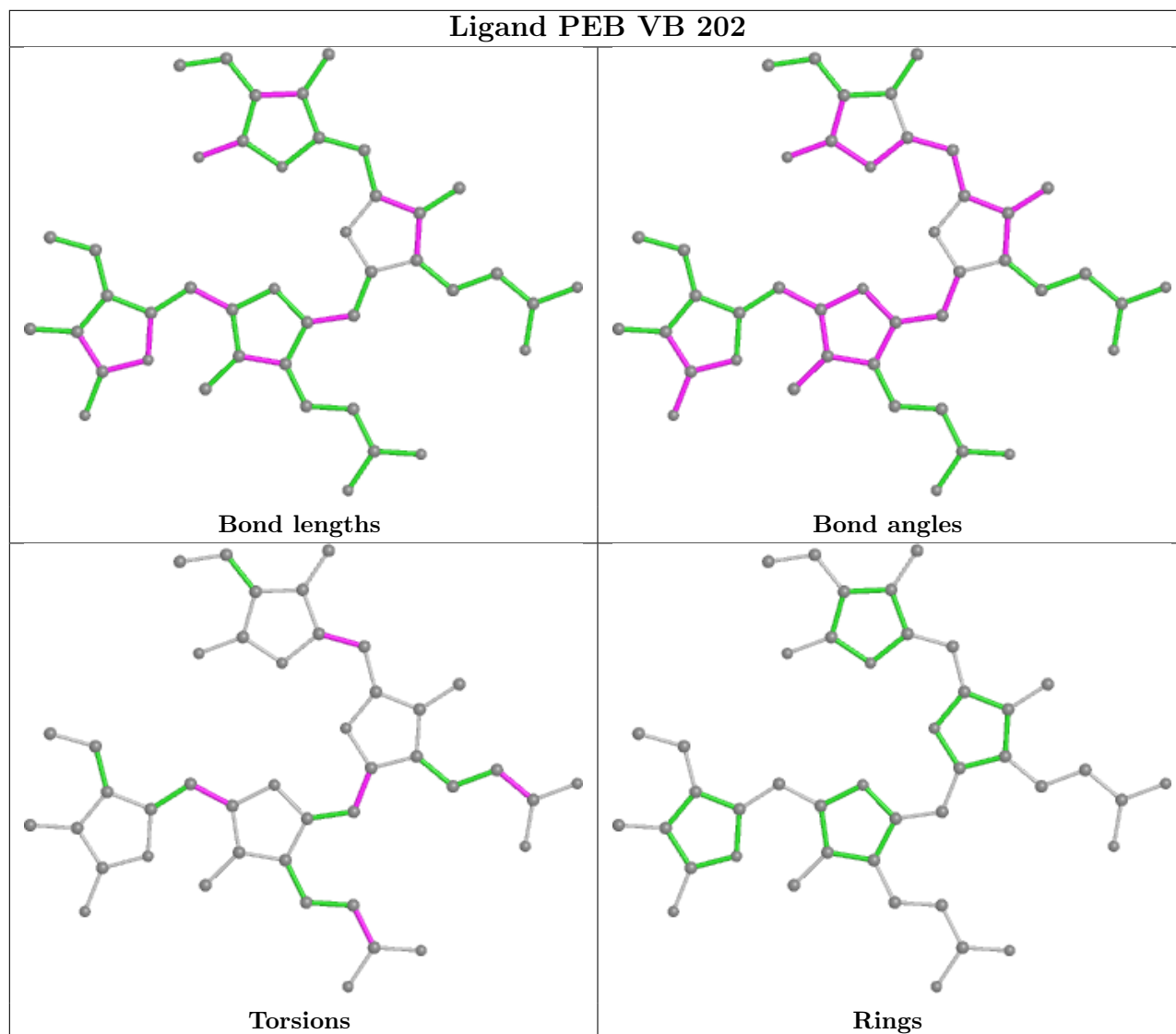


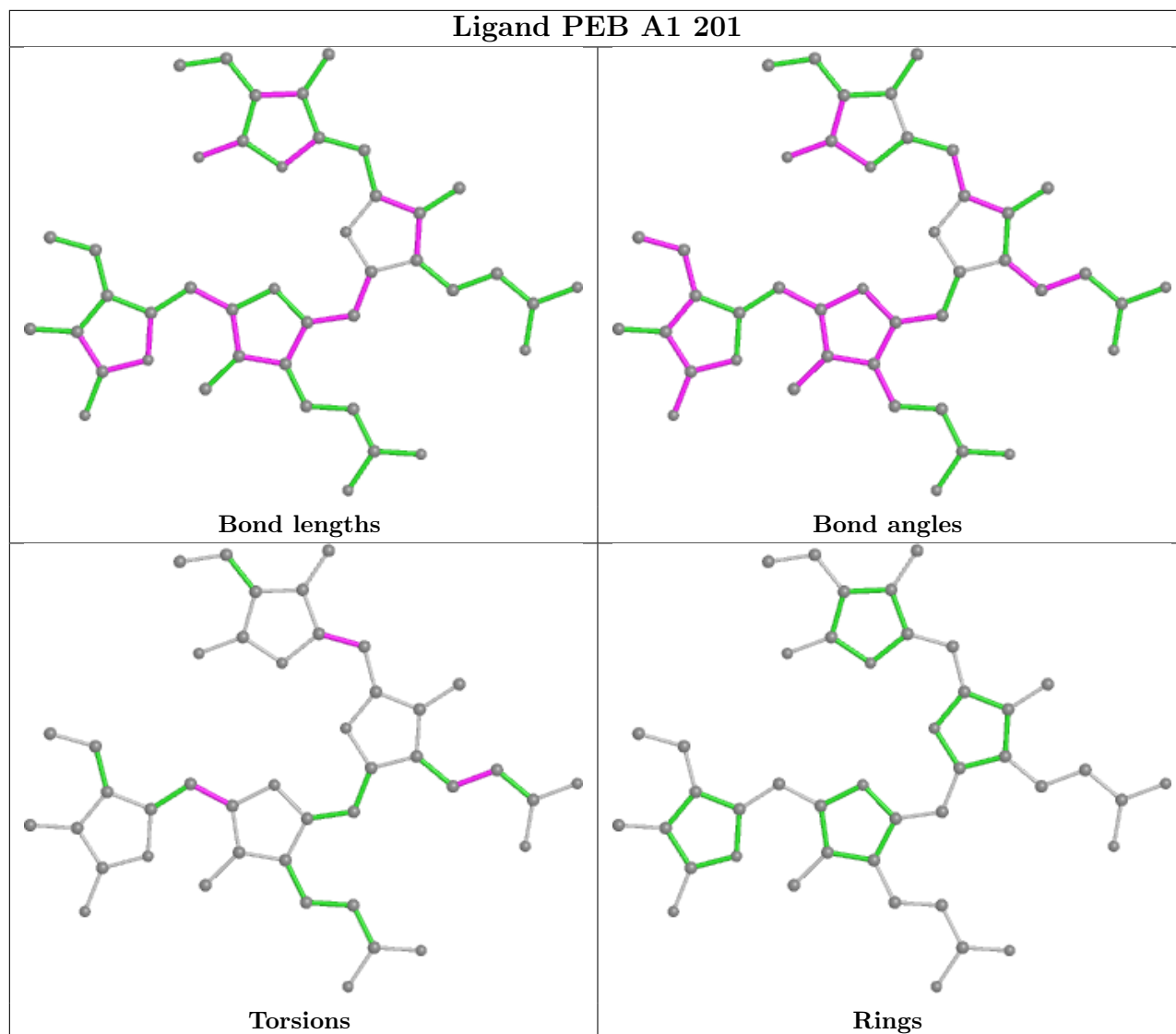


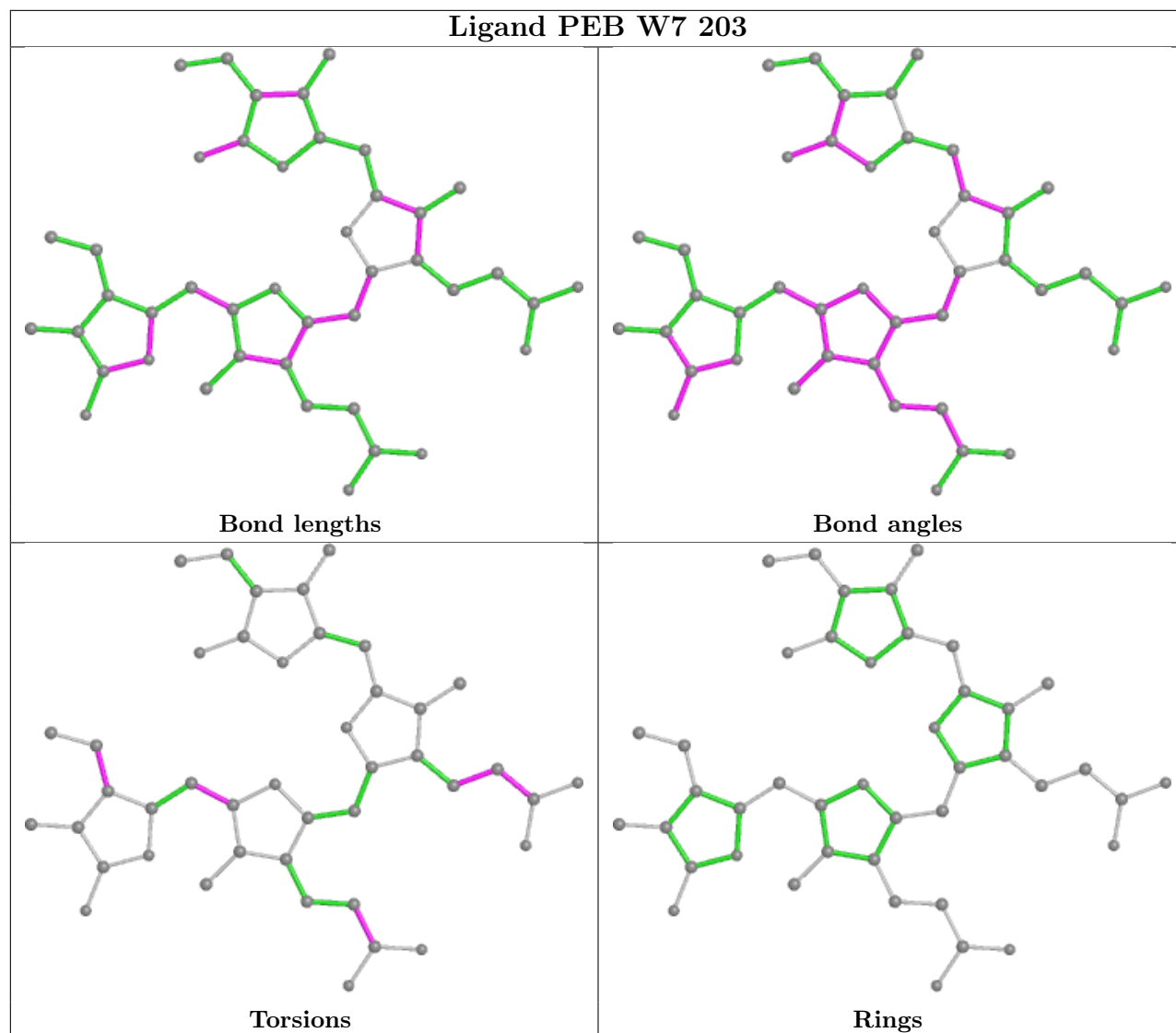


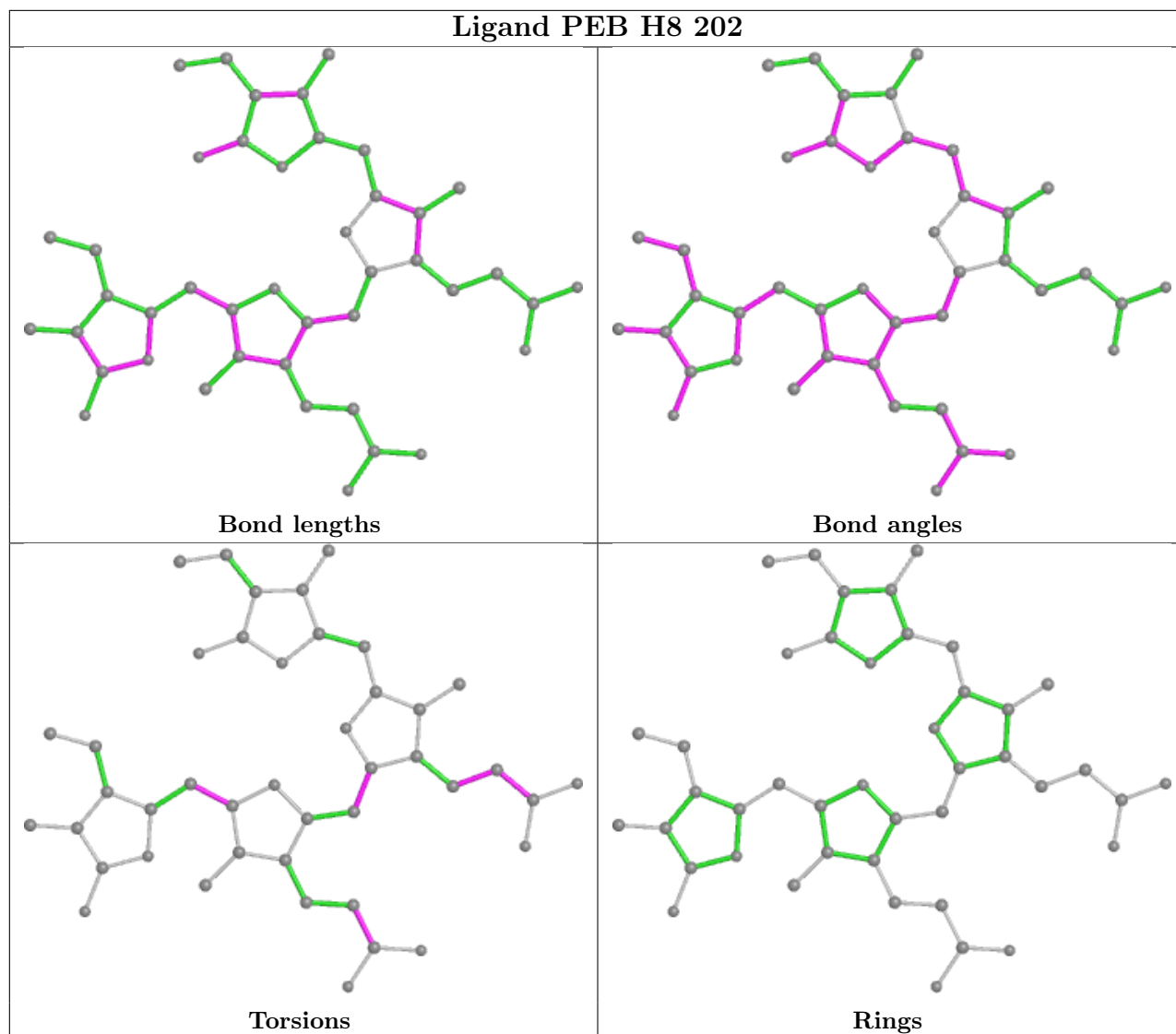


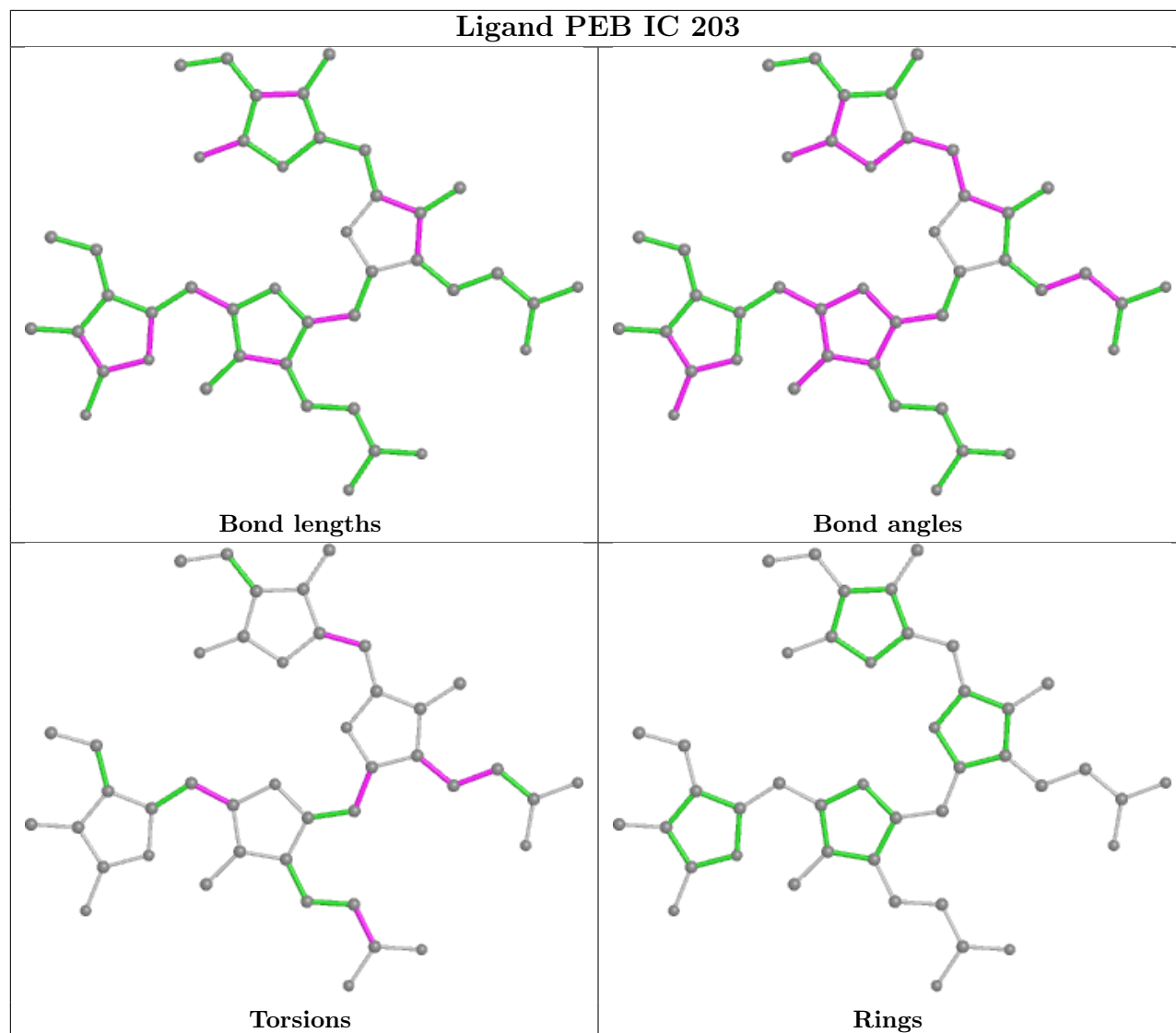


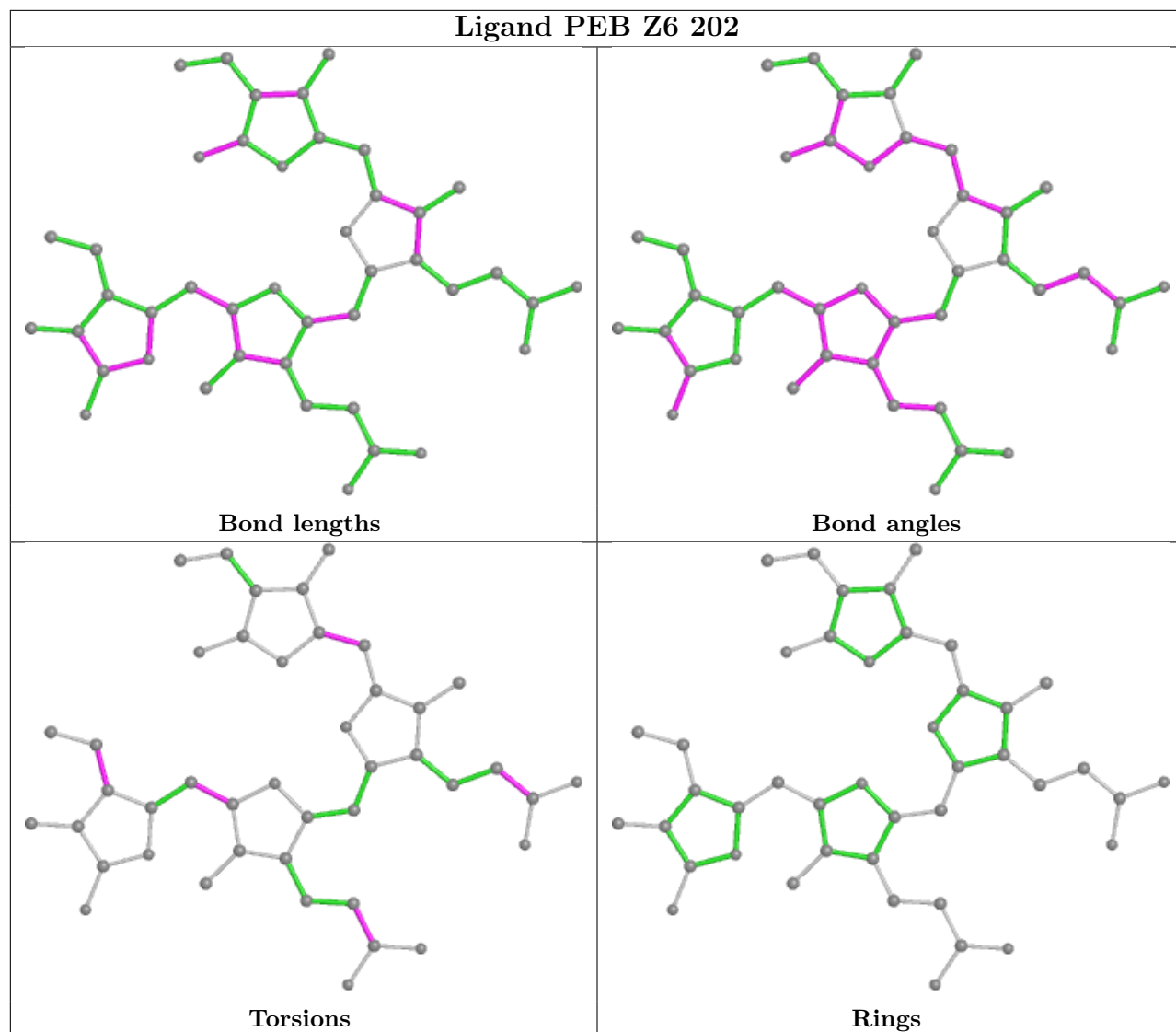


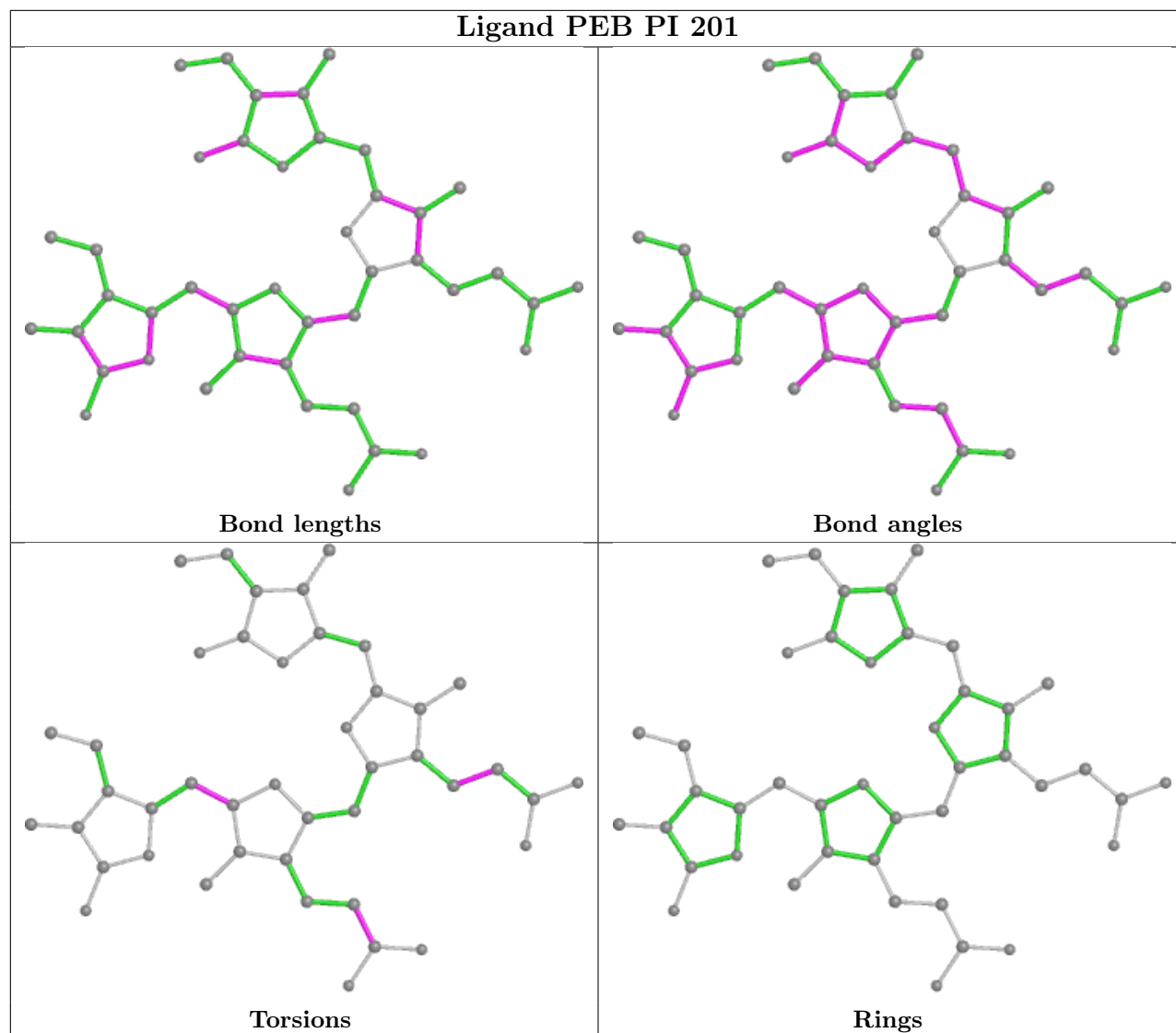


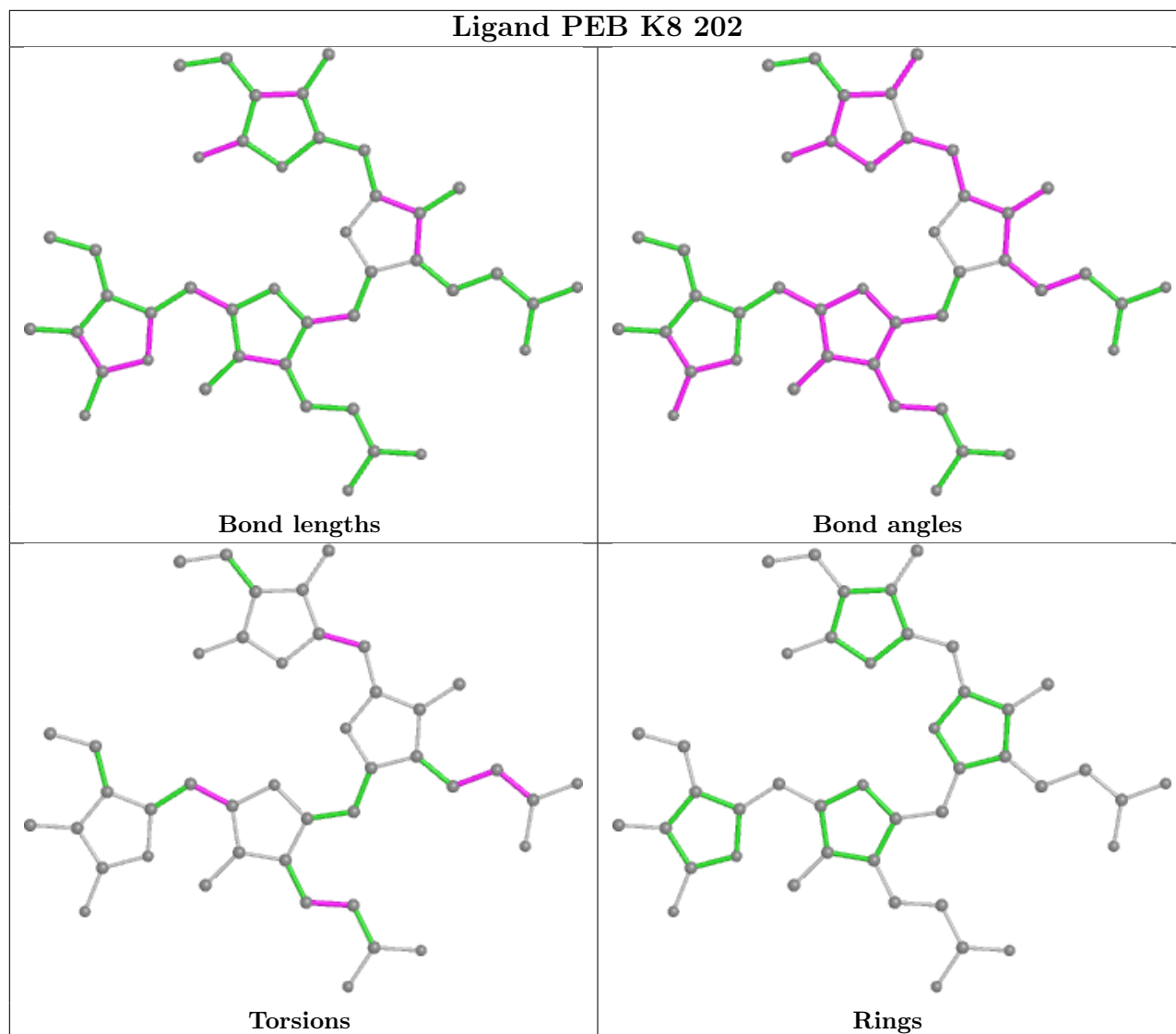


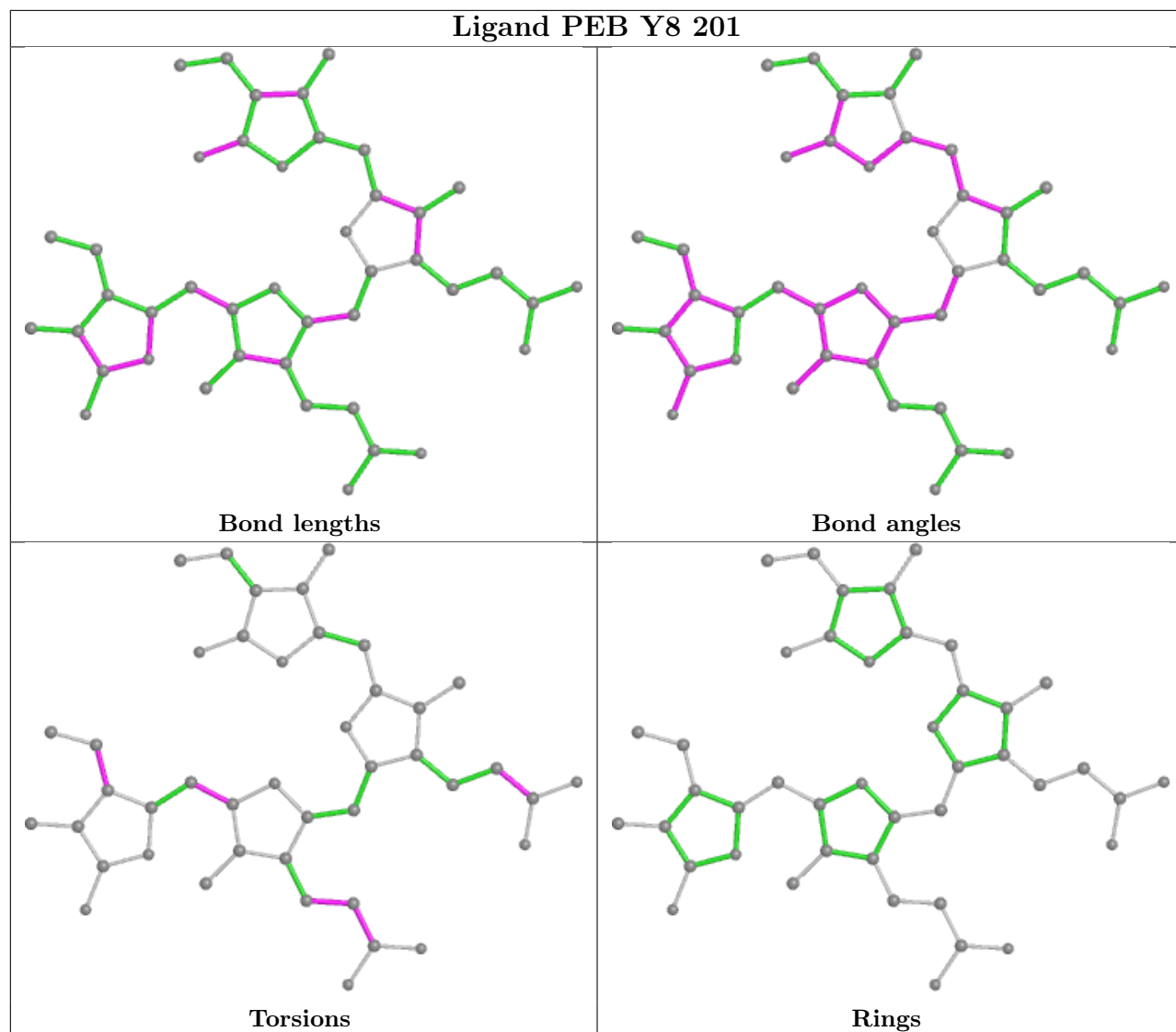


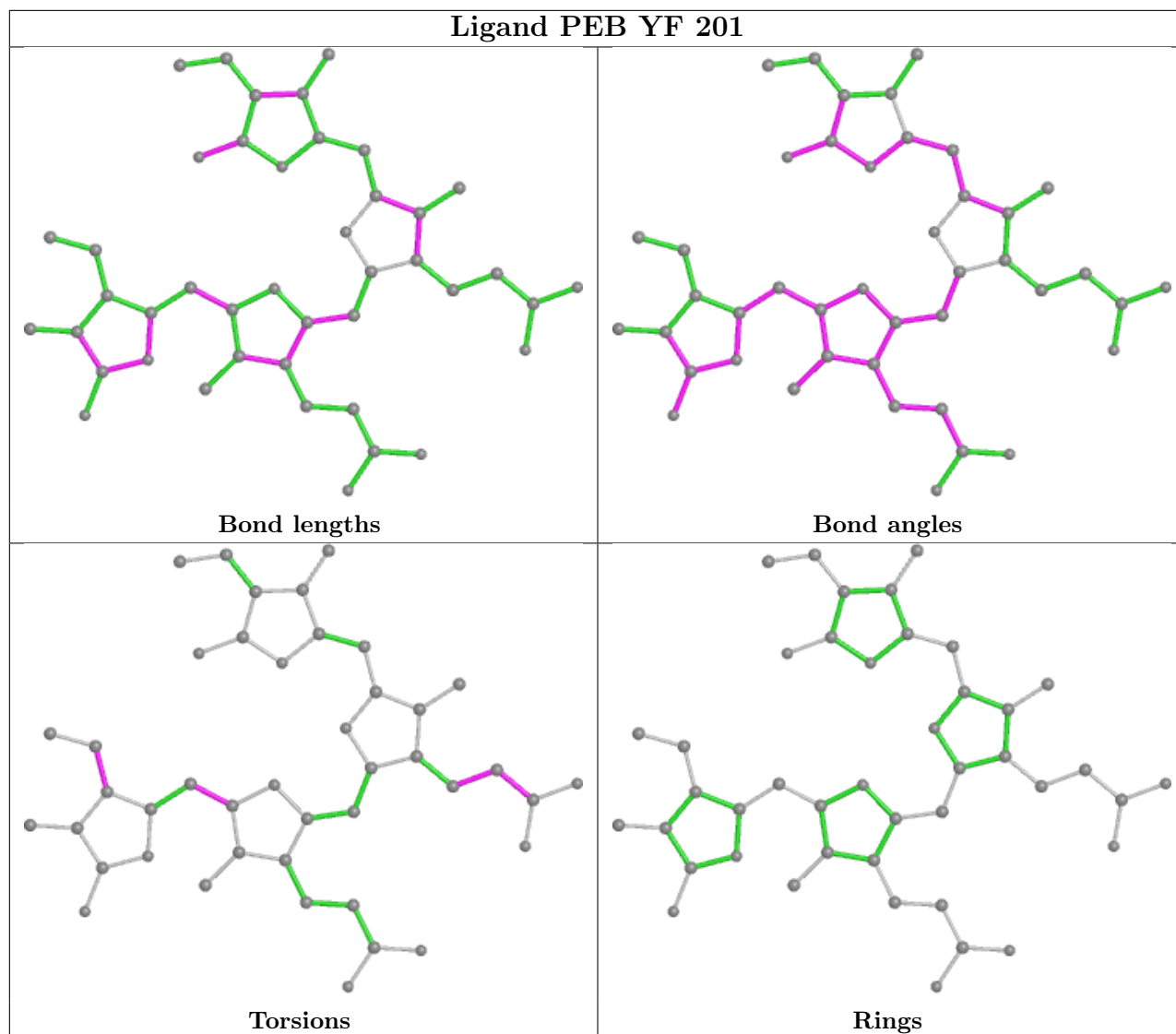


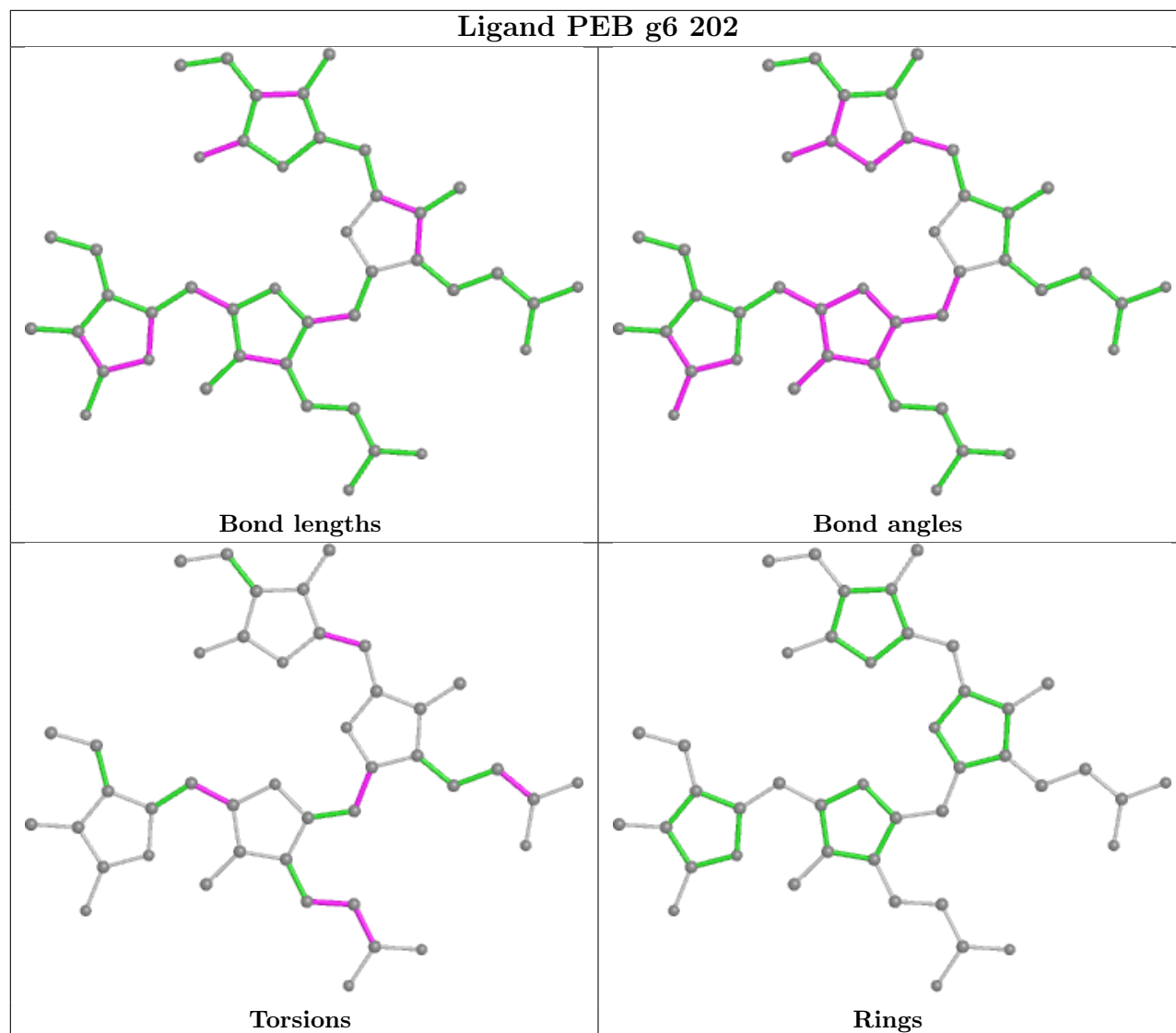


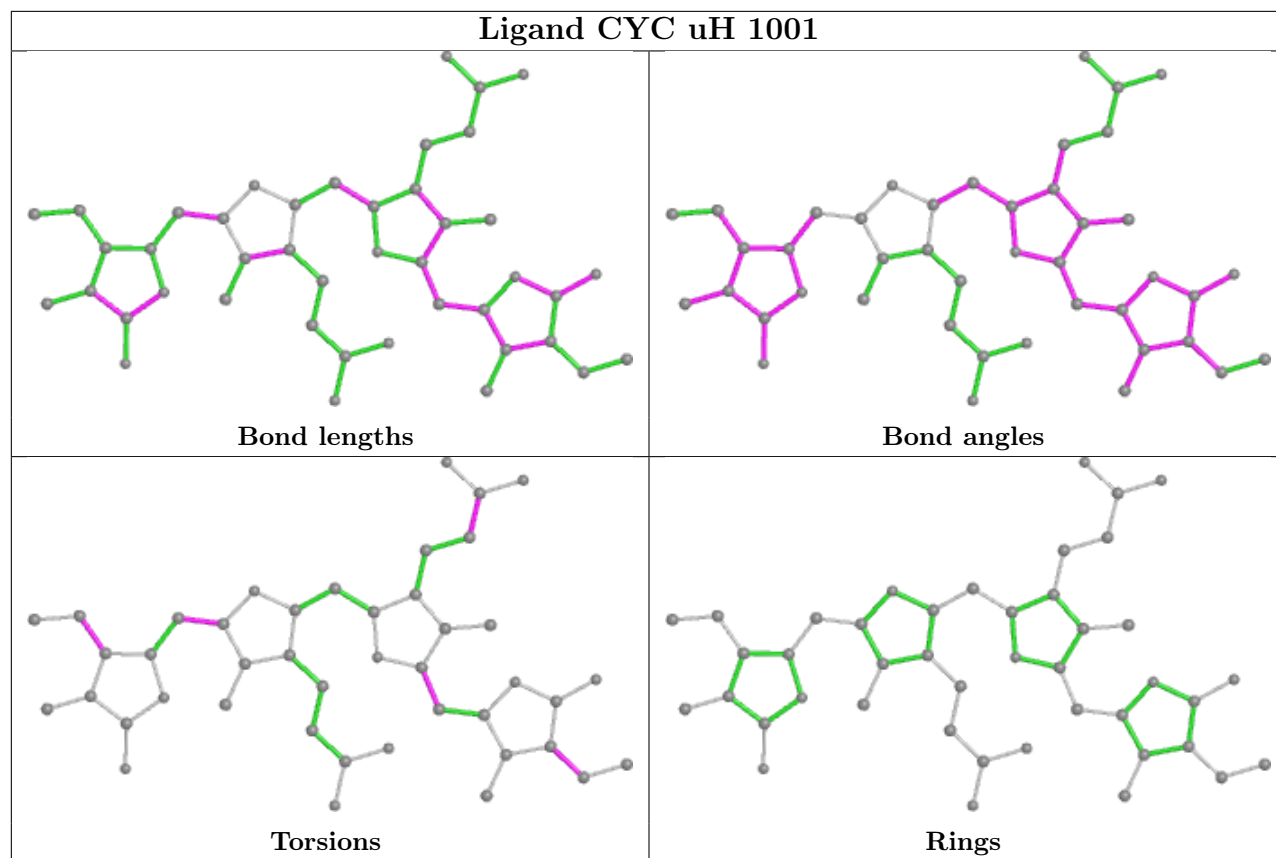


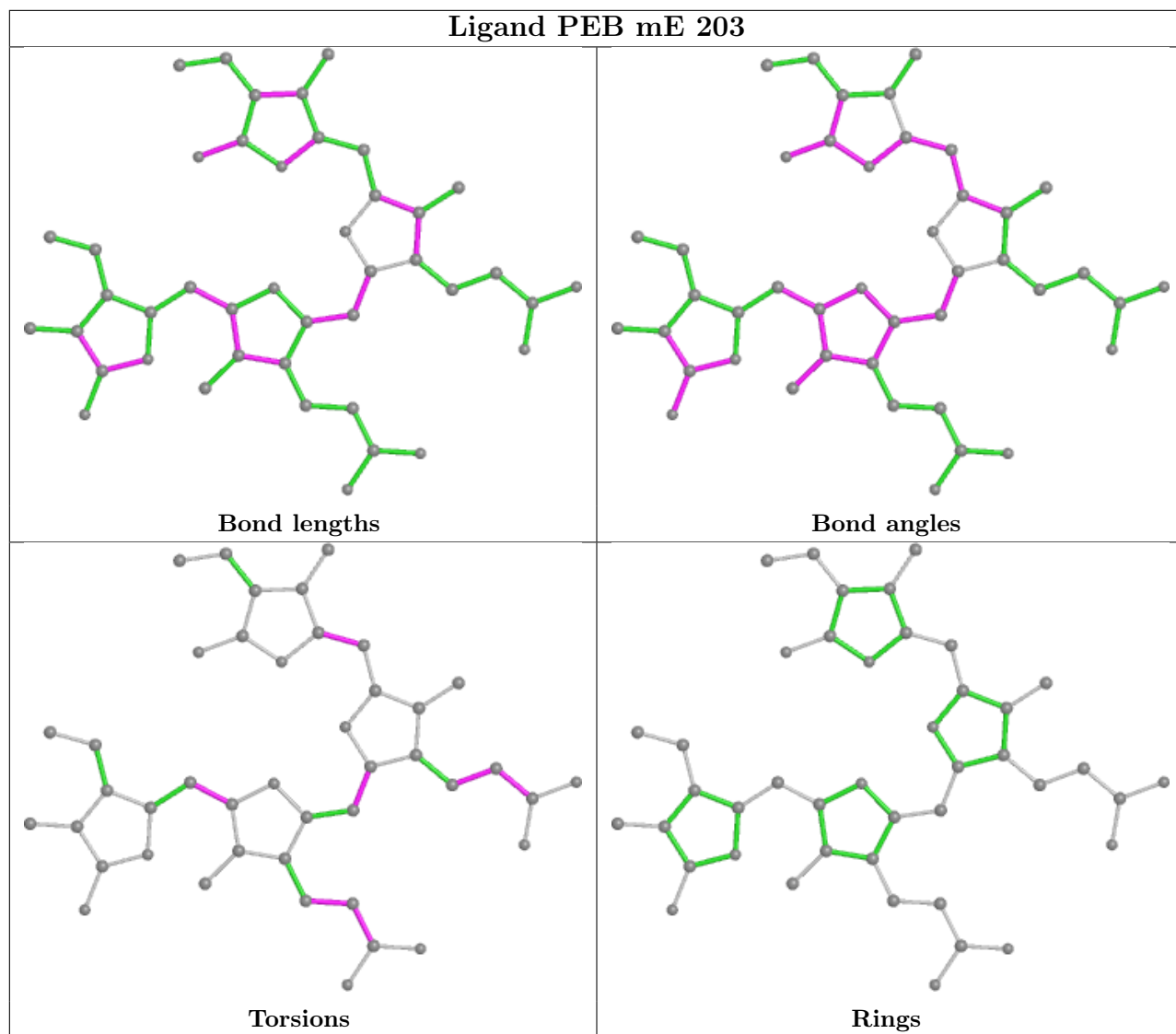


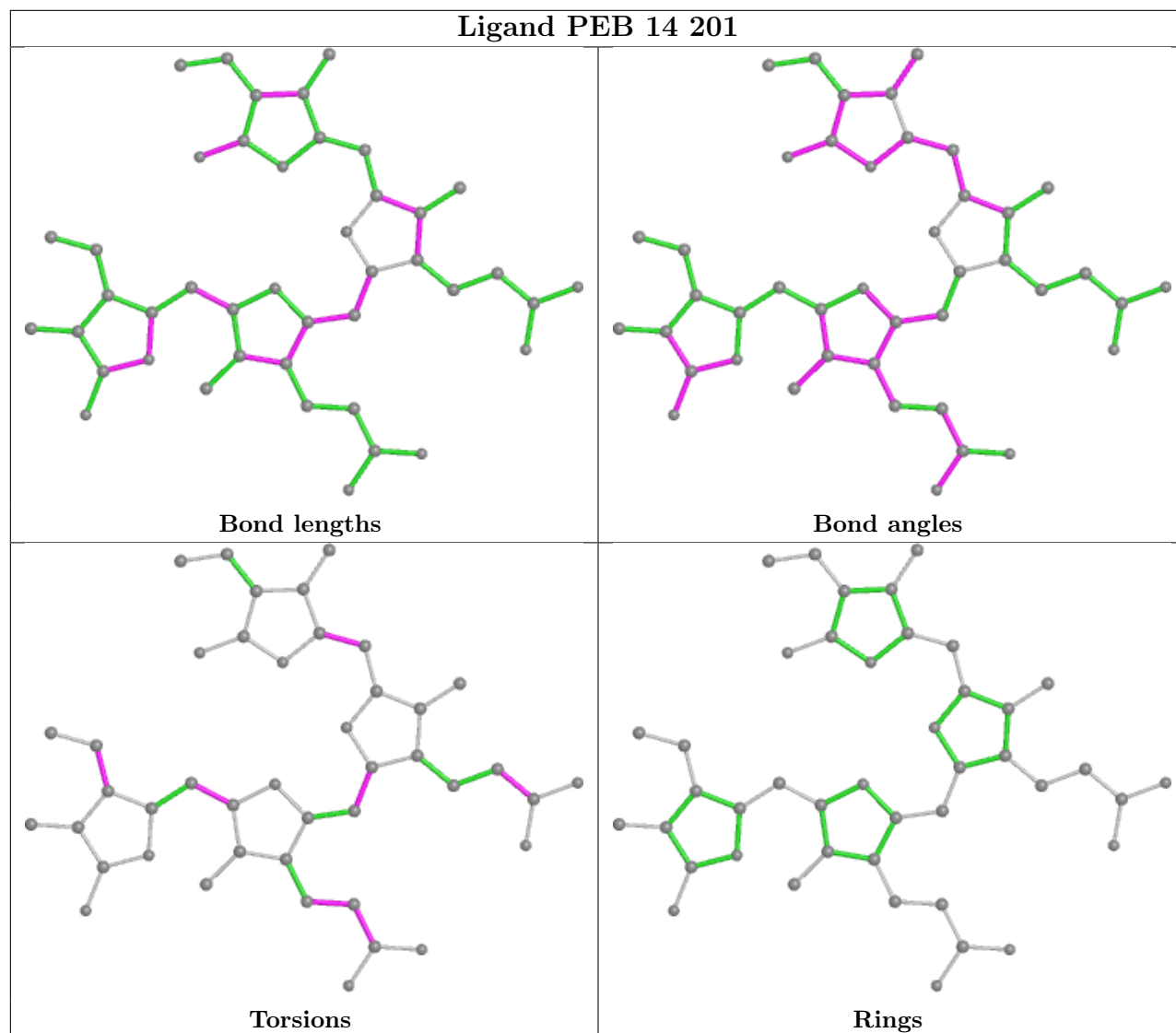


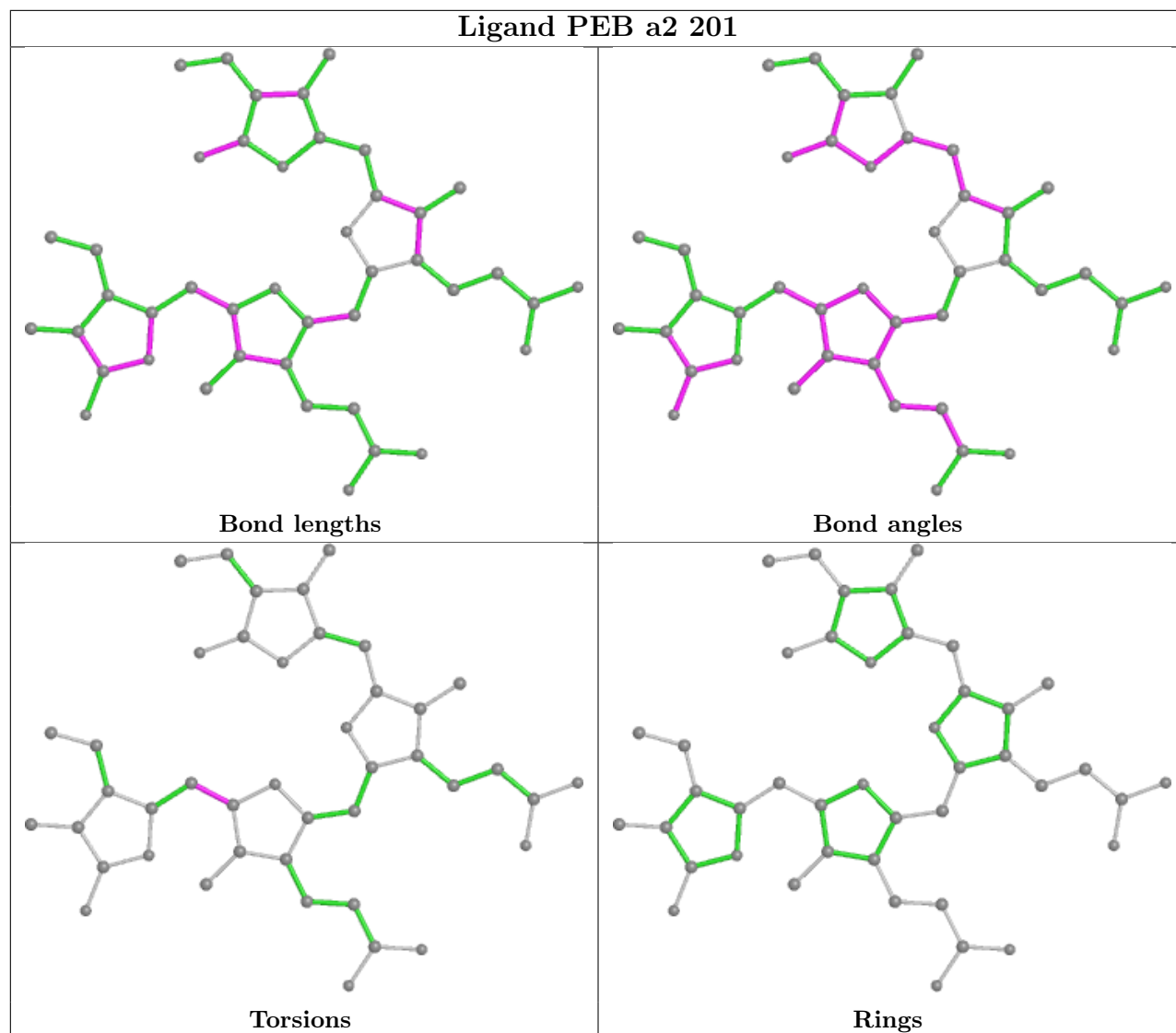


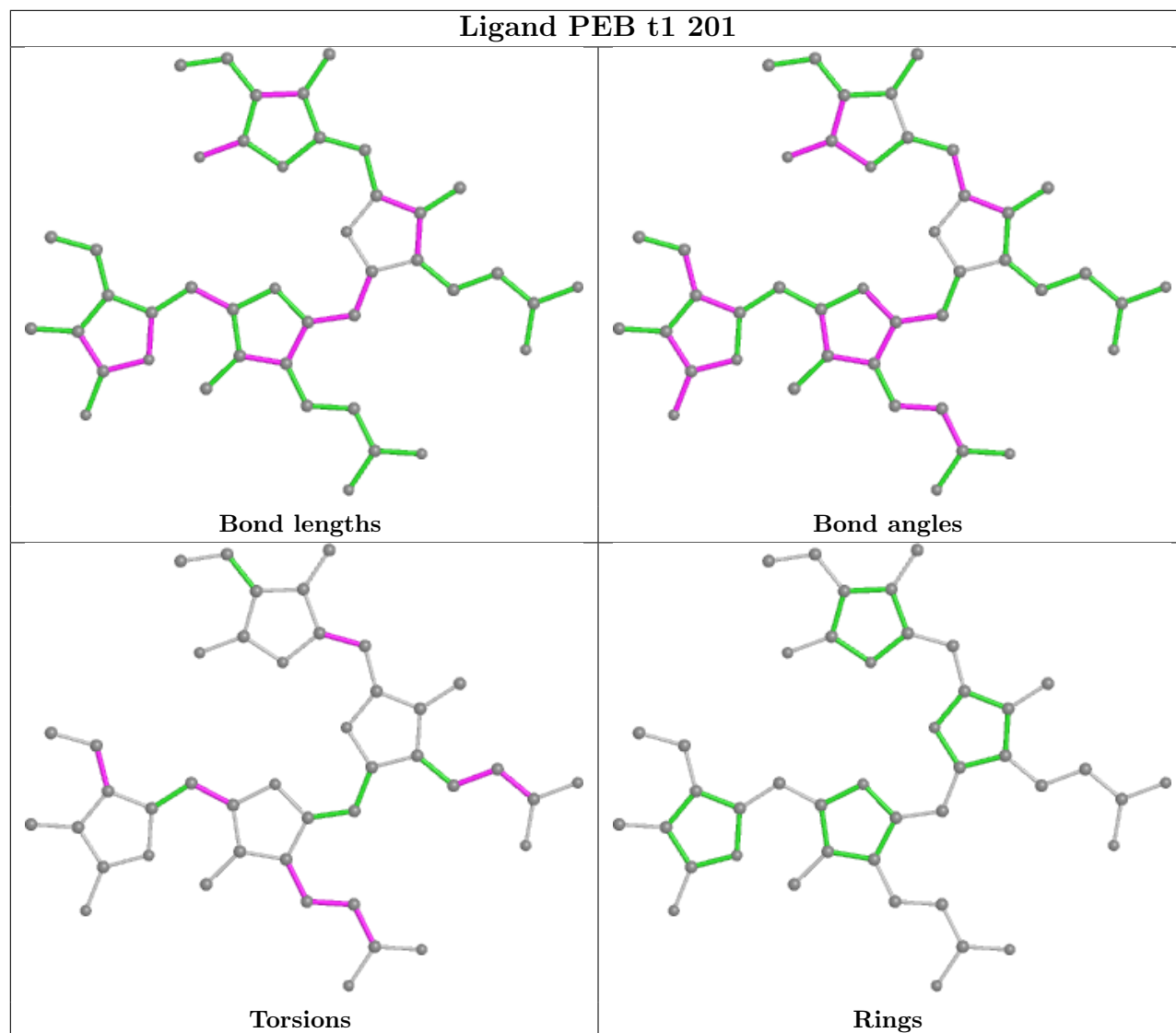


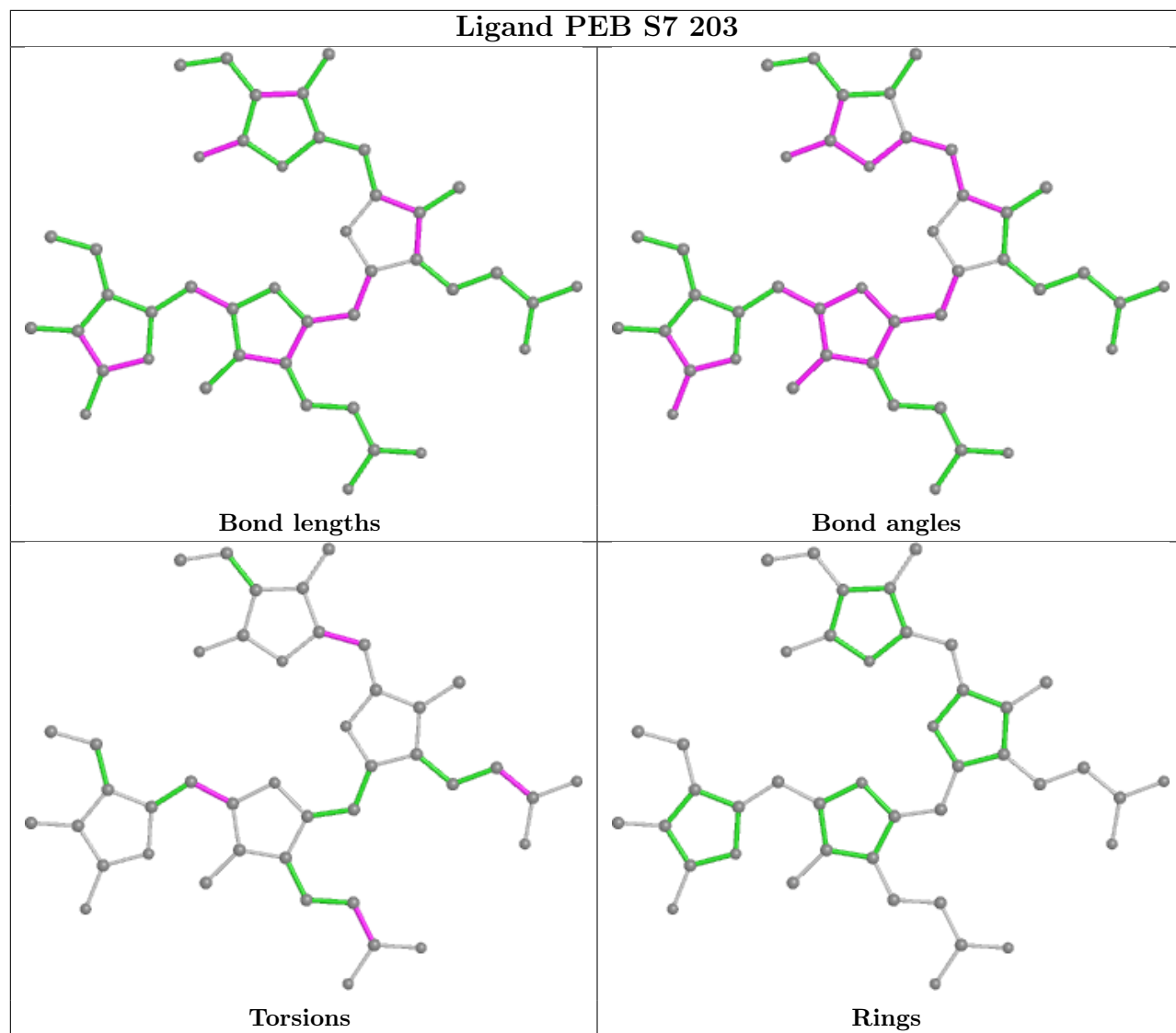


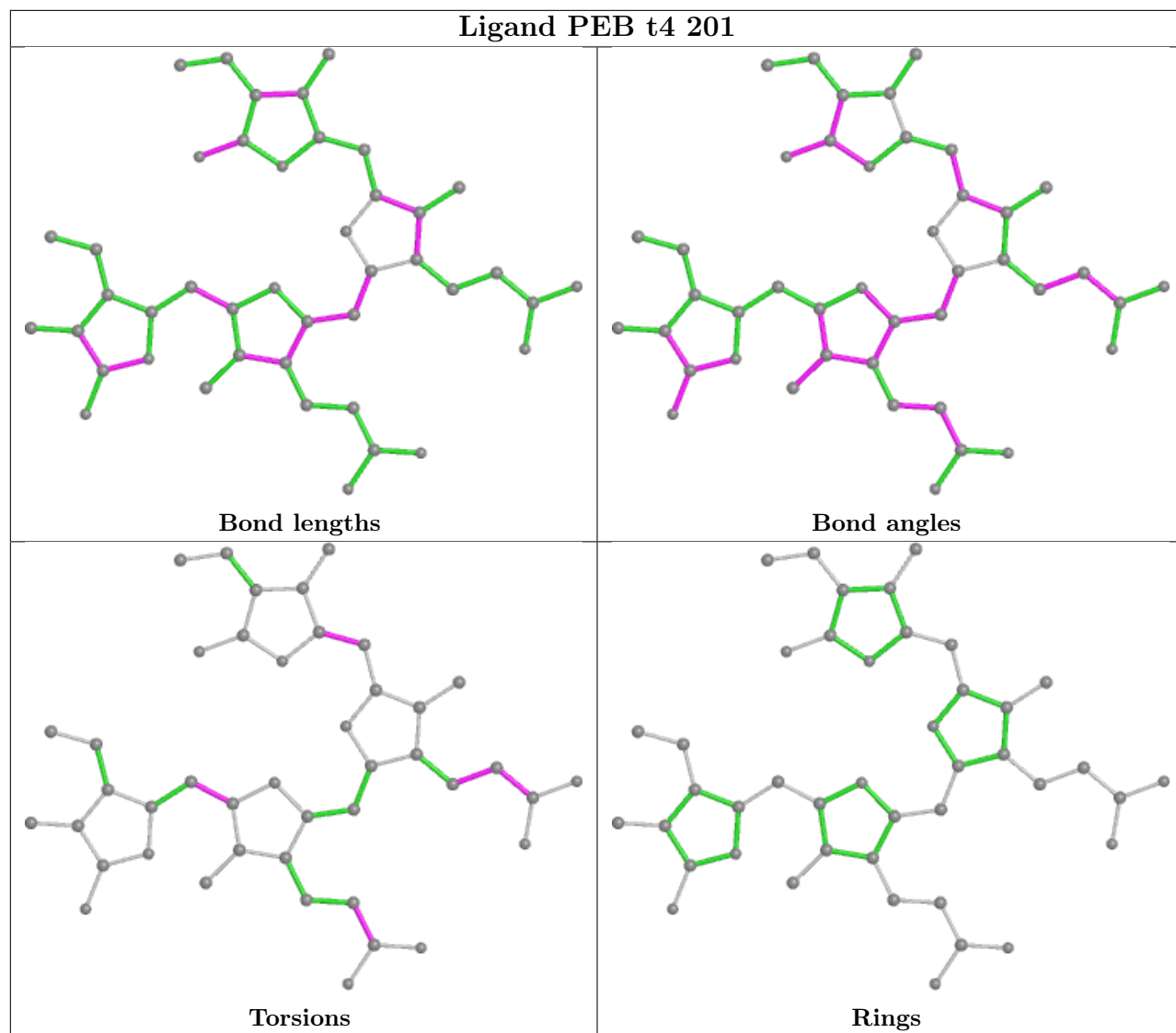


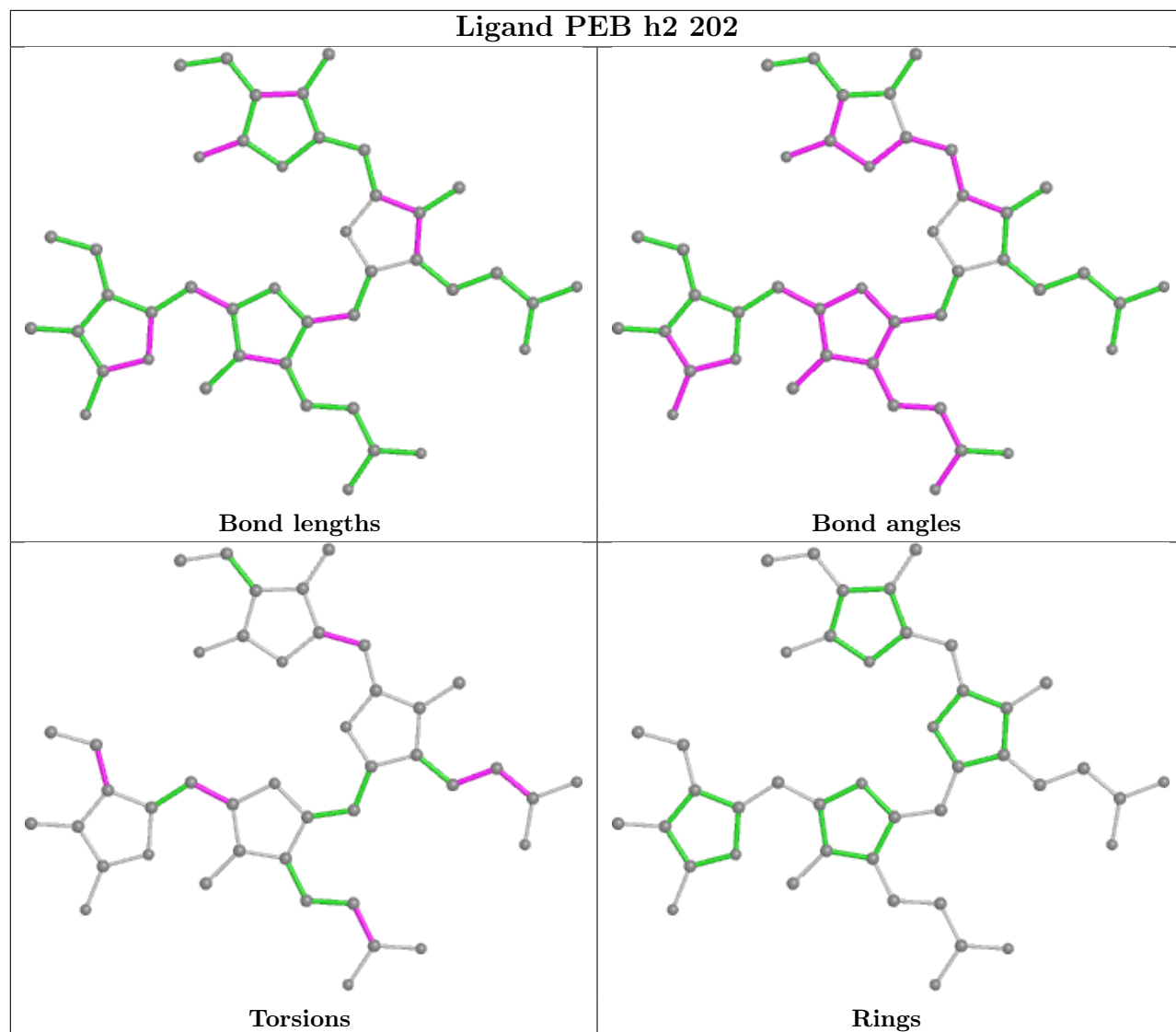


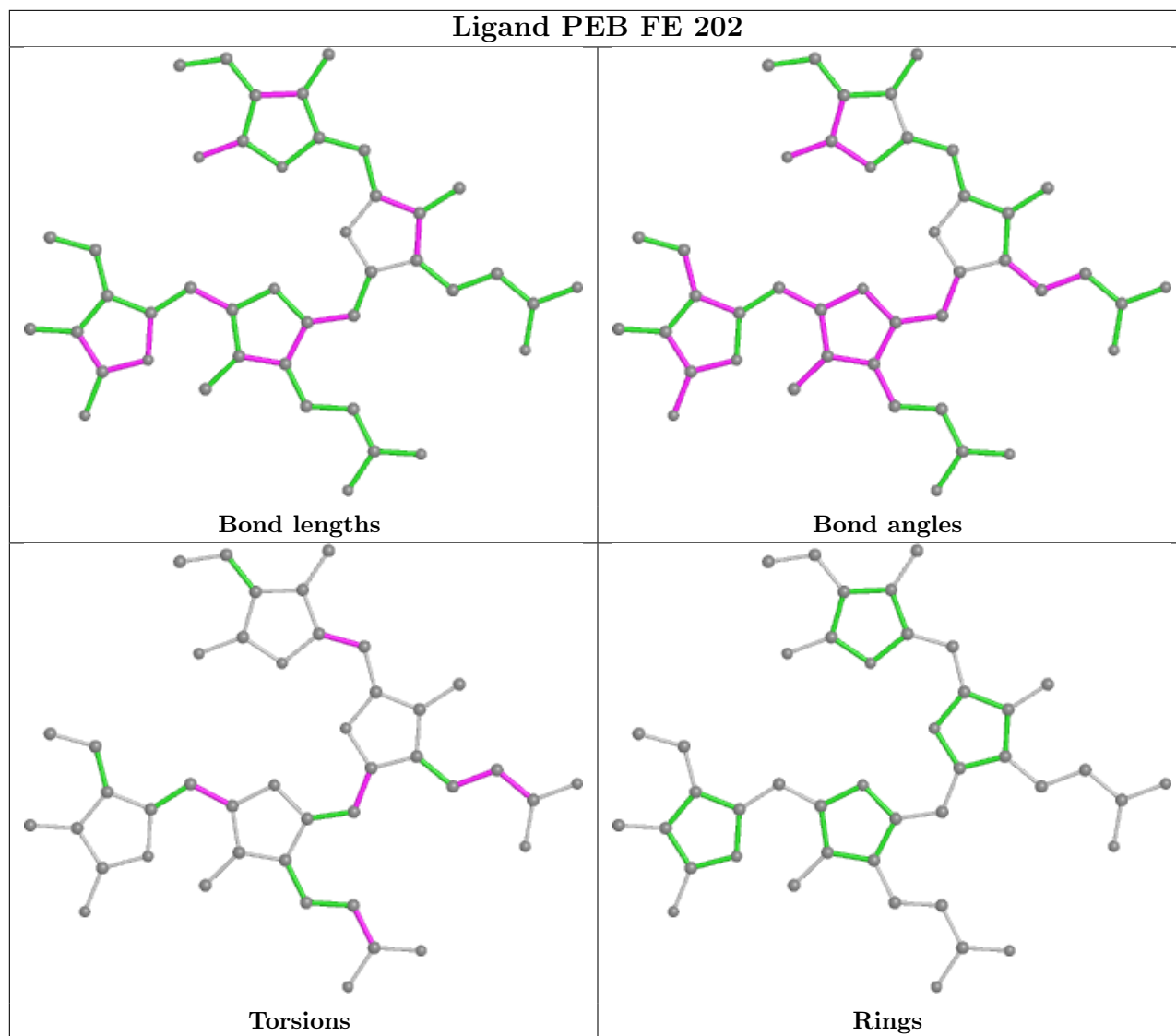


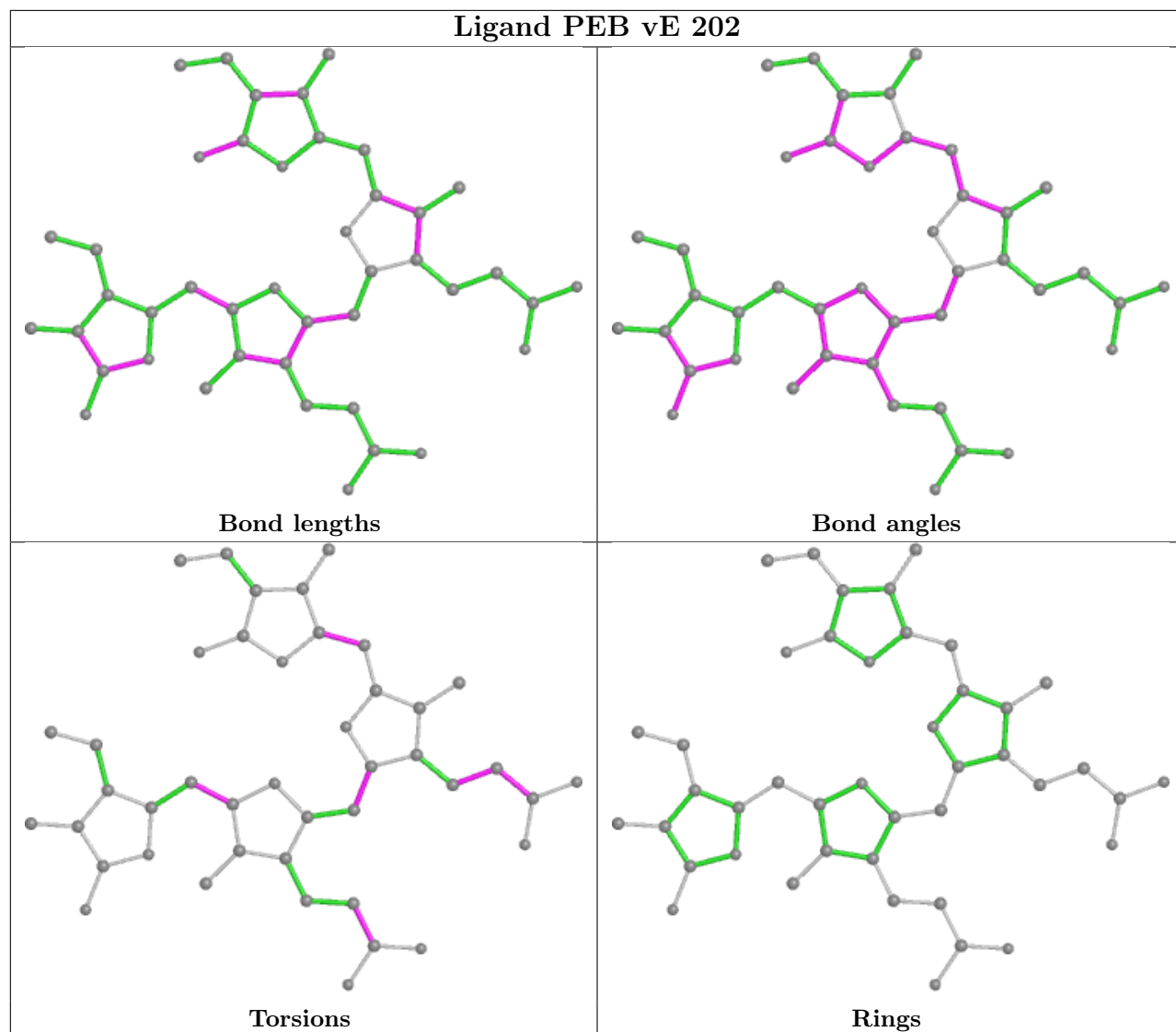


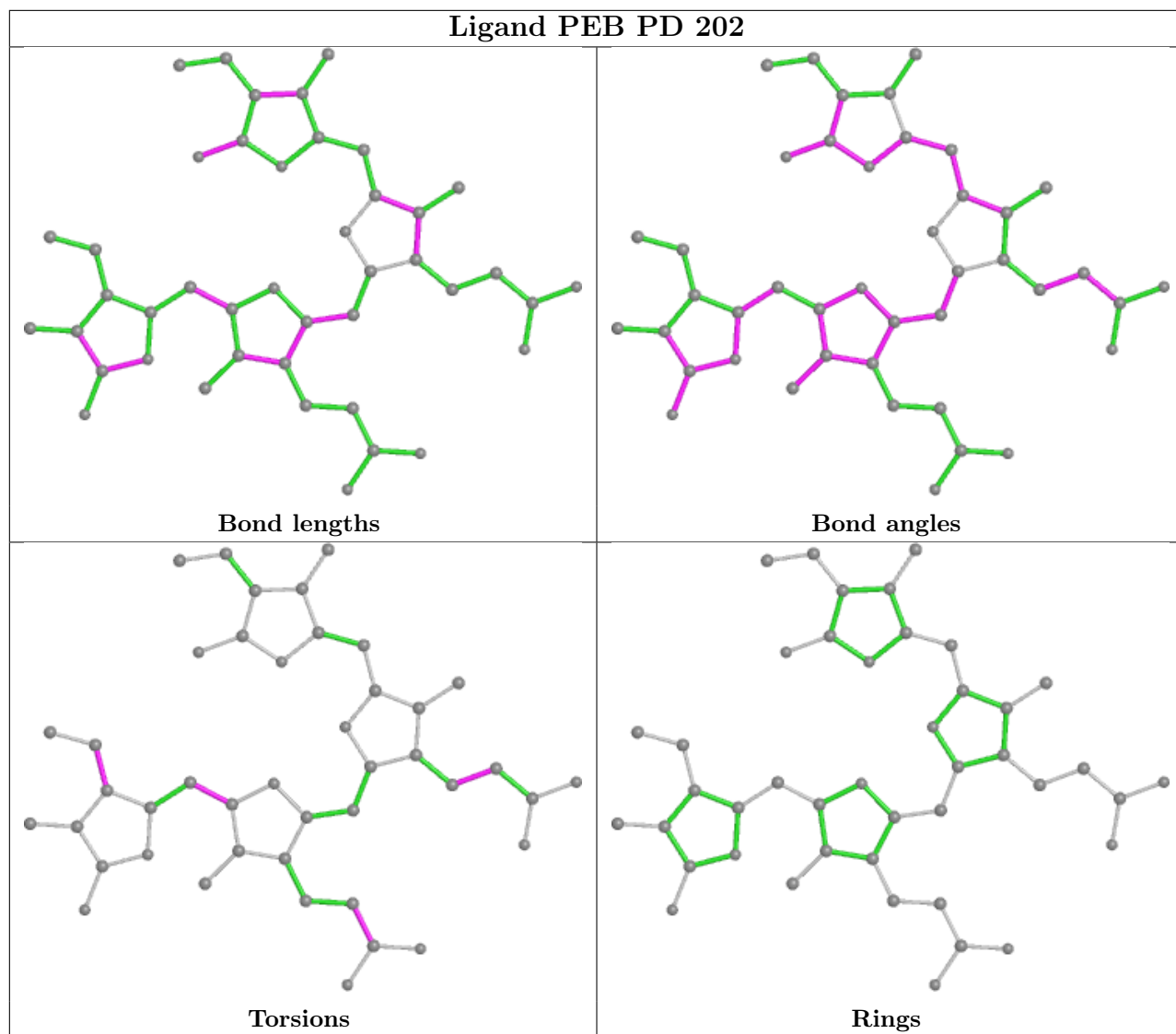


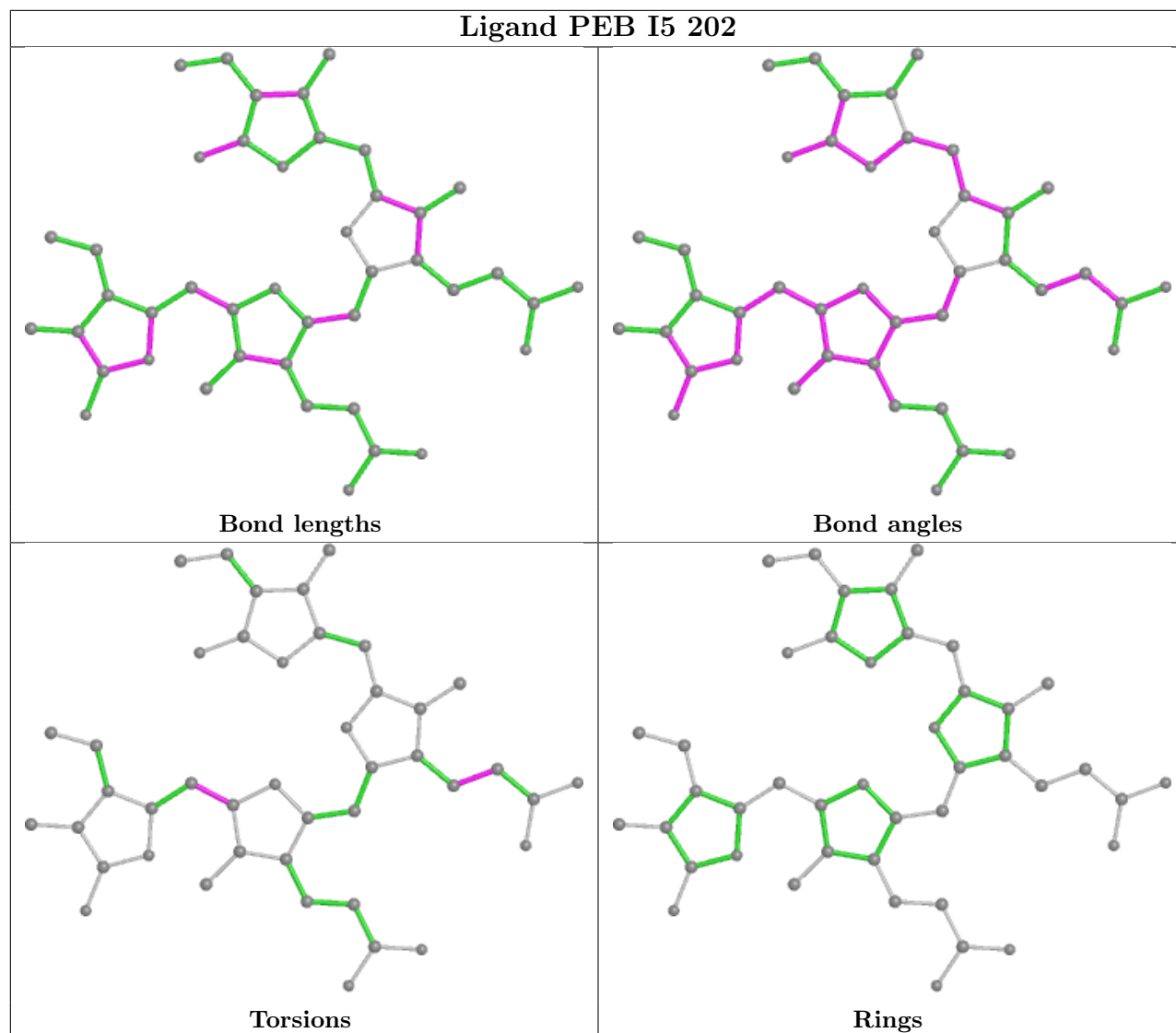


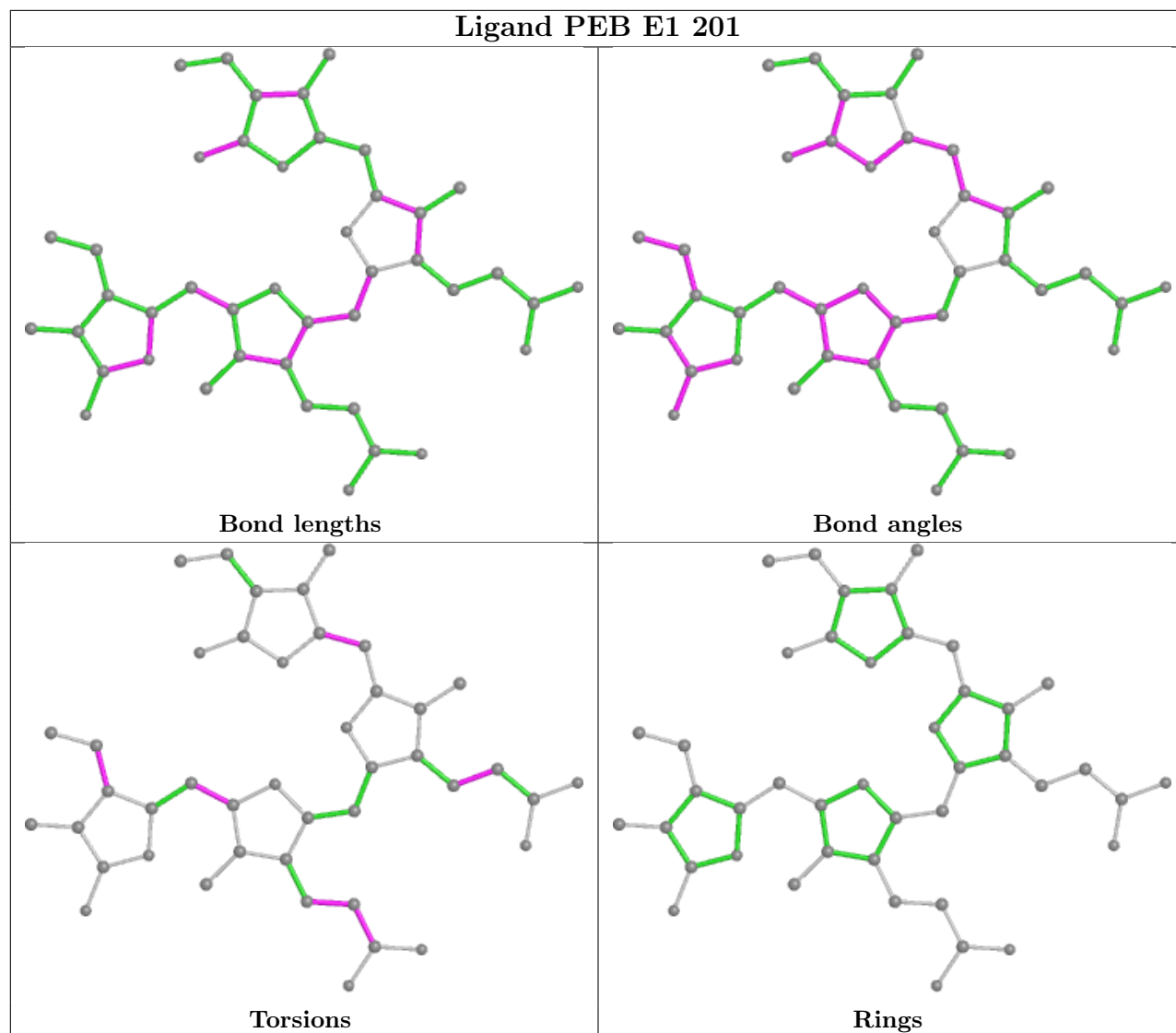


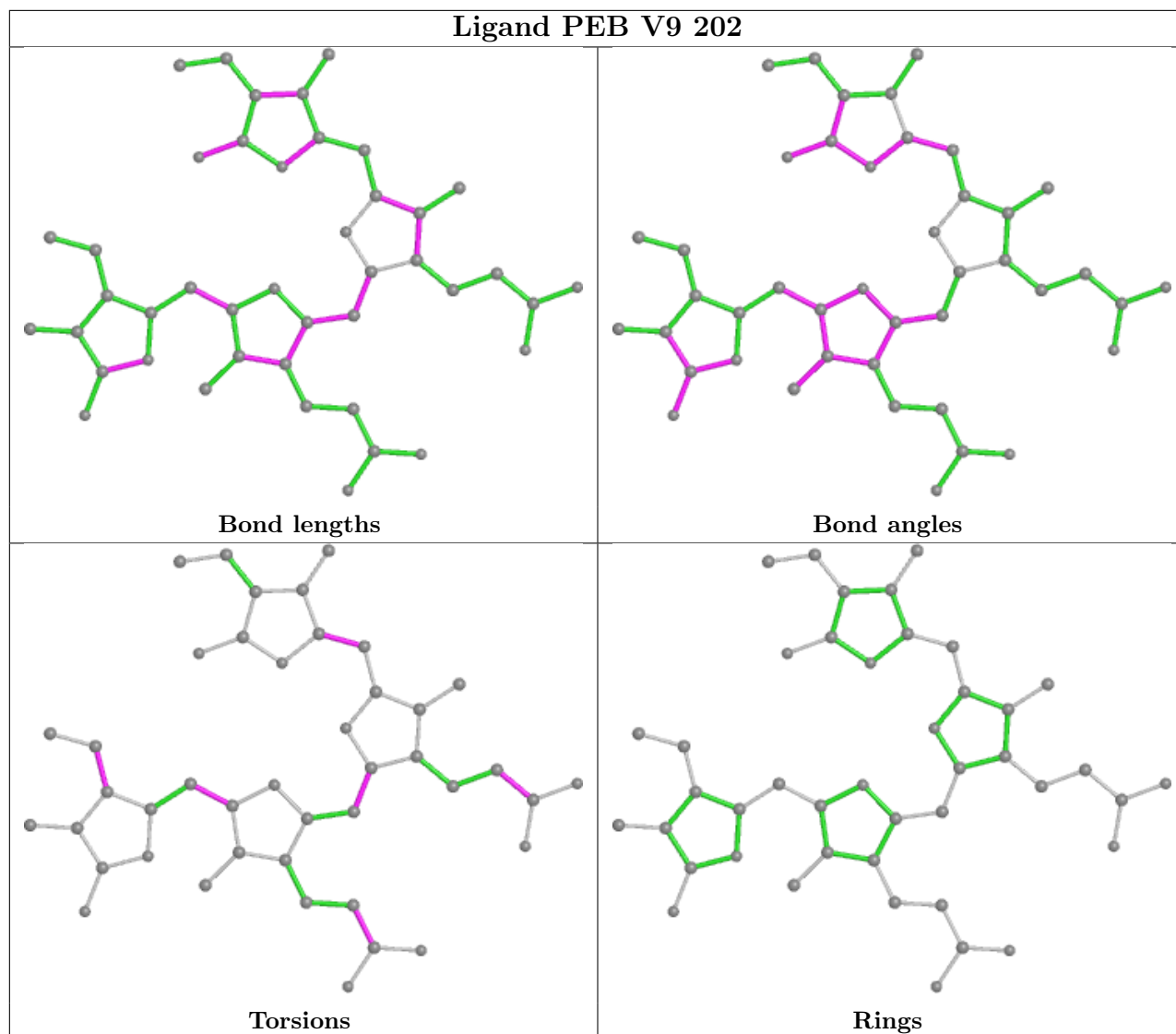


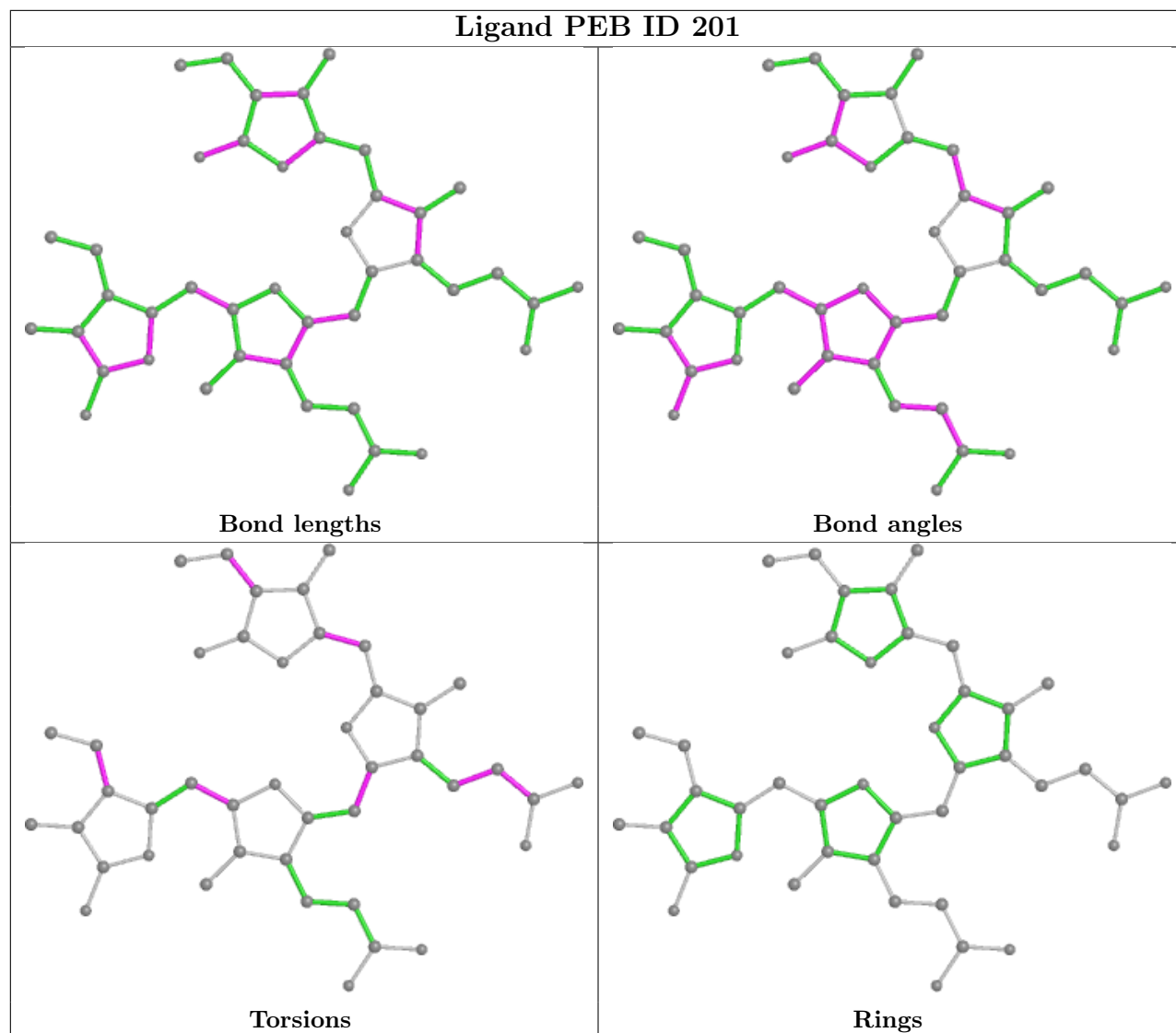


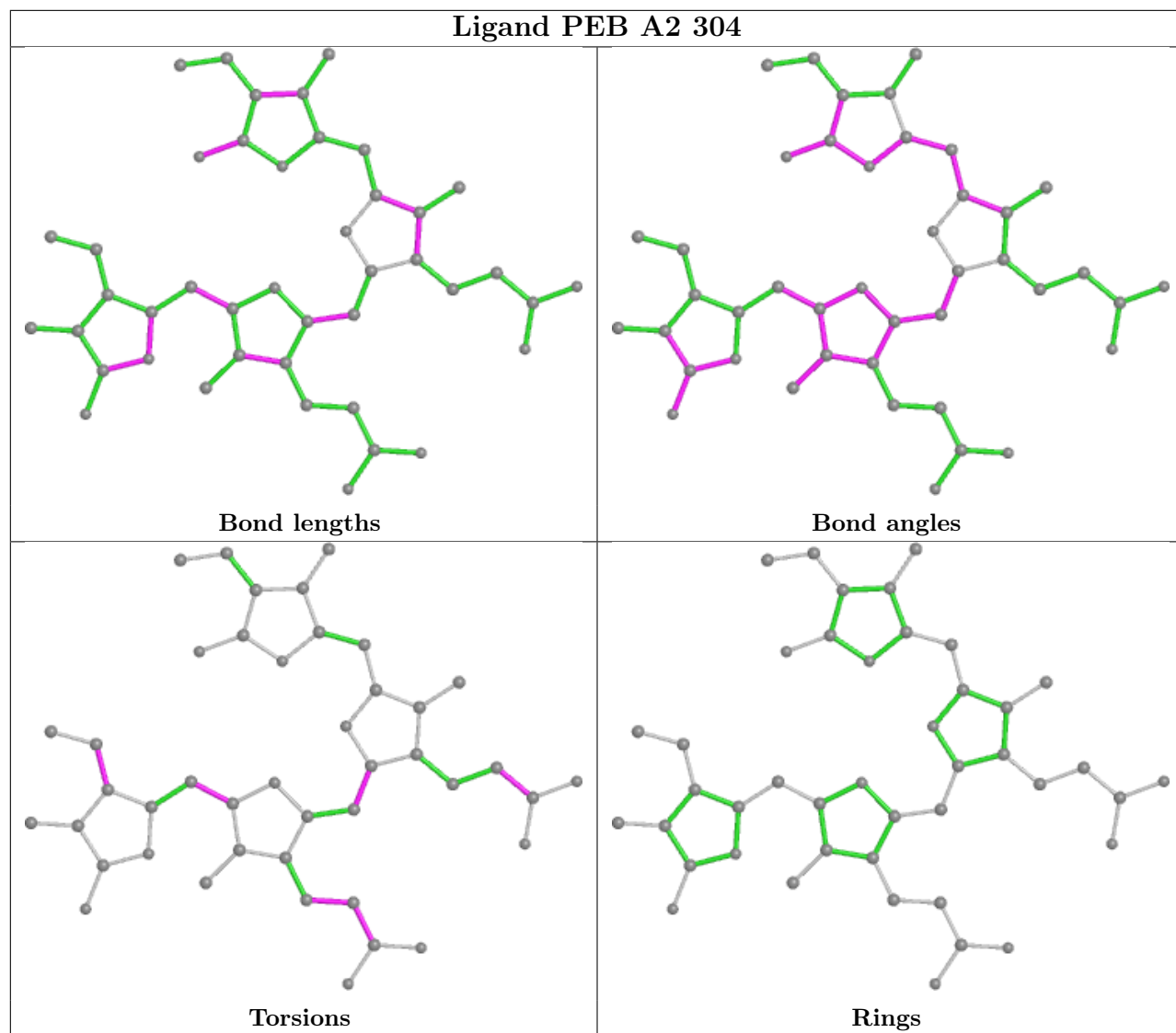


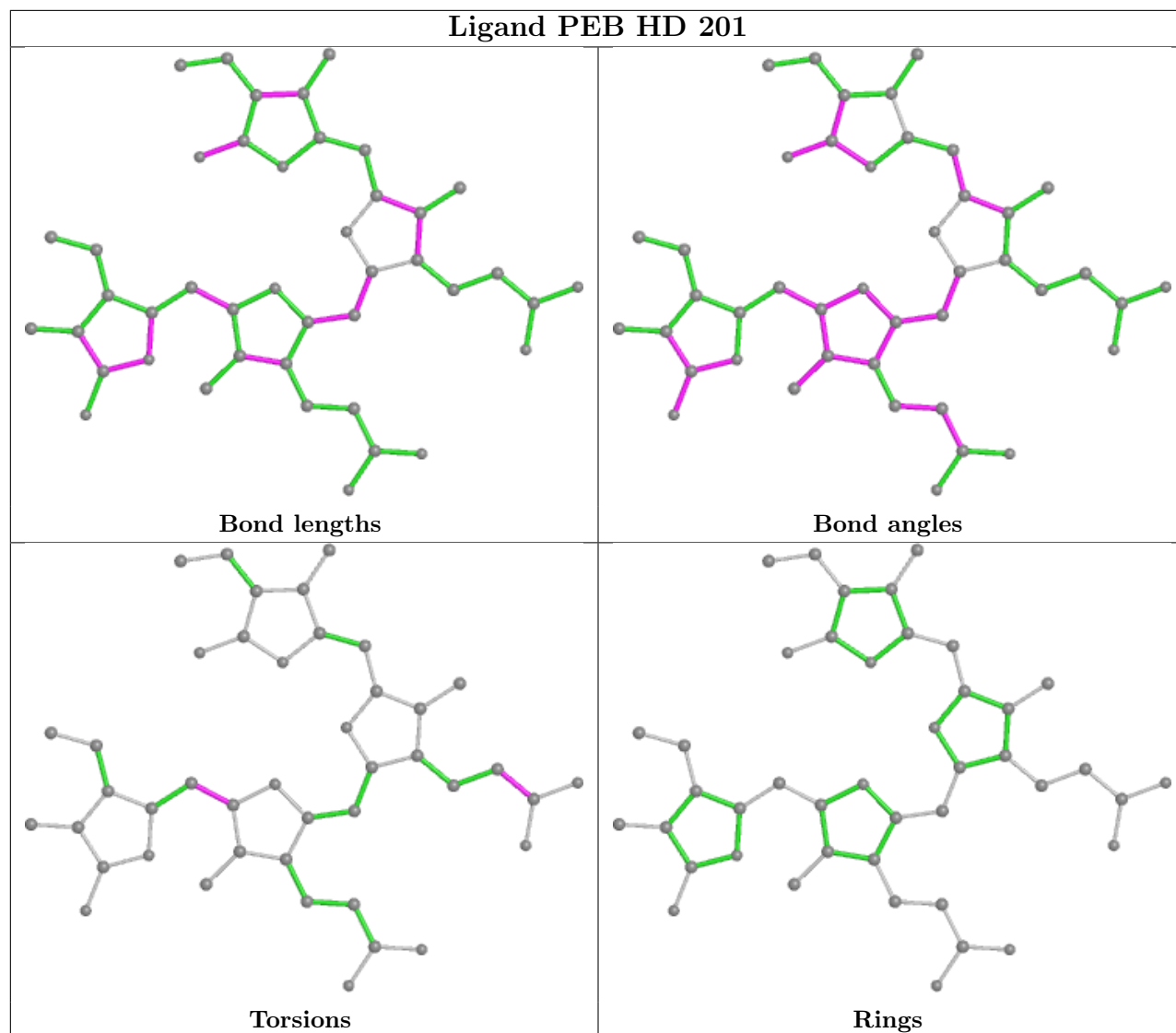


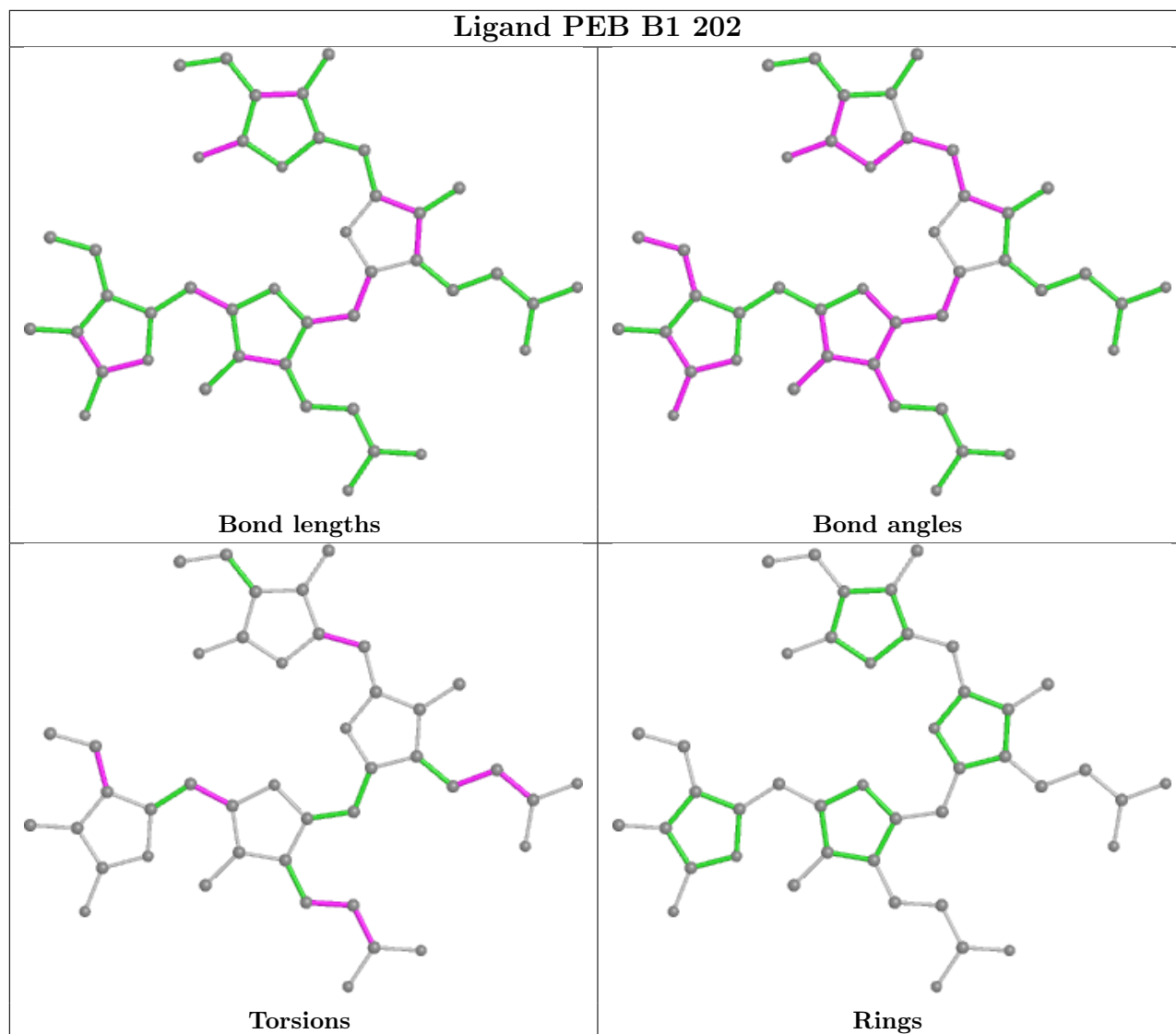


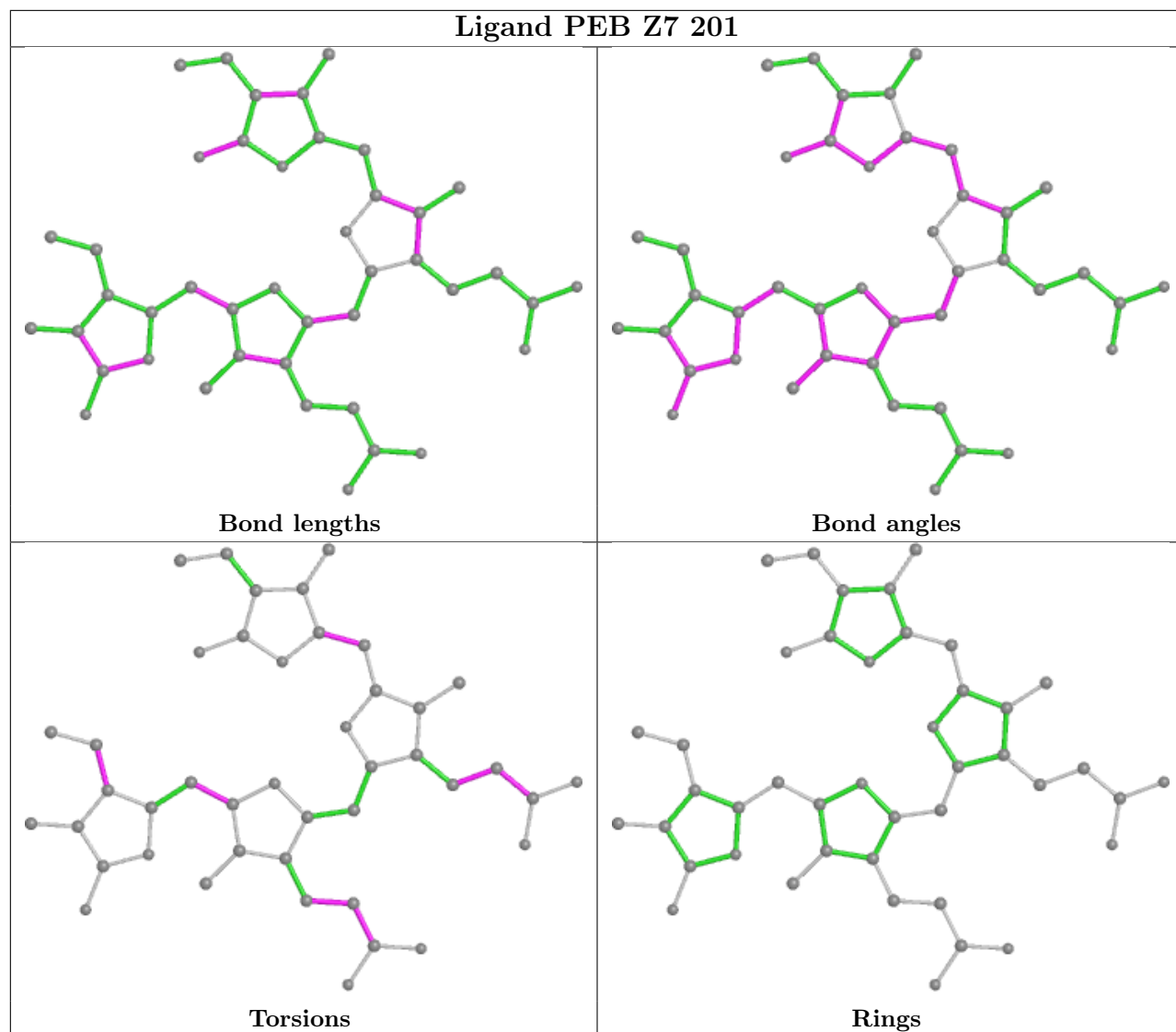


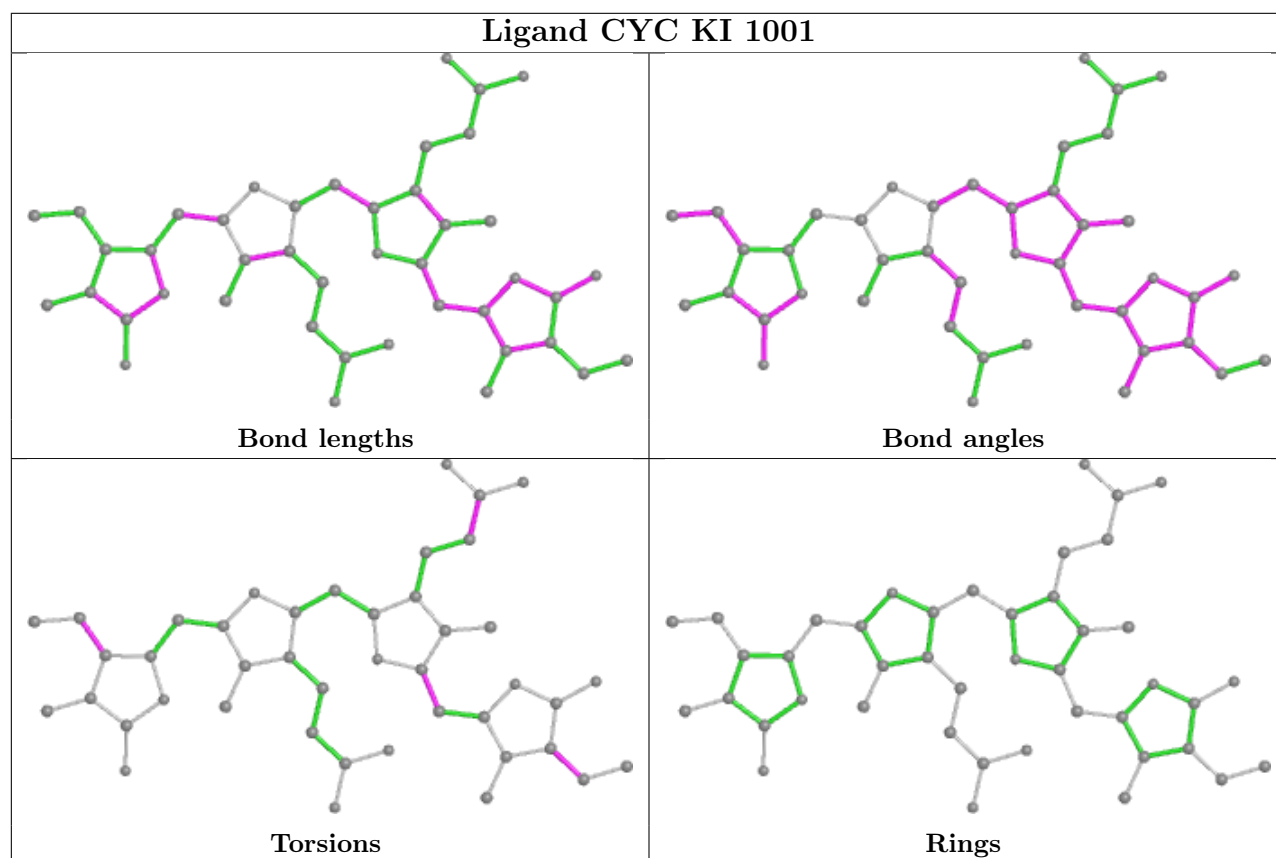
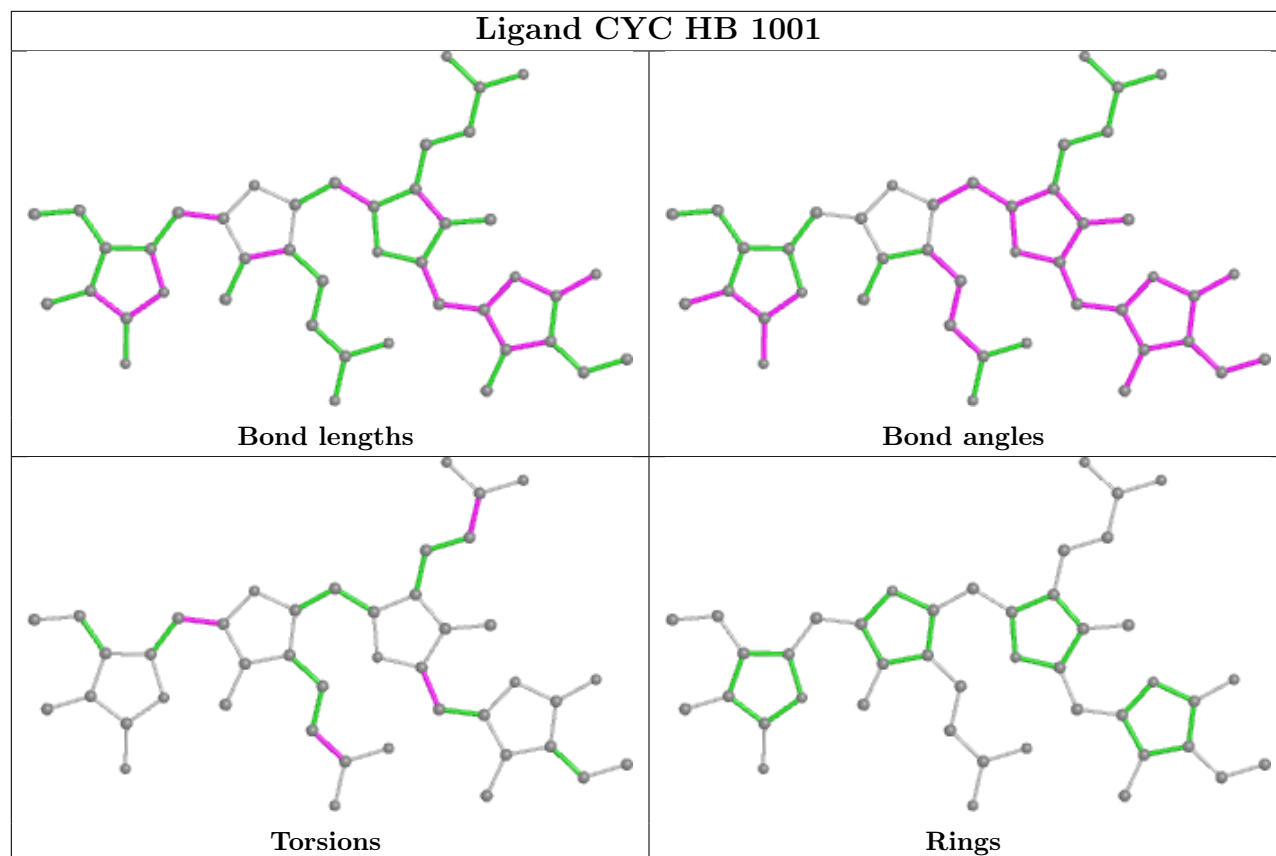


