



Full wwPDB EM Validation Report ⓘ

Mar 26, 2024 – 02:14 PM JST

PDB ID : 7EZK
EMDB ID : EMD-31393
Title : Structure of the phycobilisome from the red alga *Porphyridium purpureum* in Middle Light
Authors : Ma, J.F.; Sui, S.-F.
Deposited on : 2021-06-02
Resolution : 3.00 Å (reported)
Based on initial model : 6KGX

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:

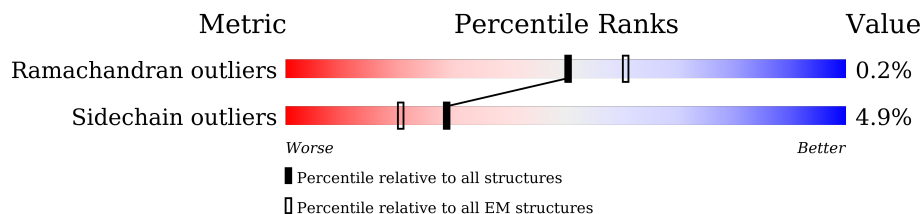
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.00 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	X1	363	
1	X7	363	
1	X9	363	
1	XF	363	
1	XI	363	
1	XK	363	
2	A1	290	
2	A7	290	
2	A9	290	

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Mol	Chain	Length	Quality of chain
2	AF	290	51% 88% 11%
2	AI	290	52% 88% 11%
2	AK	290	88% 87% 11%
3	B1	232	21% 94%
3	B7	232	93% 6%
3	B9	232	93% 6%
3	BF	232	10% 99%
3	BI	232	10% 98%
3	BK	232	21% 94%
4	C1	162	74% 94% 6%
4	C7	162	93% 7%
4	C9	162	93% 7%
4	CF	162	99%
4	CI	162	99%
4	CK	162	77% 94% 6%
4	E1	162	7% 95% 5%
4	E7	162	94% 6%
4	E9	162	94% 6%
4	EF	162	99%
4	EI	162	99%
4	EK	162	7% 95% 5%
4	G1	162	53% 98%
4	G7	162	94% 6%
4	G9	162	94% 6%
4	GF	162	99%

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Mol	Chain	Length	Quality of chain
4	GI	162	99%
4	GK	162	52% 98%
4	I1	162	6% 99%
4	I7	162	93% 6%
4	I9	162	93% 6%
4	IF	162	99%
4	II	162	99%
4	IK	162	6% 99%
4	K1	162	36% 99%
4	K7	162	93% 7%
4	K9	162	93% 7%
4	KF	162	99%
4	KI	162	99%
4	KK	162	35% 98%
4	M1	162	73% 96%
4	M7	162	94% 6%
4	M9	162	94% 6%
4	MF	162	99%
4	MI	162	99%
4	MK	162	73% 96%
5	D1	172	85% 96%
5	D7	172	86% 14%
5	D9	172	86% 14%
5	DF	172	13% 99%
5	DI	172	12% 99%

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Mol	Chain	Length	Quality of chain
5	DK	172	84% 96% ..
5	F1	172	39% 94% 6% .
5	F7	172	5% 87% 13%
5	F9	172	5% 88% 12%
5	FF	172	10% 99% .
5	FI	172	9% 100%
5	FK	172	36% 93% 6% .
5	H1	172	33% 97% ..
5	H7	172	. 87% 13% .
5	H9	172	. 87% 13% .
5	HF	172	. 99% .
5	HI	172	. 99% .
5	HK	172	26% 97% ..
5	J1	172	31% 94% 6% .
5	J7	172	. 88% 12%
5	J9	172	. 88% 12%
5	JF	172	. 99% .
5	JI	172	. 99% .
5	JK	172	33% 93% 6% .
5	L1	172	10% 97% ..
5	L7	172	. 87% 13%
5	L9	172	. 87% 13%
5	LF	172	8% 98% .
5	LI	172	6% 98% .
5	LK	172	12% 97% ..

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Mol	Chain	Length	Quality of chain
5	N1	172	62% 95% 5%
5	N7	172	88% 12%
5	N9	172	88% 12%
5	NF	172	7% 98%
5	NI	172	6% 98%
5	NK	172	58% 95% 5%
6	A3	164	10% 96%
6	AA	164	100% 95% 5%
6	AC	164	100% 95%
6	AE	164	100% 95%
6	AG	164	100% 90% 9%
6	AJ	164	27% 95% 5%
6	AL	164	27% 95% 5%
6	AN	164	100% 95% 5%
6	AO	164	9% 96%
6	AQ	164	100% 90% 8%
6	B4	164	86% 89% 10%
6	BD	164	84% 89% 10%
6	C3	164	41% 95% 5%
6	CA	164	100% 95% 5%
6	CB	164	10% 99%
6	CC	164	99% 94% 5%
6	CE	164	99% 94% 5%
6	CG	164	100% 87% 11%
6	CJ	164	25% 98%

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Mol	Chain	Length	Quality of chain
6	CL	164	28% 98%
6	CM	164	11% 99%
6	CN	164	100% 95% 5%
6	CO	164	41% 95% 5%
6	CQ	164	100% 87% 11%
6	D4	164	55% 85% 14%
6	DD	164	55% 85% 14%
6	E3	164	48% 93% 7%
6	EA	164	100% 96%
6	EB	164	34% 99%
6	EC	164	100% 93% 6%
6	EE	164	100% 93% 6%
6	EG	164	100% 88% 10%
6	EJ	164	18% 99%
6	EL	164	17% 99%
6	EM	164	32% 99%
6	EN	164	100% 96%
6	EO	164	47% 93% 7%
6	EQ	164	100% 88% 10%
6	F4	164	71% 84% 16%
6	FD	164	68% 83% 16%
6	G3	164	41% 96%
6	GA	164	100% 95% 5%
6	GB	164	42% 96%
6	GC	164	96% 93% 6%

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Mol	Chain	Length	Quality of chain
6	GE	164	98% 93% 6%
6	GG	164	100% 88% 10%
6	GJ	164	6% 94% 6%
6	GL	164	5% 95% 5%
6	GM	164	41% 96% .
6	GN	164	100% 95% 5%
6	GO	164	41% 96% .
6	GQ	164	100% 88% 10%
6	H4	164	82% 85% 14%
6	HD	164	81% 85% 15%
6	I3	164	14% 93% 7%
6	IA	164	100% 95% 5%
6	IB	164	13% 99% .
6	IC	164	99% 95% ..
6	IE	164	99% 95% ..
6	IG	164	100% 89% 9%
6	IJ	164	5% 93% 7%
6	IL	164	5% 93% 7%
6	IM	164	15% 99% .
6	IN	164	100% 95% 5%
6	IO	164	16% 93% 7%
6	IQ	164	100% 89% 9%
6	J4	164	95% 87% 13%
6	J5	164	8% 97% .
6	J8	164	8% 96% .

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Mol	Chain	Length	Quality of chain
6	JD	164	95% 87% 12%
6	K3	164	94% 6%
6	KA	164	100% 95% 5%
6	KB	164	7% 99%
6	KC	164	99% 94% 6%
6	KE	164	100% 94% 6%
6	KG	164	100% 88% 10%
6	KJ	164	12% 95% 5%
6	KL	164	12% 95% 5%
6	KM	164	6% 99%
6	KN	164	100% 95% 5%
6	KO	164	94% 6%
6	KQ	164	100% 88% 10%
6	L4	164	88% 85% 13%
6	LD	164	89% 86% 13%
6	M2	164	56% 95% 5%
6	MB	164	6% 99%
6	MJ	164	46% 96%
6	ML	164	46% 96%
6	MM	164	5% 99%
6	MR	164	55% 95% 5%
6	O1	164	84% 99%
6	O2	164	13% 93% 7%
6	O7	164	6% 95% 5%
6	O9	164	9% 95% 5%

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Mol	Chain	Length	Quality of chain
6	OB	164	30% 99%
6	OF	164	10% 98%
6	OI	164	9% 98%
6	OJ	164	27% 99%
6	OK	164	85% 99%
6	OL	164	25% 99%
6	OM	164	31% 99%
6	OR	164	12% 95% 5%
6	Q1	164	77% 99%
6	Q2	164	23% 94% 6%
6	Q7	164	95% 5%
6	Q9	164	95% 5%
6	QB	164	51% 98%
6	QF	164	27% 98%
6	QI	164	26% 98%
6	QJ	164	32% 98%
6	QK	164	78% 99%
6	QL	164	33% 98%
6	QM	164	48% 98%
6	QR	164	24% 96%
6	S1	164	85% 99%
6	S2	164	18% 98%
6	S7	164	96%
6	S9	164	96%
6	SB	164	58% 99%

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Mol	Chain	Length	Quality of chain
6	SF	164	22% 98%
6	SI	164	24% 98%
6	SJ	164	16% 96%
6	SK	164	84% 99%
6	SL	164	16% 96%
6	SM	164	57% 99%
6	SR	164	19% 96%
6	U1	164	96% 99%
6	U2	164	41% 95%
6	U7	164	5% 95%
6	U9	164	7% 95%
6	UB	164	20% 99%
6	UF	164	24% 98%
6	UI	164	24% 98%
6	UJ	164	15% 96%
6	UK	164	97% 99%
6	UL	164	17% 96%
6	UM	164	18% 99%
6	UR	164	41% 95%
6	W1	164	96% 99%
6	W2	164	52% 97%
6	W7	164	96%
6	W9	164	96%
6	WB	164	8% 99%
6	WF	164	12% 98%

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Mol	Chain	Length	Quality of chain
6	WI	164	13% 98%
6	WJ	164	30% 97%
6	WK	164	96% 99%
6	WL	164	27% 97%
6	WM	164	9% 99%
6	WR	164	54% 96%
6	YB	164	11% 99%
6	YJ	164	98% 98%
6	YL	164	98% 98%
6	YM	164	10% 99%
6	Z1	164	99% 99%
6	Z7	164	5% 96%
6	Z9	164	5% 96%
6	ZF	164	8% 99%
6	ZI	164	9% 99%
6	ZK	164	99% 99%
6	aB	164	92% 99%
6	aJ	164	89% 96%
6	aL	164	87% 96%
6	aM	164	91% 99%
6	b1	164	100% 99%
6	b7	164	29% 95%
6	b9	164	29% 95%
6	bF	164	37% 98%
6	bI	164	36% 98%

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Mol	Chain	Length	Quality of chain
6	bK	164	100% 99%
6	cJ	164	93% 96%
6	cL	164	93% 95% 5%
6	d1	164	99% 99%
6	d7	164	24% 95% 5%
6	d9	164	25% 95% 5%
6	dB	164	93% 99%
6	dF	164	66% 98%
6	dI	164	68% 98%
6	dK	164	99% 99%
6	dM	164	92% 99%
6	eJ	164	90% 98%
6	eL	164	91% 98%
6	f1	164	99% 99%
6	f7	164	35% 96%
6	f9	164	37% 96%
6	fB	164	98% 99%
6	fF	164	79% 97%
6	fI	164	77% 97%
6	fK	164	99% 99%
6	fM	164	98% 99%
6	gJ	164	93% 98%
6	gL	164	93% 98%
6	h1	164	100% 98%
6	h7	164	30% 95% 5%

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Mol	Chain	Length	Quality of chain
6	h9	164	28% 95% 5%
6	hB	164	98% 99%
6	hF	164	91% 98%
6	hI	164	91% 98%
6	hK	164	100% 99%
6	hM	164	96% 99%
6	iJ	164	85% 96%
6	iL	164	86% 96%
6	j1	164	99% 99%
6	j7	164	43% 96%
6	j9	164	45% 96%
6	jB	164	98% 98%
6	jF	164	65% 98%
6	jI	164	68% 98%
6	jK	164	99% 99%
6	jM	164	97% 99%
6	kJ	164	100% 96%
6	kL	164	100% 96%
6	l1	164	100% 99%
6	l7	164	27% 95% 5%
6	l9	164	25% 96%
6	lB	164	73% 98%
6	lF	164	57% 98%
6	lI	164	57% 98%
6	lK	164	99% 99%

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Mol	Chain	Length	Quality of chain
6	lM	164	73% 97% 100%
6	mJ	164	97% 100%
6	mL	164	100% 97%
6	oJ	164	100% 98%
6	oL	164	100% 98%
6	qJ	164	100% 96%
6	qL	164	100% 96%
6	sJ	164	100% 96%
6	sL	164	100% 96%
6	uJ	164	100% 97%
6	uL	164	100% 97%
7	A5	177	100% 90% 10%
7	A8	177	100% 90% 10%
7	B3	177	18% 95% 5%
7	B5	177	79% 80% 18%
7	B8	177	80% 80% 18%
7	BA	177	100% 94% 5%
7	BC	177	100% 93% 7%
7	BE	177	100% 93% 7%
7	BG	177	100% 94% 6%
7	BJ	177	35% 97%
7	BL	177	34% 97%
7	BN	177	100% 94% 5%
7	BO	177	18% 95% 5%
7	BQ	177	100% 94% 6%

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Mol	Chain	Length	Quality of chain
7	C4	177	82% 82% 16% .
7	C5	177	100% 91% 8% .
7	C8	177	100% 91% 8% .
7	CD	177	82% 82% 16% .
7	D3	177	17% 92% 8%
7	DA	177	100% 95% . .
7	DB	177	29% 98% .
7	DC	177	98% 92% 8%
7	DE	177	98% 92% 8%
7	DG	177	100% 93% 7%
7	DJ	177	27% 98% .
7	DL	177	28% 98% .
7	DM	177	29% 98% .
7	DN	177	100% 95% . .
7	DO	177	19% 92% 8%
7	DQ	177	100% 93% 7%
7	E4	177	69% 82% 17% .
7	ED	177	69% 82% 16% .
7	F3	177	31% 93% 7%
7	F5	177	27% 80% . 18%
7	F8	177	25% 80% . 18%
7	FA	177	100% 94% 6%
7	FB	177	16% 98% .
7	FC	177	99% 90% 10%
7	FE	177	99% 90% 10%

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Mol	Chain	Length	Quality of chain
7	FG	177	100% 93% 7%
7	FJ	177	11% 93% 7%
7	FL	177	10% 93% 7%
7	FM	177	16% 98% .
7	FN	177	100% 94% 6%
7	FO	177	32% 93% 7%
7	FQ	177	100% 93% 7%
7	G4	177	90% 80% 18% .
7	G5	177	59% 80% . 18%
7	G8	177	58% 80% . 18%
7	GD	177	90% 81% 18% .
7	H3	177	46% 92% 8%
7	H5	177	24% 80% . 18%
7	H8	177	24% 80% . 18%
7	HA	177	100% 94% 6% .
7	HB	177	24% 97% .
7	HC	177	99% 90% 10%
7	HE	177	99% 90% 10%
7	HG	177	100% 93% 7%
7	HJ	177	9% 88% 12%
7	HL	177	9% 88% 12%
7	HM	177	25% 97% .
7	HN	177	100% 94% 6% .
7	HO	177	46% 92% 8%
7	HQ	177	100% 93% 7%

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Mol	Chain	Length	Quality of chain
7	I4	177	45% 88% 11%
7	I5	177	15% 89% 11%
7	I8	177	16% 89% 11%
7	ID	177	44% 88% 11%
7	J3	177	7% 93% 7%
7	JA	177	100% 95% 5%
7	JB	177	27% 97% .
7	JC	177	100% 92% 8%
7	JE	177	100% 92% 8%
7	JG	177	100% 93% 7%
7	JJ	177	12% 96% .
7	JL	177	11% 96% .
7	JM	177	27% 97% .
7	JN	177	100% 95% 5%
7	JO	177	8% 93% 7%
7	JQ	177	100% 93% 7%
7	K4	177	95% 82% 17%
7	K5	177	42% 89% 11%
7	K8	177	42% 89% 11%
7	KD	177	95% 82% 16%
7	L3	177	12% 93% 7%
7	L5	177	23% 80% 18%
7	L8	177	23% 80% 18%
7	LA	177	100% 96% ..
7	LB	177	10% 99% .

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Mol	Chain	Length	Quality of chain
7	LC	177	94% 92% 8%
7	LE	177	95% 92% 8%
7	LG	177	100% 93% 7%
7	LJ	177	10% 98% .
7	LL	177	10% 98% .
7	LM	177	10% 99% .
7	LN	177	100% 96% ..
7	LO	177	13% 93% 7%
7	LQ	177	100% 93% 7%
7	M3	177	24% 76% 7% 18%
7	M4	177	85% 83% 15% .
7	MD	177	85% 82% 16% .
7	MO	177	24% 76% 7% 18%
7	N2	177	38% 96% .
7	N3	177	48% 76% 6% 18%
7	NB	177	6% 96% .
7	NJ	177	42% 98% .
7	NL	177	44% 98% .
7	NM	177	6% 97% .
7	NO	177	47% 76% 6% 18%
7	NR	177	38% 96% .
7	P1	177	51% 98% .
7	P2	177	24% 97% ..
7	P7	177	9% 93% 7%
7	P9	177	8% 93% 7%

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Mol	Chain	Length	Quality of chain
7	PB	177	53% 99%
7	PF	177	18% 99%
7	PI	177	17% 99%
7	PJ	177	26% 95% 5%
7	PK	177	54% 98%
7	PL	177	23% 95% 5%
7	PM	177	50% 99%
7	PR	177	24% 97%
7	R1	177	94% 98%
7	R2	177	33% 98%
7	R7	177	93% 7%
7	R9	177	93% 7%
7	RB	177	27% 96%
7	RF	177	15% 99%
7	RI	177	15% 99%
7	RJ	177	26% 98%
7	RK	177	93% 98%
7	RL	177	25% 98%
7	RM	177	26% 96%
7	RR	177	34% 98%
7	T1	177	85% 99%
7	T2	177	10% 97%
7	T7	177	12% 93% 7%
7	T9	177	8% 93% 7%
7	TB	177	31% 97%

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Mol	Chain	Length	Quality of chain
7	TF	177	11% 98%
7	TI	177	12% 98%
7	TJ	177	13% 98%
7	TK	177	85% 99%
7	TL	177	14% 98%
7	TM	177	32% 97%
7	TR	177	10% 97%
7	V1	177	90% 98%
7	V2	177	64% 96%
7	V7	177	5% 94% 6%
7	V9	177	5% 94% 6%
7	VB	177	40% 97%
7	VF	177	24% 98%
7	VI	177	26% 98%
7	VJ	177	31% 99%
7	VK	177	88% 98%
7	VL	177	30% 99%
7	VM	177	41% 97%
7	VR	177	64% 96%
7	X2	177	24% 95% 5%
7	XB	177	16% 99%
7	XJ	177	16% 99%
7	XL	177	16% 99%
7	XM	177	14% 99%
7	XR	177	24% 95% 5%

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Mol	Chain	Length	Quality of chain
7	Y1	177	92%
7	Y7	177	10% 99% 7%
7	Y9	177	10% 93% 7%
7	YF	177	8% 99% 0%
7	YI	177	8% 99% 0%
7	YK	177	93% 99% 0%
7	ZB	177	10% 97% 0%
7	ZJ	177	97% 98% 0%
7	ZL	177	96% 98% 0%
7	ZM	177	10% 97% 0%
7	a1	177	98% 98% 0%
7	a7	177	10% 93% 7%
7	a9	177	11% 92% 8%
7	aF	177	22% 98% 0%
7	aI	177	21% 98% 0%
7	aK	177	98% 98% 0%
7	bJ	177	89% 97% 0%
7	bL	177	87% 97% 0%
7	c1	177	100% 99% 0%
7	c7	177	49% 93% 7%
7	c9	177	44% 93% 7%
7	cB	177	97% 98% 0%
7	cF	177	46% 97% 0%
7	cI	177	46% 97% 0%
7	cK	177	100% 99% 0%

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Mol	Chain	Length	Quality of chain
7	cM	177	97% 98%
7	dJ	177	95% 98%
7	dL	177	96% 98%
7	e1	177	100% 99%
7	e7	177	16% 92% 8%
7	e9	177	16% 92% 8%
7	eB	177	64% 96%
7	eF	177	60% 98%
7	eI	177	59% 98%
7	eK	177	100% 99%
7	eM	177	66% 96%
7	fJ	177	80% 97%
7	fL	177	79% 97%
7	g1	177	99% 99%
7	g7	177	48% 93% 7%
7	g9	177	47% 93% 7%
7	gB	177	99% 96%
7	gF	177	59% 99%
7	gI	177	56% 99%
7	gK	177	99% 99%
7	gM	177	99% 96%
7	hJ	177	96% 97%
7	hL	177	96% 97%
7	i1	177	100% 99%
7	i7	177	14% 93% 7%

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Mol	Chain	Length	Quality of chain
7	i9	177	15% 93% 7%
7	iB	177	88% 98%
7	iF	177	86% 98%
7	iI	177	86% 98%
7	iK	177	100% 99%
7	iM	177	87% 98%
7	jJ	177	80% 97%
7	jL	177	81% 97%
7	k1	177	100% 99%
7	k7	177	40% 93% 7%
7	k9	177	40% 93% 7%
7	kB	177	95% 95% 5%
7	kF	177	38% 98%
7	kI	177	40% 98%
7	kK	177	100% 99%
7	kM	177	98% 95% 5%
7	lJ	177	100% 94% 6%
7	lL	177	100% 94% 6%
7	m1	177	100% 99%
7	m7	177	21% 94% 6%
7	m9	177	23% 94% 6%
7	mB	177	85% 98%
7	mF	177	80% 98%
7	mI	177	80% 98%
7	mK	177	100% 99%

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Mol	Chain	Length	Quality of chain
7	mM	177	86% 98% 100%
7	nJ	177	95% 100%
7	nL	177	95% 100%
7	pJ	177	95% 100%
7	pL	177	95% 100%
7	rJ	177	96% 100%
7	rL	177	96% 100%
7	tJ	177	95% 100%
7	tL	177	95% 100%
7	vJ	177	95% 100%
7	vL	177	95% 100%
8	e2	303	33% 79% 18%
8	eR	303	33% 79% 18%
9	O3	405	27% 91% 7%
9	OO	405	27% 91% 7%
10	d4	342	58% 85% 13%
10	dD	342	52% 85% 13%
11	D5	327	25% 75%
11	D8	327	25% 75%
12	E5	288	27% 71% 29%
12	E8	288	26% 71% 29%
13	k6	288	6% 93% 6%
13	kH	288	6% 93% 6%
14	MA	333	71% 69% 29%
14	MG	333	71% 67% 29%

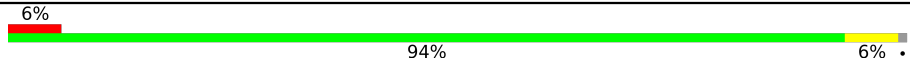
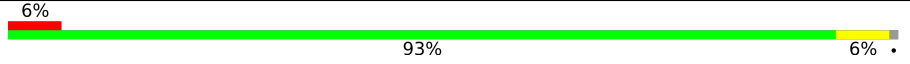
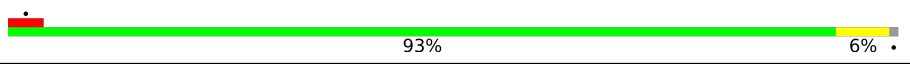
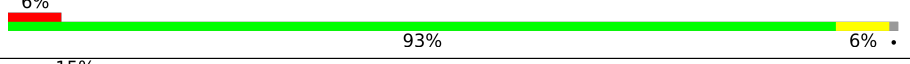
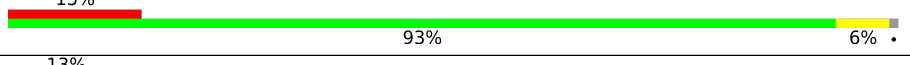
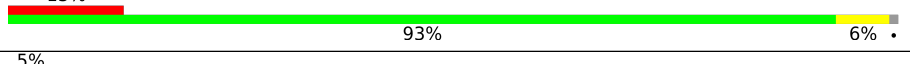
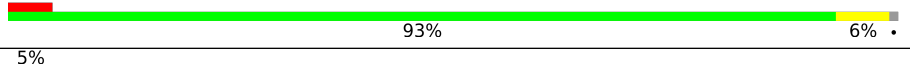
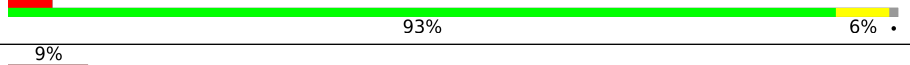
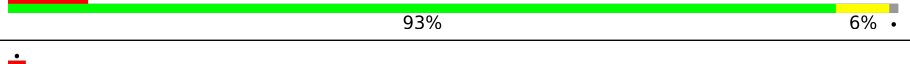
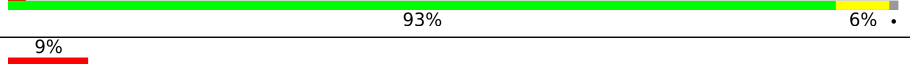
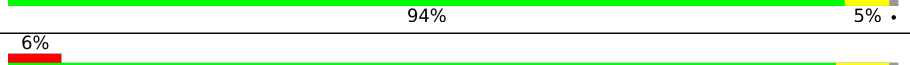
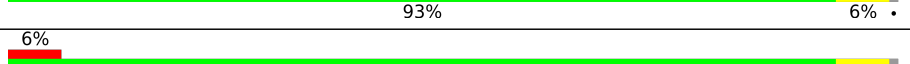
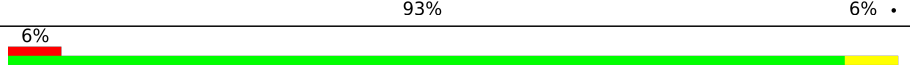
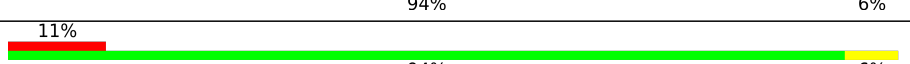
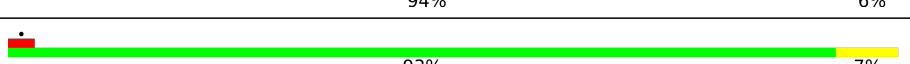
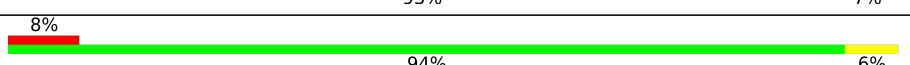
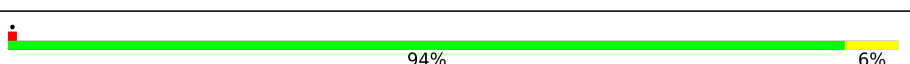
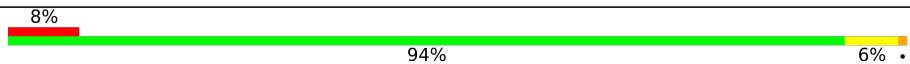
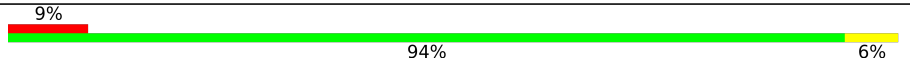
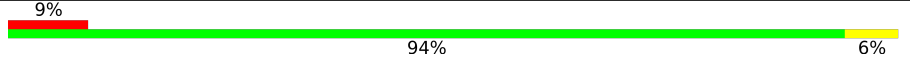
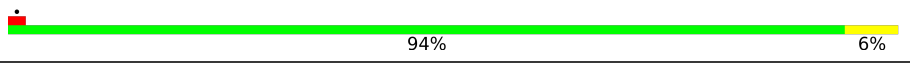
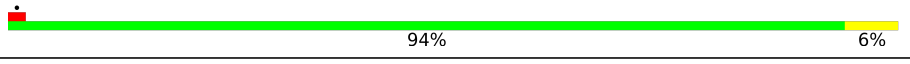
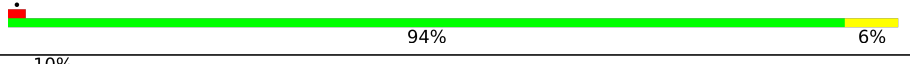
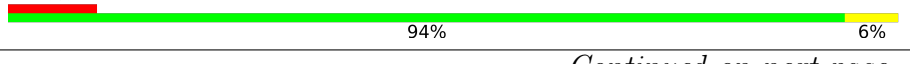

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Mol	Chain	Length	Quality of chain
14	MN	333	71% 69% 29%
14	MQ	333	71% 68% 29%
15	bB	490	9% 76% 22%
15	bM	490	9% 75% 22%
16	AB	273	76% 86% 13%
16	AM	273	77% 86% 13%
16	wJ	273	69% 79% 7% 13%
16	wL	273	68% 79% 7% 13%
16	xJ	273	87% 79% 7% 13%
16	xL	273	87% 80% 7% 13%
17	BB	290	17% 86% 14%
17	BM	290	16% 86% 14%
17	yJ	290	11% 86% 14%
17	yL	290	11% 86% 14%
18	MC	316	79% 78% 10% 11%
18	ME	316	80% 78% 9% 11%
19	zJ	498	8% 73% 26%
19	zL	498	7% 72% 26%
20	AP	161	7% 93% 6%
20	CP	161	14% 93% 6%
20	EP	161	12% 93% 6%
20	GP	161	6% 93% 6%
20	JP	161	6% 94% 6%
20	KP	161	7% 93% 6%
20	NP	161	• 93% 6%

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Mol	Chain	Length	Quality of chain
20	PP	161	 6% 94% 6%
20	RP	161	 6% 93% 6%
20	TP	161	 6% 93% 6%
20	cP	161	 6% 93% 6%
20	eP	161	 15% 93% 6%
20	gP	161	 13% 93% 6%
20	iP	161	 5% 93% 6%
20	lP	161	 5% 93% 6%
20	mP	161	 9% 93% 6%
20	pP	161	 6% 93% 6%
20	rP	161	 9% 94% 5%
20	tP	161	 6% 93% 6%
20	vP	161	 6% 93% 6%
21	BP	161	 6% 94% 6%
21	DP	161	 11% 94% 6%
21	FP	161	 6% 93% 7%
21	HP	161	 8% 94% 6%
21	IP	161	 6% 94% 6%
21	LP	161	 8% 94% 6%
21	MP	161	 9% 94% 6%
21	OP	161	 9% 94% 6%
21	QP	161	 6% 94% 6%
21	SP	161	 6% 94% 6%
21	UP	161	 6% 94% 6%
21	dP	161	 10% 94% 6%

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Mol	Chain	Length	Quality of chain
21	fP	161	94% 6%
21	hP	161	94% 6%
21	jP	161	94% 6%
21	kP	161	94% 6%
21	nP	161	94% 6%
21	oP	161	93% 7%
21	qP	161	94% 6%
21	sP	161	94% 6%
21	uP	161	94% 6%
21	wP	161	94% 6%
22	VP	161	98% ...
22	xP	161	98% ...
23	WP	173	100%
23	yP	173	100%
24	XP	132	69% 30%
24	zP	132	69% 30%
25	1P	879	95% ..
25	YP	879	95% ..
26	2P	159	82% 17%
26	ZP	159	81% 17%
27	3P	288	85% 12%
27	aP	288	85% 12%
28	4P	253	80% 18%
28	bP	253	80% 18%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	MEN	LP	71	-	X	-	-
21	MEN	jP	71	-	X	-	-
21	MEN	kP	71	-	X	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 944670 atoms, of which 0 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 Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X1	324	2527	1603	431	486	7	0	0
1	X7	324	2527	1603	431	486	7	0	0
1	X9	324	2527	1603	431	486	7	0	0
1	XF	324	2527	1603	431	486	7	0	0
1	XI	324	2523	1600	430	486	7	0	0
1	XK	324	2527	1603	431	486	7	0	0

- Molecule 2 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A1	257	1987	1226	368	378	15	0	0
2	A7	257	1987	1226	368	378	15	0	0
2	A9	257	1987	1226	368	378	15	0	0
2	AF	257	1987	1226	368	378	15	0	0
2	AI	257	1987	1226	368	378	15	0	0
2	AK	257	1987	1226	368	378	15	0	0

- Molecule 3 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B1	227	Total	C	N	O	S	0	0
			1874	1197	328	345	4		
3	B7	230	Total	C	N	O	S	0	0
			1889	1206	331	348	4		
3	B9	230	Total	C	N	O	S	0	0
			1889	1206	331	348	4		
3	BF	231	Total	C	N	O	S	0	0
			1897	1212	332	349	4		
3	BI	231	Total	C	N	O	S	0	0
			1897	1212	332	349	4		
3	BK	227	Total	C	N	O	S	0	0
			1874	1197	328	345	4		

- Molecule 4 is a protein called C-phycoyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	E1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	G1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	I1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	K1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	M1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	C7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	E7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	G7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	I7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	K7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	M7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	C9	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	E9	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G9	162	1228	773	209	240	6	0	0
4	I9	162	1228	773	209	240	6	0	0
4	K9	162	1228	773	209	240	6	0	0
4	M9	162	1228	773	209	240	6	0	0
4	CF	162	1228	773	209	240	6	0	0
4	EF	162	1228	773	209	240	6	0	0
4	GF	162	1228	773	209	240	6	0	0
4	IF	162	1228	773	209	240	6	0	0
4	KF	162	1228	773	209	240	6	0	0
4	MF	162	1228	773	209	240	6	0	0
4	CI	162	1228	773	209	240	6	0	0
4	EI	162	1228	773	209	240	6	0	0
4	GI	162	1228	773	209	240	6	0	0
4	II	162	1228	773	209	240	6	0	0
4	KI	162	1228	773	209	240	6	0	0
4	MI	162	1228	773	209	240	6	0	0
4	CK	162	1228	773	209	240	6	0	0
4	EK	162	1228	773	209	240	6	0	0
4	GK	162	1228	773	209	240	6	0	0
4	IK	162	1228	773	209	240	6	0	0
4	KK	162	1228	773	209	240	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	MK	162	1228	773	209	240	6	0	0

- Molecule 5 is a protein called C-phycoyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D1	172	1272	786	224	253	9	0	0
5	F1	172	1272	786	224	253	9	0	0
5	H1	172	1272	786	224	253	9	0	0
5	J1	172	1272	786	224	253	9	0	0
5	L1	172	1272	786	224	253	9	0	0
5	N1	172	1272	786	224	253	9	0	0
5	D7	172	1272	786	224	253	9	0	0
5	F7	172	1272	786	224	253	9	0	0
5	H7	172	1272	786	224	253	9	0	0
5	J7	172	1272	786	224	253	9	0	0
5	L7	172	1272	786	224	253	9	0	0
5	N7	172	1272	786	224	253	9	0	0
5	D9	172	1272	786	224	253	9	0	0
5	F9	172	1272	786	224	253	9	0	0
5	H9	172	1272	786	224	253	9	0	0
5	J9	172	1272	786	224	253	9	0	0
5	L9	172	1272	786	224	253	9	0	0
5	N9	172	1272	786	224	253	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	DF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	FF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	HF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	JF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	LF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	NF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	DI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	FI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	HI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	JI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	LI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	NI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	DK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	FK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	HK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	JK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	LK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	NK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

- Molecule 6 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	U1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	W1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Z1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	b1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	d1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	f1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	h1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	j1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	l1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	M2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	O2	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	Q2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S2	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	U2	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	W2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	A3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	C3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	E3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	G3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	I3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	K3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	B4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	D4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	F4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	H4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	J4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	L4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	J5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	O7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Q7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	U7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	W7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Z7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	b7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	d7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	f7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	h7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	j7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	l7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	J8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	O9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Q9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	U9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	W9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Z9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	b9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	d9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	f9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	h9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	j9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	l9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	GB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	KC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	BD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	DD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	FD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	HD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	JD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	LD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ZF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	bF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	fF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ZI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	bI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	II	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	cJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	eJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	gJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	iJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	kJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	mJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	oJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	qJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	sJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	uJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ZK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	bK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	KL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ML	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	cL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	eL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	gL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	iL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	kL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	mL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	oL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	qL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	sL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	uL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	GM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	KN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MR	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OR	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	QR	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SR	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	UR	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	WR	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 7 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	R1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	T1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	V1	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	Y1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	a1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	c1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	e1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	g1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	i1	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	k1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	m1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	N2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	P2	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	R2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	T2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	V2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	X2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	B3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	D3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	F3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	H3	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		
7	J3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	L3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	M3	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	N3	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	C4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	E4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	G4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	I4	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	K4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	M4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	B5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	F5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	G5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	H5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	I5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	K5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	L5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	A5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	C5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	P7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	R7	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		
7	T7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	V7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	Y7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	a7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	c7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	e7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	g7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	i7	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	k7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	m7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	B8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	F8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	G8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	H8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	I8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	K8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	L8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	A8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	C8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	P9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	R9	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		
7	T9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	V9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	Y9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	a9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	c9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	e9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	g9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	i9	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	k9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	m9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HA	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	FB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	HB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	JB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	LB	177	Total 1300	C 804	N 225	O 259	S 12	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	NB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	PB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	TB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	VB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	XB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	ZB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	cB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	eB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	gB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	iB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	kB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	mB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	BC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	CD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	ED	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		
7	GD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	ID	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	KD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	MD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	YF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	aF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	cF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	eF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	gF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	iF	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	kF	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		
7	mF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HG	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VI	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	YI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	aI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	cI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	eI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	gI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	iI	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	kI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	mI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DJ	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		
7	FJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	NJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PJ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	RJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	XJ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	ZJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	bJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	dJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	fJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	hJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	jJ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	lJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	nJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	pJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	rJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	tJ	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		
7	vJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VK	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	YK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	aK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	cK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	eK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	gK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	iK	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	kK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	mK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	NL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PL	177	Total 1297	C 802	N 225	O 258	S 12	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	RL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	XL	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	ZL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	bL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	dL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	fL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	hL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	jL	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	lL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	nL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	pL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	rL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	tL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	vL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	FM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	HM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	JM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	LM	177	Total 1300	C 804	N 225	O 259	S 12	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	NM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	PM	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	TM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	VM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	XM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	ZM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	cM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	eM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	gM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	iM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	kM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	mM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	BN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HN	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DO	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		
7	FO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	MO	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	NO	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	BQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HQ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	NR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PR	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	RR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	XR	177	Total 1294	C 800	N 225	O 257	S 12	0	0

- Molecule 8 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	e2	248	Total 1932	C 1217	N 336	O 369	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	eR	248	Total	C	N	O	S	0	0
			1932	1217	336	369	10		

- Molecule 9 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O3	375	Total	C	N	O	S	0	0
			2873	1809	488	563	13		
9	OO	375	Total	C	N	O	S	0	0
			2873	1809	488	563	13		

- Molecule 10 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d4	297	Total	C	N	O	S	0	0
			2293	1425	407	450	11		
10	dD	297	Total	C	N	O	S	0	0
			2293	1425	407	450	11		

- Molecule 11 is a protein called CaRSPs2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D5	81	Total	C	N	O	S	0	0
			654	417	113	122	2		
11	D8	81	Total	C	N	O	S	0	0
			654	417	113	122	2		

- Molecule 12 is a protein called CaRSPs1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E5	205	Total	C	N	O	S	0	0
			1580	1004	278	289	9		
12	E8	205	Total	C	N	O	S	0	0
			1580	1004	278	289	9		

- Molecule 13 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	k6	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	kH	285	2182	1399	369	404	10	0	0

- Molecule 14 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	MA	238	1851	1140	348	348	15	0	0
14	MG	238	1851	1140	348	348	15	0	0
14	MN	238	1851	1140	348	348	15	0	0
14	MQ	238	1851	1140	348	348	15	0	0

- Molecule 15 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	bB	380	2961	1867	514	565	15	0	0
15	bM	380	2961	1867	514	565	15	0	0

- Molecule 16 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AB	238	1814	1122	335	342	15	0	0
16	wJ	238	1814	1122	335	342	15	0	0
16	xJ	238	1814	1122	335	342	15	0	0
16	wL	238	1814	1122	335	342	15	0	0
16	xL	238	1814	1122	335	342	15	0	0
16	AM	238	1814	1122	335	342	15	0	0

- Molecule 17 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BB	250	Total 1902	C 1184	N 346	O 358	S 14	0	0
17	yJ	250	Total 1902	C 1184	N 346	O 358	S 14	0	0
17	yL	250	Total 1902	C 1184	N 346	O 358	S 14	0	0
17	BM	250	Total 1902	C 1184	N 346	O 358	S 14	0	0

- Molecule 18 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	MC	280	Total 2196	C 1391	N 382	O 413	S 10	0	0
18	ME	280	Total 2196	C 1391	N 382	O 413	S 10	0	0

- Molecule 19 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	zJ	370	Total 2901	C 1833	N 514	O 540	S 14	0	0
19	zL	370	Total 2901	C 1833	N 514	O 540	S 14	0	0

- Molecule 20 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	CP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	EP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	GP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	JP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	KP	160	Total 1225	C 768	N 211	O 239	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	NP	160	1225	768	211	239	7	0	0
20	PP	160	1225	768	211	239	7	0	0
20	RP	160	1225	768	211	239	7	0	0
20	TP	160	1225	768	211	239	7	0	0
20	cP	160	1225	768	211	239	7	0	0
20	eP	160	1225	768	211	239	7	0	0
20	gP	160	1225	768	211	239	7	0	0
20	iP	160	1225	768	211	239	7	0	0
20	lP	160	1225	768	211	239	7	0	0
20	mP	160	1225	768	211	239	7	0	0
20	pP	160	1225	768	211	239	7	0	0
20	rP	160	1225	768	211	239	7	0	0
20	tP	160	1225	768	211	239	7	0	0
20	vP	160	1225	768	211	239	7	0	0

- Molecule 21 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	DP	161	1220	767	206	240	7	0	0
21	FP	161	1220	767	206	240	7	0	0
21	BP	161	1220	767	206	240	7	0	0
21	HP	161	1220	767	206	240	7	0	0
21	IP	161	1220	767	206	240	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	LP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	MP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	OP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	QP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	SP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	UP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	dP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	fP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	hP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	jP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	kP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	nP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	oP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	qP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	sP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	uP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	wP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 22 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	VP	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
22	xP	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 23 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	WP	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		
23	yP	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

- Molecule 24 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	XP	92	Total	C	N	O	S	0	0
			720	453	127	135	5		
24	zP	92	Total	C	N	O	S	0	0
			720	453	127	135	5		

- Molecule 25 is a protein called Phycobilisome linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	YP	844	Total	C	N	O	S	0	0
			6756	4328	1169	1245	14		
25	1P	844	Total	C	N	O	S	0	0
			6756	4328	1169	1245	14		

- Molecule 26 is a protein called Lrc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	ZP	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		
26	2P	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		

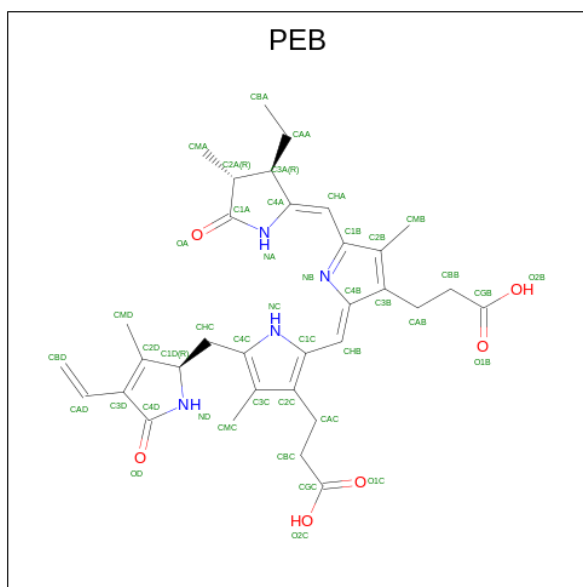
- Molecule 27 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	aP	253	Total	C	N	O	S	0	0
			1897	1190	325	375	7		
27	3P	253	Total	C	N	O	S	0	0
			1897	1190	325	375	7		

- Molecule 28 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	bP	207	1537	985	260	287	5	0	0
28	4P	207	1537	985	260	287	5	0	0

- Molecule 29 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	A1	1	43	33	4	6	0
29	A1	1	43	33	4	6	0
29	A1	1	43	33	4	6	0
29	D1	1	43	33	4	6	0
29	F1	1	43	33	4	6	0
29	H1	1	43	33	4	6	0
29	J1	1	43	33	4	6	0
29	L1	1	43	33	4	6	0
29	N1	1	43	33	4	6	0
29	O1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	O1	1	43	33	4	6	0
29	P1	1	43	33	4	6	0
29	P1	1	43	33	4	6	0
29	P1	1	43	33	4	6	0
29	Q1	1	43	33	4	6	0
29	Q1	1	43	33	4	6	0
29	R1	1	43	33	4	6	0
29	R1	1	43	33	4	6	0
29	R1	1	43	33	4	6	0
29	S1	1	43	33	4	6	0
29	S1	1	43	33	4	6	0
29	T1	1	43	33	4	6	0
29	T1	1	43	33	4	6	0
29	U1	1	43	33	4	6	0
29	U1	1	43	33	4	6	0
29	U1	1	43	33	4	6	0
29	V1	1	43	33	4	6	0
29	V1	1	43	33	4	6	0
29	V1	1	43	33	4	6	0
29	W1	1	43	33	4	6	0
29	W1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	Y1	1	43	33	4	6	0
29	Y1	1	43	33	4	6	0
29	Z1	1	43	33	4	6	0
29	Z1	1	43	33	4	6	0
29	Z1	1	43	33	4	6	0
29	a1	1	43	33	4	6	0
29	a1	1	43	33	4	6	0
29	a1	1	43	33	4	6	0
29	b1	1	43	33	4	6	0
29	b1	1	43	33	4	6	0
29	c1	1	43	33	4	6	0
29	c1	1	43	33	4	6	0
29	c1	1	43	33	4	6	0
29	d1	1	43	33	4	6	0
29	d1	1	43	33	4	6	0
29	e1	1	43	33	4	6	0
29	e1	1	43	33	4	6	0
29	e1	1	43	33	4	6	0
29	f1	1	43	33	4	6	0
29	f1	1	43	33	4	6	0
29	g1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	g1	1	43	33	4	6	0
29	g1	1	43	33	4	6	0
29	h1	1	43	33	4	6	0
29	h1	1	43	33	4	6	0
29	i1	1	43	33	4	6	0
29	i1	1	43	33	4	6	0
29	i1	1	43	33	4	6	0
29	j1	1	43	33	4	6	0
29	j1	1	43	33	4	6	0
29	j1	1	43	33	4	6	0
29	k1	1	43	33	4	6	0
29	k1	1	43	33	4	6	0
29	k1	1	43	33	4	6	0
29	l1	1	43	33	4	6	0
29	l1	1	43	33	4	6	0
29	m1	1	43	33	4	6	0
29	m1	1	43	33	4	6	0
29	e2	1	43	33	4	6	0
29	e2	1	43	33	4	6	0
29	M2	1	43	33	4	6	0
29	M2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	N2	1	43	33	4	6	0
29	N2	1	43	33	4	6	0
29	N2	1	43	33	4	6	0
29	O2	1	43	33	4	6	0
29	O2	1	43	33	4	6	0
29	P2	1	43	33	4	6	0
29	P2	1	43	33	4	6	0
29	Q2	1	43	33	4	6	0
29	Q2	1	43	33	4	6	0
29	R2	1	43	33	4	6	0
29	R2	1	43	33	4	6	0
29	R2	1	43	33	4	6	0
29	S2	1	43	33	4	6	0
29	S2	1	43	33	4	6	0
29	T2	1	43	33	4	6	0
29	T2	1	43	33	4	6	0
29	T2	1	43	33	4	6	0
29	U2	1	43	33	4	6	0
29	U2	1	43	33	4	6	0
29	V2	1	43	33	4	6	0
29	V2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	V2	1	43	33	4	6	0
29	W2	1	43	33	4	6	0
29	W2	1	43	33	4	6	0
29	X2	1	43	33	4	6	0
29	X2	1	43	33	4	6	0
29	A3	1	43	33	4	6	0
29	A3	1	43	33	4	6	0
29	B3	1	43	33	4	6	0
29	B3	1	43	33	4	6	0
29	B3	1	43	33	4	6	0
29	C3	1	43	33	4	6	0
29	C3	1	43	33	4	6	0
29	D3	1	43	33	4	6	0
29	D3	1	43	33	4	6	0
29	D3	1	43	33	4	6	0
29	E3	1	43	33	4	6	0
29	E3	1	43	33	4	6	0
29	F3	1	43	33	4	6	0
29	F3	1	43	33	4	6	0
29	F3	1	43	33	4	6	0
29	G3	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	G3	1	Total 43	C 33	N 4	O 6	0
29	H3	1	Total 43	C 33	N 4	O 6	0
29	H3	1	Total 43	C 33	N 4	O 6	0
29	H3	1	Total 43	C 33	N 4	O 6	0
29	I3	1	Total 43	C 33	N 4	O 6	0
29	I3	1	Total 43	C 33	N 4	O 6	0
29	I3	1	Total 43	C 33	N 4	O 6	0
29	J3	1	Total 43	C 33	N 4	O 6	0
29	J3	1	Total 43	C 33	N 4	O 6	0
29	J3	1	Total 43	C 33	N 4	O 6	0
29	K3	1	Total 43	C 33	N 4	O 6	0
29	K3	1	Total 43	C 33	N 4	O 6	0
29	L3	1	Total 43	C 33	N 4	O 6	0
29	L3	1	Total 43	C 33	N 4	O 6	0
29	M3	1	Total 43	C 33	N 4	O 6	0
29	M3	1	Total 43	C 33	N 4	O 6	0
29	M3	1	Total 43	C 33	N 4	O 6	0
29	N3	1	Total 43	C 33	N 4	O 6	0
29	N3	1	Total 43	C 33	N 4	O 6	0
29	N3	1	Total 43	C 33	N 4	O 6	0
29	B4	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	B4	1	43	33	4	6	0
29	C4	1	43	33	4	6	0
29	C4	1	43	33	4	6	0
29	C4	1	43	33	4	6	0
29	D4	1	43	33	4	6	0
29	D4	1	43	33	4	6	0
29	E4	1	43	33	4	6	0
29	E4	1	43	33	4	6	0
29	E4	1	43	33	4	6	0
29	F4	1	43	33	4	6	0
29	F4	1	43	33	4	6	0
29	G4	1	43	33	4	6	0
29	G4	1	43	33	4	6	0
29	G4	1	43	33	4	6	0
29	H4	1	43	33	4	6	0
29	H4	1	43	33	4	6	0
29	I4	1	43	33	4	6	0
29	I4	1	43	33	4	6	0
29	I4	1	43	33	4	6	0
29	J4	1	43	33	4	6	0
29	J4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	K4	1	Total 43	C 33	N 4	O 6	0
29	K4	1	Total 43	C 33	N 4	O 6	0
29	K4	1	Total 43	C 33	N 4	O 6	0
29	L4	1	Total 43	C 33	N 4	O 6	0
29	L4	1	Total 43	C 33	N 4	O 6	0
29	M4	1	Total 43	C 33	N 4	O 6	0
29	M4	1	Total 43	C 33	N 4	O 6	0
29	M4	1	Total 43	C 33	N 4	O 6	0
29	B5	1	Total 43	C 33	N 4	O 6	0
29	B5	1	Total 43	C 33	N 4	O 6	0
29	B5	1	Total 43	C 33	N 4	O 6	0
29	F5	1	Total 43	C 33	N 4	O 6	0
29	F5	1	Total 43	C 33	N 4	O 6	0
29	F5	1	Total 43	C 33	N 4	O 6	0
29	G5	1	Total 43	C 33	N 4	O 6	0
29	G5	1	Total 43	C 33	N 4	O 6	0
29	G5	1	Total 43	C 33	N 4	O 6	0
29	H5	1	Total 43	C 33	N 4	O 6	0
29	H5	1	Total 43	C 33	N 4	O 6	0
29	H5	1	Total 43	C 33	N 4	O 6	0
29	I5	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	I5	1	43	33	4	6	0
29	I5	1	43	33	4	6	0
29	J5	1	43	33	4	6	0
29	J5	1	43	33	4	6	0
29	K5	1	43	33	4	6	0
29	K5	1	43	33	4	6	0
29	K5	1	43	33	4	6	0
29	L5	1	43	33	4	6	0
29	L5	1	43	33	4	6	0
29	L5	1	43	33	4	6	0
29	A5	1	43	33	4	6	0
29	A5	1	43	33	4	6	0
29	A5	1	43	33	4	6	0
29	C5	1	43	33	4	6	0
29	C5	1	43	33	4	6	0
29	C5	1	43	33	4	6	0
29	A7	1	43	33	4	6	0
29	A7	1	43	33	4	6	0
29	A7	1	43	33	4	6	0
29	D7	1	43	33	4	6	0
29	F7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	H7	1	43	33	4	6	0
29	J7	1	43	33	4	6	0
29	L7	1	43	33	4	6	0
29	N7	1	43	33	4	6	0
29	O7	1	43	33	4	6	0
29	O7	1	43	33	4	6	0
29	P7	1	43	33	4	6	0
29	P7	1	43	33	4	6	0
29	P7	1	43	33	4	6	0
29	Q7	1	43	33	4	6	0
29	Q7	1	43	33	4	6	0
29	R7	1	43	33	4	6	0
29	R7	1	43	33	4	6	0
29	R7	1	43	33	4	6	0
29	S7	1	43	33	4	6	0
29	S7	1	43	33	4	6	0
29	T7	1	43	33	4	6	0
29	T7	1	43	33	4	6	0
29	T7	1	43	33	4	6	0
29	U7	1	43	33	4	6	0
29	U7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	V7	1	43	33	4	6	0
29	V7	1	43	33	4	6	0
29	V7	1	43	33	4	6	0
29	W7	1	43	33	4	6	0
29	W7	1	43	33	4	6	0
29	Y7	1	43	33	4	6	0
29	Y7	1	43	33	4	6	0
29	Y7	1	43	33	4	6	0
29	Z7	1	43	33	4	6	0
29	Z7	1	43	33	4	6	0
29	a7	1	43	33	4	6	0
29	a7	1	43	33	4	6	0
29	a7	1	43	33	4	6	0
29	b7	1	43	33	4	6	0
29	b7	1	43	33	4	6	0
29	c7	1	43	33	4	6	0
29	c7	1	43	33	4	6	0
29	c7	1	43	33	4	6	0
29	d7	1	43	33	4	6	0
29	d7	1	43	33	4	6	0
29	e7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	e7	1	Total 43	C 33	N 4	O 6	0
29	e7	1	Total 43	C 33	N 4	O 6	0
29	f7	1	Total 43	C 33	N 4	O 6	0
29	f7	1	Total 43	C 33	N 4	O 6	0
29	g7	1	Total 43	C 33	N 4	O 6	0
29	g7	1	Total 43	C 33	N 4	O 6	0
29	g7	1	Total 43	C 33	N 4	O 6	0
29	h7	1	Total 43	C 33	N 4	O 6	0
29	h7	1	Total 43	C 33	N 4	O 6	0
29	i7	1	Total 43	C 33	N 4	O 6	0
29	i7	1	Total 43	C 33	N 4	O 6	0
29	i7	1	Total 43	C 33	N 4	O 6	0
29	j7	1	Total 43	C 33	N 4	O 6	0
29	j7	1	Total 43	C 33	N 4	O 6	0
29	k7	1	Total 43	C 33	N 4	O 6	0
29	k7	1	Total 43	C 33	N 4	O 6	0
29	k7	1	Total 43	C 33	N 4	O 6	0
29	l7	1	Total 43	C 33	N 4	O 6	0
29	l7	1	Total 43	C 33	N 4	O 6	0
29	m7	1	Total 43	C 33	N 4	O 6	0
29	m7	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	m7	1	43	33	4	6	0
29	B8	1	43	33	4	6	0
29	B8	1	43	33	4	6	0
29	B8	1	43	33	4	6	0
29	F8	1	43	33	4	6	0
29	F8	1	43	33	4	6	0
29	F8	1	43	33	4	6	0
29	G8	1	43	33	4	6	0
29	G8	1	43	33	4	6	0
29	G8	1	43	33	4	6	0
29	H8	1	43	33	4	6	0
29	H8	1	43	33	4	6	0
29	H8	1	43	33	4	6	0
29	I8	1	43	33	4	6	0
29	I8	1	43	33	4	6	0
29	I8	1	43	33	4	6	0
29	J8	1	43	33	4	6	0
29	J8	1	43	33	4	6	0
29	K8	1	43	33	4	6	0
29	K8	1	43	33	4	6	0
29	K8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	L8	1	Total 43	C 33	N 4	O 6	0
29	L8	1	Total 43	C 33	N 4	O 6	0
29	L8	1	Total 43	C 33	N 4	O 6	0
29	A8	1	Total 43	C 33	N 4	O 6	0
29	A8	1	Total 43	C 33	N 4	O 6	0
29	A8	1	Total 43	C 33	N 4	O 6	0
29	C8	1	Total 43	C 33	N 4	O 6	0
29	C8	1	Total 43	C 33	N 4	O 6	0
29	C8	1	Total 43	C 33	N 4	O 6	0
29	A9	1	Total 43	C 33	N 4	O 6	0
29	A9	1	Total 43	C 33	N 4	O 6	0
29	A9	1	Total 43	C 33	N 4	O 6	0
29	D9	1	Total 43	C 33	N 4	O 6	0
29	F9	1	Total 43	C 33	N 4	O 6	0
29	H9	1	Total 43	C 33	N 4	O 6	0
29	J9	1	Total 43	C 33	N 4	O 6	0
29	L9	1	Total 43	C 33	N 4	O 6	0
29	N9	1	Total 43	C 33	N 4	O 6	0
29	O9	1	Total 43	C 33	N 4	O 6	0
29	O9	1	Total 43	C 33	N 4	O 6	0
29	P9	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	P9	1	43	33	4	6	0
29	P9	1	43	33	4	6	0
29	Q9	1	43	33	4	6	0
29	Q9	1	43	33	4	6	0
29	R9	1	43	33	4	6	0
29	R9	1	43	33	4	6	0
29	R9	1	43	33	4	6	0
29	S9	1	43	33	4	6	0
29	S9	1	43	33	4	6	0
29	T9	1	43	33	4	6	0
29	T9	1	43	33	4	6	0
29	T9	1	43	33	4	6	0
29	U9	1	43	33	4	6	0
29	U9	1	43	33	4	6	0
29	V9	1	43	33	4	6	0
29	V9	1	43	33	4	6	0
29	V9	1	43	33	4	6	0
29	W9	1	43	33	4	6	0
29	W9	1	43	33	4	6	0
29	Y9	1	43	33	4	6	0
29	Y9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	Y9	1	Total 43	C 33	N 4	O 6	0
29	Z9	1	Total 43	C 33	N 4	O 6	0
29	Z9	1	Total 43	C 33	N 4	O 6	0
29	a9	1	Total 43	C 33	N 4	O 6	0
29	a9	1	Total 43	C 33	N 4	O 6	0
29	a9	1	Total 43	C 33	N 4	O 6	0
29	b9	1	Total 43	C 33	N 4	O 6	0
29	b9	1	Total 43	C 33	N 4	O 6	0
29	c9	1	Total 43	C 33	N 4	O 6	0
29	c9	1	Total 43	C 33	N 4	O 6	0
29	c9	1	Total 43	C 33	N 4	O 6	0
29	d9	1	Total 43	C 33	N 4	O 6	0
29	d9	1	Total 43	C 33	N 4	O 6	0
29	e9	1	Total 43	C 33	N 4	O 6	0
29	e9	1	Total 43	C 33	N 4	O 6	0
29	e9	1	Total 43	C 33	N 4	O 6	0
29	f9	1	Total 43	C 33	N 4	O 6	0
29	f9	1	Total 43	C 33	N 4	O 6	0
29	g9	1	Total 43	C 33	N 4	O 6	0
29	g9	1	Total 43	C 33	N 4	O 6	0
29	g9	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	h9	1	43	33	4	6	0
29	h9	1	43	33	4	6	0
29	i9	1	43	33	4	6	0
29	i9	1	43	33	4	6	0
29	i9	1	43	33	4	6	0
29	j9	1	43	33	4	6	0
29	j9	1	43	33	4	6	0
29	k9	1	43	33	4	6	0
29	k9	1	43	33	4	6	0
29	k9	1	43	33	4	6	0
29	l9	1	43	33	4	6	0
29	l9	1	43	33	4	6	0
29	m9	1	43	33	4	6	0
29	m9	1	43	33	4	6	0
29	m9	1	43	33	4	6	0
29	AA	1	43	33	4	6	0
29	AA	1	43	33	4	6	0
29	BA	1	43	33	4	6	0
29	BA	1	43	33	4	6	0
29	BA	1	43	33	4	6	0
29	CA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	CA	1	43	33	4	6	0
29	DA	1	43	33	4	6	0
29	DA	1	43	33	4	6	0
29	DA	1	43	33	4	6	0
29	EA	1	43	33	4	6	0
29	EA	1	43	33	4	6	0
29	FA	1	43	33	4	6	0
29	FA	1	43	33	4	6	0
29	FA	1	43	33	4	6	0
29	GA	1	43	33	4	6	0
29	GA	1	43	33	4	6	0
29	HA	1	43	33	4	6	0
29	HA	1	43	33	4	6	0
29	HA	1	43	33	4	6	0
29	IA	1	43	33	4	6	0
29	IA	1	43	33	4	6	0
29	JA	1	43	33	4	6	0
29	JA	1	43	33	4	6	0
29	JA	1	43	33	4	6	0
29	KA	1	43	33	4	6	0
29	KA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	LA	1	43	33	4	6	0
29	LA	1	43	33	4	6	0
29	LA	1	43	33	4	6	0
29	MA	1	43	33	4	6	0
29	MA	1	43	33	4	6	0
29	MA	1	43	33	4	6	0
29	AB	1	43	33	4	6	0
29	AB	1	43	33	4	6	0
29	AB	1	43	33	4	6	0
29	BB	1	43	33	4	6	0
29	CB	1	43	33	4	6	0
29	CB	1	43	33	4	6	0
29	DB	1	43	33	4	6	0
29	DB	1	43	33	4	6	0
29	DB	1	43	33	4	6	0
29	EB	1	43	33	4	6	0
29	EB	1	43	33	4	6	0
29	FB	1	43	33	4	6	0
29	FB	1	43	33	4	6	0
29	FB	1	43	33	4	6	0
29	GB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	GB	1	Total 43	C 33	N 4	O 6	0
29	HB	1	Total 43	C 33	N 4	O 6	0
29	HB	1	Total 43	C 33	N 4	O 6	0
29	HB	1	Total 43	C 33	N 4	O 6	0
29	IB	1	Total 43	C 33	N 4	O 6	0
29	IB	1	Total 43	C 33	N 4	O 6	0
29	JB	1	Total 43	C 33	N 4	O 6	0
29	JB	1	Total 43	C 33	N 4	O 6	0
29	JB	1	Total 43	C 33	N 4	O 6	0
29	KB	1	Total 43	C 33	N 4	O 6	0
29	KB	1	Total 43	C 33	N 4	O 6	0
29	KB	1	Total 43	C 33	N 4	O 6	0
29	LB	1	Total 43	C 33	N 4	O 6	0
29	LB	1	Total 43	C 33	N 4	O 6	0
29	LB	1	Total 43	C 33	N 4	O 6	0
29	MB	1	Total 43	C 33	N 4	O 6	0
29	MB	1	Total 43	C 33	N 4	O 6	0
29	NB	1	Total 43	C 33	N 4	O 6	0
29	NB	1	Total 43	C 33	N 4	O 6	0
29	OB	1	Total 43	C 33	N 4	O 6	0
29	OB	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	PB	1	43	33	4	6	0
29	PB	1	43	33	4	6	0
29	QB	1	43	33	4	6	0
29	QB	1	43	33	4	6	0
29	QB	1	43	33	4	6	0
29	RB	1	43	33	4	6	0
29	RB	1	43	33	4	6	0
29	RB	1	43	33	4	6	0
29	SB	1	43	33	4	6	0
29	SB	1	43	33	4	6	0
29	TB	1	43	33	4	6	0
29	TB	1	43	33	4	6	0
29	TB	1	43	33	4	6	0
29	UB	1	43	33	4	6	0
29	UB	1	43	33	4	6	0
29	VB	1	43	33	4	6	0
29	VB	1	43	33	4	6	0
29	VB	1	43	33	4	6	0
29	WB	1	43	33	4	6	0
29	WB	1	43	33	4	6	0
29	XB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	XB	1	43	33	4	6	0
29	YB	1	43	33	4	6	0
29	YB	1	43	33	4	6	0
29	YB	1	43	33	4	6	0
29	ZB	1	43	33	4	6	0
29	ZB	1	43	33	4	6	0
29	ZB	1	43	33	4	6	0
29	aB	1	43	33	4	6	0
29	aB	1	43	33	4	6	0
29	aB	1	43	33	4	6	0
29	cB	1	43	33	4	6	0
29	cB	1	43	33	4	6	0
29	cB	1	43	33	4	6	0
29	dB	1	43	33	4	6	0
29	dB	1	43	33	4	6	0
29	eB	1	43	33	4	6	0
29	eB	1	43	33	4	6	0
29	fB	1	43	33	4	6	0
29	fB	1	43	33	4	6	0
29	gB	1	43	33	4	6	0
29	gB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	gB	1	43	33	4	6	0
29	hB	1	43	33	4	6	0
29	hB	1	43	33	4	6	0
29	iB	1	43	33	4	6	0
29	iB	1	43	33	4	6	0
29	iB	1	43	33	4	6	0
29	jB	1	43	33	4	6	0
29	jB	1	43	33	4	6	0
29	kB	1	43	33	4	6	0
29	kB	1	43	33	4	6	0
29	kB	1	43	33	4	6	0
29	lB	1	43	33	4	6	0
29	lB	1	43	33	4	6	0
29	mB	1	43	33	4	6	0
29	mB	1	43	33	4	6	0
29	mB	1	43	33	4	6	0
29	AC	1	43	33	4	6	0
29	AC	1	43	33	4	6	0
29	AC	1	43	33	4	6	0
29	BC	1	43	33	4	6	0
29	BC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	BC	1	43	33	4	6	0
29	CC	1	43	33	4	6	0
29	CC	1	43	33	4	6	0
29	DC	1	43	33	4	6	0
29	DC	1	43	33	4	6	0
29	EC	1	43	33	4	6	0
29	EC	1	43	33	4	6	0
29	FC	1	43	33	4	6	0
29	FC	1	43	33	4	6	0
29	FC	1	43	33	4	6	0
29	GC	1	43	33	4	6	0
29	GC	1	43	33	4	6	0
29	HC	1	43	33	4	6	0
29	HC	1	43	33	4	6	0
29	HC	1	43	33	4	6	0
29	IC	1	43	33	4	6	0
29	IC	1	43	33	4	6	0
29	JC	1	43	33	4	6	0
29	JC	1	43	33	4	6	0
29	KC	1	43	33	4	6	0
29	KC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	KC	1	43	33	4	6	0
29	LC	1	43	33	4	6	0
29	LC	1	43	33	4	6	0
29	LC	1	43	33	4	6	0
29	dD	1	43	33	4	6	0
29	BD	1	43	33	4	6	0
29	BD	1	43	33	4	6	0
29	CD	1	43	33	4	6	0
29	CD	1	43	33	4	6	0
29	CD	1	43	33	4	6	0
29	DD	1	43	33	4	6	0
29	DD	1	43	33	4	6	0
29	ED	1	43	33	4	6	0
29	ED	1	43	33	4	6	0
29	FD	1	43	33	4	6	0
29	FD	1	43	33	4	6	0
29	GD	1	43	33	4	6	0
29	GD	1	43	33	4	6	0
29	GD	1	43	33	4	6	0
29	HD	1	43	33	4	6	0
29	HD	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	ID	1	43	33	4	6	0
29	ID	1	43	33	4	6	0
29	ID	1	43	33	4	6	0
29	JD	1	43	33	4	6	0
29	JD	1	43	33	4	6	0
29	KD	1	43	33	4	6	0
29	KD	1	43	33	4	6	0
29	KD	1	43	33	4	6	0
29	LD	1	43	33	4	6	0
29	LD	1	43	33	4	6	0
29	MD	1	43	33	4	6	0
29	MD	1	43	33	4	6	0
29	MD	1	43	33	4	6	0
29	AE	1	43	33	4	6	0
29	AE	1	43	33	4	6	0
29	AE	1	43	33	4	6	0
29	BE	1	43	33	4	6	0
29	BE	1	43	33	4	6	0
29	BE	1	43	33	4	6	0
29	CE	1	43	33	4	6	0
29	CE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	DE	1	43	33	4	6	0
29	DE	1	43	33	4	6	0
29	EE	1	43	33	4	6	0
29	EE	1	43	33	4	6	0
29	FE	1	43	33	4	6	0
29	FE	1	43	33	4	6	0
29	FE	1	43	33	4	6	0
29	GE	1	43	33	4	6	0
29	GE	1	43	33	4	6	0
29	HE	1	43	33	4	6	0
29	HE	1	43	33	4	6	0
29	HE	1	43	33	4	6	0
29	IE	1	43	33	4	6	0
29	IE	1	43	33	4	6	0
29	JE	1	43	33	4	6	0
29	JE	1	43	33	4	6	0
29	KE	1	43	33	4	6	0
29	KE	1	43	33	4	6	0
29	KE	1	43	33	4	6	0
29	LE	1	43	33	4	6	0
29	LE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	LE	1	43	33	4	6	0
29	AF	1	43	33	4	6	0
29	AF	1	43	33	4	6	0
29	AF	1	43	33	4	6	0
29	DF	1	43	33	4	6	0
29	FF	1	43	33	4	6	0
29	HF	1	43	33	4	6	0
29	JF	1	43	33	4	6	0
29	LF	1	43	33	4	6	0
29	NF	1	43	33	4	6	0
29	OF	1	43	33	4	6	0
29	OF	1	43	33	4	6	0
29	OF	1	43	33	4	6	0
29	PF	1	43	33	4	6	0
29	PF	1	43	33	4	6	0
29	PF	1	43	33	4	6	0
29	QF	1	43	33	4	6	0
29	QF	1	43	33	4	6	0
29	RF	1	43	33	4	6	0
29	RF	1	43	33	4	6	0
29	SF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	SF	1	43	33	4	6	0
29	TF	1	43	33	4	6	0
29	TF	1	43	33	4	6	0
29	UF	1	43	33	4	6	0
29	UF	1	43	33	4	6	0
29	UF	1	43	33	4	6	0
29	VF	1	43	33	4	6	0
29	VF	1	43	33	4	6	0
29	VF	1	43	33	4	6	0
29	WF	1	43	33	4	6	0
29	WF	1	43	33	4	6	0
29	YF	1	43	33	4	6	0
29	YF	1	43	33	4	6	0
29	YF	1	43	33	4	6	0
29	ZF	1	43	33	4	6	0
29	ZF	1	43	33	4	6	0
29	aF	1	43	33	4	6	0
29	aF	1	43	33	4	6	0
29	aF	1	43	33	4	6	0
29	bF	1	43	33	4	6	0
29	bF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	cF	1	43	33	4	6	0
29	cF	1	43	33	4	6	0
29	dF	1	43	33	4	6	0
29	dF	1	43	33	4	6	0
29	dF	1	43	33	4	6	0
29	eF	1	43	33	4	6	0
29	eF	1	43	33	4	6	0
29	eF	1	43	33	4	6	0
29	fF	1	43	33	4	6	0
29	fF	1	43	33	4	6	0
29	gF	1	43	33	4	6	0
29	gF	1	43	33	4	6	0
29	gF	1	43	33	4	6	0
29	hF	1	43	33	4	6	0
29	hF	1	43	33	4	6	0
29	iF	1	43	33	4	6	0
29	iF	1	43	33	4	6	0
29	iF	1	43	33	4	6	0
29	jF	1	43	33	4	6	0
29	jF	1	43	33	4	6	0
29	kF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	kF	1	43	33	4	6	0
29	kF	1	43	33	4	6	0
29	lF	1	43	33	4	6	0
29	lF	1	43	33	4	6	0
29	mF	1	43	33	4	6	0
29	mF	1	43	33	4	6	0
29	mF	1	43	33	4	6	0
29	AG	1	43	33	4	6	0
29	AG	1	43	33	4	6	0
29	BG	1	43	33	4	6	0
29	BG	1	43	33	4	6	0
29	BG	1	43	33	4	6	0
29	CG	1	43	33	4	6	0
29	CG	1	43	33	4	6	0
29	DG	1	43	33	4	6	0
29	DG	1	43	33	4	6	0
29	DG	1	43	33	4	6	0
29	EG	1	43	33	4	6	0
29	EG	1	43	33	4	6	0
29	FG	1	43	33	4	6	0
29	FG	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	FG	1	Total 43	C 33	N 4	O 6	0
29	GG	1	Total 43	C 33	N 4	O 6	0
29	GG	1	Total 43	C 33	N 4	O 6	0
29	HG	1	Total 43	C 33	N 4	O 6	0
29	HG	1	Total 43	C 33	N 4	O 6	0
29	HG	1	Total 43	C 33	N 4	O 6	0
29	IG	1	Total 43	C 33	N 4	O 6	0
29	IG	1	Total 43	C 33	N 4	O 6	0
29	JG	1	Total 43	C 33	N 4	O 6	0
29	JG	1	Total 43	C 33	N 4	O 6	0
29	JG	1	Total 43	C 33	N 4	O 6	0
29	KG	1	Total 43	C 33	N 4	O 6	0
29	KG	1	Total 43	C 33	N 4	O 6	0
29	LG	1	Total 43	C 33	N 4	O 6	0
29	LG	1	Total 43	C 33	N 4	O 6	0
29	LG	1	Total 43	C 33	N 4	O 6	0
29	MG	1	Total 43	C 33	N 4	O 6	0
29	MG	1	Total 43	C 33	N 4	O 6	0
29	MG	1	Total 43	C 33	N 4	O 6	0
29	AI	1	Total 43	C 33	N 4	O 6	0
29	AI	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	AI	1	Total 43	C 33	N 4	O 6	0
29	DI	1	Total 43	C 33	N 4	O 6	0
29	FI	1	Total 43	C 33	N 4	O 6	0
29	HI	1	Total 43	C 33	N 4	O 6	0
29	JI	1	Total 43	C 33	N 4	O 6	0
29	LI	1	Total 43	C 33	N 4	O 6	0
29	NI	1	Total 43	C 33	N 4	O 6	0
29	OI	1	Total 43	C 33	N 4	O 6	0
29	OI	1	Total 43	C 33	N 4	O 6	0
29	OI	1	Total 43	C 33	N 4	O 6	0
29	PI	1	Total 43	C 33	N 4	O 6	0
29	PI	1	Total 43	C 33	N 4	O 6	0
29	PI	1	Total 43	C 33	N 4	O 6	0
29	QI	1	Total 43	C 33	N 4	O 6	0
29	QI	1	Total 43	C 33	N 4	O 6	0
29	RI	1	Total 43	C 33	N 4	O 6	0
29	RI	1	Total 43	C 33	N 4	O 6	0
29	SI	1	Total 43	C 33	N 4	O 6	0
29	SI	1	Total 43	C 33	N 4	O 6	0
29	TI	1	Total 43	C 33	N 4	O 6	0
29	TI	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	UI	1	43	33	4	6	0
29	UI	1	43	33	4	6	0
29	UI	1	43	33	4	6	0
29	VI	1	43	33	4	6	0
29	VI	1	43	33	4	6	0
29	VI	1	43	33	4	6	0
29	WI	1	43	33	4	6	0
29	WI	1	43	33	4	6	0
29	YI	1	43	33	4	6	0
29	YI	1	43	33	4	6	0
29	YI	1	43	33	4	6	0
29	ZI	1	43	33	4	6	0
29	ZI	1	43	33	4	6	0
29	aI	1	43	33	4	6	0
29	aI	1	43	33	4	6	0
29	aI	1	43	33	4	6	0
29	bI	1	43	33	4	6	0
29	bI	1	43	33	4	6	0
29	cI	1	43	33	4	6	0
29	cI	1	43	33	4	6	0
29	dI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	dI	1	43	33	4	6	0
29	dI	1	43	33	4	6	0
29	eI	1	43	33	4	6	0
29	eI	1	43	33	4	6	0
29	eI	1	43	33	4	6	0
29	fI	1	43	33	4	6	0
29	fI	1	43	33	4	6	0
29	gI	1	43	33	4	6	0
29	gI	1	43	33	4	6	0
29	gI	1	43	33	4	6	0
29	hI	1	43	33	4	6	0
29	hI	1	43	33	4	6	0
29	iI	1	43	33	4	6	0
29	iI	1	43	33	4	6	0
29	iI	1	43	33	4	6	0
29	jI	1	43	33	4	6	0
29	jI	1	43	33	4	6	0
29	kI	1	43	33	4	6	0
29	kI	1	43	33	4	6	0
29	kI	1	43	33	4	6	0
29	lI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	lI	1	Total 43	C 33	N 4	O 6	0
29	mI	1	Total 43	C 33	N 4	O 6	0
29	mI	1	Total 43	C 33	N 4	O 6	0
29	mI	1	Total 43	C 33	N 4	O 6	0
29	AJ	1	Total 43	C 33	N 4	O 6	0
29	AJ	1	Total 43	C 33	N 4	O 6	0
29	AJ	1	Total 43	C 33	N 4	O 6	0
29	BJ	1	Total 43	C 33	N 4	O 6	0
29	BJ	1	Total 43	C 33	N 4	O 6	0
29	BJ	1	Total 43	C 33	N 4	O 6	0
29	CJ	1	Total 43	C 33	N 4	O 6	0
29	CJ	1	Total 43	C 33	N 4	O 6	0
29	DJ	1	Total 43	C 33	N 4	O 6	0
29	DJ	1	Total 43	C 33	N 4	O 6	0
29	EJ	1	Total 43	C 33	N 4	O 6	0
29	EJ	1	Total 43	C 33	N 4	O 6	0
29	FJ	1	Total 43	C 33	N 4	O 6	0
29	FJ	1	Total 43	C 33	N 4	O 6	0
29	FJ	1	Total 43	C 33	N 4	O 6	0
29	GJ	1	Total 43	C 33	N 4	O 6	0
29	GJ	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	HJ	1	Total 43	C 33	N 4	O 6	0
29	HJ	1	Total 43	C 33	N 4	O 6	0
29	IJ	1	Total 43	C 33	N 4	O 6	0
29	IJ	1	Total 43	C 33	N 4	O 6	0
29	IJ	1	Total 43	C 33	N 4	O 6	0
29	JJ	1	Total 43	C 33	N 4	O 6	0
29	JJ	1	Total 43	C 33	N 4	O 6	0
29	JJ	1	Total 43	C 33	N 4	O 6	0
29	KJ	1	Total 43	C 33	N 4	O 6	0
29	KJ	1	Total 43	C 33	N 4	O 6	0
29	LJ	1	Total 43	C 33	N 4	O 6	0
29	LJ	1	Total 43	C 33	N 4	O 6	0
29	MJ	1	Total 43	C 33	N 4	O 6	0
29	MJ	1	Total 43	C 33	N 4	O 6	0
29	NJ	1	Total 43	C 33	N 4	O 6	0
29	NJ	1	Total 43	C 33	N 4	O 6	0
29	NJ	1	Total 43	C 33	N 4	O 6	0
29	OJ	1	Total 43	C 33	N 4	O 6	0
29	OJ	1	Total 43	C 33	N 4	O 6	0
29	PJ	1	Total 43	C 33	N 4	O 6	0
29	PJ	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	PJ	1	43	33	4	6	0
29	QJ	1	43	33	4	6	0
29	QJ	1	43	33	4	6	0
29	RJ	1	43	33	4	6	0
29	RJ	1	43	33	4	6	0
29	RJ	1	43	33	4	6	0
29	SJ	1	43	33	4	6	0
29	SJ	1	43	33	4	6	0
29	TJ	1	43	33	4	6	0
29	TJ	1	43	33	4	6	0
29	TJ	1	43	33	4	6	0
29	UJ	1	43	33	4	6	0
29	UJ	1	43	33	4	6	0
29	VJ	1	43	33	4	6	0
29	VJ	1	43	33	4	6	0
29	WJ	1	43	33	4	6	0
29	WJ	1	43	33	4	6	0
29	WJ	1	43	33	4	6	0
29	XJ	1	43	33	4	6	0
29	XJ	1	43	33	4	6	0
29	XJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	YJ	1	43	33	4	6	0
29	YJ	1	43	33	4	6	0
29	ZJ	1	43	33	4	6	0
29	ZJ	1	43	33	4	6	0
29	ZJ	1	43	33	4	6	0
29	aJ	1	43	33	4	6	0
29	aJ	1	43	33	4	6	0
29	bJ	1	43	33	4	6	0
29	bJ	1	43	33	4	6	0
29	bJ	1	43	33	4	6	0
29	cJ	1	43	33	4	6	0
29	cJ	1	43	33	4	6	0
29	dJ	1	43	33	4	6	0
29	dJ	1	43	33	4	6	0
29	dJ	1	43	33	4	6	0
29	eJ	1	43	33	4	6	0
29	eJ	1	43	33	4	6	0
29	fJ	1	43	33	4	6	0
29	fJ	1	43	33	4	6	0
29	fJ	1	43	33	4	6	0
29	gJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	gJ	1	43	33	4	6	0
29	hJ	1	43	33	4	6	0
29	hJ	1	43	33	4	6	0
29	hJ	1	43	33	4	6	0
29	iJ	1	43	33	4	6	0
29	iJ	1	43	33	4	6	0
29	jJ	1	43	33	4	6	0
29	jJ	1	43	33	4	6	0
29	jJ	1	43	33	4	6	0
29	kJ	1	43	33	4	6	0
29	kJ	1	43	33	4	6	0
29	lJ	1	43	33	4	6	0
29	lJ	1	43	33	4	6	0
29	lJ	1	43	33	4	6	0
29	mJ	1	43	33	4	6	0
29	mJ	1	43	33	4	6	0
29	nJ	1	43	33	4	6	0
29	nJ	1	43	33	4	6	0
29	nJ	1	43	33	4	6	0
29	oJ	1	43	33	4	6	0
29	oJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	pJ	1	Total 43	C 33	N 4	O 6	0
29	pJ	1	Total 43	C 33	N 4	O 6	0
29	pJ	1	Total 43	C 33	N 4	O 6	0
29	qJ	1	Total 43	C 33	N 4	O 6	0
29	qJ	1	Total 43	C 33	N 4	O 6	0
29	rJ	1	Total 43	C 33	N 4	O 6	0
29	rJ	1	Total 43	C 33	N 4	O 6	0
29	rJ	1	Total 43	C 33	N 4	O 6	0
29	sJ	1	Total 43	C 33	N 4	O 6	0
29	sJ	1	Total 43	C 33	N 4	O 6	0
29	sJ	1	Total 43	C 33	N 4	O 6	0
29	tJ	1	Total 43	C 33	N 4	O 6	0
29	tJ	1	Total 43	C 33	N 4	O 6	0
29	uJ	1	Total 43	C 33	N 4	O 6	0
29	uJ	1	Total 43	C 33	N 4	O 6	0
29	uJ	1	Total 43	C 33	N 4	O 6	0
29	vJ	1	Total 43	C 33	N 4	O 6	0
29	vJ	1	Total 43	C 33	N 4	O 6	0
29	wJ	1	Total 43	C 33	N 4	O 6	0
29	wJ	1	Total 43	C 33	N 4	O 6	0
29	wJ	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	xJ	1	Total 43	C 33	N 4	O 6	0
29	xJ	1	Total 43	C 33	N 4	O 6	0
29	xJ	1	Total 43	C 33	N 4	O 6	0
29	yJ	1	Total 43	C 33	N 4	O 6	0
29	zJ	1	Total 43	C 33	N 4	O 6	0
29	AK	1	Total 43	C 33	N 4	O 6	0
29	AK	1	Total 43	C 33	N 4	O 6	0
29	AK	1	Total 43	C 33	N 4	O 6	0
29	DK	1	Total 43	C 33	N 4	O 6	0
29	FK	1	Total 43	C 33	N 4	O 6	0
29	HK	1	Total 43	C 33	N 4	O 6	0
29	JK	1	Total 43	C 33	N 4	O 6	0
29	LK	1	Total 43	C 33	N 4	O 6	0
29	NK	1	Total 43	C 33	N 4	O 6	0
29	OK	1	Total 43	C 33	N 4	O 6	0
29	OK	1	Total 43	C 33	N 4	O 6	0
29	PK	1	Total 43	C 33	N 4	O 6	0
29	PK	1	Total 43	C 33	N 4	O 6	0
29	PK	1	Total 43	C 33	N 4	O 6	0
29	QK	1	Total 43	C 33	N 4	O 6	0
29	QK	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	RK	1	43	33	4	6	0
29	RK	1	43	33	4	6	0
29	RK	1	43	33	4	6	0
29	SK	1	43	33	4	6	0
29	SK	1	43	33	4	6	0
29	TK	1	43	33	4	6	0
29	TK	1	43	33	4	6	0
29	UK	1	43	33	4	6	0
29	UK	1	43	33	4	6	0
29	UK	1	43	33	4	6	0
29	VK	1	43	33	4	6	0
29	VK	1	43	33	4	6	0
29	VK	1	43	33	4	6	0
29	WK	1	43	33	4	6	0
29	WK	1	43	33	4	6	0
29	YK	1	43	33	4	6	0
29	YK	1	43	33	4	6	0
29	ZK	1	43	33	4	6	0
29	ZK	1	43	33	4	6	0
29	ZK	1	43	33	4	6	0
29	aK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	aK	1	43	33	4	6	0
29	aK	1	43	33	4	6	0
29	bK	1	43	33	4	6	0
29	bK	1	43	33	4	6	0
29	cK	1	43	33	4	6	0
29	cK	1	43	33	4	6	0
29	cK	1	43	33	4	6	0
29	dK	1	43	33	4	6	0
29	dK	1	43	33	4	6	0
29	eK	1	43	33	4	6	0
29	eK	1	43	33	4	6	0
29	eK	1	43	33	4	6	0
29	fK	1	43	33	4	6	0
29	fK	1	43	33	4	6	0
29	gK	1	43	33	4	6	0
29	gK	1	43	33	4	6	0
29	gK	1	43	33	4	6	0
29	hK	1	43	33	4	6	0
29	hK	1	43	33	4	6	0
29	iK	1	43	33	4	6	0
29	iK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	iK	1	Total 43	C 33	N 4	O 6	0
29	jK	1	Total 43	C 33	N 4	O 6	0
29	jK	1	Total 43	C 33	N 4	O 6	0
29	jK	1	Total 43	C 33	N 4	O 6	0
29	kK	1	Total 43	C 33	N 4	O 6	0
29	kK	1	Total 43	C 33	N 4	O 6	0
29	kK	1	Total 43	C 33	N 4	O 6	0
29	lK	1	Total 43	C 33	N 4	O 6	0
29	lK	1	Total 43	C 33	N 4	O 6	0
29	mK	1	Total 43	C 33	N 4	O 6	0
29	mK	1	Total 43	C 33	N 4	O 6	0
29	AL	1	Total 43	C 33	N 4	O 6	0
29	AL	1	Total 43	C 33	N 4	O 6	0
29	AL	1	Total 43	C 33	N 4	O 6	0
29	BL	1	Total 43	C 33	N 4	O 6	0
29	BL	1	Total 43	C 33	N 4	O 6	0
29	BL	1	Total 43	C 33	N 4	O 6	0
29	CL	1	Total 43	C 33	N 4	O 6	0
29	CL	1	Total 43	C 33	N 4	O 6	0
29	DL	1	Total 43	C 33	N 4	O 6	0
29	DL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	EL	1	Total 43	C 33	N 4	O 6	0
29	EL	1	Total 43	C 33	N 4	O 6	0
29	FL	1	Total 43	C 33	N 4	O 6	0
29	FL	1	Total 43	C 33	N 4	O 6	0
29	FL	1	Total 43	C 33	N 4	O 6	0
29	GL	1	Total 43	C 33	N 4	O 6	0
29	GL	1	Total 43	C 33	N 4	O 6	0
29	HL	1	Total 43	C 33	N 4	O 6	0
29	HL	1	Total 43	C 33	N 4	O 6	0
29	IL	1	Total 43	C 33	N 4	O 6	0
29	IL	1	Total 43	C 33	N 4	O 6	0
29	IL	1	Total 43	C 33	N 4	O 6	0
29	JL	1	Total 43	C 33	N 4	O 6	0
29	JL	1	Total 43	C 33	N 4	O 6	0
29	JL	1	Total 43	C 33	N 4	O 6	0
29	KL	1	Total 43	C 33	N 4	O 6	0
29	KL	1	Total 43	C 33	N 4	O 6	0
29	LL	1	Total 43	C 33	N 4	O 6	0
29	LL	1	Total 43	C 33	N 4	O 6	0
29	ML	1	Total 43	C 33	N 4	O 6	0
29	ML	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	NL	1	Total 43	C 33	N 4	O 6	0
29	NL	1	Total 43	C 33	N 4	O 6	0
29	NL	1	Total 43	C 33	N 4	O 6	0
29	OL	1	Total 43	C 33	N 4	O 6	0
29	OL	1	Total 43	C 33	N 4	O 6	0
29	PL	1	Total 43	C 33	N 4	O 6	0
29	PL	1	Total 43	C 33	N 4	O 6	0
29	PL	1	Total 43	C 33	N 4	O 6	0
29	QL	1	Total 43	C 33	N 4	O 6	0
29	QL	1	Total 43	C 33	N 4	O 6	0
29	RL	1	Total 43	C 33	N 4	O 6	0
29	RL	1	Total 43	C 33	N 4	O 6	0
29	RL	1	Total 43	C 33	N 4	O 6	0
29	SL	1	Total 43	C 33	N 4	O 6	0
29	SL	1	Total 43	C 33	N 4	O 6	0
29	TL	1	Total 43	C 33	N 4	O 6	0
29	TL	1	Total 43	C 33	N 4	O 6	0
29	TL	1	Total 43	C 33	N 4	O 6	0
29	UL	1	Total 43	C 33	N 4	O 6	0
29	UL	1	Total 43	C 33	N 4	O 6	0
29	VL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	VL	1	43	33	4	6	0
29	WL	1	43	33	4	6	0
29	WL	1	43	33	4	6	0
29	WL	1	43	33	4	6	0
29	XL	1	43	33	4	6	0
29	XL	1	43	33	4	6	0
29	XL	1	43	33	4	6	0
29	YL	1	43	33	4	6	0
29	YL	1	43	33	4	6	0
29	ZL	1	43	33	4	6	0
29	ZL	1	43	33	4	6	0
29	ZL	1	43	33	4	6	0
29	aL	1	43	33	4	6	0
29	aL	1	43	33	4	6	0
29	bL	1	43	33	4	6	0
29	bL	1	43	33	4	6	0
29	bL	1	43	33	4	6	0
29	cL	1	43	33	4	6	0
29	cL	1	43	33	4	6	0
29	dL	1	43	33	4	6	0
29	dL	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	dL	1	Total 43	C 33	N 4	O 6	0
29	eL	1	Total 43	C 33	N 4	O 6	0
29	eL	1	Total 43	C 33	N 4	O 6	0
29	fL	1	Total 43	C 33	N 4	O 6	0
29	fL	1	Total 43	C 33	N 4	O 6	0
29	fL	1	Total 43	C 33	N 4	O 6	0
29	gL	1	Total 43	C 33	N 4	O 6	0
29	gL	1	Total 43	C 33	N 4	O 6	0
29	hL	1	Total 43	C 33	N 4	O 6	0
29	hL	1	Total 43	C 33	N 4	O 6	0
29	hL	1	Total 43	C 33	N 4	O 6	0
29	iL	1	Total 43	C 33	N 4	O 6	0
29	iL	1	Total 43	C 33	N 4	O 6	0
29	jL	1	Total 43	C 33	N 4	O 6	0
29	jL	1	Total 43	C 33	N 4	O 6	0
29	jL	1	Total 43	C 33	N 4	O 6	0
29	kL	1	Total 43	C 33	N 4	O 6	0
29	kL	1	Total 43	C 33	N 4	O 6	0
29	lL	1	Total 43	C 33	N 4	O 6	0
29	lL	1	Total 43	C 33	N 4	O 6	0
29	lL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	mL	1	Total 43	C 33	N 4	O 6	0
29	mL	1	Total 43	C 33	N 4	O 6	0
29	nL	1	Total 43	C 33	N 4	O 6	0
29	nL	1	Total 43	C 33	N 4	O 6	0
29	nL	1	Total 43	C 33	N 4	O 6	0
29	oL	1	Total 43	C 33	N 4	O 6	0
29	oL	1	Total 43	C 33	N 4	O 6	0
29	pL	1	Total 43	C 33	N 4	O 6	0
29	pL	1	Total 43	C 33	N 4	O 6	0
29	pL	1	Total 43	C 33	N 4	O 6	0
29	qL	1	Total 43	C 33	N 4	O 6	0
29	qL	1	Total 43	C 33	N 4	O 6	0
29	rL	1	Total 43	C 33	N 4	O 6	0
29	rL	1	Total 43	C 33	N 4	O 6	0
29	rL	1	Total 43	C 33	N 4	O 6	0
29	sL	1	Total 43	C 33	N 4	O 6	0
29	sL	1	Total 43	C 33	N 4	O 6	0
29	sL	1	Total 43	C 33	N 4	O 6	0
29	tL	1	Total 43	C 33	N 4	O 6	0
29	tL	1	Total 43	C 33	N 4	O 6	0
29	uL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	uL	1	43	33	4	6	0
29	uL	1	43	33	4	6	0
29	vL	1	43	33	4	6	0
29	vL	1	43	33	4	6	0
29	wL	1	43	33	4	6	0
29	wL	1	43	33	4	6	0
29	wL	1	43	33	4	6	0
29	xL	1	43	33	4	6	0
29	xL	1	43	33	4	6	0
29	xL	1	43	33	4	6	0
29	yL	1	43	33	4	6	0
29	zL	1	43	33	4	6	0
29	AM	1	43	33	4	6	0
29	AM	1	43	33	4	6	0
29	AM	1	43	33	4	6	0
29	BM	1	43	33	4	6	0
29	CM	1	43	33	4	6	0
29	CM	1	43	33	4	6	0
29	DM	1	43	33	4	6	0
29	DM	1	43	33	4	6	0
29	DM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	EM	1	43	33	4	6	0
29	EM	1	43	33	4	6	0
29	FM	1	43	33	4	6	0
29	FM	1	43	33	4	6	0
29	FM	1	43	33	4	6	0
29	GM	1	43	33	4	6	0
29	GM	1	43	33	4	6	0
29	HM	1	43	33	4	6	0
29	HM	1	43	33	4	6	0
29	HM	1	43	33	4	6	0
29	IM	1	43	33	4	6	0
29	IM	1	43	33	4	6	0
29	JM	1	43	33	4	6	0
29	JM	1	43	33	4	6	0
29	JM	1	43	33	4	6	0
29	KM	1	43	33	4	6	0
29	KM	1	43	33	4	6	0
29	KM	1	43	33	4	6	0
29	LM	1	43	33	4	6	0
29	LM	1	43	33	4	6	0
29	LM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	MM	1	43	33	4	6	0
29	MM	1	43	33	4	6	0
29	NM	1	43	33	4	6	0
29	NM	1	43	33	4	6	0
29	OM	1	43	33	4	6	0
29	OM	1	43	33	4	6	0
29	PM	1	43	33	4	6	0
29	PM	1	43	33	4	6	0
29	QM	1	43	33	4	6	0
29	QM	1	43	33	4	6	0
29	QM	1	43	33	4	6	0
29	RM	1	43	33	4	6	0
29	RM	1	43	33	4	6	0
29	RM	1	43	33	4	6	0
29	SM	1	43	33	4	6	0
29	SM	1	43	33	4	6	0
29	TM	1	43	33	4	6	0
29	TM	1	43	33	4	6	0
29	TM	1	43	33	4	6	0
29	UM	1	43	33	4	6	0
29	VM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	VM	1	43	33	4	6	0
29	VM	1	43	33	4	6	0
29	WM	1	43	33	4	6	0
29	WM	1	43	33	4	6	0
29	XM	1	43	33	4	6	0
29	XM	1	43	33	4	6	0
29	YM	1	43	33	4	6	0
29	YM	1	43	33	4	6	0
29	YM	1	43	33	4	6	0
29	ZM	1	43	33	4	6	0
29	ZM	1	43	33	4	6	0
29	ZM	1	43	33	4	6	0
29	aM	1	43	33	4	6	0
29	aM	1	43	33	4	6	0
29	aM	1	43	33	4	6	0
29	cM	1	43	33	4	6	0
29	cM	1	43	33	4	6	0
29	cM	1	43	33	4	6	0
29	dM	1	43	33	4	6	0
29	dM	1	43	33	4	6	0
29	eM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	eM	1	Total 43	C 33	N 4	O 6	0
29	fM	1	Total 43	C 33	N 4	O 6	0
29	fM	1	Total 43	C 33	N 4	O 6	0
29	gM	1	Total 43	C 33	N 4	O 6	0
29	gM	1	Total 43	C 33	N 4	O 6	0
29	gM	1	Total 43	C 33	N 4	O 6	0
29	hM	1	Total 43	C 33	N 4	O 6	0
29	hM	1	Total 43	C 33	N 4	O 6	0
29	iM	1	Total 43	C 33	N 4	O 6	0
29	iM	1	Total 43	C 33	N 4	O 6	0
29	iM	1	Total 43	C 33	N 4	O 6	0
29	jM	1	Total 43	C 33	N 4	O 6	0
29	jM	1	Total 43	C 33	N 4	O 6	0
29	kM	1	Total 43	C 33	N 4	O 6	0
29	kM	1	Total 43	C 33	N 4	O 6	0
29	kM	1	Total 43	C 33	N 4	O 6	0
29	lM	1	Total 43	C 33	N 4	O 6	0
29	lM	1	Total 43	C 33	N 4	O 6	0
29	mM	1	Total 43	C 33	N 4	O 6	0
29	mM	1	Total 43	C 33	N 4	O 6	0
29	mM	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	AN	1	43	33	4	6	0
29	AN	1	43	33	4	6	0
29	BN	1	43	33	4	6	0
29	BN	1	43	33	4	6	0
29	BN	1	43	33	4	6	0
29	CN	1	43	33	4	6	0
29	CN	1	43	33	4	6	0
29	DN	1	43	33	4	6	0
29	DN	1	43	33	4	6	0
29	DN	1	43	33	4	6	0
29	EN	1	43	33	4	6	0
29	EN	1	43	33	4	6	0
29	FN	1	43	33	4	6	0
29	FN	1	43	33	4	6	0
29	FN	1	43	33	4	6	0
29	GN	1	43	33	4	6	0
29	GN	1	43	33	4	6	0
29	HN	1	43	33	4	6	0
29	HN	1	43	33	4	6	0
29	HN	1	43	33	4	6	0
29	IN	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	IN	1	43	33	4	6	0
29	JN	1	43	33	4	6	0
29	JN	1	43	33	4	6	0
29	JN	1	43	33	4	6	0
29	KN	1	43	33	4	6	0
29	KN	1	43	33	4	6	0
29	LN	1	43	33	4	6	0
29	LN	1	43	33	4	6	0
29	LN	1	43	33	4	6	0
29	MN	1	43	33	4	6	0
29	MN	1	43	33	4	6	0
29	MN	1	43	33	4	6	0
29	AO	1	43	33	4	6	0
29	AO	1	43	33	4	6	0
29	BO	1	43	33	4	6	0
29	BO	1	43	33	4	6	0
29	BO	1	43	33	4	6	0
29	CO	1	43	33	4	6	0
29	CO	1	43	33	4	6	0
29	DO	1	43	33	4	6	0
29	DO	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	DO	1	Total 43	C 33	N 4	O 6	0
29	EO	1	Total 43	C 33	N 4	O 6	0
29	EO	1	Total 43	C 33	N 4	O 6	0
29	FO	1	Total 43	C 33	N 4	O 6	0
29	FO	1	Total 43	C 33	N 4	O 6	0
29	FO	1	Total 43	C 33	N 4	O 6	0
29	GO	1	Total 43	C 33	N 4	O 6	0
29	GO	1	Total 43	C 33	N 4	O 6	0
29	HO	1	Total 43	C 33	N 4	O 6	0
29	HO	1	Total 43	C 33	N 4	O 6	0
29	HO	1	Total 43	C 33	N 4	O 6	0
29	IO	1	Total 43	C 33	N 4	O 6	0
29	IO	1	Total 43	C 33	N 4	O 6	0
29	IO	1	Total 43	C 33	N 4	O 6	0
29	JO	1	Total 43	C 33	N 4	O 6	0
29	JO	1	Total 43	C 33	N 4	O 6	0
29	JO	1	Total 43	C 33	N 4	O 6	0
29	KO	1	Total 43	C 33	N 4	O 6	0
29	KO	1	Total 43	C 33	N 4	O 6	0
29	LO	1	Total 43	C 33	N 4	O 6	0
29	LO	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	MO	1	43	33	4	6	0
29	MO	1	43	33	4	6	0
29	MO	1	43	33	4	6	0
29	NO	1	43	33	4	6	0
29	NO	1	43	33	4	6	0
29	NO	1	43	33	4	6	0
29	AQ	1	43	33	4	6	0
29	AQ	1	43	33	4	6	0
29	BQ	1	43	33	4	6	0
29	BQ	1	43	33	4	6	0
29	BQ	1	43	33	4	6	0
29	CQ	1	43	33	4	6	0
29	CQ	1	43	33	4	6	0
29	DQ	1	43	33	4	6	0
29	DQ	1	43	33	4	6	0
29	DQ	1	43	33	4	6	0
29	EQ	1	43	33	4	6	0
29	EQ	1	43	33	4	6	0
29	FQ	1	43	33	4	6	0
29	FQ	1	43	33	4	6	0
29	FQ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	GQ	1	43	33	4	6	0
29	GQ	1	43	33	4	6	0
29	HQ	1	43	33	4	6	0
29	HQ	1	43	33	4	6	0
29	HQ	1	43	33	4	6	0
29	IQ	1	43	33	4	6	0
29	IQ	1	43	33	4	6	0
29	JQ	1	43	33	4	6	0
29	JQ	1	43	33	4	6	0
29	JQ	1	43	33	4	6	0
29	KQ	1	43	33	4	6	0
29	KQ	1	43	33	4	6	0
29	LQ	1	43	33	4	6	0
29	LQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	eR	1	43	33	4	6	0
29	MR	1	43	33	4	6	0

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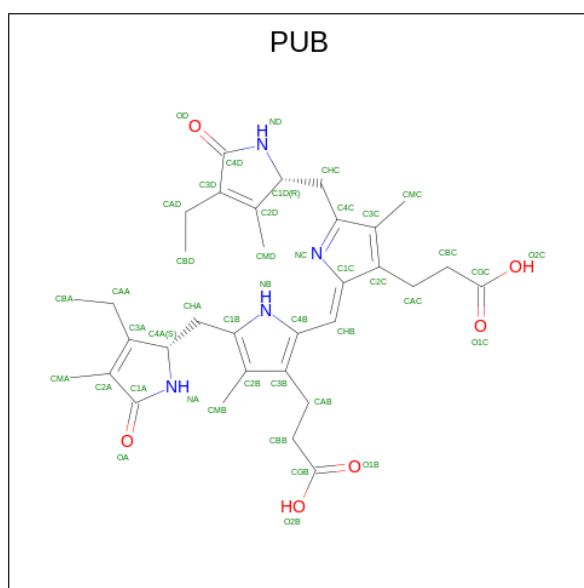
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	MR	1	43	33	4	6	0
29	NR	1	43	33	4	6	0
29	NR	1	43	33	4	6	0
29	NR	1	43	33	4	6	0
29	OR	1	43	33	4	6	0
29	OR	1	43	33	4	6	0
29	PR	1	43	33	4	6	0
29	PR	1	43	33	4	6	0
29	QR	1	43	33	4	6	0
29	QR	1	43	33	4	6	0
29	RR	1	43	33	4	6	0
29	RR	1	43	33	4	6	0
29	RR	1	43	33	4	6	0
29	SR	1	43	33	4	6	0
29	SR	1	43	33	4	6	0
29	TR	1	43	33	4	6	0
29	TR	1	43	33	4	6	0
29	TR	1	43	33	4	6	0
29	UR	1	43	33	4	6	0
29	UR	1	43	33	4	6	0
29	VR	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	VR	1	Total 43	C 33	N 4	O 6	0
29	VR	1	Total 43	C 33	N 4	O 6	0
29	WR	1	Total 43	C 33	N 4	O 6	0
29	WR	1	Total 43	C 33	N 4	O 6	0
29	XR	1	Total 43	C 33	N 4	O 6	0
29	XR	1	Total 43	C 33	N 4	O 6	0
29	XR	1	Total 43	C 33	N 4	O 6	0

- Molecule 30 is PHYCOUROBILIN (three-letter code: PUB) (formula: $C_{33}H_{42}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	A1	1	Total 43	C 33	N 4	O 6	0
30	A1	1	Total 43	C 33	N 4	O 6	0
30	A7	1	Total 43	C 33	N 4	O 6	0
30	A7	1	Total 43	C 33	N 4	O 6	0

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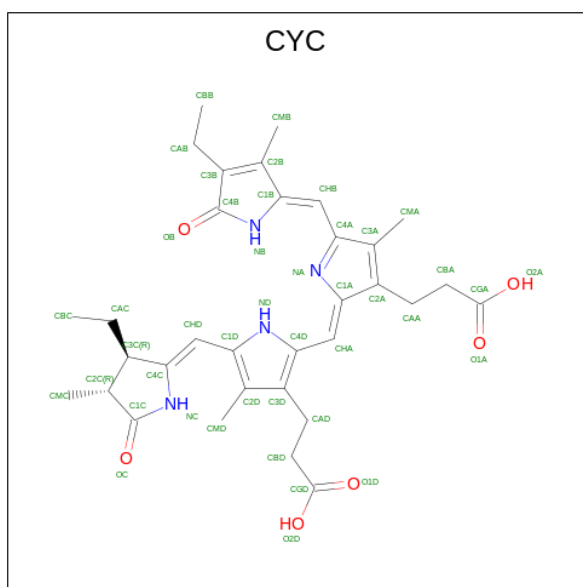
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	A9	1	Total 43	C 33	N 4	O 6	0
30	A9	1	Total 43	C 33	N 4	O 6	0
30	MA	1	Total 43	C 33	N 4	O 6	0
30	MA	1	Total 43	C 33	N 4	O 6	0
30	AB	1	Total 43	C 33	N 4	O 6	0
30	AB	1	Total 43	C 33	N 4	O 6	0
30	BB	1	Total 43	C 33	N 4	O 6	0
30	QB	1	Total 43	C 33	N 4	O 6	0
30	AF	1	Total 43	C 33	N 4	O 6	0
30	AF	1	Total 43	C 33	N 4	O 6	0
30	MG	1	Total 43	C 33	N 4	O 6	0
30	MG	1	Total 43	C 33	N 4	O 6	0
30	AI	1	Total 43	C 33	N 4	O 6	0
30	AI	1	Total 43	C 33	N 4	O 6	0
30	wJ	1	Total 43	C 33	N 4	O 6	0
30	wJ	1	Total 43	C 33	N 4	O 6	0
30	xJ	1	Total 43	C 33	N 4	O 6	0
30	xJ	1	Total 43	C 33	N 4	O 6	0
30	yJ	1	Total 43	C 33	N 4	O 6	0
30	yJ	1	Total 43	C 33	N 4	O 6	0
30	AK	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	AK	1	43	33	4	6	0
30	wL	1	43	33	4	6	0
30	wL	1	43	33	4	6	0
30	xL	1	43	33	4	6	0
30	xL	1	43	33	4	6	0
30	yL	1	43	33	4	6	0
30	yL	1	43	33	4	6	0
30	AM	1	43	33	4	6	0
30	AM	1	43	33	4	6	0
30	BM	1	43	33	4	6	0
30	QM	1	43	33	4	6	0
30	MN	1	43	33	4	6	0
30	MN	1	43	33	4	6	0
30	MQ	1	43	33	4	6	0
30	MQ	1	43	33	4	6	0

- Molecule 31 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
31	C1	1	43	33	4	6	0
31	D1	1	43	33	4	6	0
31	D1	1	43	33	4	6	0
31	E1	1	43	33	4	6	0
31	F1	1	43	33	4	6	0
31	H1	1	43	33	4	6	0
31	I1	1	43	33	4	6	0
31	J1	1	43	33	4	6	0
31	K1	1	43	33	4	6	0
31	L1	1	43	33	4	6	0
31	M1	1	43	33	4	6	0
31	N1	1	43	33	4	6	0
31	C7	1	43	33	4	6	0
31	D7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	E7	1	Total 43	C 33	N 4	O 6	0
31	F7	1	Total 43	C 33	N 4	O 6	0
31	G7	1	Total 43	C 33	N 4	O 6	0
31	H7	1	Total 43	C 33	N 4	O 6	0
31	I7	1	Total 43	C 33	N 4	O 6	0
31	J7	1	Total 43	C 33	N 4	O 6	0
31	K7	1	Total 43	C 33	N 4	O 6	0
31	L7	1	Total 43	C 33	N 4	O 6	0
31	M7	1	Total 43	C 33	N 4	O 6	0
31	N7	1	Total 43	C 33	N 4	O 6	0
31	C9	1	Total 43	C 33	N 4	O 6	0
31	D9	1	Total 43	C 33	N 4	O 6	0
31	E9	1	Total 43	C 33	N 4	O 6	0
31	F9	1	Total 43	C 33	N 4	O 6	0
31	G9	1	Total 43	C 33	N 4	O 6	0
31	H9	1	Total 43	C 33	N 4	O 6	0
31	I9	1	Total 43	C 33	N 4	O 6	0
31	J9	1	Total 43	C 33	N 4	O 6	0
31	K9	1	Total 43	C 33	N 4	O 6	0
31	L9	1	Total 43	C 33	N 4	O 6	0
31	M9	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	N9	1	Total 43	C 33	N 4	O 6	0
31	CF	1	Total 43	C 33	N 4	O 6	0
31	DF	1	Total 43	C 33	N 4	O 6	0
31	EF	1	Total 43	C 33	N 4	O 6	0
31	FF	1	Total 43	C 33	N 4	O 6	0
31	GF	1	Total 43	C 33	N 4	O 6	0
31	HF	1	Total 43	C 33	N 4	O 6	0
31	IF	1	Total 43	C 33	N 4	O 6	0
31	JF	1	Total 43	C 33	N 4	O 6	0
31	KF	1	Total 43	C 33	N 4	O 6	0
31	LF	1	Total 43	C 33	N 4	O 6	0
31	MF	1	Total 43	C 33	N 4	O 6	0
31	NF	1	Total 43	C 33	N 4	O 6	0
31	CI	1	Total 43	C 33	N 4	O 6	0
31	DI	1	Total 43	C 33	N 4	O 6	0
31	EI	1	Total 43	C 33	N 4	O 6	0
31	FI	1	Total 43	C 33	N 4	O 6	0
31	GI	1	Total 43	C 33	N 4	O 6	0
31	HI	1	Total 43	C 33	N 4	O 6	0
31	II	1	Total 43	C 33	N 4	O 6	0
31	JI	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	KI	1	43	33	4	6	0
31	LI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	NI	1	43	33	4	6	0
31	CK	1	43	33	4	6	0
31	DK	1	43	33	4	6	0
31	EK	1	43	33	4	6	0
31	FK	1	43	33	4	6	0
31	GK	1	43	33	4	6	0
31	HK	1	43	33	4	6	0
31	IK	1	43	33	4	6	0
31	JK	1	43	33	4	6	0
31	KK	1	43	33	4	6	0
31	LK	1	43	33	4	6	0
31	MK	1	43	33	4	6	0
31	NK	1	43	33	4	6	0
31	AP	1	43	33	4	6	0
31	DP	1	43	33	4	6	0
31	CP	1	43	33	4	6	0
31	FP	1	43	33	4	6	0
31	EP	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	BP	1	43	33	4	6	0
31	GP	1	43	33	4	6	0
31	HP	1	43	33	4	6	0
31	IP	1	43	33	4	6	0
31	JP	1	43	33	4	6	0
31	KP	1	43	33	4	6	0
31	MP	1	43	33	4	6	0
31	NP	1	43	33	4	6	0
31	OP	1	43	33	4	6	0
31	PP	1	43	33	4	6	0
31	QP	1	43	33	4	6	0
31	RP	1	43	33	4	6	0
31	SP	1	43	33	4	6	0
31	TP	1	43	33	4	6	0
31	UP	1	43	33	4	6	0
31	VP	1	43	33	4	6	0
31	WP	1	43	33	4	6	0
31	XP	1	43	33	4	6	0
31	YP	1	43	33	4	6	0
31	cP	1	43	33	4	6	0
31	eP	1	43	33	4	6	0

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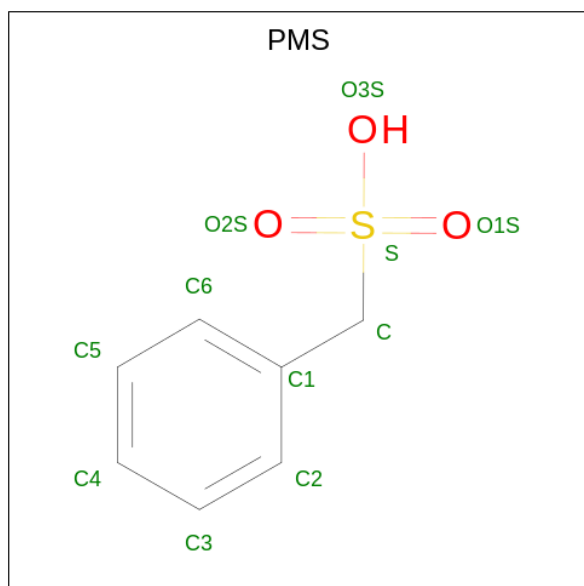
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	fP	1	Total 43	C 33	N 4	O 6	0
31	gP	1	Total 43	C 33	N 4	O 6	0
31	hP	1	Total 43	C 33	N 4	O 6	0
31	iP	1	Total 43	C 33	N 4	O 6	0
31	jP	1	Total 43	C 33	N 4	O 6	0
31	kP	1	Total 43	C 33	N 4	O 6	0
31	lP	1	Total 43	C 33	N 4	O 6	0
31	mP	1	Total 43	C 33	N 4	O 6	0
31	nP	1	Total 43	C 33	N 4	O 6	0
31	oP	1	Total 43	C 33	N 4	O 6	0
31	pP	1	Total 43	C 33	N 4	O 6	0
31	qP	1	Total 43	C 33	N 4	O 6	0
31	rP	1	Total 43	C 33	N 4	O 6	0
31	sP	1	Total 43	C 33	N 4	O 6	0
31	tP	1	Total 43	C 33	N 4	O 6	0
31	uP	1	Total 43	C 33	N 4	O 6	0
31	vP	1	Total 43	C 33	N 4	O 6	0
31	wP	1	Total 43	C 33	N 4	O 6	0
31	xP	1	Total 43	C 33	N 4	O 6	0
31	yP	1	Total 43	C 33	N 4	O 6	0
31	1P	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	1P	1	43	33	4	6	0

- Molecule 32 is phenylmethanesulfonic acid (three-letter code: PMS) (formula: $C_7H_8O_3S$).

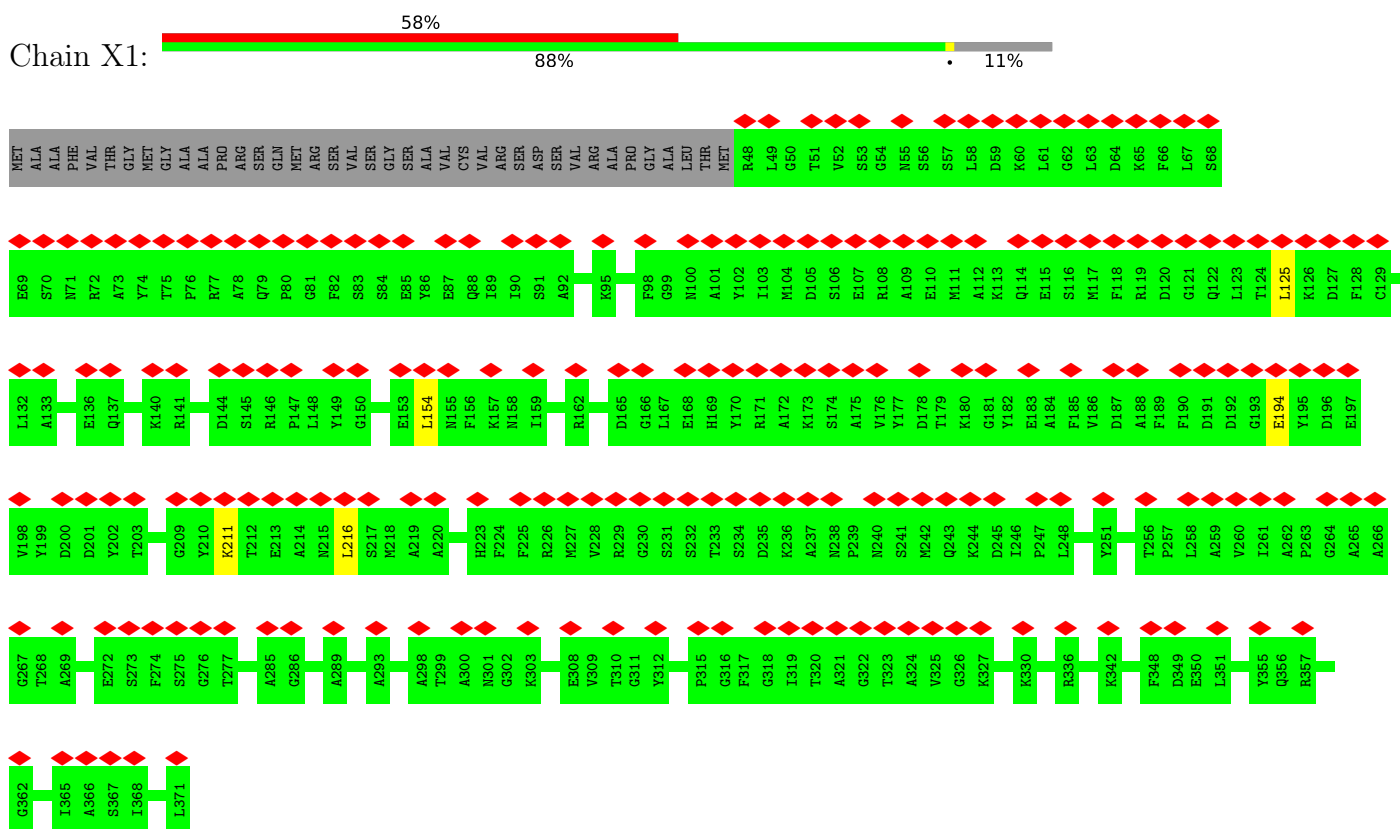


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	k6	1	11	7	3	1	0
32	k6	1	11	7	3	1	0
32	kH	1	11	7	3	1	0
32	kH	1	11	7	3	1	0

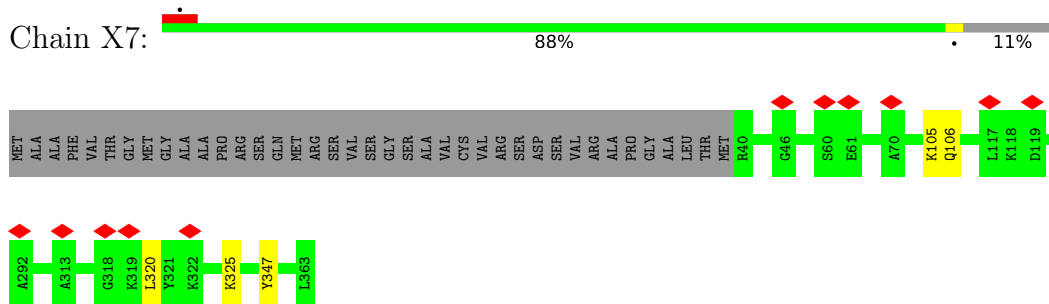
3 Residue-property plots [i](#)

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.

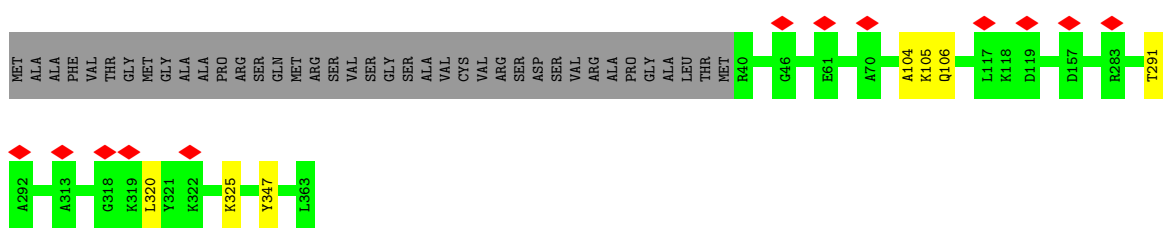
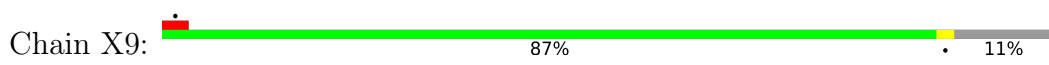
- Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



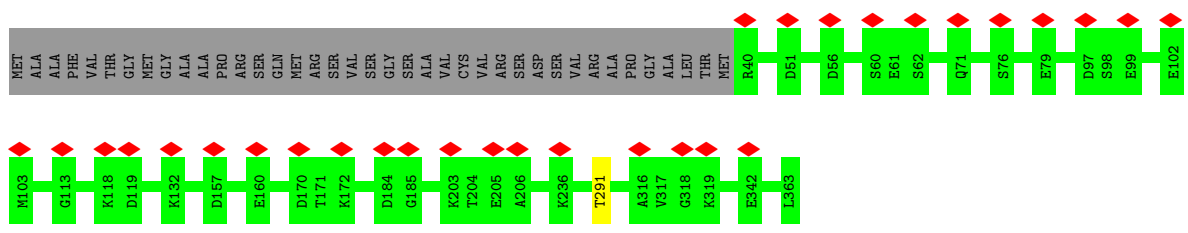
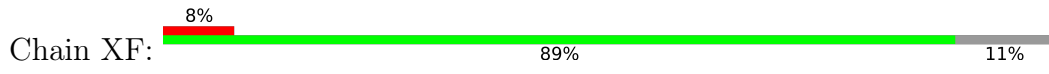
- Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



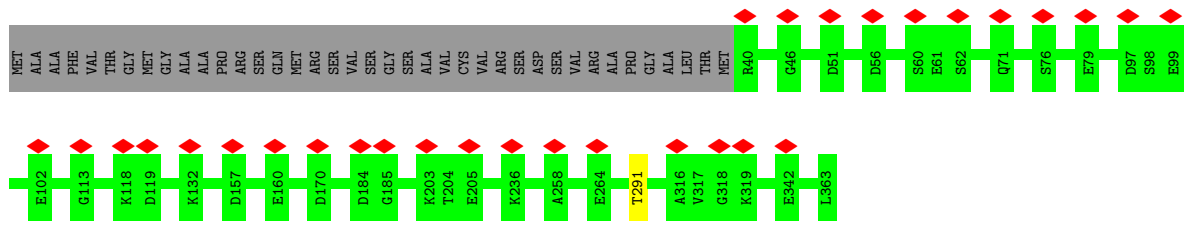
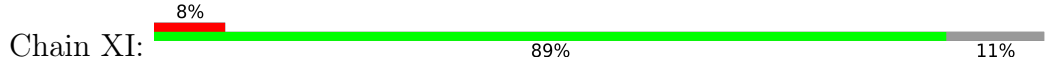
- Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



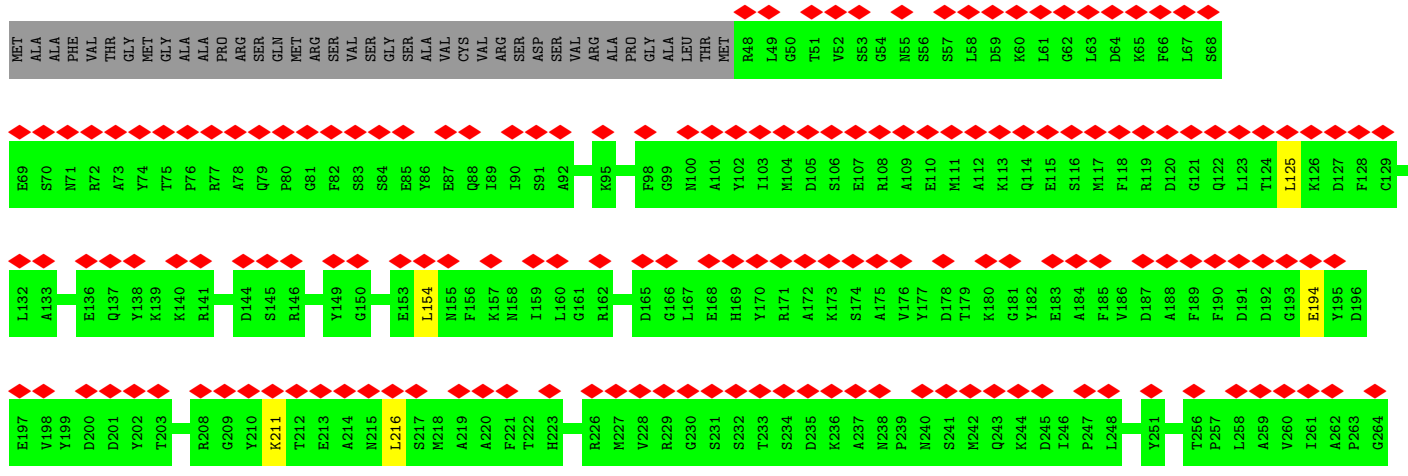
• Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

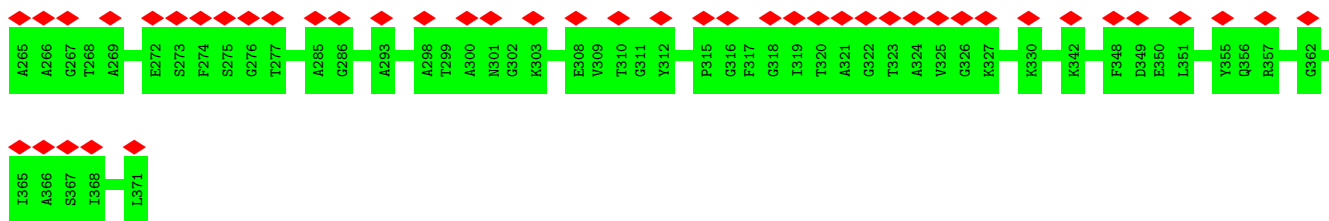


• Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

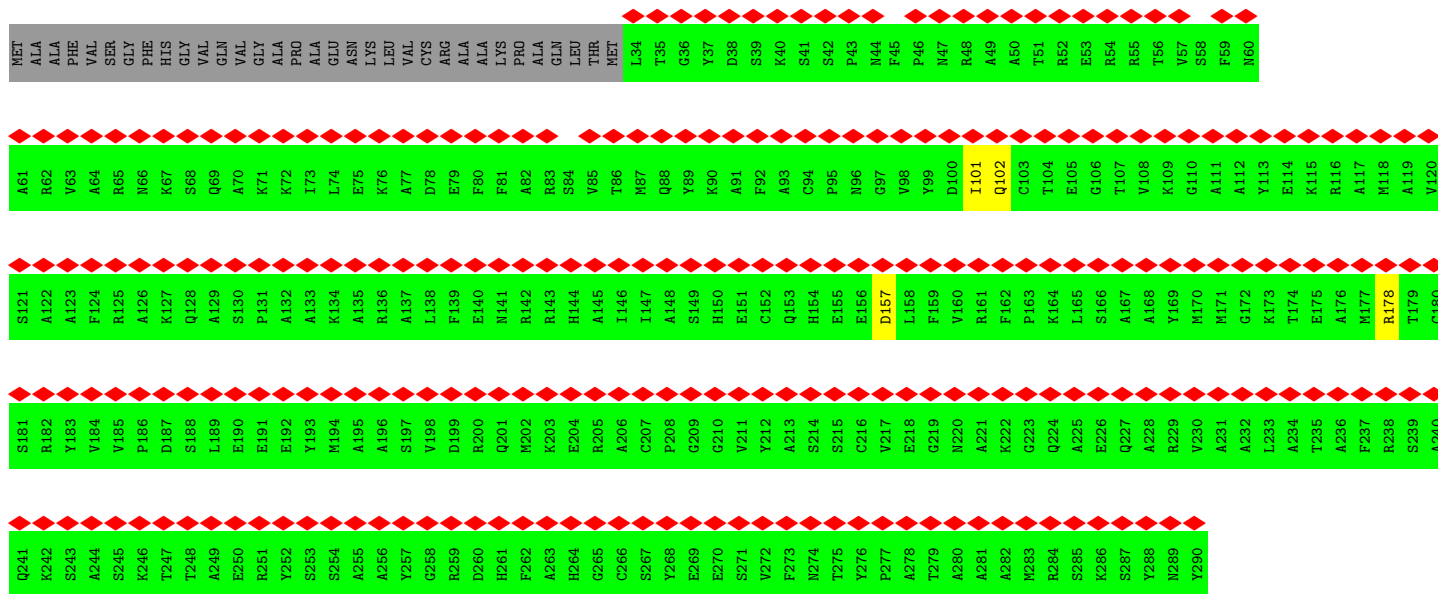
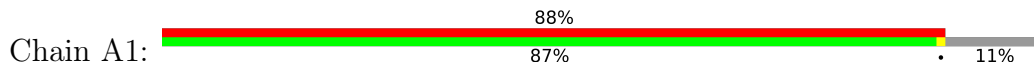


• Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

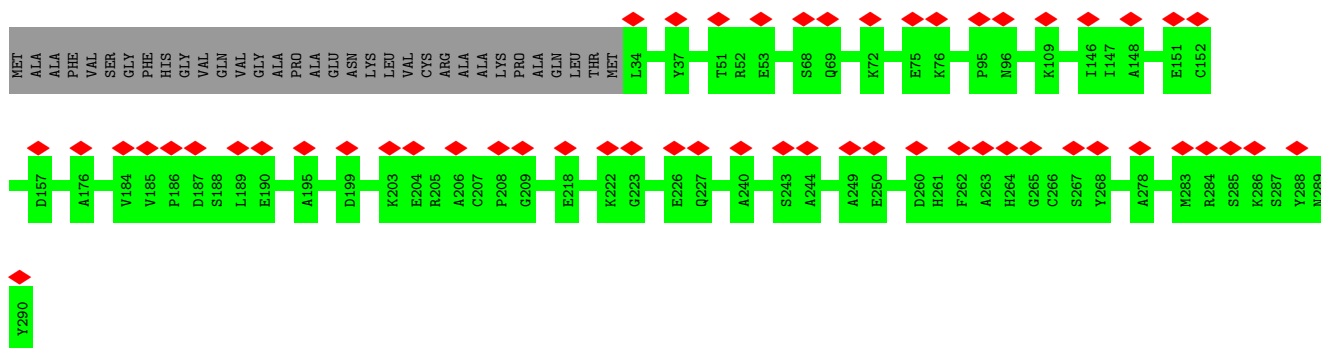
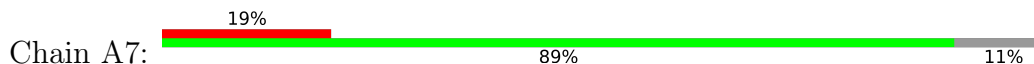




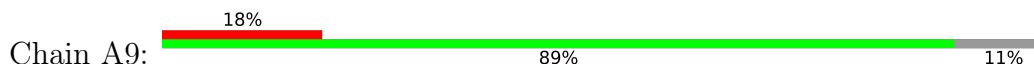
• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

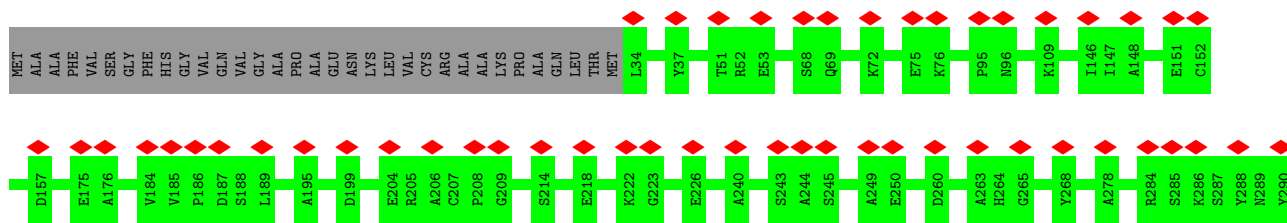


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

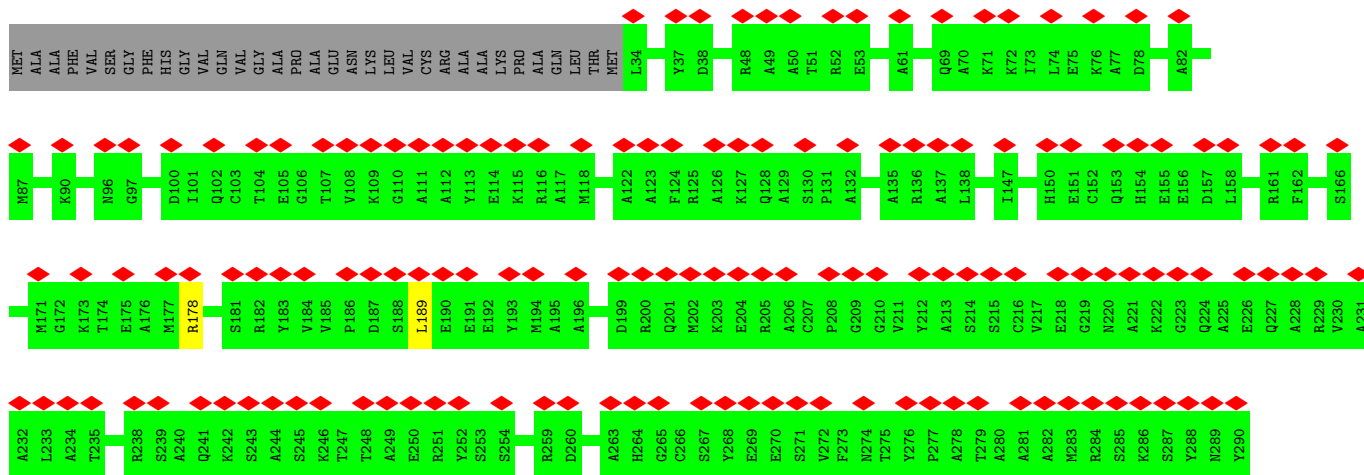
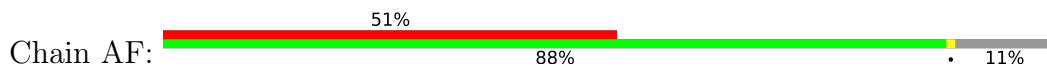


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

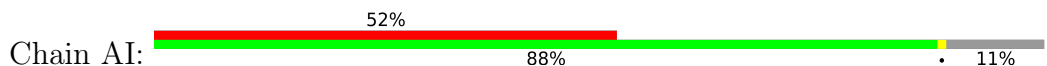




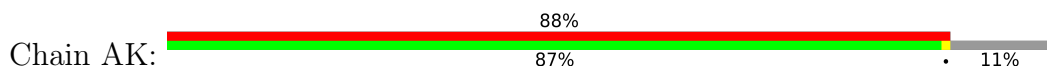
• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

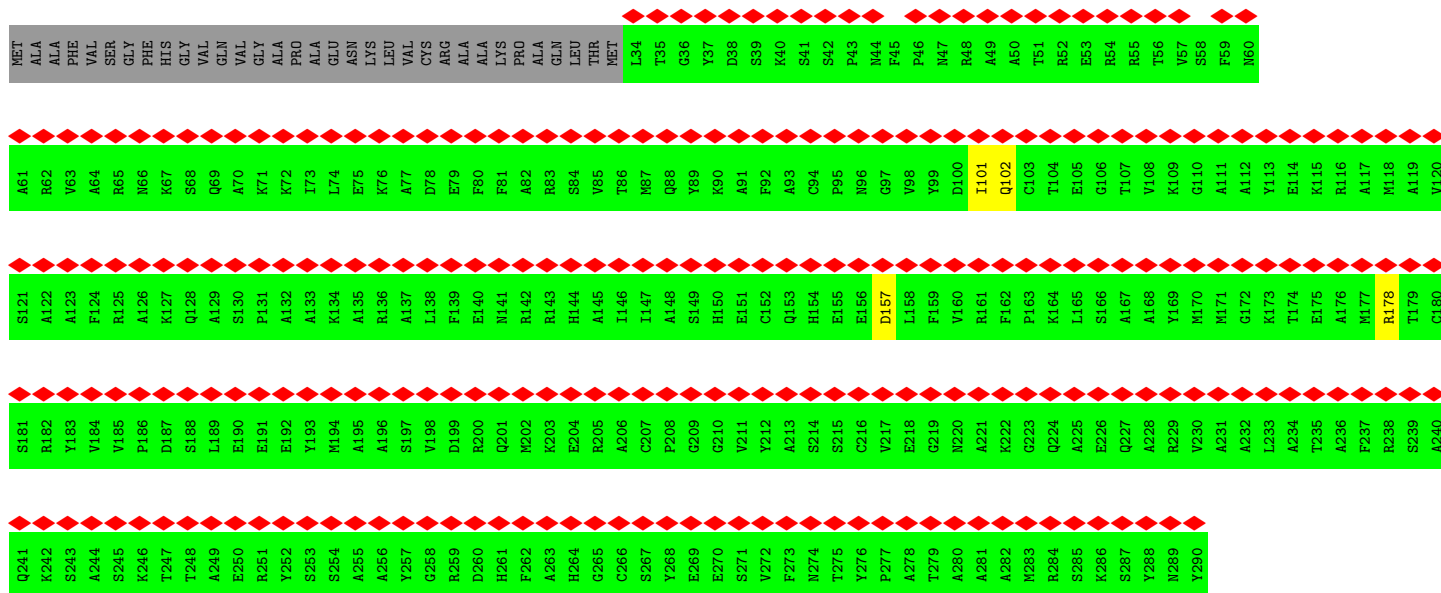


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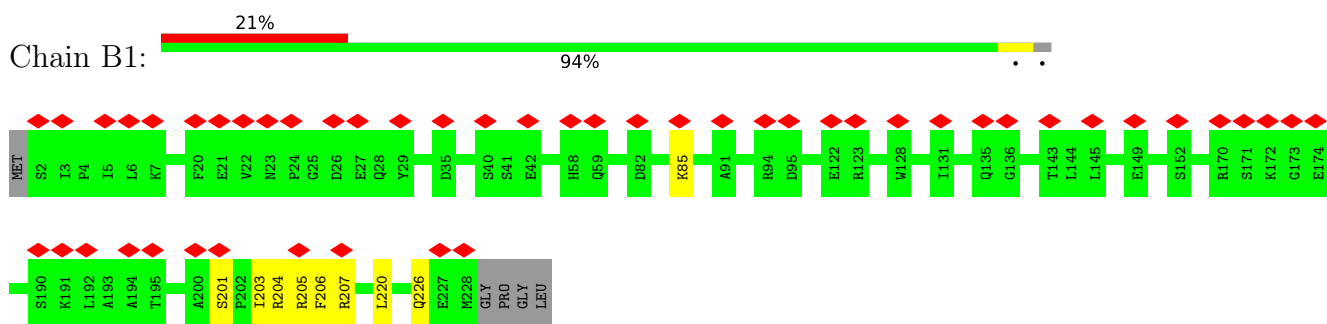


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

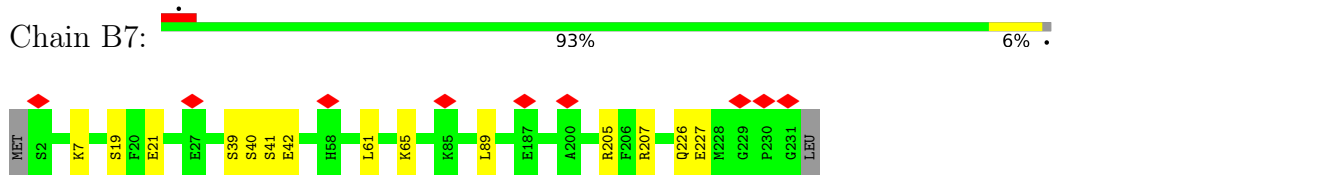




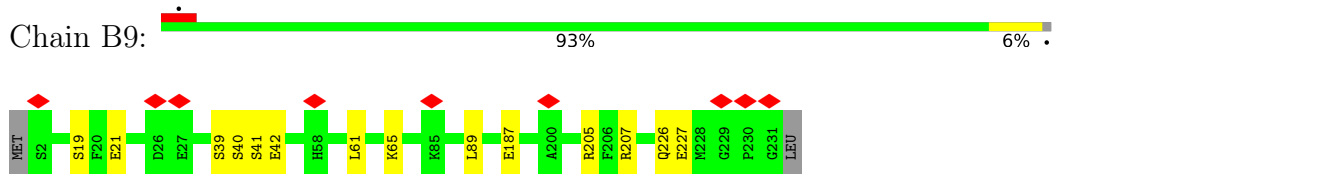
• Molecule 3: Phycobilisome rod-core linker polypeptide



• Molecule 3: Phycobilisome rod-core linker polypeptide

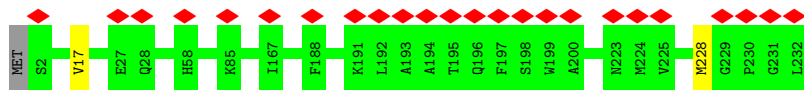


• Molecule 3: Phycobilisome rod-core linker polypeptide

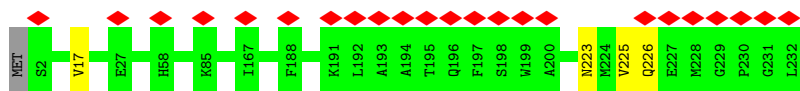


• Molecule 3: Phycobilisome rod-core linker polypeptide

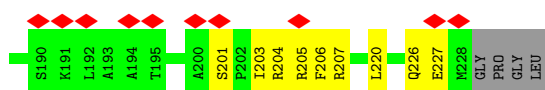
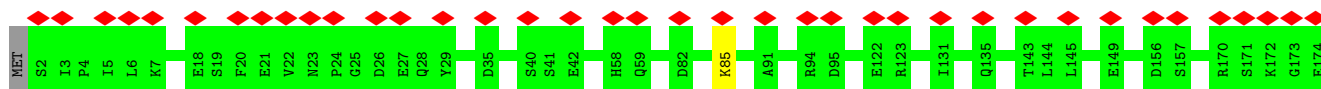




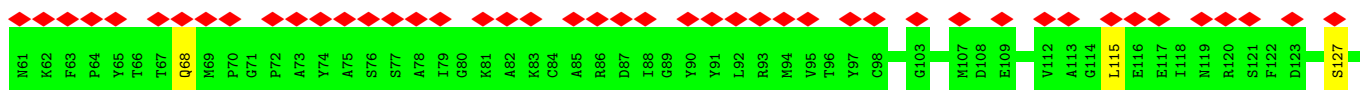
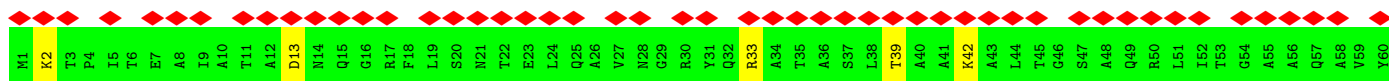
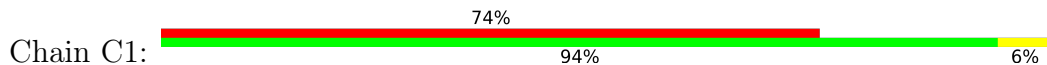
• Molecule 3: Phycobilisome rod-core linker polypeptide



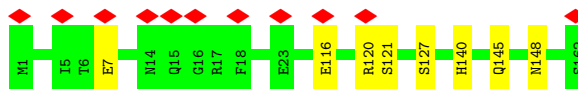
• Molecule 3: Phycobilisome rod-core linker polypeptide



• Molecule 4: C-phycoerythrin alpha subunit

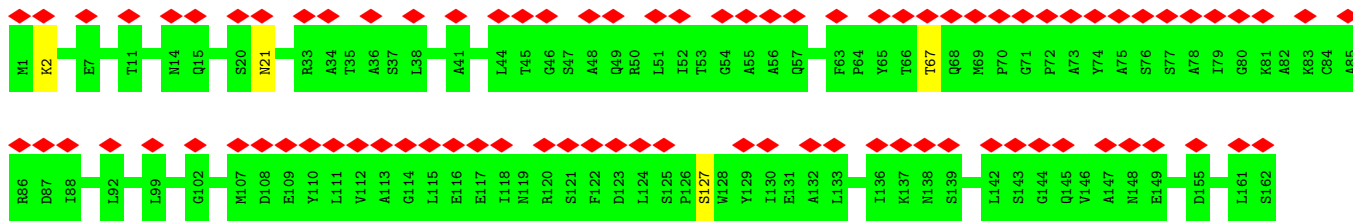


• Molecule 4: C-phycoerythrin alpha subunit

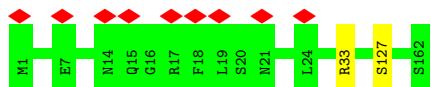


• Molecule 4: C-phycoerythrin alpha subunit

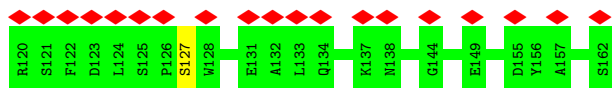
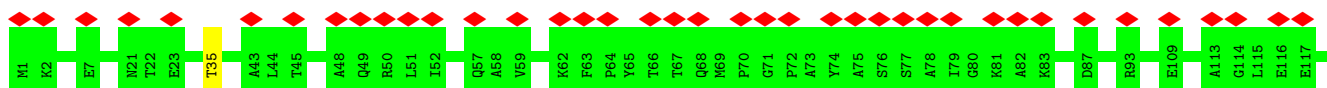




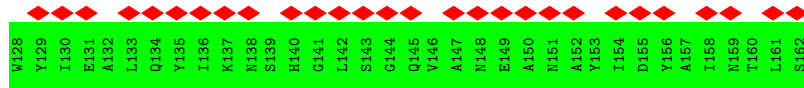
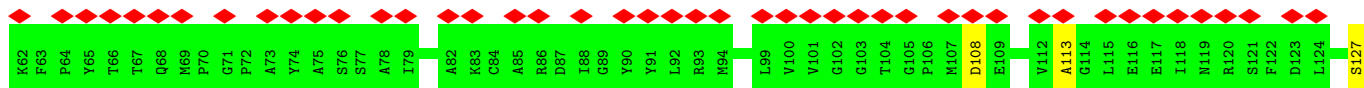
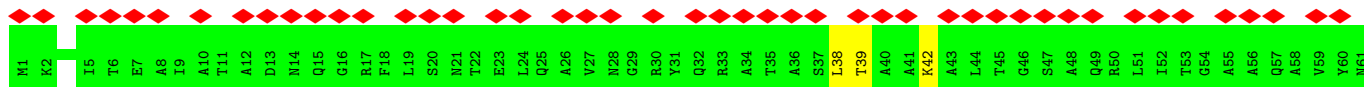
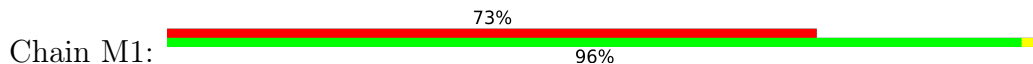
• Molecule 4: C-phycoerythrin alpha subunit



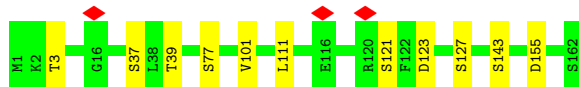
• Molecule 4: C-phycoerythrin alpha subunit



• Molecule 4: C-phycoerythrin alpha subunit



• Molecule 4: C-phycoerythrin alpha subunit



• Molecule 4: C-phycoerythrin alpha subunit

Chain E7:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain G7:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain I7:  93% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain K7:  93% 7%



• Molecule 4: C-phyco cyanin alpha subunit

Chain M7:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain C9:  93% 7%



• Molecule 4: C-phyco cyanin alpha subunit

Chain E9:  94% 6%




• Molecule 4: C-phyco cyanin alpha subunit

Chain G9:  94% 6%



● Molecule 4: C-phycoerythrin alpha subunit

Chain I9:  93% 6%



● Molecule 4: C-phycoerythrin alpha subunit

Chain K9:  93% 7%



● Molecule 4: C-phycoerythrin alpha subunit

Chain M9:  94% 6%



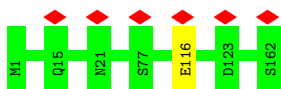
● Molecule 4: C-phycoerythrin alpha subunit

Chain CF:  99%



● Molecule 4: C-phycoerythrin alpha subunit

Chain EF:  99%



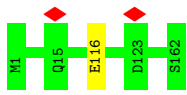
● Molecule 4: C-phycoerythrin alpha subunit

Chain GF:  99%



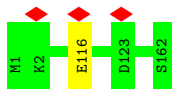
- Molecule 4: C-phycoerythrin alpha subunit

Chain IF:  99%



- Molecule 4: C-phycoerythrin alpha subunit

Chain KF:  99%



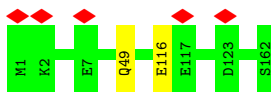
- Molecule 4: C-phycoerythrin alpha subunit

Chain MF:  99%



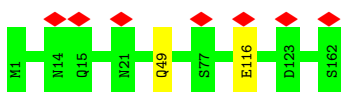
- Molecule 4: C-phycoerythrin alpha subunit

Chain CI:  99%



- Molecule 4: C-phycoerythrin alpha subunit

Chain EI:  99%



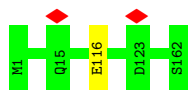
- Molecule 4: C-phycoerythrin alpha subunit

Chain GI:  99%

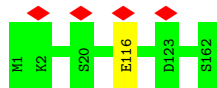


- Molecule 4: C-phycoerythrin alpha subunit

Chain II:  99%



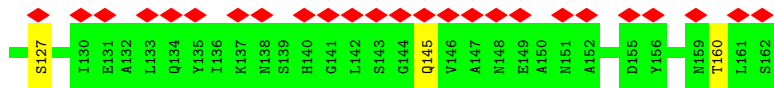
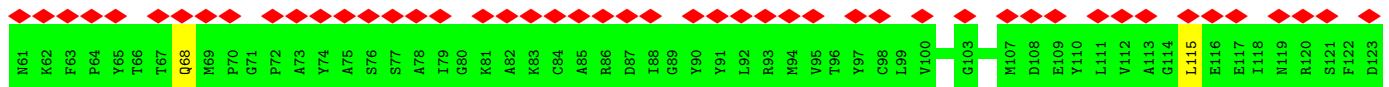
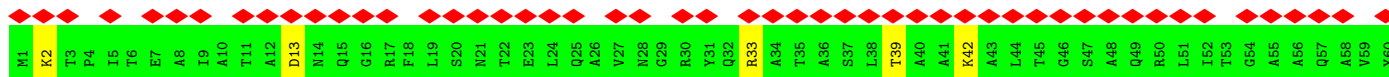
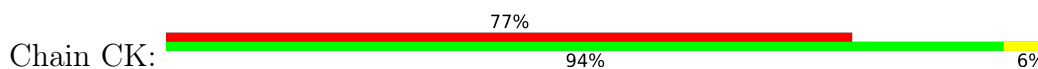
• Molecule 4: C-phycoerythrin alpha subunit



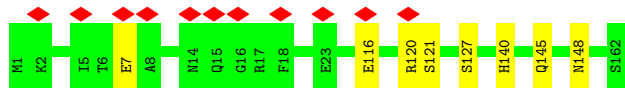
• Molecule 4: C-phycoerythrin alpha subunit



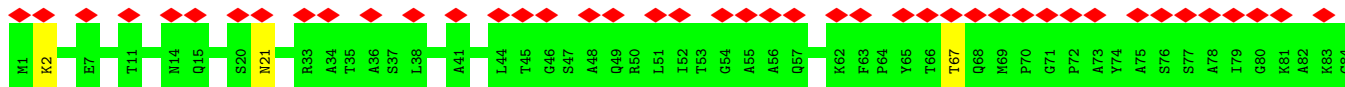
• Molecule 4: C-phycoerythrin alpha subunit

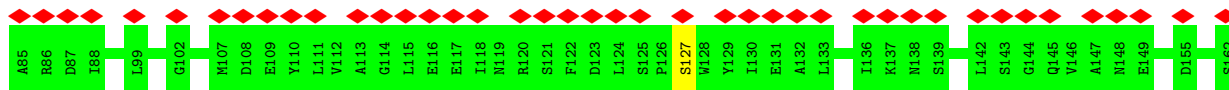


• Molecule 4: C-phycoerythrin alpha subunit

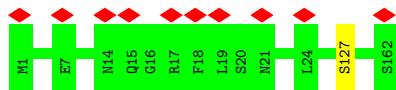


• Molecule 4: C-phycoerythrin alpha subunit

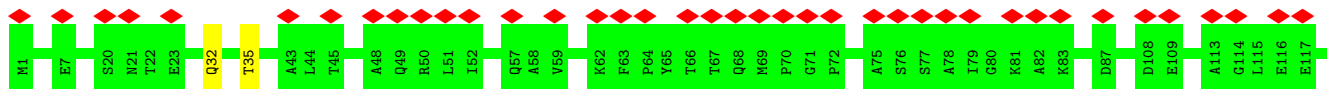




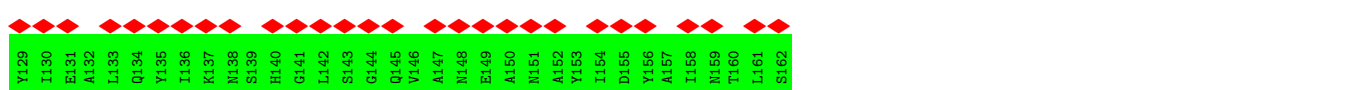
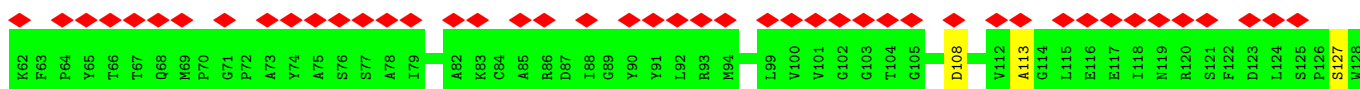
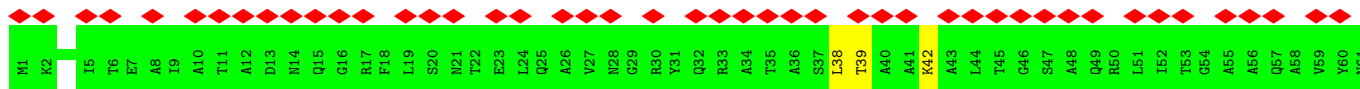
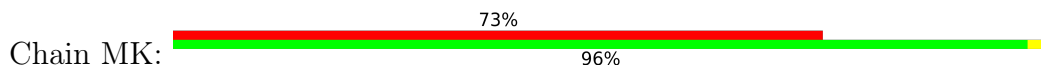
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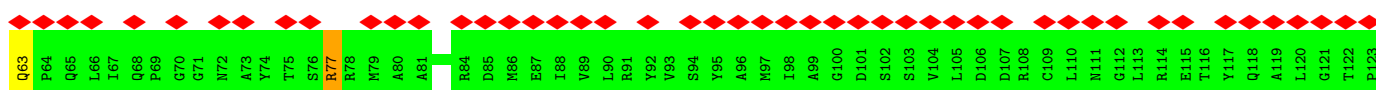
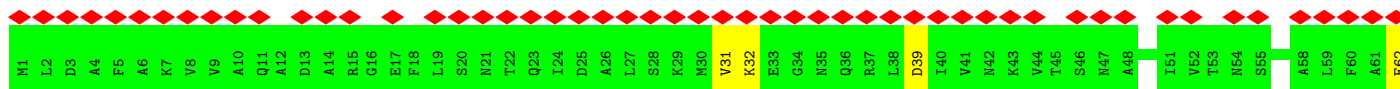
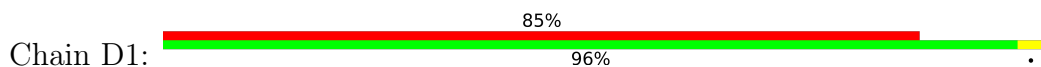
• Molecule 4: C-phycoerythrin alpha subunit

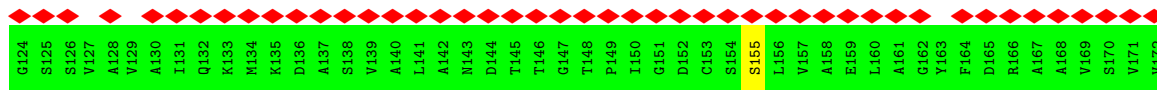


• Molecule 4: C-phycoerythrin alpha subunit

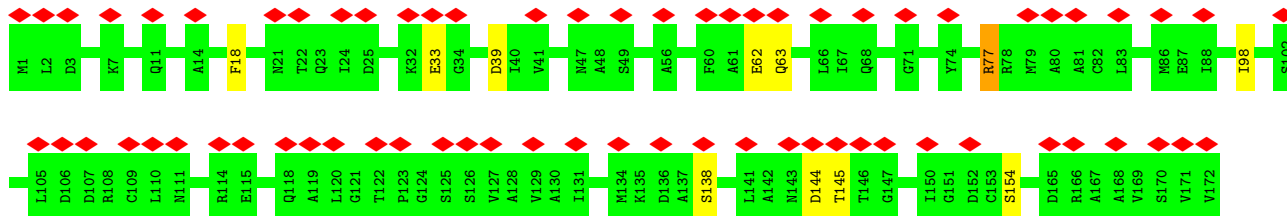
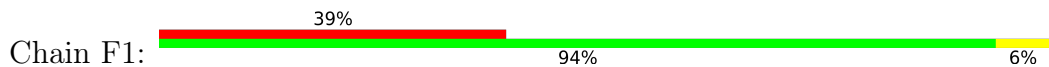


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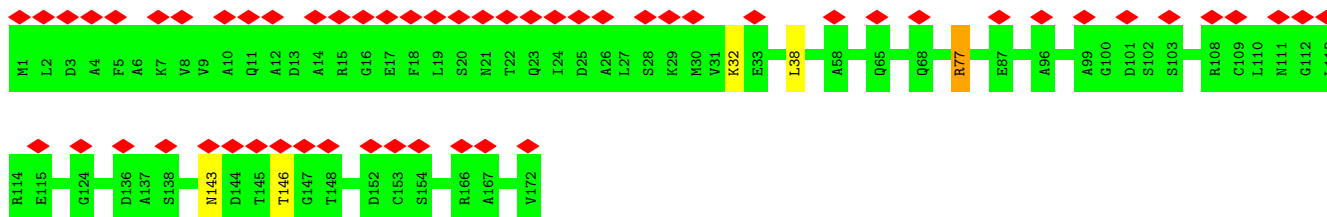




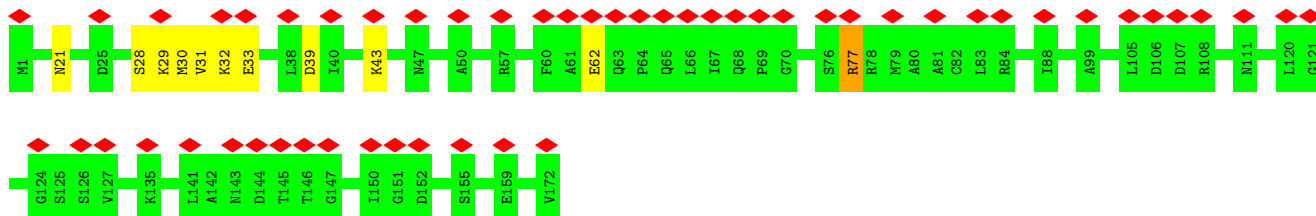
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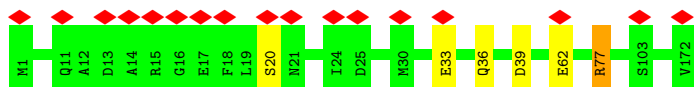
• Molecule 5: C-phycoerythrin beta subunit



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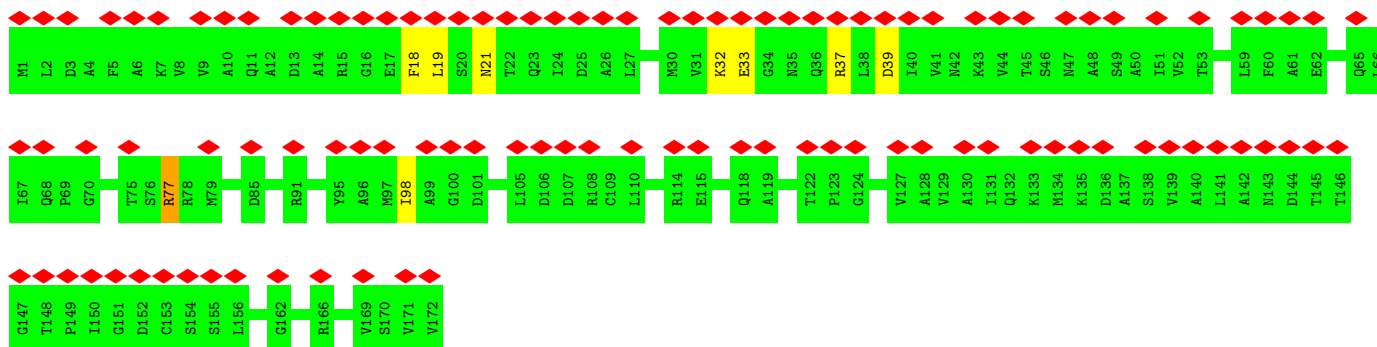


• Molecule 5: C-phycoerythrin beta subunit



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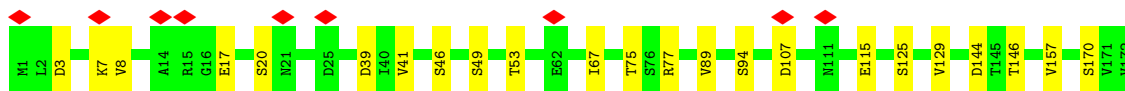
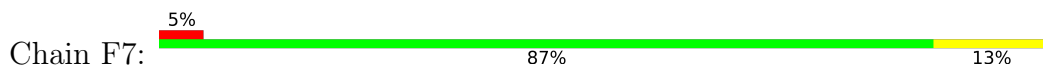




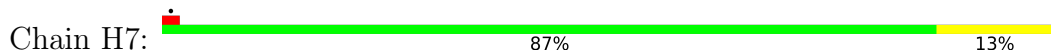
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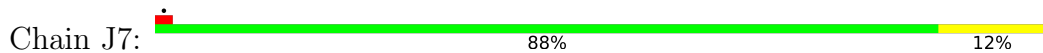
- Molecule 5: C-phycoerythrin beta subunit



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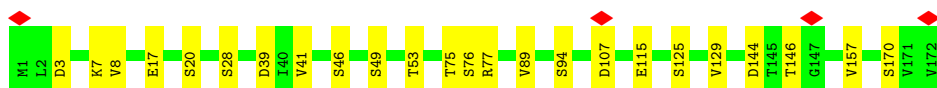
- Molecule 5: C-phycoerythrin beta subunit

Chain N7:  88% 12%




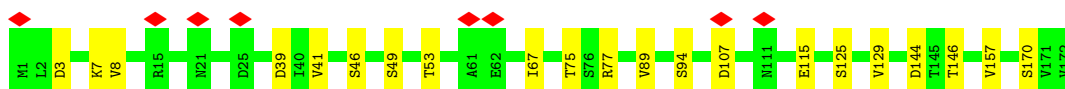
• Molecule 5: C-phycoyanin beta subunit

Chain D9:  86% 14%




• Molecule 5: C-phycoyanin beta subunit

Chain F9:  88% 12% 5%




• Molecule 5: C-phycoyanin beta subunit

Chain H9:  87% 13%



• Molecule 5: C-phycoyanin beta subunit

Chain J9:  88% 12%




• Molecule 5: C-phycoyanin beta subunit

Chain L9:  87% 13%

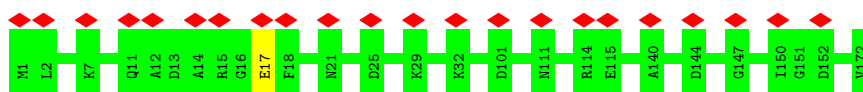


• Molecule 5: C-phycoyanin beta subunit

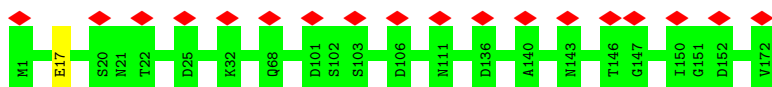
Chain N9:  88% 12%



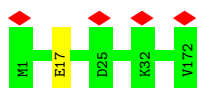
- Molecule 5: C-phycoerythrin beta subunit



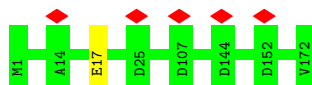
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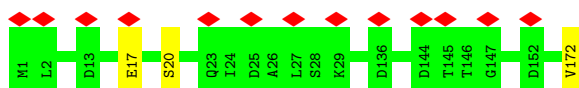
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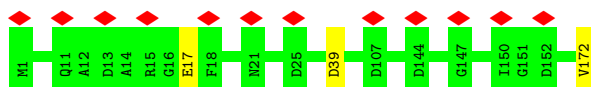
- Molecule 5: C-phycoerythrin beta subunit



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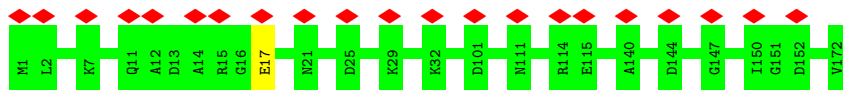


- Molecule 5: C-phycoerythrin beta subunit

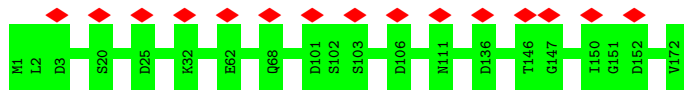


- Molecule 5: C-phycoerythrin beta subunit

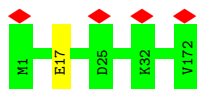




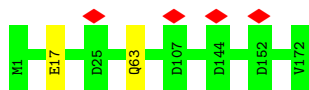
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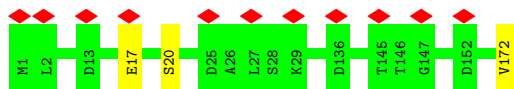
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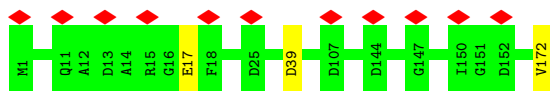
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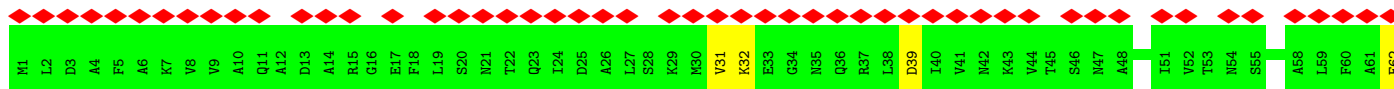
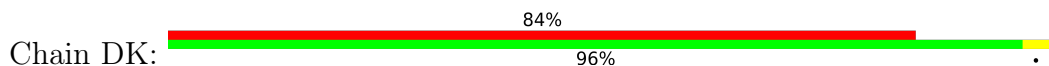
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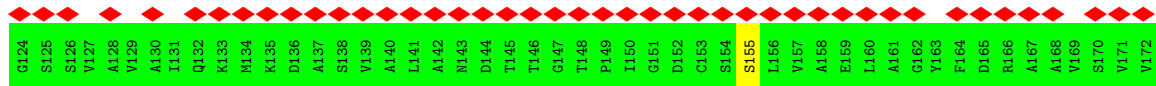
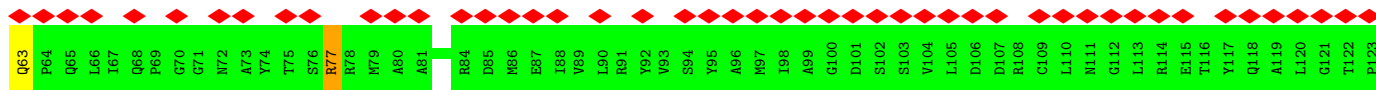


• Molecule 5: C-phycoerythrin beta subunit

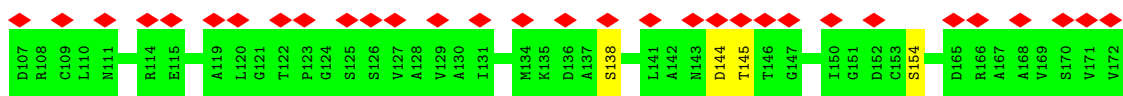
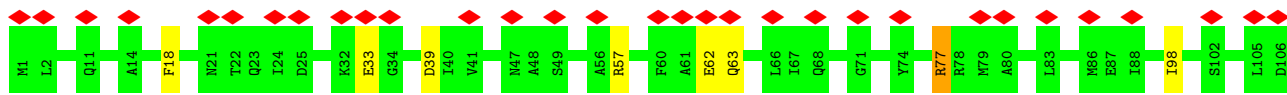
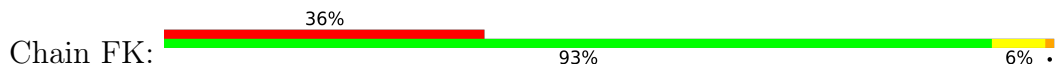


• Molecule 5: C-phycoerythrin beta subunit

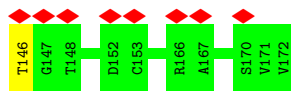
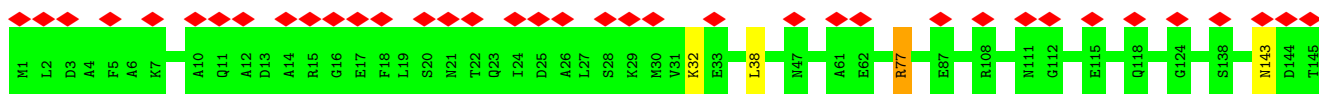




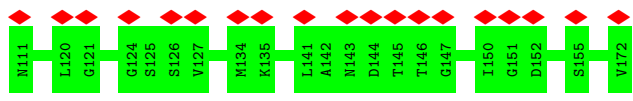
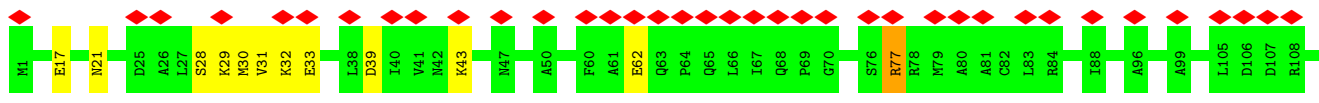
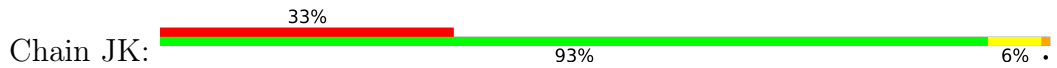
• Molecule 5: C-phycoerythrin beta subunit



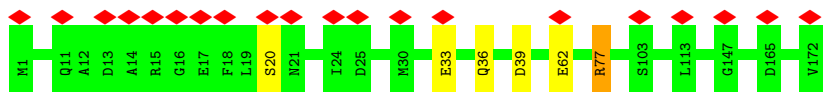
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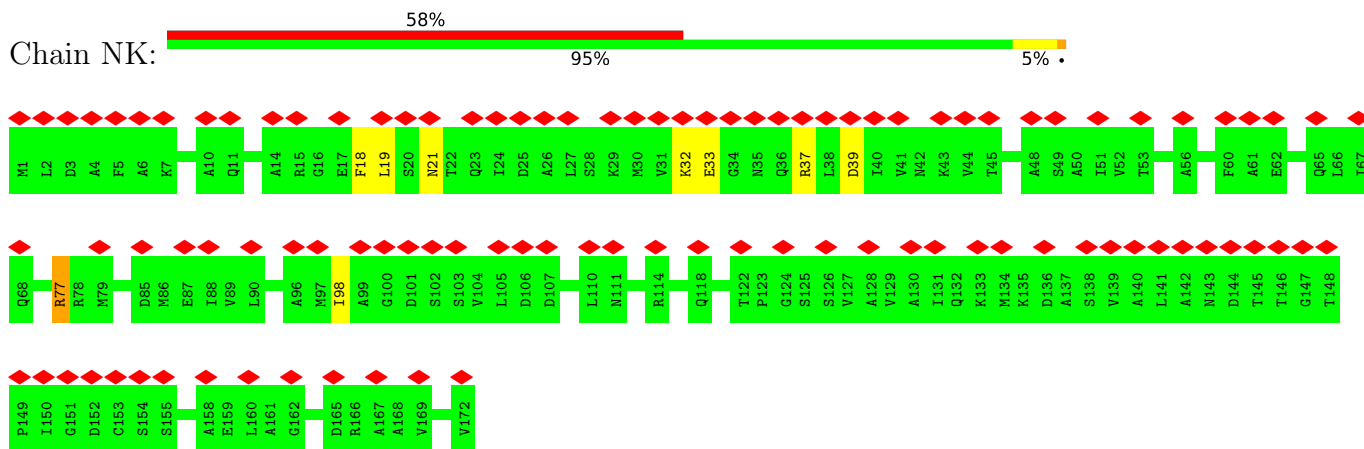
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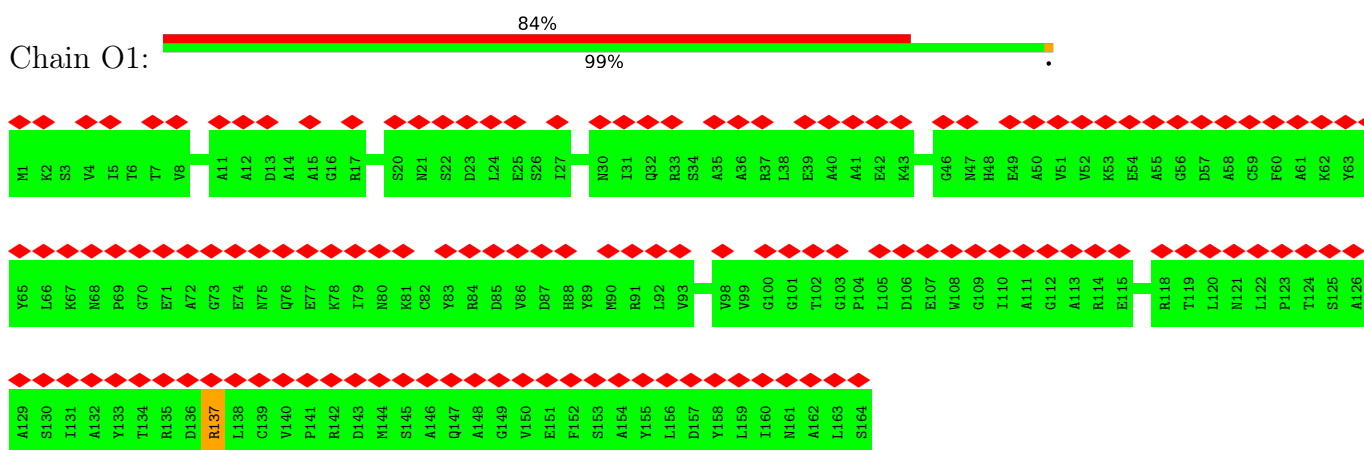
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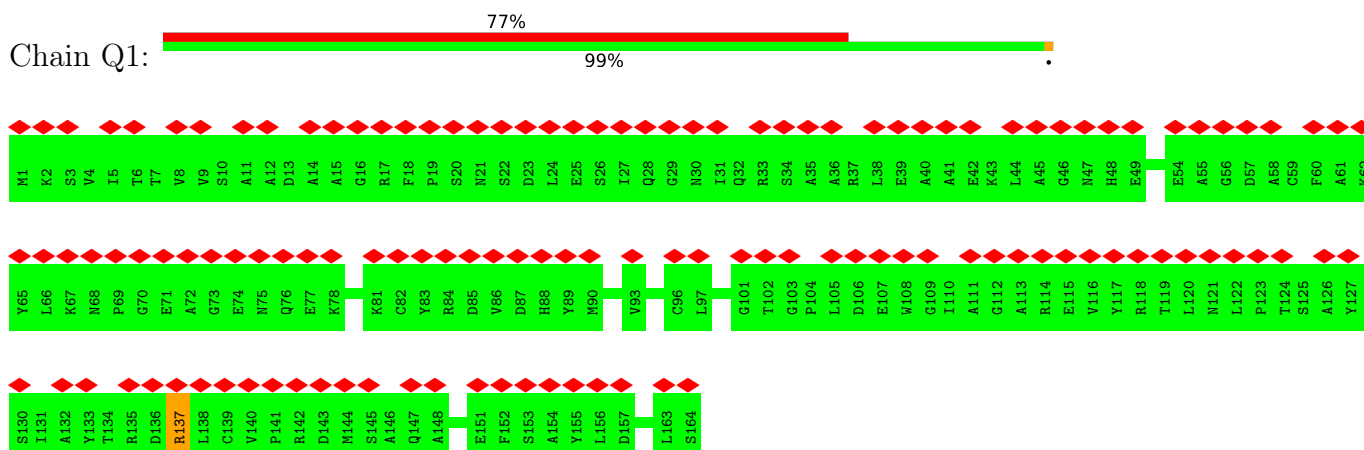
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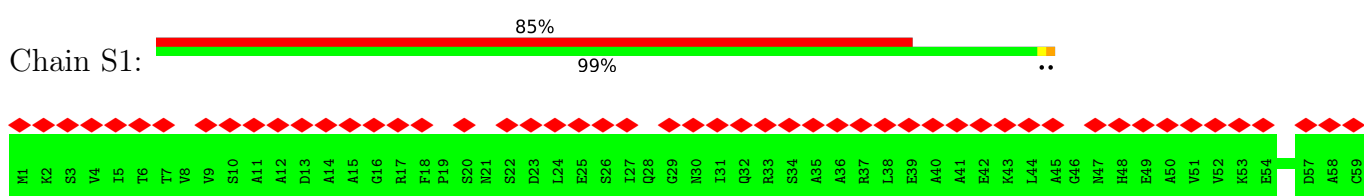
• Molecule 6: Phycoerythrin alpha subunit

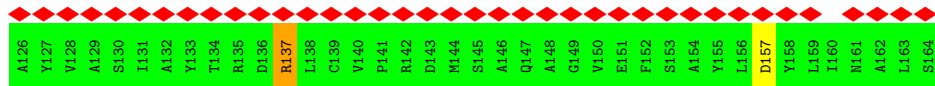
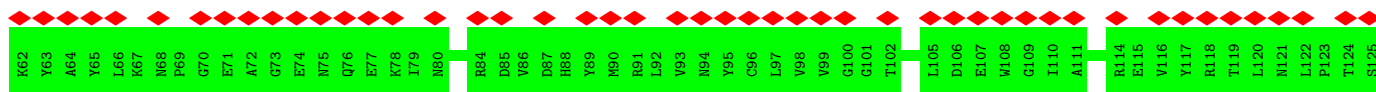


• Molecule 6: Phycoerythrin alpha subunit

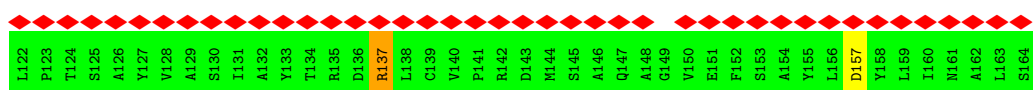
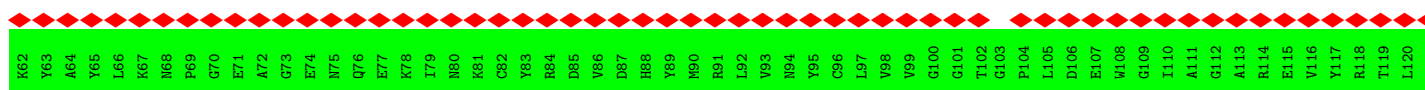


• Molecule 6: Phycoerythrin alpha subunit

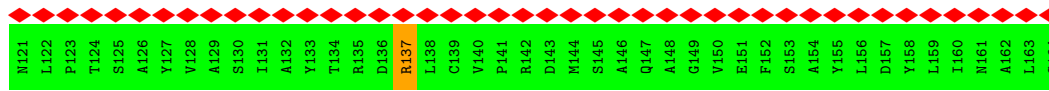
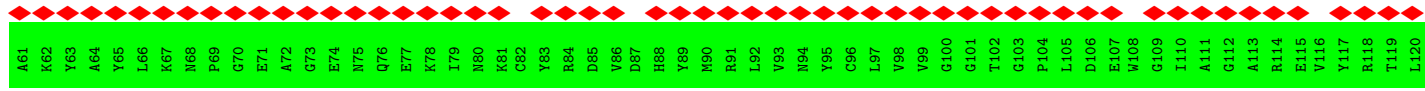
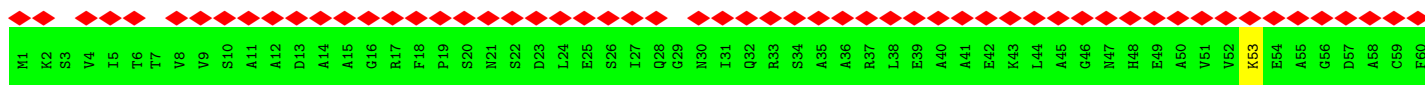




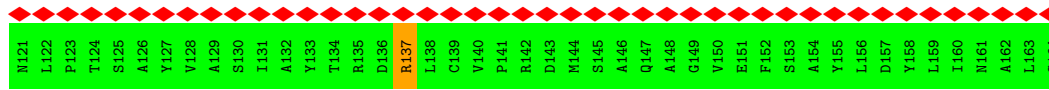
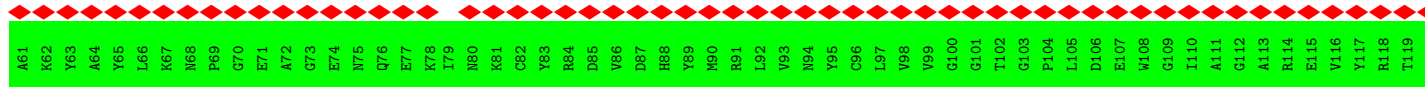
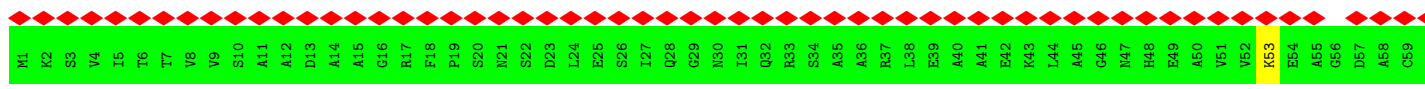
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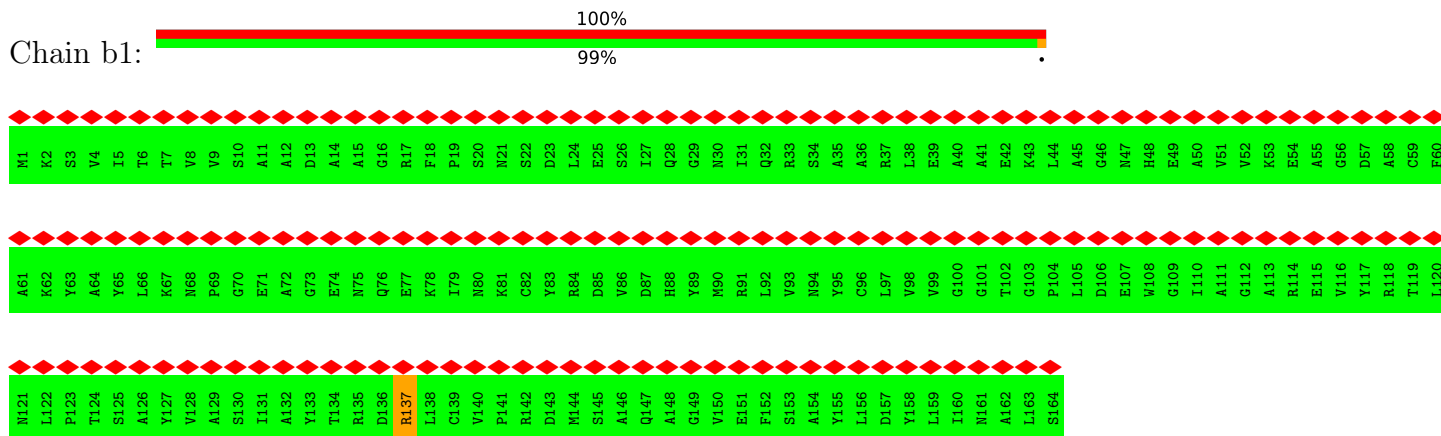
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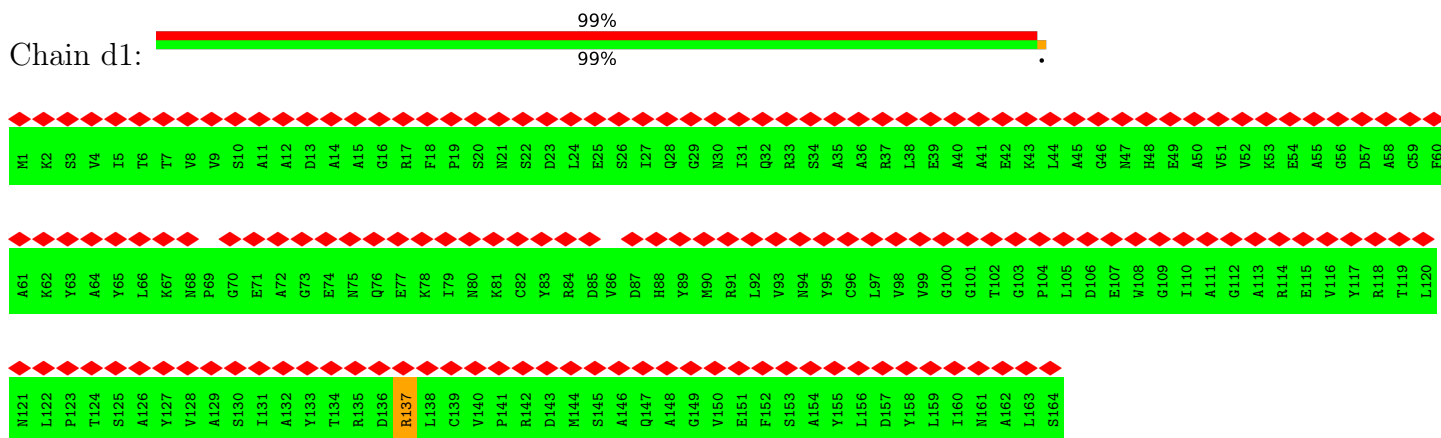
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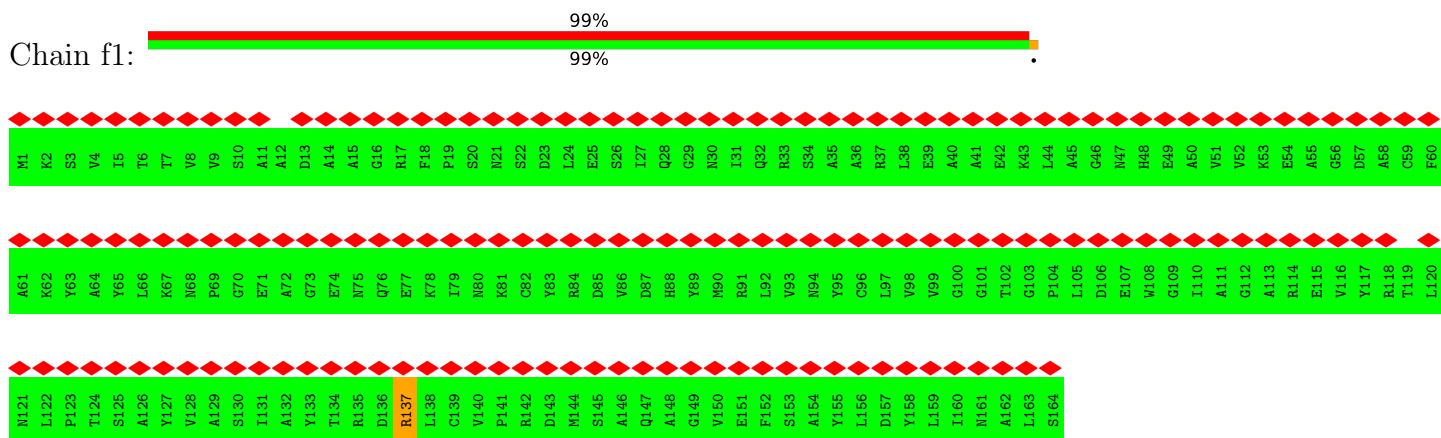
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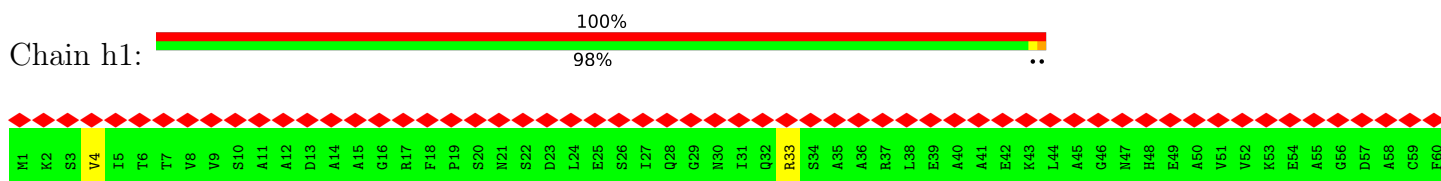
• Molecule 6: Phycoerythrin alpha subunit

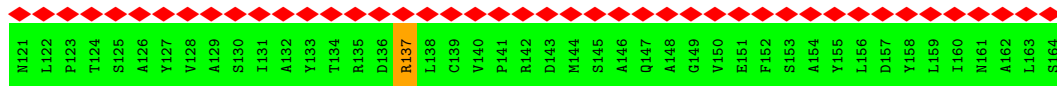
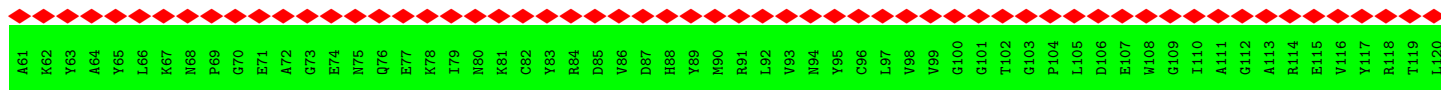


• Molecule 6: Phycoerythrin alpha subunit

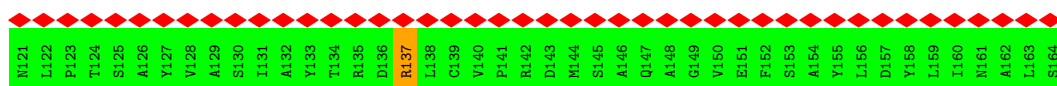
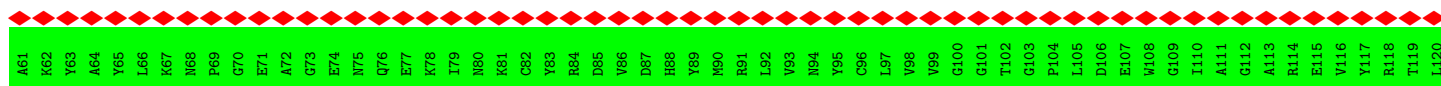
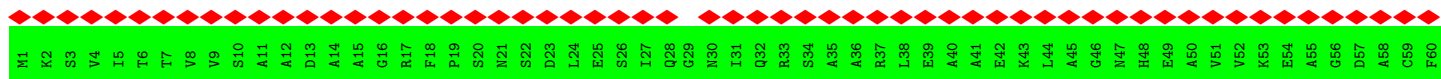


• Molecule 6: Phycoerythrin alpha subunit

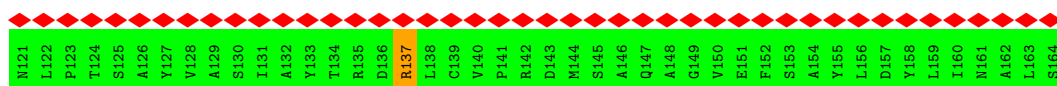
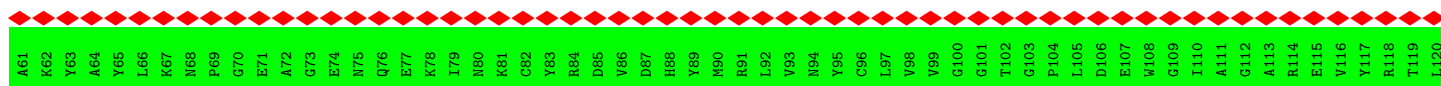
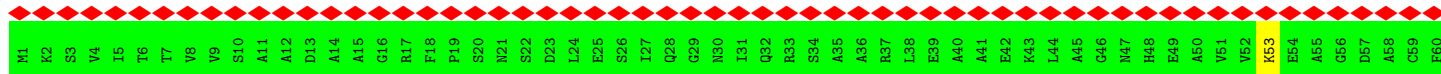




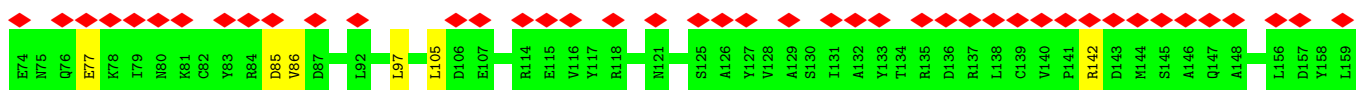
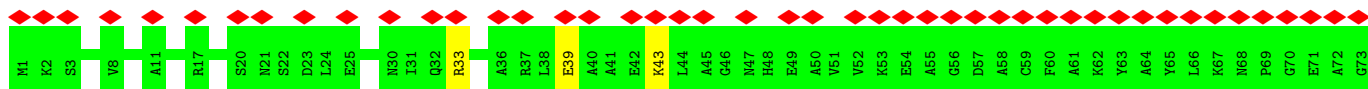
• Molecule 6: Phycoerythrin alpha subunit

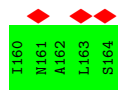


• Molecule 6: Phycoerythrin alpha subunit

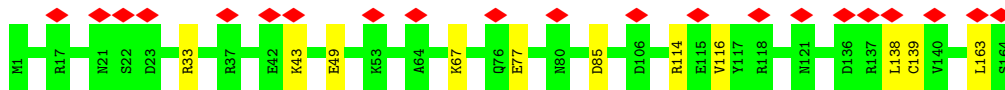


• Molecule 6: Phycoerythrin alpha subunit

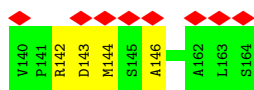
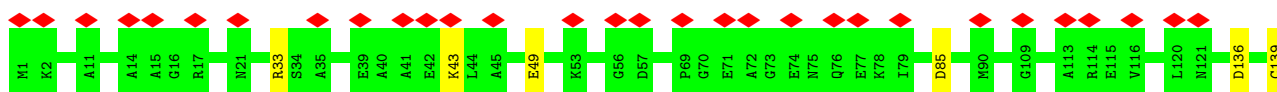




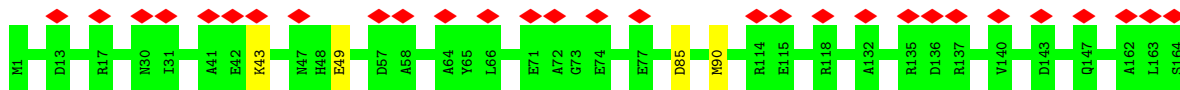
• Molecule 6: Phycoerythrin alpha subunit



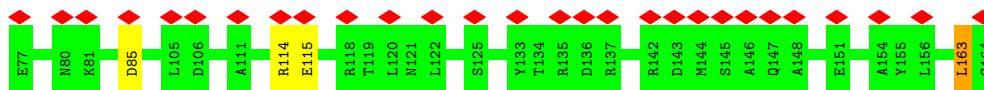
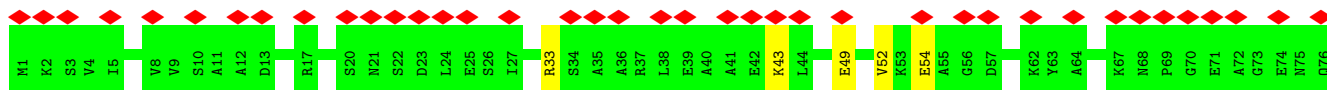
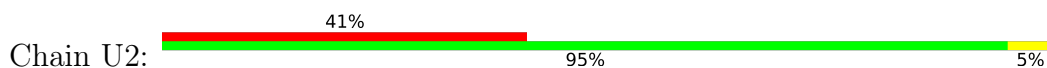
• Molecule 6: Phycoerythrin alpha subunit



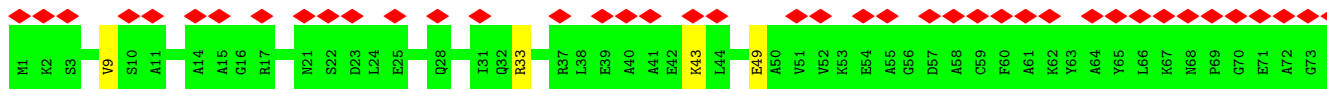
• Molecule 6: Phycoerythrin alpha subunit



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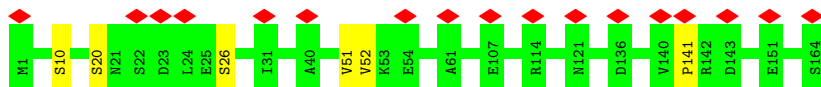


• Molecule 6: Phycoerythrin alpha subunit

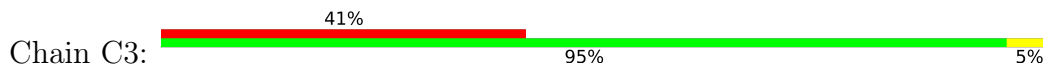




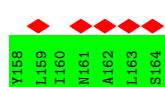
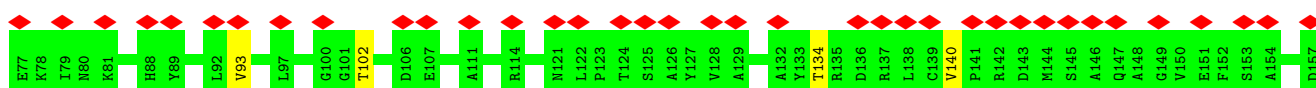
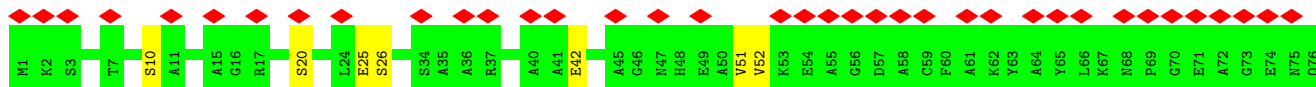
• Molecule 6: Phycoerythrin alpha subunit



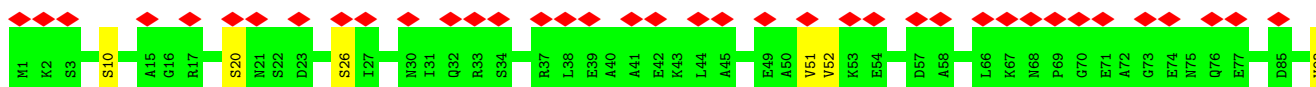
• Molecule 6: Phycoerythrin alpha subunit

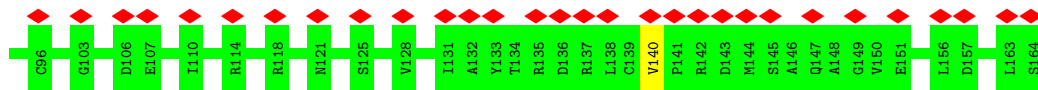


• Molecule 6: Phycoerythrin alpha subunit

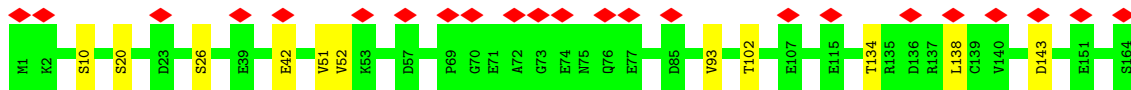
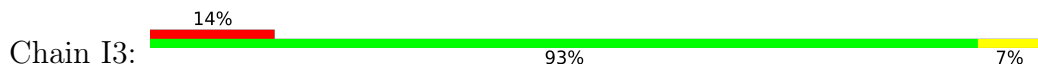


• Molecule 6: Phycoerythrin alpha subunit





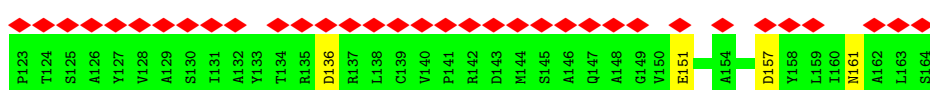
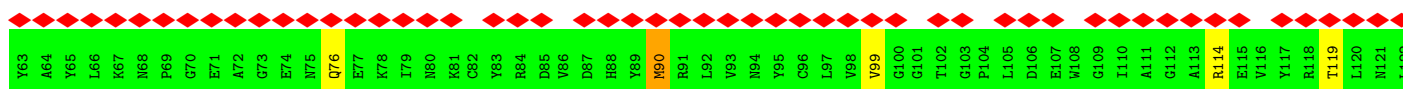
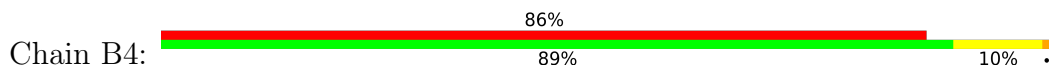
• Molecule 6: Phycoerythrin alpha subunit



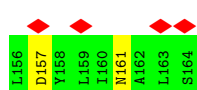
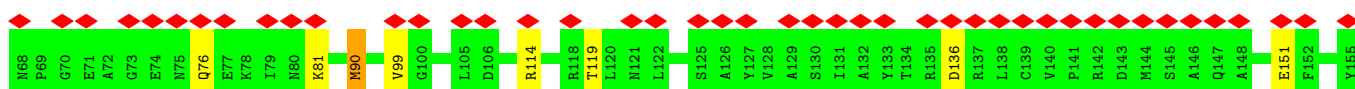
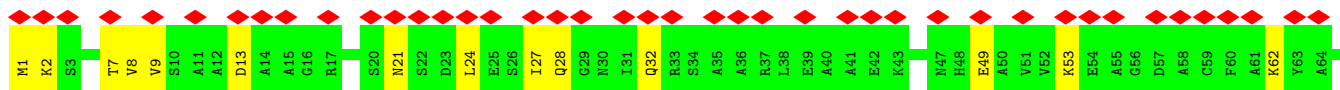
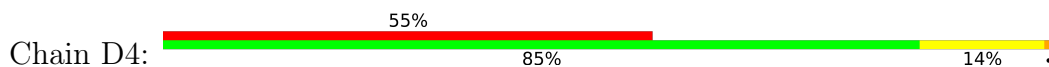
• Molecule 6: Phycoerythrin alpha subunit



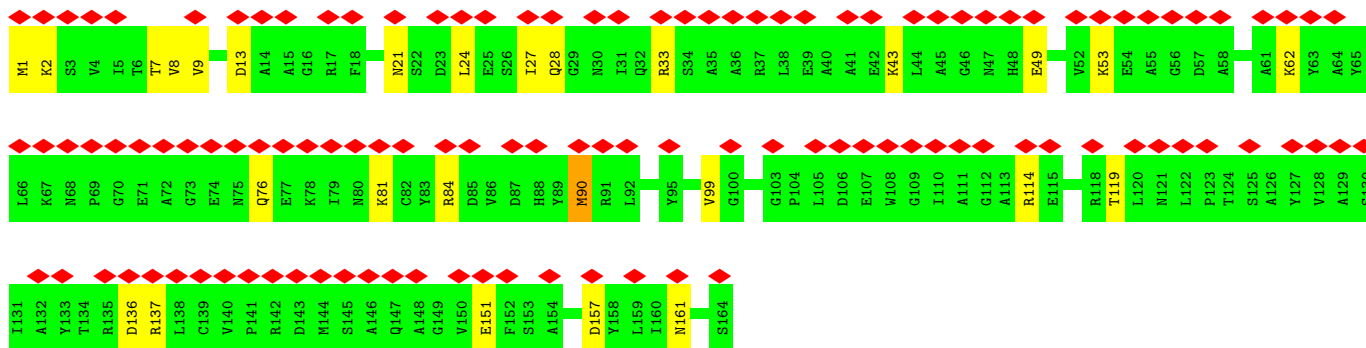
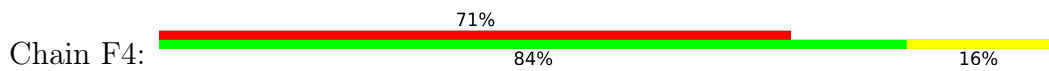
• Molecule 6: Phycoerythrin alpha subunit



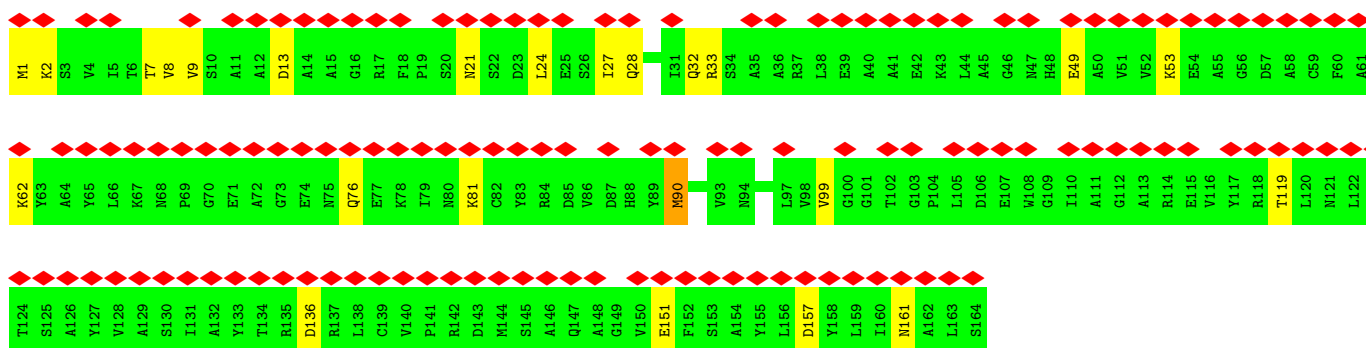
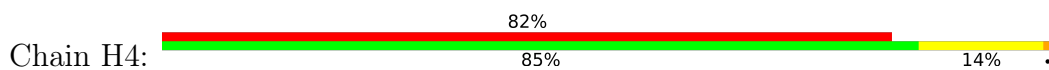
• Molecule 6: Phycoerythrin alpha subunit



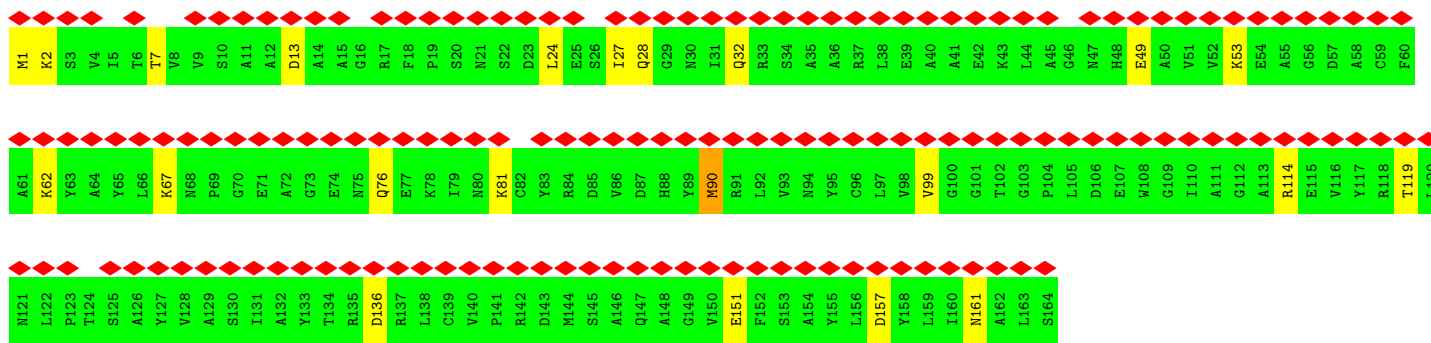
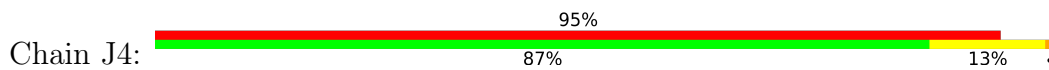
• Molecule 6: Phycoerythrin alpha subunit



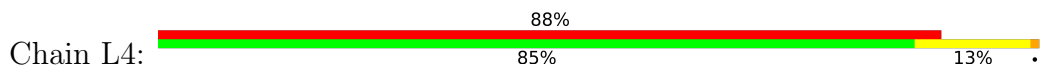
• Molecule 6: Phycoerythrin alpha subunit

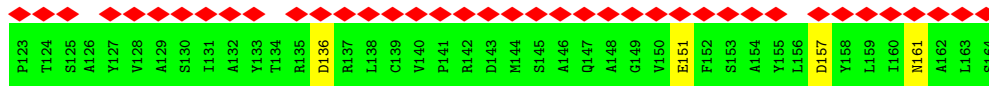
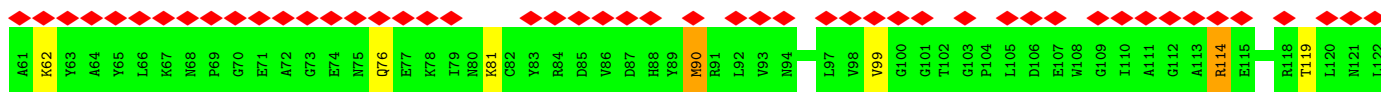


• Molecule 6: Phycoerythrin alpha subunit

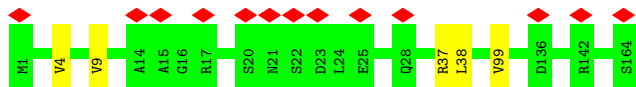


• Molecule 6: Phycoerythrin alpha subunit





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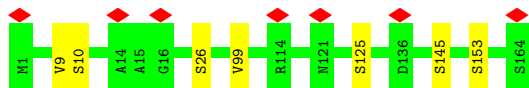
• Molecule 6: Phycoerythrin alpha subunit



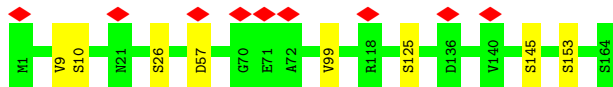
• Molecule 6: Phycoerythrin alpha subunit



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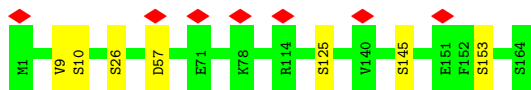


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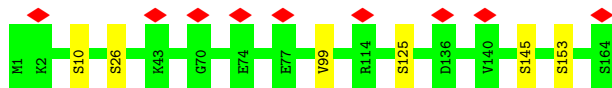


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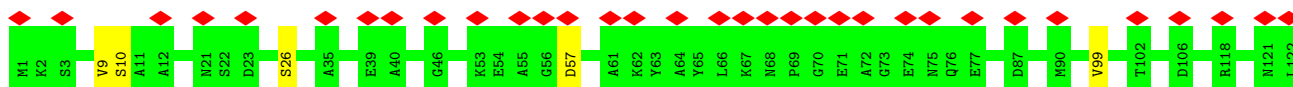




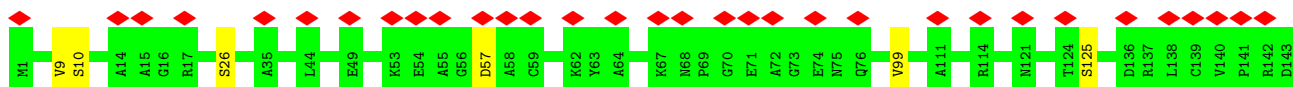
- Molecule 6: Phycoerythrin alpha subunit



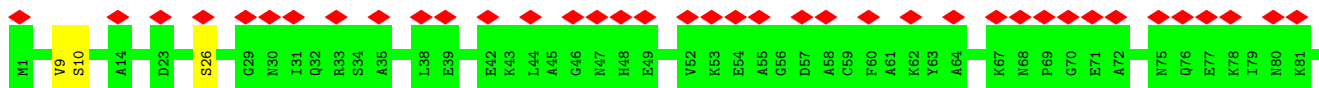
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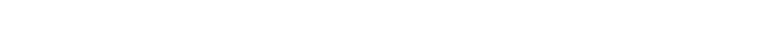
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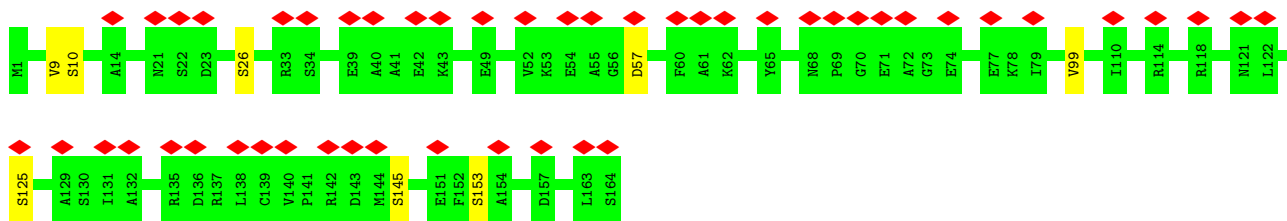


- Molecule 6: Phycoerythrin alpha subunit

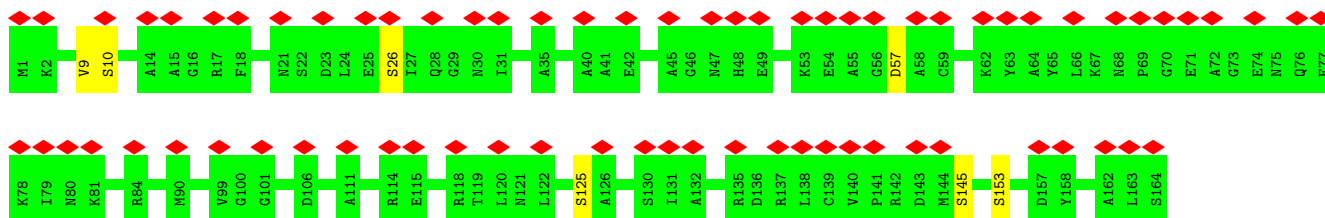
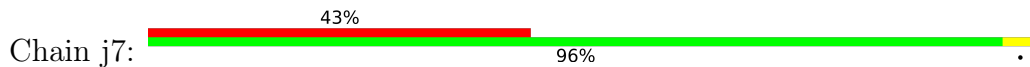


- Molecule 6: Phycoerythrin alpha subunit

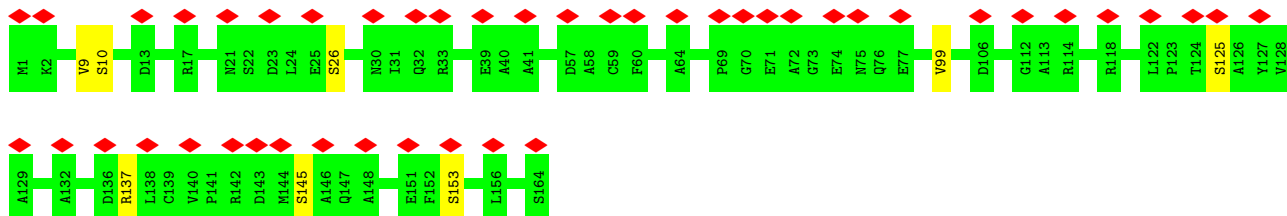




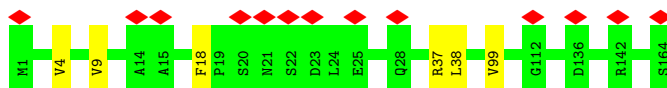
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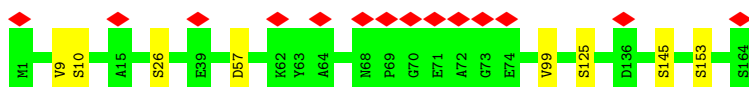
- Molecule 6: Phycoerythrin alpha subunit



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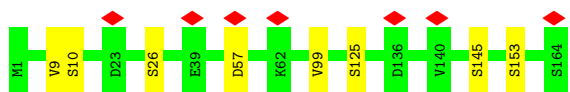


- Molecule 6: Phycoerythrin alpha subunit

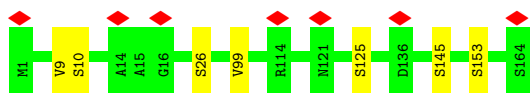


- Molecule 6: Phycoerythrin alpha subunit

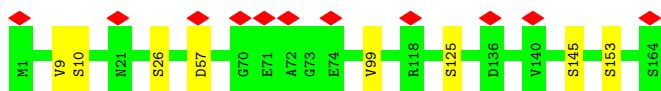




- Molecule 6: Phycoerythrin alpha subunit



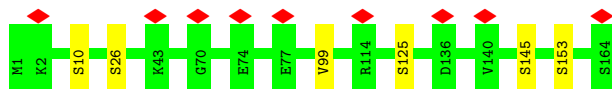
- Molecule 6: Phycoerythrin alpha subunit



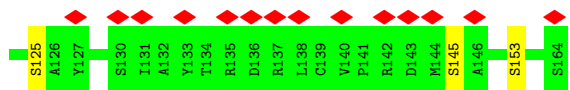
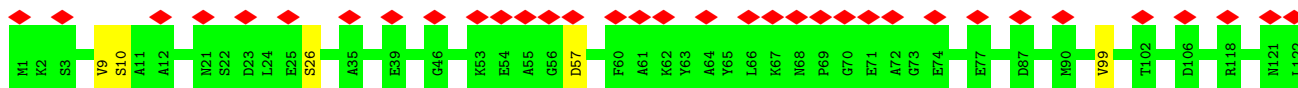
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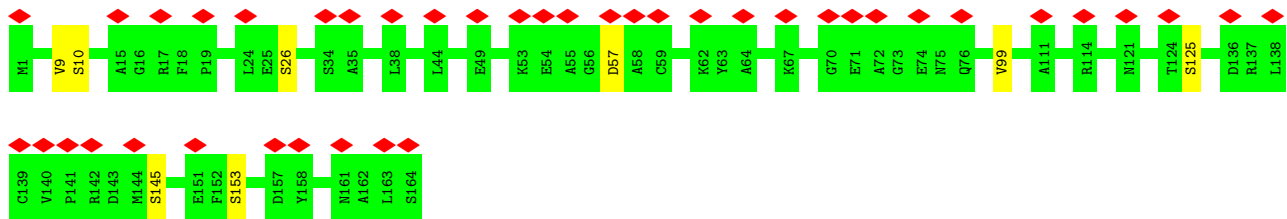


- Molecule 6: Phycoerythrin alpha subunit



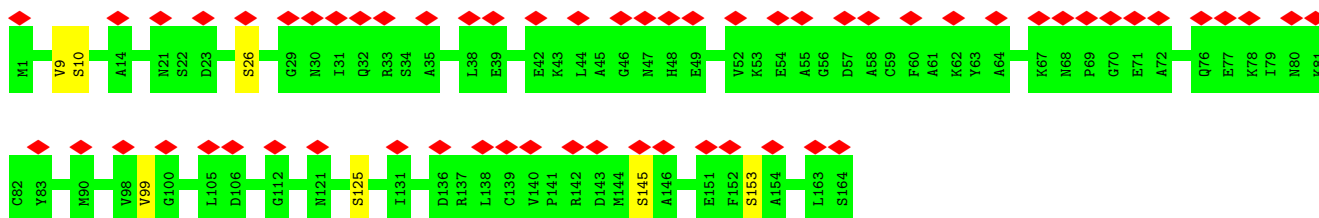
- Molecule 6: Phycoerythrin alpha subunit





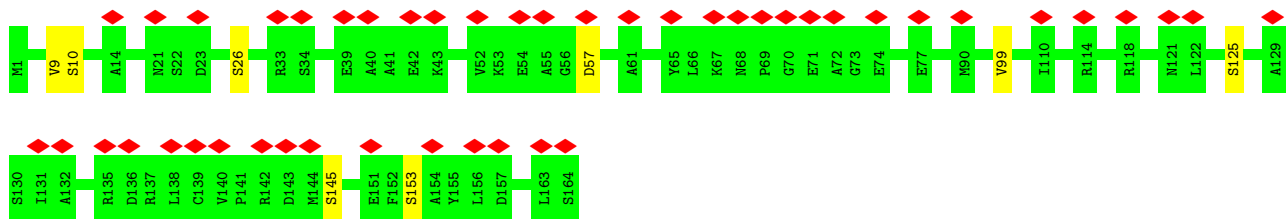
- Molecule 6: Phycoerythrin alpha subunit

Chain f9: 37% 96%



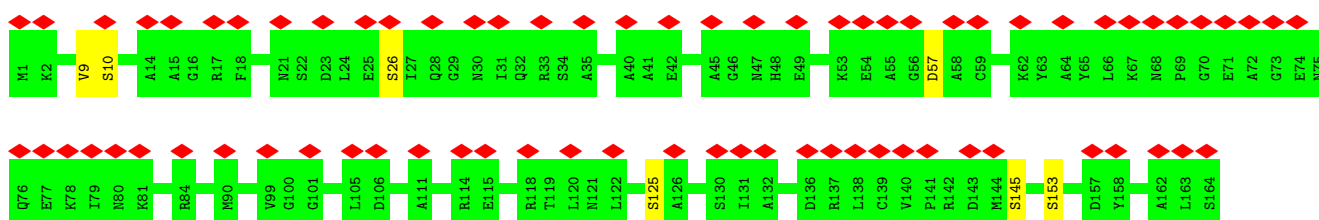
- Molecule 6: Phycoerythrin alpha subunit

Chain h9: 28% 95% 5%



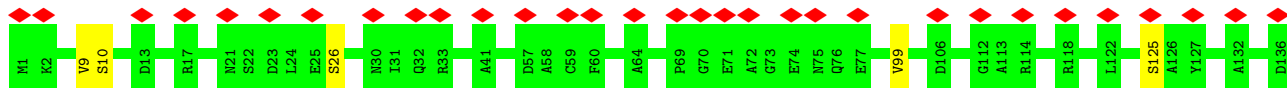
- Molecule 6: Phycoerythrin alpha subunit

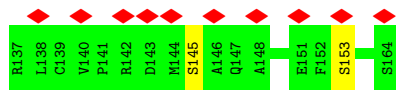
Chain j9: 45% 96% 5%



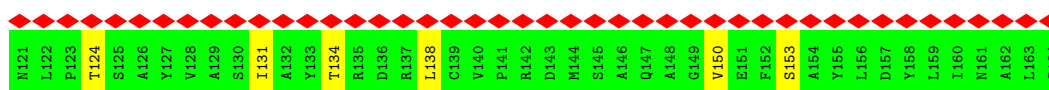
- Molecule 6: Phycoerythrin alpha subunit

Chain l9: 25% 96% 5%

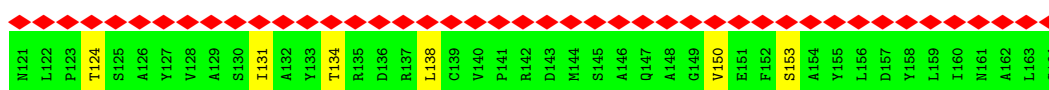




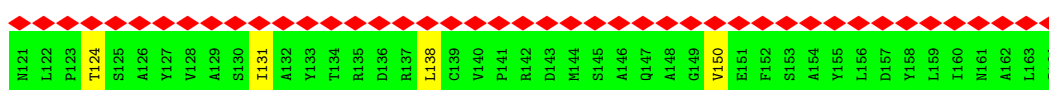
• Molecule 6: Phycoerythrin alpha subunit



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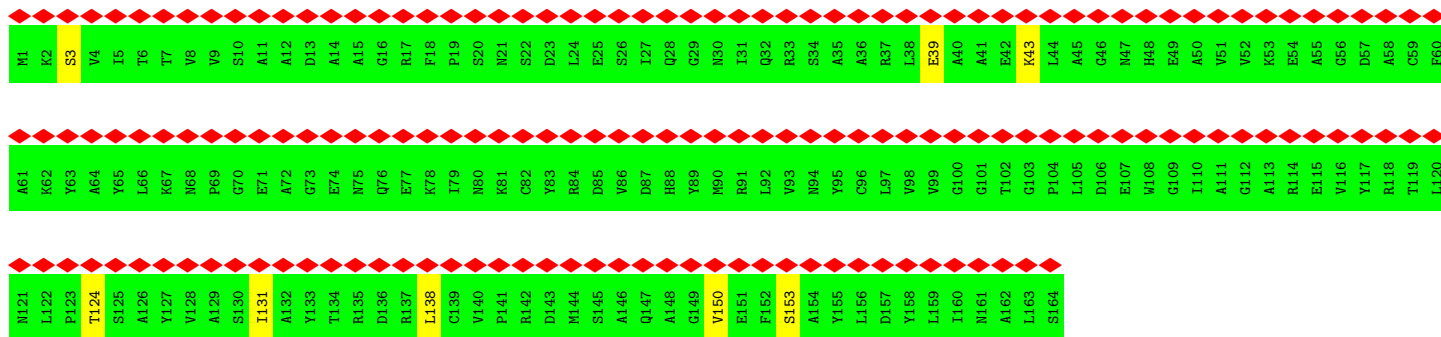


• Molecule 6: Phycoerythrin alpha subunit

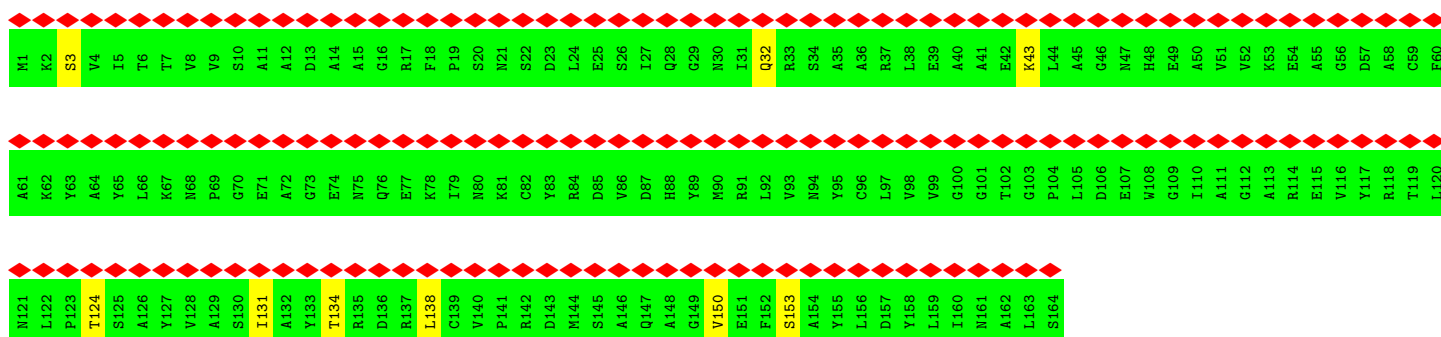


• Molecule 6: Phycoerythrin alpha subunit

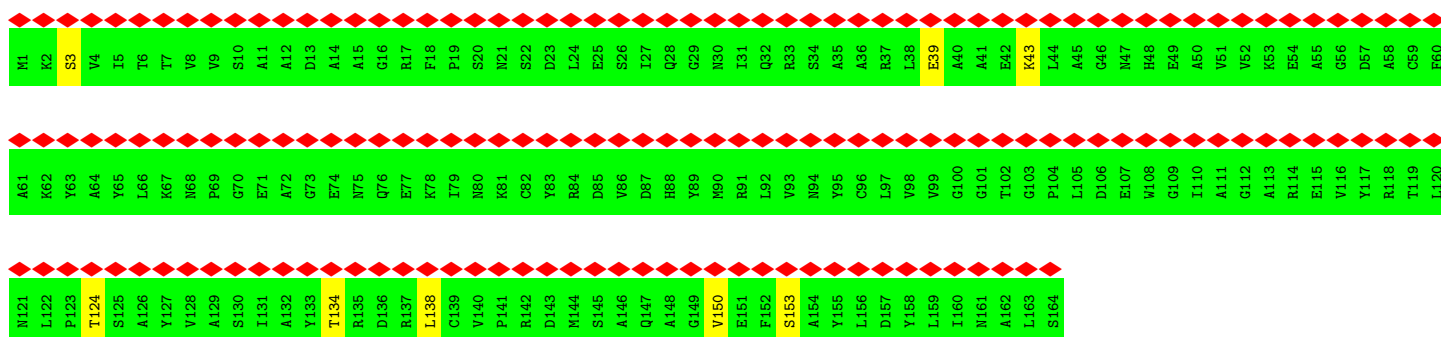




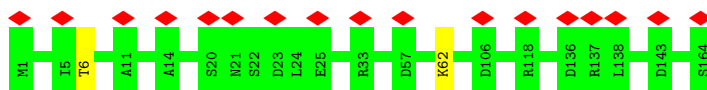
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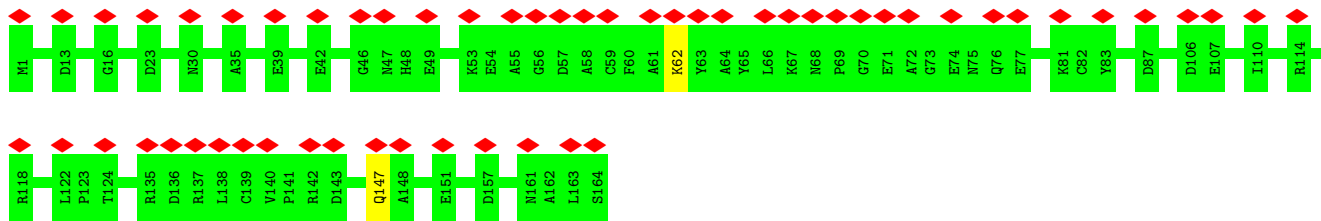


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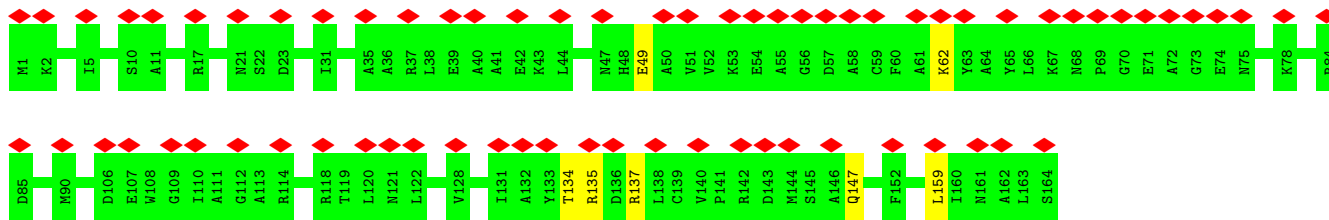
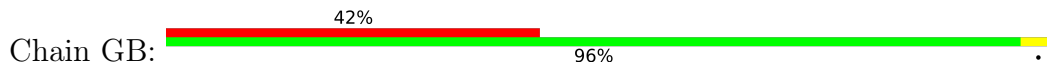


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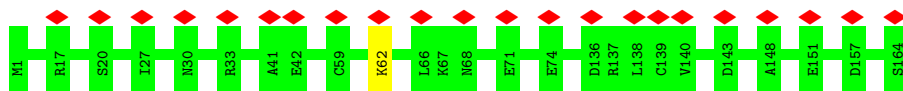




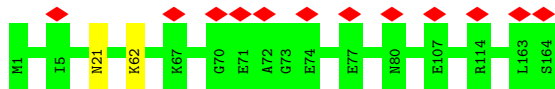
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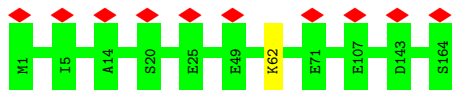
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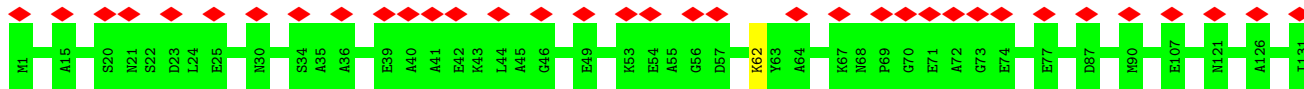
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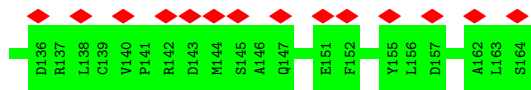


• Molecule 6: Phycoerythrin alpha subunit

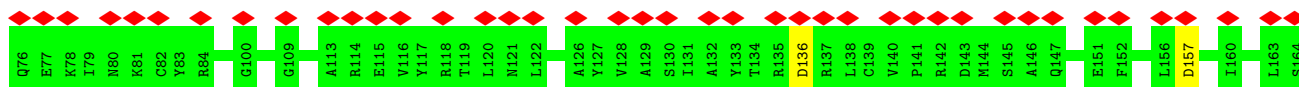
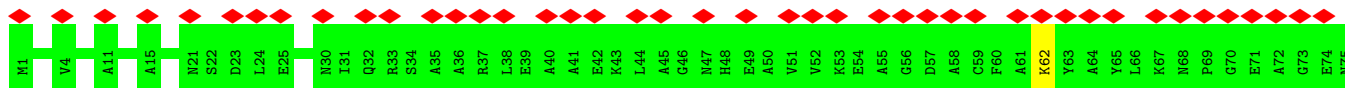


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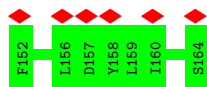
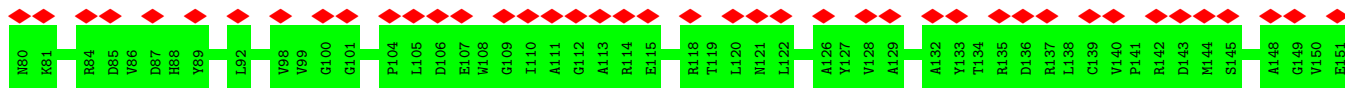
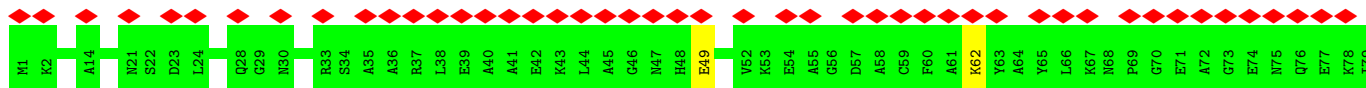




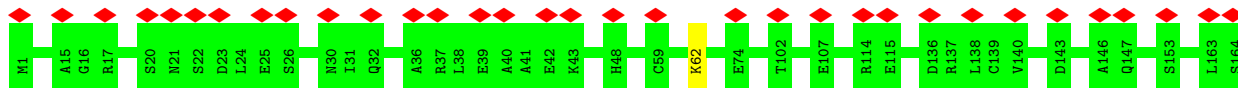
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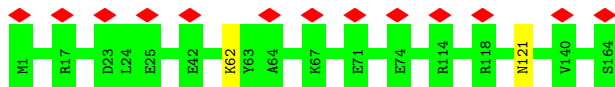
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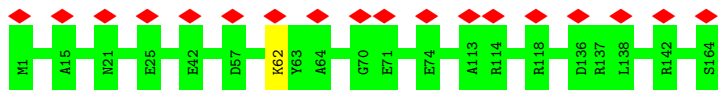


• Molecule 6: Phycoerythrin alpha subunit

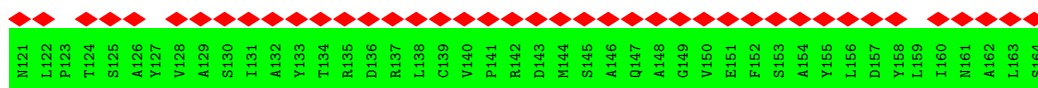
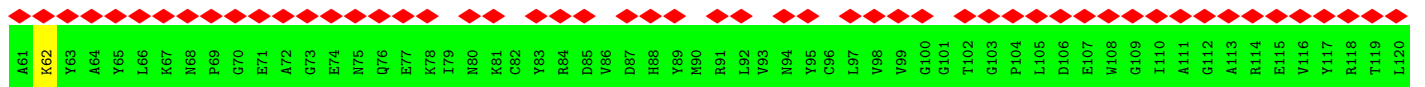
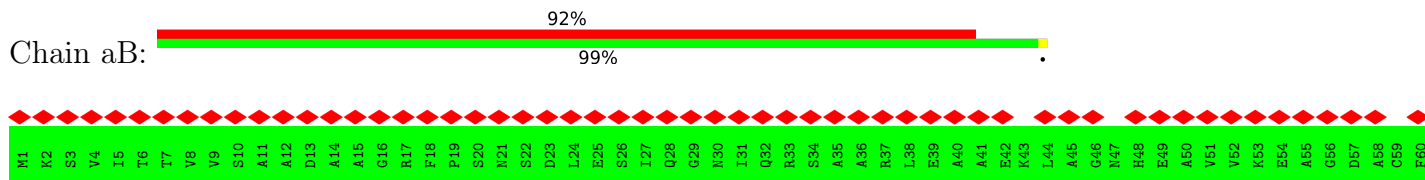


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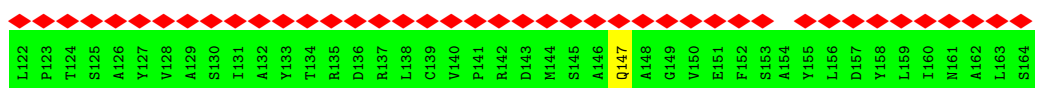
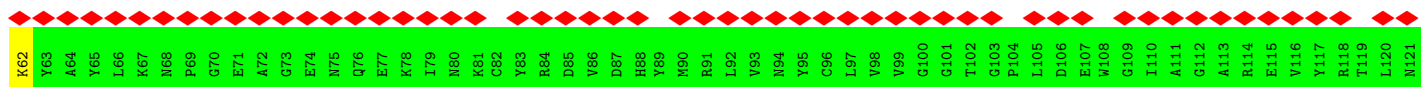
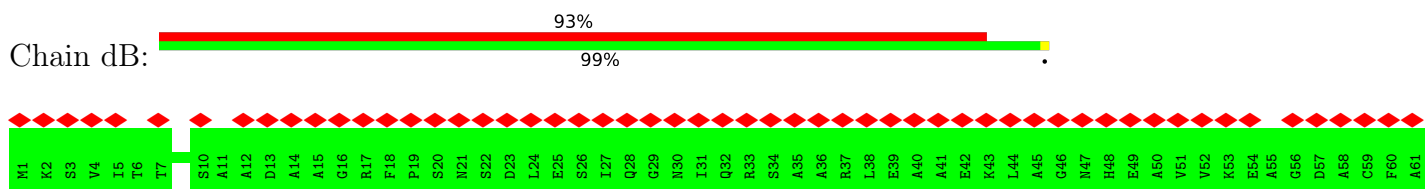




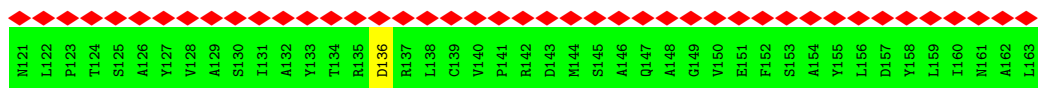
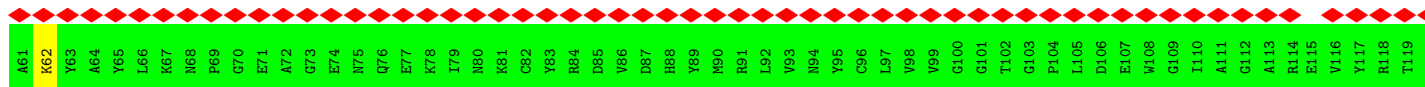
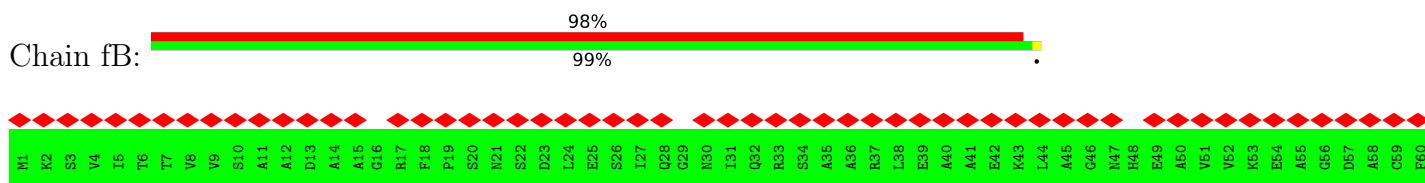
• Molecule 6: Phycoerythrin alpha subunit



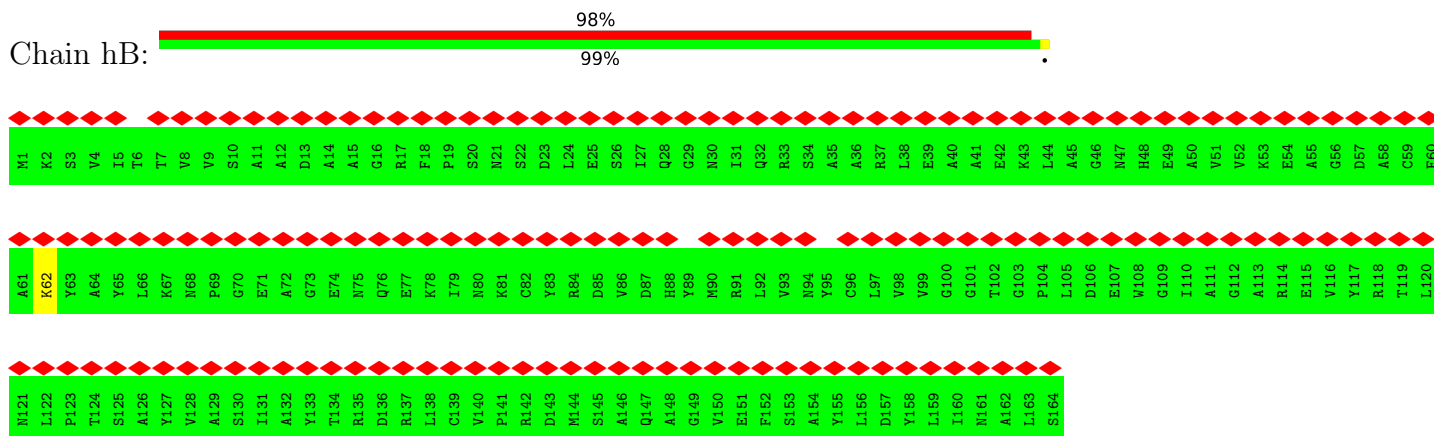
• Molecule 6: Phycoerythrin alpha subunit



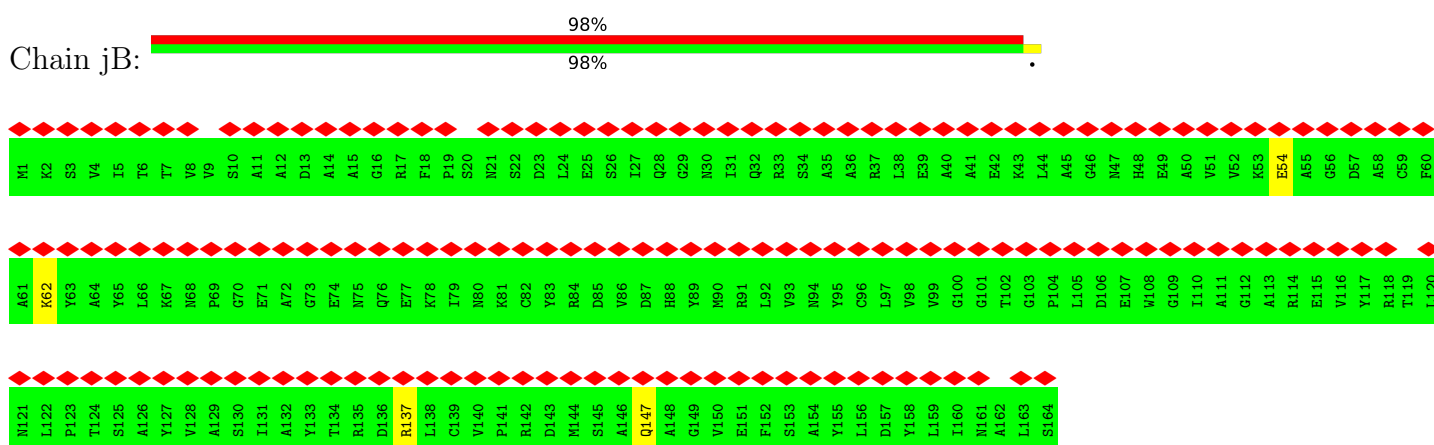
• Molecule 6: Phycoerythrin alpha subunit



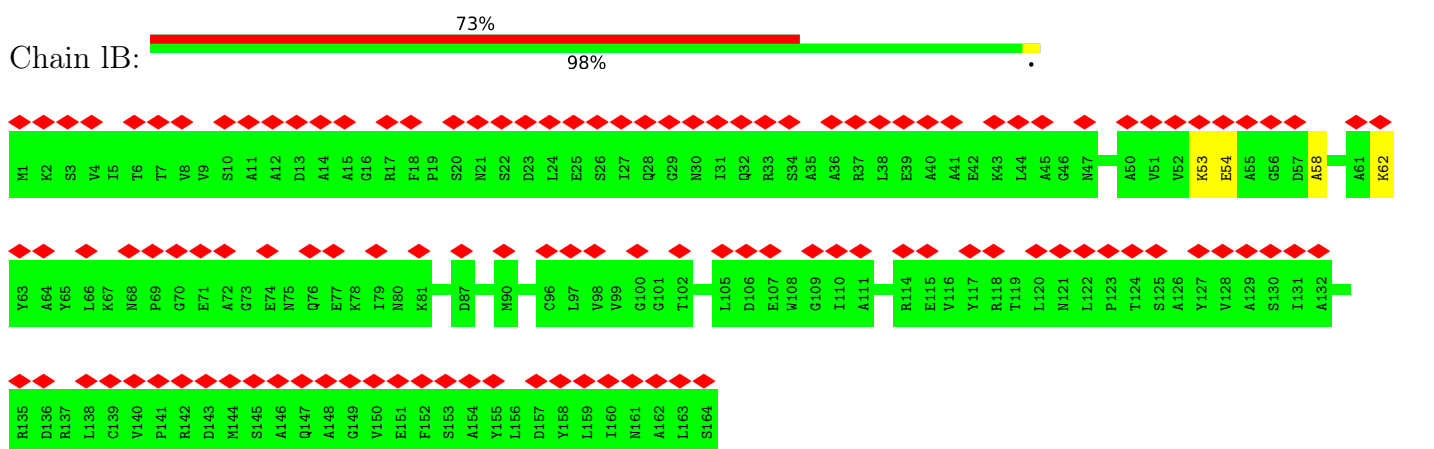
• Molecule 6: Phycoerythrin alpha subunit



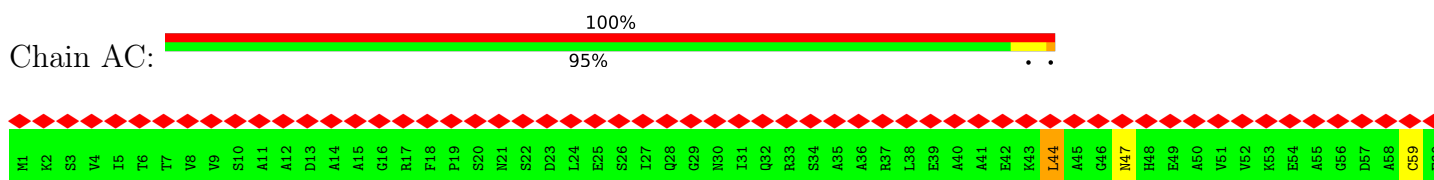
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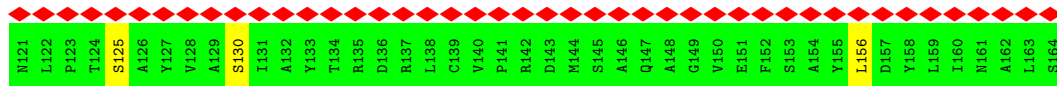
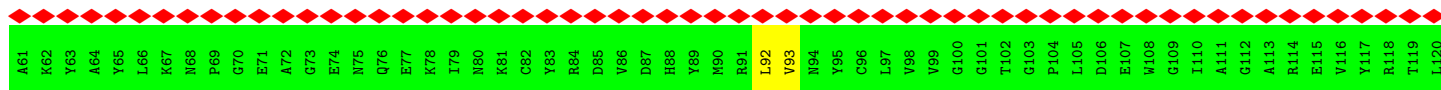


• Molecule 6: Phycoerythrin alpha subunit

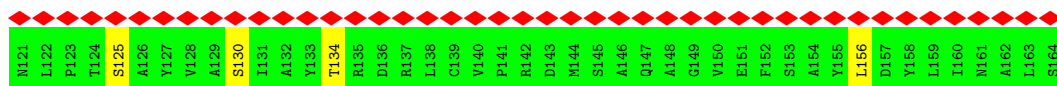
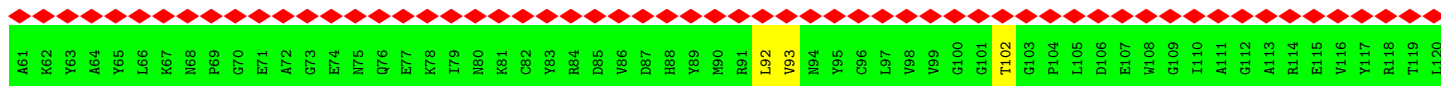
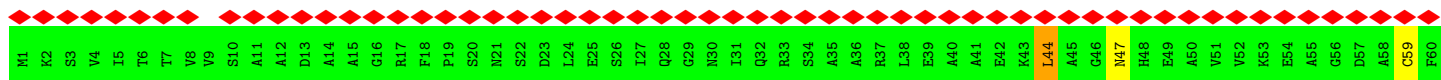


• Molecule 6: Phycoerythrin alpha subunit

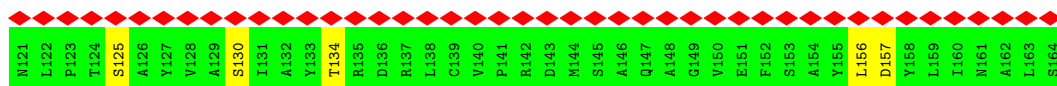
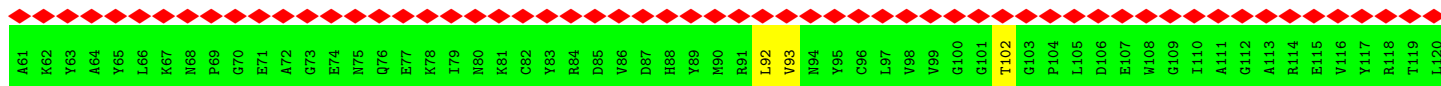
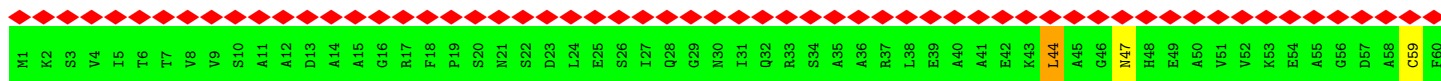
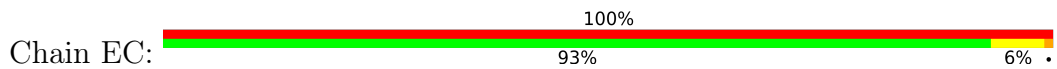




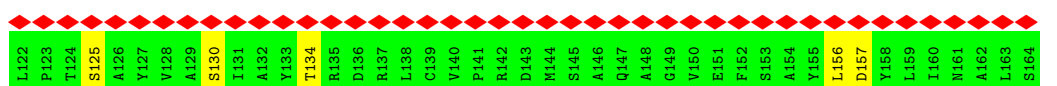
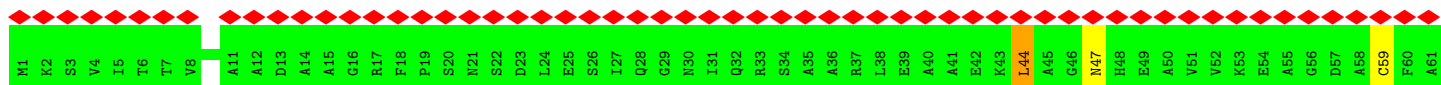
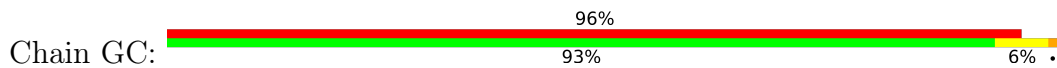
• Molecule 6: Phycoerythrin alpha subunit



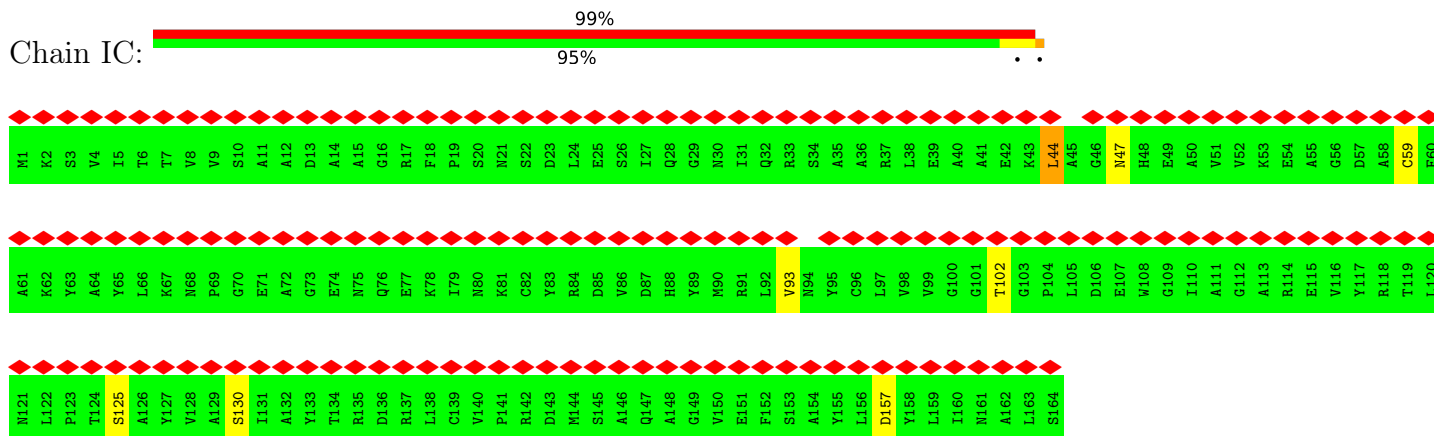
• Molecule 6: Phycoerythrin alpha subunit



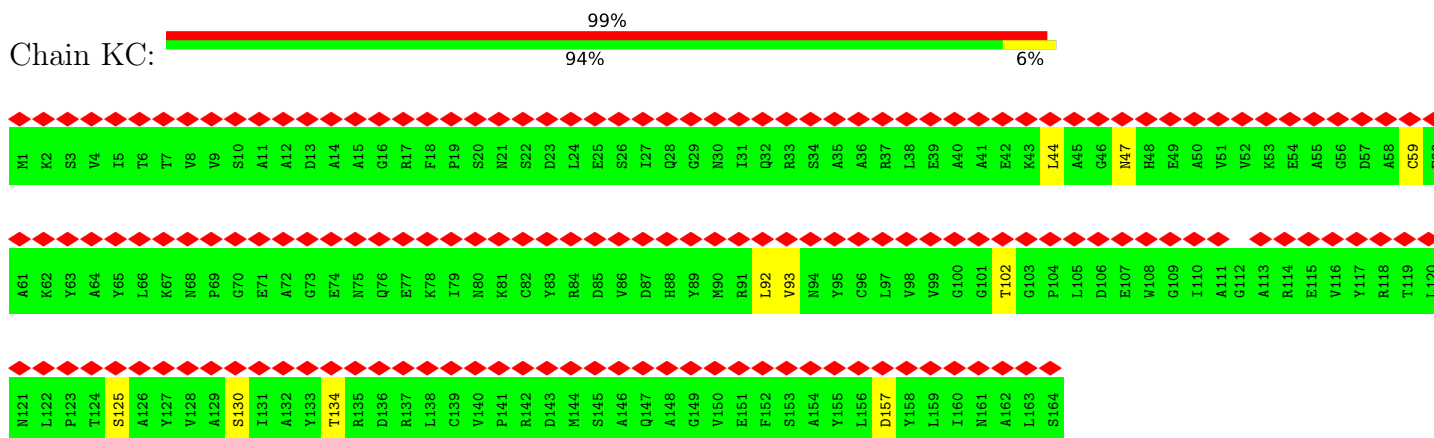
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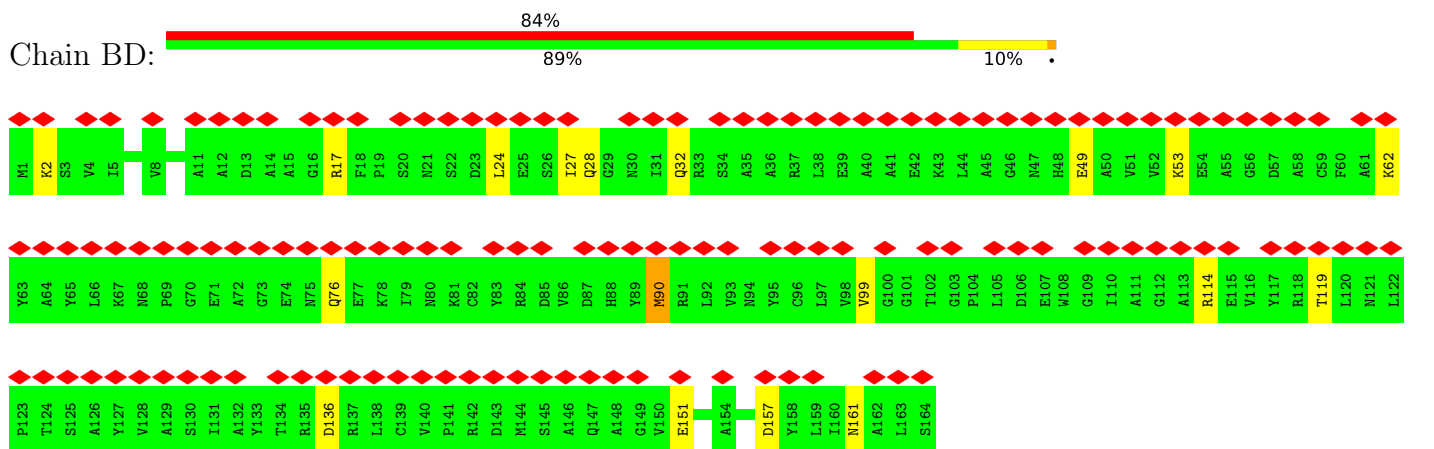
• Molecule 6: Phycoerythrin alpha subunit



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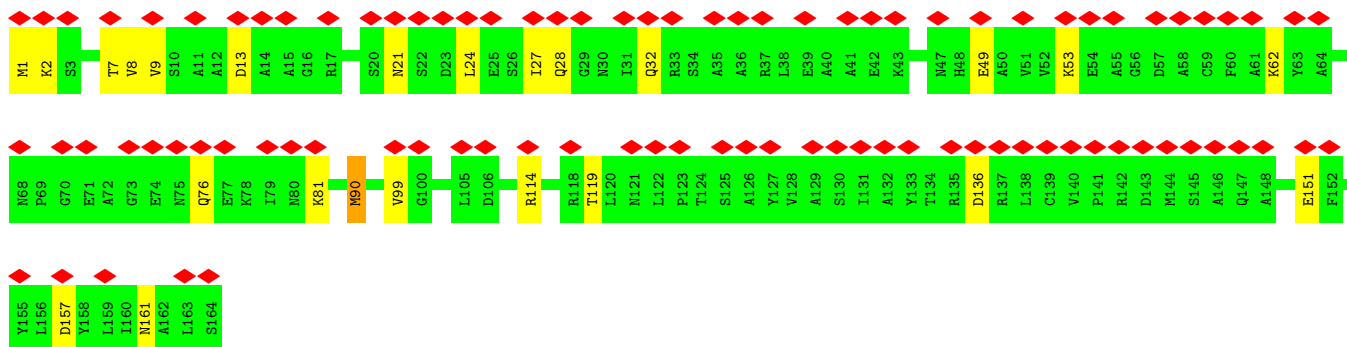


• Molecule 6: Phycoerythrin alpha subunit

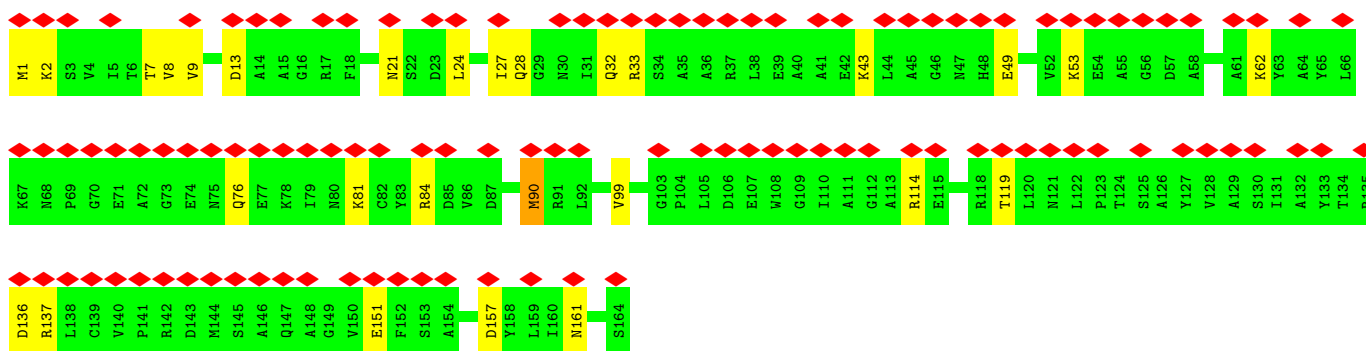
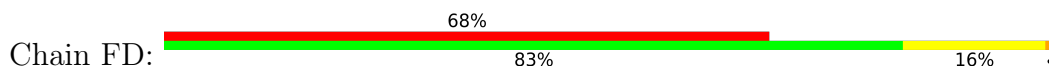


• Molecule 6: Phycoerythrin alpha subunit

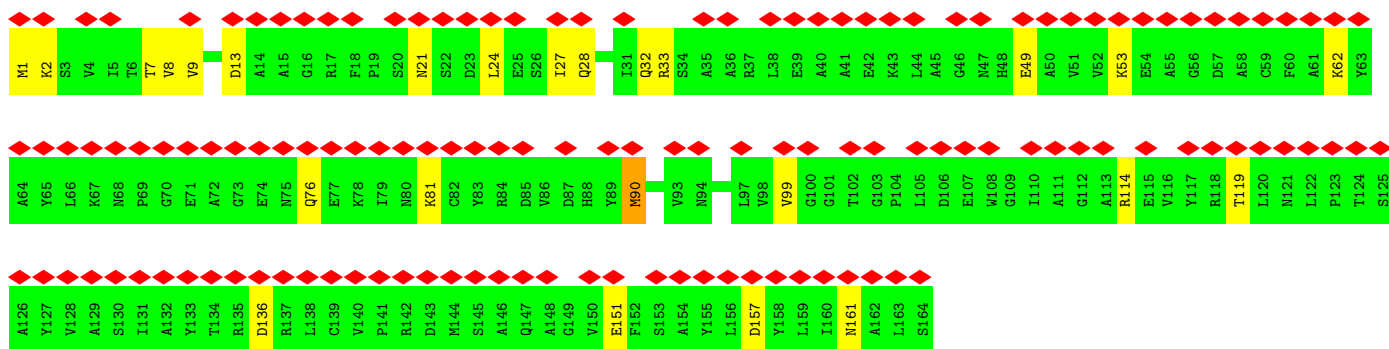
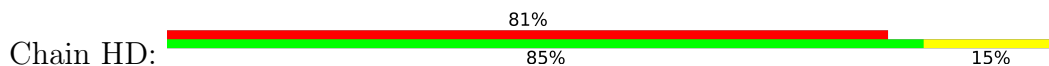




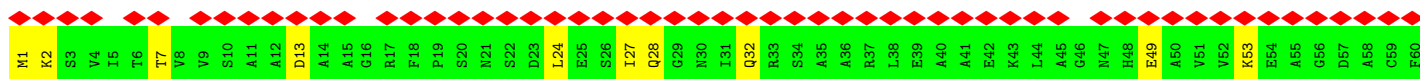
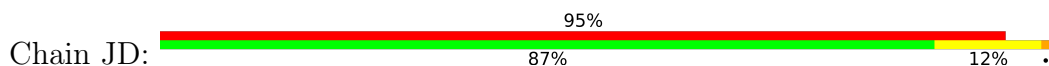
• Molecule 6: Phycoerythrin alpha subunit

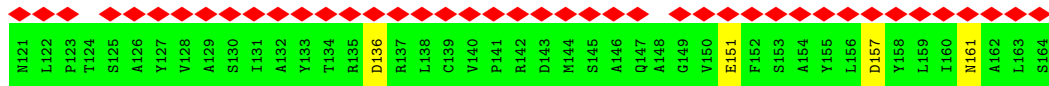
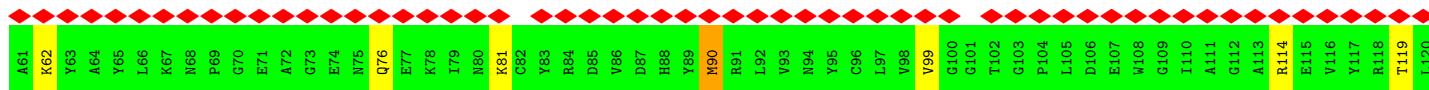


• Molecule 6: Phycoerythrin alpha subunit

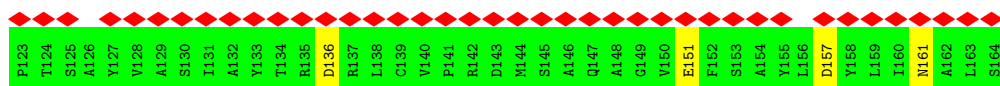
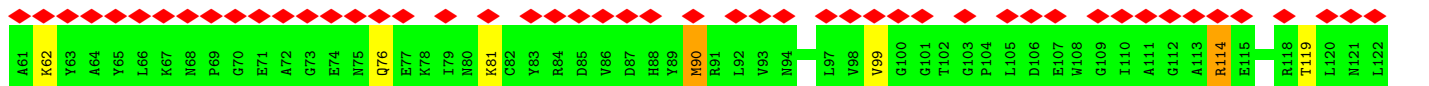
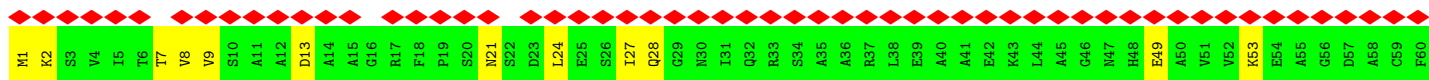
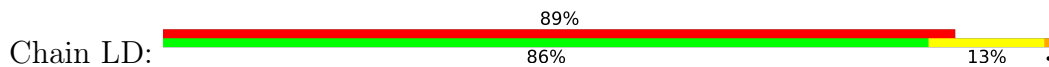


• Molecule 6: Phycoerythrin alpha subunit

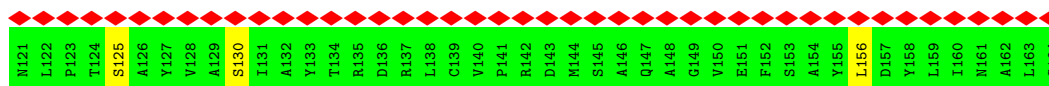
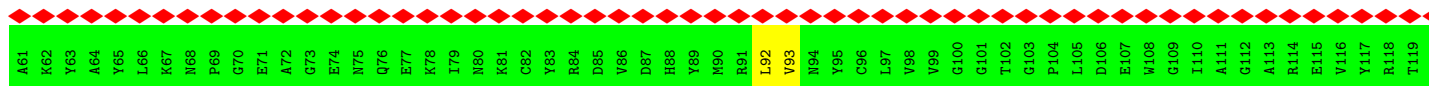
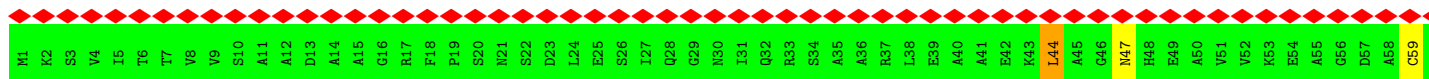




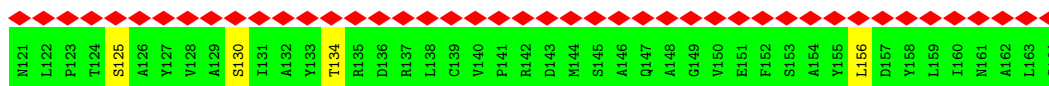
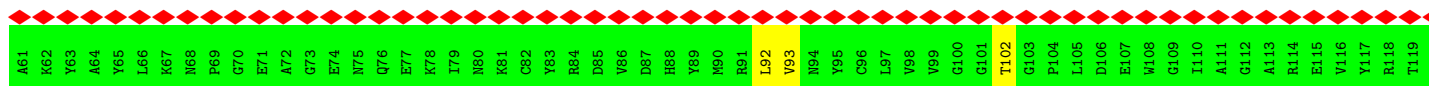
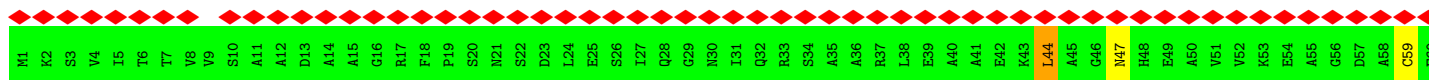
• Molecule 6: Phycoerythrin alpha subunit



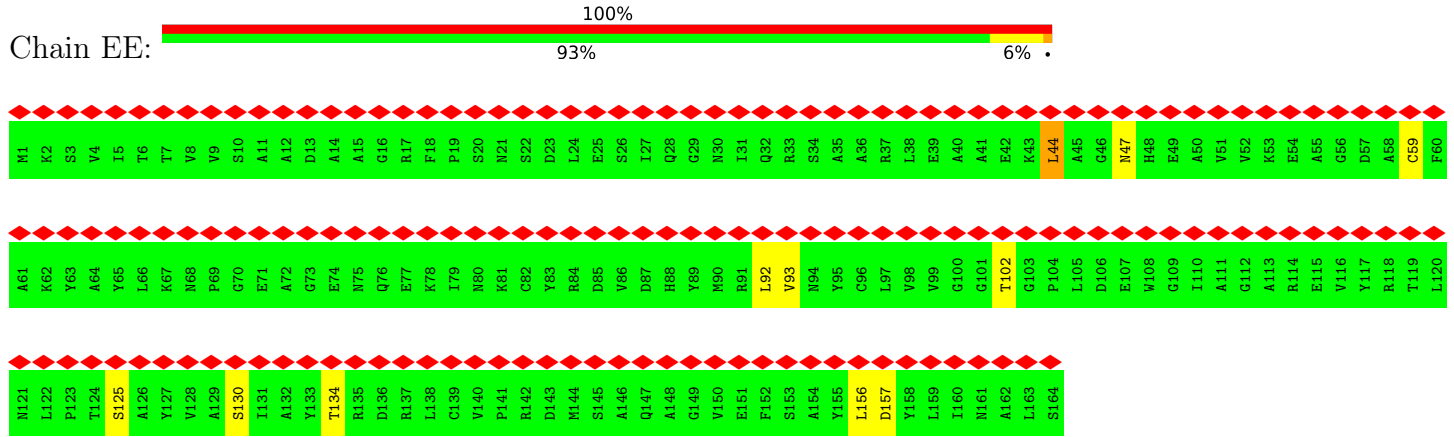
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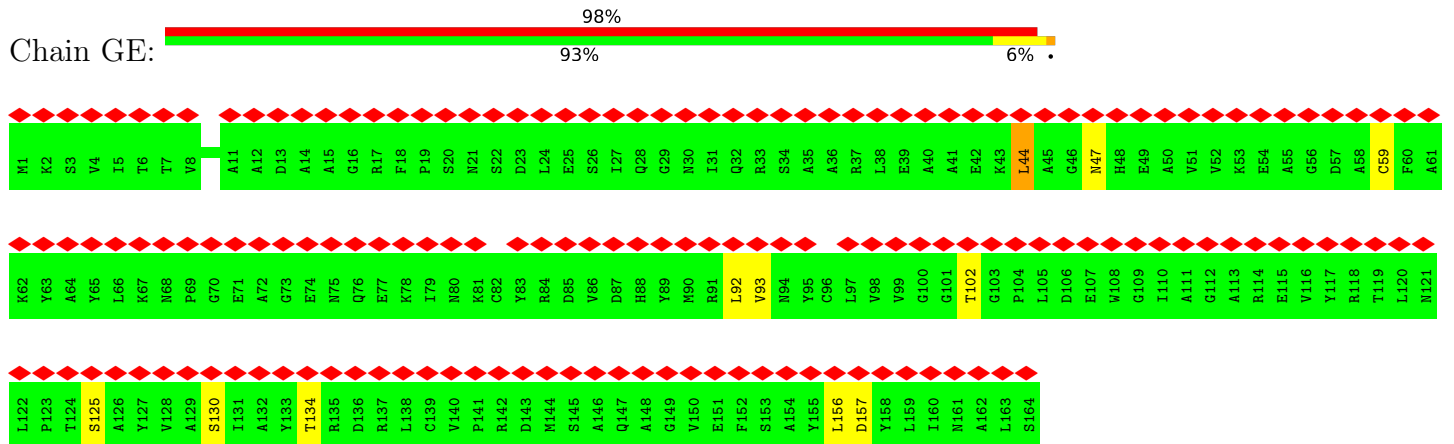
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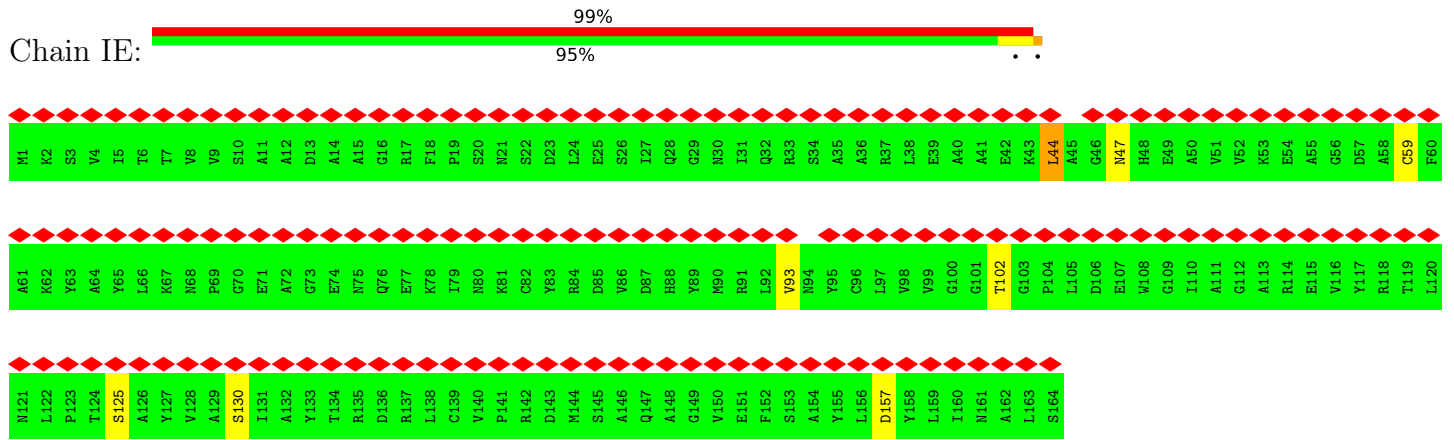
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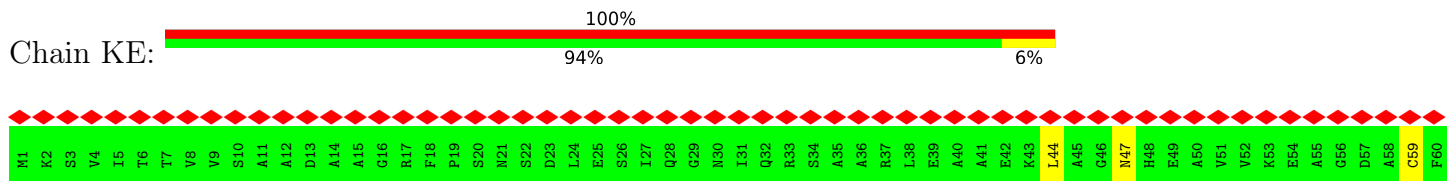
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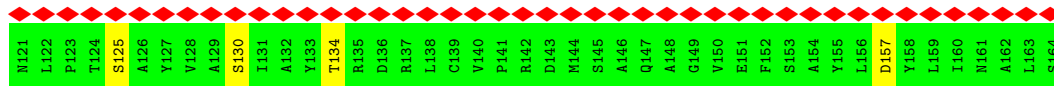
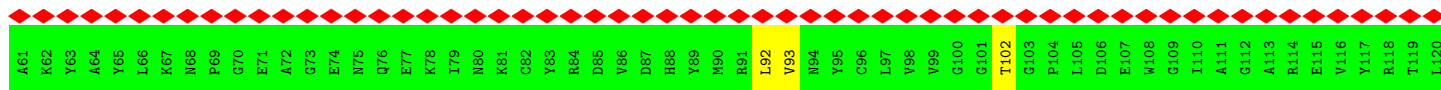


• Molecule 6: Phycoerythrin alpha subunit

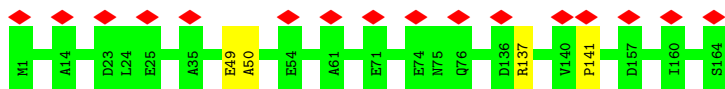


• Molecule 6: Phycoerythrin alpha subunit

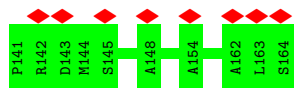
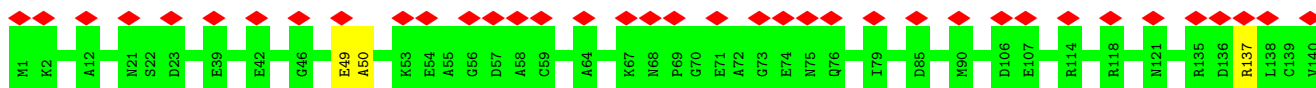




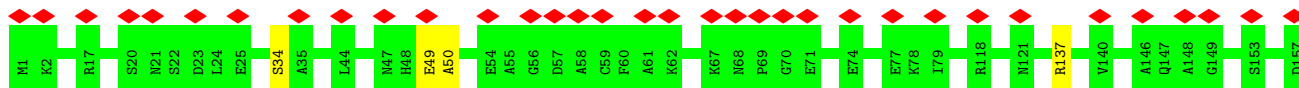
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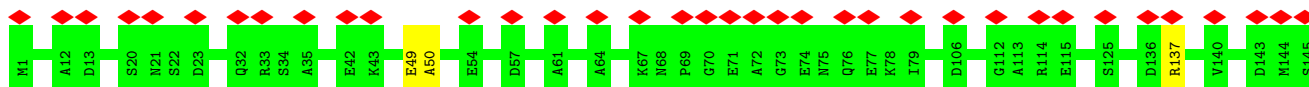
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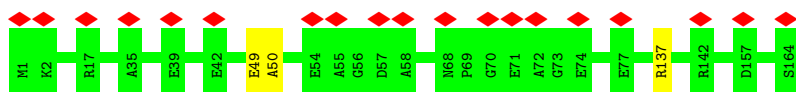
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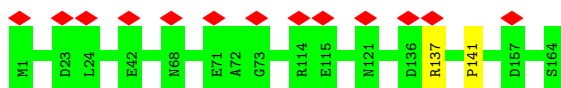
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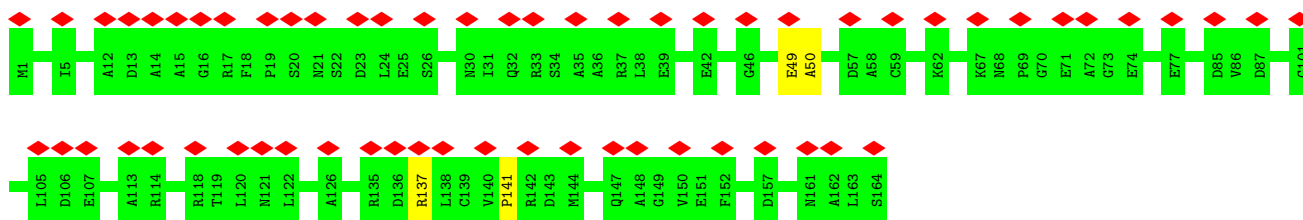
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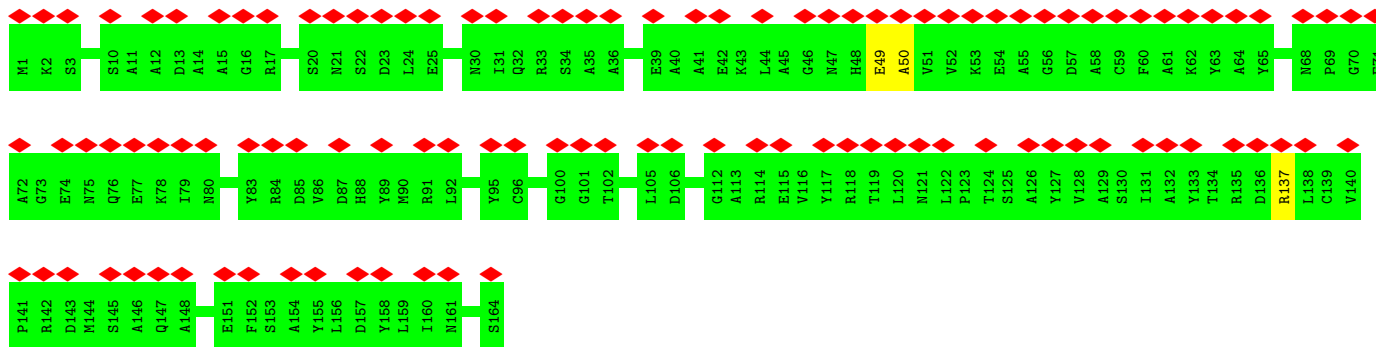
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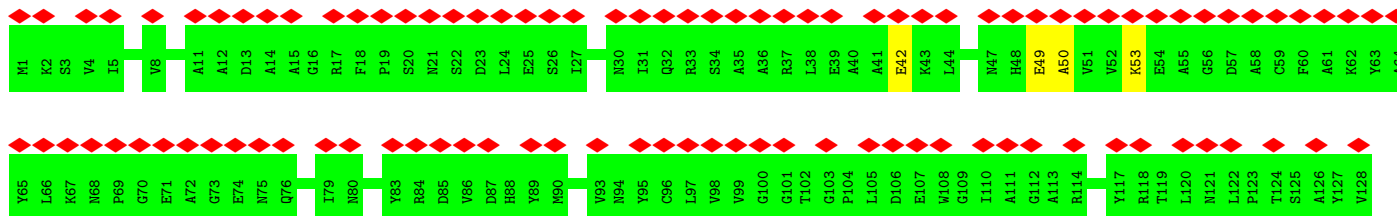
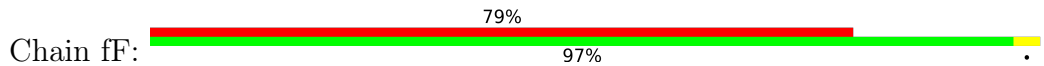
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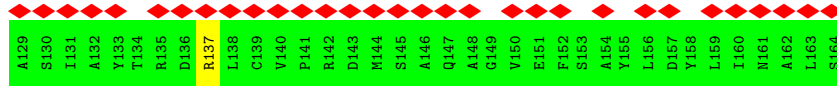


- Molecule 6: Phycoerythrin alpha subunit

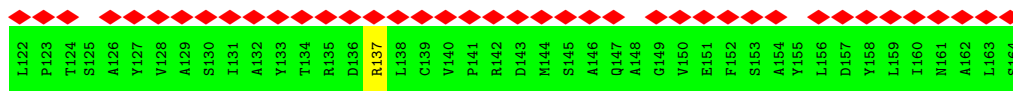
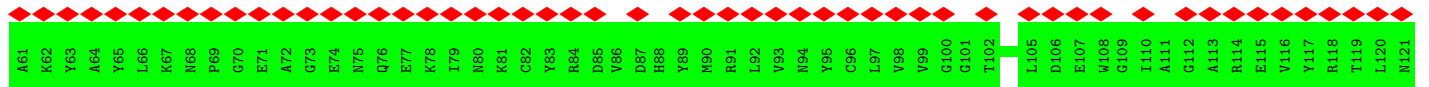
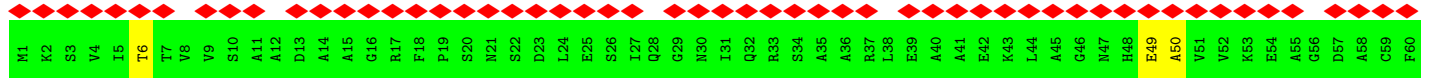
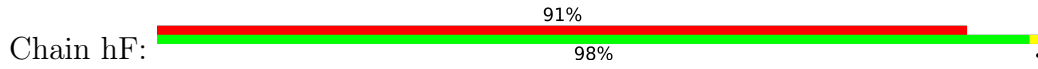


- Molecule 6: Phycoerythrin alpha subunit

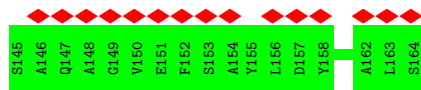
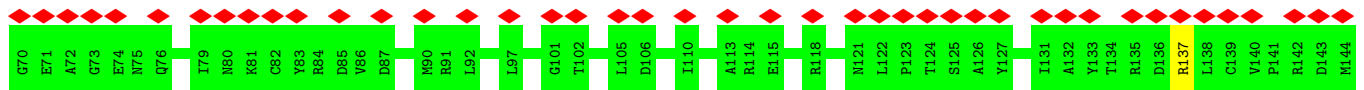
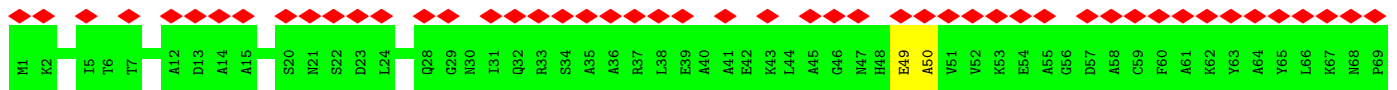




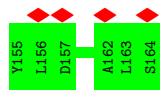
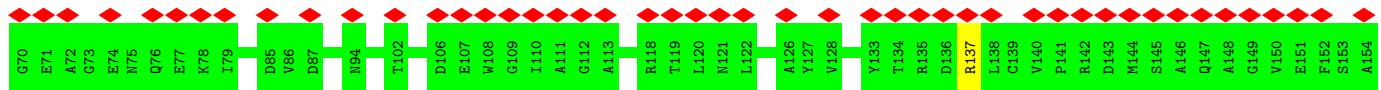
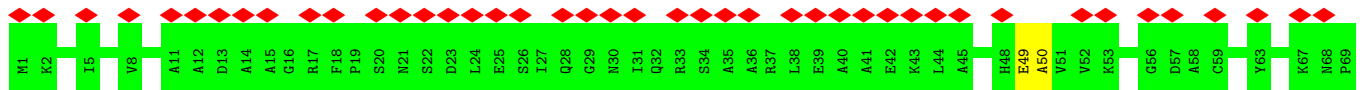
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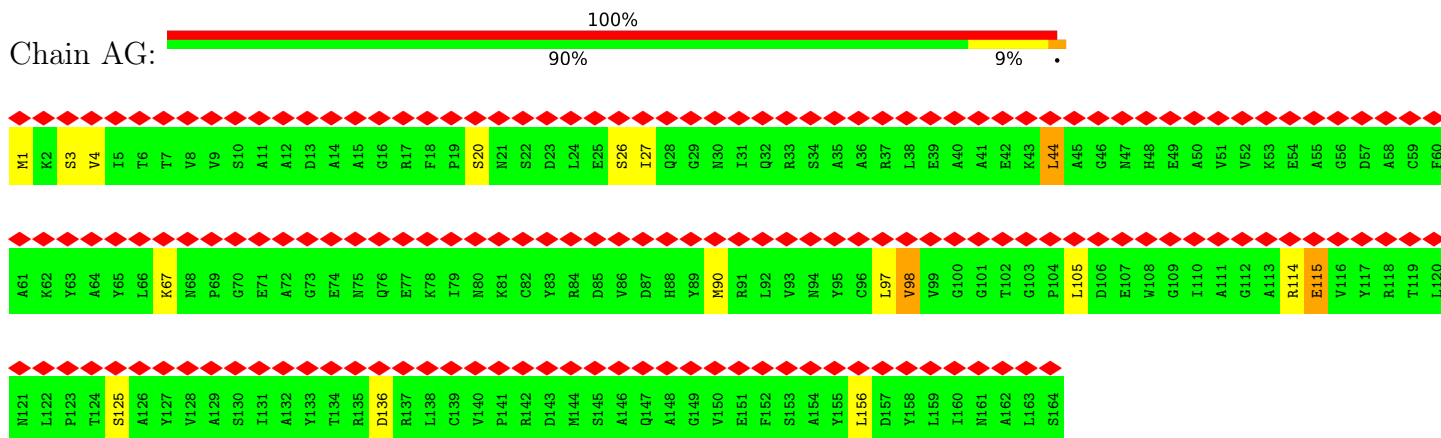
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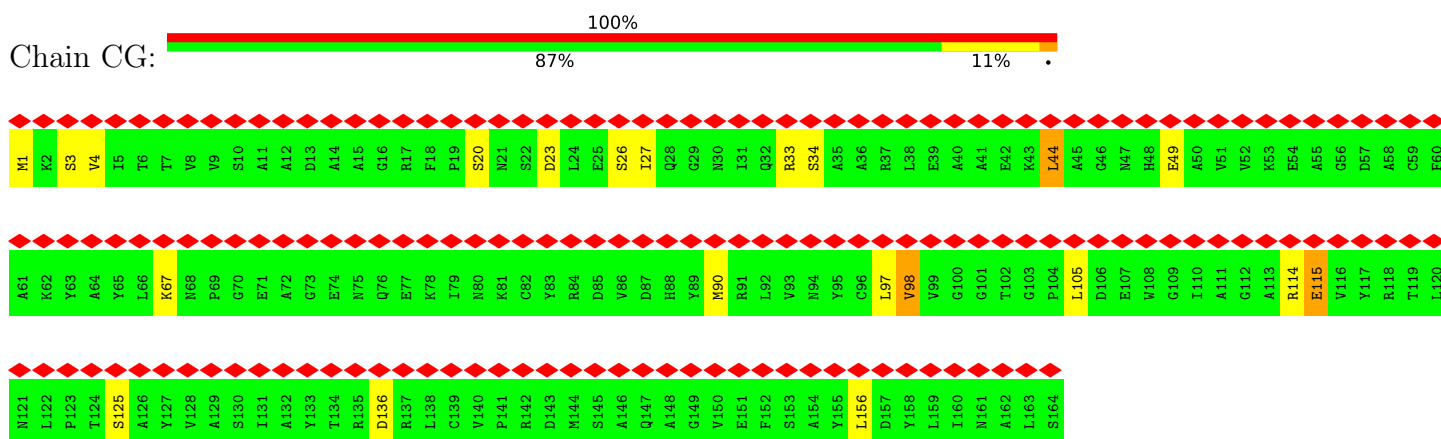
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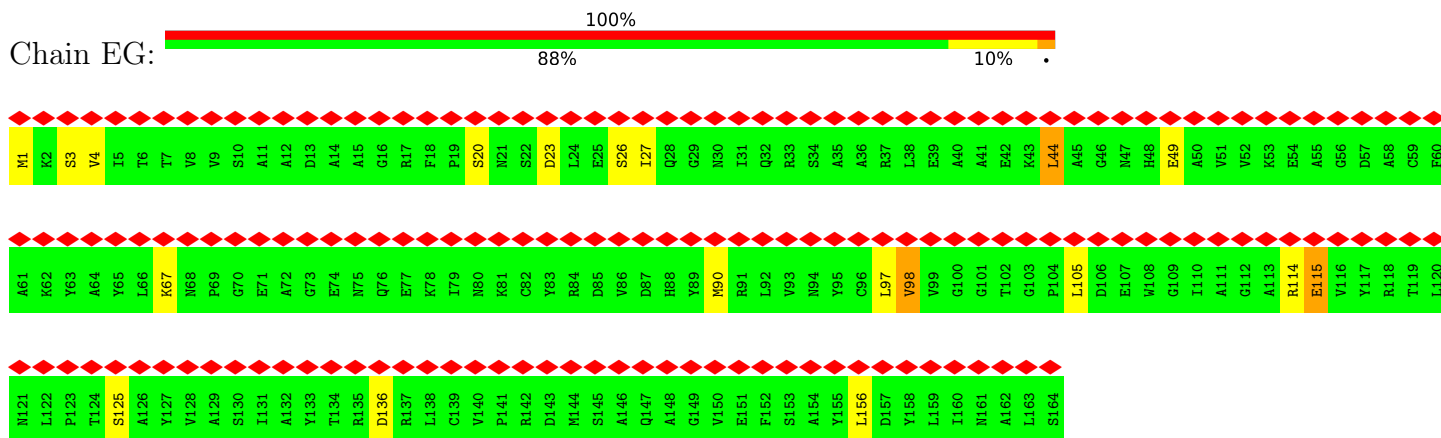
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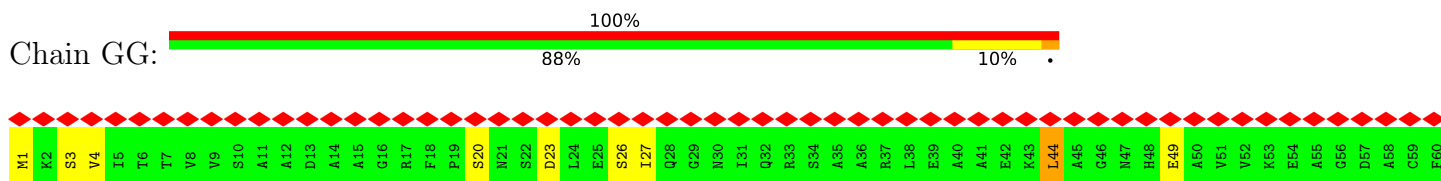
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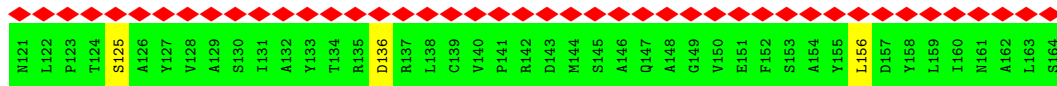
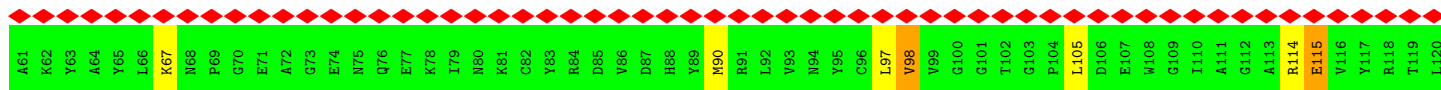


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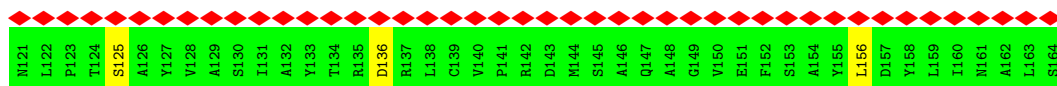
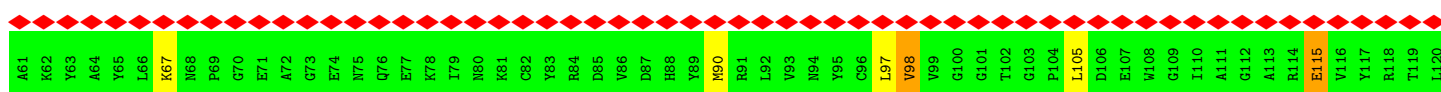
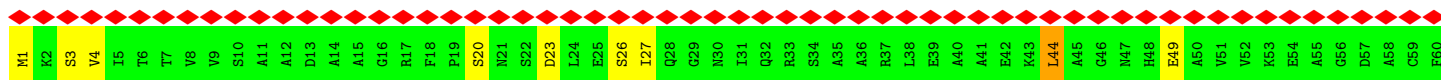
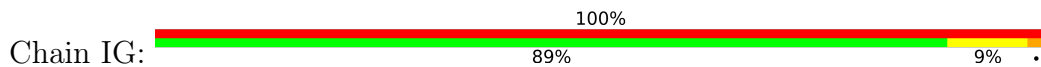


• Molecule 6: Phycoerythrin alpha subunit

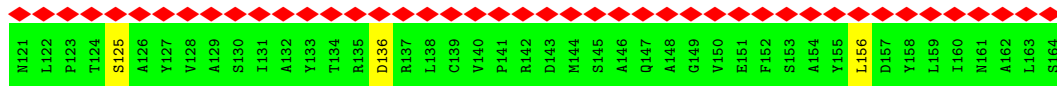
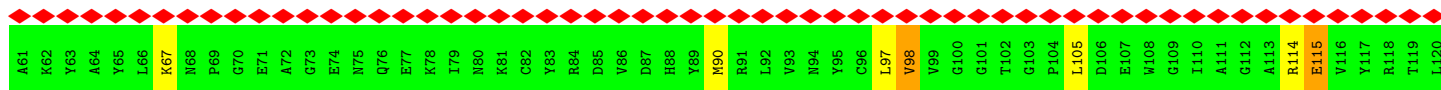
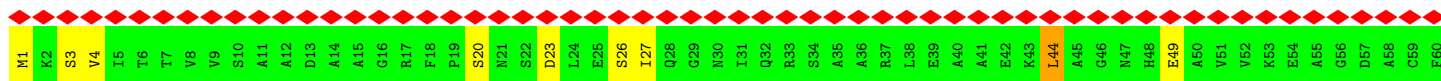
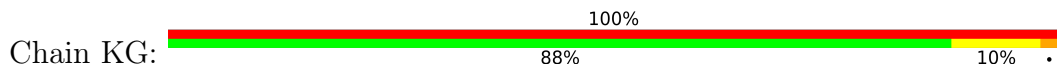




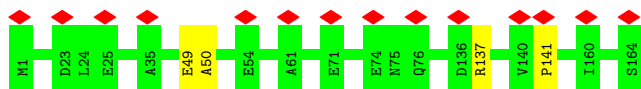
• Molecule 6: Phycoerythrin alpha subunit



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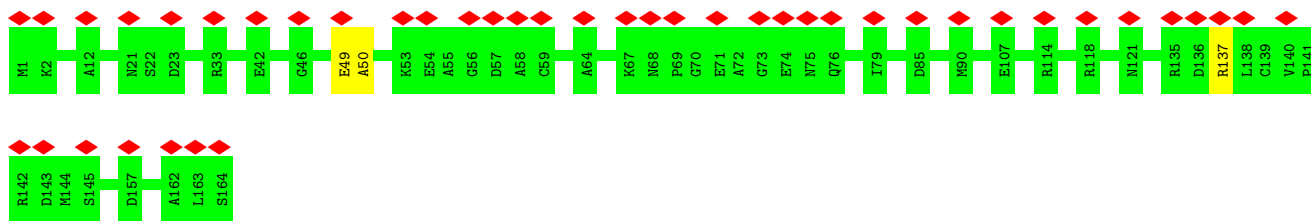


• Molecule 6: Phycoerythrin alpha subunit

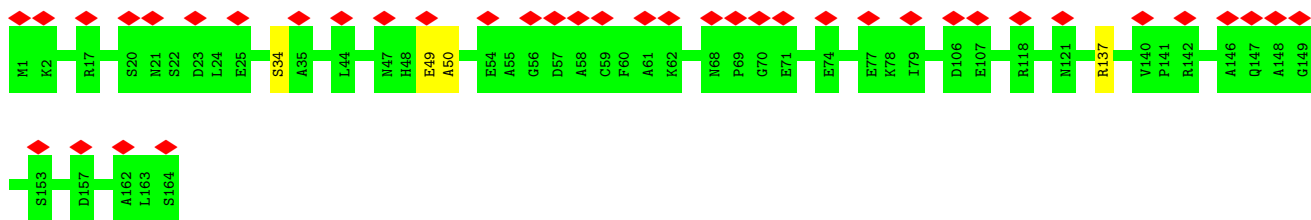


• Molecule 6: Phycoerythrin alpha subunit

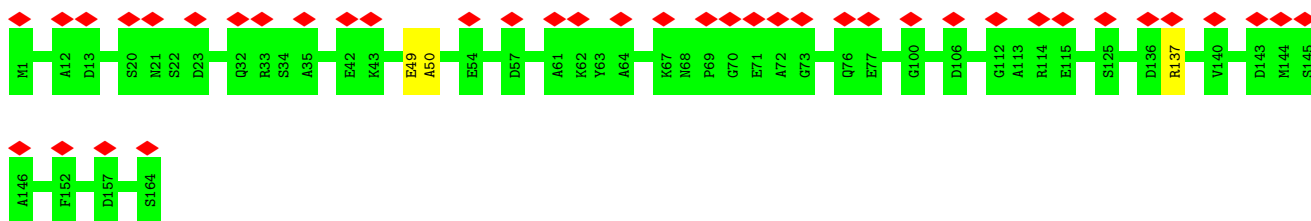




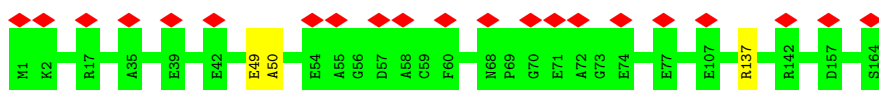
• Molecule 6: Phycoerythrin alpha subunit



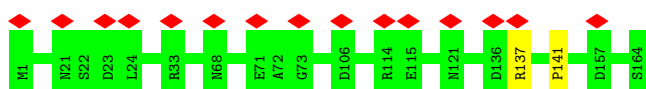
• Molecule 6: Phycoerythrin alpha subunit



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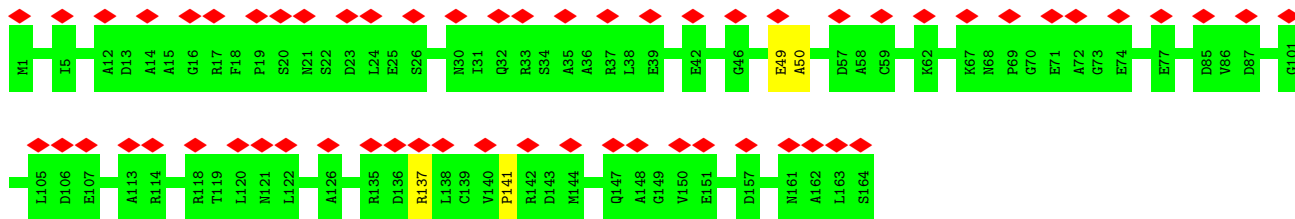


• Molecule 6: Phycoerythrin alpha subunit

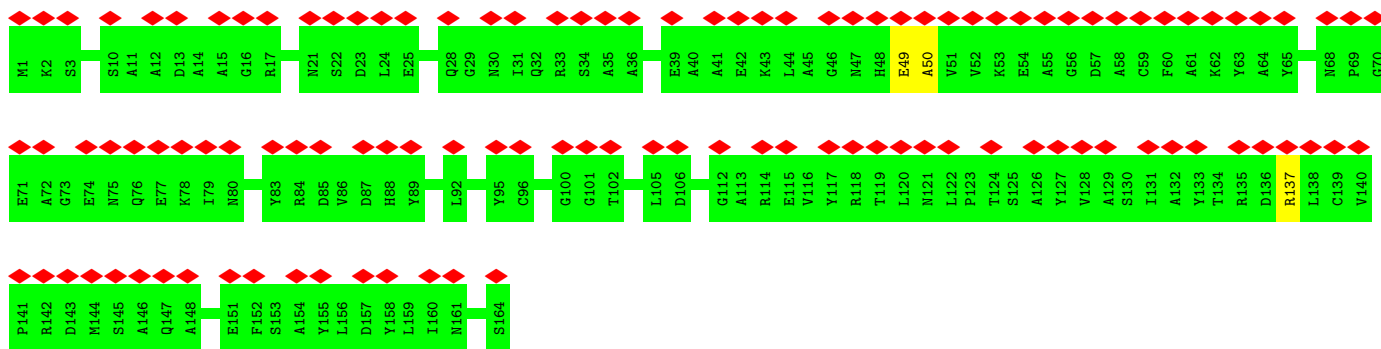


• Molecule 6: Phycoerythrin alpha subunit

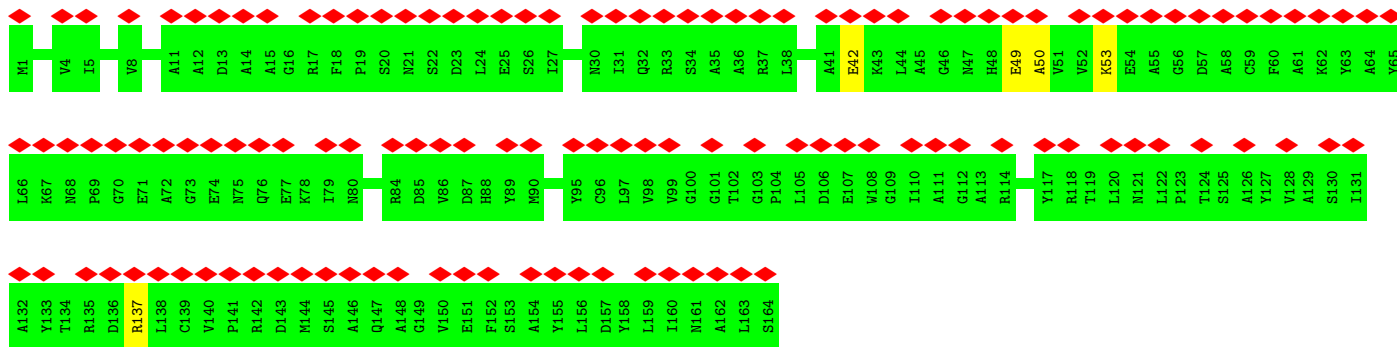
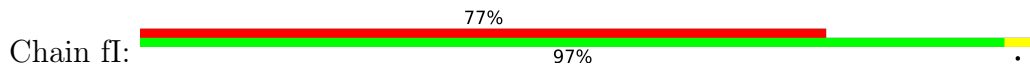




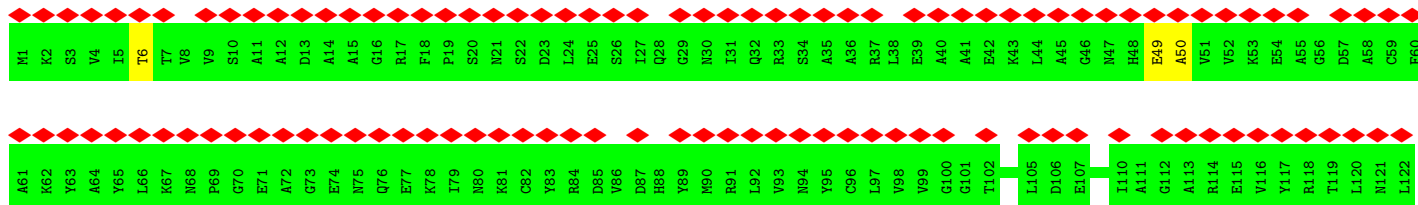
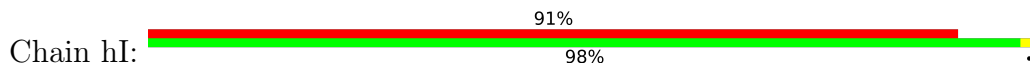
- Molecule 6: Phycoerythrin alpha subunit

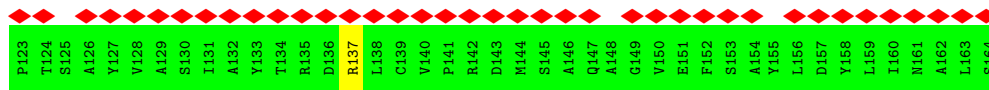


- Molecule 6: Phycoerythrin alpha subunit

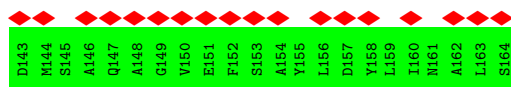
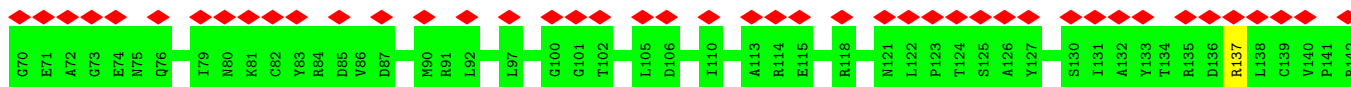
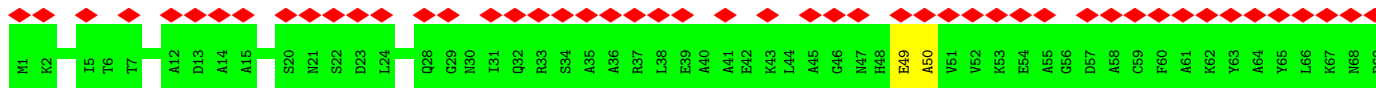


- Molecule 6: Phycoerythrin alpha subunit

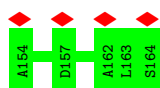
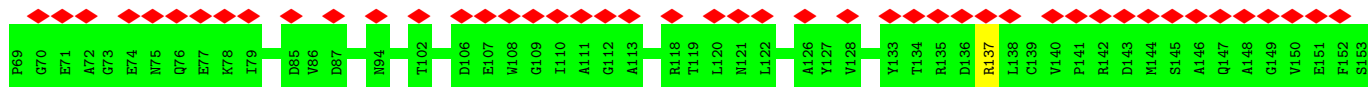
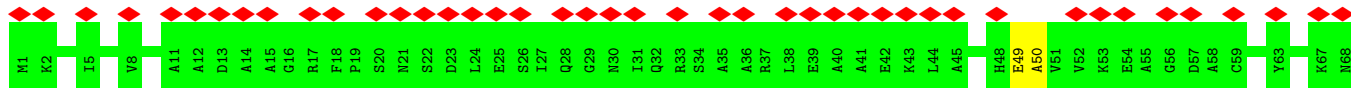




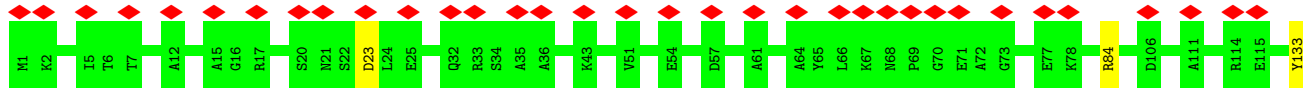
• Molecule 6: Phycoerythrin alpha subunit



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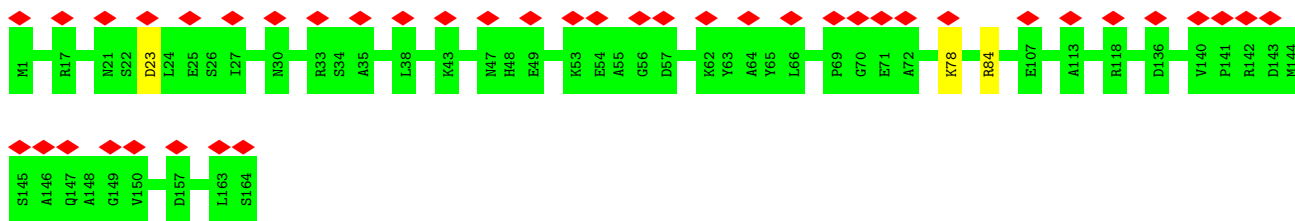


• Molecule 6: Phycoerythrin alpha subunit

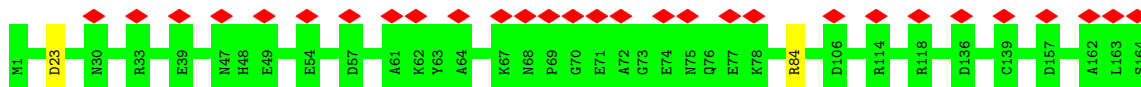


• Molecule 6: Phycoerythrin alpha subunit

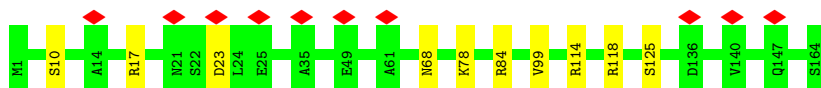




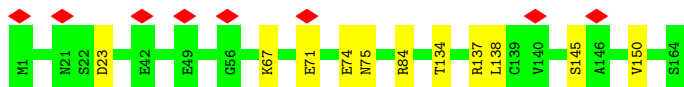
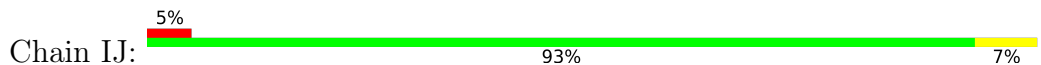
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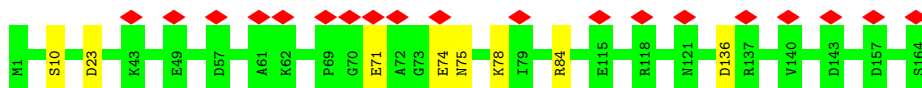
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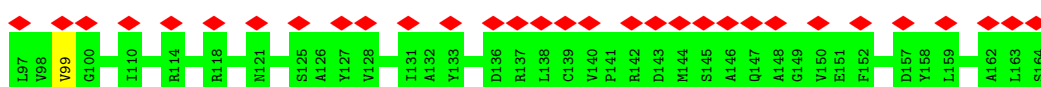
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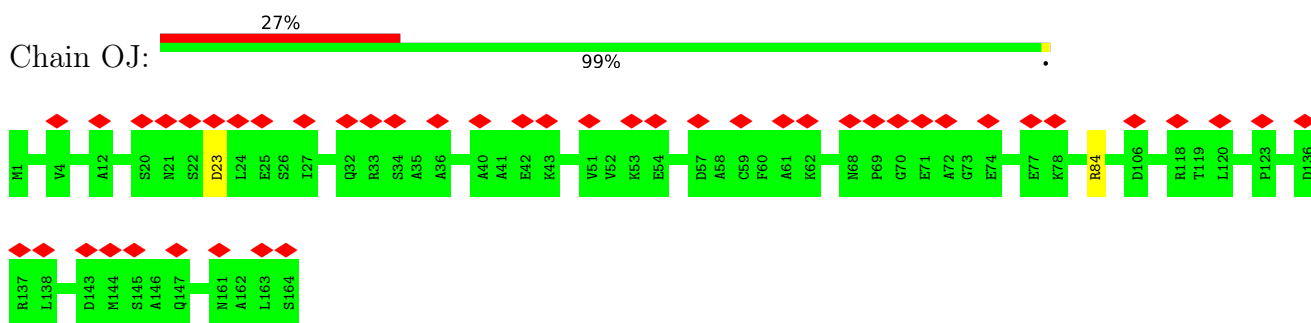
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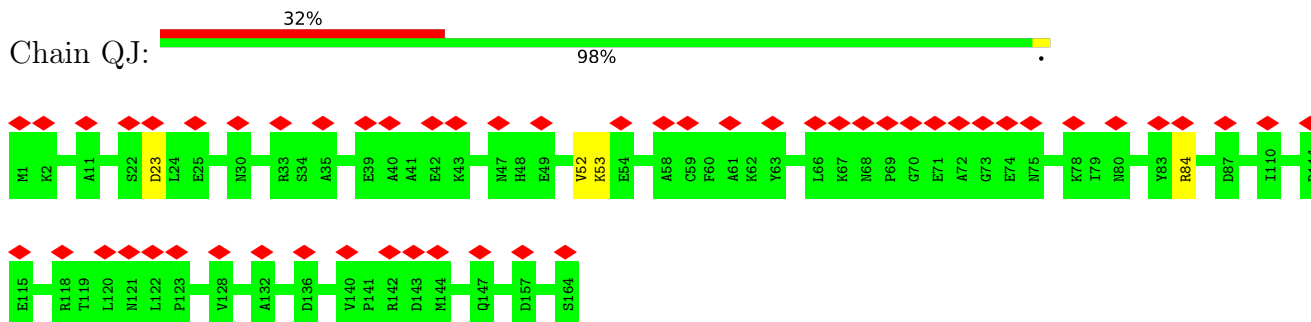
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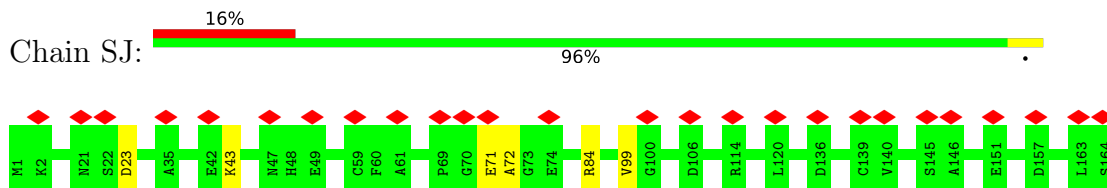
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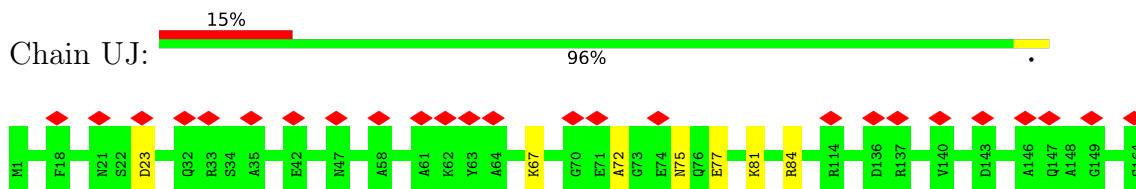
- Molecule 6: Phycoerythrin alpha subunit



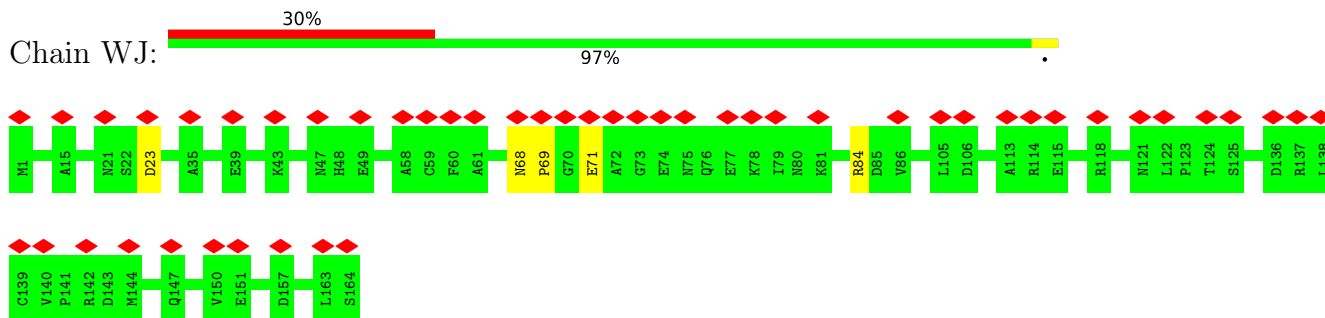
- Molecule 6: Phycoerythrin alpha subunit



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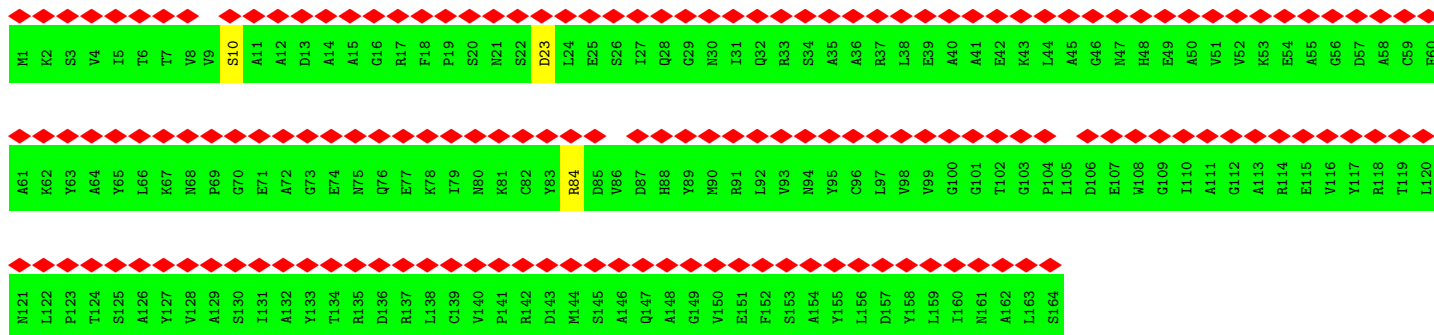


- Molecule 6: Phycoerythrin alpha subunit

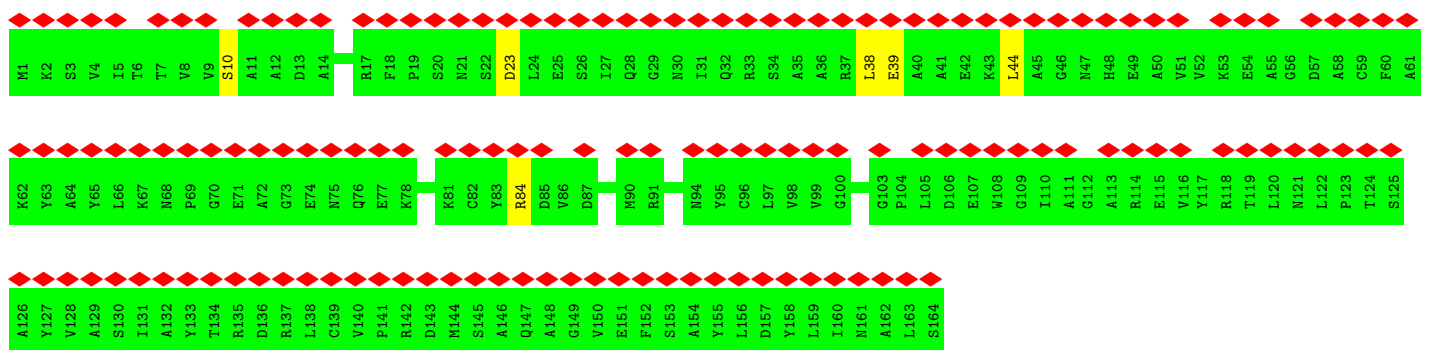
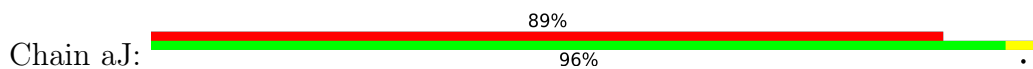


- Molecule 6: Phycoerythrin alpha subunit

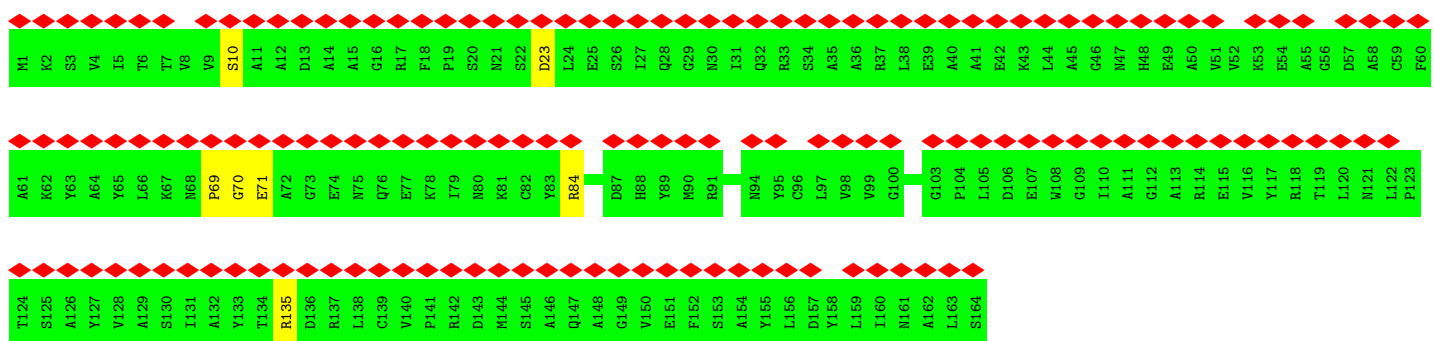




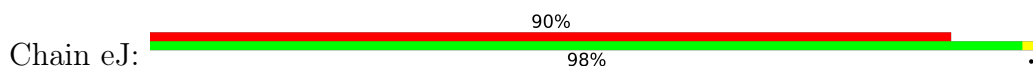
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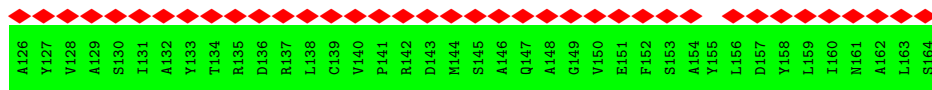


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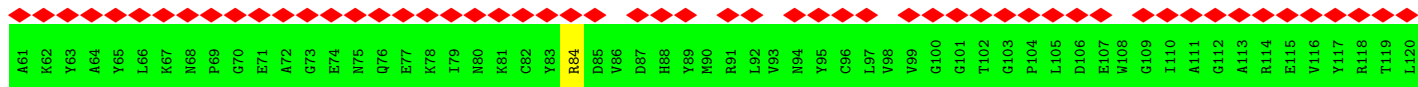
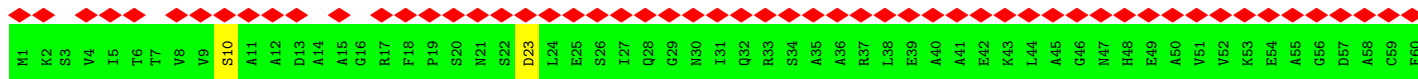


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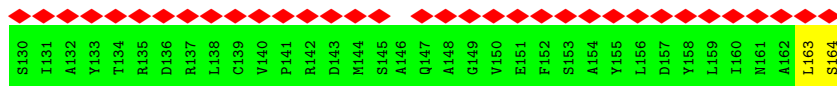
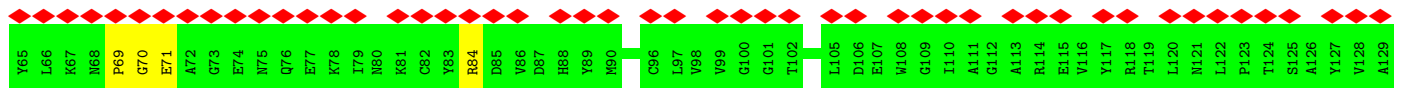
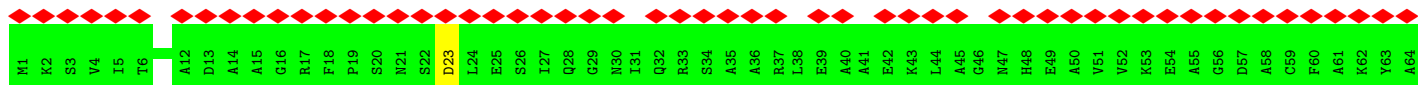
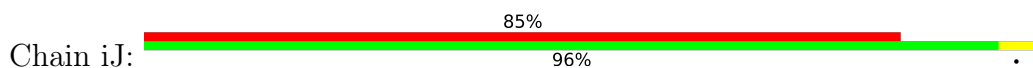




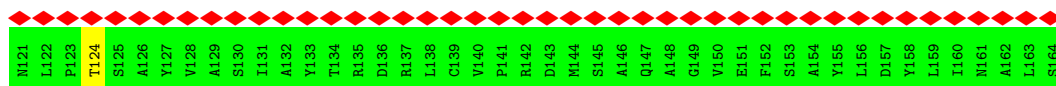
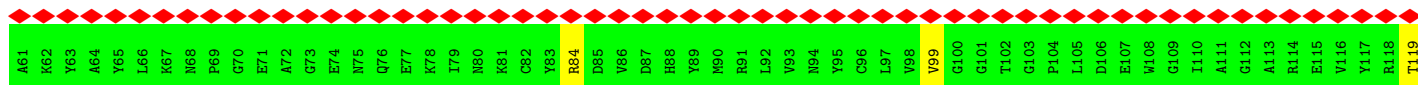
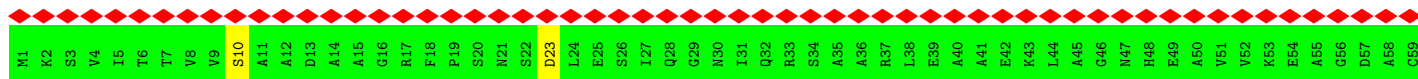
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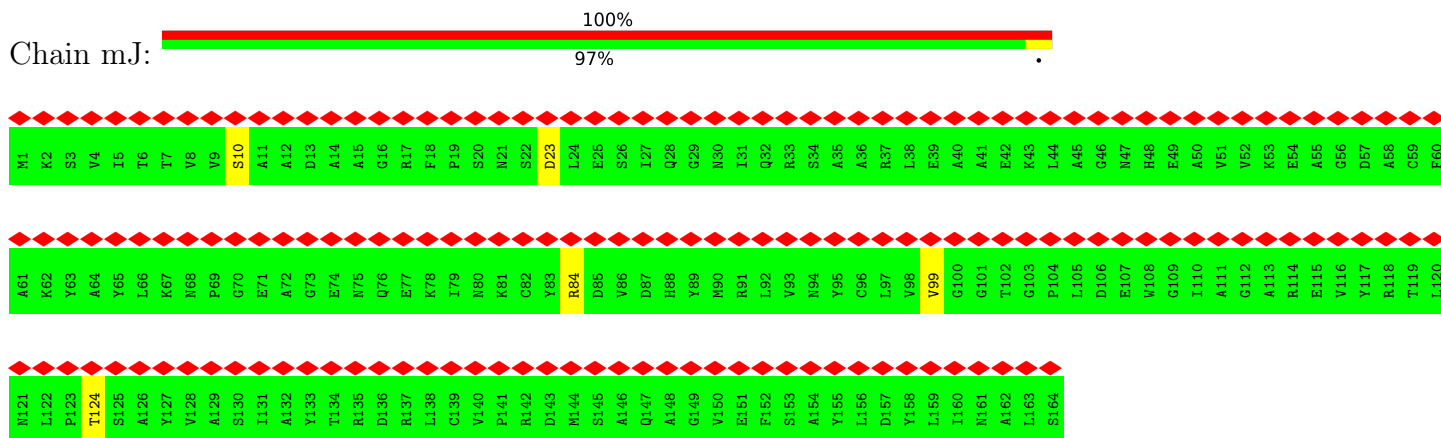
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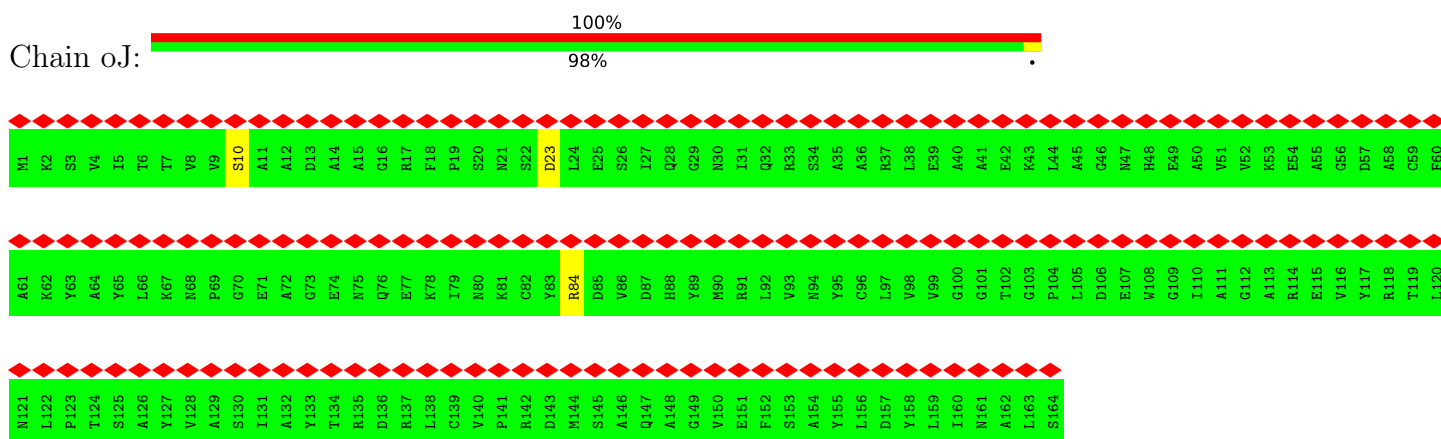
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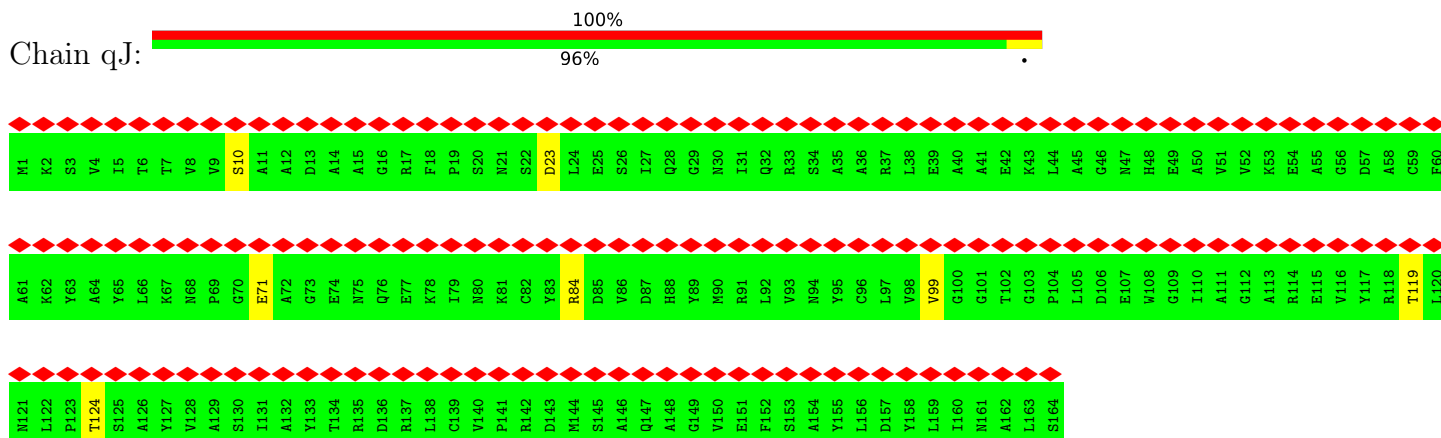
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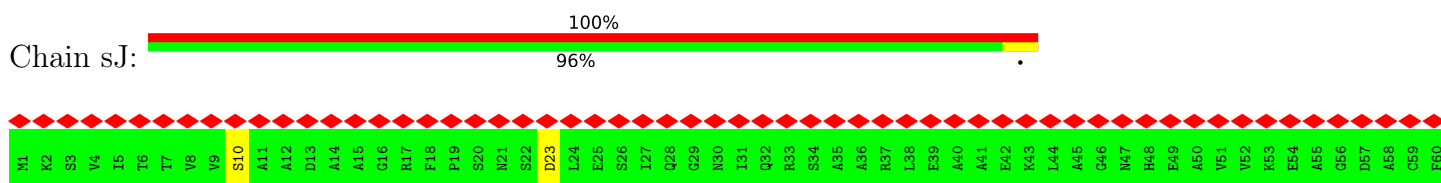
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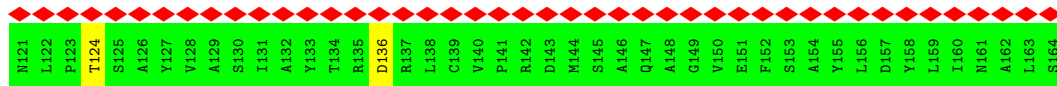
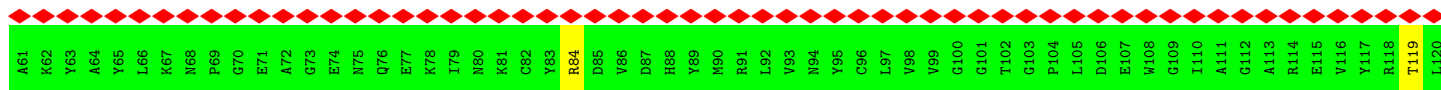


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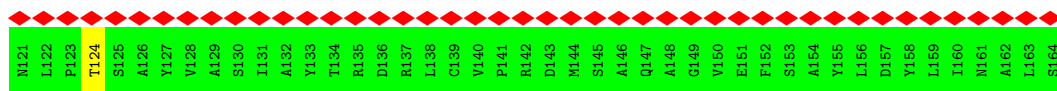
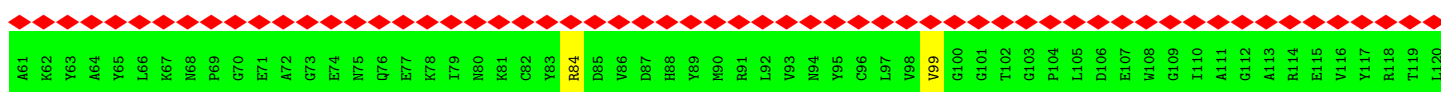
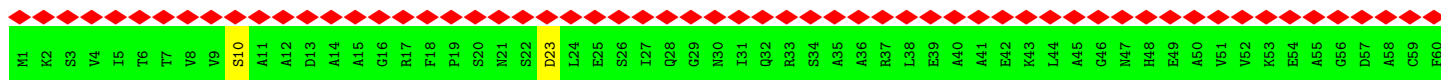


• Molecule 6: Phycoerythrin alpha subunit

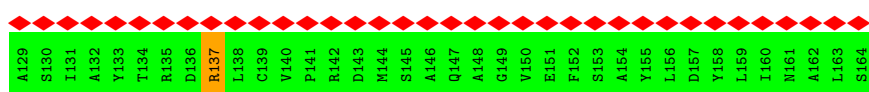
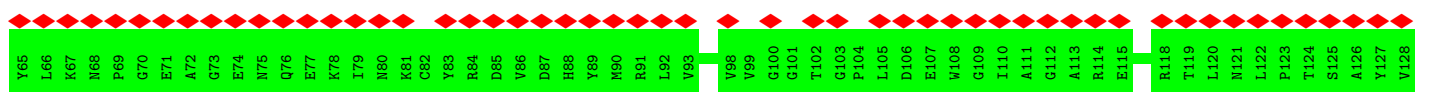
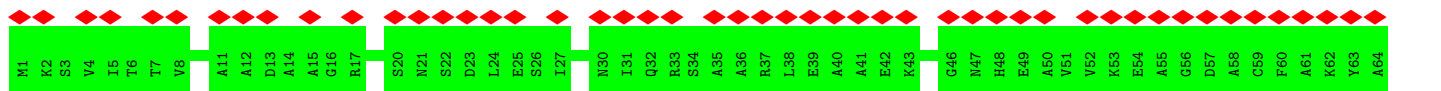
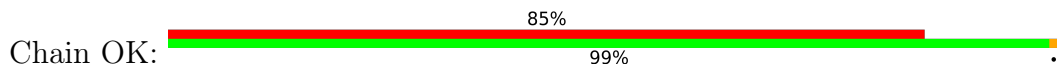




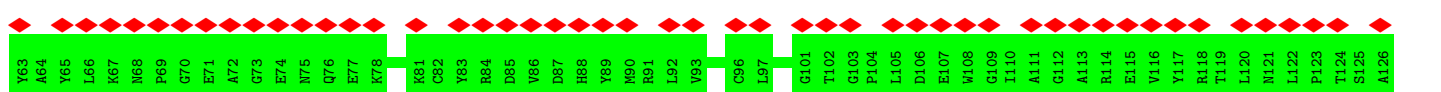
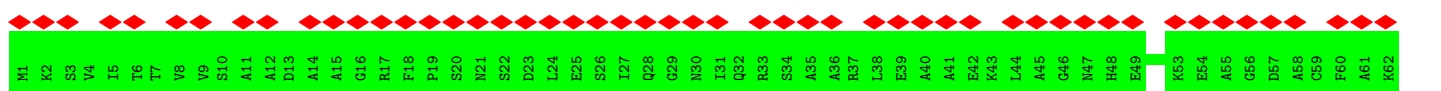
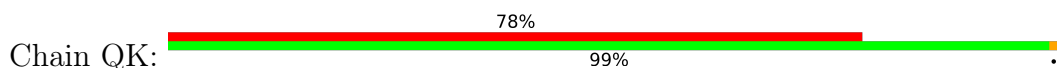
• Molecule 6: Phycoerythrin alpha subunit

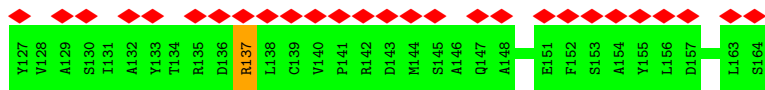


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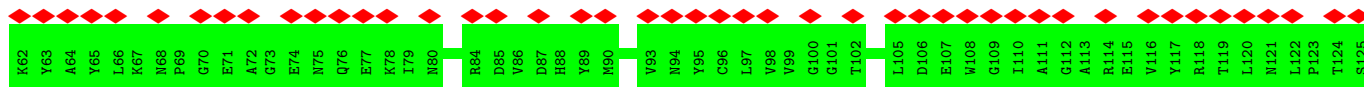
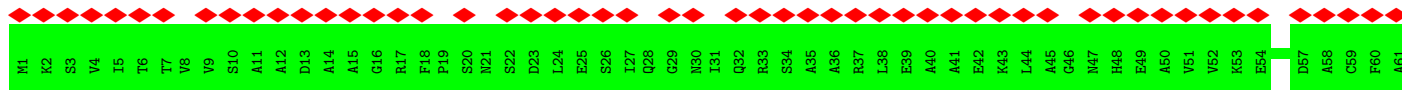
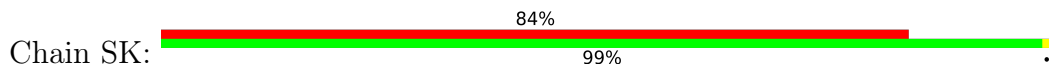


• Molecule 6: Phycoerythrin alpha subunit

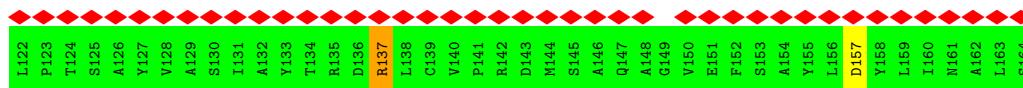
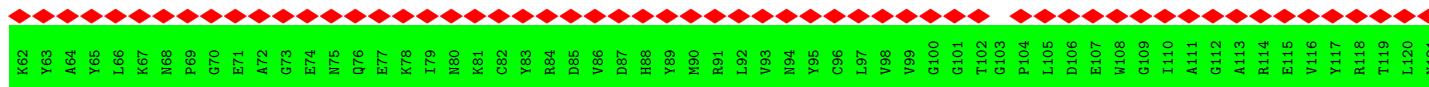
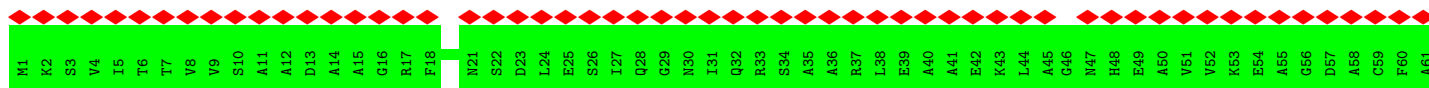




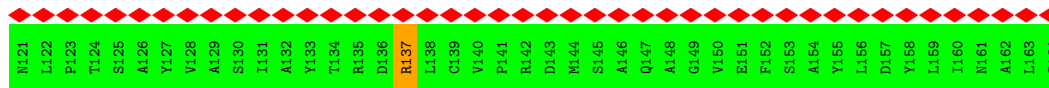
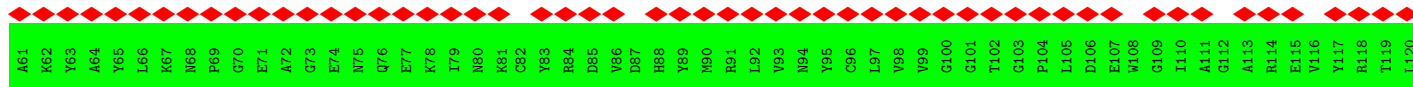
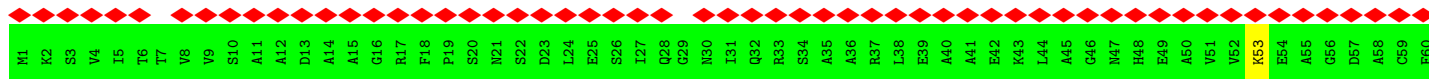
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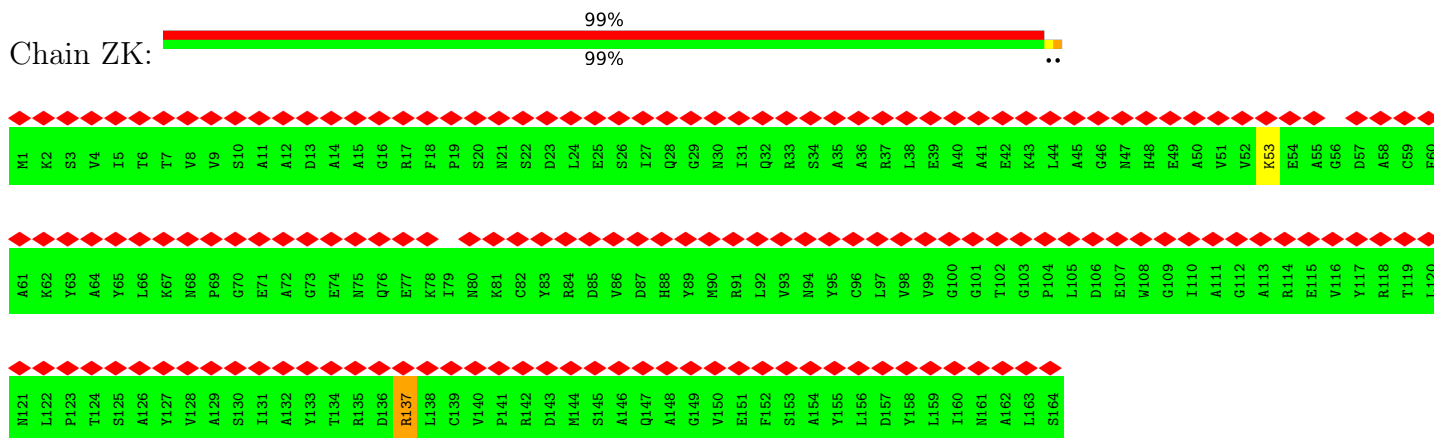
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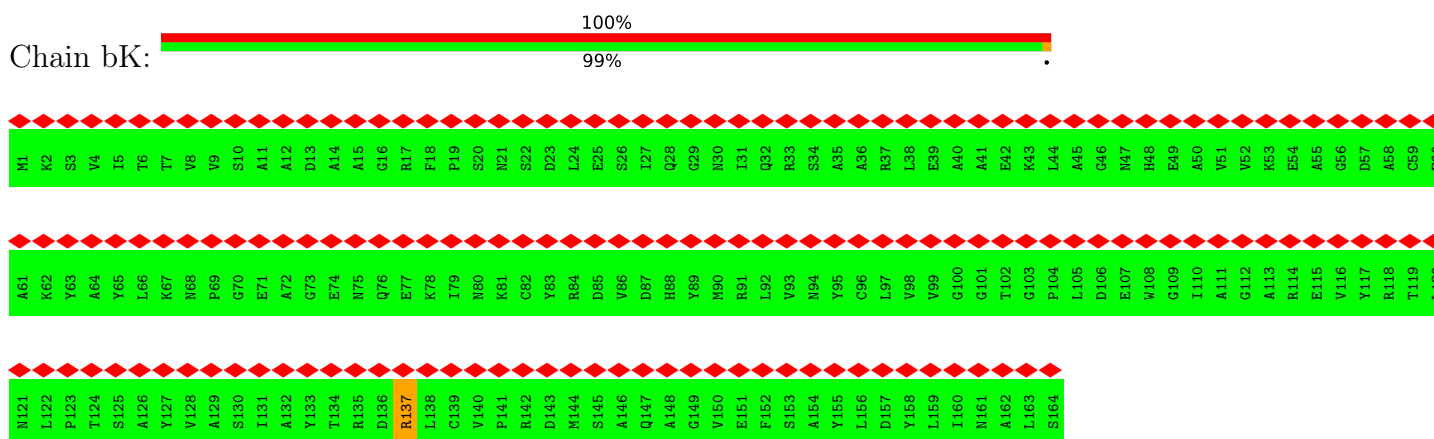
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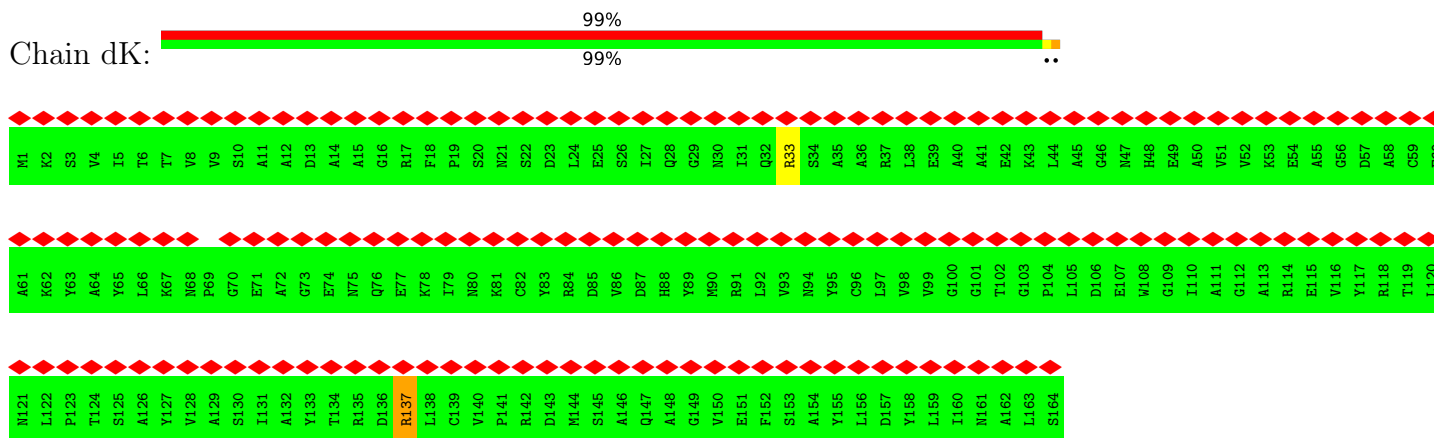
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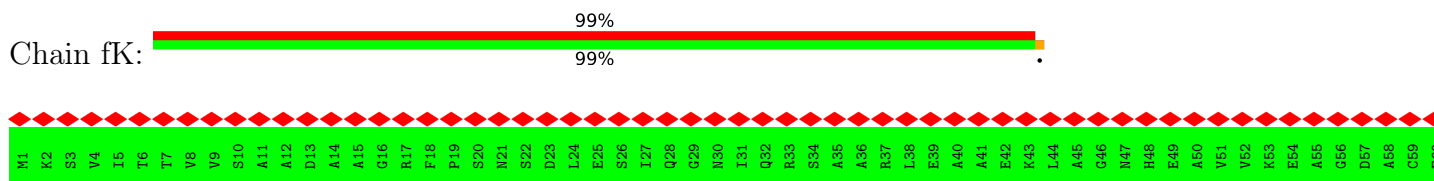
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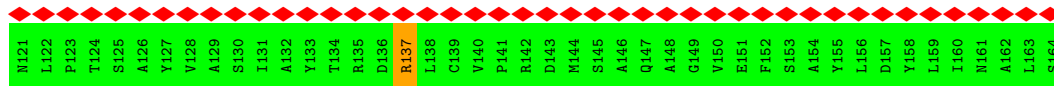
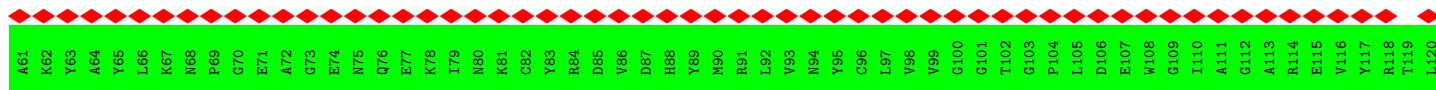


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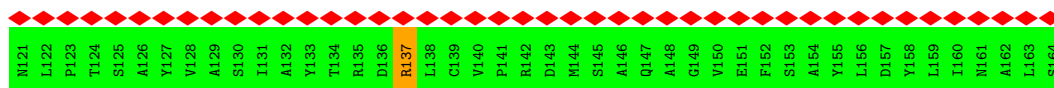
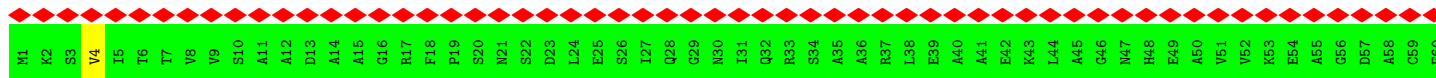


• Molecule 6: Phycoerythrin alpha subunit

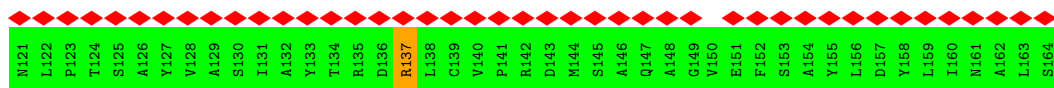
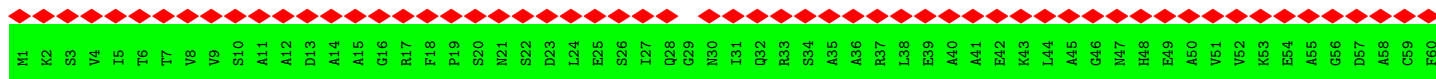




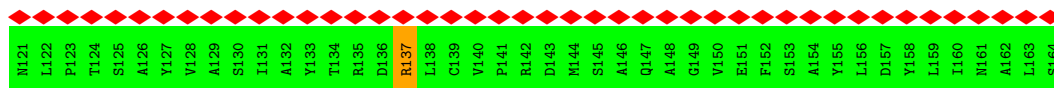
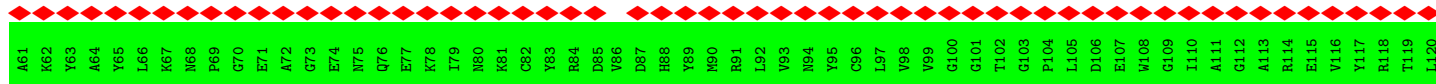
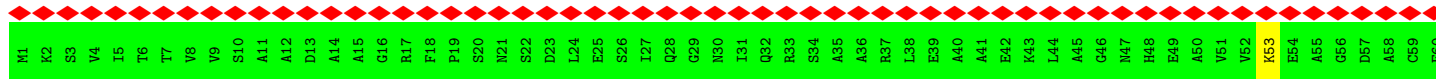
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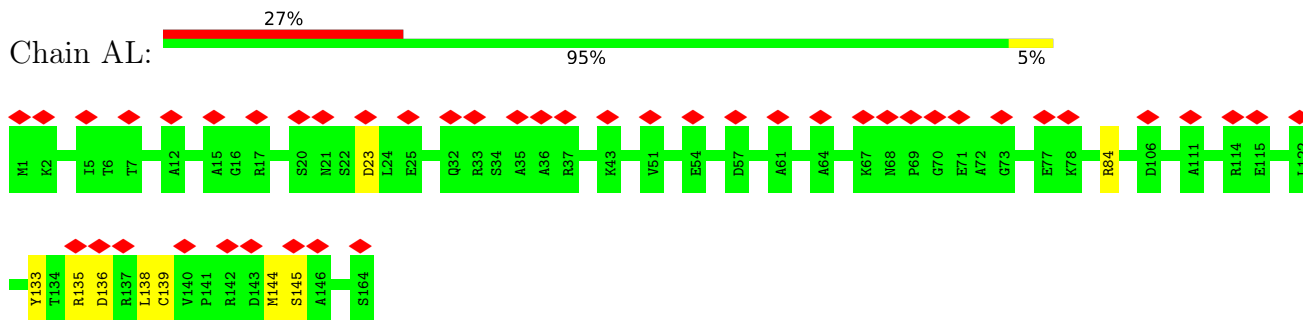
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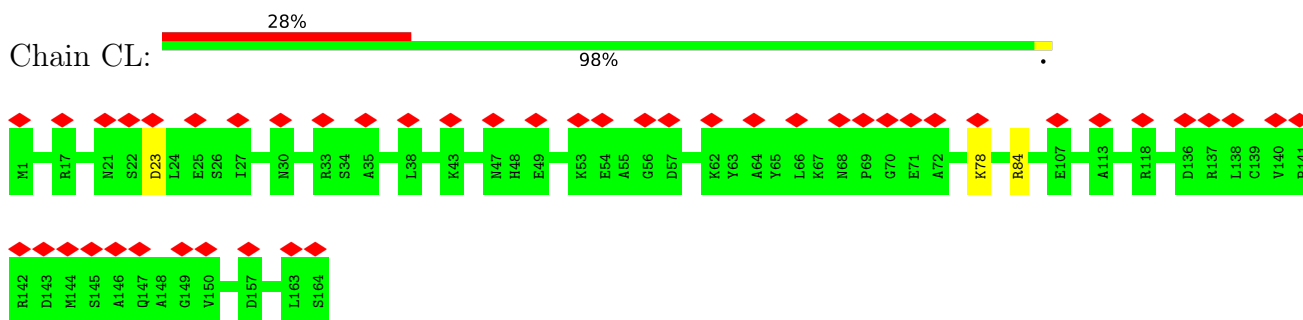
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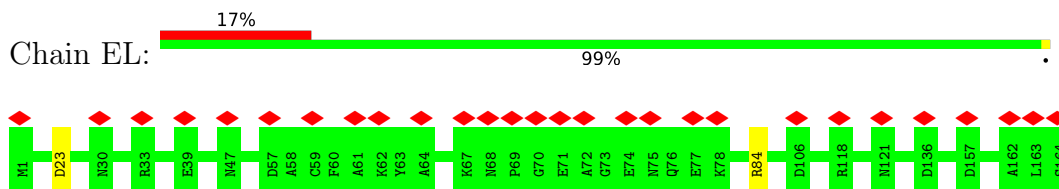
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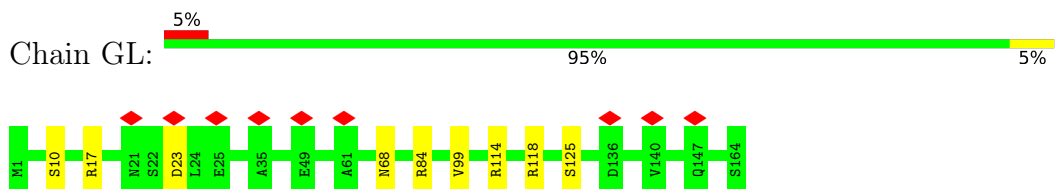
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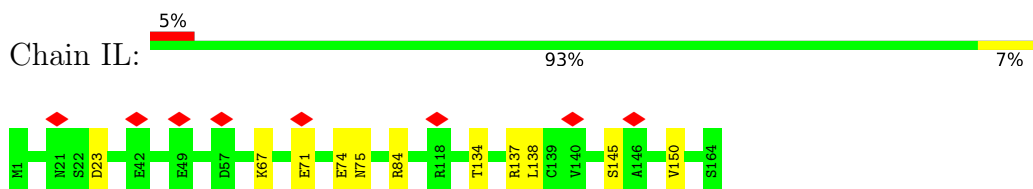
- Molecule 6: Phycoerythrin alpha subunit



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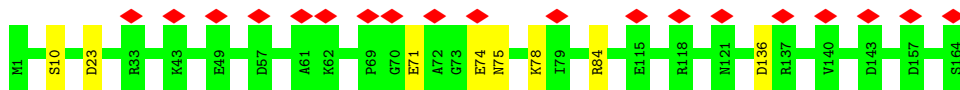


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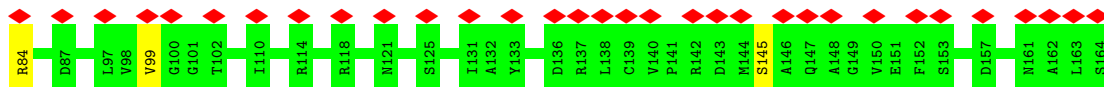
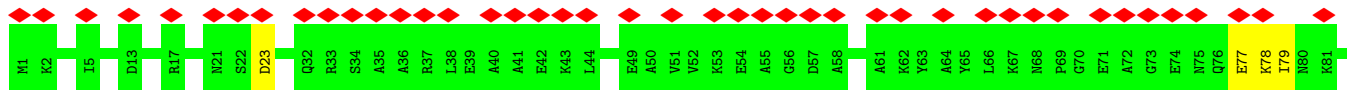


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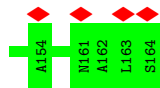
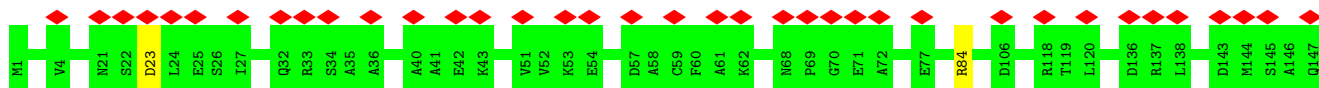




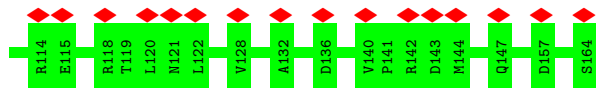
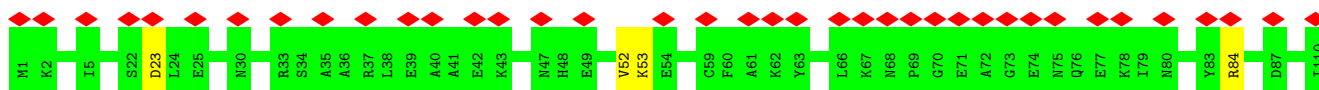
• Molecule 6: Phycoerythrin alpha subunit



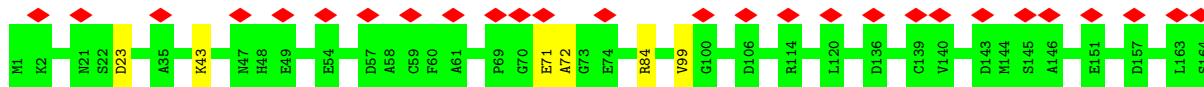
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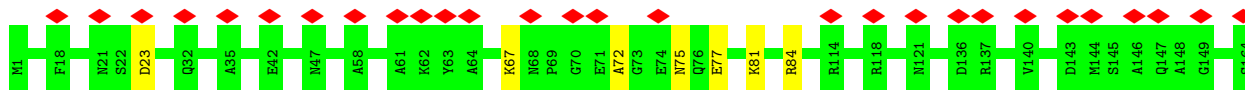


• Molecule 6: Phycoerythrin alpha subunit

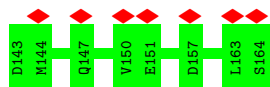
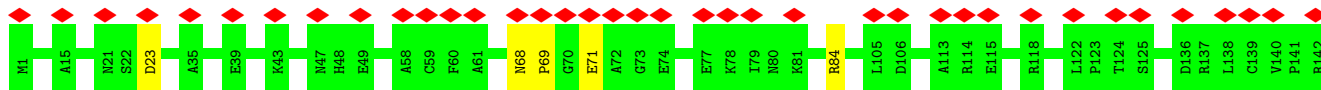


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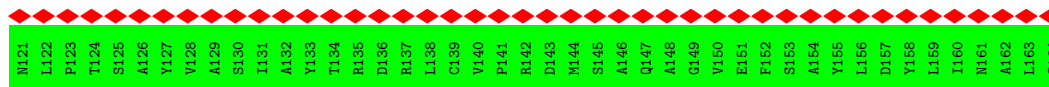
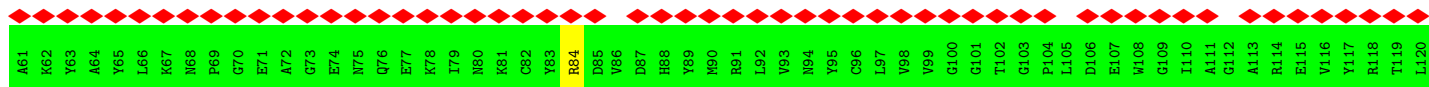
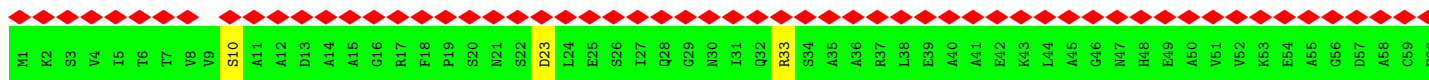




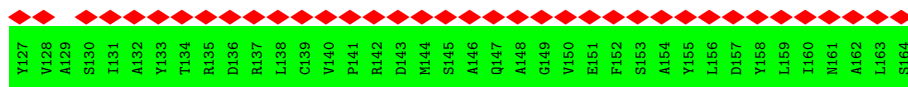
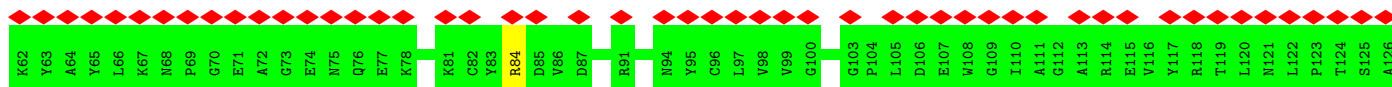
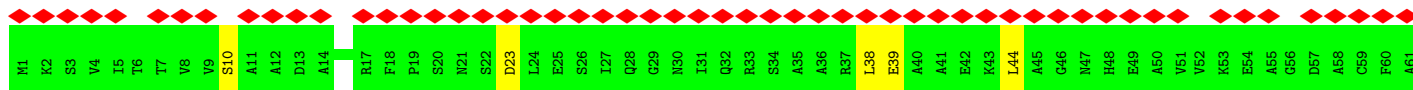
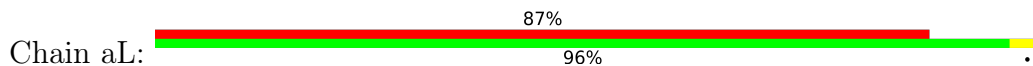
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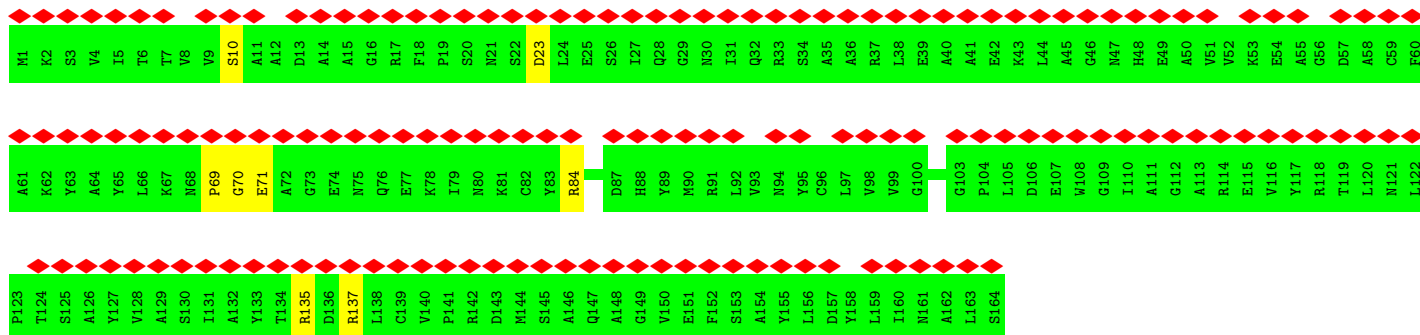


• Molecule 6: Phycoerythrin alpha subunit

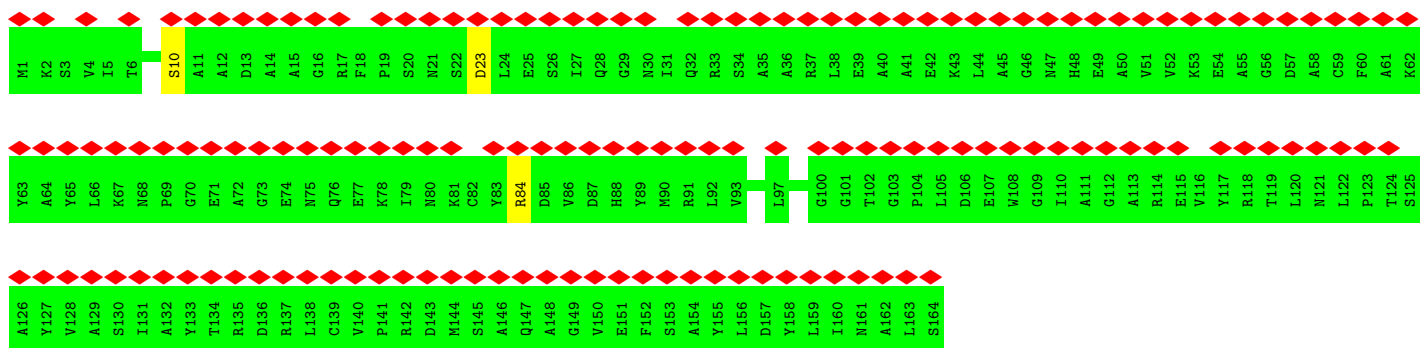


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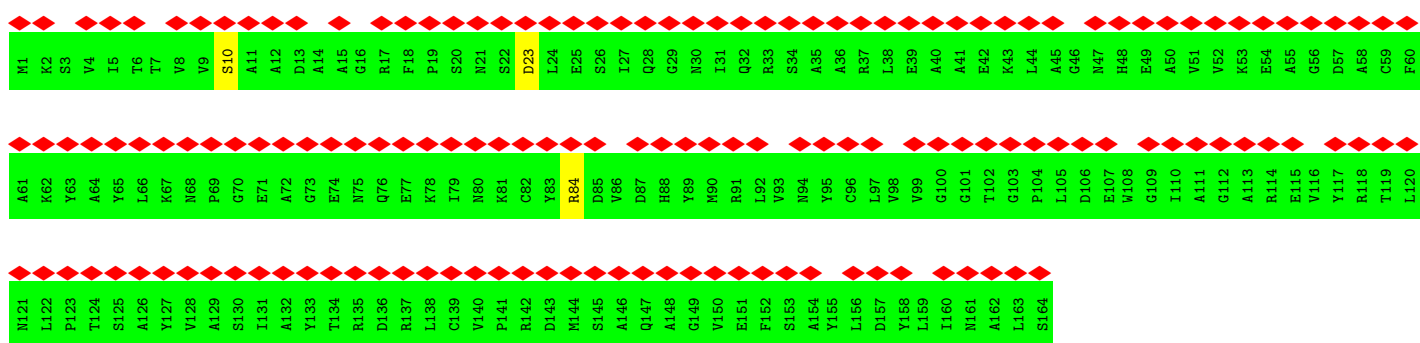




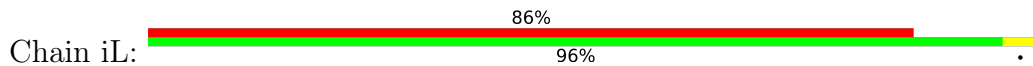
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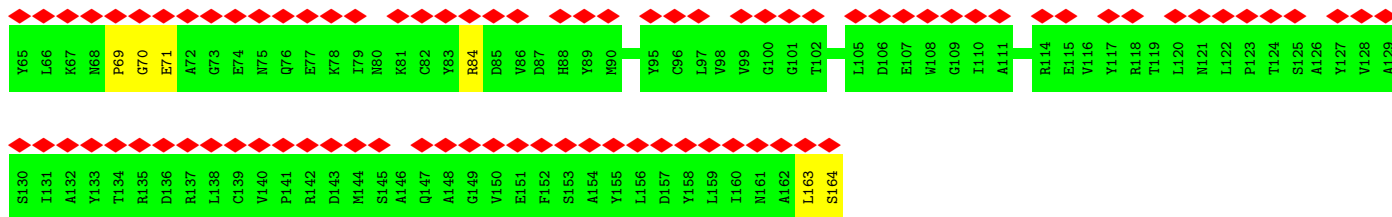


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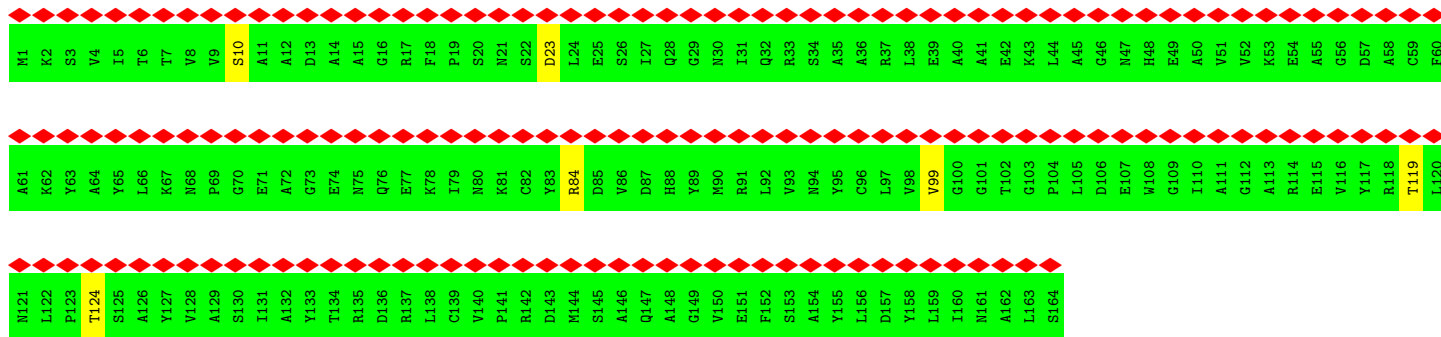


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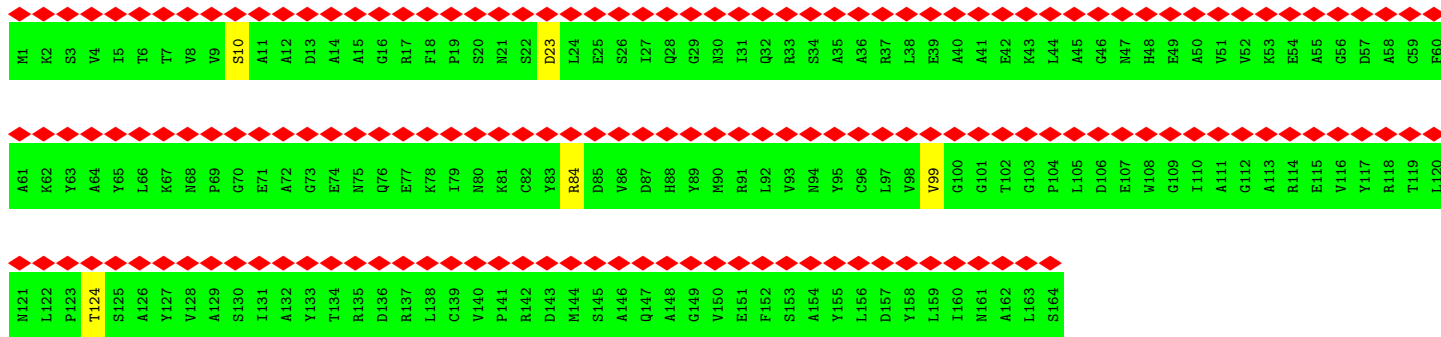




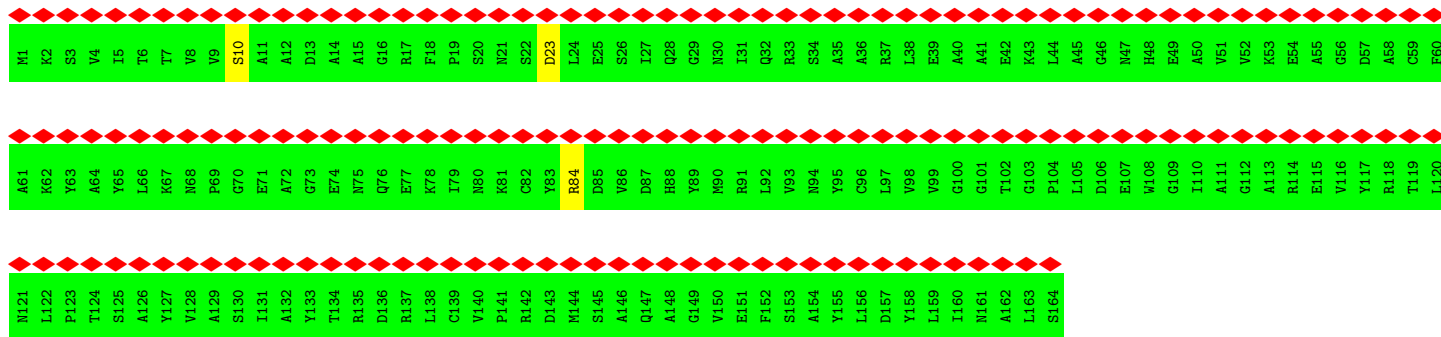
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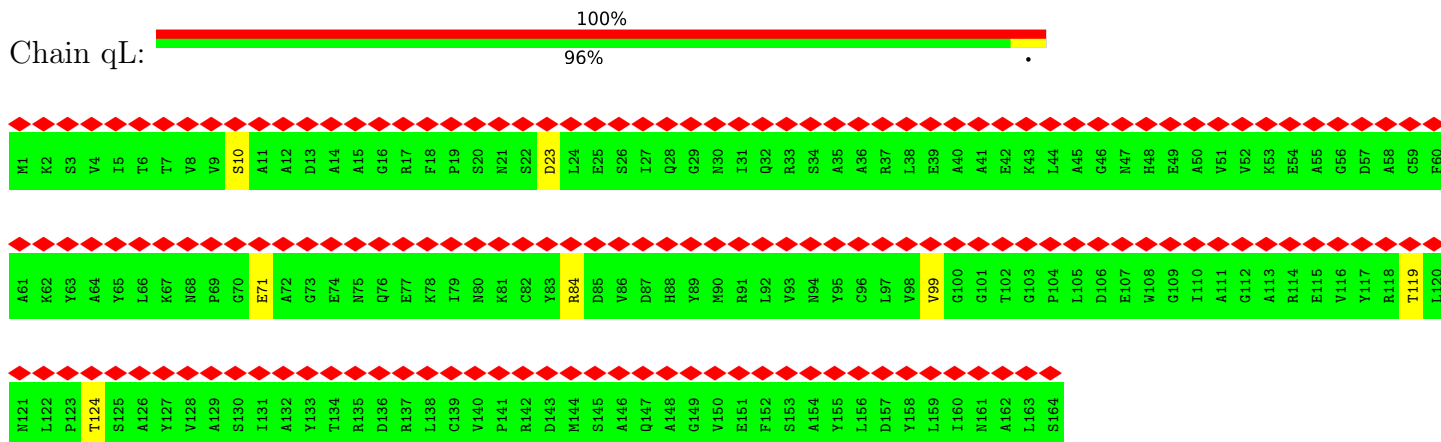
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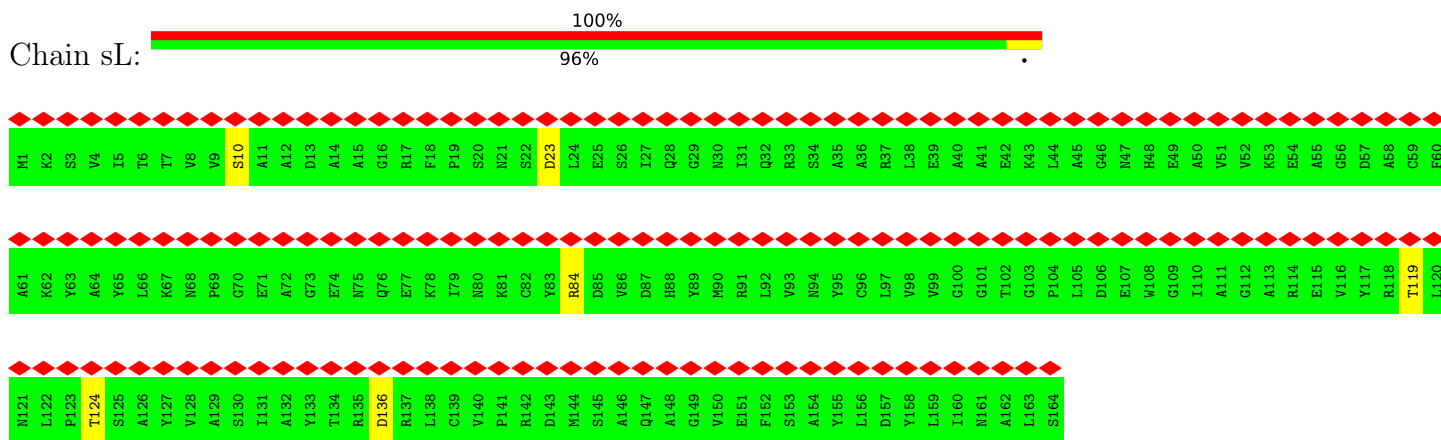
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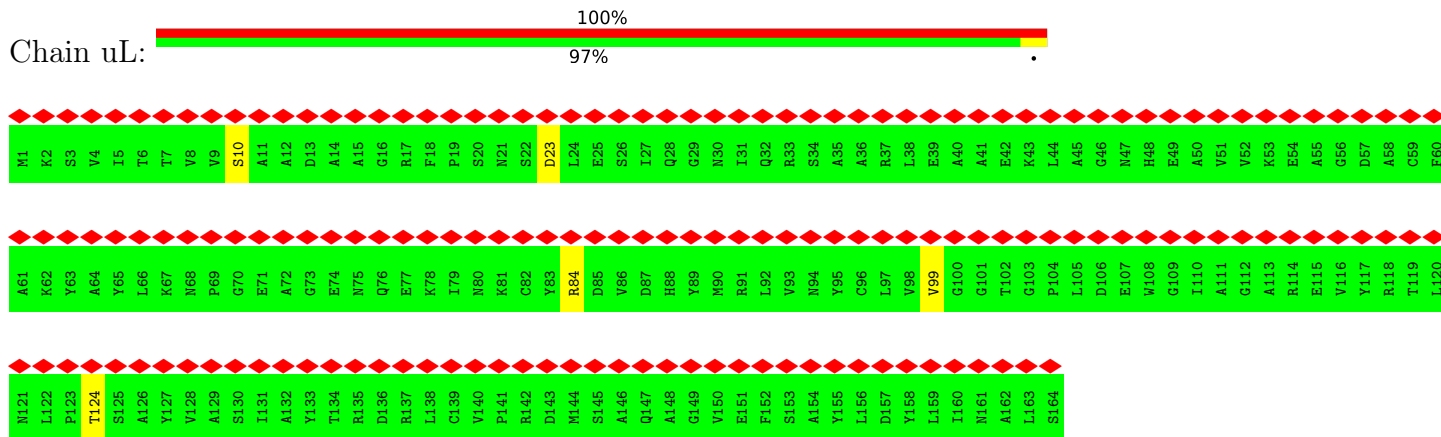
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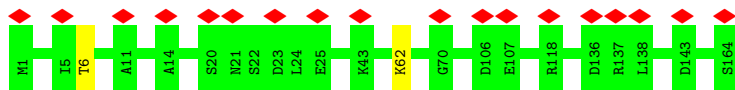


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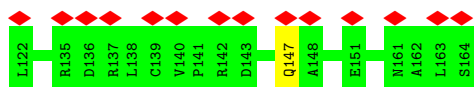
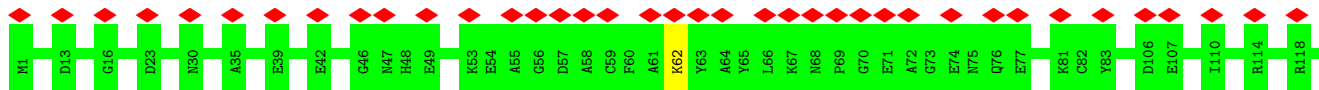


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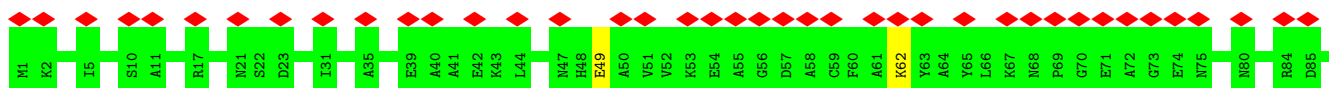
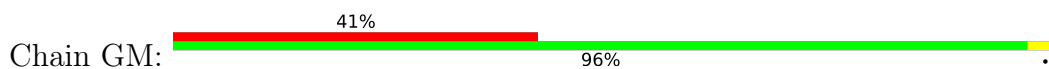




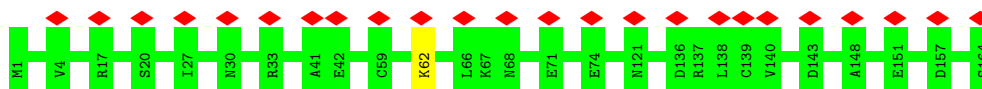
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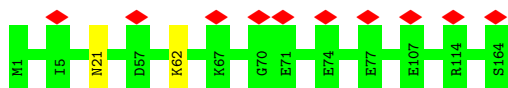
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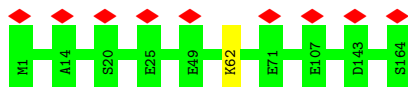
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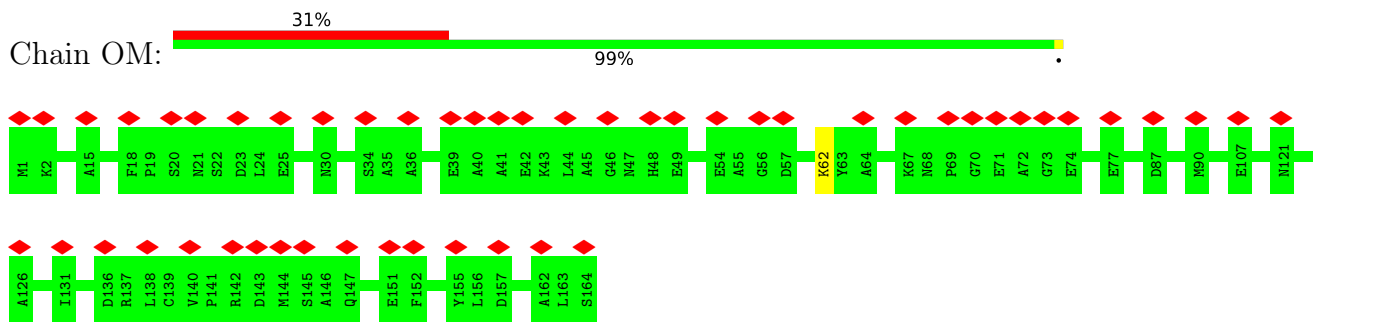
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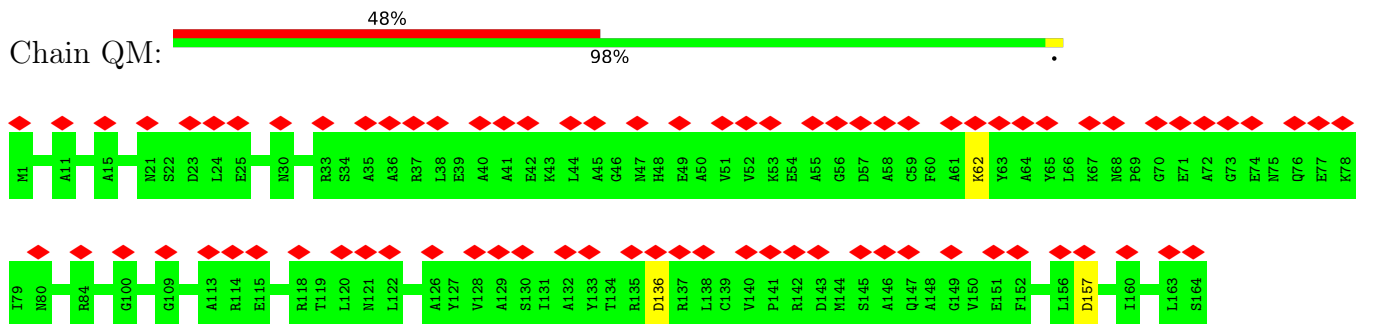
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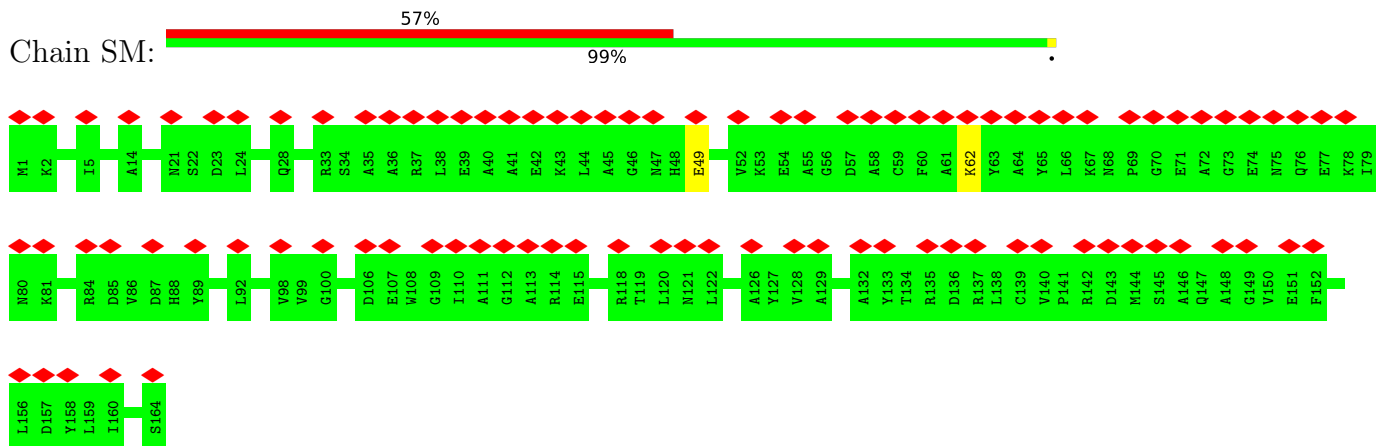
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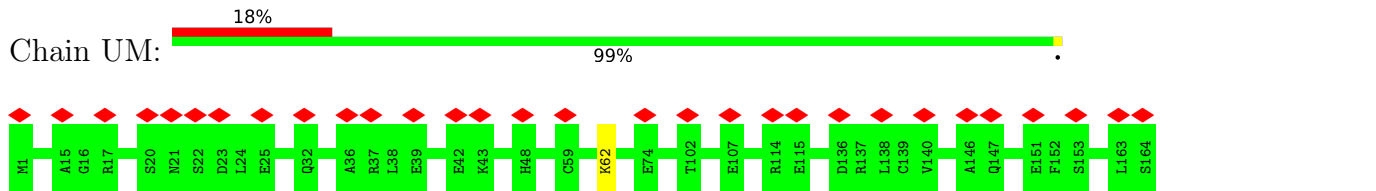
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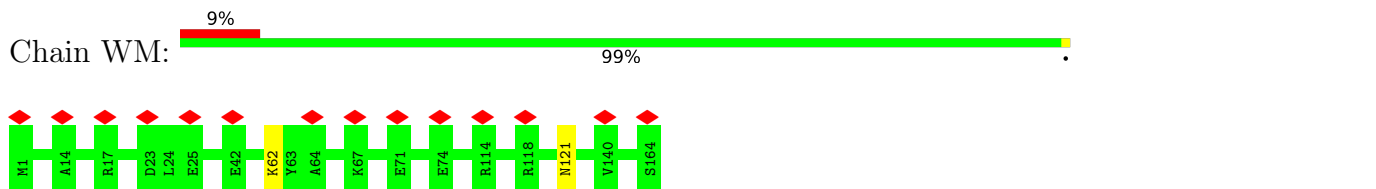
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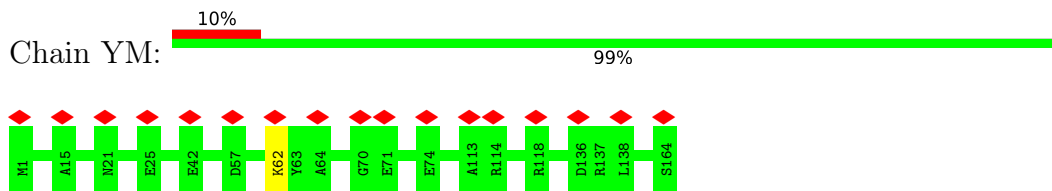
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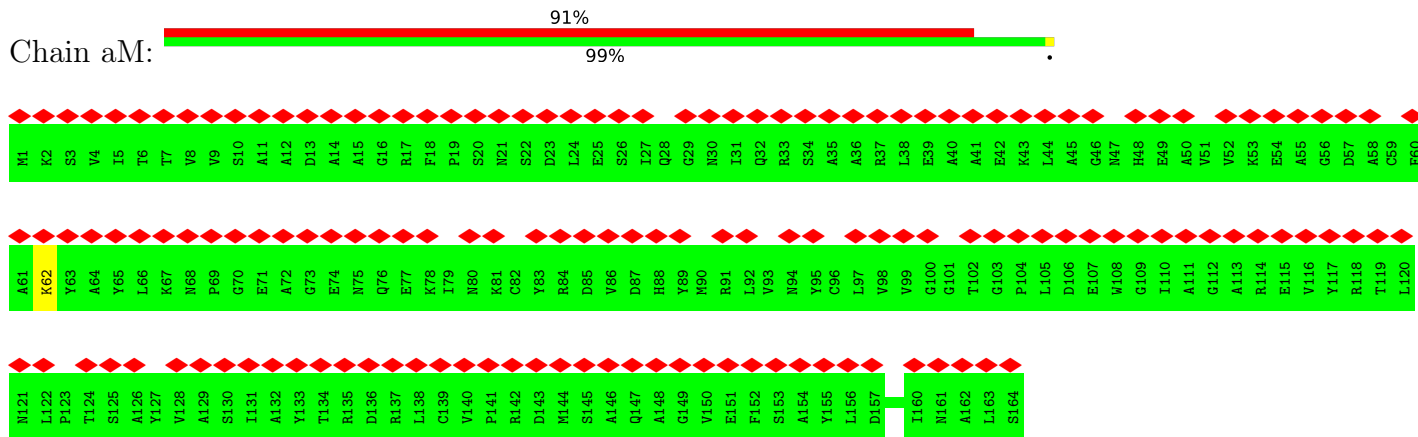
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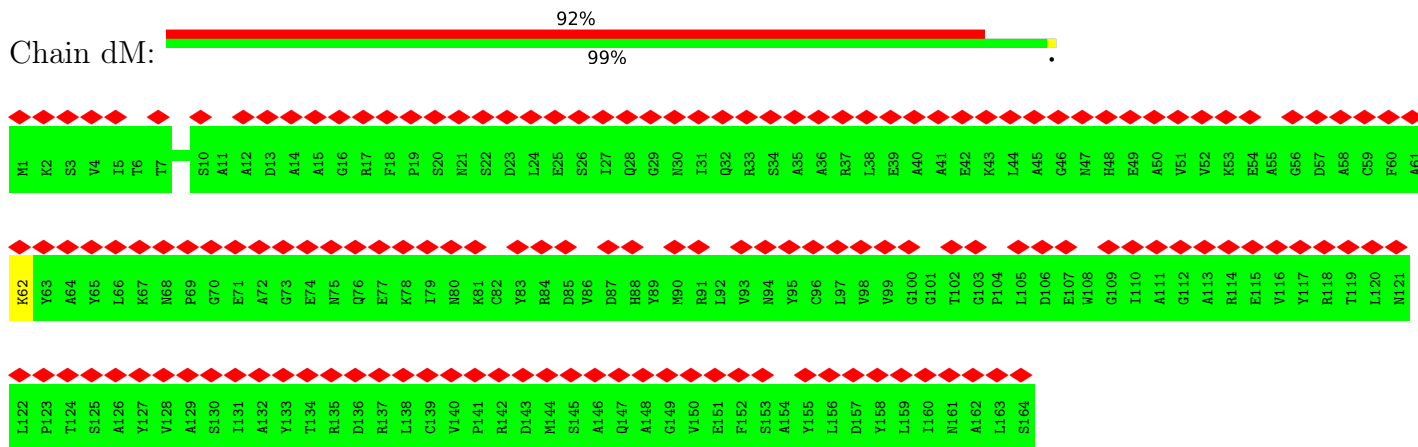
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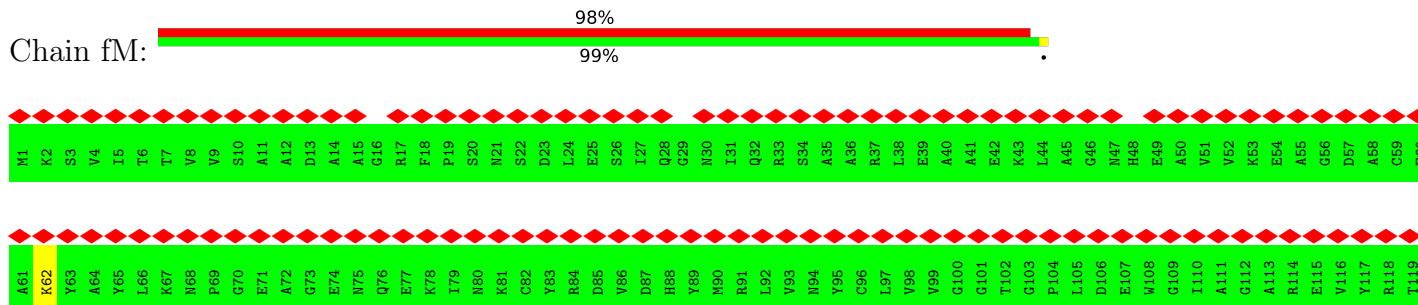
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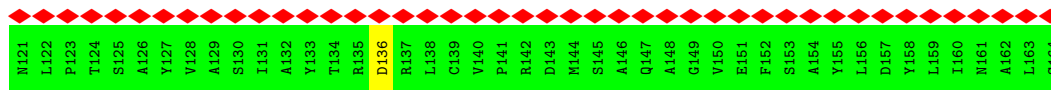


- Molecule 6: Phycoerythrin alpha subunit

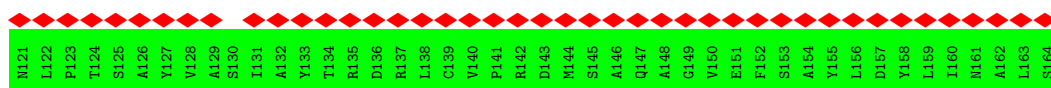
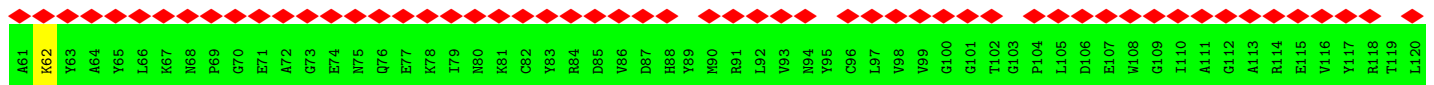
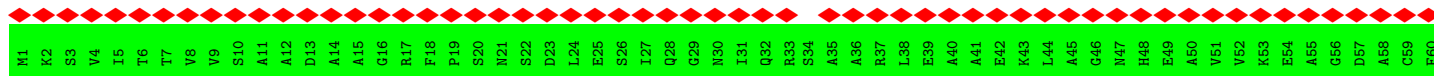


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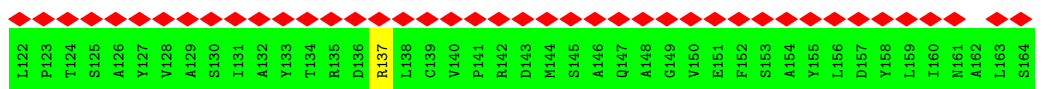
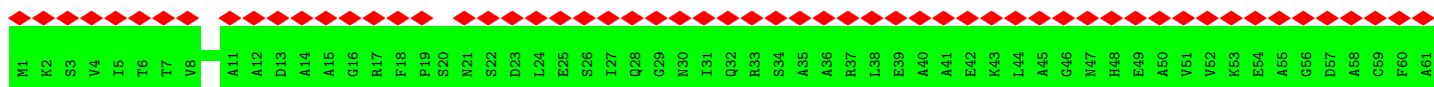




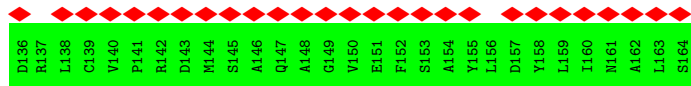
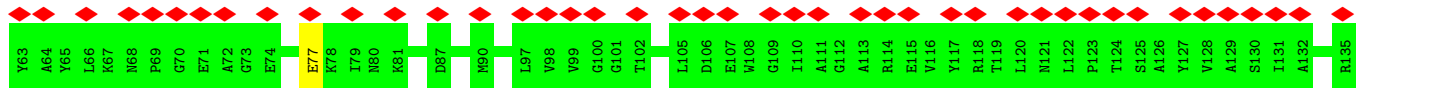
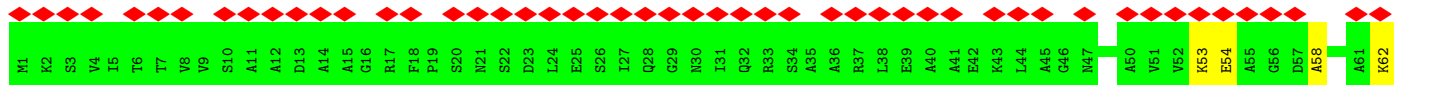
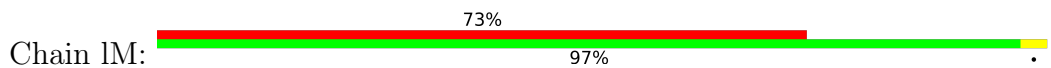
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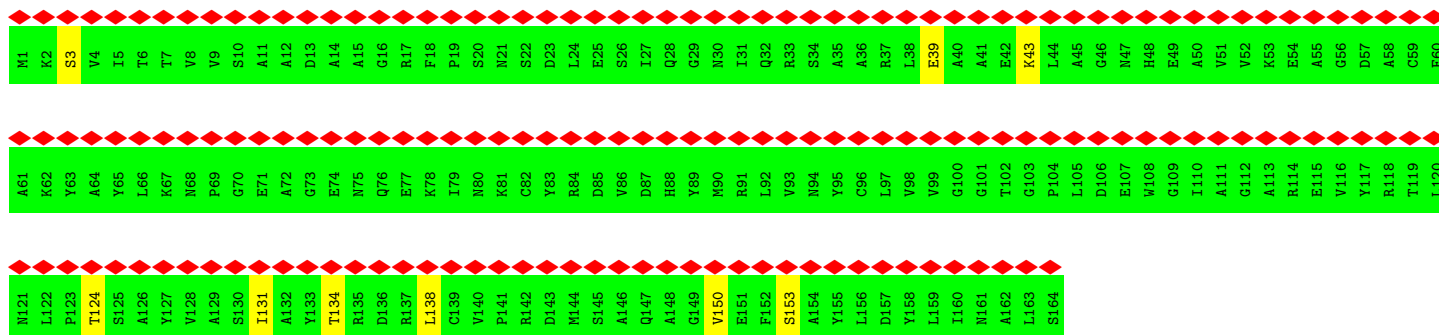


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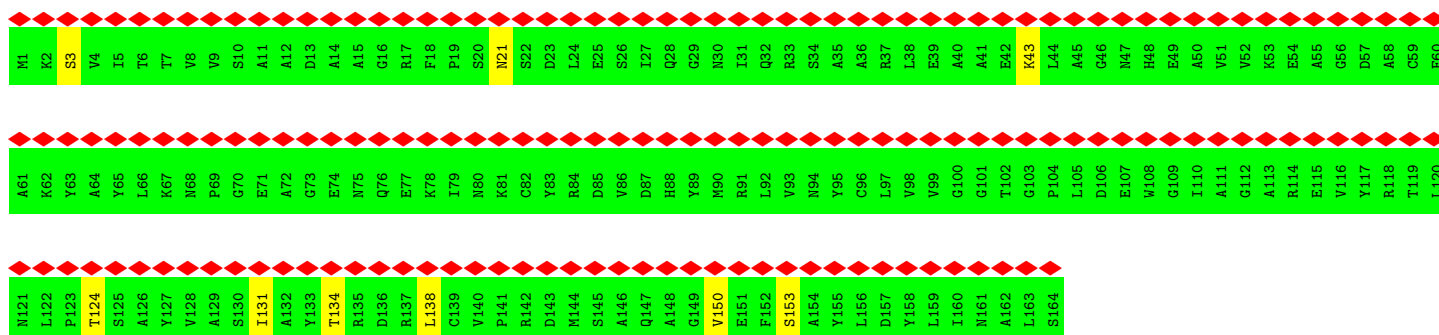
• Molecule 6: Phycoerythrin alpha subunit

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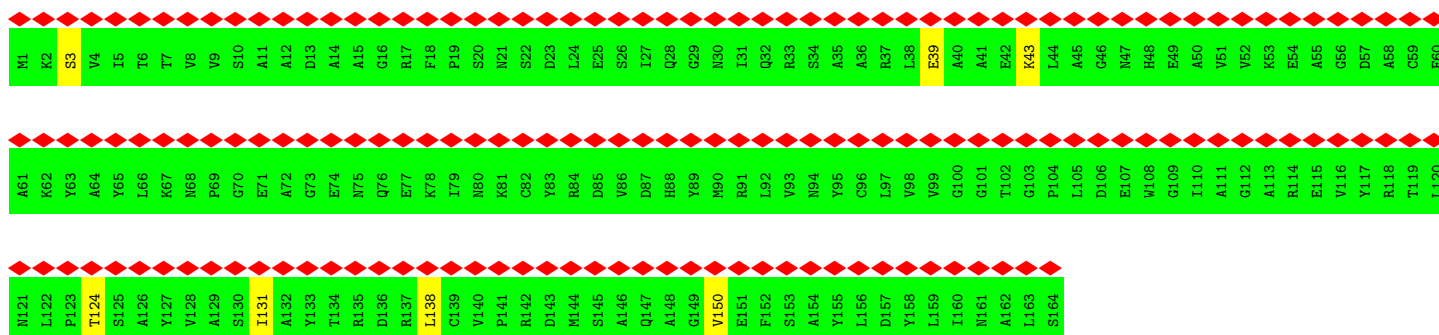
• Molecule 6: Phycoerythrin alpha subunit

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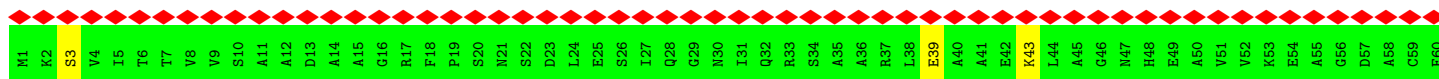
• Molecule 6: Phycoerythrin alpha subunit

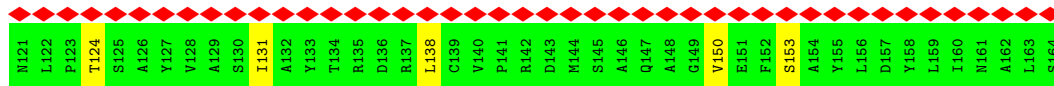
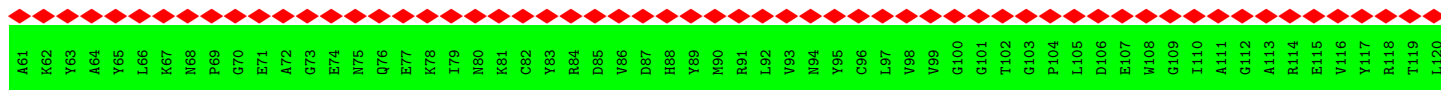
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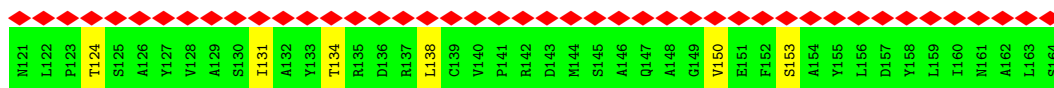
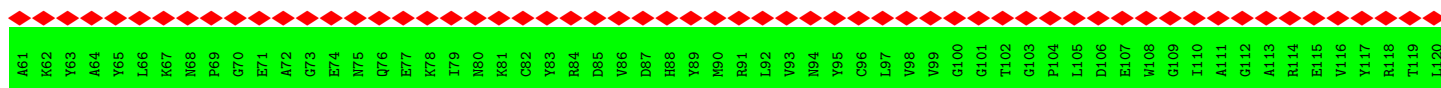
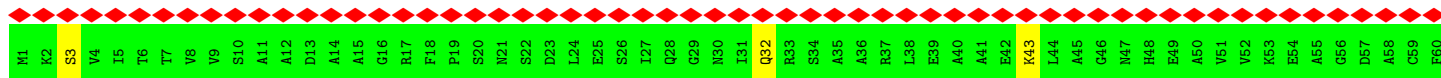
• Molecule 6: Phycoerythrin alpha subunit

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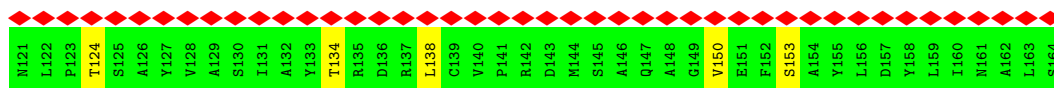
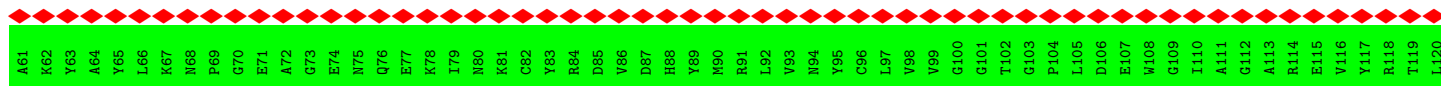
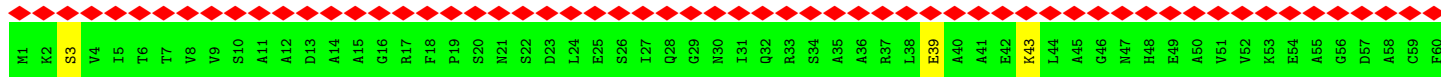




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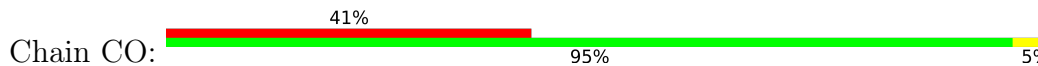
• Molecule 6: Phycoerythrin alpha subunit

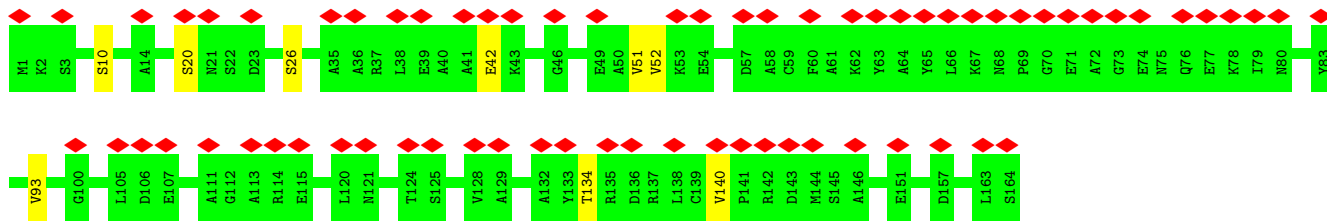


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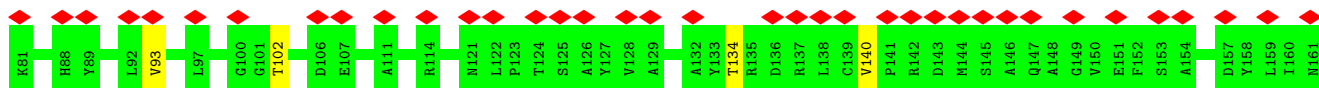
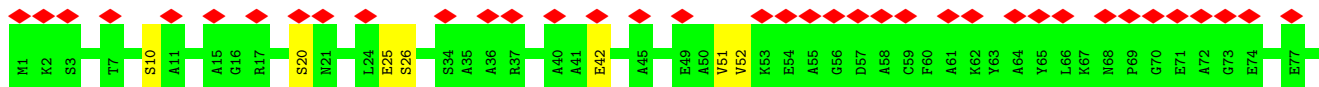


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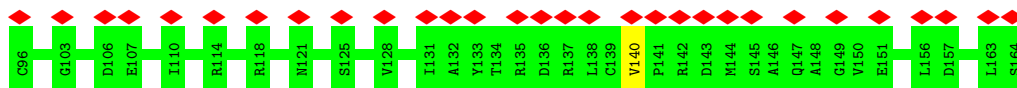
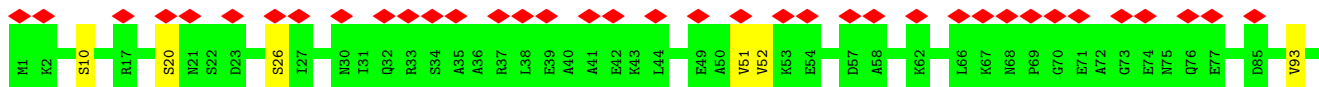
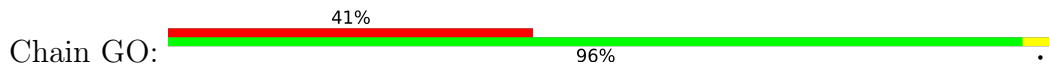




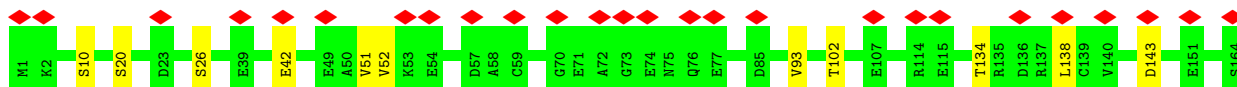
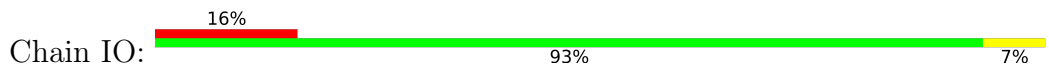
• Molecule 6: Phycoerythrin alpha subunit



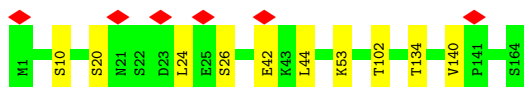
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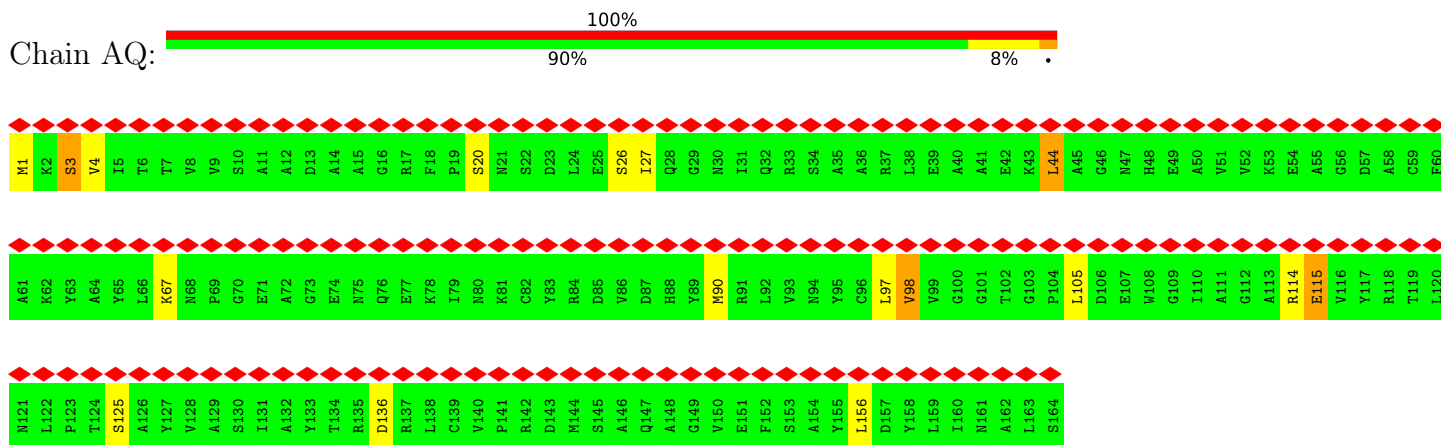
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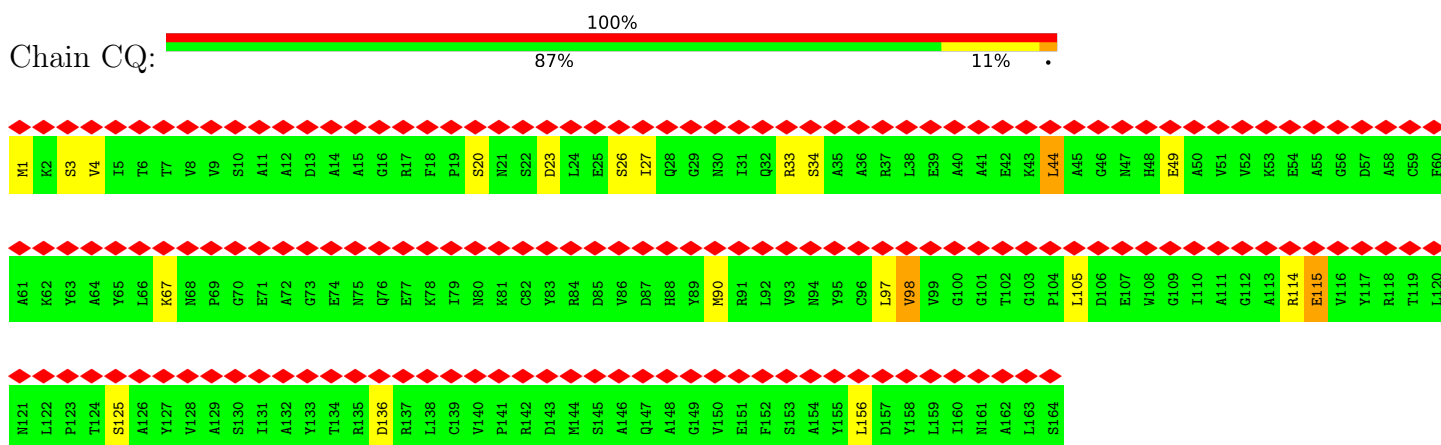
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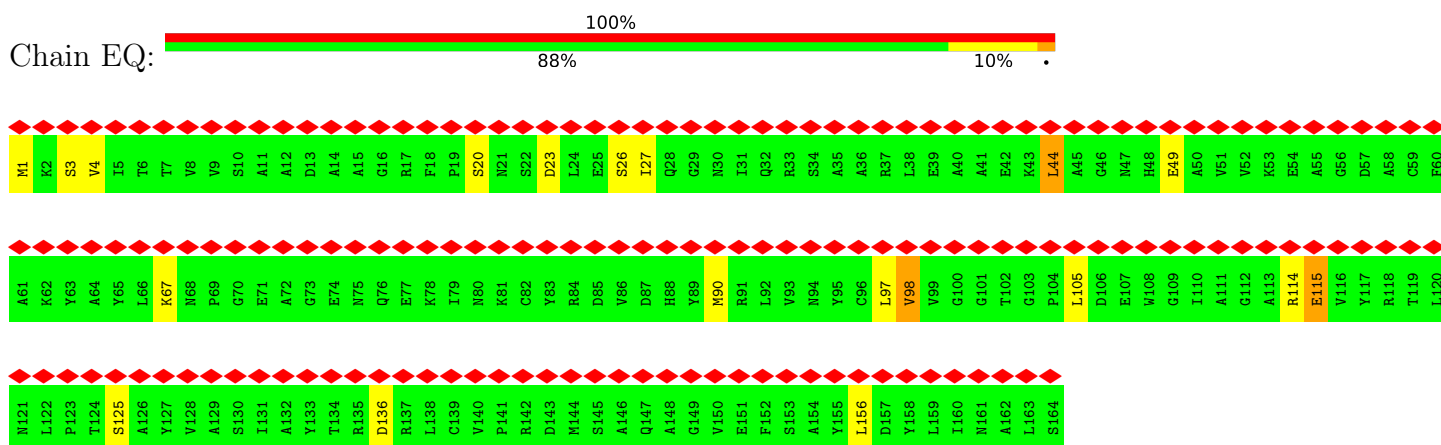
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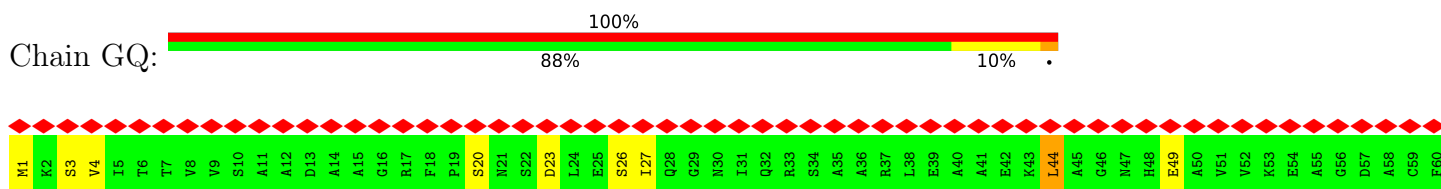
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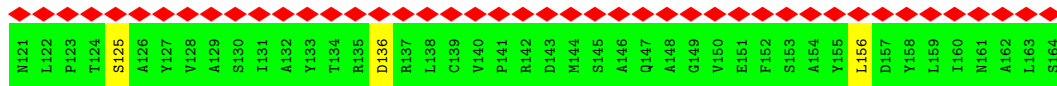
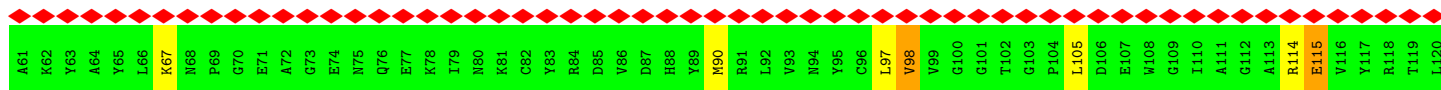


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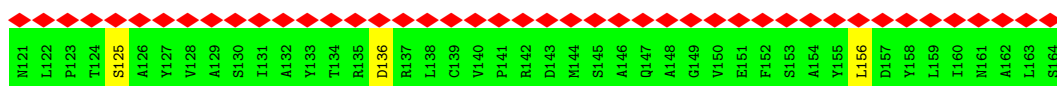
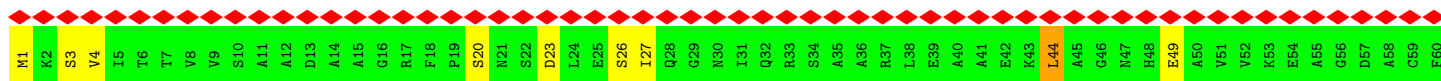
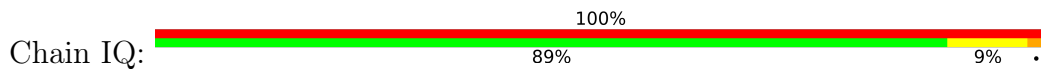


• Molecule 6: Phycoerythrin alpha subunit

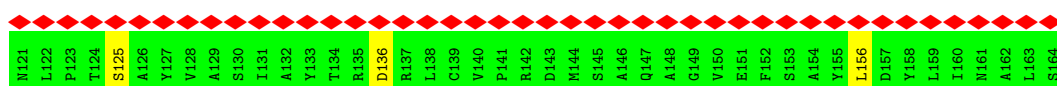
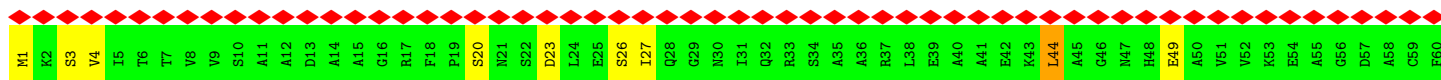
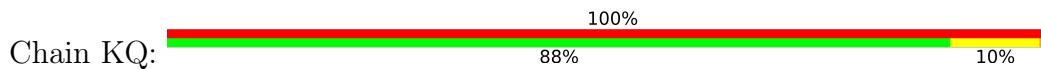




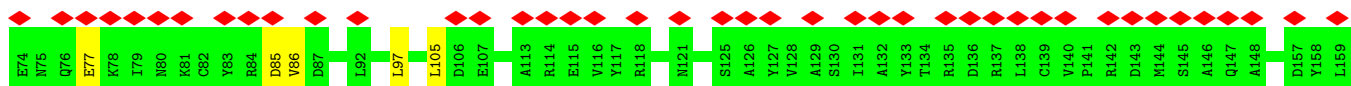
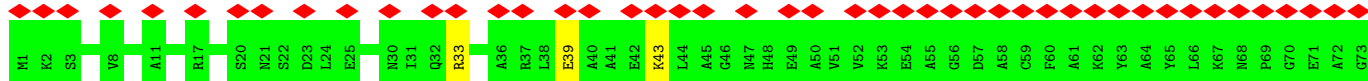
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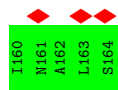


• Molecule 6: Phycoerythrin alpha subunit

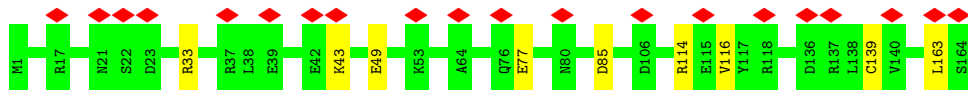


• Molecule 6: Phycoerythrin alpha subunit

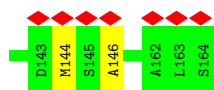
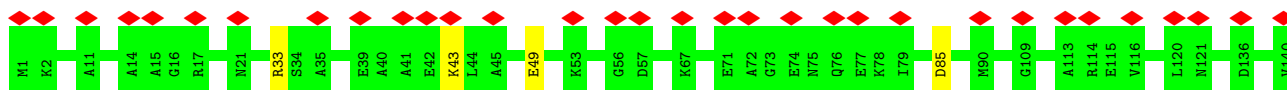




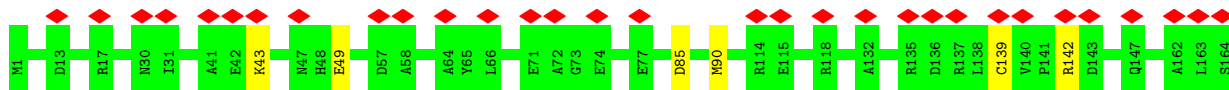
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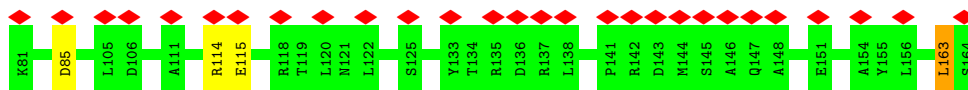
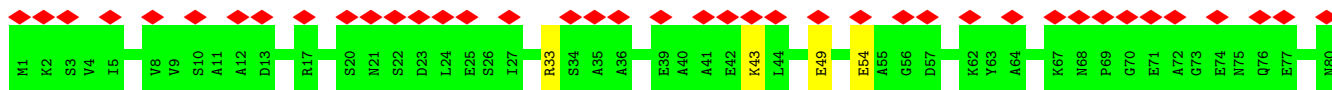
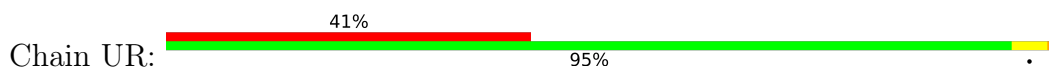
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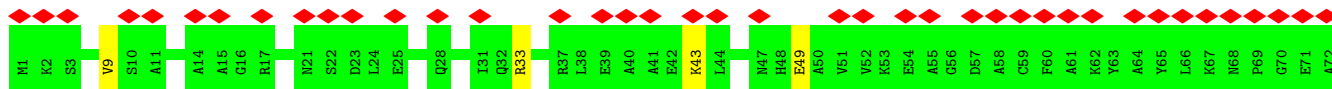
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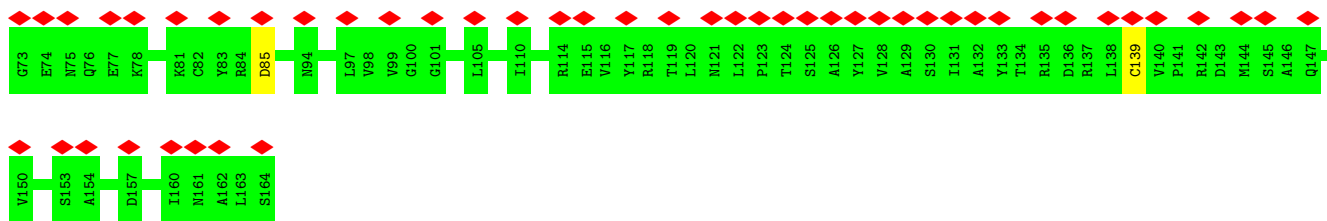


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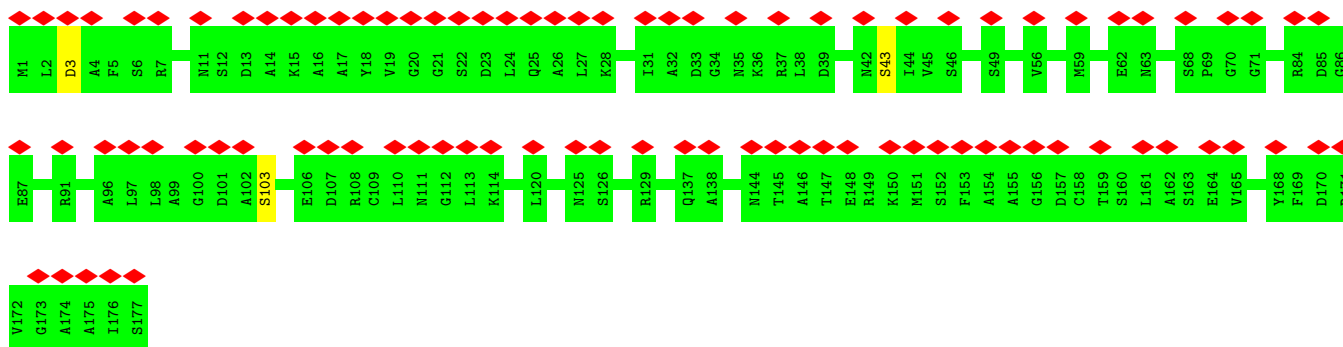


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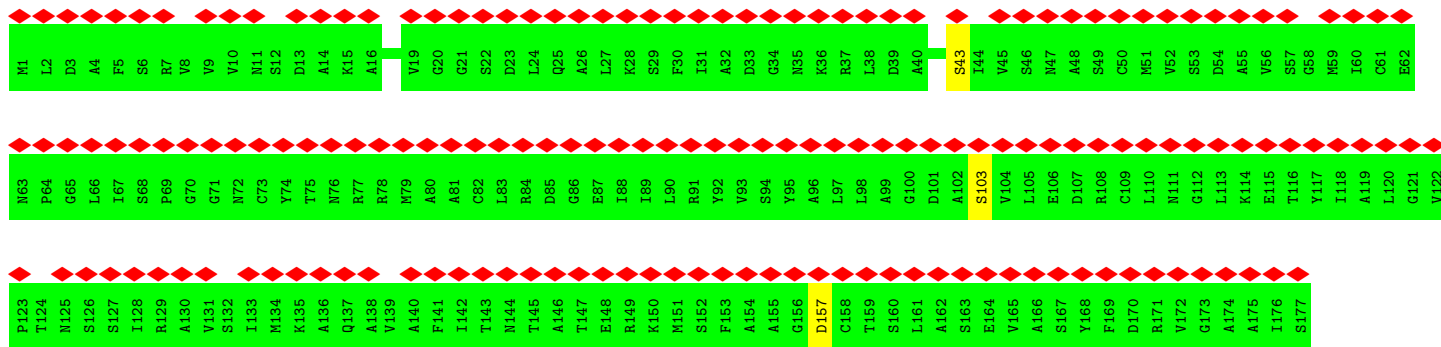




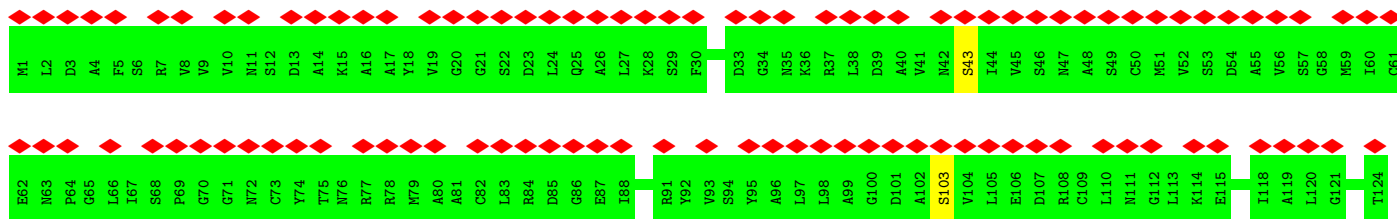
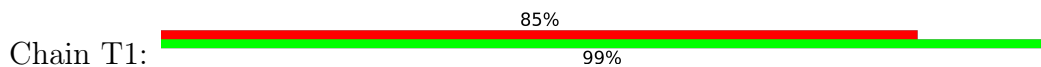
• Molecule 7: B-phycoerythrin beta chain

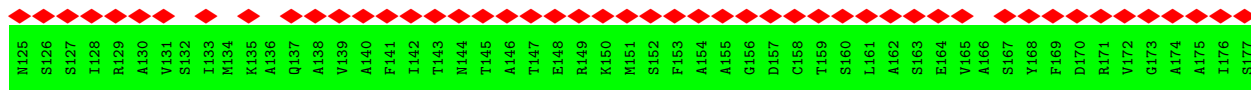


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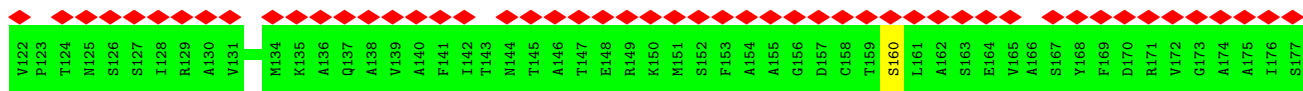
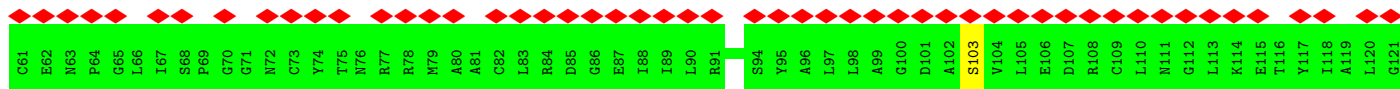
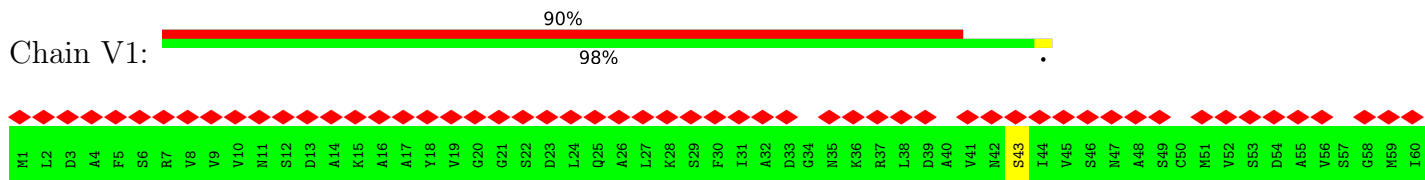


• Molecule 7: B-phycoerythrin beta chain

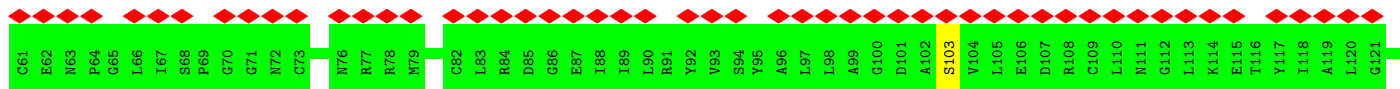
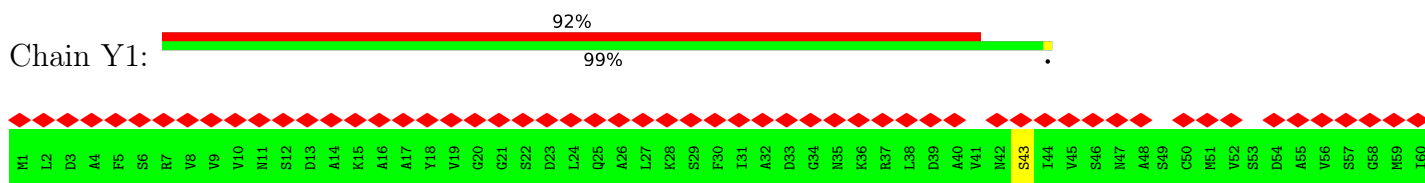




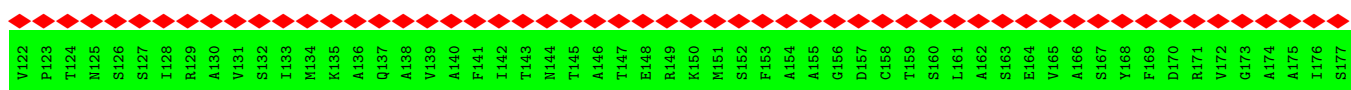
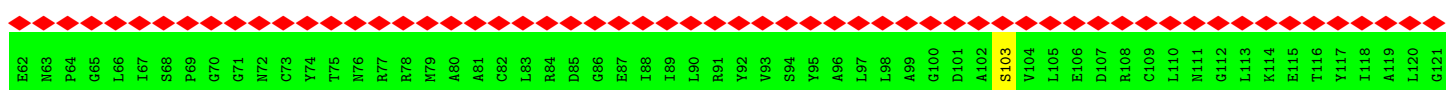
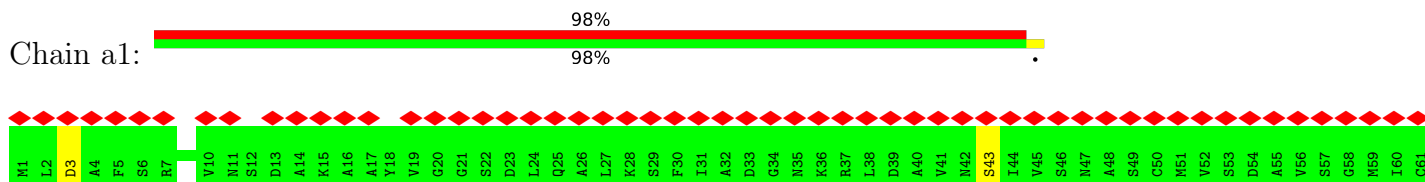
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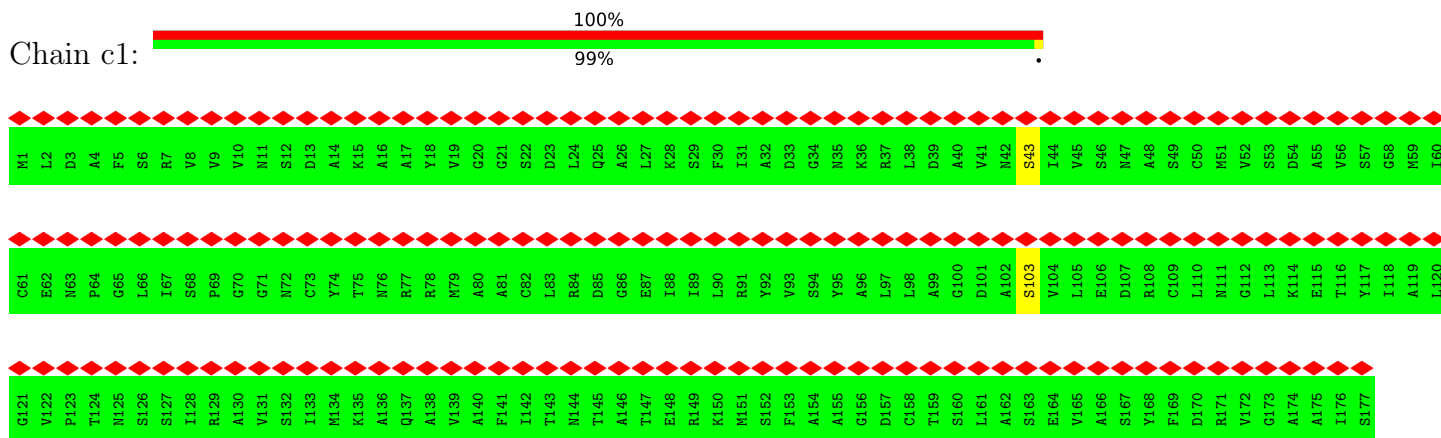
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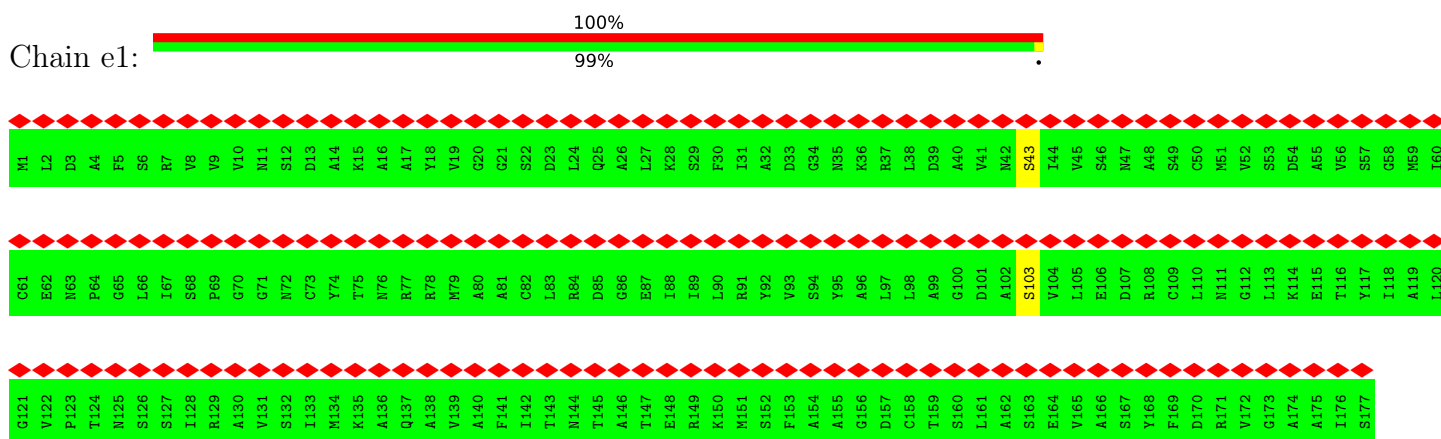
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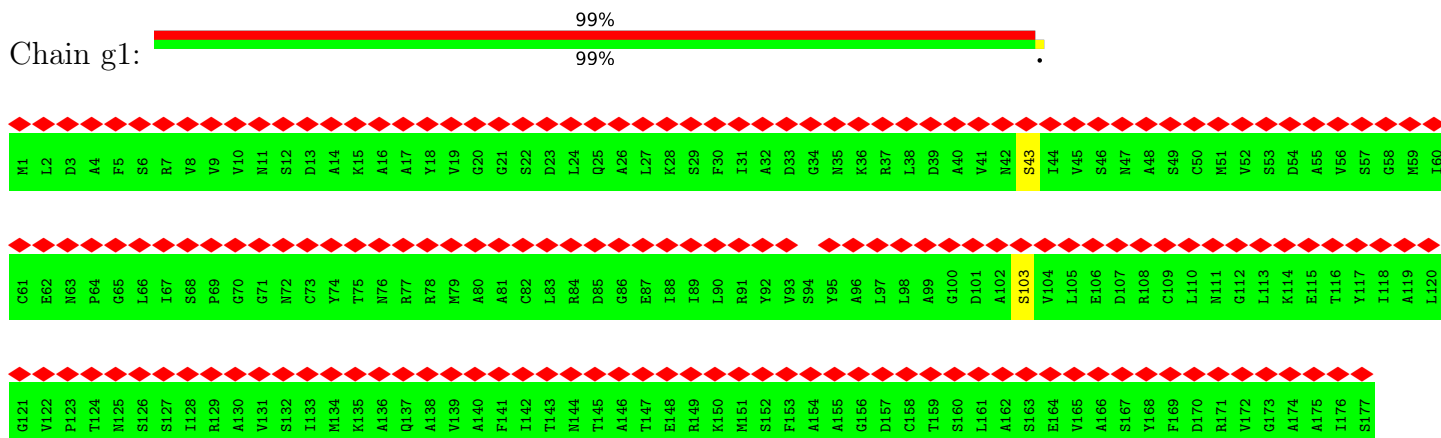
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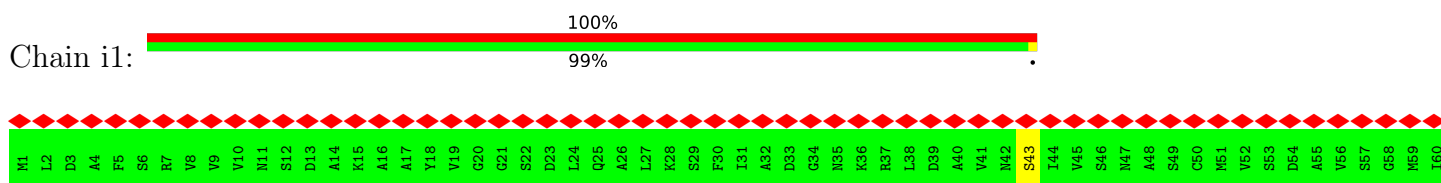
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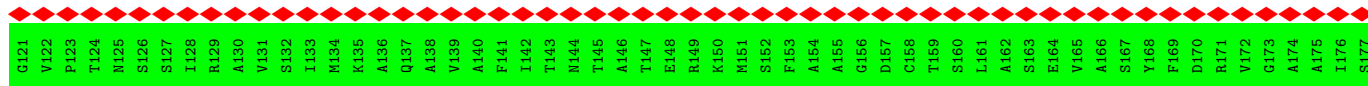
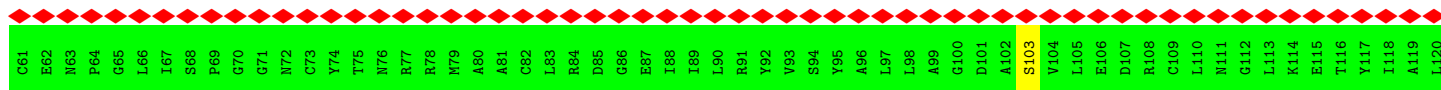


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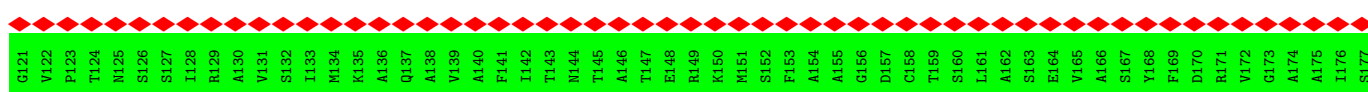
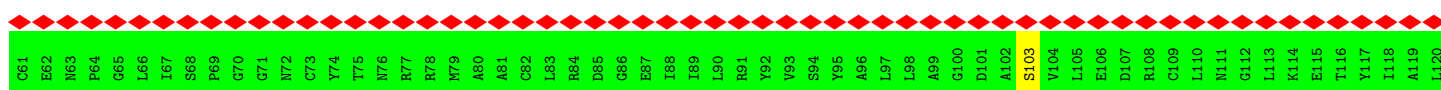


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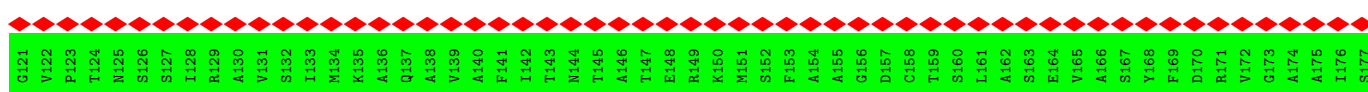
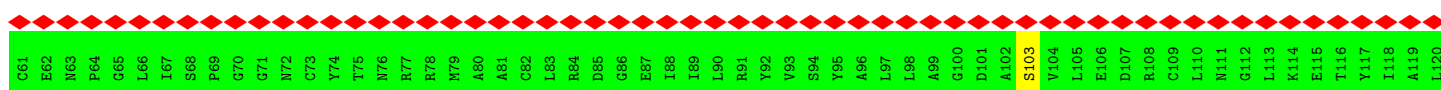




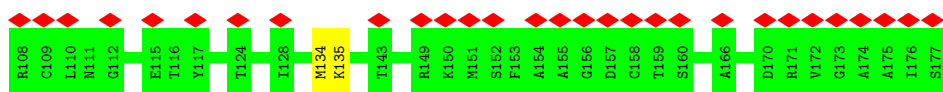
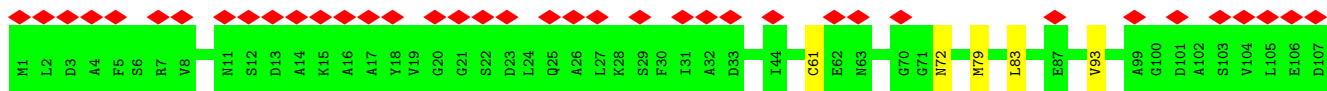
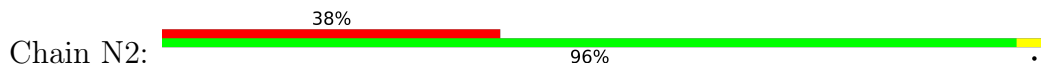
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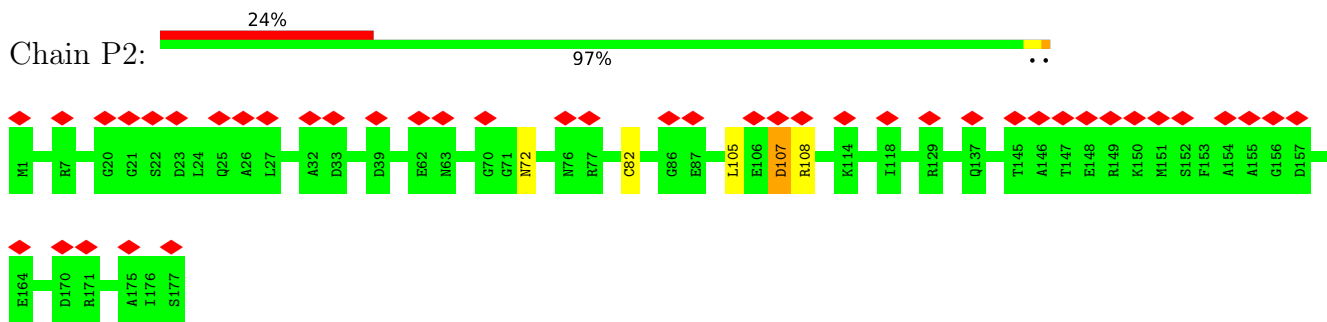
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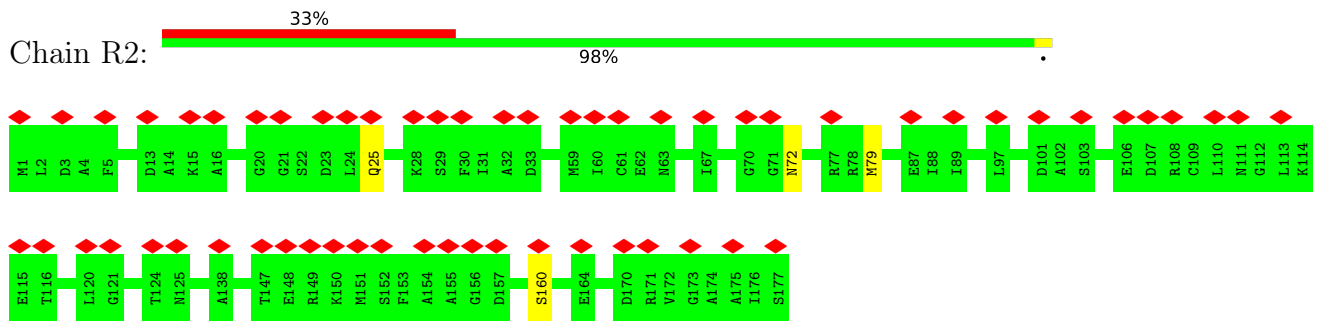
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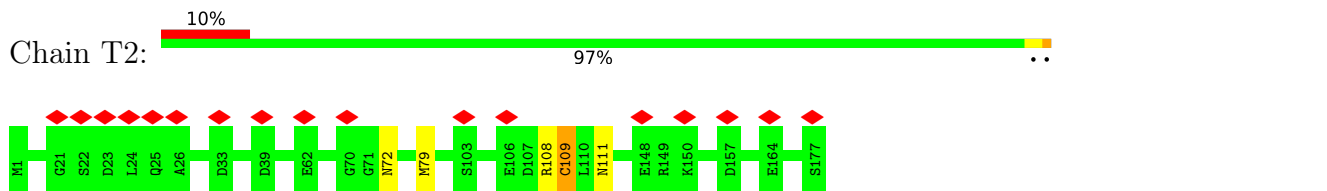
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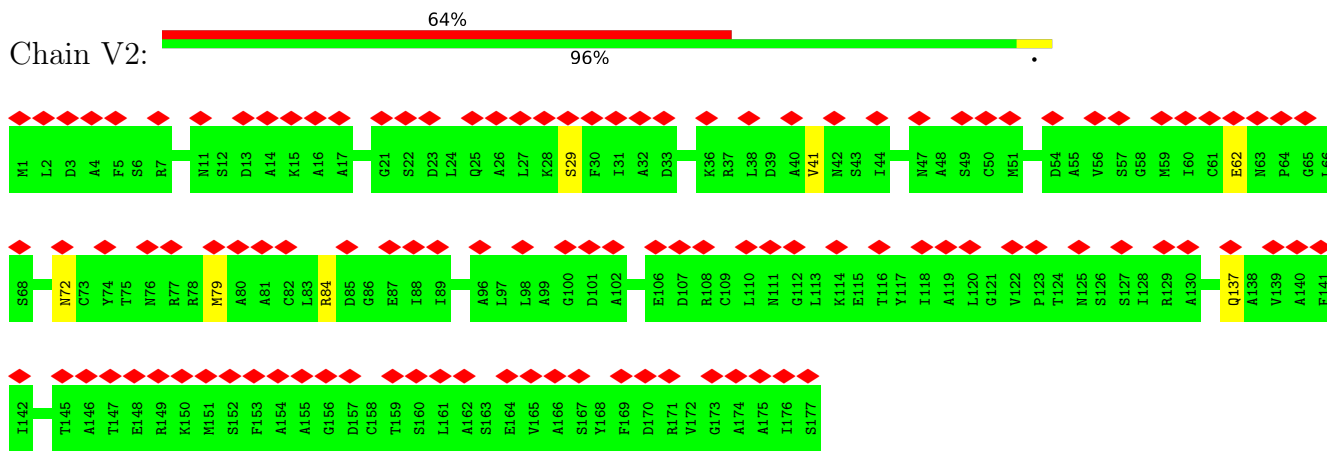
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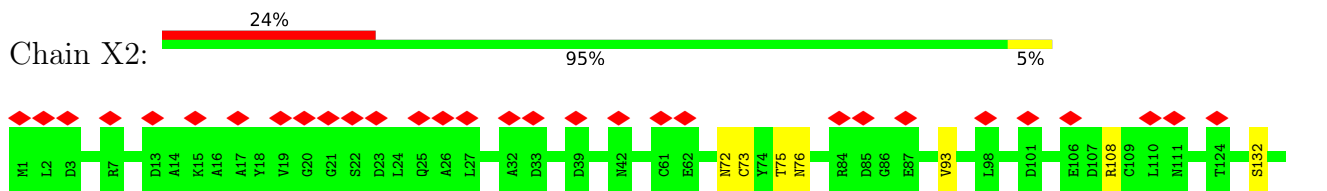
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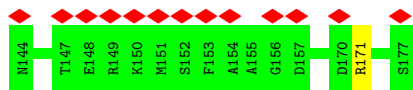


● Molecule 7: B-phycoerythrin beta chain



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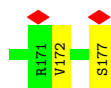
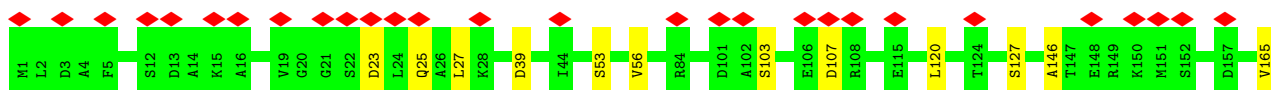




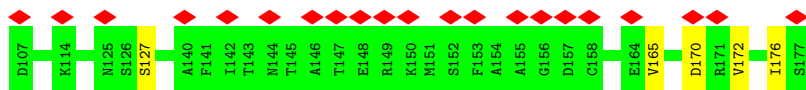
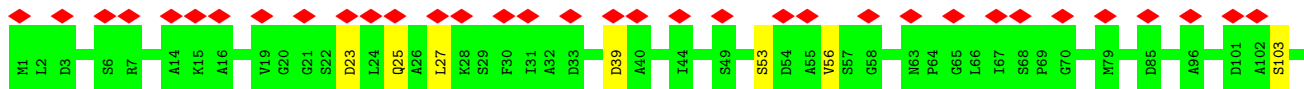
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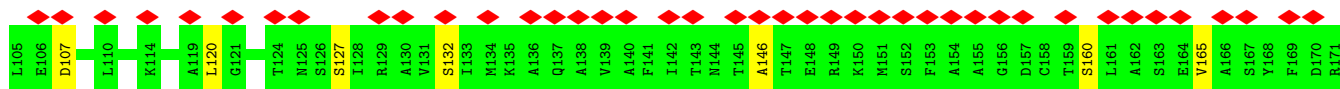
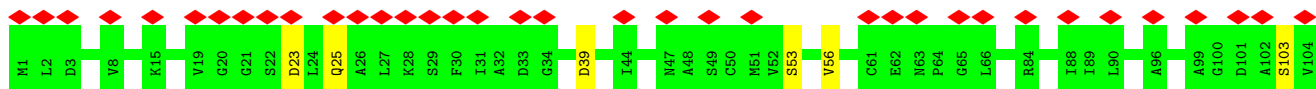
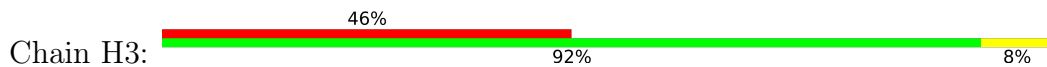
• Molecule 7: B-phycoerythrin beta chain



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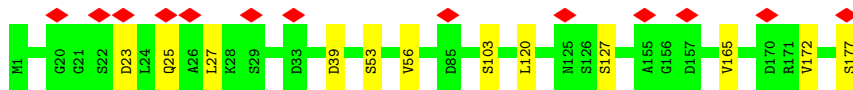


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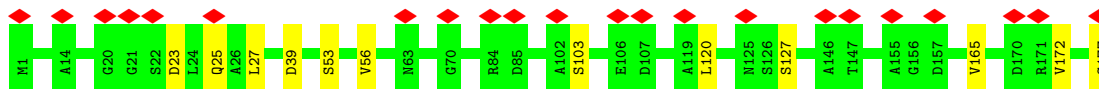




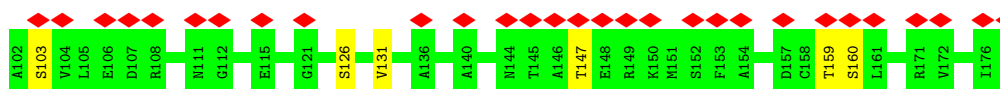
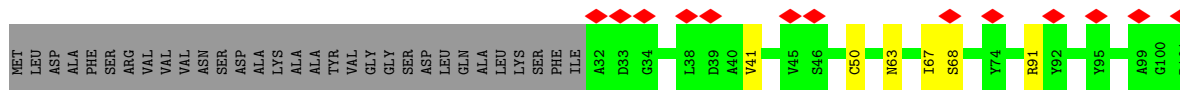
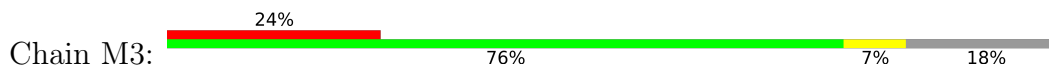
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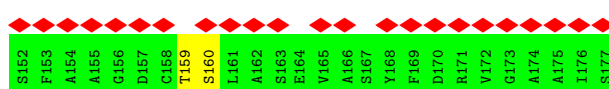
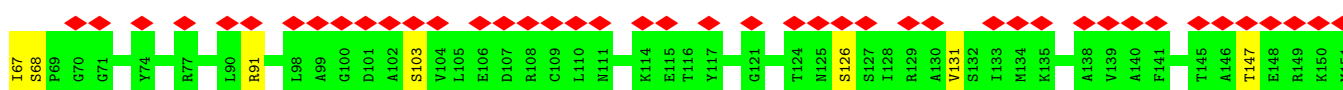
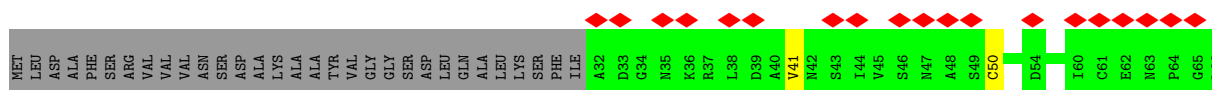
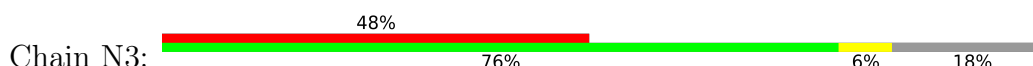
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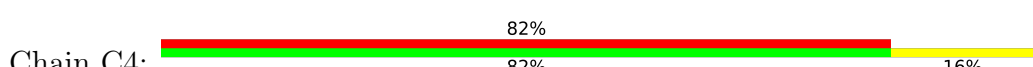
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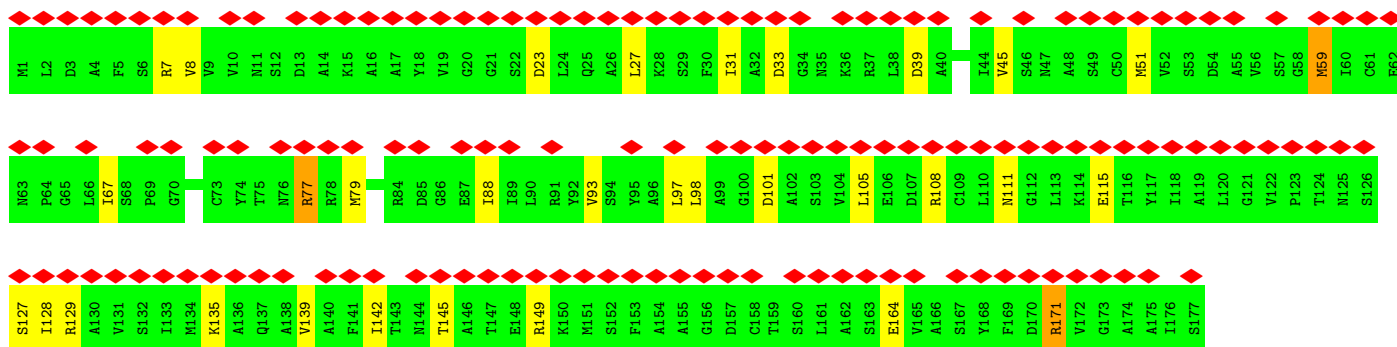


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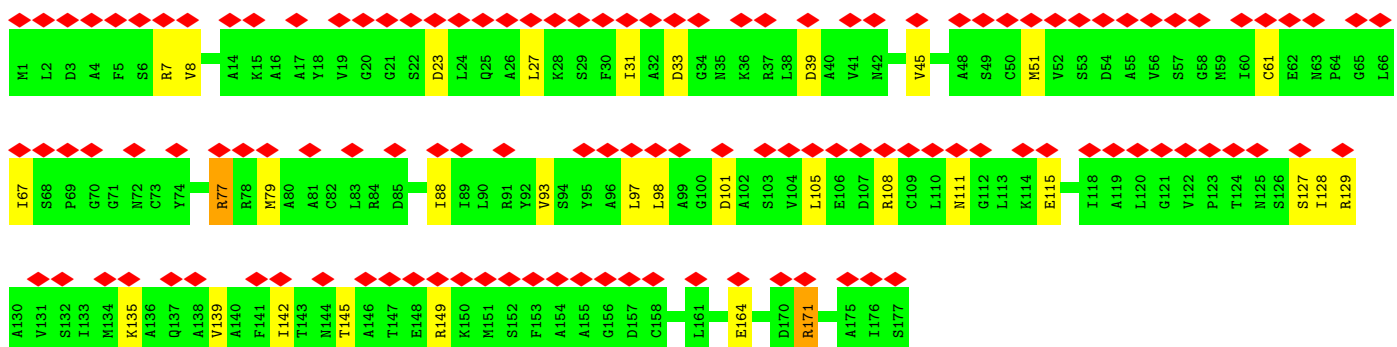
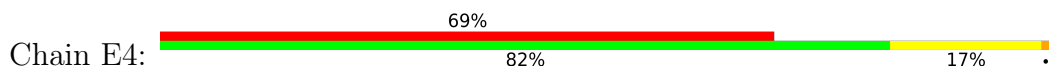


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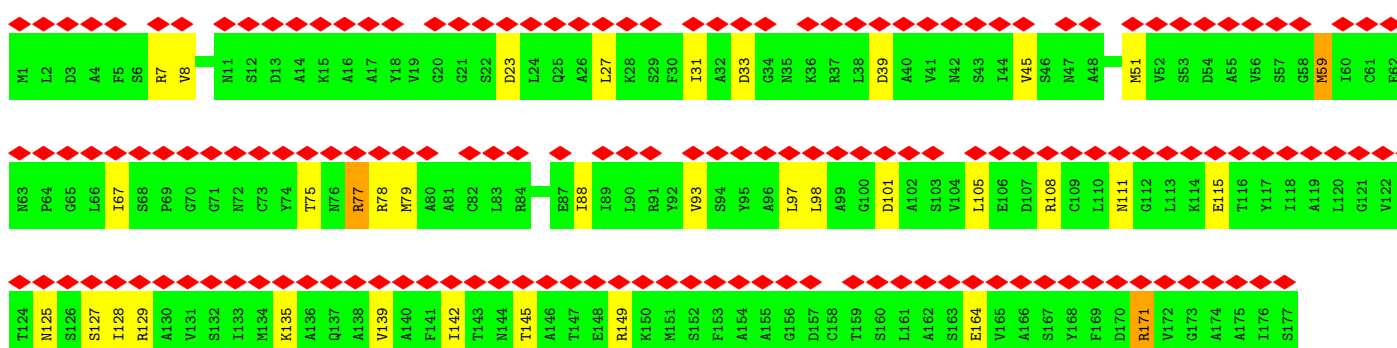
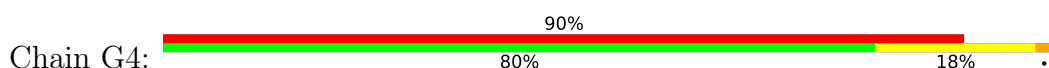




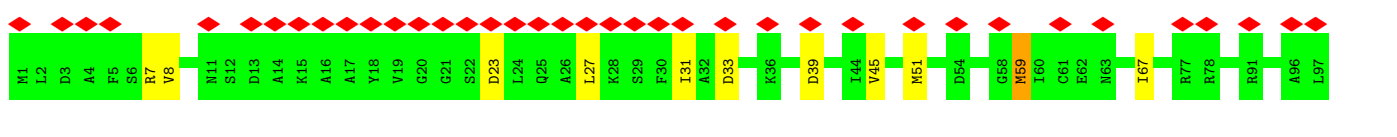
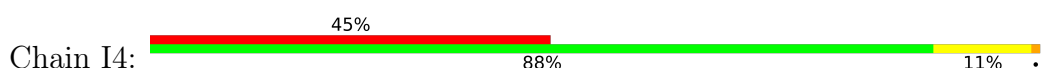
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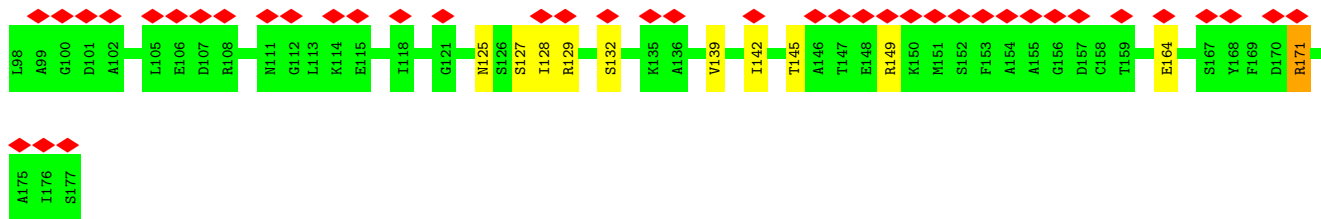


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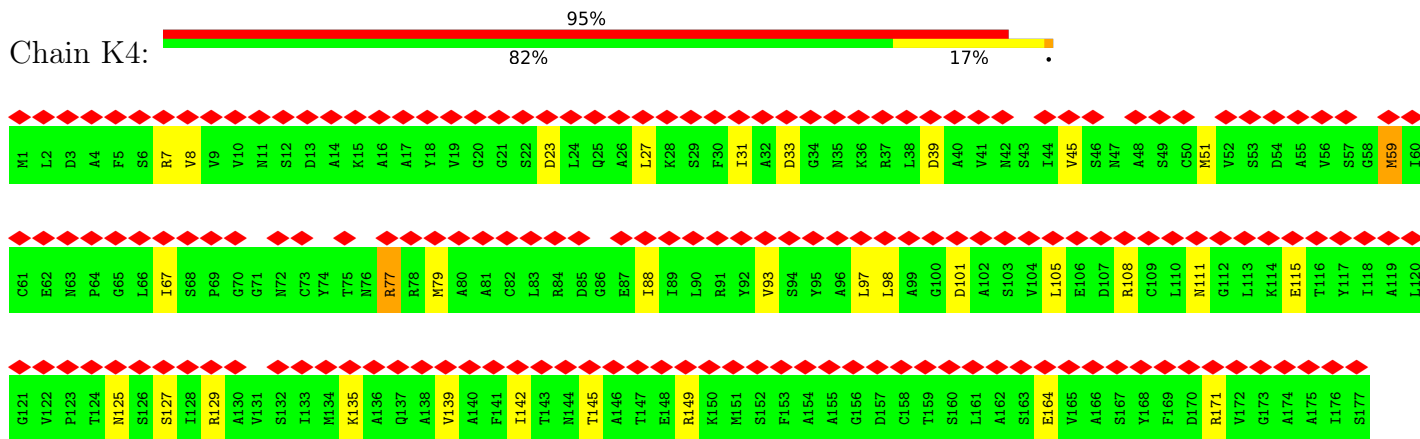


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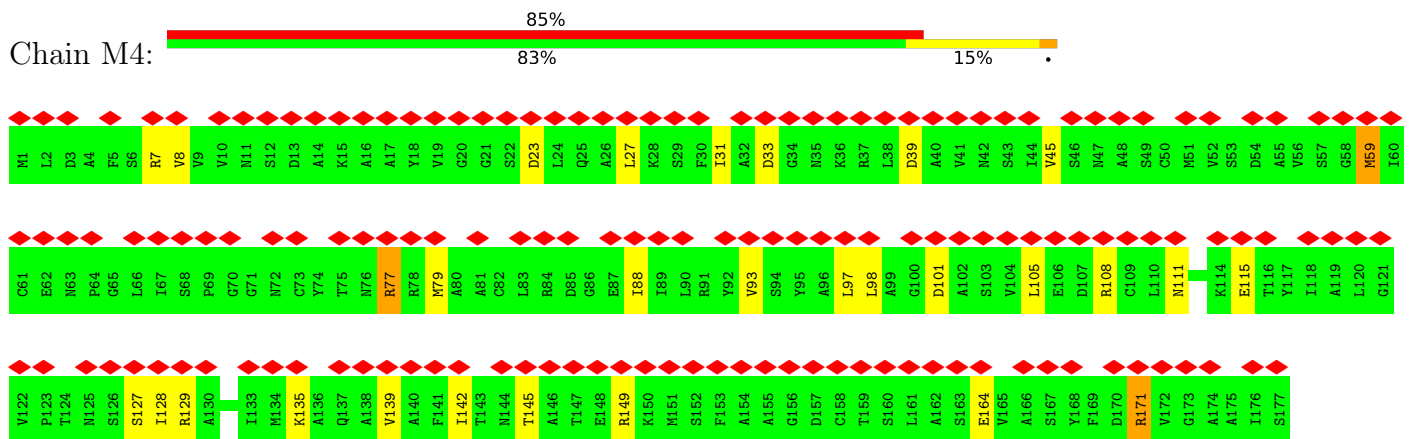




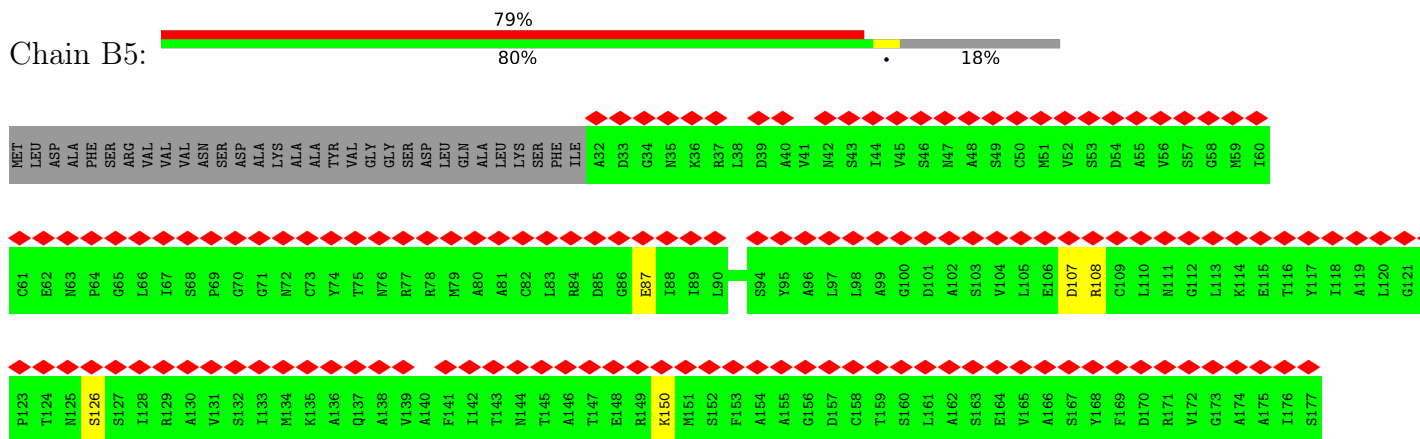
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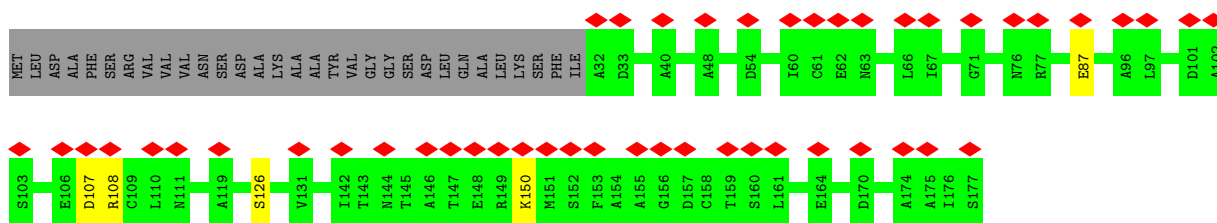
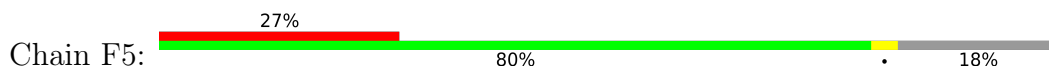
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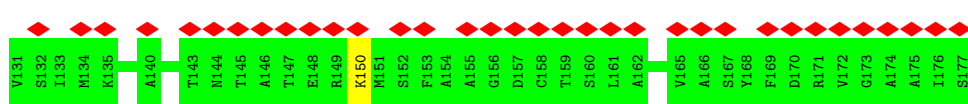
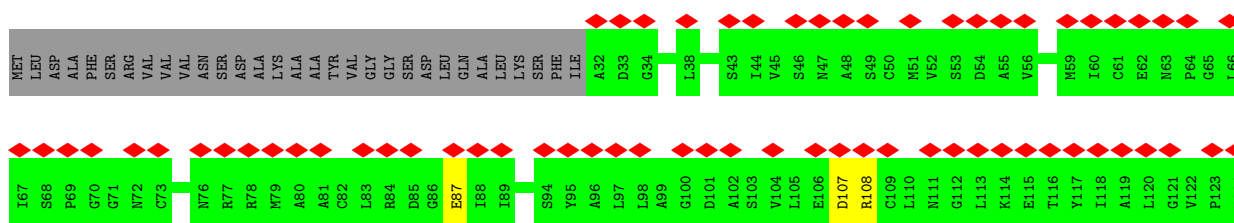
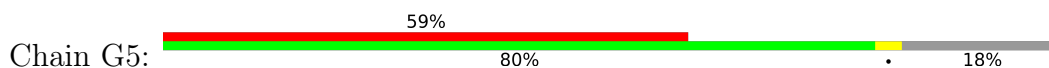
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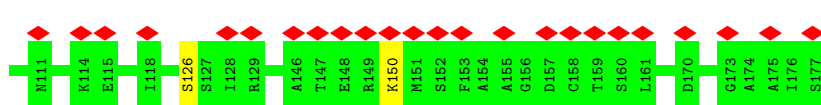
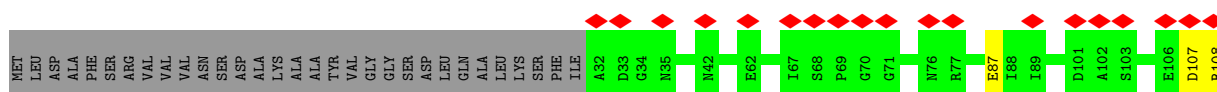
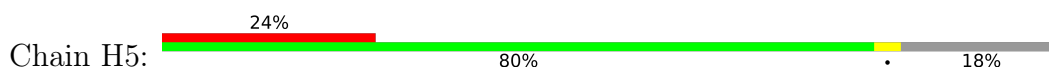
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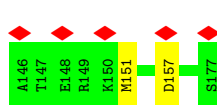
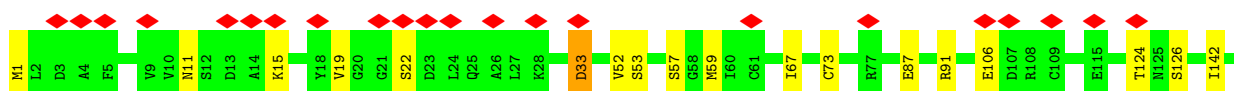
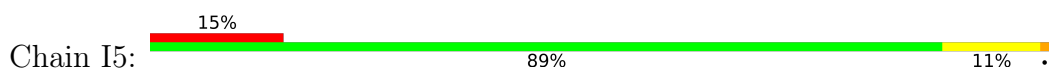
• Molecule 7: B-phycoerythrin beta chain



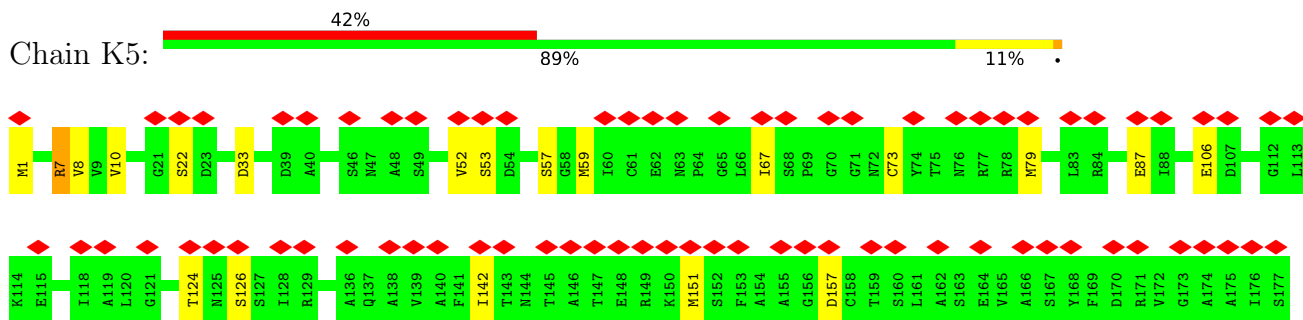
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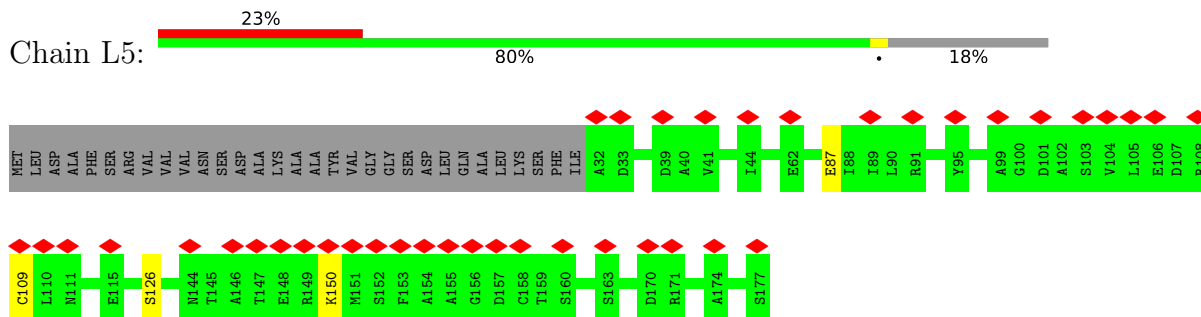
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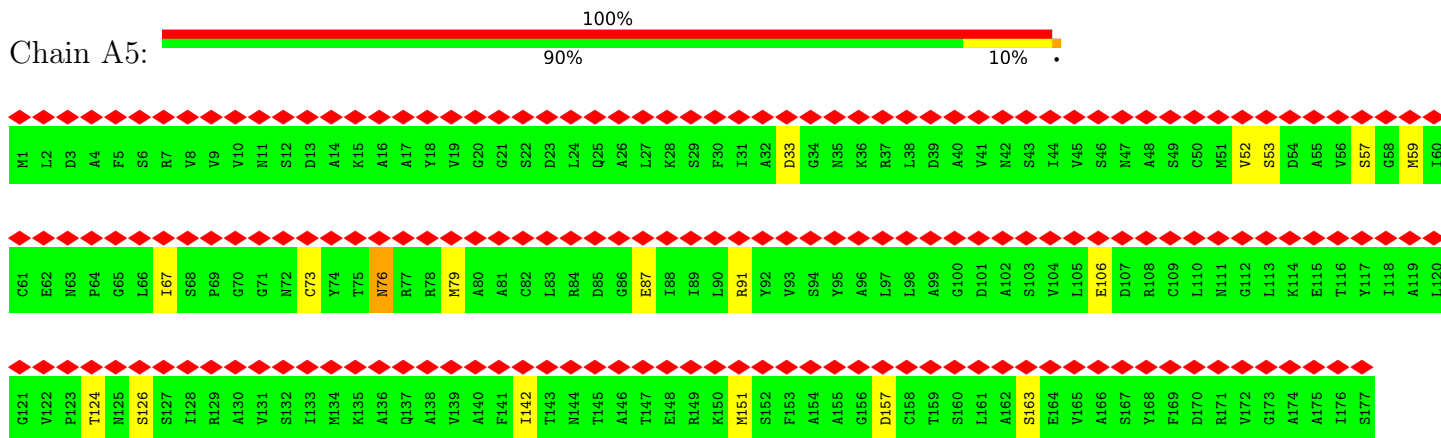
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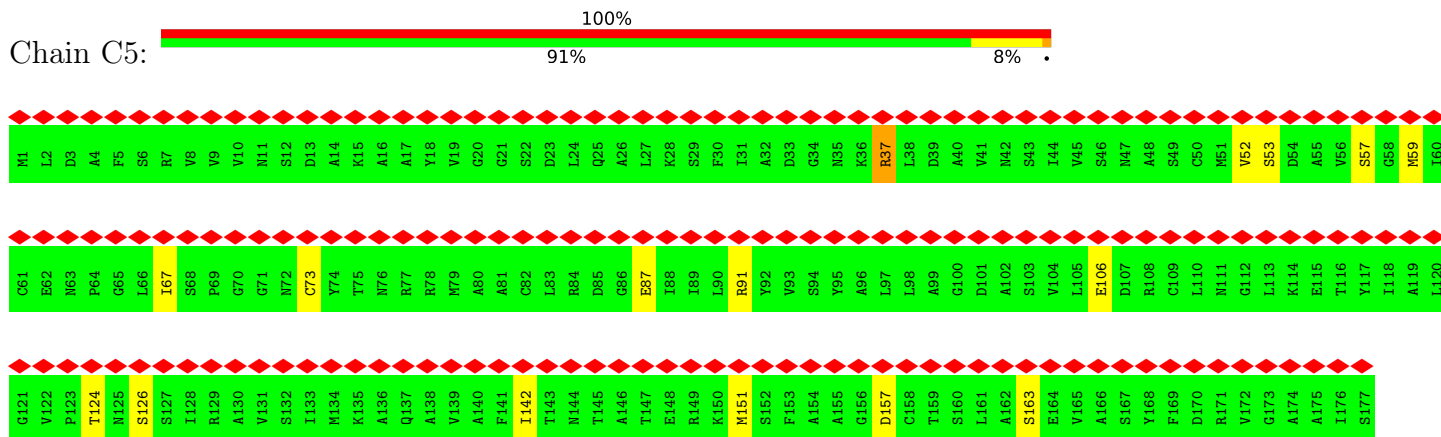
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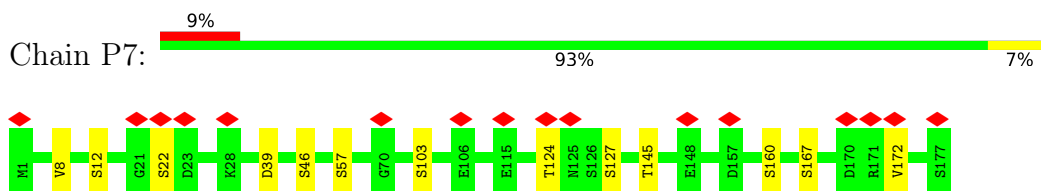
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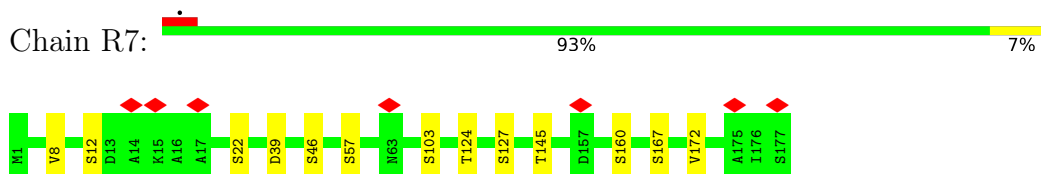
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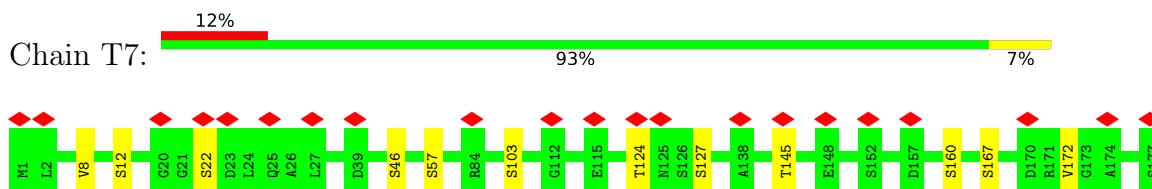
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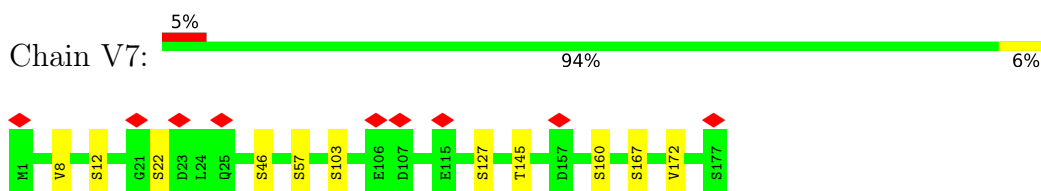
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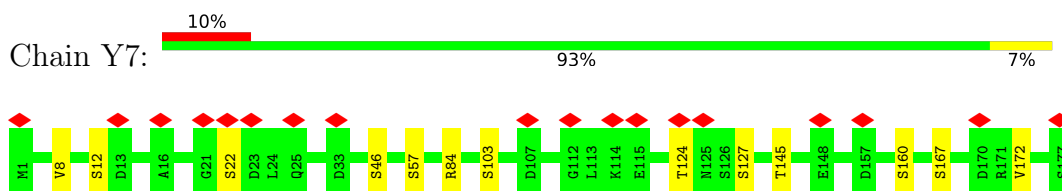
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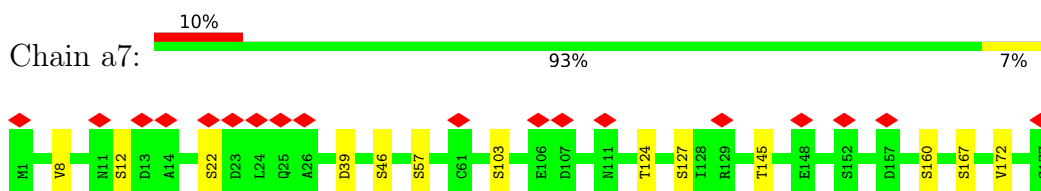
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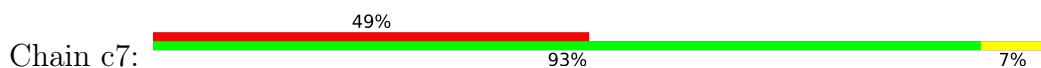
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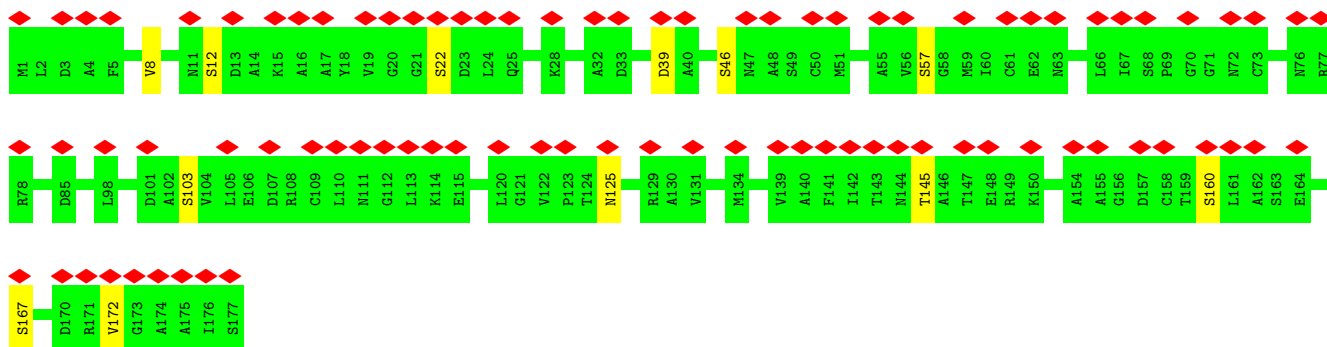


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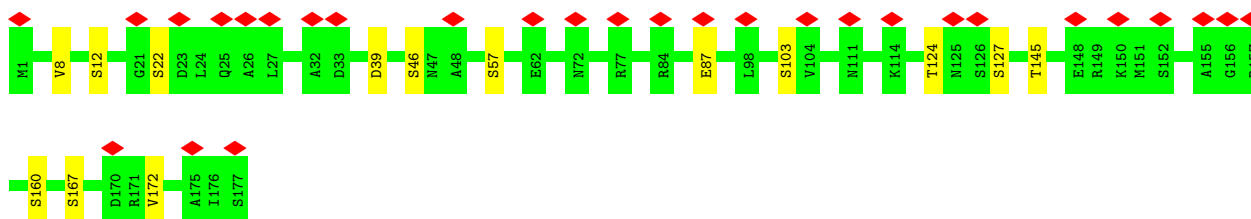


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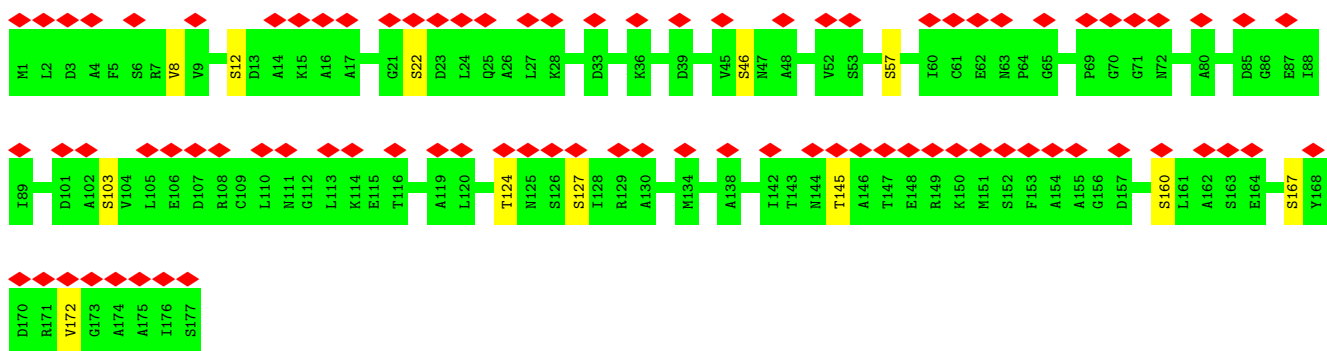
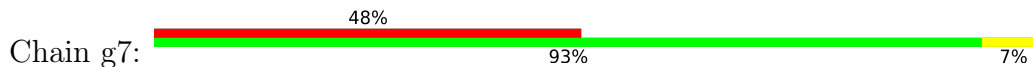




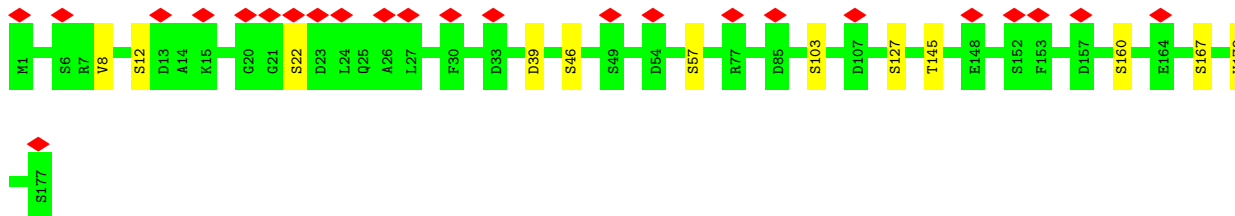
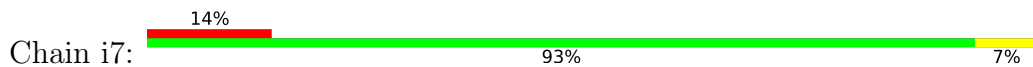
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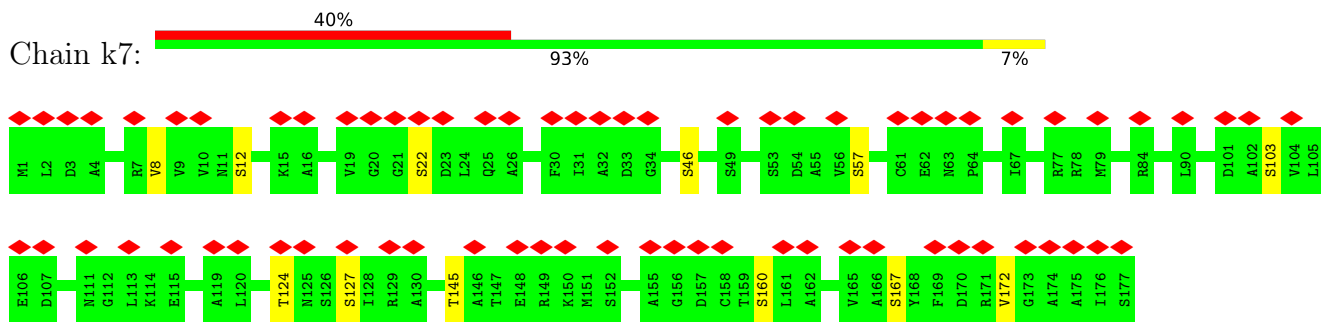
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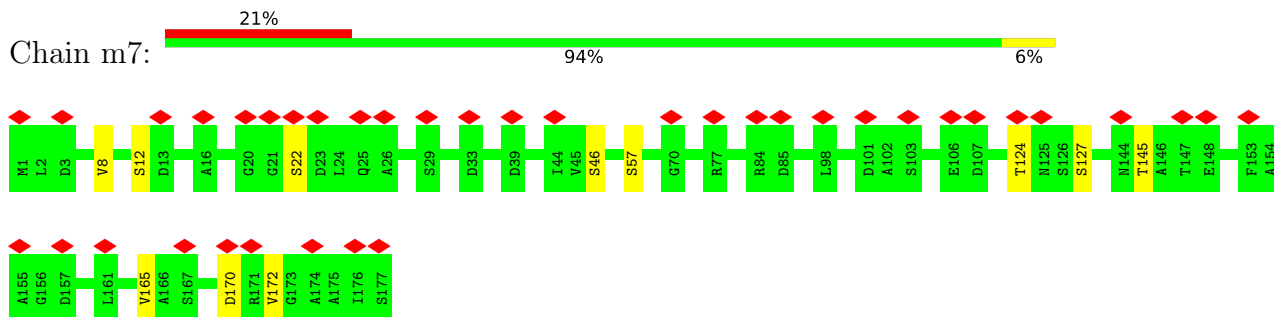
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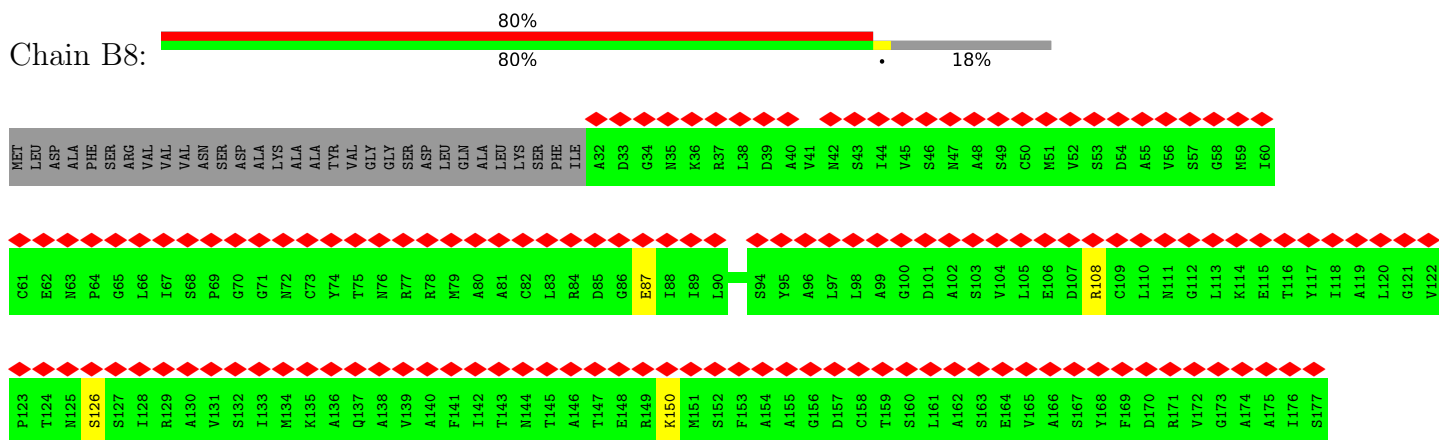
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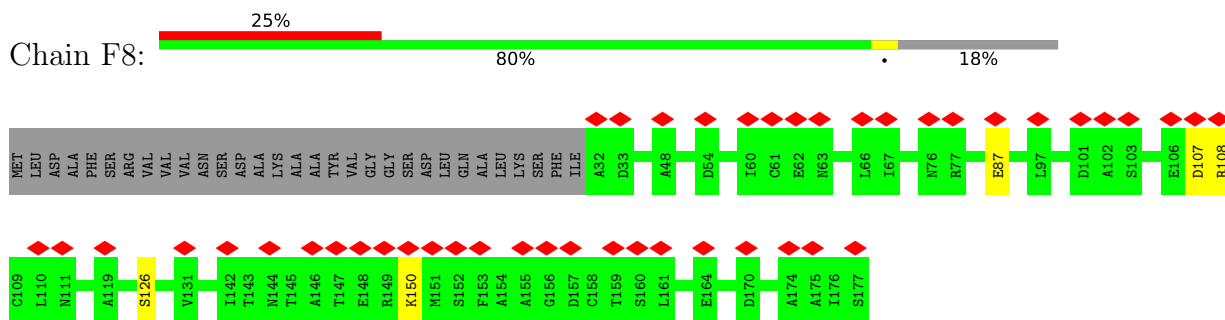
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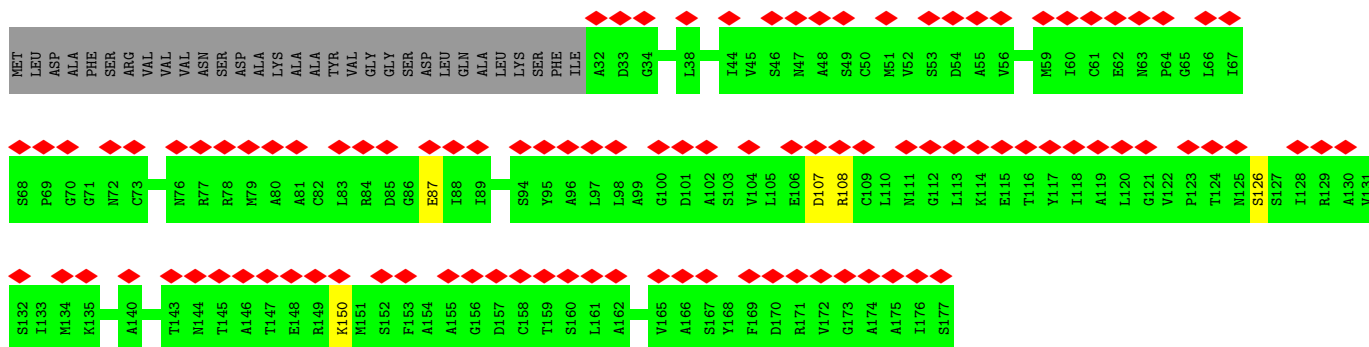


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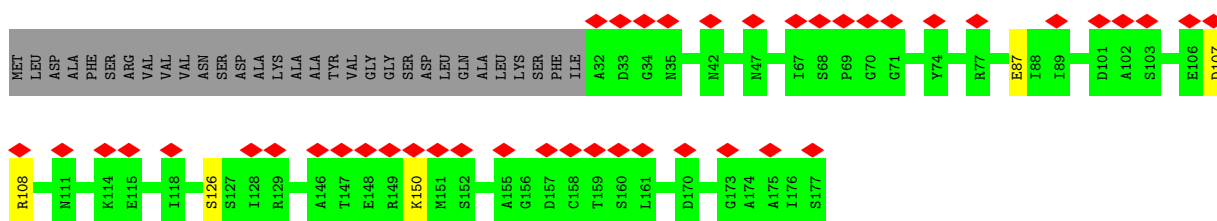
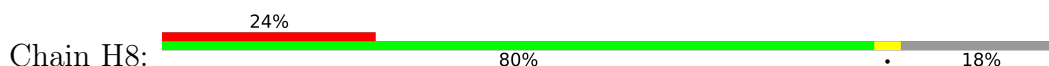


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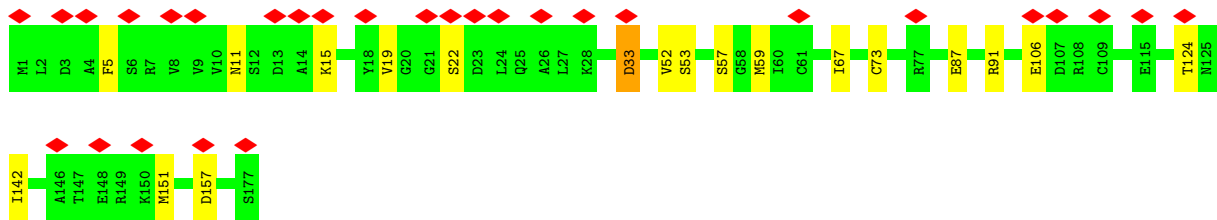
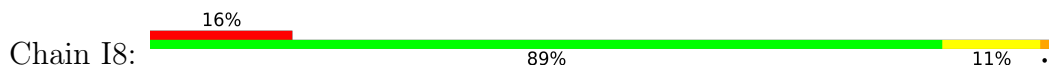




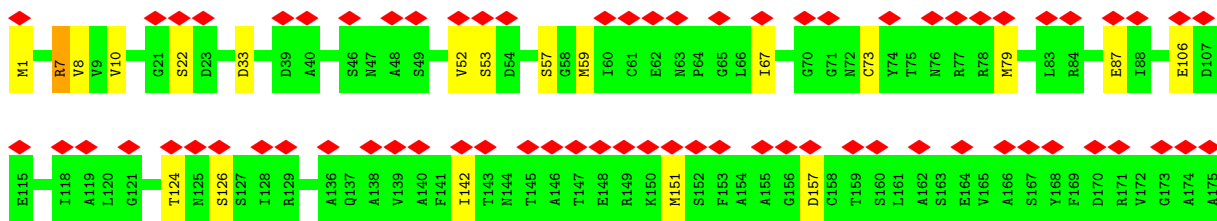
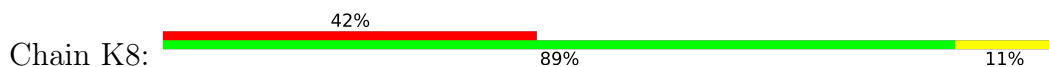
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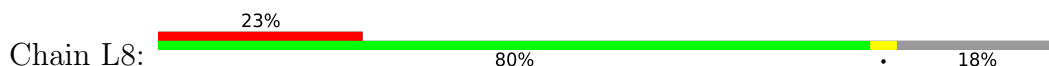
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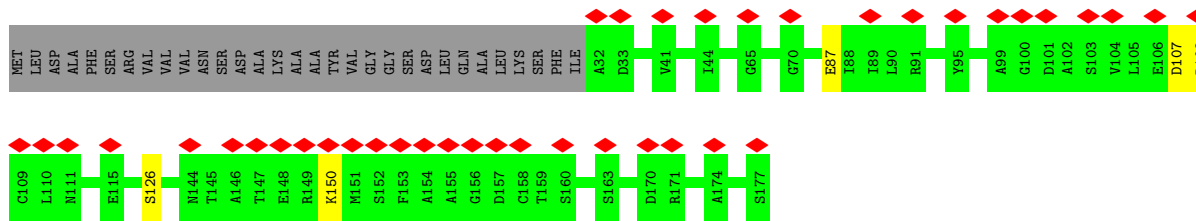


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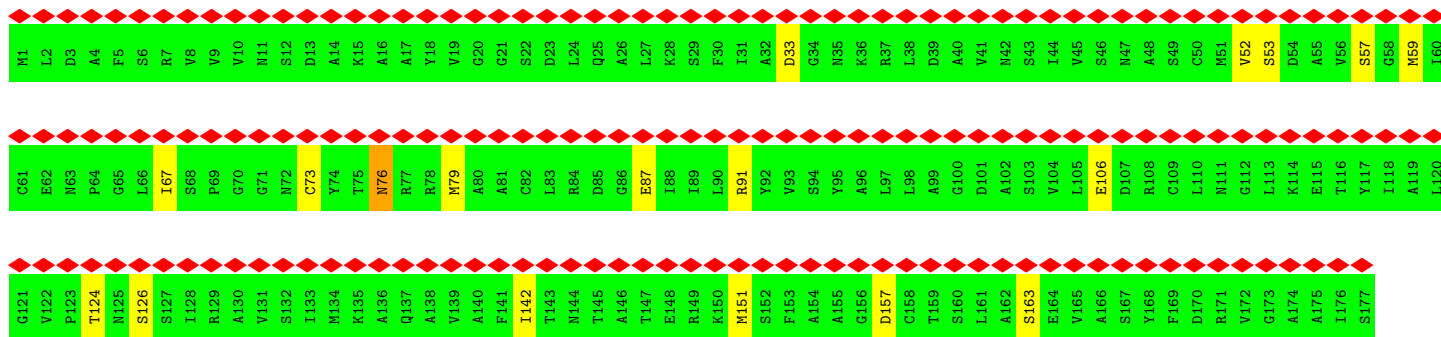
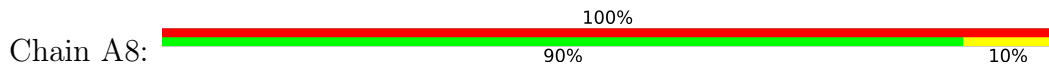


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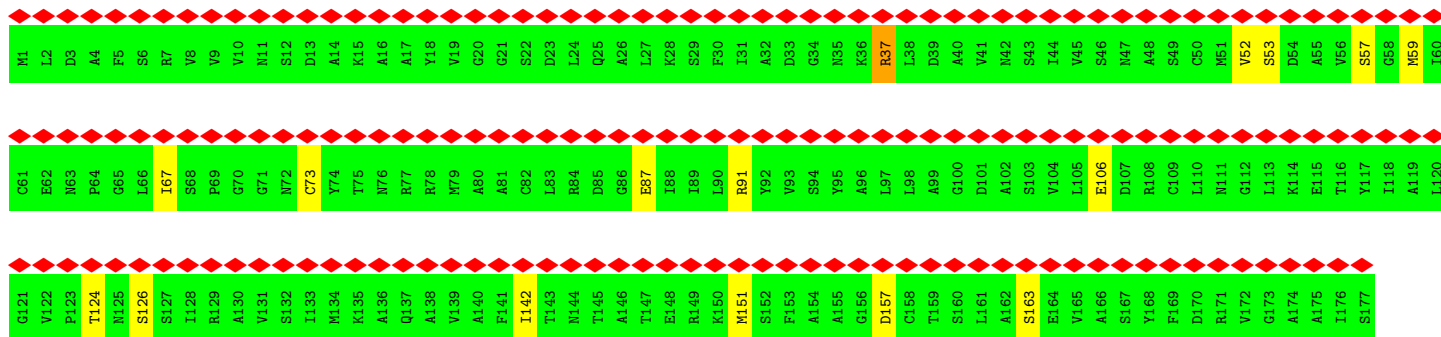
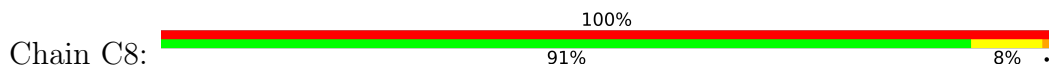




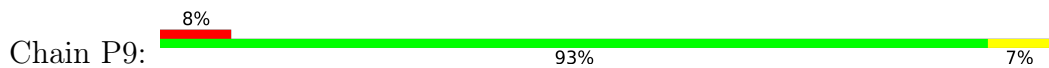
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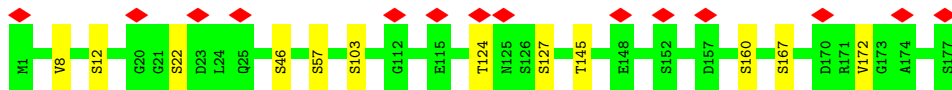


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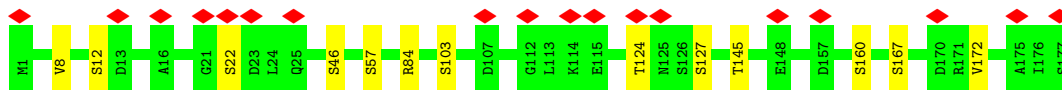
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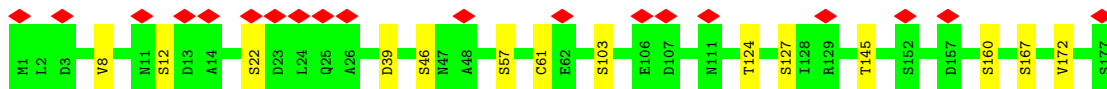
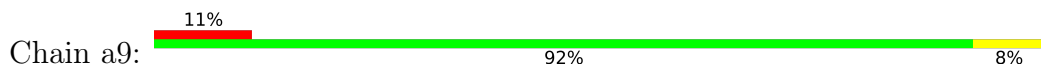
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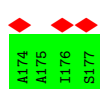
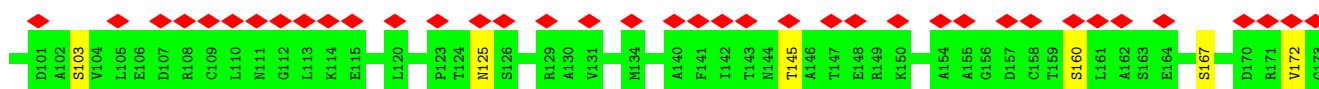
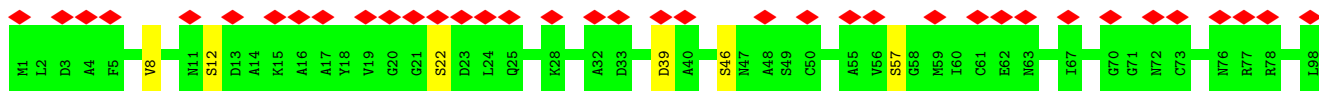
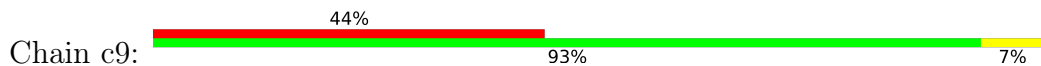
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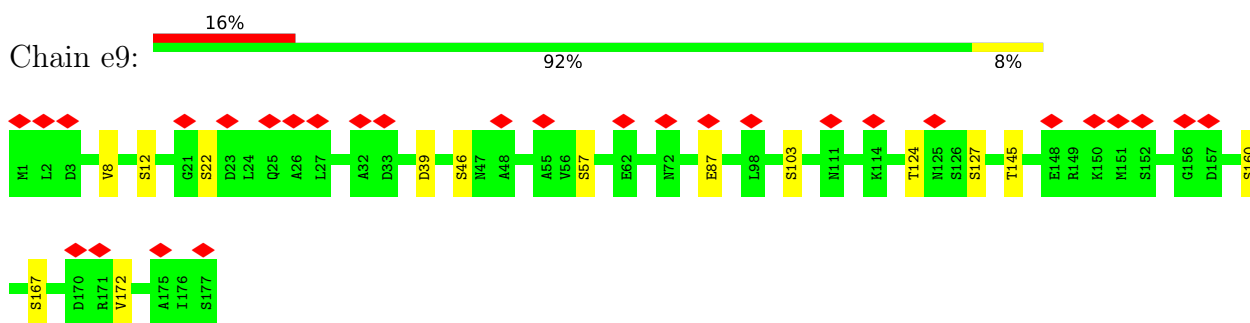
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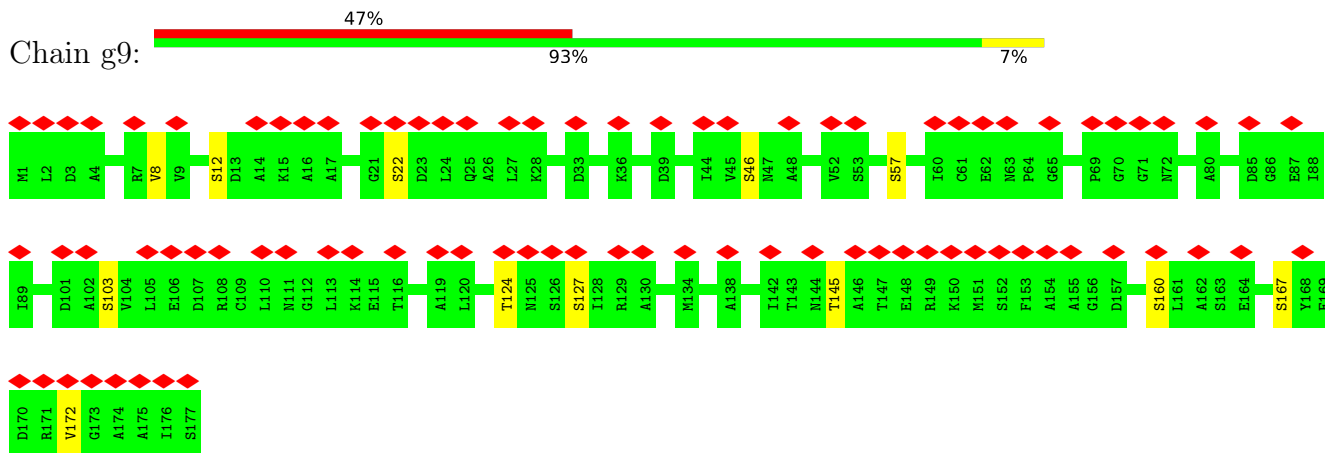
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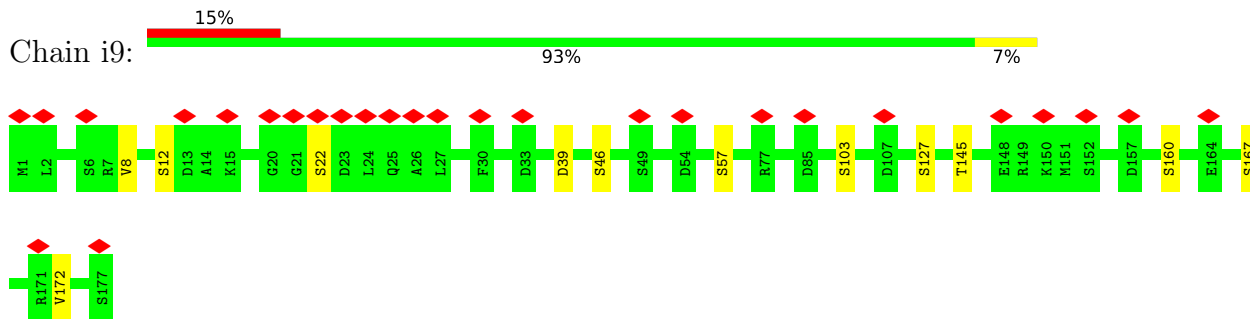
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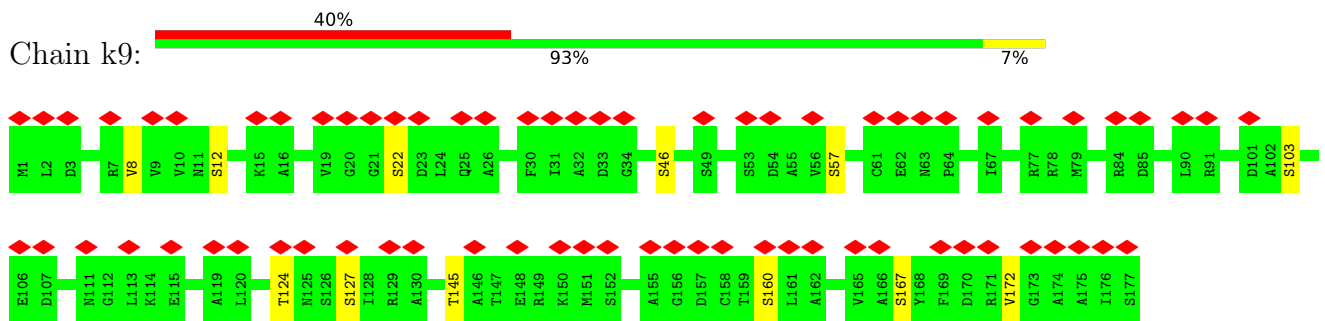
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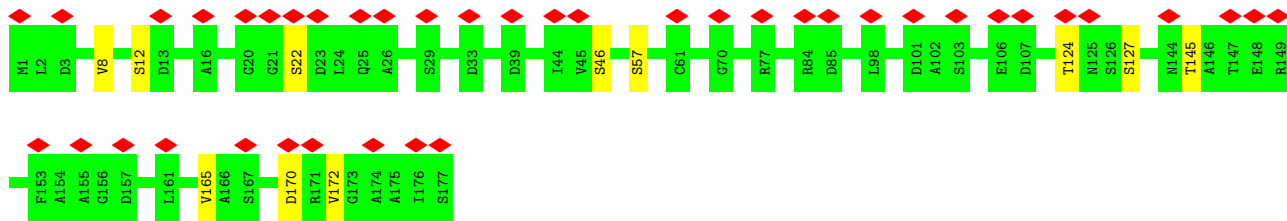


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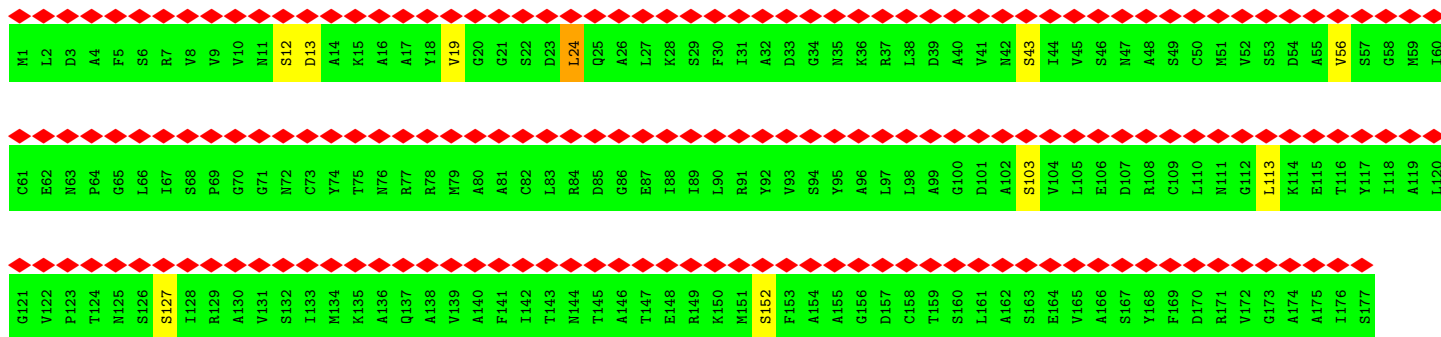


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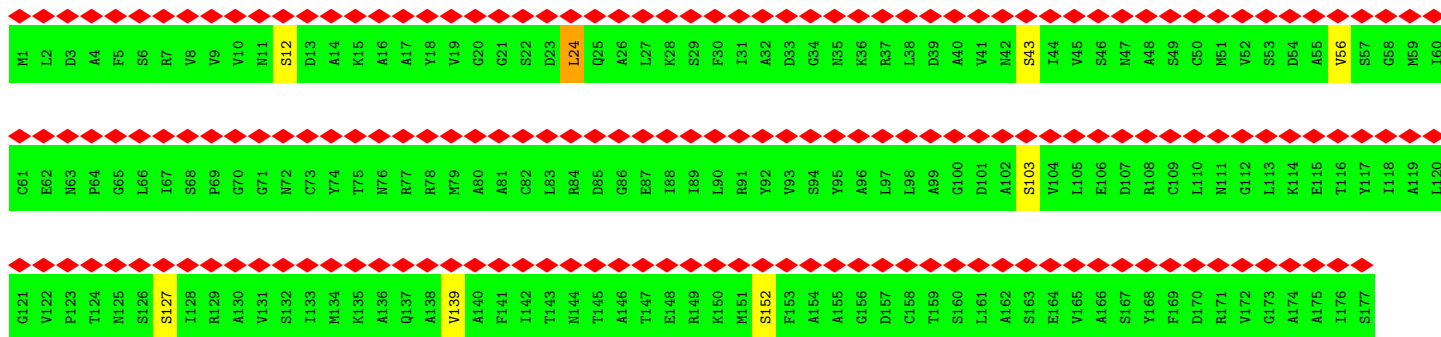




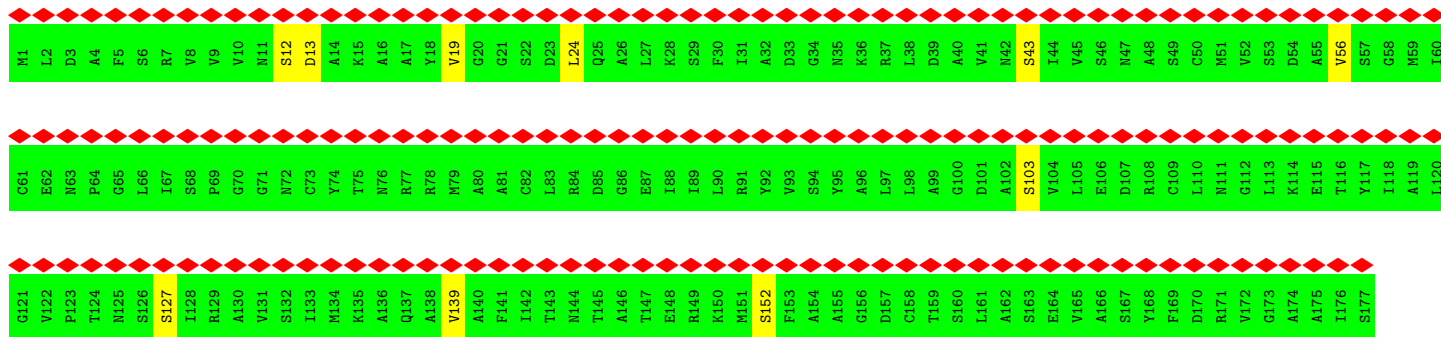
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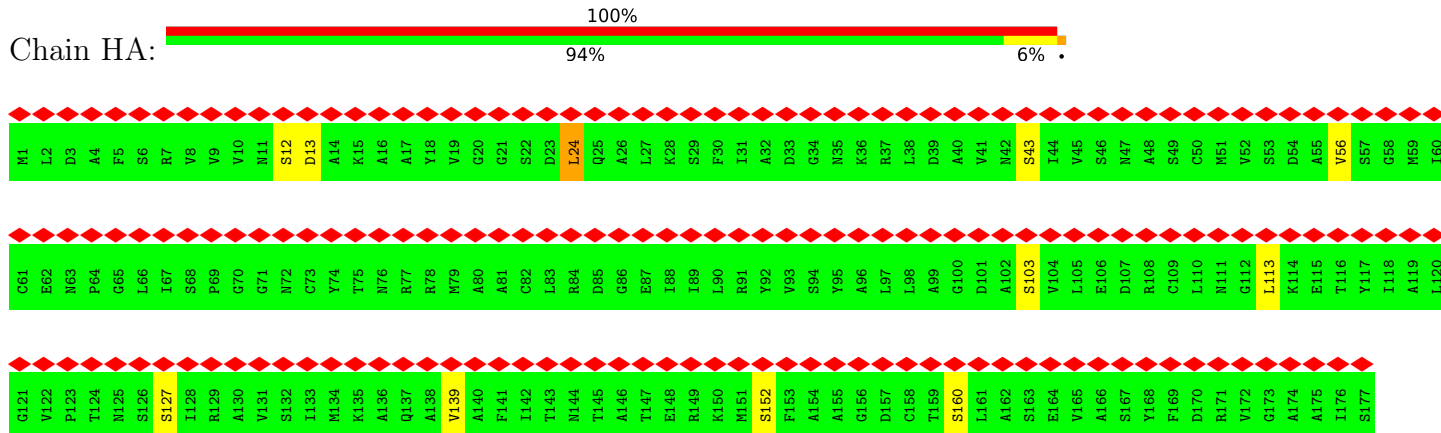
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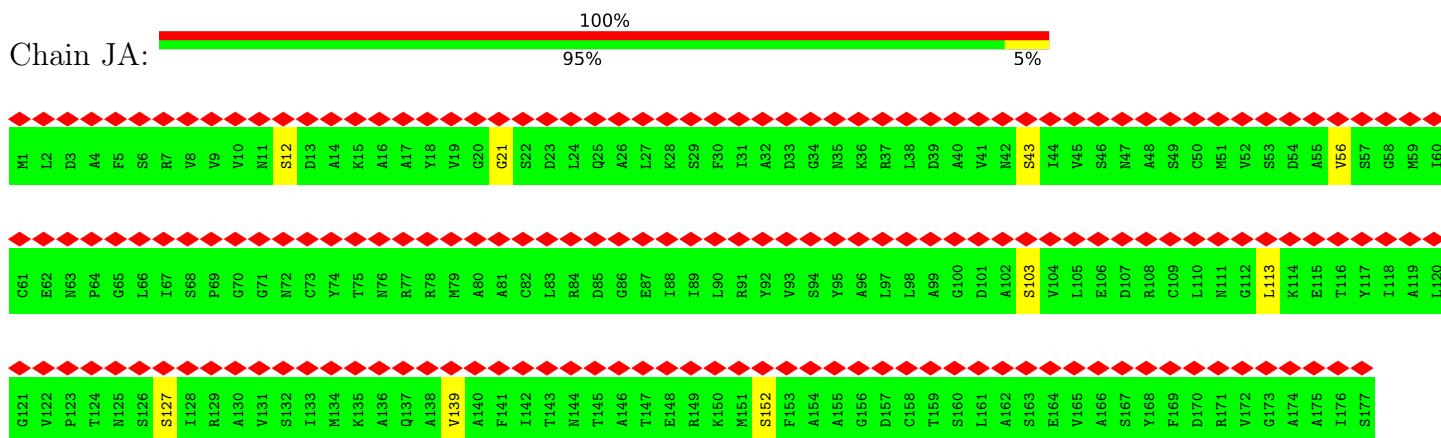
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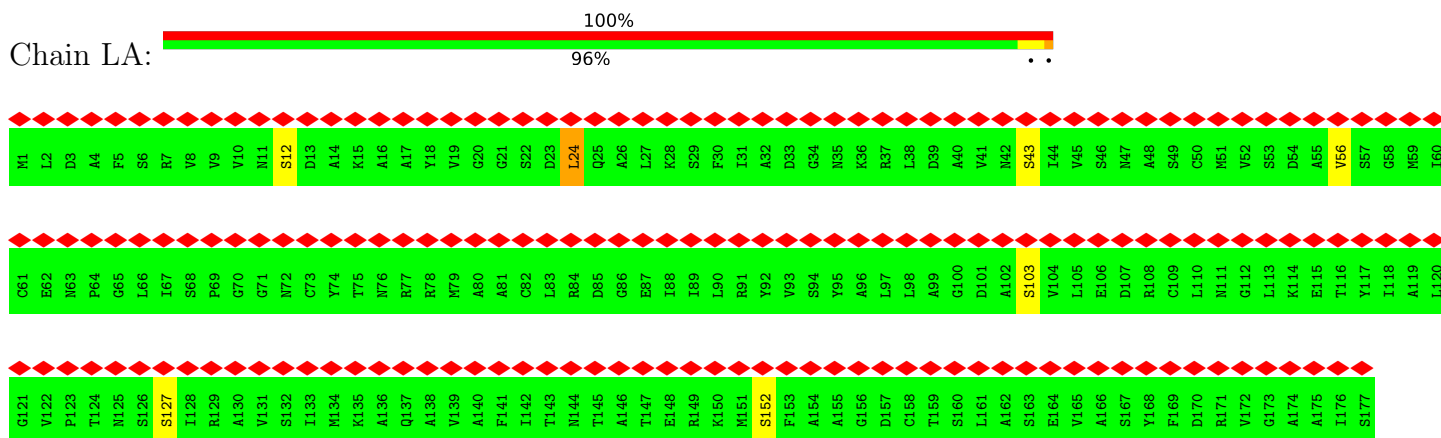
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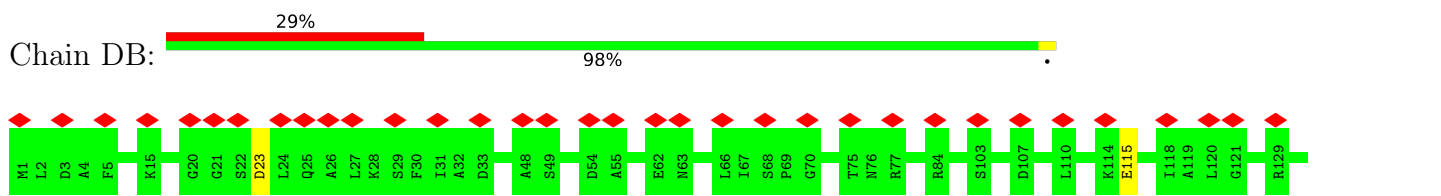
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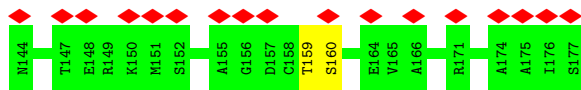


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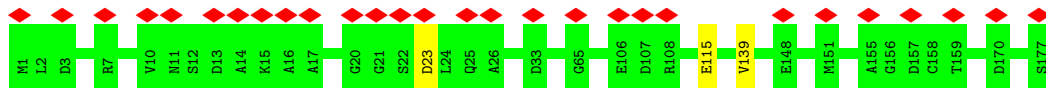


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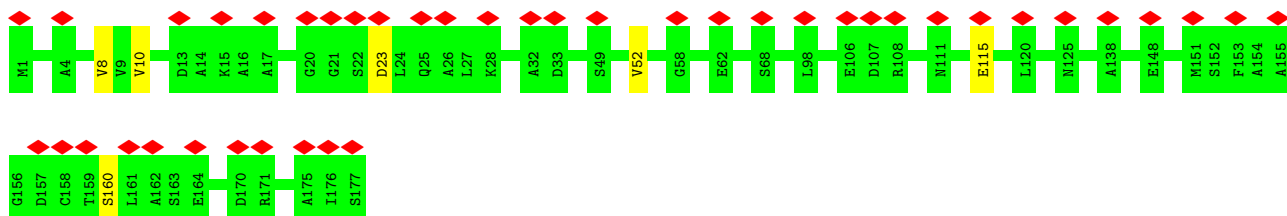




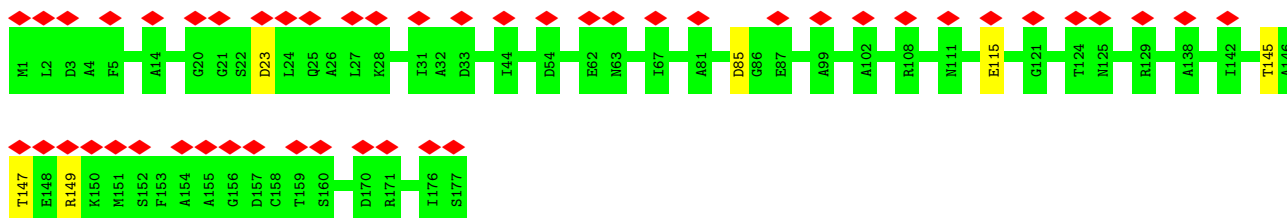
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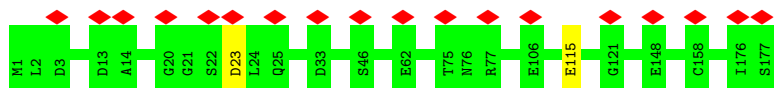
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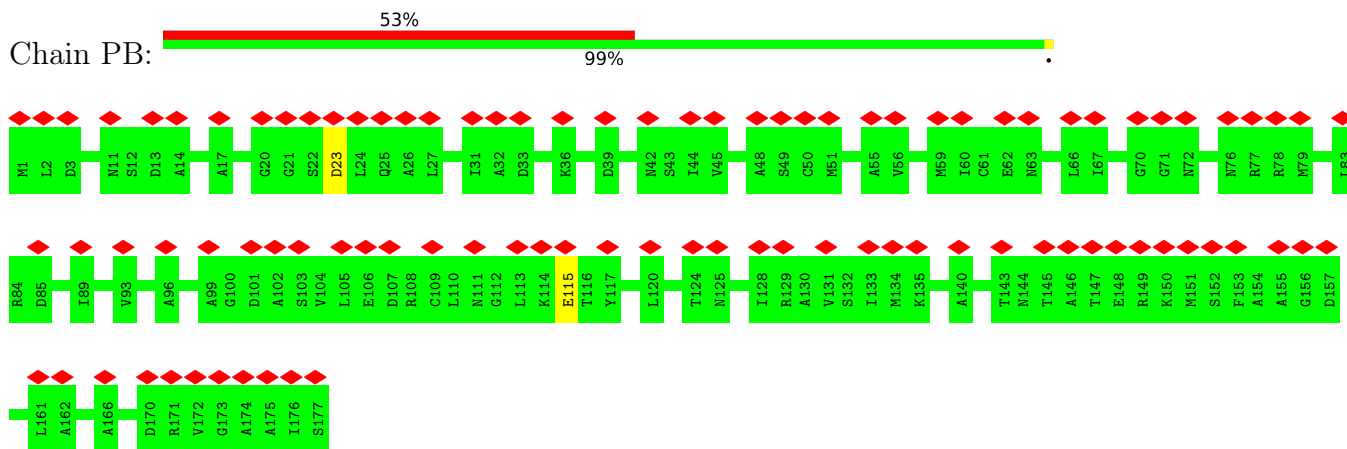
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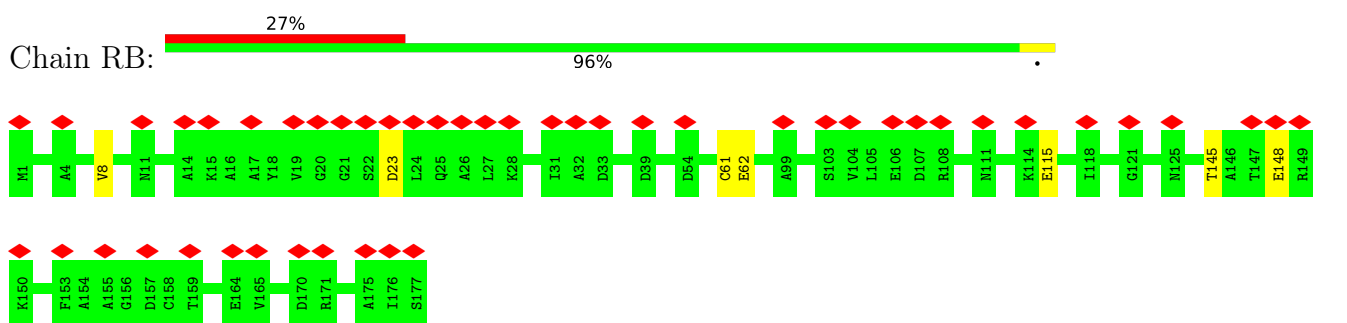
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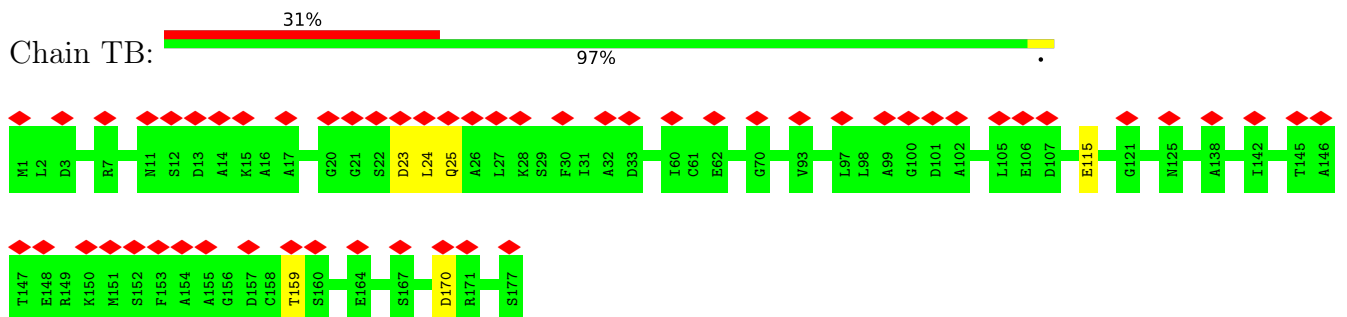
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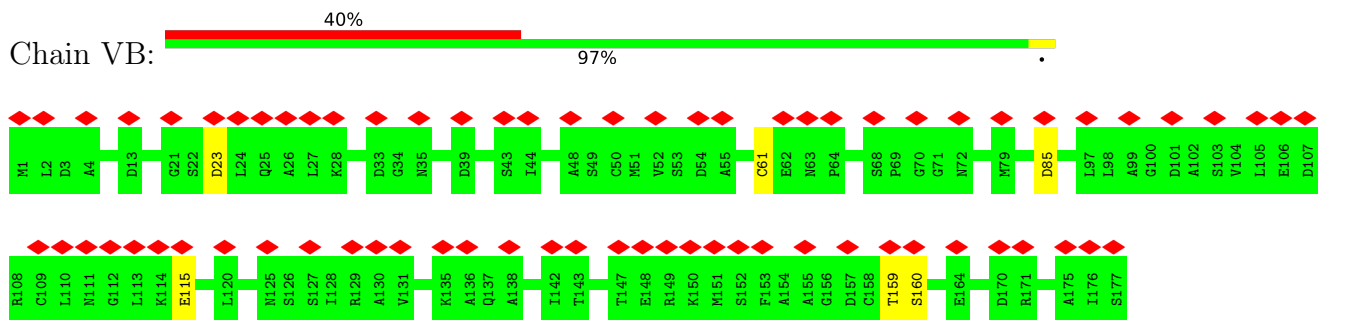
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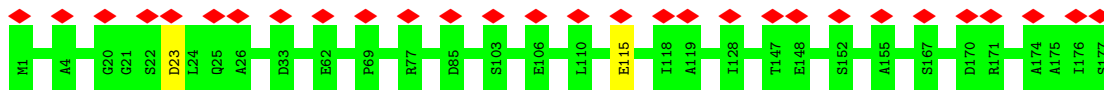


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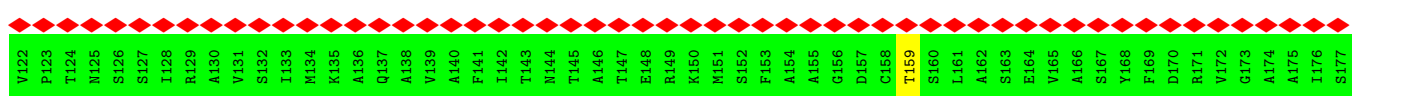
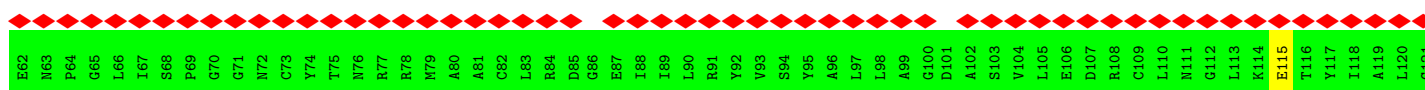
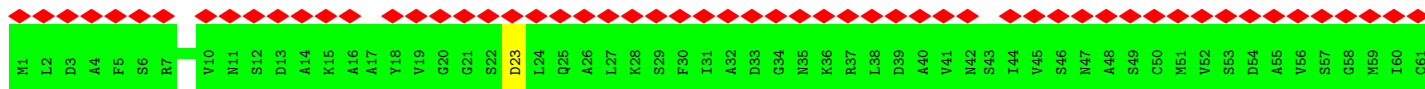




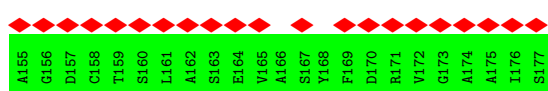
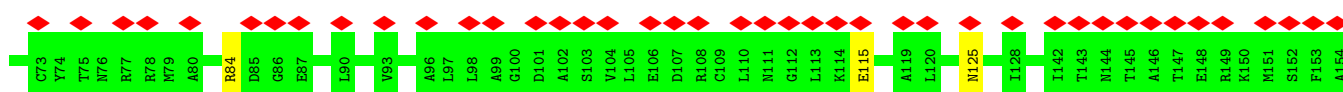
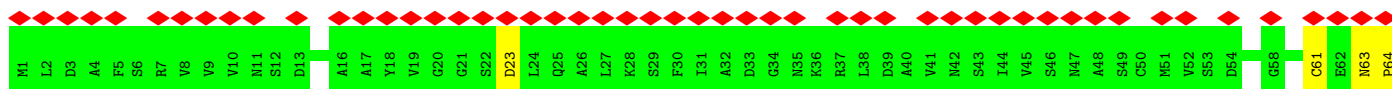
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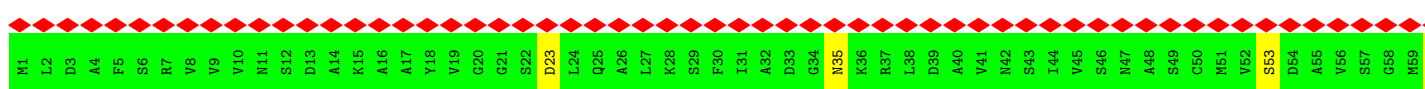
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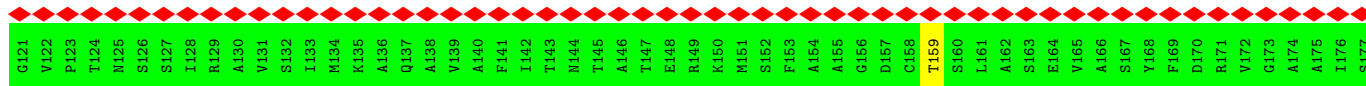
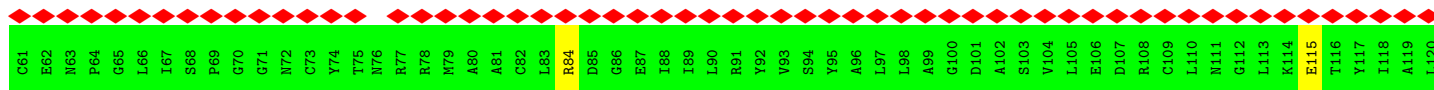


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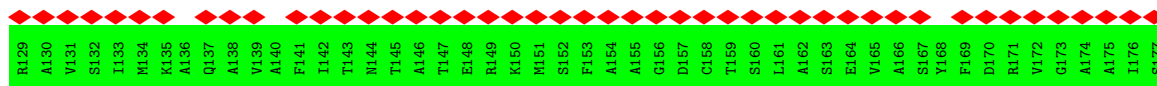
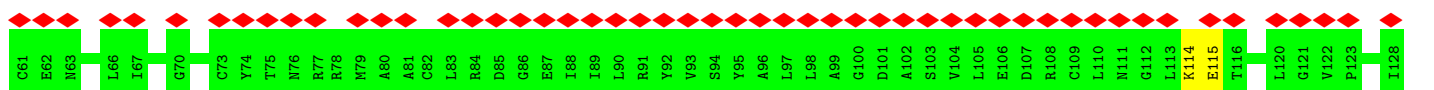
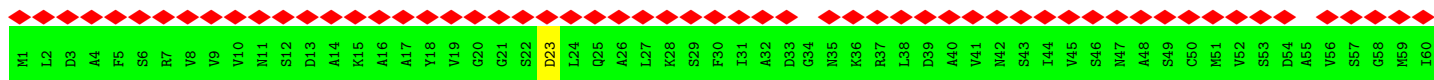
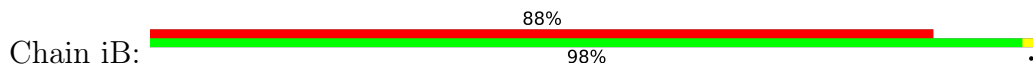