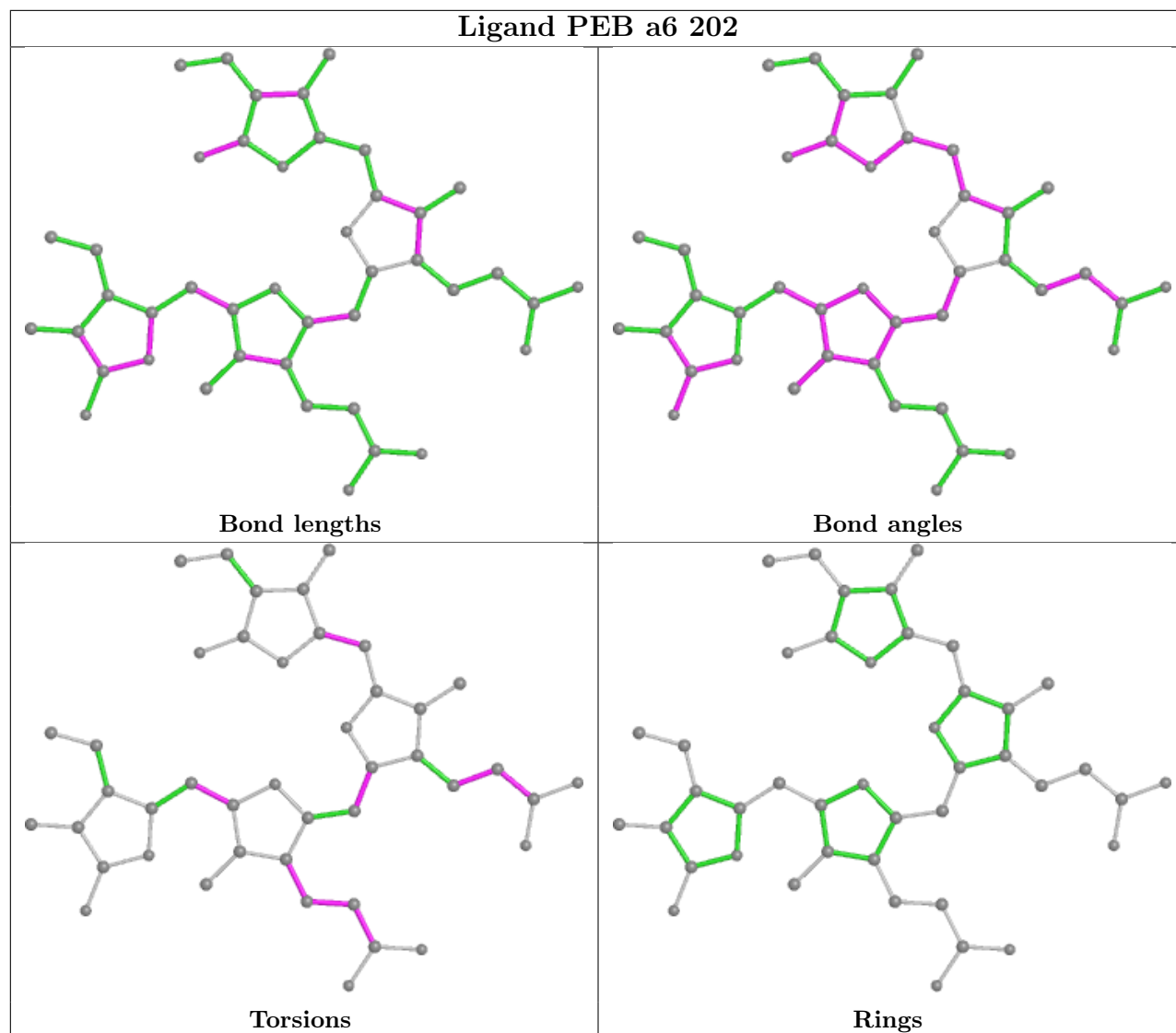


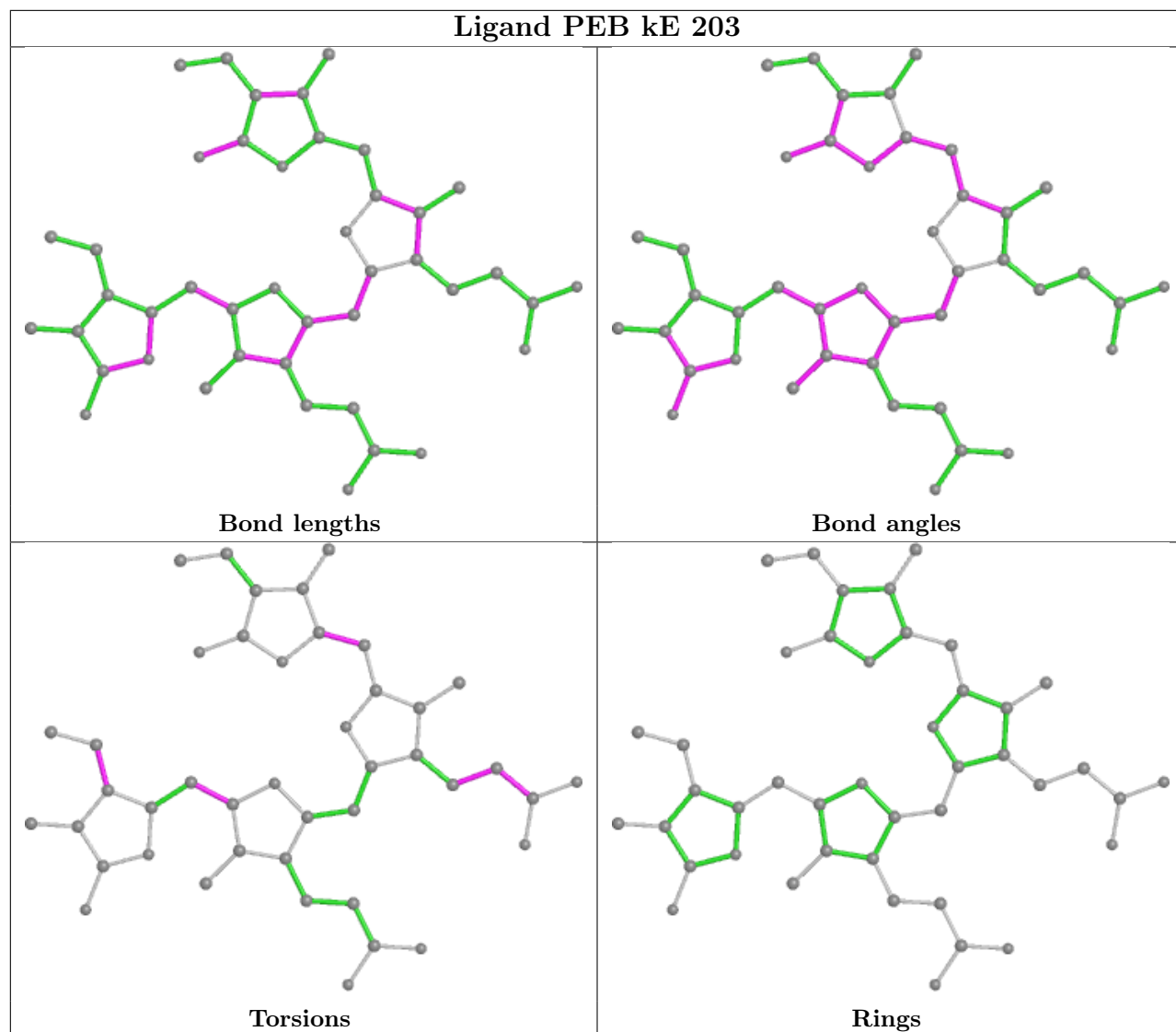


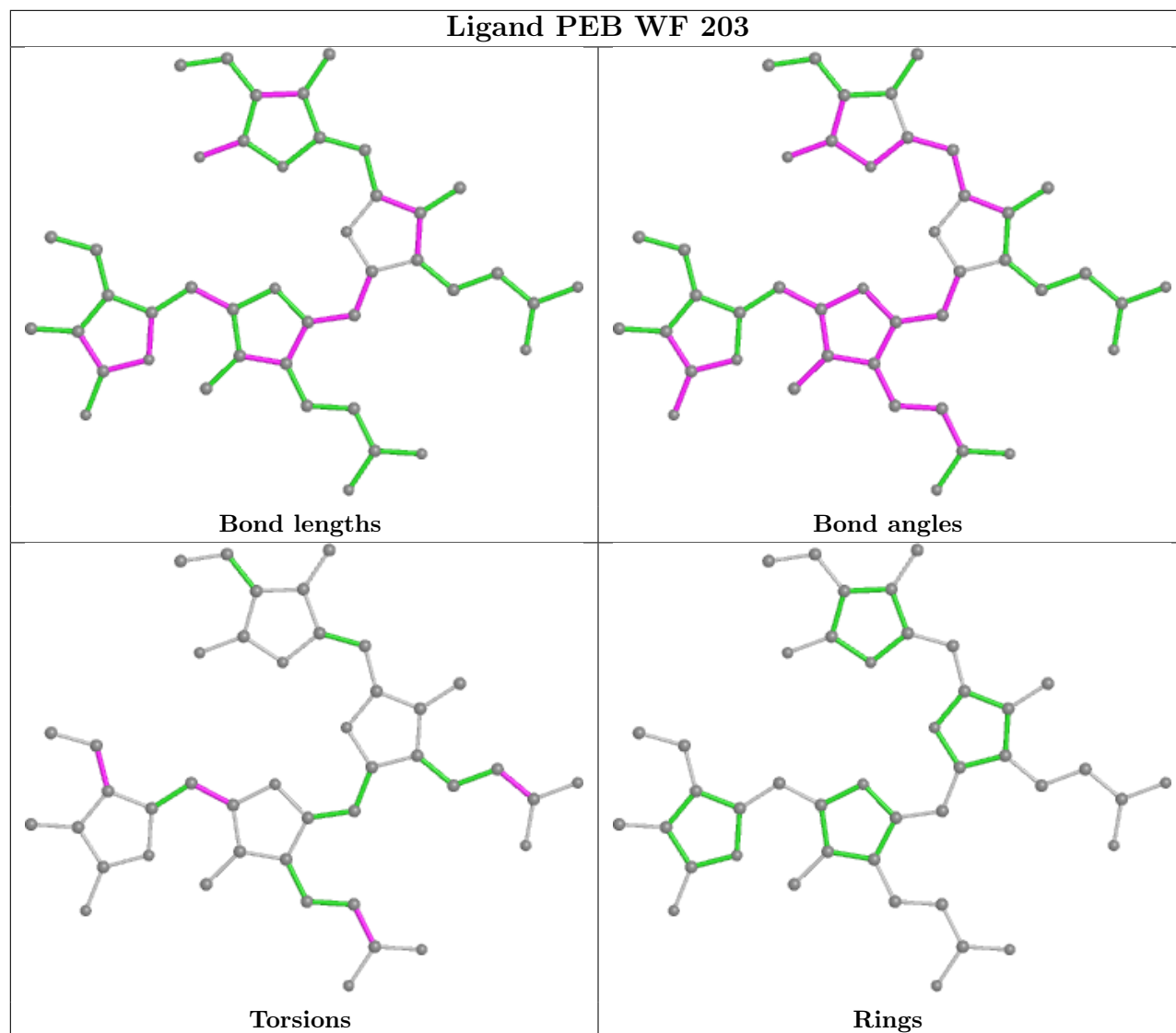


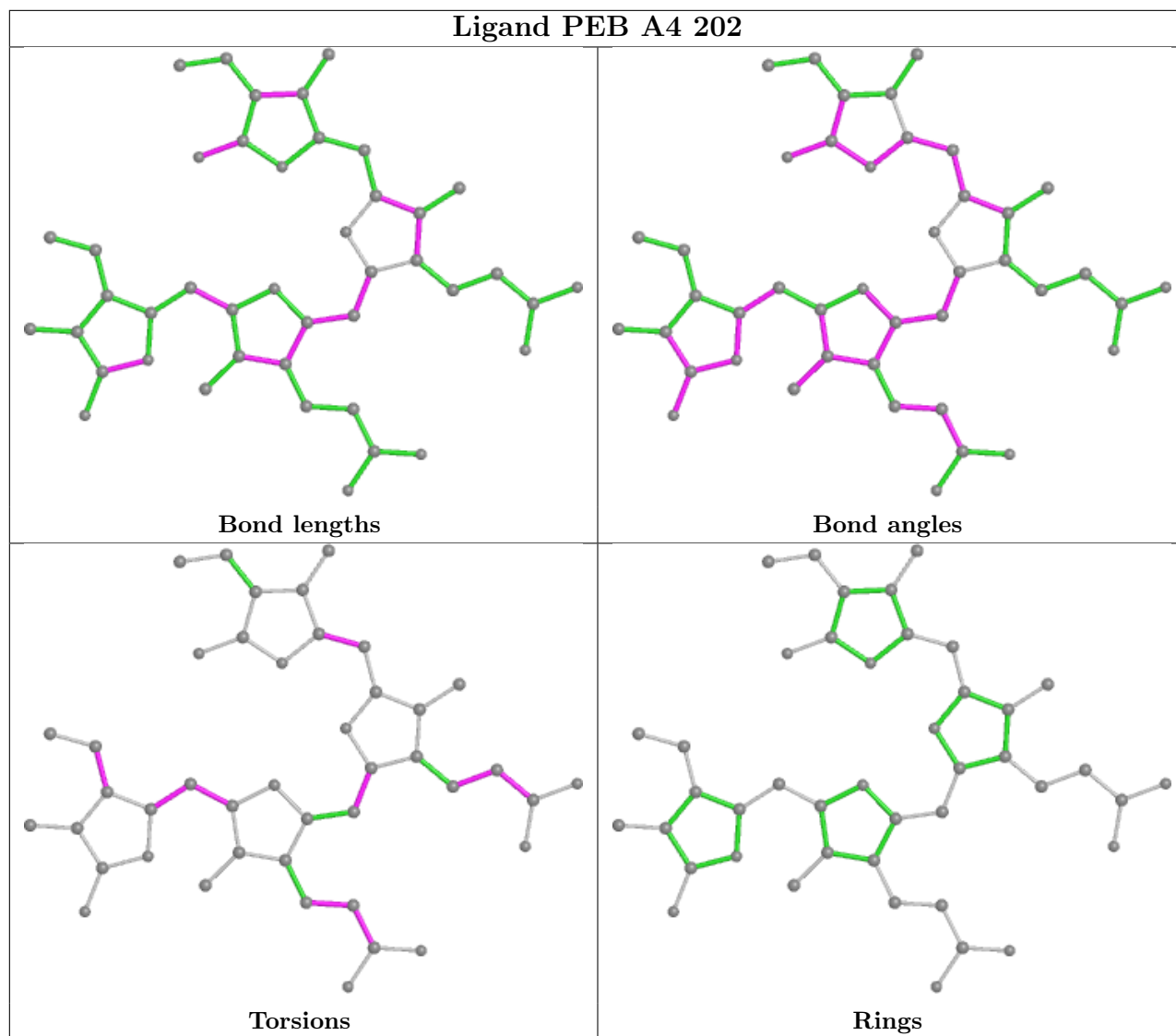


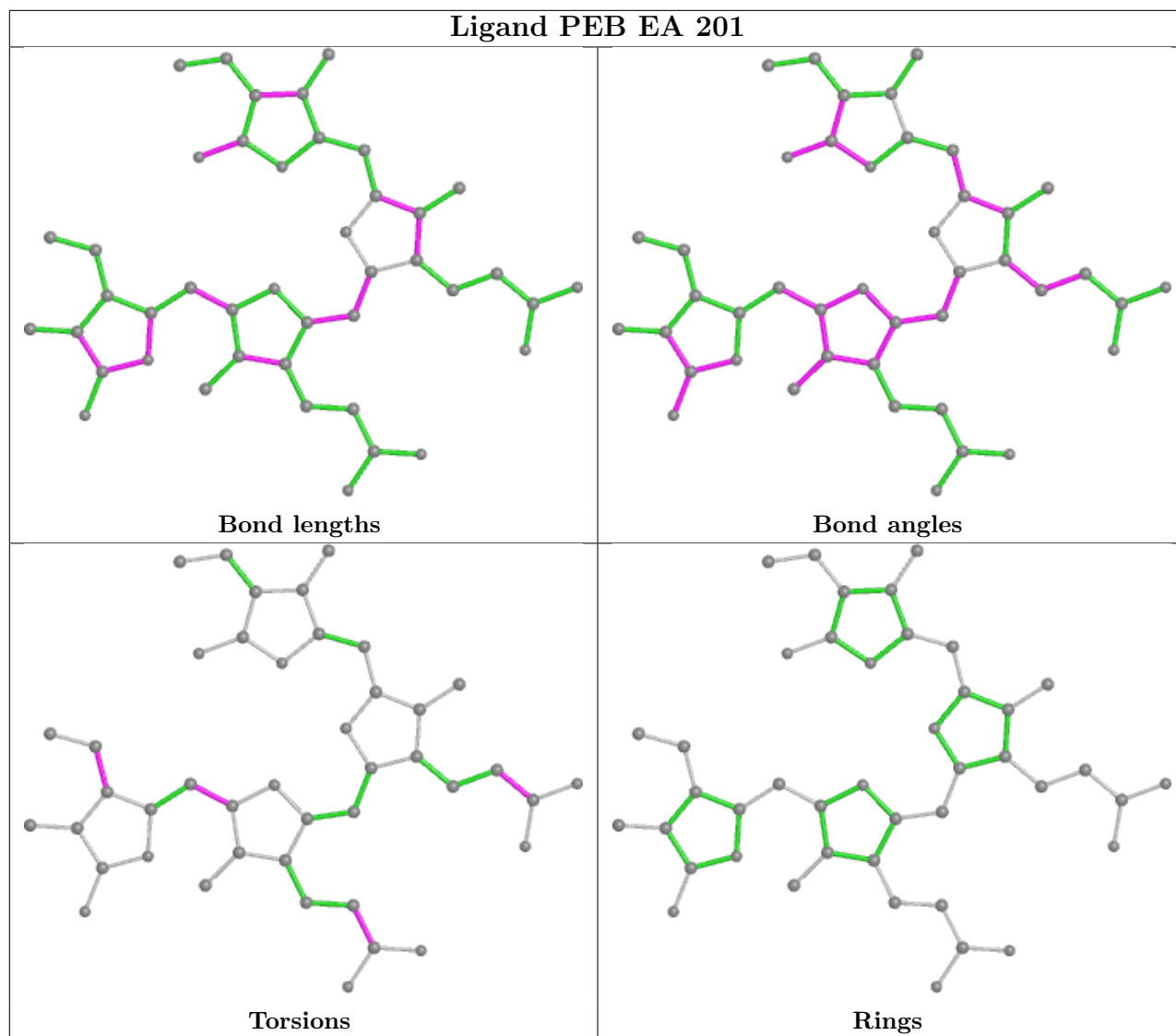


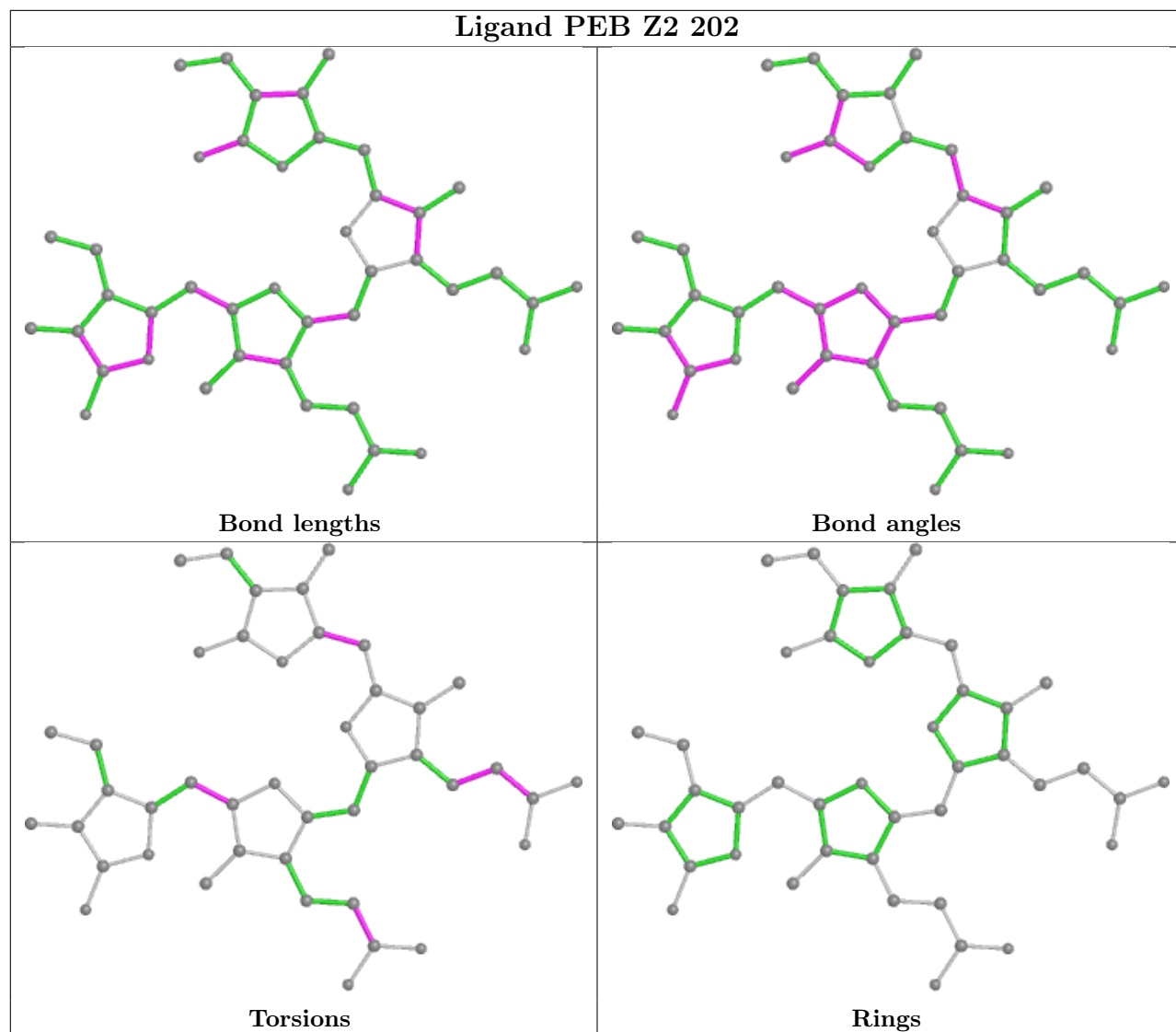


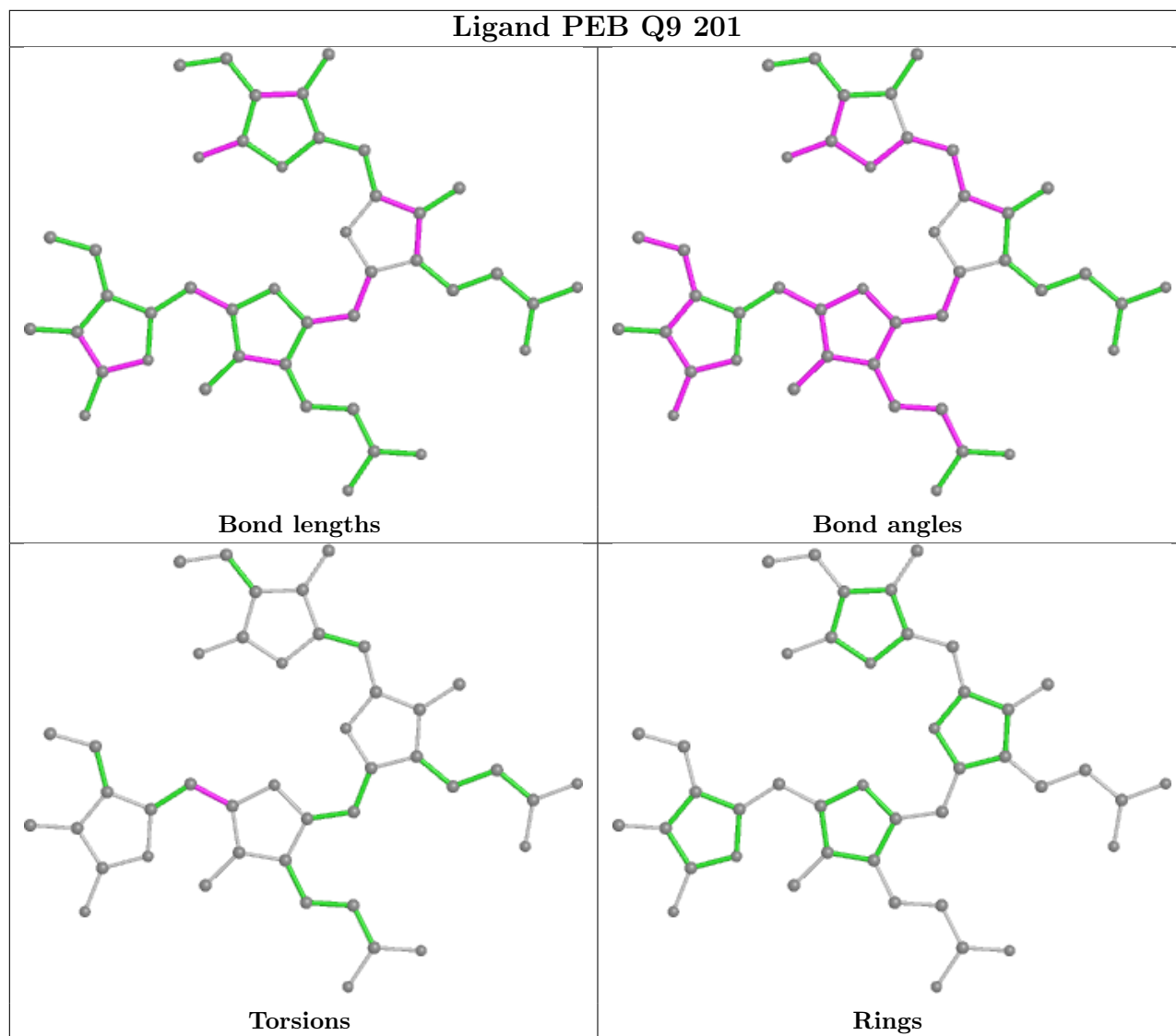


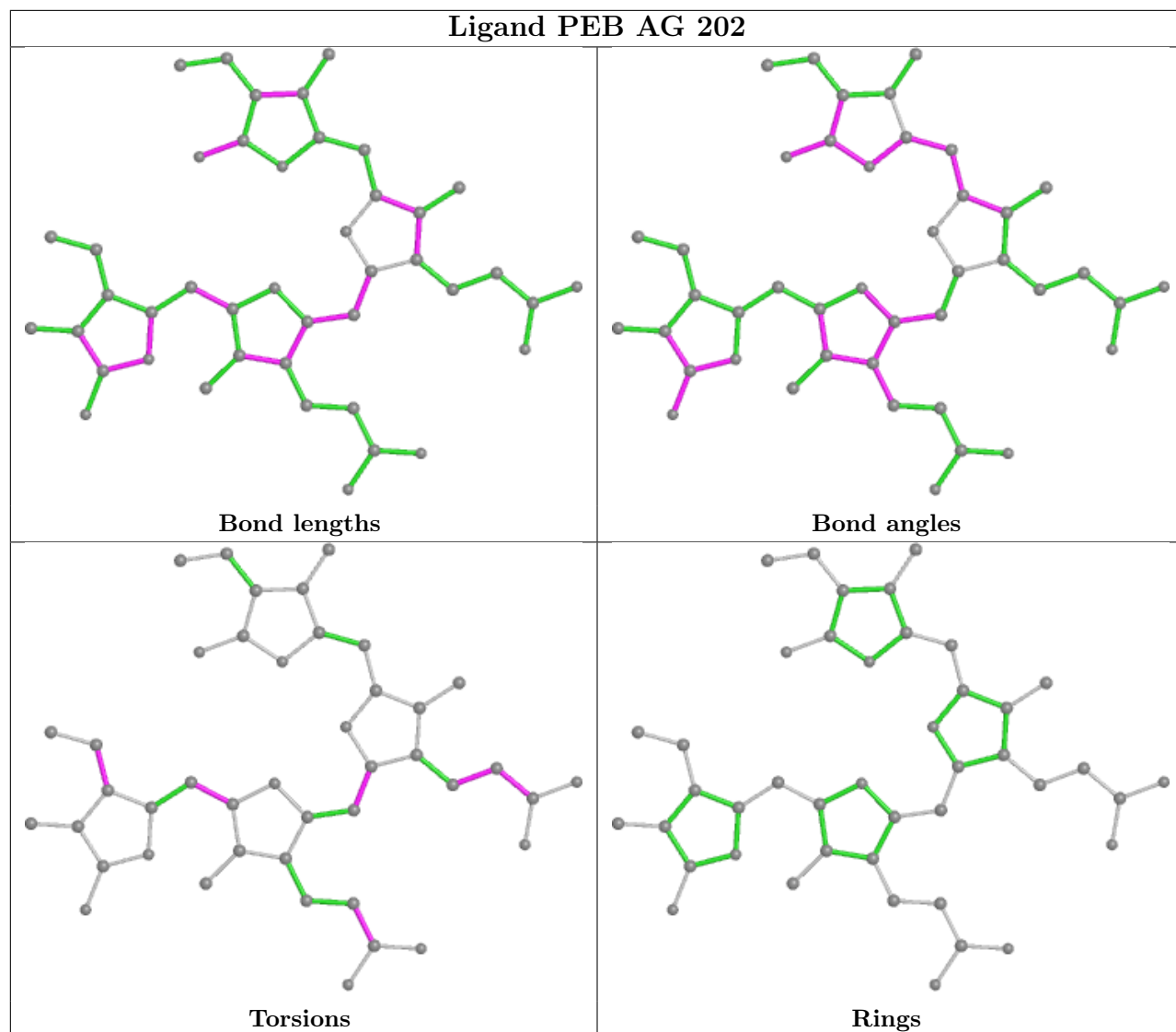


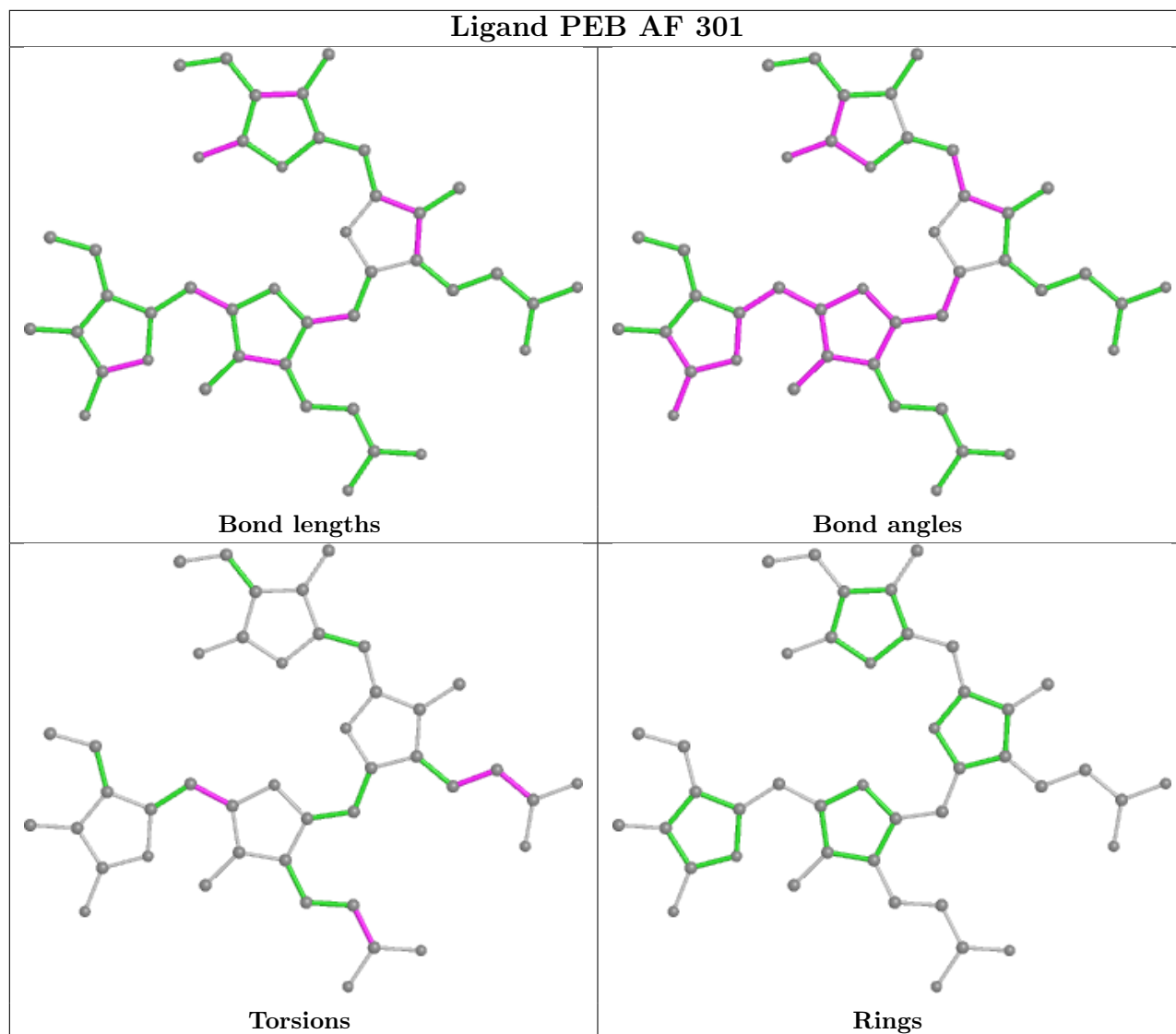


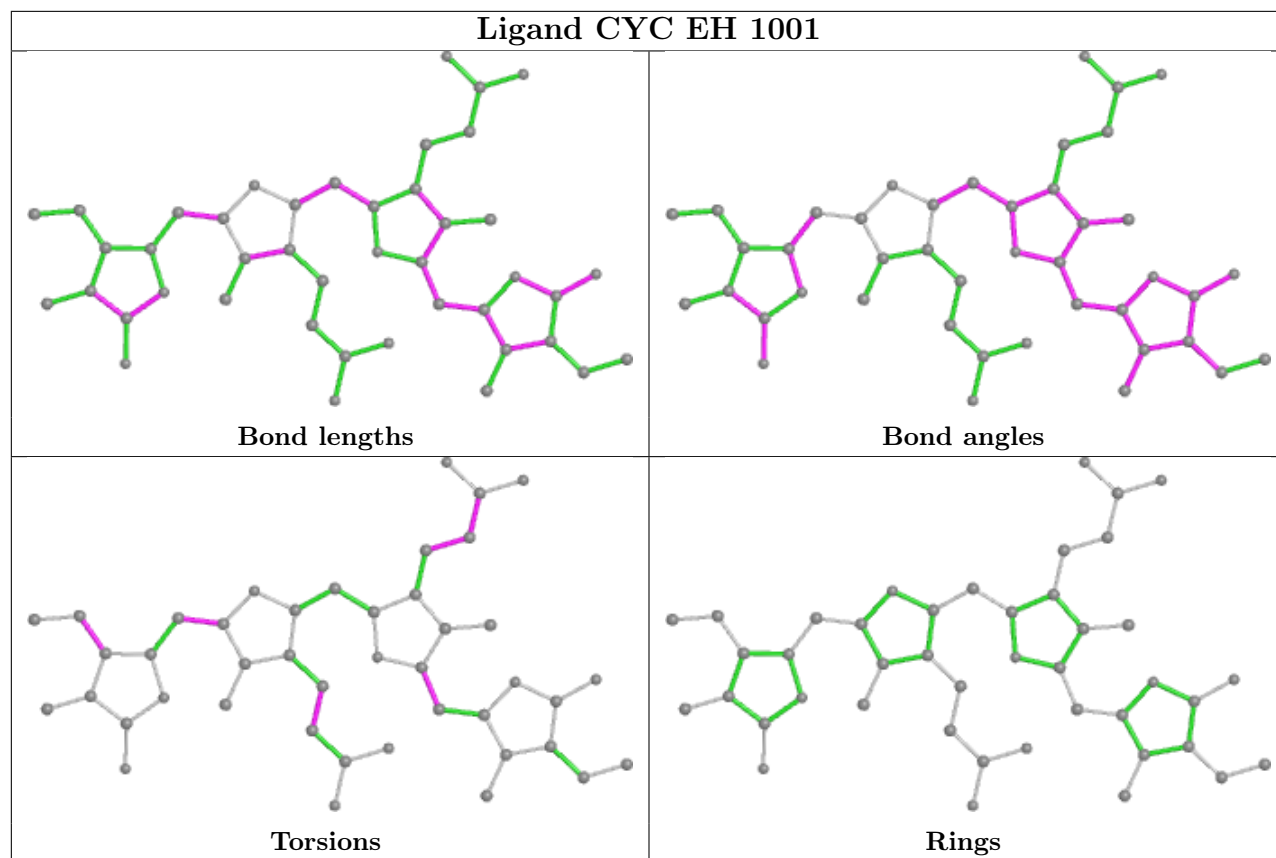


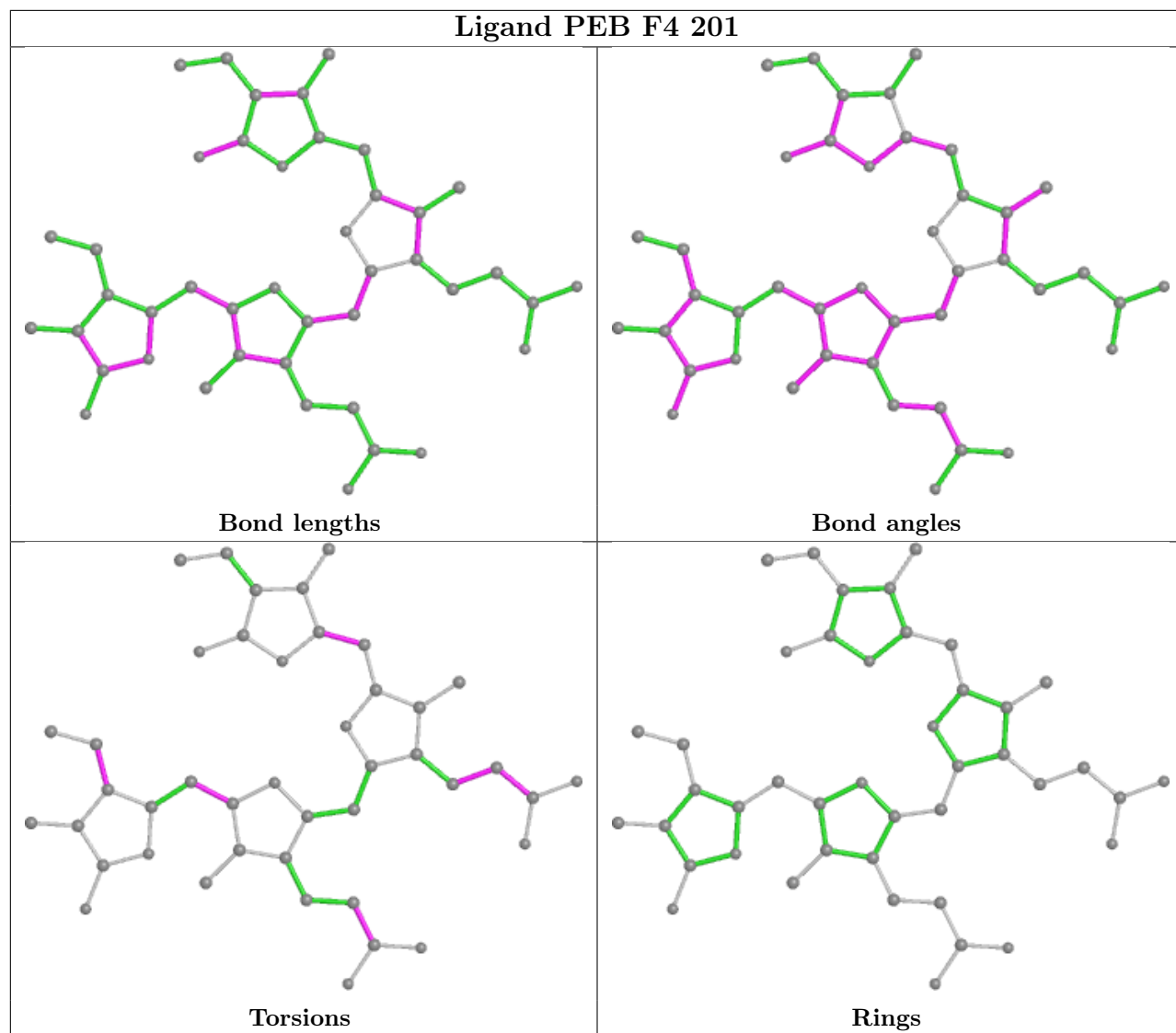


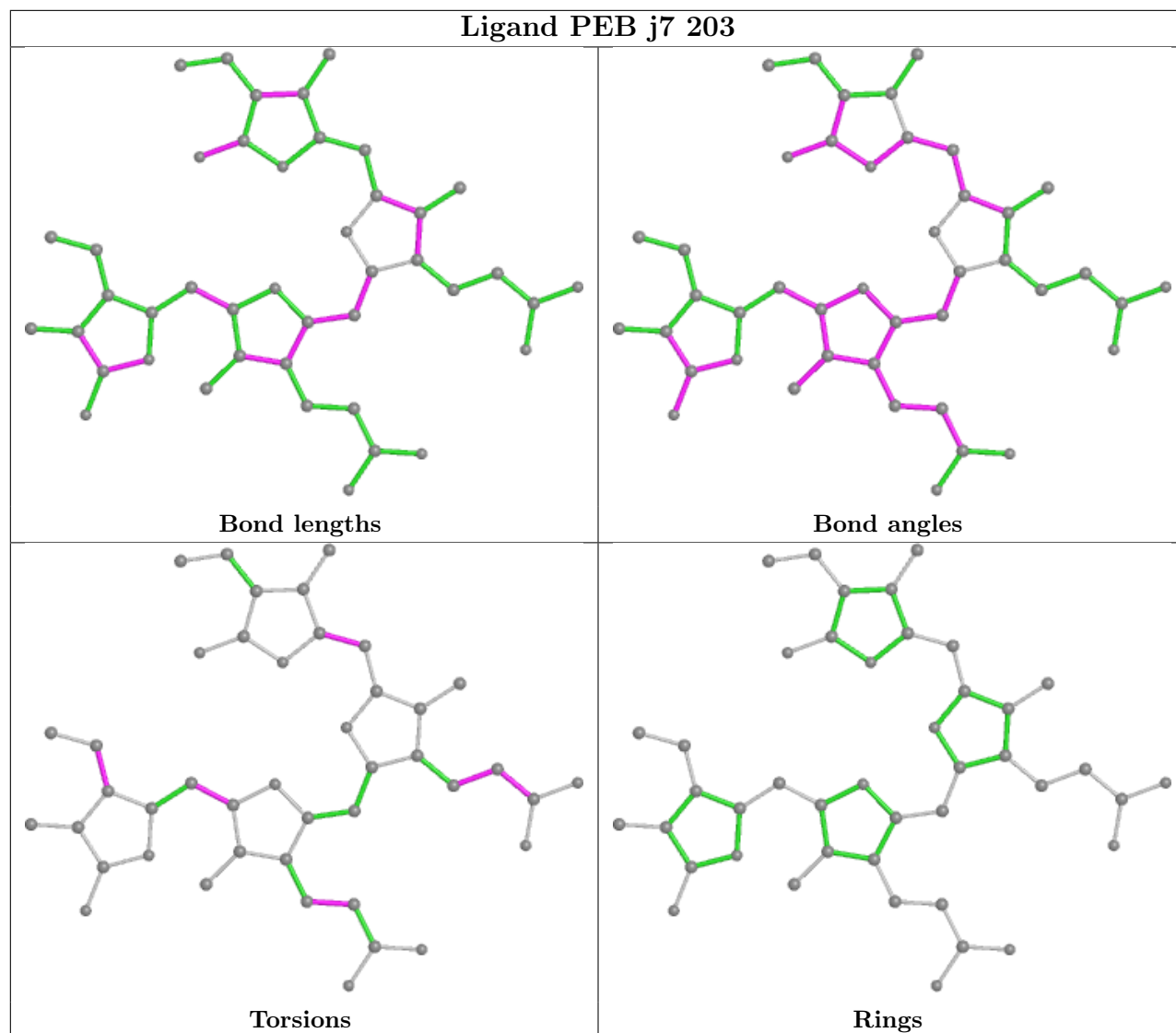


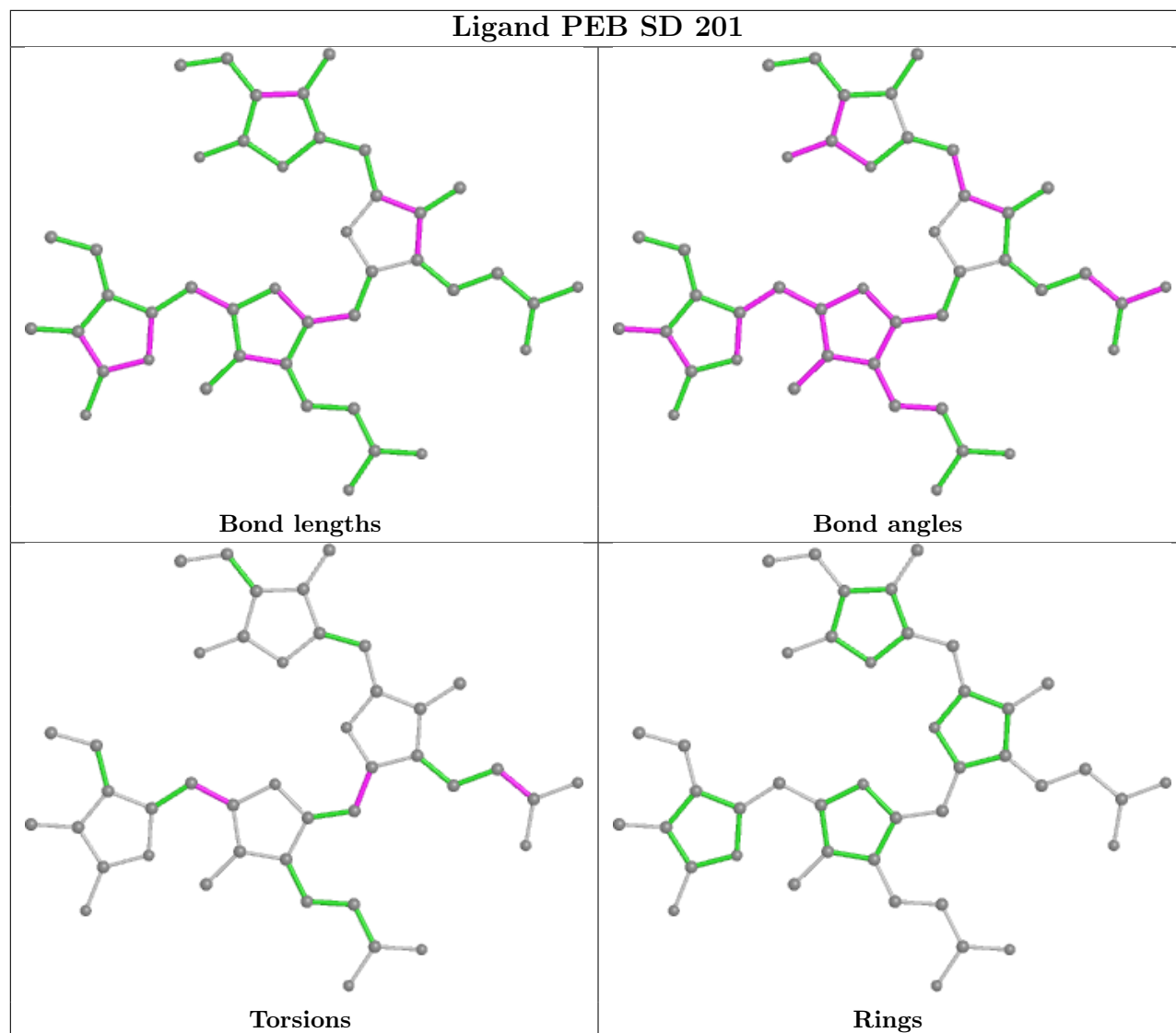


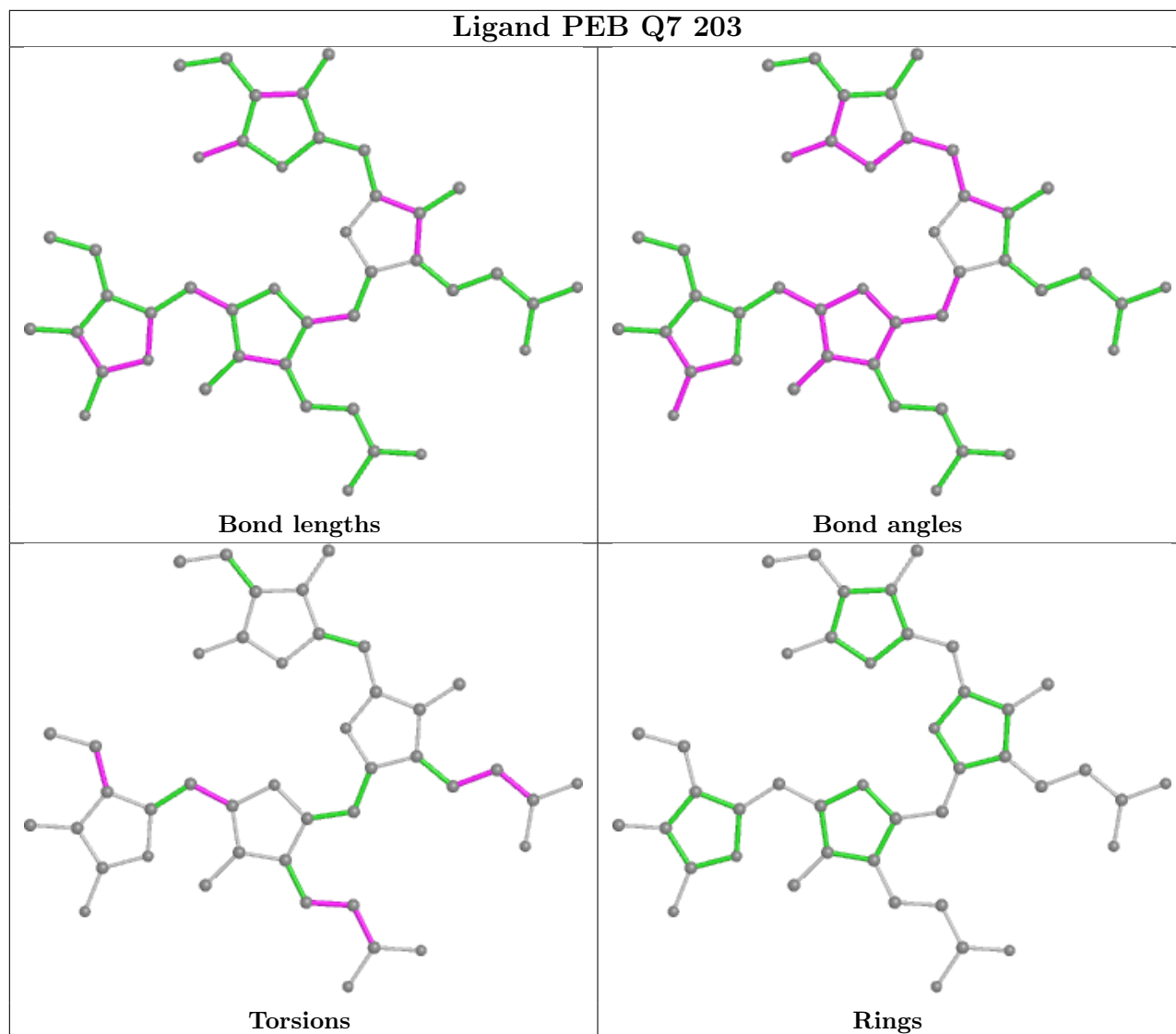


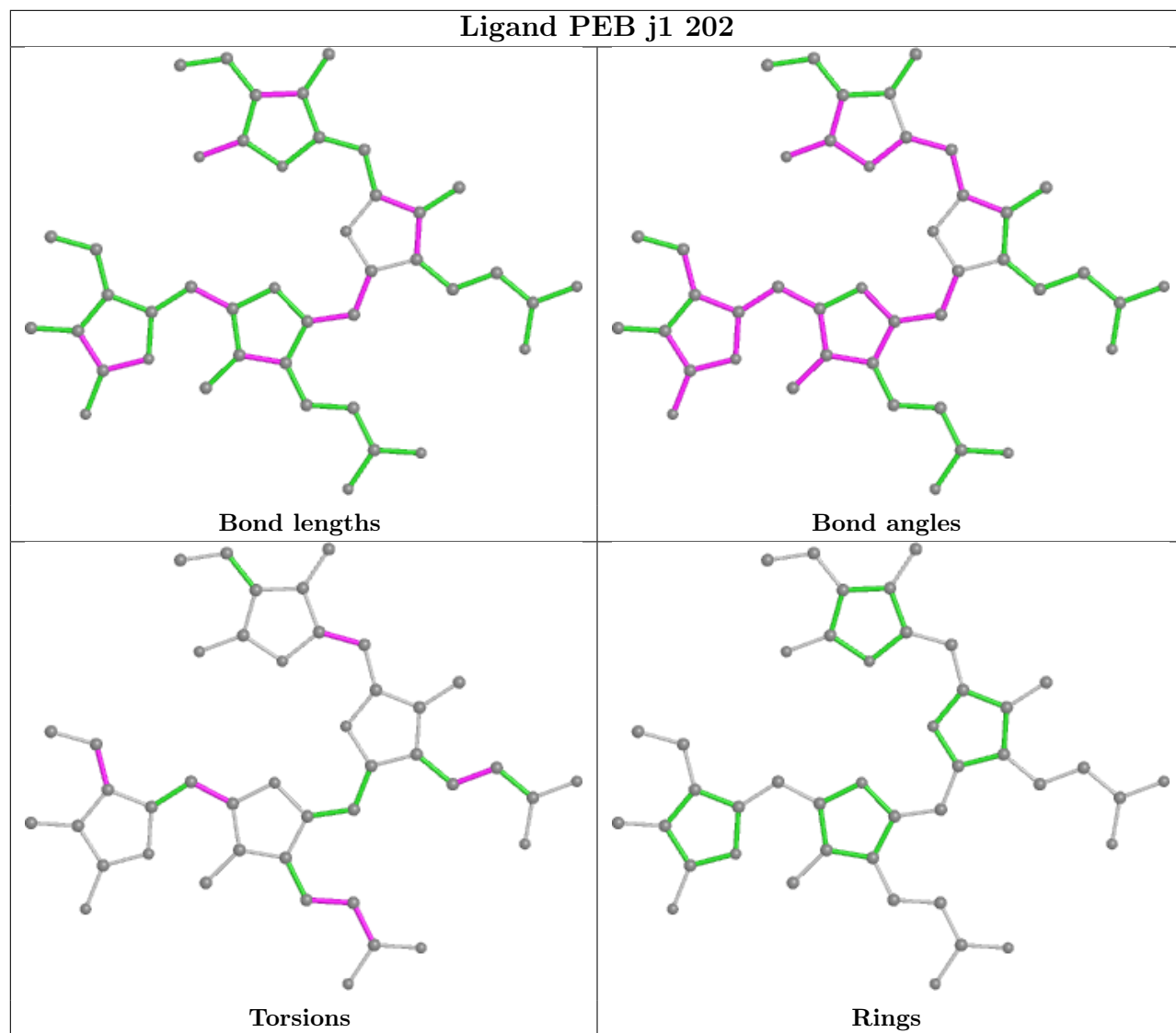


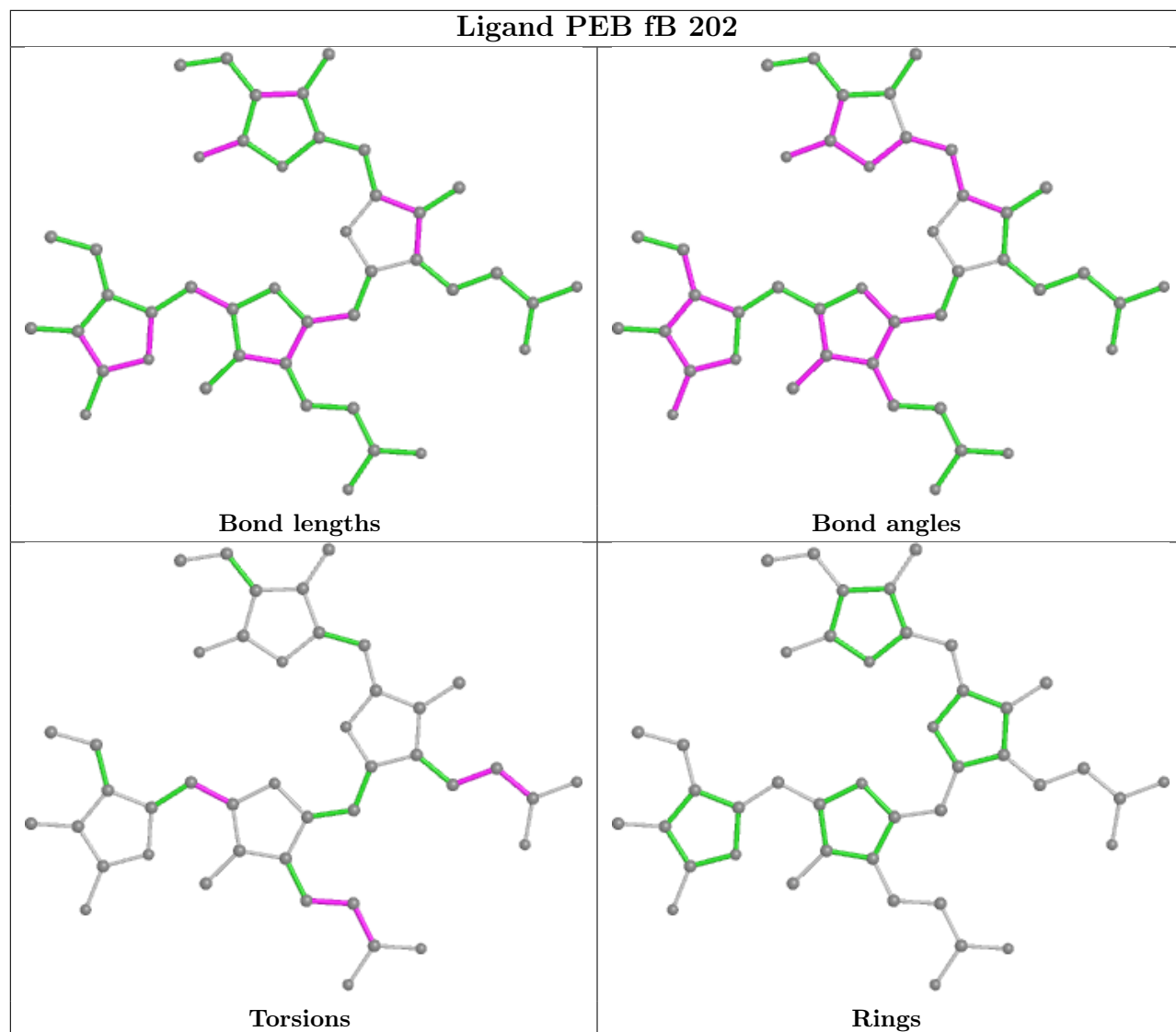


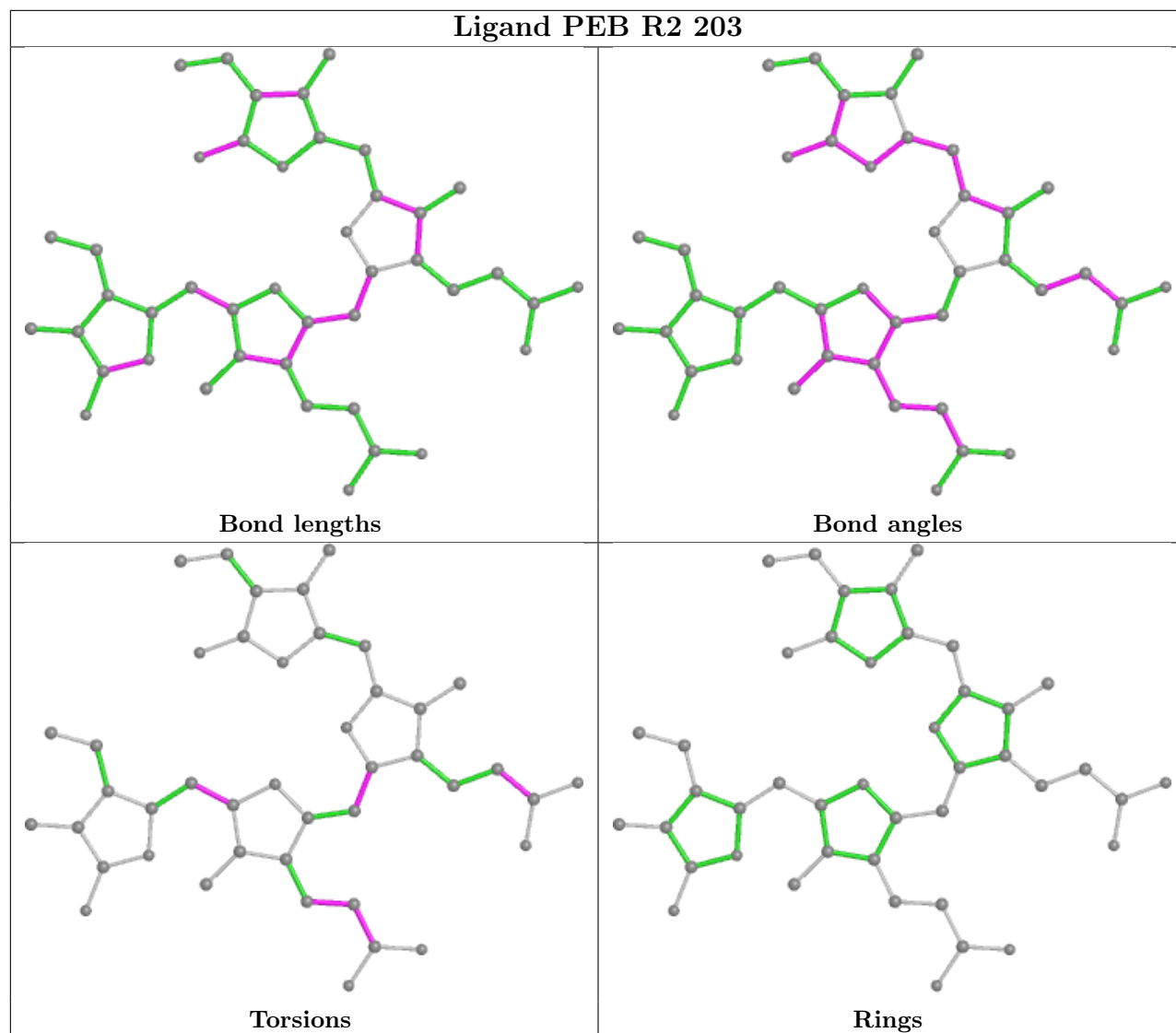


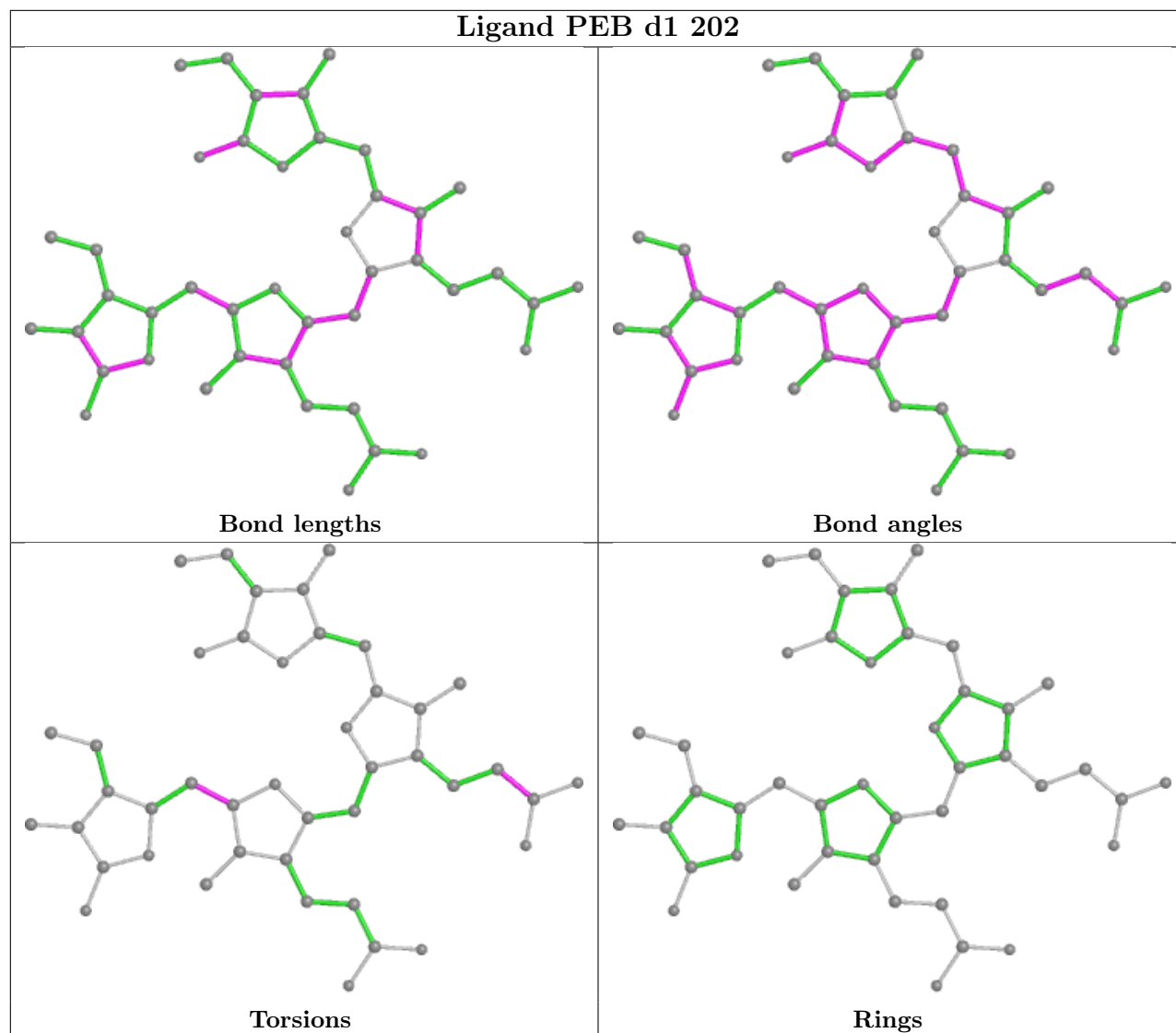


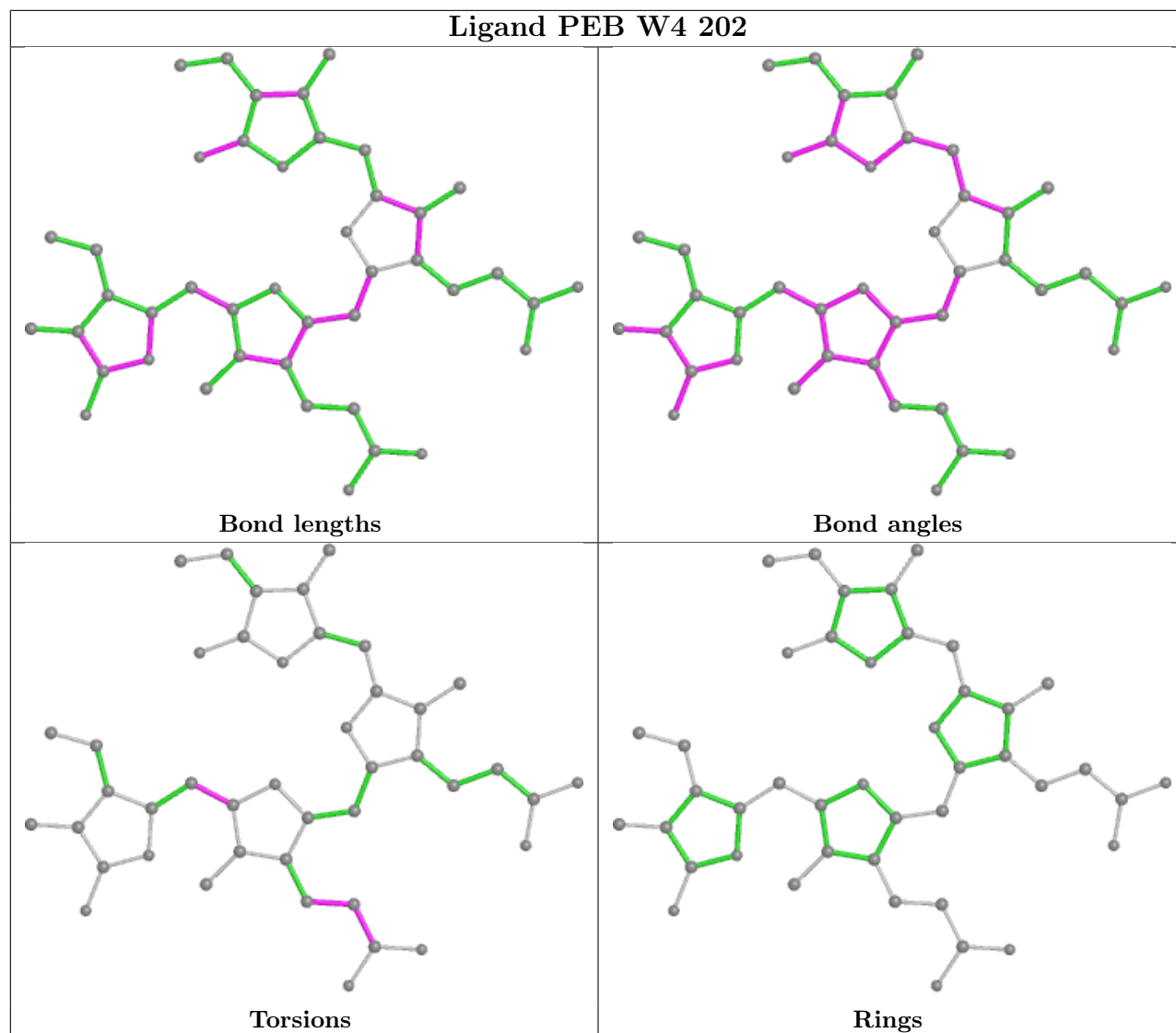


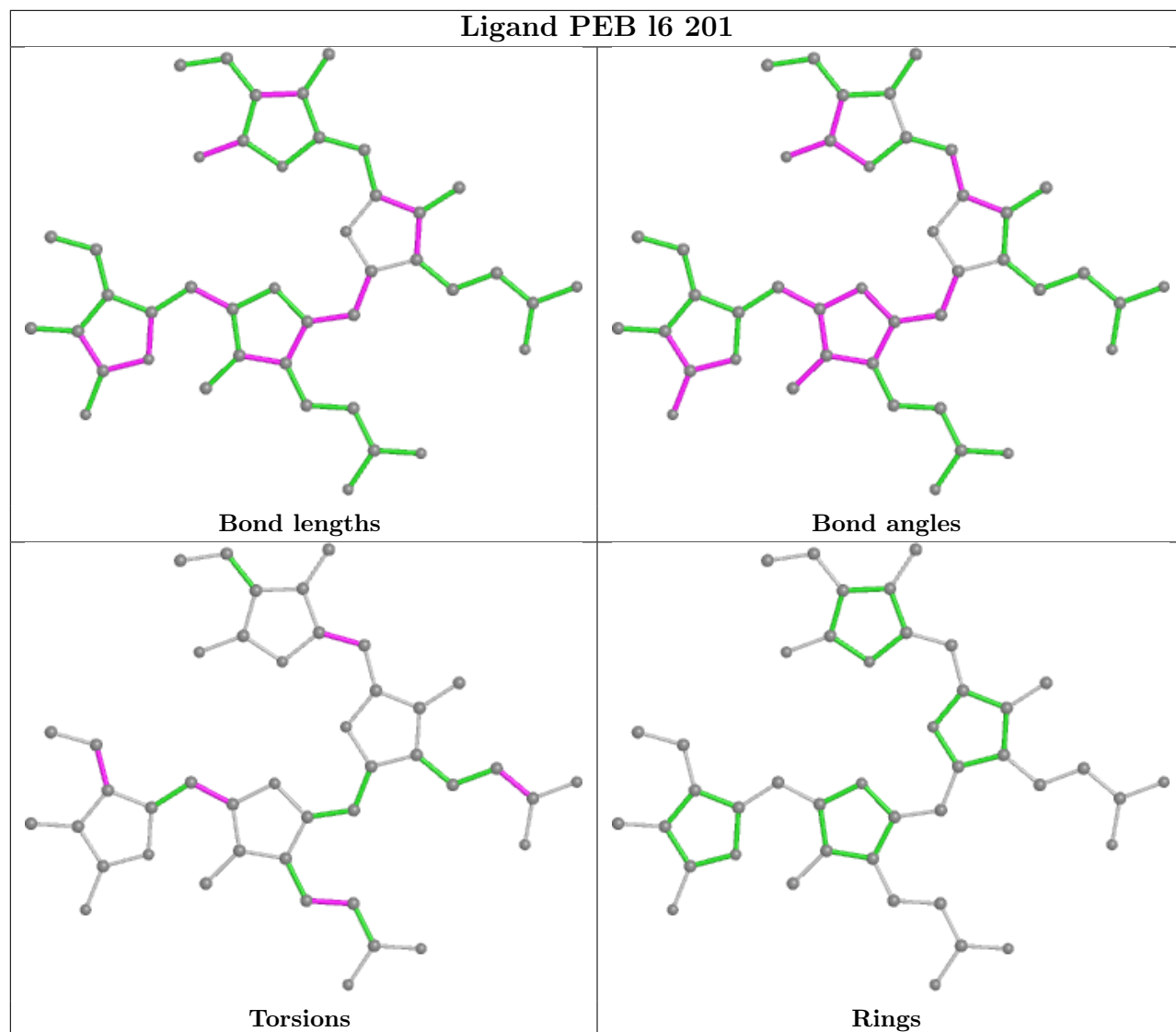


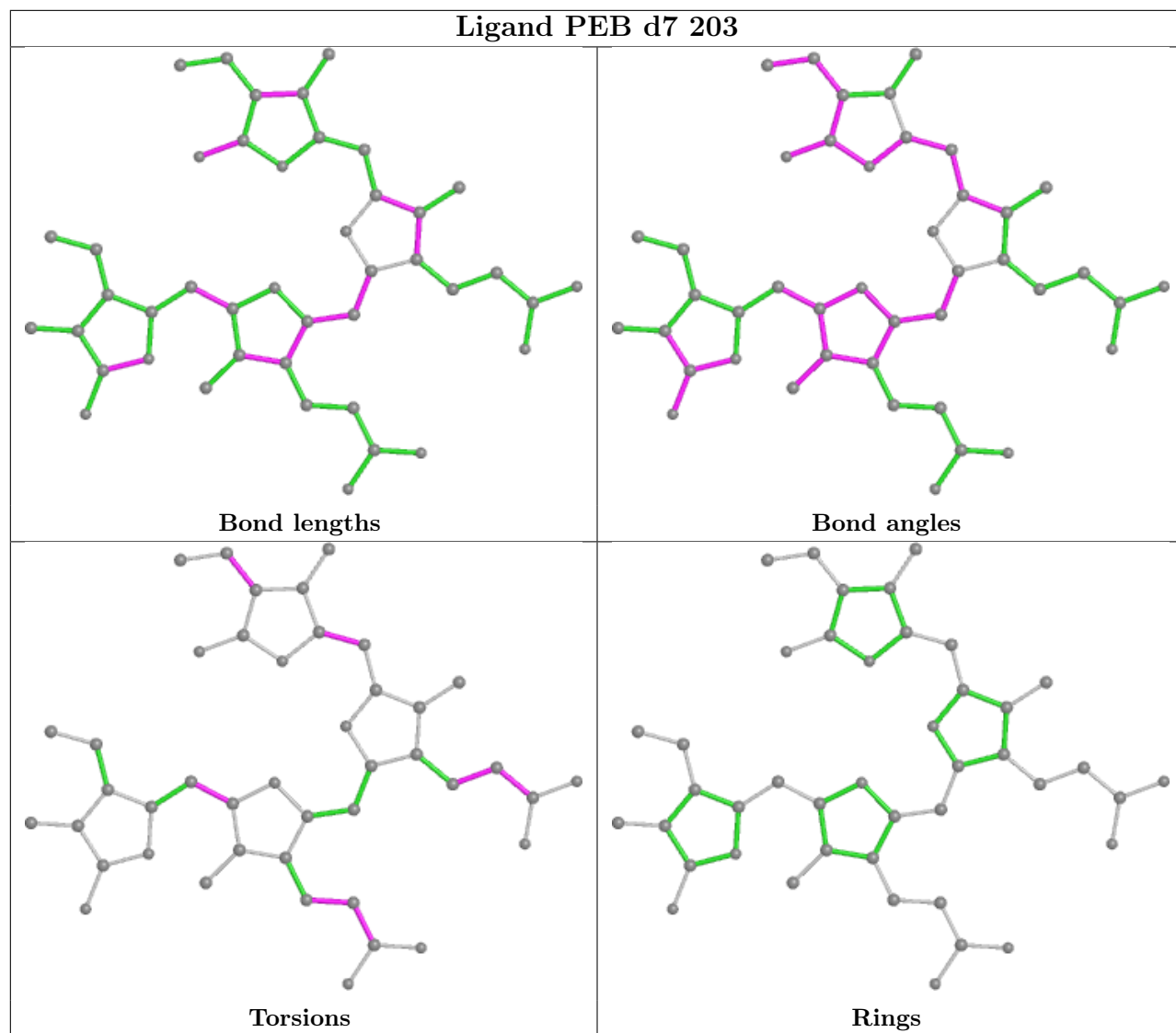


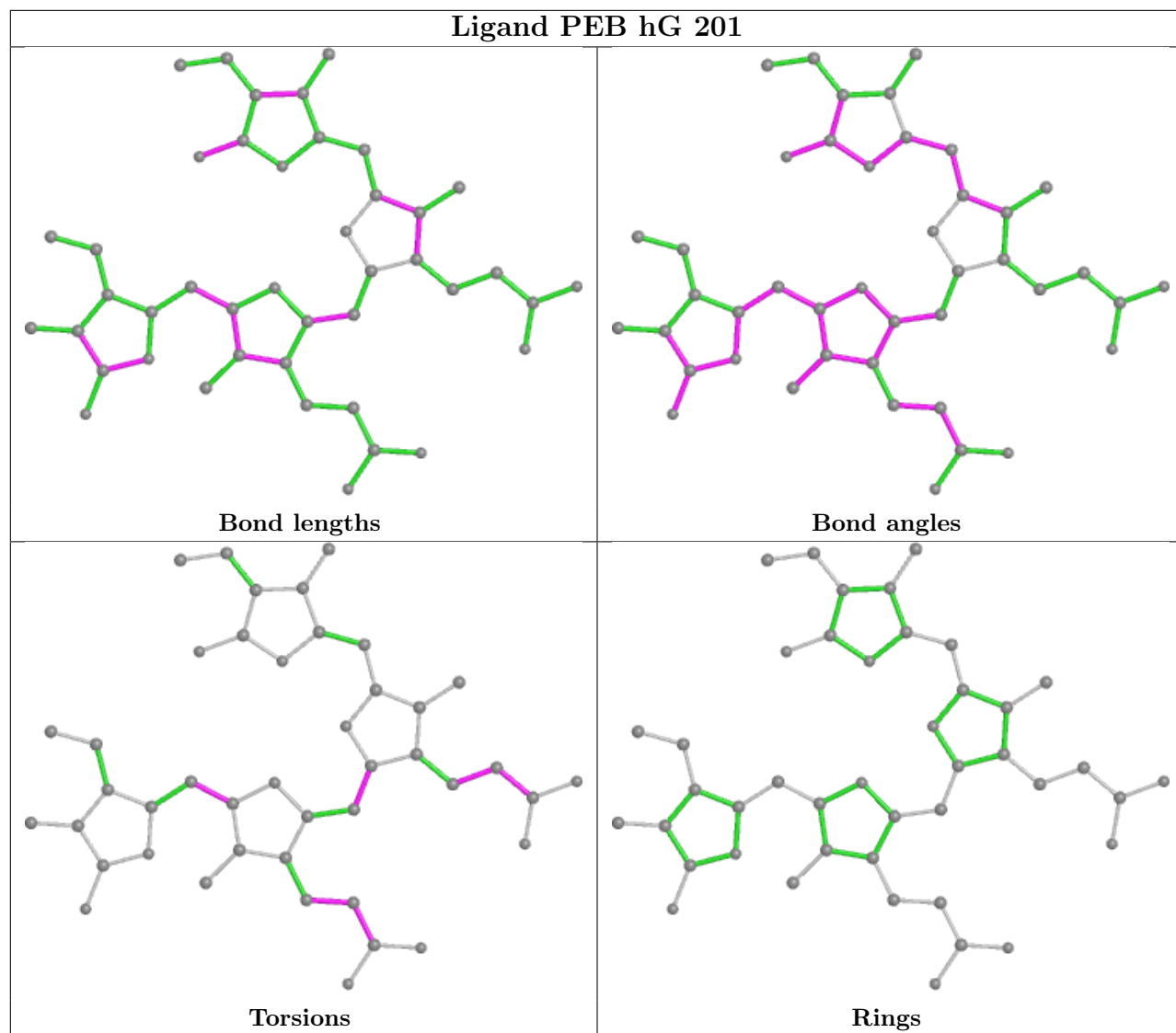


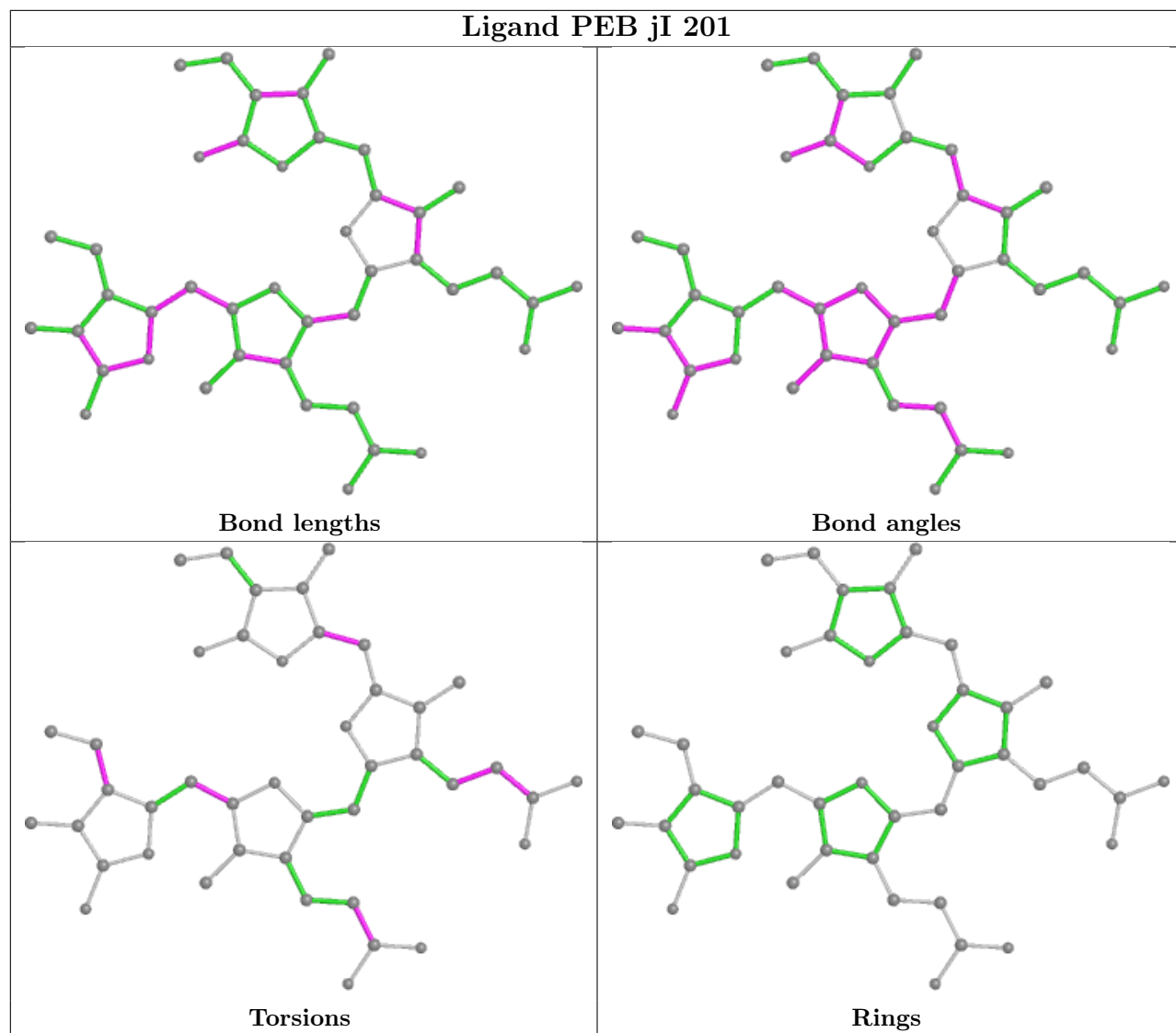


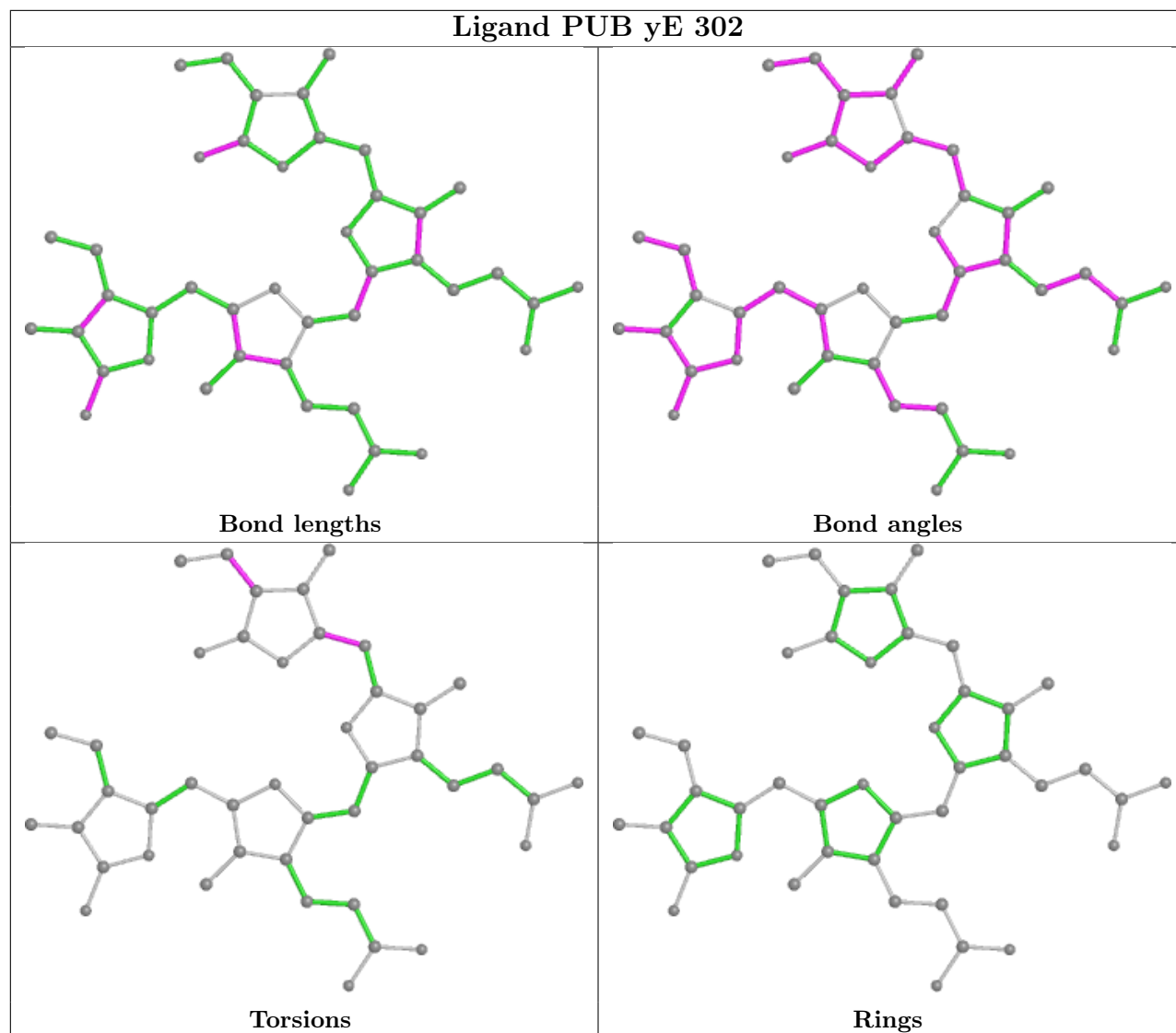


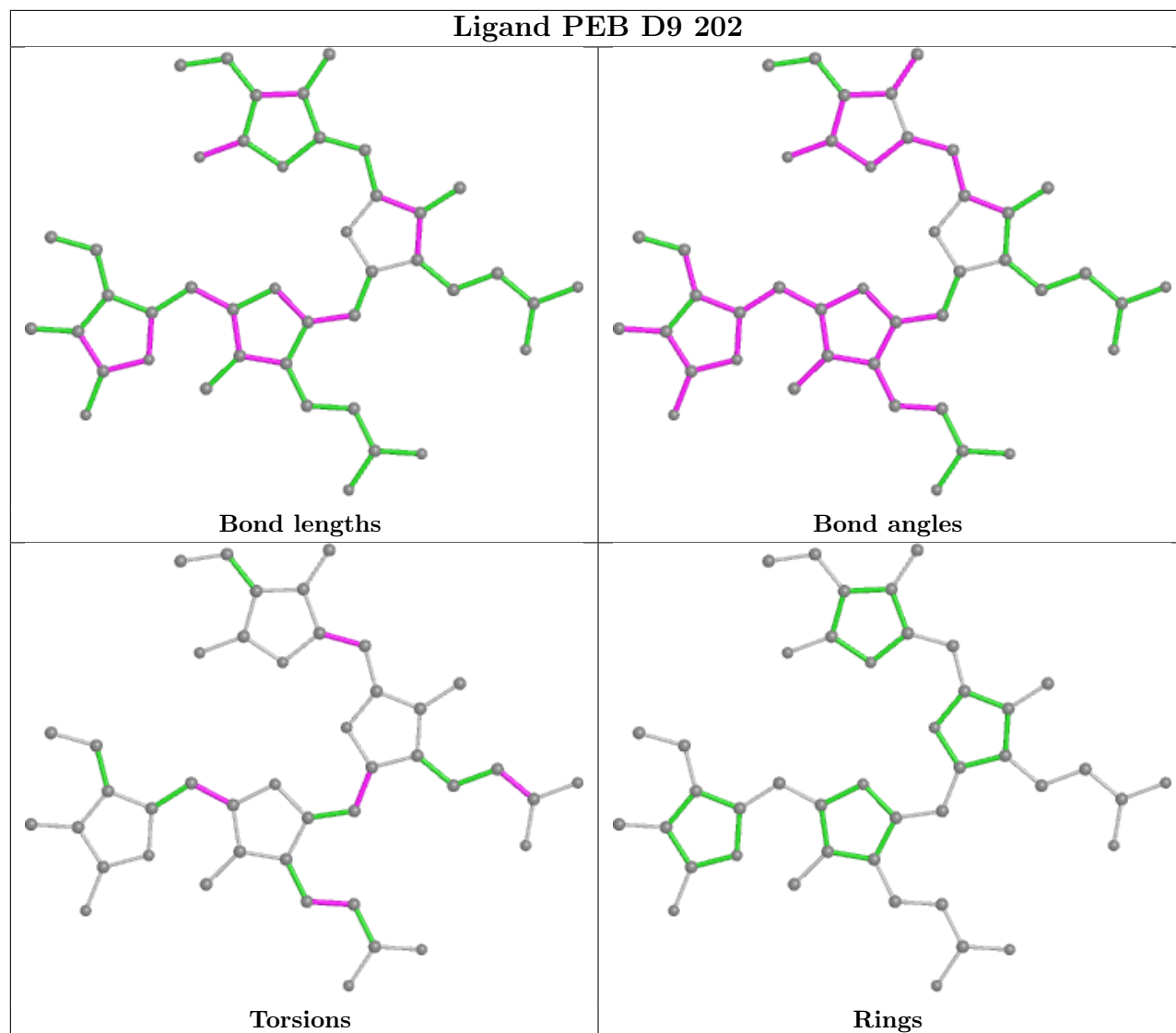


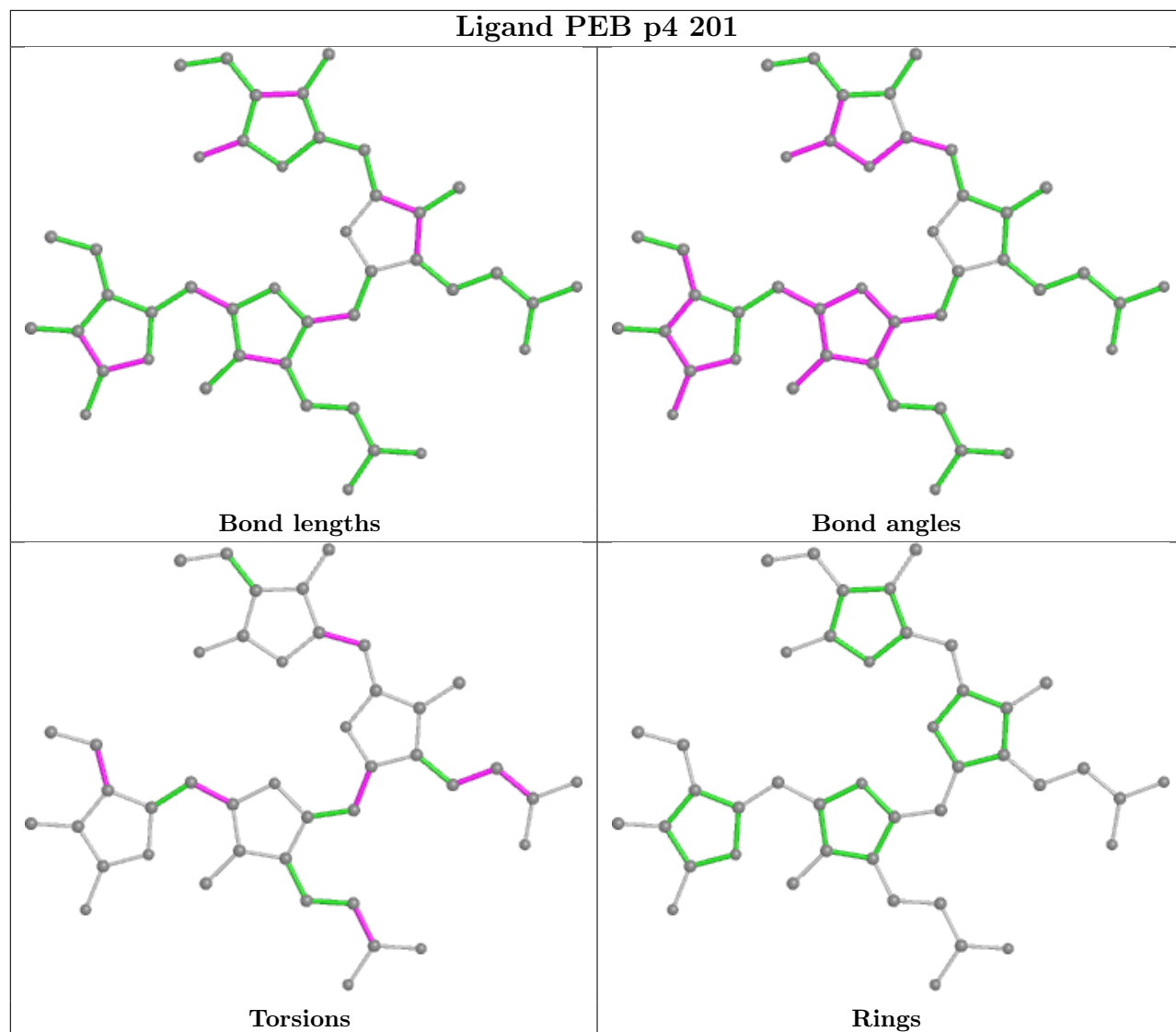


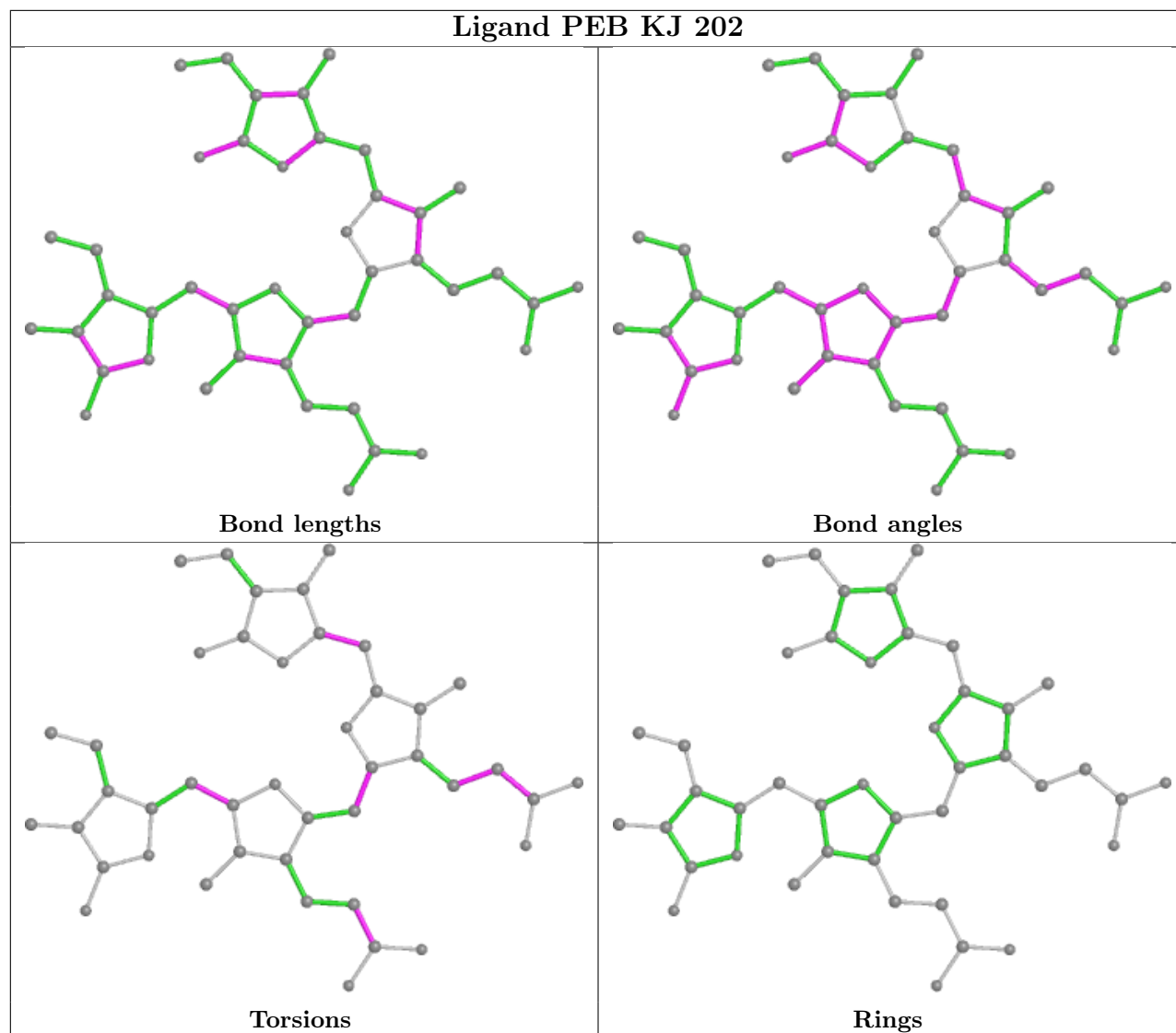


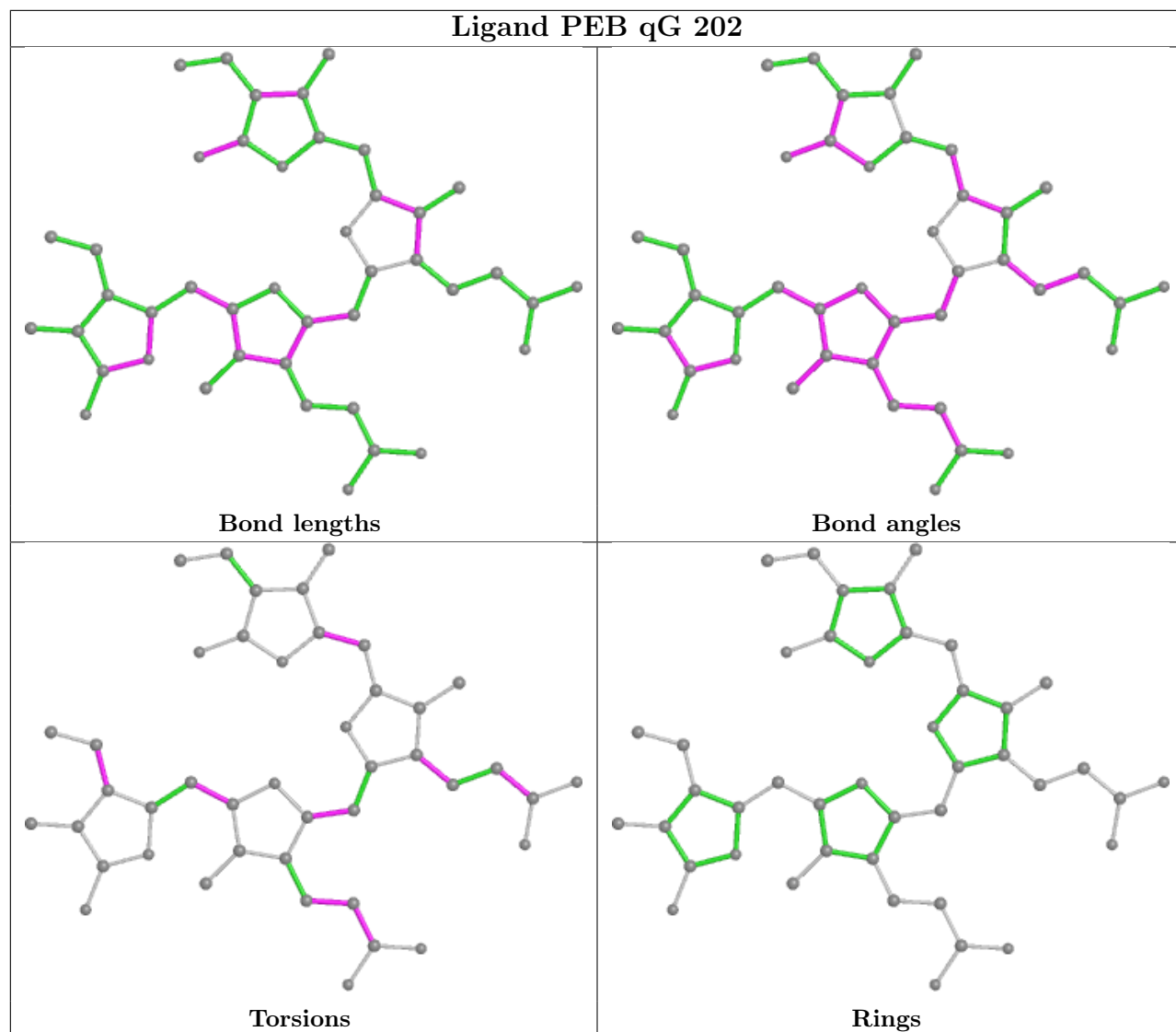


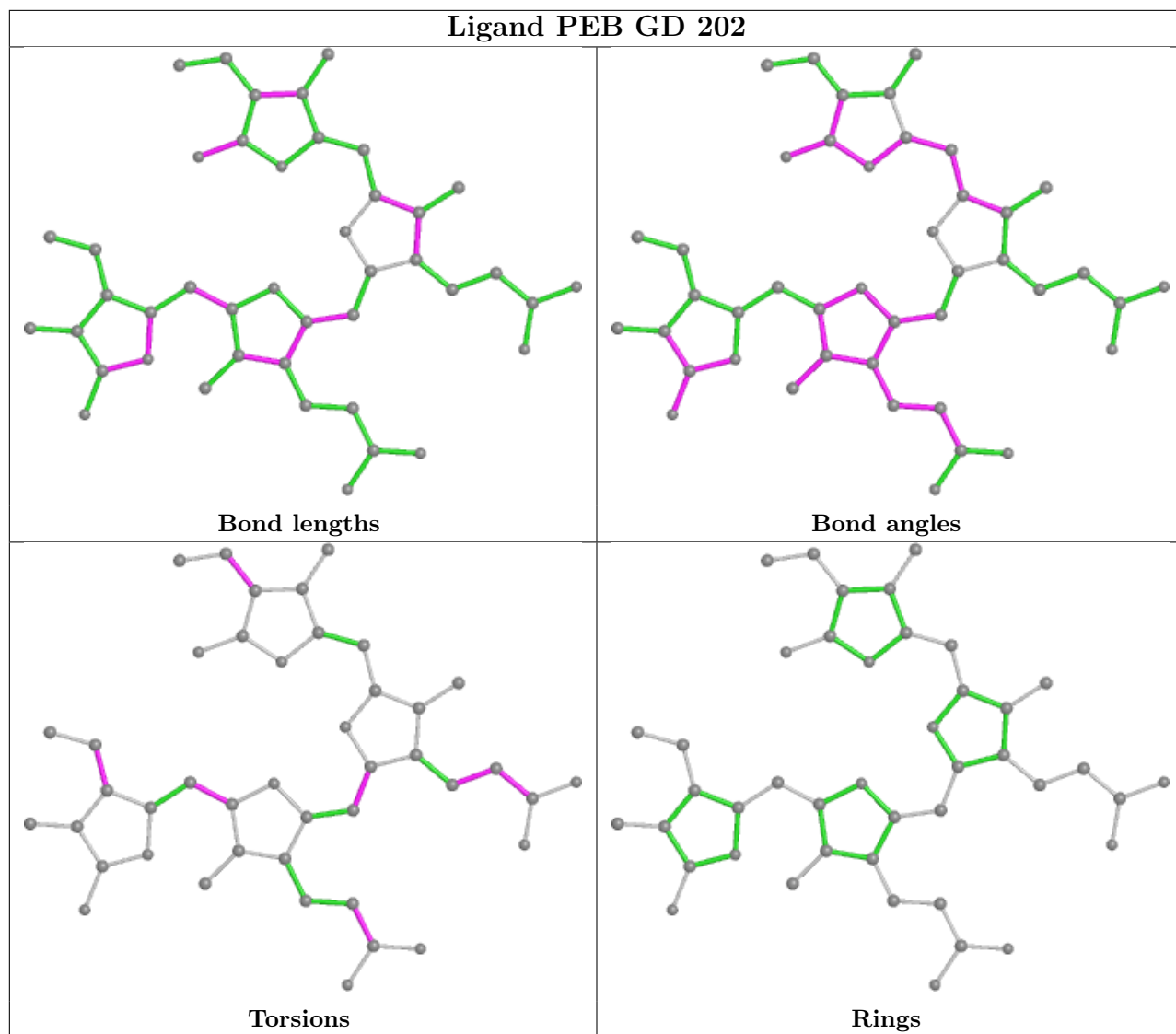


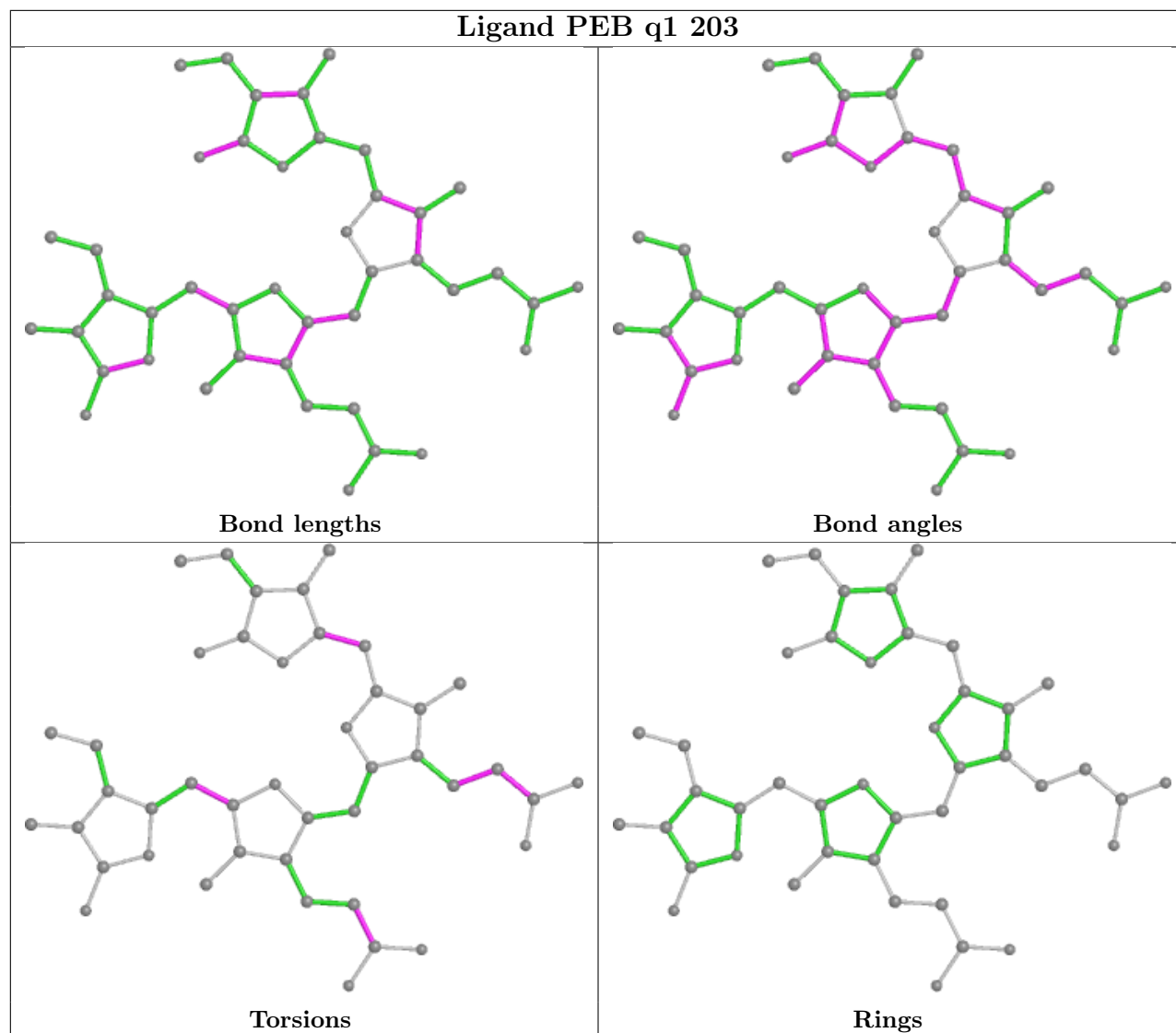


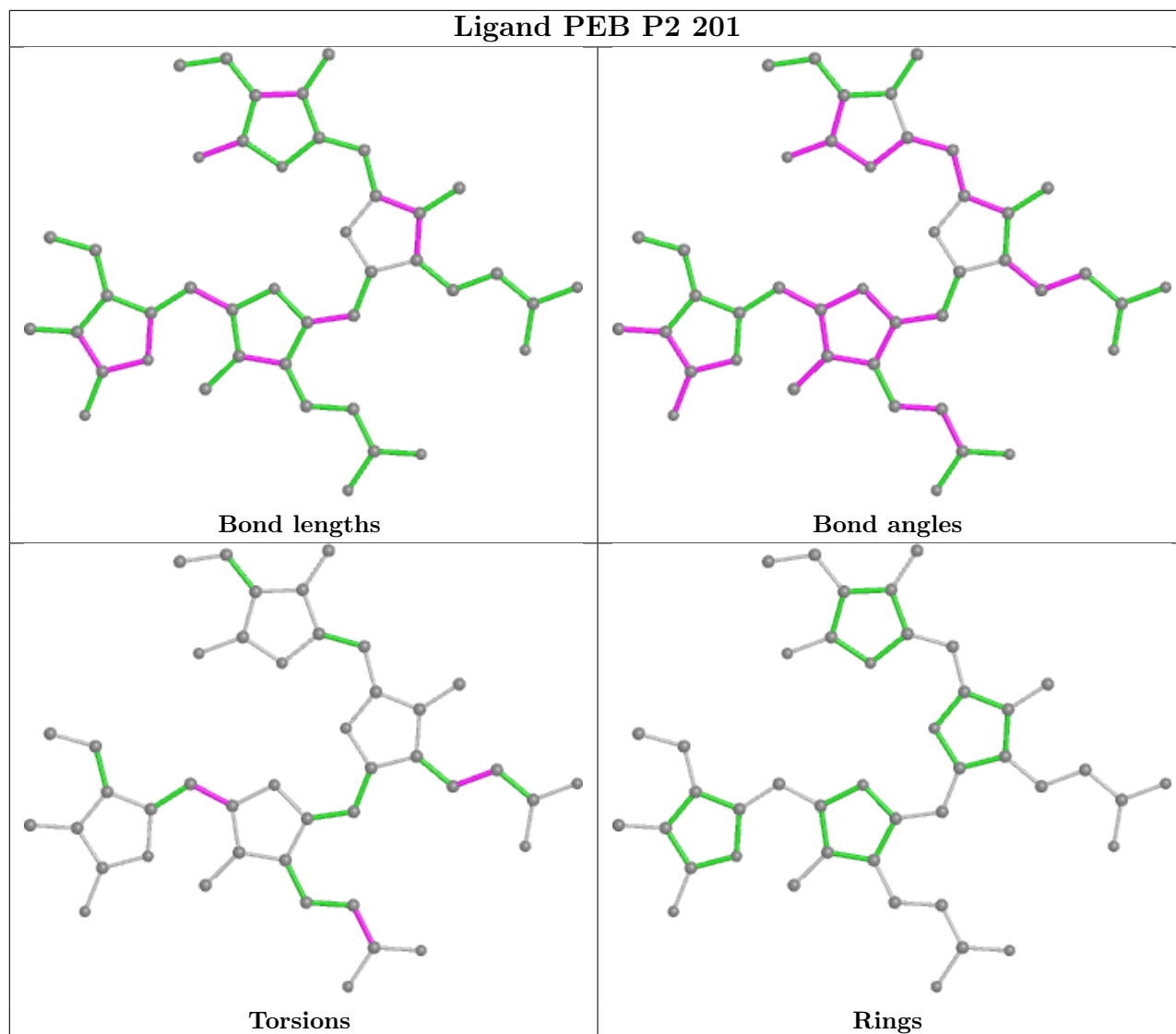


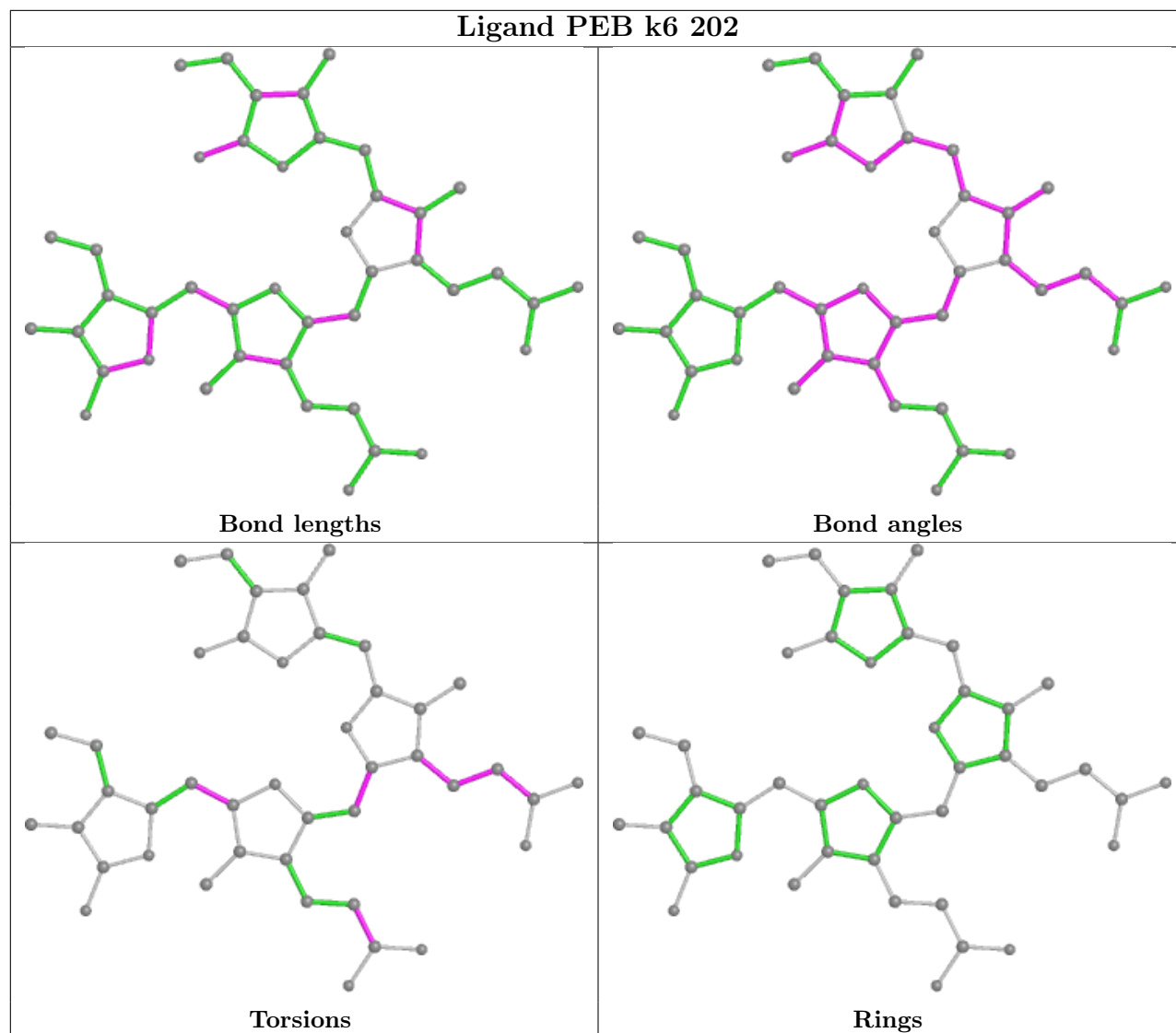


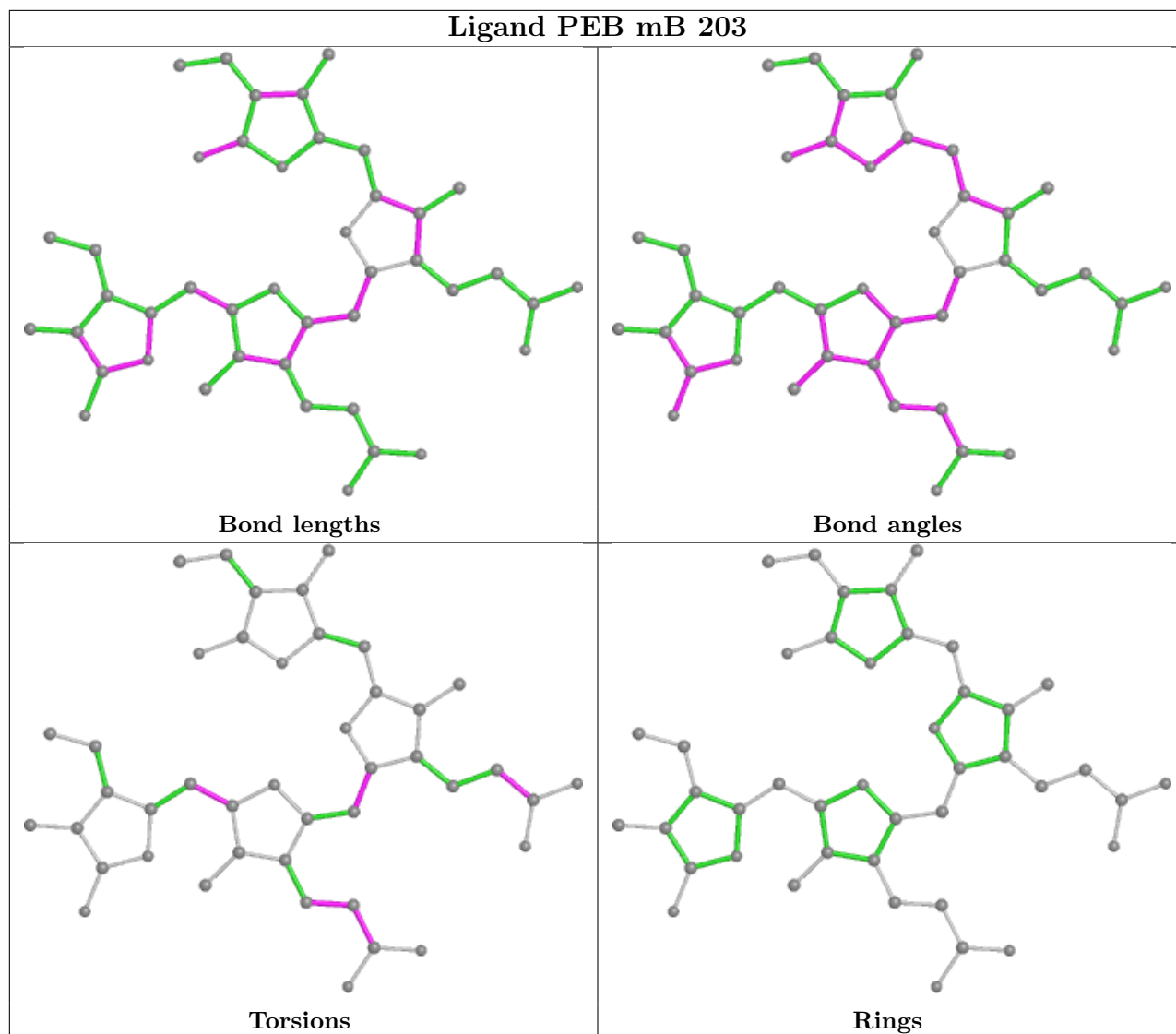


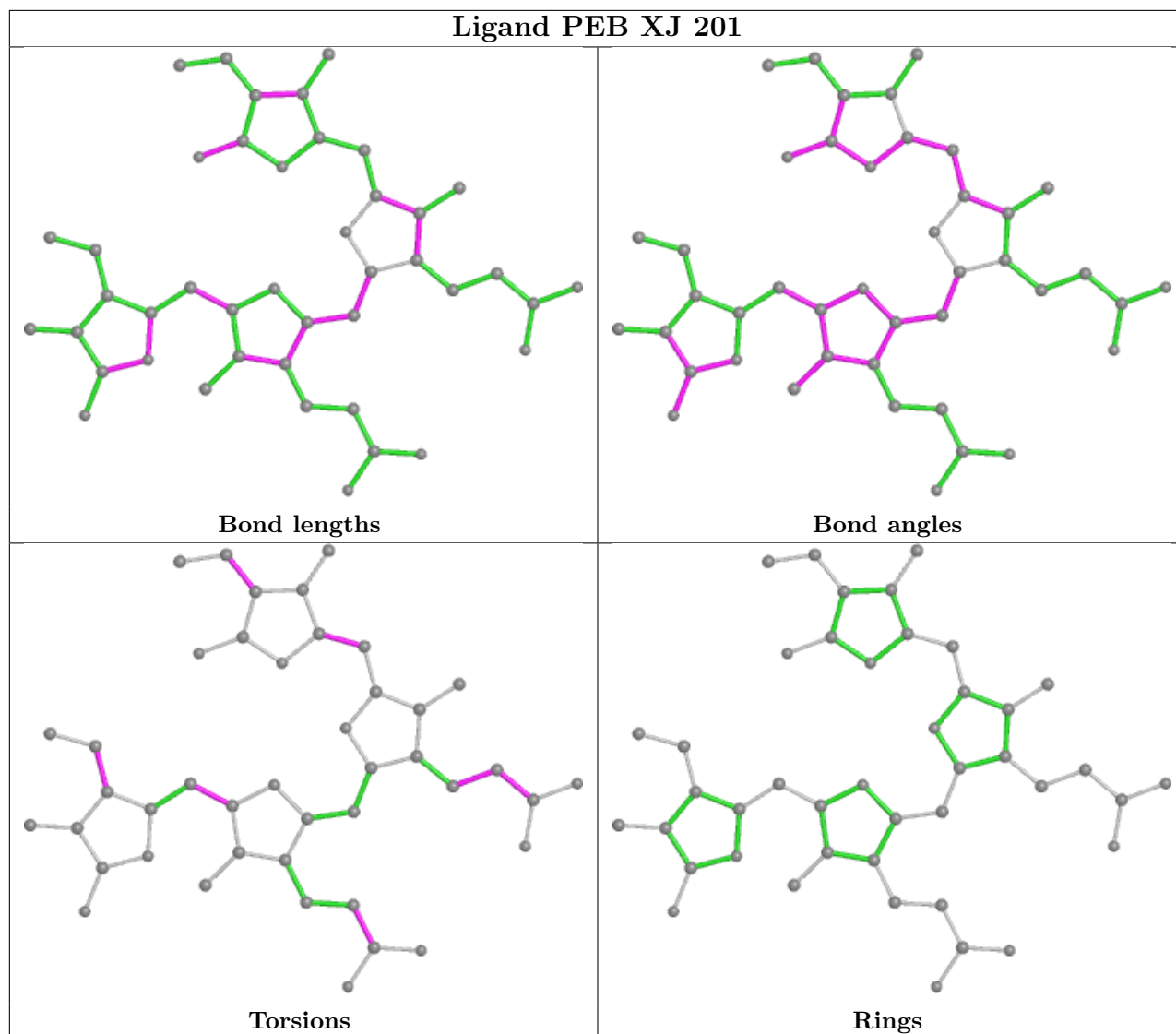


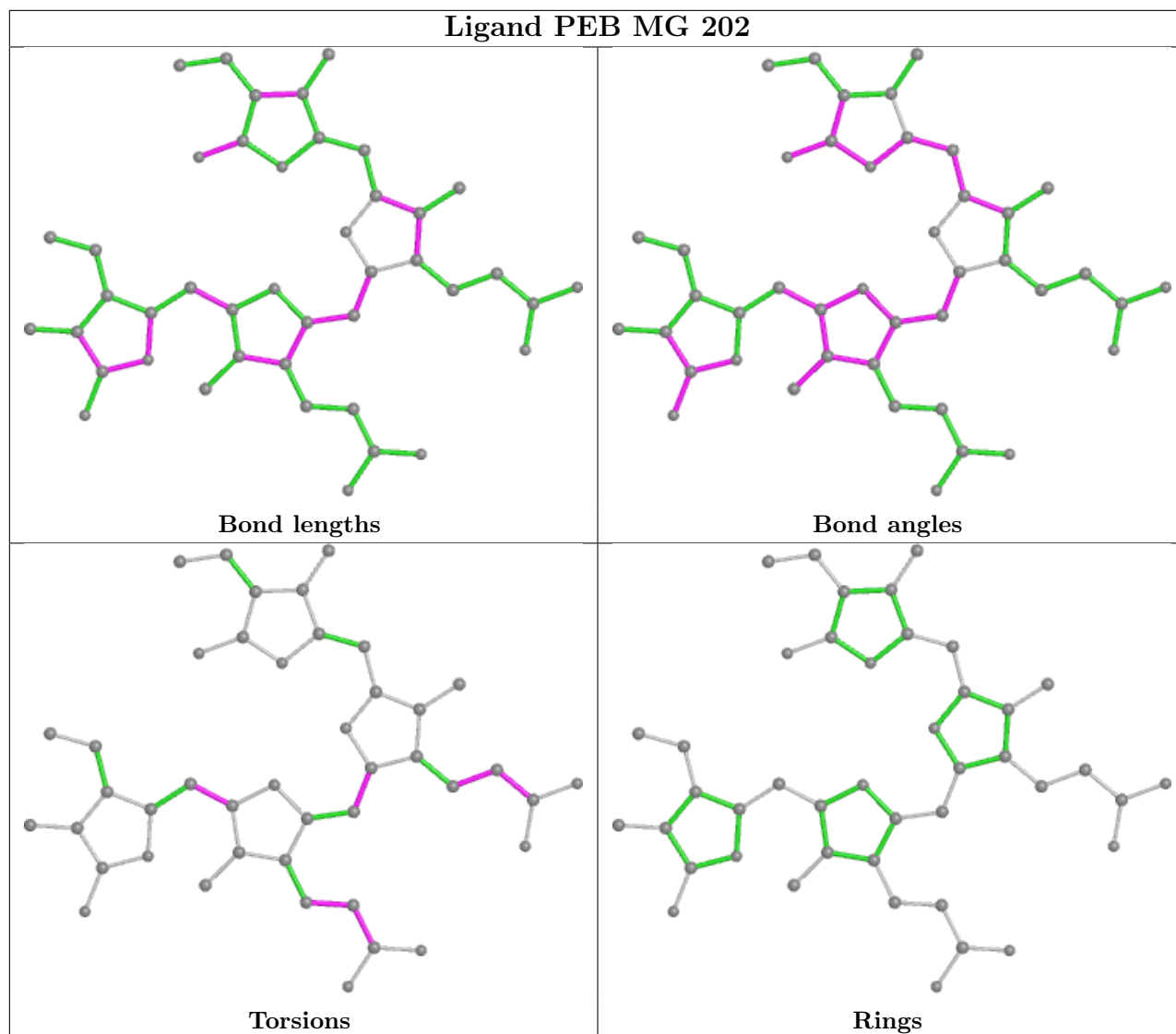


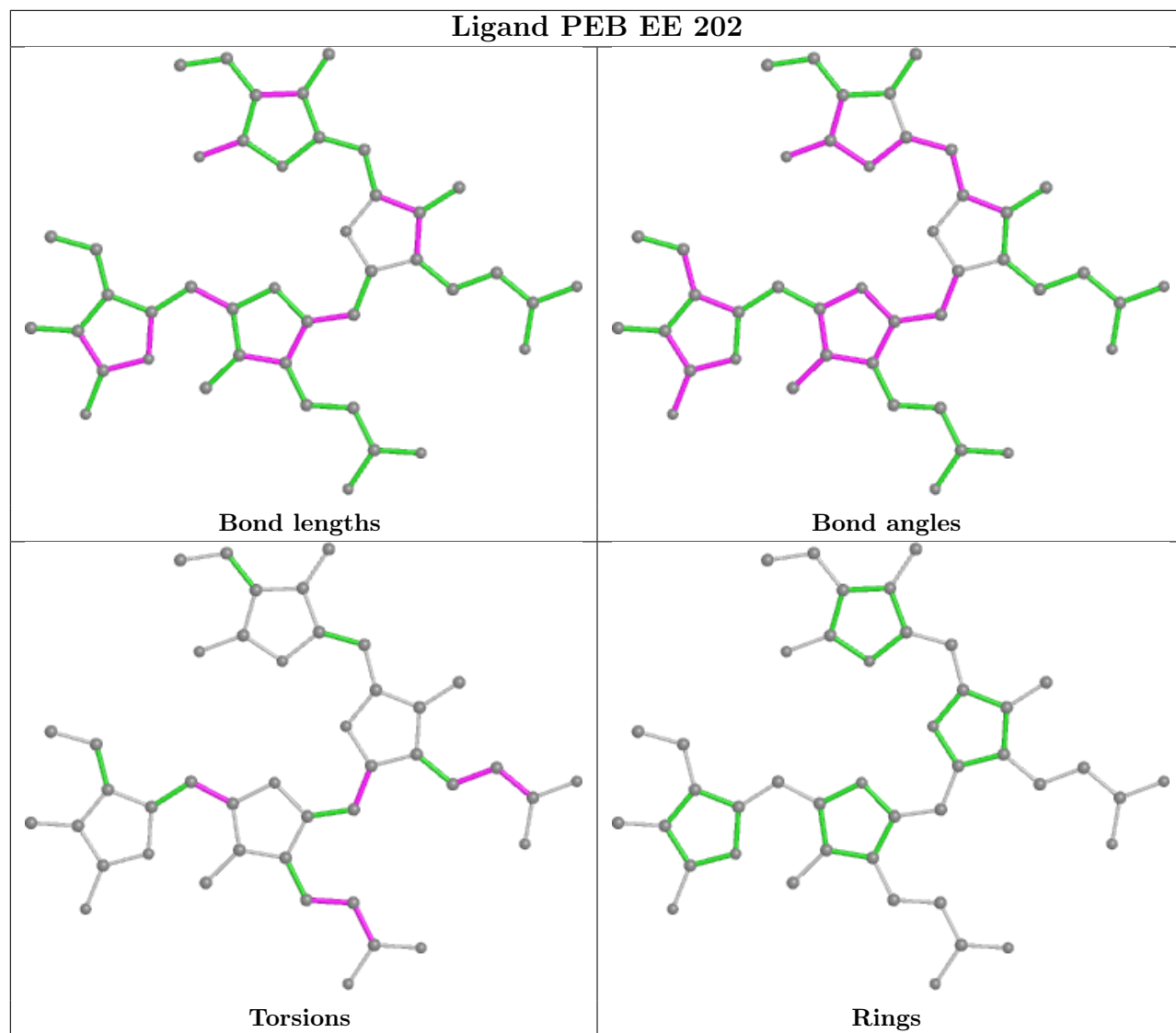


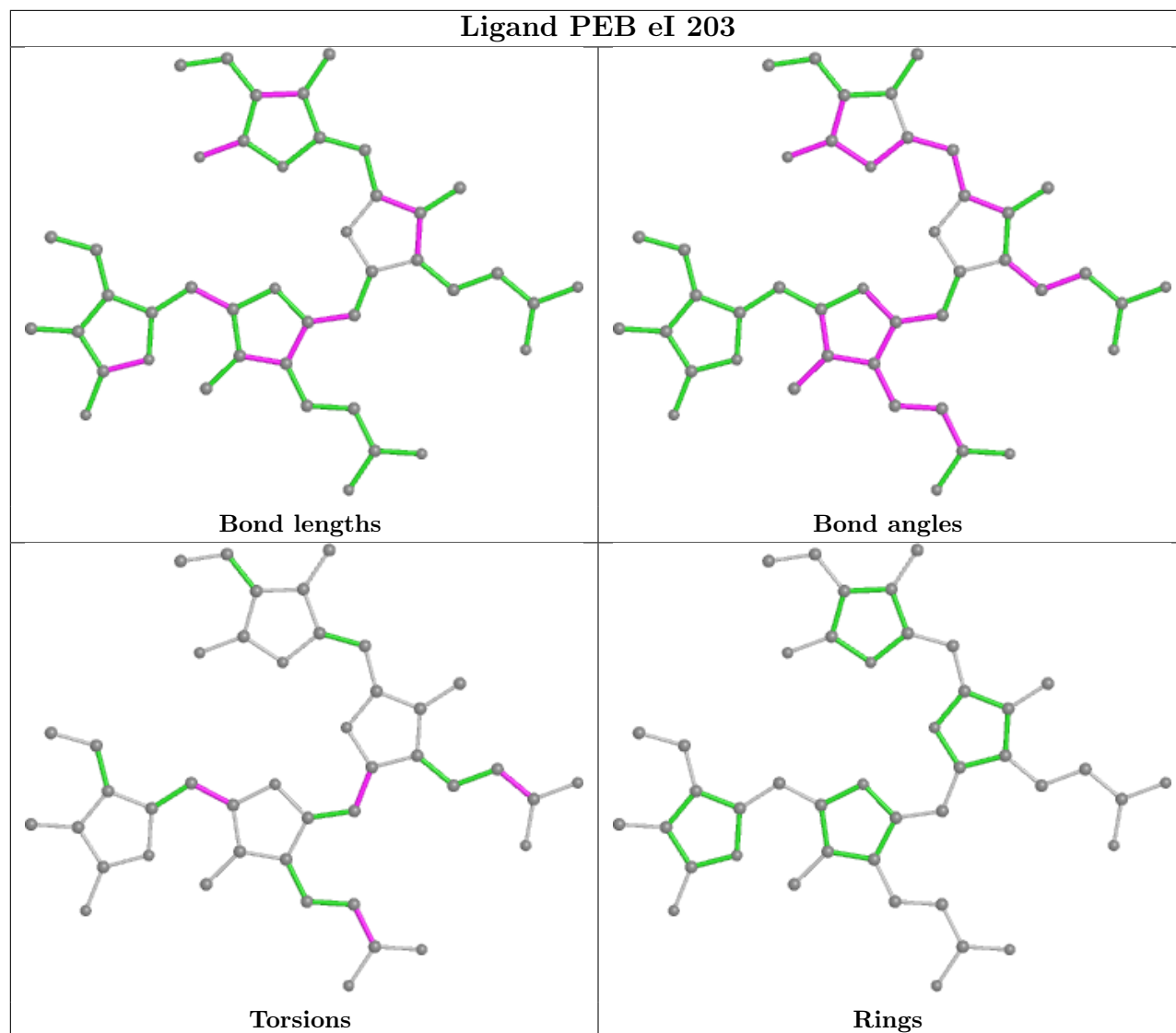


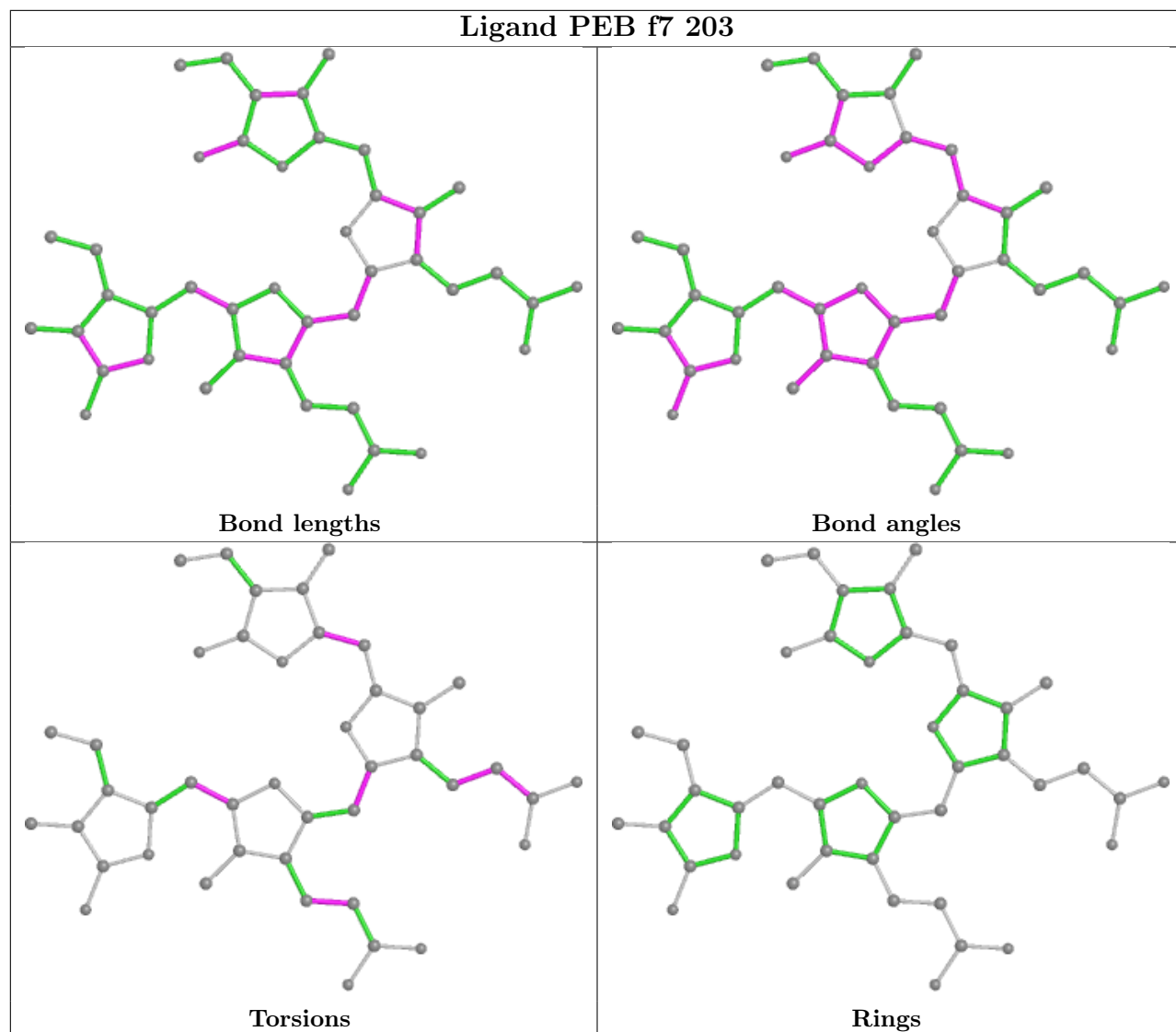


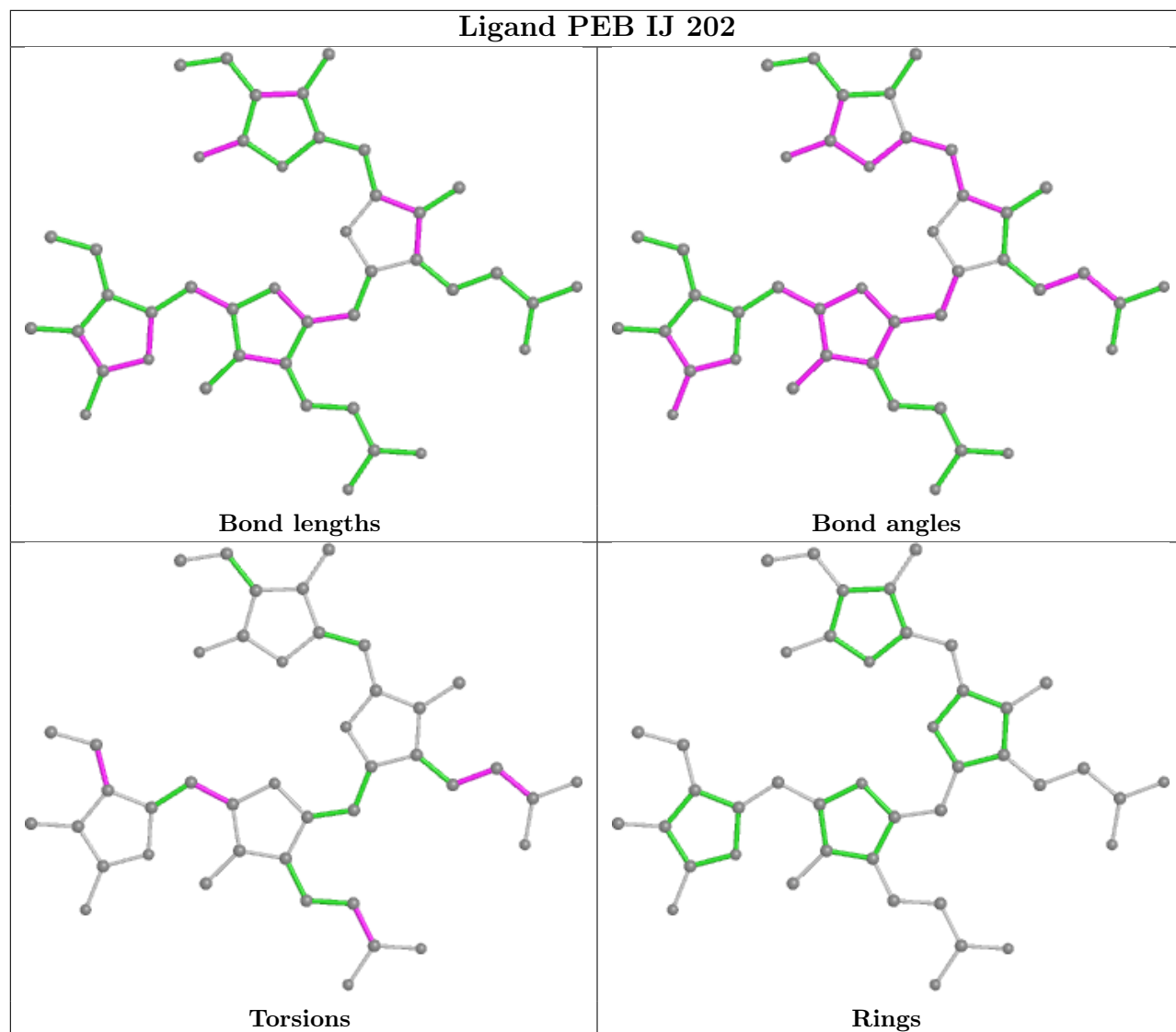


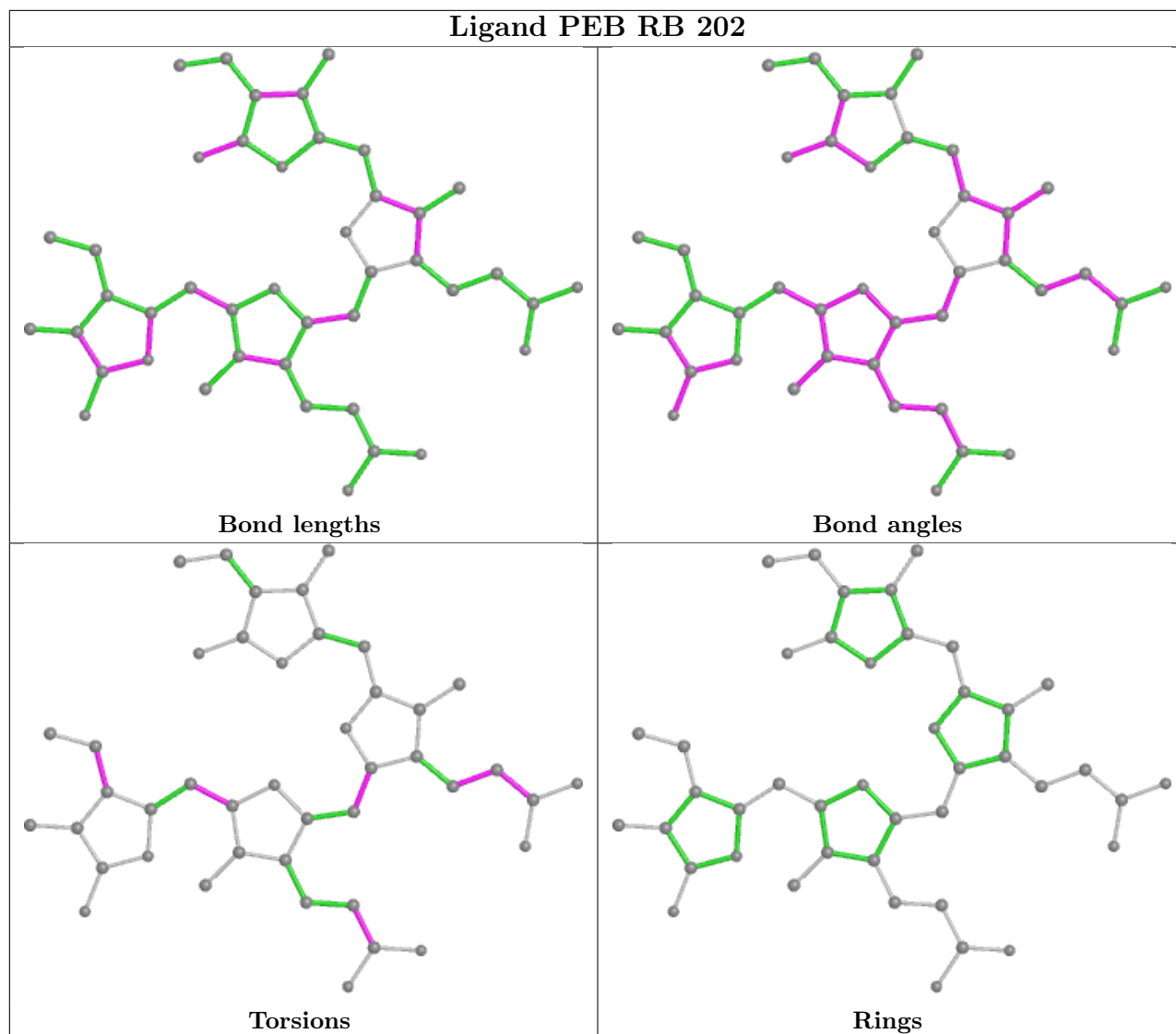


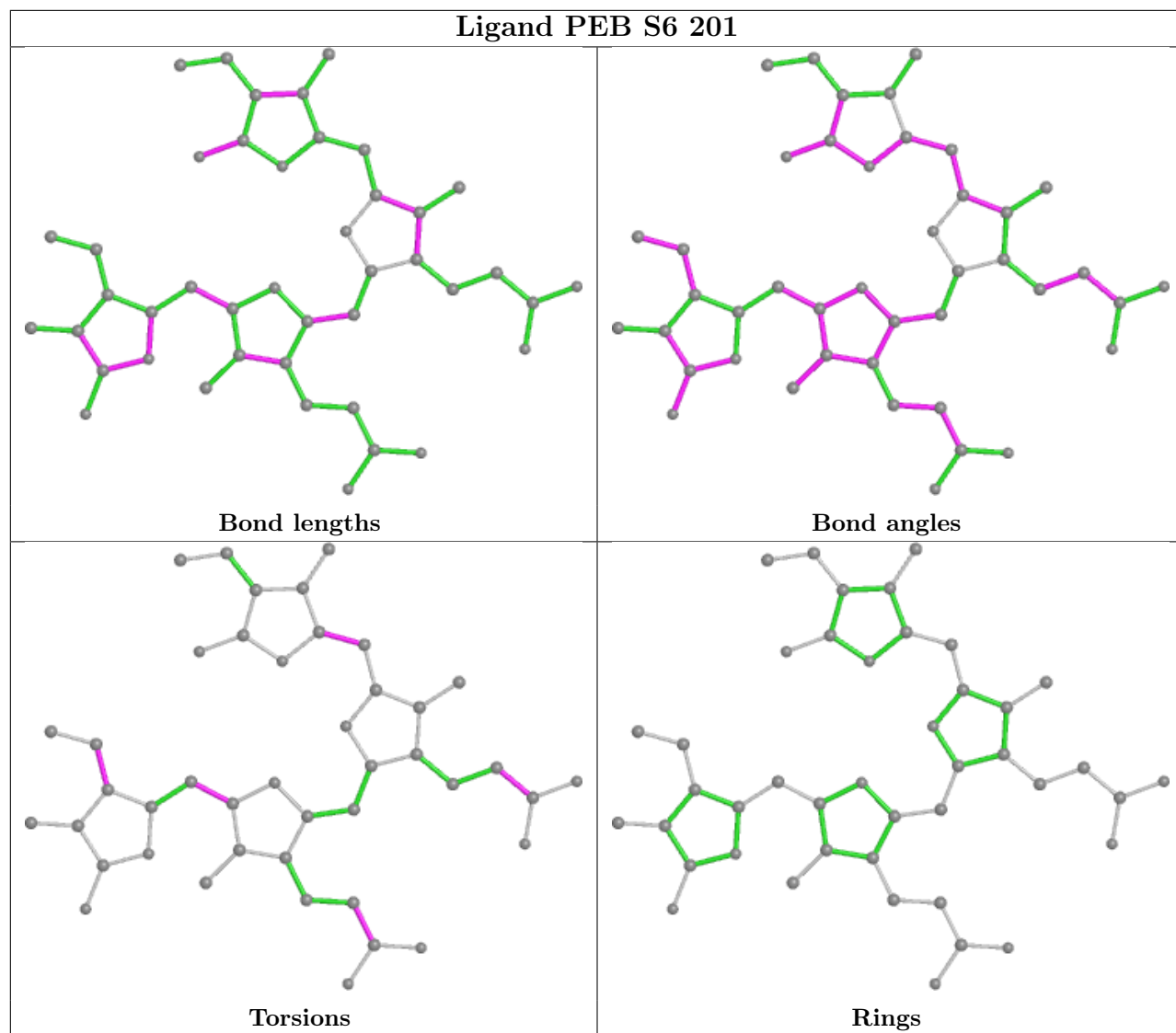


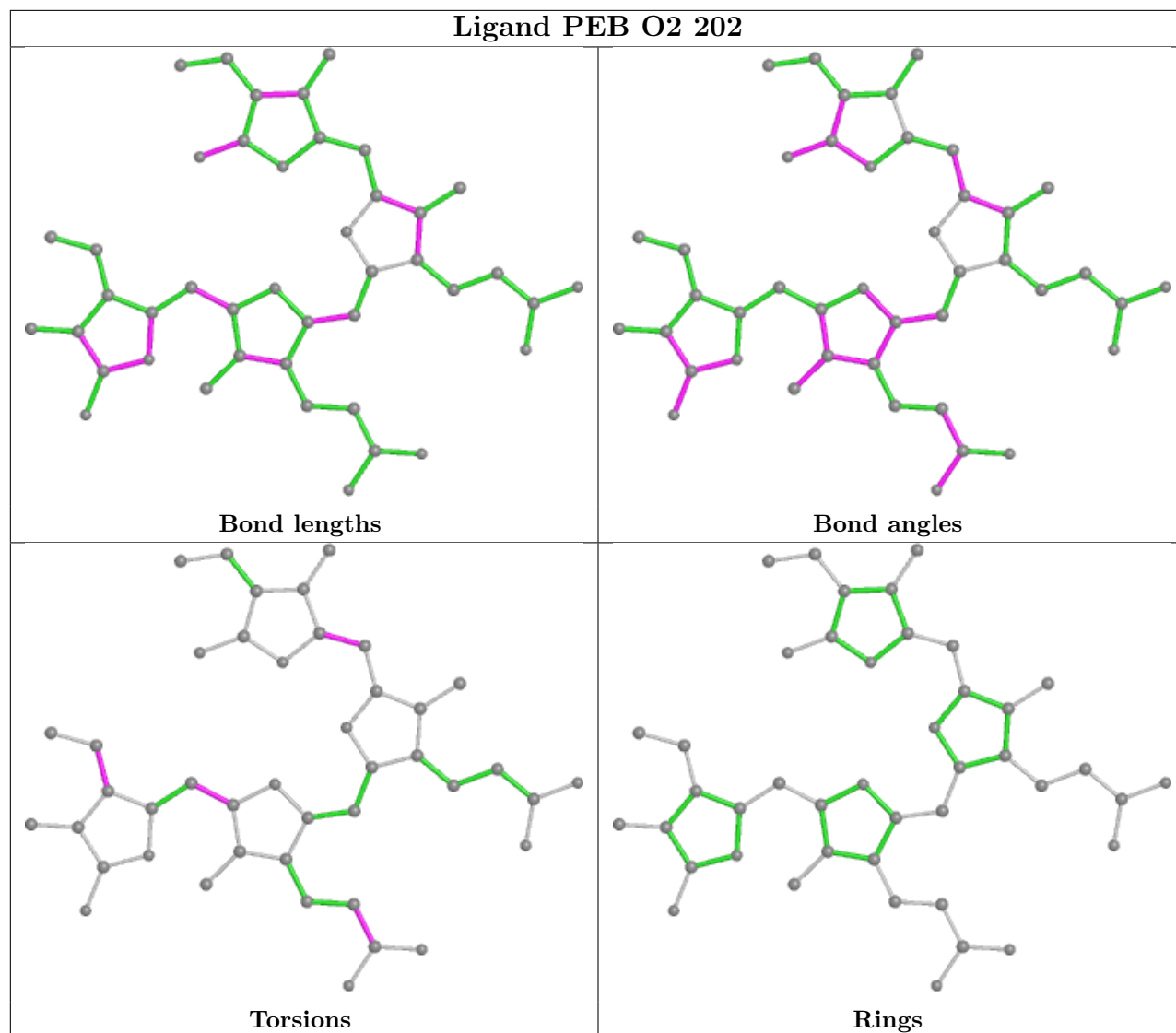


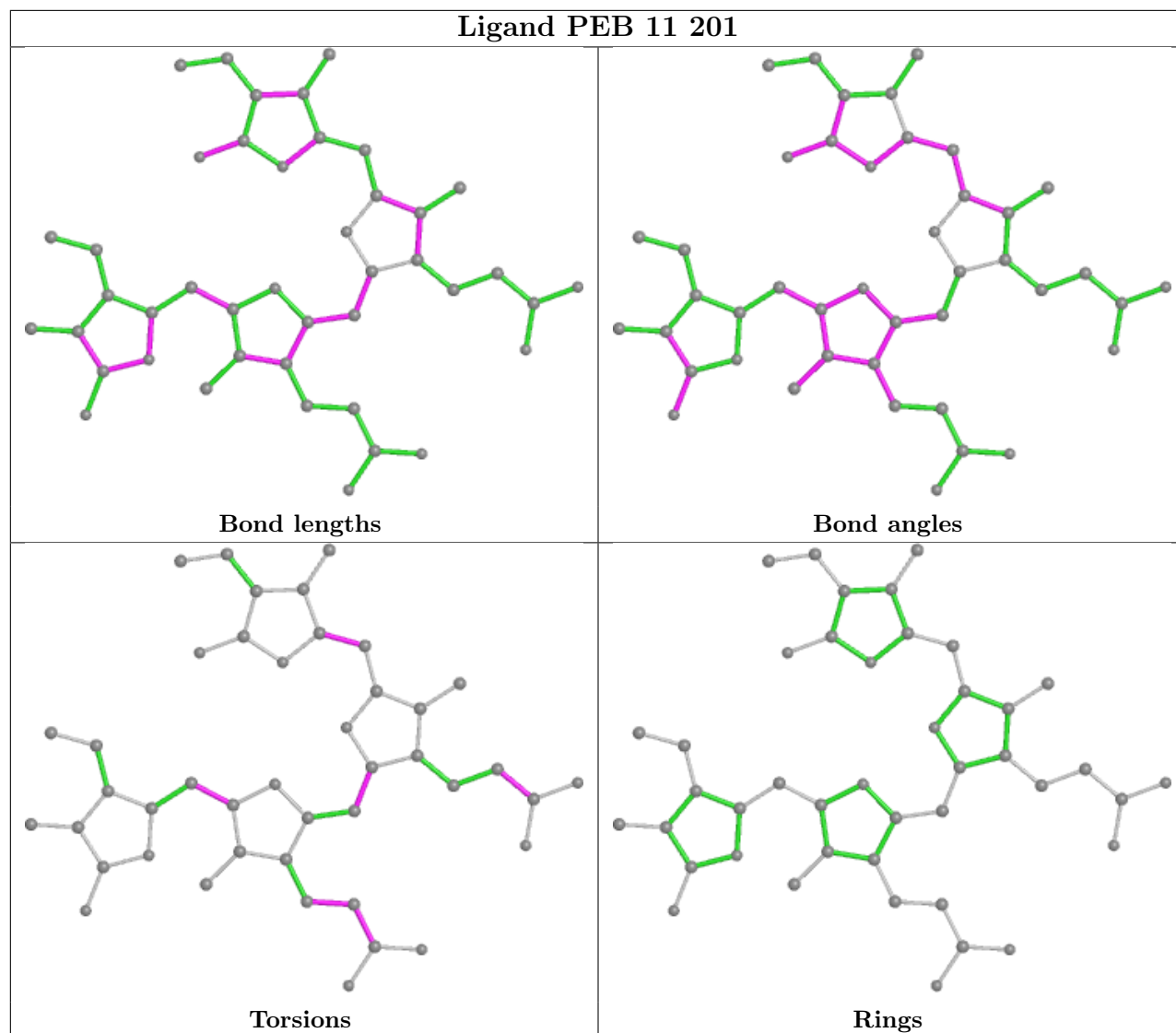


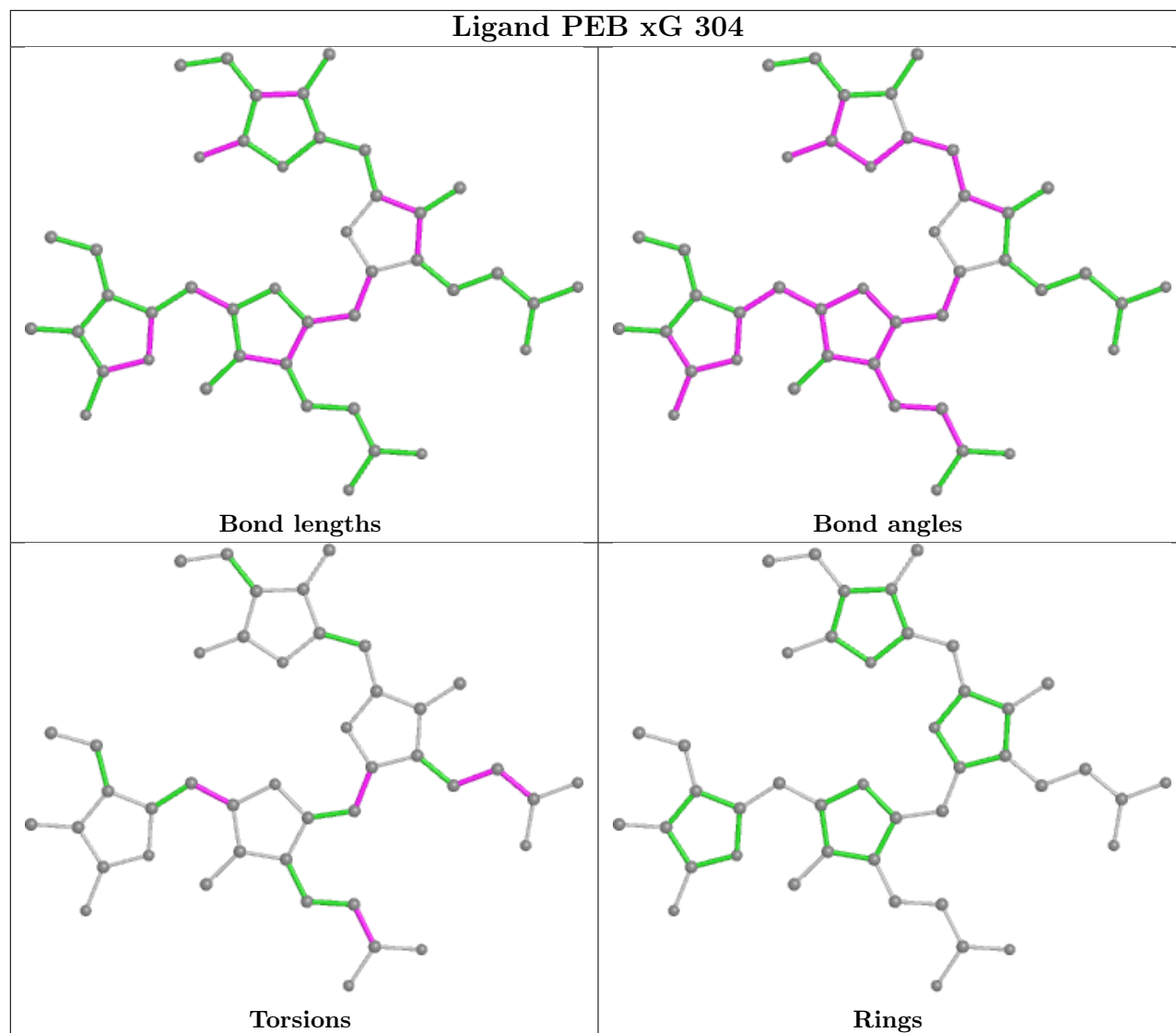


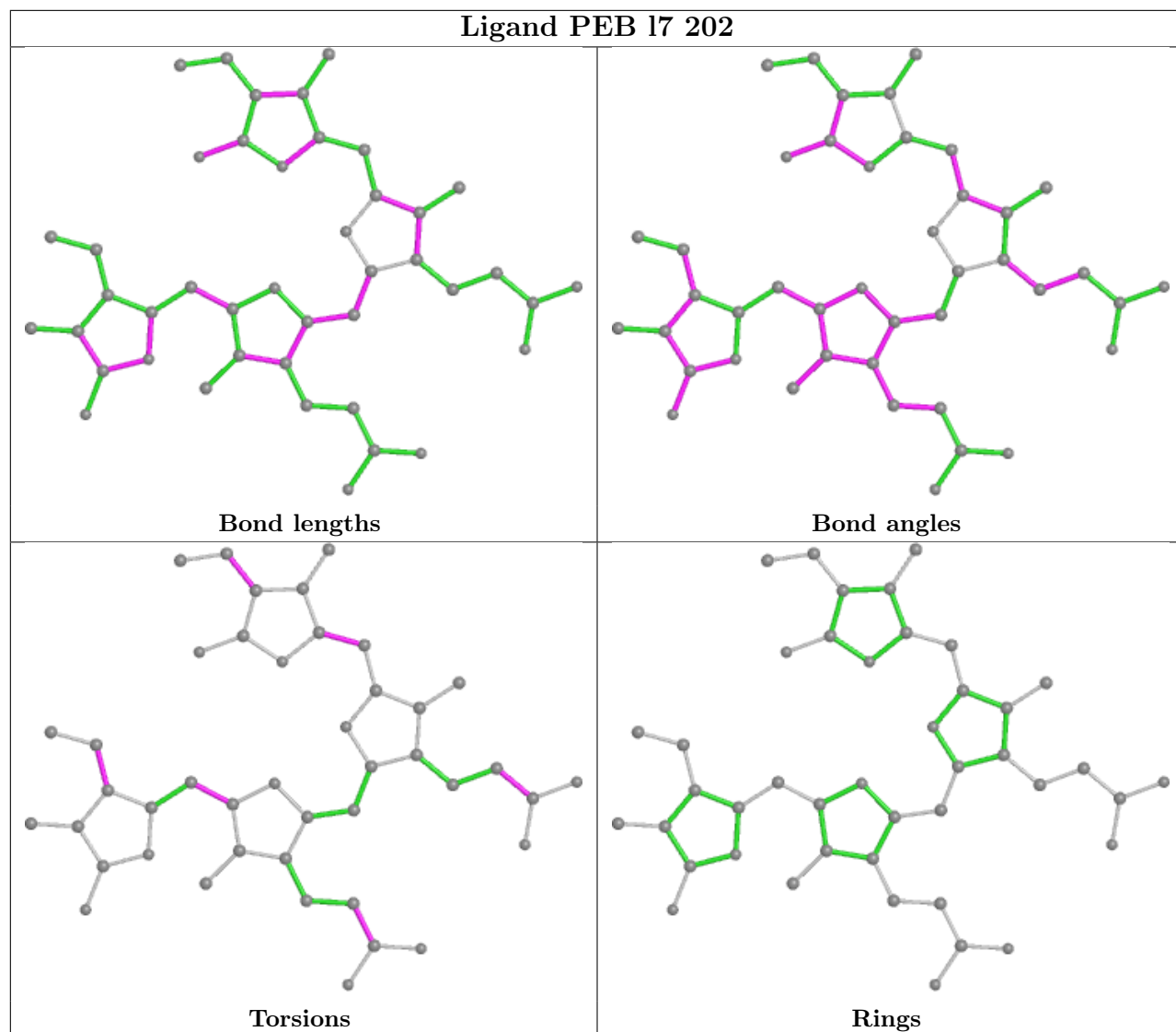


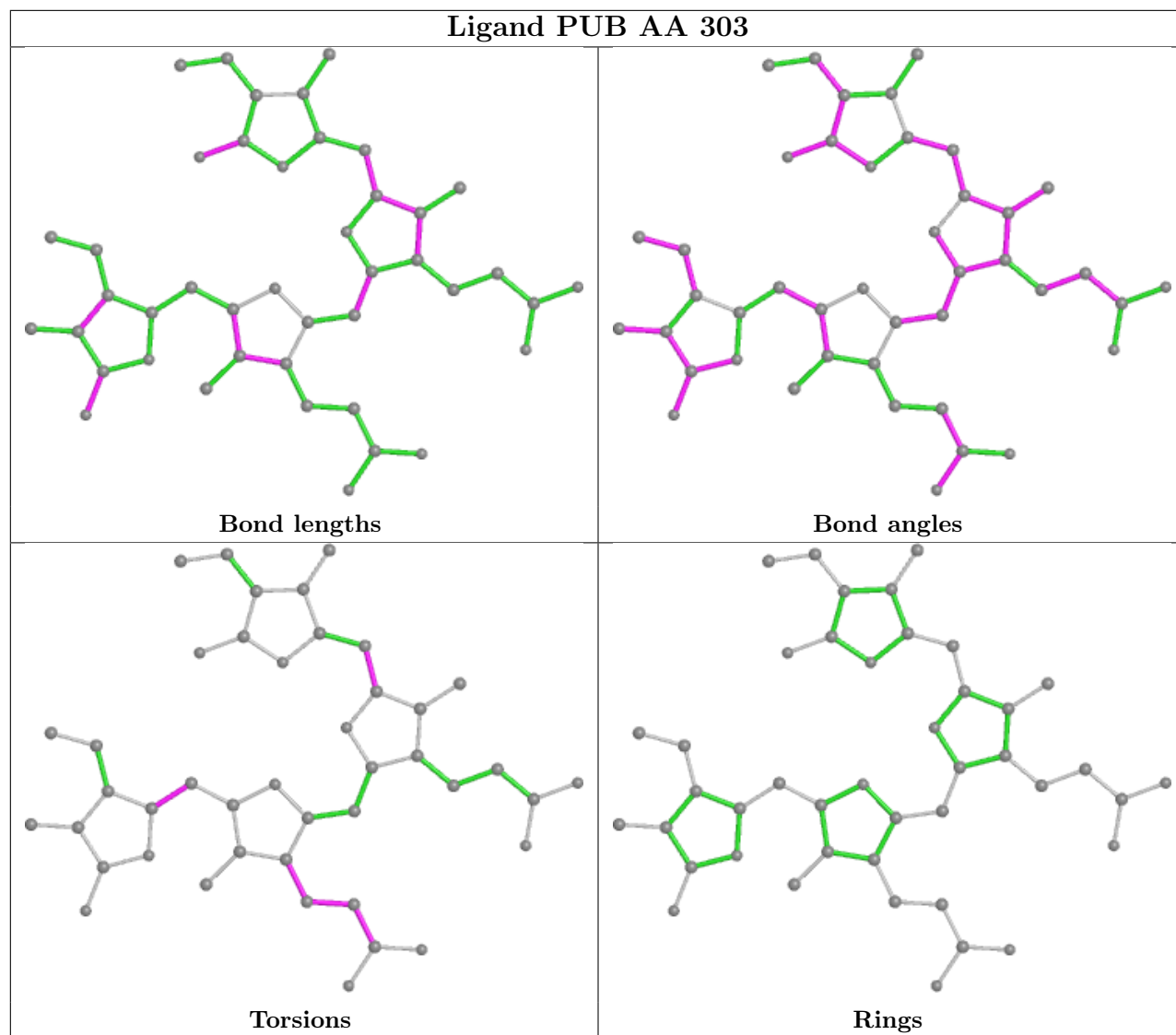


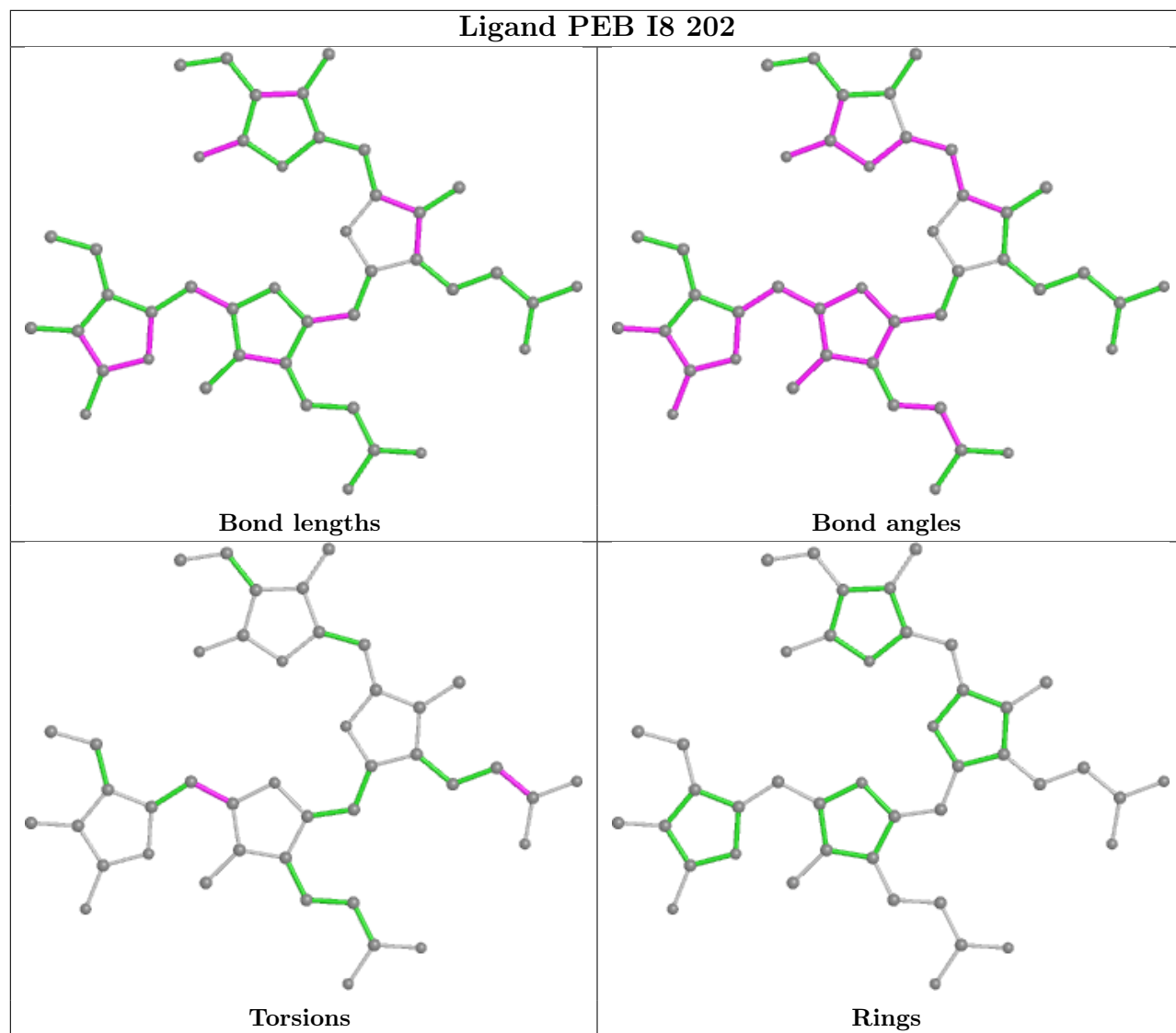


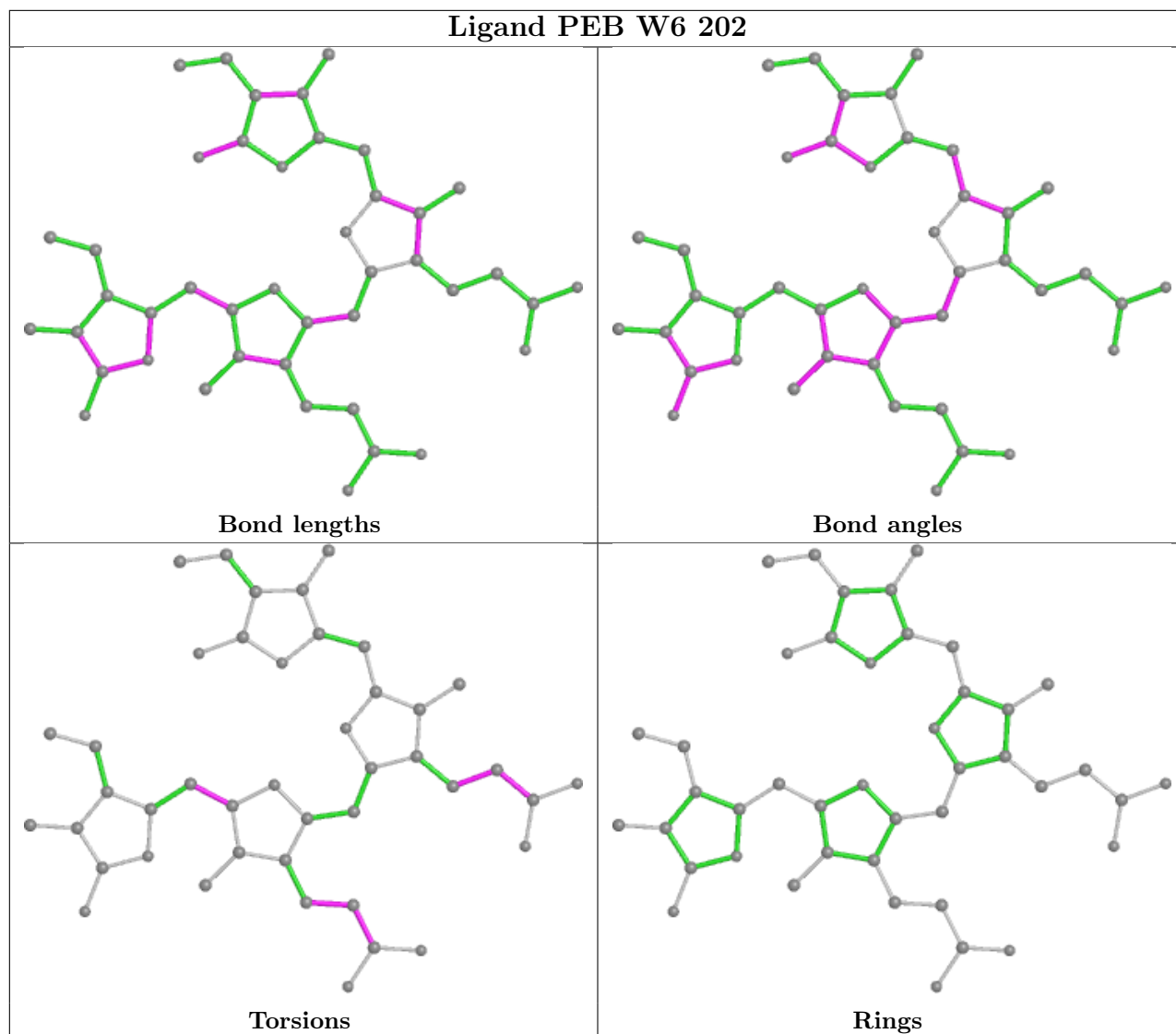


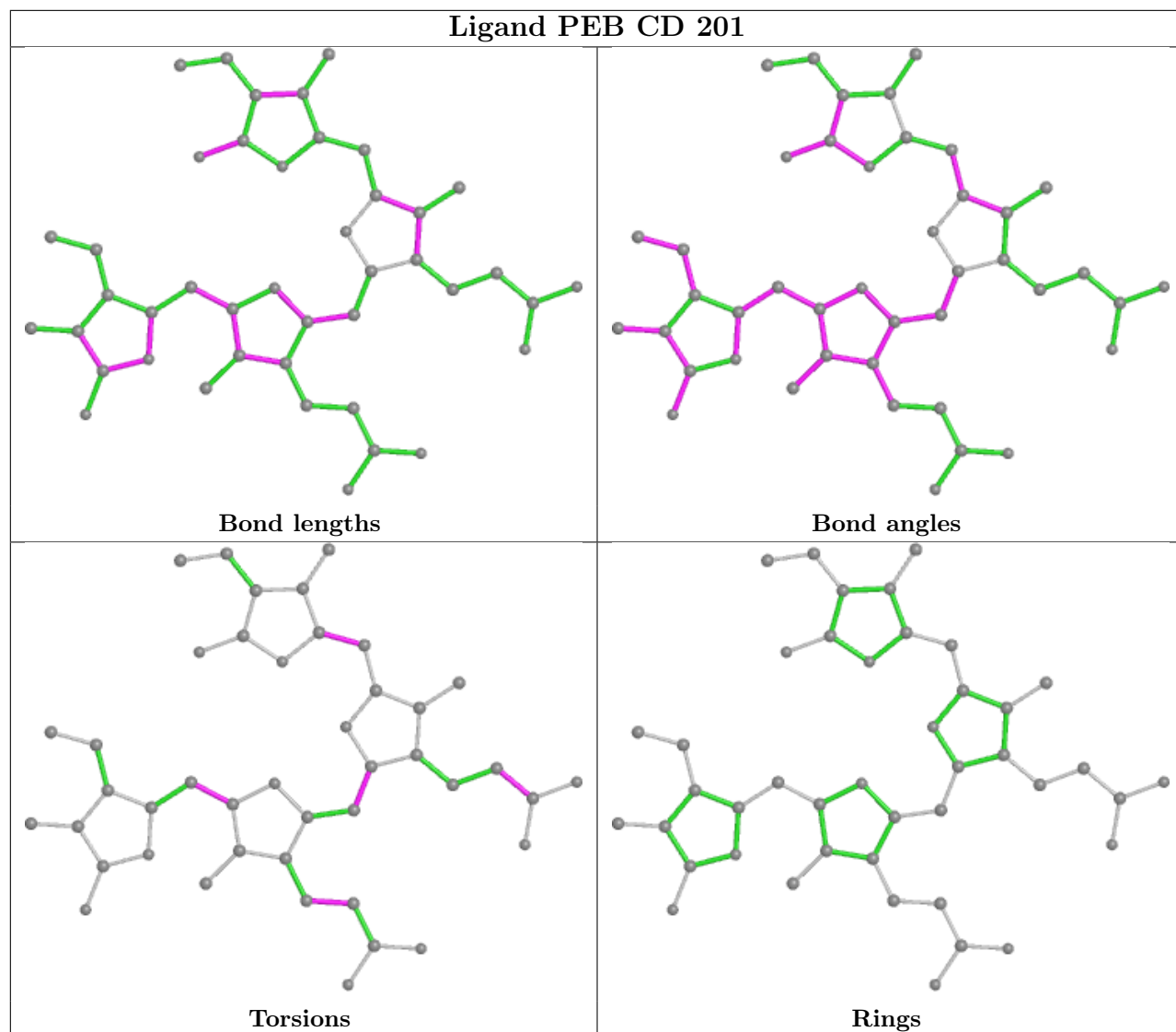


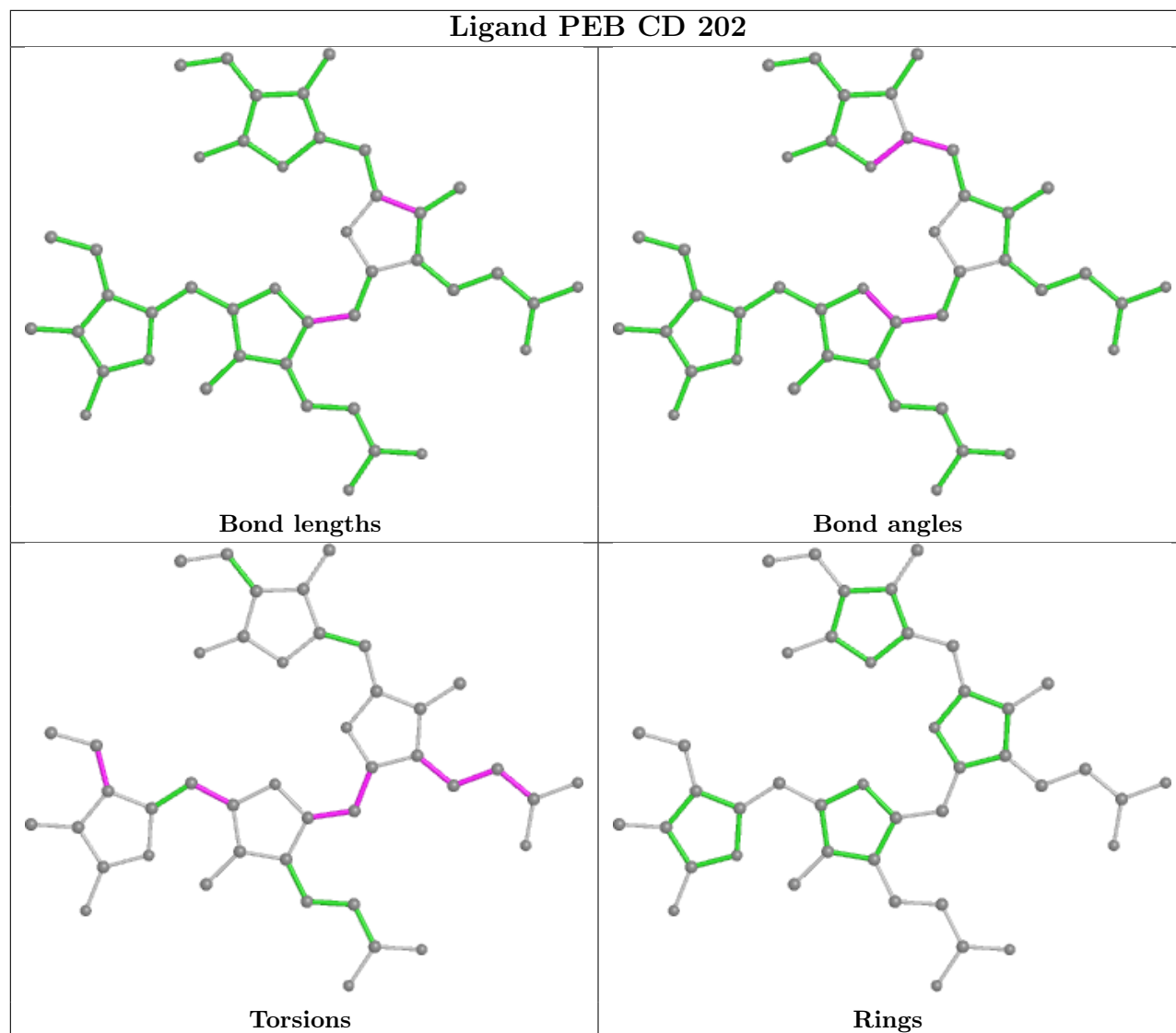


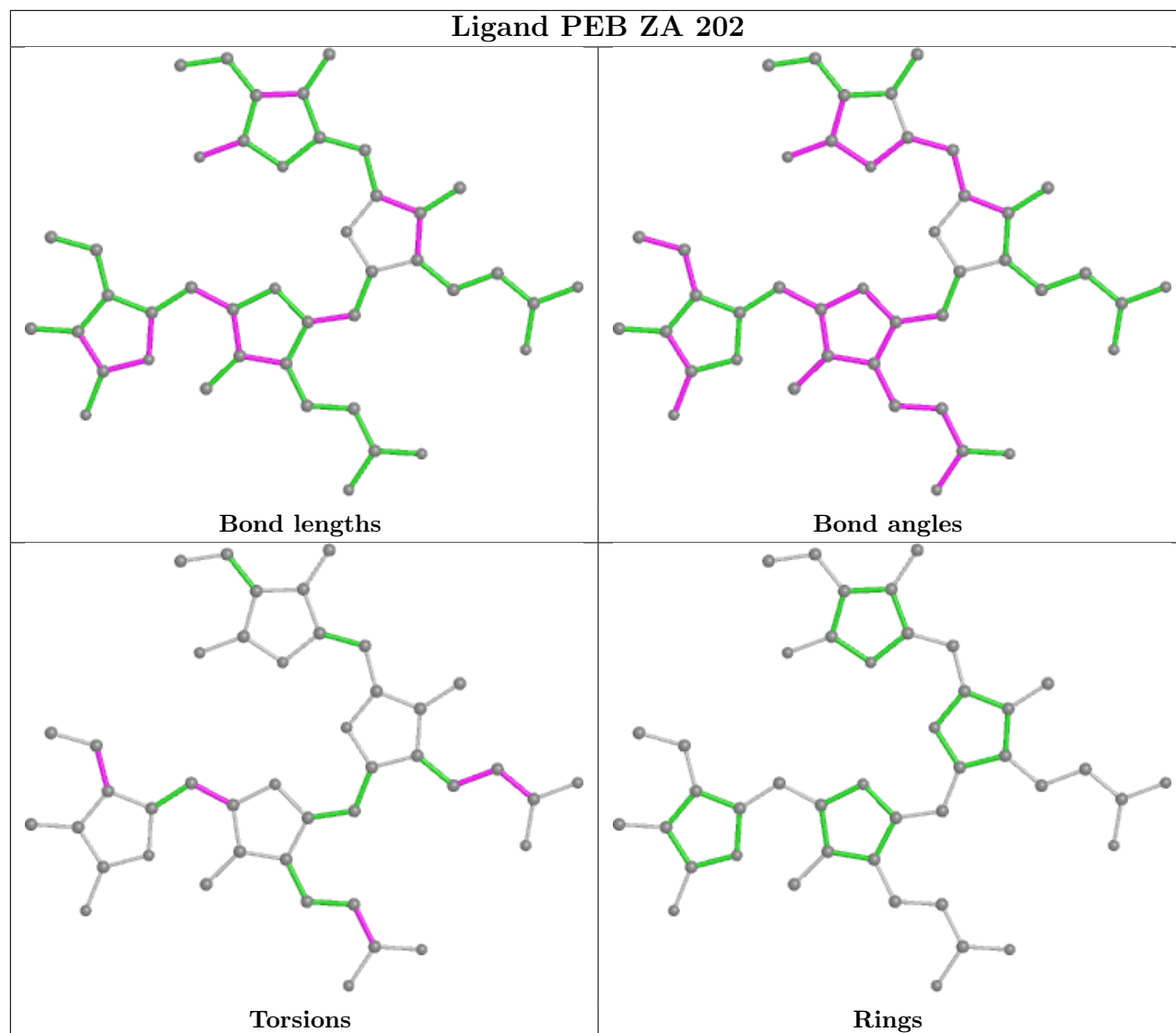


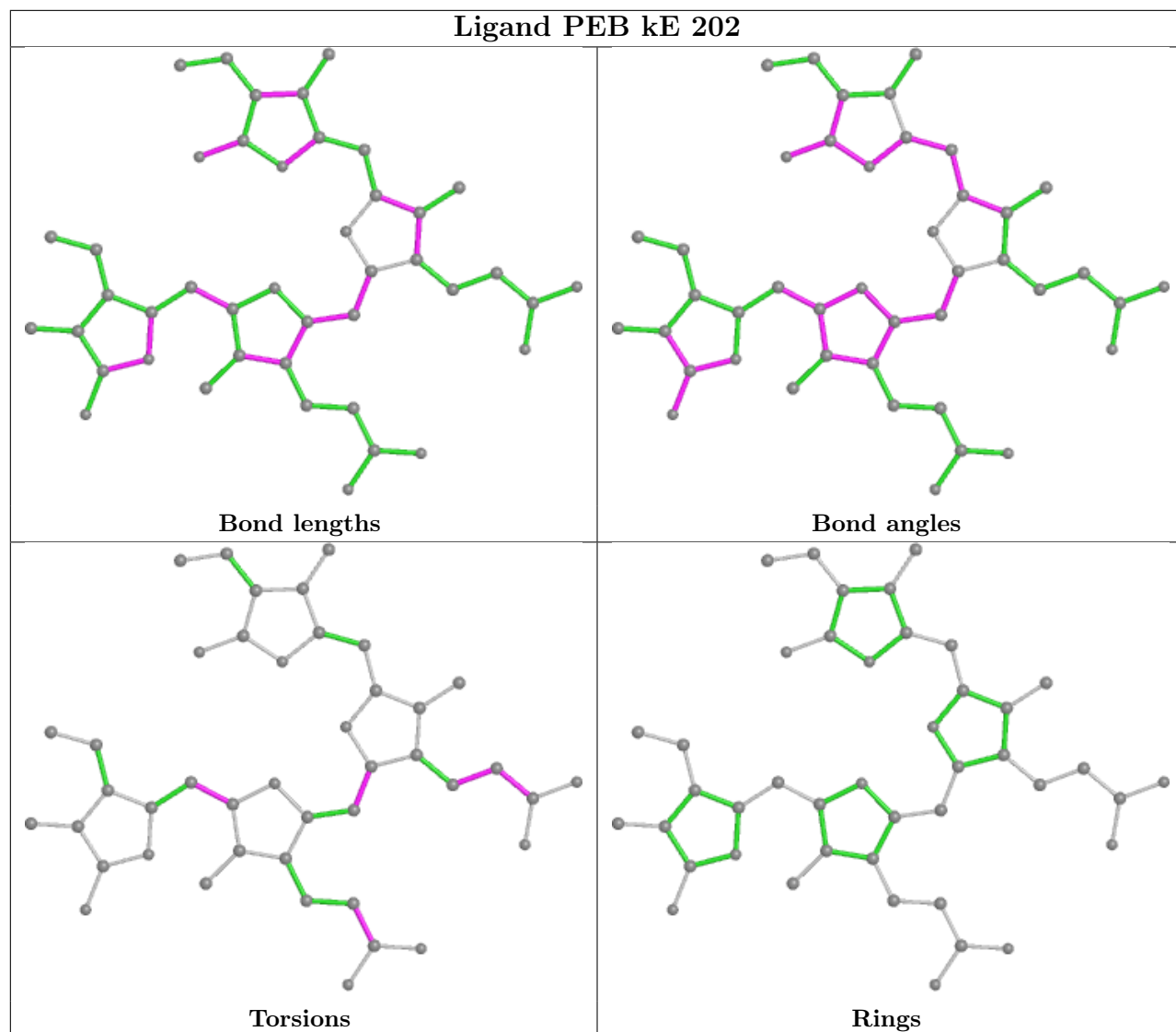


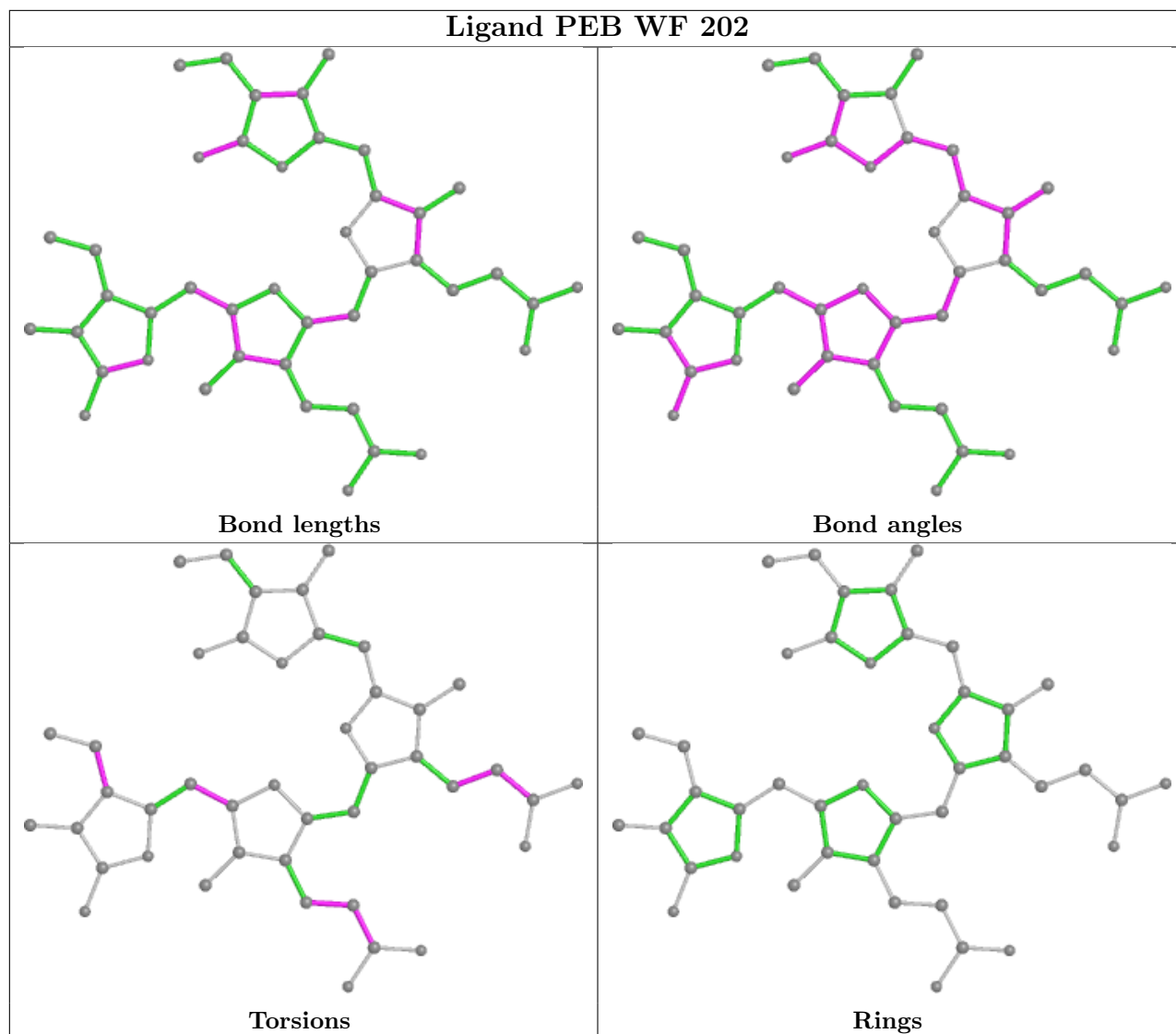


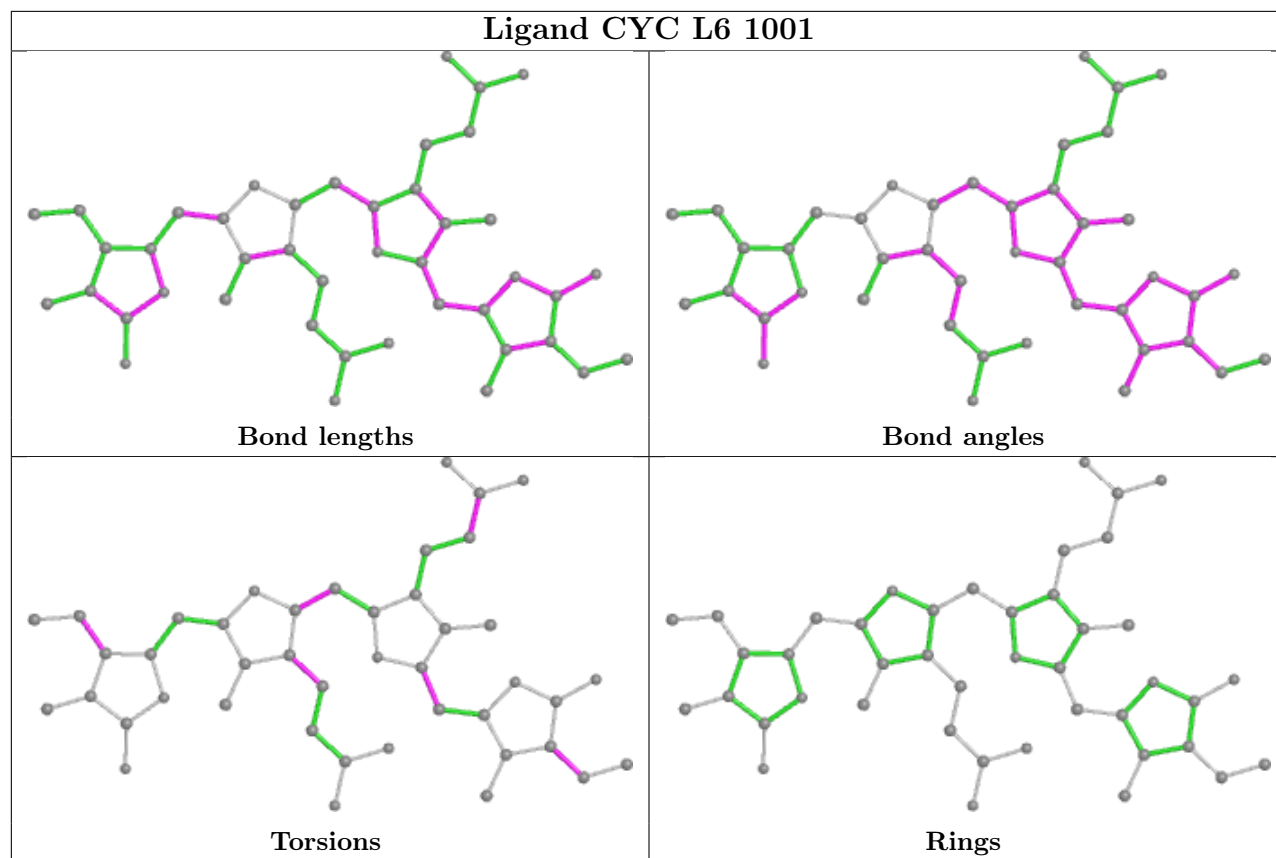


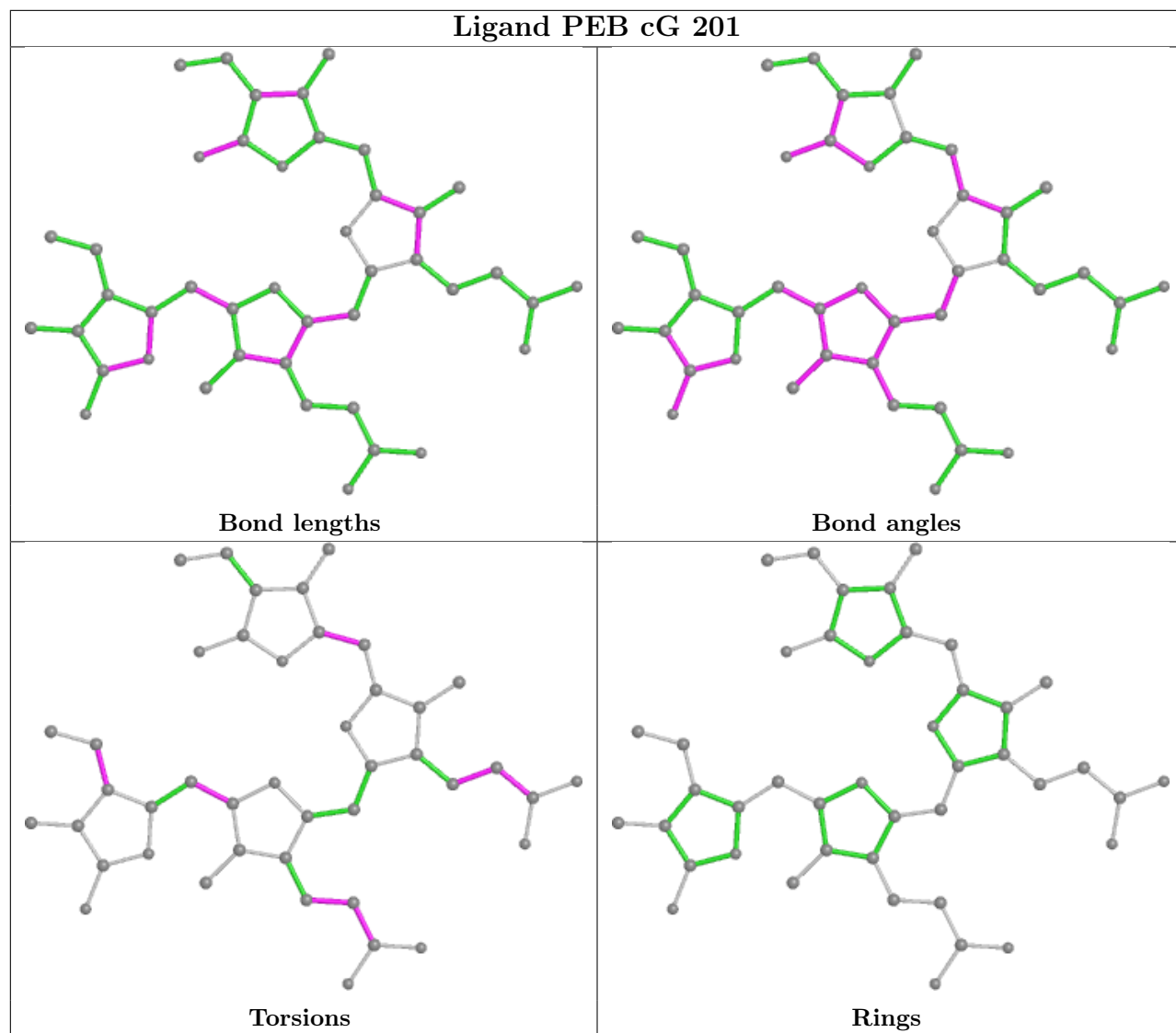


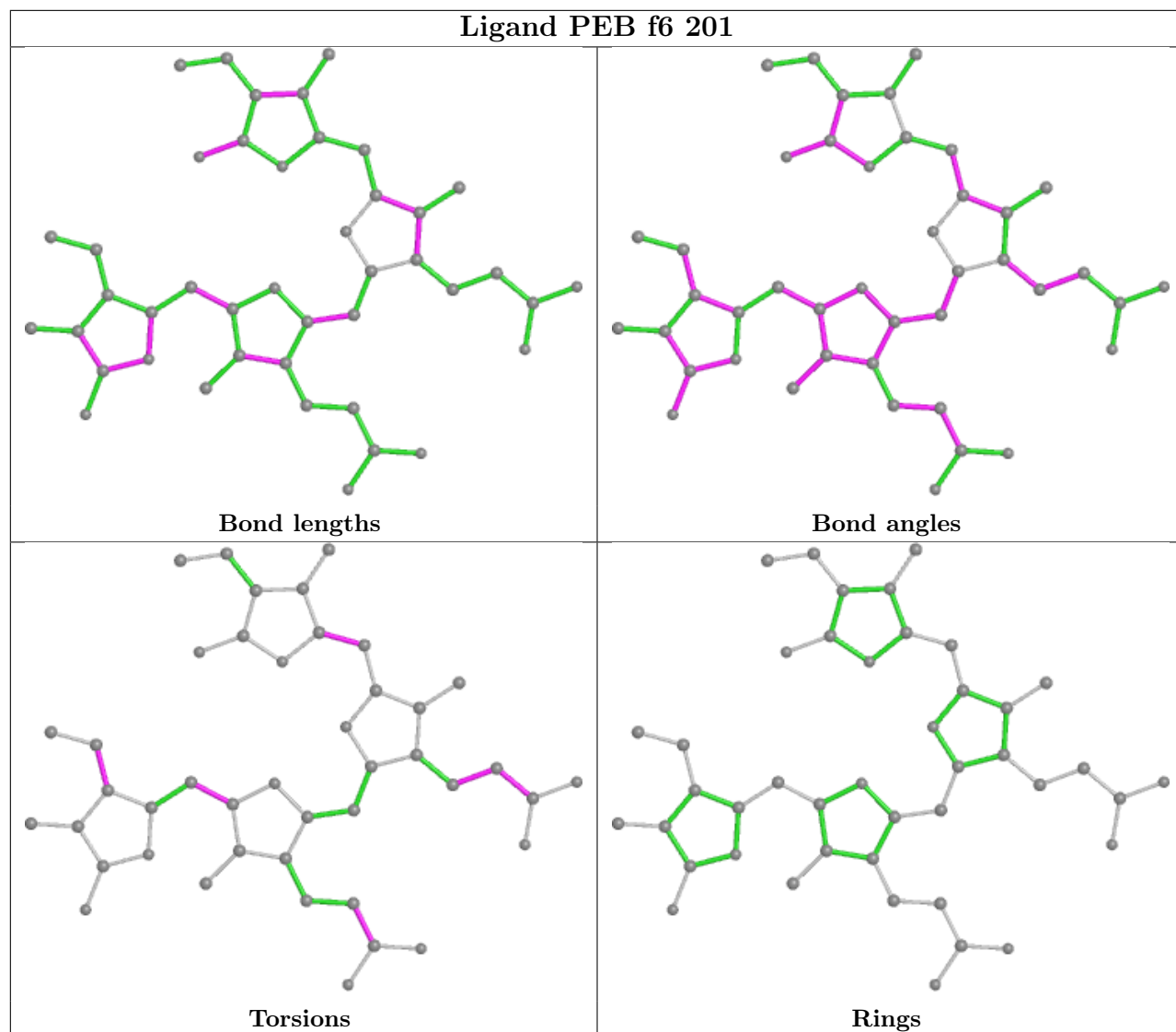


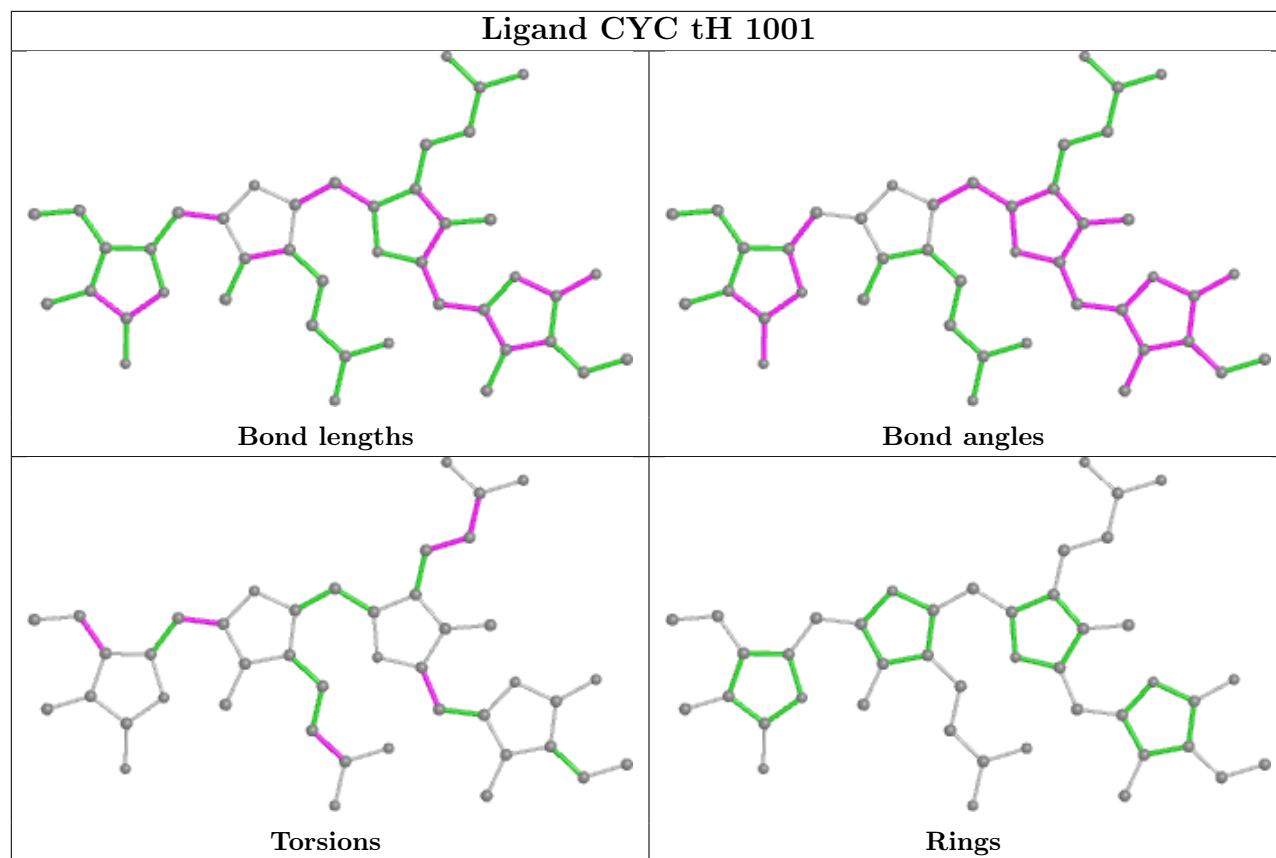


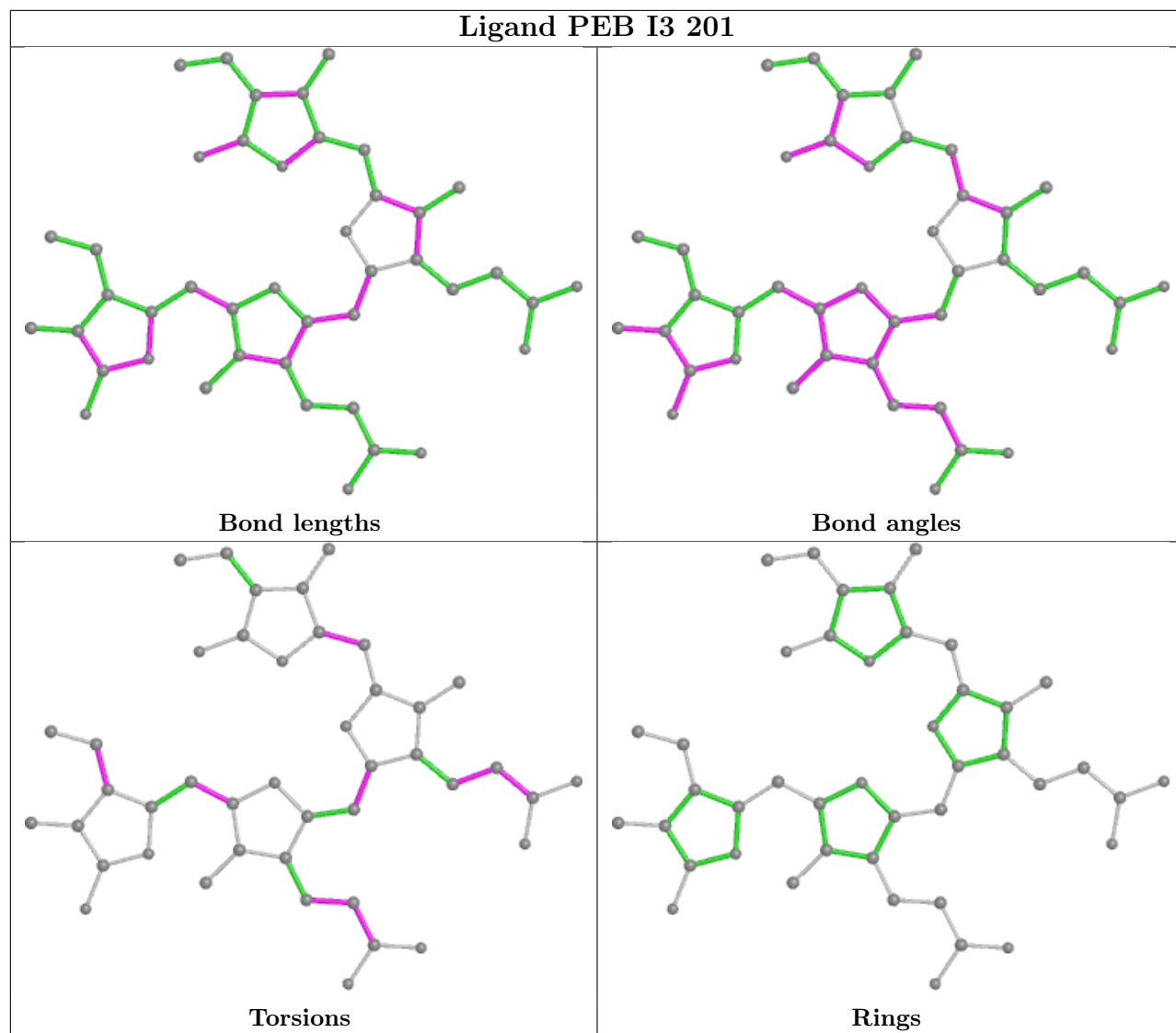


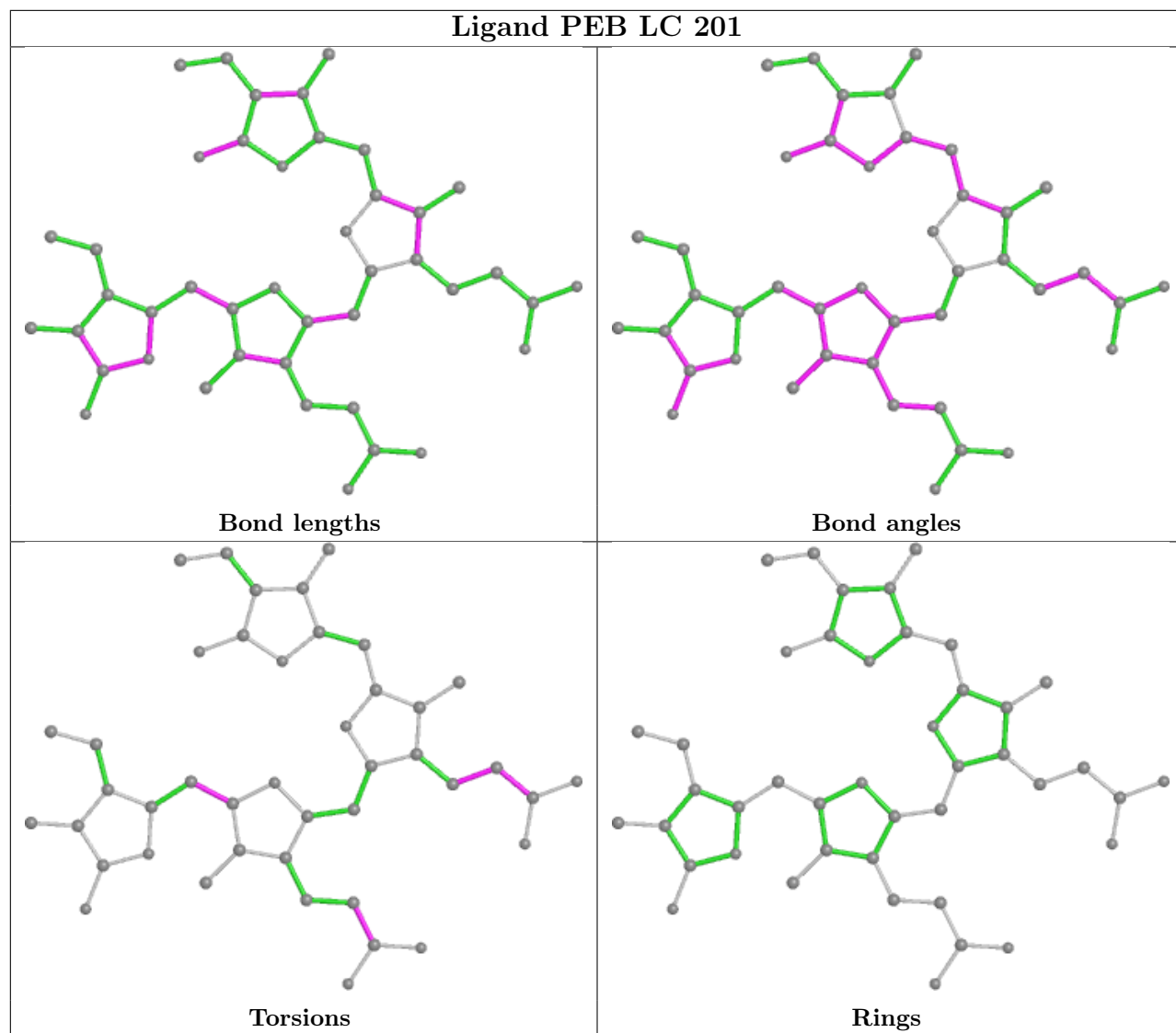


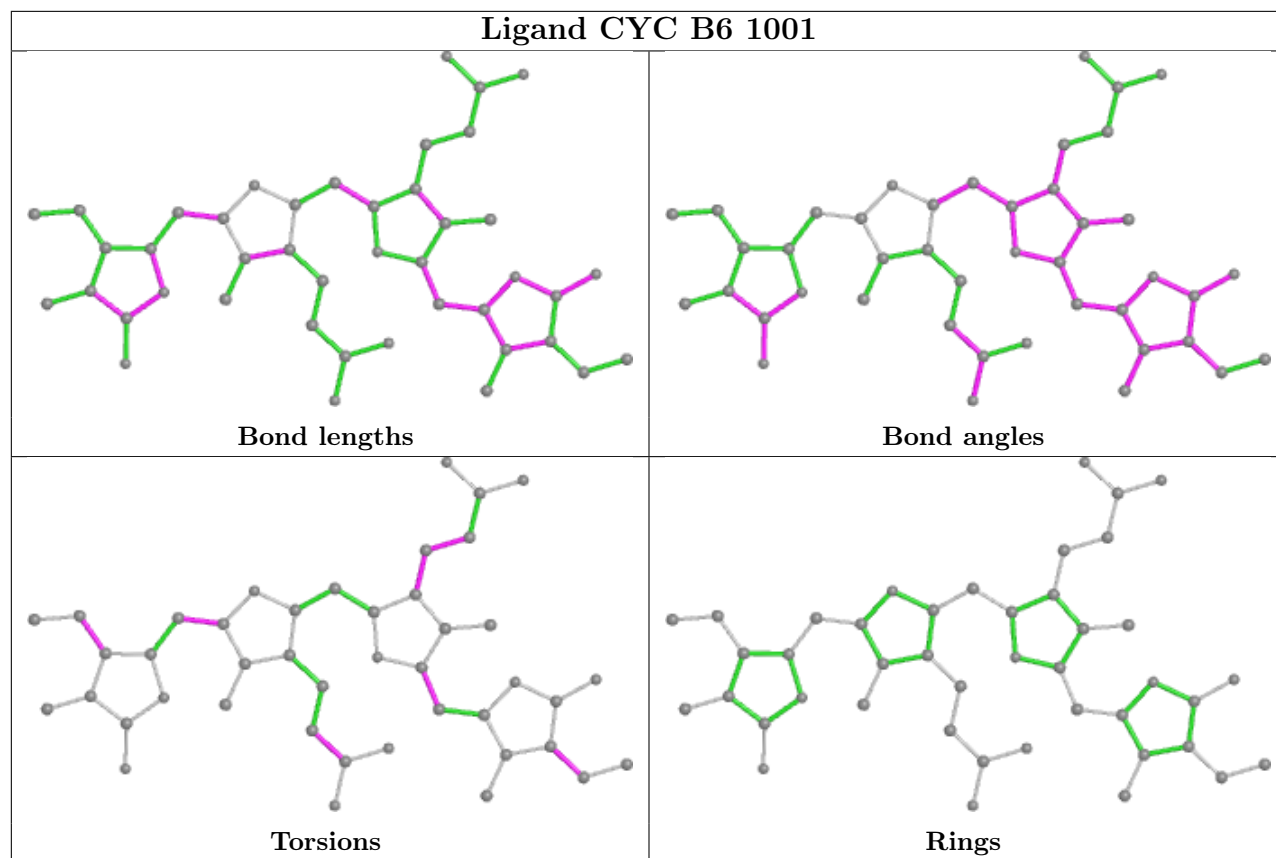


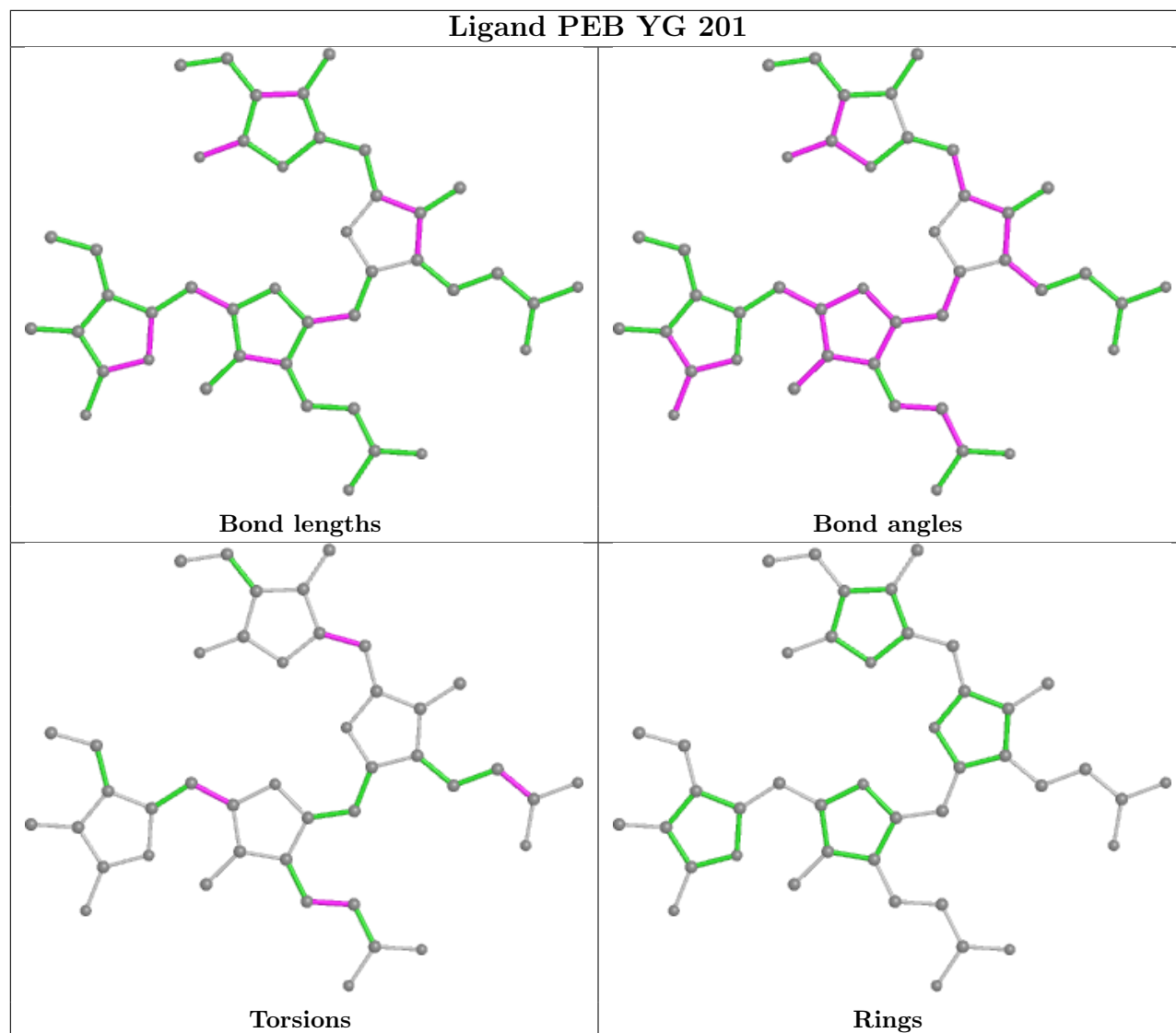


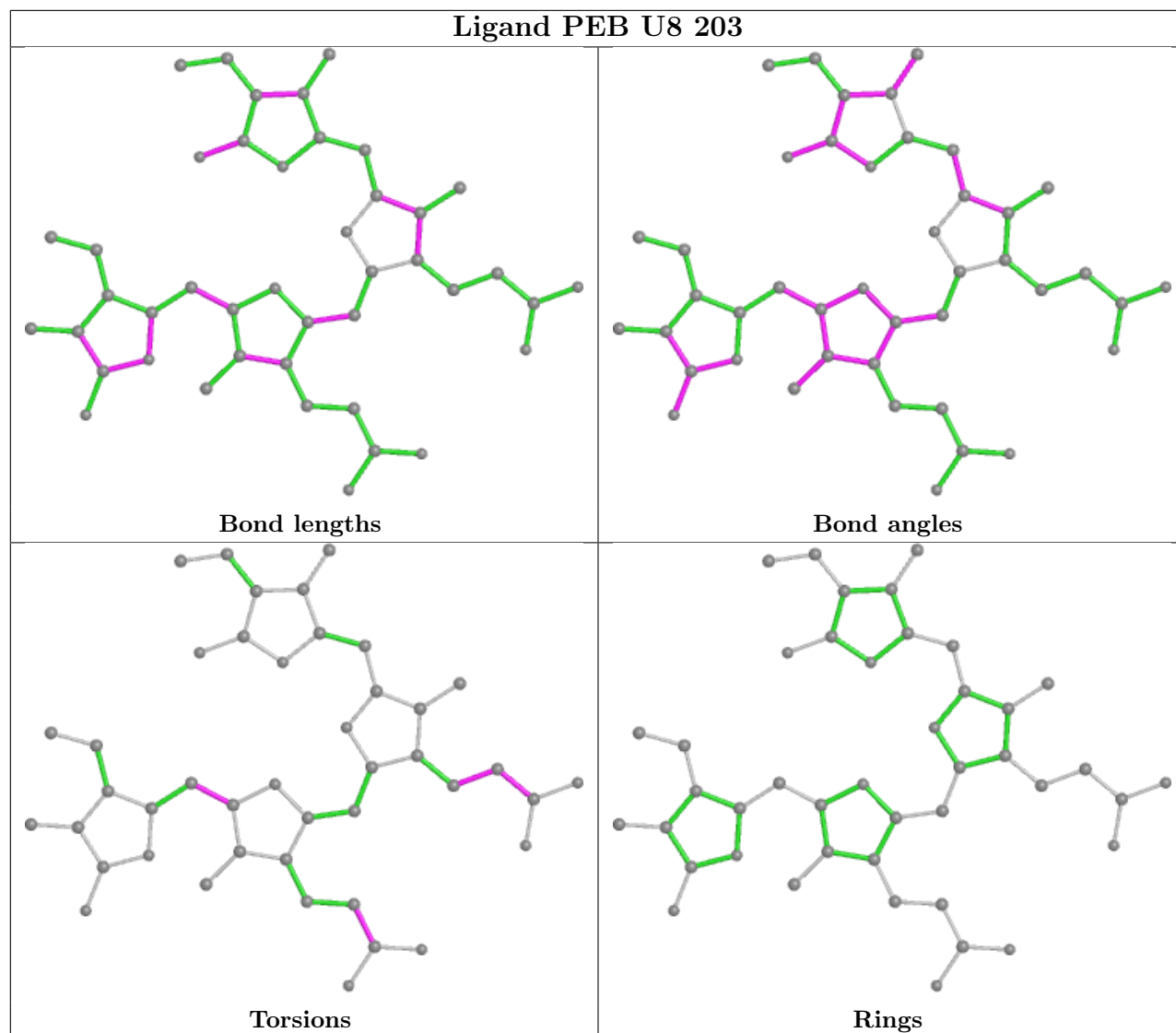


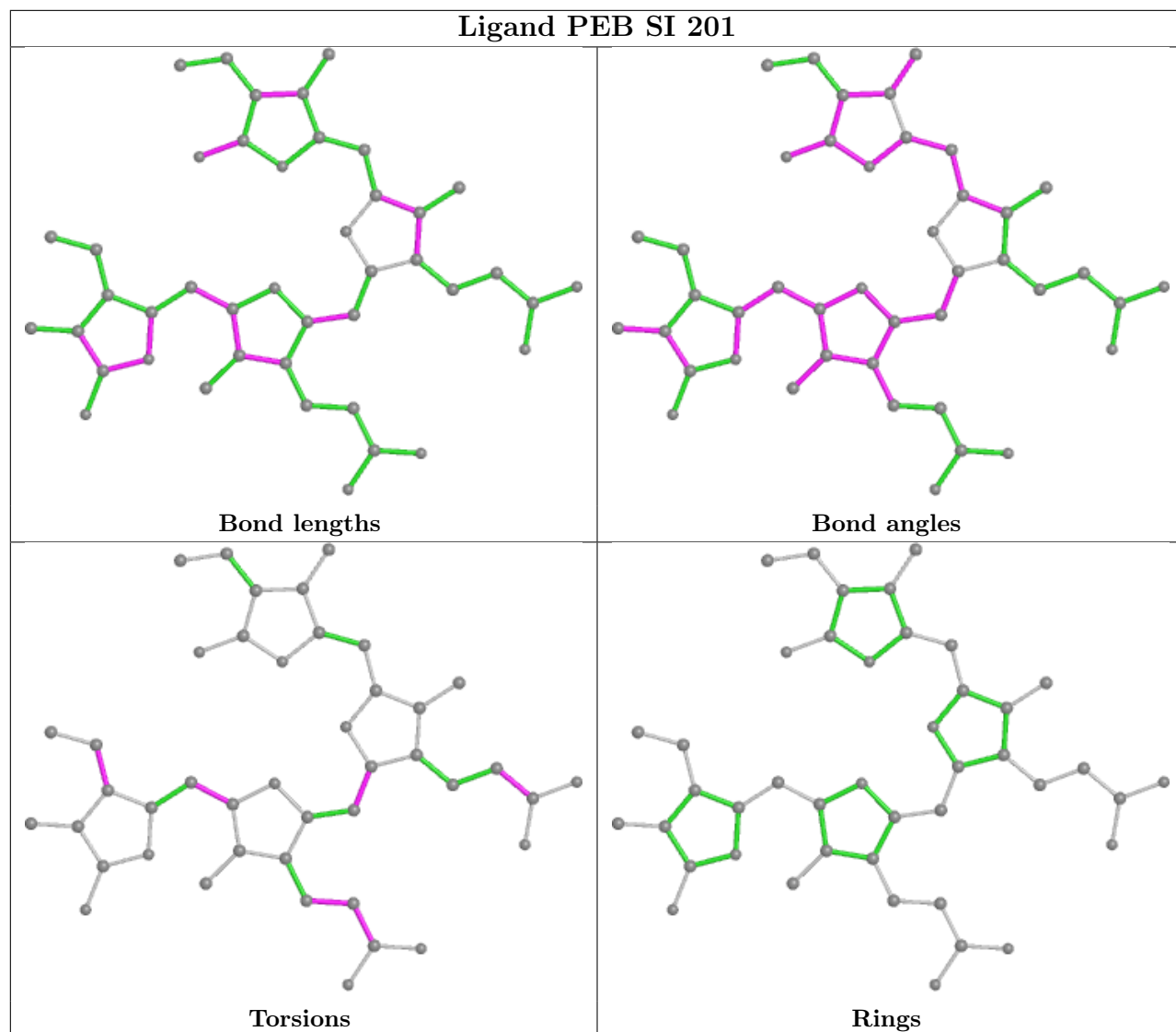


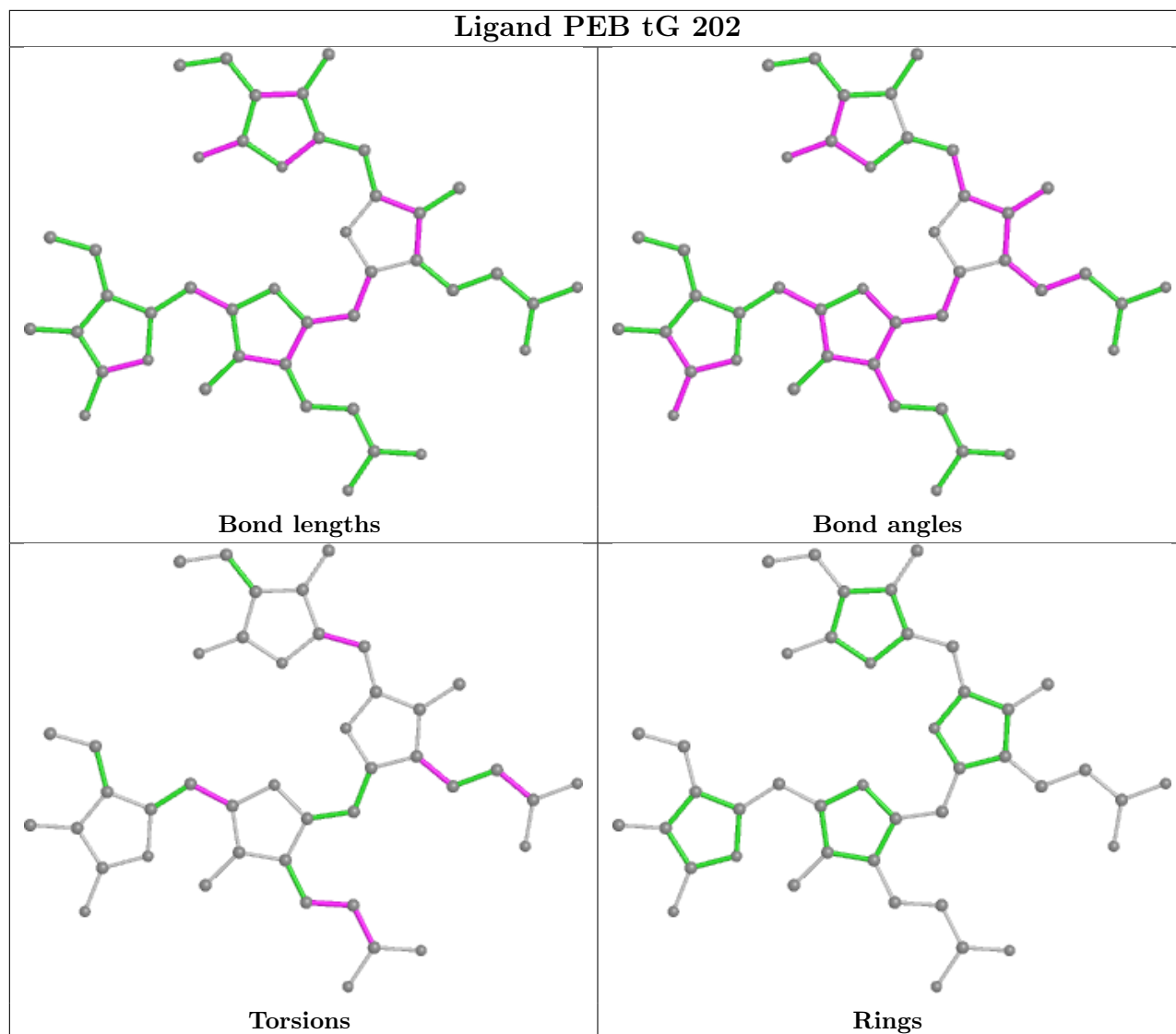


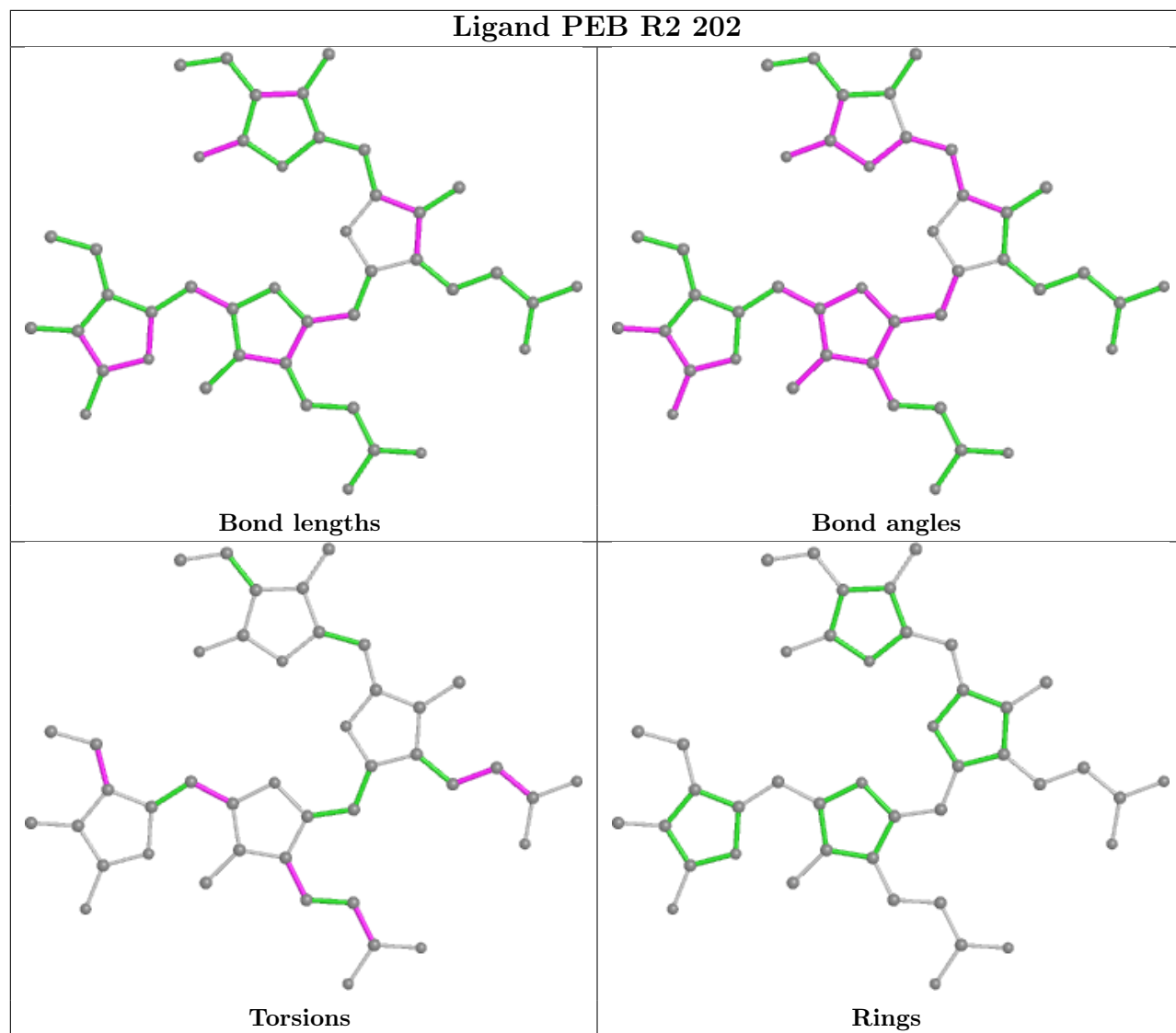


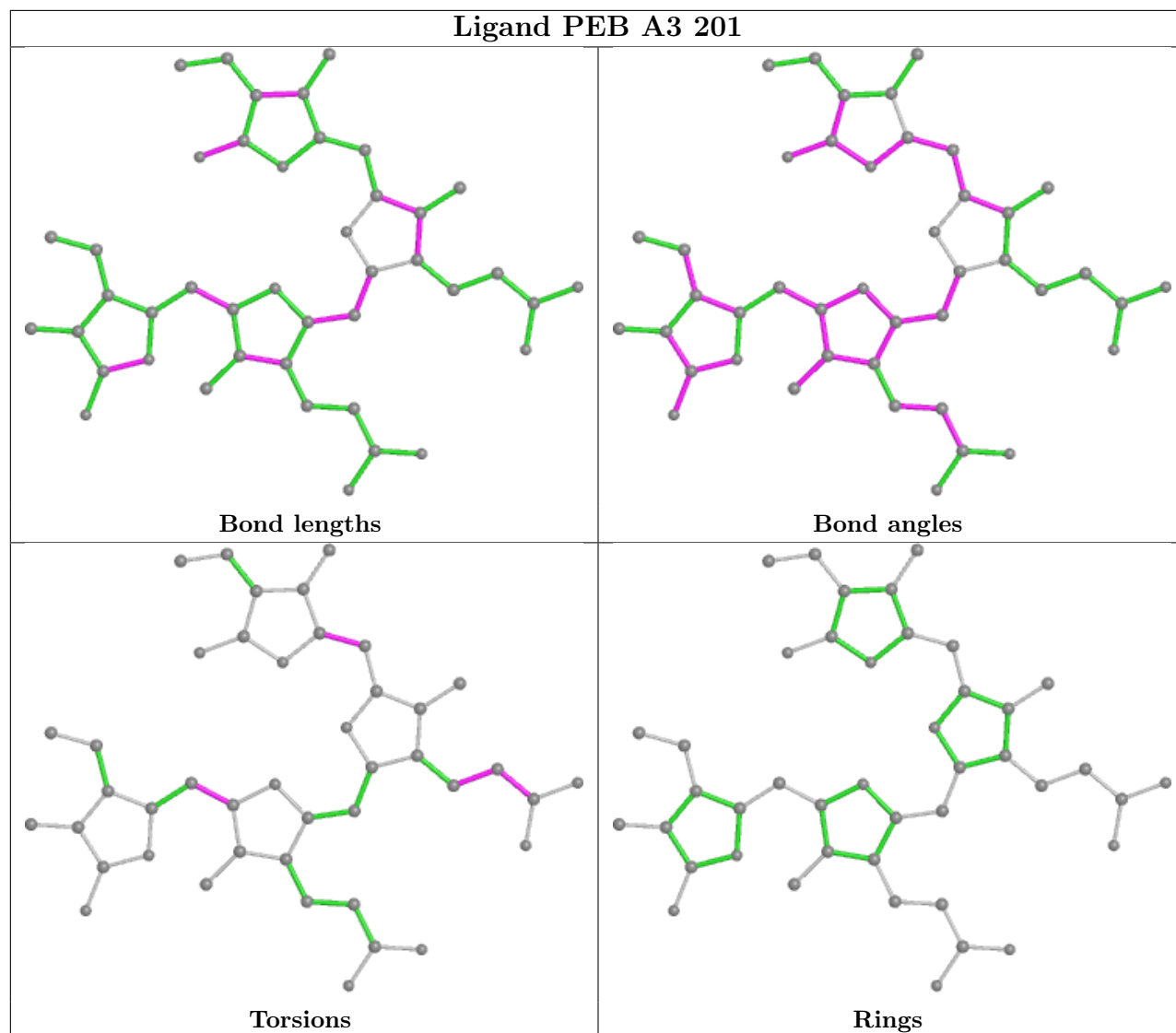


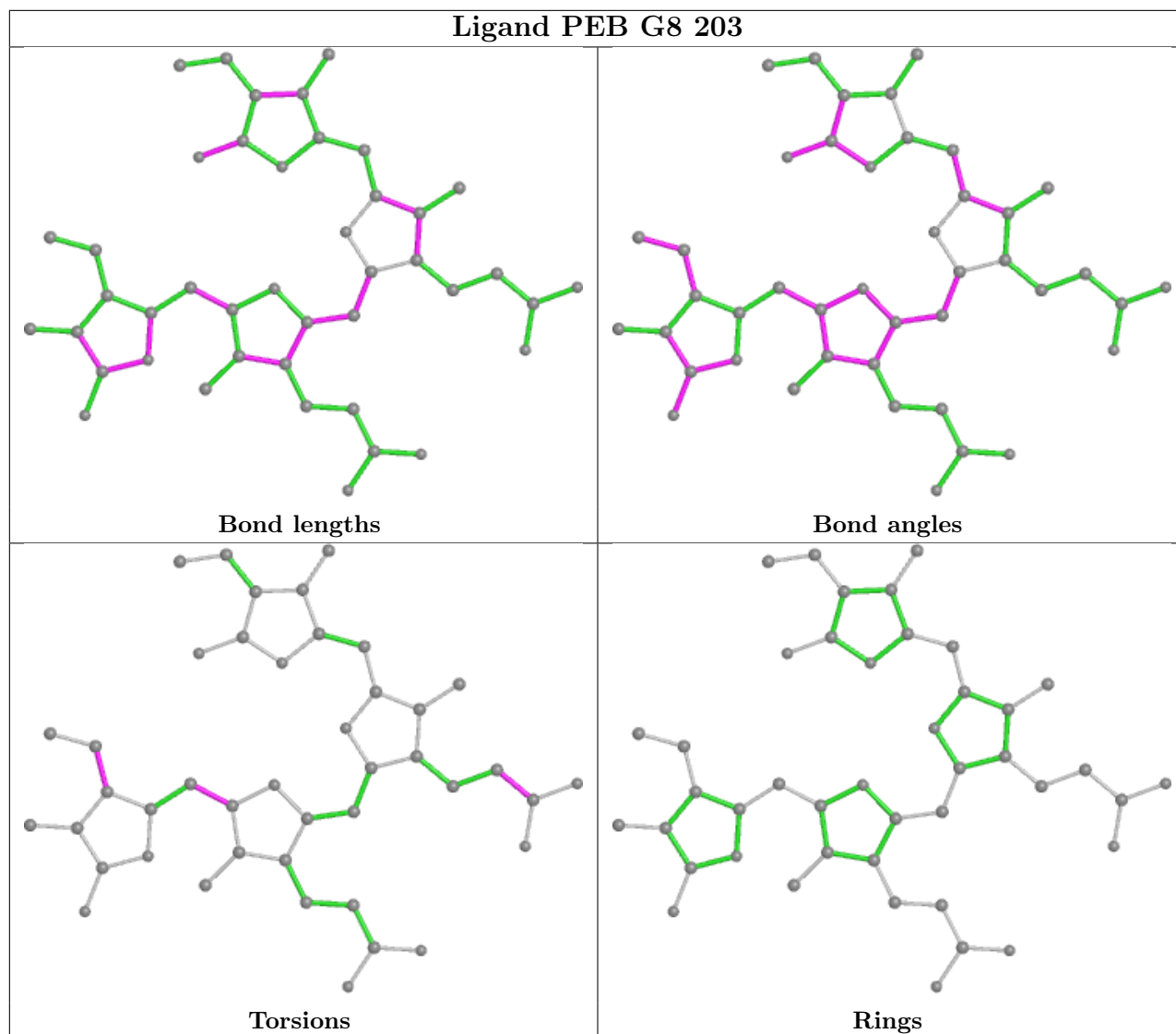


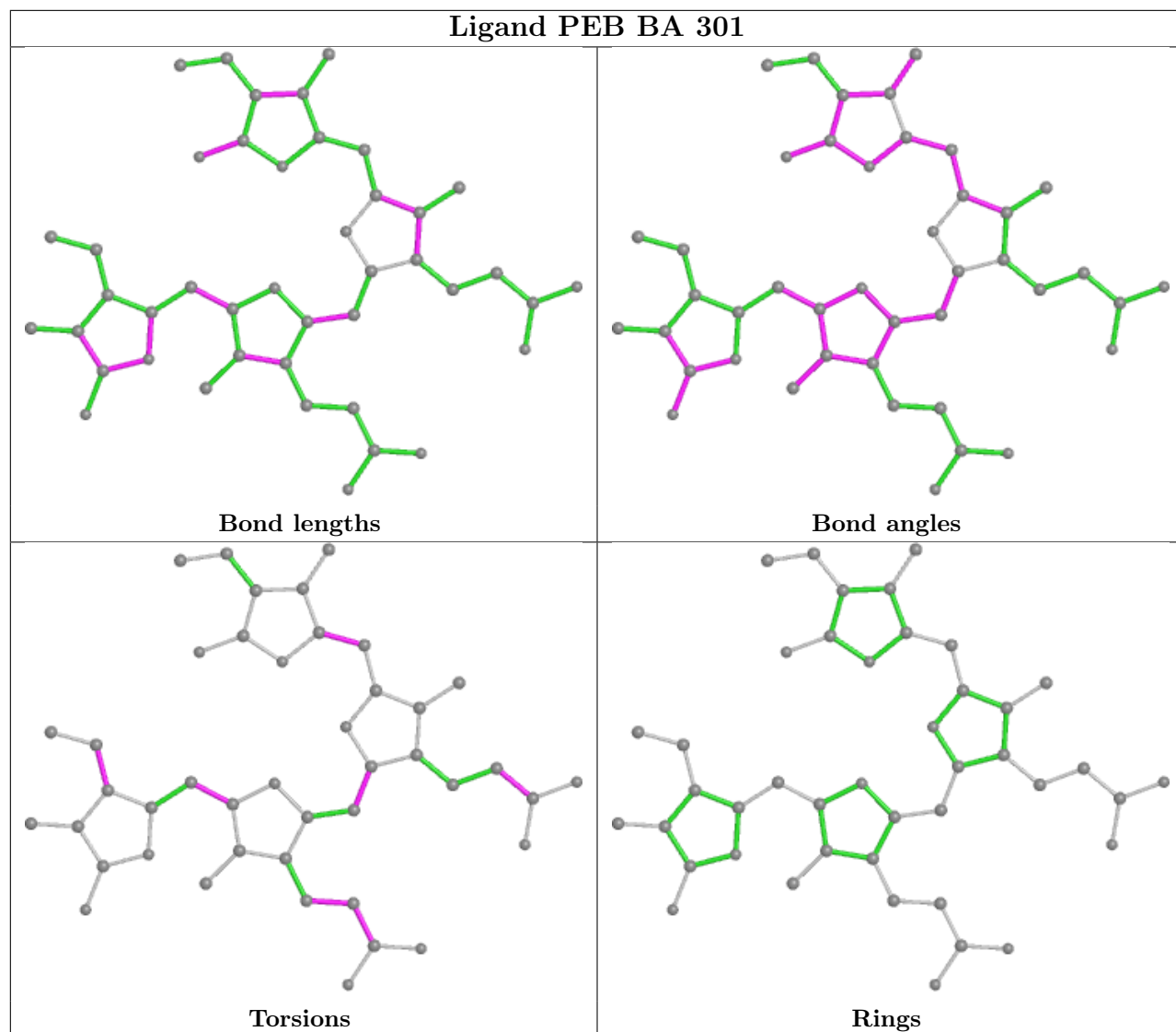


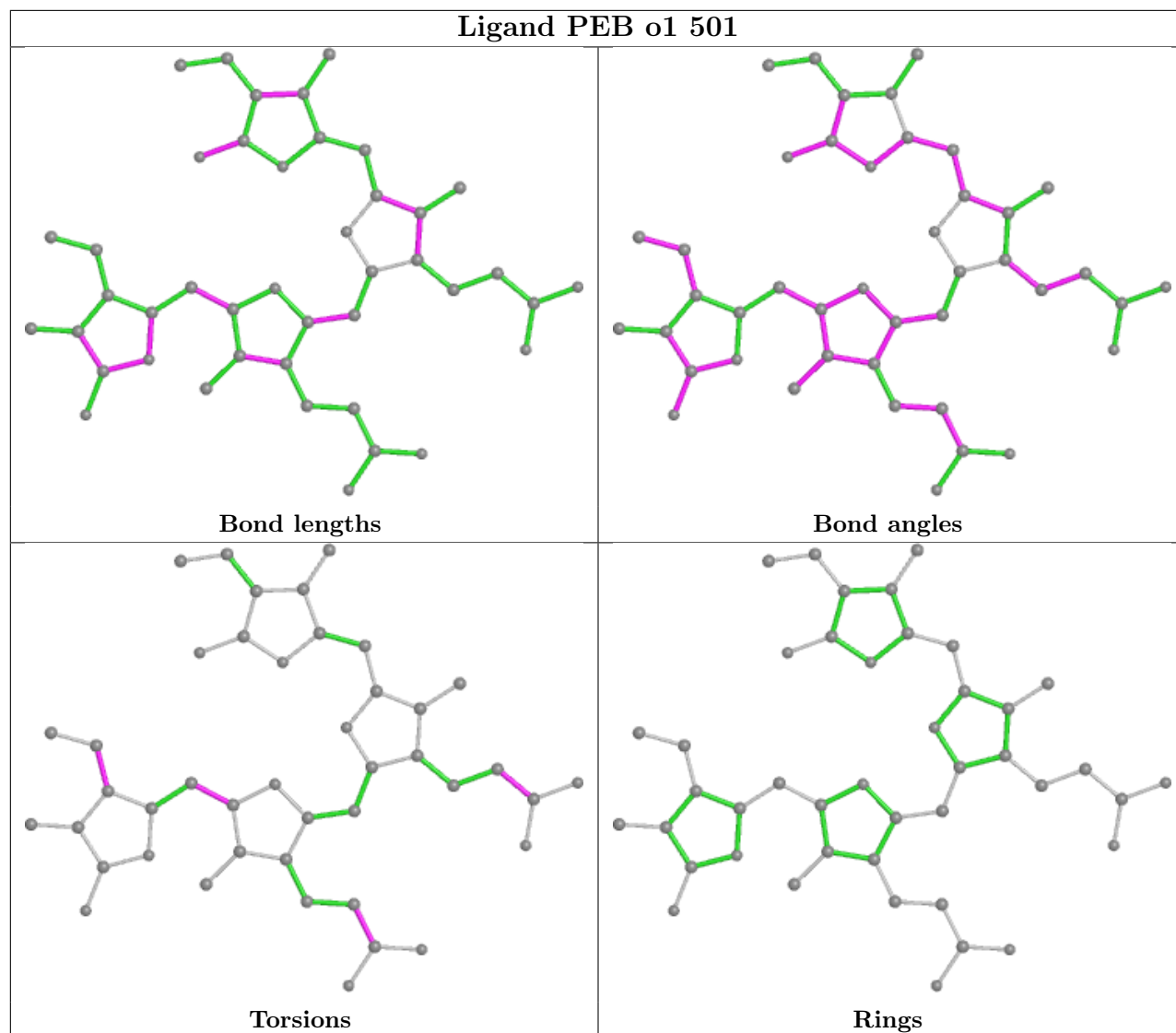


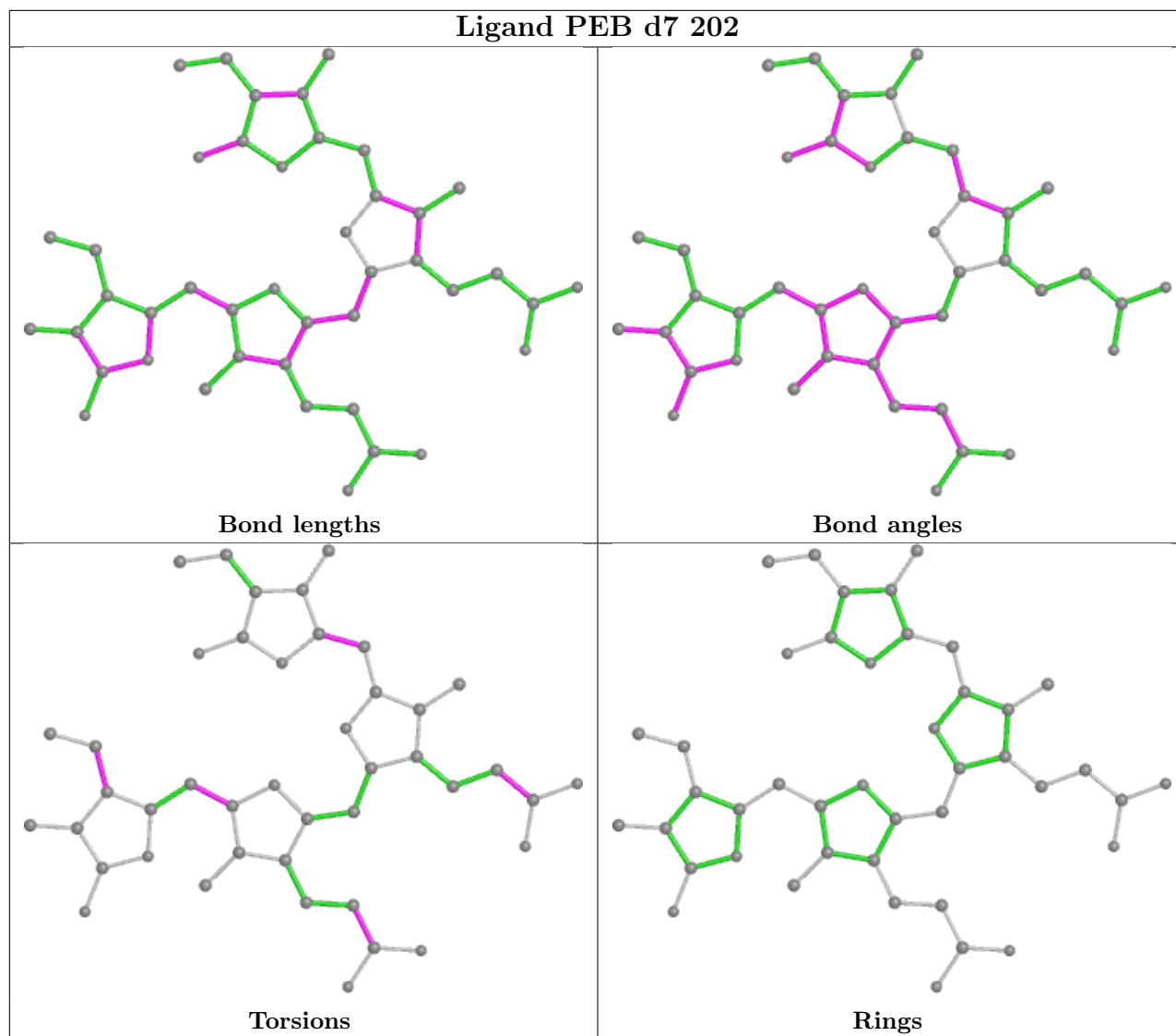


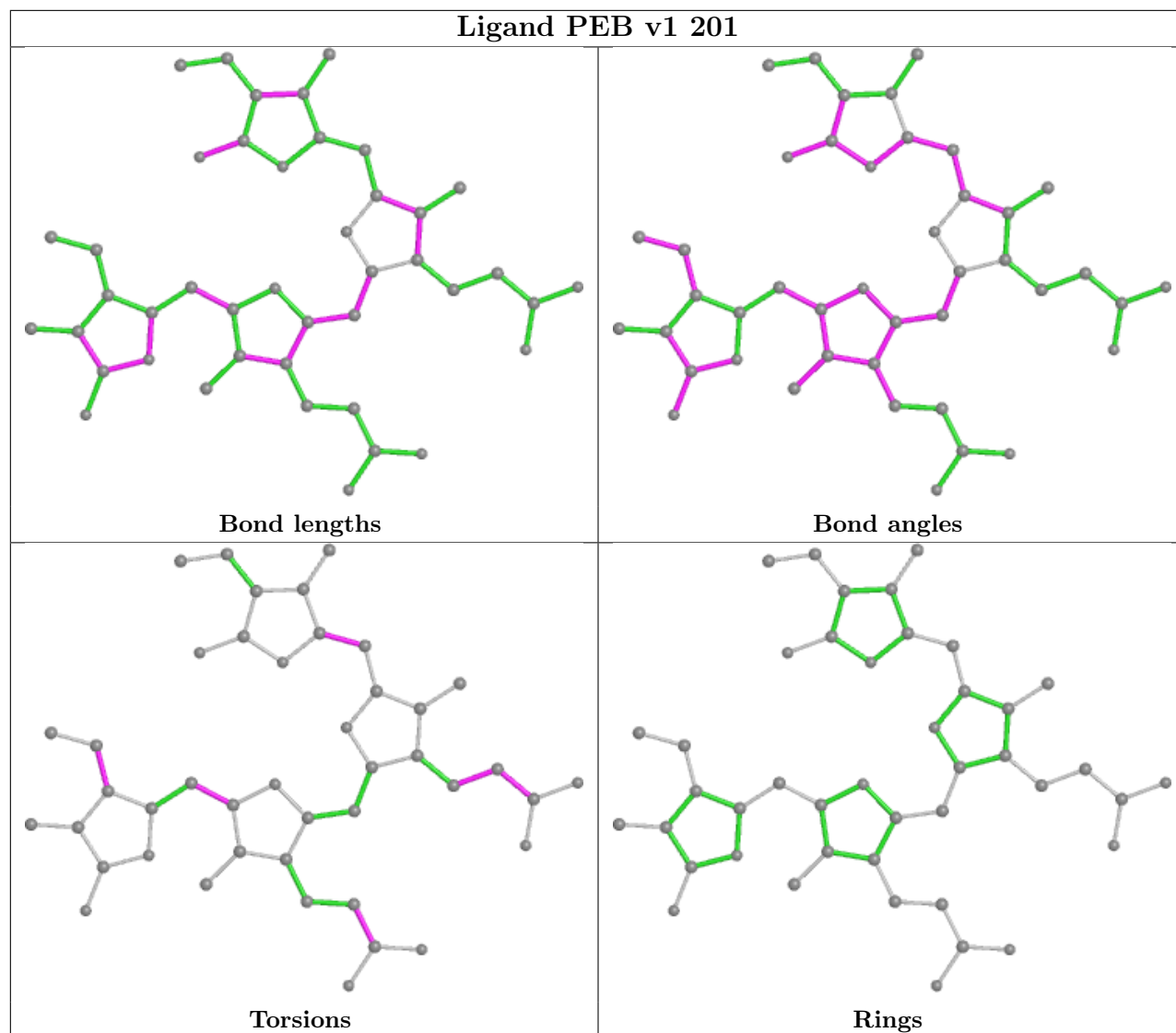


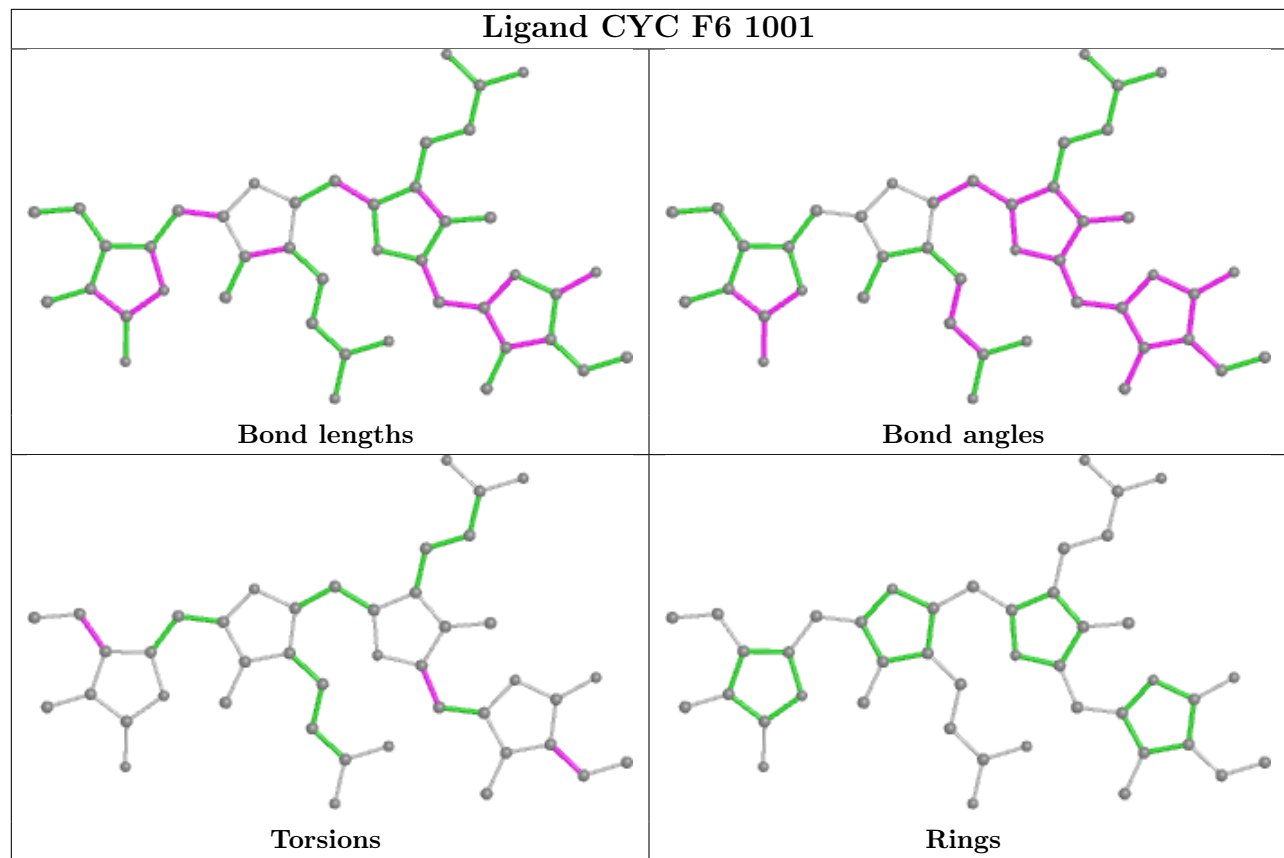


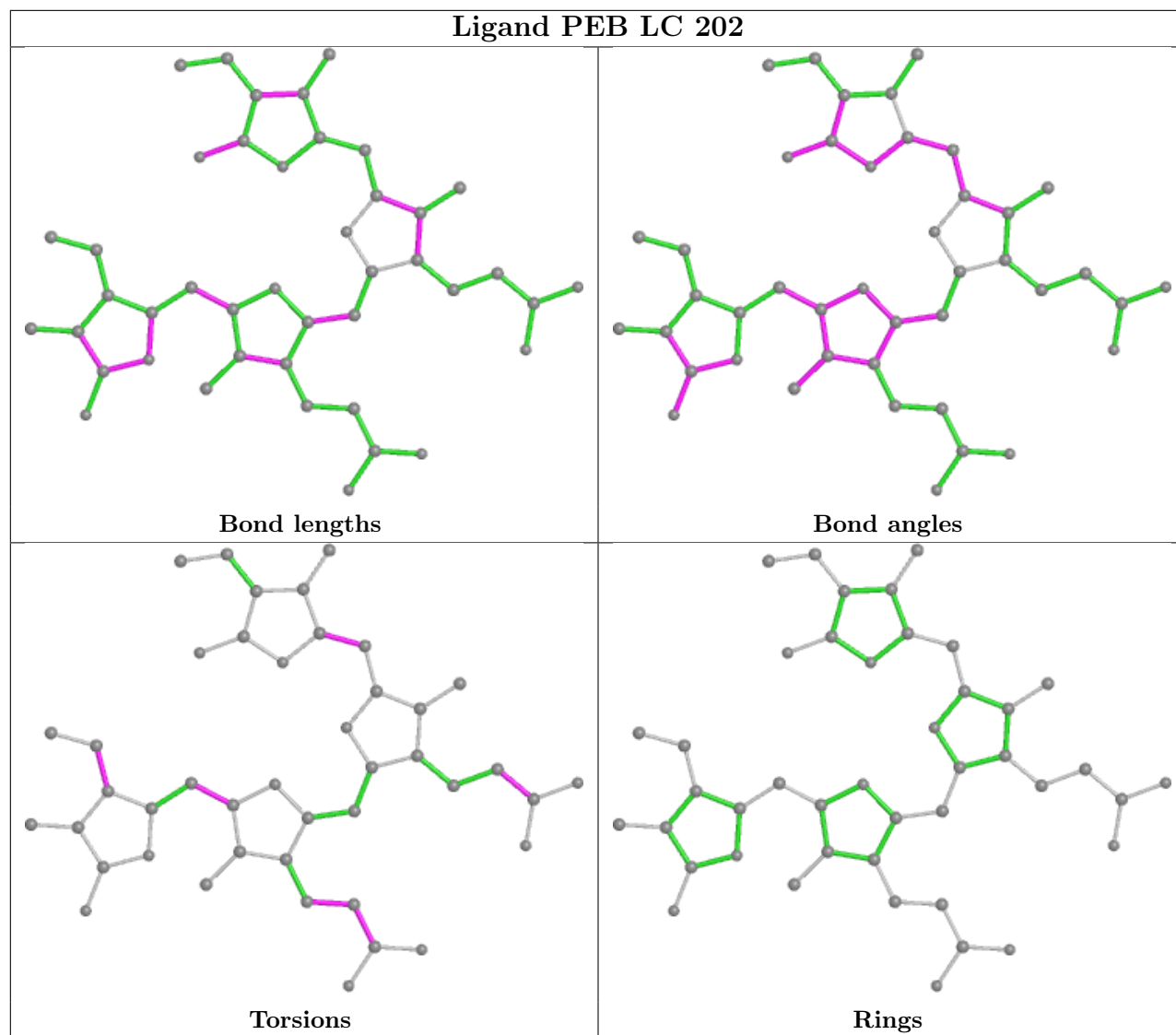


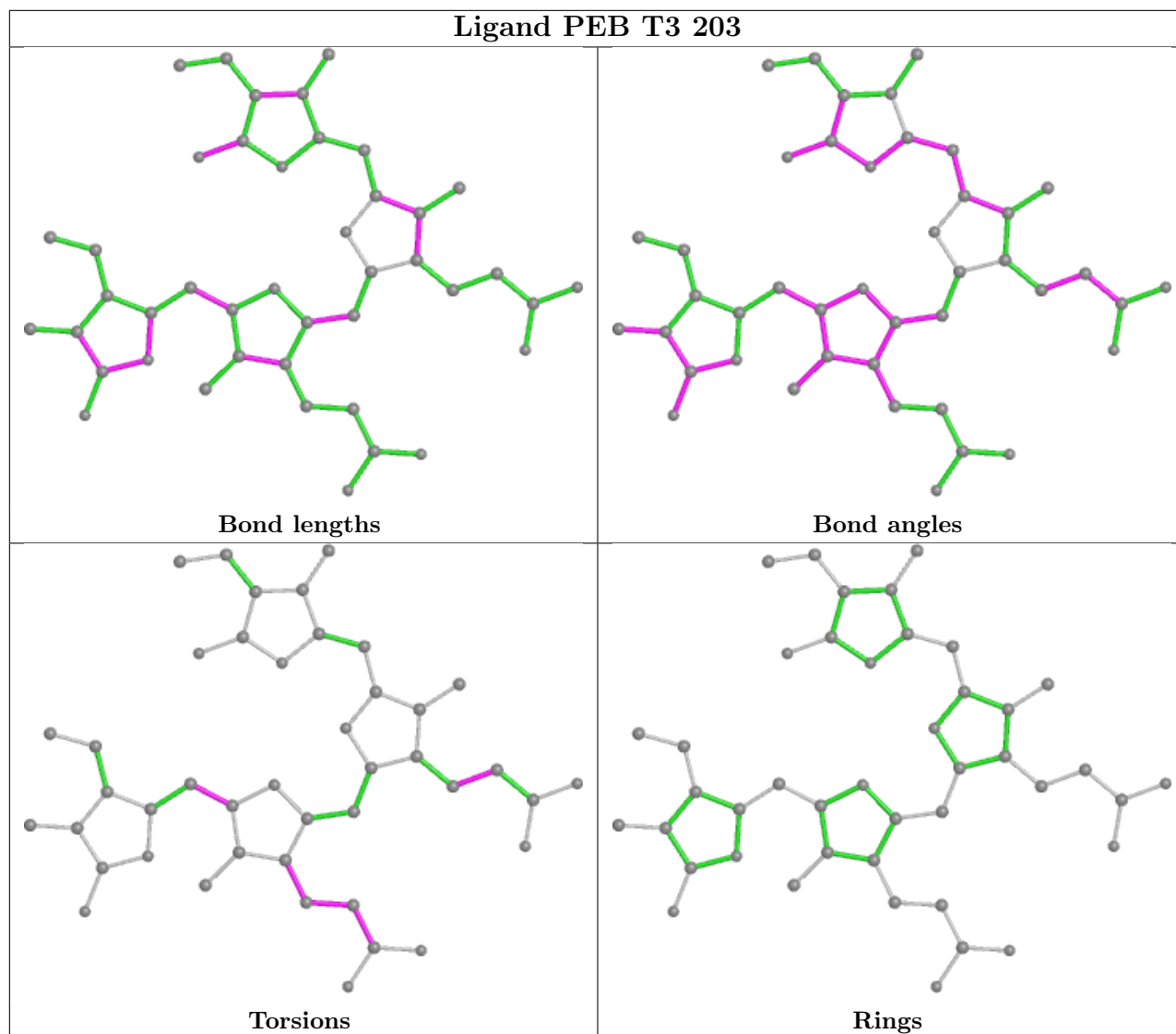


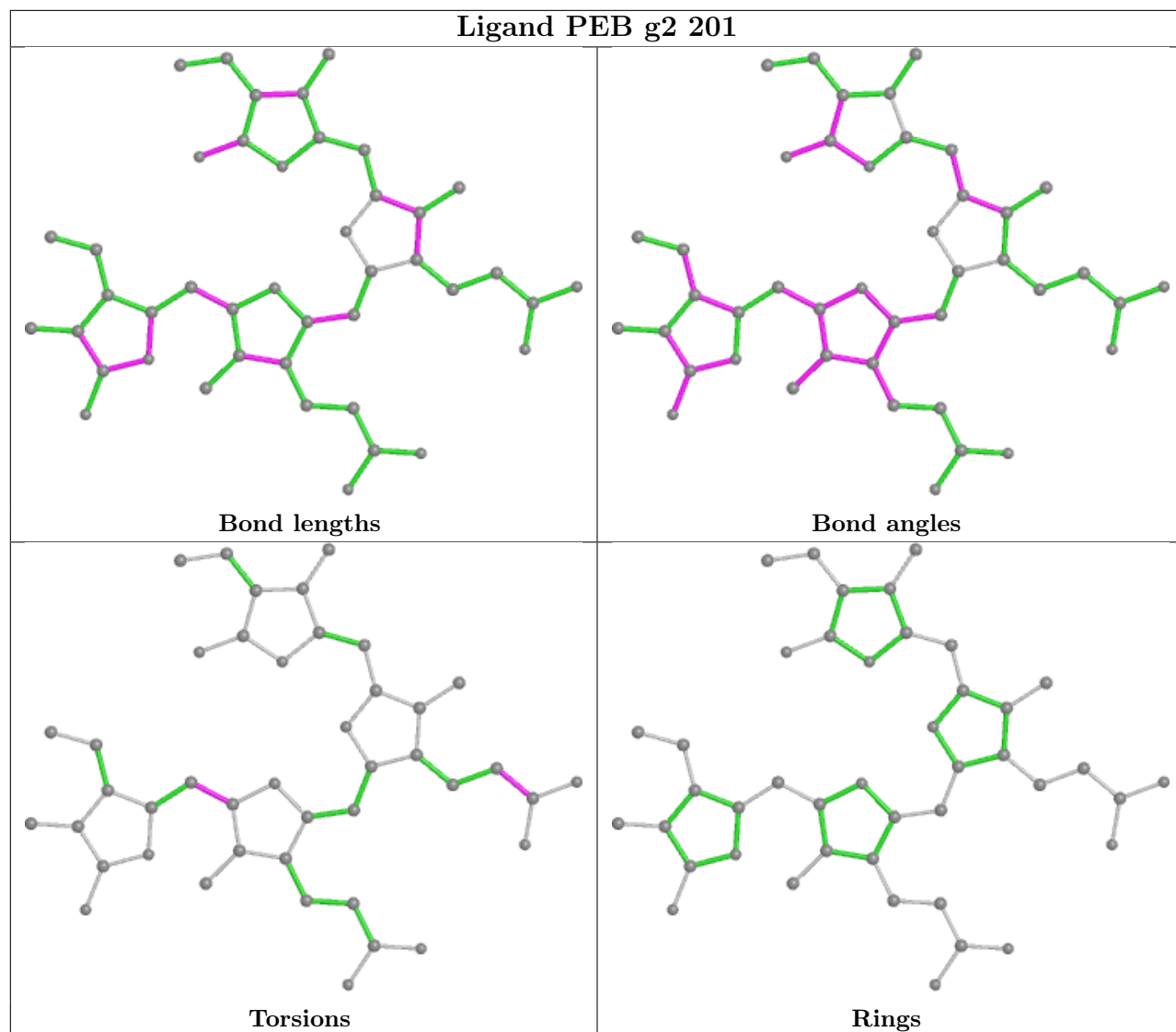


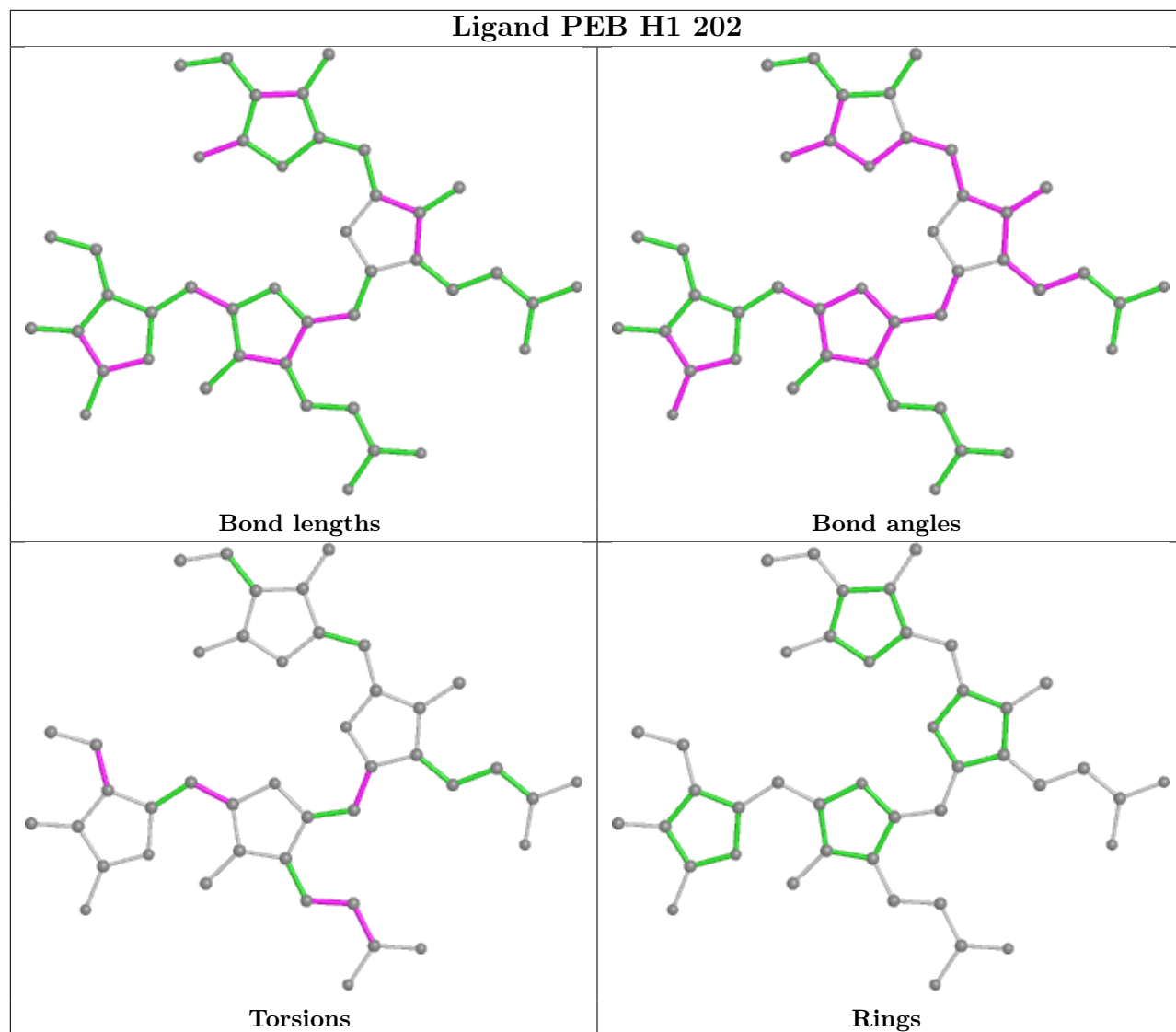


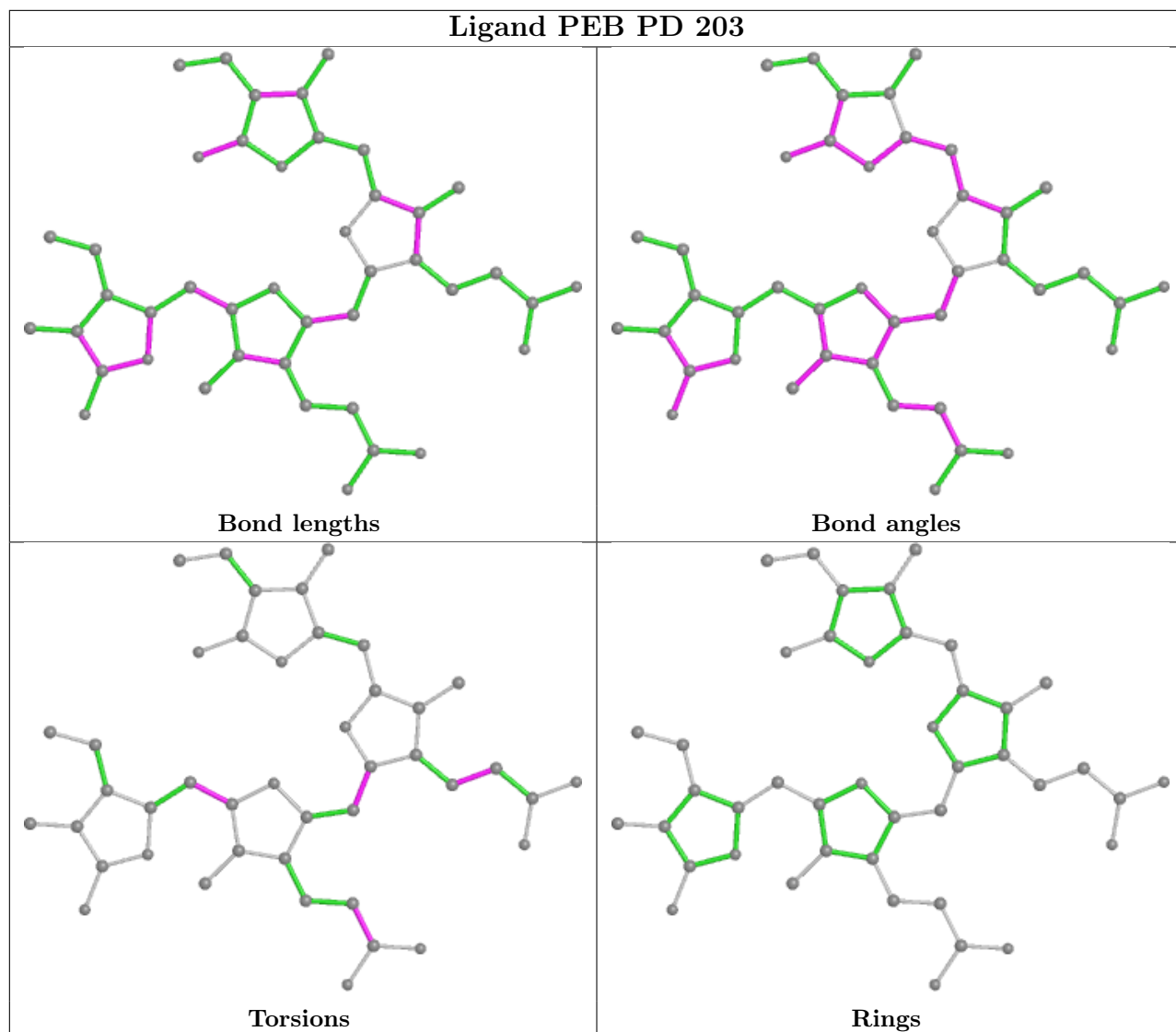


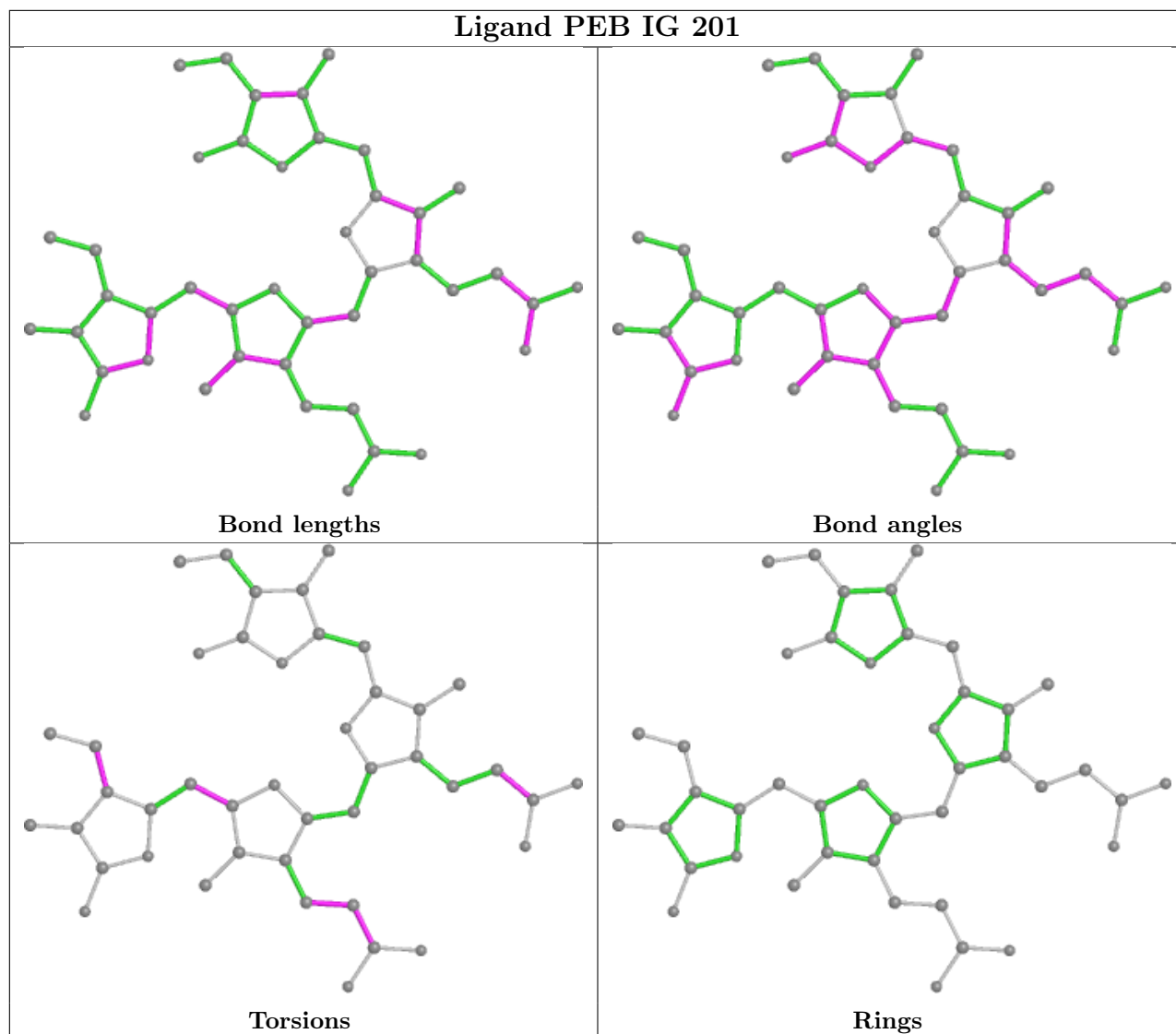


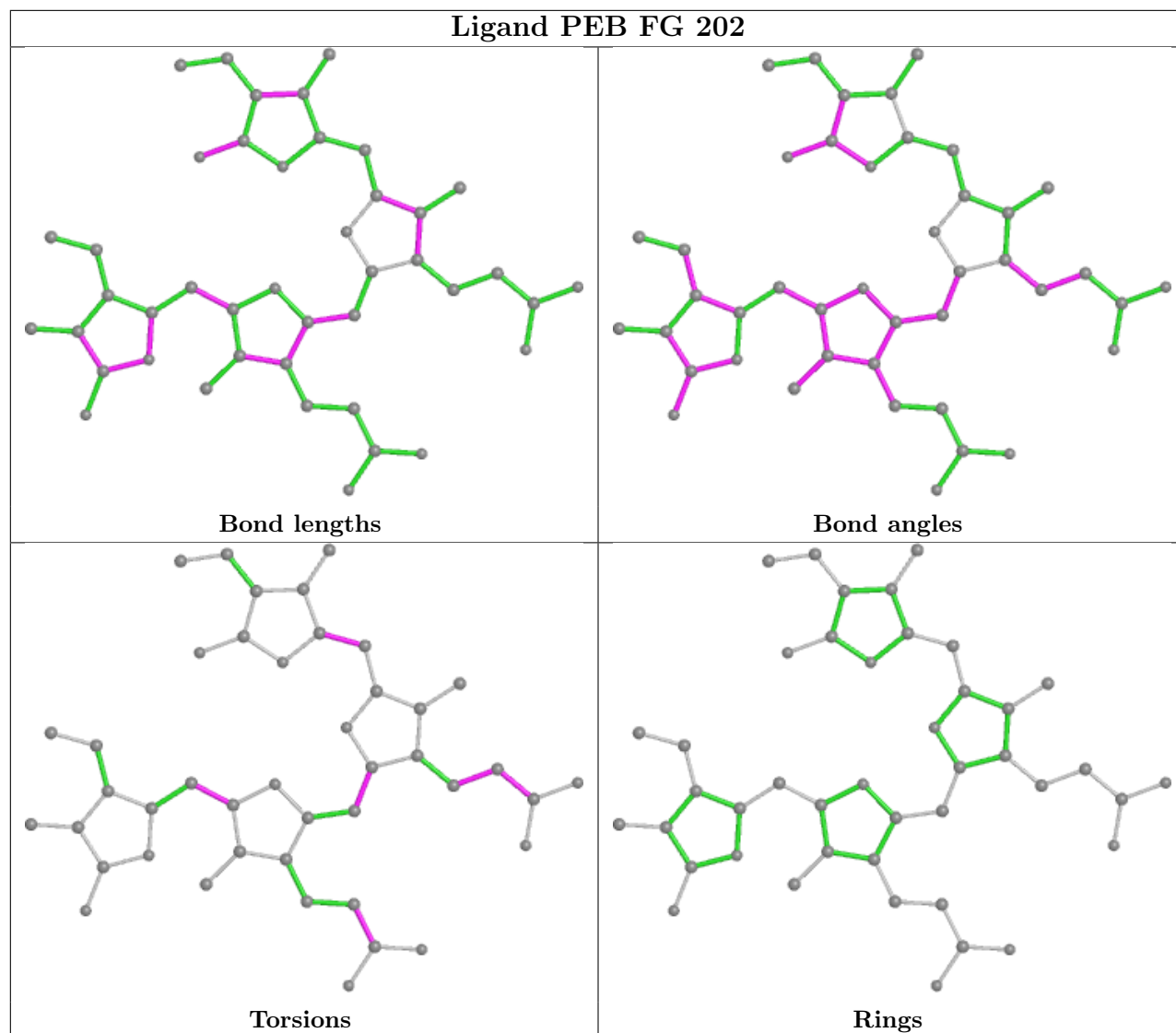


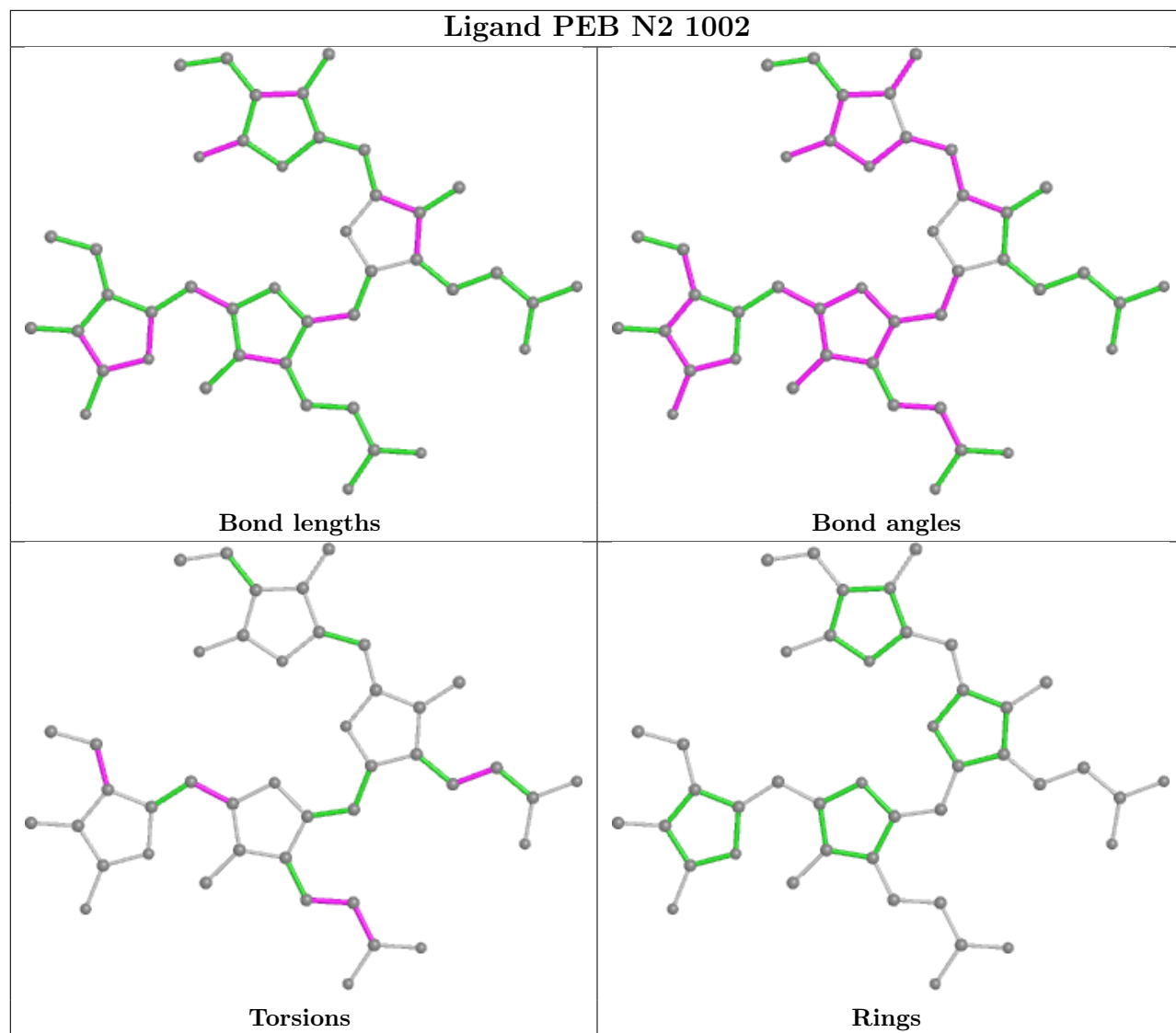


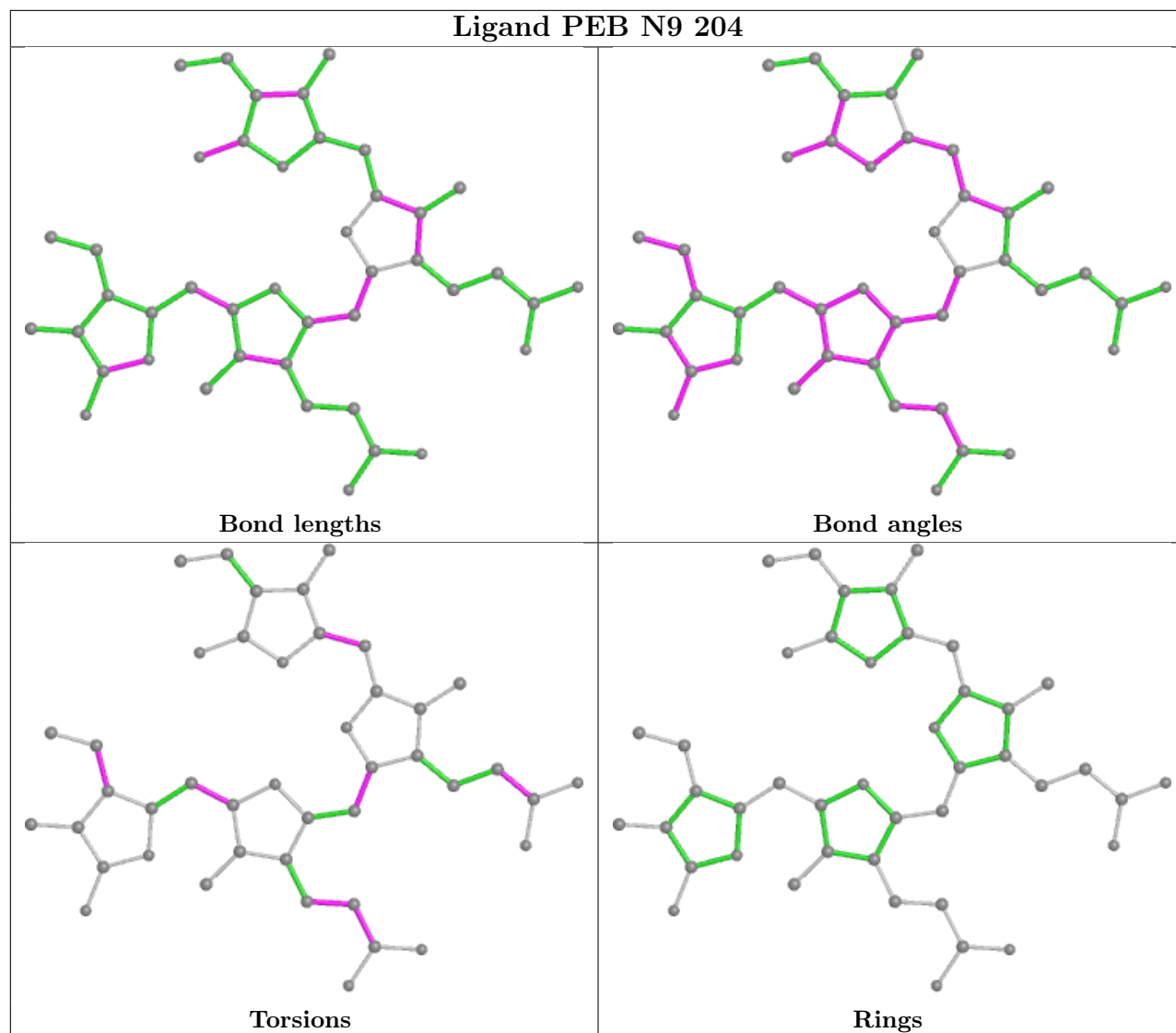


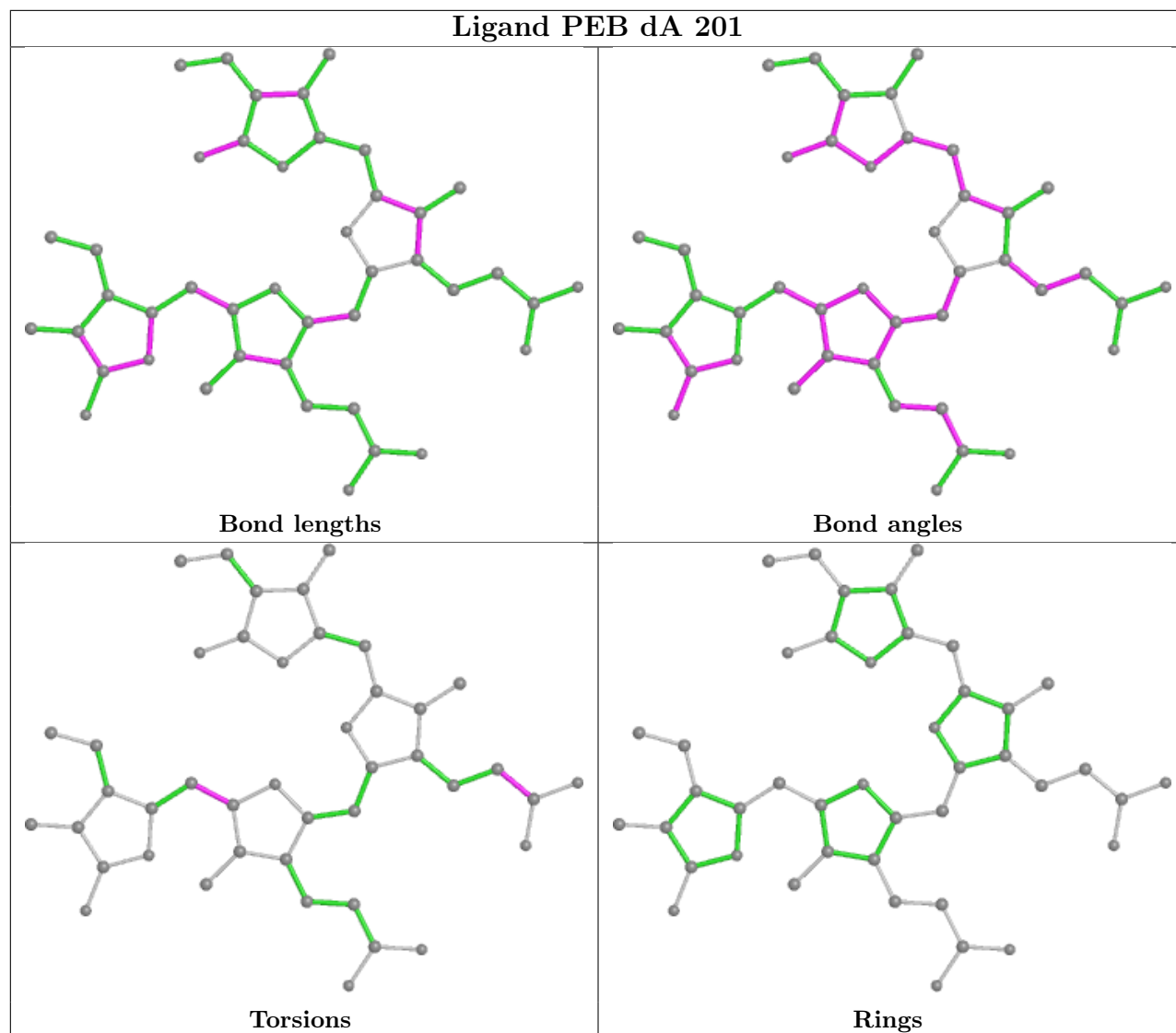


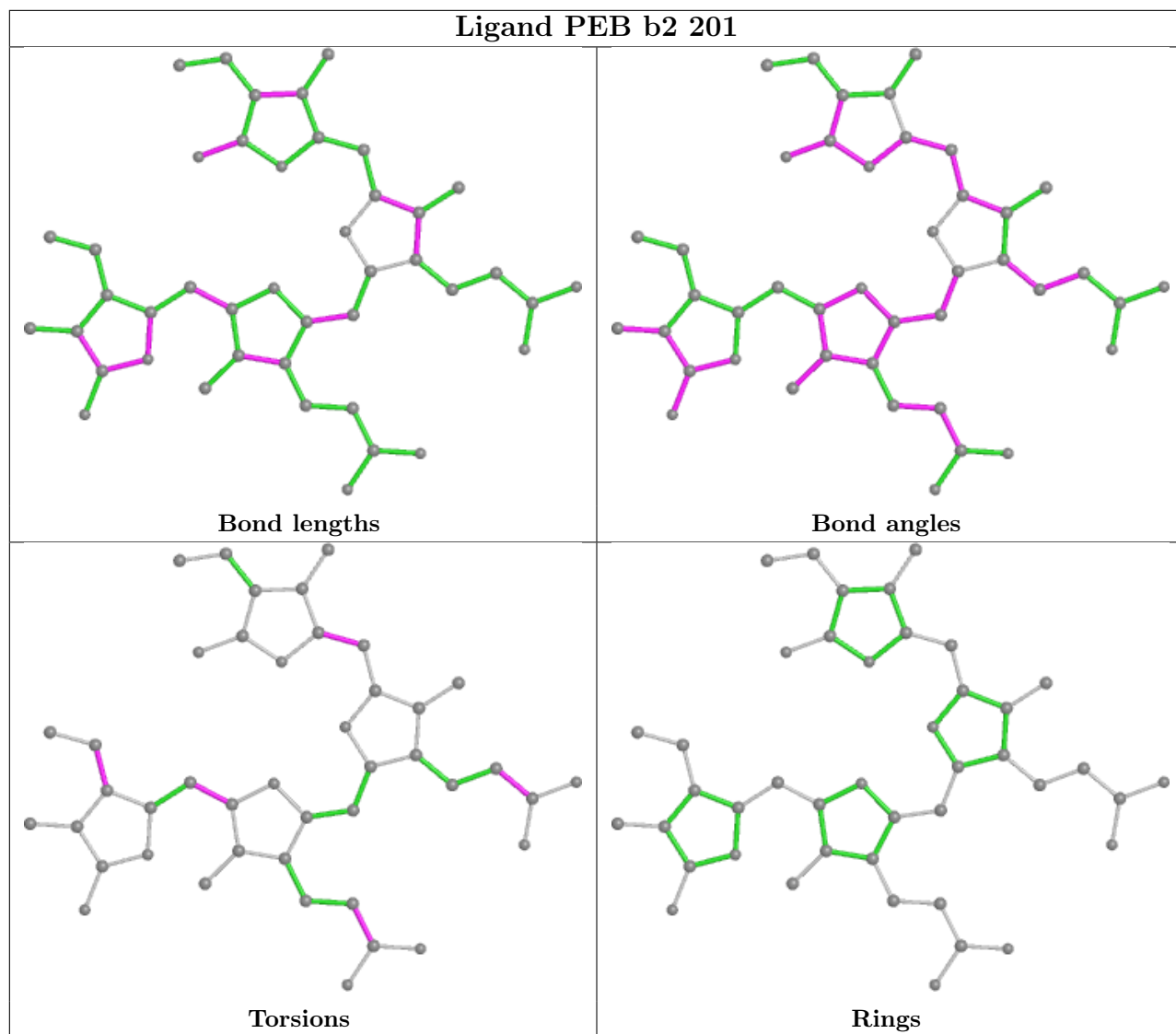


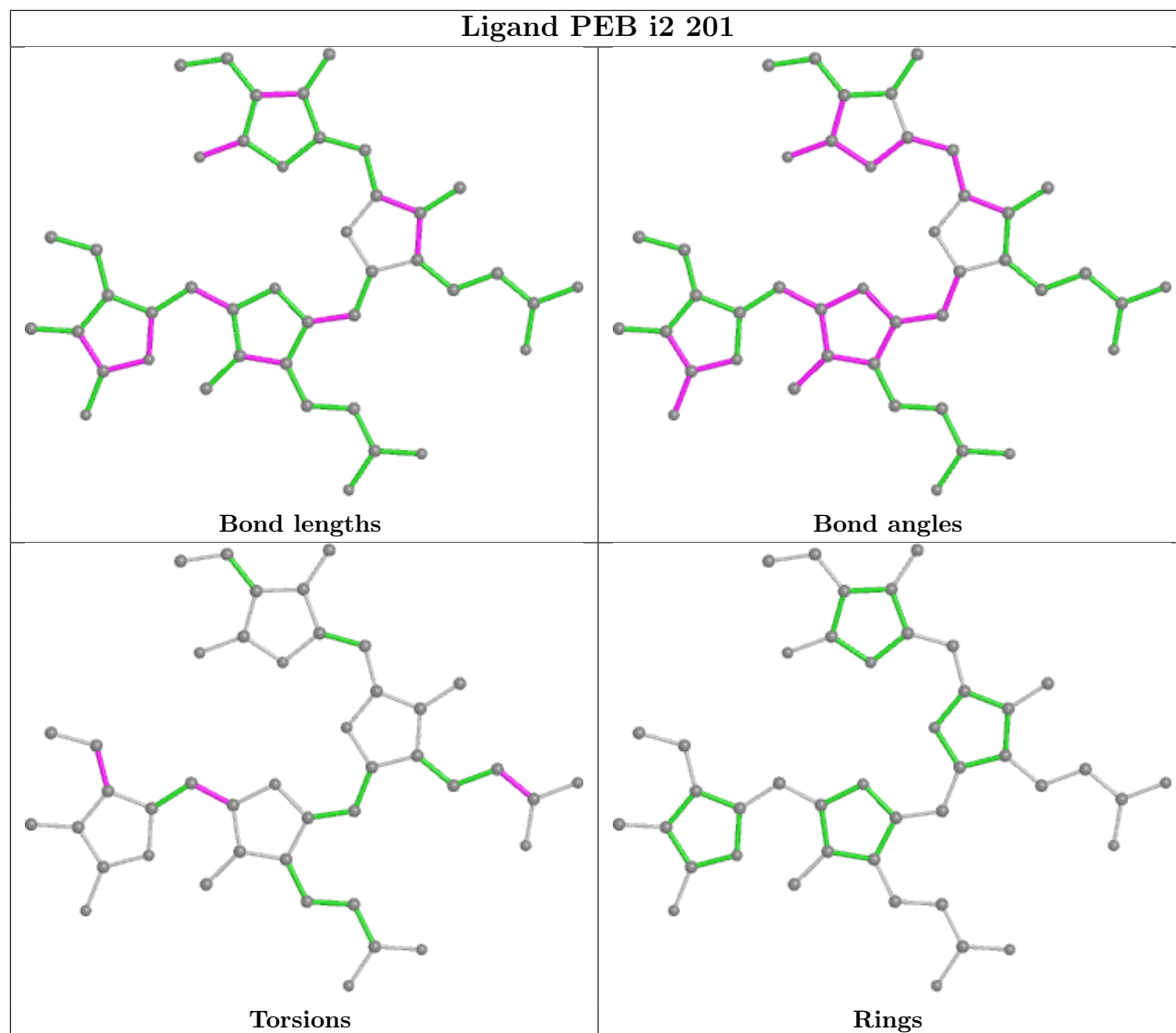


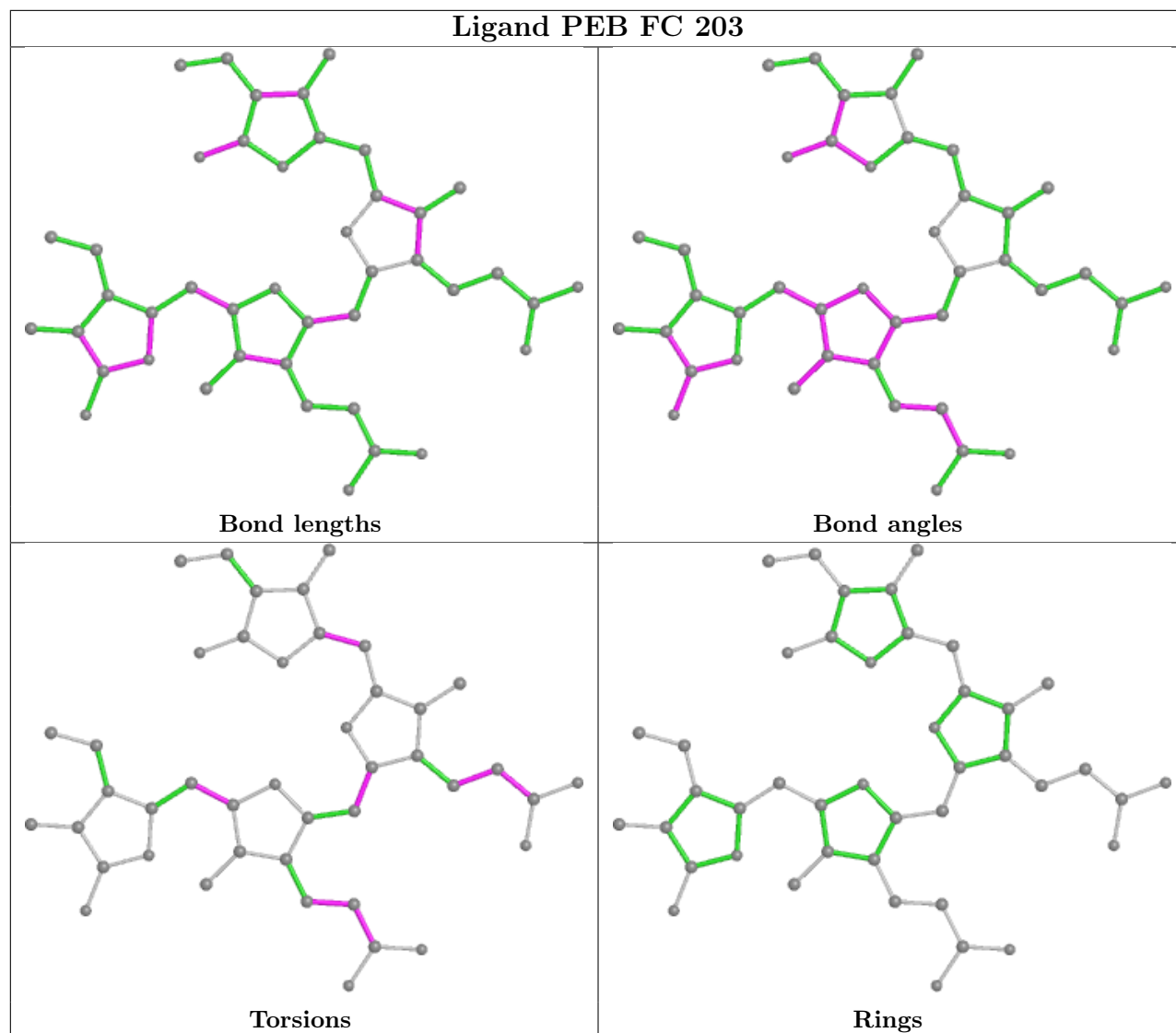


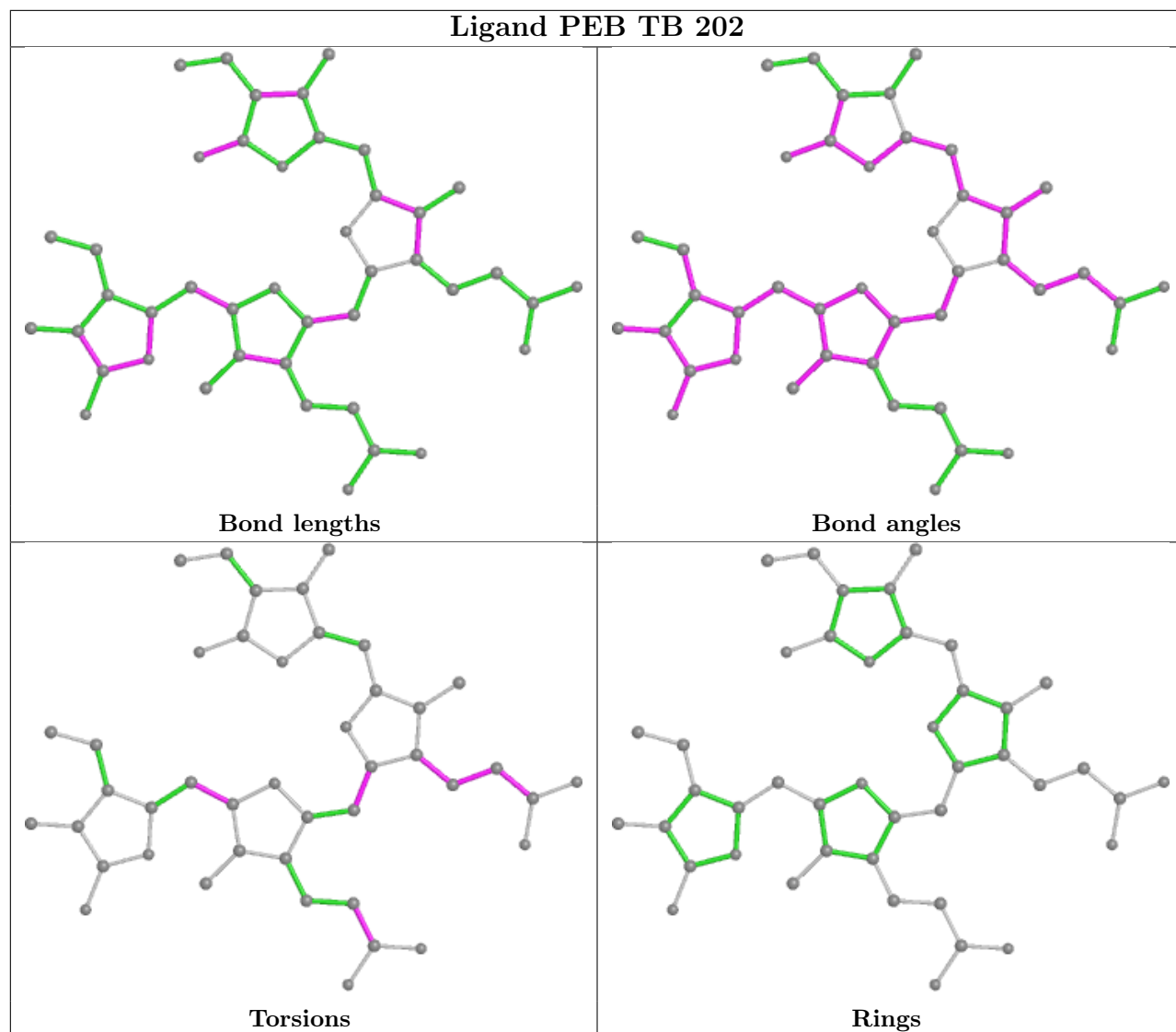


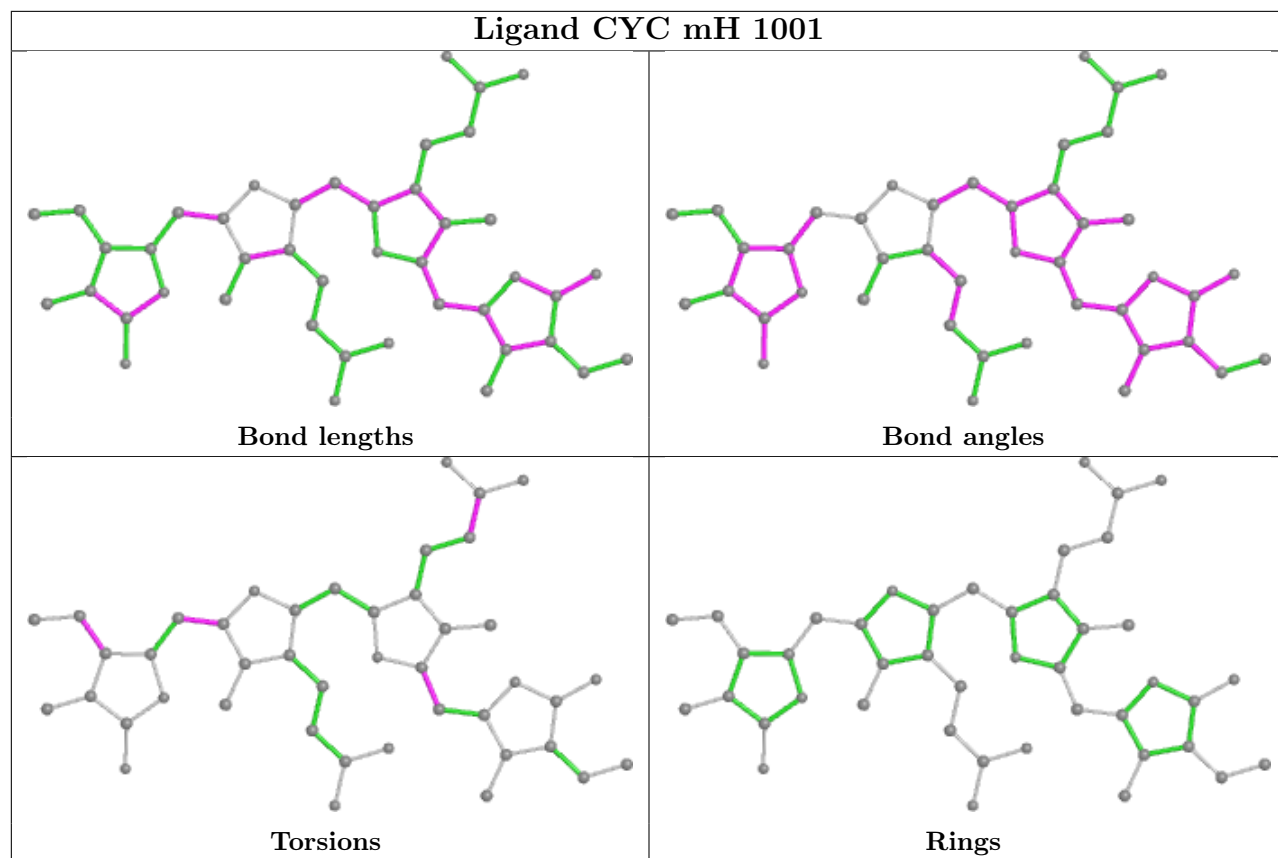


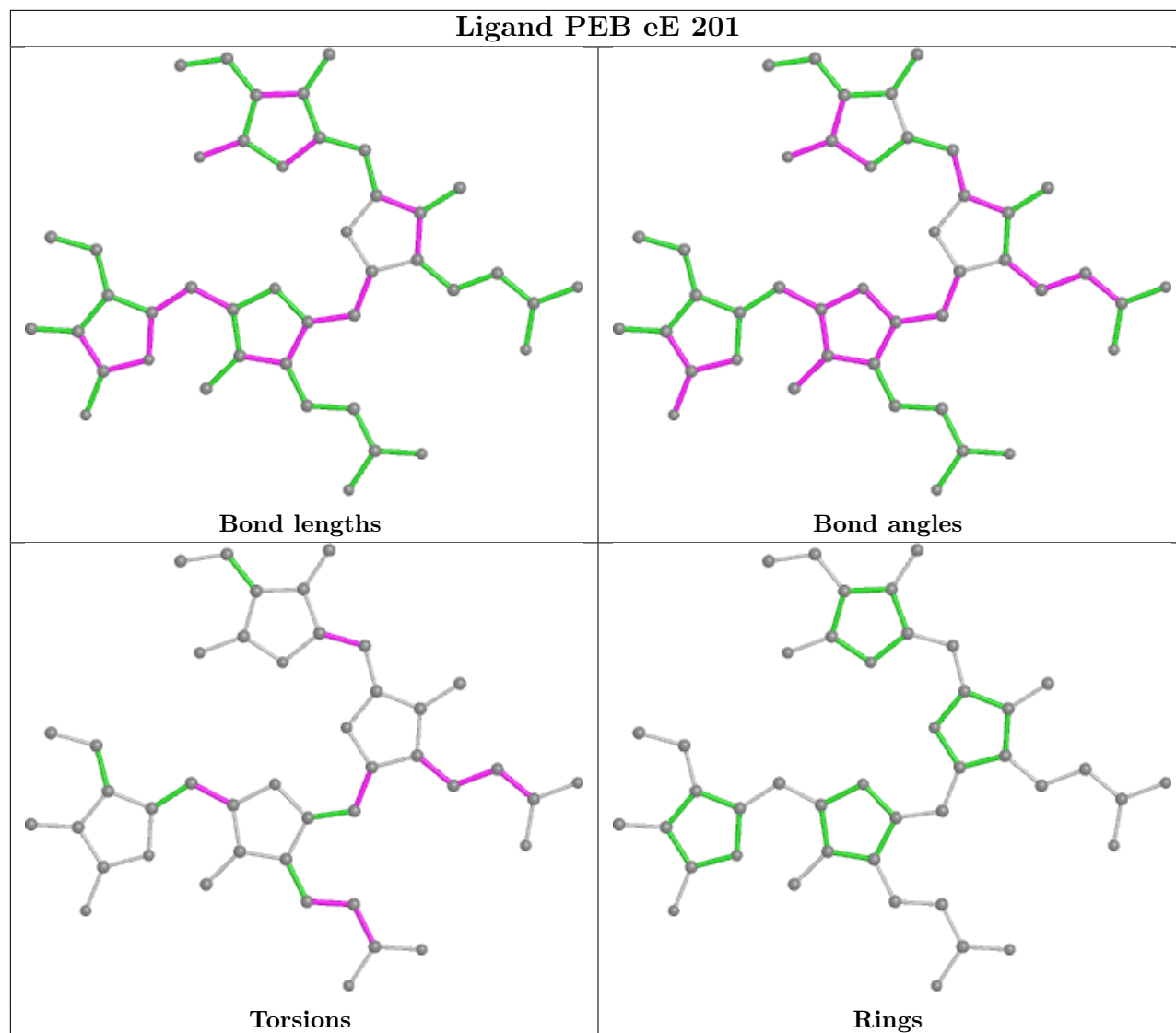