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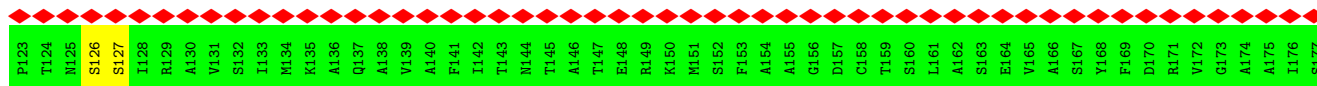
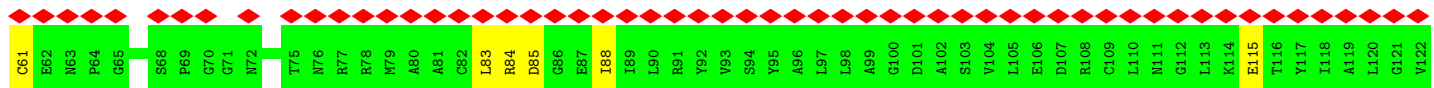
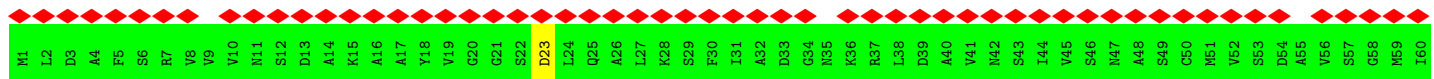




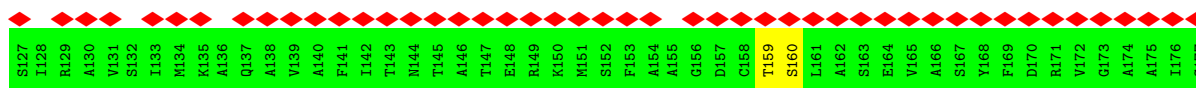
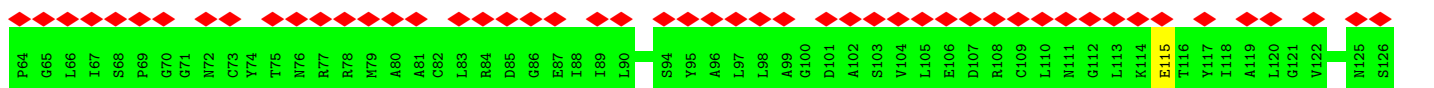
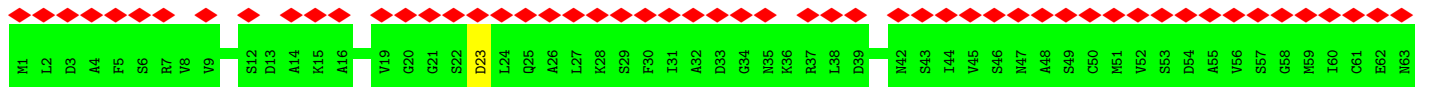
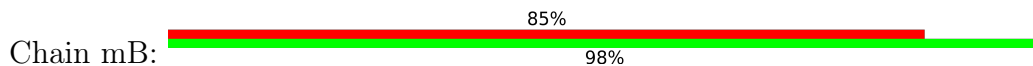
• Molecule 7: B-phycoerythrin beta chain



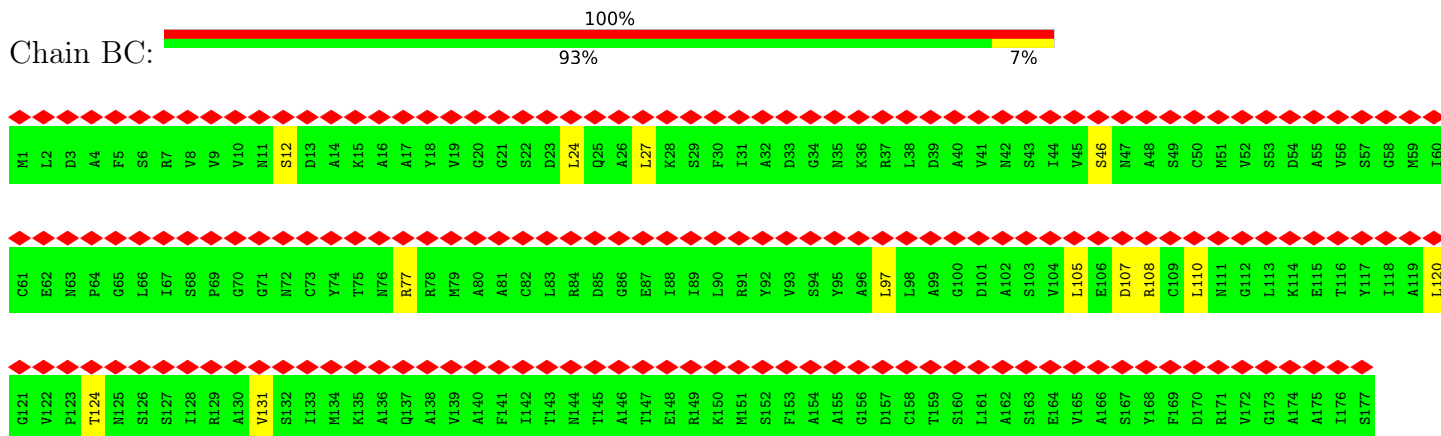
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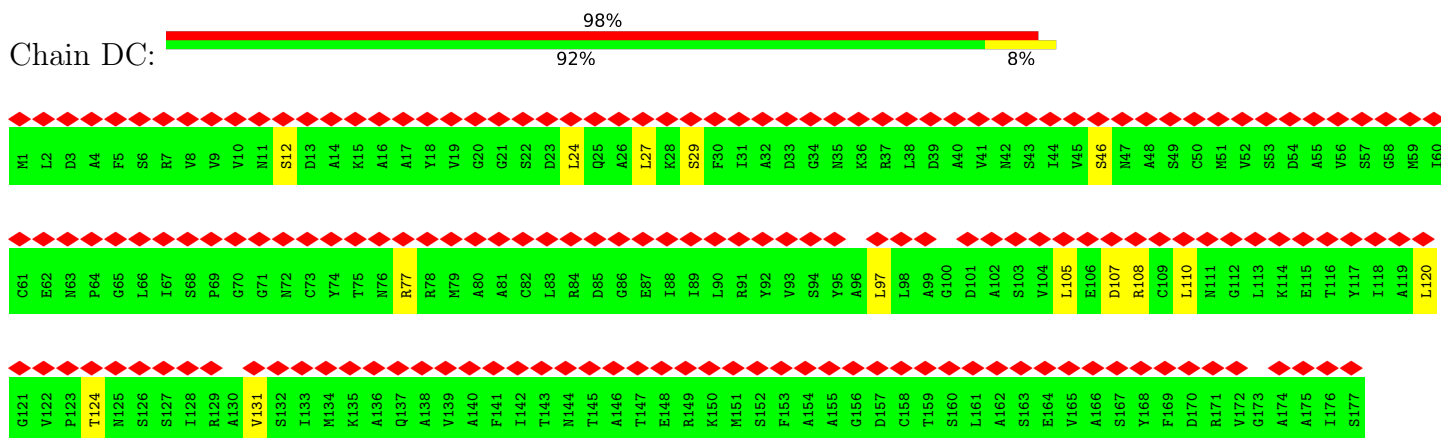
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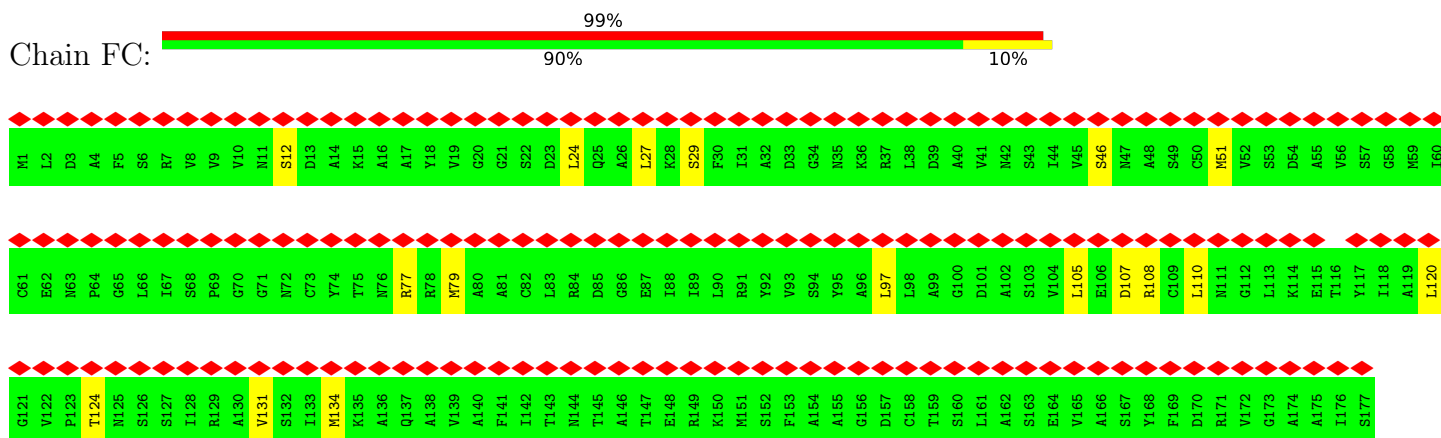
- Molecule 7: B-phycoerythrin beta chain



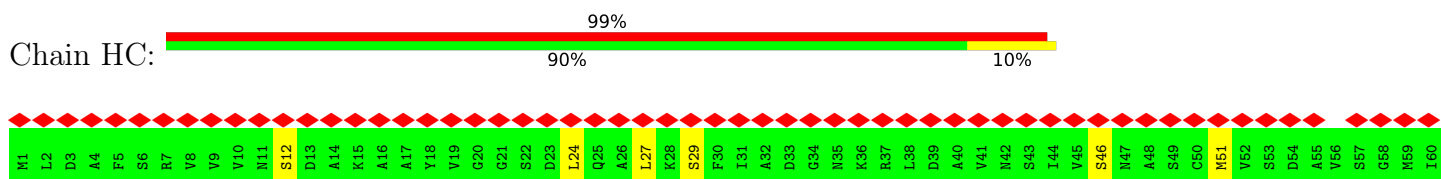
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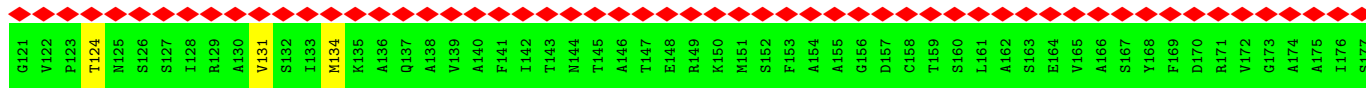
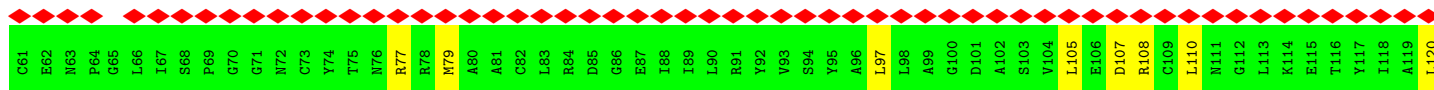


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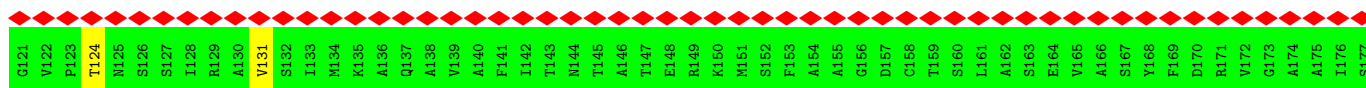
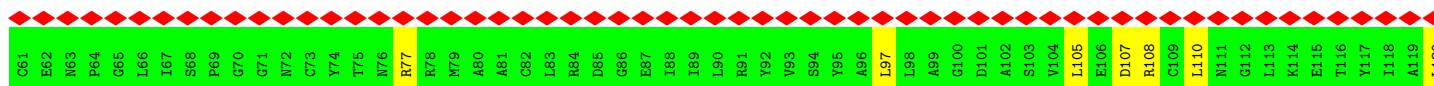
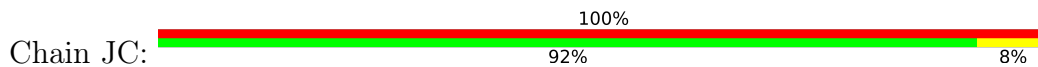


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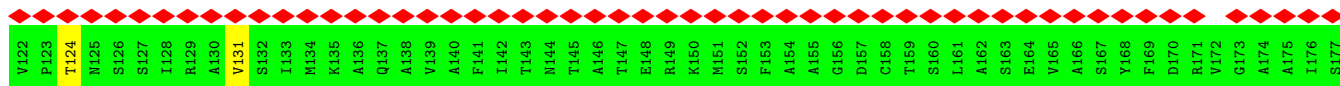
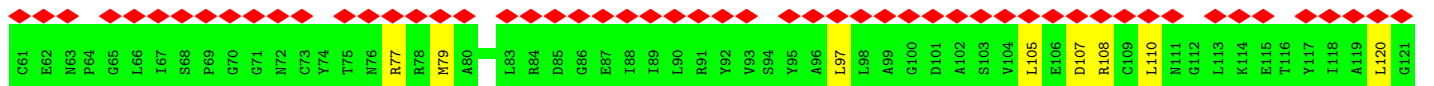




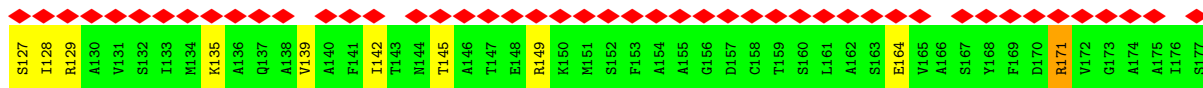
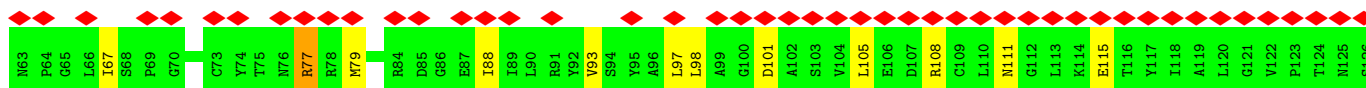
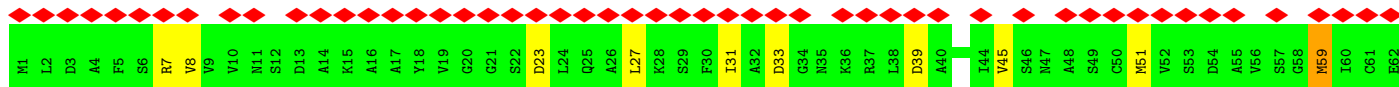
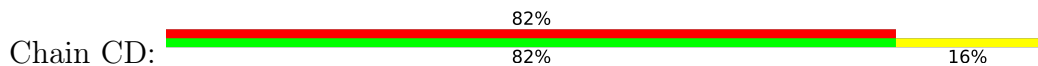
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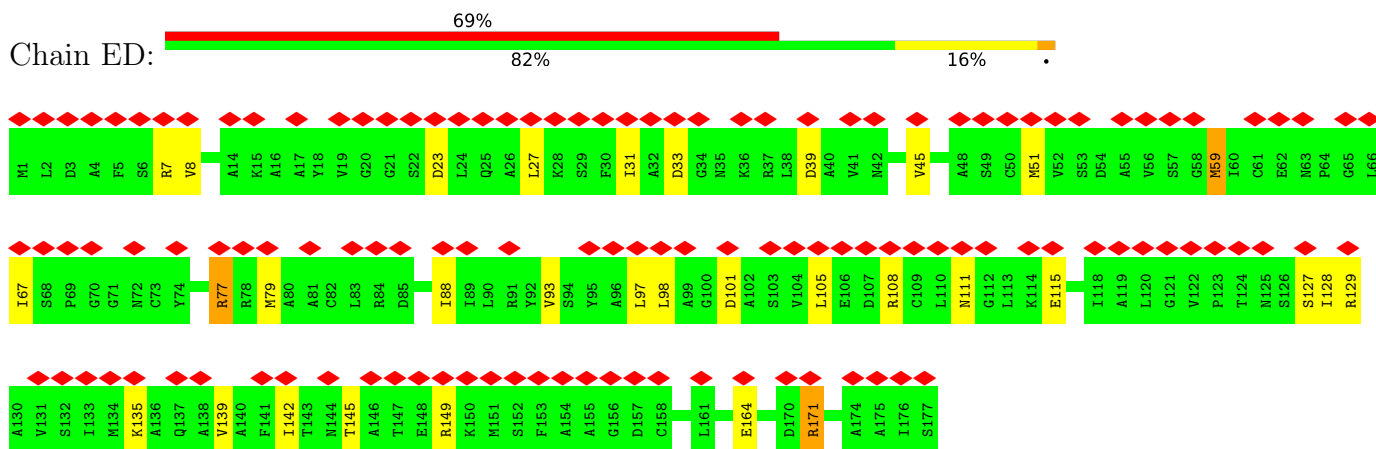
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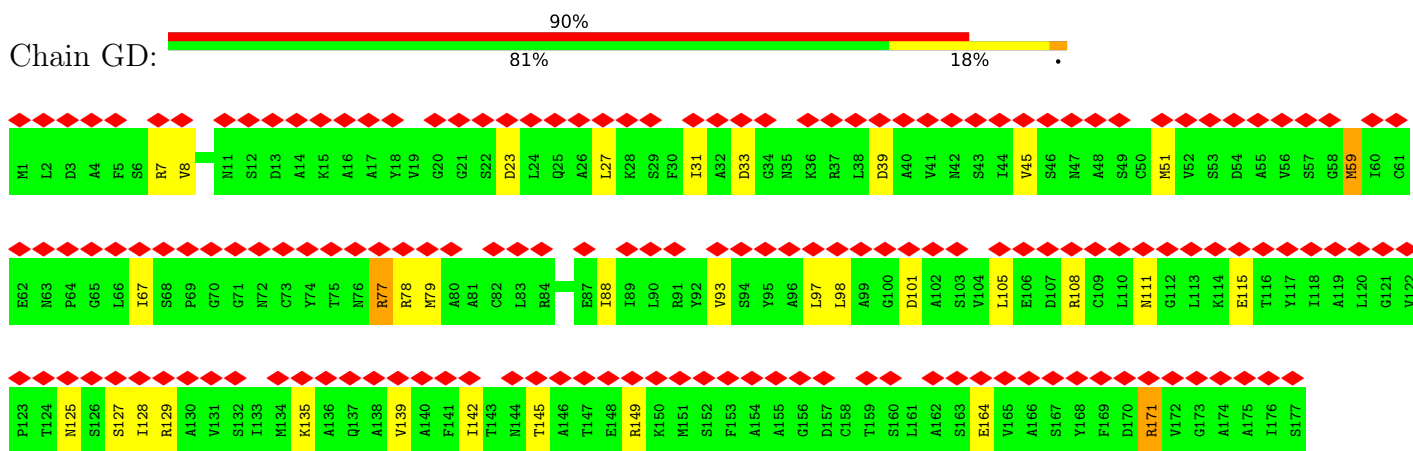
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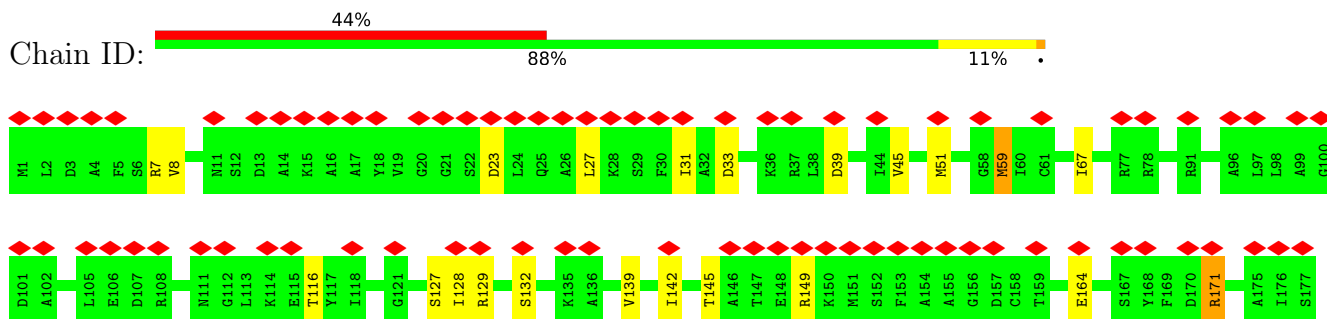
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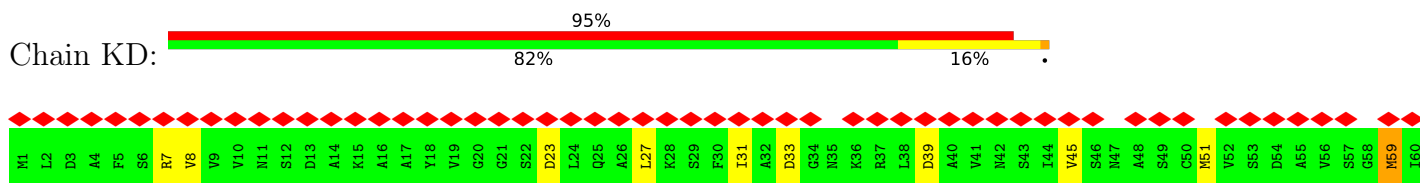
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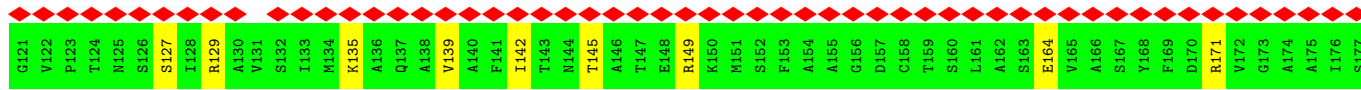
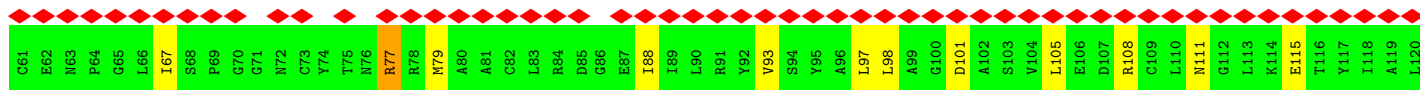


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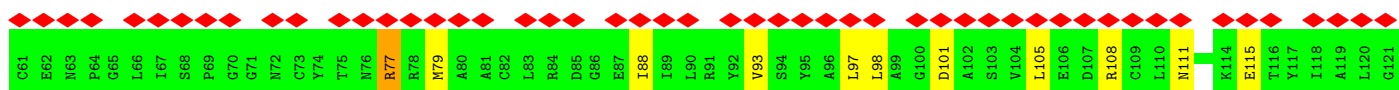
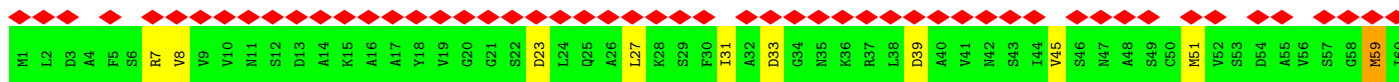
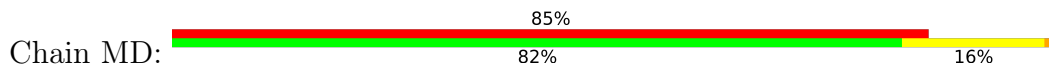


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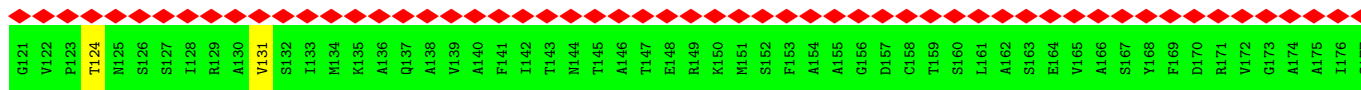
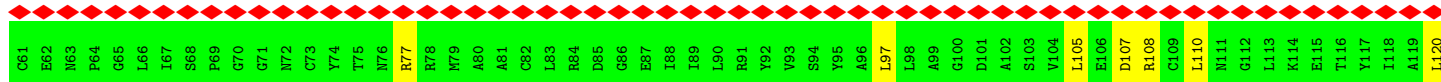
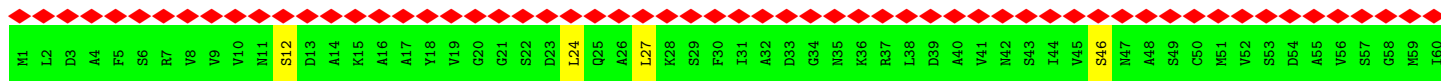
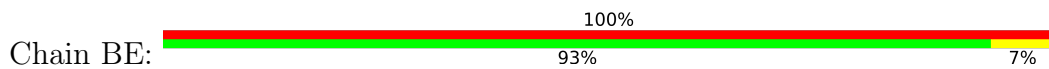




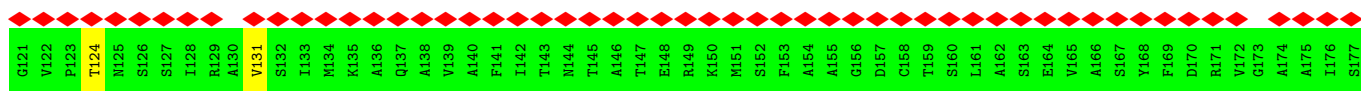
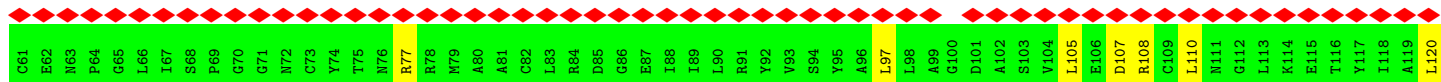
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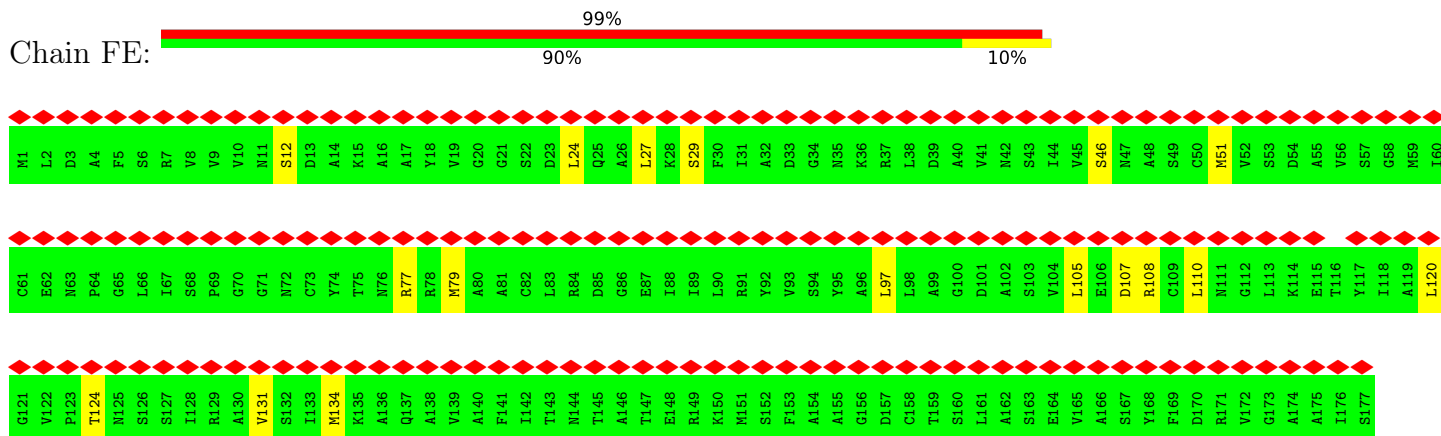
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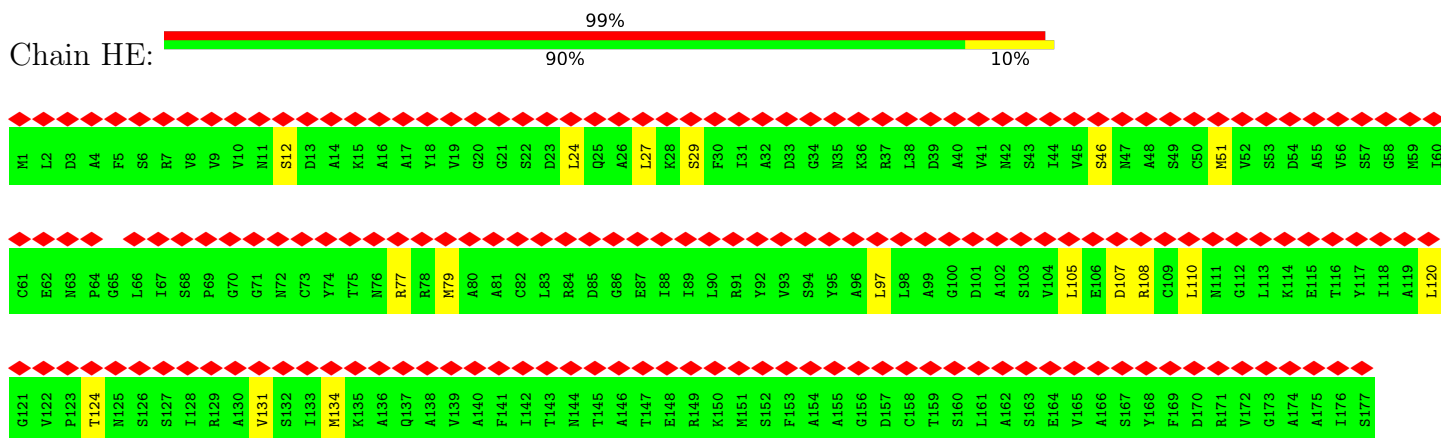
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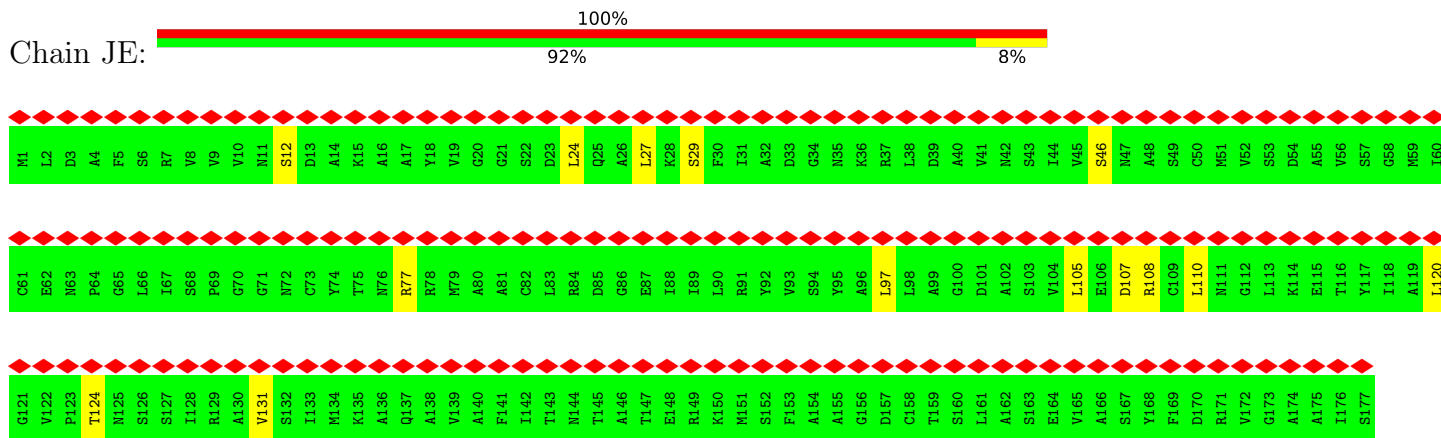
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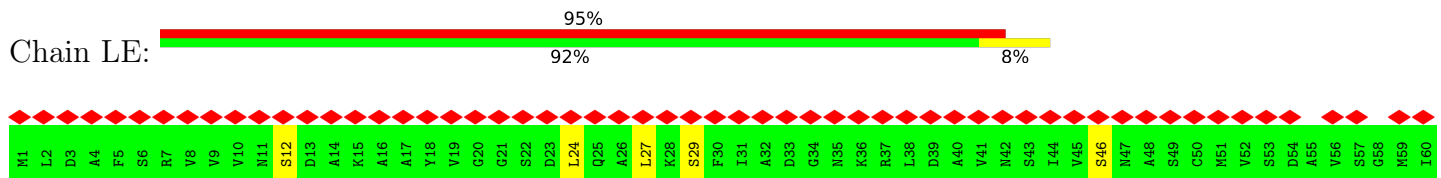
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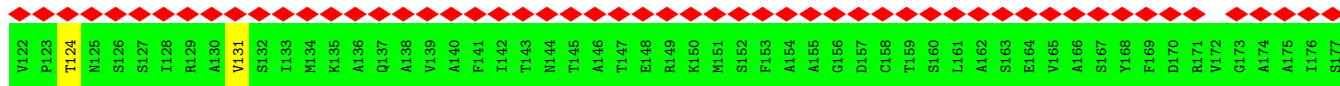
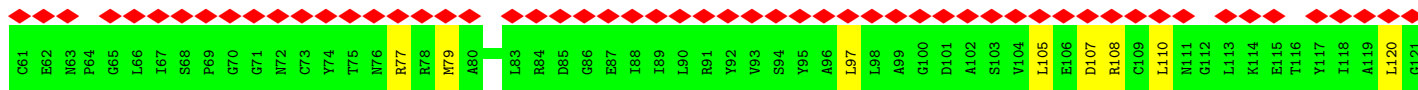


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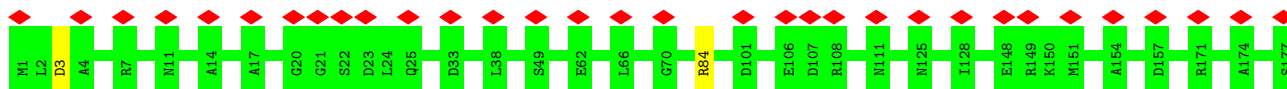


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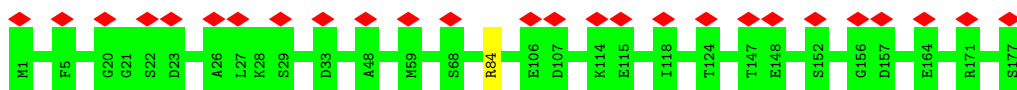




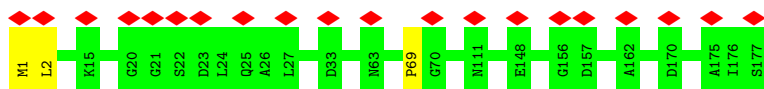
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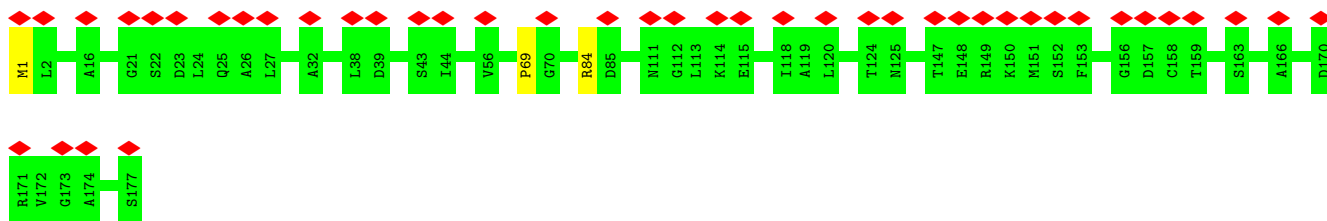
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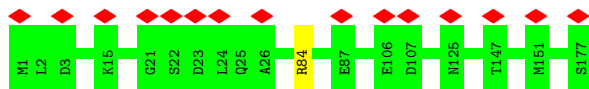
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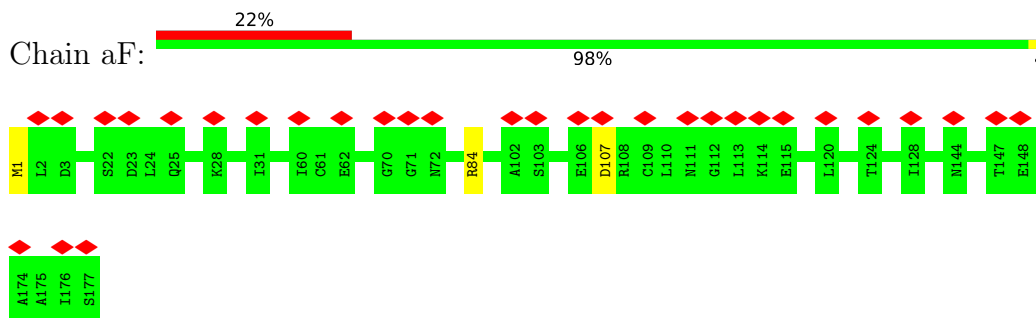
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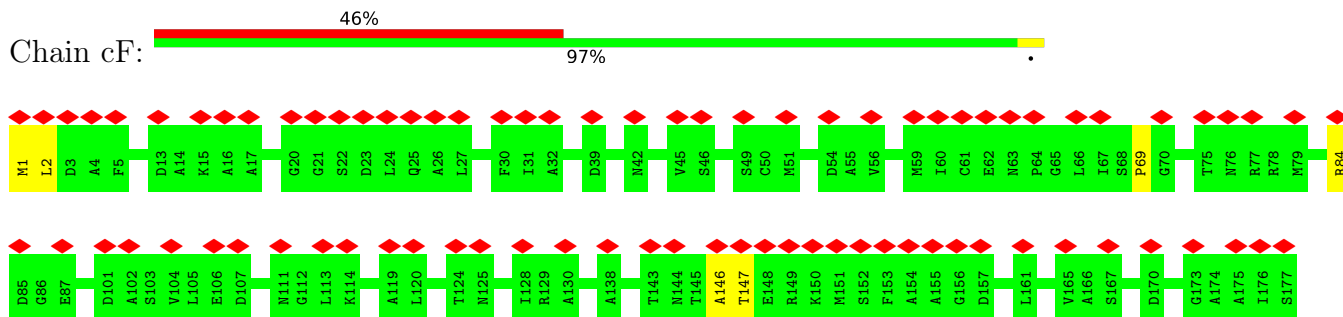
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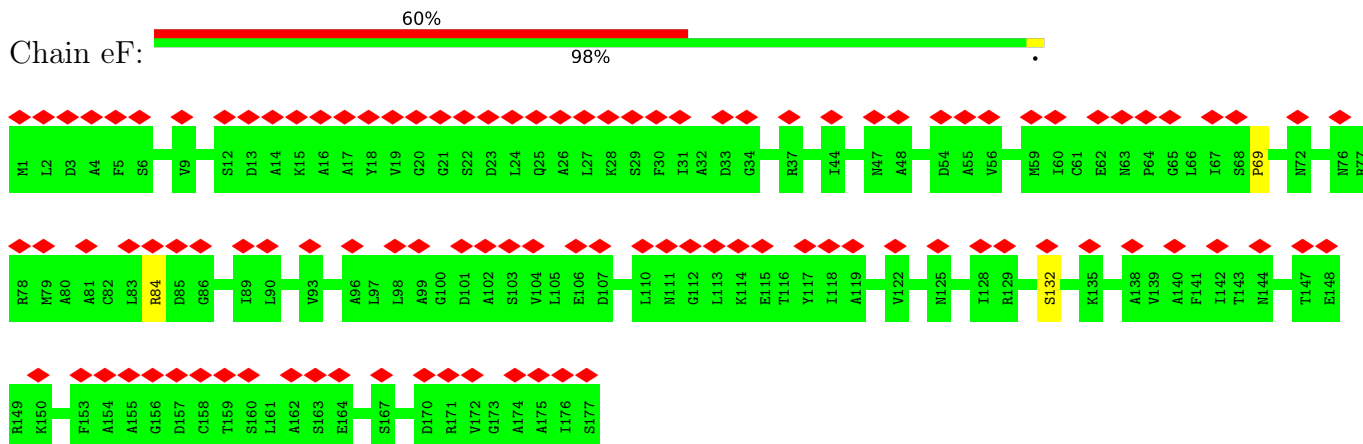
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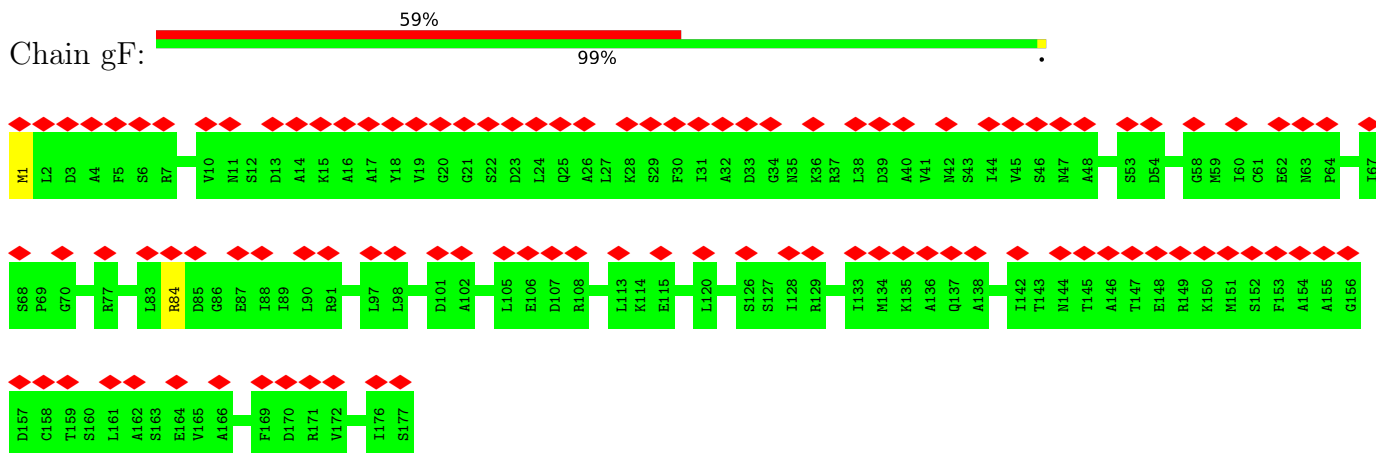
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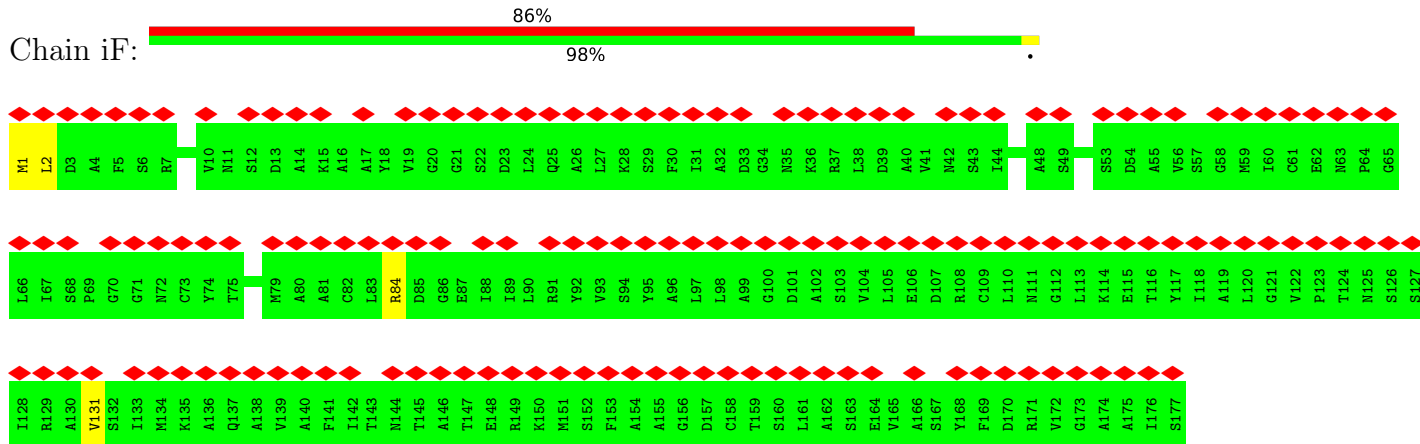
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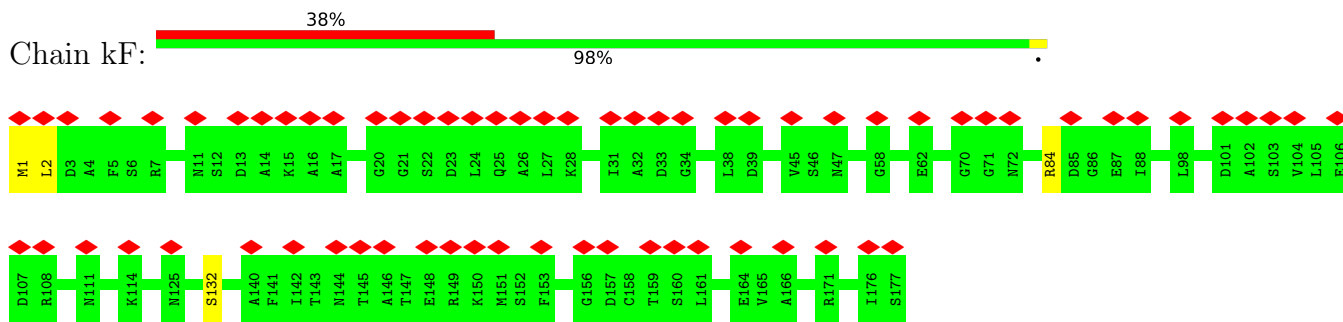
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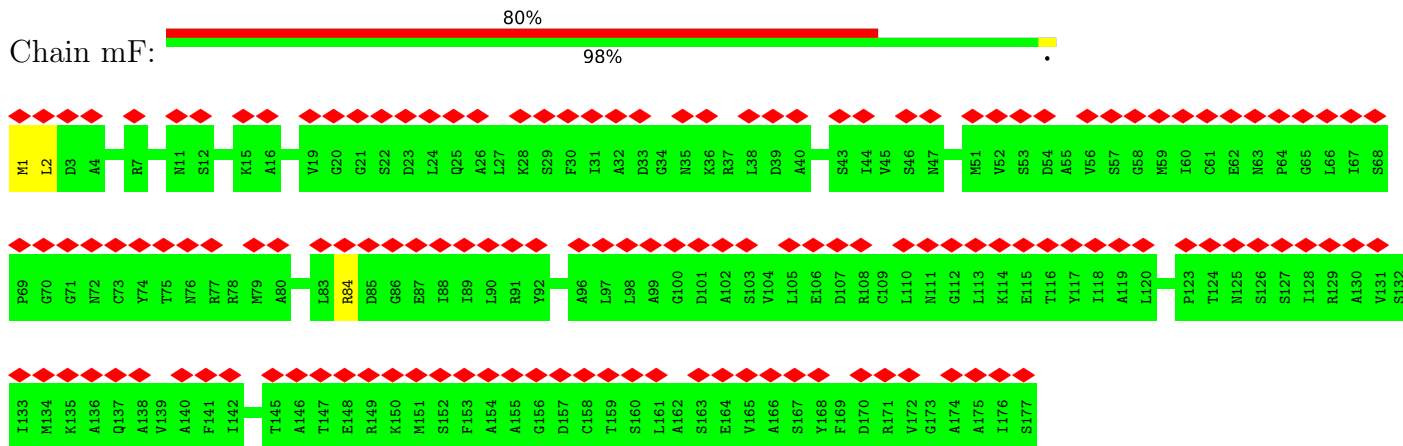
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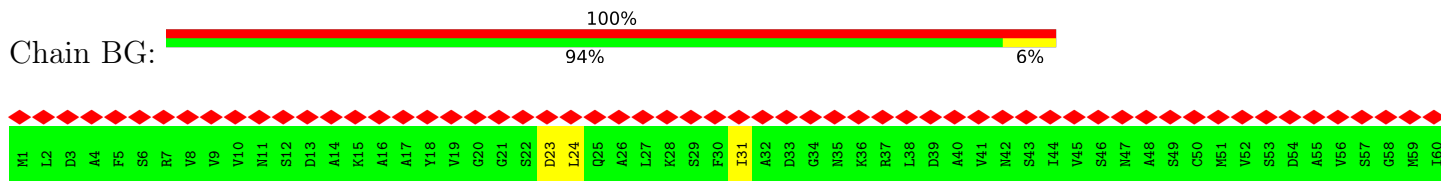
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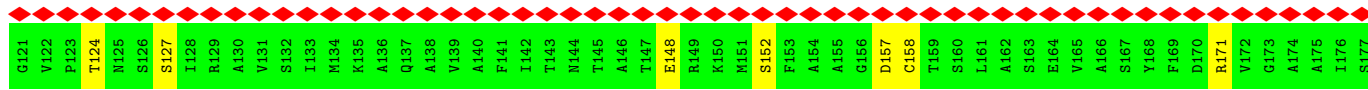
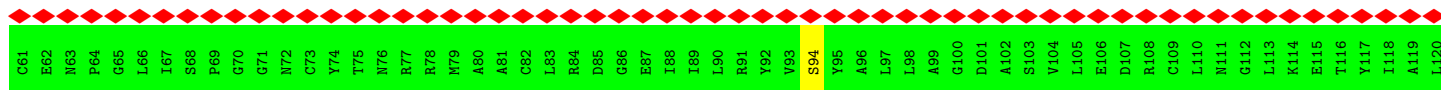


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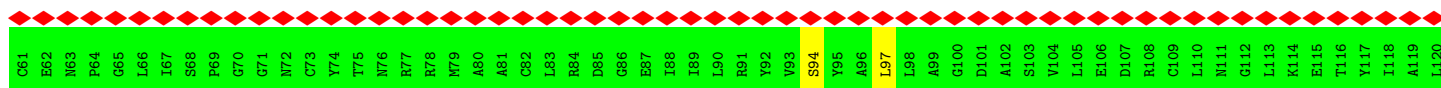


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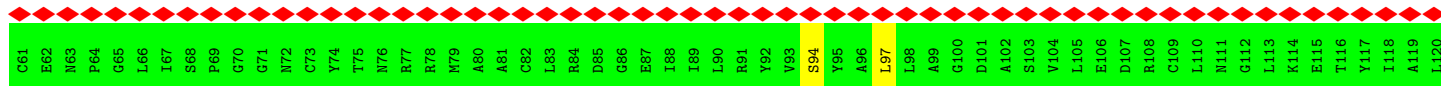




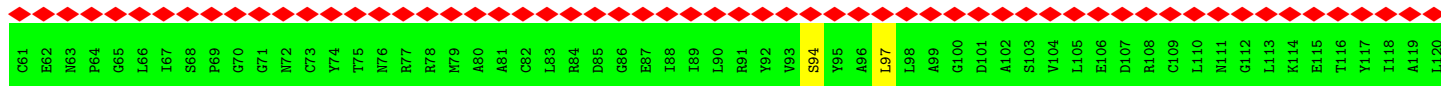
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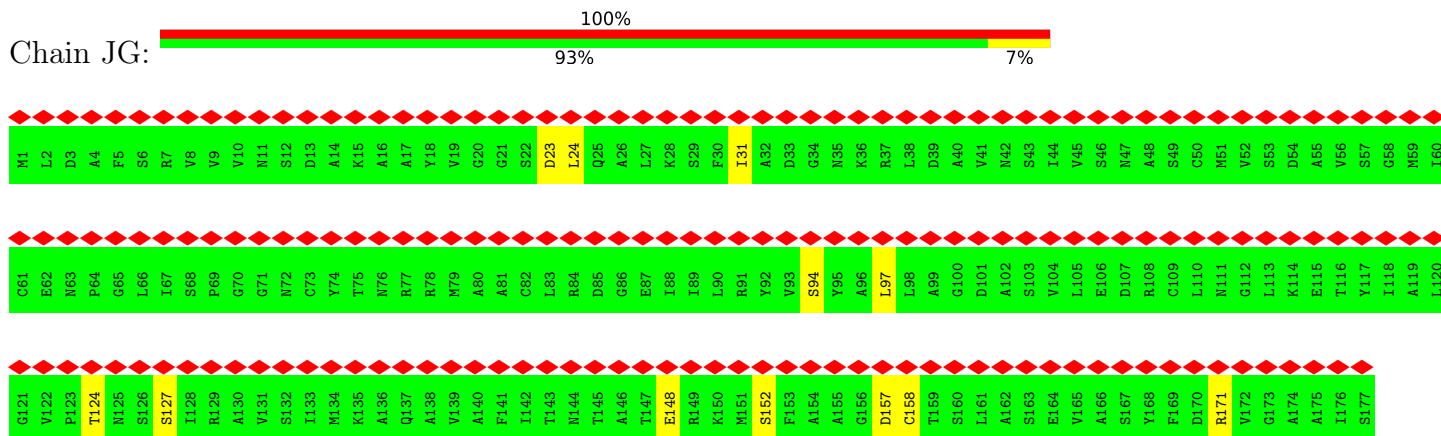
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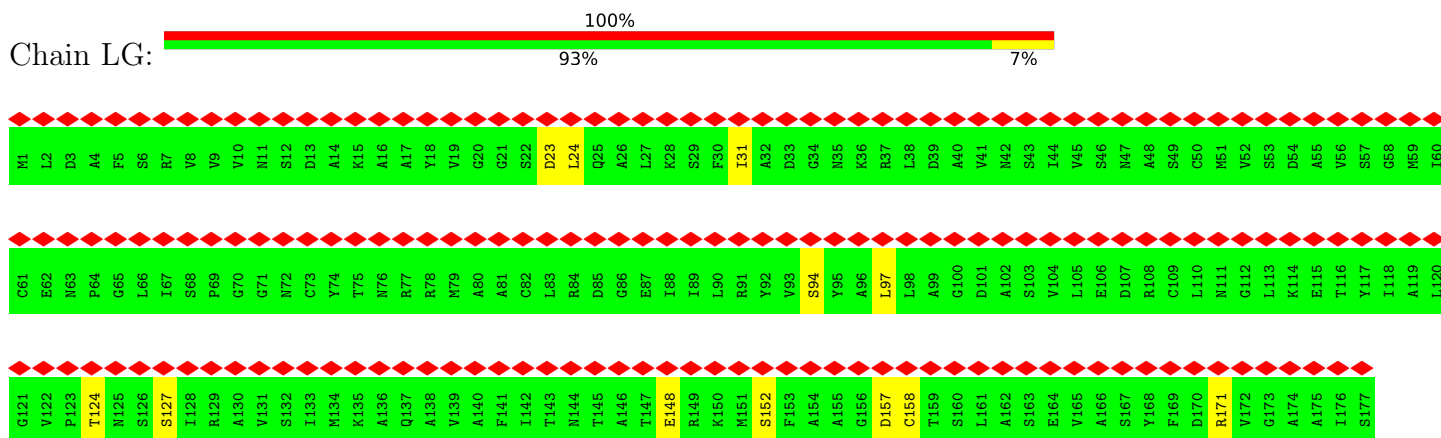
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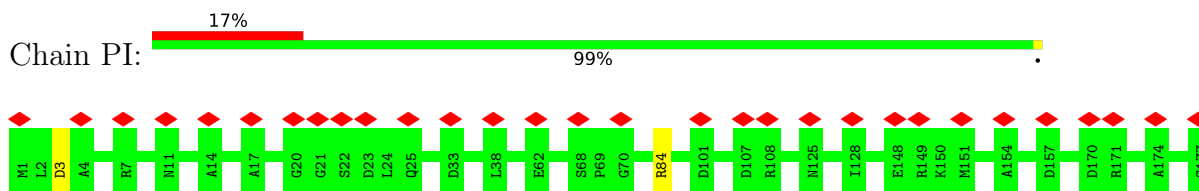
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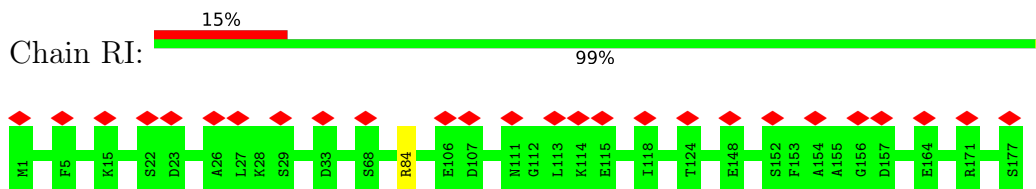
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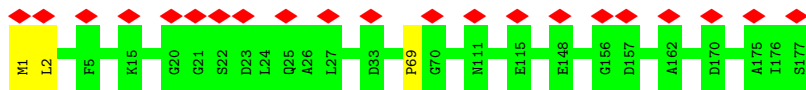


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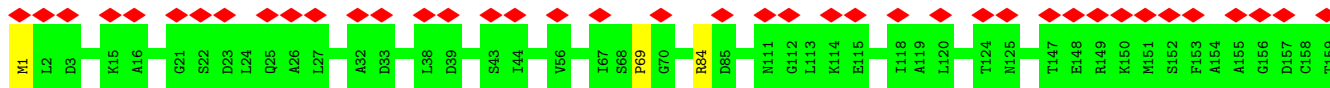


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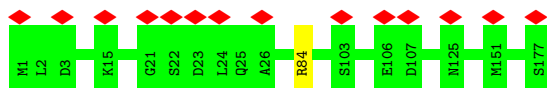




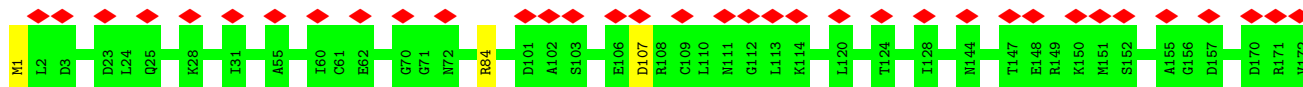
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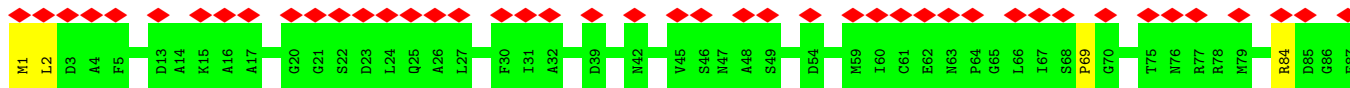
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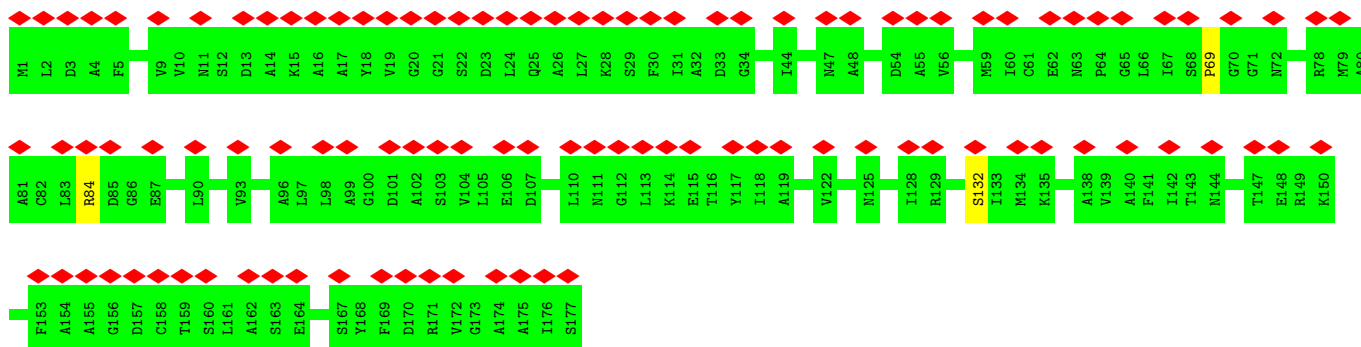


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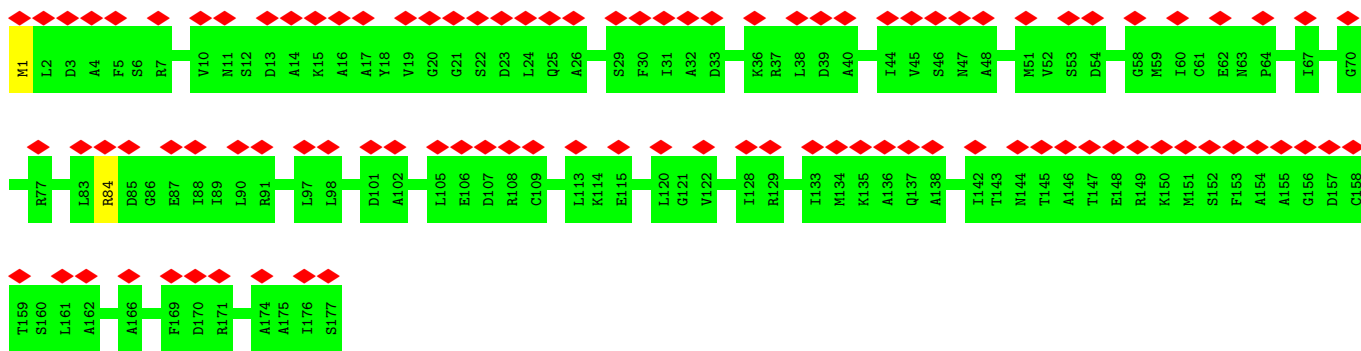


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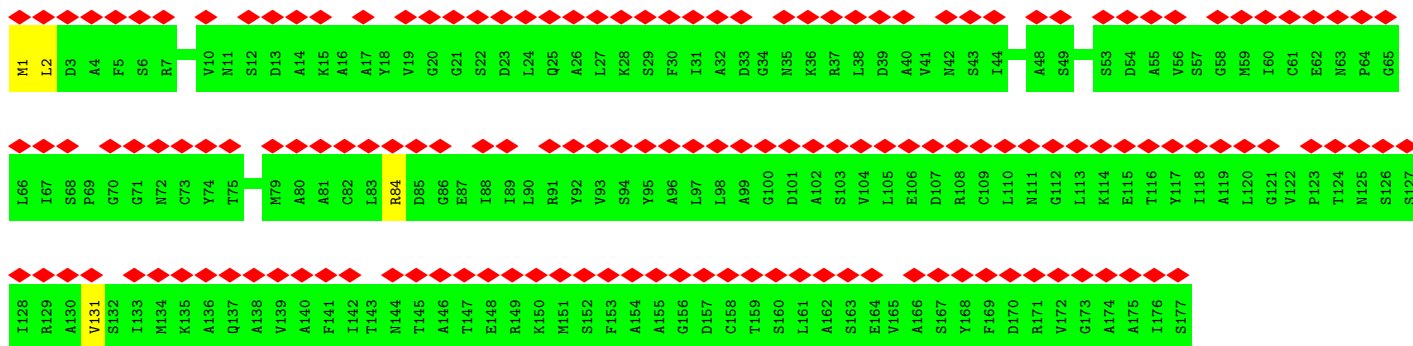
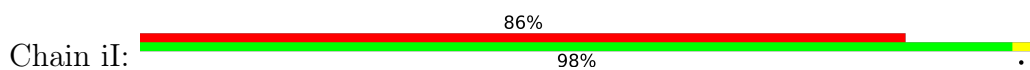




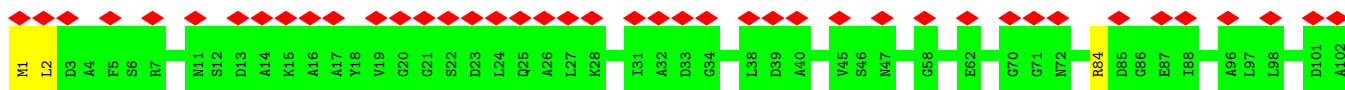
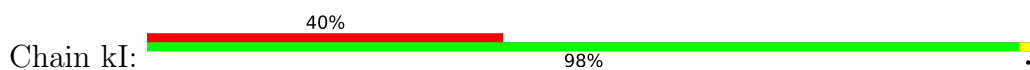
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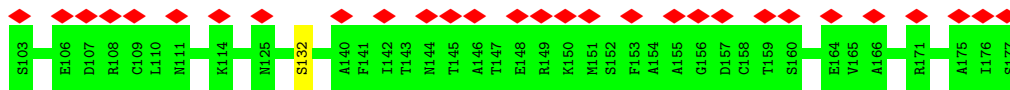


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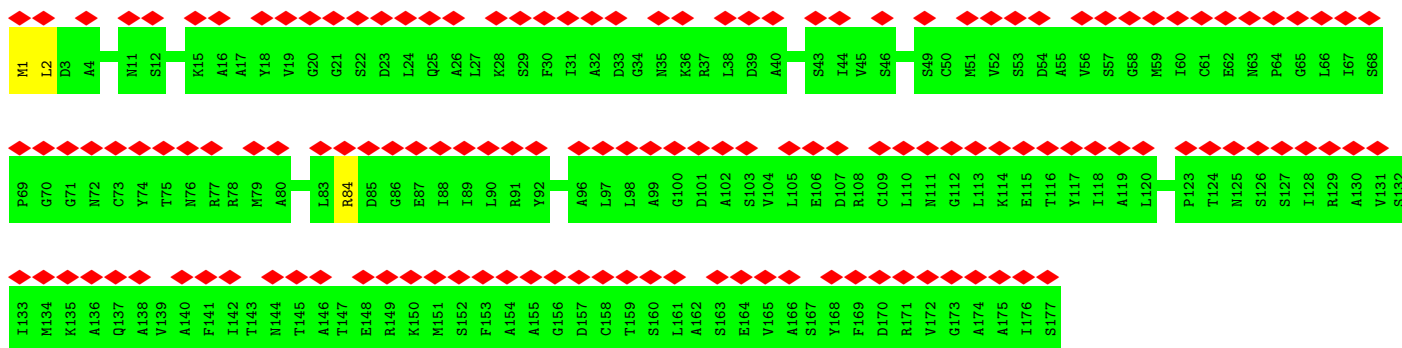
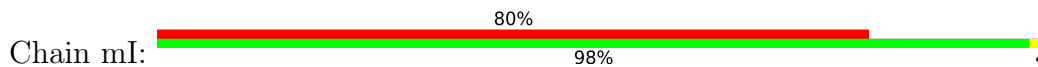


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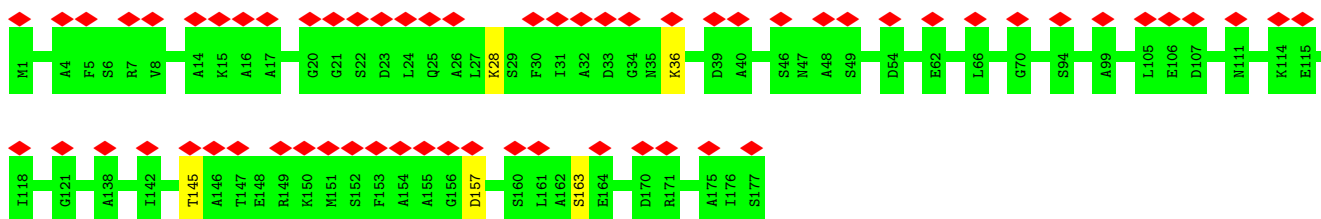




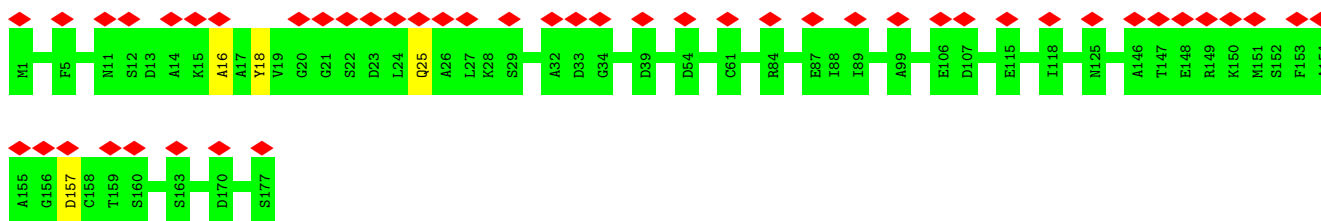
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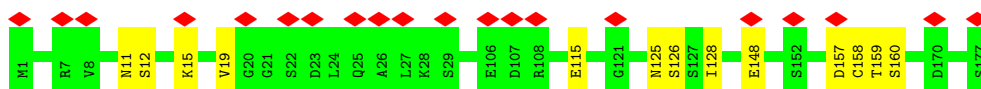
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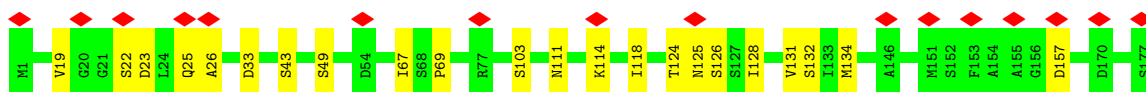
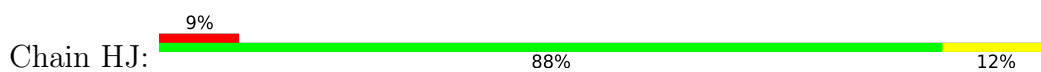
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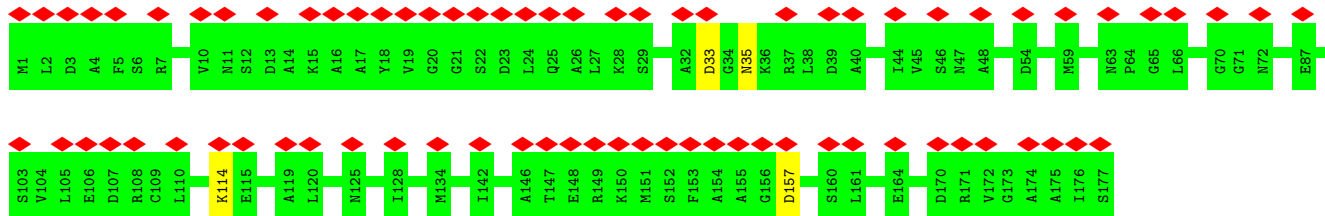
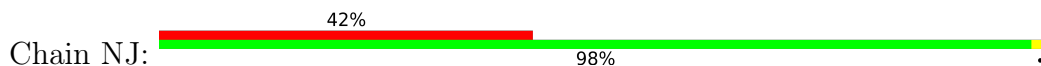
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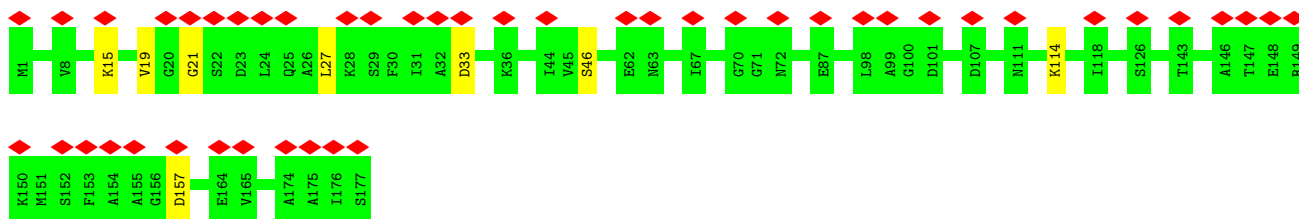
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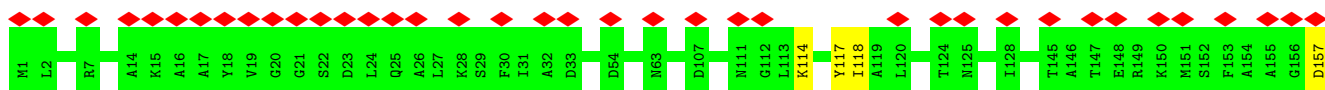
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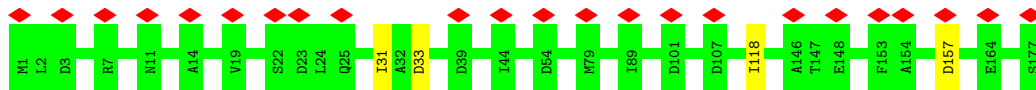


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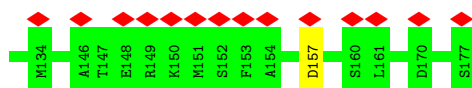
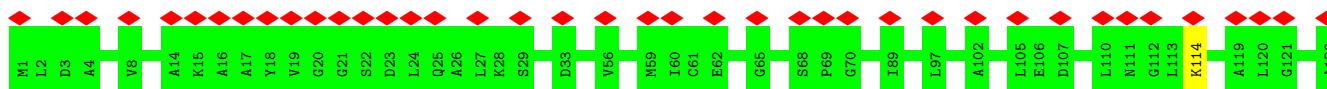




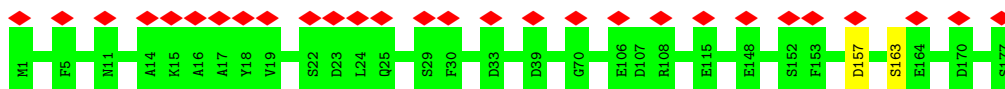
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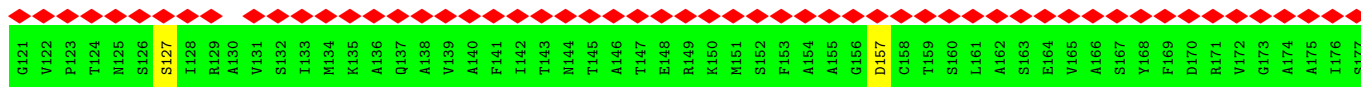
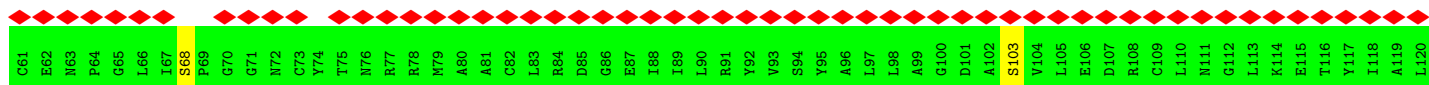
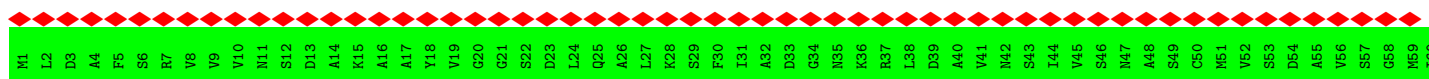
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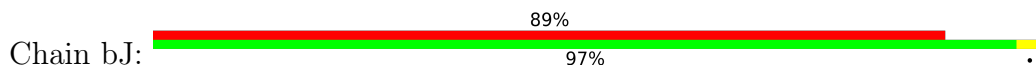
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- Molecule 7: B-phycoerythrin beta chain

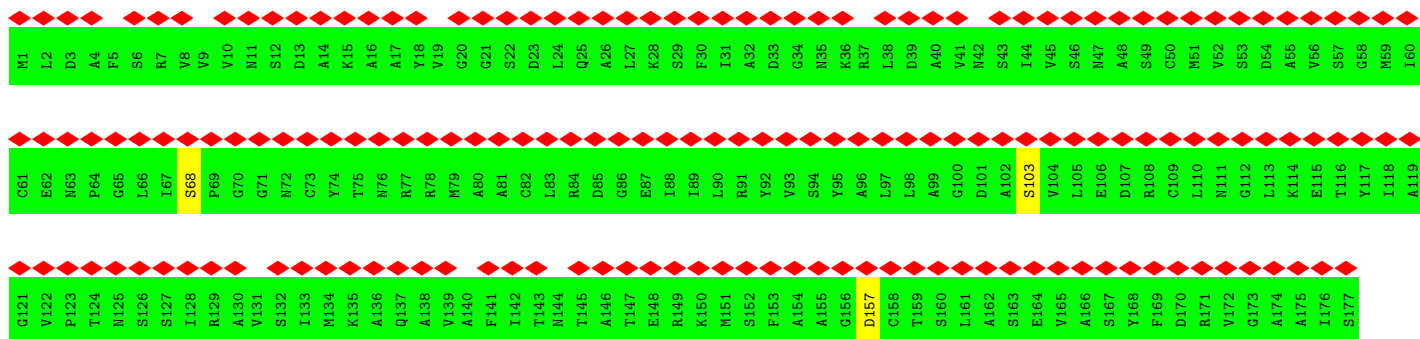


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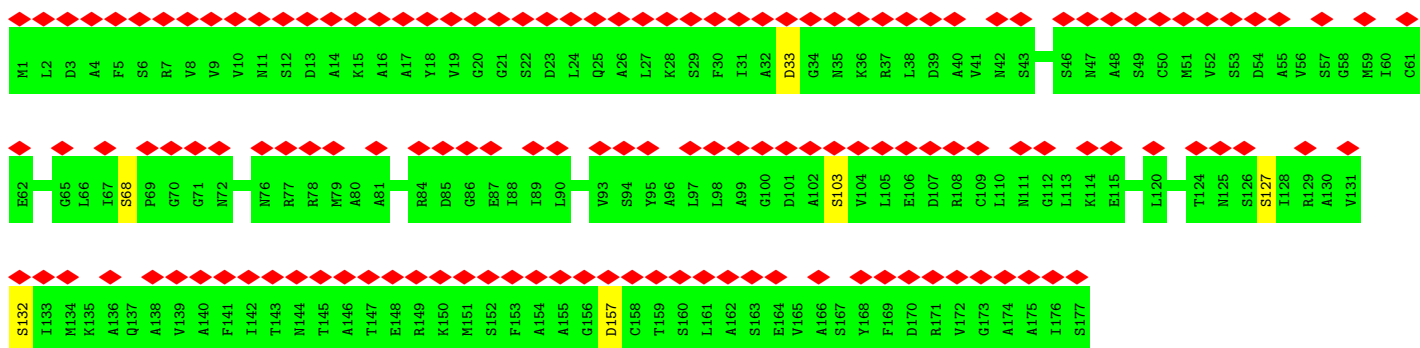
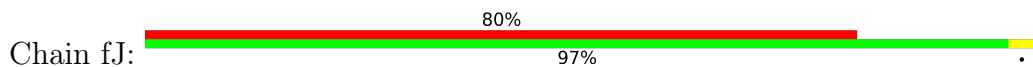




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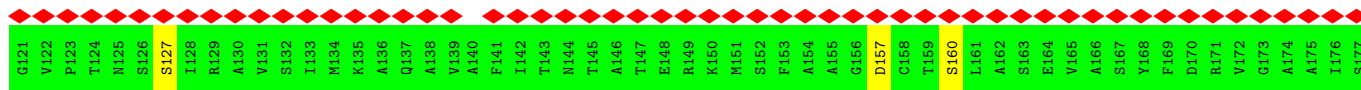


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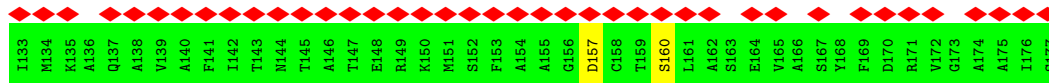
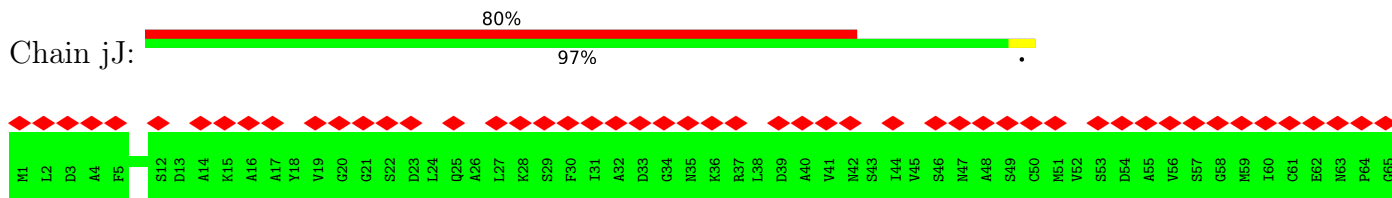


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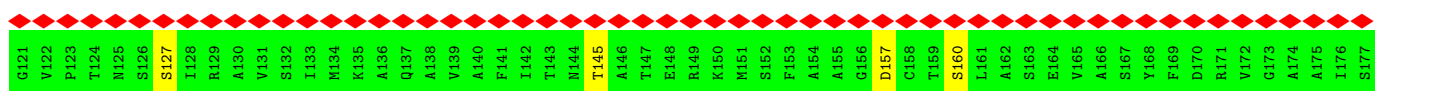
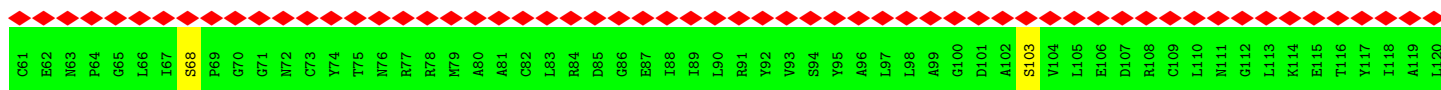
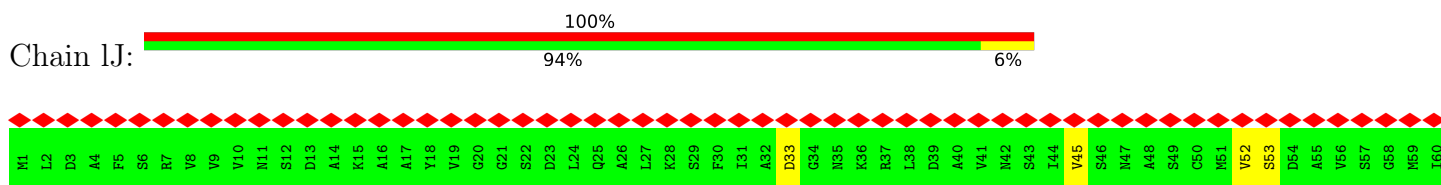




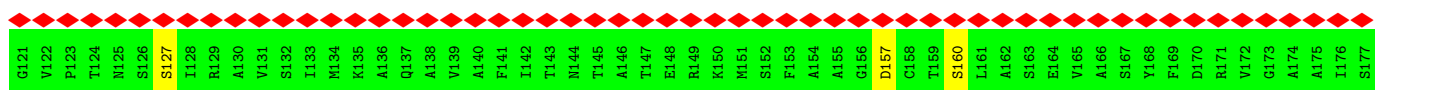
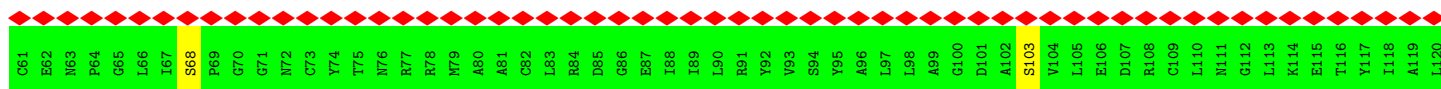
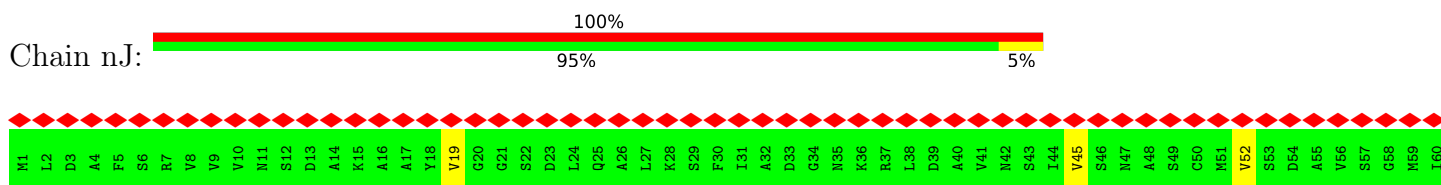
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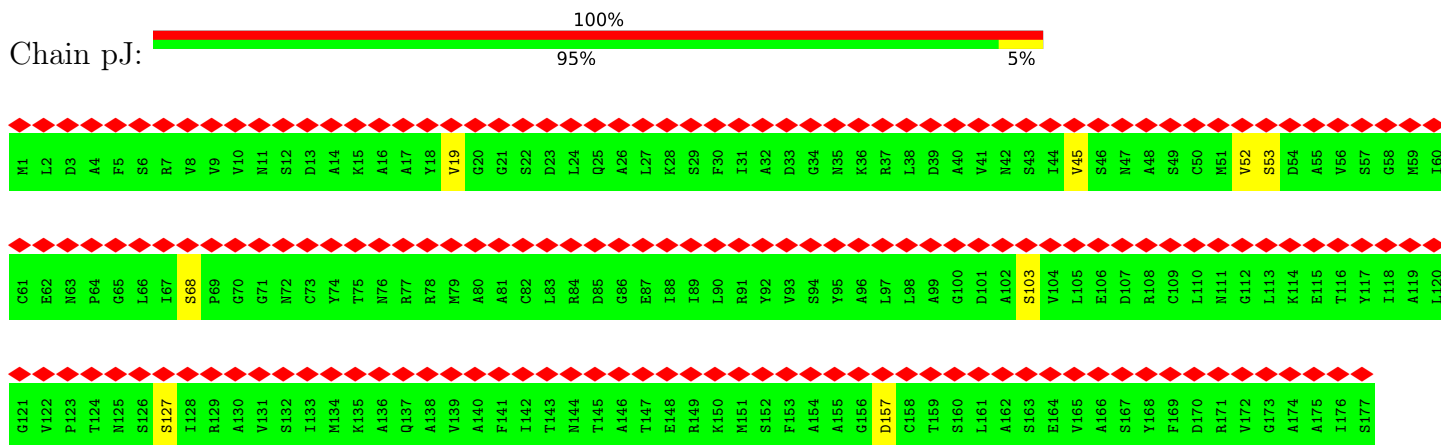
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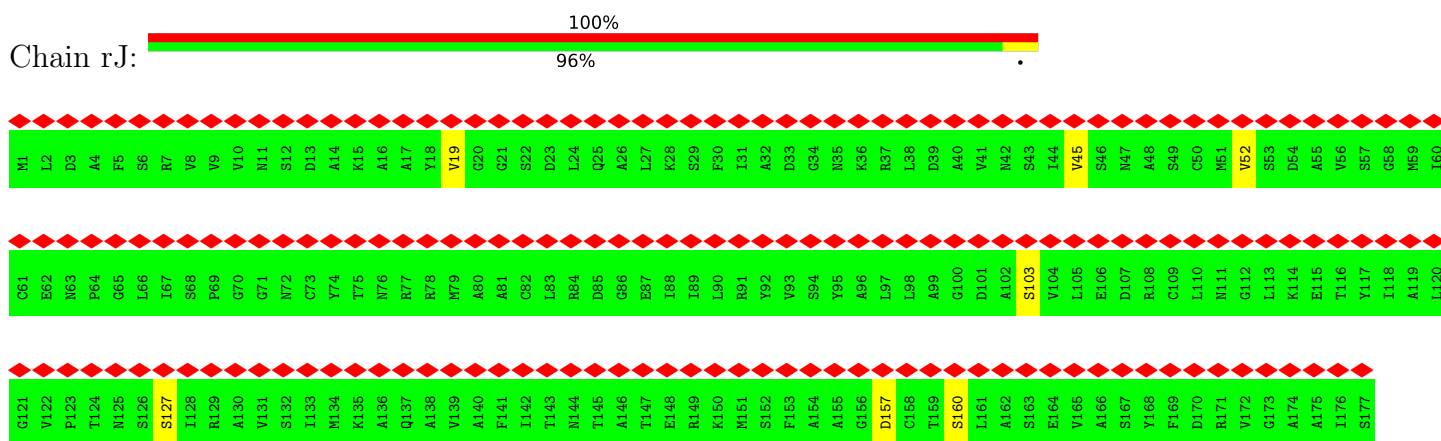
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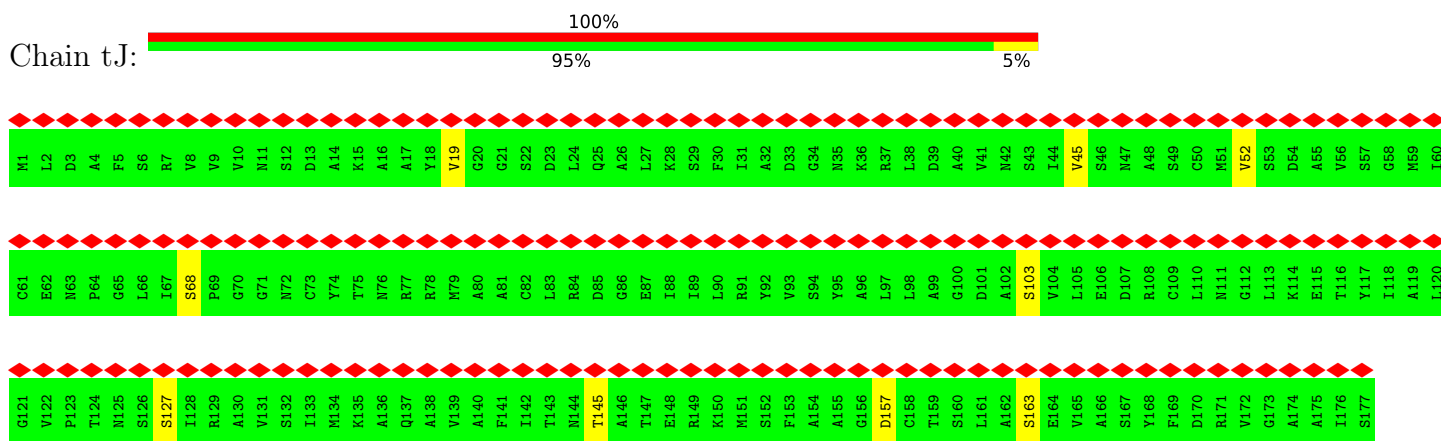
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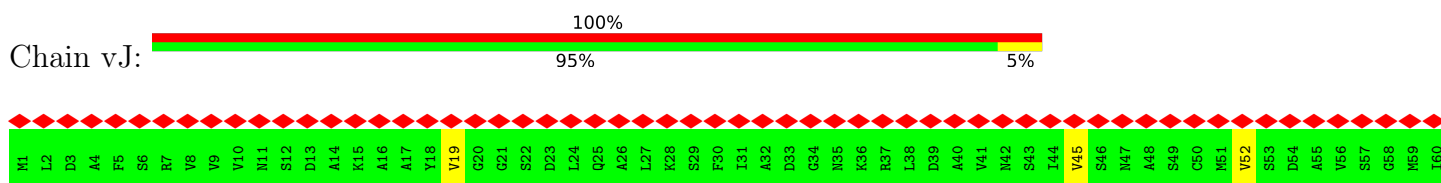
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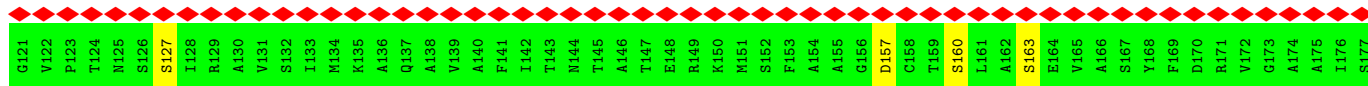
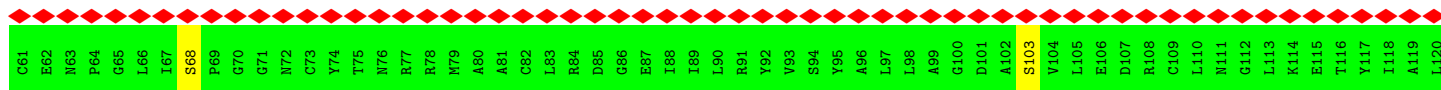


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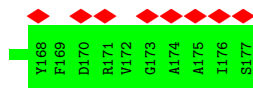
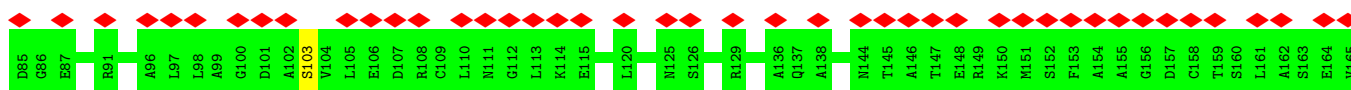


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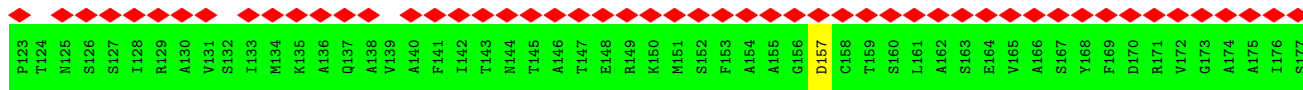
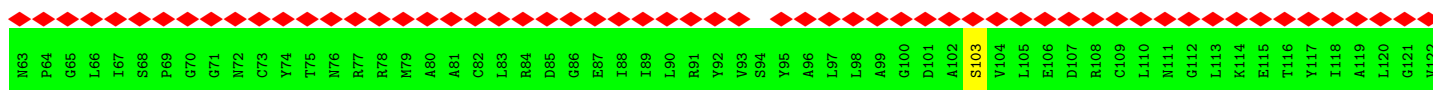
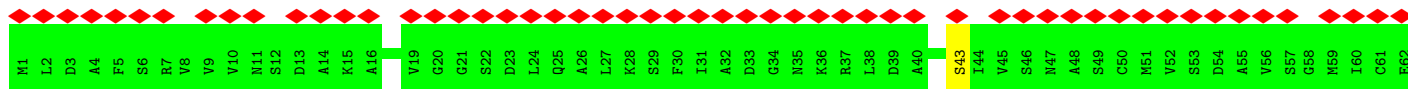




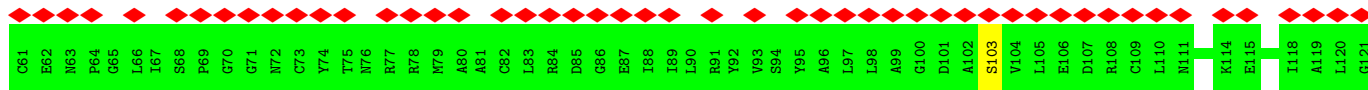
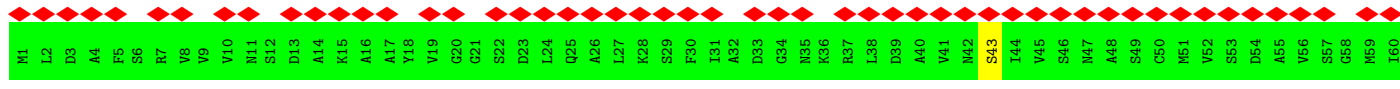
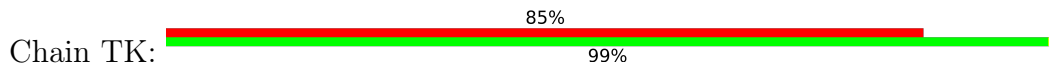
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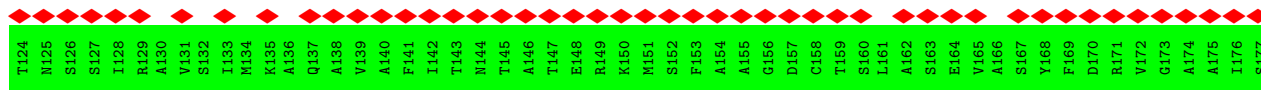


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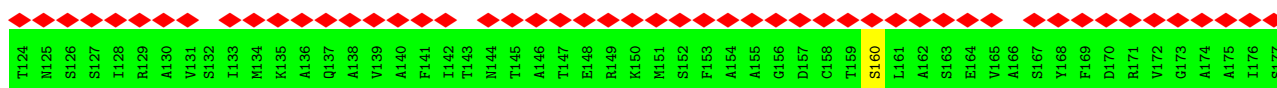
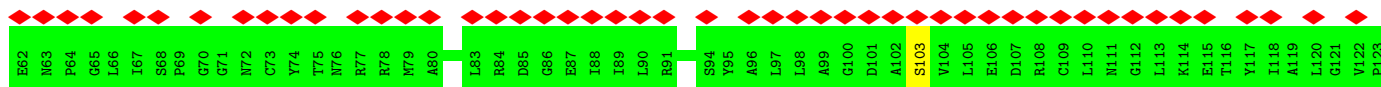
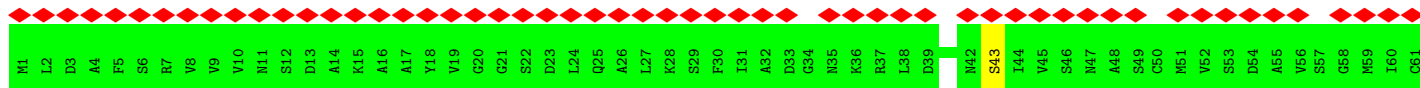


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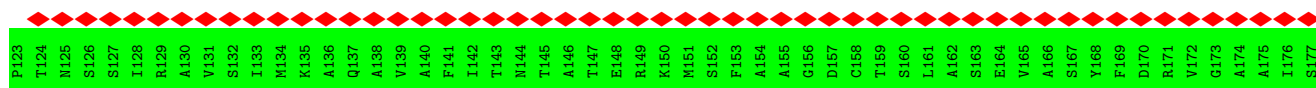
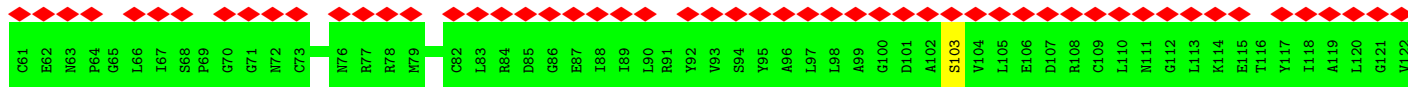
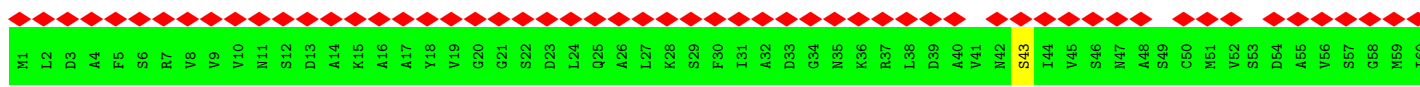




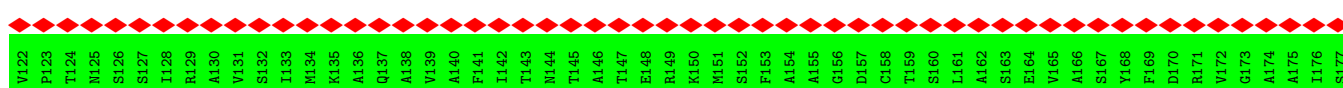
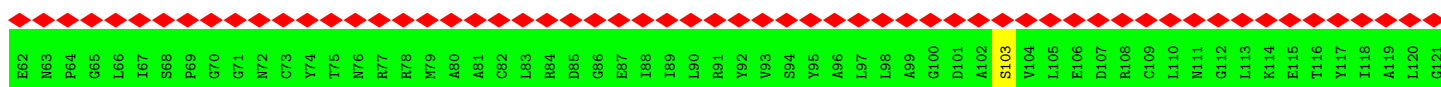
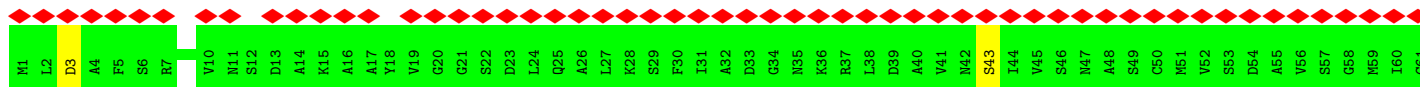
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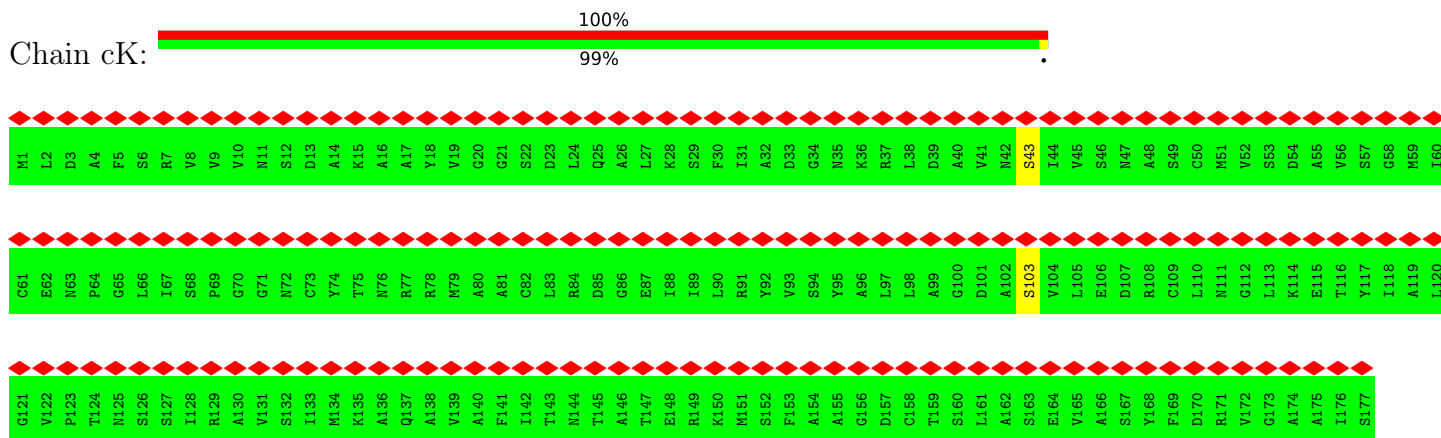
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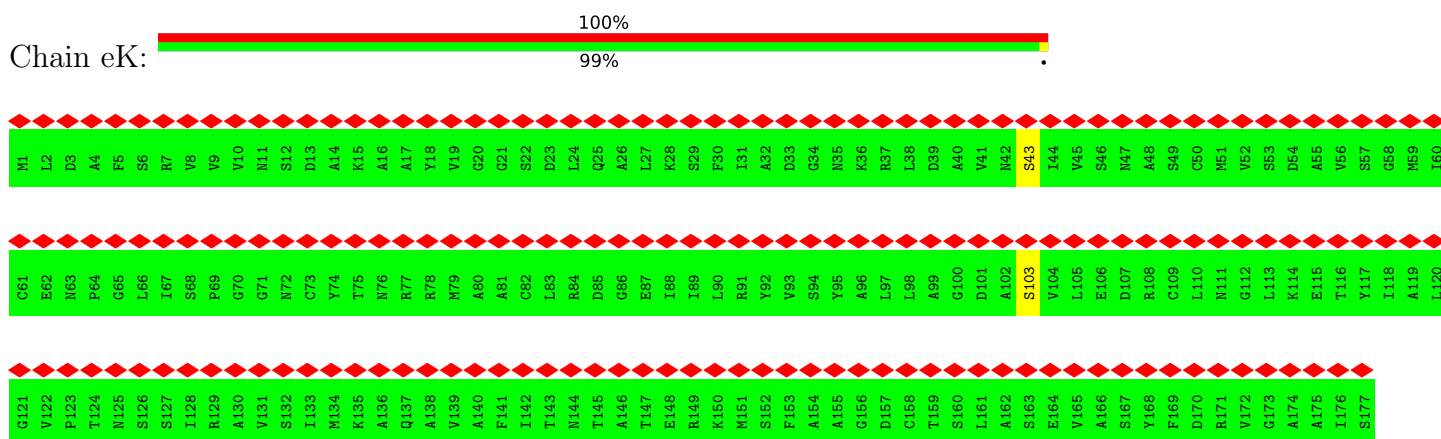
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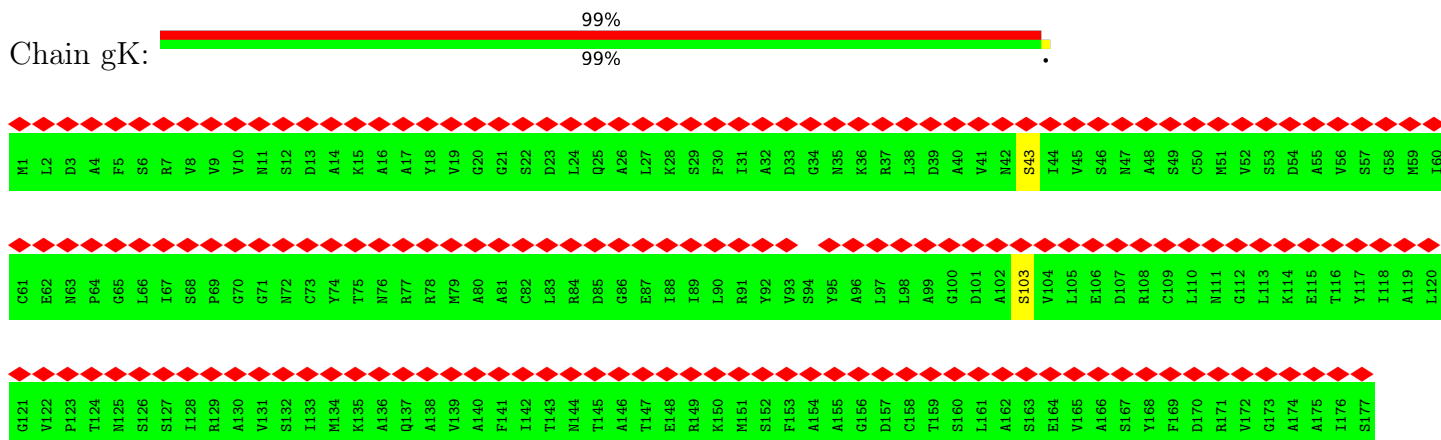
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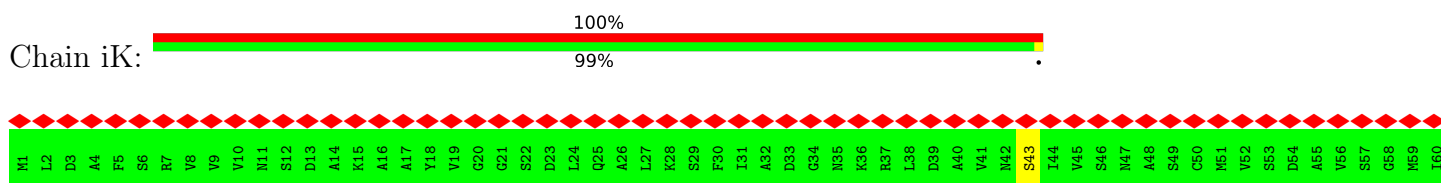
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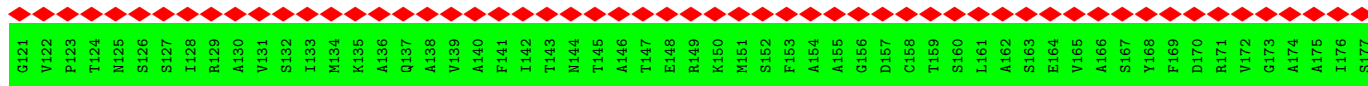
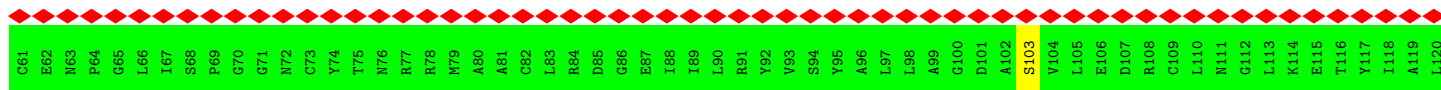


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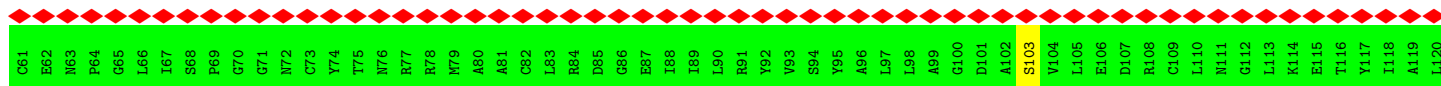


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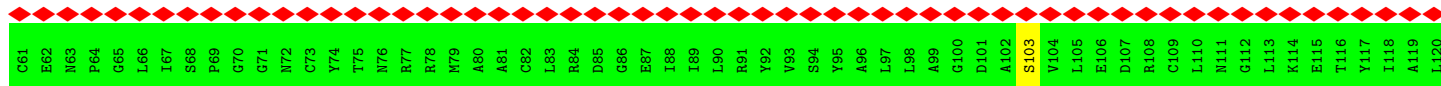




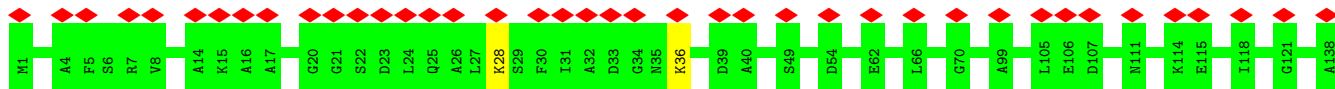
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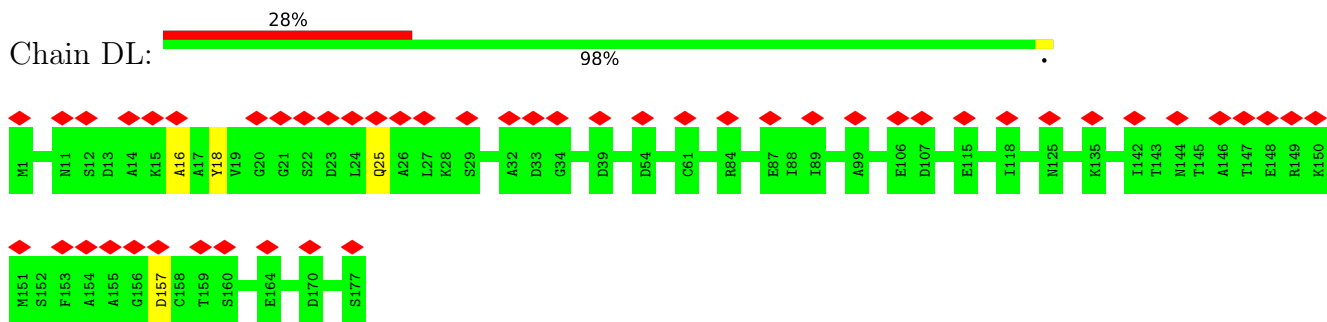
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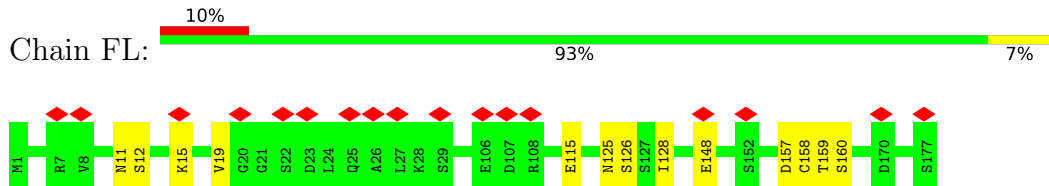
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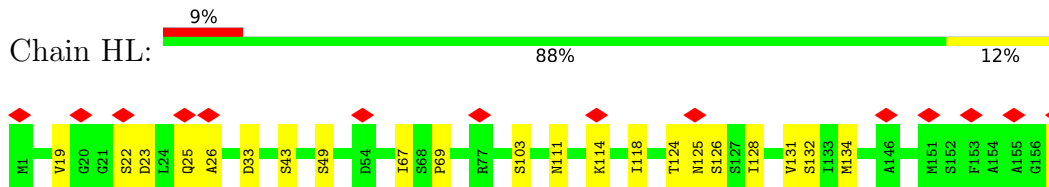
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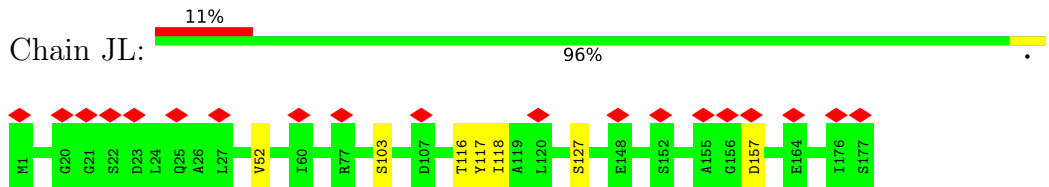
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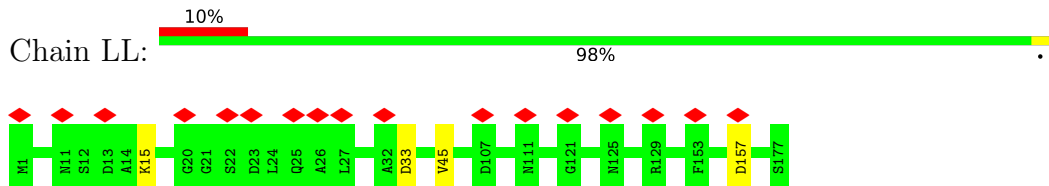
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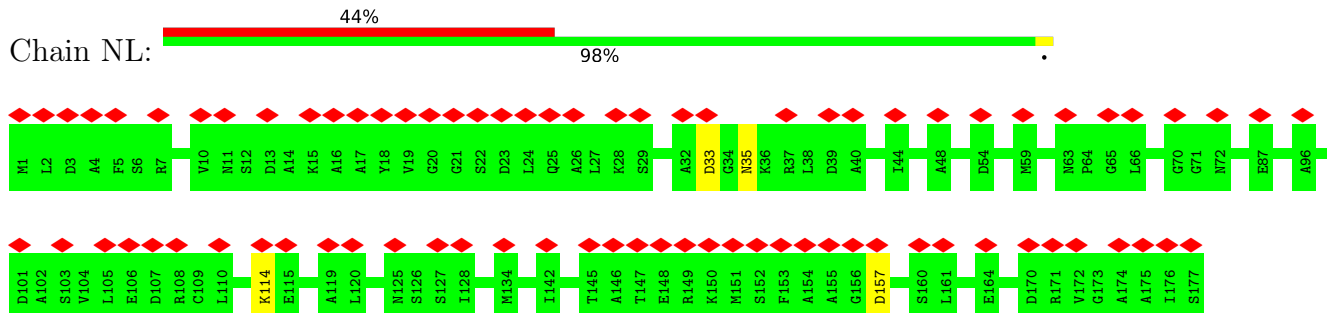
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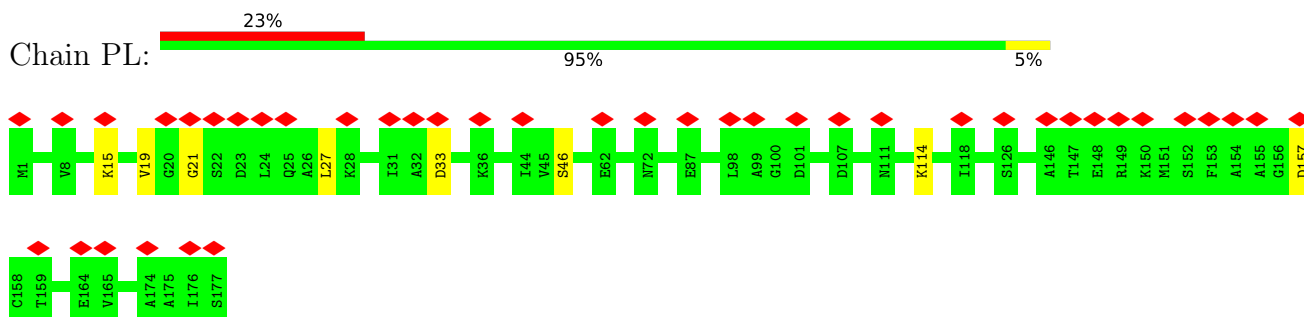
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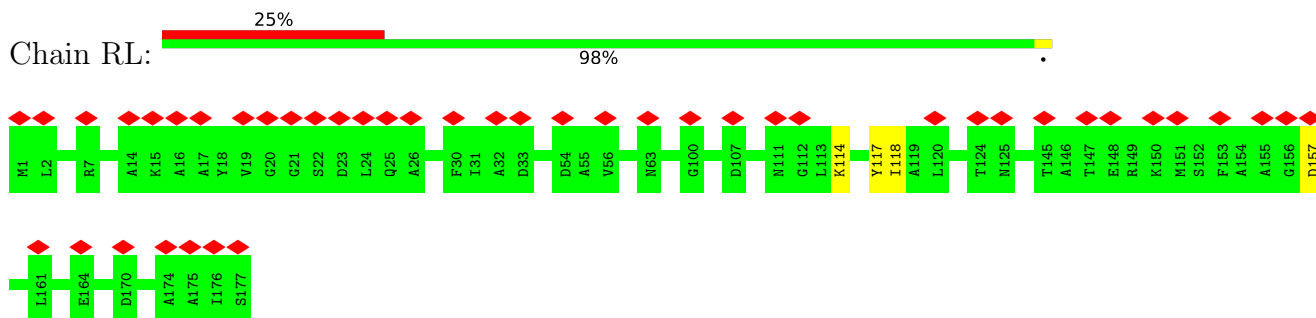
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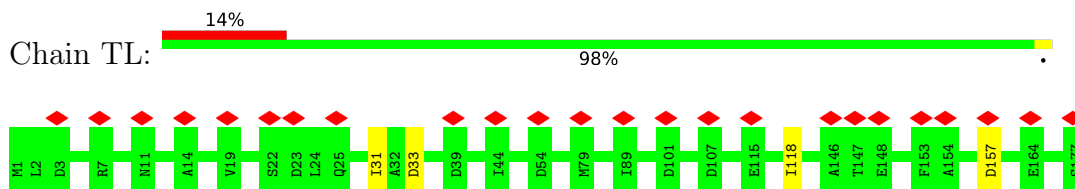
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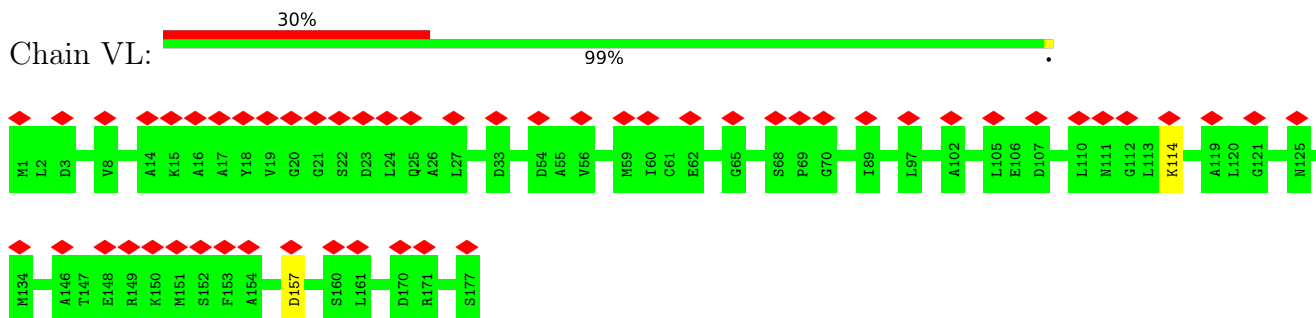
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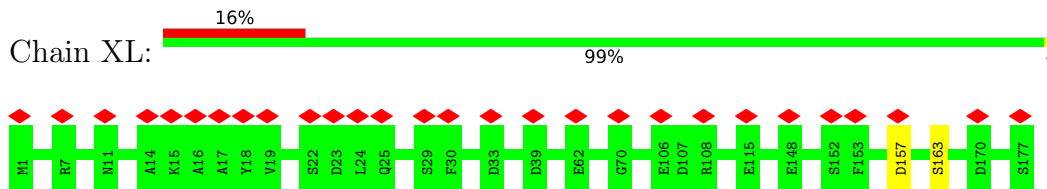
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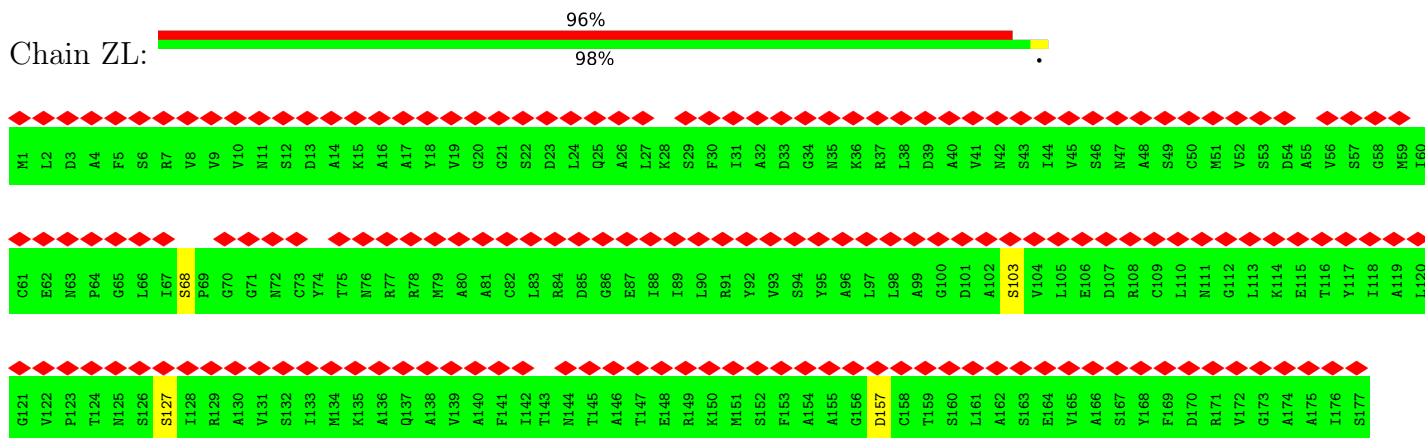
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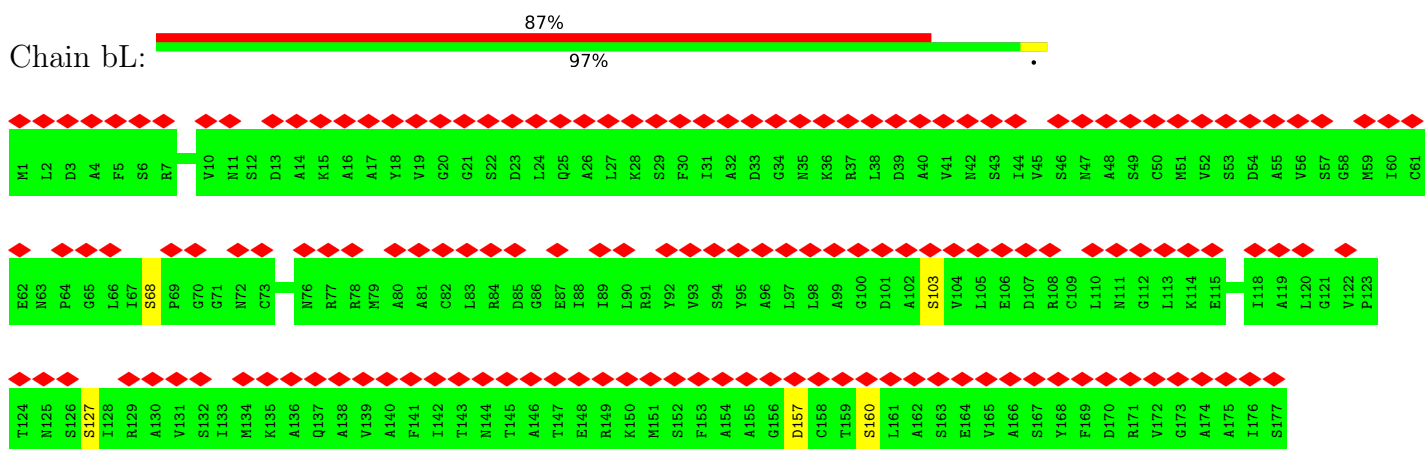
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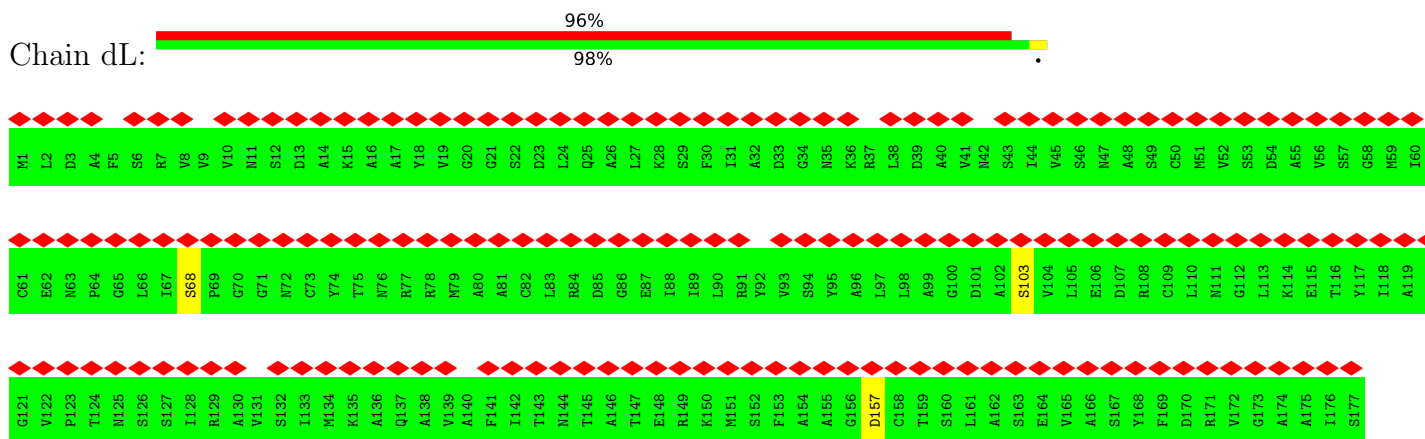
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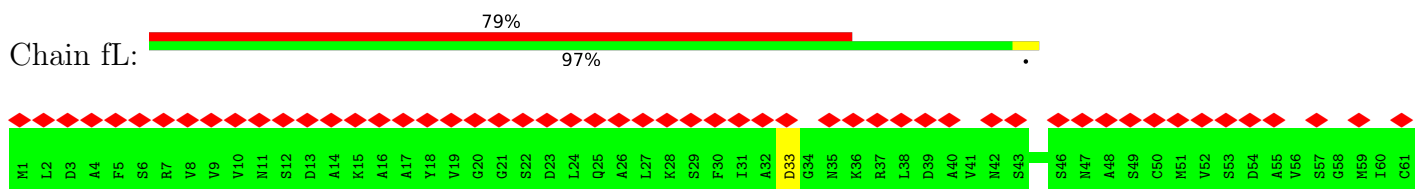
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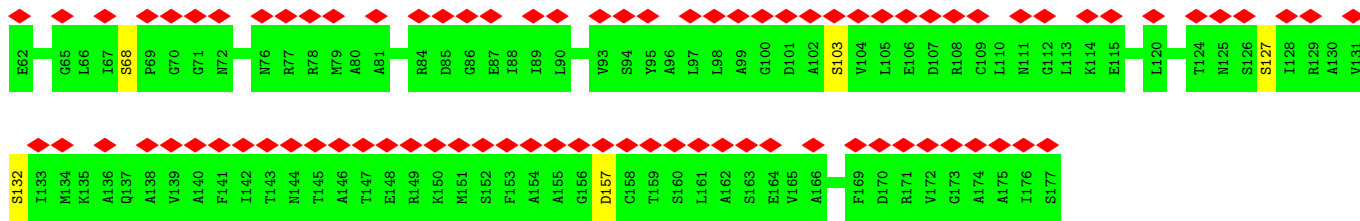


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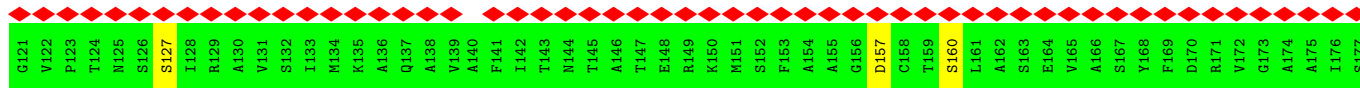
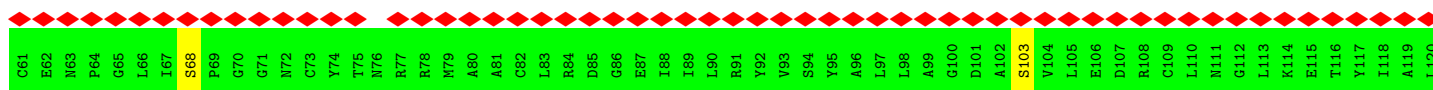
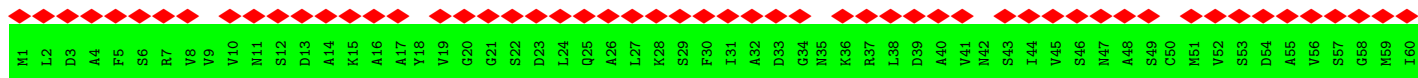


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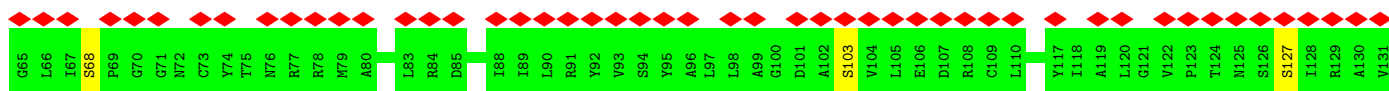
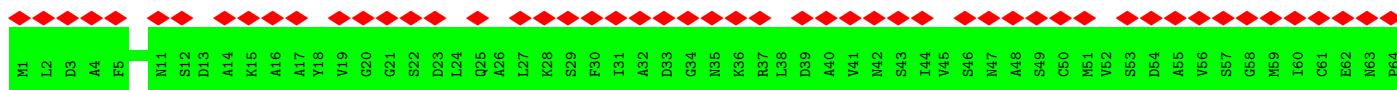
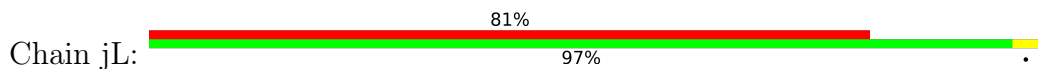




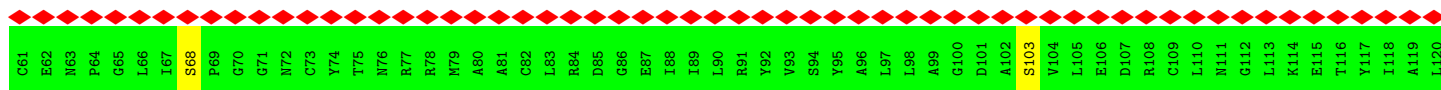
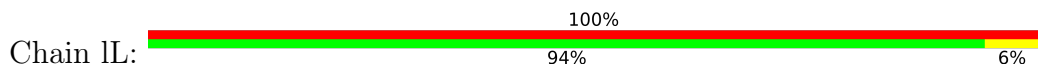
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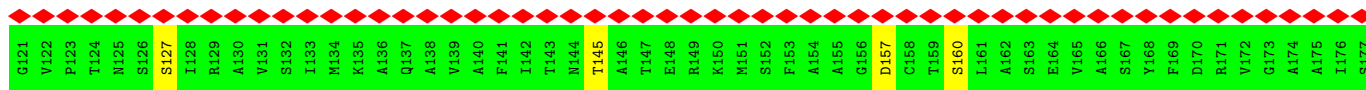


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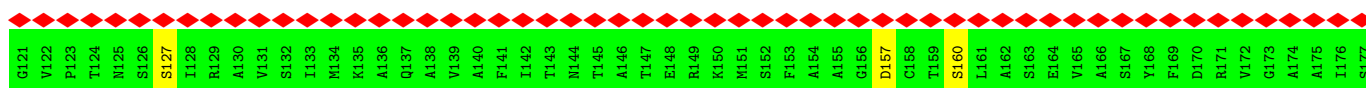
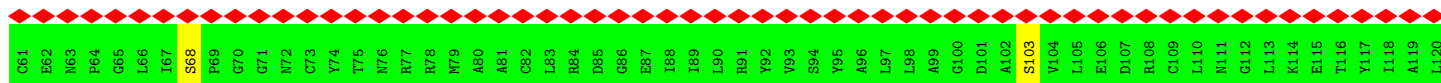
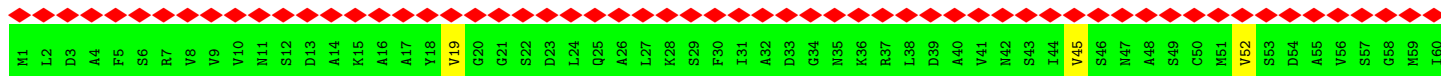


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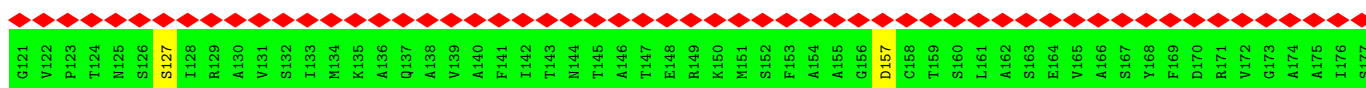
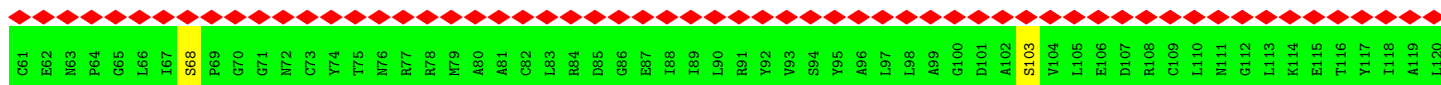




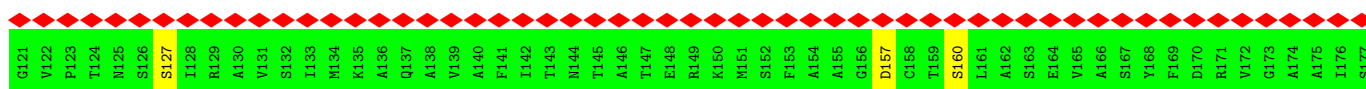
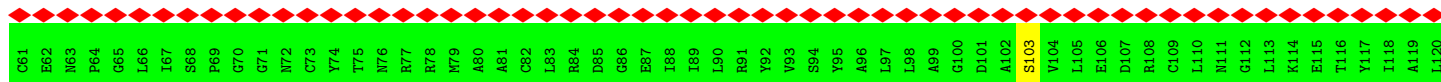
• Molecule 7: B-phycoerythrin beta chain



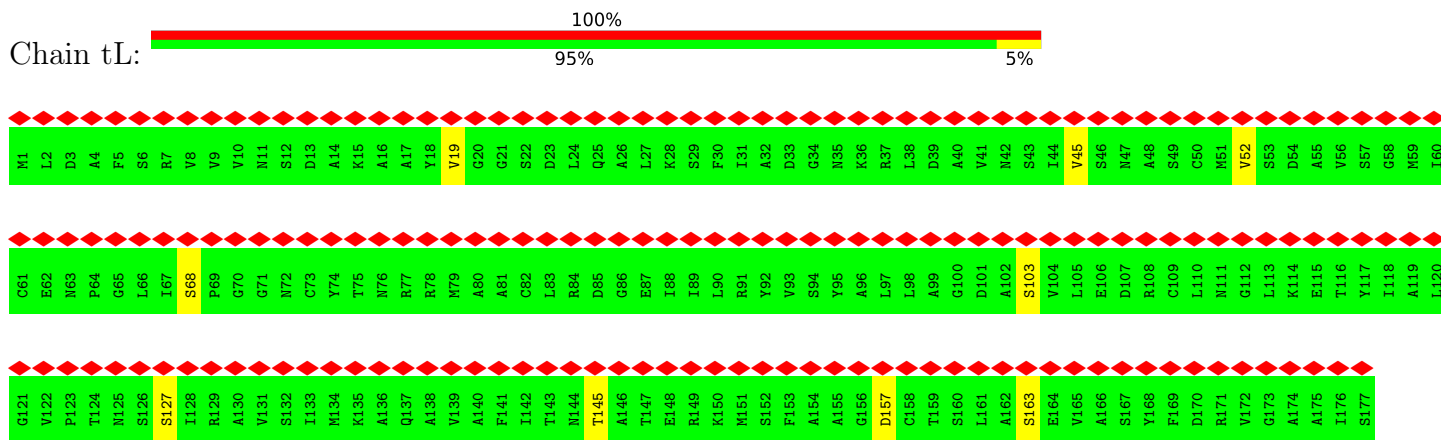
• Molecule 7: B-phycoerythrin beta chain



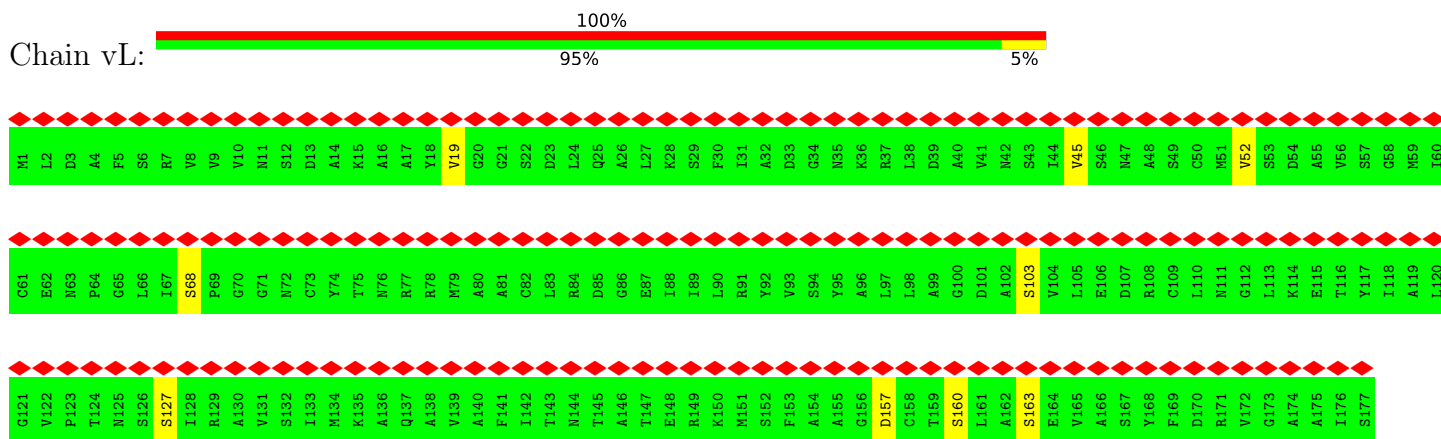
• Molecule 7: B-phycoerythrin beta chain



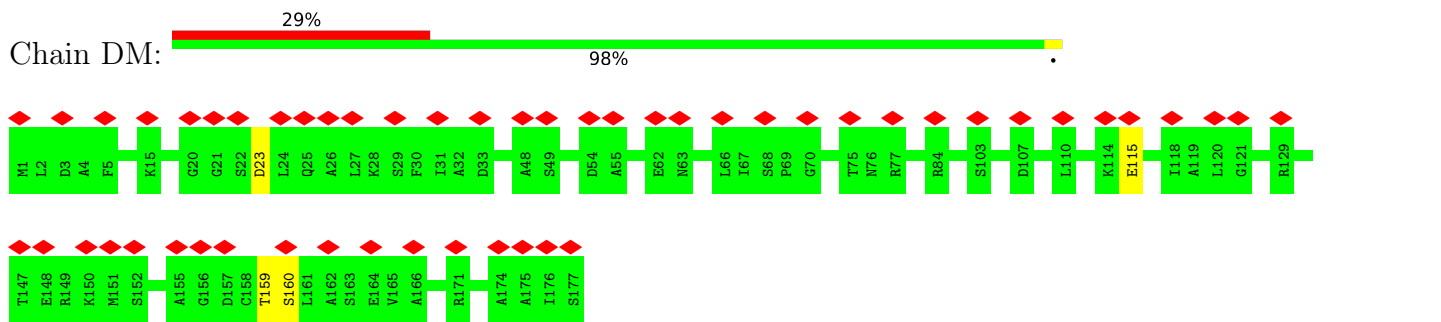
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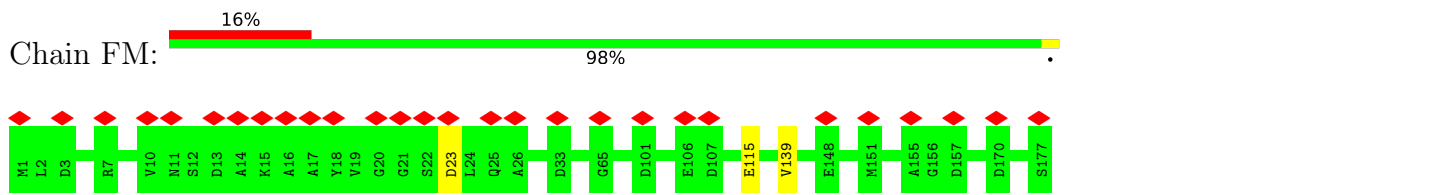
• Molecule 7: B-phycoerythrin beta chain



• Molecule 7: B-phycoerythrin beta chain

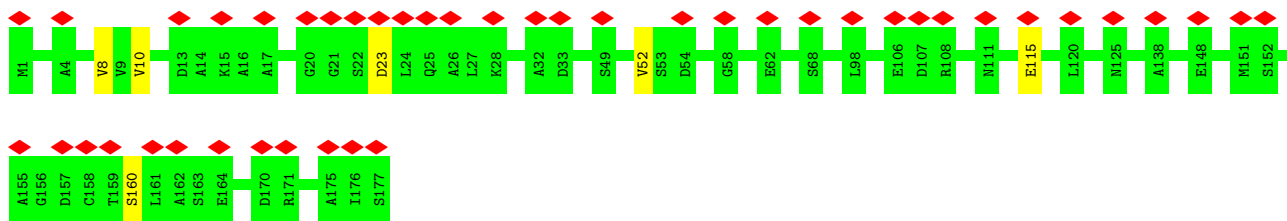


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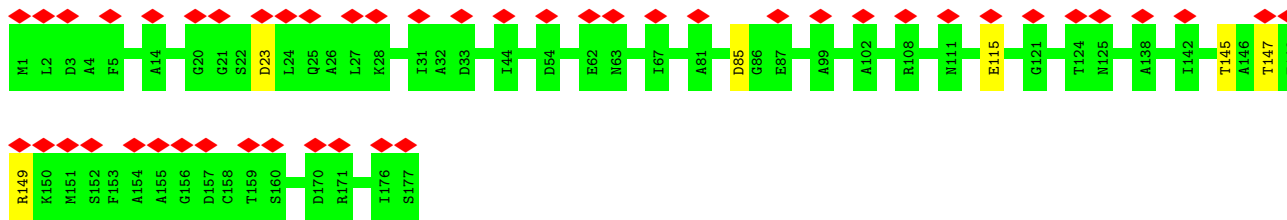


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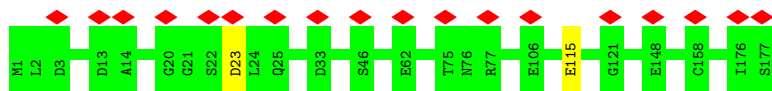




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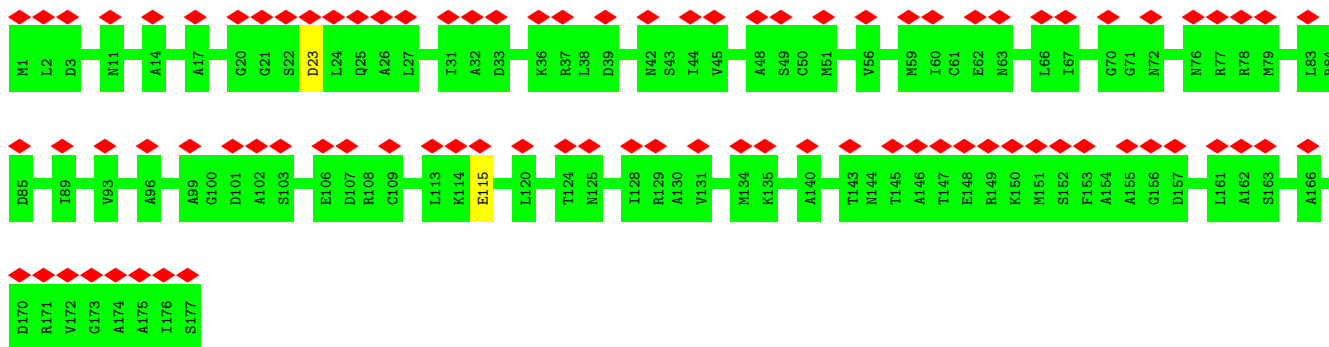
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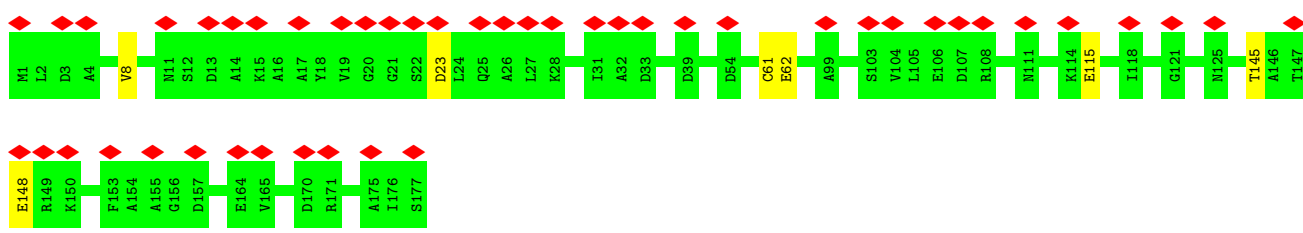
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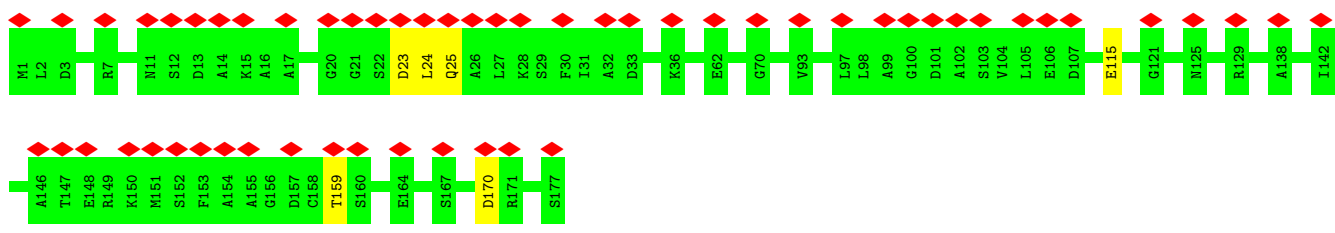
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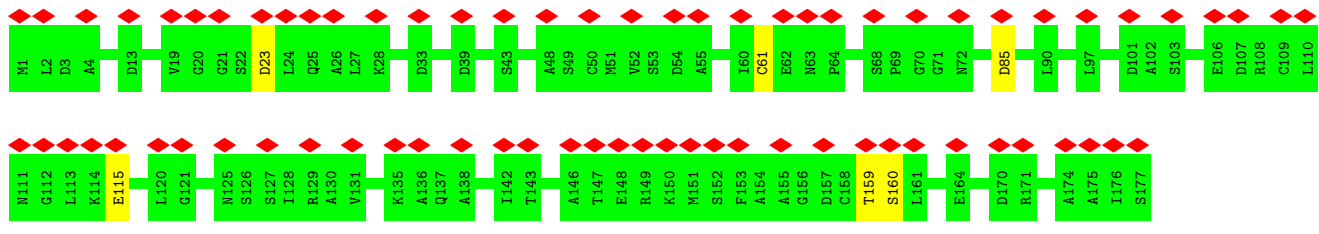
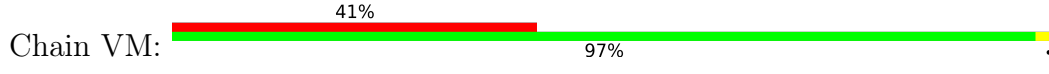
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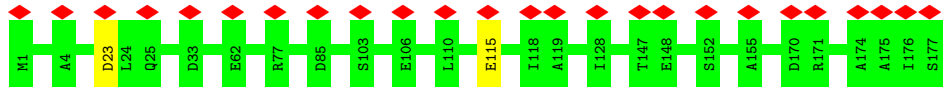
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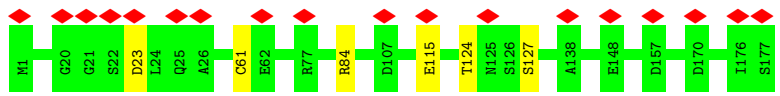
• Molecule 7: B-phycoerythrin beta chain



• Molecule 7: B-phycoerythrin beta chain

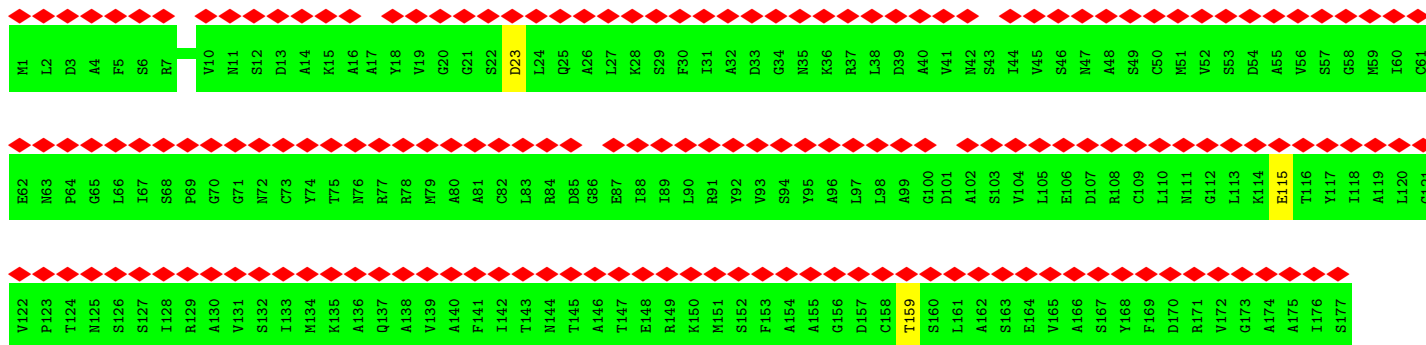


• Molecule 7: B-phycoerythrin beta chain

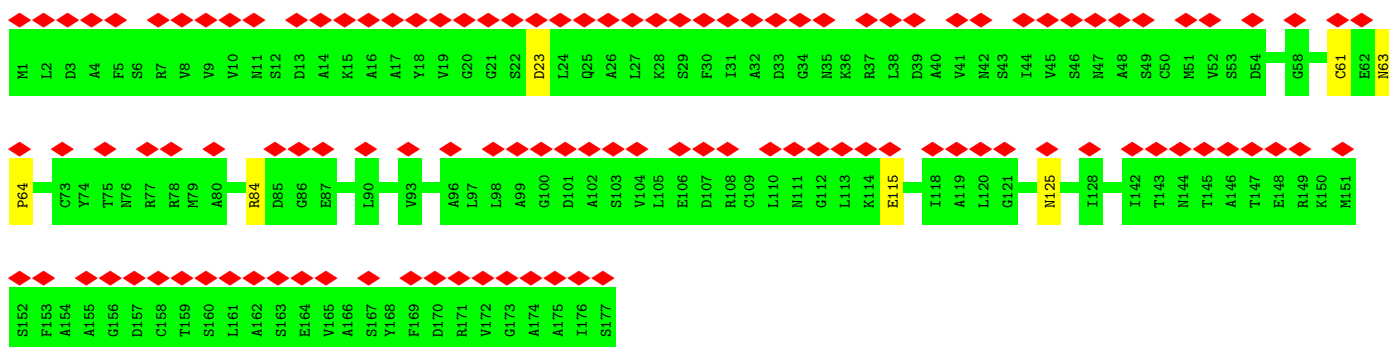


• Molecule 7: B-phycoerythrin beta chain

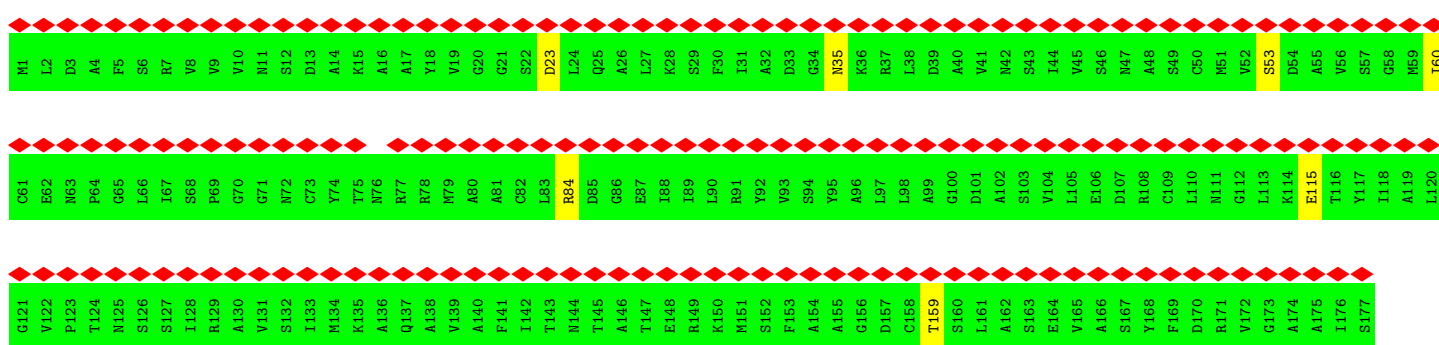




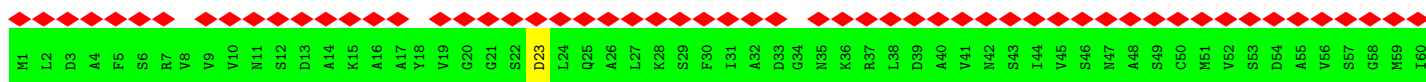
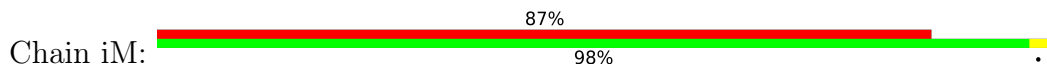
• Molecule 7: B-phycoerythrin beta chain

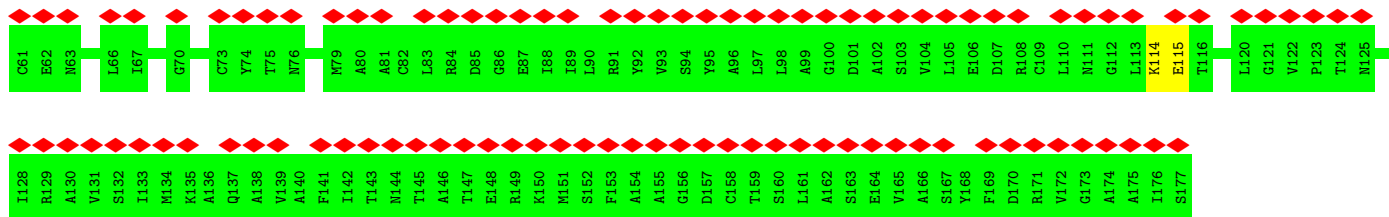


• Molecule 7: B-phycoerythrin beta chain

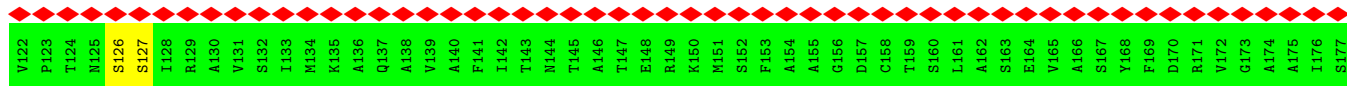
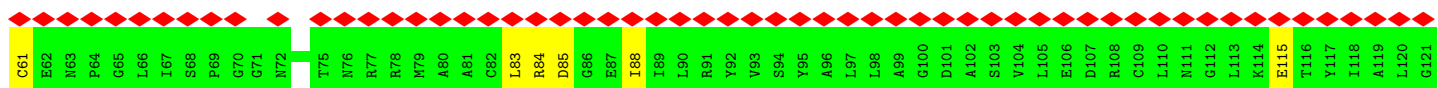
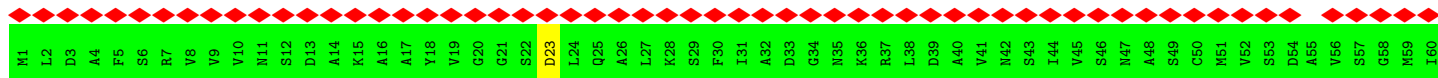


• Molecule 7: B-phycoerythrin beta chain

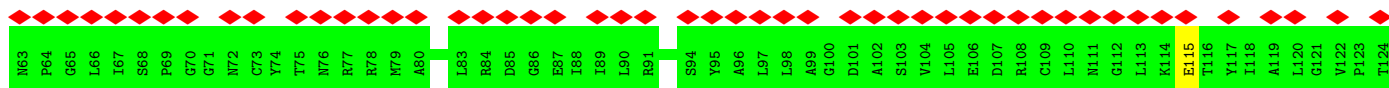
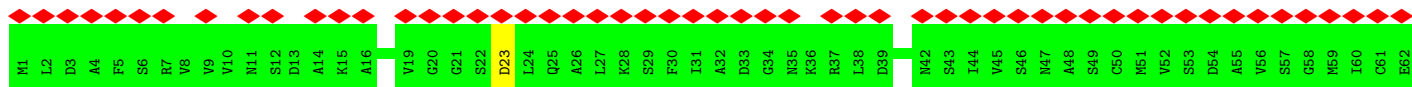




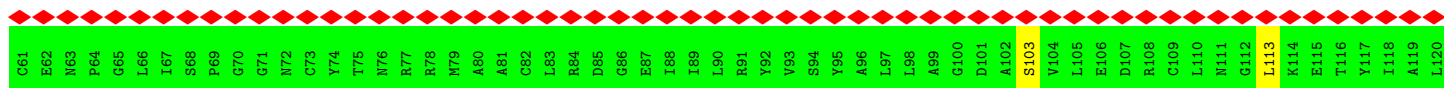
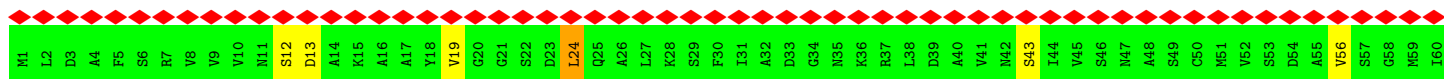
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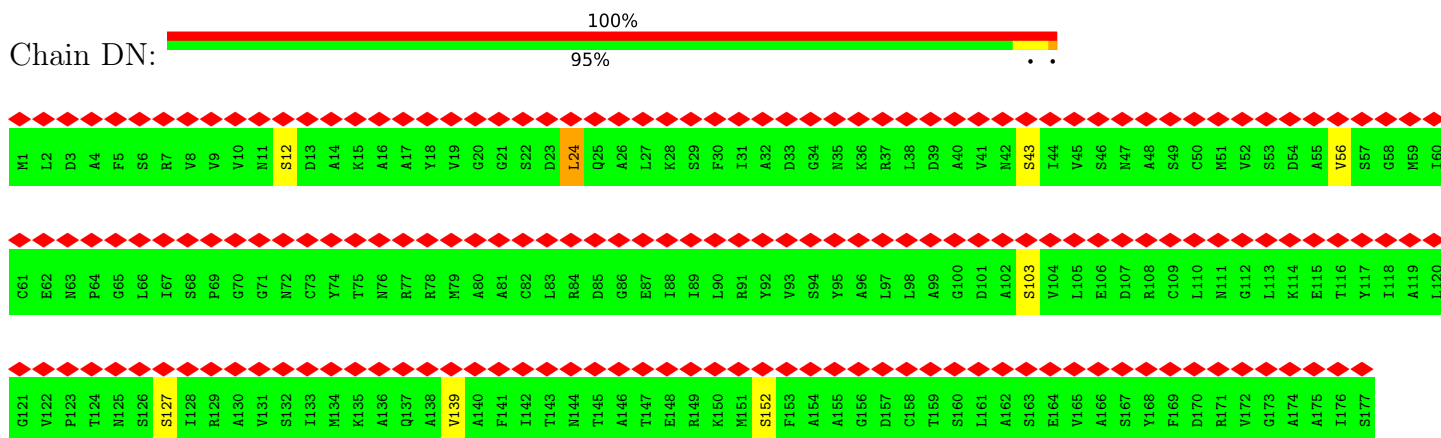
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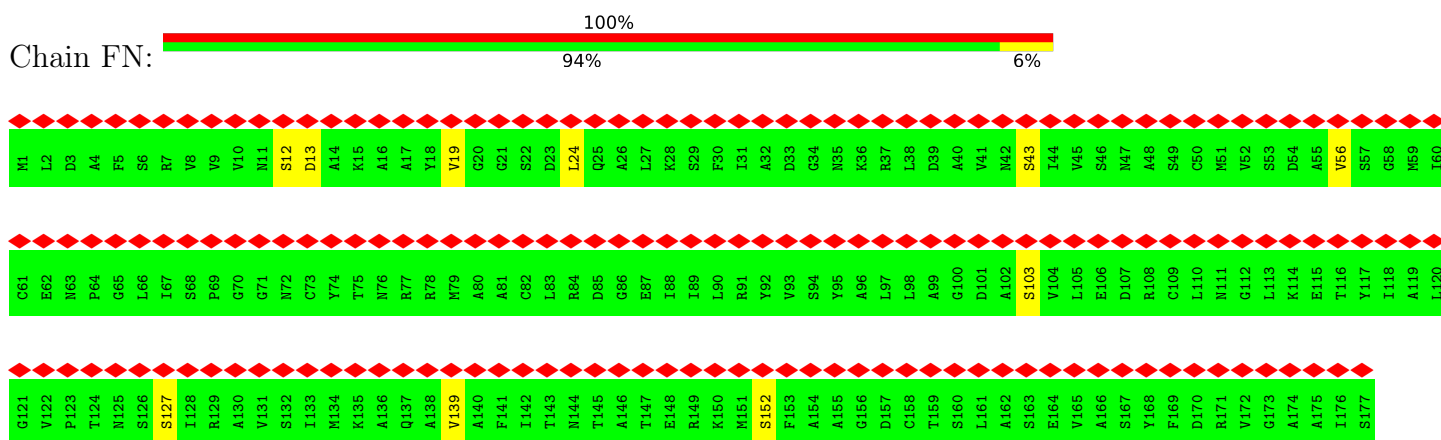
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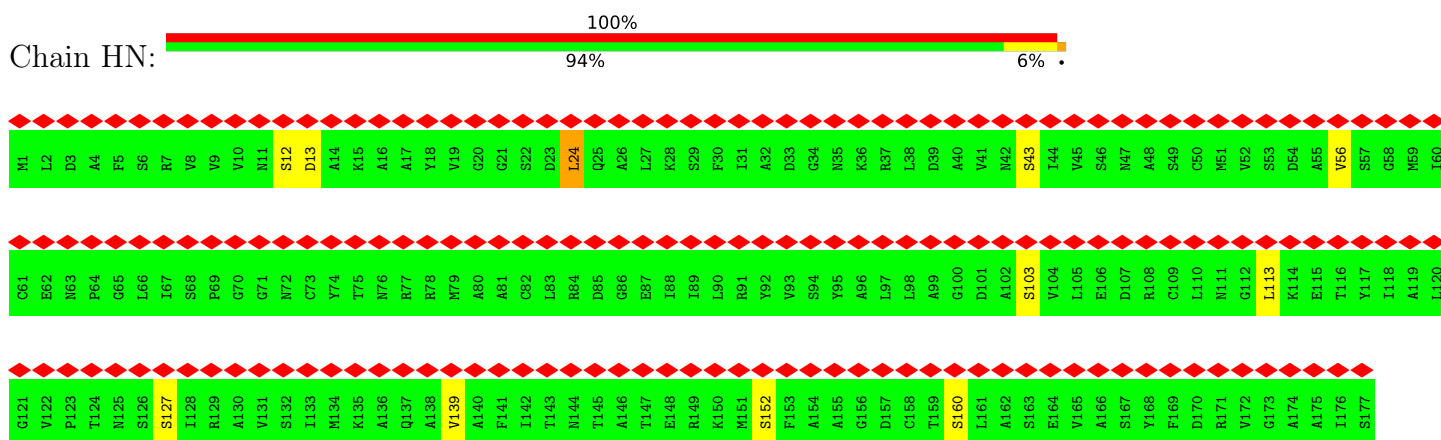
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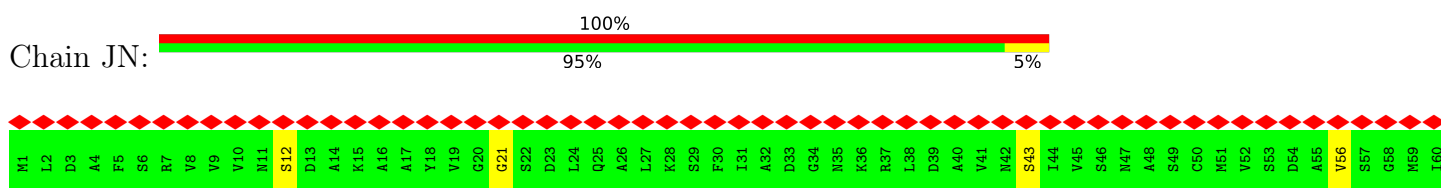
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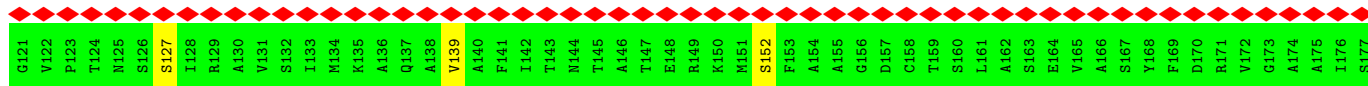
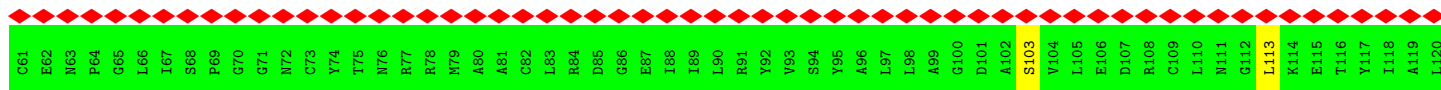


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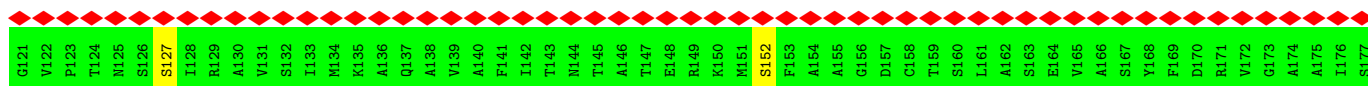
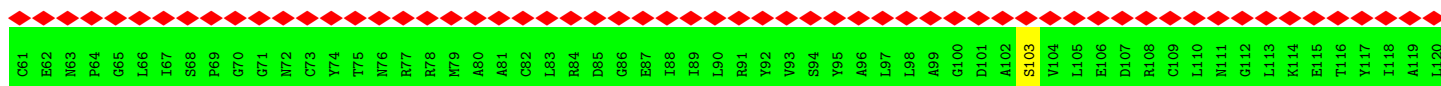


• Molecule 7: B-phycoerythrin beta chain





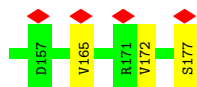
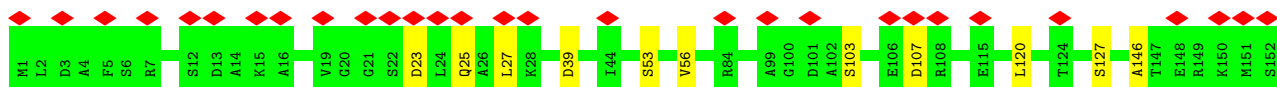
• Molecule 7: B-phycoerythrin beta chain



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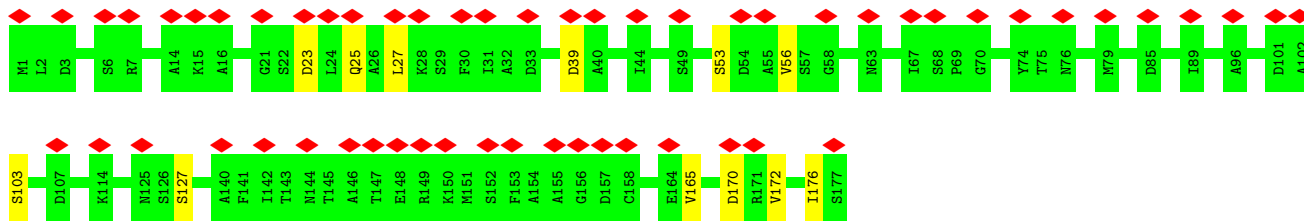


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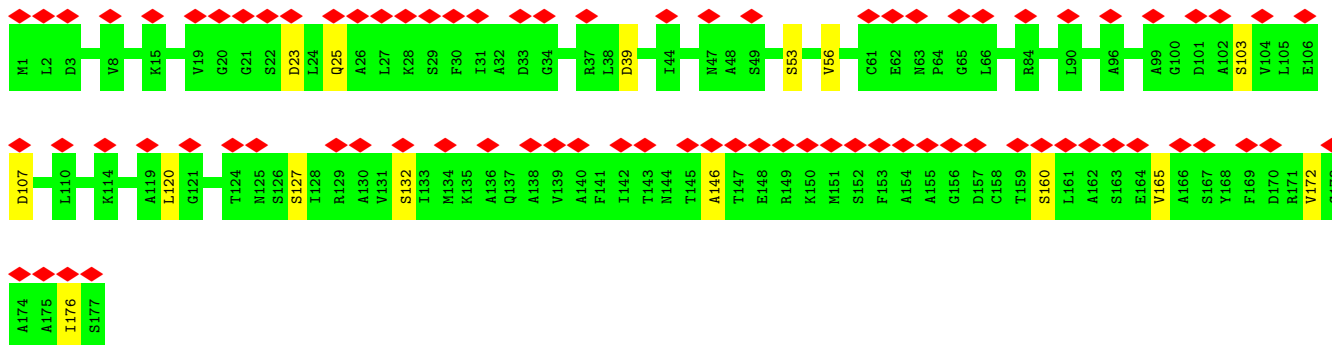


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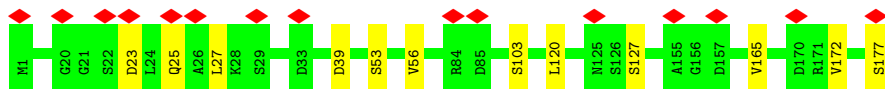




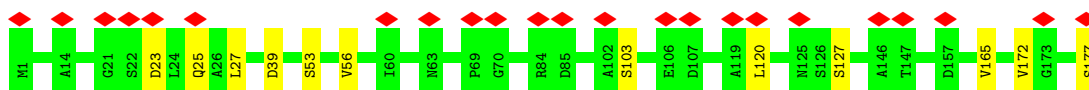
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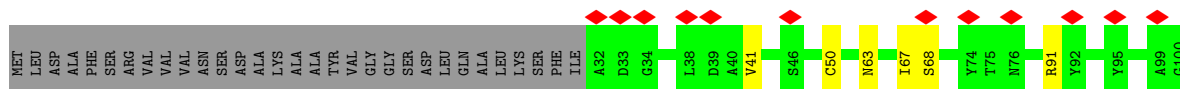
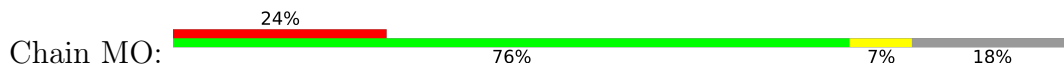
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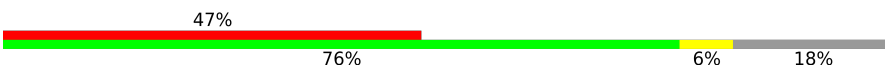
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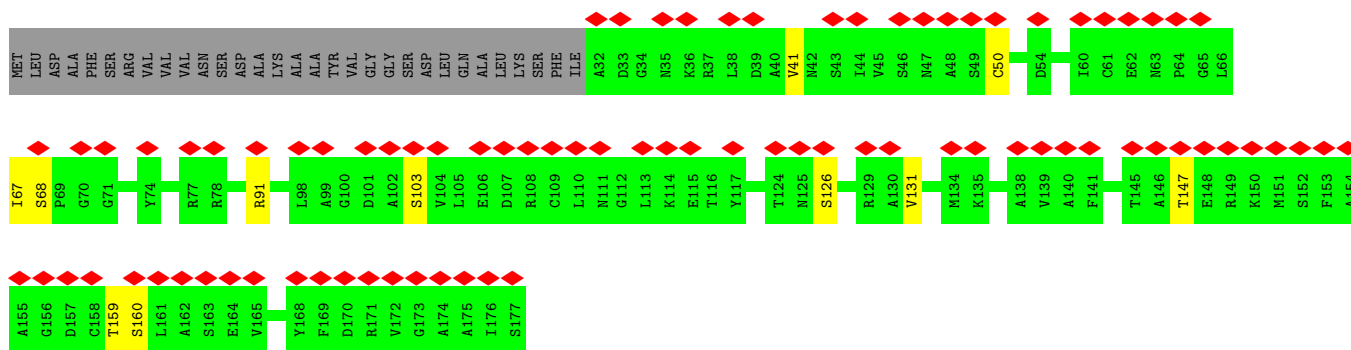


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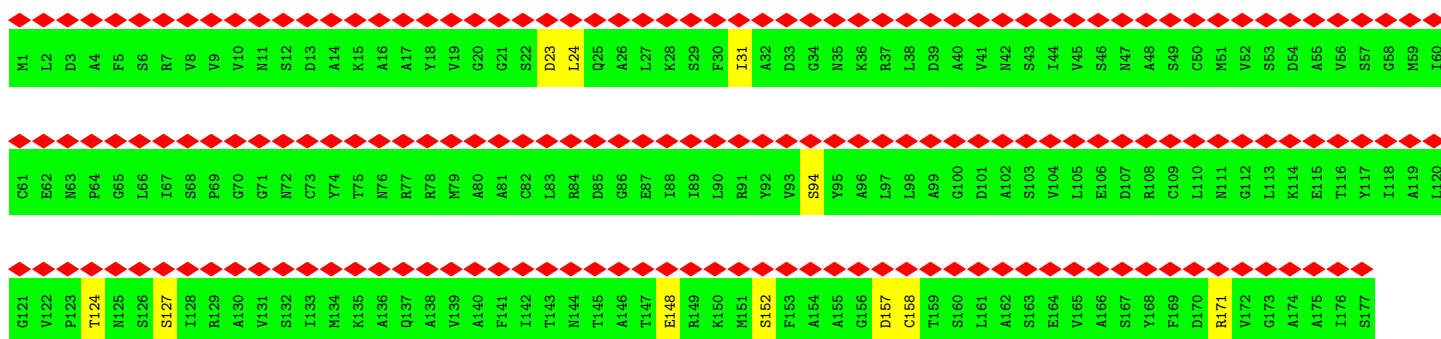
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Chain NO: 



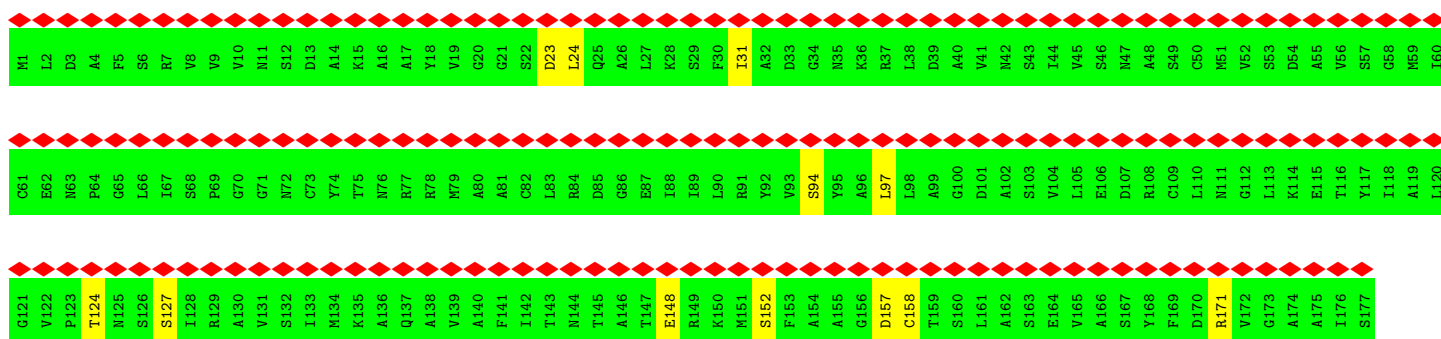
• Molecule 7: B-phycoerythrin beta chain

Chain BQ: 



• Molecule 7: B-phycoerythrin beta chain

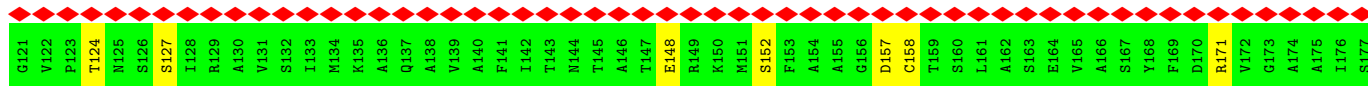
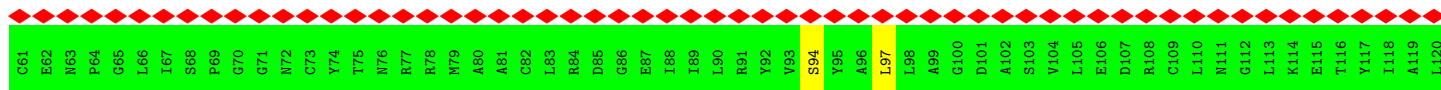
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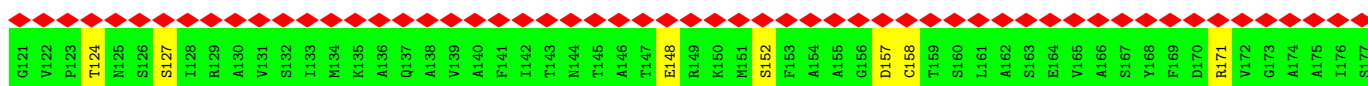
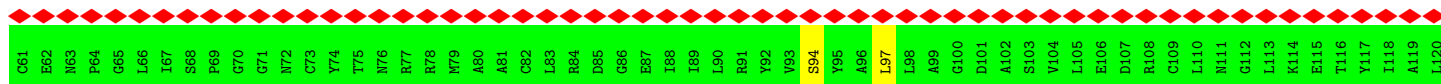
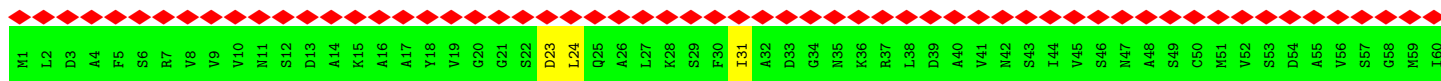
• Molecule 7: B-phycoerythrin beta chain

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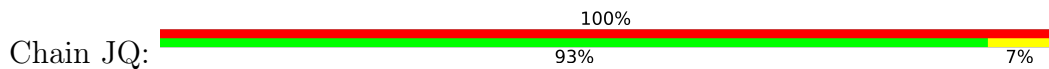




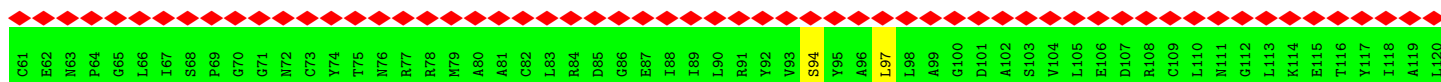
• Molecule 7: B-phycoerythrin beta chain



• Molecule 7: B-phycoerythrin beta chain

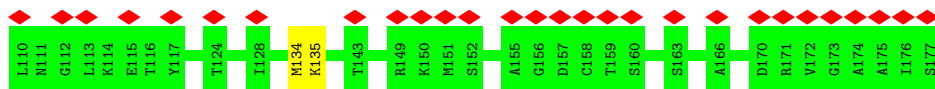
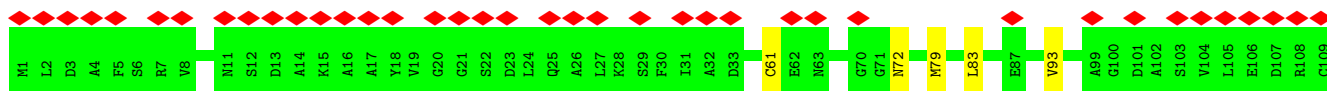
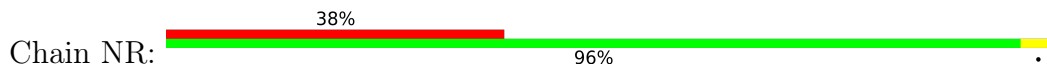


• Molecule 7: B-phycoerythrin beta chain

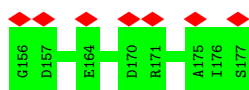
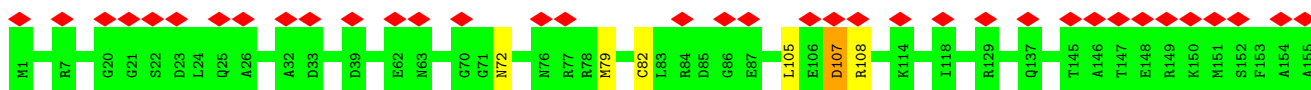




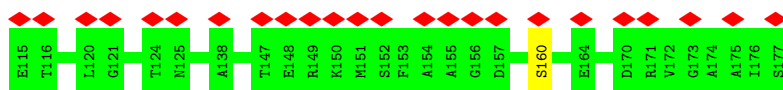
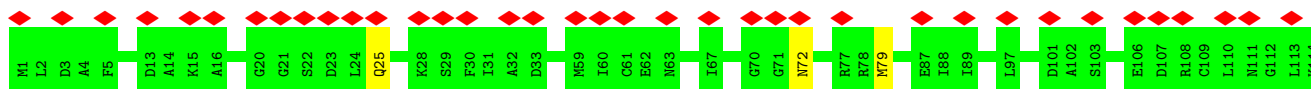
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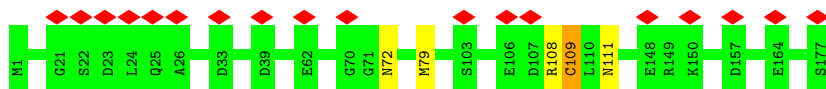
- Molecule 7: B-phycoerythrin beta chain



- Molecule 7: B-phycoerythrin beta chain

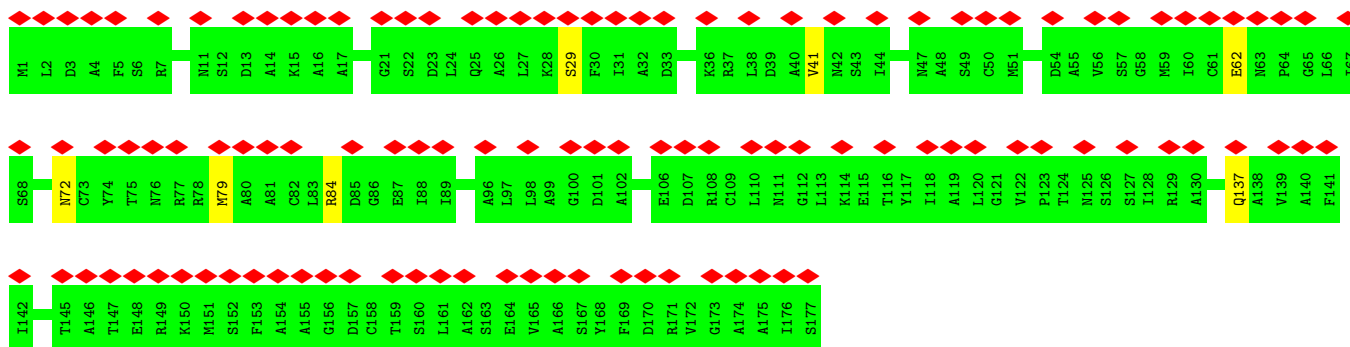


- Molecule 7: B-phycoerythrin beta chain

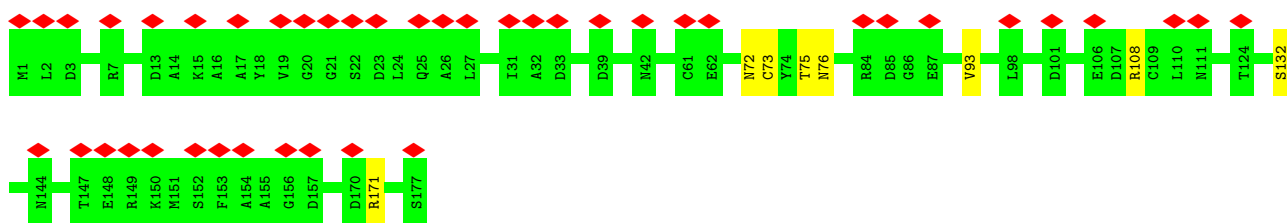


- Molecule 7: B-phycoerythrin beta chain

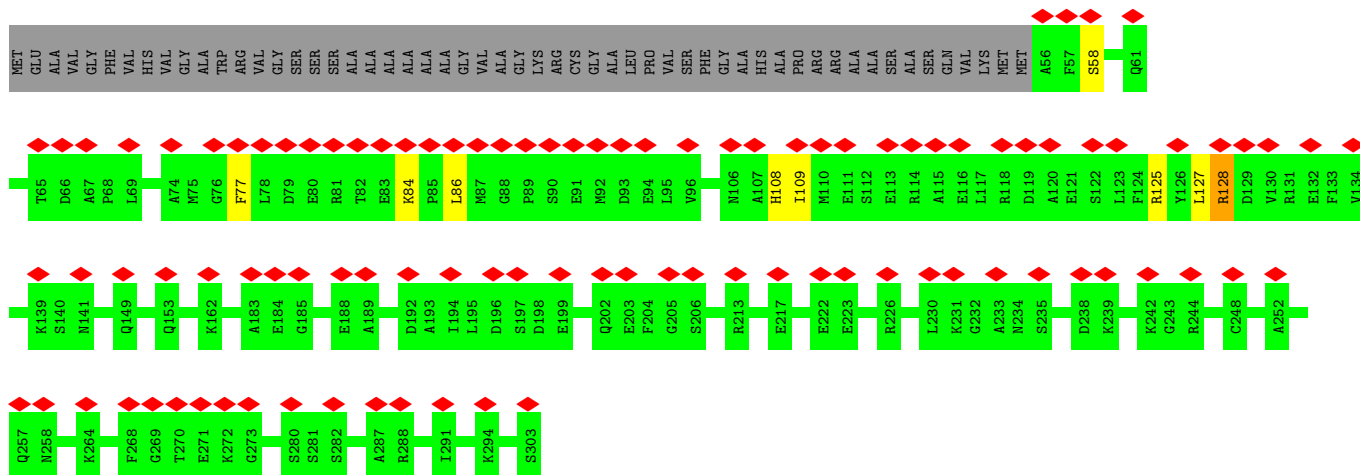
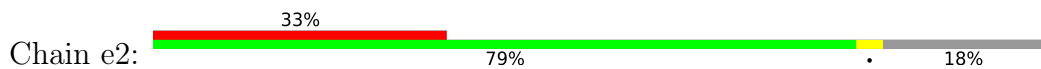




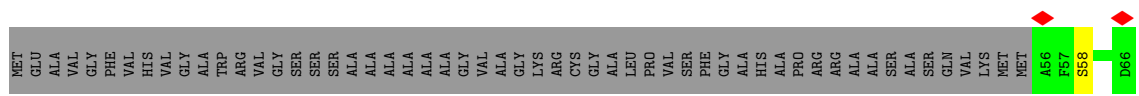
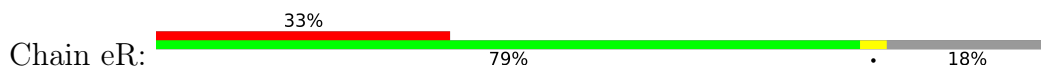
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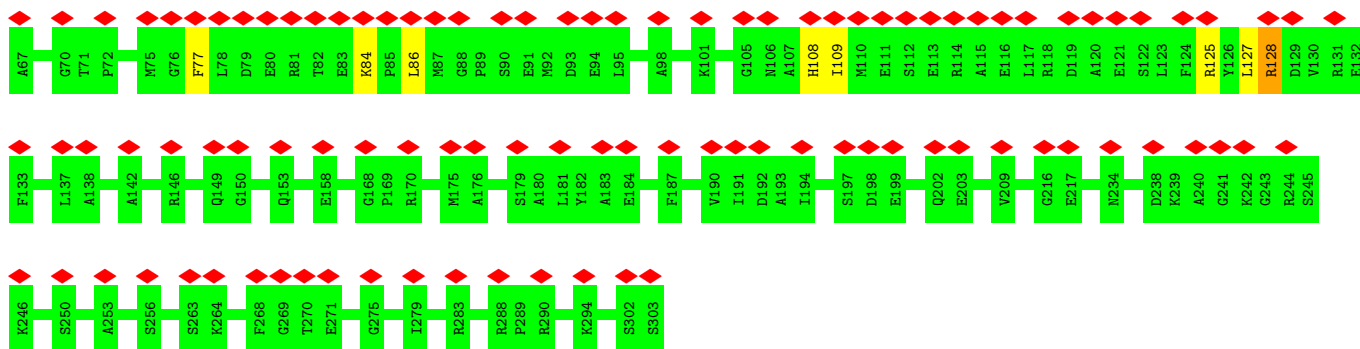


• Molecule 8: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

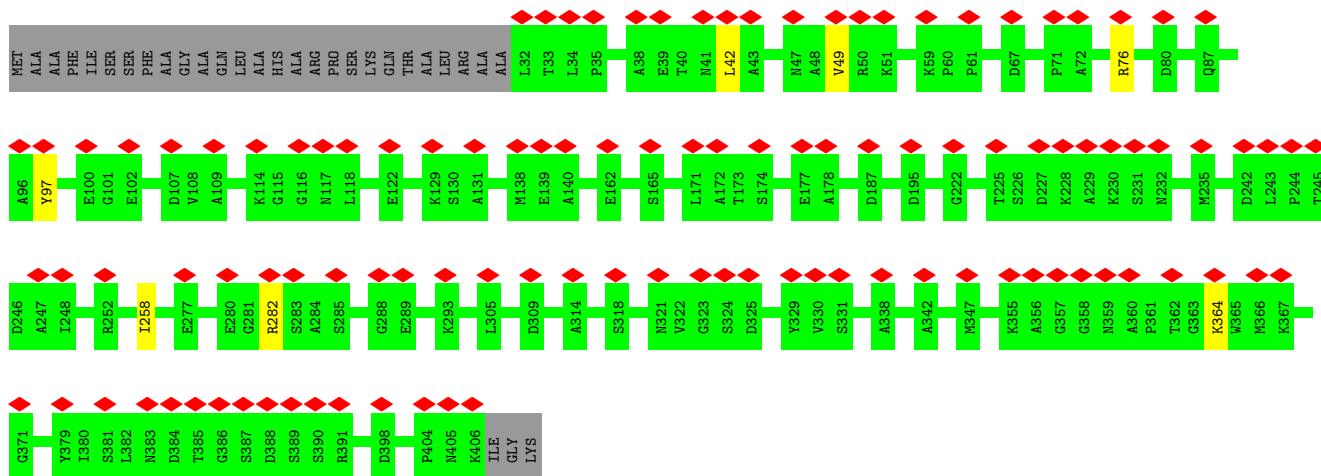


• Molecule 8: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

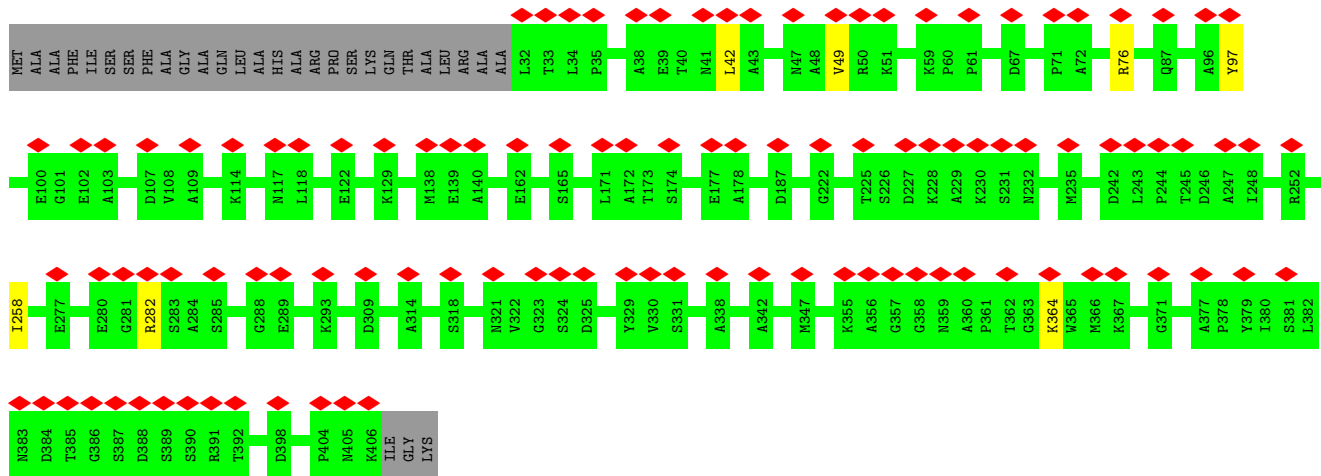




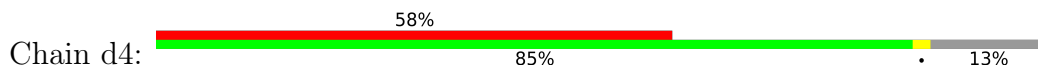
• Molecule 9: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



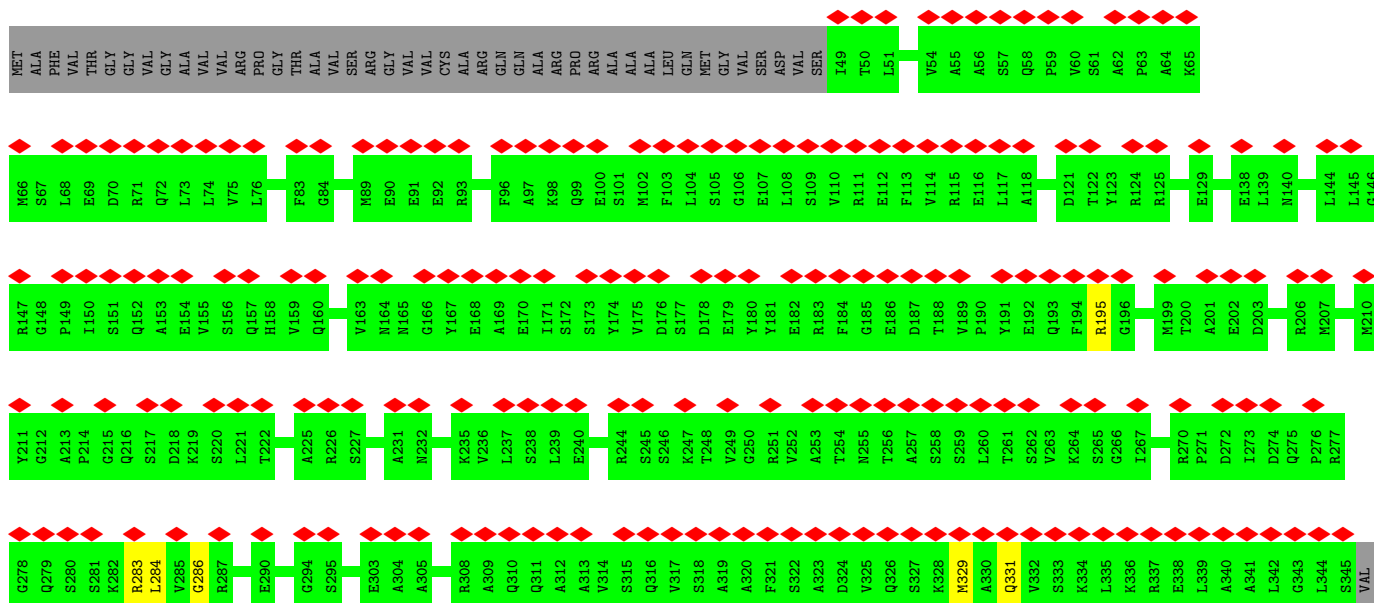
• Molecule 9: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



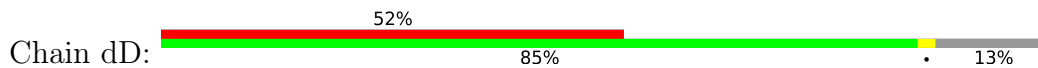
• Molecule 10: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod



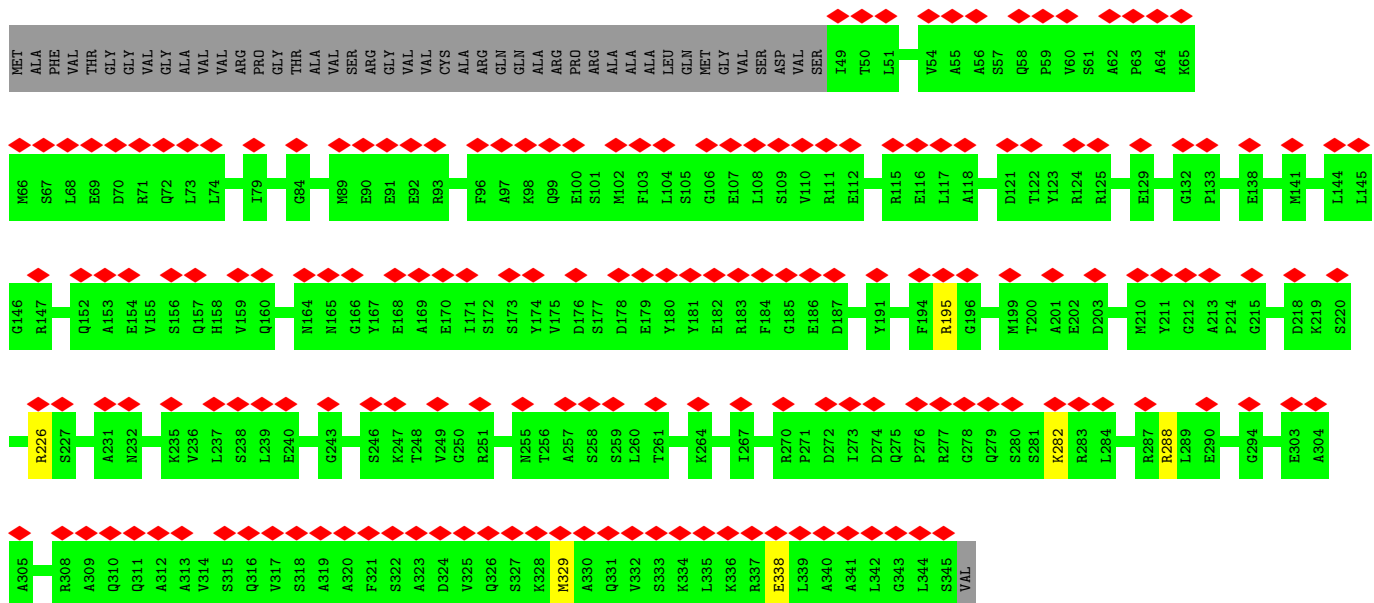
Chain d4:



• Molecule 10: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod



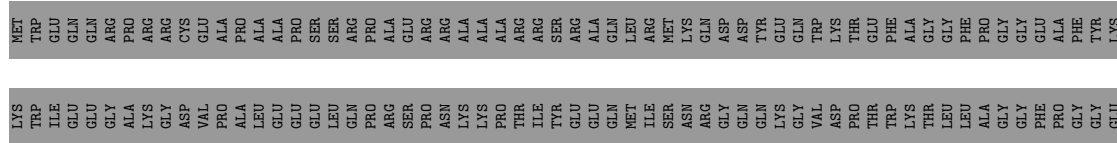
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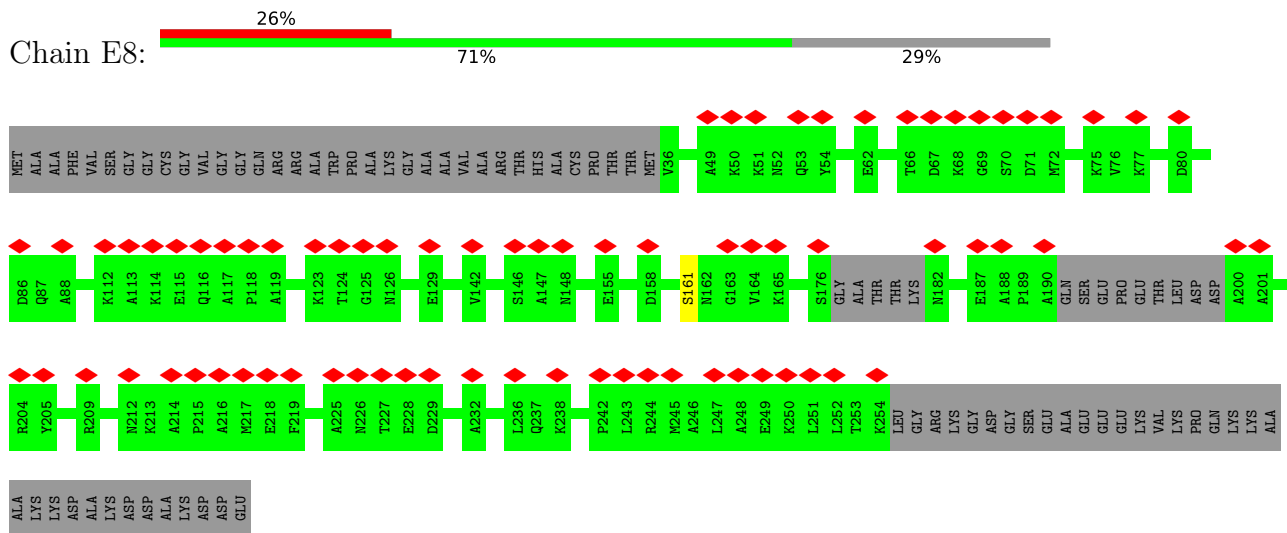
• Molecule 11: CaRSPs2



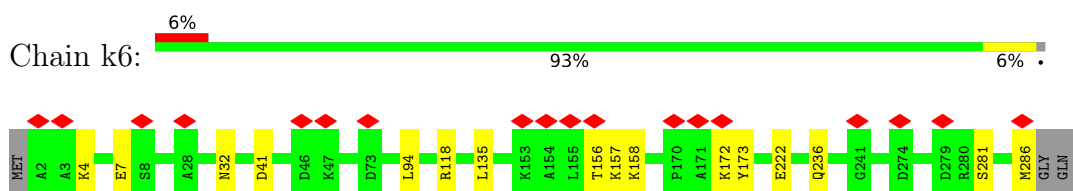
Chain D5:



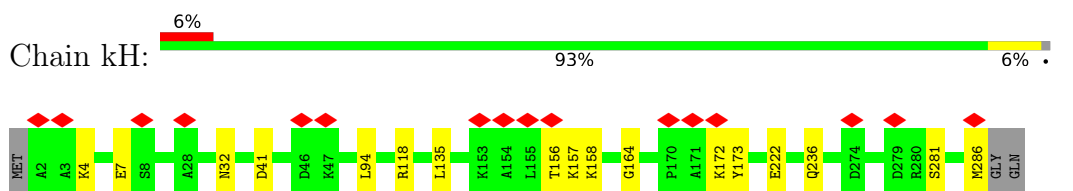
• Molecule 12: CaRSPs1



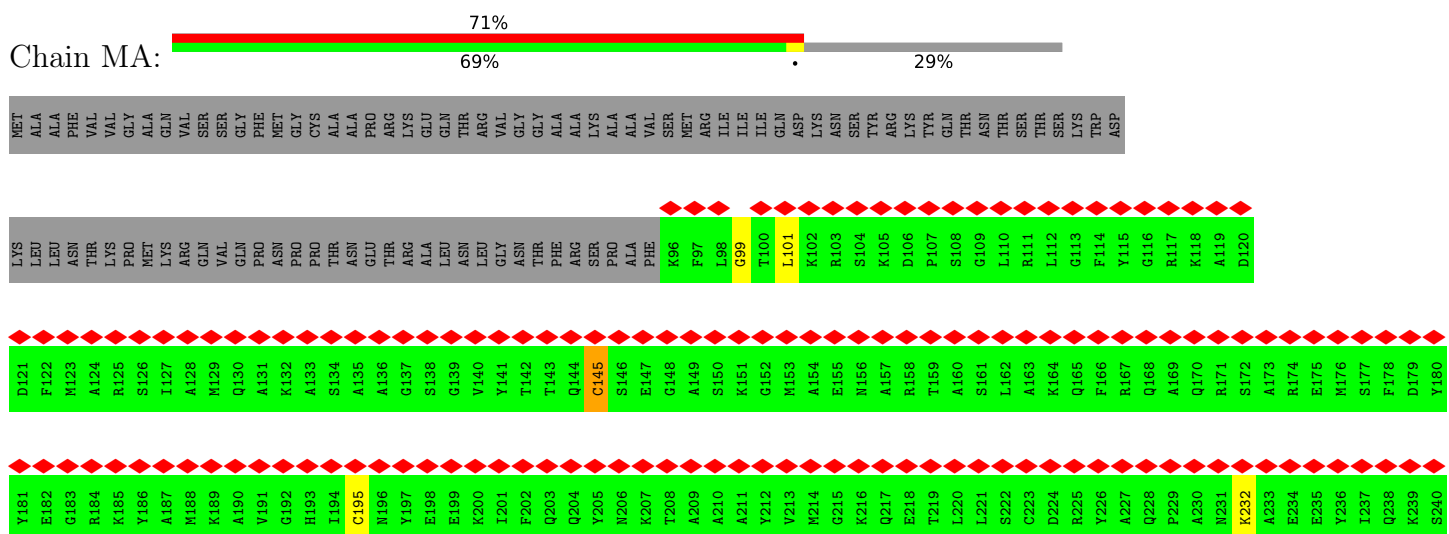
• Molecule 13: FAS1 domain-containing protein



• Molecule 13: FAS1 domain-containing protein



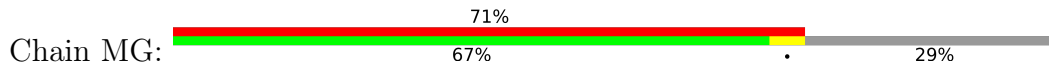
• Molecule 14: R-phycoerythrin gamma chain, chloroplastic



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A301	N302	D303	W304	H305	N306	N307	G308	C309	N310	Y311	E312	E313	K314	L315	T316	S317	R318	F319	P320	A321	A322	A323	S324	S325	V326	R327	P328	T329	T330	N331	R332	Y333
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• Molecule 14: R-phycoerythrin gamma chain, chloroplastic



MET	ALA	ALA	PHE	VAL	VAL	GLY	ALA	GLN	VAL	ARG	SER	GLN	VAL	SER	GLY	VAL	THR	THR	ARG	VAL	GLY	GLY	ALA	ALA	LYS	ALA	ALA	VAL	PHE	MET	ARG	ARG	ILE	ILE	ILE	GLN	LYS	ASP	ASN	TYR	ARG	LYS	TYR	GLN	THR	THR	THR	SER	LYS	LYS	TRP	ASP
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LYS	LEU	LEU	ASN	THR	LYS	PRO	MET	LYS	ARG	ARG	GLN	VAL	VAL	GLN	PRO	ASN	PRO	THR	ASN	LEU	GLY	ASN	THR	PHE	ALA	ARG	SER	PRO	ALA	ALA	PHE	K96	F97	L98	G99	T100	L101	K102	R103	S104	K105	P107	G109	S108	G109	L110	R111	L112	G113	F114	Y115	G116	R117	K118	A119	D120
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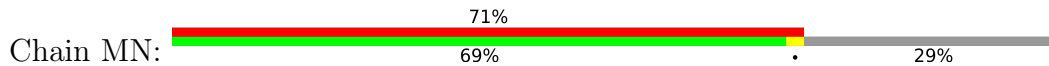
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Y181	E182	G183	R184	K185	Y186	A187	M188	K189	A190	V191	G192	A193	H194	C195	N196	Y197	E198	E199	K200	I201	F202	Q203	Q204	Y205	N206	K207	T208	A209	A210	A211	Y212	Y213	M214	G215	K216	Q217	E218	T219	L220	L221	S222	C223	D224	R225	Y226	A227	Q228	P229	A230	M231	K232	A233	E234	E235	Y236	I237	Q238	K239	S240
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W241	Q242	M243	Q244	M245	K246	K247	R248	S249	I250	P251	Y252	G253	V254	Y255	T256	T257	S258	C259	A260	D261	G262	T263	V264	K265	G266	M267	A268	E269	N270	A271	R272	V273	A274	K275	E276	S277	A278	N279	F280	R281	A282	R283	Q284	M285	S286	A287	G288	A289	K290	A291	A292	A293	R294	F295	N296	A297	R298	R299	V300
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A301	N302	D303	W304	H305	N306	N307	G308	C309	N310	Y311	E312	E313	K314	L315	T316	S317	R318	F319	P320	A321	A322	A323	S324	S325	V326	R327	P328	T329	T330	N331	R332	Y333
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• Molecule 14: R-phycoerythrin gamma chain, chloroplastic



MET	ALA	ALA	PHE	VAL	VAL	GLY	ALA	GLN	VAL	ARG	SER	GLN	VAL	SER	GLY	VAL	THR	THR	ARG	VAL	GLY	GLY	ALA	ALA	LYS	ALA	ALA	VAL	PHE	MET	ARG	ARG	ILE	ILE	ILE	GLN	LYS	ASP	ASN	TYR	ARG	LYS	TYR	GLN	THR	THR	THR	SER	LYS	LYS	TRP	ASP
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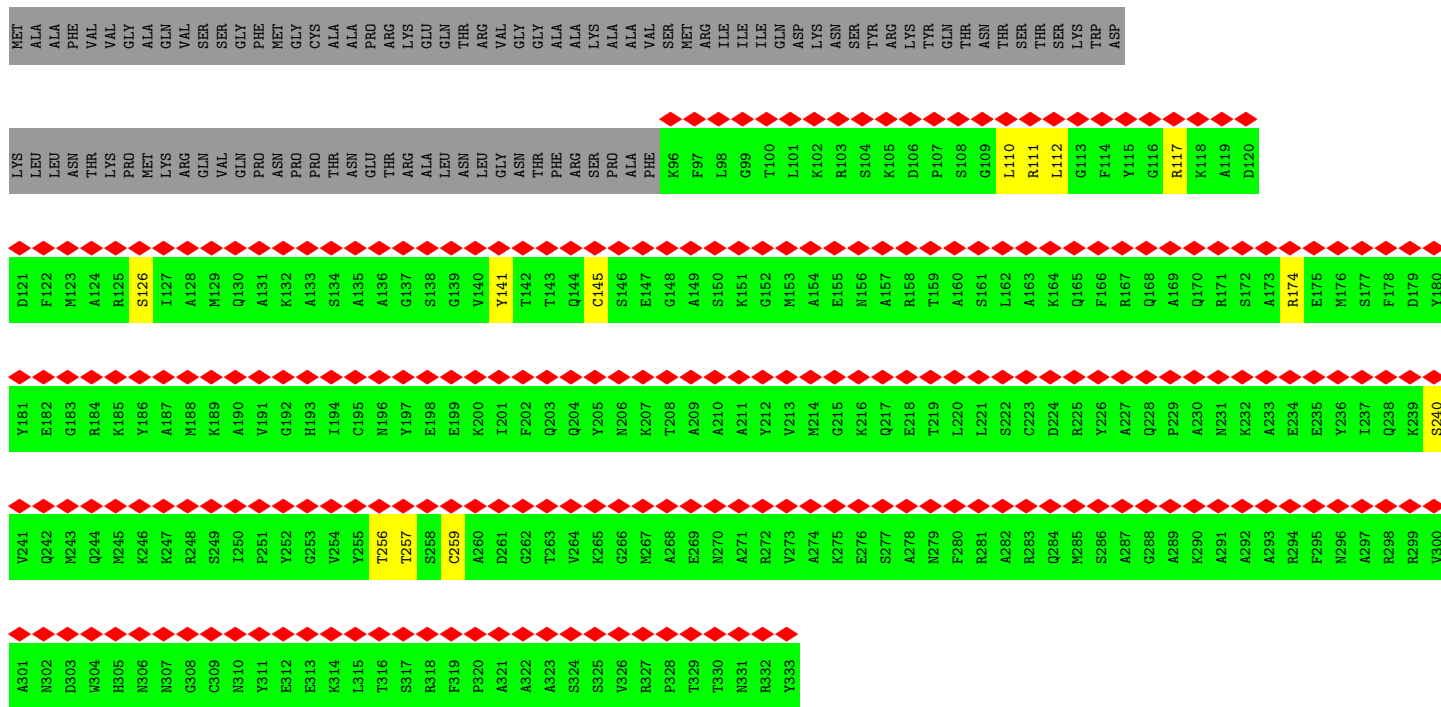
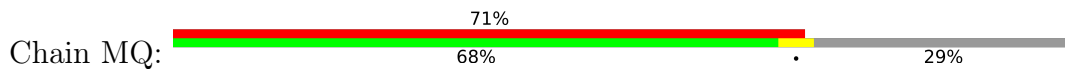
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D121	F122	M123	A124	R125	S126	I127	A128	M129	Q130	A131	K132	A133	S134	A135	A136	G137	S138	G139	V140	Y141	T142	Q203	T143	Q204	Y205	N206	K207	T208	A209	A210	A211	Y212	Y213	M214	G215	K216	Q217	E218	T219	L220	L221	S222	C223	D224	R225	Y226	F227	R228	Q229	A230	M231	K232	A233	E234	E235	Y236	I237	Q238	K239	S240
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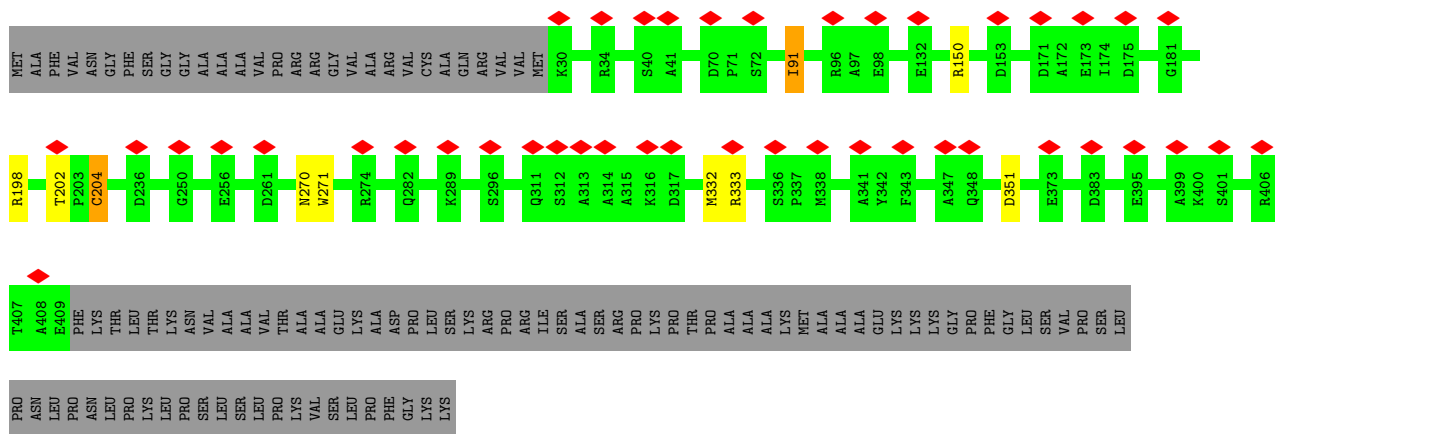
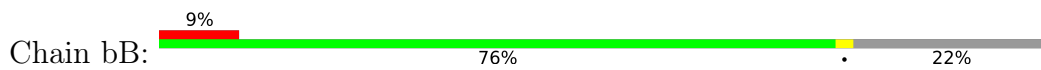
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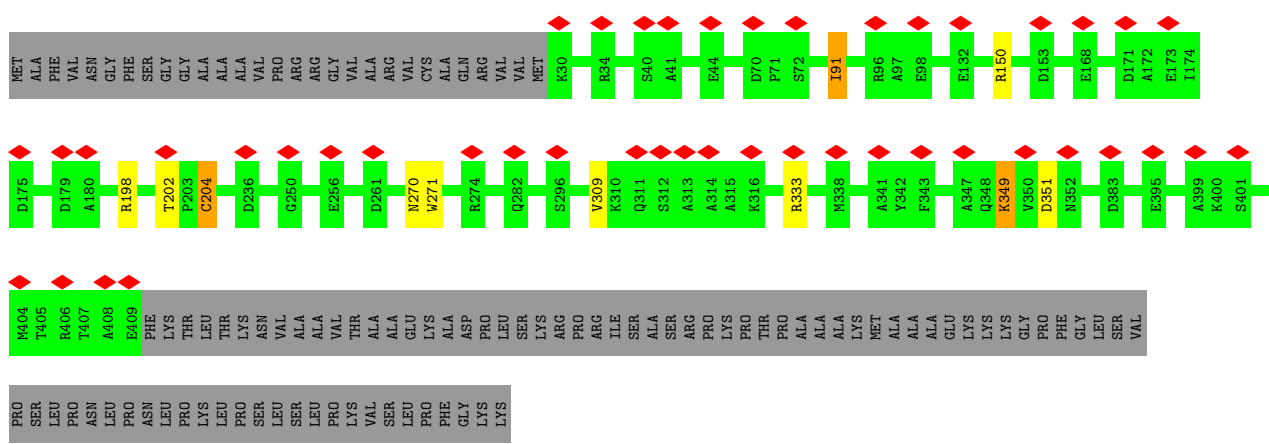
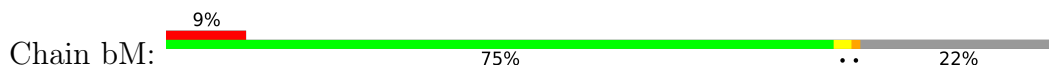
• Molecule 14: R-phycoerythrin gamma chain, chloroplastic



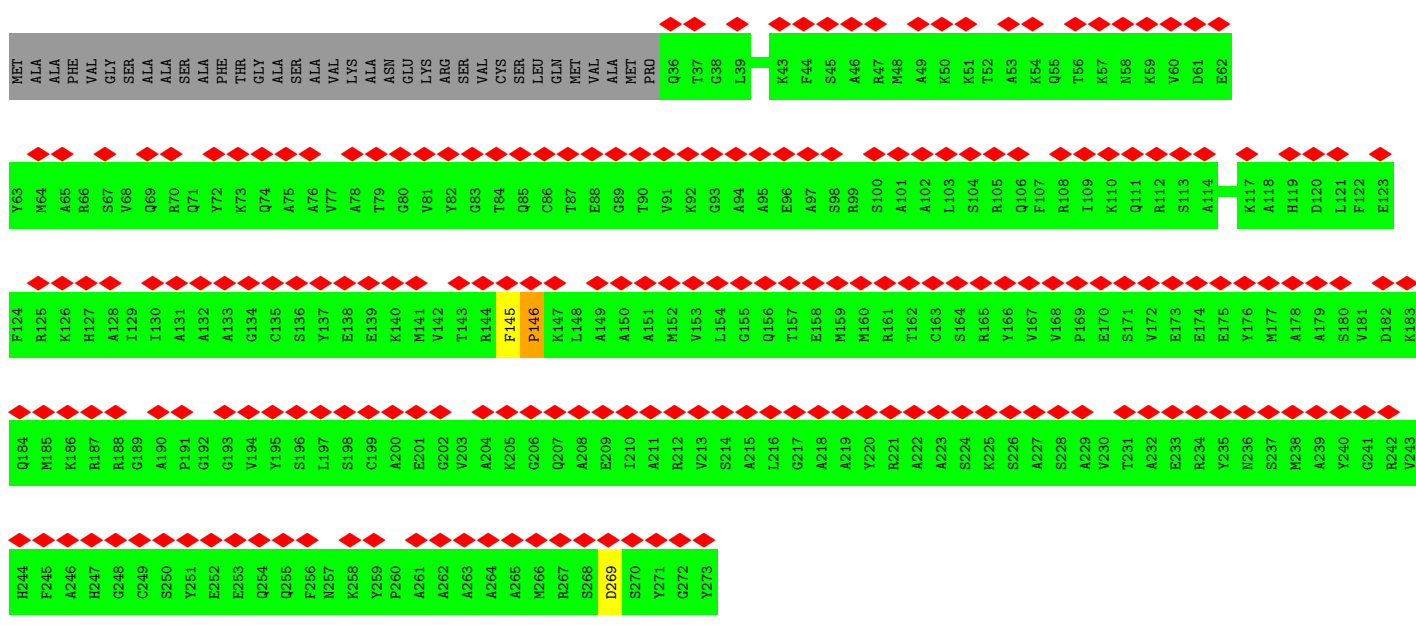
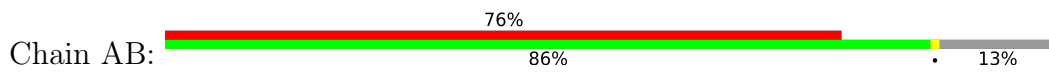
• Molecule 15: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod



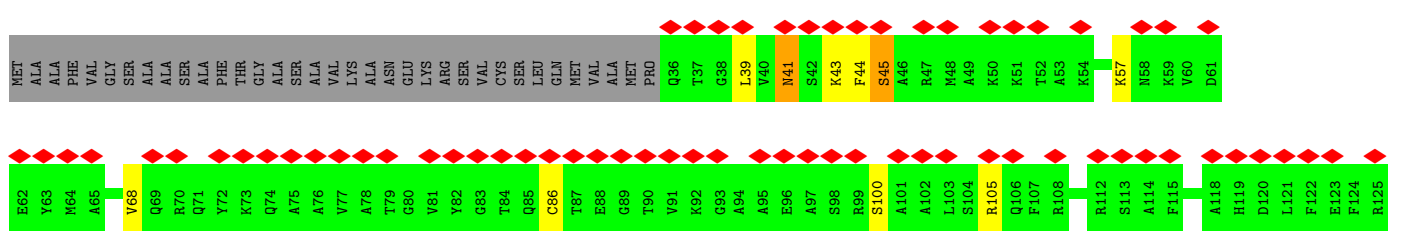
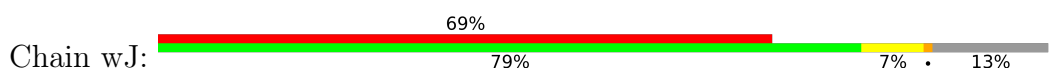
• Molecule 15: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

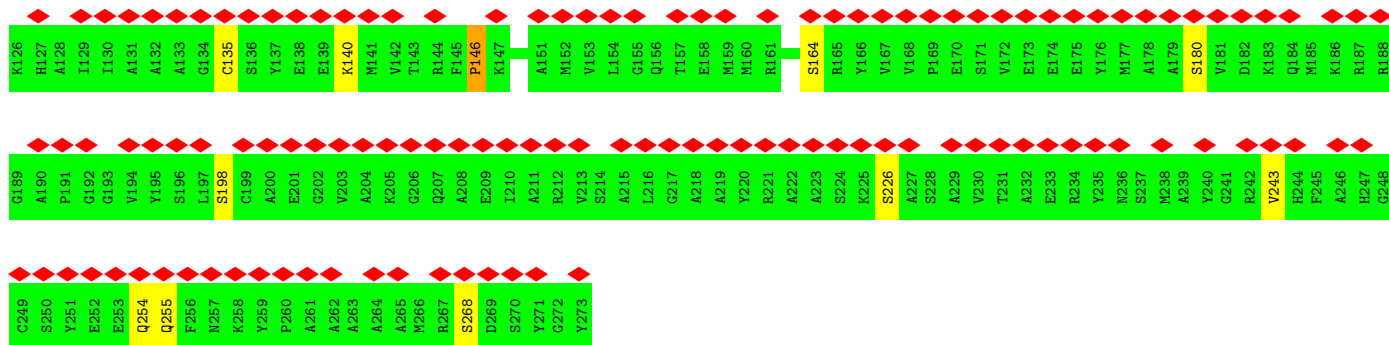


• Molecule 16: R-phycoerythrin gamma chain, chloroplastic

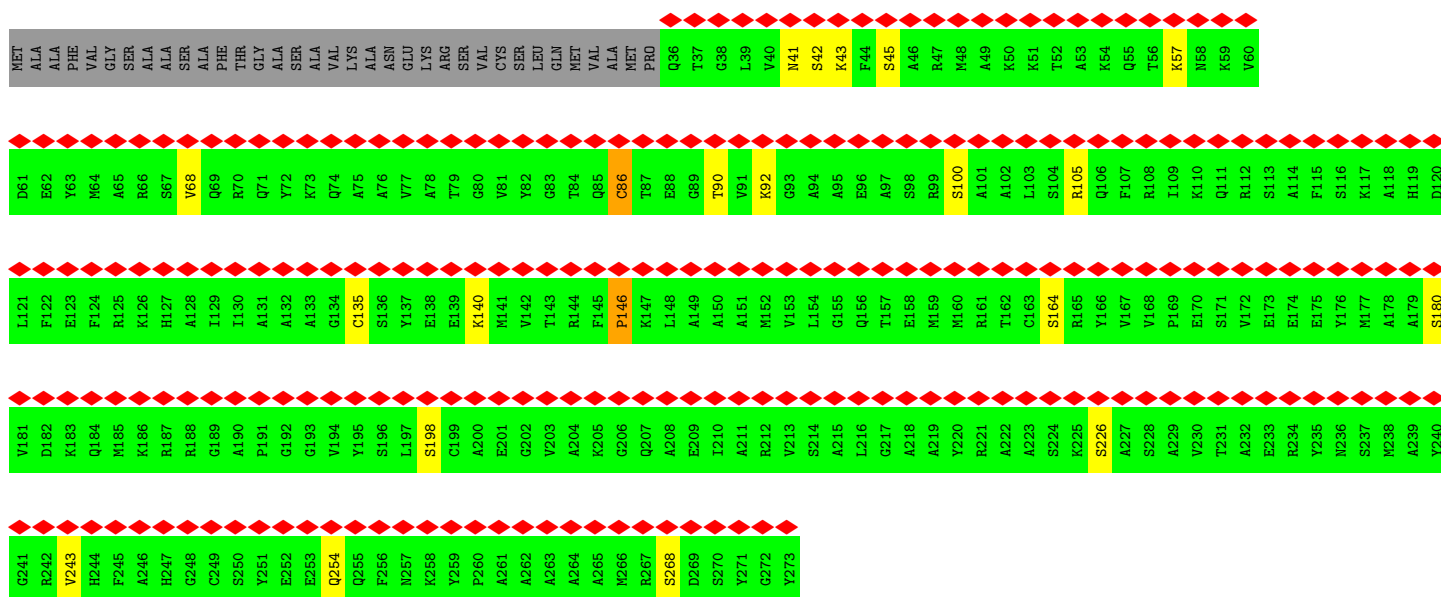
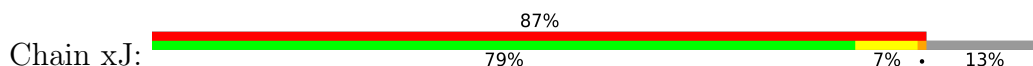


• Molecule 16: R-phycoerythrin gamma chain, chloroplastic

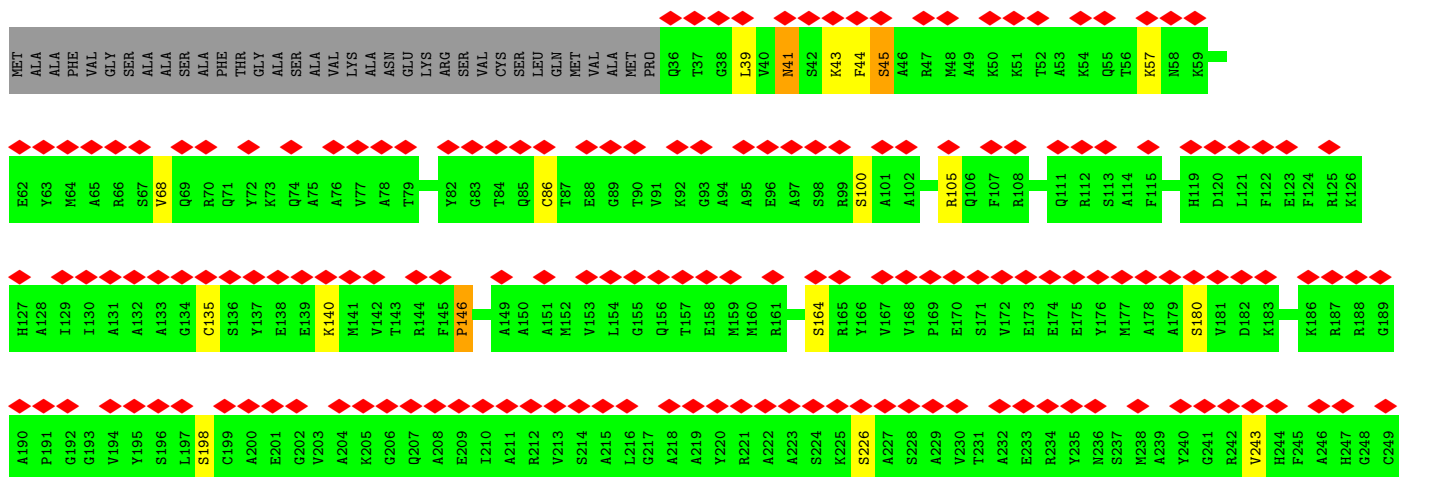
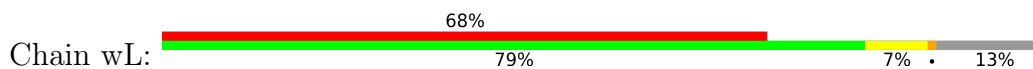


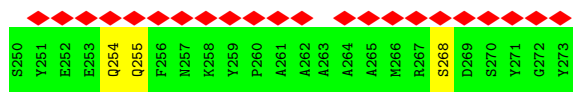


• Molecule 16: R-phycoerythrin gamma chain, chloroplastic

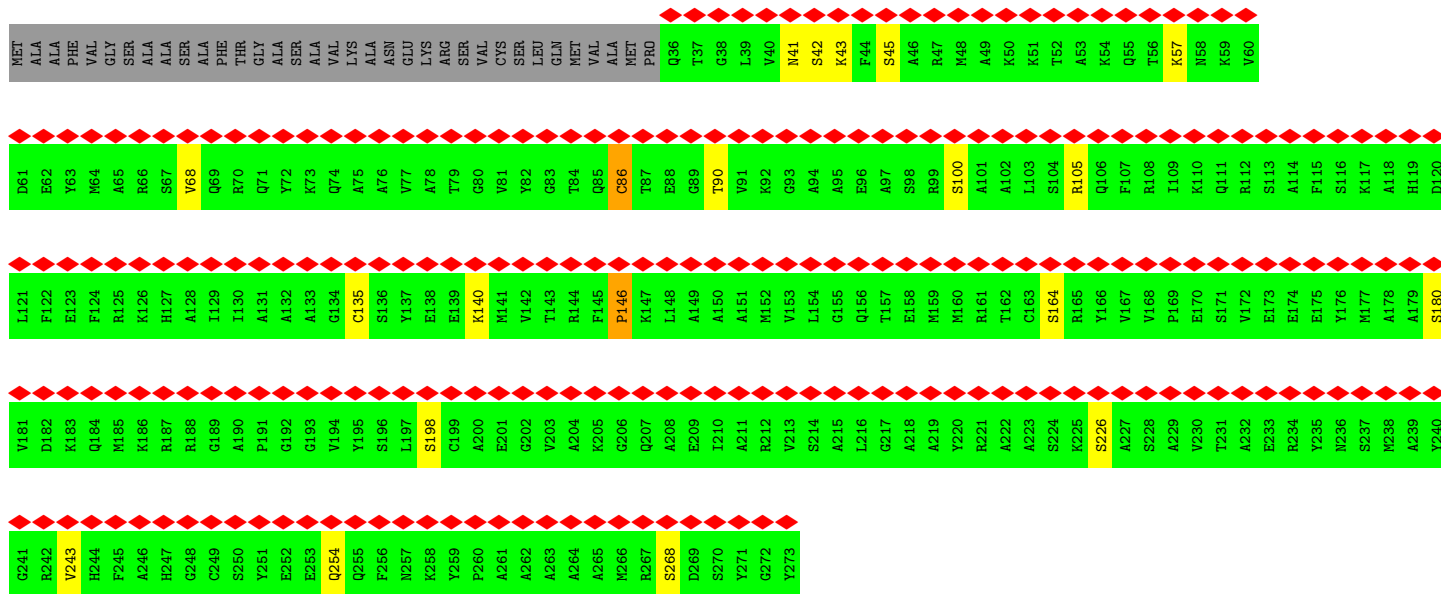
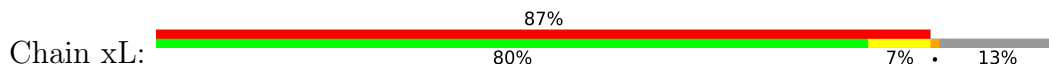


• Molecule 16: R-phycoerythrin gamma chain, chloroplastic

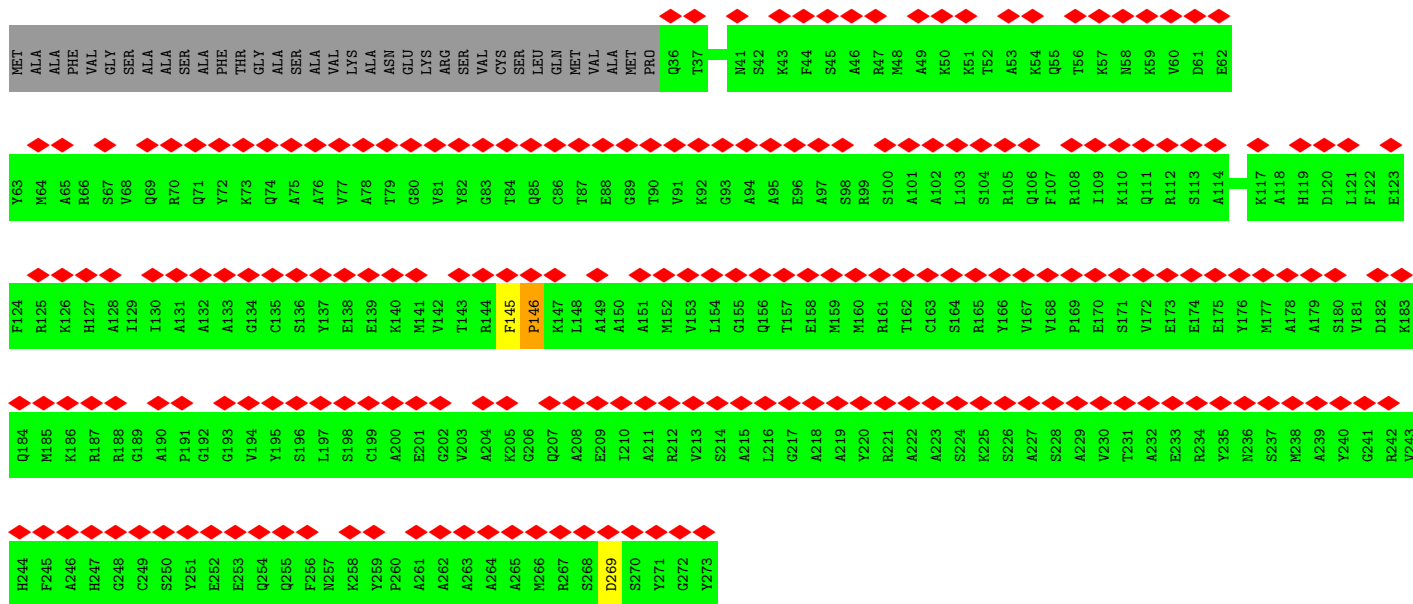
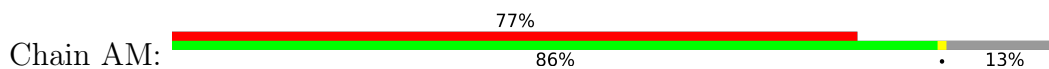




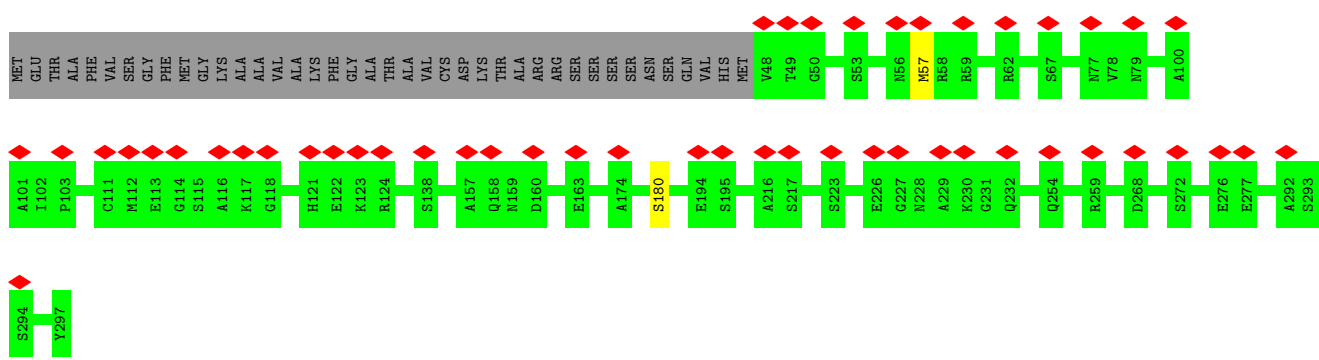
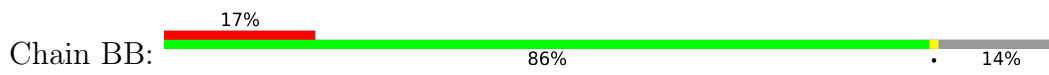
• Molecule 16: R-phycoerythrin gamma chain, chloroplastic



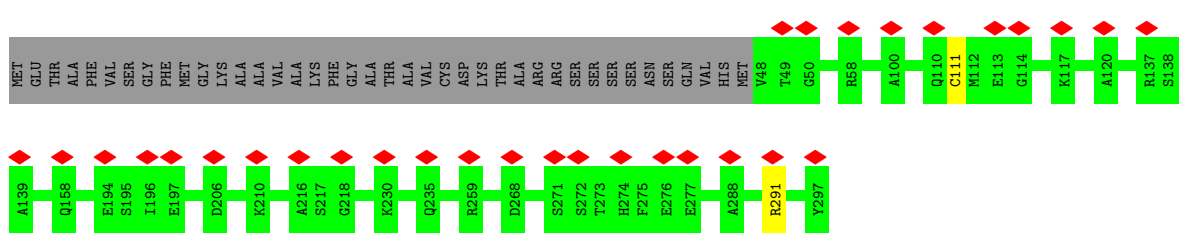
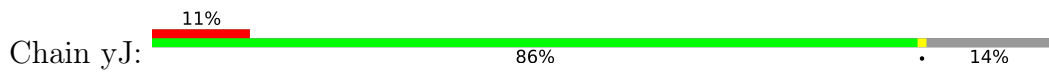
• Molecule 16: R-phycoerythrin gamma chain, chloroplastic



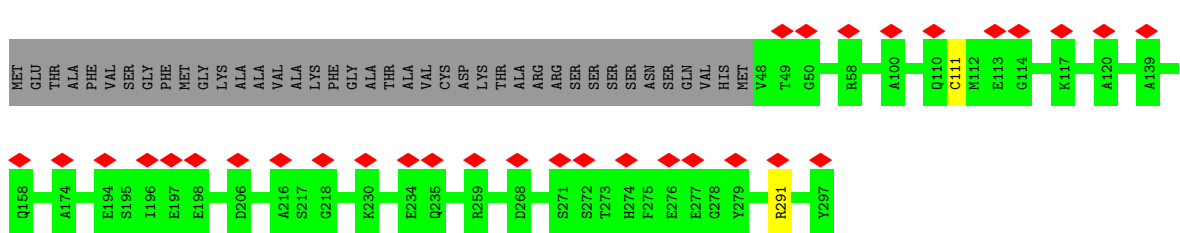
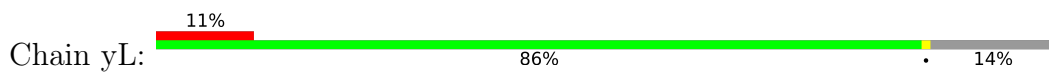
• Molecule 17: R-phycoerythrin gamma chain, chloroplastic



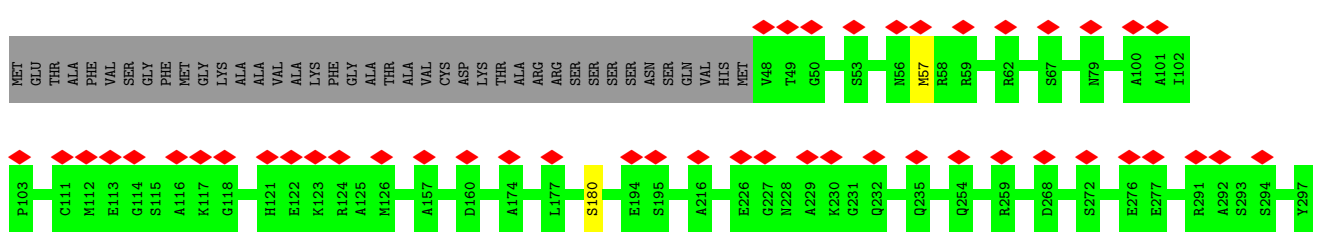
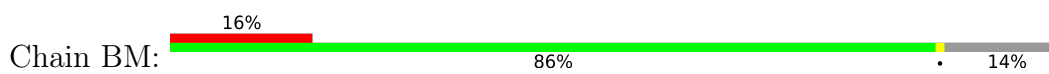
• Molecule 17: R-phycoerythrin gamma chain, chloroplastic



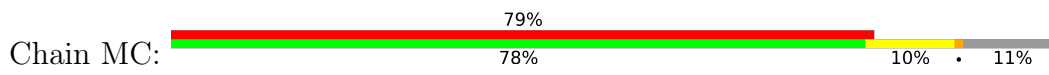
• Molecule 17: R-phycoerythrin gamma chain, chloroplastic

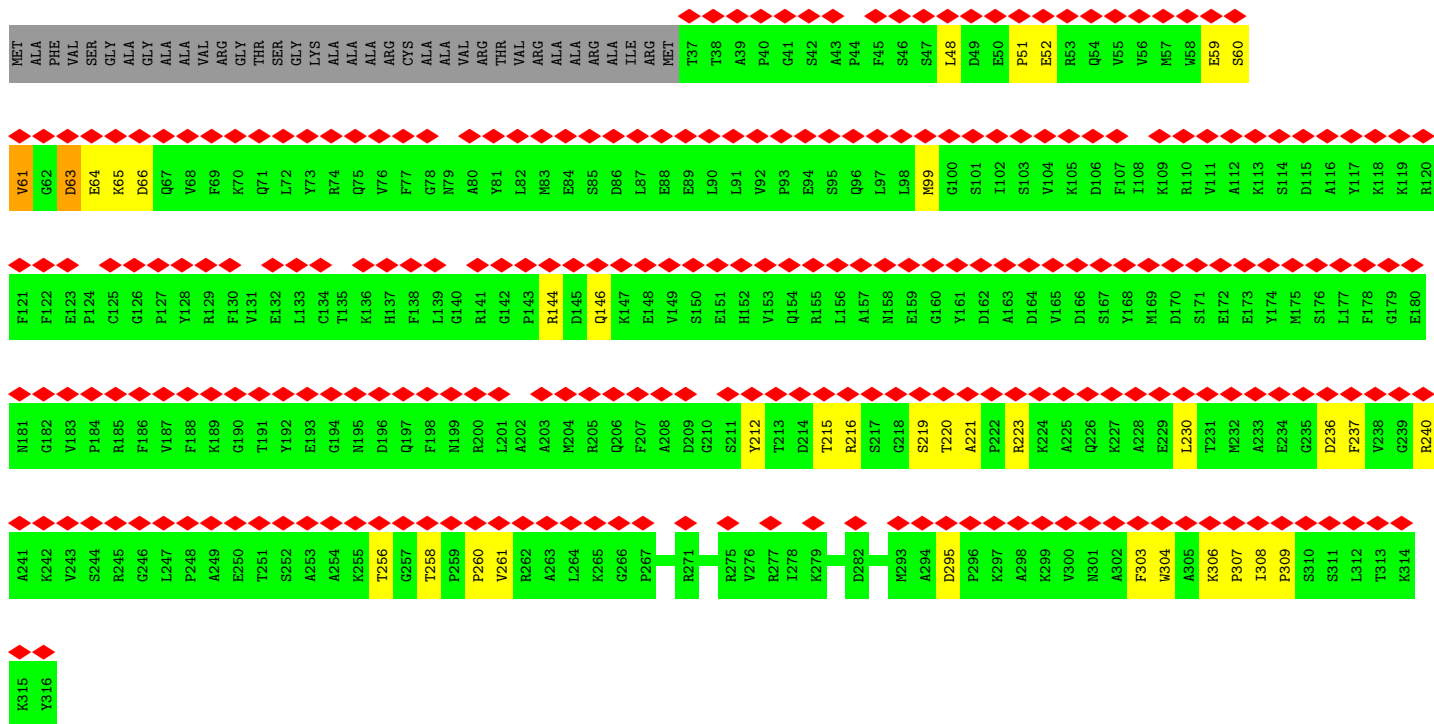


• Molecule 17: R-phycoerythrin gamma chain, chloroplastic

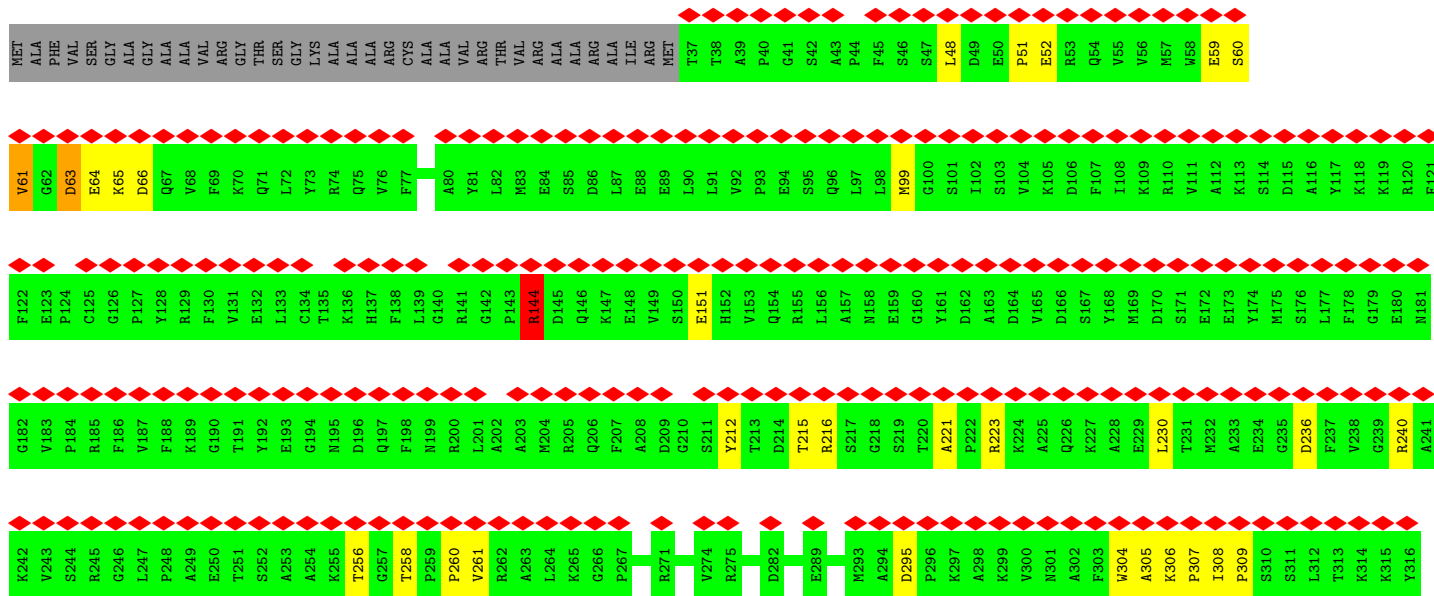
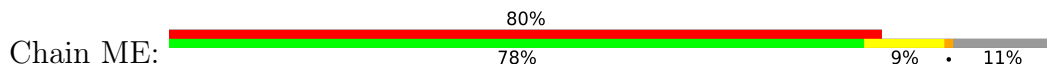


• Molecule 18: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

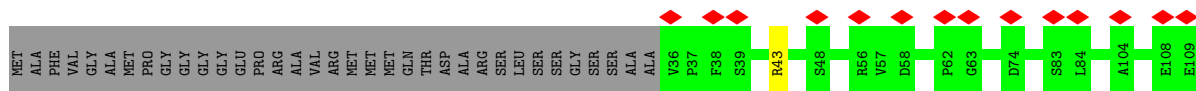
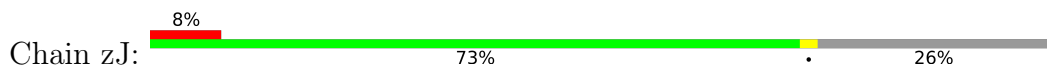


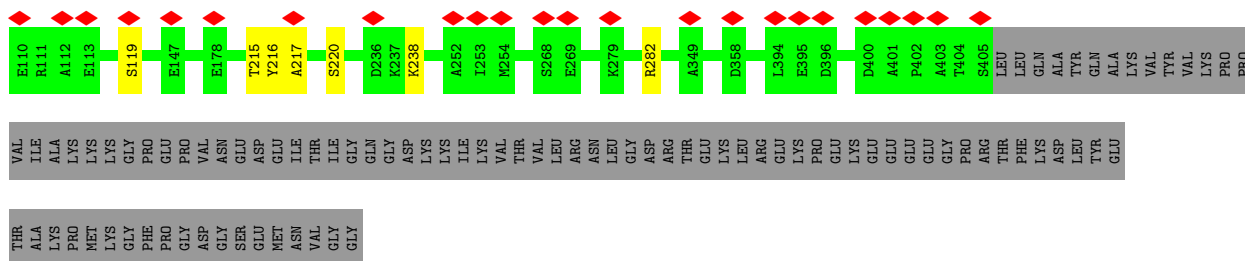


• Molecule 18: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

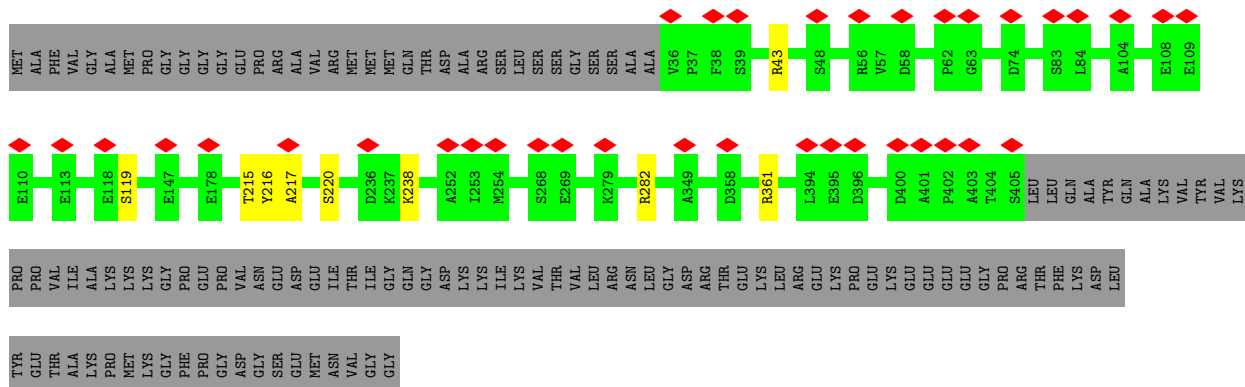
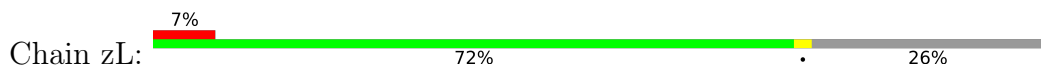


• Molecule 19: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

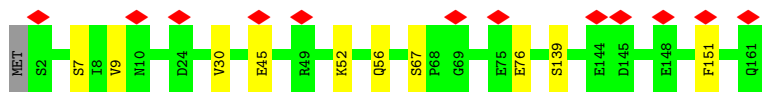




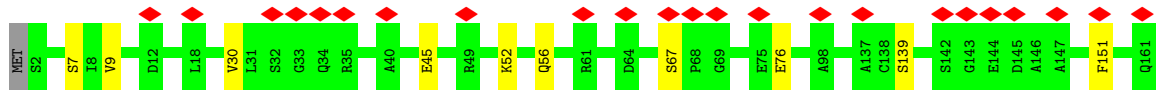
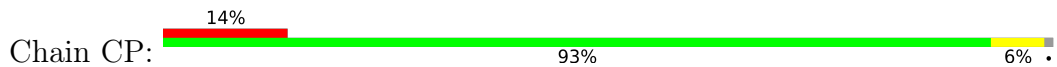
• Molecule 19: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



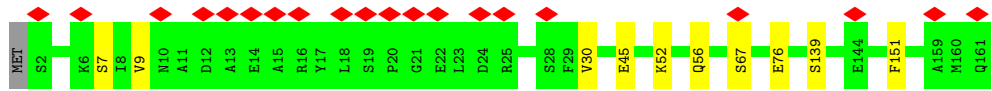
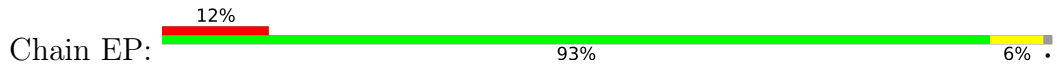
• Molecule 20: Allophycocyanin alpha subunit



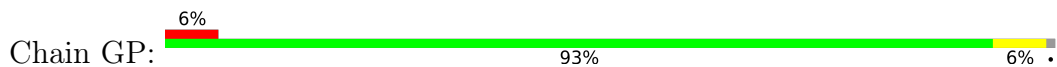
• Molecule 20: Allophycocyanin alpha subunit

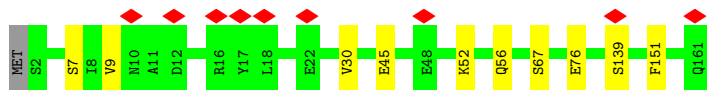


• Molecule 20: Allophycocyanin alpha subunit

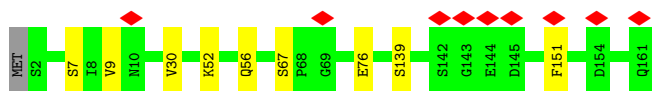
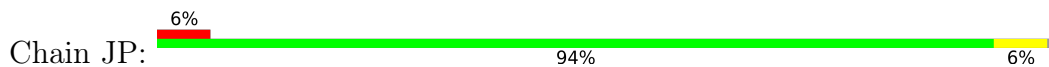


• Molecule 20: Allophycocyanin alpha subunit





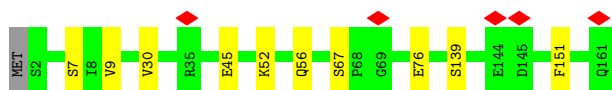
- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



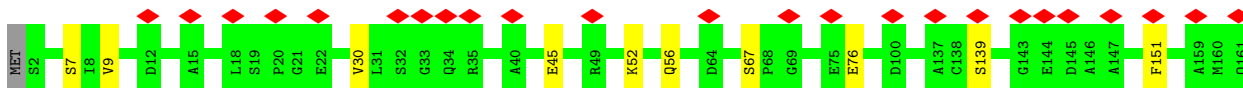
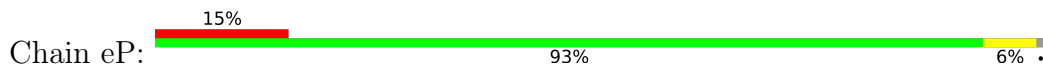
- Molecule 20: Allophycocyanin alpha subunit



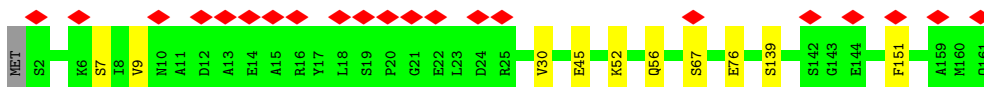
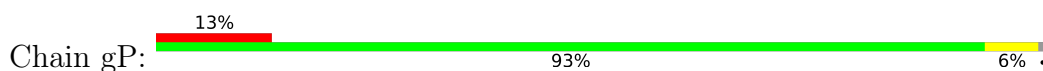
- Molecule 20: Allophycocyanin alpha subunit



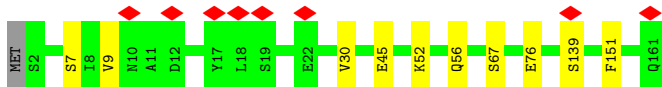
- Molecule 20: Allophycocyanin alpha subunit



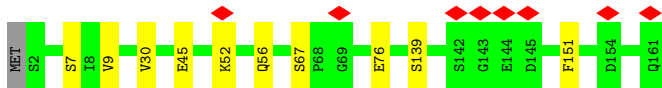
- Molecule 20: Allophycocyanin alpha subunit



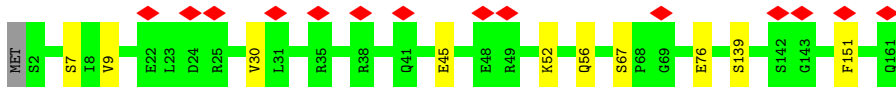
- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit

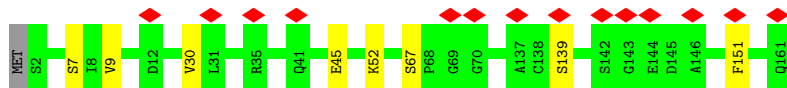
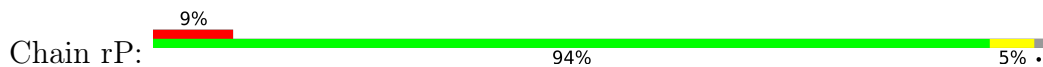


- Molecule 20: Allophycocyanin alpha subunit

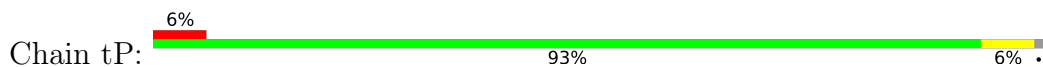




- Molecule 20: Allophycocyanin alpha subunit



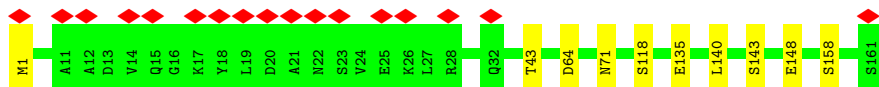
- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



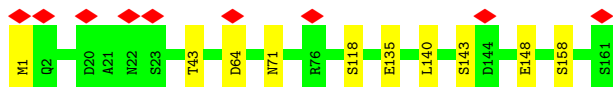
- Molecule 21: Allophycocyanin beta subunit



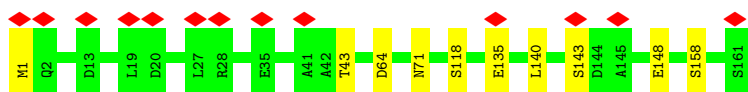
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



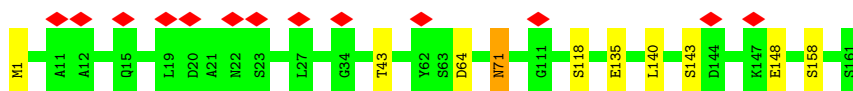
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



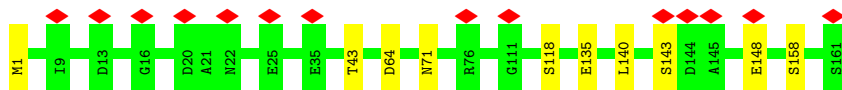
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



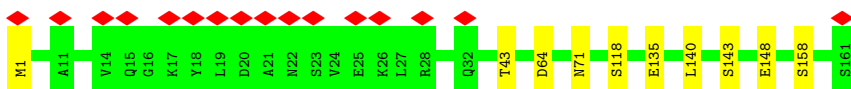
- Molecule 21: Allophycocyanin beta subunit

Chain UP:  94% 6%



- Molecule 21: Allophycocyanin beta subunit

Chain dP:  10% 94% 6%



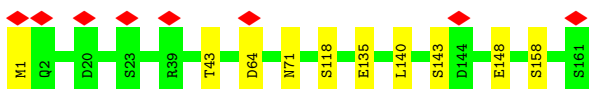
- Molecule 21: Allophycocyanin beta subunit

Chain fP:  94% 6%

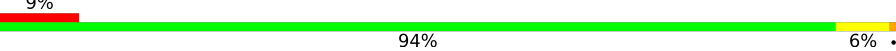


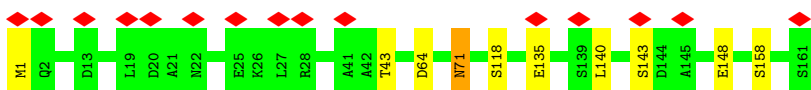
- Molecule 21: Allophycocyanin beta subunit

Chain hP:  5% 94% 6%



- Molecule 21: Allophycocyanin beta subunit

Chain jP:  9% 94% 6%



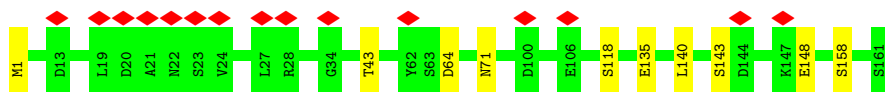
- Molecule 21: Allophycocyanin beta subunit

Chain kP:  94% 6%

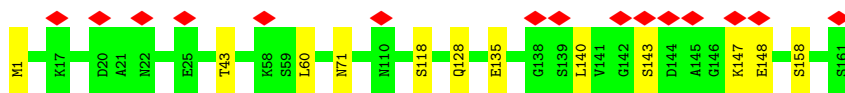


- Molecule 21: Allophycocyanin beta subunit

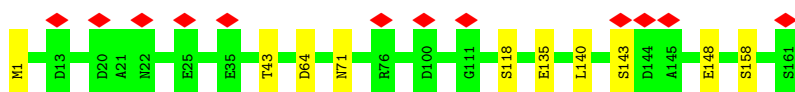
Chain nP:  9% 94% 6%



- Molecule 21: Allophycocyanin beta subunit



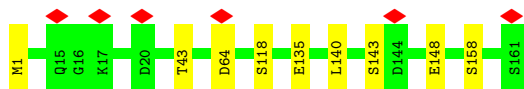
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



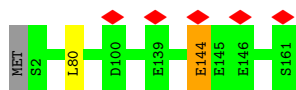
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit

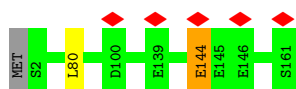


- Molecule 22: Allophycocyanin gamma subunit



- Molecule 22: Allophycocyanin gamma subunit

Chain xP:  98%



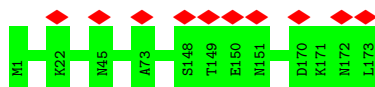
- Molecule 23: Allophycocyanin beta 18 subunit

Chain WP:  5% 100%



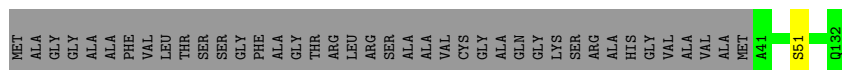
- Molecule 23: Allophycocyanin beta 18 subunit

Chain yP:  6% 100%



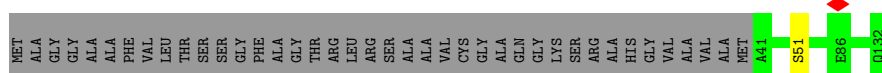
- Molecule 24: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain XP:  69% 30%



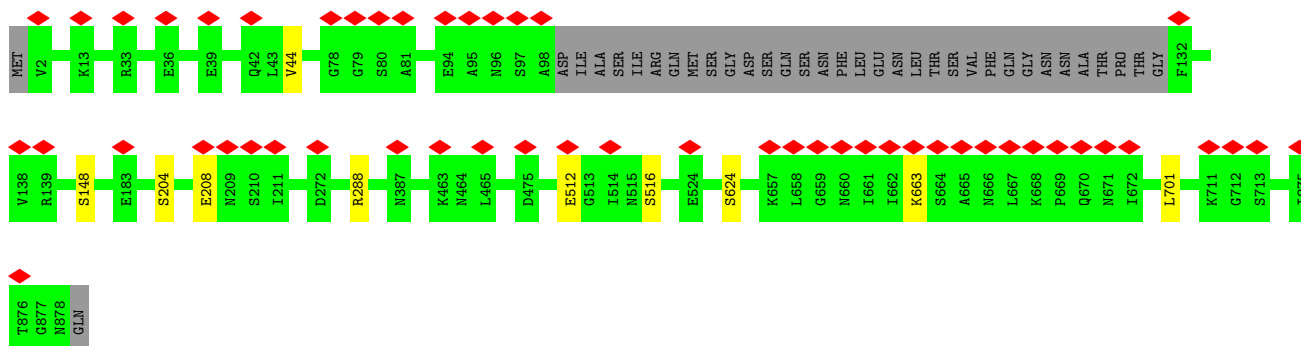
- Molecule 24: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain zP:  69% 30%

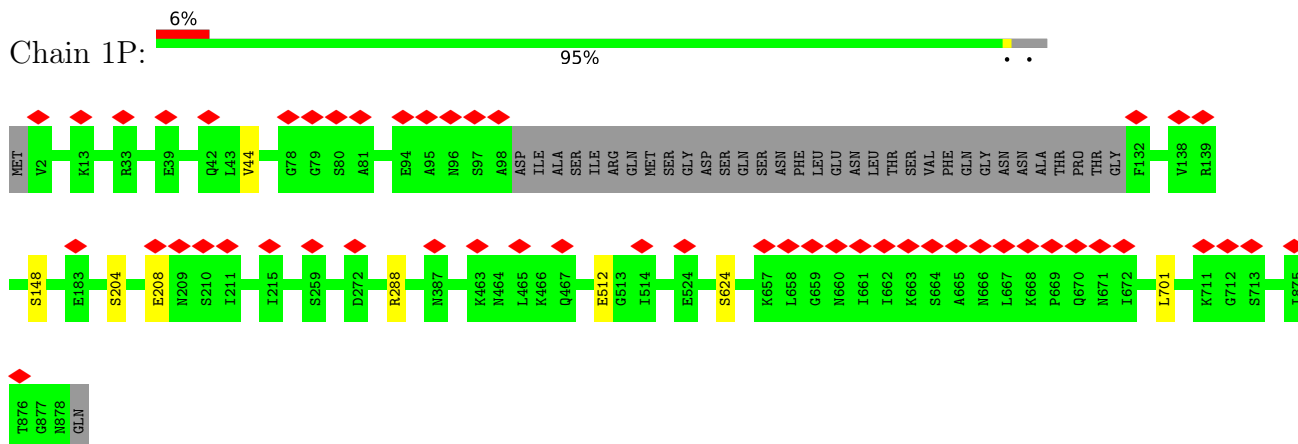


- Molecule 25: Phycobilisome linker polypeptide

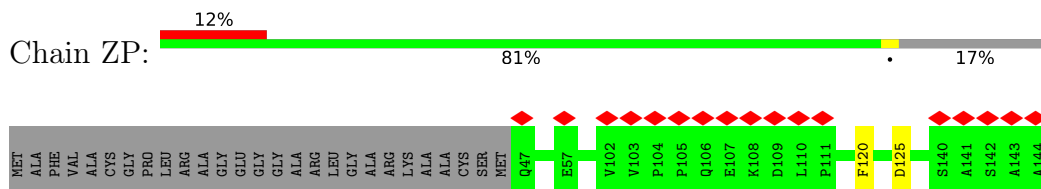
Chain yP:  6% 95%



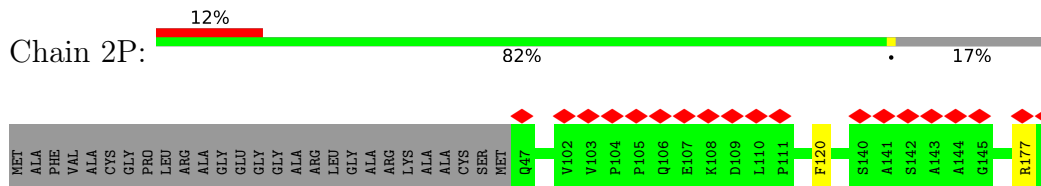
- Molecule 25: Phycobilisome linker polypeptide



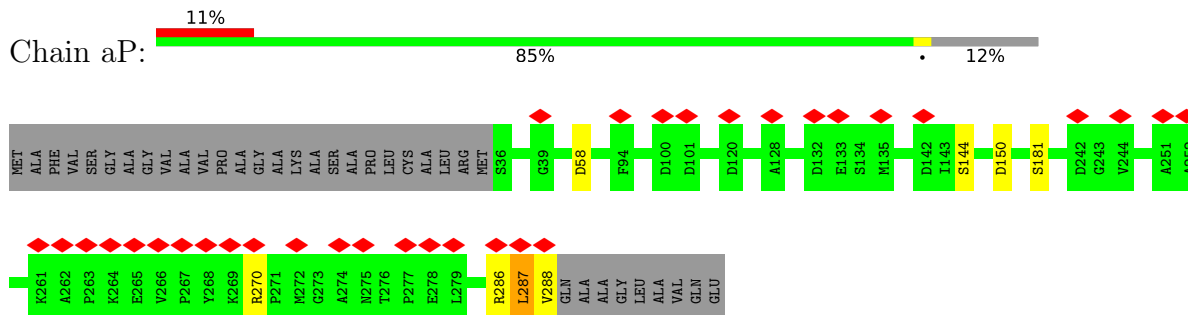
- Molecule 26: Lrc4



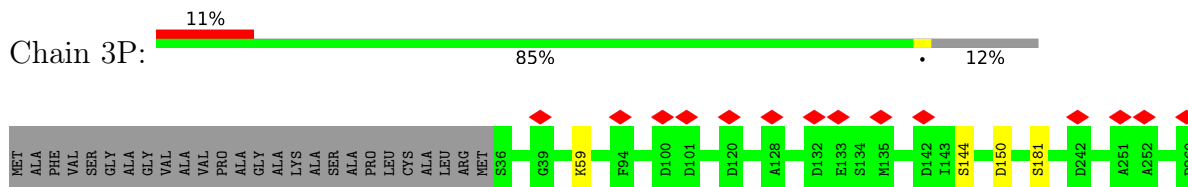
- Molecule 26: Lrc4

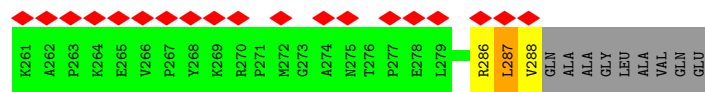


- Molecule 27: LRC5

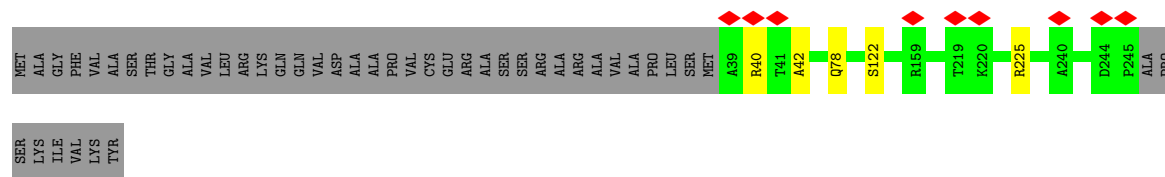
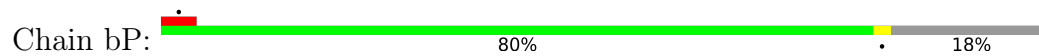


- Molecule 27: LRC5

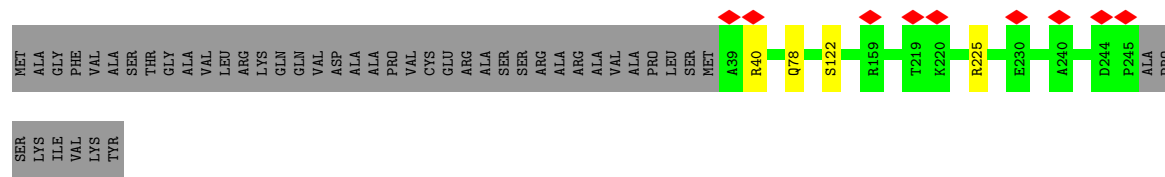
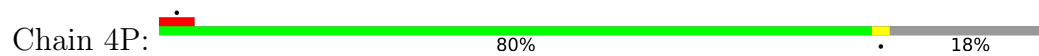