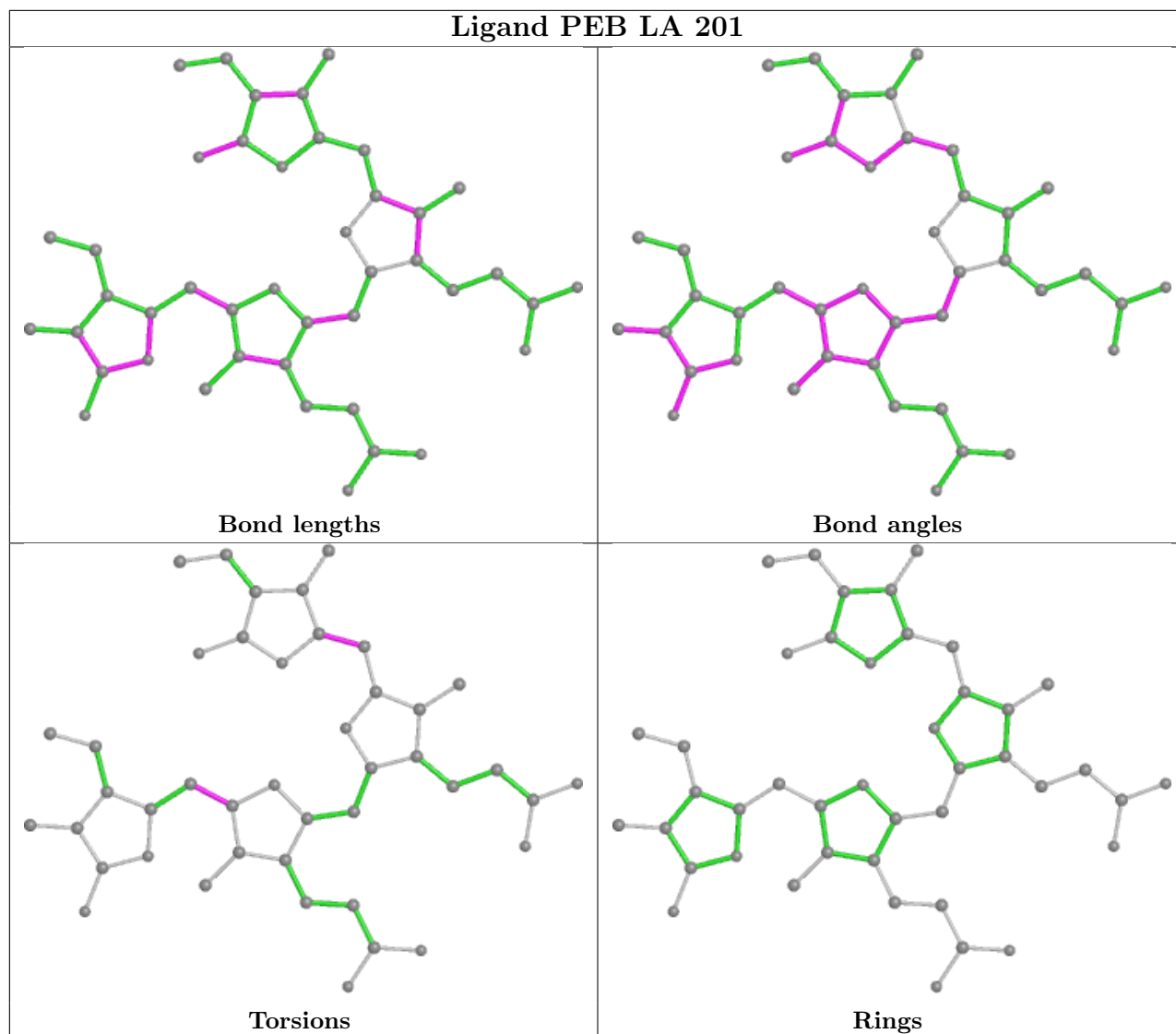


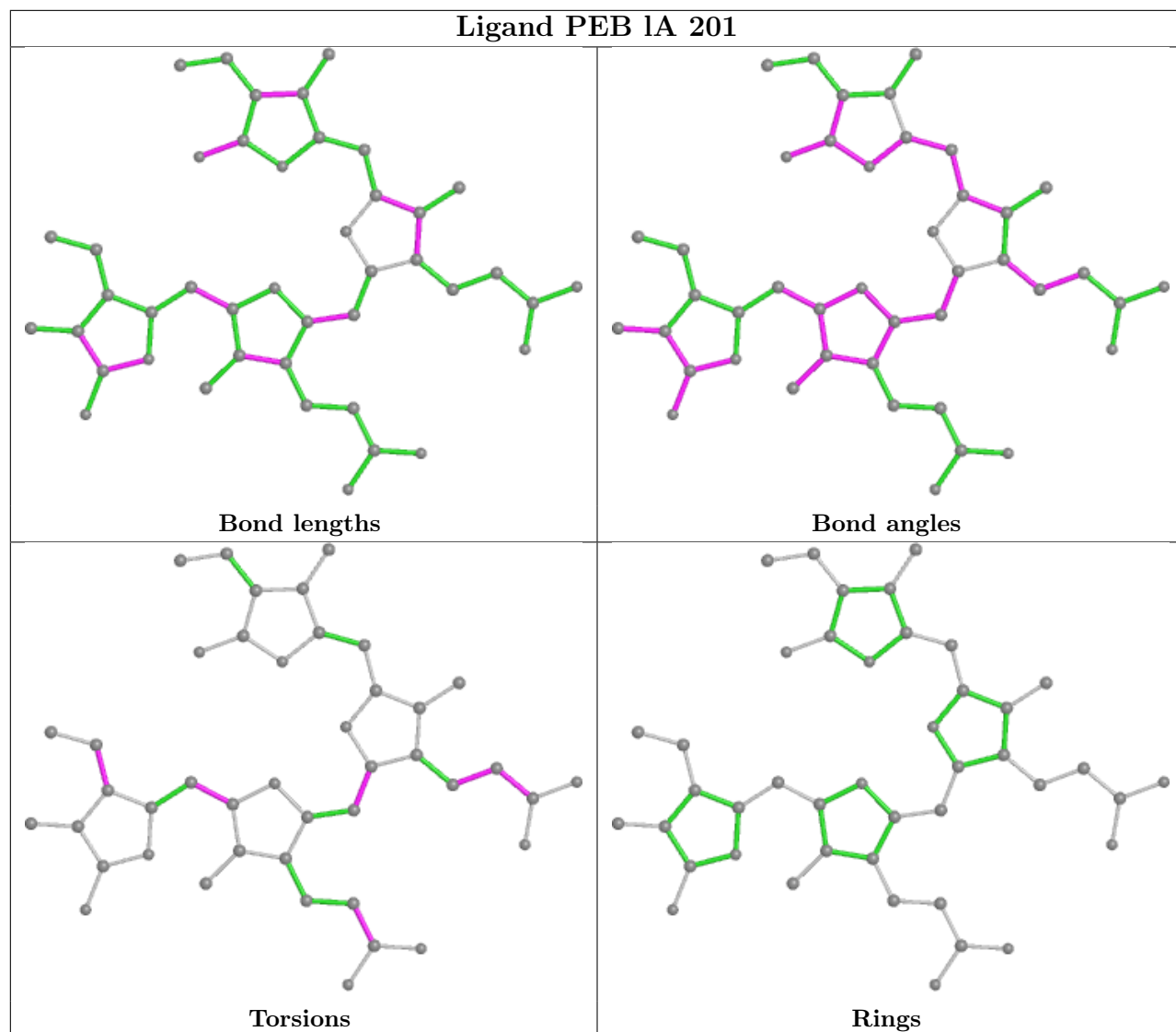


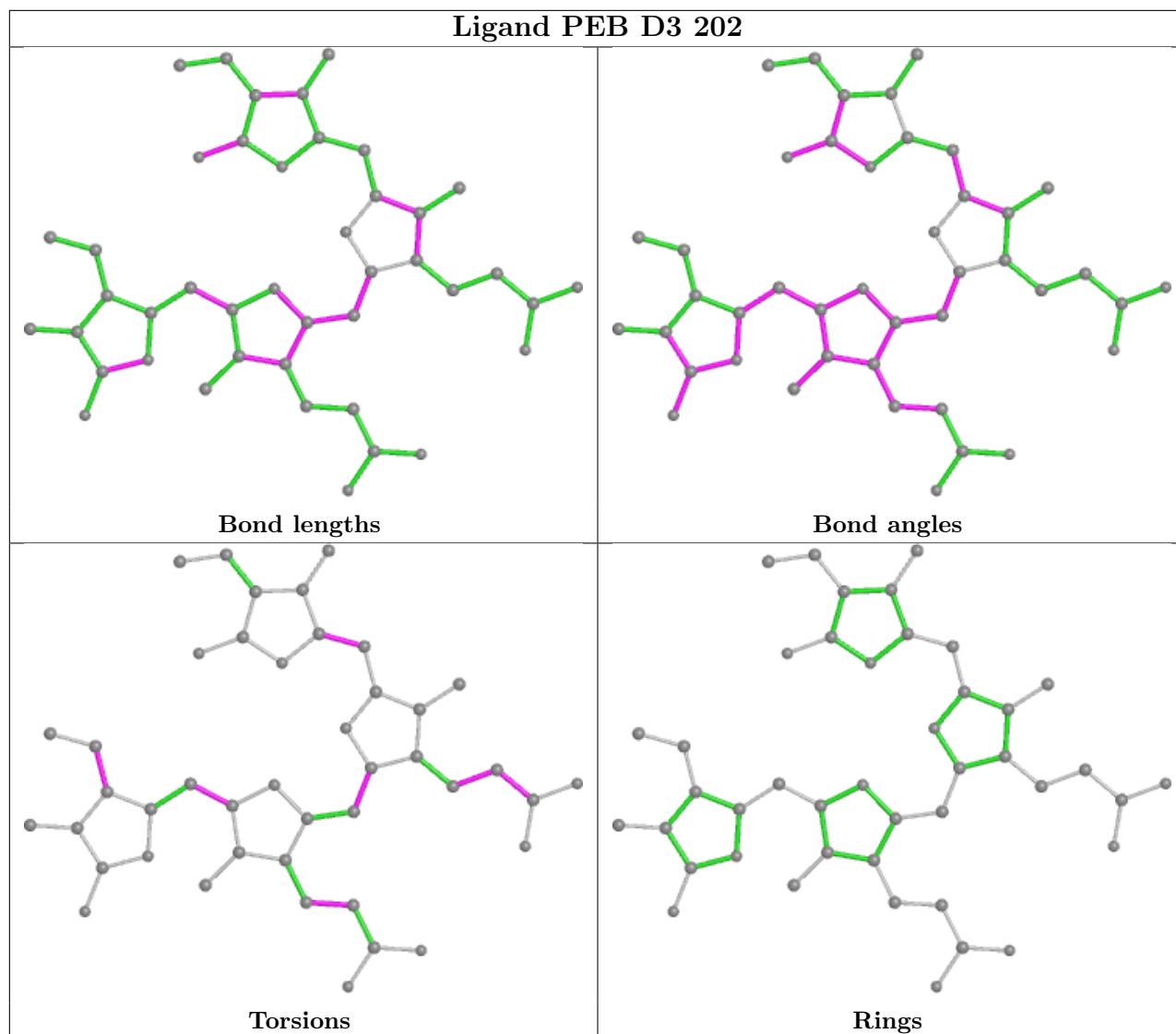


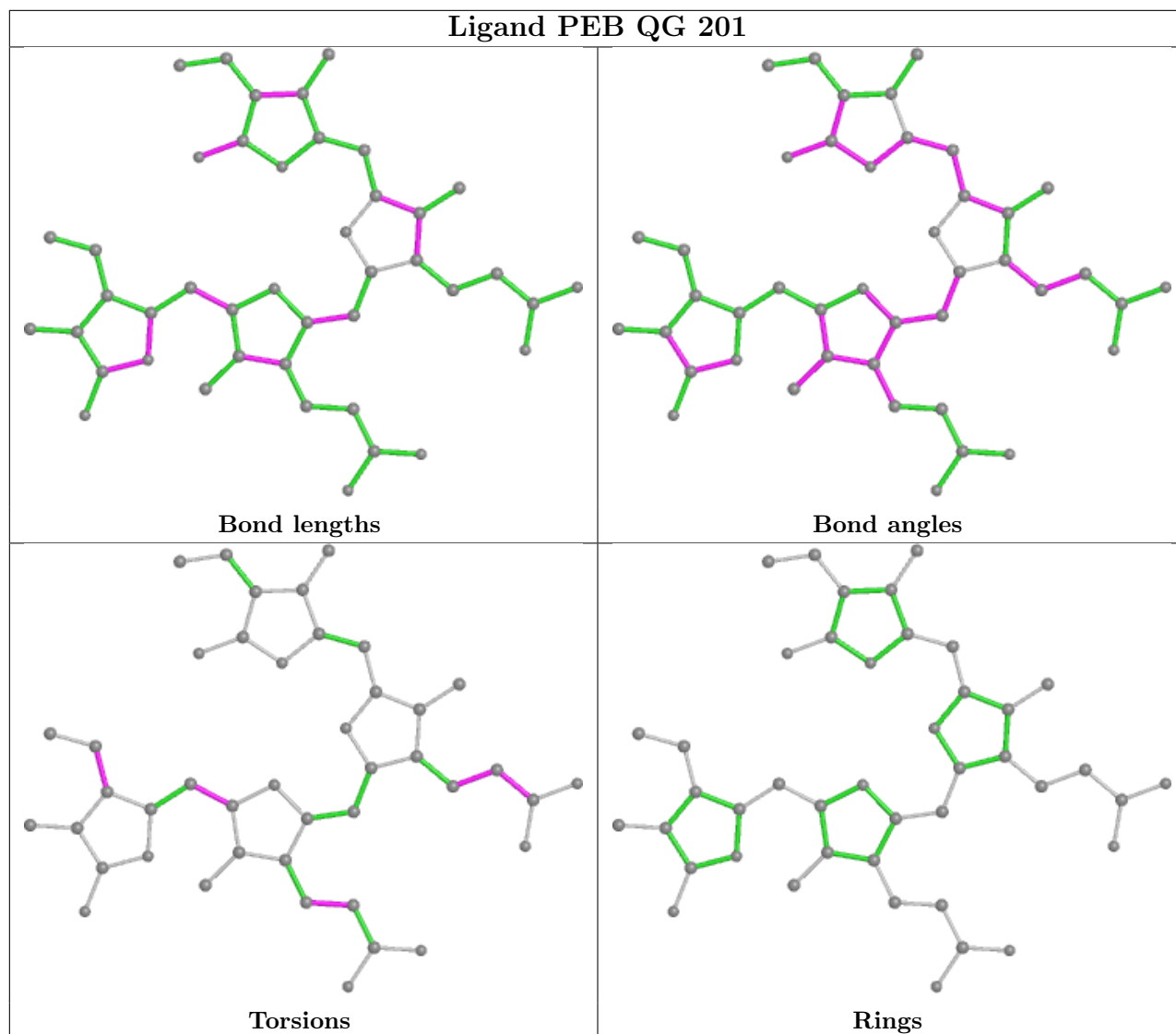


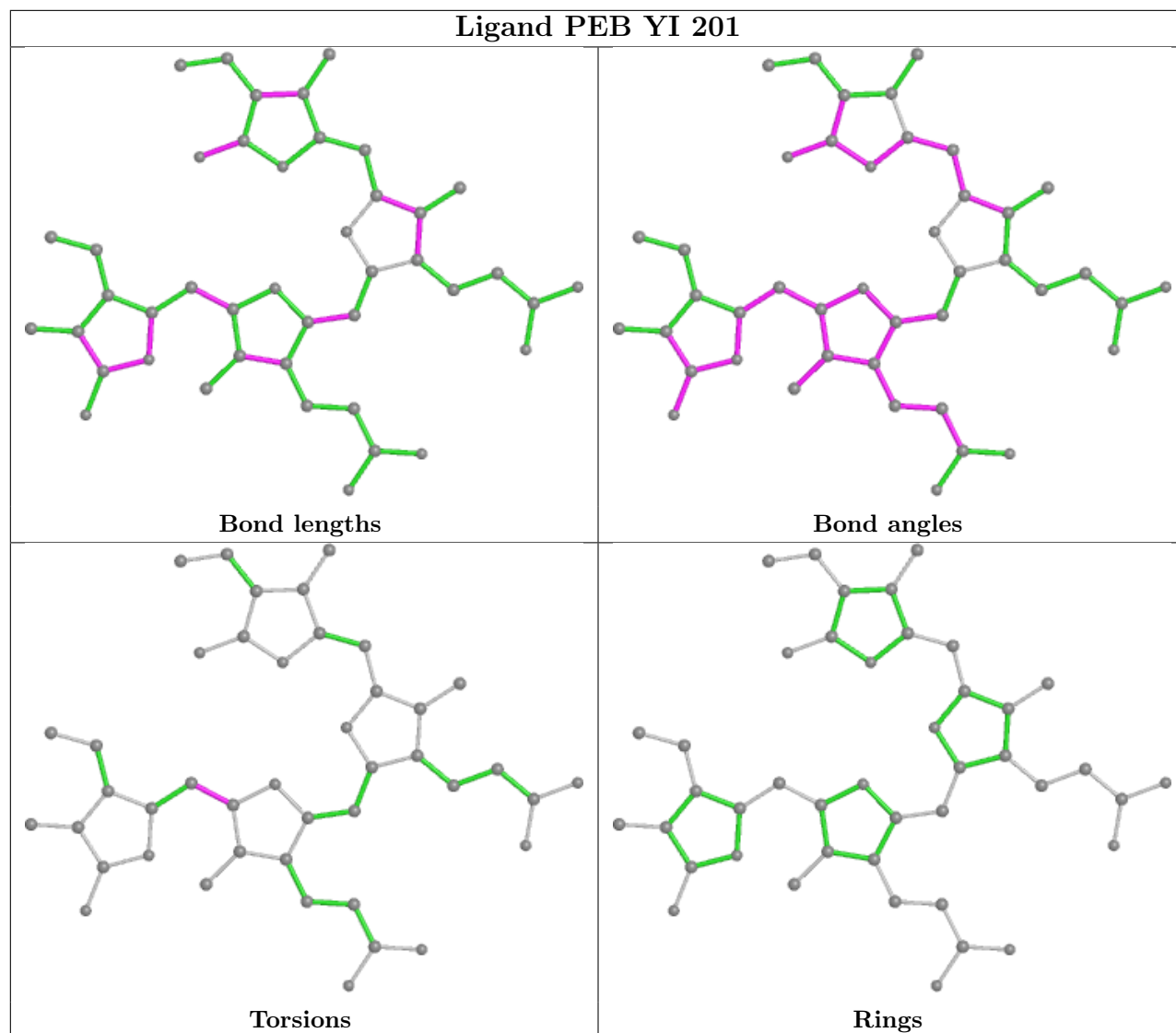


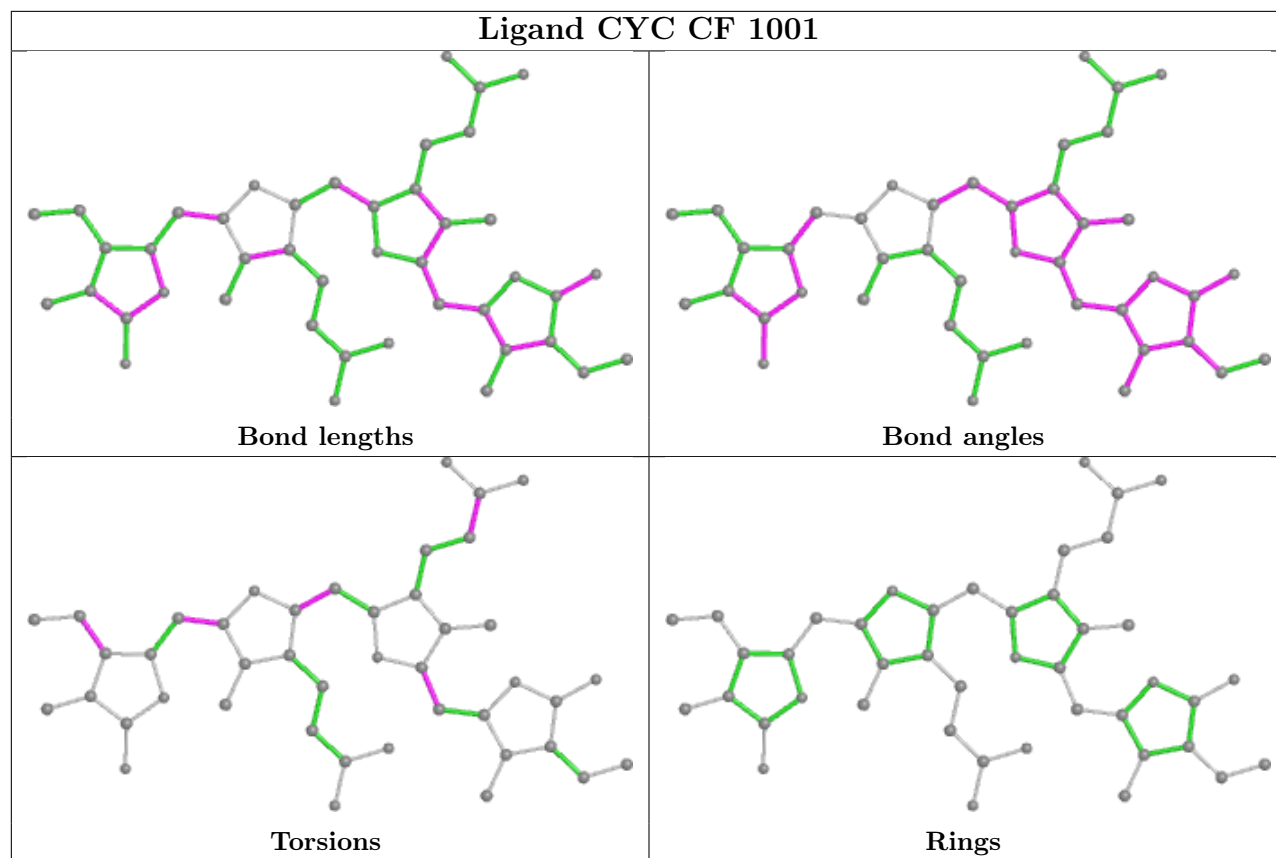


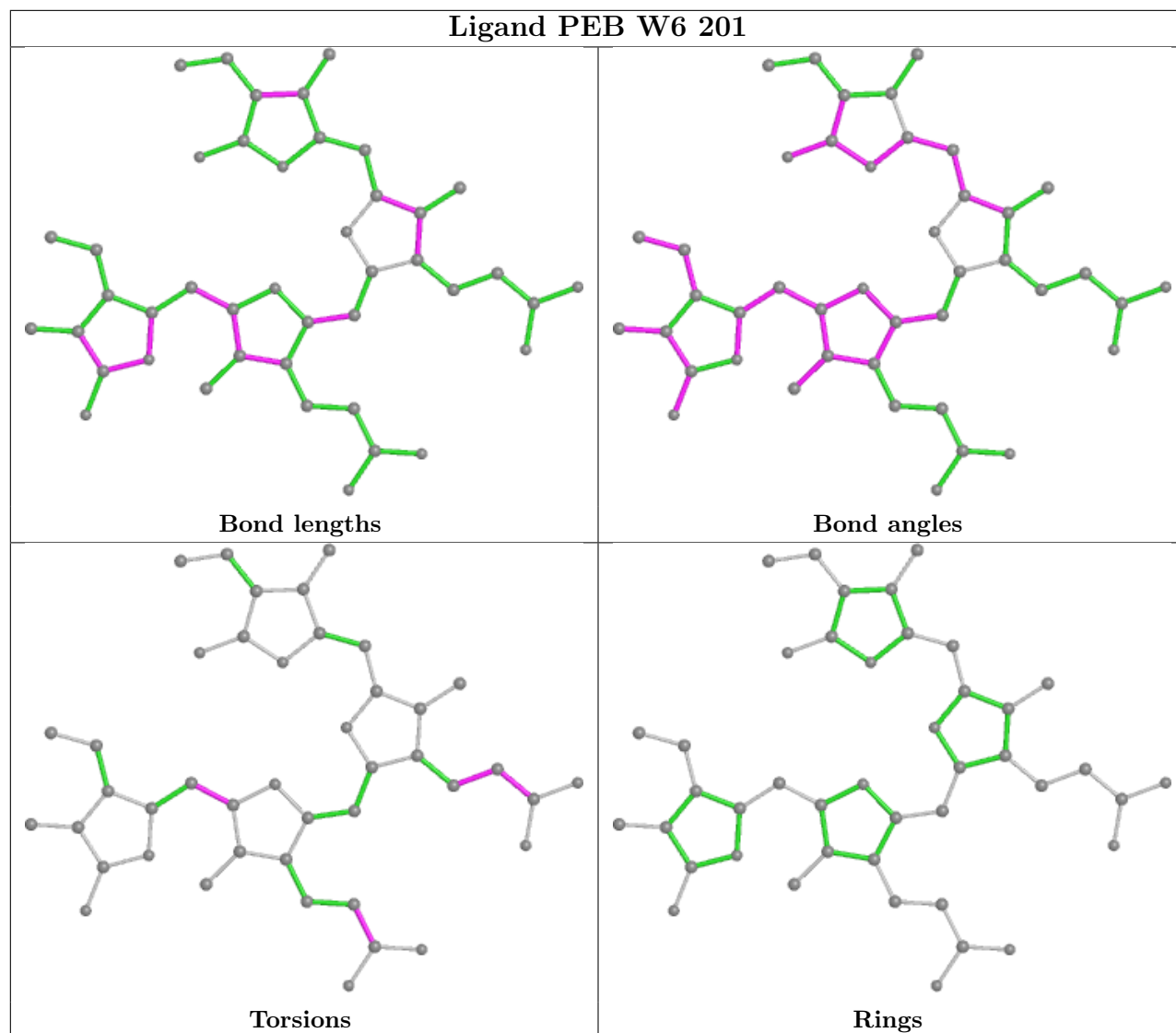


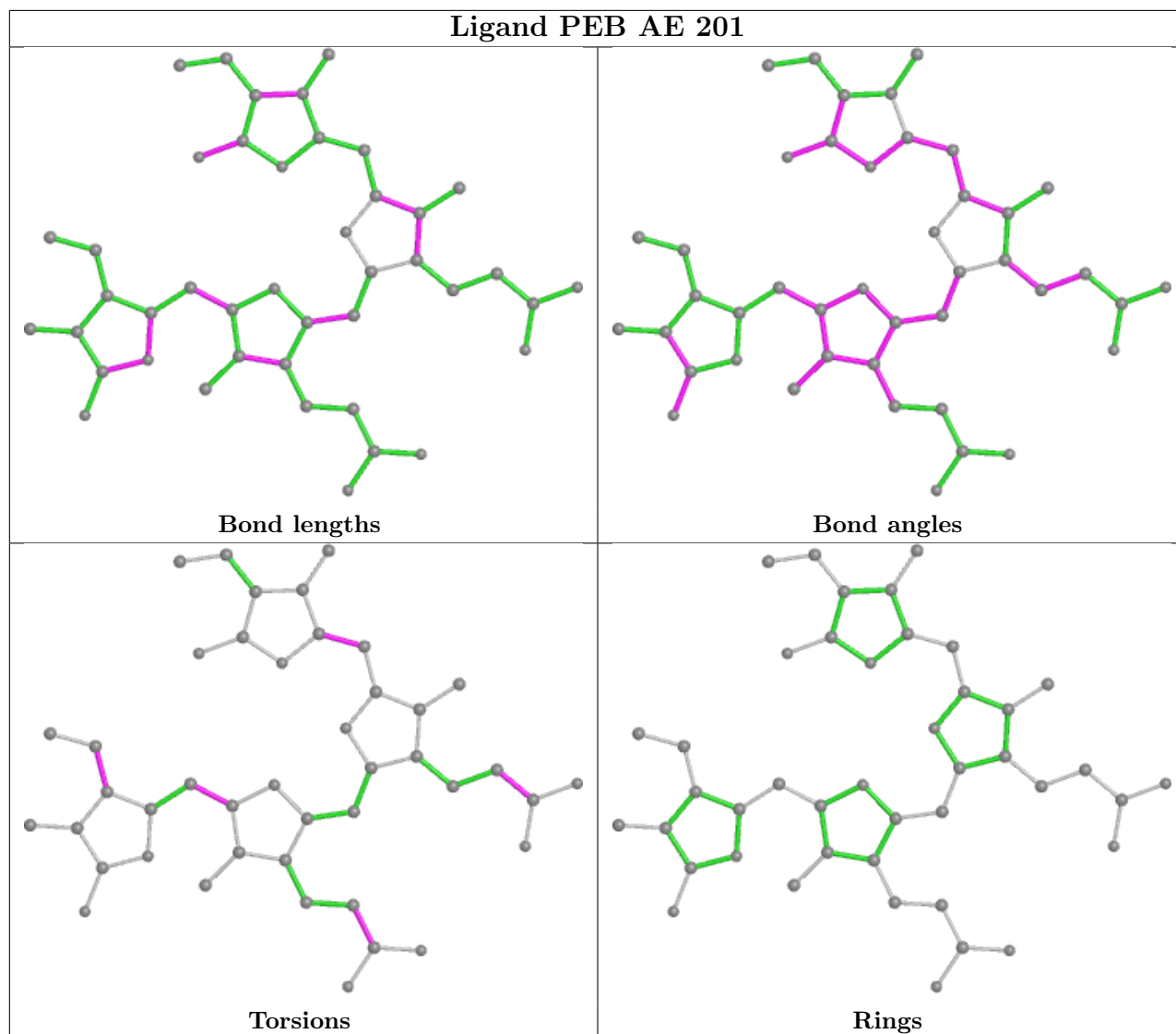


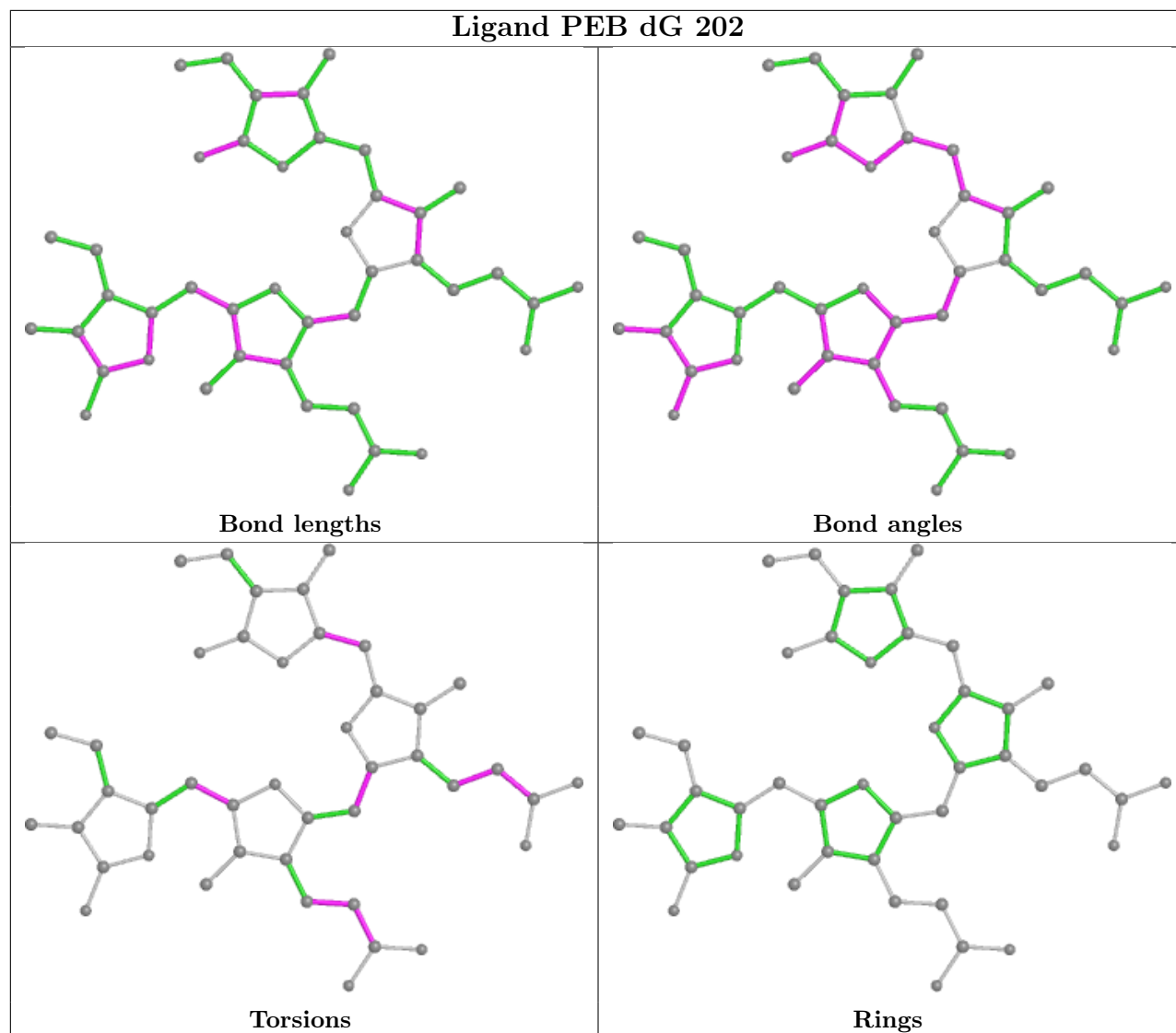


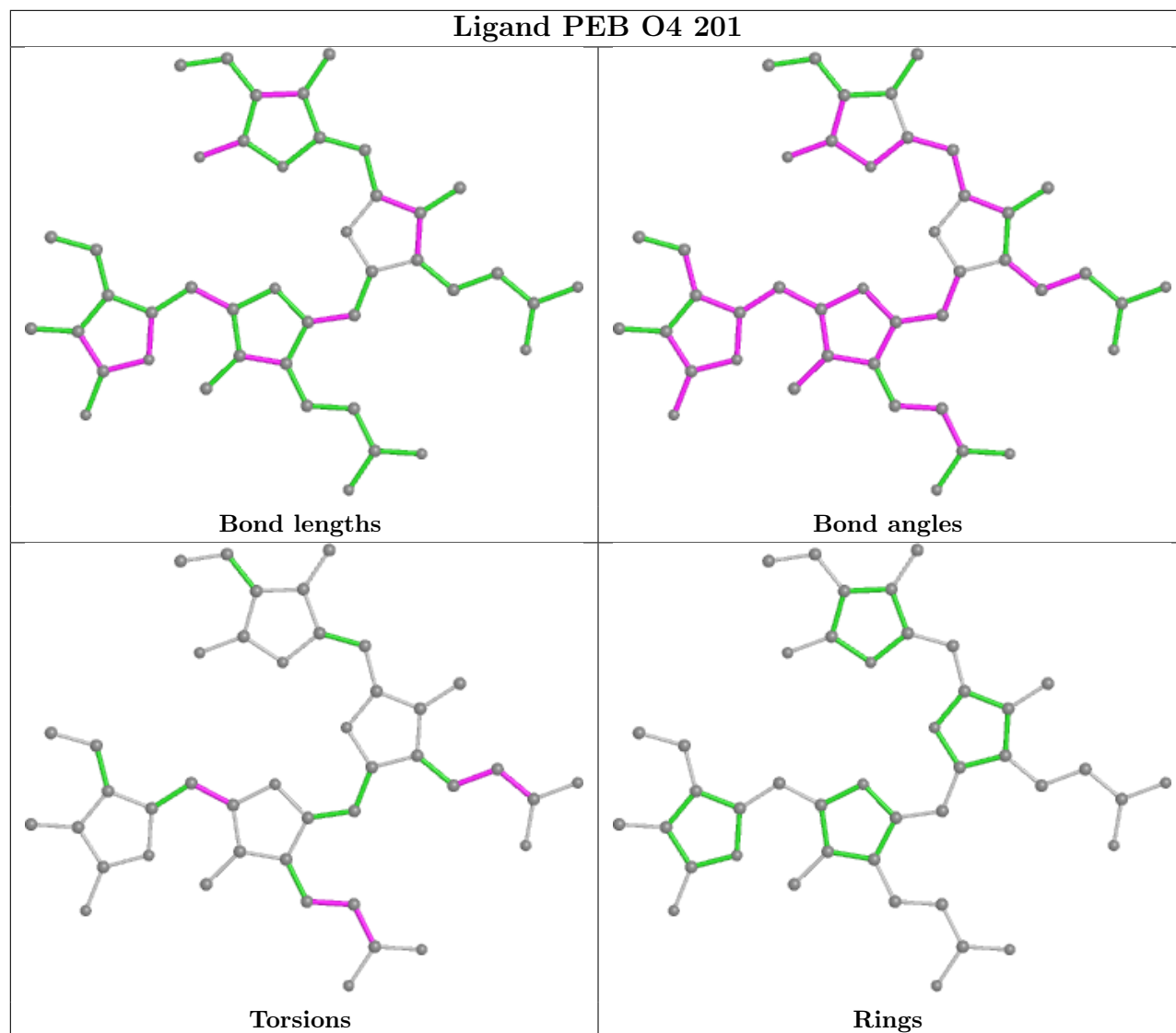


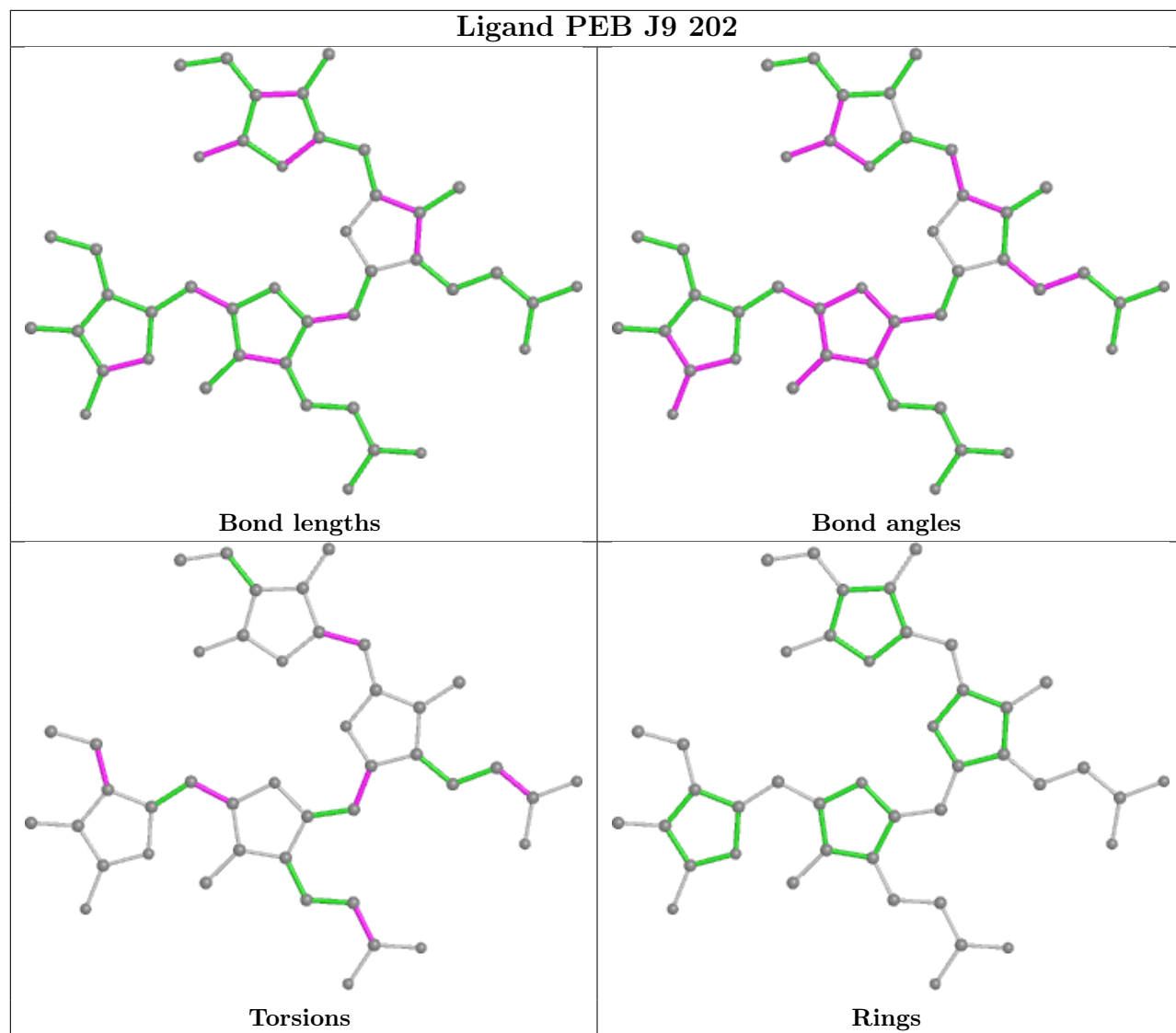


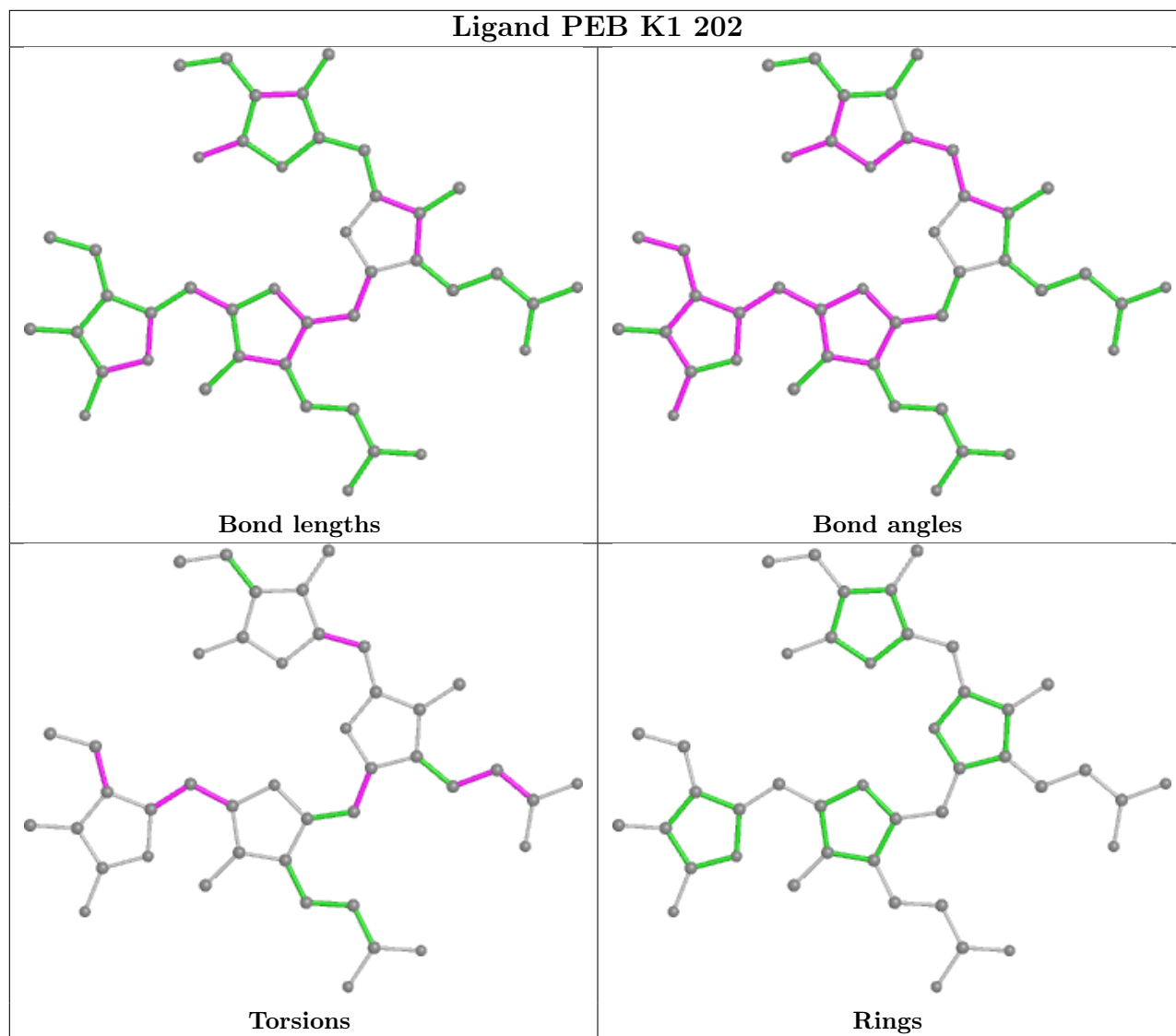


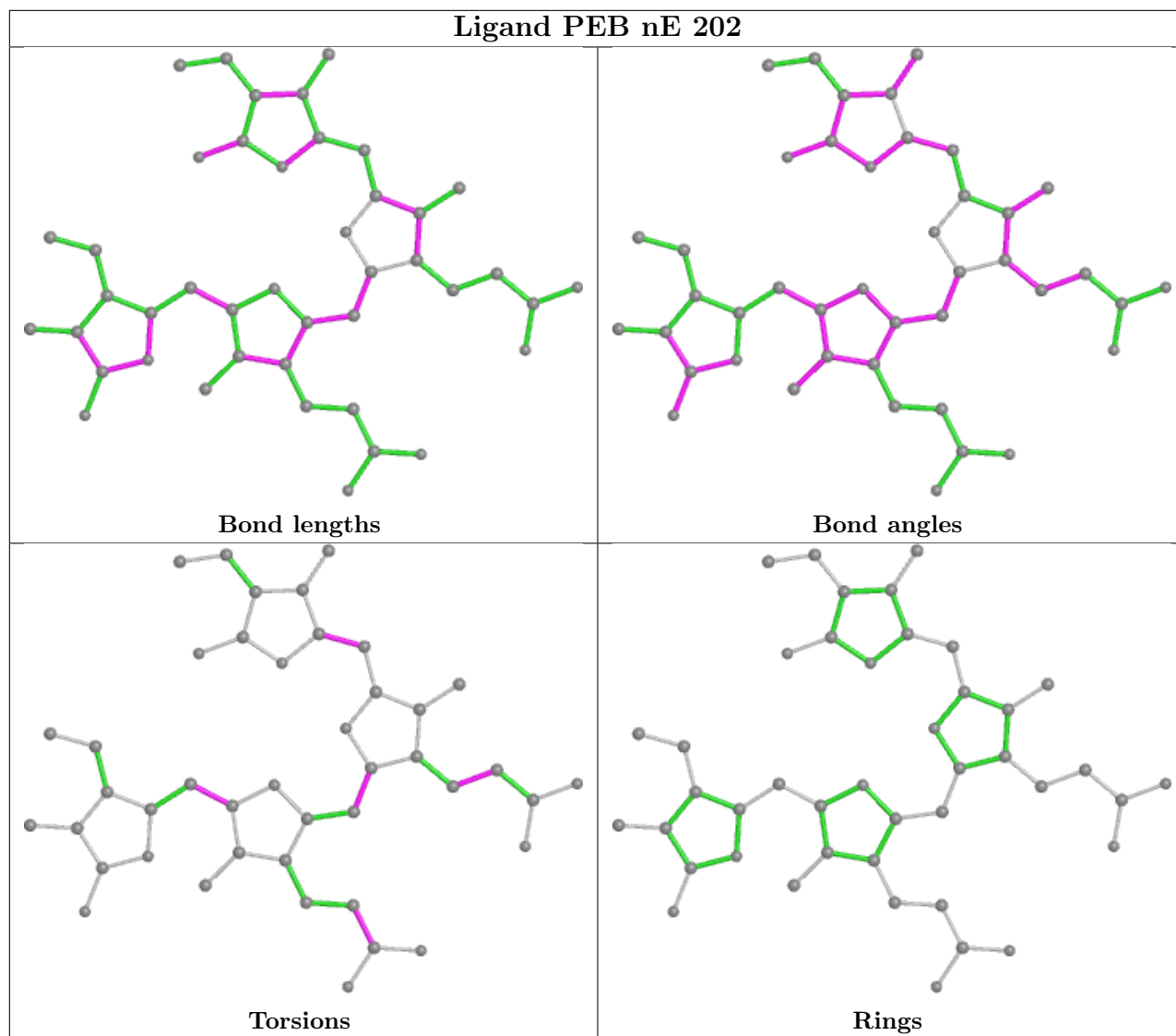


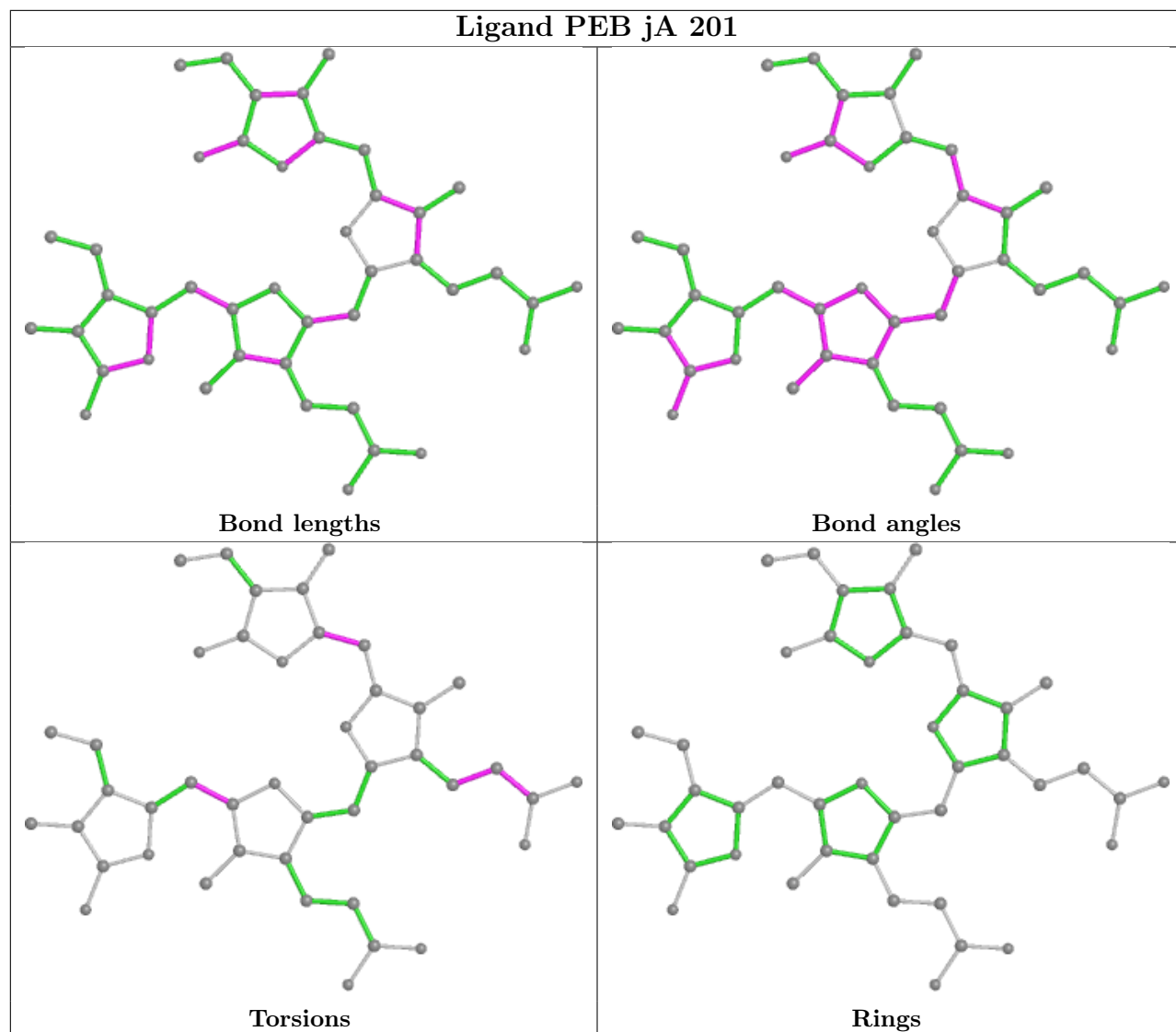


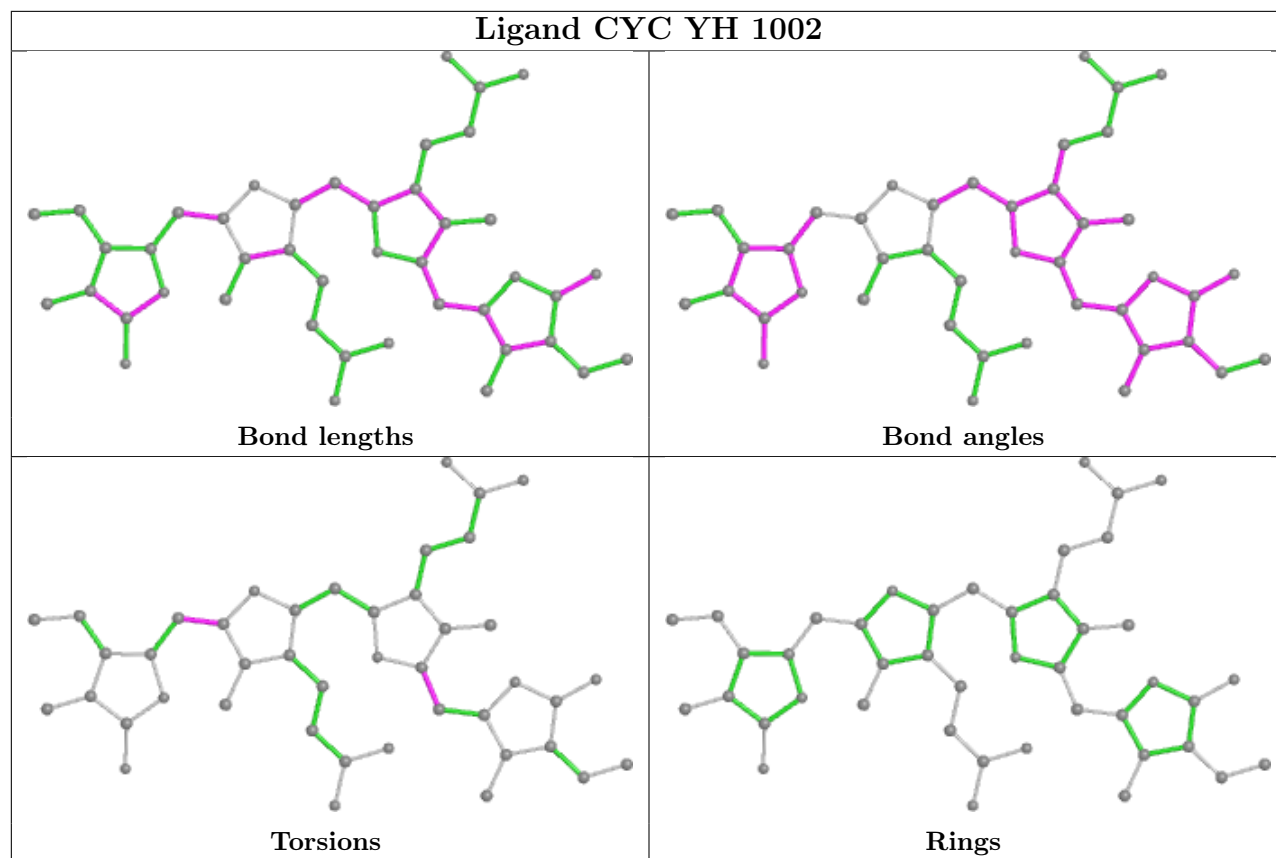


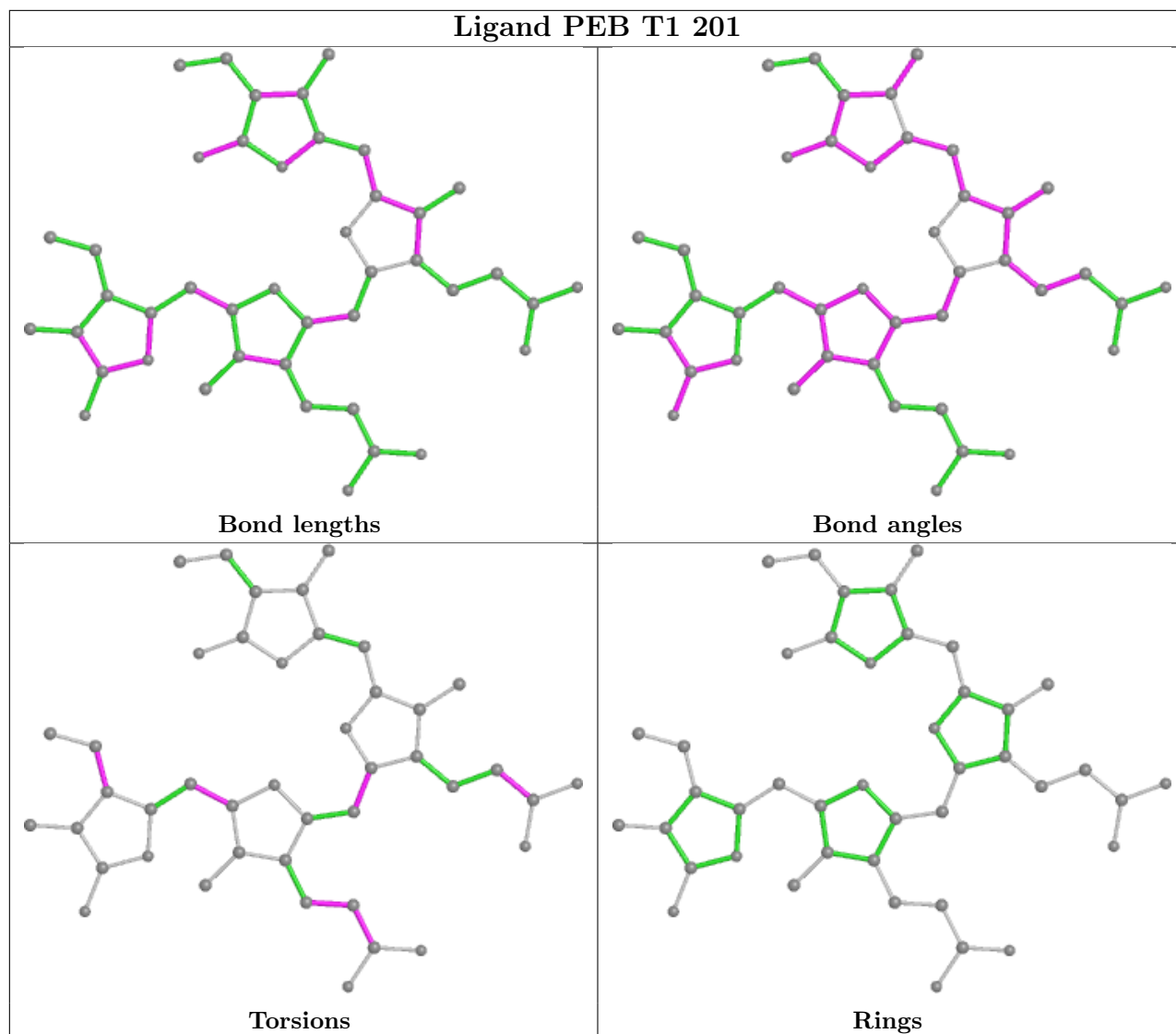


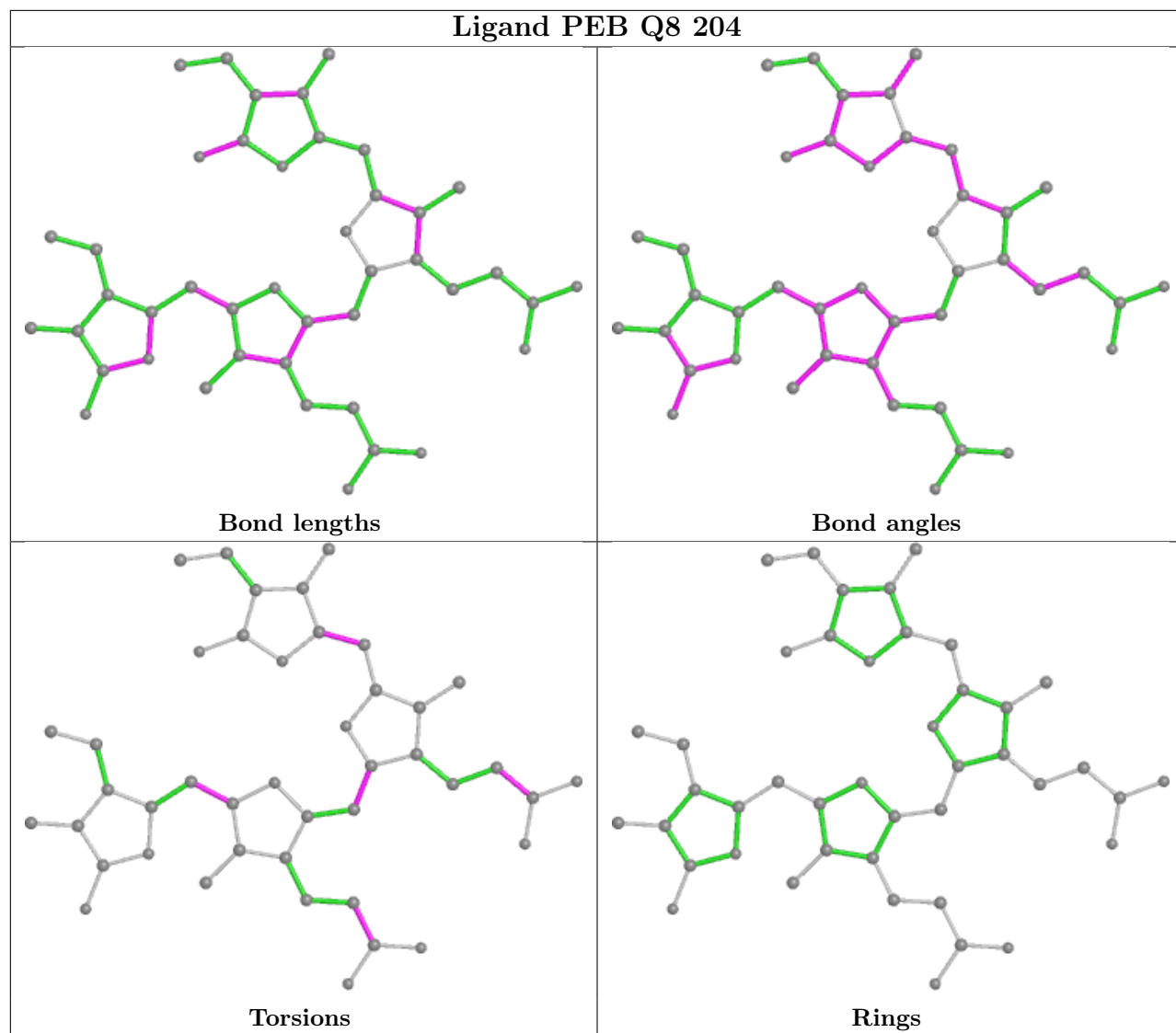


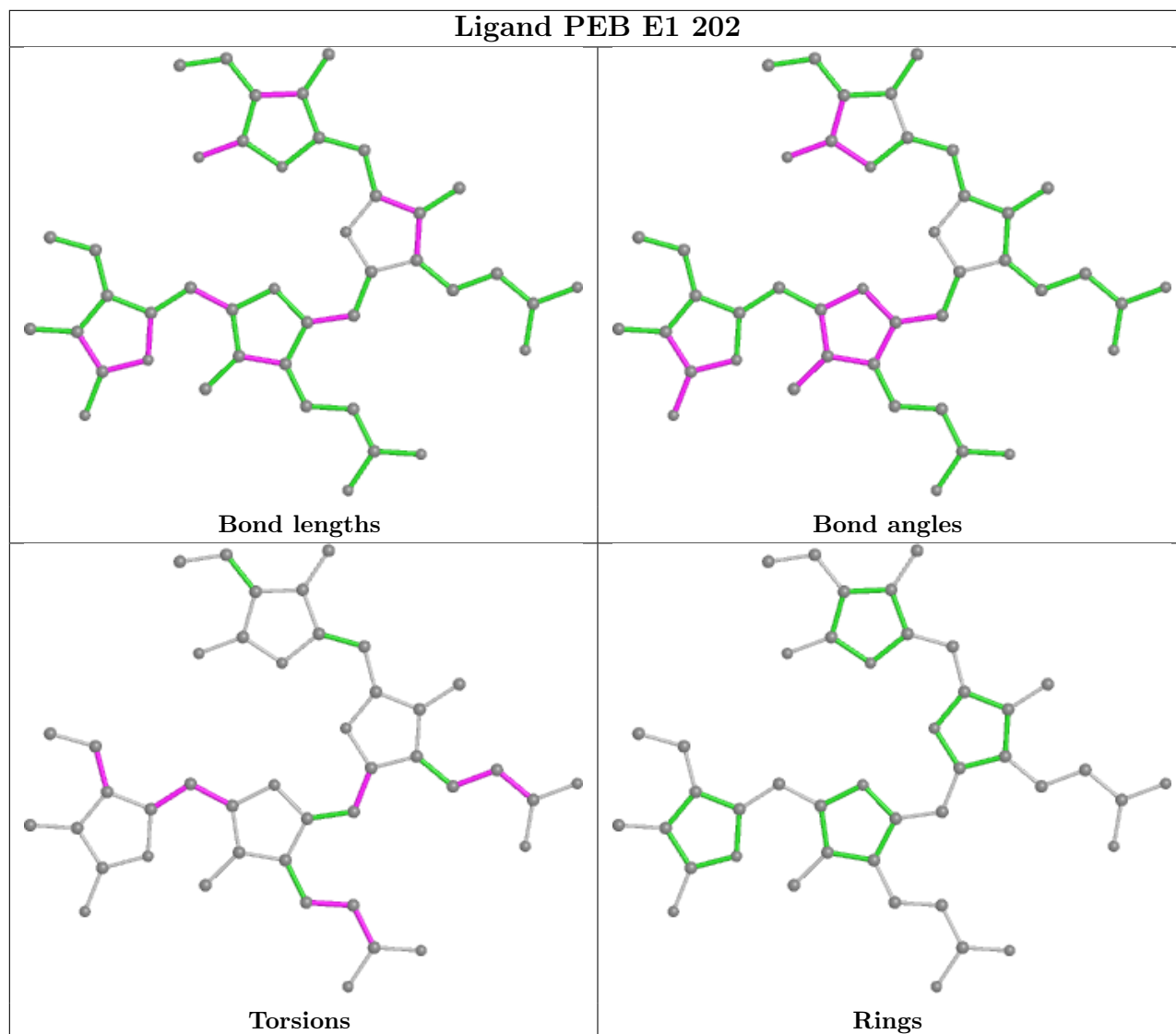


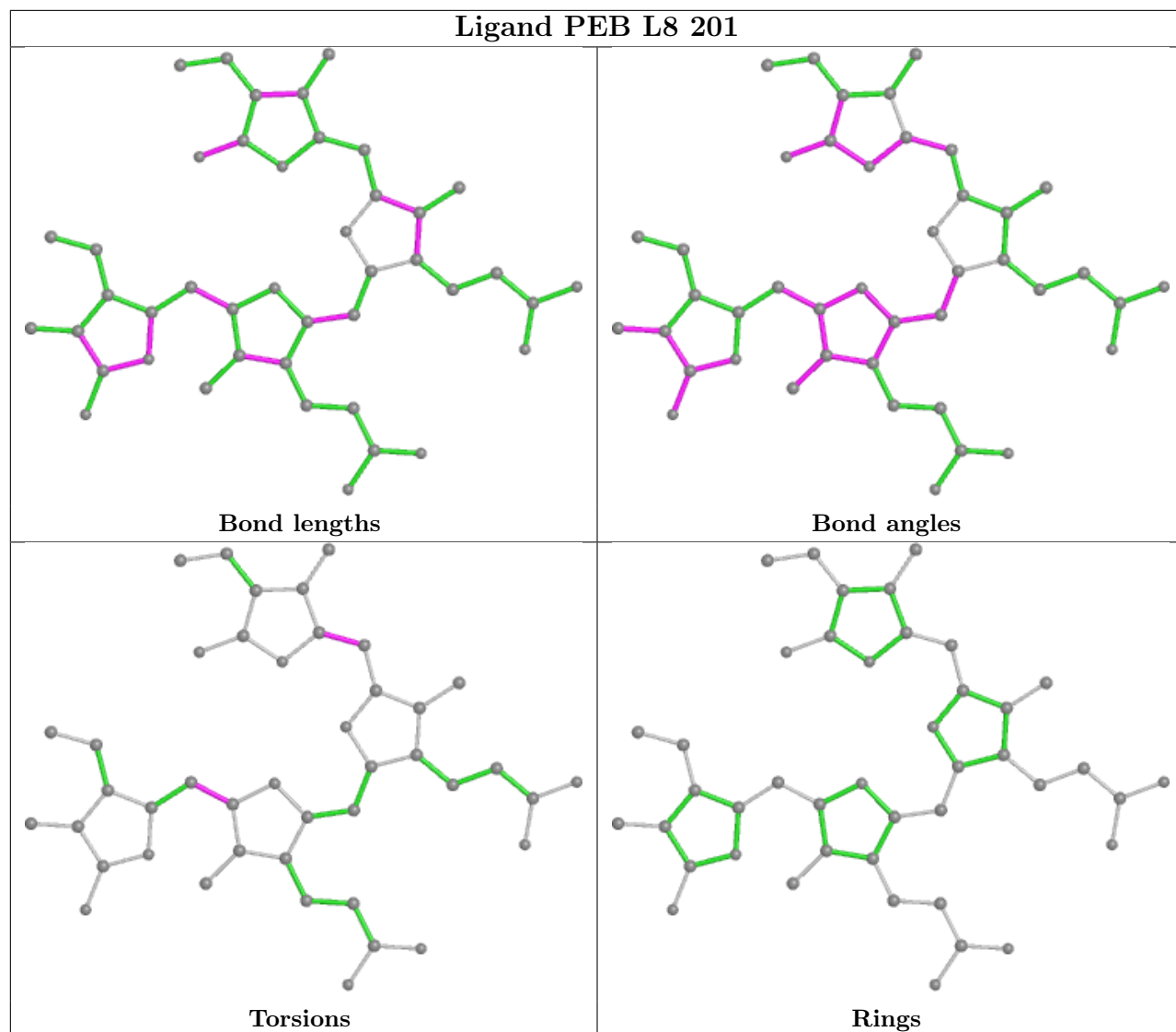


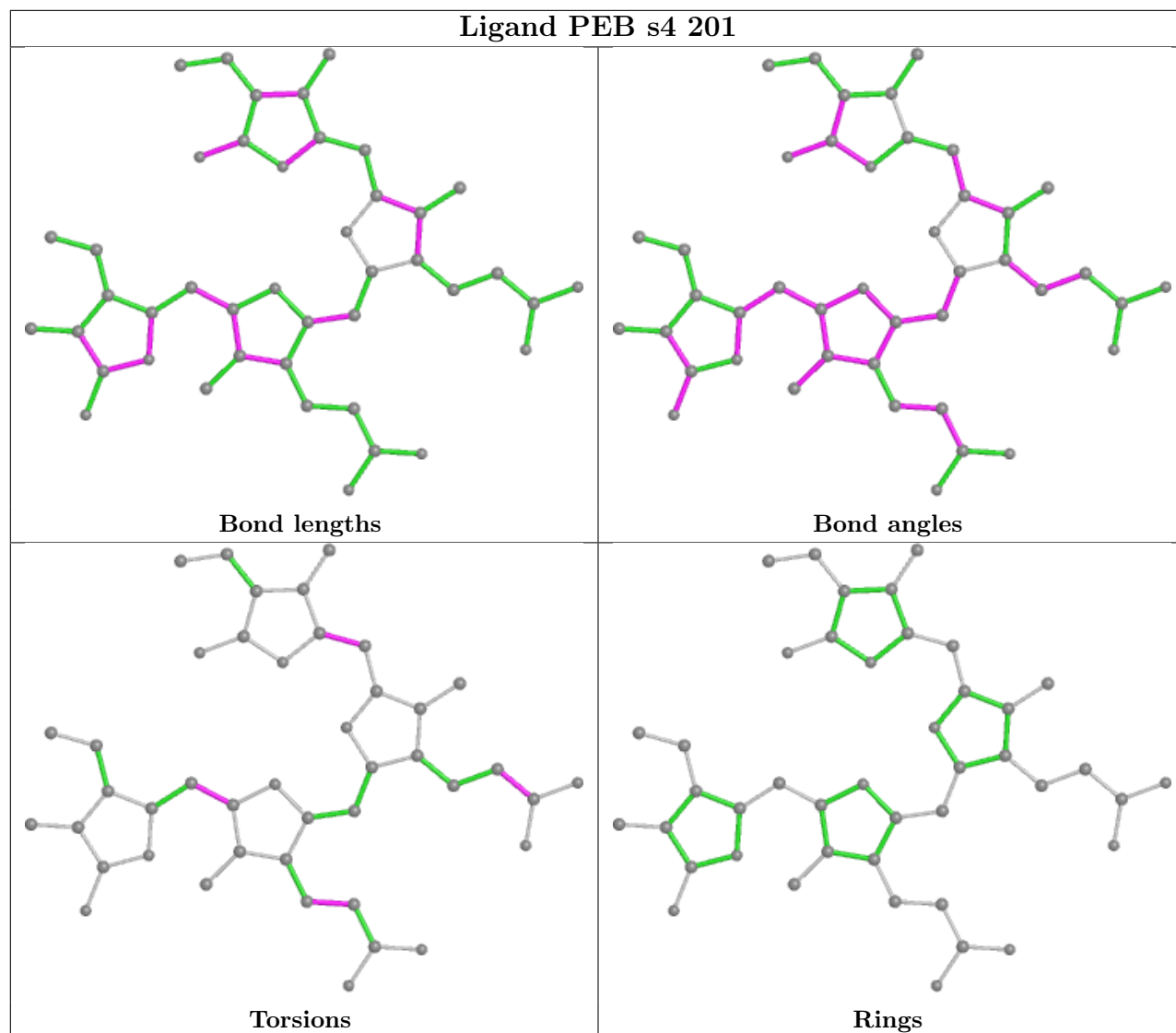


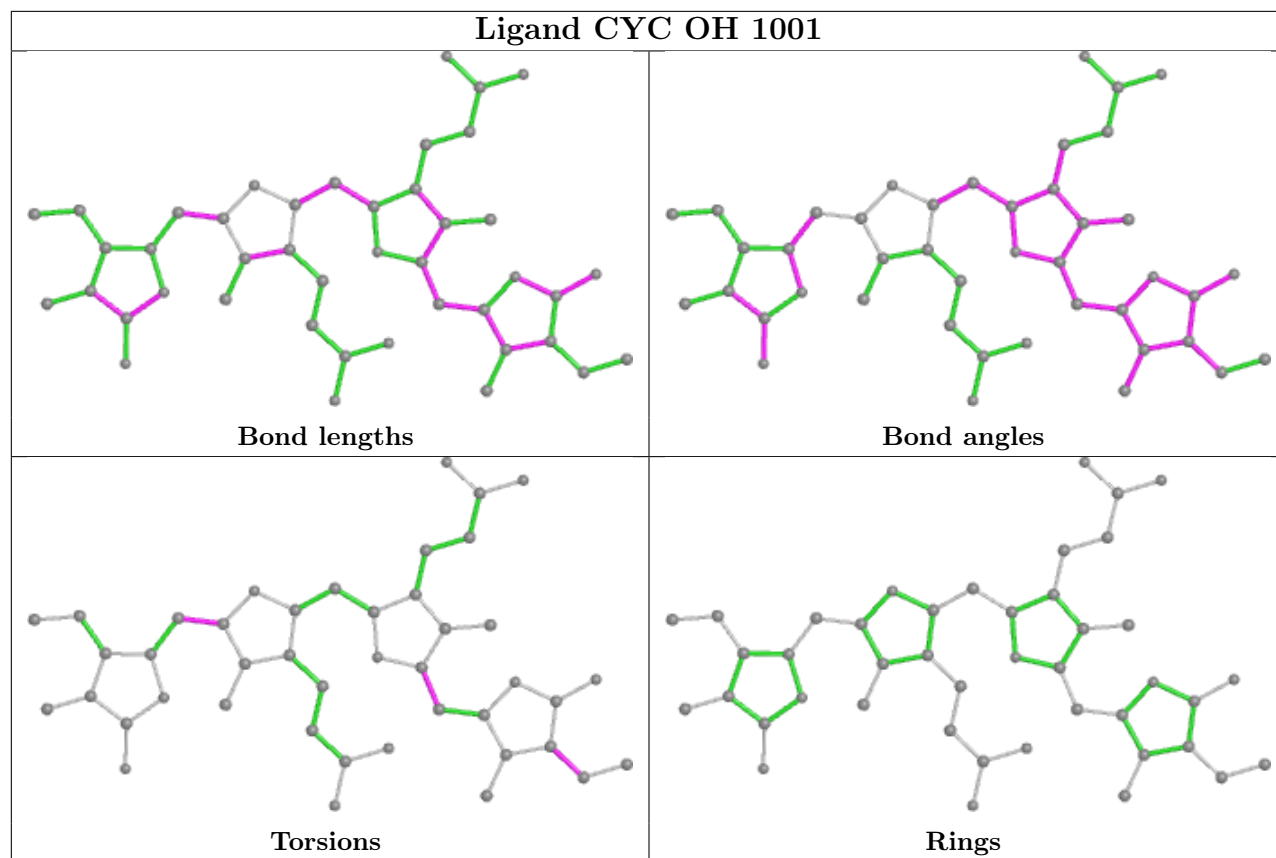


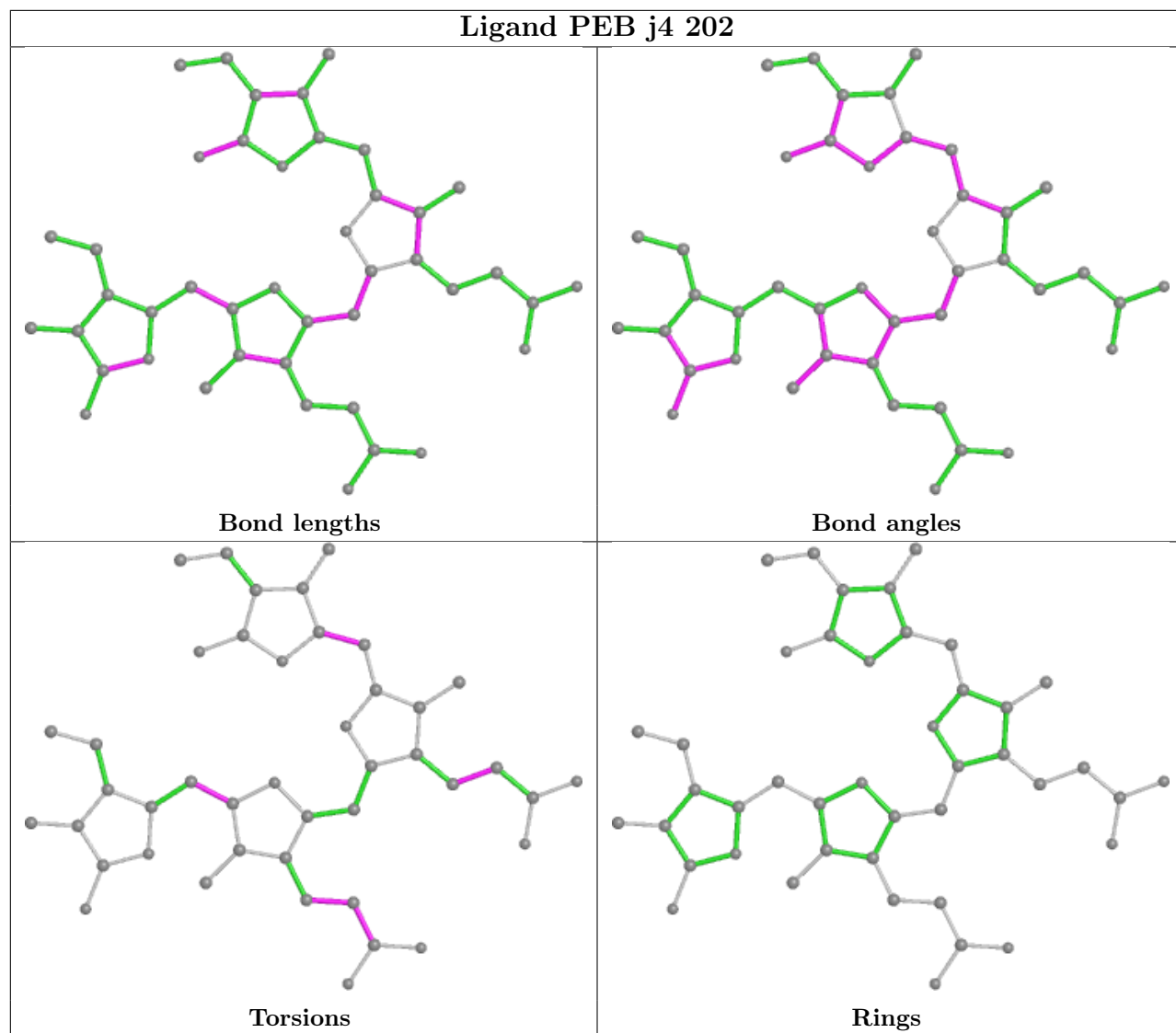


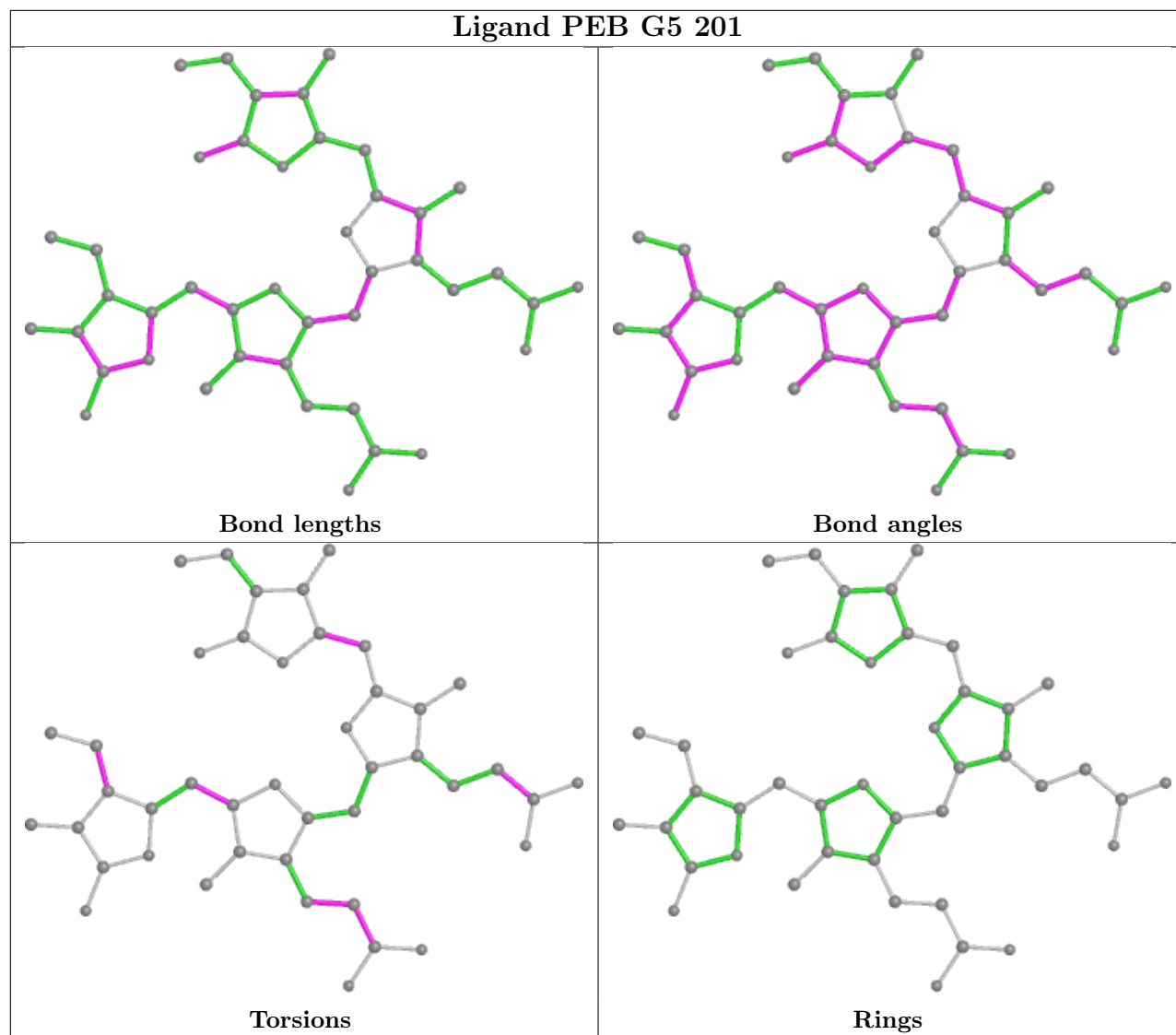


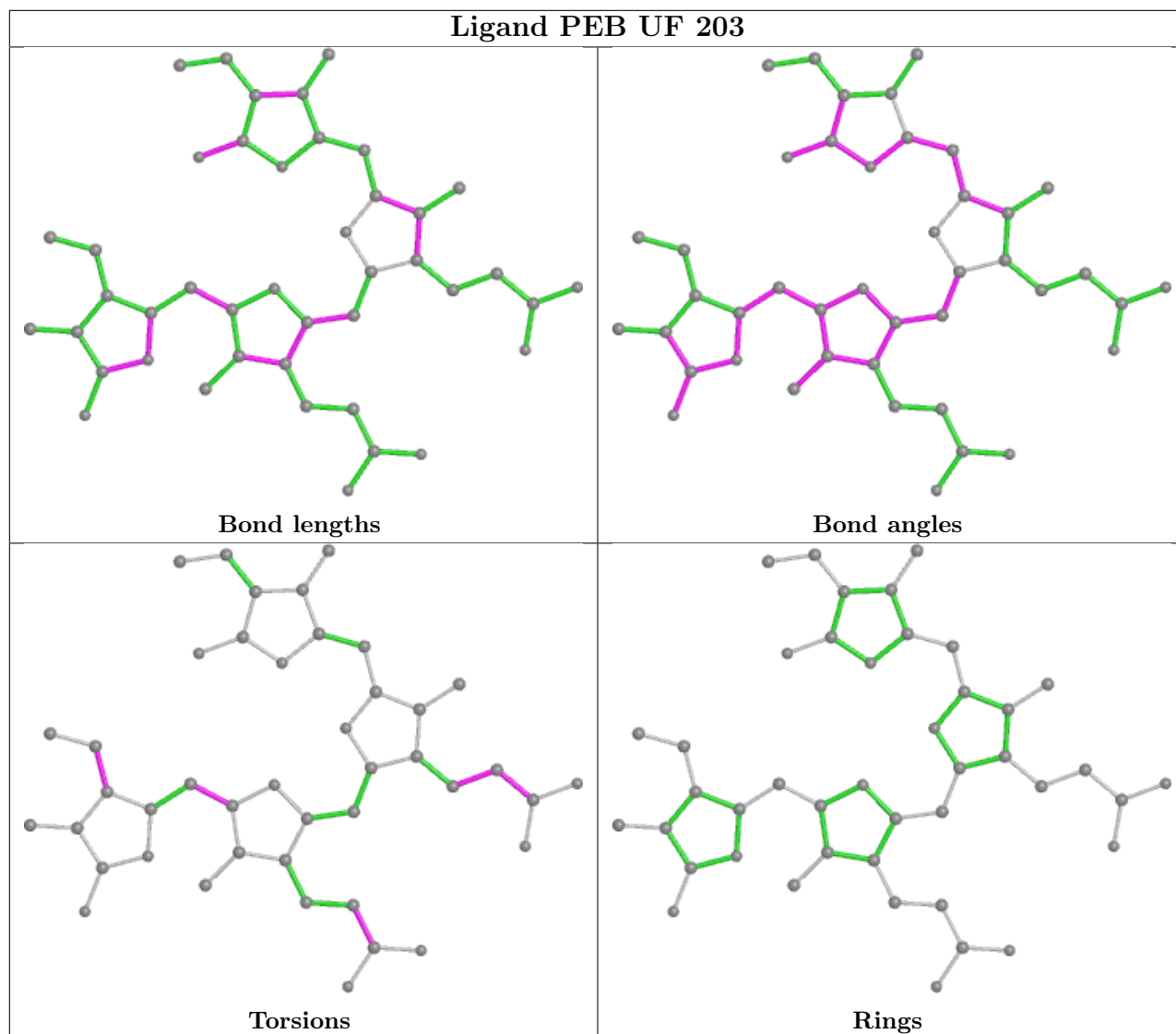


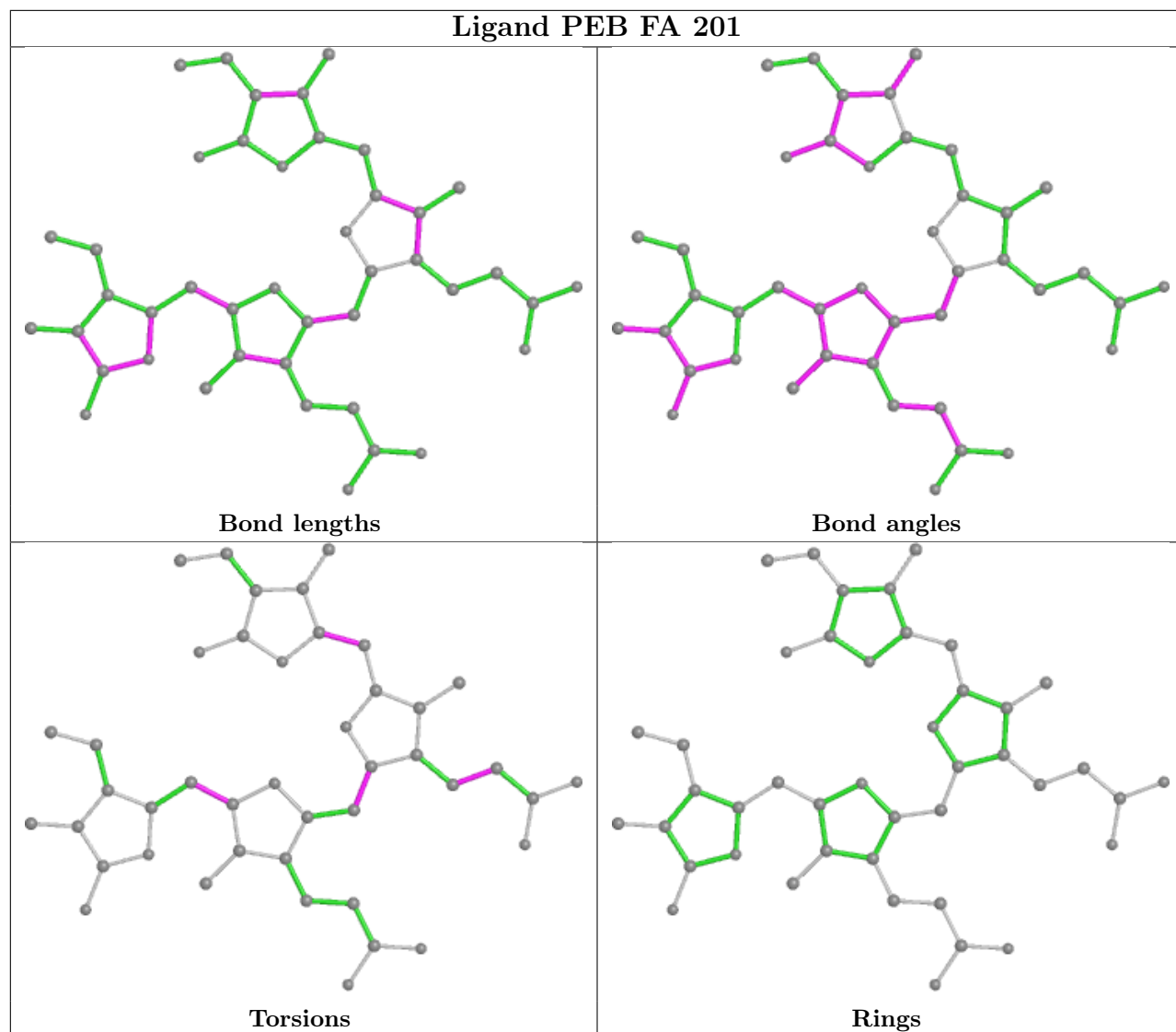


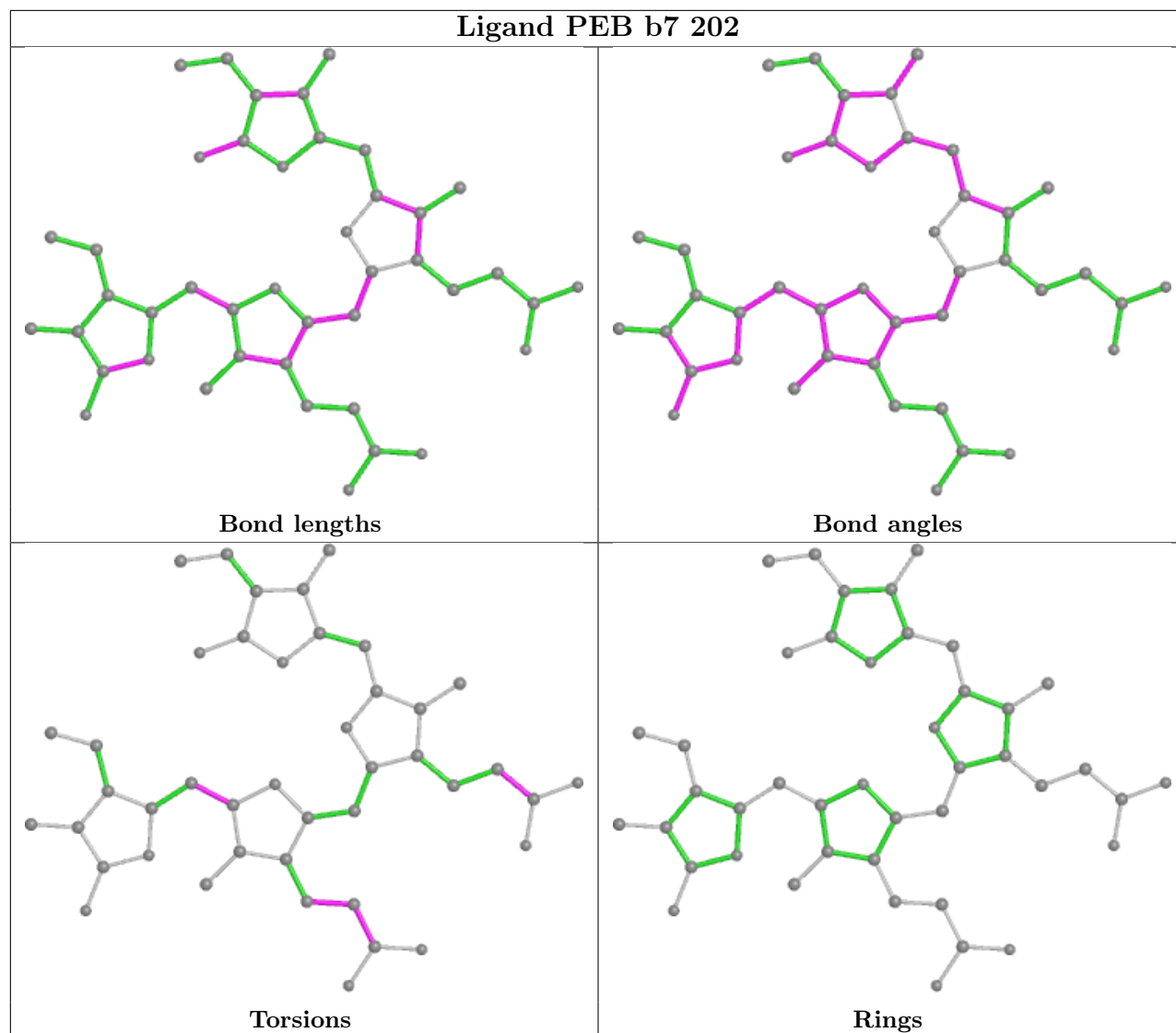


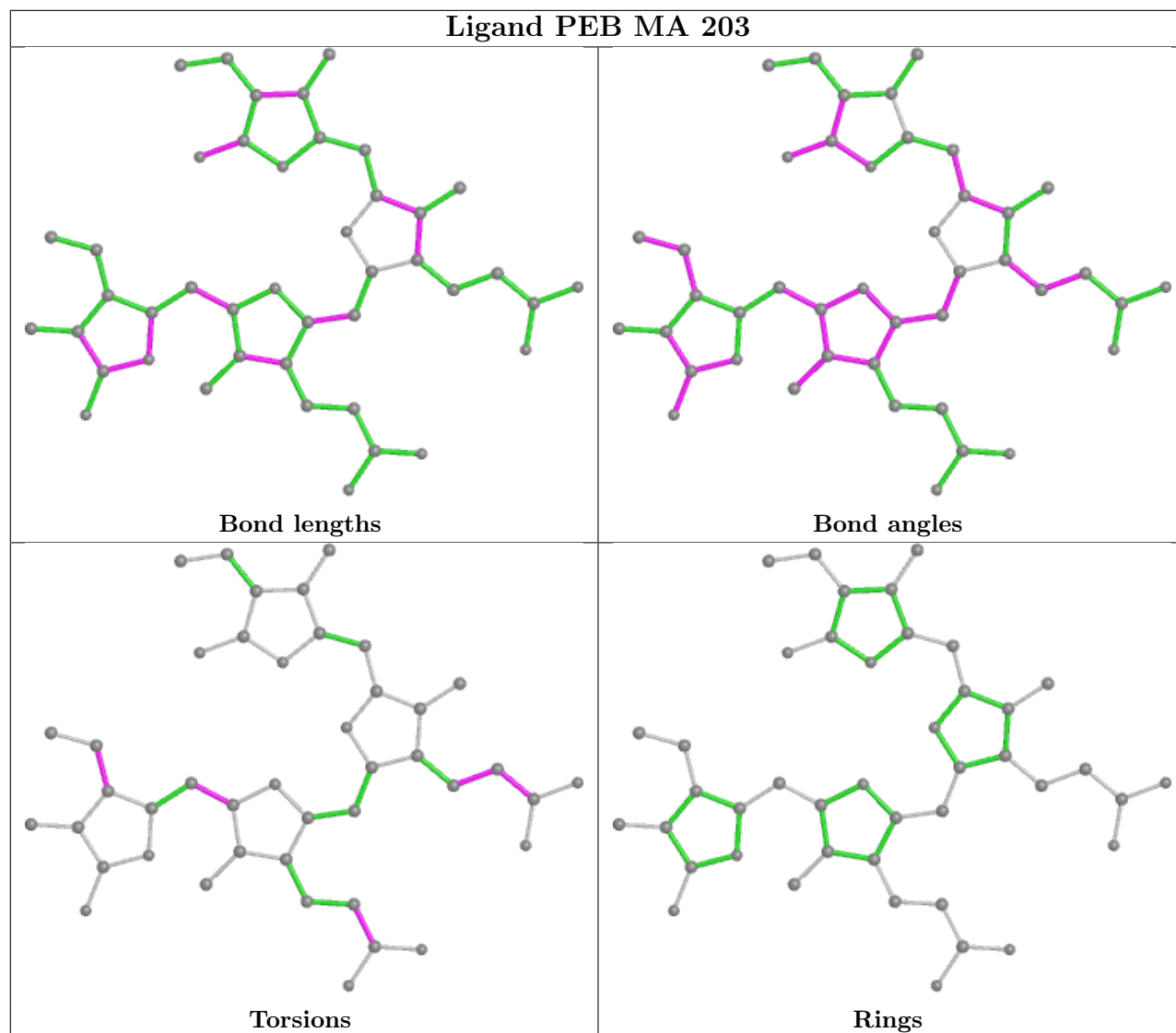


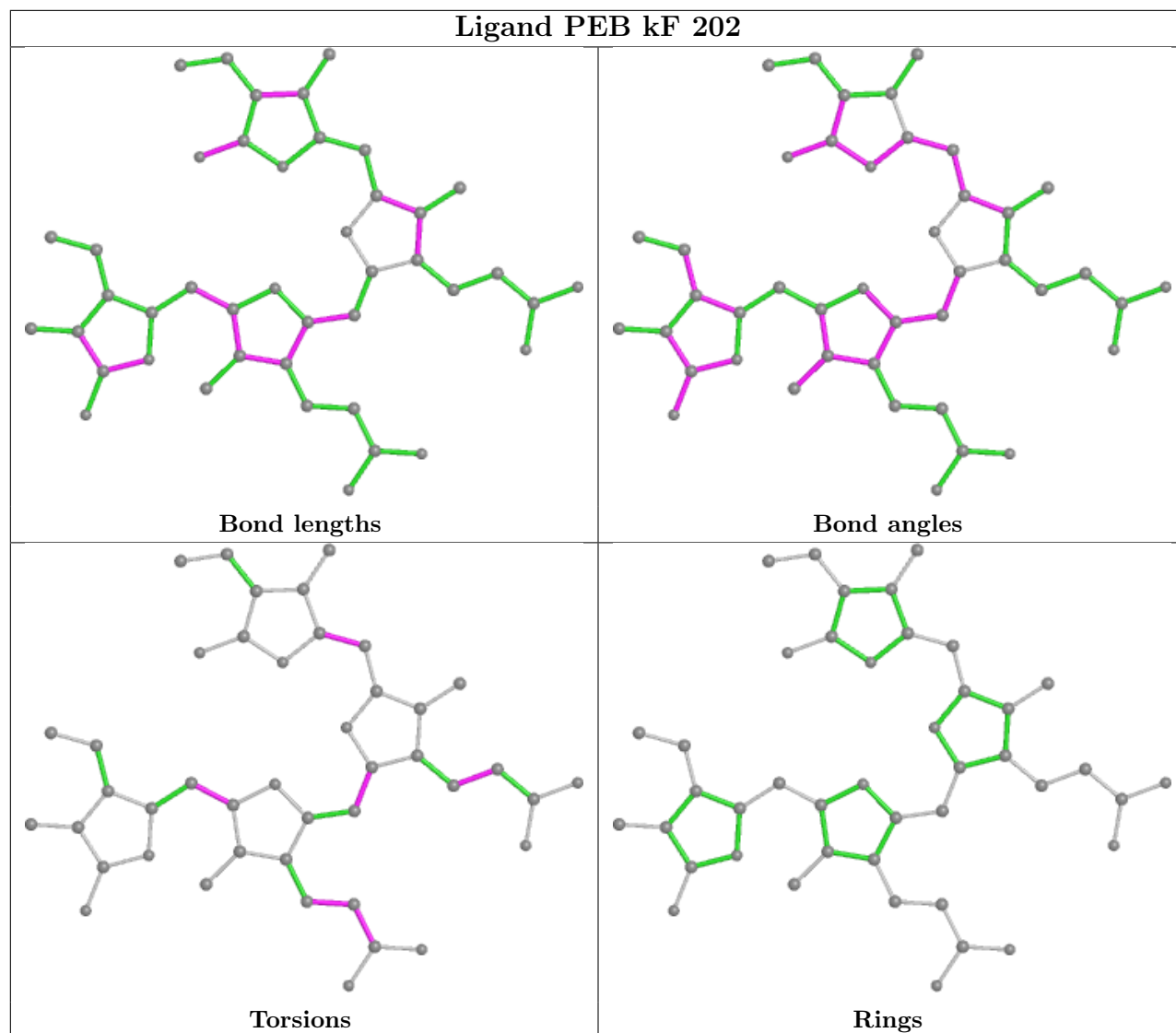


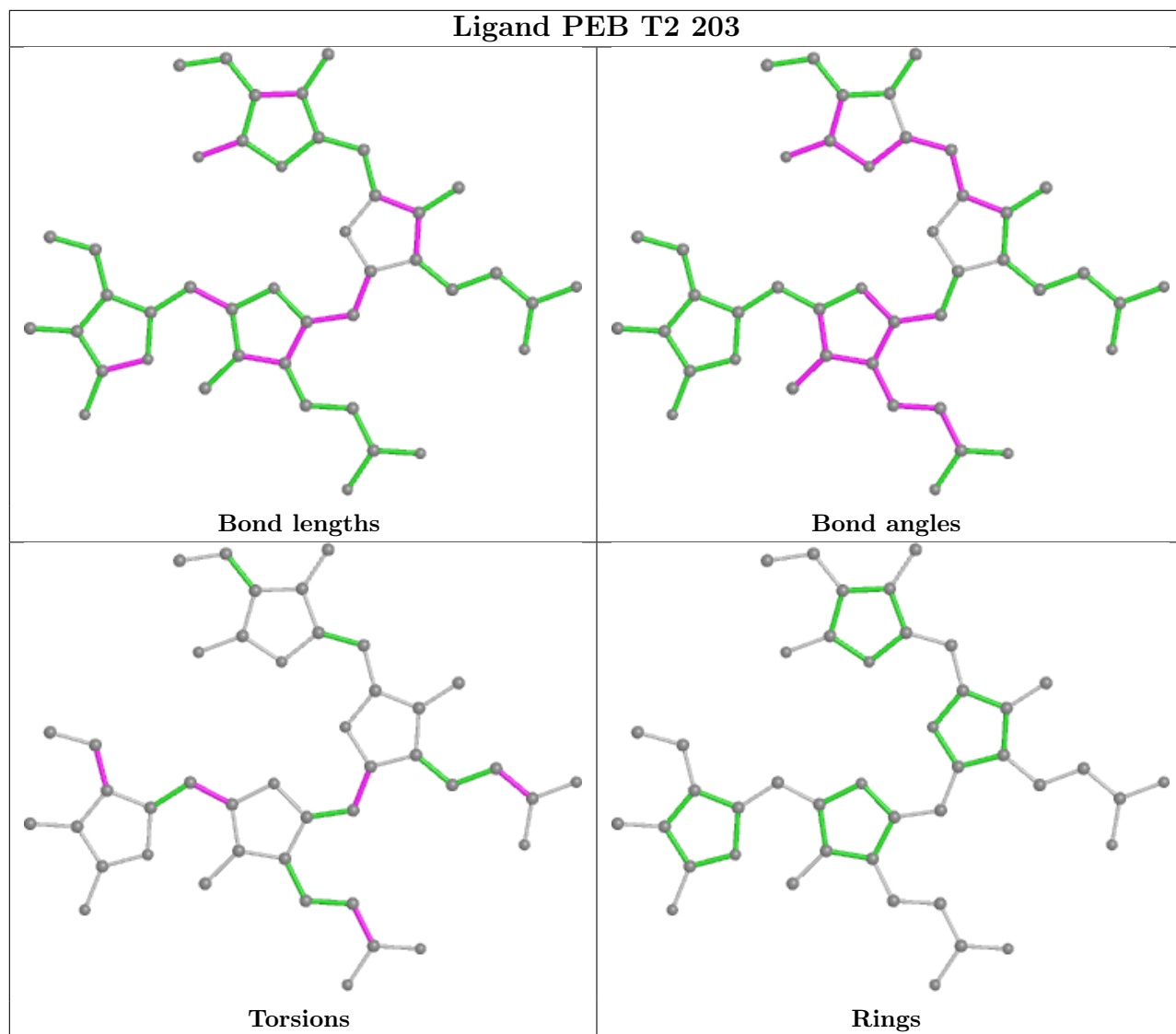


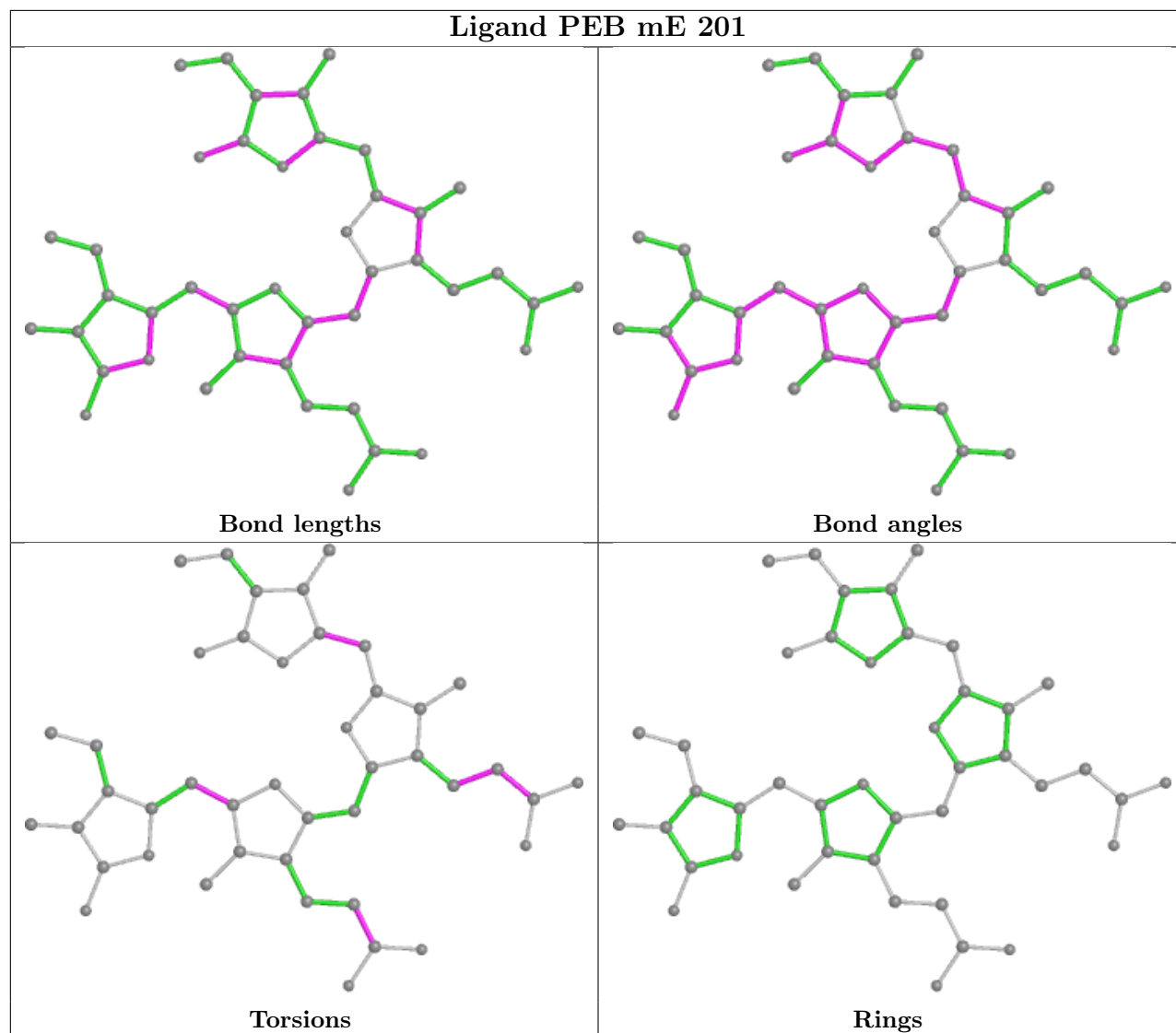


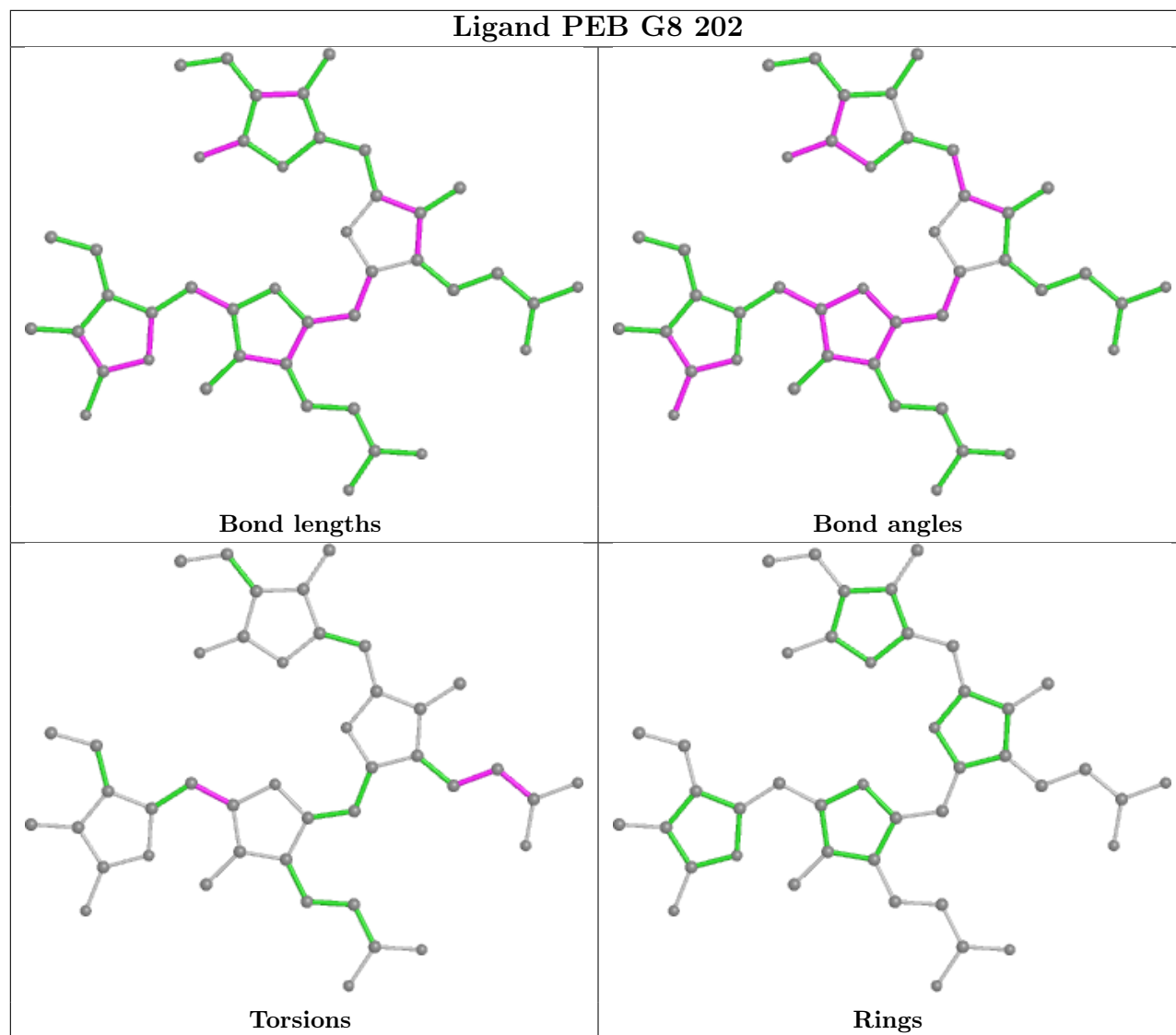


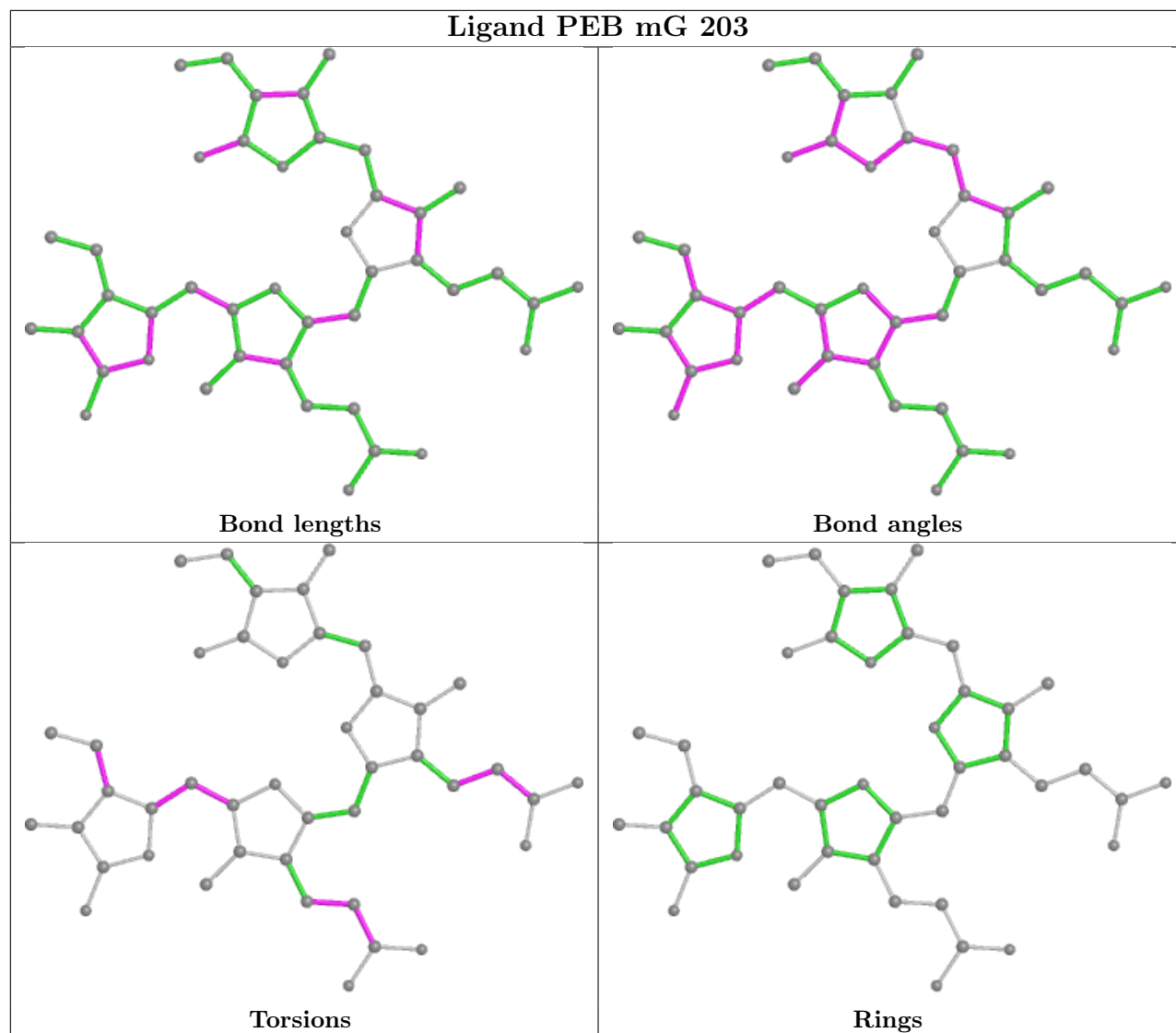


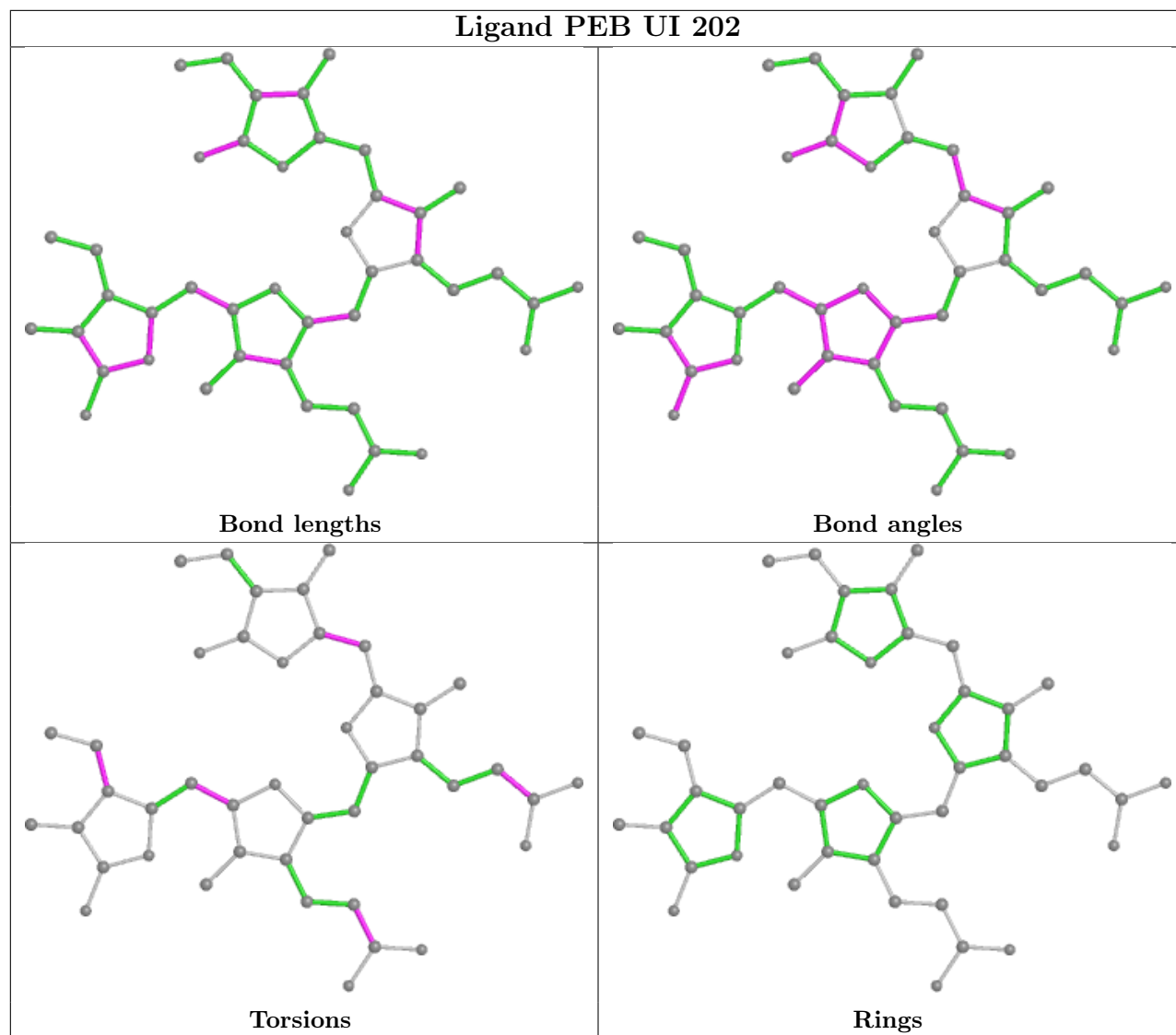


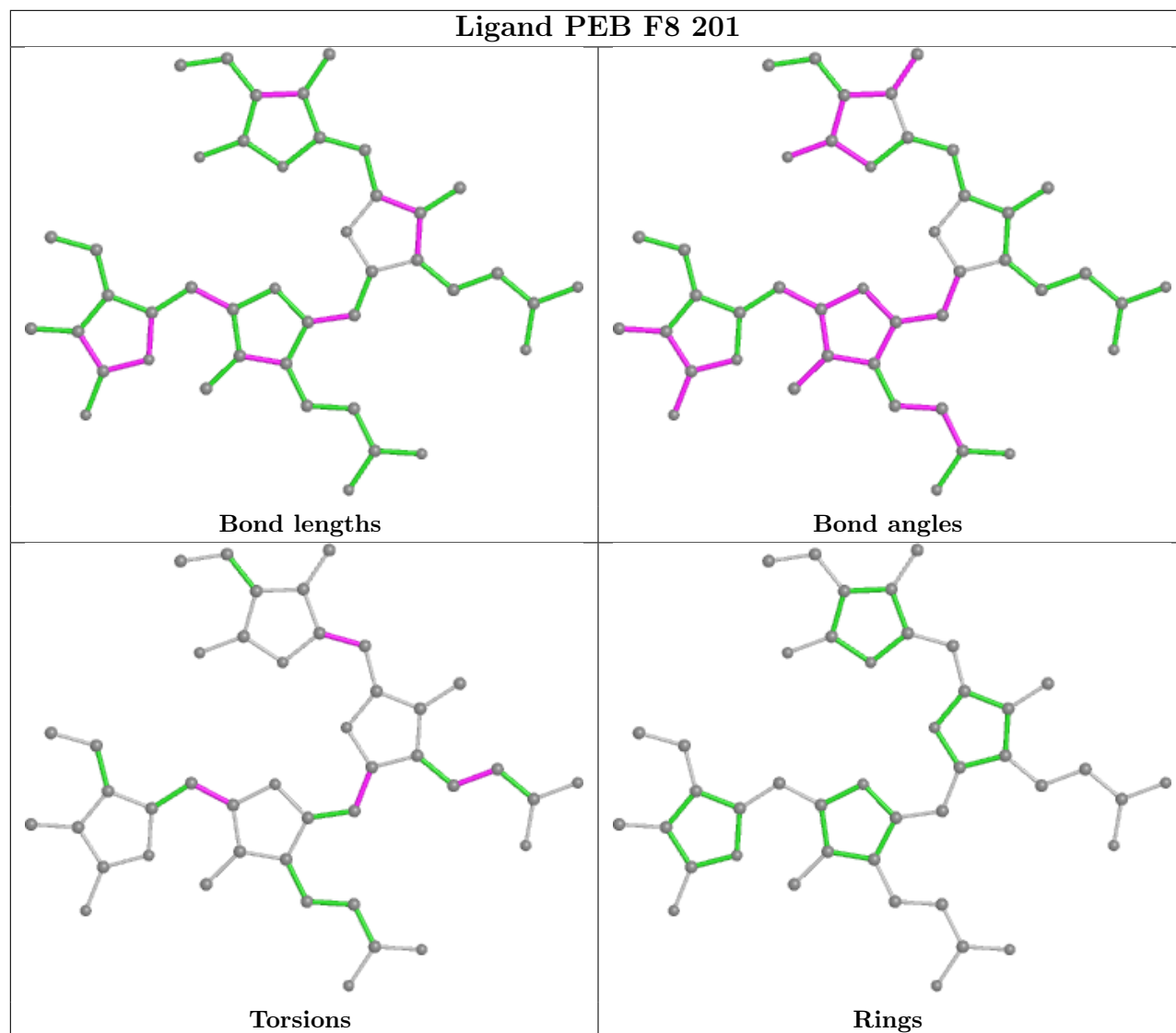


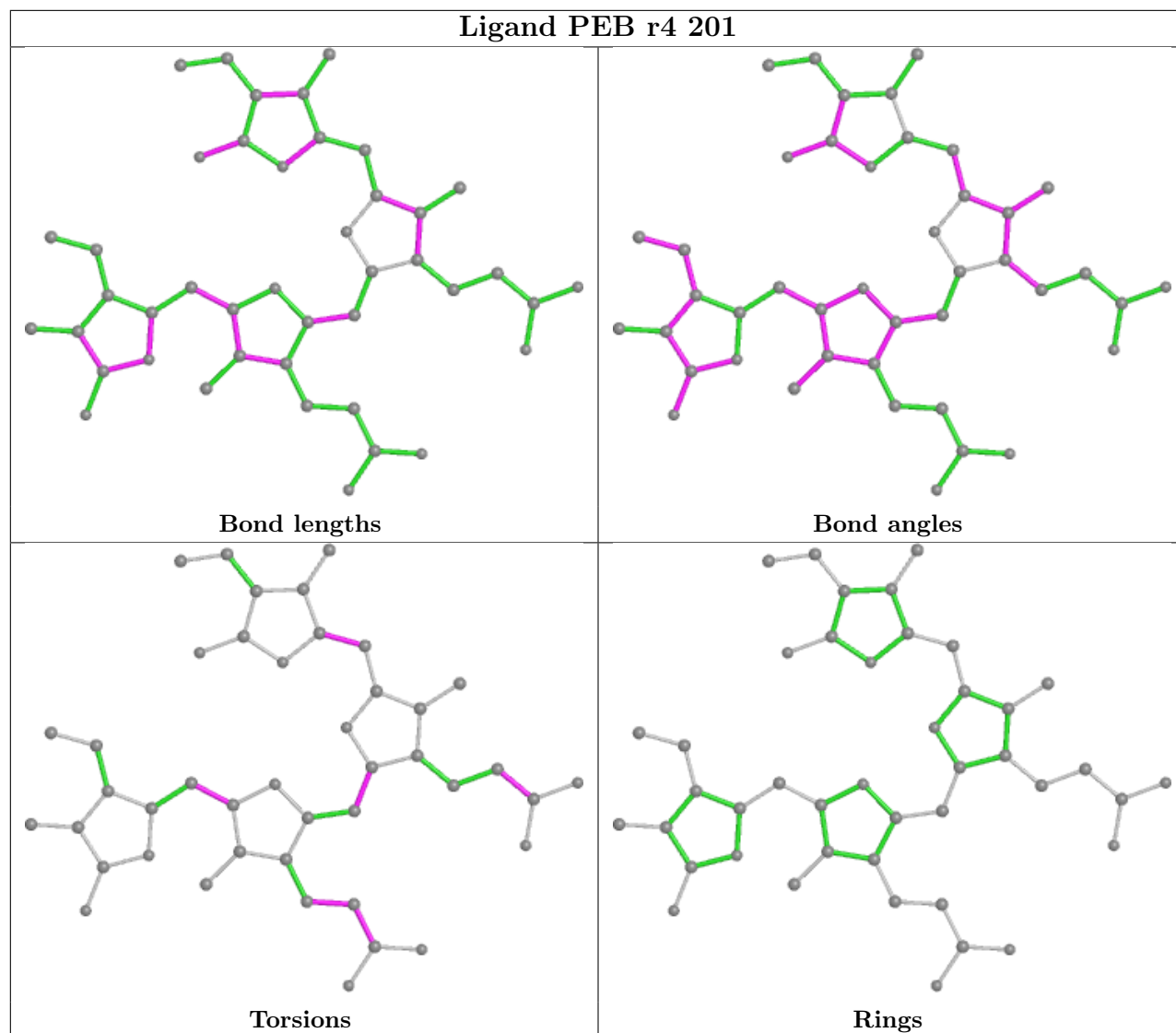


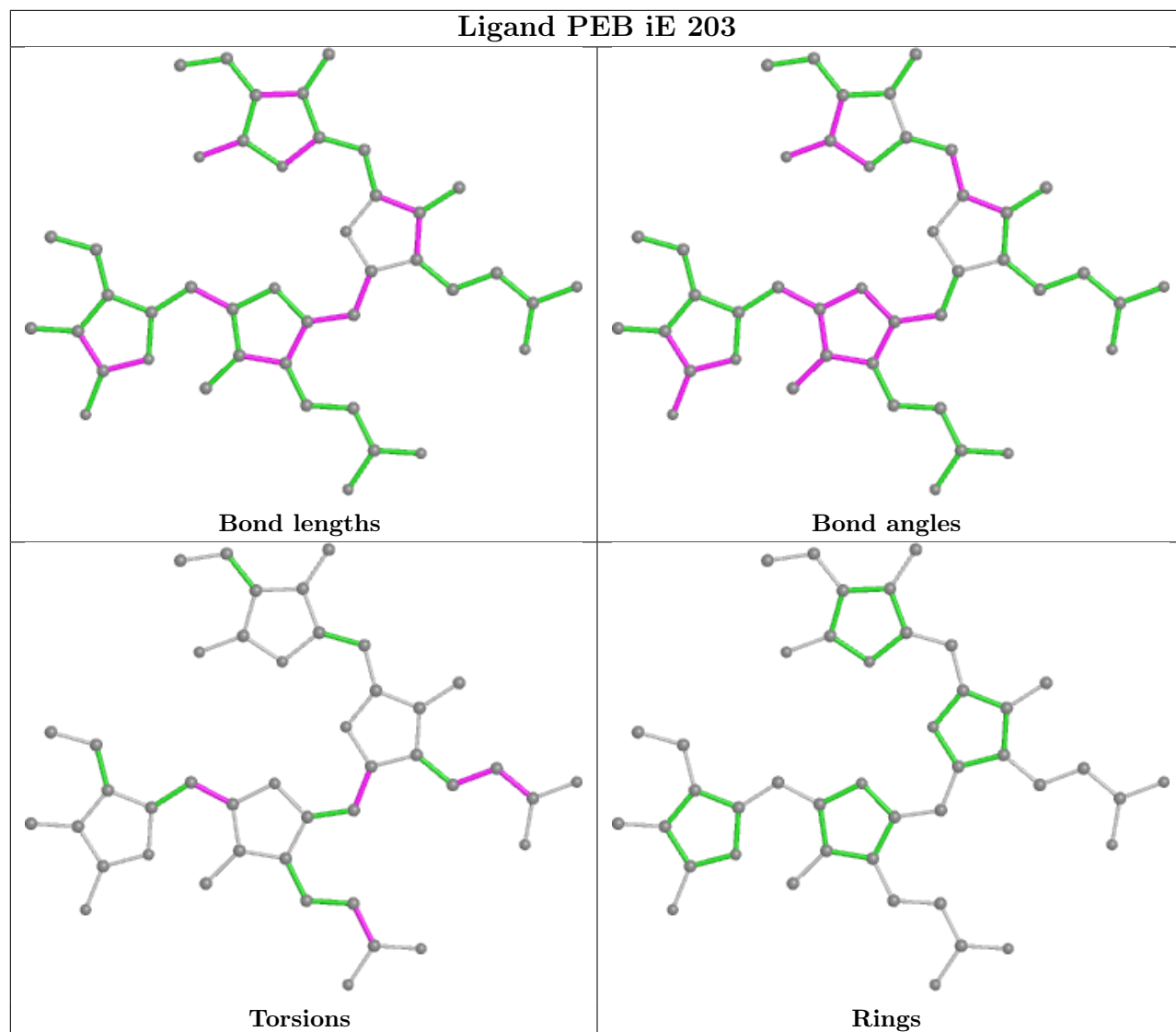


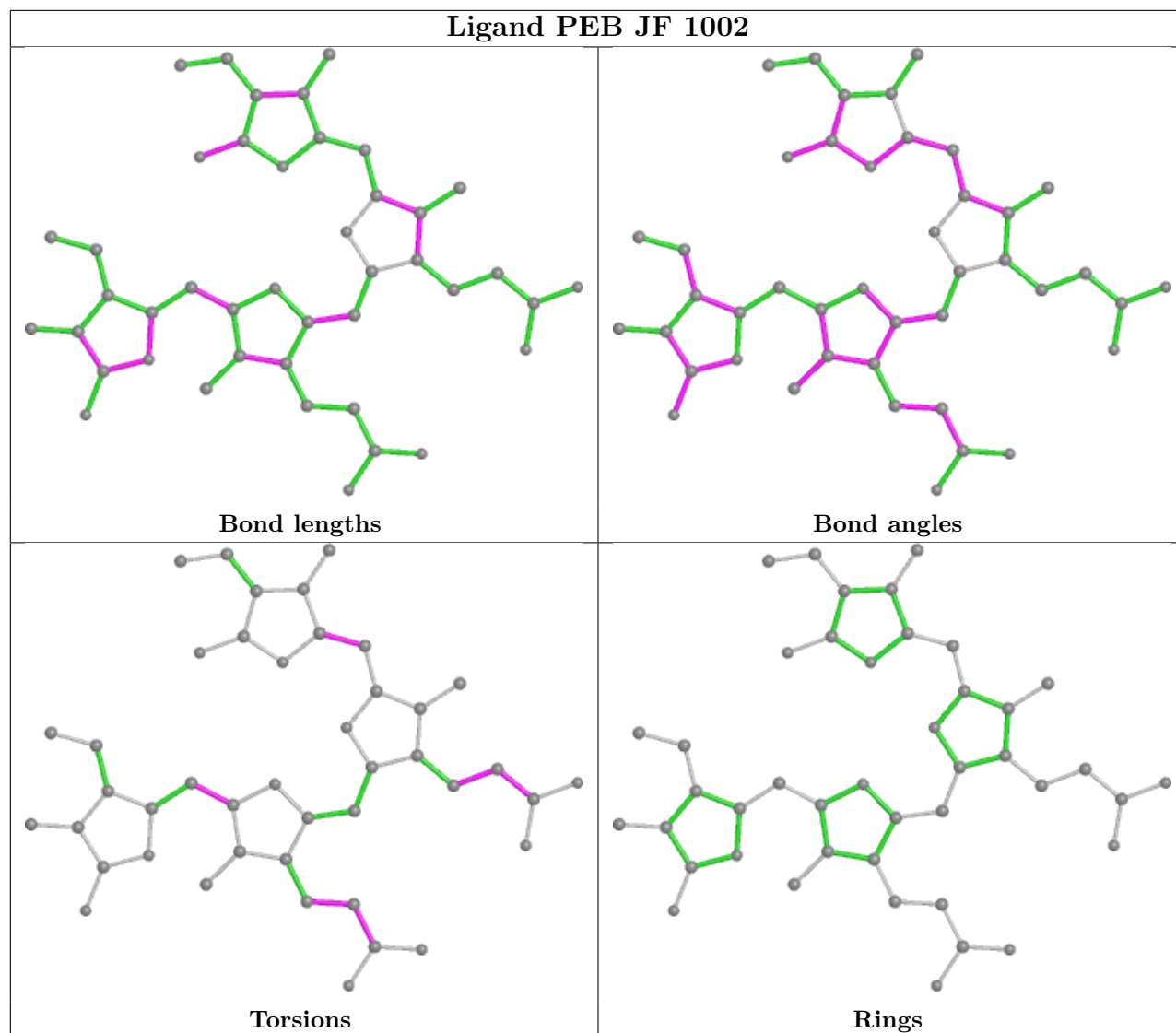


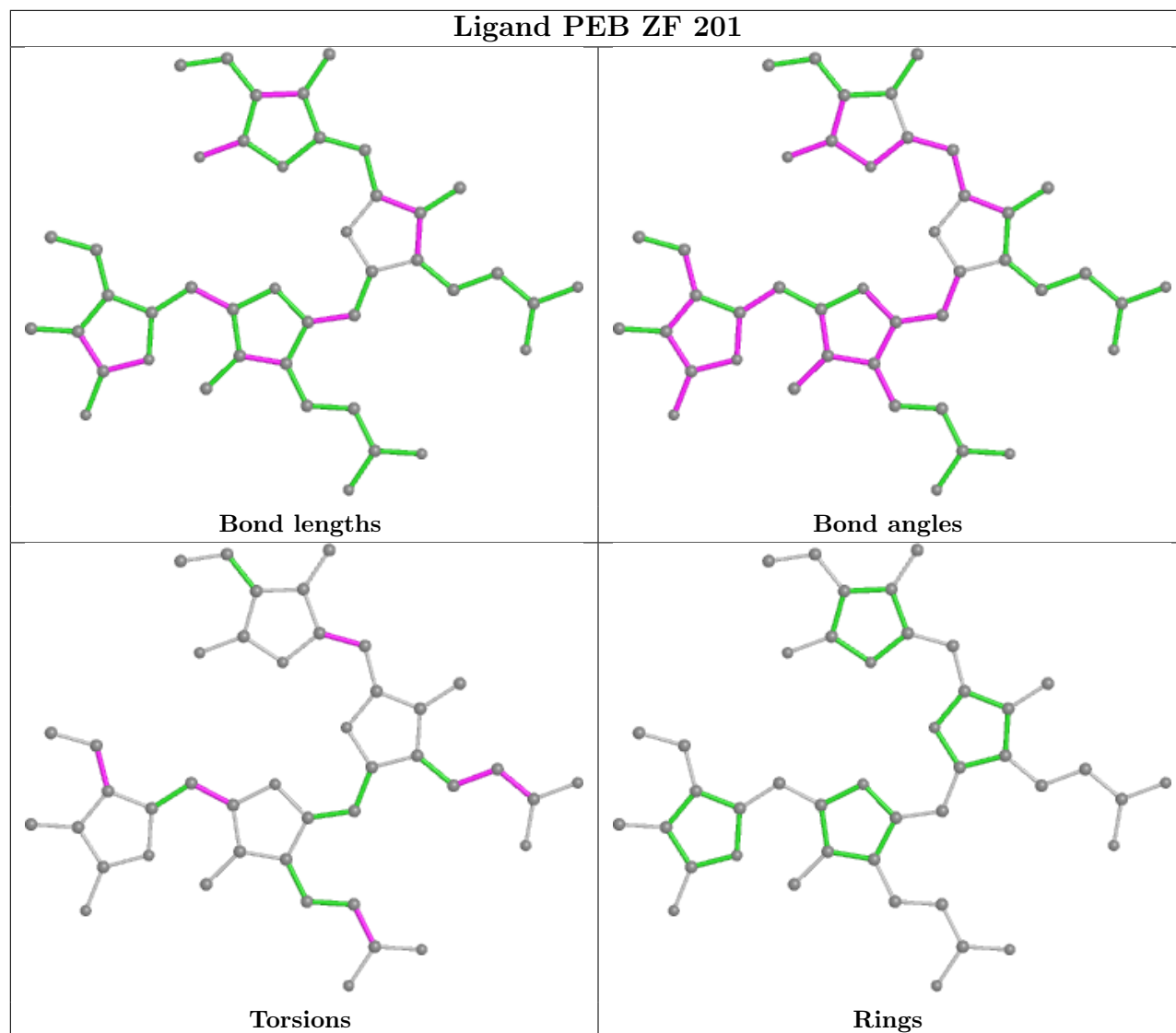


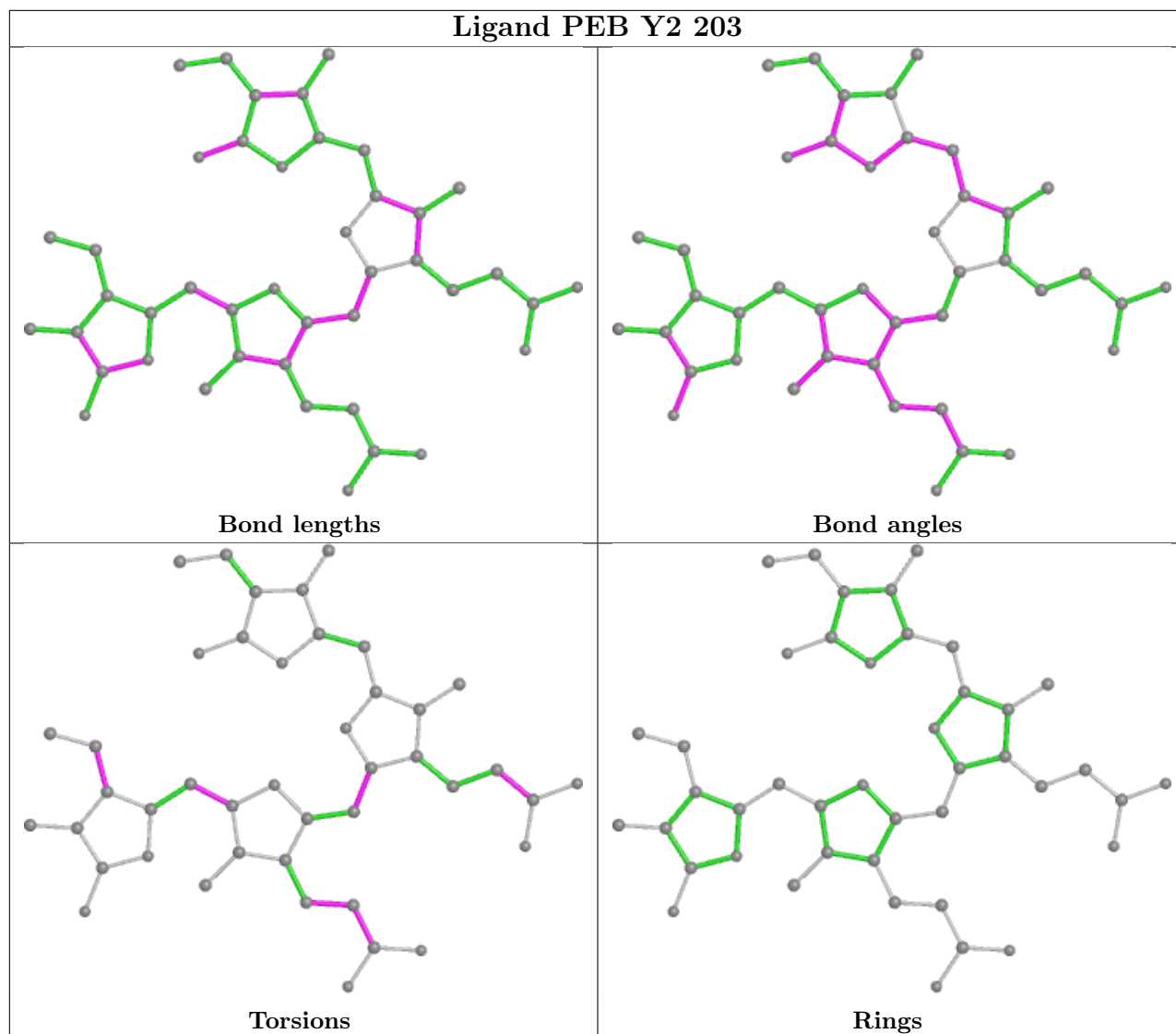


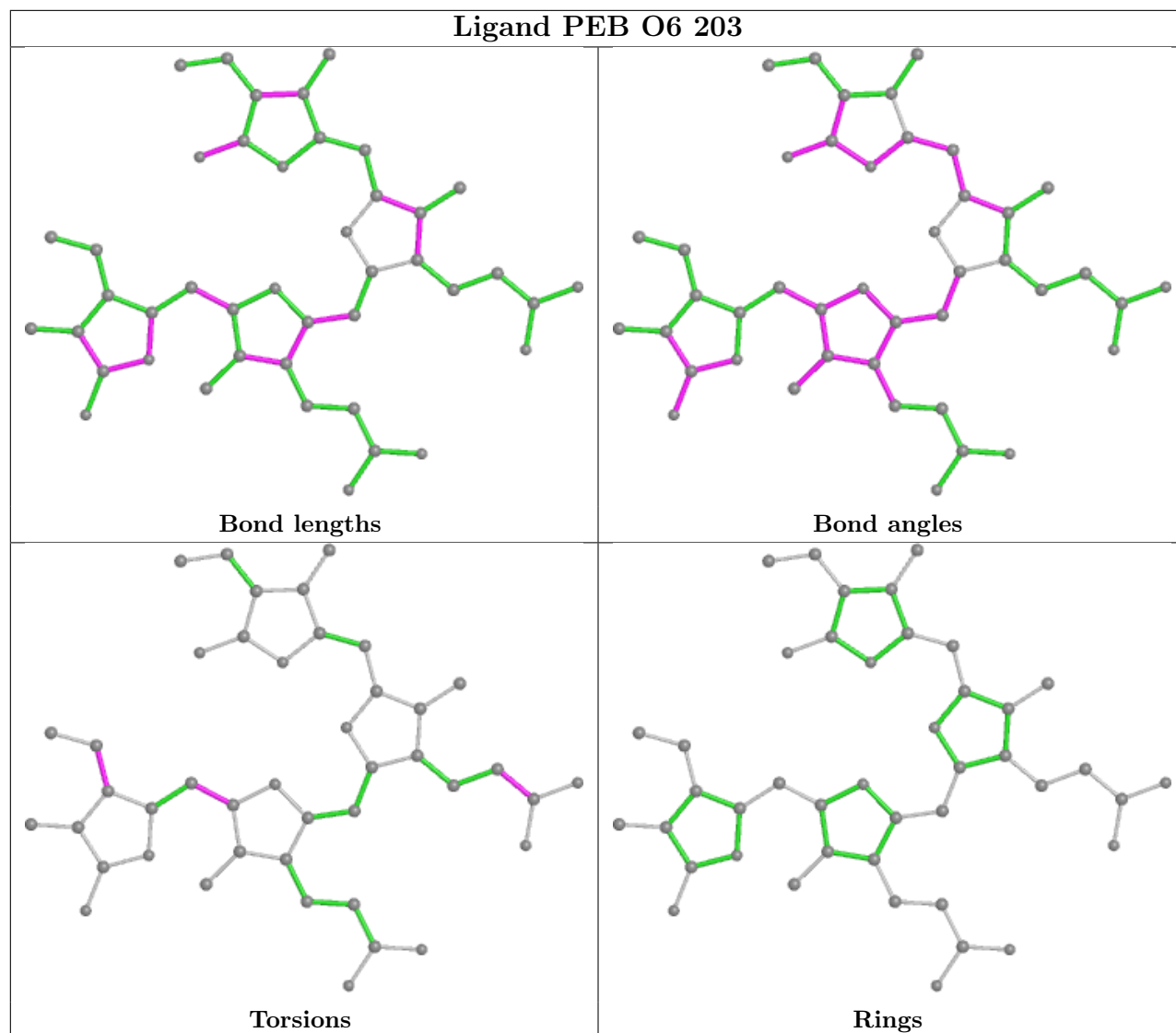


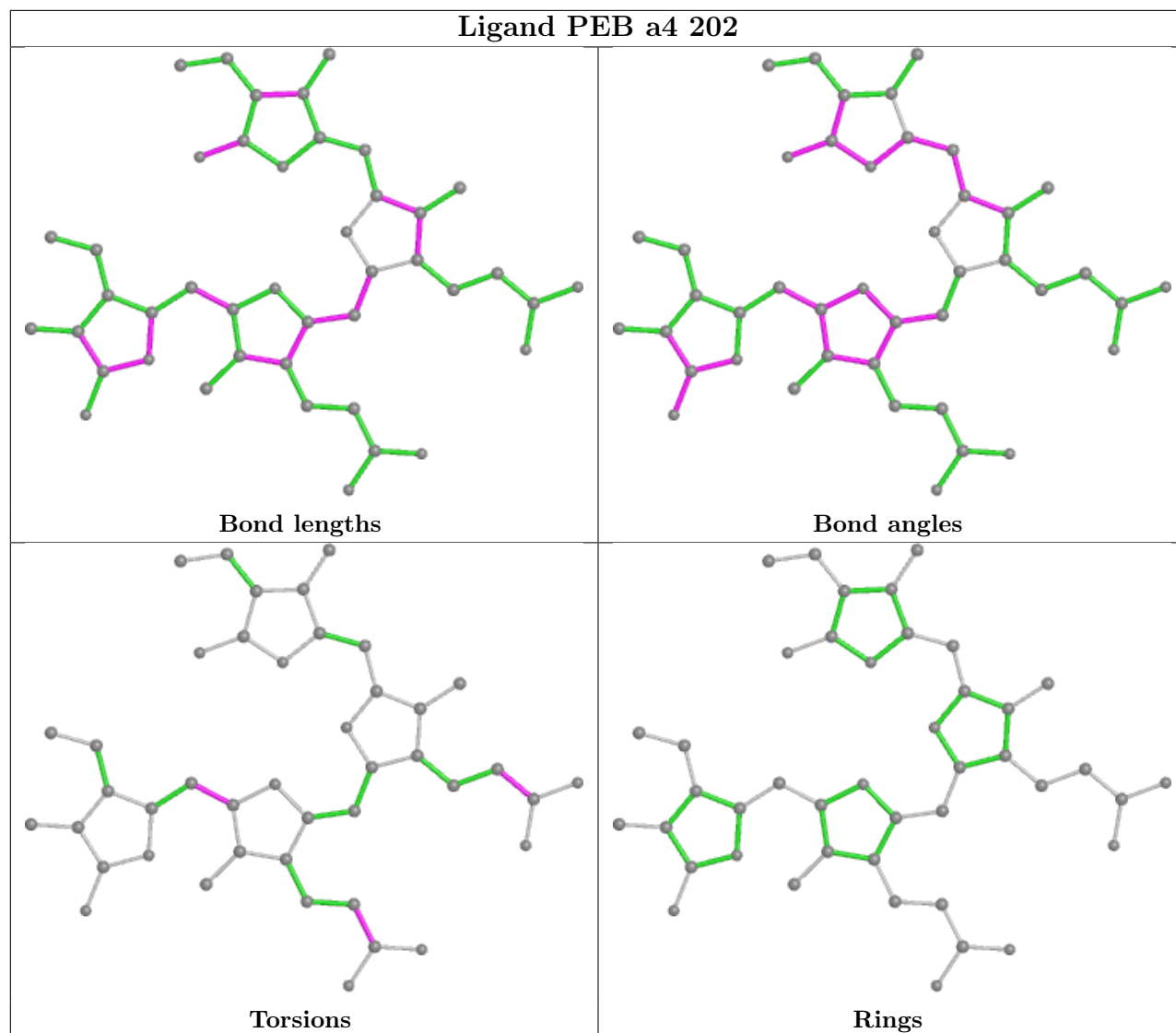


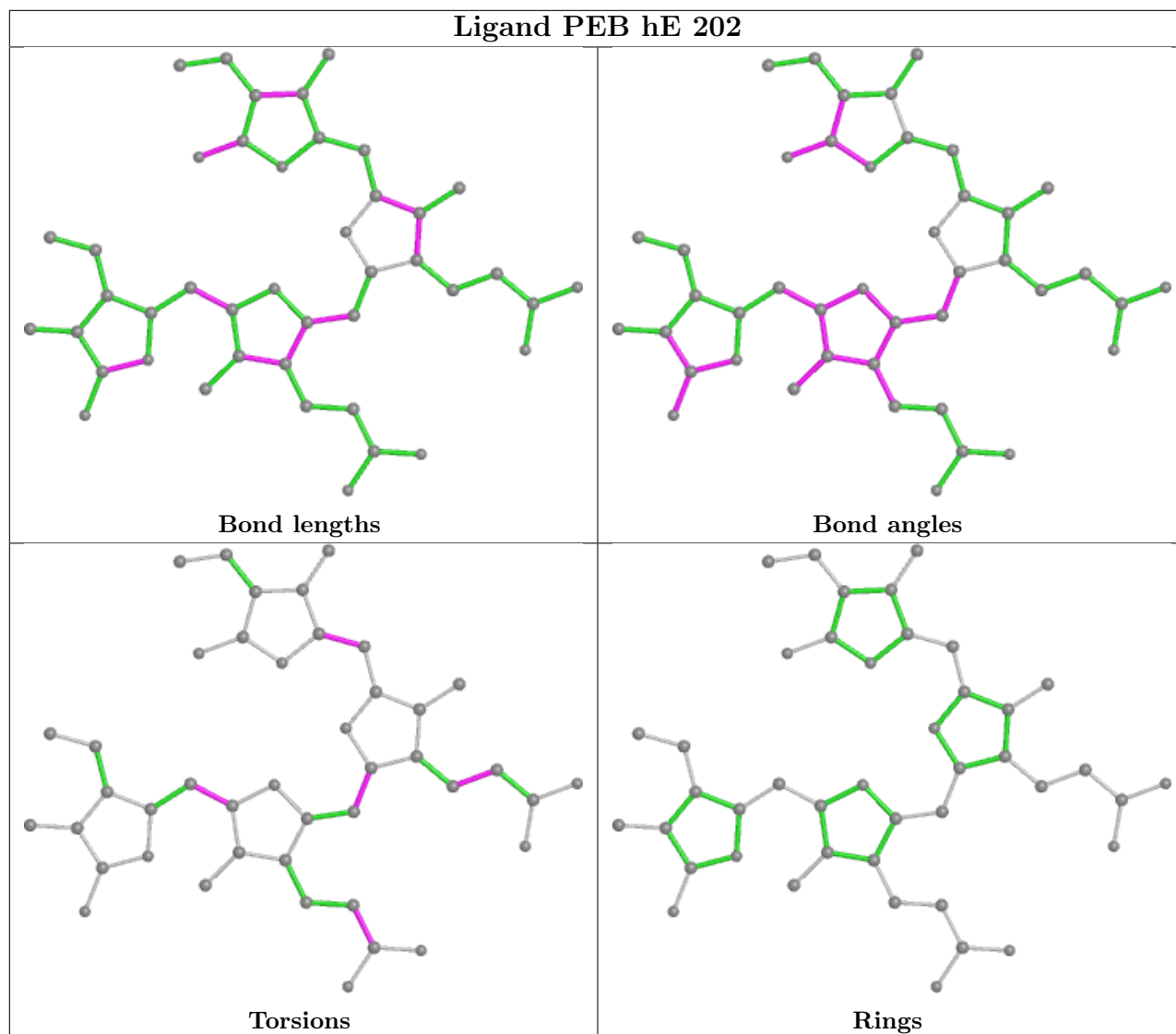


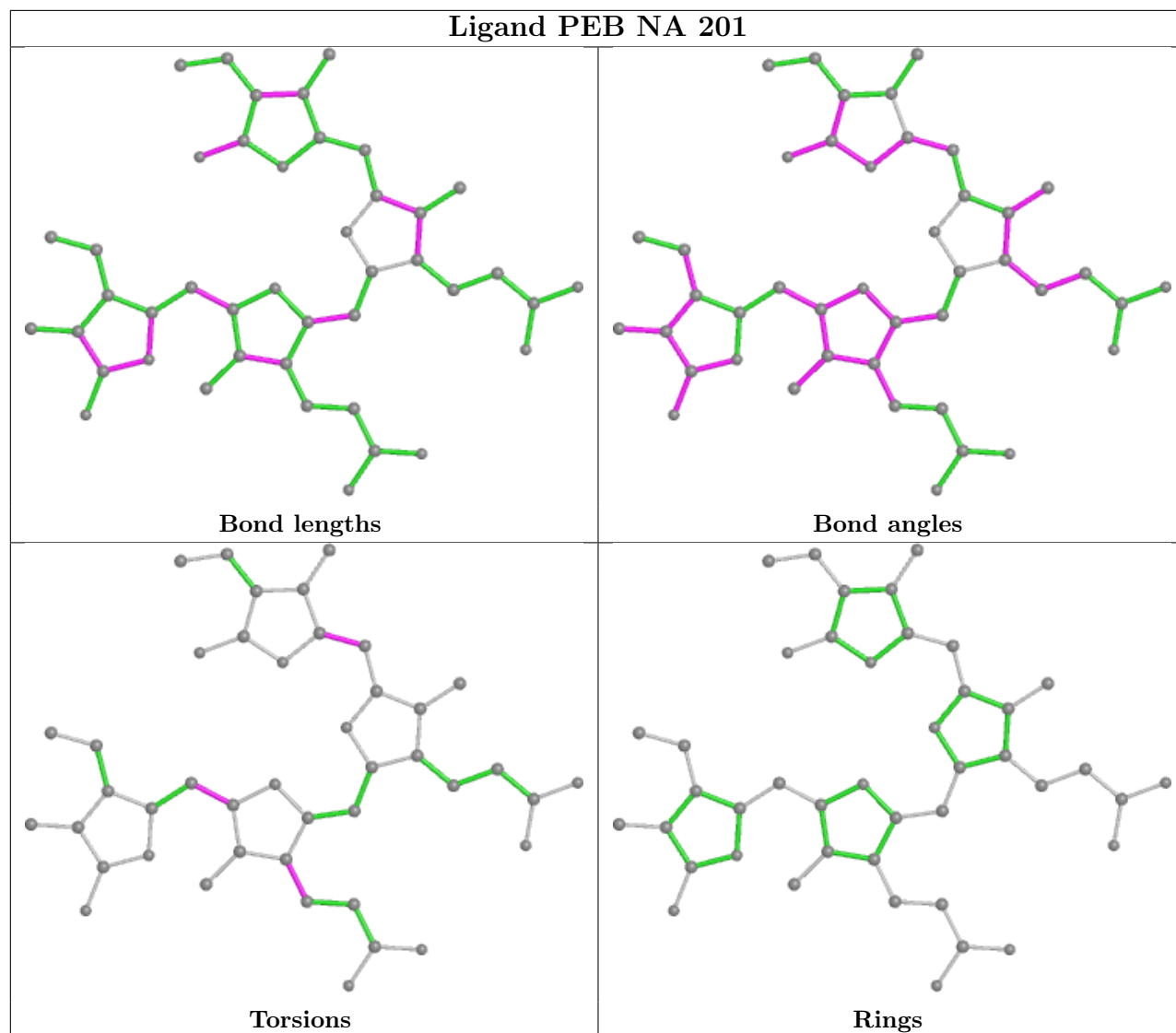


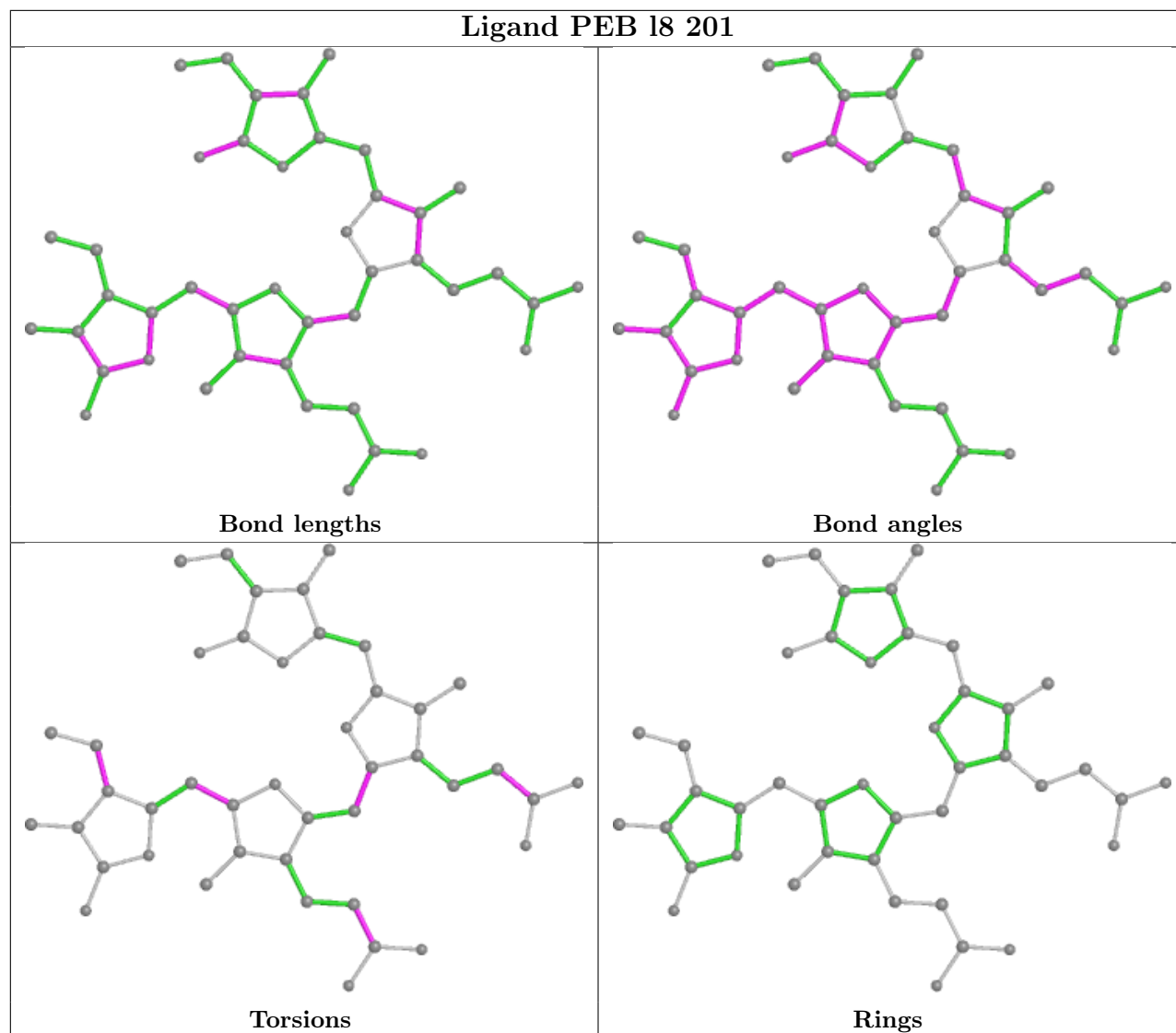


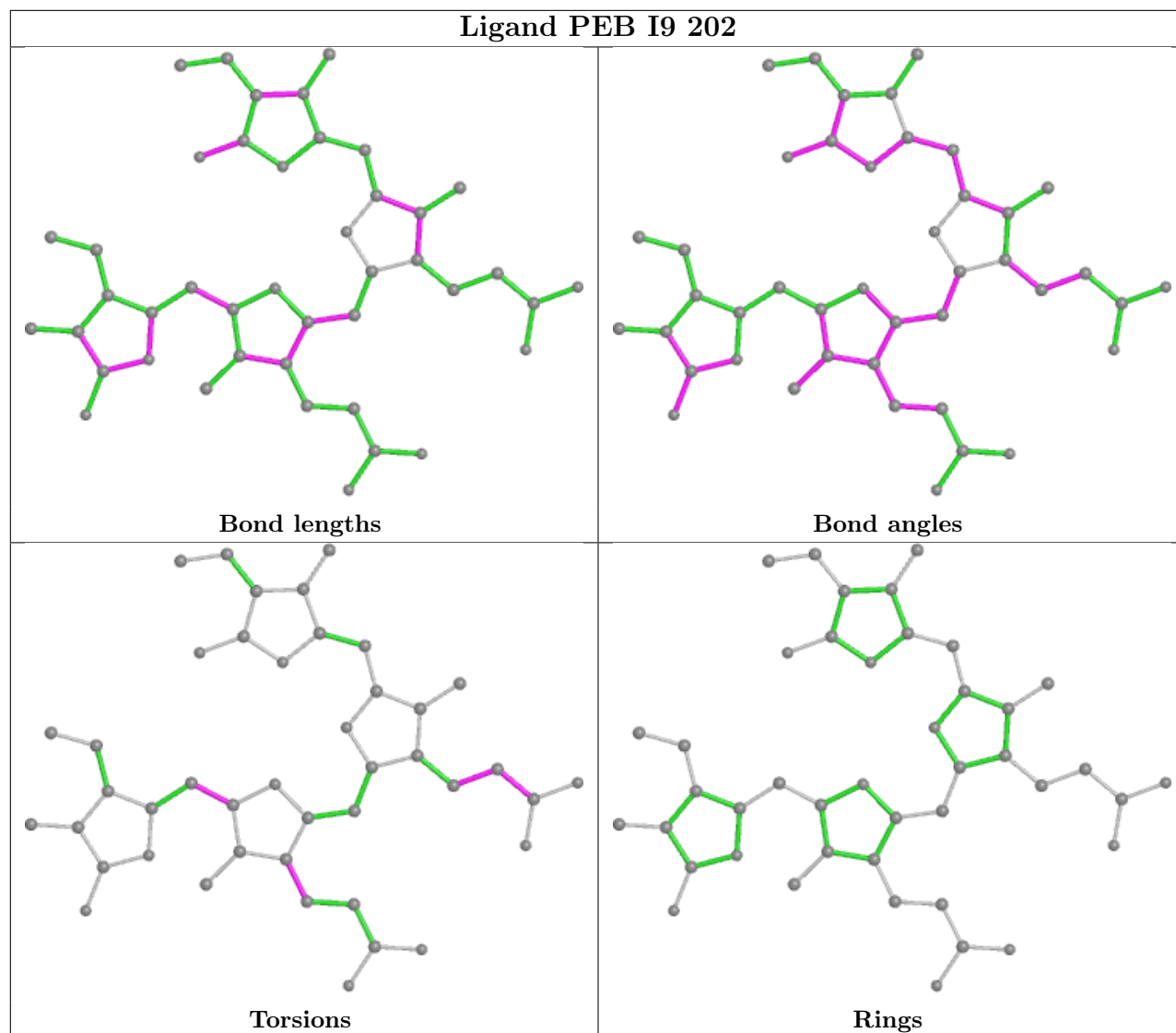


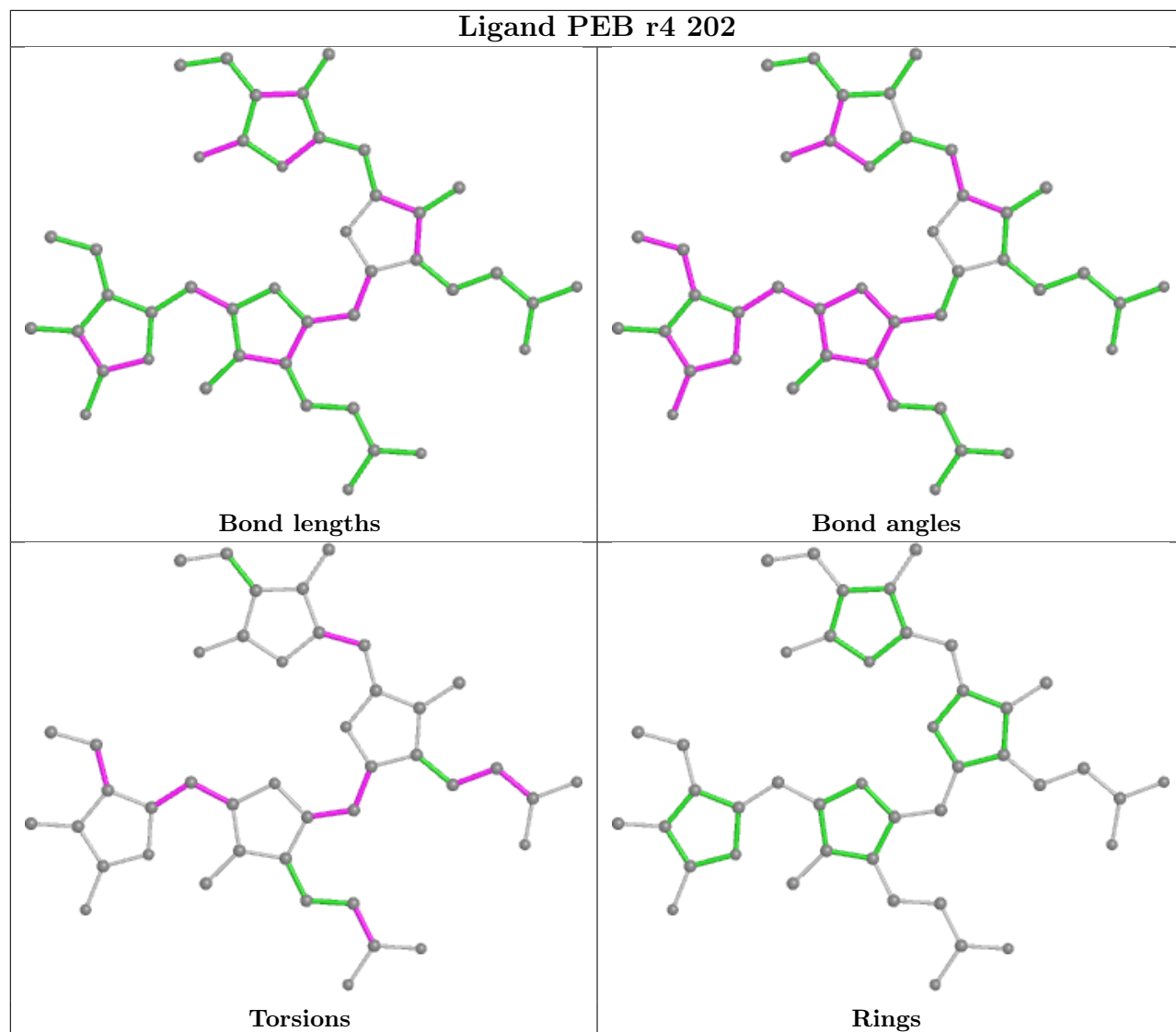


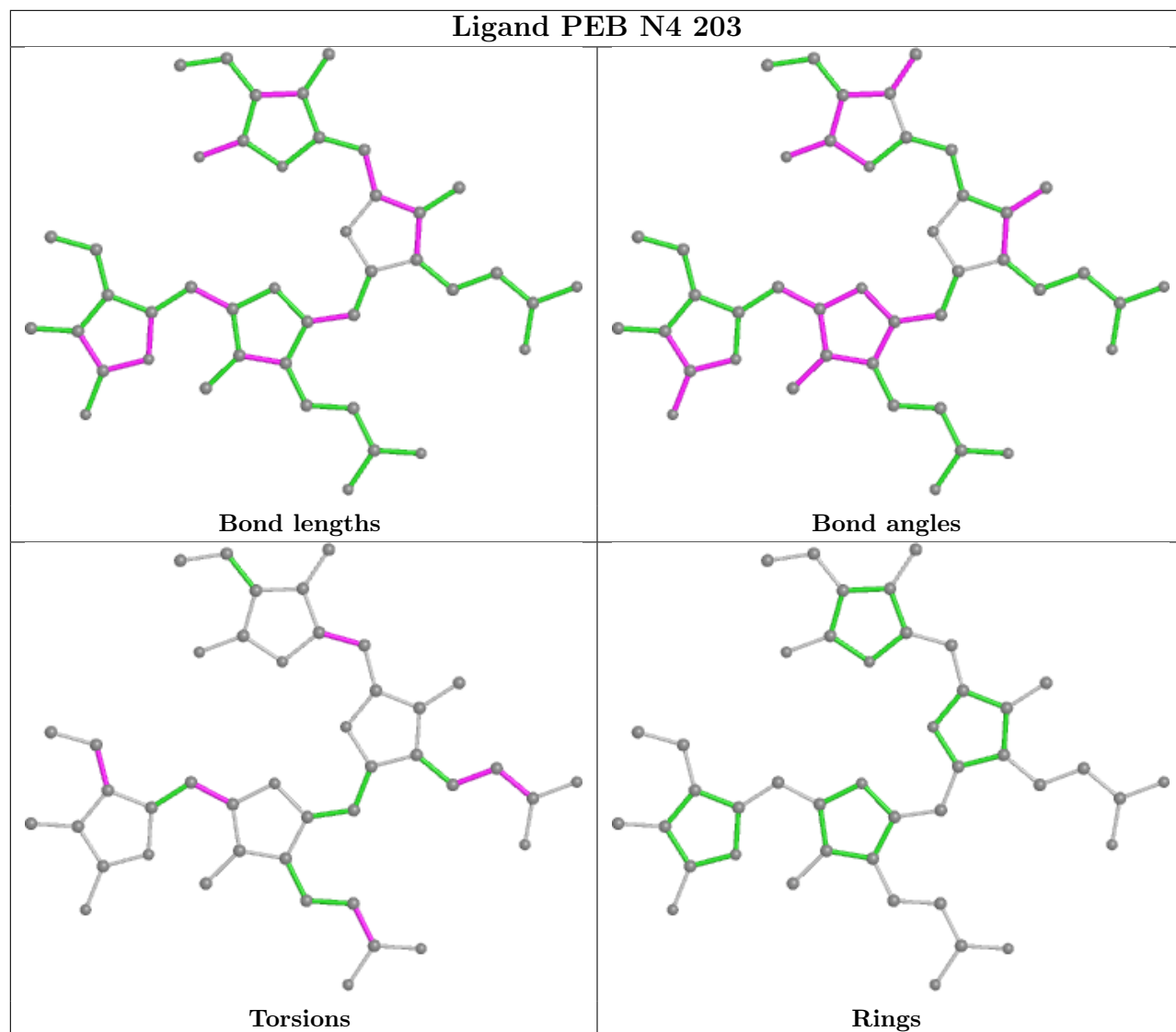


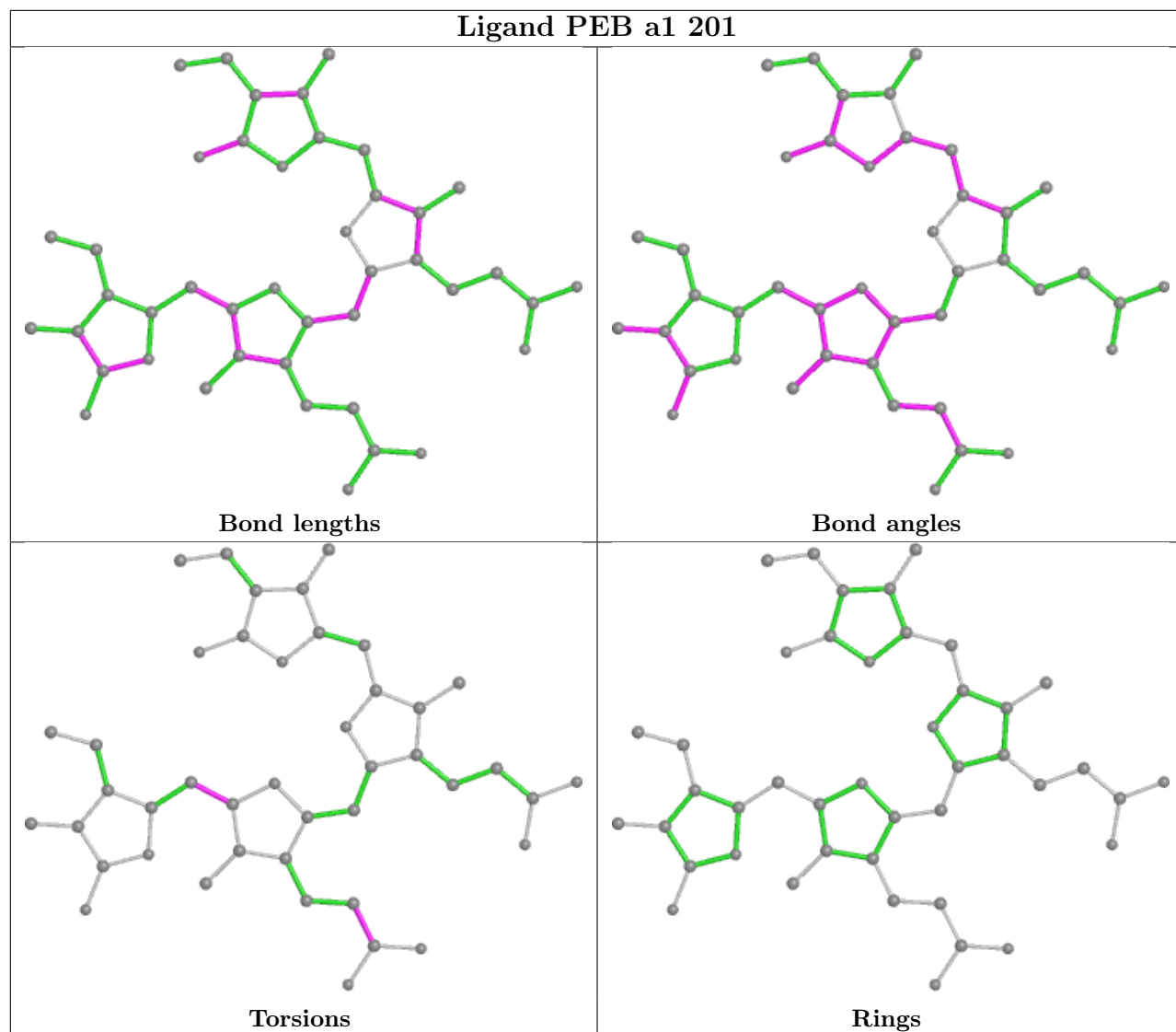


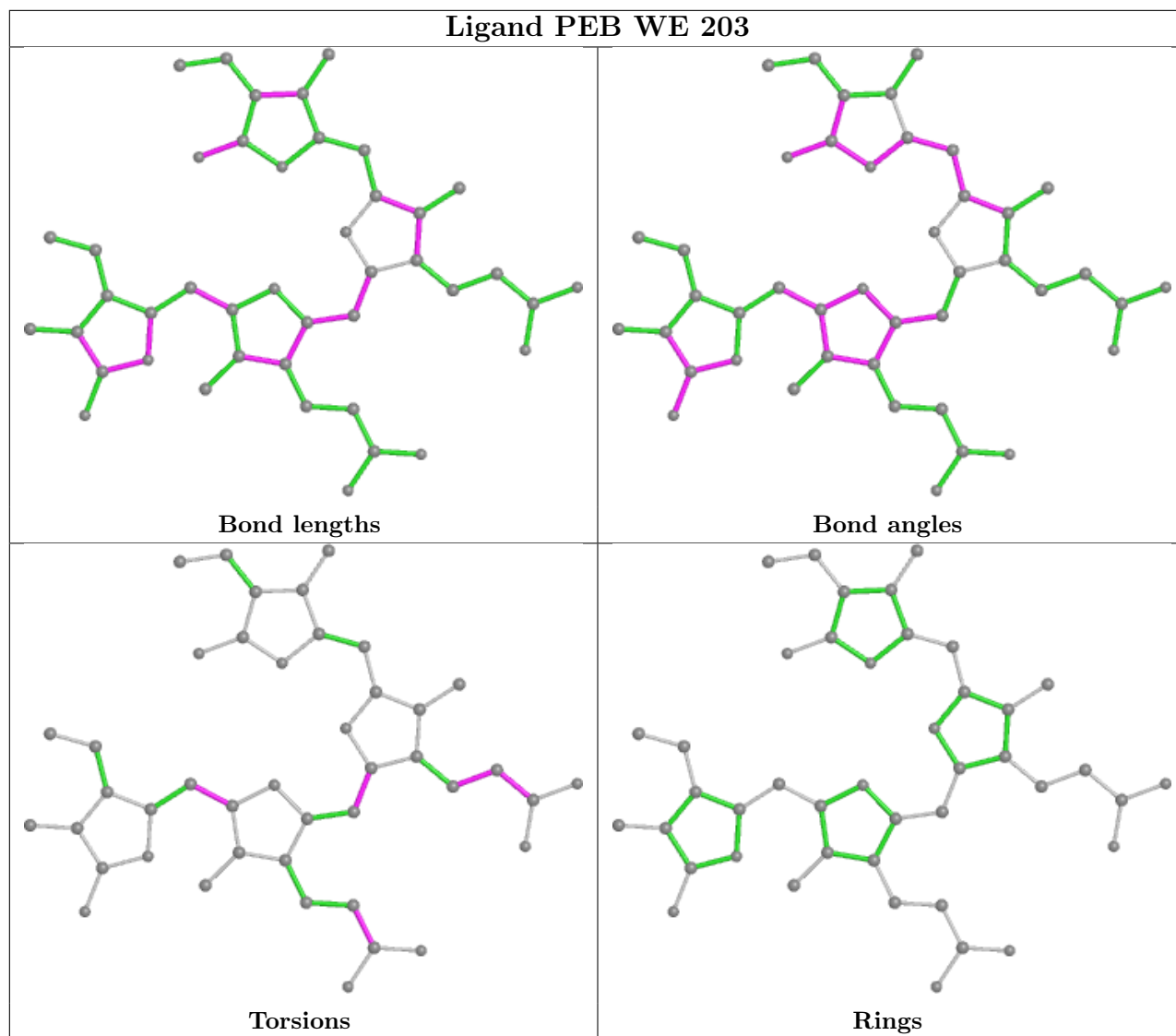


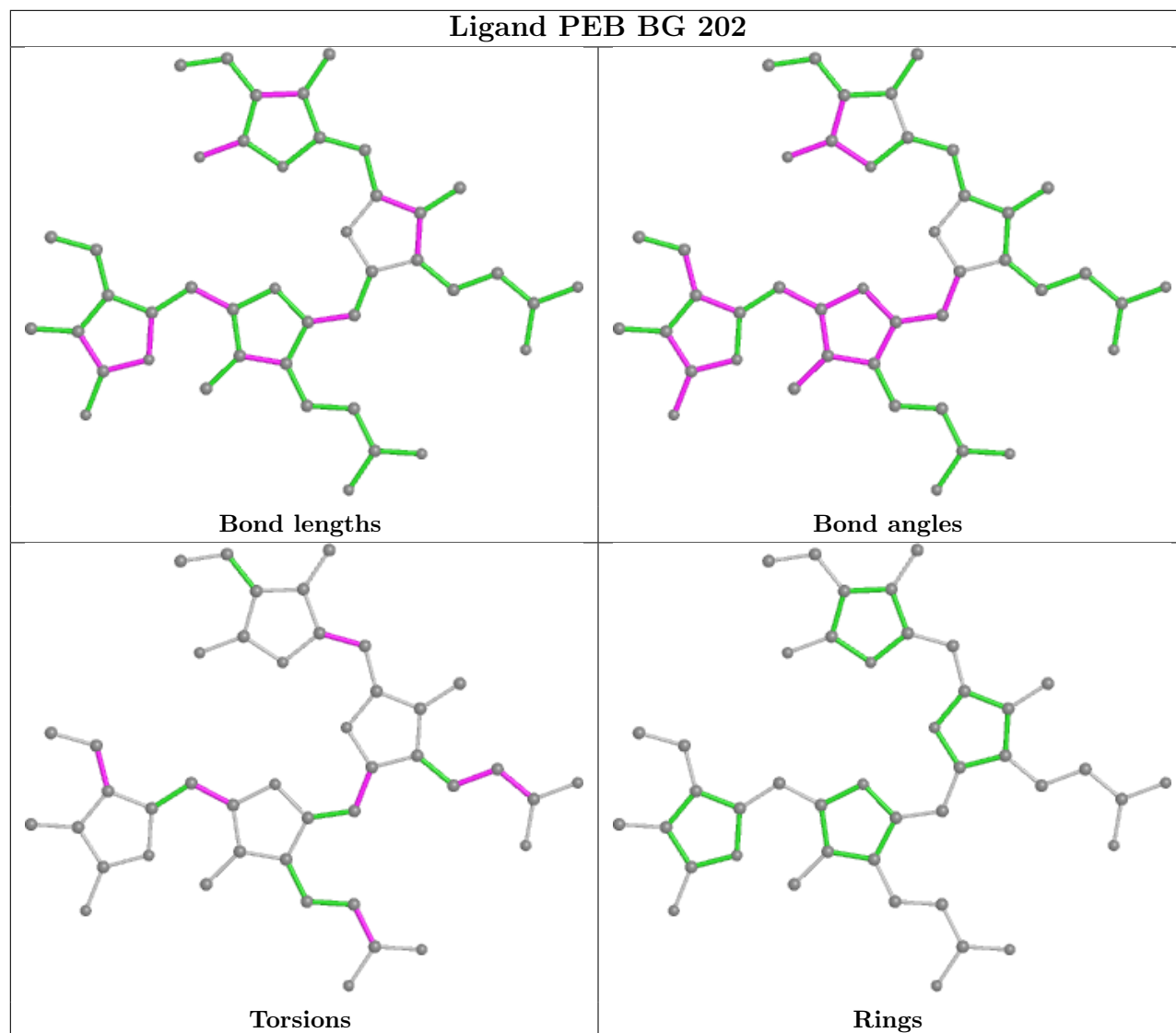


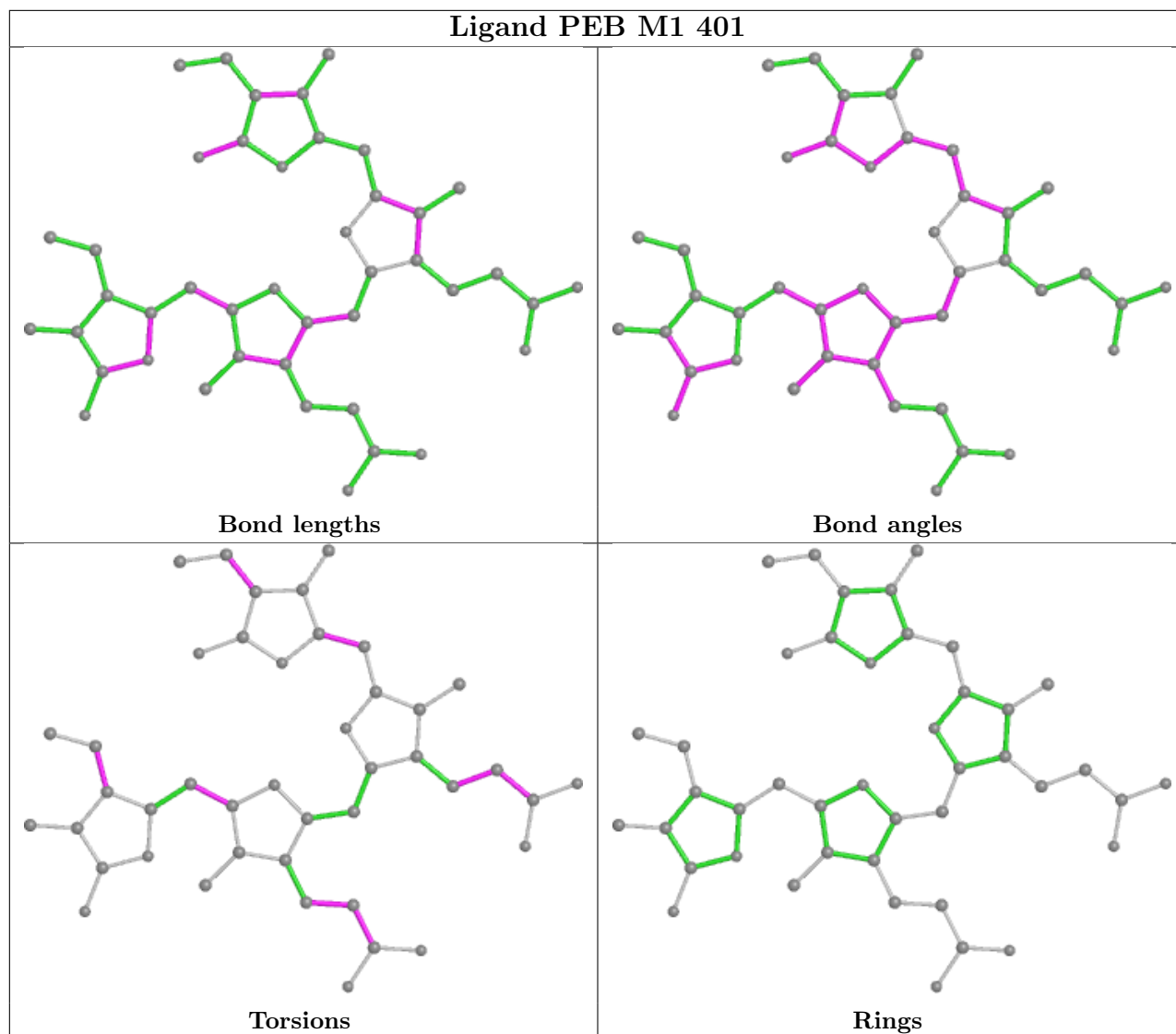


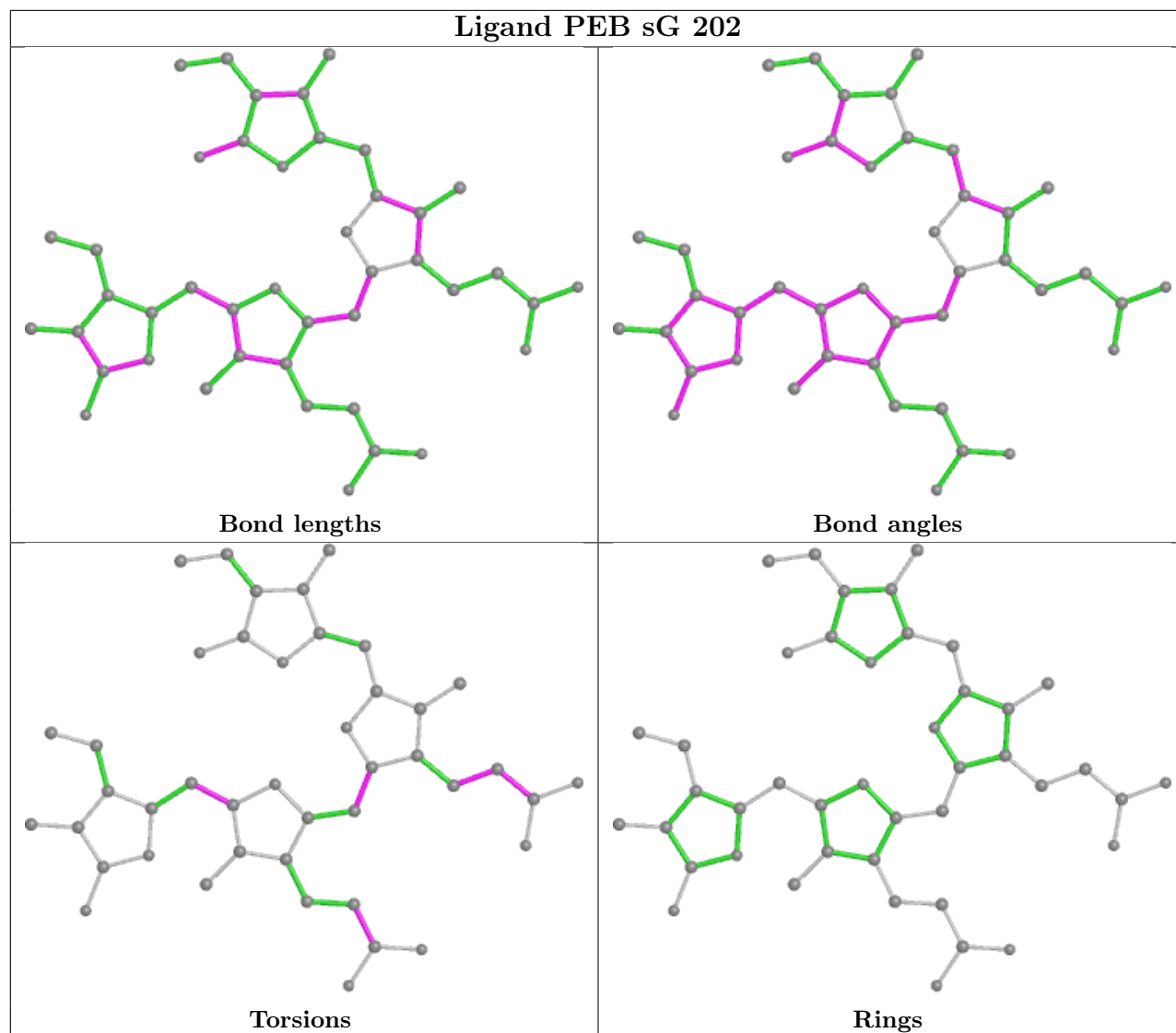


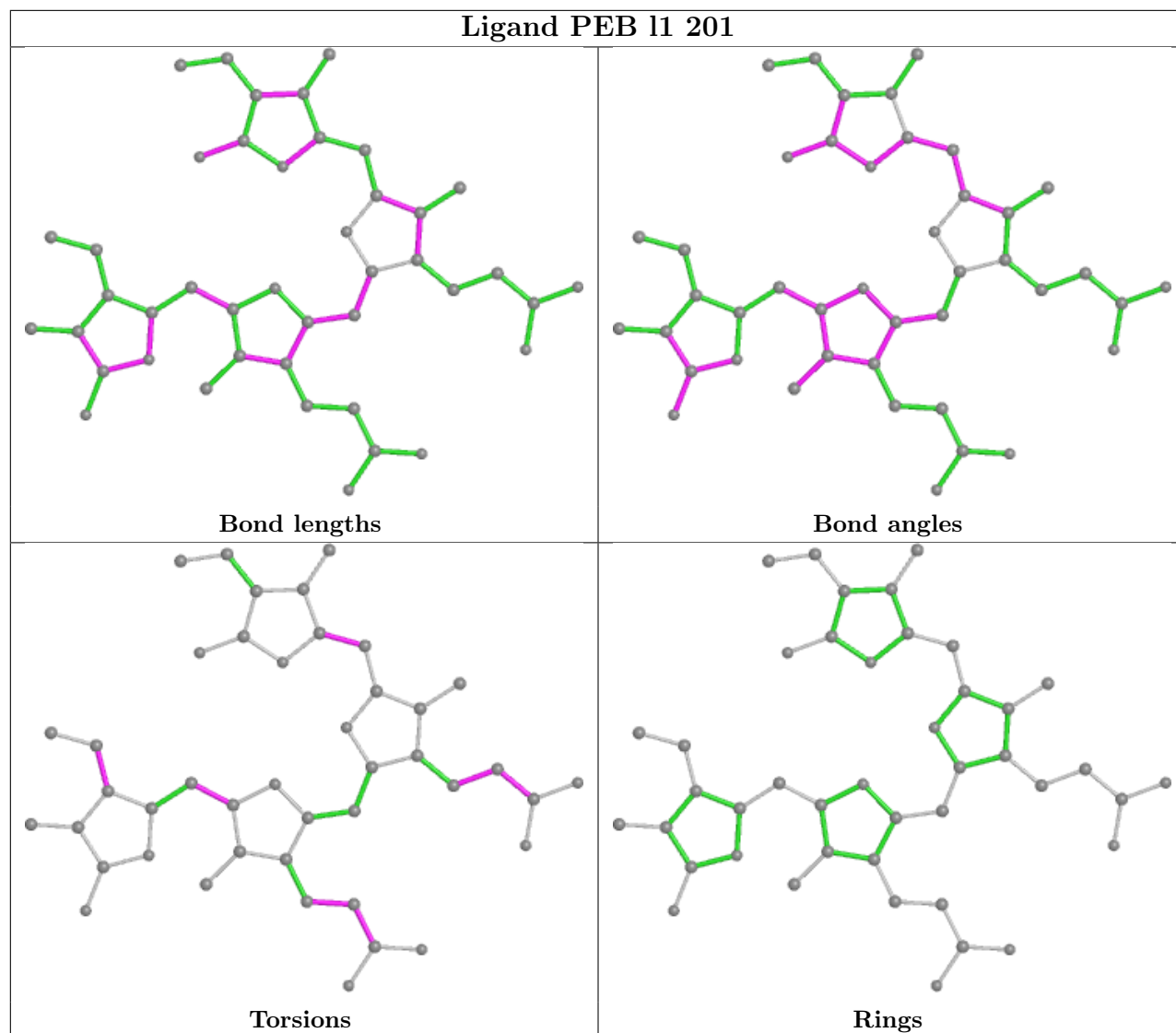


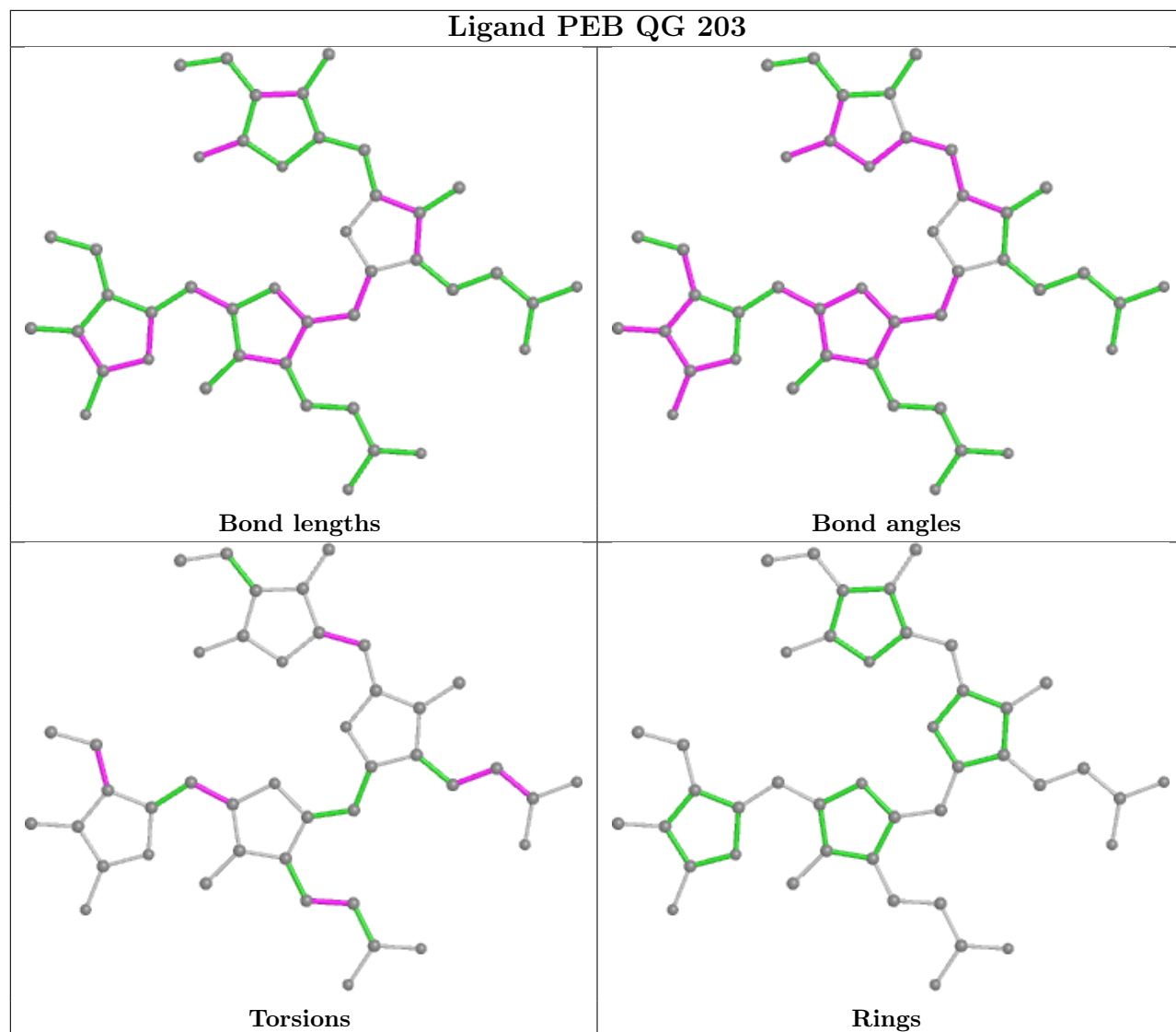


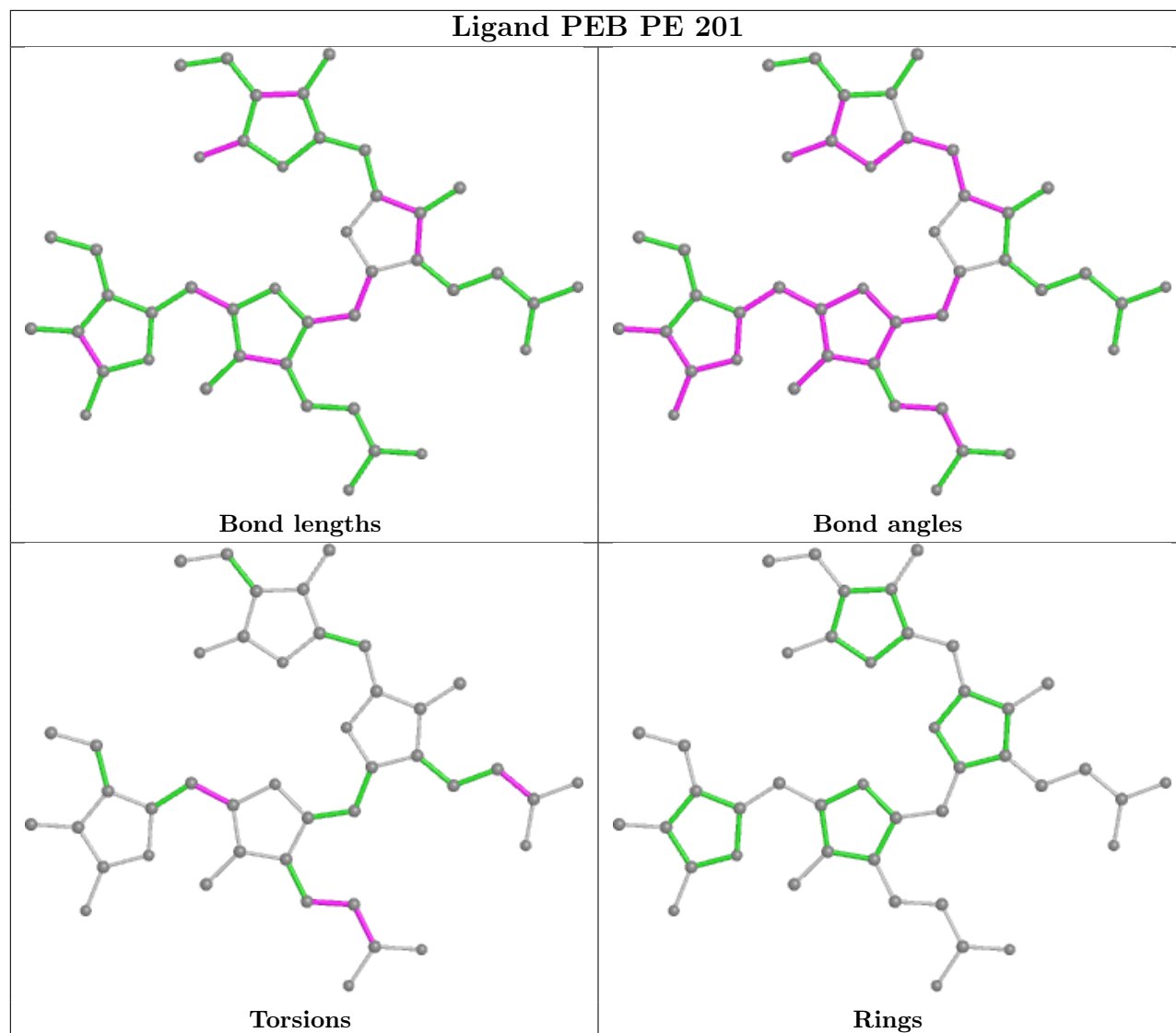


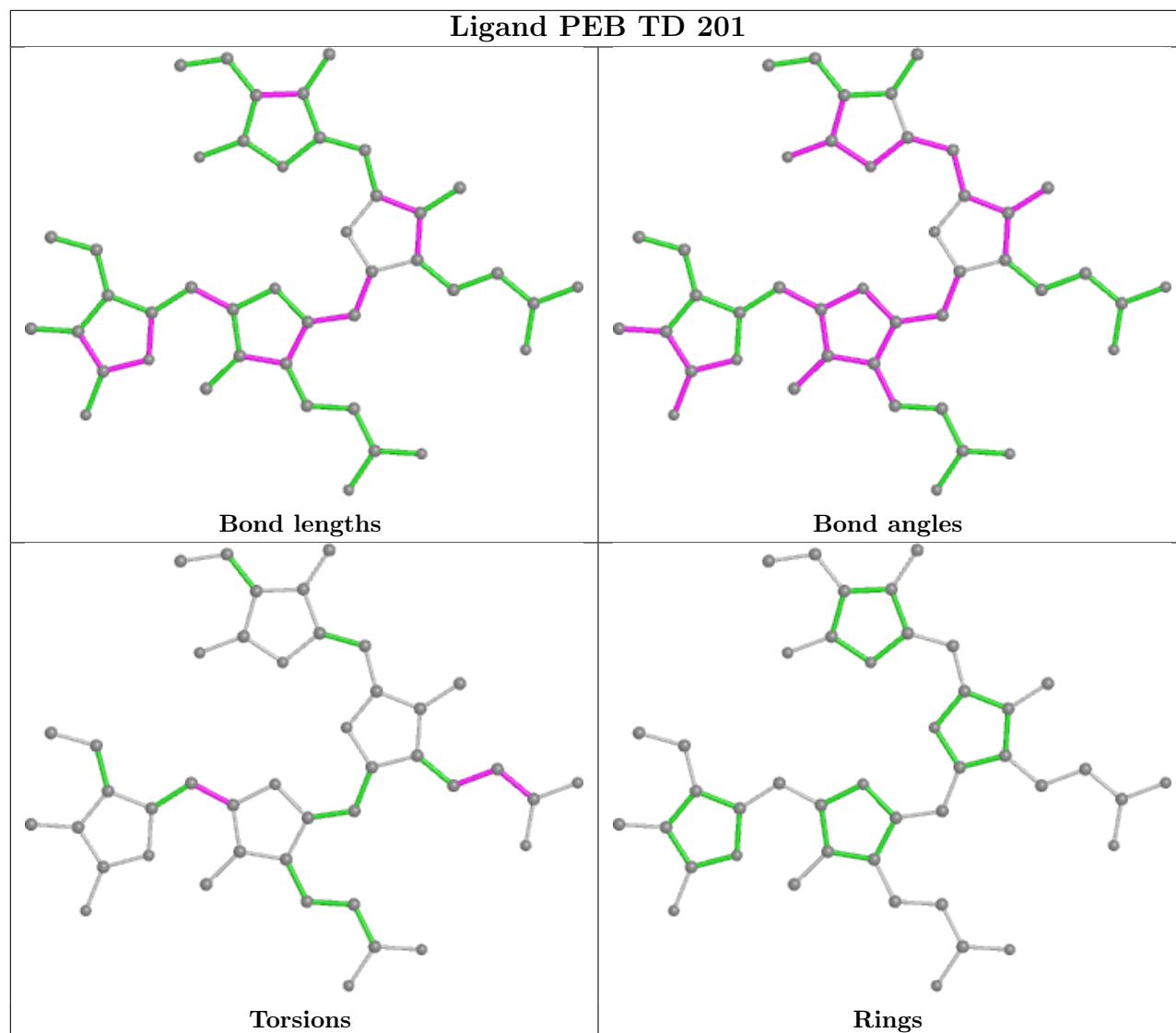


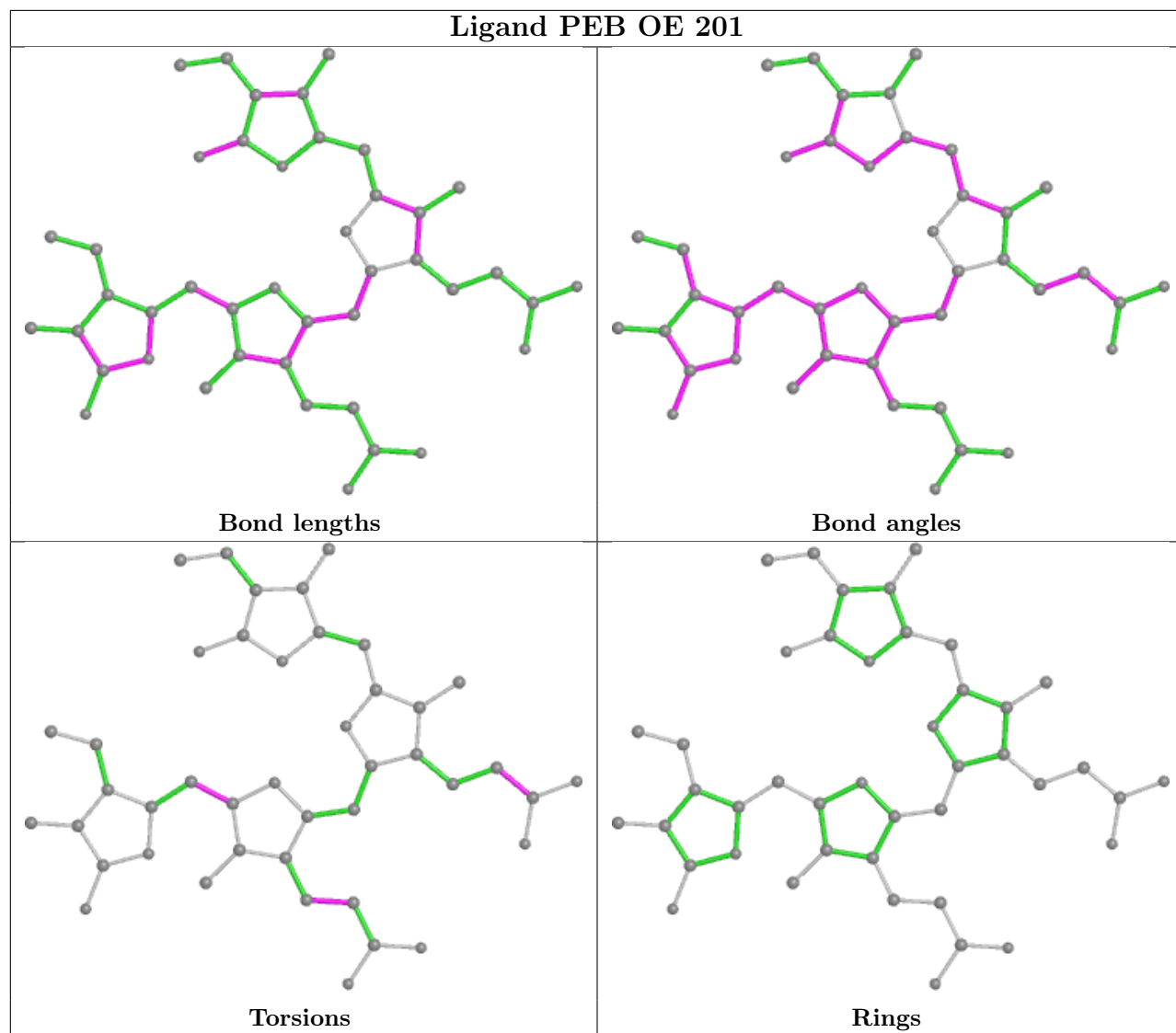


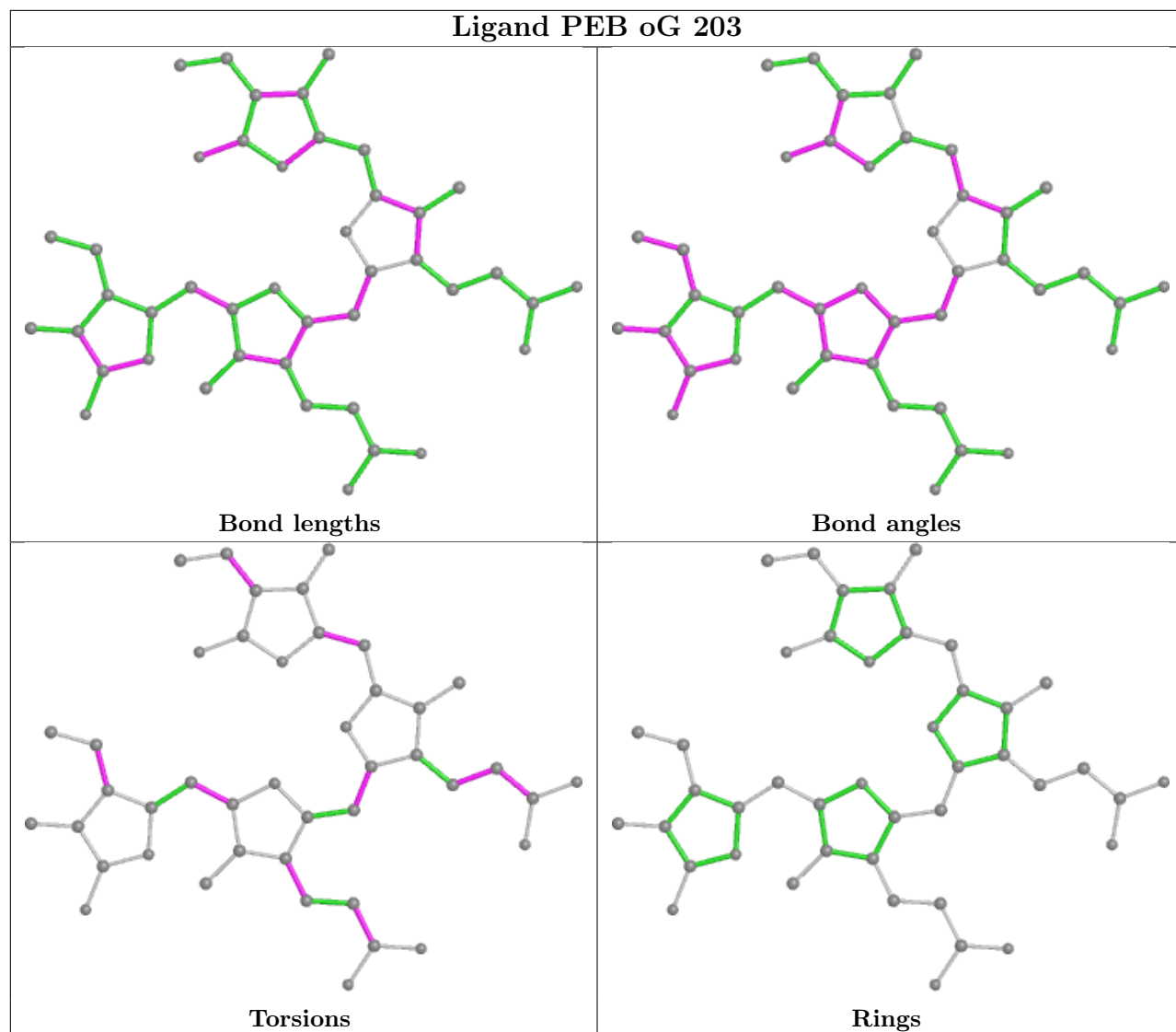


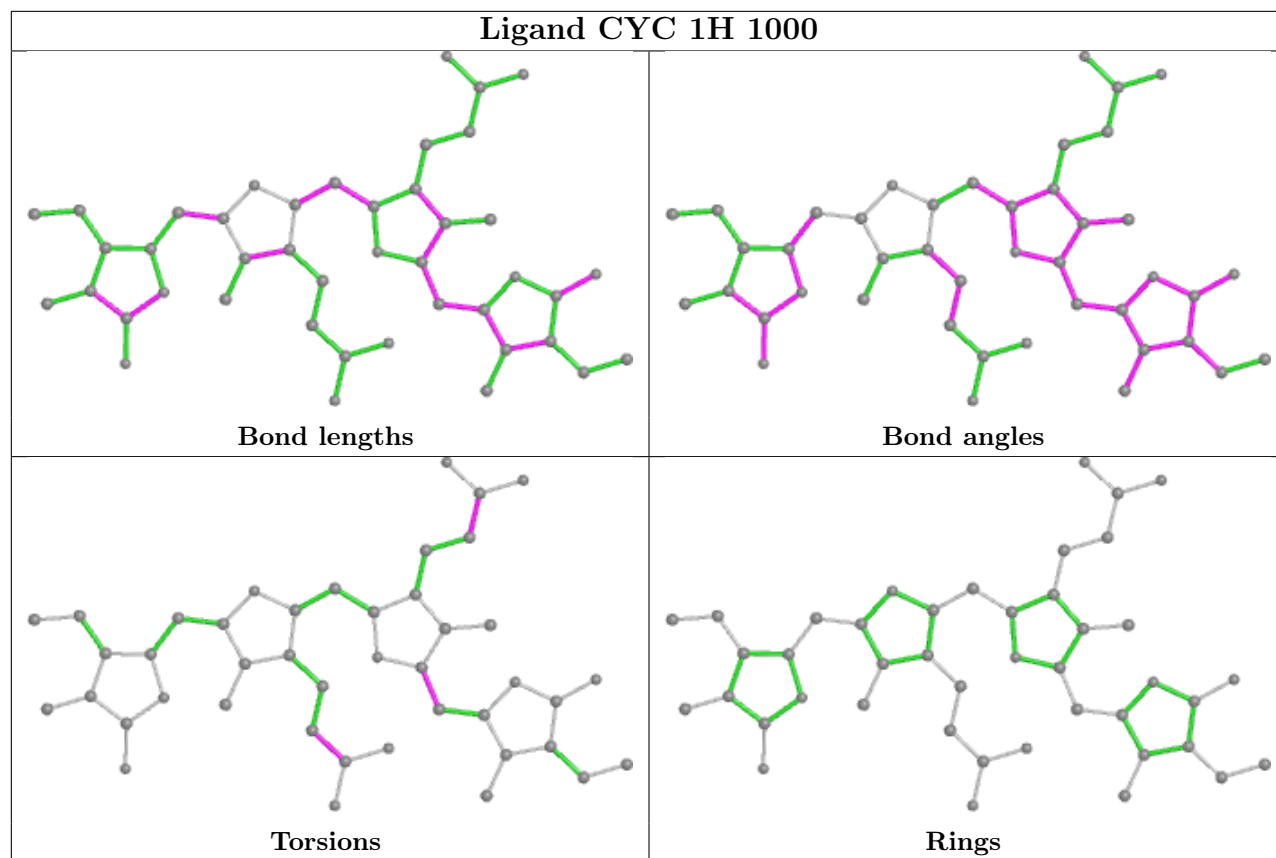


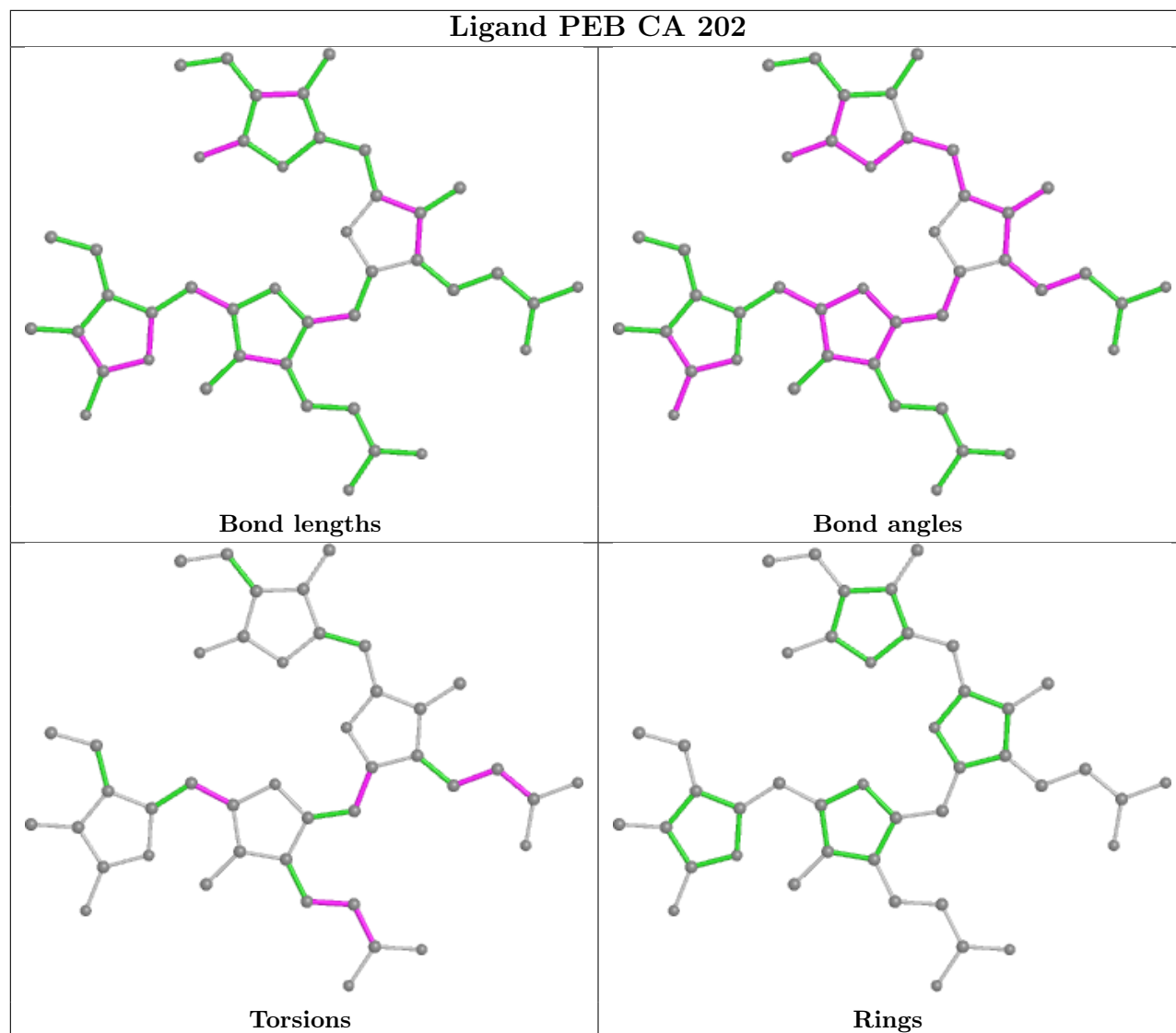


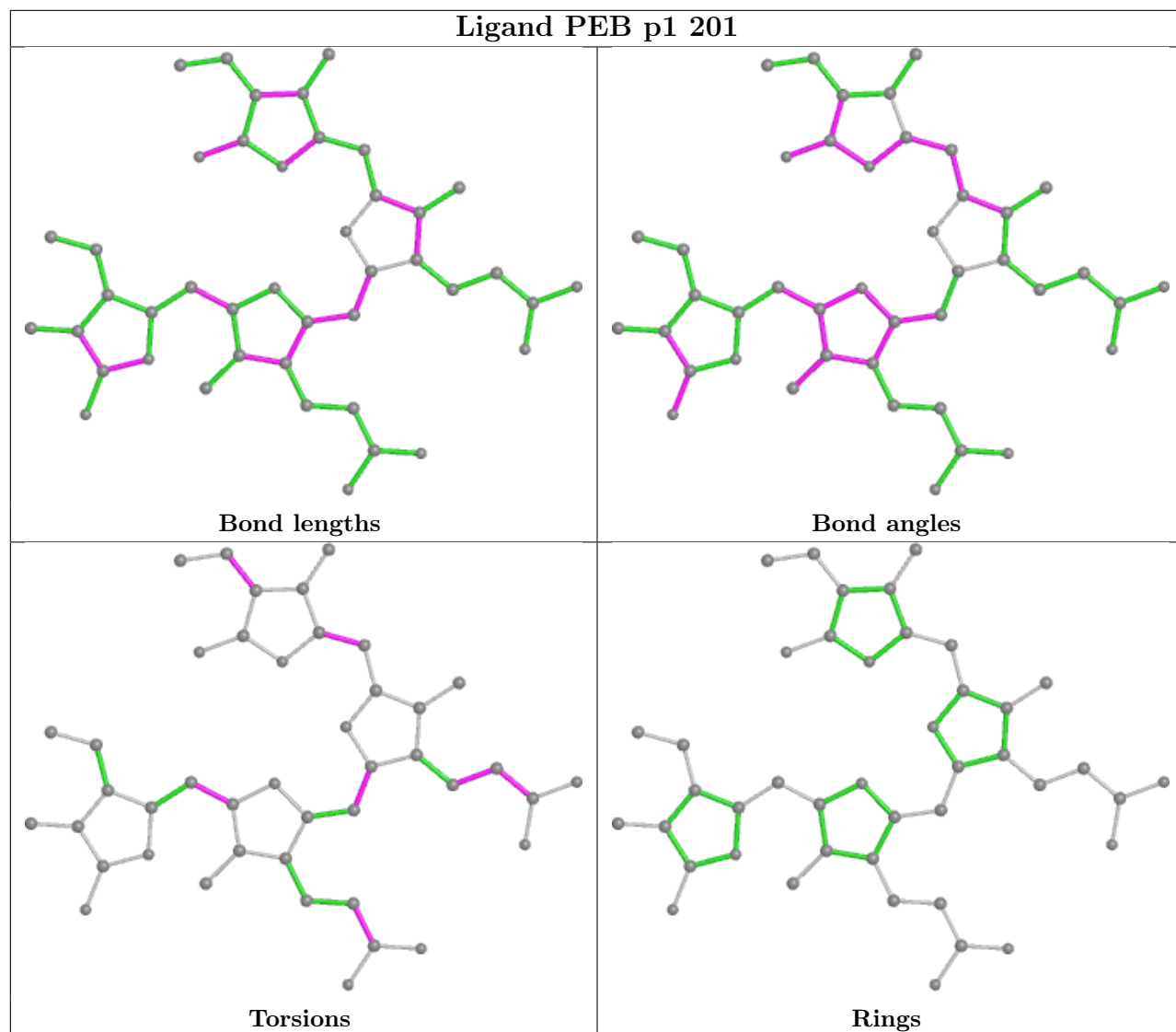


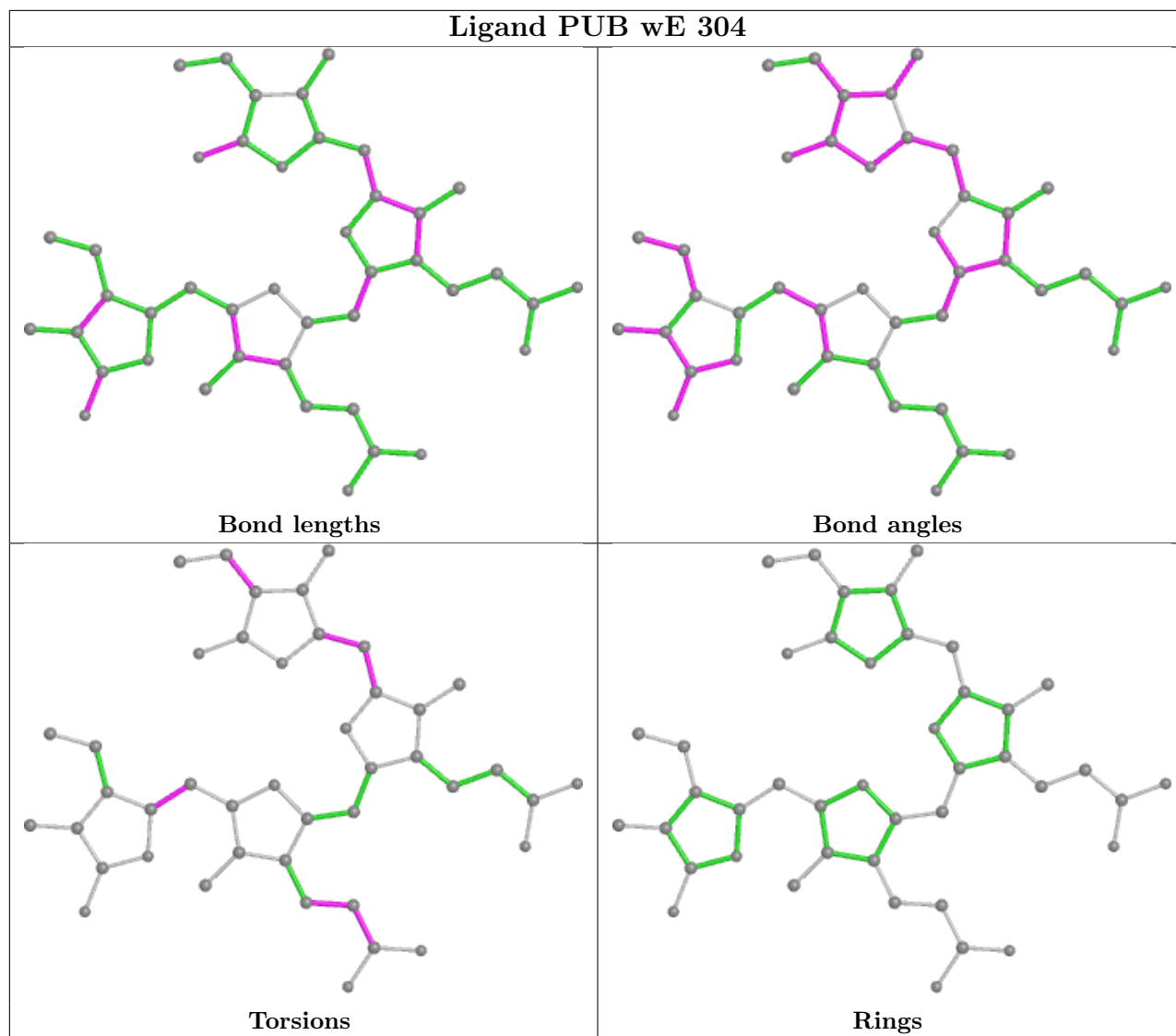


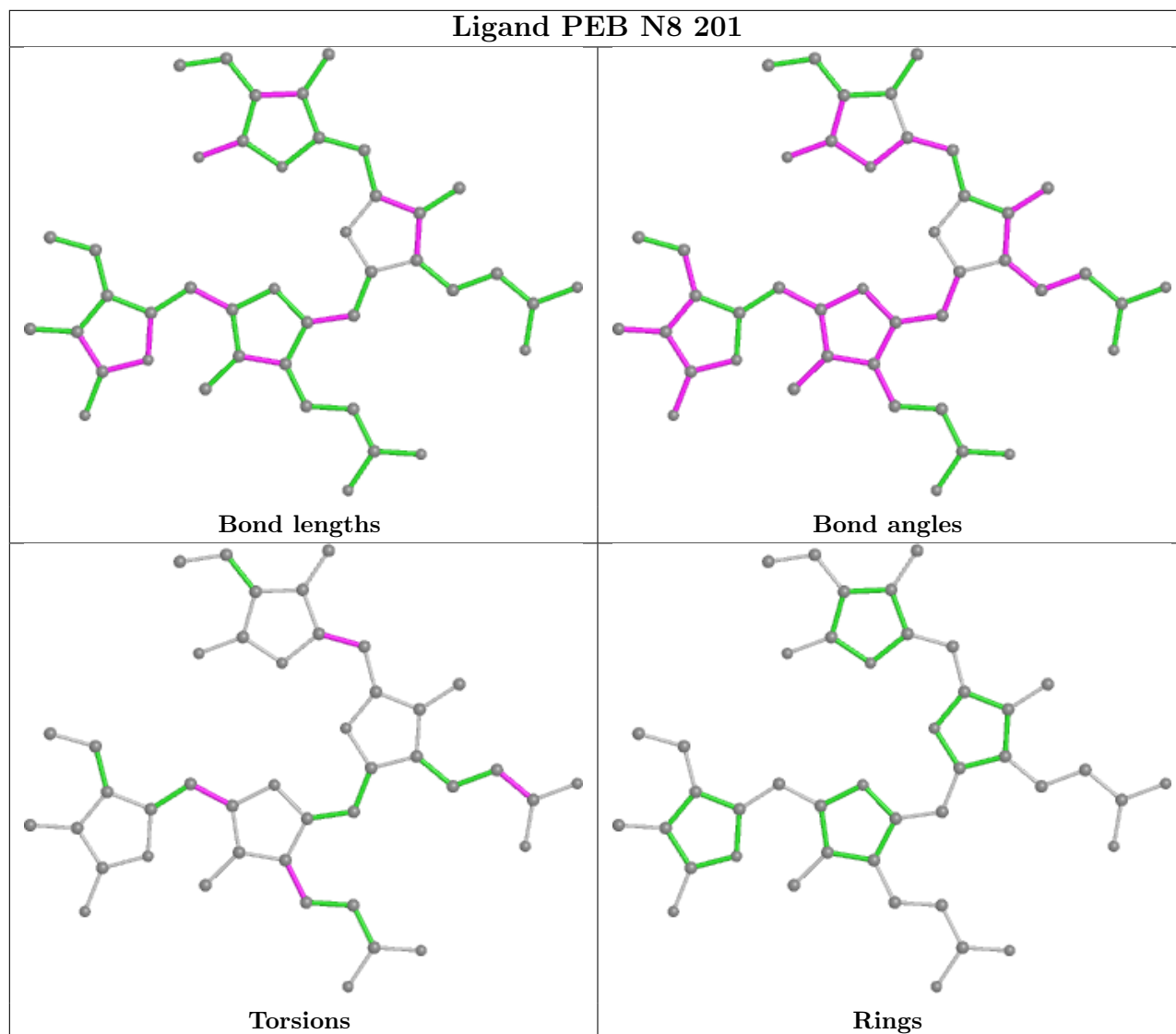


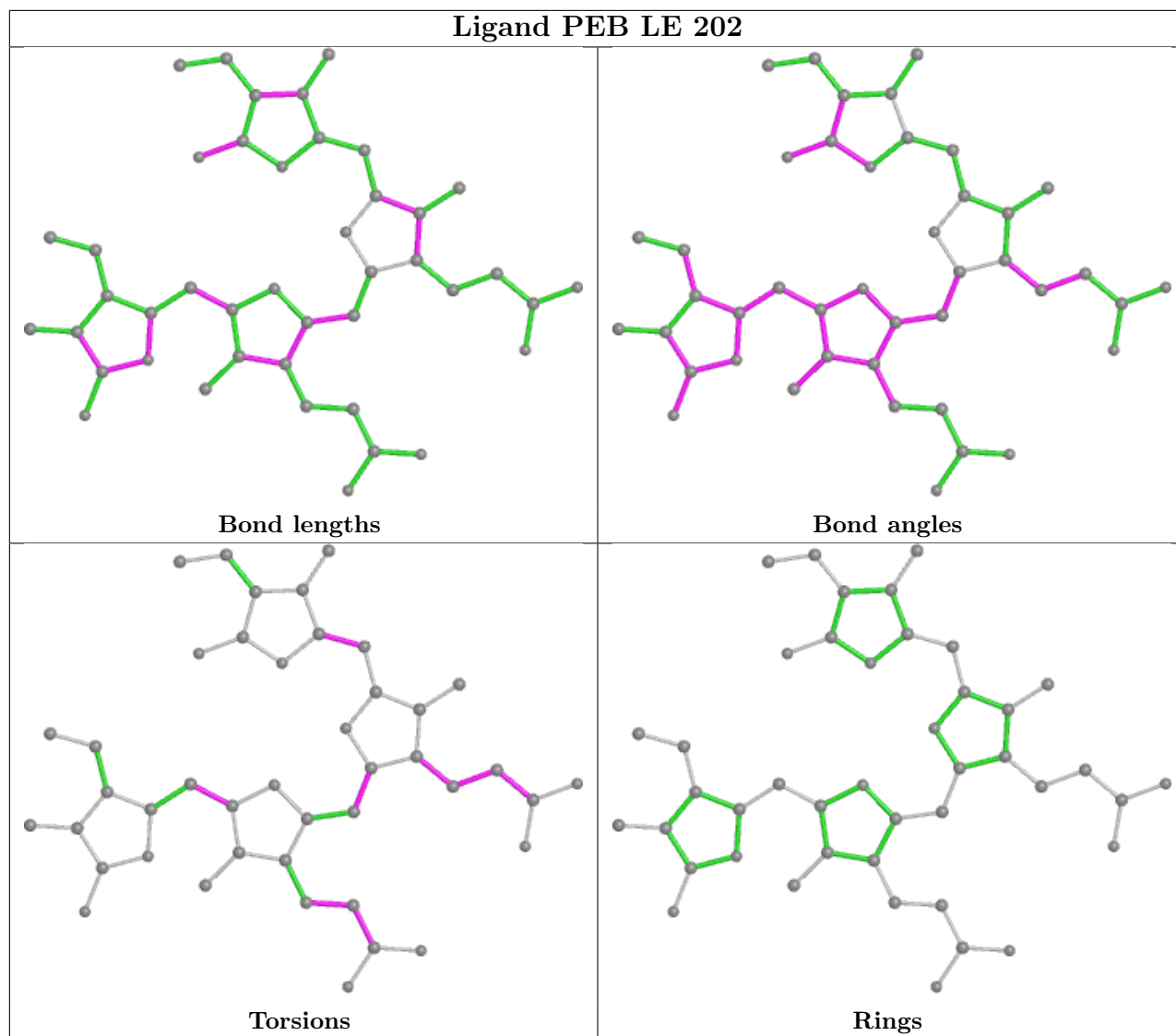


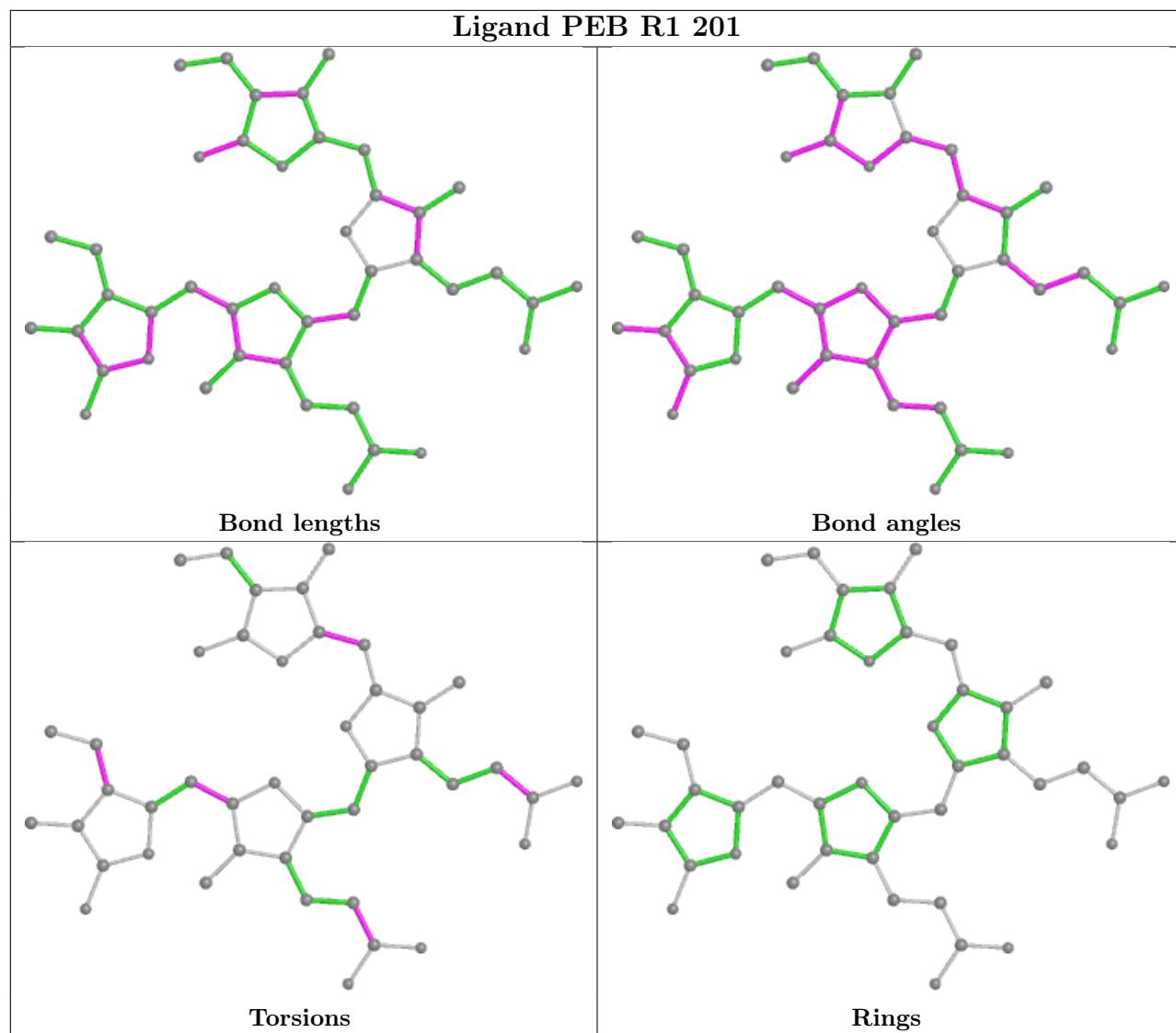


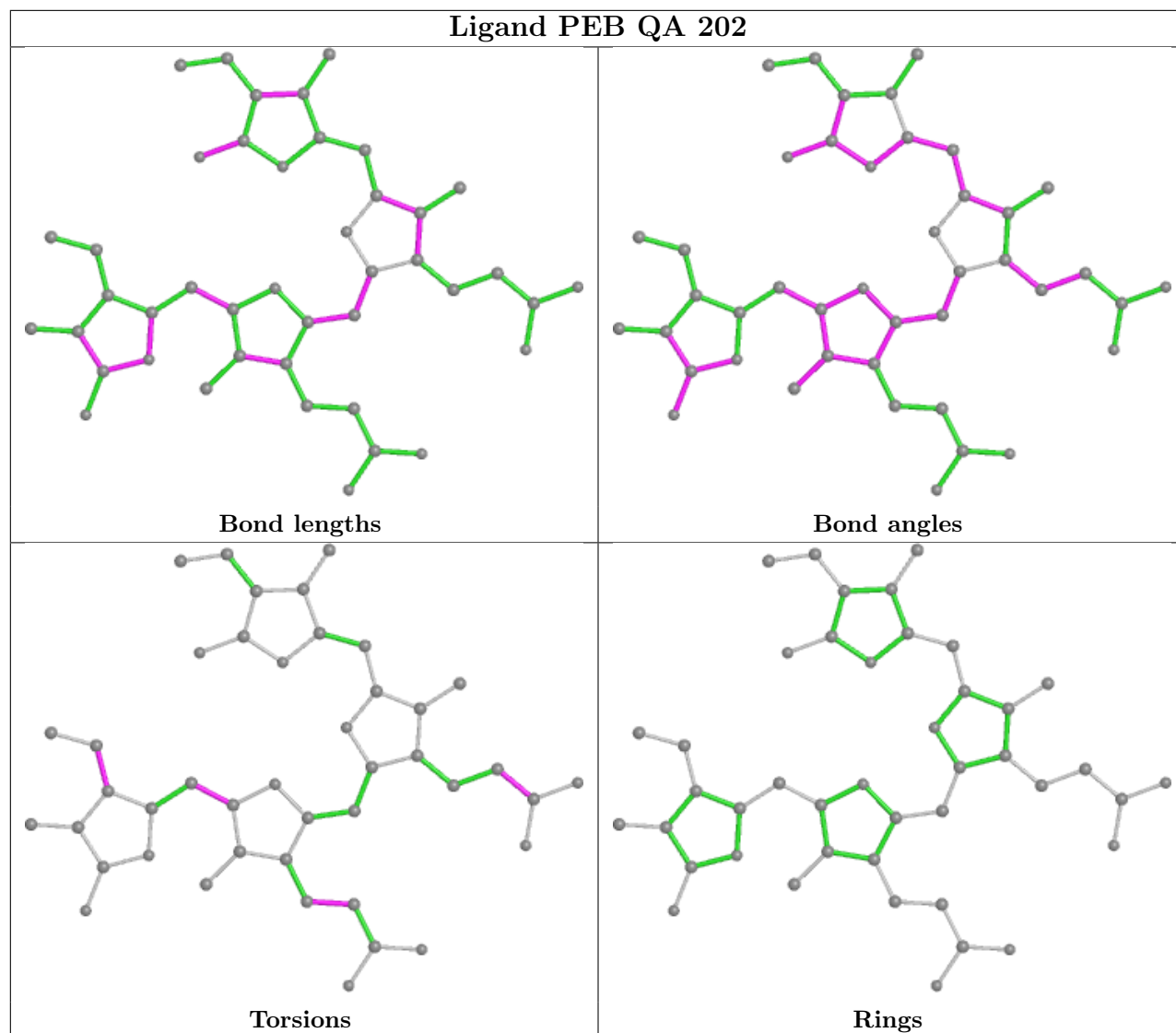


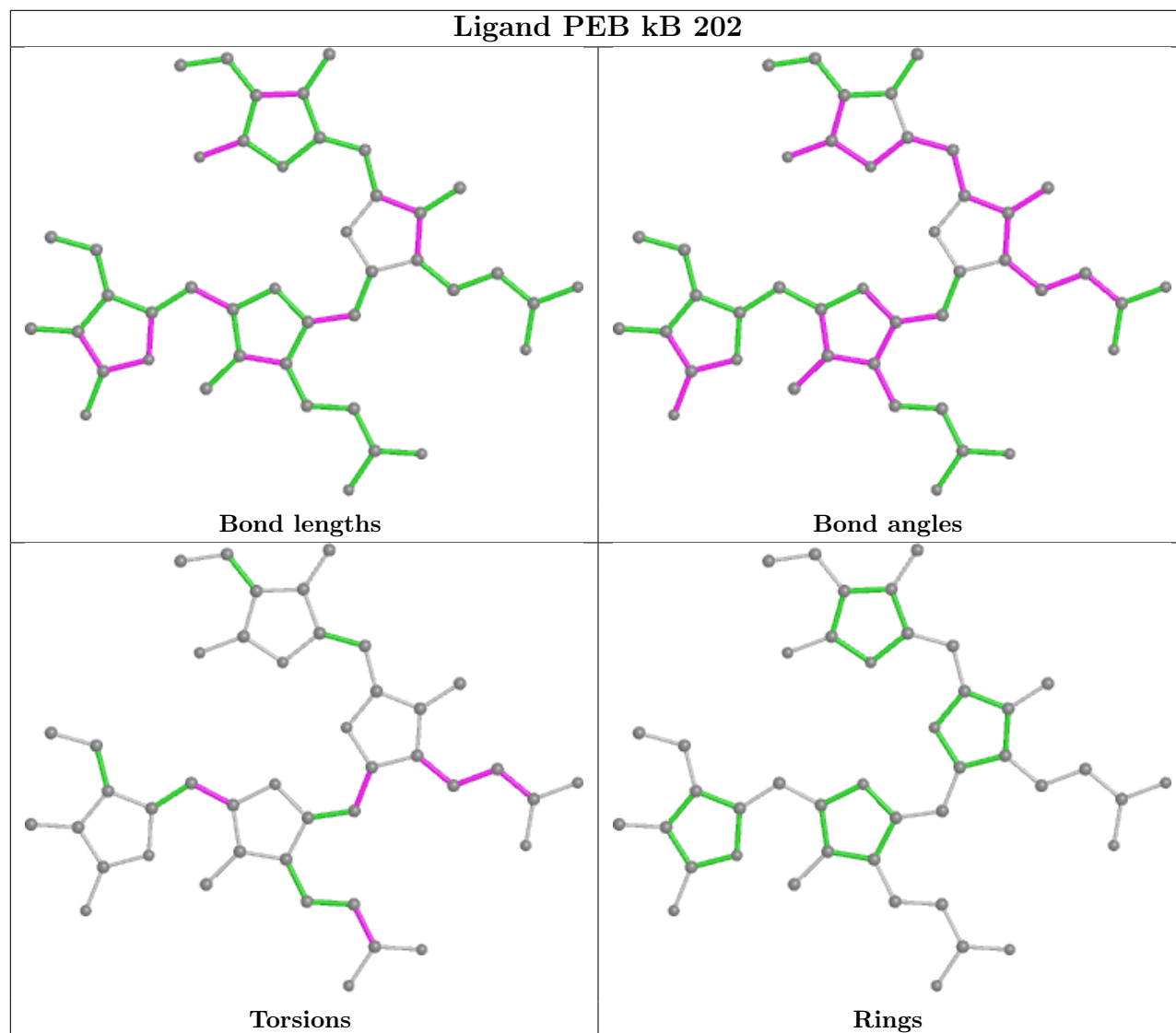


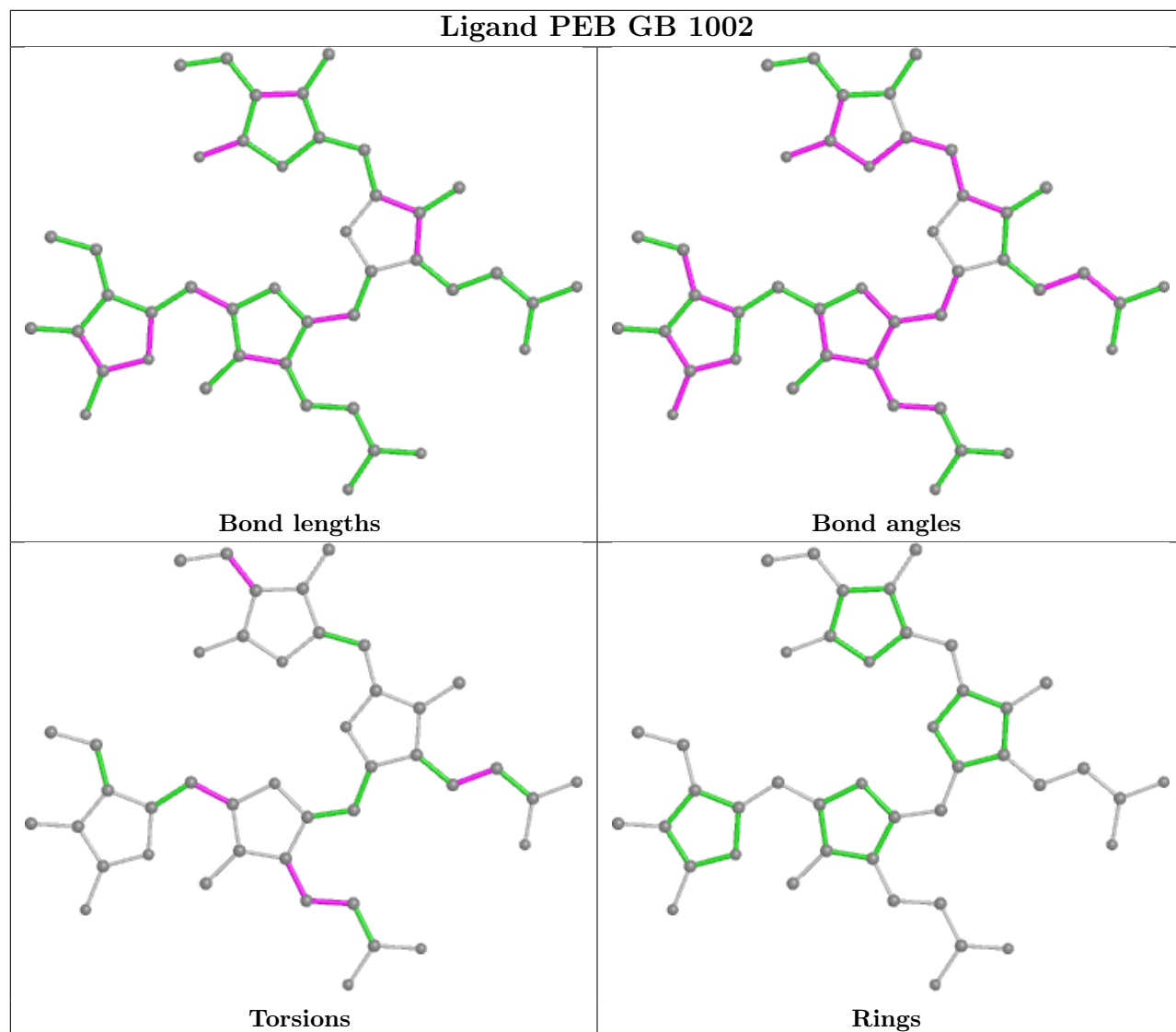


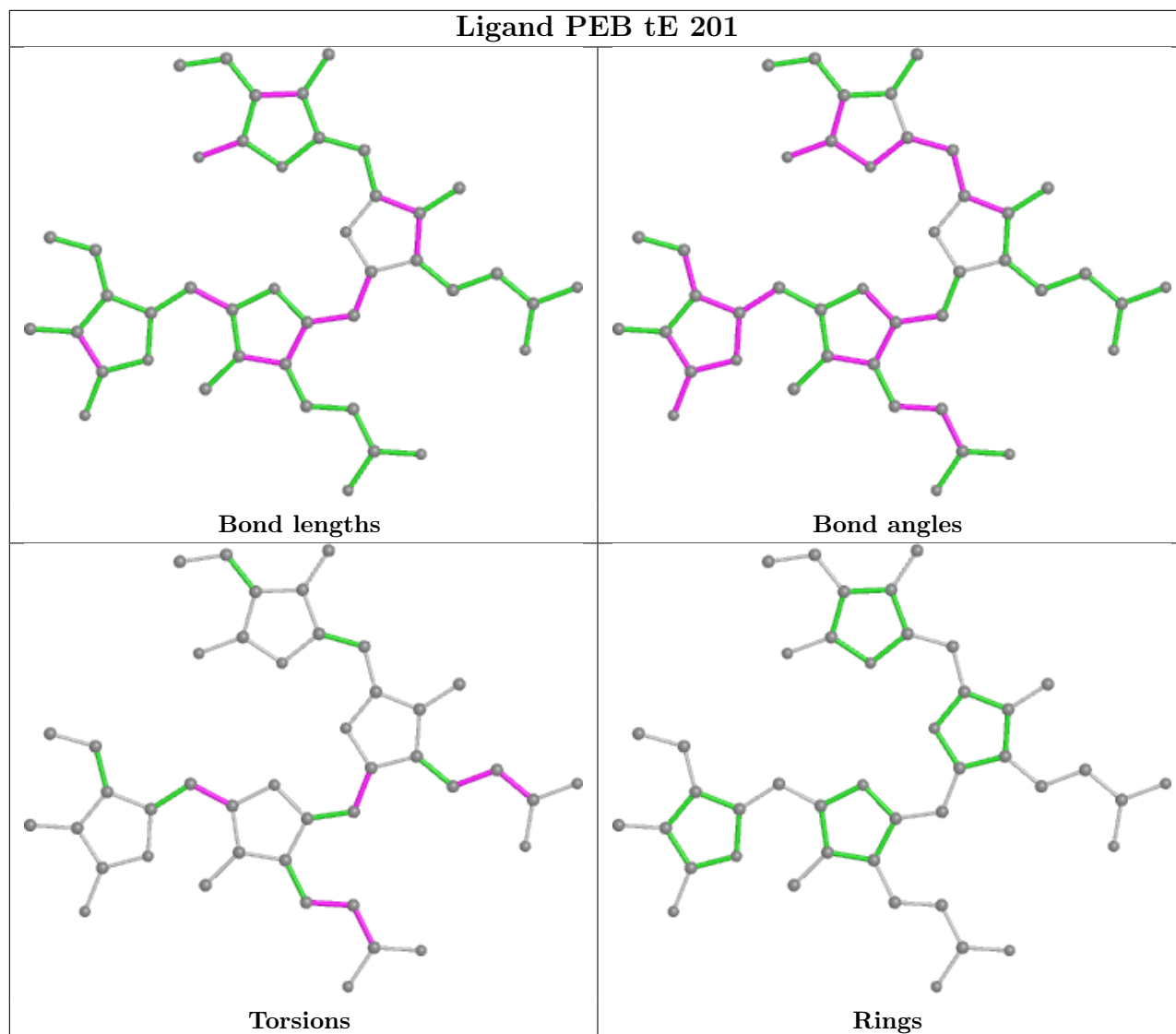


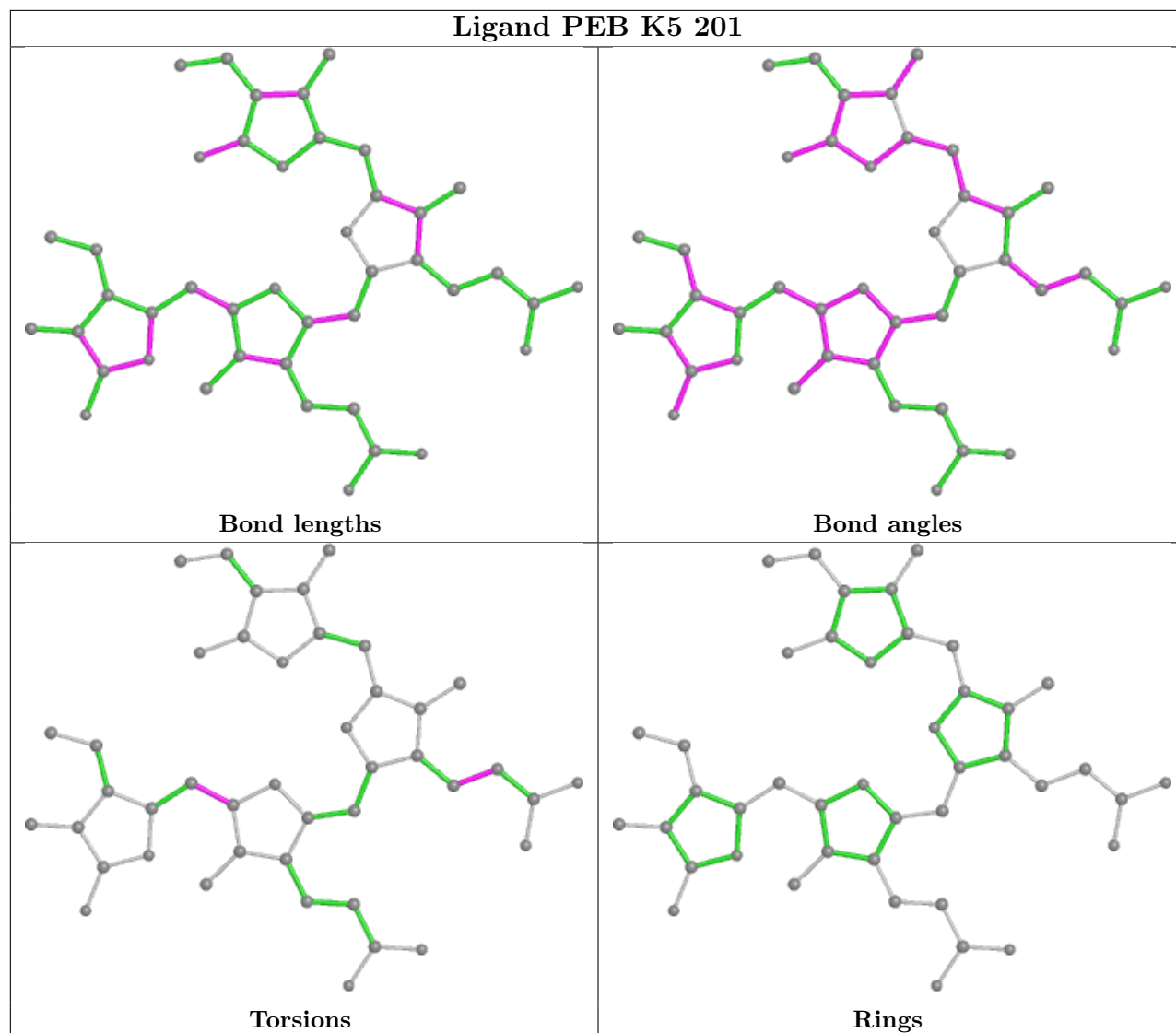


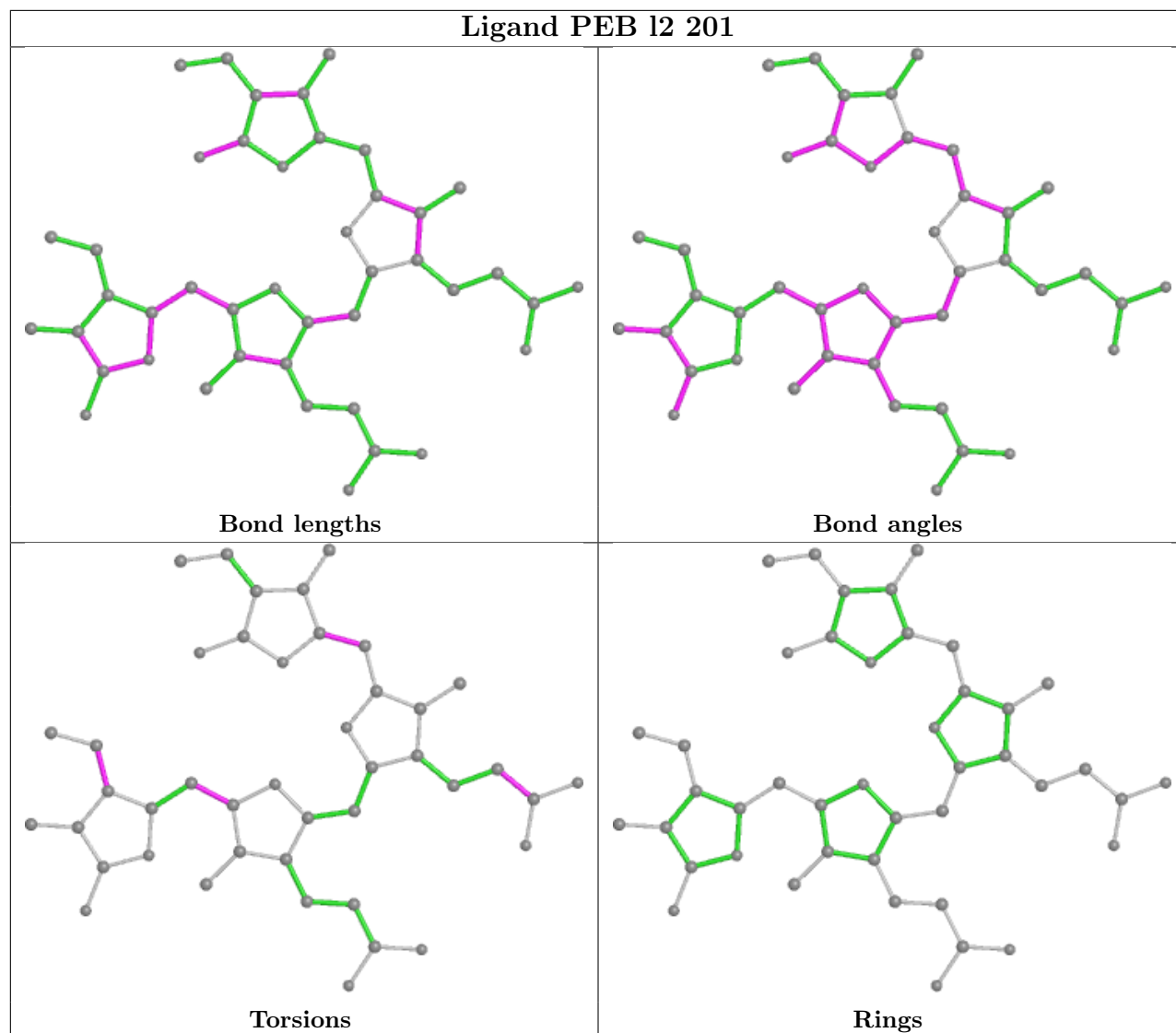


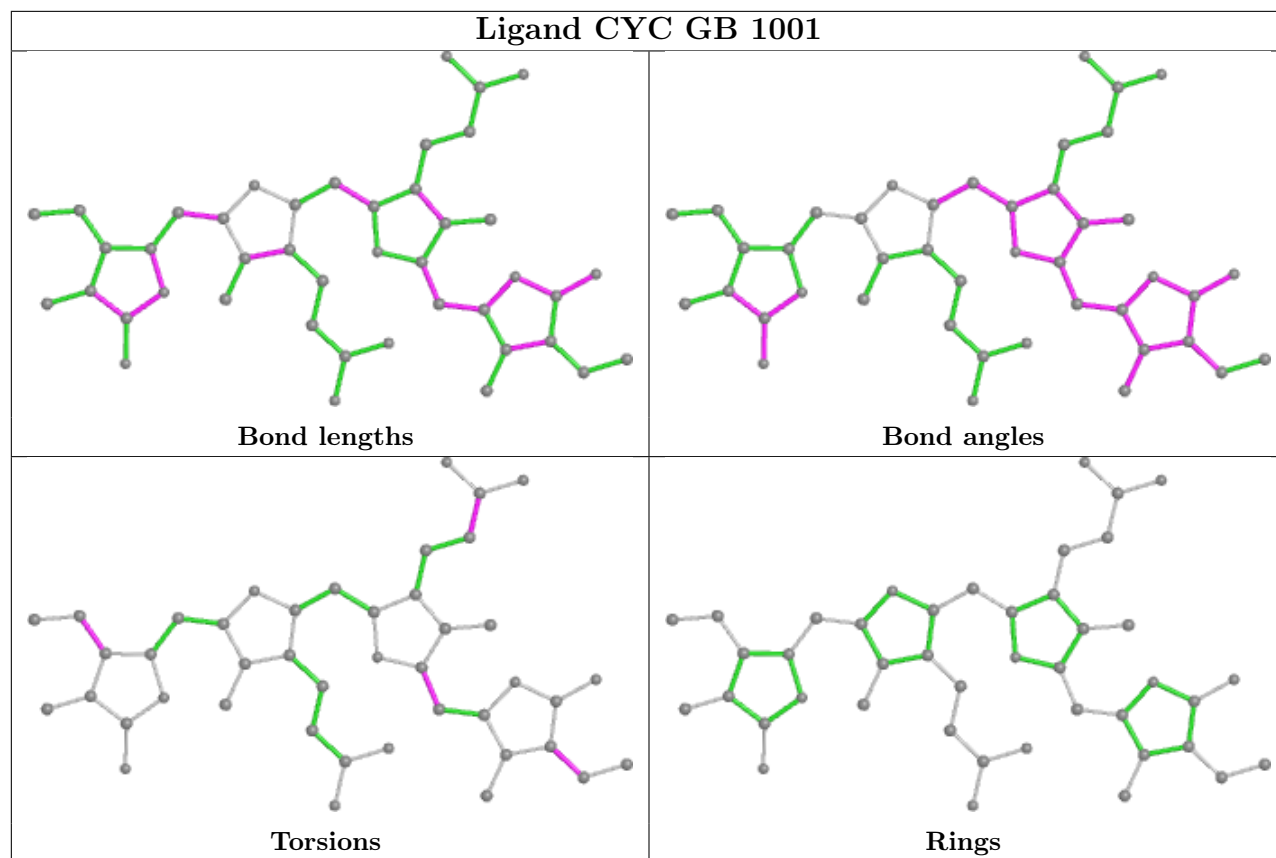


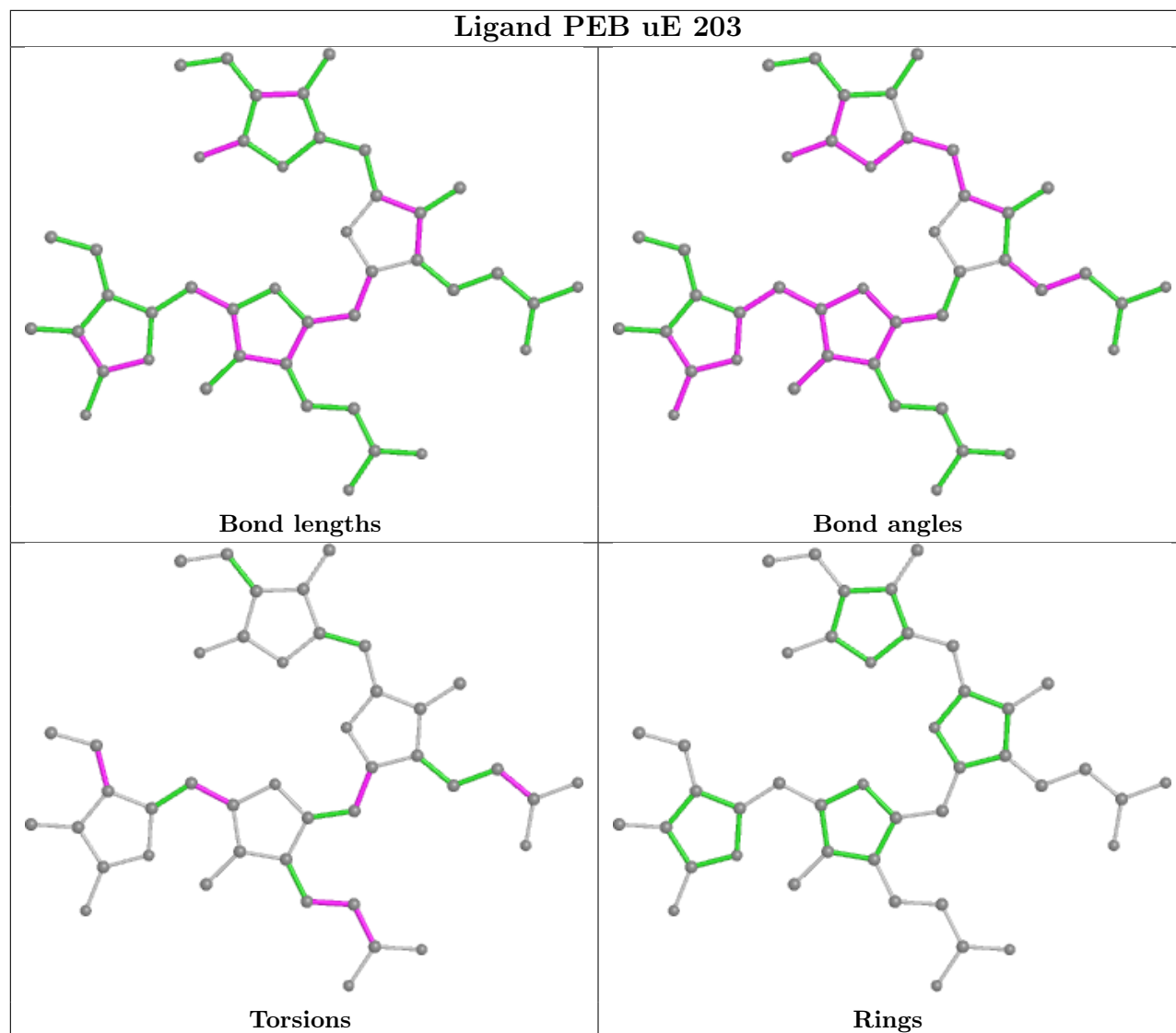


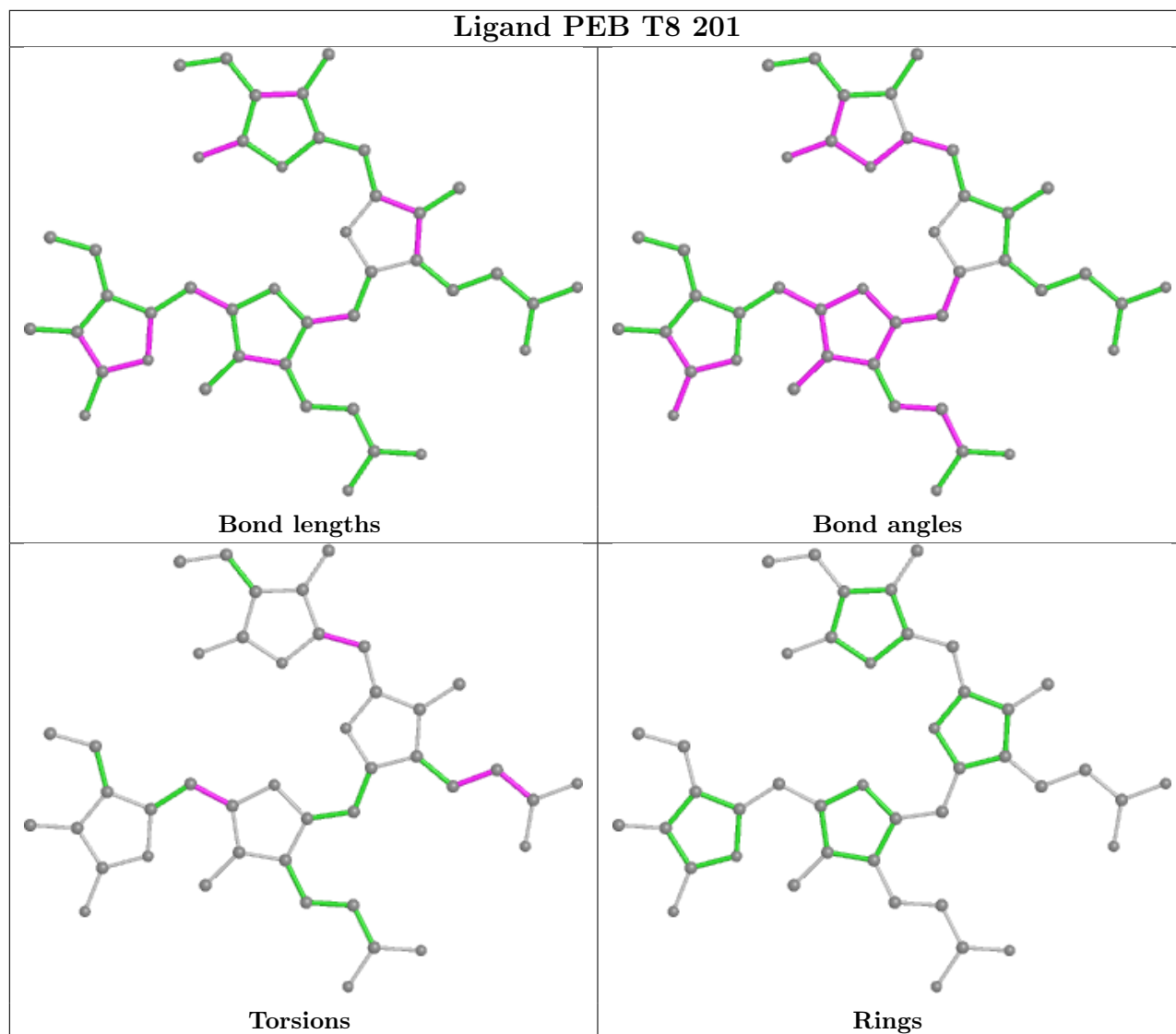


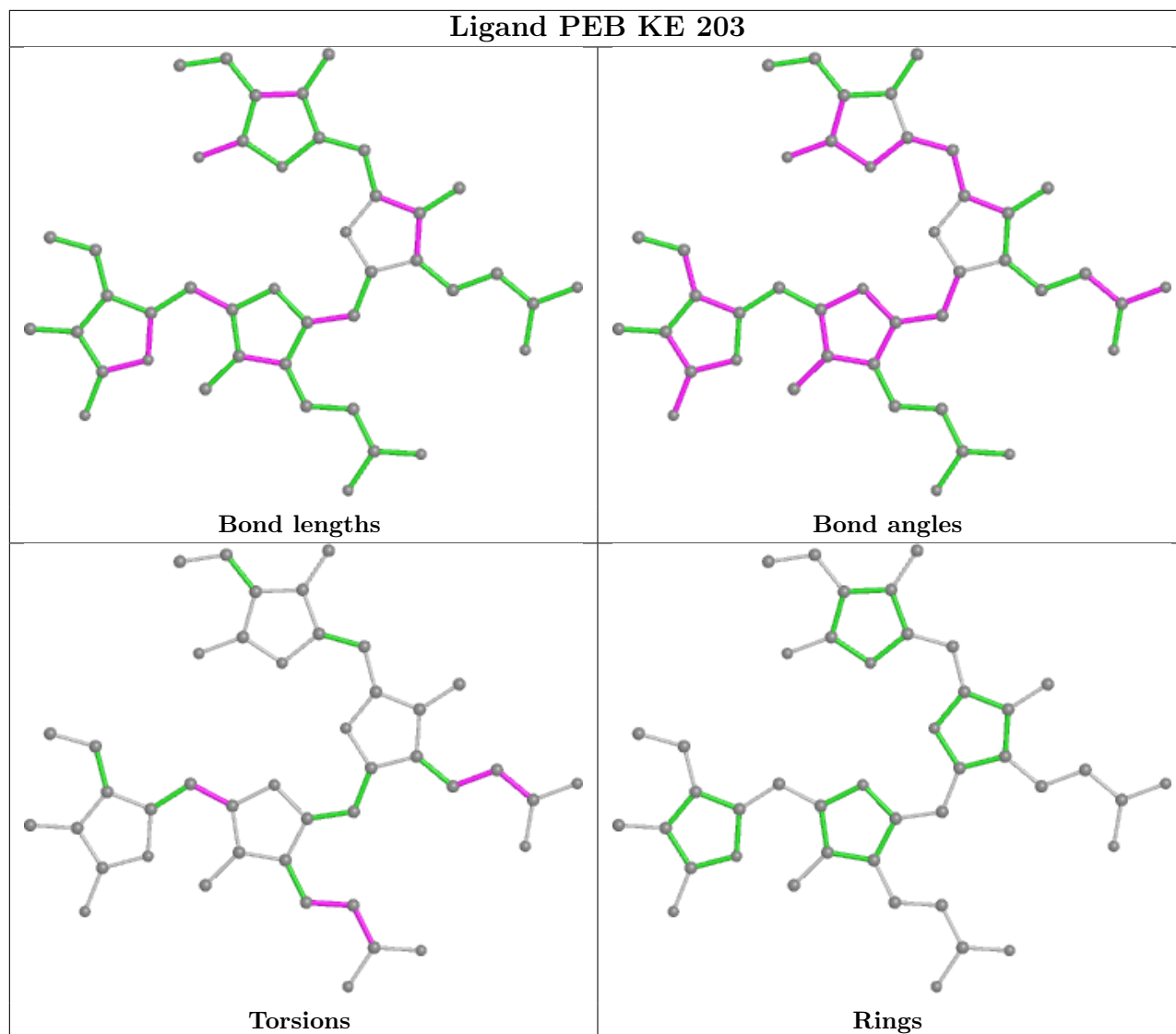


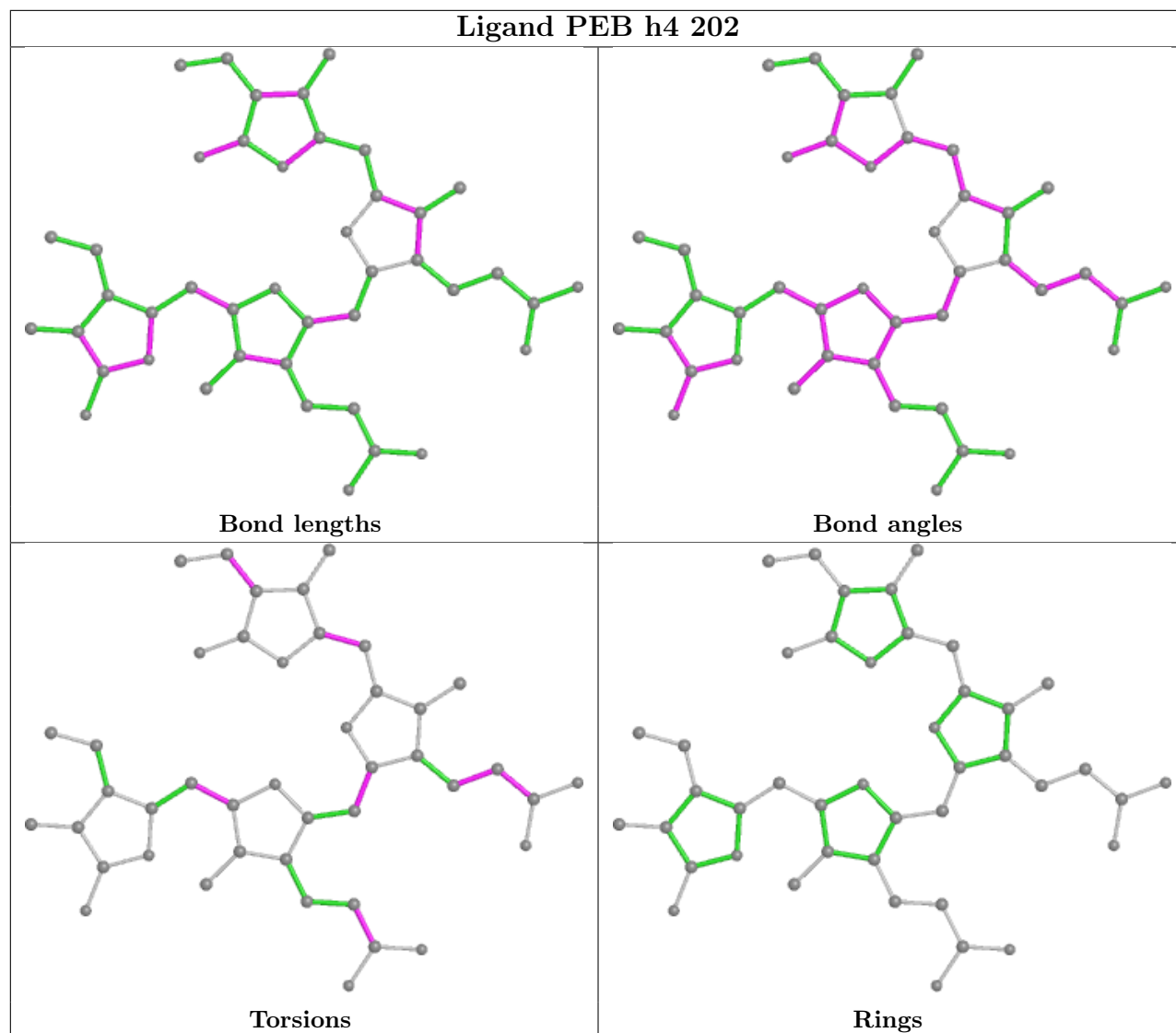


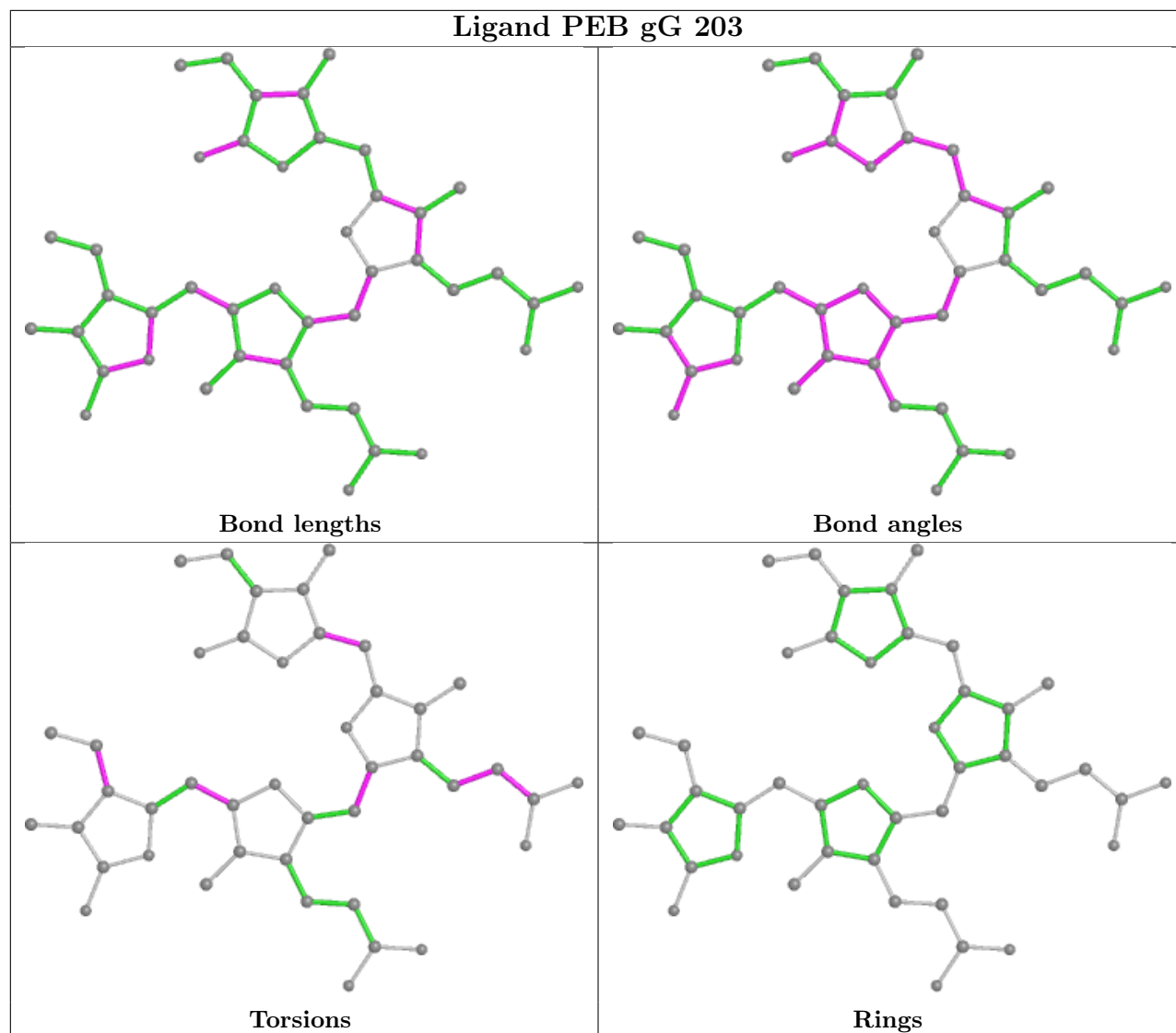


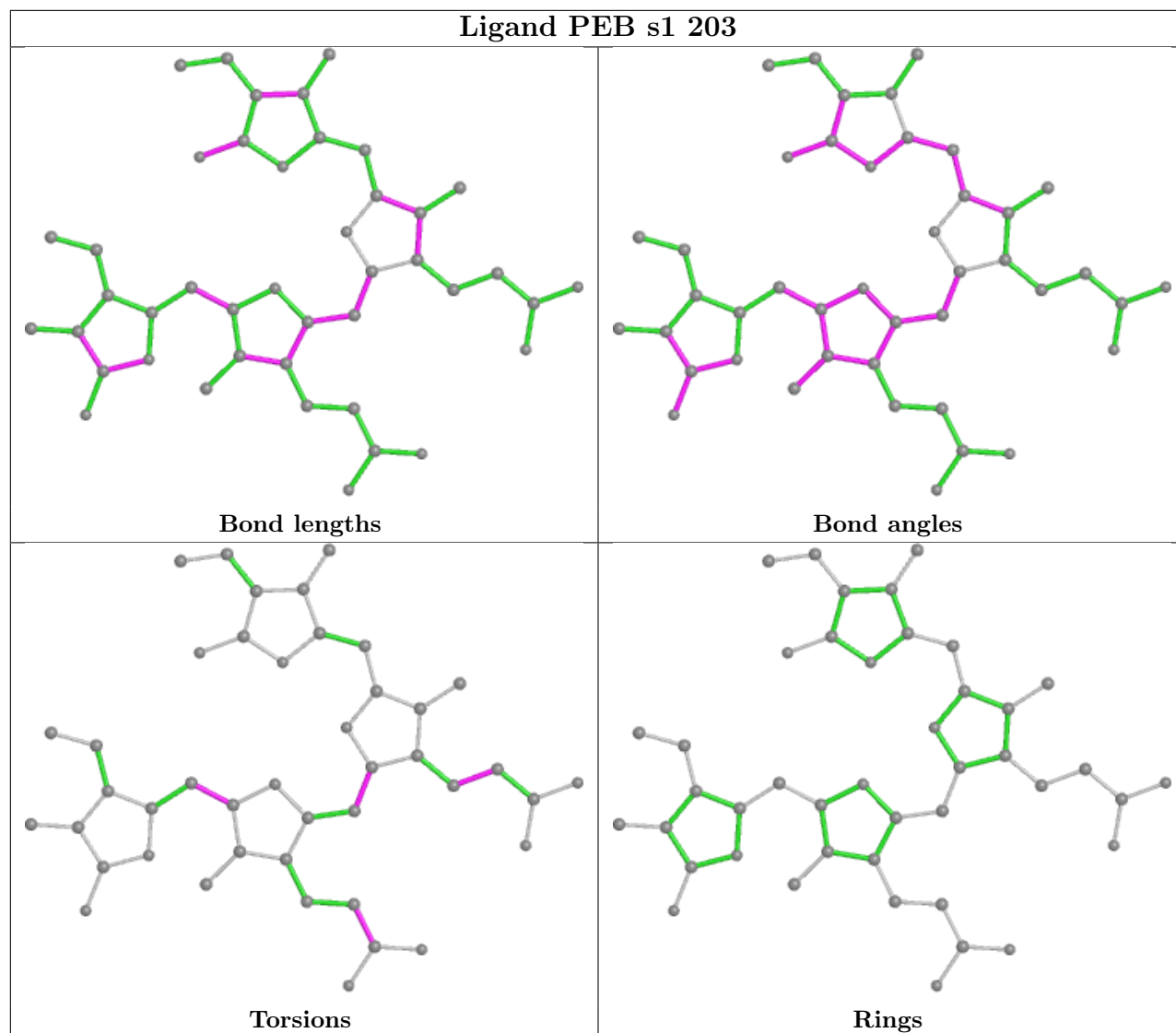


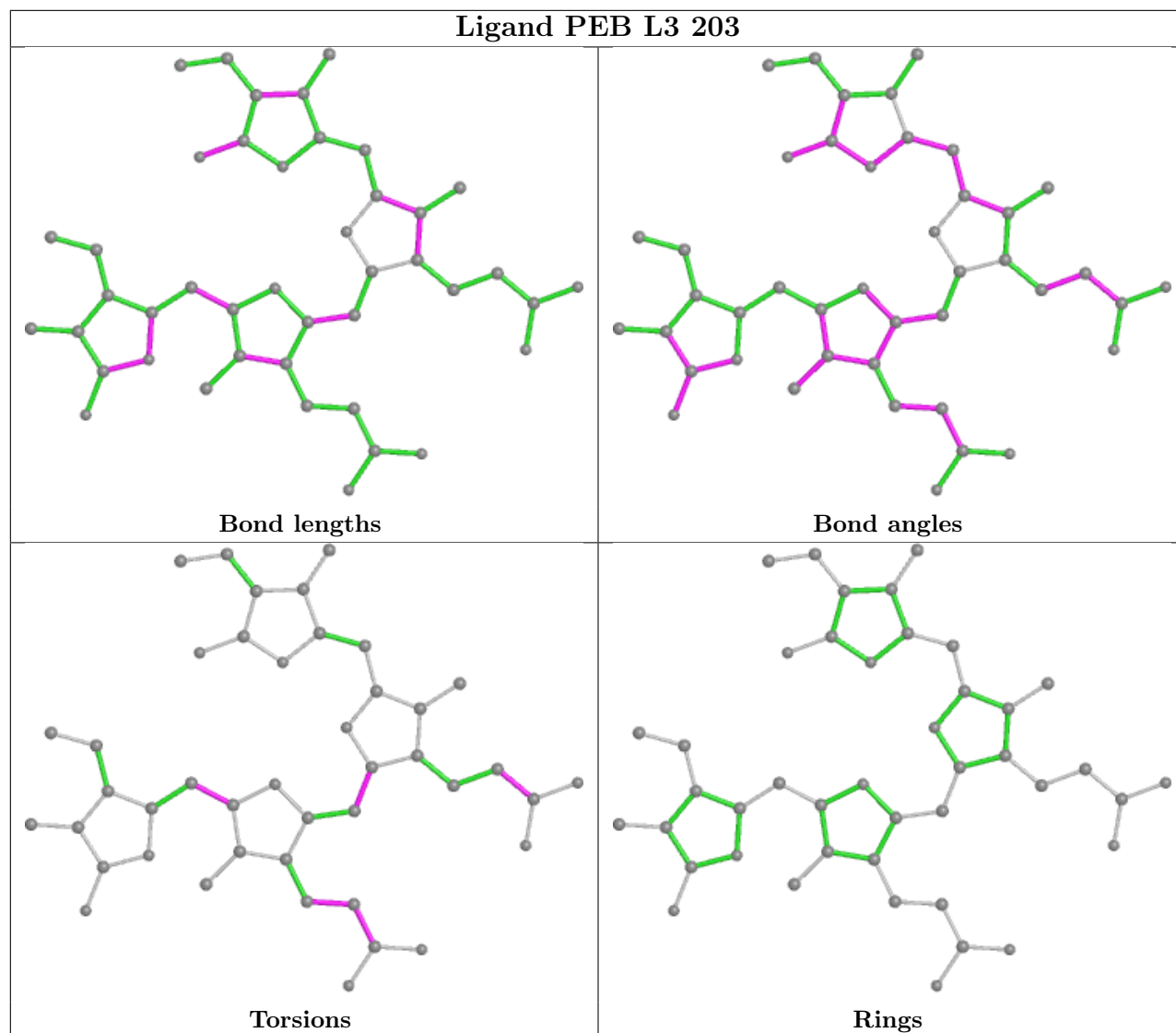


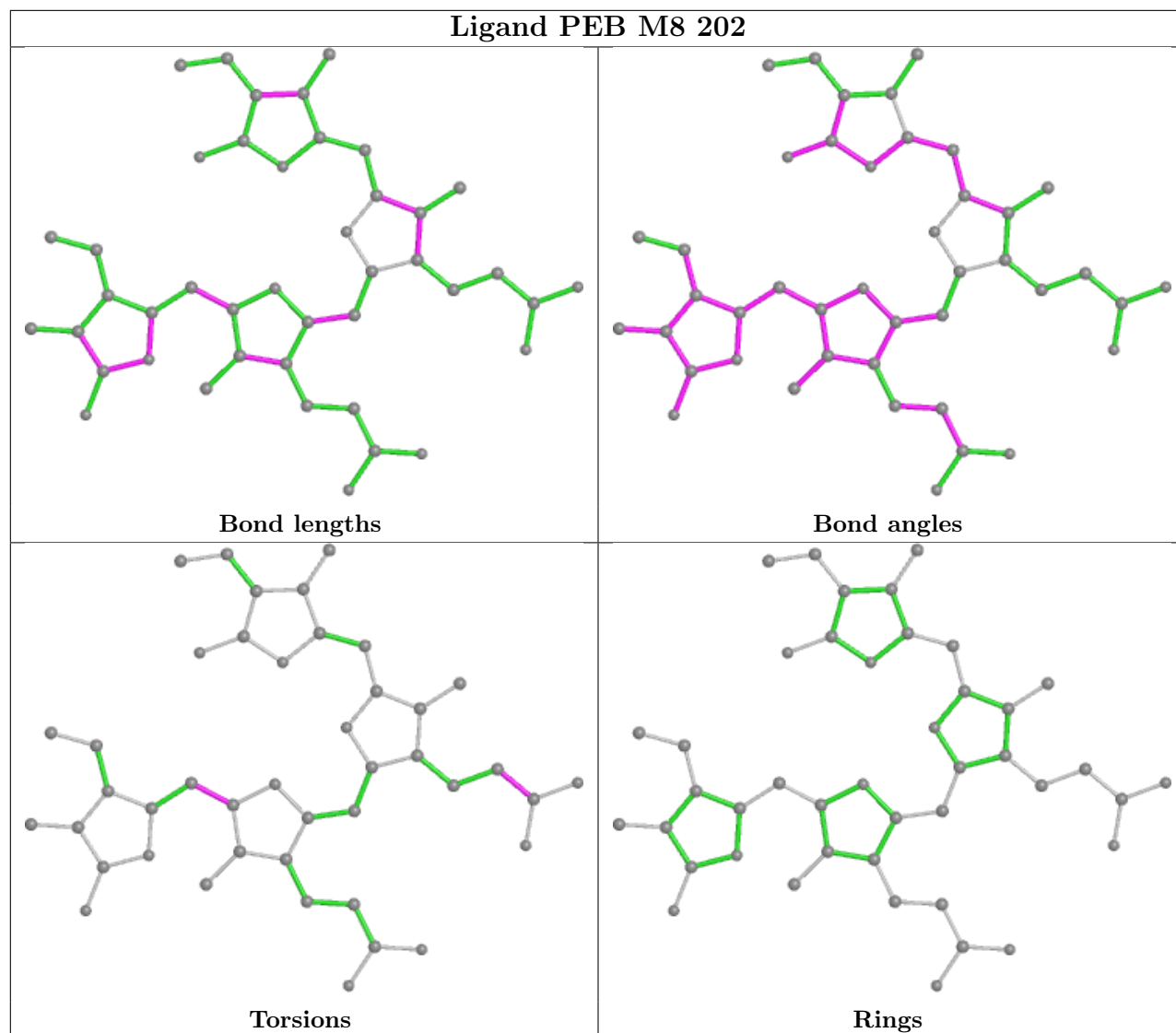


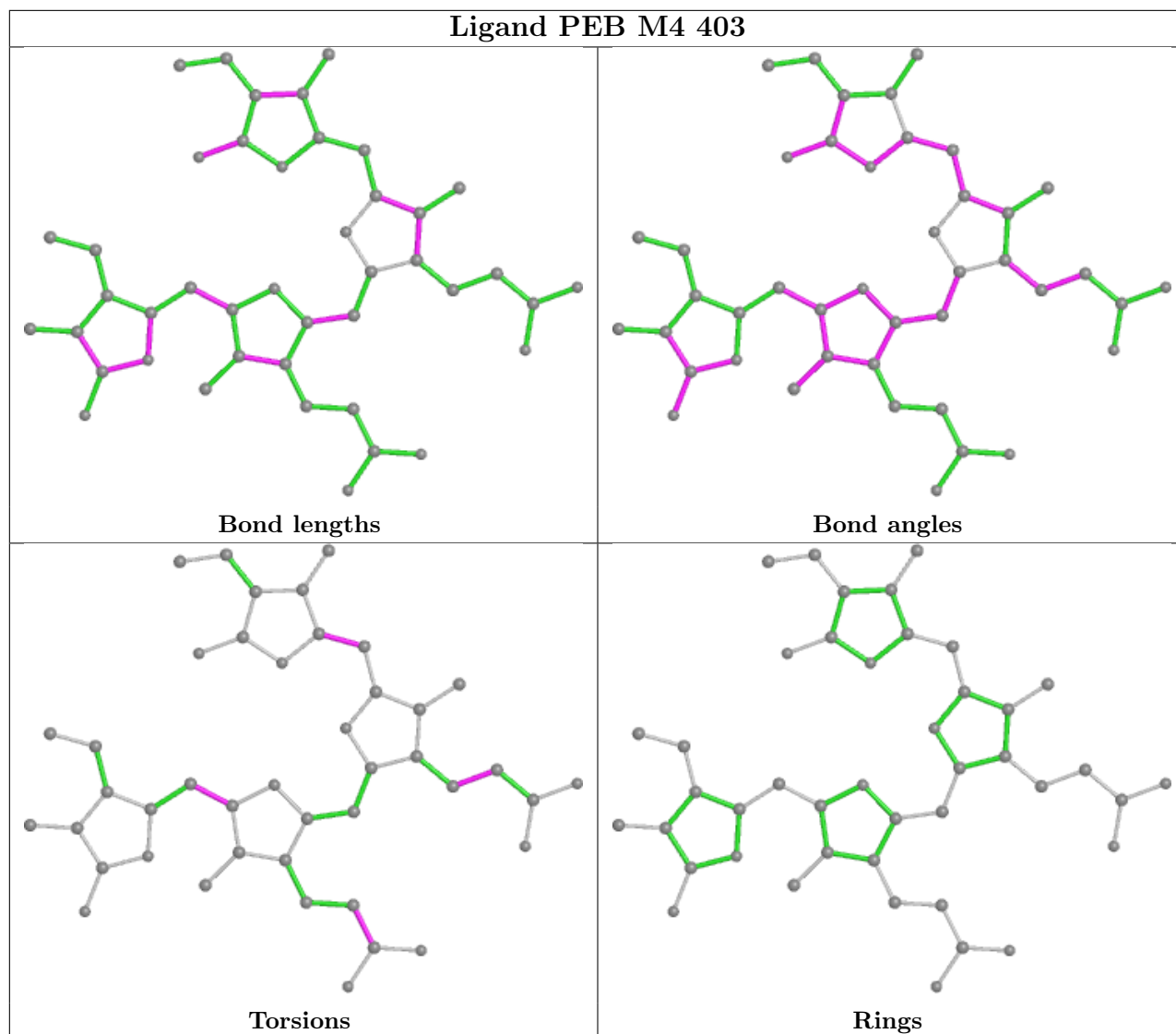


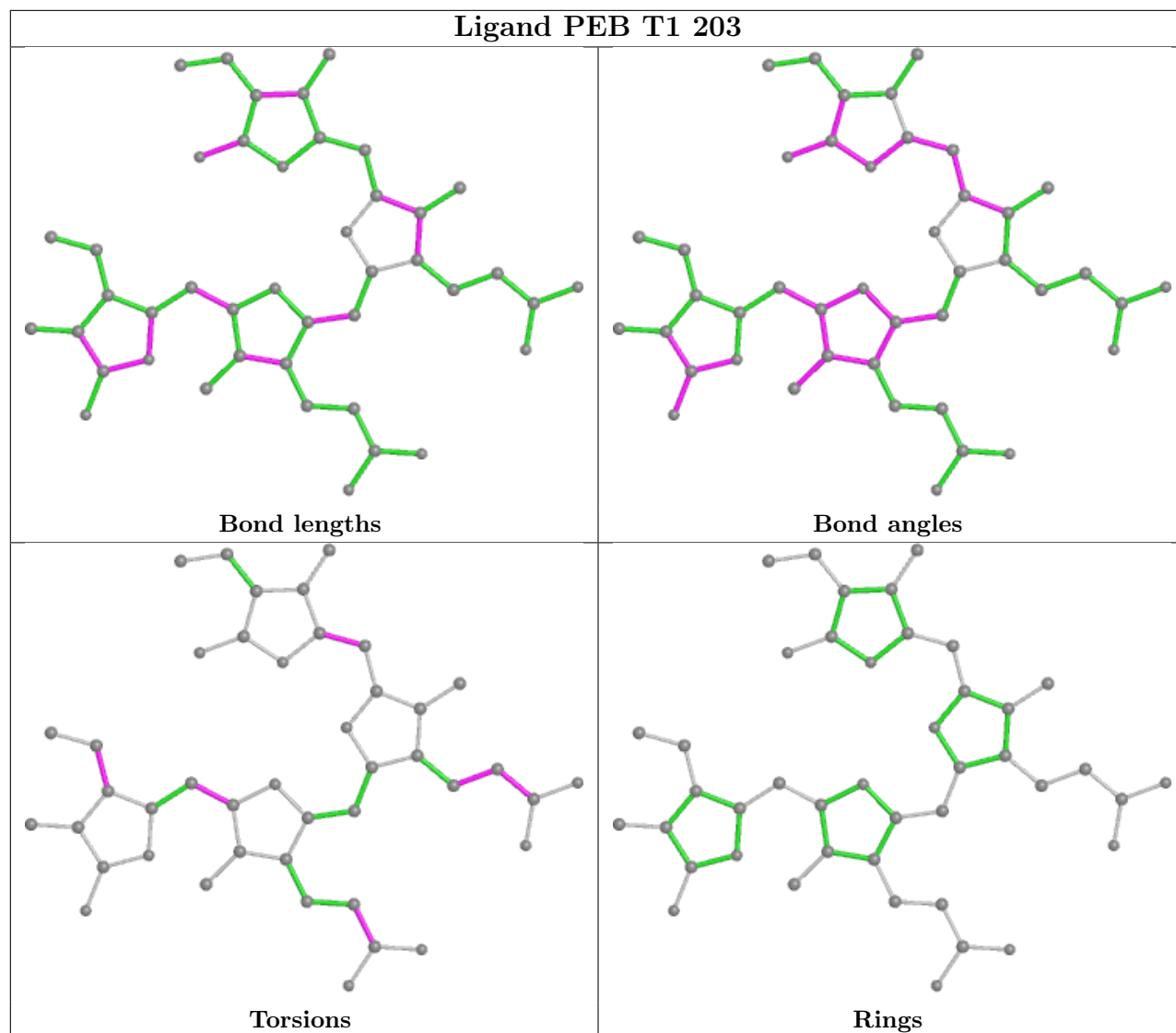


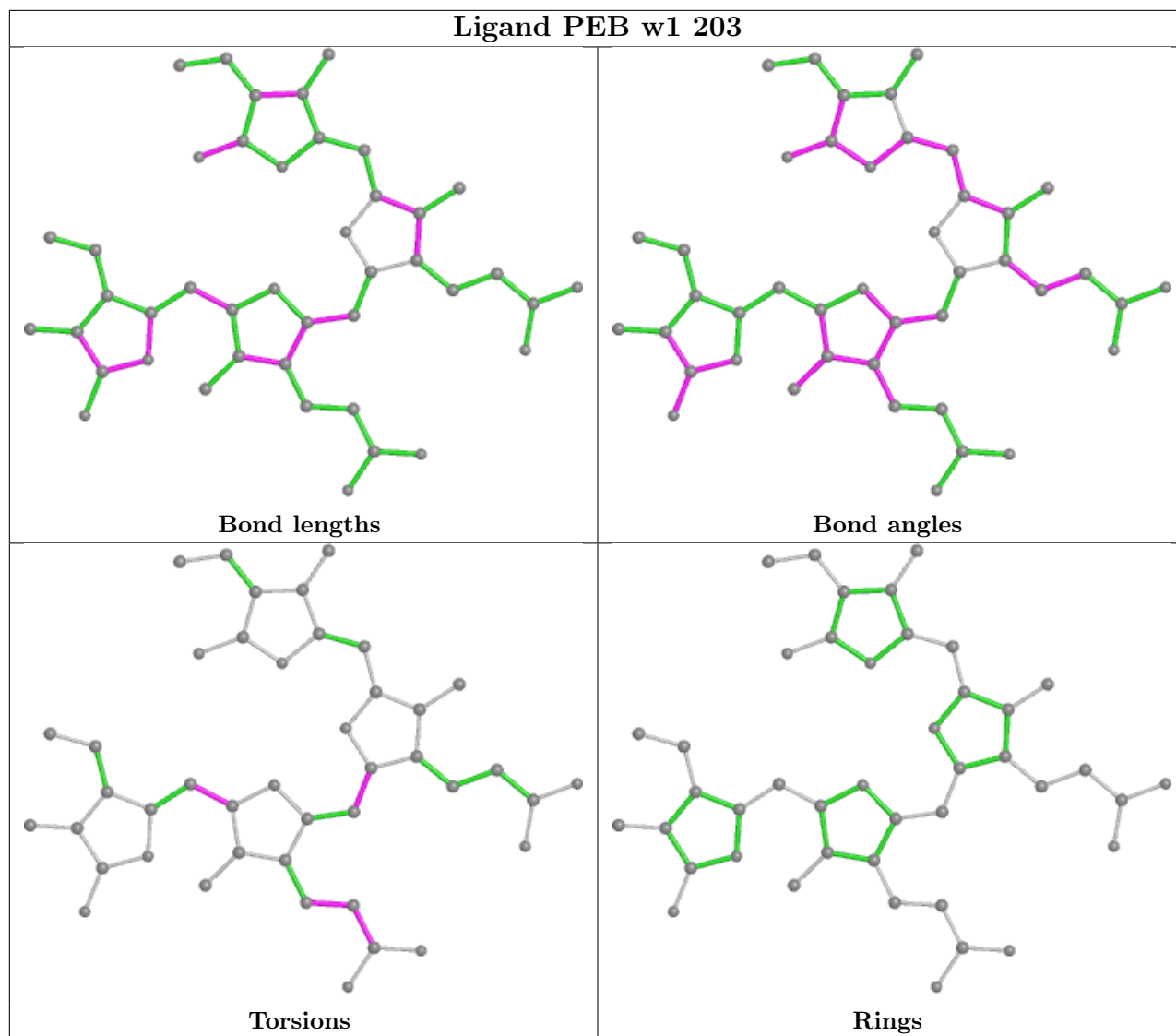


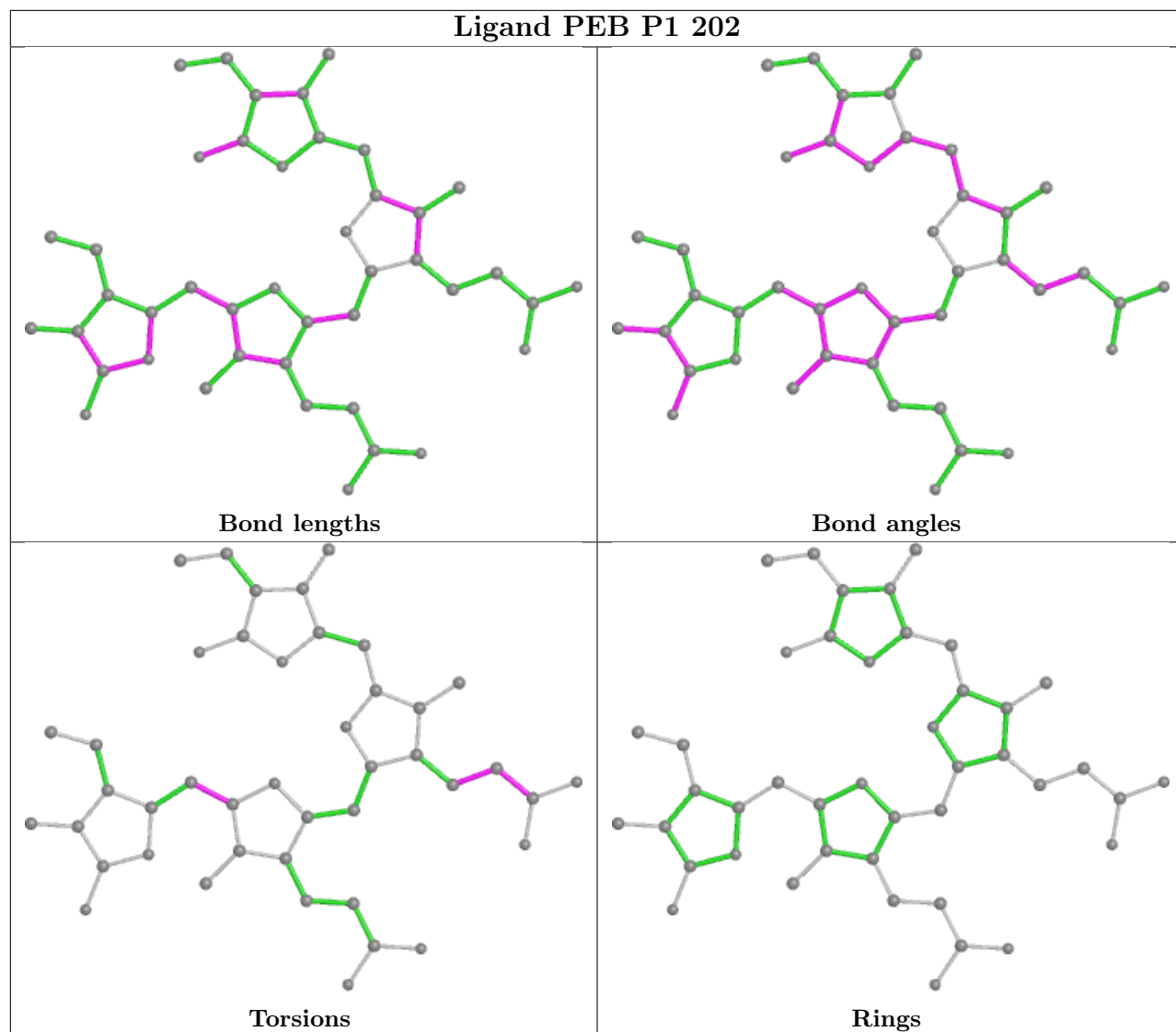


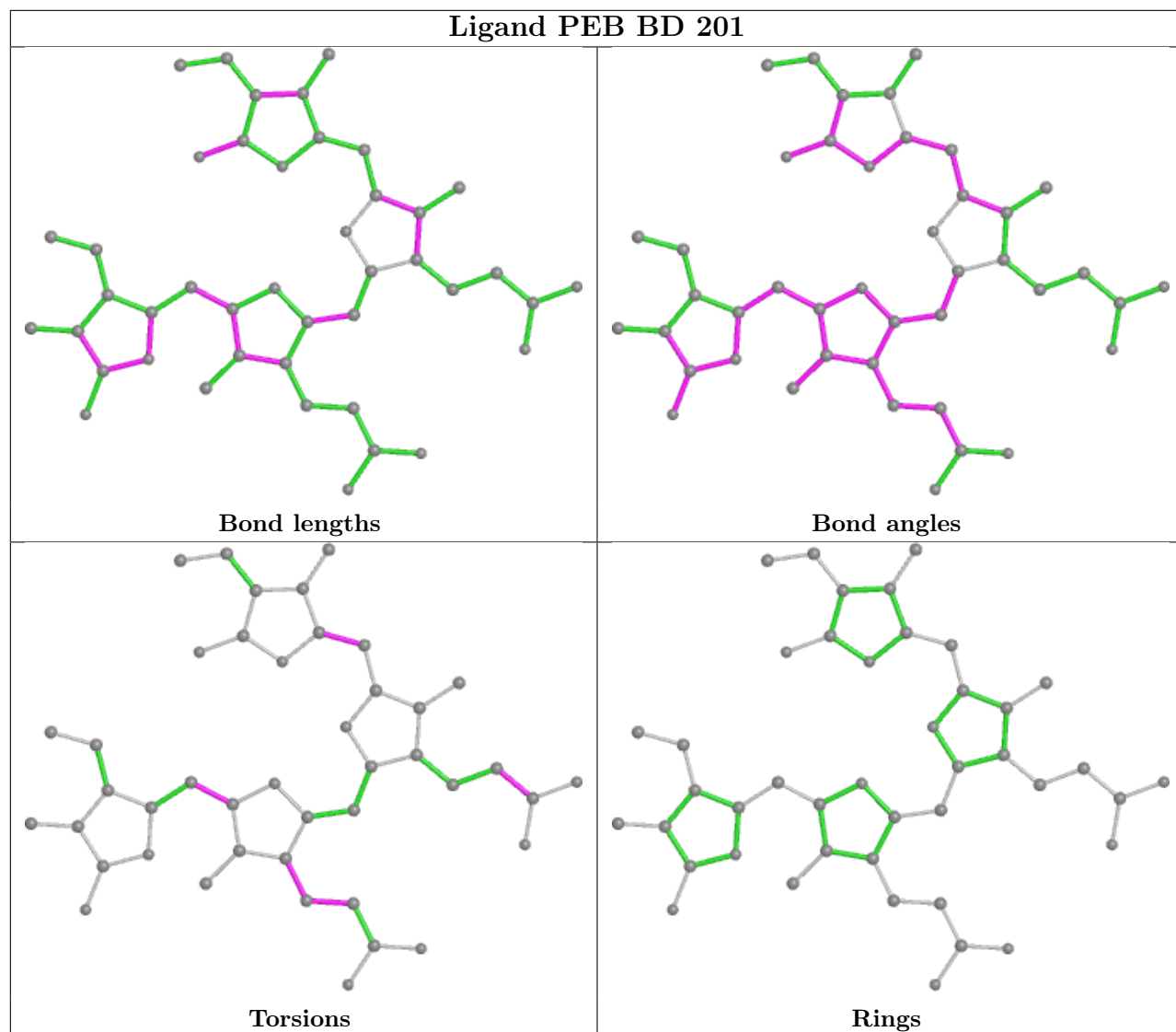


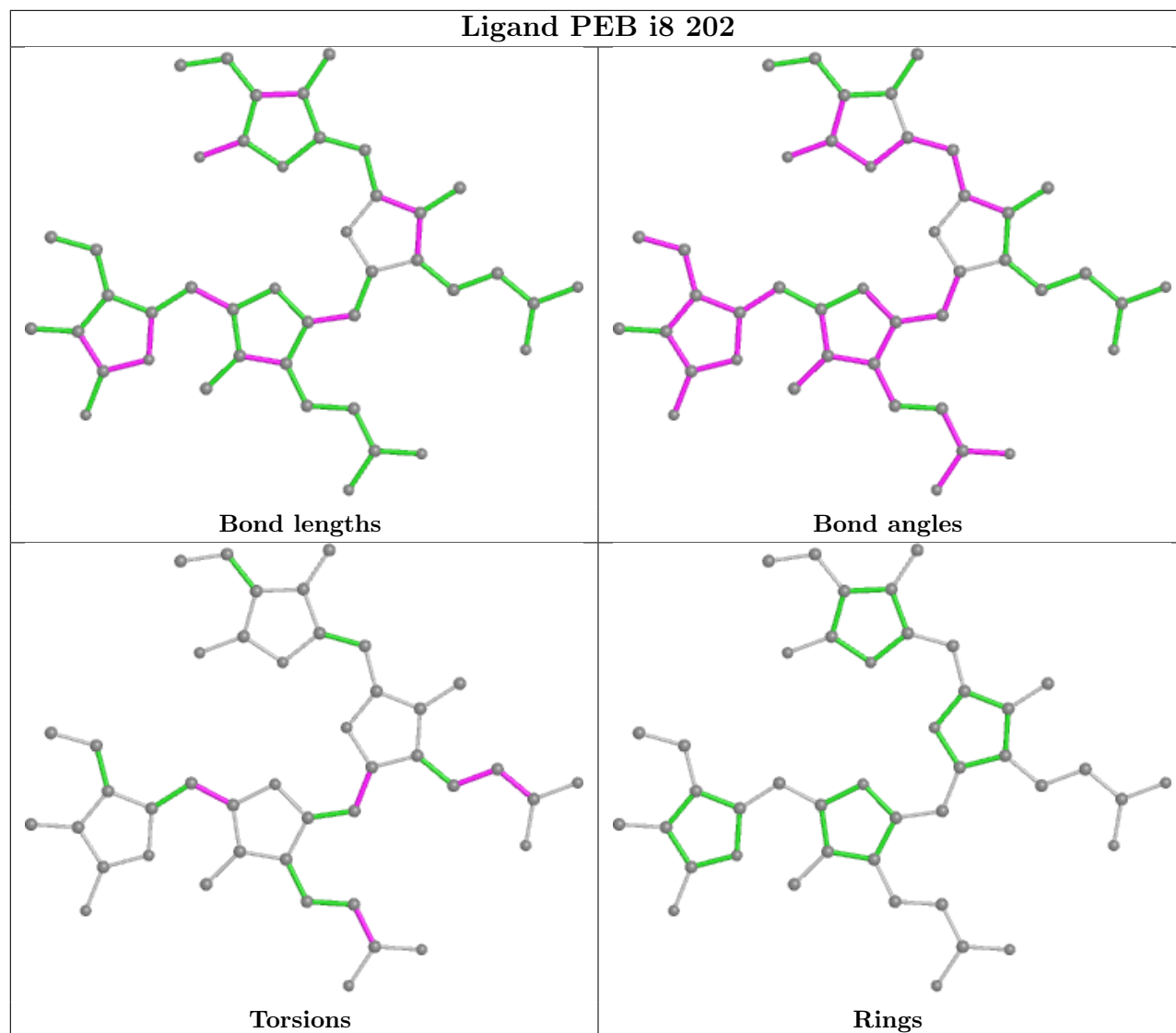


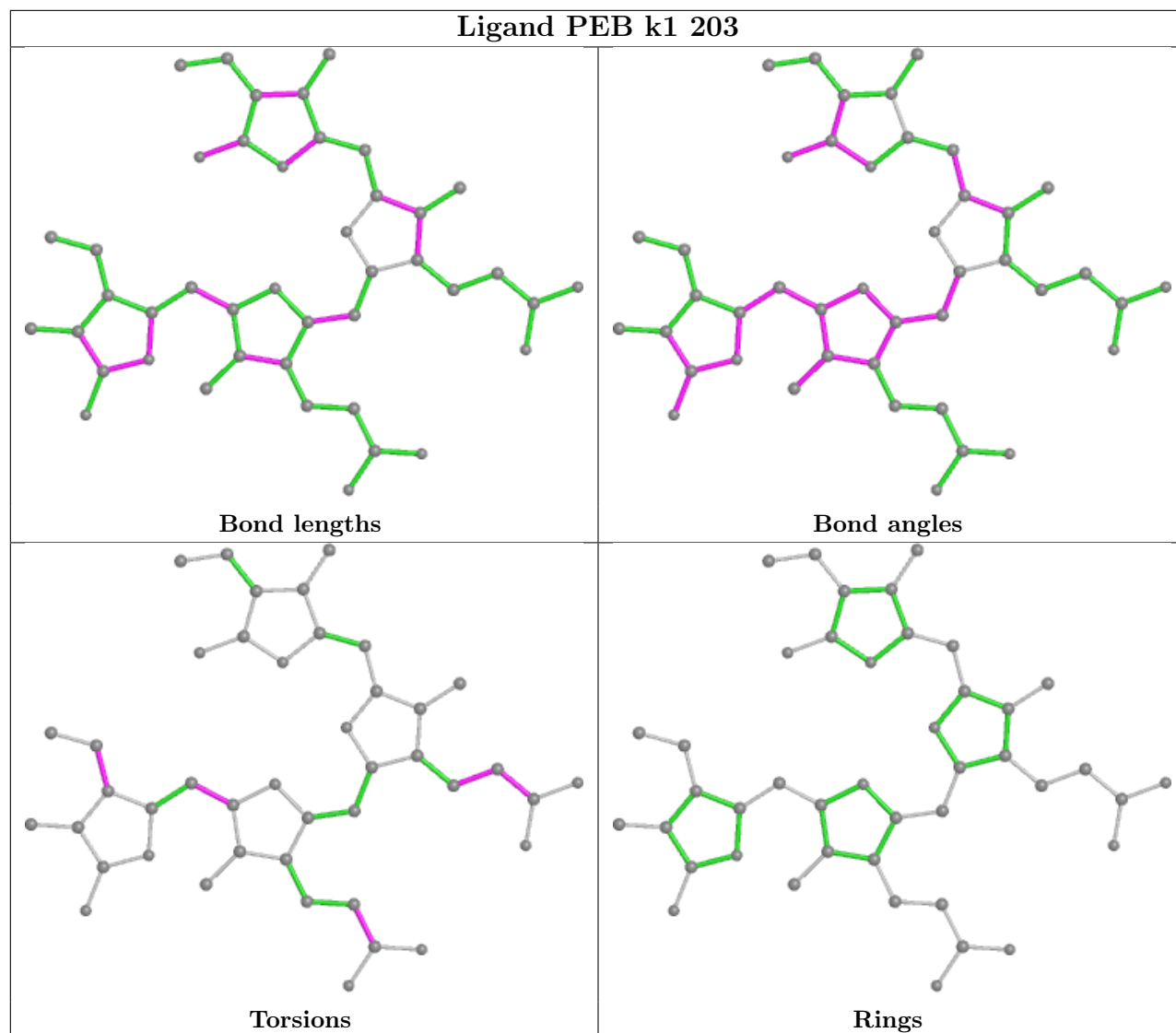


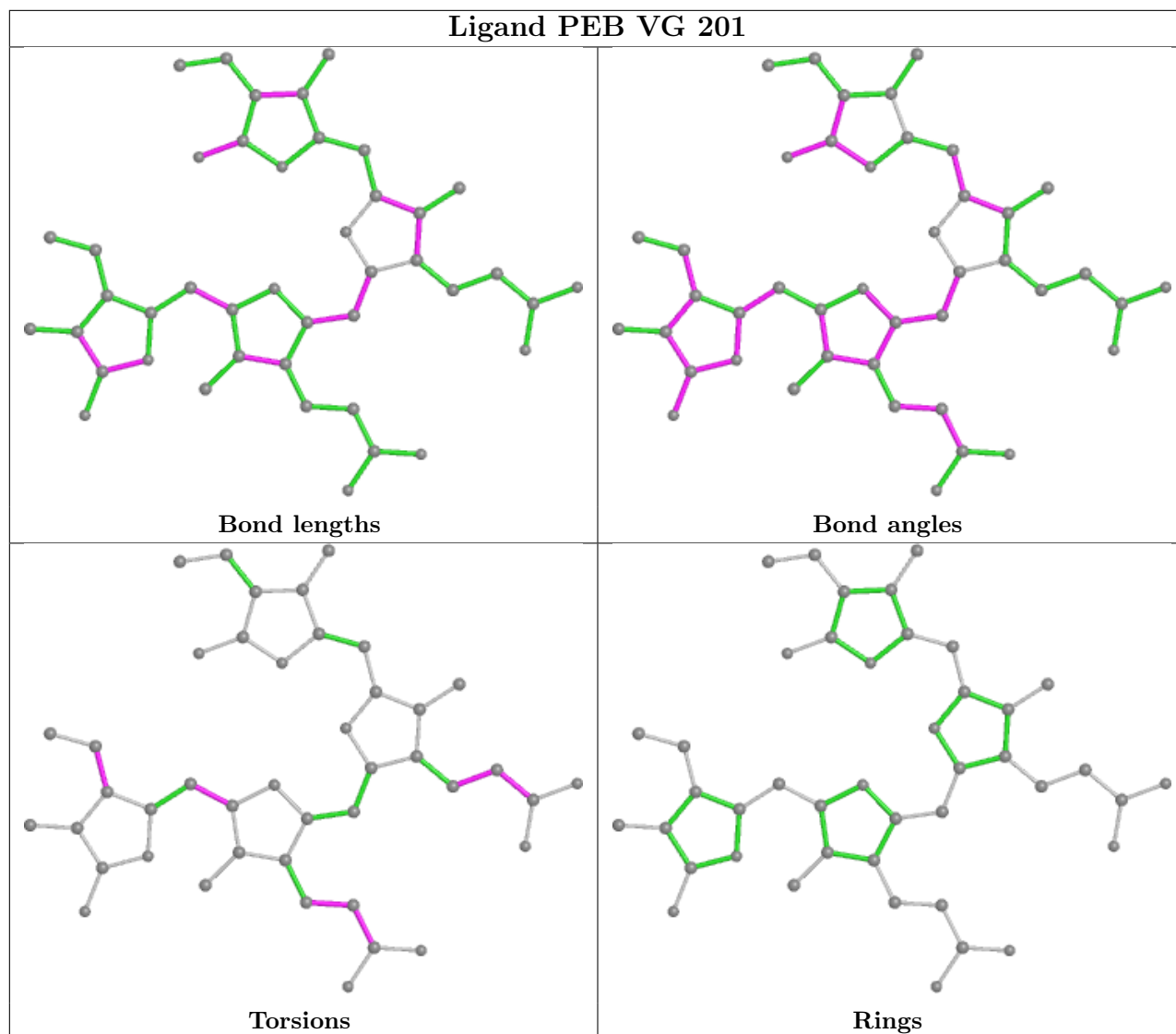


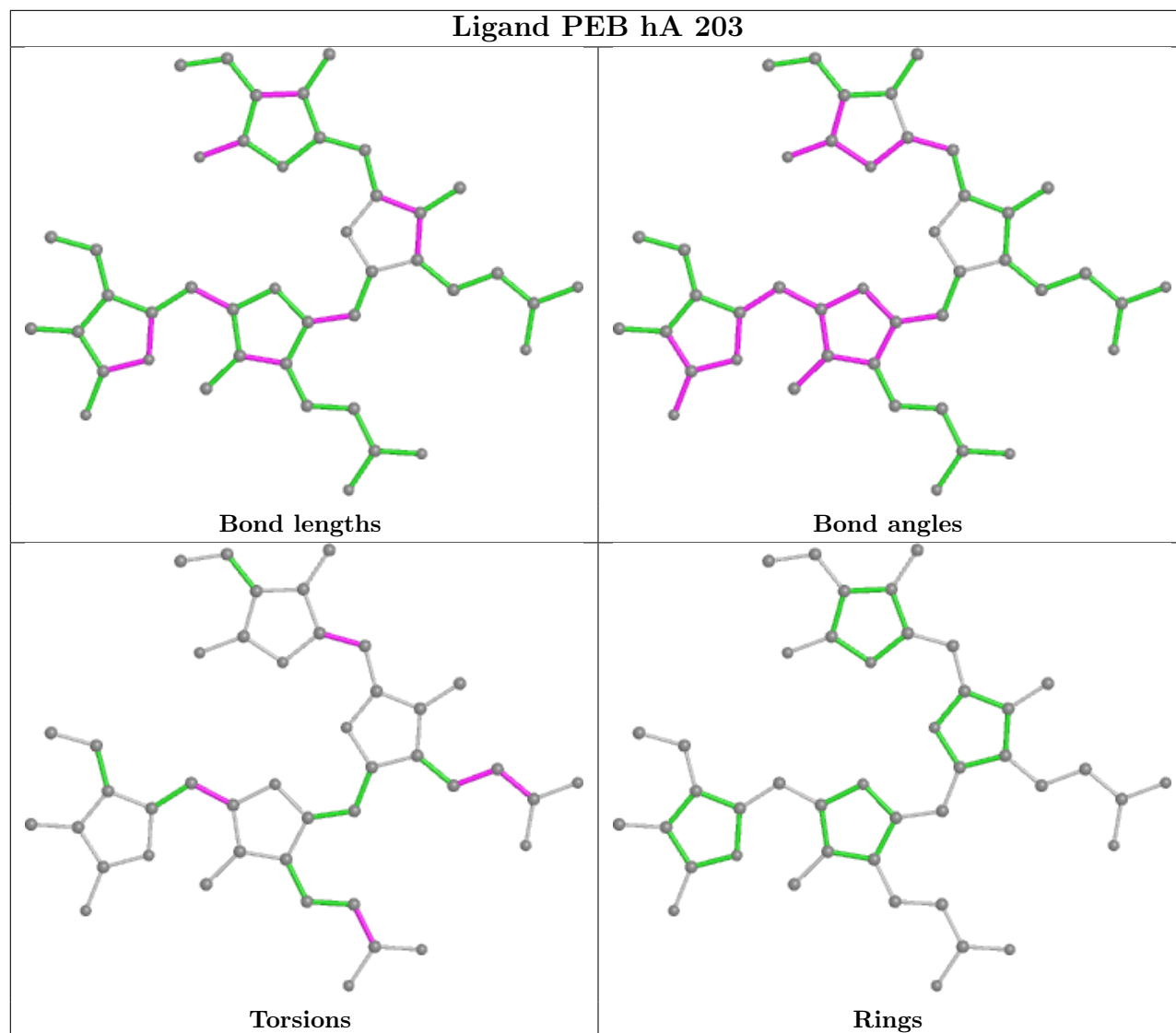


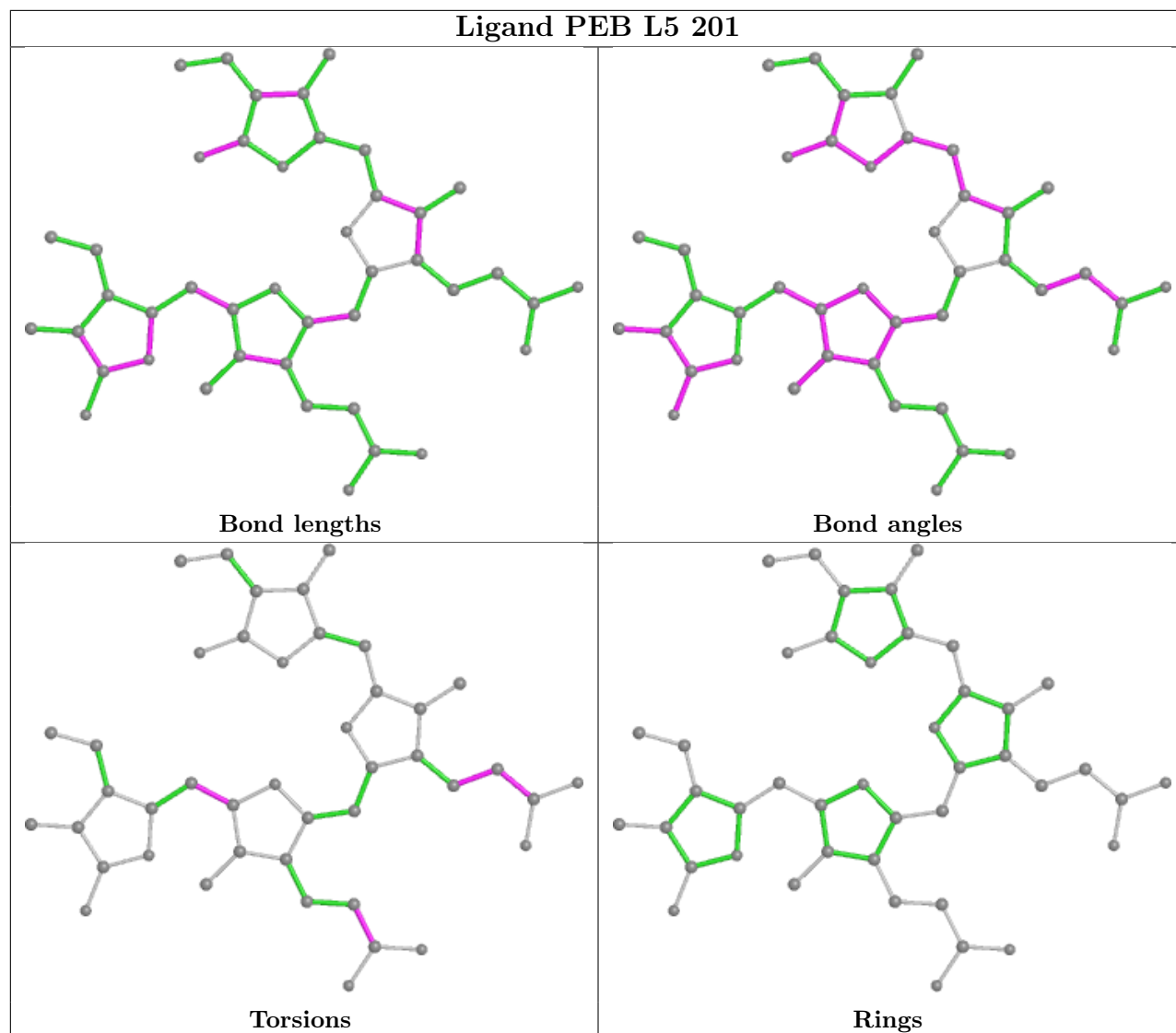


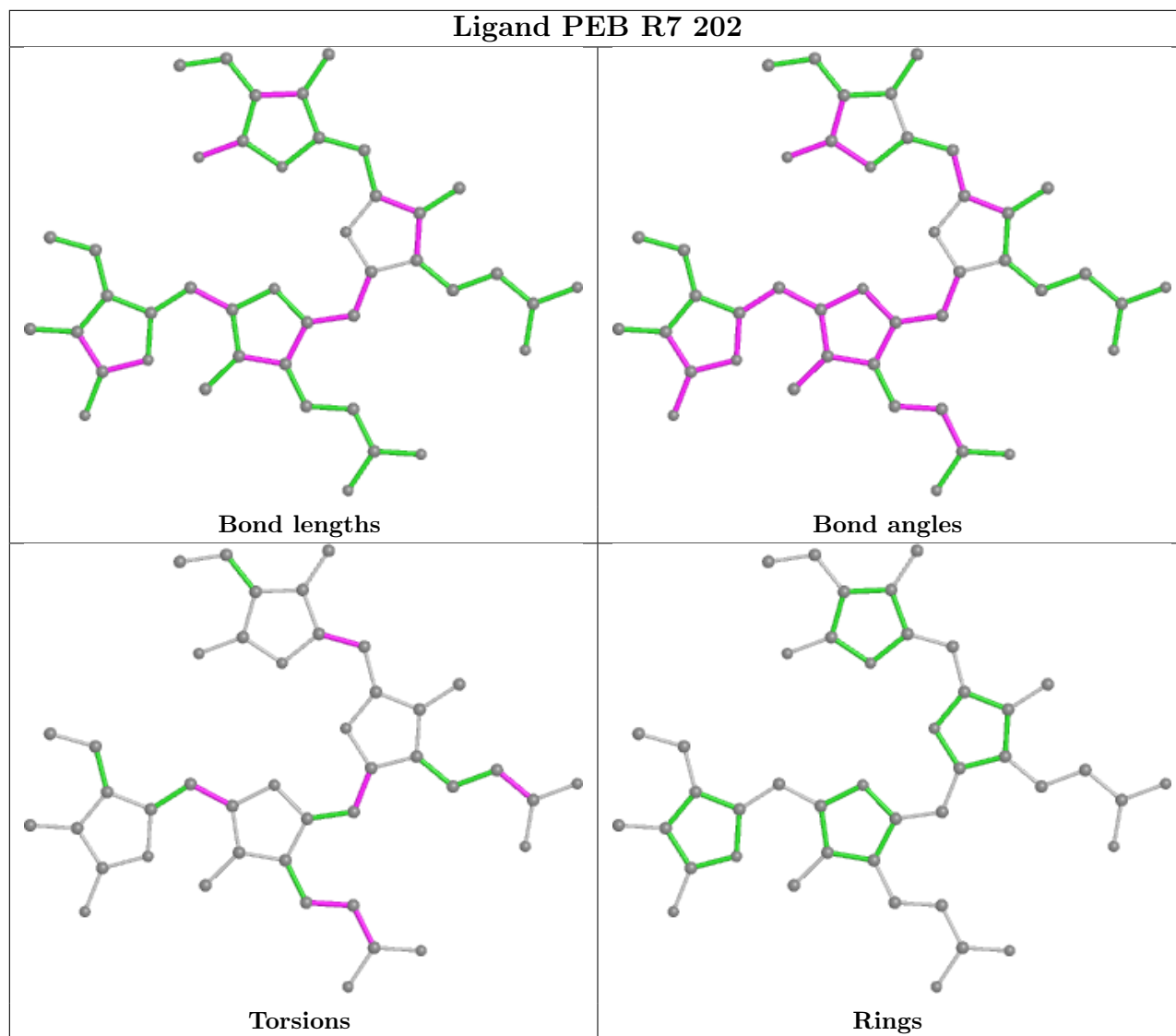


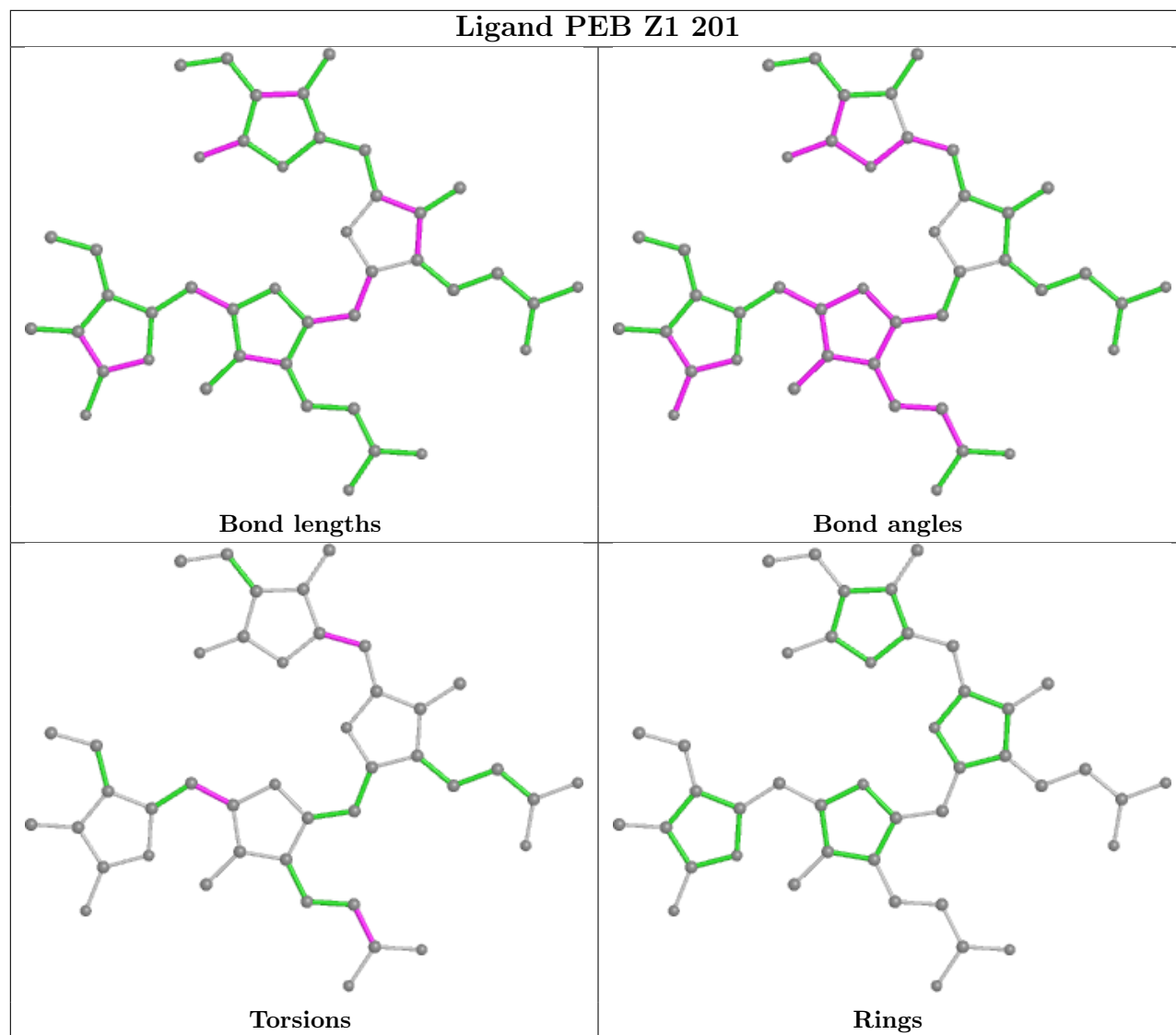


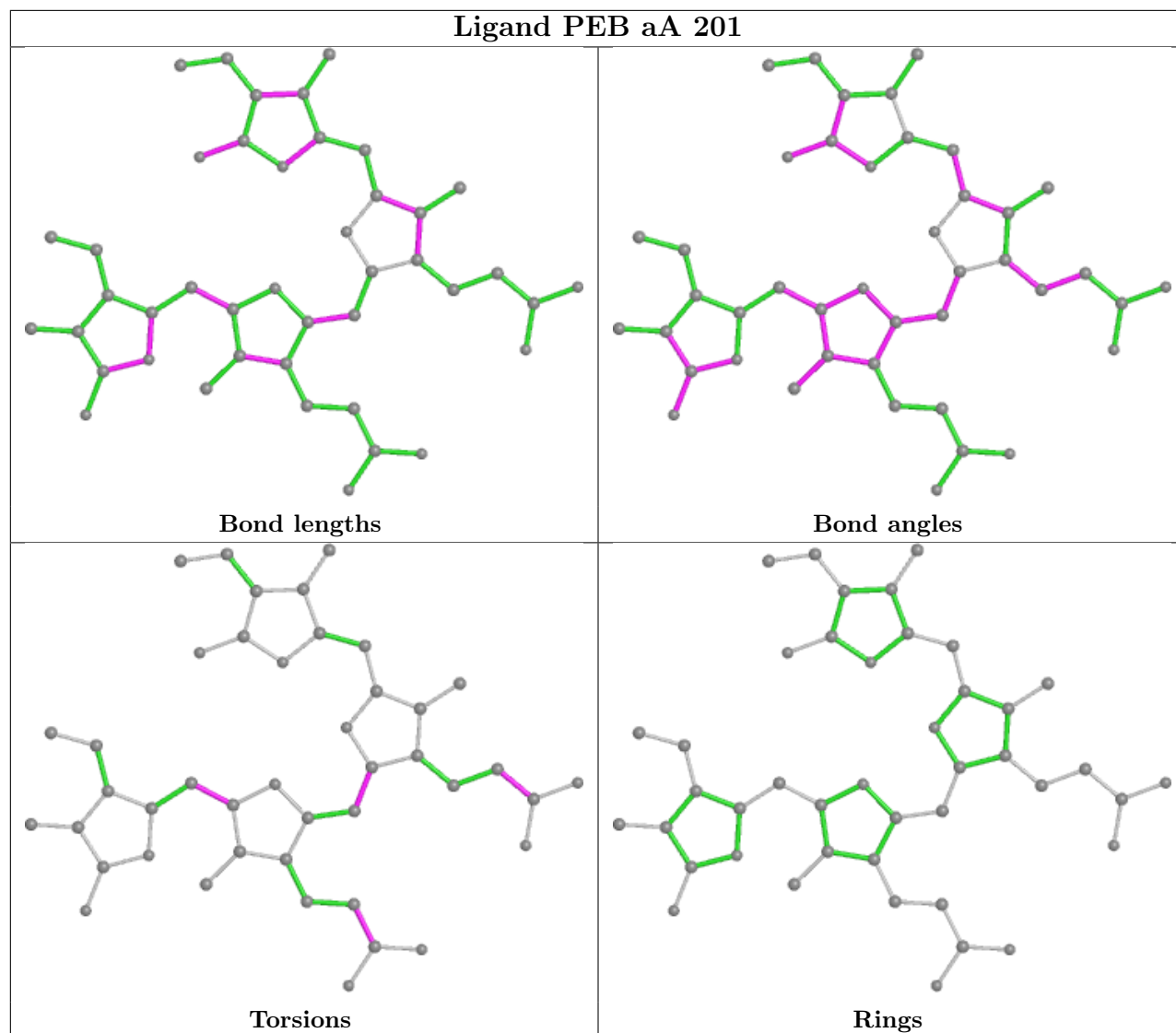


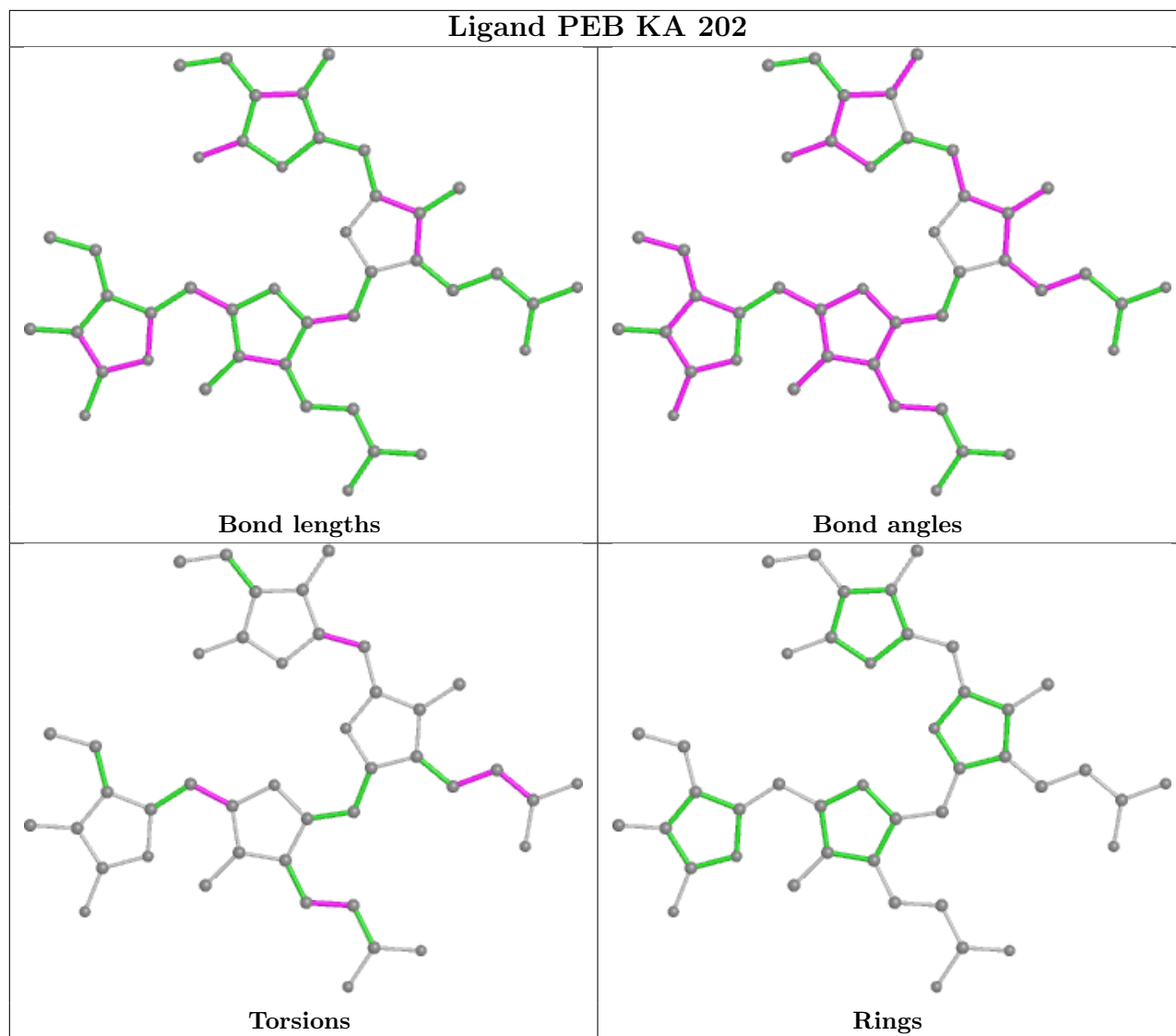


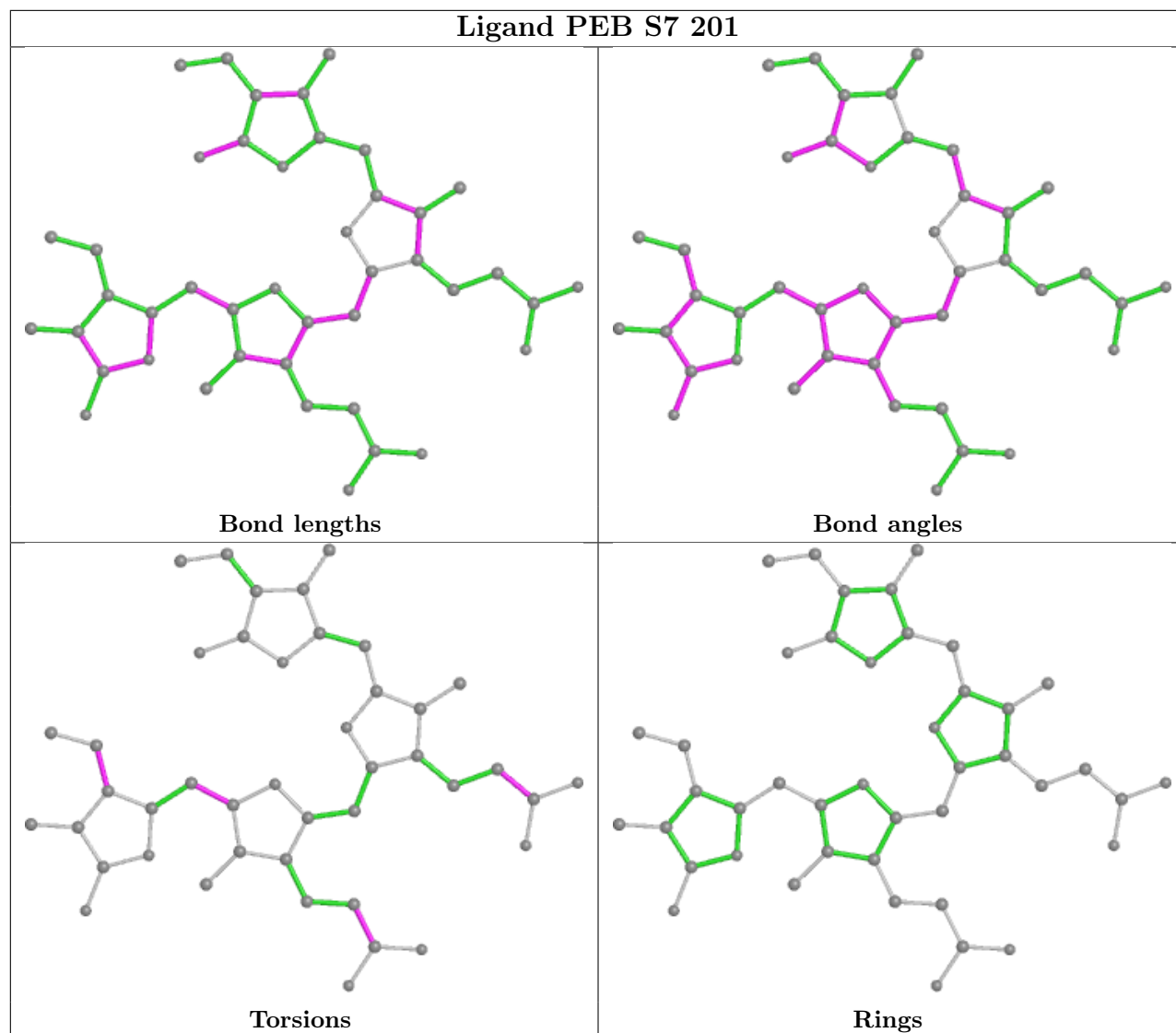


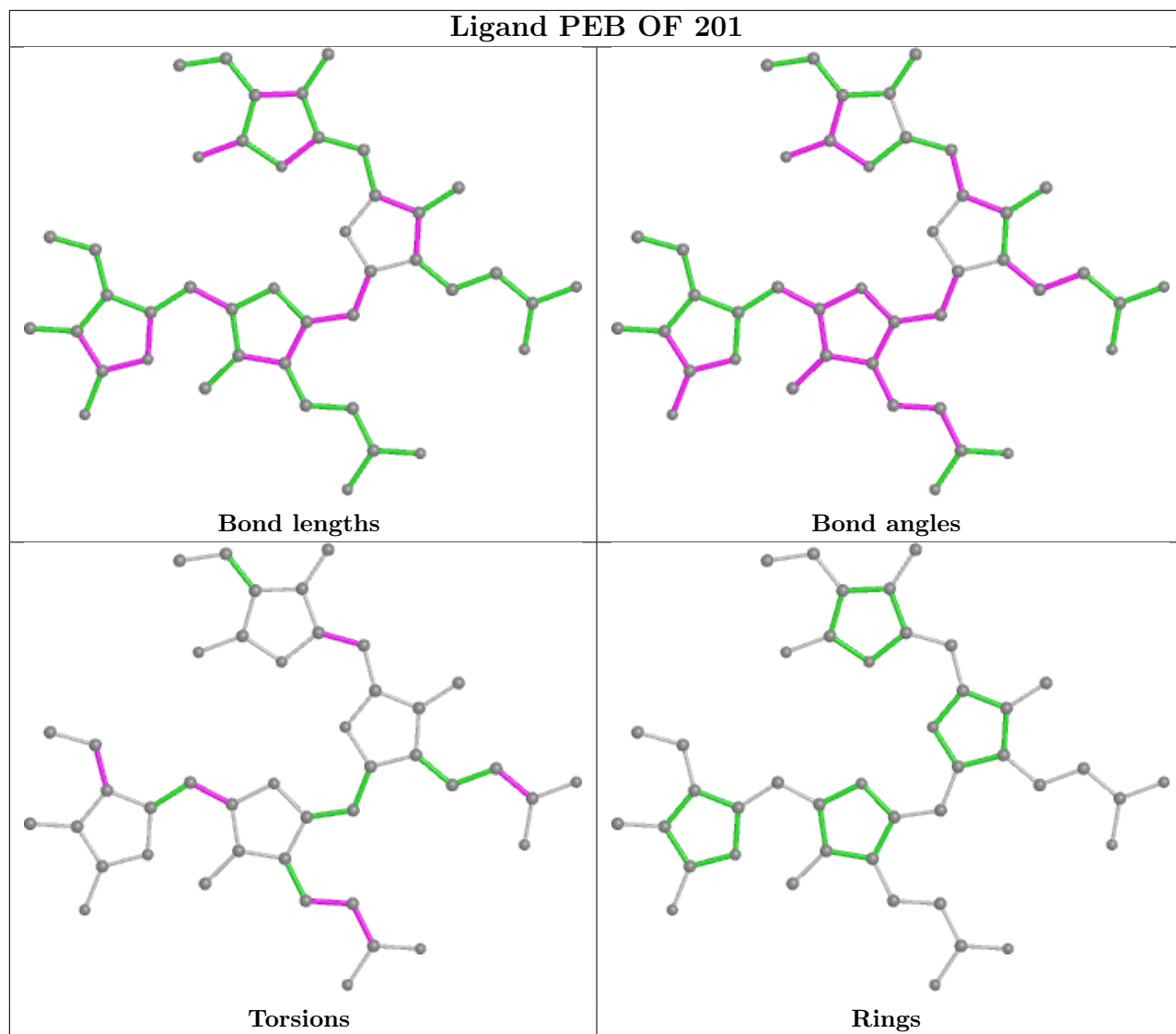


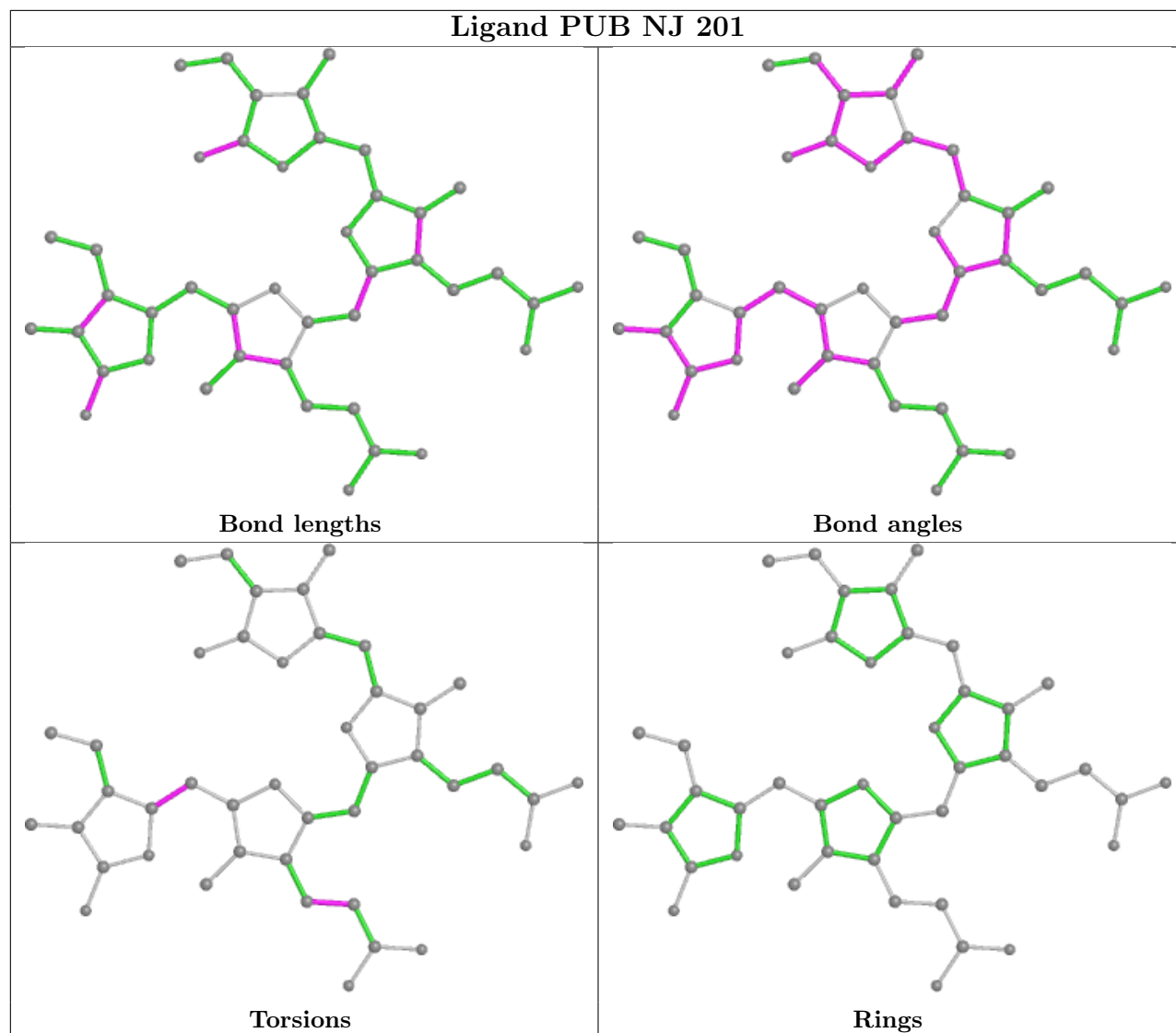


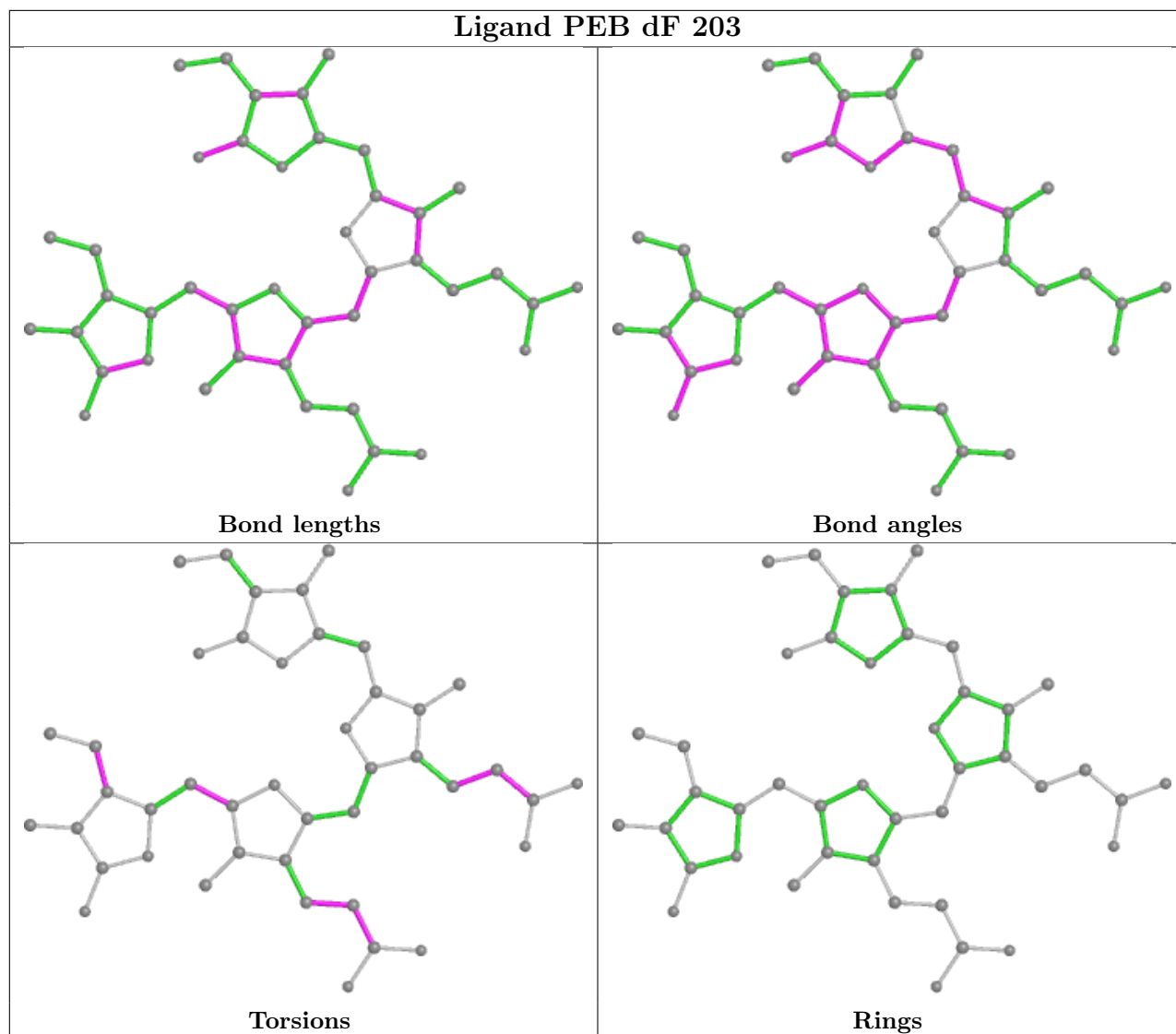


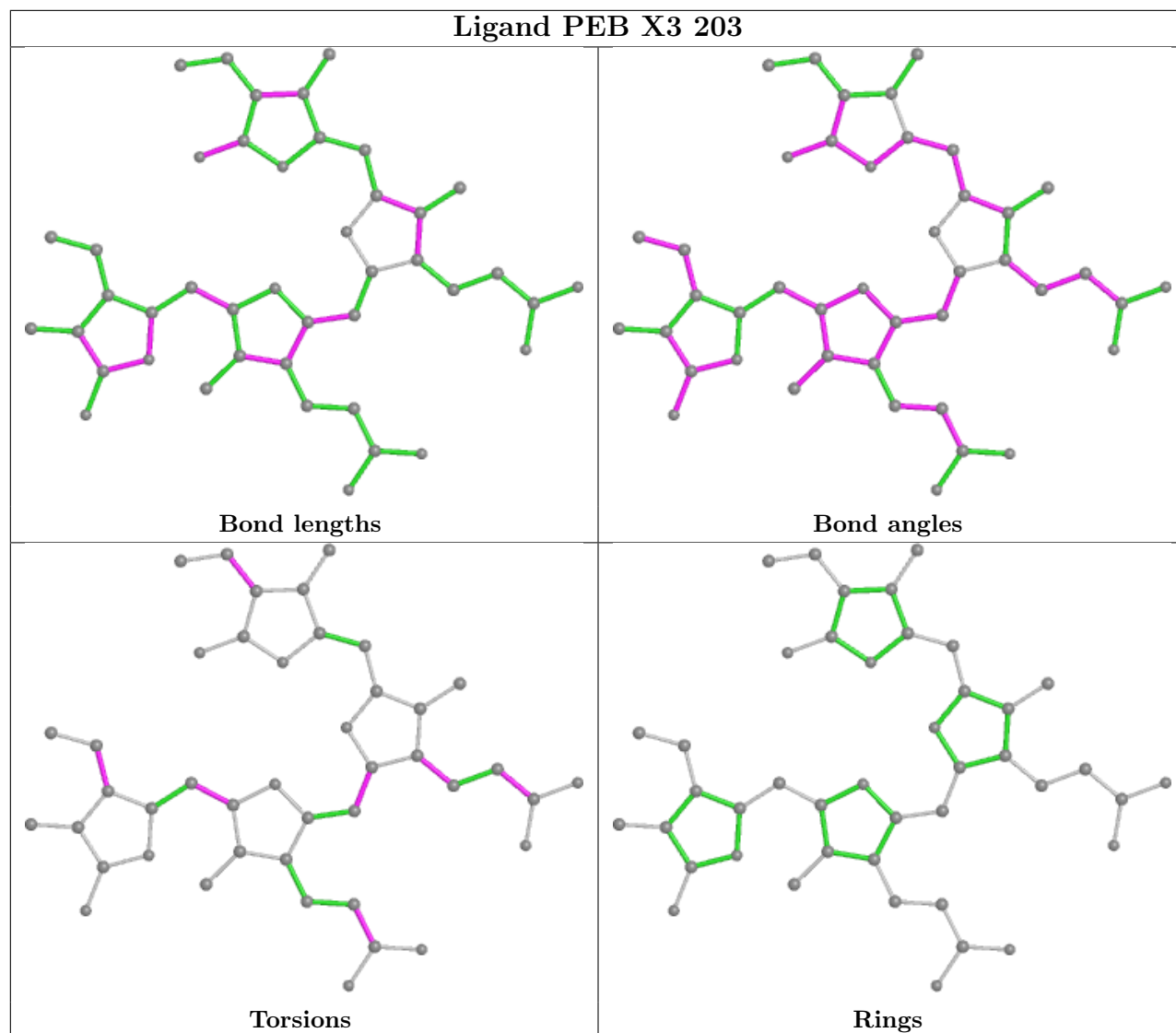


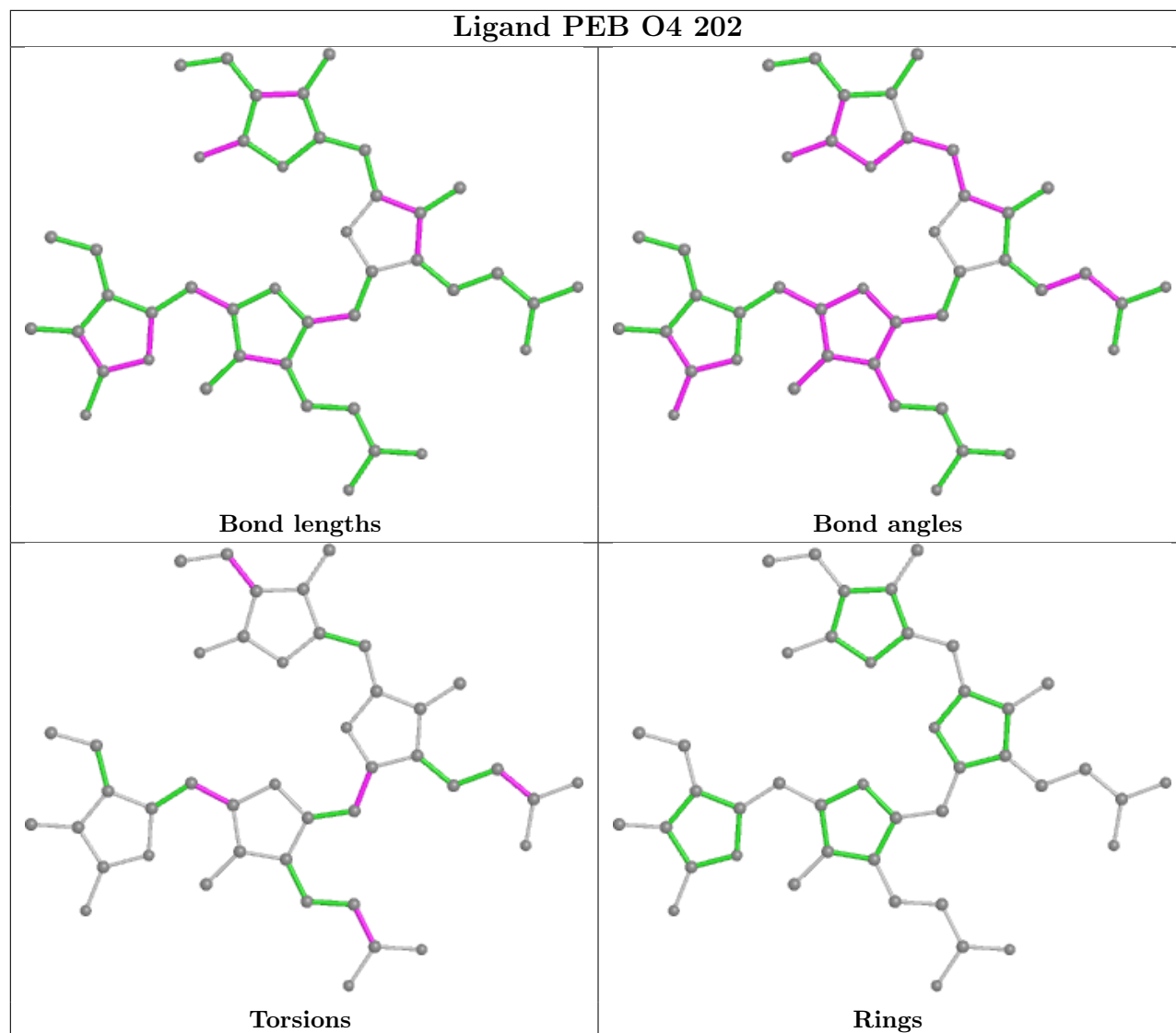


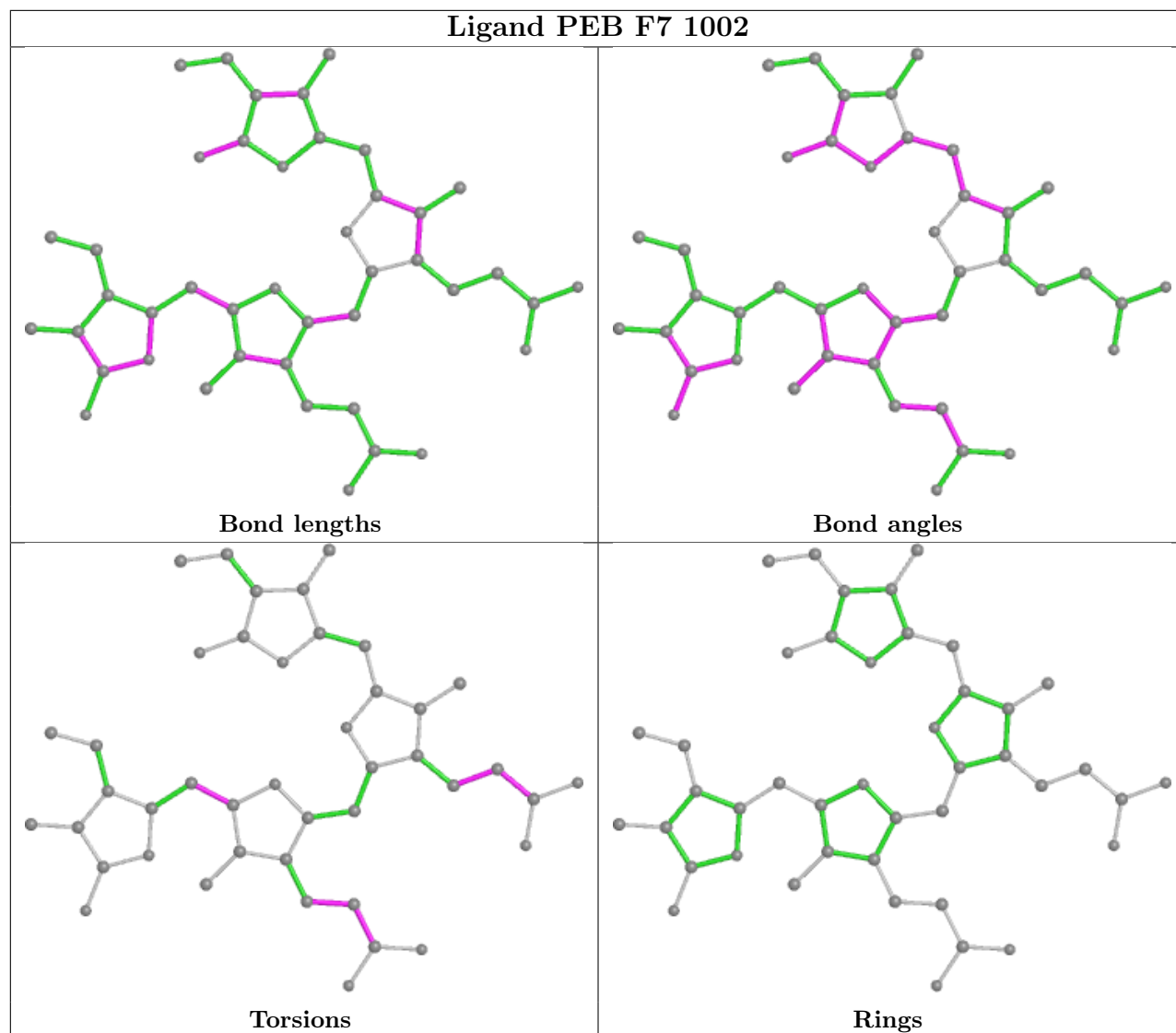


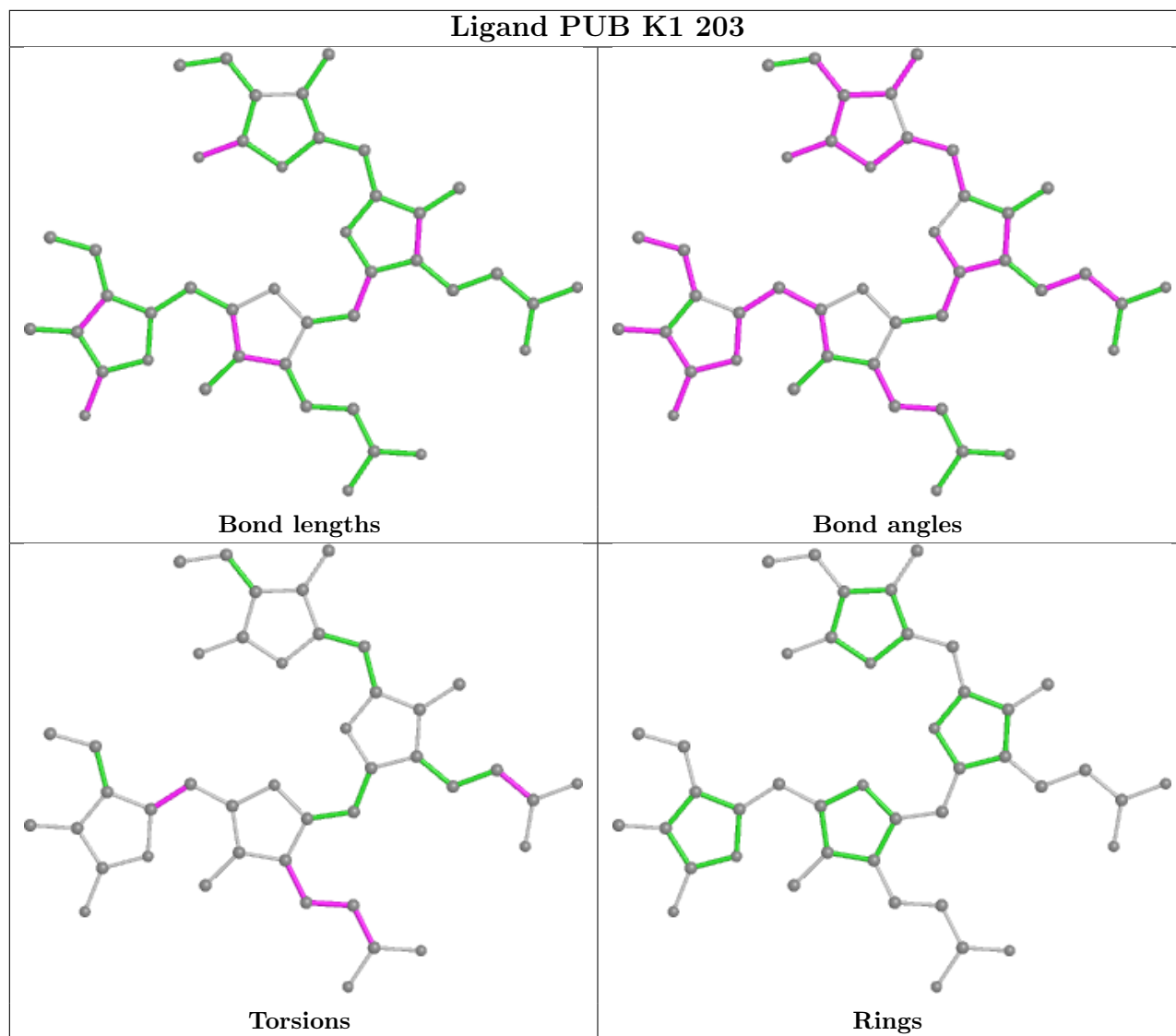


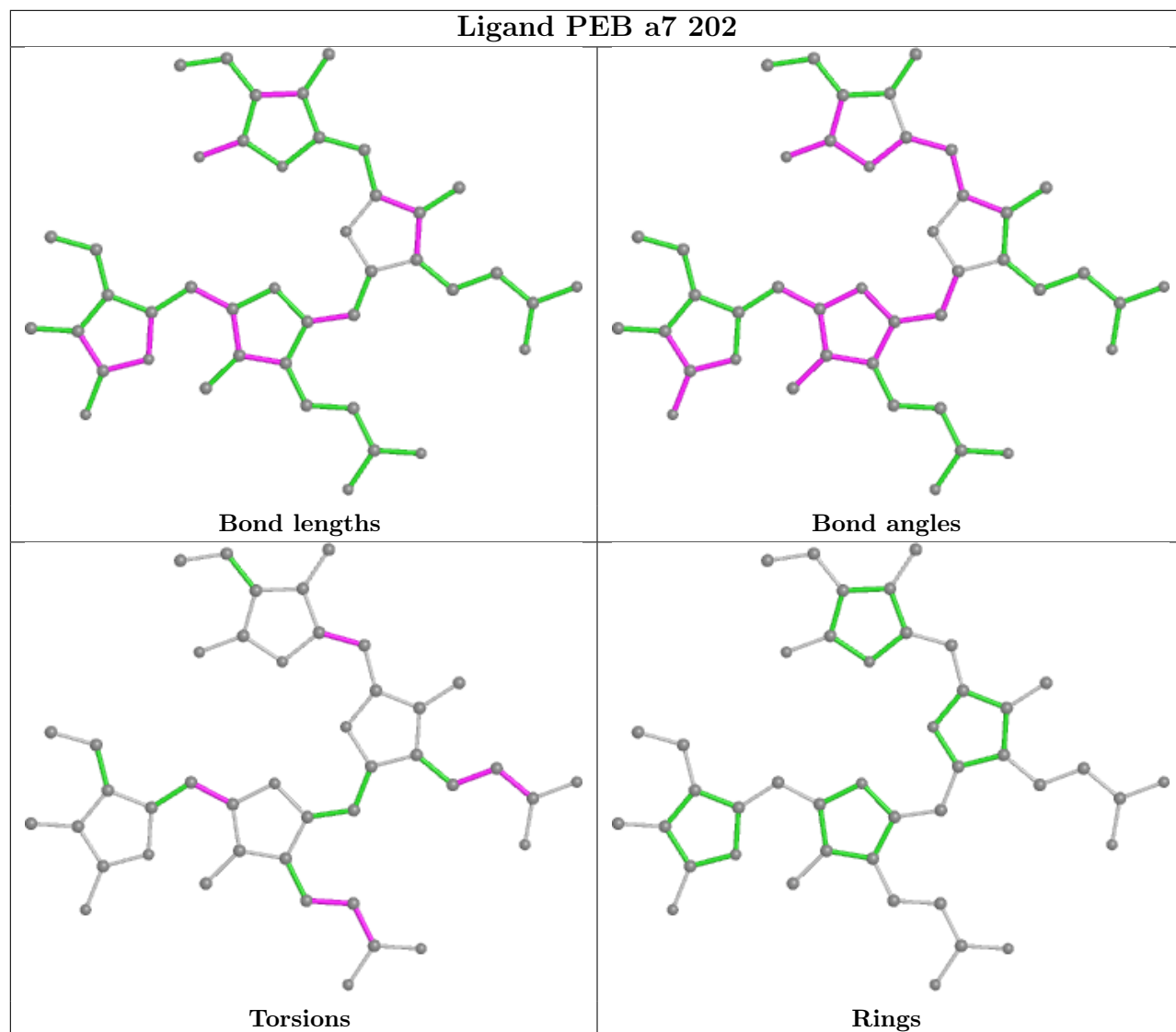


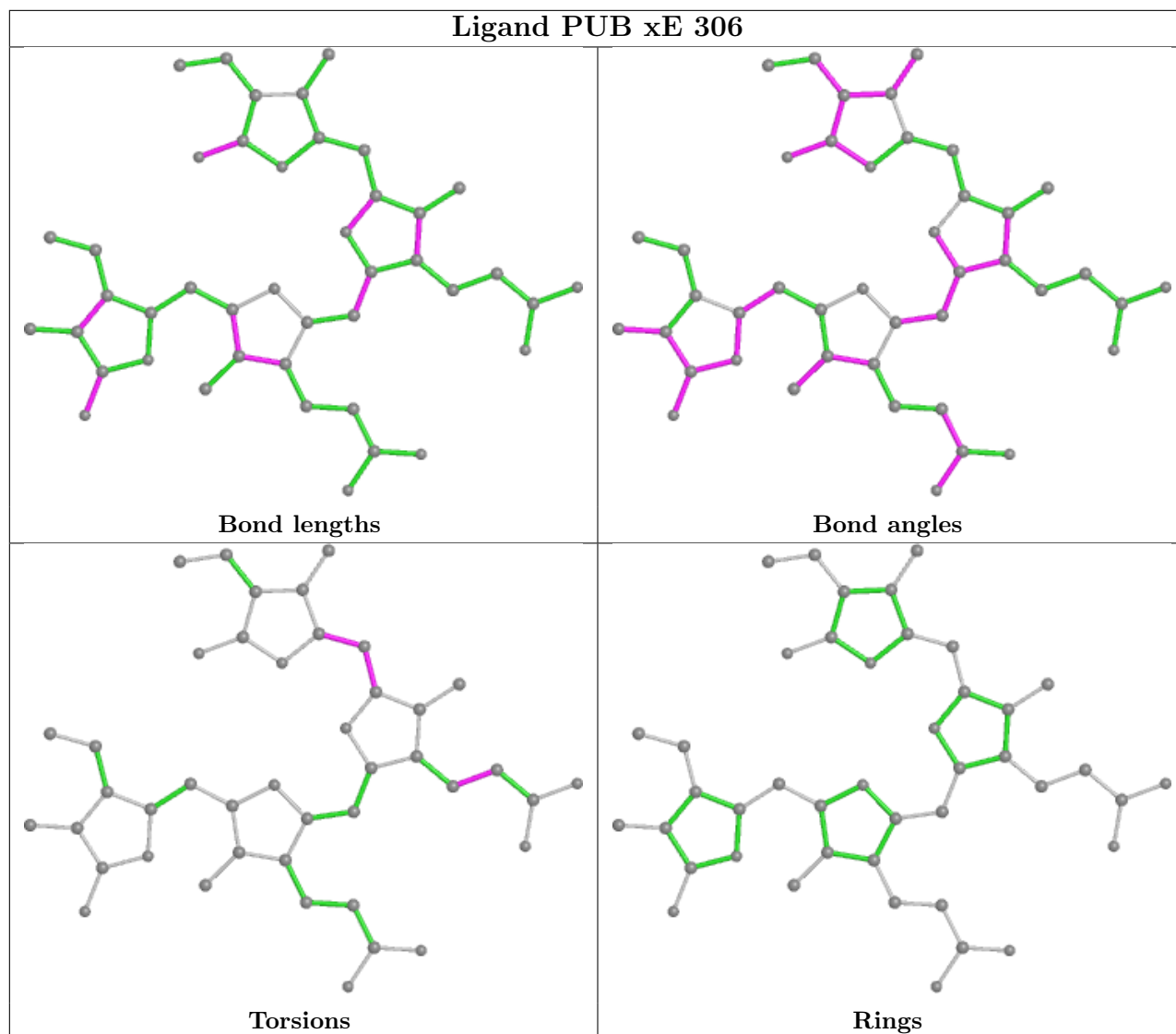


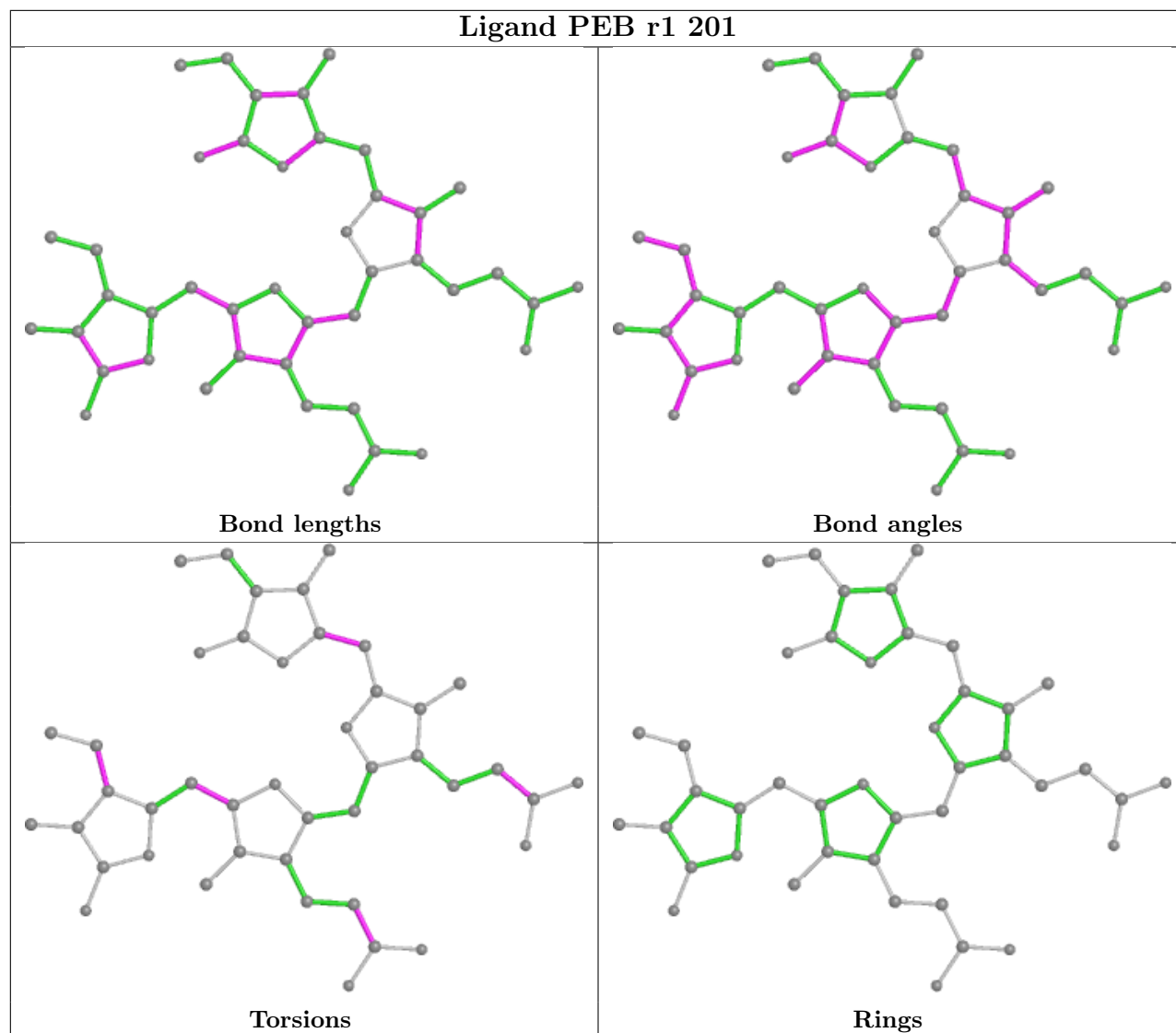


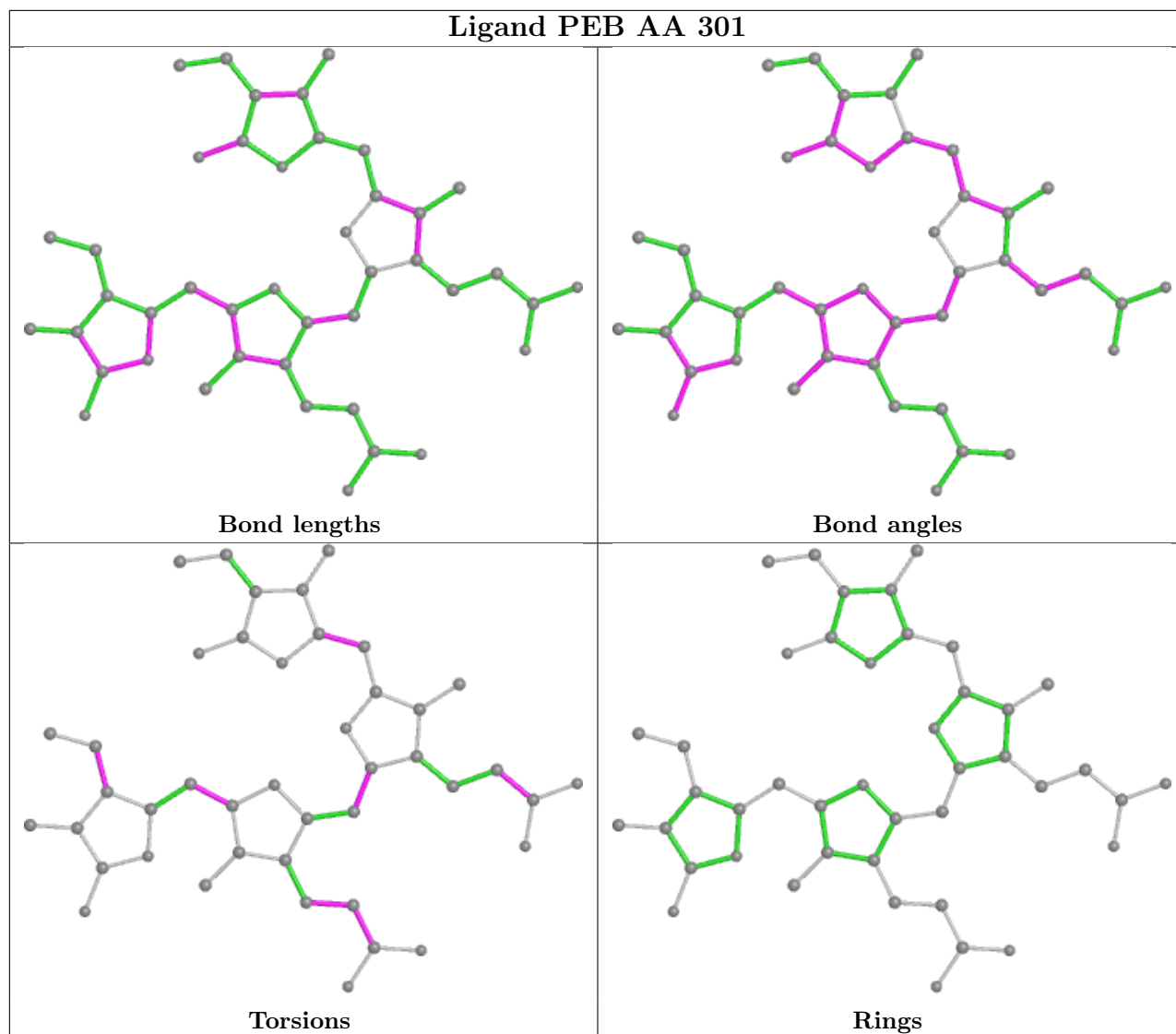


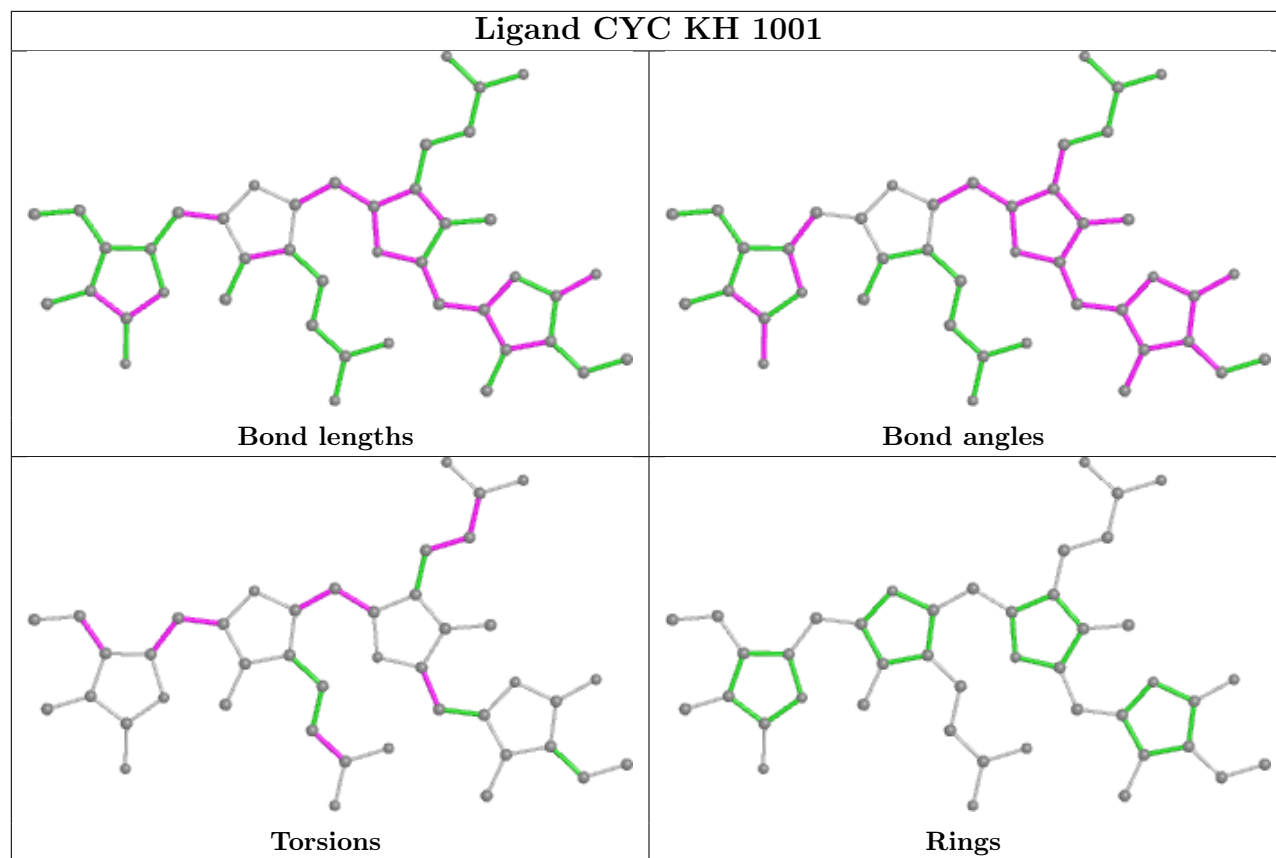


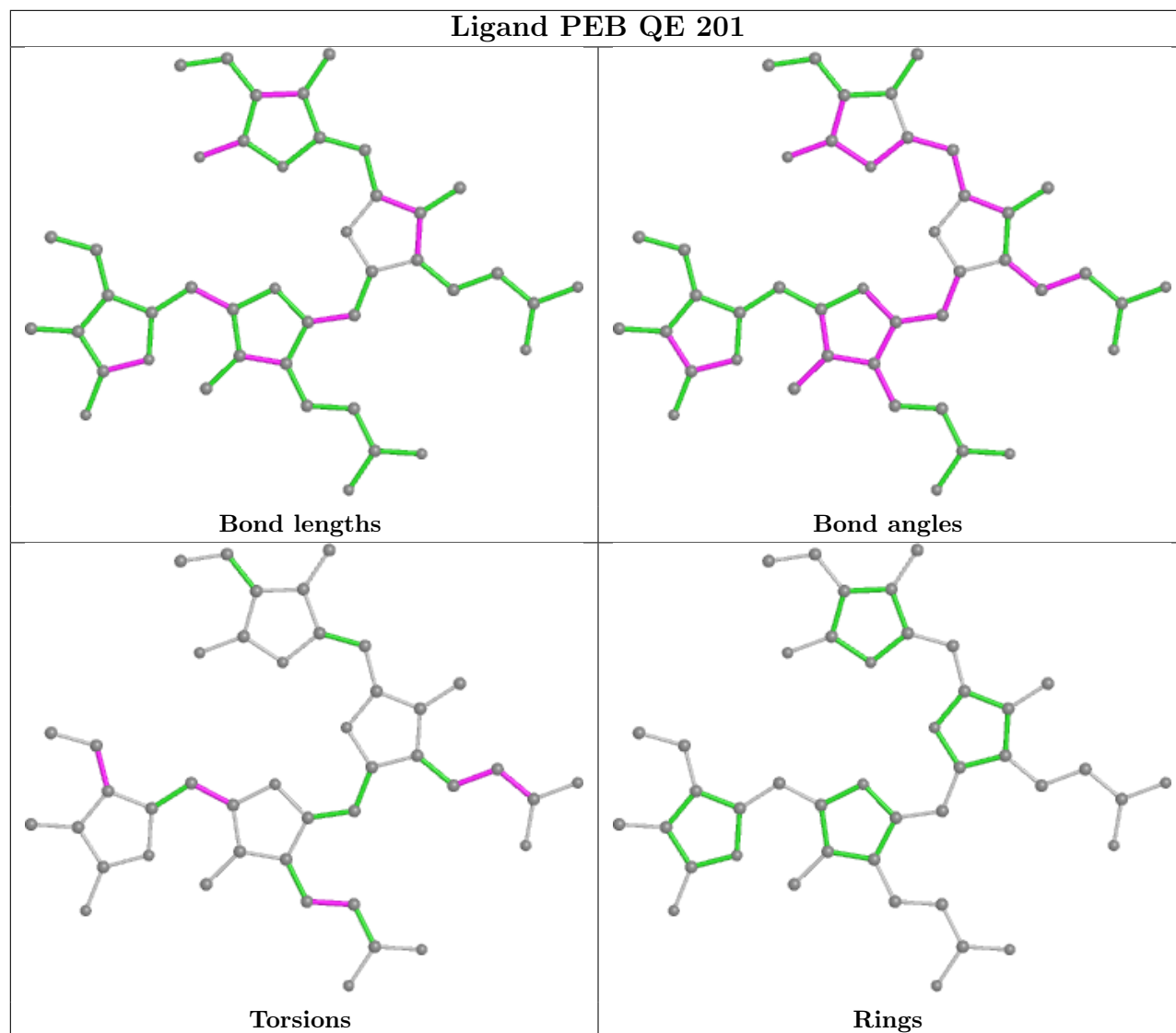


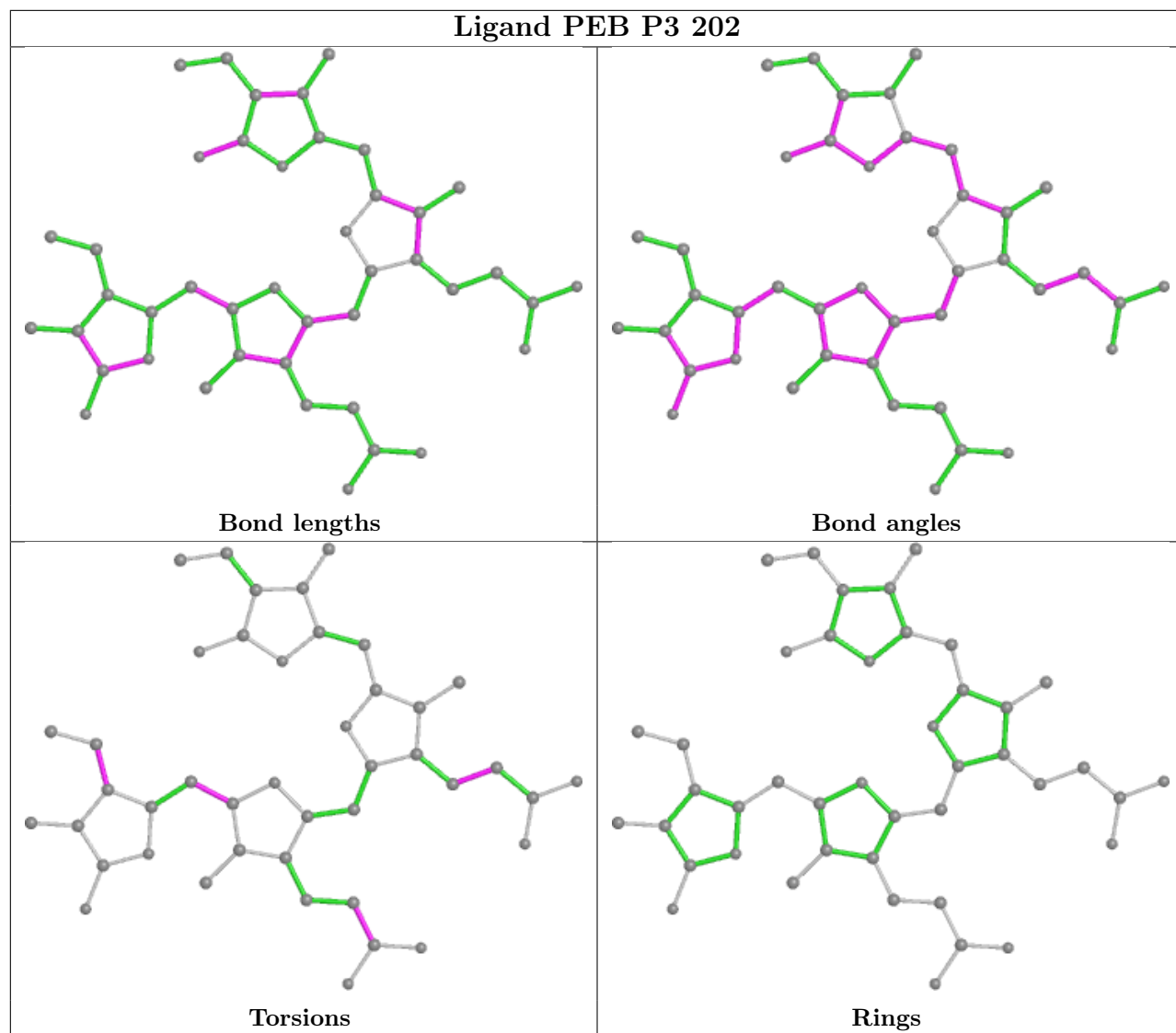


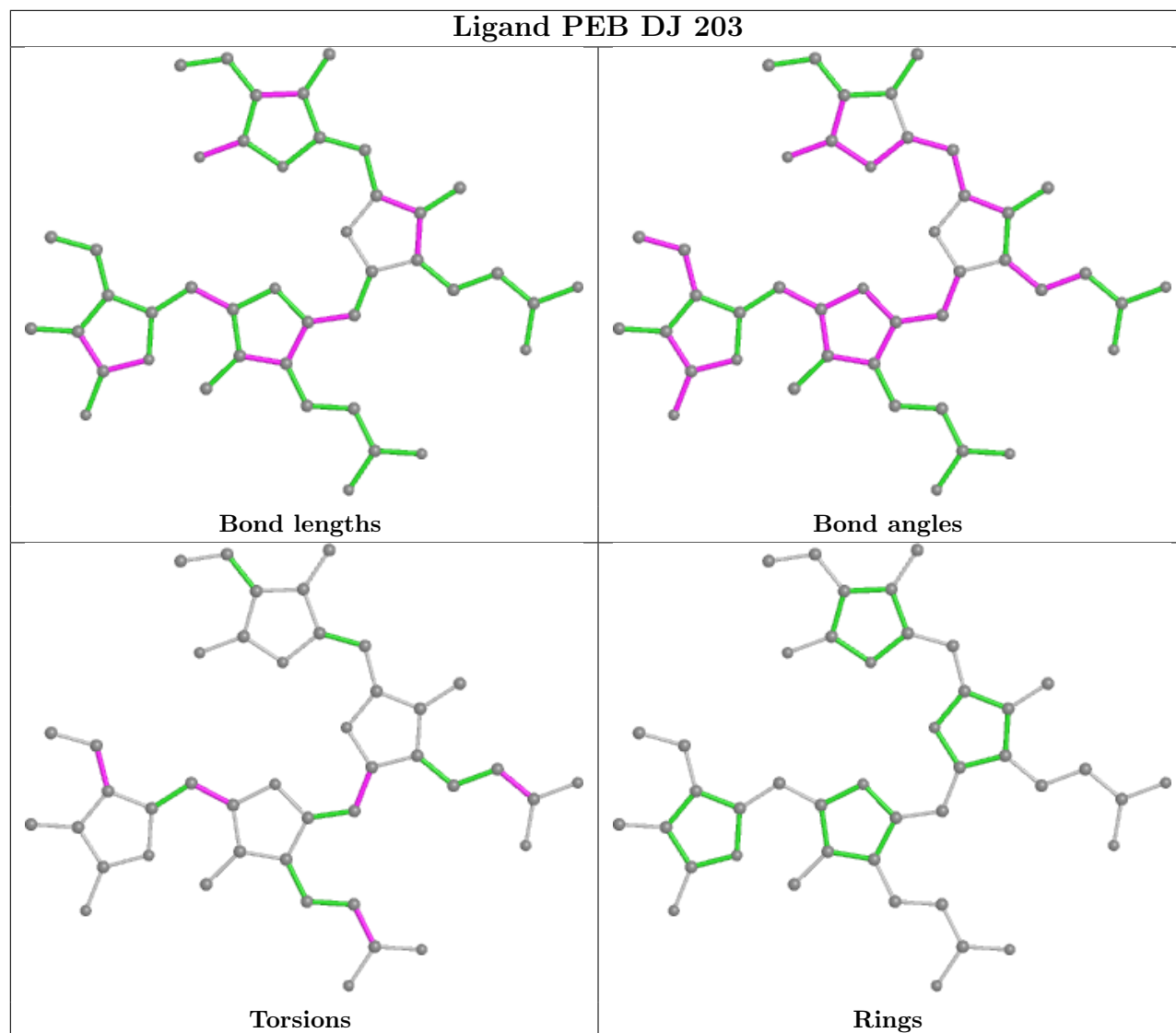


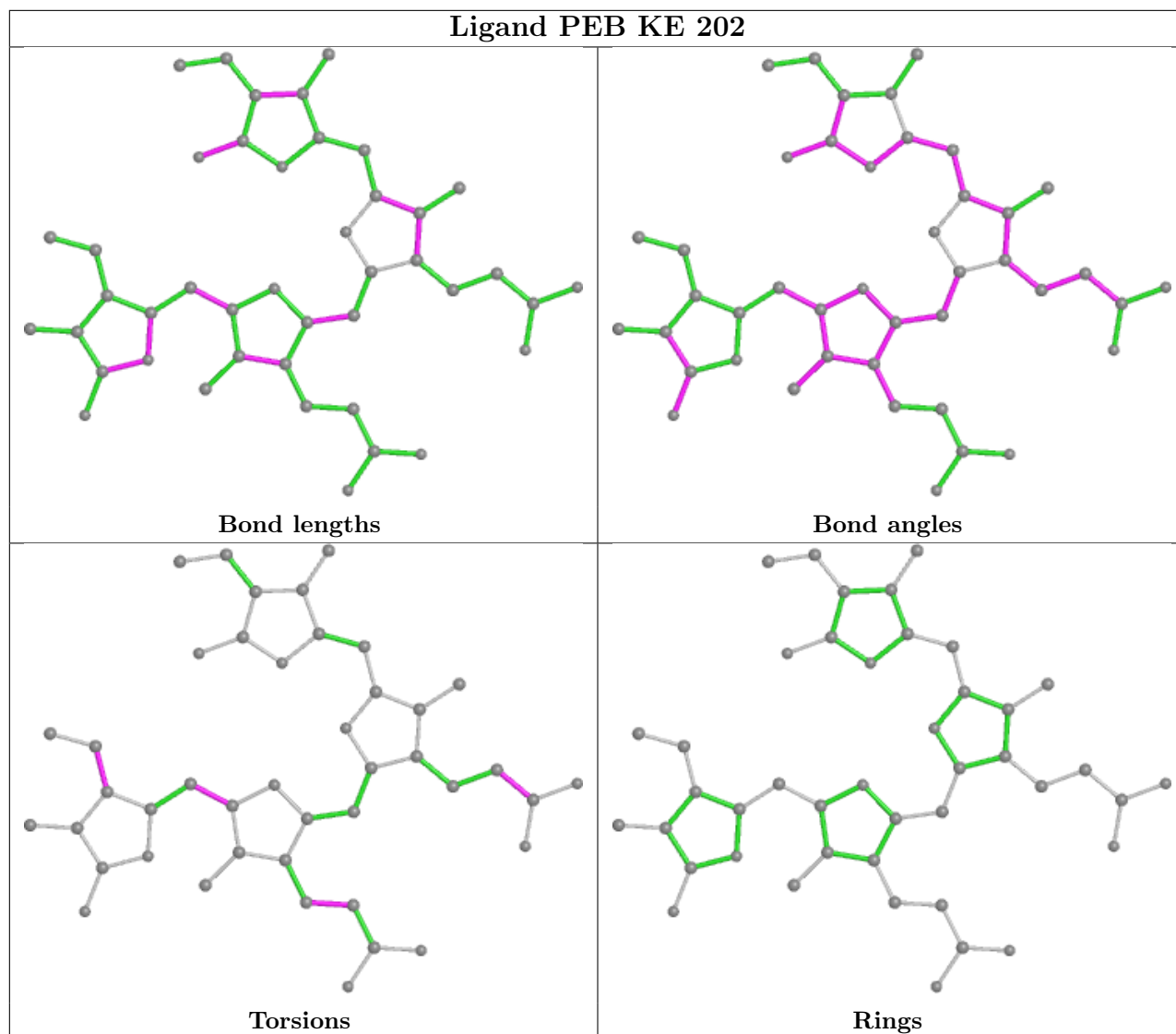


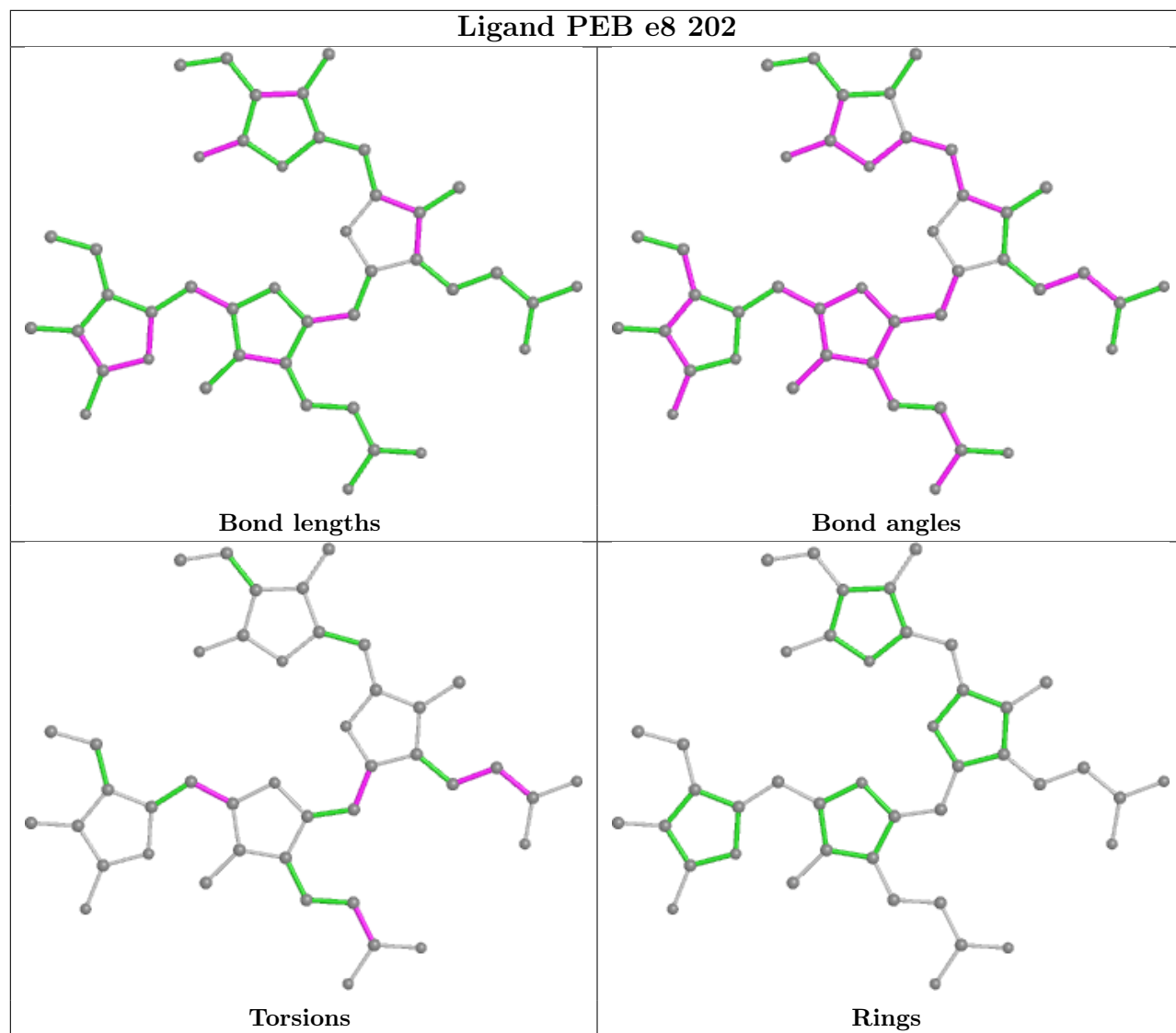


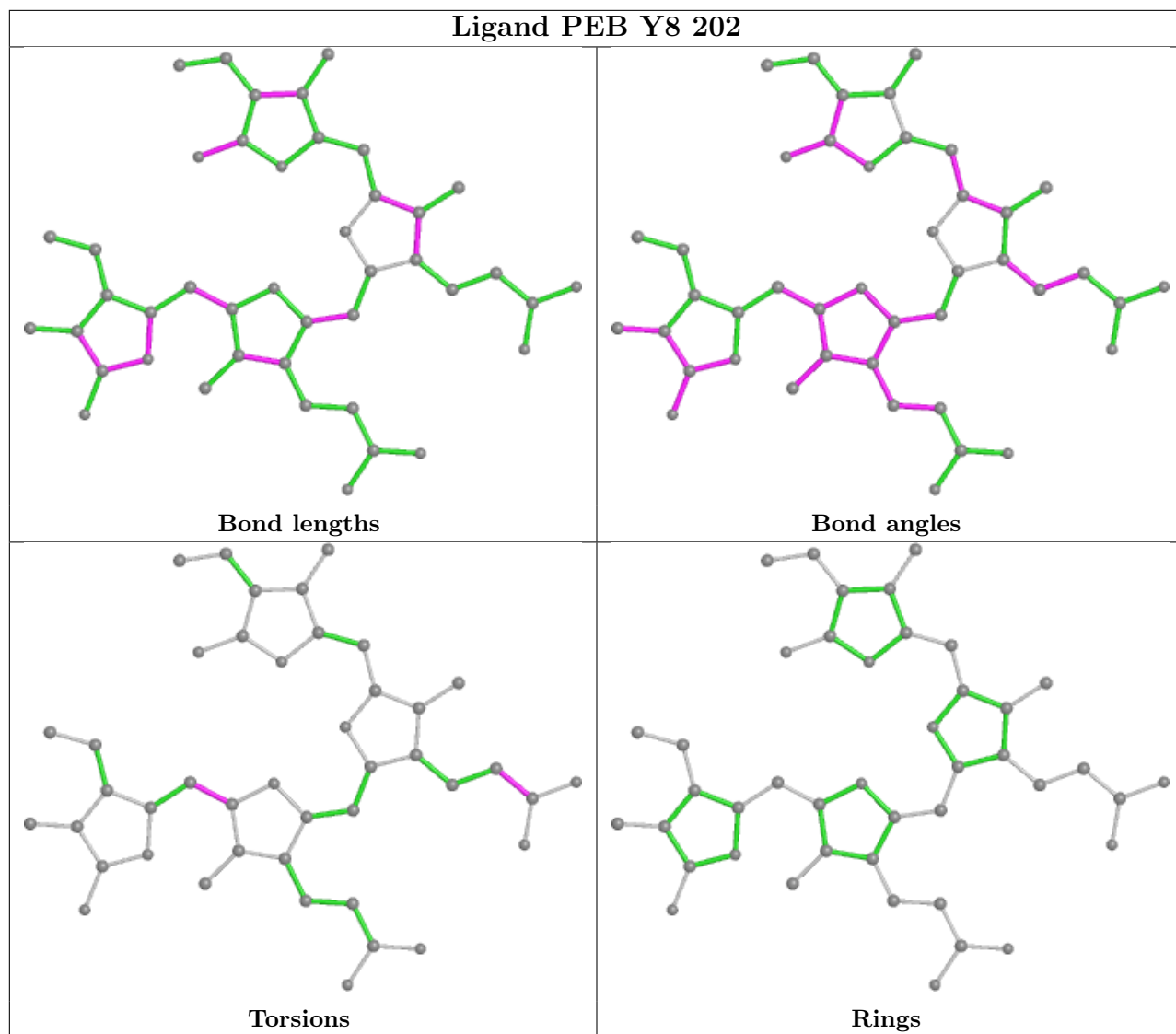


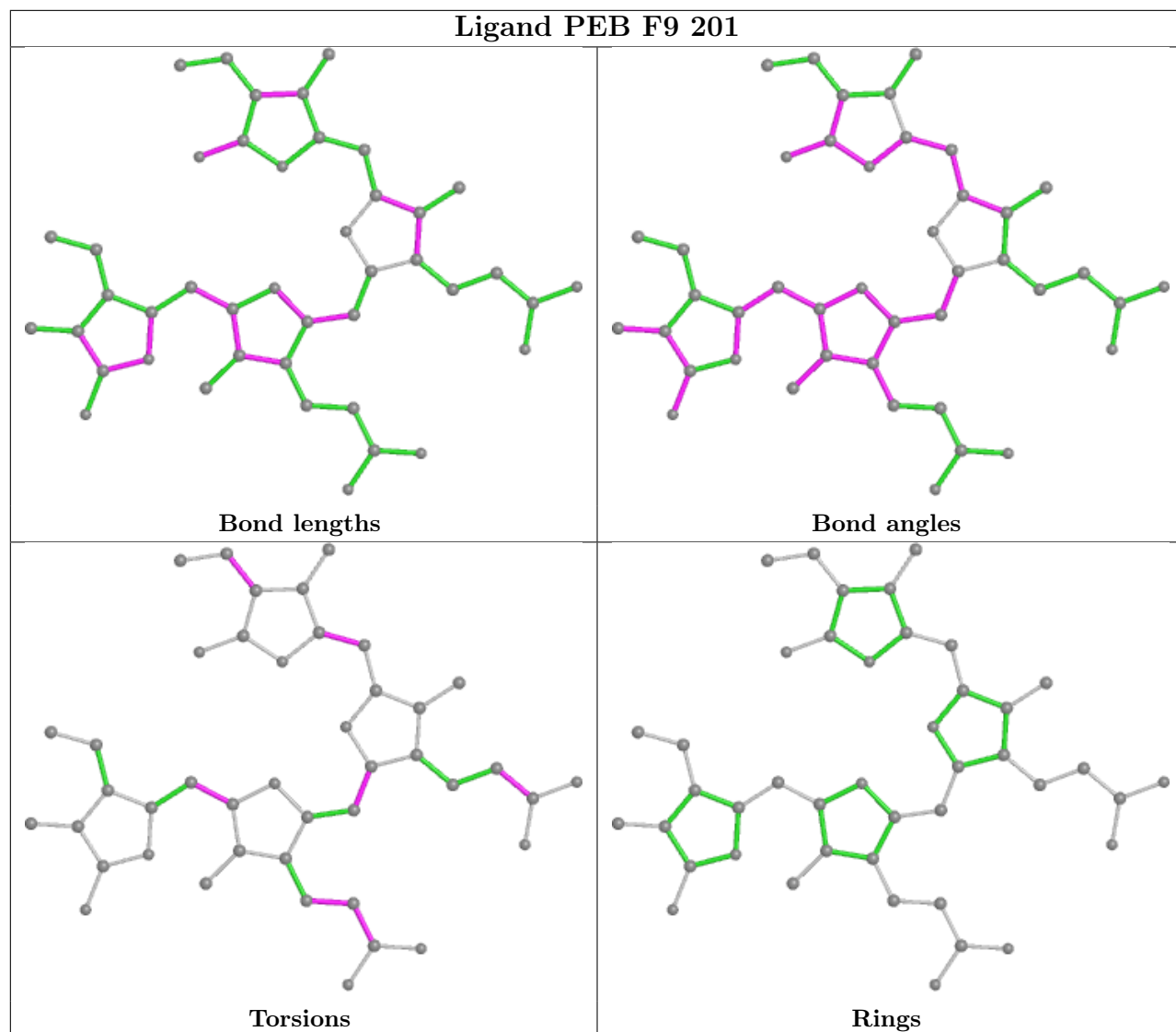


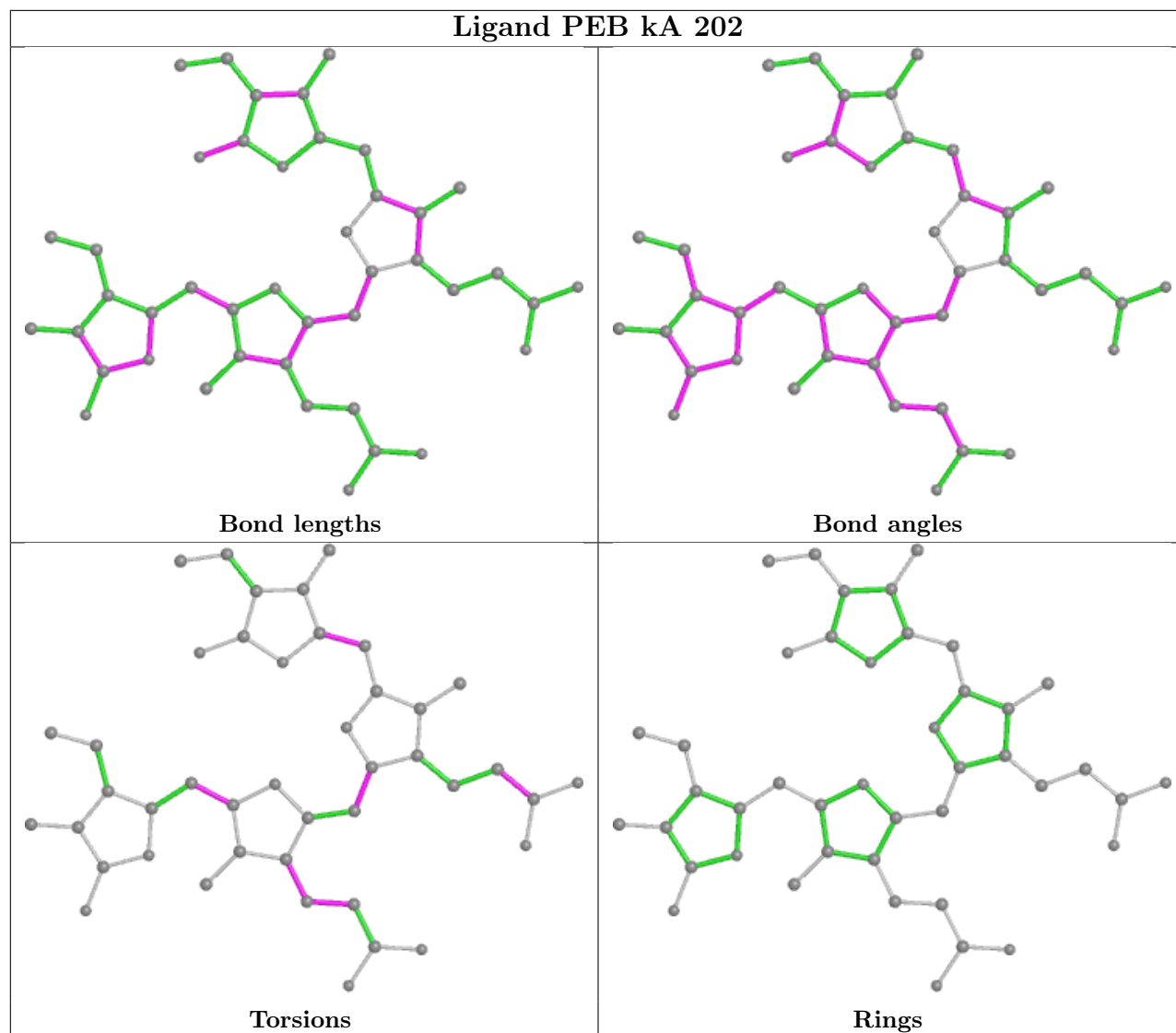


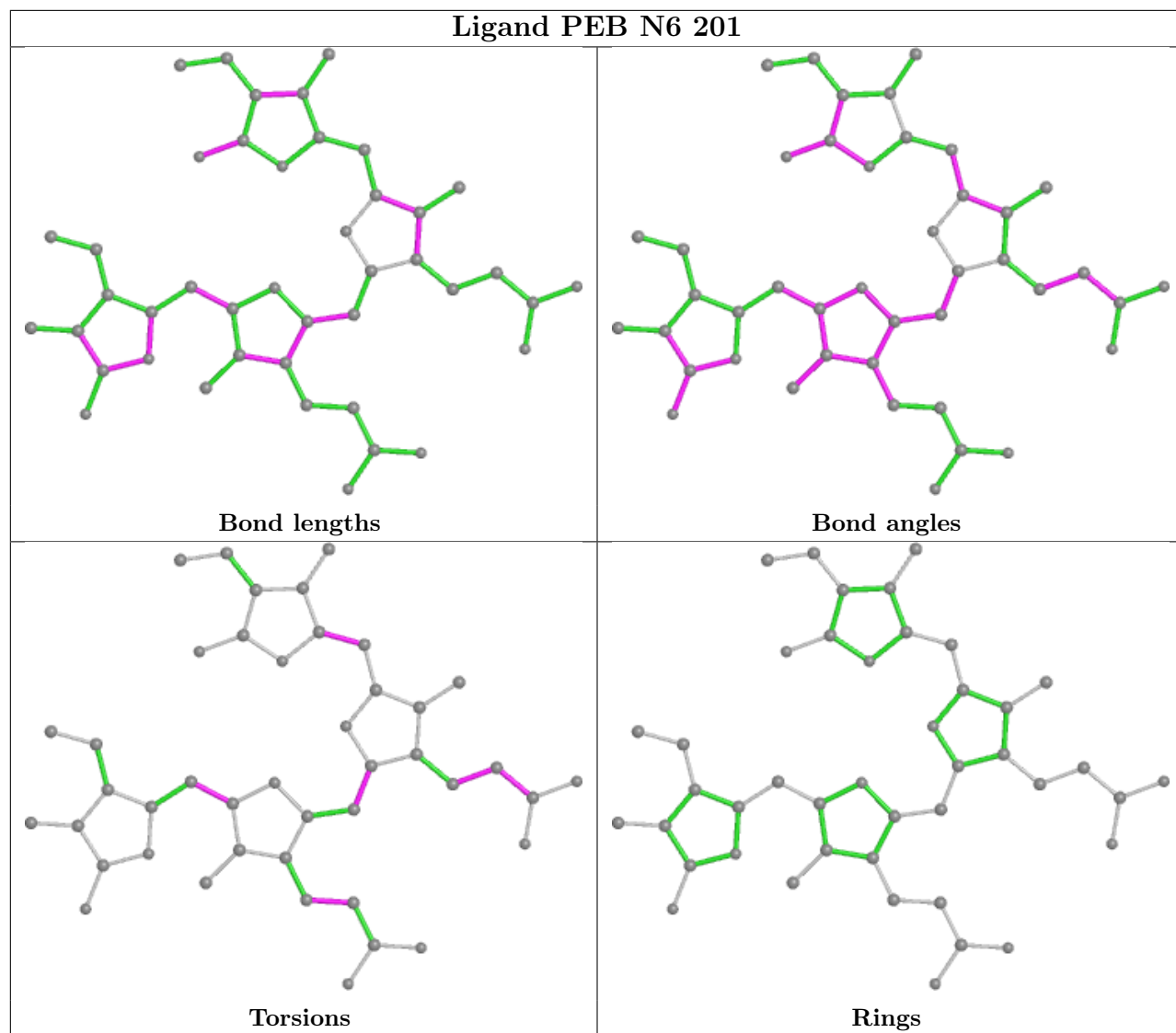


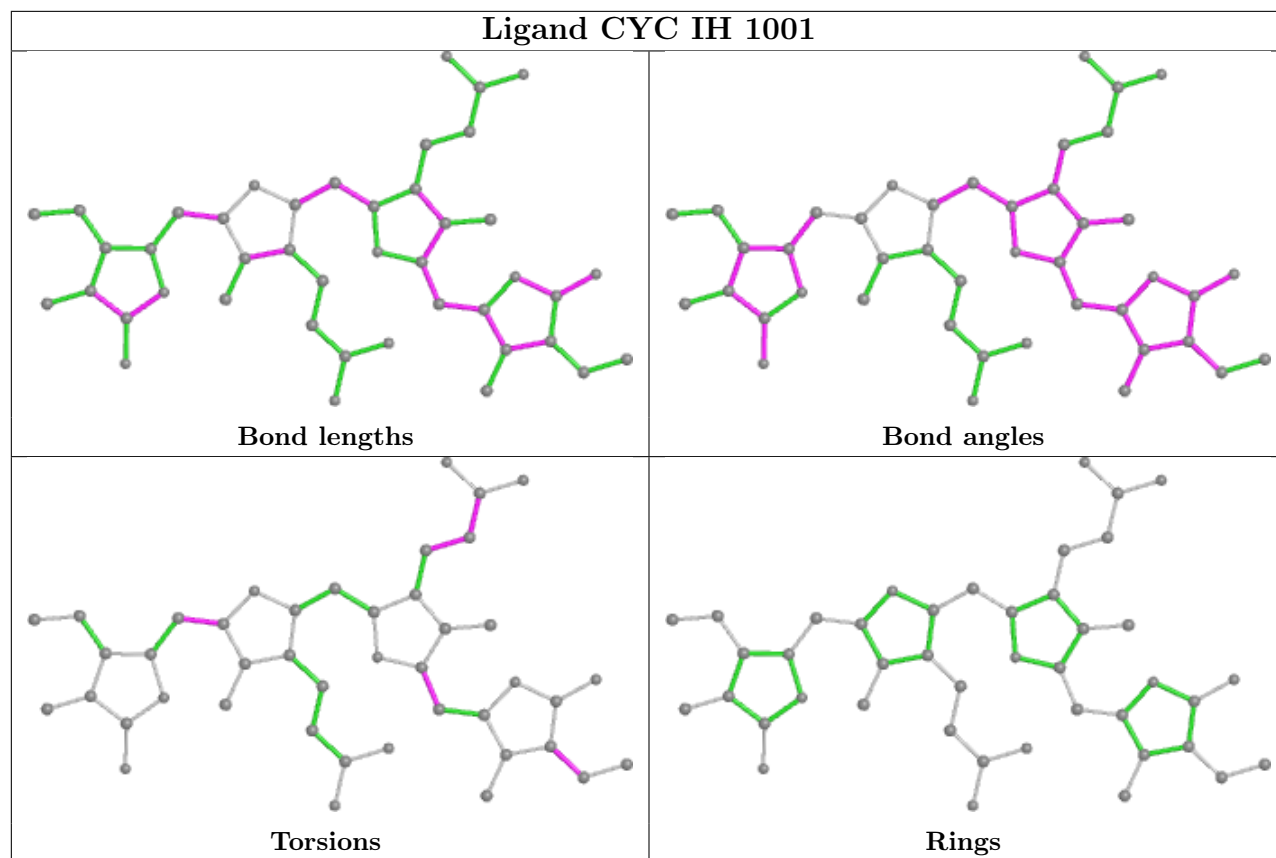


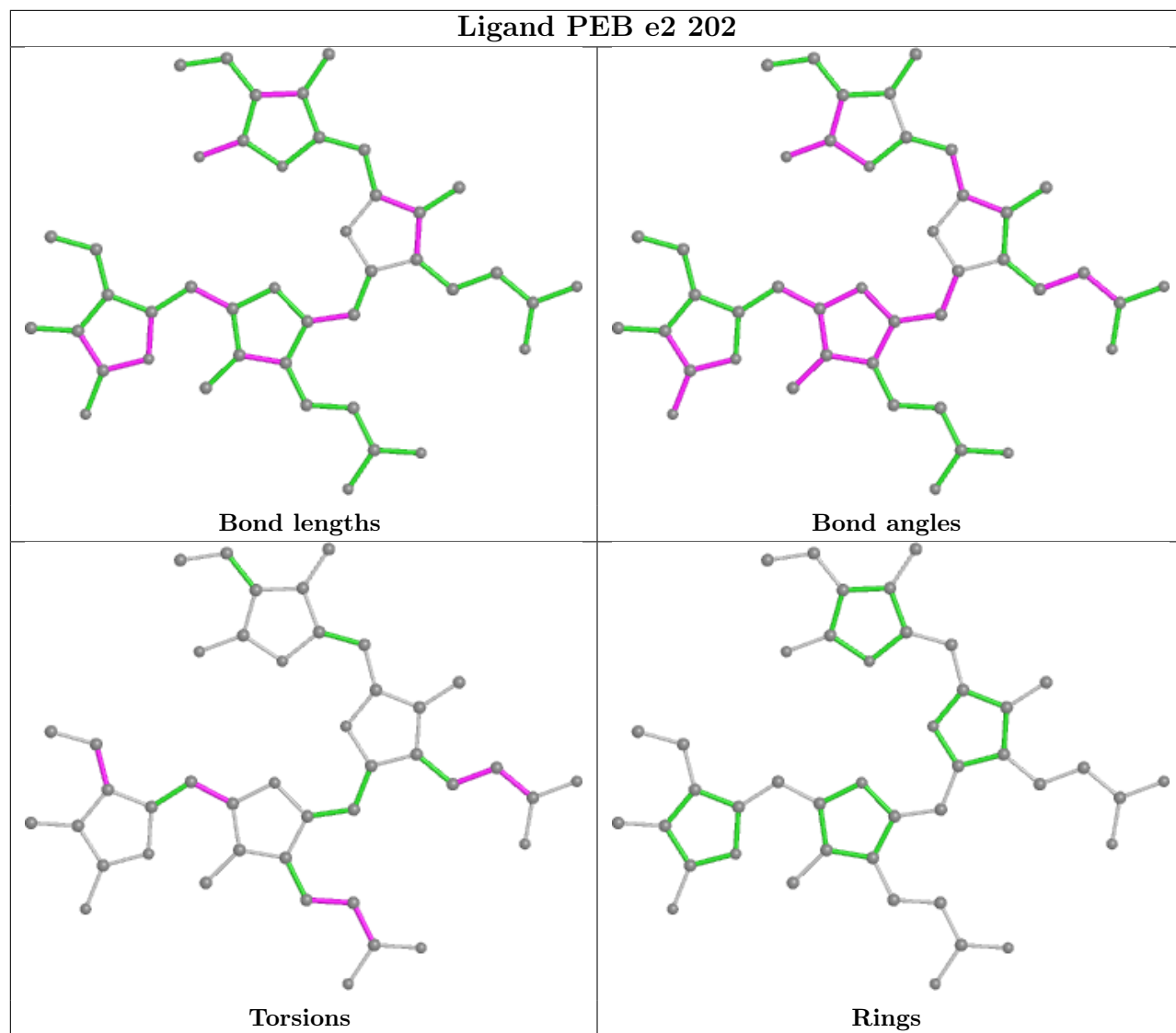


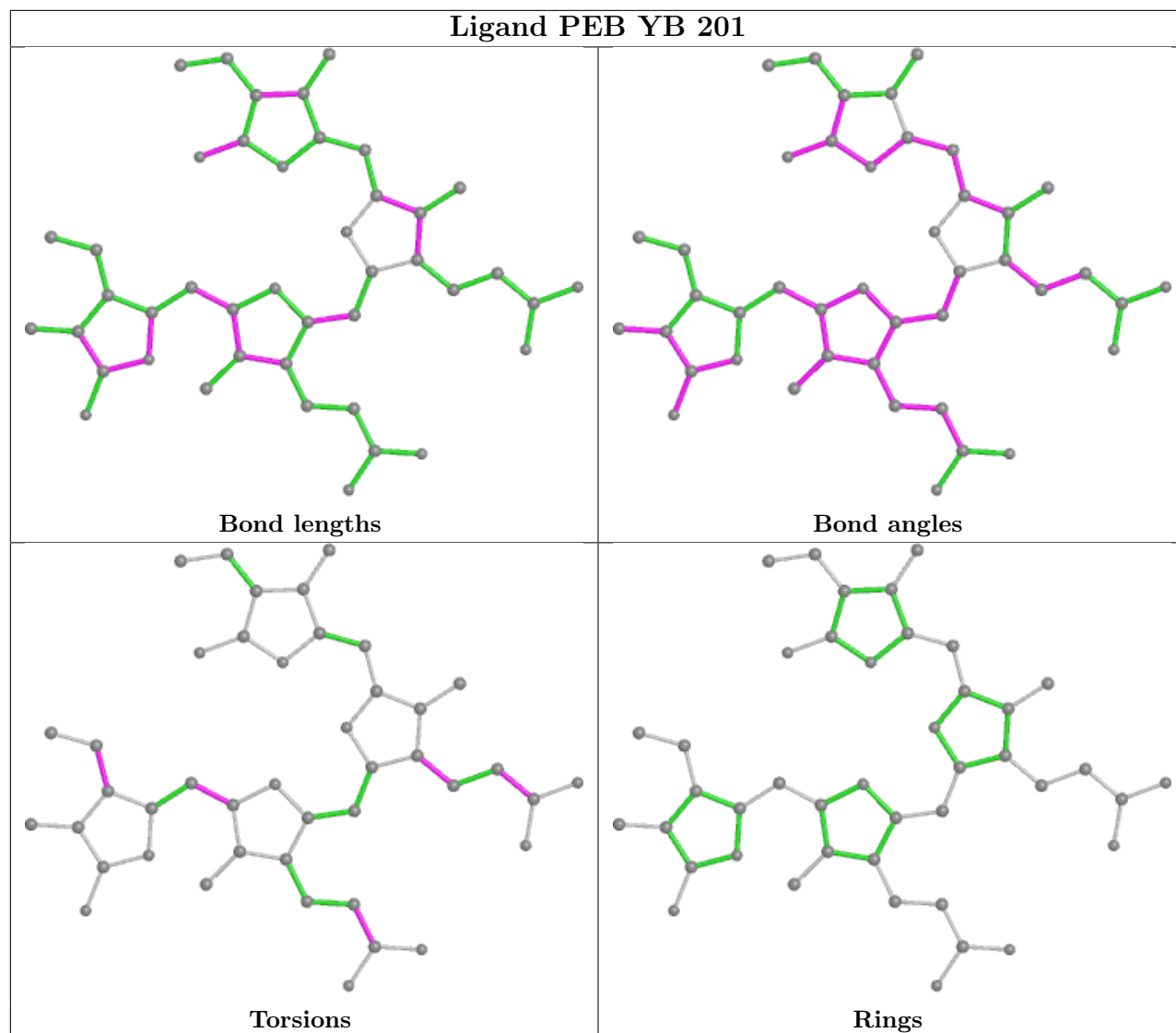


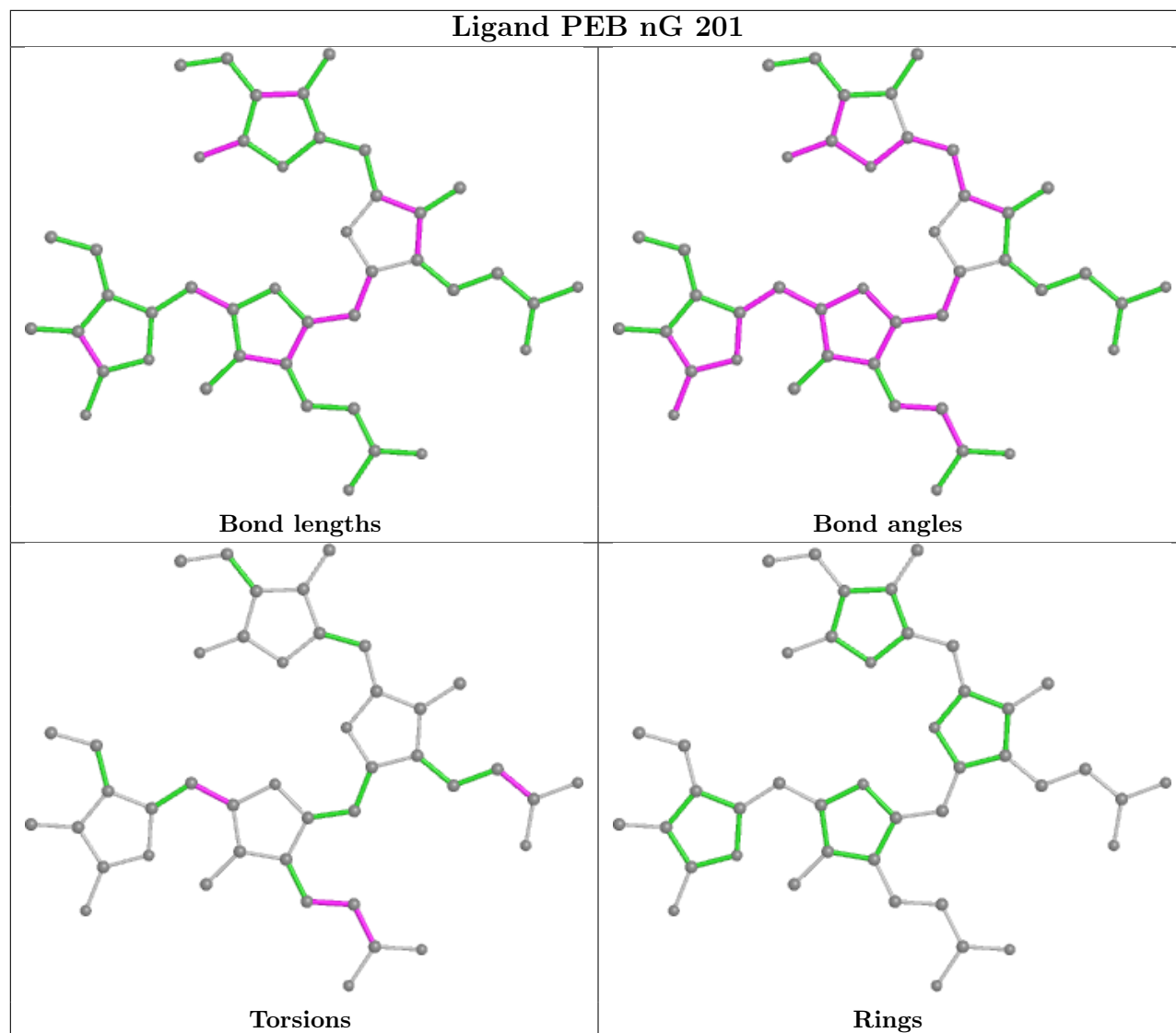


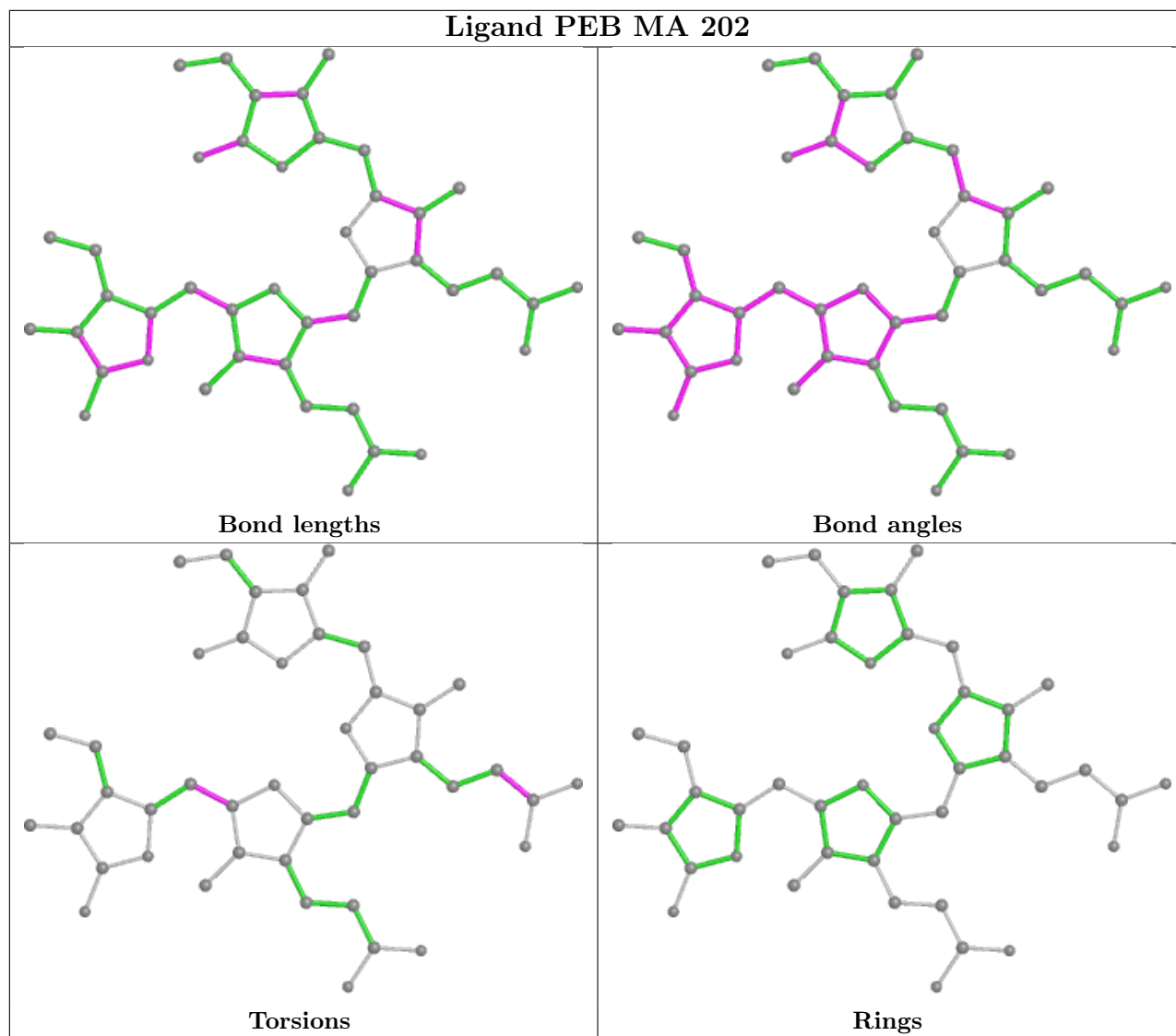


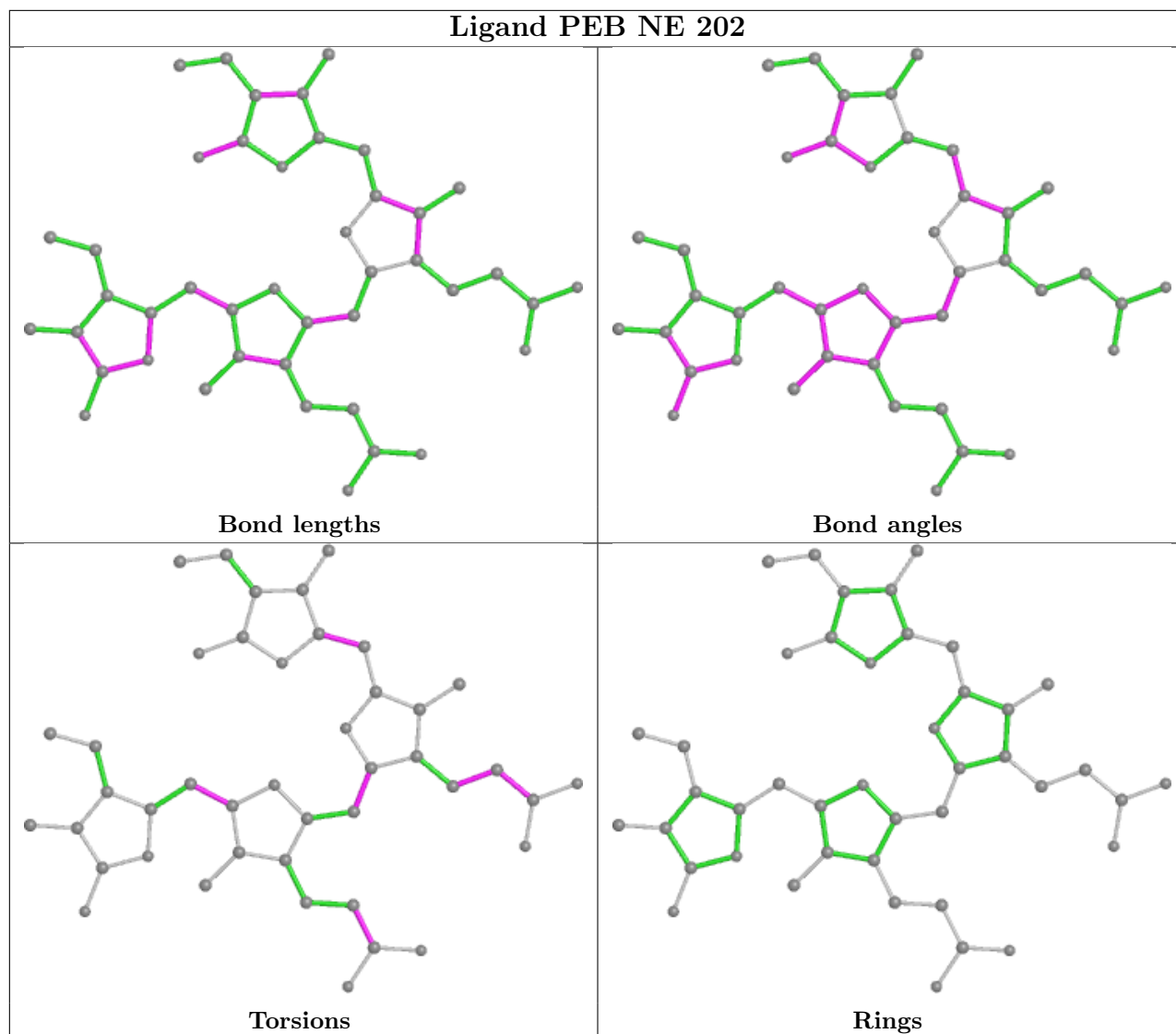


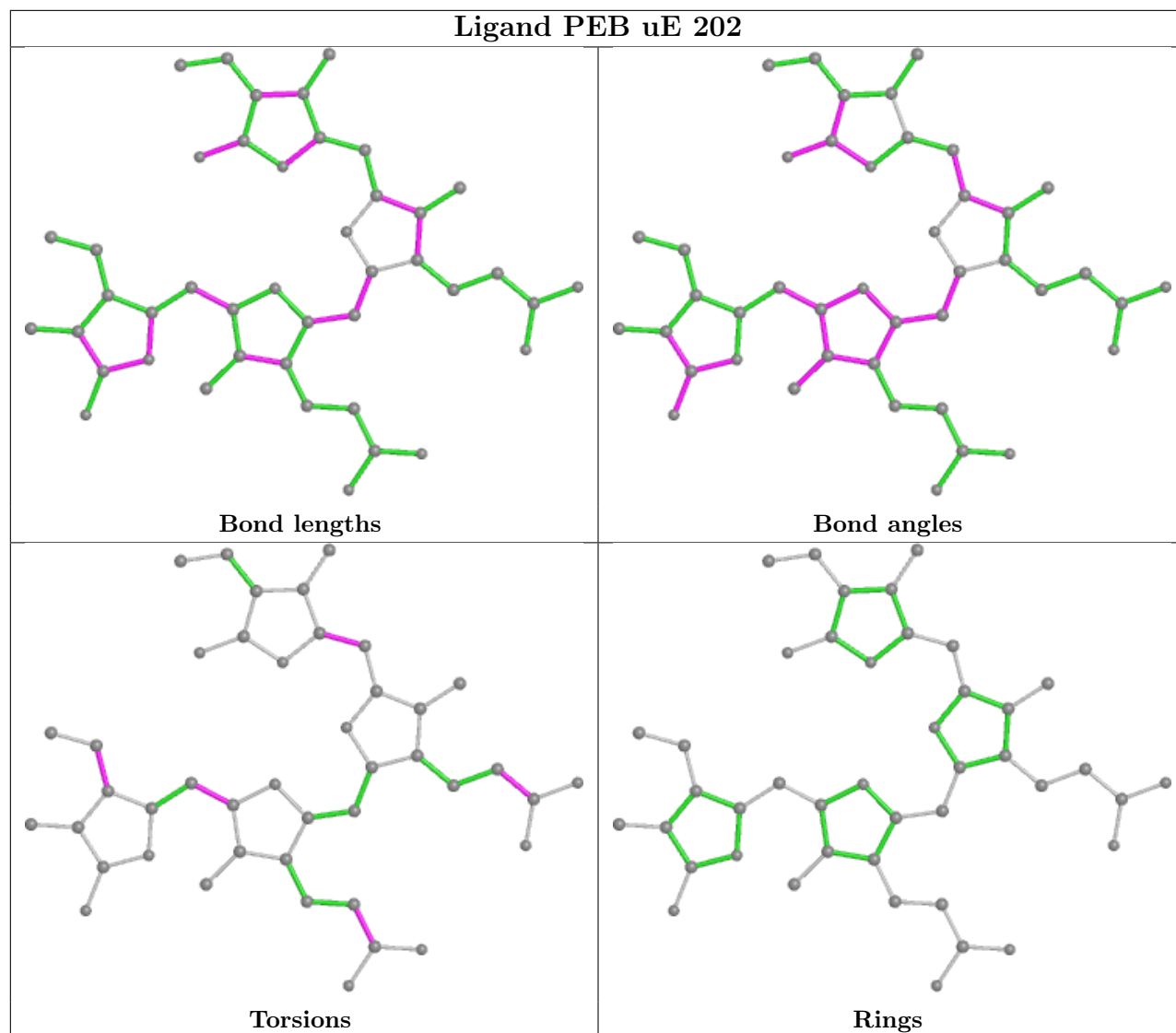


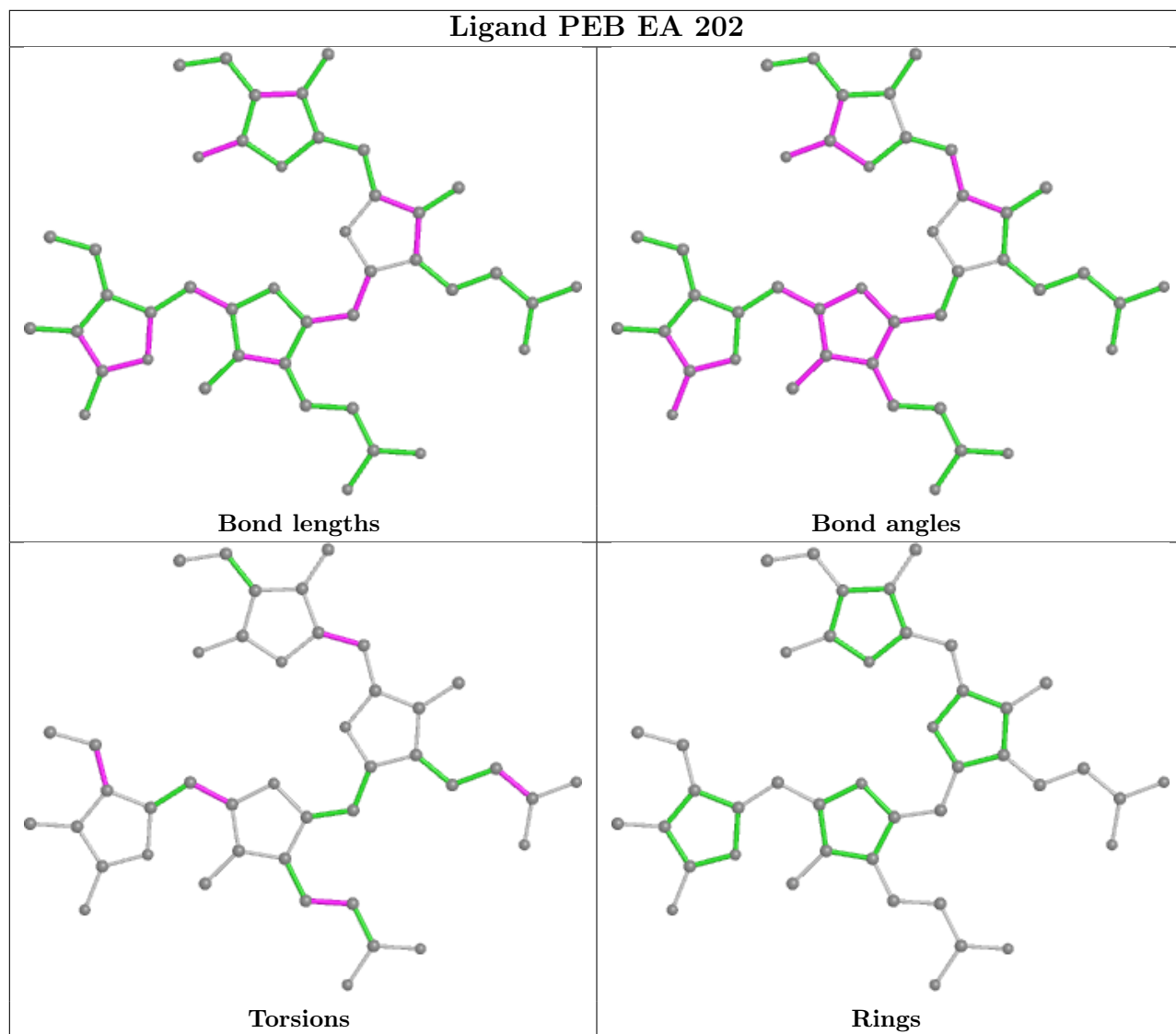


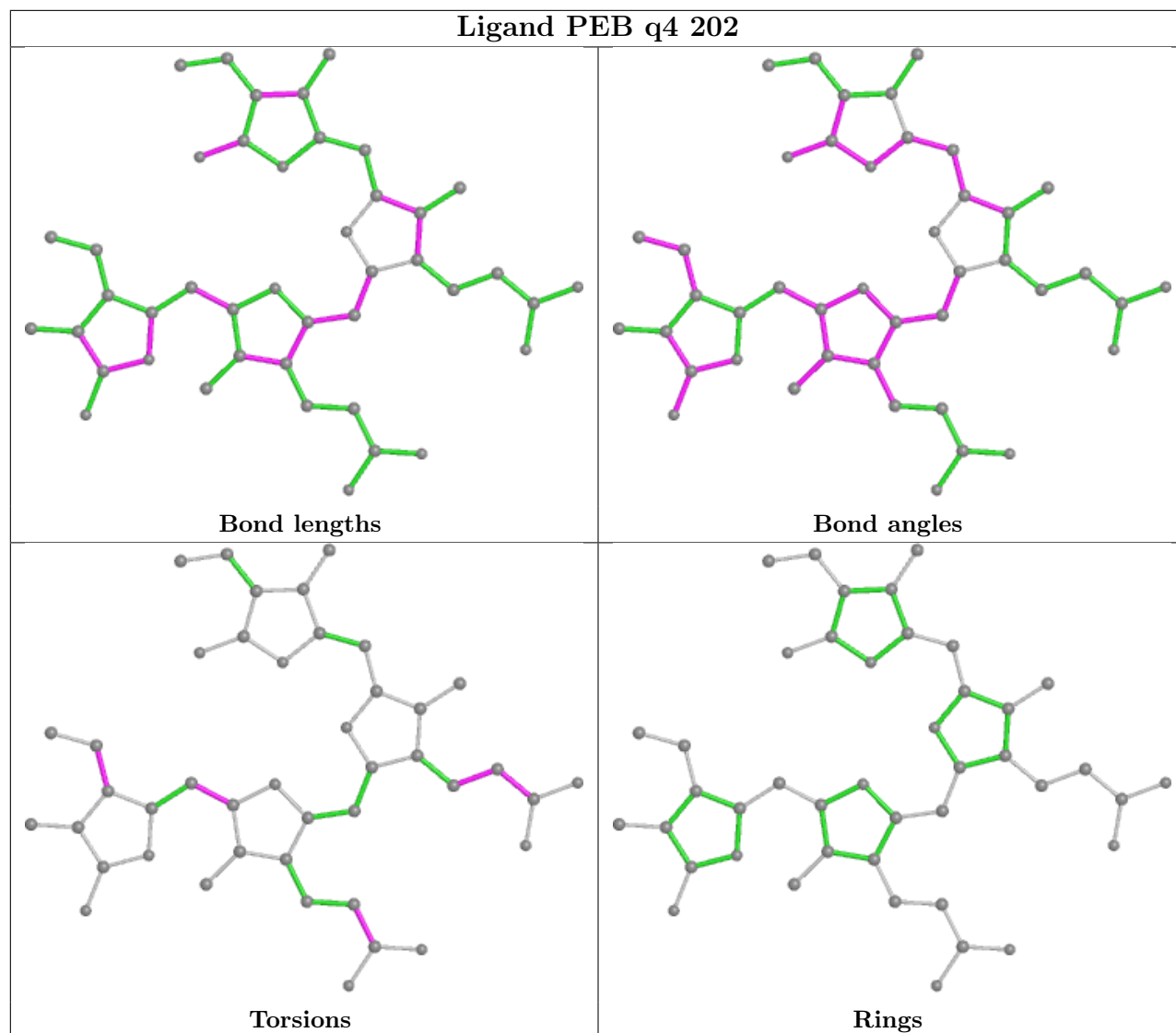


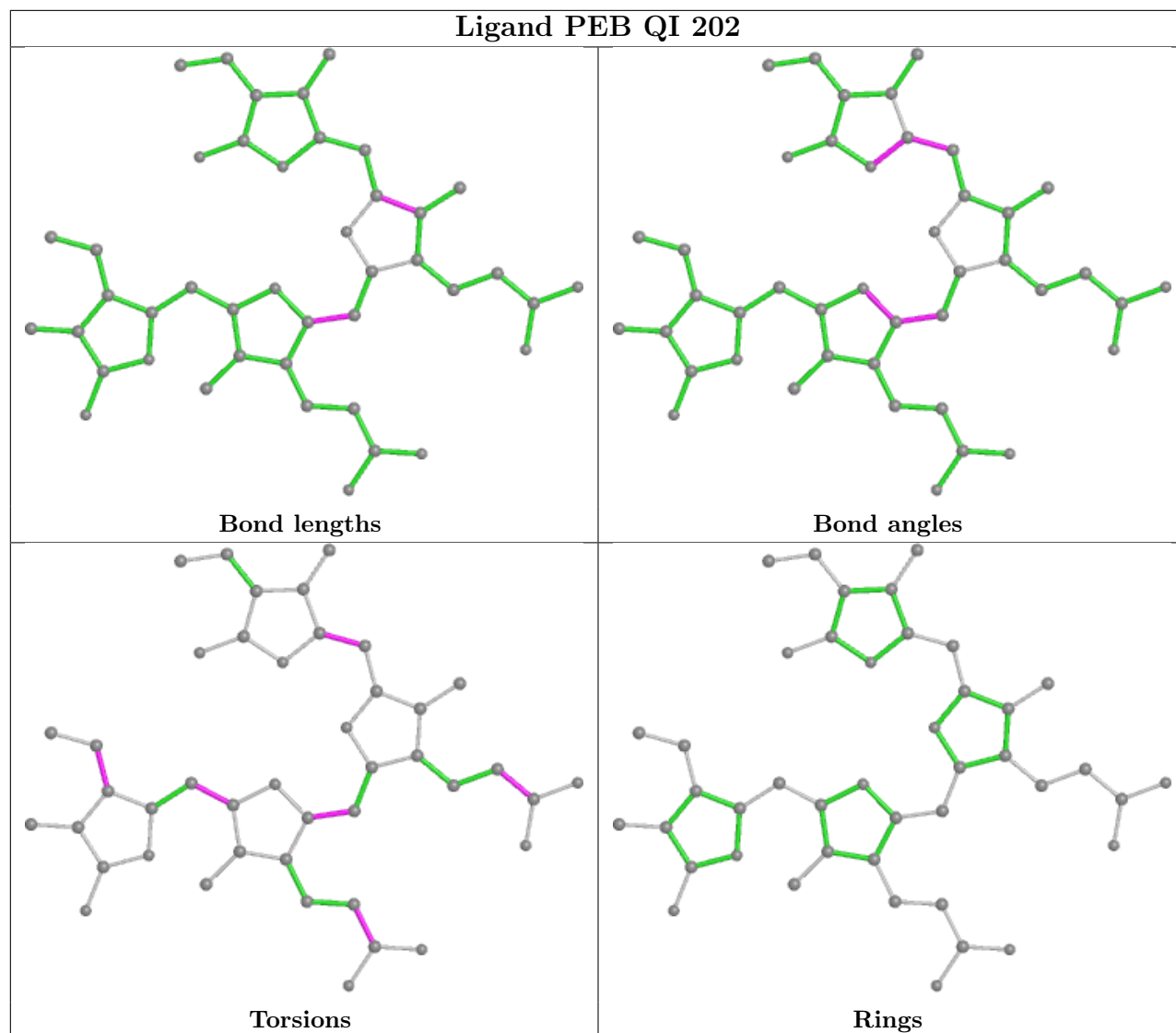


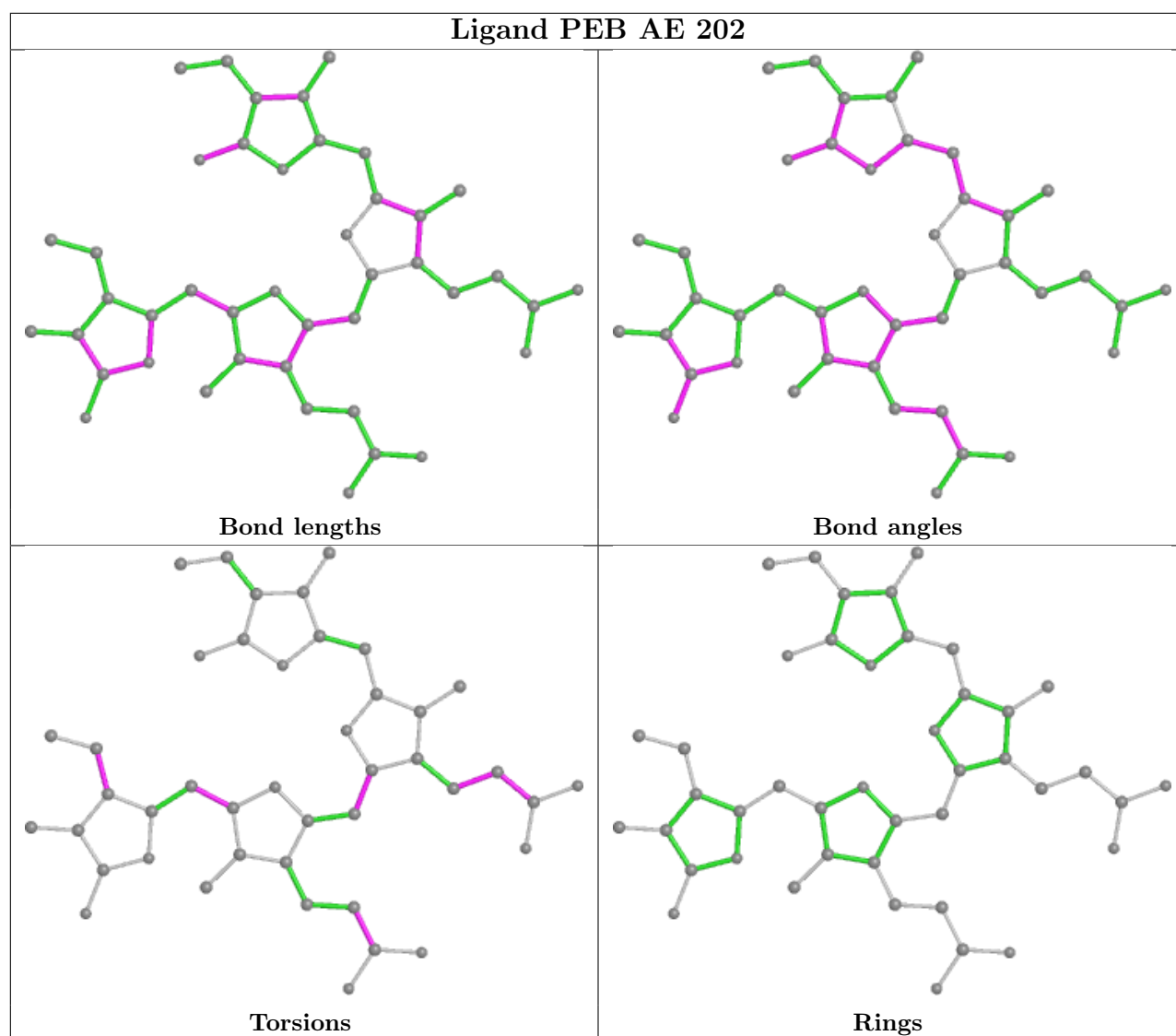












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

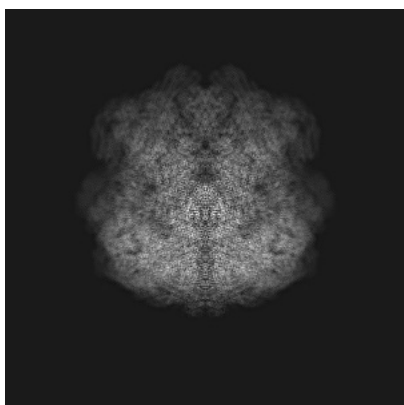
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9976. These allow visual inspection of the internal detail of the map and identification of artifacts.

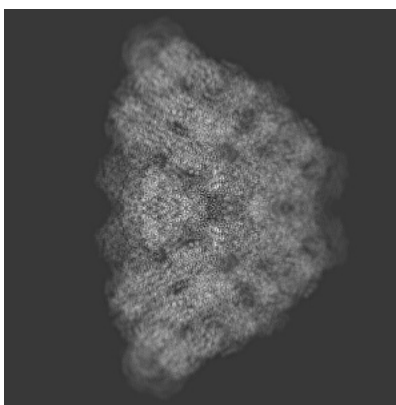
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

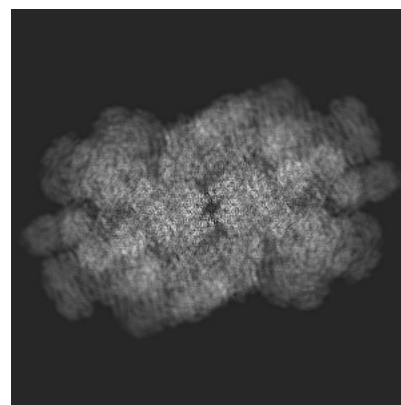
6.1.1 Primary map



X



Y



Z

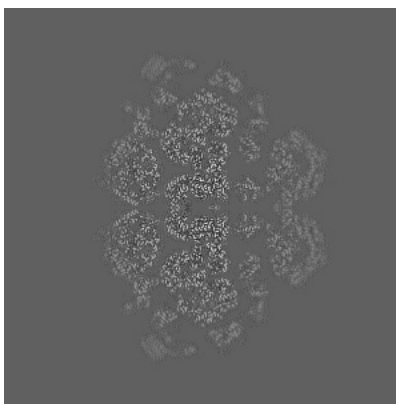
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

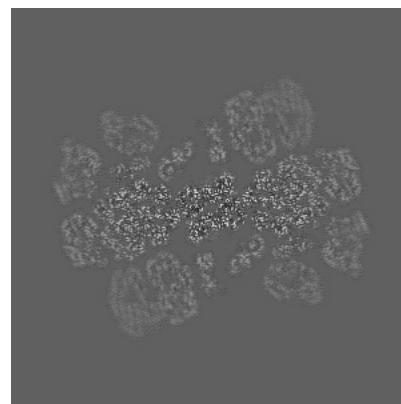
6.2.1 Primary map



X Index: 280



Y Index: 280

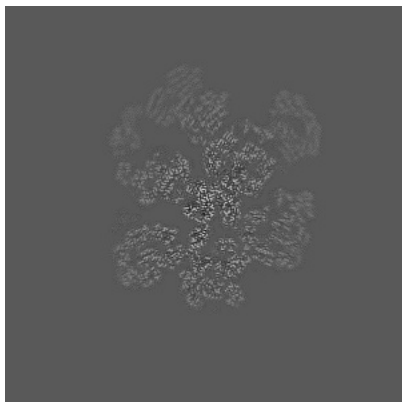


Z Index: 280

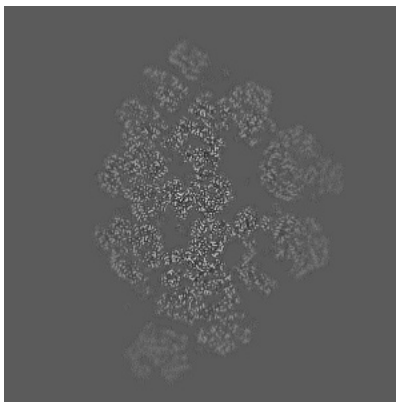
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

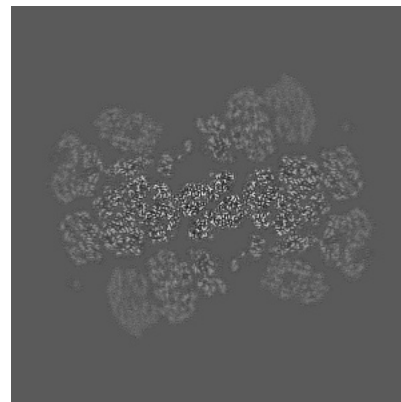
6.3.1 Primary map



X Index: 305



Y Index: 268

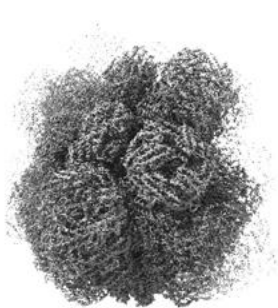


Z Index: 275

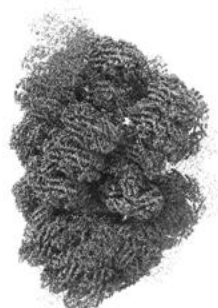
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

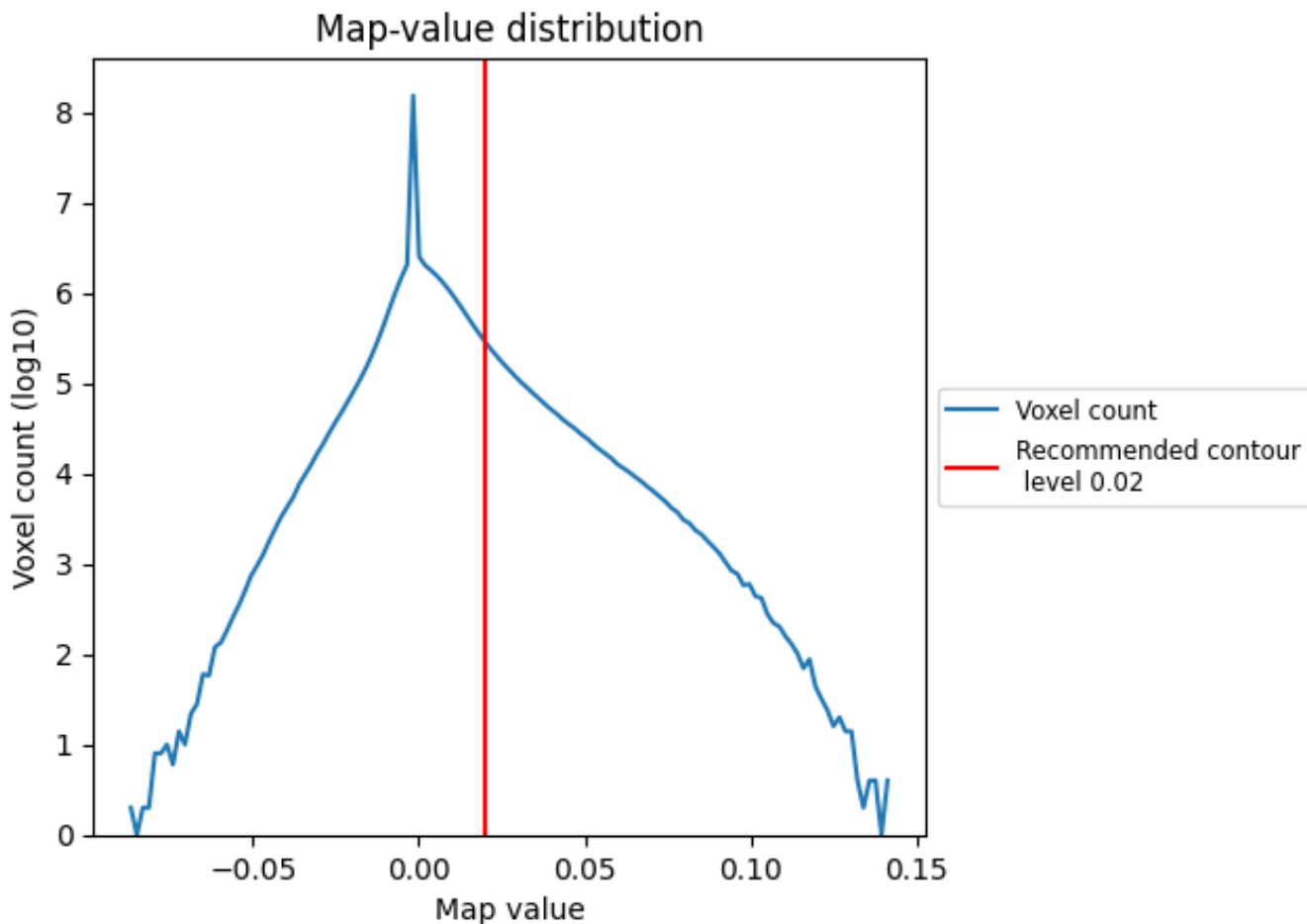
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

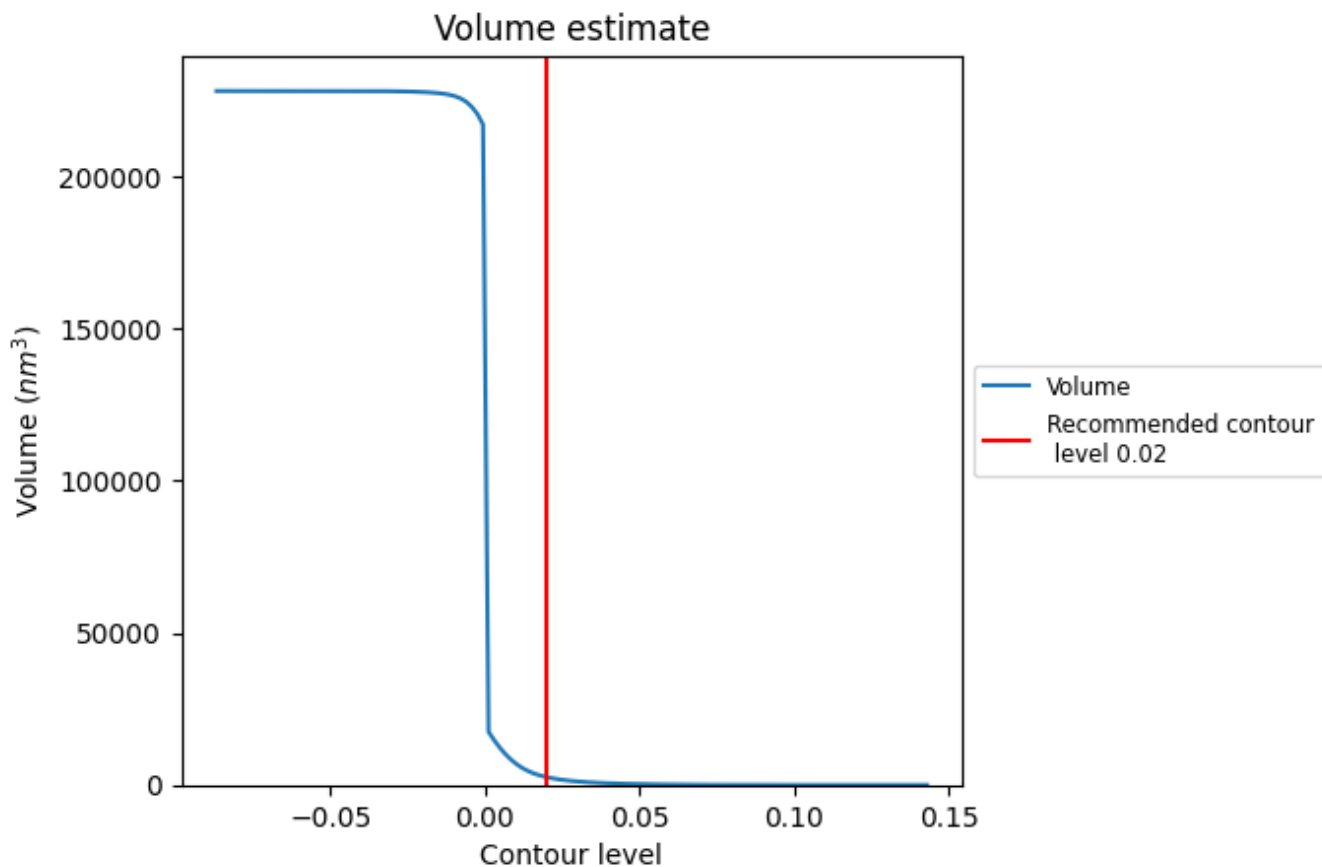
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

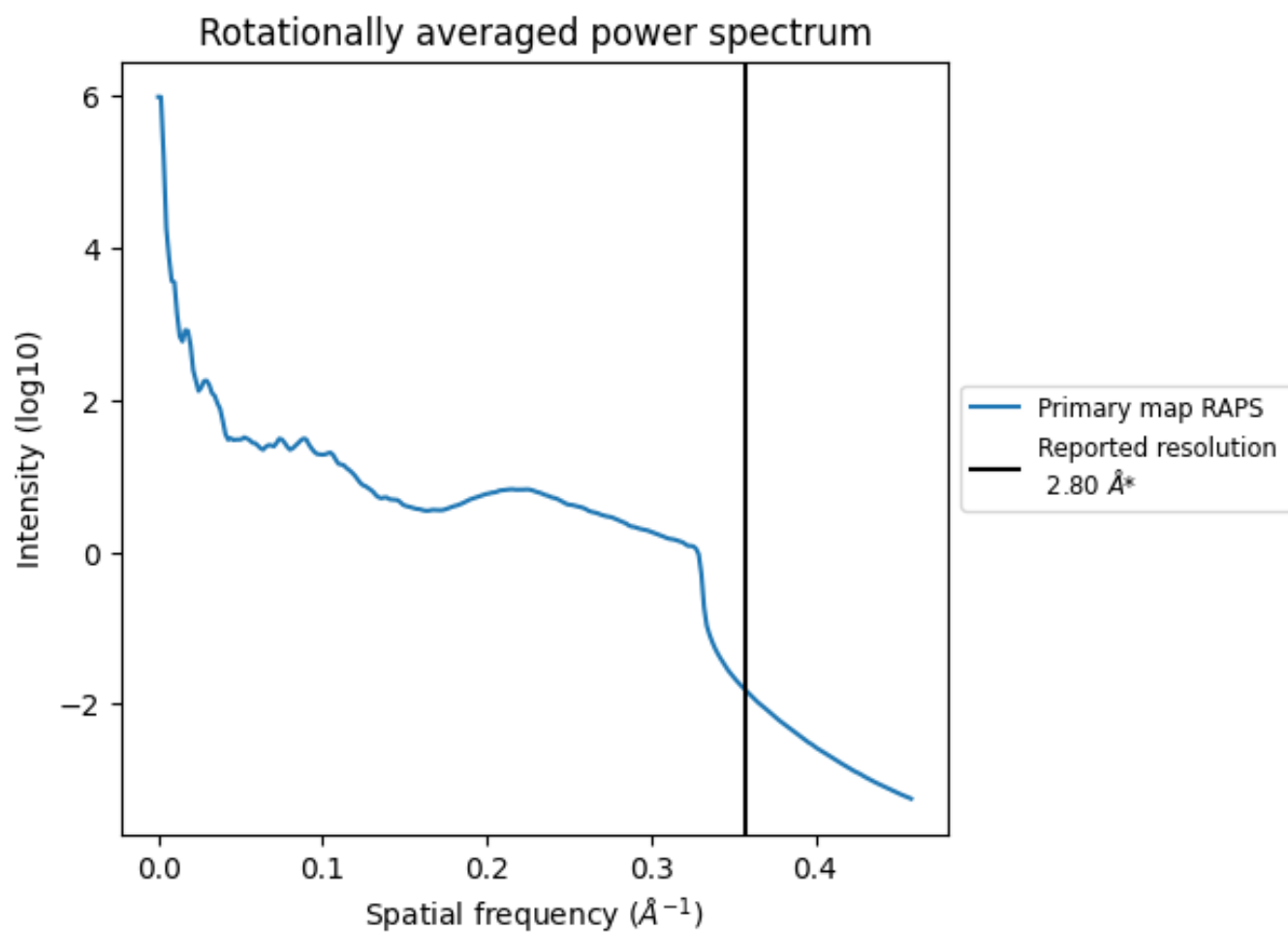
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2573 nm^3 ; this corresponds to an approximate mass of 2324 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

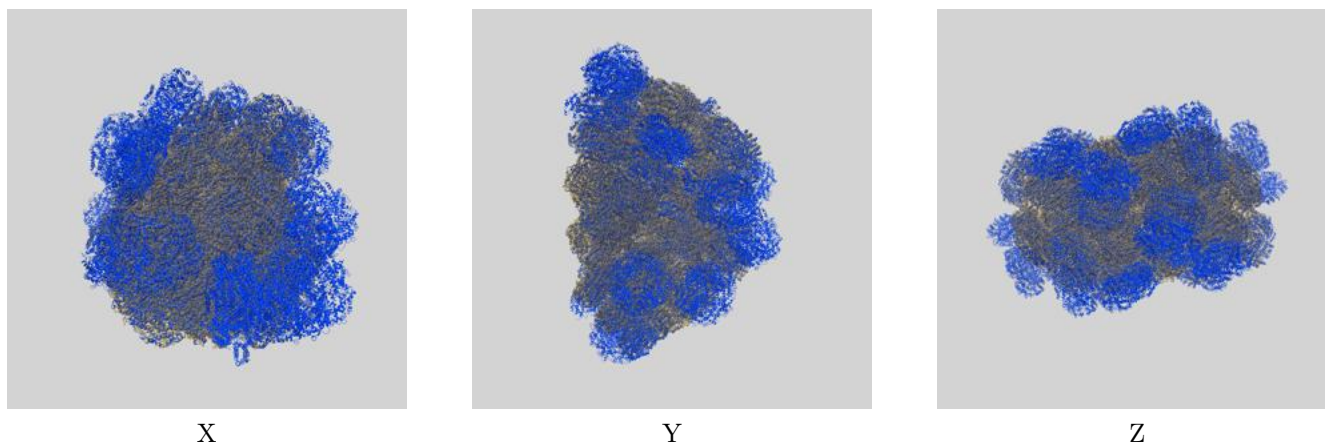
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

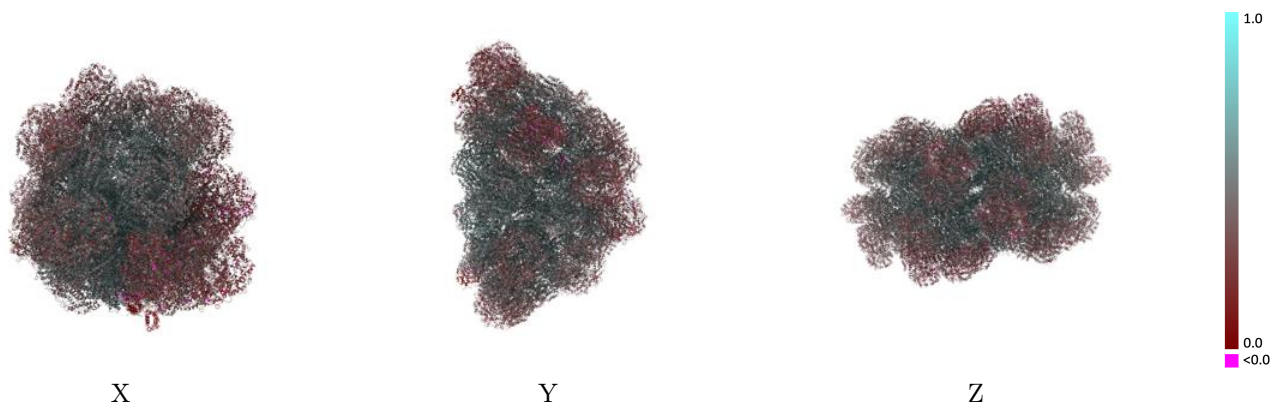
This section contains information regarding the fit between EMDB map EMD-9976 and PDB model 6KGX. Per-residue inclusion information can be found in section [3](#) on page [145](#).

9.1 Map-model overlay [i](#)



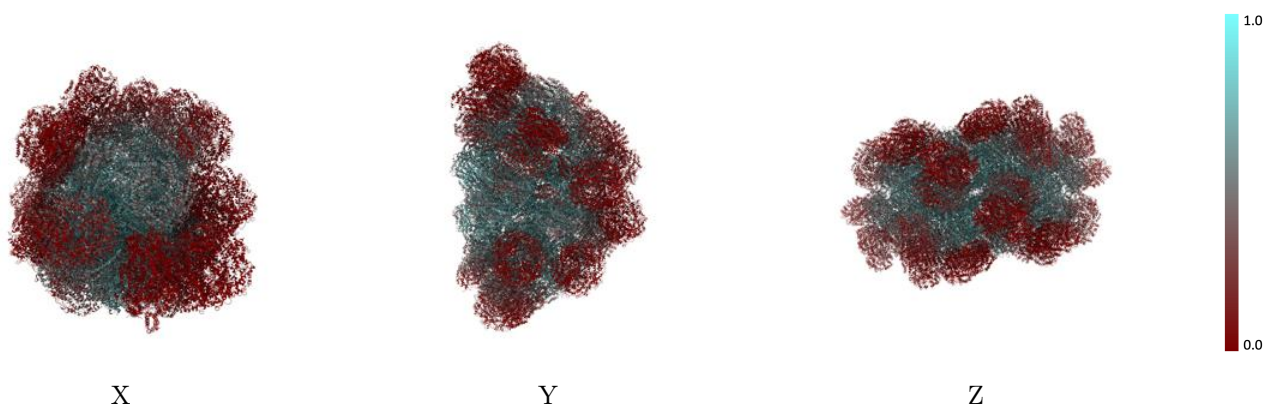
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



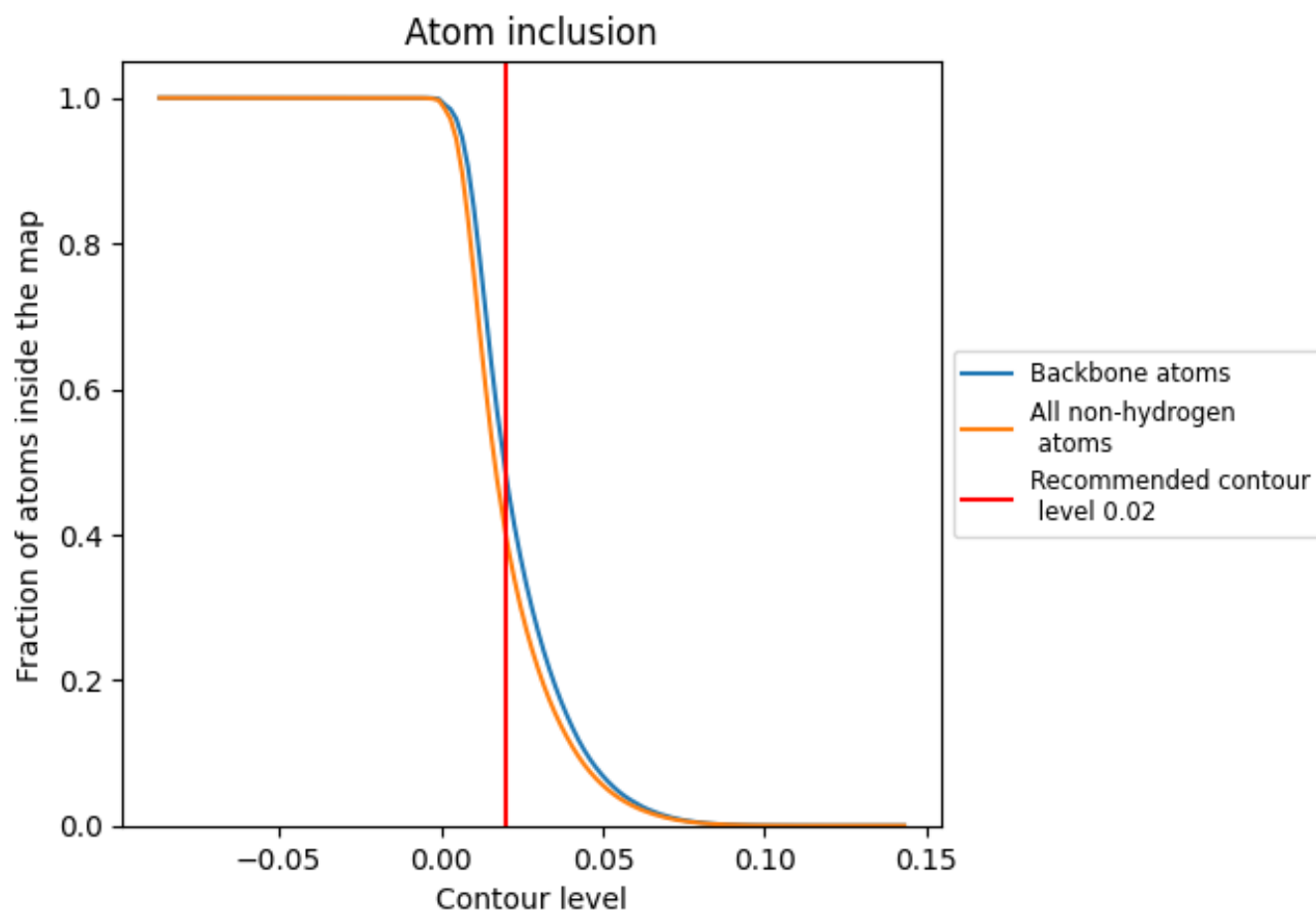
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4018	 0.4550
11	 0.0014	 0.2860
14	 0.0036	 0.2720
1H	 0.7734	 0.5840
21	 0.0100	 0.2690
24	 0.0080	 0.2650
2H	 0.7276	 0.5700
31	 0.7462	 0.5720
34	 0.7457	 0.5740