- Molecule 28: FAS1 domain-containing protein



- Molecule 28: FAS1 domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	87399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	618.2801, 618.2801, 618.2801	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0660001, 1.0660001, 1.0660001	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: MEN, PEB, PMS, PUB, 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	X1	0.50	0/2585	0.69	3/3492 (0.1%)
1	X7	0.48	1/2585 (0.0%)	0.66	0/3492
1	X9	0.48	1/2585 (0.0%)	0.66	0/3492
1	XF	0.54	0/2585	0.66	0/3492
1	XI	0.54	0/2581	0.66	0/3488
1	XK	0.50	0/2585	0.69	3/3492 (0.1%)
2	A1	0.44	0/2025	0.59	1/2722 (0.0%)
2	A7	0.42	0/2025	0.56	0/2722
2	A9	0.42	0/2025	0.56	0/2722
2	AF	0.44	0/2025	0.60	1/2722 (0.0%)
2	AI	0.44	0/2025	0.60	1/2722 (0.0%)
2	AK	0.44	0/2025	0.59	1/2722 (0.0%)
3	B1	0.48	0/1917	0.64	1/2592 (0.0%)
3	B7	0.44	0/1933	0.65	1/2614 (0.0%)
3	B9	0.44	0/1933	0.65	1/2614 (0.0%)
3	BF	0.56	1/1941 (0.1%)	0.63	0/2625
3	BI	0.56	1/1941 (0.1%)	0.64	0/2625
3	BK	0.49	0/1917	0.65	1/2592 (0.0%)
4	C1	0.37	0/1251	0.49	0/1699
4	C7	0.41	0/1251	0.53	0/1699
4	C9	0.41	0/1251	0.53	0/1699
4	CF	0.50	0/1251	0.56	1/1699 (0.1%)
4	CI	0.50	0/1251	0.56	1/1699 (0.1%)
4	CK	0.37	0/1251	0.48	0/1699
4	E1	0.36	0/1251	0.48	0/1699
4	E7	0.41	0/1251	0.53	0/1699
4	E9	0.41	0/1251	0.53	0/1699
4	EF	0.50	0/1251	0.56	1/1699 (0.1%)
4	EI	0.50	0/1251	0.56	1/1699 (0.1%)
4	EK	0.36	0/1251	0.48	0/1699
4	G1	0.38	0/1251	0.50	0/1699
4	G7	0.41	0/1251	0.53	0/1699

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	G9	0.41	0/1251	0.53	0/1699
4	GF	0.50	0/1251	0.56	1/1699 (0.1%)
4	GI	0.50	0/1251	0.56	1/1699 (0.1%)
4	GK	0.38	0/1251	0.50	0/1699
4	I1	0.40	0/1251	0.52	0/1699
4	I7	0.39	0/1251	0.54	0/1699
4	I9	0.39	0/1251	0.54	0/1699
4	IF	0.50	0/1251	0.56	1/1699 (0.1%)
4	II	0.50	0/1251	0.56	1/1699 (0.1%)
4	IK	0.40	0/1251	0.52	0/1699
4	K1	0.40	0/1251	0.52	0/1699
4	K7	0.41	0/1251	0.53	0/1699
4	K9	0.41	0/1251	0.53	0/1699
4	KF	0.49	0/1251	0.58	1/1699 (0.1%)
4	KI	0.50	0/1251	0.58	1/1699 (0.1%)
4	KK	0.40	0/1251	0.52	0/1699
4	M1	0.38	0/1251	0.51	0/1699
4	M7	0.41	0/1251	0.53	0/1699
4	M9	0.41	0/1251	0.53	0/1699
4	MF	0.50	0/1251	0.64	2/1699 (0.1%)
4	MI	0.50	0/1251	0.64	2/1699 (0.1%)
4	MK	0.38	0/1251	0.51	0/1699
5	D1	0.39	0/1274	0.64	1/1723 (0.1%)
5	D7	0.49	0/1274	0.70	4/1723 (0.2%)
5	D9	0.49	0/1274	0.70	4/1723 (0.2%)
5	DF	0.47	0/1274	0.59	0/1723
5	DI	0.47	0/1274	0.59	0/1723
5	DK	0.39	0/1274	0.64	1/1723 (0.1%)
5	F1	0.42	0/1274	0.68	2/1723 (0.1%)
5	F7	0.46	0/1274	0.61	1/1723 (0.1%)
5	F9	0.46	0/1274	0.61	1/1723 (0.1%)
5	FF	0.46	0/1274	0.60	0/1723
5	FI	0.47	0/1274	0.60	0/1723
5	FK	0.42	0/1274	0.68	2/1723 (0.1%)
5	H1	0.40	0/1274	0.65	1/1723 (0.1%)
5	H7	0.49	0/1274	0.66	2/1723 (0.1%)
5	H9	0.49	0/1274	0.66	2/1723 (0.1%)
5	HF	0.46	0/1274	0.59	0/1723
5	HI	0.46	0/1274	0.59	0/1723
5	HK	0.40	0/1274	0.65	1/1723 (0.1%)
5	J1	0.44	0/1274	0.70	3/1723 (0.2%)
5	J7	0.49	0/1274	0.67	2/1723 (0.1%)
5	J9	0.49	0/1274	0.67	2/1723 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	JF	0.47	0/1274	0.63	0/1723
5	JI	0.47	0/1274	0.63	0/1723
5	JK	0.44	0/1274	0.70	3/1723 (0.2%)
5	L1	0.45	0/1274	0.72	3/1723 (0.2%)
5	L7	0.49	0/1274	0.70	4/1723 (0.2%)
5	L9	0.49	0/1274	0.70	4/1723 (0.2%)
5	LF	0.46	0/1274	0.60	0/1723
5	LI	0.46	0/1274	0.60	0/1723
5	LK	0.45	0/1274	0.72	3/1723 (0.2%)
5	N1	0.41	0/1274	0.67	2/1723 (0.1%)
5	N7	0.49	0/1274	0.69	4/1723 (0.2%)
5	N9	0.49	0/1274	0.69	4/1723 (0.2%)
5	NF	0.46	0/1274	0.63	0/1723
5	NI	0.46	0/1274	0.63	0/1723
5	NK	0.41	0/1274	0.67	2/1723 (0.1%)
6	A3	0.42	1/1271 (0.1%)	0.63	3/1721 (0.2%)
6	AA	0.38	0/1271	0.58	0/1721
6	AC	0.28	0/1271	0.51	1/1721 (0.1%)
6	AE	0.28	0/1271	0.51	1/1721 (0.1%)
6	AG	0.46	0/1271	0.75	4/1721 (0.2%)
6	AJ	0.39	0/1271	0.57	2/1721 (0.1%)
6	AL	0.39	0/1271	0.57	2/1721 (0.1%)
6	AN	0.38	0/1271	0.58	0/1721
6	AO	0.42	1/1271 (0.1%)	0.63	3/1721 (0.2%)
6	AQ	0.46	0/1271	0.76	4/1721 (0.2%)
6	B4	0.61	0/1271	0.82	3/1721 (0.2%)
6	BD	0.61	0/1271	0.82	3/1721 (0.2%)
6	C3	0.40	0/1271	0.68	2/1721 (0.1%)
6	CA	0.38	0/1271	0.59	0/1721
6	CB	0.33	0/1271	0.50	0/1721
6	CC	0.28	0/1271	0.51	1/1721 (0.1%)
6	CE	0.28	0/1271	0.51	1/1721 (0.1%)
6	CG	0.45	0/1271	0.75	4/1721 (0.2%)
6	CJ	0.39	0/1271	0.58	2/1721 (0.1%)
6	CL	0.39	0/1271	0.58	2/1721 (0.1%)
6	CM	0.33	0/1271	0.50	0/1721
6	CN	0.38	0/1271	0.59	0/1721
6	CO	0.40	0/1271	0.68	2/1721 (0.1%)
6	CQ	0.45	0/1271	0.75	4/1721 (0.2%)
6	D4	0.61	0/1271	0.82	3/1721 (0.2%)
6	DD	0.61	0/1271	0.83	3/1721 (0.2%)
6	E3	0.40	0/1271	0.70	2/1721 (0.1%)
6	EA	0.38	0/1271	0.58	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	EB	0.35	0/1271	0.52	0/1721
6	EC	0.28	0/1271	0.51	1/1721 (0.1%)
6	EE	0.28	0/1271	0.51	1/1721 (0.1%)
6	EG	0.46	0/1271	0.75	4/1721 (0.2%)
6	EJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	EL	0.40	0/1271	0.59	2/1721 (0.1%)
6	EM	0.35	0/1271	0.52	0/1721
6	EN	0.38	0/1271	0.58	0/1721
6	EO	0.40	0/1271	0.70	2/1721 (0.1%)
6	EQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	F4	0.61	0/1271	0.83	3/1721 (0.2%)
6	FD	0.61	0/1271	0.83	3/1721 (0.2%)
6	G3	0.39	0/1271	0.69	0/1721
6	GA	0.38	0/1271	0.58	0/1721
6	GB	0.34	0/1271	0.45	0/1721
6	GC	0.28	0/1271	0.51	1/1721 (0.1%)
6	GE	0.28	0/1271	0.51	1/1721 (0.1%)
6	GG	0.46	0/1271	0.75	4/1721 (0.2%)
6	GJ	0.35	0/1271	0.56	2/1721 (0.1%)
6	GL	0.35	0/1271	0.56	2/1721 (0.1%)
6	GM	0.34	0/1271	0.45	0/1721
6	GN	0.38	0/1271	0.58	0/1721
6	GO	0.39	0/1271	0.69	0/1721
6	GQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	H4	0.60	0/1271	0.81	3/1721 (0.2%)
6	HD	0.61	0/1271	0.82	3/1721 (0.2%)
6	I3	0.39	0/1271	0.69	2/1721 (0.1%)
6	IA	0.39	0/1271	0.60	0/1721
6	IB	0.35	0/1271	0.52	0/1721
6	IC	0.28	0/1271	0.51	1/1721 (0.1%)
6	IE	0.28	0/1271	0.51	1/1721 (0.1%)
6	IG	0.46	0/1271	0.75	4/1721 (0.2%)
6	IJ	0.39	0/1271	0.56	2/1721 (0.1%)
6	IL	0.39	0/1271	0.56	2/1721 (0.1%)
6	IM	0.35	0/1271	0.52	0/1721
6	IN	0.39	0/1271	0.60	0/1721
6	IO	0.39	0/1271	0.69	2/1721 (0.1%)
6	IQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	J4	0.63	0/1271	0.84	3/1721 (0.2%)
6	J5	0.95	6/1271 (0.5%)	0.70	1/1721 (0.1%)
6	J8	0.95	6/1271 (0.5%)	0.70	1/1721 (0.1%)
6	JD	0.63	0/1271	0.84	3/1721 (0.2%)
6	K3	0.40	0/1271	0.68	3/1721 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	KA	0.38	0/1271	0.58	0/1721
6	KB	0.34	0/1271	0.49	0/1721
6	KC	0.28	0/1271	0.51	1/1721 (0.1%)
6	KE	0.28	0/1271	0.51	1/1721 (0.1%)
6	KG	0.46	0/1271	0.75	4/1721 (0.2%)
6	KJ	0.40	0/1271	0.57	2/1721 (0.1%)
6	KL	0.40	0/1271	0.57	2/1721 (0.1%)
6	KM	0.34	0/1271	0.49	0/1721
6	KN	0.38	0/1271	0.58	0/1721
6	KO	0.40	0/1271	0.68	3/1721 (0.2%)
6	KQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	L4	0.61	0/1271	0.85	4/1721 (0.2%)
6	LD	0.62	0/1271	0.86	4/1721 (0.2%)
6	M2	0.49	0/1271	0.83	8/1721 (0.5%)
6	MB	0.34	0/1271	0.50	0/1721
6	MJ	0.39	0/1271	0.58	2/1721 (0.1%)
6	ML	0.38	0/1271	0.57	2/1721 (0.1%)
6	MM	0.34	0/1271	0.50	0/1721
6	MR	0.48	0/1271	0.68	3/1721 (0.2%)
6	O1	0.37	0/1271	0.56	1/1721 (0.1%)
6	O2	0.46	0/1270	0.71	4/1721 (0.2%)
6	O7	0.39	0/1271	0.52	0/1721
6	O9	0.39	0/1271	0.52	0/1721
6	OB	0.36	0/1271	0.52	0/1721
6	OF	0.44	1/1271 (0.1%)	0.70	4/1721 (0.2%)
6	OI	0.44	1/1271 (0.1%)	0.70	4/1721 (0.2%)
6	OJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	OK	0.37	0/1271	0.56	1/1721 (0.1%)
6	OL	0.40	0/1271	0.59	2/1721 (0.1%)
6	OM	0.36	0/1271	0.52	0/1721
6	OR	0.46	0/1270	0.71	4/1721 (0.2%)
6	Q1	0.37	0/1271	0.56	1/1721 (0.1%)
6	Q2	0.47	0/1271	0.71	4/1721 (0.2%)
6	Q7	0.39	0/1271	0.52	0/1721
6	Q9	0.39	0/1271	0.52	0/1721
6	QB	0.35	0/1271	0.52	0/1721
6	QF	0.40	0/1271	0.63	2/1721 (0.1%)
6	QI	0.40	0/1271	0.63	2/1721 (0.1%)
6	QJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	QK	0.37	0/1271	0.56	1/1721 (0.1%)
6	QL	0.40	0/1271	0.58	2/1721 (0.1%)
6	QM	0.35	0/1271	0.52	0/1721
6	QR	0.47	0/1271	0.71	4/1721 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	S1	0.37	0/1271	0.56	1/1721 (0.1%)
6	S2	0.46	0/1270	0.73	3/1721 (0.2%)
6	S7	0.39	0/1271	0.51	0/1721
6	S9	0.39	0/1271	0.51	0/1721
6	SB	0.34	0/1271	0.50	0/1721
6	SF	0.40	0/1271	0.63	2/1721 (0.1%)
6	SI	0.40	0/1271	0.63	2/1721 (0.1%)
6	SJ	0.38	0/1271	0.57	2/1721 (0.1%)
6	SK	0.37	0/1271	0.56	1/1721 (0.1%)
6	SL	0.38	0/1271	0.57	2/1721 (0.1%)
6	SM	0.34	0/1271	0.50	0/1721
6	SR	0.47	0/1270	0.87	8/1721 (0.5%)
6	U1	0.37	0/1271	0.56	1/1721 (0.1%)
6	U2	0.46	0/1270	0.72	5/1721 (0.3%)
6	U7	0.39	0/1271	0.52	0/1721
6	U9	0.39	0/1271	0.52	0/1721
6	UB	0.35	0/1271	0.52	0/1721
6	UF	0.40	0/1271	0.65	2/1721 (0.1%)
6	UI	0.40	0/1271	0.65	2/1721 (0.1%)
6	UJ	0.39	0/1271	0.58	2/1721 (0.1%)
6	UK	0.37	0/1271	0.56	1/1721 (0.1%)
6	UL	0.39	0/1271	0.58	2/1721 (0.1%)
6	UM	0.35	0/1271	0.52	0/1721
6	UR	0.46	0/1270	0.71	5/1721 (0.3%)
6	W1	0.36	0/1271	0.54	1/1721 (0.1%)
6	W2	0.47	0/1271	0.73	4/1721 (0.2%)
6	W7	0.38	0/1271	0.52	0/1721
6	W9	0.38	0/1271	0.52	0/1721
6	WB	0.35	0/1271	0.52	0/1721
6	WF	0.40	0/1271	0.63	2/1721 (0.1%)
6	WI	0.40	0/1271	0.63	2/1721 (0.1%)
6	WJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	WK	0.36	0/1271	0.54	1/1721 (0.1%)
6	WL	0.40	0/1271	0.59	2/1721 (0.1%)
6	WM	0.35	0/1271	0.52	0/1721
6	WR	0.46	0/1271	0.74	4/1721 (0.2%)
6	YB	0.34	0/1271	0.50	0/1721
6	YJ	0.39	0/1271	0.59	2/1721 (0.1%)
6	YL	0.39	0/1271	0.58	2/1721 (0.1%)
6	YM	0.34	0/1271	0.51	0/1721
6	Z1	0.37	0/1271	0.55	1/1721 (0.1%)
6	Z7	0.39	0/1271	0.52	0/1721
6	Z9	0.39	0/1271	0.52	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	ZF	0.43	1/1271 (0.1%)	0.59	0/1721
6	ZI	0.43	1/1271 (0.1%)	0.61	0/1721
6	ZK	0.37	0/1271	0.55	1/1721 (0.1%)
6	aB	0.35	0/1271	0.52	0/1721
6	aJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	aL	0.40	0/1271	0.58	2/1721 (0.1%)
6	aM	0.35	0/1271	0.52	0/1721
6	b1	0.37	0/1271	0.56	1/1721 (0.1%)
6	b7	0.39	0/1271	0.52	0/1721
6	b9	0.39	0/1271	0.52	0/1721
6	bF	0.44	1/1271 (0.1%)	0.68	4/1721 (0.2%)
6	bI	0.44	1/1271 (0.1%)	0.68	4/1721 (0.2%)
6	bK	0.37	0/1271	0.56	1/1721 (0.1%)
6	cJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	cL	0.40	0/1271	0.58	2/1721 (0.1%)
6	d1	0.36	0/1271	0.56	1/1721 (0.1%)
6	d7	0.39	0/1271	0.52	0/1721
6	d9	0.39	0/1271	0.52	0/1721
6	dB	0.35	0/1271	0.52	0/1721
6	dF	0.41	0/1271	0.68	2/1721 (0.1%)
6	dI	0.41	0/1271	0.68	2/1721 (0.1%)
6	dK	0.36	0/1271	0.56	1/1721 (0.1%)
6	dM	0.35	0/1271	0.52	0/1721
6	eJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	eL	0.40	0/1271	0.59	2/1721 (0.1%)
6	f1	0.37	0/1271	0.56	1/1721 (0.1%)
6	f7	0.39	0/1271	0.52	0/1721
6	f9	0.39	0/1271	0.52	0/1721
6	fB	0.35	0/1271	0.53	0/1721
6	fF	0.40	0/1271	0.67	3/1721 (0.2%)
6	fI	0.40	0/1271	0.67	3/1721 (0.2%)
6	fK	0.37	0/1271	0.56	1/1721 (0.1%)
6	fM	0.35	0/1271	0.53	0/1721
6	gJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	gL	0.40	0/1271	0.59	2/1721 (0.1%)
6	h1	0.36	0/1271	0.55	1/1721 (0.1%)
6	h7	0.39	0/1271	0.52	0/1721
6	h9	0.39	0/1271	0.52	0/1721
6	hB	0.35	0/1271	0.52	0/1721
6	hF	0.40	0/1271	0.64	2/1721 (0.1%)
6	hI	0.40	0/1271	0.64	2/1721 (0.1%)
6	hK	0.36	0/1271	0.56	1/1721 (0.1%)
6	hM	0.35	0/1271	0.52	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	iJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	iL	0.40	0/1271	0.59	2/1721 (0.1%)
6	j1	0.37	0/1271	0.56	1/1721 (0.1%)
6	j7	0.39	0/1271	0.52	0/1721
6	j9	0.39	0/1271	0.52	0/1721
6	jB	0.35	0/1271	0.50	0/1721
6	jF	0.39	0/1271	0.59	1/1721 (0.1%)
6	jI	0.39	0/1271	0.59	1/1721 (0.1%)
6	jK	0.37	0/1271	0.56	1/1721 (0.1%)
6	jM	0.33	0/1271	0.49	0/1721
6	kJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	kL	0.40	0/1271	0.59	2/1721 (0.1%)
6	l1	0.37	0/1271	0.55	1/1721 (0.1%)
6	l7	0.39	0/1271	0.52	0/1721
6	l9	0.39	0/1271	0.52	0/1721
6	lB	0.34	0/1271	0.50	0/1721
6	lF	0.40	0/1271	0.66	2/1721 (0.1%)
6	lI	0.40	0/1271	0.66	2/1721 (0.1%)
6	lK	0.37	0/1271	0.55	1/1721 (0.1%)
6	lM	0.33	0/1271	0.51	0/1721
6	mJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	mL	0.40	0/1271	0.59	2/1721 (0.1%)
6	oJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	oL	0.40	0/1271	0.59	2/1721 (0.1%)
6	qJ	0.39	0/1271	0.59	2/1721 (0.1%)
6	qL	0.39	0/1271	0.59	2/1721 (0.1%)
6	sJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	sL	0.40	0/1271	0.59	2/1721 (0.1%)
6	uJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	uL	0.40	0/1271	0.59	2/1721 (0.1%)
7	A5	0.42	0/1297	0.63	1/1750 (0.1%)
7	A8	0.42	0/1297	0.63	1/1750 (0.1%)
7	B3	0.40	0/1297	0.78	6/1750 (0.3%)
7	B5	0.33	0/1065	0.51	0/1437
7	B8	0.33	0/1065	0.52	0/1437
7	BA	0.37	0/1297	0.62	2/1750 (0.1%)
7	BC	0.30	0/1297	0.56	0/1750
7	BE	0.30	0/1297	0.56	0/1750
7	BG	0.37	0/1297	0.62	0/1750
7	BJ	0.40	0/1297	0.62	1/1750 (0.1%)
7	BL	0.40	0/1297	0.62	1/1750 (0.1%)
7	BN	0.37	0/1297	0.62	2/1750 (0.1%)
7	BO	0.40	0/1297	0.78	6/1750 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	BQ	0.37	0/1297	0.62	0/1750
7	C4	0.68	0/1297	1.09	10/1750 (0.6%)
7	C5	0.44	0/1297	0.66	2/1750 (0.1%)
7	C8	0.44	0/1297	0.66	2/1750 (0.1%)
7	CD	0.68	0/1297	1.09	10/1750 (0.6%)
7	D3	0.39	0/1297	0.74	6/1750 (0.3%)
7	DA	0.37	0/1297	0.62	2/1750 (0.1%)
7	DB	0.38	0/1309	0.61	1/1766 (0.1%)
7	DC	0.29	0/1297	0.56	0/1750
7	DE	0.29	0/1297	0.56	0/1750
7	DG	0.37	0/1297	0.62	0/1750
7	DJ	0.39	0/1297	0.60	1/1750 (0.1%)
7	DL	0.39	0/1297	0.60	1/1750 (0.1%)
7	DM	0.38	0/1309	0.61	1/1766 (0.1%)
7	DN	0.37	0/1297	0.62	2/1750 (0.1%)
7	DO	0.39	0/1297	0.74	6/1750 (0.3%)
7	DQ	0.37	0/1297	0.62	0/1750
7	E4	0.65	0/1297	1.00	8/1750 (0.5%)
7	ED	0.68	0/1297	1.09	10/1750 (0.6%)
7	F3	0.37	0/1297	0.64	3/1750 (0.2%)
7	F5	0.33	0/1065	0.51	0/1437
7	F8	0.33	0/1065	0.51	0/1437
7	FA	0.36	0/1297	0.62	2/1750 (0.1%)
7	FB	0.38	0/1303	0.62	1/1758 (0.1%)
7	FC	0.30	0/1297	0.56	0/1750
7	FE	0.30	0/1297	0.56	0/1750
7	FG	0.36	0/1297	0.62	0/1750
7	FJ	0.37	0/1297	0.57	1/1750 (0.1%)
7	FL	0.37	0/1297	0.57	1/1750 (0.1%)
7	FM	0.38	0/1303	0.62	1/1758 (0.1%)
7	FN	0.36	0/1297	0.62	2/1750 (0.1%)
7	FO	0.37	0/1297	0.64	3/1750 (0.2%)
7	FQ	0.37	0/1297	0.62	0/1750
7	G4	0.67	0/1297	1.09	10/1750 (0.6%)
7	G5	0.33	0/1065	0.51	0/1437
7	G8	0.33	0/1065	0.51	0/1437
7	GD	0.67	0/1297	1.09	10/1750 (0.6%)
7	H3	0.38	0/1297	0.71	5/1750 (0.3%)
7	H5	0.33	0/1065	0.51	0/1437
7	H8	0.33	0/1065	0.51	0/1437
7	HA	0.37	0/1303	0.62	2/1758 (0.1%)
7	HB	0.38	0/1309	0.62	1/1766 (0.1%)
7	HC	0.30	0/1297	0.56	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	HE	0.30	0/1297	0.56	0/1750
7	HG	0.37	0/1303	0.62	0/1758
7	HJ	0.33	0/1297	0.54	1/1750 (0.1%)
7	HL	0.33	0/1297	0.54	1/1750 (0.1%)
7	HM	0.38	0/1309	0.62	1/1766 (0.1%)
7	HN	0.37	0/1303	0.62	2/1758 (0.1%)
7	HO	0.38	0/1297	0.71	5/1750 (0.3%)
7	HQ	0.37	0/1303	0.62	0/1758
7	I4	0.67	0/1303	1.05	8/1758 (0.5%)
7	I5	0.33	0/1297	0.61	1/1750 (0.1%)
7	I8	0.33	0/1297	0.60	1/1750 (0.1%)
7	ID	0.66	0/1303	1.05	8/1758 (0.5%)
7	J3	0.37	0/1297	0.66	4/1750 (0.2%)
7	JA	0.36	0/1297	0.55	0/1750
7	JB	0.38	0/1309	0.60	1/1766 (0.1%)
7	JC	0.30	0/1297	0.56	0/1750
7	JE	0.30	0/1297	0.56	0/1750
7	JG	0.37	0/1297	0.62	0/1750
7	JJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	JL	0.40	0/1297	0.61	1/1750 (0.1%)
7	JM	0.38	0/1309	0.60	1/1766 (0.1%)
7	JN	0.36	0/1297	0.55	0/1750
7	JO	0.37	0/1297	0.66	4/1750 (0.2%)
7	JQ	0.37	0/1297	0.62	0/1750
7	K4	0.68	0/1297	1.09	10/1750 (0.6%)
7	K5	0.71	2/1297 (0.2%)	0.76	2/1750 (0.1%)
7	K8	0.71	2/1297 (0.2%)	0.76	2/1750 (0.1%)
7	KD	0.68	0/1297	1.09	10/1750 (0.6%)
7	L3	0.38	0/1297	0.68	4/1750 (0.2%)
7	L5	0.33	0/1065	0.52	0/1437
7	L8	0.33	0/1065	0.51	0/1437
7	LA	0.37	0/1297	0.62	2/1750 (0.1%)
7	LB	0.38	0/1309	0.62	1/1766 (0.1%)
7	LC	0.30	0/1297	0.56	0/1750
7	LE	0.30	0/1297	0.56	0/1750
7	LG	0.37	0/1297	0.62	0/1750
7	LJ	0.39	0/1297	0.60	1/1750 (0.1%)
7	LL	0.39	0/1297	0.60	1/1750 (0.1%)
7	LM	0.38	0/1309	0.62	1/1766 (0.1%)
7	LN	0.37	0/1297	0.62	2/1750 (0.1%)
7	LO	0.38	0/1297	0.68	4/1750 (0.2%)
7	LQ	0.36	0/1297	0.62	0/1750
7	M3	0.33	0/1065	0.69	1/1437 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	M4	0.67	0/1297	1.07	8/1750 (0.5%)
7	MD	0.68	0/1297	1.09	10/1750 (0.6%)
7	MO	0.33	0/1065	0.69	1/1437 (0.1%)
7	N2	0.42	0/1297	0.62	0/1750
7	N3	0.32	0/1065	0.63	0/1437
7	NB	0.35	0/1309	0.55	0/1766
7	NJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	NL	0.40	0/1297	0.61	1/1750 (0.1%)
7	NM	0.35	0/1309	0.55	0/1766
7	NO	0.32	0/1065	0.63	0/1437
7	NR	0.42	0/1297	0.62	0/1750
7	P1	0.37	0/1297	0.57	0/1750
7	P2	0.43	0/1303	0.58	0/1758
7	P7	0.37	0/1297	0.51	0/1750
7	P9	0.37	0/1297	0.51	0/1750
7	PB	0.37	0/1297	0.60	1/1750 (0.1%)
7	PF	0.41	0/1297	0.66	2/1750 (0.1%)
7	PI	0.41	0/1297	0.66	2/1750 (0.1%)
7	PJ	0.38	0/1303	0.59	1/1758 (0.1%)
7	PK	0.37	0/1297	0.57	0/1750
7	PL	0.38	0/1303	0.59	1/1758 (0.1%)
7	PM	0.37	0/1297	0.60	1/1750 (0.1%)
7	PR	0.43	0/1303	0.63	1/1758 (0.1%)
7	R1	0.37	0/1297	0.56	0/1750
7	R2	0.41	0/1297	0.63	1/1750 (0.1%)
7	R7	0.38	0/1297	0.53	0/1750
7	R9	0.38	0/1297	0.53	0/1750
7	RB	0.38	0/1303	0.59	1/1758 (0.1%)
7	RF	0.41	0/1297	0.65	2/1750 (0.1%)
7	RI	0.41	0/1297	0.65	2/1750 (0.1%)
7	RJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	RK	0.37	0/1297	0.56	0/1750
7	RL	0.40	0/1297	0.61	1/1750 (0.1%)
7	RM	0.38	0/1303	0.59	1/1758 (0.1%)
7	RR	0.41	0/1297	0.63	1/1750 (0.1%)
7	T1	0.37	0/1297	0.57	0/1750
7	T2	0.43	0/1297	0.62	1/1750 (0.1%)
7	T7	0.37	0/1297	0.52	0/1750
7	T9	0.37	0/1297	0.52	0/1750
7	TB	0.37	0/1303	0.59	1/1758 (0.1%)
7	TF	0.48	1/1297 (0.1%)	0.59	0/1750
7	TI	0.48	1/1297 (0.1%)	0.59	0/1750
7	TJ	0.40	0/1297	0.61	1/1750 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	TK	0.37	0/1297	0.57	0/1750
7	TL	0.40	0/1297	0.61	1/1750 (0.1%)
7	TM	0.37	0/1303	0.59	1/1758 (0.1%)
7	TR	0.43	0/1297	0.62	1/1750 (0.1%)
7	V1	0.37	0/1309	0.56	0/1766
7	V2	0.46	0/1297	0.64	2/1750 (0.1%)
7	V7	0.37	0/1297	0.53	0/1750
7	V9	0.37	0/1297	0.53	0/1750
7	VB	0.37	0/1309	0.59	1/1766 (0.1%)
7	VF	0.44	1/1309 (0.1%)	0.68	2/1766 (0.1%)
7	VI	0.44	1/1309 (0.1%)	0.68	2/1766 (0.1%)
7	VJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	VK	0.37	0/1309	0.56	0/1766
7	VL	0.40	0/1297	0.61	1/1750 (0.1%)
7	VM	0.37	0/1309	0.59	1/1766 (0.1%)
7	VR	0.46	0/1297	0.64	2/1750 (0.1%)
7	X2	0.42	0/1297	0.62	0/1750
7	XB	0.38	0/1309	0.62	1/1766 (0.1%)
7	XJ	0.41	0/1303	0.62	1/1758 (0.1%)
7	XL	0.41	0/1303	0.62	1/1758 (0.1%)
7	XM	0.38	0/1309	0.62	1/1766 (0.1%)
7	XR	0.42	0/1297	0.62	0/1750
7	Y1	0.37	0/1297	0.57	0/1750
7	Y7	0.38	0/1297	0.53	0/1750
7	Y9	0.38	0/1297	0.53	0/1750
7	YF	0.41	0/1297	0.67	2/1750 (0.1%)
7	YI	0.41	0/1297	0.67	2/1750 (0.1%)
7	YK	0.37	0/1297	0.57	0/1750
7	ZB	0.37	0/1309	0.59	1/1766 (0.1%)
7	ZJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	ZL	0.41	0/1297	0.62	1/1750 (0.1%)
7	ZM	0.37	0/1309	0.59	1/1766 (0.1%)
7	a1	0.37	0/1297	0.57	0/1750
7	a7	0.36	0/1297	0.55	0/1750
7	a9	0.36	0/1297	0.55	0/1750
7	aF	0.41	0/1297	0.69	3/1750 (0.2%)
7	aI	0.41	0/1297	0.69	3/1750 (0.2%)
7	aK	0.37	0/1297	0.57	0/1750
7	bJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	bL	0.41	0/1297	0.62	1/1750 (0.1%)
7	c1	0.37	0/1297	0.57	0/1750
7	c7	0.38	0/1297	0.53	0/1750
7	c9	0.38	0/1297	0.53	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	cB	0.38	0/1303	0.62	1/1758 (0.1%)
7	cF	0.43	1/1297 (0.1%)	0.70	2/1750 (0.1%)
7	cI	0.43	1/1297 (0.1%)	0.70	2/1750 (0.1%)
7	cK	0.37	0/1297	0.57	0/1750
7	cM	0.38	0/1303	0.62	1/1758 (0.1%)
7	dJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	dL	0.41	0/1297	0.62	1/1750 (0.1%)
7	e1	0.37	0/1297	0.57	0/1750
7	e7	0.38	0/1297	0.53	0/1750
7	e9	0.38	0/1297	0.53	0/1750
7	eB	0.37	0/1309	0.59	1/1766 (0.1%)
7	eF	0.49	1/1297 (0.1%)	0.73	3/1750 (0.2%)
7	eI	0.49	1/1297 (0.1%)	0.73	3/1750 (0.2%)
7	eK	0.37	0/1297	0.57	0/1750
7	eM	0.37	0/1309	0.59	1/1766 (0.1%)
7	fJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	fL	0.41	0/1297	0.62	1/1750 (0.1%)
7	g1	0.37	0/1297	0.57	0/1750
7	g7	0.38	0/1297	0.53	0/1750
7	g9	0.38	0/1297	0.53	0/1750
7	gB	0.37	0/1309	0.59	1/1766 (0.1%)
7	gF	0.42	0/1297	0.70	2/1750 (0.1%)
7	gI	0.42	0/1297	0.70	2/1750 (0.1%)
7	gK	0.37	0/1297	0.57	0/1750
7	gM	0.37	0/1309	0.59	1/1766 (0.1%)
7	hJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	hL	0.41	0/1297	0.62	1/1750 (0.1%)
7	i1	0.37	0/1303	0.57	0/1758
7	i7	0.37	0/1303	0.52	0/1758
7	i9	0.37	0/1303	0.52	0/1758
7	iB	0.36	0/1309	0.59	0/1766
7	iF	0.42	0/1303	0.68	2/1758 (0.1%)
7	iI	0.42	0/1303	0.68	2/1758 (0.1%)
7	iK	0.37	0/1303	0.57	0/1758
7	iM	0.36	0/1309	0.59	0/1766
7	jJ	0.41	0/1303	0.62	1/1758 (0.1%)
7	jL	0.41	0/1303	0.62	1/1758 (0.1%)
7	k1	0.37	0/1297	0.58	0/1750
7	k7	0.38	0/1297	0.53	0/1750
7	k9	0.38	0/1297	0.53	0/1750
7	kB	0.37	0/1309	0.59	1/1766 (0.1%)
7	kF	0.42	0/1297	0.69	3/1750 (0.2%)
7	kI	0.42	0/1297	0.69	3/1750 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	kK	0.37	0/1297	0.58	0/1750
7	kM	0.37	0/1309	0.59	1/1766 (0.1%)
7	lJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	lL	0.41	0/1297	0.62	1/1750 (0.1%)
7	m1	0.37	0/1297	0.59	0/1750
7	m7	0.37	0/1297	0.53	0/1750
7	m9	0.37	0/1297	0.53	0/1750
7	mB	0.38	0/1309	0.61	1/1766 (0.1%)
7	mF	0.42	0/1297	0.67	2/1750 (0.1%)
7	mI	0.42	0/1297	0.67	2/1750 (0.1%)
7	mK	0.37	0/1297	0.59	0/1750
7	mM	0.38	0/1309	0.61	1/1766 (0.1%)
7	nJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	nL	0.41	0/1297	0.62	1/1750 (0.1%)
7	pJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	pL	0.41	0/1297	0.62	1/1750 (0.1%)
7	rJ	0.40	0/1297	0.62	1/1750 (0.1%)
7	rL	0.40	0/1297	0.62	1/1750 (0.1%)
7	tJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	tL	0.41	0/1297	0.62	1/1750 (0.1%)
7	vJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	vL	0.40	0/1297	0.62	1/1750 (0.1%)
8	e2	0.59	0/1973	0.64	2/2657 (0.1%)
8	eR	0.61	0/1973	0.64	2/2657 (0.1%)
9	O3	0.40	1/2936 (0.0%)	0.61	2/3989 (0.1%)
9	OO	0.40	1/2936 (0.0%)	0.61	2/3989 (0.1%)
10	d4	0.79	0/2332	0.71	1/3145 (0.0%)
10	dD	0.80	0/2332	0.71	1/3145 (0.0%)
11	D5	0.34	0/670	0.58	0/904
11	D8	0.35	0/670	0.58	0/904
12	E5	0.33	0/1612	0.51	0/2179
12	E8	0.34	0/1612	0.50	0/2179
13	k6	0.38	0/2233	0.49	0/3024
13	kH	0.37	0/2233	0.50	0/3024
14	MA	0.43	0/1882	0.64	1/2518 (0.0%)
14	MG	0.51	2/1882 (0.1%)	0.70	5/2518 (0.2%)
14	MN	0.43	0/1882	0.65	2/2518 (0.1%)
14	MQ	0.51	1/1882 (0.1%)	0.70	5/2518 (0.2%)
15	bB	0.44	0/3022	0.60	0/4084
15	bM	0.44	1/3022 (0.0%)	0.60	0/4084
16	AB	0.40	0/1843	0.62	3/2469 (0.1%)
16	AM	0.40	0/1843	0.62	3/2469 (0.1%)
16	wJ	0.47	0/1843	0.85	8/2469 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	wL	0.47	0/1843	0.85	8/2469 (0.3%)
16	xJ	0.47	0/1843	0.85	8/2469 (0.3%)
16	xL	0.48	0/1843	0.86	8/2469 (0.3%)
17	BB	0.42	0/1932	0.60	1/2590 (0.0%)
17	BM	0.42	0/1932	0.60	1/2590 (0.0%)
17	yJ	0.45	0/1932	0.59	1/2590 (0.0%)
17	yL	0.45	0/1932	0.59	1/2590 (0.0%)
18	MC	0.36	0/2247	0.73	6/3036 (0.2%)
18	ME	0.36	0/2247	0.74	7/3036 (0.2%)
19	zJ	0.45	1/2964 (0.0%)	0.60	0/4003
19	zL	0.45	1/2964 (0.0%)	0.59	0/4003
20	AP	0.34	0/1241	0.48	0/1676
20	CP	0.34	0/1241	0.48	0/1676
20	EP	0.34	0/1241	0.48	0/1676
20	GP	0.34	0/1241	0.48	0/1676
20	JP	0.34	0/1241	0.47	0/1676
20	KP	0.34	0/1241	0.48	0/1676
20	NP	0.34	0/1241	0.48	0/1676
20	PP	0.33	0/1241	0.48	0/1676
20	RP	0.34	0/1241	0.48	0/1676
20	TP	0.34	0/1241	0.48	0/1676
20	cP	0.34	0/1241	0.48	0/1676
20	eP	0.34	0/1241	0.48	0/1676
20	gP	0.34	0/1241	0.48	0/1676
20	iP	0.34	0/1241	0.48	0/1676
20	lP	0.34	0/1241	0.48	0/1676
20	mP	0.34	0/1241	0.48	0/1676
20	pP	0.34	0/1241	0.48	0/1676
20	rP	0.33	0/1241	0.47	0/1676
20	tP	0.34	0/1241	0.49	0/1676
20	vP	0.34	0/1241	0.48	0/1676
21	BP	0.33	0/1226	0.46	0/1655
21	DP	0.34	0/1226	0.47	0/1655
21	FP	0.33	0/1226	0.47	0/1655
21	HP	0.34	0/1226	0.47	0/1655
21	IP	0.34	0/1226	0.47	0/1655
21	LP	0.34	0/1226	0.47	0/1655
21	MP	0.33	0/1226	0.46	0/1655
21	OP	0.34	0/1226	0.47	0/1655
21	QP	0.34	0/1226	0.47	0/1655
21	SP	0.34	0/1226	0.47	0/1655
21	UP	0.34	0/1226	0.47	0/1655
21	dP	0.34	0/1226	0.47	0/1655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	fP	0.34	0/1226	0.47	0/1655
21	hP	0.33	0/1226	0.46	0/1655
21	jP	0.34	0/1226	0.47	0/1655
21	kP	0.34	0/1226	0.47	0/1655
21	nP	0.34	0/1226	0.47	0/1655
21	oP	0.33	0/1226	0.47	0/1655
21	qP	0.34	0/1226	0.47	0/1655
21	sP	0.34	0/1226	0.47	0/1655
21	uP	0.34	0/1226	0.46	0/1655
21	wP	0.34	0/1226	0.47	0/1655
22	VP	0.34	0/1281	0.50	2/1731 (0.1%)
22	xP	0.34	0/1281	0.50	2/1731 (0.1%)
23	WP	0.31	0/1396	0.44	0/1886
23	yP	0.31	0/1396	0.44	0/1886
24	XP	0.39	0/732	0.52	0/981
24	zP	0.39	0/732	0.52	0/981
25	1P	0.31	0/6891	0.47	0/9305
25	YP	0.31	0/6891	0.47	0/9305
26	2P	0.33	0/1027	0.54	0/1399
26	ZP	0.33	0/1027	0.54	0/1399
27	3P	0.30	0/1940	0.51	0/2637
27	aP	0.30	0/1940	0.51	0/2637
28	4P	0.29	0/1574	0.48	0/2154
28	bP	0.29	0/1574	0.47	0/2154
All	All	0.41	44/891758 (0.0%)	0.61	861/1205190 (0.1%)

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
6	U2	0	1
6	UR	0	1
7	A5	0	1
7	A8	0	1
7	C5	0	1
7	C8	0	1
12	E5	0	1
12	E8	0	1
21	LP	0	1
21	jP	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	kP	0	1
All	All	0	11

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	eF	69	PRO	N-CD	-9.95	1.33	1.47
7	eI	69	PRO	N-CD	-9.95	1.33	1.47
7	TF	69	PRO	N-CD	-9.94	1.33	1.47
7	TI	69	PRO	N-CD	-9.94	1.33	1.47
6	J5	4	VAL	CB-CG2	-8.97	1.34	1.52
6	J8	4	VAL	CB-CG2	-8.97	1.34	1.52
1	X7	347	TYR	CD1-CE1	-7.46	1.28	1.39
1	X9	347	TYR	CD1-CE1	-7.46	1.28	1.39
6	J5	4	VAL	CB-CG1	-7.33	1.37	1.52
6	J8	4	VAL	CB-CG1	-7.33	1.37	1.52
6	J5	37	ARG	CB-CG	-7.18	1.33	1.52
6	J8	37	ARG	CB-CG	-7.15	1.33	1.52
19	zJ	119	SER	CB-OG	6.95	1.51	1.42
19	zL	119	SER	CB-OG	6.95	1.51	1.42
7	VF	69	PRO	N-CD	-6.55	1.38	1.47
7	VI	69	PRO	N-CD	-6.55	1.38	1.47
6	OF	141	PRO	N-CD	-6.47	1.38	1.47
6	bF	141	PRO	N-CD	-6.47	1.38	1.47
6	OI	141	PRO	N-CD	-6.47	1.38	1.47
6	bI	141	PRO	N-CD	-6.47	1.38	1.47
3	BF	17	VAL	CB-CG2	-6.31	1.39	1.52
3	BI	17	VAL	CB-CG2	-6.31	1.39	1.52
7	K8	8	VAL	CB-CG2	-6.26	1.39	1.52
7	K5	8	VAL	CB-CG2	-6.25	1.39	1.52
7	K5	10	VAL	CB-CG2	-5.73	1.40	1.52
7	K8	10	VAL	CB-CG2	-5.73	1.40	1.52
6	J5	9	VAL	CB-CG2	-5.72	1.40	1.52
6	J8	9	VAL	CB-CG2	-5.72	1.40	1.52
6	J5	9	VAL	CB-CG1	-5.64	1.41	1.52
6	J8	9	VAL	CB-CG1	-5.64	1.41	1.52
9	O3	97	TYR	CD2-CE2	-5.43	1.31	1.39
9	OO	97	TYR	CD2-CE2	-5.43	1.31	1.39
6	A3	141	PRO	N-CD	-5.39	1.40	1.47
6	AO	141	PRO	N-CD	-5.39	1.40	1.47
7	cF	69	PRO	N-CD	-5.28	1.40	1.47
7	cI	69	PRO	N-CD	-5.28	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	MQ	141	TYR	CD2-CE2	-5.21	1.31	1.39
14	MG	141	TYR	CD2-CE2	-5.19	1.31	1.39
6	J5	99	VAL	CB-CG1	-5.17	1.42	1.52
6	J8	99	VAL	CB-CG1	-5.17	1.42	1.52
6	ZF	141	PRO	N-CD	-5.08	1.40	1.47
6	ZI	141	PRO	N-CD	-5.08	1.40	1.47
15	bM	309	VAL	CB-CG2	-5.01	1.42	1.52
14	MG	255	TYR	CD2-CE2	5.00	1.46	1.39

All (861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I4	59	MET	CG-SD-CE	-14.92	76.33	100.20
7	K4	59	MET	CG-SD-CE	-14.91	76.34	100.20
7	ED	59	MET	CG-SD-CE	-14.91	76.34	100.20
7	G4	59	MET	CG-SD-CE	-14.91	76.35	100.20
7	GD	59	MET	CG-SD-CE	-14.90	76.36	100.20
7	KD	59	MET	CG-SD-CE	-14.90	76.36	100.20
7	CD	59	MET	CG-SD-CE	-14.90	76.36	100.20
7	ID	59	MET	CG-SD-CE	-14.90	76.36	100.20
7	C4	59	MET	CG-SD-CE	-14.89	76.38	100.20
7	M4	59	MET	CG-SD-CE	-14.89	76.38	100.20
7	MD	59	MET	CG-SD-CE	-14.87	76.41	100.20
7	GD	39	ASP	CB-CG-OD1	-12.11	107.40	118.30
7	K4	39	ASP	CB-CG-OD1	-12.09	107.42	118.30
7	G4	39	ASP	CB-CG-OD1	-12.08	107.43	118.30
7	C4	39	ASP	CB-CG-OD1	-12.07	107.44	118.30
7	CD	39	ASP	CB-CG-OD1	-12.07	107.44	118.30
7	KD	39	ASP	CB-CG-OD1	-12.07	107.44	118.30
7	M4	39	ASP	CB-CG-OD1	-12.04	107.47	118.30
7	MD	39	ASP	CB-CG-OD1	-12.04	107.47	118.30
7	E4	39	ASP	CB-CG-OD1	-12.02	107.49	118.30
7	ID	39	ASP	CB-CG-OD1	-12.01	107.49	118.30
7	ED	39	ASP	CB-CG-OD1	-11.99	107.51	118.30
7	I4	39	ASP	CB-CG-OD1	-11.98	107.51	118.30
6	SR	142	ARG	NE-CZ-NH2	-11.82	114.39	120.30
6	M2	142	ARG	NE-CZ-NH2	-11.62	114.49	120.30
7	YF	84	ARG	NE-CZ-NH1	11.47	126.04	120.30
7	YI	84	ARG	NE-CZ-NH1	11.47	126.04	120.30
7	RF	84	ARG	NE-CZ-NH1	11.46	126.03	120.30
7	RI	84	ARG	NE-CZ-NH1	11.46	126.03	120.30
7	C4	39	ASP	CB-CG-OD2	11.45	128.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	CD	39	ASP	CB-CG-OD2	11.43	128.59	118.30
7	VF	84	ARG	NE-CZ-NH1	11.43	126.01	120.30
7	VI	84	ARG	NE-CZ-NH1	11.43	126.01	120.30
7	M4	39	ASP	CB-CG-OD2	11.42	128.58	118.30
7	GD	39	ASP	CB-CG-OD2	11.42	128.58	118.30
7	ED	39	ASP	CB-CG-OD2	11.41	128.57	118.30
7	K4	39	ASP	CB-CG-OD2	11.41	128.57	118.30
7	G4	39	ASP	CB-CG-OD2	11.41	128.57	118.30
7	cF	84	ARG	NE-CZ-NH1	11.41	126.00	120.30
7	cI	84	ARG	NE-CZ-NH1	11.41	126.00	120.30
7	E4	39	ASP	CB-CG-OD2	11.40	128.56	118.30
7	KD	39	ASP	CB-CG-OD2	11.38	128.54	118.30
7	mF	84	ARG	NE-CZ-NH1	11.38	125.99	120.30
7	mI	84	ARG	NE-CZ-NH1	11.38	125.99	120.30
7	gF	84	ARG	NE-CZ-NH1	11.38	125.99	120.30
7	gI	84	ARG	NE-CZ-NH1	11.38	125.99	120.30
7	MD	39	ASP	CB-CG-OD2	11.36	128.52	118.30
7	ID	39	ASP	CB-CG-OD2	11.35	128.52	118.30
7	I4	39	ASP	CB-CG-OD2	11.33	128.50	118.30
7	PF	84	ARG	NE-CZ-NH1	11.33	125.97	120.30
7	PI	84	ARG	NE-CZ-NH1	11.33	125.97	120.30
7	eF	84	ARG	NE-CZ-NH1	11.32	125.96	120.30
7	eI	84	ARG	NE-CZ-NH1	11.32	125.96	120.30
7	kF	84	ARG	NE-CZ-NH1	11.32	125.96	120.30
7	kI	84	ARG	NE-CZ-NH1	11.32	125.96	120.30
7	iF	84	ARG	NE-CZ-NH1	11.31	125.96	120.30
7	iI	84	ARG	NE-CZ-NH1	11.31	125.96	120.30
7	aF	84	ARG	NE-CZ-NH1	11.28	125.94	120.30
7	aI	84	ARG	NE-CZ-NH1	11.28	125.94	120.30
16	xJ	86	CYS	CA-CB-SG	10.14	132.26	114.00
16	wL	86	CYS	CA-CB-SG	10.13	132.24	114.00
16	wJ	86	CYS	CA-CB-SG	10.13	132.24	114.00
16	xL	86	CYS	CA-CB-SG	10.13	132.23	114.00
5	N1	77	ARG	NE-CZ-NH2	10.04	125.32	120.30
5	NK	77	ARG	NE-CZ-NH2	10.01	125.31	120.30
5	D1	77	ARG	NE-CZ-NH2	10.00	125.30	120.30
5	DK	77	ARG	NE-CZ-NH2	9.97	125.29	120.30
5	J1	77	ARG	NE-CZ-NH2	9.96	125.28	120.30
5	JK	77	ARG	NE-CZ-NH2	9.96	125.28	120.30
5	L1	77	ARG	NE-CZ-NH2	9.94	125.27	120.30
5	LK	77	ARG	NE-CZ-NH2	9.94	125.27	120.30
5	H1	77	ARG	NE-CZ-NH2	9.91	125.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F1	77	ARG	NE-CZ-NH2	9.89	125.25	120.30
5	FK	77	ARG	NE-CZ-NH2	9.89	125.25	120.30
5	HK	77	ARG	NE-CZ-NH2	9.87	125.24	120.30
7	H3	39	ASP	CB-CG-OD1	9.45	126.80	118.30
7	HO	39	ASP	CB-CG-OD1	9.45	126.80	118.30
7	BA	24	LEU	CB-CG-CD2	-9.43	94.97	111.00
7	DA	24	LEU	CB-CG-CD2	-9.43	94.97	111.00
7	BN	24	LEU	CB-CG-CD2	-9.43	94.97	111.00
7	DN	24	LEU	CB-CG-CD2	-9.43	94.97	111.00
7	B3	39	ASP	CB-CG-OD1	9.42	126.78	118.30
7	BO	39	ASP	CB-CG-OD1	9.42	126.78	118.30
7	LA	24	LEU	CB-CG-CD2	-9.42	94.98	111.00
7	LN	24	LEU	CB-CG-CD2	-9.42	94.98	111.00
7	L3	39	ASP	CB-CG-OD1	9.41	126.77	118.30
7	LO	39	ASP	CB-CG-OD1	9.41	126.77	118.30
7	J3	39	ASP	CB-CG-OD1	9.41	126.77	118.30
7	HA	24	LEU	CB-CG-CD2	-9.41	95.00	111.00
7	HN	24	LEU	CB-CG-CD2	-9.41	95.00	111.00
7	JO	39	ASP	CB-CG-OD1	9.41	126.77	118.30
7	D3	39	ASP	CB-CG-OD1	9.41	126.77	118.30
7	DO	39	ASP	CB-CG-OD1	9.41	126.77	118.30
7	F3	39	ASP	CB-CG-OD1	9.40	126.76	118.30
7	FO	39	ASP	CB-CG-OD1	9.40	126.76	118.30
7	FA	24	LEU	CB-CG-CD2	-9.40	95.03	111.00
7	FN	24	LEU	CB-CG-CD2	-9.40	95.03	111.00
14	MA	145	CYS	CA-CB-SG	9.39	130.90	114.00
14	MN	145	CYS	CA-CB-SG	9.37	130.87	114.00
7	K8	33	ASP	CB-CG-OD1	9.23	126.61	118.30
7	K5	33	ASP	CB-CG-OD1	9.20	126.58	118.30
7	I5	33	ASP	CB-CG-OD1	9.18	126.56	118.30
7	I8	33	ASP	CB-CG-OD1	9.16	126.55	118.30
7	C8	37	ARG	O-C-N	-9.15	108.06	122.70
6	SR	142	ARG	NE-CZ-NH1	9.15	124.87	120.30
7	C5	37	ARG	O-C-N	-9.14	108.08	122.70
6	M2	142	ARG	NE-CZ-NH1	9.06	124.83	120.30
6	SR	142	ARG	CG-CD-NE	8.96	130.62	111.80
6	M2	142	ARG	CG-CD-NE	8.92	130.53	111.80
16	AB	146	PRO	CA-N-CD	-8.90	99.03	111.50
16	AM	146	PRO	CA-N-CD	-8.90	99.04	111.50
16	wJ	146	PRO	CA-N-CD	-8.87	99.08	111.50
16	wL	146	PRO	CA-N-CD	-8.86	99.09	111.50
16	xL	146	PRO	CA-N-CD	-8.86	99.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	ME	309	PRO	CA-N-CD	-8.86	99.10	111.50
16	xJ	146	PRO	CA-N-CD	-8.85	99.11	111.50
18	MC	309	PRO	CA-N-CD	-8.84	99.13	111.50
16	xL	105	ARG	CA-CB-CG	8.55	132.21	113.40
16	xJ	105	ARG	CA-CB-CG	8.55	132.20	113.40
16	wL	105	ARG	CA-CB-CG	8.53	132.17	113.40
16	wJ	105	ARG	CA-CB-CG	8.52	132.15	113.40
8	eR	127	LEU	CB-CG-CD2	-8.51	96.53	111.00
8	e2	127	LEU	CB-CG-CD2	-8.47	96.61	111.00
18	ME	230	LEU	CA-CB-CG	8.38	134.56	115.30
18	MC	230	LEU	CA-CB-CG	8.37	134.54	115.30
6	M2	85	ASP	CB-CG-OD2	8.36	125.82	118.30
6	U2	85	ASP	CB-CG-OD2	8.36	125.82	118.30
6	UR	85	ASP	CB-CG-OD2	8.32	125.79	118.30
6	MR	85	ASP	CB-CG-OD2	8.32	125.79	118.30
6	SR	85	ASP	CB-CG-OD2	8.32	125.79	118.30
6	Q2	85	ASP	CB-CG-OD2	8.29	125.76	118.30
6	QR	85	ASP	CB-CG-OD2	8.26	125.73	118.30
6	WR	85	ASP	CB-CG-OD2	8.25	125.72	118.30
6	O2	85	ASP	CB-CG-OD2	8.24	125.72	118.30
6	S2	85	ASP	CB-CG-OD2	8.24	125.72	118.30
6	OR	85	ASP	CB-CG-OD2	8.24	125.72	118.30
6	W2	85	ASP	CB-CG-OD2	8.22	125.69	118.30
1	X1	216	LEU	CA-CB-CG	7.95	133.58	115.30
1	XK	216	LEU	CA-CB-CG	7.95	133.58	115.30
6	M2	142	ARG	CB-CG-CD	7.87	132.07	111.60
6	SR	142	ARG	CB-CG-CD	7.87	132.06	111.60
9	O3	42	LEU	CA-CB-CG	7.84	133.34	115.30
9	OO	42	LEU	CA-CB-CG	7.84	133.34	115.30
5	L1	33	GLU	CA-CB-CG	7.77	130.49	113.40
7	aF	84	ARG	CD-NE-CZ	7.77	134.47	123.60
7	aI	84	ARG	CD-NE-CZ	7.77	134.47	123.60
5	LK	33	GLU	CA-CB-CG	7.77	130.49	113.40
5	N1	33	GLU	CA-CB-CG	7.76	130.48	113.40
7	iF	84	ARG	CD-NE-CZ	7.76	134.47	123.60
7	iI	84	ARG	CD-NE-CZ	7.76	134.47	123.60
7	kF	84	ARG	CD-NE-CZ	7.76	134.46	123.60
7	kI	84	ARG	CD-NE-CZ	7.76	134.46	123.60
7	eF	84	ARG	CD-NE-CZ	7.75	134.46	123.60
7	eI	84	ARG	CD-NE-CZ	7.75	134.46	123.60
5	NK	33	GLU	CA-CB-CG	7.75	130.45	113.40
4	MF	116	GLU	CA-CB-CG	7.75	130.44	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	MI	116	GLU	CA-CB-CG	7.75	130.44	113.40
5	F1	33	GLU	CA-CB-CG	7.74	130.43	113.40
4	KI	116	GLU	CA-CB-CG	7.74	130.43	113.40
5	FK	33	GLU	CA-CB-CG	7.74	130.43	113.40
4	GF	116	GLU	CA-CB-CG	7.74	130.42	113.40
4	GI	116	GLU	CA-CB-CG	7.74	130.42	113.40
4	KF	116	GLU	CA-CB-CG	7.74	130.42	113.40
7	gF	84	ARG	CD-NE-CZ	7.74	134.43	123.60
7	mF	84	ARG	CD-NE-CZ	7.74	134.43	123.60
7	gI	84	ARG	CD-NE-CZ	7.74	134.43	123.60
7	mI	84	ARG	CD-NE-CZ	7.74	134.43	123.60
5	J1	33	GLU	CA-CB-CG	7.73	130.41	113.40
5	JK	33	GLU	CA-CB-CG	7.73	130.41	113.40
4	CF	116	GLU	CA-CB-CG	7.73	130.40	113.40
7	PF	84	ARG	CD-NE-CZ	7.73	134.42	123.60
4	CI	116	GLU	CA-CB-CG	7.73	130.40	113.40
7	PI	84	ARG	CD-NE-CZ	7.73	134.42	123.60
4	EF	116	GLU	CA-CB-CG	7.72	130.39	113.40
7	VF	84	ARG	CD-NE-CZ	7.72	134.41	123.60
4	EI	116	GLU	CA-CB-CG	7.72	130.39	113.40
7	VI	84	ARG	CD-NE-CZ	7.72	134.41	123.60
7	cF	84	ARG	CD-NE-CZ	7.72	134.41	123.60
7	cI	84	ARG	CD-NE-CZ	7.72	134.41	123.60
4	IF	116	GLU	CA-CB-CG	7.72	130.39	113.40
4	II	116	GLU	CA-CB-CG	7.72	130.39	113.40
7	RF	84	ARG	CD-NE-CZ	7.71	134.40	123.60
7	RI	84	ARG	CD-NE-CZ	7.71	134.40	123.60
7	YF	84	ARG	CD-NE-CZ	7.70	134.38	123.60
7	YI	84	ARG	CD-NE-CZ	7.70	134.38	123.60
5	F9	39	ASP	CB-CG-OD1	7.69	125.22	118.30
5	F7	39	ASP	CB-CG-OD1	7.68	125.22	118.30
5	D7	39	ASP	CB-CG-OD1	7.65	125.18	118.30
5	D9	39	ASP	CB-CG-OD1	7.65	125.18	118.30
5	H7	39	ASP	CB-CG-OD1	7.64	125.18	118.30
5	H9	39	ASP	CB-CG-OD1	7.64	125.18	118.30
5	J7	39	ASP	CB-CG-OD1	7.63	125.17	118.30
5	J9	39	ASP	CB-CG-OD1	7.63	125.17	118.30
5	L9	39	ASP	CB-CG-OD1	7.59	125.13	118.30
5	N7	39	ASP	CB-CG-OD1	7.59	125.13	118.30
5	N9	39	ASP	CB-CG-OD1	7.59	125.13	118.30
5	L7	39	ASP	CB-CG-OD1	7.58	125.12	118.30
6	AG	98	VAL	CA-CB-CG2	7.57	122.25	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AQ	98	VAL	CA-CB-CG2	7.57	122.25	110.90
6	EG	98	VAL	CA-CB-CG2	7.55	122.22	110.90
6	EQ	98	VAL	CA-CB-CG2	7.55	122.22	110.90
6	IG	98	VAL	CA-CB-CG2	7.54	122.21	110.90
6	IQ	98	VAL	CA-CB-CG2	7.54	122.21	110.90
6	GG	98	VAL	CA-CB-CG2	7.54	122.21	110.90
6	GQ	98	VAL	CA-CB-CG2	7.54	122.21	110.90
6	CG	98	VAL	CA-CB-CG2	7.54	122.20	110.90
6	CQ	98	VAL	CA-CB-CG2	7.54	122.20	110.90
6	KG	98	VAL	CA-CB-CG2	7.53	122.20	110.90
6	KQ	98	VAL	CA-CB-CG2	7.53	122.20	110.90
16	xJ	140	LYS	CD-CE-NZ	-7.51	94.43	111.70
16	xL	140	LYS	CD-CE-NZ	-7.51	94.43	111.70
5	L9	115	GLU	CA-CB-CG	7.50	129.90	113.40
5	L7	115	GLU	CA-CB-CG	7.49	129.88	113.40
16	wL	140	LYS	CD-CE-NZ	-7.49	94.48	111.70
5	J9	115	GLU	CA-CB-CG	7.48	129.86	113.40
5	D7	115	GLU	CA-CB-CG	7.48	129.86	113.40
5	D9	115	GLU	CA-CB-CG	7.48	129.86	113.40
5	H7	115	GLU	CA-CB-CG	7.48	129.85	113.40
5	H9	115	GLU	CA-CB-CG	7.48	129.85	113.40
5	J7	115	GLU	CA-CB-CG	7.48	129.85	113.40
16	wJ	140	LYS	CD-CE-NZ	-7.47	94.51	111.70
5	N7	115	GLU	CA-CB-CG	7.47	129.84	113.40
5	N9	115	GLU	CA-CB-CG	7.47	129.84	113.40
16	xL	105	ARG	CB-CG-CD	7.42	130.90	111.60
16	xJ	105	ARG	CB-CG-CD	7.39	130.82	111.60
16	wL	105	ARG	CB-CG-CD	7.39	130.81	111.60
16	wJ	105	ARG	CB-CG-CD	7.38	130.80	111.60
16	AB	269	ASP	CB-CG-OD1	7.38	124.94	118.30
7	nJ	157	ASP	CB-CG-OD1	7.37	124.93	118.30
7	nL	157	ASP	CB-CG-OD1	7.37	124.93	118.30
7	dJ	157	ASP	CB-CG-OD1	7.37	124.93	118.30
7	dL	157	ASP	CB-CG-OD1	7.37	124.93	118.30
7	NJ	157	ASP	CB-CG-OD1	7.36	124.92	118.30
7	IJ	157	ASP	CB-CG-OD1	7.36	124.92	118.30
7	NL	157	ASP	CB-CG-OD1	7.36	124.92	118.30
7	IL	157	ASP	CB-CG-OD1	7.36	124.92	118.30
7	ZJ	157	ASP	CB-CG-OD1	7.35	124.92	118.30
7	ZL	157	ASP	CB-CG-OD1	7.35	124.92	118.30
7	HJ	157	ASP	CB-CG-OD1	7.35	124.92	118.30
7	HL	157	ASP	CB-CG-OD1	7.35	124.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AM	269	ASP	CB-CG-OD1	7.34	124.91	118.30
7	M4	59	MET	CA-CB-CG	-7.34	100.83	113.30
7	DJ	157	ASP	CB-CG-OD1	7.34	124.90	118.30
7	XJ	157	ASP	CB-CG-OD1	7.34	124.90	118.30
7	DL	157	ASP	CB-CG-OD1	7.34	124.90	118.30
7	XL	157	ASP	CB-CG-OD1	7.34	124.90	118.30
7	JJ	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	JL	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	PJ	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	fJ	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	PL	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	fL	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	bJ	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	bL	157	ASP	CB-CG-OD1	7.33	124.90	118.30
7	ED	59	MET	CA-CB-CG	-7.33	100.85	113.30
7	GD	59	MET	CA-CB-CG	-7.33	100.85	113.30
7	LJ	157	ASP	CB-CG-OD1	7.32	124.89	118.30
7	LL	157	ASP	CB-CG-OD1	7.32	124.89	118.30
7	VJ	157	ASP	CB-CG-OD1	7.32	124.89	118.30
7	VL	157	ASP	CB-CG-OD1	7.32	124.89	118.30
7	MD	59	MET	CA-CB-CG	-7.32	100.86	113.30
7	rJ	157	ASP	CB-CG-OD1	7.32	124.89	118.30
7	rL	157	ASP	CB-CG-OD1	7.32	124.89	118.30
7	C4	59	MET	CA-CB-CG	-7.32	100.86	113.30
7	K4	59	MET	CA-CB-CG	-7.32	100.86	113.30
7	BJ	157	ASP	CB-CG-OD1	7.32	124.88	118.30
7	BL	157	ASP	CB-CG-OD1	7.32	124.88	118.30
7	RJ	157	ASP	CB-CG-OD1	7.31	124.88	118.30
7	RL	157	ASP	CB-CG-OD1	7.31	124.88	118.30
7	TJ	157	ASP	CB-CG-OD1	7.31	124.88	118.30
7	TL	157	ASP	CB-CG-OD1	7.31	124.88	118.30
7	KD	59	MET	CA-CB-CG	-7.31	100.88	113.30
7	jJ	157	ASP	CB-CG-OD1	7.31	124.88	118.30
7	jL	157	ASP	CB-CG-OD1	7.31	124.88	118.30
7	hJ	157	ASP	CB-CG-OD1	7.30	124.87	118.30
7	hL	157	ASP	CB-CG-OD1	7.30	124.87	118.30
7	G4	59	MET	CA-CB-CG	-7.30	100.89	113.30
7	CD	59	MET	CA-CB-CG	-7.30	100.90	113.30
7	vJ	157	ASP	CB-CG-OD1	7.29	124.86	118.30
7	vL	157	ASP	CB-CG-OD1	7.29	124.86	118.30
7	FJ	157	ASP	CB-CG-OD1	7.29	124.86	118.30
7	pJ	157	ASP	CB-CG-OD1	7.29	124.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	FL	157	ASP	CB-CG-OD1	7.29	124.86	118.30
7	pL	157	ASP	CB-CG-OD1	7.29	124.86	118.30
7	I4	59	MET	CA-CB-CG	-7.29	100.91	113.30
7	ID	59	MET	CA-CB-CG	-7.28	100.92	113.30
6	CG	44	LEU	CA-CB-CG	7.23	131.94	115.30
6	CQ	44	LEU	CA-CB-CG	7.23	131.94	115.30
7	tJ	157	ASP	CB-CG-OD1	7.23	124.81	118.30
7	tL	157	ASP	CB-CG-OD1	7.23	124.81	118.30
14	MQ	145	CYS	CA-CB-SG	7.22	127.00	114.00
7	CD	51	MET	CA-CB-CG	-7.21	101.04	113.30
6	IG	44	LEU	CA-CB-CG	7.21	131.88	115.30
6	IQ	44	LEU	CA-CB-CG	7.21	131.88	115.30
6	KG	44	LEU	CA-CB-CG	7.21	131.87	115.30
6	KQ	44	LEU	CA-CB-CG	7.21	131.87	115.30
6	GG	44	LEU	CA-CB-CG	7.21	131.87	115.30
6	GQ	44	LEU	CA-CB-CG	7.21	131.87	115.30
6	AG	44	LEU	CA-CB-CG	7.20	131.87	115.30
6	AQ	44	LEU	CA-CB-CG	7.20	131.87	115.30
6	EG	44	LEU	CA-CB-CG	7.19	131.84	115.30
6	EQ	44	LEU	CA-CB-CG	7.19	131.84	115.30
18	MC	48	LEU	CA-CB-CG	7.19	131.84	115.30
14	MG	145	CYS	CA-CB-SG	7.19	126.94	114.00
18	ME	48	LEU	CA-CB-CG	7.19	131.83	115.30
7	I4	51	MET	CA-CB-CG	-7.17	101.11	113.30
7	C4	51	MET	CA-CB-CG	-7.16	101.12	113.30
7	ID	51	MET	CA-CB-CG	-7.16	101.13	113.30
7	E4	51	MET	CA-CB-CG	-7.15	101.14	113.30
7	K4	51	MET	CA-CB-CG	-7.14	101.16	113.30
7	G4	51	MET	CA-CB-CG	-7.14	101.17	113.30
7	ED	51	MET	CA-CB-CG	-7.13	101.18	113.30
7	GD	51	MET	CA-CB-CG	-7.12	101.20	113.30
7	KD	51	MET	CA-CB-CG	-7.11	101.21	113.30
7	MD	51	MET	CA-CB-CG	-7.11	101.21	113.30
6	U2	85	ASP	CB-CG-OD1	-7.11	111.90	118.30
6	SR	85	ASP	CB-CG-OD1	-7.11	111.90	118.30
6	QR	85	ASP	CB-CG-OD1	-7.08	111.93	118.30
6	M2	85	ASP	CB-CG-OD1	-7.07	111.94	118.30
6	W2	85	ASP	CB-CG-OD1	-7.06	111.94	118.30
7	CD	171	ARG	CG-CD-NE	7.05	126.61	111.80
6	O2	85	ASP	CB-CG-OD1	-7.05	111.96	118.30
6	Q2	85	ASP	CB-CG-OD1	-7.05	111.96	118.30
6	S2	85	ASP	CB-CG-OD1	-7.04	111.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	GD	171	ARG	CG-CD-NE	7.04	126.59	111.80
7	C4	171	ARG	CG-CD-NE	7.04	126.58	111.80
7	ED	171	ARG	CG-CD-NE	7.03	126.57	111.80
7	K4	171	ARG	CG-CD-NE	7.03	126.56	111.80
6	MR	85	ASP	CB-CG-OD1	-7.03	111.97	118.30
7	E4	171	ARG	CG-CD-NE	7.03	126.56	111.80
6	OR	85	ASP	CB-CG-OD1	-7.03	111.98	118.30
6	UR	85	ASP	CB-CG-OD1	-7.03	111.98	118.30
7	G4	171	ARG	CG-CD-NE	7.02	126.55	111.80
7	I4	171	ARG	CG-CD-NE	7.02	126.55	111.80
7	MD	171	ARG	CG-CD-NE	7.02	126.55	111.80
7	M4	171	ARG	CG-CD-NE	7.02	126.54	111.80
7	KD	171	ARG	CG-CD-NE	7.02	126.54	111.80
7	ID	171	ARG	CG-CD-NE	7.01	126.52	111.80
6	WR	85	ASP	CB-CG-OD1	-7.01	111.99	118.30
7	B3	177	SER	N-CA-CB	6.98	120.97	110.50
7	BO	177	SER	N-CA-CB	6.98	120.97	110.50
7	L3	177	SER	N-CA-CB	6.98	120.97	110.50
7	LO	177	SER	N-CA-CB	6.98	120.97	110.50
7	D3	177	SER	N-CA-CB	6.97	120.95	110.50
7	DO	177	SER	N-CA-CB	6.97	120.95	110.50
6	fF	50	ALA	N-CA-CB	6.93	119.80	110.10
6	fI	50	ALA	N-CA-CB	6.93	119.80	110.10
6	dF	50	ALA	N-CA-CB	6.92	119.80	110.10
6	dI	50	ALA	N-CA-CB	6.92	119.80	110.10
6	lF	50	ALA	N-CA-CB	6.92	119.78	110.10
6	lI	50	ALA	N-CA-CB	6.92	119.78	110.10
6	oF	50	ALA	N-CA-CB	6.91	119.77	110.10
6	oI	50	ALA	N-CA-CB	6.91	119.77	110.10
6	jF	50	ALA	N-CA-CB	6.90	119.76	110.10
6	jI	50	ALA	N-CA-CB	6.90	119.76	110.10
18	MC	99	MET	CA-CB-CG	6.90	125.03	113.30
6	qF	50	ALA	N-CA-CB	6.90	119.76	110.10
6	qI	50	ALA	N-CA-CB	6.90	119.76	110.10
6	sF	50	ALA	N-CA-CB	6.89	119.75	110.10
6	hF	50	ALA	N-CA-CB	6.89	119.75	110.10
6	sI	50	ALA	N-CA-CB	6.89	119.75	110.10
6	hI	50	ALA	N-CA-CB	6.89	119.75	110.10
18	ME	99	MET	CA-CB-CG	6.89	125.01	113.30
6	uF	50	ALA	N-CA-CB	6.88	119.74	110.10
6	uI	50	ALA	N-CA-CB	6.88	119.74	110.10
7	I4	171	ARG	NE-CZ-NH1	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C4	171	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	X1	125	LEU	CB-CG-CD2	-6.86	99.34	111.00
6	WF	50	ALA	N-CA-CB	6.86	119.70	110.10
6	bF	50	ALA	N-CA-CB	6.86	119.70	110.10
6	WI	50	ALA	N-CA-CB	6.86	119.70	110.10
6	bI	50	ALA	N-CA-CB	6.86	119.70	110.10
1	XK	125	LEU	CB-CG-CD2	-6.86	99.34	111.00
7	CD	171	ARG	NE-CZ-NH1	6.86	123.73	120.30
7	ID	171	ARG	NE-CZ-NH1	6.86	123.73	120.30
3	B7	89	LEU	CA-CB-CG	6.83	131.01	115.30
3	B9	89	LEU	CA-CB-CG	6.83	131.01	115.30
6	OF	141	PRO	N-CD-CG	-6.83	92.95	103.20
6	OI	141	PRO	N-CD-CG	-6.83	92.95	103.20
7	M4	171	ARG	NE-CZ-NH1	6.81	123.70	120.30
6	bF	141	PRO	N-CD-CG	-6.80	93.00	103.20
6	bI	141	PRO	N-CD-CG	-6.80	93.00	103.20
7	E4	171	ARG	NE-CZ-NH1	6.76	123.68	120.30
6	LD	114	ARG	CA-CB-CG	-6.74	98.57	113.40
6	L4	114	ARG	CA-CB-CG	-6.71	98.63	113.40
7	K4	171	ARG	NE-CZ-NH1	6.71	123.66	120.30
7	G4	171	ARG	NE-CZ-NH1	6.71	123.65	120.30
7	GD	171	ARG	NE-CZ-NH1	6.71	123.65	120.30
7	KD	171	ARG	NE-CZ-NH1	6.70	123.65	120.30
7	MD	171	ARG	NE-CZ-NH1	6.69	123.65	120.30
7	H3	107	ASP	N-CA-CB	-6.65	98.64	110.60
7	HO	107	ASP	N-CA-CB	-6.65	98.64	110.60
7	ED	171	ARG	NE-CZ-NH1	6.63	123.62	120.30
6	OR	33	ARG	CG-CD-NE	-6.48	98.19	111.80
6	M2	33	ARG	CG-CD-NE	-6.48	98.20	111.80
6	UR	33	ARG	CG-CD-NE	-6.47	98.21	111.80
2	A1	157	ASP	CB-CG-OD1	-6.47	112.48	118.30
2	AK	157	ASP	CB-CG-OD1	-6.47	112.48	118.30
6	J5	38	LEU	CB-CG-CD1	-6.47	100.00	111.00
6	J8	38	LEU	CB-CG-CD1	-6.47	100.00	111.00
6	MR	33	ARG	CG-CD-NE	-6.47	98.22	111.80
6	Q2	33	ARG	CG-CD-NE	-6.46	98.23	111.80
6	U2	33	ARG	CG-CD-NE	-6.46	98.23	111.80
6	O2	33	ARG	CG-CD-NE	-6.45	98.25	111.80
6	QR	33	ARG	CG-CD-NE	-6.45	98.25	111.80
6	W2	33	ARG	CG-CD-NE	-6.44	98.28	111.80
6	A3	141	PRO	N-CD-CG	-6.43	93.55	103.20
6	AO	141	PRO	N-CD-CG	-6.43	93.55	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	WR	33	ARG	CG-CD-NE	-6.43	98.30	111.80
2	AF	189	LEU	CA-CB-CG	6.34	129.87	115.30
2	AI	189	LEU	CA-CB-CG	6.34	129.87	115.30
6	A3	141	PRO	N-CA-CB	-6.31	95.66	102.60
6	AO	141	PRO	N-CA-CB	-6.31	95.66	102.60
7	M3	63	ASN	N-CA-CB	-6.30	99.26	110.60
7	MO	63	ASN	N-CA-CB	-6.30	99.26	110.60
6	iJ	84	ARG	NE-CZ-NH1	6.21	123.41	120.30
6	iL	84	ARG	NE-CZ-NH1	6.21	123.41	120.30
6	SJ	84	ARG	NE-CZ-NH1	6.19	123.39	120.30
6	SL	84	ARG	NE-CZ-NH1	6.19	123.39	120.30
6	CJ	84	ARG	NE-CZ-NH1	6.18	123.39	120.30
6	CL	84	ARG	NE-CZ-NH1	6.18	123.39	120.30
22	VP	144	GLU	CA-CB-CG	6.18	127.00	113.40
22	xP	144	GLU	CA-CB-CG	6.16	126.96	113.40
6	OJ	84	ARG	NE-CZ-NH1	6.16	123.38	120.30
6	OL	84	ARG	NE-CZ-NH1	6.16	123.38	120.30
6	qJ	84	ARG	NE-CZ-NH1	6.15	123.38	120.30
6	qL	84	ARG	NE-CZ-NH1	6.15	123.38	120.30
6	I3	42	GLU	CB-CA-C	-6.15	98.11	110.40
6	IO	42	GLU	CB-CA-C	-6.15	98.11	110.40
6	aJ	84	ARG	NE-CZ-NH1	6.14	123.37	120.30
6	aL	84	ARG	NE-CZ-NH1	6.14	123.37	120.30
6	cJ	84	ARG	NE-CZ-NH1	6.13	123.37	120.30
6	cL	84	ARG	NE-CZ-NH1	6.13	123.37	120.30
6	AJ	84	ARG	NE-CZ-NH1	6.13	123.36	120.30
6	AL	84	ARG	NE-CZ-NH1	6.13	123.36	120.30
7	aF	107	ASP	N-CA-CB	-6.12	99.58	110.60
7	aI	107	ASP	N-CA-CB	-6.12	99.58	110.60
6	UJ	84	ARG	NE-CZ-NH1	6.12	123.36	120.30
6	UL	84	ARG	NE-CZ-NH1	6.12	123.36	120.30
6	MJ	84	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	YJ	84	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	ML	84	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	YL	84	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	kJ	84	ARG	NE-CZ-NH1	6.09	123.34	120.30
6	kL	84	ARG	NE-CZ-NH1	6.09	123.34	120.30
6	QJ	84	ARG	NE-CZ-NH1	6.08	123.34	120.30
6	QL	84	ARG	NE-CZ-NH1	6.08	123.34	120.30
6	IJ	84	ARG	NE-CZ-NH1	6.07	123.34	120.30
6	IL	84	ARG	NE-CZ-NH1	6.07	123.34	120.30
6	uJ	84	ARG	NE-CZ-NH1	6.07	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	uL	84	ARG	NE-CZ-NH1	6.07	123.33	120.30
6	KJ	84	ARG	NE-CZ-NH1	6.06	123.33	120.30
6	KL	84	ARG	NE-CZ-NH1	6.06	123.33	120.30
6	EJ	84	ARG	NE-CZ-NH1	6.04	123.32	120.30
6	EL	84	ARG	NE-CZ-NH1	6.04	123.32	120.30
6	WJ	84	ARG	NE-CZ-NH1	6.03	123.32	120.30
6	WL	84	ARG	NE-CZ-NH1	6.03	123.32	120.30
6	sJ	84	ARG	NE-CZ-NH1	6.02	123.31	120.30
6	sL	84	ARG	NE-CZ-NH1	6.02	123.31	120.30
6	mJ	84	ARG	NE-CZ-NH1	6.00	123.30	120.30
6	mL	84	ARG	NE-CZ-NH1	6.00	123.30	120.30
6	GJ	84	ARG	NE-CZ-NH1	6.00	123.30	120.30
6	GL	84	ARG	NE-CZ-NH1	6.00	123.30	120.30
6	oJ	84	ARG	NE-CZ-NH1	5.99	123.29	120.30
6	oL	84	ARG	NE-CZ-NH1	5.99	123.29	120.30
9	O3	258	ILE	C-N-CA	5.98	136.65	121.70
6	OF	141	PRO	N-CA-CB	-5.98	96.02	102.60
6	OI	141	PRO	N-CA-CB	-5.98	96.02	102.60
9	OO	258	ILE	C-N-CA	5.98	136.65	121.70
6	bF	141	PRO	N-CA-CB	-5.97	96.03	102.60
6	bI	141	PRO	N-CA-CB	-5.97	96.03	102.60
6	gJ	84	ARG	NE-CZ-NH1	5.97	123.28	120.30
6	gL	84	ARG	NE-CZ-NH1	5.97	123.28	120.30
16	xL	57	LYS	CA-CB-CG	5.97	126.53	113.40
7	eF	132	SER	N-CA-CB	5.97	119.45	110.50
7	eI	132	SER	N-CA-CB	5.97	119.45	110.50
6	eJ	84	ARG	NE-CZ-NH1	5.97	123.28	120.30
6	eL	84	ARG	NE-CZ-NH1	5.97	123.28	120.30
16	xJ	57	LYS	CA-CB-CG	5.95	126.48	113.40
16	wL	57	LYS	CA-CB-CG	5.94	126.47	113.40
16	wJ	57	LYS	CA-CB-CG	5.94	126.46	113.40
7	B3	25	GLN	CA-CB-CG	5.92	126.43	113.40
7	BO	25	GLN	CA-CB-CG	5.92	126.43	113.40
7	F3	25	GLN	CA-CB-CG	5.92	126.42	113.40
7	FO	25	GLN	CA-CB-CG	5.92	126.42	113.40
7	H3	25	GLN	CA-CB-CG	5.91	126.40	113.40
7	HO	25	GLN	CA-CB-CG	5.91	126.40	113.40
7	J3	25	GLN	CA-CB-CG	5.91	126.39	113.40
7	JO	25	GLN	CA-CB-CG	5.91	126.39	113.40
7	L3	25	GLN	CA-CB-CG	5.90	126.38	113.40
7	LO	25	GLN	CA-CB-CG	5.90	126.38	113.40
7	D3	25	GLN	CA-CB-CG	5.89	126.36	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	DO	25	GLN	CA-CB-CG	5.89	126.36	113.40
6	EG	156	LEU	CA-CB-CG	5.87	128.80	115.30
6	EQ	156	LEU	CA-CB-CG	5.87	128.80	115.30
6	CG	156	LEU	CA-CB-CG	5.87	128.79	115.30
6	CQ	156	LEU	CA-CB-CG	5.87	128.79	115.30
7	D3	39	ASP	CB-CG-OD2	-5.86	113.02	118.30
7	DO	39	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	X1	154	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	XK	154	LEU	CB-CG-CD2	-5.86	101.03	111.00
7	FA	24	LEU	CB-CG-CD1	5.85	120.95	111.00
7	FN	24	LEU	CB-CG-CD1	5.85	120.95	111.00
7	C5	37	ARG	C-N-CA	5.85	136.32	121.70
7	C8	37	ARG	C-N-CA	5.84	136.31	121.70
6	GG	156	LEU	CA-CB-CG	5.84	128.74	115.30
6	GQ	156	LEU	CA-CB-CG	5.84	128.74	115.30
6	IG	156	LEU	CA-CB-CG	5.84	128.73	115.30
6	IQ	156	LEU	CA-CB-CG	5.84	128.73	115.30
7	B3	39	ASP	CB-CG-OD2	-5.84	113.05	118.30
7	BO	39	ASP	CB-CG-OD2	-5.84	113.05	118.30
6	KG	156	LEU	CA-CB-CG	5.83	128.71	115.30
6	KQ	156	LEU	CA-CB-CG	5.83	128.71	115.30
6	AG	156	LEU	CA-CB-CG	5.82	128.70	115.30
6	AQ	156	LEU	CA-CB-CG	5.82	128.70	115.30
14	MN	101	LEU	CA-CB-CG	5.82	128.69	115.30
7	H3	39	ASP	CB-CG-OD2	-5.81	113.07	118.30
7	L3	39	ASP	CB-CG-OD2	-5.81	113.07	118.30
7	HO	39	ASP	CB-CG-OD2	-5.81	113.07	118.30
7	LO	39	ASP	CB-CG-OD2	-5.81	113.07	118.30
7	F3	39	ASP	CB-CG-OD2	-5.80	113.08	118.30
7	BA	24	LEU	CB-CG-CD1	5.80	120.87	111.00
7	BN	24	LEU	CB-CG-CD1	5.80	120.87	111.00
7	FO	39	ASP	CB-CG-OD2	-5.80	113.08	118.30
7	HA	24	LEU	CB-CG-CD1	5.80	120.86	111.00
7	HN	24	LEU	CB-CG-CD1	5.80	120.86	111.00
7	DA	24	LEU	CB-CG-CD1	5.80	120.86	111.00
7	DN	24	LEU	CB-CG-CD1	5.80	120.86	111.00
7	LA	24	LEU	CB-CG-CD1	5.79	120.85	111.00
7	LN	24	LEU	CB-CG-CD1	5.79	120.85	111.00
6	C3	42	GLU	CB-CA-C	-5.78	98.84	110.40
6	CO	42	GLU	CB-CA-C	-5.78	98.84	110.40
7	J3	39	ASP	CB-CG-OD2	-5.77	113.11	118.30
7	JO	39	ASP	CB-CG-OD2	-5.77	113.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L7	77	ARG	NE-CZ-NH2	5.74	123.17	120.30
7	RR	79	MET	CB-CG-SD	5.73	129.58	112.40
7	R2	79	MET	CB-CG-SD	5.72	129.56	112.40
7	T2	79	MET	CB-CG-SD	5.72	129.56	112.40
5	N7	77	ARG	NE-CZ-NH2	5.71	123.16	120.30
5	N9	77	ARG	NE-CZ-NH2	5.71	123.16	120.30
7	V2	62	GLU	N-CA-CB	5.71	120.88	110.60
7	PR	79	MET	CB-CG-SD	5.71	129.53	112.40
7	VR	62	GLU	N-CA-CB	5.71	120.88	110.60
7	E4	77	ARG	NE-CZ-NH1	5.70	123.15	120.30
7	TR	79	MET	CB-CG-SD	5.70	129.51	112.40
7	ED	77	ARG	NE-CZ-NH1	5.70	123.15	120.30
7	V2	79	MET	CB-CG-SD	5.69	129.48	112.40
7	VR	79	MET	CB-CG-SD	5.69	129.47	112.40
7	CD	77	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	LB	115	GLU	CA-CB-CG	5.67	125.87	113.40
7	LM	115	GLU	CA-CB-CG	5.67	125.87	113.40
7	PB	115	GLU	CA-CB-CG	5.67	125.87	113.40
7	PM	115	GLU	CA-CB-CG	5.67	125.87	113.40
7	VB	115	GLU	CA-CB-CG	5.67	125.87	113.40
7	eB	115	GLU	CA-CB-CG	5.67	125.86	113.40
7	VM	115	GLU	CA-CB-CG	5.67	125.87	113.40
7	eM	115	GLU	CA-CB-CG	5.67	125.86	113.40
7	TB	115	GLU	CA-CB-CG	5.66	125.85	113.40
7	cB	115	GLU	CA-CB-CG	5.66	125.85	113.40
7	TM	115	GLU	CA-CB-CG	5.66	125.85	113.40
7	cM	115	GLU	CA-CB-CG	5.66	125.85	113.40
6	Q1	137	ARG	NE-CZ-NH2	-5.66	117.47	120.30
6	QK	137	ARG	NE-CZ-NH2	-5.66	117.47	120.30
7	JB	115	GLU	CA-CB-CG	5.65	125.84	113.40
7	JM	115	GLU	CA-CB-CG	5.65	125.84	113.40
6	Z1	137	ARG	NE-CZ-NH2	-5.65	117.47	120.30
7	K4	77	ARG	NE-CZ-NH1	5.65	123.13	120.30
6	ZK	137	ARG	NE-CZ-NH2	-5.65	117.47	120.30
7	G4	77	ARG	NE-CZ-NH1	5.65	123.13	120.30
5	L9	77	ARG	NE-CZ-NH2	5.65	123.12	120.30
7	ZB	115	GLU	CA-CB-CG	5.65	125.83	113.40
7	kB	115	GLU	CA-CB-CG	5.65	125.83	113.40
7	ZM	115	GLU	CA-CB-CG	5.65	125.83	113.40
7	kM	115	GLU	CA-CB-CG	5.65	125.83	113.40
7	gB	115	GLU	CA-CB-CG	5.65	125.82	113.40
7	gM	115	GLU	CA-CB-CG	5.65	125.82	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	mB	115	GLU	CA-CB-CG	5.64	125.81	113.40
7	mM	115	GLU	CA-CB-CG	5.64	125.81	113.40
7	FB	115	GLU	CA-CB-CG	5.64	125.81	113.40
7	RB	115	GLU	CA-CB-CG	5.64	125.81	113.40
7	FM	115	GLU	CA-CB-CG	5.64	125.81	113.40
7	RM	115	GLU	CA-CB-CG	5.64	125.81	113.40
7	DB	115	GLU	CA-CB-CG	5.64	125.80	113.40
7	DM	115	GLU	CA-CB-CG	5.64	125.80	113.40
6	l1	137	ARG	NE-CZ-NH2	-5.63	117.49	120.30
7	HB	115	GLU	CA-CB-CG	5.63	125.78	113.40
7	XB	115	GLU	CA-CB-CG	5.63	125.78	113.40
6	lK	137	ARG	NE-CZ-NH2	-5.63	117.49	120.30
7	HM	115	GLU	CA-CB-CG	5.63	125.78	113.40
7	XM	115	GLU	CA-CB-CG	5.63	125.78	113.40
7	C4	77	ARG	NE-CZ-NH1	5.63	123.11	120.30
6	b1	137	ARG	NE-CZ-NH2	-5.62	117.49	120.30
6	bK	137	ARG	NE-CZ-NH2	-5.62	117.49	120.30
6	d1	137	ARG	NE-CZ-NH2	-5.61	117.50	120.30
5	D7	77	ARG	NE-CZ-NH2	5.61	123.11	120.30
5	D9	77	ARG	NE-CZ-NH2	5.61	123.11	120.30
6	dK	137	ARG	NE-CZ-NH2	-5.61	117.50	120.30
7	KD	77	ARG	NE-CZ-NH1	5.60	123.10	120.30
6	S1	137	ARG	NE-CZ-NH2	-5.59	117.50	120.30
6	SK	137	ARG	NE-CZ-NH2	-5.59	117.50	120.30
7	kF	132	SER	N-CA-CB	5.59	118.88	110.50
7	kI	132	SER	N-CA-CB	5.59	118.88	110.50
10	d4	329	MET	CG-SD-CE	5.58	109.14	100.20
22	VP	80	LEU	CA-CB-CG	-5.58	102.46	115.30
10	dD	329	MET	CG-SD-CE	5.58	109.13	100.20
6	K3	42	GLU	CB-CA-C	-5.57	99.26	110.40
6	KO	42	GLU	CB-CA-C	-5.57	99.26	110.40
7	GD	77	ARG	NE-CZ-NH1	5.57	123.08	120.30
14	MG	110	LEU	CA-CB-CG	5.56	128.10	115.30
6	j1	137	ARG	NE-CZ-NH2	-5.56	117.52	120.30
6	jK	137	ARG	NE-CZ-NH2	-5.56	117.52	120.30
22	xP	80	LEU	CA-CB-CG	-5.55	102.53	115.30
14	MQ	110	LEU	CA-CB-CG	5.55	128.07	115.30
6	U1	137	ARG	NE-CZ-NH2	-5.55	117.53	120.30
6	UK	137	ARG	NE-CZ-NH2	-5.55	117.53	120.30
6	f1	137	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	fK	137	ARG	NE-CZ-NH2	-5.54	117.53	120.30
7	J3	177	SER	N-CA-CB	5.54	118.81	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M4	77	ARG	NE-CZ-NH1	5.54	123.07	120.30
7	JO	177	SER	N-CA-CB	5.54	118.81	110.50
3	B1	85	LYS	CB-CG-CD	-5.54	97.20	111.60
3	BK	85	LYS	CB-CG-CD	-5.54	97.20	111.60
7	MD	77	ARG	NE-CZ-NH1	5.54	123.07	120.30
6	W1	137	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	WK	137	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	M2	142	ARG	CD-NE-CZ	-5.53	115.86	123.60
5	N7	77	ARG	NE-CZ-NH1	-5.51	117.55	120.30
5	N9	77	ARG	NE-CZ-NH1	-5.51	117.55	120.30
6	U2	163	LEU	O-C-N	-5.49	113.92	122.70
5	L7	77	ARG	NE-CZ-NH1	-5.48	117.56	120.30
6	UR	163	LEU	O-C-N	-5.48	113.93	122.70
6	O1	137	ARG	NE-CZ-NH2	-5.48	117.56	120.30
6	OK	137	ARG	NE-CZ-NH2	-5.48	117.56	120.30
6	LD	157	ASP	CB-CG-OD2	-5.47	113.38	118.30
6	h1	137	ARG	NE-CZ-NH2	-5.47	117.56	120.30
6	hK	137	ARG	NE-CZ-NH2	-5.47	117.56	120.30
6	L4	157	ASP	CB-CG-OD2	-5.45	113.39	118.30
6	SR	142	ARG	CD-NE-CZ	-5.45	115.97	123.60
6	D4	157	ASP	CB-CG-OD2	-5.43	113.41	118.30
17	BB	57	MET	CA-CB-CG	5.43	122.53	113.30
17	BM	57	MET	CA-CB-CG	5.43	122.53	113.30
7	D3	107	ASP	N-CA-CB	-5.43	100.83	110.60
7	DO	107	ASP	N-CA-CB	-5.43	100.83	110.60
5	D7	77	ARG	NE-CZ-NH1	-5.42	117.59	120.30
5	D9	77	ARG	NE-CZ-NH1	-5.42	117.59	120.30
6	H4	157	ASP	CB-CG-OD2	-5.42	113.42	118.30
17	yJ	111	CYS	CA-CB-SG	5.41	123.74	114.00
17	yL	111	CYS	CA-CB-SG	5.41	123.74	114.00
6	DD	157	ASP	CB-CG-OD2	-5.41	113.43	118.30
6	J4	157	ASP	CB-CG-OD2	-5.40	113.44	118.30
6	JD	157	ASP	CB-CG-OD2	-5.39	113.44	118.30
5	L9	77	ARG	NE-CZ-NH1	-5.39	117.60	120.30
6	FD	157	ASP	CB-CG-OD2	-5.39	113.45	118.30
6	JD	2	LYS	CD-CE-NZ	5.39	124.10	111.70
6	F4	2	LYS	CD-CE-NZ	5.39	124.09	111.70
6	HD	157	ASP	CB-CG-OD2	-5.39	113.45	118.30
6	J4	2	LYS	CD-CE-NZ	5.38	124.09	111.70
7	B3	173	GLY	N-CA-C	-5.38	99.66	113.10
6	F4	157	ASP	CB-CG-OD2	-5.38	113.46	118.30
7	BO	173	GLY	N-CA-C	-5.38	99.66	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H4	2	LYS	CD-CE-NZ	5.37	124.06	111.70
6	E3	25	GLU	N-CA-CB	5.37	120.26	110.60
6	E3	42	GLU	CB-CA-C	-5.37	99.66	110.40
6	B4	2	LYS	CD-CE-NZ	5.37	124.05	111.70
6	L4	2	LYS	CD-CE-NZ	5.37	124.05	111.70
6	EO	25	GLU	N-CA-CB	5.37	120.26	110.60
6	EO	42	GLU	CB-CA-C	-5.37	99.66	110.40
6	FD	2	LYS	CD-CE-NZ	5.37	124.04	111.70
6	D4	2	LYS	CD-CE-NZ	5.36	124.03	111.70
6	K3	42	GLU	N-CA-C	5.36	125.47	111.00
6	KO	42	GLU	N-CA-C	5.36	125.47	111.00
7	D3	146	ALA	N-CA-C	-5.36	96.54	111.00
6	BD	2	LYS	CD-CE-NZ	5.36	124.02	111.70
7	DO	146	ALA	N-CA-C	-5.36	96.54	111.00
7	H3	146	ALA	N-CA-C	-5.35	96.54	111.00
7	HO	146	ALA	N-CA-C	-5.35	96.54	111.00
6	LD	2	LYS	CD-CE-NZ	5.35	124.01	111.70
6	DD	2	LYS	CD-CE-NZ	5.35	124.00	111.70
6	HD	2	LYS	CD-CE-NZ	5.35	124.00	111.70
7	B3	146	ALA	N-CA-C	-5.34	96.58	111.00
7	BO	146	ALA	N-CA-C	-5.34	96.58	111.00
7	ED	171	ARG	CD-NE-CZ	5.33	131.06	123.60
7	MD	171	ARG	CD-NE-CZ	5.33	131.05	123.60
6	fF	53	LYS	N-CA-CB	5.33	120.19	110.60
6	fI	53	LYS	N-CA-CB	5.33	120.19	110.60
7	K4	171	ARG	CD-NE-CZ	5.32	131.05	123.60
6	GG	115	GLU	CA-CB-CG	5.32	125.11	113.40
6	GQ	115	GLU	CA-CB-CG	5.32	125.11	113.40
7	KD	171	ARG	CD-NE-CZ	5.32	131.05	123.60
6	IG	115	GLU	CA-CB-CG	5.32	125.10	113.40
6	IQ	115	GLU	CA-CB-CG	5.32	125.10	113.40
6	BD	157	ASP	CB-CG-OD2	-5.32	113.51	118.30
7	ID	171	ARG	CD-NE-CZ	5.32	131.04	123.60
6	B4	157	ASP	CB-CG-OD2	-5.32	113.52	118.30
6	EG	115	GLU	CA-CB-CG	5.31	125.08	113.40
6	EQ	115	GLU	CA-CB-CG	5.31	125.08	113.40
6	QF	49	GLU	CB-CA-C	-5.30	99.79	110.40
6	QI	49	GLU	CB-CA-C	-5.30	99.79	110.40
7	E4	171	ARG	CD-NE-CZ	5.30	131.02	123.60
6	AG	115	GLU	CA-CB-CG	5.30	125.06	113.40
6	AQ	115	GLU	CA-CB-CG	5.30	125.06	113.40
7	G4	171	ARG	CD-NE-CZ	5.30	131.02	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	bF	49	GLU	CB-CA-C	-5.30	99.80	110.40
6	bI	49	GLU	CB-CA-C	-5.30	99.80	110.40
6	OF	49	GLU	CB-CA-C	-5.30	99.81	110.40
6	OI	49	GLU	CB-CA-C	-5.30	99.81	110.40
7	M4	171	ARG	CD-NE-CZ	5.29	131.01	123.60
16	wL	68	VAL	CG1-CB-CG2	-5.29	102.44	110.90
6	WF	49	GLU	CB-CA-C	-5.29	99.83	110.40
6	WI	49	GLU	CB-CA-C	-5.29	99.83	110.40
6	hF	49	GLU	CB-CA-C	-5.29	99.83	110.40
6	CG	115	GLU	CA-CB-CG	5.29	125.03	113.40
6	hI	49	GLU	CB-CA-C	-5.29	99.83	110.40
6	CQ	115	GLU	CA-CB-CG	5.29	125.03	113.40
4	MF	110	TYR	N-CA-CB	5.28	120.11	110.60
4	MI	110	TYR	N-CA-CB	5.28	120.11	110.60
6	lF	49	GLU	CB-CA-C	-5.28	99.84	110.40
6	KG	115	GLU	CA-CB-CG	5.28	125.02	113.40
6	II	49	GLU	CB-CA-C	-5.28	99.84	110.40
6	KQ	115	GLU	CA-CB-CG	5.28	125.02	113.40
7	I4	171	ARG	CD-NE-CZ	5.28	130.99	123.60
6	dF	49	GLU	CB-CA-C	-5.28	99.84	110.40
6	dI	49	GLU	CB-CA-C	-5.28	99.84	110.40
6	UF	49	GLU	CB-CA-C	-5.27	99.85	110.40
6	UI	49	GLU	CB-CA-C	-5.27	99.85	110.40
6	fF	49	GLU	CB-CA-C	-5.27	99.85	110.40
6	fI	49	GLU	CB-CA-C	-5.27	99.85	110.40
7	GD	171	ARG	CD-NE-CZ	5.26	130.97	123.60
16	wJ	68	VAL	CG1-CB-CG2	-5.26	102.48	110.90
6	C3	42	GLU	N-CA-C	5.26	125.20	111.00
7	A8	76	ASN	N-CA-C	5.26	125.20	111.00
6	CO	42	GLU	N-CA-C	5.26	125.20	111.00
6	SF	49	GLU	CB-CA-C	-5.26	99.89	110.40
6	SI	49	GLU	CB-CA-C	-5.26	99.89	110.40
7	A5	76	ASN	N-CA-C	5.25	125.18	111.00
16	xJ	68	VAL	CG1-CB-CG2	-5.24	102.52	110.90
7	C4	171	ARG	CD-NE-CZ	5.24	130.93	123.60
7	CD	171	ARG	CD-NE-CZ	5.24	130.93	123.60
16	wL	254	GLN	CA-CB-CG	5.24	124.92	113.40
16	wJ	254	GLN	CA-CB-CG	5.23	124.91	113.40
16	xL	68	VAL	CG1-CB-CG2	-5.23	102.54	110.90
18	MC	295	ASP	CB-CG-OD2	5.22	123.00	118.30
18	ME	295	ASP	CB-CG-OD2	5.21	122.99	118.30
16	xJ	254	GLN	CA-CB-CG	5.20	124.85	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	MG	141	TYR	CB-CG-CD2	-5.20	117.88	121.00
6	qJ	84	ARG	NE-CZ-NH2	-5.20	117.70	120.30
6	qL	84	ARG	NE-CZ-NH2	-5.20	117.70	120.30
16	xL	254	GLN	CA-CB-CG	5.19	124.82	113.40
18	ME	144	ARG	N-CA-C	5.19	125.01	111.00
6	CJ	84	ARG	NE-CZ-NH2	-5.18	117.71	120.30
6	CL	84	ARG	NE-CZ-NH2	-5.18	117.71	120.30
6	cJ	84	ARG	NE-CZ-NH2	-5.18	117.71	120.30
6	cL	84	ARG	NE-CZ-NH2	-5.18	117.71	120.30
6	EC	44	LEU	CA-CB-CG	5.16	127.16	115.30
6	EE	44	LEU	CA-CB-CG	5.16	127.16	115.30
14	MQ	141	TYR	CB-CG-CD2	-5.15	117.91	121.00
8	e2	127	LEU	CA-CB-CG	5.15	127.15	115.30
6	IC	44	LEU	CA-CB-CG	5.15	127.14	115.30
6	IE	44	LEU	CA-CB-CG	5.15	127.14	115.30
6	I3	42	GLU	N-CA-C	5.15	124.89	111.00
6	IO	42	GLU	N-CA-C	5.15	124.89	111.00
6	AC	44	LEU	CA-CB-CG	5.14	127.13	115.30
7	MD	77	ARG	NE-CZ-NH2	-5.14	117.73	120.30
6	AE	44	LEU	CA-CB-CG	5.14	127.13	115.30
6	GC	44	LEU	CA-CB-CG	5.13	127.11	115.30
6	GE	44	LEU	CA-CB-CG	5.13	127.11	115.30
6	kJ	84	ARG	NE-CZ-NH2	-5.13	117.73	120.30
6	kL	84	ARG	NE-CZ-NH2	-5.13	117.73	120.30
6	S2	49	GLU	CA-CB-CG	5.13	124.68	113.40
6	IJ	84	ARG	NE-CZ-NH2	-5.13	117.74	120.30
6	IL	84	ARG	NE-CZ-NH2	-5.13	117.74	120.30
6	CC	44	LEU	CA-CB-CG	5.13	127.09	115.30
6	CE	44	LEU	CA-CB-CG	5.13	127.09	115.30
6	U2	49	GLU	CA-CB-CG	5.12	124.68	113.40
6	KC	44	LEU	CA-CB-CG	5.12	127.08	115.30
6	KE	44	LEU	CA-CB-CG	5.12	127.08	115.30
6	SR	49	GLU	CA-CB-CG	5.12	124.67	113.40
6	OR	49	GLU	CA-CB-CG	5.12	124.67	113.40
6	OJ	84	ARG	NE-CZ-NH2	-5.12	117.74	120.30
6	OL	84	ARG	NE-CZ-NH2	-5.12	117.74	120.30
6	SJ	84	ARG	NE-CZ-NH2	-5.12	117.74	120.30
6	SL	84	ARG	NE-CZ-NH2	-5.12	117.74	120.30
6	iJ	84	ARG	NE-CZ-NH2	-5.11	117.74	120.30
6	uJ	84	ARG	NE-CZ-NH2	-5.11	117.74	120.30
6	iL	84	ARG	NE-CZ-NH2	-5.11	117.74	120.30
6	uL	84	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	WR	49	GLU	CA-CB-CG	5.11	124.65	113.40
6	W2	49	GLU	CA-CB-CG	5.10	124.62	113.40
6	QR	49	GLU	CA-CB-CG	5.10	124.61	113.40
8	eR	127	LEU	CA-CB-CG	5.10	127.02	115.30
6	O2	49	GLU	CA-CB-CG	5.09	124.60	113.40
6	UJ	84	ARG	NE-CZ-NH2	-5.09	117.75	120.30
6	UL	84	ARG	NE-CZ-NH2	-5.09	117.75	120.30
7	ED	77	ARG	NE-CZ-NH2	-5.09	117.75	120.30
7	KD	77	ARG	NE-CZ-NH2	-5.09	117.76	120.30
6	AJ	84	ARG	NE-CZ-NH2	-5.09	117.76	120.30
6	AL	84	ARG	NE-CZ-NH2	-5.09	117.76	120.30
6	K3	44	LEU	N-CA-CB	5.08	120.57	110.40
6	KO	44	LEU	N-CA-CB	5.08	120.57	110.40
6	Q2	49	GLU	CA-CB-CG	5.08	124.58	113.40
16	AB	145	PHE	C-N-CD	5.08	139.08	128.40
6	UR	49	GLU	CA-CB-CG	5.08	124.58	113.40
5	J1	62	GLU	CA-CB-CG	5.08	124.57	113.40
5	JK	62	GLU	CA-CB-CG	5.08	124.57	113.40
6	eJ	84	ARG	NE-CZ-NH2	-5.08	117.76	120.30
6	eL	84	ARG	NE-CZ-NH2	-5.08	117.76	120.30
7	K4	77	ARG	NE-CZ-NH2	-5.07	117.77	120.30
6	oJ	84	ARG	NE-CZ-NH2	-5.07	117.77	120.30
6	oL	84	ARG	NE-CZ-NH2	-5.07	117.77	120.30
16	AM	145	PHE	C-N-CD	5.07	139.04	128.40
7	G4	77	ARG	NE-CZ-NH2	-5.06	117.77	120.30
5	L1	62	GLU	CA-CB-CG	5.06	124.54	113.40
6	KJ	84	ARG	NE-CZ-NH2	-5.06	117.77	120.30
6	WJ	84	ARG	NE-CZ-NH2	-5.06	117.77	120.30
5	LK	62	GLU	CA-CB-CG	5.06	124.54	113.40
6	KL	84	ARG	NE-CZ-NH2	-5.06	117.77	120.30
6	WL	84	ARG	NE-CZ-NH2	-5.06	117.77	120.30
14	MG	112	LEU	CA-CB-CG	5.06	126.94	115.30
7	GD	77	ARG	NE-CZ-NH2	-5.06	117.77	120.30
6	F4	90	MET	CG-SD-CE	5.04	108.27	100.20
18	ME	230	LEU	CB-CG-CD2	-5.04	102.42	111.00
7	K8	7	ARG	CG-CD-NE	-5.04	101.21	111.80
6	HD	90	MET	CG-SD-CE	5.04	108.27	100.20
6	mJ	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
6	mL	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
14	MQ	112	LEU	CA-CB-CG	5.04	126.90	115.30
14	MQ	259	CYS	CA-CB-SG	5.04	123.08	114.00
6	sJ	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	sL	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
14	MG	259	CYS	CA-CB-SG	5.04	123.07	114.00
6	EJ	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
6	EL	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
6	YJ	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
6	YL	84	ARG	NE-CZ-NH2	-5.04	117.78	120.30
18	MC	230	LEU	CB-CG-CD2	-5.03	102.45	111.00
6	FD	90	MET	CG-SD-CE	5.03	108.25	100.20
6	J4	90	MET	CG-SD-CE	5.03	108.24	100.20
6	MJ	84	ARG	NE-CZ-NH2	-5.03	117.79	120.30
6	ML	84	ARG	NE-CZ-NH2	-5.03	117.79	120.30
7	E4	77	ARG	NE-CZ-NH2	-5.03	117.79	120.30
6	H4	90	MET	CG-SD-CE	5.03	108.24	100.20
7	K5	7	ARG	CG-CD-NE	-5.03	101.25	111.80
6	A3	141	PRO	N-CA-C	5.02	125.16	112.10
6	JD	90	MET	CG-SD-CE	5.02	108.23	100.20
6	QJ	84	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	QL	84	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	AO	141	PRO	N-CA-C	5.02	125.16	112.10
6	GJ	84	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	aJ	84	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	GL	84	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	aL	84	ARG	NE-CZ-NH2	-5.02	117.79	120.30
6	D4	90	MET	CG-SD-CE	5.01	108.22	100.20
6	L4	90	MET	CG-SD-CE	5.01	108.22	100.20
6	BD	90	MET	CG-SD-CE	5.01	108.22	100.20
6	DD	90	MET	CG-SD-CE	5.01	108.22	100.20
7	C4	77	ARG	NE-CZ-NH2	-5.01	117.80	120.30
6	gJ	84	ARG	NE-CZ-NH2	-5.01	117.80	120.30
6	gL	84	ARG	NE-CZ-NH2	-5.01	117.80	120.30
6	LD	90	MET	CG-SD-CE	5.00	108.21	100.20
7	CD	77	ARG	NE-CZ-NH2	-5.00	117.80	120.30
6	B4	90	MET	CG-SD-CE	5.00	108.20	100.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A5	33	ASP	Mainchain
7	A8	33	ASP	Mainchain
7	C5	37	ARG	Mainchain
7	C8	37	ARG	Mainchain

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Mol	Chain	Res	Type	Group
12	E5	161	SER	Peptide
12	E8	161	SER	Peptide
21	LP	71	MEN	Mainchain
6	U2	163	LEU	Mainchain
6	UR	163	LEU	Mainchain
21	jP	71	MEN	Mainchain
21	kP	71	MEN	Mainchain

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	X1	322/363 (89%)	296 (92%)	26 (8%)	0	100	100
1	X7	322/363 (89%)	283 (88%)	38 (12%)	1 (0%)	41	76
1	X9	322/363 (89%)	283 (88%)	37 (12%)	2 (1%)	25	64
1	XF	322/363 (89%)	283 (88%)	39 (12%)	0	100	100
1	XI	322/363 (89%)	283 (88%)	39 (12%)	0	100	100
1	XK	322/363 (89%)	296 (92%)	26 (8%)	0	100	100
2	A1	255/290 (88%)	241 (94%)	14 (6%)	0	100	100
2	A7	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
2	A9	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
2	AF	255/290 (88%)	239 (94%)	16 (6%)	0	100	100
2	AI	255/290 (88%)	239 (94%)	16 (6%)	0	100	100
2	AK	255/290 (88%)	241 (94%)	14 (6%)	0	100	100
3	B1	225/232 (97%)	207 (92%)	17 (8%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B7	228/232 (98%)	206 (90%)	21 (9%)	1 (0%)	34	72
3	B9	228/232 (98%)	205 (90%)	22 (10%)	1 (0%)	34	72
3	BF	229/232 (99%)	207 (90%)	22 (10%)	0	100	100
3	BI	229/232 (99%)	208 (91%)	21 (9%)	0	100	100
3	BK	225/232 (97%)	207 (92%)	17 (8%)	1 (0%)	34	72
4	C1	160/162 (99%)	146 (91%)	12 (8%)	2 (1%)	12	45
4	C7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	C9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	CF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	CI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	CK	160/162 (99%)	146 (91%)	12 (8%)	2 (1%)	12	45
4	E1	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
4	E7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	E9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	EF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	EI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	EK	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
4	G1	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
4	G7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	G9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	GF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	GI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	GK	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
4	I1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	I7	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25	64
4	I9	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25	64
4	IF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	II	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	IK	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	K1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	K7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	KF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	KI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	KK	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	M1	160/162 (99%)	152 (95%)	7 (4%)	1 (1%)	25	64
4	M7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	M9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	MF	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	MI	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	MK	160/162 (99%)	152 (95%)	7 (4%)	1 (1%)	25	64
5	D1	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
5	D7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	D9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	DF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	DI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	DK	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
5	F1	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
5	F7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	F9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	FF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	FI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	FK	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
5	H1	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	64
5	H7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	H9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	HF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	HI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	HK	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	25	64
5	J1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
5	J7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	J9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	JF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	JI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	JK	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
5	L1	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
5	L7	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	25	64
5	L9	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	25	64
5	LF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	LI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	LK	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
5	N1	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
5	N7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	N9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	NF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	NI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	NK	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
6	A3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	AA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	AC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	AJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AL	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	AO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	AQ	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	B4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	BD	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	C3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	CA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	CB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	CC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CG	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	CJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CL	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CM	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	CN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	CO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	CQ	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	D4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	DD	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	E3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	EA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	EB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	EC	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
6	EE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	EG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	EJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	EL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	EM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	EN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	EO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	EQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	F4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	FD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	G3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	GA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	GB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	GC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	GE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	GG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	GJ	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	GL	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	GM	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	GN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	GO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	GQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	H4	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	HD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	I3	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	IA	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
6	IB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	IE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	IG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	IJ	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IL	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IN	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
6	IO	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	IQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	J4	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	J5	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	J8	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	JD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	K3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	KA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	KB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	KC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	KE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	KG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	KJ	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	KL	162/164 (99%)	154 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	KM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	KN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	KO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	KQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	L4	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	LD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	M2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	MB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	MJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	ML	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	MM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	MR	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	O1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	O2	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
6	O7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	O9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	OB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	OF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	OI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	OJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	OK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	OL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	OM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	OR	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
6	Q1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	Q2	162/164 (99%)	155 (96%)	5 (3%)	2 (1%)	13	48
6	Q7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	Q9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	QB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	QF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	QI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	QJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
6	QK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	QL	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
6	QM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	QR	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
6	S1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	S2	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
6	S7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	S9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	SB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SJ	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
6	SK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	SL	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
6	SM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SR	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
6	U1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	U2	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	U7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	U9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	UB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	UF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	UI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	UJ	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	UK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	UL	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	UM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	UR	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	W1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	W2	162/164 (99%)	156 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	W7	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	W9	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	WB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WJ	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	WK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	WL	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	WM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WR	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
6	YB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	YJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	YL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	YM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	Z1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	Z7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	Z9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	ZF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	ZI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	ZK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	aB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	aJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	aL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	aM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	b1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	b7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	b9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	bF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	bI	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	bK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	cJ	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	cL	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	48
6	d1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	d7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	d9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	dB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	dF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	dI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	dK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	dM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	eJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	eL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	f1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	f7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	f9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	fB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	fF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	fI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	fK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	fM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	gJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	gL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	h1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	h7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	h9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	hB	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	hF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	hI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	hK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	hM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	iJ	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	48
6	iL	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	j1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	j7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	j9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	jB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	jF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	jI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	jK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	jM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	kJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	kL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	l1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	l7	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	l9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	lB	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	lF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	lI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	lK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	lM	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
6	mJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	mL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	oJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	oL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	qJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	qL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	sJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	sL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	uJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	uL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
7	A5	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	64
7	A8	174/177 (98%)	170 (98%)	3 (2%)	1 (1%)	25	64
7	B3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	B8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	BA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	BC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	BE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	BJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	BL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	BN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	BO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	BQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	C4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	C5	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	C8	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	CD	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	D3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	DA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	DB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	DC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	DE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	DG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	DJ	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	DL	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	DM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	DN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	DO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	DQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	E4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	ED	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	F3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	F5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	FA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	FB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	FC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	FE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	FG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	FJ	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
7	FL	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
7	FM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	FN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	FO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	FQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	G4	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
7	G5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	G8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	GD	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
7	H3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	H5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	H8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	HA	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
7	HB	176/177 (99%)	176 (100%)	0	0	100	100
7	HC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	HE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	HG	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
7	HJ	174/177 (98%)	160 (92%)	11 (6%)	3 (2%)	9	39
7	HL	174/177 (98%)	160 (92%)	11 (6%)	3 (2%)	9	39
7	HM	176/177 (99%)	176 (100%)	0	0	100	100
7	HN	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
7	HO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	HQ	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
7	I4	175/177 (99%)	159 (91%)	16 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I5	174/177 (98%)	167 (96%)	4 (2%)	3 (2%)	9	39
7	I8	174/177 (98%)	168 (97%)	3 (2%)	3 (2%)	9	39
7	ID	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
7	J3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	JA	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	25	64
7	JB	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	JC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	JJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JL	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JM	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	JN	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	25	64
7	JO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	JQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	K4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	K5	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	K8	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	KD	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	L3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	L5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	L8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	LA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	LB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	LC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	LJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LL	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	LN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	LO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	LQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	M3	143/177 (81%)	128 (90%)	15 (10%)	0	100	100
7	M4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	MD	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	MO	143/177 (81%)	128 (90%)	15 (10%)	0	100	100
7	N2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	N3	143/177 (81%)	130 (91%)	13 (9%)	0	100	100
7	NB	176/177 (99%)	173 (98%)	2 (1%)	1 (1%)	25	64
7	NJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	NL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	NM	176/177 (99%)	173 (98%)	2 (1%)	1 (1%)	25	64
7	NO	143/177 (81%)	130 (91%)	13 (9%)	0	100	100
7	NR	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	P1	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	P2	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	P7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	P9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	PB	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
7	PF	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	64
7	PI	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	64
7	PJ	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	PK	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	PL	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	PM	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
7	PR	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	R1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	R2	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	R7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	R9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	RB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	RF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	RI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	RJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	RK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	RL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	RM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	RR	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	T1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	T2	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	T7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	T9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	TB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	TF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	TI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	TJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	TK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	TL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	TM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	TR	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	V1	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
7	V2	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	V7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	V9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	VB	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	VF	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
7	VI	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
7	VJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	VK	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
7	VL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	VM	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	VR	174/177 (98%)	169 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	X2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	XB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	XJ	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	XL	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	XM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	XR	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	Y1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	Y7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	Y9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	YF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	YI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	YK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	ZB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	ZJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	ZL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	ZM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	a1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	a7	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	a9	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	aF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	aI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	aK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	bJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	bL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	c1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	c7	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	25	64
7	c9	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	25	64
7	cB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	cF	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	64
7	cI	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	64
7	cK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	cM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	dJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	dL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	e1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	e7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	e9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	eB	176/177 (99%)	172 (98%)	2 (1%)	2 (1%)	14	50
7	eF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	eI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	eK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	eM	176/177 (99%)	172 (98%)	2 (1%)	2 (1%)	14	50
7	fJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	fL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	g1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	g7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	g9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	gB	176/177 (99%)	176 (100%)	0	0	100	100
7	gF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	gI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	gK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	gM	176/177 (99%)	176 (100%)	0	0	100	100
7	hJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	hL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	i1	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
7	i7	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	i9	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	iB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	iF	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	iI	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	iK	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
7	iM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	jJ	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	jL	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	k1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	k7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	k9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	kB	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	kF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	kI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	kK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	kM	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	lJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	lL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	m1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	m7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	m9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	mB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	mF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	mI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	mK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	mM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	nJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	nL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	pJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	pL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	rJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	rL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	tJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	tL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	vJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	vL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
8	e2	246/303 (81%)	223 (91%)	21 (8%)	2 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	eR	246/303 (81%)	224 (91%)	20 (8%)	2 (1%)	19	57
9	O3	373/405 (92%)	344 (92%)	29 (8%)	0	100	100
9	OO	373/405 (92%)	344 (92%)	29 (8%)	0	100	100
10	d4	295/342 (86%)	260 (88%)	33 (11%)	2 (1%)	22	60
10	dD	295/342 (86%)	260 (88%)	34 (12%)	1 (0%)	41	76
11	D5	79/327 (24%)	73 (92%)	6 (8%)	0	100	100
11	D8	79/327 (24%)	73 (92%)	6 (8%)	0	100	100
12	E5	199/288 (69%)	192 (96%)	7 (4%)	0	100	100
12	E8	199/288 (69%)	192 (96%)	7 (4%)	0	100	100
13	k6	283/288 (98%)	257 (91%)	26 (9%)	0	100	100
13	kH	283/288 (98%)	257 (91%)	25 (9%)	1 (0%)	34	72
14	MA	236/333 (71%)	221 (94%)	14 (6%)	1 (0%)	34	72
14	MG	236/333 (71%)	208 (88%)	24 (10%)	4 (2%)	9	39
14	MN	236/333 (71%)	220 (93%)	16 (7%)	0	100	100
14	MQ	236/333 (71%)	209 (89%)	25 (11%)	2 (1%)	19	57
15	bB	378/490 (77%)	352 (93%)	23 (6%)	3 (1%)	19	57
15	bM	378/490 (77%)	351 (93%)	24 (6%)	3 (1%)	19	57
16	AB	236/273 (86%)	229 (97%)	6 (2%)	1 (0%)	34	72
16	AM	236/273 (86%)	229 (97%)	6 (2%)	1 (0%)	34	72
16	wJ	236/273 (86%)	221 (94%)	12 (5%)	3 (1%)	12	45
16	wL	236/273 (86%)	221 (94%)	12 (5%)	3 (1%)	12	45
16	xJ	236/273 (86%)	221 (94%)	13 (6%)	2 (1%)	19	57
16	xL	236/273 (86%)	221 (94%)	13 (6%)	2 (1%)	19	57
17	BB	248/290 (86%)	241 (97%)	7 (3%)	0	100	100
17	BM	248/290 (86%)	241 (97%)	7 (3%)	0	100	100
17	yJ	248/290 (86%)	239 (96%)	9 (4%)	0	100	100
17	yL	248/290 (86%)	239 (96%)	9 (4%)	0	100	100
18	MC	278/316 (88%)	214 (77%)	50 (18%)	14 (5%)	2	12
18	ME	278/316 (88%)	210 (76%)	51 (18%)	17 (6%)	1	8
19	zJ	368/498 (74%)	339 (92%)	26 (7%)	3 (1%)	19	57
19	zL	368/498 (74%)	339 (92%)	26 (7%)	3 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	CP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	EP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	GP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	JP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
20	KP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	NP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	PP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	RP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	TP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	cP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	eP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	gP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	iP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	lP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	mP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	pP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	rP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	tP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	vP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	BP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	DP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	FP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	HP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	IP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	LP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	MP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	OP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	QP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	SP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	UP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	dP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	fP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	hP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	jP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	kP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	nP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	oP	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
21	qP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	sP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	uP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	wP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
22	VP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
22	xP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
23	WP	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
23	yP	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
24	XP	90/132 (68%)	87 (97%)	3 (3%)	0	100	100
24	zP	90/132 (68%)	87 (97%)	3 (3%)	0	100	100
25	1P	840/879 (96%)	787 (94%)	53 (6%)	0	100	100
25	YP	840/879 (96%)	788 (94%)	50 (6%)	2 (0%)	47	82
26	2P	130/159 (82%)	119 (92%)	11 (8%)	0	100	100
26	ZP	130/159 (82%)	117 (90%)	13 (10%)	0	100	100
27	3P	251/288 (87%)	228 (91%)	22 (9%)	1 (0%)	34	72
27	aP	251/288 (87%)	229 (91%)	21 (8%)	1 (0%)	34	72
28	4P	205/253 (81%)	191 (93%)	14 (7%)	0	100	100
28	bP	205/253 (81%)	191 (93%)	13 (6%)	1 (0%)	29	68
All	All	115760/120800 (96%)	110526 (96%)	5057 (4%)	177 (0%)	50	82

All (177) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C1	13	ASP
5	N1	18	PHE
6	Q2	146	ALA

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Mol	Chain	Res	Type
6	I3	143	ASP
10	d4	284	LEU
6	B4	114	ARG
6	D4	114	ARG
6	F4	114	ARG
6	J4	114	ARG
6	L4	114	ARG
7	I5	33	ASP
7	A5	76	ASN
1	X7	325	LYS
7	I8	33	ASP
7	A8	76	ASN
1	X9	325	LYS
6	lB	58	ALA
18	MC	51	PRO
18	MC	63	ASP
18	MC	66	ASP
18	MC	216	ARG
18	MC	256	THR
18	MC	258	THR
10	dD	288	ARG
6	BD	114	ARG
6	DD	114	ARG
6	FD	114	ARG
6	HD	114	ARG
6	JD	114	ARG
6	LD	114	ARG
18	ME	51	PRO
18	ME	63	ASP
18	ME	66	ASP
18	ME	144	ARG
18	ME	216	ARG
18	ME	256	THR
18	ME	258	THR
18	ME	305	ALA
14	MG	256	THR
14	MG	257	THR
7	HJ	134	MET
7	PJ	21	GLY
6	UJ	72	ALA
16	xJ	43	LYS
19	zJ	216	TYR

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Mol	Chain	Res	Type
19	zJ	217	ALA
4	CK	13	ASP
5	NK	18	PHE
7	HL	134	MET
7	PL	21	GLY
6	UL	72	ALA
16	xL	43	LYS
19	zL	216	TYR
19	zL	217	ALA
15	bM	349	LYS
6	lM	58	ALA
6	IO	143	ASP
28	bP	42	ALA
14	MQ	256	THR
14	MQ	257	THR
6	QR	146	ALA
5	F1	18	PHE
5	H1	146	THR
4	M1	113	ALA
8	e2	86	LEU
7	I5	15	LYS
7	I5	22	SER
4	I7	112	VAL
7	I8	15	LYS
7	I8	22	SER
4	I9	112	VAL
7	JA	21	GLY
14	MA	99	GLY
18	MC	52	GLU
18	MC	215	THR
18	MC	221	ALA
18	MC	260	PRO
18	ME	52	GLU
18	ME	215	THR
18	ME	221	ALA
18	ME	260	PRO
7	PF	3	ASP
7	cF	146	ALA
14	MG	105	LYS
7	PI	3	ASP
7	cI	146	ALA
6	GJ	68	ASN

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Mol	Chain	Res	Type
16	wJ	41	ASN
16	wJ	45	SER
5	FK	18	PHE
5	HK	146	THR
4	MK	113	ALA
6	GL	68	ASN
16	wL	41	ASN
16	wL	45	SER
7	JN	21	GLY
25	YP	516	SER
8	eR	86	LEU
3	B1	201	SER
6	O2	114	ARG
7	T2	109	CYS
7	c7	125	ASN
7	c9	125	ASN
16	AB	146	PRO
7	eB	64	PRO
18	ME	151	GLU
13	kH	164	GLY
7	DJ	25	GLN
7	HJ	26	ALA
6	iJ	70	GLY
19	zJ	238	LYS
3	BK	201	SER
7	DL	25	GLN
7	HL	26	ALA
6	iL	70	GLY
19	zL	238	LYS
16	AM	146	PRO
7	eM	64	PRO
27	aP	287	LEU
27	3P	287	LEU
6	AQ	3	SER
6	OR	114	ARG
7	TR	109	CYS
8	e2	128	ARG
7	P2	107	ASP
3	B7	39	SER
3	B9	39	SER
15	bB	204	CYS
7	eB	61	CYS

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Mol	Chain	Res	Type
18	MC	307	PRO
18	ME	307	PRO
6	CG	34	SER
7	HJ	69	PRO
6	SJ	72	ALA
6	WJ	69	PRO
7	HL	69	PRO
6	SL	72	ALA
6	WL	69	PRO
15	bM	204	CYS
7	eM	61	CYS
6	CQ	34	SER
8	eR	128	ARG
7	PR	107	ASP
4	C1	115	LEU
6	Q2	143	ASP
10	d4	286	GLY
15	bB	351	ASP
7	NB	61	CYS
7	DJ	16	ALA
6	cJ	70	GLY
16	wJ	146	PRO
16	xJ	146	PRO
4	CK	115	LEU
7	DL	16	ALA
6	cL	70	GLY
16	wL	146	PRO
16	xL	146	PRO
7	NM	61	CYS
25	YP	663	LYS
7	T2	111	ASN
5	L7	75	THR
1	X9	104	ALA
5	L9	75	THR
6	iJ	69	PRO
6	iL	69	PRO
7	TR	111	ASN
18	MC	306	LYS
18	ME	306	LYS
15	bB	91	ILE
18	MC	308	ILE
18	ME	308	ILE

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Mol	Chain	Res	Type
14	MG	106	ASP
15	bM	91	ILE
18	MC	61	VAL
18	ME	61	VAL
6	cJ	69	PRO
6	cL	69	PRO

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	X1	261/290 (90%)	259 (99%)	2 (1%)	81	93
1	X7	261/290 (90%)	257 (98%)	4 (2%)	65	87
1	X9	261/290 (90%)	257 (98%)	4 (2%)	65	87
1	XF	261/290 (90%)	260 (100%)	1 (0%)	91	97
1	XI	260/290 (90%)	259 (100%)	1 (0%)	91	97
1	XK	261/290 (90%)	259 (99%)	2 (1%)	81	93
2	A1	199/222 (90%)	196 (98%)	3 (2%)	65	87
2	A7	199/222 (90%)	199 (100%)	0	100	100
2	A9	199/222 (90%)	199 (100%)	0	100	100
2	AF	199/222 (90%)	198 (100%)	1 (0%)	88	96
2	AI	199/222 (90%)	198 (100%)	1 (0%)	88	96
2	AK	199/222 (90%)	196 (98%)	3 (2%)	65	87
3	B1	208/211 (99%)	201 (97%)	7 (3%)	37	72
3	B7	209/211 (99%)	197 (94%)	12 (6%)	20	56
3	B9	209/211 (99%)	197 (94%)	12 (6%)	20	56
3	BF	210/211 (100%)	209 (100%)	1 (0%)	88	96
3	BI	210/211 (100%)	207 (99%)	3 (1%)	67	88
3	BK	208/211 (99%)	200 (96%)	8 (4%)	33	69
4	C1	125/125 (100%)	117 (94%)	8 (6%)	17	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C7	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	C9	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	CF	125/125 (100%)	125 (100%)	0	100	100
4	CI	125/125 (100%)	124 (99%)	1 (1%)	81	93
4	CK	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	E1	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	E7	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	E9	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	EF	125/125 (100%)	125 (100%)	0	100	100
4	EI	125/125 (100%)	124 (99%)	1 (1%)	81	93
4	EK	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	G1	125/125 (100%)	121 (97%)	4 (3%)	39	74
4	G7	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	G9	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	GF	125/125 (100%)	125 (100%)	0	100	100
4	GI	125/125 (100%)	125 (100%)	0	100	100
4	GK	125/125 (100%)	121 (97%)	4 (3%)	39	74
4	I1	125/125 (100%)	123 (98%)	2 (2%)	62	86
4	I7	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	I9	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	IF	125/125 (100%)	125 (100%)	0	100	100
4	II	125/125 (100%)	125 (100%)	0	100	100
4	IK	125/125 (100%)	124 (99%)	1 (1%)	81	93
4	K1	125/125 (100%)	123 (98%)	2 (2%)	62	86
4	K7	125/125 (100%)	113 (90%)	12 (10%)	8	32
4	K9	125/125 (100%)	113 (90%)	12 (10%)	8	32
4	KF	125/125 (100%)	125 (100%)	0	100	100
4	KI	125/125 (100%)	125 (100%)	0	100	100
4	KK	125/125 (100%)	122 (98%)	3 (2%)	49	79
4	M1	125/125 (100%)	120 (96%)	5 (4%)	31	68
4	M7	125/125 (100%)	116 (93%)	9 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M9	125/125 (100%)	116 (93%)	9 (7%)	14	45
4	MF	125/125 (100%)	125 (100%)	0	100	100
4	MI	125/125 (100%)	125 (100%)	0	100	100
4	MK	125/125 (100%)	120 (96%)	5 (4%)	31	68
5	D1	134/134 (100%)	127 (95%)	7 (5%)	23	59
5	D7	134/134 (100%)	113 (84%)	21 (16%)	2	13
5	D9	134/134 (100%)	113 (84%)	21 (16%)	2	13
5	DF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	DI	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	DK	134/134 (100%)	127 (95%)	7 (5%)	23	59
5	F1	134/134 (100%)	125 (93%)	9 (7%)	16	49
5	F7	134/134 (100%)	112 (84%)	22 (16%)	2	11
5	F9	134/134 (100%)	114 (85%)	20 (15%)	3	14
5	FF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	FI	134/134 (100%)	134 (100%)	0	100	100
5	FK	134/134 (100%)	124 (92%)	10 (8%)	13	43
5	H1	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	H7	134/134 (100%)	112 (84%)	22 (16%)	2	11
5	H9	134/134 (100%)	112 (84%)	22 (16%)	2	11
5	HF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	HI	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	HK	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	J1	134/134 (100%)	125 (93%)	9 (7%)	16	49
5	J7	134/134 (100%)	115 (86%)	19 (14%)	3	16
5	J9	134/134 (100%)	115 (86%)	19 (14%)	3	16
5	JF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	JI	134/134 (100%)	132 (98%)	2 (2%)	65	87
5	JK	134/134 (100%)	124 (92%)	10 (8%)	13	43
5	L1	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	L7	134/134 (100%)	116 (87%)	18 (13%)	4	17
5	L9	134/134 (100%)	116 (87%)	18 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LF	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	LI	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	LK	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	N1	134/134 (100%)	127 (95%)	7 (5%)	23	59
5	N7	134/134 (100%)	117 (87%)	17 (13%)	4	19
5	N9	134/134 (100%)	117 (87%)	17 (13%)	4	19
5	NF	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	NI	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	NK	134/134 (100%)	127 (95%)	7 (5%)	23	59
6	A3	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	AA	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	AC	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AE	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AG	128/128 (100%)	112 (88%)	16 (12%)	4	20
6	AJ	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AL	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AN	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	AO	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	AQ	128/128 (100%)	112 (88%)	16 (12%)	4	20
6	B4	128/128 (100%)	113 (88%)	15 (12%)	5	22
6	BD	128/128 (100%)	113 (88%)	15 (12%)	5	22
6	C3	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	CA	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	CB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CC	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	CE	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	CG	128/128 (100%)	109 (85%)	19 (15%)	3	14
6	CJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CN	128/128 (100%)	119 (93%)	9 (7%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CO	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	CQ	128/128 (100%)	109 (85%)	19 (15%)	3	14
6	D4	128/128 (100%)	107 (84%)	21 (16%)	2	11
6	DD	128/128 (100%)	107 (84%)	21 (16%)	2	11
6	E3	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	EA	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	EB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	EC	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	EE	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	EG	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	EJ	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	EL	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	EM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	EN	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	EO	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	EQ	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	F4	128/128 (100%)	104 (81%)	24 (19%)	1	8
6	FD	128/128 (100%)	103 (80%)	25 (20%)	1	7
6	G3	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GA	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	GB	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GC	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	GE	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	GG	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	GJ	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	GL	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GM	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GN	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	GO	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GQ	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	H4	128/128 (100%)	106 (83%)	22 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	HD	128/128 (100%)	106 (83%)	22 (17%)	2	10
6	I3	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IA	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	IC	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	IE	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	IG	128/128 (100%)	111 (87%)	17 (13%)	4	17
6	IJ	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	IL	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	IM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	IN	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IO	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IQ	128/128 (100%)	111 (87%)	17 (13%)	4	17
6	J4	128/128 (100%)	109 (85%)	19 (15%)	3	14
6	J5	128/128 (100%)	128 (100%)	0	100	100
6	J8	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	JD	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	K3	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KA	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	KC	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	KE	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	KG	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	KJ	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	KL	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	KM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	KN	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KO	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KQ	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	L4	128/128 (100%)	107 (84%)	21 (16%)	2	11
6	LD	128/128 (100%)	108 (84%)	20 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M2	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	MB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	MJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	ML	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	MM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	MR	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	O1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	O2	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	O7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	O9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	OB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OJ	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OL	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OR	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	Q1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	Q2	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	Q7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	Q9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	QB	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	QI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	QJ	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	QL	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QM	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QR	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	S1	128/128 (100%)	126 (98%)	2 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S2	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	S7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	S9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	SB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	SK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SL	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	SM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SR	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	U1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	U2	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	U7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	U9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	UB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	UK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	UL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	UM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UR	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	W1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	W2	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	W7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	W9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	WB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	WF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	WI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	WJ	128/128 (100%)	125 (98%)	3 (2%)	50	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	WK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	WL	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	WM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	WR	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	YB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	YJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	YL	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	YM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	Z1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	Z7	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	Z9	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	ZF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	ZI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	ZK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	aB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	aJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	aL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	aM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	b1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	b7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	b9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	bF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	bI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	bK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	cJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	cL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	d1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	d7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	d9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	dB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	dF	128/128 (100%)	127 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	dI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	dK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	dM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	eJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	eL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	f7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	f9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	fB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	fM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	gJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	gL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	h1	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	h7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	h9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	hB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	hF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	hI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	hK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	hM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	iJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	iL	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	j1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	j7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	j9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	jB	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	jF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	jI	128/128 (100%)	126 (98%)	2 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	jK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	jM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	kJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	kL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	l1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	l7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	l9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	lB	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	lF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	lI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	lK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	lM	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	mJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	mL	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	oJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	oL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	qJ	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	qL	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	sJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	sL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	uJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	uL	128/128 (100%)	124 (97%)	4 (3%)	40	75
7	A5	137/137 (100%)	121 (88%)	16 (12%)	5	22
7	A8	137/137 (100%)	121 (88%)	16 (12%)	5	22
7	B3	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	B5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	B8	113/137 (82%)	109 (96%)	4 (4%)	36	71
7	BA	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	BC	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	BE	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	BG	137/137 (100%)	126 (92%)	11 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BJ	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	BL	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	BN	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	BO	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	BQ	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	C4	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	C5	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	C8	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	CD	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	D3	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	DA	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	DB	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	DC	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	DE	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	DG	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	DJ	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	DL	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	DM	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	DN	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	DO	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	DQ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	E4	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	ED	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	F3	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	F5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	F8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	FA	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	FB	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	FC	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	FE	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	FG	137/137 (100%)	125 (91%)	12 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	FJ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	FL	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	FM	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	FN	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	FO	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	FQ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	G4	137/137 (100%)	104 (76%)	33 (24%)	0	3
7	G5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	G8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	GD	137/137 (100%)	105 (77%)	32 (23%)	1	4
7	H3	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	H5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	H8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	HA	138/137 (101%)	127 (92%)	11 (8%)	12	40
7	HB	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	HC	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	HE	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	HG	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	HJ	137/137 (100%)	119 (87%)	18 (13%)	4	18
7	HL	137/137 (100%)	119 (87%)	18 (13%)	4	18
7	HM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	HN	138/137 (101%)	127 (92%)	11 (8%)	12	40
7	HO	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	HQ	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	I4	138/137 (101%)	118 (86%)	20 (14%)	3	15
7	I5	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	I8	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	ID	138/137 (101%)	118 (86%)	20 (14%)	3	15
7	J3	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	JA	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	JB	139/137 (102%)	134 (96%)	5 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	JC	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	JE	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	JG	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	JJ	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	JL	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	JM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	JN	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	JO	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	JQ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	K4	137/137 (100%)	108 (79%)	29 (21%)	1	5
7	K5	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	K8	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	KD	137/137 (100%)	109 (80%)	28 (20%)	1	6
7	L3	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	L5	113/137 (82%)	109 (96%)	4 (4%)	36	71
7	L8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	LA	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	LB	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	LC	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	LE	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	LG	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	LJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	LL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	LM	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	LN	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	LO	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	LQ	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	M3	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	M4	137/137 (100%)	108 (79%)	29 (21%)	1	5
7	MD	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	MO	113/137 (82%)	102 (90%)	11 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	N2	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	N3	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	NB	139/137 (102%)	133 (96%)	6 (4%)	29	66
7	NJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	NL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	NM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	NO	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	NR	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	P1	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	P2	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	P7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	P9	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	PB	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	PF	137/137 (100%)	137 (100%)	0	100	100
7	PI	137/137 (100%)	137 (100%)	0	100	100
7	PJ	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	PK	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	PL	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	PM	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	PR	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	R1	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	R2	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	R7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	R9	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	RB	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	RF	137/137 (100%)	137 (100%)	0	100	100
7	RI	137/137 (100%)	137 (100%)	0	100	100
7	RJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	RK	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	RL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	RM	138/137 (101%)	132 (96%)	6 (4%)	29	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	RR	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	T1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	T2	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	T7	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	T9	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	TB	138/137 (101%)	133 (96%)	5 (4%)	35	70
7	TF	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	TI	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	TJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	TK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	TL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	TM	138/137 (101%)	133 (96%)	5 (4%)	35	70
7	TR	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	V1	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	V2	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	V7	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	V9	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	VB	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	VF	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	VI	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	VJ	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	VK	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	VL	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	VM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	VR	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	X2	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	XB	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	XJ	138/137 (101%)	137 (99%)	1 (1%)	84	94
7	XL	138/137 (101%)	137 (99%)	1 (1%)	84	94
7	XM	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	XR	137/137 (100%)	130 (95%)	7 (5%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Y1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	Y7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	Y9	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	YF	137/137 (100%)	137 (100%)	0	100	100
7	YI	137/137 (100%)	137 (100%)	0	100	100
7	YK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	ZB	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	ZJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	ZL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	ZM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	a1	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	a7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	a9	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	aF	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	aI	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	aK	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	bJ	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	bL	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	c1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	c7	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	c9	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	cB	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	cF	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	cI	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	cK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	cM	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	dJ	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	dL	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	e1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	e7	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	e9	137/137 (100%)	123 (90%)	14 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	eB	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	eF	137/137 (100%)	137 (100%)	0	100	100
7	eI	137/137 (100%)	137 (100%)	0	100	100
7	eK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	eM	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	fJ	137/137 (100%)	132 (96%)	5 (4%)	35	70
7	fL	137/137 (100%)	132 (96%)	5 (4%)	35	70
7	g1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	g7	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	g9	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	gB	139/137 (102%)	132 (95%)	7 (5%)	24	60
7	gF	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	gI	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	gK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	gM	139/137 (102%)	132 (95%)	7 (5%)	24	60
7	hJ	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	hL	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	i1	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	i7	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	i9	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	iB	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	iF	138/137 (101%)	135 (98%)	3 (2%)	52	81
7	iI	138/137 (101%)	135 (98%)	3 (2%)	52	81
7	iK	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	iM	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	jJ	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	jL	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	k1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	k7	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	k9	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	kB	139/137 (102%)	131 (94%)	8 (6%)	20	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	kF	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	kI	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	kK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	kM	139/137 (102%)	131 (94%)	8 (6%)	20	55
7	lJ	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	lL	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	m1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	m7	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	m9	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	mB	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	mF	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	mI	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	mK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	mM	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	nJ	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	nL	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	pJ	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	pL	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	rJ	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	rL	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	tJ	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	tL	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	vJ	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	vL	137/137 (100%)	129 (94%)	8 (6%)	20	55
8	e2	204/237 (86%)	197 (97%)	7 (3%)	37	72
8	eR	204/237 (86%)	197 (97%)	7 (3%)	37	72
9	O3	312/331 (94%)	308 (99%)	4 (1%)	69	89
9	OO	312/331 (94%)	308 (99%)	4 (1%)	69	89
10	d4	247/278 (89%)	244 (99%)	3 (1%)	71	90
10	dD	247/278 (89%)	243 (98%)	4 (2%)	62	86
11	D5	72/268 (27%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	D8	72/268 (27%)	72 (100%)	0	100	100
12	E5	164/223 (74%)	164 (100%)	0	100	100
12	E8	164/223 (74%)	164 (100%)	0	100	100
13	k6	227/229 (99%)	211 (93%)	16 (7%)	15	47
13	kH	227/229 (99%)	211 (93%)	16 (7%)	15	47
14	MA	184/262 (70%)	178 (97%)	6 (3%)	38	73
14	MG	184/262 (70%)	180 (98%)	4 (2%)	52	81
14	MN	184/262 (70%)	177 (96%)	7 (4%)	33	69
14	MQ	184/262 (70%)	179 (97%)	5 (3%)	44	77
15	bB	304/389 (78%)	295 (97%)	9 (3%)	41	75
15	bM	304/389 (78%)	294 (97%)	10 (3%)	38	73
16	AB	179/203 (88%)	179 (100%)	0	100	100
16	AM	179/203 (88%)	179 (100%)	0	100	100
16	wJ	179/203 (88%)	165 (92%)	14 (8%)	12	42
16	wL	179/203 (88%)	165 (92%)	14 (8%)	12	42
16	xJ	179/203 (88%)	165 (92%)	14 (8%)	12	42
16	xL	179/203 (88%)	166 (93%)	13 (7%)	14	44
17	BB	188/218 (86%)	187 (100%)	1 (0%)	88	96
17	BM	188/218 (86%)	187 (100%)	1 (0%)	88	96
17	yJ	188/218 (86%)	187 (100%)	1 (0%)	88	96
17	yL	188/218 (86%)	187 (100%)	1 (0%)	88	96
18	MC	231/256 (90%)	213 (92%)	18 (8%)	12	42
18	ME	231/256 (90%)	218 (94%)	13 (6%)	21	56
19	zJ	303/406 (75%)	299 (99%)	4 (1%)	69	89
19	zL	303/406 (75%)	298 (98%)	5 (2%)	60	85
20	AP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	CP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	EP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	GP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	JP	130/131 (99%)	121 (93%)	9 (7%)	15	48
20	KP	130/131 (99%)	120 (92%)	10 (8%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	NP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	PP	130/131 (99%)	121 (93%)	9 (7%)	15	48
20	RP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	TP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	cP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	eP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	gP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	iP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	lP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	mP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	pP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	rP	130/131 (99%)	122 (94%)	8 (6%)	18	52
20	tP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	vP	130/131 (99%)	120 (92%)	10 (8%)	13	42
21	BP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	DP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	FP	124/124 (100%)	113 (91%)	11 (9%)	9	35
21	HP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	IP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	LP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	MP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	OP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	QP	124/124 (100%)	114 (92%)	10 (8%)	11	40
21	SP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	UP	124/124 (100%)	114 (92%)	10 (8%)	11	40
21	dP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	fP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	hP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	jP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	kP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	nP	124/124 (100%)	115 (93%)	9 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	oP	124/124 (100%)	113 (91%)	11 (9%)	9	35
21	qP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	sP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	uP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	wP	124/124 (100%)	114 (92%)	10 (8%)	11	40
22	VP	133/136 (98%)	132 (99%)	1 (1%)	81	93
22	xP	133/136 (98%)	132 (99%)	1 (1%)	81	93
23	WP	147/153 (96%)	147 (100%)	0	100	100
23	yP	147/153 (96%)	147 (100%)	0	100	100
24	XP	78/101 (77%)	77 (99%)	1 (1%)	69	89
24	zP	78/101 (77%)	77 (99%)	1 (1%)	69	89
25	1P	742/772 (96%)	734 (99%)	8 (1%)	73	90
25	YP	742/772 (96%)	734 (99%)	8 (1%)	73	90
26	2P	106/121 (88%)	104 (98%)	2 (2%)	57	84
26	ZP	106/121 (88%)	103 (97%)	3 (3%)	43	77
27	3P	194/214 (91%)	187 (96%)	7 (4%)	35	70
27	aP	194/214 (91%)	186 (96%)	8 (4%)	30	67
28	4P	165/199 (83%)	161 (98%)	4 (2%)	49	79
28	bP	165/199 (83%)	161 (98%)	4 (2%)	49	79
All	All	91927/94464 (97%)	87419 (95%)	4508 (5%)	29	61

All (4508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X1	194	GLU
1	X1	211	LYS
2	A1	101	ILE
2	A1	102	GLN
2	A1	178	ARG
3	B1	203	ILE
3	B1	204	ARG
3	B1	205	ARG
3	B1	206	PHE
3	B1	207	ARG
3	B1	220	LEU

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Mol	Chain	Res	Type
3	B1	226	GLN
4	C1	2	LYS
4	C1	33	ARG
4	C1	39	THR
4	C1	42	LYS
4	C1	68	GLN
4	C1	127	SER
4	C1	145	GLN
4	C1	160	THR
5	D1	31	VAL
5	D1	32	LYS
5	D1	39	ASP
5	D1	62	GLU
5	D1	63	GLN
5	D1	77	ARG
5	D1	155	SER
4	E1	7	GLU
4	E1	116	GLU
4	E1	120	ARG
4	E1	121	SER
4	E1	127	SER
4	E1	140	HIS
4	E1	145	GLN
4	E1	148	ASN
5	F1	39	ASP
5	F1	62	GLU
5	F1	63	GLN
5	F1	77	ARG
5	F1	98	ILE
5	F1	138	SER
5	F1	144	ASP
5	F1	145	THR
5	F1	154	SER
4	G1	2	LYS
4	G1	21	ASN
4	G1	67	THR
4	G1	127	SER
5	H1	32	LYS
5	H1	38	LEU
5	H1	77	ARG
5	H1	143	ASN
4	I1	33	ARG

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Mol	Chain	Res	Type
4	I1	127	SER
5	J1	21	ASN
5	J1	28	SER
5	J1	29	LYS
5	J1	30	MET
5	J1	31	VAL
5	J1	32	LYS
5	J1	39	ASP
5	J1	43	LYS
5	J1	77	ARG
4	K1	35	THR
4	K1	127	SER
5	L1	20	SER
5	L1	36	GLN
5	L1	39	ASP
5	L1	77	ARG
4	M1	38	LEU
4	M1	39	THR
4	M1	42	LYS
4	M1	108	ASP
4	M1	127	SER
5	N1	19	LEU
5	N1	21	ASN
5	N1	32	LYS
5	N1	37	ARG
5	N1	39	ASP
5	N1	77	ARG
5	N1	98	ILE
6	O1	137	ARG
7	P1	3	ASP
7	P1	43	SER
7	P1	103	SER
6	Q1	137	ARG
7	R1	43	SER
7	R1	103	SER
7	R1	157	ASP
6	S1	137	ARG
6	S1	157	ASP
7	T1	43	SER
7	T1	103	SER
6	U1	137	ARG
6	U1	157	ASP

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Mol	Chain	Res	Type
7	V1	43	SER
7	V1	103	SER
7	V1	160[A]	SER
7	V1	160[B]	SER
6	W1	53	LYS
6	W1	137	ARG
7	Y1	43	SER
7	Y1	103	SER
6	Z1	53	LYS
6	Z1	137	ARG
7	a1	3	ASP
7	a1	43	SER
7	a1	103	SER
6	b1	137	ARG
7	c1	43	SER
7	c1	103	SER
6	d1	137	ARG
7	e1	43	SER
7	e1	103	SER
6	f1	137	ARG
7	g1	43	SER
7	g1	103	SER
6	h1	4	VAL
6	h1	33	ARG
6	h1	137	ARG
7	i1	43	SER
7	i1	103	SER
6	j1	137	ARG
7	k1	43	SER
7	k1	103	SER
6	l1	53	LYS
6	l1	137	ARG
7	m1	43	SER
7	m1	103	SER
8	e2	58	SER
8	e2	77	PHE
8	e2	84	LYS
8	e2	108	HIS
8	e2	109	ILE
8	e2	125	ARG
8	e2	128	ARG
6	M2	39	GLU

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Mol	Chain	Res	Type
6	M2	43	LYS
6	M2	77	GLU
6	M2	86	VAL
6	M2	97	LEU
6	M2	105	LEU
7	N2	61	CYS
7	N2	79	MET
7	N2	83	LEU
7	N2	93	VAL
7	N2	134	MET
7	N2	135	LYS
6	O2	43	LYS
6	O2	67	LYS
6	O2	77	GLU
6	O2	116	VAL
6	O2	138	LEU
6	O2	139	CYS
6	O2	163	LEU
7	P2	82	CYS
7	P2	105	LEU
7	P2	107	ASP
7	P2	108	ARG
6	Q2	43	LYS
6	Q2	136	ASP
6	Q2	139	CYS
6	Q2	142	ARG
6	Q2	144	MET
7	R2	25	GLN
7	R2	160	SER
6	S2	43	LYS
6	S2	90	MET
7	T2	108	ARG
7	T2	109	CYS
6	U2	43	LYS
6	U2	52	VAL
6	U2	54	GLU
6	U2	114	ARG
6	U2	115	GLU
7	V2	29	SER
7	V2	41	VAL
7	V2	84	ARG
7	V2	137	GLN

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Mol	Chain	Res	Type
6	W2	9	VAL
6	W2	43	LYS
7	X2	73	CYS
7	X2	75	THR
7	X2	76	ASN
7	X2	93	VAL
7	X2	108	ARG
7	X2	132	SER
7	X2	171	ARG
6	A3	10	SER
6	A3	20	SER
6	A3	26	SER
6	A3	51	VAL
6	A3	52	VAL
7	B3	23	ASP
7	B3	53	SER
7	B3	103	SER
7	B3	127	SER
6	C3	10	SER
6	C3	20	SER
6	C3	26	SER
6	C3	51	VAL
6	C3	52	VAL
6	C3	93	VAL
6	C3	134	THR
6	C3	140	VAL
7	D3	23	ASP
7	D3	27	LEU
7	D3	53	SER
7	D3	56	VAL
7	D3	103	SER
7	D3	120	LEU
7	D3	127	SER
7	D3	165	VAL
7	D3	172	VAL
6	E3	10	SER
6	E3	20	SER
6	E3	26	SER
6	E3	51	VAL
6	E3	52	VAL
6	E3	93	VAL
6	E3	102	THR

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Mol	Chain	Res	Type
6	E3	134	THR
6	E3	140	VAL
7	F3	23	ASP
7	F3	27	LEU
7	F3	53	SER
7	F3	56	VAL
7	F3	103	SER
7	F3	127	SER
7	F3	165	VAL
7	F3	170	ASP
7	F3	172	VAL
7	F3	176	ILE
6	G3	10	SER
6	G3	20	SER
6	G3	26	SER
6	G3	51	VAL
6	G3	52	VAL
6	G3	93	VAL
6	G3	140	VAL
7	H3	23	ASP
7	H3	53	SER
7	H3	56	VAL
7	H3	103	SER
7	H3	120	LEU
7	H3	127	SER
7	H3	132	SER
7	H3	160	SER
7	H3	165	VAL
7	H3	172	VAL
7	H3	176	ILE
6	I3	10	SER
6	I3	20	SER
6	I3	26	SER
6	I3	51	VAL
6	I3	52	VAL
6	I3	93	VAL
6	I3	102	THR
6	I3	134	THR
6	I3	138	LEU
7	J3	23	ASP
7	J3	27	LEU
7	J3	53	SER

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Mol	Chain	Res	Type
7	J3	56	VAL
7	J3	103	SER
7	J3	120	LEU
7	J3	127	SER
7	J3	165	VAL
7	J3	172	VAL
6	K3	10	SER
6	K3	20	SER
6	K3	24	LEU
6	K3	26	SER
6	K3	53	LYS
6	K3	102	THR
6	K3	134	THR
6	K3	140	VAL
7	L3	23	ASP
7	L3	27	LEU
7	L3	53	SER
7	L3	56	VAL
7	L3	103	SER
7	L3	120	LEU
7	L3	127	SER
7	L3	165	VAL
7	L3	172	VAL
7	M3	41	VAL
7	M3	50	CYS
7	M3	67	ILE
7	M3	68	SER
7	M3	91	ARG
7	M3	103	SER
7	M3	126	SER
7	M3	131	VAL
7	M3	147	THR
7	M3	159	THR
7	M3	160	SER
7	N3	41	VAL
7	N3	50	CYS
7	N3	67	ILE
7	N3	68	SER
7	N3	91	ARG
7	N3	103	SER
7	N3	126	SER
7	N3	131	VAL

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Mol	Chain	Res	Type
7	N3	147	THR
7	N3	159	THR
7	N3	160	SER
9	O3	49	VAL
9	O3	76	ARG
9	O3	282	ARG
9	O3	364	LYS
10	d4	195	ARG
10	d4	283	ARG
10	d4	331	GLN
6	B4	17	ARG
6	B4	24	LEU
6	B4	27	ILE
6	B4	28	GLN
6	B4	32	GLN
6	B4	49	GLU
6	B4	53	LYS
6	B4	62	LYS
6	B4	76	GLN
6	B4	90	MET
6	B4	99	VAL
6	B4	119	THR
6	B4	136	ASP
6	B4	151	GLU
6	B4	161	ASN
7	C4	7	ARG
7	C4	8	VAL
7	C4	23	ASP
7	C4	27	LEU
7	C4	31	ILE
7	C4	33	ASP
7	C4	45	VAL
7	C4	59	MET
7	C4	67	ILE
7	C4	77	ARG
7	C4	79	MET
7	C4	88	ILE
7	C4	93	VAL
7	C4	97	LEU
7	C4	98	LEU
7	C4	101	ASP
7	C4	105	LEU

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Mol	Chain	Res	Type
7	C4	108	ARG
7	C4	111	ASN
7	C4	115	GLU
7	C4	127	SER
7	C4	128	ILE
7	C4	129	ARG
7	C4	135	LYS
7	C4	139	VAL
7	C4	142	ILE
7	C4	145	THR
7	C4	149	ARG
7	C4	164	GLU
7	C4	171	ARG
6	D4	1	MET
6	D4	7	THR
6	D4	8	VAL
6	D4	9	VAL
6	D4	13	ASP
6	D4	21	ASN
6	D4	24	LEU
6	D4	27	ILE
6	D4	28	GLN
6	D4	32	GLN
6	D4	49	GLU
6	D4	53	LYS
6	D4	62	LYS
6	D4	76	GLN
6	D4	81	LYS
6	D4	90	MET
6	D4	99	VAL
6	D4	119	THR
6	D4	136	ASP
6	D4	151	GLU
6	D4	161	ASN
7	E4	7	ARG
7	E4	8	VAL
7	E4	23	ASP
7	E4	27	LEU
7	E4	31	ILE
7	E4	33	ASP
7	E4	45	VAL
7	E4	61	CYS

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Mol	Chain	Res	Type
7	E4	67	ILE
7	E4	77	ARG
7	E4	79	MET
7	E4	88	ILE
7	E4	93	VAL
7	E4	97	LEU
7	E4	98	LEU
7	E4	101	ASP
7	E4	105	LEU
7	E4	108	ARG
7	E4	111	ASN
7	E4	115	GLU
7	E4	127	SER
7	E4	128	ILE
7	E4	129	ARG
7	E4	135	LYS
7	E4	139	VAL
7	E4	142	ILE
7	E4	145	THR
7	E4	149	ARG
7	E4	164	GLU
7	E4	171	ARG
6	F4	1	MET
6	F4	7	THR
6	F4	8	VAL
6	F4	9	VAL
6	F4	13	ASP
6	F4	21	ASN
6	F4	24	LEU
6	F4	27	ILE
6	F4	28	GLN
6	F4	33	ARG
6	F4	43	LYS
6	F4	49	GLU
6	F4	53	LYS
6	F4	62	LYS
6	F4	76	GLN
6	F4	81	LYS
6	F4	84	ARG
6	F4	90	MET
6	F4	99	VAL
6	F4	119	THR

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Mol	Chain	Res	Type
6	F4	136	ASP
6	F4	137	ARG
6	F4	151	GLU
6	F4	161	ASN
7	G4	7	ARG
7	G4	8	VAL
7	G4	23	ASP
7	G4	27	LEU
7	G4	31	ILE
7	G4	33	ASP
7	G4	45	VAL
7	G4	59	MET
7	G4	67	ILE
7	G4	75	THR
7	G4	77	ARG
7	G4	78	ARG
7	G4	79	MET
7	G4	88	ILE
7	G4	93	VAL
7	G4	97	LEU
7	G4	98	LEU
7	G4	101	ASP
7	G4	105	LEU
7	G4	108	ARG
7	G4	111	ASN
7	G4	115	GLU
7	G4	125	ASN
7	G4	127	SER
7	G4	128	ILE
7	G4	129	ARG
7	G4	135	LYS
7	G4	139	VAL
7	G4	142	ILE
7	G4	145	THR
7	G4	149	ARG
7	G4	164	GLU
7	G4	171	ARG
6	H4	1	MET
6	H4	7	THR
6	H4	8	VAL
6	H4	9	VAL
6	H4	13	ASP

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Mol	Chain	Res	Type
6	H4	21	ASN
6	H4	24	LEU
6	H4	27	ILE
6	H4	28	GLN
6	H4	32	GLN
6	H4	33	ARG
6	H4	49	GLU
6	H4	53	LYS
6	H4	62	LYS
6	H4	76	GLN
6	H4	81	LYS
6	H4	90	MET
6	H4	99	VAL
6	H4	119	THR
6	H4	136	ASP
6	H4	151	GLU
6	H4	161	ASN
7	I4	7	ARG
7	I4	8	VAL
7	I4	23	ASP
7	I4	27	LEU
7	I4	31	ILE
7	I4	33	ASP
7	I4	45	VAL
7	I4	59	MET
7	I4	67	ILE
7	I4	125	ASN
7	I4	127	SER
7	I4	128	ILE
7	I4	129	ARG
7	I4	132	SER
7	I4	139	VAL
7	I4	142	ILE
7	I4	145	THR
7	I4	149	ARG
7	I4	164	GLU
7	I4	171	ARG
6	J4	1	MET
6	J4	7	THR
6	J4	13	ASP
6	J4	24	LEU
6	J4	27	ILE

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Mol	Chain	Res	Type
6	J4	28	GLN
6	J4	32	GLN
6	J4	49	GLU
6	J4	53	LYS
6	J4	62	LYS
6	J4	67	LYS
6	J4	76	GLN
6	J4	81	LYS
6	J4	90	MET
6	J4	99	VAL
6	J4	119	THR
6	J4	136	ASP
6	J4	151	GLU
6	J4	161	ASN
7	K4	7	ARG
7	K4	8	VAL
7	K4	23	ASP
7	K4	27	LEU
7	K4	31	ILE
7	K4	33	ASP
7	K4	45	VAL
7	K4	59	MET
7	K4	67	ILE
7	K4	77	ARG
7	K4	79	MET
7	K4	88	ILE
7	K4	93	VAL
7	K4	97	LEU
7	K4	98	LEU
7	K4	101	ASP
7	K4	105	LEU
7	K4	108	ARG
7	K4	111	ASN
7	K4	115	GLU
7	K4	125	ASN
7	K4	127	SER
7	K4	129	ARG
7	K4	135	LYS
7	K4	139	VAL
7	K4	142	ILE
7	K4	145	THR
7	K4	149	ARG

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Mol	Chain	Res	Type
7	K4	164	GLU
6	L4	1	MET
6	L4	7	THR
6	L4	8	VAL
6	L4	9	VAL
6	L4	13	ASP
6	L4	21	ASN
6	L4	24	LEU
6	L4	27	ILE
6	L4	28	GLN
6	L4	33	ARG
6	L4	49	GLU
6	L4	53	LYS
6	L4	62	LYS
6	L4	76	GLN
6	L4	81	LYS
6	L4	90	MET
6	L4	99	VAL
6	L4	119	THR
6	L4	136	ASP
6	L4	151	GLU
6	L4	161	ASN
7	M4	7	ARG
7	M4	8	VAL
7	M4	23	ASP
7	M4	27	LEU
7	M4	31	ILE
7	M4	33	ASP
7	M4	45	VAL
7	M4	59	MET
7	M4	77	ARG
7	M4	79	MET
7	M4	88	ILE
7	M4	93	VAL
7	M4	97	LEU
7	M4	98	LEU
7	M4	101	ASP
7	M4	105	LEU
7	M4	108	ARG
7	M4	111	ASN
7	M4	115	GLU
7	M4	127	SER

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Mol	Chain	Res	Type
7	M4	128	ILE
7	M4	129	ARG
7	M4	135	LYS
7	M4	139	VAL
7	M4	142	ILE
7	M4	145	THR
7	M4	149	ARG
7	M4	164	GLU
7	M4	171	ARG
7	B5	87	GLU
7	B5	107	ASP
7	B5	108	ARG
7	B5	126	SER
7	B5	150	LYS
7	F5	87	GLU
7	F5	107	ASP
7	F5	108	ARG
7	F5	126	SER
7	F5	150	LYS
7	G5	87	GLU
7	G5	107	ASP
7	G5	108	ARG
7	G5	126	SER
7	G5	150	LYS
7	H5	87	GLU
7	H5	107	ASP
7	H5	108	ARG
7	H5	126	SER
7	H5	150	LYS
7	I5	1	MET
7	I5	11	ASN
7	I5	19	VAL
7	I5	52	VAL
7	I5	53	SER
7	I5	57	SER
7	I5	59	MET
7	I5	67	ILE
7	I5	73	CYS
7	I5	87	GLU
7	I5	91	ARG
7	I5	106	GLU
7	I5	124	THR

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Mol	Chain	Res	Type
7	I5	126	SER
7	I5	142	ILE
7	I5	151	MET
7	I5	157	ASP
7	K5	1	MET
7	K5	7	ARG
7	K5	22	SER
7	K5	52	VAL
7	K5	53	SER
7	K5	57	SER
7	K5	59	MET
7	K5	67	ILE
7	K5	73	CYS
7	K5	79	MET
7	K5	87	GLU
7	K5	106	GLU
7	K5	124	THR
7	K5	126	SER
7	K5	142	ILE
7	K5	151	MET
7	K5	157	ASP
7	L5	87	GLU
7	L5	109	CYS
7	L5	126	SER
7	L5	150	LYS
7	A5	52	VAL
7	A5	53	SER
7	A5	57	SER
7	A5	59	MET
7	A5	67	ILE
7	A5	73	CYS
7	A5	79	MET
7	A5	87	GLU
7	A5	91	ARG
7	A5	106	GLU
7	A5	124	THR
7	A5	126	SER
7	A5	142	ILE
7	A5	151	MET
7	A5	157	ASP
7	A5	163	SER
7	C5	52	VAL

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Mol	Chain	Res	Type
7	C5	53	SER
7	C5	57	SER
7	C5	59	MET
7	C5	67	ILE
7	C5	73	CYS
7	C5	87	GLU
7	C5	91	ARG
7	C5	106	GLU
7	C5	124	THR
7	C5	126	SER
7	C5	142	ILE
7	C5	151	MET
7	C5	157	ASP
7	C5	163	SER
13	k6	4	LYS
13	k6	7	GLU
13	k6	32	ASN
13	k6	41	ASP
13	k6	94	LEU
13	k6	118	ARG
13	k6	135	LEU
13	k6	156	THR
13	k6	157	LYS
13	k6	158	LYS
13	k6	172	LYS
13	k6	173	TYR
13	k6	222	GLU
13	k6	236	GLN
13	k6	281	SER
13	k6	286	MET
1	X7	105	LYS
1	X7	106	GLN
1	X7	291	THR
1	X7	320	LEU
3	B7	7	LYS
3	B7	19	SER
3	B7	21	GLU
3	B7	40	SER
3	B7	41	SER
3	B7	42	GLU
3	B7	61	LEU
3	B7	65	LYS

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Mol	Chain	Res	Type
3	B7	205	ARG
3	B7	207	ARG
3	B7	226	GLN
3	B7	227	GLU
4	C7	3	THR
4	C7	37	SER
4	C7	39	THR
4	C7	77	SER
4	C7	101	VAL
4	C7	111	LEU
4	C7	121	SER
4	C7	123	ASP
4	C7	127	SER
4	C7	143	SER
4	C7	155	ASP
5	D7	3	ASP
5	D7	7	LYS
5	D7	8	VAL
5	D7	17	GLU
5	D7	20	SER
5	D7	28	SER
5	D7	41	VAL
5	D7	46	SER
5	D7	49	SER
5	D7	53	THR
5	D7	75	THR
5	D7	76	SER
5	D7	89	VAL
5	D7	94	SER
5	D7	107	ASP
5	D7	125	SER
5	D7	129	VAL
5	D7	144	ASP
5	D7	146	THR
5	D7	157	VAL
5	D7	170	SER
4	E7	3	THR
4	E7	37	SER
4	E7	39	THR
4	E7	77	SER
4	E7	101	VAL
4	E7	111	LEU

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Mol	Chain	Res	Type
4	E7	121	SER
4	E7	127	SER
4	E7	143	SER
4	E7	155	ASP
5	F7	3	ASP
5	F7	7	LYS
5	F7	8	VAL
5	F7	17	GLU
5	F7	20	SER
5	F7	41	VAL
5	F7	46	SER
5	F7	49	SER
5	F7	53	THR
5	F7	67	ILE
5	F7	75	THR
5	F7	77	ARG
5	F7	89	VAL
5	F7	94	SER
5	F7	107	ASP
5	F7	115	GLU
5	F7	125	SER
5	F7	129	VAL
5	F7	144	ASP
5	F7	146	THR
5	F7	157	VAL
5	F7	170	SER
4	G7	3	THR
4	G7	37	SER
4	G7	39	THR
4	G7	77	SER
4	G7	101	VAL
4	G7	111	LEU
4	G7	121	SER
4	G7	127	SER
4	G7	143	SER
4	G7	155	ASP
5	H7	3	ASP
5	H7	7	LYS
5	H7	8	VAL
5	H7	17	GLU
5	H7	20	SER
5	H7	28	SER

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Mol	Chain	Res	Type
5	H7	41	VAL
5	H7	46	SER
5	H7	49	SER
5	H7	53	THR
5	H7	77	ARG
5	H7	78	ARG
5	H7	89	VAL
5	H7	94	SER
5	H7	107	ASP
5	H7	115	GLU
5	H7	125	SER
5	H7	129	VAL
5	H7	144	ASP
5	H7	146	THR
5	H7	157	VAL
5	H7	170	SER
4	I7	3	THR
4	I7	37	SER
4	I7	39	THR
4	I7	77	SER
4	I7	101	VAL
4	I7	112	VAL
4	I7	121	SER
4	I7	123	ASP
4	I7	127	SER
4	I7	143	SER
4	I7	155	ASP
5	J7	3	ASP
5	J7	8	VAL
5	J7	17	GLU
5	J7	20	SER
5	J7	28	SER
5	J7	41	VAL
5	J7	46	SER
5	J7	49	SER
5	J7	53	THR
5	J7	77	ARG
5	J7	89	VAL
5	J7	94	SER
5	J7	107	ASP
5	J7	125	SER
5	J7	129	VAL

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Mol	Chain	Res	Type
5	J7	144	ASP
5	J7	146	THR
5	J7	157	VAL
5	J7	170	SER
4	K7	3	THR
4	K7	37	SER
4	K7	39	THR
4	K7	49	GLN
4	K7	77	SER
4	K7	101	VAL
4	K7	111	LEU
4	K7	121	SER
4	K7	123	ASP
4	K7	127	SER
4	K7	143	SER
4	K7	155	ASP
5	L7	3	ASP
5	L7	8	VAL
5	L7	17	GLU
5	L7	20	SER
5	L7	28	SER
5	L7	41	VAL
5	L7	46	SER
5	L7	49	SER
5	L7	53	THR
5	L7	76	SER
5	L7	89	VAL
5	L7	94	SER
5	L7	125	SER
5	L7	129	VAL
5	L7	144	ASP
5	L7	146	THR
5	L7	157	VAL
5	L7	170	SER
4	M7	3	THR
4	M7	37	SER
4	M7	39	THR
4	M7	77	SER
4	M7	101	VAL
4	M7	111	LEU
4	M7	121	SER
4	M7	127	SER

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Mol	Chain	Res	Type
4	M7	143	SER
5	N7	7	LYS
5	N7	8	VAL
5	N7	17	GLU
5	N7	20	SER
5	N7	28	SER
5	N7	41	VAL
5	N7	46	SER
5	N7	49	SER
5	N7	53	THR
5	N7	76	SER
5	N7	89	VAL
5	N7	94	SER
5	N7	107	ASP
5	N7	125	SER
5	N7	129	VAL
5	N7	157	VAL
5	N7	170	SER
6	O7	9	VAL
6	O7	10	SER
6	O7	26	SER
6	O7	57	ASP
6	O7	99	VAL
6	O7	125	SER
6	O7	145	SER
6	O7	153	SER
7	P7	8	VAL
7	P7	12	SER
7	P7	22	SER
7	P7	39	ASP
7	P7	46	SER
7	P7	57	SER
7	P7	103	SER
7	P7	124	THR
7	P7	127	SER
7	P7	145	THR
7	P7	160	SER
7	P7	167	SER
7	P7	172	VAL
6	Q7	9	VAL
6	Q7	10	SER
6	Q7	26	SER

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Mol	Chain	Res	Type
6	Q7	57	ASP
6	Q7	99	VAL
6	Q7	125	SER
6	Q7	145	SER
6	Q7	153	SER
7	R7	8	VAL
7	R7	12	SER
7	R7	22	SER
7	R7	39	ASP
7	R7	46	SER
7	R7	57	SER
7	R7	103	SER
7	R7	124	THR
7	R7	127	SER
7	R7	145	THR
7	R7	160	SER
7	R7	167	SER
7	R7	172	VAL
6	S7	9	VAL
6	S7	10	SER
6	S7	26	SER
6	S7	99	VAL
6	S7	125	SER
6	S7	145	SER
6	S7	153	SER
7	T7	8	VAL
7	T7	12	SER
7	T7	22	SER
7	T7	46	SER
7	T7	57	SER
7	T7	103	SER
7	T7	124	THR
7	T7	127	SER
7	T7	145	THR
7	T7	160	SER
7	T7	167	SER
7	T7	172	VAL
6	U7	9	VAL
6	U7	10	SER
6	U7	26	SER
6	U7	57	ASP
6	U7	99	VAL

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Mol	Chain	Res	Type
6	U7	125	SER
6	U7	145	SER
6	U7	153	SER
7	V7	8	VAL
7	V7	12	SER
7	V7	22	SER
7	V7	46	SER
7	V7	57	SER
7	V7	103	SER
7	V7	127	SER
7	V7	145	THR
7	V7	160	SER
7	V7	167	SER
7	V7	172	VAL
6	W7	9	VAL
6	W7	10	SER
6	W7	26	SER
6	W7	57	ASP
6	W7	125	SER
6	W7	145	SER
6	W7	153	SER
7	Y7	8	VAL
7	Y7	12	SER
7	Y7	22	SER
7	Y7	46	SER
7	Y7	57	SER
7	Y7	84	ARG
7	Y7	103	SER
7	Y7	124	THR
7	Y7	127	SER
7	Y7	145	THR
7	Y7	160	SER
7	Y7	167	SER
7	Y7	172	VAL
6	Z7	10	SER
6	Z7	26	SER
6	Z7	99	VAL
6	Z7	125	SER
6	Z7	145	SER
6	Z7	153	SER
7	a7	8	VAL
7	a7	12	SER

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Mol	Chain	Res	Type
7	a7	22	SER
7	a7	39	ASP
7	a7	46	SER
7	a7	57	SER
7	a7	103	SER
7	a7	124	THR
7	a7	127	SER
7	a7	145	THR
7	a7	160	SER
7	a7	167	SER
7	a7	172	VAL
6	b7	9	VAL
6	b7	10	SER
6	b7	26	SER
6	b7	57	ASP
6	b7	99	VAL
6	b7	125	SER
6	b7	145	SER
6	b7	153	SER
7	c7	8	VAL
7	c7	12	SER
7	c7	22	SER
7	c7	39	ASP
7	c7	46	SER
7	c7	57	SER
7	c7	103	SER
7	c7	145	THR
7	c7	160	SER
7	c7	167	SER
7	c7	172	VAL
6	d7	9	VAL
6	d7	10	SER
6	d7	26	SER
6	d7	57	ASP
6	d7	99	VAL
6	d7	125	SER
6	d7	145	SER
6	d7	153	SER
7	e7	8	VAL
7	e7	12	SER
7	e7	22	SER
7	e7	39	ASP

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Mol	Chain	Res	Type
7	e7	46	SER
7	e7	57	SER
7	e7	87	GLU
7	e7	103	SER
7	e7	124	THR
7	e7	127	SER
7	e7	145	THR
7	e7	160	SER
7	e7	167	SER
7	e7	172	VAL
6	f7	9	VAL
6	f7	10	SER
6	f7	26	SER
6	f7	99	VAL
6	f7	125	SER
6	f7	145	SER
6	f7	153	SER
7	g7	8	VAL
7	g7	12	SER
7	g7	22	SER
7	g7	46	SER
7	g7	57	SER
7	g7	103	SER
7	g7	124	THR
7	g7	127	SER
7	g7	145	THR
7	g7	160	SER
7	g7	167	SER
7	g7	172	VAL
6	h7	9	VAL
6	h7	10	SER
6	h7	26	SER
6	h7	57	ASP
6	h7	99	VAL
6	h7	125	SER
6	h7	145	SER
6	h7	153	SER
7	i7	8	VAL
7	i7	12	SER
7	i7	22	SER
7	i7	39	ASP
7	i7	46	SER

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Mol	Chain	Res	Type
7	i7	57	SER
7	i7	103	SER
7	i7	127	SER
7	i7	145	THR
7	i7	160	SER
7	i7	167	SER
7	i7	172	VAL
6	j7	9	VAL
6	j7	10	SER
6	j7	26	SER
6	j7	57	ASP
6	j7	125	SER
6	j7	145	SER
6	j7	153	SER
7	k7	8	VAL
7	k7	12	SER
7	k7	22	SER
7	k7	46	SER
7	k7	57	SER
7	k7	103	SER
7	k7	124	THR
7	k7	127	SER
7	k7	145	THR
7	k7	160	SER
7	k7	167	SER
7	k7	172	VAL
6	l7	9	VAL
6	l7	10	SER
6	l7	26	SER
6	l7	99	VAL
6	l7	125	SER
6	l7	137	ARG
6	l7	145	SER
6	l7	153	SER
7	m7	8	VAL
7	m7	12	SER
7	m7	22	SER
7	m7	46	SER
7	m7	57	SER
7	m7	124	THR
7	m7	127	SER
7	m7	145	THR

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Mol	Chain	Res	Type
7	m7	165	VAL
7	m7	170	ASP
7	m7	172	VAL
7	B8	87	GLU
7	B8	108	ARG
7	B8	126	SER
7	B8	150	LYS
7	F8	87	GLU
7	F8	107	ASP
7	F8	108	ARG
7	F8	126	SER
7	F8	150	LYS
7	G8	87	GLU
7	G8	107	ASP
7	G8	108	ARG
7	G8	126	SER
7	G8	150	LYS
7	H8	87	GLU
7	H8	107	ASP
7	H8	108	ARG
7	H8	126	SER
7	H8	150	LYS
7	I8	5	PHE
7	I8	11	ASN
7	I8	19	VAL
7	I8	52	VAL
7	I8	53	SER
7	I8	57	SER
7	I8	59	MET
7	I8	67	ILE
7	I8	73	CYS
7	I8	87	GLU
7	I8	91	ARG
7	I8	106	GLU
7	I8	124	THR
7	I8	126	SER
7	I8	142	ILE
7	I8	151	MET
7	I8	157	ASP
6	J8	18	PHE
7	K8	1	MET
7	K8	7	ARG

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Mol	Chain	Res	Type
7	K8	22	SER
7	K8	52	VAL
7	K8	53	SER
7	K8	57	SER
7	K8	59	MET
7	K8	67	ILE
7	K8	73	CYS
7	K8	79	MET
7	K8	87	GLU
7	K8	106	GLU
7	K8	124	THR
7	K8	126	SER
7	K8	142	ILE
7	K8	151	MET
7	K8	157	ASP
7	L8	87	GLU
7	L8	107	ASP
7	L8	108	ARG
7	L8	126	SER
7	L8	150	LYS
7	A8	52	VAL
7	A8	53	SER
7	A8	57	SER
7	A8	59	MET
7	A8	67	ILE
7	A8	73	CYS
7	A8	79	MET
7	A8	87	GLU
7	A8	91	ARG
7	A8	106	GLU
7	A8	124	THR
7	A8	126	SER
7	A8	142	ILE
7	A8	151	MET
7	A8	157	ASP
7	A8	163	SER
7	C8	52	VAL
7	C8	53	SER
7	C8	57	SER
7	C8	59	MET
7	C8	67	ILE
7	C8	73	CYS

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Mol	Chain	Res	Type
7	C8	87	GLU
7	C8	91	ARG
7	C8	106	GLU
7	C8	124	THR
7	C8	126	SER
7	C8	142	ILE
7	C8	151	MET
7	C8	157	ASP
7	C8	163	SER
1	X9	105	LYS
1	X9	106	GLN
1	X9	291	THR
1	X9	320	LEU
3	B9	19	SER
3	B9	21	GLU
3	B9	40	SER
3	B9	41	SER
3	B9	42	GLU
3	B9	61	LEU
3	B9	65	LYS
3	B9	187	GLU
3	B9	205	ARG
3	B9	207	ARG
3	B9	226	GLN
3	B9	227	GLU
4	C9	3	THR
4	C9	37	SER
4	C9	39	THR
4	C9	77	SER
4	C9	101	VAL
4	C9	111	LEU
4	C9	121	SER
4	C9	123	ASP
4	C9	127	SER
4	C9	143	SER
4	C9	155	ASP
5	D9	3	ASP
5	D9	7	LYS
5	D9	8	VAL
5	D9	17	GLU
5	D9	20	SER
5	D9	28	SER

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Mol	Chain	Res	Type
5	D9	41	VAL
5	D9	46	SER
5	D9	49	SER
5	D9	53	THR
5	D9	75	THR
5	D9	76	SER
5	D9	89	VAL
5	D9	94	SER
5	D9	107	ASP
5	D9	125	SER
5	D9	129	VAL
5	D9	144	ASP
5	D9	146	THR
5	D9	157	VAL
5	D9	170	SER
4	E9	3	THR
4	E9	37	SER
4	E9	39	THR
4	E9	77	SER
4	E9	101	VAL
4	E9	111	LEU
4	E9	121	SER
4	E9	127	SER
4	E9	143	SER
4	E9	155	ASP
5	F9	3	ASP
5	F9	7	LYS
5	F9	8	VAL
5	F9	41	VAL
5	F9	46	SER
5	F9	49	SER
5	F9	53	THR
5	F9	67	ILE
5	F9	75	THR
5	F9	77	ARG
5	F9	89	VAL
5	F9	94	SER
5	F9	107	ASP
5	F9	115	GLU
5	F9	125	SER
5	F9	129	VAL
5	F9	144	ASP

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Mol	Chain	Res	Type
5	F9	146	THR
5	F9	157	VAL
5	F9	170	SER
4	G9	3	THR
4	G9	37	SER
4	G9	39	THR
4	G9	77	SER
4	G9	101	VAL
4	G9	111	LEU
4	G9	121	SER
4	G9	127	SER
4	G9	143	SER
4	G9	155	ASP
5	H9	3	ASP
5	H9	7	LYS
5	H9	8	VAL
5	H9	17	GLU
5	H9	20	SER
5	H9	28	SER
5	H9	41	VAL
5	H9	46	SER
5	H9	49	SER
5	H9	53	THR
5	H9	77	ARG
5	H9	78	ARG
5	H9	89	VAL
5	H9	94	SER
5	H9	107	ASP
5	H9	115	GLU
5	H9	125	SER
5	H9	129	VAL
5	H9	144	ASP
5	H9	146	THR
5	H9	157	VAL
5	H9	170	SER
4	I9	3	THR
4	I9	37	SER
4	I9	39	THR
4	I9	77	SER
4	I9	101	VAL
4	I9	112	VAL
4	I9	121	SER

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Mol	Chain	Res	Type
4	I9	123	ASP
4	I9	127	SER
4	I9	143	SER
4	I9	155	ASP
5	J9	3	ASP
5	J9	8	VAL
5	J9	17	GLU
5	J9	20	SER
5	J9	28	SER
5	J9	41	VAL
5	J9	46	SER
5	J9	49	SER
5	J9	53	THR
5	J9	77	ARG
5	J9	89	VAL
5	J9	94	SER
5	J9	107	ASP
5	J9	125	SER
5	J9	129	VAL
5	J9	144	ASP
5	J9	146	THR
5	J9	157	VAL
5	J9	170	SER
4	K9	3	THR
4	K9	37	SER
4	K9	39	THR
4	K9	49	GLN
4	K9	77	SER
4	K9	101	VAL
4	K9	111	LEU
4	K9	121	SER
4	K9	123	ASP
4	K9	127	SER
4	K9	143	SER
4	K9	155	ASP
5	L9	3	ASP
5	L9	8	VAL
5	L9	17	GLU
5	L9	20	SER
5	L9	28	SER
5	L9	41	VAL
5	L9	46	SER

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Mol	Chain	Res	Type
5	L9	49	SER
5	L9	53	THR
5	L9	76	SER
5	L9	89	VAL
5	L9	94	SER
5	L9	125	SER
5	L9	129	VAL
5	L9	144	ASP
5	L9	146	THR
5	L9	157	VAL
5	L9	170	SER
4	M9	3	THR
4	M9	37	SER
4	M9	39	THR
4	M9	77	SER
4	M9	101	VAL
4	M9	111	LEU
4	M9	121	SER
4	M9	127	SER
4	M9	143	SER
5	N9	7	LYS
5	N9	8	VAL
5	N9	17	GLU
5	N9	20	SER
5	N9	28	SER
5	N9	41	VAL
5	N9	46	SER
5	N9	49	SER
5	N9	53	THR
5	N9	76	SER
5	N9	89	VAL
5	N9	94	SER
5	N9	107	ASP
5	N9	125	SER
5	N9	129	VAL
5	N9	157	VAL
5	N9	170	SER
6	O9	9	VAL
6	O9	10	SER
6	O9	26	SER
6	O9	57	ASP
6	O9	99	VAL

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Mol	Chain	Res	Type
6	O9	125	SER
6	O9	145	SER
6	O9	153	SER
7	P9	8	VAL
7	P9	12	SER
7	P9	22	SER
7	P9	39	ASP
7	P9	46	SER
7	P9	57	SER
7	P9	103	SER
7	P9	124	THR
7	P9	127	SER
7	P9	145	THR
7	P9	160	SER
7	P9	167	SER
7	P9	172	VAL
6	Q9	9	VAL
6	Q9	10	SER
6	Q9	26	SER
6	Q9	57	ASP
6	Q9	99	VAL
6	Q9	125	SER
6	Q9	145	SER
6	Q9	153	SER
7	R9	8	VAL
7	R9	12	SER
7	R9	22	SER
7	R9	39	ASP
7	R9	46	SER
7	R9	57	SER
7	R9	103	SER
7	R9	124	THR
7	R9	127	SER
7	R9	145	THR
7	R9	160	SER
7	R9	167	SER
7	R9	172	VAL
6	S9	9	VAL
6	S9	10	SER
6	S9	26	SER
6	S9	99	VAL
6	S9	125	SER

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Mol	Chain	Res	Type
6	S9	145	SER
6	S9	153	SER
7	T9	8	VAL
7	T9	12	SER
7	T9	22	SER
7	T9	46	SER
7	T9	57	SER
7	T9	103	SER
7	T9	124	THR
7	T9	127	SER
7	T9	145	THR
7	T9	160	SER
7	T9	167	SER
7	T9	172	VAL
6	U9	9	VAL
6	U9	10	SER
6	U9	26	SER
6	U9	57	ASP
6	U9	99	VAL
6	U9	125	SER
6	U9	145	SER
6	U9	153	SER
7	V9	8	VAL
7	V9	12	SER
7	V9	22	SER
7	V9	46	SER
7	V9	57	SER
7	V9	103	SER
7	V9	127	SER
7	V9	145	THR
7	V9	160	SER
7	V9	167	SER
7	V9	172	VAL
6	W9	9	VAL
6	W9	10	SER
6	W9	26	SER
6	W9	57	ASP
6	W9	125	SER
6	W9	145	SER
6	W9	153	SER
7	Y9	8	VAL
7	Y9	12	SER

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Mol	Chain	Res	Type
7	Y9	22	SER
7	Y9	46	SER
7	Y9	57	SER
7	Y9	84	ARG
7	Y9	103	SER
7	Y9	124	THR
7	Y9	127	SER
7	Y9	145	THR
7	Y9	160	SER
7	Y9	167	SER
7	Y9	172	VAL
6	Z9	10	SER
6	Z9	26	SER
6	Z9	99	VAL
6	Z9	125	SER
6	Z9	145	SER
6	Z9	153	SER
7	a9	8	VAL
7	a9	12	SER
7	a9	22	SER
7	a9	39	ASP
7	a9	46	SER
7	a9	57	SER
7	a9	61	CYS
7	a9	103	SER
7	a9	124	THR
7	a9	127	SER
7	a9	145	THR
7	a9	160	SER
7	a9	167	SER
7	a9	172	VAL
6	b9	9	VAL
6	b9	10	SER
6	b9	26	SER
6	b9	57	ASP
6	b9	99	VAL
6	b9	125	SER
6	b9	145	SER
6	b9	153	SER
7	c9	8	VAL
7	c9	12	SER
7	c9	22	SER

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Mol	Chain	Res	Type
7	c9	39	ASP
7	c9	46	SER
7	c9	57	SER
7	c9	103	SER
7	c9	145	THR
7	c9	160	SER
7	c9	167	SER
7	c9	172	VAL
6	d9	9	VAL
6	d9	10	SER
6	d9	26	SER
6	d9	57	ASP
6	d9	99	VAL
6	d9	125	SER
6	d9	145	SER
6	d9	153	SER
7	e9	8	VAL
7	e9	12	SER
7	e9	22	SER
7	e9	39	ASP
7	e9	46	SER
7	e9	57	SER
7	e9	87	GLU
7	e9	103	SER
7	e9	124	THR
7	e9	127	SER
7	e9	145	THR
7	e9	160	SER
7	e9	167	SER
7	e9	172	VAL
6	f9	9	VAL
6	f9	10	SER
6	f9	26	SER
6	f9	99	VAL
6	f9	125	SER
6	f9	145	SER
6	f9	153	SER
7	g9	8	VAL
7	g9	12	SER
7	g9	22	SER
7	g9	46	SER
7	g9	57	SER

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Mol	Chain	Res	Type
7	g9	103	SER
7	g9	124	THR
7	g9	127	SER
7	g9	145	THR
7	g9	160	SER
7	g9	167	SER
7	g9	172	VAL
6	h9	9	VAL
6	h9	10	SER
6	h9	26	SER
6	h9	57	ASP
6	h9	99	VAL
6	h9	125	SER
6	h9	145	SER
6	h9	153	SER
7	i9	8	VAL
7	i9	12	SER
7	i9	22	SER
7	i9	39	ASP
7	i9	46	SER
7	i9	57	SER
7	i9	103	SER
7	i9	127	SER
7	i9	145	THR
7	i9	160	SER
7	i9	167	SER
7	i9	172	VAL
6	j9	9	VAL
6	j9	10	SER
6	j9	26	SER
6	j9	57	ASP
6	j9	125	SER
6	j9	145	SER
6	j9	153	SER
7	k9	8	VAL
7	k9	12	SER
7	k9	22	SER
7	k9	46	SER
7	k9	57	SER
7	k9	103	SER
7	k9	124	THR
7	k9	127	SER

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Mol	Chain	Res	Type
7	k9	145	THR
7	k9	160	SER
7	k9	167	SER
7	k9	172	VAL
6	l9	9	VAL
6	l9	10	SER
6	l9	26	SER
6	l9	99	VAL
6	l9	125	SER
6	l9	145	SER
6	l9	153	SER
7	m9	8	VAL
7	m9	12	SER
7	m9	22	SER
7	m9	46	SER
7	m9	57	SER
7	m9	124	THR
7	m9	127	SER
7	m9	145	THR
7	m9	165	VAL
7	m9	170	ASP
7	m9	172	VAL
6	AA	3	SER
6	AA	39	GLU
6	AA	43	LYS
6	AA	124	THR
6	AA	131	ILE
6	AA	134	THR
6	AA	138	LEU
6	AA	150	VAL
6	AA	153	SER
7	BA	12	SER
7	BA	13	ASP
7	BA	19	VAL
7	BA	24	LEU
7	BA	43	SER
7	BA	56	VAL
7	BA	103	SER
7	BA	113	LEU
7	BA	127	SER
7	BA	152	SER
6	CA	3	SER

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Mol	Chain	Res	Type
6	CA	21	ASN
6	CA	43	LYS
6	CA	124	THR
6	CA	131	ILE
6	CA	134	THR
6	CA	138	LEU
6	CA	150	VAL
6	CA	153	SER
7	DA	12	SER
7	DA	24	LEU
7	DA	43	SER
7	DA	56	VAL
7	DA	103	SER
7	DA	127	SER
7	DA	139	VAL
7	DA	152	SER
6	EA	3	SER
6	EA	39	GLU
6	EA	43	LYS
6	EA	124	THR
6	EA	131	ILE
6	EA	138	LEU
6	EA	150	VAL
7	FA	12	SER
7	FA	13	ASP
7	FA	19	VAL
7	FA	43	SER
7	FA	56	VAL
7	FA	103	SER
7	FA	127	SER
7	FA	139	VAL
7	FA	152	SER
6	GA	3	SER
6	GA	39	GLU
6	GA	43	LYS
6	GA	124	THR
6	GA	131	ILE
6	GA	138	LEU
6	GA	150	VAL
6	GA	153	SER
7	HA	12	SER
7	HA	13	ASP

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Mol	Chain	Res	Type
7	HA	24	LEU
7	HA	43	SER
7	HA	56	VAL
7	HA	103	SER
7	HA	113	LEU
7	HA	127	SER
7	HA	139	VAL
7	HA	152	SER
7	HA	160	SER
6	IA	3	SER
6	IA	32	GLN
6	IA	43	LYS
6	IA	124	THR
6	IA	131	ILE
6	IA	134	THR
6	IA	138	LEU
6	IA	150	VAL
6	IA	153	SER
7	JA	12	SER
7	JA	43	SER
7	JA	56	VAL
7	JA	103	SER
7	JA	113	LEU
7	JA	127	SER
7	JA	139	VAL
7	JA	152	SER
6	KA	3	SER
6	KA	39	GLU
6	KA	43	LYS
6	KA	124	THR
6	KA	134	THR
6	KA	138	LEU
6	KA	150	VAL
6	KA	153	SER
7	LA	12	SER
7	LA	24	LEU
7	LA	43	SER
7	LA	56	VAL
7	LA	103	SER
7	LA	127	SER
7	LA	152	SER
14	MA	101	LEU

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Mol	Chain	Res	Type
14	MA	145	CYS
14	MA	195	CYS
14	MA	232	LYS
14	MA	259	CYS
14	MA	314	LYS
15	bB	91	ILE
15	bB	150	ARG
15	bB	198	ARG
15	bB	202	THR
15	bB	204	CYS
15	bB	270	ASN
15	bB	271	TRP
15	bB	332	MET
15	bB	333	ARG
17	BB	180	SER
6	CB	6	THR
6	CB	62	LYS
7	DB	23	ASP
7	DB	159	THR
7	DB	160	SER
6	EB	62	LYS
6	EB	147	GLN
7	FB	23	ASP
7	FB	139	VAL
6	GB	49	GLU
6	GB	62	LYS
6	GB	134	THR
6	GB	135	ARG
6	GB	137	ARG
6	GB	147	GLN
6	GB	159	LEU
7	HB	8	VAL
7	HB	10	VAL
7	HB	23	ASP
7	HB	52	VAL
7	HB	160	SER
6	IB	62	LYS
7	JB	23	ASP
7	JB	85	ASP
7	JB	145	THR
7	JB	147	THR
7	JB	149	ARG

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Mol	Chain	Res	Type
6	KB	21	ASN
6	KB	62	LYS
7	LB	23	ASP
6	MB	62	LYS
7	NB	23	ASP
7	NB	25	GLN
7	NB	62	GLU
7	NB	85	ASP
7	NB	114	LYS
7	NB	159	THR
6	OB	62	LYS
7	PB	23	ASP
6	QB	62	LYS
6	QB	136	ASP
6	QB	157	ASP
7	RB	8	VAL
7	RB	23	ASP
7	RB	61	CYS
7	RB	62	GLU
7	RB	145	THR
7	RB	148	GLU
6	SB	49	GLU
6	SB	62	LYS
7	TB	23	ASP
7	TB	24	LEU
7	TB	25	GLN
7	TB	159	THR
7	TB	170	ASP
6	UB	62	LYS
7	VB	23	ASP
7	VB	61	CYS
7	VB	85	ASP
7	VB	159	THR
7	VB	160	SER
6	WB	62	LYS
6	WB	121	ASN
7	XB	23	ASP
6	YB	62	LYS
7	ZB	23	ASP
7	ZB	61	CYS
7	ZB	84	ARG
7	ZB	124	THR

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Mol	Chain	Res	Type
7	ZB	127	SER
6	aB	62	LYS
7	cB	23	ASP
7	cB	159	THR
6	dB	62	LYS
6	dB	147	GLN
7	eB	23	ASP
7	eB	63	ASN
7	eB	84	ARG
7	eB	125	ASN
6	fB	62	LYS
6	fB	136	ASP
7	gB	23	ASP
7	gB	35	ASN
7	gB	53[A]	SER
7	gB	53[B]	SER
7	gB	60	ILE
7	gB	84	ARG
7	gB	159	THR
6	hB	62	LYS
7	iB	23	ASP
7	iB	114	LYS
7	iB	115	GLU
6	jB	54	GLU
6	jB	62	LYS
6	jB	137	ARG
6	jB	147	GLN
7	kB	23	ASP
7	kB	61	CYS
7	kB	83	LEU
7	kB	84	ARG
7	kB	85	ASP
7	kB	88	ILE
7	kB	126	SER
7	kB	127	SER
6	lB	53	LYS
6	lB	54	GLU
6	lB	62	LYS
7	mB	23	ASP
7	mB	159	THR
7	mB	160	SER
6	AC	44	LEU

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Mol	Chain	Res	Type
6	AC	47	ASN
6	AC	59	CYS
6	AC	92	LEU
6	AC	93	VAL
6	AC	125	SER
6	AC	130	SER
6	AC	156	LEU
7	BC	12	SER
7	BC	24	LEU
7	BC	27	LEU
7	BC	46	SER
7	BC	77	ARG
7	BC	97	LEU
7	BC	105	LEU
7	BC	107	ASP
7	BC	108	ARG
7	BC	110	LEU
7	BC	120	LEU
7	BC	124	THR
7	BC	131	VAL
6	CC	44	LEU
6	CC	47	ASN
6	CC	59	CYS
6	CC	92	LEU
6	CC	93	VAL
6	CC	102	THR
6	CC	125	SER
6	CC	130	SER
6	CC	134	THR
6	CC	156	LEU
7	DC	12	SER
7	DC	24	LEU
7	DC	27	LEU
7	DC	29	SER
7	DC	46	SER
7	DC	77	ARG
7	DC	97	LEU
7	DC	105	LEU
7	DC	107	ASP
7	DC	108	ARG
7	DC	110	LEU
7	DC	120	LEU

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Mol	Chain	Res	Type
7	DC	124	THR
7	DC	131	VAL
6	EC	44	LEU
6	EC	47	ASN
6	EC	59	CYS
6	EC	92	LEU
6	EC	93	VAL
6	EC	102	THR
6	EC	125	SER
6	EC	130	SER
6	EC	134	THR
6	EC	156	LEU
6	EC	157	ASP
7	FC	12	SER
7	FC	24	LEU
7	FC	27	LEU
7	FC	29	SER
7	FC	46	SER
7	FC	51	MET
7	FC	77	ARG
7	FC	79	MET
7	FC	97	LEU
7	FC	105	LEU
7	FC	107	ASP
7	FC	108	ARG
7	FC	110	LEU
7	FC	120	LEU
7	FC	124	THR
7	FC	131	VAL
7	FC	134	MET
6	GC	44	LEU
6	GC	47	ASN
6	GC	59	CYS
6	GC	92	LEU
6	GC	93	VAL
6	GC	102	THR
6	GC	125	SER
6	GC	130	SER
6	GC	134	THR
6	GC	156	LEU
6	GC	157	ASP
7	HC	12	SER

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Mol	Chain	Res	Type
7	HC	24	LEU
7	HC	27	LEU
7	HC	29	SER
7	HC	46	SER
7	HC	51	MET
7	HC	77	ARG
7	HC	79	MET
7	HC	97	LEU
7	HC	105	LEU
7	HC	107	ASP
7	HC	108	ARG
7	HC	110	LEU
7	HC	120	LEU
7	HC	124	THR
7	HC	131	VAL
7	HC	134	MET
6	IC	44	LEU
6	IC	47	ASN
6	IC	59	CYS
6	IC	93	VAL
6	IC	102	THR
6	IC	125	SER
6	IC	130	SER
6	IC	157	ASP
7	JC	12	SER
7	JC	24	LEU
7	JC	27	LEU
7	JC	29	SER
7	JC	46	SER
7	JC	77	ARG
7	JC	97	LEU
7	JC	105	LEU
7	JC	107	ASP
7	JC	108	ARG
7	JC	110	LEU
7	JC	120	LEU
7	JC	124	THR
7	JC	131	VAL
6	KC	47	ASN
6	KC	59	CYS
6	KC	92	LEU
6	KC	93	VAL

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Mol	Chain	Res	Type
6	KC	102	THR
6	KC	125	SER
6	KC	130	SER
6	KC	134	THR
6	KC	157	ASP
7	LC	12	SER
7	LC	24	LEU
7	LC	27	LEU
7	LC	29	SER
7	LC	46	SER
7	LC	77	ARG
7	LC	79	MET
7	LC	97	LEU
7	LC	105	LEU
7	LC	107	ASP
7	LC	108	ARG
7	LC	110	LEU
7	LC	120	LEU
7	LC	124	THR
7	LC	131	VAL
18	MC	59	GLU
18	MC	60	SER
18	MC	61	VAL
18	MC	63	ASP
18	MC	64	GLU
18	MC	65	LYS
18	MC	144	ARG
18	MC	146	GLN
18	MC	212	TYR
18	MC	219	SER
18	MC	220	THR
18	MC	223	ARG
18	MC	236	ASP
18	MC	237	PHE
18	MC	240	ARG
18	MC	261	VAL
18	MC	303	PHE
18	MC	304	TRP
10	dD	195	ARG
10	dD	226	ARG
10	dD	282	LYS
10	dD	338	GLU

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Mol	Chain	Res	Type
6	BD	17	ARG
6	BD	24	LEU
6	BD	27	ILE
6	BD	28	GLN
6	BD	32	GLN
6	BD	49	GLU
6	BD	53	LYS
6	BD	62	LYS
6	BD	76	GLN
6	BD	90	MET
6	BD	99	VAL
6	BD	119	THR
6	BD	136	ASP
6	BD	151	GLU
6	BD	161	ASN
7	CD	7	ARG
7	CD	8	VAL
7	CD	23	ASP
7	CD	27	LEU
7	CD	31	ILE
7	CD	33	ASP
7	CD	45	VAL
7	CD	59	MET
7	CD	67	ILE
7	CD	77	ARG
7	CD	79	MET
7	CD	88	ILE
7	CD	93	VAL
7	CD	97	LEU
7	CD	98	LEU
7	CD	101	ASP
7	CD	105	LEU
7	CD	108	ARG
7	CD	111	ASN
7	CD	115	GLU
7	CD	127	SER
7	CD	128	ILE
7	CD	129	ARG
7	CD	135	LYS
7	CD	139	VAL
7	CD	142	ILE
7	CD	145	THR

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Mol	Chain	Res	Type
7	CD	149	ARG
7	CD	164	GLU
7	CD	171	ARG
6	DD	1	MET
6	DD	7	THR
6	DD	8	VAL
6	DD	9	VAL
6	DD	13	ASP
6	DD	21	ASN
6	DD	24	LEU
6	DD	27	ILE
6	DD	28	GLN
6	DD	32	GLN
6	DD	49	GLU
6	DD	53	LYS
6	DD	62	LYS
6	DD	76	GLN
6	DD	81	LYS
6	DD	90	MET
6	DD	99	VAL
6	DD	119	THR
6	DD	136	ASP
6	DD	151	GLU
6	DD	161	ASN
7	ED	7	ARG
7	ED	8	VAL
7	ED	23	ASP
7	ED	27	LEU
7	ED	31	ILE
7	ED	33	ASP
7	ED	45	VAL
7	ED	59	MET
7	ED	67	ILE
7	ED	77	ARG
7	ED	79	MET
7	ED	88	ILE
7	ED	93	VAL
7	ED	97	LEU
7	ED	98	LEU
7	ED	101	ASP
7	ED	105	LEU
7	ED	108	ARG

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Mol	Chain	Res	Type
7	ED	111	ASN
7	ED	115	GLU
7	ED	127	SER
7	ED	128	ILE
7	ED	129	ARG
7	ED	135	LYS
7	ED	139	VAL
7	ED	142	ILE
7	ED	145	THR
7	ED	149	ARG
7	ED	164	GLU
7	ED	171	ARG
6	FD	1	MET
6	FD	7	THR
6	FD	8	VAL
6	FD	9	VAL
6	FD	13	ASP
6	FD	21	ASN
6	FD	24	LEU
6	FD	27	ILE
6	FD	28	GLN
6	FD	32	GLN
6	FD	33	ARG
6	FD	43	LYS
6	FD	49	GLU
6	FD	53	LYS
6	FD	62	LYS
6	FD	76	GLN
6	FD	81	LYS
6	FD	84	ARG
6	FD	90	MET
6	FD	99	VAL
6	FD	119	THR
6	FD	136	ASP
6	FD	137	ARG
6	FD	151	GLU
6	FD	161	ASN
7	GD	7	ARG
7	GD	8	VAL
7	GD	23	ASP
7	GD	27	LEU
7	GD	31	ILE

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Mol	Chain	Res	Type
7	GD	33	ASP
7	GD	45	VAL
7	GD	59	MET
7	GD	67	ILE
7	GD	77	ARG
7	GD	78	ARG
7	GD	79	MET
7	GD	88	ILE
7	GD	93	VAL
7	GD	97	LEU
7	GD	98	LEU
7	GD	101	ASP
7	GD	105	LEU
7	GD	108	ARG
7	GD	111	ASN
7	GD	115	GLU
7	GD	125	ASN
7	GD	127	SER
7	GD	128	ILE
7	GD	129	ARG
7	GD	135	LYS
7	GD	139	VAL
7	GD	142	ILE
7	GD	145	THR
7	GD	149	ARG
7	GD	164	GLU
7	GD	171	ARG
6	HD	1	MET
6	HD	7	THR
6	HD	8	VAL
6	HD	9	VAL
6	HD	13	ASP
6	HD	21	ASN
6	HD	24	LEU
6	HD	27	ILE
6	HD	28	GLN
6	HD	32	GLN
6	HD	33	ARG
6	HD	49	GLU
6	HD	53	LYS
6	HD	62	LYS
6	HD	76	GLN

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Mol	Chain	Res	Type
6	HD	81	LYS
6	HD	90	MET
6	HD	99	VAL
6	HD	119	THR
6	HD	136	ASP
6	HD	151	GLU
6	HD	161	ASN
7	ID	7	ARG
7	ID	8	VAL
7	ID	23	ASP
7	ID	27	LEU
7	ID	31	ILE
7	ID	33	ASP
7	ID	45	VAL
7	ID	59	MET
7	ID	67	ILE
7	ID	116	THR
7	ID	127	SER
7	ID	128	ILE
7	ID	129	ARG
7	ID	132	SER
7	ID	139	VAL
7	ID	142	ILE
7	ID	145	THR
7	ID	149	ARG
7	ID	164	GLU
7	ID	171	ARG
6	JD	1	MET
6	JD	7	THR
6	JD	13	ASP
6	JD	24	LEU
6	JD	27	ILE
6	JD	28	GLN
6	JD	32	GLN
6	JD	49	GLU
6	JD	53	LYS
6	JD	62	LYS
6	JD	76	GLN
6	JD	81	LYS
6	JD	90	MET
6	JD	99	VAL
6	JD	119	THR

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Mol	Chain	Res	Type
6	JD	136	ASP
6	JD	151	GLU
6	JD	161	ASN
7	KD	7	ARG
7	KD	8	VAL
7	KD	23	ASP
7	KD	27	LEU
7	KD	31	ILE
7	KD	33	ASP
7	KD	45	VAL
7	KD	59	MET
7	KD	67	ILE
7	KD	77	ARG
7	KD	79	MET
7	KD	88	ILE
7	KD	93	VAL
7	KD	97	LEU
7	KD	98	LEU
7	KD	101	ASP
7	KD	105	LEU
7	KD	108	ARG
7	KD	111	ASN
7	KD	115	GLU
7	KD	127	SER
7	KD	129	ARG
7	KD	135	LYS
7	KD	139	VAL
7	KD	142	ILE
7	KD	145	THR
7	KD	149	ARG
7	KD	164	GLU
6	LD	1	MET
6	LD	7	THR
6	LD	8	VAL
6	LD	9	VAL
6	LD	13	ASP
6	LD	21	ASN
6	LD	24	LEU
6	LD	27	ILE
6	LD	28	GLN
6	LD	49	GLU
6	LD	53	LYS

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Mol	Chain	Res	Type
6	LD	62	LYS
6	LD	76	GLN
6	LD	81	LYS
6	LD	90	MET
6	LD	99	VAL
6	LD	119	THR
6	LD	136	ASP
6	LD	151	GLU
6	LD	161	ASN
7	MD	7	ARG
7	MD	8	VAL
7	MD	23	ASP
7	MD	27	LEU
7	MD	31	ILE
7	MD	33	ASP
7	MD	45	VAL
7	MD	59	MET
7	MD	77	ARG
7	MD	79	MET
7	MD	88	ILE
7	MD	93	VAL
7	MD	97	LEU
7	MD	98	LEU
7	MD	101	ASP
7	MD	105	LEU
7	MD	108	ARG
7	MD	111	ASN
7	MD	115	GLU
7	MD	125	ASN
7	MD	127	SER
7	MD	128	ILE
7	MD	129	ARG
7	MD	135	LYS
7	MD	139	VAL
7	MD	142	ILE
7	MD	145	THR
7	MD	149	ARG
7	MD	164	GLU
7	MD	171	ARG
6	AE	44	LEU
6	AE	47	ASN
6	AE	59	CYS

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Mol	Chain	Res	Type
6	AE	92	LEU
6	AE	93	VAL
6	AE	125	SER
6	AE	130	SER
6	AE	156	LEU
7	BE	12	SER
7	BE	24	LEU
7	BE	27	LEU
7	BE	46	SER
7	BE	77	ARG
7	BE	97	LEU
7	BE	105	LEU
7	BE	107	ASP
7	BE	108	ARG
7	BE	110	LEU
7	BE	120	LEU
7	BE	124	THR
7	BE	131	VAL
6	CE	44	LEU
6	CE	47	ASN
6	CE	59	CYS
6	CE	92	LEU
6	CE	93	VAL
6	CE	102	THR
6	CE	125	SER
6	CE	130	SER
6	CE	134	THR
6	CE	156	LEU
7	DE	12	SER
7	DE	24	LEU
7	DE	27	LEU
7	DE	29	SER
7	DE	46	SER
7	DE	77	ARG
7	DE	97	LEU
7	DE	105	LEU
7	DE	107	ASP
7	DE	108	ARG
7	DE	110	LEU
7	DE	120	LEU
7	DE	124	THR
7	DE	131	VAL

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Mol	Chain	Res	Type
6	EE	44	LEU
6	EE	47	ASN
6	EE	59	CYS
6	EE	92	LEU
6	EE	93	VAL
6	EE	102	THR
6	EE	125	SER
6	EE	130	SER
6	EE	134	THR
6	EE	156	LEU
6	EE	157	ASP
7	FE	12	SER
7	FE	24	LEU
7	FE	27	LEU
7	FE	29	SER
7	FE	46	SER
7	FE	51	MET
7	FE	77	ARG
7	FE	79	MET
7	FE	97	LEU
7	FE	105	LEU
7	FE	107	ASP
7	FE	108	ARG
7	FE	110	LEU
7	FE	120	LEU
7	FE	124	THR
7	FE	131	VAL
7	FE	134	MET
6	GE	44	LEU
6	GE	47	ASN
6	GE	59	CYS
6	GE	92	LEU
6	GE	93	VAL
6	GE	102	THR
6	GE	125	SER
6	GE	130	SER
6	GE	134	THR
6	GE	156	LEU
6	GE	157	ASP
7	HE	12	SER
7	HE	24	LEU
7	HE	27	LEU

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Mol	Chain	Res	Type
7	HE	29	SER
7	HE	46	SER
7	HE	51	MET
7	HE	77	ARG
7	HE	79	MET
7	HE	97	LEU
7	HE	105	LEU
7	HE	107	ASP
7	HE	108	ARG
7	HE	110	LEU
7	HE	120	LEU
7	HE	124	THR
7	HE	131	VAL
7	HE	134	MET
6	IE	44	LEU
6	IE	47	ASN
6	IE	59	CYS
6	IE	93	VAL
6	IE	102	THR
6	IE	125	SER
6	IE	130	SER
6	IE	157	ASP
7	JE	12	SER
7	JE	24	LEU
7	JE	27	LEU
7	JE	29	SER
7	JE	46	SER
7	JE	77	ARG
7	JE	97	LEU
7	JE	105	LEU
7	JE	107	ASP
7	JE	108	ARG
7	JE	110	LEU
7	JE	120	LEU
7	JE	124	THR
7	JE	131	VAL
6	KE	47	ASN
6	KE	59	CYS
6	KE	92	LEU
6	KE	93	VAL
6	KE	102	THR
6	KE	125	SER

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Mol	Chain	Res	Type
6	KE	130	SER
6	KE	134	THR
6	KE	157	ASP
7	LE	12	SER
7	LE	24	LEU
7	LE	27	LEU
7	LE	29	SER
7	LE	46	SER
7	LE	77	ARG
7	LE	79	MET
7	LE	97	LEU
7	LE	105	LEU
7	LE	107	ASP
7	LE	108	ARG
7	LE	110	LEU
7	LE	120	LEU
7	LE	124	THR
7	LE	131	VAL
18	ME	59	GLU
18	ME	60	SER
18	ME	61	VAL
18	ME	63	ASP
18	ME	64	GLU
18	ME	65	LYS
18	ME	144	ARG
18	ME	212	TYR
18	ME	223	ARG
18	ME	236	ASP
18	ME	240	ARG
18	ME	261	VAL
18	ME	304	TRP
1	XF	291	THR
2	AF	178	ARG
3	BF	228	MET
5	DF	17	GLU
5	FF	17	GLU
5	HF	17	GLU
5	JF	17	GLU
5	LF	17	GLU
5	LF	20	SER
5	LF	172	VAL
5	NF	17	GLU

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Mol	Chain	Res	Type
5	NF	39	ASP
5	NF	172	VAL
6	OF	137	ARG
6	QF	137	ARG
6	SF	34	SER
6	SF	137	ARG
7	TF	1	MET
7	TF	2	LEU
6	UF	137	ARG
7	VF	1	MET
6	WF	137	ARG
6	ZF	137	ARG
7	aF	1	MET
6	bF	137	ARG
7	cF	1	MET
7	cF	2	LEU
7	cF	147	THR
6	dF	137	ARG
6	fF	42	GLU
6	fF	137	ARG
7	gF	1	MET
6	hF	6	THR
6	hF	137	ARG
7	iF	1	MET
7	iF	2	LEU
7	iF	131	VAL
6	jF	49	GLU
6	jF	137	ARG
7	kF	1	MET
7	kF	2	LEU
6	lF	137	ARG
7	mF	1	MET
7	mF	2	LEU
6	AG	1	MET
6	AG	3	SER
6	AG	4	VAL
6	AG	20	SER
6	AG	26	SER
6	AG	27	ILE
6	AG	44	LEU
6	AG	67	LYS
6	AG	90	MET

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Mol	Chain	Res	Type
6	AG	97	LEU
6	AG	98	VAL
6	AG	105	LEU
6	AG	114	ARG
6	AG	115	GLU
6	AG	125	SER
6	AG	136	ASP
7	BG	23	ASP
7	BG	24	LEU
7	BG	31	ILE
7	BG	94	SER
7	BG	124	THR
7	BG	127	SER
7	BG	148	GLU
7	BG	152	SER
7	BG	157	ASP
7	BG	158	CYS
7	BG	171	ARG
6	CG	1	MET
6	CG	3	SER
6	CG	4	VAL
6	CG	20	SER
6	CG	23	ASP
6	CG	26	SER
6	CG	27	ILE
6	CG	33	ARG
6	CG	44	LEU
6	CG	49	GLU
6	CG	67	LYS
6	CG	90	MET
6	CG	97	LEU
6	CG	98	VAL
6	CG	105	LEU
6	CG	114	ARG
6	CG	115	GLU
6	CG	125	SER
6	CG	136	ASP
7	DG	23	ASP
7	DG	24	LEU
7	DG	31	ILE
7	DG	94	SER
7	DG	97	LEU

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Mol	Chain	Res	Type
7	DG	124	THR
7	DG	127	SER
7	DG	148	GLU
7	DG	152	SER
7	DG	157	ASP
7	DG	158	CYS
7	DG	171	ARG
6	EG	1	MET
6	EG	3	SER
6	EG	4	VAL
6	EG	20	SER
6	EG	23	ASP
6	EG	26	SER
6	EG	27	ILE
6	EG	44	LEU
6	EG	49	GLU
6	EG	67	LYS
6	EG	90	MET
6	EG	97	LEU
6	EG	98	VAL
6	EG	105	LEU
6	EG	114	ARG
6	EG	115	GLU
6	EG	125	SER
6	EG	136	ASP
7	FG	23	ASP
7	FG	24	LEU
7	FG	31	ILE
7	FG	94	SER
7	FG	97	LEU
7	FG	124	THR
7	FG	127	SER
7	FG	148	GLU
7	FG	152	SER
7	FG	157	ASP
7	FG	158	CYS
7	FG	171	ARG
6	GG	1	MET
6	GG	3	SER
6	GG	4	VAL
6	GG	20	SER
6	GG	23	ASP

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Mol	Chain	Res	Type
6	GG	26	SER
6	GG	27	ILE
6	GG	44	LEU
6	GG	49	GLU
6	GG	67	LYS
6	GG	90	MET
6	GG	97	LEU
6	GG	98	VAL
6	GG	105	LEU
6	GG	114	ARG
6	GG	115	GLU
6	GG	125	SER
6	GG	136	ASP
7	HG	23	ASP
7	HG	24	LEU
7	HG	31	ILE
7	HG	94	SER
7	HG	97	LEU
7	HG	124	THR
7	HG	127	SER
7	HG	148	GLU
7	HG	152	SER
7	HG	157	ASP
7	HG	158	CYS
7	HG	171	ARG
6	IG	1	MET
6	IG	3	SER
6	IG	4	VAL
6	IG	20	SER
6	IG	23	ASP
6	IG	26	SER
6	IG	27	ILE
6	IG	44	LEU
6	IG	49	GLU
6	IG	67	LYS
6	IG	90	MET
6	IG	97	LEU
6	IG	98	VAL
6	IG	105	LEU
6	IG	115	GLU
6	IG	125	SER
6	IG	136	ASP

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Mol	Chain	Res	Type
7	JG	23	ASP
7	JG	24	LEU
7	JG	31	ILE
7	JG	94	SER
7	JG	97	LEU
7	JG	124	THR
7	JG	127	SER
7	JG	148	GLU
7	JG	152	SER
7	JG	157	ASP
7	JG	158	CYS
7	JG	171	ARG
6	KG	1	MET
6	KG	3	SER
6	KG	4	VAL
6	KG	20	SER
6	KG	23	ASP
6	KG	26	SER
6	KG	27	ILE
6	KG	44	LEU
6	KG	49	GLU
6	KG	67	LYS
6	KG	90	MET
6	KG	97	LEU
6	KG	98	VAL
6	KG	105	LEU
6	KG	114	ARG
6	KG	115	GLU
6	KG	125	SER
6	KG	136	ASP
7	LG	23	ASP
7	LG	24	LEU
7	LG	31	ILE
7	LG	94	SER
7	LG	97	LEU
7	LG	124	THR
7	LG	127	SER
7	LG	148	GLU
7	LG	152	SER
7	LG	157	ASP
7	LG	158	CYS
7	LG	171	ARG

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Mol	Chain	Res	Type
14	MG	96	LYS
14	MG	117	ARG
14	MG	126	SER
14	MG	243	MET
13	kH	4	LYS
13	kH	7	GLU
13	kH	32	ASN
13	kH	41	ASP
13	kH	94	LEU
13	kH	118	ARG
13	kH	135	LEU
13	kH	156	THR
13	kH	157	LYS
13	kH	158	LYS
13	kH	172	LYS
13	kH	173	TYR
13	kH	222	GLU
13	kH	236	GLN
13	kH	281	SER
13	kH	286	MET
1	XI	291	THR
2	AI	178	ARG
3	BI	223	ASN
3	BI	225	VAL
3	BI	226	GLN
4	CI	49	GLN
5	DI	17	GLU
4	EI	49	GLN
5	HI	17	GLU
5	JI	17	GLU
5	JI	63	GLN
5	LI	17	GLU
5	LI	20	SER
5	LI	172	VAL
5	NI	17	GLU
5	NI	39	ASP
5	NI	172	VAL
6	OI	137	ARG
6	QI	137	ARG
6	SI	34	SER
6	SI	137	ARG
7	TI	1	MET

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Mol	Chain	Res	Type
7	TI	2	LEU
6	UI	137	ARG
7	VI	1	MET
6	WI	137	ARG
6	ZI	137	ARG
7	aI	1	MET
6	bI	137	ARG
7	cI	1	MET
7	cI	2	LEU
7	cI	147	THR
6	dI	137	ARG
6	fI	42	GLU
6	fI	137	ARG
7	gI	1	MET
6	hI	6	THR
6	hI	137	ARG
7	iI	1	MET
7	iI	2	LEU
7	iI	131	VAL
6	jI	49	GLU
6	jI	137	ARG
7	kI	1	MET
7	kI	2	LEU
6	lI	137	ARG
7	mI	1	MET
7	mI	2	LEU
6	AJ	23	ASP
6	AJ	133	TYR
6	AJ	135	ARG
6	AJ	136	ASP
6	AJ	138	LEU
6	AJ	139	CYS
6	AJ	144	MET
6	AJ	145	SER
7	BJ	28	LYS
7	BJ	36	LYS
7	BJ	145	THR
7	BJ	163	SER
6	CJ	23	ASP
6	CJ	78	LYS
7	DJ	18	TYR
6	EJ	23	ASP

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Mol	Chain	Res	Type
7	FJ	11	ASN
7	FJ	12	SER
7	FJ	15	LYS
7	FJ	19	VAL
7	FJ	115	GLU
7	FJ	125	ASN
7	FJ	126	SER
7	FJ	128	ILE
7	FJ	148	GLU
7	FJ	158	CYS
7	FJ	159	THR
7	FJ	160	SER
6	GJ	10	SER
6	GJ	17	ARG
6	GJ	23	ASP
6	GJ	78	LYS
6	GJ	99	VAL
6	GJ	114	ARG
6	GJ	118	ARG
6	GJ	125	SER
7	HJ	19	VAL
7	HJ	22	SER
7	HJ	23	ASP
7	HJ	25	GLN
7	HJ	33	ASP
7	HJ	43	SER
7	HJ	49	SER
7	HJ	67	ILE
7	HJ	103	SER
7	HJ	111	ASN
7	HJ	114	LYS
7	HJ	118	ILE
7	HJ	124	THR
7	HJ	125	ASN
7	HJ	126	SER
7	HJ	128	ILE
7	HJ	131	VAL
7	HJ	132	SER
6	IJ	23	ASP
6	IJ	67	LYS
6	IJ	71	GLU
6	IJ	74	GLU

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Mol	Chain	Res	Type
6	IJ	75	ASN
6	IJ	134	THR
6	IJ	137	ARG
6	IJ	138	LEU
6	IJ	145	SER
6	IJ	150	VAL
7	JJ	52	VAL
7	JJ	103	SER
7	JJ	116	THR
7	JJ	117	TYR
7	JJ	118	ILE
7	JJ	127	SER
6	KJ	10	SER
6	KJ	23	ASP
6	KJ	71	GLU
6	KJ	74	GLU
6	KJ	75	ASN
6	KJ	78	LYS
6	KJ	136	ASP
7	LJ	15	LYS
7	LJ	33	ASP
7	LJ	45	VAL
6	MJ	23	ASP
6	MJ	77	GLU
6	MJ	78	LYS
6	MJ	79	ILE
6	MJ	99	VAL
7	NJ	33	ASP
7	NJ	35	ASN
7	NJ	114	LYS
6	OJ	23	ASP
7	PJ	15	LYS
7	PJ	19	VAL
7	PJ	27	LEU
7	PJ	33	ASP
7	PJ	46	SER
7	PJ	114	LYS
6	QJ	23	ASP
6	QJ	52	VAL
6	QJ	53	LYS
7	RJ	114	LYS
7	RJ	117	TYR

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Mol	Chain	Res	Type
7	RJ	118	ILE
6	SJ	23	ASP
6	SJ	43	LYS
6	SJ	71	GLU
6	SJ	99	VAL
7	TJ	31	ILE
7	TJ	33	ASP
7	TJ	118	ILE
6	UJ	23	ASP
6	UJ	67	LYS
6	UJ	75	ASN
6	UJ	77	GLU
6	UJ	81	LYS
7	VJ	114	LYS
6	WJ	23	ASP
6	WJ	68	ASN
6	WJ	71	GLU
7	XJ	163	SER
6	YJ	10	SER
6	YJ	23	ASP
7	ZJ	68	SER
7	ZJ	103	SER
7	ZJ	127	SER
6	aJ	10	SER
6	aJ	23	ASP
6	aJ	38	LEU
6	aJ	39	GLU
6	aJ	44	LEU
7	bJ	68	SER
7	bJ	103	SER
7	bJ	127	SER
7	bJ	160	SER
6	cJ	10	SER
6	cJ	23	ASP
6	cJ	71	GLU
6	cJ	135	ARG
7	dJ	68	SER
7	dJ	103	SER
6	eJ	10	SER
6	eJ	23	ASP
7	fJ	33	ASP
7	fJ	68	SER

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Mol	Chain	Res	Type
7	fJ	103	SER
7	fJ	127	SER
7	fJ	132	SER
6	gJ	10	SER
6	gJ	23	ASP
7	hJ	68	SER
7	hJ	103	SER
7	hJ	127	SER
7	hJ	160	SER
6	iJ	23	ASP
6	iJ	71	GLU
6	iJ	163	LEU
6	iJ	164	SER
7	jJ	68	SER
7	jJ	103	SER
7	jJ	127	SER
7	jJ	160	SER
6	kJ	10	SER
6	kJ	23	ASP
6	kJ	99	VAL
6	kJ	119	THR
6	kJ	124	THR
7	lJ	33	ASP
7	lJ	45	VAL
7	lJ	52	VAL
7	lJ	53	SER
7	lJ	68	SER
7	lJ	103	SER
7	lJ	127	SER
7	lJ	145	THR
7	lJ	160	SER
6	mJ	10	SER
6	mJ	23	ASP
6	mJ	99	VAL
6	mJ	124	THR
7	nJ	19	VAL
7	nJ	45	VAL
7	nJ	52	VAL
7	nJ	68	SER
7	nJ	103	SER
7	nJ	127	SER
7	nJ	160	SER

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Mol	Chain	Res	Type
6	oJ	10	SER
6	oJ	23	ASP
7	pJ	19	VAL
7	pJ	45	VAL
7	pJ	52	VAL
7	pJ	53	SER
7	pJ	68	SER
7	pJ	103	SER
7	pJ	127	SER
6	qJ	10	SER
6	qJ	23	ASP
6	qJ	71	GLU
6	qJ	99	VAL
6	qJ	119	THR
6	qJ	124	THR
7	rJ	19	VAL
7	rJ	45	VAL
7	rJ	52	VAL
7	rJ	103	SER
7	rJ	127	SER
7	rJ	160	SER
6	sJ	10	SER
6	sJ	23	ASP
6	sJ	119	THR
6	sJ	124	THR
6	sJ	136	ASP
7	tJ	19	VAL
7	tJ	45	VAL
7	tJ	52	VAL
7	tJ	68	SER
7	tJ	103	SER
7	tJ	127	SER
7	tJ	145	THR
7	tJ	163	SER
6	uJ	10	SER
6	uJ	23	ASP
6	uJ	99	VAL
6	uJ	124	THR
7	vJ	19	VAL
7	vJ	45	VAL
7	vJ	52	VAL
7	vJ	68	SER

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Mol	Chain	Res	Type
7	vJ	103	SER
7	vJ	127	SER
7	vJ	160	SER
7	vJ	163	SER
16	wJ	39	LEU
16	wJ	41	ASN
16	wJ	43	LYS
16	wJ	44	PHE
16	wJ	45	SER
16	wJ	100	SER
16	wJ	135	CYS
16	wJ	164	SER
16	wJ	180	SER
16	wJ	198	SER
16	wJ	226	SER
16	wJ	243	VAL
16	wJ	255	GLN
16	wJ	268	SER
16	xJ	41	ASN
16	xJ	42	SER
16	xJ	45	SER
16	xJ	86	CYS
16	xJ	90	THR
16	xJ	92	LYS
16	xJ	100	SER
16	xJ	135	CYS
16	xJ	164	SER
16	xJ	180	SER
16	xJ	198	SER
16	xJ	226	SER
16	xJ	243	VAL
16	xJ	268	SER
17	yJ	291	ARG
19	zJ	43	ARG
19	zJ	215	THR
19	zJ	220	SER
19	zJ	282	ARG
1	XK	194	GLU
1	XK	211	LYS
2	AK	101	ILE
2	AK	102	GLN
2	AK	178	ARG

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Mol	Chain	Res	Type
3	BK	203	ILE
3	BK	204	ARG
3	BK	205	ARG
3	BK	206	PHE
3	BK	207	ARG
3	BK	220	LEU
3	BK	226	GLN
3	BK	227	GLU
4	CK	2	LYS
4	CK	33	ARG
4	CK	39	THR
4	CK	42	LYS
4	CK	68	GLN
4	CK	127	SER
4	CK	145	GLN
4	CK	160	THR
5	DK	31	VAL
5	DK	32	LYS
5	DK	39	ASP
5	DK	62	GLU
5	DK	63	GLN
5	DK	77	ARG
5	DK	155	SER
4	EK	7	GLU
4	EK	116	GLU
4	EK	120	ARG
4	EK	121	SER
4	EK	127	SER
4	EK	140	HIS
4	EK	145	GLN
4	EK	148	ASN
5	FK	39	ASP
5	FK	57	ARG
5	FK	62	GLU
5	FK	63	GLN
5	FK	77	ARG
5	FK	98	ILE
5	FK	138	SER
5	FK	144	ASP
5	FK	145	THR
5	FK	154	SER
4	GK	2	LYS

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Mol	Chain	Res	Type
4	GK	21	ASN
4	GK	67	THR
4	GK	127	SER
5	HK	32	LYS
5	HK	38	LEU
5	HK	77	ARG
5	HK	143	ASN
4	IK	127	SER
5	JK	17	GLU
5	JK	21	ASN
5	JK	28	SER
5	JK	29	LYS
5	JK	30	MET
5	JK	31	VAL
5	JK	32	LYS
5	JK	39	ASP
5	JK	43	LYS
5	JK	77	ARG
4	KK	32	GLN
4	KK	35	THR
4	KK	127	SER
5	LK	20	SER
5	LK	36	GLN
5	LK	39	ASP
5	LK	77	ARG
4	MK	38	LEU
4	MK	39	THR
4	MK	42	LYS
4	MK	108	ASP
4	MK	127	SER
5	NK	19	LEU
5	NK	21	ASN
5	NK	32	LYS
5	NK	37	ARG
5	NK	39	ASP
5	NK	77	ARG
5	NK	98	ILE
6	OK	137	ARG
7	PK	3	ASP
7	PK	43	SER
7	PK	103	SER
6	QK	137	ARG

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Mol	Chain	Res	Type
7	RK	43	SER
7	RK	103	SER
7	RK	157	ASP
6	SK	137	ARG
6	SK	157	ASP
7	TK	43	SER
7	TK	103	SER
6	UK	137	ARG
6	UK	157	ASP
7	VK	43	SER
7	VK	103	SER
7	VK	160[A]	SER
7	VK	160[B]	SER
6	WK	53	LYS
6	WK	137	ARG
7	YK	43	SER
7	YK	103	SER
6	ZK	53	LYS
6	ZK	137	ARG
7	aK	3	ASP
7	aK	43	SER
7	aK	103	SER
6	bK	137	ARG
7	cK	43	SER
7	cK	103	SER
6	dK	33	ARG
6	dK	137	ARG
7	eK	43	SER
7	eK	103	SER
6	fK	137	ARG
7	gK	43	SER
7	gK	103	SER
6	hK	4	VAL
6	hK	137	ARG
7	iK	43	SER
7	iK	103	SER
6	jK	137	ARG
7	kK	43	SER
7	kK	103	SER
6	lK	53	LYS
6	lK	137	ARG
7	mK	43	SER

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Mol	Chain	Res	Type
7	mK	103	SER
6	AL	23	ASP
6	AL	133	TYR
6	AL	135	ARG
6	AL	136	ASP
6	AL	138	LEU
6	AL	139	CYS
6	AL	144	MET
6	AL	145	SER
7	BL	28	LYS
7	BL	36	LYS
7	BL	145	THR
7	BL	163	SER
6	CL	23	ASP
6	CL	78	LYS
7	DL	18	TYR
6	EL	23	ASP
7	FL	11	ASN
7	FL	12	SER
7	FL	15	LYS
7	FL	19	VAL
7	FL	115	GLU
7	FL	125	ASN
7	FL	126	SER
7	FL	128	ILE
7	FL	148	GLU
7	FL	158	CYS
7	FL	159	THR
7	FL	160	SER
6	GL	10	SER
6	GL	17	ARG
6	GL	23	ASP
6	GL	99	VAL
6	GL	114	ARG
6	GL	118	ARG
6	GL	125	SER
7	HL	19	VAL
7	HL	22	SER
7	HL	23	ASP
7	HL	25	GLN
7	HL	33	ASP
7	HL	43	SER

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Mol	Chain	Res	Type
7	HL	49	SER
7	HL	67	ILE
7	HL	103	SER
7	HL	111	ASN
7	HL	114	LYS
7	HL	118	ILE
7	HL	124	THR
7	HL	125	ASN
7	HL	126	SER
7	HL	128	ILE
7	HL	131	VAL
7	HL	132	SER
6	IL	23	ASP
6	IL	67	LYS
6	IL	71	GLU
6	IL	74	GLU
6	IL	75	ASN
6	IL	134	THR
6	IL	137	ARG
6	IL	138	LEU
6	IL	145	SER
6	IL	150	VAL
7	JL	52	VAL
7	JL	103	SER
7	JL	116	THR
7	JL	117	TYR
7	JL	118	ILE
7	JL	127	SER
6	KL	10	SER
6	KL	23	ASP
6	KL	71	GLU
6	KL	74	GLU
6	KL	75	ASN
6	KL	78	LYS
6	KL	136	ASP
7	LL	15	LYS
7	LL	33	ASP
7	LL	45	VAL
6	ML	23	ASP
6	ML	77	GLU
6	ML	78	LYS
6	ML	79	ILE

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Mol	Chain	Res	Type
6	ML	99	VAL
6	ML	145	SER
7	NL	33	ASP
7	NL	35	ASN
7	NL	114	LYS
6	OL	23	ASP
7	PL	15	LYS
7	PL	19	VAL
7	PL	27	LEU
7	PL	33	ASP
7	PL	46	SER
7	PL	114	LYS
6	QL	23	ASP
6	QL	52	VAL
6	QL	53	LYS
7	RL	114	LYS
7	RL	117	TYR
7	RL	118	ILE
6	SL	23	ASP
6	SL	43	LYS
6	SL	71	GLU
6	SL	99	VAL
7	TL	31	ILE
7	TL	33	ASP
7	TL	118	ILE
6	UL	23	ASP
6	UL	67	LYS
6	UL	75	ASN
6	UL	77	GLU
6	UL	81	LYS
7	VL	114	LYS
6	WL	23	ASP
6	WL	68	ASN
6	WL	71	GLU
7	XL	163	SER
6	YL	10	SER
6	YL	23	ASP
6	YL	33	ARG
7	ZL	68	SER
7	ZL	103	SER
7	ZL	127	SER
6	aL	10	SER

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Mol	Chain	Res	Type
6	aL	23	ASP
6	aL	38	LEU
6	aL	39	GLU
6	aL	44	LEU
7	bL	68	SER
7	bL	103	SER
7	bL	127	SER
7	bL	160	SER
6	cL	10	SER
6	cL	23	ASP
6	cL	71	GLU
6	cL	135	ARG
6	cL	137	ARG
7	dL	68	SER
7	dL	103	SER
6	eL	10	SER
6	eL	23	ASP
7	fL	33	ASP
7	fL	68	SER
7	fL	103	SER
7	fL	127	SER
7	fL	132	SER
6	gL	10	SER
6	gL	23	ASP
7	hL	68	SER
7	hL	103	SER
7	hL	127	SER
7	hL	160	SER
6	iL	23	ASP
6	iL	71	GLU
6	iL	163	LEU
6	iL	164	SER
7	jL	68	SER
7	jL	103	SER
7	jL	127	SER
7	jL	160	SER
6	kL	10	SER
6	kL	23	ASP
6	kL	99	VAL
6	kL	119	THR
6	kL	124	THR
7	lL	33	ASP

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Mol	Chain	Res	Type
7	lL	45	VAL
7	lL	52	VAL
7	lL	53	SER
7	lL	68	SER
7	lL	103	SER
7	lL	127	SER
7	lL	145	THR
7	lL	160	SER
6	mL	10	SER
6	mL	23	ASP
6	mL	99	VAL
6	mL	124	THR
7	nL	19	VAL
7	nL	45	VAL
7	nL	52	VAL
7	nL	68	SER
7	nL	103	SER
7	nL	127	SER
7	nL	160	SER
6	oL	10	SER
6	oL	23	ASP
7	pL	19	VAL
7	pL	45	VAL
7	pL	52	VAL
7	pL	53	SER
7	pL	68	SER
7	pL	103	SER
7	pL	127	SER
6	qL	10	SER
6	qL	23	ASP
6	qL	71	GLU
6	qL	99	VAL
6	qL	119	THR
6	qL	124	THR
7	rL	19	VAL
7	rL	45	VAL
7	rL	52	VAL
7	rL	103	SER
7	rL	127	SER
7	rL	160	SER
6	sL	10	SER
6	sL	23	ASP

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Mol	Chain	Res	Type
6	sL	119	THR
6	sL	124	THR
6	sL	136	ASP
7	tL	19	VAL
7	tL	45	VAL
7	tL	52	VAL
7	tL	68	SER
7	tL	103	SER
7	tL	127	SER
7	tL	145	THR
7	tL	163	SER
6	uL	10	SER
6	uL	23	ASP
6	uL	99	VAL
6	uL	124	THR
7	vL	19	VAL
7	vL	45	VAL
7	vL	52	VAL
7	vL	68	SER
7	vL	103	SER
7	vL	127	SER
7	vL	160	SER
7	vL	163	SER
16	wL	39	LEU
16	wL	41	ASN
16	wL	43	LYS
16	wL	44	PHE
16	wL	45	SER
16	wL	100	SER
16	wL	135	CYS
16	wL	164	SER
16	wL	180	SER
16	wL	198	SER
16	wL	226	SER
16	wL	243	VAL
16	wL	255	GLN
16	wL	268	SER
16	xL	41	ASN
16	xL	42	SER
16	xL	45	SER
16	xL	86	CYS
16	xL	90	THR

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Mol	Chain	Res	Type
16	xL	100	SER
16	xL	135	CYS
16	xL	164	SER
16	xL	180	SER
16	xL	198	SER
16	xL	226	SER
16	xL	243	VAL
16	xL	268	SER
17	yL	291	ARG
19	zL	43	ARG
19	zL	215	THR
19	zL	220	SER
19	zL	282	ARG
19	zL	361	ARG
15	bM	91	ILE
15	bM	150	ARG
15	bM	198	ARG
15	bM	202	THR
15	bM	204	CYS
15	bM	270	ASN
15	bM	271	TRP
15	bM	333	ARG
15	bM	349	LYS
15	bM	351	ASP
17	BM	180	SER
6	CM	6	THR
6	CM	62	LYS
7	DM	23	ASP
7	DM	159	THR
7	DM	160	SER
6	EM	62	LYS
6	EM	147	GLN
7	FM	23	ASP
7	FM	139	VAL
6	GM	49	GLU
6	GM	62	LYS
6	GM	134	THR
6	GM	135	ARG
6	GM	137	ARG
6	GM	147	GLN
6	GM	159	LEU
7	HM	8	VAL

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Mol	Chain	Res	Type
7	HM	10	VAL
7	HM	23	ASP
7	HM	52	VAL
7	HM	160	SER
6	IM	62	LYS
7	JM	23	ASP
7	JM	85	ASP
7	JM	145	THR
7	JM	147	THR
7	JM	149	ARG
6	KM	21	ASN
6	KM	62	LYS
7	LM	23	ASP
6	MM	62	LYS
7	NM	23	ASP
7	NM	62	GLU
7	NM	85	ASP
7	NM	114	LYS
7	NM	159	THR
6	OM	62	LYS
7	PM	23	ASP
6	QM	62	LYS
6	QM	136	ASP
6	QM	157	ASP
7	RM	8	VAL
7	RM	23	ASP
7	RM	61	CYS
7	RM	62	GLU
7	RM	145	THR
7	RM	148	GLU
6	SM	49	GLU
6	SM	62	LYS
7	TM	23	ASP
7	TM	24	LEU
7	TM	25	GLN
7	TM	159	THR
7	TM	170	ASP
6	UM	62	LYS
7	VM	23	ASP
7	VM	61	CYS
7	VM	85	ASP
7	VM	159	THR

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Mol	Chain	Res	Type
7	VM	160	SER
6	WM	62	LYS
6	WM	121	ASN
7	XM	23	ASP
6	YM	62	LYS
7	ZM	23	ASP
7	ZM	61	CYS
7	ZM	84	ARG
7	ZM	124	THR
7	ZM	127	SER
6	aM	62	LYS
7	cM	23	ASP
7	cM	159	THR
6	dM	62	LYS
7	eM	23	ASP
7	eM	63	ASN
7	eM	84	ARG
7	eM	125	ASN
6	fM	62	LYS
6	fM	136	ASP
7	gM	23	ASP
7	gM	35	ASN
7	gM	53[A]	SER
7	gM	53[B]	SER
7	gM	60	ILE
7	gM	84	ARG
7	gM	159	THR
6	hM	62	LYS
7	iM	23	ASP
7	iM	114	LYS
7	iM	115	GLU
6	jM	62	LYS
6	jM	137	ARG
7	kM	23	ASP
7	kM	61	CYS
7	kM	83	LEU
7	kM	84	ARG
7	kM	85	ASP
7	kM	88	ILE
7	kM	126	SER
7	kM	127	SER
6	lM	53	LYS

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Mol	Chain	Res	Type
6	IM	54	GLU
6	IM	62	LYS
6	IM	77	GLU
7	mM	23	ASP
7	mM	159	THR
7	mM	160	SER
6	AN	3	SER
6	AN	39	GLU
6	AN	43	LYS
6	AN	124	THR
6	AN	131	ILE
6	AN	134	THR
6	AN	138	LEU
6	AN	150	VAL
6	AN	153	SER
7	BN	12	SER
7	BN	13	ASP
7	BN	19	VAL
7	BN	24	LEU
7	BN	43	SER
7	BN	56	VAL
7	BN	103	SER
7	BN	113	LEU
7	BN	127	SER
7	BN	152	SER
6	CN	3	SER
6	CN	21	ASN
6	CN	43	LYS
6	CN	124	THR
6	CN	131	ILE
6	CN	134	THR
6	CN	138	LEU
6	CN	150	VAL
6	CN	153	SER
7	DN	12	SER
7	DN	24	LEU
7	DN	43	SER
7	DN	56	VAL
7	DN	103	SER
7	DN	127	SER
7	DN	139	VAL
7	DN	152	SER

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Mol	Chain	Res	Type
6	EN	3	SER
6	EN	39	GLU
6	EN	43	LYS
6	EN	124	THR
6	EN	131	ILE
6	EN	138	LEU
6	EN	150	VAL
7	FN	12	SER
7	FN	13	ASP
7	FN	19	VAL
7	FN	43	SER
7	FN	56	VAL
7	FN	103	SER
7	FN	127	SER
7	FN	139	VAL
7	FN	152	SER
6	GN	3	SER
6	GN	39	GLU
6	GN	43	LYS
6	GN	124	THR
6	GN	131	ILE
6	GN	138	LEU
6	GN	150	VAL
6	GN	153	SER
7	HN	12	SER
7	HN	13	ASP
7	HN	24	LEU
7	HN	43	SER
7	HN	56	VAL
7	HN	103	SER
7	HN	113	LEU
7	HN	127	SER
7	HN	139	VAL
7	HN	152	SER
7	HN	160	SER
6	IN	3	SER
6	IN	32	GLN
6	IN	43	LYS
6	IN	124	THR
6	IN	131	ILE
6	IN	134	THR
6	IN	138	LEU

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Mol	Chain	Res	Type
6	IN	150	VAL
6	IN	153	SER
7	JN	12	SER
7	JN	43	SER
7	JN	56	VAL
7	JN	103	SER
7	JN	113	LEU
7	JN	127	SER
7	JN	139	VAL
7	JN	152	SER
6	KN	3	SER
6	KN	39	GLU
6	KN	43	LYS
6	KN	124	THR
6	KN	134	THR
6	KN	138	LEU
6	KN	150	VAL
6	KN	153	SER
7	LN	12	SER
7	LN	24	LEU
7	LN	43	SER
7	LN	56	VAL
7	LN	103	SER
7	LN	127	SER
7	LN	152	SER
14	MN	96	LYS
14	MN	103	ARG
14	MN	145	CYS
14	MN	195	CYS
14	MN	232	LYS
14	MN	259	CYS
14	MN	314	LYS
6	AO	10	SER
6	AO	20	SER
6	AO	26	SER
6	AO	51	VAL
6	AO	52	VAL
7	BO	23	ASP
7	BO	53	SER
7	BO	103	SER
7	BO	127	SER
6	CO	10	SER

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Mol	Chain	Res	Type
6	CO	20	SER
6	CO	26	SER
6	CO	51	VAL
6	CO	52	VAL
6	CO	93	VAL
6	CO	134	THR
6	CO	140	VAL
7	DO	23	ASP
7	DO	27	LEU
7	DO	53	SER
7	DO	56	VAL
7	DO	103	SER
7	DO	120	LEU
7	DO	127	SER
7	DO	165	VAL
7	DO	172	VAL
6	EO	10	SER
6	EO	20	SER
6	EO	26	SER
6	EO	51	VAL
6	EO	52	VAL
6	EO	93	VAL
6	EO	102	THR
6	EO	134	THR
6	EO	140	VAL
7	FO	23	ASP
7	FO	27	LEU
7	FO	53	SER
7	FO	56	VAL
7	FO	103	SER
7	FO	127	SER
7	FO	165	VAL
7	FO	170	ASP
7	FO	172	VAL
7	FO	176	ILE
6	GO	10	SER
6	GO	20	SER
6	GO	26	SER
6	GO	51	VAL
6	GO	52	VAL
6	GO	93	VAL
6	GO	140	VAL

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Mol	Chain	Res	Type
7	HO	23	ASP
7	HO	53	SER
7	HO	56	VAL
7	HO	103	SER
7	HO	120	LEU
7	HO	127	SER
7	HO	132	SER
7	HO	160	SER
7	HO	165	VAL
7	HO	172	VAL
7	HO	176	ILE
6	IO	10	SER
6	IO	20	SER
6	IO	26	SER
6	IO	51	VAL
6	IO	52	VAL
6	IO	93	VAL
6	IO	102	THR
6	IO	134	THR
6	IO	138	LEU
7	JO	23	ASP
7	JO	27	LEU
7	JO	53	SER
7	JO	56	VAL
7	JO	103	SER
7	JO	120	LEU
7	JO	127	SER
7	JO	165	VAL
7	JO	172	VAL
6	KO	10	SER
6	KO	20	SER
6	KO	24	LEU
6	KO	26	SER
6	KO	53	LYS
6	KO	102	THR
6	KO	134	THR
6	KO	140	VAL
7	LO	23	ASP
7	LO	27	LEU
7	LO	53	SER
7	LO	56	VAL
7	LO	103	SER

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Mol	Chain	Res	Type
7	LO	120	LEU
7	LO	127	SER
7	LO	165	VAL
7	LO	172	VAL
7	MO	41	VAL
7	MO	50	CYS
7	MO	67	ILE
7	MO	68	SER
7	MO	91	ARG
7	MO	103	SER
7	MO	126	SER
7	MO	131	VAL
7	MO	147	THR
7	MO	159	THR
7	MO	160	SER
7	NO	41	VAL
7	NO	50	CYS
7	NO	67	ILE
7	NO	68	SER
7	NO	91	ARG
7	NO	103	SER
7	NO	126	SER
7	NO	131	VAL
7	NO	147	THR
7	NO	159	THR
7	NO	160	SER
9	OO	49	VAL
9	OO	76	ARG
9	OO	282	ARG
9	OO	364	LYS
20	AP	7	SER
20	AP	9	VAL
20	AP	30	VAL
20	AP	45	GLU
20	AP	52	LYS
20	AP	56	GLN
20	AP	67	SER
20	AP	76	GLU
20	AP	139	SER
20	AP	151	PHE
21	DP	1	MET
21	DP	43	THR

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Mol	Chain	Res	Type
21	DP	64	ASP
21	DP	118	SER
21	DP	135	GLU
21	DP	140	LEU
21	DP	143	SER
21	DP	148	GLU
21	DP	158	SER
20	CP	7	SER
20	CP	9	VAL
20	CP	30	VAL
20	CP	45	GLU
20	CP	52	LYS
20	CP	56	GLN
20	CP	67	SER
20	CP	76	GLU
20	CP	139	SER
20	CP	151	PHE
21	FP	1	MET
21	FP	43	THR
21	FP	64	ASP
21	FP	65	ILE
21	FP	67	ARG
21	FP	118	SER
21	FP	135	GLU
21	FP	140	LEU
21	FP	143	SER
21	FP	148	GLU
21	FP	158	SER
20	EP	7	SER
20	EP	9	VAL
20	EP	30	VAL
20	EP	45	GLU
20	EP	52	LYS
20	EP	56	GLN
20	EP	67	SER
20	EP	76	GLU
20	EP	139	SER
20	EP	151	PHE
21	BP	1	MET
21	BP	43	THR
21	BP	64	ASP
21	BP	118	SER

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Mol	Chain	Res	Type
21	BP	135	GLU
21	BP	140	LEU
21	BP	143	SER
21	BP	148	GLU
21	BP	158	SER
20	GP	7	SER
20	GP	9	VAL
20	GP	30	VAL
20	GP	45	GLU
20	GP	52	LYS
20	GP	56	GLN
20	GP	67	SER
20	GP	76	GLU
20	GP	139	SER
20	GP	151	PHE
21	HP	1	MET
21	HP	43	THR
21	HP	64	ASP
21	HP	118	SER
21	HP	135	GLU
21	HP	140	LEU
21	HP	143	SER
21	HP	148	GLU
21	HP	158	SER
21	IP	1	MET
21	IP	43	THR
21	IP	64	ASP
21	IP	118	SER
21	IP	135	GLU
21	IP	140	LEU
21	IP	143	SER
21	IP	148	GLU
21	IP	158	SER
20	JP	7	SER
20	JP	9	VAL
20	JP	30	VAL
20	JP	52	LYS
20	JP	56	GLN
20	JP	67	SER
20	JP	76	GLU
20	JP	139	SER
20	JP	151	PHE

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Mol	Chain	Res	Type
20	KP	7	SER
20	KP	9	VAL
20	KP	30	VAL
20	KP	45	GLU
20	KP	52	LYS
20	KP	56	GLN
20	KP	67	SER
20	KP	76	GLU
20	KP	139	SER
20	KP	151	PHE
21	LP	1	MET
21	LP	43	THR
21	LP	64	ASP
21	LP	118	SER
21	LP	135	GLU
21	LP	140	LEU
21	LP	143	SER
21	LP	148	GLU
21	LP	158	SER
21	MP	1	MET
21	MP	43	THR
21	MP	64	ASP
21	MP	118	SER
21	MP	135	GLU
21	MP	140	LEU
21	MP	143	SER
21	MP	148	GLU
21	MP	158	SER
20	NP	7	SER
20	NP	9	VAL
20	NP	30	VAL
20	NP	45	GLU
20	NP	52	LYS
20	NP	56	GLN
20	NP	67	SER
20	NP	76	GLU
20	NP	139	SER
20	NP	151	PHE
21	OP	1	MET
21	OP	43	THR
21	OP	64	ASP
21	OP	118	SER

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Mol	Chain	Res	Type
21	OP	135	GLU
21	OP	140	LEU
21	OP	143	SER
21	OP	148	GLU
21	OP	158	SER
20	PP	7	SER
20	PP	9	VAL
20	PP	30	VAL
20	PP	45	GLU
20	PP	52	LYS
20	PP	56	GLN
20	PP	67	SER
20	PP	139	SER
20	PP	151	PHE
21	QP	1	MET
21	QP	43	THR
21	QP	64	ASP
21	QP	67	ARG
21	QP	118	SER
21	QP	135	GLU
21	QP	140	LEU
21	QP	143	SER
21	QP	148	GLU
21	QP	158	SER
20	RP	7	SER
20	RP	9	VAL
20	RP	30	VAL
20	RP	45	GLU
20	RP	52	LYS
20	RP	56	GLN
20	RP	67	SER
20	RP	76	GLU
20	RP	139	SER
20	RP	151	PHE
21	SP	1	MET
21	SP	43	THR
21	SP	64	ASP
21	SP	118	SER
21	SP	135	GLU
21	SP	140	LEU
21	SP	143	SER
21	SP	148	GLU

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Mol	Chain	Res	Type
21	SP	158	SER
20	TP	7	SER
20	TP	9	VAL
20	TP	30	VAL
20	TP	45	GLU
20	TP	52	LYS
20	TP	56	GLN
20	TP	67	SER
20	TP	76	GLU
20	TP	139	SER
20	TP	151	PHE
21	UP	1	MET
21	UP	43	THR
21	UP	64	ASP
21	UP	72	MET
21	UP	118	SER
21	UP	135	GLU
21	UP	140	LEU
21	UP	143	SER
21	UP	148	GLU
21	UP	158	SER
22	VP	144	GLU
24	XP	51	SER
25	YP	44	VAL
25	YP	148	SER
25	YP	204	SER
25	YP	208	GLU
25	YP	288	ARG
25	YP	512	GLU
25	YP	624	SER
25	YP	701	LEU
26	ZP	120	PHE
26	ZP	125	ASP
26	ZP	177	ARG
27	aP	58	ASP
27	aP	144	SER
27	aP	150	ASP
27	aP	181	SER
27	aP	270	ARG
27	aP	286	ARG
27	aP	287	LEU
27	aP	288	VAL

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Mol	Chain	Res	Type
28	bP	40	ARG
28	bP	78	GLN
28	bP	122	SER
28	bP	225	ARG
20	cP	7	SER
20	cP	9	VAL
20	cP	30	VAL
20	cP	45	GLU
20	cP	52	LYS
20	cP	56	GLN
20	cP	67	SER
20	cP	76	GLU
20	cP	139	SER
20	cP	151	PHE
21	dP	1	MET
21	dP	43	THR
21	dP	64	ASP
21	dP	118	SER
21	dP	135	GLU
21	dP	140	LEU
21	dP	143	SER
21	dP	148	GLU
21	dP	158	SER
20	eP	7	SER
20	eP	9	VAL
20	eP	30	VAL
20	eP	45	GLU
20	eP	52	LYS
20	eP	56	GLN
20	eP	67	SER
20	eP	76	GLU
20	eP	139	SER
20	eP	151	PHE
21	fP	1	MET
21	fP	43	THR
21	fP	64	ASP
21	fP	118	SER
21	fP	135	GLU
21	fP	140	LEU
21	fP	143	SER
21	fP	148	GLU
21	fP	158	SER

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Mol	Chain	Res	Type
20	gP	7	SER
20	gP	9	VAL
20	gP	30	VAL
20	gP	45	GLU
20	gP	52	LYS
20	gP	56	GLN
20	gP	67	SER
20	gP	76	GLU
20	gP	139	SER
20	gP	151	PHE
21	hP	1	MET
21	hP	43	THR
21	hP	64	ASP
21	hP	118	SER
21	hP	135	GLU
21	hP	140	LEU
21	hP	143	SER
21	hP	148	GLU
21	hP	158	SER
20	iP	7	SER
20	iP	9	VAL
20	iP	30	VAL
20	iP	45	GLU
20	iP	52	LYS
20	iP	56	GLN
20	iP	67	SER
20	iP	76	GLU
20	iP	139	SER
20	iP	151	PHE
21	jP	1	MET
21	jP	43	THR
21	jP	64	ASP
21	jP	118	SER
21	jP	135	GLU
21	jP	140	LEU
21	jP	143	SER
21	jP	148	GLU
21	jP	158	SER
21	kP	1	MET
21	kP	43	THR
21	kP	64	ASP
21	kP	118	SER

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Mol	Chain	Res	Type
21	kP	135	GLU
21	kP	140	LEU
21	kP	143	SER
21	kP	148	GLU
21	kP	158	SER
20	lP	7	SER
20	lP	9	VAL
20	lP	30	VAL
20	lP	45	GLU
20	lP	52	LYS
20	lP	56	GLN
20	lP	67	SER
20	lP	76	GLU
20	lP	139	SER
20	lP	151	PHE
20	mP	7	SER
20	mP	9	VAL
20	mP	30	VAL
20	mP	45	GLU
20	mP	52	LYS
20	mP	56	GLN
20	mP	67	SER
20	mP	76	GLU
20	mP	139	SER
20	mP	151	PHE
21	nP	1	MET
21	nP	43	THR
21	nP	64	ASP
21	nP	118	SER
21	nP	135	GLU
21	nP	140	LEU
21	nP	143	SER
21	nP	148	GLU
21	nP	158	SER
21	oP	1	MET
21	oP	43	THR
21	oP	60	LEU
21	oP	118	SER
21	oP	128	GLN
21	oP	135	GLU
21	oP	140	LEU
21	oP	143	SER

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Mol	Chain	Res	Type
21	oP	147	LYS
21	oP	148	GLU
21	oP	158	SER
20	pP	7	SER
20	pP	9	VAL
20	pP	30	VAL
20	pP	45	GLU
20	pP	52	LYS
20	pP	56	GLN
20	pP	67	SER
20	pP	76	GLU
20	pP	139	SER
20	pP	151	PHE
21	qP	1	MET
21	qP	43	THR
21	qP	64	ASP
21	qP	118	SER
21	qP	135	GLU
21	qP	140	LEU
21	qP	143	SER
21	qP	148	GLU
21	qP	158	SER
20	rP	7	SER
20	rP	9	VAL
20	rP	30	VAL
20	rP	45	GLU
20	rP	52	LYS
20	rP	67	SER
20	rP	139	SER
20	rP	151	PHE
21	sP	1	MET
21	sP	43	THR
21	sP	64	ASP
21	sP	118	SER
21	sP	135	GLU
21	sP	140	LEU
21	sP	143	SER
21	sP	148	GLU
21	sP	158	SER
20	tP	7	SER
20	tP	9	VAL
20	tP	30	VAL

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Mol	Chain	Res	Type
20	tP	45	GLU
20	tP	52	LYS
20	tP	56	GLN
20	tP	67	SER
20	tP	76	GLU
20	tP	139	SER
20	tP	151	PHE
21	uP	1	MET
21	uP	43	THR
21	uP	64	ASP
21	uP	118	SER
21	uP	135	GLU
21	uP	140	LEU
21	uP	143	SER
21	uP	148	GLU
21	uP	158	SER
20	vP	7	SER
20	vP	9	VAL
20	vP	30	VAL
20	vP	45	GLU
20	vP	52	LYS
20	vP	56	GLN
20	vP	67	SER
20	vP	76	GLU
20	vP	139	SER
20	vP	151	PHE
21	wP	1	MET
21	wP	43	THR
21	wP	64	ASP
21	wP	72	MET
21	wP	118	SER
21	wP	135	GLU
21	wP	140	LEU
21	wP	143	SER
21	wP	148	GLU
21	wP	158	SER
22	xP	144	GLU
24	zP	51	SER
25	1P	44	VAL
25	1P	148	SER
25	1P	204	SER
25	1P	208	GLU

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Mol	Chain	Res	Type
25	1P	288	ARG
25	1P	512	GLU
25	1P	624	SER
25	1P	701	LEU
26	2P	120	PHE
26	2P	177	ARG
27	3P	59	LYS
27	3P	144	SER
27	3P	150	ASP
27	3P	181	SER
27	3P	286	ARG
27	3P	287	LEU
27	3P	288	VAL
28	4P	40	ARG
28	4P	78	GLN
28	4P	122	SER
28	4P	225	ARG
6	AQ	1	MET
6	AQ	3	SER
6	AQ	4	VAL
6	AQ	20	SER
6	AQ	26	SER
6	AQ	27	ILE
6	AQ	44	LEU
6	AQ	67	LYS
6	AQ	90	MET
6	AQ	97	LEU
6	AQ	98	VAL
6	AQ	105	LEU
6	AQ	114	ARG
6	AQ	115	GLU
6	AQ	125	SER
6	AQ	136	ASP
7	BQ	23	ASP
7	BQ	24	LEU
7	BQ	31	ILE
7	BQ	94	SER
7	BQ	124	THR
7	BQ	127	SER
7	BQ	148	GLU
7	BQ	152	SER
7	BQ	157	ASP

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Mol	Chain	Res	Type
7	BQ	158	CYS
7	BQ	171	ARG
6	CQ	1	MET
6	CQ	3	SER
6	CQ	4	VAL
6	CQ	20	SER
6	CQ	23	ASP
6	CQ	26	SER
6	CQ	27	ILE
6	CQ	33	ARG
6	CQ	44	LEU
6	CQ	49	GLU
6	CQ	67	LYS
6	CQ	90	MET
6	CQ	97	LEU
6	CQ	98	VAL
6	CQ	105	LEU
6	CQ	114	ARG
6	CQ	115	GLU
6	CQ	125	SER
6	CQ	136	ASP
7	DQ	23	ASP
7	DQ	24	LEU
7	DQ	31	ILE
7	DQ	94	SER
7	DQ	97	LEU
7	DQ	124	THR
7	DQ	127	SER
7	DQ	148	GLU
7	DQ	152	SER
7	DQ	157	ASP
7	DQ	158	CYS
7	DQ	171	ARG
6	EQ	1	MET
6	EQ	3	SER
6	EQ	4	VAL
6	EQ	20	SER
6	EQ	23	ASP
6	EQ	26	SER
6	EQ	27	ILE
6	EQ	44	LEU
6	EQ	49	GLU

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Mol	Chain	Res	Type
6	EQ	67	LYS
6	EQ	90	MET
6	EQ	97	LEU
6	EQ	98	VAL
6	EQ	105	LEU
6	EQ	114	ARG
6	EQ	115	GLU
6	EQ	125	SER
6	EQ	136	ASP
7	FQ	23	ASP
7	FQ	24	LEU
7	FQ	31	ILE
7	FQ	94	SER
7	FQ	97	LEU
7	FQ	124	THR
7	FQ	127	SER
7	FQ	148	GLU
7	FQ	152	SER
7	FQ	157	ASP
7	FQ	158	CYS
7	FQ	171	ARG
6	GQ	1	MET
6	GQ	3	SER
6	GQ	4	VAL
6	GQ	20	SER
6	GQ	23	ASP
6	GQ	26	SER
6	GQ	27	ILE
6	GQ	44	LEU
6	GQ	49	GLU
6	GQ	67	LYS
6	GQ	90	MET
6	GQ	97	LEU
6	GQ	98	VAL
6	GQ	105	LEU
6	GQ	114	ARG
6	GQ	115	GLU
6	GQ	125	SER
6	GQ	136	ASP
7	HQ	23	ASP
7	HQ	24	LEU
7	HQ	31	ILE

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Mol	Chain	Res	Type
7	HQ	94	SER
7	HQ	97	LEU
7	HQ	124	THR
7	HQ	127	SER
7	HQ	148	GLU
7	HQ	152	SER
7	HQ	157	ASP
7	HQ	158	CYS
7	HQ	171	ARG
6	IQ	1	MET
6	IQ	3	SER
6	IQ	4	VAL
6	IQ	20	SER
6	IQ	23	ASP
6	IQ	26	SER
6	IQ	27	ILE
6	IQ	44	LEU
6	IQ	49	GLU
6	IQ	67	LYS
6	IQ	90	MET
6	IQ	97	LEU
6	IQ	98	VAL
6	IQ	105	LEU
6	IQ	115	GLU
6	IQ	125	SER
6	IQ	136	ASP
7	JQ	23	ASP
7	JQ	24	LEU
7	JQ	31	ILE
7	JQ	94	SER
7	JQ	97	LEU
7	JQ	124	THR
7	JQ	127	SER
7	JQ	148	GLU
7	JQ	152	SER
7	JQ	157	ASP
7	JQ	158	CYS
7	JQ	171	ARG
6	KQ	1	MET
6	KQ	3	SER
6	KQ	4	VAL
6	KQ	20	SER

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Mol	Chain	Res	Type
6	KQ	23	ASP
6	KQ	26	SER
6	KQ	27	ILE
6	KQ	44	LEU
6	KQ	49	GLU
6	KQ	67	LYS
6	KQ	90	MET
6	KQ	97	LEU
6	KQ	98	VAL
6	KQ	105	LEU
6	KQ	114	ARG
6	KQ	115	GLU
6	KQ	125	SER
6	KQ	136	ASP
7	LQ	23	ASP
7	LQ	24	LEU
7	LQ	31	ILE
7	LQ	60	ILE
7	LQ	94	SER
7	LQ	97	LEU
7	LQ	124	THR
7	LQ	127	SER
7	LQ	148	GLU
7	LQ	152	SER
7	LQ	157	ASP
7	LQ	158	CYS
7	LQ	171	ARG
14	MQ	111	ARG
14	MQ	117	ARG
14	MQ	126	SER
14	MQ	174	ARG
14	MQ	240	SER
8	eR	58	SER
8	eR	77	PHE
8	eR	84	LYS
8	eR	108	HIS
8	eR	109	ILE
8	eR	125	ARG
8	eR	128	ARG
6	MR	39	GLU
6	MR	43	LYS
6	MR	77	GLU

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Mol	Chain	Res	Type
6	MR	86	VAL
6	MR	97	LEU
6	MR	105	LEU
7	NR	61	CYS
7	NR	79	MET
7	NR	83	LEU
7	NR	93	VAL
7	NR	134	MET
7	NR	135	LYS
6	OR	43	LYS
6	OR	77	GLU
6	OR	116	VAL
6	OR	139	CYS
6	OR	163	LEU
7	PR	82	CYS
7	PR	105	LEU
7	PR	107	ASP
7	PR	108	ARG
6	QR	43	LYS
6	QR	144	MET
7	RR	25	GLN
7	RR	160	SER
6	SR	43	LYS
6	SR	90	MET
6	SR	139	CYS
7	TR	108	ARG
7	TR	109	CYS
6	UR	43	LYS
6	UR	54	GLU
6	UR	114	ARG
6	UR	115	GLU
7	VR	29	SER
7	VR	41	VAL
7	VR	84	ARG
7	VR	137	GLN
6	WR	9	VAL
6	WR	43	LYS
6	WR	139	CYS
7	XR	73	CYS
7	XR	75	THR
7	XR	76	ASN
7	XR	93	VAL

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Mol	Chain	Res	Type
7	XR	108	ARG
7	XR	132	SER
7	XR	171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1080) such sidechains are listed below:

Mol	Chain	Res	Type
1	X1	71	ASN
1	X1	332	ASN
1	X1	341	ASN
2	A1	47	ASN
2	A1	88	GLN
2	A1	224	GLN
2	A1	261	HIS
2	A1	289	ASN
3	B1	13	GLN
3	B1	14	ASN
3	B1	15	GLN
3	B1	23	ASN
3	B1	28	GLN
3	B1	59	GLN
3	B1	72	GLN
3	B1	169	GLN
3	B1	211	GLN
3	B1	226	GLN
5	D1	23	GLN
5	D1	63	GLN
5	D1	143	ASN
4	E1	25	GLN
4	E1	140	HIS
4	E1	145	GLN
4	E1	151	ASN
5	F1	21	ASN
5	F1	23	GLN
5	F1	47	ASN
5	F1	63	GLN
5	F1	111	ASN
5	F1	143	ASN
4	G1	15	GLN
5	H1	23	GLN
5	H1	35	ASN
5	H1	143	ASN

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Mol	Chain	Res	Type
5	J1	23	GLN
5	J1	63	GLN
5	J1	111	ASN
5	J1	143	ASN
4	K1	32	GLN
5	L1	23	GLN
5	L1	36	GLN
5	L1	63	GLN
5	L1	68	GLN
5	L1	143	ASN
4	M1	15	GLN
5	N1	21	ASN
5	N1	23	GLN
5	N1	63	GLN
5	N1	143	ASN
6	O1	88	HIS
7	P1	63	ASN
7	P1	76	ASN
6	Q1	88	HIS
7	R1	63	ASN
6	S1	94	ASN
6	S1	147	GLN
7	T1	63	ASN
6	U1	21	ASN
6	U1	88	HIS
6	U1	147	GLN
7	V1	63	ASN
6	W1	21	ASN
6	W1	88	HIS
6	W1	94	ASN
7	Y1	63	ASN
6	Z1	88	HIS
7	a1	63	ASN
6	b1	21	ASN
6	b1	88	HIS
7	c1	63	ASN
6	d1	88	HIS
7	e1	63	ASN
6	f1	88	HIS
7	g1	63	ASN
6	h1	88	HIS
7	i1	63	ASN

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Mol	Chain	Res	Type
6	j1	88	HIS
7	k1	63	ASN
6	l1	88	HIS
6	l1	147	GLN
7	m1	63	ASN
8	e2	153	GLN
8	e2	225	ASN
7	N2	137	GLN
7	V2	47	ASN
6	W2	47	ASN
7	X2	137	GLN
6	A3	68	ASN
6	A3	88	HIS
6	C3	68	ASN
6	C3	88	HIS
6	C3	147	GLN
7	D3	25	GLN
6	E3	68	ASN
6	E3	88	HIS
6	G3	68	ASN
6	G3	88	HIS
6	I3	68	ASN
6	I3	88	HIS
6	K3	68	ASN
6	K3	88	HIS
10	d4	72	GLN
10	d4	311	GLN
6	B4	48	HIS
7	C4	35	ASN
6	D4	147	GLN
7	E4	35	ASN
7	G4	35	ASN
7	G4	76	ASN
6	H4	48	HIS
7	I4	35	ASN
7	I4	76	ASN
6	J4	48	HIS
7	K4	35	ASN
7	K4	76	ASN
6	L4	32	GLN
7	M4	35	ASN
7	M4	76	ASN

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Mol	Chain	Res	Type
7	B5	35	ASN
7	F5	35	ASN
7	F5	137	GLN
7	G5	35	ASN
7	G5	137	GLN
7	H5	35	ASN
7	H5	137	GLN
7	I5	11	ASN
6	J5	28	GLN
6	J5	68	ASN
7	L5	35	ASN
7	L5	76	ASN
7	L5	137	GLN
7	A5	76	ASN
12	E5	162	ASN
12	E5	182	ASN
13	k6	32	ASN
13	k6	104	GLN
13	k6	124	ASN
13	k6	236	GLN
1	X7	47	ASN
1	X7	63	ASN
1	X7	88	GLN
1	X7	306	GLN
2	A7	60	ASN
2	A7	274	ASN
3	B7	53	GLN
3	B7	99	ASN
3	B7	121	ASN
3	B7	135	GLN
3	B7	146	ASN
3	B7	169	GLN
3	B7	209	GLN
4	C7	14	ASN
4	C7	57	GLN
4	C7	148	ASN
4	E7	148	ASN
5	F7	35	ASN
4	G7	148	ASN
5	H7	35	ASN
4	I7	68	GLN
4	I7	134	GLN

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Mol	Chain	Res	Type
4	I7	148	ASN
5	J7	11	GLN
5	J7	35	ASN
4	K7	57	GLN
4	K7	148	ASN
5	L7	35	ASN
4	M7	148	ASN
5	N7	35	ASN
5	N7	111	ASN
6	O7	28	GLN
6	O7	32	GLN
6	Q7	76	GLN
6	S7	28	GLN
6	S7	32	GLN
6	U7	28	GLN
6	U7	32	GLN
6	W7	76	GLN
7	i7	125	ASN
7	B8	35	ASN
7	F8	35	ASN
7	F8	137	GLN
7	G8	35	ASN
7	H8	35	ASN
7	I8	11	ASN
6	J8	28	GLN
6	J8	68	ASN
7	L8	35	ASN
7	L8	76	ASN
7	L8	137	GLN
7	A8	76	ASN
12	E8	162	ASN
12	E8	182	ASN
1	X9	47	ASN
1	X9	63	ASN
1	X9	80	GLN
1	X9	88	GLN
1	X9	306	GLN
2	A9	60	ASN
2	A9	274	ASN
3	B9	53	GLN
3	B9	99	ASN
3	B9	121	ASN

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Mol	Chain	Res	Type
3	B9	135	GLN
3	B9	146	ASN
3	B9	169	GLN
4	C9	14	ASN
4	C9	57	GLN
4	C9	148	ASN
5	D9	35	ASN
4	E9	148	ASN
5	F9	35	ASN
4	G9	148	ASN
5	H9	35	ASN
4	I9	68	GLN
4	I9	134	GLN
4	I9	148	ASN
5	J9	11	GLN
5	J9	35	ASN
4	K9	14	ASN
4	K9	49	GLN
4	K9	57	GLN
4	K9	148	ASN
5	L9	35	ASN
4	M9	148	ASN
5	N9	35	ASN
5	N9	111	ASN
6	O9	28	GLN
6	O9	32	GLN
6	Q9	76	GLN
6	S9	28	GLN
6	S9	32	GLN
6	U9	28	GLN
6	U9	32	GLN
6	U9	68	ASN
6	W9	76	GLN
7	i9	125	ASN
6	AA	28	GLN
6	AA	76	GLN
6	AA	80	ASN
6	CA	28	GLN
6	CA	76	GLN
6	CA	80	ASN
6	EA	76	GLN
6	EA	80	ASN

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Mol	Chain	Res	Type
7	FA	42	ASN
6	GA	76	GLN
6	GA	80	ASN
7	HA	111	ASN
6	IA	32	GLN
6	IA	76	GLN
6	IA	80	ASN
6	KA	76	GLN
6	KA	80	ASN
14	MA	156	ASN
14	MA	196	ASN
14	MA	238	GLN
14	MA	242	GLN
14	MA	279	ASN
14	MA	331	ASN
15	bB	60	HIS
15	bB	84	GLN
15	bB	146	HIS
15	bB	155	HIS
15	bB	270	ASN
15	bB	360	ASN
16	AB	106	GLN
16	AB	119	HIS
16	AB	236	ASN
17	BB	61	GLN
17	BB	136	GLN
17	BB	235	GLN
17	BB	274	HIS
6	CB	32	GLN
6	CB	48	HIS
6	EB	32	GLN
7	FB	76	ASN
7	FB	125	ASN
6	GB	32	GLN
7	HB	125	ASN
6	IB	32	GLN
6	KB	21	ASN
6	KB	32	GLN
6	MB	32	GLN
6	MB	48	HIS
6	MB	80	ASN
7	NB	25	GLN