3H	 0.8233	 0.5980
4H	 0.6788	 0.5760
A1	 0.0299	 0.3560
A2	 0.5533	 0.4990
A3	 0.0077	 0.3530
A4	 0.0261	 0.3500
A5	 0.0000	 -0.0070
A6	 0.2494	 0.4250
A7	 0.0193	 0.3250
A8	 0.1939	 0.4300
A9	 0.0048	 0.3270
AA	 0.1959	 0.4270
AB	 0.2504	 0.4240
AC	 0.0000	 0.0030
AD	 0.0054	 0.3350
AE	 0.4888	 0.4690
AF	 0.0155	 0.3290
AG	 0.4865	 0.4750
AH	 0.6983	 0.5630
AI	 0.5575	 0.5000
AJ	 0.0052	 0.3350
B1	 0.0468	 0.3710
B2	 0.9125	 0.6200
B3	 0.0115	 0.3600
B4	 0.0548	 0.3660
B5	 0.0052	 0.2100























































































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Chain	Atom inclusion	Q-score
B6	 0.8331	 0.5950
B7	 0.5465	 0.5370
B8	 0.4997	 0.5200
B9	 0.2666	 0.4540
BA	 0.4951	 0.5170
BB	 0.8311	 0.5950
BC	 0.0034	 0.1960
BD	 0.0137	 0.3500
BE	 0.4800	 0.4880
BF	 0.5433	 0.5380
BG	 0.4829	 0.4960
BH	 0.7368	 0.5640
BI	 0.9169	 0.6200
BJ	 0.2659	 0.4580
C1	 0.0139	 0.3120
C2	 0.9186	 0.6240
C3	 0.0339	 0.4040
C4	 0.0123	 0.3050
C5	 0.0000	 -0.0000
C6	 0.7317	 0.5820
C7	 0.1716	 0.3940
C8	 0.5400	 0.5220
C9	 0.3516	 0.4790
CA	 0.5385	 0.5200
CB	 0.7301	 0.5780
CC	 0.0000	 -0.0050
CD	 0.0339	 0.3980
CE	 0.4384	 0.4610
CF	 0.1684	 0.3950
CG	 0.4421	 0.4650
CH	 0.6780	 0.5500
CI	 0.9186	 0.6260
CJ	 0.3561	 0.4790
D1	 0.0209	 0.3510
D2	 0.8696	 0.6110
D3	 0.0231	 0.4000
D4	 0.0202	 0.3390
D6	 0.7438	 0.5860
D7	 0.1341	 0.3700
D8	 0.3650	 0.4680
D9	 0.5161	 0.5270
DA	 0.3657	 0.4680





















































































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Chain	Atom inclusion	Q-score
DB	 0.7423	 0.5860
DD	 0.0281	 0.3990
DE	 0.5281	 0.5010
DF	 0.1361	 0.3670
DG	 0.5267	 0.5060
DH	 0.8066	 0.5950
DI	 0.8711	 0.6120
DJ	 0.5116	 0.5300
E1	 0.0277	 0.3380
E2	 0.8928	 0.6220
E3	 0.0177	 0.3850
E4	 0.0293	 0.3340
E6	 0.8187	 0.5950
E7	 0.7260	 0.5840
E8	 0.3256	 0.4390
E9	 0.4533	 0.5120
EA	 0.3286	 0.4430
EB	 0.8203	 0.5930
ED	 0.0146	 0.3780
EE	 0.5774	 0.5100
EF	 0.7228	 0.5860
EG	 0.5720	 0.5120
EH	 0.8654	 0.6100
EI	 0.8936	 0.6230
EJ	 0.4599	 0.5190
F1	 0.1477	 0.4320
F2	 0.8742	 0.6140
F3	 0.0036	 0.3450
F4	 0.1455	 0.4280
F5	 0.4406	 0.5120
F6	 0.7234	 0.5730
F7	 0.4333	 0.4900
F8	 0.5809	 0.5210
F9	 0.4205	 0.4880
FA	 0.5823	 0.5210
FB	 0.7226	 0.5720
FC	 0.4355	 0.5030
FD	 0.0029	 0.3310
FE	 0.7589	 0.5820
FF	 0.4348	 0.4970
FG	 0.7656	 0.5830
FH	 0.8324	 0.6000





















































































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Chain	Atom inclusion	Q-score
FI	 0.8772	 0.6120
FJ	 0.4196	 0.4930
G1	 0.0739	 0.3820
G2	 0.9025	 0.6190
G3	 0.0185	 0.3860
G4	 0.0708	 0.3760
G5	 0.0947	 0.3870
G6	 0.8931	 0.6220
G7	 0.2853	 0.4260
G8	 0.2704	 0.4300
G9	 0.1869	 0.4080
GA	 0.2681	 0.4270
GB	 0.8907	 0.6220
GC	 0.0921	 0.3790
GD	 0.0169	 0.3810
GE	 0.7976	 0.5880
GF	 0.2889	 0.4240
GG	 0.8051	 0.5930
GH	 0.8337	 0.6010
GI	 0.9033	 0.6200
GJ	 0.1847	 0.4090
H1	 0.0317	 0.3460
H2	 0.8659	 0.6110
H3	 0.0605	 0.4420
H4	 0.0281	 0.3290
H5	 0.6119	 0.5690
H6	 0.8199	 0.6000
H7	 0.4906	 0.4960
H8	 0.4228	 0.4900
H9	 0.2524	 0.4240
HA	 0.4295	 0.4930
HB	 0.8199	 0.6020
HC	 0.6033	 0.5640
HD	 0.0634	 0.4360
HE	 0.6669	 0.5420
HF	 0.4928	 0.4950
HG	 0.6677	 0.5470
HH	 0.7124	 0.5640
HI	 0.8644	 0.6100
HJ	 0.2524	 0.4270
I1	 0.1432	 0.4330
I2	 0.8920	 0.6250

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Chain	Atom inclusion	Q-score
I3	 0.0069	 0.3510
I4	 0.1393	 0.4270
I5	 0.5591	 0.5540
I6	 0.8977	 0.6180
I7	 0.6970	 0.5660
I8	 0.4981	 0.5210
I9	 0.5593	 0.5340
IA	 0.4974	 0.5200
IB	 0.8993	 0.6180
IC	 0.5529	 0.5520
ID	 0.0023	 0.3410
IE	 0.7931	 0.5900
IF	 0.6946	 0.5660
IG	 0.7909	 0.5910
IH	 0.8535	 0.6050
II	 0.8912	 0.6210
IJ	 0.5605	 0.5400