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Mol	Chain	Res	Type
6	OB	32	GLN
6	QB	32	GLN
7	RB	125	ASN
6	SB	32	GLN
7	TB	25	GLN
6	UB	32	GLN
6	WB	32	GLN
6	WB	147	GLN
7	XB	25	GLN
6	YB	32	GLN
6	aB	32	GLN
6	dB	32	GLN
6	dB	147	GLN
6	fB	32	GLN
7	gB	35	ASN
7	gB	76	ASN
6	hB	21	ASN
6	hB	32	GLN
6	jB	32	GLN
6	lB	32	GLN
7	mB	125	ASN
6	AC	30	ASN
6	AC	147	GLN
7	BC	137	GLN
6	CC	30	ASN
6	CC	147	GLN
7	DC	137	GLN
6	EC	21	ASN
6	EC	30	ASN
7	FC	137	GLN
6	GC	21	ASN
6	GC	30	ASN
6	GC	147	GLN
7	HC	137	GLN
6	IC	30	ASN
6	IC	121	ASN
6	IC	147	GLN
7	JC	137	GLN
6	KC	30	ASN
6	KC	147	GLN
7	LC	137	GLN
18	MC	152	HIS

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Mol	Chain	Res	Type
10	dD	72	GLN
10	dD	311	GLN
10	dD	331	GLN
6	BD	32	GLN
6	BD	48	HIS
7	CD	35	ASN
6	DD	147	GLN
7	ED	35	ASN
7	ED	76	ASN
6	FD	48	HIS
7	GD	35	ASN
7	GD	76	ASN
6	HD	48	HIS
7	ID	35	ASN
7	ID	76	ASN
6	JD	48	HIS
7	KD	35	ASN
7	KD	76	ASN
7	MD	35	ASN
7	MD	76	ASN
6	AE	30	ASN
6	AE	147	GLN
7	BE	137	GLN
6	CE	30	ASN
6	CE	147	GLN
7	DE	137	GLN
6	EE	21	ASN
6	EE	30	ASN
7	FE	137	GLN
6	GE	21	ASN
6	GE	30	ASN
6	GE	147	GLN
7	HE	137	GLN
6	IE	30	ASN
6	IE	121	ASN
6	IE	147	GLN
7	JE	137	GLN
6	KE	30	ASN
6	KE	147	GLN
7	LE	137	GLN
18	ME	301	ASN
1	XF	306	GLN

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Mol	Chain	Res	Type
1	XF	333	ASN
2	AF	60	ASN
2	AF	88	GLN
2	AF	154	HIS
2	AF	264	HIS
3	BF	146	ASN
3	BF	169	GLN
3	BF	178	ASN
3	BF	209	GLN
3	BF	226	GLN
4	CF	145	GLN
4	CF	148	ASN
4	CF	159	ASN
5	DF	35	ASN
5	DF	118	GLN
4	EF	28	ASN
4	EF	49	GLN
4	EF	145	GLN
4	EF	148	ASN
5	FF	35	ASN
5	FF	42	ASN
5	FF	118	GLN
4	GF	14	ASN
4	GF	57	GLN
4	GF	145	GLN
4	GF	148	ASN
5	HF	11	GLN
5	HF	35	ASN
5	HF	118	GLN
4	IF	14	ASN
4	IF	28	ASN
4	IF	145	GLN
4	IF	148	ASN
5	JF	35	ASN
5	JF	118	GLN
4	KF	49	GLN
4	KF	145	GLN
4	KF	148	ASN
5	LF	35	ASN
5	LF	118	GLN
4	MF	15	GLN
4	MF	145	GLN

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Mol	Chain	Res	Type
4	MF	148	ASN
5	NF	21	ASN
5	NF	35	ASN
5	NF	118	GLN
6	OF	88	HIS
6	OF	147	GLN
7	PF	144	ASN
6	QF	88	HIS
6	QF	147	GLN
7	RF	144	ASN
6	SF	88	HIS
7	TF	144	ASN
6	UF	88	HIS
7	VF	144	ASN
6	WF	88	HIS
7	YF	144	ASN
6	ZF	88	HIS
7	aF	144	ASN
6	bF	76	GLN
6	bF	80	ASN
6	bF	88	HIS
7	cF	144	ASN
6	dF	88	HIS
7	eF	144	ASN
6	fF	88	HIS
7	gF	144	ASN
6	hF	88	HIS
7	iF	144	ASN
6	jF	88	HIS
7	kF	144	ASN
6	lF	88	HIS
7	mF	144	ASN
6	AG	28	GLN
7	BG	11	ASN
7	BG	25	GLN
7	BG	35	ASN
7	BG	111	ASN
7	BG	137	GLN
7	BG	144	ASN
7	DG	11	ASN
7	DG	25	GLN
7	DG	35	ASN

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Mol	Chain	Res	Type
7	DG	111	ASN
7	DG	137	GLN
7	DG	144	ASN
7	FG	11	ASN
7	FG	25	GLN
7	FG	35	ASN
7	FG	111	ASN
7	FG	137	GLN
7	FG	144	ASN
6	GG	28	GLN
7	HG	11	ASN
7	HG	25	GLN
7	HG	35	ASN
7	HG	47	ASN
7	HG	111	ASN
7	HG	137	GLN
7	HG	144	ASN
7	JG	11	ASN
7	JG	25	GLN
7	JG	35	ASN
7	JG	111	ASN
7	JG	137	GLN
7	JG	144	ASN
6	KG	28	GLN
6	KG	121	ASN
7	LG	11	ASN
7	LG	25	GLN
7	LG	35	ASN
7	LG	111	ASN
7	LG	137	GLN
7	LG	144	ASN
14	MG	130	GLN
14	MG	196	ASN
14	MG	203	GLN
14	MG	217	GLN
14	MG	228	GLN
14	MG	270	ASN
14	MG	302	ASN
14	MG	307	ASN
13	kH	32	ASN
13	kH	104	GLN
13	kH	124	ASN

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Mol	Chain	Res	Type
13	kH	236	GLN
1	XI	306	GLN
1	XI	333	ASN
2	AI	60	ASN
2	AI	88	GLN
2	AI	154	HIS
2	AI	264	HIS
3	BI	146	ASN
3	BI	169	GLN
3	BI	178	ASN
3	BI	209	GLN
3	BI	223	ASN
3	BI	226	GLN
4	CI	49	GLN
4	CI	145	GLN
4	CI	148	ASN
4	CI	159	ASN
5	DI	35	ASN
5	DI	118	GLN
4	EI	14	ASN
4	EI	15	GLN
4	EI	28	ASN
4	EI	49	GLN
4	EI	145	GLN
4	EI	148	ASN
5	FI	35	ASN
5	FI	42	ASN
5	FI	118	GLN
4	GI	14	ASN
4	GI	145	GLN
4	GI	148	ASN
5	HI	11	GLN
5	HI	35	ASN
5	HI	118	GLN
4	II	14	ASN
4	II	28	ASN
4	II	145	GLN
4	II	148	ASN
5	JI	35	ASN
5	JI	111	ASN
5	JI	118	GLN
4	KI	15	GLN

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Mol	Chain	Res	Type
4	KI	49	GLN
4	KI	145	GLN
4	KI	148	ASN
5	LI	35	ASN
5	LI	118	GLN
4	MI	15	GLN
4	MI	145	GLN
4	MI	148	ASN
5	NI	21	ASN
5	NI	35	ASN
5	NI	118	GLN
6	OI	88	HIS
6	OI	94	ASN
6	OI	147	GLN
7	PI	144	ASN
6	QI	88	HIS
7	RI	144	ASN
6	SI	88	HIS
7	TI	144	ASN
6	UI	88	HIS
7	VI	144	ASN
6	WI	88	HIS
7	YI	144	ASN
6	ZI	88	HIS
7	aI	144	ASN
6	bI	76	GLN
6	bI	80	ASN
6	bI	88	HIS
7	cI	144	ASN
6	dI	88	HIS
7	eI	144	ASN
6	fI	88	HIS
7	gI	144	ASN
6	hI	88	HIS
7	iI	144	ASN
6	jI	88	HIS
7	kI	144	ASN
6	lI	88	HIS
7	mI	144	ASN
6	AJ	80	ASN
7	BJ	47	ASN
6	CJ	80	ASN

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Mol	Chain	Res	Type
6	CJ	94	ASN
7	DJ	47	ASN
6	EJ	80	ASN
7	FJ	47	ASN
7	FJ	125	ASN
6	GJ	76	GLN
6	GJ	94	ASN
7	HJ	47	ASN
6	IJ	75	ASN
7	JJ	47	ASN
6	KJ	47	ASN
6	KJ	80	ASN
6	KJ	161	ASN
7	LJ	47	ASN
6	MJ	80	ASN
6	MJ	147	GLN
7	NJ	47	ASN
6	OJ	80	ASN
6	OJ	94	ASN
7	PJ	47	ASN
6	QJ	47	ASN
6	QJ	80	ASN
7	RJ	47	ASN
6	SJ	80	ASN
7	TJ	47	ASN
6	UJ	80	ASN
7	VJ	47	ASN
6	WJ	68	ASN
6	WJ	80	ASN
7	XJ	47	ASN
6	YJ	80	ASN
7	ZJ	47	ASN
6	aJ	80	ASN
7	bJ	47	ASN
6	cJ	80	ASN
7	dJ	47	ASN
6	eJ	80	ASN
7	fJ	47	ASN
6	gJ	80	ASN
7	hJ	47	ASN
6	iJ	80	ASN
7	jJ	47	ASN

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Mol	Chain	Res	Type
6	kJ	80	ASN
6	kJ	161	ASN
7	lJ	42	ASN
7	lJ	47	ASN
7	lJ	76	ASN
6	mJ	80	ASN
6	mJ	161	ASN
7	nJ	47	ASN
6	oJ	80	ASN
7	pJ	47	ASN
6	qJ	80	ASN
6	qJ	147	GLN
7	rJ	47	ASN
6	sJ	80	ASN
7	tJ	47	ASN
7	tJ	76	ASN
6	uJ	80	ASN
6	uJ	161	ASN
7	vJ	47	ASN
16	xJ	41	ASN
17	yJ	61	GLN
17	yJ	79	ASN
17	yJ	235	GLN
17	yJ	274	HIS
19	zJ	248	ASN
19	zJ	256	HIS
19	zJ	273	GLN
19	zJ	276	ASN
19	zJ	343	GLN
19	zJ	351	GLN
1	XK	71	ASN
1	XK	96	GLN
1	XK	332	ASN
1	XK	341	ASN
2	AK	47	ASN
2	AK	88	GLN
2	AK	224	GLN
2	AK	261	HIS
2	AK	289	ASN
3	BK	23	ASN
3	BK	28	GLN
3	BK	59	GLN

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Mol	Chain	Res	Type
3	BK	72	GLN
3	BK	169	GLN
3	BK	223	ASN
3	BK	226	GLN
5	DK	23	GLN
5	DK	63	GLN
5	DK	143	ASN
4	EK	21	ASN
4	EK	25	GLN
4	EK	140	HIS
4	EK	145	GLN
4	EK	151	ASN
5	FK	21	ASN
5	FK	23	GLN
5	FK	63	GLN
5	FK	111	ASN
5	FK	143	ASN
4	GK	15	GLN
5	HK	23	GLN
5	HK	35	ASN
5	HK	143	ASN
4	IK	49	GLN
5	JK	23	GLN
5	JK	47	ASN
5	JK	63	GLN
5	JK	111	ASN
5	JK	143	ASN
4	KK	32	GLN
5	LK	23	GLN
5	LK	36	GLN
5	LK	63	GLN
5	LK	65	GLN
5	LK	68	GLN
5	LK	143	ASN
4	MK	15	GLN
5	NK	21	ASN
5	NK	63	GLN
5	NK	143	ASN
6	OK	88	HIS
7	PK	63	ASN
7	PK	76	ASN
6	QK	88	HIS

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Mol	Chain	Res	Type
7	RK	63	ASN
6	SK	147	GLN
7	TK	63	ASN
6	UK	21	ASN
6	UK	88	HIS
6	UK	147	GLN
7	VK	63	ASN
6	WK	21	ASN
6	WK	88	HIS
7	YK	63	ASN
6	ZK	88	HIS
7	aK	63	ASN
6	bK	21	ASN
6	bK	88	HIS
6	bK	94	ASN
7	cK	63	ASN
6	dK	88	HIS
7	eK	63	ASN
6	fK	88	HIS
7	gK	63	ASN
6	hK	88	HIS
7	iK	63	ASN
6	jK	88	HIS
7	kK	63	ASN
6	lK	88	HIS
6	lK	147	GLN
7	mK	63	ASN
6	AL	80	ASN
6	AL	147	GLN
7	BL	47	ASN
6	CL	80	ASN
6	CL	94	ASN
7	DL	47	ASN
6	EL	80	ASN
7	FL	47	ASN
7	FL	125	ASN
6	GL	76	GLN
6	GL	94	ASN
7	HL	47	ASN
7	HL	111	ASN
6	IL	75	ASN
7	JL	47	ASN

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Mol	Chain	Res	Type
6	KL	47	ASN
6	KL	80	ASN
6	KL	161	ASN
7	LL	47	ASN
6	ML	80	ASN
6	ML	147	GLN
7	NL	47	ASN
6	OL	80	ASN
6	OL	94	ASN
7	PL	47	ASN
6	QL	47	ASN
6	QL	80	ASN
7	RL	47	ASN
6	SL	80	ASN
6	SL	147	GLN
7	TL	47	ASN
6	UL	80	ASN
7	VL	47	ASN
6	WL	68	ASN
6	WL	80	ASN
7	XL	47	ASN
6	YL	80	ASN
7	ZL	47	ASN
6	aL	80	ASN
7	bL	47	ASN
6	cL	80	ASN
7	dL	47	ASN
6	eL	80	ASN
7	fL	47	ASN
6	gL	80	ASN
7	hL	47	ASN
6	iL	80	ASN
7	jL	47	ASN
6	kL	80	ASN
6	kL	161	ASN
7	lL	42	ASN
7	lL	47	ASN
7	lL	76	ASN
6	mL	80	ASN
6	mL	161	ASN
7	nL	47	ASN
6	oL	80	ASN

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Mol	Chain	Res	Type
7	pL	47	ASN
7	pL	111	ASN
6	qL	21	ASN
6	qL	80	ASN
7	rL	47	ASN
6	sL	80	ASN
7	tL	47	ASN
7	tL	76	ASN
6	uL	80	ASN
6	uL	161	ASN
7	vL	47	ASN
16	xL	41	ASN
17	yL	61	GLN
17	yL	79	ASN
17	yL	235	GLN
17	yL	274	HIS
19	zL	248	ASN
19	zL	256	HIS
19	zL	273	GLN
19	zL	276	ASN
19	zL	343	GLN
19	zL	351	GLN
15	bM	60	HIS
15	bM	84	GLN
15	bM	146	HIS
15	bM	155	HIS
15	bM	360	ASN
16	AM	106	GLN
16	AM	119	HIS
16	AM	236	ASN
17	BM	61	GLN
17	BM	136	GLN
17	BM	235	GLN
17	BM	274	HIS
6	CM	32	GLN
6	CM	48	HIS
6	EM	32	GLN
6	EM	147	GLN
7	FM	76	ASN
7	FM	125	ASN
6	GM	32	GLN
6	GM	147	GLN

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Mol	Chain	Res	Type
7	HM	125	ASN
6	IM	32	GLN
6	KM	21	ASN
6	KM	32	GLN
6	MM	32	GLN
6	MM	48	HIS
6	MM	80	ASN
6	OM	32	GLN
6	QM	32	GLN
7	RM	125	ASN
6	SM	32	GLN
7	TM	25	GLN
6	UM	32	GLN
6	WM	32	GLN
6	WM	147	GLN
7	XM	25	GLN
6	YM	32	GLN
6	aM	32	GLN
6	dM	32	GLN
6	fM	32	GLN
7	gM	35	ASN
7	gM	76	ASN
6	hM	21	ASN
6	hM	32	GLN
6	jM	32	GLN
6	lM	32	GLN
6	lM	76	GLN
7	mM	125	ASN
6	AN	28	GLN
6	AN	76	GLN
6	AN	80	ASN
6	CN	28	GLN
6	CN	76	GLN
6	CN	80	ASN
6	EN	76	GLN
6	EN	80	ASN
7	FN	42	ASN
6	GN	76	GLN
6	GN	80	ASN
7	HN	111	ASN
6	IN	32	GLN
6	IN	76	GLN

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Mol	Chain	Res	Type
6	IN	80	ASN
6	KN	76	GLN
6	KN	80	ASN
14	MN	156	ASN
14	MN	196	ASN
14	MN	238	GLN
14	MN	242	GLN
14	MN	279	ASN
14	MN	331	ASN
6	AO	68	ASN
6	AO	88	HIS
6	CO	68	ASN
6	CO	88	HIS
6	CO	147	GLN
7	DO	25	GLN
6	EO	68	ASN
6	EO	88	HIS
6	GO	68	ASN
6	GO	88	HIS
6	IO	68	ASN
6	IO	88	HIS
6	KO	68	ASN
6	KO	88	HIS
20	AP	71	ASN
21	DP	15	GLN
21	DP	22	ASN
21	DP	110	ASN
20	CP	71	ASN
21	FP	15	GLN
20	EP	71	ASN
21	BP	15	GLN
20	GP	71	ASN
21	HP	15	GLN
21	HP	117	ASN
21	IP	15	GLN
21	IP	110	ASN
20	JP	41	GLN
20	JP	71	ASN
20	KP	71	ASN
21	LP	15	GLN
21	LP	110	ASN
21	LP	128	GLN

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Mol	Chain	Res	Type
21	MP	15	GLN
21	MP	110	ASN
21	MP	128	GLN
20	NP	41	GLN
20	NP	71	ASN
21	OP	15	GLN
20	PP	71	ASN
21	QP	15	GLN
20	RP	71	ASN
21	SP	15	GLN
20	TP	71	ASN
21	UP	15	GLN
22	VP	44	GLN
23	WP	50	ASN
23	WP	137	GLN
23	WP	154	ASN
24	XP	106	GLN
24	XP	109	GLN
25	YP	51	ASN
25	YP	169	ASN
25	YP	221	ASN
25	YP	229	ASN
25	YP	307	ASN
25	YP	331	GLN
25	YP	410	GLN
25	YP	415	GLN
25	YP	447	ASN
25	YP	557	ASN
25	YP	558	ASN
25	YP	655	GLN
25	YP	705	GLN
25	YP	724	GLN
25	YP	755	GLN
25	YP	800	GLN
25	YP	807	ASN
25	YP	816	GLN
25	YP	849	ASN
26	ZP	47	GLN
26	ZP	61	ASN
27	aP	54	GLN
27	aP	275	ASN
28	bP	78	GLN

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Mol	Chain	Res	Type
28	bP	135	ASN
28	bP	145	HIS
28	bP	211	ASN
20	cP	71	ASN
21	dP	15	GLN
21	dP	22	ASN
21	dP	110	ASN
20	eP	71	ASN
21	fP	15	GLN
20	gP	71	ASN
21	hP	15	GLN
21	hP	128	GLN
20	iP	71	ASN
21	jP	15	GLN
21	jP	117	ASN
21	kP	15	GLN
21	kP	110	ASN
21	kP	128	GLN
20	lP	71	ASN
20	mP	71	ASN
21	nP	15	GLN
21	nP	110	ASN
21	nP	128	GLN
21	oP	15	GLN
21	oP	110	ASN
21	oP	128	GLN
20	pP	41	GLN
20	pP	71	ASN
21	qP	15	GLN
20	rP	71	ASN
21	sP	15	GLN
21	sP	128	GLN
20	tP	71	ASN
21	uP	15	GLN
20	vP	60	GLN
20	vP	71	ASN
21	wP	15	GLN
22	xP	44	GLN
23	yP	45	ASN
23	yP	50	ASN
23	yP	137	GLN
23	yP	154	ASN

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Mol	Chain	Res	Type
24	zP	109	GLN
25	1P	169	ASN
25	1P	221	ASN
25	1P	229	ASN
25	1P	307	ASN
25	1P	331	GLN
25	1P	410	GLN
25	1P	415	GLN
25	1P	447	ASN
25	1P	557	ASN
25	1P	655	GLN
25	1P	705	GLN
25	1P	724	GLN
25	1P	755	GLN
25	1P	800	GLN
25	1P	816	GLN
25	1P	849	ASN
26	2P	47	GLN
26	2P	61	ASN
27	3P	275	ASN
28	4P	78	GLN
28	4P	135	ASN
28	4P	145	HIS
28	4P	211	ASN
7	BQ	11	ASN
7	BQ	25	GLN
7	BQ	35	ASN
7	BQ	111	ASN
7	BQ	137	GLN
7	BQ	144	ASN
7	DQ	11	ASN
7	DQ	25	GLN
7	DQ	35	ASN
7	DQ	111	ASN
7	DQ	137	GLN
7	DQ	144	ASN
6	EQ	28	GLN
7	FQ	11	ASN
7	FQ	25	GLN
7	FQ	35	ASN
7	FQ	111	ASN
7	FQ	137	GLN

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Mol	Chain	Res	Type
7	FQ	144	ASN
6	GQ	28	GLN
7	HQ	11	ASN
7	HQ	25	GLN
7	HQ	35	ASN
7	HQ	111	ASN
7	HQ	137	GLN
7	HQ	144	ASN
6	IQ	28	GLN
7	JQ	11	ASN
7	JQ	25	GLN
7	JQ	35	ASN
7	JQ	111	ASN
7	JQ	137	GLN
7	JQ	144	ASN
6	KQ	28	GLN
6	KQ	121	ASN
7	LQ	11	ASN
7	LQ	25	GLN
7	LQ	35	ASN
7	LQ	111	ASN
7	LQ	144	ASN
14	MQ	130	GLN
14	MQ	196	ASN
14	MQ	203	GLN
14	MQ	217	GLN
14	MQ	228	GLN
14	MQ	270	ASN
8	eR	108	HIS
8	eR	153	GLN
8	eR	221	ASN
8	eR	225	ASN
8	eR	258	ASN
8	eR	284	ASN
7	NR	137	GLN
7	VR	47	ASN
7	XR	137	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

308 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
7	MEN	VJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	RJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	a9	72	7	7,8,9	0.70	0	6,9,11	0.80	0
7	MEN	DO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	PI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
21	MEN	oP	71	21	7,8,9	1.13	1 (14%)	6,9,11	0.94	0
7	MEN	rL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	V1	72	7	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	Y9	72	7	7,8,9	0.72	0	6,9,11	0.77	0
7	MEN	L3	72	7	7,8,9	0.72	0	6,9,11	0.66	0
7	MEN	e9	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	kK	72	7	7,8,9	0.70	0	6,9,11	0.91	0
7	MEN	i1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	V9	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	iM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	mF	72	7	7,8,9	0.77	0	6,9,11	0.81	0
7	MEN	FB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	cB	72	7	7,8,9	0.68	0	6,9,11	0.87	0
7	MEN	iK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	NR	72	7	7,8,9	0.75	0	6,9,11	1.15	1 (16%)
7	MEN	FL	72	7,29	7,8,9	0.75	0	6,9,11	0.89	0
7	MEN	kI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	eI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	vJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	kB	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	H5	72	7	7,8,9	0.72	0	6,9,11	0.65	0
7	MEN	gM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	XB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	PM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
5	MEN	HK	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	HM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	ZB	72	7	7,8,9	0.68	0	6,9,11	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MEN	HI	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	LJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
5	MEN	L7	72	5	7,8,9	0.62	0	6,9,11	0.71	0
7	MEN	iI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	PJ	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	BO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	NJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	F5	72	7	7,8,9	0.72	0	6,9,11	0.64	0
7	MEN	fL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	aK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	DA	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	FG	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	jJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	mB	72	7	7,8,9	0.67	0	6,9,11	0.87	0
7	MEN	BJ	72	7,29	7,8,9	0.75	0	6,9,11	0.91	0
7	MEN	TM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	L8	72	7	7,8,9	0.72	0	6,9,11	0.63	0
7	MEN	HC	72	7	7,8,9	0.66	0	6,9,11	0.75	0
5	MEN	L9	72	5	7,8,9	0.62	0	6,9,11	0.72	0
7	MEN	HL	72	7	7,8,9	0.62	0	6,9,11	1.08	0
5	MEN	JF	72	5	7,8,9	0.70	0	6,9,11	0.90	0
7	MEN	aF	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	Y1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	VK	72	7	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	LE	72	7	7,8,9	0.67	0	6,9,11	0.74	0
7	MEN	iB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	VF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	cM	72	7	7,8,9	0.68	0	6,9,11	0.87	0
7	MEN	TI	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	dL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	m1	72	7	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	YK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	fJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	C4	72	7	7,8,9	0.64	0	6,9,11	0.51	0
7	MEN	E4	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	nL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	BC	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	k9	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	J3	72	7	7,8,9	0.74	0	6,9,11	0.67	0
21	MEN	LP	71	21	7,8,9	8.57	4 (57%)	6,9,11	12.38	5 (83%)
7	MEN	k1	72	7	7,8,9	0.70	0	6,9,11	0.91	0
7	MEN	C8	72	7	7,8,9	0.67	0	6,9,11	0.79	0
7	MEN	NB	72	7	7,8,9	0.68	0	6,9,11	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	PR	72	7	7,8,9	0.75	0	6,9,11	1.15	1 (16%)
7	MEN	tJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	HO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	GD	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	CD	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	DL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
5	MEN	DI	72	5,1	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	LG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	bL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	gB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	VR	72	7	7,8,9	0.74	0	6,9,11	1.16	1 (16%)
21	MEN	OP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.97	0
7	MEN	vL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	lJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	HG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	HA	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	ED	72	7	7,8,9	0.63	0	6,9,11	0.53	0
5	MEN	H9	72	5	7,8,9	0.67	0	6,9,11	0.83	0
7	MEN	TF	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	ID	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	HE	72	7	7,8,9	0.66	0	6,9,11	0.75	0
7	MEN	Y7	72	7	7,8,9	0.72	0	6,9,11	0.77	0
5	MEN	FK	72	5	7,8,9	0.71	0	6,9,11	0.88	0
7	MEN	gF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	cF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	G8	72	7	7,8,9	0.72	0	6,9,11	0.64	0
7	MEN	F8	72	7	7,8,9	0.72	0	6,9,11	0.64	0
5	MEN	H7	72	5	7,8,9	0.67	0	6,9,11	0.83	0
7	MEN	TB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	LL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
21	MEN	qP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.99	0
7	MEN	V7	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	eM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	KD	72	7	7,8,9	0.62	0	6,9,11	0.52	0
7	MEN	m7	72	7	7,8,9	0.71	0	6,9,11	0.77	0
7	MEN	FO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	NL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	H3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	g1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
5	MEN	L1	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	HN	72	7	7,8,9	0.74	0	6,9,11	0.83	0
5	MEN	JK	72	5	7,8,9	0.71	0	6,9,11	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	MEN	fP	71	21	7,8,9	1.16	1 (14%)	6,9,11	1.10	0
7	MEN	B5	72	7	7,8,9	0.73	0	6,9,11	0.65	0
7	MEN	DJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
21	MEN	UP	71	21	7,8,9	0.80	0	6,9,11	0.61	0
7	MEN	JC	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	I4	72	7	7,8,9	0.63	0	6,9,11	0.53	0
7	MEN	FQ	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	LN	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	hL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	BG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	PK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	FJ	72	7,29	7,8,9	0.75	0	6,9,11	0.89	0
7	MEN	XM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	MO	72	7	7,8,9	0.69	0	6,9,11	0.75	0
5	MEN	F7	72	5	7,8,9	0.65	0	6,9,11	0.79	0
7	MEN	FM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	e1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	RI	72	7	7,8,9	0.76	0	6,9,11	0.81	0
5	MEN	N1	72	5	7,8,9	0.70	0	6,9,11	0.87	0
7	MEN	R7	72	7	7,8,9	0.72	0	6,9,11	0.77	0
7	MEN	JB	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	rJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	A5	72	7	7,8,9	0.68	0	6,9,11	0.78	0
7	MEN	DQ	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	c9	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	C5	72	7	7,8,9	0.67	0	6,9,11	0.79	0
5	MEN	N9	72	5	7,8,9	0.63	0	6,9,11	0.70	0
7	MEN	JE	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	HQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	tL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
5	MEN	J7	72	5	7,8,9	0.66	0	6,9,11	0.84	0
7	MEN	VB	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	LB	72	7	7,8,9	0.67	0	6,9,11	0.87	0
21	MEN	DP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.95	0
7	MEN	VI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	LC	72	7	7,8,9	0.67	0	6,9,11	0.74	0
7	MEN	T1	72	7	7,8,9	0.72	0	6,9,11	0.92	0
7	MEN	e7	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	aI	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	FN	72	7	7,8,9	0.74	0	6,9,11	0.82	0
7	MEN	DC	72	7	7,8,9	0.67	0	6,9,11	0.73	0
21	MEN	IP	71	21	7,8,9	1.17	1 (14%)	6,9,11	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	BL	72	7,29	7,8,9	0.75	0	6,9,11	0.91	0
7	MEN	DM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	DG	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	eB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	G4	72	7	7,8,9	0.63	0	6,9,11	0.53	0
7	MEN	JA	72	7	7,8,9	0.73	0	6,9,11	0.82	0
21	MEN	kP	71	21	7,8,9	8.57	4 (57%)	6,9,11	12.37	5 (83%)
7	MEN	HJ	72	7	7,8,9	0.61	0	6,9,11	1.13	0
7	MEN	L5	72	7	7,8,9	0.72	0	6,9,11	0.64	0
7	MEN	NM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	TJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	k7	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	JO	72	7	7,8,9	0.74	0	6,9,11	0.67	0
7	MEN	ZJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	cK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
5	MEN	FF	72	5	7,8,9	0.71	0	6,9,11	0.89	0
7	MEN	RB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	gK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	c1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	JL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	i7	72	7	7,8,9	0.70	0	6,9,11	0.78	0
5	MEN	D1	72	5	7,8,9	0.70	0	6,9,11	0.87	0
7	MEN	JJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	NO	72	7	7,8,9	0.70	0	6,9,11	0.75	0
5	MEN	H1	72	5	7,8,9	0.71	0	6,9,11	0.85	0
7	MEN	V2	72	7	7,8,9	0.75	0	6,9,11	1.15	1 (16%)
21	MEN	BP	71	21	7,8,9	1.16	1 (14%)	6,9,11	1.29	1 (16%)
7	MEN	B3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	nJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	PB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	G5	72	7	7,8,9	0.73	0	6,9,11	0.63	0
7	MEN	gI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	bJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	T9	72	7	7,8,9	0.71	0	6,9,11	0.79	0
7	MEN	LO	72	7	7,8,9	0.72	0	6,9,11	0.66	0
7	MEN	RK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	I8	72	7	7,8,9	0.69	0	6,9,11	0.76	0
7	MEN	M4	72	7	7,8,9	0.61	0	6,9,11	0.53	0
7	MEN	A8	72	7	7,8,9	0.68	0	6,9,11	0.77	0
7	MEN	g7	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	T7	72	7	7,8,9	0.71	0	6,9,11	0.79	0
5	MEN	F1	72	5	7,8,9	0.71	0	6,9,11	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	K5	72	7	7,8,9	0.68	0	6,9,11	0.78	0
5	MEN	JI	72	5	7,8,9	0.70	0	6,9,11	0.90	0
5	MEN	LF	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	PL	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	YI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	VM	72	7	7,8,9	0.68	0	6,9,11	0.85	0
5	MEN	LI	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	dJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	PF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	kF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	g9	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	P2	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
21	MEN	MP	71	21	7,8,9	1.13	1 (14%)	6,9,11	0.96	0
7	MEN	DB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	XJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	K8	72	7	7,8,9	0.68	0	6,9,11	0.78	0
21	MEN	uP	71	21	7,8,9	0.64	0	6,9,11	0.96	0
7	MEN	i9	72	7	7,8,9	0.70	0	6,9,11	0.78	0
7	MEN	BE	72	7	7,8,9	0.66	0	6,9,11	0.74	0
5	MEN	LK	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	TK	72	7	7,8,9	0.72	0	6,9,11	0.92	0
7	MEN	BQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	BA	72	7	7,8,9	0.73	0	6,9,11	0.82	0
7	MEN	FA	72	7	7,8,9	0.74	0	6,9,11	0.82	0
7	MEN	DN	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	jL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
5	MEN	NI	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	pL	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	c7	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	ZM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
5	MEN	D7	72	5	7,8,9	0.65	0	6,9,11	0.87	0
7	MEN	YF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	K4	72	7	7,8,9	0.62	0	6,9,11	0.52	0
5	MEN	DK	72	5	7,8,9	0.71	0	6,9,11	0.86	0
7	MEN	cI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	mI	72	7	7,8,9	0.77	0	6,9,11	0.81	0
7	MEN	R2	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
7	MEN	FC	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	MD	72	7	7,8,9	0.62	0	6,9,11	0.54	0
7	MEN	HB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
21	MEN	jP	71	21	7,8,9	8.57	4 (57%)	6,9,11	12.38	5 (83%)
7	MEN	I5	72	7	7,8,9	0.69	0	6,9,11	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	H8	72	7	7,8,9	0.74	0	6,9,11	0.64	0
5	MEN	J1	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	mM	72	7	7,8,9	0.67	0	6,9,11	0.87	0
7	MEN	D3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	N3	72	7	7,8,9	0.69	0	6,9,11	0.73	0
7	MEN	XR	72	7	7,8,9	0.76	0	6,9,11	1.14	1 (16%)
7	MEN	eK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	F3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
5	MEN	HF	72	5	7,8,9	0.71	0	6,9,11	0.90	0
5	MEN	NK	72	5	7,8,9	0.70	0	6,9,11	0.87	0
7	MEN	VL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	LQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
5	MEN	NF	72	5	7,8,9	0.71	0	6,9,11	0.90	0
5	MEN	FI	72	5	7,8,9	0.71	0	6,9,11	0.89	0
7	MEN	P9	72	7	7,8,9	0.72	0	6,9,11	0.79	0
5	MEN	D9	72	5	7,8,9	0.65	0	6,9,11	0.87	0
7	MEN	kM	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	P1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	RM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	XL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	TL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	M3	72	7	7,8,9	0.69	0	6,9,11	0.75	0
7	MEN	TR	72	7	7,8,9	0.74	0	6,9,11	1.16	1 (16%)
21	MEN	HP	71	21	7,8,9	1.18	1 (14%)	6,9,11	0.97	0
7	MEN	a7	72	7	7,8,9	0.70	0	6,9,11	0.80	0
7	MEN	JQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	DE	72	7	7,8,9	0.67	0	6,9,11	0.73	0
21	MEN	sP	71	21	7,8,9	0.63	0	6,9,11	0.78	0
7	MEN	hJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	N2	72	7	7,8,9	0.74	0	6,9,11	1.15	1 (16%)
7	MEN	iF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	BN	72	7	7,8,9	0.73	0	6,9,11	0.82	0
7	MEN	T2	72	7	7,8,9	0.75	0	6,9,11	1.14	1 (16%)
21	MEN	nP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.91	0
7	MEN	m9	72	7	7,8,9	0.71	0	6,9,11	0.77	0
7	MEN	P7	72	7	7,8,9	0.72	0	6,9,11	0.79	0
7	MEN	B8	72	7	7,8,9	0.73	0	6,9,11	0.65	0
7	MEN	RL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	IL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	R9	72	7	7,8,9	0.72	0	6,9,11	0.77	0
7	MEN	LA	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	pJ	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	a1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
21	MEN	dP	71	21	7,8,9	1.14	1 (14%)	6,9,11	0.93	0
5	MEN	N7	72	5	7,8,9	0.63	0	6,9,11	0.70	0
5	MEN	J9	72	5	7,8,9	0.65	0	6,9,11	0.84	0
7	MEN	R1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
21	MEN	wP	71	21	7,8,9	0.79	0	6,9,11	0.63	0
7	MEN	JN	72	7	7,8,9	0.73	0	6,9,11	0.82	0
7	MEN	RF	72	7	7,8,9	0.76	0	6,9,11	0.81	0
7	MEN	JG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	JM	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	mK	72	7	7,8,9	0.71	0	6,9,11	0.91	0
21	MEN	FP	71	21	7,8,9	1.14	1 (14%)	6,9,11	0.86	0
5	MEN	DF	72	5,1	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	X2	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
21	MEN	hP	71	21	7,8,9	1.14	1 (14%)	6,9,11	0.96	0
7	MEN	eF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
21	MEN	SP	71	21	7,8,9	0.63	0	6,9,11	0.99	0
7	MEN	RR	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
7	MEN	ZL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	LM	72	7	7,8,9	0.67	0	6,9,11	0.87	0
7	MEN	FE	72	7	7,8,9	0.66	0	6,9,11	0.74	0
5	MEN	F9	72	5	7,8,9	0.65	0	6,9,11	0.78	0
21	MEN	QP	71	21	7,8,9	0.63	0	6,9,11	0.76	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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	VJ	72	7,29	-	4/7/8/10	-
7	MEN	RJ	72	7,29	-	4/7/8/10	-
7	MEN	a9	72	7	-	6/7/8/10	-
7	MEN	DO	72	7	-	4/7/8/10	-
7	MEN	PI	72	7	-	6/7/8/10	-
21	MEN	oP	71	21	-	6/7/8/10	-
7	MEN	rL	72	7,29	-	4/7/8/10	-
7	MEN	V1	72	7	-	6/7/8/10	-
7	MEN	Y9	72	7	-	6/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	L3	72	7	-	4/7/8/10	-
7	MEN	e9	72	7	-	6/7/8/10	-
7	MEN	kK	72	7	-	6/7/8/10	-
7	MEN	i1	72	7	-	6/7/8/10	-
7	MEN	V9	72	7	-	6/7/8/10	-
7	MEN	iM	72	7	-	6/7/8/10	-
7	MEN	mF	72	7	-	6/7/8/10	-
7	MEN	FB	72	7	-	6/7/8/10	-
7	MEN	cB	72	7	-	6/7/8/10	-
7	MEN	iK	72	7	-	6/7/8/10	-
7	MEN	NR	72	7	-	3/7/8/10	-
7	MEN	FL	72	7,29	-	4/7/8/10	-
7	MEN	kI	72	7	-	6/7/8/10	-
7	MEN	eI	72	7	-	6/7/8/10	-
7	MEN	vJ	72	7,29	-	4/7/8/10	-
7	MEN	kB	72	7	-	6/7/8/10	-
7	MEN	H5	72	7	-	2/7/8/10	-
7	MEN	gM	72	7	-	6/7/8/10	-
7	MEN	XB	72	7	-	6/7/8/10	-
7	MEN	PM	72	7	-	6/7/8/10	-
5	MEN	HK	72	5	-	2/7/8/10	-
7	MEN	HM	72	7	-	6/7/8/10	-
7	MEN	ZB	72	7	-	6/7/8/10	-
5	MEN	HI	72	5	-	4/7/8/10	-
7	MEN	LJ	72	7,29	-	4/7/8/10	-
5	MEN	L7	72	5	-	2/7/8/10	-
7	MEN	iI	72	7	-	6/7/8/10	-
7	MEN	PJ	72	7,29	-	4/7/8/10	-
7	MEN	BO	72	7	-	4/7/8/10	-
7	MEN	NJ	72	7,29	-	4/7/8/10	-
7	MEN	F5	72	7	-	2/7/8/10	-
7	MEN	fL	72	7,29	-	4/7/8/10	-
7	MEN	aK	72	7	-	6/7/8/10	-
7	MEN	DA	72	7	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	FG	72	7	-	4/7/8/10	-
7	MEN	jJ	72	7,29	-	4/7/8/10	-
7	MEN	mB	72	7	-	6/7/8/10	-
7	MEN	BJ	72	7,29	-	4/7/8/10	-
7	MEN	TM	72	7	-	6/7/8/10	-
7	MEN	L8	72	7	-	2/7/8/10	-
7	MEN	HC	72	7	-	2/7/8/10	-
5	MEN	L9	72	5	-	2/7/8/10	-
7	MEN	HL	72	7	-	5/7/8/10	-
5	MEN	JF	72	5	-	4/7/8/10	-
7	MEN	aF	72	7	-	6/7/8/10	-
7	MEN	Y1	72	7	-	6/7/8/10	-
7	MEN	VK	72	7	-	6/7/8/10	-
7	MEN	LE	72	7	-	2/7/8/10	-
7	MEN	iB	72	7	-	6/7/8/10	-
7	MEN	VF	72	7	-	6/7/8/10	-
7	MEN	cM	72	7	-	6/7/8/10	-
7	MEN	TI	72	7	-	6/7/8/10	-
7	MEN	dL	72	7,29	-	4/7/8/10	-
7	MEN	m1	72	7	-	6/7/8/10	-
7	MEN	YK	72	7	-	6/7/8/10	-
7	MEN	fJ	72	7,29	-	4/7/8/10	-
7	MEN	C4	72	7	-	5/7/8/10	-
7	MEN	E4	72	7	-	5/7/8/10	-
7	MEN	nL	72	7,29	-	4/7/8/10	-
7	MEN	BC	72	7	-	2/7/8/10	-
7	MEN	k9	72	7	-	6/7/8/10	-
7	MEN	J3	72	7	-	4/7/8/10	-
21	MEN	LP	71	21	-	6/7/8/10	-
7	MEN	k1	72	7	-	6/7/8/10	-
7	MEN	C8	72	7	-	6/7/8/10	-
7	MEN	NB	72	7	-	6/7/8/10	-
7	MEN	PR	72	7	-	3/7/8/10	-
7	MEN	tJ	72	7,29	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	HO	72	7	-	4/7/8/10	-
7	MEN	GD	72	7	-	5/7/8/10	-
7	MEN	CD	72	7	-	5/7/8/10	-
7	MEN	DL	72	7,29	-	4/7/8/10	-
5	MEN	DI	72	5,1	-	5/7/8/10	-
7	MEN	LG	72	7	-	4/7/8/10	-
7	MEN	bL	72	7,29	-	4/7/8/10	-
7	MEN	gB	72	7	-	6/7/8/10	-
7	MEN	VR	72	7	-	3/7/8/10	-
21	MEN	OP	71	21	-	4/7/8/10	-
7	MEN	vL	72	7,29	-	4/7/8/10	-
7	MEN	lJ	72	7,29	-	4/7/8/10	-
7	MEN	HG	72	7	-	4/7/8/10	-
7	MEN	HA	72	7	-	2/7/8/10	-
7	MEN	ED	72	7	-	5/7/8/10	-
5	MEN	H9	72	5	-	6/7/8/10	-
7	MEN	TF	72	7	-	6/7/8/10	-
7	MEN	ID	72	7	-	5/7/8/10	-
7	MEN	HE	72	7	-	2/7/8/10	-
7	MEN	Y7	72	7	-	6/7/8/10	-
5	MEN	FK	72	5	-	2/7/8/10	-
7	MEN	gF	72	7	-	6/7/8/10	-
7	MEN	cF	72	7	-	6/7/8/10	-
7	MEN	G8	72	7	-	2/7/8/10	-
7	MEN	F8	72	7	-	2/7/8/10	-
5	MEN	H7	72	5	-	6/7/8/10	-
7	MEN	TB	72	7	-	6/7/8/10	-
7	MEN	LL	72	7,29	-	4/7/8/10	-
21	MEN	qP	71	21	-	4/7/8/10	-
7	MEN	V7	72	7	-	6/7/8/10	-
7	MEN	eM	72	7	-	6/7/8/10	-
7	MEN	KD	72	7	-	5/7/8/10	-
7	MEN	m7	72	7	-	6/7/8/10	-
7	MEN	FO	72	7	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	NL	72	7,29	-	4/7/8/10	-
7	MEN	H3	72	7	-	4/7/8/10	-
7	MEN	g1	72	7	-	6/7/8/10	-
5	MEN	L1	72	5	-	2/7/8/10	-
7	MEN	HN	72	7	-	2/7/8/10	-
5	MEN	JK	72	5	-	2/7/8/10	-
21	MEN	fP	71	21	-	4/7/8/10	-
7	MEN	B5	72	7	-	2/7/8/10	-
7	MEN	DJ	72	7,29	-	4/7/8/10	-
21	MEN	UP	71	21	-	4/7/8/10	-
7	MEN	JC	72	7	-	2/7/8/10	-
7	MEN	I4	72	7	-	5/7/8/10	-
7	MEN	FQ	72	7	-	4/7/8/10	-
7	MEN	LN	72	7	-	2/7/8/10	-
7	MEN	hL	72	7,29	-	4/7/8/10	-
7	MEN	BG	72	7	-	4/7/8/10	-
7	MEN	PK	72	7	-	6/7/8/10	-
7	MEN	FJ	72	7,29	-	4/7/8/10	-
7	MEN	XM	72	7	-	6/7/8/10	-
7	MEN	MO	72	7	-	2/7/8/10	-
5	MEN	F7	72	5	-	4/7/8/10	-
7	MEN	FM	72	7	-	6/7/8/10	-
7	MEN	e1	72	7	-	6/7/8/10	-
7	MEN	RI	72	7	-	6/7/8/10	-
5	MEN	N1	72	5	-	2/7/8/10	-
7	MEN	R7	72	7	-	6/7/8/10	-
7	MEN	JB	72	7	-	6/7/8/10	-
7	MEN	rJ	72	7,29	-	4/7/8/10	-
7	MEN	A5	72	7	-	6/7/8/10	-
7	MEN	DQ	72	7	-	4/7/8/10	-
7	MEN	c9	72	7	-	6/7/8/10	-
7	MEN	C5	72	7	-	6/7/8/10	-
5	MEN	N9	72	5	-	4/7/8/10	-
7	MEN	JE	72	7	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	HQ	72	7	-	4/7/8/10	-
7	MEN	tL	72	7,29	-	4/7/8/10	-
5	MEN	J7	72	5	-	4/7/8/10	-
7	MEN	VB	72	7	-	6/7/8/10	-
7	MEN	LB	72	7	-	6/7/8/10	-
21	MEN	DP	71	21	-	2/7/8/10	-
7	MEN	VI	72	7	-	6/7/8/10	-
7	MEN	LC	72	7	-	2/7/8/10	-
7	MEN	T1	72	7	-	6/7/8/10	-
7	MEN	e7	72	7	-	6/7/8/10	-
7	MEN	aI	72	7	-	6/7/8/10	-
7	MEN	FN	72	7	-	2/7/8/10	-
7	MEN	DC	72	7	-	2/7/8/10	-
21	MEN	IP	71	21	-	2/7/8/10	-
7	MEN	BL	72	7,29	-	4/7/8/10	-
7	MEN	DM	72	7	-	6/7/8/10	-
7	MEN	DG	72	7	-	4/7/8/10	-
7	MEN	eB	72	7	-	6/7/8/10	-
7	MEN	G4	72	7	-	5/7/8/10	-
7	MEN	JA	72	7	-	2/7/8/10	-
21	MEN	kP	71	21	-	6/7/8/10	-
7	MEN	HJ	72	7	-	4/7/8/10	-
7	MEN	L5	72	7	-	2/7/8/10	-
7	MEN	NM	72	7	-	6/7/8/10	-
7	MEN	TJ	72	7,29	-	4/7/8/10	-
7	MEN	k7	72	7	-	6/7/8/10	-
7	MEN	JO	72	7	-	4/7/8/10	-
7	MEN	ZJ	72	7,29	-	4/7/8/10	-
7	MEN	cK	72	7	-	6/7/8/10	-
5	MEN	FF	72	5	-	4/7/8/10	-
7	MEN	RB	72	7	-	6/7/8/10	-
7	MEN	gK	72	7	-	6/7/8/10	-
7	MEN	c1	72	7	-	6/7/8/10	-
7	MEN	JL	72	7,29	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	i7	72	7	-	6/7/8/10	-
5	MEN	D1	72	5	-	2/7/8/10	-
7	MEN	JJ	72	7,29	-	4/7/8/10	-
7	MEN	NO	72	7	-	2/7/8/10	-
5	MEN	H1	72	5	-	2/7/8/10	-
7	MEN	V2	72	7	-	3/7/8/10	-
21	MEN	BP	71	21	-	4/7/8/10	-
7	MEN	B3	72	7	-	4/7/8/10	-
7	MEN	nJ	72	7,29	-	4/7/8/10	-
7	MEN	PB	72	7	-	6/7/8/10	-
7	MEN	G5	72	7	-	2/7/8/10	-
7	MEN	gI	72	7	-	6/7/8/10	-
7	MEN	bJ	72	7,29	-	4/7/8/10	-
7	MEN	T9	72	7	-	6/7/8/10	-
7	MEN	LO	72	7	-	4/7/8/10	-
7	MEN	RK	72	7	-	6/7/8/10	-
7	MEN	I8	72	7	-	6/7/8/10	-
7	MEN	M4	72	7	-	5/7/8/10	-
7	MEN	A8	72	7	-	6/7/8/10	-
7	MEN	g7	72	7	-	6/7/8/10	-
7	MEN	T7	72	7	-	6/7/8/10	-
5	MEN	F1	72	5	-	2/7/8/10	-
7	MEN	K5	72	7	-	6/7/8/10	-
5	MEN	JI	72	5	-	4/7/8/10	-
5	MEN	LF	72	5	-	4/7/8/10	-
7	MEN	PL	72	7,29	-	4/7/8/10	-
7	MEN	YI	72	7	-	6/7/8/10	-
7	MEN	VM	72	7	-	6/7/8/10	-
5	MEN	LI	72	5	-	4/7/8/10	-
7	MEN	dJ	72	7,29	-	4/7/8/10	-
7	MEN	PF	72	7	-	6/7/8/10	-
7	MEN	kF	72	7	-	6/7/8/10	-
7	MEN	g9	72	7	-	6/7/8/10	-
7	MEN	P2	72	7	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	MEN	MP	71	21	-	6/7/8/10	-
7	MEN	DB	72	7	-	6/7/8/10	-
7	MEN	XJ	72	7,29	-	4/7/8/10	-
7	MEN	K8	72	7	-	6/7/8/10	-
21	MEN	uP	71	21	-	5/7/8/10	-
7	MEN	i9	72	7	-	6/7/8/10	-
7	MEN	BE	72	7	-	2/7/8/10	-
5	MEN	LK	72	5	-	2/7/8/10	-
7	MEN	TK	72	7	-	6/7/8/10	-
7	MEN	BQ	72	7	-	4/7/8/10	-
7	MEN	BA	72	7	-	2/7/8/10	-
7	MEN	FA	72	7	-	2/7/8/10	-
7	MEN	DN	72	7	-	2/7/8/10	-
7	MEN	jL	72	7,29	-	4/7/8/10	-
5	MEN	NI	72	5	-	4/7/8/10	-
7	MEN	pL	72	7,29	-	4/7/8/10	-
7	MEN	c7	72	7	-	6/7/8/10	-
7	MEN	ZM	72	7	-	6/7/8/10	-
5	MEN	D7	72	5	-	2/7/8/10	-
7	MEN	YF	72	7	-	6/7/8/10	-
7	MEN	K4	72	7	-	5/7/8/10	-
5	MEN	DK	72	5	-	2/7/8/10	-
7	MEN	cI	72	7	-	6/7/8/10	-
7	MEN	mI	72	7	-	6/7/8/10	-
7	MEN	R2	72	7	-	3/7/8/10	-
7	MEN	FC	72	7	-	2/7/8/10	-
7	MEN	MD	72	7	-	5/7/8/10	-
7	MEN	HB	72	7	-	6/7/8/10	-
21	MEN	jP	71	21	-	6/7/8/10	-
7	MEN	I5	72	7	-	6/7/8/10	-
7	MEN	H8	72	7	-	2/7/8/10	-
5	MEN	J1	72	5	-	2/7/8/10	-
7	MEN	mM	72	7	-	6/7/8/10	-
7	MEN	D3	72	7	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	N3	72	7	-	2/7/8/10	-
7	MEN	XR	72	7	-	3/7/8/10	-
7	MEN	eK	72	7	-	6/7/8/10	-
7	MEN	F3	72	7	-	4/7/8/10	-
5	MEN	HF	72	5	-	4/7/8/10	-
5	MEN	NK	72	5	-	2/7/8/10	-
7	MEN	VL	72	7,29	-	4/7/8/10	-
7	MEN	LQ	72	7	-	4/7/8/10	-
5	MEN	NF	72	5	-	4/7/8/10	-
5	MEN	FI	72	5	-	4/7/8/10	-
7	MEN	P9	72	7	-	6/7/8/10	-
5	MEN	D9	72	5	-	2/7/8/10	-
7	MEN	kM	72	7	-	6/7/8/10	-
7	MEN	P1	72	7	-	6/7/8/10	-
7	MEN	RM	72	7	-	6/7/8/10	-
7	MEN	XL	72	7,29	-	4/7/8/10	-
7	MEN	TL	72	7,29	-	4/7/8/10	-
7	MEN	M3	72	7	-	2/7/8/10	-
7	MEN	TR	72	7	-	3/7/8/10	-
21	MEN	HP	71	21	-	4/7/8/10	-
7	MEN	a7	72	7	-	6/7/8/10	-
7	MEN	JQ	72	7	-	4/7/8/10	-
7	MEN	DE	72	7	-	2/7/8/10	-
21	MEN	sP	71	21	-	2/7/8/10	-
7	MEN	hJ	72	7,29	-	4/7/8/10	-
7	MEN	N2	72	7	-	3/7/8/10	-
7	MEN	iF	72	7	-	6/7/8/10	-
7	MEN	BN	72	7	-	2/7/8/10	-
7	MEN	T2	72	7	-	3/7/8/10	-
21	MEN	nP	71	21	-	4/7/8/10	-
7	MEN	m9	72	7	-	6/7/8/10	-
7	MEN	P7	72	7	-	6/7/8/10	-
7	MEN	B8	72	7	-	2/7/8/10	-
7	MEN	RL	72	7,29	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	lL	72	7,29	-	4/7/8/10	-
7	MEN	R9	72	7	-	6/7/8/10	-
7	MEN	LA	72	7	-	2/7/8/10	-
7	MEN	pJ	72	7,29	-	4/7/8/10	-
7	MEN	a1	72	7	-	6/7/8/10	-
21	MEN	dP	71	21	-	2/7/8/10	-
5	MEN	N7	72	5	-	4/7/8/10	-
5	MEN	J9	72	5	-	4/7/8/10	-
7	MEN	R1	72	7	-	6/7/8/10	-
21	MEN	wP	71	21	-	4/7/8/10	-
7	MEN	JN	72	7	-	2/7/8/10	-
7	MEN	RF	72	7	-	6/7/8/10	-
7	MEN	JG	72	7	-	4/7/8/10	-
7	MEN	JM	72	7	-	6/7/8/10	-
7	MEN	mK	72	7	-	6/7/8/10	-
21	MEN	FP	71	21	-	6/7/8/10	-
5	MEN	DF	72	5,1	-	5/7/8/10	-
7	MEN	X2	72	7	-	3/7/8/10	-
21	MEN	hP	71	21	-	5/7/8/10	-
7	MEN	eF	72	7	-	6/7/8/10	-
21	MEN	SP	71	21	-	5/7/8/10	-
7	MEN	RR	72	7	-	3/7/8/10	-
7	MEN	ZL	72	7,29	-	4/7/8/10	-
7	MEN	LM	72	7	-	6/7/8/10	-
7	MEN	FE	72	7	-	2/7/8/10	-
5	MEN	F9	72	5	-	4/7/8/10	-
21	MEN	QP	71	21	-	2/7/8/10	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	LP	71	MEN	O-C	21.59	2.06	1.19
21	kP	71	MEN	O-C	21.59	2.06	1.19
21	jP	71	MEN	O-C	21.58	2.06	1.19
21	jP	71	MEN	CB-CA	-5.16	1.42	1.53
21	kP	71	MEN	CB-CA	-5.16	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	LP	71	MEN	CB-CA	-5.16	1.42	1.53
21	kP	71	MEN	CB-CG	3.65	1.60	1.51
21	LP	71	MEN	CB-CG	3.63	1.59	1.51
21	jP	71	MEN	CB-CG	3.61	1.59	1.51
21	IP	71	MEN	O-C	2.91	1.31	1.19
21	OP	71	MEN	O-C	2.87	1.31	1.19
21	qP	71	MEN	O-C	2.87	1.31	1.19
21	nP	71	MEN	O-C	2.87	1.31	1.19
21	BP	71	MEN	O-C	2.87	1.31	1.19
21	HP	71	MEN	O-C	2.86	1.31	1.19
21	fP	71	MEN	O-C	2.85	1.31	1.19
21	DP	71	MEN	O-C	2.84	1.31	1.19
21	hP	71	MEN	O-C	2.84	1.31	1.19
21	dP	71	MEN	O-C	2.83	1.31	1.19
21	oP	71	MEN	O-C	2.82	1.31	1.19
21	MP	71	MEN	O-C	2.81	1.31	1.19
21	FP	71	MEN	O-C	2.80	1.31	1.19
21	kP	71	MEN	CE2-ND2	2.47	1.50	1.45
21	jP	71	MEN	CE2-ND2	2.44	1.49	1.45
21	LP	71	MEN	CE2-ND2	2.40	1.49	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	jP	71	MEN	CB-CA-C	-19.45	75.00	111.47
21	LP	71	MEN	CB-CA-C	-19.45	75.00	111.47
21	kP	71	MEN	CB-CA-C	-19.44	75.03	111.47
21	LP	71	MEN	CB-CG-ND2	14.88	135.50	115.48
21	kP	71	MEN	CB-CG-ND2	14.88	135.50	115.48
21	jP	71	MEN	CB-CG-ND2	14.86	135.47	115.48
21	LP	71	MEN	CA-CB-CG	-11.44	80.14	112.70
21	jP	71	MEN	CA-CB-CG	-11.44	80.16	112.70
21	kP	71	MEN	CA-CB-CG	-11.44	80.16	112.70
21	jP	71	MEN	OD1-CG-CB	10.17	136.40	121.50
21	LP	71	MEN	OD1-CG-CB	10.13	136.34	121.50
21	kP	71	MEN	OD1-CG-CB	10.13	136.33	121.50
21	kP	71	MEN	OD1-CG-ND2	-9.27	74.08	122.36
21	jP	71	MEN	OD1-CG-ND2	-9.27	74.10	122.36
21	LP	71	MEN	OD1-CG-ND2	-9.27	74.11	122.36
7	TR	72	MEN	CA-CB-CG	-2.49	105.61	112.70
7	PR	72	MEN	CA-CB-CG	-2.48	105.65	112.70
7	P2	72	MEN	CA-CB-CG	-2.47	105.66	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N2	72	MEN	CA-CB-CG	-2.47	105.66	112.70
7	NR	72	MEN	CA-CB-CG	-2.47	105.66	112.70
7	RR	72	MEN	CA-CB-CG	-2.47	105.67	112.70
7	T2	72	MEN	CA-CB-CG	-2.47	105.68	112.70
7	R2	72	MEN	CA-CB-CG	-2.46	105.70	112.70
7	V2	72	MEN	CA-CB-CG	-2.46	105.70	112.70
7	VR	72	MEN	CA-CB-CG	-2.46	105.70	112.70
7	X2	72	MEN	CA-CB-CG	-2.46	105.70	112.70
7	XR	72	MEN	CA-CB-CG	-2.45	105.72	112.70
21	BP	71	MEN	CA-CB-CG	-2.45	105.73	112.70

There are no chirality outliers.

All (1368) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P1	72	MEN	C-CA-CB-CG
7	R1	72	MEN	C-CA-CB-CG
7	T1	72	MEN	C-CA-CB-CG
7	V1	72	MEN	C-CA-CB-CG
7	Y1	72	MEN	C-CA-CB-CG
7	a1	72	MEN	C-CA-CB-CG
7	c1	72	MEN	C-CA-CB-CG
7	e1	72	MEN	C-CA-CB-CG
7	g1	72	MEN	C-CA-CB-CG
7	i1	72	MEN	C-CA-CB-CG
7	k1	72	MEN	C-CA-CB-CG
7	m1	72	MEN	C-CA-CB-CG
7	N2	72	MEN	CB-CG-ND2-CE2
7	P2	72	MEN	CB-CG-ND2-CE2
7	R2	72	MEN	CB-CG-ND2-CE2
7	T2	72	MEN	CB-CG-ND2-CE2
7	V2	72	MEN	CB-CG-ND2-CE2
7	X2	72	MEN	CB-CG-ND2-CE2
7	C4	72	MEN	O-C-CA-CB
7	C4	72	MEN	CB-CG-ND2-CE2
7	E4	72	MEN	O-C-CA-CB
7	E4	72	MEN	CB-CG-ND2-CE2
7	G4	72	MEN	O-C-CA-CB
7	G4	72	MEN	CB-CG-ND2-CE2
7	I4	72	MEN	O-C-CA-CB
7	I4	72	MEN	CB-CG-ND2-CE2
7	K4	72	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
7	K4	72	MEN	CB-CG-ND2-CE2
7	M4	72	MEN	O-C-CA-CB
7	M4	72	MEN	CB-CG-ND2-CE2
7	B5	72	MEN	CB-CG-ND2-CE2
7	B5	72	MEN	OD1-CG-ND2-CE2
7	F5	72	MEN	CB-CG-ND2-CE2
7	F5	72	MEN	OD1-CG-ND2-CE2
7	G5	72	MEN	CB-CG-ND2-CE2
7	G5	72	MEN	OD1-CG-ND2-CE2
7	H5	72	MEN	CB-CG-ND2-CE2
7	H5	72	MEN	OD1-CG-ND2-CE2
7	I5	72	MEN	CB-CG-ND2-CE2
7	K5	72	MEN	CB-CG-ND2-CE2
7	L5	72	MEN	CB-CG-ND2-CE2
7	L5	72	MEN	OD1-CG-ND2-CE2
7	A5	72	MEN	CB-CG-ND2-CE2
7	C5	72	MEN	CB-CG-ND2-CE2
5	D7	72	MEN	CB-CG-ND2-CE2
5	F7	72	MEN	C-CA-CB-CG
5	H7	72	MEN	C-CA-CB-CG
5	H7	72	MEN	CB-CG-ND2-CE2
5	J7	72	MEN	C-CA-CB-CG
7	P7	72	MEN	C-CA-CB-CG
7	R7	72	MEN	C-CA-CB-CG
7	T7	72	MEN	C-CA-CB-CG
7	V7	72	MEN	C-CA-CB-CG
7	Y7	72	MEN	C-CA-CB-CG
7	a7	72	MEN	C-CA-CB-CG
7	c7	72	MEN	C-CA-CB-CG
7	e7	72	MEN	C-CA-CB-CG
7	g7	72	MEN	C-CA-CB-CG
7	i7	72	MEN	C-CA-CB-CG
7	k7	72	MEN	C-CA-CB-CG
7	m7	72	MEN	C-CA-CB-CG
7	B8	72	MEN	CB-CG-ND2-CE2
7	B8	72	MEN	OD1-CG-ND2-CE2
7	F8	72	MEN	CB-CG-ND2-CE2
7	F8	72	MEN	OD1-CG-ND2-CE2
7	G8	72	MEN	CB-CG-ND2-CE2
7	G8	72	MEN	OD1-CG-ND2-CE2
7	H8	72	MEN	CB-CG-ND2-CE2
7	H8	72	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	I8	72	MEN	CB-CG-ND2-CE2
7	K8	72	MEN	CB-CG-ND2-CE2
7	L8	72	MEN	CB-CG-ND2-CE2
7	L8	72	MEN	OD1-CG-ND2-CE2
7	A8	72	MEN	CB-CG-ND2-CE2
7	C8	72	MEN	CB-CG-ND2-CE2
5	D9	72	MEN	CB-CG-ND2-CE2
5	F9	72	MEN	C-CA-CB-CG
5	H9	72	MEN	C-CA-CB-CG
5	H9	72	MEN	CB-CG-ND2-CE2
5	J9	72	MEN	C-CA-CB-CG
7	P9	72	MEN	C-CA-CB-CG
7	R9	72	MEN	C-CA-CB-CG
7	T9	72	MEN	C-CA-CB-CG
7	V9	72	MEN	C-CA-CB-CG
7	Y9	72	MEN	C-CA-CB-CG
7	a9	72	MEN	C-CA-CB-CG
7	c9	72	MEN	C-CA-CB-CG
7	e9	72	MEN	C-CA-CB-CG
7	g9	72	MEN	C-CA-CB-CG
7	i9	72	MEN	C-CA-CB-CG
7	k9	72	MEN	C-CA-CB-CG
7	m9	72	MEN	C-CA-CB-CG
7	DB	72	MEN	C-CA-CB-CG
7	DB	72	MEN	CB-CG-ND2-CE2
7	FB	72	MEN	C-CA-CB-CG
7	FB	72	MEN	CB-CG-ND2-CE2
7	HB	72	MEN	C-CA-CB-CG
7	HB	72	MEN	CB-CG-ND2-CE2
7	JB	72	MEN	C-CA-CB-CG
7	JB	72	MEN	CB-CG-ND2-CE2
7	LB	72	MEN	C-CA-CB-CG
7	LB	72	MEN	CB-CG-ND2-CE2
7	NB	72	MEN	C-CA-CB-CG
7	NB	72	MEN	CB-CG-ND2-CE2
7	PB	72	MEN	C-CA-CB-CG
7	PB	72	MEN	CB-CG-ND2-CE2
7	RB	72	MEN	C-CA-CB-CG
7	RB	72	MEN	CB-CG-ND2-CE2
7	TB	72	MEN	C-CA-CB-CG
7	TB	72	MEN	CB-CG-ND2-CE2
7	VB	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	VB	72	MEN	CB-CG-ND2-CE2
7	XB	72	MEN	C-CA-CB-CG
7	XB	72	MEN	CB-CG-ND2-CE2
7	ZB	72	MEN	C-CA-CB-CG
7	ZB	72	MEN	CB-CG-ND2-CE2
7	cB	72	MEN	C-CA-CB-CG
7	cB	72	MEN	CB-CG-ND2-CE2
7	eB	72	MEN	C-CA-CB-CG
7	eB	72	MEN	CB-CG-ND2-CE2
7	gB	72	MEN	C-CA-CB-CG
7	gB	72	MEN	CB-CG-ND2-CE2
7	iB	72	MEN	C-CA-CB-CG
7	iB	72	MEN	CB-CG-ND2-CE2
7	kB	72	MEN	C-CA-CB-CG
7	kB	72	MEN	CB-CG-ND2-CE2
7	mB	72	MEN	C-CA-CB-CG
7	mB	72	MEN	CB-CG-ND2-CE2
7	BC	72	MEN	C-CA-CB-CG
7	DC	72	MEN	C-CA-CB-CG
7	FC	72	MEN	C-CA-CB-CG
7	HC	72	MEN	C-CA-CB-CG
7	JC	72	MEN	C-CA-CB-CG
7	LC	72	MEN	C-CA-CB-CG
7	CD	72	MEN	O-C-CA-CB
7	CD	72	MEN	CB-CG-ND2-CE2
7	ED	72	MEN	O-C-CA-CB
7	ED	72	MEN	CB-CG-ND2-CE2
7	GD	72	MEN	O-C-CA-CB
7	GD	72	MEN	CB-CG-ND2-CE2
7	ID	72	MEN	O-C-CA-CB
7	ID	72	MEN	CB-CG-ND2-CE2
7	KD	72	MEN	O-C-CA-CB
7	KD	72	MEN	CB-CG-ND2-CE2
7	MD	72	MEN	O-C-CA-CB
7	MD	72	MEN	CB-CG-ND2-CE2
7	BE	72	MEN	C-CA-CB-CG
7	DE	72	MEN	C-CA-CB-CG
7	FE	72	MEN	C-CA-CB-CG
7	HE	72	MEN	C-CA-CB-CG
7	JE	72	MEN	C-CA-CB-CG
7	LE	72	MEN	C-CA-CB-CG
5	DF	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
5	DF	72	MEN	CB-CG-ND2-CE2
5	DF	72	MEN	OD1-CG-ND2-CE2
5	FF	72	MEN	C-CA-CB-CG
5	FF	72	MEN	CB-CG-ND2-CE2
5	FF	72	MEN	OD1-CG-ND2-CE2
5	HF	72	MEN	C-CA-CB-CG
5	HF	72	MEN	CB-CG-ND2-CE2
5	HF	72	MEN	OD1-CG-ND2-CE2
5	JF	72	MEN	C-CA-CB-CG
5	JF	72	MEN	CB-CG-ND2-CE2
5	JF	72	MEN	OD1-CG-ND2-CE2
5	LF	72	MEN	C-CA-CB-CG
5	LF	72	MEN	CB-CG-ND2-CE2
5	LF	72	MEN	OD1-CG-ND2-CE2
5	NF	72	MEN	C-CA-CB-CG
5	NF	72	MEN	CB-CG-ND2-CE2
5	NF	72	MEN	OD1-CG-ND2-CE2
7	BG	72	MEN	C-CA-CB-CG
7	DG	72	MEN	C-CA-CB-CG
7	FG	72	MEN	C-CA-CB-CG
7	HG	72	MEN	C-CA-CB-CG
7	JG	72	MEN	C-CA-CB-CG
7	LG	72	MEN	C-CA-CB-CG
5	DI	72	MEN	C-CA-CB-CG
5	DI	72	MEN	CB-CG-ND2-CE2
5	DI	72	MEN	OD1-CG-ND2-CE2
5	FI	72	MEN	C-CA-CB-CG
5	FI	72	MEN	CB-CG-ND2-CE2
5	FI	72	MEN	OD1-CG-ND2-CE2
5	HI	72	MEN	C-CA-CB-CG
5	HI	72	MEN	CB-CG-ND2-CE2
5	HI	72	MEN	OD1-CG-ND2-CE2
5	JI	72	MEN	C-CA-CB-CG
5	JI	72	MEN	CB-CG-ND2-CE2
5	JI	72	MEN	OD1-CG-ND2-CE2
5	LI	72	MEN	C-CA-CB-CG
5	LI	72	MEN	CB-CG-ND2-CE2
5	LI	72	MEN	OD1-CG-ND2-CE2
5	NI	72	MEN	C-CA-CB-CG
5	NI	72	MEN	CB-CG-ND2-CE2
5	NI	72	MEN	OD1-CG-ND2-CE2
7	BJ	72	MEN	CB-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	BJ	72	MEN	OD1-CG-ND2-CE2
7	DJ	72	MEN	CB-CG-ND2-CE2
7	DJ	72	MEN	OD1-CG-ND2-CE2
7	FJ	72	MEN	CB-CG-ND2-CE2
7	FJ	72	MEN	OD1-CG-ND2-CE2
7	HJ	72	MEN	C-CA-CB-CG
7	HJ	72	MEN	CB-CG-ND2-CE2
7	JJ	72	MEN	CB-CG-ND2-CE2
7	JJ	72	MEN	OD1-CG-ND2-CE2
7	LJ	72	MEN	CB-CG-ND2-CE2
7	LJ	72	MEN	OD1-CG-ND2-CE2
7	NJ	72	MEN	CB-CG-ND2-CE2
7	NJ	72	MEN	OD1-CG-ND2-CE2
7	PJ	72	MEN	CB-CG-ND2-CE2
7	PJ	72	MEN	OD1-CG-ND2-CE2
7	RJ	72	MEN	CB-CG-ND2-CE2
7	RJ	72	MEN	OD1-CG-ND2-CE2
7	TJ	72	MEN	CB-CG-ND2-CE2
7	TJ	72	MEN	OD1-CG-ND2-CE2
7	VJ	72	MEN	CB-CG-ND2-CE2
7	VJ	72	MEN	OD1-CG-ND2-CE2
7	XJ	72	MEN	CB-CG-ND2-CE2
7	XJ	72	MEN	OD1-CG-ND2-CE2
7	ZJ	72	MEN	CB-CG-ND2-CE2
7	ZJ	72	MEN	OD1-CG-ND2-CE2
7	bJ	72	MEN	CB-CG-ND2-CE2
7	bJ	72	MEN	OD1-CG-ND2-CE2
7	dJ	72	MEN	CB-CG-ND2-CE2
7	dJ	72	MEN	OD1-CG-ND2-CE2
7	fJ	72	MEN	CB-CG-ND2-CE2
7	fJ	72	MEN	OD1-CG-ND2-CE2
7	hJ	72	MEN	CB-CG-ND2-CE2
7	hJ	72	MEN	OD1-CG-ND2-CE2
7	jJ	72	MEN	CB-CG-ND2-CE2
7	jJ	72	MEN	OD1-CG-ND2-CE2
7	lJ	72	MEN	CB-CG-ND2-CE2
7	lJ	72	MEN	OD1-CG-ND2-CE2
7	nJ	72	MEN	CB-CG-ND2-CE2
7	nJ	72	MEN	OD1-CG-ND2-CE2
7	pJ	72	MEN	CB-CG-ND2-CE2
7	pJ	72	MEN	OD1-CG-ND2-CE2
7	rJ	72	MEN	CB-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	rJ	72	MEN	OD1-CG-ND2-CE2
7	tJ	72	MEN	CB-CG-ND2-CE2
7	tJ	72	MEN	OD1-CG-ND2-CE2
7	vJ	72	MEN	CB-CG-ND2-CE2
7	vJ	72	MEN	OD1-CG-ND2-CE2
7	PK	72	MEN	C-CA-CB-CG
7	RK	72	MEN	C-CA-CB-CG
7	TK	72	MEN	C-CA-CB-CG
7	VK	72	MEN	C-CA-CB-CG
7	YK	72	MEN	C-CA-CB-CG
7	aK	72	MEN	C-CA-CB-CG
7	cK	72	MEN	C-CA-CB-CG
7	eK	72	MEN	C-CA-CB-CG
7	gK	72	MEN	C-CA-CB-CG
7	iK	72	MEN	C-CA-CB-CG
7	kK	72	MEN	C-CA-CB-CG
7	mK	72	MEN	C-CA-CB-CG
7	BL	72	MEN	CB-CG-ND2-CE2
7	BL	72	MEN	OD1-CG-ND2-CE2
7	DL	72	MEN	CB-CG-ND2-CE2
7	DL	72	MEN	OD1-CG-ND2-CE2
7	FL	72	MEN	CB-CG-ND2-CE2
7	FL	72	MEN	OD1-CG-ND2-CE2
7	JL	72	MEN	CB-CG-ND2-CE2
7	JL	72	MEN	OD1-CG-ND2-CE2
7	LL	72	MEN	CB-CG-ND2-CE2
7	LL	72	MEN	OD1-CG-ND2-CE2
7	NL	72	MEN	CB-CG-ND2-CE2
7	NL	72	MEN	OD1-CG-ND2-CE2
7	PL	72	MEN	CB-CG-ND2-CE2
7	PL	72	MEN	OD1-CG-ND2-CE2
7	RL	72	MEN	CB-CG-ND2-CE2
7	RL	72	MEN	OD1-CG-ND2-CE2
7	TL	72	MEN	CB-CG-ND2-CE2
7	TL	72	MEN	OD1-CG-ND2-CE2
7	VL	72	MEN	CB-CG-ND2-CE2
7	VL	72	MEN	OD1-CG-ND2-CE2
7	XL	72	MEN	CB-CG-ND2-CE2
7	XL	72	MEN	OD1-CG-ND2-CE2
7	ZL	72	MEN	CB-CG-ND2-CE2
7	ZL	72	MEN	OD1-CG-ND2-CE2
7	bL	72	MEN	CB-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	bL	72	MEN	OD1-CG-ND2-CE2
7	dL	72	MEN	CB-CG-ND2-CE2
7	dL	72	MEN	OD1-CG-ND2-CE2
7	fL	72	MEN	CB-CG-ND2-CE2
7	fL	72	MEN	OD1-CG-ND2-CE2
7	hL	72	MEN	CB-CG-ND2-CE2
7	hL	72	MEN	OD1-CG-ND2-CE2
7	jL	72	MEN	CB-CG-ND2-CE2
7	jL	72	MEN	OD1-CG-ND2-CE2
7	lL	72	MEN	CB-CG-ND2-CE2
7	lL	72	MEN	OD1-CG-ND2-CE2
7	nL	72	MEN	CB-CG-ND2-CE2
7	nL	72	MEN	OD1-CG-ND2-CE2
7	pL	72	MEN	CB-CG-ND2-CE2
7	pL	72	MEN	OD1-CG-ND2-CE2
7	rL	72	MEN	CB-CG-ND2-CE2
7	rL	72	MEN	OD1-CG-ND2-CE2
7	tL	72	MEN	CB-CG-ND2-CE2
7	tL	72	MEN	OD1-CG-ND2-CE2
7	vL	72	MEN	CB-CG-ND2-CE2
7	vL	72	MEN	OD1-CG-ND2-CE2
7	DM	72	MEN	C-CA-CB-CG
7	DM	72	MEN	CB-CG-ND2-CE2
7	FM	72	MEN	C-CA-CB-CG
7	FM	72	MEN	CB-CG-ND2-CE2
7	HM	72	MEN	C-CA-CB-CG
7	HM	72	MEN	CB-CG-ND2-CE2
7	JM	72	MEN	C-CA-CB-CG
7	JM	72	MEN	CB-CG-ND2-CE2
7	LM	72	MEN	C-CA-CB-CG
7	LM	72	MEN	CB-CG-ND2-CE2
7	NM	72	MEN	C-CA-CB-CG
7	NM	72	MEN	CB-CG-ND2-CE2
7	PM	72	MEN	C-CA-CB-CG
7	PM	72	MEN	CB-CG-ND2-CE2
7	RM	72	MEN	C-CA-CB-CG
7	RM	72	MEN	CB-CG-ND2-CE2
7	TM	72	MEN	C-CA-CB-CG
7	TM	72	MEN	CB-CG-ND2-CE2
7	VM	72	MEN	C-CA-CB-CG
7	VM	72	MEN	CB-CG-ND2-CE2
7	XM	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	XM	72	MEN	CB-CG-ND2-CE2
7	ZM	72	MEN	C-CA-CB-CG
7	ZM	72	MEN	CB-CG-ND2-CE2
7	cM	72	MEN	C-CA-CB-CG
7	cM	72	MEN	CB-CG-ND2-CE2
7	eM	72	MEN	C-CA-CB-CG
7	eM	72	MEN	CB-CG-ND2-CE2
7	gM	72	MEN	C-CA-CB-CG
7	gM	72	MEN	CB-CG-ND2-CE2
7	iM	72	MEN	C-CA-CB-CG
7	iM	72	MEN	CB-CG-ND2-CE2
7	kM	72	MEN	C-CA-CB-CG
7	kM	72	MEN	CB-CG-ND2-CE2
7	mM	72	MEN	C-CA-CB-CG
7	mM	72	MEN	CB-CG-ND2-CE2
21	FP	71	MEN	C-CA-CB-CG
21	FP	71	MEN	CB-CG-ND2-CE2
21	BP	71	MEN	N-CA-CB-CG
21	BP	71	MEN	C-CA-CB-CG
21	BP	71	MEN	CB-CG-ND2-CE2
21	HP	71	MEN	CB-CG-ND2-CE2
21	LP	71	MEN	C-CA-CB-CG
21	LP	71	MEN	CB-CG-ND2-CE2
21	MP	71	MEN	C-CA-CB-CG
21	MP	71	MEN	CB-CG-ND2-CE2
21	OP	71	MEN	CB-CG-ND2-CE2
21	UP	71	MEN	C-CA-CB-CG
21	fP	71	MEN	C-CA-CB-CG
21	fP	71	MEN	CB-CG-ND2-CE2
21	hP	71	MEN	C-CA-CB-CG
21	hP	71	MEN	CB-CG-ND2-CE2
21	jP	71	MEN	C-CA-CB-CG
21	jP	71	MEN	CB-CG-ND2-CE2
21	kP	71	MEN	C-CA-CB-CG
21	kP	71	MEN	CB-CG-ND2-CE2
21	nP	71	MEN	CB-CG-ND2-CE2
21	oP	71	MEN	C-CA-CB-CG
21	oP	71	MEN	CB-CG-ND2-CE2
21	qP	71	MEN	CB-CG-ND2-CE2
21	uP	71	MEN	CB-CG-ND2-CE2
21	wP	71	MEN	C-CA-CB-CG
7	BQ	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	DQ	72	MEN	C-CA-CB-CG
7	FQ	72	MEN	C-CA-CB-CG
7	HQ	72	MEN	C-CA-CB-CG
7	JQ	72	MEN	C-CA-CB-CG
7	LQ	72	MEN	C-CA-CB-CG
7	NR	72	MEN	CB-CG-ND2-CE2
7	PR	72	MEN	CB-CG-ND2-CE2
7	RR	72	MEN	CB-CG-ND2-CE2
7	TR	72	MEN	CB-CG-ND2-CE2
7	VR	72	MEN	CB-CG-ND2-CE2
7	XR	72	MEN	CB-CG-ND2-CE2
21	LP	71	MEN	CA-CB-CG-ND2
21	jP	71	MEN	CA-CB-CG-ND2
21	kP	71	MEN	CA-CB-CG-ND2
7	C4	72	MEN	OD1-CG-ND2-CE2
7	E4	72	MEN	OD1-CG-ND2-CE2
7	G4	72	MEN	OD1-CG-ND2-CE2
7	I4	72	MEN	OD1-CG-ND2-CE2
7	K4	72	MEN	OD1-CG-ND2-CE2
7	M4	72	MEN	OD1-CG-ND2-CE2
7	I5	72	MEN	OD1-CG-ND2-CE2
7	K5	72	MEN	OD1-CG-ND2-CE2
7	A5	72	MEN	OD1-CG-ND2-CE2
7	C5	72	MEN	OD1-CG-ND2-CE2
5	H7	72	MEN	OD1-CG-ND2-CE2
5	N7	72	MEN	OD1-CG-ND2-CE2
7	I8	72	MEN	OD1-CG-ND2-CE2
7	K8	72	MEN	OD1-CG-ND2-CE2
7	A8	72	MEN	OD1-CG-ND2-CE2
7	C8	72	MEN	OD1-CG-ND2-CE2
5	H9	72	MEN	OD1-CG-ND2-CE2
5	N9	72	MEN	OD1-CG-ND2-CE2
7	CD	72	MEN	OD1-CG-ND2-CE2
7	ED	72	MEN	OD1-CG-ND2-CE2
7	GD	72	MEN	OD1-CG-ND2-CE2
7	ID	72	MEN	OD1-CG-ND2-CE2
7	KD	72	MEN	OD1-CG-ND2-CE2
7	MD	72	MEN	OD1-CG-ND2-CE2
7	HJ	72	MEN	OD1-CG-ND2-CE2
7	HL	72	MEN	OD1-CG-ND2-CE2
21	FP	71	MEN	OD1-CG-ND2-CE2
21	HP	71	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
21	LP	71	MEN	OD1-CG-ND2-CE2
21	MP	71	MEN	OD1-CG-ND2-CE2
21	OP	71	MEN	OD1-CG-ND2-CE2
21	hP	71	MEN	OD1-CG-ND2-CE2
21	jP	71	MEN	OD1-CG-ND2-CE2
21	kP	71	MEN	OD1-CG-ND2-CE2
21	nP	71	MEN	OD1-CG-ND2-CE2
21	uP	71	MEN	OD1-CG-ND2-CE2
7	P1	72	MEN	N-CA-CB-CG
7	R1	72	MEN	N-CA-CB-CG
7	T1	72	MEN	N-CA-CB-CG
7	V1	72	MEN	N-CA-CB-CG
7	Y1	72	MEN	N-CA-CB-CG
7	a1	72	MEN	N-CA-CB-CG
7	c1	72	MEN	N-CA-CB-CG
7	e1	72	MEN	N-CA-CB-CG
7	g1	72	MEN	N-CA-CB-CG
7	i1	72	MEN	N-CA-CB-CG
7	k1	72	MEN	N-CA-CB-CG
7	m1	72	MEN	N-CA-CB-CG
7	I5	72	MEN	N-CA-CB-CG
7	K5	72	MEN	N-CA-CB-CG
7	A5	72	MEN	N-CA-CB-CG
7	C5	72	MEN	N-CA-CB-CG
5	H7	72	MEN	N-CA-CB-CG
7	I8	72	MEN	N-CA-CB-CG
7	K8	72	MEN	N-CA-CB-CG
7	A8	72	MEN	N-CA-CB-CG
7	C8	72	MEN	N-CA-CB-CG
5	H9	72	MEN	N-CA-CB-CG
7	DB	72	MEN	N-CA-CB-CG
7	FB	72	MEN	N-CA-CB-CG
7	HB	72	MEN	N-CA-CB-CG
7	JB	72	MEN	N-CA-CB-CG
7	LB	72	MEN	N-CA-CB-CG
7	NB	72	MEN	N-CA-CB-CG
7	PB	72	MEN	N-CA-CB-CG
7	RB	72	MEN	N-CA-CB-CG
7	TB	72	MEN	N-CA-CB-CG
7	VB	72	MEN	N-CA-CB-CG
7	XB	72	MEN	N-CA-CB-CG
7	ZB	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	cB	72	MEN	N-CA-CB-CG
7	eB	72	MEN	N-CA-CB-CG
7	gB	72	MEN	N-CA-CB-CG
7	iB	72	MEN	N-CA-CB-CG
7	kB	72	MEN	N-CA-CB-CG
7	mB	72	MEN	N-CA-CB-CG
7	BC	72	MEN	N-CA-CB-CG
7	DC	72	MEN	N-CA-CB-CG
7	FC	72	MEN	N-CA-CB-CG
7	HC	72	MEN	N-CA-CB-CG
7	JC	72	MEN	N-CA-CB-CG
7	LC	72	MEN	N-CA-CB-CG
7	BE	72	MEN	N-CA-CB-CG
7	DE	72	MEN	N-CA-CB-CG
7	FE	72	MEN	N-CA-CB-CG
7	HE	72	MEN	N-CA-CB-CG
7	JE	72	MEN	N-CA-CB-CG
7	LE	72	MEN	N-CA-CB-CG
5	DF	72	MEN	N-CA-CB-CG
5	FF	72	MEN	N-CA-CB-CG
5	HF	72	MEN	N-CA-CB-CG
5	JF	72	MEN	N-CA-CB-CG
5	LF	72	MEN	N-CA-CB-CG
5	NF	72	MEN	N-CA-CB-CG
7	BG	72	MEN	N-CA-CB-CG
7	DG	72	MEN	N-CA-CB-CG
7	FG	72	MEN	N-CA-CB-CG
7	HG	72	MEN	N-CA-CB-CG
7	JG	72	MEN	N-CA-CB-CG
7	LG	72	MEN	N-CA-CB-CG
5	DI	72	MEN	N-CA-CB-CG
5	FI	72	MEN	N-CA-CB-CG
5	HI	72	MEN	N-CA-CB-CG
5	JI	72	MEN	N-CA-CB-CG
5	LI	72	MEN	N-CA-CB-CG
5	NI	72	MEN	N-CA-CB-CG
7	HJ	72	MEN	N-CA-CB-CG
7	PK	72	MEN	N-CA-CB-CG
7	RK	72	MEN	N-CA-CB-CG
7	TK	72	MEN	N-CA-CB-CG
7	VK	72	MEN	N-CA-CB-CG
7	YK	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	aK	72	MEN	N-CA-CB-CG
7	cK	72	MEN	N-CA-CB-CG
7	eK	72	MEN	N-CA-CB-CG
7	gK	72	MEN	N-CA-CB-CG
7	iK	72	MEN	N-CA-CB-CG
7	kK	72	MEN	N-CA-CB-CG
7	mK	72	MEN	N-CA-CB-CG
7	HL	72	MEN	N-CA-CB-CG
7	DM	72	MEN	N-CA-CB-CG
7	FM	72	MEN	N-CA-CB-CG
7	HM	72	MEN	N-CA-CB-CG
7	JM	72	MEN	N-CA-CB-CG
7	LM	72	MEN	N-CA-CB-CG
7	NM	72	MEN	N-CA-CB-CG
7	PM	72	MEN	N-CA-CB-CG
7	RM	72	MEN	N-CA-CB-CG
7	TM	72	MEN	N-CA-CB-CG
7	VM	72	MEN	N-CA-CB-CG
7	XM	72	MEN	N-CA-CB-CG
7	ZM	72	MEN	N-CA-CB-CG
7	cM	72	MEN	N-CA-CB-CG
7	eM	72	MEN	N-CA-CB-CG
7	gM	72	MEN	N-CA-CB-CG
7	iM	72	MEN	N-CA-CB-CG
7	kM	72	MEN	N-CA-CB-CG
7	mM	72	MEN	N-CA-CB-CG
21	FP	71	MEN	N-CA-CB-CG
21	LP	71	MEN	N-CA-CB-CG
21	MP	71	MEN	N-CA-CB-CG
21	fP	71	MEN	N-CA-CB-CG
21	hP	71	MEN	N-CA-CB-CG
21	jP	71	MEN	N-CA-CB-CG
21	kP	71	MEN	N-CA-CB-CG
21	oP	71	MEN	N-CA-CB-CG
7	BQ	72	MEN	N-CA-CB-CG
7	DQ	72	MEN	N-CA-CB-CG
7	FQ	72	MEN	N-CA-CB-CG
7	HQ	72	MEN	N-CA-CB-CG
7	JQ	72	MEN	N-CA-CB-CG
7	LQ	72	MEN	N-CA-CB-CG
5	N7	72	MEN	CB-CG-ND2-CE2
5	N9	72	MEN	CB-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	HL	72	MEN	CB-CG-ND2-CE2
7	N2	72	MEN	OD1-CG-ND2-CE2
7	P2	72	MEN	OD1-CG-ND2-CE2
7	R2	72	MEN	OD1-CG-ND2-CE2
7	T2	72	MEN	OD1-CG-ND2-CE2
7	V2	72	MEN	OD1-CG-ND2-CE2
7	X2	72	MEN	OD1-CG-ND2-CE2
5	D7	72	MEN	OD1-CG-ND2-CE2
5	D9	72	MEN	OD1-CG-ND2-CE2
7	DB	72	MEN	OD1-CG-ND2-CE2
7	FB	72	MEN	OD1-CG-ND2-CE2
7	HB	72	MEN	OD1-CG-ND2-CE2
7	JB	72	MEN	OD1-CG-ND2-CE2
7	LB	72	MEN	OD1-CG-ND2-CE2
7	NB	72	MEN	OD1-CG-ND2-CE2
7	PB	72	MEN	OD1-CG-ND2-CE2
7	RB	72	MEN	OD1-CG-ND2-CE2
7	TB	72	MEN	OD1-CG-ND2-CE2
7	VB	72	MEN	OD1-CG-ND2-CE2
7	XB	72	MEN	OD1-CG-ND2-CE2
7	ZB	72	MEN	OD1-CG-ND2-CE2
7	cB	72	MEN	OD1-CG-ND2-CE2
7	eB	72	MEN	OD1-CG-ND2-CE2
7	gB	72	MEN	OD1-CG-ND2-CE2
7	iB	72	MEN	OD1-CG-ND2-CE2
7	kB	72	MEN	OD1-CG-ND2-CE2
7	mB	72	MEN	OD1-CG-ND2-CE2
7	DM	72	MEN	OD1-CG-ND2-CE2
7	FM	72	MEN	OD1-CG-ND2-CE2
7	HM	72	MEN	OD1-CG-ND2-CE2
7	JM	72	MEN	OD1-CG-ND2-CE2
7	LM	72	MEN	OD1-CG-ND2-CE2
7	NM	72	MEN	OD1-CG-ND2-CE2
7	PM	72	MEN	OD1-CG-ND2-CE2
7	RM	72	MEN	OD1-CG-ND2-CE2
7	TM	72	MEN	OD1-CG-ND2-CE2
7	VM	72	MEN	OD1-CG-ND2-CE2
7	XM	72	MEN	OD1-CG-ND2-CE2
7	ZM	72	MEN	OD1-CG-ND2-CE2
7	cM	72	MEN	OD1-CG-ND2-CE2
7	eM	72	MEN	OD1-CG-ND2-CE2
7	gM	72	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	iM	72	MEN	OD1-CG-ND2-CE2
7	kM	72	MEN	OD1-CG-ND2-CE2
7	mM	72	MEN	OD1-CG-ND2-CE2
21	BP	71	MEN	OD1-CG-ND2-CE2
21	fP	71	MEN	OD1-CG-ND2-CE2
21	oP	71	MEN	OD1-CG-ND2-CE2
21	qP	71	MEN	OD1-CG-ND2-CE2
7	NR	72	MEN	OD1-CG-ND2-CE2
7	PR	72	MEN	OD1-CG-ND2-CE2
7	RR	72	MEN	OD1-CG-ND2-CE2
7	TR	72	MEN	OD1-CG-ND2-CE2
7	VR	72	MEN	OD1-CG-ND2-CE2
7	XR	72	MEN	OD1-CG-ND2-CE2
7	P1	72	MEN	CA-CB-CG-OD1
7	R1	72	MEN	CA-CB-CG-OD1
7	T1	72	MEN	CA-CB-CG-OD1
7	V1	72	MEN	CA-CB-CG-OD1
7	Y1	72	MEN	CA-CB-CG-OD1
7	a1	72	MEN	CA-CB-CG-OD1
7	c1	72	MEN	CA-CB-CG-OD1
7	e1	72	MEN	CA-CB-CG-OD1
7	g1	72	MEN	CA-CB-CG-OD1
7	i1	72	MEN	CA-CB-CG-OD1
7	k1	72	MEN	CA-CB-CG-OD1
7	m1	72	MEN	CA-CB-CG-OD1
7	B3	72	MEN	CA-CB-CG-OD1
7	D3	72	MEN	CA-CB-CG-OD1
7	F3	72	MEN	CA-CB-CG-OD1
7	H3	72	MEN	CA-CB-CG-OD1
7	J3	72	MEN	CA-CB-CG-OD1
7	L3	72	MEN	CA-CB-CG-OD1
7	M3	72	MEN	CA-CB-CG-OD1
7	N3	72	MEN	CA-CB-CG-OD1
5	F7	72	MEN	CA-CB-CG-OD1
5	L7	72	MEN	CA-CB-CG-OD1
5	N7	72	MEN	CA-CB-CG-OD1
5	F9	72	MEN	CA-CB-CG-OD1
5	L9	72	MEN	CA-CB-CG-OD1
5	N9	72	MEN	CA-CB-CG-OD1
7	FB	72	MEN	CA-CB-CG-OD1
7	JB	72	MEN	CA-CB-CG-OD1
7	PB	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
7	TB	72	MEN	CA-CB-CG-OD1
7	VB	72	MEN	CA-CB-CG-OD1
7	XB	72	MEN	CA-CB-CG-OD1
7	ZB	72	MEN	CA-CB-CG-OD1
7	eB	72	MEN	CA-CB-CG-OD1
7	gB	72	MEN	CA-CB-CG-OD1
7	iB	72	MEN	CA-CB-CG-OD1
7	kB	72	MEN	CA-CB-CG-OD1
7	PF	72	MEN	CA-CB-CG-OD1
7	RF	72	MEN	CA-CB-CG-OD1
7	TF	72	MEN	CA-CB-CG-OD1
7	VF	72	MEN	CA-CB-CG-OD1
7	YF	72	MEN	CA-CB-CG-OD1
7	aF	72	MEN	CA-CB-CG-OD1
7	cF	72	MEN	CA-CB-CG-OD1
7	eF	72	MEN	CA-CB-CG-OD1
7	gF	72	MEN	CA-CB-CG-OD1
7	iF	72	MEN	CA-CB-CG-OD1
7	kF	72	MEN	CA-CB-CG-OD1
7	mF	72	MEN	CA-CB-CG-OD1
7	BG	72	MEN	CA-CB-CG-OD1
7	DG	72	MEN	CA-CB-CG-OD1
7	FG	72	MEN	CA-CB-CG-OD1
7	HG	72	MEN	CA-CB-CG-OD1
7	JG	72	MEN	CA-CB-CG-OD1
7	LG	72	MEN	CA-CB-CG-OD1
7	PI	72	MEN	CA-CB-CG-OD1
7	RI	72	MEN	CA-CB-CG-OD1
7	TI	72	MEN	CA-CB-CG-OD1
7	VI	72	MEN	CA-CB-CG-OD1
7	YI	72	MEN	CA-CB-CG-OD1
7	aI	72	MEN	CA-CB-CG-OD1
7	cI	72	MEN	CA-CB-CG-OD1
7	eI	72	MEN	CA-CB-CG-OD1
7	gI	72	MEN	CA-CB-CG-OD1
7	iI	72	MEN	CA-CB-CG-OD1
7	kI	72	MEN	CA-CB-CG-OD1
7	mI	72	MEN	CA-CB-CG-OD1
7	BJ	72	MEN	CA-CB-CG-OD1
7	DJ	72	MEN	CA-CB-CG-OD1
7	FJ	72	MEN	CA-CB-CG-OD1
7	JJ	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
7	LJ	72	MEN	CA-CB-CG-OD1
7	NJ	72	MEN	CA-CB-CG-OD1
7	PJ	72	MEN	CA-CB-CG-OD1
7	RJ	72	MEN	CA-CB-CG-OD1
7	TJ	72	MEN	CA-CB-CG-OD1
7	VJ	72	MEN	CA-CB-CG-OD1
7	XJ	72	MEN	CA-CB-CG-OD1
7	ZJ	72	MEN	CA-CB-CG-OD1
7	bJ	72	MEN	CA-CB-CG-OD1
7	dJ	72	MEN	CA-CB-CG-OD1
7	fJ	72	MEN	CA-CB-CG-OD1
7	hJ	72	MEN	CA-CB-CG-OD1
7	jJ	72	MEN	CA-CB-CG-OD1
7	lJ	72	MEN	CA-CB-CG-OD1
7	nJ	72	MEN	CA-CB-CG-OD1
7	pJ	72	MEN	CA-CB-CG-OD1
7	rJ	72	MEN	CA-CB-CG-OD1
7	tJ	72	MEN	CA-CB-CG-OD1
7	vJ	72	MEN	CA-CB-CG-OD1
7	PK	72	MEN	CA-CB-CG-OD1
7	RK	72	MEN	CA-CB-CG-OD1
7	TK	72	MEN	CA-CB-CG-OD1
7	VK	72	MEN	CA-CB-CG-OD1
7	YK	72	MEN	CA-CB-CG-OD1
7	aK	72	MEN	CA-CB-CG-OD1
7	cK	72	MEN	CA-CB-CG-OD1
7	eK	72	MEN	CA-CB-CG-OD1
7	gK	72	MEN	CA-CB-CG-OD1
7	iK	72	MEN	CA-CB-CG-OD1
7	kK	72	MEN	CA-CB-CG-OD1
7	mK	72	MEN	CA-CB-CG-OD1
7	BL	72	MEN	CA-CB-CG-OD1
7	DL	72	MEN	CA-CB-CG-OD1
7	FL	72	MEN	CA-CB-CG-OD1
7	JL	72	MEN	CA-CB-CG-OD1
7	LL	72	MEN	CA-CB-CG-OD1
7	NL	72	MEN	CA-CB-CG-OD1
7	PL	72	MEN	CA-CB-CG-OD1
7	RL	72	MEN	CA-CB-CG-OD1
7	TL	72	MEN	CA-CB-CG-OD1
7	VL	72	MEN	CA-CB-CG-OD1
7	XL	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
7	ZL	72	MEN	CA-CB-CG-OD1
7	bL	72	MEN	CA-CB-CG-OD1
7	dL	72	MEN	CA-CB-CG-OD1
7	fL	72	MEN	CA-CB-CG-OD1
7	hL	72	MEN	CA-CB-CG-OD1
7	jL	72	MEN	CA-CB-CG-OD1
7	lL	72	MEN	CA-CB-CG-OD1
7	nL	72	MEN	CA-CB-CG-OD1
7	pL	72	MEN	CA-CB-CG-OD1
7	rL	72	MEN	CA-CB-CG-OD1
7	tL	72	MEN	CA-CB-CG-OD1
7	vL	72	MEN	CA-CB-CG-OD1
7	FM	72	MEN	CA-CB-CG-OD1
7	JM	72	MEN	CA-CB-CG-OD1
7	PM	72	MEN	CA-CB-CG-OD1
7	TM	72	MEN	CA-CB-CG-OD1
7	VM	72	MEN	CA-CB-CG-OD1
7	XM	72	MEN	CA-CB-CG-OD1
7	ZM	72	MEN	CA-CB-CG-OD1
7	eM	72	MEN	CA-CB-CG-OD1
7	gM	72	MEN	CA-CB-CG-OD1
7	iM	72	MEN	CA-CB-CG-OD1
7	kM	72	MEN	CA-CB-CG-OD1
7	BO	72	MEN	CA-CB-CG-OD1
7	DO	72	MEN	CA-CB-CG-OD1
7	FO	72	MEN	CA-CB-CG-OD1
7	HO	72	MEN	CA-CB-CG-OD1
7	JO	72	MEN	CA-CB-CG-OD1
7	LO	72	MEN	CA-CB-CG-OD1
7	MO	72	MEN	CA-CB-CG-OD1
7	NO	72	MEN	CA-CB-CG-OD1
21	FP	71	MEN	CA-CB-CG-OD1
21	QP	71	MEN	CA-CB-CG-OD1
21	kP	71	MEN	CA-CB-CG-OD1
21	nP	71	MEN	CA-CB-CG-OD1
21	sP	71	MEN	CA-CB-CG-OD1
7	BQ	72	MEN	CA-CB-CG-OD1
7	DQ	72	MEN	CA-CB-CG-OD1
7	FQ	72	MEN	CA-CB-CG-OD1
7	HQ	72	MEN	CA-CB-CG-OD1
7	JQ	72	MEN	CA-CB-CG-OD1
7	LQ	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
5	D1	72	MEN	CA-CB-CG-ND2
5	F1	72	MEN	CA-CB-CG-ND2
5	H1	72	MEN	CA-CB-CG-ND2
5	J1	72	MEN	CA-CB-CG-ND2
5	L1	72	MEN	CA-CB-CG-ND2
5	N1	72	MEN	CA-CB-CG-ND2
7	B3	72	MEN	CA-CB-CG-ND2
7	D3	72	MEN	CA-CB-CG-ND2
7	F3	72	MEN	CA-CB-CG-ND2
7	H3	72	MEN	CA-CB-CG-ND2
7	J3	72	MEN	CA-CB-CG-ND2
7	L3	72	MEN	CA-CB-CG-ND2
7	M3	72	MEN	CA-CB-CG-ND2
7	N3	72	MEN	CA-CB-CG-ND2
5	J7	72	MEN	CA-CB-CG-ND2
5	L7	72	MEN	CA-CB-CG-ND2
7	P7	72	MEN	CA-CB-CG-ND2
7	R7	72	MEN	CA-CB-CG-ND2
7	T7	72	MEN	CA-CB-CG-ND2
7	V7	72	MEN	CA-CB-CG-ND2
7	Y7	72	MEN	CA-CB-CG-ND2
7	a7	72	MEN	CA-CB-CG-ND2
7	c7	72	MEN	CA-CB-CG-ND2
7	e7	72	MEN	CA-CB-CG-ND2
7	g7	72	MEN	CA-CB-CG-ND2
7	i7	72	MEN	CA-CB-CG-ND2
7	k7	72	MEN	CA-CB-CG-ND2
7	m7	72	MEN	CA-CB-CG-ND2
5	J9	72	MEN	CA-CB-CG-ND2
5	L9	72	MEN	CA-CB-CG-ND2
7	P9	72	MEN	CA-CB-CG-ND2
7	R9	72	MEN	CA-CB-CG-ND2
7	T9	72	MEN	CA-CB-CG-ND2
7	V9	72	MEN	CA-CB-CG-ND2
7	Y9	72	MEN	CA-CB-CG-ND2
7	a9	72	MEN	CA-CB-CG-ND2
7	c9	72	MEN	CA-CB-CG-ND2
7	e9	72	MEN	CA-CB-CG-ND2
7	g9	72	MEN	CA-CB-CG-ND2
7	i9	72	MEN	CA-CB-CG-ND2
7	k9	72	MEN	CA-CB-CG-ND2
7	m9	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
7	BA	72	MEN	CA-CB-CG-ND2
7	DA	72	MEN	CA-CB-CG-ND2
7	FA	72	MEN	CA-CB-CG-ND2
7	HA	72	MEN	CA-CB-CG-ND2
7	JA	72	MEN	CA-CB-CG-ND2
7	LA	72	MEN	CA-CB-CG-ND2
7	PF	72	MEN	CA-CB-CG-ND2
7	RF	72	MEN	CA-CB-CG-ND2
7	TF	72	MEN	CA-CB-CG-ND2
7	VF	72	MEN	CA-CB-CG-ND2
7	YF	72	MEN	CA-CB-CG-ND2
7	aF	72	MEN	CA-CB-CG-ND2
7	cF	72	MEN	CA-CB-CG-ND2
7	eF	72	MEN	CA-CB-CG-ND2
7	gF	72	MEN	CA-CB-CG-ND2
7	iF	72	MEN	CA-CB-CG-ND2
7	kF	72	MEN	CA-CB-CG-ND2
7	mF	72	MEN	CA-CB-CG-ND2
7	BG	72	MEN	CA-CB-CG-ND2
7	DG	72	MEN	CA-CB-CG-ND2
7	FG	72	MEN	CA-CB-CG-ND2
7	HG	72	MEN	CA-CB-CG-ND2
7	JG	72	MEN	CA-CB-CG-ND2
7	LG	72	MEN	CA-CB-CG-ND2
7	PI	72	MEN	CA-CB-CG-ND2
7	RI	72	MEN	CA-CB-CG-ND2
7	TI	72	MEN	CA-CB-CG-ND2
7	VI	72	MEN	CA-CB-CG-ND2
7	YI	72	MEN	CA-CB-CG-ND2
7	aI	72	MEN	CA-CB-CG-ND2
7	cI	72	MEN	CA-CB-CG-ND2
7	eI	72	MEN	CA-CB-CG-ND2
7	gI	72	MEN	CA-CB-CG-ND2
7	iI	72	MEN	CA-CB-CG-ND2
7	kI	72	MEN	CA-CB-CG-ND2
7	mI	72	MEN	CA-CB-CG-ND2
7	BJ	72	MEN	CA-CB-CG-ND2
7	DJ	72	MEN	CA-CB-CG-ND2
7	FJ	72	MEN	CA-CB-CG-ND2
7	JJ	72	MEN	CA-CB-CG-ND2
7	LJ	72	MEN	CA-CB-CG-ND2
7	NJ	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
7	PJ	72	MEN	CA-CB-CG-ND2
7	RJ	72	MEN	CA-CB-CG-ND2
7	TJ	72	MEN	CA-CB-CG-ND2
7	VJ	72	MEN	CA-CB-CG-ND2
7	XJ	72	MEN	CA-CB-CG-ND2
7	ZJ	72	MEN	CA-CB-CG-ND2
7	bJ	72	MEN	CA-CB-CG-ND2
7	dJ	72	MEN	CA-CB-CG-ND2
7	fJ	72	MEN	CA-CB-CG-ND2
7	hJ	72	MEN	CA-CB-CG-ND2
7	jJ	72	MEN	CA-CB-CG-ND2
7	lJ	72	MEN	CA-CB-CG-ND2
7	nJ	72	MEN	CA-CB-CG-ND2
7	pJ	72	MEN	CA-CB-CG-ND2
7	rJ	72	MEN	CA-CB-CG-ND2
7	tJ	72	MEN	CA-CB-CG-ND2
7	vJ	72	MEN	CA-CB-CG-ND2
5	DK	72	MEN	CA-CB-CG-ND2
5	FK	72	MEN	CA-CB-CG-ND2
5	HK	72	MEN	CA-CB-CG-ND2
5	JK	72	MEN	CA-CB-CG-ND2
5	LK	72	MEN	CA-CB-CG-ND2
5	NK	72	MEN	CA-CB-CG-ND2
7	BL	72	MEN	CA-CB-CG-ND2
7	DL	72	MEN	CA-CB-CG-ND2
7	FL	72	MEN	CA-CB-CG-ND2
7	JL	72	MEN	CA-CB-CG-ND2
7	LL	72	MEN	CA-CB-CG-ND2
7	NL	72	MEN	CA-CB-CG-ND2
7	PL	72	MEN	CA-CB-CG-ND2
7	RL	72	MEN	CA-CB-CG-ND2
7	TL	72	MEN	CA-CB-CG-ND2
7	VL	72	MEN	CA-CB-CG-ND2
7	XL	72	MEN	CA-CB-CG-ND2
7	ZL	72	MEN	CA-CB-CG-ND2
7	bL	72	MEN	CA-CB-CG-ND2
7	dL	72	MEN	CA-CB-CG-ND2
7	fL	72	MEN	CA-CB-CG-ND2
7	hL	72	MEN	CA-CB-CG-ND2
7	jL	72	MEN	CA-CB-CG-ND2
7	lL	72	MEN	CA-CB-CG-ND2
7	nL	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
7	pL	72	MEN	CA-CB-CG-ND2
7	rL	72	MEN	CA-CB-CG-ND2
7	tL	72	MEN	CA-CB-CG-ND2
7	vL	72	MEN	CA-CB-CG-ND2
7	BN	72	MEN	CA-CB-CG-ND2
7	DN	72	MEN	CA-CB-CG-ND2
7	FN	72	MEN	CA-CB-CG-ND2
7	HN	72	MEN	CA-CB-CG-ND2
7	JN	72	MEN	CA-CB-CG-ND2
7	LN	72	MEN	CA-CB-CG-ND2
7	BO	72	MEN	CA-CB-CG-ND2
7	DO	72	MEN	CA-CB-CG-ND2
7	FO	72	MEN	CA-CB-CG-ND2
7	HO	72	MEN	CA-CB-CG-ND2
7	JO	72	MEN	CA-CB-CG-ND2
7	LO	72	MEN	CA-CB-CG-ND2
7	MO	72	MEN	CA-CB-CG-ND2
7	NO	72	MEN	CA-CB-CG-ND2
21	DP	71	MEN	CA-CB-CG-ND2
21	FP	71	MEN	CA-CB-CG-ND2
21	IP	71	MEN	CA-CB-CG-ND2
21	MP	71	MEN	CA-CB-CG-ND2
21	OP	71	MEN	CA-CB-CG-ND2
21	QP	71	MEN	CA-CB-CG-ND2
21	SP	71	MEN	CA-CB-CG-ND2
21	dP	71	MEN	CA-CB-CG-ND2
21	nP	71	MEN	CA-CB-CG-ND2
21	oP	71	MEN	CA-CB-CG-ND2
21	qP	71	MEN	CA-CB-CG-ND2
21	sP	71	MEN	CA-CB-CG-ND2
21	uP	71	MEN	CA-CB-CG-ND2
7	BQ	72	MEN	CA-CB-CG-ND2
7	DQ	72	MEN	CA-CB-CG-ND2
7	FQ	72	MEN	CA-CB-CG-ND2
7	HQ	72	MEN	CA-CB-CG-ND2
7	JQ	72	MEN	CA-CB-CG-ND2
7	LQ	72	MEN	CA-CB-CG-ND2
5	D1	72	MEN	CA-CB-CG-OD1
5	F1	72	MEN	CA-CB-CG-OD1
5	H1	72	MEN	CA-CB-CG-OD1
5	J1	72	MEN	CA-CB-CG-OD1
5	L1	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
5	N1	72	MEN	CA-CB-CG-OD1
7	C4	72	MEN	CA-CB-CG-OD1
7	E4	72	MEN	CA-CB-CG-OD1
7	G4	72	MEN	CA-CB-CG-OD1
7	I4	72	MEN	CA-CB-CG-OD1
7	K4	72	MEN	CA-CB-CG-OD1
7	M4	72	MEN	CA-CB-CG-OD1
7	I5	72	MEN	CA-CB-CG-OD1
7	K5	72	MEN	CA-CB-CG-OD1
7	A5	72	MEN	CA-CB-CG-OD1
7	C5	72	MEN	CA-CB-CG-OD1
5	H7	72	MEN	CA-CB-CG-OD1
5	J7	72	MEN	CA-CB-CG-OD1
7	P7	72	MEN	CA-CB-CG-OD1
7	R7	72	MEN	CA-CB-CG-OD1
7	T7	72	MEN	CA-CB-CG-OD1
7	V7	72	MEN	CA-CB-CG-OD1
7	Y7	72	MEN	CA-CB-CG-OD1
7	a7	72	MEN	CA-CB-CG-OD1
7	c7	72	MEN	CA-CB-CG-OD1
7	e7	72	MEN	CA-CB-CG-OD1
7	g7	72	MEN	CA-CB-CG-OD1
7	i7	72	MEN	CA-CB-CG-OD1
7	k7	72	MEN	CA-CB-CG-OD1
7	m7	72	MEN	CA-CB-CG-OD1
7	I8	72	MEN	CA-CB-CG-OD1
7	K8	72	MEN	CA-CB-CG-OD1
7	A8	72	MEN	CA-CB-CG-OD1
7	C8	72	MEN	CA-CB-CG-OD1
5	H9	72	MEN	CA-CB-CG-OD1
5	J9	72	MEN	CA-CB-CG-OD1
7	P9	72	MEN	CA-CB-CG-OD1
7	R9	72	MEN	CA-CB-CG-OD1
7	T9	72	MEN	CA-CB-CG-OD1
7	V9	72	MEN	CA-CB-CG-OD1
7	Y9	72	MEN	CA-CB-CG-OD1
7	a9	72	MEN	CA-CB-CG-OD1
7	c9	72	MEN	CA-CB-CG-OD1
7	e9	72	MEN	CA-CB-CG-OD1
7	g9	72	MEN	CA-CB-CG-OD1
7	i9	72	MEN	CA-CB-CG-OD1
7	k9	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
7	m9	72	MEN	CA-CB-CG-OD1
7	BA	72	MEN	CA-CB-CG-OD1
7	DA	72	MEN	CA-CB-CG-OD1
7	FA	72	MEN	CA-CB-CG-OD1
7	HA	72	MEN	CA-CB-CG-OD1
7	JA	72	MEN	CA-CB-CG-OD1
7	LA	72	MEN	CA-CB-CG-OD1
7	DB	72	MEN	CA-CB-CG-OD1
7	HB	72	MEN	CA-CB-CG-OD1
7	LB	72	MEN	CA-CB-CG-OD1
7	NB	72	MEN	CA-CB-CG-OD1
7	RB	72	MEN	CA-CB-CG-OD1
7	cB	72	MEN	CA-CB-CG-OD1
7	mB	72	MEN	CA-CB-CG-OD1
7	CD	72	MEN	CA-CB-CG-OD1
7	ED	72	MEN	CA-CB-CG-OD1
7	GD	72	MEN	CA-CB-CG-OD1
7	ID	72	MEN	CA-CB-CG-OD1
7	KD	72	MEN	CA-CB-CG-OD1
7	MD	72	MEN	CA-CB-CG-OD1
5	DK	72	MEN	CA-CB-CG-OD1
5	FK	72	MEN	CA-CB-CG-OD1
5	HK	72	MEN	CA-CB-CG-OD1
5	JK	72	MEN	CA-CB-CG-OD1
5	LK	72	MEN	CA-CB-CG-OD1
5	NK	72	MEN	CA-CB-CG-OD1
7	DM	72	MEN	CA-CB-CG-OD1
7	HM	72	MEN	CA-CB-CG-OD1
7	LM	72	MEN	CA-CB-CG-OD1
7	NM	72	MEN	CA-CB-CG-OD1
7	RM	72	MEN	CA-CB-CG-OD1
7	cM	72	MEN	CA-CB-CG-OD1
7	mM	72	MEN	CA-CB-CG-OD1
7	BN	72	MEN	CA-CB-CG-OD1
7	DN	72	MEN	CA-CB-CG-OD1
7	FN	72	MEN	CA-CB-CG-OD1
7	HN	72	MEN	CA-CB-CG-OD1
7	JN	72	MEN	CA-CB-CG-OD1
7	LN	72	MEN	CA-CB-CG-OD1
21	DP	71	MEN	CA-CB-CG-OD1
21	HP	71	MEN	CA-CB-CG-OD1
21	IP	71	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
21	LP	71	MEN	CA-CB-CG-OD1
21	MP	71	MEN	CA-CB-CG-OD1
21	SP	71	MEN	CA-CB-CG-OD1
21	dP	71	MEN	CA-CB-CG-OD1
21	jP	71	MEN	CA-CB-CG-OD1
21	oP	71	MEN	CA-CB-CG-OD1
21	qP	71	MEN	CA-CB-CG-OD1
21	uP	71	MEN	CA-CB-CG-OD1
7	P1	72	MEN	CA-CB-CG-ND2
7	R1	72	MEN	CA-CB-CG-ND2
7	T1	72	MEN	CA-CB-CG-ND2
7	V1	72	MEN	CA-CB-CG-ND2
7	Y1	72	MEN	CA-CB-CG-ND2
7	a1	72	MEN	CA-CB-CG-ND2
7	c1	72	MEN	CA-CB-CG-ND2
7	e1	72	MEN	CA-CB-CG-ND2
7	g1	72	MEN	CA-CB-CG-ND2
7	i1	72	MEN	CA-CB-CG-ND2
7	k1	72	MEN	CA-CB-CG-ND2
7	m1	72	MEN	CA-CB-CG-ND2
7	DB	72	MEN	CA-CB-CG-ND2
7	FB	72	MEN	CA-CB-CG-ND2
7	HB	72	MEN	CA-CB-CG-ND2
7	JB	72	MEN	CA-CB-CG-ND2
7	LB	72	MEN	CA-CB-CG-ND2
7	NB	72	MEN	CA-CB-CG-ND2
7	PB	72	MEN	CA-CB-CG-ND2
7	RB	72	MEN	CA-CB-CG-ND2
7	TB	72	MEN	CA-CB-CG-ND2
7	VB	72	MEN	CA-CB-CG-ND2
7	XB	72	MEN	CA-CB-CG-ND2
7	ZB	72	MEN	CA-CB-CG-ND2
7	cB	72	MEN	CA-CB-CG-ND2
7	eB	72	MEN	CA-CB-CG-ND2
7	gB	72	MEN	CA-CB-CG-ND2
7	iB	72	MEN	CA-CB-CG-ND2
7	kB	72	MEN	CA-CB-CG-ND2
7	mB	72	MEN	CA-CB-CG-ND2
7	PK	72	MEN	CA-CB-CG-ND2
7	RK	72	MEN	CA-CB-CG-ND2
7	TK	72	MEN	CA-CB-CG-ND2
7	VK	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
7	YK	72	MEN	CA-CB-CG-ND2
7	aK	72	MEN	CA-CB-CG-ND2
7	cK	72	MEN	CA-CB-CG-ND2
7	eK	72	MEN	CA-CB-CG-ND2
7	gK	72	MEN	CA-CB-CG-ND2
7	iK	72	MEN	CA-CB-CG-ND2
7	kK	72	MEN	CA-CB-CG-ND2
7	mK	72	MEN	CA-CB-CG-ND2
7	DM	72	MEN	CA-CB-CG-ND2
7	FM	72	MEN	CA-CB-CG-ND2
7	HM	72	MEN	CA-CB-CG-ND2
7	JM	72	MEN	CA-CB-CG-ND2
7	LM	72	MEN	CA-CB-CG-ND2
7	NM	72	MEN	CA-CB-CG-ND2
7	PM	72	MEN	CA-CB-CG-ND2
7	RM	72	MEN	CA-CB-CG-ND2
7	TM	72	MEN	CA-CB-CG-ND2
7	VM	72	MEN	CA-CB-CG-ND2
7	XM	72	MEN	CA-CB-CG-ND2
7	ZM	72	MEN	CA-CB-CG-ND2
7	cM	72	MEN	CA-CB-CG-ND2
7	eM	72	MEN	CA-CB-CG-ND2
7	gM	72	MEN	CA-CB-CG-ND2
7	iM	72	MEN	CA-CB-CG-ND2
7	kM	72	MEN	CA-CB-CG-ND2
7	mM	72	MEN	CA-CB-CG-ND2
21	HP	71	MEN	CA-CB-CG-ND2
7	P1	72	MEN	CB-CG-ND2-CE2
7	R1	72	MEN	CB-CG-ND2-CE2
7	T1	72	MEN	CB-CG-ND2-CE2
7	V1	72	MEN	CB-CG-ND2-CE2
7	Y1	72	MEN	CB-CG-ND2-CE2
7	a1	72	MEN	CB-CG-ND2-CE2
7	c1	72	MEN	CB-CG-ND2-CE2
7	e1	72	MEN	CB-CG-ND2-CE2
7	g1	72	MEN	CB-CG-ND2-CE2
7	i1	72	MEN	CB-CG-ND2-CE2
7	k1	72	MEN	CB-CG-ND2-CE2
7	m1	72	MEN	CB-CG-ND2-CE2
7	PF	72	MEN	CB-CG-ND2-CE2
7	RF	72	MEN	CB-CG-ND2-CE2
7	TF	72	MEN	CB-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	VF	72	MEN	CB-CG-ND2-CE2
7	YF	72	MEN	CB-CG-ND2-CE2
7	aF	72	MEN	CB-CG-ND2-CE2
7	cF	72	MEN	CB-CG-ND2-CE2
7	eF	72	MEN	CB-CG-ND2-CE2
7	gF	72	MEN	CB-CG-ND2-CE2
7	iF	72	MEN	CB-CG-ND2-CE2
7	kF	72	MEN	CB-CG-ND2-CE2
7	mF	72	MEN	CB-CG-ND2-CE2
7	PI	72	MEN	CB-CG-ND2-CE2
7	RI	72	MEN	CB-CG-ND2-CE2
7	TI	72	MEN	CB-CG-ND2-CE2
7	VI	72	MEN	CB-CG-ND2-CE2
7	YI	72	MEN	CB-CG-ND2-CE2
7	aI	72	MEN	CB-CG-ND2-CE2
7	cI	72	MEN	CB-CG-ND2-CE2
7	eI	72	MEN	CB-CG-ND2-CE2
7	gI	72	MEN	CB-CG-ND2-CE2
7	iI	72	MEN	CB-CG-ND2-CE2
7	kI	72	MEN	CB-CG-ND2-CE2
7	mI	72	MEN	CB-CG-ND2-CE2
7	PK	72	MEN	CB-CG-ND2-CE2
7	RK	72	MEN	CB-CG-ND2-CE2
7	TK	72	MEN	CB-CG-ND2-CE2
7	VK	72	MEN	CB-CG-ND2-CE2
7	YK	72	MEN	CB-CG-ND2-CE2
7	aK	72	MEN	CB-CG-ND2-CE2
7	cK	72	MEN	CB-CG-ND2-CE2
7	eK	72	MEN	CB-CG-ND2-CE2
7	gK	72	MEN	CB-CG-ND2-CE2
7	iK	72	MEN	CB-CG-ND2-CE2
7	kK	72	MEN	CB-CG-ND2-CE2
7	mK	72	MEN	CB-CG-ND2-CE2
21	SP	71	MEN	CB-CG-ND2-CE2
7	B3	72	MEN	C-CA-CB-CG
7	D3	72	MEN	C-CA-CB-CG
7	F3	72	MEN	C-CA-CB-CG
7	H3	72	MEN	C-CA-CB-CG
7	J3	72	MEN	C-CA-CB-CG
7	L3	72	MEN	C-CA-CB-CG
7	I5	72	MEN	C-CA-CB-CG
7	K5	72	MEN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	A5	72	MEN	C-CA-CB-CG
7	C5	72	MEN	C-CA-CB-CG
7	I8	72	MEN	C-CA-CB-CG
7	K8	72	MEN	C-CA-CB-CG
7	A8	72	MEN	C-CA-CB-CG
7	C8	72	MEN	C-CA-CB-CG
7	PF	72	MEN	C-CA-CB-CG
7	RF	72	MEN	C-CA-CB-CG
7	TF	72	MEN	C-CA-CB-CG
7	VF	72	MEN	C-CA-CB-CG
7	YF	72	MEN	C-CA-CB-CG
7	aF	72	MEN	C-CA-CB-CG
7	cF	72	MEN	C-CA-CB-CG
7	eF	72	MEN	C-CA-CB-CG
7	gF	72	MEN	C-CA-CB-CG
7	iF	72	MEN	C-CA-CB-CG
7	kF	72	MEN	C-CA-CB-CG
7	mF	72	MEN	C-CA-CB-CG
7	PI	72	MEN	C-CA-CB-CG
7	RI	72	MEN	C-CA-CB-CG
7	TI	72	MEN	C-CA-CB-CG
7	VI	72	MEN	C-CA-CB-CG
7	YI	72	MEN	C-CA-CB-CG
7	aI	72	MEN	C-CA-CB-CG
7	cI	72	MEN	C-CA-CB-CG
7	eI	72	MEN	C-CA-CB-CG
7	gI	72	MEN	C-CA-CB-CG
7	iI	72	MEN	C-CA-CB-CG
7	kI	72	MEN	C-CA-CB-CG
7	mI	72	MEN	C-CA-CB-CG
7	HL	72	MEN	C-CA-CB-CG
7	BO	72	MEN	C-CA-CB-CG
7	DO	72	MEN	C-CA-CB-CG
7	FO	72	MEN	C-CA-CB-CG
7	HO	72	MEN	C-CA-CB-CG
7	JO	72	MEN	C-CA-CB-CG
7	LO	72	MEN	C-CA-CB-CG
7	PF	72	MEN	OD1-CG-ND2-CE2
7	RF	72	MEN	OD1-CG-ND2-CE2
7	TF	72	MEN	OD1-CG-ND2-CE2
7	VF	72	MEN	OD1-CG-ND2-CE2
7	YF	72	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	aF	72	MEN	OD1-CG-ND2-CE2
7	cF	72	MEN	OD1-CG-ND2-CE2
7	eF	72	MEN	OD1-CG-ND2-CE2
7	gF	72	MEN	OD1-CG-ND2-CE2
7	iF	72	MEN	OD1-CG-ND2-CE2
7	kF	72	MEN	OD1-CG-ND2-CE2
7	mF	72	MEN	OD1-CG-ND2-CE2
7	PI	72	MEN	OD1-CG-ND2-CE2
7	RI	72	MEN	OD1-CG-ND2-CE2
7	TI	72	MEN	OD1-CG-ND2-CE2
7	VI	72	MEN	OD1-CG-ND2-CE2
7	YI	72	MEN	OD1-CG-ND2-CE2
7	aI	72	MEN	OD1-CG-ND2-CE2
7	cI	72	MEN	OD1-CG-ND2-CE2
7	eI	72	MEN	OD1-CG-ND2-CE2
7	gI	72	MEN	OD1-CG-ND2-CE2
7	iI	72	MEN	OD1-CG-ND2-CE2
7	kI	72	MEN	OD1-CG-ND2-CE2
7	mI	72	MEN	OD1-CG-ND2-CE2
21	OP	71	MEN	CA-CB-CG-OD1
7	C4	72	MEN	CA-CB-CG-ND2
7	E4	72	MEN	CA-CB-CG-ND2
7	G4	72	MEN	CA-CB-CG-ND2
7	I4	72	MEN	CA-CB-CG-ND2
7	K4	72	MEN	CA-CB-CG-ND2
7	M4	72	MEN	CA-CB-CG-ND2
7	I5	72	MEN	CA-CB-CG-ND2
7	K5	72	MEN	CA-CB-CG-ND2
7	A5	72	MEN	CA-CB-CG-ND2
7	C5	72	MEN	CA-CB-CG-ND2
5	F7	72	MEN	CA-CB-CG-ND2
5	H7	72	MEN	CA-CB-CG-ND2
5	N7	72	MEN	CA-CB-CG-ND2
7	I8	72	MEN	CA-CB-CG-ND2
7	K8	72	MEN	CA-CB-CG-ND2
7	A8	72	MEN	CA-CB-CG-ND2
7	C8	72	MEN	CA-CB-CG-ND2
5	F9	72	MEN	CA-CB-CG-ND2
5	H9	72	MEN	CA-CB-CG-ND2
5	N9	72	MEN	CA-CB-CG-ND2
7	CD	72	MEN	CA-CB-CG-ND2
7	ED	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
7	GD	72	MEN	CA-CB-CG-ND2
7	ID	72	MEN	CA-CB-CG-ND2
7	KD	72	MEN	CA-CB-CG-ND2
7	MD	72	MEN	CA-CB-CG-ND2
21	UP	71	MEN	CA-CB-CG-ND2
21	wP	71	MEN	CA-CB-CG-ND2
5	F7	72	MEN	N-CA-CB-CG
5	J7	72	MEN	N-CA-CB-CG
7	P7	72	MEN	N-CA-CB-CG
7	R7	72	MEN	N-CA-CB-CG
7	T7	72	MEN	N-CA-CB-CG
7	V7	72	MEN	N-CA-CB-CG
7	Y7	72	MEN	N-CA-CB-CG
7	a7	72	MEN	N-CA-CB-CG
7	c7	72	MEN	N-CA-CB-CG
7	e7	72	MEN	N-CA-CB-CG
7	g7	72	MEN	N-CA-CB-CG
7	i7	72	MEN	N-CA-CB-CG
7	k7	72	MEN	N-CA-CB-CG
7	m7	72	MEN	N-CA-CB-CG
5	F9	72	MEN	N-CA-CB-CG
5	J9	72	MEN	N-CA-CB-CG
7	P9	72	MEN	N-CA-CB-CG
7	R9	72	MEN	N-CA-CB-CG
7	T9	72	MEN	N-CA-CB-CG
7	V9	72	MEN	N-CA-CB-CG
7	Y9	72	MEN	N-CA-CB-CG
7	a9	72	MEN	N-CA-CB-CG
7	c9	72	MEN	N-CA-CB-CG
7	e9	72	MEN	N-CA-CB-CG
7	g9	72	MEN	N-CA-CB-CG
7	i9	72	MEN	N-CA-CB-CG
7	k9	72	MEN	N-CA-CB-CG
7	m9	72	MEN	N-CA-CB-CG
21	UP	71	MEN	N-CA-CB-CG
21	wP	71	MEN	N-CA-CB-CG
21	SP	71	MEN	OD1-CG-ND2-CE2
7	P7	72	MEN	CB-CG-ND2-CE2
7	R7	72	MEN	CB-CG-ND2-CE2
7	T7	72	MEN	CB-CG-ND2-CE2
7	V7	72	MEN	CB-CG-ND2-CE2
7	Y7	72	MEN	CB-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	a7	72	MEN	CB-CG-ND2-CE2
7	c7	72	MEN	CB-CG-ND2-CE2
7	e7	72	MEN	CB-CG-ND2-CE2
7	g7	72	MEN	CB-CG-ND2-CE2
7	i7	72	MEN	CB-CG-ND2-CE2
7	k7	72	MEN	CB-CG-ND2-CE2
7	m7	72	MEN	CB-CG-ND2-CE2
7	P9	72	MEN	CB-CG-ND2-CE2
7	R9	72	MEN	CB-CG-ND2-CE2
7	T9	72	MEN	CB-CG-ND2-CE2
7	V9	72	MEN	CB-CG-ND2-CE2
7	Y9	72	MEN	CB-CG-ND2-CE2
7	a9	72	MEN	CB-CG-ND2-CE2
7	c9	72	MEN	CB-CG-ND2-CE2
7	e9	72	MEN	CB-CG-ND2-CE2
7	g9	72	MEN	CB-CG-ND2-CE2
7	i9	72	MEN	CB-CG-ND2-CE2
7	k9	72	MEN	CB-CG-ND2-CE2
7	m9	72	MEN	CB-CG-ND2-CE2
21	UP	71	MEN	CA-CB-CG-OD1
21	wP	71	MEN	CA-CB-CG-OD1
7	P1	72	MEN	OD1-CG-ND2-CE2
7	R1	72	MEN	OD1-CG-ND2-CE2
7	T1	72	MEN	OD1-CG-ND2-CE2
7	V1	72	MEN	OD1-CG-ND2-CE2
7	Y1	72	MEN	OD1-CG-ND2-CE2
7	a1	72	MEN	OD1-CG-ND2-CE2
7	c1	72	MEN	OD1-CG-ND2-CE2
7	e1	72	MEN	OD1-CG-ND2-CE2
7	g1	72	MEN	OD1-CG-ND2-CE2
7	i1	72	MEN	OD1-CG-ND2-CE2
7	k1	72	MEN	OD1-CG-ND2-CE2
7	m1	72	MEN	OD1-CG-ND2-CE2
7	P7	72	MEN	OD1-CG-ND2-CE2
7	R7	72	MEN	OD1-CG-ND2-CE2
7	T7	72	MEN	OD1-CG-ND2-CE2
7	V7	72	MEN	OD1-CG-ND2-CE2
7	Y7	72	MEN	OD1-CG-ND2-CE2
7	a7	72	MEN	OD1-CG-ND2-CE2
7	c7	72	MEN	OD1-CG-ND2-CE2
7	e7	72	MEN	OD1-CG-ND2-CE2
7	g7	72	MEN	OD1-CG-ND2-CE2

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Mol	Chain	Res	Type	Atoms
7	i7	72	MEN	OD1-CG-ND2-CE2
7	k7	72	MEN	OD1-CG-ND2-CE2
7	m7	72	MEN	OD1-CG-ND2-CE2
7	P9	72	MEN	OD1-CG-ND2-CE2
7	R9	72	MEN	OD1-CG-ND2-CE2
7	T9	72	MEN	OD1-CG-ND2-CE2
7	V9	72	MEN	OD1-CG-ND2-CE2
7	Y9	72	MEN	OD1-CG-ND2-CE2
7	a9	72	MEN	OD1-CG-ND2-CE2
7	c9	72	MEN	OD1-CG-ND2-CE2
7	e9	72	MEN	OD1-CG-ND2-CE2
7	g9	72	MEN	OD1-CG-ND2-CE2
7	i9	72	MEN	OD1-CG-ND2-CE2
7	k9	72	MEN	OD1-CG-ND2-CE2
7	m9	72	MEN	OD1-CG-ND2-CE2
7	PK	72	MEN	OD1-CG-ND2-CE2
7	RK	72	MEN	OD1-CG-ND2-CE2
7	TK	72	MEN	OD1-CG-ND2-CE2
7	VK	72	MEN	OD1-CG-ND2-CE2
7	YK	72	MEN	OD1-CG-ND2-CE2
7	aK	72	MEN	OD1-CG-ND2-CE2
7	cK	72	MEN	OD1-CG-ND2-CE2
7	eK	72	MEN	OD1-CG-ND2-CE2
7	gK	72	MEN	OD1-CG-ND2-CE2
7	iK	72	MEN	OD1-CG-ND2-CE2
7	kK	72	MEN	OD1-CG-ND2-CE2
7	mK	72	MEN	OD1-CG-ND2-CE2
7	B3	72	MEN	N-CA-CB-CG
7	D3	72	MEN	N-CA-CB-CG
7	F3	72	MEN	N-CA-CB-CG
7	H3	72	MEN	N-CA-CB-CG
7	J3	72	MEN	N-CA-CB-CG
7	L3	72	MEN	N-CA-CB-CG
7	PF	72	MEN	N-CA-CB-CG
7	RF	72	MEN	N-CA-CB-CG
7	TF	72	MEN	N-CA-CB-CG
7	VF	72	MEN	N-CA-CB-CG
7	YF	72	MEN	N-CA-CB-CG
7	aF	72	MEN	N-CA-CB-CG
7	cF	72	MEN	N-CA-CB-CG
7	eF	72	MEN	N-CA-CB-CG
7	gF	72	MEN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	iF	72	MEN	N-CA-CB-CG
7	kF	72	MEN	N-CA-CB-CG
7	mF	72	MEN	N-CA-CB-CG
7	PI	72	MEN	N-CA-CB-CG
7	RI	72	MEN	N-CA-CB-CG
7	TI	72	MEN	N-CA-CB-CG
7	VI	72	MEN	N-CA-CB-CG
7	YI	72	MEN	N-CA-CB-CG
7	aI	72	MEN	N-CA-CB-CG
7	cI	72	MEN	N-CA-CB-CG
7	eI	72	MEN	N-CA-CB-CG
7	gI	72	MEN	N-CA-CB-CG
7	iI	72	MEN	N-CA-CB-CG
7	kI	72	MEN	N-CA-CB-CG
7	mI	72	MEN	N-CA-CB-CG
7	BO	72	MEN	N-CA-CB-CG
7	DO	72	MEN	N-CA-CB-CG
7	FO	72	MEN	N-CA-CB-CG
7	HO	72	MEN	N-CA-CB-CG
7	JO	72	MEN	N-CA-CB-CG
7	LO	72	MEN	N-CA-CB-CG
21	SP	71	MEN	N-CA-CB-CG
21	uP	71	MEN	N-CA-CB-CG
21	hP	71	MEN	CA-CB-CG-OD1
7	N2	72	MEN	CA-CB-CG-OD1
7	P2	72	MEN	CA-CB-CG-OD1
7	R2	72	MEN	CA-CB-CG-OD1
7	T2	72	MEN	CA-CB-CG-OD1
7	V2	72	MEN	CA-CB-CG-OD1
7	X2	72	MEN	CA-CB-CG-OD1
5	DF	72	MEN	CA-CB-CG-OD1
5	DI	72	MEN	CA-CB-CG-OD1
7	HL	72	MEN	CA-CB-CG-OD1
7	NR	72	MEN	CA-CB-CG-OD1
7	PR	72	MEN	CA-CB-CG-OD1
7	RR	72	MEN	CA-CB-CG-OD1
7	TR	72	MEN	CA-CB-CG-OD1
7	VR	72	MEN	CA-CB-CG-OD1
7	XR	72	MEN	CA-CB-CG-OD1

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](#)

1462 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
31	CYC	GI	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	fB	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	gF	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	PB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	c7	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	S9	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	FN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	A1	303	2	43,46,46	3.24	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	T7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	AL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	QK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
31	CYC	M7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	DA	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	mF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	RM	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	FB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	a7	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	qL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	eK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	S1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	MP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	e9	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	NL	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	16 (35%)
29	PEB	aI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	aK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	Q1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	dB	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	E4	203	-	43,46,46	3.30	10 (23%)	45,67,67	2.63	18 (40%)
29	PEB	LL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	J5	201	6	43,46,46	3.37	11 (25%)	45,67,67	2.77	16 (35%)
29	PEB	NO	202	7	43,46,46	3.36	10 (23%)	45,67,67	2.25	13 (28%)
29	PEB	iL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	C9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.81	21 (42%)
29	PEB	CA	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	JC	202	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
31	CYC	I9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	IN	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
31	CYC	E1	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	LN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	B3	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	f9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	A1	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.13	15 (33%)
29	PEB	iJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	VM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	gL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
32	PMS	kH	301	-	11,11,11	0.83	1 (9%)	14,15,15	0.65	0
29	PEB	VL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	H8	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	dK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	RB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
31	CYC	CF	1001	4,5	42,46,46	3.08	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	RI	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	AM	303	16	43,46,46	3.34	10 (23%)	45,67,67	2.18	14 (31%)
29	PEB	R1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	R7	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	IM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	JB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	AF	304	2	43,46,46	3.29	10 (23%)	45,67,67	2.25	15 (33%)
29	PEB	L7	1002	-	43,46,46	3.24	11 (25%)	45,67,67	2.21	17 (37%)
29	PEB	W7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	k9	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	c1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	LK	1002	-	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	kM	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	bL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	RL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	mI	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	OR	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.55	18 (40%)
29	PEB	UJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	tL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	EG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	kF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	rL	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	mM	201	7,16	43,46,46	3.36	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	cF	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	MG	405	14	43,46,46	3.11	10 (23%)	45,67,67	2.98	17 (37%)
29	PEB	VM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	UK	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
32	PMS	kH	302	-	11,11,11	1.23	1 (9%)	14,15,15	1.08	1 (7%)
31	CYC	sP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	SL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
30	PUB	QB	201	6,17	42,46,46	3.60	8 (19%)	37,67,67	3.06	14 (37%)
29	PEB	B8	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	BE	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	PL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	S7	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	g1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	ZK	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	I4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	bK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	MN	404	14	43,46,46	3.15	12 (27%)	45,67,67	2.49	13 (28%)
29	PEB	HA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	mI	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
31	CYC	tP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	hJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	A9	303	-	42,46,46	3.34	7 (16%)	37,67,67	3.09	14 (37%)
29	PEB	H5	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	IG	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	M3	203	7	43,46,46	3.23	11 (25%)	45,67,67	2.14	14 (31%)
29	PEB	P1	201	7,1	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	cF	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	dJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	CO	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	TL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	gF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	WF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	NR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.36	14 (31%)
31	CYC	I1	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	C4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	K3	202	6	43,46,46	3.61	12 (27%)	45,67,67	1.97	15 (33%)
29	PEB	KB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	A7	305	-	43,46,46	3.31	10 (23%)	45,67,67	2.24	17 (37%)
31	CYC	EF	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	UF	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	M9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	IE	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	N7	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	H3	203	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	L5	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	AE	201	6	43,46,46	3.45	9 (20%)	45,67,67	2.08	15 (33%)
29	PEB	B4	201	6	43,46,46	3.12	14 (32%)	45,67,67	2.73	21 (46%)
29	PEB	nL	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
31	CYC	eP	1001	20	42,46,46	3.37	14 (33%)	50,67,67	3.10	22 (44%)
29	PEB	KB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	U7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	DO	201	7	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	eM	202	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PUB	AI	303	2	42,46,46	3.29	7 (16%)	37,67,67	3.30	14 (37%)
29	PEB	dI	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	sJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	DL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	E7	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	JD	201	6	43,46,46	3.11	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	iI	202	6,7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	RR	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.47	17 (37%)
31	CYC	CP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	D1	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	WK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	A1	302	-	43,46,46	3.36	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	l9	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
31	CYC	oP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
30	PUB	A1	305	-	42,46,46	3.40	8 (19%)	37,67,67	4.48	16 (43%)
29	PEB	FA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.27	16 (35%)
29	PEB	LI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	LG	203	-	43,46,46	3.44	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	M2	202	6	43,46,46	3.63	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	JA	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	kI	202	7,6	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
31	CYC	PP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.12	22 (44%)
29	PEB	ED	202	7	43,46,46	3.31	10 (23%)	45,67,67	2.62	18 (40%)
29	PEB	hJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	U2	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.55	18 (40%)
29	PEB	hF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	FF	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	e1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	l7	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	LJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	A9	302	2	42,46,46	3.35	7 (16%)	37,67,67	3.17	18 (48%)
29	PEB	iI	202	6,7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	R9	201	7,1	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	HG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	SK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	k1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	cJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	FE	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	16 (35%)
29	PEB	HQ	203	7	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	DA	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.25	16 (35%)
29	PEB	YL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	mF	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	SR	202	6	43,46,46	3.59	12 (27%)	45,67,67	2.04	15 (33%)
29	PEB	LF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	J1	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	K8	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	DG	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.07	16 (35%)
29	PEB	eK	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
31	CYC	EP	1001	20	42,46,46	3.39	14 (33%)	50,67,67	3.10	22 (44%)
29	PEB	dF	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	f1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	YK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	MR	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.55	18 (40%)
29	PEB	g7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	dB	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	YF	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	UR	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.55	18 (40%)
30	PUB	yJ	303	-	42,46,46	3.50	7 (16%)	37,67,67	3.28	16 (43%)
29	PEB	WR	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	sL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	Y1	202	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	FO	202	7,6	43,46,46	3.53	12 (27%)	45,67,67	2.12	15 (33%)
30	PUB	MQ	404	14	42,46,46	3.70	9 (21%)	37,67,67	4.02	21 (56%)
29	PEB	DN	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	H3	202	6,7	43,46,46	3.53	13 (30%)	45,67,67	2.12	15 (33%)
30	PUB	AK	305	-	42,46,46	3.40	8 (19%)	37,67,67	4.48	16 (43%)
29	PEB	B5	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	TF	202	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
31	CYC	XP	1001	24,21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
30	PUB	BB	302	17	42,46,46	3.40	7 (16%)	37,67,67	3.33	12 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	BJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LG	201	7,14	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	lB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	oL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	h7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	SJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	GO	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	17 (37%)
29	PEB	K5	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.10	15 (33%)
29	PEB	VR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
30	PUB	MG	403	14	42,46,46	3.55	8 (19%)	37,67,67	3.60	19 (51%)
29	PEB	JF	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.12	16 (35%)
31	CYC	DF	1001	5	42,46,46	3.20	14 (33%)	50,67,67	3.02	21 (42%)
29	PEB	PR	202	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
31	CYC	M1	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	R2	201	7	43,46,46	3.37	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	VK	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	L4	201	6	43,46,46	3.13	13 (30%)	45,67,67	2.72	21 (46%)
29	PEB	PJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	N2	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.36	14 (31%)
29	PEB	fl	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	WM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	MQ	401	6,14	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	PB	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	QI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	JP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	Q9	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	sJ	203	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
30	PUB	xL	305	16	42,46,46	3.29	8 (19%)	37,67,67	3.75	15 (40%)
31	CYC	JK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	SM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	kI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	JN	203	-	43,46,46	3.29	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	UI	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	Z1	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	hJ	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	bJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	O9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	QI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	RP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	A5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	DB	201	7,17	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	W2	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	JL	203	7	43,46,46	3.41	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	AQ	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
31	CYC	BP	1001	25,21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	wL	303	16	43,46,46	3.43	12 (27%)	45,67,67	2.28	18 (40%)
29	PEB	LL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	CB	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	CN	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	LA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	H4	201	6	43,46,46	3.14	14 (32%)	45,67,67	2.73	21 (46%)
29	PEB	vL	201	7	43,46,46	3.33	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	IC	201	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	g1	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	g7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	jM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	PI	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	aL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	iL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	CM	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	NJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	16 (35%)
29	PEB	kK	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	jL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	R7	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	DE	201	7,18	43,46,46	3.55	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	h1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	SF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	fP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	GA	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	21 (46%)
29	PEB	XJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	EA	201	6	43,46,46	3.04	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	Q7	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	fB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
30	PUB	AI	302	2	42,46,46	3.54	8 (19%)	37,67,67	3.18	15 (40%)
29	PEB	IC	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	IF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
29	PEB	KD	202	7,6	43,46,46	3.05	11 (25%)	45,67,67	2.59	16 (35%)
29	PEB	WM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	WJ	202	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	DC	201	7	43,46,46	3.55	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	jL	202	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	F5	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	GD	202	7	43,46,46	3.05	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	G3	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	I3	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	jK	203	6,7	43,46,46	3.10	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	lB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	XJ	202	6,7	43,46,46	3.07	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	G8	203	7	43,46,46	3.33	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	GN	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	B4	202	6	43,46,46	3.14	10 (23%)	45,67,67	2.40	20 (44%)
31	CYC	GF	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	HO	203	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	hM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	VF	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	lF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	PR	201	7	43,46,46	3.04	8 (18%)	45,67,67	2.47	18 (40%)
29	PEB	BE	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.42	15 (33%)
29	PEB	hB	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	m7	203	7	43,46,46	3.50	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	N2	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	VR	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	17 (37%)
29	PEB	KA	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	FC	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	16 (35%)
31	CYC	KI	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
31	CYC	IK	1001	4,5	42,46,46	3.10	14 (33%)	50,67,67	2.78	18 (36%)
29	PEB	VB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	d9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
32	PMS	k6	301	-	11,11,11	0.83	1 (9%)	14,15,15	0.65	0
29	PEB	F8	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	FG	203	-	43,46,46	3.45	9 (20%)	45,67,67	2.17	16 (35%)
29	PEB	wL	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.26	19 (42%)
30	PUB	yJ	302	-	42,46,46	3.35	7 (16%)	37,67,67	3.26	15 (40%)
29	PEB	uJ	203	6	43,46,46	3.29	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	iK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	CG	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.06	14 (31%)
29	PEB	m7	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	BL	201	7,19	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	FQ	203	-	43,46,46	3.46	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	eR	401	-	43,46,46	1.07	2 (4%)	45,67,67	1.02	2 (4%)
29	PEB	A8	202	-	43,46,46	3.28	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	JB	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	GA	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	c9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	KJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	OM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.42	16 (35%)
29	PEB	I8	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.12	14 (31%)
29	PEB	KG	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	14 (31%)
29	PEB	DB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	NL	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	m1	202	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	aI	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	DG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	KD	201	7	43,46,46	3.15	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	V7	203	7	43,46,46	3.47	12 (27%)	45,67,67	2.10	14 (31%)
31	CYC	J9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	25 (50%)
30	PUB	xJ	304	-	42,46,46	3.35	7 (16%)	37,67,67	3.30	16 (43%)
29	PEB	EJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	iM	201	7,16	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	CA	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	AK	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.13	15 (33%)
29	PEB	HN	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
30	PUB	xL	304	-	42,46,46	3.36	7 (16%)	37,67,67	3.30	16 (43%)
31	CYC	H7	1001	5	42,46,46	3.03	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	YB	203	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	Y9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	c1	202	7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	T7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	hM	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	WB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	HO	201	7,9	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	YK	202	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
31	CYC	1P	1001	25,21	42,46,46	3.28	14 (33%)	50,67,67	3.10	21 (42%)
29	PEB	C5	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	15 (33%)
30	PUB	MQ	405	14	42,46,46	3.56	8 (19%)	37,67,67	3.60	19 (51%)
29	PEB	EB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	lM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	SI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	sJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	WI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	IA	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.90	20 (44%)
29	PEB	BA	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	Q9	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	EL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	i1	203	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	lJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	jB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	OI	203	6,7	43,46,46	3.15	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	G3	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	17 (37%)
29	PEB	BN	203	-	43,46,46	3.29	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	ZJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	hK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	MM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	IB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	W1	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	ZF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	L4	202	6	43,46,46	3.14	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	GQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	OM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	H1	1002	-	43,46,46	3.44	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	AA	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.89	20 (44%)
29	PEB	mL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	mB	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	gB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	QM	204	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	L8	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	IB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	HG	203	7	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
31	CYC	F7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	f9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	tJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	R9	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	iB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	BL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	DF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	eK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	uL	201	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	DB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	C3	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	16 (35%)
30	PUB	yL	303	-	42,46,46	3.51	7 (16%)	37,67,67	3.28	16 (43%)
29	PEB	K8	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	W2	202	6	43,46,46	3.62	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	H4	202	6	43,46,46	3.11	10 (23%)	45,67,67	2.39	19 (42%)
29	PEB	OL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	KG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	KD	203	-	43,46,46	3.30	10 (23%)	45,67,67	2.62	18 (40%)
30	PUB	AM	305	16	42,46,46	3.40	7 (16%)	37,67,67	3.00	15 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CYC	pP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	HJ	201	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	QB	204	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	LB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	d1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	VI	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	EO	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.17	16 (35%)
31	CYC	L1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	Y9	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	kJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
30	PUB	MA	402	14	42,46,46	3.43	7 (16%)	37,67,67	3.77	19 (51%)
29	PEB	U1	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	e1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	j7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
30	PUB	wJ	305	16	42,46,46	3.29	8 (19%)	37,67,67	3.74	15 (40%)
29	PEB	JC	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	D3	203	-	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	EA	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	20 (44%)
29	PEB	kL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	bI	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	WP	1001	-	42,46,46	3.50	15 (35%)	50,67,67	2.92	20 (40%)
29	PEB	qJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	LB	202	7,6	43,46,46	3.18	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	OI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
29	PEB	DO	202	-	43,46,46	3.41	11 (25%)	45,67,67	2.10	13 (28%)
29	PEB	hL	201	7	43,46,46	3.31	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	c7	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	S7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	JM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	T7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	F3	202	7,6	43,46,46	3.53	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	DN	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.25	16 (35%)
29	PEB	YJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	XR	202	7	43,46,46	3.04	8 (18%)	45,67,67	2.48	17 (37%)
29	PEB	c1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	CE	202	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	UM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	GM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	gI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	fM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
31	CYC	NI	1001	5,3	42,46,46	3.21	15 (35%)	50,67,67	3.03	21 (42%)
31	CYC	D1	1003	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
31	CYC	D7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	JG	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	WF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	HL	201	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	NB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	eL	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.12	13 (28%)
29	PEB	J5	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.17	16 (35%)
29	PEB	TR	202	7	43,46,46	3.04	8 (18%)	45,67,67	2.47	17 (37%)
29	PEB	kJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	J3	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	iB	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	SK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	mK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	tL	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	HP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	D3	201	7	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
31	CYC	LI	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.03	21 (42%)
29	PEB	MQ	407	14	43,46,46	3.13	9 (20%)	45,67,67	2.99	17 (37%)
29	PEB	iK	202	6,7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	YL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	F3	201	7,9	43,46,46	3.44	11 (25%)	45,67,67	2.08	16 (35%)
31	CYC	NF	1001	5,3	42,46,46	3.21	15 (35%)	50,67,67	3.03	21 (42%)
29	PEB	HC	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	eM	201	7,16	43,46,46	3.35	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	pJ	202	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	a1	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	cK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	TL	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	OB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	NR	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	WL	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	IN	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.90	20 (44%)
29	PEB	bJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	FA	201	7	43,46,46	3.23	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	M2	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.55	18 (40%)
31	CYC	OP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	FJ	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	mI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	eF	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	e9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	rJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	F5	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	SB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	AC	201	6	43,46,46	3.45	9 (20%)	45,67,67	2.08	15 (33%)
29	PEB	WL	202	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	K3	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.16	16 (35%)
30	PUB	BM	302	17	42,46,46	3.40	7 (16%)	37,67,67	3.33	12 (32%)
29	PEB	fJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
31	CYC	QP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	LB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	pL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	dI	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	HI	1001	5	42,46,46	3.20	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	a9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	FG	201	7,14	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	eL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	J9	1002	-	43,46,46	3.25	10 (23%)	45,67,67	2.22	16 (35%)
29	PEB	N3	203	7	43,46,46	3.23	10 (23%)	45,67,67	2.14	14 (31%)
29	PEB	nJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	XR	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	N2	202	7	43,46,46	3.02	8 (18%)	45,67,67	2.48	18 (40%)
29	PEB	FQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	IJ	202	7	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CYC	AP	1001	20	42,46,46	3.37	15 (35%)	50,67,67	3.12	22 (44%)
29	PEB	b7	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	dL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	BO	201	7,9	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
31	CYC	K1	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	MA	401	14	43,46,46	3.16	9 (20%)	45,67,67	2.86	14 (31%)
29	PEB	b9	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	J3	202	7,6	43,46,46	3.55	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	oJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	A7	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.15	14 (31%)
29	PEB	QL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	eJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	gB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	EM	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	aJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	HM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	JI	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.12	16 (35%)
29	PEB	CQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	l1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	PM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	OF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	xJ	301	-	43,46,46	3.18	10 (23%)	45,67,67	2.55	17 (37%)
29	PEB	PJ	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	M4	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	AE	203	6,7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	NO	203	7	43,46,46	3.23	11 (25%)	45,67,67	2.13	14 (31%)
29	PEB	C3	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	bL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	D3	202	-	43,46,46	3.41	9 (20%)	45,67,67	2.10	13 (28%)
29	PEB	CM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	FB	201	7,15	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
31	CYC	EI	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	e7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	DO	203	-	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	m9	203	7	43,46,46	3.50	13 (30%)	45,67,67	2.11	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	F7	1002	-	43,46,46	3.24	10 (23%)	45,67,67	2.22	17 (37%)
29	PEB	g9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	GJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	DN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	IO	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	G4	203	7	43,46,46	3.29	10 (23%)	45,67,67	2.61	18 (40%)
29	PEB	L3	202	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
31	CYC	jP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	JJ	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	N1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	bF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	HI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.10	16 (35%)
29	PEB	HA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	k1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	MN	401	14	43,46,46	3.16	9 (20%)	45,67,67	2.86	14 (31%)
29	PEB	J4	201	6	43,46,46	3.11	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	EL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	D1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.01	24 (48%)
29	PEB	I5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	JJ	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	K4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	R2	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	dD	401	7,10	43,46,46	3.17	10 (23%)	45,67,67	2.23	20 (44%)
29	PEB	DL	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	TJ	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	cB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	GC	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	YB	201	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	g7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	NF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	aF	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	H8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	kK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	S9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	BC	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.98	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	mF	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	BD	202	6	43,46,46	3.15	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	Z9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	AL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	FL	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	cM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
30	PUB	AM	304	16	42,46,46	3.14	9 (21%)	37,67,67	3.65	18 (48%)
31	CYC	FI	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	IJ	203	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	JB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	OL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	c9	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	iF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	AE	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	GB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	wL	301	-	43,46,46	3.18	10 (23%)	45,67,67	2.54	17 (37%)
29	PEB	IA	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	J8	201	6	43,46,46	3.37	11 (25%)	45,67,67	2.77	16 (35%)
29	PEB	bL	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	JE	202	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	L3	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.07	14 (31%)
29	PEB	Z7	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	eJ	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.12	13 (28%)
29	PEB	U1	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.61	14 (31%)
29	PEB	IJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
30	PUB	wJ	304	-	42,46,46	3.35	7 (16%)	37,67,67	3.30	16 (43%)
29	PEB	G5	203	7	43,46,46	3.34	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	LJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	HB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	cB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	LQ	201	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	iI	201	7	43,46,46	3.32	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	WR	202	6	43,46,46	3.60	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	U7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	HG	201	7,14	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	HE	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	C8	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	N1	1002	5	43,46,46	3.41	13 (30%)	45,67,67	2.33	18 (40%)
29	PEB	uJ	202	6	43,46,46	2.93	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	SL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	O1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	W1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	I4	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	lK	202	6	43,46,46	3.25	10 (23%)	45,67,67	2.61	15 (33%)
29	PEB	aB	203	6,7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	cL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	RR	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	FD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.72	21 (46%)
31	CYC	GP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.10	22 (44%)
29	PEB	TK	202	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	G8	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	F9	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	ZL	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.00	12 (26%)
29	PEB	lL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	ZI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	QK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	P2	202	7	43,46,46	3.42	10 (23%)	45,67,67	2.20	16 (35%)
31	CYC	vP	1001	20	42,46,46	3.40	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	fK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	JO	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	XL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	XM	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	MA	404	14	43,46,46	3.14	12 (27%)	45,67,67	2.49	13 (28%)
29	PEB	WJ	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	mB	201	7,16	43,46,46	3.36	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	gJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
30	PUB	A7	302	2	42,46,46	3.35	7 (16%)	37,67,67	3.17	18 (48%)
29	PEB	k7	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	aF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	l7	202	6	43,46,46	3.21	9 (20%)	45,67,67	2.07	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	A7	304	-	43,46,46	3.30	9 (20%)	45,67,67	2.23	14 (31%)
31	CYC	G9	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	QF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	VK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	gJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	P7	203	7	43,46,46	3.47	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	Z9	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	MQ	402	7,14	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	AK	303	2	43,46,46	3.24	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	iK	203	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	MQ	406	29,14	43,46,46	3.22	10 (23%)	45,67,67	2.48	20 (44%)
29	PEB	IJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	R1	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	VI	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	kP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	LC	202	6,7	43,46,46	3.26	11 (25%)	45,67,67	2.43	16 (35%)
29	PEB	kB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	jK	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	pJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	aB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	G8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	MJ	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	aM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	BQ	201	7,29,14	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	MR	202	6	43,46,46	3.44	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	KM	203	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	e7	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	CB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	SI	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	KN	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	OF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
31	CYC	DP	1001	25,21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	I8	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	Q2	202	6	43,46,46	3.60	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	O2	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.54	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	A3	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.16	17 (37%)
29	PEB	UI	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	CO	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	16 (35%)
29	PEB	CL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	IF	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	gM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	JA	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.26	16 (35%)
31	CYC	HK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	RF	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	F4	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	I3	203	6,7	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	D4	201	6	43,46,46	3.12	13 (30%)	45,67,67	2.72	21 (46%)
29	PEB	JQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	iM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	HN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	NM	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	C8	202	-	43,46,46	3.28	10 (23%)	45,67,67	2.21	12 (26%)
31	CYC	nP	1001	24,21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	HQ	201	7,14	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
31	CYC	gP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	YI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	UB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	AC	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	I4	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.39	15 (33%)
29	PEB	IL	202	7	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	JL	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	KQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
30	PUB	yL	302	-	42,46,46	3.35	7 (16%)	37,67,67	3.26	15 (40%)
29	PEB	PI	201	7,1	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	zJ	501	7	43,46,46	3.38	9 (20%)	45,67,67	2.03	14 (31%)
29	PEB	qJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	iP	1001	20	42,46,46	3.39	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	H5	203	7	43,46,46	3.33	10 (23%)	45,67,67	1.90	12 (26%)
30	PUB	MN	403	14	42,46,46	3.46	10 (23%)	37,67,67	3.90	16 (43%)
29	PEB	V2	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.19	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	MJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	mM	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	nJ	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	EN	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	20 (44%)
31	CYC	LF	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.03	21 (42%)
31	CYC	N7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	k1	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
31	CYC	GK	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	GL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	YF	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	BO	202	7,6	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	FJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	CJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	nL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	c9	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	TI	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
30	PUB	A7	303	-	42,46,46	3.34	7 (16%)	37,67,67	3.09	14 (37%)
29	PEB	CD	201	7	43,46,46	3.15	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	H8	202	-	43,46,46	3.25	10 (23%)	45,67,67	2.05	13 (28%)
31	CYC	FP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	EQ	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.05	13 (28%)
29	PEB	KE	203	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	BL	202	7,6	43,46,46	3.07	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	pJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	EM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
31	CYC	CK	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	UL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	LC	203	-	43,46,46	3.45	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	FJ	202	7,6	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	T9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	uL	203	6	43,46,46	3.29	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	T2	202	7	43,46,46	3.04	8 (18%)	45,67,67	2.47	17 (37%)
29	PEB	Z7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
30	PUB	AF	303	2	42,46,46	3.29	7 (16%)	37,67,67	3.30	14 (37%)
29	PEB	PJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CYC	xP	1001	21	42,46,46	3.95	18 (42%)	50,67,67	3.57	28 (56%)
29	PEB	ED	201	7	43,46,46	3.07	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	V1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	FB	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	HE	201	7	43,46,46	3.56	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	eF	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	YJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	kL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	KC	202	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	OB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.42	16 (35%)
31	CYC	EK	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	J8	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.17	16 (35%)
29	PEB	hL	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	qL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	R2	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.46	17 (37%)
29	PEB	TK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
30	PUB	MA	403	14	42,46,46	3.46	10 (23%)	37,67,67	3.89	16 (43%)
29	PEB	TR	201	7	43,46,46	3.37	12 (27%)	45,67,67	2.36	14 (31%)
29	PEB	LD	202	6	43,46,46	3.14	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	l1	202	6	43,46,46	3.25	10 (23%)	45,67,67	2.61	15 (33%)
29	PEB	bJ	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	GD	203	7	43,46,46	3.30	10 (23%)	45,67,67	2.63	18 (40%)
29	PEB	j1	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	LE	202	6,7	43,46,46	3.26	11 (25%)	45,67,67	2.43	16 (35%)
29	PEB	i7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	l1	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	vL	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	K4	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	AK	302	-	43,46,46	3.36	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	VB	202	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	LA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	K8	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	hL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	BG	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	AN	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	FG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	L8	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.89	12 (26%)
29	PEB	cI	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	i9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	QL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	FD	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	RI	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
31	CYC	YP	1000	25	42,46,46	3.41	13 (30%)	50,67,67	2.92	19 (38%)
29	PEB	WB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	QR	202	6	43,46,46	3.60	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	FL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	gI	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	xJ	303	16	43,46,46	3.43	11 (25%)	45,67,67	2.27	18 (40%)
29	PEB	BM	301	17	43,46,46	3.38	11 (25%)	45,67,67	2.41	17 (37%)
29	PEB	PF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	d7	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	S2	202	6	43,46,46	3.61	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	JG	203	7	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	e2	401	-	43,46,46	1.07	2 (4%)	45,67,67	1.01	2 (4%)
31	CYC	HF	1001	5	42,46,46	3.20	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	QB	203	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	JD	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.39	20 (44%)
29	PEB	HJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	GM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	O7	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
31	CYC	C1	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	DM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	RM	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	MG	401	14	43,46,46	3.11	11 (25%)	45,67,67	2.44	14 (31%)
29	PEB	RJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	nL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	rL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	TI	202	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	TJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	NI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	O1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	a9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	A9	305	-	43,46,46	3.31	10 (23%)	45,67,67	2.24	17 (37%)
29	PEB	aM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	BQ	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	AG	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	LQ	202	-	43,46,46	3.44	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	gF	202	7,6	43,46,46	3.15	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	J4	202	6	43,46,46	3.12	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	fJ	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	FQ	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
31	CYC	SP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.10	21 (42%)
31	CYC	D9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	FA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	FM	201	7,15	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	AG	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	dF	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	E4	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.23	20 (44%)
29	PEB	KC	201	7,6	43,46,46	3.26	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	bF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	17 (37%)
29	PEB	IM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	UB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	iF	201	7	43,46,46	3.32	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	cK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	GL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	GC	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	pL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
31	CYC	N9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	RL	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	LM	202	7,6	43,46,46	3.18	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	LE	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	BJ	202	7,6	43,46,46	3.07	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	DK	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	B3	201	7,9	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	U1	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	hI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	gI	202	7,6	43,46,46	3.15	10 (23%)	45,67,67	2.59	14 (31%)
31	CYC	hP	1001	25,21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
31	CYC	LK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	FC	201	7,18	43,46,46	3.57	12 (27%)	45,67,67	2.18	16 (35%)
29	PEB	V1	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	RK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	DM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	eB	202	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	FN	201	7	43,46,46	3.23	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	a1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	g9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	N3	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	mJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	fJ	201	7,16	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	ZL	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	E3	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	dJ	202	7,6	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	fL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
29	PEB	KN	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	I5	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.12	14 (31%)
29	PEB	FO	201	7,9	43,46,46	3.44	11 (25%)	45,67,67	2.08	16 (35%)
30	PUB	A1	304	2	42,46,46	3.54	8 (19%)	37,67,67	3.22	16 (43%)
29	PEB	BN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	P9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	j7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	gM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
31	CYC	KK	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	ZB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	T2	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	UF	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	NK	1001	5,3	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	Y7	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	k7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	iB	201	7,16	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	HQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
31	CYC	1P	1002	25	42,46,46	3.42	13 (30%)	50,67,67	2.93	19 (38%)
29	PEB	VK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	NM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	dK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	bI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	17 (37%)
29	PEB	DD	201	6	43,46,46	3.11	13 (30%)	45,67,67	2.72	21 (46%)
29	PEB	BD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.73	21 (46%)
29	PEB	AO	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.16	17 (37%)
29	PEB	YM	201	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	MA	405	14	43,46,46	3.20	12 (27%)	45,67,67	2.60	16 (35%)
29	PEB	GQ	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	O2	202	6	43,46,46	3.61	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	h9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
30	PUB	AF	302	2	42,46,46	3.54	8 (19%)	37,67,67	3.18	15 (40%)
29	PEB	AJ	203	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
30	PUB	xJ	305	16	42,46,46	3.28	8 (19%)	37,67,67	3.74	15 (40%)
29	PEB	CN	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	m9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	U2	202	-	43,46,46	3.60	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	oJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	K7	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	K4	203	7	43,46,46	3.29	10 (23%)	45,67,67	2.62	18 (40%)
30	PUB	MN	402	14	42,46,46	3.43	7 (16%)	37,67,67	3.76	19 (51%)
29	PEB	QJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	L1	1002	-	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	j9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
31	CYC	mP	1001	20	42,46,46	3.39	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	d1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	C7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.81	21 (42%)
29	PEB	HD	202	6	43,46,46	3.12	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	HB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	GE	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	JM	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	IO	203	6,7	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	AL	203	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	VL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	ZM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	V2	201	7,8	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	mL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	h1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	lK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	JM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	YI	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	CQ	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.06	14 (31%)
29	PEB	OI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	cL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	HA	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	DA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
31	CYC	H1	1001	5	42,46,46	3.20	13 (30%)	50,67,67	2.98	24 (48%)
29	PEB	NK	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	L5	201	7	43,46,46	3.27	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	M3	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	J3	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	XM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	SB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	UK	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.61	14 (31%)
29	PEB	oL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	ZB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	aK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	bK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	V7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	d7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	V9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	QJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	KE	201	7,6	43,46,46	3.26	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	RF	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	HC	201	7	43,46,46	3.56	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	jF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	cP	1001	20	42,46,46	3.39	15 (35%)	50,67,67	3.10	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	GG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	fM	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	gL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	PL	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	JN	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	KQ	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	14 (31%)
29	PEB	mK	202	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	X2	202	7	43,46,46	3.42	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	E4	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	YF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	i9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	FL	202	7,6	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
31	CYC	MI	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	GG	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	WJ	203	6	43,46,46	3.29	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	dM	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	TL	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	BA	203	-	43,46,46	3.29	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	kM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	NR	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	18 (40%)
29	PEB	A8	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	IJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
31	CYC	I7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	MD	202	6,7	43,46,46	3.07	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	DQ	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.07	16 (35%)
29	PEB	jK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	MO	202	7	43,46,46	3.35	10 (23%)	45,67,67	2.24	13 (28%)
29	PEB	F4	201	6	43,46,46	3.14	13 (30%)	45,67,67	2.73	21 (46%)
29	PEB	CJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	rJ	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
32	PMS	k6	302	-	11,11,11	1.23	1 (9%)	14,15,15	1.08	1 (7%)
29	PEB	ZM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
31	CYC	MF	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	U9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	b1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	CC	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	B8	203	7	43,46,46	3.35	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	RK	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	A9	304	-	43,46,46	3.30	10 (23%)	45,67,67	2.23	14 (31%)
29	PEB	UL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	dI	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	IL	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	GO	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	iJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	dL	201	7	43,46,46	3.32	9 (20%)	45,67,67	2.99	15 (33%)
29	PEB	kI	201	7,2	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	aM	203	6,7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	N3	202	7	43,46,46	3.35	10 (23%)	45,67,67	2.24	13 (28%)
29	PEB	vJ	201	7	43,46,46	3.33	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	V9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
31	CYC	FK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	F8	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	OF	203	6,7	43,46,46	3.15	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	Q7	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	gM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	EC	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	cI	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	ZB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
30	PUB	MG	402	14	42,46,46	3.70	9 (21%)	37,67,67	4.02	21 (56%)
29	PEB	aK	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	P1	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	HM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	a7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	CL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	YI	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	L5	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.89	12 (26%)
29	PEB	P7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	AB	303	16	43,46,46	3.35	10 (23%)	45,67,67	2.18	14 (31%)
30	PUB	AK	304	2	42,46,46	3.54	8 (19%)	37,67,67	3.22	16 (43%)
29	PEB	jM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	QM	203	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	JQ	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	VI	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	PI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	rL	201	7,16	43,46,46	3.30	9 (20%)	45,67,67	2.98	15 (33%)
29	PEB	gK	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
31	CYC	JI	1001	5,3	42,46,46	3.19	14 (33%)	50,67,67	3.02	21 (42%)
29	PEB	e7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	F5	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	aF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	HK	1002	-	43,46,46	3.44	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	AN	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.89	20 (44%)
29	PEB	JJ	203	7	43,46,46	3.41	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	RJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	C5	202	-	43,46,46	3.28	10 (23%)	45,67,67	2.21	12 (26%)
29	PEB	BA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	TB	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	EC	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	VF	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	G5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	I3	201	6	43,46,46	3.28	11 (25%)	45,67,67	2.17	17 (37%)
29	PEB	GJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	m9	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	I8	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.21	12 (26%)
29	PEB	FF	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	PK	201	7,1	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	T1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	AC	203	6,7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	mJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	GB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	ZL	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	E3	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	CD	203	-	43,46,46	3.29	10 (23%)	45,67,67	2.60	18 (40%)
29	PEB	JA	203	-	43,46,46	3.29	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	i7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	MM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	T1	202	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	FK	1002	5	43,46,46	3.43	13 (30%)	45,67,67	2.35	17 (37%)
29	PEB	BG	201	7	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	T9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	eI	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	IQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	m1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	P2	201	7	43,46,46	3.04	9 (20%)	45,67,67	2.48	17 (37%)
29	PEB	cJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	VM	202	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	UK	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	VB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	LO	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.07	14 (31%)
30	PUB	wL	304	-	42,46,46	3.33	7 (16%)	37,67,67	3.30	16 (43%)
29	PEB	DC	202	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	H7	1002	-	43,46,46	3.22	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	R9	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
31	CYC	J7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	HE	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	kF	202	7,6	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	PM	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
31	CYC	H9	1001	5	42,46,46	3.03	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	eI	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	c7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	P1	202	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	yJ	301	-	43,46,46	3.29	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	cM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	TJ	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	OK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	AB	302	6,16	43,46,46	3.34	8 (18%)	45,67,67	2.01	13 (28%)
29	PEB	ID	203	7	43,46,46	3.29	10 (23%)	45,67,67	2.62	18 (40%)
29	PEB	C4	202	7,6	43,46,46	3.06	11 (25%)	45,67,67	2.58	15 (33%)
29	PEB	gK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	jJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.98	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	QM	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	a7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	fL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	sL	203	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	TR	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	QF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	iF	202	6,7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	j1	203	6,7	43,46,46	3.10	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	M4	203	7	43,46,46	3.41	9 (20%)	45,67,67	2.28	14 (31%)
29	PEB	jF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	OJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
31	CYC	E9	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	fF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	V1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	i9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	JK	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
31	CYC	TP	1001	20	42,46,46	3.39	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	f7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	G5	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
31	CYC	CI	1001	4,5	42,46,46	3.08	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	LN	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	AA	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	SM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	QB	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	JO	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	DQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	XL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	A5	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	EN	201	6	43,46,46	3.04	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	QR	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	RB	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	uJ	201	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	D7	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	g1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	N9	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	i7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	XL	202	6,7	43,46,46	3.07	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	BC	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.42	15 (33%)
29	PEB	k9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	DD	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.39	20 (44%)
29	PEB	M3	202	7	43,46,46	3.35	10 (23%)	45,67,67	2.24	13 (28%)
29	PEB	e1	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	J7	1002	-	43,46,46	3.24	10 (23%)	45,67,67	2.22	17 (37%)
29	PEB	P9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	U9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	KO	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	ID	201	7	43,46,46	3.15	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	CC	202	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	RL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	DJ	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	wL	305	16	42,46,46	3.28	7 (16%)	37,67,67	3.74	15 (40%)
29	PEB	kK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	k7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	HF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.10	16 (35%)
29	PEB	PF	201	7,1	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	kF	201	7,2	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	ID	202	7	43,46,46	3.07	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	cM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	HC	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	KM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	h9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	AI	305	6,2	43,46,46	3.26	8 (18%)	45,67,67	1.98	13 (28%)
29	PEB	C4	203	7	43,46,46	3.28	10 (23%)	45,67,67	2.61	18 (40%)
29	PEB	FM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	BE	201	7	43,46,46	3.56	11 (25%)	45,67,67	2.18	16 (35%)
29	PEB	DM	201	7,17	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	EQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	LG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	R1	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	ZK	201	7,6	43,46,46	3.08	9 (20%)	45,67,67	2.59	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	cK	202	7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	eB	201	7,16	43,46,46	3.35	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	A5	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	YM	202	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	JE	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
31	CYC	IP	1001	20	42,46,46	3.37	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	j1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	TM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	wJ	303	16	43,46,46	3.44	12 (27%)	45,67,67	2.28	18 (40%)
29	PEB	XB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	EE	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	JG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	ZI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	pL	202	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	mM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	GE	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	XJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	TB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	dJ	201	7	43,46,46	3.32	9 (20%)	45,67,67	2.99	15 (33%)
29	PEB	OK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	gK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	KE	202	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	UJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	WK	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
31	CYC	DK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	CD	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	K5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	EG	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.05	13 (28%)
29	PEB	iI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	HN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	OR	202	6	43,46,46	3.39	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	ML	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	UF	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	RJ	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	FC	203	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	MD	203	7	43,46,46	3.30	10 (23%)	45,67,67	2.63	18 (40%)
29	PEB	H3	201	7,9	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	e2	402	7,8	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	A9	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.15	14 (31%)
29	PEB	RK	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	SR	201	6	43,46,46	3.43	11 (25%)	45,67,67	2.52	14 (31%)
29	PEB	xL	301	-	43,46,46	3.18	10 (23%)	45,67,67	2.56	17 (37%)
29	PEB	g9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	D9	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	IM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
31	CYC	KF	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	H5	202	-	43,46,46	3.25	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	dL	202	7,6	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	A8	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	KA	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	JL	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	I5	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	FO	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	MB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	B5	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
31	CYC	UP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	P9	203	7	43,46,46	3.47	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	NL	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	aI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	DG	203	-	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	F1	1002	5	43,46,46	3.43	13 (30%)	45,67,67	2.35	17 (37%)
29	PEB	hK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	J1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	TF	201	7	43,46,46	3.41	11 (25%)	45,67,67	2.10	15 (33%)
29	PEB	hI	201	6	43,46,46	3.24	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	BB	301	17	43,46,46	3.38	11 (25%)	45,67,67	2.41	17 (37%)
29	PEB	KC	203	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	FN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.27	16 (35%)
29	PEB	HM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	EE	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	jI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	MD	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	Y9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	aJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	FM	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	NJ	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	SF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	T9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	JN	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	jB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	YM	203	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	EB	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	TM	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	VR	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	CG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	FE	203	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	WI	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	NP	1001	20,19	42,46,46	3.39	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	AM	301	16	43,46,46	3.29	11 (25%)	45,67,67	2.34	19 (42%)
29	PEB	l9	202	6	43,46,46	3.21	9 (20%)	45,67,67	2.07	13 (28%)
31	CYC	JF	1001	5,3	42,46,46	3.19	14 (33%)	50,67,67	3.02	21 (42%)
31	CYC	II	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	G4	202	7	43,46,46	3.05	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	Q1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
30	PUB	AB	305	16	42,46,46	3.41	7 (16%)	37,67,67	3.01	15 (40%)
29	PEB	T2	201	7	43,46,46	3.37	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	dM	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	Y7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	16 (35%)
31	CYC	DI	1001	5	42,46,46	3.20	14 (33%)	50,67,67	3.02	21 (42%)
29	PEB	OJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	GN	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	21 (46%)
29	PEB	yL	301	-	43,46,46	3.29	10 (23%)	45,67,67	2.21	16 (35%)
31	CYC	yP	1001	-	42,46,46	3.49	15 (35%)	50,67,67	2.92	20 (40%)
29	PEB	Z1	201	7,6	43,46,46	3.08	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	ZJ	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.00	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	O9	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	IE	201	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	KL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	B5	201	7	43,46,46	3.27	10 (23%)	45,67,67	2.15	16 (35%)
31	CYC	IP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	L9	1002	-	43,46,46	3.24	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	mB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	HB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	IG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	IL	203	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	BJ	201	7,19	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	L8	201	7	43,46,46	3.27	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	HL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	fl	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	NB	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	cB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	D4	202	6	43,46,46	3.12	10 (23%)	45,67,67	2.39	20 (44%)
29	PEB	GD	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	K5	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.13	14 (31%)
31	CYC	MK	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	tJ	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	KL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	gB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	JO	202	7,6	43,46,46	3.55	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	b9	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	RB	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	AM	302	6,16	43,46,46	3.35	8 (18%)	45,67,67	2.01	13 (28%)
29	PEB	dF	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	F9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	25 (50%)
29	PEB	VF	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	vJ	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	IL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	xJ	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.25	19 (42%)
29	PEB	W7	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	jJ	202	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	AI	301	2	43,46,46	3.23	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	zL	501	7	43,46,46	3.36	9 (20%)	45,67,67	2.02	14 (31%)
29	PEB	sL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	BQ	203	-	43,46,46	3.45	9 (20%)	45,67,67	2.18	16 (35%)
31	CYC	F1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	k9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	xL	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.26	19 (42%)
29	PEB	MO	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	AF	305	6,2	43,46,46	3.26	8 (18%)	45,67,67	1.98	13 (28%)
29	PEB	UI	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	rP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.10	22 (44%)
29	PEB	S1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	TB	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	wJ	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.26	19 (42%)
29	PEB	C5	201	7	43,46,46	3.32	10 (23%)	45,67,67	2.12	14 (31%)
29	PEB	NJ	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	QM	201	6,17	42,46,46	3.60	8 (19%)	37,67,67	3.06	14 (37%)
31	CYC	G7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	P7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	PF	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
30	PUB	AB	304	16	42,46,46	3.14	9 (21%)	37,67,67	3.65	18 (48%)
29	PEB	m7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	fF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	rJ	201	7	43,46,46	3.30	9 (20%)	45,67,67	2.98	15 (33%)
29	PEB	kB	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	jJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
29	PEB	ZM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	NO	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	O7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	FE	201	7,18	43,46,46	3.57	12 (27%)	45,67,67	2.18	16 (35%)
29	PEB	MG	404	14	43,46,46	3.22	10 (23%)	45,67,67	2.49	20 (44%)
29	PEB	KJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	II	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
31	CYC	qP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	HO	202	6,7	43,46,46	3.53	13 (30%)	45,67,67	2.12	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	LA	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	b1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	wJ	301	-	43,46,46	3.17	10 (23%)	45,67,67	2.54	17 (37%)
29	PEB	IO	201	6	43,46,46	3.28	11 (25%)	45,67,67	2.17	17 (37%)
29	PEB	H9	1002	-	43,46,46	3.22	10 (23%)	45,67,67	2.21	17 (37%)
31	CYC	uP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	ZK	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	DI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	f1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	XR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	aB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	G4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	Y1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	X2	201	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	17 (37%)
29	PEB	DQ	203	-	43,46,46	3.45	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	Q2	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.54	18 (40%)
31	CYC	KP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	PK	202	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	IL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	V7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	ZF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	UR	202	6	43,46,46	3.61	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	aL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	jL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
29	PEB	W9	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	V2	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	18 (40%)
29	PEB	kM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	KB	203	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	Z1	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	KO	202	6	43,46,46	3.61	12 (27%)	45,67,67	1.97	15 (33%)
29	PEB	j9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	W9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	BC	201	7	43,46,46	3.56	11 (25%)	45,67,67	2.18	16 (35%)
29	PEB	V9	203	7	43,46,46	3.47	12 (27%)	45,67,67	2.10	14 (31%)
29	PEB	AF	301	2	43,46,46	3.23	10 (23%)	45,67,67	2.14	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	HD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	LO	202	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	AI	304	2	43,46,46	3.29	10 (23%)	45,67,67	2.25	15 (33%)
29	PEB	RR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	a1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	M4	202	6,7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	A3	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	DE	202	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	YB	202	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	TM	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	B8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	ML	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	xL	303	16	43,46,46	3.43	10 (23%)	45,67,67	2.28	18 (40%)
29	PEB	XB	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	F8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	LC	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	F3	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	fK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	AO	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	eF	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	hF	201	6	43,46,46	3.24	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	RM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	WL	203	6	43,46,46	3.29	10 (23%)	45,67,67	2.12	13 (28%)
31	CYC	L7	1001	5	42,46,46	3.03	15 (35%)	50,67,67	3.23	26 (52%)
29	PEB	EJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	EO	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	fL	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	AQ	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	b7	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	JQ	203	7	43,46,46	3.46	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	uL	202	6	43,46,46	2.93	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	MO	203	7	43,46,46	3.23	11 (25%)	45,67,67	2.14	14 (31%)
29	PEB	AB	301	16	43,46,46	3.29	11 (25%)	45,67,67	2.34	19 (42%)
29	PEB	MQ	403	14	43,46,46	3.10	12 (27%)	45,67,67	2.44	14 (31%)
31	CYC	K9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.81	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	e9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	ZJ	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	hB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	a9	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	C8	201	7	43,46,46	3.32	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	LM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
31	CYC	L9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.23	26 (52%)
29	PEB	kB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	S2	201	6	43,46,46	3.45	11 (25%)	45,67,67	2.17	14 (31%)
29	PEB	PL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	d9	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
31	CYC	VP	1001	21	42,46,46	3.95	18 (42%)	50,67,67	3.57	28 (56%)
29	PEB	MN	405	14	43,46,46	3.19	12 (27%)	45,67,67	2.60	16 (35%)
29	PEB	R7	201	7,1	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	f7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	B3	202	7,6	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	nJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	IQ	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	AJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	Y7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	jI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	PK	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	h7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	VJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	iI	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	BO	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	AJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	DJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	LE	203	-	43,46,46	3.45	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	MB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	KM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	BN	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	SJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	BG	203	-	43,46,46	3.46	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	eI	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CYC	wP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	iM	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	VJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	CE	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	FI	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)

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
31	CYC	GI	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	fB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	PB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	c7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	S9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	FN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	A1	303	2	-	9/24/74/74	0/4/4/4
29	PEB	T7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	AL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	QK	201	6	-	8/24/74/74	0/4/4/4
31	CYC	M7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	DA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	mF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	RM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	FB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	a7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	qL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	eK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	S1	202	6	-	9/24/74/74	0/4/4/4
31	CYC	MP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	e9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	NL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	aI	201	7	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	aK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	Q1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	dB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	E4	203	-	-	11/24/74/74	0/4/4/4
29	PEB	LL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	J5	201	6	-	5/24/74/74	0/4/4/4
29	PEB	NO	202	7	-	10/24/74/74	0/4/4/4
29	PEB	iL	202	6	-	10/24/74/74	0/4/4/4
31	CYC	C9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	CA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	JC	202	-	-	9/24/74/74	0/4/4/4
31	CYC	I9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	IN	201	6	-	10/24/74/74	0/4/4/4
31	CYC	E1	1001	4,5	-	9/25/74/74	0/4/4/4
29	PEB	LN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	B3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	f9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	A1	301	2	-	10/24/74/74	0/4/4/4
29	PEB	iJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	VM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	gL	202	6	-	10/24/74/74	0/4/4/4
32	PMS	kH	301	-	-	2/5/5/5	0/1/1/1
29	PEB	VL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	H8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	dK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	RB	203	7	-	13/24/74/74	0/4/4/4
31	CYC	CF	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	RI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	AM	303	16	-	13/24/74/74	0/4/4/4
29	PEB	R1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	R7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	IM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	JB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	AF	304	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	L7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	W7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	k9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	c1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LK	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	kM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	bL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	RL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	mI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	OR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	UJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	tL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	EG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	kF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	rL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	mM	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	cF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	MG	405	14	-	11/24/74/74	0/4/4/4
29	PEB	VM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	UK	201	7,6	-	6/24/74/74	0/4/4/4
32	PMS	kH	302	-	-	2/5/5/5	0/1/1/1
31	CYC	sP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	SL	201	6	-	9/24/74/74	0/4/4/4
30	PUB	QB	201	6,17	-	6/24/74/74	0/4/4/4
29	PEB	B8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	BE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	PL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	S7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	g1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	ZK	203	6	-	9/24/74/74	0/4/4/4
29	PEB	I4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	bK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	MN	404	14	-	11/24/74/74	0/4/4/4
29	PEB	HA	203	-	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	mI	203	7	-	14/24/74/74	0/4/4/4
31	CYC	tP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	hJ	203	7	-	13/24/74/74	0/4/4/4
30	PUB	A9	303	-	-	8/24/74/74	0/4/4/4
29	PEB	H5	201	7	-	7/24/74/74	0/4/4/4
29	PEB	IG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	M3	203	7	-	10/24/74/74	0/4/4/4
29	PEB	P1	201	7,1	-	6/24/74/74	0/4/4/4
29	PEB	cF	202	7	-	14/24/74/74	0/4/4/4
29	PEB	dJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	CO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	TL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	gF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	WF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	NR	201	7	-	9/24/74/74	0/4/4/4
31	CYC	I1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	C4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	K3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	KB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	A7	305	-	-	10/24/74/74	0/4/4/4
31	CYC	EF	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	UF	203	6	-	8/24/74/74	0/4/4/4
31	CYC	M9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	IE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	N7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	H3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	L5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	AE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	B4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	nL	202	6,7	-	9/24/74/74	0/4/4/4
31	CYC	eP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	KB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	U7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	DO	201	7	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	eM	202	7	-	13/24/74/74	0/4/4/4
30	PUB	AI	303	2	-	6/24/74/74	0/4/4/4
29	PEB	dI	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	sJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	DL	201	7	-	7/24/74/74	0/4/4/4
31	CYC	E7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	JD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	iI	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	RR	202	7	-	7/24/74/74	0/4/4/4
31	CYC	CP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	D1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	WK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	A1	302	-	-	9/24/74/74	0/4/4/4
29	PEB	l9	201	6	-	8/24/74/74	0/4/4/4
31	CYC	oP	1001	21	-	8/25/74/74	0/4/4/4
30	PUB	A1	305	-	-	13/24/74/74	0/4/4/4
29	PEB	FA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	LI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	LG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	M2	202	6	-	10/24/74/74	0/4/4/4
29	PEB	JA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	kI	202	7,6	-	7/24/74/74	0/4/4/4
31	CYC	PP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	ED	202	7	-	11/24/74/74	0/4/4/4
29	PEB	hJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	U2	201	6	-	7/24/74/74	0/4/4/4
29	PEB	hF	202	6	-	8/24/74/74	0/4/4/4
31	CYC	FF	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	e1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	l7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	LJ	202	7	-	13/24/74/74	0/4/4/4
30	PUB	A9	302	2	-	5/24/74/74	0/4/4/4
29	PEB	iI	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	R9	201	7,1	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	HG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	SK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	k1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	cJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	FE	202	7	-	8/24/74/74	0/4/4/4
29	PEB	HQ	203	7	-	12/24/74/74	0/4/4/4
29	PEB	DA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	YL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	mF	202	7	-	7/24/74/74	0/4/4/4
29	PEB	SR	202	6	-	10/24/74/74	0/4/4/4
29	PEB	LF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	J1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	K8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	DG	201	7	-	10/24/74/74	0/4/4/4
29	PEB	eK	202	6,7	-	6/24/74/74	0/4/4/4
31	CYC	EP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	dF	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	f1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	YK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	MR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	g7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	dB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	YF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	UR	201	6	-	7/24/74/74	0/4/4/4
30	PUB	yJ	303	-	-	5/24/74/74	0/4/4/4
29	PEB	WR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	sL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	Y1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	FO	202	7,6	-	9/24/74/74	0/4/4/4
30	PUB	MQ	404	14	-	15/24/74/74	0/4/4/4
29	PEB	DN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	H3	202	6,7	-	9/24/74/74	0/4/4/4
30	PUB	AK	305	-	-	13/24/74/74	0/4/4/4
29	PEB	B5	203	7	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	TF	202	7	-	14/24/74/74	0/4/4/4
31	CYC	XP	1001	24,21	-	8/25/74/74	0/4/4/4
30	PUB	BB	302	17	-	7/24/74/74	0/4/4/4
29	PEB	BJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	LG	201	7,14	-	10/24/74/74	0/4/4/4
29	PEB	lB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	oL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	h7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	SJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	GO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	K5	203	7	-	9/24/74/74	0/4/4/4
29	PEB	VR	201	7	-	9/24/74/74	0/4/4/4
30	PUB	MG	403	14	-	10/24/74/74	0/4/4/4
29	PEB	JF	1002	4	-	13/24/74/74	0/4/4/4
31	CYC	DF	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	PR	202	7	-	12/24/74/74	0/4/4/4
31	CYC	M1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	R2	201	7	-	9/24/74/74	0/4/4/4
29	PEB	VK	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	L4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	PJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	LM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	N2	201	7	-	9/24/74/74	0/4/4/4
29	PEB	fl	201	6	-	6/24/74/74	0/4/4/4
29	PEB	WM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	MQ	401	6,14	-	10/24/74/74	0/4/4/4
29	PEB	PB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	QI	201	6	-	6/24/74/74	0/4/4/4
31	CYC	JP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	Q9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	sJ	203	6,7	-	9/24/74/74	0/4/4/4
30	PUB	xL	305	16	-	5/24/74/74	0/4/4/4
31	CYC	JK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	SM	202	6	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	kI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	JN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	UI	202	6	-	6/24/74/74	0/4/4/4
29	PEB	Z1	202	6	-	8/24/74/74	0/4/4/4
29	PEB	hJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	bJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	O9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	QI	202	6	-	8/24/74/74	0/4/4/4
31	CYC	RP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	A5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	DB	201	7,17	-	6/24/74/74	0/4/4/4
29	PEB	W2	201	6	-	7/24/74/74	0/4/4/4
29	PEB	JL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	AQ	202	6	-	12/24/74/74	0/4/4/4
31	CYC	BP	1001	25,21	-	8/25/74/74	0/4/4/4
29	PEB	wL	303	16	-	14/24/74/74	0/4/4/4
29	PEB	LL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	LD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	CB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	CN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	LA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	H4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	vL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	IC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	g1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	g7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	jM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	PI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	aL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	iL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	CM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	NJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	jL	201	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	R7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	DE	201	7,18	-	6/24/74/74	0/4/4/4
29	PEB	h1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	SF	201	6	-	6/24/74/74	0/4/4/4
31	CYC	fP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	GA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	XJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	EA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	Q7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	fB	201	6	-	5/24/74/74	0/4/4/4
30	PUB	AI	302	2	-	9/24/74/74	0/4/4/4
29	PEB	IC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	lF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	KD	202	7,6	-	12/24/74/74	0/4/4/4
29	PEB	WM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	WJ	202	6	-	9/24/74/74	0/4/4/4
29	PEB	DC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	jL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	F5	201	7	-	7/24/74/74	0/4/4/4
29	PEB	GD	202	7	-	12/24/74/74	0/4/4/4
29	PEB	G3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	I3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	jK	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	lB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	XJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	G8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	GN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	B4	202	6	-	11/24/74/74	0/4/4/4
31	CYC	GF	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	HO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	hM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	VF	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	lF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	PR	201	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	BE	202	7	-	8/24/74/74	0/4/4/4
29	PEB	hB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	m7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	N2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	VR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	KA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	FC	202	7	-	8/24/74/74	0/4/4/4
31	CYC	KI	1001	4	-	8/25/74/74	0/4/4/4
31	CYC	IK	1001	4,5	-	9/25/74/74	0/4/4/4
29	PEB	VB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	d9	201	6	-	8/24/74/74	0/4/4/4
32	PMS	k6	301	-	-	2/5/5/5	0/1/1/1
29	PEB	F8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	FG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	wL	302	-	-	7/24/74/74	0/4/4/4
30	PUB	yJ	302	-	-	7/24/74/74	0/4/4/4
29	PEB	uJ	203	6	-	10/24/74/74	0/4/4/4
29	PEB	iK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	CG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	m7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	BL	201	7,19	-	7/24/74/74	0/4/4/4
29	PEB	FQ	203	-	-	12/24/74/74	0/4/4/4
29	PEB	eR	401	-	-	9/24/74/74	0/4/4/4
29	PEB	A8	202	-	-	9/24/74/74	0/4/4/4
29	PEB	JB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	GA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	c9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	KJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	OM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	I8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	KG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	DB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	NL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	m1	202	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	aI	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	DG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	KD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	V7	203	7	-	12/24/74/74	0/4/4/4
31	CYC	J9	1001	5	-	9/25/74/74	0/4/4/4
30	PUB	xJ	304	-	-	9/24/74/74	0/4/4/4
29	PEB	EJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	iM	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	CA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	AK	301	2	-	10/24/74/74	0/4/4/4
29	PEB	HN	201	7	-	12/24/74/74	0/4/4/4
30	PUB	xL	304	-	-	9/24/74/74	0/4/4/4
31	CYC	H7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	YB	203	6	-	10/24/74/74	0/4/4/4
29	PEB	Y9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	c1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	T7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	hM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	WB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	HO	201	7,9	-	5/24/74/74	0/4/4/4
29	PEB	YK	202	7	-	6/24/74/74	0/4/4/4
31	CYC	1P	1001	25,21	-	8/25/74/74	0/4/4/4
29	PEB	C5	203	7	-	9/24/74/74	0/4/4/4
30	PUB	MQ	405	14	-	10/24/74/74	0/4/4/4
29	PEB	EB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	lM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	SI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	sJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	WI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	BA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	Q9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	EL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	i1	203	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	lJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	jB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	OI	203	6,7	-	7/24/74/74	0/4/4/4
29	PEB	G3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	BN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	ZJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	hK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	MM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	IB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	W1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	ZF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	L4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	GQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	OM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	H1	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	AA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	mL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	mB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	gB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	QM	204	6	-	10/24/74/74	0/4/4/4
29	PEB	L8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	IB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	HG	203	7	-	12/24/74/74	0/4/4/4
31	CYC	F7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	f9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	tJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	R9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	iB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	LN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	DF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	eK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	uL	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	DB	202	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	C3	201	6	-	4/24/74/74	0/4/4/4
30	PUB	yL	303	-	-	5/24/74/74	0/4/4/4
29	PEB	K8	202	-	-	9/24/74/74	0/4/4/4
29	PEB	W2	202	6	-	10/24/74/74	0/4/4/4
29	PEB	H4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	OL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	KG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	KD	203	-	-	11/24/74/74	0/4/4/4
30	PUB	AM	305	16	-	7/24/74/74	0/4/4/4
31	CYC	pP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	HJ	201	7	-	9/24/74/74	0/4/4/4
29	PEB	QB	204	6	-	10/24/74/74	0/4/4/4
29	PEB	LB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	d1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	VI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	EO	201	6	-	4/24/74/74	0/4/4/4
31	CYC	L1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	Y9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	kJ	202	6	-	10/24/74/74	0/4/4/4
30	PUB	MA	402	14	-	8/24/74/74	0/4/4/4
29	PEB	U1	202	6	-	8/24/74/74	0/4/4/4
29	PEB	e1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	j7	201	6	-	8/24/74/74	0/4/4/4
30	PUB	wJ	305	16	-	5/24/74/74	0/4/4/4
29	PEB	JC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	D3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	EA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	kL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	bI	201	6	-	6/24/74/74	0/4/4/4
31	CYC	WP	1001	-	-	8/25/74/74	0/4/4/4
29	PEB	qJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	LB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	OI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	DO	202	-	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	hL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	c7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	S7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	T7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	F3	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	DN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	YJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	XR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	c1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	CE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	UM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	GM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	fM	201	6	-	5/24/74/74	0/4/4/4
31	CYC	NI	1001	5,3	-	7/25/74/74	0/4/4/4
31	CYC	D1	1003	4,5	-	9/25/74/74	0/4/4/4
31	CYC	D7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	JG	201	7	-	10/24/74/74	0/4/4/4
29	PEB	WF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	HL	201	7	-	9/24/74/74	0/4/4/4
29	PEB	NB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	eL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	J5	202	6	-	8/24/74/74	0/4/4/4
29	PEB	TR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	kJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	J3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	iB	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	SK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	mK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	tL	201	7	-	7/24/74/74	0/4/4/4
31	CYC	HP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	D3	201	7	-	5/24/74/74	0/4/4/4
31	CYC	LI	1001	5	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	MQ	407	14	-	11/24/74/74	0/4/4/4
29	PEB	iK	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	YL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	F3	201	7,9	-	5/24/74/74	0/4/4/4
31	CYC	NF	1001	5,3	-	7/25/74/74	0/4/4/4
29	PEB	HC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	eM	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	pJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	a1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	cK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	TL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	OB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	NR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	WL	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	IN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	bJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	FA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	M2	201	6	-	7/24/74/74	0/4/4/4
31	CYC	OP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	FJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	mI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	eF	202	7	-	7/24/74/74	0/4/4/4
29	PEB	e9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	rJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	F5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	SB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	AC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	WL	202	6	-	9/24/74/74	0/4/4/4
29	PEB	K3	201	6	-	4/24/74/74	0/4/4/4
30	PUB	BM	302	17	-	7/24/74/74	0/4/4/4
29	PEB	fJ	203	7	-	13/24/74/74	0/4/4/4
31	CYC	QP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	LB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	pL	201	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	dI	203	6	-	8/24/74/74	0/4/4/4
31	CYC	HI	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	a9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	FG	201	7,14	-	10/24/74/74	0/4/4/4
29	PEB	eL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	J9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	N3	203	7	-	10/24/74/74	0/4/4/4
29	PEB	nJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	XR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	N2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	FQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	lJ	202	7	-	9/24/74/74	0/4/4/4
31	CYC	AP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	b7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	dL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BO	201	7,9	-	5/24/74/74	0/4/4/4
31	CYC	K1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	MA	401	14	-	12/24/74/74	0/4/4/4
29	PEB	b9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	J3	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	oJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	A7	301	2	-	9/24/74/74	0/4/4/4
29	PEB	QL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	eJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	gB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	EM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	aJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	HM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	JI	1002	4	-	13/24/74/74	0/4/4/4
29	PEB	CQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	l1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	PM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	OF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	xJ	301	-	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	PJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	M4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	AE	203	6,7	-	8/24/74/74	0/4/4/4
29	PEB	NO	203	7	-	10/24/74/74	0/4/4/4
29	PEB	C3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	bL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	D3	202	-	-	12/24/74/74	0/4/4/4
29	PEB	CM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	FB	201	7,15	-	6/24/74/74	0/4/4/4
31	CYC	EI	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	e7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	DO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	m9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	F7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	g9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	GJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	DN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	IO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	G4	203	7	-	11/24/74/74	0/4/4/4
29	PEB	L3	202	-	-	10/24/74/74	0/4/4/4
31	CYC	jP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	JJ	201	7	-	7/24/74/74	0/4/4/4
31	CYC	N1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	bF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	HI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	HA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	k1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	MN	401	14	-	12/24/74/74	0/4/4/4
29	PEB	J4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	EL	202	6	-	10/24/74/74	0/4/4/4
31	CYC	D1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	I5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	JJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	K4	201	7	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	R2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	dD	401	7,10	-	9/24/74/74	0/4/4/4
29	PEB	DL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	TJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	cB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	GC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	YB	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	g7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	NF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	aF	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	H8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	S9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	BC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	mF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	BD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	Z9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	AL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	FL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	cM	201	7	-	6/24/74/74	0/4/4/4
30	PUB	AM	304	16	-	13/24/74/74	0/4/4/4
31	CYC	FI	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	IJ	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	JB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	OL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	c9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	iF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	AE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	GB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	wL	301	-	-	12/24/74/74	0/4/4/4
29	PEB	IA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	J8	201	6	-	5/24/74/74	0/4/4/4
29	PEB	bL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JE	202	-	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	L3	201	7	-	5/24/74/74	0/4/4/4
29	PEB	Z7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	eJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	U1	203	6	-	9/24/74/74	0/4/4/4
29	PEB	IJ	202	6	-	10/24/74/74	0/4/4/4
30	PUB	wJ	304	-	-	9/24/74/74	0/4/4/4
29	PEB	G5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	LJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	HB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	cB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LQ	201	7	-	6/24/74/74	0/4/4/4
29	PEB	iI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	WR	202	6	-	10/24/74/74	0/4/4/4
29	PEB	U7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	HG	201	7,14	-	10/24/74/74	0/4/4/4
29	PEB	HE	202	7	-	8/24/74/74	0/4/4/4
29	PEB	C8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	N1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	uJ	202	6	-	9/24/74/74	0/4/4/4
29	PEB	SL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	O1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	W1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	I4	202	7	-	12/24/74/74	0/4/4/4
29	PEB	lK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	aB	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	cL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	RR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	FD	201	6	-	9/24/74/74	0/4/4/4
31	CYC	GP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	TK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	G8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	F9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	ZL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	lL	203	7	-	13/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	ZI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	QK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	P2	202	7	-	12/24/74/74	0/4/4/4
31	CYC	vP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	fK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	XL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	XM	202	7	-	13/24/74/74	0/4/4/4
29	PEB	MA	404	14	-	11/24/74/74	0/4/4/4
29	PEB	WJ	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	mB	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	gJ	201	6	-	9/24/74/74	0/4/4/4
30	PUB	A7	302	2	-	5/24/74/74	0/4/4/4
29	PEB	k7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	aF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	l7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	A7	304	-	-	10/24/74/74	0/4/4/4
31	CYC	G9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	QF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	VK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	gJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	P7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	Z9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	MQ	402	7,14	-	10/24/74/74	0/4/4/4
29	PEB	AK	303	2	-	9/24/74/74	0/4/4/4
29	PEB	iK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	MQ	406	29,14	-	10/24/74/74	0/4/4/4
29	PEB	IJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	R1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	VI	202	6,7	-	7/24/74/74	0/4/4/4
31	CYC	kP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	LC	202	6,7	-	8/24/74/74	0/4/4/4
29	PEB	kB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	jk	201	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	pJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	aB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	G8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	MJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	aM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	BQ	201	7,29,14	-	10/24/74/74	0/4/4/4
29	PEB	MR	202	6	-	5/24/74/74	0/4/4/4
29	PEB	KM	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	e7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	CB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	SI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	KN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	OF	201	6	-	6/24/74/74	0/4/4/4
31	CYC	DP	1001	25,21	-	8/25/74/74	0/4/4/4
29	PEB	I8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	Q2	202	6	-	11/24/74/74	0/4/4/4
29	PEB	O2	201	6	-	7/24/74/74	0/4/4/4
29	PEB	A3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	UI	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	CO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	CL	202	6	-	10/24/74/74	0/4/4/4
31	CYC	IF	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	gM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	JA	202	7	-	11/24/74/74	0/4/4/4
31	CYC	HK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	RF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	F4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	I3	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	D4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	JQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	iM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	HN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	NM	202	7	-	13/24/74/74	0/4/4/4
29	PEB	C8	202	-	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CYC	nP	1001	24,21	-	8/25/74/74	0/4/4/4
29	PEB	HQ	201	7,14	-	10/24/74/74	0/4/4/4
31	CYC	gP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	YI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	UB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	AC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	I4	203	7	-	8/24/74/74	0/4/4/4
29	PEB	IL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	KQ	201	6	-	7/24/74/74	0/4/4/4
30	PUB	yL	302	-	-	7/24/74/74	0/4/4/4
29	PEB	PI	201	7,1	-	11/24/74/74	0/4/4/4
29	PEB	zJ	501	7	-	8/24/74/74	0/4/4/4
29	PEB	qJ	202	6	-	10/24/74/74	0/4/4/4
31	CYC	iP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	H5	203	7	-	12/24/74/74	0/4/4/4
30	PUB	MN	403	14	-	10/24/74/74	0/4/4/4
29	PEB	V2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	MJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	mM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	nJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	EN	202	6	-	16/24/74/74	0/4/4/4
31	CYC	LF	1001	5	-	7/25/74/74	0/4/4/4
31	CYC	N7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	k1	202	7	-	6/24/74/74	0/4/4/4
31	CYC	GK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	GL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	YF	202	7	-	7/24/74/74	0/4/4/4
29	PEB	BO	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	FJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	CJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	nL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	c9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	TI	201	7	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PUB	A7	303	-	-	8/24/74/74	0/4/4/4
29	PEB	CD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	H8	202	-	-	10/24/74/74	0/4/4/4
31	CYC	FP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	EQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	KE	203	6	-	8/24/74/74	0/4/4/4
29	PEB	BL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	pJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	EM	202	6	-	10/24/74/74	0/4/4/4
31	CYC	CK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	UL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	LC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	FJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	T9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	uL	203	6	-	10/24/74/74	0/4/4/4
29	PEB	T2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	Z7	202	6	-	8/24/74/74	0/4/4/4
30	PUB	AF	303	2	-	6/24/74/74	0/4/4/4
29	PEB	PJ	201	7	-	7/24/74/74	0/4/4/4
31	CYC	xP	1001	21	-	10/25/74/74	0/4/4/4
29	PEB	ED	201	7	-	12/24/74/74	0/4/4/4
29	PEB	V1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	FB	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	HE	201	7	-	6/24/74/74	0/4/4/4
29	PEB	eF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	YJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	kL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	KC	202	6	-	6/24/74/74	0/4/4/4
29	PEB	OB	202	6	-	10/24/74/74	0/4/4/4
31	CYC	EK	1001	4,5	-	9/25/74/74	0/4/4/4
29	PEB	J8	202	6	-	8/24/74/74	0/4/4/4
29	PEB	hL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	qL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	R2	202	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	TK	201	7	-	6/24/74/74	0/4/4/4
30	PUB	MA	403	14	-	10/24/74/74	0/4/4/4
29	PEB	TR	201	7	-	9/24/74/74	0/4/4/4
29	PEB	LD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	l1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	bJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	GD	203	7	-	11/24/74/74	0/4/4/4
29	PEB	j1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	LE	202	6,7	-	8/24/74/74	0/4/4/4
29	PEB	i7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	lI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	vL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	K4	202	7	-	12/24/74/74	0/4/4/4
29	PEB	AK	302	-	-	9/24/74/74	0/4/4/4
29	PEB	VB	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	LA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	K8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	hL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	AN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	FG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	L8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	cI	202	7	-	14/24/74/74	0/4/4/4
29	PEB	i9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	QL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	FD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	RI	202	7	-	14/24/74/74	0/4/4/4
31	CYC	YP	1000	25	-	7/25/74/74	0/4/4/4
29	PEB	WB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	QR	202	6	-	10/24/74/74	0/4/4/4
29	PEB	FL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	gI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	xJ	303	16	-	14/24/74/74	0/4/4/4
29	PEB	BM	301	17	-	13/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	PF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	d7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	S2	202	6	-	10/24/74/74	0/4/4/4
29	PEB	JG	203	7	-	12/24/74/74	0/4/4/4
29	PEB	e2	401	-	-	9/24/74/74	0/4/4/4
31	CYC	HF	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	QB	203	6	-	5/24/74/74	0/4/4/4
29	PEB	JD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	HJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	GM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	O7	202	6	-	8/24/74/74	0/4/4/4
31	CYC	C1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	DM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	RM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	MG	401	14	-	9/24/74/74	0/4/4/4
29	PEB	RJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	nL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	rL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	TI	202	7	-	14/24/74/74	0/4/4/4
29	PEB	TJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	NI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	O1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	a9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	A9	305	-	-	10/24/74/74	0/4/4/4
29	PEB	aM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	BQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	AG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	LQ	202	-	-	12/24/74/74	0/4/4/4
29	PEB	gF	202	7,6	-	7/24/74/74	0/4/4/4
29	PEB	J4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	fJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	FQ	201	7	-	10/24/74/74	0/4/4/4
31	CYC	SP	1001	21	-	8/25/74/74	0/4/4/4
31	CYC	D9	1001	5	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	FA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	FM	201	7,15	-	6/24/74/74	0/4/4/4
29	PEB	AG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	dF	203	6	-	8/24/74/74	0/4/4/4
29	PEB	E4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	KC	201	7,6	-	8/24/74/74	0/4/4/4
29	PEB	bF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	UB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	iF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	cK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	GL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	GC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	pL	203	7	-	13/24/74/74	0/4/4/4
31	CYC	N9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	RL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	LM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	LE	201	7	-	6/24/74/74	0/4/4/4
29	PEB	BJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	DK	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	B3	201	7,9	-	5/24/74/74	0/4/4/4
29	PEB	U1	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	hI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	gI	202	7,6	-	7/24/74/74	0/4/4/4
31	CYC	hP	1001	25,21	-	8/25/74/74	0/4/4/4
31	CYC	LK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	FC	201	7,18	-	6/24/74/74	0/4/4/4
29	PEB	V1	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	RK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	DM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	eB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	FN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	a1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	g9	201	7	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	N3	201	-	-	6/24/74/74	0/4/4/4
29	PEB	mJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	fJ	201	7,16	-	7/24/74/74	0/4/4/4
29	PEB	ZL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	E3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	dJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	fL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	KN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	I5	201	7	-	6/24/74/74	0/4/4/4
29	PEB	FO	201	7,9	-	5/24/74/74	0/4/4/4
30	PUB	A1	304	2	-	4/24/74/74	0/4/4/4
29	PEB	BN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	P9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	j7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	gM	202	7	-	6/24/74/74	0/4/4/4
31	CYC	KK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	ZB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	T2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	UF	202	6	-	6/24/74/74	0/4/4/4
31	CYC	NK	1001	5,3	-	7/25/74/74	0/4/4/4
29	PEB	Y7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	k7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	iB	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	HQ	202	7	-	6/24/74/74	0/4/4/4
31	CYC	1P	1002	25	-	7/25/74/74	0/4/4/4
29	PEB	VK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	NM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	dK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	bI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	DD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	BD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	AO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	YM	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	MA	405	14	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	GQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	O2	202	6	-	11/24/74/74	0/4/4/4
29	PEB	h9	202	6	-	8/24/74/74	0/4/4/4
30	PUB	AF	302	2	-	9/24/74/74	0/4/4/4
29	PEB	AJ	203	6,7	-	9/24/74/74	0/4/4/4
30	PUB	xJ	305	16	-	5/24/74/74	0/4/4/4
29	PEB	CN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	m9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	U2	202	-	-	10/24/74/74	0/4/4/4
29	PEB	oJ	202	6	-	10/24/74/74	0/4/4/4
31	CYC	K7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	K4	203	7	-	11/24/74/74	0/4/4/4
30	PUB	MN	402	14	-	8/24/74/74	0/4/4/4
29	PEB	QJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	L1	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	j9	202	6	-	8/24/74/74	0/4/4/4
31	CYC	mP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	d1	202	6	-	9/24/74/74	0/4/4/4
31	CYC	C7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	HD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	HB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	GE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	JM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	IO	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	AL	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	VL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	ZM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	V2	201	7,8	-	9/24/74/74	0/4/4/4
29	PEB	mL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	h1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	lK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	YI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	CQ	202	6	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	OI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	cL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	HA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	DA	203	-	-	9/24/74/74	0/4/4/4
31	CYC	H1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	NK	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	L5	201	7	-	7/24/74/74	0/4/4/4
29	PEB	M3	201	-	-	6/24/74/74	0/4/4/4
29	PEB	J3	201	7	-	5/24/74/74	0/4/4/4
29	PEB	XM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	SB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	UK	203	6	-	9/24/74/74	0/4/4/4
29	PEB	oL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	ZB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	aK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	bK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	V7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	d7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	V9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	QJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	KE	201	7,6	-	8/24/74/74	0/4/4/4
29	PEB	RF	202	7	-	14/24/74/74	0/4/4/4
29	PEB	HC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	jF	201	6	-	6/24/74/74	0/4/4/4
31	CYC	cP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	GG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	fM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	PL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	KQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	mK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	X2	202	7	-	12/24/74/74	0/4/4/4
29	PEB	E4	202	7	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	YF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	i9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	FL	202	7,6	-	9/24/74/74	0/4/4/4
31	CYC	MI	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	GG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	WJ	203	6	-	10/24/74/74	0/4/4/4
29	PEB	dM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	TL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	BA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	kM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	NR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	A8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	lJ	203	7	-	13/24/74/74	0/4/4/4
31	CYC	I7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	MD	202	6,7	-	12/24/74/74	0/4/4/4
29	PEB	DQ	201	7	-	10/24/74/74	0/4/4/4
29	PEB	jK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	MO	202	7	-	10/24/74/74	0/4/4/4
29	PEB	F4	201	6	-	8/24/74/74	0/4/4/4
29	PEB	CJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	rJ	202	6,7	-	9/24/74/74	0/4/4/4
32	PMS	k6	302	-	-	2/5/5/5	0/1/1/1
29	PEB	ZM	202	7	-	6/24/74/74	0/4/4/4
31	CYC	MF	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	U9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	b1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	CC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	B8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	RK	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	A9	304	-	-	10/24/74/74	0/4/4/4
29	PEB	UL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	dI	202	6	-	6/24/74/74	0/4/4/4
29	PEB	lL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	GO	202	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	iJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	dL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kI	201	7,2	-	11/24/74/74	0/4/4/4
29	PEB	aM	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	N3	202	7	-	10/24/74/74	0/4/4/4
29	PEB	vJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	V9	201	7	-	4/24/74/74	0/4/4/4
31	CYC	FK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	F8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	OF	203	6,7	-	7/24/74/74	0/4/4/4
29	PEB	Q7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	gM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	EC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	cI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	ZB	203	7	-	13/24/74/74	0/4/4/4
30	PUB	MG	402	14	-	15/24/74/74	0/4/4/4
29	PEB	aK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	P1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	HM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	a7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	CL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	YI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	L5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	P7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	AB	303	16	-	13/24/74/74	0/4/4/4
30	PUB	AK	304	2	-	4/24/74/74	0/4/4/4
29	PEB	jM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	QM	203	6	-	5/24/74/74	0/4/4/4
29	PEB	JQ	201	7	-	10/24/74/74	0/4/4/4
29	PEB	VI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	PI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	rL	201	7,16	-	7/24/74/74	0/4/4/4
29	PEB	gK	202	7	-	6/24/74/74	0/4/4/4
31	CYC	JI	1001	5,3	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	e7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	F5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	aF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	HK	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	AN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	JJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	RJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	C5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	BA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	TB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	EC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	VF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	G5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	I3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	GJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	m9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	I8	202	-	-	9/24/74/74	0/4/4/4
29	PEB	FF	1002	4	-	13/24/74/74	0/4/4/4
29	PEB	PK	201	7,1	-	6/24/74/74	0/4/4/4
29	PEB	T1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	AC	203	6,7	-	8/24/74/74	0/4/4/4
29	PEB	mJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	GB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	ZL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	E3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	CD	203	-	-	11/24/74/74	0/4/4/4
29	PEB	JA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	i7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	MM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	T1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	FK	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	BG	201	7	-	10/24/74/74	0/4/4/4
29	PEB	T9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	eI	201	7	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	IQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	m1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	P2	201	7	-	7/24/74/74	0/4/4/4
29	PEB	cJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	VM	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	UK	202	6	-	8/24/74/74	0/4/4/4
29	PEB	VB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LO	201	7	-	5/24/74/74	0/4/4/4
30	PUB	wL	304	-	-	9/24/74/74	0/4/4/4
29	PEB	DC	202	-	-	9/24/74/74	0/4/4/4
29	PEB	H7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	R9	203	7	-	12/24/74/74	0/4/4/4
31	CYC	J7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	HE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	kF	202	7,6	-	7/24/74/74	0/4/4/4
29	PEB	PM	202	7	-	13/24/74/74	0/4/4/4
31	CYC	H9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	eI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	c7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	P1	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	yJ	301	-	-	9/24/74/74	0/4/4/4
29	PEB	cM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	TJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	OK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	AB	302	6,16	-	8/24/74/74	0/4/4/4
29	PEB	ID	203	7	-	11/24/74/74	0/4/4/4
29	PEB	C4	202	7,6	-	12/24/74/74	0/4/4/4
29	PEB	gK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	jJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	QM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	a7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	fL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	sL	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	TR	203	7	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	QF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	iF	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	j1	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	M4	203	7	-	12/24/74/74	0/4/4/4
29	PEB	jF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	OJ	201	6	-	9/24/74/74	0/4/4/4
31	CYC	E9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	fF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	V1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	i9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	JK	1002	5	-	8/24/74/74	0/4/4/4
31	CYC	TP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	f7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	G5	201	7	-	7/24/74/74	0/4/4/4
31	CYC	CI	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	LN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	AA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	SM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	QB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	JO	201	7	-	5/24/74/74	0/4/4/4
29	PEB	DQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	XL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	A5	203	7	-	9/24/74/74	0/4/4/4
29	PEB	EN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	QR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	RB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	uJ	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	D7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	g1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	N9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	i7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	XL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	BC	202	7	-	8/24/74/74	0/4/4/4
29	PEB	k9	201	7	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	DD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	M3	202	7	-	10/24/74/74	0/4/4/4
29	PEB	e1	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	J7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	P9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	U9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	KO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	ID	201	7	-	9/24/74/74	0/4/4/4
29	PEB	CC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	RL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	DJ	202	7	-	13/24/74/74	0/4/4/4
30	PUB	wL	305	16	-	5/24/74/74	0/4/4/4
29	PEB	kK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	k7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	HF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	PF	201	7,1	-	11/24/74/74	0/4/4/4
29	PEB	kF	201	7,2	-	11/24/74/74	0/4/4/4
29	PEB	ID	202	7	-	12/24/74/74	0/4/4/4
29	PEB	cM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	HC	202	7	-	8/24/74/74	0/4/4/4
29	PEB	KM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	h9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	AI	305	6,2	-	7/24/74/74	0/4/4/4
29	PEB	C4	203	7	-	11/24/74/74	0/4/4/4
29	PEB	FM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BE	201	7	-	6/24/74/74	0/4/4/4
29	PEB	DM	201	7,17	-	6/24/74/74	0/4/4/4
29	PEB	EQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	LG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	R1	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	ZK	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	cK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	eB	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	A5	201	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	YM	202	6	-	5/24/74/74	0/4/4/4
29	PEB	JE	201	7	-	6/24/74/74	0/4/4/4
31	CYC	IP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	j1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	TM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	wJ	303	16	-	14/24/74/74	0/4/4/4
29	PEB	XB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	EE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	JG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	ZI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	pL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	mM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	GE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	XJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	TB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	dJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	OK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	gK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	KE	202	6	-	6/24/74/74	0/4/4/4
29	PEB	UJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	WK	201	6	-	8/24/74/74	0/4/4/4
31	CYC	DK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	CD	202	7	-	12/24/74/74	0/4/4/4
29	PEB	K5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	EG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	iI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	HN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	OR	202	6	-	8/24/74/74	0/4/4/4
29	PEB	ML	202	6	-	10/24/74/74	0/4/4/4
29	PEB	UF	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	RJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	FC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	MD	203	7	-	11/24/74/74	0/4/4/4
29	PEB	H3	201	7,9	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	e2	402	7,8	-	9/24/74/74	0/4/4/4
29	PEB	A9	301	2	-	9/24/74/74	0/4/4/4
29	PEB	RK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	SR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	xL	301	-	-	12/24/74/74	0/4/4/4
29	PEB	g9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	D9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	lM	202	6	-	10/24/74/74	0/4/4/4
31	CYC	KF	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	H5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	dL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	A8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	KA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	JL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	I5	203	7	-	9/24/74/74	0/4/4/4
29	PEB	FO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	MB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	B5	202	-	-	10/24/74/74	0/4/4/4
31	CYC	UP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	P9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	NL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	aI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	DG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	F1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	hK	202	6	-	9/24/74/74	0/4/4/4
31	CYC	J1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	TF	201	7	-	6/24/74/74	0/4/4/4
29	PEB	hI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	BB	301	17	-	13/24/74/74	0/4/4/4
29	PEB	KC	203	6	-	8/24/74/74	0/4/4/4
29	PEB	FN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	HM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	EE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	jI	202	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	MD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	Y9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	aJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	FM	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	NJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	SF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	T9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	jB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	YM	203	6	-	10/24/74/74	0/4/4/4
29	PEB	EB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	TM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	VR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	CG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	FE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	WI	201	6	-	6/24/74/74	0/4/4/4
31	CYC	NP	1001	20,19	-	8/25/74/74	0/4/4/4
29	PEB	AM	301	16	-	10/24/74/74	0/4/4/4
29	PEB	l9	202	6	-	8/24/74/74	0/4/4/4
31	CYC	JF	1001	5,3	-	7/25/74/74	0/4/4/4
31	CYC	II	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	G4	202	7	-	12/24/74/74	0/4/4/4
29	PEB	Q1	201	6	-	8/24/74/74	0/4/4/4
30	PUB	AB	305	16	-	7/24/74/74	0/4/4/4
29	PEB	T2	201	7	-	9/24/74/74	0/4/4/4
29	PEB	dM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	Y7	201	7	-	4/24/74/74	0/4/4/4
31	CYC	DI	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	OJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	GN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	yL	301	-	-	9/24/74/74	0/4/4/4
31	CYC	yP	1001	-	-	8/25/74/74	0/4/4/4
29	PEB	Z1	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	ZJ	203	7	-	13/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	O9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	KL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	B5	201	7	-	7/24/74/74	0/4/4/4
31	CYC	IP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	L9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	mB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	HB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	IG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	IL	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	BJ	201	7,19	-	7/24/74/74	0/4/4/4
29	PEB	L8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	HL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	fl	202	6	-	8/24/74/74	0/4/4/4
29	PEB	NB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	cB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	D4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	GD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	K5	201	7	-	6/24/74/74	0/4/4/4
31	CYC	MK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	tJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	KL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	JO	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	b9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	RB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	AM	302	6,16	-	8/24/74/74	0/4/4/4
29	PEB	dF	202	6	-	6/24/74/74	0/4/4/4
31	CYC	F9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	VF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	vJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	IL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	xJ	302	-	-	7/24/74/74	0/4/4/4
29	PEB	W7	201	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	jJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	AI	301	2	-	12/24/74/74	0/4/4/4
29	PEB	zL	501	7	-	8/24/74/74	0/4/4/4
29	PEB	sL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	BQ	203	-	-	12/24/74/74	0/4/4/4
31	CYC	F1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	k9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	xL	302	-	-	7/24/74/74	0/4/4/4
29	PEB	MO	201	-	-	6/24/74/74	0/4/4/4
29	PEB	AF	305	6,2	-	7/24/74/74	0/4/4/4
29	PEB	UI	203	6	-	8/24/74/74	0/4/4/4
31	CYC	rP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	S1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	TB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	wJ	302	-	-	7/24/74/74	0/4/4/4
29	PEB	C5	201	7	-	6/24/74/74	0/4/4/4
29	PEB	NJ	203	7	-	13/24/74/74	0/4/4/4
30	PUB	QM	201	6,17	-	6/24/74/74	0/4/4/4
31	CYC	G7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	P7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	PF	202	7	-	7/24/74/74	0/4/4/4
30	PUB	AB	304	16	-	13/24/74/74	0/4/4/4
29	PEB	m7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	fF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	rJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	jJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	ZM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	NO	201	-	-	6/24/74/74	0/4/4/4
29	PEB	O7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	FE	201	7,18	-	6/24/74/74	0/4/4/4
29	PEB	MG	404	14	-	10/24/74/74	0/4/4/4
29	PEB	KJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	II	201	6	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CYC	qP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	HO	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	LA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	b1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	wJ	301	-	-	12/24/74/74	0/4/4/4
29	PEB	IO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	H9	1002	-	-	12/24/74/74	0/4/4/4
31	CYC	uP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	ZK	202	6	-	8/24/74/74	0/4/4/4
29	PEB	DI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	f1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	XR	201	7	-	9/24/74/74	0/4/4/4
29	PEB	aB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	G4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	Y1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	X2	201	7	-	7/24/74/74	0/4/4/4
29	PEB	DQ	203	-	-	12/24/74/74	0/4/4/4
29	PEB	Q2	201	6	-	7/24/74/74	0/4/4/4
31	CYC	KP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	PK	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	IL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	V7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	ZF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	UR	202	6	-	11/24/74/74	0/4/4/4
29	PEB	aL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	jL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	W9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	V2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	kM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	KB	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	Z1	203	6	-	9/24/74/74	0/4/4/4
29	PEB	KO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	j9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	W9	202	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	BC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	V9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	AF	301	2	-	12/24/74/74	0/4/4/4
29	PEB	HD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	LO	202	-	-	10/24/74/74	0/4/4/4
29	PEB	AI	304	2	-	9/24/74/74	0/4/4/4
29	PEB	RR	201	7	-	9/24/74/74	0/4/4/4
29	PEB	a1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	M4	202	6,7	-	12/24/74/74	0/4/4/4
29	PEB	A3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	DE	202	-	-	9/24/74/74	0/4/4/4
29	PEB	YB	202	6	-	5/24/74/74	0/4/4/4
29	PEB	TM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	B8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	ML	201	6	-	9/24/74/74	0/4/4/4
29	PEB	xL	303	16	-	14/24/74/74	0/4/4/4
29	PEB	XB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	F8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	LC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	F3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	fK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	AO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	eF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	hF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	RM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	WL	203	6	-	10/24/74/74	0/4/4/4
31	CYC	L7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	EJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	EO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	fL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	AQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	b7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JQ	203	7	-	12/24/74/74	0/4/4/4
29	PEB	uL	202	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	MO	203	7	-	10/24/74/74	0/4/4/4
29	PEB	AB	301	16	-	10/24/74/74	0/4/4/4
29	PEB	MQ	403	14	-	9/24/74/74	0/4/4/4
31	CYC	K9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	e9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	ZJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	hB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	a9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	C8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LM	203	7	-	13/24/74/74	0/4/4/4
31	CYC	L9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	kB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	S2	201	6	-	4/24/74/74	0/4/4/4
29	PEB	PL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	d9	202	6	-	8/24/74/74	0/4/4/4
31	CYC	VP	1001	21	-	10/25/74/74	0/4/4/4
29	PEB	MN	405	14	-	9/24/74/74	0/4/4/4
29	PEB	R7	201	7,1	-	4/24/74/74	0/4/4/4
29	PEB	f7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	B3	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	nJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	IQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	AJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	Y7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	jI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	PK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	h7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	VJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	i1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	BO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	AJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	DJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	LE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	MB	202	6	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	KM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	BN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	SJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	BG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	eI	203	7	-	14/24/74/74	0/4/4/4
31	CYC	wP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	iM	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	VJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	CE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	FI	1002	4	-	13/24/74/74	0/4/4/4

All (15197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	VP	1001	CYC	CHA-C1A	19.85	1.51	1.35
31	xP	1001	CYC	CHA-C1A	19.80	1.51	1.35
29	C3	202	PEB	CHB-C4B	18.15	1.50	1.35
29	CO	202	PEB	CHB-C4B	18.15	1.50	1.35
29	A3	202	PEB	CHB-C4B	18.14	1.50	1.35
29	AO	202	PEB	CHB-C4B	18.14	1.50	1.35
29	E3	202	PEB	CHB-C4B	18.12	1.50	1.35
29	EO	202	PEB	CHB-C4B	18.12	1.50	1.35
29	I3	202	PEB	CHB-C4B	18.04	1.50	1.35
29	IO	202	PEB	CHB-C4B	18.04	1.50	1.35
29	G3	202	PEB	CHB-C4B	18.04	1.50	1.35
29	GO	202	PEB	CHB-C4B	18.04	1.50	1.35
29	K3	202	PEB	CHB-C4B	18.00	1.50	1.35
29	KO	202	PEB	CHB-C4B	18.00	1.50	1.35
29	M2	202	PEB	CHB-C4B	17.93	1.50	1.35
29	W2	202	PEB	CHB-C4B	17.92	1.50	1.35
29	S2	202	PEB	CHB-C4B	17.87	1.50	1.35
29	UR	202	PEB	CHB-C4B	17.84	1.50	1.35
29	O2	202	PEB	CHB-C4B	17.84	1.50	1.35
29	Q2	202	PEB	CHB-C4B	17.79	1.50	1.35
29	U2	202	PEB	CHB-C4B	17.74	1.49	1.35
29	QR	202	PEB	CHB-C4B	17.74	1.49	1.35
29	SR	202	PEB	CHB-C4B	17.74	1.49	1.35
29	WR	202	PEB	CHB-C4B	17.74	1.49	1.35
29	FC	201	PEB	CHB-C4B	17.61	1.49	1.35
29	FE	201	PEB	CHB-C4B	17.61	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	WP	1001	CYC	CHA-C1A	17.56	1.49	1.35
29	BC	201	PEB	CHB-C4B	17.55	1.49	1.35
29	BE	201	PEB	CHB-C4B	17.55	1.49	1.35
29	HC	201	PEB	CHB-C4B	17.53	1.49	1.35
29	HE	201	PEB	CHB-C4B	17.53	1.49	1.35
31	yP	1001	CYC	CHA-C1A	17.51	1.49	1.35
29	DC	201	PEB	CHB-C4B	17.50	1.49	1.35
29	DE	201	PEB	CHB-C4B	17.50	1.49	1.35
29	JC	201	PEB	CHB-C4B	17.45	1.49	1.35
29	JE	201	PEB	CHB-C4B	17.45	1.49	1.35
29	LC	201	PEB	CHB-C4B	17.42	1.49	1.35
29	LE	201	PEB	CHB-C4B	17.42	1.49	1.35
31	1P	1002	CYC	CHA-C1A	17.32	1.49	1.35
31	YP	1000	CYC	CHA-C1A	17.23	1.49	1.35
30	A1	304	PUB	CHB-C1C	17.11	1.49	1.35
30	AK	304	PUB	CHB-C1C	17.11	1.49	1.35
31	vP	1001	CYC	CHA-C1A	17.05	1.49	1.35
31	cP	1001	CYC	CHA-C1A	17.03	1.49	1.35
31	TP	1001	CYC	CHA-C1A	17.01	1.49	1.35
31	mP	1001	CYC	CHA-C1A	17.01	1.49	1.35
29	m7	203	PEB	CHB-C4B	17.00	1.49	1.35
29	m9	203	PEB	CHB-C4B	17.00	1.49	1.35
31	EP	1001	CYC	CHA-C1A	16.99	1.49	1.35
31	NP	1001	CYC	CHA-C1A	16.99	1.49	1.35
31	iP	1001	CYC	CHA-C1A	16.99	1.49	1.35
31	JP	1001	CYC	CHA-C1A	16.96	1.49	1.35
31	pP	1001	CYC	CHA-C1A	16.95	1.49	1.35
29	T7	203	PEB	CHB-C4B	16.94	1.49	1.35
29	T9	203	PEB	CHB-C4B	16.94	1.49	1.35
29	Y7	203	PEB	CHB-C4B	16.94	1.49	1.35
29	Y9	203	PEB	CHB-C4B	16.94	1.49	1.35
31	CP	1001	CYC	CHA-C1A	16.93	1.49	1.35
31	tP	1001	CYC	CHA-C1A	16.92	1.49	1.35
31	GP	1001	CYC	CHA-C1A	16.92	1.49	1.35
31	rP	1001	CYC	CHA-C1A	16.91	1.49	1.35
29	c7	203	PEB	CHB-C4B	16.90	1.49	1.35
29	c9	203	PEB	CHB-C4B	16.90	1.49	1.35
31	eP	1001	CYC	CHA-C1A	16.90	1.49	1.35
31	RP	1001	CYC	CHA-C1A	16.90	1.49	1.35
31	PP	1001	CYC	CHA-C1A	16.89	1.49	1.35
29	i7	203	PEB	CHB-C4B	16.89	1.49	1.35
29	i9	203	PEB	CHB-C4B	16.89	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	gP	1001	CYC	CHA-C1A	16.89	1.49	1.35
29	g7	203	PEB	CHB-C4B	16.88	1.49	1.35
29	g9	203	PEB	CHB-C4B	16.88	1.49	1.35
31	KP	1001	CYC	CHA-C1A	16.88	1.49	1.35
31	AP	1001	CYC	CHA-C1A	16.88	1.49	1.35
31	lP	1001	CYC	CHA-C1A	16.87	1.49	1.35
29	e7	203	PEB	CHB-C4B	16.86	1.49	1.35
29	e9	203	PEB	CHB-C4B	16.86	1.49	1.35
29	a7	203	PEB	CHB-C4B	16.84	1.49	1.35
29	k7	203	PEB	CHB-C4B	16.84	1.49	1.35
29	a9	203	PEB	CHB-C4B	16.84	1.49	1.35
29	k9	203	PEB	CHB-C4B	16.84	1.49	1.35
29	R7	203	PEB	CHB-C4B	16.80	1.49	1.35
29	R9	203	PEB	CHB-C4B	16.80	1.49	1.35
29	P7	203	PEB	CHB-C4B	16.80	1.49	1.35
29	P9	203	PEB	CHB-C4B	16.80	1.49	1.35
30	QB	201	PUB	CHB-C1C	16.79	1.49	1.35
30	QM	201	PUB	CHB-C1C	16.79	1.49	1.35
29	V7	203	PEB	CHB-C4B	16.78	1.49	1.35
29	V9	203	PEB	CHB-C4B	16.78	1.49	1.35
29	F3	201	PEB	CHB-C4B	16.77	1.49	1.35
29	FO	201	PEB	CHB-C4B	16.77	1.49	1.35
29	B3	201	PEB	CHB-C4B	16.77	1.49	1.35
29	BO	201	PEB	CHB-C4B	16.77	1.49	1.35
29	wJ	303	PEB	CHB-C4B	16.76	1.49	1.35
29	xJ	303	PEB	CHB-C4B	16.75	1.49	1.35
29	AC	201	PEB	CHB-C4B	16.74	1.49	1.35
29	AE	201	PEB	CHB-C4B	16.74	1.49	1.35
29	D3	201	PEB	CHB-C4B	16.73	1.49	1.35
29	DO	201	PEB	CHB-C4B	16.73	1.49	1.35
29	wL	303	PEB	CHB-C4B	16.72	1.49	1.35
29	xL	303	PEB	CHB-C4B	16.72	1.49	1.35
29	J3	201	PEB	CHB-C4B	16.71	1.49	1.35
29	CC	201	PEB	CHB-C4B	16.71	1.49	1.35
29	CE	201	PEB	CHB-C4B	16.71	1.49	1.35
29	JO	201	PEB	CHB-C4B	16.71	1.49	1.35
29	L3	201	PEB	CHB-C4B	16.69	1.49	1.35
29	LO	201	PEB	CHB-C4B	16.69	1.49	1.35
29	H3	201	PEB	CHB-C4B	16.68	1.49	1.35
29	HO	201	PEB	CHB-C4B	16.68	1.49	1.35
29	GC	201	PEB	CHB-C4B	16.68	1.49	1.35
29	GE	201	PEB	CHB-C4B	16.68	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EC	201	PEB	CHB-C4B	16.67	1.49	1.35
29	EE	201	PEB	CHB-C4B	16.67	1.49	1.35
29	S2	201	PEB	CHB-C4B	16.65	1.49	1.35
29	P2	202	PEB	CHB-C4B	16.65	1.49	1.35
29	IC	201	PEB	CHB-C4B	16.64	1.49	1.35
29	IE	201	PEB	CHB-C4B	16.64	1.49	1.35
29	X2	202	PEB	CHB-C4B	16.63	1.49	1.35
29	XR	203	PEB	CHB-C4B	16.63	1.49	1.35
29	NR	203	PEB	CHB-C4B	16.62	1.49	1.35
29	RR	203	PEB	CHB-C4B	16.61	1.49	1.35
29	KC	202	PEB	CHB-C4B	16.60	1.49	1.35
29	KE	202	PEB	CHB-C4B	16.60	1.49	1.35
29	MR	202	PEB	CHB-C4B	16.58	1.49	1.35
29	KG	202	PEB	CHB-C4B	16.58	1.49	1.35
29	KQ	202	PEB	CHB-C4B	16.58	1.49	1.35
29	VR	203	PEB	CHB-C4B	16.58	1.49	1.35
29	R2	203	PEB	CHB-C4B	16.57	1.49	1.35
29	gF	203	PEB	CHB-C4B	16.57	1.49	1.35
29	gI	203	PEB	CHB-C4B	16.57	1.49	1.35
29	wJ	302	PEB	CHB-C4B	16.56	1.49	1.35
29	wL	302	PEB	CHB-C4B	16.55	1.48	1.35
29	PR	202	PEB	CHB-C4B	16.55	1.48	1.35
29	xL	302	PEB	CHB-C4B	16.55	1.48	1.35
29	IG	202	PEB	CHB-C4B	16.54	1.48	1.35
29	IQ	202	PEB	CHB-C4B	16.54	1.48	1.35
29	T2	203	PEB	CHB-C4B	16.53	1.48	1.35
29	kF	203	PEB	CHB-C4B	16.53	1.48	1.35
29	kI	203	PEB	CHB-C4B	16.53	1.48	1.35
29	TR	203	PEB	CHB-C4B	16.53	1.48	1.35
29	iF	203	PEB	CHB-C4B	16.53	1.48	1.35
29	iI	203	PEB	CHB-C4B	16.53	1.48	1.35
29	AG	202	PEB	CHB-C4B	16.52	1.48	1.35
29	EG	202	PEB	CHB-C4B	16.52	1.48	1.35
29	AQ	202	PEB	CHB-C4B	16.52	1.48	1.35
29	EQ	202	PEB	CHB-C4B	16.52	1.48	1.35
29	N2	203	PEB	CHB-C4B	16.52	1.48	1.35
29	TF	202	PEB	CHB-C4B	16.52	1.48	1.35
29	TI	202	PEB	CHB-C4B	16.52	1.48	1.35
29	A1	302	PEB	CHB-C4B	16.51	1.48	1.35
29	AK	302	PEB	CHB-C4B	16.51	1.48	1.35
29	xJ	302	PEB	CHB-C4B	16.50	1.48	1.35
29	YF	203	PEB	CHB-C4B	16.49	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YI	203	PEB	CHB-C4B	16.49	1.48	1.35
29	GC	202	PEB	CHB-C4B	16.49	1.48	1.35
29	GE	202	PEB	CHB-C4B	16.49	1.48	1.35
29	eF	203	PEB	CHB-C4B	16.48	1.48	1.35
29	eI	203	PEB	CHB-C4B	16.48	1.48	1.35
29	CG	202	PEB	CHB-C4B	16.48	1.48	1.35
29	CQ	202	PEB	CHB-C4B	16.48	1.48	1.35
29	D3	202	PEB	CHB-C4B	16.48	1.48	1.35
29	GG	202	PEB	CHB-C4B	16.47	1.48	1.35
29	GQ	202	PEB	CHB-C4B	16.47	1.48	1.35
29	AC	202	PEB	CHB-C4B	16.47	1.48	1.35
29	AE	202	PEB	CHB-C4B	16.47	1.48	1.35
29	RF	202	PEB	CHB-C4B	16.47	1.48	1.35
29	RI	202	PEB	CHB-C4B	16.47	1.48	1.35
29	SR	201	PEB	CHB-C4B	16.47	1.48	1.35
29	cF	202	PEB	CHB-C4B	16.46	1.48	1.35
29	cI	202	PEB	CHB-C4B	16.46	1.48	1.35
29	V2	203	PEB	CHB-C4B	16.46	1.48	1.35
29	EC	202	PEB	CHB-C4B	16.46	1.48	1.35
29	EE	202	PEB	CHB-C4B	16.46	1.48	1.35
30	MQ	405	PUB	CHB-C1C	16.45	1.48	1.35
29	TF	201	PEB	CHB-C4B	16.43	1.48	1.35
29	CC	202	PEB	CHB-C4B	16.43	1.48	1.35
29	CE	202	PEB	CHB-C4B	16.43	1.48	1.35
29	PF	203	PEB	CHB-C4B	16.43	1.48	1.35
29	PI	203	PEB	CHB-C4B	16.43	1.48	1.35
29	DO	202	PEB	CHB-C4B	16.43	1.48	1.35
29	aF	203	PEB	CHB-C4B	16.42	1.48	1.35
29	aI	203	PEB	CHB-C4B	16.42	1.48	1.35
29	LC	203	PEB	CHB-C4B	16.42	1.48	1.35
29	LE	203	PEB	CHB-C4B	16.42	1.48	1.35
29	mF	203	PEB	CHB-C4B	16.42	1.48	1.35
29	mI	203	PEB	CHB-C4B	16.42	1.48	1.35
29	KC	203	PEB	CHB-C4B	16.41	1.48	1.35
29	KE	203	PEB	CHB-C4B	16.41	1.48	1.35
29	IC	202	PEB	CHB-C4B	16.40	1.48	1.35
29	IE	202	PEB	CHB-C4B	16.40	1.48	1.35
29	cF	201	PEB	CHB-C4B	16.40	1.48	1.35
29	cI	201	PEB	CHB-C4B	16.40	1.48	1.35
29	VF	203	PEB	CHB-C4B	16.39	1.48	1.35
29	VI	203	PEB	CHB-C4B	16.39	1.48	1.35
29	VF	201	PEB	CHB-C4B	16.37	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VI	201	PEB	CHB-C4B	16.37	1.48	1.35
30	MG	403	PUB	CHB-C1C	16.37	1.48	1.35
29	HC	203	PEB	CHB-C4B	16.36	1.48	1.35
29	HE	203	PEB	CHB-C4B	16.36	1.48	1.35
29	AM	302	PEB	CHB-C4B	16.36	1.48	1.35
29	BC	203	PEB	CHB-C4B	16.36	1.48	1.35
29	BE	203	PEB	CHB-C4B	16.36	1.48	1.35
30	AF	302	PUB	CHB-C1C	16.36	1.48	1.35
30	AI	302	PUB	CHB-C1C	16.36	1.48	1.35
29	mF	201	PEB	CHB-C4B	16.35	1.48	1.35
29	mI	201	PEB	CHB-C4B	16.35	1.48	1.35
29	HQ	203	PEB	CHB-C4B	16.35	1.48	1.35
29	AB	302	PEB	CHB-C4B	16.35	1.48	1.35
30	yL	303	PUB	CHB-C1C	16.34	1.48	1.35
29	M4	203	PEB	CHB-C4B	16.34	1.48	1.35
29	HG	203	PEB	CHB-C4B	16.34	1.48	1.35
29	NJ	203	PEB	CHB-C4B	16.34	1.48	1.35
29	NL	203	PEB	CHB-C4B	16.34	1.48	1.35
29	JC	202	PEB	CHB-C4B	16.34	1.48	1.35
29	JE	202	PEB	CHB-C4B	16.34	1.48	1.35
29	gF	201	PEB	CHB-C4B	16.34	1.48	1.35
29	gI	201	PEB	CHB-C4B	16.34	1.48	1.35
29	JG	203	PEB	CHB-C4B	16.33	1.48	1.35
29	L3	202	PEB	CHB-C4B	16.33	1.48	1.35
29	tJ	201	PEB	CHB-C4B	16.33	1.48	1.35
29	tL	201	PEB	CHB-C4B	16.33	1.48	1.35
29	LO	202	PEB	CHB-C4B	16.33	1.48	1.35
29	DG	203	PEB	CHB-C4B	16.33	1.48	1.35
29	JJ	201	PEB	CHB-C4B	16.33	1.48	1.35
29	JL	201	PEB	CHB-C4B	16.33	1.48	1.35
29	vJ	201	PEB	CHB-C4B	16.32	1.48	1.35
29	vL	201	PEB	CHB-C4B	16.32	1.48	1.35
29	F3	203	PEB	CHB-C4B	16.32	1.48	1.35
29	FO	203	PEB	CHB-C4B	16.32	1.48	1.35
29	BJ	201	PEB	CHB-C4B	16.31	1.48	1.35
29	BL	201	PEB	CHB-C4B	16.31	1.48	1.35
29	H3	203	PEB	CHB-C4B	16.31	1.48	1.35
29	HO	203	PEB	CHB-C4B	16.31	1.48	1.35
29	YF	201	PEB	CHB-C4B	16.31	1.48	1.35
29	YI	201	PEB	CHB-C4B	16.31	1.48	1.35
29	YB	203	PEB	CHB-C4B	16.30	1.48	1.35
29	YM	203	PEB	CHB-C4B	16.30	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	vJ	202	PEB	CHB-C4B	16.30	1.48	1.35
29	vL	202	PEB	CHB-C4B	16.30	1.48	1.35
29	J3	203	PEB	CHB-C4B	16.30	1.48	1.35
29	lB	202	PEB	CHB-C4B	16.30	1.48	1.35
29	RF	201	PEB	CHB-C4B	16.30	1.48	1.35
29	RI	201	PEB	CHB-C4B	16.30	1.48	1.35
29	lM	202	PEB	CHB-C4B	16.30	1.48	1.35
29	JO	203	PEB	CHB-C4B	16.30	1.48	1.35
29	JQ	203	PEB	CHB-C4B	16.30	1.48	1.35
29	QB	204	PEB	CHB-C4B	16.30	1.48	1.35
29	QM	204	PEB	CHB-C4B	16.30	1.48	1.35
29	J3	202	PEB	CHB-C4B	16.29	1.48	1.35
29	ZJ	201	PEB	CHB-C4B	16.29	1.48	1.35
29	ZL	201	PEB	CHB-C4B	16.29	1.48	1.35
29	JO	202	PEB	CHB-C4B	16.29	1.48	1.35
29	TI	201	PEB	CHB-C4B	16.29	1.48	1.35
29	B3	202	PEB	CHB-C4B	16.29	1.48	1.35
29	BO	202	PEB	CHB-C4B	16.29	1.48	1.35
29	BG	203	PEB	CHB-C4B	16.29	1.48	1.35
29	aF	201	PEB	CHB-C4B	16.29	1.48	1.35
29	aI	201	PEB	CHB-C4B	16.29	1.48	1.35
29	DC	202	PEB	CHB-C4B	16.29	1.48	1.35
29	DE	202	PEB	CHB-C4B	16.29	1.48	1.35
29	hF	202	PEB	CHB-C4B	16.28	1.48	1.35
29	hI	202	PEB	CHB-C4B	16.28	1.48	1.35
29	TJ	203	PEB	CHB-C4B	16.28	1.48	1.35
29	TL	203	PEB	CHB-C4B	16.28	1.48	1.35
29	DQ	203	PEB	CHB-C4B	16.28	1.48	1.35
29	FC	203	PEB	CHB-C4B	16.28	1.48	1.35
29	FE	203	PEB	CHB-C4B	16.28	1.48	1.35
29	DJ	202	PEB	CHB-C4B	16.28	1.48	1.35
29	DL	202	PEB	CHB-C4B	16.28	1.48	1.35
29	PF	201	PEB	CHB-C4B	16.28	1.48	1.35
29	PI	201	PEB	CHB-C4B	16.28	1.48	1.35
29	FQ	203	PEB	CHB-C4B	16.28	1.48	1.35
29	FJ	203	PEB	CHB-C4B	16.28	1.48	1.35
29	FL	203	PEB	CHB-C4B	16.28	1.48	1.35
29	NJ	201	PEB	CHB-C4B	16.27	1.48	1.35
29	NL	201	PEB	CHB-C4B	16.27	1.48	1.35
29	RJ	203	PEB	CHB-C4B	16.27	1.48	1.35
29	RL	203	PEB	CHB-C4B	16.27	1.48	1.35
29	OB	202	PEB	CHB-C4B	16.27	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	OM	202	PEB	CHB-C4B	16.27	1.48	1.35
29	eF	201	PEB	CHB-C4B	16.27	1.48	1.35
29	eI	201	PEB	CHB-C4B	16.27	1.48	1.35
29	tJ	202	PEB	CHB-C4B	16.27	1.48	1.35
29	tL	202	PEB	CHB-C4B	16.27	1.48	1.35
29	kF	201	PEB	CHB-C4B	16.27	1.48	1.35
29	kI	201	PEB	CHB-C4B	16.27	1.48	1.35
29	FJ	201	PEB	CHB-C4B	16.26	1.48	1.35
29	FL	201	PEB	CHB-C4B	16.26	1.48	1.35
29	NO	202	PEB	CHB-C4B	16.26	1.48	1.35
29	fJ	201	PEB	CHB-C4B	16.26	1.48	1.35
29	nJ	201	PEB	CHB-C4B	16.26	1.48	1.35
29	fL	201	PEB	CHB-C4B	16.26	1.48	1.35
29	nL	201	PEB	CHB-C4B	16.26	1.48	1.35
29	AB	303	PEB	CHB-C4B	16.26	1.48	1.35
29	jJ	201	PEB	CHB-C4B	16.26	1.48	1.35
29	lJ	201	PEB	CHB-C4B	16.26	1.48	1.35
29	jL	201	PEB	CHB-C4B	16.26	1.48	1.35
29	lL	201	PEB	CHB-C4B	16.26	1.48	1.35
29	LJ	201	PEB	CHB-C4B	16.26	1.48	1.35
29	fJ	203	PEB	CHB-C4B	16.26	1.48	1.35
29	LL	201	PEB	CHB-C4B	16.26	1.48	1.35
29	fL	203	PEB	CHB-C4B	16.26	1.48	1.35
29	OR	202	PEB	CHB-C4B	16.26	1.48	1.35
29	KB	202	PEB	CHB-C4B	16.25	1.48	1.35
29	bF	202	PEB	CHB-C4B	16.25	1.48	1.35
29	bI	202	PEB	CHB-C4B	16.25	1.48	1.35
29	HJ	202	PEB	CHB-C4B	16.25	1.48	1.35
29	HL	202	PEB	CHB-C4B	16.25	1.48	1.35
29	KM	202	PEB	CHB-C4B	16.25	1.48	1.35
29	WF	202	PEB	CHB-C4B	16.25	1.48	1.35
29	WI	202	PEB	CHB-C4B	16.25	1.48	1.35
29	VJ	202	PEB	CHB-C4B	16.25	1.48	1.35
29	VL	202	PEB	CHB-C4B	16.25	1.48	1.35
29	RJ	201	PEB	CHB-C4B	16.25	1.48	1.35
29	RL	201	PEB	CHB-C4B	16.25	1.48	1.35
29	dJ	203	PEB	CHB-C4B	16.25	1.48	1.35
29	dL	203	PEB	CHB-C4B	16.25	1.48	1.35
29	CB	202	PEB	CHB-C4B	16.25	1.48	1.35
29	CM	202	PEB	CHB-C4B	16.25	1.48	1.35
29	SB	202	PEB	CHB-C4B	16.25	1.48	1.35
29	SM	202	PEB	CHB-C4B	16.25	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	jJ	203	PEB	CHB-C4B	16.25	1.48	1.35
29	jL	203	PEB	CHB-C4B	16.25	1.48	1.35
29	jB	202	PEB	CHB-C4B	16.24	1.48	1.35
29	jM	202	PEB	CHB-C4B	16.24	1.48	1.35
29	K5	203	PEB	CHB-C4B	16.24	1.48	1.35
29	K8	203	PEB	CHB-C4B	16.24	1.48	1.35
29	B3	203	PEB	CHB-C4B	16.24	1.48	1.35
29	XJ	203	PEB	CHB-C4B	16.24	1.48	1.35
29	XL	203	PEB	CHB-C4B	16.24	1.48	1.35
29	BO	203	PEB	CHB-C4B	16.24	1.48	1.35
29	dJ	201	PEB	CHB-C4B	16.24	1.48	1.35
29	dL	201	PEB	CHB-C4B	16.24	1.48	1.35
30	yJ	303	PUB	CHB-C1C	16.24	1.48	1.35
29	FG	203	PEB	CHB-C4B	16.23	1.48	1.35
29	MB	202	PEB	CHB-C4B	16.23	1.48	1.35
29	MM	202	PEB	CHB-C4B	16.23	1.48	1.35
29	SF	202	PEB	CHB-C4B	16.23	1.48	1.35
29	iF	201	PEB	CHB-C4B	16.23	1.48	1.35
29	SI	202	PEB	CHB-C4B	16.23	1.48	1.35
29	iI	201	PEB	CHB-C4B	16.23	1.48	1.35
29	BQ	203	PEB	CHB-C4B	16.23	1.48	1.35
29	PJ	201	PEB	CHB-C4B	16.22	1.48	1.35
29	rJ	203	PEB	CHB-C4B	16.22	1.48	1.35
29	PL	201	PEB	CHB-C4B	16.22	1.48	1.35
29	rL	203	PEB	CHB-C4B	16.22	1.48	1.35
29	hB	202	PEB	CHB-C4B	16.22	1.48	1.35
29	hM	202	PEB	CHB-C4B	16.22	1.48	1.35
29	N3	202	PEB	CHB-C4B	16.22	1.48	1.35
29	bJ	201	PEB	CHB-C4B	16.22	1.48	1.35
29	bL	201	PEB	CHB-C4B	16.22	1.48	1.35
29	BJ	203	PEB	CHB-C4B	16.22	1.48	1.35
29	BL	203	PEB	CHB-C4B	16.22	1.48	1.35
29	pJ	203	PEB	CHB-C4B	16.22	1.48	1.35
29	pL	203	PEB	CHB-C4B	16.22	1.48	1.35
29	hJ	201	PEB	CHB-C4B	16.22	1.48	1.35
29	hL	201	PEB	CHB-C4B	16.22	1.48	1.35
29	aB	202	PEB	CHB-C4B	16.21	1.48	1.35
29	aM	202	PEB	CHB-C4B	16.21	1.48	1.35
29	F3	202	PEB	CHB-C4B	16.21	1.48	1.35
29	bJ	203	PEB	CHB-C4B	16.21	1.48	1.35
29	bL	203	PEB	CHB-C4B	16.21	1.48	1.35
29	FO	202	PEB	CHB-C4B	16.21	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	nJ	203	PEB	CHB-C4B	16.21	1.48	1.35
29	zJ	501	PEB	CHB-C4B	16.21	1.48	1.35
29	nL	203	PEB	CHB-C4B	16.21	1.48	1.35
29	VJ	201	PEB	CHB-C4B	16.21	1.48	1.35
29	VL	201	PEB	CHB-C4B	16.21	1.48	1.35
29	I5	203	PEB	CHB-C4B	16.21	1.48	1.35
29	I8	203	PEB	CHB-C4B	16.21	1.48	1.35
29	M3	202	PEB	CHB-C4B	16.21	1.48	1.35
29	dF	203	PEB	CHB-C4B	16.21	1.48	1.35
29	dI	203	PEB	CHB-C4B	16.21	1.48	1.35
29	PJ	203	PEB	CHB-C4B	16.21	1.48	1.35
29	PL	203	PEB	CHB-C4B	16.21	1.48	1.35
29	MO	202	PEB	CHB-C4B	16.21	1.48	1.35
29	A5	203	PEB	CHB-C4B	16.20	1.48	1.35
29	A8	203	PEB	CHB-C4B	16.20	1.48	1.35
29	IB	202	PEB	CHB-C4B	16.20	1.48	1.35
29	TJ	201	PEB	CHB-C4B	16.20	1.48	1.35
29	TL	201	PEB	CHB-C4B	16.20	1.48	1.35
29	IM	202	PEB	CHB-C4B	16.20	1.48	1.35
29	IF	202	PEB	CHB-C4B	16.20	1.48	1.35
29	II	202	PEB	CHB-C4B	16.20	1.48	1.35
29	dB	202	PEB	CHB-C4B	16.20	1.48	1.35
29	dM	202	PEB	CHB-C4B	16.20	1.48	1.35
29	D3	203	PEB	CHB-C4B	16.20	1.48	1.35
29	DO	203	PEB	CHB-C4B	16.20	1.48	1.35
29	I3	203	PEB	CHB-C4B	16.20	1.48	1.35
29	IO	203	PEB	CHB-C4B	16.20	1.48	1.35
29	WB	202	PEB	CHB-C4B	16.20	1.48	1.35
29	WM	202	PEB	CHB-C4B	16.20	1.48	1.35
29	jF	202	PEB	CHB-C4B	16.19	1.48	1.35
29	jI	202	PEB	CHB-C4B	16.19	1.48	1.35
30	AB	305	PUB	CHB-C1C	16.19	1.48	1.35
29	DJ	201	PEB	CHB-C4B	16.19	1.48	1.35
29	DL	201	PEB	CHB-C4B	16.19	1.48	1.35
29	AM	303	PEB	CHB-C4B	16.18	1.48	1.35
29	H3	202	PEB	CHB-C4B	16.18	1.48	1.35
29	GB	202	PEB	CHB-C4B	16.18	1.48	1.35
29	GM	202	PEB	CHB-C4B	16.18	1.48	1.35
29	HO	202	PEB	CHB-C4B	16.18	1.48	1.35
29	OF	202	PEB	CHB-C4B	16.18	1.48	1.35
29	OI	202	PEB	CHB-C4B	16.18	1.48	1.35
29	LJ	202	PEB	CHB-C4B	16.18	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	hJ	203	PEB	CHB-C4B	16.18	1.48	1.35
29	LL	202	PEB	CHB-C4B	16.18	1.48	1.35
29	hL	203	PEB	CHB-C4B	16.18	1.48	1.35
29	lJ	203	PEB	CHB-C4B	16.18	1.48	1.35
29	lL	203	PEB	CHB-C4B	16.18	1.48	1.35
29	LQ	202	PEB	CHB-C4B	16.17	1.48	1.35
29	UB	202	PEB	CHB-C4B	16.17	1.48	1.35
29	MQ	401	PEB	CHB-C4B	16.17	1.48	1.35
29	EB	202	PEB	CHB-C4B	16.17	1.48	1.35
29	EM	202	PEB	CHB-C4B	16.17	1.48	1.35
29	XJ	201	PEB	CHB-C4B	16.17	1.48	1.35
29	XL	201	PEB	CHB-C4B	16.17	1.48	1.35
29	C5	203	PEB	CHB-C4B	16.16	1.48	1.35
29	fB	202	PEB	CHB-C4B	16.16	1.48	1.35
29	fM	202	PEB	CHB-C4B	16.16	1.48	1.35
29	UF	203	PEB	CHB-C4B	16.15	1.48	1.35
29	UI	203	PEB	CHB-C4B	16.15	1.48	1.35
29	ZF	202	PEB	CHB-C4B	16.15	1.48	1.35
29	ZI	202	PEB	CHB-C4B	16.15	1.48	1.35
29	pJ	201	PEB	CHB-C4B	16.14	1.48	1.35
29	pL	201	PEB	CHB-C4B	16.14	1.48	1.35
29	C8	203	PEB	CHB-C4B	16.14	1.48	1.35
29	QF	202	PEB	CHB-C4B	16.14	1.48	1.35
29	QI	202	PEB	CHB-C4B	16.14	1.48	1.35
29	RR	201	PEB	CHB-C4B	16.13	1.48	1.35
29	ZJ	203	PEB	CHB-C4B	16.13	1.48	1.35
29	ZL	203	PEB	CHB-C4B	16.13	1.48	1.35
29	JJ	203	PEB	CHB-C4B	16.13	1.48	1.35
29	JL	203	PEB	CHB-C4B	16.13	1.48	1.35
29	fF	202	PEB	CHB-C4B	16.13	1.48	1.35
29	fI	202	PEB	CHB-C4B	16.13	1.48	1.35
30	AM	305	PUB	CHB-C1C	16.13	1.48	1.35
29	LG	203	PEB	CHB-C4B	16.12	1.48	1.35
29	rJ	201	PEB	CHB-C4B	16.11	1.48	1.35
29	rL	201	PEB	CHB-C4B	16.11	1.48	1.35
29	P1	203	PEB	CHB-C4B	16.10	1.48	1.35
29	PK	203	PEB	CHB-C4B	16.10	1.48	1.35
29	e2	402	PEB	CHB-C4B	16.09	1.48	1.35
29	V2	201	PEB	CHB-C4B	16.07	1.48	1.35
29	VR	201	PEB	CHB-C4B	16.07	1.48	1.35
29	N2	201	PEB	CHB-C4B	16.06	1.48	1.35
29	NR	201	PEB	CHB-C4B	16.06	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	zL	501	PEB	CHB-C4B	16.06	1.48	1.35
29	T2	201	PEB	CHB-C4B	16.05	1.48	1.35
29	TR	201	PEB	CHB-C4B	16.05	1.48	1.35
29	Y1	202	PEB	CHB-C4B	16.05	1.48	1.35
29	R2	201	PEB	CHB-C4B	16.05	1.48	1.35
29	YK	202	PEB	CHB-C4B	16.05	1.48	1.35
29	XR	201	PEB	CHB-C4B	16.03	1.48	1.35
29	e1	203	PEB	CHB-C4B	16.03	1.48	1.35
29	eK	203	PEB	CHB-C4B	16.03	1.48	1.35
29	DF	1002	PEB	CHB-C4B	16.03	1.48	1.35
29	DI	1002	PEB	CHB-C4B	16.03	1.48	1.35
29	R1	203	PEB	CHB-C4B	16.01	1.48	1.35
29	RK	203	PEB	CHB-C4B	16.01	1.48	1.35
29	g1	203	PEB	CHB-C4B	16.00	1.48	1.35
29	gK	203	PEB	CHB-C4B	16.00	1.48	1.35
29	I4	203	PEB	CHB-C4B	16.00	1.48	1.35
29	V1	203	PEB	CHB-C4B	16.00	1.48	1.35
29	VK	203	PEB	CHB-C4B	16.00	1.48	1.35
29	HF	1002	PEB	CHB-C4B	16.00	1.48	1.35
29	HI	1002	PEB	CHB-C4B	16.00	1.48	1.35
29	FF	1002	PEB	CHB-C4B	15.98	1.48	1.35
29	FI	1002	PEB	CHB-C4B	15.98	1.48	1.35
29	m1	202	PEB	CHB-C4B	15.98	1.48	1.35
29	K5	201	PEB	CHB-C4B	15.98	1.48	1.35
29	K8	201	PEB	CHB-C4B	15.98	1.48	1.35
29	mK	202	PEB	CHB-C4B	15.98	1.48	1.35
29	JF	1002	PEB	CHB-C4B	15.97	1.48	1.35
29	JI	1002	PEB	CHB-C4B	15.97	1.48	1.35
29	k1	203	PEB	CHB-C4B	15.97	1.48	1.35
29	kK	203	PEB	CHB-C4B	15.97	1.48	1.35
29	a1	203	PEB	CHB-C4B	15.97	1.48	1.35
29	aK	203	PEB	CHB-C4B	15.97	1.48	1.35
29	LF	1002	PEB	CHB-C4B	15.96	1.48	1.35
29	LI	1002	PEB	CHB-C4B	15.96	1.48	1.35
29	T1	202	PEB	CHB-C4B	15.95	1.48	1.35
29	I5	201	PEB	CHB-C4B	15.95	1.48	1.35
29	I8	201	PEB	CHB-C4B	15.95	1.48	1.35
29	TK	202	PEB	CHB-C4B	15.95	1.48	1.35
29	c1	203	PEB	CHB-C4B	15.94	1.48	1.35
29	cK	203	PEB	CHB-C4B	15.94	1.48	1.35
29	NF	1002	PEB	CHB-C4B	15.94	1.48	1.35
29	NI	1002	PEB	CHB-C4B	15.94	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A7	305	PEB	CHB-C4B	15.94	1.48	1.35
29	A9	305	PEB	CHB-C4B	15.94	1.48	1.35
29	i1	203	PEB	CHB-C4B	15.91	1.48	1.35
29	iK	203	PEB	CHB-C4B	15.91	1.48	1.35
29	mB	201	PEB	CHB-C4B	15.91	1.48	1.35
29	mM	201	PEB	CHB-C4B	15.91	1.48	1.35
29	A5	201	PEB	CHB-C4B	15.91	1.48	1.35
29	A8	201	PEB	CHB-C4B	15.91	1.48	1.35
29	A7	304	PEB	CHB-C4B	15.91	1.48	1.35
29	A9	304	PEB	CHB-C4B	15.84	1.48	1.35
29	XB	201	PEB	CHB-C4B	15.84	1.48	1.35
29	XM	201	PEB	CHB-C4B	15.84	1.48	1.35
29	PB	201	PEB	CHB-C4B	15.84	1.48	1.35
29	PM	201	PEB	CHB-C4B	15.84	1.48	1.35
29	eB	201	PEB	CHB-C4B	15.83	1.48	1.35
29	eM	201	PEB	CHB-C4B	15.83	1.48	1.35
29	gB	201	PEB	CHB-C4B	15.83	1.48	1.35
29	gM	201	PEB	CHB-C4B	15.83	1.48	1.35
29	LB	201	PEB	CHB-C4B	15.83	1.48	1.35
29	LM	201	PEB	CHB-C4B	15.83	1.48	1.35
29	ZB	201	PEB	CHB-C4B	15.82	1.48	1.35
29	ZM	201	PEB	CHB-C4B	15.82	1.48	1.35
29	C5	201	PEB	CHB-C4B	15.80	1.48	1.35
29	C8	201	PEB	CHB-C4B	15.80	1.48	1.35
29	cB	201	PEB	CHB-C4B	15.80	1.48	1.35
29	cM	201	PEB	CHB-C4B	15.80	1.48	1.35
29	DG	201	PEB	CHB-C4B	15.80	1.48	1.35
29	DQ	201	PEB	CHB-C4B	15.80	1.48	1.35
29	B8	203	PEB	CHB-C4B	15.80	1.48	1.35
29	kB	201	PEB	CHB-C4B	15.78	1.48	1.35
29	kM	201	PEB	CHB-C4B	15.78	1.48	1.35
29	AF	305	PEB	CHB-C4B	15.78	1.48	1.35
29	AI	305	PEB	CHB-C4B	15.78	1.48	1.35
29	HB	201	PEB	CHB-C4B	15.78	1.48	1.35
29	NB	202	PEB	CHB-C4B	15.78	1.48	1.35
29	HM	201	PEB	CHB-C4B	15.78	1.48	1.35
29	NM	202	PEB	CHB-C4B	15.78	1.48	1.35
29	iB	201	PEB	CHB-C4B	15.77	1.48	1.35
29	iM	201	PEB	CHB-C4B	15.77	1.48	1.35
30	BB	302	PUB	CHB-C1C	15.77	1.48	1.35
30	BM	302	PUB	CHB-C1C	15.77	1.48	1.35
29	JB	201	PEB	CHB-C4B	15.77	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JM	201	PEB	CHB-C4B	15.77	1.48	1.35
29	iB	203	PEB	CHB-C4B	15.77	1.48	1.35
29	iM	203	PEB	CHB-C4B	15.77	1.48	1.35
29	RB	203	PEB	CHB-C4B	15.77	1.48	1.35
29	RM	203	PEB	CHB-C4B	15.77	1.48	1.35
29	AF	304	PEB	CHB-C4B	15.76	1.48	1.35
29	AI	304	PEB	CHB-C4B	15.76	1.48	1.35
29	VB	201	PEB	CHB-C4B	15.76	1.48	1.35
29	VM	201	PEB	CHB-C4B	15.76	1.48	1.35
29	DB	203	PEB	CHB-C4B	15.76	1.48	1.35
29	HB	203	PEB	CHB-C4B	15.76	1.48	1.35
29	DM	203	PEB	CHB-C4B	15.76	1.48	1.35
29	HM	203	PEB	CHB-C4B	15.76	1.48	1.35
29	NB	201	PEB	CHB-C4B	15.76	1.48	1.35
29	NM	201	PEB	CHB-C4B	15.76	1.48	1.35
29	ZB	203	PEB	CHB-C4B	15.76	1.48	1.35
29	ZM	203	PEB	CHB-C4B	15.76	1.48	1.35
29	XB	202	PEB	CHB-C4B	15.76	1.48	1.35
29	XM	202	PEB	CHB-C4B	15.76	1.48	1.35
29	FB	201	PEB	CHB-C4B	15.75	1.48	1.35
29	FM	201	PEB	CHB-C4B	15.75	1.48	1.35
29	gB	203	PEB	CHB-C4B	15.75	1.48	1.35
29	gM	203	PEB	CHB-C4B	15.75	1.48	1.35
29	G5	203	PEB	CHB-C4B	15.75	1.48	1.35
29	HK	1002	PEB	CHB-C4B	15.74	1.48	1.35
31	NK	1001	CYC	CHA-C1A	15.74	1.48	1.35
29	PB	202	PEB	CHB-C4B	15.74	1.48	1.35
29	PM	202	PEB	CHB-C4B	15.74	1.48	1.35
29	B8	201	PEB	CHB-C4B	15.73	1.48	1.35
31	D1	1001	CYC	CHA-C1A	15.73	1.48	1.35
29	LB	203	PEB	CHB-C4B	15.73	1.48	1.35
29	LM	203	PEB	CHB-C4B	15.73	1.48	1.35
29	gI	201	PEB	CHB-C4B	15.73	1.48	1.35
29	gK	201	PEB	CHB-C4B	15.73	1.48	1.35
29	H1	1002	PEB	CHB-C4B	15.73	1.48	1.35
31	L1	1001	CYC	CHA-C1A	15.73	1.48	1.35
31	LK	1001	CYC	CHA-C1A	15.73	1.48	1.35
31	N1	1001	CYC	CHA-C1A	15.72	1.48	1.35
29	RB	201	PEB	CHB-C4B	15.72	1.48	1.35
29	RM	201	PEB	CHB-C4B	15.72	1.48	1.35
29	H5	203	PEB	CHB-C4B	15.72	1.48	1.35
29	mB	203	PEB	CHB-C4B	15.72	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	mM	203	PEB	CHB-C4B	15.72	1.48	1.35
29	H8	201	PEB	CHB-C4B	15.71	1.48	1.35
29	HA	203	PEB	CHB-C4B	15.71	1.48	1.35
29	HN	203	PEB	CHB-C4B	15.71	1.48	1.35
29	DA	203	PEB	CHB-C4B	15.71	1.48	1.35
29	TB	203	PEB	CHB-C4B	15.71	1.48	1.35
29	TM	203	PEB	CHB-C4B	15.71	1.48	1.35
29	DN	203	PEB	CHB-C4B	15.71	1.48	1.35
29	e1	201	PEB	CHB-C4B	15.71	1.48	1.35
29	eK	201	PEB	CHB-C4B	15.71	1.48	1.35
31	OP	1001	CYC	CHA-C1A	15.71	1.48	1.35
29	I5	202	PEB	CHB-C4B	15.71	1.48	1.35
29	I8	202	PEB	CHB-C4B	15.71	1.48	1.35
29	G8	203	PEB	CHB-C4B	15.71	1.48	1.35
29	A8	202	PEB	CHB-C4B	15.71	1.48	1.35
29	FA	203	PEB	CHB-C4B	15.71	1.48	1.35
29	FN	203	PEB	CHB-C4B	15.71	1.48	1.35
31	F1	1001	CYC	CHA-C1A	15.71	1.48	1.35
31	FK	1001	CYC	CHA-C1A	15.71	1.48	1.35
29	DB	201	PEB	CHB-C4B	15.70	1.48	1.35
29	cB	203	PEB	CHB-C4B	15.70	1.48	1.35
29	kB	203	PEB	CHB-C4B	15.70	1.48	1.35
29	DM	201	PEB	CHB-C4B	15.70	1.48	1.35
29	cM	203	PEB	CHB-C4B	15.70	1.48	1.35
29	kM	203	PEB	CHB-C4B	15.70	1.48	1.35
29	B8	202	PEB	CHB-C4B	15.70	1.48	1.35
31	DK	1001	CYC	CHA-C1A	15.70	1.48	1.35
31	HK	1001	CYC	CHA-C1A	15.70	1.48	1.35
31	sP	1001	CYC	CHA-C1A	15.70	1.48	1.35
31	oP	1001	CYC	CHA-C1A	15.70	1.48	1.35
29	BA	203	PEB	CHB-C4B	15.70	1.48	1.35
29	VB	203	PEB	CHB-C4B	15.70	1.48	1.35
29	VM	203	PEB	CHB-C4B	15.70	1.48	1.35
29	BN	203	PEB	CHB-C4B	15.70	1.48	1.35
29	V1	201	PEB	CHB-C4B	15.70	1.48	1.35
29	Y1	201	PEB	CHB-C4B	15.70	1.48	1.35
29	TB	201	PEB	CHB-C4B	15.70	1.48	1.35
29	VK	201	PEB	CHB-C4B	15.70	1.48	1.35
29	YK	201	PEB	CHB-C4B	15.70	1.48	1.35
29	TM	201	PEB	CHB-C4B	15.70	1.48	1.35
31	QP	1001	CYC	CHA-C1A	15.70	1.48	1.35
29	eB	202	PEB	CHB-C4B	15.69	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	eM	202	PEB	CHB-C4B	15.69	1.48	1.35
29	LA	203	PEB	CHB-C4B	15.69	1.48	1.35
29	LN	203	PEB	CHB-C4B	15.69	1.48	1.35
31	J1	1001	CYC	CHA-C1A	15.69	1.48	1.35
31	JK	1001	CYC	CHA-C1A	15.69	1.48	1.35
29	L8	203	PEB	CHB-C4B	15.69	1.48	1.35
29	FB	203	PEB	CHB-C4B	15.68	1.48	1.35
29	FM	203	PEB	CHB-C4B	15.68	1.48	1.35
29	B5	202	PEB	CHB-C4B	15.68	1.48	1.35
29	HG	201	PEB	CHB-C4B	15.68	1.48	1.35
29	HQ	201	PEB	CHB-C4B	15.68	1.48	1.35
29	F5	201	PEB	CHB-C4B	15.68	1.48	1.35
29	F8	201	PEB	CHB-C4B	15.68	1.48	1.35
29	G8	202	PEB	CHB-C4B	15.68	1.48	1.35
29	BG	201	PEB	CHB-C4B	15.68	1.48	1.35
29	BQ	201	PEB	CHB-C4B	15.68	1.48	1.35
31	fP	1001	CYC	CHA-C1A	15.68	1.48	1.35
29	FG	201	PEB	CHB-C4B	15.67	1.48	1.35
29	FQ	201	PEB	CHB-C4B	15.67	1.48	1.35
31	H1	1001	CYC	CHA-C1A	15.67	1.48	1.35
29	C5	202	PEB	CHB-C4B	15.67	1.48	1.35
29	C8	202	PEB	CHB-C4B	15.67	1.48	1.35
29	c1	201	PEB	CHB-C4B	15.67	1.48	1.35
29	cK	201	PEB	CHB-C4B	15.67	1.48	1.35
29	G5	201	PEB	CHB-C4B	15.67	1.48	1.35
29	H5	201	PEB	CHB-C4B	15.67	1.48	1.35
29	L5	202	PEB	CHB-C4B	15.67	1.48	1.35
29	JA	203	PEB	CHB-C4B	15.67	1.48	1.35
29	JN	203	PEB	CHB-C4B	15.67	1.48	1.35
31	HP	1001	CYC	CHA-C1A	15.67	1.48	1.35
29	m1	201	PEB	CHB-C4B	15.66	1.48	1.35
29	mK	201	PEB	CHB-C4B	15.66	1.48	1.35
31	XP	1001	CYC	CHA-C1A	15.66	1.48	1.35
29	JG	201	PEB	CHB-C4B	15.66	1.48	1.35
29	JQ	201	PEB	CHB-C4B	15.66	1.48	1.35
30	yJ	302	PUB	CHB-C1C	15.66	1.48	1.35
30	yL	302	PUB	CHB-C1C	15.66	1.48	1.35
29	L5	203	PEB	CHB-C4B	15.66	1.48	1.35
31	FP	1001	CYC	CHA-C1A	15.66	1.48	1.35
31	MP	1001	CYC	CHA-C1A	15.65	1.48	1.35
29	K5	202	PEB	CHB-C4B	15.65	1.48	1.35
29	F1	1002	PEB	CHB-C4B	15.65	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FK	1002	PEB	CHB-C4B	15.65	1.48	1.35
29	k1	201	PEB	CHB-C4B	15.65	1.48	1.35
29	JB	203	PEB	CHB-C4B	15.65	1.48	1.35
29	kK	201	PEB	CHB-C4B	15.65	1.48	1.35
29	JM	203	PEB	CHB-C4B	15.65	1.48	1.35
29	G8	201	PEB	CHB-C4B	15.65	1.48	1.35
31	DP	1001	CYC	CHA-C1A	15.65	1.48	1.35
29	T1	201	PEB	CHB-C4B	15.64	1.48	1.35
29	LG	201	PEB	CHB-C4B	15.64	1.48	1.35
29	TK	201	PEB	CHB-C4B	15.64	1.48	1.35
29	MQ	402	PEB	CHB-C4B	15.64	1.48	1.35
29	G5	202	PEB	CHB-C4B	15.64	1.48	1.35
29	dB	201	PEB	CHB-C4B	15.64	1.48	1.35
29	dM	201	PEB	CHB-C4B	15.64	1.48	1.35
29	A5	202	PEB	CHB-C4B	15.64	1.48	1.35
29	EB	201	PEB	CHB-C4B	15.64	1.48	1.35
29	EM	201	PEB	CHB-C4B	15.64	1.48	1.35
29	a1	201	PEB	CHB-C4B	15.64	1.48	1.35
29	aK	201	PEB	CHB-C4B	15.64	1.48	1.35
29	B5	203	PEB	CHB-C4B	15.64	1.48	1.35
29	AM	301	PEB	CHB-C4B	15.63	1.48	1.35
29	P1	201	PEB	CHB-C4B	15.63	1.48	1.35
29	PK	201	PEB	CHB-C4B	15.63	1.48	1.35
31	IP	1001	CYC	CHA-C1A	15.63	1.48	1.35
31	nP	1001	CYC	CHA-C1A	15.63	1.48	1.35
31	kP	1001	CYC	CHA-C1A	15.63	1.48	1.35
29	R1	201	PEB	CHB-C4B	15.62	1.48	1.35
29	H8	203	PEB	CHB-C4B	15.62	1.48	1.35
29	RK	201	PEB	CHB-C4B	15.62	1.48	1.35
31	SP	1001	CYC	CHA-C1A	15.62	1.48	1.35
29	i1	201	PEB	CHB-C4B	15.62	1.48	1.35
29	AB	301	PEB	CHB-C4B	15.62	1.48	1.35
29	iK	201	PEB	CHB-C4B	15.62	1.48	1.35
31	jP	1001	CYC	CHA-C1A	15.61	1.48	1.35
29	hF	201	PEB	CHB-C4B	15.61	1.48	1.35
29	hI	201	PEB	CHB-C4B	15.61	1.48	1.35
29	L8	202	PEB	CHB-C4B	15.61	1.48	1.35
29	D1	1002	PEB	CHB-C4B	15.61	1.48	1.35
31	wP	1001	CYC	CHA-C1A	15.61	1.48	1.35
29	DK	1002	PEB	CHB-C4B	15.60	1.48	1.35
31	uP	1001	CYC	CHA-C1A	15.60	1.48	1.35
29	lB	201	PEB	CHB-C4B	15.59	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	lM	201	PEB	CHB-C4B	15.59	1.48	1.35
29	F5	202	PEB	CHB-C4B	15.59	1.48	1.35
29	F8	202	PEB	CHB-C4B	15.59	1.48	1.35
29	hB	201	PEB	CHB-C4B	15.59	1.48	1.35
29	hM	201	PEB	CHB-C4B	15.59	1.48	1.35
29	B5	201	PEB	CHB-C4B	15.59	1.48	1.35
29	Y7	201	PEB	CHB-C4B	15.58	1.48	1.35
29	Y9	201	PEB	CHB-C4B	15.58	1.48	1.35
31	BP	1001	CYC	CHA-C1A	15.58	1.48	1.35
29	J1	1002	PEB	CHB-C4B	15.58	1.48	1.35
29	BB	301	PEB	CHB-C4B	15.58	1.48	1.35
29	JK	1002	PEB	CHB-C4B	15.58	1.48	1.35
29	BM	301	PEB	CHB-C4B	15.58	1.48	1.35
29	fF	201	PEB	CHB-C4B	15.58	1.48	1.35
29	fI	201	PEB	CHB-C4B	15.58	1.48	1.35
31	UP	1001	CYC	CHA-C1A	15.58	1.48	1.35
30	A7	303	PUB	CHB-C1C	15.58	1.48	1.35
30	A9	303	PUB	CHB-C1C	15.58	1.48	1.35
31	qP	1001	CYC	CHA-C1A	15.58	1.48	1.35
29	L1	1002	PEB	CHB-C4B	15.58	1.48	1.35
29	K8	202	PEB	CHB-C4B	15.58	1.48	1.35
29	LK	1002	PEB	CHB-C4B	15.58	1.48	1.35
29	F5	203	PEB	CHB-C4B	15.57	1.48	1.35
31	hP	1001	CYC	CHA-C1A	15.57	1.48	1.35
31	lP	1001	CYC	CHA-C1A	15.57	1.48	1.35
29	AG	201	PEB	CHB-C4B	15.57	1.48	1.35
29	AQ	201	PEB	CHB-C4B	15.57	1.48	1.35
29	F8	203	PEB	CHB-C4B	15.57	1.48	1.35
29	H8	202	PEB	CHB-C4B	15.57	1.48	1.35
29	MB	201	PEB	CHB-C4B	15.55	1.48	1.35
29	MM	201	PEB	CHB-C4B	15.55	1.48	1.35
29	lF	201	PEB	CHB-C4B	15.55	1.48	1.35
29	lI	201	PEB	CHB-C4B	15.55	1.48	1.35
30	A7	302	PUB	CHB-C1C	15.55	1.48	1.35
30	A9	302	PUB	CHB-C1C	15.55	1.48	1.35
29	UB	201	PEB	CHB-C4B	15.55	1.48	1.35
29	UM	201	PEB	CHB-C4B	15.55	1.48	1.35
29	K3	201	PEB	CHB-C4B	15.54	1.48	1.35
29	KO	201	PEB	CHB-C4B	15.54	1.48	1.35
29	OB	201	PEB	CHB-C4B	15.54	1.48	1.35
29	OM	201	PEB	CHB-C4B	15.54	1.48	1.35
29	NO	201	PEB	CHB-C4B	15.54	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	aB	201	PEB	CHB-C4B	15.54	1.48	1.35
29	aM	201	PEB	CHB-C4B	15.54	1.48	1.35
29	g7	201	PEB	CHB-C4B	15.54	1.48	1.35
29	g9	201	PEB	CHB-C4B	15.54	1.48	1.35
29	c7	201	PEB	CHB-C4B	15.53	1.48	1.35
29	c9	201	PEB	CHB-C4B	15.53	1.48	1.35
29	YB	202	PEB	CHB-C4B	15.53	1.48	1.35
29	CG	201	PEB	CHB-C4B	15.53	1.48	1.35
29	YM	202	PEB	CHB-C4B	15.53	1.48	1.35
29	CQ	201	PEB	CHB-C4B	15.53	1.48	1.35
29	P7	201	PEB	CHB-C4B	15.53	1.48	1.35
29	P9	201	PEB	CHB-C4B	15.53	1.48	1.35
29	WB	201	PEB	CHB-C4B	15.53	1.48	1.35
29	WM	201	PEB	CHB-C4B	15.53	1.48	1.35
29	k7	201	PEB	CHB-C4B	15.53	1.48	1.35
29	k9	201	PEB	CHB-C4B	15.53	1.48	1.35
29	SF	201	PEB	CHB-C4B	15.53	1.48	1.35
29	bF	201	PEB	CHB-C4B	15.53	1.48	1.35
29	SI	201	PEB	CHB-C4B	15.53	1.48	1.35
29	bI	201	PEB	CHB-C4B	15.53	1.48	1.35
29	WF	201	PEB	CHB-C4B	15.52	1.48	1.35
29	WI	201	PEB	CHB-C4B	15.52	1.48	1.35
29	KG	201	PEB	CHB-C4B	15.52	1.48	1.35
29	KQ	201	PEB	CHB-C4B	15.52	1.48	1.35
29	SB	201	PEB	CHB-C4B	15.52	1.48	1.35
29	SM	201	PEB	CHB-C4B	15.52	1.48	1.35
29	EG	201	PEB	CHB-C4B	15.52	1.48	1.35
29	EQ	201	PEB	CHB-C4B	15.52	1.48	1.35
29	KB	201	PEB	CHB-C4B	15.52	1.48	1.35
29	KM	201	PEB	CHB-C4B	15.52	1.48	1.35
29	H5	202	PEB	CHB-C4B	15.52	1.48	1.35
29	jB	201	PEB	CHB-C4B	15.51	1.48	1.35
29	jM	201	PEB	CHB-C4B	15.51	1.48	1.35
29	m7	201	PEB	CHB-C4B	15.51	1.48	1.35
29	m9	201	PEB	CHB-C4B	15.51	1.48	1.35
29	IG	201	PEB	CHB-C4B	15.51	1.48	1.35
29	kJ	202	PEB	CHB-C4B	15.51	1.48	1.35
29	NK	1002	PEB	CHB-C4B	15.51	1.48	1.35
29	kL	202	PEB	CHB-C4B	15.51	1.48	1.35
29	IQ	201	PEB	CHB-C4B	15.51	1.48	1.35
29	GG	201	PEB	CHB-C4B	15.50	1.48	1.35
29	GQ	201	PEB	CHB-C4B	15.50	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E3	201	PEB	CHB-C4B	15.50	1.48	1.35
29	EO	201	PEB	CHB-C4B	15.50	1.48	1.35
29	I3	201	PEB	CHB-C4B	15.50	1.48	1.35
29	a7	201	PEB	CHB-C4B	15.50	1.48	1.35
29	a9	201	PEB	CHB-C4B	15.50	1.48	1.35
29	QB	203	PEB	CHB-C4B	15.50	1.48	1.35
29	QM	203	PEB	CHB-C4B	15.50	1.48	1.35
29	IO	201	PEB	CHB-C4B	15.50	1.48	1.35
29	CB	201	PEB	CHB-C4B	15.49	1.48	1.35
29	CM	201	PEB	CHB-C4B	15.49	1.48	1.35
29	UF	202	PEB	CHB-C4B	15.49	1.48	1.35
29	UI	202	PEB	CHB-C4B	15.49	1.48	1.35
30	xL	304	PUB	CHB-C1C	15.49	1.48	1.35
29	C3	201	PEB	CHB-C4B	15.49	1.48	1.35
29	T7	201	PEB	CHB-C4B	15.49	1.48	1.35
29	e7	201	PEB	CHB-C4B	15.49	1.48	1.35
29	L8	201	PEB	CHB-C4B	15.49	1.48	1.35
29	T9	201	PEB	CHB-C4B	15.49	1.48	1.35
29	e9	201	PEB	CHB-C4B	15.49	1.48	1.35
29	IB	201	PEB	CHB-C4B	15.49	1.48	1.35
29	IM	201	PEB	CHB-C4B	15.49	1.48	1.35
29	CO	201	PEB	CHB-C4B	15.49	1.48	1.35
29	IJ	202	PEB	CHB-C4B	15.49	1.48	1.35
29	IL	202	PEB	CHB-C4B	15.49	1.48	1.35
29	OF	201	PEB	CHB-C4B	15.49	1.48	1.35
29	OI	201	PEB	CHB-C4B	15.49	1.48	1.35
29	iJ	202	PEB	CHB-C4B	15.49	1.48	1.35
29	iL	202	PEB	CHB-C4B	15.49	1.48	1.35
29	GB	201	PEB	CHB-C4B	15.49	1.48	1.35
29	GM	201	PEB	CHB-C4B	15.49	1.48	1.35
29	GJ	202	PEB	CHB-C4B	15.48	1.48	1.35
29	GL	202	PEB	CHB-C4B	15.48	1.48	1.35
29	N3	201	PEB	CHB-C4B	15.48	1.48	1.35
29	fB	201	PEB	CHB-C4B	15.48	1.48	1.35
29	fM	201	PEB	CHB-C4B	15.48	1.48	1.35
29	aJ	202	PEB	CHB-C4B	15.48	1.48	1.35
29	aL	202	PEB	CHB-C4B	15.48	1.48	1.35
29	G3	201	PEB	CHB-C4B	15.47	1.48	1.35
29	QF	201	PEB	CHB-C4B	15.47	1.48	1.35
29	QI	201	PEB	CHB-C4B	15.47	1.48	1.35
29	GO	201	PEB	CHB-C4B	15.47	1.48	1.35
29	R7	201	PEB	CHB-C4B	15.47	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R9	201	PEB	CHB-C4B	15.47	1.48	1.35
29	L5	201	PEB	CHB-C4B	15.47	1.48	1.35
29	i7	201	PEB	CHB-C4B	15.47	1.48	1.35
29	i9	201	PEB	CHB-C4B	15.47	1.48	1.35
29	AJ	202	PEB	CHB-C4B	15.47	1.48	1.35
29	AL	202	PEB	CHB-C4B	15.47	1.48	1.35
29	V7	201	PEB	CHB-C4B	15.47	1.48	1.35
29	V9	201	PEB	CHB-C4B	15.47	1.48	1.35
29	EJ	202	PEB	CHB-C4B	15.47	1.48	1.35
29	EL	202	PEB	CHB-C4B	15.47	1.48	1.35
29	SJ	202	PEB	CHB-C4B	15.46	1.48	1.35
29	SL	202	PEB	CHB-C4B	15.46	1.48	1.35
29	N1	1002	PEB	CHB-C4B	15.46	1.48	1.35
29	jF	201	PEB	CHB-C4B	15.46	1.48	1.35
29	jI	201	PEB	CHB-C4B	15.46	1.48	1.35
29	A1	303	PEB	CHB-C4B	15.46	1.48	1.35
29	sJ	202	PEB	CHB-C4B	15.46	1.48	1.35
29	AK	303	PEB	CHB-C4B	15.46	1.48	1.35
29	sL	202	PEB	CHB-C4B	15.46	1.48	1.35
29	dF	202	PEB	CHB-C4B	15.46	1.48	1.35
29	dI	202	PEB	CHB-C4B	15.46	1.48	1.35
30	AF	303	PUB	CHB-C1C	15.46	1.48	1.35
30	AI	303	PUB	CHB-C1C	15.46	1.48	1.35
29	A3	201	PEB	CHB-C4B	15.46	1.48	1.35
29	AO	201	PEB	CHB-C4B	15.46	1.48	1.35
29	KJ	202	PEB	CHB-C4B	15.45	1.48	1.35
29	KL	202	PEB	CHB-C4B	15.45	1.48	1.35
29	M3	201	PEB	CHB-C4B	15.45	1.48	1.35
29	MO	201	PEB	CHB-C4B	15.45	1.48	1.35
29	CJ	202	PEB	CHB-C4B	15.44	1.48	1.35
29	CL	202	PEB	CHB-C4B	15.44	1.48	1.35
29	mJ	202	PEB	CHB-C4B	15.44	1.48	1.35
29	uJ	203	PEB	CHB-C4B	15.44	1.48	1.35
29	mL	202	PEB	CHB-C4B	15.44	1.48	1.35
29	uL	203	PEB	CHB-C4B	15.44	1.48	1.35
29	QJ	202	PEB	CHB-C4B	15.44	1.48	1.35
29	QL	202	PEB	CHB-C4B	15.44	1.48	1.35
29	oJ	202	PEB	CHB-C4B	15.43	1.48	1.35
29	oL	202	PEB	CHB-C4B	15.43	1.48	1.35
29	ZF	201	PEB	CHB-C4B	15.43	1.48	1.35
29	ZI	201	PEB	CHB-C4B	15.43	1.48	1.35
30	xJ	304	PUB	CHB-C1C	15.43	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M9	1001	CYC	CHA-C1A	15.43	1.48	1.35
29	KC	201	PEB	CHB-C4B	15.42	1.48	1.35
29	KE	201	PEB	CHB-C4B	15.42	1.48	1.35
29	UJ	202	PEB	CHB-C4B	15.42	1.48	1.35
29	UL	202	PEB	CHB-C4B	15.42	1.48	1.35
30	wJ	304	PUB	CHB-C1C	15.41	1.48	1.35
29	cJ	202	PEB	CHB-C4B	15.41	1.48	1.35
29	cL	202	PEB	CHB-C4B	15.41	1.48	1.35
31	C7	1001	CYC	CHA-C1A	15.41	1.48	1.35
31	C9	1001	CYC	CHA-C1A	15.41	1.48	1.35
29	A1	301	PEB	CHB-C4B	15.41	1.48	1.35
29	OJ	202	PEB	CHB-C4B	15.41	1.48	1.35
29	WJ	203	PEB	CHB-C4B	15.41	1.48	1.35
29	YJ	202	PEB	CHB-C4B	15.41	1.48	1.35
29	AK	301	PEB	CHB-C4B	15.41	1.48	1.35
29	OL	202	PEB	CHB-C4B	15.41	1.48	1.35
29	WL	203	PEB	CHB-C4B	15.41	1.48	1.35
29	YL	202	PEB	CHB-C4B	15.41	1.48	1.35
31	G7	1001	CYC	CHA-C1A	15.40	1.48	1.35
31	M7	1001	CYC	CHA-C1A	15.40	1.48	1.35
29	MJ	202	PEB	CHB-C4B	15.39	1.48	1.35
29	ML	202	PEB	CHB-C4B	15.39	1.48	1.35
29	gJ	202	PEB	CHB-C4B	15.39	1.48	1.35
29	gL	202	PEB	CHB-C4B	15.39	1.48	1.35
29	LC	202	PEB	CHB-C4B	15.38	1.48	1.35
29	LE	202	PEB	CHB-C4B	15.38	1.48	1.35
29	qJ	202	PEB	CHB-C4B	15.37	1.48	1.35
29	qL	202	PEB	CHB-C4B	15.37	1.48	1.35
31	K9	1001	CYC	CHA-C1A	15.37	1.48	1.35
29	HC	202	PEB	CHB-C4B	15.36	1.48	1.35
29	HE	202	PEB	CHB-C4B	15.36	1.48	1.35
29	BC	202	PEB	CHB-C4B	15.36	1.48	1.35
29	BE	202	PEB	CHB-C4B	15.36	1.48	1.35
31	K7	1001	CYC	CHA-C1A	15.36	1.47	1.35
29	eJ	202	PEB	CHB-C4B	15.35	1.47	1.35
29	eL	202	PEB	CHB-C4B	15.35	1.47	1.35
31	NF	1001	CYC	CHA-C1A	15.35	1.47	1.35
31	NI	1001	CYC	CHA-C1A	15.35	1.47	1.35
29	FC	202	PEB	CHB-C4B	15.34	1.47	1.35
29	FE	202	PEB	CHB-C4B	15.34	1.47	1.35
31	HF	1001	CYC	CHA-C1A	15.34	1.47	1.35
31	HI	1001	CYC	CHA-C1A	15.34	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I7	1001	CYC	CHA-C1A	15.34	1.47	1.35
31	I9	1001	CYC	CHA-C1A	15.34	1.47	1.35
31	E7	1001	CYC	CHA-C1A	15.33	1.47	1.35
31	E9	1001	CYC	CHA-C1A	15.33	1.47	1.35
31	G9	1001	CYC	CHA-C1A	15.32	1.47	1.35
29	EA	202	PEB	CHB-C4B	15.31	1.47	1.35
29	EN	202	PEB	CHB-C4B	15.31	1.47	1.35
30	wL	304	PUB	CHB-C1C	15.31	1.47	1.35
29	AC	203	PEB	CHB-C4B	15.30	1.47	1.35
29	AE	203	PEB	CHB-C4B	15.30	1.47	1.35
31	JF	1001	CYC	CHA-C1A	15.29	1.47	1.35
31	JI	1001	CYC	CHA-C1A	15.29	1.47	1.35
31	DF	1001	CYC	CHA-C1A	15.29	1.47	1.35
31	DI	1001	CYC	CHA-C1A	15.29	1.47	1.35
31	FF	1001	CYC	CHA-C1A	15.29	1.47	1.35
31	FI	1001	CYC	CHA-C1A	15.29	1.47	1.35
29	AF	301	PEB	CHB-C4B	15.28	1.47	1.35
29	AI	301	PEB	CHB-C4B	15.28	1.47	1.35
29	KA	202	PEB	CHB-C4B	15.26	1.47	1.35
29	KN	202	PEB	CHB-C4B	15.26	1.47	1.35
31	LF	1001	CYC	CHA-C1A	15.26	1.47	1.35
31	LI	1001	CYC	CHA-C1A	15.26	1.47	1.35
29	A7	301	PEB	CHB-C4B	15.26	1.47	1.35
29	A9	301	PEB	CHB-C4B	15.26	1.47	1.35
29	CA	202	PEB	CHB-C4B	15.26	1.47	1.35
29	CN	202	PEB	CHB-C4B	15.26	1.47	1.35
29	IA	202	PEB	CHB-C4B	15.25	1.47	1.35
29	IN	202	PEB	CHB-C4B	15.25	1.47	1.35
29	yJ	301	PEB	CHB-C4B	15.23	1.47	1.35
29	yL	301	PEB	CHB-C4B	15.23	1.47	1.35
29	d7	202	PEB	CHB-C4B	15.21	1.47	1.35
29	d9	202	PEB	CHB-C4B	15.21	1.47	1.35
29	GA	202	PEB	CHB-C4B	15.20	1.47	1.35
29	GN	202	PEB	CHB-C4B	15.20	1.47	1.35
29	S7	202	PEB	CHB-C4B	15.17	1.47	1.35
29	h7	202	PEB	CHB-C4B	15.17	1.47	1.35
29	S9	202	PEB	CHB-C4B	15.17	1.47	1.35
29	h9	202	PEB	CHB-C4B	15.17	1.47	1.35
29	AA	202	PEB	CHB-C4B	15.17	1.47	1.35
29	AN	202	PEB	CHB-C4B	15.17	1.47	1.35
31	K1	1001	CYC	CHA-C1A	15.17	1.47	1.35
31	KK	1001	CYC	CHA-C1A	15.17	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	KB	203	PEB	CHB-C4B	15.17	1.47	1.35
29	KM	203	PEB	CHB-C4B	15.17	1.47	1.35
29	J5	201	PEB	CHB-C4B	15.16	1.47	1.35
29	J8	201	PEB	CHB-C4B	15.16	1.47	1.35
29	U7	202	PEB	CHB-C4B	15.16	1.47	1.35
29	U9	202	PEB	CHB-C4B	15.16	1.47	1.35
29	l7	202	PEB	CHB-C4B	15.15	1.47	1.35
29	l9	202	PEB	CHB-C4B	15.15	1.47	1.35
29	Z7	202	PEB	CHB-C4B	15.14	1.47	1.35
29	Z9	202	PEB	CHB-C4B	15.14	1.47	1.35
29	W7	202	PEB	CHB-C4B	15.13	1.47	1.35
29	W9	202	PEB	CHB-C4B	15.13	1.47	1.35
29	f7	202	PEB	CHB-C4B	15.12	1.47	1.35
29	f9	202	PEB	CHB-C4B	15.12	1.47	1.35
29	Z7	201	PEB	CHB-C4B	15.12	1.47	1.35
29	Z9	201	PEB	CHB-C4B	15.12	1.47	1.35
29	W7	201	PEB	CHB-C4B	15.12	1.47	1.35
29	W9	201	PEB	CHB-C4B	15.12	1.47	1.35
30	wJ	305	PUB	CHB-C1C	15.11	1.47	1.35
29	J8	202	PEB	CHB-C4B	15.10	1.47	1.35
31	EK	1001	CYC	CHA-C1A	15.10	1.47	1.35
29	mB	202	PEB	CHB-C4B	15.10	1.47	1.35
29	mM	202	PEB	CHB-C4B	15.10	1.47	1.35
31	IK	1001	CYC	CHA-C1A	15.09	1.47	1.35
29	h7	201	PEB	CHB-C4B	15.09	1.47	1.35
29	h9	201	PEB	CHB-C4B	15.09	1.47	1.35
29	HB	202	PEB	CHB-C4B	15.09	1.47	1.35
29	HM	202	PEB	CHB-C4B	15.09	1.47	1.35
29	j7	202	PEB	CHB-C4B	15.09	1.47	1.35
29	j9	202	PEB	CHB-C4B	15.09	1.47	1.35
29	LG	202	PEB	CHB-C4B	15.09	1.47	1.35
29	LQ	201	PEB	CHB-C4B	15.09	1.47	1.35
31	M1	1001	CYC	CHA-C1A	15.09	1.47	1.35
31	CK	1001	CYC	CHA-C1A	15.09	1.47	1.35
31	MK	1001	CYC	CHA-C1A	15.09	1.47	1.35
29	U7	201	PEB	CHB-C4B	15.08	1.47	1.35
29	U9	201	PEB	CHB-C4B	15.08	1.47	1.35
29	RB	202	PEB	CHB-C4B	15.08	1.47	1.35
29	RM	202	PEB	CHB-C4B	15.08	1.47	1.35
29	b7	202	PEB	CHB-C4B	15.08	1.47	1.35
29	b9	202	PEB	CHB-C4B	15.08	1.47	1.35
29	f7	201	PEB	CHB-C4B	15.08	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f9	201	PEB	CHB-C4B	15.08	1.47	1.35
31	C1	1001	CYC	CHA-C1A	15.08	1.47	1.35
29	b7	201	PEB	CHB-C4B	15.08	1.47	1.35
29	b9	201	PEB	CHB-C4B	15.08	1.47	1.35
31	D1	1003	CYC	CHA-C1A	15.08	1.47	1.35
29	LA	201	PEB	CHB-C4B	15.07	1.47	1.35
29	LN	201	PEB	CHB-C4B	15.07	1.47	1.35
31	GK	1001	CYC	CHA-C1A	15.07	1.47	1.35
30	xL	305	PUB	CHB-C1C	15.07	1.47	1.35
31	I1	1001	CYC	CHA-C1A	15.06	1.47	1.35
29	O7	202	PEB	CHB-C4B	15.06	1.47	1.35
29	O9	202	PEB	CHB-C4B	15.06	1.47	1.35
29	VB	202	PEB	CHB-C4B	15.05	1.47	1.35
29	VM	202	PEB	CHB-C4B	15.05	1.47	1.35
29	ZB	202	PEB	CHB-C4B	15.05	1.47	1.35
29	cB	202	PEB	CHB-C4B	15.05	1.47	1.35
29	ZM	202	PEB	CHB-C4B	15.05	1.47	1.35
29	cM	202	PEB	CHB-C4B	15.05	1.47	1.35
29	FG	202	PEB	CHB-C4B	15.05	1.47	1.35
29	FQ	202	PEB	CHB-C4B	15.05	1.47	1.35
29	QB	202	PEB	CHB-C4B	15.04	1.47	1.35
29	TB	202	PEB	CHB-C4B	15.04	1.47	1.35
29	QM	202	PEB	CHB-C4B	15.04	1.47	1.35
29	TM	202	PEB	CHB-C4B	15.04	1.47	1.35
29	DB	202	PEB	CHB-C4B	15.04	1.47	1.35
29	DM	202	PEB	CHB-C4B	15.04	1.47	1.35
31	E1	1001	CYC	CHA-C1A	15.04	1.47	1.35
29	gB	202	PEB	CHB-C4B	15.04	1.47	1.35
29	gM	202	PEB	CHB-C4B	15.04	1.47	1.35
29	aB	203	PEB	CHB-C4B	15.04	1.47	1.35
29	aM	203	PEB	CHB-C4B	15.04	1.47	1.35
30	xJ	305	PUB	CHB-C1C	15.04	1.47	1.35
29	O7	201	PEB	CHB-C4B	15.03	1.47	1.35
29	O9	201	PEB	CHB-C4B	15.03	1.47	1.35
29	JB	202	PEB	CHB-C4B	15.03	1.47	1.35
29	JM	202	PEB	CHB-C4B	15.03	1.47	1.35
29	iB	202	PEB	CHB-C4B	15.03	1.47	1.35
29	iM	202	PEB	CHB-C4B	15.03	1.47	1.35
29	j7	201	PEB	CHB-C4B	15.03	1.47	1.35
29	j9	201	PEB	CHB-C4B	15.03	1.47	1.35
29	DA	201	PEB	CHB-C4B	15.03	1.47	1.35
29	DN	201	PEB	CHB-C4B	15.03	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q7	202	PEB	CHB-C4B	15.02	1.47	1.35
29	Q9	202	PEB	CHB-C4B	15.02	1.47	1.35
29	kB	202	PEB	CHB-C4B	15.02	1.47	1.35
29	kM	202	PEB	CHB-C4B	15.02	1.47	1.35
29	DG	202	PEB	CHB-C4B	15.02	1.47	1.35
29	DQ	202	PEB	CHB-C4B	15.02	1.47	1.35
29	S7	201	PEB	CHB-C4B	15.02	1.47	1.35
29	d7	201	PEB	CHB-C4B	15.02	1.47	1.35
29	S9	201	PEB	CHB-C4B	15.02	1.47	1.35
29	d9	201	PEB	CHB-C4B	15.02	1.47	1.35
29	HG	202	PEB	CHB-C4B	15.02	1.47	1.35
29	HQ	202	PEB	CHB-C4B	15.02	1.47	1.35
29	LB	202	PEB	CHB-C4B	15.01	1.47	1.35
29	LM	202	PEB	CHB-C4B	15.01	1.47	1.35
29	YB	201	PEB	CHB-C4B	15.01	1.47	1.35
29	YM	201	PEB	CHB-C4B	15.01	1.47	1.35
29	J5	202	PEB	CHB-C4B	15.01	1.47	1.35
30	MN	403	PUB	CHB-C1C	15.00	1.47	1.35
29	Q7	201	PEB	CHB-C4B	15.00	1.47	1.35
29	Q9	201	PEB	CHB-C4B	15.00	1.47	1.35
30	MA	403	PUB	CHB-C1C	15.00	1.47	1.35
29	HA	201	PEB	CHB-C4B	14.99	1.47	1.35
29	HN	201	PEB	CHB-C4B	14.99	1.47	1.35
29	JG	202	PEB	CHB-C4B	14.99	1.47	1.35
29	JQ	202	PEB	CHB-C4B	14.99	1.47	1.35
29	l7	201	PEB	CHB-C4B	14.98	1.47	1.35
29	l9	201	PEB	CHB-C4B	14.98	1.47	1.35
29	W2	201	PEB	CHB-C4B	14.98	1.47	1.35
29	FB	202	PEB	CHB-C4B	14.98	1.47	1.35
29	FM	202	PEB	CHB-C4B	14.98	1.47	1.35
29	JA	201	PEB	CHB-C4B	14.97	1.47	1.35
29	JN	201	PEB	CHB-C4B	14.97	1.47	1.35
29	O2	201	PEB	CHB-C4B	14.96	1.47	1.35
30	wL	305	PUB	CHB-C1C	14.96	1.47	1.35
29	M2	201	PEB	CHB-C4B	14.95	1.47	1.35
29	MR	201	PEB	CHB-C4B	14.95	1.47	1.35
29	ED	202	PEB	CHB-C4B	14.95	1.47	1.35
30	A1	305	PUB	CHB-C1C	14.94	1.47	1.35
30	AK	305	PUB	CHB-C1C	14.94	1.47	1.35
29	GD	203	PEB	CHB-C4B	14.94	1.47	1.35
29	BA	201	PEB	CHB-C4B	14.92	1.47	1.35
29	BN	201	PEB	CHB-C4B	14.92	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FA	201	PEB	CHB-C4B	14.92	1.47	1.35
29	FN	201	PEB	CHB-C4B	14.92	1.47	1.35
29	BG	202	PEB	CHB-C4B	14.92	1.47	1.35
29	BQ	202	PEB	CHB-C4B	14.92	1.47	1.35
29	wL	301	PEB	CHB-C4B	14.90	1.47	1.35
29	J9	1002	PEB	CHB-C4B	14.90	1.47	1.35
29	WR	201	PEB	CHB-C4B	14.90	1.47	1.35
29	OR	201	PEB	CHB-C4B	14.90	1.47	1.35
29	MD	203	PEB	CHB-C4B	14.90	1.47	1.35
31	MF	1001	CYC	CHA-C1A	14.89	1.47	1.35
31	MI	1001	CYC	CHA-C1A	14.89	1.47	1.35
29	L9	1002	PEB	CHB-C4B	14.89	1.47	1.35
29	E4	203	PEB	CHB-C4B	14.88	1.47	1.35
29	CD	203	PEB	CHB-C4B	14.88	1.47	1.35
29	MD	201	PEB	CHB-C4B	14.88	1.47	1.35
29	xL	301	PEB	CHB-C4B	14.87	1.47	1.35
29	UR	201	PEB	CHB-C4B	14.86	1.47	1.35
29	F7	1002	PEB	CHB-C4B	14.86	1.47	1.35
29	MA	405	PEB	CHB-C4B	14.85	1.47	1.35
29	M4	201	PEB	CHB-C4B	14.84	1.47	1.35
29	MN	405	PEB	CHB-C4B	14.84	1.47	1.35
29	QR	201	PEB	CHB-C4B	14.84	1.47	1.35
29	dD	401	PEB	CHB-C4B	14.84	1.47	1.35
29	U1	203	PEB	CHB-C4B	14.84	1.47	1.35
29	UK	203	PEB	CHB-C4B	14.84	1.47	1.35
29	K4	201	PEB	CHB-C4B	14.84	1.47	1.35
31	GF	1001	CYC	CHA-C1A	14.84	1.47	1.35
31	GI	1001	CYC	CHA-C1A	14.84	1.47	1.35
29	Q2	201	PEB	CHB-C4B	14.84	1.47	1.35
29	GD	201	PEB	CHB-C4B	14.84	1.47	1.35
29	l1	202	PEB	CHB-C4B	14.84	1.47	1.35
29	lK	202	PEB	CHB-C4B	14.84	1.47	1.35
29	J7	1002	PEB	CHB-C4B	14.83	1.47	1.35
29	G4	203	PEB	CHB-C4B	14.82	1.47	1.35
29	C4	201	PEB	CHB-C4B	14.81	1.47	1.35
30	MG	402	PUB	CHB-C1C	14.81	1.47	1.35
31	KI	1001	CYC	CHA-C1A	14.81	1.47	1.35
29	wJ	301	PEB	CHB-C4B	14.81	1.47	1.35
29	f1	202	PEB	CHB-C4B	14.80	1.47	1.35
29	fK	202	PEB	CHB-C4B	14.80	1.47	1.35
29	G4	201	PEB	CHB-C4B	14.80	1.47	1.35
31	KF	1001	CYC	CHA-C1A	14.80	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z1	203	PEB	CHB-C4B	14.80	1.47	1.35
29	ZK	203	PEB	CHB-C4B	14.80	1.47	1.35
31	IF	1001	CYC	CHA-C1A	14.80	1.47	1.35
31	II	1001	CYC	CHA-C1A	14.80	1.47	1.35
29	ID	203	PEB	CHB-C4B	14.80	1.47	1.35
29	L7	1002	PEB	CHB-C4B	14.79	1.47	1.35
29	C4	203	PEB	CHB-C4B	14.79	1.47	1.35
29	KD	203	PEB	CHB-C4B	14.79	1.47	1.35
29	xJ	301	PEB	CHB-C4B	14.79	1.47	1.35
31	EF	1001	CYC	CHA-C1A	14.79	1.47	1.35
31	EI	1001	CYC	CHA-C1A	14.79	1.47	1.35
29	K4	203	PEB	CHB-C4B	14.79	1.47	1.35
29	W1	202	PEB	CHB-C4B	14.79	1.47	1.35
29	E4	201	PEB	CHB-C4B	14.79	1.47	1.35
29	WK	202	PEB	CHB-C4B	14.79	1.47	1.35
29	R7	202	PEB	CHB-C4B	14.78	1.47	1.35
29	R9	202	PEB	CHB-C4B	14.78	1.47	1.35
29	Q1	202	PEB	CHB-C4B	14.78	1.47	1.35
29	h1	202	PEB	CHB-C4B	14.78	1.47	1.35
29	QK	202	PEB	CHB-C4B	14.78	1.47	1.35
29	hK	202	PEB	CHB-C4B	14.78	1.47	1.35
29	d1	202	PEB	CHB-C4B	14.78	1.47	1.35
29	dK	202	PEB	CHB-C4B	14.78	1.47	1.35
29	b1	202	PEB	CHB-C4B	14.78	1.47	1.35
29	bK	202	PEB	CHB-C4B	14.78	1.47	1.35
29	j1	202	PEB	CHB-C4B	14.77	1.47	1.35
29	I4	201	PEB	CHB-C4B	14.77	1.47	1.35
29	jK	202	PEB	CHB-C4B	14.77	1.47	1.35
29	F9	1002	PEB	CHB-C4B	14.77	1.47	1.35
29	V7	202	PEB	CHB-C4B	14.76	1.47	1.35
29	V9	202	PEB	CHB-C4B	14.76	1.47	1.35
29	JA	202	PEB	CHB-C4B	14.75	1.47	1.35
29	JN	202	PEB	CHB-C4B	14.75	1.47	1.35
29	T7	202	PEB	CHB-C4B	14.75	1.47	1.35
29	k7	202	PEB	CHB-C4B	14.75	1.47	1.35
29	T9	202	PEB	CHB-C4B	14.75	1.47	1.35
29	k9	202	PEB	CHB-C4B	14.75	1.47	1.35
31	CF	1001	CYC	CHA-C1A	14.75	1.47	1.35
31	CI	1001	CYC	CHA-C1A	14.75	1.47	1.35
29	DA	202	PEB	CHB-C4B	14.74	1.47	1.35
29	DN	202	PEB	CHB-C4B	14.74	1.47	1.35
29	P7	202	PEB	CHB-C4B	14.74	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P9	202	PEB	CHB-C4B	14.74	1.47	1.35
29	S1	202	PEB	CHB-C4B	14.72	1.47	1.35
29	Y7	202	PEB	CHB-C4B	14.72	1.47	1.35
29	Y9	202	PEB	CHB-C4B	14.72	1.47	1.35
29	SK	202	PEB	CHB-C4B	14.72	1.47	1.35
29	NO	203	PEB	CHB-C4B	14.72	1.47	1.35
29	a7	202	PEB	CHB-C4B	14.71	1.47	1.35
29	a9	202	PEB	CHB-C4B	14.71	1.47	1.35
29	FA	202	PEB	CHB-C4B	14.71	1.47	1.35
29	FN	202	PEB	CHB-C4B	14.71	1.47	1.35
29	H7	1002	PEB	CHB-C4B	14.71	1.47	1.35
29	H9	1002	PEB	CHB-C4B	14.71	1.47	1.35
29	LA	202	PEB	CHB-C4B	14.71	1.47	1.35
29	LN	202	PEB	CHB-C4B	14.71	1.47	1.35
29	O1	202	PEB	CHB-C4B	14.71	1.47	1.35
29	OK	202	PEB	CHB-C4B	14.71	1.47	1.35
29	U2	201	PEB	CHB-C4B	14.70	1.47	1.35
29	N7	1002	PEB	CHB-C4B	14.70	1.47	1.35
29	N9	1002	PEB	CHB-C4B	14.70	1.47	1.35
29	HA	202	PEB	CHB-C4B	14.69	1.47	1.35
29	HN	202	PEB	CHB-C4B	14.69	1.47	1.35
29	D7	1002	PEB	CHB-C4B	14.68	1.47	1.35
29	D9	1002	PEB	CHB-C4B	14.68	1.47	1.35
29	ID	201	PEB	CHB-C4B	14.68	1.47	1.35
29	IJ	202	PEB	CHB-C4B	14.68	1.47	1.35
29	IL	202	PEB	CHB-C4B	14.68	1.47	1.35
29	KD	201	PEB	CHB-C4B	14.67	1.47	1.35
29	CD	201	PEB	CHB-C4B	14.67	1.47	1.35
29	dJ	202	PEB	CHB-C4B	14.67	1.47	1.35
29	dL	202	PEB	CHB-C4B	14.67	1.47	1.35
30	MQ	404	PUB	CHB-C1C	14.67	1.47	1.35
29	i7	202	PEB	CHB-C4B	14.66	1.47	1.35
29	i9	202	PEB	CHB-C4B	14.66	1.47	1.35
29	g7	202	PEB	CHB-C4B	14.66	1.47	1.35
29	g9	202	PEB	CHB-C4B	14.66	1.47	1.35
29	BA	202	PEB	CHB-C4B	14.66	1.47	1.35
29	BN	202	PEB	CHB-C4B	14.66	1.47	1.35
29	c7	202	PEB	CHB-C4B	14.65	1.47	1.35
29	m7	202	PEB	CHB-C4B	14.65	1.47	1.35
29	c9	202	PEB	CHB-C4B	14.65	1.47	1.35
29	m9	202	PEB	CHB-C4B	14.65	1.47	1.35
29	e7	202	PEB	CHB-C4B	14.64	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e9	202	PEB	CHB-C4B	14.64	1.47	1.35
29	FJ	202	PEB	CHB-C4B	14.64	1.47	1.35
29	FL	202	PEB	CHB-C4B	14.64	1.47	1.35
29	M3	203	PEB	CHB-C4B	14.64	1.47	1.35
29	MO	203	PEB	CHB-C4B	14.64	1.47	1.35
29	jJ	202	PEB	CHB-C4B	14.62	1.47	1.35
29	jL	202	PEB	CHB-C4B	14.62	1.47	1.35
29	N3	203	PEB	CHB-C4B	14.62	1.47	1.35
29	hJ	202	PEB	CHB-C4B	14.62	1.47	1.35
29	hL	202	PEB	CHB-C4B	14.62	1.47	1.35
29	fJ	202	PEB	CHB-C4B	14.61	1.47	1.35
29	sJ	203	PEB	CHB-C4B	14.61	1.47	1.35
29	fL	202	PEB	CHB-C4B	14.61	1.47	1.35
29	sL	203	PEB	CHB-C4B	14.61	1.47	1.35
29	bJ	202	PEB	CHB-C4B	14.61	1.47	1.35
29	bL	202	PEB	CHB-C4B	14.61	1.47	1.35
29	WJ	201	PEB	CHB-C4B	14.60	1.47	1.35
29	WL	201	PEB	CHB-C4B	14.60	1.47	1.35
29	j1	201	PEB	CHB-C4B	14.59	1.47	1.35
29	jK	201	PEB	CHB-C4B	14.59	1.47	1.35
29	PJ	202	PEB	CHB-C4B	14.58	1.47	1.35
29	PL	202	PEB	CHB-C4B	14.58	1.47	1.35
29	JJ	202	PEB	CHB-C4B	14.57	1.47	1.35
29	JL	202	PEB	CHB-C4B	14.57	1.47	1.35
29	NJ	202	PEB	CHB-C4B	14.57	1.47	1.35
29	NL	202	PEB	CHB-C4B	14.57	1.47	1.35
29	AJ	203	PEB	CHB-C4B	14.56	1.47	1.35
29	RJ	202	PEB	CHB-C4B	14.56	1.47	1.35
29	AL	203	PEB	CHB-C4B	14.56	1.47	1.35
29	RL	202	PEB	CHB-C4B	14.56	1.47	1.35
29	IJ	203	PEB	CHB-C4B	14.56	1.47	1.35
29	IL	203	PEB	CHB-C4B	14.56	1.47	1.35
29	U1	202	PEB	CHB-C4B	14.56	1.47	1.35
29	UK	202	PEB	CHB-C4B	14.56	1.47	1.35
29	T2	202	PEB	CHB-C4B	14.56	1.47	1.35
29	pJ	202	PEB	CHB-C4B	14.56	1.47	1.35
29	pL	202	PEB	CHB-C4B	14.56	1.47	1.35
29	TR	202	PEB	CHB-C4B	14.56	1.47	1.35
29	HJ	201	PEB	CHB-C4B	14.56	1.47	1.35
29	HL	201	PEB	CHB-C4B	14.56	1.47	1.35
29	nJ	202	PEB	CHB-C4B	14.55	1.47	1.35
29	uJ	201	PEB	CHB-C4B	14.55	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	nL	202	PEB	CHB-C4B	14.55	1.47	1.35
29	uL	201	PEB	CHB-C4B	14.55	1.47	1.35
29	rJ	202	PEB	CHB-C4B	14.54	1.47	1.35
29	rL	202	PEB	CHB-C4B	14.54	1.47	1.35
29	W1	201	PEB	CHB-C4B	14.54	1.47	1.35
29	WK	201	PEB	CHB-C4B	14.54	1.47	1.35
29	MQ	406	PEB	CHB-C4B	14.54	1.47	1.35
29	h1	201	PEB	CHB-C4B	14.53	1.47	1.35
29	hK	201	PEB	CHB-C4B	14.53	1.47	1.35
29	S1	201	PEB	CHB-C4B	14.52	1.47	1.35
29	gF	202	PEB	CHB-C4B	14.52	1.47	1.35
29	gI	202	PEB	CHB-C4B	14.52	1.47	1.35
29	SK	201	PEB	CHB-C4B	14.52	1.47	1.35
29	OF	203	PEB	CHB-C4B	14.52	1.47	1.35
29	OI	203	PEB	CHB-C4B	14.52	1.47	1.35
29	ZJ	202	PEB	CHB-C4B	14.52	1.47	1.35
29	ZL	202	PEB	CHB-C4B	14.52	1.47	1.35
29	f1	201	PEB	CHB-C4B	14.52	1.47	1.35
29	BJ	202	PEB	CHB-C4B	14.52	1.47	1.35
29	fK	201	PEB	CHB-C4B	14.52	1.47	1.35
29	BL	202	PEB	CHB-C4B	14.52	1.47	1.35
29	XR	202	PEB	CHB-C4B	14.51	1.47	1.35
29	TJ	202	PEB	CHB-C4B	14.50	1.47	1.35
29	TL	202	PEB	CHB-C4B	14.50	1.47	1.35
29	Q1	201	PEB	CHB-C4B	14.49	1.47	1.35
29	QK	201	PEB	CHB-C4B	14.49	1.47	1.35
29	b1	201	PEB	CHB-C4B	14.49	1.47	1.35
29	bK	201	PEB	CHB-C4B	14.49	1.47	1.35
29	VF	202	PEB	CHB-C4B	14.48	1.47	1.35
29	VI	202	PEB	CHB-C4B	14.48	1.47	1.35
29	MQ	403	PEB	CHB-C4B	14.48	1.47	1.35
29	O1	201	PEB	CHB-C4B	14.47	1.47	1.35
29	Z1	202	PEB	CHB-C4B	14.47	1.47	1.35
29	OK	201	PEB	CHB-C4B	14.47	1.47	1.35
29	ZK	202	PEB	CHB-C4B	14.47	1.47	1.35
29	P2	201	PEB	CHB-C4B	14.47	1.47	1.35
29	PR	201	PEB	CHB-C4B	14.47	1.47	1.35
29	MG	401	PEB	CHB-C4B	14.46	1.47	1.35
29	l1	201	PEB	CHB-C4B	14.46	1.47	1.35
29	lK	201	PEB	CHB-C4B	14.46	1.47	1.35
29	R2	202	PEB	CHB-C4B	14.45	1.47	1.35
29	RR	202	PEB	CHB-C4B	14.45	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	XJ	202	PEB	CHB-C4B	14.45	1.47	1.35
29	XL	202	PEB	CHB-C4B	14.45	1.47	1.35
29	MG	404	PEB	CHB-C4B	14.45	1.47	1.35
29	d1	201	PEB	CHB-C4B	14.45	1.47	1.35
29	dK	201	PEB	CHB-C4B	14.45	1.47	1.35
29	kF	202	PEB	CHB-C4B	14.45	1.47	1.35
29	kI	202	PEB	CHB-C4B	14.45	1.47	1.35
30	MA	402	PUB	CHB-C1C	14.45	1.47	1.35
29	X2	201	PEB	CHB-C4B	14.45	1.47	1.35
29	NR	202	PEB	CHB-C4B	14.44	1.47	1.35
29	eF	202	PEB	CHB-C4B	14.43	1.47	1.35
29	eI	202	PEB	CHB-C4B	14.43	1.47	1.35
29	aF	202	PEB	CHB-C4B	14.43	1.47	1.35
29	aI	202	PEB	CHB-C4B	14.43	1.47	1.35
29	iF	202	PEB	CHB-C4B	14.42	1.47	1.35
29	iI	202	PEB	CHB-C4B	14.42	1.47	1.35
29	V2	202	PEB	CHB-C4B	14.42	1.47	1.35
29	mF	202	PEB	CHB-C4B	14.42	1.47	1.35
29	mI	202	PEB	CHB-C4B	14.42	1.47	1.35
30	MN	402	PUB	CHB-C1C	14.41	1.47	1.35
29	PF	202	PEB	CHB-C4B	14.40	1.47	1.35
29	PI	202	PEB	CHB-C4B	14.40	1.47	1.35
29	YF	202	PEB	CHB-C4B	14.40	1.47	1.35
29	YI	202	PEB	CHB-C4B	14.40	1.47	1.35
29	dF	201	PEB	CHB-C4B	14.38	1.47	1.35
29	dI	201	PEB	CHB-C4B	14.38	1.47	1.35
29	UF	201	PEB	CHB-C4B	14.37	1.47	1.35
29	UI	201	PEB	CHB-C4B	14.37	1.47	1.35
29	VR	202	PEB	CHB-C4B	14.36	1.47	1.35
29	N2	202	PEB	CHB-C4B	14.31	1.47	1.35
29	F4	201	PEB	CHB-C4B	14.27	1.47	1.35
29	HD	201	PEB	CHB-C4B	14.24	1.47	1.35
29	LD	201	PEB	CHB-C4B	14.22	1.47	1.35
29	L4	201	PEB	CHB-C4B	14.21	1.47	1.35
29	BD	201	PEB	CHB-C4B	14.21	1.47	1.35
29	H4	201	PEB	CHB-C4B	14.20	1.47	1.35
29	MD	202	PEB	CHB-C4B	14.20	1.47	1.35
29	FD	201	PEB	CHB-C4B	14.20	1.47	1.35
29	ID	202	PEB	CHB-C4B	14.19	1.47	1.35
29	ED	201	PEB	CHB-C4B	14.14	1.46	1.35
29	I4	202	PEB	CHB-C4B	14.14	1.46	1.35
29	B4	201	PEB	CHB-C4B	14.14	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K4	202	PEB	CHB-C4B	14.13	1.46	1.35
29	M4	202	PEB	CHB-C4B	14.13	1.46	1.35
29	D4	201	PEB	CHB-C4B	14.11	1.46	1.35
29	MQ	407	PEB	CHB-C4B	14.11	1.46	1.35
29	E4	202	PEB	CHB-C4B	14.09	1.46	1.35
29	C4	202	PEB	CHB-C4B	14.08	1.46	1.35
29	MN	404	PEB	CHB-C4B	14.08	1.46	1.35
29	CD	202	PEB	CHB-C4B	14.08	1.46	1.35
29	DD	201	PEB	CHB-C4B	14.07	1.46	1.35
29	MA	404	PEB	CHB-C4B	14.06	1.46	1.35
29	BD	202	PEB	CHB-C4B	14.06	1.46	1.35
29	G4	202	PEB	CHB-C4B	14.06	1.46	1.35
29	J4	201	PEB	CHB-C4B	14.06	1.46	1.35
29	JD	201	PEB	CHB-C4B	14.06	1.46	1.35
31	N7	1001	CYC	CHA-C1A	14.04	1.46	1.35
31	N9	1001	CYC	CHA-C1A	14.04	1.46	1.35
31	L9	1001	CYC	CHA-C1A	14.03	1.46	1.35
29	KD	202	PEB	CHB-C4B	14.03	1.46	1.35
31	F7	1001	CYC	CHA-C1A	14.02	1.46	1.35
31	F9	1001	CYC	CHA-C1A	14.01	1.46	1.35
29	LD	202	PEB	CHB-C4B	14.01	1.46	1.35
31	D7	1001	CYC	CHA-C1A	14.00	1.46	1.35
31	D9	1001	CYC	CHA-C1A	14.00	1.46	1.35
31	J9	1001	CYC	CHA-C1A	14.00	1.46	1.35
29	GD	202	PEB	CHB-C4B	13.98	1.46	1.35
31	J7	1001	CYC	CHA-C1A	13.98	1.46	1.35
29	L4	202	PEB	CHB-C4B	13.96	1.46	1.35
29	FD	202	PEB	CHB-C4B	13.96	1.46	1.35
31	L7	1001	CYC	CHA-C1A	13.96	1.46	1.35
29	B4	202	PEB	CHB-C4B	13.95	1.46	1.35
29	MG	405	PEB	CHB-C4B	13.95	1.46	1.35
31	H7	1001	CYC	CHA-C1A	13.94	1.46	1.35
31	H9	1001	CYC	CHA-C1A	13.94	1.46	1.35
29	F4	202	PEB	CHB-C4B	13.94	1.46	1.35
29	DD	202	PEB	CHB-C4B	13.93	1.46	1.35
29	P1	202	PEB	CHB-C4B	13.91	1.46	1.35
29	PK	202	PEB	CHB-C4B	13.91	1.46	1.35
29	g1	202	PEB	CHB-C4B	13.91	1.46	1.35
29	gK	202	PEB	CHB-C4B	13.91	1.46	1.35
29	JD	202	PEB	CHB-C4B	13.90	1.46	1.35
29	V1	202	PEB	CHB-C4B	13.89	1.46	1.35
29	j1	203	PEB	CHB-C4B	13.89	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VK	202	PEB	CHB-C4B	13.89	1.46	1.35
29	jK	203	PEB	CHB-C4B	13.89	1.46	1.35
29	i1	202	PEB	CHB-C4B	13.86	1.46	1.35
29	iK	202	PEB	CHB-C4B	13.86	1.46	1.35
29	J4	202	PEB	CHB-C4B	13.86	1.46	1.35
29	c1	202	PEB	CHB-C4B	13.85	1.46	1.35
29	cK	202	PEB	CHB-C4B	13.85	1.46	1.35
29	KA	201	PEB	CHB-C4B	13.84	1.46	1.35
29	KN	201	PEB	CHB-C4B	13.84	1.46	1.35
29	e1	202	PEB	CHB-C4B	13.84	1.46	1.35
29	eK	202	PEB	CHB-C4B	13.84	1.46	1.35
29	IA	201	PEB	CHB-C4B	13.83	1.46	1.35
29	IN	201	PEB	CHB-C4B	13.83	1.46	1.35
29	HD	202	PEB	CHB-C4B	13.83	1.46	1.35
29	GA	201	PEB	CHB-C4B	13.82	1.46	1.35
29	GN	201	PEB	CHB-C4B	13.82	1.46	1.35
29	U1	201	PEB	CHB-C4B	13.82	1.46	1.35
29	UK	201	PEB	CHB-C4B	13.82	1.46	1.35
29	D4	202	PEB	CHB-C4B	13.79	1.46	1.35
29	MN	401	PEB	CHB-C4B	13.79	1.46	1.35
29	a1	202	PEB	CHB-C4B	13.79	1.46	1.35
29	aK	202	PEB	CHB-C4B	13.79	1.46	1.35
29	R1	202	PEB	CHB-C4B	13.78	1.46	1.35
29	RK	202	PEB	CHB-C4B	13.78	1.46	1.35
29	Z1	201	PEB	CHB-C4B	13.78	1.46	1.35
29	ZK	201	PEB	CHB-C4B	13.78	1.46	1.35
29	CA	201	PEB	CHB-C4B	13.77	1.46	1.35
29	EA	201	PEB	CHB-C4B	13.77	1.46	1.35
29	CN	201	PEB	CHB-C4B	13.77	1.46	1.35
29	EN	201	PEB	CHB-C4B	13.77	1.46	1.35
29	AA	201	PEB	CHB-C4B	13.77	1.46	1.35
29	AN	201	PEB	CHB-C4B	13.77	1.46	1.35
29	H4	202	PEB	CHB-C4B	13.75	1.46	1.35
29	k1	202	PEB	CHB-C4B	13.74	1.46	1.35
29	kK	202	PEB	CHB-C4B	13.74	1.46	1.35
29	MA	401	PEB	CHB-C4B	13.73	1.46	1.35
30	MN	402	PUB	C3A-C2A	13.52	1.49	1.34
30	MA	402	PUB	C3A-C2A	13.44	1.49	1.34
30	AB	304	PUB	CHB-C1C	13.33	1.46	1.35
30	AM	304	PUB	CHB-C1C	13.32	1.46	1.35
30	MQ	404	PUB	C3A-C2A	13.20	1.49	1.34
30	MG	402	PUB	C3A-C2A	13.06	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	uJ	202	PEB	CHB-C4B	12.84	1.45	1.35
29	uL	202	PEB	CHB-C4B	12.84	1.45	1.35
29	qJ	201	PEB	CHB-C4B	12.81	1.45	1.35
29	qL	201	PEB	CHB-C4B	12.81	1.45	1.35
29	IJ	201	PEB	CHB-C4B	12.81	1.45	1.35
29	IL	201	PEB	CHB-C4B	12.81	1.45	1.35
29	KJ	201	PEB	CHB-C4B	12.79	1.45	1.35
29	KL	201	PEB	CHB-C4B	12.79	1.45	1.35
29	MJ	201	PEB	CHB-C4B	12.79	1.45	1.35
29	ML	201	PEB	CHB-C4B	12.79	1.45	1.35
29	gJ	201	PEB	CHB-C4B	12.78	1.45	1.35
29	gL	201	PEB	CHB-C4B	12.78	1.45	1.35
29	UJ	201	PEB	CHB-C4B	12.77	1.45	1.35
29	UL	201	PEB	CHB-C4B	12.77	1.45	1.35
29	OJ	201	PEB	CHB-C4B	12.77	1.45	1.35
29	OL	201	PEB	CHB-C4B	12.77	1.45	1.35
29	WJ	202	PEB	CHB-C4B	12.75	1.45	1.35
29	WL	202	PEB	CHB-C4B	12.75	1.45	1.35
29	mJ	201	PEB	CHB-C4B	12.75	1.45	1.35
29	mL	201	PEB	CHB-C4B	12.75	1.45	1.35
29	EJ	201	PEB	CHB-C4B	12.75	1.45	1.35
29	kJ	201	PEB	CHB-C4B	12.75	1.45	1.35
29	EL	201	PEB	CHB-C4B	12.75	1.45	1.35
29	kL	201	PEB	CHB-C4B	12.75	1.45	1.35
29	sJ	201	PEB	CHB-C4B	12.74	1.45	1.35
29	sL	201	PEB	CHB-C4B	12.74	1.45	1.35
29	CJ	201	PEB	CHB-C4B	12.74	1.45	1.35
29	CL	201	PEB	CHB-C4B	12.74	1.45	1.35
29	aJ	201	PEB	CHB-C4B	12.73	1.45	1.35
29	aL	201	PEB	CHB-C4B	12.73	1.45	1.35
29	QJ	201	PEB	CHB-C4B	12.73	1.45	1.35
29	QL	201	PEB	CHB-C4B	12.73	1.45	1.35
29	SJ	201	PEB	CHB-C4B	12.72	1.45	1.35
29	SL	201	PEB	CHB-C4B	12.72	1.45	1.35
29	cJ	201	PEB	CHB-C4B	12.72	1.45	1.35
29	cL	201	PEB	CHB-C4B	12.72	1.45	1.35
29	iJ	201	PEB	CHB-C4B	12.72	1.45	1.35
29	iL	201	PEB	CHB-C4B	12.72	1.45	1.35
29	YJ	201	PEB	CHB-C4B	12.71	1.45	1.35
29	YL	201	PEB	CHB-C4B	12.71	1.45	1.35
29	oJ	201	PEB	CHB-C4B	12.70	1.45	1.35
29	oL	201	PEB	CHB-C4B	12.70	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GJ	201	PEB	CHB-C4B	12.69	1.45	1.35
29	GL	201	PEB	CHB-C4B	12.69	1.45	1.35
29	eJ	201	PEB	CHB-C4B	12.68	1.45	1.35
29	eL	201	PEB	CHB-C4B	12.68	1.45	1.35
29	AJ	201	PEB	CHB-C4B	12.65	1.45	1.35
29	AL	201	PEB	CHB-C4B	12.65	1.45	1.35
30	A1	305	PUB	C3A-C2A	12.38	1.48	1.34
30	AK	305	PUB	C3A-C2A	12.38	1.48	1.34
30	QB	201	PUB	C3A-C2A	12.14	1.48	1.34
30	QM	201	PUB	C3A-C2A	12.14	1.48	1.34
30	MQ	405	PUB	C3A-C2A	11.97	1.48	1.34
30	MG	403	PUB	C3A-C2A	11.91	1.47	1.34
30	yL	303	PUB	C3A-C2A	11.65	1.47	1.34
30	yJ	303	PUB	C3A-C2A	11.64	1.47	1.34
30	xL	304	PUB	C3A-C2A	11.60	1.47	1.34
30	xJ	304	PUB	C3A-C2A	11.58	1.47	1.34
30	wJ	304	PUB	C3A-C2A	11.52	1.47	1.34
30	BB	302	PUB	C3A-C2A	11.50	1.47	1.34
30	wL	304	PUB	C3A-C2A	11.50	1.47	1.34
30	BM	302	PUB	C3A-C2A	11.50	1.47	1.34
30	MA	403	PUB	C3A-C2A	11.38	1.47	1.34
30	MN	403	PUB	C3A-C2A	11.36	1.47	1.34
30	AF	302	PUB	C3A-C2A	11.33	1.47	1.34
30	AI	302	PUB	C3A-C2A	11.33	1.47	1.34
30	AM	304	PUB	C3A-C2A	11.32	1.47	1.34
30	AB	304	PUB	C3A-C2A	11.29	1.47	1.34
30	A7	303	PUB	C3A-C2A	11.28	1.47	1.34
30	A9	303	PUB	C3A-C2A	11.28	1.47	1.34
30	A1	304	PUB	C3A-C2A	11.21	1.47	1.34
30	AK	304	PUB	C3A-C2A	11.21	1.47	1.34
30	xL	305	PUB	C3A-C2A	11.16	1.47	1.34
30	A7	302	PUB	C3A-C2A	11.15	1.47	1.34
30	A9	302	PUB	C3A-C2A	11.15	1.47	1.34
30	wL	305	PUB	C3A-C2A	11.14	1.47	1.34
30	yJ	302	PUB	C3A-C2A	11.13	1.47	1.34
30	yL	302	PUB	C3A-C2A	11.13	1.47	1.34
30	AM	305	PUB	C3A-C2A	11.11	1.47	1.34
30	xJ	305	PUB	C3A-C2A	11.10	1.47	1.34
30	AB	305	PUB	C3A-C2A	11.09	1.47	1.34
30	wJ	305	PUB	C3A-C2A	11.08	1.46	1.34
30	AF	303	PUB	C3A-C2A	10.88	1.46	1.34
30	AI	303	PUB	C3A-C2A	10.88	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HQ	203	PEB	C2D-C3D	10.30	1.47	1.34
29	JG	203	PEB	C2D-C3D	10.26	1.47	1.34
29	FQ	203	PEB	C2D-C3D	10.24	1.47	1.34
29	BQ	203	PEB	C2D-C3D	10.23	1.47	1.34
29	HG	203	PEB	C2D-C3D	10.23	1.47	1.34
29	BG	203	PEB	C2D-C3D	10.22	1.47	1.34
29	DG	203	PEB	C2D-C3D	10.21	1.47	1.34
29	JQ	203	PEB	C2D-C3D	10.18	1.47	1.34
29	LG	203	PEB	C2D-C3D	10.17	1.47	1.34
29	LQ	202	PEB	C2D-C3D	10.17	1.47	1.34
29	FG	203	PEB	C2D-C3D	10.16	1.47	1.34
29	MG	404	PEB	C2D-C3D	10.13	1.47	1.34
29	KD	203	PEB	C2D-C3D	10.13	1.47	1.34
29	DQ	203	PEB	C2D-C3D	10.13	1.47	1.34
29	MQ	406	PEB	C2D-C3D	10.08	1.47	1.34
29	DC	202	PEB	C2D-C3D	10.06	1.47	1.34
29	DE	202	PEB	C2D-C3D	10.06	1.47	1.34
29	K4	203	PEB	C2D-C3D	10.05	1.47	1.34
29	LC	203	PEB	C2D-C3D	10.04	1.47	1.34
29	LE	203	PEB	C2D-C3D	10.04	1.47	1.34
29	HC	203	PEB	C2D-C3D	10.03	1.47	1.34
29	HE	203	PEB	C2D-C3D	10.03	1.47	1.34
29	FC	203	PEB	C2D-C3D	10.03	1.47	1.34
29	FE	203	PEB	C2D-C3D	10.03	1.47	1.34
29	JC	202	PEB	C2D-C3D	10.02	1.47	1.34
29	JE	202	PEB	C2D-C3D	10.02	1.47	1.34
29	ED	202	PEB	C2D-C3D	10.02	1.47	1.34
29	MD	203	PEB	C2D-C3D	10.02	1.47	1.34
29	ID	203	PEB	C2D-C3D	10.01	1.47	1.34
29	BC	203	PEB	C2D-C3D	10.01	1.47	1.34
29	BE	203	PEB	C2D-C3D	10.01	1.47	1.34
29	G4	203	PEB	C2D-C3D	9.97	1.47	1.34
29	E4	203	PEB	C2D-C3D	9.95	1.47	1.34
29	GD	203	PEB	C2D-C3D	9.94	1.47	1.34
29	CD	203	PEB	C2D-C3D	9.93	1.47	1.34
29	C4	203	PEB	C2D-C3D	9.92	1.47	1.34
29	Y7	203	PEB	C2D-C3D	9.91	1.47	1.34
29	Y9	203	PEB	C2D-C3D	9.91	1.47	1.34
29	m7	203	PEB	C2D-C3D	9.91	1.47	1.34
29	m9	203	PEB	C2D-C3D	9.91	1.47	1.34
29	i7	203	PEB	C2D-C3D	9.89	1.47	1.34
29	i9	203	PEB	C2D-C3D	9.89	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V7	203	PEB	C2D-C3D	9.86	1.47	1.34
29	V9	203	PEB	C2D-C3D	9.86	1.47	1.34
29	A3	202	PEB	C2D-C3D	9.86	1.47	1.34
29	AO	202	PEB	C2D-C3D	9.86	1.47	1.34
29	c7	203	PEB	C2D-C3D	9.86	1.47	1.34
29	c9	203	PEB	C2D-C3D	9.86	1.47	1.34
29	e7	203	PEB	C2D-C3D	9.86	1.47	1.34
29	e9	203	PEB	C2D-C3D	9.86	1.47	1.34
29	k7	203	PEB	C2D-C3D	9.86	1.47	1.34
29	k9	203	PEB	C2D-C3D	9.86	1.47	1.34
29	R7	203	PEB	C2D-C3D	9.86	1.47	1.34
29	R9	203	PEB	C2D-C3D	9.86	1.47	1.34
29	I4	203	PEB	C2D-C3D	9.85	1.47	1.34
29	a7	203	PEB	C2D-C3D	9.84	1.47	1.34
29	a9	203	PEB	C2D-C3D	9.84	1.47	1.34
29	g7	203	PEB	C2D-C3D	9.84	1.47	1.34
29	g9	203	PEB	C2D-C3D	9.84	1.47	1.34
29	C3	202	PEB	C2D-C3D	9.83	1.47	1.34
29	CO	202	PEB	C2D-C3D	9.83	1.47	1.34
29	T7	203	PEB	C2D-C3D	9.81	1.47	1.34
29	T9	203	PEB	C2D-C3D	9.81	1.47	1.34
29	P7	203	PEB	C2D-C3D	9.80	1.47	1.34
29	P9	203	PEB	C2D-C3D	9.80	1.47	1.34
29	I3	202	PEB	C2D-C3D	9.80	1.47	1.34
29	IO	202	PEB	C2D-C3D	9.80	1.47	1.34
29	KC	202	PEB	C2D-C3D	9.80	1.47	1.34
29	KE	202	PEB	C2D-C3D	9.80	1.47	1.34
29	BC	201	PEB	C2D-C3D	9.80	1.47	1.34
29	BE	201	PEB	C2D-C3D	9.80	1.47	1.34
29	E3	202	PEB	C2D-C3D	9.79	1.47	1.34
29	EO	202	PEB	C2D-C3D	9.79	1.47	1.34
29	G3	202	PEB	C2D-C3D	9.79	1.47	1.34
29	GO	202	PEB	C2D-C3D	9.79	1.47	1.34
29	JC	201	PEB	C2D-C3D	9.77	1.47	1.34
29	JE	201	PEB	C2D-C3D	9.77	1.47	1.34
29	HC	201	PEB	C2D-C3D	9.76	1.47	1.34
29	HE	201	PEB	C2D-C3D	9.76	1.47	1.34
29	BB	301	PEB	C2D-C3D	9.76	1.47	1.34
29	BM	301	PEB	C2D-C3D	9.76	1.47	1.34
29	NB	202	PEB	C2D-C3D	9.76	1.47	1.34
29	NM	202	PEB	C2D-C3D	9.76	1.47	1.34
29	kB	203	PEB	C2D-C3D	9.76	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	kM	203	PEB	C2D-C3D	9.76	1.47	1.34
29	LB	203	PEB	C2D-C3D	9.76	1.47	1.34
29	LM	203	PEB	C2D-C3D	9.76	1.47	1.34
29	H3	202	PEB	C2D-C3D	9.75	1.47	1.34
29	J3	202	PEB	C2D-C3D	9.75	1.47	1.34
29	HO	202	PEB	C2D-C3D	9.75	1.47	1.34
29	JO	202	PEB	C2D-C3D	9.75	1.47	1.34
29	XB	202	PEB	C2D-C3D	9.75	1.47	1.34
29	XM	202	PEB	C2D-C3D	9.75	1.47	1.34
29	PB	202	PEB	C2D-C3D	9.75	1.47	1.34
29	PM	202	PEB	C2D-C3D	9.75	1.47	1.34
29	mB	203	PEB	C2D-C3D	9.75	1.47	1.34
29	mM	203	PEB	C2D-C3D	9.75	1.47	1.34
29	I3	203	PEB	C2D-C3D	9.74	1.47	1.34
29	DC	201	PEB	C2D-C3D	9.74	1.47	1.34
29	GC	201	PEB	C2D-C3D	9.74	1.47	1.34
29	DE	201	PEB	C2D-C3D	9.74	1.47	1.34
29	GE	201	PEB	C2D-C3D	9.74	1.47	1.34
29	IO	203	PEB	C2D-C3D	9.74	1.47	1.34
29	c1	203	PEB	C2D-C3D	9.74	1.47	1.34
29	cK	203	PEB	C2D-C3D	9.74	1.47	1.34
29	K3	202	PEB	C2D-C3D	9.74	1.47	1.34
29	KO	202	PEB	C2D-C3D	9.74	1.47	1.34
29	MA	401	PEB	C2D-C3D	9.74	1.47	1.34
29	FC	201	PEB	C2D-C3D	9.73	1.47	1.34
29	FE	201	PEB	C2D-C3D	9.73	1.47	1.34
29	TB	203	PEB	C2D-C3D	9.72	1.47	1.34
29	TM	203	PEB	C2D-C3D	9.72	1.47	1.34
29	JB	203	PEB	C2D-C3D	9.72	1.47	1.34
29	JM	203	PEB	C2D-C3D	9.72	1.47	1.34
29	ZB	203	PEB	C2D-C3D	9.72	1.47	1.34
29	CC	201	PEB	C2D-C3D	9.72	1.47	1.34
29	CE	201	PEB	C2D-C3D	9.72	1.47	1.34
29	ZM	203	PEB	C2D-C3D	9.72	1.47	1.34
29	gB	203	PEB	C2D-C3D	9.72	1.47	1.34
29	gM	203	PEB	C2D-C3D	9.72	1.47	1.34
29	MR	202	PEB	C2D-C3D	9.72	1.47	1.34
29	DB	203	PEB	C2D-C3D	9.72	1.47	1.34
29	DM	203	PEB	C2D-C3D	9.72	1.47	1.34
29	cB	203	PEB	C2D-C3D	9.71	1.47	1.34
29	cM	203	PEB	C2D-C3D	9.71	1.47	1.34
29	IC	201	PEB	C2D-C3D	9.71	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IE	201	PEB	C2D-C3D	9.71	1.47	1.34
29	Y1	202	PEB	C2D-C3D	9.71	1.47	1.34
29	YK	202	PEB	C2D-C3D	9.71	1.47	1.34
29	FB	203	PEB	C2D-C3D	9.71	1.47	1.34
29	FM	203	PEB	C2D-C3D	9.71	1.47	1.34
29	VB	203	PEB	C2D-C3D	9.70	1.47	1.34
29	VM	203	PEB	C2D-C3D	9.70	1.47	1.34
29	MN	401	PEB	C2D-C3D	9.70	1.47	1.34
29	LC	201	PEB	C2D-C3D	9.70	1.47	1.34
29	LE	201	PEB	C2D-C3D	9.70	1.47	1.34
29	SR	201	PEB	C2D-C3D	9.70	1.47	1.34
29	k1	203	PEB	C2D-C3D	9.70	1.47	1.34
29	kK	203	PEB	C2D-C3D	9.70	1.47	1.34
29	H3	203	PEB	C2D-C3D	9.70	1.47	1.34
29	HO	203	PEB	C2D-C3D	9.70	1.47	1.34
29	B3	202	PEB	C2D-C3D	9.69	1.47	1.34
29	BO	202	PEB	C2D-C3D	9.69	1.47	1.34
29	L3	202	PEB	C2D-C3D	9.69	1.47	1.34
29	RB	203	PEB	C2D-C3D	9.69	1.47	1.34
29	RM	203	PEB	C2D-C3D	9.69	1.47	1.34
29	LO	202	PEB	C2D-C3D	9.69	1.47	1.34
29	P1	203	PEB	C2D-C3D	9.69	1.47	1.34
29	PK	203	PEB	C2D-C3D	9.69	1.47	1.34
29	R1	203	PEB	C2D-C3D	9.69	1.47	1.34
29	LA	203	PEB	C2D-C3D	9.69	1.47	1.34
29	RK	203	PEB	C2D-C3D	9.69	1.47	1.34
29	LN	203	PEB	C2D-C3D	9.69	1.47	1.34
29	J3	203	PEB	C2D-C3D	9.69	1.47	1.34
29	JO	203	PEB	C2D-C3D	9.69	1.47	1.34
29	F3	202	PEB	C2D-C3D	9.69	1.47	1.34
29	FO	202	PEB	C2D-C3D	9.69	1.47	1.34
29	e1	203	PEB	C2D-C3D	9.68	1.47	1.34
29	eK	203	PEB	C2D-C3D	9.68	1.47	1.34
29	OR	202	PEB	C2D-C3D	9.68	1.47	1.34
29	HB	203	PEB	C2D-C3D	9.68	1.47	1.34
29	EC	201	PEB	C2D-C3D	9.68	1.47	1.34
29	EE	201	PEB	C2D-C3D	9.68	1.47	1.34
29	HM	203	PEB	C2D-C3D	9.68	1.47	1.34
29	M4	203	PEB	C2D-C3D	9.68	1.47	1.34
29	LA	202	PEB	C2D-C3D	9.67	1.47	1.34
29	LN	202	PEB	C2D-C3D	9.67	1.47	1.34
29	C5	203	PEB	C2D-C3D	9.67	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C8	203	PEB	C2D-C3D	9.67	1.47	1.34
29	JA	202	PEB	C2D-C3D	9.67	1.47	1.34
29	JN	202	PEB	C2D-C3D	9.67	1.47	1.34
29	eB	202	PEB	C2D-C3D	9.67	1.47	1.34
29	eM	202	PEB	C2D-C3D	9.67	1.47	1.34
29	iB	203	PEB	C2D-C3D	9.67	1.47	1.34
29	iM	203	PEB	C2D-C3D	9.67	1.47	1.34
29	HA	202	PEB	C2D-C3D	9.67	1.47	1.34
29	HN	202	PEB	C2D-C3D	9.67	1.47	1.34
29	S2	201	PEB	C2D-C3D	9.67	1.47	1.34
29	AC	201	PEB	C2D-C3D	9.66	1.47	1.34
29	AE	201	PEB	C2D-C3D	9.66	1.47	1.34
29	DA	202	PEB	C2D-C3D	9.66	1.47	1.34
29	DN	202	PEB	C2D-C3D	9.66	1.47	1.34
29	FA	203	PEB	C2D-C3D	9.66	1.47	1.34
29	FN	203	PEB	C2D-C3D	9.66	1.47	1.34
29	T1	202	PEB	C2D-C3D	9.66	1.47	1.34
29	TK	202	PEB	C2D-C3D	9.66	1.47	1.34
29	V1	203	PEB	C2D-C3D	9.65	1.46	1.34
29	VK	203	PEB	C2D-C3D	9.65	1.46	1.34
29	FA	202	PEB	C2D-C3D	9.65	1.46	1.34
29	FN	202	PEB	C2D-C3D	9.65	1.46	1.34
29	HA	203	PEB	C2D-C3D	9.64	1.46	1.34
29	HN	203	PEB	C2D-C3D	9.64	1.46	1.34
29	m1	202	PEB	C2D-C3D	9.64	1.46	1.34
29	AA	202	PEB	C2D-C3D	9.64	1.46	1.34
29	BA	202	PEB	C2D-C3D	9.64	1.46	1.34
29	mK	202	PEB	C2D-C3D	9.64	1.46	1.34
29	AN	202	PEB	C2D-C3D	9.64	1.46	1.34
29	BN	202	PEB	C2D-C3D	9.64	1.46	1.34
29	a1	203	PEB	C2D-C3D	9.64	1.46	1.34
29	aK	203	PEB	C2D-C3D	9.64	1.46	1.34
29	DA	203	PEB	C2D-C3D	9.63	1.46	1.34
29	DN	203	PEB	C2D-C3D	9.63	1.46	1.34
29	g1	203	PEB	C2D-C3D	9.63	1.46	1.34
29	gK	203	PEB	C2D-C3D	9.63	1.46	1.34
29	F3	203	PEB	C2D-C3D	9.63	1.46	1.34
29	FO	203	PEB	C2D-C3D	9.63	1.46	1.34
29	JA	203	PEB	C2D-C3D	9.63	1.46	1.34
29	JN	203	PEB	C2D-C3D	9.63	1.46	1.34
29	DO	202	PEB	C2D-C3D	9.62	1.46	1.34
29	GA	202	PEB	C2D-C3D	9.62	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GN	202	PEB	C2D-C3D	9.62	1.46	1.34
29	D3	203	PEB	C2D-C3D	9.62	1.46	1.34
29	DO	203	PEB	C2D-C3D	9.62	1.46	1.34
29	i1	203	PEB	C2D-C3D	9.62	1.46	1.34
29	iK	203	PEB	C2D-C3D	9.62	1.46	1.34
29	I5	203	PEB	C2D-C3D	9.61	1.46	1.34
29	I8	203	PEB	C2D-C3D	9.61	1.46	1.34
29	B3	203	PEB	C2D-C3D	9.61	1.46	1.34
29	TF	201	PEB	C2D-C3D	9.61	1.46	1.34
29	BO	203	PEB	C2D-C3D	9.61	1.46	1.34
29	K8	203	PEB	C2D-C3D	9.61	1.46	1.34
29	K5	203	PEB	C2D-C3D	9.60	1.46	1.34
29	A5	203	PEB	C2D-C3D	9.59	1.46	1.34
29	A8	203	PEB	C2D-C3D	9.59	1.46	1.34
29	M3	201	PEB	C2D-C3D	9.59	1.46	1.34
29	MO	201	PEB	C2D-C3D	9.59	1.46	1.34
29	EJ	202	PEB	C2D-C3D	9.58	1.46	1.34
29	EL	202	PEB	C2D-C3D	9.58	1.46	1.34
29	CA	202	PEB	C2D-C3D	9.58	1.46	1.34
29	CN	202	PEB	C2D-C3D	9.58	1.46	1.34
29	BA	203	PEB	C2D-C3D	9.57	1.46	1.34
29	BN	203	PEB	C2D-C3D	9.57	1.46	1.34
29	EC	202	PEB	C2D-C3D	9.56	1.46	1.34
29	EE	202	PEB	C2D-C3D	9.56	1.46	1.34
29	D3	202	PEB	C2D-C3D	9.56	1.46	1.34
29	IA	202	PEB	C2D-C3D	9.56	1.46	1.34
29	IN	202	PEB	C2D-C3D	9.56	1.46	1.34
29	cJ	202	PEB	C2D-C3D	9.55	1.46	1.34
29	cL	202	PEB	C2D-C3D	9.55	1.46	1.34
29	AC	202	PEB	C2D-C3D	9.55	1.46	1.34
29	AE	202	PEB	C2D-C3D	9.55	1.46	1.34
29	zJ	501	PEB	C2D-C3D	9.55	1.46	1.34
29	GC	202	PEB	C2D-C3D	9.54	1.46	1.34
29	GE	202	PEB	C2D-C3D	9.54	1.46	1.34
29	KJ	202	PEB	C2D-C3D	9.54	1.46	1.34
29	KL	202	PEB	C2D-C3D	9.54	1.46	1.34
29	h1	202	PEB	C2D-C3D	9.54	1.46	1.34
29	hK	202	PEB	C2D-C3D	9.54	1.46	1.34
29	WJ	203	PEB	C2D-C3D	9.53	1.46	1.34
29	WL	203	PEB	C2D-C3D	9.53	1.46	1.34
29	l1	202	PEB	C2D-C3D	9.53	1.46	1.34
29	lK	202	PEB	C2D-C3D	9.53	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	KA	202	PEB	C2D-C3D	9.53	1.46	1.34
29	SJ	202	PEB	C2D-C3D	9.53	1.46	1.34
29	SL	202	PEB	C2D-C3D	9.53	1.46	1.34
29	KN	202	PEB	C2D-C3D	9.53	1.46	1.34
29	b1	202	PEB	C2D-C3D	9.53	1.46	1.34
29	bK	202	PEB	C2D-C3D	9.53	1.46	1.34
29	EA	202	PEB	C2D-C3D	9.53	1.46	1.34
29	IJ	202	PEB	C2D-C3D	9.53	1.46	1.34
29	IL	202	PEB	C2D-C3D	9.53	1.46	1.34
29	EN	202	PEB	C2D-C3D	9.53	1.46	1.34
29	KC	203	PEB	C2D-C3D	9.53	1.46	1.34
29	KE	203	PEB	C2D-C3D	9.53	1.46	1.34
29	zL	501	PEB	C2D-C3D	9.53	1.46	1.34
29	sJ	202	PEB	C2D-C3D	9.53	1.46	1.34
29	sL	202	PEB	C2D-C3D	9.53	1.46	1.34
29	aJ	202	PEB	C2D-C3D	9.53	1.46	1.34
29	aL	202	PEB	C2D-C3D	9.53	1.46	1.34
29	Q1	202	PEB	C2D-C3D	9.52	1.46	1.34
29	CC	202	PEB	C2D-C3D	9.52	1.46	1.34
29	CE	202	PEB	C2D-C3D	9.52	1.46	1.34
29	YJ	202	PEB	C2D-C3D	9.52	1.46	1.34
29	QK	202	PEB	C2D-C3D	9.52	1.46	1.34
29	YL	202	PEB	C2D-C3D	9.52	1.46	1.34
29	OJ	202	PEB	C2D-C3D	9.52	1.46	1.34
29	OL	202	PEB	C2D-C3D	9.52	1.46	1.34
29	S1	202	PEB	C2D-C3D	9.51	1.46	1.34
29	eJ	202	PEB	C2D-C3D	9.51	1.46	1.34
29	SK	202	PEB	C2D-C3D	9.51	1.46	1.34
29	eL	202	PEB	C2D-C3D	9.51	1.46	1.34
29	N3	201	PEB	C2D-C3D	9.51	1.46	1.34
29	W1	202	PEB	C2D-C3D	9.50	1.46	1.34
29	WK	202	PEB	C2D-C3D	9.50	1.46	1.34
29	O1	202	PEB	C2D-C3D	9.50	1.46	1.34
29	OK	202	PEB	C2D-C3D	9.50	1.46	1.34
29	CJ	202	PEB	C2D-C3D	9.50	1.46	1.34
29	CL	202	PEB	C2D-C3D	9.50	1.46	1.34
29	MJ	202	PEB	C2D-C3D	9.50	1.46	1.34
29	ML	202	PEB	C2D-C3D	9.50	1.46	1.34
29	U1	203	PEB	C2D-C3D	9.49	1.46	1.34
29	d1	202	PEB	C2D-C3D	9.49	1.46	1.34
29	UK	203	PEB	C2D-C3D	9.49	1.46	1.34
29	dK	202	PEB	C2D-C3D	9.49	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	uJ	203	PEB	C2D-C3D	9.49	1.46	1.34
29	uL	203	PEB	C2D-C3D	9.49	1.46	1.34
29	qJ	202	PEB	C2D-C3D	9.49	1.46	1.34
29	qL	202	PEB	C2D-C3D	9.49	1.46	1.34
29	NO	201	PEB	C2D-C3D	9.48	1.46	1.34
29	fI	202	PEB	C2D-C3D	9.48	1.46	1.34
29	fK	202	PEB	C2D-C3D	9.48	1.46	1.34
29	AJ	202	PEB	C2D-C3D	9.48	1.46	1.34
29	AL	202	PEB	C2D-C3D	9.48	1.46	1.34
29	oJ	202	PEB	C2D-C3D	9.48	1.46	1.34
29	oL	202	PEB	C2D-C3D	9.48	1.46	1.34
29	ZI	203	PEB	C2D-C3D	9.47	1.46	1.34
29	ZK	203	PEB	C2D-C3D	9.47	1.46	1.34
29	IC	202	PEB	C2D-C3D	9.47	1.46	1.34
29	IE	202	PEB	C2D-C3D	9.47	1.46	1.34
29	BC	202	PEB	C2D-C3D	9.47	1.46	1.34
29	BE	202	PEB	C2D-C3D	9.47	1.46	1.34
29	kJ	202	PEB	C2D-C3D	9.47	1.46	1.34
29	kL	202	PEB	C2D-C3D	9.47	1.46	1.34
29	AC	203	PEB	C2D-C3D	9.47	1.46	1.34
29	AE	203	PEB	C2D-C3D	9.47	1.46	1.34
29	gJ	202	PEB	C2D-C3D	9.47	1.46	1.34
29	gL	202	PEB	C2D-C3D	9.47	1.46	1.34
29	UJ	202	PEB	C2D-C3D	9.46	1.46	1.34
29	UL	202	PEB	C2D-C3D	9.46	1.46	1.34
29	iI	202	PEB	C2D-C3D	9.46	1.46	1.34
29	LC	202	PEB	C2D-C3D	9.46	1.46	1.34
29	LE	202	PEB	C2D-C3D	9.46	1.46	1.34
29	iK	202	PEB	C2D-C3D	9.46	1.46	1.34
29	QJ	202	PEB	C2D-C3D	9.46	1.46	1.34
29	QL	202	PEB	C2D-C3D	9.46	1.46	1.34
29	GJ	202	PEB	C2D-C3D	9.46	1.46	1.34
29	GL	202	PEB	C2D-C3D	9.46	1.46	1.34
29	FC	202	PEB	C2D-C3D	9.46	1.46	1.34
29	FE	202	PEB	C2D-C3D	9.46	1.46	1.34
29	cI	202	PEB	C2D-C3D	9.45	1.46	1.34
29	cK	202	PEB	C2D-C3D	9.45	1.46	1.34
29	jI	202	PEB	C2D-C3D	9.45	1.46	1.34
29	jK	202	PEB	C2D-C3D	9.45	1.46	1.34
29	iJ	202	PEB	C2D-C3D	9.45	1.46	1.34
29	iL	202	PEB	C2D-C3D	9.45	1.46	1.34
29	mJ	202	PEB	C2D-C3D	9.45	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	mL	202	PEB	C2D-C3D	9.45	1.46	1.34
29	j1	203	PEB	C2D-C3D	9.44	1.46	1.34
29	jK	203	PEB	C2D-C3D	9.44	1.46	1.34
29	Z1	201	PEB	C2D-C3D	9.44	1.46	1.34
29	e1	202	PEB	C2D-C3D	9.44	1.46	1.34
29	ZK	201	PEB	C2D-C3D	9.44	1.46	1.34
29	eK	202	PEB	C2D-C3D	9.44	1.46	1.34
29	NB	201	PEB	C2D-C3D	9.44	1.46	1.34
29	NM	201	PEB	C2D-C3D	9.44	1.46	1.34
29	KC	201	PEB	C2D-C3D	9.43	1.46	1.34
29	KE	201	PEB	C2D-C3D	9.43	1.46	1.34
29	AF	305	PEB	C2D-C3D	9.43	1.46	1.34
29	AI	305	PEB	C2D-C3D	9.43	1.46	1.34
29	HC	202	PEB	C2D-C3D	9.42	1.46	1.34
29	HE	202	PEB	C2D-C3D	9.42	1.46	1.34
29	a1	202	PEB	C2D-C3D	9.42	1.46	1.34
29	aK	202	PEB	C2D-C3D	9.42	1.46	1.34
29	iB	201	PEB	C2D-C3D	9.42	1.46	1.34
29	iM	201	PEB	C2D-C3D	9.42	1.46	1.34
29	K5	201	PEB	C2D-C3D	9.42	1.46	1.34
29	K8	201	PEB	C2D-C3D	9.42	1.46	1.34
29	PB	201	PEB	C2D-C3D	9.42	1.46	1.34
29	mB	201	PEB	C2D-C3D	9.42	1.46	1.34
29	PM	201	PEB	C2D-C3D	9.42	1.46	1.34
29	mM	201	PEB	C2D-C3D	9.42	1.46	1.34
29	I5	201	PEB	C2D-C3D	9.42	1.46	1.34
29	I8	201	PEB	C2D-C3D	9.42	1.46	1.34
29	DB	201	PEB	C2D-C3D	9.42	1.46	1.34
29	DM	201	PEB	C2D-C3D	9.42	1.46	1.34
29	C5	201	PEB	C2D-C3D	9.41	1.46	1.34
29	k1	202	PEB	C2D-C3D	9.41	1.46	1.34
29	kK	202	PEB	C2D-C3D	9.41	1.46	1.34
29	U1	201	PEB	C2D-C3D	9.40	1.46	1.34
29	UK	201	PEB	C2D-C3D	9.40	1.46	1.34
29	V1	202	PEB	C2D-C3D	9.40	1.46	1.34
29	VK	202	PEB	C2D-C3D	9.40	1.46	1.34
29	FB	201	PEB	C2D-C3D	9.40	1.46	1.34
29	FM	201	PEB	C2D-C3D	9.40	1.46	1.34
29	RB	201	PEB	C2D-C3D	9.40	1.46	1.34
29	RM	201	PEB	C2D-C3D	9.40	1.46	1.34
29	R1	202	PEB	C2D-C3D	9.40	1.46	1.34
29	RK	202	PEB	C2D-C3D	9.40	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	cB	201	PEB	C2D-C3D	9.39	1.46	1.34
29	cM	201	PEB	C2D-C3D	9.39	1.46	1.34
29	eB	201	PEB	C2D-C3D	9.39	1.46	1.34
29	eM	201	PEB	C2D-C3D	9.39	1.46	1.34
29	LB	201	PEB	C2D-C3D	9.38	1.46	1.34
29	LM	201	PEB	C2D-C3D	9.38	1.46	1.34
29	g1	202	PEB	C2D-C3D	9.38	1.46	1.34
29	A5	201	PEB	C2D-C3D	9.38	1.46	1.34
29	A8	201	PEB	C2D-C3D	9.38	1.46	1.34
29	C8	201	PEB	C2D-C3D	9.38	1.46	1.34
29	gK	202	PEB	C2D-C3D	9.38	1.46	1.34
29	JB	201	PEB	C2D-C3D	9.38	1.46	1.34
29	JM	201	PEB	C2D-C3D	9.38	1.46	1.34
29	B3	201	PEB	C2D-C3D	9.36	1.46	1.34
29	BO	201	PEB	C2D-C3D	9.36	1.46	1.34
29	F3	201	PEB	C2D-C3D	9.36	1.46	1.34
29	FO	201	PEB	C2D-C3D	9.36	1.46	1.34
29	P1	202	PEB	C2D-C3D	9.36	1.46	1.34
29	H3	201	PEB	C2D-C3D	9.36	1.46	1.34
29	PK	202	PEB	C2D-C3D	9.36	1.46	1.34
29	HO	201	PEB	C2D-C3D	9.36	1.46	1.34
29	kB	201	PEB	C2D-C3D	9.36	1.46	1.34
29	kM	201	PEB	C2D-C3D	9.36	1.46	1.34
29	VB	201	PEB	C2D-C3D	9.36	1.46	1.34
29	VM	201	PEB	C2D-C3D	9.36	1.46	1.34
29	ZJ	203	PEB	C2D-C3D	9.35	1.46	1.34
29	ZL	203	PEB	C2D-C3D	9.35	1.46	1.34
29	XB	201	PEB	C2D-C3D	9.35	1.46	1.34
29	XM	201	PEB	C2D-C3D	9.35	1.46	1.34
29	TB	201	PEB	C2D-C3D	9.35	1.46	1.34
29	TM	201	PEB	C2D-C3D	9.35	1.46	1.34
29	ZB	201	PEB	C2D-C3D	9.35	1.46	1.34
29	ZM	201	PEB	C2D-C3D	9.35	1.46	1.34
29	gB	201	PEB	C2D-C3D	9.34	1.46	1.34
29	gM	201	PEB	C2D-C3D	9.34	1.46	1.34
29	HB	201	PEB	C2D-C3D	9.34	1.46	1.34
29	HM	201	PEB	C2D-C3D	9.34	1.46	1.34
29	L3	201	PEB	C2D-C3D	9.33	1.46	1.34
29	LO	201	PEB	C2D-C3D	9.33	1.46	1.34
29	NO	202	PEB	C2D-C3D	9.32	1.46	1.34
29	TR	203	PEB	C2D-C3D	9.32	1.46	1.34
29	PJ	203	PEB	C2D-C3D	9.32	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	PL	203	PEB	C2D-C3D	9.32	1.46	1.34
29	VR	201	PEB	C2D-C3D	9.32	1.46	1.34
29	lJ	203	PEB	C2D-C3D	9.32	1.46	1.34
29	lL	203	PEB	C2D-C3D	9.32	1.46	1.34
29	FJ	203	PEB	C2D-C3D	9.31	1.46	1.34
29	FL	203	PEB	C2D-C3D	9.31	1.46	1.34
29	MQ	407	PEB	C2D-C3D	9.31	1.46	1.34
29	e2	402	PEB	C2D-C3D	9.31	1.46	1.34
29	XR	201	PEB	C2D-C3D	9.31	1.46	1.34
29	fJ	203	PEB	C2D-C3D	9.31	1.46	1.34
29	fL	203	PEB	C2D-C3D	9.31	1.46	1.34
29	pJ	203	PEB	C2D-C3D	9.31	1.46	1.34
29	pL	203	PEB	C2D-C3D	9.31	1.46	1.34
29	G8	202	PEB	C2D-C3D	9.31	1.46	1.34
29	G5	202	PEB	C2D-C3D	9.30	1.46	1.34
29	jJ	203	PEB	C2D-C3D	9.30	1.46	1.34
29	jL	203	PEB	C2D-C3D	9.30	1.46	1.34
29	dJ	203	PEB	C2D-C3D	9.30	1.46	1.34
29	vJ	202	PEB	C2D-C3D	9.30	1.46	1.34
29	dL	203	PEB	C2D-C3D	9.30	1.46	1.34
29	vL	202	PEB	C2D-C3D	9.30	1.46	1.34
29	rJ	203	PEB	C2D-C3D	9.30	1.46	1.34
29	rL	203	PEB	C2D-C3D	9.30	1.46	1.34
29	D3	201	PEB	C2D-C3D	9.30	1.46	1.34
29	FA	201	PEB	C2D-C3D	9.30	1.46	1.34
29	VJ	202	PEB	C2D-C3D	9.30	1.46	1.34
29	VL	202	PEB	C2D-C3D	9.30	1.46	1.34
29	FN	201	PEB	C2D-C3D	9.30	1.46	1.34
29	DO	201	PEB	C2D-C3D	9.30	1.46	1.34
29	RR	203	PEB	C2D-C3D	9.29	1.46	1.34
29	N2	201	PEB	C2D-C3D	9.29	1.46	1.34
29	LJ	202	PEB	C2D-C3D	9.29	1.46	1.34
29	LL	202	PEB	C2D-C3D	9.29	1.46	1.34
29	cF	202	PEB	C2D-C3D	9.29	1.46	1.34
29	cI	202	PEB	C2D-C3D	9.29	1.46	1.34
29	HA	201	PEB	C2D-C3D	9.29	1.46	1.34
29	TJ	203	PEB	C2D-C3D	9.29	1.46	1.34
29	TL	203	PEB	C2D-C3D	9.29	1.46	1.34
29	HN	201	PEB	C2D-C3D	9.29	1.46	1.34
29	bJ	203	PEB	C2D-C3D	9.29	1.46	1.34
29	bL	203	PEB	C2D-C3D	9.29	1.46	1.34
29	A7	301	PEB	C2D-C3D	9.28	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A9	301	PEB	C2D-C3D	9.28	1.46	1.34
29	K8	202	PEB	C2D-C3D	9.28	1.46	1.34
29	M3	202	PEB	C2D-C3D	9.28	1.46	1.34
29	MO	202	PEB	C2D-C3D	9.28	1.46	1.34
29	HJ	202	PEB	C2D-C3D	9.28	1.46	1.34
29	RJ	203	PEB	C2D-C3D	9.28	1.46	1.34
29	HL	202	PEB	C2D-C3D	9.28	1.46	1.34
29	RL	203	PEB	C2D-C3D	9.28	1.46	1.34
29	J3	201	PEB	C2D-C3D	9.28	1.46	1.34
29	DA	201	PEB	C2D-C3D	9.28	1.46	1.34
29	AM	301	PEB	C2D-C3D	9.28	1.46	1.34
29	DN	201	PEB	C2D-C3D	9.28	1.46	1.34
29	JO	201	PEB	C2D-C3D	9.28	1.46	1.34
29	DJ	202	PEB	C2D-C3D	9.28	1.46	1.34
29	DL	202	PEB	C2D-C3D	9.28	1.46	1.34
29	NJ	203	PEB	C2D-C3D	9.28	1.46	1.34
29	NL	203	PEB	C2D-C3D	9.28	1.46	1.34
29	MG	405	PEB	C2D-C3D	9.27	1.46	1.34
29	XJ	203	PEB	C2D-C3D	9.27	1.46	1.34
29	XL	203	PEB	C2D-C3D	9.27	1.46	1.34
29	BJ	203	PEB	C2D-C3D	9.27	1.46	1.34
29	BL	203	PEB	C2D-C3D	9.27	1.46	1.34
29	JA	201	PEB	C2D-C3D	9.27	1.46	1.34
29	RF	202	PEB	C2D-C3D	9.27	1.46	1.34
29	RI	202	PEB	C2D-C3D	9.27	1.46	1.34
29	JN	201	PEB	C2D-C3D	9.27	1.46	1.34
29	LA	201	PEB	C2D-C3D	9.27	1.46	1.34
29	AB	301	PEB	C2D-C3D	9.27	1.46	1.34
29	gF	203	PEB	C2D-C3D	9.27	1.46	1.34
29	gI	203	PEB	C2D-C3D	9.27	1.46	1.34
29	LN	201	PEB	C2D-C3D	9.27	1.46	1.34
29	N3	202	PEB	C2D-C3D	9.27	1.46	1.34
29	B4	202	PEB	C2D-C3D	9.27	1.46	1.34
29	xJ	301	PEB	C2D-C3D	9.27	1.46	1.34
29	N2	203	PEB	C2D-C3D	9.26	1.46	1.34
29	V2	201	PEB	C2D-C3D	9.26	1.46	1.34
29	bF	202	PEB	C2D-C3D	9.26	1.46	1.34
29	bI	202	PEB	C2D-C3D	9.26	1.46	1.34
29	eF	203	PEB	C2D-C3D	9.26	1.46	1.34
29	eI	203	PEB	C2D-C3D	9.26	1.46	1.34
29	nJ	203	PEB	C2D-C3D	9.26	1.46	1.34
29	nL	203	PEB	C2D-C3D	9.26	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	hJ	203	PEB	C2D-C3D	9.26	1.46	1.34
29	hL	203	PEB	C2D-C3D	9.26	1.46	1.34
29	JD	202	PEB	C2D-C3D	9.26	1.46	1.34
29	NR	203	PEB	C2D-C3D	9.26	1.46	1.34
29	T2	203	PEB	C2D-C3D	9.26	1.46	1.34
29	I3	201	PEB	C2D-C3D	9.26	1.46	1.34
29	IO	201	PEB	C2D-C3D	9.26	1.46	1.34
29	C5	202	PEB	C2D-C3D	9.26	1.46	1.34
29	aF	203	PEB	C2D-C3D	9.26	1.46	1.34
29	aI	203	PEB	C2D-C3D	9.26	1.46	1.34
29	BD	202	PEB	C2D-C3D	9.26	1.46	1.34
29	F5	202	PEB	C2D-C3D	9.25	1.46	1.34
29	F8	202	PEB	C2D-C3D	9.25	1.46	1.34
29	AG	201	PEB	C2D-C3D	9.25	1.46	1.34
29	AQ	201	PEB	C2D-C3D	9.25	1.46	1.34
29	BA	201	PEB	C2D-C3D	9.25	1.46	1.34
29	BN	201	PEB	C2D-C3D	9.25	1.46	1.34
29	tJ	202	PEB	C2D-C3D	9.25	1.46	1.34
29	tL	202	PEB	C2D-C3D	9.25	1.46	1.34
29	A5	202	PEB	C2D-C3D	9.25	1.46	1.34
29	A8	202	PEB	C2D-C3D	9.25	1.46	1.34
29	TF	202	PEB	C2D-C3D	9.25	1.46	1.34
29	TI	202	PEB	C2D-C3D	9.25	1.46	1.34
29	PF	203	PEB	C2D-C3D	9.24	1.46	1.34
29	PI	203	PEB	C2D-C3D	9.24	1.46	1.34
29	GG	201	PEB	C2D-C3D	9.24	1.46	1.34
29	xL	301	PEB	C2D-C3D	9.24	1.46	1.34
29	GQ	201	PEB	C2D-C3D	9.24	1.46	1.34
29	LJ	201	PEB	C2D-C3D	9.24	1.46	1.34
29	LL	201	PEB	C2D-C3D	9.24	1.46	1.34
29	L4	202	PEB	C2D-C3D	9.24	1.46	1.34
29	YB	201	PEB	C2D-C3D	9.24	1.46	1.34
29	YM	201	PEB	C2D-C3D	9.24	1.46	1.34
29	ZF	202	PEB	C2D-C3D	9.24	1.46	1.34
29	ZI	202	PEB	C2D-C3D	9.24	1.46	1.34
29	R2	203	PEB	C2D-C3D	9.24	1.46	1.34
29	F4	202	PEB	C2D-C3D	9.24	1.46	1.34
29	QF	202	PEB	C2D-C3D	9.24	1.46	1.34
29	QI	202	PEB	C2D-C3D	9.24	1.46	1.34
29	K5	202	PEB	C2D-C3D	9.24	1.46	1.34
29	IG	201	PEB	C2D-C3D	9.23	1.46	1.34
29	IQ	201	PEB	C2D-C3D	9.23	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JJ	203	PEB	C2D-C3D	9.23	1.46	1.34
29	JL	203	PEB	C2D-C3D	9.23	1.46	1.34
29	VB	202	PEB	C2D-C3D	9.23	1.46	1.34
29	VM	202	PEB	C2D-C3D	9.23	1.46	1.34
29	mB	202	PEB	C2D-C3D	9.23	1.46	1.34
29	mM	202	PEB	C2D-C3D	9.23	1.46	1.34
29	HG	202	PEB	C2D-C3D	9.23	1.46	1.34
29	HQ	202	PEB	C2D-C3D	9.23	1.46	1.34
29	NR	201	PEB	C2D-C3D	9.23	1.46	1.34
29	H5	202	PEB	C2D-C3D	9.23	1.46	1.34
29	YF	203	PEB	C2D-C3D	9.23	1.46	1.34
29	YI	203	PEB	C2D-C3D	9.23	1.46	1.34
29	LD	202	PEB	C2D-C3D	9.22	1.46	1.34
29	EG	201	PEB	C2D-C3D	9.22	1.46	1.34
29	EQ	201	PEB	C2D-C3D	9.22	1.46	1.34
29	O7	202	PEB	C2D-C3D	9.22	1.46	1.34
29	O9	202	PEB	C2D-C3D	9.22	1.46	1.34
29	VR	203	PEB	C2D-C3D	9.22	1.46	1.34
29	rJ	201	PEB	C2D-C3D	9.22	1.46	1.34
29	rL	201	PEB	C2D-C3D	9.22	1.46	1.34
29	L8	202	PEB	C2D-C3D	9.22	1.46	1.34
29	C8	202	PEB	C2D-C3D	9.22	1.46	1.34
29	TB	202	PEB	C2D-C3D	9.22	1.46	1.34
29	TM	202	PEB	C2D-C3D	9.22	1.46	1.34
29	Z7	201	PEB	C2D-C3D	9.22	1.46	1.34
29	Z9	201	PEB	C2D-C3D	9.22	1.46	1.34
29	j7	202	PEB	C2D-C3D	9.22	1.46	1.34
29	j9	202	PEB	C2D-C3D	9.22	1.46	1.34
29	mF	203	PEB	C2D-C3D	9.22	1.46	1.34
29	mI	203	PEB	C2D-C3D	9.22	1.46	1.34
29	B5	202	PEB	C2D-C3D	9.22	1.46	1.34
29	FD	202	PEB	C2D-C3D	9.22	1.46	1.34
29	JG	202	PEB	C2D-C3D	9.21	1.46	1.34
29	JQ	202	PEB	C2D-C3D	9.21	1.46	1.34
29	f7	202	PEB	C2D-C3D	9.21	1.46	1.34
29	f9	202	PEB	C2D-C3D	9.21	1.46	1.34
29	X2	202	PEB	C2D-C3D	9.21	1.46	1.34
29	wJ	301	PEB	C2D-C3D	9.21	1.46	1.34
29	XR	203	PEB	C2D-C3D	9.21	1.46	1.34
29	RJ	201	PEB	C2D-C3D	9.21	1.46	1.34
29	RL	201	PEB	C2D-C3D	9.21	1.46	1.34
29	RB	202	PEB	C2D-C3D	9.21	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gB	202	PEB	C2D-C3D	9.21	1.46	1.34
29	UF	203	PEB	C2D-C3D	9.21	1.46	1.34
29	UI	203	PEB	C2D-C3D	9.21	1.46	1.34
29	fJ	201	PEB	C2D-C3D	9.21	1.46	1.34
29	fL	201	PEB	C2D-C3D	9.21	1.46	1.34
29	RM	202	PEB	C2D-C3D	9.21	1.46	1.34
29	gM	202	PEB	C2D-C3D	9.21	1.46	1.34
29	fF	202	PEB	C2D-C3D	9.21	1.46	1.34
29	fI	202	PEB	C2D-C3D	9.21	1.46	1.34
29	DJ	201	PEB	C2D-C3D	9.21	1.46	1.34
29	DL	201	PEB	C2D-C3D	9.21	1.46	1.34
29	aB	203	PEB	C2D-C3D	9.20	1.46	1.34
29	aM	203	PEB	C2D-C3D	9.20	1.46	1.34
29	DG	202	PEB	C2D-C3D	9.20	1.46	1.34
29	DQ	202	PEB	C2D-C3D	9.20	1.46	1.34
29	PJ	201	PEB	C2D-C3D	9.20	1.46	1.34
29	IJ	201	PEB	C2D-C3D	9.20	1.46	1.34
29	PL	201	PEB	C2D-C3D	9.20	1.46	1.34
29	IL	201	PEB	C2D-C3D	9.20	1.46	1.34
29	OF	202	PEB	C2D-C3D	9.20	1.46	1.34
29	FG	202	PEB	C2D-C3D	9.20	1.46	1.34
29	OI	202	PEB	C2D-C3D	9.20	1.46	1.34
29	FQ	202	PEB	C2D-C3D	9.20	1.46	1.34
29	d7	202	PEB	C2D-C3D	9.20	1.46	1.34
29	d9	202	PEB	C2D-C3D	9.20	1.46	1.34
29	A3	201	PEB	C2D-C3D	9.20	1.46	1.34
29	HB	202	PEB	C2D-C3D	9.20	1.46	1.34
29	PF	201	PEB	C2D-C3D	9.20	1.46	1.34
29	eF	201	PEB	C2D-C3D	9.20	1.46	1.34
29	PI	201	PEB	C2D-C3D	9.20	1.46	1.34
29	eI	201	PEB	C2D-C3D	9.20	1.46	1.34
29	HM	202	PEB	C2D-C3D	9.20	1.46	1.34
29	AO	201	PEB	C2D-C3D	9.20	1.46	1.34
29	VF	203	PEB	C2D-C3D	9.20	1.46	1.34
29	VI	203	PEB	C2D-C3D	9.20	1.46	1.34
29	BG	202	PEB	C2D-C3D	9.20	1.46	1.34
29	wL	301	PEB	C2D-C3D	9.20	1.46	1.34
29	BQ	202	PEB	C2D-C3D	9.20	1.46	1.34
29	QR	202	PEB	C2D-C3D	9.20	1.46	1.34
29	D4	202	PEB	C2D-C3D	9.20	1.46	1.34
29	L5	202	PEB	C2D-C3D	9.20	1.46	1.34
29	SF	202	PEB	C2D-C3D	9.19	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SI	202	PEB	C2D-C3D	9.19	1.46	1.34
29	TR	201	PEB	C2D-C3D	9.19	1.46	1.34
29	tJ	201	PEB	C2D-C3D	9.19	1.46	1.34
29	tL	201	PEB	C2D-C3D	9.19	1.46	1.34
29	G3	201	PEB	C2D-C3D	9.19	1.46	1.34
29	kB	202	PEB	C2D-C3D	9.19	1.46	1.34
29	kM	202	PEB	C2D-C3D	9.19	1.46	1.34
29	GO	201	PEB	C2D-C3D	9.19	1.46	1.34
29	H4	202	PEB	C2D-C3D	9.19	1.46	1.34
29	W7	202	PEB	C2D-C3D	9.19	1.46	1.34
29	W9	202	PEB	C2D-C3D	9.19	1.46	1.34
29	Z7	202	PEB	C2D-C3D	9.19	1.46	1.34
29	Z9	202	PEB	C2D-C3D	9.19	1.46	1.34
29	HD	202	PEB	C2D-C3D	9.19	1.46	1.34
29	pJ	201	PEB	C2D-C3D	9.19	1.46	1.34
29	pL	201	PEB	C2D-C3D	9.19	1.46	1.34
29	QB	202	PEB	C2D-C3D	9.19	1.46	1.34
29	QM	202	PEB	C2D-C3D	9.19	1.46	1.34
29	V2	203	PEB	C2D-C3D	9.19	1.46	1.34
29	S7	202	PEB	C2D-C3D	9.19	1.46	1.34
29	S9	202	PEB	C2D-C3D	9.19	1.46	1.34
29	FB	202	PEB	C2D-C3D	9.19	1.46	1.34
29	FM	202	PEB	C2D-C3D	9.19	1.46	1.34
29	J4	202	PEB	C2D-C3D	9.18	1.46	1.34
29	hF	202	PEB	C2D-C3D	9.18	1.46	1.34
29	hI	202	PEB	C2D-C3D	9.18	1.46	1.34
29	I8	202	PEB	C2D-C3D	9.18	1.46	1.34
29	DB	202	PEB	C2D-C3D	9.18	1.46	1.34
29	FJ	201	PEB	C2D-C3D	9.18	1.46	1.34
29	FL	201	PEB	C2D-C3D	9.18	1.46	1.34
29	DM	202	PEB	C2D-C3D	9.18	1.46	1.34
29	CG	201	PEB	C2D-C3D	9.18	1.46	1.34
29	CQ	201	PEB	C2D-C3D	9.18	1.46	1.34
29	F5	203	PEB	C2D-C3D	9.18	1.46	1.34
29	L5	201	PEB	C2D-C3D	9.18	1.46	1.34
29	b7	202	PEB	C2D-C3D	9.18	1.46	1.34
29	F8	203	PEB	C2D-C3D	9.18	1.46	1.34
29	b9	202	PEB	C2D-C3D	9.18	1.46	1.34
29	M2	202	PEB	C2D-C3D	9.18	1.46	1.34
29	kF	203	PEB	C2D-C3D	9.18	1.46	1.34
29	kI	203	PEB	C2D-C3D	9.18	1.46	1.34
29	T2	201	PEB	C2D-C3D	9.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	cB	202	PEB	C2D-C3D	9.18	1.46	1.34
29	cM	202	PEB	C2D-C3D	9.18	1.46	1.34
29	b7	201	PEB	C2D-C3D	9.18	1.46	1.34
29	j7	201	PEB	C2D-C3D	9.18	1.46	1.34
29	b9	201	PEB	C2D-C3D	9.18	1.46	1.34
29	j9	201	PEB	C2D-C3D	9.18	1.46	1.34
29	NJ	201	PEB	C2D-C3D	9.18	1.46	1.34
29	NL	201	PEB	C2D-C3D	9.18	1.46	1.34
29	JJ	201	PEB	C2D-C3D	9.18	1.46	1.34
29	JL	201	PEB	C2D-C3D	9.18	1.46	1.34
29	WF	202	PEB	C2D-C3D	9.18	1.46	1.34
29	iF	203	PEB	C2D-C3D	9.18	1.46	1.34
29	WI	202	PEB	C2D-C3D	9.18	1.46	1.34
29	iI	203	PEB	C2D-C3D	9.18	1.46	1.34
29	K3	201	PEB	C2D-C3D	9.18	1.46	1.34
29	KO	201	PEB	C2D-C3D	9.18	1.46	1.34
29	C3	201	PEB	C2D-C3D	9.17	1.46	1.34
29	CO	201	PEB	C2D-C3D	9.17	1.46	1.34
29	I5	202	PEB	C2D-C3D	9.17	1.46	1.34
29	bJ	201	PEB	C2D-C3D	9.17	1.46	1.34
29	bL	201	PEB	C2D-C3D	9.17	1.46	1.34
29	O2	202	PEB	C2D-C3D	9.17	1.46	1.34
29	R2	201	PEB	C2D-C3D	9.17	1.46	1.34
29	jF	202	PEB	C2D-C3D	9.17	1.46	1.34
29	jI	202	PEB	C2D-C3D	9.17	1.46	1.34
29	dJ	201	PEB	C2D-C3D	9.17	1.46	1.34
29	dL	201	PEB	C2D-C3D	9.17	1.46	1.34
29	iB	202	PEB	C2D-C3D	9.17	1.46	1.34
29	iM	202	PEB	C2D-C3D	9.17	1.46	1.34
29	l7	201	PEB	C2D-C3D	9.17	1.46	1.34
29	l9	201	PEB	C2D-C3D	9.17	1.46	1.34
29	YF	201	PEB	C2D-C3D	9.17	1.46	1.34
29	dF	203	PEB	C2D-C3D	9.17	1.46	1.34
29	LG	202	PEB	C2D-C3D	9.17	1.46	1.34
29	YI	201	PEB	C2D-C3D	9.17	1.46	1.34
29	dI	203	PEB	C2D-C3D	9.17	1.46	1.34
29	LQ	201	PEB	C2D-C3D	9.17	1.46	1.34
29	h7	202	PEB	C2D-C3D	9.17	1.46	1.34
29	H8	202	PEB	C2D-C3D	9.17	1.46	1.34
29	h9	202	PEB	C2D-C3D	9.17	1.46	1.34
29	ZB	202	PEB	C2D-C3D	9.17	1.46	1.34
29	ZM	202	PEB	C2D-C3D	9.17	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q7	202	PEB	C2D-C3D	9.16	1.46	1.34
29	Q9	202	PEB	C2D-C3D	9.16	1.46	1.34
29	P2	202	PEB	C2D-C3D	9.16	1.46	1.34
29	JB	202	PEB	C2D-C3D	9.16	1.46	1.34
29	vJ	201	PEB	C2D-C3D	9.16	1.46	1.34
29	vL	201	PEB	C2D-C3D	9.16	1.46	1.34
29	JM	202	PEB	C2D-C3D	9.16	1.46	1.34
29	VF	201	PEB	C2D-C3D	9.16	1.46	1.34
29	VI	201	PEB	C2D-C3D	9.16	1.46	1.34
29	U7	201	PEB	C2D-C3D	9.16	1.46	1.34
29	U9	201	PEB	C2D-C3D	9.16	1.46	1.34
29	l7	202	PEB	C2D-C3D	9.16	1.46	1.34
29	l9	202	PEB	C2D-C3D	9.16	1.46	1.34
29	G5	203	PEB	C2D-C3D	9.16	1.46	1.34
29	YF	202	PEB	C2D-C3D	9.16	1.46	1.34
29	KG	201	PEB	C2D-C3D	9.16	1.46	1.34
29	YI	202	PEB	C2D-C3D	9.16	1.46	1.34
29	VJ	201	PEB	C2D-C3D	9.16	1.46	1.34
29	VL	201	PEB	C2D-C3D	9.16	1.46	1.34
29	KQ	201	PEB	C2D-C3D	9.16	1.46	1.34
29	lF	202	PEB	C2D-C3D	9.16	1.46	1.34
29	lI	202	PEB	C2D-C3D	9.16	1.46	1.34
29	TJ	201	PEB	C2D-C3D	9.15	1.46	1.34
29	TL	201	PEB	C2D-C3D	9.15	1.46	1.34
29	gF	201	PEB	C2D-C3D	9.15	1.46	1.34
29	gI	201	PEB	C2D-C3D	9.15	1.46	1.34
29	PR	202	PEB	C2D-C3D	9.15	1.46	1.34
29	d7	201	PEB	C2D-C3D	9.15	1.46	1.34
29	f7	201	PEB	C2D-C3D	9.15	1.46	1.34
29	B8	202	PEB	C2D-C3D	9.15	1.46	1.34
29	d9	201	PEB	C2D-C3D	9.15	1.46	1.34
29	f9	201	PEB	C2D-C3D	9.15	1.46	1.34
29	jJ	201	PEB	C2D-C3D	9.15	1.46	1.34
29	jL	201	PEB	C2D-C3D	9.15	1.46	1.34
29	WR	202	PEB	C2D-C3D	9.15	1.46	1.34
29	RR	201	PEB	C2D-C3D	9.15	1.46	1.34
29	kF	201	PEB	C2D-C3D	9.15	1.46	1.34
29	kI	201	PEB	C2D-C3D	9.15	1.46	1.34
29	E3	201	PEB	C2D-C3D	9.15	1.46	1.34
29	EO	201	PEB	C2D-C3D	9.15	1.46	1.34
29	KB	203	PEB	C2D-C3D	9.15	1.46	1.34
29	KM	203	PEB	C2D-C3D	9.15	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DD	202	PEB	C2D-C3D	9.15	1.46	1.34
29	O7	201	PEB	C2D-C3D	9.15	1.46	1.34
29	O9	201	PEB	C2D-C3D	9.15	1.46	1.34
29	Q7	201	PEB	C2D-C3D	9.15	1.46	1.34
29	Q9	201	PEB	C2D-C3D	9.15	1.46	1.34
29	cF	201	PEB	C2D-C3D	9.14	1.46	1.34
29	mF	201	PEB	C2D-C3D	9.14	1.46	1.34
29	cI	201	PEB	C2D-C3D	9.14	1.46	1.34
29	mI	201	PEB	C2D-C3D	9.14	1.46	1.34
29	A9	304	PEB	C2D-C3D	9.14	1.46	1.34
29	aF	201	PEB	C2D-C3D	9.14	1.46	1.34
29	aI	201	PEB	C2D-C3D	9.14	1.46	1.34
29	LB	202	PEB	C2D-C3D	9.14	1.46	1.34
29	LM	202	PEB	C2D-C3D	9.14	1.46	1.34
29	S2	202	PEB	C2D-C3D	9.14	1.46	1.34
29	FG	201	PEB	C2D-C3D	9.14	1.46	1.34
29	TI	201	PEB	C2D-C3D	9.14	1.46	1.34
29	FQ	201	PEB	C2D-C3D	9.14	1.46	1.34
29	S7	201	PEB	C2D-C3D	9.14	1.46	1.34
29	h7	201	PEB	C2D-C3D	9.14	1.46	1.34
29	G8	203	PEB	C2D-C3D	9.14	1.46	1.34
29	S9	201	PEB	C2D-C3D	9.14	1.46	1.34
29	h9	201	PEB	C2D-C3D	9.14	1.46	1.34
29	MB	202	PEB	C2D-C3D	9.14	1.46	1.34
29	MM	202	PEB	C2D-C3D	9.14	1.46	1.34
29	BJ	201	PEB	C2D-C3D	9.14	1.46	1.34
29	nJ	201	PEB	C2D-C3D	9.14	1.46	1.34
29	BL	201	PEB	C2D-C3D	9.14	1.46	1.34
29	nL	201	PEB	C2D-C3D	9.14	1.46	1.34
29	Y7	201	PEB	C2D-C3D	9.14	1.46	1.34
29	Y9	201	PEB	C2D-C3D	9.14	1.46	1.34
29	b1	201	PEB	C2D-C3D	9.14	1.46	1.34
29	bK	201	PEB	C2D-C3D	9.14	1.46	1.34
29	hJ	201	PEB	C2D-C3D	9.13	1.46	1.34
29	hL	201	PEB	C2D-C3D	9.13	1.46	1.34
29	H5	203	PEB	C2D-C3D	9.13	1.46	1.34
29	XJ	201	PEB	C2D-C3D	9.13	1.46	1.34
29	XL	201	PEB	C2D-C3D	9.13	1.46	1.34
29	ZJ	201	PEB	C2D-C3D	9.13	1.46	1.34
29	ZL	201	PEB	C2D-C3D	9.13	1.46	1.34
29	B8	203	PEB	C2D-C3D	9.13	1.46	1.34
29	Q2	202	PEB	C2D-C3D	9.13	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R7	201	PEB	C2D-C3D	9.13	1.46	1.34
29	R9	201	PEB	C2D-C3D	9.13	1.46	1.34
29	B5	203	PEB	C2D-C3D	9.12	1.46	1.34
29	U7	202	PEB	C2D-C3D	9.12	1.46	1.34
29	U9	202	PEB	C2D-C3D	9.12	1.46	1.34
29	HG	201	PEB	C2D-C3D	9.12	1.46	1.34
29	HQ	201	PEB	C2D-C3D	9.12	1.46	1.34
29	Z1	202	PEB	C2D-C3D	9.12	1.46	1.34
29	ZK	202	PEB	C2D-C3D	9.12	1.46	1.34
29	CB	202	PEB	C2D-C3D	9.12	1.46	1.34
29	CM	202	PEB	C2D-C3D	9.12	1.46	1.34
29	RF	201	PEB	C2D-C3D	9.12	1.46	1.34
29	RI	201	PEB	C2D-C3D	9.12	1.46	1.34
29	SR	202	PEB	C2D-C3D	9.12	1.46	1.34
29	A7	305	PEB	C2D-C3D	9.11	1.46	1.34
29	A9	305	PEB	C2D-C3D	9.11	1.46	1.34
29	e7	201	PEB	C2D-C3D	9.11	1.46	1.34
29	e9	201	PEB	C2D-C3D	9.11	1.46	1.34
29	a7	201	PEB	C2D-C3D	9.11	1.46	1.34
29	a9	201	PEB	C2D-C3D	9.11	1.46	1.34
29	A7	304	PEB	C2D-C3D	9.11	1.46	1.34
29	g7	201	PEB	C2D-C3D	9.11	1.46	1.34
29	g9	201	PEB	C2D-C3D	9.11	1.46	1.34
29	c7	201	PEB	C2D-C3D	9.11	1.46	1.34
29	c9	201	PEB	C2D-C3D	9.11	1.46	1.34
29	G8	201	PEB	C2D-C3D	9.11	1.46	1.34
29	aB	202	PEB	C2D-C3D	9.11	1.46	1.34
29	aM	202	PEB	C2D-C3D	9.11	1.46	1.34
29	W7	201	PEB	C2D-C3D	9.11	1.46	1.34
29	W9	201	PEB	C2D-C3D	9.11	1.46	1.34
29	d1	201	PEB	C2D-C3D	9.11	1.46	1.34
29	dK	201	PEB	C2D-C3D	9.11	1.46	1.34
29	iF	201	PEB	C2D-C3D	9.11	1.46	1.34
29	iI	201	PEB	C2D-C3D	9.11	1.46	1.34
29	UB	202	PEB	C2D-C3D	9.10	1.46	1.34
29	MQ	401	PEB	C2D-C3D	9.10	1.46	1.34
29	OB	202	PEB	C2D-C3D	9.10	1.46	1.34
29	OM	202	PEB	C2D-C3D	9.10	1.46	1.34
29	CJ	201	PEB	C2D-C3D	9.10	1.46	1.34
29	CL	201	PEB	C2D-C3D	9.10	1.46	1.34
29	V7	201	PEB	C2D-C3D	9.10	1.46	1.34
29	V9	201	PEB	C2D-C3D	9.10	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IB	202	PEB	C2D-C3D	9.10	1.46	1.34
29	IM	202	PEB	C2D-C3D	9.10	1.46	1.34
29	f1	201	PEB	C2D-C3D	9.10	1.46	1.34
29	fK	201	PEB	C2D-C3D	9.10	1.46	1.34
29	W1	201	PEB	C2D-C3D	9.10	1.46	1.34
29	WK	201	PEB	C2D-C3D	9.10	1.46	1.34
29	H8	201	PEB	C2D-C3D	9.10	1.46	1.34
29	mF	202	PEB	C2D-C3D	9.10	1.46	1.34
29	mI	202	PEB	C2D-C3D	9.10	1.46	1.34
29	OF	203	PEB	C2D-C3D	9.09	1.46	1.34
29	OI	203	PEB	C2D-C3D	9.09	1.46	1.34
29	mJ	201	PEB	C2D-C3D	9.09	1.46	1.34
29	mL	201	PEB	C2D-C3D	9.09	1.46	1.34
29	A1	301	PEB	C2D-C3D	9.09	1.46	1.34
29	j1	201	PEB	C2D-C3D	9.09	1.46	1.34
29	m7	201	PEB	C2D-C3D	9.09	1.46	1.34
29	m9	201	PEB	C2D-C3D	9.09	1.46	1.34
29	AK	301	PEB	C2D-C3D	9.09	1.46	1.34
29	jK	201	PEB	C2D-C3D	9.09	1.46	1.34
29	LG	201	PEB	C2D-C3D	9.09	1.46	1.34
29	MQ	402	PEB	C2D-C3D	9.09	1.46	1.34
29	W2	202	PEB	C2D-C3D	9.09	1.46	1.34
29	PF	202	PEB	C2D-C3D	9.09	1.46	1.34
29	PI	202	PEB	C2D-C3D	9.09	1.46	1.34
29	L8	201	PEB	C2D-C3D	9.09	1.46	1.34
29	AJ	201	PEB	C2D-C3D	9.09	1.46	1.34
29	AL	201	PEB	C2D-C3D	9.09	1.46	1.34
29	P7	201	PEB	C2D-C3D	9.09	1.46	1.34
29	k7	201	PEB	C2D-C3D	9.09	1.46	1.34
29	P9	201	PEB	C2D-C3D	9.09	1.46	1.34
29	k9	201	PEB	C2D-C3D	9.09	1.46	1.34
29	h1	201	PEB	C2D-C3D	9.09	1.46	1.34
29	hK	201	PEB	C2D-C3D	9.09	1.46	1.34
29	gF	202	PEB	C2D-C3D	9.08	1.46	1.34
29	gI	202	PEB	C2D-C3D	9.08	1.46	1.34
29	H5	201	PEB	C2D-C3D	9.08	1.46	1.34
29	EB	202	PEB	C2D-C3D	9.08	1.46	1.34
29	GJ	201	PEB	C2D-C3D	9.08	1.46	1.34
29	GL	201	PEB	C2D-C3D	9.08	1.46	1.34
29	EM	202	PEB	C2D-C3D	9.08	1.46	1.34
29	i7	201	PEB	C2D-C3D	9.08	1.46	1.34
29	i9	201	PEB	C2D-C3D	9.08	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G5	201	PEB	C2D-C3D	9.08	1.46	1.34
29	T7	201	PEB	C2D-C3D	9.08	1.46	1.34
29	T9	201	PEB	C2D-C3D	9.08	1.46	1.34
29	F5	201	PEB	C2D-C3D	9.08	1.46	1.34
29	F8	201	PEB	C2D-C3D	9.08	1.46	1.34
29	fB	201	PEB	C2D-C3D	9.08	1.46	1.34
29	fM	201	PEB	C2D-C3D	9.08	1.46	1.34
29	kF	202	PEB	C2D-C3D	9.08	1.46	1.34
29	kI	202	PEB	C2D-C3D	9.08	1.46	1.34
29	YB	203	PEB	C2D-C3D	9.07	1.46	1.34
29	aF	202	PEB	C2D-C3D	9.07	1.46	1.34
29	aI	202	PEB	C2D-C3D	9.07	1.46	1.34
29	YM	203	PEB	C2D-C3D	9.07	1.46	1.34
29	JG	201	PEB	C2D-C3D	9.07	1.46	1.34
29	JQ	201	PEB	C2D-C3D	9.07	1.46	1.34
29	Q1	201	PEB	C2D-C3D	9.07	1.46	1.34
29	QK	201	PEB	C2D-C3D	9.07	1.46	1.34
29	L5	203	PEB	C2D-C3D	9.07	1.46	1.34
29	OB	201	PEB	C2D-C3D	9.07	1.46	1.34
29	OM	201	PEB	C2D-C3D	9.07	1.46	1.34
29	l1	201	PEB	C2D-C3D	9.07	1.46	1.34
29	WB	202	PEB	C2D-C3D	9.07	1.46	1.34
29	lK	201	PEB	C2D-C3D	9.07	1.46	1.34
29	WM	202	PEB	C2D-C3D	9.07	1.46	1.34
29	H8	203	PEB	C2D-C3D	9.07	1.46	1.34
29	EJ	201	PEB	C2D-C3D	9.07	1.46	1.34
29	EL	201	PEB	C2D-C3D	9.07	1.46	1.34
29	UR	202	PEB	C2D-C3D	9.07	1.46	1.34
29	GB	202	PEB	C2D-C3D	9.07	1.46	1.34
29	cJ	201	PEB	C2D-C3D	9.07	1.46	1.34
29	cL	201	PEB	C2D-C3D	9.07	1.46	1.34
29	GM	202	PEB	C2D-C3D	9.07	1.46	1.34
29	QB	204	PEB	C2D-C3D	9.06	1.46	1.34
29	AF	304	PEB	C2D-C3D	9.06	1.46	1.34
29	AI	304	PEB	C2D-C3D	9.06	1.46	1.34
29	AM	302	PEB	C2D-C3D	9.06	1.46	1.34
29	QM	204	PEB	C2D-C3D	9.06	1.46	1.34
29	iF	202	PEB	C2D-C3D	9.06	1.46	1.34
29	iI	202	PEB	C2D-C3D	9.06	1.46	1.34
29	sJ	201	PEB	C2D-C3D	9.06	1.46	1.34
29	sL	201	PEB	C2D-C3D	9.06	1.46	1.34
29	hB	201	PEB	C2D-C3D	9.06	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	hM	201	PEB	C2D-C3D	9.06	1.46	1.34
29	M2	201	PEB	C2D-C3D	9.06	1.46	1.34
29	U1	202	PEB	C2D-C3D	9.06	1.46	1.34
29	UF	201	PEB	C2D-C3D	9.06	1.46	1.34
29	UI	201	PEB	C2D-C3D	9.06	1.46	1.34
29	UK	202	PEB	C2D-C3D	9.06	1.46	1.34
29	OJ	201	PEB	C2D-C3D	9.06	1.46	1.34
29	WJ	202	PEB	C2D-C3D	9.06	1.46	1.34
29	YJ	201	PEB	C2D-C3D	9.06	1.46	1.34
29	gJ	201	PEB	C2D-C3D	9.06	1.46	1.34
29	OL	201	PEB	C2D-C3D	9.06	1.46	1.34
29	WL	202	PEB	C2D-C3D	9.06	1.46	1.34
29	YL	201	PEB	C2D-C3D	9.06	1.46	1.34
29	gL	201	PEB	C2D-C3D	9.06	1.46	1.34
29	jB	202	PEB	C2D-C3D	9.06	1.46	1.34
29	jM	202	PEB	C2D-C3D	9.06	1.46	1.34
29	hB	202	PEB	C2D-C3D	9.06	1.46	1.34
29	hM	202	PEB	C2D-C3D	9.06	1.46	1.34
29	GB	201	PEB	C2D-C3D	9.06	1.46	1.34
29	QJ	201	PEB	C2D-C3D	9.06	1.46	1.34
29	QL	201	PEB	C2D-C3D	9.06	1.46	1.34
29	GM	201	PEB	C2D-C3D	9.06	1.46	1.34
29	dF	201	PEB	C2D-C3D	9.05	1.46	1.34
29	dI	201	PEB	C2D-C3D	9.05	1.46	1.34
29	xJ	302	PEB	C2D-C3D	9.05	1.46	1.34
29	wJ	302	PEB	C2D-C3D	9.05	1.46	1.34
29	aB	201	PEB	C2D-C3D	9.05	1.46	1.34
29	KJ	201	PEB	C2D-C3D	9.05	1.46	1.34
29	KL	201	PEB	C2D-C3D	9.05	1.46	1.34
29	aM	201	PEB	C2D-C3D	9.05	1.46	1.34
29	xL	302	PEB	C2D-C3D	9.05	1.46	1.34
29	BG	201	PEB	C2D-C3D	9.05	1.46	1.34
29	eJ	201	PEB	C2D-C3D	9.05	1.46	1.34
29	eL	201	PEB	C2D-C3D	9.05	1.46	1.34
29	BQ	201	PEB	C2D-C3D	9.05	1.46	1.34
29	O1	201	PEB	C2D-C3D	9.05	1.46	1.34
29	OK	201	PEB	C2D-C3D	9.05	1.46	1.34
29	fB	202	PEB	C2D-C3D	9.05	1.46	1.34
29	fM	202	PEB	C2D-C3D	9.05	1.46	1.34
29	DG	201	PEB	C2D-C3D	9.04	1.46	1.34
29	DQ	201	PEB	C2D-C3D	9.04	1.46	1.34
29	L8	203	PEB	C2D-C3D	9.04	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	kJ	201	PEB	C2D-C3D	9.04	1.46	1.34
29	kL	201	PEB	C2D-C3D	9.04	1.46	1.34
29	S1	201	PEB	C2D-C3D	9.04	1.46	1.34
29	SK	201	PEB	C2D-C3D	9.04	1.46	1.34
29	VF	202	PEB	C2D-C3D	9.04	1.46	1.34
29	eF	202	PEB	C2D-C3D	9.04	1.46	1.34
29	VI	202	PEB	C2D-C3D	9.04	1.46	1.34
29	eI	202	PEB	C2D-C3D	9.04	1.46	1.34
29	KB	202	PEB	C2D-C3D	9.04	1.46	1.34
29	KM	202	PEB	C2D-C3D	9.04	1.46	1.34
29	WR	201	PEB	C2D-C3D	9.04	1.46	1.34
29	uJ	202	PEB	C2D-C3D	9.04	1.46	1.34
29	uL	202	PEB	C2D-C3D	9.04	1.46	1.34
29	B5	201	PEB	C2D-C3D	9.04	1.46	1.34
29	IJ	201	PEB	C2D-C3D	9.04	1.46	1.34
29	UJ	201	PEB	C2D-C3D	9.04	1.46	1.34
29	IL	201	PEB	C2D-C3D	9.04	1.46	1.34
29	UL	201	PEB	C2D-C3D	9.04	1.46	1.34
29	CB	201	PEB	C2D-C3D	9.04	1.46	1.34
29	CM	201	PEB	C2D-C3D	9.04	1.46	1.34
29	yJ	301	PEB	C2D-C3D	9.04	1.46	1.34
29	yL	301	PEB	C2D-C3D	9.04	1.46	1.34
29	MR	201	PEB	C2D-C3D	9.04	1.46	1.34
29	AB	302	PEB	C2D-C3D	9.04	1.46	1.34
29	SJ	201	PEB	C2D-C3D	9.04	1.46	1.34
29	SL	201	PEB	C2D-C3D	9.04	1.46	1.34
29	U2	202	PEB	C2D-C3D	9.04	1.46	1.34
29	dB	202	PEB	C2D-C3D	9.04	1.46	1.34
29	dM	202	PEB	C2D-C3D	9.04	1.46	1.34
29	WB	201	PEB	C2D-C3D	9.03	1.46	1.34
29	WM	201	PEB	C2D-C3D	9.03	1.46	1.34
29	SB	201	PEB	C2D-C3D	9.03	1.46	1.34
29	SM	201	PEB	C2D-C3D	9.03	1.46	1.34
29	QB	203	PEB	C2D-C3D	9.03	1.46	1.34
29	QM	203	PEB	C2D-C3D	9.03	1.46	1.34
29	wL	302	PEB	C2D-C3D	9.03	1.46	1.34
29	N3	203	PEB	C2D-C3D	9.02	1.46	1.34
29	oJ	201	PEB	C2D-C3D	9.02	1.46	1.34
29	oL	201	PEB	C2D-C3D	9.02	1.46	1.34
29	MA	405	PEB	C2D-C3D	9.02	1.46	1.34
29	B8	201	PEB	C2D-C3D	9.02	1.46	1.34
29	YB	202	PEB	C2D-C3D	9.02	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YM	202	PEB	C2D-C3D	9.02	1.46	1.34
29	UR	201	PEB	C2D-C3D	9.02	1.46	1.34
29	Q2	201	PEB	C2D-C3D	9.01	1.46	1.34
29	UB	201	PEB	C2D-C3D	9.01	1.46	1.34
29	UM	201	PEB	C2D-C3D	9.01	1.46	1.34
29	MJ	201	PEB	C2D-C3D	9.01	1.46	1.34
29	ML	201	PEB	C2D-C3D	9.01	1.46	1.34
29	J9	1002	PEB	C2D-C3D	9.01	1.46	1.34
29	IB	202	PEB	C2D-C3D	9.01	1.46	1.34
29	IM	202	PEB	C2D-C3D	9.01	1.46	1.34
29	W2	201	PEB	C2D-C3D	9.01	1.46	1.34
29	IB	201	PEB	C2D-C3D	9.01	1.46	1.34
29	IM	201	PEB	C2D-C3D	9.01	1.46	1.34
29	MB	201	PEB	C2D-C3D	9.00	1.46	1.34
29	MM	201	PEB	C2D-C3D	9.00	1.46	1.34
29	jB	201	PEB	C2D-C3D	9.00	1.46	1.34
29	jM	201	PEB	C2D-C3D	9.00	1.46	1.34
29	lB	201	PEB	C2D-C3D	9.00	1.46	1.34
29	lM	201	PEB	C2D-C3D	9.00	1.46	1.34
29	qJ	201	PEB	C2D-C3D	9.00	1.46	1.34
29	qL	201	PEB	C2D-C3D	9.00	1.46	1.34
29	iJ	201	PEB	C2D-C3D	8.99	1.46	1.34
29	iL	201	PEB	C2D-C3D	8.99	1.46	1.34
29	QR	201	PEB	C2D-C3D	8.99	1.46	1.34
29	SB	202	PEB	C2D-C3D	8.99	1.46	1.34
29	SM	202	PEB	C2D-C3D	8.99	1.46	1.34
29	aJ	201	PEB	C2D-C3D	8.99	1.46	1.34
29	aL	201	PEB	C2D-C3D	8.99	1.46	1.34
29	A1	302	PEB	C2D-C3D	8.99	1.46	1.34
29	AK	302	PEB	C2D-C3D	8.99	1.46	1.34
29	M3	203	PEB	C2D-C3D	8.99	1.46	1.34
29	MO	203	PEB	C2D-C3D	8.99	1.46	1.34
29	KB	201	PEB	C2D-C3D	8.98	1.46	1.34
29	KM	201	PEB	C2D-C3D	8.98	1.46	1.34
29	D7	1002	PEB	C2D-C3D	8.97	1.46	1.34
29	D9	1002	PEB	C2D-C3D	8.97	1.46	1.34
29	NO	203	PEB	C2D-C3D	8.97	1.46	1.34
29	dB	201	PEB	C2D-C3D	8.97	1.46	1.34
29	dM	201	PEB	C2D-C3D	8.97	1.46	1.34
29	L7	1002	PEB	C2D-C3D	8.97	1.46	1.34
29	EB	201	PEB	C2D-C3D	8.97	1.46	1.34
29	EM	201	PEB	C2D-C3D	8.97	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O2	201	PEB	C2D-C3D	8.96	1.46	1.34
29	OR	201	PEB	C2D-C3D	8.96	1.46	1.34
29	L9	1002	PEB	C2D-C3D	8.96	1.46	1.34
29	J7	1002	PEB	C2D-C3D	8.96	1.46	1.34
29	MN	405	PEB	C2D-C3D	8.95	1.46	1.34
29	N1	1002	PEB	C2D-C3D	8.95	1.46	1.34
29	N7	1002	PEB	C2D-C3D	8.95	1.46	1.34
29	N9	1002	PEB	C2D-C3D	8.95	1.46	1.34
29	U2	201	PEB	C2D-C3D	8.95	1.46	1.34
29	J1	1002	PEB	C2D-C3D	8.94	1.46	1.34
29	JK	1002	PEB	C2D-C3D	8.94	1.46	1.34
29	GA	201	PEB	C2D-C3D	8.94	1.46	1.34
29	GN	201	PEB	C2D-C3D	8.94	1.46	1.34
29	xJ	303	PEB	C2D-C3D	8.94	1.46	1.34
29	NK	1002	PEB	C2D-C3D	8.94	1.46	1.34
29	wL	303	PEB	C2D-C3D	8.93	1.46	1.34
29	HK	1002	PEB	C2D-C3D	8.93	1.46	1.34
29	H1	1002	PEB	C2D-C3D	8.92	1.46	1.34
29	CA	201	PEB	C2D-C3D	8.91	1.46	1.34
29	CN	201	PEB	C2D-C3D	8.91	1.46	1.34
29	KA	201	PEB	C2D-C3D	8.91	1.46	1.34
29	KN	201	PEB	C2D-C3D	8.91	1.46	1.34
29	xL	303	PEB	C2D-C3D	8.91	1.46	1.34
29	AA	201	PEB	C2D-C3D	8.90	1.46	1.34
29	AN	201	PEB	C2D-C3D	8.90	1.46	1.34
29	L1	1002	PEB	C2D-C3D	8.90	1.46	1.34
29	LK	1002	PEB	C2D-C3D	8.90	1.46	1.34
29	wJ	303	PEB	C2D-C3D	8.90	1.46	1.34
29	AM	303	PEB	C2D-C3D	8.89	1.46	1.34
29	N2	202	PEB	C2D-C3D	8.89	1.46	1.34
29	P2	201	PEB	C2D-C3D	8.88	1.46	1.34
29	X2	201	PEB	C2D-C3D	8.88	1.46	1.34
29	XR	202	PEB	C2D-C3D	8.88	1.46	1.34
29	F1	1002	PEB	C2D-C3D	8.88	1.46	1.34
29	FK	1002	PEB	C2D-C3D	8.88	1.46	1.34
29	PR	201	PEB	C2D-C3D	8.88	1.46	1.34
29	F7	1002	PEB	C2D-C3D	8.88	1.46	1.34
29	H7	1002	PEB	C2D-C3D	8.87	1.45	1.34
29	H9	1002	PEB	C2D-C3D	8.87	1.45	1.34
29	F9	1002	PEB	C2D-C3D	8.87	1.45	1.34
29	AB	303	PEB	C2D-C3D	8.86	1.45	1.34
29	DK	1002	PEB	C2D-C3D	8.86	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NR	202	PEB	C2D-C3D	8.86	1.45	1.34
29	IA	201	PEB	C2D-C3D	8.85	1.45	1.34
29	IN	201	PEB	C2D-C3D	8.85	1.45	1.34
29	EA	201	PEB	C2D-C3D	8.85	1.45	1.34
29	EN	201	PEB	C2D-C3D	8.85	1.45	1.34
29	D1	1002	PEB	C2D-C3D	8.84	1.45	1.34
29	J5	202	PEB	C2D-C3D	8.84	1.45	1.34
29	J8	202	PEB	C2D-C3D	8.84	1.45	1.34
29	R2	202	PEB	C2D-C3D	8.84	1.45	1.34
29	VR	202	PEB	C2D-C3D	8.84	1.45	1.34
29	a7	202	PEB	C2D-C3D	8.82	1.45	1.34
29	a9	202	PEB	C2D-C3D	8.82	1.45	1.34
29	ZF	201	PEB	C2D-C3D	8.82	1.45	1.34
29	ZI	201	PEB	C2D-C3D	8.82	1.45	1.34
29	UF	202	PEB	C2D-C3D	8.81	1.45	1.34
29	UI	202	PEB	C2D-C3D	8.81	1.45	1.34
29	T2	202	PEB	C2D-C3D	8.80	1.45	1.34
29	TR	202	PEB	C2D-C3D	8.80	1.45	1.34
29	AF	301	PEB	C2D-C3D	8.80	1.45	1.34
29	AI	301	PEB	C2D-C3D	8.80	1.45	1.34
29	g7	202	PEB	C2D-C3D	8.79	1.45	1.34
29	g9	202	PEB	C2D-C3D	8.79	1.45	1.34
29	T7	202	PEB	C2D-C3D	8.79	1.45	1.34
29	T9	202	PEB	C2D-C3D	8.79	1.45	1.34
29	SF	201	PEB	C2D-C3D	8.79	1.45	1.34
29	SI	201	PEB	C2D-C3D	8.79	1.45	1.34
29	c7	202	PEB	C2D-C3D	8.78	1.45	1.34
29	c9	202	PEB	C2D-C3D	8.78	1.45	1.34
29	hF	201	PEB	C2D-C3D	8.78	1.45	1.34
29	hI	201	PEB	C2D-C3D	8.78	1.45	1.34
29	V2	202	PEB	C2D-C3D	8.78	1.45	1.34
29	e7	202	PEB	C2D-C3D	8.78	1.45	1.34
29	e9	202	PEB	C2D-C3D	8.78	1.45	1.34
29	WF	201	PEB	C2D-C3D	8.77	1.45	1.34
29	WI	201	PEB	C2D-C3D	8.77	1.45	1.34
29	H4	201	PEB	C2D-C3D	8.77	1.45	1.34
29	MN	404	PEB	C2D-C3D	8.77	1.45	1.34
29	R7	202	PEB	C2D-C3D	8.77	1.45	1.34
29	R9	202	PEB	C2D-C3D	8.77	1.45	1.34
29	MA	404	PEB	C2D-C3D	8.77	1.45	1.34
29	fF	201	PEB	C2D-C3D	8.77	1.45	1.34
29	fI	201	PEB	C2D-C3D	8.77	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y7	202	PEB	C2D-C3D	8.76	1.45	1.34
29	Y9	202	PEB	C2D-C3D	8.76	1.45	1.34
29	bF	201	PEB	C2D-C3D	8.76	1.45	1.34
29	bI	201	PEB	C2D-C3D	8.76	1.45	1.34
29	P7	202	PEB	C2D-C3D	8.76	1.45	1.34
29	P9	202	PEB	C2D-C3D	8.76	1.45	1.34
29	OF	201	PEB	C2D-C3D	8.76	1.45	1.34
29	OI	201	PEB	C2D-C3D	8.76	1.45	1.34
29	HD	201	PEB	C2D-C3D	8.76	1.45	1.34
29	B4	201	PEB	C2D-C3D	8.75	1.45	1.34
29	RR	202	PEB	C2D-C3D	8.75	1.45	1.34
29	k7	202	PEB	C2D-C3D	8.75	1.45	1.34
29	k9	202	PEB	C2D-C3D	8.75	1.45	1.34
29	i7	202	PEB	C2D-C3D	8.74	1.45	1.34
29	i9	202	PEB	C2D-C3D	8.74	1.45	1.34
29	BD	201	PEB	C2D-C3D	8.74	1.45	1.34
29	V7	202	PEB	C2D-C3D	8.73	1.45	1.34
29	V9	202	PEB	C2D-C3D	8.73	1.45	1.34
29	a1	201	PEB	C2D-C3D	8.73	1.45	1.34
29	aK	201	PEB	C2D-C3D	8.73	1.45	1.34
29	lF	201	PEB	C2D-C3D	8.73	1.45	1.34
29	lI	201	PEB	C2D-C3D	8.73	1.45	1.34
29	F4	201	PEB	C2D-C3D	8.73	1.45	1.34
29	FD	201	PEB	C2D-C3D	8.73	1.45	1.34
29	jF	201	PEB	C2D-C3D	8.73	1.45	1.34
29	jI	201	PEB	C2D-C3D	8.73	1.45	1.34
29	QF	201	PEB	C2D-C3D	8.72	1.45	1.34
29	QI	201	PEB	C2D-C3D	8.72	1.45	1.34
29	m7	202	PEB	C2D-C3D	8.72	1.45	1.34
29	m9	202	PEB	C2D-C3D	8.72	1.45	1.34
29	dF	202	PEB	C2D-C3D	8.72	1.45	1.34
29	dI	202	PEB	C2D-C3D	8.72	1.45	1.34
29	J4	201	PEB	C2D-C3D	8.72	1.45	1.34
29	L4	201	PEB	C2D-C3D	8.71	1.45	1.34
29	LD	201	PEB	C2D-C3D	8.71	1.45	1.34
29	i1	201	PEB	C2D-C3D	8.69	1.45	1.34
29	iK	201	PEB	C2D-C3D	8.69	1.45	1.34
29	g1	201	PEB	C2D-C3D	8.69	1.45	1.34
29	gK	201	PEB	C2D-C3D	8.69	1.45	1.34
29	V1	201	PEB	C2D-C3D	8.69	1.45	1.34
29	VK	201	PEB	C2D-C3D	8.69	1.45	1.34
29	JD	201	PEB	C2D-C3D	8.68	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e1	201	PEB	C2D-C3D	8.67	1.45	1.34
29	eK	201	PEB	C2D-C3D	8.67	1.45	1.34
29	D4	201	PEB	C2D-C3D	8.66	1.45	1.34
29	DD	201	PEB	C2D-C3D	8.66	1.45	1.34
29	m1	201	PEB	C2D-C3D	8.65	1.45	1.34
29	mK	201	PEB	C2D-C3D	8.65	1.45	1.34
29	T1	201	PEB	C2D-C3D	8.64	1.45	1.34
29	TK	201	PEB	C2D-C3D	8.64	1.45	1.34
29	P1	201	PEB	C2D-C3D	8.64	1.45	1.34
29	PK	201	PEB	C2D-C3D	8.64	1.45	1.34
29	A1	303	PEB	C2D-C3D	8.63	1.45	1.34
29	AK	303	PEB	C2D-C3D	8.63	1.45	1.34
29	k1	201	PEB	C2D-C3D	8.62	1.45	1.34
29	kK	201	PEB	C2D-C3D	8.62	1.45	1.34
29	Y1	201	PEB	C2D-C3D	8.62	1.45	1.34
29	YK	201	PEB	C2D-C3D	8.62	1.45	1.34
29	R1	201	PEB	C2D-C3D	8.61	1.45	1.34
29	RK	201	PEB	C2D-C3D	8.61	1.45	1.34
29	J5	201	PEB	C2D-C3D	8.61	1.45	1.34
29	J8	201	PEB	C2D-C3D	8.61	1.45	1.34
29	c1	201	PEB	C2D-C3D	8.61	1.45	1.34
29	cK	201	PEB	C2D-C3D	8.61	1.45	1.34
29	IG	202	PEB	C2D-C3D	8.61	1.45	1.34
29	IQ	202	PEB	C2D-C3D	8.61	1.45	1.34
29	GG	202	PEB	C2D-C3D	8.60	1.45	1.34
29	GQ	202	PEB	C2D-C3D	8.60	1.45	1.34
29	KG	202	PEB	C2D-C3D	8.56	1.45	1.34
29	KQ	202	PEB	C2D-C3D	8.56	1.45	1.34
29	EG	202	PEB	C2D-C3D	8.53	1.45	1.34
29	EQ	202	PEB	C2D-C3D	8.53	1.45	1.34
29	CG	202	PEB	C2D-C3D	8.53	1.45	1.34
29	CQ	202	PEB	C2D-C3D	8.53	1.45	1.34
29	AG	202	PEB	C2D-C3D	8.52	1.45	1.34
29	AQ	202	PEB	C2D-C3D	8.52	1.45	1.34
29	MG	401	PEB	C2D-C3D	8.51	1.45	1.34
29	G4	201	PEB	C2D-C3D	8.46	1.45	1.34
29	GD	201	PEB	C2D-C3D	8.46	1.45	1.34
29	dD	401	PEB	C2D-C3D	8.44	1.45	1.34
29	MQ	403	PEB	C2D-C3D	8.44	1.45	1.34
29	E4	201	PEB	C2D-C3D	8.41	1.45	1.34
29	MD	201	PEB	C2D-C3D	8.41	1.45	1.34
29	I4	201	PEB	C2D-C3D	8.39	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	CD	201	PEB	C2D-C3D	8.38	1.45	1.34
29	ID	201	PEB	C2D-C3D	8.37	1.45	1.34
29	K4	201	PEB	C2D-C3D	8.37	1.45	1.34
29	KD	201	PEB	C2D-C3D	8.37	1.45	1.34
29	C4	201	PEB	C2D-C3D	8.36	1.45	1.34
29	M4	201	PEB	C2D-C3D	8.35	1.45	1.34
29	GD	202	PEB	C2D-C3D	8.33	1.45	1.34
29	ED	201	PEB	C2D-C3D	8.31	1.45	1.34
29	K4	202	PEB	C2D-C3D	8.30	1.45	1.34
29	M4	202	PEB	C2D-C3D	8.28	1.45	1.34
29	CD	202	PEB	C2D-C3D	8.28	1.45	1.34
29	C4	202	PEB	C2D-C3D	8.28	1.45	1.34
29	ID	202	PEB	C2D-C3D	8.26	1.45	1.34
29	G4	202	PEB	C2D-C3D	8.24	1.45	1.34
29	KD	202	PEB	C2D-C3D	8.24	1.45	1.34
29	E4	202	PEB	C2D-C3D	8.23	1.45	1.34
29	MD	202	PEB	C2D-C3D	8.23	1.45	1.34
29	I4	202	PEB	C2D-C3D	8.23	1.45	1.34
29	NF	1002	PEB	C2D-C3D	8.22	1.45	1.34
29	NI	1002	PEB	C2D-C3D	8.22	1.45	1.34
29	DF	1002	PEB	C2D-C3D	8.21	1.45	1.34
29	DI	1002	PEB	C2D-C3D	8.21	1.45	1.34
29	JF	1002	PEB	C2D-C3D	8.19	1.45	1.34
29	JI	1002	PEB	C2D-C3D	8.19	1.45	1.34
29	LF	1002	PEB	C2D-C3D	8.18	1.45	1.34
29	LI	1002	PEB	C2D-C3D	8.18	1.45	1.34
29	HF	1002	PEB	C2D-C3D	8.18	1.45	1.34
29	HI	1002	PEB	C2D-C3D	8.18	1.45	1.34
29	FF	1002	PEB	C2D-C3D	8.12	1.45	1.34
29	FI	1002	PEB	C2D-C3D	8.12	1.45	1.34
29	ZJ	202	PEB	C2D-C3D	7.83	1.44	1.34
29	ZL	202	PEB	C2D-C3D	7.83	1.44	1.34
29	RJ	202	PEB	C2D-C3D	7.83	1.44	1.34
29	RL	202	PEB	C2D-C3D	7.83	1.44	1.34
29	IJ	203	PEB	C2D-C3D	7.82	1.44	1.34
29	IL	203	PEB	C2D-C3D	7.82	1.44	1.34
29	dJ	202	PEB	C2D-C3D	7.82	1.44	1.34
29	dL	202	PEB	C2D-C3D	7.82	1.44	1.34
29	HJ	201	PEB	C2D-C3D	7.82	1.44	1.34
29	TJ	202	PEB	C2D-C3D	7.82	1.44	1.34
29	HL	201	PEB	C2D-C3D	7.82	1.44	1.34
29	TL	202	PEB	C2D-C3D	7.82	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	XJ	202	PEB	C2D-C3D	7.82	1.44	1.34
29	XL	202	PEB	C2D-C3D	7.82	1.44	1.34
29	hJ	202	PEB	C2D-C3D	7.81	1.44	1.34
29	nJ	202	PEB	C2D-C3D	7.81	1.44	1.34
29	hL	202	PEB	C2D-C3D	7.81	1.44	1.34
29	nL	202	PEB	C2D-C3D	7.81	1.44	1.34
29	lJ	202	PEB	C2D-C3D	7.81	1.44	1.34
29	lL	202	PEB	C2D-C3D	7.81	1.44	1.34
29	WJ	201	PEB	C2D-C3D	7.80	1.44	1.34
29	WL	201	PEB	C2D-C3D	7.80	1.44	1.34
29	NJ	202	PEB	C2D-C3D	7.80	1.44	1.34
29	NL	202	PEB	C2D-C3D	7.80	1.44	1.34
29	PJ	202	PEB	C2D-C3D	7.80	1.44	1.34
29	fJ	202	PEB	C2D-C3D	7.80	1.44	1.34
29	PL	202	PEB	C2D-C3D	7.80	1.44	1.34
29	fL	202	PEB	C2D-C3D	7.80	1.44	1.34
29	jJ	202	PEB	C2D-C3D	7.79	1.44	1.34
29	jL	202	PEB	C2D-C3D	7.79	1.44	1.34
29	sJ	203	PEB	C2D-C3D	7.79	1.44	1.34
29	sL	203	PEB	C2D-C3D	7.79	1.44	1.34
29	bJ	202	PEB	C2D-C3D	7.78	1.44	1.34
29	bL	202	PEB	C2D-C3D	7.78	1.44	1.34
29	JJ	202	PEB	C2D-C3D	7.78	1.44	1.34
29	JL	202	PEB	C2D-C3D	7.78	1.44	1.34
29	pJ	202	PEB	C2D-C3D	7.78	1.44	1.34
29	pL	202	PEB	C2D-C3D	7.78	1.44	1.34
29	I3	203	PEB	C3C-C4C	7.77	1.54	1.42
29	IO	203	PEB	C3C-C4C	7.77	1.54	1.42
29	AJ	203	PEB	C2D-C3D	7.77	1.44	1.34
29	AL	203	PEB	C2D-C3D	7.77	1.44	1.34
29	F3	202	PEB	C3C-C4C	7.76	1.54	1.42
29	FO	202	PEB	C3C-C4C	7.76	1.54	1.42
29	FJ	202	PEB	C2D-C3D	7.76	1.44	1.34
29	FL	202	PEB	C2D-C3D	7.76	1.44	1.34
29	BJ	202	PEB	C2D-C3D	7.76	1.44	1.34
29	BL	202	PEB	C2D-C3D	7.76	1.44	1.34
29	uJ	201	PEB	C2D-C3D	7.75	1.44	1.34
29	uL	201	PEB	C2D-C3D	7.75	1.44	1.34
29	B3	202	PEB	C3C-C4C	7.75	1.54	1.42
29	H3	202	PEB	C3C-C4C	7.75	1.54	1.42
29	BO	202	PEB	C3C-C4C	7.75	1.54	1.42
29	HO	202	PEB	C3C-C4C	7.75	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J3	202	PEB	C3C-C4C	7.74	1.54	1.42
29	JO	202	PEB	C3C-C4C	7.74	1.54	1.42
29	rJ	202	PEB	C2D-C3D	7.72	1.44	1.34
29	rL	202	PEB	C2D-C3D	7.72	1.44	1.34
30	MG	402	PUB	C3B-C2B	6.75	1.57	1.37
30	MQ	404	PUB	C3B-C2B	6.74	1.57	1.37
29	J5	202	PEB	C3C-C4C	6.53	1.52	1.42
29	J8	202	PEB	C3C-C4C	6.53	1.52	1.42
30	AF	302	PUB	C2B-C1B	6.44	1.52	1.42
30	AI	302	PUB	C2B-C1B	6.44	1.52	1.42
29	hJ	203	PEB	C3C-C4C	6.41	1.52	1.42
29	hL	203	PEB	C3C-C4C	6.41	1.52	1.42
29	HJ	202	PEB	C3C-C4C	6.41	1.52	1.42
29	HL	202	PEB	C3C-C4C	6.41	1.52	1.42
29	wJ	303	PEB	C3B-C2B	6.40	1.50	1.36
29	TJ	203	PEB	C3C-C4C	6.40	1.52	1.42
29	TL	203	PEB	C3C-C4C	6.40	1.52	1.42
29	IJ	203	PEB	C3C-C4C	6.40	1.52	1.42
29	IL	203	PEB	C3C-C4C	6.40	1.52	1.42
29	PJ	203	PEB	C3C-C4C	6.38	1.52	1.42
29	PL	203	PEB	C3C-C4C	6.38	1.52	1.42
29	wL	303	PEB	C3B-C2B	6.38	1.50	1.36
29	nJ	203	PEB	C3C-C4C	6.38	1.52	1.42
29	nL	203	PEB	C3C-C4C	6.38	1.52	1.42
29	pJ	203	PEB	C3C-C4C	6.38	1.52	1.42
29	pL	203	PEB	C3C-C4C	6.38	1.52	1.42
29	FJ	203	PEB	C3C-C4C	6.38	1.52	1.42
29	FL	203	PEB	C3C-C4C	6.38	1.52	1.42
30	MQ	404	PUB	C2B-C1B	6.38	1.52	1.42
29	fJ	203	PEB	C3C-C4C	6.36	1.52	1.42
29	fL	203	PEB	C3C-C4C	6.36	1.52	1.42
29	dJ	203	PEB	C3C-C4C	6.36	1.52	1.42
29	dL	203	PEB	C3C-C4C	6.36	1.52	1.42
29	XJ	203	PEB	C3C-C4C	6.36	1.52	1.42
29	XL	203	PEB	C3C-C4C	6.36	1.52	1.42
30	MG	402	PUB	C2B-C1B	6.35	1.52	1.42
29	bJ	203	PEB	C3C-C4C	6.35	1.52	1.42
29	bL	203	PEB	C3C-C4C	6.35	1.52	1.42
29	VJ	202	PEB	C3C-C4C	6.34	1.52	1.42
29	VL	202	PEB	C3C-C4C	6.34	1.52	1.42
29	ZJ	203	PEB	C3C-C4C	6.34	1.51	1.42
29	ZL	203	PEB	C3C-C4C	6.34	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	rJ	203	PEB	C3C-C4C	6.34	1.51	1.42
29	rL	203	PEB	C3C-C4C	6.34	1.51	1.42
29	DJ	202	PEB	C3C-C4C	6.33	1.51	1.42
29	DL	202	PEB	C3C-C4C	6.33	1.51	1.42
29	xL	303	PEB	C3B-C2B	6.33	1.50	1.36
29	jJ	203	PEB	C3C-C4C	6.33	1.51	1.42
29	jL	203	PEB	C3C-C4C	6.33	1.51	1.42
29	LJ	202	PEB	C3C-C4C	6.33	1.51	1.42
29	LL	202	PEB	C3C-C4C	6.33	1.51	1.42
29	JJ	203	PEB	C3C-C4C	6.32	1.51	1.42
29	JL	203	PEB	C3C-C4C	6.32	1.51	1.42
29	RJ	203	PEB	C3C-C4C	6.32	1.51	1.42
29	RL	203	PEB	C3C-C4C	6.32	1.51	1.42
29	NJ	203	PEB	C3C-C4C	6.32	1.51	1.42
29	NL	203	PEB	C3C-C4C	6.32	1.51	1.42
29	BJ	203	PEB	C3C-C4C	6.32	1.51	1.42
29	BL	203	PEB	C3C-C4C	6.32	1.51	1.42
29	vJ	202	PEB	C3C-C4C	6.31	1.51	1.42
29	vL	202	PEB	C3C-C4C	6.31	1.51	1.42
29	NF	1002	PEB	C3C-C4C	6.31	1.51	1.42
29	NI	1002	PEB	C3C-C4C	6.31	1.51	1.42
29	tJ	202	PEB	C3C-C4C	6.30	1.51	1.42
29	tL	202	PEB	C3C-C4C	6.30	1.51	1.42
29	HF	1002	PEB	C3C-C4C	6.29	1.51	1.42
29	HI	1002	PEB	C3C-C4C	6.29	1.51	1.42
29	xJ	303	PEB	C3B-C2B	6.28	1.50	1.36
29	LF	1002	PEB	C3C-C4C	6.28	1.51	1.42
29	LI	1002	PEB	C3C-C4C	6.28	1.51	1.42
29	JF	1002	PEB	C3C-C4C	6.26	1.51	1.42
29	JI	1002	PEB	C3C-C4C	6.26	1.51	1.42
29	FF	1002	PEB	C3C-C4C	6.25	1.51	1.42
29	FI	1002	PEB	C3C-C4C	6.25	1.51	1.42
29	DF	1002	PEB	C3C-C4C	6.23	1.51	1.42
29	DI	1002	PEB	C3C-C4C	6.23	1.51	1.42
29	J9	1002	PEB	C3C-C4C	6.17	1.51	1.42
29	L9	1002	PEB	C3C-C4C	6.14	1.51	1.42
29	J7	1002	PEB	C3C-C4C	6.13	1.51	1.42
29	L7	1002	PEB	C3C-C4C	6.12	1.51	1.42
29	H7	1002	PEB	C3C-C4C	6.11	1.51	1.42
29	H9	1002	PEB	C3C-C4C	6.11	1.51	1.42
29	F9	1002	PEB	C3C-C4C	6.11	1.51	1.42
29	N7	1002	PEB	C3C-C4C	6.11	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N9	1002	PEB	C3C-C4C	6.11	1.51	1.42
29	D7	1002	PEB	C3C-C4C	6.10	1.51	1.42
29	D9	1002	PEB	C3C-C4C	6.10	1.51	1.42
29	F7	1002	PEB	C3C-C4C	6.08	1.51	1.42
29	Q2	202	PEB	C3B-C2B	6.06	1.49	1.36
29	S2	202	PEB	C3B-C2B	6.04	1.49	1.36
29	M2	202	PEB	C3B-C2B	6.03	1.49	1.36
29	g7	202	PEB	C3C-C4C	6.03	1.51	1.42
29	g9	202	PEB	C3C-C4C	6.03	1.51	1.42
29	R7	202	PEB	C3C-C4C	6.02	1.51	1.42
29	R9	202	PEB	C3C-C4C	6.02	1.51	1.42
29	UR	202	PEB	C3B-C2B	6.01	1.49	1.36
29	SR	202	PEB	C3B-C2B	6.01	1.49	1.36
29	O2	202	PEB	C3B-C2B	6.00	1.49	1.36
29	QR	202	PEB	C3B-C2B	6.00	1.49	1.36
29	W2	202	PEB	C3B-C2B	6.00	1.49	1.36
29	m7	202	PEB	C3C-C4C	5.99	1.51	1.42
29	m9	202	PEB	C3C-C4C	5.99	1.51	1.42
29	NO	203	PEB	C3C-C4C	5.99	1.51	1.42
29	N3	203	PEB	C3C-C4C	5.99	1.51	1.42
29	i7	202	PEB	C3C-C4C	5.99	1.51	1.42
29	i9	202	PEB	C3C-C4C	5.99	1.51	1.42
29	Y7	202	PEB	C3C-C4C	5.99	1.51	1.42
29	Y9	202	PEB	C3C-C4C	5.99	1.51	1.42
29	T7	202	PEB	C3C-C4C	5.98	1.51	1.42
29	T9	202	PEB	C3C-C4C	5.98	1.51	1.42
29	U2	202	PEB	C3B-C2B	5.98	1.49	1.36
29	k7	202	PEB	C3C-C4C	5.98	1.51	1.42
29	k9	202	PEB	C3C-C4C	5.98	1.51	1.42
29	M3	203	PEB	C3C-C4C	5.97	1.51	1.42
29	MO	203	PEB	C3C-C4C	5.97	1.51	1.42
29	V7	202	PEB	C3C-C4C	5.97	1.51	1.42
29	V9	202	PEB	C3C-C4C	5.97	1.51	1.42
29	a7	202	PEB	C3C-C4C	5.97	1.51	1.42
29	a9	202	PEB	C3C-C4C	5.97	1.51	1.42
29	WR	202	PEB	C3B-C2B	5.95	1.49	1.36
29	c7	202	PEB	C3C-C4C	5.95	1.51	1.42
29	c9	202	PEB	C3C-C4C	5.95	1.51	1.42
29	P7	202	PEB	C3C-C4C	5.94	1.51	1.42
29	P9	202	PEB	C3C-C4C	5.94	1.51	1.42
29	F5	203	PEB	C3C-C4C	5.91	1.51	1.42
29	F8	203	PEB	C3C-C4C	5.91	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e7	202	PEB	C3C-C4C	5.91	1.51	1.42
29	e9	202	PEB	C3C-C4C	5.91	1.51	1.42
29	MN	401	PEB	C3C-C4C	5.90	1.51	1.42
29	L8	203	PEB	C3C-C4C	5.88	1.51	1.42
29	H5	203	PEB	C3C-C4C	5.87	1.51	1.42
29	B8	203	PEB	C3C-C4C	5.87	1.51	1.42
29	e2	402	PEB	C3B-C2B	5.87	1.49	1.36
29	H8	203	PEB	C3C-C4C	5.86	1.51	1.42
29	B5	203	PEB	C3C-C4C	5.86	1.51	1.42
29	L5	203	PEB	C3C-C4C	5.86	1.51	1.42
29	G5	203	PEB	C3C-C4C	5.86	1.51	1.42
29	XR	201	PEB	C3B-C2B	5.85	1.49	1.36
29	T2	201	PEB	C3B-C2B	5.85	1.49	1.36
31	VP	1001	CYC	C2A-C3A	5.84	1.49	1.36
29	m7	203	PEB	C3B-C2B	5.84	1.49	1.36
29	m9	203	PEB	C3B-C2B	5.84	1.49	1.36
29	MA	401	PEB	C3C-C4C	5.83	1.51	1.42
29	g7	203	PEB	C3B-C2B	5.83	1.49	1.36
29	g9	203	PEB	C3B-C2B	5.83	1.49	1.36
31	xP	1001	CYC	C2A-C3A	5.83	1.49	1.36
29	TR	201	PEB	C3B-C2B	5.83	1.49	1.36
30	MA	403	PUB	C2B-C1B	5.82	1.51	1.42
29	VR	201	PEB	C3B-C2B	5.82	1.49	1.36
29	c7	203	PEB	C3B-C2B	5.82	1.49	1.36
29	c9	203	PEB	C3B-C2B	5.82	1.49	1.36
29	G8	203	PEB	C3C-C4C	5.81	1.51	1.42
29	R7	203	PEB	C3B-C2B	5.81	1.49	1.36
29	R9	203	PEB	C3B-C2B	5.81	1.49	1.36
29	N2	201	PEB	C3B-C2B	5.81	1.49	1.36
29	NR	201	PEB	C3B-C2B	5.81	1.49	1.36
29	a7	203	PEB	C3B-C2B	5.81	1.49	1.36
29	a9	203	PEB	C3B-C2B	5.81	1.49	1.36
31	L9	1001	CYC	C3B-C2B	5.81	1.49	1.36
29	e7	203	PEB	C3B-C2B	5.81	1.49	1.36
29	e9	203	PEB	C3B-C2B	5.81	1.49	1.36
31	N7	1001	CYC	C3B-C2B	5.81	1.49	1.36
31	N9	1001	CYC	C3B-C2B	5.81	1.49	1.36
29	R2	201	PEB	C3B-C2B	5.80	1.49	1.36
29	RR	201	PEB	C3B-C2B	5.80	1.49	1.36
29	k7	203	PEB	C3B-C2B	5.80	1.49	1.36
29	k9	203	PEB	C3B-C2B	5.80	1.49	1.36
30	MN	403	PUB	C2B-C1B	5.79	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T7	203	PEB	C3B-C2B	5.79	1.49	1.36
29	T9	203	PEB	C3B-C2B	5.79	1.49	1.36
29	V2	201	PEB	C3B-C2B	5.79	1.49	1.36
31	J7	1001	CYC	C3B-C2B	5.79	1.49	1.36
29	Y7	203	PEB	C3B-C2B	5.79	1.49	1.36
29	i7	203	PEB	C3B-C2B	5.79	1.49	1.36
29	Y9	203	PEB	C3B-C2B	5.79	1.49	1.36
29	i9	203	PEB	C3B-C2B	5.79	1.49	1.36
31	DF	1001	CYC	C3B-C2B	5.79	1.49	1.36
31	DI	1001	CYC	C3B-C2B	5.79	1.49	1.36
29	V7	203	PEB	C3B-C2B	5.78	1.49	1.36
29	V9	203	PEB	C3B-C2B	5.78	1.49	1.36
31	L7	1001	CYC	C3B-C2B	5.77	1.49	1.36
29	P7	203	PEB	C3B-C2B	5.77	1.49	1.36
29	P9	203	PEB	C3B-C2B	5.77	1.49	1.36
31	FF	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	FI	1001	CYC	C3B-C2B	5.76	1.49	1.36
29	SR	201	PEB	C3B-C2B	5.76	1.49	1.36
31	NF	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	NI	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	F9	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	D7	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	D9	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	F7	1001	CYC	C3B-C2B	5.76	1.49	1.36
31	HF	1001	CYC	C3B-C2B	5.75	1.49	1.36
31	HI	1001	CYC	C3B-C2B	5.75	1.49	1.36
31	JF	1001	CYC	C3B-C2B	5.75	1.49	1.36
31	JI	1001	CYC	C3B-C2B	5.75	1.49	1.36
31	J9	1001	CYC	C3B-C2B	5.75	1.49	1.36
31	LF	1001	CYC	C3B-C2B	5.75	1.48	1.36
31	LI	1001	CYC	C3B-C2B	5.75	1.48	1.36
31	H7	1001	CYC	C3B-C2B	5.74	1.48	1.36
31	H9	1001	CYC	C3B-C2B	5.74	1.48	1.36
29	M4	203	PEB	C3B-C2B	5.74	1.48	1.36
29	AM	302	PEB	C3B-C2B	5.71	1.48	1.36
29	AB	302	PEB	C3B-C2B	5.71	1.48	1.36
29	J5	201	PEB	CHA-C1B	5.70	1.53	1.40
29	J8	201	PEB	CHA-C1B	5.70	1.53	1.40
29	I4	203	PEB	C3B-C2B	5.70	1.48	1.36
29	xJ	301	PEB	C3B-C2B	5.68	1.48	1.36
31	I1	1001	CYC	C3B-C2B	5.67	1.48	1.36
29	AC	202	PEB	C3B-C2B	5.67	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AE	202	PEB	C3B-C2B	5.67	1.48	1.36
30	MA	403	PUB	C2C-C3C	5.67	1.48	1.36
31	E1	1001	CYC	C3B-C2B	5.66	1.48	1.36
29	wL	302	PEB	C3B-C2B	5.66	1.48	1.36
29	wJ	302	PEB	C3B-C2B	5.66	1.48	1.36
30	MN	403	PUB	C2C-C3C	5.66	1.48	1.36
29	xL	301	PEB	C3B-C2B	5.66	1.48	1.36
29	S2	201	PEB	C3B-C2B	5.66	1.48	1.36
29	IC	202	PEB	C3B-C2B	5.66	1.48	1.36
29	IE	202	PEB	C3B-C2B	5.66	1.48	1.36
29	xL	302	PEB	C3B-C2B	5.65	1.48	1.36
29	xJ	302	PEB	C3B-C2B	5.64	1.48	1.36
29	KC	203	PEB	C3B-C2B	5.64	1.48	1.36
29	KE	203	PEB	C3B-C2B	5.64	1.48	1.36
29	U1	201	PEB	C3C-C4C	5.63	1.50	1.42
29	UK	201	PEB	C3C-C4C	5.63	1.50	1.42
29	g1	202	PEB	C3C-C4C	5.63	1.50	1.42
29	gK	202	PEB	C3C-C4C	5.63	1.50	1.42
29	BG	203	PEB	C3B-C2B	5.63	1.48	1.36
29	wJ	301	PEB	C3B-C2B	5.63	1.48	1.36
31	IK	1001	CYC	C3B-C2B	5.62	1.48	1.36
29	e1	202	PEB	C3C-C4C	5.62	1.50	1.42
29	eK	202	PEB	C3C-C4C	5.62	1.50	1.42
29	P1	202	PEB	C3C-C4C	5.62	1.50	1.42
29	PK	202	PEB	C3C-C4C	5.62	1.50	1.42
29	c1	202	PEB	C3C-C4C	5.62	1.50	1.42
29	cK	202	PEB	C3C-C4C	5.62	1.50	1.42
29	LG	203	PEB	C3B-C2B	5.62	1.48	1.36
31	CK	1001	CYC	C3B-C2B	5.62	1.48	1.36
29	R1	202	PEB	C3C-C4C	5.62	1.50	1.42
29	RK	202	PEB	C3C-C4C	5.62	1.50	1.42
29	a1	202	PEB	C3C-C4C	5.62	1.50	1.42
29	aK	202	PEB	C3C-C4C	5.62	1.50	1.42
29	GC	202	PEB	C3B-C2B	5.61	1.48	1.36
29	GE	202	PEB	C3B-C2B	5.61	1.48	1.36
29	Z1	201	PEB	C3C-C4C	5.61	1.50	1.42
29	ZK	201	PEB	C3C-C4C	5.61	1.50	1.42
29	EC	202	PEB	C3B-C2B	5.61	1.48	1.36
29	EE	202	PEB	C3B-C2B	5.61	1.48	1.36
29	CC	202	PEB	C3B-C2B	5.61	1.48	1.36
29	CE	202	PEB	C3B-C2B	5.61	1.48	1.36
29	j1	203	PEB	C3C-C4C	5.60	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	jK	203	PEB	C3C-C4C	5.60	1.50	1.42
29	EB	202	PEB	C3B-C2B	5.60	1.48	1.36
29	EM	202	PEB	C3B-C2B	5.60	1.48	1.36
29	A1	302	PEB	C3B-C2B	5.60	1.48	1.36
29	AK	302	PEB	C3B-C2B	5.60	1.48	1.36
29	OB	202	PEB	C3B-C2B	5.60	1.48	1.36
29	OM	202	PEB	C3B-C2B	5.60	1.48	1.36
29	V1	202	PEB	C3C-C4C	5.60	1.50	1.42
29	VK	202	PEB	C3C-C4C	5.60	1.50	1.42
29	DG	203	PEB	C3B-C2B	5.60	1.48	1.36
29	i1	202	PEB	C3C-C4C	5.60	1.50	1.42
29	iK	202	PEB	C3C-C4C	5.60	1.50	1.42
29	SB	202	PEB	C3B-C2B	5.60	1.48	1.36
29	SM	202	PEB	C3B-C2B	5.60	1.48	1.36
29	k1	202	PEB	C3C-C4C	5.60	1.50	1.42
29	kK	202	PEB	C3C-C4C	5.60	1.50	1.42
29	QB	204	PEB	C3B-C2B	5.59	1.48	1.36
29	QM	204	PEB	C3B-C2B	5.59	1.48	1.36
29	NR	203	PEB	C3B-C2B	5.59	1.48	1.36
29	hB	202	PEB	C3B-C2B	5.59	1.48	1.36
29	hM	202	PEB	C3B-C2B	5.59	1.48	1.36
29	CB	202	PEB	C3B-C2B	5.59	1.48	1.36
29	CM	202	PEB	C3B-C2B	5.59	1.48	1.36
29	N2	203	PEB	C3B-C2B	5.59	1.48	1.36
29	BQ	203	PEB	C3B-C2B	5.59	1.48	1.36
29	wL	301	PEB	C3B-C2B	5.59	1.48	1.36
31	D1	1003	CYC	C3B-C2B	5.59	1.48	1.36
31	M1	1001	CYC	C3B-C2B	5.59	1.48	1.36
31	MK	1001	CYC	C3B-C2B	5.59	1.48	1.36
29	LQ	202	PEB	C3B-C2B	5.59	1.48	1.36
31	wP	1001	CYC	C2A-C3A	5.59	1.48	1.36
29	AM	301	PEB	C3B-C2B	5.59	1.48	1.36
31	EK	1001	CYC	C3B-C2B	5.59	1.48	1.36
31	C1	1001	CYC	C3B-C2B	5.59	1.48	1.36
29	GB	202	PEB	C3B-C2B	5.59	1.48	1.36
29	IB	202	PEB	C3B-C2B	5.59	1.48	1.36
29	GM	202	PEB	C3B-C2B	5.59	1.48	1.36
29	IM	202	PEB	C3B-C2B	5.59	1.48	1.36
31	GK	1001	CYC	C3B-C2B	5.59	1.48	1.36
29	WB	202	PEB	C3B-C2B	5.58	1.48	1.36
29	WM	202	PEB	C3B-C2B	5.58	1.48	1.36
29	DD	202	PEB	C3C-C4C	5.58	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	MB	202	PEB	C3B-C2B	5.58	1.48	1.36
29	MM	202	PEB	C3B-C2B	5.58	1.48	1.36
31	UP	1001	CYC	C2A-C3A	5.58	1.48	1.36
29	fB	202	PEB	C3B-C2B	5.58	1.48	1.36
29	fM	202	PEB	C3B-C2B	5.58	1.48	1.36
31	K1	1001	CYC	C3B-C2B	5.58	1.48	1.36
31	KK	1001	CYC	C3B-C2B	5.58	1.48	1.36
29	JQ	203	PEB	C3B-C2B	5.58	1.48	1.36
29	JG	203	PEB	C3B-C2B	5.58	1.48	1.36
29	X2	202	PEB	C3B-C2B	5.57	1.48	1.36
29	FC	202	PEB	C3B-C2B	5.57	1.48	1.36
29	FE	202	PEB	C3B-C2B	5.57	1.48	1.36
29	XR	203	PEB	C3B-C2B	5.57	1.48	1.36
29	MR	202	PEB	C3B-C2B	5.57	1.48	1.36
29	P2	202	PEB	C3B-C2B	5.57	1.48	1.36
29	UB	202	PEB	C3B-C2B	5.57	1.48	1.36
29	MQ	401	PEB	C3B-C2B	5.57	1.48	1.36
29	aB	202	PEB	C3B-C2B	5.57	1.48	1.36
29	jB	202	PEB	C3B-C2B	5.57	1.48	1.36
29	aM	202	PEB	C3B-C2B	5.57	1.48	1.36
29	jM	202	PEB	C3B-C2B	5.57	1.48	1.36
29	JQ	203	PEB	C3C-C4C	5.57	1.50	1.42
31	uP	1001	CYC	C2A-C3A	5.57	1.48	1.36
31	FP	1001	CYC	C2A-C3A	5.57	1.48	1.36
29	AB	301	PEB	C3B-C2B	5.57	1.48	1.36
29	PR	202	PEB	C3B-C2B	5.57	1.48	1.36
29	LD	202	PEB	C3C-C4C	5.56	1.50	1.42
31	MP	1001	CYC	C2A-C3A	5.56	1.48	1.36
29	YB	203	PEB	C3B-C2B	5.56	1.48	1.36
29	YM	203	PEB	C3B-C2B	5.56	1.48	1.36
29	HG	203	PEB	C3B-C2B	5.56	1.48	1.36
29	BC	203	PEB	C3C-C4C	5.56	1.50	1.42
29	BE	203	PEB	C3C-C4C	5.56	1.50	1.42
29	HQ	203	PEB	C3B-C2B	5.56	1.48	1.36
31	sP	1001	CYC	C2A-C3A	5.56	1.48	1.36
29	dB	202	PEB	C3B-C2B	5.56	1.48	1.36
29	dM	202	PEB	C3B-C2B	5.56	1.48	1.36
31	XP	1001	CYC	C2A-C3A	5.56	1.48	1.36
29	JD	202	PEB	C3C-C4C	5.55	1.50	1.42
29	KB	202	PEB	C3B-C2B	5.55	1.48	1.36
29	KM	202	PEB	C3B-C2B	5.55	1.48	1.36
29	FG	203	PEB	C3B-C2B	5.55	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	nP	1001	CYC	C2A-C3A	5.55	1.48	1.36
31	QP	1001	CYC	C2A-C3A	5.55	1.48	1.36
31	BP	1001	CYC	C2A-C3A	5.55	1.48	1.36
31	1P	1001	CYC	C2A-C3A	5.55	1.48	1.36
29	J4	202	PEB	C3C-C4C	5.55	1.50	1.42
29	HC	202	PEB	C3B-C2B	5.55	1.48	1.36
29	HE	202	PEB	C3B-C2B	5.55	1.48	1.36
31	jP	1001	CYC	C2A-C3A	5.55	1.48	1.36
29	V2	203	PEB	C3B-C2B	5.54	1.48	1.36
29	VR	203	PEB	C3B-C2B	5.54	1.48	1.36
29	lB	202	PEB	C3B-C2B	5.54	1.48	1.36
29	lM	202	PEB	C3B-C2B	5.54	1.48	1.36
31	SP	1001	CYC	C2A-C3A	5.54	1.48	1.36
29	DQ	203	PEB	C3C-C4C	5.54	1.50	1.42
29	H4	202	PEB	C3C-C4C	5.54	1.50	1.42
29	OR	202	PEB	C3B-C2B	5.54	1.48	1.36
31	HP	1001	CYC	C2A-C3A	5.54	1.48	1.36
31	oP	1001	CYC	C2A-C3A	5.54	1.48	1.36
29	FQ	203	PEB	C3B-C2B	5.54	1.48	1.36
29	DQ	203	PEB	C3B-C2B	5.54	1.48	1.36
29	BQ	203	PEB	C3C-C4C	5.54	1.50	1.42
31	IP	1001	CYC	C2A-C3A	5.54	1.48	1.36
31	qP	1001	CYC	C2A-C3A	5.54	1.48	1.36
29	AB	303	PEB	C3B-C2B	5.54	1.48	1.36
31	kP	1001	CYC	C2A-C3A	5.54	1.48	1.36
31	DP	1001	CYC	C2A-C3A	5.54	1.48	1.36
29	DG	203	PEB	C3C-C4C	5.53	1.50	1.42
29	TR	203	PEB	C3B-C2B	5.53	1.48	1.36
30	yJ	303	PUB	C2C-C3C	5.53	1.48	1.36
31	fP	1001	CYC	C2A-C3A	5.53	1.48	1.36
29	LC	202	PEB	C3B-C2B	5.53	1.48	1.36
29	LE	202	PEB	C3B-C2B	5.53	1.48	1.36
31	OP	1001	CYC	C2A-C3A	5.53	1.48	1.36
29	l1	202	PEB	C3B-C2B	5.53	1.48	1.36
29	lK	202	PEB	C3B-C2B	5.53	1.48	1.36
29	LQ	202	PEB	C3C-C4C	5.52	1.50	1.42
29	D4	202	PEB	C3C-C4C	5.52	1.50	1.42
30	MG	402	PUB	CAB-C3B	5.52	1.60	1.52
29	W1	202	PEB	C3B-C2B	5.52	1.48	1.36
29	WK	202	PEB	C3B-C2B	5.52	1.48	1.36
29	BC	202	PEB	C3B-C2B	5.52	1.48	1.36
29	KC	201	PEB	C3B-C2B	5.52	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BE	202	PEB	C3B-C2B	5.52	1.48	1.36
29	KE	201	PEB	C3B-C2B	5.52	1.48	1.36
29	HC	203	PEB	C3C-C4C	5.52	1.50	1.42
29	HE	203	PEB	C3C-C4C	5.52	1.50	1.42
31	WP	1001	CYC	CHB-C1B	5.52	1.51	1.38
29	BG	203	PEB	C3C-C4C	5.52	1.50	1.42
29	R2	203	PEB	C3B-C2B	5.51	1.48	1.36
29	RR	203	PEB	C3B-C2B	5.51	1.48	1.36
31	hP	1001	CYC	C2A-C3A	5.51	1.48	1.36
29	AM	303	PEB	C3B-C2B	5.51	1.48	1.36
29	JG	203	PEB	C3C-C4C	5.51	1.50	1.42
29	E3	202	PEB	C3C-C4C	5.51	1.50	1.42
29	EO	202	PEB	C3C-C4C	5.51	1.50	1.42
31	yP	1001	CYC	CHB-C1B	5.51	1.51	1.38
29	A7	305	PEB	C3B-C2B	5.51	1.48	1.36
29	A9	305	PEB	C3B-C2B	5.51	1.48	1.36
29	AC	203	PEB	C3B-C2B	5.51	1.48	1.36
29	AE	203	PEB	C3B-C2B	5.51	1.48	1.36
29	LC	203	PEB	C3C-C4C	5.51	1.50	1.42
29	LE	203	PEB	C3C-C4C	5.51	1.50	1.42
30	MQ	405	PUB	C2B-C1B	5.51	1.50	1.42
29	FD	202	PEB	C3C-C4C	5.51	1.50	1.42
29	MA	401	PEB	C3B-C2B	5.50	1.48	1.36
29	T2	203	PEB	C3B-C2B	5.50	1.48	1.36
30	yL	303	PUB	C2C-C3C	5.50	1.48	1.36
29	B4	202	PEB	C3C-C4C	5.50	1.50	1.42
29	BD	202	PEB	C3C-C4C	5.50	1.50	1.42
29	FC	203	PEB	C3C-C4C	5.50	1.50	1.42
29	FE	203	PEB	C3C-C4C	5.50	1.50	1.42
29	HD	202	PEB	C3C-C4C	5.50	1.50	1.42
29	Q1	202	PEB	C3B-C2B	5.50	1.48	1.36
29	AF	301	PEB	C3B-C2B	5.50	1.48	1.36
29	AF	304	PEB	C3B-C2B	5.50	1.48	1.36
29	AI	301	PEB	C3B-C2B	5.50	1.48	1.36
29	AI	304	PEB	C3B-C2B	5.50	1.48	1.36
29	QK	202	PEB	C3B-C2B	5.50	1.48	1.36
29	sJ	203	PEB	C3B-C2B	5.50	1.48	1.36
29	sL	203	PEB	C3B-C2B	5.50	1.48	1.36
29	b1	202	PEB	C3B-C2B	5.50	1.48	1.36
29	MG	405	PEB	C3B-C2B	5.50	1.48	1.36
29	bK	202	PEB	C3B-C2B	5.50	1.48	1.36
31	YP	1000	CYC	CHB-C1B	5.50	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IJ	203	PEB	C3B-C2B	5.49	1.48	1.36
29	IL	203	PEB	C3B-C2B	5.49	1.48	1.36
29	HG	203	PEB	C3C-C4C	5.49	1.50	1.42
30	MQ	404	PUB	CAB-C3B	5.49	1.60	1.52
29	U1	203	PEB	C3B-C2B	5.49	1.48	1.36
29	UK	203	PEB	C3B-C2B	5.49	1.48	1.36
29	RB	201	PEB	C3C-C4C	5.49	1.50	1.42
29	RM	201	PEB	C3C-C4C	5.49	1.50	1.42
29	j1	202	PEB	C3B-C2B	5.49	1.48	1.36
29	jK	202	PEB	C3B-C2B	5.49	1.48	1.36
29	MQ	407	PEB	C3B-C2B	5.49	1.48	1.36
29	DC	202	PEB	C3C-C4C	5.48	1.50	1.42
29	DE	202	PEB	C3C-C4C	5.48	1.50	1.42
29	PJ	202	PEB	C3B-C2B	5.48	1.48	1.36
29	PL	202	PEB	C3B-C2B	5.48	1.48	1.36
31	1P	1002	CYC	CHB-C1B	5.48	1.51	1.38
29	JC	202	PEB	C3C-C4C	5.48	1.50	1.42
29	JE	202	PEB	C3C-C4C	5.48	1.50	1.42
29	f1	202	PEB	C3B-C2B	5.48	1.48	1.36
29	fK	202	PEB	C3B-C2B	5.48	1.48	1.36
29	F4	202	PEB	C3C-C4C	5.48	1.50	1.42
29	mB	201	PEB	C3C-C4C	5.48	1.50	1.42
29	mM	201	PEB	C3C-C4C	5.48	1.50	1.42
29	AJ	203	PEB	C3B-C2B	5.48	1.48	1.36
29	AL	203	PEB	C3B-C2B	5.48	1.48	1.36
29	rJ	202	PEB	C3B-C2B	5.48	1.48	1.36
29	rL	202	PEB	C3B-C2B	5.48	1.48	1.36
29	HQ	203	PEB	C3C-C4C	5.48	1.50	1.42
29	lJ	202	PEB	C3B-C2B	5.48	1.48	1.36
29	lL	202	PEB	C3B-C2B	5.48	1.48	1.36
29	S1	202	PEB	C3B-C2B	5.48	1.48	1.36
29	SK	202	PEB	C3B-C2B	5.48	1.48	1.36
29	h1	202	PEB	C3B-C2B	5.48	1.48	1.36
29	hK	202	PEB	C3B-C2B	5.48	1.48	1.36
29	LG	203	PEB	C3C-C4C	5.47	1.50	1.42
29	O1	202	PEB	C3B-C2B	5.47	1.48	1.36
29	OK	202	PEB	C3B-C2B	5.47	1.48	1.36
29	FB	201	PEB	C3C-C4C	5.47	1.50	1.42
29	FM	201	PEB	C3C-C4C	5.47	1.50	1.42
29	FJ	202	PEB	C3B-C2B	5.47	1.48	1.36
29	FL	202	PEB	C3B-C2B	5.47	1.48	1.36
29	d1	202	PEB	C3B-C2B	5.47	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	dK	202	PEB	C3B-C2B	5.47	1.48	1.36
29	HB	201	PEB	C3C-C4C	5.47	1.50	1.42
29	HM	201	PEB	C3C-C4C	5.47	1.50	1.42
29	MN	401	PEB	C3B-C2B	5.47	1.48	1.36
29	G3	202	PEB	C3C-C4C	5.47	1.50	1.42
29	GO	202	PEB	C3C-C4C	5.47	1.50	1.42
29	GD	203	PEB	C3C-C4C	5.47	1.50	1.42
29	TJ	202	PEB	C3B-C2B	5.47	1.48	1.36
29	TL	202	PEB	C3B-C2B	5.47	1.48	1.36
29	DB	201	PEB	C3C-C4C	5.47	1.50	1.42
29	DM	201	PEB	C3C-C4C	5.47	1.50	1.42
29	zL	501	PEB	C3B-C2B	5.47	1.48	1.36
29	VB	201	PEB	C3C-C4C	5.47	1.50	1.42
29	VM	201	PEB	C3C-C4C	5.47	1.50	1.42
29	FQ	203	PEB	C3C-C4C	5.47	1.50	1.42
29	hJ	202	PEB	C3B-C2B	5.47	1.48	1.36
29	hL	202	PEB	C3B-C2B	5.47	1.48	1.36
29	jJ	202	PEB	C3B-C2B	5.47	1.48	1.36
29	jL	202	PEB	C3B-C2B	5.47	1.48	1.36
29	L4	202	PEB	C3C-C4C	5.47	1.50	1.42
29	KD	203	PEB	C3C-C4C	5.47	1.50	1.42
29	iB	201	PEB	C3C-C4C	5.46	1.50	1.42
29	iM	201	PEB	C3C-C4C	5.46	1.50	1.42
29	Z1	203	PEB	C3B-C2B	5.46	1.48	1.36
29	BC	201	PEB	C3B-C2B	5.46	1.48	1.36
29	BE	201	PEB	C3B-C2B	5.46	1.48	1.36
29	ZK	203	PEB	C3B-C2B	5.46	1.48	1.36
31	yP	1001	CYC	C3B-C2B	5.46	1.48	1.36
29	MN	405	PEB	C3B-C2B	5.46	1.48	1.36
29	NO	202	PEB	C3B-C2B	5.46	1.48	1.36
29	JJ	202	PEB	C3B-C2B	5.46	1.48	1.36
29	JL	202	PEB	C3B-C2B	5.46	1.48	1.36
31	K9	1001	CYC	C3B-C2B	5.46	1.48	1.36
29	uJ	201	PEB	C3B-C2B	5.46	1.48	1.36
29	uL	201	PEB	C3B-C2B	5.46	1.48	1.36
29	BJ	202	PEB	C3B-C2B	5.46	1.48	1.36
29	BL	202	PEB	C3B-C2B	5.46	1.48	1.36
29	bJ	202	PEB	C3B-C2B	5.46	1.48	1.36
29	dJ	202	PEB	C3B-C2B	5.46	1.48	1.36
29	bL	202	PEB	C3B-C2B	5.46	1.48	1.36
29	dL	202	PEB	C3B-C2B	5.46	1.48	1.36
29	ZJ	202	PEB	C3B-C2B	5.46	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZL	202	PEB	C3B-C2B	5.46	1.48	1.36
29	HJ	201	PEB	C3B-C2B	5.46	1.48	1.36
29	HL	201	PEB	C3B-C2B	5.46	1.48	1.36
29	ZB	201	PEB	C3C-C4C	5.46	1.50	1.42
29	ZM	201	PEB	C3C-C4C	5.46	1.50	1.42
29	N3	202	PEB	C3B-C2B	5.46	1.48	1.36
29	I3	202	PEB	C3C-C4C	5.45	1.50	1.42
29	IO	202	PEB	C3C-C4C	5.45	1.50	1.42
29	fJ	202	PEB	C3B-C2B	5.45	1.48	1.36
29	fL	202	PEB	C3B-C2B	5.45	1.48	1.36
29	XJ	202	PEB	C3B-C2B	5.45	1.48	1.36
29	XL	202	PEB	C3B-C2B	5.45	1.48	1.36
29	pJ	202	PEB	C3B-C2B	5.45	1.48	1.36
29	pL	202	PEB	C3B-C2B	5.45	1.48	1.36
29	C3	202	PEB	C3C-C4C	5.45	1.50	1.42
29	CO	202	PEB	C3C-C4C	5.45	1.50	1.42
30	MG	403	PUB	C2B-C1B	5.45	1.50	1.42
31	E7	1001	CYC	C3B-C2B	5.45	1.48	1.36
31	E9	1001	CYC	C3B-C2B	5.45	1.48	1.36
29	MA	405	PEB	C3B-C2B	5.45	1.48	1.36
29	g1	203	PEB	C3C-C4C	5.45	1.50	1.42
29	cB	201	PEB	C3C-C4C	5.45	1.50	1.42
29	gK	203	PEB	C3C-C4C	5.45	1.50	1.42
29	cM	201	PEB	C3C-C4C	5.45	1.50	1.42
29	kB	201	PEB	C3C-C4C	5.44	1.50	1.42
29	kM	201	PEB	C3C-C4C	5.44	1.50	1.42
29	Y1	202	PEB	C3C-C4C	5.44	1.50	1.42
29	YK	202	PEB	C3C-C4C	5.44	1.50	1.42
29	TF	201	PEB	C3B-C2B	5.44	1.48	1.36
29	WJ	201	PEB	C3B-C2B	5.44	1.48	1.36
29	WL	201	PEB	C3B-C2B	5.44	1.48	1.36
29	S7	201	PEB	C3C-C4C	5.44	1.50	1.42
29	S9	201	PEB	C3C-C4C	5.44	1.50	1.42
31	I7	1001	CYC	C3B-C2B	5.44	1.48	1.36
31	I9	1001	CYC	C3B-C2B	5.44	1.48	1.36
29	E4	203	PEB	C3C-C4C	5.44	1.50	1.42
29	JB	201	PEB	C3C-C4C	5.44	1.50	1.42
29	JM	201	PEB	C3C-C4C	5.44	1.50	1.42
29	Q7	201	PEB	C3C-C4C	5.44	1.50	1.42
29	Q9	201	PEB	C3C-C4C	5.44	1.50	1.42
29	e1	203	PEB	C3C-C4C	5.44	1.50	1.42
29	eK	203	PEB	C3C-C4C	5.44	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	zJ	501	PEB	C3B-C2B	5.44	1.48	1.36
29	DC	201	PEB	C3B-C2B	5.44	1.48	1.36
29	DE	201	PEB	C3B-C2B	5.44	1.48	1.36
29	T1	202	PEB	C3C-C4C	5.44	1.50	1.42
29	TK	202	PEB	C3C-C4C	5.44	1.50	1.42
29	nJ	202	PEB	C3B-C2B	5.43	1.48	1.36
29	nL	202	PEB	C3B-C2B	5.43	1.48	1.36
29	eB	201	PEB	C3C-C4C	5.43	1.50	1.42
29	eM	201	PEB	C3C-C4C	5.43	1.50	1.42
29	HC	201	PEB	C3B-C2B	5.43	1.48	1.36
29	HE	201	PEB	C3B-C2B	5.43	1.48	1.36
29	RJ	202	PEB	C3B-C2B	5.43	1.48	1.36
29	RL	202	PEB	C3B-C2B	5.43	1.48	1.36
29	JC	201	PEB	C3B-C2B	5.43	1.48	1.36
29	JE	201	PEB	C3B-C2B	5.43	1.48	1.36
29	M3	202	PEB	C3B-C2B	5.43	1.48	1.36
29	MO	202	PEB	C3B-C2B	5.43	1.48	1.36
29	i1	203	PEB	C3C-C4C	5.43	1.50	1.42
29	iK	203	PEB	C3C-C4C	5.43	1.50	1.42
29	FC	201	PEB	C3B-C2B	5.43	1.48	1.36
29	FE	201	PEB	C3B-C2B	5.43	1.48	1.36
31	G9	1001	CYC	C3B-C2B	5.43	1.48	1.36
29	FG	203	PEB	C3C-C4C	5.43	1.50	1.42
31	K7	1001	CYC	C3B-C2B	5.43	1.48	1.36
29	G4	203	PEB	C3C-C4C	5.43	1.50	1.42
29	DA	203	PEB	C3C-C4C	5.43	1.50	1.42
29	DN	203	PEB	C3C-C4C	5.43	1.50	1.42
29	A3	202	PEB	C3C-C4C	5.43	1.50	1.42
29	AO	202	PEB	C3C-C4C	5.43	1.50	1.42
29	P1	203	PEB	C3C-C4C	5.42	1.50	1.42
29	TB	201	PEB	C3C-C4C	5.42	1.50	1.42
29	PK	203	PEB	C3C-C4C	5.42	1.50	1.42
29	TM	201	PEB	C3C-C4C	5.42	1.50	1.42
29	LC	201	PEB	C3B-C2B	5.42	1.48	1.36
29	LE	201	PEB	C3B-C2B	5.42	1.48	1.36
29	V1	203	PEB	C3C-C4C	5.42	1.50	1.42
29	VK	203	PEB	C3C-C4C	5.42	1.50	1.42
29	NJ	202	PEB	C3B-C2B	5.42	1.48	1.36
29	NL	202	PEB	C3B-C2B	5.42	1.48	1.36
29	NB	201	PEB	C3C-C4C	5.42	1.50	1.42
29	NM	201	PEB	C3C-C4C	5.42	1.50	1.42
29	BA	203	PEB	C3C-C4C	5.42	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BN	203	PEB	C3C-C4C	5.42	1.50	1.42
29	D3	202	PEB	C3B-C2B	5.42	1.48	1.36
29	b7	201	PEB	C3C-C4C	5.42	1.50	1.42
29	b9	201	PEB	C3C-C4C	5.42	1.50	1.42
29	XB	201	PEB	C3C-C4C	5.42	1.50	1.42
29	XM	201	PEB	C3C-C4C	5.42	1.50	1.42
29	gB	201	PEB	C3C-C4C	5.42	1.50	1.42
29	gM	201	PEB	C3C-C4C	5.42	1.50	1.42
31	G7	1001	CYC	C3B-C2B	5.42	1.48	1.36
29	C4	203	PEB	C3C-C4C	5.41	1.50	1.42
29	Z7	201	PEB	C3C-C4C	5.41	1.50	1.42
29	Z9	201	PEB	C3C-C4C	5.41	1.50	1.42
29	m1	202	PEB	C3C-C4C	5.41	1.50	1.42
29	mK	202	PEB	C3C-C4C	5.41	1.50	1.42
29	ID	203	PEB	C3C-C4C	5.41	1.50	1.42
29	K4	203	PEB	C3C-C4C	5.41	1.50	1.42
29	CD	203	PEB	C3C-C4C	5.41	1.50	1.42
29	MD	203	PEB	C3C-C4C	5.41	1.50	1.42
29	j7	201	PEB	C3C-C4C	5.41	1.50	1.42
29	j9	201	PEB	C3C-C4C	5.41	1.50	1.42
29	DA	202	PEB	C3C-C4C	5.41	1.50	1.42
29	DN	202	PEB	C3C-C4C	5.41	1.50	1.42
31	WP	1001	CYC	C3B-C2B	5.40	1.48	1.36
31	M7	1001	CYC	C3B-C2B	5.40	1.48	1.36
29	PB	201	PEB	C3C-C4C	5.40	1.50	1.42
29	PM	201	PEB	C3C-C4C	5.40	1.50	1.42
29	l7	201	PEB	C3C-C4C	5.40	1.50	1.42
29	l9	201	PEB	C3C-C4C	5.40	1.50	1.42
29	WJ	202	PEB	C3C-C4C	5.40	1.50	1.42
29	WL	202	PEB	C3C-C4C	5.40	1.50	1.42
29	A7	304	PEB	C3B-C2B	5.40	1.48	1.36
31	C7	1001	CYC	C3B-C2B	5.40	1.48	1.36
31	C9	1001	CYC	C3B-C2B	5.40	1.48	1.36
29	k1	203	PEB	C3C-C4C	5.40	1.50	1.42
29	kK	203	PEB	C3C-C4C	5.40	1.50	1.42
29	W7	201	PEB	C3C-C4C	5.40	1.50	1.42
29	W9	201	PEB	C3C-C4C	5.40	1.50	1.42
29	JA	203	PEB	C3C-C4C	5.40	1.50	1.42
29	JN	203	PEB	C3C-C4C	5.40	1.50	1.42
31	M9	1001	CYC	C3B-C2B	5.40	1.48	1.36
29	ED	202	PEB	C3C-C4C	5.40	1.50	1.42
29	LA	203	PEB	C3C-C4C	5.39	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LN	203	PEB	C3C-C4C	5.39	1.50	1.42
29	LC	203	PEB	C3B-C2B	5.39	1.48	1.36
29	LE	203	PEB	C3B-C2B	5.39	1.48	1.36
29	f7	201	PEB	C3C-C4C	5.39	1.50	1.42
29	h7	201	PEB	C3C-C4C	5.39	1.50	1.42
29	f9	201	PEB	C3C-C4C	5.39	1.50	1.42
29	h9	201	PEB	C3C-C4C	5.39	1.50	1.42
29	K3	202	PEB	C3C-C4C	5.39	1.50	1.42
29	KO	202	PEB	C3C-C4C	5.39	1.50	1.42
29	R1	203	PEB	C3C-C4C	5.39	1.50	1.42
29	FA	202	PEB	C3C-C4C	5.39	1.50	1.42
29	RK	203	PEB	C3C-C4C	5.39	1.50	1.42
29	FN	202	PEB	C3C-C4C	5.39	1.50	1.42
29	O7	201	PEB	C3C-C4C	5.39	1.50	1.42
29	d7	201	PEB	C3C-C4C	5.39	1.50	1.42
29	O9	201	PEB	C3C-C4C	5.39	1.50	1.42
29	d9	201	PEB	C3C-C4C	5.39	1.50	1.42
29	DO	202	PEB	C3B-C2B	5.39	1.48	1.36
29	a1	203	PEB	C3C-C4C	5.39	1.50	1.42
29	LB	201	PEB	C3C-C4C	5.39	1.50	1.42
29	aK	203	PEB	C3C-C4C	5.39	1.50	1.42
29	LM	201	PEB	C3C-C4C	5.39	1.50	1.42
29	KA	202	PEB	C3B-C2B	5.39	1.48	1.36
29	KN	202	PEB	C3B-C2B	5.39	1.48	1.36
29	FC	203	PEB	C3B-C2B	5.39	1.48	1.36
29	FE	203	PEB	C3B-C2B	5.39	1.48	1.36
29	c1	203	PEB	C3C-C4C	5.38	1.50	1.42
29	oJ	201	PEB	C3C-C4C	5.38	1.50	1.42
29	cK	203	PEB	C3C-C4C	5.38	1.50	1.42
29	oL	201	PEB	C3C-C4C	5.38	1.50	1.42
30	MA	402	PUB	C2C-C3C	5.38	1.48	1.36
29	cJ	201	PEB	C3C-C4C	5.38	1.50	1.42
29	cL	201	PEB	C3C-C4C	5.38	1.50	1.42
29	OJ	201	PEB	C3C-C4C	5.38	1.50	1.42
29	kJ	201	PEB	C3C-C4C	5.38	1.50	1.42
29	OL	201	PEB	C3C-C4C	5.38	1.50	1.42
29	kL	201	PEB	C3C-C4C	5.38	1.50	1.42
29	IA	202	PEB	C3B-C2B	5.37	1.48	1.36
29	IN	202	PEB	C3B-C2B	5.37	1.48	1.36
29	FA	203	PEB	C3C-C4C	5.37	1.50	1.42
29	JA	202	PEB	C3C-C4C	5.37	1.50	1.42
29	CJ	201	PEB	C3C-C4C	5.37	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	CL	201	PEB	C3C-C4C	5.37	1.50	1.42
29	FN	203	PEB	C3C-C4C	5.37	1.50	1.42
29	JN	202	PEB	C3C-C4C	5.37	1.50	1.42
29	mJ	201	PEB	C3C-C4C	5.37	1.50	1.42
29	mL	201	PEB	C3C-C4C	5.37	1.50	1.42
29	uJ	202	PEB	C3C-C4C	5.37	1.50	1.42
29	uL	202	PEB	C3C-C4C	5.37	1.50	1.42
29	HC	203	PEB	C3B-C2B	5.36	1.48	1.36
29	HE	203	PEB	C3B-C2B	5.36	1.48	1.36
29	JC	202	PEB	C3B-C2B	5.36	1.48	1.36
29	JE	202	PEB	C3B-C2B	5.36	1.48	1.36
29	eJ	202	PEB	C3B-C2B	5.36	1.48	1.36
29	eL	202	PEB	C3B-C2B	5.36	1.48	1.36
29	A1	303	PEB	C3B-C2B	5.36	1.48	1.36
29	AK	303	PEB	C3B-C2B	5.36	1.48	1.36
29	HA	203	PEB	C3C-C4C	5.36	1.50	1.42
29	HN	203	PEB	C3C-C4C	5.36	1.50	1.42
30	MN	402	PUB	C2C-C3C	5.36	1.48	1.36
29	GA	202	PEB	C3B-C2B	5.36	1.48	1.36
29	GN	202	PEB	C3B-C2B	5.36	1.48	1.36
29	aJ	201	PEB	C3C-C4C	5.36	1.50	1.42
29	qJ	201	PEB	C3C-C4C	5.36	1.50	1.42
29	aL	201	PEB	C3C-C4C	5.36	1.50	1.42
29	qL	201	PEB	C3C-C4C	5.36	1.50	1.42
29	A9	304	PEB	C3B-C2B	5.36	1.48	1.36
29	YF	203	PEB	C3B-C2B	5.36	1.48	1.36
29	YI	203	PEB	C3B-C2B	5.36	1.48	1.36
29	BC	203	PEB	C3B-C2B	5.36	1.48	1.36
29	BE	203	PEB	C3B-C2B	5.36	1.48	1.36
29	iJ	201	PEB	C3C-C4C	5.36	1.50	1.42
29	iL	201	PEB	C3C-C4C	5.36	1.50	1.42
29	N7	1002	PEB	C3B-C2B	5.36	1.48	1.36
29	N9	1002	PEB	C3B-C2B	5.36	1.48	1.36
29	BA	202	PEB	C3C-C4C	5.35	1.50	1.42
29	BN	202	PEB	C3C-C4C	5.35	1.50	1.42
29	cJ	202	PEB	C3B-C2B	5.35	1.48	1.36
29	cL	202	PEB	C3B-C2B	5.35	1.48	1.36
29	HA	202	PEB	C3C-C4C	5.35	1.50	1.42
29	HN	202	PEB	C3C-C4C	5.35	1.50	1.42
29	AA	202	PEB	C3B-C2B	5.35	1.48	1.36
29	cF	202	PEB	C3B-C2B	5.35	1.48	1.36
29	cI	202	PEB	C3B-C2B	5.35	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AN	202	PEB	C3B-C2B	5.35	1.48	1.36
29	U7	201	PEB	C3C-C4C	5.35	1.50	1.42
29	U9	201	PEB	C3C-C4C	5.35	1.50	1.42
29	gJ	201	PEB	C3C-C4C	5.35	1.50	1.42
29	gL	201	PEB	C3C-C4C	5.35	1.50	1.42
29	TF	202	PEB	C3B-C2B	5.35	1.48	1.36
29	TI	202	PEB	C3B-C2B	5.35	1.48	1.36
29	oJ	202	PEB	C3B-C2B	5.35	1.48	1.36
29	oL	202	PEB	C3B-C2B	5.35	1.48	1.36
30	A1	305	PUB	C2C-C3C	5.35	1.48	1.36
30	AK	305	PUB	C2C-C3C	5.35	1.48	1.36
29	QJ	201	PEB	C3C-C4C	5.34	1.50	1.42
29	QL	201	PEB	C3C-C4C	5.34	1.50	1.42
31	KF	1001	CYC	C3B-C2B	5.34	1.48	1.36
29	DC	202	PEB	C3B-C2B	5.34	1.48	1.36
29	DE	202	PEB	C3B-C2B	5.34	1.48	1.36
29	GJ	201	PEB	C3C-C4C	5.34	1.50	1.42
29	GL	201	PEB	C3C-C4C	5.34	1.50	1.42
29	W2	201	PEB	C3B-C2B	5.34	1.48	1.36
29	M3	201	PEB	C3B-C2B	5.34	1.48	1.36
29	eF	203	PEB	C3B-C2B	5.34	1.48	1.36
29	eI	203	PEB	C3B-C2B	5.34	1.48	1.36
29	MO	201	PEB	C3B-C2B	5.34	1.48	1.36
29	kJ	202	PEB	C3B-C2B	5.34	1.48	1.36
29	kL	202	PEB	C3B-C2B	5.34	1.48	1.36
29	UJ	201	PEB	C3C-C4C	5.34	1.50	1.42
29	UL	201	PEB	C3C-C4C	5.34	1.50	1.42
31	KI	1001	CYC	C3B-C2B	5.34	1.48	1.36
29	QJ	202	PEB	C3B-C2B	5.34	1.48	1.36
29	QL	202	PEB	C3B-C2B	5.34	1.48	1.36
29	F7	1002	PEB	C3B-C2B	5.34	1.48	1.36
29	J7	1002	PEB	C3B-C2B	5.34	1.48	1.36
29	PF	203	PEB	C3B-C2B	5.33	1.48	1.36
29	PI	203	PEB	C3B-C2B	5.33	1.48	1.36
29	LA	202	PEB	C3C-C4C	5.33	1.50	1.42
29	LN	202	PEB	C3C-C4C	5.33	1.50	1.42
29	mJ	202	PEB	C3B-C2B	5.33	1.48	1.36
29	mL	202	PEB	C3B-C2B	5.33	1.48	1.36
29	kF	203	PEB	C3B-C2B	5.33	1.48	1.36
29	kI	203	PEB	C3B-C2B	5.33	1.48	1.36
29	WJ	203	PEB	C3B-C2B	5.33	1.48	1.36
29	WL	203	PEB	C3B-C2B	5.33	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SJ	201	PEB	C3C-C4C	5.33	1.50	1.42
29	SL	201	PEB	C3C-C4C	5.33	1.50	1.42
29	H7	1002	PEB	C3B-C2B	5.33	1.48	1.36
29	H9	1002	PEB	C3B-C2B	5.33	1.48	1.36
29	YJ	202	PEB	C3B-C2B	5.33	1.48	1.36
29	YL	202	PEB	C3B-C2B	5.33	1.48	1.36
29	iJ	202	PEB	C3B-C2B	5.33	1.48	1.36
29	qJ	202	PEB	C3B-C2B	5.33	1.48	1.36
29	iL	202	PEB	C3B-C2B	5.33	1.48	1.36
29	qL	202	PEB	C3B-C2B	5.33	1.48	1.36
29	YJ	201	PEB	C3C-C4C	5.33	1.50	1.42
29	YL	201	PEB	C3C-C4C	5.33	1.50	1.42
29	L7	1002	PEB	C3B-C2B	5.33	1.48	1.36
29	RF	202	PEB	C3B-C2B	5.33	1.48	1.36
29	RI	202	PEB	C3B-C2B	5.33	1.48	1.36
29	AJ	201	PEB	C3C-C4C	5.33	1.50	1.42
29	AL	201	PEB	C3C-C4C	5.33	1.50	1.42
31	GF	1001	CYC	C3B-C2B	5.33	1.48	1.36
31	GI	1001	CYC	C3B-C2B	5.33	1.48	1.36
31	1P	1002	CYC	C2A-C3A	5.33	1.48	1.36
29	MN	404	PEB	C3C-C4C	5.33	1.50	1.42
29	MA	404	PEB	C3C-C4C	5.33	1.50	1.42
29	uJ	203	PEB	C3B-C2B	5.33	1.48	1.36
29	uL	203	PEB	C3B-C2B	5.33	1.48	1.36
29	F9	1002	PEB	C3B-C2B	5.33	1.48	1.36
29	DJ	201	PEB	C3B-C2B	5.33	1.48	1.36
29	DL	201	PEB	C3B-C2B	5.33	1.48	1.36
29	VF	203	PEB	C3B-C2B	5.33	1.48	1.36
29	VI	203	PEB	C3B-C2B	5.33	1.48	1.36
29	CA	202	PEB	C3B-C2B	5.33	1.48	1.36
29	CN	202	PEB	C3B-C2B	5.33	1.48	1.36
31	MF	1001	CYC	C3B-C2B	5.32	1.48	1.36
31	MI	1001	CYC	C3B-C2B	5.32	1.48	1.36
29	EA	202	PEB	C3B-C2B	5.32	1.48	1.36
29	EN	202	PEB	C3B-C2B	5.32	1.48	1.36
29	KJ	201	PEB	C3C-C4C	5.32	1.50	1.42
29	KL	201	PEB	C3C-C4C	5.32	1.50	1.42
29	aF	203	PEB	C3B-C2B	5.32	1.48	1.36
29	aI	203	PEB	C3B-C2B	5.32	1.48	1.36
29	gJ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	gL	202	PEB	C3B-C2B	5.32	1.48	1.36
29	U2	201	PEB	C3B-C2B	5.32	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	UR	201	PEB	C3B-C2B	5.32	1.48	1.36
31	EF	1001	CYC	C3B-C2B	5.32	1.48	1.36
31	EI	1001	CYC	C3B-C2B	5.32	1.48	1.36
31	CP	1001	CYC	C2A-C3A	5.32	1.48	1.36
31	YP	1000	CYC	C2A-C3A	5.32	1.48	1.36
29	CG	202	PEB	C3B-C2B	5.32	1.48	1.36
29	CQ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	WR	201	PEB	C3B-C2B	5.32	1.48	1.36
31	IF	1001	CYC	C3B-C2B	5.32	1.48	1.36
31	II	1001	CYC	C3B-C2B	5.32	1.48	1.36
29	H4	201	PEB	C3B-C2B	5.32	1.48	1.36
29	EJ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	EL	202	PEB	C3B-C2B	5.32	1.48	1.36
31	F7	1001	CYC	C2A-C3A	5.32	1.48	1.36
29	M2	201	PEB	C3B-C2B	5.32	1.48	1.36
29	IJ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	sJ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	IL	202	PEB	C3B-C2B	5.32	1.48	1.36
29	sL	202	PEB	C3B-C2B	5.32	1.48	1.36
29	MR	201	PEB	C3B-C2B	5.32	1.48	1.36
29	eJ	201	PEB	C3C-C4C	5.32	1.50	1.42
29	eL	201	PEB	C3C-C4C	5.32	1.50	1.42
29	AJ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	AL	202	PEB	C3B-C2B	5.32	1.48	1.36
29	OJ	202	PEB	C3B-C2B	5.32	1.48	1.36
29	OL	202	PEB	C3B-C2B	5.32	1.48	1.36
29	L3	202	PEB	C3B-C2B	5.32	1.48	1.36
29	LO	202	PEB	C3B-C2B	5.32	1.48	1.36
29	CJ	202	PEB	C3B-C2B	5.31	1.48	1.36
29	CL	202	PEB	C3B-C2B	5.31	1.48	1.36
29	MJ	201	PEB	C3C-C4C	5.31	1.50	1.42
29	ML	201	PEB	C3C-C4C	5.31	1.50	1.42
29	KJ	202	PEB	C3B-C2B	5.31	1.48	1.36
29	KL	202	PEB	C3B-C2B	5.31	1.48	1.36
31	H7	1001	CYC	C2A-C3A	5.31	1.48	1.36
31	H9	1001	CYC	C2A-C3A	5.31	1.48	1.36
29	J9	1002	PEB	C3B-C2B	5.31	1.48	1.36
29	KG	202	PEB	C3B-C2B	5.31	1.48	1.36
29	KQ	202	PEB	C3B-C2B	5.31	1.48	1.36
29	D3	203	PEB	C3B-C2B	5.31	1.48	1.36
29	IG	202	PEB	C3B-C2B	5.31	1.48	1.36
29	DO	203	PEB	C3B-C2B	5.31	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IQ	202	PEB	C3B-C2B	5.31	1.48	1.36
31	L7	1001	CYC	C2A-C3A	5.31	1.48	1.36
29	AG	202	PEB	C3B-C2B	5.31	1.48	1.36
29	tJ	201	PEB	C3B-C2B	5.31	1.48	1.36
29	tL	201	PEB	C3B-C2B	5.31	1.48	1.36
29	AQ	202	PEB	C3B-C2B	5.31	1.48	1.36
29	QR	201	PEB	C3B-C2B	5.31	1.48	1.36
29	iF	203	PEB	C3B-C2B	5.31	1.48	1.36
29	iI	203	PEB	C3B-C2B	5.31	1.48	1.36
29	IJ	201	PEB	C3C-C4C	5.31	1.50	1.42
29	IL	201	PEB	C3C-C4C	5.31	1.50	1.42
29	D7	1002	PEB	C3B-C2B	5.31	1.48	1.36
29	D9	1002	PEB	C3B-C2B	5.31	1.48	1.36
29	UJ	202	PEB	C3B-C2B	5.31	1.48	1.36
29	UL	202	PEB	C3B-C2B	5.31	1.48	1.36
29	c1	203	PEB	C3B-C2B	5.31	1.48	1.36
29	cK	203	PEB	C3B-C2B	5.31	1.48	1.36
29	MG	404	PEB	C3C-C4C	5.31	1.50	1.42
29	N3	201	PEB	C3B-C2B	5.31	1.48	1.36
29	sJ	201	PEB	C3C-C4C	5.31	1.50	1.42
29	sL	201	PEB	C3C-C4C	5.31	1.50	1.42
29	mF	203	PEB	C3B-C2B	5.31	1.48	1.36
29	mI	203	PEB	C3B-C2B	5.31	1.48	1.36
29	hJ	201	PEB	C3B-C2B	5.31	1.48	1.36
29	hL	201	PEB	C3B-C2B	5.31	1.48	1.36
31	RP	1001	CYC	C2A-C3A	5.31	1.48	1.36
29	GJ	202	PEB	C3B-C2B	5.30	1.48	1.36
29	GL	202	PEB	C3B-C2B	5.30	1.48	1.36
29	FD	201	PEB	C3B-C2B	5.30	1.48	1.36
29	MQ	406	PEB	C3C-C4C	5.30	1.50	1.42
31	F9	1001	CYC	C2A-C3A	5.30	1.48	1.36
29	SJ	202	PEB	C3B-C2B	5.30	1.48	1.36
29	SL	202	PEB	C3B-C2B	5.30	1.48	1.36
29	B3	203	PEB	C3B-C2B	5.30	1.48	1.36
29	BO	203	PEB	C3B-C2B	5.30	1.48	1.36
29	gF	203	PEB	C3B-C2B	5.30	1.48	1.36
29	gI	203	PEB	C3B-C2B	5.30	1.48	1.36
29	L9	1002	PEB	C3B-C2B	5.30	1.48	1.36
29	R1	203	PEB	C3B-C2B	5.30	1.48	1.36
29	RK	203	PEB	C3B-C2B	5.30	1.48	1.36
29	Y1	202	PEB	C3B-C2B	5.30	1.48	1.36
29	aJ	202	PEB	C3B-C2B	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YK	202	PEB	C3B-C2B	5.30	1.48	1.36
29	aL	202	PEB	C3B-C2B	5.30	1.48	1.36
29	MA	404	PEB	C3B-C2B	5.30	1.48	1.36
29	O2	201	PEB	C3B-C2B	5.30	1.48	1.36
29	OR	201	PEB	C3B-C2B	5.30	1.48	1.36
31	vP	1001	CYC	C2A-C3A	5.30	1.48	1.36
29	A7	301	PEB	C3B-C2B	5.29	1.48	1.36
29	A9	301	PEB	C3B-C2B	5.29	1.48	1.36
31	iP	1001	CYC	C2A-C3A	5.29	1.48	1.36
31	iP	1001	CYC	C3B-C2B	5.29	1.48	1.36
31	PP	1001	CYC	C2A-C3A	5.29	1.48	1.36
29	I8	203	PEB	C3C-C4C	5.29	1.50	1.42
29	PJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	PL	201	PEB	C3B-C2B	5.29	1.48	1.36
31	KP	1001	CYC	C2A-C3A	5.29	1.48	1.36
29	EG	202	PEB	C3B-C2B	5.29	1.48	1.36
29	NO	201	PEB	C3B-C2B	5.29	1.48	1.36
29	EQ	202	PEB	C3B-C2B	5.29	1.48	1.36
29	ZJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	vJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	ZL	201	PEB	C3B-C2B	5.29	1.48	1.36
29	vL	201	PEB	C3B-C2B	5.29	1.48	1.36
31	D7	1001	CYC	C2A-C3A	5.29	1.48	1.36
31	D9	1001	CYC	C2A-C3A	5.29	1.48	1.36
29	EJ	201	PEB	C3C-C4C	5.29	1.50	1.42
29	EL	201	PEB	C3C-C4C	5.29	1.50	1.42
29	NJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	NL	201	PEB	C3B-C2B	5.29	1.48	1.36
29	T1	202	PEB	C3B-C2B	5.29	1.48	1.36
29	VJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	TK	202	PEB	C3B-C2B	5.29	1.48	1.36
29	VL	201	PEB	C3B-C2B	5.29	1.48	1.36
30	BB	302	PUB	C2C-C3C	5.29	1.48	1.36
30	BM	302	PUB	C2C-C3C	5.29	1.48	1.36
31	CF	1001	CYC	C3B-C2B	5.29	1.48	1.36
31	CI	1001	CYC	C3B-C2B	5.29	1.48	1.36
31	eP	1001	CYC	C2A-C3A	5.29	1.48	1.36
30	QB	201	PUB	C2B-C1B	5.29	1.50	1.42
30	QM	201	PUB	C2B-C1B	5.29	1.50	1.42
29	B4	201	PEB	C3B-C2B	5.29	1.48	1.36
29	JJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	JL	201	PEB	C3B-C2B	5.29	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fJ	201	PEB	C3B-C2B	5.29	1.48	1.36
29	fL	201	PEB	C3B-C2B	5.29	1.48	1.36
31	WP	1001	CYC	C2A-C3A	5.28	1.48	1.36
31	NP	1001	CYC	C2A-C3A	5.28	1.48	1.36
31	J9	1001	CYC	C2A-C3A	5.28	1.48	1.36
31	L9	1001	CYC	C2A-C3A	5.28	1.48	1.36
29	D4	201	PEB	C3B-C2B	5.28	1.48	1.36
31	N7	1001	CYC	C2A-C3A	5.28	1.48	1.36
31	N9	1001	CYC	C2A-C3A	5.28	1.48	1.36
29	i1	203	PEB	C3B-C2B	5.28	1.48	1.36
29	iK	203	PEB	C3B-C2B	5.28	1.48	1.36
31	J7	1001	CYC	C2A-C3A	5.28	1.48	1.36
29	J3	203	PEB	C3B-C2B	5.28	1.48	1.36
29	JO	203	PEB	C3B-C2B	5.28	1.48	1.36
31	cP	1001	CYC	C2A-C3A	5.28	1.48	1.36
29	MN	404	PEB	C3B-C2B	5.28	1.47	1.36
29	MJ	202	PEB	C3B-C2B	5.28	1.47	1.36
29	ML	202	PEB	C3B-C2B	5.28	1.47	1.36
29	bJ	201	PEB	C3B-C2B	5.28	1.47	1.36
29	bL	201	PEB	C3B-C2B	5.28	1.47	1.36
29	A1	301	PEB	C3B-C2B	5.28	1.47	1.36
29	AK	301	PEB	C3B-C2B	5.28	1.47	1.36
31	rP	1001	CYC	C2A-C3A	5.28	1.47	1.36
29	GG	202	PEB	C3B-C2B	5.28	1.47	1.36
29	GQ	202	PEB	C3B-C2B	5.28	1.47	1.36
29	C8	203	PEB	C3C-C4C	5.28	1.50	1.42
29	nJ	201	PEB	C3B-C2B	5.27	1.47	1.36
29	nL	201	PEB	C3B-C2B	5.27	1.47	1.36
29	V1	203	PEB	C3B-C2B	5.27	1.47	1.36
29	Q2	201	PEB	C3B-C2B	5.27	1.47	1.36
29	F3	203	PEB	C3B-C2B	5.27	1.47	1.36
29	VK	203	PEB	C3B-C2B	5.27	1.47	1.36
29	FO	203	PEB	C3B-C2B	5.27	1.47	1.36
30	A1	304	PUB	C2C-C3C	5.27	1.47	1.36
30	AK	304	PUB	C2C-C3C	5.27	1.47	1.36
29	MG	401	PEB	C3B-C2B	5.27	1.47	1.36
29	RJ	201	PEB	C3B-C2B	5.27	1.47	1.36
29	RL	201	PEB	C3B-C2B	5.27	1.47	1.36
29	JA	201	PEB	C3B-C2B	5.27	1.47	1.36
29	JN	201	PEB	C3B-C2B	5.27	1.47	1.36
29	H3	203	PEB	C3B-C2B	5.27	1.47	1.36
29	HA	201	PEB	C3B-C2B	5.27	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HN	201	PEB	C3B-C2B	5.27	1.47	1.36
29	HO	203	PEB	C3B-C2B	5.27	1.47	1.36
29	k1	203	PEB	C3B-C2B	5.27	1.47	1.36
29	kK	203	PEB	C3B-C2B	5.27	1.47	1.36
31	xP	1001	CYC	C1A-C2A	5.27	1.54	1.45
30	yJ	302	PUB	C2C-C3C	5.27	1.47	1.36
30	yL	302	PUB	C2C-C3C	5.27	1.47	1.36
29	BJ	201	PEB	C3B-C2B	5.27	1.47	1.36
29	BL	201	PEB	C3B-C2B	5.27	1.47	1.36
29	DD	201	PEB	C3B-C2B	5.27	1.47	1.36
29	LJ	201	PEB	C3B-C2B	5.26	1.47	1.36
29	LL	201	PEB	C3B-C2B	5.26	1.47	1.36
29	TJ	201	PEB	C3B-C2B	5.26	1.47	1.36
29	TL	201	PEB	C3B-C2B	5.26	1.47	1.36
31	mP	1001	CYC	C2A-C3A	5.26	1.47	1.36
29	m1	202	PEB	C3B-C2B	5.26	1.47	1.36
29	mK	202	PEB	C3B-C2B	5.26	1.47	1.36
31	TP	1001	CYC	C2A-C3A	5.26	1.47	1.36
29	BA	201	PEB	C3B-C2B	5.26	1.47	1.36
29	BN	201	PEB	C3B-C2B	5.26	1.47	1.36
29	dF	201	PEB	C3C-C4C	5.26	1.50	1.42
29	dI	201	PEB	C3C-C4C	5.26	1.50	1.42
29	lJ	201	PEB	C3B-C2B	5.26	1.47	1.36
29	lL	201	PEB	C3B-C2B	5.26	1.47	1.36
31	KP	1001	CYC	C3B-C2B	5.26	1.47	1.36
30	yJ	302	PUB	C2B-C1B	5.26	1.50	1.42
30	yL	302	PUB	C2B-C1B	5.26	1.50	1.42
29	P1	203	PEB	C3B-C2B	5.26	1.47	1.36
29	PK	203	PEB	C3B-C2B	5.26	1.47	1.36
31	EP	1001	CYC	C2A-C3A	5.26	1.47	1.36
29	e1	203	PEB	C3B-C2B	5.26	1.47	1.36
29	eK	203	PEB	C3B-C2B	5.26	1.47	1.36
29	L4	201	PEB	C3B-C2B	5.26	1.47	1.36
29	MQ	403	PEB	C3B-C2B	5.26	1.47	1.36
29	HD	201	PEB	C3B-C2B	5.26	1.47	1.36
31	1P	1002	CYC	C3B-C2B	5.26	1.47	1.36
29	BD	201	PEB	C3B-C2B	5.26	1.47	1.36
29	XJ	201	PEB	C3B-C2B	5.26	1.47	1.36
29	jJ	201	PEB	C3B-C2B	5.26	1.47	1.36
29	XL	201	PEB	C3B-C2B	5.26	1.47	1.36
29	jL	201	PEB	C3B-C2B	5.26	1.47	1.36
29	LD	201	PEB	C3B-C2B	5.25	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	pP	1001	CYC	C2A-C3A	5.25	1.47	1.36
30	wL	305	PUB	C2B-C1B	5.25	1.50	1.42
31	tP	1001	CYC	C2A-C3A	5.25	1.47	1.36
29	AF	305	PEB	C3B-C2B	5.25	1.47	1.36
29	AI	305	PEB	C3B-C2B	5.25	1.47	1.36
29	L3	202	PEB	C3C-C4C	5.25	1.50	1.42
29	LO	202	PEB	C3C-C4C	5.25	1.50	1.42
31	NP	1001	CYC	C3B-C2B	5.25	1.47	1.36
31	gP	1001	CYC	C2A-C3A	5.25	1.47	1.36
29	mF	202	PEB	C3C-C4C	5.25	1.50	1.42
29	mI	202	PEB	C3C-C4C	5.25	1.50	1.42
29	A5	203	PEB	C3C-C4C	5.25	1.50	1.42
29	A8	203	PEB	C3C-C4C	5.25	1.50	1.42
31	cP	1001	CYC	C3B-C2B	5.25	1.47	1.36
29	a1	203	PEB	C3B-C2B	5.25	1.47	1.36
29	F4	201	PEB	C3B-C2B	5.25	1.47	1.36
29	aK	203	PEB	C3B-C2B	5.25	1.47	1.36
29	aJ	202	PEB	C3C-C4C	5.25	1.50	1.42
29	aL	202	PEB	C3C-C4C	5.25	1.50	1.42
29	V1	201	PEB	C3B-C2B	5.25	1.47	1.36
29	VK	201	PEB	C3B-C2B	5.25	1.47	1.36
29	g1	203	PEB	C3B-C2B	5.25	1.47	1.36
29	gK	203	PEB	C3B-C2B	5.25	1.47	1.36
31	JP	1001	CYC	C3B-C2B	5.25	1.47	1.36
29	k1	201	PEB	C3B-C2B	5.24	1.47	1.36
29	kK	201	PEB	C3B-C2B	5.24	1.47	1.36
29	C5	203	PEB	C3C-C4C	5.24	1.50	1.42
29	YF	202	PEB	C3C-C4C	5.24	1.50	1.42
29	YI	202	PEB	C3C-C4C	5.24	1.50	1.42
29	A3	202	PEB	C3B-C2B	5.24	1.47	1.36
29	AO	202	PEB	C3B-C2B	5.24	1.47	1.36
29	I5	203	PEB	C3C-C4C	5.24	1.50	1.42
29	F1	1002	PEB	C1D-ND	5.24	1.53	1.45
29	FK	1002	PEB	C1D-ND	5.24	1.53	1.45
31	VP	1001	CYC	C1A-C2A	5.24	1.54	1.45
29	DA	201	PEB	C3B-C2B	5.24	1.47	1.36
29	rJ	201	PEB	C3B-C2B	5.24	1.47	1.36
29	rL	201	PEB	C3B-C2B	5.24	1.47	1.36
29	DN	201	PEB	C3B-C2B	5.24	1.47	1.36
31	G7	1001	CYC	C2A-C3A	5.24	1.47	1.36
31	AP	1001	CYC	C3B-C2B	5.24	1.47	1.36
31	PP	1001	CYC	C3B-C2B	5.24	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	pJ	201	PEB	C3B-C2B	5.24	1.47	1.36
29	pL	201	PEB	C3B-C2B	5.24	1.47	1.36
31	tP	1001	CYC	C3B-C2B	5.24	1.47	1.36
29	CC	201	PEB	C3C-C4C	5.24	1.50	1.42
29	CE	201	PEB	C3C-C4C	5.24	1.50	1.42
30	wJ	305	PUB	C2B-C1B	5.24	1.50	1.42
31	RP	1001	CYC	C3B-C2B	5.24	1.47	1.36
31	yP	1001	CYC	C2A-C3A	5.24	1.47	1.36
29	AC	201	PEB	C3C-C4C	5.24	1.50	1.42
29	AE	201	PEB	C3C-C4C	5.24	1.50	1.42
29	J1	1002	PEB	C3B-C2B	5.24	1.47	1.36
29	JK	1002	PEB	C3B-C2B	5.24	1.47	1.36
31	E7	1001	CYC	C2A-C3A	5.24	1.47	1.36
31	E9	1001	CYC	C2A-C3A	5.24	1.47	1.36
30	A7	303	PUB	C2C-C3C	5.24	1.47	1.36
30	A9	303	PUB	C2C-C3C	5.24	1.47	1.36
29	I3	202	PEB	C3B-C2B	5.24	1.47	1.36
29	IO	202	PEB	C3B-C2B	5.24	1.47	1.36
29	a1	201	PEB	C3B-C2B	5.24	1.47	1.36
29	LA	201	PEB	C3B-C2B	5.24	1.47	1.36
29	aK	201	PEB	C3B-C2B	5.24	1.47	1.36
29	LN	201	PEB	C3B-C2B	5.24	1.47	1.36
29	OF	203	PEB	C3C-C4C	5.24	1.50	1.42
29	OI	203	PEB	C3C-C4C	5.24	1.50	1.42
30	AF	302	PUB	C2C-C3C	5.23	1.47	1.36
30	AI	302	PUB	C2C-C3C	5.23	1.47	1.36
31	JP	1001	CYC	C2A-C3A	5.23	1.47	1.36
31	IP	1001	CYC	C2A-C3A	5.23	1.47	1.36
31	GP	1001	CYC	C3B-C2B	5.23	1.47	1.36
29	UF	201	PEB	C3C-C4C	5.23	1.50	1.42
29	UI	201	PEB	C3C-C4C	5.23	1.50	1.42
29	gJ	202	PEB	C3C-C4C	5.23	1.50	1.42
29	gL	202	PEB	C3C-C4C	5.23	1.50	1.42
29	NO	201	PEB	C3C-C4C	5.23	1.50	1.42
29	dJ	201	PEB	C3B-C2B	5.23	1.47	1.36
29	dL	201	PEB	C3B-C2B	5.23	1.47	1.36
29	R1	201	PEB	C3B-C2B	5.23	1.47	1.36
29	RK	201	PEB	C3B-C2B	5.23	1.47	1.36
31	1P	1001	CYC	CHB-C1B	5.23	1.50	1.38
29	M3	201	PEB	C3C-C4C	5.23	1.50	1.42
29	MO	201	PEB	C3C-C4C	5.23	1.50	1.42
29	D3	203	PEB	C3C-C4C	5.23	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	UB	201	PEB	C3C-C4C	5.23	1.50	1.42
29	UM	201	PEB	C3C-C4C	5.23	1.50	1.42
29	DO	203	PEB	C3C-C4C	5.23	1.50	1.42
31	rP	1001	CYC	C3B-C2B	5.23	1.47	1.36
29	kF	202	PEB	C3C-C4C	5.23	1.50	1.42
29	kI	202	PEB	C3C-C4C	5.23	1.50	1.42
29	K5	203	PEB	C3C-C4C	5.23	1.50	1.42
29	K8	203	PEB	C3C-C4C	5.23	1.50	1.42
29	JA	201	PEB	C3C-C4C	5.23	1.50	1.42
29	JN	201	PEB	C3C-C4C	5.23	1.50	1.42
29	FJ	201	PEB	C3B-C2B	5.23	1.47	1.36
29	FL	201	PEB	C3B-C2B	5.23	1.47	1.36
31	I7	1001	CYC	C2A-C3A	5.23	1.47	1.36
31	I9	1001	CYC	C2A-C3A	5.23	1.47	1.36
29	P1	201	PEB	C3B-C2B	5.23	1.47	1.36
29	PK	201	PEB	C3B-C2B	5.23	1.47	1.36
29	N3	201	PEB	C3C-C4C	5.23	1.50	1.42
29	N1	1002	PEB	C3B-C2B	5.23	1.47	1.36
29	NK	1002	PEB	C3B-C2B	5.22	1.47	1.36
29	G3	202	PEB	C3B-C2B	5.22	1.47	1.36
29	GO	202	PEB	C3B-C2B	5.22	1.47	1.36
29	BC	201	PEB	C3C-C4C	5.22	1.50	1.42
29	BE	201	PEB	C3C-C4C	5.22	1.50	1.42
31	K7	1001	CYC	C2A-C3A	5.22	1.47	1.36
31	YP	1000	CYC	C3B-C2B	5.22	1.47	1.36
31	IP	1001	CYC	C3B-C2B	5.22	1.47	1.36
29	H3	203	PEB	C3C-C4C	5.22	1.50	1.42
29	HO	203	PEB	C3C-C4C	5.22	1.50	1.42
29	J4	201	PEB	C3B-C2B	5.22	1.47	1.36
29	VF	202	PEB	C3C-C4C	5.22	1.50	1.42
29	VI	202	PEB	C3C-C4C	5.22	1.50	1.42
31	gP	1001	CYC	C3B-C2B	5.22	1.47	1.36
31	pP	1001	CYC	C3B-C2B	5.22	1.47	1.36
29	FA	201	PEB	C3B-C2B	5.22	1.47	1.36
29	FN	201	PEB	C3B-C2B	5.22	1.47	1.36
31	AP	1001	CYC	C2A-C3A	5.22	1.47	1.36
29	L1	1002	PEB	C1D-ND	5.22	1.53	1.45
29	LK	1002	PEB	C1D-ND	5.22	1.53	1.45
31	G9	1001	CYC	C2A-C3A	5.22	1.47	1.36
29	F1	1002	PEB	C3B-C2B	5.22	1.47	1.36
29	FK	1002	PEB	C3B-C2B	5.22	1.47	1.36
31	CP	1001	CYC	C3B-C2B	5.22	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	xP	1001	CYC	CHB-C1B	5.22	1.50	1.38
31	CP	1001	CYC	CHB-C1B	5.22	1.50	1.38
29	DA	201	PEB	C3C-C4C	5.22	1.50	1.42
29	DN	201	PEB	C3C-C4C	5.22	1.50	1.42
29	kJ	202	PEB	C3C-C4C	5.22	1.50	1.42
29	kL	202	PEB	C3C-C4C	5.22	1.50	1.42
31	EP	1001	CYC	CHB-C1B	5.22	1.50	1.38
29	iJ	202	PEB	C3C-C4C	5.21	1.50	1.42
29	iL	202	PEB	C3C-C4C	5.21	1.50	1.42
29	C5	201	PEB	C3B-C2B	5.21	1.47	1.36
29	C8	201	PEB	C3B-C2B	5.21	1.47	1.36
29	K5	202	PEB	C3C-C4C	5.21	1.50	1.42
29	E3	202	PEB	C3B-C2B	5.21	1.47	1.36
29	EO	202	PEB	C3B-C2B	5.21	1.47	1.36
29	QB	203	PEB	C3C-C4C	5.21	1.50	1.42
29	CJ	202	PEB	C3C-C4C	5.21	1.50	1.42
29	CL	202	PEB	C3C-C4C	5.21	1.50	1.42
29	QM	203	PEB	C3C-C4C	5.21	1.50	1.42
31	kP	1001	CYC	CHB-C1B	5.21	1.50	1.38
29	g1	201	PEB	C3B-C2B	5.21	1.47	1.36
29	gK	201	PEB	C3B-C2B	5.21	1.47	1.36
31	QP	1001	CYC	CHB-C1B	5.21	1.50	1.38
29	DK	1002	PEB	C1D-ND	5.21	1.53	1.45
29	e1	201	PEB	C3B-C2B	5.21	1.47	1.36
29	eK	201	PEB	C3B-C2B	5.21	1.47	1.36
30	xJ	304	PUB	C2C-C3C	5.21	1.47	1.36
29	C5	202	PEB	C3C-C4C	5.21	1.50	1.42
29	C8	202	PEB	C3C-C4C	5.21	1.50	1.42
29	OJ	202	PEB	C3C-C4C	5.21	1.50	1.42
29	SJ	202	PEB	C3C-C4C	5.21	1.50	1.42
29	OL	202	PEB	C3C-C4C	5.21	1.50	1.42
29	SL	202	PEB	C3C-C4C	5.21	1.50	1.42
29	NK	1002	PEB	C1D-ND	5.21	1.53	1.45
31	mP	1001	CYC	C3B-C2B	5.21	1.47	1.36
29	K8	202	PEB	C3C-C4C	5.21	1.50	1.42
29	HK	1002	PEB	C3B-C2B	5.21	1.47	1.36
31	C7	1001	CYC	C2A-C3A	5.21	1.47	1.36
31	C9	1001	CYC	C2A-C3A	5.21	1.47	1.36
31	M9	1001	CYC	C2A-C3A	5.21	1.47	1.36
29	C3	202	PEB	C3B-C2B	5.21	1.47	1.36
29	CO	202	PEB	C3B-C2B	5.21	1.47	1.36
29	eF	202	PEB	C3C-C4C	5.21	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	eI	202	PEB	C3C-C4C	5.21	1.50	1.42
29	Y1	201	PEB	C3B-C2B	5.21	1.47	1.36
29	YK	201	PEB	C3B-C2B	5.21	1.47	1.36
29	gF	202	PEB	C3C-C4C	5.21	1.50	1.42
29	gI	202	PEB	C3C-C4C	5.21	1.50	1.42
31	VP	1001	CYC	CHB-C1B	5.21	1.50	1.38
29	WJ	203	PEB	C3C-C4C	5.21	1.50	1.42
29	WL	203	PEB	C3C-C4C	5.21	1.50	1.42
29	i1	201	PEB	C3B-C2B	5.20	1.47	1.36
29	iK	201	PEB	C3B-C2B	5.20	1.47	1.36
29	MB	201	PEB	C3C-C4C	5.20	1.50	1.42
29	MM	201	PEB	C3C-C4C	5.20	1.50	1.42