J1	 0.1037	 0.4350
J2	 0.8998	 0.6190
J3	 0.0029	 0.3520
J4	 0.1059	 0.4310
J5	 0.8068	 0.5960
J6	 0.9118	 0.6290
J7	 0.4587	 0.4790
J8	 0.3865	 0.4770
J9	 0.1001	 0.3530
JA	 0.3828	 0.4770
JB	 0.9086	 0.6290
JC	 0.7914	 0.5940
JD	 0.0022	 0.3330
JE	 0.7025	 0.5590
JF	 0.4565	 0.4790
JG	 0.7033	 0.5610
JH	 0.8005	 0.5900
JI	 0.8990	 0.6190
JJ	 0.0934	 0.3540
K1	 0.0702	 0.3770
K2	 0.9291	 0.6330
K3	 0.0052	 0.3480
K4	 0.0702	 0.3740
K5	 0.6707	 0.5730
K6	 0.7721	 0.5890

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Chain	Atom inclusion	Q-score
K7	0.4488	0.4920
K8	0.6632	0.5630
K9	0.1417	0.3900
KA	0.6624	0.5650
KB	0.7705	0.5860
KC	0.6693	0.5700
KD	0.0067	0.3360
KE	0.6535	0.5370
KF	0.4553	0.4950
KG	0.6587	0.5450
KH	0.6626	0.5520
KI	0.9251	0.6340
KJ	0.1432	0.3920
L1	0.0807	0.3890
L2	0.9013	0.6230
L3	0.0259	0.3890
L4	0.0836	0.3830
L5	0.6411	0.5550
L6	0.8320	0.6030
L7	0.6895	0.5710
L8	0.6625	0.5690
L9	0.1822	0.4090
LA	0.6617	0.5690
LB	0.8320	0.6040
LC	0.6429	0.5540
LD	0.0238	0.3800
LE	0.7975	0.5900
LF	0.6895	0.5750
LG	0.7990	0.5940
LH	0.7893	0.5900
LI	0.9035	0.6240
LJ	0.1792	0.4150
M1	0.1031	0.4080
M2	0.9041	0.6210
M3	0.4488	0.4610
M4	0.1099	0.3970
M6	0.8582	0.6130
M7	0.1749	0.3870
M8	0.7438	0.5870
M9	0.2136	0.4280
MA	0.7476	0.5870
MB	0.8630	0.6140





















































































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Chain	Atom inclusion	Q-score
MD	0.4450	0.4580
ME	0.3391	0.4370
MF	0.1707	0.3900
MG	0.3413	0.4420
MH	0.7705	0.5780
MI	0.9049	0.6220
MJ	0.2159	0.4310
N1	0.7715	0.5920
N2	0.9073	0.6230
N3	0.5843	0.5170
N4	0.7737	0.5910
N6	0.8104	0.5990
N7	0.2743	0.4180
N8	0.7322	0.5870
N9	0.0000	0.3080
NA	0.7315	0.5840
NB	0.8124	0.6000
ND	0.5836	0.5160
NE	0.3947	0.4530
NF	0.2645	0.4260
NG	0.3976	0.4560
NH	0.8475	0.6120
NI	0.9088	0.6230
NJ	0.0015	0.3160
O1	0.6387	0.5470
O2	0.7290	0.5560
O3	0.7067	0.5600
O4	0.6358	0.5450
O6	0.6714	0.5490
O7	0.1105	0.3840
O8	0.4571	0.4750
O9	0.0015	0.2870
OA	0.4571	0.4730
OB	0.6774	0.5500
OD	0.6975	0.5580
OE	0.4683	0.4630
OF	0.1083	0.3880
OG	0.4683	0.4690
OH	0.6509	0.5480
OI	0.7267	0.5560
OJ	0.0015	0.2900
P1	0.5302	0.5080

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Chain	Atom inclusion	Q-score
P2	 0.7003	 0.5560
P3	 0.6045	 0.5290
P4	 0.5310	 0.5030
P6	 0.6424	 0.5560
P7	 0.3464	 0.4770
P8	 0.3375	 0.4490
P9	 0.0119	 0.3540
PA	 0.3316	 0.4430
PB	 0.6461	 0.5580
PD	 0.5980	 0.5290
PE	 0.4711	 0.4800
PF	 0.3464	 0.4810
PG	 0.4748	 0.4830
PH	 0.8921	 0.6120
PI	 0.7017	 0.5540
PJ	 0.0075	 0.3540
Q1	 0.7122	 0.5760
Q2	 0.7490	 0.5650
Q3	 0.6975	 0.5700
Q4	 0.7122	 0.5720
Q6	 0.4959	 0.4850
Q7	 0.2181	 0.4250
Q8	 0.3452	 0.4410
Q9	 0.0163	 0.3480
QA	 0.3474	 0.4430
QB	 0.4974	 0.4890
QD	 0.6913	 0.5660
QE	 0.5474	 0.4880
QF	 0.2143	 0.4280
QG	 0.5467	 0.4940
QH	 0.9146	 0.6160
QI	 0.7560	 0.5660
QJ	 0.0141	 0.3580
R1	 0.4406	 0.4590
R2	 0.8213	 0.5910
R3	 0.6427	 0.5430
R4	 0.4406	 0.4620
R6	 0.5586	 0.5100
R7	 0.0660	 0.3560
R8	 0.4985	 0.4980
R9	 0.0030	 0.3030
RA	 0.4948	 0.4950

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Chain	Atom inclusion	Q-score
RB	0.5564	0.5100
RD	0.6398	0.5380
RE	0.6157	0.5390
RF	0.0690	0.3620
RG	0.6202	0.5400
RH	0.9051	0.6150
RI	0.8249	0.5920
RJ	0.0037	0.3070
S1	0.5312	0.5140
S2	0.7475	0.5600
S3	0.7206	0.5730
S4	0.5319	0.5130
S6	0.5235	0.4950
S7	0.1710	0.4110
S8	0.3323	0.4370
S9	0.0007	0.2820
SA	0.3331	0.4350
SB	0.5250	0.4950
SD	0.7182	0.5690
SE	0.7184	0.5650
SF	0.1694	0.4110
SG	0.7282	0.5740
SH	0.9195	0.6240
SI	0.7444	0.5580
SJ	0.0015	0.2800
T1	0.4518	0.4680
T2	0.7320	0.5670
T3	0.7889	0.6000
T4	0.4548	0.4700
T6	0.6907	0.5550
T7	0.1261	0.3680
T8	0.5289	0.4970
T9	0.0045	0.3070
TA	0.5289	0.4980
TB	0.6936	0.5570
TD	0.7824	0.5960
TE	0.6766	0.5560
TF	0.1269	0.3670
TG	0.6758	0.5570
TH	0.9108	0.6190