30	A7	302	PUB	C2B-C1B	5.20	1.50	1.42
30	A9	302	PUB	C2B-C1B	5.20	1.50	1.42
29	JD	201	PEB	C3B-C2B	5.20	1.47	1.36
29	PF	202	PEB	C3C-C4C	5.20	1.50	1.42
29	PI	202	PEB	C3C-C4C	5.20	1.50	1.42
29	T1	201	PEB	C3B-C2B	5.20	1.47	1.36
29	TK	201	PEB	C3B-C2B	5.20	1.47	1.36
29	J1	1002	PEB	C1D-ND	5.20	1.53	1.45
29	JK	1002	PEB	C1D-ND	5.20	1.53	1.45
29	GD	203	PEB	C3B-C2B	5.20	1.47	1.36
31	EP	1001	CYC	C3B-C2B	5.20	1.47	1.36
29	I5	201	PEB	C3B-C2B	5.20	1.47	1.36
29	I8	201	PEB	C3B-C2B	5.20	1.47	1.36
29	sJ	202	PEB	C3C-C4C	5.20	1.50	1.42
29	sL	202	PEB	C3C-C4C	5.20	1.50	1.42
29	LC	201	PEB	C3C-C4C	5.20	1.50	1.42
29	LE	201	PEB	C3C-C4C	5.20	1.50	1.42
29	J3	203	PEB	C3C-C4C	5.20	1.50	1.42
29	KB	201	PEB	C3C-C4C	5.20	1.50	1.42
29	KM	201	PEB	C3C-C4C	5.20	1.50	1.42
29	JO	203	PEB	C3C-C4C	5.20	1.50	1.42
31	M7	1001	CYC	C2A-C3A	5.20	1.47	1.36
31	K9	1001	CYC	C2A-C3A	5.20	1.47	1.36
29	qJ	202	PEB	C3C-C4C	5.20	1.50	1.42
29	qL	202	PEB	C3C-C4C	5.20	1.50	1.42
29	L1	1002	PEB	C3B-C2B	5.20	1.47	1.36
29	LK	1002	PEB	C3B-C2B	5.20	1.47	1.36
29	F3	203	PEB	C3C-C4C	5.20	1.50	1.42
29	FO	203	PEB	C3C-C4C	5.20	1.50	1.42
29	A5	201	PEB	C3B-C2B	5.20	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A8	201	PEB	C3B-C2B	5.20	1.47	1.36
29	cJ	202	PEB	C3C-C4C	5.20	1.50	1.42
29	cL	202	PEB	C3C-C4C	5.20	1.50	1.42
31	GP	1001	CYC	C2A-C3A	5.20	1.47	1.36
29	c1	201	PEB	C3B-C2B	5.20	1.47	1.36
29	cK	201	PEB	C3B-C2B	5.20	1.47	1.36
29	QJ	202	PEB	C3C-C4C	5.20	1.50	1.42
29	QL	202	PEB	C3C-C4C	5.20	1.50	1.42
29	aF	202	PEB	C3C-C4C	5.20	1.50	1.42
29	aI	202	PEB	C3C-C4C	5.20	1.50	1.42
29	KJ	202	PEB	C3C-C4C	5.20	1.50	1.42
29	KL	202	PEB	C3C-C4C	5.20	1.50	1.42
31	XP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	DP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	wP	1001	CYC	CHB-C1B	5.19	1.50	1.38
29	jB	201	PEB	C3B-C2B	5.19	1.47	1.36
29	jM	201	PEB	C3B-C2B	5.19	1.47	1.36
31	vP	1001	CYC	C3B-C2B	5.19	1.47	1.36
31	JP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	MP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	VP	1001	CYC	C3B-C2B	5.19	1.47	1.36
29	jB	201	PEB	C3C-C4C	5.19	1.50	1.42
29	jM	201	PEB	C3C-C4C	5.19	1.50	1.42
31	jP	1001	CYC	CHB-C1B	5.19	1.50	1.38
29	KB	201	PEB	C3B-C2B	5.19	1.47	1.36
29	KM	201	PEB	C3B-C2B	5.19	1.47	1.36
29	eJ	202	PEB	C3C-C4C	5.19	1.50	1.42
29	eL	202	PEB	C3C-C4C	5.19	1.50	1.42
31	oP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	AP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	mP	1001	CYC	CHB-C1B	5.19	1.50	1.38
29	EJ	202	PEB	C3C-C4C	5.19	1.50	1.42
29	EL	202	PEB	C3C-C4C	5.19	1.50	1.42
31	nP	1001	CYC	CHB-C1B	5.19	1.50	1.38
31	pP	1001	CYC	CHB-C1B	5.19	1.50	1.38
30	wL	304	PUB	C2C-C3C	5.19	1.47	1.36
29	GC	201	PEB	C3C-C4C	5.19	1.50	1.42
29	GE	201	PEB	C3C-C4C	5.19	1.50	1.42
29	iF	202	PEB	C3C-C4C	5.19	1.50	1.42
29	iI	202	PEB	C3C-C4C	5.19	1.50	1.42
29	D1	1002	PEB	C3B-C2B	5.19	1.47	1.36
29	K3	202	PEB	C3B-C2B	5.19	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IC	201	PEB	C3B-C2B	5.19	1.47	1.36
29	IE	201	PEB	C3B-C2B	5.19	1.47	1.36
29	KO	202	PEB	C3B-C2B	5.19	1.47	1.36
30	xJ	305	PUB	C2B-C1B	5.19	1.50	1.42
29	B3	203	PEB	C3C-C4C	5.19	1.50	1.42
29	GB	201	PEB	C3C-C4C	5.19	1.50	1.42
29	GM	201	PEB	C3C-C4C	5.19	1.50	1.42
29	BO	203	PEB	C3C-C4C	5.19	1.50	1.42
31	hP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	KP	1001	CYC	CHB-C1B	5.18	1.50	1.38
29	QB	203	PEB	C3B-C2B	5.18	1.47	1.36
29	QM	203	PEB	C3B-C2B	5.18	1.47	1.36
29	b1	202	PEB	C3C-C4C	5.18	1.50	1.42
29	bK	202	PEB	C3C-C4C	5.18	1.50	1.42
31	eP	1001	CYC	C3B-C2B	5.18	1.47	1.36
29	Q1	202	PEB	C3C-C4C	5.18	1.50	1.42
29	QK	202	PEB	C3C-C4C	5.18	1.50	1.42
29	IB	201	PEB	C3C-C4C	5.18	1.50	1.42
29	uJ	203	PEB	C3C-C4C	5.18	1.50	1.42
29	uL	203	PEB	C3C-C4C	5.18	1.50	1.42
29	IM	201	PEB	C3C-C4C	5.18	1.50	1.42
30	xL	304	PUB	C2C-C3C	5.18	1.47	1.36
29	H1	1002	PEB	C3B-C2B	5.18	1.47	1.36
31	HP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	rP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	tP	1001	CYC	CHB-C1B	5.18	1.50	1.38
29	lB	201	PEB	C3C-C4C	5.18	1.50	1.42
29	lM	201	PEB	C3C-C4C	5.18	1.50	1.42
31	FP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	lP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	TP	1001	CYC	C3B-C2B	5.18	1.47	1.36
29	K5	201	PEB	C3B-C2B	5.18	1.47	1.36
29	K8	201	PEB	C3B-C2B	5.18	1.47	1.36
29	BA	201	PEB	C3C-C4C	5.18	1.50	1.42
29	BN	201	PEB	C3C-C4C	5.18	1.50	1.42
29	hB	201	PEB	C3C-C4C	5.18	1.50	1.42
29	hM	201	PEB	C3C-C4C	5.18	1.50	1.42
31	GP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	qP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	RP	1001	CYC	CHB-C1B	5.18	1.50	1.38
30	xL	305	PUB	C2B-C1B	5.18	1.50	1.42
29	A5	203	PEB	C3B-C2B	5.18	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A8	203	PEB	C3B-C2B	5.18	1.47	1.36
29	EB	201	PEB	C3C-C4C	5.18	1.50	1.42
29	EM	201	PEB	C3C-C4C	5.18	1.50	1.42
31	cP	1001	CYC	CHB-C1B	5.18	1.50	1.38
31	UP	1001	CYC	CHB-C1B	5.18	1.50	1.38
29	I5	203	PEB	C3B-C2B	5.18	1.47	1.36
29	UB	201	PEB	C3B-C2B	5.18	1.47	1.36
29	UM	201	PEB	C3B-C2B	5.18	1.47	1.36
29	N1	1002	PEB	C1D-ND	5.18	1.53	1.45
29	AJ	202	PEB	C3C-C4C	5.18	1.50	1.42
29	MJ	202	PEB	C3C-C4C	5.18	1.50	1.42
29	mJ	202	PEB	C3C-C4C	5.18	1.50	1.42
29	AL	202	PEB	C3C-C4C	5.18	1.50	1.42
29	ML	202	PEB	C3C-C4C	5.18	1.50	1.42
29	mL	202	PEB	C3C-C4C	5.18	1.50	1.42
29	HA	201	PEB	C3C-C4C	5.18	1.50	1.42
29	LA	201	PEB	C3C-C4C	5.18	1.50	1.42
29	HN	201	PEB	C3C-C4C	5.18	1.50	1.42
29	LN	201	PEB	C3C-C4C	5.18	1.50	1.42
29	I8	203	PEB	C3B-C2B	5.17	1.47	1.36
29	KC	202	PEB	C3B-C2B	5.17	1.47	1.36
29	KE	202	PEB	C3B-C2B	5.17	1.47	1.36
29	FA	201	PEB	C3C-C4C	5.17	1.50	1.42
29	IJ	202	PEB	C3C-C4C	5.17	1.50	1.42
29	IL	202	PEB	C3C-C4C	5.17	1.50	1.42
29	FN	201	PEB	C3C-C4C	5.17	1.50	1.42
29	M4	203	PEB	C3C-C4C	5.17	1.50	1.42
31	gP	1001	CYC	CHB-C1B	5.17	1.50	1.38
31	BP	1001	CYC	CHB-C1B	5.17	1.50	1.38
29	EC	201	PEB	C3B-C2B	5.17	1.47	1.36
29	EE	201	PEB	C3B-C2B	5.17	1.47	1.36
29	D1	1002	PEB	C1D-ND	5.17	1.53	1.45
29	WB	201	PEB	C3B-C2B	5.17	1.47	1.36
29	WM	201	PEB	C3B-C2B	5.17	1.47	1.36
30	AF	303	PUB	C2C-C3C	5.17	1.47	1.36
30	AI	303	PUB	C2C-C3C	5.17	1.47	1.36
29	CB	201	PEB	C3C-C4C	5.17	1.50	1.42
29	CM	201	PEB	C3C-C4C	5.17	1.50	1.42
29	H1	1002	PEB	C1D-ND	5.17	1.53	1.45
31	fP	1001	CYC	CHB-C1B	5.17	1.50	1.38
29	DK	1002	PEB	C3B-C2B	5.17	1.47	1.36
29	EC	201	PEB	C3C-C4C	5.17	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EE	201	PEB	C3C-C4C	5.17	1.50	1.42
31	eP	1001	CYC	CHB-C1B	5.17	1.50	1.38
29	IB	201	PEB	C3B-C2B	5.17	1.47	1.36
29	IM	201	PEB	C3B-C2B	5.17	1.47	1.36
29	OB	201	PEB	C3C-C4C	5.17	1.50	1.42
29	OM	201	PEB	C3C-C4C	5.17	1.50	1.42
29	A5	202	PEB	C3C-C4C	5.17	1.50	1.42
29	A8	202	PEB	C3C-C4C	5.17	1.50	1.42
29	GJ	202	PEB	C3C-C4C	5.17	1.50	1.42
29	GL	202	PEB	C3C-C4C	5.17	1.50	1.42
30	yJ	303	PUB	C2B-C1B	5.17	1.50	1.42
29	MB	201	PEB	C3B-C2B	5.17	1.47	1.36
29	MM	201	PEB	C3B-C2B	5.17	1.47	1.36
30	wJ	304	PUB	C2C-C3C	5.17	1.47	1.36
29	m1	201	PEB	C3B-C2B	5.17	1.47	1.36
29	mK	201	PEB	C3B-C2B	5.17	1.47	1.36
29	WB	201	PEB	C3C-C4C	5.17	1.50	1.42
29	FC	201	PEB	C3C-C4C	5.17	1.50	1.42
29	FE	201	PEB	C3C-C4C	5.17	1.50	1.42
29	WM	201	PEB	C3C-C4C	5.17	1.50	1.42
31	IP	1001	CYC	CHB-C1B	5.17	1.50	1.38
31	TP	1001	CYC	CHB-C1B	5.17	1.50	1.38
29	j1	202	PEB	C3C-C4C	5.16	1.50	1.42
29	jK	202	PEB	C3C-C4C	5.16	1.50	1.42
29	IC	201	PEB	C3C-C4C	5.16	1.50	1.42
29	IE	201	PEB	C3C-C4C	5.16	1.50	1.42
31	iP	1001	CYC	CHB-C1B	5.16	1.50	1.38
31	PP	1001	CYC	CHB-C1B	5.16	1.50	1.38
31	SP	1001	CYC	CHB-C1B	5.16	1.50	1.38
29	WF	202	PEB	C3B-C2B	5.16	1.47	1.36
29	WI	202	PEB	C3B-C2B	5.16	1.47	1.36
29	I5	202	PEB	C3C-C4C	5.16	1.50	1.42
29	I8	202	PEB	C3C-C4C	5.16	1.50	1.42
29	HK	1002	PEB	C1D-ND	5.16	1.53	1.45
29	oJ	202	PEB	C3C-C4C	5.16	1.50	1.42
29	oL	202	PEB	C3C-C4C	5.16	1.50	1.42
29	CB	201	PEB	C3B-C2B	5.16	1.47	1.36
29	CM	201	PEB	C3B-C2B	5.16	1.47	1.36
29	dB	201	PEB	C3C-C4C	5.16	1.50	1.42
29	dM	201	PEB	C3C-C4C	5.16	1.50	1.42
29	SB	201	PEB	C3B-C2B	5.16	1.47	1.36
29	SM	201	PEB	C3B-C2B	5.16	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YB	202	PEB	C3C-C4C	5.16	1.50	1.42
29	YM	202	PEB	C3C-C4C	5.16	1.50	1.42
29	SB	201	PEB	C3C-C4C	5.16	1.50	1.42
29	SM	201	PEB	C3C-C4C	5.16	1.50	1.42
29	K8	203	PEB	C3B-C2B	5.16	1.47	1.36
29	KD	203	PEB	C3B-C2B	5.16	1.47	1.36
29	GC	201	PEB	C3B-C2B	5.16	1.47	1.36
29	GE	201	PEB	C3B-C2B	5.16	1.47	1.36
29	GB	201	PEB	C3B-C2B	5.16	1.47	1.36
29	dB	201	PEB	C3B-C2B	5.16	1.47	1.36
29	GM	201	PEB	C3B-C2B	5.16	1.47	1.36
29	dM	201	PEB	C3B-C2B	5.16	1.47	1.36
29	d1	202	PEB	C3C-C4C	5.16	1.50	1.42
29	dK	202	PEB	C3C-C4C	5.16	1.50	1.42
29	K4	203	PEB	C3B-C2B	5.16	1.47	1.36
29	E4	203	PEB	C3B-C2B	5.15	1.47	1.36
29	AC	201	PEB	C3B-C2B	5.15	1.47	1.36
29	AE	201	PEB	C3B-C2B	5.15	1.47	1.36
29	K5	203	PEB	C3B-C2B	5.15	1.47	1.36
29	UJ	202	PEB	C3C-C4C	5.15	1.50	1.42
29	UL	202	PEB	C3C-C4C	5.15	1.50	1.42
29	H3	202	PEB	C3B-C2B	5.15	1.47	1.36
29	HO	202	PEB	C3B-C2B	5.15	1.47	1.36
29	Q2	201	PEB	C3C-C4C	5.15	1.50	1.42
29	CC	201	PEB	C3B-C2B	5.15	1.47	1.36
29	CE	201	PEB	C3B-C2B	5.15	1.47	1.36
31	vP	1001	CYC	CHB-C1B	5.15	1.50	1.38
31	sP	1001	CYC	CHB-C1B	5.15	1.50	1.38
29	MG	404	PEB	C3B-C2B	5.15	1.47	1.36
31	xP	1001	CYC	C3B-C2B	5.15	1.47	1.36
29	OR	201	PEB	C3C-C4C	5.15	1.50	1.42
29	YB	202	PEB	C3B-C2B	5.15	1.47	1.36
29	YM	202	PEB	C3B-C2B	5.15	1.47	1.36
29	Z1	203	PEB	C3C-C4C	5.15	1.50	1.42
29	ZK	203	PEB	C3C-C4C	5.15	1.50	1.42
29	lB	201	PEB	C3B-C2B	5.15	1.47	1.36
29	lM	201	PEB	C3B-C2B	5.15	1.47	1.36
29	HC	201	PEB	C3C-C4C	5.15	1.50	1.42
29	HE	201	PEB	C3C-C4C	5.15	1.50	1.42
29	MD	203	PEB	C3B-C2B	5.15	1.47	1.36
29	SF	202	PEB	C3B-C2B	5.15	1.47	1.36
29	SI	202	PEB	C3B-C2B	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IG	202	PEB	C3C-C4C	5.15	1.50	1.42
29	IQ	202	PEB	C3C-C4C	5.15	1.50	1.42
29	MR	202	PEB	C3C-C4C	5.15	1.50	1.42
31	OP	1001	CYC	CHB-C1B	5.15	1.50	1.38
29	C5	203	PEB	C3B-C2B	5.15	1.47	1.36
29	C8	203	PEB	C3B-C2B	5.15	1.47	1.36
29	U2	201	PEB	C3C-C4C	5.15	1.50	1.42
29	JC	201	PEB	C3C-C4C	5.15	1.50	1.42
29	JE	201	PEB	C3C-C4C	5.15	1.50	1.42
29	h1	202	PEB	C3C-C4C	5.14	1.50	1.42
29	YJ	202	PEB	C3C-C4C	5.14	1.50	1.42
29	hK	202	PEB	C3C-C4C	5.14	1.50	1.42
29	YL	202	PEB	C3C-C4C	5.14	1.50	1.42
29	lF	202	PEB	C3B-C2B	5.14	1.47	1.36
29	lI	202	PEB	C3B-C2B	5.14	1.47	1.36
29	UF	203	PEB	C3B-C2B	5.14	1.47	1.36
29	hF	202	PEB	C3B-C2B	5.14	1.47	1.36
29	UI	203	PEB	C3B-C2B	5.14	1.47	1.36
29	hI	202	PEB	C3B-C2B	5.14	1.47	1.36
29	DO	202	PEB	C3C-C4C	5.14	1.50	1.42
29	fB	201	PEB	C3B-C2B	5.14	1.47	1.36
29	fM	201	PEB	C3B-C2B	5.14	1.47	1.36
29	BB	301	PEB	C3B-C2B	5.14	1.47	1.36
29	BM	301	PEB	C3B-C2B	5.14	1.47	1.36
29	fB	201	PEB	C3C-C4C	5.14	1.50	1.42
29	KC	202	PEB	C3C-C4C	5.14	1.50	1.42
29	KE	202	PEB	C3C-C4C	5.14	1.50	1.42
29	CG	202	PEB	C3C-C4C	5.14	1.50	1.42
29	fM	201	PEB	C3C-C4C	5.14	1.50	1.42
29	CQ	202	PEB	C3C-C4C	5.14	1.50	1.42
29	dF	203	PEB	C3B-C2B	5.14	1.47	1.36
29	dI	203	PEB	C3B-C2B	5.14	1.47	1.36
29	LB	203	PEB	C3B-C2B	5.14	1.47	1.36
29	LM	203	PEB	C3B-C2B	5.14	1.47	1.36
29	EG	202	PEB	C3C-C4C	5.14	1.50	1.42
29	EQ	202	PEB	C3C-C4C	5.14	1.50	1.42
29	hB	201	PEB	C3B-C2B	5.14	1.47	1.36
29	hM	201	PEB	C3B-C2B	5.14	1.47	1.36
29	OB	201	PEB	C3B-C2B	5.14	1.47	1.36
29	OM	201	PEB	C3B-C2B	5.14	1.47	1.36
31	NP	1001	CYC	CHB-C1B	5.14	1.50	1.38
29	ED	202	PEB	C3B-C2B	5.14	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EB	201	PEB	C3B-C2B	5.14	1.47	1.36
29	EM	201	PEB	C3B-C2B	5.14	1.47	1.36
30	yL	303	PUB	C2B-C1B	5.14	1.50	1.42
29	QF	202	PEB	C3B-C2B	5.14	1.47	1.36
29	QI	202	PEB	C3B-C2B	5.14	1.47	1.36
31	uP	1001	CYC	CHB-C1B	5.14	1.50	1.38
29	aB	201	PEB	C3B-C2B	5.14	1.47	1.36
29	aM	201	PEB	C3B-C2B	5.14	1.47	1.36
29	OF	202	PEB	C3B-C2B	5.13	1.47	1.36
29	OI	202	PEB	C3B-C2B	5.13	1.47	1.36
29	yJ	301	PEB	C3C-C4C	5.13	1.50	1.42
29	yL	301	PEB	C3C-C4C	5.13	1.50	1.42
29	G5	201	PEB	C3B-C2B	5.13	1.47	1.36
29	HB	203	PEB	C3B-C2B	5.13	1.47	1.36
29	RB	203	PEB	C3B-C2B	5.13	1.47	1.36
29	HM	203	PEB	C3B-C2B	5.13	1.47	1.36
29	RM	203	PEB	C3B-C2B	5.13	1.47	1.36
29	aB	201	PEB	C3C-C4C	5.13	1.50	1.42
29	DC	201	PEB	C3C-C4C	5.13	1.50	1.42
29	DE	201	PEB	C3C-C4C	5.13	1.50	1.42
29	aM	201	PEB	C3C-C4C	5.13	1.50	1.42
30	QB	201	PUB	C2C-C3C	5.13	1.47	1.36
30	QM	201	PUB	C2C-C3C	5.13	1.47	1.36
29	VB	203	PEB	C3B-C2B	5.13	1.47	1.36
29	VM	203	PEB	C3B-C2B	5.13	1.47	1.36
29	NB	201	PEB	C3B-C2B	5.13	1.47	1.36
29	NM	201	PEB	C3B-C2B	5.13	1.47	1.36
29	F8	201	PEB	C3B-C2B	5.13	1.47	1.36
29	JF	1002	PEB	C3B-C2B	5.13	1.47	1.36
29	JI	1002	PEB	C3B-C2B	5.13	1.47	1.36
29	DF	1002	PEB	C3B-C2B	5.13	1.47	1.36
29	DI	1002	PEB	C3B-C2B	5.13	1.47	1.36
29	AG	202	PEB	C3C-C4C	5.13	1.50	1.42
29	AQ	202	PEB	C3C-C4C	5.13	1.50	1.42
29	ZF	202	PEB	C3B-C2B	5.13	1.47	1.36
29	ZI	202	PEB	C3B-C2B	5.13	1.47	1.36
29	l1	202	PEB	C3C-C4C	5.12	1.50	1.42
29	lK	202	PEB	C3C-C4C	5.12	1.50	1.42
29	O2	201	PEB	C3C-C4C	5.12	1.50	1.42
29	HF	1002	PEB	C3B-C2B	5.12	1.47	1.36
29	HI	1002	PEB	C3B-C2B	5.12	1.47	1.36
29	NF	1002	PEB	C3B-C2B	5.12	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NI	1002	PEB	C3B-C2B	5.12	1.47	1.36
29	S1	202	PEB	C3C-C4C	5.12	1.50	1.42
29	SK	202	PEB	C3C-C4C	5.12	1.50	1.42
29	G4	203	PEB	C3B-C2B	5.12	1.47	1.36
29	M2	201	PEB	C3C-C4C	5.12	1.50	1.42
29	fF	202	PEB	C3B-C2B	5.12	1.47	1.36
29	jF	202	PEB	C3B-C2B	5.12	1.47	1.36
29	fI	202	PEB	C3B-C2B	5.12	1.47	1.36
29	jI	202	PEB	C3B-C2B	5.12	1.47	1.36
29	FB	201	PEB	C3B-C2B	5.12	1.47	1.36
29	FM	201	PEB	C3B-C2B	5.12	1.47	1.36
29	MQ	406	PEB	C3B-C2B	5.12	1.47	1.36
29	B3	202	PEB	C3B-C2B	5.12	1.47	1.36
29	F3	202	PEB	C3B-C2B	5.12	1.47	1.36
29	BO	202	PEB	C3B-C2B	5.12	1.47	1.36
29	FO	202	PEB	C3B-C2B	5.12	1.47	1.36
31	F1	1001	CYC	C3B-C2B	5.12	1.47	1.36
31	FK	1001	CYC	C3B-C2B	5.12	1.47	1.36
29	ID	203	PEB	C3B-C2B	5.12	1.47	1.36
31	NK	1001	CYC	C3B-C2B	5.11	1.47	1.36
29	PB	202	PEB	C3B-C2B	5.11	1.47	1.36
29	PM	202	PEB	C3B-C2B	5.11	1.47	1.36
29	C4	203	PEB	C3B-C2B	5.11	1.47	1.36
29	LF	1002	PEB	C3B-C2B	5.11	1.47	1.36
29	LI	1002	PEB	C3B-C2B	5.11	1.47	1.36
29	O1	202	PEB	C3C-C4C	5.11	1.50	1.42
29	OK	202	PEB	C3C-C4C	5.11	1.50	1.42
29	OR	202	PEB	C3C-C4C	5.11	1.50	1.42
29	H5	201	PEB	C3B-C2B	5.11	1.47	1.36
29	G8	201	PEB	C3B-C2B	5.11	1.47	1.36
29	I3	203	PEB	C3B-C2B	5.11	1.47	1.36
29	IO	203	PEB	C3B-C2B	5.11	1.47	1.36
29	D3	202	PEB	C3C-C4C	5.11	1.50	1.42
29	NB	202	PEB	C3B-C2B	5.11	1.47	1.36
29	NM	202	PEB	C3B-C2B	5.11	1.47	1.36
29	eB	201	PEB	C3B-C2B	5.11	1.47	1.36
29	eM	201	PEB	C3B-C2B	5.11	1.47	1.36
29	JG	201	PEB	C3B-C2B	5.11	1.47	1.36
29	JQ	201	PEB	C3B-C2B	5.11	1.47	1.36
29	fI	202	PEB	C3C-C4C	5.11	1.50	1.42
29	fK	202	PEB	C3C-C4C	5.11	1.50	1.42
29	CD	203	PEB	C3B-C2B	5.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	HK	1001	CYC	C3B-C2B	5.11	1.47	1.36
29	U1	203	PEB	C3C-C4C	5.11	1.50	1.42
29	UK	203	PEB	C3C-C4C	5.11	1.50	1.42
29	eB	202	PEB	C3B-C2B	5.10	1.47	1.36
29	eM	202	PEB	C3B-C2B	5.10	1.47	1.36
29	MR	201	PEB	C3C-C4C	5.10	1.50	1.42
29	FB	203	PEB	C3B-C2B	5.10	1.47	1.36
29	FM	203	PEB	C3B-C2B	5.10	1.47	1.36
31	L1	1001	CYC	C3B-C2B	5.10	1.47	1.36
31	LK	1001	CYC	C3B-C2B	5.10	1.47	1.36
29	cB	203	PEB	C3B-C2B	5.10	1.47	1.36
29	cM	203	PEB	C3B-C2B	5.10	1.47	1.36
29	W1	202	PEB	C3C-C4C	5.10	1.50	1.42
29	WK	202	PEB	C3C-C4C	5.10	1.50	1.42
29	QR	201	PEB	C3C-C4C	5.10	1.50	1.42
29	J3	202	PEB	C3B-C2B	5.10	1.47	1.36
29	XB	202	PEB	C3B-C2B	5.10	1.47	1.36
29	iB	201	PEB	C3B-C2B	5.10	1.47	1.36
29	iB	203	PEB	C3B-C2B	5.10	1.47	1.36
29	XM	202	PEB	C3B-C2B	5.10	1.47	1.36
29	iM	201	PEB	C3B-C2B	5.10	1.47	1.36
29	iM	203	PEB	C3B-C2B	5.10	1.47	1.36
29	JO	202	PEB	C3B-C2B	5.10	1.47	1.36
29	TB	203	PEB	C3B-C2B	5.10	1.47	1.36
29	TM	203	PEB	C3B-C2B	5.10	1.47	1.36
29	gB	203	PEB	C3B-C2B	5.10	1.47	1.36
29	bF	202	PEB	C3B-C2B	5.10	1.47	1.36
29	bI	202	PEB	C3B-C2B	5.10	1.47	1.36
29	gM	203	PEB	C3B-C2B	5.10	1.47	1.36
29	S2	201	PEB	C3C-C4C	5.10	1.50	1.42
29	W2	201	PEB	C3C-C4C	5.10	1.50	1.42
29	I4	203	PEB	C3C-C4C	5.10	1.50	1.42
29	WR	201	PEB	C3C-C4C	5.10	1.50	1.42
29	DB	201	PEB	C3B-C2B	5.10	1.47	1.36
29	DM	201	PEB	C3B-C2B	5.10	1.47	1.36
29	mB	201	PEB	C3B-C2B	5.10	1.47	1.36
29	mM	201	PEB	C3B-C2B	5.10	1.47	1.36
29	JB	203	PEB	C3B-C2B	5.09	1.47	1.36
29	JM	203	PEB	C3B-C2B	5.09	1.47	1.36
29	DG	201	PEB	C3B-C2B	5.09	1.47	1.36
29	DQ	201	PEB	C3B-C2B	5.09	1.47	1.36
29	Q1	201	PEB	C3C-C4C	5.09	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QK	201	PEB	C3C-C4C	5.09	1.50	1.42
29	H8	203	PEB	C3B-C2B	5.09	1.47	1.36
29	DB	203	PEB	C3B-C2B	5.09	1.47	1.36
29	DM	203	PEB	C3B-C2B	5.09	1.47	1.36
29	J3	201	PEB	C3B-C2B	5.09	1.47	1.36
29	JO	201	PEB	C3B-C2B	5.09	1.47	1.36
29	FF	1002	PEB	C3B-C2B	5.09	1.47	1.36
29	FI	1002	PEB	C3B-C2B	5.09	1.47	1.36
29	F3	201	PEB	C3B-C2B	5.09	1.47	1.36
29	FO	201	PEB	C3B-C2B	5.09	1.47	1.36
29	UR	201	PEB	C3C-C4C	5.09	1.50	1.42
29	S1	201	PEB	C3C-C4C	5.09	1.50	1.42
29	d1	201	PEB	C3C-C4C	5.09	1.50	1.42
29	SK	201	PEB	C3C-C4C	5.09	1.50	1.42
29	dK	201	PEB	C3C-C4C	5.09	1.50	1.42
29	kB	203	PEB	C3B-C2B	5.09	1.47	1.36
29	kM	203	PEB	C3B-C2B	5.09	1.47	1.36
29	H5	203	PEB	C3B-C2B	5.09	1.47	1.36
29	DB	203	PEB	C3C-C4C	5.09	1.50	1.42
29	DM	203	PEB	C3C-C4C	5.09	1.50	1.42
29	AB	302	PEB	C3C-C4C	5.09	1.50	1.42
29	LB	201	PEB	C3B-C2B	5.09	1.47	1.36
29	ZB	203	PEB	C3B-C2B	5.09	1.47	1.36
29	LM	201	PEB	C3B-C2B	5.09	1.47	1.36
29	ZM	203	PEB	C3B-C2B	5.09	1.47	1.36
29	ZB	201	PEB	C3B-C2B	5.09	1.47	1.36
29	yJ	301	PEB	C3B-C2B	5.09	1.47	1.36
29	yL	301	PEB	C3B-C2B	5.09	1.47	1.36
29	ZM	201	PEB	C3B-C2B	5.09	1.47	1.36
31	J1	1001	CYC	C3B-C2B	5.09	1.47	1.36
31	JK	1001	CYC	C3B-C2B	5.09	1.47	1.36
29	GG	202	PEB	C3C-C4C	5.09	1.50	1.42
29	GQ	202	PEB	C3C-C4C	5.09	1.50	1.42
29	FG	201	PEB	C3B-C2B	5.09	1.47	1.36
29	FQ	201	PEB	C3B-C2B	5.09	1.47	1.36
29	H5	202	PEB	C3B-C2B	5.08	1.47	1.36
29	KG	202	PEB	C3C-C4C	5.08	1.50	1.42
29	KQ	202	PEB	C3C-C4C	5.08	1.50	1.42
29	F5	201	PEB	C3B-C2B	5.08	1.47	1.36
29	JB	203	PEB	C3C-C4C	5.08	1.50	1.42
29	JM	203	PEB	C3C-C4C	5.08	1.50	1.42
31	D1	1001	CYC	C3B-C2B	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G5	202	PEB	C3B-C2B	5.08	1.47	1.36
29	cB	201	PEB	C3B-C2B	5.08	1.47	1.36
29	cM	201	PEB	C3B-C2B	5.08	1.47	1.36
29	kB	203	PEB	C3C-C4C	5.08	1.50	1.42
29	kM	203	PEB	C3C-C4C	5.08	1.50	1.42
29	H3	201	PEB	C3B-C2B	5.08	1.47	1.36
29	HO	201	PEB	C3B-C2B	5.08	1.47	1.36
31	H1	1001	CYC	C3B-C2B	5.08	1.47	1.36
29	FB	203	PEB	C3C-C4C	5.08	1.50	1.42
29	FM	203	PEB	C3C-C4C	5.08	1.50	1.42
29	W7	202	PEB	C3B-C2B	5.08	1.47	1.36
29	W9	202	PEB	C3B-C2B	5.08	1.47	1.36
29	PB	201	PEB	C3B-C2B	5.08	1.47	1.36
29	gB	201	PEB	C3B-C2B	5.08	1.47	1.36
29	PM	201	PEB	C3B-C2B	5.08	1.47	1.36
29	gM	201	PEB	C3B-C2B	5.08	1.47	1.36
29	Z7	202	PEB	C3B-C2B	5.08	1.47	1.36
29	Z9	202	PEB	C3B-C2B	5.08	1.47	1.36
29	D3	201	PEB	C3B-C2B	5.08	1.47	1.36
29	DO	201	PEB	C3B-C2B	5.08	1.47	1.36
31	DK	1001	CYC	C3B-C2B	5.08	1.47	1.36
29	kB	201	PEB	C3B-C2B	5.08	1.47	1.36
29	kM	201	PEB	C3B-C2B	5.08	1.47	1.36
29	G8	202	PEB	C3B-C2B	5.08	1.47	1.36
29	LG	201	PEB	C3B-C2B	5.08	1.47	1.36
29	MQ	402	PEB	C3B-C2B	5.08	1.47	1.36
29	L5	203	PEB	C3B-C2B	5.08	1.47	1.36
31	N1	1001	CYC	C3B-C2B	5.08	1.47	1.36
29	L5	201	PEB	C3B-C2B	5.08	1.47	1.36
29	H8	201	PEB	C3B-C2B	5.08	1.47	1.36
29	h7	202	PEB	C3B-C2B	5.07	1.47	1.36
29	h9	202	PEB	C3B-C2B	5.07	1.47	1.36
29	eB	202	PEB	C3C-C4C	5.07	1.50	1.42
29	eM	202	PEB	C3C-C4C	5.07	1.50	1.42
29	TB	201	PEB	C3B-C2B	5.07	1.47	1.36
29	TM	201	PEB	C3B-C2B	5.07	1.47	1.36
29	HB	203	PEB	C3C-C4C	5.07	1.50	1.42
29	HM	203	PEB	C3C-C4C	5.07	1.50	1.42
29	H8	202	PEB	C3B-C2B	5.07	1.47	1.36
29	RB	201	PEB	C3B-C2B	5.07	1.47	1.36
29	RM	201	PEB	C3B-C2B	5.07	1.47	1.36
29	JB	201	PEB	C3B-C2B	5.07	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JM	201	PEB	C3B-C2B	5.07	1.47	1.36
29	B5	201	PEB	C3B-C2B	5.07	1.47	1.36
29	BG	201	PEB	C3B-C2B	5.07	1.47	1.36
29	BQ	201	PEB	C3B-C2B	5.07	1.47	1.36
29	HB	201	PEB	C3B-C2B	5.07	1.47	1.36
29	HM	201	PEB	C3B-C2B	5.07	1.47	1.36
29	TB	203	PEB	C3C-C4C	5.07	1.50	1.42
29	TM	203	PEB	C3C-C4C	5.07	1.50	1.42
29	XB	201	PEB	C3B-C2B	5.07	1.47	1.36
29	XM	201	PEB	C3B-C2B	5.07	1.47	1.36
29	f7	202	PEB	C3B-C2B	5.07	1.47	1.36
29	f9	202	PEB	C3B-C2B	5.07	1.47	1.36
29	F5	203	PEB	C3B-C2B	5.07	1.47	1.36
29	F8	203	PEB	C3B-C2B	5.07	1.47	1.36
29	K4	202	PEB	C3B-C2B	5.06	1.47	1.36
29	L8	201	PEB	C3B-C2B	5.06	1.47	1.36
29	KD	202	PEB	C3B-C2B	5.06	1.47	1.36
29	W1	201	PEB	C3C-C4C	5.06	1.49	1.42
29	VB	203	PEB	C3C-C4C	5.06	1.49	1.42
29	WK	201	PEB	C3C-C4C	5.06	1.49	1.42
29	VM	203	PEB	C3C-C4C	5.06	1.49	1.42
29	j7	202	PEB	C3B-C2B	5.06	1.47	1.36
29	j9	202	PEB	C3B-C2B	5.06	1.47	1.36
29	mB	203	PEB	C3B-C2B	5.06	1.47	1.36
29	mM	203	PEB	C3B-C2B	5.06	1.47	1.36
29	L3	201	PEB	C3B-C2B	5.06	1.47	1.36
29	LO	201	PEB	C3B-C2B	5.06	1.47	1.36
29	wJ	302	PEB	C3C-C4C	5.06	1.49	1.42
29	JB	202	PEB	C3B-C2B	5.06	1.47	1.36
29	JM	202	PEB	C3B-C2B	5.06	1.47	1.36
29	Z1	202	PEB	C3B-C2B	5.06	1.47	1.36
29	ZK	202	PEB	C3B-C2B	5.06	1.47	1.36
29	h1	201	PEB	C3C-C4C	5.06	1.49	1.42
29	hK	201	PEB	C3C-C4C	5.06	1.49	1.42
29	F5	202	PEB	C3B-C2B	5.06	1.47	1.36
29	B8	202	PEB	C3B-C2B	5.06	1.47	1.36
29	XB	202	PEB	C3C-C4C	5.06	1.49	1.42
29	XM	202	PEB	C3C-C4C	5.06	1.49	1.42
29	B3	201	PEB	C3B-C2B	5.06	1.47	1.36
29	BO	201	PEB	C3B-C2B	5.06	1.47	1.36
29	AB	303	PEB	C3C-C4C	5.06	1.49	1.42
29	f1	201	PEB	C3C-C4C	5.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fK	201	PEB	C3C-C4C	5.05	1.49	1.42
29	YB	201	PEB	C3B-C2B	5.05	1.47	1.36
29	YM	201	PEB	C3B-C2B	5.05	1.47	1.36
29	AM	303	PEB	C3C-C4C	5.05	1.49	1.42
29	NB	202	PEB	C3C-C4C	5.05	1.49	1.42
29	NM	202	PEB	C3C-C4C	5.05	1.49	1.42
29	PB	202	PEB	C3C-C4C	5.05	1.49	1.42
29	PM	202	PEB	C3C-C4C	5.05	1.49	1.42
29	O7	202	PEB	C3B-C2B	5.05	1.47	1.36
29	O9	202	PEB	C3B-C2B	5.05	1.47	1.36
29	L8	202	PEB	C3B-C2B	5.05	1.47	1.36
29	L8	203	PEB	C3B-C2B	5.05	1.47	1.36
31	MP	1001	CYC	C3B-C2B	5.05	1.47	1.36
29	j1	201	PEB	C3C-C4C	5.05	1.49	1.42
29	LB	203	PEB	C3C-C4C	5.05	1.49	1.42
29	jK	201	PEB	C3C-C4C	5.05	1.49	1.42
29	LM	203	PEB	C3C-C4C	5.05	1.49	1.42
29	b1	201	PEB	C3B-C2B	5.05	1.47	1.36
29	bK	201	PEB	C3B-C2B	5.05	1.47	1.36
29	f1	201	PEB	C3B-C2B	5.05	1.47	1.36
29	HG	201	PEB	C3B-C2B	5.05	1.47	1.36
29	fK	201	PEB	C3B-C2B	5.05	1.47	1.36
29	HQ	201	PEB	C3B-C2B	5.05	1.47	1.36
29	AM	302	PEB	C3C-C4C	5.05	1.49	1.42
30	AM	305	PUB	C2C-C3C	5.05	1.47	1.36
29	A5	201	PEB	C3C-C4C	5.05	1.49	1.42
29	A8	201	PEB	C3C-C4C	5.05	1.49	1.42
29	iB	203	PEB	C3C-C4C	5.05	1.49	1.42
29	iM	203	PEB	C3C-C4C	5.05	1.49	1.42
29	b7	202	PEB	C3B-C2B	5.05	1.47	1.36
29	b9	202	PEB	C3B-C2B	5.05	1.47	1.36
29	U7	202	PEB	C3B-C2B	5.05	1.47	1.36
29	U9	202	PEB	C3B-C2B	5.05	1.47	1.36
29	S7	202	PEB	C3B-C2B	5.04	1.47	1.36
29	S9	202	PEB	C3B-C2B	5.04	1.47	1.36
29	RB	203	PEB	C3C-C4C	5.04	1.49	1.42
29	RM	203	PEB	C3C-C4C	5.04	1.49	1.42
30	AB	305	PUB	C2C-C3C	5.04	1.47	1.36
29	L5	202	PEB	C3B-C2B	5.04	1.47	1.36
29	B5	202	PEB	C3B-C2B	5.04	1.47	1.36
29	A5	202	PEB	C3B-C2B	5.04	1.47	1.36
29	A8	202	PEB	C3B-C2B	5.04	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	U1	202	PEB	C3C-C4C	5.04	1.49	1.42
29	ZB	203	PEB	C3C-C4C	5.04	1.49	1.42
29	UK	202	PEB	C3C-C4C	5.04	1.49	1.42
29	ZM	203	PEB	C3C-C4C	5.04	1.49	1.42
29	B8	201	PEB	C3B-C2B	5.04	1.47	1.36
29	C5	201	PEB	C3C-C4C	5.04	1.49	1.42
29	mB	203	PEB	C3C-C4C	5.04	1.49	1.42
29	mM	203	PEB	C3C-C4C	5.04	1.49	1.42
29	F8	202	PEB	C3B-C2B	5.04	1.47	1.36
29	TF	201	PEB	C3C-C4C	5.04	1.49	1.42
30	A7	302	PUB	C2C-C3C	5.04	1.47	1.36
30	A9	302	PUB	C2C-C3C	5.04	1.47	1.36
29	Q7	202	PEB	C3B-C2B	5.04	1.47	1.36
29	Q9	202	PEB	C3B-C2B	5.04	1.47	1.36
31	GK	1001	CYC	C2A-C3A	5.04	1.47	1.36
31	OP	1001	CYC	C3B-C2B	5.04	1.47	1.36
29	l7	202	PEB	C3B-C2B	5.04	1.47	1.36
29	l9	202	PEB	C3B-C2B	5.04	1.47	1.36
29	O1	201	PEB	C3B-C2B	5.04	1.47	1.36
29	OK	201	PEB	C3B-C2B	5.04	1.47	1.36
29	cB	203	PEB	C3C-C4C	5.04	1.49	1.42
29	cM	203	PEB	C3C-C4C	5.04	1.49	1.42
29	h1	201	PEB	C3B-C2B	5.03	1.47	1.36
29	l1	201	PEB	C3B-C2B	5.03	1.47	1.36
29	hK	201	PEB	C3B-C2B	5.03	1.47	1.36
29	lK	201	PEB	C3B-C2B	5.03	1.47	1.36
29	U1	202	PEB	C3B-C2B	5.03	1.47	1.36
29	UK	202	PEB	C3B-C2B	5.03	1.47	1.36
29	G8	203	PEB	C3B-C2B	5.03	1.47	1.36
29	mF	202	PEB	C3B-C2B	5.03	1.47	1.36
29	mI	202	PEB	C3B-C2B	5.03	1.47	1.36
29	S7	202	PEB	C3C-C4C	5.03	1.49	1.42
29	S9	202	PEB	C3C-C4C	5.03	1.49	1.42
29	kB	202	PEB	C3B-C2B	5.03	1.47	1.36
29	kM	202	PEB	C3B-C2B	5.03	1.47	1.36
29	G5	203	PEB	C3B-C2B	5.03	1.47	1.36
29	d7	202	PEB	C3B-C2B	5.03	1.47	1.36
29	d9	202	PEB	C3B-C2B	5.03	1.47	1.36
29	VB	201	PEB	C3B-C2B	5.03	1.47	1.36
29	VM	201	PEB	C3B-C2B	5.03	1.47	1.36
29	gB	203	PEB	C3C-C4C	5.03	1.49	1.42
29	gM	203	PEB	C3C-C4C	5.03	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d1	201	PEB	C3B-C2B	5.03	1.47	1.36
29	FB	202	PEB	C3B-C2B	5.03	1.47	1.36
29	dK	201	PEB	C3B-C2B	5.03	1.47	1.36
29	FM	202	PEB	C3B-C2B	5.03	1.47	1.36
29	K5	201	PEB	C3C-C4C	5.03	1.49	1.42
29	U7	202	PEB	C3C-C4C	5.03	1.49	1.42
29	K8	201	PEB	C3C-C4C	5.03	1.49	1.42
29	U9	202	PEB	C3C-C4C	5.03	1.49	1.42
29	Q1	201	PEB	C3B-C2B	5.03	1.47	1.36
29	HB	202	PEB	C3B-C2B	5.03	1.47	1.36
29	QK	201	PEB	C3B-C2B	5.03	1.47	1.36
29	HM	202	PEB	C3B-C2B	5.03	1.47	1.36
31	D1	1003	CYC	C2A-C3A	5.03	1.47	1.36
29	cB	202	PEB	C3B-C2B	5.03	1.47	1.36
29	cM	202	PEB	C3B-C2B	5.03	1.47	1.36
31	oP	1001	CYC	C3B-C2B	5.03	1.47	1.36
29	W1	201	PEB	C3B-C2B	5.03	1.47	1.36
29	VF	202	PEB	C3B-C2B	5.03	1.47	1.36
29	VI	202	PEB	C3B-C2B	5.03	1.47	1.36
29	WK	201	PEB	C3B-C2B	5.03	1.47	1.36
31	jP	1001	CYC	C3B-C2B	5.03	1.47	1.36
29	Q7	202	PEB	C3C-C4C	5.03	1.49	1.42
29	Q9	202	PEB	C3C-C4C	5.03	1.49	1.42
29	S1	201	PEB	C3B-C2B	5.03	1.47	1.36
29	SK	201	PEB	C3B-C2B	5.03	1.47	1.36
29	l1	201	PEB	C3C-C4C	5.03	1.49	1.42
29	lK	201	PEB	C3C-C4C	5.03	1.49	1.42
29	iB	202	PEB	C3B-C2B	5.03	1.47	1.36
29	iM	202	PEB	C3B-C2B	5.03	1.47	1.36
29	VB	202	PEB	C3B-C2B	5.02	1.47	1.36
29	VM	202	PEB	C3B-C2B	5.02	1.47	1.36
29	gB	202	PEB	C3B-C2B	5.02	1.47	1.36
29	mB	202	PEB	C3B-C2B	5.02	1.47	1.36
29	gM	202	PEB	C3B-C2B	5.02	1.47	1.36
29	mM	202	PEB	C3B-C2B	5.02	1.47	1.36
29	MA	405	PEB	C3C-C4C	5.02	1.49	1.42
29	O1	201	PEB	C3C-C4C	5.02	1.49	1.42
29	OK	201	PEB	C3C-C4C	5.02	1.49	1.42
29	N3	203	PEB	C3B-C2B	5.02	1.47	1.36
29	TB	202	PEB	C3B-C2B	5.02	1.47	1.36
29	TM	202	PEB	C3B-C2B	5.02	1.47	1.36
29	b1	201	PEB	C3C-C4C	5.02	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	bK	201	PEB	C3C-C4C	5.02	1.49	1.42
31	FP	1001	CYC	C3B-C2B	5.02	1.47	1.36
29	DB	202	PEB	C3B-C2B	5.02	1.47	1.36
29	DM	202	PEB	C3B-C2B	5.02	1.47	1.36
29	dF	201	PEB	C3B-C2B	5.02	1.47	1.36
29	dI	201	PEB	C3B-C2B	5.02	1.47	1.36
29	RB	202	PEB	C3B-C2B	5.02	1.47	1.36
29	RM	202	PEB	C3B-C2B	5.02	1.47	1.36
29	b7	202	PEB	C3C-C4C	5.02	1.49	1.42
29	j7	202	PEB	C3C-C4C	5.02	1.49	1.42
29	b9	202	PEB	C3C-C4C	5.02	1.49	1.42
29	j9	202	PEB	C3C-C4C	5.02	1.49	1.42
29	MQ	407	PEB	C3C-C4C	5.02	1.49	1.42
29	Z1	202	PEB	C3C-C4C	5.02	1.49	1.42
29	ZK	202	PEB	C3C-C4C	5.02	1.49	1.42
29	ID	202	PEB	C3B-C2B	5.02	1.47	1.36
31	QP	1001	CYC	C3B-C2B	5.02	1.47	1.36
31	hP	1001	CYC	C3B-C2B	5.02	1.47	1.36
29	GD	202	PEB	C3B-C2B	5.01	1.47	1.36
29	G4	202	PEB	C3B-C2B	5.01	1.47	1.36
29	E4	202	PEB	C3B-C2B	5.01	1.47	1.36
29	ED	201	PEB	C3B-C2B	5.01	1.47	1.36
31	qP	1001	CYC	C3B-C2B	5.01	1.47	1.36
31	E1	1001	CYC	C2A-C3A	5.01	1.47	1.36
29	MG	405	PEB	C3C-C4C	5.01	1.49	1.42
31	sP	1001	CYC	C3B-C2B	5.01	1.47	1.36
29	C8	201	PEB	C3C-C4C	5.01	1.49	1.42
31	K1	1001	CYC	C2A-C3A	5.01	1.47	1.36
31	KK	1001	CYC	C2A-C3A	5.01	1.47	1.36
29	OF	203	PEB	C3B-C2B	5.01	1.47	1.36
29	OI	203	PEB	C3B-C2B	5.01	1.47	1.36
31	1P	1001	CYC	C3B-C2B	5.01	1.47	1.36
29	B8	203	PEB	C3B-C2B	5.01	1.47	1.36
29	wL	302	PEB	C3C-C4C	5.01	1.49	1.42
29	j1	201	PEB	C3B-C2B	5.01	1.47	1.36
29	B5	203	PEB	C3B-C2B	5.01	1.47	1.36
29	YF	202	PEB	C3B-C2B	5.01	1.47	1.36
29	YI	202	PEB	C3B-C2B	5.01	1.47	1.36
29	jK	201	PEB	C3B-C2B	5.01	1.47	1.36
29	C4	202	PEB	C3B-C2B	5.01	1.47	1.36
29	CD	202	PEB	C3B-C2B	5.01	1.47	1.36
31	M1	1001	CYC	C2A-C3A	5.01	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	MK	1001	CYC	C2A-C3A	5.01	1.47	1.36
31	SP	1001	CYC	C3B-C2B	5.01	1.47	1.36
31	nP	1001	CYC	C3B-C2B	5.01	1.47	1.36
29	M4	202	PEB	C3B-C2B	5.01	1.47	1.36
29	MD	202	PEB	C3B-C2B	5.01	1.47	1.36
31	HP	1001	CYC	C3B-C2B	5.01	1.47	1.36
31	wP	1001	CYC	C3B-C2B	5.01	1.47	1.36
29	LB	202	PEB	C3B-C2B	5.00	1.47	1.36
29	LM	202	PEB	C3B-C2B	5.00	1.47	1.36
31	fP	1001	CYC	C3B-C2B	5.00	1.47	1.36
29	aB	203	PEB	C3B-C2B	5.00	1.47	1.36
29	aF	202	PEB	C3B-C2B	5.00	1.47	1.36
29	aI	202	PEB	C3B-C2B	5.00	1.47	1.36
29	aM	203	PEB	C3B-C2B	5.00	1.47	1.36
29	I5	202	PEB	C3B-C2B	5.00	1.47	1.36
29	I8	202	PEB	C3B-C2B	5.00	1.47	1.36
29	KB	203	PEB	C3B-C2B	5.00	1.47	1.36
29	KM	203	PEB	C3B-C2B	5.00	1.47	1.36
29	f7	202	PEB	C3C-C4C	5.00	1.49	1.42
29	f9	202	PEB	C3C-C4C	5.00	1.49	1.42
29	FG	201	PEB	C3C-C4C	5.00	1.49	1.42
29	FQ	201	PEB	C3C-C4C	5.00	1.49	1.42
29	HG	201	PEB	C3C-C4C	5.00	1.49	1.42
29	HQ	201	PEB	C3C-C4C	5.00	1.49	1.42
29	UF	201	PEB	C3B-C2B	5.00	1.47	1.36
29	UI	201	PEB	C3B-C2B	5.00	1.47	1.36
29	gF	202	PEB	C3B-C2B	5.00	1.47	1.36
29	gI	202	PEB	C3B-C2B	5.00	1.47	1.36
29	zJ	501	PEB	C3C-C4C	5.00	1.49	1.42
31	DP	1001	CYC	C3B-C2B	5.00	1.47	1.36
29	HG	202	PEB	C3C-C4C	5.00	1.49	1.42
29	HQ	202	PEB	C3C-C4C	5.00	1.49	1.42
31	kP	1001	CYC	C3B-C2B	5.00	1.47	1.36
29	zL	501	PEB	C3C-C4C	5.00	1.49	1.42
29	J5	201	PEB	C2A-C1A	-4.99	1.47	1.52
29	J8	201	PEB	C2A-C1A	-4.99	1.47	1.52
31	CK	1001	CYC	C2A-C3A	4.99	1.47	1.36
29	W7	202	PEB	C3C-C4C	4.99	1.49	1.42
29	W9	202	PEB	C3C-C4C	4.99	1.49	1.42
29	C5	202	PEB	C3B-C2B	4.99	1.47	1.36
29	C8	202	PEB	C3B-C2B	4.99	1.47	1.36
29	ZB	202	PEB	C3B-C2B	4.99	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZM	202	PEB	C3B-C2B	4.99	1.47	1.36
29	JG	201	PEB	C3C-C4C	4.99	1.49	1.42
29	JQ	201	PEB	C3C-C4C	4.99	1.49	1.42
29	BB	301	PEB	C3C-C4C	4.99	1.49	1.42
29	BM	301	PEB	C3C-C4C	4.99	1.49	1.42
29	kF	202	PEB	C3B-C2B	4.99	1.47	1.36
29	kI	202	PEB	C3B-C2B	4.99	1.47	1.36
29	h7	202	PEB	C3C-C4C	4.99	1.49	1.42
29	h9	202	PEB	C3C-C4C	4.99	1.49	1.42
29	iF	202	PEB	C3B-C2B	4.99	1.47	1.36
29	iI	202	PEB	C3B-C2B	4.99	1.47	1.36
29	I4	202	PEB	C3B-C2B	4.99	1.47	1.36
29	PF	202	PEB	C3B-C2B	4.99	1.47	1.36
29	PI	202	PEB	C3B-C2B	4.99	1.47	1.36
31	I1	1001	CYC	C2A-C3A	4.99	1.47	1.36
29	xJ	302	PEB	C3C-C4C	4.99	1.49	1.42
31	C1	1001	CYC	C2A-C3A	4.98	1.47	1.36
29	K5	202	PEB	C3B-C2B	4.98	1.47	1.36
29	K8	202	PEB	C3B-C2B	4.98	1.47	1.36
29	I5	201	PEB	C3C-C4C	4.98	1.49	1.42
29	I8	201	PEB	C3C-C4C	4.98	1.49	1.42
31	BP	1001	CYC	C3B-C2B	4.98	1.47	1.36
31	uP	1001	CYC	C3B-C2B	4.98	1.47	1.36
29	DG	201	PEB	C3C-C4C	4.98	1.49	1.42
29	DQ	201	PEB	C3C-C4C	4.98	1.49	1.42
29	QB	202	PEB	C3B-C2B	4.98	1.47	1.36
29	QM	202	PEB	C3B-C2B	4.98	1.47	1.36
29	MN	405	PEB	C3C-C4C	4.98	1.49	1.42
29	BA	202	PEB	C3B-C2B	4.98	1.47	1.36
29	BN	202	PEB	C3B-C2B	4.98	1.47	1.36
29	NO	203	PEB	C3B-C2B	4.98	1.47	1.36
29	O7	202	PEB	C3C-C4C	4.98	1.49	1.42
29	O9	202	PEB	C3C-C4C	4.98	1.49	1.42
31	UP	1001	CYC	C3B-C2B	4.98	1.47	1.36
31	IK	1001	CYC	C2A-C3A	4.98	1.47	1.36
29	eF	202	PEB	C3B-C2B	4.98	1.47	1.36
29	eI	202	PEB	C3B-C2B	4.98	1.47	1.36
31	XP	1001	CYC	C3B-C2B	4.98	1.47	1.36
29	d7	202	PEB	C3C-C4C	4.98	1.49	1.42
29	d9	202	PEB	C3C-C4C	4.98	1.49	1.42
31	EK	1001	CYC	C2A-C3A	4.97	1.47	1.36
29	WF	202	PEB	C3C-C4C	4.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	WI	202	PEB	C3C-C4C	4.97	1.49	1.42
29	A1	301	PEB	C3C-C4C	4.97	1.49	1.42
29	AK	301	PEB	C3C-C4C	4.97	1.49	1.42
29	Z7	202	PEB	C3C-C4C	4.96	1.49	1.42
29	Z9	202	PEB	C3C-C4C	4.96	1.49	1.42
29	SF	202	PEB	C3C-C4C	4.96	1.49	1.42
29	SI	202	PEB	C3C-C4C	4.96	1.49	1.42
30	A1	304	PUB	C2B-C1B	4.96	1.49	1.42
30	AK	304	PUB	C2B-C1B	4.96	1.49	1.42
31	IP	1001	CYC	C3B-C2B	4.96	1.47	1.36
29	xL	302	PEB	C3C-C4C	4.96	1.49	1.42
29	M3	203	PEB	C3B-C2B	4.96	1.47	1.36
29	MO	203	PEB	C3B-C2B	4.96	1.47	1.36
29	HA	202	PEB	C3B-C2B	4.96	1.47	1.36
29	LA	202	PEB	C3B-C2B	4.96	1.47	1.36
29	HN	202	PEB	C3B-C2B	4.96	1.47	1.36
29	LN	202	PEB	C3B-C2B	4.96	1.47	1.36
29	l7	202	PEB	C3C-C4C	4.95	1.49	1.42
29	l9	202	PEB	C3C-C4C	4.95	1.49	1.42
29	LG	201	PEB	C3C-C4C	4.95	1.49	1.42
29	MQ	402	PEB	C3C-C4C	4.95	1.49	1.42
29	OF	202	PEB	C3C-C4C	4.95	1.49	1.42
29	BG	201	PEB	C3C-C4C	4.95	1.49	1.42
29	OI	202	PEB	C3C-C4C	4.95	1.49	1.42
29	BQ	201	PEB	C3C-C4C	4.95	1.49	1.42
29	FA	202	PEB	C3B-C2B	4.95	1.47	1.36
29	FN	202	PEB	C3B-C2B	4.95	1.47	1.36
29	AA	202	PEB	C3C-C4C	4.95	1.49	1.42
29	AN	202	PEB	C3C-C4C	4.95	1.49	1.42
29	MQ	403	PEB	C3C-C4C	4.95	1.49	1.42
29	MG	401	PEB	C3C-C4C	4.95	1.49	1.42
30	AB	304	PUB	C2C-C3C	4.95	1.47	1.36
29	dF	203	PEB	C3C-C4C	4.95	1.49	1.42
29	dI	203	PEB	C3C-C4C	4.95	1.49	1.42
29	fF	202	PEB	C3C-C4C	4.95	1.49	1.42
29	fI	202	PEB	C3C-C4C	4.95	1.49	1.42
29	JA	202	PEB	C3B-C2B	4.95	1.47	1.36
29	JN	202	PEB	C3B-C2B	4.95	1.47	1.36
29	hF	202	PEB	C3C-C4C	4.95	1.49	1.42
29	hI	202	PEB	C3C-C4C	4.95	1.49	1.42
29	bF	202	PEB	C3C-C4C	4.94	1.49	1.42
29	bI	202	PEB	C3C-C4C	4.94	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	J1	1001	CYC	C2A-C3A	4.94	1.47	1.36
31	JK	1001	CYC	C2A-C3A	4.94	1.47	1.36
29	BG	202	PEB	C3C-C4C	4.94	1.49	1.42
29	BQ	202	PEB	C3C-C4C	4.94	1.49	1.42
29	HK	1002	PEB	C3C-C4C	4.94	1.49	1.42
29	JG	202	PEB	C3C-C4C	4.94	1.49	1.42
29	JQ	202	PEB	C3C-C4C	4.94	1.49	1.42
31	DK	1001	CYC	C2A-C3A	4.94	1.47	1.36
31	D1	1001	CYC	C2A-C3A	4.94	1.47	1.36
29	AF	301	PEB	C3C-C4C	4.94	1.49	1.42
29	AI	301	PEB	C3C-C4C	4.94	1.49	1.42
29	i1	202	PEB	C3B-C2B	4.94	1.47	1.36
29	iK	202	PEB	C3B-C2B	4.94	1.47	1.36
29	V1	202	PEB	C3B-C2B	4.94	1.47	1.36
29	VK	202	PEB	C3B-C2B	4.94	1.47	1.36
29	GC	202	PEB	C3C-C4C	4.94	1.49	1.42
29	GE	202	PEB	C3C-C4C	4.94	1.49	1.42
29	UF	203	PEB	C3C-C4C	4.93	1.49	1.42
29	UI	203	PEB	C3C-C4C	4.93	1.49	1.42
29	Z1	201	PEB	C3B-C2B	4.93	1.47	1.36
29	e1	202	PEB	C3B-C2B	4.93	1.47	1.36
29	ZK	201	PEB	C3B-C2B	4.93	1.47	1.36
29	eK	202	PEB	C3B-C2B	4.93	1.47	1.36
29	lF	202	PEB	C3C-C4C	4.93	1.49	1.42
29	lI	202	PEB	C3C-C4C	4.93	1.49	1.42
29	FG	202	PEB	C3C-C4C	4.93	1.49	1.42
29	FQ	202	PEB	C3C-C4C	4.93	1.49	1.42
31	F1	1001	CYC	C2A-C3A	4.93	1.47	1.36
31	FK	1001	CYC	C2A-C3A	4.93	1.47	1.36
29	AC	202	PEB	C3C-C4C	4.93	1.49	1.42
29	AE	202	PEB	C3C-C4C	4.93	1.49	1.42
29	L1	1002	PEB	C3C-C4C	4.93	1.49	1.42
29	LK	1002	PEB	C3C-C4C	4.93	1.49	1.42
30	AM	304	PUB	C2C-C3C	4.93	1.47	1.36
29	N1	1002	PEB	C3C-C4C	4.92	1.49	1.42
31	N1	1001	CYC	C2A-C3A	4.92	1.47	1.36
29	DA	202	PEB	C3B-C2B	4.92	1.47	1.36
29	DN	202	PEB	C3B-C2B	4.92	1.47	1.36
29	NK	1002	PEB	C3C-C4C	4.92	1.49	1.42
29	H1	1002	PEB	C3C-C4C	4.92	1.49	1.42
29	A7	301	PEB	C3C-C4C	4.92	1.49	1.42
29	A9	301	PEB	C3C-C4C	4.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	NK	1001	CYC	C2A-C3A	4.92	1.47	1.36
31	DF	1001	CYC	C2A-C3A	4.92	1.47	1.36
31	DI	1001	CYC	C2A-C3A	4.92	1.47	1.36
29	B3	201	PEB	C3C-C4C	4.92	1.49	1.42
29	BO	201	PEB	C3C-C4C	4.92	1.49	1.42
29	U1	201	PEB	C3B-C2B	4.92	1.47	1.36
29	UK	201	PEB	C3B-C2B	4.92	1.47	1.36
31	HK	1001	CYC	C2A-C3A	4.92	1.47	1.36
29	QF	202	PEB	C3C-C4C	4.91	1.49	1.42
29	QI	202	PEB	C3C-C4C	4.91	1.49	1.42
29	IC	202	PEB	C3C-C4C	4.91	1.49	1.42
29	IE	202	PEB	C3C-C4C	4.91	1.49	1.42
29	KA	202	PEB	C3C-C4C	4.91	1.49	1.42
29	KN	202	PEB	C3C-C4C	4.91	1.49	1.42
29	D1	1002	PEB	C3C-C4C	4.91	1.49	1.42
31	L1	1001	CYC	C2A-C3A	4.91	1.47	1.36
31	LK	1001	CYC	C2A-C3A	4.91	1.47	1.36
29	c1	202	PEB	C3B-C2B	4.91	1.47	1.36
29	g1	202	PEB	C3B-C2B	4.91	1.47	1.36
29	cK	202	PEB	C3B-C2B	4.91	1.47	1.36
29	gK	202	PEB	C3B-C2B	4.91	1.47	1.36
31	HF	1001	CYC	C2A-C3A	4.91	1.47	1.36
31	HI	1001	CYC	C2A-C3A	4.91	1.47	1.36
29	CC	202	PEB	C3C-C4C	4.91	1.49	1.42
29	CE	202	PEB	C3C-C4C	4.91	1.49	1.42
29	DG	202	PEB	C3C-C4C	4.91	1.49	1.42
29	DQ	202	PEB	C3C-C4C	4.91	1.49	1.42
29	GG	201	PEB	C3B-C2B	4.91	1.47	1.36
29	GQ	201	PEB	C3B-C2B	4.91	1.47	1.36
29	j1	203	PEB	C3B-C2B	4.90	1.47	1.36
29	jK	203	PEB	C3B-C2B	4.90	1.47	1.36
29	LG	202	PEB	C3C-C4C	4.90	1.49	1.42
29	LQ	201	PEB	C3C-C4C	4.90	1.49	1.42
29	e2	401	PEB	CHB-C4B	4.90	1.39	1.35
29	R1	202	PEB	C3B-C2B	4.90	1.47	1.36
29	RK	202	PEB	C3B-C2B	4.90	1.47	1.36
29	FG	202	PEB	C3B-C2B	4.90	1.47	1.36
29	FQ	202	PEB	C3B-C2B	4.90	1.47	1.36
29	a1	202	PEB	C3B-C2B	4.90	1.47	1.36
29	aK	202	PEB	C3B-C2B	4.90	1.47	1.36
29	EC	202	PEB	C3C-C4C	4.90	1.49	1.42
29	EE	202	PEB	C3C-C4C	4.90	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EA	202	PEB	C3C-C4C	4.90	1.49	1.42
29	EN	202	PEB	C3C-C4C	4.90	1.49	1.42
29	P1	202	PEB	C3B-C2B	4.90	1.47	1.36
29	PK	202	PEB	C3B-C2B	4.90	1.47	1.36
31	LF	1001	CYC	C2A-C3A	4.90	1.47	1.36
31	LI	1001	CYC	C2A-C3A	4.90	1.47	1.36
29	e7	203	PEB	C3C-C4C	4.90	1.49	1.42
29	e9	203	PEB	C3C-C4C	4.90	1.49	1.42
29	jF	202	PEB	C3C-C4C	4.90	1.49	1.42
29	jI	202	PEB	C3C-C4C	4.90	1.49	1.42
29	DG	202	PEB	C3B-C2B	4.90	1.47	1.36
29	DQ	202	PEB	C3B-C2B	4.90	1.47	1.36
29	P7	203	PEB	C3C-C4C	4.90	1.49	1.42
29	P9	203	PEB	C3C-C4C	4.90	1.49	1.42
29	CA	201	PEB	C3B-C2B	4.90	1.47	1.36
29	CN	201	PEB	C3B-C2B	4.90	1.47	1.36
31	JF	1001	CYC	C2A-C3A	4.90	1.47	1.36
31	JI	1001	CYC	C2A-C3A	4.90	1.47	1.36
31	NF	1001	CYC	C2A-C3A	4.90	1.47	1.36
31	NI	1001	CYC	C2A-C3A	4.90	1.47	1.36
29	AG	201	PEB	C3B-C2B	4.89	1.47	1.36
29	AQ	201	PEB	C3B-C2B	4.89	1.47	1.36
29	H3	201	PEB	C3C-C4C	4.89	1.49	1.42
29	HO	201	PEB	C3C-C4C	4.89	1.49	1.42
29	AB	301	PEB	C3C-C4C	4.89	1.49	1.42
29	DK	1002	PEB	C3C-C4C	4.89	1.49	1.42
31	H1	1001	CYC	C2A-C3A	4.89	1.47	1.36
29	EG	201	PEB	C3B-C2B	4.89	1.47	1.36
29	EQ	201	PEB	C3B-C2B	4.89	1.47	1.36
29	A1	303	PEB	C3C-C4C	4.89	1.49	1.42
29	AK	303	PEB	C3C-C4C	4.89	1.49	1.42
29	B5	201	PEB	C3C-C4C	4.88	1.49	1.42
29	SR	201	PEB	C3C-C4C	4.88	1.49	1.42
29	CG	201	PEB	C3B-C2B	4.88	1.47	1.36
29	CQ	201	PEB	C3B-C2B	4.88	1.47	1.36
29	KC	203	PEB	C3C-C4C	4.88	1.49	1.42
29	KE	203	PEB	C3C-C4C	4.88	1.49	1.42
29	k1	202	PEB	C3B-C2B	4.88	1.47	1.36
29	LG	202	PEB	C3B-C2B	4.88	1.47	1.36
29	kK	202	PEB	C3B-C2B	4.88	1.47	1.36
29	LQ	201	PEB	C3B-C2B	4.88	1.47	1.36
31	FF	1001	CYC	C2A-C3A	4.88	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	FI	1001	CYC	C2A-C3A	4.88	1.47	1.36
29	F1	1002	PEB	C3C-C4C	4.88	1.49	1.42
29	FK	1002	PEB	C3C-C4C	4.88	1.49	1.42
29	IG	201	PEB	C3B-C2B	4.88	1.47	1.36
29	IQ	201	PEB	C3B-C2B	4.88	1.47	1.36
29	KG	201	PEB	C3B-C2B	4.87	1.47	1.36
29	KQ	201	PEB	C3B-C2B	4.87	1.47	1.36
29	ZF	202	PEB	C3C-C4C	4.87	1.49	1.42
29	ZI	202	PEB	C3C-C4C	4.87	1.49	1.42
29	JG	202	PEB	C3B-C2B	4.87	1.47	1.36
29	JQ	202	PEB	C3B-C2B	4.87	1.47	1.36
29	J1	1002	PEB	C3C-C4C	4.87	1.49	1.42
29	JK	1002	PEB	C3C-C4C	4.87	1.49	1.42
29	k7	203	PEB	C3C-C4C	4.87	1.49	1.42
29	k9	203	PEB	C3C-C4C	4.87	1.49	1.42
29	F3	201	PEB	C3C-C4C	4.87	1.49	1.42
29	G5	201	PEB	C3C-C4C	4.87	1.49	1.42
29	FO	201	PEB	C3C-C4C	4.87	1.49	1.42
29	R7	203	PEB	C3C-C4C	4.86	1.49	1.42
29	Y7	203	PEB	C3C-C4C	4.86	1.49	1.42
29	R9	203	PEB	C3C-C4C	4.86	1.49	1.42
29	Y9	203	PEB	C3C-C4C	4.86	1.49	1.42
29	eR	401	PEB	CHB-C4B	4.86	1.39	1.35
29	g7	203	PEB	C3C-C4C	4.86	1.49	1.42
29	g9	203	PEB	C3C-C4C	4.86	1.49	1.42
29	LJ	202	PEB	C3B-C2B	4.86	1.47	1.36
29	LL	202	PEB	C3B-C2B	4.86	1.47	1.36
29	m7	203	PEB	C3C-C4C	4.86	1.49	1.42
29	m9	203	PEB	C3C-C4C	4.86	1.49	1.42
31	F1	1001	CYC	CHB-C1B	4.86	1.49	1.38
31	FK	1001	CYC	CHB-C1B	4.86	1.49	1.38
29	T7	203	PEB	C3C-C4C	4.85	1.49	1.42
29	T9	203	PEB	C3C-C4C	4.85	1.49	1.42
29	J3	201	PEB	C3C-C4C	4.85	1.49	1.42
29	JO	201	PEB	C3C-C4C	4.85	1.49	1.42
29	HG	202	PEB	C3B-C2B	4.85	1.47	1.36
29	HQ	202	PEB	C3B-C2B	4.85	1.47	1.36
29	BG	202	PEB	C3B-C2B	4.85	1.47	1.36
29	BQ	202	PEB	C3B-C2B	4.85	1.47	1.36
29	CA	202	PEB	C3C-C4C	4.85	1.49	1.42
29	CN	202	PEB	C3C-C4C	4.85	1.49	1.42
29	L8	201	PEB	C3C-C4C	4.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a7	203	PEB	C3C-C4C	4.85	1.49	1.42
29	a9	203	PEB	C3C-C4C	4.85	1.49	1.42
31	NK	1001	CYC	CHB-C1B	4.85	1.49	1.38
29	V7	203	PEB	C3C-C4C	4.85	1.49	1.42
29	V9	203	PEB	C3C-C4C	4.85	1.49	1.42
29	B8	201	PEB	C3C-C4C	4.85	1.49	1.42
31	L1	1001	CYC	CHB-C1B	4.85	1.49	1.38
31	LK	1001	CYC	CHB-C1B	4.85	1.49	1.38
29	D3	201	PEB	C3C-C4C	4.85	1.49	1.42
29	J5	201	PEB	C3C-C4C	4.85	1.49	1.42
29	J8	201	PEB	C3C-C4C	4.85	1.49	1.42
29	GA	202	PEB	C3C-C4C	4.85	1.49	1.42
29	GN	202	PEB	C3C-C4C	4.85	1.49	1.42
29	DO	201	PEB	C3C-C4C	4.85	1.49	1.42
29	kB	202	PEB	C3C-C4C	4.84	1.49	1.42
29	kM	202	PEB	C3C-C4C	4.84	1.49	1.42
29	mB	202	PEB	C3C-C4C	4.84	1.49	1.42
29	mM	202	PEB	C3C-C4C	4.84	1.49	1.42
29	AM	301	PEB	C3C-C4C	4.84	1.49	1.42
29	BJ	203	PEB	C3B-C2B	4.84	1.47	1.36
29	BL	203	PEB	C3B-C2B	4.84	1.47	1.36
29	c7	203	PEB	C3C-C4C	4.84	1.49	1.42
29	c9	203	PEB	C3C-C4C	4.84	1.49	1.42
29	I4	201	PEB	C3B-C2B	4.84	1.47	1.36
31	KI	1001	CYC	C2A-C3A	4.84	1.47	1.36
31	D1	1001	CYC	CHB-C1B	4.84	1.49	1.38
29	G8	201	PEB	C3C-C4C	4.84	1.49	1.42
31	N1	1001	CYC	CHB-C1B	4.84	1.49	1.38
29	aB	203	PEB	C3C-C4C	4.84	1.49	1.42
29	aM	203	PEB	C3C-C4C	4.84	1.49	1.42
29	ZJ	203	PEB	C3B-C2B	4.84	1.47	1.36
29	ZL	203	PEB	C3B-C2B	4.84	1.47	1.36
29	L3	201	PEB	C3C-C4C	4.83	1.49	1.42
29	LO	201	PEB	C3C-C4C	4.83	1.49	1.42
29	C4	201	PEB	C3B-C2B	4.83	1.47	1.36
29	TJ	203	PEB	C3B-C2B	4.83	1.47	1.36
29	TL	203	PEB	C3B-C2B	4.83	1.47	1.36
29	TR	203	PEB	C3C-C4C	4.83	1.49	1.42
31	DK	1001	CYC	CHB-C1B	4.83	1.49	1.38
29	XJ	203	PEB	C3B-C2B	4.83	1.47	1.36
29	XL	203	PEB	C3B-C2B	4.83	1.47	1.36
29	QB	202	PEB	C3C-C4C	4.83	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QM	202	PEB	C3C-C4C	4.83	1.49	1.42
29	VJ	202	PEB	C3B-C2B	4.83	1.47	1.36
29	VL	202	PEB	C3B-C2B	4.83	1.47	1.36
29	jJ	203	PEB	C3B-C2B	4.82	1.47	1.36
29	jL	203	PEB	C3B-C2B	4.82	1.47	1.36
29	MD	201	PEB	C3B-C2B	4.82	1.47	1.36
29	P2	201	PEB	C3B-C2B	4.82	1.47	1.36
29	ID	201	PEB	C3B-C2B	4.82	1.47	1.36
29	VB	202	PEB	C3C-C4C	4.82	1.49	1.42
29	VM	202	PEB	C3C-C4C	4.82	1.49	1.42
29	iB	202	PEB	C3C-C4C	4.82	1.49	1.42
29	iM	202	PEB	C3C-C4C	4.82	1.49	1.42
29	KA	201	PEB	C3B-C2B	4.82	1.47	1.36
29	KN	201	PEB	C3B-C2B	4.82	1.47	1.36
29	HB	202	PEB	C3C-C4C	4.82	1.49	1.42
29	HM	202	PEB	C3C-C4C	4.82	1.49	1.42
29	bJ	203	PEB	C3B-C2B	4.82	1.47	1.36
29	dJ	203	PEB	C3B-C2B	4.82	1.47	1.36
29	bL	203	PEB	C3B-C2B	4.82	1.47	1.36
29	dL	203	PEB	C3B-C2B	4.82	1.47	1.36
29	hJ	203	PEB	C3B-C2B	4.82	1.47	1.36
29	hL	203	PEB	C3B-C2B	4.82	1.47	1.36
29	F5	201	PEB	C3C-C4C	4.82	1.49	1.42
29	F8	201	PEB	C3C-C4C	4.82	1.49	1.42
29	IA	202	PEB	C3C-C4C	4.82	1.49	1.42
29	IN	202	PEB	C3C-C4C	4.82	1.49	1.42
29	dD	401	PEB	C3B-C2B	4.82	1.47	1.36
29	pJ	203	PEB	C3B-C2B	4.82	1.47	1.36
29	pL	203	PEB	C3B-C2B	4.82	1.47	1.36
29	PJ	203	PEB	C3B-C2B	4.82	1.47	1.36
29	PL	203	PEB	C3B-C2B	4.82	1.47	1.36
29	i7	203	PEB	C3C-C4C	4.82	1.49	1.42
29	i9	203	PEB	C3C-C4C	4.82	1.49	1.42
29	AA	201	PEB	C3B-C2B	4.82	1.47	1.36
29	AN	201	PEB	C3B-C2B	4.82	1.47	1.36
29	GA	201	PEB	C3B-C2B	4.82	1.47	1.36
29	GN	201	PEB	C3B-C2B	4.82	1.47	1.36
29	V2	202	PEB	C3B-C2B	4.81	1.47	1.36
31	MF	1001	CYC	C2A-C3A	4.81	1.47	1.36
31	MI	1001	CYC	C2A-C3A	4.81	1.47	1.36
29	VR	202	PEB	C3B-C2B	4.81	1.47	1.36
29	EA	201	PEB	C3B-C2B	4.81	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EN	201	PEB	C3B-C2B	4.81	1.47	1.36
31	KF	1001	CYC	C2A-C3A	4.81	1.47	1.36
29	L5	201	PEB	C3C-C4C	4.81	1.49	1.42
31	HK	1001	CYC	CHB-C1B	4.81	1.49	1.38
29	vJ	202	PEB	C3B-C2B	4.81	1.47	1.36
29	vL	202	PEB	C3B-C2B	4.81	1.47	1.36
29	LB	202	PEB	C3C-C4C	4.81	1.49	1.42
29	LM	202	PEB	C3C-C4C	4.81	1.49	1.42
29	DJ	202	PEB	C3B-C2B	4.81	1.47	1.36
29	tJ	202	PEB	C3B-C2B	4.81	1.47	1.36
29	DL	202	PEB	C3B-C2B	4.81	1.47	1.36
29	tL	202	PEB	C3B-C2B	4.81	1.47	1.36
29	FJ	203	PEB	C3B-C2B	4.81	1.47	1.36
29	JJ	203	PEB	C3B-C2B	4.81	1.47	1.36
29	FL	203	PEB	C3B-C2B	4.81	1.47	1.36
29	JL	203	PEB	C3B-C2B	4.81	1.47	1.36
31	J1	1001	CYC	CHB-C1B	4.81	1.49	1.38
31	JK	1001	CYC	CHB-C1B	4.81	1.49	1.38
29	lJ	203	PEB	C3B-C2B	4.81	1.46	1.36
29	lL	203	PEB	C3B-C2B	4.81	1.46	1.36
29	cB	202	PEB	C3C-C4C	4.81	1.49	1.42
29	cM	202	PEB	C3C-C4C	4.81	1.49	1.42
29	nJ	203	PEB	C3B-C2B	4.81	1.46	1.36
29	nL	203	PEB	C3B-C2B	4.81	1.46	1.36
29	IA	201	PEB	C3B-C2B	4.81	1.46	1.36
29	CD	201	PEB	C3B-C2B	4.81	1.46	1.36
29	IN	201	PEB	C3B-C2B	4.81	1.46	1.36
29	N2	202	PEB	C3B-C2B	4.81	1.46	1.36
29	AG	201	PEB	C3C-C4C	4.81	1.49	1.42
29	AQ	201	PEB	C3C-C4C	4.81	1.49	1.42
31	EF	1001	CYC	C2A-C3A	4.80	1.46	1.36
31	GF	1001	CYC	C2A-C3A	4.80	1.46	1.36
31	EI	1001	CYC	C2A-C3A	4.80	1.46	1.36
31	GI	1001	CYC	C2A-C3A	4.80	1.46	1.36
31	H1	1001	CYC	CHB-C1B	4.80	1.49	1.38
29	RJ	203	PEB	C3B-C2B	4.80	1.46	1.36
29	RL	203	PEB	C3B-C2B	4.80	1.46	1.36
29	E4	201	PEB	C3B-C2B	4.80	1.46	1.36
29	N2	203	PEB	C3C-C4C	4.80	1.49	1.42
29	rJ	203	PEB	C3B-C2B	4.80	1.46	1.36
29	rL	203	PEB	C3B-C2B	4.80	1.46	1.36
29	NJ	203	PEB	C3B-C2B	4.80	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NL	203	PEB	C3B-C2B	4.80	1.46	1.36
29	M4	201	PEB	C3B-C2B	4.80	1.46	1.36
29	DB	202	PEB	C3C-C4C	4.80	1.49	1.42
29	ZB	202	PEB	C3C-C4C	4.80	1.49	1.42
29	DM	202	PEB	C3C-C4C	4.80	1.49	1.42
29	ZM	202	PEB	C3C-C4C	4.80	1.49	1.42
31	CF	1001	CYC	C2A-C3A	4.80	1.46	1.36
31	CI	1001	CYC	C2A-C3A	4.80	1.46	1.36
29	RB	202	PEB	C3C-C4C	4.80	1.49	1.42
29	RM	202	PEB	C3C-C4C	4.80	1.49	1.42
29	TB	202	PEB	C3C-C4C	4.79	1.49	1.42
29	TM	202	PEB	C3C-C4C	4.79	1.49	1.42
29	JB	202	PEB	C3C-C4C	4.79	1.49	1.42
29	KB	203	PEB	C3C-C4C	4.79	1.49	1.42
29	JM	202	PEB	C3C-C4C	4.79	1.49	1.42
29	KM	203	PEB	C3C-C4C	4.79	1.49	1.42
29	YB	201	PEB	C3C-C4C	4.79	1.49	1.42
29	YM	201	PEB	C3C-C4C	4.79	1.49	1.42
29	PR	201	PEB	C3B-C2B	4.79	1.46	1.36
29	B4	202	PEB	C3B-C2B	4.78	1.46	1.36
29	H5	201	PEB	C3C-C4C	4.78	1.49	1.42
29	W2	202	PEB	C3C-C4C	4.78	1.49	1.42
29	FB	202	PEB	C3C-C4C	4.78	1.49	1.42
29	FM	202	PEB	C3C-C4C	4.78	1.49	1.42
29	I3	201	PEB	C3B-C2B	4.78	1.46	1.36
29	IO	201	PEB	C3B-C2B	4.78	1.46	1.36
29	X2	201	PEB	C3B-C2B	4.78	1.46	1.36
29	XR	202	PEB	C3B-C2B	4.78	1.46	1.36
29	nJ	201	PEB	C3C-C4C	4.78	1.49	1.42
29	nL	201	PEB	C3C-C4C	4.78	1.49	1.42
29	C3	201	PEB	C3B-C2B	4.78	1.46	1.36
29	CO	201	PEB	C3B-C2B	4.78	1.46	1.36
29	HJ	202	PEB	C3B-C2B	4.78	1.46	1.36
29	HL	202	PEB	C3B-C2B	4.78	1.46	1.36
29	TR	202	PEB	C3B-C2B	4.78	1.46	1.36
29	KG	201	PEB	C3C-C4C	4.77	1.49	1.42
29	KQ	201	PEB	C3C-C4C	4.77	1.49	1.42
29	RR	203	PEB	C3C-C4C	4.77	1.49	1.42
29	T2	202	PEB	C3B-C2B	4.77	1.46	1.36
29	NR	202	PEB	C3B-C2B	4.77	1.46	1.36
29	K4	201	PEB	C3B-C2B	4.77	1.46	1.36
29	KD	201	PEB	C3B-C2B	4.77	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fJ	203	PEB	C3B-C2B	4.77	1.46	1.36
29	fL	203	PEB	C3B-C2B	4.77	1.46	1.36
29	QR	202	PEB	CHA-C1B	4.77	1.51	1.40
29	H8	201	PEB	C3C-C4C	4.76	1.49	1.42
29	GD	201	PEB	C3B-C2B	4.76	1.46	1.36
29	D4	202	PEB	C3B-C2B	4.76	1.46	1.36
29	A3	201	PEB	C3B-C2B	4.76	1.46	1.36
29	AO	201	PEB	C3B-C2B	4.76	1.46	1.36
29	BD	202	PEB	C3B-C2B	4.76	1.46	1.36
29	GG	201	PEB	C3C-C4C	4.76	1.49	1.42
29	GQ	201	PEB	C3C-C4C	4.76	1.49	1.42
29	T2	203	PEB	C3C-C4C	4.76	1.49	1.42
29	RR	202	PEB	C3B-C2B	4.76	1.46	1.36
29	gB	202	PEB	C3C-C4C	4.76	1.49	1.42
29	gM	202	PEB	C3C-C4C	4.76	1.49	1.42
29	R2	203	PEB	C3C-C4C	4.76	1.49	1.42
30	wL	304	PUB	C2B-C1B	4.76	1.49	1.42
29	tJ	201	PEB	C3C-C4C	4.76	1.49	1.42
29	tL	201	PEB	C3C-C4C	4.76	1.49	1.42
31	IF	1001	CYC	C2A-C3A	4.76	1.46	1.36
31	II	1001	CYC	C2A-C3A	4.76	1.46	1.36
29	VR	203	PEB	C3C-C4C	4.75	1.49	1.42
29	O2	202	PEB	C3C-C4C	4.75	1.49	1.42
29	dJ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	dL	201	PEB	C3C-C4C	4.75	1.49	1.42
29	IG	201	PEB	C3C-C4C	4.75	1.49	1.42
29	IQ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	G3	201	PEB	C3B-C2B	4.75	1.46	1.36
29	G4	201	PEB	C3B-C2B	4.75	1.46	1.36
29	GO	201	PEB	C3B-C2B	4.75	1.46	1.36
29	vJ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	vL	201	PEB	C3C-C4C	4.75	1.49	1.42
29	EG	201	PEB	C3C-C4C	4.75	1.49	1.42
29	EQ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	RJ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	RL	201	PEB	C3C-C4C	4.75	1.49	1.42
29	hJ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	hL	201	PEB	C3C-C4C	4.75	1.49	1.42
29	bJ	201	PEB	C3C-C4C	4.75	1.49	1.42
29	bL	201	PEB	C3C-C4C	4.75	1.49	1.42
29	X2	202	PEB	C3C-C4C	4.74	1.49	1.42
29	XR	203	PEB	C3C-C4C	4.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FJ	201	PEB	C3C-C4C	4.74	1.49	1.42
29	FL	201	PEB	C3C-C4C	4.74	1.49	1.42
29	NR	203	PEB	C3C-C4C	4.74	1.49	1.42
29	K3	201	PEB	C3B-C2B	4.74	1.46	1.36
29	KO	201	PEB	C3B-C2B	4.74	1.46	1.36
29	E3	201	PEB	C3B-C2B	4.74	1.46	1.36
29	EO	201	PEB	C3B-C2B	4.74	1.46	1.36
29	L4	202	PEB	C3B-C2B	4.74	1.46	1.36
29	M3	202	PEB	C3C-C4C	4.74	1.49	1.42
29	MO	202	PEB	C3C-C4C	4.74	1.49	1.42
30	wJ	304	PUB	C2B-C1B	4.74	1.49	1.42
29	N3	202	PEB	C3C-C4C	4.74	1.49	1.42
29	R2	202	PEB	C3B-C2B	4.74	1.46	1.36
29	H4	202	PEB	C3B-C2B	4.74	1.46	1.36
29	F4	202	PEB	C3B-C2B	4.73	1.46	1.36
29	P2	202	PEB	C3C-C4C	4.73	1.49	1.42
29	jJ	201	PEB	C3C-C4C	4.73	1.49	1.42
29	jL	201	PEB	C3C-C4C	4.73	1.49	1.42
29	NO	202	PEB	C3C-C4C	4.73	1.49	1.42
29	PR	202	PEB	C3C-C4C	4.73	1.49	1.42
29	HA	203	PEB	C3B-C2B	4.73	1.46	1.36
29	HN	203	PEB	C3B-C2B	4.73	1.46	1.36
29	CG	201	PEB	C3C-C4C	4.73	1.49	1.42
29	CQ	201	PEB	C3C-C4C	4.73	1.49	1.42
29	m7	201	PEB	C3B-C2B	4.73	1.46	1.36
29	m9	201	PEB	C3B-C2B	4.73	1.46	1.36
29	U2	202	PEB	CHA-C1B	4.73	1.51	1.40
29	wL	303	PEB	C3C-C4C	4.73	1.49	1.42
29	lJ	201	PEB	C3C-C4C	4.73	1.49	1.42
29	lL	201	PEB	C3C-C4C	4.73	1.49	1.42
29	rJ	201	PEB	C3C-C4C	4.73	1.49	1.42
29	rL	201	PEB	C3C-C4C	4.73	1.49	1.42
29	Y7	201	PEB	C3B-C2B	4.73	1.46	1.36
29	Y9	201	PEB	C3B-C2B	4.73	1.46	1.36
29	wJ	303	PEB	C3C-C4C	4.73	1.49	1.42
29	LD	202	PEB	C3B-C2B	4.73	1.46	1.36
29	V2	203	PEB	C3C-C4C	4.72	1.49	1.42
29	J5	202	PEB	C3B-C2B	4.72	1.46	1.36
29	J8	202	PEB	C3B-C2B	4.72	1.46	1.36
29	c7	201	PEB	C3B-C2B	4.72	1.46	1.36
29	c9	201	PEB	C3B-C2B	4.72	1.46	1.36
29	TJ	201	PEB	C3C-C4C	4.72	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TL	201	PEB	C3C-C4C	4.72	1.49	1.42
29	pJ	201	PEB	C3C-C4C	4.72	1.49	1.42
29	pL	201	PEB	C3C-C4C	4.72	1.49	1.42
29	g7	201	PEB	C3B-C2B	4.72	1.46	1.36
29	g9	201	PEB	C3B-C2B	4.72	1.46	1.36
29	R7	201	PEB	C3B-C2B	4.72	1.46	1.36
29	R9	201	PEB	C3B-C2B	4.72	1.46	1.36
29	c7	201	PEB	C3C-C4C	4.72	1.49	1.42
29	c9	201	PEB	C3C-C4C	4.72	1.49	1.42
29	PJ	201	PEB	C3C-C4C	4.72	1.49	1.42
29	PL	201	PEB	C3C-C4C	4.72	1.49	1.42
29	V7	201	PEB	C3B-C2B	4.72	1.46	1.36
29	V9	201	PEB	C3B-C2B	4.72	1.46	1.36
29	Q2	202	PEB	C3C-C4C	4.72	1.49	1.42
29	J4	202	PEB	C3B-C2B	4.72	1.46	1.36
29	LA	203	PEB	C3B-C2B	4.72	1.46	1.36
29	DD	202	PEB	C3B-C2B	4.72	1.46	1.36
29	LN	203	PEB	C3B-C2B	4.72	1.46	1.36
29	W2	202	PEB	CHA-C1B	4.72	1.51	1.40
29	XJ	201	PEB	C3C-C4C	4.72	1.49	1.42
29	XL	201	PEB	C3C-C4C	4.72	1.49	1.42
29	BA	203	PEB	C3B-C2B	4.72	1.46	1.36
29	BN	203	PEB	C3B-C2B	4.72	1.46	1.36
29	WR	202	PEB	C3C-C4C	4.72	1.49	1.42
29	FA	203	PEB	C3B-C2B	4.72	1.46	1.36
29	FN	203	PEB	C3B-C2B	4.72	1.46	1.36
29	P7	201	PEB	C3B-C2B	4.71	1.46	1.36
29	P9	201	PEB	C3B-C2B	4.71	1.46	1.36
29	VJ	201	PEB	C3C-C4C	4.71	1.49	1.42
29	VL	201	PEB	C3C-C4C	4.71	1.49	1.42
29	M2	202	PEB	CHA-C1B	4.71	1.51	1.40
29	NJ	201	PEB	C3C-C4C	4.71	1.49	1.42
29	NL	201	PEB	C3C-C4C	4.71	1.49	1.42
29	HD	202	PEB	C3B-C2B	4.71	1.46	1.36
29	S2	202	PEB	CHA-C1B	4.71	1.51	1.40
29	UR	202	PEB	CHA-C1B	4.70	1.51	1.40
29	a7	201	PEB	C3C-C4C	4.70	1.49	1.42
29	a9	201	PEB	C3C-C4C	4.70	1.49	1.42
29	V7	201	PEB	C3C-C4C	4.70	1.49	1.42
29	V9	201	PEB	C3C-C4C	4.70	1.49	1.42
29	LJ	201	PEB	C3C-C4C	4.70	1.49	1.42
29	LL	201	PEB	C3C-C4C	4.70	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QR	202	PEB	C3C-C4C	4.70	1.49	1.42
30	xJ	304	PUB	C2B-C1B	4.70	1.49	1.42
29	SR	202	PEB	CHA-C1B	4.70	1.51	1.40
29	m7	201	PEB	C3C-C4C	4.70	1.49	1.42
29	m9	201	PEB	C3C-C4C	4.70	1.49	1.42
29	a7	201	PEB	C3B-C2B	4.70	1.46	1.36
29	a9	201	PEB	C3B-C2B	4.70	1.46	1.36
29	g7	201	PEB	C3C-C4C	4.70	1.49	1.42
29	g9	201	PEB	C3C-C4C	4.70	1.49	1.42
29	P7	201	PEB	C3C-C4C	4.69	1.49	1.42
29	P9	201	PEB	C3C-C4C	4.69	1.49	1.42
29	JJ	201	PEB	C3C-C4C	4.69	1.49	1.42
29	JL	201	PEB	C3C-C4C	4.69	1.49	1.42
29	UR	202	PEB	C3C-C4C	4.69	1.49	1.42
29	BJ	201	PEB	C3C-C4C	4.69	1.49	1.42
29	ZJ	201	PEB	C3C-C4C	4.69	1.49	1.42
29	BL	201	PEB	C3C-C4C	4.69	1.49	1.42
29	ZL	201	PEB	C3C-C4C	4.69	1.49	1.42
29	DA	203	PEB	C3B-C2B	4.69	1.46	1.36
29	DN	203	PEB	C3B-C2B	4.69	1.46	1.36
29	O2	202	PEB	CHA-C1B	4.69	1.51	1.40
29	N2	201	PEB	C3C-C4C	4.69	1.49	1.42
29	k7	201	PEB	C3B-C2B	4.69	1.46	1.36
29	k9	201	PEB	C3B-C2B	4.69	1.46	1.36
30	A7	303	PUB	C2B-C1B	4.69	1.49	1.42
30	A9	303	PUB	C2B-C1B	4.69	1.49	1.42
29	WR	202	PEB	CHA-C1B	4.69	1.51	1.40
29	i7	201	PEB	C3B-C2B	4.69	1.46	1.36
29	i9	201	PEB	C3B-C2B	4.69	1.46	1.36
29	xL	303	PEB	C3C-C4C	4.69	1.49	1.42
29	e7	201	PEB	C3B-C2B	4.69	1.46	1.36
29	e9	201	PEB	C3B-C2B	4.69	1.46	1.36
29	M2	202	PEB	C3C-C4C	4.69	1.49	1.42
29	e7	201	PEB	C3C-C4C	4.69	1.49	1.42
29	e9	201	PEB	C3C-C4C	4.69	1.49	1.42
29	T7	201	PEB	C3B-C2B	4.69	1.46	1.36
29	T9	201	PEB	C3B-C2B	4.69	1.46	1.36
29	DJ	201	PEB	C3C-C4C	4.69	1.49	1.42
29	DL	201	PEB	C3C-C4C	4.69	1.49	1.42
29	FD	202	PEB	C3B-C2B	4.69	1.46	1.36
29	JD	202	PEB	C3B-C2B	4.69	1.46	1.36
29	k7	201	PEB	C3C-C4C	4.68	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	k9	201	PEB	C3C-C4C	4.68	1.49	1.42
29	xJ	303	PEB	C3C-C4C	4.68	1.49	1.42
30	xL	304	PUB	C2B-C1B	4.68	1.49	1.42
29	A9	304	PEB	C3C-C4C	4.68	1.49	1.42
29	T7	201	PEB	C3C-C4C	4.68	1.49	1.42
29	T9	201	PEB	C3C-C4C	4.68	1.49	1.42
29	AF	304	PEB	C3C-C4C	4.68	1.49	1.42
29	AI	304	PEB	C3C-C4C	4.68	1.49	1.42
29	fJ	201	PEB	C3C-C4C	4.68	1.49	1.42
29	fL	201	PEB	C3C-C4C	4.68	1.49	1.42
29	JA	203	PEB	C3B-C2B	4.68	1.46	1.36
29	JN	203	PEB	C3B-C2B	4.68	1.46	1.36
29	Q2	202	PEB	CHA-C1B	4.68	1.51	1.40
29	R7	201	PEB	C3C-C4C	4.68	1.49	1.42
29	R9	201	PEB	C3C-C4C	4.68	1.49	1.42
29	NR	201	PEB	C3C-C4C	4.67	1.49	1.42
29	SR	202	PEB	C3C-C4C	4.67	1.49	1.42
29	i7	201	PEB	C3C-C4C	4.67	1.49	1.42
29	i9	201	PEB	C3C-C4C	4.67	1.49	1.42
30	BB	302	PUB	C2B-C1B	4.67	1.49	1.42
30	BM	302	PUB	C2B-C1B	4.67	1.49	1.42
29	Y7	201	PEB	C3C-C4C	4.66	1.49	1.42
29	Y9	201	PEB	C3C-C4C	4.66	1.49	1.42
29	A7	304	PEB	C3C-C4C	4.66	1.49	1.42
31	J9	1001	CYC	C1C-NC	-4.66	1.31	1.37
29	S2	202	PEB	C3C-C4C	4.66	1.49	1.42
29	TF	202	PEB	C3C-C4C	4.66	1.49	1.42
29	TI	202	PEB	C3C-C4C	4.66	1.49	1.42
29	H5	202	PEB	C3C-C4C	4.65	1.49	1.42
30	A1	305	PUB	C2B-C1B	4.65	1.49	1.42
30	AK	305	PUB	C2B-C1B	4.65	1.49	1.42
29	kF	203	PEB	C3C-C4C	4.65	1.49	1.42
29	kI	203	PEB	C3C-C4C	4.65	1.49	1.42
29	VR	202	PEB	C3C-C4C	4.65	1.49	1.42
29	V2	201	PEB	C3C-C4C	4.65	1.49	1.42
29	eF	203	PEB	C3C-C4C	4.64	1.49	1.42
29	eI	203	PEB	C3C-C4C	4.64	1.49	1.42
29	T2	201	PEB	C3C-C4C	4.64	1.49	1.42
29	cF	202	PEB	C3C-C4C	4.64	1.49	1.42
29	cI	202	PEB	C3C-C4C	4.64	1.49	1.42
29	TR	201	PEB	C3C-C4C	4.64	1.49	1.42
29	U2	202	PEB	C3C-C4C	4.64	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	iF	203	PEB	C3C-C4C	4.64	1.49	1.42
29	iI	203	PEB	C3C-C4C	4.64	1.49	1.42
29	gF	203	PEB	C3C-C4C	4.64	1.49	1.42
29	gI	203	PEB	C3C-C4C	4.64	1.49	1.42
29	mF	203	PEB	C3C-C4C	4.63	1.49	1.42
29	mI	203	PEB	C3C-C4C	4.63	1.49	1.42
29	VF	203	PEB	C3C-C4C	4.63	1.49	1.42
29	VI	203	PEB	C3C-C4C	4.63	1.49	1.42
29	L8	202	PEB	C3C-C4C	4.63	1.49	1.42
29	L5	202	PEB	C3C-C4C	4.62	1.49	1.42
29	YF	203	PEB	C3C-C4C	4.62	1.49	1.42
29	YI	203	PEB	C3C-C4C	4.62	1.49	1.42
29	V2	202	PEB	C3C-C4C	4.61	1.49	1.42
29	B5	202	PEB	C3C-C4C	4.61	1.49	1.42
29	H8	202	PEB	C3C-C4C	4.61	1.49	1.42
29	T2	202	PEB	C3C-C4C	4.61	1.49	1.42
29	RF	202	PEB	C3C-C4C	4.61	1.49	1.42
29	RI	202	PEB	C3C-C4C	4.61	1.49	1.42
29	V7	202	PEB	C3B-C2B	4.61	1.46	1.36
29	V9	202	PEB	C3B-C2B	4.61	1.46	1.36
31	J7	1001	CYC	C1C-NC	-4.61	1.31	1.37
29	B8	202	PEB	C3C-C4C	4.60	1.49	1.42
29	G8	202	PEB	C3C-C4C	4.60	1.49	1.42
29	UF	202	PEB	C3C-C4C	4.60	1.49	1.42
29	UI	202	PEB	C3C-C4C	4.60	1.49	1.42
29	g7	202	PEB	C3B-C2B	4.60	1.46	1.36
29	g9	202	PEB	C3B-C2B	4.60	1.46	1.36
29	VR	201	PEB	C3C-C4C	4.60	1.49	1.42
29	XR	202	PEB	C3C-C4C	4.60	1.49	1.42
30	AM	305	PUB	C2B-C1B	4.60	1.49	1.42
29	NR	202	PEB	C3C-C4C	4.60	1.49	1.42
29	e2	402	PEB	C3C-C4C	4.59	1.49	1.42
30	MQ	404	PUB	C2C-C3C	4.59	1.46	1.36
29	E4	201	PEB	C3C-C4C	4.59	1.49	1.42
29	G5	202	PEB	C3C-C4C	4.59	1.49	1.42
29	WF	201	PEB	C3C-C4C	4.59	1.49	1.42
29	WI	201	PEB	C3C-C4C	4.59	1.49	1.42
29	P7	202	PEB	C3B-C2B	4.59	1.46	1.36
29	P9	202	PEB	C3B-C2B	4.59	1.46	1.36
29	P2	201	PEB	C3C-C4C	4.59	1.49	1.42
29	aF	203	PEB	C3C-C4C	4.59	1.49	1.42
29	aI	203	PEB	C3C-C4C	4.59	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	PR	201	PEB	C3C-C4C	4.59	1.49	1.42
30	AB	305	PUB	C2B-C1B	4.59	1.49	1.42
29	k7	202	PEB	C3B-C2B	4.59	1.46	1.36
29	k9	202	PEB	C3B-C2B	4.59	1.46	1.36
29	bF	201	PEB	C3C-C4C	4.59	1.49	1.42
29	bI	201	PEB	C3C-C4C	4.59	1.49	1.42
29	GD	201	PEB	C3C-C4C	4.59	1.49	1.42
29	N2	202	PEB	C3C-C4C	4.59	1.49	1.42
29	m7	202	PEB	C3B-C2B	4.59	1.46	1.36
29	m9	202	PEB	C3B-C2B	4.59	1.46	1.36
29	ID	201	PEB	C3C-C4C	4.59	1.49	1.42
29	RR	201	PEB	C3C-C4C	4.59	1.49	1.42
29	S7	201	PEB	C1A-NA	-4.58	1.31	1.37
29	S9	201	PEB	C1A-NA	-4.58	1.31	1.37
29	c7	202	PEB	C3B-C2B	4.58	1.46	1.36
29	c9	202	PEB	C3B-C2B	4.58	1.46	1.36
29	IA	201	PEB	C3C-C4C	4.58	1.49	1.42
29	IN	201	PEB	C3C-C4C	4.58	1.49	1.42
29	j7	201	PEB	C1A-NA	-4.58	1.31	1.37
29	j9	201	PEB	C1A-NA	-4.58	1.31	1.37
29	F5	202	PEB	C3C-C4C	4.58	1.49	1.42
29	F8	202	PEB	C3C-C4C	4.58	1.49	1.42
29	W7	201	PEB	C1A-NA	-4.58	1.31	1.37
29	W9	201	PEB	C1A-NA	-4.58	1.31	1.37
29	RR	202	PEB	C3C-C4C	4.58	1.49	1.42
29	KD	201	PEB	C3C-C4C	4.58	1.49	1.42
30	MG	402	PUB	C2C-C3C	4.58	1.46	1.36
29	h7	201	PEB	C1A-NA	-4.57	1.31	1.37
29	h9	201	PEB	C1A-NA	-4.57	1.31	1.37
29	jF	201	PEB	C3C-C4C	4.57	1.49	1.42
29	jI	201	PEB	C3C-C4C	4.57	1.49	1.42
29	KA	201	PEB	C3C-C4C	4.57	1.49	1.42
29	KN	201	PEB	C3C-C4C	4.57	1.49	1.42
29	a7	202	PEB	C3B-C2B	4.57	1.46	1.36
29	a9	202	PEB	C3B-C2B	4.57	1.46	1.36
31	F9	1001	CYC	C1C-NC	-4.57	1.31	1.37
31	L7	1001	CYC	C1C-NC	-4.57	1.31	1.37
29	R2	201	PEB	C3C-C4C	4.57	1.49	1.42
29	PF	203	PEB	C3C-C4C	4.57	1.49	1.42
29	IF	201	PEB	C3C-C4C	4.57	1.49	1.42
29	PI	203	PEB	C3C-C4C	4.57	1.49	1.42
29	II	201	PEB	C3C-C4C	4.57	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SF	201	PEB	C3C-C4C	4.57	1.49	1.42
29	SI	201	PEB	C3C-C4C	4.57	1.49	1.42
29	J5	201	PEB	C1A-NA	-4.56	1.31	1.37
29	J8	201	PEB	C1A-NA	-4.56	1.31	1.37
29	CA	201	PEB	C3C-C4C	4.56	1.49	1.42
29	CN	201	PEB	C3C-C4C	4.56	1.49	1.42
29	EA	201	PEB	C3C-C4C	4.56	1.49	1.42
29	EN	201	PEB	C3C-C4C	4.56	1.49	1.42
29	T7	202	PEB	C3B-C2B	4.56	1.46	1.36
29	T9	202	PEB	C3B-C2B	4.56	1.46	1.36
29	E4	202	PEB	C1A-NA	-4.56	1.31	1.37
29	Y7	202	PEB	C3B-C2B	4.56	1.46	1.36
29	Y9	202	PEB	C3B-C2B	4.56	1.46	1.36
29	dF	202	PEB	C3C-C4C	4.56	1.49	1.42
29	dI	202	PEB	C3C-C4C	4.56	1.49	1.42
29	i7	202	PEB	C3B-C2B	4.56	1.46	1.36
29	i9	202	PEB	C3B-C2B	4.56	1.46	1.36
29	B4	202	PEB	C1A-NA	-4.56	1.31	1.37
29	H4	202	PEB	C1A-NA	-4.56	1.31	1.37
29	f7	201	PEB	C1A-NA	-4.56	1.31	1.37
29	f9	201	PEB	C1A-NA	-4.56	1.31	1.37
29	BD	202	PEB	C1A-NA	-4.56	1.31	1.37
29	HD	202	PEB	C1A-NA	-4.56	1.31	1.37
29	XR	201	PEB	C3C-C4C	4.56	1.49	1.42
29	GA	201	PEB	C3C-C4C	4.55	1.49	1.42
29	GN	201	PEB	C3C-C4C	4.55	1.49	1.42
29	TR	202	PEB	C3C-C4C	4.55	1.49	1.42
29	TI	201	PEB	C3B-C2B	4.55	1.46	1.36
29	Z7	201	PEB	C1A-NA	-4.55	1.31	1.37
29	Z9	201	PEB	C1A-NA	-4.55	1.31	1.37
29	X2	201	PEB	C3C-C4C	4.55	1.49	1.42
29	d7	201	PEB	C1A-NA	-4.55	1.31	1.37
29	d9	201	PEB	C1A-NA	-4.55	1.31	1.37
29	C4	201	PEB	C3C-C4C	4.55	1.49	1.42
29	CD	201	PEB	C3C-C4C	4.55	1.49	1.42
29	xL	301	PEB	C3C-C4C	4.55	1.49	1.42
29	b7	201	PEB	C1A-NA	-4.55	1.31	1.37
29	b9	201	PEB	C1A-NA	-4.55	1.31	1.37
29	QF	201	PEB	C3C-C4C	4.55	1.49	1.42
29	QI	201	PEB	C3C-C4C	4.55	1.49	1.42
31	C1	1001	CYC	CHB-C1B	4.55	1.48	1.38
31	M1	1001	CYC	CHB-C1B	4.55	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	MK	1001	CYC	CHB-C1B	4.55	1.48	1.38
29	e7	202	PEB	C3B-C2B	4.54	1.46	1.36
29	e9	202	PEB	C3B-C2B	4.54	1.46	1.36
29	K4	201	PEB	C3C-C4C	4.54	1.49	1.42
29	AA	201	PEB	C3C-C4C	4.54	1.49	1.42
29	AN	201	PEB	C3C-C4C	4.54	1.49	1.42
29	R7	202	PEB	C3B-C2B	4.54	1.46	1.36
29	R9	202	PEB	C3B-C2B	4.54	1.46	1.36
29	U7	201	PEB	C1A-NA	-4.54	1.31	1.37
29	U9	201	PEB	C1A-NA	-4.54	1.31	1.37
31	H7	1001	CYC	C1C-NC	-4.54	1.31	1.37
31	N7	1001	CYC	C1C-NC	-4.54	1.31	1.37
31	H9	1001	CYC	C1C-NC	-4.54	1.31	1.37
31	N9	1001	CYC	C1C-NC	-4.54	1.31	1.37
29	dD	401	PEB	C3C-C4C	4.54	1.49	1.42
29	wJ	301	PEB	C3C-C4C	4.54	1.49	1.42
29	MB	202	PEB	C3C-C4C	4.54	1.49	1.42
29	fF	201	PEB	C3C-C4C	4.54	1.49	1.42
29	fI	201	PEB	C3C-C4C	4.54	1.49	1.42
29	MM	202	PEB	C3C-C4C	4.54	1.49	1.42
31	EK	1001	CYC	CHB-C1B	4.54	1.48	1.38
29	kF	201	PEB	C3B-C2B	4.54	1.46	1.36
29	kI	201	PEB	C3B-C2B	4.54	1.46	1.36
29	l7	201	PEB	C1A-NA	-4.54	1.31	1.37
29	l9	201	PEB	C1A-NA	-4.54	1.31	1.37
29	hF	201	PEB	C3C-C4C	4.54	1.49	1.42
29	hI	201	PEB	C3C-C4C	4.54	1.49	1.42
31	K1	1001	CYC	CHB-C1B	4.54	1.48	1.38
31	KK	1001	CYC	CHB-C1B	4.54	1.48	1.38
31	GK	1001	CYC	CHB-C1B	4.54	1.48	1.38
29	I4	201	PEB	C3C-C4C	4.54	1.49	1.42
31	D7	1001	CYC	C1C-NC	-4.53	1.31	1.37
31	D9	1001	CYC	C1C-NC	-4.53	1.31	1.37
29	G4	201	PEB	C3C-C4C	4.53	1.49	1.42
29	gF	201	PEB	C3B-C2B	4.53	1.46	1.36
29	gI	201	PEB	C3B-C2B	4.53	1.46	1.36
29	eF	201	PEB	C3B-C2B	4.53	1.46	1.36
29	eI	201	PEB	C3B-C2B	4.53	1.46	1.36
29	OF	201	PEB	C3C-C4C	4.53	1.49	1.42
29	OI	201	PEB	C3C-C4C	4.53	1.49	1.42
31	D1	1003	CYC	CHB-C1B	4.53	1.48	1.38
29	fB	202	PEB	C3C-C4C	4.53	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fM	202	PEB	C3C-C4C	4.53	1.49	1.42
29	MD	201	PEB	C3C-C4C	4.53	1.49	1.42
31	E1	1001	CYC	CHB-C1B	4.53	1.48	1.38
29	YF	201	PEB	C3B-C2B	4.53	1.46	1.36
29	YI	201	PEB	C3B-C2B	4.53	1.46	1.36
29	A1	302	PEB	C3C-C4C	4.53	1.49	1.42
29	AK	302	PEB	C3C-C4C	4.53	1.49	1.42
29	OB	202	PEB	C3C-C4C	4.53	1.49	1.42
29	OM	202	PEB	C3C-C4C	4.53	1.49	1.42
29	VF	201	PEB	C3B-C2B	4.52	1.46	1.36
29	VI	201	PEB	C3B-C2B	4.52	1.46	1.36
29	ZF	201	PEB	C3C-C4C	4.52	1.49	1.42
29	ZI	201	PEB	C3C-C4C	4.52	1.49	1.42
31	L9	1001	CYC	C1C-NC	-4.52	1.31	1.37
31	CK	1001	CYC	CHB-C1B	4.52	1.48	1.38
29	RF	201	PEB	C3B-C2B	4.52	1.46	1.36
29	RI	201	PEB	C3B-C2B	4.52	1.46	1.36
29	aF	201	PEB	C3B-C2B	4.52	1.46	1.36
29	aI	201	PEB	C3B-C2B	4.52	1.46	1.36
29	hB	202	PEB	C3C-C4C	4.52	1.49	1.42
29	hM	202	PEB	C3C-C4C	4.52	1.49	1.42
29	xJ	301	PEB	C3C-C4C	4.52	1.49	1.42
29	SB	202	PEB	C3C-C4C	4.51	1.49	1.42
29	SM	202	PEB	C3C-C4C	4.51	1.49	1.42
29	YB	203	PEB	C3C-C4C	4.51	1.49	1.42
29	YM	203	PEB	C3C-C4C	4.51	1.49	1.42
31	F7	1001	CYC	C1C-NC	-4.51	1.31	1.37
29	M4	201	PEB	C3C-C4C	4.51	1.49	1.42
29	ED	201	PEB	C1A-NA	-4.51	1.31	1.37
29	iF	201	PEB	C3B-C2B	4.51	1.46	1.36
29	iI	201	PEB	C3B-C2B	4.51	1.46	1.36
29	UB	202	PEB	C3C-C4C	4.51	1.49	1.42
29	MQ	401	PEB	C3C-C4C	4.51	1.49	1.42
29	EB	202	PEB	C3C-C4C	4.50	1.49	1.42
29	EM	202	PEB	C3C-C4C	4.50	1.49	1.42
29	DD	202	PEB	C1A-NA	-4.50	1.31	1.37
29	QB	204	PEB	C3C-C4C	4.50	1.49	1.42
29	QM	204	PEB	C3C-C4C	4.50	1.49	1.42
29	Q7	201	PEB	C1A-NA	-4.50	1.31	1.37
29	Q9	201	PEB	C1A-NA	-4.50	1.31	1.37
31	IK	1001	CYC	CHB-C1B	4.50	1.48	1.38
29	FD	202	PEB	C1A-NA	-4.50	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	wJ	305	PUB	C2C-C3C	4.50	1.46	1.36
29	GB	202	PEB	C3C-C4C	4.50	1.49	1.42
29	GM	202	PEB	C3C-C4C	4.50	1.49	1.42
31	I1	1001	CYC	CHB-C1B	4.50	1.48	1.38
29	mF	201	PEB	C3B-C2B	4.50	1.46	1.36
29	mI	201	PEB	C3B-C2B	4.50	1.46	1.36
29	cF	201	PEB	C3B-C2B	4.50	1.46	1.36
29	cI	201	PEB	C3B-C2B	4.50	1.46	1.36
29	R2	202	PEB	C3C-C4C	4.49	1.49	1.42
29	PF	201	PEB	C3B-C2B	4.49	1.46	1.36
29	PI	201	PEB	C3B-C2B	4.49	1.46	1.36
29	jB	202	PEB	C3C-C4C	4.49	1.49	1.42
29	jM	202	PEB	C3C-C4C	4.49	1.49	1.42
29	F4	202	PEB	C1A-NA	-4.49	1.31	1.37
29	KD	202	PEB	C1A-NA	-4.49	1.31	1.37
29	aB	202	PEB	C3C-C4C	4.48	1.49	1.42
29	aM	202	PEB	C3C-C4C	4.48	1.49	1.42
29	K3	201	PEB	C3C-C4C	4.48	1.49	1.42
29	KO	201	PEB	C3C-C4C	4.48	1.49	1.42
29	KB	202	PEB	C3C-C4C	4.48	1.49	1.42
29	KM	202	PEB	C3C-C4C	4.48	1.49	1.42
29	M2	201	PEB	C1A-NA	-4.48	1.31	1.37
29	MR	201	PEB	C1A-NA	-4.48	1.31	1.37
29	wL	301	PEB	C3C-C4C	4.48	1.49	1.42
29	U2	201	PEB	C1A-NA	-4.47	1.31	1.37
29	lB	202	PEB	C3C-C4C	4.47	1.49	1.42
29	lM	202	PEB	C3C-C4C	4.47	1.49	1.42
30	wL	305	PUB	C2C-C3C	4.47	1.46	1.36
29	O7	201	PEB	C1A-NA	-4.47	1.31	1.37
29	O9	201	PEB	C1A-NA	-4.47	1.31	1.37
29	CB	202	PEB	C3C-C4C	4.47	1.49	1.42
29	CM	202	PEB	C3C-C4C	4.47	1.49	1.42
29	lB	202	PEB	C3C-C4C	4.47	1.49	1.42
29	lM	202	PEB	C3C-C4C	4.47	1.49	1.42
29	A3	201	PEB	C3C-C4C	4.47	1.49	1.42
29	AO	201	PEB	C3C-C4C	4.47	1.49	1.42
29	K4	202	PEB	C1A-NA	-4.46	1.31	1.37
29	M4	202	PEB	C1A-NA	-4.46	1.31	1.37
29	JD	202	PEB	C1A-NA	-4.46	1.31	1.37
29	MD	202	PEB	C1A-NA	-4.46	1.31	1.37
29	dB	202	PEB	C3C-C4C	4.46	1.49	1.42
29	dM	202	PEB	C3C-C4C	4.46	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D4	202	PEB	C1A-NA	-4.46	1.31	1.37
29	I4	202	PEB	C1A-NA	-4.46	1.31	1.37
29	ID	202	PEB	C1A-NA	-4.46	1.31	1.37
30	xJ	305	PUB	C2C-C3C	4.46	1.46	1.36
29	H4	201	PEB	C3C-C4C	4.46	1.49	1.42
29	L4	202	PEB	C1A-NA	-4.46	1.31	1.37
30	MN	403	PUB	OD-C4D	4.45	1.32	1.23
29	G3	201	PEB	C3C-C4C	4.45	1.49	1.42
29	GO	201	PEB	C3C-C4C	4.45	1.49	1.42
30	MA	403	PUB	OD-C4D	4.45	1.32	1.23
29	hF	201	PEB	C3B-C2B	4.45	1.46	1.36
29	hI	201	PEB	C3B-C2B	4.45	1.46	1.36
29	E3	201	PEB	C3C-C4C	4.45	1.49	1.42
29	EO	201	PEB	C3C-C4C	4.45	1.49	1.42
29	UF	202	PEB	C3B-C2B	4.45	1.46	1.36
29	UI	202	PEB	C3B-C2B	4.45	1.46	1.36
30	MQ	405	PUB	C2C-C3C	4.45	1.46	1.36
30	MG	403	PUB	C2C-C3C	4.44	1.46	1.36
30	xL	305	PUB	C2C-C3C	4.44	1.46	1.36
30	AF	303	PUB	C2B-C1B	4.44	1.49	1.42
30	AI	303	PUB	C2B-C1B	4.44	1.49	1.42
29	fF	201	PEB	C3B-C2B	4.44	1.46	1.36
29	fI	201	PEB	C3B-C2B	4.44	1.46	1.36
29	G4	202	PEB	C1A-NA	-4.44	1.31	1.37
29	GD	202	PEB	C1A-NA	-4.44	1.31	1.37
29	QR	201	PEB	C1A-NA	-4.44	1.31	1.37
29	BC	202	PEB	C3C-C4C	4.44	1.49	1.42
29	BE	202	PEB	C3C-C4C	4.44	1.49	1.42
29	bF	201	PEB	C3B-C2B	4.43	1.46	1.36
29	bI	201	PEB	C3B-C2B	4.43	1.46	1.36
29	WB	202	PEB	C3C-C4C	4.43	1.49	1.42
29	WM	202	PEB	C3C-C4C	4.43	1.49	1.42
29	LD	202	PEB	C1A-NA	-4.43	1.31	1.37
29	C3	201	PEB	C3C-C4C	4.43	1.49	1.42
29	CO	201	PEB	C3C-C4C	4.43	1.49	1.42
29	QF	201	PEB	C3B-C2B	4.43	1.46	1.36
29	QI	201	PEB	C3B-C2B	4.43	1.46	1.36
29	jF	201	PEB	C3B-C2B	4.43	1.46	1.36
29	jI	201	PEB	C3B-C2B	4.43	1.46	1.36
29	WF	201	PEB	C3B-C2B	4.43	1.46	1.36
29	WI	201	PEB	C3B-C2B	4.43	1.46	1.36
31	F9	1001	CYC	CHB-C1B	4.43	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	F7	1001	CYC	CHB-C1B	4.42	1.48	1.38
29	O2	201	PEB	C1A-NA	-4.42	1.31	1.37
31	H7	1001	CYC	CHB-C1B	4.42	1.48	1.38
31	H9	1001	CYC	CHB-C1B	4.42	1.48	1.38
31	D7	1001	CYC	CHB-C1B	4.42	1.48	1.38
31	D9	1001	CYC	CHB-C1B	4.42	1.48	1.38
31	N7	1001	CYC	CHB-C1B	4.42	1.48	1.38
31	N9	1001	CYC	CHB-C1B	4.42	1.48	1.38
29	J4	202	PEB	C1A-NA	-4.42	1.31	1.37
29	SF	201	PEB	C3B-C2B	4.41	1.46	1.36
29	SI	201	PEB	C3B-C2B	4.41	1.46	1.36
29	MA	404	PEB	C1A-NA	-4.41	1.31	1.37
29	I3	201	PEB	C3C-C4C	4.41	1.48	1.42
29	IO	201	PEB	C3C-C4C	4.41	1.48	1.42
29	FC	202	PEB	C3C-C4C	4.41	1.48	1.42
29	FE	202	PEB	C3C-C4C	4.41	1.48	1.42
31	KF	1001	CYC	CHB-C1B	4.41	1.48	1.38
29	UR	201	PEB	C1A-NA	-4.41	1.31	1.37
31	CF	1001	CYC	CHB-C1B	4.40	1.48	1.38
31	CI	1001	CYC	CHB-C1B	4.40	1.48	1.38
29	OR	201	PEB	C1A-NA	-4.40	1.31	1.37
29	WR	201	PEB	C1A-NA	-4.40	1.31	1.37
29	J5	201	PEB	C3B-C2B	4.40	1.46	1.36
29	J8	201	PEB	C3B-C2B	4.40	1.46	1.36
29	B4	201	PEB	C3C-C4C	4.40	1.48	1.42
29	JB	203	PEB	CHA-C1B	4.40	1.50	1.40
29	JM	203	PEB	CHA-C1B	4.40	1.50	1.40
29	BD	201	PEB	C3C-C4C	4.40	1.48	1.42
31	KI	1001	CYC	CHB-C1B	4.40	1.48	1.38
31	J7	1001	CYC	CHB-C1B	4.40	1.48	1.38
29	DB	203	PEB	CHA-C1B	4.40	1.50	1.40
29	DM	203	PEB	CHA-C1B	4.40	1.50	1.40
29	dF	202	PEB	C3B-C2B	4.40	1.46	1.36
29	dI	202	PEB	C3B-C2B	4.40	1.46	1.36
31	L7	1001	CYC	CHB-C1B	4.40	1.48	1.38
29	ZF	201	PEB	C3B-C2B	4.40	1.46	1.36
29	ZI	201	PEB	C3B-C2B	4.40	1.46	1.36
31	J9	1001	CYC	CHB-C1B	4.39	1.48	1.38
29	iB	203	PEB	CHA-C1B	4.39	1.50	1.40
29	iM	203	PEB	CHA-C1B	4.39	1.50	1.40
29	MN	404	PEB	C1A-NA	-4.39	1.31	1.37
29	L4	201	PEB	C3C-C4C	4.39	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LD	201	PEB	C3C-C4C	4.39	1.48	1.42
29	YF	201	PEB	C3C-C4C	4.39	1.48	1.42
29	YI	201	PEB	C3C-C4C	4.39	1.48	1.42
29	NB	202	PEB	CHA-C1B	4.39	1.50	1.40
29	NM	202	PEB	CHA-C1B	4.39	1.50	1.40
29	jJ	202	PEB	C3C-C4C	4.39	1.48	1.42
29	jL	202	PEB	C3C-C4C	4.39	1.48	1.42
29	PB	202	PEB	CHA-C1B	4.39	1.50	1.40
29	PM	202	PEB	CHA-C1B	4.39	1.50	1.40
29	Q2	201	PEB	C1A-NA	-4.38	1.31	1.37
29	HC	202	PEB	C3C-C4C	4.38	1.48	1.42
29	DD	201	PEB	C3C-C4C	4.38	1.48	1.42
29	HE	202	PEB	C3C-C4C	4.38	1.48	1.42
29	TJ	202	PEB	C3C-C4C	4.38	1.48	1.42
29	TL	202	PEB	C3C-C4C	4.38	1.48	1.42
29	OF	201	PEB	C3B-C2B	4.38	1.46	1.36
29	OI	201	PEB	C3B-C2B	4.38	1.46	1.36
29	eB	202	PEB	CHA-C1B	4.38	1.50	1.40
29	eM	202	PEB	CHA-C1B	4.38	1.50	1.40
29	lF	201	PEB	C3B-C2B	4.38	1.46	1.36
29	lI	201	PEB	C3B-C2B	4.38	1.46	1.36
31	MF	1001	CYC	CHB-C1B	4.38	1.48	1.38
31	MI	1001	CYC	CHB-C1B	4.38	1.48	1.38
29	fJ	202	PEB	C3C-C4C	4.38	1.48	1.42
29	fL	202	PEB	C3C-C4C	4.38	1.48	1.42
29	cB	203	PEB	CHA-C1B	4.38	1.50	1.40
29	cM	203	PEB	CHA-C1B	4.38	1.50	1.40
31	lF	1001	CYC	CHB-C1B	4.38	1.48	1.38
31	lI	1001	CYC	CHB-C1B	4.38	1.48	1.38
29	kB	203	PEB	CHA-C1B	4.38	1.50	1.40
29	kM	203	PEB	CHA-C1B	4.38	1.50	1.40
29	HB	203	PEB	CHA-C1B	4.37	1.50	1.40
29	HM	203	PEB	CHA-C1B	4.37	1.50	1.40
29	JD	201	PEB	C3C-C4C	4.37	1.48	1.42
29	HD	201	PEB	C3C-C4C	4.37	1.48	1.42
31	L9	1001	CYC	CHB-C1B	4.37	1.48	1.38
29	PF	201	PEB	C3C-C4C	4.37	1.48	1.42
29	PI	201	PEB	C3C-C4C	4.37	1.48	1.42
29	ZJ	202	PEB	C3C-C4C	4.37	1.48	1.42
29	ZL	202	PEB	C3C-C4C	4.37	1.48	1.42
29	VB	203	PEB	CHA-C1B	4.37	1.50	1.40
29	gB	203	PEB	CHA-C1B	4.37	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VM	203	PEB	CHA-C1B	4.37	1.50	1.40
29	gM	203	PEB	CHA-C1B	4.37	1.50	1.40
29	PJ	202	PEB	C3C-C4C	4.37	1.48	1.42
29	PL	202	PEB	C3C-C4C	4.37	1.48	1.42
29	TB	203	PEB	CHA-C1B	4.37	1.50	1.40
29	TM	203	PEB	CHA-C1B	4.37	1.50	1.40
29	C4	202	PEB	C1A-NA	-4.37	1.31	1.37
31	EF	1001	CYC	CHB-C1B	4.37	1.48	1.38
31	EI	1001	CYC	CHB-C1B	4.37	1.48	1.38
29	FB	203	PEB	CHA-C1B	4.37	1.50	1.40
29	FM	203	PEB	CHA-C1B	4.37	1.50	1.40
29	AC	203	PEB	C3C-C4C	4.36	1.48	1.42
29	AE	203	PEB	C3C-C4C	4.36	1.48	1.42
29	IJ	202	PEB	C3C-C4C	4.36	1.48	1.42
29	IL	202	PEB	C3C-C4C	4.36	1.48	1.42
29	BJ	202	PEB	C3C-C4C	4.36	1.48	1.42
29	hJ	202	PEB	C3C-C4C	4.36	1.48	1.42
29	BL	202	PEB	C3C-C4C	4.36	1.48	1.42
29	hL	202	PEB	C3C-C4C	4.36	1.48	1.42
29	CD	202	PEB	C1A-NA	-4.36	1.32	1.37
31	DF	1001	CYC	C1C-NC	-4.36	1.32	1.37
31	DI	1001	CYC	C1C-NC	-4.36	1.32	1.37
29	LB	203	PEB	CHA-C1B	4.36	1.50	1.40
29	LM	203	PEB	CHA-C1B	4.36	1.50	1.40
29	IJ	203	PEB	C3C-C4C	4.36	1.48	1.42
29	IL	203	PEB	C3C-C4C	4.36	1.48	1.42
29	pJ	202	PEB	C3C-C4C	4.36	1.48	1.42
29	pL	202	PEB	C3C-C4C	4.36	1.48	1.42
29	RB	203	PEB	CHA-C1B	4.36	1.50	1.40
29	RM	203	PEB	CHA-C1B	4.36	1.50	1.40
29	mB	203	PEB	CHA-C1B	4.36	1.50	1.40
29	mM	203	PEB	CHA-C1B	4.36	1.50	1.40
29	sJ	203	PEB	C3C-C4C	4.36	1.48	1.42
29	sL	203	PEB	C3C-C4C	4.36	1.48	1.42
31	GF	1001	CYC	CHB-C1B	4.35	1.48	1.38
31	GI	1001	CYC	CHB-C1B	4.35	1.48	1.38
29	cF	201	PEB	C3C-C4C	4.35	1.48	1.42
29	cI	201	PEB	C3C-C4C	4.35	1.48	1.42
29	XB	202	PEB	CHA-C1B	4.35	1.50	1.40
29	XM	202	PEB	CHA-C1B	4.35	1.50	1.40
29	gF	201	PEB	C3C-C4C	4.35	1.48	1.42
29	gI	201	PEB	C3C-C4C	4.35	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LC	202	PEB	C3C-C4C	4.35	1.48	1.42
29	LE	202	PEB	C3C-C4C	4.35	1.48	1.42
29	nJ	202	PEB	C3C-C4C	4.35	1.48	1.42
29	nL	202	PEB	C3C-C4C	4.35	1.48	1.42
31	JF	1001	CYC	C1C-NC	-4.35	1.32	1.37
31	JI	1001	CYC	C1C-NC	-4.35	1.32	1.37
31	NF	1001	CYC	C1C-NC	-4.35	1.32	1.37
31	NI	1001	CYC	C1C-NC	-4.35	1.32	1.37
31	LF	1001	CYC	C1C-NC	-4.35	1.32	1.37
31	LI	1001	CYC	C1C-NC	-4.35	1.32	1.37
29	aF	201	PEB	C3C-C4C	4.35	1.48	1.42
29	aI	201	PEB	C3C-C4C	4.35	1.48	1.42
29	ED	202	PEB	C2A-C1A	-4.34	1.48	1.52
29	W2	201	PEB	C1A-NA	-4.34	1.32	1.37
29	rJ	202	PEB	C3C-C4C	4.34	1.48	1.42
29	rL	202	PEB	C3C-C4C	4.34	1.48	1.42
29	WJ	201	PEB	C3C-C4C	4.34	1.48	1.42
29	WL	201	PEB	C3C-C4C	4.34	1.48	1.42
29	ZB	203	PEB	CHA-C1B	4.34	1.50	1.40
29	ZM	203	PEB	CHA-C1B	4.34	1.50	1.40
29	VF	201	PEB	C3C-C4C	4.34	1.48	1.42
29	VI	201	PEB	C3C-C4C	4.34	1.48	1.42
29	CD	203	PEB	C2A-C1A	-4.34	1.48	1.52
29	J4	201	PEB	C3C-C4C	4.34	1.48	1.42
29	uJ	201	PEB	C3C-C4C	4.34	1.48	1.42
29	uL	201	PEB	C3C-C4C	4.34	1.48	1.42
29	NJ	202	PEB	C3C-C4C	4.34	1.48	1.42
29	NL	202	PEB	C3C-C4C	4.34	1.48	1.42
29	ID	203	PEB	C2A-C1A	-4.34	1.48	1.52
29	HJ	201	PEB	C3C-C4C	4.34	1.48	1.42
29	HL	201	PEB	C3C-C4C	4.34	1.48	1.42
29	KC	201	PEB	C3C-C4C	4.33	1.48	1.42
29	KE	201	PEB	C3C-C4C	4.33	1.48	1.42
29	bJ	202	PEB	C3C-C4C	4.33	1.48	1.42
29	bL	202	PEB	C3C-C4C	4.33	1.48	1.42
29	dJ	202	PEB	C3C-C4C	4.33	1.48	1.42
29	dL	202	PEB	C3C-C4C	4.33	1.48	1.42
29	F4	201	PEB	C3C-C4C	4.32	1.48	1.42
29	TI	201	PEB	C3C-C4C	4.32	1.48	1.42
29	D4	201	PEB	C3C-C4C	4.32	1.48	1.42
29	XJ	202	PEB	C3C-C4C	4.32	1.48	1.42
29	XL	202	PEB	C3C-C4C	4.32	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	WJ	202	PEB	C1A-NA	-4.31	1.32	1.37
29	WL	202	PEB	C1A-NA	-4.31	1.32	1.37
31	nP	1001	CYC	C1C-NC	-4.31	1.32	1.37
31	HF	1001	CYC	C1C-NC	-4.31	1.32	1.37
31	HI	1001	CYC	C1C-NC	-4.31	1.32	1.37
29	RJ	202	PEB	C3C-C4C	4.31	1.48	1.42
29	RL	202	PEB	C3C-C4C	4.31	1.48	1.42
29	RF	201	PEB	C3C-C4C	4.31	1.48	1.42
29	RI	201	PEB	C3C-C4C	4.31	1.48	1.42
31	MP	1001	CYC	C1C-NC	-4.31	1.32	1.37
30	MG	403	PUB	OD-C4D	4.30	1.31	1.23
29	JJ	202	PEB	C3C-C4C	4.30	1.48	1.42
29	JL	202	PEB	C3C-C4C	4.30	1.48	1.42
29	AJ	203	PEB	C3C-C4C	4.30	1.48	1.42
29	AL	203	PEB	C3C-C4C	4.30	1.48	1.42
29	BB	301	PEB	CHA-C1B	4.30	1.50	1.40
29	BM	301	PEB	CHA-C1B	4.30	1.50	1.40
29	FJ	202	PEB	C3C-C4C	4.30	1.48	1.42
29	FL	202	PEB	C3C-C4C	4.30	1.48	1.42
29	kF	201	PEB	C3C-C4C	4.29	1.48	1.42
29	kI	201	PEB	C3C-C4C	4.29	1.48	1.42
31	UP	1001	CYC	C1C-NC	-4.29	1.32	1.37
31	hP	1001	CYC	C1C-NC	-4.29	1.32	1.37
29	OJ	201	PEB	C1A-NA	-4.29	1.32	1.37
29	OL	201	PEB	C1A-NA	-4.29	1.32	1.37
31	XP	1001	CYC	C1C-NC	-4.29	1.32	1.37
29	iF	201	PEB	C3C-C4C	4.29	1.48	1.42
29	iI	201	PEB	C3C-C4C	4.29	1.48	1.42
31	FF	1001	CYC	C1C-NC	-4.29	1.32	1.37
31	FI	1001	CYC	C1C-NC	-4.29	1.32	1.37
31	qP	1001	CYC	C1C-NC	-4.28	1.32	1.37
29	C4	203	PEB	C2A-C1A	-4.28	1.48	1.52
29	eF	201	PEB	C3C-C4C	4.28	1.48	1.42
29	eI	201	PEB	C3C-C4C	4.28	1.48	1.42
29	YJ	201	PEB	C1A-NA	-4.28	1.32	1.37
29	YL	201	PEB	C1A-NA	-4.28	1.32	1.37
30	MQ	405	PUB	OD-C4D	4.27	1.31	1.23
29	mF	201	PEB	C3C-C4C	4.27	1.48	1.42
29	mI	201	PEB	C3C-C4C	4.27	1.48	1.42
29	mJ	201	PEB	C1A-NA	-4.27	1.32	1.37
29	mL	201	PEB	C1A-NA	-4.27	1.32	1.37
29	oJ	201	PEB	C1A-NA	-4.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	oL	201	PEB	C1A-NA	-4.27	1.32	1.37
29	FD	201	PEB	C3C-C4C	4.27	1.48	1.42
29	SJ	201	PEB	C1A-NA	-4.27	1.32	1.37
29	SL	201	PEB	C1A-NA	-4.27	1.32	1.37
29	gJ	201	PEB	C1A-NA	-4.27	1.32	1.37
29	gL	201	PEB	C1A-NA	-4.27	1.32	1.37
29	CJ	201	PEB	C1A-NA	-4.27	1.32	1.37
29	CL	201	PEB	C1A-NA	-4.27	1.32	1.37
31	DP	1001	CYC	C1C-NC	-4.27	1.32	1.37
29	uJ	202	PEB	C1A-NA	-4.26	1.32	1.37
29	uL	202	PEB	C1A-NA	-4.26	1.32	1.37
31	IP	1001	CYC	C1C-NC	-4.26	1.32	1.37
31	BP	1001	CYC	C1C-NC	-4.26	1.32	1.37
31	VP	1001	CYC	C2C-C1C	-4.26	1.48	1.52
29	qJ	201	PEB	C1A-NA	-4.26	1.32	1.37
29	qL	201	PEB	C1A-NA	-4.26	1.32	1.37
31	LF	1001	CYC	CHB-C1B	4.26	1.48	1.38
31	LI	1001	CYC	CHB-C1B	4.26	1.48	1.38
31	FP	1001	CYC	C1C-NC	-4.26	1.32	1.37
31	K9	1001	CYC	CHB-C1B	4.26	1.48	1.38
29	KJ	201	PEB	C1A-NA	-4.26	1.32	1.37
29	KL	201	PEB	C1A-NA	-4.26	1.32	1.37
31	1P	1002	CYC	CHB-C4A	4.26	1.50	1.40
29	IJ	201	PEB	C1A-NA	-4.25	1.32	1.37
29	IL	201	PEB	C1A-NA	-4.25	1.32	1.37
31	jP	1001	CYC	C1C-NC	-4.25	1.32	1.37
29	G4	203	PEB	C2A-C1A	-4.25	1.48	1.52
29	MJ	201	PEB	C1A-NA	-4.25	1.32	1.37
29	ML	201	PEB	C1A-NA	-4.25	1.32	1.37
31	G9	1001	CYC	CHB-C1B	4.25	1.48	1.38
29	K4	203	PEB	C2A-C1A	-4.25	1.48	1.52
31	K7	1001	CYC	CHB-C1B	4.25	1.48	1.38
29	D4	201	PEB	C1A-NA	-4.25	1.32	1.37
29	DD	201	PEB	C1A-NA	-4.25	1.32	1.37
31	HP	1001	CYC	C1C-NC	-4.25	1.32	1.37
31	NF	1001	CYC	CHB-C1B	4.25	1.48	1.38
31	NI	1001	CYC	CHB-C1B	4.25	1.48	1.38
29	kJ	201	PEB	C1A-NA	-4.25	1.32	1.37
29	kL	201	PEB	C1A-NA	-4.25	1.32	1.37
29	EJ	201	PEB	C1A-NA	-4.25	1.32	1.37
29	EL	201	PEB	C1A-NA	-4.25	1.32	1.37
31	HF	1001	CYC	CHB-C1B	4.25	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	HI	1001	CYC	CHB-C1B	4.25	1.48	1.38
31	OP	1001	CYC	C1C-NC	-4.25	1.32	1.37
31	G7	1001	CYC	CHB-C1B	4.24	1.48	1.38
31	M9	1001	CYC	CHB-C1B	4.24	1.48	1.38
29	iJ	201	PEB	C1A-NA	-4.24	1.32	1.37
29	iL	201	PEB	C1A-NA	-4.24	1.32	1.37
29	AJ	201	PEB	C1A-NA	-4.24	1.32	1.37
29	AL	201	PEB	C1A-NA	-4.24	1.32	1.37
31	DF	1001	CYC	CHB-C1B	4.24	1.48	1.38
31	DI	1001	CYC	CHB-C1B	4.24	1.48	1.38
29	E4	203	PEB	C2A-C1A	-4.24	1.48	1.52
31	WP	1001	CYC	CHB-C4A	4.24	1.50	1.40
29	eJ	201	PEB	C1A-NA	-4.24	1.32	1.37
29	eL	201	PEB	C1A-NA	-4.24	1.32	1.37
31	uP	1001	CYC	C1C-NC	-4.24	1.32	1.37
31	oP	1001	CYC	C1C-NC	-4.24	1.32	1.37
29	E4	201	PEB	C1A-NA	-4.24	1.32	1.37
29	UJ	201	PEB	C1A-NA	-4.24	1.32	1.37
29	UL	201	PEB	C1A-NA	-4.24	1.32	1.37
31	FF	1001	CYC	CHB-C1B	4.24	1.48	1.38
31	FI	1001	CYC	CHB-C1B	4.24	1.48	1.38
29	mB	203	PEB	C1A-NA	-4.24	1.32	1.37
29	mM	203	PEB	C1A-NA	-4.24	1.32	1.37
31	M7	1001	CYC	CHB-C1B	4.24	1.48	1.38
31	yP	1001	CYC	CHB-C4A	4.24	1.50	1.40
29	BD	201	PEB	C1A-NA	-4.24	1.32	1.37
31	1P	1001	CYC	C1C-NC	-4.24	1.32	1.37
29	j7	201	PEB	C2A-C1A	-4.23	1.48	1.52
29	j9	201	PEB	C2A-C1A	-4.23	1.48	1.52
29	aJ	201	PEB	C1A-NA	-4.23	1.32	1.37
29	aL	201	PEB	C1A-NA	-4.23	1.32	1.37
31	JF	1001	CYC	CHB-C1B	4.23	1.48	1.38
31	JI	1001	CYC	CHB-C1B	4.23	1.48	1.38
29	BA	201	PEB	C1A-NA	-4.23	1.32	1.37
29	BN	201	PEB	C1A-NA	-4.23	1.32	1.37
29	sJ	201	PEB	C1A-NA	-4.23	1.32	1.37
29	sL	201	PEB	C1A-NA	-4.23	1.32	1.37
31	QP	1001	CYC	C1C-NC	-4.23	1.32	1.37
30	AB	304	PUB	C2B-C1B	4.23	1.48	1.42
31	fP	1001	CYC	C1C-NC	-4.23	1.32	1.37
29	GD	203	PEB	C2A-C1A	-4.23	1.48	1.52
31	xP	1001	CYC	C2C-C1C	-4.23	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E7	1001	CYC	CHB-C1B	4.23	1.48	1.38
31	E9	1001	CYC	CHB-C1B	4.23	1.48	1.38
29	DA	201	PEB	C1A-NA	-4.23	1.32	1.37
29	DN	201	PEB	C1A-NA	-4.23	1.32	1.37
31	C7	1001	CYC	CHB-C1B	4.22	1.48	1.38
31	C9	1001	CYC	CHB-C1B	4.22	1.48	1.38
29	QJ	201	PEB	C1A-NA	-4.22	1.32	1.37
29	QL	201	PEB	C1A-NA	-4.22	1.32	1.37
31	wP	1001	CYC	C1C-NC	-4.22	1.32	1.37
31	I7	1001	CYC	CHB-C1B	4.22	1.48	1.38
31	I9	1001	CYC	CHB-C1B	4.22	1.48	1.38
29	GJ	201	PEB	C1A-NA	-4.22	1.32	1.37
29	GL	201	PEB	C1A-NA	-4.22	1.32	1.37
31	SP	1001	CYC	C1C-NC	-4.22	1.32	1.37
31	sP	1001	CYC	C1C-NC	-4.22	1.32	1.37
29	J4	201	PEB	C1A-NA	-4.22	1.32	1.37
31	YP	1000	CYC	CHB-C4A	4.22	1.50	1.40
29	HA	201	PEB	C1A-NA	-4.21	1.32	1.37
29	HN	201	PEB	C1A-NA	-4.21	1.32	1.37
31	kP	1001	CYC	C1C-NC	-4.21	1.32	1.37
29	LA	201	PEB	C1A-NA	-4.21	1.32	1.37
29	LN	201	PEB	C1A-NA	-4.21	1.32	1.37
29	K4	201	PEB	C1A-NA	-4.21	1.32	1.37
29	KD	201	PEB	C1A-NA	-4.21	1.32	1.37
29	O7	201	PEB	C2A-C1A	-4.21	1.48	1.52
29	O9	201	PEB	C2A-C1A	-4.21	1.48	1.52
29	FD	201	PEB	C1A-NA	-4.21	1.32	1.37
29	BB	301	PEB	C1A-NA	-4.21	1.32	1.37
29	BM	301	PEB	C1A-NA	-4.21	1.32	1.37
29	L4	201	PEB	C1A-NA	-4.21	1.32	1.37
29	CD	201	PEB	C1A-NA	-4.21	1.32	1.37
29	JD	201	PEB	C1A-NA	-4.21	1.32	1.37
29	H4	201	PEB	C1A-NA	-4.20	1.32	1.37
29	dD	401	PEB	C1A-NA	-4.20	1.32	1.37
29	cJ	201	PEB	C1A-NA	-4.20	1.32	1.37
29	cL	201	PEB	C1A-NA	-4.20	1.32	1.37
29	b7	201	PEB	C2A-C1A	-4.20	1.48	1.52
29	b9	201	PEB	C2A-C1A	-4.20	1.48	1.52
29	PB	202	PEB	C1A-NA	-4.20	1.32	1.37
29	PM	202	PEB	C1A-NA	-4.20	1.32	1.37
29	MD	201	PEB	C1A-NA	-4.20	1.32	1.37
30	AM	304	PUB	C2B-C1B	4.19	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZB	203	PEB	C1A-NA	-4.19	1.32	1.37
29	ZM	203	PEB	C1A-NA	-4.19	1.32	1.37
29	JA	201	PEB	C1A-NA	-4.19	1.32	1.37
29	JN	201	PEB	C1A-NA	-4.19	1.32	1.37
29	I4	201	PEB	C1A-NA	-4.19	1.32	1.37
29	d7	201	PEB	C2A-C1A	-4.18	1.48	1.52
29	d9	201	PEB	C2A-C1A	-4.18	1.48	1.52
29	M4	201	PEB	C1A-NA	-4.18	1.32	1.37
29	FB	203	PEB	C1A-NA	-4.18	1.32	1.37
29	FM	203	PEB	C1A-NA	-4.18	1.32	1.37
29	HQ	203	PEB	C1A-NA	-4.18	1.32	1.37
29	J5	202	PEB	C1A-NA	-4.17	1.32	1.37
29	J8	202	PEB	C1A-NA	-4.17	1.32	1.37
29	FA	201	PEB	C1A-NA	-4.17	1.32	1.37
29	eB	202	PEB	C1A-NA	-4.17	1.32	1.37
29	eM	202	PEB	C1A-NA	-4.17	1.32	1.37
29	FN	201	PEB	C1A-NA	-4.17	1.32	1.37
29	F4	201	PEB	C1A-NA	-4.17	1.32	1.37
29	HB	203	PEB	C1A-NA	-4.17	1.32	1.37
29	HM	203	PEB	C1A-NA	-4.17	1.32	1.37
29	h7	201	PEB	C2A-C1A	-4.17	1.48	1.52
29	h9	201	PEB	C2A-C1A	-4.17	1.48	1.52
29	C3	202	PEB	C2C-C3C	4.17	1.50	1.37
29	CO	202	PEB	C2C-C3C	4.17	1.50	1.37
29	f7	201	PEB	C2A-C1A	-4.17	1.48	1.52
29	f9	201	PEB	C2A-C1A	-4.17	1.48	1.52
29	TB	203	PEB	C1A-NA	-4.16	1.32	1.37
29	TM	203	PEB	C1A-NA	-4.16	1.32	1.37
29	Q7	201	PEB	C2A-C1A	-4.16	1.48	1.52
29	Q9	201	PEB	C2A-C1A	-4.16	1.48	1.52
29	G3	202	PEB	C2C-C3C	4.16	1.50	1.37
29	GO	202	PEB	C2C-C3C	4.16	1.50	1.37
29	LB	203	PEB	C1A-NA	-4.16	1.32	1.37
29	LM	203	PEB	C1A-NA	-4.16	1.32	1.37
29	B4	201	PEB	C1A-NA	-4.16	1.32	1.37
29	cB	203	PEB	C1A-NA	-4.16	1.32	1.37
29	iB	203	PEB	C1A-NA	-4.16	1.32	1.37
29	cM	203	PEB	C1A-NA	-4.16	1.32	1.37
29	iM	203	PEB	C1A-NA	-4.16	1.32	1.37
30	MA	402	PUB	C2B-C1B	4.15	1.48	1.42
29	MD	203	PEB	C2A-C1A	-4.15	1.48	1.52
29	XB	202	PEB	C1A-NA	-4.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	XM	202	PEB	C1A-NA	-4.15	1.32	1.37
29	I3	202	PEB	C2C-C3C	4.15	1.50	1.37
29	IO	202	PEB	C2C-C3C	4.15	1.50	1.37
29	W7	201	PEB	C2A-C1A	-4.15	1.48	1.52
29	W9	201	PEB	C2A-C1A	-4.15	1.48	1.52
29	gB	203	PEB	C1A-NA	-4.15	1.32	1.37
29	gM	203	PEB	C1A-NA	-4.15	1.32	1.37
29	A7	305	PEB	C3C-C4C	4.14	1.48	1.42
29	A9	305	PEB	C3C-C4C	4.14	1.48	1.42
29	JB	203	PEB	C1A-NA	-4.14	1.32	1.37
29	kB	203	PEB	C1A-NA	-4.14	1.32	1.37
29	JM	203	PEB	C1A-NA	-4.14	1.32	1.37
29	kM	203	PEB	C1A-NA	-4.14	1.32	1.37
29	AF	305	PEB	C3C-C4C	4.14	1.48	1.42
29	AI	305	PEB	C3C-C4C	4.14	1.48	1.42
29	l7	201	PEB	C2A-C1A	-4.14	1.48	1.52
29	l9	201	PEB	C2A-C1A	-4.14	1.48	1.52
29	A3	202	PEB	C2C-C3C	4.14	1.49	1.37
29	AO	202	PEB	C2C-C3C	4.14	1.49	1.37
29	VB	203	PEB	C1A-NA	-4.14	1.32	1.37
29	VM	203	PEB	C1A-NA	-4.14	1.32	1.37
29	E3	202	PEB	C2C-C3C	4.14	1.49	1.37
29	EO	202	PEB	C2C-C3C	4.14	1.49	1.37
29	LD	201	PEB	C1A-NA	-4.14	1.32	1.37
29	S7	201	PEB	C2A-C1A	-4.14	1.48	1.52
29	S9	201	PEB	C2A-C1A	-4.14	1.48	1.52
29	HD	201	PEB	C1A-NA	-4.14	1.32	1.37
29	C4	201	PEB	C1A-NA	-4.13	1.32	1.37
29	NB	202	PEB	C1A-NA	-4.13	1.32	1.37
29	NM	202	PEB	C1A-NA	-4.13	1.32	1.37
29	HG	203	PEB	C1A-NA	-4.13	1.32	1.37
31	TP	1001	CYC	C1C-NC	-4.13	1.32	1.37
29	JQ	203	PEB	C1A-NA	-4.13	1.32	1.37
29	KD	203	PEB	C2A-C1A	-4.13	1.48	1.52
29	U7	201	PEB	C2A-C1A	-4.13	1.48	1.52
29	U9	201	PEB	C2A-C1A	-4.13	1.48	1.52
30	MN	402	PUB	C2B-C1B	4.13	1.48	1.42
29	K3	202	PEB	C2C-C3C	4.13	1.49	1.37
29	KO	202	PEB	C2C-C3C	4.13	1.49	1.37
29	FQ	203	PEB	C1A-NA	-4.12	1.32	1.37
31	pP	1001	CYC	C1C-NC	-4.12	1.32	1.37
29	DG	203	PEB	C1A-NA	-4.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	lP	1001	CYC	C1C-NC	-4.12	1.32	1.37
29	R1	201	PEB	C3C-C4C	4.12	1.48	1.42
29	RK	201	PEB	C3C-C4C	4.12	1.48	1.42
29	bJ	203	PEB	C1A-NA	-4.12	1.32	1.37
29	bL	203	PEB	C1A-NA	-4.12	1.32	1.37
29	GD	201	PEB	C1A-NA	-4.12	1.32	1.37
31	RP	1001	CYC	C1C-NC	-4.12	1.32	1.37
29	DB	203	PEB	C1A-NA	-4.11	1.32	1.37
29	DM	203	PEB	C1A-NA	-4.11	1.32	1.37
29	G4	201	PEB	C1A-NA	-4.11	1.32	1.37
31	N1	1001	CYC	C1C-NC	-4.11	1.32	1.37
29	JG	203	PEB	C1A-NA	-4.11	1.32	1.37
31	D1	1001	CYC	C1C-NC	-4.11	1.32	1.37
31	NF	1001	CYC	C2C-C1C	-4.11	1.48	1.52
31	NI	1001	CYC	C2C-C1C	-4.11	1.48	1.52
31	rP	1001	CYC	C1C-NC	-4.11	1.32	1.37
29	RB	203	PEB	C1A-NA	-4.11	1.32	1.37
29	RM	203	PEB	C1A-NA	-4.11	1.32	1.37
29	K3	201	PEB	C1A-NA	-4.11	1.32	1.37
29	KO	201	PEB	C1A-NA	-4.11	1.32	1.37
31	JP	1001	CYC	C1C-NC	-4.11	1.32	1.37
29	DQ	203	PEB	C1A-NA	-4.11	1.32	1.37
29	FJ	203	PEB	C1A-NA	-4.10	1.32	1.37
29	FL	203	PEB	C1A-NA	-4.10	1.32	1.37
31	H1	1001	CYC	C1C-NC	-4.10	1.32	1.37
31	iP	1001	CYC	C1C-NC	-4.10	1.32	1.37
29	nJ	203	PEB	C1A-NA	-4.10	1.32	1.37
29	nL	203	PEB	C1A-NA	-4.10	1.32	1.37
29	Z7	201	PEB	C2A-C1A	-4.10	1.48	1.52
29	Z9	201	PEB	C2A-C1A	-4.10	1.48	1.52
31	PP	1001	CYC	C1C-NC	-4.09	1.32	1.37
31	DK	1001	CYC	C1C-NC	-4.09	1.32	1.37
29	i7	202	PEB	C1A-NA	-4.09	1.32	1.37
29	i9	202	PEB	C1A-NA	-4.09	1.32	1.37
31	AP	1001	CYC	C1C-NC	-4.09	1.32	1.37
31	GP	1001	CYC	C1C-NC	-4.09	1.32	1.37
31	J1	1001	CYC	C1C-NC	-4.09	1.32	1.37
31	JK	1001	CYC	C1C-NC	-4.09	1.32	1.37
31	gP	1001	CYC	C1C-NC	-4.09	1.32	1.37
29	ID	201	PEB	C1A-NA	-4.09	1.32	1.37
29	HJ	202	PEB	C1A-NA	-4.09	1.32	1.37
29	HL	202	PEB	C1A-NA	-4.09	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V7	202	PEB	C1A-NA	-4.08	1.32	1.37
29	V9	202	PEB	C1A-NA	-4.08	1.32	1.37
31	NK	1001	CYC	C1C-NC	-4.08	1.32	1.37
31	vP	1001	CYC	C1C-NC	-4.08	1.32	1.37
29	E3	201	PEB	C1A-NA	-4.08	1.32	1.37
29	EO	201	PEB	C1A-NA	-4.08	1.32	1.37
29	LJ	202	PEB	C1A-NA	-4.08	1.32	1.37
29	LL	202	PEB	C1A-NA	-4.08	1.32	1.37
29	DJ	202	PEB	C1A-NA	-4.08	1.32	1.37
29	DL	202	PEB	C1A-NA	-4.08	1.32	1.37
29	BG	203	PEB	C1A-NA	-4.08	1.32	1.37
31	KP	1001	CYC	C1C-NC	-4.07	1.32	1.37
29	aF	201	PEB	C1A-NA	-4.07	1.32	1.37
29	aI	201	PEB	C1A-NA	-4.07	1.32	1.37
29	vJ	202	PEB	C1A-NA	-4.07	1.32	1.37
29	vL	202	PEB	C1A-NA	-4.07	1.32	1.37
31	IF	1001	CYC	C1C-NC	-4.07	1.32	1.37
31	II	1001	CYC	C1C-NC	-4.07	1.32	1.37
31	EP	1001	CYC	C1C-NC	-4.07	1.32	1.37
29	T1	202	PEB	CHA-C1B	4.07	1.49	1.40
29	TK	202	PEB	CHA-C1B	4.07	1.49	1.40
29	G3	201	PEB	C1A-NA	-4.07	1.32	1.37
29	GO	201	PEB	C1A-NA	-4.07	1.32	1.37
29	V1	203	PEB	CHA-C1B	4.07	1.49	1.40
29	VK	203	PEB	CHA-C1B	4.07	1.49	1.40
29	P1	201	PEB	C3C-C4C	4.07	1.48	1.42
29	PK	201	PEB	C3C-C4C	4.07	1.48	1.42
29	FG	203	PEB	C1A-NA	-4.07	1.32	1.37
31	CF	1001	CYC	C1C-NC	-4.07	1.32	1.37
31	CI	1001	CYC	C1C-NC	-4.07	1.32	1.37
29	IJ	203	PEB	C1A-NA	-4.06	1.32	1.37
29	rJ	203	PEB	C1A-NA	-4.06	1.32	1.37
29	IL	203	PEB	C1A-NA	-4.06	1.32	1.37
29	rL	203	PEB	C1A-NA	-4.06	1.32	1.37
29	IF	201	PEB	C1A-NA	-4.06	1.32	1.37
29	II	201	PEB	C1A-NA	-4.06	1.32	1.37
31	F1	1001	CYC	C1C-NC	-4.06	1.32	1.37
31	FK	1001	CYC	C1C-NC	-4.06	1.32	1.37
31	eP	1001	CYC	C1C-NC	-4.06	1.32	1.37
29	RJ	203	PEB	C1A-NA	-4.06	1.32	1.37
29	RL	203	PEB	C1A-NA	-4.06	1.32	1.37
29	Y1	202	PEB	CHA-C1B	4.06	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YK	202	PEB	CHA-C1B	4.06	1.49	1.40
29	pJ	203	PEB	C1A-NA	-4.06	1.32	1.37
29	pL	203	PEB	C1A-NA	-4.06	1.32	1.37
29	MD	202	PEB	OD-C4D	4.06	1.31	1.23
29	VJ	202	PEB	C1A-NA	-4.06	1.32	1.37
29	VL	202	PEB	C1A-NA	-4.06	1.32	1.37
31	mP	1001	CYC	C1C-NC	-4.06	1.32	1.37
29	R1	203	PEB	CHA-C1B	4.06	1.49	1.40
29	RK	203	PEB	CHA-C1B	4.06	1.49	1.40
29	m7	202	PEB	C1A-NA	-4.06	1.32	1.37
29	m9	202	PEB	C1A-NA	-4.06	1.32	1.37
29	gF	201	PEB	C1A-NA	-4.06	1.32	1.37
29	gI	201	PEB	C1A-NA	-4.06	1.32	1.37
29	LG	203	PEB	C1A-NA	-4.06	1.32	1.37
29	P1	203	PEB	CHA-C1B	4.06	1.49	1.40
29	PK	203	PEB	CHA-C1B	4.06	1.49	1.40
31	CP	1001	CYC	C1C-NC	-4.05	1.32	1.37
29	YF	201	PEB	C1A-NA	-4.05	1.32	1.37
29	YI	201	PEB	C1A-NA	-4.05	1.32	1.37
29	Y7	202	PEB	C1A-NA	-4.05	1.32	1.37
29	Y9	202	PEB	C1A-NA	-4.05	1.32	1.37
31	EF	1001	CYC	C1C-NC	-4.05	1.32	1.37
31	EI	1001	CYC	C1C-NC	-4.05	1.32	1.37
29	ED	201	PEB	OD-C4D	4.05	1.31	1.23
29	c1	203	PEB	CHA-C1B	4.05	1.49	1.40
29	cK	203	PEB	CHA-C1B	4.05	1.49	1.40
29	QF	201	PEB	C1A-NA	-4.05	1.32	1.37
29	QI	201	PEB	C1A-NA	-4.05	1.32	1.37
29	g1	203	PEB	CHA-C1B	4.05	1.49	1.40
29	gK	203	PEB	CHA-C1B	4.05	1.49	1.40
30	QB	201	PUB	C3B-C2B	4.05	1.49	1.37
30	QM	201	PUB	C3B-C2B	4.05	1.49	1.37
29	ZJ	203	PEB	C1A-NA	-4.05	1.32	1.37
29	ZL	203	PEB	C1A-NA	-4.05	1.32	1.37
31	tP	1001	CYC	C1C-NC	-4.05	1.32	1.37
29	i1	201	PEB	C3C-C4C	4.05	1.48	1.42
29	iK	201	PEB	C3C-C4C	4.05	1.48	1.42
29	I4	202	PEB	OD-C4D	4.05	1.31	1.23
29	ID	202	PEB	OD-C4D	4.05	1.31	1.23
29	hF	201	PEB	C1A-NA	-4.05	1.32	1.37
29	hI	201	PEB	C1A-NA	-4.05	1.32	1.37
29	BQ	203	PEB	C1A-NA	-4.05	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JJ	203	PEB	C1A-NA	-4.04	1.32	1.37
29	JL	203	PEB	C1A-NA	-4.04	1.32	1.37
29	k1	203	PEB	CHA-C1B	4.04	1.49	1.40
29	kK	203	PEB	CHA-C1B	4.04	1.49	1.40
29	i1	203	PEB	CHA-C1B	4.04	1.49	1.40
29	iK	203	PEB	CHA-C1B	4.04	1.49	1.40
29	bF	201	PEB	C1A-NA	-4.04	1.32	1.37
29	bI	201	PEB	C1A-NA	-4.04	1.32	1.37
29	R7	202	PEB	C1A-NA	-4.04	1.32	1.37
29	e7	202	PEB	C1A-NA	-4.04	1.32	1.37
29	R9	202	PEB	C1A-NA	-4.04	1.32	1.37
29	e9	202	PEB	C1A-NA	-4.04	1.32	1.37
29	a1	203	PEB	CHA-C1B	4.04	1.49	1.40
29	aK	203	PEB	CHA-C1B	4.04	1.49	1.40
29	PJ	203	PEB	C1A-NA	-4.04	1.32	1.37
29	TJ	203	PEB	C1A-NA	-4.04	1.32	1.37
29	PL	203	PEB	C1A-NA	-4.04	1.32	1.37
29	TL	203	PEB	C1A-NA	-4.04	1.32	1.37
31	LF	1001	CYC	C2C-C1C	-4.04	1.48	1.52
31	LI	1001	CYC	C2C-C1C	-4.04	1.48	1.52
29	N3	203	PEB	CHA-C1B	4.04	1.49	1.40
29	T1	201	PEB	C3C-C4C	4.04	1.48	1.42
29	k1	201	PEB	C3C-C4C	4.04	1.48	1.42
29	TK	201	PEB	C3C-C4C	4.04	1.48	1.42
29	kK	201	PEB	C3C-C4C	4.04	1.48	1.42
29	dJ	203	PEB	C1A-NA	-4.04	1.32	1.37
29	dL	203	PEB	C1A-NA	-4.04	1.32	1.37
31	HK	1001	CYC	C1C-NC	-4.04	1.32	1.37
29	NO	203	PEB	CHA-C1B	4.04	1.49	1.40
31	NP	1001	CYC	C1C-NC	-4.04	1.32	1.37
29	Y1	201	PEB	C3C-C4C	4.04	1.48	1.42
29	YK	201	PEB	C3C-C4C	4.04	1.48	1.42
29	Z1	202	PEB	C1A-NA	-4.04	1.32	1.37
29	CA	201	PEB	C1A-NA	-4.04	1.32	1.37
29	ZK	202	PEB	C1A-NA	-4.04	1.32	1.37
29	CN	201	PEB	C1A-NA	-4.04	1.32	1.37
29	k7	202	PEB	C1A-NA	-4.04	1.32	1.37
29	k9	202	PEB	C1A-NA	-4.04	1.32	1.37
29	BJ	203	PEB	C1A-NA	-4.04	1.32	1.37
29	BL	203	PEB	C1A-NA	-4.04	1.32	1.37
29	e1	203	PEB	CHA-C1B	4.04	1.49	1.40
29	eK	203	PEB	CHA-C1B	4.04	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a1	201	PEB	C3C-C4C	4.04	1.48	1.42
29	aK	201	PEB	C3C-C4C	4.04	1.48	1.42
31	L1	1001	CYC	C1C-NC	-4.03	1.32	1.37
31	LK	1001	CYC	C1C-NC	-4.03	1.32	1.37
29	S1	201	PEB	C1A-NA	-4.03	1.32	1.37
29	kF	201	PEB	C1A-NA	-4.03	1.32	1.37
29	kI	201	PEB	C1A-NA	-4.03	1.32	1.37
29	SK	201	PEB	C1A-NA	-4.03	1.32	1.37
29	M3	203	PEB	CHA-C1B	4.03	1.49	1.40
29	MO	203	PEB	CHA-C1B	4.03	1.49	1.40
29	a7	202	PEB	C1A-NA	-4.03	1.32	1.37
29	a9	202	PEB	C1A-NA	-4.03	1.32	1.37
29	OF	201	PEB	C1A-NA	-4.03	1.32	1.37
29	mF	201	PEB	C1A-NA	-4.03	1.32	1.37
29	OI	201	PEB	C1A-NA	-4.03	1.32	1.37
29	mI	201	PEB	C1A-NA	-4.03	1.32	1.37
29	PF	201	PEB	C1A-NA	-4.03	1.32	1.37
29	PI	201	PEB	C1A-NA	-4.03	1.32	1.37
29	XJ	203	PEB	C1A-NA	-4.03	1.32	1.37
29	XL	203	PEB	C1A-NA	-4.03	1.32	1.37
29	C4	202	PEB	OD-C4D	4.03	1.31	1.23
29	CD	202	PEB	OD-C4D	4.03	1.31	1.23
31	cP	1001	CYC	C1C-NC	-4.03	1.32	1.37
29	f1	201	PEB	C1A-NA	-4.03	1.32	1.37
29	fK	201	PEB	C1A-NA	-4.03	1.32	1.37
29	m1	202	PEB	CHA-C1B	4.03	1.49	1.40
29	mK	202	PEB	CHA-C1B	4.03	1.49	1.40
29	TI	201	PEB	C1A-NA	-4.03	1.32	1.37
31	MF	1001	CYC	C1C-NC	-4.03	1.32	1.37
31	MI	1001	CYC	C1C-NC	-4.03	1.32	1.37
29	NJ	203	PEB	C1A-NA	-4.02	1.32	1.37
29	NL	203	PEB	C1A-NA	-4.02	1.32	1.37
31	JF	1001	CYC	C2C-C1C	-4.02	1.48	1.52
31	JI	1001	CYC	C2C-C1C	-4.02	1.48	1.52
29	fJ	203	PEB	C1A-NA	-4.02	1.32	1.37
29	fL	203	PEB	C1A-NA	-4.02	1.32	1.37
29	E4	202	PEB	OD-C4D	4.02	1.31	1.23
29	iF	201	PEB	C1A-NA	-4.02	1.32	1.37
29	iI	201	PEB	C1A-NA	-4.02	1.32	1.37
29	tJ	202	PEB	C1A-NA	-4.02	1.32	1.37
29	tL	202	PEB	C1A-NA	-4.02	1.32	1.37
29	J3	203	PEB	CHA-C1B	4.02	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JO	203	PEB	CHA-C1B	4.02	1.49	1.40
29	jF	201	PEB	C1A-NA	-4.02	1.32	1.37
29	jI	201	PEB	C1A-NA	-4.02	1.32	1.37
29	LQ	202	PEB	C1A-NA	-4.02	1.32	1.37
29	M4	202	PEB	OD-C4D	4.02	1.31	1.23
29	jJ	203	PEB	C1A-NA	-4.02	1.32	1.37
29	jL	203	PEB	C1A-NA	-4.02	1.32	1.37
29	e1	201	PEB	C3C-C4C	4.01	1.48	1.42
29	eK	201	PEB	C3C-C4C	4.01	1.48	1.42
29	C3	201	PEB	C1A-NA	-4.01	1.32	1.37
29	CO	201	PEB	C1A-NA	-4.01	1.32	1.37
29	G4	202	PEB	OD-C4D	4.01	1.31	1.23
29	m1	201	PEB	C3C-C4C	4.01	1.48	1.42
29	mK	201	PEB	C3C-C4C	4.01	1.48	1.42
29	I3	201	PEB	C1A-NA	-4.01	1.32	1.37
29	IO	201	PEB	C1A-NA	-4.01	1.32	1.37
29	fF	201	PEB	C1A-NA	-4.01	1.32	1.37
29	fI	201	PEB	C1A-NA	-4.01	1.32	1.37
29	D3	203	PEB	CHA-C1B	4.01	1.49	1.40
29	DO	203	PEB	CHA-C1B	4.01	1.49	1.40
29	g1	201	PEB	C3C-C4C	4.01	1.48	1.42
29	gK	201	PEB	C3C-C4C	4.01	1.48	1.42
29	j1	201	PEB	C1A-NA	-4.01	1.32	1.37
29	jK	201	PEB	C1A-NA	-4.01	1.32	1.37
29	VF	201	PEB	C1A-NA	-4.01	1.32	1.37
29	VI	201	PEB	C1A-NA	-4.01	1.32	1.37
29	c1	201	PEB	C3C-C4C	4.01	1.48	1.42
29	cK	201	PEB	C3C-C4C	4.01	1.48	1.42
29	cF	201	PEB	C1A-NA	-4.01	1.32	1.37
29	cI	201	PEB	C1A-NA	-4.01	1.32	1.37
29	V1	201	PEB	C3C-C4C	4.01	1.48	1.42
29	VK	201	PEB	C3C-C4C	4.01	1.48	1.42
29	A3	201	PEB	C1A-NA	-4.01	1.32	1.37
29	SF	201	PEB	C1A-NA	-4.01	1.32	1.37
29	SI	201	PEB	C1A-NA	-4.01	1.32	1.37
29	AO	201	PEB	C1A-NA	-4.01	1.32	1.37
29	GD	202	PEB	OD-C4D	4.00	1.31	1.23
29	hJ	203	PEB	C1A-NA	-4.00	1.32	1.37
29	hL	203	PEB	C1A-NA	-4.00	1.32	1.37
29	L3	202	PEB	CHA-C1B	4.00	1.49	1.40
29	LO	202	PEB	CHA-C1B	4.00	1.49	1.40
29	O1	201	PEB	C1A-NA	-4.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W1	201	PEB	C1A-NA	-4.00	1.32	1.37
29	c7	202	PEB	C1A-NA	-4.00	1.32	1.37
29	c9	202	PEB	C1A-NA	-4.00	1.32	1.37
29	OK	201	PEB	C1A-NA	-4.00	1.32	1.37
29	WK	201	PEB	C1A-NA	-4.00	1.32	1.37
31	KF	1001	CYC	C1C-NC	-4.00	1.32	1.37
31	FF	1001	CYC	C2C-C1C	-4.00	1.48	1.52
31	FI	1001	CYC	C2C-C1C	-4.00	1.48	1.52
29	F3	203	PEB	CHA-C1B	4.00	1.49	1.40
29	FO	203	PEB	CHA-C1B	4.00	1.49	1.40
29	B3	203	PEB	CHA-C1B	4.00	1.49	1.40
29	BO	203	PEB	CHA-C1B	4.00	1.49	1.40
29	AA	201	PEB	C1A-NA	-4.00	1.32	1.37
29	AN	201	PEB	C1A-NA	-4.00	1.32	1.37
31	GF	1001	CYC	C1C-NC	-4.00	1.32	1.37
31	GI	1001	CYC	C1C-NC	-4.00	1.32	1.37
31	HF	1001	CYC	C2C-C1C	-3.99	1.48	1.52
31	HI	1001	CYC	C2C-C1C	-3.99	1.48	1.52
29	P7	202	PEB	C1A-NA	-3.99	1.32	1.37
29	P9	202	PEB	C1A-NA	-3.99	1.32	1.37
31	qP	1001	CYC	C2C-C1C	-3.99	1.48	1.52
29	eF	201	PEB	C1A-NA	-3.99	1.32	1.37
29	eI	201	PEB	C1A-NA	-3.99	1.32	1.37
29	g7	202	PEB	C1A-NA	-3.99	1.32	1.37
29	g9	202	PEB	C1A-NA	-3.99	1.32	1.37
29	K4	202	PEB	OD-C4D	3.99	1.31	1.23
29	KD	202	PEB	OD-C4D	3.99	1.31	1.23
29	dF	202	PEB	C1A-NA	-3.99	1.32	1.37
29	dI	202	PEB	C1A-NA	-3.99	1.32	1.37
29	U1	202	PEB	C1A-NA	-3.99	1.32	1.37
29	UK	202	PEB	C1A-NA	-3.99	1.32	1.37
29	WF	201	PEB	C1A-NA	-3.98	1.32	1.37
29	WI	201	PEB	C1A-NA	-3.98	1.32	1.37
31	KI	1001	CYC	C1C-NC	-3.98	1.32	1.37
31	HP	1001	CYC	C2C-C1C	-3.98	1.48	1.52
29	UF	202	PEB	C1A-NA	-3.98	1.32	1.37
29	UI	202	PEB	C1A-NA	-3.98	1.32	1.37
29	l1	201	PEB	C1A-NA	-3.98	1.32	1.37
29	lK	201	PEB	C1A-NA	-3.98	1.32	1.37
30	AB	304	PUB	OD-C4D	3.98	1.31	1.23
29	GA	201	PEB	C1A-NA	-3.98	1.32	1.37
29	ZF	201	PEB	C1A-NA	-3.98	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZI	201	PEB	C1A-NA	-3.98	1.32	1.37
29	GN	201	PEB	C1A-NA	-3.98	1.32	1.37
29	yJ	301	PEB	C1A-NA	-3.98	1.32	1.37
29	yL	301	PEB	C1A-NA	-3.98	1.32	1.37
31	DF	1001	CYC	C2C-C1C	-3.98	1.48	1.52
31	DI	1001	CYC	C2C-C1C	-3.98	1.48	1.52
31	VP	1001	CYC	CHB-C4A	3.98	1.49	1.40
29	GD	202	PEB	C3C-C4C	3.98	1.48	1.42
29	T7	202	PEB	C1A-NA	-3.98	1.32	1.37
29	T9	202	PEB	C1A-NA	-3.98	1.32	1.37
31	vP	1001	CYC	CHB-C4A	3.98	1.49	1.40
29	RF	201	PEB	C1A-NA	-3.98	1.32	1.37
29	RI	201	PEB	C1A-NA	-3.98	1.32	1.37
29	H3	203	PEB	CHA-C1B	3.97	1.49	1.40
29	HO	203	PEB	CHA-C1B	3.97	1.49	1.40
29	C4	202	PEB	C3C-C4C	3.97	1.48	1.42
29	xJ	302	PEB	CHA-C1B	3.96	1.49	1.40
31	NP	1001	CYC	CHB-C4A	3.96	1.49	1.40
31	PP	1001	CYC	CHB-C4A	3.96	1.49	1.40
29	wJ	302	PEB	CHA-C1B	3.96	1.49	1.40
29	xL	302	PEB	CHA-C1B	3.96	1.49	1.40
29	DC	202	PEB	CHA-C1B	3.96	1.49	1.40
29	DE	202	PEB	CHA-C1B	3.96	1.49	1.40
29	KA	201	PEB	C1A-NA	-3.96	1.32	1.37
29	KN	201	PEB	C1A-NA	-3.96	1.32	1.37
30	AM	304	PUB	OD-C4D	3.95	1.31	1.23
29	EA	201	PEB	C1A-NA	-3.95	1.32	1.37
29	EN	201	PEB	C1A-NA	-3.95	1.32	1.37
31	fP	1001	CYC	C2C-C1C	-3.95	1.48	1.52
29	d1	201	PEB	C1A-NA	-3.95	1.32	1.37
29	JF	1002	PEB	C1A-NA	-3.95	1.32	1.37
29	JI	1002	PEB	C1A-NA	-3.95	1.32	1.37
29	dK	201	PEB	C1A-NA	-3.95	1.32	1.37
29	wL	302	PEB	CHA-C1B	3.95	1.49	1.40
29	yJ	301	PEB	C2A-C1A	-3.95	1.48	1.52
29	yL	301	PEB	C2A-C1A	-3.95	1.48	1.52
29	JC	202	PEB	CHA-C1B	3.95	1.49	1.40
29	JE	202	PEB	CHA-C1B	3.95	1.49	1.40
29	CD	202	PEB	C3C-C4C	3.95	1.48	1.42
29	b1	201	PEB	C1A-NA	-3.95	1.32	1.37
29	bK	201	PEB	C1A-NA	-3.95	1.32	1.37
31	lP	1001	CYC	CHB-C4A	3.95	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	rP	1001	CYC	CHB-C4A	3.95	1.49	1.40
29	M4	202	PEB	C3C-C4C	3.95	1.48	1.42
31	pP	1001	CYC	CHB-C4A	3.94	1.49	1.40
31	xP	1001	CYC	CHB-C4A	3.94	1.49	1.40
31	WP	1001	CYC	C1C-NC	-3.94	1.32	1.37
29	UF	203	PEB	CHA-C1B	3.94	1.49	1.40
29	UI	203	PEB	CHA-C1B	3.94	1.49	1.40
29	A7	305	PEB	CHA-C1B	3.94	1.49	1.40
29	A9	305	PEB	CHA-C1B	3.94	1.49	1.40
31	GP	1001	CYC	CHB-C4A	3.94	1.49	1.40
31	JP	1001	CYC	CHB-C4A	3.94	1.49	1.40
29	QF	202	PEB	CHA-C1B	3.94	1.49	1.40
29	QI	202	PEB	CHA-C1B	3.94	1.49	1.40
29	MD	202	PEB	C3C-C4C	3.94	1.48	1.42
31	iP	1001	CYC	CHB-C4A	3.94	1.49	1.40
31	IP	1001	CYC	C2C-C1C	-3.93	1.48	1.52
31	SP	1001	CYC	C2C-C1C	-3.93	1.48	1.52
31	yP	1001	CYC	C1C-NC	-3.93	1.32	1.37
29	h1	201	PEB	C1A-NA	-3.93	1.32	1.37
29	hK	201	PEB	C1A-NA	-3.93	1.32	1.37
29	ID	202	PEB	C3C-C4C	3.93	1.48	1.42
29	BJ	202	PEB	OD-C4D	3.93	1.31	1.23
29	BL	202	PEB	OD-C4D	3.93	1.31	1.23
29	LC	203	PEB	CHA-C1B	3.93	1.49	1.40
29	LE	203	PEB	CHA-C1B	3.93	1.49	1.40
29	BC	203	PEB	CHA-C1B	3.93	1.49	1.40
29	BE	203	PEB	CHA-C1B	3.93	1.49	1.40
31	RP	1001	CYC	CHB-C4A	3.93	1.49	1.40
29	EA	202	PEB	C2C-C3C	3.93	1.49	1.37
29	EN	202	PEB	C2C-C3C	3.93	1.49	1.37
29	G4	202	PEB	C3C-C4C	3.93	1.48	1.42
29	fJ	202	PEB	OD-C4D	3.93	1.31	1.23
29	fL	202	PEB	OD-C4D	3.93	1.31	1.23
29	XJ	202	PEB	OD-C4D	3.92	1.31	1.23
29	XL	202	PEB	OD-C4D	3.92	1.31	1.23
29	ED	201	PEB	C3C-C4C	3.92	1.48	1.42
31	tP	1001	CYC	CHB-C4A	3.92	1.49	1.40
31	TP	1001	CYC	CHB-C4A	3.92	1.49	1.40
29	h7	201	PEB	C3B-C2B	3.92	1.45	1.36
29	h9	201	PEB	C3B-C2B	3.92	1.45	1.36
31	EP	1001	CYC	CHB-C4A	3.92	1.49	1.40
29	Z7	201	PEB	C3B-C2B	3.92	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z9	201	PEB	C3B-C2B	3.92	1.45	1.36
29	Q1	201	PEB	C1A-NA	-3.92	1.32	1.37
29	QK	201	PEB	C1A-NA	-3.92	1.32	1.37
29	E4	202	PEB	C3C-C4C	3.92	1.48	1.42
29	nJ	202	PEB	OD-C4D	3.92	1.31	1.23
29	nL	202	PEB	OD-C4D	3.92	1.31	1.23
31	gP	1001	CYC	CHB-C4A	3.92	1.49	1.40
29	U7	201	PEB	C3B-C2B	3.92	1.45	1.36
29	W7	201	PEB	C3B-C2B	3.92	1.45	1.36
29	b7	201	PEB	C3B-C2B	3.92	1.45	1.36
29	U9	201	PEB	C3B-C2B	3.92	1.45	1.36
29	W9	201	PEB	C3B-C2B	3.92	1.45	1.36
29	b9	201	PEB	C3B-C2B	3.92	1.45	1.36
31	BP	1001	CYC	C2C-C1C	-3.92	1.48	1.52
29	Q7	201	PEB	C3B-C2B	3.92	1.45	1.36
29	Q9	201	PEB	C3B-C2B	3.92	1.45	1.36
29	FF	1002	PEB	C1A-NA	-3.92	1.32	1.37
29	FI	1002	PEB	C1A-NA	-3.92	1.32	1.37
29	CA	202	PEB	C2C-C3C	3.92	1.49	1.37
29	CN	202	PEB	C2C-C3C	3.92	1.49	1.37
31	KP	1001	CYC	CHB-C4A	3.92	1.49	1.40
29	dJ	202	PEB	OD-C4D	3.92	1.31	1.23
29	dL	202	PEB	OD-C4D	3.92	1.31	1.23
31	AP	1001	CYC	CHB-C4A	3.92	1.49	1.40
29	IA	201	PEB	C1A-NA	-3.92	1.32	1.37
29	IN	201	PEB	C1A-NA	-3.92	1.32	1.37
29	AA	202	PEB	C2C-C3C	3.92	1.49	1.37
29	AN	202	PEB	C2C-C3C	3.92	1.49	1.37
29	HC	203	PEB	CHA-C1B	3.92	1.49	1.40
29	HE	203	PEB	CHA-C1B	3.92	1.49	1.40
31	cP	1001	CYC	CHB-C4A	3.92	1.49	1.40
29	KD	202	PEB	C3C-C4C	3.91	1.48	1.42
30	AF	302	PUB	C3B-C2B	3.91	1.49	1.37
30	AI	302	PUB	C3B-C2B	3.91	1.49	1.37
29	O7	201	PEB	C3B-C2B	3.91	1.45	1.36
29	O9	201	PEB	C3B-C2B	3.91	1.45	1.36
29	ZF	202	PEB	CHA-C1B	3.91	1.49	1.40
29	ZI	202	PEB	CHA-C1B	3.91	1.49	1.40
31	eP	1001	CYC	CHB-C4A	3.91	1.49	1.40
31	nP	1001	CYC	C2C-C1C	-3.91	1.48	1.52
29	j7	201	PEB	C3B-C2B	3.91	1.45	1.36
29	j9	201	PEB	C3B-C2B	3.91	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	wP	1001	CYC	C2C-C1C	-3.91	1.48	1.52
31	kP	1001	CYC	C2C-C1C	-3.91	1.48	1.52
29	lJ	202	PEB	OD-C4D	3.91	1.31	1.23
29	lL	202	PEB	OD-C4D	3.91	1.31	1.23
29	lF	202	PEB	CHA-C1B	3.91	1.49	1.40
29	lI	202	PEB	CHA-C1B	3.91	1.49	1.40
31	DK	1001	CYC	C2C-C1C	-3.91	1.48	1.52
29	KA	202	PEB	C2C-C3C	3.91	1.49	1.37
29	KN	202	PEB	C2C-C3C	3.91	1.49	1.37
29	J3	201	PEB	C1A-NA	-3.91	1.32	1.37
29	JO	201	PEB	C1A-NA	-3.91	1.32	1.37
29	I4	202	PEB	C3C-C4C	3.91	1.48	1.42
29	dF	203	PEB	CHA-C1B	3.91	1.49	1.40
29	dI	203	PEB	CHA-C1B	3.91	1.49	1.40
29	JJ	202	PEB	OD-C4D	3.91	1.31	1.23
29	JL	202	PEB	OD-C4D	3.91	1.31	1.23
29	HJ	201	PEB	OD-C4D	3.91	1.31	1.23
29	HL	201	PEB	OD-C4D	3.91	1.31	1.23
29	bJ	202	PEB	OD-C4D	3.90	1.31	1.23
29	bL	202	PEB	OD-C4D	3.90	1.31	1.23
29	K4	202	PEB	C3C-C4C	3.90	1.48	1.42
29	rJ	202	PEB	OD-C4D	3.90	1.31	1.23
29	rL	202	PEB	OD-C4D	3.90	1.31	1.23
29	FC	203	PEB	CHA-C1B	3.90	1.49	1.40
29	FE	203	PEB	CHA-C1B	3.90	1.49	1.40
29	hJ	202	PEB	OD-C4D	3.90	1.31	1.23
29	hL	202	PEB	OD-C4D	3.90	1.31	1.23
29	SF	202	PEB	CHA-C1B	3.90	1.49	1.40
29	SI	202	PEB	CHA-C1B	3.90	1.49	1.40
31	mP	1001	CYC	CHB-C4A	3.90	1.49	1.40
29	WJ	201	PEB	OD-C4D	3.90	1.31	1.23
29	WL	201	PEB	OD-C4D	3.90	1.31	1.23
29	AJ	203	PEB	OD-C4D	3.90	1.31	1.23
29	IJ	203	PEB	OD-C4D	3.90	1.31	1.23
29	AL	203	PEB	OD-C4D	3.90	1.31	1.23
29	IL	203	PEB	OD-C4D	3.90	1.31	1.23
29	pJ	202	PEB	OD-C4D	3.90	1.31	1.23
29	pL	202	PEB	OD-C4D	3.90	1.31	1.23
29	jF	202	PEB	CHA-C1B	3.90	1.49	1.40
29	jI	202	PEB	CHA-C1B	3.90	1.49	1.40
31	UP	1001	CYC	C2C-C1C	-3.90	1.48	1.52
29	GA	202	PEB	C2C-C3C	3.90	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GN	202	PEB	C2C-C3C	3.90	1.49	1.37
29	d7	201	PEB	C3B-C2B	3.90	1.45	1.36
29	d9	201	PEB	C3B-C2B	3.90	1.45	1.36
31	CP	1001	CYC	CHB-C4A	3.90	1.49	1.40
29	sJ	203	PEB	OD-C4D	3.90	1.31	1.23
29	sL	203	PEB	OD-C4D	3.90	1.31	1.23
29	hF	202	PEB	CHA-C1B	3.90	1.49	1.40
29	hI	202	PEB	CHA-C1B	3.90	1.49	1.40
29	IA	202	PEB	C2C-C3C	3.90	1.49	1.37
29	IN	202	PEB	C2C-C3C	3.90	1.49	1.37
29	D3	201	PEB	C1A-NA	-3.90	1.32	1.37
29	DO	201	PEB	C1A-NA	-3.90	1.32	1.37
29	OF	202	PEB	CHA-C1B	3.90	1.49	1.40
29	OI	202	PEB	CHA-C1B	3.90	1.49	1.40
29	OF	203	PEB	C1A-NA	-3.90	1.32	1.37
29	OI	203	PEB	C1A-NA	-3.90	1.32	1.37
29	bF	202	PEB	CHA-C1B	3.89	1.49	1.40
29	bI	202	PEB	CHA-C1B	3.89	1.49	1.40
29	FJ	202	PEB	OD-C4D	3.89	1.31	1.23
29	FL	202	PEB	OD-C4D	3.89	1.31	1.23
29	NF	1002	PEB	C1A-NA	-3.89	1.32	1.37
29	NI	1002	PEB	C1A-NA	-3.89	1.32	1.37
29	PJ	202	PEB	OD-C4D	3.89	1.31	1.23
29	PL	202	PEB	OD-C4D	3.89	1.31	1.23
29	f7	201	PEB	C3B-C2B	3.89	1.45	1.36
29	f9	201	PEB	C3B-C2B	3.89	1.45	1.36
29	uJ	201	PEB	OD-C4D	3.89	1.31	1.23
29	uL	201	PEB	OD-C4D	3.89	1.31	1.23
29	S7	201	PEB	C3B-C2B	3.89	1.45	1.36
29	S9	201	PEB	C3B-C2B	3.89	1.45	1.36
29	fF	202	PEB	CHA-C1B	3.89	1.49	1.40
29	fI	202	PEB	CHA-C1B	3.89	1.49	1.40
29	eF	203	PEB	CHA-C1B	3.89	1.49	1.40
29	eI	203	PEB	CHA-C1B	3.89	1.49	1.40
29	DF	1002	PEB	C1A-NA	-3.89	1.32	1.37
29	DI	1002	PEB	C1A-NA	-3.89	1.32	1.37
29	l7	201	PEB	C3B-C2B	3.89	1.45	1.36
29	l9	201	PEB	C3B-C2B	3.89	1.45	1.36
31	M9	1001	CYC	C1C-NC	-3.89	1.32	1.37
29	RJ	202	PEB	OD-C4D	3.89	1.31	1.23
29	TJ	202	PEB	OD-C4D	3.89	1.31	1.23
29	RL	202	PEB	OD-C4D	3.89	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TL	202	PEB	OD-C4D	3.89	1.31	1.23
29	F3	201	PEB	C1A-NA	-3.89	1.32	1.37
29	FO	201	PEB	C1A-NA	-3.89	1.32	1.37
29	gF	203	PEB	CHA-C1B	3.89	1.49	1.40
29	gI	203	PEB	CHA-C1B	3.89	1.49	1.40
31	L1	1001	CYC	C2C-C1C	-3.88	1.48	1.52
31	LK	1001	CYC	C2C-C1C	-3.88	1.48	1.52
31	MP	1001	CYC	C2C-C1C	-3.88	1.48	1.52
29	TF	202	PEB	CHA-C1B	3.88	1.49	1.40
29	TI	202	PEB	CHA-C1B	3.88	1.49	1.40
29	ZJ	202	PEB	OD-C4D	3.88	1.31	1.23
29	ZL	202	PEB	OD-C4D	3.88	1.31	1.23
29	A1	302	PEB	CHA-C1B	3.88	1.49	1.40
29	AK	302	PEB	CHA-C1B	3.88	1.49	1.40
29	QR	202	PEB	C1A-NA	-3.88	1.32	1.37
29	WF	202	PEB	CHA-C1B	3.88	1.49	1.40
29	WI	202	PEB	CHA-C1B	3.88	1.49	1.40
29	HF	1002	PEB	C1A-NA	-3.87	1.32	1.37
29	HI	1002	PEB	C1A-NA	-3.87	1.32	1.37
29	NJ	202	PEB	OD-C4D	3.87	1.31	1.23
29	NL	202	PEB	OD-C4D	3.87	1.31	1.23
29	jJ	202	PEB	OD-C4D	3.87	1.31	1.23
29	jL	202	PEB	OD-C4D	3.87	1.31	1.23
29	LF	1002	PEB	C1A-NA	-3.87	1.32	1.37
29	LI	1002	PEB	C1A-NA	-3.87	1.32	1.37
29	G8	203	PEB	CHA-C1B	3.87	1.49	1.40
29	W2	202	PEB	C1A-NA	-3.87	1.32	1.37
29	mF	203	PEB	CHA-C1B	3.87	1.49	1.40
29	mI	203	PEB	CHA-C1B	3.87	1.49	1.40
31	OP	1001	CYC	C2C-C1C	-3.87	1.48	1.52
31	QP	1001	CYC	C2C-C1C	-3.87	1.48	1.52
29	VF	203	PEB	CHA-C1B	3.87	1.49	1.40
29	VI	203	PEB	CHA-C1B	3.87	1.49	1.40
29	TB	201	PEB	CHA-C1B	3.87	1.49	1.40
29	TM	201	PEB	CHA-C1B	3.87	1.49	1.40
31	DP	1001	CYC	C2C-C1C	-3.87	1.48	1.52
29	g1	201	PEB	C1A-NA	-3.87	1.32	1.37
29	gK	201	PEB	C1A-NA	-3.87	1.32	1.37
29	PF	203	PEB	CHA-C1B	3.87	1.49	1.40
29	PI	203	PEB	CHA-C1B	3.87	1.49	1.40
31	oP	1001	CYC	C2C-C1C	-3.86	1.48	1.52
29	aF	202	PEB	C1A-NA	-3.86	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	aI	202	PEB	C1A-NA	-3.86	1.32	1.37
31	HK	1001	CYC	CHB-C4A	3.86	1.49	1.40
31	jP	1001	CYC	C2C-C1C	-3.86	1.48	1.52
29	aF	203	PEB	CHA-C1B	3.86	1.49	1.40
29	aI	203	PEB	CHA-C1B	3.86	1.49	1.40
29	L3	201	PEB	C1A-NA	-3.86	1.32	1.37
29	LO	201	PEB	C1A-NA	-3.86	1.32	1.37
29	m7	201	PEB	C1A-NA	-3.86	1.32	1.37
29	m9	201	PEB	C1A-NA	-3.86	1.32	1.37
29	iB	201	PEB	CHA-C1B	3.86	1.49	1.40
29	RF	202	PEB	CHA-C1B	3.86	1.49	1.40
29	RI	202	PEB	CHA-C1B	3.86	1.49	1.40
29	iM	201	PEB	CHA-C1B	3.86	1.49	1.40
31	M7	1001	CYC	C1C-NC	-3.85	1.32	1.37
31	1P	1002	CYC	C1C-NC	-3.85	1.32	1.37
29	i7	201	PEB	C1A-NA	-3.85	1.32	1.37
29	i9	201	PEB	C1A-NA	-3.85	1.32	1.37
31	uP	1001	CYC	C2C-C1C	-3.85	1.48	1.52
29	PB	201	PEB	CHA-C1B	3.85	1.49	1.40
29	PM	201	PEB	CHA-C1B	3.85	1.49	1.40
29	NB	201	PEB	CHA-C1B	3.85	1.49	1.40
29	NM	201	PEB	CHA-C1B	3.85	1.49	1.40
31	H1	1001	CYC	CHB-C4A	3.85	1.49	1.40
29	cF	202	PEB	CHA-C1B	3.85	1.49	1.40
29	cI	202	PEB	CHA-C1B	3.85	1.49	1.40
29	L8	203	PEB	CHA-C1B	3.85	1.49	1.40
29	iF	203	PEB	CHA-C1B	3.85	1.49	1.40
29	iI	203	PEB	CHA-C1B	3.85	1.49	1.40
29	kF	203	PEB	CHA-C1B	3.85	1.49	1.40
29	kI	203	PEB	CHA-C1B	3.85	1.49	1.40
29	V7	201	PEB	C1A-NA	-3.85	1.32	1.37
29	V9	201	PEB	C1A-NA	-3.85	1.32	1.37
29	B8	203	PEB	CHA-C1B	3.85	1.49	1.40
31	XP	1001	CYC	C2C-C1C	-3.84	1.48	1.52
29	H3	201	PEB	C1A-NA	-3.84	1.32	1.37
29	HO	201	PEB	C1A-NA	-3.84	1.32	1.37
29	g7	201	PEB	C1A-NA	-3.84	1.32	1.37
29	g9	201	PEB	C1A-NA	-3.84	1.32	1.37
29	RB	201	PEB	CHA-C1B	3.84	1.49	1.40
29	RM	201	PEB	CHA-C1B	3.84	1.49	1.40
29	YF	203	PEB	CHA-C1B	3.84	1.49	1.40
29	YI	203	PEB	CHA-C1B	3.84	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c7	201	PEB	C1A-NA	-3.84	1.32	1.37
29	e7	201	PEB	C1A-NA	-3.84	1.32	1.37
29	c9	201	PEB	C1A-NA	-3.84	1.32	1.37
29	e9	201	PEB	C1A-NA	-3.84	1.32	1.37
29	G5	203	PEB	CHA-C1B	3.84	1.49	1.40
29	i1	201	PEB	C1A-NA	-3.84	1.32	1.37
29	iK	201	PEB	C1A-NA	-3.84	1.32	1.37
31	hP	1001	CYC	C2C-C1C	-3.84	1.48	1.52
29	VF	202	PEB	C1A-NA	-3.84	1.32	1.37
29	VI	202	PEB	C1A-NA	-3.84	1.32	1.37
31	NK	1001	CYC	C2C-C1C	-3.84	1.48	1.52
29	B5	203	PEB	CHA-C1B	3.83	1.49	1.40
29	O2	202	PEB	C1A-NA	-3.83	1.32	1.37
29	FB	201	PEB	CHA-C1B	3.83	1.49	1.40
29	FM	201	PEB	CHA-C1B	3.83	1.49	1.40
29	U2	202	PEB	C1A-NA	-3.83	1.32	1.37
29	B3	201	PEB	C1A-NA	-3.83	1.32	1.37
29	BO	201	PEB	C1A-NA	-3.83	1.32	1.37
29	JB	201	PEB	CHA-C1B	3.83	1.49	1.40
29	JM	201	PEB	CHA-C1B	3.83	1.49	1.40
29	YF	202	PEB	C1A-NA	-3.83	1.32	1.37
29	YI	202	PEB	C1A-NA	-3.83	1.32	1.37
29	xL	302	PEB	C1A-NA	-3.83	1.32	1.37
31	NK	1001	CYC	CHB-C4A	3.83	1.49	1.40
29	L5	203	PEB	CHA-C1B	3.83	1.49	1.40
31	HK	1001	CYC	C2C-C1C	-3.83	1.48	1.52
29	kF	202	PEB	C1A-NA	-3.83	1.32	1.37
29	kI	202	PEB	C1A-NA	-3.83	1.32	1.37
31	xP	1001	CYC	C1C-NC	-3.83	1.32	1.37
31	J1	1001	CYC	CHB-C4A	3.83	1.49	1.40
31	JK	1001	CYC	CHB-C4A	3.83	1.49	1.40
29	cB	201	PEB	CHA-C1B	3.83	1.49	1.40
29	kB	201	PEB	CHA-C1B	3.83	1.49	1.40
29	cM	201	PEB	CHA-C1B	3.83	1.49	1.40
29	kM	201	PEB	CHA-C1B	3.83	1.49	1.40
29	VB	201	PEB	CHA-C1B	3.83	1.49	1.40
29	VM	201	PEB	CHA-C1B	3.83	1.49	1.40
31	VP	1001	CYC	C1C-NC	-3.83	1.32	1.37
29	mB	201	PEB	CHA-C1B	3.82	1.49	1.40
29	mM	201	PEB	CHA-C1B	3.82	1.49	1.40
31	F1	1001	CYC	C2C-C1C	-3.82	1.48	1.52
31	FK	1001	CYC	C2C-C1C	-3.82	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	XB	201	PEB	CHA-C1B	3.82	1.49	1.40
29	XM	201	PEB	CHA-C1B	3.82	1.49	1.40
31	F1	1001	CYC	CHB-C4A	3.82	1.49	1.40
31	FK	1001	CYC	CHB-C4A	3.82	1.49	1.40
29	nJ	203	PEB	CHA-C1B	3.82	1.49	1.40
29	nL	203	PEB	CHA-C1B	3.82	1.49	1.40
29	m1	201	PEB	C1A-NA	-3.82	1.32	1.37
29	xJ	302	PEB	C1A-NA	-3.82	1.32	1.37
29	mK	201	PEB	C1A-NA	-3.82	1.32	1.37
29	HB	201	PEB	CHA-C1B	3.82	1.49	1.40
29	HM	201	PEB	CHA-C1B	3.82	1.49	1.40
31	FP	1001	CYC	C2C-C1C	-3.82	1.48	1.52
29	eB	201	PEB	CHA-C1B	3.82	1.49	1.40
29	eM	201	PEB	CHA-C1B	3.82	1.49	1.40
29	F5	203	PEB	CHA-C1B	3.82	1.49	1.40
29	F8	203	PEB	CHA-C1B	3.82	1.49	1.40
31	D1	1001	CYC	CHB-C4A	3.82	1.49	1.40
31	DK	1001	CYC	CHB-C4A	3.82	1.49	1.40
29	UF	201	PEB	C1A-NA	-3.82	1.32	1.37
29	UI	201	PEB	C1A-NA	-3.82	1.32	1.37
31	J1	1001	CYC	C2C-C1C	-3.82	1.48	1.52
31	JK	1001	CYC	C2C-C1C	-3.82	1.48	1.52
29	A1	301	PEB	C1A-NA	-3.82	1.32	1.37
29	AK	301	PEB	C1A-NA	-3.82	1.32	1.37
29	ZB	201	PEB	CHA-C1B	3.82	1.49	1.40
29	ZM	201	PEB	CHA-C1B	3.82	1.49	1.40
31	H1	1001	CYC	C2C-C1C	-3.82	1.48	1.52
29	P7	201	PEB	C1A-NA	-3.82	1.32	1.37
29	P9	201	PEB	C1A-NA	-3.82	1.32	1.37
31	YP	1000	CYC	C1C-NC	-3.82	1.32	1.37
29	H8	203	PEB	CHA-C1B	3.82	1.49	1.40
31	I7	1001	CYC	C1C-NC	-3.81	1.32	1.37
31	I9	1001	CYC	C1C-NC	-3.81	1.32	1.37
31	C7	1001	CYC	C1C-NC	-3.81	1.32	1.37
31	C9	1001	CYC	C1C-NC	-3.81	1.32	1.37
29	mF	202	PEB	C1A-NA	-3.81	1.32	1.37
29	mI	202	PEB	C1A-NA	-3.81	1.32	1.37
31	N1	1001	CYC	C2C-C1C	-3.81	1.48	1.52
29	P2	202	PEB	CHA-C1B	3.81	1.49	1.40
29	PR	202	PEB	CHA-C1B	3.81	1.49	1.40
29	LB	201	PEB	CHA-C1B	3.81	1.49	1.40
29	LM	201	PEB	CHA-C1B	3.81	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S2	202	PEB	C1A-NA	-3.81	1.32	1.37
31	N1	1001	CYC	CHB-C4A	3.81	1.49	1.40
29	T7	201	PEB	C1A-NA	-3.81	1.32	1.37
29	T9	201	PEB	C1A-NA	-3.81	1.32	1.37
31	L1	1001	CYC	CHB-C4A	3.81	1.49	1.40
31	LK	1001	CYC	CHB-C4A	3.81	1.49	1.40
29	dF	201	PEB	C1A-NA	-3.81	1.32	1.37
29	dI	201	PEB	C1A-NA	-3.81	1.32	1.37
29	R7	201	PEB	C1A-NA	-3.81	1.32	1.37
29	R9	201	PEB	C1A-NA	-3.81	1.32	1.37
29	gF	202	PEB	C1A-NA	-3.81	1.32	1.37
29	gI	202	PEB	C1A-NA	-3.81	1.32	1.37
29	k7	201	PEB	C1A-NA	-3.81	1.32	1.37
29	k9	201	PEB	C1A-NA	-3.81	1.32	1.37
29	iF	202	PEB	C1A-NA	-3.81	1.32	1.37
29	iI	202	PEB	C1A-NA	-3.81	1.32	1.37
29	vJ	202	PEB	CHA-C1B	3.81	1.49	1.40
29	vL	202	PEB	CHA-C1B	3.81	1.49	1.40
29	DB	201	PEB	CHA-C1B	3.80	1.49	1.40
29	DM	201	PEB	CHA-C1B	3.80	1.49	1.40
29	VR	203	PEB	CHA-C1B	3.80	1.49	1.40
29	WR	202	PEB	C1A-NA	-3.80	1.32	1.37
29	dJ	203	PEB	CHA-C1B	3.80	1.49	1.40
29	dL	203	PEB	CHA-C1B	3.80	1.49	1.40
29	MG	404	PEB	C1A-NA	-3.80	1.32	1.37
29	R1	201	PEB	C1A-NA	-3.80	1.32	1.37
29	RK	201	PEB	C1A-NA	-3.80	1.32	1.37
29	V2	203	PEB	CHA-C1B	3.80	1.49	1.40
29	a7	201	PEB	C1A-NA	-3.80	1.32	1.37
29	a9	201	PEB	C1A-NA	-3.80	1.32	1.37
29	DJ	202	PEB	CHA-C1B	3.80	1.49	1.40
29	DL	202	PEB	CHA-C1B	3.80	1.49	1.40
29	V1	201	PEB	C1A-NA	-3.80	1.32	1.37
29	c1	201	PEB	C1A-NA	-3.80	1.32	1.37
29	VK	201	PEB	C1A-NA	-3.80	1.32	1.37
29	cK	201	PEB	C1A-NA	-3.80	1.32	1.37
31	sP	1001	CYC	C2C-C1C	-3.80	1.48	1.52
31	oP	1001	CYC	CHB-C4A	3.79	1.49	1.40
29	UJ	201	PEB	C3B-C2B	3.79	1.44	1.36
29	UL	201	PEB	C3B-C2B	3.79	1.44	1.36
29	M3	203	PEB	C1A-NA	-3.79	1.32	1.37
29	MO	203	PEB	C1A-NA	-3.79	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JJ	203	PEB	CHA-C1B	3.79	1.49	1.40
29	JL	203	PEB	CHA-C1B	3.79	1.49	1.40
31	fP	1001	CYC	CHB-C4A	3.79	1.49	1.40
29	a1	201	PEB	C1A-NA	-3.79	1.32	1.37
29	aK	201	PEB	C1A-NA	-3.79	1.32	1.37
29	SJ	201	PEB	C3B-C2B	3.79	1.44	1.36
29	SL	201	PEB	C3B-C2B	3.79	1.44	1.36
29	X2	202	PEB	CHA-C1B	3.79	1.49	1.40
29	XR	203	PEB	CHA-C1B	3.79	1.49	1.40
29	eF	202	PEB	C1A-NA	-3.79	1.32	1.37
29	eI	202	PEB	C1A-NA	-3.79	1.32	1.37
29	fJ	203	PEB	CHA-C1B	3.79	1.49	1.40
29	fL	203	PEB	CHA-C1B	3.79	1.49	1.40
31	sP	1001	CYC	CHB-C4A	3.79	1.49	1.40
29	H5	203	PEB	CHA-C1B	3.79	1.49	1.40
29	e1	201	PEB	C1A-NA	-3.79	1.32	1.37
29	Y7	201	PEB	C1A-NA	-3.79	1.32	1.37
29	Y9	201	PEB	C1A-NA	-3.79	1.32	1.37
29	PF	202	PEB	C1A-NA	-3.79	1.32	1.37
29	PI	202	PEB	C1A-NA	-3.79	1.32	1.37
29	eK	201	PEB	C1A-NA	-3.79	1.32	1.37
29	T1	201	PEB	C1A-NA	-3.79	1.32	1.37
29	TK	201	PEB	C1A-NA	-3.79	1.32	1.37
31	E7	1001	CYC	C1C-NC	-3.79	1.32	1.37
31	E9	1001	CYC	C1C-NC	-3.79	1.32	1.37
31	UP	1001	CYC	CHB-C4A	3.79	1.49	1.40
29	gB	201	PEB	CHA-C1B	3.79	1.49	1.40
29	gM	201	PEB	CHA-C1B	3.79	1.49	1.40
29	k1	201	PEB	C1A-NA	-3.79	1.32	1.37
29	kK	201	PEB	C1A-NA	-3.79	1.32	1.37
31	K7	1001	CYC	C1C-NC	-3.79	1.32	1.37
31	K9	1001	CYC	C1C-NC	-3.78	1.32	1.37
29	K5	203	PEB	CHA-C1B	3.78	1.49	1.40
29	K8	203	PEB	CHA-C1B	3.78	1.49	1.40
31	SP	1001	CYC	CHB-C4A	3.78	1.49	1.40
29	MJ	201	PEB	C3B-C2B	3.78	1.44	1.36
29	ML	201	PEB	C3B-C2B	3.78	1.44	1.36
29	VJ	202	PEB	CHA-C1B	3.78	1.49	1.40
29	ZJ	203	PEB	CHA-C1B	3.78	1.49	1.40
29	VL	202	PEB	CHA-C1B	3.78	1.49	1.40
29	ZL	203	PEB	CHA-C1B	3.78	1.49	1.40
31	IP	1001	CYC	CHB-C4A	3.78	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1P	1001	CYC	C2C-C1C	-3.78	1.48	1.52
29	SR	202	PEB	C1A-NA	-3.78	1.32	1.37
31	G7	1001	CYC	C1C-NC	-3.78	1.32	1.37
29	N3	203	PEB	C1A-NA	-3.78	1.32	1.37
31	OP	1001	CYC	CHB-C4A	3.78	1.49	1.40
29	sJ	201	PEB	C3B-C2B	3.78	1.44	1.36
29	sL	201	PEB	C3B-C2B	3.78	1.44	1.36
29	FJ	203	PEB	CHA-C1B	3.78	1.49	1.40
29	FL	203	PEB	CHA-C1B	3.78	1.49	1.40
31	MP	1001	CYC	CHB-C4A	3.78	1.49	1.40
31	uP	1001	CYC	CHB-C4A	3.78	1.49	1.40
29	PJ	203	PEB	CHA-C1B	3.78	1.49	1.40
29	PL	203	PEB	CHA-C1B	3.78	1.49	1.40
29	N2	203	PEB	CHA-C1B	3.78	1.49	1.40
29	NR	203	PEB	CHA-C1B	3.78	1.49	1.40
31	FP	1001	CYC	CHB-C4A	3.78	1.49	1.40
31	jP	1001	CYC	CHB-C4A	3.77	1.49	1.40
31	DP	1001	CYC	CHB-C4A	3.77	1.49	1.40
31	BP	1001	CYC	CHB-C4A	3.77	1.49	1.40
29	wL	302	PEB	C1A-NA	-3.77	1.32	1.37
29	hJ	203	PEB	CHA-C1B	3.77	1.49	1.40
29	tJ	202	PEB	CHA-C1B	3.77	1.49	1.40
29	hL	203	PEB	CHA-C1B	3.77	1.49	1.40
29	tL	202	PEB	CHA-C1B	3.77	1.49	1.40
31	nP	1001	CYC	CHB-C4A	3.77	1.49	1.40
29	TJ	203	PEB	CHA-C1B	3.77	1.49	1.40
29	TL	203	PEB	CHA-C1B	3.77	1.49	1.40
29	Q2	202	PEB	C1A-NA	-3.77	1.32	1.37
29	IJ	203	PEB	CHA-C1B	3.77	1.49	1.40
29	IL	203	PEB	CHA-C1B	3.77	1.49	1.40
29	MQ	406	PEB	C1A-NA	-3.77	1.32	1.37
31	hP	1001	CYC	CHB-C4A	3.77	1.49	1.40
29	NO	203	PEB	C1A-NA	-3.77	1.32	1.37
29	QJ	201	PEB	C3B-C2B	3.77	1.44	1.36
29	QL	201	PEB	C3B-C2B	3.77	1.44	1.36
29	BJ	203	PEB	CHA-C1B	3.77	1.49	1.40
29	BL	203	PEB	CHA-C1B	3.77	1.49	1.40
29	KJ	201	PEB	C3B-C2B	3.77	1.44	1.36
29	KL	201	PEB	C3B-C2B	3.77	1.44	1.36
29	bJ	203	PEB	CHA-C1B	3.77	1.49	1.40
29	bL	203	PEB	CHA-C1B	3.77	1.49	1.40
29	wJ	302	PEB	C1A-NA	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HJ	202	PEB	CHA-C1B	3.76	1.49	1.40
29	HL	202	PEB	CHA-C1B	3.76	1.49	1.40
29	A7	304	PEB	CHA-C1B	3.76	1.49	1.40
29	A9	304	PEB	CHA-C1B	3.76	1.49	1.40
31	HP	1001	CYC	CHB-C4A	3.76	1.49	1.40
31	kP	1001	CYC	CHB-C4A	3.76	1.49	1.40
29	LJ	202	PEB	CHA-C1B	3.76	1.49	1.40
29	LL	202	PEB	CHA-C1B	3.76	1.49	1.40
29	AB	303	PEB	CHA-C1B	3.76	1.49	1.40
29	uJ	202	PEB	C3B-C2B	3.76	1.44	1.36
29	uL	202	PEB	C3B-C2B	3.76	1.44	1.36
31	G9	1001	CYC	C1C-NC	-3.76	1.32	1.37
29	AM	303	PEB	CHA-C1B	3.75	1.49	1.40
31	qP	1001	CYC	CHB-C4A	3.75	1.49	1.40
31	lP	1001	CYC	CHB-C4A	3.75	1.49	1.40
31	XP	1001	CYC	CHB-C4A	3.75	1.49	1.40
29	oJ	201	PEB	C3B-C2B	3.75	1.44	1.36
29	oL	201	PEB	C3B-C2B	3.75	1.44	1.36
29	AJ	201	PEB	C3B-C2B	3.75	1.44	1.36
29	AL	201	PEB	C3B-C2B	3.75	1.44	1.36
29	T2	203	PEB	CHA-C1B	3.75	1.49	1.40
29	A5	203	PEB	CHA-C1B	3.75	1.49	1.40
29	A8	203	PEB	CHA-C1B	3.75	1.49	1.40
29	RJ	203	PEB	CHA-C1B	3.75	1.49	1.40
29	pJ	203	PEB	CHA-C1B	3.75	1.49	1.40
29	RL	203	PEB	CHA-C1B	3.75	1.49	1.40
29	pL	203	PEB	CHA-C1B	3.75	1.49	1.40
31	QP	1001	CYC	CHB-C4A	3.75	1.49	1.40
31	D1	1001	CYC	C2C-C1C	-3.75	1.48	1.52
29	aJ	201	PEB	C3B-C2B	3.75	1.44	1.36
29	aL	201	PEB	C3B-C2B	3.75	1.44	1.36
29	J1	1002	PEB	CHA-C1B	3.75	1.49	1.40
29	NJ	203	PEB	CHA-C1B	3.75	1.49	1.40
29	JK	1002	PEB	CHA-C1B	3.75	1.49	1.40
29	NL	203	PEB	CHA-C1B	3.75	1.49	1.40
29	GB	201	PEB	C1A-NA	-3.75	1.32	1.37
29	GM	201	PEB	C1A-NA	-3.75	1.32	1.37
29	EJ	201	PEB	C3B-C2B	3.75	1.44	1.36
29	EL	201	PEB	C3B-C2B	3.75	1.44	1.36
29	R2	203	PEB	CHA-C1B	3.75	1.49	1.40
29	MN	405	PEB	CHA-C1B	3.75	1.49	1.40
29	GJ	201	PEB	C3B-C2B	3.75	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GL	201	PEB	C3B-C2B	3.75	1.44	1.36
29	CJ	201	PEB	C3B-C2B	3.75	1.44	1.36
29	CL	201	PEB	C3B-C2B	3.75	1.44	1.36
29	XJ	203	PEB	CHA-C1B	3.74	1.49	1.40
29	XL	203	PEB	CHA-C1B	3.74	1.49	1.40
29	MA	405	PEB	CHA-C1B	3.74	1.49	1.40
31	wP	1001	CYC	CHB-C4A	3.74	1.49	1.40
29	jB	201	PEB	C1A-NA	-3.74	1.32	1.37
29	jM	201	PEB	C1A-NA	-3.74	1.32	1.37
29	TR	203	PEB	CHA-C1B	3.74	1.49	1.40
29	cJ	201	PEB	C3B-C2B	3.74	1.44	1.36
29	cL	201	PEB	C3B-C2B	3.74	1.44	1.36
29	Y1	201	PEB	C1A-NA	-3.74	1.32	1.37
29	YK	201	PEB	C1A-NA	-3.74	1.32	1.37
29	YJ	201	PEB	C3B-C2B	3.74	1.44	1.36
29	YL	201	PEB	C3B-C2B	3.74	1.44	1.36
29	OJ	201	PEB	C3B-C2B	3.74	1.44	1.36
29	OL	201	PEB	C3B-C2B	3.74	1.44	1.36
29	IJ	201	PEB	C3B-C2B	3.74	1.44	1.36
29	IL	201	PEB	C3B-C2B	3.74	1.44	1.36
29	C5	203	PEB	CHA-C1B	3.74	1.49	1.40
29	C8	203	PEB	CHA-C1B	3.74	1.49	1.40
29	WJ	202	PEB	C3B-C2B	3.74	1.44	1.36
29	WL	202	PEB	C3B-C2B	3.74	1.44	1.36
29	jJ	203	PEB	CHA-C1B	3.74	1.49	1.40
29	jL	203	PEB	CHA-C1B	3.74	1.49	1.40
29	P1	201	PEB	C1A-NA	-3.74	1.32	1.37
29	PK	201	PEB	C1A-NA	-3.74	1.32	1.37
29	I5	203	PEB	CHA-C1B	3.74	1.49	1.40
29	I8	203	PEB	CHA-C1B	3.74	1.49	1.40
29	qJ	201	PEB	C3B-C2B	3.73	1.44	1.36
29	qL	201	PEB	C3B-C2B	3.73	1.44	1.36
29	rJ	203	PEB	CHA-C1B	3.73	1.49	1.40
29	rL	203	PEB	CHA-C1B	3.73	1.49	1.40
29	RR	203	PEB	CHA-C1B	3.73	1.49	1.40
29	OF	201	PEB	C2A-C1A	-3.73	1.48	1.52
29	OI	201	PEB	C2A-C1A	-3.73	1.48	1.52
29	H1	1002	PEB	CHA-C1B	3.73	1.49	1.40
29	eJ	201	PEB	C3B-C2B	3.72	1.44	1.36
29	eL	201	PEB	C3B-C2B	3.72	1.44	1.36
29	kJ	201	PEB	C3B-C2B	3.72	1.44	1.36
29	kL	201	PEB	C3B-C2B	3.72	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NK	1002	PEB	CHA-C1B	3.72	1.49	1.40
29	TF	202	PEB	C2C-C3C	3.72	1.48	1.37
29	TI	202	PEB	C2C-C3C	3.72	1.48	1.37
29	fB	201	PEB	C1A-NA	-3.72	1.32	1.37
29	fM	201	PEB	C1A-NA	-3.72	1.32	1.37
29	N1	1002	PEB	CHA-C1B	3.72	1.49	1.40
29	LG	203	PEB	CHA-C1B	3.72	1.49	1.40
29	iJ	201	PEB	C3B-C2B	3.72	1.44	1.36
29	iL	201	PEB	C3B-C2B	3.72	1.44	1.36
29	mJ	201	PEB	C3B-C2B	3.72	1.44	1.36
29	mL	201	PEB	C3B-C2B	3.72	1.44	1.36
29	LQ	202	PEB	CHA-C1B	3.72	1.49	1.40
29	RF	202	PEB	C2C-C3C	3.72	1.48	1.37
29	RI	202	PEB	C2C-C3C	3.72	1.48	1.37
29	UR	202	PEB	C1A-NA	-3.72	1.32	1.37
29	QB	203	PEB	C1A-NA	-3.72	1.32	1.37
29	QM	203	PEB	C1A-NA	-3.72	1.32	1.37
29	FQ	203	PEB	CHA-C1B	3.72	1.49	1.40
29	MB	201	PEB	C1A-NA	-3.71	1.32	1.37
29	MM	201	PEB	C1A-NA	-3.71	1.32	1.37
29	WF	201	PEB	C2A-C1A	-3.71	1.48	1.52
29	WI	201	PEB	C2A-C1A	-3.71	1.48	1.52
29	RF	202	PEB	C1A-NA	-3.71	1.32	1.37
29	RI	202	PEB	C1A-NA	-3.71	1.32	1.37
29	SB	201	PEB	C1A-NA	-3.71	1.32	1.37
29	SM	201	PEB	C1A-NA	-3.71	1.32	1.37
29	eF	203	PEB	C2C-C3C	3.71	1.48	1.37
29	eI	203	PEB	C2C-C3C	3.71	1.48	1.37
29	gJ	201	PEB	C3B-C2B	3.71	1.44	1.36
29	gL	201	PEB	C3B-C2B	3.71	1.44	1.36
29	KC	202	PEB	C2C-C3C	3.71	1.48	1.37
29	KE	202	PEB	C2C-C3C	3.71	1.48	1.37
29	UF	202	PEB	C2A-C1A	-3.71	1.48	1.52
29	UI	202	PEB	C2A-C1A	-3.71	1.48	1.52
29	IB	201	PEB	C1A-NA	-3.71	1.32	1.37
29	IM	201	PEB	C1A-NA	-3.71	1.32	1.37
29	J5	201	PEB	C1B-C2B	3.71	1.53	1.45
29	J8	201	PEB	C1B-C2B	3.71	1.53	1.45
29	F1	1002	PEB	CHA-C1B	3.71	1.49	1.40
29	FK	1002	PEB	CHA-C1B	3.71	1.49	1.40
29	Y1	202	PEB	C1A-NA	-3.71	1.32	1.37
29	YK	202	PEB	C1A-NA	-3.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L8	201	PEB	C1A-NA	-3.70	1.32	1.37
29	L1	1002	PEB	CHA-C1B	3.70	1.49	1.40
29	LK	1002	PEB	CHA-C1B	3.70	1.49	1.40
29	FG	203	PEB	CHA-C1B	3.70	1.49	1.40
29	B8	201	PEB	C1A-NA	-3.70	1.32	1.37
29	HQ	203	PEB	CHA-C1B	3.70	1.49	1.40
29	MA	401	PEB	C1A-NA	-3.70	1.32	1.37
29	LC	201	PEB	CHA-C1B	3.70	1.49	1.40
29	LE	201	PEB	CHA-C1B	3.70	1.49	1.40
29	GC	201	PEB	C2C-C3C	3.70	1.48	1.37
29	GE	201	PEB	C2C-C3C	3.70	1.48	1.37
29	CB	201	PEB	C1A-NA	-3.70	1.32	1.37
29	CM	201	PEB	C1A-NA	-3.70	1.32	1.37
29	eF	203	PEB	C1A-NA	-3.70	1.32	1.37
29	eI	203	PEB	C1A-NA	-3.70	1.32	1.37
29	EB	201	PEB	C1A-NA	-3.70	1.32	1.37
29	EM	201	PEB	C1A-NA	-3.70	1.32	1.37
29	aF	203	PEB	C2C-C3C	3.70	1.48	1.37
29	aI	203	PEB	C2C-C3C	3.70	1.48	1.37
29	h1	202	PEB	C1A-NA	-3.70	1.32	1.37
29	L5	201	PEB	C1A-NA	-3.70	1.32	1.37
29	hK	202	PEB	C1A-NA	-3.70	1.32	1.37
29	HG	203	PEB	CHA-C1B	3.69	1.49	1.40
29	DK	1002	PEB	CHA-C1B	3.69	1.49	1.40
29	DB	202	PEB	C1A-NA	-3.69	1.32	1.37
29	WB	201	PEB	C1A-NA	-3.69	1.32	1.37
29	DM	202	PEB	C1A-NA	-3.69	1.32	1.37
29	WM	201	PEB	C1A-NA	-3.69	1.32	1.37
29	c7	203	PEB	CHA-C1B	3.69	1.49	1.40
29	c9	203	PEB	CHA-C1B	3.69	1.49	1.40
29	VF	203	PEB	C2C-C3C	3.69	1.48	1.37
29	VI	203	PEB	C2C-C3C	3.69	1.48	1.37
29	M2	202	PEB	C1A-NA	-3.69	1.32	1.37
29	ID	203	PEB	C1A-NA	-3.69	1.32	1.37
29	KD	203	PEB	C1A-NA	-3.69	1.32	1.37
29	D1	1002	PEB	CHA-C1B	3.69	1.49	1.40
29	BA	202	PEB	C1A-NA	-3.69	1.32	1.37
29	BN	202	PEB	C1A-NA	-3.69	1.32	1.37
29	iF	203	PEB	C2C-C3C	3.69	1.48	1.37
29	iI	203	PEB	C2C-C3C	3.69	1.48	1.37
29	iF	203	PEB	C1A-NA	-3.69	1.32	1.37
29	iI	203	PEB	C1A-NA	-3.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	hJ	202	PEB	C1A-NA	-3.69	1.32	1.37
29	hL	202	PEB	C1A-NA	-3.69	1.32	1.37
29	W1	201	PEB	C2A-C1A	-3.69	1.48	1.52
29	l1	201	PEB	C2A-C1A	-3.69	1.48	1.52
29	WK	201	PEB	C2A-C1A	-3.69	1.48	1.52
29	lK	201	PEB	C2A-C1A	-3.69	1.48	1.52
29	DG	203	PEB	CHA-C1B	3.69	1.49	1.40
29	AC	201	PEB	C2C-C3C	3.69	1.48	1.37
29	AE	201	PEB	C2C-C3C	3.69	1.48	1.37
29	dB	201	PEB	C1A-NA	-3.69	1.32	1.37
29	lB	201	PEB	C1A-NA	-3.69	1.32	1.37
29	dM	201	PEB	C1A-NA	-3.69	1.32	1.37
29	lM	201	PEB	C1A-NA	-3.69	1.32	1.37
29	l1	202	PEB	C1A-NA	-3.69	1.32	1.37
29	N3	201	PEB	C1A-NA	-3.69	1.32	1.37
29	KB	203	PEB	C1A-NA	-3.69	1.32	1.37
29	RJ	202	PEB	C1A-NA	-3.69	1.32	1.37
29	lK	202	PEB	C1A-NA	-3.69	1.32	1.37
29	RL	202	PEB	C1A-NA	-3.69	1.32	1.37
29	KM	203	PEB	C1A-NA	-3.69	1.32	1.37
29	EA	201	PEB	C2C-C3C	3.69	1.48	1.37
29	cF	202	PEB	C2C-C3C	3.69	1.48	1.37
29	cI	202	PEB	C2C-C3C	3.69	1.48	1.37
29	EN	201	PEB	C2C-C3C	3.69	1.48	1.37
29	MN	401	PEB	C1A-NA	-3.69	1.32	1.37
29	BQ	203	PEB	CHA-C1B	3.69	1.49	1.40
29	h1	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	hK	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	IC	201	PEB	C2C-C3C	3.68	1.48	1.37
29	IE	201	PEB	C2C-C3C	3.68	1.48	1.37
29	YF	203	PEB	C2C-C3C	3.68	1.48	1.37
29	YI	203	PEB	C2C-C3C	3.68	1.48	1.37
29	E4	203	PEB	C1A-NA	-3.68	1.32	1.37
29	MD	203	PEB	C1A-NA	-3.68	1.32	1.37
29	IA	201	PEB	C2C-C3C	3.68	1.48	1.37
29	IN	201	PEB	C2C-C3C	3.68	1.48	1.37
29	FA	202	PEB	C1A-NA	-3.68	1.32	1.37
29	FN	202	PEB	C1A-NA	-3.68	1.32	1.37
29	PF	203	PEB	C2C-C3C	3.68	1.48	1.37
29	PI	203	PEB	C2C-C3C	3.68	1.48	1.37
29	KA	201	PEB	C2C-C3C	3.68	1.48	1.37
29	KN	201	PEB	C2C-C3C	3.68	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F5	201	PEB	C1A-NA	-3.68	1.32	1.37
29	F8	201	PEB	C1A-NA	-3.68	1.32	1.37
29	i7	203	PEB	CHA-C1B	3.68	1.49	1.40
29	i9	203	PEB	CHA-C1B	3.68	1.49	1.40
29	BG	203	PEB	CHA-C1B	3.68	1.49	1.40
29	FC	201	PEB	CHA-C1B	3.68	1.49	1.40
29	FE	201	PEB	CHA-C1B	3.68	1.49	1.40
29	C3	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	CO	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	kF	203	PEB	C2C-C3C	3.68	1.48	1.37
29	kI	203	PEB	C2C-C3C	3.68	1.48	1.37
29	CA	201	PEB	C2C-C3C	3.68	1.48	1.37
29	gF	203	PEB	C2C-C3C	3.68	1.48	1.37
29	gI	203	PEB	C2C-C3C	3.68	1.48	1.37
29	CN	201	PEB	C2C-C3C	3.68	1.48	1.37
29	AF	305	PEB	CHA-C1B	3.68	1.49	1.40
29	AI	305	PEB	CHA-C1B	3.68	1.49	1.40
29	YB	202	PEB	C1A-NA	-3.68	1.32	1.37
29	YM	202	PEB	C1A-NA	-3.68	1.32	1.37
29	RB	202	PEB	C1A-NA	-3.68	1.32	1.37
29	RM	202	PEB	C1A-NA	-3.68	1.32	1.37
29	AA	201	PEB	C2C-C3C	3.68	1.48	1.37
29	AN	201	PEB	C2C-C3C	3.68	1.48	1.37
29	O1	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	d1	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	OK	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	dK	201	PEB	C2A-C1A	-3.68	1.48	1.52
29	b1	202	PEB	C1A-NA	-3.67	1.32	1.37
29	A5	201	PEB	C1A-NA	-3.67	1.32	1.37
29	A8	201	PEB	C1A-NA	-3.67	1.32	1.37
29	bK	202	PEB	C1A-NA	-3.67	1.32	1.37
29	AB	302	PEB	CHA-C1B	3.67	1.49	1.40
29	R1	203	PEB	C1A-NA	-3.67	1.32	1.37
29	jJ	202	PEB	C1A-NA	-3.67	1.32	1.37
29	RK	203	PEB	C1A-NA	-3.67	1.32	1.37
29	jL	202	PEB	C1A-NA	-3.67	1.32	1.37
29	QF	201	PEB	C2A-C1A	-3.67	1.48	1.52
29	QI	201	PEB	C2A-C1A	-3.67	1.48	1.52
29	EC	201	PEB	C2C-C3C	3.67	1.48	1.37
29	EE	201	PEB	C2C-C3C	3.67	1.48	1.37
29	a7	203	PEB	CHA-C1B	3.67	1.49	1.40
29	a9	203	PEB	CHA-C1B	3.67	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f1	202	PEB	C1A-NA	-3.67	1.32	1.37
29	A7	301	PEB	C1A-NA	-3.67	1.32	1.37
29	A9	301	PEB	C1A-NA	-3.67	1.32	1.37
29	JA	202	PEB	C1A-NA	-3.67	1.32	1.37
29	fK	202	PEB	C1A-NA	-3.67	1.32	1.37
29	JN	202	PEB	C1A-NA	-3.67	1.32	1.37
29	CC	201	PEB	C2C-C3C	3.67	1.48	1.37
29	CE	201	PEB	C2C-C3C	3.67	1.48	1.37
29	i1	203	PEB	C1A-NA	-3.67	1.32	1.37
29	YF	203	PEB	C1A-NA	-3.67	1.32	1.37
29	YI	203	PEB	C1A-NA	-3.67	1.32	1.37
29	fJ	202	PEB	C1A-NA	-3.67	1.32	1.37
29	iK	203	PEB	C1A-NA	-3.67	1.32	1.37
29	fL	202	PEB	C1A-NA	-3.67	1.32	1.37
29	UB	201	PEB	C1A-NA	-3.67	1.32	1.37
29	UM	201	PEB	C1A-NA	-3.67	1.32	1.37
29	JG	203	PEB	CHA-C1B	3.67	1.49	1.40
29	G5	201	PEB	C1A-NA	-3.67	1.32	1.37
29	mF	203	PEB	C2C-C3C	3.67	1.48	1.37
29	mI	203	PEB	C2C-C3C	3.67	1.48	1.37
29	HK	1002	PEB	CHA-C1B	3.67	1.49	1.40
29	hB	201	PEB	C1A-NA	-3.67	1.32	1.37
29	hM	201	PEB	C1A-NA	-3.67	1.32	1.37
29	TB	202	PEB	C1A-NA	-3.67	1.32	1.37
29	PF	203	PEB	C1A-NA	-3.67	1.32	1.37
29	PI	203	PEB	C1A-NA	-3.67	1.32	1.37
29	TM	202	PEB	C1A-NA	-3.67	1.32	1.37
29	T7	203	PEB	CHA-C1B	3.67	1.49	1.40
29	T9	203	PEB	CHA-C1B	3.67	1.49	1.40
29	LA	203	PEB	CHA-C1B	3.66	1.49	1.40
29	LN	203	PEB	CHA-C1B	3.66	1.49	1.40
29	e7	203	PEB	CHA-C1B	3.66	1.49	1.40
29	e9	203	PEB	CHA-C1B	3.66	1.49	1.40
29	A3	201	PEB	C2A-C1A	-3.66	1.48	1.52
29	AO	201	PEB	C2A-C1A	-3.66	1.48	1.52
29	P1	203	PEB	C1A-NA	-3.66	1.32	1.37
29	AJ	203	PEB	C1A-NA	-3.66	1.32	1.37
29	PK	203	PEB	C1A-NA	-3.66	1.32	1.37
29	AL	203	PEB	C1A-NA	-3.66	1.32	1.37
29	JC	201	PEB	CHA-C1B	3.66	1.49	1.40
29	JE	201	PEB	CHA-C1B	3.66	1.49	1.40
29	K5	201	PEB	C1A-NA	-3.66	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NJ	202	PEB	C1A-NA	-3.66	1.32	1.37
29	NL	202	PEB	C1A-NA	-3.66	1.32	1.37
29	JQ	203	PEB	CHA-C1B	3.66	1.49	1.40
29	C5	203	PEB	C1A-NA	-3.66	1.32	1.37
29	G8	201	PEB	C1A-NA	-3.66	1.32	1.37
29	DQ	203	PEB	CHA-C1B	3.66	1.49	1.40
29	Q1	202	PEB	C1A-NA	-3.66	1.32	1.37
29	IJ	202	PEB	C1A-NA	-3.66	1.32	1.37
29	QK	202	PEB	C1A-NA	-3.66	1.32	1.37
29	IL	202	PEB	C1A-NA	-3.66	1.32	1.37
29	GA	201	PEB	C2C-C3C	3.66	1.48	1.37
29	GN	201	PEB	C2C-C3C	3.66	1.48	1.37
29	NJ	201	PEB	CHA-C1B	3.66	1.49	1.40
29	NL	201	PEB	CHA-C1B	3.66	1.49	1.40
29	aB	201	PEB	C1A-NA	-3.66	1.32	1.37
29	aM	201	PEB	C1A-NA	-3.66	1.32	1.37
29	NO	201	PEB	C1A-NA	-3.66	1.32	1.37
31	M1	1001	CYC	C1C-NC	-3.66	1.32	1.37
31	MK	1001	CYC	C1C-NC	-3.66	1.32	1.37
29	HA	202	PEB	C1A-NA	-3.66	1.32	1.37
29	PJ	202	PEB	C1A-NA	-3.66	1.32	1.37
29	PL	202	PEB	C1A-NA	-3.66	1.32	1.37
29	HN	202	PEB	C1A-NA	-3.66	1.32	1.37
29	H8	203	PEB	C1A-NA	-3.66	1.32	1.37
29	AM	302	PEB	CHA-C1B	3.66	1.49	1.40
29	g1	203	PEB	C1A-NA	-3.66	1.32	1.37
29	FJ	202	PEB	C1A-NA	-3.66	1.32	1.37
29	gK	203	PEB	C1A-NA	-3.66	1.32	1.37
29	FL	202	PEB	C1A-NA	-3.66	1.32	1.37
29	DA	203	PEB	CHA-C1B	3.66	1.49	1.40
29	DN	203	PEB	CHA-C1B	3.66	1.49	1.40
29	cF	202	PEB	C1A-NA	-3.65	1.32	1.37
29	cI	202	PEB	C1A-NA	-3.65	1.32	1.37
29	HJ	201	PEB	C1A-NA	-3.65	1.32	1.37
29	HL	201	PEB	C1A-NA	-3.65	1.32	1.37
29	a1	203	PEB	C1A-NA	-3.65	1.32	1.37
29	DA	202	PEB	C1A-NA	-3.65	1.32	1.37
29	ED	202	PEB	C1A-NA	-3.65	1.32	1.37
29	HG	201	PEB	C1A-NA	-3.65	1.32	1.37
29	aK	203	PEB	C1A-NA	-3.65	1.32	1.37
29	DN	202	PEB	C1A-NA	-3.65	1.32	1.37
29	HQ	201	PEB	C1A-NA	-3.65	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e1	203	PEB	C1A-NA	-3.65	1.32	1.37
29	FB	202	PEB	C1A-NA	-3.65	1.32	1.37
29	uJ	201	PEB	C1A-NA	-3.65	1.32	1.37
29	eK	203	PEB	C1A-NA	-3.65	1.32	1.37
29	uL	201	PEB	C1A-NA	-3.65	1.32	1.37
29	FM	202	PEB	C1A-NA	-3.65	1.32	1.37
29	DC	201	PEB	CHA-C1B	3.65	1.49	1.40
29	DE	201	PEB	CHA-C1B	3.65	1.49	1.40
29	QB	202	PEB	C1A-NA	-3.65	1.32	1.37
29	QM	202	PEB	C1A-NA	-3.65	1.32	1.37
29	j1	202	PEB	C1A-NA	-3.65	1.32	1.37
29	jK	202	PEB	C1A-NA	-3.65	1.32	1.37
29	K4	203	PEB	C1A-NA	-3.65	1.32	1.37
29	SF	201	PEB	C2A-C1A	-3.65	1.48	1.52
29	SI	201	PEB	C2A-C1A	-3.65	1.48	1.52
29	H5	201	PEB	C1A-NA	-3.65	1.32	1.37
29	A5	203	PEB	C1A-NA	-3.65	1.32	1.37
29	A8	203	PEB	C1A-NA	-3.65	1.32	1.37
29	KB	201	PEB	C1A-NA	-3.65	1.32	1.37
29	XJ	202	PEB	C1A-NA	-3.65	1.32	1.37
29	XL	202	PEB	C1A-NA	-3.65	1.32	1.37
29	KM	201	PEB	C1A-NA	-3.65	1.32	1.37
31	C1	1001	CYC	C1C-NC	-3.65	1.32	1.37
29	c1	203	PEB	C1A-NA	-3.65	1.32	1.37
29	M3	201	PEB	C1A-NA	-3.65	1.32	1.37
29	LB	202	PEB	C1A-NA	-3.65	1.32	1.37
29	TF	202	PEB	C1A-NA	-3.65	1.32	1.37
29	TI	202	PEB	C1A-NA	-3.65	1.32	1.37
29	cK	203	PEB	C1A-NA	-3.65	1.32	1.37
29	LM	202	PEB	C1A-NA	-3.65	1.32	1.37
29	MO	201	PEB	C1A-NA	-3.65	1.32	1.37
29	FG	201	PEB	C2C-C3C	3.65	1.48	1.37
29	FQ	201	PEB	C2C-C3C	3.65	1.48	1.37
29	LJ	201	PEB	CHA-C1B	3.65	1.49	1.40
29	LL	201	PEB	CHA-C1B	3.65	1.49	1.40
29	k1	203	PEB	C1A-NA	-3.65	1.32	1.37
29	H8	201	PEB	C1A-NA	-3.65	1.32	1.37
29	kK	203	PEB	C1A-NA	-3.65	1.32	1.37
29	L1	1002	PEB	C2C-C3C	3.64	1.48	1.37
29	LK	1002	PEB	C2C-C3C	3.64	1.48	1.37
29	U1	203	PEB	C1A-NA	-3.64	1.32	1.37
29	UK	203	PEB	C1A-NA	-3.64	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	vJ	201	PEB	CHA-C1B	3.64	1.49	1.40
29	vL	201	PEB	CHA-C1B	3.64	1.49	1.40
29	F1	1002	PEB	C4D-ND	3.64	1.40	1.35
29	FK	1002	PEB	C4D-ND	3.64	1.40	1.35
29	lF	201	PEB	C2A-C1A	-3.64	1.48	1.52
29	lI	201	PEB	C2A-C1A	-3.64	1.48	1.52
29	VB	202	PEB	C1A-NA	-3.64	1.32	1.37
29	kB	202	PEB	C1A-NA	-3.64	1.32	1.37
29	VM	202	PEB	C1A-NA	-3.64	1.32	1.37
29	kM	202	PEB	C1A-NA	-3.64	1.32	1.37
29	HC	201	PEB	CHA-C1B	3.64	1.48	1.40
29	HE	201	PEB	CHA-C1B	3.64	1.48	1.40
29	HG	201	PEB	C2C-C3C	3.64	1.48	1.37
29	HQ	201	PEB	C2C-C3C	3.64	1.48	1.37
29	l8	201	PEB	C1A-NA	-3.64	1.32	1.37
29	MG	401	PEB	C1A-NA	-3.64	1.32	1.37
29	sJ	203	PEB	C1A-NA	-3.64	1.32	1.37
29	sL	203	PEB	C1A-NA	-3.64	1.32	1.37
29	bJ	201	PEB	CHA-C1B	3.64	1.48	1.40
29	bL	201	PEB	CHA-C1B	3.64	1.48	1.40
30	yJ	303	PUB	C3B-C2B	3.64	1.48	1.37
29	l5	201	PEB	C1A-NA	-3.64	1.32	1.37
29	m7	203	PEB	CHA-C1B	3.64	1.48	1.40
29	m9	203	PEB	CHA-C1B	3.64	1.48	1.40
29	LA	202	PEB	C1A-NA	-3.64	1.32	1.37
29	LN	202	PEB	C1A-NA	-3.64	1.32	1.37
29	PJ	201	PEB	CHA-C1B	3.64	1.48	1.40
29	VJ	201	PEB	CHA-C1B	3.64	1.48	1.40
29	PL	201	PEB	CHA-C1B	3.64	1.48	1.40
29	VL	201	PEB	CHA-C1B	3.64	1.48	1.40
29	l5	203	PEB	C1A-NA	-3.64	1.32	1.37
29	l8	203	PEB	C1A-NA	-3.64	1.32	1.37
29	gB	202	PEB	C1A-NA	-3.64	1.32	1.37
29	gM	202	PEB	C1A-NA	-3.64	1.32	1.37
29	T1	202	PEB	C1A-NA	-3.64	1.32	1.37
29	BJ	202	PEB	C1A-NA	-3.64	1.32	1.37
29	TK	202	PEB	C1A-NA	-3.64	1.32	1.37
29	BL	202	PEB	C1A-NA	-3.64	1.32	1.37
29	dJ	201	PEB	CHA-C1B	3.64	1.48	1.40
29	dL	201	PEB	CHA-C1B	3.64	1.48	1.40
29	GG	201	PEB	C1A-NA	-3.64	1.32	1.37
29	GQ	201	PEB	C1A-NA	-3.64	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L1	1002	PEB	C4D-ND	3.64	1.40	1.35
29	LK	1002	PEB	C4D-ND	3.64	1.40	1.35
29	F1	1002	PEB	C2C-C3C	3.64	1.48	1.37
29	FK	1002	PEB	C2C-C3C	3.64	1.48	1.37
29	LG	201	PEB	C2C-C3C	3.64	1.48	1.37
29	MQ	402	PEB	C2C-C3C	3.64	1.48	1.37
29	ZB	202	PEB	C1A-NA	-3.64	1.32	1.37
29	aB	203	PEB	C1A-NA	-3.64	1.32	1.37
29	ZM	202	PEB	C1A-NA	-3.64	1.32	1.37
29	aM	203	PEB	C1A-NA	-3.64	1.32	1.37
29	N2	203	PEB	C1A-NA	-3.64	1.32	1.37
29	cB	202	PEB	C1A-NA	-3.63	1.32	1.37
29	cM	202	PEB	C1A-NA	-3.63	1.32	1.37
29	jJ	201	PEB	CHA-C1B	3.63	1.48	1.40
29	jL	201	PEB	CHA-C1B	3.63	1.48	1.40
29	MQ	403	PEB	C1A-NA	-3.63	1.32	1.37
29	hJ	201	PEB	CHA-C1B	3.63	1.48	1.40
29	hL	201	PEB	CHA-C1B	3.63	1.48	1.40
29	DK	1002	PEB	C2C-C3C	3.63	1.48	1.37
29	G5	203	PEB	C1A-NA	-3.63	1.32	1.37
29	TJ	202	PEB	C1A-NA	-3.63	1.32	1.37
29	TL	202	PEB	C1A-NA	-3.63	1.32	1.37
29	B5	201	PEB	C1A-NA	-3.63	1.32	1.37
29	MR	202	PEB	C2C-C3C	3.63	1.48	1.37
29	OB	201	PEB	C1A-NA	-3.63	1.32	1.37
29	OM	201	PEB	C1A-NA	-3.63	1.32	1.37
29	Y7	203	PEB	CHA-C1B	3.63	1.48	1.40
29	Y9	203	PEB	CHA-C1B	3.63	1.48	1.40
31	CF	1001	CYC	C2C-C1C	-3.63	1.48	1.52
31	CI	1001	CYC	C2C-C1C	-3.63	1.48	1.52
29	g7	203	PEB	CHA-C1B	3.63	1.48	1.40
29	g9	203	PEB	CHA-C1B	3.63	1.48	1.40
29	JA	203	PEB	CHA-C1B	3.63	1.48	1.40
29	JN	203	PEB	CHA-C1B	3.63	1.48	1.40
29	mF	203	PEB	C1A-NA	-3.63	1.32	1.37
29	mI	203	PEB	C1A-NA	-3.63	1.32	1.37
29	JG	201	PEB	C2C-C3C	3.63	1.48	1.37
29	JQ	201	PEB	C2C-C3C	3.63	1.48	1.37
29	R7	203	PEB	CHA-C1B	3.63	1.48	1.40
29	R9	203	PEB	CHA-C1B	3.63	1.48	1.40
29	BC	201	PEB	CHA-C1B	3.63	1.48	1.40
29	BE	201	PEB	CHA-C1B	3.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	pJ	201	PEB	CHA-C1B	3.63	1.48	1.40
29	pL	201	PEB	CHA-C1B	3.63	1.48	1.40
29	ZJ	202	PEB	C1A-NA	-3.63	1.32	1.37
29	ZL	202	PEB	C1A-NA	-3.63	1.32	1.37
29	JG	201	PEB	C1A-NA	-3.63	1.32	1.37
29	dJ	202	PEB	C1A-NA	-3.63	1.32	1.37
29	dL	202	PEB	C1A-NA	-3.63	1.32	1.37
29	JQ	201	PEB	C1A-NA	-3.63	1.32	1.37
29	B3	201	PEB	CHA-C1B	3.63	1.48	1.40
29	BO	201	PEB	CHA-C1B	3.63	1.48	1.40
29	rJ	202	PEB	C1A-NA	-3.63	1.32	1.37
29	rL	202	PEB	C1A-NA	-3.63	1.32	1.37
29	J1	1002	PEB	C2C-C3C	3.63	1.48	1.37
29	JK	1002	PEB	C2C-C3C	3.63	1.48	1.37
29	I3	201	PEB	C2A-C1A	-3.63	1.48	1.52
29	IO	201	PEB	C2A-C1A	-3.63	1.48	1.52
29	DJ	201	PEB	CHA-C1B	3.63	1.48	1.40
29	zJ	501	PEB	CHA-C1B	3.63	1.48	1.40
29	DL	201	PEB	CHA-C1B	3.63	1.48	1.40
29	Z1	203	PEB	C1A-NA	-3.63	1.32	1.37
29	K5	203	PEB	C1A-NA	-3.63	1.32	1.37
29	K8	203	PEB	C1A-NA	-3.63	1.32	1.37
29	VF	203	PEB	C1A-NA	-3.63	1.32	1.37
29	VI	203	PEB	C1A-NA	-3.63	1.32	1.37
29	ZK	203	PEB	C1A-NA	-3.63	1.32	1.37
29	D1	1002	PEB	C2C-C3C	3.63	1.48	1.37
30	A1	304	PUB	C3B-C2B	3.63	1.48	1.37
30	AK	304	PUB	C3B-C2B	3.63	1.48	1.37
29	M4	203	PEB	CHA-C1B	3.63	1.48	1.40
29	BA	203	PEB	CHA-C1B	3.63	1.48	1.40
29	BN	203	PEB	CHA-C1B	3.63	1.48	1.40
29	F3	201	PEB	CHA-C1B	3.62	1.48	1.40
29	XJ	201	PEB	CHA-C1B	3.62	1.48	1.40
29	XL	201	PEB	CHA-C1B	3.62	1.48	1.40
29	FO	201	PEB	CHA-C1B	3.62	1.48	1.40
29	BG	201	PEB	C2C-C3C	3.62	1.48	1.37
29	BQ	201	PEB	C2C-C3C	3.62	1.48	1.37
29	V1	203	PEB	C1A-NA	-3.62	1.32	1.37
29	B8	203	PEB	C1A-NA	-3.62	1.32	1.37
29	C8	203	PEB	C1A-NA	-3.62	1.32	1.37
29	VK	203	PEB	C1A-NA	-3.62	1.32	1.37
29	bJ	202	PEB	C1A-NA	-3.62	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	bL	202	PEB	C1A-NA	-3.62	1.32	1.37
29	FJ	201	PEB	CHA-C1B	3.62	1.48	1.40
29	IJ	201	PEB	CHA-C1B	3.62	1.48	1.40
29	FL	201	PEB	CHA-C1B	3.62	1.48	1.40
29	IL	201	PEB	CHA-C1B	3.62	1.48	1.40
29	rJ	201	PEB	CHA-C1B	3.62	1.48	1.40
29	rL	201	PEB	CHA-C1B	3.62	1.48	1.40
29	S1	202	PEB	C1A-NA	-3.62	1.32	1.37
29	BG	201	PEB	C1A-NA	-3.62	1.32	1.37
29	SK	202	PEB	C1A-NA	-3.62	1.32	1.37
29	BQ	201	PEB	C1A-NA	-3.62	1.32	1.37
29	PR	202	PEB	C1A-NA	-3.62	1.32	1.37
29	DG	201	PEB	C2C-C3C	3.62	1.48	1.37
29	DQ	201	PEB	C2C-C3C	3.62	1.48	1.37
29	H3	201	PEB	CHA-C1B	3.62	1.48	1.40
29	zL	501	PEB	CHA-C1B	3.62	1.48	1.40
29	HO	201	PEB	CHA-C1B	3.62	1.48	1.40
29	S2	201	PEB	CHA-C1B	3.62	1.48	1.40
29	P7	203	PEB	CHA-C1B	3.62	1.48	1.40
29	P9	203	PEB	CHA-C1B	3.62	1.48	1.40
29	FA	203	PEB	CHA-C1B	3.62	1.48	1.40
29	FN	203	PEB	CHA-C1B	3.62	1.48	1.40
29	iB	202	PEB	C1A-NA	-3.62	1.32	1.37
29	iM	202	PEB	C1A-NA	-3.62	1.32	1.37
29	aF	203	PEB	C1A-NA	-3.62	1.32	1.37
29	kF	203	PEB	C1A-NA	-3.62	1.32	1.37
29	aI	203	PEB	C1A-NA	-3.62	1.32	1.37
29	kI	203	PEB	C1A-NA	-3.62	1.32	1.37
29	nJ	202	PEB	C1A-NA	-3.62	1.32	1.37
29	pJ	202	PEB	C1A-NA	-3.62	1.32	1.37
29	nL	202	PEB	C1A-NA	-3.62	1.32	1.37
29	pL	202	PEB	C1A-NA	-3.62	1.32	1.37
29	N1	1002	PEB	C2C-C3C	3.62	1.48	1.37
29	TF	201	PEB	CHA-C1B	3.62	1.48	1.40
29	fF	201	PEB	C2A-C1A	-3.62	1.48	1.52
29	fI	201	PEB	C2A-C1A	-3.62	1.48	1.52
29	NK	1002	PEB	C2C-C3C	3.62	1.48	1.37
29	HB	202	PEB	C1A-NA	-3.62	1.32	1.37
29	HM	202	PEB	C1A-NA	-3.62	1.32	1.37
29	HK	1002	PEB	C2C-C3C	3.62	1.48	1.37
29	fJ	201	PEB	CHA-C1B	3.62	1.48	1.40
29	fL	201	PEB	CHA-C1B	3.62	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H1	1002	PEB	C2C-C3C	3.62	1.48	1.37
29	K8	201	PEB	CHA-C1B	3.62	1.48	1.40
29	b1	201	PEB	C2A-C1A	-3.62	1.48	1.52
29	ZF	201	PEB	C2A-C1A	-3.62	1.48	1.52
29	ZI	201	PEB	C2A-C1A	-3.62	1.48	1.52
29	bK	201	PEB	C2A-C1A	-3.62	1.48	1.52
29	mB	202	PEB	C1A-NA	-3.61	1.32	1.37
29	mM	202	PEB	C1A-NA	-3.61	1.32	1.37
29	V7	203	PEB	CHA-C1B	3.61	1.48	1.40
29	V9	203	PEB	CHA-C1B	3.61	1.48	1.40
29	Z1	202	PEB	C2A-C1A	-3.61	1.48	1.52
29	j1	201	PEB	C2A-C1A	-3.61	1.48	1.52
29	ZK	202	PEB	C2A-C1A	-3.61	1.48	1.52
29	jK	201	PEB	C2A-C1A	-3.61	1.48	1.52
29	JB	202	PEB	C1A-NA	-3.61	1.32	1.37
29	JM	202	PEB	C1A-NA	-3.61	1.32	1.37
29	k7	203	PEB	CHA-C1B	3.61	1.48	1.40
29	k9	203	PEB	CHA-C1B	3.61	1.48	1.40
29	TJ	201	PEB	CHA-C1B	3.61	1.48	1.40
29	TL	201	PEB	CHA-C1B	3.61	1.48	1.40
29	ZJ	201	PEB	CHA-C1B	3.61	1.48	1.40
29	ZL	201	PEB	CHA-C1B	3.61	1.48	1.40
29	jF	201	PEB	C2A-C1A	-3.61	1.48	1.52
29	jI	201	PEB	C2A-C1A	-3.61	1.48	1.52
29	YB	201	PEB	C1A-NA	-3.61	1.32	1.37
29	LG	201	PEB	C1A-NA	-3.61	1.32	1.37
29	YM	201	PEB	C1A-NA	-3.61	1.32	1.37
29	MQ	402	PEB	C1A-NA	-3.61	1.32	1.37
29	JJ	202	PEB	C1A-NA	-3.61	1.32	1.37
29	JL	202	PEB	C1A-NA	-3.61	1.32	1.37
29	tJ	201	PEB	CHA-C1B	3.61	1.48	1.40
29	tL	201	PEB	CHA-C1B	3.61	1.48	1.40
29	JC	201	PEB	C2C-C3C	3.61	1.48	1.37
29	JE	201	PEB	C2C-C3C	3.61	1.48	1.37
29	N1	1002	PEB	C4D-ND	3.61	1.40	1.35
29	j1	203	PEB	C1A-NA	-3.61	1.32	1.37
29	KG	201	PEB	C1A-NA	-3.61	1.32	1.37
29	WJ	201	PEB	C1A-NA	-3.61	1.32	1.37
29	jK	203	PEB	C1A-NA	-3.61	1.32	1.37
29	WL	201	PEB	C1A-NA	-3.61	1.32	1.37
29	KQ	201	PEB	C1A-NA	-3.61	1.32	1.37
30	yL	303	PUB	C3B-C2B	3.61	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C4	203	PEB	C1A-NA	-3.61	1.32	1.37
29	K8	201	PEB	C1A-NA	-3.61	1.32	1.37
29	d1	202	PEB	C1A-NA	-3.61	1.32	1.37
29	dK	202	PEB	C1A-NA	-3.61	1.32	1.37
29	HA	203	PEB	CHA-C1B	3.61	1.48	1.40
29	HN	203	PEB	CHA-C1B	3.61	1.48	1.40
29	DC	201	PEB	C2C-C3C	3.61	1.48	1.37
29	DE	201	PEB	C2C-C3C	3.61	1.48	1.37
29	m1	202	PEB	C1A-NA	-3.61	1.32	1.37
29	mK	202	PEB	C1A-NA	-3.61	1.32	1.37
29	A1	303	PEB	CHA-C1B	3.60	1.48	1.40
29	L3	201	PEB	CHA-C1B	3.60	1.48	1.40
29	AK	303	PEB	CHA-C1B	3.60	1.48	1.40
29	LO	201	PEB	CHA-C1B	3.60	1.48	1.40
29	BJ	201	PEB	CHA-C1B	3.60	1.48	1.40
29	BL	201	PEB	CHA-C1B	3.60	1.48	1.40
29	LC	201	PEB	C2C-C3C	3.60	1.48	1.37
29	LE	201	PEB	C2C-C3C	3.60	1.48	1.37
29	FG	201	PEB	C1A-NA	-3.60	1.32	1.37
29	FQ	201	PEB	C1A-NA	-3.60	1.32	1.37
29	CD	203	PEB	C1A-NA	-3.60	1.32	1.37
29	SR	201	PEB	C2C-C3C	3.60	1.48	1.37
29	O1	202	PEB	C1A-NA	-3.60	1.32	1.37
29	W1	202	PEB	C1A-NA	-3.60	1.32	1.37
29	CG	201	PEB	C1A-NA	-3.60	1.32	1.37
29	OK	202	PEB	C1A-NA	-3.60	1.32	1.37
29	WK	202	PEB	C1A-NA	-3.60	1.32	1.37
29	CQ	201	PEB	C1A-NA	-3.60	1.32	1.37
29	K5	201	PEB	CHA-C1B	3.60	1.48	1.40
29	C5	201	PEB	C1A-NA	-3.60	1.32	1.37
29	nJ	201	PEB	CHA-C1B	3.60	1.48	1.40
29	nL	201	PEB	CHA-C1B	3.60	1.48	1.40
31	EK	1001	CYC	C1C-NC	-3.60	1.32	1.37
29	JJ	201	PEB	CHA-C1B	3.60	1.48	1.40
29	JL	201	PEB	CHA-C1B	3.60	1.48	1.40
29	A7	305	PEB	C1A-NA	-3.60	1.32	1.37
29	A9	305	PEB	C1A-NA	-3.60	1.32	1.37
31	I1	1001	CYC	C1C-NC	-3.60	1.32	1.37
29	HC	201	PEB	C2C-C3C	3.60	1.48	1.37
29	HE	201	PEB	C2C-C3C	3.60	1.48	1.37
29	NK	1002	PEB	C4D-ND	3.60	1.40	1.35
31	GK	1001	CYC	C1C-NC	-3.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	RJ	201	PEB	CHA-C1B	3.60	1.48	1.40
29	RL	201	PEB	CHA-C1B	3.60	1.48	1.40
31	vP	1001	CYC	C2C-C1C	-3.60	1.48	1.52
29	AF	304	PEB	C1A-NA	-3.60	1.32	1.37
29	AI	304	PEB	C1A-NA	-3.60	1.32	1.37
29	KC	203	PEB	C2C-C3C	3.60	1.48	1.37
29	KE	203	PEB	C2C-C3C	3.60	1.48	1.37
29	AF	304	PEB	CHA-C1B	3.60	1.48	1.40
29	AI	304	PEB	CHA-C1B	3.60	1.48	1.40
29	hF	201	PEB	C2A-C1A	-3.60	1.48	1.52
29	hI	201	PEB	C2A-C1A	-3.60	1.48	1.52
29	vJ	201	PEB	C2A-C1A	-3.60	1.48	1.52
29	vL	201	PEB	C2A-C1A	-3.60	1.48	1.52
31	gP	1001	CYC	C2C-C1C	-3.60	1.48	1.52
29	FC	201	PEB	C2C-C3C	3.59	1.48	1.37
29	FE	201	PEB	C2C-C3C	3.59	1.48	1.37
29	H5	203	PEB	C1A-NA	-3.59	1.32	1.37
29	DK	1002	PEB	C1A-NA	-3.59	1.32	1.37
29	BC	201	PEB	C2C-C3C	3.59	1.48	1.37
29	BE	201	PEB	C2C-C3C	3.59	1.48	1.37
29	D3	201	PEB	CHA-C1B	3.59	1.48	1.40
29	M3	202	PEB	CHA-C1B	3.59	1.48	1.40
29	DO	201	PEB	CHA-C1B	3.59	1.48	1.40
29	MO	202	PEB	CHA-C1B	3.59	1.48	1.40
29	IC	202	PEB	C2C-C3C	3.59	1.48	1.37
29	IE	202	PEB	C2C-C3C	3.59	1.48	1.37
29	e1	202	PEB	C1A-NA	-3.59	1.33	1.37
29	eK	202	PEB	C1A-NA	-3.59	1.33	1.37
29	C5	201	PEB	CHA-C1B	3.59	1.48	1.40
29	C8	201	PEB	CHA-C1B	3.59	1.48	1.40
29	gB	201	PEB	C1A-NA	-3.59	1.33	1.37
29	gM	201	PEB	C1A-NA	-3.59	1.33	1.37
29	KC	203	PEB	CHA-C1B	3.59	1.48	1.40
29	KE	203	PEB	CHA-C1B	3.59	1.48	1.40
29	dF	202	PEB	C2A-C1A	-3.59	1.48	1.52
29	dI	202	PEB	C2A-C1A	-3.59	1.48	1.52
29	A1	303	PEB	C1A-NA	-3.59	1.33	1.37
29	C8	201	PEB	C1A-NA	-3.59	1.33	1.37
29	AK	303	PEB	C1A-NA	-3.59	1.33	1.37
29	f1	201	PEB	C2A-C1A	-3.59	1.48	1.52
29	fK	201	PEB	C2A-C1A	-3.59	1.48	1.52
29	D1	1002	PEB	C4D-ND	3.59	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B5	203	PEB	C1A-NA	-3.59	1.33	1.37
29	gF	203	PEB	C1A-NA	-3.59	1.33	1.37
29	gI	203	PEB	C1A-NA	-3.59	1.33	1.37
29	IC	202	PEB	CHA-C1B	3.59	1.48	1.40
29	IE	202	PEB	CHA-C1B	3.59	1.48	1.40
31	tP	1001	CYC	C2C-C1C	-3.58	1.48	1.52
29	g1	202	PEB	C1A-NA	-3.58	1.33	1.37
29	gK	202	PEB	C1A-NA	-3.58	1.33	1.37
29	L5	201	PEB	CHA-C1B	3.58	1.48	1.40
29	Q1	201	PEB	C2A-C1A	-3.58	1.48	1.52
29	bF	201	PEB	C2A-C1A	-3.58	1.48	1.52
29	bI	201	PEB	C2A-C1A	-3.58	1.48	1.52
29	QK	201	PEB	C2A-C1A	-3.58	1.48	1.52
29	CC	202	PEB	C2C-C3C	3.58	1.48	1.37
29	CE	202	PEB	C2C-C3C	3.58	1.48	1.37
29	J3	201	PEB	CHA-C1B	3.58	1.48	1.40
29	JO	201	PEB	CHA-C1B	3.58	1.48	1.40
29	AC	202	PEB	C2C-C3C	3.58	1.48	1.37
29	AE	202	PEB	C2C-C3C	3.58	1.48	1.37
29	Q7	202	PEB	C1A-NA	-3.58	1.33	1.37
29	Q9	202	PEB	C1A-NA	-3.58	1.33	1.37
29	HK	1002	PEB	C4D-ND	3.58	1.39	1.35
29	EC	202	PEB	C2C-C3C	3.58	1.48	1.37
29	EE	202	PEB	C2C-C3C	3.58	1.48	1.37
29	EG	201	PEB	C1A-NA	-3.58	1.33	1.37
29	EQ	201	PEB	C1A-NA	-3.58	1.33	1.37
29	g7	201	PEB	CHA-C1B	3.58	1.48	1.40
29	g9	201	PEB	CHA-C1B	3.58	1.48	1.40
29	G3	201	PEB	C2A-C1A	-3.58	1.48	1.52
29	GO	201	PEB	C2A-C1A	-3.58	1.48	1.52
29	DK	1002	PEB	C4D-ND	3.58	1.39	1.35
30	MQ	405	PUB	C3B-C2B	3.58	1.48	1.37
29	V1	202	PEB	C1A-NA	-3.58	1.33	1.37
29	G4	203	PEB	C1A-NA	-3.58	1.33	1.37
29	G8	203	PEB	C1A-NA	-3.58	1.33	1.37
29	VK	202	PEB	C1A-NA	-3.58	1.33	1.37
29	O7	202	PEB	C1A-NA	-3.58	1.33	1.37
29	O9	202	PEB	C1A-NA	-3.58	1.33	1.37
29	IJ	203	PEB	C1A-NA	-3.58	1.33	1.37
29	IL	203	PEB	C1A-NA	-3.58	1.33	1.37
29	GC	202	PEB	C2C-C3C	3.57	1.48	1.37
29	GE	202	PEB	C2C-C3C	3.57	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E1	1001	CYC	C1C-NC	-3.57	1.33	1.37
29	fJ	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	fL	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	I4	203	PEB	C2C-C3C	3.57	1.48	1.37
29	TF	201	PEB	C2C-C3C	3.57	1.48	1.37
29	GJ	202	PEB	C1A-NA	-3.57	1.33	1.37
29	GL	202	PEB	C1A-NA	-3.57	1.33	1.37
31	CK	1001	CYC	C1C-NC	-3.57	1.33	1.37
29	F5	201	PEB	CHA-C1B	3.57	1.48	1.40
29	L8	201	PEB	CHA-C1B	3.57	1.48	1.40
30	MG	403	PUB	C3B-C2B	3.57	1.48	1.37
29	d7	202	PEB	C1A-NA	-3.57	1.33	1.37
29	d9	202	PEB	C1A-NA	-3.57	1.33	1.37
29	AB	301	PEB	C1A-NA	-3.57	1.33	1.37
29	FJ	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	FL	201	PEB	C2A-C1A	-3.57	1.48	1.52
31	NP	1001	CYC	C2C-C1C	-3.57	1.48	1.52
31	HF	1001	CYC	CHB-C4A	3.57	1.48	1.40
31	HI	1001	CYC	CHB-C4A	3.57	1.48	1.40
29	cB	201	PEB	C1A-NA	-3.57	1.33	1.37
29	cM	201	PEB	C1A-NA	-3.57	1.33	1.37
29	J1	1002	PEB	C4D-ND	3.57	1.39	1.35
29	JK	1002	PEB	C4D-ND	3.57	1.39	1.35
29	EC	202	PEB	CHA-C1B	3.57	1.48	1.40
29	EE	202	PEB	CHA-C1B	3.57	1.48	1.40
29	U1	202	PEB	C2A-C1A	-3.57	1.48	1.52
29	UK	202	PEB	C2A-C1A	-3.57	1.48	1.52
31	RP	1001	CYC	C2C-C1C	-3.57	1.48	1.52
31	pP	1001	CYC	C2C-C1C	-3.57	1.48	1.52
29	a7	201	PEB	CHA-C1B	3.57	1.48	1.40
29	a9	201	PEB	CHA-C1B	3.57	1.48	1.40
29	eB	201	PEB	C1A-NA	-3.57	1.33	1.37
29	eM	201	PEB	C1A-NA	-3.57	1.33	1.37
29	S1	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	K3	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	SK	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	KO	201	PEB	C2A-C1A	-3.57	1.48	1.52
29	QJ	202	PEB	C1A-NA	-3.57	1.33	1.37
29	QL	202	PEB	C1A-NA	-3.57	1.33	1.37
29	F8	201	PEB	CHA-C1B	3.57	1.48	1.40
29	EC	201	PEB	CHA-C1B	3.57	1.48	1.40
29	EE	201	PEB	CHA-C1B	3.57	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I5	201	PEB	CHA-C1B	3.57	1.48	1.40
29	I8	201	PEB	CHA-C1B	3.57	1.48	1.40
29	AC	202	PEB	CHA-C1B	3.57	1.48	1.40
29	AE	202	PEB	CHA-C1B	3.57	1.48	1.40
29	GC	202	PEB	CHA-C1B	3.56	1.48	1.40
29	GE	202	PEB	CHA-C1B	3.56	1.48	1.40
31	yP	1001	CYC	C2C-C1C	-3.56	1.48	1.52
29	L8	203	PEB	C1A-NA	-3.56	1.33	1.37
29	pJ	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	pL	201	PEB	C2A-C1A	-3.56	1.48	1.52
31	JF	1001	CYC	CHB-C4A	3.56	1.48	1.40
31	NF	1001	CYC	CHB-C4A	3.56	1.48	1.40
31	JI	1001	CYC	CHB-C4A	3.56	1.48	1.40
31	NI	1001	CYC	CHB-C4A	3.56	1.48	1.40
29	M4	203	PEB	C2C-C3C	3.56	1.48	1.37
29	c7	201	PEB	CHA-C1B	3.56	1.48	1.40
29	c9	201	PEB	CHA-C1B	3.56	1.48	1.40
29	A5	201	PEB	CHA-C1B	3.56	1.48	1.40
29	A8	201	PEB	CHA-C1B	3.56	1.48	1.40
29	I4	203	PEB	CHA-C1B	3.56	1.48	1.40
29	AM	301	PEB	C1A-NA	-3.56	1.33	1.37
29	XJ	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	bJ	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	jJ	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	XL	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	bL	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	jL	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	R7	201	PEB	CHA-C1B	3.56	1.48	1.40
29	R9	201	PEB	CHA-C1B	3.56	1.48	1.40
31	DF	1001	CYC	CHB-C4A	3.56	1.48	1.40
31	DI	1001	CYC	CHB-C4A	3.56	1.48	1.40
29	IG	201	PEB	C1A-NA	-3.56	1.33	1.37
29	IQ	201	PEB	C1A-NA	-3.56	1.33	1.37
31	mP	1001	CYC	C2C-C1C	-3.56	1.48	1.52
29	S2	201	PEB	C2C-C3C	3.56	1.48	1.37
29	H1	1002	PEB	C4D-ND	3.56	1.39	1.35
31	xP	1001	CYC	C4D-CHA	3.56	1.54	1.41
29	PJ	201	PEB	C2A-C1A	-3.56	1.48	1.52
29	PL	201	PEB	C2A-C1A	-3.56	1.48	1.52
31	WP	1001	CYC	C2C-C1C	-3.56	1.48	1.52
29	H5	201	PEB	CHA-C1B	3.56	1.48	1.40
29	k7	201	PEB	CHA-C1B	3.56	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	m7	201	PEB	CHA-C1B	3.56	1.48	1.40
29	k9	201	PEB	CHA-C1B	3.56	1.48	1.40
29	m9	201	PEB	CHA-C1B	3.56	1.48	1.40
29	e7	201	PEB	CHA-C1B	3.56	1.48	1.40
29	e9	201	PEB	CHA-C1B	3.56	1.48	1.40
31	VP	1001	CYC	C4D-CHA	3.56	1.54	1.41
29	f7	202	PEB	C1A-NA	-3.56	1.33	1.37
29	l7	202	PEB	C1A-NA	-3.56	1.33	1.37
29	f9	202	PEB	C1A-NA	-3.56	1.33	1.37
29	l9	202	PEB	C1A-NA	-3.56	1.33	1.37
29	GD	203	PEB	C1A-NA	-3.56	1.33	1.37
29	T7	201	PEB	CHA-C1B	3.56	1.48	1.40
29	T9	201	PEB	CHA-C1B	3.56	1.48	1.40
29	c1	202	PEB	C1A-NA	-3.56	1.33	1.37
29	i1	202	PEB	C1A-NA	-3.56	1.33	1.37
29	cK	202	PEB	C1A-NA	-3.56	1.33	1.37
29	iK	202	PEB	C1A-NA	-3.56	1.33	1.37
29	F5	203	PEB	C1A-NA	-3.55	1.33	1.37
29	F8	203	PEB	C1A-NA	-3.55	1.33	1.37
29	L8	202	PEB	C1A-NA	-3.55	1.33	1.37
29	uJ	203	PEB	C1A-NA	-3.55	1.33	1.37
29	uL	203	PEB	C1A-NA	-3.55	1.33	1.37
29	D3	202	PEB	C1A-NA	-3.55	1.33	1.37
29	F3	203	PEB	C1A-NA	-3.55	1.33	1.37
29	FO	203	PEB	C1A-NA	-3.55	1.33	1.37
29	GC	201	PEB	CHA-C1B	3.55	1.48	1.40
29	GE	201	PEB	CHA-C1B	3.55	1.48	1.40
31	IK	1001	CYC	C1C-NC	-3.55	1.33	1.37
29	Y7	201	PEB	CHA-C1B	3.55	1.48	1.40
29	Y9	201	PEB	CHA-C1B	3.55	1.48	1.40
29	JJ	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	JL	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	P2	202	PEB	C1A-NA	-3.55	1.33	1.37
29	gJ	202	PEB	C1A-NA	-3.55	1.33	1.37
29	zJ	501	PEB	C1A-NA	-3.55	1.33	1.37
29	gL	202	PEB	C1A-NA	-3.55	1.33	1.37
29	i7	201	PEB	CHA-C1B	3.55	1.48	1.40
29	i9	201	PEB	CHA-C1B	3.55	1.48	1.40
29	OR	202	PEB	C2C-C3C	3.55	1.48	1.37
29	P7	201	PEB	CHA-C1B	3.55	1.48	1.40
29	P9	201	PEB	CHA-C1B	3.55	1.48	1.40
29	F1	1002	PEB	C1A-NA	-3.55	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FK	1002	PEB	C1A-NA	-3.55	1.33	1.37
29	CC	202	PEB	CHA-C1B	3.55	1.48	1.40
29	CE	202	PEB	CHA-C1B	3.55	1.48	1.40
29	V7	201	PEB	CHA-C1B	3.55	1.48	1.40
29	V9	201	PEB	CHA-C1B	3.55	1.48	1.40
31	D1	1003	CYC	C1C-NC	-3.55	1.33	1.37
29	BJ	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	DJ	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	BL	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	DL	201	PEB	C2A-C1A	-3.55	1.48	1.52
31	KP	1001	CYC	C2C-C1C	-3.55	1.48	1.52
29	SR	201	PEB	CHA-C1B	3.55	1.48	1.40
29	N3	202	PEB	CHA-C1B	3.55	1.48	1.40
29	tJ	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	tL	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	A1	302	PEB	C2C-C3C	3.55	1.48	1.37
29	AK	302	PEB	C2C-C3C	3.55	1.48	1.37
29	T2	203	PEB	C1A-NA	-3.55	1.33	1.37
29	IJ	201	PEB	C2A-C1A	-3.55	1.48	1.52
29	IL	201	PEB	C2A-C1A	-3.55	1.48	1.52
31	VP	1001	CYC	C3D-C2D	3.55	1.48	1.37
29	RJ	201	PEB	C2A-C1A	-3.54	1.48	1.52
29	RL	201	PEB	C2A-C1A	-3.54	1.48	1.52
31	xP	1001	CYC	C3D-C2D	3.54	1.48	1.37
29	G5	202	PEB	CHA-C1B	3.54	1.48	1.40
29	G5	202	PEB	C1A-NA	-3.54	1.33	1.37
29	a1	202	PEB	C1A-NA	-3.54	1.33	1.37
29	aK	202	PEB	C1A-NA	-3.54	1.33	1.37
29	HB	201	PEB	C1A-NA	-3.54	1.33	1.37
29	HM	201	PEB	C1A-NA	-3.54	1.33	1.37
29	NO	202	PEB	CHA-C1B	3.54	1.48	1.40
29	NR	203	PEB	C1A-NA	-3.54	1.33	1.37
29	D3	202	PEB	C2C-C3C	3.54	1.48	1.37
29	VR	203	PEB	C1A-NA	-3.54	1.33	1.37
29	zJ	501	PEB	C2C-C3C	3.54	1.48	1.37
29	H8	201	PEB	CHA-C1B	3.54	1.48	1.40
29	TJ	201	PEB	C2A-C1A	-3.54	1.48	1.52
29	TL	201	PEB	C2A-C1A	-3.54	1.48	1.52
29	Z1	201	PEB	C1A-NA	-3.54	1.33	1.37
29	U7	202	PEB	C1A-NA	-3.54	1.33	1.37
29	U9	202	PEB	C1A-NA	-3.54	1.33	1.37
29	ZK	201	PEB	C1A-NA	-3.54	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HF	1002	PEB	CHA-C1B	3.54	1.48	1.40
29	HI	1002	PEB	CHA-C1B	3.54	1.48	1.40
31	cP	1001	CYC	C2C-C1C	-3.54	1.48	1.52
29	k1	202	PEB	C1A-NA	-3.54	1.33	1.37
29	kK	202	PEB	C1A-NA	-3.54	1.33	1.37
29	AM	303	PEB	C2C-C3C	3.54	1.48	1.37
29	DG	201	PEB	C1A-NA	-3.54	1.33	1.37
29	DQ	201	PEB	C1A-NA	-3.54	1.33	1.37
31	FF	1001	CYC	CHB-C4A	3.54	1.48	1.40
31	FI	1001	CYC	CHB-C4A	3.54	1.48	1.40
29	D1	1002	PEB	C1A-NA	-3.54	1.33	1.37
29	AJ	202	PEB	C1A-NA	-3.54	1.33	1.37
29	AL	202	PEB	C1A-NA	-3.54	1.33	1.37
29	DO	202	PEB	C2C-C3C	3.54	1.48	1.37
29	R1	202	PEB	C1A-NA	-3.54	1.33	1.37
29	RK	202	PEB	C1A-NA	-3.54	1.33	1.37
29	C5	202	PEB	C1A-NA	-3.54	1.33	1.37
29	C8	202	PEB	C1A-NA	-3.54	1.33	1.37
29	AG	201	PEB	C1A-NA	-3.54	1.33	1.37
29	AQ	201	PEB	C1A-NA	-3.54	1.33	1.37
31	K1	1001	CYC	C1C-NC	-3.54	1.33	1.37
31	KK	1001	CYC	C1C-NC	-3.54	1.33	1.37
31	rP	1001	CYC	C2C-C1C	-3.54	1.48	1.52
29	L5	203	PEB	C1A-NA	-3.54	1.33	1.37
29	b7	202	PEB	C1A-NA	-3.54	1.33	1.37
29	b9	202	PEB	C1A-NA	-3.54	1.33	1.37
29	TB	201	PEB	C1A-NA	-3.53	1.33	1.37
29	TM	201	PEB	C1A-NA	-3.53	1.33	1.37
29	B8	201	PEB	CHA-C1B	3.53	1.48	1.40
31	MF	1001	CYC	C2C-C1C	-3.53	1.48	1.52
31	MI	1001	CYC	C2C-C1C	-3.53	1.48	1.52
29	TR	203	PEB	C1A-NA	-3.53	1.33	1.37
29	B5	201	PEB	CHA-C1B	3.53	1.48	1.40
29	G5	201	PEB	CHA-C1B	3.53	1.48	1.40
29	L5	202	PEB	CHA-C1B	3.53	1.48	1.40
29	L8	202	PEB	CHA-C1B	3.53	1.48	1.40
29	A3	201	PEB	CHA-C1B	3.53	1.48	1.40
29	AO	201	PEB	CHA-C1B	3.53	1.48	1.40
29	MA	404	PEB	C2C-C3C	3.53	1.48	1.37
29	MN	404	PEB	C2C-C3C	3.53	1.48	1.37
29	LJ	201	PEB	C2A-C1A	-3.53	1.48	1.52
29	LL	201	PEB	C2A-C1A	-3.53	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H3	203	PEB	C1A-NA	-3.53	1.33	1.37
29	HO	203	PEB	C1A-NA	-3.53	1.33	1.37
29	XB	201	PEB	C1A-NA	-3.53	1.33	1.37
29	XM	201	PEB	C1A-NA	-3.53	1.33	1.37
29	AB	303	PEB	C2C-C3C	3.53	1.48	1.37
31	PP	1001	CYC	C2C-C1C	-3.53	1.48	1.52
29	F8	202	PEB	C1A-NA	-3.53	1.33	1.37
29	LB	201	PEB	C1A-NA	-3.53	1.33	1.37
29	LM	201	PEB	C1A-NA	-3.53	1.33	1.37
29	MG	401	PEB	C2C-C3C	3.53	1.48	1.37
29	L3	202	PEB	C1A-NA	-3.52	1.33	1.37
29	DO	202	PEB	C1A-NA	-3.52	1.33	1.37
29	LO	202	PEB	C1A-NA	-3.52	1.33	1.37
29	G8	201	PEB	CHA-C1B	3.52	1.48	1.40
29	G8	202	PEB	CHA-C1B	3.52	1.48	1.40
29	I3	203	PEB	CHA-C1B	3.52	1.48	1.40
29	IO	203	PEB	CHA-C1B	3.52	1.48	1.40
31	TP	1001	CYC	C2C-C1C	-3.52	1.48	1.52
29	D3	203	PEB	C1A-NA	-3.52	1.33	1.37
29	DO	203	PEB	C1A-NA	-3.52	1.33	1.37
29	OJ	202	PEB	C1A-NA	-3.52	1.33	1.37
29	OL	202	PEB	C1A-NA	-3.52	1.33	1.37
29	rJ	201	PEB	C2A-C1A	-3.52	1.48	1.52
29	rL	201	PEB	C2A-C1A	-3.52	1.48	1.52
29	wJ	303	PEB	C2C-C3C	3.52	1.48	1.37
29	S7	202	PEB	C1A-NA	-3.52	1.33	1.37
29	S9	202	PEB	C1A-NA	-3.52	1.33	1.37
29	MJ	202	PEB	C1A-NA	-3.52	1.33	1.37
29	iJ	202	PEB	C1A-NA	-3.52	1.33	1.37
29	ML	202	PEB	C1A-NA	-3.52	1.33	1.37
29	iL	202	PEB	C1A-NA	-3.52	1.33	1.37
32	k6	302	PMS	O1S-S	3.52	1.55	1.45
32	kH	302	PMS	O1S-S	3.52	1.55	1.45
29	aJ	202	PEB	C1A-NA	-3.52	1.33	1.37
29	aL	202	PEB	C1A-NA	-3.52	1.33	1.37
29	IC	201	PEB	CHA-C1B	3.52	1.48	1.40
29	KC	202	PEB	CHA-C1B	3.52	1.48	1.40
29	IE	201	PEB	CHA-C1B	3.52	1.48	1.40
29	KE	202	PEB	CHA-C1B	3.52	1.48	1.40
29	LF	1002	PEB	CHA-C1B	3.52	1.48	1.40
29	LI	1002	PEB	CHA-C1B	3.52	1.48	1.40
29	CC	201	PEB	CHA-C1B	3.52	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	CE	201	PEB	CHA-C1B	3.52	1.48	1.40
29	H1	1002	PEB	C1A-NA	-3.52	1.33	1.37
29	JB	201	PEB	C1A-NA	-3.52	1.33	1.37
29	JM	201	PEB	C1A-NA	-3.52	1.33	1.37
29	A1	301	PEB	CHA-C1B	3.52	1.48	1.40
29	NF	1002	PEB	CHA-C1B	3.52	1.48	1.40
29	NI	1002	PEB	CHA-C1B	3.52	1.48	1.40
29	AK	301	PEB	CHA-C1B	3.52	1.48	1.40
31	CP	1001	CYC	C2C-C1C	-3.52	1.49	1.52
29	RB	201	PEB	C1A-NA	-3.52	1.33	1.37
29	YB	203	PEB	C1A-NA	-3.52	1.33	1.37
29	RM	201	PEB	C1A-NA	-3.52	1.33	1.37
29	YM	203	PEB	C1A-NA	-3.52	1.33	1.37
29	AC	201	PEB	CHA-C1B	3.52	1.48	1.40
29	AE	201	PEB	CHA-C1B	3.52	1.48	1.40
29	F5	202	PEB	C1A-NA	-3.52	1.33	1.37
31	LF	1001	CYC	CHB-C4A	3.52	1.48	1.40
31	LI	1001	CYC	CHB-C4A	3.52	1.48	1.40
29	I3	201	PEB	CHA-C1B	3.52	1.48	1.40
29	IO	201	PEB	CHA-C1B	3.52	1.48	1.40
29	EJ	202	PEB	C1A-NA	-3.51	1.33	1.37
29	EL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	CA	202	PEB	C1A-NA	-3.51	1.33	1.37
29	DB	201	PEB	C1A-NA	-3.51	1.33	1.37
29	DM	201	PEB	C1A-NA	-3.51	1.33	1.37
29	CN	202	PEB	C1A-NA	-3.51	1.33	1.37
29	ZJ	201	PEB	C2A-C1A	-3.51	1.49	1.52
29	ZL	201	PEB	C2A-C1A	-3.51	1.49	1.52
29	h7	202	PEB	C1A-NA	-3.51	1.33	1.37
29	h9	202	PEB	C1A-NA	-3.51	1.33	1.37
31	EF	1001	CYC	C2C-C1C	-3.51	1.49	1.52
31	EI	1001	CYC	C2C-C1C	-3.51	1.49	1.52
31	GP	1001	CYC	C2C-C1C	-3.51	1.49	1.52
29	B3	202	PEB	CHA-C1B	3.51	1.48	1.40
29	BO	202	PEB	CHA-C1B	3.51	1.48	1.40
29	SJ	202	PEB	C1A-NA	-3.51	1.33	1.37
29	oJ	202	PEB	C1A-NA	-3.51	1.33	1.37
29	qJ	202	PEB	C1A-NA	-3.51	1.33	1.37
29	SL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	oL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	qL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	YJ	202	PEB	C1A-NA	-3.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	kJ	202	PEB	C1A-NA	-3.51	1.33	1.37
29	YL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	kL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	A9	304	PEB	C2C-C3C	3.51	1.48	1.37
31	KF	1001	CYC	C2C-C1C	-3.51	1.49	1.52
29	L1	1002	PEB	C1A-NA	-3.51	1.33	1.37
29	CJ	202	PEB	C1A-NA	-3.51	1.33	1.37
29	LK	1002	PEB	C1A-NA	-3.51	1.33	1.37
29	CL	202	PEB	C1A-NA	-3.51	1.33	1.37
29	zL	501	PEB	C2C-C3C	3.51	1.48	1.37
31	IF	1001	CYC	C2C-C1C	-3.51	1.49	1.52
31	II	1001	CYC	C2C-C1C	-3.51	1.49	1.52
29	F5	202	PEB	CHA-C1B	3.51	1.48	1.40
29	F8	202	PEB	CHA-C1B	3.51	1.48	1.40
29	dJ	201	PEB	C2A-C1A	-3.50	1.49	1.52
29	dL	201	PEB	C2A-C1A	-3.50	1.49	1.52
29	L5	202	PEB	C1A-NA	-3.50	1.33	1.37
29	NK	1002	PEB	C1A-NA	-3.50	1.33	1.37
29	JF	1002	PEB	CHA-C1B	3.50	1.48	1.40
29	JI	1002	PEB	CHA-C1B	3.50	1.48	1.40
29	H5	202	PEB	C1A-NA	-3.50	1.33	1.37
29	MQ	403	PEB	C2C-C3C	3.50	1.48	1.37
29	B8	202	PEB	CHA-C1B	3.50	1.48	1.40
29	H8	202	PEB	C1A-NA	-3.50	1.33	1.37
29	UB	202	PEB	C1A-NA	-3.50	1.33	1.37
29	sJ	202	PEB	C1A-NA	-3.50	1.33	1.37
29	sL	202	PEB	C1A-NA	-3.50	1.33	1.37
29	MQ	401	PEB	C1A-NA	-3.50	1.33	1.37
29	J3	202	PEB	CHA-C1B	3.50	1.48	1.40
29	JO	202	PEB	CHA-C1B	3.50	1.48	1.40
29	B3	203	PEB	C1A-NA	-3.50	1.33	1.37
29	mB	201	PEB	C1A-NA	-3.50	1.33	1.37
29	mM	201	PEB	C1A-NA	-3.50	1.33	1.37
29	BO	203	PEB	C1A-NA	-3.50	1.33	1.37
29	NR	201	PEB	C1A-NA	-3.50	1.33	1.37
29	nJ	201	PEB	C2A-C1A	-3.50	1.49	1.52
29	nL	201	PEB	C2A-C1A	-3.50	1.49	1.52
29	J1	1002	PEB	C1A-NA	-3.50	1.33	1.37
29	JK	1002	PEB	C1A-NA	-3.50	1.33	1.37
29	A7	304	PEB	C2C-C3C	3.50	1.48	1.37
29	GB	201	PEB	CHA-C1B	3.50	1.48	1.40
29	FF	1002	PEB	CHA-C1B	3.50	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FI	1002	PEB	CHA-C1B	3.50	1.48	1.40
29	GM	201	PEB	CHA-C1B	3.50	1.48	1.40
29	QB	203	PEB	CHA-C1B	3.50	1.48	1.40
29	DF	1002	PEB	CHA-C1B	3.50	1.48	1.40
29	DI	1002	PEB	CHA-C1B	3.50	1.48	1.40
29	QM	203	PEB	CHA-C1B	3.50	1.48	1.40
29	VB	201	PEB	C1A-NA	-3.50	1.33	1.37
29	KJ	202	PEB	C1A-NA	-3.50	1.33	1.37
29	KL	202	PEB	C1A-NA	-3.50	1.33	1.37
29	VM	201	PEB	C1A-NA	-3.50	1.33	1.37
29	MA	404	PEB	CHA-C1B	3.50	1.48	1.40
29	GC	201	PEB	C1A-NA	-3.50	1.33	1.37
29	GE	201	PEB	C1A-NA	-3.50	1.33	1.37
29	eJ	202	PEB	C1A-NA	-3.50	1.33	1.37
29	eL	202	PEB	C1A-NA	-3.50	1.33	1.37
29	MB	202	PEB	C1A-NA	-3.50	1.33	1.37
29	MM	202	PEB	C1A-NA	-3.50	1.33	1.37
31	EP	1001	CYC	C2C-C1C	-3.50	1.49	1.52
29	j7	202	PEB	C1A-NA	-3.50	1.33	1.37
29	j9	202	PEB	C1A-NA	-3.50	1.33	1.37
29	VJ	201	PEB	C2A-C1A	-3.50	1.49	1.52
29	VL	201	PEB	C2A-C1A	-3.50	1.49	1.52
29	U1	201	PEB	C1A-NA	-3.49	1.33	1.37
29	lB	202	PEB	C1A-NA	-3.49	1.33	1.37
29	UK	201	PEB	C1A-NA	-3.49	1.33	1.37
29	lM	202	PEB	C1A-NA	-3.49	1.33	1.37
29	TR	201	PEB	C1A-NA	-3.49	1.33	1.37
29	NR	201	PEB	CHA-C1B	3.49	1.48	1.40
29	dB	202	PEB	C1A-NA	-3.49	1.33	1.37
29	dM	202	PEB	C1A-NA	-3.49	1.33	1.37
29	OB	201	PEB	CHA-C1B	3.49	1.48	1.40
29	OM	201	PEB	CHA-C1B	3.49	1.48	1.40
29	dJ	203	PEB	C2C-C3C	3.49	1.48	1.37
29	dL	203	PEB	C2C-C3C	3.49	1.48	1.37
29	DB	203	PEB	C2C-C3C	3.49	1.48	1.37
29	DM	203	PEB	C2C-C3C	3.49	1.48	1.37
29	aB	201	PEB	CHA-C1B	3.49	1.48	1.40
29	aM	201	PEB	CHA-C1B	3.49	1.48	1.40
29	G3	202	PEB	C1A-NA	-3.49	1.33	1.37
29	GO	202	PEB	C1A-NA	-3.49	1.33	1.37
29	E3	201	PEB	CHA-C1B	3.49	1.48	1.40
29	EO	201	PEB	CHA-C1B	3.49	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W7	202	PEB	C1A-NA	-3.49	1.33	1.37
29	W9	202	PEB	C1A-NA	-3.49	1.33	1.37
29	CB	202	PEB	C1A-NA	-3.49	1.33	1.37
29	CM	202	PEB	C1A-NA	-3.49	1.33	1.37
29	M3	201	PEB	C2A-C1A	-3.49	1.49	1.52
29	MO	201	PEB	C2A-C1A	-3.49	1.49	1.52
29	F7	1002	PEB	C1A-NA	-3.49	1.33	1.37
29	DG	202	PEB	CHA-C1B	3.49	1.48	1.40
29	DQ	202	PEB	CHA-C1B	3.49	1.48	1.40
29	Z7	202	PEB	C1A-NA	-3.49	1.33	1.37
29	Z9	202	PEB	C1A-NA	-3.49	1.33	1.37
29	PB	201	PEB	C1A-NA	-3.49	1.33	1.37
29	PM	201	PEB	C1A-NA	-3.49	1.33	1.37
31	cP	1001	CYC	C3D-C2D	3.49	1.48	1.37
29	H8	202	PEB	CHA-C1B	3.49	1.48	1.40
29	hB	201	PEB	CHA-C1B	3.49	1.48	1.40
29	hM	201	PEB	CHA-C1B	3.49	1.48	1.40
29	MN	401	PEB	CHA-C1B	3.49	1.48	1.40
29	E3	201	PEB	C2A-C1A	-3.49	1.49	1.52
29	EO	201	PEB	C2A-C1A	-3.49	1.49	1.52
29	P1	202	PEB	C1A-NA	-3.49	1.33	1.37
29	PK	202	PEB	C1A-NA	-3.49	1.33	1.37
29	I5	202	PEB	C1A-NA	-3.49	1.33	1.37
29	G8	202	PEB	C1A-NA	-3.49	1.33	1.37
29	I8	202	PEB	C1A-NA	-3.49	1.33	1.37
29	F9	1002	PEB	C1A-NA	-3.49	1.33	1.37
29	WB	202	PEB	C1A-NA	-3.49	1.33	1.37
29	WM	202	PEB	C1A-NA	-3.49	1.33	1.37