TI	0.7370	0.5670
TJ	0.0022	0.3090





















































































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Chain	Atom inclusion	Q-score
U1	0.4651	0.4850
U2	0.8029	0.5860
U3	0.5912	0.5110
U4	0.4666	0.4820
U6	0.5497	0.4920
U7	0.0515	0.3330
U8	0.5489	0.5200
U9	0.0245	0.3590
UA	0.5444	0.5230
UB	0.5497	0.4890
UD	0.5843	0.5090
UE	0.6826	0.5480
UF	0.0485	0.3260
UG	0.6882	0.5560
UH	0.9081	0.6190
UI	0.8045	0.5890
UJ	0.0245	0.3650
V1	0.6527	0.5470
V2	0.8343	0.5960
V3	0.4171	0.4520
V4	0.6542	0.5500
V6	0.4310	0.4710
V7	0.1009	0.3790
V8	0.4058	0.4670
V9	0.0030	0.2740
VA	0.4028	0.4670
VB	0.4295	0.4730
VD	0.4186	0.4520
VE	0.5245	0.4910
VF	0.1016	0.3810
VG	0.5274	0.4990
VH	0.6591	0.5510
VI	0.8307	0.5970
VJ	0.0045	0.2720
W1	0.7886	0.5980
W2	0.7768	0.5790
W3	0.4965	0.4840
W4	0.7938	0.5970
W6	0.6781	0.5530
W7	0.0530	0.3280
W8	0.7095	0.5700
W9	0.0022	0.2820





















































































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Chain	Atom inclusion	Q-score
WA	 0.7087	 0.5670
WB	 0.6781	 0.5530
WD	 0.4927	 0.4830
WE	 0.5235	 0.4880
WF	 0.0530	 0.3240
WG	 0.5190	 0.4940
WH	 0.7282	 0.5830
WI	 0.7760	 0.5770
WJ	 0.0015	 0.2820
X1	 0.8297	 0.6030
X2	 0.8532	 0.6040
X3	 0.6383	 0.5410
X4	 0.8364	 0.6040
X6	 0.7393	 0.5740
X7	 0.1914	 0.4470
X8	 0.5964	 0.5300
X9	 0.0015	 0.2970
XA	 0.5972	 0.5310
XB	 0.7413	 0.5750
XD	 0.6390	 0.5380
XE	 0.7077	 0.5650
XF	 0.1955	 0.4460
XG	 0.7097	 0.5700
XH	 0.8151	 0.6100
XI	 0.8516	 0.6040
XJ	 0.0037	 0.2980
Y1	 0.6721	 0.5660
Y2	 0.7378	 0.5680
Y3	 0.0397	 0.4090
Y4	 0.6795	 0.5660
Y6	 0.7641	 0.5880
Y7	 0.0675	 0.3630
Y8	 0.6438	 0.5440
Y9	 0.0015	 0.3150
YA	 0.6415	 0.5460
YB	 0.7671	 0.5900
YD	 0.0428	 0.4050
YE	 0.0993	 0.3130
YF	 0.0697	 0.3640
YG	 0.1001	 0.3190
YH	 0.7735	 0.5840
YI	 0.7363	 0.5680





















































































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Chain	Atom inclusion	Q-score
YJ	 0.0030	 0.3190
Z1	 0.3565	 0.5110
Z2	 0.7991	 0.5780
Z4	 0.3565	 0.5040
Z6	 0.6916	 0.5520
Z7	 0.0254	 0.3010
Z8	 0.6855	 0.5670
ZA	 0.6862	 0.5690
ZB	 0.6960	 0.5520
ZE	 0.1343	 0.3150
ZF	 0.0194	 0.3090
ZG	 0.1335	 0.3220
ZH	 0.7276	 0.5760
ZI	 0.7983	 0.5780
a1	 0.0981	 0.4560
a2	 0.8314	 0.5990
a4	 0.0990	 0.4460
a6	 0.5757	 0.5170
a7	 0.0364	 0.3110
a8	 0.2828	 0.4430
aA	 0.2857	 0.4430
aB	 0.5757	 0.5210
aE	 0.1964	 0.3610
aF	 0.0364	 0.3090
aG	 0.2009	 0.3750
aH	 0.8200	 0.5960
aI	 0.8293	 0.6010
b1	 0.5932	 0.5320
b2	 0.4503	 0.4370
b4	 0.5900	 0.5300
b6	 0.3795	 0.4490
b7	 0.0134	 0.3070
b8	 0.6324	 0.5450
bA	 0.6300	 0.5440
bB	 0.3857	 0.4470
bE	 0.2448	 0.3890
bF	 0.0119	 0.3060
bG	 0.2500	 0.3950
bH	 0.6828	 0.5760
bI	 0.4480	 0.4400
c1	 0.0060	 0.2740
c2	 0.3977	 0.4150





















































































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Chain	Atom inclusion	Q-score
c4	 0.0022	 0.2560
c6	 0.2930	 0.4300
c7	 0.0289	 0.3320
c8	 0.1335	 0.3740
cA	 0.1304	 0.3750
cB	 0.3027	 0.4330
cE	 0.2054	 0.3580
cF	 0.0312	 0.3340
cG	 0.2270	 0.3750
cH	 0.6983	 0.5590
cI	 0.3991	 0.4230
d1	 0.0029	 0.2940
d2	 0.5035	 0.4600
d4	 0.0036	 0.2720
d6	 0.1762	 0.3580
d7	 0.0172	 0.2950
d8	 0.2091	 0.4090
d9	 0.4597	 0.5030
dA	 0.2176	 0.4140
dB	 0.1668	 0.3620
dE	 0.2418	 0.4080
dF	 0.0209	 0.2950
dG	 0.2374	 0.4160
dH	 0.7966	 0.5900
dI	 0.5019	 0.4620
dJ	 0.4573	 0.5020
e1	 0.0069	 0.2900
e2	 0.5720	 0.5070
e3	 0.6824	 0.5560
e4	 0.0085	 0.2910
e6	 0.2032	 0.3710
e7	 0.0126	 0.2740
e8	 0.4384	 0.4980
eA	 0.4369	 0.5000
eB	 0.2046	 0.3700
eD	 0.6798	 0.5560
eE	 0.2517	 0.4140
eF	 0.0104	 0.2840
eG	 0.2502	 0.4220
eH	 0.6788	 0.5530
eI	 0.5648	 0.5110
f1	 0.0200	 0.3310





















































































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Chain	Atom inclusion	Q-score
f2	 0.4273	 0.4260
f4	 0.0163	 0.3060
f6	 0.1501	 0.3440
f7	 0.0284	 0.3240
f8	 0.1001	 0.3430
fA	 0.1023	 0.3440
fB	 0.1486	 0.3540
fE	 0.3086	 0.4280
fF	 0.0321	 0.3170
fG	 0.3093	 0.4340
fH	 0.8340	 0.6000
fI	 0.4249	 0.4280
g1	 0.0022	 0.2940
g2	 0.4114	 0.4290
g4	 0.0015	 0.2860
g6	 0.2596	 0.4140
g7	 0.0163	 0.3090
g8	 0.0519	 0.3340
gA	 0.0512	 0.3320
gB	 0.2648	 0.4160
gE	 0.3032	 0.4430
gF	 0.0185	 0.3140
gG	 0.3122	 0.4510
gH	 0.8605	 0.6070
gI	 0.4193	 0.4340
h1	 0.0134	 0.3020
h2	 0.5258	 0.4760
h4	 0.0144	 0.2970
h6	 0.1232	 0.3390
h7	 0.0112	 0.2780
h8	 0.1031	 0.3590
hA	 0.0926	 0.3520
hB	 0.1180	 0.3420
hE	 0.1610	 0.3640
hF	 0.0112	 0.2860
hG	 0.1588	 0.3720
hH	 0.7331	 0.5620
hI	 0.5281	 0.4710
i1	 0.0381	 0.3480
i2	 0.5742	 0.5010
i4	 0.0339	 0.3440
i6	 0.0935	 0.3300





















































































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Chain	Atom inclusion	Q-score
i7	 0.0119	 0.2920
i8	 0.2070	 0.3980
iA	 0.2047	 0.3970
iB	 0.0987	 0.3340
iE	 0.2263	 0.3680
iF	 0.0104	 0.2920
iG	 0.2270	 0.3760
iH	 0.8345	 0.5970
iI	 0.5713	 0.5030
j1	 0.0274	 0.3410
j2	 0.4796	 0.4540
j4	 0.0252	 0.3400
j6	 0.2510	 0.3900
j7	 0.0127	 0.2630
j8	 0.1255	 0.3710
jA	 0.1217	 0.3700
jB	 0.2494	 0.3970
jE	 0.3828	 0.4640
jF	 0.0105	 0.2710
jG	 0.3850	 0.4680
jH	 0.7095	 0.5620
jI	 0.4804	 0.4560
k1	 0.0164	 0.3180
k2	 0.4316	 0.4300
k4	 0.0127	 0.3070
k6	 0.4473	 0.4730
k7	 0.0037	 0.3000
k8	 0.1877	 0.3820
kA	 0.1936	 0.3840
kB	 0.4444	 0.4730
kE	 0.0037	 0.2160
kF	 0.0030	 0.2910
kG	 0.0015	 0.2380
kH	 0.8552	 0.6040
kI	 0.4337	 0.4290
l1	 0.0059	 0.2950
l2	 0.5473	 0.4750
l4	 0.0067	 0.2900
l6	 0.2726	 0.4040
l7	 0.0030	 0.2470
l8	 0.3883	 0.4630
lA	 0.3883	 0.4660





















































































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Chain	Atom inclusion	Q-score
lB	 0.2763	 0.4030
lE	 0.0007	 0.2300
lF	 0.0015	 0.2480
lG	 0.0037	 0.2440
lH	 0.8021	 0.5910
lI	 0.5450	 0.4710
m1	 0.0112	 0.2870
m2	 0.6001	 0.5240
m4	 0.0112	 0.2810
m6	 0.1455	 0.3380
m7	 0.0052	 0.2550
m8	 0.2507	 0.4450
mA	 0.2463	 0.4450
mB	 0.1513	 0.3470
mE	 0.0134	 0.2350
mF	 0.0037	 0.2560
mG	 0.0134	 0.2710
mH	 0.6618	 0.5580
mI	 0.6102	 0.5230
n1	 0.0635	 0.3760
n4	 0.0645	 0.3610
nE	 0.0059	 0.2510
nG	 0.0067	 0.2680
nH	 0.7925	 0.5910
o1	 0.0383	 0.3390
o4	 0.0380	 0.3230
oE	 0.0022	 0.2340
oG	 0.0060	 0.2500
oH	 0.7730	 0.5790
p1	 0.0015	 0.2710
p4	 0.0038	 0.2510
pE	 0.0134	 0.2540
pG	 0.0111	 0.2720
pH	 0.8443	 0.6100
q1	 0.0022	 0.2650
q4	 0.0014	 0.2680
qE	 0.0224	 0.2950
qG	 0.0246	 0.3120
qH	 0.6446	 0.5320
r1	 0.0031	 0.2610
r4	 0.0023	 0.2340
rE	 0.0178	 0.2830

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Chain	Atom inclusion	Q-score
rG	 0.0193	 0.2960
rH	 0.8897	 0.6080
s1	 0.0000	 0.2580
s4	 0.0007	 0.2370
sE	 0.0052	 0.2580
sG	 0.0075	 0.2750
sH	 0.9211	 0.6220
t1	 0.0054	 0.3010
t4	 0.0054	 0.2680
tE	 0.0022	 0.2210
tG	 0.0007	 0.2430
tH	 0.9002	 0.6160
u1	 0.0339	 0.3320
u4	 0.0310	 0.3290
uE	 0.0037	 0.2300
uG	 0.0022	 0.2410
uH	 0.9138	 0.6200
v1	 0.0192	 0.3270
v4	 0.0154	 0.3080
vE	 0.0438	 0.3110
vG	 0.0460	 0.3220
vH	 0.9148	 0.6210
w1	 0.0072	 0.2790
w4	 0.0063	 0.2650
wE	 0.3316	 0.4490
wG	 0.3337	 0.4540
wH	 0.9073	 0.6190
x1	 0.0177	 0.3110
x4	 0.0154	 0.2940
xE	 0.0140	 0.2790
xG	 0.0125	 0.2900
xH	 0.5935	 0.4930
y1	 0.0036	 0.2740
y4	 0.0014	 0.2580
yE	 0.6287	 0.5480
yG	 0.6328	 0.5480
yH	 0.7253	 0.5770
z1	 0.0000	 0.2640
z4	 0.0000	 0.2490
zE	 0.7216	 0.5710
zG	 0.7219	 0.5760
zH	 0.8137	 0.6050