29	T2	201	PEB	CHA-C1B	3.49	1.48	1.40
29	TR	201	PEB	CHA-C1B	3.49	1.48	1.40
29	UJ	202	PEB	C1A-NA	-3.49	1.33	1.37
29	UL	202	PEB	C1A-NA	-3.49	1.33	1.37
29	UB	201	PEB	CHA-C1B	3.49	1.48	1.40
29	UM	201	PEB	CHA-C1B	3.49	1.48	1.40
29	JG	202	PEB	CHA-C1B	3.49	1.48	1.40
29	JQ	202	PEB	CHA-C1B	3.49	1.48	1.40
29	R7	202	PEB	CHA-C1B	3.49	1.48	1.40
29	R9	202	PEB	CHA-C1B	3.49	1.48	1.40
29	KB	201	PEB	CHA-C1B	3.49	1.48	1.40
29	FG	202	PEB	CHA-C1B	3.49	1.48	1.40
29	KM	201	PEB	CHA-C1B	3.49	1.48	1.40
29	FQ	202	PEB	CHA-C1B	3.49	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	RR	201	PEB	CHA-C1B	3.49	1.48	1.40
31	C7	1001	CYC	CHB-C4A	3.48	1.48	1.40
31	C9	1001	CYC	CHB-C4A	3.48	1.48	1.40
29	eB	202	PEB	C2C-C3C	3.48	1.48	1.37
29	wL	303	PEB	C2C-C3C	3.48	1.48	1.37
29	eM	202	PEB	C2C-C3C	3.48	1.48	1.37
31	tP	1001	CYC	C3D-C2D	3.48	1.48	1.37
31	KI	1001	CYC	C2C-C1C	-3.48	1.49	1.52
29	HB	203	PEB	C2C-C3C	3.48	1.48	1.37
29	HM	203	PEB	C2C-C3C	3.48	1.48	1.37
29	dB	201	PEB	CHA-C1B	3.48	1.48	1.40
29	dM	201	PEB	CHA-C1B	3.48	1.48	1.40
29	A5	202	PEB	C1A-NA	-3.48	1.33	1.37
29	J9	1002	PEB	C1A-NA	-3.48	1.33	1.37
29	OB	202	PEB	C1A-NA	-3.48	1.33	1.37
29	OM	202	PEB	C1A-NA	-3.48	1.33	1.37
29	V2	201	PEB	CHA-C1B	3.48	1.48	1.40
29	VR	201	PEB	CHA-C1B	3.48	1.48	1.40
31	vP	1001	CYC	C3D-C2D	3.48	1.48	1.37
29	KG	202	PEB	CHA-C1B	3.48	1.48	1.40
29	KQ	202	PEB	CHA-C1B	3.48	1.48	1.40
31	pP	1001	CYC	C3D-C2D	3.48	1.48	1.37
29	hJ	201	PEB	C2A-C1A	-3.48	1.49	1.52
29	hL	201	PEB	C2A-C1A	-3.48	1.49	1.52
29	A8	202	PEB	C1A-NA	-3.48	1.33	1.37
29	fB	201	PEB	CHA-C1B	3.48	1.48	1.40
29	fM	201	PEB	CHA-C1B	3.48	1.48	1.40
29	AC	201	PEB	C1A-NA	-3.48	1.33	1.37
29	AE	201	PEB	C1A-NA	-3.48	1.33	1.37
29	NJ	201	PEB	C2A-C1A	-3.48	1.49	1.52
29	NL	201	PEB	C2A-C1A	-3.48	1.49	1.52
29	J3	203	PEB	C1A-NA	-3.48	1.33	1.37
29	SB	202	PEB	C1A-NA	-3.48	1.33	1.37
29	SM	202	PEB	C1A-NA	-3.48	1.33	1.37
29	JO	203	PEB	C1A-NA	-3.48	1.33	1.37
29	K3	201	PEB	CHA-C1B	3.48	1.48	1.40
29	KO	201	PEB	CHA-C1B	3.48	1.48	1.40
29	H3	202	PEB	CHA-C1B	3.48	1.48	1.40
29	HO	202	PEB	CHA-C1B	3.48	1.48	1.40
29	V1	201	PEB	CHA-C1B	3.47	1.48	1.40
29	VK	201	PEB	CHA-C1B	3.47	1.48	1.40
29	T2	201	PEB	C1A-NA	-3.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JB	203	PEB	C2C-C3C	3.47	1.48	1.37
29	ZB	203	PEB	C2C-C3C	3.47	1.48	1.37
29	JM	203	PEB	C2C-C3C	3.47	1.48	1.37
29	ZM	203	PEB	C2C-C3C	3.47	1.48	1.37
31	lP	1001	CYC	C2C-C1C	-3.47	1.49	1.52
29	J7	1002	PEB	C1A-NA	-3.47	1.33	1.37
29	QB	204	PEB	C1A-NA	-3.47	1.33	1.37
29	QM	204	PEB	C1A-NA	-3.47	1.33	1.37
29	A7	305	PEB	C2C-C3C	3.47	1.48	1.37
29	A9	305	PEB	C2C-C3C	3.47	1.48	1.37
29	PB	202	PEB	C2C-C3C	3.47	1.48	1.37
29	rJ	203	PEB	C2C-C3C	3.47	1.48	1.37
29	rL	203	PEB	C2C-C3C	3.47	1.48	1.37
29	PM	202	PEB	C2C-C3C	3.47	1.48	1.37
31	eP	1001	CYC	C2C-C1C	-3.47	1.49	1.52
29	R2	203	PEB	C1A-NA	-3.47	1.33	1.37
29	RR	203	PEB	C1A-NA	-3.47	1.33	1.37
29	tJ	202	PEB	C2C-C3C	3.47	1.48	1.37
29	tL	202	PEB	C2C-C3C	3.47	1.48	1.37
29	F3	202	PEB	CHA-C1B	3.47	1.48	1.40
29	FO	202	PEB	CHA-C1B	3.47	1.48	1.40
31	RP	1001	CYC	C3D-C2D	3.47	1.48	1.37
29	IB	201	PEB	CHA-C1B	3.47	1.48	1.40
29	IM	201	PEB	CHA-C1B	3.47	1.48	1.40
31	GF	1001	CYC	C2C-C1C	-3.47	1.49	1.52
31	GI	1001	CYC	C2C-C1C	-3.47	1.49	1.52
29	D3	202	PEB	CHA-C1B	3.47	1.48	1.40
29	kB	203	PEB	C2C-C3C	3.47	1.48	1.37
29	kM	203	PEB	C2C-C3C	3.47	1.48	1.37
29	MB	201	PEB	CHA-C1B	3.47	1.48	1.40
29	MM	201	PEB	CHA-C1B	3.47	1.48	1.40
29	VB	203	PEB	C2C-C3C	3.47	1.48	1.37
29	ZJ	203	PEB	C2C-C3C	3.47	1.48	1.37
29	ZL	203	PEB	C2C-C3C	3.47	1.48	1.37
29	VM	203	PEB	C2C-C3C	3.47	1.48	1.37
29	iB	201	PEB	C1A-NA	-3.47	1.33	1.37
29	WJ	203	PEB	C1A-NA	-3.47	1.33	1.37
29	WL	203	PEB	C1A-NA	-3.47	1.33	1.37
29	iM	201	PEB	C1A-NA	-3.47	1.33	1.37
29	MQ	407	PEB	C1A-NA	-3.47	1.33	1.37
29	k7	202	PEB	CHA-C1B	3.47	1.48	1.40
29	k9	202	PEB	CHA-C1B	3.47	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	m1	201	PEB	CHA-C1B	3.47	1.48	1.40
29	AG	202	PEB	CHA-C1B	3.47	1.48	1.40
29	mK	201	PEB	CHA-C1B	3.47	1.48	1.40
29	AQ	202	PEB	CHA-C1B	3.47	1.48	1.40
29	F3	202	PEB	C1A-NA	-3.47	1.33	1.37
29	FO	202	PEB	C1A-NA	-3.47	1.33	1.37
29	G3	201	PEB	CHA-C1B	3.47	1.48	1.40
29	GO	201	PEB	CHA-C1B	3.47	1.48	1.40
29	FJ	203	PEB	C2C-C3C	3.47	1.47	1.37
29	FL	203	PEB	C2C-C3C	3.47	1.47	1.37
29	R2	201	PEB	CHA-C1B	3.47	1.48	1.40
29	MN	404	PEB	CHA-C1B	3.47	1.48	1.40
29	cB	203	PEB	C2C-C3C	3.47	1.47	1.37
29	cM	203	PEB	C2C-C3C	3.47	1.47	1.37
29	V2	201	PEB	C1A-NA	-3.47	1.33	1.37
29	XR	201	PEB	C1A-NA	-3.47	1.33	1.37
29	N2	201	PEB	CHA-C1B	3.47	1.48	1.40
31	JP	1001	CYC	C2C-C1C	-3.47	1.49	1.52
29	R2	201	PEB	C1A-NA	-3.47	1.33	1.37
29	NB	201	PEB	C1A-NA	-3.47	1.33	1.37
29	NM	201	PEB	C1A-NA	-3.47	1.33	1.37
29	RR	201	PEB	C1A-NA	-3.47	1.33	1.37
29	V2	203	PEB	C1A-NA	-3.47	1.33	1.37
29	kB	201	PEB	C1A-NA	-3.47	1.33	1.37
29	kM	201	PEB	C1A-NA	-3.47	1.33	1.37
31	mP	1001	CYC	C3D-C2D	3.47	1.47	1.37
29	a1	201	PEB	CHA-C1B	3.47	1.48	1.40
29	k1	201	PEB	CHA-C1B	3.47	1.48	1.40
29	aK	201	PEB	CHA-C1B	3.47	1.48	1.40
29	kK	201	PEB	CHA-C1B	3.47	1.48	1.40
29	MR	202	PEB	CHA-C1B	3.47	1.48	1.40
29	Y1	201	PEB	CHA-C1B	3.46	1.48	1.40
29	aF	201	PEB	CHA-C1B	3.46	1.48	1.40
29	aI	201	PEB	CHA-C1B	3.46	1.48	1.40
29	YK	201	PEB	CHA-C1B	3.46	1.48	1.40
29	IJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	IL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	hJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	hL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	CB	201	PEB	CHA-C1B	3.46	1.48	1.40
29	CM	201	PEB	CHA-C1B	3.46	1.48	1.40
31	EP	1001	CYC	C3D-C2D	3.46	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A3	202	PEB	C1A-NA	-3.46	1.33	1.37
29	AO	202	PEB	C1A-NA	-3.46	1.33	1.37
29	SB	201	PEB	CHA-C1B	3.46	1.48	1.40
29	SM	201	PEB	CHA-C1B	3.46	1.48	1.40
31	PP	1001	CYC	C3D-C2D	3.46	1.47	1.37
29	nJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	nL	203	PEB	C2C-C3C	3.46	1.47	1.37
31	D7	1001	CYC	C2C-C1C	-3.46	1.49	1.52
31	D9	1001	CYC	C2C-C1C	-3.46	1.49	1.52
29	KB	202	PEB	C1A-NA	-3.46	1.33	1.37
29	KM	202	PEB	C1A-NA	-3.46	1.33	1.37
29	mB	203	PEB	C2C-C3C	3.46	1.47	1.37
29	mM	203	PEB	C2C-C3C	3.46	1.47	1.37
29	LG	202	PEB	CHA-C1B	3.46	1.48	1.40
29	LQ	201	PEB	CHA-C1B	3.46	1.48	1.40
29	TB	203	PEB	C2C-C3C	3.46	1.47	1.37
29	TM	203	PEB	C2C-C3C	3.46	1.47	1.37
29	K5	202	PEB	C1A-NA	-3.46	1.33	1.37
29	K8	202	PEB	C1A-NA	-3.46	1.33	1.37
29	fB	202	PEB	C1A-NA	-3.46	1.33	1.37
29	mJ	202	PEB	C1A-NA	-3.46	1.33	1.37
29	mL	202	PEB	C1A-NA	-3.46	1.33	1.37
29	fM	202	PEB	C1A-NA	-3.46	1.33	1.37
29	RJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	RL	203	PEB	C2C-C3C	3.46	1.47	1.37
31	NP	1001	CYC	C3D-C2D	3.46	1.47	1.37
29	jB	201	PEB	C2C-C3C	3.46	1.47	1.37
29	fJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	jJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	fL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	jL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	jM	201	PEB	C2C-C3C	3.46	1.47	1.37
31	gP	1001	CYC	C3D-C2D	3.46	1.47	1.37
29	H5	202	PEB	CHA-C1B	3.46	1.48	1.40
29	m7	202	PEB	CHA-C1B	3.46	1.48	1.40
29	m9	202	PEB	CHA-C1B	3.46	1.48	1.40
29	TJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	TL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	e2	402	PEB	CHA-C1B	3.46	1.48	1.40
29	P7	202	PEB	CHA-C1B	3.46	1.48	1.40
29	P9	202	PEB	CHA-C1B	3.46	1.48	1.40
29	VJ	202	PEB	C2C-C3C	3.46	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VL	202	PEB	C2C-C3C	3.46	1.47	1.37
29	GB	202	PEB	C1A-NA	-3.46	1.33	1.37
29	GM	202	PEB	C1A-NA	-3.46	1.33	1.37
29	XJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	XL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	xL	303	PEB	C2C-C3C	3.46	1.47	1.37
29	IJ	202	PEB	C1A-NA	-3.46	1.33	1.37
29	IL	202	PEB	C1A-NA	-3.46	1.33	1.37
29	vJ	202	PEB	C2C-C3C	3.46	1.47	1.37
29	vL	202	PEB	C2C-C3C	3.46	1.47	1.37
29	N3	201	PEB	C2A-C1A	-3.46	1.49	1.52
29	JJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	pJ	203	PEB	C2C-C3C	3.46	1.47	1.37
29	JL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	pL	203	PEB	C2C-C3C	3.46	1.47	1.37
29	NB	202	PEB	C2C-C3C	3.46	1.47	1.37
29	NM	202	PEB	C2C-C3C	3.46	1.47	1.37
31	M7	1001	CYC	CHB-C4A	3.46	1.48	1.40
29	DJ	202	PEB	C2C-C3C	3.46	1.47	1.37
29	DL	202	PEB	C2C-C3C	3.46	1.47	1.37
29	B5	202	PEB	C1A-NA	-3.46	1.33	1.37
29	ZB	201	PEB	C1A-NA	-3.46	1.33	1.37
29	ZM	201	PEB	C1A-NA	-3.46	1.33	1.37
31	iP	1001	CYC	C2C-C1C	-3.46	1.49	1.52
29	gB	203	PEB	C2C-C3C	3.46	1.47	1.37
29	gM	203	PEB	C2C-C3C	3.46	1.47	1.37
29	xJ	303	PEB	C2C-C3C	3.46	1.47	1.37
29	xL	302	PEB	C2C-C3C	3.46	1.47	1.37
29	XR	201	PEB	CHA-C1B	3.46	1.48	1.40
29	N1	1002	PEB	C1A-NA	-3.46	1.33	1.37
29	CG	202	PEB	CHA-C1B	3.46	1.48	1.40
29	CQ	202	PEB	CHA-C1B	3.46	1.48	1.40
31	JP	1001	CYC	C3D-C2D	3.46	1.47	1.37
29	WB	201	PEB	CHA-C1B	3.46	1.48	1.40
29	WM	201	PEB	CHA-C1B	3.46	1.48	1.40
29	e1	201	PEB	CHA-C1B	3.45	1.48	1.40
29	RF	201	PEB	CHA-C1B	3.45	1.48	1.40
29	RI	201	PEB	CHA-C1B	3.45	1.48	1.40
29	eK	201	PEB	CHA-C1B	3.45	1.48	1.40
29	B3	202	PEB	C1A-NA	-3.45	1.33	1.37
29	K3	202	PEB	C1A-NA	-3.45	1.33	1.37
29	FB	201	PEB	C1A-NA	-3.45	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	cJ	202	PEB	C1A-NA	-3.45	1.33	1.37
29	cL	202	PEB	C1A-NA	-3.45	1.33	1.37
29	FM	201	PEB	C1A-NA	-3.45	1.33	1.37
29	BO	202	PEB	C1A-NA	-3.45	1.33	1.37
29	KO	202	PEB	C1A-NA	-3.45	1.33	1.37
29	PJ	203	PEB	C2C-C3C	3.45	1.47	1.37
29	PL	203	PEB	C2C-C3C	3.45	1.47	1.37
29	IB	201	PEB	CHA-C1B	3.45	1.48	1.40
29	IM	201	PEB	CHA-C1B	3.45	1.48	1.40
29	iB	203	PEB	C2C-C3C	3.45	1.47	1.37
29	iM	203	PEB	C2C-C3C	3.45	1.47	1.37
29	N2	201	PEB	C1A-NA	-3.45	1.33	1.37
29	MG	405	PEB	C1A-NA	-3.45	1.33	1.37
29	LB	203	PEB	C2C-C3C	3.45	1.47	1.37
29	LM	203	PEB	C2C-C3C	3.45	1.47	1.37
29	X2	202	PEB	C1A-NA	-3.45	1.33	1.37
29	XR	203	PEB	C1A-NA	-3.45	1.33	1.37
29	c1	201	PEB	CHA-C1B	3.45	1.48	1.40
29	cK	201	PEB	CHA-C1B	3.45	1.48	1.40
29	XB	202	PEB	C2C-C3C	3.45	1.47	1.37
29	XM	202	PEB	C2C-C3C	3.45	1.47	1.37
31	iP	1001	CYC	C3D-C2D	3.45	1.47	1.37
29	P1	201	PEB	CHA-C1B	3.45	1.48	1.40
29	PK	201	PEB	CHA-C1B	3.45	1.48	1.40
29	EC	201	PEB	C1A-NA	-3.45	1.33	1.37
29	EE	201	PEB	C1A-NA	-3.45	1.33	1.37
31	AP	1001	CYC	C3D-C2D	3.45	1.47	1.37
31	rP	1001	CYC	C3D-C2D	3.45	1.47	1.37
29	VF	201	PEB	CHA-C1B	3.45	1.48	1.40
29	VI	201	PEB	CHA-C1B	3.45	1.48	1.40
29	A1	302	PEB	C1A-NA	-3.45	1.33	1.37
29	AK	302	PEB	C1A-NA	-3.45	1.33	1.37
29	NO	202	PEB	C2C-C3C	3.45	1.47	1.37
29	T7	202	PEB	CHA-C1B	3.45	1.48	1.40
29	a7	202	PEB	CHA-C1B	3.45	1.48	1.40
29	T9	202	PEB	CHA-C1B	3.45	1.48	1.40
29	a9	202	PEB	CHA-C1B	3.45	1.48	1.40
29	LJ	202	PEB	C2C-C3C	3.45	1.47	1.37
29	LL	202	PEB	C2C-C3C	3.45	1.47	1.37
29	Y7	202	PEB	CHA-C1B	3.45	1.48	1.40
29	Y9	202	PEB	CHA-C1B	3.45	1.48	1.40
29	GG	202	PEB	CHA-C1B	3.45	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GQ	202	PEB	CHA-C1B	3.45	1.48	1.40
29	hB	202	PEB	C1A-NA	-3.45	1.33	1.37
29	hM	202	PEB	C1A-NA	-3.45	1.33	1.37
29	BG	202	PEB	CHA-C1B	3.45	1.48	1.40
29	BQ	202	PEB	CHA-C1B	3.45	1.48	1.40
29	D7	1002	PEB	C1A-NA	-3.45	1.33	1.37
29	D9	1002	PEB	C1A-NA	-3.45	1.33	1.37
29	WR	201	PEB	C2A-C1A	-3.45	1.49	1.52
29	RB	203	PEB	C2C-C3C	3.45	1.47	1.37
29	NJ	203	PEB	C2C-C3C	3.45	1.47	1.37
29	NL	203	PEB	C2C-C3C	3.45	1.47	1.37
29	RM	203	PEB	C2C-C3C	3.45	1.47	1.37
29	mF	201	PEB	CHA-C1B	3.45	1.48	1.40
29	mI	201	PEB	CHA-C1B	3.45	1.48	1.40
29	J3	202	PEB	C1A-NA	-3.45	1.33	1.37
29	IB	202	PEB	C1A-NA	-3.45	1.33	1.37
29	zL	501	PEB	C1A-NA	-3.45	1.33	1.37
29	IM	202	PEB	C1A-NA	-3.45	1.33	1.37
29	JO	202	PEB	C1A-NA	-3.45	1.33	1.37
29	W1	202	PEB	C2C-C3C	3.45	1.47	1.37
29	NB	201	PEB	C2C-C3C	3.45	1.47	1.37
29	WK	202	PEB	C2C-C3C	3.45	1.47	1.37
29	NM	201	PEB	C2C-C3C	3.45	1.47	1.37
29	QR	201	PEB	C2A-C1A	-3.45	1.49	1.52
29	HJ	202	PEB	C2C-C3C	3.45	1.47	1.37
29	HL	202	PEB	C2C-C3C	3.45	1.47	1.37
31	KP	1001	CYC	C3D-C2D	3.45	1.47	1.37
29	HG	202	PEB	CHA-C1B	3.45	1.48	1.40
29	HQ	202	PEB	CHA-C1B	3.45	1.48	1.40
29	C3	201	PEB	CHA-C1B	3.45	1.48	1.40
29	CO	201	PEB	CHA-C1B	3.45	1.48	1.40
31	K7	1001	CYC	CHB-C4A	3.45	1.48	1.40
31	L9	1001	CYC	CHB-C4A	3.45	1.48	1.40
31	M9	1001	CYC	CHB-C4A	3.45	1.48	1.40
31	IP	1001	CYC	C3D-C2D	3.45	1.47	1.37
31	E7	1001	CYC	CHB-C4A	3.45	1.48	1.40
31	E9	1001	CYC	CHB-C4A	3.45	1.48	1.40
29	MA	401	PEB	CHA-C1B	3.45	1.48	1.40
29	VB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	WB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	VM	201	PEB	C2C-C3C	3.44	1.47	1.37
29	WM	201	PEB	C2C-C3C	3.44	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B5	202	PEB	CHA-C1B	3.44	1.48	1.40
29	OR	202	PEB	CHA-C1B	3.44	1.48	1.40
29	MQ	407	PEB	C2C-C3C	3.44	1.47	1.37
29	g1	201	PEB	CHA-C1B	3.44	1.48	1.40
29	gK	201	PEB	CHA-C1B	3.44	1.48	1.40
29	bJ	203	PEB	C2C-C3C	3.44	1.47	1.37
29	bL	203	PEB	C2C-C3C	3.44	1.47	1.37
29	I5	202	PEB	CHA-C1B	3.44	1.48	1.40
29	e7	202	PEB	CHA-C1B	3.44	1.48	1.40
29	I8	202	PEB	CHA-C1B	3.44	1.48	1.40
29	e9	202	PEB	CHA-C1B	3.44	1.48	1.40
29	WR	202	PEB	C2C-C3C	3.44	1.47	1.37
29	i7	202	PEB	CHA-C1B	3.44	1.48	1.40
29	i9	202	PEB	CHA-C1B	3.44	1.48	1.40
29	IG	202	PEB	CHA-C1B	3.44	1.48	1.40
29	IQ	202	PEB	CHA-C1B	3.44	1.48	1.40
29	Q2	201	PEB	C2A-C1A	-3.44	1.49	1.52
29	dB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	BJ	203	PEB	C2C-C3C	3.44	1.47	1.37
29	BL	203	PEB	C2C-C3C	3.44	1.47	1.37
29	dM	201	PEB	C2C-C3C	3.44	1.47	1.37
29	DO	202	PEB	CHA-C1B	3.44	1.48	1.40
29	IC	201	PEB	C1A-NA	-3.44	1.33	1.37
29	IE	201	PEB	C1A-NA	-3.44	1.33	1.37
29	FB	203	PEB	C2C-C3C	3.44	1.47	1.37
29	FM	203	PEB	C2C-C3C	3.44	1.47	1.37
31	TP	1001	CYC	C3D-C2D	3.44	1.47	1.37
29	C5	202	PEB	CHA-C1B	3.44	1.48	1.40
29	g7	202	PEB	CHA-C1B	3.44	1.48	1.40
29	C8	202	PEB	CHA-C1B	3.44	1.48	1.40
29	g9	202	PEB	CHA-C1B	3.44	1.48	1.40
29	B8	202	PEB	C1A-NA	-3.44	1.33	1.37
29	IA	202	PEB	C1A-NA	-3.44	1.33	1.37
29	IN	202	PEB	C1A-NA	-3.44	1.33	1.37
29	l1	202	PEB	C2C-C3C	3.44	1.47	1.37
29	N3	202	PEB	C2C-C3C	3.44	1.47	1.37
29	lK	202	PEB	C2C-C3C	3.44	1.47	1.37
29	HK	1002	PEB	C1A-NA	-3.44	1.33	1.37
29	gF	201	PEB	CHA-C1B	3.44	1.48	1.40
29	gI	201	PEB	CHA-C1B	3.44	1.48	1.40
31	CP	1001	CYC	C3D-C2D	3.44	1.47	1.37
29	VR	201	PEB	C1A-NA	-3.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	xJ	302	PEB	C2C-C3C	3.44	1.47	1.37
29	jB	201	PEB	CHA-C1B	3.44	1.48	1.40
29	jM	201	PEB	CHA-C1B	3.44	1.48	1.40
29	GA	202	PEB	C1A-NA	-3.44	1.33	1.37
29	AF	301	PEB	C1A-NA	-3.44	1.33	1.37
29	AI	301	PEB	C1A-NA	-3.44	1.33	1.37
29	GN	202	PEB	C1A-NA	-3.44	1.33	1.37
29	mB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	IG	201	PEB	C2C-C3C	3.44	1.47	1.37
29	mM	201	PEB	C2C-C3C	3.44	1.47	1.37
29	IQ	201	PEB	C2C-C3C	3.44	1.47	1.37
29	EG	201	PEB	C2C-C3C	3.44	1.47	1.37
29	EQ	201	PEB	C2C-C3C	3.44	1.47	1.37
29	c7	202	PEB	CHA-C1B	3.44	1.48	1.40
29	c9	202	PEB	CHA-C1B	3.44	1.48	1.40
29	M2	202	PEB	C2C-C3C	3.44	1.47	1.37
29	E3	202	PEB	C1A-NA	-3.44	1.33	1.37
29	EO	202	PEB	C1A-NA	-3.44	1.33	1.37
29	YB	202	PEB	CHA-C1B	3.44	1.48	1.40
29	YM	202	PEB	CHA-C1B	3.44	1.48	1.40
29	KA	202	PEB	C1A-NA	-3.44	1.33	1.37
29	EB	202	PEB	C1A-NA	-3.44	1.33	1.37
29	EM	202	PEB	C1A-NA	-3.44	1.33	1.37
29	KN	202	PEB	C1A-NA	-3.44	1.33	1.37
29	IB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	CG	201	PEB	C2C-C3C	3.44	1.47	1.37
29	IM	201	PEB	C2C-C3C	3.44	1.47	1.37
29	CQ	201	PEB	C2C-C3C	3.44	1.47	1.37
31	eP	1001	CYC	C3D-C2D	3.44	1.47	1.37
29	eB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	eM	201	PEB	C2C-C3C	3.44	1.47	1.37
29	kF	201	PEB	CHA-C1B	3.44	1.48	1.40
29	kI	201	PEB	CHA-C1B	3.44	1.48	1.40
29	KB	201	PEB	C2C-C3C	3.44	1.47	1.37
29	KM	201	PEB	C2C-C3C	3.44	1.47	1.37
29	eJ	201	PEB	CHA-C1B	3.43	1.48	1.40
29	eL	201	PEB	CHA-C1B	3.43	1.48	1.40
29	GB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	GM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	jB	202	PEB	C1A-NA	-3.43	1.33	1.37
29	jM	202	PEB	C1A-NA	-3.43	1.33	1.37
29	N3	203	PEB	C2A-C1A	-3.43	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EG	202	PEB	CHA-C1B	3.43	1.48	1.40
29	EQ	202	PEB	CHA-C1B	3.43	1.48	1.40
29	MG	405	PEB	C2C-C3C	3.43	1.47	1.37
29	OB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	OM	201	PEB	C2C-C3C	3.43	1.47	1.37
31	GP	1001	CYC	C3D-C2D	3.43	1.47	1.37
29	UB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	UM	201	PEB	C2C-C3C	3.43	1.47	1.37
31	I1	1001	CYC	CHB-C4A	3.43	1.48	1.40
29	F7	1002	PEB	CHA-C1B	3.43	1.48	1.40
29	EB	201	PEB	CHA-C1B	3.43	1.48	1.40
29	EM	201	PEB	CHA-C1B	3.43	1.48	1.40
31	MF	1001	CYC	C3D-C2D	3.43	1.47	1.37
31	MI	1001	CYC	C3D-C2D	3.43	1.47	1.37
29	M3	201	PEB	C2C-C3C	3.43	1.47	1.37
29	MO	201	PEB	C2C-C3C	3.43	1.47	1.37
29	hB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	hM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	W2	202	PEB	C2C-C3C	3.43	1.47	1.37
31	G9	1001	CYC	CHB-C4A	3.43	1.48	1.40
29	DB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	DM	201	PEB	C2C-C3C	3.43	1.47	1.37
31	D1	1003	CYC	CHB-C4A	3.43	1.48	1.40
31	I7	1001	CYC	CHB-C4A	3.43	1.48	1.40
31	I9	1001	CYC	CHB-C4A	3.43	1.48	1.40
29	FB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	HC	203	PEB	C2C-C3C	3.43	1.47	1.37
29	HE	203	PEB	C2C-C3C	3.43	1.47	1.37
29	FM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	BA	201	PEB	C2C-C3C	3.43	1.47	1.37
29	BN	201	PEB	C2C-C3C	3.43	1.47	1.37
29	M3	202	PEB	C2C-C3C	3.43	1.47	1.37
29	KG	201	PEB	C2C-C3C	3.43	1.47	1.37
29	MO	202	PEB	C2C-C3C	3.43	1.47	1.37
29	KQ	201	PEB	C2C-C3C	3.43	1.47	1.37
29	EA	202	PEB	C1A-NA	-3.43	1.33	1.37
29	EN	202	PEB	C1A-NA	-3.43	1.33	1.37
29	V7	202	PEB	CHA-C1B	3.43	1.48	1.40
29	V9	202	PEB	CHA-C1B	3.43	1.48	1.40
29	aB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	aM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	LA	203	PEB	C1A-NA	-3.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LN	203	PEB	C1A-NA	-3.43	1.33	1.37
29	YB	202	PEB	C2C-C3C	3.43	1.47	1.37
29	YM	202	PEB	C2C-C3C	3.43	1.47	1.37
29	JB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	LB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	JM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	LM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	U1	203	PEB	C2C-C3C	3.43	1.47	1.37
29	MB	201	PEB	C2C-C3C	3.43	1.47	1.37
29	AG	201	PEB	C2C-C3C	3.43	1.47	1.37
29	UK	203	PEB	C2C-C3C	3.43	1.47	1.37
29	MM	201	PEB	C2C-C3C	3.43	1.47	1.37
29	AQ	201	PEB	C2C-C3C	3.43	1.47	1.37
29	N7	1002	PEB	C1A-NA	-3.43	1.33	1.37
29	N9	1002	PEB	C1A-NA	-3.43	1.33	1.37
30	AB	305	PUB	C3B-C2B	3.42	1.47	1.37
29	L9	1002	PEB	C1A-NA	-3.42	1.33	1.37
31	H7	1001	CYC	C2C-C1C	-3.42	1.49	1.52
31	H9	1001	CYC	C2C-C1C	-3.42	1.49	1.52
29	XB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	AM	302	PEB	C2C-C3C	3.42	1.47	1.37
29	XM	201	PEB	C2C-C3C	3.42	1.47	1.37
29	MR	202	PEB	C1A-NA	-3.42	1.33	1.37
29	GJ	201	PEB	CHA-C1B	3.42	1.48	1.40
29	GL	201	PEB	CHA-C1B	3.42	1.48	1.40
29	T1	201	PEB	CHA-C1B	3.42	1.48	1.40
29	cF	201	PEB	CHA-C1B	3.42	1.48	1.40
29	cI	201	PEB	CHA-C1B	3.42	1.48	1.40
29	oJ	201	PEB	CHA-C1B	3.42	1.48	1.40
29	TK	201	PEB	CHA-C1B	3.42	1.48	1.40
29	oL	201	PEB	CHA-C1B	3.42	1.48	1.40
29	L7	1002	PEB	C1A-NA	-3.42	1.33	1.37
29	H7	1002	PEB	CHA-C1B	3.42	1.48	1.40
29	H9	1002	PEB	CHA-C1B	3.42	1.48	1.40
29	SJ	201	PEB	CHA-C1B	3.42	1.48	1.40
29	SL	201	PEB	CHA-C1B	3.42	1.48	1.40
29	R1	201	PEB	CHA-C1B	3.42	1.48	1.40
29	RK	201	PEB	CHA-C1B	3.42	1.48	1.40
29	b1	202	PEB	C2C-C3C	3.42	1.47	1.37
29	cB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	bK	202	PEB	C2C-C3C	3.42	1.47	1.37
29	cM	201	PEB	C2C-C3C	3.42	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	MJ	201	PEB	CHA-C1B	3.42	1.48	1.40
29	ML	201	PEB	CHA-C1B	3.42	1.48	1.40
31	L7	1001	CYC	CHB-C4A	3.42	1.48	1.40
31	CK	1001	CYC	CHB-C4A	3.42	1.48	1.40
29	j1	202	PEB	C2C-C3C	3.42	1.47	1.37
29	jK	202	PEB	C2C-C3C	3.42	1.47	1.37
29	P1	203	PEB	C2A-C1A	-3.42	1.49	1.52
29	PK	203	PEB	C2A-C1A	-3.42	1.49	1.52
31	J9	1001	CYC	CHB-C4A	3.42	1.48	1.40
29	h1	202	PEB	C2C-C3C	3.42	1.47	1.37
29	hK	202	PEB	C2C-C3C	3.42	1.47	1.37
29	fB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	fM	201	PEB	C2C-C3C	3.42	1.47	1.37
29	D7	1002	PEB	CHA-C1B	3.42	1.48	1.40
29	D9	1002	PEB	CHA-C1B	3.42	1.48	1.40
29	Q1	202	PEB	C2C-C3C	3.42	1.47	1.37
29	wJ	302	PEB	C2C-C3C	3.42	1.47	1.37
29	QK	202	PEB	C2C-C3C	3.42	1.47	1.37
31	IF	1001	CYC	C3D-C2D	3.42	1.47	1.37
31	II	1001	CYC	C3D-C2D	3.42	1.47	1.37
29	N3	201	PEB	C2C-C3C	3.42	1.47	1.37
29	SB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	ZB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	SM	201	PEB	C2C-C3C	3.42	1.47	1.37
29	ZM	201	PEB	C2C-C3C	3.42	1.47	1.37
31	J7	1001	CYC	C2C-C1C	-3.42	1.49	1.52
29	HB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	HM	201	PEB	C2C-C3C	3.42	1.47	1.37
31	K1	1001	CYC	CHB-C4A	3.42	1.48	1.40
31	KK	1001	CYC	CHB-C4A	3.42	1.48	1.40
29	GG	201	PEB	C2C-C3C	3.42	1.47	1.37
29	GQ	201	PEB	C2C-C3C	3.42	1.47	1.37
31	AP	1001	CYC	C2C-C1C	-3.42	1.49	1.52
29	FC	203	PEB	C2C-C3C	3.42	1.47	1.37
29	FE	203	PEB	C2C-C3C	3.42	1.47	1.37
30	AM	305	PUB	C3B-C2B	3.42	1.47	1.37
29	uJ	202	PEB	CHA-C1B	3.42	1.48	1.40
29	uL	202	PEB	CHA-C1B	3.42	1.48	1.40
29	A5	202	PEB	CHA-C1B	3.42	1.48	1.40
29	L7	1002	PEB	CHA-C1B	3.42	1.48	1.40
29	A8	202	PEB	CHA-C1B	3.42	1.48	1.40
31	G7	1001	CYC	CHB-C4A	3.42	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EB	201	PEB	C2C-C3C	3.42	1.47	1.37
29	EM	201	PEB	C2C-C3C	3.42	1.47	1.37
29	HA	203	PEB	C1A-NA	-3.42	1.33	1.37
29	HN	203	PEB	C1A-NA	-3.42	1.33	1.37
29	JC	202	PEB	C2C-C3C	3.42	1.47	1.37
29	JE	202	PEB	C2C-C3C	3.42	1.47	1.37
29	RB	201	PEB	C2C-C3C	3.41	1.47	1.37
29	kB	201	PEB	C2C-C3C	3.41	1.47	1.37
29	RM	201	PEB	C2C-C3C	3.41	1.47	1.37
29	kM	201	PEB	C2C-C3C	3.41	1.47	1.37
31	E1	1001	CYC	CHB-C4A	3.41	1.48	1.40
29	DA	201	PEB	C2C-C3C	3.41	1.47	1.37
29	DN	201	PEB	C2C-C3C	3.41	1.47	1.37
29	f1	202	PEB	C2C-C3C	3.41	1.47	1.37
29	fK	202	PEB	C2C-C3C	3.41	1.47	1.37
29	NO	201	PEB	C2A-C1A	-3.41	1.49	1.52
31	K9	1001	CYC	CHB-C4A	3.41	1.48	1.40
29	LA	201	PEB	C2C-C3C	3.41	1.47	1.37
29	LN	201	PEB	C2C-C3C	3.41	1.47	1.37
29	TI	201	PEB	CHA-C1B	3.41	1.48	1.40
31	KI	1001	CYC	C3D-C2D	3.41	1.47	1.37
29	i1	201	PEB	CHA-C1B	3.41	1.48	1.40
29	iK	201	PEB	CHA-C1B	3.41	1.48	1.40
29	a1	203	PEB	C2A-C1A	-3.41	1.49	1.52
29	aK	203	PEB	C2A-C1A	-3.41	1.49	1.52
29	JA	201	PEB	C2C-C3C	3.41	1.47	1.37
29	iB	201	PEB	C2C-C3C	3.41	1.47	1.37
29	iM	201	PEB	C2C-C3C	3.41	1.47	1.37
29	JN	201	PEB	C2C-C3C	3.41	1.47	1.37
31	M1	1001	CYC	CHB-C4A	3.41	1.48	1.40
31	MK	1001	CYC	CHB-C4A	3.41	1.48	1.40
29	GB	202	PEB	C2C-C3C	3.41	1.47	1.37
29	GM	202	PEB	C2C-C3C	3.41	1.47	1.37
31	IK	1001	CYC	CHB-C4A	3.41	1.48	1.40
29	LC	203	PEB	C2C-C3C	3.41	1.47	1.37
29	LE	203	PEB	C2C-C3C	3.41	1.47	1.37
29	CB	201	PEB	C2C-C3C	3.41	1.47	1.37
29	CM	201	PEB	C2C-C3C	3.41	1.47	1.37
29	eF	201	PEB	CHA-C1B	3.41	1.48	1.40
29	eI	201	PEB	CHA-C1B	3.41	1.48	1.40
29	mJ	201	PEB	CHA-C1B	3.41	1.48	1.40
29	mL	201	PEB	CHA-C1B	3.41	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	1001	CYC	CHB-C4A	3.41	1.48	1.40
31	N7	1001	CYC	CHB-C4A	3.41	1.48	1.40
31	N9	1001	CYC	CHB-C4A	3.41	1.48	1.40
31	GK	1001	CYC	CHB-C4A	3.41	1.48	1.40
31	J7	1001	CYC	CHB-C4A	3.41	1.48	1.40
29	KB	202	PEB	C2C-C3C	3.41	1.47	1.37
29	gB	201	PEB	C2C-C3C	3.41	1.47	1.37
29	KM	202	PEB	C2C-C3C	3.41	1.47	1.37
29	gM	201	PEB	C2C-C3C	3.41	1.47	1.37
29	FA	203	PEB	C1A-NA	-3.41	1.33	1.37
29	FN	203	PEB	C1A-NA	-3.41	1.33	1.37
31	EK	1001	CYC	CHB-C4A	3.41	1.48	1.40
29	S2	202	PEB	C2C-C3C	3.41	1.47	1.37
29	AJ	201	PEB	CHA-C1B	3.41	1.48	1.40
29	AL	201	PEB	CHA-C1B	3.41	1.48	1.40
29	PF	201	PEB	CHA-C1B	3.41	1.48	1.40
29	PI	201	PEB	CHA-C1B	3.41	1.48	1.40
29	aB	202	PEB	C1A-NA	-3.41	1.33	1.37
29	aM	202	PEB	C1A-NA	-3.41	1.33	1.37
31	EF	1001	CYC	C3D-C2D	3.41	1.47	1.37
31	EI	1001	CYC	C3D-C2D	3.41	1.47	1.37
29	I3	203	PEB	C1A-NA	-3.41	1.33	1.37
29	IO	203	PEB	C1A-NA	-3.41	1.33	1.37
29	NO	201	PEB	C2C-C3C	3.41	1.47	1.37
29	iF	201	PEB	CHA-C1B	3.40	1.48	1.40
29	iI	201	PEB	CHA-C1B	3.40	1.48	1.40
29	U2	202	PEB	C2C-C3C	3.40	1.47	1.37
29	AB	302	PEB	C2C-C3C	3.40	1.47	1.37
29	I3	202	PEB	C1A-NA	-3.40	1.33	1.37
29	IO	202	PEB	C1A-NA	-3.40	1.33	1.37
29	O1	202	PEB	C2C-C3C	3.40	1.47	1.37
29	d1	202	PEB	C2C-C3C	3.40	1.47	1.37
29	OK	202	PEB	C2C-C3C	3.40	1.47	1.37
29	dK	202	PEB	C2C-C3C	3.40	1.47	1.37
29	PB	201	PEB	C2C-C3C	3.40	1.47	1.37
29	PM	201	PEB	C2C-C3C	3.40	1.47	1.37
29	Z1	203	PEB	C2C-C3C	3.40	1.47	1.37
29	Q2	202	PEB	C2C-C3C	3.40	1.47	1.37
29	ZK	203	PEB	C2C-C3C	3.40	1.47	1.37
31	CF	1001	CYC	C3D-C2D	3.40	1.47	1.37
31	CI	1001	CYC	C3D-C2D	3.40	1.47	1.37
29	YJ	201	PEB	CHA-C1B	3.40	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YL	201	PEB	CHA-C1B	3.40	1.48	1.40
29	AF	304	PEB	C2C-C3C	3.40	1.47	1.37
29	AI	304	PEB	C2C-C3C	3.40	1.47	1.37
29	H7	1002	PEB	C1A-NA	-3.40	1.33	1.37
29	H9	1002	PEB	C1A-NA	-3.40	1.33	1.37
29	KC	202	PEB	C1A-NA	-3.40	1.33	1.37
29	KE	202	PEB	C1A-NA	-3.40	1.33	1.37
29	IB	201	PEB	C2C-C3C	3.40	1.47	1.37
29	BC	203	PEB	C2C-C3C	3.40	1.47	1.37
29	BE	203	PEB	C2C-C3C	3.40	1.47	1.37
29	IM	201	PEB	C2C-C3C	3.40	1.47	1.37
29	Q1	202	PEB	CHA-C1B	3.40	1.48	1.40
29	QK	202	PEB	CHA-C1B	3.40	1.48	1.40
29	S1	202	PEB	C2C-C3C	3.40	1.47	1.37
29	SK	202	PEB	C2C-C3C	3.40	1.47	1.37
29	UR	202	PEB	C2C-C3C	3.40	1.47	1.37
29	HA	201	PEB	C2C-C3C	3.40	1.47	1.37
29	HN	201	PEB	C2C-C3C	3.40	1.47	1.37
30	A7	302	PUB	C3B-C2B	3.40	1.47	1.37
30	A9	302	PUB	C3B-C2B	3.40	1.47	1.37
29	EJ	201	PEB	CHA-C1B	3.40	1.48	1.40
29	EL	201	PEB	CHA-C1B	3.40	1.48	1.40
29	TB	201	PEB	C2C-C3C	3.40	1.47	1.37
29	TM	201	PEB	C2C-C3C	3.40	1.47	1.37
29	H3	202	PEB	C1A-NA	-3.40	1.33	1.37
29	HO	202	PEB	C1A-NA	-3.40	1.33	1.37
29	YB	203	PEB	C2C-C3C	3.40	1.47	1.37
29	YM	203	PEB	C2C-C3C	3.40	1.47	1.37
31	E1	1001	CYC	C3D-C2D	3.40	1.47	1.37
29	b1	202	PEB	CHA-C1B	3.40	1.48	1.40
29	J7	1002	PEB	CHA-C1B	3.40	1.48	1.40
29	bK	202	PEB	CHA-C1B	3.40	1.48	1.40
29	FA	201	PEB	C2C-C3C	3.40	1.47	1.37
29	FN	201	PEB	C2C-C3C	3.40	1.47	1.37
29	qJ	201	PEB	CHA-C1B	3.40	1.48	1.40
29	qL	201	PEB	CHA-C1B	3.40	1.48	1.40
29	jB	202	PEB	C2C-C3C	3.40	1.47	1.37
29	jM	202	PEB	C2C-C3C	3.40	1.47	1.37
29	j1	202	PEB	CHA-C1B	3.40	1.48	1.40
29	IJ	201	PEB	CHA-C1B	3.40	1.48	1.40
29	jK	202	PEB	CHA-C1B	3.40	1.48	1.40
29	IL	201	PEB	CHA-C1B	3.40	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K5	202	PEB	CHA-C1B	3.40	1.48	1.40
29	K8	202	PEB	CHA-C1B	3.40	1.48	1.40
31	D1	1003	CYC	C3D-C2D	3.40	1.47	1.37
31	IK	1001	CYC	C3D-C2D	3.40	1.47	1.37
29	YF	201	PEB	CHA-C1B	3.40	1.48	1.40
29	YI	201	PEB	CHA-C1B	3.40	1.48	1.40
29	WB	202	PEB	C2C-C3C	3.40	1.47	1.37
29	WM	202	PEB	C2C-C3C	3.40	1.47	1.37
29	C3	202	PEB	C1A-NA	-3.40	1.33	1.37
29	BA	203	PEB	C1A-NA	-3.40	1.33	1.37
29	BN	203	PEB	C1A-NA	-3.40	1.33	1.37
29	CO	202	PEB	C1A-NA	-3.40	1.33	1.37
29	wL	302	PEB	C2C-C3C	3.40	1.47	1.37
29	OJ	201	PEB	CHA-C1B	3.40	1.48	1.40
29	OL	201	PEB	CHA-C1B	3.40	1.48	1.40
31	D7	1001	CYC	CHB-C4A	3.40	1.48	1.40
31	D9	1001	CYC	CHB-C4A	3.40	1.48	1.40
29	F9	1002	PEB	CHA-C1B	3.39	1.48	1.40
29	QB	203	PEB	C2C-C3C	3.39	1.47	1.37
29	QB	204	PEB	C2C-C3C	3.39	1.47	1.37
29	QM	203	PEB	C2C-C3C	3.39	1.47	1.37
29	QM	204	PEB	C2C-C3C	3.39	1.47	1.37
29	KJ	201	PEB	CHA-C1B	3.39	1.48	1.40
29	KL	201	PEB	CHA-C1B	3.39	1.48	1.40
29	g1	203	PEB	C2A-C1A	-3.39	1.49	1.52
29	gK	203	PEB	C2A-C1A	-3.39	1.49	1.52
29	kJ	201	PEB	CHA-C1B	3.39	1.48	1.40
29	kL	201	PEB	CHA-C1B	3.39	1.48	1.40
31	WP	1001	CYC	C3D-C2D	3.39	1.47	1.37
29	S1	202	PEB	CHA-C1B	3.39	1.48	1.40
29	gJ	201	PEB	CHA-C1B	3.39	1.48	1.40
29	SK	202	PEB	CHA-C1B	3.39	1.48	1.40
29	gL	201	PEB	CHA-C1B	3.39	1.48	1.40
31	GF	1001	CYC	C3D-C2D	3.39	1.47	1.37
31	GI	1001	CYC	C3D-C2D	3.39	1.47	1.37
29	L9	1002	PEB	CHA-C1B	3.39	1.48	1.40
29	sJ	201	PEB	CHA-C1B	3.39	1.48	1.40
29	sL	201	PEB	CHA-C1B	3.39	1.48	1.40
29	DA	203	PEB	C1A-NA	-3.39	1.33	1.37
29	xL	303	PEB	C1A-NA	-3.39	1.33	1.37
29	DN	203	PEB	C1A-NA	-3.39	1.33	1.37
29	iJ	202	PEB	C2C-C3C	3.39	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	iL	202	PEB	C2C-C3C	3.39	1.47	1.37
29	O2	202	PEB	C2C-C3C	3.39	1.47	1.37
29	EB	202	PEB	C2C-C3C	3.39	1.47	1.37
29	EM	202	PEB	C2C-C3C	3.39	1.47	1.37
29	kJ	202	PEB	C2C-C3C	3.39	1.47	1.37
29	kL	202	PEB	C2C-C3C	3.39	1.47	1.37
31	J9	1001	CYC	C2C-C1C	-3.39	1.49	1.52
29	e2	402	PEB	C1A-NA	-3.39	1.33	1.37
31	F9	1001	CYC	CHB-C4A	3.39	1.48	1.40
31	KF	1001	CYC	C3D-C2D	3.39	1.47	1.37
29	AA	202	PEB	C1A-NA	-3.39	1.33	1.37
29	AN	202	PEB	C1A-NA	-3.39	1.33	1.37
29	SB	202	PEB	C2C-C3C	3.39	1.47	1.37
29	eJ	202	PEB	C2C-C3C	3.39	1.47	1.37
29	eL	202	PEB	C2C-C3C	3.39	1.47	1.37
29	SM	202	PEB	C2C-C3C	3.39	1.47	1.37
29	C3	201	PEB	C2C-C3C	3.39	1.47	1.37
29	oJ	202	PEB	C2C-C3C	3.39	1.47	1.37
29	oL	202	PEB	C2C-C3C	3.39	1.47	1.37
29	CO	201	PEB	C2C-C3C	3.39	1.47	1.37
29	QJ	201	PEB	CHA-C1B	3.39	1.48	1.40
29	QL	201	PEB	CHA-C1B	3.39	1.48	1.40
29	AM	301	PEB	C2C-C3C	3.39	1.47	1.37
29	cJ	202	PEB	C2C-C3C	3.39	1.47	1.37
29	cL	202	PEB	C2C-C3C	3.39	1.47	1.37
29	OJ	202	PEB	C2C-C3C	3.39	1.47	1.37
29	OL	202	PEB	C2C-C3C	3.39	1.47	1.37
31	H7	1001	CYC	CHB-C4A	3.39	1.48	1.40
31	H9	1001	CYC	CHB-C4A	3.39	1.48	1.40
29	P2	202	PEB	C2C-C3C	3.39	1.47	1.37
29	PR	202	PEB	C2C-C3C	3.39	1.47	1.37
29	QR	202	PEB	C2C-C3C	3.39	1.47	1.37
29	R2	203	PEB	C2C-C3C	3.38	1.47	1.37
29	RR	203	PEB	C2C-C3C	3.38	1.47	1.37
29	JA	203	PEB	C2C-C3C	3.38	1.47	1.37
29	JN	203	PEB	C2C-C3C	3.38	1.47	1.37
29	GG	202	PEB	C1A-NA	-3.38	1.33	1.37
29	GQ	202	PEB	C1A-NA	-3.38	1.33	1.37
29	U1	203	PEB	CHA-C1B	3.38	1.48	1.40
29	UK	203	PEB	CHA-C1B	3.38	1.48	1.40
29	CB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	CM	202	PEB	C2C-C3C	3.38	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d1	202	PEB	CHA-C1B	3.38	1.48	1.40
29	dK	202	PEB	CHA-C1B	3.38	1.48	1.40
29	J9	1002	PEB	CHA-C1B	3.38	1.48	1.40
29	h1	202	PEB	CHA-C1B	3.38	1.48	1.40
29	hK	202	PEB	CHA-C1B	3.38	1.48	1.40
29	hB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	hM	202	PEB	C2C-C3C	3.38	1.47	1.37
29	NR	203	PEB	C2C-C3C	3.38	1.47	1.37
29	KJ	202	PEB	C2C-C3C	3.38	1.47	1.37
29	KL	202	PEB	C2C-C3C	3.38	1.47	1.37
29	DC	202	PEB	C2C-C3C	3.38	1.47	1.37
29	DE	202	PEB	C2C-C3C	3.38	1.47	1.37
29	MJ	202	PEB	C2C-C3C	3.38	1.47	1.37
29	ML	202	PEB	C2C-C3C	3.38	1.47	1.37
29	JA	203	PEB	C1A-NA	-3.38	1.33	1.37
29	JN	203	PEB	C1A-NA	-3.38	1.33	1.37
29	OB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	OM	202	PEB	C2C-C3C	3.38	1.47	1.37
31	M1	1001	CYC	C3D-C2D	3.38	1.47	1.37
31	MK	1001	CYC	C3D-C2D	3.38	1.47	1.37
29	MN	405	PEB	C1A-NA	-3.38	1.33	1.37
29	W1	202	PEB	CHA-C1B	3.38	1.48	1.40
29	CJ	201	PEB	CHA-C1B	3.38	1.48	1.40
29	WK	202	PEB	CHA-C1B	3.38	1.48	1.40
29	CL	201	PEB	CHA-C1B	3.38	1.48	1.40
29	X2	202	PEB	C2C-C3C	3.38	1.47	1.37
29	XR	203	PEB	C2C-C3C	3.38	1.47	1.37
29	O2	201	PEB	C2A-C1A	-3.38	1.49	1.52
29	lB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	BG	202	PEB	C2C-C3C	3.38	1.47	1.37
29	lM	202	PEB	C2C-C3C	3.38	1.47	1.37
29	BQ	202	PEB	C2C-C3C	3.38	1.47	1.37
29	fB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	uJ	203	PEB	C2C-C3C	3.38	1.47	1.37
29	uL	203	PEB	C2C-C3C	3.38	1.47	1.37
29	fM	202	PEB	C2C-C3C	3.38	1.47	1.37
29	T1	202	PEB	C2A-C1A	-3.38	1.49	1.52
29	TK	202	PEB	C2A-C1A	-3.38	1.49	1.52
29	UB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	EJ	202	PEB	C2C-C3C	3.38	1.47	1.37
29	EL	202	PEB	C2C-C3C	3.38	1.47	1.37
29	MQ	401	PEB	C2C-C3C	3.38	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LA	203	PEB	C2C-C3C	3.38	1.47	1.37
29	LN	203	PEB	C2C-C3C	3.38	1.47	1.37
29	N7	1002	PEB	CHA-C1B	3.38	1.48	1.40
29	N9	1002	PEB	CHA-C1B	3.38	1.48	1.40
29	V2	203	PEB	C2C-C3C	3.38	1.47	1.37
29	mJ	202	PEB	C2C-C3C	3.38	1.47	1.37
29	mL	202	PEB	C2C-C3C	3.38	1.47	1.37
29	fI	202	PEB	CHA-C1B	3.38	1.48	1.40
29	fK	202	PEB	CHA-C1B	3.38	1.48	1.40
29	MB	202	PEB	C2C-C3C	3.38	1.47	1.37
29	MM	202	PEB	C2C-C3C	3.38	1.47	1.37
29	sJ	202	PEB	C2C-C3C	3.38	1.47	1.37
29	sL	202	PEB	C2C-C3C	3.38	1.47	1.37
29	WJ	202	PEB	CHA-C1B	3.38	1.48	1.40
29	WL	202	PEB	CHA-C1B	3.38	1.48	1.40
29	lF	202	PEB	C2C-C3C	3.37	1.47	1.37
29	lI	202	PEB	C2C-C3C	3.37	1.47	1.37
29	aJ	201	PEB	CHA-C1B	3.37	1.48	1.40
29	aL	201	PEB	CHA-C1B	3.37	1.48	1.40
31	lI	1001	CYC	C3D-C2D	3.37	1.47	1.37
31	GK	1001	CYC	C3D-C2D	3.37	1.47	1.37
29	KG	202	PEB	C2C-C3C	3.37	1.47	1.37
29	KQ	202	PEB	C2C-C3C	3.37	1.47	1.37
29	QJ	202	PEB	C2C-C3C	3.37	1.47	1.37
29	QL	202	PEB	C2C-C3C	3.37	1.47	1.37
29	aB	202	PEB	C2C-C3C	3.37	1.47	1.37
29	aM	202	PEB	C2C-C3C	3.37	1.47	1.37
29	R1	203	PEB	C2A-C1A	-3.37	1.49	1.52
29	RK	203	PEB	C2A-C1A	-3.37	1.49	1.52
29	K3	201	PEB	C2C-C3C	3.37	1.47	1.37
29	KO	201	PEB	C2C-C3C	3.37	1.47	1.37
29	Z1	203	PEB	CHA-C1B	3.37	1.48	1.40
29	ZK	203	PEB	CHA-C1B	3.37	1.48	1.40
29	E3	201	PEB	C2C-C3C	3.37	1.47	1.37
29	IB	202	PEB	C2C-C3C	3.37	1.47	1.37
29	CJ	202	PEB	C2C-C3C	3.37	1.47	1.37
29	CL	202	PEB	C2C-C3C	3.37	1.47	1.37
29	IM	202	PEB	C2C-C3C	3.37	1.47	1.37
29	EO	201	PEB	C2C-C3C	3.37	1.47	1.37
30	MN	403	PUB	C3B-C2B	3.37	1.47	1.37
29	I3	203	PEB	C2C-C3C	3.37	1.47	1.37
29	DA	203	PEB	C2C-C3C	3.37	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	WJ	203	PEB	C2C-C3C	3.37	1.47	1.37
29	WL	203	PEB	C2C-C3C	3.37	1.47	1.37
29	DN	203	PEB	C2C-C3C	3.37	1.47	1.37
29	IO	203	PEB	C2C-C3C	3.37	1.47	1.37
29	CC	201	PEB	C1A-NA	-3.37	1.33	1.37
29	CE	201	PEB	C1A-NA	-3.37	1.33	1.37
29	cJ	201	PEB	CHA-C1B	3.37	1.48	1.40
29	cL	201	PEB	CHA-C1B	3.37	1.48	1.40
29	NO	203	PEB	C2A-C1A	-3.37	1.49	1.52
29	OR	201	PEB	C2A-C1A	-3.37	1.49	1.52
29	EG	202	PEB	C2C-C3C	3.37	1.47	1.37
29	EQ	202	PEB	C2C-C3C	3.37	1.47	1.37
31	yP	1001	CYC	C3D-C2D	3.37	1.47	1.37
29	A1	303	PEB	C2C-C3C	3.37	1.47	1.37
29	dB	202	PEB	C2C-C3C	3.37	1.47	1.37
29	AK	303	PEB	C2C-C3C	3.37	1.47	1.37
29	dM	202	PEB	C2C-C3C	3.37	1.47	1.37
31	EK	1001	CYC	C3D-C2D	3.37	1.47	1.37
29	I3	201	PEB	C2C-C3C	3.37	1.47	1.37
29	IO	201	PEB	C2C-C3C	3.37	1.47	1.37
29	UJ	201	PEB	CHA-C1B	3.37	1.48	1.40
29	UL	201	PEB	CHA-C1B	3.37	1.48	1.40
29	SJ	202	PEB	C2C-C3C	3.37	1.47	1.37
29	SL	202	PEB	C2C-C3C	3.37	1.47	1.37
29	iJ	201	PEB	CHA-C1B	3.37	1.48	1.40
29	iL	201	PEB	CHA-C1B	3.37	1.48	1.40
31	K1	1001	CYC	C3D-C2D	3.37	1.47	1.37
31	KK	1001	CYC	C3D-C2D	3.37	1.47	1.37
29	GJ	202	PEB	C2C-C3C	3.37	1.47	1.37
29	GL	202	PEB	C2C-C3C	3.37	1.47	1.37
29	AB	301	PEB	C2C-C3C	3.37	1.47	1.37
29	WF	201	PEB	CHA-C1B	3.37	1.48	1.40
29	WI	201	PEB	CHA-C1B	3.37	1.48	1.40
29	l1	201	PEB	CHA-C1B	3.37	1.48	1.40
29	SF	201	PEB	CHA-C1B	3.37	1.48	1.40
29	SI	201	PEB	CHA-C1B	3.37	1.48	1.40
29	lK	201	PEB	CHA-C1B	3.37	1.48	1.40
29	UJ	202	PEB	C2C-C3C	3.36	1.47	1.37
29	UL	202	PEB	C2C-C3C	3.36	1.47	1.37
29	FA	203	PEB	C2C-C3C	3.36	1.47	1.37
29	FN	203	PEB	C2C-C3C	3.36	1.47	1.37
29	gJ	202	PEB	C2C-C3C	3.36	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gL	202	PEB	C2C-C3C	3.36	1.47	1.37
31	F7	1001	CYC	C2C-C1C	-3.36	1.49	1.52
29	YJ	202	PEB	C2C-C3C	3.36	1.47	1.37
29	YL	202	PEB	C2C-C3C	3.36	1.47	1.37
29	yJ	301	PEB	CHA-C1B	3.36	1.48	1.40
29	yL	301	PEB	CHA-C1B	3.36	1.48	1.40
29	IJ	202	PEB	C2C-C3C	3.36	1.47	1.37
29	IL	202	PEB	C2C-C3C	3.36	1.47	1.37
29	I4	203	PEB	C1A-NA	-3.36	1.33	1.37
29	A3	201	PEB	C2C-C3C	3.36	1.47	1.37
29	aJ	202	PEB	C2C-C3C	3.36	1.47	1.37
29	aL	202	PEB	C2C-C3C	3.36	1.47	1.37
29	AO	201	PEB	C2C-C3C	3.36	1.47	1.37
29	MA	401	PEB	C2C-C3C	3.36	1.47	1.37
29	ZF	202	PEB	C2C-C3C	3.36	1.47	1.37
29	ZI	202	PEB	C2C-C3C	3.36	1.47	1.37
29	O1	201	PEB	CHA-C1B	3.36	1.48	1.40
29	OK	201	PEB	CHA-C1B	3.36	1.48	1.40
31	F7	1001	CYC	CHB-C4A	3.36	1.48	1.40
29	fB	202	PEB	CHA-C1B	3.36	1.48	1.40
29	fM	202	PEB	CHA-C1B	3.36	1.48	1.40
29	AG	202	PEB	C2C-C3C	3.36	1.47	1.37
29	AQ	202	PEB	C2C-C3C	3.36	1.47	1.37
29	QF	202	PEB	C2C-C3C	3.36	1.47	1.37
29	QI	202	PEB	C2C-C3C	3.36	1.47	1.37
29	LC	201	PEB	C1A-NA	-3.36	1.33	1.37
29	LE	201	PEB	C1A-NA	-3.36	1.33	1.37
29	G3	201	PEB	C2C-C3C	3.36	1.47	1.37
29	GO	201	PEB	C2C-C3C	3.36	1.47	1.37
29	O1	202	PEB	CHA-C1B	3.36	1.48	1.40
29	OK	202	PEB	CHA-C1B	3.36	1.48	1.40
29	MA	405	PEB	C2C-C3C	3.36	1.47	1.37
29	VR	203	PEB	C2C-C3C	3.36	1.47	1.37
29	l1	202	PEB	CHA-C1B	3.36	1.48	1.40
29	lK	202	PEB	CHA-C1B	3.36	1.48	1.40
30	BB	302	PUB	OD-C4D	3.36	1.30	1.23
30	BM	302	PUB	OD-C4D	3.36	1.30	1.23
29	Y1	202	PEB	C2A-C1A	-3.36	1.49	1.52
29	YK	202	PEB	C2A-C1A	-3.36	1.49	1.52
29	J3	202	PEB	C2C-C3C	3.36	1.47	1.37
29	JO	202	PEB	C2C-C3C	3.36	1.47	1.37
29	EB	202	PEB	CHA-C1B	3.36	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EM	202	PEB	CHA-C1B	3.36	1.48	1.40
29	fF	201	PEB	CHA-C1B	3.35	1.48	1.40
29	fI	201	PEB	CHA-C1B	3.35	1.48	1.40
29	BA	203	PEB	C2C-C3C	3.35	1.47	1.37
29	BN	203	PEB	C2C-C3C	3.35	1.47	1.37
30	MA	403	PUB	C3B-C2B	3.35	1.47	1.37
29	T2	203	PEB	C2C-C3C	3.35	1.47	1.37
29	b7	202	PEB	C2C-C3C	3.35	1.47	1.37
29	b9	202	PEB	C2C-C3C	3.35	1.47	1.37
29	HA	203	PEB	C2C-C3C	3.35	1.47	1.37
29	HN	203	PEB	C2C-C3C	3.35	1.47	1.37
29	LG	202	PEB	C2C-C3C	3.35	1.47	1.37
29	LQ	201	PEB	C2C-C3C	3.35	1.47	1.37
29	jF	202	PEB	C2C-C3C	3.35	1.47	1.37
29	jI	202	PEB	C2C-C3C	3.35	1.47	1.37
29	AJ	202	PEB	C2C-C3C	3.35	1.47	1.37
29	AL	202	PEB	C2C-C3C	3.35	1.47	1.37
29	TR	203	PEB	C2C-C3C	3.35	1.47	1.37
29	FC	201	PEB	C1A-NA	-3.35	1.33	1.37
29	FE	201	PEB	C1A-NA	-3.35	1.33	1.37
29	IG	202	PEB	C2C-C3C	3.35	1.47	1.37
29	IQ	202	PEB	C2C-C3C	3.35	1.47	1.37
29	N2	203	PEB	C2C-C3C	3.35	1.47	1.37
29	B3	202	PEB	C2C-C3C	3.35	1.47	1.37
29	BO	202	PEB	C2C-C3C	3.35	1.47	1.37
29	wL	303	PEB	C1A-NA	-3.35	1.33	1.37
29	dF	202	PEB	CHA-C1B	3.35	1.48	1.40
29	dI	202	PEB	CHA-C1B	3.35	1.48	1.40
29	fI	201	PEB	CHA-C1B	3.35	1.48	1.40
29	fK	201	PEB	CHA-C1B	3.35	1.48	1.40
29	H3	202	PEB	C2C-C3C	3.35	1.47	1.37
29	HO	202	PEB	C2C-C3C	3.35	1.47	1.37
29	j7	202	PEB	C2C-C3C	3.35	1.47	1.37
29	j9	202	PEB	C2C-C3C	3.35	1.47	1.37
29	hF	202	PEB	C2C-C3C	3.35	1.47	1.37
29	hI	202	PEB	C2C-C3C	3.35	1.47	1.37
29	BC	203	PEB	C1A-NA	-3.35	1.33	1.37
29	BE	203	PEB	C1A-NA	-3.35	1.33	1.37
29	JG	202	PEB	C1A-NA	-3.35	1.33	1.37
29	JQ	202	PEB	C1A-NA	-3.35	1.33	1.37
29	OF	202	PEB	C2C-C3C	3.35	1.47	1.37
29	OI	202	PEB	C2C-C3C	3.35	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	bF	201	PEB	CHA-C1B	3.35	1.48	1.40
29	bI	201	PEB	CHA-C1B	3.35	1.48	1.40
29	G5	201	PEB	C2C-C3C	3.35	1.47	1.37
29	QF	201	PEB	CHA-C1B	3.35	1.48	1.40
29	QI	201	PEB	CHA-C1B	3.35	1.48	1.40
29	F5	201	PEB	C2C-C3C	3.35	1.47	1.37
29	F8	201	PEB	C2C-C3C	3.35	1.47	1.37
29	Z1	202	PEB	CHA-C1B	3.34	1.48	1.40
29	ZK	202	PEB	CHA-C1B	3.34	1.48	1.40
29	l7	202	PEB	C2C-C3C	3.34	1.47	1.37
29	l9	202	PEB	C2C-C3C	3.34	1.47	1.37
29	HG	202	PEB	C2C-C3C	3.34	1.47	1.37
29	HQ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	AG	202	PEB	C1A-NA	-3.34	1.33	1.37
29	AQ	202	PEB	C1A-NA	-3.34	1.33	1.37
29	MN	401	PEB	C2C-C3C	3.34	1.47	1.37
29	W1	201	PEB	CHA-C1B	3.34	1.48	1.40
29	IB	202	PEB	CHA-C1B	3.34	1.48	1.40
29	WK	201	PEB	CHA-C1B	3.34	1.48	1.40
29	IM	202	PEB	CHA-C1B	3.34	1.48	1.40
31	C1	1001	CYC	C3D-C2D	3.34	1.47	1.37
31	I7	1001	CYC	C3D-C2D	3.34	1.47	1.37
31	I9	1001	CYC	C3D-C2D	3.34	1.47	1.37
29	bF	202	PEB	C2C-C3C	3.34	1.47	1.37
29	GG	202	PEB	C2C-C3C	3.34	1.47	1.37
29	bI	202	PEB	C2C-C3C	3.34	1.47	1.37
29	qJ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	qL	202	PEB	C2C-C3C	3.34	1.47	1.37
29	GQ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	HC	203	PEB	C1A-NA	-3.34	1.33	1.37
29	HE	203	PEB	C1A-NA	-3.34	1.33	1.37
29	F3	202	PEB	C2C-C3C	3.34	1.47	1.37
29	FO	202	PEB	C2C-C3C	3.34	1.47	1.37
29	AF	305	PEB	C2C-C3C	3.34	1.47	1.37
29	dF	203	PEB	C2C-C3C	3.34	1.47	1.37
29	CG	202	PEB	C2C-C3C	3.34	1.47	1.37
29	AI	305	PEB	C2C-C3C	3.34	1.47	1.37
29	dI	203	PEB	C2C-C3C	3.34	1.47	1.37
29	CQ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	b1	201	PEB	CHA-C1B	3.34	1.48	1.40
29	bK	201	PEB	CHA-C1B	3.34	1.48	1.40
29	DC	202	PEB	C1A-NA	-3.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DE	202	PEB	C1A-NA	-3.34	1.33	1.37
29	AF	301	PEB	CHA-C1B	3.34	1.48	1.40
29	AI	301	PEB	CHA-C1B	3.34	1.48	1.40
29	G8	201	PEB	C2C-C3C	3.34	1.47	1.37
29	A1	301	PEB	C2C-C3C	3.34	1.47	1.37
29	AK	301	PEB	C2C-C3C	3.34	1.47	1.37
31	N7	1001	CYC	C2C-C1C	-3.34	1.49	1.52
31	N9	1001	CYC	C2C-C1C	-3.34	1.49	1.52
31	CK	1001	CYC	C3D-C2D	3.34	1.47	1.37
29	g1	203	PEB	C2C-C3C	3.34	1.47	1.37
29	h7	202	PEB	C2C-C3C	3.34	1.47	1.37
29	h9	202	PEB	C2C-C3C	3.34	1.47	1.37
29	DG	202	PEB	C2C-C3C	3.34	1.47	1.37
29	gK	203	PEB	C2C-C3C	3.34	1.47	1.37
29	DQ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	V1	203	PEB	C2A-C1A	-3.34	1.49	1.52
29	VK	203	PEB	C2A-C1A	-3.34	1.49	1.52
29	FG	202	PEB	C2C-C3C	3.34	1.47	1.37
29	FQ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	wJ	303	PEB	C1A-NA	-3.34	1.33	1.37
29	B5	201	PEB	C2C-C3C	3.34	1.47	1.37
29	wJ	303	PEB	CHA-C1B	3.34	1.48	1.40
29	JG	202	PEB	C2C-C3C	3.34	1.47	1.37
29	JQ	202	PEB	C2C-C3C	3.34	1.47	1.37
29	J3	201	PEB	C2C-C3C	3.34	1.47	1.37
29	B8	201	PEB	C2C-C3C	3.34	1.47	1.37
29	JO	201	PEB	C2C-C3C	3.34	1.47	1.37
29	SR	202	PEB	C2C-C3C	3.34	1.47	1.37
29	OB	202	PEB	CHA-C1B	3.33	1.48	1.40
29	OM	202	PEB	CHA-C1B	3.33	1.48	1.40
31	K9	1001	CYC	C3D-C2D	3.33	1.47	1.37
29	h1	201	PEB	CHA-C1B	3.33	1.48	1.40
29	hK	201	PEB	CHA-C1B	3.33	1.48	1.40
29	f7	202	PEB	C2C-C3C	3.33	1.47	1.37
29	f9	202	PEB	C2C-C3C	3.33	1.47	1.37
29	L5	202	PEB	C2C-C3C	3.33	1.47	1.37
29	d7	202	PEB	C2C-C3C	3.33	1.47	1.37
29	d9	202	PEB	C2C-C3C	3.33	1.47	1.37
29	L3	201	PEB	C2C-C3C	3.33	1.47	1.37
29	LO	201	PEB	C2C-C3C	3.33	1.47	1.37
29	xJ	303	PEB	CHA-C1B	3.33	1.48	1.40
31	E7	1001	CYC	C3D-C2D	3.33	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E9	1001	CYC	C3D-C2D	3.33	1.47	1.37
29	MB	202	PEB	CHA-C1B	3.33	1.48	1.40
29	MM	202	PEB	CHA-C1B	3.33	1.48	1.40
29	SF	202	PEB	C2C-C3C	3.33	1.47	1.37
29	UF	203	PEB	C2C-C3C	3.33	1.47	1.37
29	SI	202	PEB	C2C-C3C	3.33	1.47	1.37
29	UI	203	PEB	C2C-C3C	3.33	1.47	1.37
29	jF	201	PEB	CHA-C1B	3.33	1.48	1.40
29	jI	201	PEB	CHA-C1B	3.33	1.48	1.40
29	hB	202	PEB	CHA-C1B	3.33	1.48	1.40
29	hM	202	PEB	CHA-C1B	3.33	1.48	1.40
29	YB	203	PEB	CHA-C1B	3.33	1.48	1.40
29	YM	203	PEB	CHA-C1B	3.33	1.48	1.40
31	K7	1001	CYC	C3D-C2D	3.33	1.47	1.37
29	WF	202	PEB	C2C-C3C	3.33	1.47	1.37
29	WI	202	PEB	C2C-C3C	3.33	1.47	1.37
29	OF	201	PEB	CHA-C1B	3.33	1.48	1.40
29	OI	201	PEB	CHA-C1B	3.33	1.48	1.40
29	R7	203	PEB	C2C-C3C	3.33	1.47	1.37
29	R9	203	PEB	C2C-C3C	3.33	1.47	1.37
29	S7	202	PEB	C2C-C3C	3.33	1.47	1.37
29	S9	202	PEB	C2C-C3C	3.33	1.47	1.37
29	ZF	201	PEB	C2C-C3C	3.33	1.47	1.37
29	ZI	201	PEB	C2C-C3C	3.33	1.47	1.37
29	aB	202	PEB	CHA-C1B	3.33	1.48	1.40
29	aM	202	PEB	CHA-C1B	3.33	1.48	1.40
29	fF	202	PEB	C2C-C3C	3.33	1.47	1.37
29	fI	202	PEB	C2C-C3C	3.33	1.47	1.37
29	MN	405	PEB	C2C-C3C	3.33	1.47	1.37
29	QF	201	PEB	C2C-C3C	3.33	1.47	1.37
29	QI	201	PEB	C2C-C3C	3.33	1.47	1.37
29	WB	202	PEB	CHA-C1B	3.33	1.48	1.40
29	xL	303	PEB	CHA-C1B	3.33	1.48	1.40
29	WM	202	PEB	CHA-C1B	3.33	1.48	1.40
31	GF	1001	CYC	CHB-C4A	3.33	1.48	1.40
31	GI	1001	CYC	CHB-C4A	3.33	1.48	1.40
29	ZF	201	PEB	CHA-C1B	3.32	1.48	1.40
29	ZI	201	PEB	CHA-C1B	3.32	1.48	1.40
29	M3	203	PEB	C2A-C1A	-3.32	1.49	1.52
29	MO	203	PEB	C2A-C1A	-3.32	1.49	1.52
29	U7	202	PEB	C2C-C3C	3.32	1.47	1.37
29	U9	202	PEB	C2C-C3C	3.32	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DC	201	PEB	C1A-NA	-3.32	1.33	1.37
29	DE	201	PEB	C1A-NA	-3.32	1.33	1.37
29	EG	202	PEB	C1A-NA	-3.32	1.33	1.37
29	EQ	202	PEB	C1A-NA	-3.32	1.33	1.37
29	P1	203	PEB	C2C-C3C	3.32	1.47	1.37
29	PK	203	PEB	C2C-C3C	3.32	1.47	1.37
29	i1	203	PEB	C2C-C3C	3.32	1.47	1.37
29	iK	203	PEB	C2C-C3C	3.32	1.47	1.37
31	YP	1000	CYC	C3D-C2D	3.32	1.47	1.37
29	SB	202	PEB	CHA-C1B	3.32	1.48	1.40
29	SM	202	PEB	CHA-C1B	3.32	1.48	1.40
29	A7	304	PEB	C1A-NA	-3.32	1.33	1.37
29	B3	201	PEB	C2C-C3C	3.32	1.47	1.37
29	F3	201	PEB	C2C-C3C	3.32	1.47	1.37
29	BO	201	PEB	C2C-C3C	3.32	1.47	1.37
29	FO	201	PEB	C2C-C3C	3.32	1.47	1.37
29	Q7	202	PEB	C2C-C3C	3.32	1.47	1.37
29	Q9	202	PEB	C2C-C3C	3.32	1.47	1.37
29	SJ	202	PEB	CHA-C1B	3.32	1.48	1.40
29	SL	202	PEB	CHA-C1B	3.32	1.48	1.40
29	e1	203	PEB	C2C-C3C	3.32	1.47	1.37
29	eK	203	PEB	C2C-C3C	3.32	1.47	1.37
29	XB	202	PEB	C2A-C1A	-3.32	1.49	1.52
29	XM	202	PEB	C2A-C1A	-3.32	1.49	1.52
29	QB	204	PEB	CHA-C1B	3.32	1.48	1.40
29	aJ	202	PEB	CHA-C1B	3.32	1.48	1.40
29	aL	202	PEB	CHA-C1B	3.32	1.48	1.40
29	QM	204	PEB	CHA-C1B	3.32	1.48	1.40
29	AM	303	PEB	C1A-NA	-3.32	1.33	1.37
29	S1	201	PEB	CHA-C1B	3.32	1.48	1.40
29	SK	201	PEB	CHA-C1B	3.32	1.48	1.40
29	wL	303	PEB	CHA-C1B	3.32	1.48	1.40
31	G7	1001	CYC	C3D-C2D	3.32	1.47	1.37
29	D3	201	PEB	C2C-C3C	3.32	1.47	1.37
29	DO	201	PEB	C2C-C3C	3.32	1.47	1.37
29	W7	202	PEB	C2C-C3C	3.32	1.47	1.37
29	W9	202	PEB	C2C-C3C	3.32	1.47	1.37
29	U1	202	PEB	CHA-C1B	3.32	1.48	1.40
29	UK	202	PEB	CHA-C1B	3.32	1.48	1.40
29	I8	203	PEB	C2C-C3C	3.32	1.47	1.37
29	lF	201	PEB	C2C-C3C	3.32	1.47	1.37
29	lI	201	PEB	C2C-C3C	3.32	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	XR	201	PEB	C2C-C3C	3.32	1.47	1.37
29	K5	203	PEB	C2C-C3C	3.32	1.47	1.37
29	O7	202	PEB	C2C-C3C	3.32	1.47	1.37
29	K8	203	PEB	C2C-C3C	3.32	1.47	1.37
29	O9	202	PEB	C2C-C3C	3.32	1.47	1.37
29	hF	201	PEB	C2C-C3C	3.32	1.47	1.37
29	hI	201	PEB	C2C-C3C	3.32	1.47	1.37
29	m1	202	PEB	C2C-C3C	3.32	1.47	1.37
29	mK	202	PEB	C2C-C3C	3.32	1.47	1.37
29	Q1	201	PEB	CHA-C1B	3.32	1.48	1.40
29	QK	201	PEB	CHA-C1B	3.32	1.48	1.40
31	IF	1001	CYC	CHB-C4A	3.32	1.48	1.40
31	II	1001	CYC	CHB-C4A	3.32	1.48	1.40
29	DG	201	PEB	CHA-C1B	3.32	1.48	1.40
29	DQ	201	PEB	CHA-C1B	3.32	1.48	1.40
29	dB	202	PEB	CHA-C1B	3.32	1.48	1.40
29	hF	201	PEB	CHA-C1B	3.32	1.48	1.40
29	hI	201	PEB	CHA-C1B	3.32	1.48	1.40
29	dM	202	PEB	CHA-C1B	3.32	1.48	1.40
29	R1	203	PEB	C2C-C3C	3.32	1.47	1.37
29	RK	203	PEB	C2C-C3C	3.32	1.47	1.37
31	1P	1002	CYC	C3D-C2D	3.31	1.47	1.37
29	mJ	202	PEB	CHA-C1B	3.31	1.48	1.40
29	mL	202	PEB	CHA-C1B	3.31	1.48	1.40
31	C7	1001	CYC	C3D-C2D	3.31	1.47	1.37
31	C9	1001	CYC	C3D-C2D	3.31	1.47	1.37
29	jF	201	PEB	C2C-C3C	3.31	1.47	1.37
29	jI	201	PEB	C2C-C3C	3.31	1.47	1.37
29	WJ	203	PEB	CHA-C1B	3.31	1.48	1.40
29	WL	203	PEB	CHA-C1B	3.31	1.48	1.40
29	UJ	202	PEB	CHA-C1B	3.31	1.48	1.40
29	UL	202	PEB	CHA-C1B	3.31	1.48	1.40
31	G9	1001	CYC	C3D-C2D	3.31	1.47	1.37
31	qP	1001	CYC	C3D-C2D	3.31	1.47	1.37
29	L8	202	PEB	C2C-C3C	3.31	1.47	1.37
29	KC	201	PEB	C1A-NA	-3.31	1.33	1.37
29	KE	201	PEB	C1A-NA	-3.31	1.33	1.37
29	c1	203	PEB	C2A-C1A	-3.31	1.49	1.52
29	cK	203	PEB	C2A-C1A	-3.31	1.49	1.52
29	d1	201	PEB	CHA-C1B	3.31	1.48	1.40
29	dK	201	PEB	CHA-C1B	3.31	1.48	1.40
29	BC	201	PEB	C1A-NA	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BE	201	PEB	C1A-NA	-3.31	1.33	1.37
29	IB	202	PEB	CHA-C1B	3.31	1.48	1.40
29	BG	201	PEB	CHA-C1B	3.31	1.48	1.40
29	IM	202	PEB	CHA-C1B	3.31	1.48	1.40
29	BQ	201	PEB	CHA-C1B	3.31	1.48	1.40
29	H8	202	PEB	C2C-C3C	3.31	1.47	1.37
29	T1	202	PEB	C2C-C3C	3.31	1.47	1.37
29	I5	203	PEB	C2C-C3C	3.31	1.47	1.37
29	TK	202	PEB	C2C-C3C	3.31	1.47	1.37
29	JG	201	PEB	CHA-C1B	3.31	1.48	1.40
29	qJ	202	PEB	CHA-C1B	3.31	1.48	1.40
29	qL	202	PEB	CHA-C1B	3.31	1.48	1.40
29	JQ	201	PEB	CHA-C1B	3.31	1.48	1.40
29	k1	203	PEB	C2A-C1A	-3.31	1.49	1.52
29	kK	203	PEB	C2A-C1A	-3.31	1.49	1.52
29	F5	202	PEB	C2C-C3C	3.31	1.47	1.37
29	Z7	202	PEB	C2C-C3C	3.31	1.47	1.37
29	Z9	202	PEB	C2C-C3C	3.31	1.47	1.37
29	SF	201	PEB	C2C-C3C	3.31	1.47	1.37
29	SI	201	PEB	C2C-C3C	3.31	1.47	1.37
31	M7	1001	CYC	C3D-C2D	3.31	1.47	1.37
29	HG	202	PEB	C1A-NA	-3.31	1.33	1.37
29	HQ	202	PEB	C1A-NA	-3.31	1.33	1.37
29	V1	203	PEB	C2C-C3C	3.31	1.47	1.37
29	H3	201	PEB	C2C-C3C	3.31	1.47	1.37
29	VK	203	PEB	C2C-C3C	3.31	1.47	1.37
29	HO	201	PEB	C2C-C3C	3.31	1.47	1.37
29	jB	202	PEB	CHA-C1B	3.31	1.48	1.40
29	jM	202	PEB	CHA-C1B	3.31	1.48	1.40
31	QP	1001	CYC	C3D-C2D	3.31	1.47	1.37
31	fP	1001	CYC	C3D-C2D	3.31	1.47	1.37
29	UB	202	PEB	CHA-C1B	3.31	1.48	1.40
29	oJ	202	PEB	CHA-C1B	3.31	1.48	1.40
29	oL	202	PEB	CHA-C1B	3.31	1.48	1.40
29	MQ	401	PEB	CHA-C1B	3.31	1.48	1.40
29	k1	203	PEB	C2C-C3C	3.31	1.47	1.37
29	bF	201	PEB	C2C-C3C	3.31	1.47	1.37
29	bI	201	PEB	C2C-C3C	3.31	1.47	1.37
29	kK	203	PEB	C2C-C3C	3.31	1.47	1.37
29	UF	202	PEB	CHA-C1B	3.31	1.48	1.40
29	UI	202	PEB	CHA-C1B	3.31	1.48	1.40
29	i7	203	PEB	C2C-C3C	3.31	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	i9	203	PEB	C2C-C3C	3.31	1.47	1.37
29	CG	202	PEB	C1A-NA	-3.30	1.33	1.37
29	CQ	202	PEB	C1A-NA	-3.30	1.33	1.37
29	L5	203	PEB	C2C-C3C	3.30	1.47	1.37
29	Y7	203	PEB	C2C-C3C	3.30	1.47	1.37
29	Y9	203	PEB	C2C-C3C	3.30	1.47	1.37
29	GB	202	PEB	CHA-C1B	3.30	1.48	1.40
29	uJ	203	PEB	CHA-C1B	3.30	1.48	1.40
29	uL	203	PEB	CHA-C1B	3.30	1.48	1.40
29	GM	202	PEB	CHA-C1B	3.30	1.48	1.40
29	m1	202	PEB	C2A-C1A	-3.30	1.49	1.52
29	mK	202	PEB	C2A-C1A	-3.30	1.49	1.52
29	G8	202	PEB	C2C-C3C	3.30	1.47	1.37
31	M9	1001	CYC	C3D-C2D	3.30	1.47	1.37
29	fF	201	PEB	C2C-C3C	3.30	1.47	1.37
29	fI	201	PEB	C2C-C3C	3.30	1.47	1.37
29	dF	202	PEB	C2C-C3C	3.30	1.47	1.37
29	dI	202	PEB	C2C-C3C	3.30	1.47	1.37
29	A5	203	PEB	C2C-C3C	3.30	1.47	1.37
29	A8	203	PEB	C2C-C3C	3.30	1.47	1.37
29	CA	202	PEB	CHA-C1B	3.30	1.48	1.40
29	CN	202	PEB	CHA-C1B	3.30	1.48	1.40
29	j1	201	PEB	CHA-C1B	3.30	1.48	1.40
29	CJ	202	PEB	CHA-C1B	3.30	1.48	1.40
29	jK	201	PEB	CHA-C1B	3.30	1.48	1.40
29	CL	202	PEB	CHA-C1B	3.30	1.48	1.40
31	FP	1001	CYC	C3D-C2D	3.30	1.47	1.37
29	FG	201	PEB	CHA-C1B	3.30	1.48	1.40
29	FQ	201	PEB	CHA-C1B	3.30	1.48	1.40
29	HC	201	PEB	C1A-NA	-3.30	1.33	1.37
29	KC	203	PEB	C1A-NA	-3.30	1.33	1.37
29	HE	201	PEB	C1A-NA	-3.30	1.33	1.37
29	KE	203	PEB	C1A-NA	-3.30	1.33	1.37
29	a1	203	PEB	C2C-C3C	3.30	1.47	1.37
29	aK	203	PEB	C2C-C3C	3.30	1.47	1.37
31	jP	1001	CYC	C3D-C2D	3.30	1.47	1.37
29	FC	203	PEB	C1A-NA	-3.30	1.33	1.37
29	FE	203	PEB	C1A-NA	-3.30	1.33	1.37
29	sJ	202	PEB	CHA-C1B	3.30	1.48	1.40
29	sL	202	PEB	CHA-C1B	3.30	1.48	1.40
29	c1	203	PEB	C2C-C3C	3.30	1.47	1.37
29	cK	203	PEB	C2C-C3C	3.30	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	UF	202	PEB	C2C-C3C	3.30	1.47	1.37
29	UI	202	PEB	C2C-C3C	3.30	1.47	1.37
29	BG	202	PEB	C1A-NA	-3.30	1.33	1.37
29	BQ	202	PEB	C1A-NA	-3.30	1.33	1.37
31	sP	1001	CYC	C3D-C2D	3.30	1.47	1.37
29	LG	202	PEB	C1A-NA	-3.30	1.33	1.37
29	LQ	201	PEB	C1A-NA	-3.30	1.33	1.37
29	T7	203	PEB	C2C-C3C	3.30	1.47	1.37
29	H8	203	PEB	C2C-C3C	3.30	1.47	1.37
29	T9	203	PEB	C2C-C3C	3.30	1.47	1.37
29	F8	202	PEB	C2C-C3C	3.30	1.47	1.37
31	DP	1001	CYC	C3D-C2D	3.30	1.47	1.37
31	IP	1001	CYC	C3D-C2D	3.30	1.47	1.37
29	cJ	202	PEB	CHA-C1B	3.30	1.48	1.40
29	cL	202	PEB	CHA-C1B	3.30	1.48	1.40
29	MA	405	PEB	C1A-NA	-3.30	1.33	1.37
29	Y1	202	PEB	C2C-C3C	3.30	1.47	1.37
29	a7	203	PEB	C2C-C3C	3.30	1.47	1.37
29	a9	203	PEB	C2C-C3C	3.30	1.47	1.37
29	YK	202	PEB	C2C-C3C	3.30	1.47	1.37
29	P7	203	PEB	C2C-C3C	3.30	1.47	1.37
29	P9	203	PEB	C2C-C3C	3.30	1.47	1.37
31	CF	1001	CYC	CHB-C4A	3.30	1.48	1.40
31	CI	1001	CYC	CHB-C4A	3.30	1.48	1.40
29	CB	202	PEB	CHA-C1B	3.30	1.48	1.40
29	CM	202	PEB	CHA-C1B	3.30	1.48	1.40
29	W2	201	PEB	C2A-C1A	-3.30	1.49	1.52
29	GC	202	PEB	C1A-NA	-3.30	1.33	1.37
29	GE	202	PEB	C1A-NA	-3.30	1.33	1.37
29	HG	201	PEB	CHA-C1B	3.30	1.48	1.40
29	HQ	201	PEB	CHA-C1B	3.30	1.48	1.40
29	L8	201	PEB	C2C-C3C	3.30	1.47	1.37
31	nP	1001	CYC	C3D-C2D	3.30	1.47	1.37
29	KG	202	PEB	C1A-NA	-3.30	1.33	1.37
29	KQ	202	PEB	C1A-NA	-3.30	1.33	1.37
29	C5	203	PEB	C2C-C3C	3.30	1.47	1.37
29	C8	203	PEB	C2C-C3C	3.30	1.47	1.37
29	IJ	202	PEB	CHA-C1B	3.30	1.48	1.40
29	IL	202	PEB	CHA-C1B	3.30	1.48	1.40
29	LG	201	PEB	CHA-C1B	3.29	1.48	1.40
29	MQ	402	PEB	CHA-C1B	3.29	1.48	1.40
31	MP	1001	CYC	C3D-C2D	3.29	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g7	201	PEB	C2C-C3C	3.29	1.47	1.37
29	g9	201	PEB	C2C-C3C	3.29	1.47	1.37
29	VR	201	PEB	C2C-C3C	3.29	1.47	1.37
29	c7	203	PEB	C2C-C3C	3.29	1.47	1.37
29	c9	203	PEB	C2C-C3C	3.29	1.47	1.37
31	hP	1001	CYC	C3D-C2D	3.29	1.47	1.37
29	EJ	202	PEB	CHA-C1B	3.29	1.48	1.40
29	EL	202	PEB	CHA-C1B	3.29	1.48	1.40
29	M2	201	PEB	C2A-C1A	-3.29	1.49	1.52
29	MR	201	PEB	C2A-C1A	-3.29	1.49	1.52
29	e2	402	PEB	C2C-C3C	3.29	1.47	1.37
29	L5	201	PEB	C2C-C3C	3.29	1.47	1.37
29	H8	201	PEB	C2C-C3C	3.29	1.47	1.37
29	OR	202	PEB	C1A-NA	-3.29	1.33	1.37
29	lF	201	PEB	CHA-C1B	3.29	1.48	1.40
29	lI	201	PEB	CHA-C1B	3.29	1.48	1.40
29	g7	203	PEB	C2C-C3C	3.29	1.47	1.37
29	g9	203	PEB	C2C-C3C	3.29	1.47	1.37
31	SP	1001	CYC	C3D-C2D	3.29	1.47	1.37
29	xJ	303	PEB	C1A-NA	-3.29	1.33	1.37
29	G5	203	PEB	C2C-C3C	3.29	1.47	1.37
29	H5	201	PEB	C2C-C3C	3.29	1.47	1.37
29	m7	203	PEB	C2C-C3C	3.29	1.47	1.37
29	m9	203	PEB	C2C-C3C	3.29	1.47	1.37
31	MF	1001	CYC	CHB-C4A	3.29	1.48	1.40
31	MI	1001	CYC	CHB-C4A	3.29	1.48	1.40
29	B8	203	PEB	C2C-C3C	3.29	1.47	1.37
31	oP	1001	CYC	C3D-C2D	3.29	1.47	1.37
31	UP	1001	CYC	C3D-C2D	3.29	1.47	1.37
29	M4	201	PEB	C2A-C1A	-3.29	1.49	1.52
29	AJ	202	PEB	CHA-C1B	3.29	1.48	1.40
29	AL	202	PEB	CHA-C1B	3.29	1.48	1.40
29	F5	203	PEB	C2C-C3C	3.29	1.47	1.37
29	F8	203	PEB	C2C-C3C	3.29	1.47	1.37
29	KA	202	PEB	CHA-C1B	3.29	1.48	1.40
29	KN	202	PEB	CHA-C1B	3.29	1.48	1.40
29	TR	201	PEB	C2C-C3C	3.29	1.47	1.37
31	BP	1001	CYC	C3D-C2D	3.29	1.47	1.37
29	OF	201	PEB	C2C-C3C	3.29	1.47	1.37
29	OI	201	PEB	C2C-C3C	3.29	1.47	1.37
29	I4	201	PEB	C2A-C1A	-3.29	1.49	1.52
29	G5	202	PEB	C2C-C3C	3.29	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HA	201	PEB	CHA-C1B	3.29	1.48	1.40
29	YJ	202	PEB	CHA-C1B	3.29	1.48	1.40
29	YL	202	PEB	CHA-C1B	3.29	1.48	1.40
29	HN	201	PEB	CHA-C1B	3.29	1.48	1.40
29	G8	203	PEB	C2C-C3C	3.29	1.47	1.37
31	wP	1001	CYC	C3D-C2D	3.29	1.47	1.37
29	wL	301	PEB	C2C-C3C	3.29	1.47	1.37
29	AB	303	PEB	C1A-NA	-3.29	1.33	1.37
29	iJ	202	PEB	CHA-C1B	3.29	1.48	1.40
29	iL	202	PEB	CHA-C1B	3.29	1.48	1.40
31	L7	1001	CYC	C2C-C1C	-3.29	1.49	1.52
29	V7	203	PEB	C2C-C3C	3.29	1.47	1.37
29	V9	203	PEB	C2C-C3C	3.29	1.47	1.37
31	XP	1001	CYC	C3D-C2D	3.28	1.47	1.37
29	JC	201	PEB	C1A-NA	-3.28	1.33	1.37
29	JE	201	PEB	C1A-NA	-3.28	1.33	1.37
31	L9	1001	CYC	C2C-C1C	-3.28	1.49	1.52
29	B8	202	PEB	C2C-C3C	3.28	1.47	1.37
29	GJ	202	PEB	CHA-C1B	3.28	1.48	1.40
29	GL	202	PEB	CHA-C1B	3.28	1.48	1.40
29	KJ	202	PEB	CHA-C1B	3.28	1.48	1.40
29	KL	202	PEB	CHA-C1B	3.28	1.48	1.40
29	A5	201	PEB	C2C-C3C	3.28	1.47	1.37
29	WF	201	PEB	C2C-C3C	3.28	1.47	1.37
29	WI	201	PEB	C2C-C3C	3.28	1.47	1.37
31	KI	1001	CYC	CHB-C4A	3.28	1.48	1.40
29	T2	201	PEB	C2C-C3C	3.28	1.47	1.37
29	H5	203	PEB	C2C-C3C	3.28	1.47	1.37
29	KB	202	PEB	CHA-C1B	3.28	1.48	1.40
29	KM	202	PEB	CHA-C1B	3.28	1.48	1.40
29	gJ	202	PEB	CHA-C1B	3.28	1.48	1.40
29	gL	202	PEB	CHA-C1B	3.28	1.48	1.40
31	EF	1001	CYC	CHB-C4A	3.28	1.48	1.40
31	KF	1001	CYC	CHB-C4A	3.28	1.48	1.40
31	EI	1001	CYC	CHB-C4A	3.28	1.48	1.40
31	kP	1001	CYC	C3D-C2D	3.28	1.47	1.37
29	GA	202	PEB	CHA-C1B	3.28	1.48	1.40
29	GN	202	PEB	CHA-C1B	3.28	1.48	1.40
29	D3	203	PEB	C2C-C3C	3.28	1.47	1.37
29	DO	203	PEB	C2C-C3C	3.28	1.47	1.37
29	eJ	202	PEB	CHA-C1B	3.28	1.48	1.40
29	eL	202	PEB	CHA-C1B	3.28	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	i1	203	PEB	C2A-C1A	-3.28	1.49	1.52
29	iK	203	PEB	C2A-C1A	-3.28	1.49	1.52
29	e7	203	PEB	C2C-C3C	3.28	1.47	1.37
29	e9	203	PEB	C2C-C3C	3.28	1.47	1.37
31	OP	1001	CYC	C3D-C2D	3.28	1.47	1.37
29	B5	203	PEB	C2C-C3C	3.28	1.47	1.37
29	LA	201	PEB	CHA-C1B	3.28	1.48	1.40
29	QJ	202	PEB	CHA-C1B	3.28	1.48	1.40
29	QL	202	PEB	CHA-C1B	3.28	1.48	1.40
29	LN	201	PEB	CHA-C1B	3.28	1.48	1.40
31	F9	1001	CYC	C2C-C1C	-3.28	1.49	1.52
29	MJ	202	PEB	CHA-C1B	3.28	1.48	1.40
29	ML	202	PEB	CHA-C1B	3.28	1.48	1.40
29	k7	203	PEB	C2C-C3C	3.28	1.47	1.37
29	k9	203	PEB	C2C-C3C	3.28	1.47	1.37
29	A8	201	PEB	C2C-C3C	3.28	1.47	1.37
29	IC	202	PEB	C1A-NA	-3.28	1.33	1.37
29	IE	202	PEB	C1A-NA	-3.28	1.33	1.37
29	kJ	202	PEB	CHA-C1B	3.27	1.48	1.40
29	kL	202	PEB	CHA-C1B	3.27	1.48	1.40
29	DA	201	PEB	CHA-C1B	3.27	1.48	1.40
29	DN	201	PEB	CHA-C1B	3.27	1.48	1.40
29	kB	203	PEB	C2A-C1A	-3.27	1.49	1.52
29	kM	203	PEB	C2A-C1A	-3.27	1.49	1.52
29	H5	202	PEB	C2C-C3C	3.27	1.47	1.37
29	e7	201	PEB	C2C-C3C	3.27	1.47	1.37
29	e9	201	PEB	C2C-C3C	3.27	1.47	1.37
31	uP	1001	CYC	C3D-C2D	3.27	1.47	1.37
29	IA	202	PEB	CHA-C1B	3.27	1.48	1.40
29	IN	202	PEB	CHA-C1B	3.27	1.48	1.40
29	AC	202	PEB	C1A-NA	-3.27	1.33	1.37
29	AE	202	PEB	C1A-NA	-3.27	1.33	1.37
29	T7	201	PEB	C2C-C3C	3.27	1.47	1.37
29	T9	201	PEB	C2C-C3C	3.27	1.47	1.37
29	A9	304	PEB	C1A-NA	-3.27	1.33	1.37
29	JC	202	PEB	C1A-NA	-3.27	1.33	1.37
29	JE	202	PEB	C1A-NA	-3.27	1.33	1.37
29	L8	203	PEB	C2C-C3C	3.27	1.47	1.37
31	1P	1001	CYC	C3D-C2D	3.27	1.47	1.37
29	B3	203	PEB	C2C-C3C	3.27	1.47	1.37
29	wJ	301	PEB	C2C-C3C	3.27	1.47	1.37
29	BO	203	PEB	C2C-C3C	3.27	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FG	202	PEB	C1A-NA	-3.27	1.33	1.37
29	FQ	202	PEB	C1A-NA	-3.27	1.33	1.37
29	V2	201	PEB	C2C-C3C	3.27	1.47	1.37
29	i7	201	PEB	C2C-C3C	3.27	1.47	1.37
29	i9	201	PEB	C2C-C3C	3.27	1.47	1.37
29	I5	201	PEB	C2C-C3C	3.27	1.47	1.37
29	I8	201	PEB	C2C-C3C	3.27	1.47	1.37
31	HP	1001	CYC	C3D-C2D	3.27	1.47	1.37
29	F3	203	PEB	C2C-C3C	3.27	1.47	1.37
29	FO	203	PEB	C2C-C3C	3.27	1.47	1.37
29	V7	201	PEB	C2C-C3C	3.27	1.47	1.37
29	V9	201	PEB	C2C-C3C	3.27	1.47	1.37
29	U2	201	PEB	C2A-C1A	-3.27	1.49	1.52
29	UR	201	PEB	C2A-C1A	-3.27	1.49	1.52
29	LC	202	PEB	C1A-NA	-3.27	1.33	1.37
29	LE	202	PEB	C1A-NA	-3.27	1.33	1.37
29	DG	202	PEB	C1A-NA	-3.27	1.33	1.37
29	DQ	202	PEB	C1A-NA	-3.27	1.33	1.37
29	Y7	201	PEB	C2C-C3C	3.27	1.47	1.37
29	k7	201	PEB	C2C-C3C	3.27	1.47	1.37
29	Y9	201	PEB	C2C-C3C	3.27	1.47	1.37
29	k9	201	PEB	C2C-C3C	3.27	1.47	1.37
29	xJ	301	PEB	C2C-C3C	3.27	1.47	1.37
29	J3	203	PEB	C2C-C3C	3.27	1.47	1.37
29	JO	203	PEB	C2C-C3C	3.27	1.47	1.37
29	OJ	202	PEB	CHA-C1B	3.26	1.48	1.40
29	OL	202	PEB	CHA-C1B	3.26	1.48	1.40
29	EA	202	PEB	CHA-C1B	3.26	1.48	1.40
29	EN	202	PEB	CHA-C1B	3.26	1.48	1.40
29	A7	301	PEB	C2C-C3C	3.26	1.47	1.37
29	K8	201	PEB	C2C-C3C	3.26	1.47	1.37
29	A9	301	PEB	C2C-C3C	3.26	1.47	1.37
29	N2	201	PEB	C2C-C3C	3.26	1.47	1.37
29	IG	202	PEB	C1A-NA	-3.26	1.33	1.37
29	IQ	202	PEB	C1A-NA	-3.26	1.33	1.37
29	NR	201	PEB	C2C-C3C	3.26	1.47	1.37
29	C4	203	PEB	CHA-C1B	3.26	1.48	1.40
29	K5	201	PEB	C2C-C3C	3.26	1.47	1.37
29	c7	201	PEB	C2C-C3C	3.26	1.47	1.37
29	c9	201	PEB	C2C-C3C	3.26	1.47	1.37
29	J5	202	PEB	C2C-C3C	3.26	1.47	1.37
29	P7	201	PEB	C2C-C3C	3.26	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	m7	201	PEB	C2C-C3C	3.26	1.47	1.37
29	J8	202	PEB	C2C-C3C	3.26	1.47	1.37
29	P9	201	PEB	C2C-C3C	3.26	1.47	1.37
29	m9	201	PEB	C2C-C3C	3.26	1.47	1.37
29	R7	201	PEB	C2C-C3C	3.26	1.47	1.37
29	R9	201	PEB	C2C-C3C	3.26	1.47	1.37
29	B5	202	PEB	C2C-C3C	3.26	1.47	1.37
29	CC	202	PEB	C1A-NA	-3.26	1.33	1.37
29	CE	202	PEB	C1A-NA	-3.26	1.33	1.37
29	e1	203	PEB	C2A-C1A	-3.26	1.49	1.52
29	eK	203	PEB	C2A-C1A	-3.26	1.49	1.52
29	G3	202	PEB	CHA-C1B	3.26	1.48	1.40
29	GO	202	PEB	CHA-C1B	3.26	1.48	1.40
29	a7	201	PEB	C2C-C3C	3.26	1.47	1.37
29	a9	201	PEB	C2C-C3C	3.26	1.47	1.37
29	NO	201	PEB	CHA-C1B	3.26	1.48	1.40
29	xL	301	PEB	C2C-C3C	3.26	1.47	1.37
29	LC	203	PEB	C1A-NA	-3.26	1.33	1.37
29	LE	203	PEB	C1A-NA	-3.26	1.33	1.37
29	TF	201	PEB	C1A-NA	-3.25	1.33	1.37
29	AA	202	PEB	CHA-C1B	3.25	1.48	1.40
29	BA	201	PEB	CHA-C1B	3.25	1.48	1.40
29	AN	202	PEB	CHA-C1B	3.25	1.48	1.40
29	BN	201	PEB	CHA-C1B	3.25	1.48	1.40
29	FA	201	PEB	CHA-C1B	3.25	1.48	1.40
29	FN	201	PEB	CHA-C1B	3.25	1.48	1.40
29	e2	402	PEB	C2A-C1A	-3.25	1.49	1.52
29	C5	201	PEB	C2C-C3C	3.25	1.47	1.37
29	C8	201	PEB	C2C-C3C	3.25	1.47	1.37
29	AC	203	PEB	C1A-NA	-3.25	1.33	1.37
29	AE	203	PEB	C1A-NA	-3.25	1.33	1.37
29	R2	201	PEB	C2C-C3C	3.25	1.47	1.37
29	RR	201	PEB	C2C-C3C	3.25	1.47	1.37
29	H3	203	PEB	C2C-C3C	3.25	1.47	1.37
29	HO	203	PEB	C2C-C3C	3.25	1.47	1.37
29	FB	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	HB	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	FM	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	HM	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	ID	201	PEB	C2A-C1A	-3.25	1.49	1.52
29	BC	202	PEB	C1A-NA	-3.25	1.33	1.37
29	BE	202	PEB	C1A-NA	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TB	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	VB	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	TM	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	VM	203	PEB	C2A-C1A	-3.25	1.49	1.52
29	SF	202	PEB	C1A-NA	-3.25	1.33	1.37
29	SI	202	PEB	C1A-NA	-3.25	1.33	1.37
29	IF	202	PEB	C1A-NA	-3.24	1.33	1.37
29	II	202	PEB	C1A-NA	-3.24	1.33	1.37
29	E4	203	PEB	CHA-C1B	3.24	1.48	1.40
29	L3	202	PEB	C2C-C3C	3.24	1.47	1.37
29	LO	202	PEB	C2C-C3C	3.24	1.47	1.37
29	KG	201	PEB	CHA-C1B	3.24	1.48	1.40
29	KQ	201	PEB	CHA-C1B	3.24	1.48	1.40
29	J5	202	PEB	CHA-C1B	3.24	1.48	1.40
29	J8	202	PEB	CHA-C1B	3.24	1.48	1.40
29	bF	202	PEB	C1A-NA	-3.24	1.33	1.37
29	bI	202	PEB	C1A-NA	-3.24	1.33	1.37
29	S2	201	PEB	C1A-NA	-3.24	1.33	1.37
29	RR	201	PEB	C2A-C1A	-3.24	1.49	1.52
29	M3	201	PEB	CHA-C1B	3.24	1.48	1.40
29	MO	201	PEB	CHA-C1B	3.24	1.48	1.40
31	uP	1001	CYC	C1B-C2B	3.24	1.50	1.45
29	gF	201	PEB	C2C-C3C	3.24	1.47	1.37
29	gI	201	PEB	C2C-C3C	3.24	1.47	1.37
29	K3	202	PEB	CHA-C1B	3.24	1.48	1.40
29	KO	202	PEB	CHA-C1B	3.24	1.48	1.40
29	FC	202	PEB	C1A-NA	-3.24	1.33	1.37
29	FE	202	PEB	C1A-NA	-3.24	1.33	1.37
29	CD	201	PEB	C2A-C1A	-3.24	1.49	1.52
29	HC	202	PEB	C1A-NA	-3.24	1.33	1.37
29	HE	202	PEB	C1A-NA	-3.24	1.33	1.37
29	SR	201	PEB	C1A-NA	-3.24	1.33	1.37
30	xJ	305	PUB	C3B-C2B	3.23	1.47	1.37
29	LF	1002	PEB	C2A-C1A	-3.23	1.49	1.52
29	LI	1002	PEB	C2A-C1A	-3.23	1.49	1.52
29	cF	201	PEB	C2C-C3C	3.23	1.47	1.37
29	cI	201	PEB	C2C-C3C	3.23	1.47	1.37
31	UP	1001	CYC	C1B-C2B	3.23	1.50	1.45
29	K5	202	PEB	C2C-C3C	3.23	1.47	1.37
29	K8	202	PEB	C2C-C3C	3.23	1.47	1.37
29	M3	203	PEB	C2C-C3C	3.23	1.47	1.37
29	MO	203	PEB	C2C-C3C	3.23	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QF	202	PEB	C1A-NA	-3.23	1.33	1.37
29	QI	202	PEB	C1A-NA	-3.23	1.33	1.37
30	wL	305	PUB	C3B-C2B	3.23	1.47	1.37
29	ED	202	PEB	CHA-C1B	3.23	1.48	1.40
29	ID	203	PEB	CHA-C1B	3.23	1.48	1.40
29	LF	1002	PEB	C2C-C3C	3.23	1.47	1.37
29	LI	1002	PEB	C2C-C3C	3.23	1.47	1.37
29	NF	1002	PEB	C2C-C3C	3.23	1.47	1.37
29	NI	1002	PEB	C2C-C3C	3.23	1.47	1.37
29	eB	202	PEB	C2A-C1A	-3.23	1.49	1.52
29	gF	201	PEB	C2A-C1A	-3.23	1.49	1.52
29	kF	201	PEB	C2A-C1A	-3.23	1.49	1.52
29	gI	201	PEB	C2A-C1A	-3.23	1.49	1.52
29	kI	201	PEB	C2A-C1A	-3.23	1.49	1.52
29	eM	202	PEB	C2A-C1A	-3.23	1.49	1.52
31	YP	1000	CYC	C2C-C1C	-3.23	1.49	1.52
31	1P	1002	CYC	C2C-C1C	-3.23	1.49	1.52
29	PF	201	PEB	C2C-C3C	3.23	1.47	1.37
29	PI	201	PEB	C2C-C3C	3.23	1.47	1.37
29	PF	201	PEB	C2A-C1A	-3.23	1.49	1.52
29	PI	201	PEB	C2A-C1A	-3.23	1.49	1.52
31	HP	1001	CYC	C1B-C2B	3.23	1.50	1.45
29	I3	202	PEB	CHA-C1B	3.22	1.48	1.40
29	AB	301	PEB	CHA-C1B	3.22	1.48	1.40
29	IO	202	PEB	CHA-C1B	3.22	1.48	1.40
29	MD	203	PEB	CHA-C1B	3.22	1.48	1.40
29	YF	201	PEB	C2C-C3C	3.22	1.47	1.37
29	YI	201	PEB	C2C-C3C	3.22	1.47	1.37
29	EC	202	PEB	C1A-NA	-3.22	1.33	1.37
29	EE	202	PEB	C1A-NA	-3.22	1.33	1.37
29	FF	1002	PEB	C2C-C3C	3.22	1.47	1.37
29	FI	1002	PEB	C2C-C3C	3.22	1.47	1.37
29	HF	1002	PEB	C2C-C3C	3.22	1.47	1.37
29	HI	1002	PEB	C2C-C3C	3.22	1.47	1.37
29	eF	201	PEB	C2C-C3C	3.22	1.47	1.37
29	eI	201	PEB	C2C-C3C	3.22	1.47	1.37
29	NO	203	PEB	C2C-C3C	3.22	1.47	1.37
29	A3	202	PEB	CHA-C1B	3.22	1.48	1.40
29	AG	201	PEB	CHA-C1B	3.22	1.48	1.40
29	AO	202	PEB	CHA-C1B	3.22	1.48	1.40
29	AQ	201	PEB	CHA-C1B	3.22	1.48	1.40
29	GG	201	PEB	CHA-C1B	3.22	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GQ	201	PEB	CHA-C1B	3.22	1.48	1.40
29	J5	201	PEB	C2C-C3C	3.22	1.47	1.37
29	J8	201	PEB	C2C-C3C	3.22	1.47	1.37
29	C5	202	PEB	C2C-C3C	3.22	1.47	1.37
29	C8	202	PEB	C2C-C3C	3.22	1.47	1.37
29	JA	201	PEB	CHA-C1B	3.22	1.48	1.40
29	JN	201	PEB	CHA-C1B	3.22	1.48	1.40
29	TI	201	PEB	C2C-C3C	3.22	1.47	1.37
29	EG	201	PEB	CHA-C1B	3.22	1.48	1.40
29	EQ	201	PEB	CHA-C1B	3.22	1.48	1.40
29	aF	201	PEB	C2C-C3C	3.22	1.47	1.37
29	aI	201	PEB	C2C-C3C	3.22	1.47	1.37
31	hP	1001	CYC	C1B-C2B	3.22	1.50	1.45
29	R2	201	PEB	C2A-C1A	-3.22	1.49	1.52
29	HD	202	PEB	C2A-C1A	-3.22	1.49	1.52
29	HF	1002	PEB	C2A-C1A	-3.22	1.49	1.52
29	HI	1002	PEB	C2A-C1A	-3.22	1.49	1.52
29	E3	202	PEB	CHA-C1B	3.22	1.47	1.40
29	N3	201	PEB	CHA-C1B	3.22	1.47	1.40
29	EO	202	PEB	CHA-C1B	3.22	1.47	1.40
29	JF	1002	PEB	C2C-C3C	3.22	1.47	1.37
29	JI	1002	PEB	C2C-C3C	3.22	1.47	1.37
29	VF	201	PEB	C2C-C3C	3.21	1.47	1.37
29	VI	201	PEB	C2C-C3C	3.21	1.47	1.37
29	CD	203	PEB	CHA-C1B	3.21	1.47	1.40
29	mF	201	PEB	C2C-C3C	3.21	1.47	1.37
29	mI	201	PEB	C2C-C3C	3.21	1.47	1.37
30	xL	305	PUB	C3B-C2B	3.21	1.47	1.37
29	OR	201	PEB	CHA-C1B	3.21	1.47	1.40
29	TI	201	PEB	C2A-C1A	-3.21	1.49	1.52
31	IP	1001	CYC	C1B-C2B	3.21	1.50	1.45
29	OF	202	PEB	C1A-NA	-3.21	1.33	1.37
29	OI	202	PEB	C1A-NA	-3.21	1.33	1.37
31	wP	1001	CYC	C1B-C2B	3.21	1.50	1.45
29	A5	202	PEB	C2C-C3C	3.21	1.47	1.37
29	DF	1002	PEB	C2C-C3C	3.21	1.47	1.37
29	DI	1002	PEB	C2C-C3C	3.21	1.47	1.37
29	XR	201	PEB	C2A-C1A	-3.21	1.49	1.52
31	FP	1001	CYC	C1B-C2B	3.21	1.50	1.45
31	XP	1001	CYC	C1B-C2B	3.21	1.50	1.45
29	Q2	201	PEB	CHA-C1B	3.21	1.47	1.40
29	QR	201	PEB	CHA-C1B	3.21	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZF	202	PEB	C1A-NA	-3.21	1.33	1.37
29	ZI	202	PEB	C1A-NA	-3.21	1.33	1.37
29	D4	202	PEB	C2A-C1A	-3.21	1.49	1.52
29	PB	202	PEB	C2A-C1A	-3.21	1.49	1.52
29	PM	202	PEB	C2A-C1A	-3.21	1.49	1.52
30	MN	402	PUB	C3B-C2B	3.21	1.47	1.37
29	C3	202	PEB	CHA-C1B	3.21	1.47	1.40
29	CO	202	PEB	CHA-C1B	3.21	1.47	1.40
29	kF	201	PEB	C2C-C3C	3.20	1.47	1.37
29	kI	201	PEB	C2C-C3C	3.20	1.47	1.37
29	iF	201	PEB	C2C-C3C	3.20	1.47	1.37
29	iI	201	PEB	C2C-C3C	3.20	1.47	1.37
29	l7	201	PEB	C2C-C3C	3.20	1.47	1.37
29	l9	201	PEB	C2C-C3C	3.20	1.47	1.37
29	dF	203	PEB	C1A-NA	-3.20	1.33	1.37
29	dI	203	PEB	C1A-NA	-3.20	1.33	1.37
29	RF	201	PEB	C2C-C3C	3.20	1.47	1.37
29	RI	201	PEB	C2C-C3C	3.20	1.47	1.37
31	fP	1001	CYC	C1B-C2B	3.20	1.50	1.45
29	G4	201	PEB	C2A-C1A	-3.20	1.49	1.52
29	GD	201	PEB	C2A-C1A	-3.20	1.49	1.52
31	jP	1001	CYC	C1B-C2B	3.20	1.50	1.45
29	RB	203	PEB	C2A-C1A	-3.20	1.49	1.52
29	MD	201	PEB	C2A-C1A	-3.20	1.49	1.52
29	RM	203	PEB	C2A-C1A	-3.20	1.49	1.52
31	OP	1001	CYC	C1B-C2B	3.20	1.50	1.45
29	I5	202	PEB	C2C-C3C	3.20	1.47	1.37
29	I8	202	PEB	C2C-C3C	3.20	1.47	1.37
29	A7	301	PEB	CHA-C1B	3.20	1.47	1.40
29	A9	301	PEB	CHA-C1B	3.20	1.47	1.40
29	jF	202	PEB	C1A-NA	-3.20	1.33	1.37
29	jI	202	PEB	C1A-NA	-3.20	1.33	1.37
29	F7	1002	PEB	C2C-C3C	3.20	1.47	1.37
29	LB	203	PEB	C2A-C1A	-3.20	1.49	1.52
29	LM	203	PEB	C2A-C1A	-3.20	1.49	1.52
29	AC	203	PEB	C2C-C3C	3.20	1.47	1.37
29	AE	203	PEB	C2C-C3C	3.20	1.47	1.37
29	FF	1002	PEB	C2A-C1A	-3.20	1.49	1.52
29	FI	1002	PEB	C2A-C1A	-3.20	1.49	1.52
30	wJ	305	PUB	C3B-C2B	3.20	1.47	1.37
30	MA	402	PUB	C3B-C2B	3.19	1.47	1.37
29	N3	203	PEB	C2C-C3C	3.19	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	nP	1001	CYC	C1B-C2B	3.19	1.50	1.45
29	CG	201	PEB	CHA-C1B	3.19	1.47	1.40
29	CQ	201	PEB	CHA-C1B	3.19	1.47	1.40
29	h7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	h9	201	PEB	C2C-C3C	3.19	1.47	1.37
29	AM	301	PEB	CHA-C1B	3.19	1.47	1.40
29	O7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	O9	201	PEB	C2C-C3C	3.19	1.47	1.37
29	C4	201	PEB	C2A-C1A	-3.19	1.49	1.52
29	cB	203	PEB	C2A-C1A	-3.19	1.49	1.52
29	cM	203	PEB	C2A-C1A	-3.19	1.49	1.52
29	G4	203	PEB	CHA-C1B	3.19	1.47	1.40
29	GD	203	PEB	CHA-C1B	3.19	1.47	1.40
29	H7	1002	PEB	C2C-C3C	3.19	1.47	1.37
29	Z7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	H9	1002	PEB	C2C-C3C	3.19	1.47	1.37
29	Z9	201	PEB	C2C-C3C	3.19	1.47	1.37
29	U7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	U9	201	PEB	C2C-C3C	3.19	1.47	1.37
31	DP	1001	CYC	C1B-C2B	3.19	1.50	1.45
29	L7	1002	PEB	C2C-C3C	3.19	1.47	1.37
31	QP	1001	CYC	C1B-C2B	3.19	1.50	1.45
29	U2	201	PEB	CHA-C1B	3.19	1.47	1.40
29	MQ	406	PEB	CHA-C1B	3.19	1.47	1.40
29	M2	201	PEB	CHA-C1B	3.19	1.47	1.40
29	MR	201	PEB	CHA-C1B	3.19	1.47	1.40
29	KD	203	PEB	CHA-C1B	3.19	1.47	1.40
29	d7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	d9	201	PEB	C2C-C3C	3.19	1.47	1.37
29	BC	202	PEB	C2C-C3C	3.19	1.47	1.37
29	BE	202	PEB	C2C-C3C	3.19	1.47	1.37
29	Q7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	Q9	201	PEB	C2C-C3C	3.19	1.47	1.37
31	oP	1001	CYC	C1B-C2B	3.19	1.50	1.45
29	W7	201	PEB	C2C-C3C	3.19	1.47	1.37
29	W9	201	PEB	C2C-C3C	3.19	1.47	1.37
29	LC	202	PEB	C2C-C3C	3.19	1.47	1.37
29	LE	202	PEB	C2C-C3C	3.19	1.47	1.37
29	AF	301	PEB	C2C-C3C	3.18	1.47	1.37
29	AI	301	PEB	C2C-C3C	3.18	1.47	1.37
29	D7	1002	PEB	C2C-C3C	3.18	1.47	1.37
29	A8	202	PEB	C2C-C3C	3.18	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D9	1002	PEB	C2C-C3C	3.18	1.47	1.37
29	yJ	301	PEB	C2C-C3C	3.18	1.47	1.37
29	yL	301	PEB	C2C-C3C	3.18	1.47	1.37
29	RF	201	PEB	C2A-C1A	-3.18	1.49	1.52
29	RI	201	PEB	C2A-C1A	-3.18	1.49	1.52
29	N7	1002	PEB	C2C-C3C	3.18	1.47	1.37
29	N9	1002	PEB	C2C-C3C	3.18	1.47	1.37
29	mF	201	PEB	C2A-C1A	-3.18	1.49	1.52
29	mI	201	PEB	C2A-C1A	-3.18	1.49	1.52
29	O2	201	PEB	CHA-C1B	3.18	1.47	1.40
29	IG	201	PEB	CHA-C1B	3.18	1.47	1.40
29	IQ	201	PEB	CHA-C1B	3.18	1.47	1.40
29	f7	201	PEB	C2C-C3C	3.18	1.47	1.37
29	f9	201	PEB	C2C-C3C	3.18	1.47	1.37
31	BP	1001	CYC	C1B-C2B	3.18	1.50	1.45
29	MG	404	PEB	CHA-C1B	3.18	1.47	1.40
29	iB	203	PEB	C2A-C1A	-3.18	1.49	1.52
29	iM	203	PEB	C2A-C1A	-3.18	1.49	1.52
29	b7	201	PEB	C2C-C3C	3.18	1.47	1.37
29	b9	201	PEB	C2C-C3C	3.18	1.47	1.37
29	UR	201	PEB	CHA-C1B	3.18	1.47	1.40
29	F9	1002	PEB	C2C-C3C	3.17	1.47	1.37
29	WR	201	PEB	CHA-C1B	3.17	1.47	1.40
31	qP	1001	CYC	C1B-C2B	3.17	1.50	1.45
31	1P	1001	CYC	C1B-C2B	3.17	1.50	1.45
29	dJ	201	PEB	C2C-C3C	3.17	1.47	1.37
29	dL	201	PEB	C2C-C3C	3.17	1.47	1.37
29	T2	201	PEB	C2A-C1A	-3.17	1.49	1.52
29	NB	202	PEB	C2A-C1A	-3.17	1.49	1.52
29	NM	202	PEB	C2A-C1A	-3.17	1.49	1.52
29	W2	201	PEB	CHA-C1B	3.17	1.47	1.40
29	B4	202	PEB	C2C-C3C	3.17	1.47	1.37
29	G4	203	PEB	C2C-C3C	3.17	1.47	1.37
29	pJ	201	PEB	C2C-C3C	3.17	1.47	1.37
29	pL	201	PEB	C2C-C3C	3.17	1.47	1.37
29	j7	201	PEB	C2C-C3C	3.17	1.47	1.37
29	j9	201	PEB	C2C-C3C	3.17	1.47	1.37
29	J7	1002	PEB	C2C-C3C	3.17	1.47	1.37
29	KC	201	PEB	C2C-C3C	3.17	1.47	1.37
29	ID	203	PEB	C2C-C3C	3.17	1.47	1.37
29	KE	201	PEB	C2C-C3C	3.17	1.47	1.37
29	PJ	201	PEB	C2C-C3C	3.17	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	PL	201	PEB	C2C-C3C	3.17	1.47	1.37
29	HC	202	PEB	C2C-C3C	3.17	1.47	1.37
29	HE	202	PEB	C2C-C3C	3.17	1.47	1.37
29	ZB	203	PEB	C2A-C1A	-3.17	1.49	1.52
29	gB	203	PEB	C2A-C1A	-3.17	1.49	1.52
29	ZM	203	PEB	C2A-C1A	-3.17	1.49	1.52
29	gM	203	PEB	C2A-C1A	-3.17	1.49	1.52
29	J9	1002	PEB	C2C-C3C	3.17	1.47	1.37
29	K4	203	PEB	CHA-C1B	3.17	1.47	1.40
31	SP	1001	CYC	C1B-C2B	3.17	1.50	1.45
29	aF	201	PEB	C2A-C1A	-3.17	1.49	1.52
29	aI	201	PEB	C2A-C1A	-3.17	1.49	1.52
29	fJ	201	PEB	C2C-C3C	3.17	1.47	1.37
29	fL	201	PEB	C2C-C3C	3.17	1.47	1.37
29	L9	1002	PEB	C2C-C3C	3.17	1.47	1.37
29	BJ	201	PEB	C2C-C3C	3.17	1.47	1.37
29	BL	201	PEB	C2C-C3C	3.17	1.47	1.37
29	FC	202	PEB	C2C-C3C	3.16	1.47	1.37
29	FE	202	PEB	C2C-C3C	3.16	1.47	1.37
29	JB	203	PEB	C2A-C1A	-3.16	1.49	1.52
29	dD	401	PEB	C2A-C1A	-3.16	1.49	1.52
29	JM	203	PEB	C2A-C1A	-3.16	1.49	1.52
29	J4	202	PEB	C2C-C3C	3.16	1.47	1.37
29	E4	203	PEB	C2C-C3C	3.16	1.47	1.37
29	JB	202	PEB	CHA-C1B	3.16	1.47	1.40
29	JM	202	PEB	CHA-C1B	3.16	1.47	1.40
29	WF	202	PEB	C1A-NA	-3.16	1.33	1.37
29	WI	202	PEB	C1A-NA	-3.16	1.33	1.37
29	CD	203	PEB	C2C-C3C	3.16	1.47	1.37
29	FB	202	PEB	CHA-C1B	3.16	1.47	1.40
29	FM	202	PEB	CHA-C1B	3.16	1.47	1.40
29	B8	203	PEB	C2A-C1A	-3.16	1.49	1.52
29	DG	203	PEB	C2C-C3C	3.16	1.47	1.37
29	HD	202	PEB	C2C-C3C	3.16	1.47	1.37
29	ZB	202	PEB	CHA-C1B	3.16	1.47	1.40
29	ZM	202	PEB	CHA-C1B	3.16	1.47	1.40
31	MP	1001	CYC	C1B-C2B	3.16	1.50	1.45
29	TB	202	PEB	CHA-C1B	3.16	1.47	1.40
29	VB	202	PEB	CHA-C1B	3.16	1.47	1.40
29	TM	202	PEB	CHA-C1B	3.16	1.47	1.40
29	VM	202	PEB	CHA-C1B	3.16	1.47	1.40
29	E4	201	PEB	C2A-C1A	-3.16	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	cF	201	PEB	C2A-C1A	-3.16	1.49	1.52
29	cI	201	PEB	C2A-C1A	-3.16	1.49	1.52
29	S7	201	PEB	C2C-C3C	3.16	1.47	1.37
29	S9	201	PEB	C2C-C3C	3.16	1.47	1.37
29	BB	301	PEB	C2C-C3C	3.16	1.47	1.37
29	BM	301	PEB	C2C-C3C	3.16	1.47	1.37
29	M2	201	PEB	C2C-C3C	3.15	1.47	1.37
29	rJ	201	PEB	C2C-C3C	3.15	1.47	1.37
29	rL	201	PEB	C2C-C3C	3.15	1.47	1.37
29	MR	201	PEB	C2C-C3C	3.15	1.47	1.37
29	DB	202	PEB	CHA-C1B	3.15	1.47	1.40
29	DM	202	PEB	CHA-C1B	3.15	1.47	1.40
29	JJ	201	PEB	C2C-C3C	3.15	1.47	1.37
29	JL	201	PEB	C2C-C3C	3.15	1.47	1.37
31	sP	1001	CYC	C1B-C2B	3.15	1.50	1.45
29	M4	203	PEB	C1A-NA	-3.15	1.33	1.37
29	VF	201	PEB	C2A-C1A	-3.15	1.49	1.52
29	VI	201	PEB	C2A-C1A	-3.15	1.49	1.52
29	ED	202	PEB	C2C-C3C	3.15	1.47	1.37
29	XJ	201	PEB	C2C-C3C	3.15	1.47	1.37
29	XL	201	PEB	C2C-C3C	3.15	1.47	1.37
30	A7	303	PUB	C3B-C2B	3.15	1.47	1.37
30	A9	303	PUB	C3B-C2B	3.15	1.47	1.37
29	N2	201	PEB	C2A-C1A	-3.15	1.49	1.52
29	L4	202	PEB	C2A-C1A	-3.15	1.49	1.52
29	LD	202	PEB	C2A-C1A	-3.15	1.49	1.52
29	NR	201	PEB	C2A-C1A	-3.15	1.49	1.52
29	YB	201	PEB	CHA-C1B	3.15	1.47	1.40
29	YM	201	PEB	CHA-C1B	3.15	1.47	1.40
29	D4	202	PEB	C2C-C3C	3.15	1.47	1.37
29	C4	203	PEB	C2C-C3C	3.15	1.47	1.37
29	JD	202	PEB	C2C-C3C	3.15	1.47	1.37
31	xP	1001	CYC	C1D-CHD	3.15	1.53	1.41
31	kP	1001	CYC	C1B-C2B	3.15	1.50	1.45
29	FD	202	PEB	C2A-C1A	-3.15	1.49	1.52
29	JG	203	PEB	C2C-C3C	3.15	1.47	1.37
29	nJ	201	PEB	C2C-C3C	3.15	1.47	1.37
29	nL	201	PEB	C2C-C3C	3.15	1.47	1.37
29	HB	202	PEB	CHA-C1B	3.15	1.47	1.40
29	HM	202	PEB	CHA-C1B	3.15	1.47	1.40
29	DB	203	PEB	C2A-C1A	-3.15	1.49	1.52
29	iF	201	PEB	C2A-C1A	-3.15	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	iI	201	PEB	C2A-C1A	-3.15	1.49	1.52
29	DM	203	PEB	C2A-C1A	-3.15	1.49	1.52
29	L4	202	PEB	C2C-C3C	3.15	1.47	1.37
29	GD	203	PEB	C2C-C3C	3.15	1.47	1.37
29	JQ	203	PEB	C2C-C3C	3.15	1.47	1.37
29	BD	202	PEB	C2C-C3C	3.15	1.47	1.37
29	NO	202	PEB	C1A-NA	-3.15	1.33	1.37
29	mB	203	PEB	C2A-C1A	-3.14	1.49	1.52
29	mM	203	PEB	C2A-C1A	-3.14	1.49	1.52
29	OF	203	PEB	CHA-C1B	3.14	1.47	1.40
29	OI	203	PEB	CHA-C1B	3.14	1.47	1.40
29	W2	201	PEB	C2C-C3C	3.14	1.47	1.37
29	RB	202	PEB	CHA-C1B	3.14	1.47	1.40
29	RM	202	PEB	CHA-C1B	3.14	1.47	1.40
30	BB	302	PUB	C3B-C2B	3.14	1.47	1.37
30	BM	302	PUB	C3B-C2B	3.14	1.47	1.37
29	NF	1002	PEB	C2A-C1A	-3.14	1.49	1.52
29	YF	201	PEB	C2A-C1A	-3.14	1.49	1.52
29	NI	1002	PEB	C2A-C1A	-3.14	1.49	1.52
29	YI	201	PEB	C2A-C1A	-3.14	1.49	1.52
29	ZJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	ZL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	tJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	tL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	M3	202	PEB	C1A-NA	-3.14	1.33	1.37
29	MO	202	PEB	C1A-NA	-3.14	1.33	1.37
29	H4	202	PEB	C2A-C1A	-3.14	1.49	1.52
29	IB	201	PEB	C2A-C1A	-3.14	1.49	1.52
29	IM	201	PEB	C2A-C1A	-3.14	1.49	1.52
29	LJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	RJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	LL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	RL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	LD	202	PEB	C2C-C3C	3.14	1.47	1.37
29	jJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	jL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	FJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	FL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	KB	203	PEB	CHA-C1B	3.14	1.47	1.40
29	KM	203	PEB	CHA-C1B	3.14	1.47	1.40
29	KD	203	PEB	C2C-C3C	3.14	1.47	1.37
29	HG	203	PEB	C2C-C3C	3.14	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	kB	202	PEB	CHA-C1B	3.14	1.47	1.40
29	kM	202	PEB	CHA-C1B	3.14	1.47	1.40
29	F4	202	PEB	C2C-C3C	3.14	1.47	1.37
29	aB	203	PEB	CHA-C1B	3.14	1.47	1.40
29	cB	202	PEB	CHA-C1B	3.14	1.47	1.40
29	aM	203	PEB	CHA-C1B	3.14	1.47	1.40
29	cM	202	PEB	CHA-C1B	3.14	1.47	1.40
29	DJ	201	PEB	C2C-C3C	3.14	1.47	1.37
29	DL	201	PEB	C2C-C3C	3.14	1.47	1.37
29	fF	202	PEB	C1A-NA	-3.14	1.33	1.37
29	fI	202	PEB	C1A-NA	-3.14	1.33	1.37
29	NJ	201	PEB	C2C-C3C	3.13	1.47	1.37
29	TJ	201	PEB	C2C-C3C	3.13	1.47	1.37
29	NL	201	PEB	C2C-C3C	3.13	1.47	1.37
29	TL	201	PEB	C2C-C3C	3.13	1.47	1.37
29	UF	203	PEB	C1A-NA	-3.13	1.33	1.37
29	hF	202	PEB	C1A-NA	-3.13	1.33	1.37
29	UI	203	PEB	C1A-NA	-3.13	1.33	1.37
29	hI	202	PEB	C1A-NA	-3.13	1.33	1.37
29	H4	202	PEB	C2C-C3C	3.13	1.47	1.37
29	bJ	201	PEB	C2C-C3C	3.13	1.47	1.37
29	bL	201	PEB	C2C-C3C	3.13	1.47	1.37
29	V2	201	PEB	C2A-C1A	-3.13	1.49	1.52
29	DD	202	PEB	C2C-C3C	3.13	1.47	1.37
29	DQ	203	PEB	C2C-C3C	3.13	1.47	1.37
29	MD	203	PEB	C2C-C3C	3.13	1.46	1.37
29	vJ	201	PEB	C2C-C3C	3.13	1.46	1.37
29	vL	201	PEB	C2C-C3C	3.13	1.46	1.37
29	FQ	203	PEB	C2C-C3C	3.13	1.46	1.37
29	iB	202	PEB	CHA-C1B	3.13	1.47	1.40
29	iM	202	PEB	CHA-C1B	3.13	1.47	1.40
29	FD	202	PEB	C2C-C3C	3.13	1.46	1.37
29	mB	202	PEB	CHA-C1B	3.13	1.47	1.40
29	mM	202	PEB	CHA-C1B	3.13	1.47	1.40
29	FG	203	PEB	C2C-C3C	3.13	1.46	1.37
29	N3	202	PEB	C1A-NA	-3.13	1.33	1.37
29	OB	201	PEB	C2A-C1A	-3.13	1.49	1.52
29	OM	201	PEB	C2A-C1A	-3.13	1.49	1.52
29	BG	203	PEB	C2C-C3C	3.13	1.46	1.37
31	VP	1001	CYC	C1D-CHD	3.13	1.53	1.41
29	LG	203	PEB	C2C-C3C	3.13	1.46	1.37
29	VJ	201	PEB	C2C-C3C	3.13	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VL	201	PEB	C2C-C3C	3.13	1.46	1.37
29	BQ	203	PEB	C2C-C3C	3.12	1.46	1.37
29	MB	201	PEB	C2A-C1A	-3.12	1.49	1.52
29	MM	201	PEB	C2A-C1A	-3.12	1.49	1.52
29	HQ	203	PEB	C2C-C3C	3.12	1.46	1.37
29	QR	201	PEB	C2C-C3C	3.12	1.46	1.37
29	VF	202	PEB	CHA-C1B	3.12	1.47	1.40
29	VI	202	PEB	CHA-C1B	3.12	1.47	1.40
29	Q2	201	PEB	C2C-C3C	3.12	1.46	1.37
29	UR	201	PEB	C2C-C3C	3.12	1.46	1.37
29	LB	202	PEB	CHA-C1B	3.12	1.47	1.40
29	LM	202	PEB	CHA-C1B	3.12	1.47	1.40
29	QB	202	PEB	CHA-C1B	3.12	1.47	1.40
29	QM	202	PEB	CHA-C1B	3.12	1.47	1.40
29	IJ	201	PEB	C2C-C3C	3.12	1.46	1.37
29	IL	201	PEB	C2C-C3C	3.12	1.46	1.37
29	hJ	201	PEB	C2C-C3C	3.12	1.46	1.37
29	hL	201	PEB	C2C-C3C	3.12	1.46	1.37
29	dF	201	PEB	CHA-C1B	3.12	1.47	1.40
29	dI	201	PEB	CHA-C1B	3.12	1.47	1.40
29	O2	201	PEB	C2C-C3C	3.12	1.46	1.37
29	OR	201	PEB	C2C-C3C	3.12	1.46	1.37
29	PF	203	PEB	C2A-C1A	-3.12	1.49	1.52
29	PI	203	PEB	C2A-C1A	-3.12	1.49	1.52
29	YF	202	PEB	CHA-C1B	3.12	1.47	1.40
29	YI	202	PEB	CHA-C1B	3.12	1.47	1.40
29	gB	202	PEB	CHA-C1B	3.11	1.47	1.40
29	gM	202	PEB	CHA-C1B	3.11	1.47	1.40
29	WR	201	PEB	C2C-C3C	3.11	1.46	1.37
29	aF	202	PEB	CHA-C1B	3.11	1.47	1.40
29	aI	202	PEB	CHA-C1B	3.11	1.47	1.40
29	gF	203	PEB	C2A-C1A	-3.11	1.49	1.52
29	gI	203	PEB	C2A-C1A	-3.11	1.49	1.52
29	DF	1002	PEB	C2A-C1A	-3.11	1.49	1.52
29	DI	1002	PEB	C2A-C1A	-3.11	1.49	1.52
29	U2	201	PEB	C2C-C3C	3.11	1.46	1.37
29	PF	202	PEB	CHA-C1B	3.11	1.47	1.40
29	PI	202	PEB	CHA-C1B	3.11	1.47	1.40
29	b1	201	PEB	C2C-C3C	3.11	1.46	1.37
29	bK	201	PEB	C2C-C3C	3.11	1.46	1.37
29	YF	203	PEB	C2A-C1A	-3.11	1.49	1.52
29	YI	203	PEB	C2A-C1A	-3.11	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	KC	201	PEB	CHA-C1B	3.11	1.47	1.40
29	KE	201	PEB	CHA-C1B	3.11	1.47	1.40
29	hB	201	PEB	C2A-C1A	-3.11	1.49	1.52
29	hM	201	PEB	C2A-C1A	-3.11	1.49	1.52
29	HC	202	PEB	CHA-C1B	3.11	1.47	1.40
29	HE	202	PEB	CHA-C1B	3.11	1.47	1.40
29	CB	201	PEB	C2A-C1A	-3.11	1.49	1.52
29	CM	201	PEB	C2A-C1A	-3.11	1.49	1.52
30	yJ	302	PUB	C3B-C2B	3.11	1.46	1.37
30	yL	302	PUB	C3B-C2B	3.11	1.46	1.37
29	K4	203	PEB	C2C-C3C	3.11	1.46	1.37
29	SB	201	PEB	C2A-C1A	-3.11	1.49	1.52
29	SM	201	PEB	C2A-C1A	-3.11	1.49	1.52
29	DD	202	PEB	C2A-C1A	-3.10	1.49	1.52
31	xP	1001	CYC	O1A-CGA	3.10	1.32	1.22
29	fI	201	PEB	C2C-C3C	3.10	1.46	1.37
29	fK	201	PEB	C2C-C3C	3.10	1.46	1.37
29	J4	202	PEB	C2A-C1A	-3.10	1.49	1.52
29	KB	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	KM	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	K4	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	KD	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	UB	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	eF	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	eI	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	UM	201	PEB	C2A-C1A	-3.10	1.49	1.52
29	kF	202	PEB	CHA-C1B	3.10	1.47	1.40
29	kI	202	PEB	CHA-C1B	3.10	1.47	1.40
29	B4	202	PEB	C2A-C1A	-3.09	1.49	1.52
29	BD	202	PEB	C2A-C1A	-3.09	1.49	1.52
29	B5	203	PEB	C2A-C1A	-3.09	1.49	1.52
29	ZB	201	PEB	C2A-C1A	-3.09	1.49	1.52
29	ZM	201	PEB	C2A-C1A	-3.09	1.49	1.52
29	iF	202	PEB	CHA-C1B	3.09	1.47	1.40
29	iI	202	PEB	CHA-C1B	3.09	1.47	1.40
29	Z1	202	PEB	C2C-C3C	3.09	1.46	1.37
29	ZK	202	PEB	C2C-C3C	3.09	1.46	1.37
29	UF	201	PEB	CHA-C1B	3.09	1.47	1.40
29	UI	201	PEB	CHA-C1B	3.09	1.47	1.40
29	LC	202	PEB	CHA-C1B	3.09	1.47	1.40
29	LE	202	PEB	CHA-C1B	3.09	1.47	1.40
29	jB	201	PEB	C2A-C1A	-3.09	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	jM	201	PEB	C2A-C1A	-3.09	1.49	1.52
29	AC	203	PEB	CHA-C1B	3.09	1.47	1.40
29	AE	203	PEB	CHA-C1B	3.09	1.47	1.40
29	eF	202	PEB	CHA-C1B	3.09	1.47	1.40
29	eI	202	PEB	CHA-C1B	3.09	1.47	1.40
29	Z7	202	PEB	CHA-C1B	3.09	1.47	1.40
29	Z9	202	PEB	CHA-C1B	3.09	1.47	1.40
29	S7	202	PEB	CHA-C1B	3.08	1.47	1.40
29	S9	202	PEB	CHA-C1B	3.08	1.47	1.40
29	EB	201	PEB	C2A-C1A	-3.08	1.49	1.52
29	EM	201	PEB	C2A-C1A	-3.08	1.49	1.52
29	Q7	202	PEB	CHA-C1B	3.08	1.47	1.40
29	Q9	202	PEB	CHA-C1B	3.08	1.47	1.40
29	d1	201	PEB	C2C-C3C	3.08	1.46	1.37
29	dK	201	PEB	C2C-C3C	3.08	1.46	1.37
30	AM	304	PUB	C3B-C2B	3.08	1.46	1.37
29	gF	202	PEB	CHA-C1B	3.08	1.47	1.40
29	gI	202	PEB	CHA-C1B	3.08	1.47	1.40
29	VF	203	PEB	C2A-C1A	-3.08	1.49	1.52
29	VI	203	PEB	C2A-C1A	-3.08	1.49	1.52
29	VR	201	PEB	C2A-C1A	-3.08	1.49	1.52
29	eF	203	PEB	C2A-C1A	-3.08	1.49	1.52
29	eI	203	PEB	C2A-C1A	-3.08	1.49	1.52
29	d7	202	PEB	CHA-C1B	3.08	1.47	1.40
29	d9	202	PEB	CHA-C1B	3.08	1.47	1.40
29	O1	201	PEB	C2C-C3C	3.08	1.46	1.37
29	OK	201	PEB	C2C-C3C	3.08	1.46	1.37
29	f7	202	PEB	CHA-C1B	3.08	1.47	1.40
29	f9	202	PEB	CHA-C1B	3.08	1.47	1.40
29	mF	202	PEB	CHA-C1B	3.08	1.47	1.40
29	mI	202	PEB	CHA-C1B	3.08	1.47	1.40
29	W7	202	PEB	CHA-C1B	3.08	1.47	1.40
29	W9	202	PEB	CHA-C1B	3.08	1.47	1.40
29	JF	1002	PEB	C2A-C1A	-3.07	1.49	1.52
29	JI	1002	PEB	C2A-C1A	-3.07	1.49	1.52
29	LQ	202	PEB	C2C-C3C	3.07	1.46	1.37
29	FC	202	PEB	CHA-C1B	3.07	1.47	1.40
29	FE	202	PEB	CHA-C1B	3.07	1.47	1.40
29	T2	203	PEB	C2A-C1A	-3.07	1.49	1.52
29	h1	201	PEB	C2C-C3C	3.07	1.46	1.37
29	hK	201	PEB	C2C-C3C	3.07	1.46	1.37
29	F5	203	PEB	C2A-C1A	-3.07	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F8	203	PEB	C2A-C1A	-3.07	1.49	1.52
30	AB	304	PUB	C3B-C2B	3.07	1.46	1.37
31	VP	1001	CYC	O1A-CGA	3.07	1.32	1.22
29	TR	201	PEB	C2A-C1A	-3.07	1.49	1.52
29	BC	202	PEB	CHA-C1B	3.07	1.47	1.40
29	BE	202	PEB	CHA-C1B	3.07	1.47	1.40
29	Q1	201	PEB	C2C-C3C	3.06	1.46	1.37
29	QK	201	PEB	C2C-C3C	3.06	1.46	1.37
29	T7	203	PEB	C1A-NA	-3.06	1.33	1.37
29	T9	203	PEB	C1A-NA	-3.06	1.33	1.37
29	VB	201	PEB	C2A-C1A	-3.06	1.49	1.52
29	VM	201	PEB	C2A-C1A	-3.06	1.49	1.52
29	S1	201	PEB	C2C-C3C	3.06	1.46	1.37
29	SK	201	PEB	C2C-C3C	3.06	1.46	1.37
29	h7	202	PEB	CHA-C1B	3.06	1.47	1.40
29	h9	202	PEB	CHA-C1B	3.06	1.47	1.40
29	W1	201	PEB	C2C-C3C	3.06	1.46	1.37
29	WK	201	PEB	C2C-C3C	3.06	1.46	1.37
29	O7	201	PEB	CHA-C1B	3.06	1.47	1.40
29	O9	201	PEB	CHA-C1B	3.06	1.47	1.40
29	j1	201	PEB	C2C-C3C	3.06	1.46	1.37
29	jK	201	PEB	C2C-C3C	3.06	1.46	1.37
29	jF	202	PEB	OD-C4D	3.06	1.29	1.23
29	jI	202	PEB	OD-C4D	3.06	1.29	1.23
29	U7	201	PEB	CHA-C1B	3.05	1.47	1.40
29	b7	202	PEB	CHA-C1B	3.05	1.47	1.40
29	U9	201	PEB	CHA-C1B	3.05	1.47	1.40
29	b9	202	PEB	CHA-C1B	3.05	1.47	1.40
29	l1	201	PEB	C2C-C3C	3.05	1.46	1.37
29	lK	201	PEB	C2C-C3C	3.05	1.46	1.37
29	aF	203	PEB	C2A-C1A	-3.05	1.49	1.52
29	aI	203	PEB	C2A-C1A	-3.05	1.49	1.52
29	OF	202	PEB	OD-C4D	3.05	1.29	1.23
29	OI	202	PEB	OD-C4D	3.05	1.29	1.23
29	iF	203	PEB	C2A-C1A	-3.05	1.49	1.52
29	iI	203	PEB	C2A-C1A	-3.05	1.49	1.52
29	R7	203	PEB	C1A-NA	-3.05	1.33	1.37
29	R9	203	PEB	C1A-NA	-3.05	1.33	1.37
29	DB	201	PEB	C2A-C1A	-3.05	1.49	1.52
29	DM	201	PEB	C2A-C1A	-3.05	1.49	1.52
29	U1	202	PEB	C2C-C3C	3.05	1.46	1.37
29	UK	202	PEB	C2C-C3C	3.05	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d7	201	PEB	CHA-C1B	3.05	1.47	1.40
29	d9	201	PEB	CHA-C1B	3.05	1.47	1.40
29	S7	201	PEB	CHA-C1B	3.05	1.47	1.40
29	S9	201	PEB	CHA-C1B	3.05	1.47	1.40
29	cF	202	PEB	C2A-C1A	-3.05	1.49	1.52
29	cI	202	PEB	C2A-C1A	-3.05	1.49	1.52
29	l7	202	PEB	CHA-C1B	3.05	1.47	1.40
29	l9	202	PEB	CHA-C1B	3.05	1.47	1.40
29	mB	201	PEB	C2A-C1A	-3.05	1.49	1.52
29	mM	201	PEB	C2A-C1A	-3.05	1.49	1.52
30	MN	402	PUB	OA-C1A	3.05	1.29	1.23
29	hF	202	PEB	OD-C4D	3.05	1.29	1.23
29	hI	202	PEB	OD-C4D	3.05	1.29	1.23
29	DJ	202	PEB	C2A-C1A	-3.05	1.49	1.52
29	DL	202	PEB	C2A-C1A	-3.05	1.49	1.52
29	W7	201	PEB	CHA-C1B	3.04	1.47	1.40
29	W9	201	PEB	CHA-C1B	3.04	1.47	1.40
29	kB	201	PEB	C2A-C1A	-3.04	1.49	1.52
29	kM	201	PEB	C2A-C1A	-3.04	1.49	1.52
29	mF	203	PEB	C2A-C1A	-3.04	1.49	1.52
29	mI	203	PEB	C2A-C1A	-3.04	1.49	1.52
30	AF	303	PUB	C3B-C2B	3.04	1.46	1.37
30	AI	303	PUB	C3B-C2B	3.04	1.46	1.37
29	tJ	202	PEB	C2A-C1A	-3.04	1.49	1.52
29	tL	202	PEB	C2A-C1A	-3.04	1.49	1.52
29	j7	201	PEB	CHA-C1B	3.04	1.47	1.40
29	j9	201	PEB	CHA-C1B	3.04	1.47	1.40
29	aB	201	PEB	C2A-C1A	-3.04	1.49	1.52
29	aM	201	PEB	C2A-C1A	-3.04	1.49	1.52
29	O7	202	PEB	CHA-C1B	3.04	1.47	1.40
29	U7	202	PEB	CHA-C1B	3.04	1.47	1.40
29	O9	202	PEB	CHA-C1B	3.04	1.47	1.40
29	U9	202	PEB	CHA-C1B	3.04	1.47	1.40
29	Y7	203	PEB	C1A-NA	-3.04	1.33	1.37
29	Y9	203	PEB	C1A-NA	-3.04	1.33	1.37
30	MA	402	PUB	OA-C1A	3.04	1.29	1.23
29	WB	201	PEB	C2A-C1A	-3.04	1.49	1.52
29	WM	201	PEB	C2A-C1A	-3.04	1.49	1.52
29	l7	201	PEB	CHA-C1B	3.04	1.47	1.40
29	l9	201	PEB	CHA-C1B	3.04	1.47	1.40
29	G5	203	PEB	C2A-C1A	-3.03	1.49	1.52
29	YB	202	PEB	C2A-C1A	-3.03	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YM	202	PEB	C2A-C1A	-3.03	1.49	1.52
29	iB	201	PEB	C2A-C1A	-3.03	1.49	1.52
29	iM	201	PEB	C2A-C1A	-3.03	1.49	1.52
29	fF	202	PEB	OD-C4D	3.03	1.29	1.23
29	fI	202	PEB	OD-C4D	3.03	1.29	1.23
29	m7	203	PEB	C1A-NA	-3.03	1.33	1.37
29	m9	203	PEB	C1A-NA	-3.03	1.33	1.37
29	ID	201	PEB	CHA-C1B	3.03	1.47	1.40
29	GD	201	PEB	CHA-C1B	3.03	1.47	1.40
29	BG	201	PEB	C2A-C1A	-3.03	1.49	1.52
29	hJ	203	PEB	C2A-C1A	-3.03	1.49	1.52
29	hL	203	PEB	C2A-C1A	-3.03	1.49	1.52
29	BQ	201	PEB	C2A-C1A	-3.03	1.49	1.52
29	fB	201	PEB	C2A-C1A	-3.03	1.49	1.52
29	fM	201	PEB	C2A-C1A	-3.03	1.49	1.52
29	P2	202	PEB	C2A-C1A	-3.03	1.49	1.52
29	TF	202	PEB	C2A-C1A	-3.03	1.49	1.52
29	kF	203	PEB	C2A-C1A	-3.03	1.49	1.52
29	TI	202	PEB	C2A-C1A	-3.03	1.49	1.52
29	kI	203	PEB	C2A-C1A	-3.03	1.49	1.52
29	lF	202	PEB	OD-C4D	3.03	1.29	1.23
29	lI	202	PEB	OD-C4D	3.03	1.29	1.23
29	b7	201	PEB	CHA-C1B	3.02	1.47	1.40
29	b9	201	PEB	CHA-C1B	3.02	1.47	1.40
29	h7	201	PEB	CHA-C1B	3.02	1.47	1.40
29	h9	201	PEB	CHA-C1B	3.02	1.47	1.40
29	GB	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	dB	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	GM	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	dM	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	ZF	202	PEB	OD-C4D	3.02	1.29	1.23
29	ZI	202	PEB	OD-C4D	3.02	1.29	1.23
29	f7	201	PEB	CHA-C1B	3.02	1.47	1.40
29	f9	201	PEB	CHA-C1B	3.02	1.47	1.40
29	ID	201	PEB	C2C-C3C	3.02	1.46	1.37
29	G4	201	PEB	CHA-C1B	3.02	1.47	1.40
29	Q7	201	PEB	CHA-C1B	3.02	1.47	1.40
29	Q9	201	PEB	CHA-C1B	3.02	1.47	1.40
29	bF	202	PEB	OD-C4D	3.02	1.29	1.23
29	bI	202	PEB	OD-C4D	3.02	1.29	1.23
29	V1	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	NB	201	PEB	C2A-C1A	-3.02	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JD	202	PEB	C2A-C1A	-3.02	1.49	1.52
29	VK	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	NM	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	dD	401	PEB	CHA-C1B	3.02	1.47	1.40
29	j7	202	PEB	CHA-C1B	3.02	1.47	1.40
29	j9	202	PEB	CHA-C1B	3.02	1.47	1.40
29	F4	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	HB	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	HM	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	gJ	202	PEB	OD-C4D	3.02	1.29	1.23
29	gL	202	PEB	OD-C4D	3.02	1.29	1.23
29	qJ	202	PEB	OD-C4D	3.02	1.29	1.23
29	qL	202	PEB	OD-C4D	3.02	1.29	1.23
29	F4	202	PEB	C2A-C1A	-3.02	1.49	1.52
29	FB	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	FM	201	PEB	C2A-C1A	-3.02	1.49	1.52
29	E4	201	PEB	CHA-C1B	3.02	1.47	1.40
29	MG	404	PEB	C2C-C3C	3.02	1.46	1.37
29	e7	203	PEB	C1A-NA	-3.02	1.33	1.37
29	e9	203	PEB	C1A-NA	-3.02	1.33	1.37
29	LJ	202	PEB	C2A-C1A	-3.01	1.49	1.52
29	LL	202	PEB	C2A-C1A	-3.01	1.49	1.52
29	RR	203	PEB	C2A-C1A	-3.01	1.49	1.52
31	I7	1001	CYC	C2C-C1C	-3.01	1.49	1.52
31	I9	1001	CYC	C2C-C1C	-3.01	1.49	1.52
29	C4	201	PEB	CHA-C1B	3.01	1.47	1.40
29	eB	201	PEB	C2A-C1A	-3.01	1.49	1.52
29	DG	202	PEB	C2A-C1A	-3.01	1.49	1.52
29	eM	201	PEB	C2A-C1A	-3.01	1.49	1.52
29	DQ	202	PEB	C2A-C1A	-3.01	1.49	1.52
29	mJ	202	PEB	OD-C4D	3.01	1.29	1.23
29	mL	202	PEB	OD-C4D	3.01	1.29	1.23
29	C4	201	PEB	C2C-C3C	3.01	1.46	1.37
29	lB	201	PEB	C2A-C1A	-3.01	1.49	1.52
29	lM	201	PEB	C2A-C1A	-3.01	1.49	1.52
29	i7	203	PEB	C1A-NA	-3.01	1.33	1.37
29	i9	203	PEB	C1A-NA	-3.01	1.33	1.37
31	E7	1001	CYC	C2C-C1C	-3.01	1.49	1.52
31	E9	1001	CYC	C2C-C1C	-3.01	1.49	1.52
29	QF	202	PEB	OD-C4D	3.01	1.29	1.23
29	QI	202	PEB	OD-C4D	3.01	1.29	1.23
29	B3	203	PEB	C2A-C1A	-3.01	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QB	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	vJ	202	PEB	C2A-C1A	-3.01	1.49	1.52
29	vL	202	PEB	C2A-C1A	-3.01	1.49	1.52
29	QM	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	BO	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	R2	202	PEB	C2C-C3C	3.01	1.46	1.37
29	JG	201	PEB	C2A-C1A	-3.01	1.49	1.52
29	JQ	201	PEB	C2A-C1A	-3.01	1.49	1.52
31	M7	1001	CYC	C2C-C1C	-3.01	1.49	1.52
29	I4	201	PEB	C2C-C3C	3.01	1.46	1.37
29	RR	202	PEB	C2C-C3C	3.01	1.46	1.37
29	UF	203	PEB	OD-C4D	3.01	1.29	1.23
29	UI	203	PEB	OD-C4D	3.01	1.29	1.23
29	FJ	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	FL	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	MD	201	PEB	C2C-C3C	3.01	1.46	1.37
29	rJ	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	rL	203	PEB	C2A-C1A	-3.01	1.49	1.52
29	nJ	203	PEB	C2A-C1A	-3.00	1.49	1.52
29	nL	203	PEB	C2A-C1A	-3.00	1.49	1.52
29	SF	202	PEB	OD-C4D	3.00	1.29	1.23
29	SI	202	PEB	OD-C4D	3.00	1.29	1.23
29	MQ	406	PEB	C2C-C3C	3.00	1.46	1.37
29	Z7	201	PEB	CHA-C1B	3.00	1.47	1.40
29	Z9	201	PEB	CHA-C1B	3.00	1.47	1.40
31	G9	1001	CYC	C2C-C1C	-3.00	1.49	1.52
29	UJ	202	PEB	OD-C4D	3.00	1.29	1.23
29	UL	202	PEB	OD-C4D	3.00	1.29	1.23
29	QJ	202	PEB	OD-C4D	3.00	1.29	1.23
29	QL	202	PEB	OD-C4D	3.00	1.29	1.23
29	X2	202	PEB	C2A-C1A	-3.00	1.49	1.52
29	k1	201	PEB	C2A-C1A	-3.00	1.49	1.52
29	RB	201	PEB	C2A-C1A	-3.00	1.49	1.52
29	kK	201	PEB	C2A-C1A	-3.00	1.49	1.52
29	RM	201	PEB	C2A-C1A	-3.00	1.49	1.52
29	MD	201	PEB	CHA-C1B	3.00	1.47	1.40
29	M4	201	PEB	CHA-C1B	3.00	1.47	1.40
29	WJ	203	PEB	OD-C4D	3.00	1.29	1.23
29	WL	203	PEB	OD-C4D	3.00	1.29	1.23
29	YJ	202	PEB	OD-C4D	3.00	1.29	1.23
29	YL	202	PEB	OD-C4D	3.00	1.29	1.23
29	jJ	203	PEB	C2A-C1A	-3.00	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	jL	203	PEB	C2A-C1A	-3.00	1.49	1.52
29	kJ	202	PEB	OD-C4D	3.00	1.29	1.23
29	kL	202	PEB	OD-C4D	3.00	1.29	1.23
31	C7	1001	CYC	C2C-C1C	-3.00	1.49	1.52
31	C9	1001	CYC	C2C-C1C	-3.00	1.49	1.52
29	MJ	202	PEB	OD-C4D	3.00	1.29	1.23
29	ML	202	PEB	OD-C4D	3.00	1.29	1.23
29	g7	203	PEB	C1A-NA	-3.00	1.33	1.37
29	g9	203	PEB	C1A-NA	-3.00	1.33	1.37
29	CD	201	PEB	CHA-C1B	3.00	1.47	1.40
29	M4	201	PEB	C2C-C3C	3.00	1.46	1.37
29	I4	201	PEB	CHA-C1B	2.99	1.47	1.40
29	dJ	203	PEB	C2A-C1A	-2.99	1.49	1.52
29	dL	203	PEB	C2A-C1A	-2.99	1.49	1.52
29	sJ	203	PEB	CHA-C1B	2.99	1.47	1.40
29	sL	203	PEB	CHA-C1B	2.99	1.47	1.40
29	U2	202	PEB	OD-C4D	2.99	1.29	1.23
29	TB	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	TM	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	P1	201	PEB	C2C-C3C	2.99	1.46	1.37
29	c1	201	PEB	C2C-C3C	2.99	1.46	1.37
29	m1	201	PEB	C2C-C3C	2.99	1.46	1.37
29	PK	201	PEB	C2C-C3C	2.99	1.46	1.37
29	cK	201	PEB	C2C-C3C	2.99	1.46	1.37
29	mK	201	PEB	C2C-C3C	2.99	1.46	1.37
29	K4	201	PEB	CHA-C1B	2.99	1.47	1.40
29	V7	203	PEB	C1A-NA	-2.99	1.33	1.37
29	k7	203	PEB	C1A-NA	-2.99	1.33	1.37
29	V9	203	PEB	C1A-NA	-2.99	1.33	1.37
29	k9	203	PEB	C1A-NA	-2.99	1.33	1.37
29	oJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	oL	202	PEB	OD-C4D	2.99	1.29	1.23
29	WF	202	PEB	OD-C4D	2.99	1.29	1.23
29	WI	202	PEB	OD-C4D	2.99	1.29	1.23
29	SJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	SL	202	PEB	OD-C4D	2.99	1.29	1.23
29	J3	202	PEB	CHC-C4C	2.99	1.57	1.50
29	JO	202	PEB	CHC-C4C	2.99	1.57	1.50
29	P7	203	PEB	C1A-NA	-2.99	1.33	1.37
29	P9	203	PEB	C1A-NA	-2.99	1.33	1.37
29	H3	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	HO	201	PEB	C2A-C1A	-2.99	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	CD	201	PEB	C2C-C3C	2.99	1.46	1.37
29	KJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	KL	202	PEB	OD-C4D	2.99	1.29	1.23
29	aJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	aL	202	PEB	OD-C4D	2.99	1.29	1.23
29	a1	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	L3	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	HJ	202	PEB	C2A-C1A	-2.99	1.49	1.52
29	aK	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	HL	202	PEB	C2A-C1A	-2.99	1.49	1.52
29	LO	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	HJ	201	PEB	CHA-C1B	2.99	1.47	1.40
29	HL	201	PEB	CHA-C1B	2.99	1.47	1.40
29	P2	201	PEB	C2C-C3C	2.99	1.46	1.37
29	TR	202	PEB	C2C-C3C	2.99	1.46	1.37
29	SJ	201	PEB	C2C-C3C	2.99	1.46	1.37
29	SL	201	PEB	C2C-C3C	2.99	1.46	1.37
29	iJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	iL	202	PEB	OD-C4D	2.99	1.29	1.23
29	V1	201	PEB	C2C-C3C	2.99	1.46	1.37
29	VK	201	PEB	C2C-C3C	2.99	1.46	1.37
29	PR	201	PEB	C2C-C3C	2.99	1.46	1.37
29	jJ	202	PEB	CHA-C1B	2.99	1.47	1.40
29	jL	202	PEB	CHA-C1B	2.99	1.47	1.40
29	UR	202	PEB	OD-C4D	2.99	1.29	1.23
29	T1	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	TK	201	PEB	C2A-C1A	-2.99	1.49	1.52
29	c7	203	PEB	C1A-NA	-2.99	1.33	1.37
29	c9	203	PEB	C1A-NA	-2.99	1.33	1.37
29	k1	201	PEB	C2C-C3C	2.99	1.46	1.37
29	kK	201	PEB	C2C-C3C	2.99	1.46	1.37
29	AJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	AL	202	PEB	OD-C4D	2.99	1.29	1.23
29	sJ	202	PEB	OD-C4D	2.99	1.29	1.23
29	sL	202	PEB	OD-C4D	2.99	1.29	1.23
29	pJ	203	PEB	C2A-C1A	-2.98	1.49	1.52
29	pL	203	PEB	C2A-C1A	-2.98	1.49	1.52
29	L3	202	PEB	C2A-C1A	-2.98	1.49	1.52
29	LO	202	PEB	C2A-C1A	-2.98	1.49	1.52
29	KD	201	PEB	CHA-C1B	2.98	1.47	1.40
29	e1	201	PEB	C2C-C3C	2.98	1.46	1.37
29	eK	201	PEB	C2C-C3C	2.98	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	EJ	201	PEB	C2C-C3C	2.98	1.46	1.37
29	EL	201	PEB	C2C-C3C	2.98	1.46	1.37
29	dF	203	PEB	OD-C4D	2.98	1.29	1.23
29	dI	203	PEB	OD-C4D	2.98	1.29	1.23
29	VJ	202	PEB	C2A-C1A	-2.98	1.49	1.52
29	VL	202	PEB	C2A-C1A	-2.98	1.49	1.52
29	KJ	201	PEB	C2C-C3C	2.98	1.46	1.37
29	KL	201	PEB	C2C-C3C	2.98	1.46	1.37
29	FG	202	PEB	C2A-C1A	-2.98	1.49	1.52
29	FQ	202	PEB	C2A-C1A	-2.98	1.49	1.52
31	K9	1001	CYC	C2C-C1C	-2.98	1.49	1.52
29	I3	203	PEB	CHC-C4C	2.98	1.57	1.50
29	IO	203	PEB	CHC-C4C	2.98	1.57	1.50
29	pJ	202	PEB	CHA-C1B	2.98	1.47	1.40
29	pL	202	PEB	CHA-C1B	2.98	1.47	1.40
29	PB	201	PEB	C2A-C1A	-2.98	1.49	1.52
29	PM	201	PEB	C2A-C1A	-2.98	1.49	1.52
29	eJ	201	PEB	C2C-C3C	2.98	1.46	1.37
29	eL	201	PEB	C2C-C3C	2.98	1.46	1.37
29	cJ	201	PEB	C2C-C3C	2.98	1.46	1.37
29	cL	201	PEB	C2C-C3C	2.98	1.46	1.37
29	FJ	202	PEB	CHA-C1B	2.98	1.47	1.40
29	FL	202	PEB	CHA-C1B	2.98	1.47	1.40
29	FG	201	PEB	C2A-C1A	-2.98	1.49	1.52
29	FQ	201	PEB	C2A-C1A	-2.98	1.49	1.52
29	Y1	201	PEB	C2C-C3C	2.98	1.46	1.37
29	g1	201	PEB	C2C-C3C	2.98	1.46	1.37
29	YK	201	PEB	C2C-C3C	2.98	1.46	1.37
29	gK	201	PEB	C2C-C3C	2.98	1.46	1.37
29	bJ	202	PEB	CHA-C1B	2.98	1.47	1.40
29	bL	202	PEB	CHA-C1B	2.98	1.47	1.40
29	Y1	201	PEB	C2A-C1A	-2.98	1.49	1.52
29	YK	201	PEB	C2A-C1A	-2.98	1.49	1.52
29	E4	201	PEB	C2C-C3C	2.98	1.46	1.37
29	dD	401	PEB	C2C-C3C	2.98	1.46	1.37
29	WJ	202	PEB	C2C-C3C	2.98	1.46	1.37
29	WL	202	PEB	C2C-C3C	2.98	1.46	1.37
29	nJ	202	PEB	CHA-C1B	2.98	1.47	1.40
29	nL	202	PEB	CHA-C1B	2.98	1.47	1.40
31	HK	1001	CYC	C3D-C2D	2.98	1.46	1.37
29	uJ	203	PEB	OD-C4D	2.98	1.29	1.23
29	uL	203	PEB	OD-C4D	2.98	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	dJ	202	PEB	CHA-C1B	2.98	1.47	1.40
29	dL	202	PEB	CHA-C1B	2.98	1.47	1.40
29	a7	203	PEB	C1A-NA	-2.98	1.33	1.37
29	a9	203	PEB	C1A-NA	-2.98	1.33	1.37
29	MJ	201	PEB	C2C-C3C	2.98	1.46	1.37
29	ML	201	PEB	C2C-C3C	2.98	1.46	1.37
29	OJ	202	PEB	OD-C4D	2.98	1.29	1.23
29	OL	202	PEB	OD-C4D	2.98	1.29	1.23
29	K4	201	PEB	C2C-C3C	2.98	1.46	1.37
30	xL	304	PUB	C3B-C2B	2.98	1.46	1.37
31	H1	1001	CYC	C3D-C2D	2.98	1.46	1.37
31	DK	1001	CYC	C3D-C2D	2.98	1.46	1.37
29	GJ	202	PEB	OD-C4D	2.98	1.29	1.23
29	GL	202	PEB	OD-C4D	2.98	1.29	1.23
29	G4	201	PEB	C2C-C3C	2.98	1.46	1.37
29	GD	201	PEB	C2C-C3C	2.98	1.46	1.37
29	fJ	202	PEB	CHA-C1B	2.97	1.47	1.40
29	fL	202	PEB	CHA-C1B	2.97	1.47	1.40
29	i1	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	iK	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	mJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	mL	201	PEB	C2C-C3C	2.97	1.46	1.37
29	WJ	201	PEB	CHA-C1B	2.97	1.47	1.40
29	WL	201	PEB	CHA-C1B	2.97	1.47	1.40
29	J3	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	H5	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	RF	202	PEB	C2A-C1A	-2.97	1.49	1.52
29	RI	202	PEB	C2A-C1A	-2.97	1.49	1.52
29	bJ	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	bL	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	JO	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	YJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	YL	201	PEB	C2C-C3C	2.97	1.46	1.37
29	NJ	202	PEB	CHA-C1B	2.97	1.47	1.40
29	NL	202	PEB	CHA-C1B	2.97	1.47	1.40
29	V2	202	PEB	C2C-C3C	2.97	1.46	1.37
29	VR	202	PEB	C2C-C3C	2.97	1.46	1.37
29	V2	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	D3	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	F3	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	fJ	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	fL	203	PEB	C2A-C1A	-2.97	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DO	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	FO	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	VR	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	B3	202	PEB	CHC-C4C	2.97	1.57	1.50
29	BO	202	PEB	CHC-C4C	2.97	1.57	1.50
29	T7	202	PEB	OD-C4D	2.97	1.29	1.23
29	T9	202	PEB	OD-C4D	2.97	1.29	1.23
29	XJ	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	XL	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	F3	202	PEB	CHC-C4C	2.97	1.57	1.50
29	FO	202	PEB	CHC-C4C	2.97	1.57	1.50
29	KD	201	PEB	C2C-C3C	2.97	1.46	1.37
29	D3	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	cB	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	FD	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	cM	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	DO	201	PEB	C2A-C1A	-2.97	1.49	1.52
29	a1	201	PEB	C2C-C3C	2.97	1.46	1.37
29	OJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	aK	201	PEB	C2C-C3C	2.97	1.46	1.37
29	OL	201	PEB	C2C-C3C	2.97	1.46	1.37
29	GJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	GL	201	PEB	C2C-C3C	2.97	1.46	1.37
30	A1	305	PUB	OA-C1A	2.97	1.29	1.23
30	AK	305	PUB	OA-C1A	2.97	1.29	1.23
29	UJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	UL	201	PEB	C2C-C3C	2.97	1.46	1.37
29	L8	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	R1	201	PEB	C2C-C3C	2.97	1.46	1.37
29	RK	201	PEB	C2C-C3C	2.97	1.46	1.37
29	IJ	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	IL	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	T1	201	PEB	C2C-C3C	2.97	1.46	1.37
29	IJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	TK	201	PEB	C2C-C3C	2.97	1.46	1.37
29	IL	201	PEB	C2C-C3C	2.97	1.46	1.37
29	N2	202	PEB	C2C-C3C	2.97	1.46	1.37
29	NR	202	PEB	C2C-C3C	2.97	1.46	1.37
29	ZJ	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	ZL	203	PEB	C2A-C1A	-2.97	1.49	1.52
29	AJ	201	PEB	C2C-C3C	2.97	1.46	1.37
29	AL	201	PEB	C2C-C3C	2.97	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	iJ	201	PEB	C2C-C3C	2.96	1.46	1.37
29	iL	201	PEB	C2C-C3C	2.96	1.46	1.37
29	PJ	202	PEB	CHA-C1B	2.96	1.47	1.40
29	PL	202	PEB	CHA-C1B	2.96	1.47	1.40
30	xJ	304	PUB	C3B-C2B	2.96	1.46	1.37
29	CJ	202	PEB	OD-C4D	2.96	1.29	1.23
29	CL	202	PEB	OD-C4D	2.96	1.29	1.23
29	IJ	202	PEB	OD-C4D	2.96	1.29	1.23
29	IL	202	PEB	OD-C4D	2.96	1.29	1.23
31	L1	1001	CYC	C3D-C2D	2.96	1.46	1.37
31	LK	1001	CYC	C3D-C2D	2.96	1.46	1.37
29	XJ	202	PEB	CHA-C1B	2.96	1.47	1.40
29	XL	202	PEB	CHA-C1B	2.96	1.47	1.40
29	aJ	201	PEB	C2C-C3C	2.96	1.46	1.37
29	kJ	201	PEB	C2C-C3C	2.96	1.46	1.37
29	aL	201	PEB	C2C-C3C	2.96	1.46	1.37
29	kL	201	PEB	C2C-C3C	2.96	1.46	1.37
29	D4	201	PEB	C2A-C1A	-2.96	1.49	1.52
29	g7	201	PEB	C2A-C1A	-2.96	1.49	1.52
29	g9	201	PEB	C2A-C1A	-2.96	1.49	1.52
29	cJ	202	PEB	OD-C4D	2.96	1.29	1.23
29	cL	202	PEB	OD-C4D	2.96	1.29	1.23
29	XR	202	PEB	C2C-C3C	2.96	1.46	1.37
29	sJ	201	PEB	C2C-C3C	2.96	1.46	1.37
29	sL	201	PEB	C2C-C3C	2.96	1.46	1.37
31	D1	1001	CYC	C3D-C2D	2.96	1.46	1.37
29	oJ	201	PEB	C2C-C3C	2.96	1.46	1.37
29	qJ	201	PEB	C2C-C3C	2.96	1.46	1.37
29	oL	201	PEB	C2C-C3C	2.96	1.46	1.37
29	qL	201	PEB	C2C-C3C	2.96	1.46	1.37
29	DG	201	PEB	C2A-C1A	-2.96	1.49	1.52
29	DQ	201	PEB	C2A-C1A	-2.96	1.49	1.52
29	e1	202	PEB	OD-C4D	2.96	1.29	1.23
29	eK	202	PEB	OD-C4D	2.96	1.29	1.23
29	ZJ	202	PEB	CHA-C1B	2.96	1.47	1.40
29	ZL	202	PEB	CHA-C1B	2.96	1.47	1.40
29	EJ	202	PEB	OD-C4D	2.96	1.29	1.23
29	EL	202	PEB	OD-C4D	2.96	1.29	1.23
31	N1	1001	CYC	C3D-C2D	2.96	1.46	1.37
29	IJ	203	PEB	CHA-C1B	2.96	1.47	1.40
29	IL	203	PEB	CHA-C1B	2.96	1.47	1.40
29	BG	202	PEB	C2A-C1A	-2.96	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LG	201	PEB	C2A-C1A	-2.96	1.49	1.52
29	BJ	203	PEB	C2A-C1A	-2.96	1.49	1.52
29	BL	203	PEB	C2A-C1A	-2.96	1.49	1.52
29	BQ	202	PEB	C2A-C1A	-2.96	1.49	1.52
29	MQ	402	PEB	C2A-C1A	-2.96	1.49	1.52
29	eJ	202	PEB	OD-C4D	2.96	1.29	1.23
29	eL	202	PEB	OD-C4D	2.96	1.29	1.23
29	WR	202	PEB	OD-C4D	2.96	1.29	1.23
31	K7	1001	CYC	C2C-C1C	-2.96	1.49	1.52
29	c1	202	PEB	OD-C4D	2.95	1.29	1.23
29	cK	202	PEB	OD-C4D	2.95	1.29	1.23
30	A1	305	PUB	C3B-C2B	2.95	1.46	1.37
30	AK	305	PUB	C3B-C2B	2.95	1.46	1.37
29	IJ	202	PEB	CHA-C1B	2.95	1.47	1.40
29	IL	202	PEB	CHA-C1B	2.95	1.47	1.40
29	m7	202	PEB	OD-C4D	2.95	1.29	1.23
29	m9	202	PEB	OD-C4D	2.95	1.29	1.23
29	QJ	201	PEB	C2C-C3C	2.95	1.46	1.37
29	QL	201	PEB	C2C-C3C	2.95	1.46	1.37
29	JJ	203	PEB	C2A-C1A	-2.95	1.49	1.52
29	JL	203	PEB	C2A-C1A	-2.95	1.49	1.52
31	G7	1001	CYC	C2C-C1C	-2.95	1.49	1.52
29	uJ	202	PEB	C2C-C3C	2.95	1.46	1.37
29	uL	202	PEB	C2C-C3C	2.95	1.46	1.37
29	M2	202	PEB	OD-C4D	2.95	1.29	1.23
29	AC	202	PEB	OD-C4D	2.95	1.29	1.23
29	AE	202	PEB	OD-C4D	2.95	1.29	1.23
29	CJ	201	PEB	C2C-C3C	2.95	1.46	1.37
29	CL	201	PEB	C2C-C3C	2.95	1.46	1.37
29	eF	202	PEB	OD-C4D	2.95	1.29	1.23
29	eI	202	PEB	OD-C4D	2.95	1.29	1.23
29	HG	202	PEB	C2A-C1A	-2.95	1.49	1.52
29	TJ	203	PEB	C2A-C1A	-2.95	1.49	1.52
29	TL	203	PEB	C2A-C1A	-2.95	1.49	1.52
29	HQ	202	PEB	C2A-C1A	-2.95	1.49	1.52
29	Z1	203	PEB	OD-C4D	2.95	1.29	1.23
29	ZK	203	PEB	OD-C4D	2.95	1.29	1.23
29	GC	202	PEB	OD-C4D	2.95	1.29	1.23
29	GE	202	PEB	OD-C4D	2.95	1.29	1.23
29	V1	202	PEB	OD-C4D	2.95	1.29	1.23
29	YF	202	PEB	OD-C4D	2.95	1.29	1.23
29	YI	202	PEB	OD-C4D	2.95	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VK	202	PEB	OD-C4D	2.95	1.29	1.23
29	LB	201	PEB	C2A-C1A	-2.95	1.49	1.52
29	JG	202	PEB	C2A-C1A	-2.95	1.49	1.52
29	RJ	203	PEB	C2A-C1A	-2.95	1.49	1.52
29	RL	203	PEB	C2A-C1A	-2.95	1.49	1.52
29	LM	201	PEB	C2A-C1A	-2.95	1.49	1.52
29	JQ	202	PEB	C2A-C1A	-2.95	1.49	1.52
31	J1	1001	CYC	C3D-C2D	2.95	1.46	1.37
31	JK	1001	CYC	C3D-C2D	2.95	1.46	1.37
29	gJ	201	PEB	C2C-C3C	2.95	1.46	1.37
29	gL	201	PEB	C2C-C3C	2.95	1.46	1.37
31	NK	1001	CYC	C3D-C2D	2.95	1.46	1.37
29	T2	202	PEB	C2C-C3C	2.95	1.46	1.37
29	P7	202	PEB	OD-C4D	2.95	1.29	1.23
29	P9	202	PEB	OD-C4D	2.95	1.29	1.23
29	P1	201	PEB	C2A-C1A	-2.95	1.49	1.52
29	PK	201	PEB	C2A-C1A	-2.95	1.49	1.52
30	wJ	304	PUB	C3B-C2B	2.95	1.46	1.37
29	TJ	202	PEB	CHA-C1B	2.95	1.47	1.40
29	TL	202	PEB	CHA-C1B	2.95	1.47	1.40
29	B3	201	PEB	C2A-C1A	-2.95	1.49	1.52
29	BO	201	PEB	C2A-C1A	-2.95	1.49	1.52
29	TR	203	PEB	C2A-C1A	-2.95	1.49	1.52
29	a1	202	PEB	OD-C4D	2.94	1.29	1.23
29	aK	202	PEB	OD-C4D	2.94	1.29	1.23
29	rJ	202	PEB	CHA-C1B	2.94	1.47	1.40
29	rL	202	PEB	CHA-C1B	2.94	1.47	1.40
29	JJ	202	PEB	CHA-C1B	2.94	1.47	1.40
29	JL	202	PEB	CHA-C1B	2.94	1.47	1.40
29	c7	202	PEB	OD-C4D	2.94	1.29	1.23
29	c9	202	PEB	OD-C4D	2.94	1.29	1.23
29	EA	202	PEB	C2A-C1A	-2.94	1.49	1.52
29	EN	202	PEB	C2A-C1A	-2.94	1.49	1.52
29	AJ	203	PEB	CHA-C1B	2.94	1.47	1.40
29	uJ	201	PEB	CHA-C1B	2.94	1.47	1.40
29	AL	203	PEB	CHA-C1B	2.94	1.47	1.40
29	uL	201	PEB	CHA-C1B	2.94	1.47	1.40
29	gB	201	PEB	C2A-C1A	-2.94	1.49	1.52
29	gM	201	PEB	C2A-C1A	-2.94	1.49	1.52
29	R7	202	PEB	OD-C4D	2.94	1.29	1.23
29	R9	202	PEB	OD-C4D	2.94	1.29	1.23
29	i1	201	PEB	C2C-C3C	2.94	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X2	201	PEB	C2C-C3C	2.94	1.46	1.37
29	iK	201	PEB	C2C-C3C	2.94	1.46	1.37
29	hJ	202	PEB	CHA-C1B	2.94	1.47	1.40
29	hL	202	PEB	CHA-C1B	2.94	1.47	1.40
29	O2	202	PEB	OD-C4D	2.94	1.29	1.23
29	H3	202	PEB	CHC-C4C	2.94	1.57	1.50
29	HO	202	PEB	CHC-C4C	2.94	1.57	1.50
31	F1	1001	CYC	C3D-C2D	2.94	1.46	1.37
31	FK	1001	CYC	C3D-C2D	2.94	1.46	1.37
29	R1	202	PEB	OD-C4D	2.94	1.29	1.23
29	RK	202	PEB	OD-C4D	2.94	1.29	1.23
29	Q2	202	PEB	OD-C4D	2.94	1.29	1.23
29	H4	201	PEB	C2A-C1A	-2.94	1.49	1.52
29	HD	201	PEB	C2A-C1A	-2.94	1.49	1.52
29	PR	202	PEB	C2A-C1A	-2.94	1.49	1.52
29	V7	202	PEB	OD-C4D	2.93	1.29	1.23
29	V9	202	PEB	OD-C4D	2.93	1.29	1.23
29	i1	202	PEB	OD-C4D	2.93	1.29	1.23
29	iK	202	PEB	OD-C4D	2.93	1.29	1.23
29	l1	202	PEB	OD-C4D	2.93	1.29	1.23
29	lK	202	PEB	OD-C4D	2.93	1.29	1.23
29	j1	202	PEB	OD-C4D	2.93	1.29	1.23
29	k7	202	PEB	OD-C4D	2.93	1.29	1.23
29	k9	202	PEB	OD-C4D	2.93	1.29	1.23
29	jK	202	PEB	OD-C4D	2.93	1.29	1.23
29	N2	203	PEB	C2A-C1A	-2.93	1.49	1.52
29	R2	203	PEB	C2A-C1A	-2.93	1.49	1.52
29	NR	203	PEB	C2A-C1A	-2.93	1.49	1.52
29	BJ	202	PEB	CHA-C1B	2.93	1.47	1.40
29	BL	202	PEB	CHA-C1B	2.93	1.47	1.40
29	RJ	202	PEB	CHA-C1B	2.93	1.47	1.40
29	RL	202	PEB	CHA-C1B	2.93	1.47	1.40
29	mF	202	PEB	OD-C4D	2.93	1.29	1.23
29	mI	202	PEB	OD-C4D	2.93	1.29	1.23
29	QR	202	PEB	OD-C4D	2.93	1.29	1.23
29	g1	201	PEB	C2A-C1A	-2.93	1.49	1.52
29	Y7	201	PEB	C2A-C1A	-2.93	1.49	1.52
29	Y9	201	PEB	C2A-C1A	-2.93	1.49	1.52
29	gK	201	PEB	C2A-C1A	-2.93	1.49	1.52
29	i7	202	PEB	OD-C4D	2.93	1.29	1.23
29	i9	202	PEB	OD-C4D	2.93	1.29	1.23
29	P1	202	PEB	OD-C4D	2.93	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	PK	202	PEB	OD-C4D	2.93	1.29	1.23
29	k1	202	PEB	OD-C4D	2.93	1.29	1.23
29	kK	202	PEB	OD-C4D	2.93	1.29	1.23
29	G8	203	PEB	C2A-C1A	-2.93	1.49	1.52
29	JB	201	PEB	C2A-C1A	-2.93	1.49	1.52
29	JM	201	PEB	C2A-C1A	-2.93	1.49	1.52
29	a7	202	PEB	OD-C4D	2.93	1.29	1.23
29	a9	202	PEB	OD-C4D	2.93	1.29	1.23
29	PF	202	PEB	OD-C4D	2.93	1.29	1.23
29	PI	202	PEB	OD-C4D	2.93	1.29	1.23
30	wL	304	PUB	C3B-C2B	2.93	1.46	1.37
29	VF	202	PEB	OD-C4D	2.93	1.29	1.23
29	VI	202	PEB	OD-C4D	2.93	1.29	1.23
30	QB	201	PUB	OD-C4D	2.93	1.29	1.23
30	QM	201	PUB	OD-C4D	2.93	1.29	1.23
29	XB	201	PEB	C2A-C1A	-2.92	1.49	1.52
29	XM	201	PEB	C2A-C1A	-2.92	1.49	1.52
29	gF	202	PEB	OD-C4D	2.92	1.29	1.23
29	gI	202	PEB	OD-C4D	2.92	1.29	1.23
29	kF	202	PEB	OD-C4D	2.92	1.29	1.23
29	kI	202	PEB	OD-C4D	2.92	1.29	1.23
29	H3	203	PEB	C2A-C1A	-2.92	1.49	1.52
29	HO	203	PEB	C2A-C1A	-2.92	1.49	1.52
29	LG	202	PEB	C2A-C1A	-2.92	1.49	1.52
29	LQ	201	PEB	C2A-C1A	-2.92	1.49	1.52
29	MQ	407	PEB	CHA-C1B	2.92	1.47	1.40
29	e7	202	PEB	OD-C4D	2.92	1.29	1.23
29	e9	202	PEB	OD-C4D	2.92	1.29	1.23
29	DB	202	PEB	C2C-C3C	2.92	1.46	1.37
29	DM	202	PEB	C2C-C3C	2.92	1.46	1.37
29	OF	203	PEB	OD-C4D	2.92	1.29	1.23
29	OI	203	PEB	OD-C4D	2.92	1.29	1.23
29	g1	202	PEB	OD-C4D	2.92	1.29	1.23
29	CC	202	PEB	OD-C4D	2.92	1.29	1.23
29	CE	202	PEB	OD-C4D	2.92	1.29	1.23
29	gK	202	PEB	OD-C4D	2.92	1.29	1.23
29	LB	202	PEB	C2C-C3C	2.92	1.46	1.37
29	LM	202	PEB	C2C-C3C	2.92	1.46	1.37
29	j1	203	PEB	OD-C4D	2.92	1.29	1.23
29	jK	203	PEB	OD-C4D	2.92	1.29	1.23
29	Q1	202	PEB	OD-C4D	2.91	1.29	1.23
29	U1	201	PEB	OD-C4D	2.91	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	UF	201	PEB	OD-C4D	2.91	1.29	1.23
29	UI	201	PEB	OD-C4D	2.91	1.29	1.23
29	QK	202	PEB	OD-C4D	2.91	1.29	1.23
29	UK	201	PEB	OD-C4D	2.91	1.29	1.23
29	R1	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	RK	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	Y7	202	PEB	OD-C4D	2.91	1.29	1.23
29	Y9	202	PEB	OD-C4D	2.91	1.29	1.23
29	F3	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	J3	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	FO	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	JO	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	YB	201	PEB	C2C-C3C	2.91	1.46	1.37
29	YM	201	PEB	C2C-C3C	2.91	1.46	1.37
29	h1	202	PEB	OD-C4D	2.91	1.29	1.23
29	g7	202	PEB	OD-C4D	2.91	1.29	1.23
29	g9	202	PEB	OD-C4D	2.91	1.29	1.23
29	IC	202	PEB	OD-C4D	2.91	1.29	1.23
29	IE	202	PEB	OD-C4D	2.91	1.29	1.23
29	hK	202	PEB	OD-C4D	2.91	1.29	1.23
29	kB	202	PEB	C2C-C3C	2.91	1.46	1.37
29	kM	202	PEB	C2C-C3C	2.91	1.46	1.37
29	iF	202	PEB	OD-C4D	2.91	1.29	1.23
29	iI	202	PEB	OD-C4D	2.91	1.29	1.23
29	H8	203	PEB	C2A-C1A	-2.91	1.49	1.52
31	M9	1001	CYC	C2C-C1C	-2.91	1.49	1.52
29	EC	202	PEB	OD-C4D	2.91	1.29	1.23
29	EE	202	PEB	OD-C4D	2.91	1.29	1.23
29	xL	303	PEB	OD-C4D	2.91	1.29	1.23
29	gB	202	PEB	C2C-C3C	2.91	1.46	1.37
29	gM	202	PEB	C2C-C3C	2.91	1.46	1.37
29	Z1	201	PEB	OD-C4D	2.91	1.29	1.23
29	ZK	201	PEB	OD-C4D	2.91	1.29	1.23
29	HB	202	PEB	C2C-C3C	2.91	1.46	1.37
29	CD	202	PEB	C2C-C3C	2.91	1.46	1.37
29	HM	202	PEB	C2C-C3C	2.91	1.46	1.37
29	U1	203	PEB	OD-C4D	2.91	1.29	1.23
29	UK	203	PEB	OD-C4D	2.91	1.29	1.23
29	e1	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	L5	203	PEB	C2A-C1A	-2.91	1.49	1.52
29	eK	201	PEB	C2A-C1A	-2.91	1.49	1.52
29	TB	202	PEB	C2C-C3C	2.90	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TM	202	PEB	C2C-C3C	2.90	1.46	1.37
29	PJ	203	PEB	C2A-C1A	-2.90	1.49	1.52
29	PL	203	PEB	C2A-C1A	-2.90	1.49	1.52
29	KB	203	PEB	C2C-C3C	2.90	1.46	1.37
29	KM	203	PEB	C2C-C3C	2.90	1.46	1.37
29	MG	405	PEB	CHA-C1B	2.90	1.47	1.40
29	KC	203	PEB	OD-C4D	2.90	1.29	1.23
29	KE	203	PEB	OD-C4D	2.90	1.29	1.23
29	HG	201	PEB	C2A-C1A	-2.90	1.49	1.52
29	HQ	201	PEB	C2A-C1A	-2.90	1.49	1.52
29	W2	202	PEB	OD-C4D	2.90	1.29	1.23
29	RB	202	PEB	C2C-C3C	2.90	1.46	1.37
29	RM	202	PEB	C2C-C3C	2.90	1.46	1.37
29	S1	202	PEB	OD-C4D	2.90	1.29	1.23
29	SK	202	PEB	OD-C4D	2.90	1.29	1.23
29	JB	202	PEB	C2C-C3C	2.90	1.46	1.37
29	JM	202	PEB	C2C-C3C	2.90	1.46	1.37
29	d1	202	PEB	OD-C4D	2.90	1.29	1.23
29	dK	202	PEB	OD-C4D	2.90	1.29	1.23
29	XR	203	PEB	C2A-C1A	-2.90	1.49	1.52
29	W1	202	PEB	OD-C4D	2.90	1.29	1.23
29	WK	202	PEB	OD-C4D	2.90	1.29	1.23
29	dF	201	PEB	OD-C4D	2.90	1.29	1.23
29	dI	201	PEB	OD-C4D	2.90	1.29	1.23
29	aB	203	PEB	C2C-C3C	2.90	1.46	1.37
29	aM	203	PEB	C2C-C3C	2.90	1.46	1.37
29	DD	201	PEB	C2A-C1A	-2.90	1.49	1.52
29	xJ	303	PEB	OD-C4D	2.90	1.29	1.23
29	QB	202	PEB	C2C-C3C	2.89	1.46	1.37
29	QM	202	PEB	C2C-C3C	2.89	1.46	1.37
29	mB	202	PEB	C2C-C3C	2.89	1.46	1.37
29	mM	202	PEB	C2C-C3C	2.89	1.46	1.37
29	R7	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	R9	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	k7	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	k9	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	J5	201	PEB	C4A-NA	-2.89	1.31	1.37
29	J8	201	PEB	C4A-NA	-2.89	1.31	1.37
29	cB	202	PEB	C2C-C3C	2.89	1.46	1.37
29	cM	202	PEB	C2C-C3C	2.89	1.46	1.37
29	SR	202	PEB	OD-C4D	2.89	1.29	1.23
29	NJ	203	PEB	C2A-C1A	-2.89	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NL	203	PEB	C2A-C1A	-2.89	1.49	1.52
29	FB	202	PEB	C2C-C3C	2.89	1.46	1.37
29	FM	202	PEB	C2C-C3C	2.89	1.46	1.37
29	T7	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	H8	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	T9	201	PEB	C2A-C1A	-2.89	1.49	1.52
29	G4	202	PEB	C2C-C3C	2.89	1.46	1.37
29	GD	202	PEB	C2C-C3C	2.89	1.46	1.37
29	B4	201	PEB	C2A-C1A	-2.88	1.49	1.52
29	BD	201	PEB	C2A-C1A	-2.88	1.49	1.52
31	1P	1001	CYC	OB-C4B	2.88	1.29	1.23
29	KD	202	PEB	C2C-C3C	2.88	1.46	1.37
29	S2	202	PEB	OD-C4D	2.88	1.29	1.23
29	ID	202	PEB	C2C-C3C	2.88	1.46	1.37
29	ZB	202	PEB	C2C-C3C	2.88	1.46	1.37
29	ZM	202	PEB	C2C-C3C	2.88	1.46	1.37
29	CA	201	PEB	CHA-C1B	2.88	1.47	1.40
29	CN	201	PEB	CHA-C1B	2.88	1.47	1.40
29	GA	202	PEB	C2A-C1A	-2.88	1.49	1.52
29	GN	202	PEB	C2A-C1A	-2.88	1.49	1.52
29	iB	202	PEB	C2C-C3C	2.88	1.46	1.37
29	iM	202	PEB	C2C-C3C	2.88	1.46	1.37
29	J3	202	PEB	OD-C4D	2.88	1.29	1.23
29	M3	203	PEB	OD-C4D	2.88	1.29	1.23
29	JO	202	PEB	OD-C4D	2.88	1.29	1.23
29	MO	203	PEB	OD-C4D	2.88	1.29	1.23
29	HA	202	PEB	C2A-C1A	-2.88	1.49	1.52
29	HN	202	PEB	C2A-C1A	-2.88	1.49	1.52
29	L4	201	PEB	C2A-C1A	-2.88	1.49	1.52
31	nP	1001	CYC	OB-C4B	2.88	1.29	1.23
29	C4	202	PEB	C2C-C3C	2.88	1.46	1.37
29	f1	202	PEB	OD-C4D	2.88	1.29	1.23
29	fK	202	PEB	OD-C4D	2.88	1.29	1.23
29	VB	202	PEB	C2C-C3C	2.87	1.46	1.37
29	VM	202	PEB	C2C-C3C	2.87	1.46	1.37
29	aF	202	PEB	OD-C4D	2.87	1.29	1.23
29	aI	202	PEB	OD-C4D	2.87	1.29	1.23
29	b1	202	PEB	OD-C4D	2.87	1.29	1.23
29	bK	202	PEB	OD-C4D	2.87	1.29	1.23
29	F5	201	PEB	C2A-C1A	-2.87	1.49	1.52
29	F8	201	PEB	C2A-C1A	-2.87	1.49	1.52
29	xL	301	PEB	C1A-NA	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	MN	402	PUB	OD-C4D	2.87	1.29	1.23
29	KA	202	PEB	C2A-C1A	-2.87	1.49	1.52
29	KN	202	PEB	C2A-C1A	-2.87	1.49	1.52
29	m1	201	PEB	C2A-C1A	-2.86	1.49	1.52
29	mK	201	PEB	C2A-C1A	-2.86	1.49	1.52
31	UP	1001	CYC	OB-C4B	2.86	1.29	1.23
29	MD	202	PEB	C2C-C3C	2.86	1.46	1.37
29	O1	202	PEB	OD-C4D	2.86	1.29	1.23
29	OK	202	PEB	OD-C4D	2.86	1.29	1.23
29	B8	201	PEB	C2A-C1A	-2.86	1.49	1.52
29	I4	202	PEB	C2C-C3C	2.86	1.46	1.37
31	SP	1001	CYC	OB-C4B	2.86	1.29	1.23
29	PR	201	PEB	CHA-C1B	2.86	1.47	1.40
31	oP	1001	CYC	OB-C4B	2.86	1.29	1.23
29	ED	201	PEB	C2C-C3C	2.86	1.46	1.37
29	P7	201	PEB	C2A-C1A	-2.86	1.49	1.52
29	P9	201	PEB	C2A-C1A	-2.86	1.49	1.52
31	kP	1001	CYC	OB-C4B	2.86	1.29	1.23
29	I3	203	PEB	OD-C4D	2.86	1.29	1.23
29	IO	203	PEB	OD-C4D	2.86	1.29	1.23
31	DP	1001	CYC	OB-C4B	2.86	1.29	1.23
29	FC	203	PEB	OD-C4D	2.86	1.29	1.23
29	FE	203	PEB	OD-C4D	2.86	1.29	1.23
29	GA	202	PEB	OD-C4D	2.86	1.29	1.23
29	GN	202	PEB	OD-C4D	2.86	1.29	1.23
29	F3	202	PEB	OD-C4D	2.86	1.29	1.23
29	FO	202	PEB	OD-C4D	2.86	1.29	1.23
29	IA	201	PEB	CHA-C1B	2.85	1.47	1.40
29	IN	201	PEB	CHA-C1B	2.85	1.47	1.40
29	g7	202	PEB	C2C-C3C	2.85	1.46	1.37
29	g9	202	PEB	C2C-C3C	2.85	1.46	1.37
29	K4	202	PEB	C2C-C3C	2.85	1.46	1.37
31	IK	1001	CYC	C2C-C1C	-2.85	1.49	1.52
29	wL	303	PEB	OD-C4D	2.85	1.29	1.23
29	EA	201	PEB	CHA-C1B	2.85	1.47	1.40
29	EN	201	PEB	CHA-C1B	2.85	1.47	1.40
29	P7	202	PEB	C2C-C3C	2.85	1.46	1.37
29	P9	202	PEB	C2C-C3C	2.85	1.46	1.37
29	LC	203	PEB	OD-C4D	2.85	1.29	1.23
29	LE	203	PEB	OD-C4D	2.85	1.29	1.23
31	BP	1001	CYC	OB-C4B	2.85	1.29	1.23
29	AF	305	PEB	C1A-NA	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AI	305	PEB	C1A-NA	-2.85	1.33	1.37
29	CA	202	PEB	C2A-C1A	-2.85	1.49	1.52
29	CN	202	PEB	C2A-C1A	-2.85	1.49	1.52
29	a7	202	PEB	C2C-C3C	2.85	1.46	1.37
29	a9	202	PEB	C2C-C3C	2.85	1.46	1.37
31	uP	1001	CYC	OB-C4B	2.85	1.29	1.23
30	AB	305	PUB	OA-C1A	2.85	1.29	1.23
31	hP	1001	CYC	OB-C4B	2.85	1.29	1.23
29	T7	202	PEB	C2C-C3C	2.85	1.46	1.37
29	T9	202	PEB	C2C-C3C	2.85	1.46	1.37
29	B3	202	PEB	OD-C4D	2.85	1.29	1.23
29	BO	202	PEB	OD-C4D	2.85	1.29	1.23
30	MA	402	PUB	OD-C4D	2.84	1.29	1.23
29	c7	202	PEB	C2C-C3C	2.84	1.46	1.37
29	c9	202	PEB	C2C-C3C	2.84	1.46	1.37
31	fP	1001	CYC	OB-C4B	2.84	1.29	1.23
29	c1	201	PEB	C2A-C1A	-2.84	1.49	1.52
29	DA	202	PEB	C2A-C1A	-2.84	1.49	1.52
29	cK	201	PEB	C2A-C1A	-2.84	1.49	1.52
29	DN	202	PEB	C2A-C1A	-2.84	1.49	1.52
29	H3	202	PEB	OD-C4D	2.84	1.29	1.23
29	HO	202	PEB	OD-C4D	2.84	1.29	1.23
29	wJ	303	PEB	OD-C4D	2.84	1.29	1.23
29	KA	201	PEB	CHA-C1B	2.84	1.47	1.40
29	KN	201	PEB	CHA-C1B	2.84	1.47	1.40
29	Y7	202	PEB	C2C-C3C	2.84	1.46	1.37
29	Y9	202	PEB	C2C-C3C	2.84	1.46	1.37
31	OP	1001	CYC	OB-C4B	2.84	1.29	1.23
29	V7	202	PEB	C2C-C3C	2.84	1.46	1.37
29	V9	202	PEB	C2C-C3C	2.84	1.46	1.37
29	GA	201	PEB	CHA-C1B	2.84	1.47	1.40
29	GN	201	PEB	CHA-C1B	2.84	1.47	1.40
29	i7	202	PEB	C2C-C3C	2.84	1.46	1.37
29	i9	202	PEB	C2C-C3C	2.84	1.46	1.37
31	FP	1001	CYC	OB-C4B	2.84	1.29	1.23
29	G8	201	PEB	C2A-C1A	-2.84	1.49	1.52
29	EA	202	PEB	OD-C4D	2.84	1.29	1.23
29	EN	202	PEB	OD-C4D	2.84	1.29	1.23
31	HP	1001	CYC	OB-C4B	2.84	1.29	1.23
29	cJ	201	PEB	C4A-NA	-2.84	1.31	1.37
29	cL	201	PEB	C4A-NA	-2.84	1.31	1.37
29	G5	201	PEB	C2A-C1A	-2.84	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LA	202	PEB	C2A-C1A	-2.84	1.49	1.52
29	LN	202	PEB	C2A-C1A	-2.84	1.49	1.52
29	c7	201	PEB	C2A-C1A	-2.83	1.49	1.52
29	c9	201	PEB	C2A-C1A	-2.83	1.49	1.52
29	AA	201	PEB	CHA-C1B	2.83	1.47	1.40
29	AN	201	PEB	CHA-C1B	2.83	1.47	1.40
29	iJ	201	PEB	C4A-NA	-2.83	1.31	1.37
29	iL	201	PEB	C4A-NA	-2.83	1.31	1.37
29	HC	203	PEB	OD-C4D	2.83	1.29	1.23
29	HE	203	PEB	OD-C4D	2.83	1.29	1.23
31	HF	1001	CYC	C3D-C2D	2.83	1.46	1.37
31	HI	1001	CYC	C3D-C2D	2.83	1.46	1.37
29	JC	202	PEB	OD-C4D	2.83	1.29	1.23
29	JE	202	PEB	OD-C4D	2.83	1.29	1.23
29	PF	202	PEB	C2A-C1A	-2.83	1.49	1.52
29	PI	202	PEB	C2A-C1A	-2.83	1.49	1.52
31	QP	1001	CYC	OB-C4B	2.83	1.29	1.23
31	sP	1001	CYC	OB-C4B	2.83	1.29	1.23
29	R7	202	PEB	C2C-C3C	2.83	1.46	1.37
29	R9	202	PEB	C2C-C3C	2.83	1.46	1.37
31	IP	1001	CYC	OB-C4B	2.83	1.29	1.23
29	i1	202	PEB	C2C-C3C	2.83	1.46	1.37
29	iK	202	PEB	C2C-C3C	2.83	1.46	1.37
29	mJ	201	PEB	C4A-NA	-2.83	1.31	1.37
29	mL	201	PEB	C4A-NA	-2.83	1.31	1.37
29	E4	202	PEB	C2C-C3C	2.83	1.46	1.37
29	aJ	201	PEB	C4A-NA	-2.83	1.31	1.37
29	aL	201	PEB	C4A-NA	-2.83	1.31	1.37
29	N3	203	PEB	OD-C4D	2.83	1.29	1.23
30	AM	305	PUB	OA-C1A	2.83	1.29	1.23
29	m7	202	PEB	C2C-C3C	2.83	1.46	1.37
29	m9	202	PEB	C2C-C3C	2.83	1.46	1.37
29	NO	203	PEB	OD-C4D	2.83	1.29	1.23
31	wP	1001	CYC	OB-C4B	2.83	1.29	1.23
29	D3	202	PEB	OD-C4D	2.83	1.29	1.23
29	k7	202	PEB	C2C-C3C	2.83	1.46	1.37
29	k9	202	PEB	C2C-C3C	2.83	1.46	1.37
29	QJ	201	PEB	C4A-NA	-2.83	1.31	1.37
29	QL	201	PEB	C4A-NA	-2.83	1.31	1.37
29	e7	202	PEB	C2C-C3C	2.83	1.46	1.37
29	e9	202	PEB	C2C-C3C	2.83	1.46	1.37
29	I5	203	PEB	C2A-C1A	-2.83	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I8	203	PEB	C2A-C1A	-2.83	1.49	1.52
29	uJ	202	PEB	C4A-NA	-2.82	1.31	1.37
29	uL	202	PEB	C4A-NA	-2.82	1.31	1.37
29	c1	202	PEB	C2C-C3C	2.82	1.46	1.37
29	cK	202	PEB	C2C-C3C	2.82	1.46	1.37
29	V7	201	PEB	C2A-C1A	-2.82	1.49	1.52
29	e7	201	PEB	C2A-C1A	-2.82	1.49	1.52
29	V9	201	PEB	C2A-C1A	-2.82	1.49	1.52
29	e9	201	PEB	C2A-C1A	-2.82	1.49	1.52
29	AJ	201	PEB	C4A-NA	-2.82	1.31	1.37
29	AL	201	PEB	C4A-NA	-2.82	1.31	1.37
29	IJ	201	PEB	C4A-NA	-2.82	1.31	1.37
29	IL	201	PEB	C4A-NA	-2.82	1.31	1.37
29	XR	202	PEB	CHA-C1B	2.82	1.47	1.40
29	SJ	201	PEB	C4A-NA	-2.82	1.31	1.37
29	SL	201	PEB	C4A-NA	-2.82	1.31	1.37
30	MA	403	PUB	OA-C1A	2.82	1.28	1.23
31	qP	1001	CYC	OB-C4B	2.82	1.28	1.23
31	DF	1001	CYC	C3D-C2D	2.82	1.46	1.37
31	DI	1001	CYC	C3D-C2D	2.82	1.46	1.37
29	JA	202	PEB	C2A-C1A	-2.82	1.49	1.52
29	JN	202	PEB	C2A-C1A	-2.82	1.49	1.52
29	g1	202	PEB	C2C-C3C	2.82	1.46	1.37
29	gK	202	PEB	C2C-C3C	2.82	1.46	1.37
29	a1	202	PEB	C2C-C3C	2.82	1.46	1.37
29	aK	202	PEB	C2C-C3C	2.82	1.46	1.37
29	DO	202	PEB	OD-C4D	2.82	1.28	1.23
29	g7	202	PEB	C2A-C1A	-2.82	1.49	1.52
29	g9	202	PEB	C2A-C1A	-2.82	1.49	1.52
29	IA	202	PEB	OD-C4D	2.82	1.28	1.23
29	DC	202	PEB	OD-C4D	2.82	1.28	1.23
29	DE	202	PEB	OD-C4D	2.82	1.28	1.23
29	IN	202	PEB	OD-C4D	2.82	1.28	1.23
31	NF	1001	CYC	C3D-C2D	2.82	1.46	1.37
31	NI	1001	CYC	C3D-C2D	2.82	1.46	1.37
31	FF	1001	CYC	C3D-C2D	2.82	1.46	1.37
31	FI	1001	CYC	C3D-C2D	2.82	1.46	1.37
29	oJ	201	PEB	C4A-NA	-2.82	1.31	1.37
29	oL	201	PEB	C4A-NA	-2.82	1.31	1.37
29	gJ	201	PEB	C4A-NA	-2.82	1.31	1.37
29	gL	201	PEB	C4A-NA	-2.82	1.31	1.37
29	OJ	201	PEB	C4A-NA	-2.81	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	OL	201	PEB	C4A-NA	-2.81	1.31	1.37
29	R2	202	PEB	CHA-C1B	2.81	1.47	1.40
29	RR	202	PEB	CHA-C1B	2.81	1.47	1.40
29	N2	202	PEB	CHA-C1B	2.81	1.47	1.40
29	NR	202	PEB	CHA-C1B	2.81	1.47	1.40
31	LF	1001	CYC	C3D-C2D	2.81	1.46	1.37
31	LI	1001	CYC	C3D-C2D	2.81	1.46	1.37
30	MQ	404	PUB	OA-C1A	2.81	1.28	1.23
30	yL	303	PUB	OD-C4D	2.81	1.28	1.23
29	B5	201	PEB	C2A-C1A	-2.81	1.49	1.52
29	AA	202	PEB	C2A-C1A	-2.81	1.49	1.52
29	AN	202	PEB	C2A-C1A	-2.81	1.49	1.52
29	CJ	201	PEB	C4A-NA	-2.81	1.31	1.37
29	CL	201	PEB	C4A-NA	-2.81	1.31	1.37
30	AF	303	PUB	OD-C4D	2.81	1.28	1.23
30	AI	303	PUB	OD-C4D	2.81	1.28	1.23
29	MJ	201	PEB	C4A-NA	-2.81	1.31	1.37
29	UJ	201	PEB	C4A-NA	-2.81	1.31	1.37
29	ML	201	PEB	C4A-NA	-2.81	1.31	1.37
29	UL	201	PEB	C4A-NA	-2.81	1.31	1.37
29	F7	1002	PEB	C2A-C1A	-2.81	1.49	1.52
29	CA	202	PEB	OD-C4D	2.81	1.28	1.23
29	CN	202	PEB	OD-C4D	2.81	1.28	1.23
29	M4	202	PEB	C2C-C3C	2.81	1.46	1.37
29	AA	202	PEB	OD-C4D	2.81	1.28	1.23
29	AN	202	PEB	OD-C4D	2.81	1.28	1.23
31	MP	1001	CYC	OB-C4B	2.81	1.28	1.23
29	eJ	201	PEB	C4A-NA	-2.81	1.31	1.37
29	eL	201	PEB	C4A-NA	-2.81	1.31	1.37
29	P2	201	PEB	CHA-C1B	2.81	1.47	1.40
29	AB	303	PEB	OD-C4D	2.81	1.28	1.23
29	sJ	201	PEB	C4A-NA	-2.81	1.31	1.37
29	sL	201	PEB	C4A-NA	-2.81	1.31	1.37
29	V2	202	PEB	CHA-C1B	2.81	1.47	1.40
29	VR	202	PEB	CHA-C1B	2.81	1.47	1.40
29	kJ	201	PEB	C4A-NA	-2.81	1.31	1.37
29	kL	201	PEB	C4A-NA	-2.81	1.31	1.37
29	Z1	201	PEB	C2C-C3C	2.81	1.46	1.37
29	ZK	201	PEB	C2C-C3C	2.81	1.46	1.37
29	e1	202	PEB	C2C-C3C	2.81	1.46	1.37
29	eK	202	PEB	C2C-C3C	2.81	1.46	1.37
30	wJ	304	PUB	OA-C1A	2.81	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H5	201	PEB	C2A-C1A	-2.80	1.49	1.52
29	xJ	301	PEB	C1A-NA	-2.80	1.34	1.37
29	KJ	201	PEB	C4A-NA	-2.80	1.31	1.37
29	KL	201	PEB	C4A-NA	-2.80	1.31	1.37
29	JA	202	PEB	C2C-C3C	2.80	1.46	1.37
29	JN	202	PEB	C2C-C3C	2.80	1.46	1.37
31	JF	1001	CYC	C3D-C2D	2.80	1.46	1.37
31	JI	1001	CYC	C3D-C2D	2.80	1.46	1.37
29	N7	1002	PEB	C2A-C1A	-2.80	1.49	1.52
29	e7	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	N9	1002	PEB	C2A-C1A	-2.80	1.49	1.52
29	e9	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	EJ	201	PEB	C4A-NA	-2.80	1.31	1.37
29	EL	201	PEB	C4A-NA	-2.80	1.31	1.37
29	M4	203	PEB	OD-C4D	2.80	1.28	1.23
29	FG	203	PEB	OD-C4D	2.80	1.28	1.23
29	FQ	203	PEB	OD-C4D	2.80	1.28	1.23
29	HA	202	PEB	C2C-C3C	2.80	1.46	1.37
29	HN	202	PEB	C2C-C3C	2.80	1.46	1.37
31	DF	1001	CYC	C1B-NB	-2.80	1.33	1.37
31	DI	1001	CYC	C1B-NB	-2.80	1.33	1.37
29	AM	302	PEB	OD-C4D	2.80	1.28	1.23
30	AB	304	PUB	OA-C1A	2.80	1.28	1.23
29	wJ	301	PEB	C1A-NA	-2.80	1.34	1.37
29	i7	201	PEB	C2A-C1A	-2.80	1.49	1.52
29	i9	201	PEB	C2A-C1A	-2.80	1.49	1.52
29	IA	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	IN	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	FA	202	PEB	C2C-C3C	2.80	1.46	1.37
29	FN	202	PEB	C2C-C3C	2.80	1.46	1.37
29	RR	202	PEB	C1A-NA	-2.80	1.34	1.37
29	FA	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	FN	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	P1	202	PEB	C2C-C3C	2.80	1.46	1.37
29	PK	202	PEB	C2C-C3C	2.80	1.46	1.37
31	XP	1001	CYC	OB-C4B	2.80	1.28	1.23
29	R1	202	PEB	C2C-C3C	2.80	1.46	1.37
29	RK	202	PEB	C2C-C3C	2.80	1.46	1.37
29	EB	202	PEB	OD-C4D	2.80	1.28	1.23
29	EM	202	PEB	OD-C4D	2.80	1.28	1.23
29	qJ	201	PEB	C4A-NA	-2.80	1.31	1.37
29	qL	201	PEB	C4A-NA	-2.80	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a7	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	a9	202	PEB	C2A-C1A	-2.80	1.49	1.52
29	F9	1002	PEB	C2A-C1A	-2.79	1.49	1.52
29	LD	201	PEB	C2A-C1A	-2.79	1.49	1.52
29	PR	201	PEB	C1A-NA	-2.79	1.34	1.37
31	E1	1001	CYC	C2C-C1C	-2.79	1.49	1.52
31	1P	1002	CYC	C1B-C2B	2.79	1.50	1.45
31	EK	1001	CYC	C2C-C1C	-2.79	1.49	1.52
29	AB	302	PEB	OD-C4D	2.79	1.28	1.23
29	xJ	301	PEB	CHA-C1B	2.79	1.47	1.40
29	BC	203	PEB	OD-C4D	2.79	1.28	1.23
29	BE	203	PEB	OD-C4D	2.79	1.28	1.23
29	OR	202	PEB	OD-C4D	2.79	1.28	1.23
30	AM	304	PUB	OA-C1A	2.79	1.28	1.23
29	WJ	202	PEB	C4A-NA	-2.79	1.31	1.37
29	WL	202	PEB	C4A-NA	-2.79	1.31	1.37
29	X2	201	PEB	CHA-C1B	2.79	1.47	1.40
29	FJ	203	PEB	OD-C4D	2.79	1.28	1.23
29	FL	203	PEB	OD-C4D	2.79	1.28	1.23
31	jP	1001	CYC	OB-C4B	2.79	1.28	1.23
29	U1	201	PEB	C2C-C3C	2.79	1.45	1.37
29	UK	201	PEB	C2C-C3C	2.79	1.45	1.37
29	BA	202	PEB	C2C-C3C	2.79	1.45	1.37
29	BN	202	PEB	C2C-C3C	2.79	1.45	1.37
29	J4	201	PEB	C2A-C1A	-2.79	1.49	1.52
29	HK	1002	PEB	C2A-C1A	-2.79	1.49	1.52
29	GJ	201	PEB	C4A-NA	-2.79	1.31	1.37
29	GL	201	PEB	C4A-NA	-2.79	1.31	1.37
29	j1	203	PEB	C2C-C3C	2.79	1.45	1.37
29	jK	203	PEB	C2C-C3C	2.79	1.45	1.37
29	k1	202	PEB	C2C-C3C	2.79	1.45	1.37
29	kK	202	PEB	C2C-C3C	2.79	1.45	1.37
29	H1	1002	PEB	C2A-C1A	-2.79	1.49	1.52
29	N2	202	PEB	C1A-NA	-2.79	1.34	1.37
29	NR	202	PEB	C1A-NA	-2.79	1.34	1.37
30	MG	402	PUB	OA-C1A	2.79	1.28	1.23
30	wL	305	PUB	OD-C4D	2.79	1.28	1.23
29	LA	202	PEB	C2C-C3C	2.78	1.45	1.37
29	LN	202	PEB	C2C-C3C	2.78	1.45	1.37
29	JD	201	PEB	C2A-C1A	-2.78	1.49	1.52
29	BG	203	PEB	OD-C4D	2.78	1.28	1.23
29	N3	202	PEB	C2A-C1A	-2.78	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	KA	202	PEB	OD-C4D	2.78	1.28	1.23
29	KN	202	PEB	OD-C4D	2.78	1.28	1.23
30	xJ	304	PUB	OA-C1A	2.78	1.28	1.23
29	i7	202	PEB	C2A-C1A	-2.78	1.49	1.52
29	i9	202	PEB	C2A-C1A	-2.78	1.49	1.52
29	V1	202	PEB	C2C-C3C	2.78	1.45	1.37
29	VK	202	PEB	C2C-C3C	2.78	1.45	1.37
29	wL	302	PEB	OD-C4D	2.78	1.28	1.23
29	DA	202	PEB	C2C-C3C	2.78	1.45	1.37
29	DN	202	PEB	C2C-C3C	2.78	1.45	1.37
29	BA	202	PEB	C2A-C1A	-2.78	1.49	1.52
29	BN	202	PEB	C2A-C1A	-2.78	1.49	1.52
29	BQ	203	PEB	OD-C4D	2.78	1.28	1.23
29	MR	202	PEB	OD-C4D	2.78	1.28	1.23
29	A7	305	PEB	OD-C4D	2.78	1.28	1.23
29	A9	305	PEB	OD-C4D	2.78	1.28	1.23
29	XB	202	PEB	OD-C4D	2.78	1.28	1.23
29	XM	202	PEB	OD-C4D	2.78	1.28	1.23
29	BB	301	PEB	C4A-NA	-2.78	1.31	1.37
29	BM	301	PEB	C4A-NA	-2.78	1.31	1.37
29	DJ	202	PEB	OD-C4D	2.77	1.28	1.23
29	DL	202	PEB	OD-C4D	2.77	1.28	1.23
29	K5	203	PEB	C2A-C1A	-2.77	1.49	1.52
29	K8	203	PEB	C2A-C1A	-2.77	1.49	1.52
29	YJ	201	PEB	C4A-NA	-2.77	1.31	1.37
29	YL	201	PEB	C4A-NA	-2.77	1.31	1.37
29	I4	203	PEB	OD-C4D	2.77	1.28	1.23
29	wJ	302	PEB	OD-C4D	2.77	1.28	1.23
29	pJ	203	PEB	OD-C4D	2.77	1.28	1.23
29	pL	203	PEB	OD-C4D	2.77	1.28	1.23
29	gF	202	PEB	C2A-C1A	-2.77	1.49	1.52
29	gI	202	PEB	C2A-C1A	-2.77	1.49	1.52
29	PB	202	PEB	OD-C4D	2.77	1.28	1.23
29	SB	202	PEB	OD-C4D	2.77	1.28	1.23
29	PM	202	PEB	OD-C4D	2.77	1.28	1.23
29	SM	202	PEB	OD-C4D	2.77	1.28	1.23
30	yL	303	PUB	OA-C1A	2.77	1.28	1.23
31	fP	1001	CYC	C1D-CHD	2.77	1.51	1.41
29	T2	202	PEB	CHA-C1B	2.77	1.46	1.40
29	TR	202	PEB	CHA-C1B	2.77	1.46	1.40
29	fJ	203	PEB	OD-C4D	2.77	1.28	1.23
29	fL	203	PEB	OD-C4D	2.77	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	eB	202	PEB	OD-C4D	2.77	1.28	1.23
29	eM	202	PEB	OD-C4D	2.77	1.28	1.23
30	MN	403	PUB	OA-C1A	2.77	1.28	1.23
29	L8	201	PEB	C2A-C1A	-2.77	1.49	1.52
30	yJ	303	PUB	OD-C4D	2.77	1.28	1.23
31	YP	1000	CYC	C1B-C2B	2.77	1.50	1.45
29	FB	203	PEB	OD-C4D	2.77	1.28	1.23
29	FM	203	PEB	OD-C4D	2.77	1.28	1.23
29	QB	204	PEB	OD-C4D	2.77	1.28	1.23
29	aB	202	PEB	OD-C4D	2.77	1.28	1.23
29	BJ	203	PEB	OD-C4D	2.77	1.28	1.23
29	BL	203	PEB	OD-C4D	2.77	1.28	1.23
29	QM	204	PEB	OD-C4D	2.77	1.28	1.23
29	aM	202	PEB	OD-C4D	2.77	1.28	1.23
29	xL	301	PEB	CHA-C1B	2.77	1.46	1.40
29	DG	202	PEB	OD-C4D	2.77	1.28	1.23
29	DQ	202	PEB	OD-C4D	2.77	1.28	1.23
29	T2	202	PEB	C1A-NA	-2.77	1.34	1.37
29	B5	203	PEB	OD-C4D	2.77	1.28	1.23
29	a7	201	PEB	C2A-C1A	-2.77	1.49	1.52
29	a9	201	PEB	C2A-C1A	-2.77	1.49	1.52
29	AM	303	PEB	OD-C4D	2.77	1.28	1.23
29	P2	201	PEB	C1A-NA	-2.76	1.34	1.37
29	m7	201	PEB	C2A-C1A	-2.76	1.49	1.52
29	m9	201	PEB	C2A-C1A	-2.76	1.49	1.52
29	MN	404	PEB	C2A-C1A	-2.76	1.49	1.52
29	mB	203	PEB	OD-C4D	2.76	1.28	1.23
29	mM	203	PEB	OD-C4D	2.76	1.28	1.23
30	xL	304	PUB	OA-C1A	2.76	1.28	1.23
29	MQ	406	PEB	C2A-C1A	-2.76	1.49	1.52
31	DP	1001	CYC	C1D-CHD	2.76	1.51	1.41
29	A5	203	PEB	C2A-C1A	-2.76	1.49	1.52
29	A8	203	PEB	C2A-C1A	-2.76	1.49	1.52
29	D1	1002	PEB	O1C-CGC	2.76	1.31	1.22
29	JJ	203	PEB	OD-C4D	2.76	1.28	1.23
29	JL	203	PEB	OD-C4D	2.76	1.28	1.23
29	IJ	203	PEB	OD-C4D	2.76	1.28	1.23
29	IL	203	PEB	OD-C4D	2.76	1.28	1.23
31	jP	1001	CYC	C1D-CHD	2.76	1.51	1.41
29	IG	201	PEB	OD-C4D	2.76	1.28	1.23
29	IQ	201	PEB	OD-C4D	2.76	1.28	1.23
29	J7	1002	PEB	C2A-C1A	-2.76	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TR	202	PEB	C1A-NA	-2.76	1.34	1.37
29	hJ	203	PEB	OD-C4D	2.76	1.28	1.23
29	hL	203	PEB	OD-C4D	2.76	1.28	1.23
29	JG	203	PEB	OD-C4D	2.76	1.28	1.23
29	wL	301	PEB	C1A-NA	-2.76	1.34	1.37
29	H4	202	PEB	OD-C4D	2.76	1.28	1.23
29	hB	202	PEB	OD-C4D	2.76	1.28	1.23
29	hM	202	PEB	OD-C4D	2.76	1.28	1.23
29	TB	203	PEB	OD-C4D	2.76	1.28	1.23
29	jB	202	PEB	OD-C4D	2.76	1.28	1.23
29	HJ	202	PEB	OD-C4D	2.76	1.28	1.23
29	TJ	203	PEB	OD-C4D	2.76	1.28	1.23
29	HL	202	PEB	OD-C4D	2.76	1.28	1.23
29	TL	203	PEB	OD-C4D	2.76	1.28	1.23
29	TM	203	PEB	OD-C4D	2.76	1.28	1.23
29	jM	202	PEB	OD-C4D	2.76	1.28	1.23
29	NB	202	PEB	OD-C4D	2.76	1.28	1.23
29	NM	202	PEB	OD-C4D	2.76	1.28	1.23
31	nP	1001	CYC	C1D-CHD	2.76	1.51	1.41
29	MG	404	PEB	C2A-C1A	-2.76	1.49	1.52
29	cB	203	PEB	OD-C4D	2.76	1.28	1.23
29	cM	203	PEB	OD-C4D	2.76	1.28	1.23
29	D4	202	PEB	OD-C4D	2.75	1.28	1.23
29	WB	202	PEB	OD-C4D	2.75	1.28	1.23
29	DD	202	PEB	OD-C4D	2.75	1.28	1.23
29	XJ	203	PEB	OD-C4D	2.75	1.28	1.23
29	XL	203	PEB	OD-C4D	2.75	1.28	1.23
29	WM	202	PEB	OD-C4D	2.75	1.28	1.23
30	yJ	303	PUB	OA-C1A	2.75	1.28	1.23
29	C5	203	PEB	C2A-C1A	-2.75	1.49	1.52
29	R7	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	T7	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	C8	203	PEB	C2A-C1A	-2.75	1.49	1.52
29	R9	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	T9	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	fB	202	PEB	OD-C4D	2.75	1.28	1.23
29	JD	202	PEB	OD-C4D	2.75	1.28	1.23
29	fM	202	PEB	OD-C4D	2.75	1.28	1.23
29	X2	201	PEB	C1A-NA	-2.75	1.34	1.37
29	ZB	203	PEB	OD-C4D	2.75	1.28	1.23
29	ZM	203	PEB	OD-C4D	2.75	1.28	1.23
29	LQ	202	PEB	OD-C4D	2.75	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NK	1002	PEB	C2A-C1A	-2.75	1.49	1.52
29	FG	202	PEB	OD-C4D	2.75	1.28	1.23
29	PJ	203	PEB	OD-C4D	2.75	1.28	1.23
29	bJ	203	PEB	OD-C4D	2.75	1.28	1.23
29	PL	203	PEB	OD-C4D	2.75	1.28	1.23
29	bL	203	PEB	OD-C4D	2.75	1.28	1.23
29	FQ	202	PEB	OD-C4D	2.75	1.28	1.23
31	sP	1001	CYC	C1D-CHD	2.75	1.51	1.41
29	LA	201	PEB	OD-C4D	2.75	1.28	1.23
29	LJ	202	PEB	OD-C4D	2.75	1.28	1.23
29	LL	202	PEB	OD-C4D	2.75	1.28	1.23
29	LN	201	PEB	OD-C4D	2.75	1.28	1.23
29	JQ	203	PEB	OD-C4D	2.75	1.28	1.23
29	vJ	202	PEB	OD-C4D	2.75	1.28	1.23
29	vL	202	PEB	OD-C4D	2.75	1.28	1.23
29	J4	202	PEB	OD-C4D	2.75	1.28	1.23
29	KB	202	PEB	OD-C4D	2.75	1.28	1.23
29	KM	202	PEB	OD-C4D	2.75	1.28	1.23
30	wL	304	PUB	OA-C1A	2.75	1.28	1.23
29	RJ	202	PEB	C2C-C3C	2.75	1.45	1.37
29	RL	202	PEB	C2C-C3C	2.75	1.45	1.37
30	wJ	305	PUB	OD-C4D	2.75	1.28	1.23
31	MP	1001	CYC	C1D-CHD	2.75	1.51	1.41
31	qP	1001	CYC	C1D-CHD	2.75	1.51	1.41
29	JG	202	PEB	OD-C4D	2.75	1.28	1.23
29	JQ	202	PEB	OD-C4D	2.75	1.28	1.23
29	D1	1002	PEB	C2A-C1A	-2.75	1.49	1.52
29	B8	203	PEB	OD-C4D	2.75	1.28	1.23
29	kB	203	PEB	OD-C4D	2.75	1.28	1.23
29	kM	203	PEB	OD-C4D	2.75	1.28	1.23
31	BP	1001	CYC	C1D-CHD	2.75	1.51	1.41
29	KC	202	PEB	OD-C4D	2.75	1.28	1.23
29	KE	202	PEB	OD-C4D	2.75	1.28	1.23
29	C3	202	PEB	OD-C4D	2.75	1.28	1.23
29	IB	202	PEB	OD-C4D	2.75	1.28	1.23
29	lB	202	PEB	OD-C4D	2.75	1.28	1.23
29	IM	202	PEB	OD-C4D	2.75	1.28	1.23
29	lM	202	PEB	OD-C4D	2.75	1.28	1.23
29	CO	202	PEB	OD-C4D	2.75	1.28	1.23
31	HP	1001	CYC	C1D-CHD	2.75	1.51	1.41
31	UP	1001	CYC	C1D-CHD	2.75	1.51	1.41
31	QP	1001	CYC	C1D-CHD	2.75	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A3	202	PEB	OD-C4D	2.75	1.28	1.23
29	BD	202	PEB	OD-C4D	2.75	1.28	1.23
29	AO	202	PEB	OD-C4D	2.75	1.28	1.23
29	P7	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	P9	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	eF	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	eI	202	PEB	C2A-C1A	-2.75	1.49	1.52
29	D3	203	PEB	OD-C4D	2.75	1.28	1.23
29	dB	202	PEB	OD-C4D	2.75	1.28	1.23
29	dM	202	PEB	OD-C4D	2.75	1.28	1.23
29	DO	203	PEB	OD-C4D	2.75	1.28	1.23
29	nJ	202	PEB	C2C-C3C	2.74	1.45	1.37
29	nL	202	PEB	C2C-C3C	2.74	1.45	1.37
29	G3	202	PEB	OD-C4D	2.74	1.28	1.23
29	GO	202	PEB	OD-C4D	2.74	1.28	1.23
29	aF	202	PEB	C2A-C1A	-2.74	1.49	1.52
29	aI	202	PEB	C2A-C1A	-2.74	1.49	1.52
29	NK	1002	PEB	O1C-CGC	2.74	1.31	1.22
29	MB	202	PEB	OD-C4D	2.74	1.28	1.23
29	UB	202	PEB	OD-C4D	2.74	1.28	1.23
29	iB	203	PEB	OD-C4D	2.74	1.28	1.23
29	rJ	203	PEB	OD-C4D	2.74	1.28	1.23
29	rL	203	PEB	OD-C4D	2.74	1.28	1.23
29	MM	202	PEB	OD-C4D	2.74	1.28	1.23
29	iM	203	PEB	OD-C4D	2.74	1.28	1.23
29	MQ	401	PEB	OD-C4D	2.74	1.28	1.23
31	oP	1001	CYC	C1D-CHD	2.74	1.51	1.41
29	L1	1002	PEB	OD-C4D	2.74	1.28	1.23
29	JA	201	PEB	OD-C4D	2.74	1.28	1.23
29	EG	202	PEB	OD-C4D	2.74	1.28	1.23
29	LK	1002	PEB	OD-C4D	2.74	1.28	1.23
29	JN	201	PEB	OD-C4D	2.74	1.28	1.23
29	EQ	202	PEB	OD-C4D	2.74	1.28	1.23
29	FJ	202	PEB	C2C-C3C	2.74	1.45	1.37
29	FL	202	PEB	C2C-C3C	2.74	1.45	1.37
29	DQ	203	PEB	OD-C4D	2.74	1.28	1.23
31	hP	1001	CYC	C1D-CHD	2.74	1.51	1.41
29	BG	202	PEB	OD-C4D	2.74	1.28	1.23
29	DG	203	PEB	OD-C4D	2.74	1.28	1.23
29	xJ	302	PEB	OD-C4D	2.74	1.28	1.23
29	BQ	202	PEB	OD-C4D	2.74	1.28	1.23
31	kP	1001	CYC	C1D-CHD	2.74	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	WJ	201	PEB	C2C-C3C	2.74	1.45	1.37
29	WL	201	PEB	C2C-C3C	2.74	1.45	1.37
29	ZJ	203	PEB	OD-C4D	2.74	1.28	1.23
29	ZL	203	PEB	OD-C4D	2.74	1.28	1.23
29	XR	202	PEB	C1A-NA	-2.74	1.34	1.37
29	c1	202	PEB	CHA-C1B	2.74	1.46	1.40
29	cK	202	PEB	CHA-C1B	2.74	1.46	1.40
29	HA	201	PEB	OD-C4D	2.74	1.28	1.23
29	HN	201	PEB	OD-C4D	2.74	1.28	1.23
31	XP	1001	CYC	C1D-CHD	2.74	1.51	1.41
29	wL	301	PEB	CHA-C1B	2.74	1.46	1.40
29	F4	202	PEB	OD-C4D	2.74	1.28	1.23
29	K5	201	PEB	OD-C4D	2.74	1.28	1.23
29	K8	201	PEB	OD-C4D	2.74	1.28	1.23
29	DA	203	PEB	OD-C4D	2.74	1.28	1.23
29	FD	202	PEB	OD-C4D	2.74	1.28	1.23
29	DN	203	PEB	OD-C4D	2.74	1.28	1.23
29	H7	1002	PEB	C2A-C1A	-2.74	1.49	1.52
29	H9	1002	PEB	C2A-C1A	-2.74	1.49	1.52
31	FF	1001	CYC	C1B-NB	-2.74	1.33	1.37
31	FI	1001	CYC	C1B-NB	-2.74	1.33	1.37
29	CC	201	PEB	OD-C4D	2.74	1.28	1.23
29	CE	201	PEB	OD-C4D	2.74	1.28	1.23
31	1P	1001	CYC	C1D-CHD	2.74	1.51	1.41
29	dJ	203	PEB	OD-C4D	2.74	1.28	1.23
29	dL	203	PEB	OD-C4D	2.74	1.28	1.23
29	IJ	203	PEB	C2C-C3C	2.74	1.45	1.37
29	IL	203	PEB	C2C-C3C	2.74	1.45	1.37
29	LB	203	PEB	OD-C4D	2.74	1.28	1.23
29	LM	203	PEB	OD-C4D	2.74	1.28	1.23
31	LF	1001	CYC	C1B-NB	-2.74	1.33	1.37
31	LI	1001	CYC	C1B-NB	-2.74	1.33	1.37
29	VF	202	PEB	C2A-C1A	-2.74	1.49	1.52
29	VI	202	PEB	C2A-C1A	-2.74	1.49	1.52
31	CK	1001	CYC	C2C-C1C	-2.74	1.49	1.52
29	N1	1002	PEB	O1C-CGC	2.74	1.31	1.22
29	RB	203	PEB	OD-C4D	2.74	1.28	1.23
29	RM	203	PEB	OD-C4D	2.74	1.28	1.23
29	AJ	203	PEB	C2C-C3C	2.74	1.45	1.37
29	AL	203	PEB	C2C-C3C	2.74	1.45	1.37
29	K3	202	PEB	OD-C4D	2.74	1.28	1.23
29	OB	202	PEB	OD-C4D	2.74	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HD	202	PEB	OD-C4D	2.74	1.28	1.23
29	LD	202	PEB	OD-C4D	2.74	1.28	1.23
29	CG	201	PEB	OD-C4D	2.74	1.28	1.23
29	OM	202	PEB	OD-C4D	2.74	1.28	1.23
29	KO	202	PEB	OD-C4D	2.74	1.28	1.23
29	CQ	201	PEB	OD-C4D	2.74	1.28	1.23
30	MQ	404	PUB	OD-C4D	2.74	1.28	1.23
29	AF	301	PEB	OD-C4D	2.74	1.28	1.23
29	AI	301	PEB	OD-C4D	2.74	1.28	1.23
29	E3	202	PEB	OD-C4D	2.74	1.28	1.23
29	EC	201	PEB	OD-C4D	2.74	1.28	1.23
29	EE	201	PEB	OD-C4D	2.74	1.28	1.23
29	EO	202	PEB	OD-C4D	2.74	1.28	1.23
31	wP	1001	CYC	C1D-CHD	2.74	1.51	1.41
29	mF	202	PEB	C2A-C1A	-2.74	1.49	1.52
29	mI	202	PEB	C2A-C1A	-2.74	1.49	1.52
29	F5	203	PEB	OD-C4D	2.74	1.28	1.23
29	F8	203	PEB	OD-C4D	2.74	1.28	1.23
29	LG	202	PEB	OD-C4D	2.74	1.28	1.23
29	LQ	201	PEB	OD-C4D	2.74	1.28	1.23
29	I5	201	PEB	OD-C4D	2.73	1.28	1.23
29	I8	201	PEB	OD-C4D	2.73	1.28	1.23
29	YB	203	PEB	OD-C4D	2.73	1.28	1.23
29	YM	203	PEB	OD-C4D	2.73	1.28	1.23
31	eP	1001	CYC	C1B-C2B	2.73	1.50	1.45
31	IP	1001	CYC	C1D-CHD	2.73	1.51	1.41
29	GC	201	PEB	OD-C4D	2.73	1.28	1.23
29	GE	201	PEB	OD-C4D	2.73	1.28	1.23
29	CG	202	PEB	OD-C4D	2.73	1.28	1.23
29	GG	202	PEB	OD-C4D	2.73	1.28	1.23
29	NK	1002	PEB	OD-C4D	2.73	1.28	1.23
29	CQ	202	PEB	OD-C4D	2.73	1.28	1.23
29	GQ	202	PEB	OD-C4D	2.73	1.28	1.23
31	mP	1001	CYC	C1B-C2B	2.73	1.50	1.45
29	KG	201	PEB	OD-C4D	2.73	1.28	1.23
29	RJ	203	PEB	OD-C4D	2.73	1.28	1.23
29	RL	203	PEB	OD-C4D	2.73	1.28	1.23
29	KQ	201	PEB	OD-C4D	2.73	1.28	1.23
31	JF	1001	CYC	C1B-NB	-2.73	1.33	1.37
31	JI	1001	CYC	C1B-NB	-2.73	1.33	1.37
31	OP	1001	CYC	C1D-CHD	2.73	1.51	1.41
29	L5	203	PEB	OD-C4D	2.73	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BA	203	PEB	OD-C4D	2.73	1.28	1.23
29	BN	203	PEB	OD-C4D	2.73	1.28	1.23
30	xL	305	PUB	OD-C4D	2.73	1.28	1.23
29	jI	203	PEB	CHA-C1B	2.73	1.46	1.40
29	jK	203	PEB	CHA-C1B	2.73	1.46	1.40
29	uJ	201	PEB	C2C-C3C	2.73	1.45	1.37
29	uL	201	PEB	C2C-C3C	2.73	1.45	1.37
29	XJ	202	PEB	C2C-C3C	2.73	1.45	1.37
29	XL	202	PEB	C2C-C3C	2.73	1.45	1.37
30	AB	305	PUB	OD-C4D	2.73	1.28	1.23
29	kI	203	PEB	OD-C4D	2.73	1.28	1.23
29	GG	201	PEB	OD-C4D	2.73	1.28	1.23
29	IG	202	PEB	OD-C4D	2.73	1.28	1.23
29	kK	203	PEB	OD-C4D	2.73	1.28	1.23
29	GQ	201	PEB	OD-C4D	2.73	1.28	1.23
29	IQ	202	PEB	OD-C4D	2.73	1.28	1.23
29	HK	1002	PEB	O1C-CGC	2.73	1.31	1.22
31	NF	1001	CYC	C1B-NB	-2.73	1.33	1.37
31	NI	1001	CYC	C1B-NB	-2.73	1.33	1.37
31	FP	1001	CYC	C1D-CHD	2.73	1.51	1.41
29	A7	304	PEB	OD-C4D	2.73	1.28	1.23
29	A9	304	PEB	OD-C4D	2.73	1.28	1.23
29	gF	202	PEB	C2C-C3C	2.73	1.45	1.37
29	gI	202	PEB	C2C-C3C	2.73	1.45	1.37
29	L5	201	PEB	C2A-C1A	-2.73	1.49	1.52
29	D7	1002	PEB	C2A-C1A	-2.73	1.49	1.52
29	D9	1002	PEB	C2A-C1A	-2.73	1.49	1.52
29	H3	203	PEB	OD-C4D	2.73	1.28	1.23
29	HO	203	PEB	OD-C4D	2.73	1.28	1.23
29	DA	201	PEB	OD-C4D	2.73	1.28	1.23
29	tJ	202	PEB	OD-C4D	2.73	1.28	1.23
29	tL	202	PEB	OD-C4D	2.73	1.28	1.23
29	DN	201	PEB	OD-C4D	2.73	1.28	1.23
31	tP	1001	CYC	C1B-C2B	2.73	1.50	1.45
29	J1	1002	PEB	O1C-CGC	2.73	1.31	1.22
29	JK	1002	PEB	O1C-CGC	2.73	1.31	1.22
29	kI	202	PEB	CHA-C1B	2.73	1.46	1.40
29	kK	202	PEB	CHA-C1B	2.73	1.46	1.40
30	AM	305	PUB	OD-C4D	2.73	1.28	1.23
31	GP	1001	CYC	C1B-C2B	2.73	1.50	1.45
29	dF	201	PEB	C2A-C1A	-2.73	1.49	1.52
29	dI	201	PEB	C2A-C1A	-2.73	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G5	202	PEB	OD-C4D	2.73	1.28	1.23
29	G8	203	PEB	OD-C4D	2.73	1.28	1.23
29	P1	202	PEB	CHA-C1B	2.73	1.46	1.40
29	PK	202	PEB	CHA-C1B	2.73	1.46	1.40
29	A1	303	PEB	C2A-C1A	-2.73	1.49	1.52
29	L9	1002	PEB	C2A-C1A	-2.73	1.49	1.52
29	AK	303	PEB	C2A-C1A	-2.73	1.49	1.52
29	L3	202	PEB	OD-C4D	2.73	1.28	1.23
29	L4	202	PEB	OD-C4D	2.73	1.28	1.23
29	NJ	203	PEB	OD-C4D	2.73	1.28	1.23
29	NL	203	PEB	OD-C4D	2.73	1.28	1.23
29	LO	202	PEB	OD-C4D	2.73	1.28	1.23
29	PJ	202	PEB	C2C-C3C	2.73	1.45	1.37
29	PL	202	PEB	C2C-C3C	2.73	1.45	1.37
31	uP	1001	CYC	C1D-CHD	2.73	1.51	1.41
29	NJ	202	PEB	C2C-C3C	2.73	1.45	1.37
29	NL	202	PEB	C2C-C3C	2.73	1.45	1.37
29	i1	203	PEB	OD-C4D	2.73	1.28	1.23
29	nJ	203	PEB	OD-C4D	2.73	1.28	1.23
29	iK	203	PEB	OD-C4D	2.73	1.28	1.23
29	nL	203	PEB	OD-C4D	2.73	1.28	1.23
30	AF	302	PUB	OD-C4D	2.73	1.28	1.23
30	AI	302	PUB	OD-C4D	2.73	1.28	1.23
31	TP	1001	CYC	C1B-C2B	2.73	1.50	1.45
29	mF	202	PEB	C2C-C3C	2.73	1.45	1.37
29	mI	202	PEB	C2C-C3C	2.73	1.45	1.37
29	JJ	202	PEB	C2C-C3C	2.73	1.45	1.37
29	JL	202	PEB	C2C-C3C	2.73	1.45	1.37
29	J1	1002	PEB	C2A-C1A	-2.73	1.49	1.52
29	V7	202	PEB	C2A-C1A	-2.73	1.49	1.52
29	V9	202	PEB	C2A-C1A	-2.73	1.49	1.52
29	JK	1002	PEB	C2A-C1A	-2.73	1.49	1.52
29	D1	1002	PEB	OD-C4D	2.72	1.28	1.23
29	B4	202	PEB	OD-C4D	2.72	1.28	1.23
29	BA	201	PEB	OD-C4D	2.72	1.28	1.23
29	CB	202	PEB	OD-C4D	2.72	1.28	1.23
29	CM	202	PEB	OD-C4D	2.72	1.28	1.23
29	BN	201	PEB	OD-C4D	2.72	1.28	1.23
29	H1	1002	PEB	O1C-CGC	2.72	1.31	1.22
29	c7	202	PEB	C2A-C1A	-2.72	1.49	1.52
29	c9	202	PEB	C2A-C1A	-2.72	1.49	1.52
29	xJ	303	PEB	C2A-C1A	-2.72	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NO	202	PEB	C2A-C1A	-2.72	1.49	1.52
29	IJ	202	PEB	C2C-C3C	2.72	1.45	1.37
29	IL	202	PEB	C2C-C3C	2.72	1.45	1.37
29	FA	202	PEB	CHA-C1B	2.72	1.46	1.40
29	FN	202	PEB	CHA-C1B	2.72	1.46	1.40
29	G8	202	PEB	OD-C4D	2.72	1.28	1.23
29	AG	202	PEB	OD-C4D	2.72	1.28	1.23
29	AQ	202	PEB	OD-C4D	2.72	1.28	1.23
29	GB	202	PEB	OD-C4D	2.72	1.28	1.23
29	HK	1002	PEB	OD-C4D	2.72	1.28	1.23
29	GM	202	PEB	OD-C4D	2.72	1.28	1.23
29	DK	1002	PEB	O1C-CGC	2.72	1.31	1.22
29	JB	203	PEB	OD-C4D	2.72	1.28	1.23
29	JM	203	PEB	OD-C4D	2.72	1.28	1.23
29	UF	201	PEB	C2A-C1A	-2.72	1.49	1.52
29	UI	201	PEB	C2A-C1A	-2.72	1.49	1.52
29	B3	203	PEB	OD-C4D	2.72	1.28	1.23
29	BO	203	PEB	OD-C4D	2.72	1.28	1.23
29	rJ	202	PEB	C2C-C3C	2.72	1.45	1.37
29	rL	202	PEB	C2C-C3C	2.72	1.45	1.37
29	YF	203	PEB	OD-C4D	2.72	1.28	1.23
29	YI	203	PEB	OD-C4D	2.72	1.28	1.23
30	xJ	305	PUB	OD-C4D	2.72	1.28	1.23
29	LG	203	PEB	OD-C4D	2.72	1.28	1.23
29	BJ	202	PEB	C2C-C3C	2.72	1.45	1.37
29	BL	202	PEB	C2C-C3C	2.72	1.45	1.37
29	e1	202	PEB	CHA-C1B	2.72	1.46	1.40
29	eK	202	PEB	CHA-C1B	2.72	1.46	1.40
29	H5	201	PEB	OD-C4D	2.72	1.28	1.23
29	A5	201	PEB	OD-C4D	2.72	1.28	1.23
29	A8	201	PEB	OD-C4D	2.72	1.28	1.23
29	L1	1002	PEB	O1C-CGC	2.72	1.31	1.22
29	LK	1002	PEB	O1C-CGC	2.72	1.31	1.22
29	aF	202	PEB	C2C-C3C	2.72	1.45	1.37
29	aI	202	PEB	C2C-C3C	2.72	1.45	1.37
29	AG	201	PEB	OD-C4D	2.72	1.28	1.23
29	KG	202	PEB	OD-C4D	2.72	1.28	1.23
29	AQ	201	PEB	OD-C4D	2.72	1.28	1.23
29	KQ	202	PEB	OD-C4D	2.72	1.28	1.23
29	VB	203	PEB	OD-C4D	2.72	1.28	1.23
29	VJ	202	PEB	OD-C4D	2.72	1.28	1.23
29	VL	202	PEB	OD-C4D	2.72	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VM	203	PEB	OD-C4D	2.72	1.28	1.23
31	SP	1001	CYC	C1D-CHD	2.72	1.51	1.41
29	Z1	201	PEB	CHA-C1B	2.72	1.46	1.40
29	ZK	201	PEB	CHA-C1B	2.72	1.46	1.40
29	a1	202	PEB	CHA-C1B	2.72	1.46	1.40
29	aK	202	PEB	CHA-C1B	2.72	1.46	1.40
29	N1	1002	PEB	OD-C4D	2.72	1.28	1.23
29	e1	203	PEB	OD-C4D	2.72	1.28	1.23
29	eK	203	PEB	OD-C4D	2.72	1.28	1.23
30	A1	305	PUB	OD-C4D	2.72	1.28	1.23
30	AK	305	PUB	OD-C4D	2.72	1.28	1.23
29	J9	1002	PEB	C2A-C1A	-2.72	1.49	1.52
29	PF	202	PEB	C2C-C3C	2.72	1.45	1.37
29	PI	202	PEB	C2C-C3C	2.72	1.45	1.37
29	H1	1002	PEB	OD-C4D	2.72	1.28	1.23
29	a1	203	PEB	OD-C4D	2.72	1.28	1.23
29	HG	202	PEB	OD-C4D	2.72	1.28	1.23
29	aK	203	PEB	OD-C4D	2.72	1.28	1.23
29	HQ	202	PEB	OD-C4D	2.72	1.28	1.23
29	Y7	202	PEB	C2A-C1A	-2.72	1.49	1.52
29	Y9	202	PEB	C2A-C1A	-2.72	1.49	1.52
29	Q2	201	PEB	C4A-NA	-2.71	1.31	1.37
29	fJ	202	PEB	C2C-C3C	2.71	1.45	1.37
29	fL	202	PEB	C2C-C3C	2.71	1.45	1.37
31	HF	1001	CYC	C1B-NB	-2.71	1.33	1.37
31	HI	1001	CYC	C1B-NB	-2.71	1.33	1.37
31	gP	1001	CYC	C1B-C2B	2.71	1.50	1.45
29	hJ	202	PEB	C2C-C3C	2.71	1.45	1.37
29	hL	202	PEB	C2C-C3C	2.71	1.45	1.37
29	HB	203	PEB	OD-C4D	2.71	1.28	1.23
29	HM	203	PEB	OD-C4D	2.71	1.28	1.23
31	K1	1001	CYC	C2C-C1C	-2.71	1.49	1.52
31	KK	1001	CYC	C2C-C1C	-2.71	1.49	1.52
29	DA	202	PEB	CHA-C1B	2.71	1.46	1.40
29	DN	202	PEB	CHA-C1B	2.71	1.46	1.40
29	R1	203	PEB	OD-C4D	2.71	1.28	1.23
29	T1	202	PEB	OD-C4D	2.71	1.28	1.23
29	c1	203	PEB	OD-C4D	2.71	1.28	1.23
29	B8	202	PEB	OD-C4D	2.71	1.28	1.23
29	RK	203	PEB	OD-C4D	2.71	1.28	1.23
29	TK	202	PEB	OD-C4D	2.71	1.28	1.23
29	cK	203	PEB	OD-C4D	2.71	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	wJ	301	PEB	CHA-C1B	2.71	1.46	1.40
29	F1	1002	PEB	OD-C4D	2.71	1.28	1.23
29	FK	1002	PEB	OD-C4D	2.71	1.28	1.23
29	AF	304	PEB	C2A-C1A	-2.71	1.49	1.52
29	AI	304	PEB	C2A-C1A	-2.71	1.49	1.52
31	NP	1001	CYC	C1B-C2B	2.71	1.50	1.45
29	pJ	202	PEB	C2C-C3C	2.71	1.45	1.37
29	pL	202	PEB	C2C-C3C	2.71	1.45	1.37
29	S2	201	PEB	OD-C4D	2.71	1.28	1.23
29	EG	201	PEB	OD-C4D	2.71	1.28	1.23
29	EQ	201	PEB	OD-C4D	2.71	1.28	1.23
29	L8	203	PEB	OD-C4D	2.71	1.28	1.23
29	jJ	203	PEB	OD-C4D	2.71	1.28	1.23
29	jL	203	PEB	OD-C4D	2.71	1.28	1.23
29	HA	203	PEB	OD-C4D	2.71	1.28	1.23
29	HN	203	PEB	OD-C4D	2.71	1.28	1.23
29	R1	202	PEB	CHA-C1B	2.71	1.46	1.40
29	RK	202	PEB	CHA-C1B	2.71	1.46	1.40
29	wJ	303	PEB	C2A-C1A	-2.71	1.49	1.52
29	AC	201	PEB	OD-C4D	2.71	1.28	1.23
29	HC	201	PEB	OD-C4D	2.71	1.28	1.23
29	AE	201	PEB	OD-C4D	2.71	1.28	1.23
29	HE	201	PEB	OD-C4D	2.71	1.28	1.23
29	I3	202	PEB	OD-C4D	2.71	1.28	1.23
29	IO	202	PEB	OD-C4D	2.71	1.28	1.23
29	J1	1002	PEB	OD-C4D	2.71	1.28	1.23
29	DB	203	PEB	OD-C4D	2.71	1.28	1.23
29	JK	1002	PEB	OD-C4D	2.71	1.28	1.23
29	DM	203	PEB	OD-C4D	2.71	1.28	1.23
29	i7	203	PEB	OD-C4D	2.71	1.28	1.23
29	i9	203	PEB	OD-C4D	2.71	1.28	1.23
29	DC	201	PEB	OD-C4D	2.71	1.28	1.23
29	DE	201	PEB	OD-C4D	2.71	1.28	1.23
29	YF	202	PEB	C2C-C3C	2.71	1.45	1.37
29	YI	202	PEB	C2C-C3C	2.71	1.45	1.37
29	LA	203	PEB	OD-C4D	2.71	1.28	1.23
29	LN	203	PEB	OD-C4D	2.71	1.28	1.23
29	iF	202	PEB	C2A-C1A	-2.71	1.49	1.52
29	iI	202	PEB	C2A-C1A	-2.71	1.49	1.52
29	F1	1002	PEB	O1C-CGC	2.71	1.31	1.22
29	FK	1002	PEB	O1C-CGC	2.71	1.31	1.22
29	iF	202	PEB	C2C-C3C	2.71	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	iI	202	PEB	C2C-C3C	2.71	1.45	1.37
29	R7	203	PEB	OD-C4D	2.71	1.28	1.23
29	R9	203	PEB	OD-C4D	2.71	1.28	1.23
29	H8	202	PEB	OD-C4D	2.71	1.28	1.23
31	I1	1001	CYC	C2C-C1C	-2.71	1.49	1.52
29	DK	1002	PEB	OD-C4D	2.71	1.28	1.23
31	RP	1001	CYC	C1B-C2B	2.71	1.50	1.45
29	Y1	202	PEB	OD-C4D	2.71	1.28	1.23
29	YK	202	PEB	OD-C4D	2.71	1.28	1.23
29	AM	301	PEB	OD-C4D	2.71	1.28	1.23
29	N1	1002	PEB	C2A-C1A	-2.71	1.49	1.52
29	OF	203	PEB	C2C-C3C	2.71	1.45	1.37
29	OI	203	PEB	C2C-C3C	2.71	1.45	1.37
29	U1	201	PEB	CHA-C1B	2.71	1.46	1.40
29	UK	201	PEB	CHA-C1B	2.71	1.46	1.40
29	HG	203	PEB	OD-C4D	2.71	1.28	1.23
29	V1	203	PEB	OD-C4D	2.71	1.28	1.23
29	VK	203	PEB	OD-C4D	2.71	1.28	1.23
29	AB	301	PEB	OD-C4D	2.70	1.28	1.23
29	LG	201	PEB	OD-C4D	2.70	1.28	1.23
29	MQ	402	PEB	OD-C4D	2.70	1.28	1.23
29	V2	202	PEB	C1A-NA	-2.70	1.34	1.37
29	VR	202	PEB	C1A-NA	-2.70	1.34	1.37
29	FA	201	PEB	OD-C4D	2.70	1.28	1.23
29	FN	201	PEB	OD-C4D	2.70	1.28	1.23
29	VF	202	PEB	C2C-C3C	2.70	1.45	1.37
29	VI	202	PEB	C2C-C3C	2.70	1.45	1.37
29	T7	203	PEB	OD-C4D	2.70	1.28	1.23
29	T9	203	PEB	OD-C4D	2.70	1.28	1.23
29	IC	201	PEB	OD-C4D	2.70	1.28	1.23
29	IE	201	PEB	OD-C4D	2.70	1.28	1.23
29	JA	202	PEB	CHA-C1B	2.70	1.46	1.40
29	JN	202	PEB	CHA-C1B	2.70	1.46	1.40
29	dJ	202	PEB	C2C-C3C	2.70	1.45	1.37
29	dL	202	PEB	C2C-C3C	2.70	1.45	1.37
29	jJ	202	PEB	C2C-C3C	2.70	1.45	1.37
29	jL	202	PEB	C2C-C3C	2.70	1.45	1.37
29	SR	201	PEB	OD-C4D	2.70	1.28	1.23
29	HA	202	PEB	CHA-C1B	2.70	1.46	1.40
29	HN	202	PEB	CHA-C1B	2.70	1.46	1.40
29	dF	201	PEB	C2C-C3C	2.70	1.45	1.37
29	dI	201	PEB	C2C-C3C	2.70	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZJ	202	PEB	C2C-C3C	2.70	1.45	1.37
29	ZL	202	PEB	C2C-C3C	2.70	1.45	1.37
29	sJ	203	PEB	C2C-C3C	2.70	1.45	1.37
29	sL	203	PEB	C2C-C3C	2.70	1.45	1.37
29	m7	202	PEB	C2A-C1A	-2.70	1.49	1.52
29	m9	202	PEB	C2A-C1A	-2.70	1.49	1.52
29	LA	202	PEB	CHA-C1B	2.70	1.46	1.40
29	LN	202	PEB	CHA-C1B	2.70	1.46	1.40
29	HJ	201	PEB	C2C-C3C	2.70	1.45	1.37
29	HL	201	PEB	C2C-C3C	2.70	1.45	1.37
29	KA	201	PEB	OD-C4D	2.70	1.28	1.23
29	KN	201	PEB	OD-C4D	2.70	1.28	1.23
30	MG	402	PUB	OD-C4D	2.70	1.28	1.23
29	i1	202	PEB	CHA-C1B	2.70	1.46	1.40
29	iK	202	PEB	CHA-C1B	2.70	1.46	1.40
29	bJ	202	PEB	C2C-C3C	2.70	1.45	1.37
29	bL	202	PEB	C2C-C3C	2.70	1.45	1.37
29	xL	302	PEB	OD-C4D	2.70	1.28	1.23
29	OF	203	PEB	C2A-C1A	-2.70	1.49	1.52
29	OI	203	PEB	C2A-C1A	-2.70	1.49	1.52
29	eF	202	PEB	C2C-C3C	2.70	1.45	1.37
29	eI	202	PEB	C2C-C3C	2.70	1.45	1.37
29	V1	202	PEB	CHA-C1B	2.70	1.46	1.40
29	VK	202	PEB	CHA-C1B	2.70	1.46	1.40
29	G5	203	PEB	OD-C4D	2.70	1.28	1.23
29	g1	202	PEB	CHA-C1B	2.70	1.46	1.40
29	gK	202	PEB	CHA-C1B	2.70	1.46	1.40
29	AA	201	PEB	OD-C4D	2.70	1.28	1.23
29	AN	201	PEB	OD-C4D	2.70	1.28	1.23
31	vP	1001	CYC	C1B-C2B	2.70	1.50	1.45
29	TJ	202	PEB	C2C-C3C	2.70	1.45	1.37
29	TL	202	PEB	C2C-C3C	2.70	1.45	1.37
29	m7	203	PEB	OD-C4D	2.70	1.28	1.23
29	m9	203	PEB	OD-C4D	2.70	1.28	1.23
29	JD	202	PEB	C4A-NA	-2.70	1.31	1.37
29	g1	203	PEB	OD-C4D	2.69	1.28	1.23
29	gB	203	PEB	OD-C4D	2.69	1.28	1.23
29	gK	203	PEB	OD-C4D	2.69	1.28	1.23
29	gM	203	PEB	OD-C4D	2.69	1.28	1.23
30	MQ	405	PUB	OA-C1A	2.69	1.28	1.23
29	F3	203	PEB	OD-C4D	2.69	1.28	1.23
29	FC	201	PEB	OD-C4D	2.69	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FE	201	PEB	OD-C4D	2.69	1.28	1.23
29	MG	404	PEB	OD-C4D	2.69	1.28	1.23
29	FO	203	PEB	OD-C4D	2.69	1.28	1.23
30	MG	403	PUB	OA-C1A	2.69	1.28	1.23
29	I5	203	PEB	OD-C4D	2.69	1.28	1.23
29	I8	203	PEB	OD-C4D	2.69	1.28	1.23
29	kF	202	PEB	C2A-C1A	-2.69	1.49	1.52
29	kI	202	PEB	C2A-C1A	-2.69	1.49	1.52
29	M3	201	PEB	OD-C4D	2.69	1.28	1.23
29	F5	202	PEB	OD-C4D	2.69	1.28	1.23
29	F8	202	PEB	OD-C4D	2.69	1.28	1.23
29	MO	201	PEB	OD-C4D	2.69	1.28	1.23
30	QB	201	PUB	OA-C1A	2.69	1.28	1.23
30	QM	201	PUB	OA-C1A	2.69	1.28	1.23
29	Y7	203	PEB	OD-C4D	2.69	1.28	1.23
29	Y9	203	PEB	OD-C4D	2.69	1.28	1.23
29	O7	202	PEB	OD-C4D	2.69	1.28	1.23
29	O9	202	PEB	OD-C4D	2.69	1.28	1.23
29	L1	1002	PEB	C2A-C1A	-2.69	1.49	1.52
29	YF	202	PEB	C2A-C1A	-2.69	1.49	1.52
29	YI	202	PEB	C2A-C1A	-2.69	1.49	1.52
29	LK	1002	PEB	C2A-C1A	-2.69	1.49	1.52
31	PP	1001	CYC	C1B-C2B	2.69	1.50	1.45
29	FA	203	PEB	OD-C4D	2.69	1.28	1.23
29	FN	203	PEB	OD-C4D	2.69	1.28	1.23
29	aF	203	PEB	OD-C4D	2.69	1.28	1.23
29	aI	203	PEB	OD-C4D	2.69	1.28	1.23
29	BA	202	PEB	CHA-C1B	2.69	1.46	1.40
29	BN	202	PEB	CHA-C1B	2.69	1.46	1.40
29	R2	202	PEB	C1A-NA	-2.69	1.34	1.37
29	f7	202	PEB	OD-C4D	2.69	1.28	1.23
29	f9	202	PEB	OD-C4D	2.69	1.28	1.23
29	J3	203	PEB	OD-C4D	2.69	1.28	1.23
29	l7	202	PEB	OD-C4D	2.69	1.28	1.23
29	l9	202	PEB	OD-C4D	2.69	1.28	1.23
29	JO	203	PEB	OD-C4D	2.69	1.28	1.23
29	L7	1002	PEB	C2A-C1A	-2.69	1.49	1.52
29	IA	201	PEB	OD-C4D	2.69	1.28	1.23
29	BC	201	PEB	OD-C4D	2.69	1.28	1.23
29	BE	201	PEB	OD-C4D	2.69	1.28	1.23
29	IN	201	PEB	OD-C4D	2.69	1.28	1.23
29	JC	201	PEB	OD-C4D	2.69	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JE	201	PEB	OD-C4D	2.69	1.28	1.23
29	PF	203	PEB	OD-C4D	2.69	1.28	1.23
29	PI	203	PEB	OD-C4D	2.69	1.28	1.23
31	J9	1001	CYC	C3D-C2D	2.69	1.45	1.37
29	m1	202	PEB	OD-C4D	2.69	1.28	1.23
29	E4	201	PEB	OD-C4D	2.69	1.28	1.23
29	mK	202	PEB	OD-C4D	2.69	1.28	1.23
29	C5	203	PEB	OD-C4D	2.69	1.28	1.23
29	C8	203	PEB	OD-C4D	2.69	1.28	1.23
31	EP	1001	CYC	C1B-C2B	2.69	1.49	1.45
30	A7	303	PUB	OA-C1A	2.69	1.28	1.23
30	A9	303	PUB	OA-C1A	2.69	1.28	1.23
31	I7	1001	CYC	OB-C4B	2.69	1.28	1.23
31	I9	1001	CYC	OB-C4B	2.69	1.28	1.23
29	A5	203	PEB	OD-C4D	2.69	1.28	1.23
29	A8	203	PEB	OD-C4D	2.69	1.28	1.23
29	JC	201	PEB	C4B-C3B	2.69	1.50	1.45
29	JE	201	PEB	C4B-C3B	2.69	1.50	1.45
29	M3	202	PEB	C2A-C1A	-2.69	1.49	1.52
29	MO	202	PEB	C2A-C1A	-2.69	1.49	1.52
29	e7	203	PEB	OD-C4D	2.69	1.28	1.23
29	e9	203	PEB	OD-C4D	2.69	1.28	1.23
29	B5	202	PEB	OD-C4D	2.68	1.28	1.23
29	kF	202	PEB	C2C-C3C	2.68	1.45	1.37
29	kI	202	PEB	C2C-C3C	2.68	1.45	1.37
29	j7	202	PEB	OD-C4D	2.68	1.28	1.23
29	j9	202	PEB	OD-C4D	2.68	1.28	1.23
29	HQ	203	PEB	OD-C4D	2.68	1.28	1.23
29	k7	203	PEB	OD-C4D	2.68	1.28	1.23
29	B8	201	PEB	OD-C4D	2.68	1.28	1.23
29	k9	203	PEB	OD-C4D	2.68	1.28	1.23
29	K5	203	PEB	OD-C4D	2.68	1.28	1.23
29	c7	203	PEB	OD-C4D	2.68	1.28	1.23
29	K8	203	PEB	OD-C4D	2.68	1.28	1.23
29	c9	203	PEB	OD-C4D	2.68	1.28	1.23
29	MQ	406	PEB	OD-C4D	2.68	1.28	1.23
29	H4	202	PEB	C4A-NA	-2.68	1.31	1.37
29	HD	202	PEB	C4A-NA	-2.68	1.31	1.37
31	M1	1001	CYC	C2C-C1C	-2.68	1.49	1.52
31	MK	1001	CYC	C2C-C1C	-2.68	1.49	1.52
29	UF	201	PEB	C2C-C3C	2.68	1.45	1.37
29	UI	201	PEB	C2C-C3C	2.68	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S7	202	PEB	OD-C4D	2.68	1.28	1.23
29	S9	202	PEB	OD-C4D	2.68	1.28	1.23
29	FD	201	PEB	C2C-C3C	2.68	1.45	1.37
31	yP	1001	CYC	C1D-CHD	2.68	1.51	1.41
29	F3	201	PEB	OD-C4D	2.68	1.28	1.23
29	FO	201	PEB	OD-C4D	2.68	1.28	1.23
29	C5	201	PEB	OD-C4D	2.68	1.28	1.23
29	Q7	202	PEB	OD-C4D	2.68	1.28	1.23
29	C8	201	PEB	OD-C4D	2.68	1.28	1.23
29	Q9	202	PEB	OD-C4D	2.68	1.28	1.23
29	cB	202	PEB	OD-C4D	2.68	1.28	1.23
29	cM	202	PEB	OD-C4D	2.68	1.28	1.23
29	eF	203	PEB	OD-C4D	2.68	1.28	1.23
29	eI	203	PEB	OD-C4D	2.68	1.28	1.23
29	JA	203	PEB	OD-C4D	2.68	1.28	1.23
29	JN	203	PEB	OD-C4D	2.68	1.28	1.23
29	DG	201	PEB	OD-C4D	2.68	1.28	1.23
29	DQ	201	PEB	OD-C4D	2.68	1.28	1.23
31	WP	1001	CYC	C1D-CHD	2.68	1.51	1.41
29	cF	202	PEB	OD-C4D	2.68	1.28	1.23
29	FG	201	PEB	OD-C4D	2.68	1.28	1.23
29	cI	202	PEB	OD-C4D	2.68	1.28	1.23
29	FQ	201	PEB	OD-C4D	2.68	1.28	1.23
29	HG	201	PEB	OD-C4D	2.68	1.28	1.23
29	HQ	201	PEB	OD-C4D	2.68	1.28	1.23
29	P1	203	PEB	OD-C4D	2.68	1.28	1.23
29	P7	203	PEB	OD-C4D	2.68	1.28	1.23
29	P9	203	PEB	OD-C4D	2.68	1.28	1.23
29	PK	203	PEB	OD-C4D	2.68	1.28	1.23
29	a7	203	PEB	OD-C4D	2.68	1.28	1.23
29	a9	203	PEB	OD-C4D	2.68	1.28	1.23
30	A7	302	PUB	OD-C4D	2.68	1.28	1.23
30	A9	302	PUB	OD-C4D	2.68	1.28	1.23
29	F4	201	PEB	C2C-C3C	2.67	1.45	1.37
31	J7	1001	CYC	C3D-C2D	2.67	1.45	1.37
31	KP	1001	CYC	C1B-C2B	2.67	1.49	1.45
29	LC	202	PEB	OD-C4D	2.67	1.28	1.23
29	LE	202	PEB	OD-C4D	2.67	1.28	1.23
29	GG	201	PEB	C2A-C1A	-2.67	1.49	1.52
29	GQ	201	PEB	C2A-C1A	-2.67	1.49	1.52
31	GK	1001	CYC	C2C-C1C	-2.67	1.49	1.52
31	H7	1001	CYC	C3D-C2D	2.67	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	H9	1001	CYC	C3D-C2D	2.67	1.45	1.37
29	J4	202	PEB	C4A-NA	-2.67	1.31	1.37
29	NO	201	PEB	OD-C4D	2.67	1.28	1.23
29	k7	202	PEB	C2A-C1A	-2.67	1.49	1.52
29	k9	202	PEB	C2A-C1A	-2.67	1.49	1.52
29	H5	202	PEB	OD-C4D	2.67	1.28	1.23
31	WP	1001	CYC	OB-C4B	2.67	1.28	1.23
31	cP	1001	CYC	C1B-C2B	2.67	1.49	1.45
29	D3	201	PEB	OD-C4D	2.67	1.28	1.23
29	DO	201	PEB	OD-C4D	2.67	1.28	1.23
31	IP	1001	CYC	C1B-C2B	2.67	1.49	1.45
29	TF	202	PEB	OD-C4D	2.67	1.28	1.23
29	TI	202	PEB	OD-C4D	2.67	1.28	1.23
29	Z7	202	PEB	OD-C4D	2.67	1.28	1.23
29	Z9	202	PEB	OD-C4D	2.67	1.28	1.23
29	LC	201	PEB	OD-C4D	2.67	1.28	1.23
29	LE	201	PEB	OD-C4D	2.67	1.28	1.23
29	MQ	403	PEB	CHA-C1B	2.67	1.46	1.40
29	L8	202	PEB	OD-C4D	2.67	1.28	1.23
29	DC	201	PEB	C4B-C3B	2.67	1.50	1.45
29	DE	201	PEB	C4B-C3B	2.67	1.50	1.45
29	VB	202	PEB	OD-C4D	2.67	1.28	1.23
29	VM	202	PEB	OD-C4D	2.67	1.28	1.23
29	F1	1002	PEB	C2A-C1A	-2.67	1.49	1.52
29	FK	1002	PEB	C2A-C1A	-2.67	1.49	1.52
29	V7	203	PEB	OD-C4D	2.67	1.28	1.23
29	V9	203	PEB	OD-C4D	2.67	1.28	1.23
29	J3	201	PEB	OD-C4D	2.67	1.28	1.23
29	GA	201	PEB	OD-C4D	2.67	1.28	1.23
29	GN	201	PEB	OD-C4D	2.67	1.28	1.23
29	JO	201	PEB	OD-C4D	2.67	1.28	1.23
29	H8	203	PEB	OD-C4D	2.67	1.28	1.23
29	AF	305	PEB	OD-C4D	2.67	1.28	1.23
29	kF	203	PEB	OD-C4D	2.67	1.28	1.23
29	AI	305	PEB	OD-C4D	2.67	1.28	1.23
29	kI	203	PEB	OD-C4D	2.67	1.28	1.23
29	LC	201	PEB	C4B-C3B	2.66	1.50	1.45
29	LE	201	PEB	C4B-C3B	2.66	1.50	1.45
29	C4	201	PEB	C4A-NA	-2.66	1.31	1.37
29	HC	202	PEB	OD-C4D	2.66	1.28	1.23
29	HE	202	PEB	OD-C4D	2.66	1.28	1.23
31	F7	1001	CYC	C3D-C2D	2.66	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	F9	1001	CYC	C3D-C2D	2.66	1.45	1.37
31	N7	1001	CYC	C3D-C2D	2.66	1.45	1.37
31	N9	1001	CYC	C3D-C2D	2.66	1.45	1.37
29	c7	201	PEB	OD-C4D	2.66	1.28	1.23
29	c9	201	PEB	OD-C4D	2.66	1.28	1.23
29	mF	203	PEB	OD-C4D	2.66	1.28	1.23
29	mI	203	PEB	OD-C4D	2.66	1.28	1.23
31	G7	1001	CYC	OB-C4B	2.66	1.28	1.23
31	AP	1001	CYC	C1B-C2B	2.66	1.49	1.45
29	g7	203	PEB	OD-C4D	2.66	1.28	1.23
29	g9	203	PEB	OD-C4D	2.66	1.28	1.23
29	H5	203	PEB	OD-C4D	2.66	1.28	1.23
29	L4	202	PEB	CHA-C1B	2.66	1.46	1.40
29	BD	202	PEB	C4A-NA	-2.66	1.31	1.37
29	U7	202	PEB	OD-C4D	2.66	1.28	1.23
29	U9	202	PEB	OD-C4D	2.66	1.28	1.23
29	CG	201	PEB	C2A-C1A	-2.66	1.49	1.52
29	CQ	201	PEB	C2A-C1A	-2.66	1.49	1.52
29	MR	201	PEB	C4A-NA	-2.66	1.31	1.37
29	N3	201	PEB	OD-C4D	2.66	1.28	1.23
29	F4	202	PEB	C4A-NA	-2.66	1.31	1.37
31	D7	1001	CYC	C3D-C2D	2.66	1.45	1.37
31	D9	1001	CYC	C3D-C2D	2.66	1.45	1.37
29	MA	404	PEB	C2A-C1A	-2.66	1.49	1.52
29	DK	1002	PEB	C2A-C1A	-2.66	1.49	1.52
31	D1	1003	CYC	C2C-C1C	-2.66	1.49	1.52
31	VP	1001	CYC	C1B-C2B	2.66	1.49	1.45
29	JB	202	PEB	OD-C4D	2.66	1.28	1.23
29	JM	202	PEB	OD-C4D	2.66	1.28	1.23
31	yP	1001	CYC	OB-C4B	2.66	1.28	1.23
31	xP	1001	CYC	C1B-C2B	2.66	1.49	1.45
29	W7	202	PEB	OD-C4D	2.66	1.28	1.23
29	h7	202	PEB	OD-C4D	2.66	1.28	1.23
29	W9	202	PEB	OD-C4D	2.66	1.28	1.23
29	h9	202	PEB	OD-C4D	2.66	1.28	1.23
29	DB	202	PEB	OD-C4D	2.66	1.28	1.23
29	DM	202	PEB	OD-C4D	2.66	1.28	1.23
29	xL	303	PEB	C2A-C1A	-2.66	1.49	1.52
29	ID	201	PEB	OD-C4D	2.66	1.28	1.23
31	JP	1001	CYC	C1B-C2B	2.66	1.49	1.45
29	d7	202	PEB	OD-C4D	2.66	1.28	1.23
29	H8	201	PEB	OD-C4D	2.66	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d9	202	PEB	OD-C4D	2.66	1.28	1.23
31	E7	1001	CYC	OB-C4B	2.66	1.28	1.23
31	E9	1001	CYC	OB-C4B	2.66	1.28	1.23
29	H3	201	PEB	OD-C4D	2.66	1.28	1.23
29	zL	501	PEB	OD-C4D	2.66	1.28	1.23
29	HO	201	PEB	OD-C4D	2.66	1.28	1.23
29	L8	201	PEB	OD-C4D	2.65	1.28	1.23
29	gB	202	PEB	OD-C4D	2.65	1.28	1.23
29	gM	202	PEB	OD-C4D	2.65	1.28	1.23
29	RB	202	PEB	OD-C4D	2.65	1.28	1.23
29	RM	202	PEB	OD-C4D	2.65	1.28	1.23
29	CA	201	PEB	C2A-C1A	-2.65	1.49	1.52
29	CN	201	PEB	C2A-C1A	-2.65	1.49	1.52
29	J4	201	PEB	C4A-NA	-2.65	1.31	1.37
29	B4	201	PEB	C2C-C3C	2.65	1.45	1.37
29	CA	201	PEB	OD-C4D	2.65	1.28	1.23
29	EA	201	PEB	OD-C4D	2.65	1.28	1.23
29	kB	202	PEB	OD-C4D	2.65	1.28	1.23
29	kM	202	PEB	OD-C4D	2.65	1.28	1.23
29	CN	201	PEB	OD-C4D	2.65	1.28	1.23
29	EN	201	PEB	OD-C4D	2.65	1.28	1.23
30	A1	304	PUB	OD-C4D	2.65	1.28	1.23
30	AK	304	PUB	OD-C4D	2.65	1.28	1.23
29	DD	202	PEB	CHA-C1B	2.65	1.46	1.40
31	pP	1001	CYC	C1B-C2B	2.65	1.49	1.45
29	M3	202	PEB	OD-C4D	2.65	1.28	1.23
29	MN	401	PEB	OD-C4D	2.65	1.28	1.23
29	MO	202	PEB	OD-C4D	2.65	1.28	1.23
29	F4	202	PEB	CHA-C1B	2.65	1.46	1.40
29	FB	202	PEB	OD-C4D	2.65	1.28	1.23
29	TF	201	PEB	OD-C4D	2.65	1.28	1.23
29	FM	202	PEB	OD-C4D	2.65	1.28	1.23
29	L5	202	PEB	OD-C4D	2.65	1.28	1.23
29	LB	202	PEB	OD-C4D	2.65	1.28	1.23
29	LM	202	PEB	OD-C4D	2.65	1.28	1.23
29	B3	202	PEB	C2A-C1A	-2.65	1.49	1.52
29	BO	202	PEB	C2A-C1A	-2.65	1.49	1.52
29	M4	202	PEB	CHA-C1B	2.65	1.46	1.40
29	b7	202	PEB	OD-C4D	2.65	1.28	1.23
29	b9	202	PEB	OD-C4D	2.65	1.28	1.23
29	QR	201	PEB	C4A-NA	-2.65	1.31	1.37
29	P2	201	PEB	OD-C4D	2.65	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	wL	303	PEB	C2A-C1A	-2.65	1.49	1.52
29	BD	201	PEB	CHA-C4A	-2.65	1.31	1.36
29	J4	202	PEB	CHA-C1B	2.65	1.46	1.40
29	HD	202	PEB	CHA-C1B	2.65	1.46	1.40
30	A7	303	PUB	OD-C4D	2.65	1.28	1.23
30	A9	303	PUB	OD-C4D	2.65	1.28	1.23
31	G9	1001	CYC	OB-C4B	2.65	1.28	1.23
29	B3	201	PEB	OD-C4D	2.65	1.28	1.23
29	YB	201	PEB	OD-C4D	2.65	1.28	1.23
29	YM	201	PEB	OD-C4D	2.65	1.28	1.23
29	BO	201	PEB	OD-C4D	2.65	1.28	1.23
29	BD	202	PEB	CHA-C1B	2.65	1.46	1.40
29	JD	202	PEB	CHA-C1B	2.64	1.46	1.40
29	P7	201	PEB	OD-C4D	2.64	1.28	1.23
29	P9	201	PEB	OD-C4D	2.64	1.28	1.23
29	VF	203	PEB	OD-C4D	2.64	1.28	1.23
29	VI	203	PEB	OD-C4D	2.64	1.28	1.23
29	D4	201	PEB	C4A-NA	-2.64	1.31	1.37
29	CD	201	PEB	C4A-NA	-2.64	1.31	1.37
29	FC	202	PEB	OD-C4D	2.64	1.28	1.23
29	FE	202	PEB	OD-C4D	2.64	1.28	1.23
29	K4	201	PEB	C4A-NA	-2.64	1.31	1.37
29	KD	201	PEB	C4A-NA	-2.64	1.31	1.37
29	LD	202	PEB	CHA-C1B	2.64	1.46	1.40
31	rP	1001	CYC	C1B-C2B	2.64	1.49	1.45
29	KG	201	PEB	C2A-C1A	-2.64	1.49	1.52
29	KQ	201	PEB	C2A-C1A	-2.64	1.49	1.52
29	LD	201	PEB	C4A-NA	-2.64	1.31	1.37
31	CP	1001	CYC	C1B-C2B	2.64	1.49	1.45
31	GP	1001	CYC	C1D-CHD	2.64	1.51	1.41
29	R1	202	PEB	C2A-C1A	-2.64	1.49	1.52
29	RK	202	PEB	C2A-C1A	-2.64	1.49	1.52
29	F5	201	PEB	OD-C4D	2.64	1.28	1.23
29	e7	201	PEB	OD-C4D	2.64	1.28	1.23
29	F8	201	PEB	OD-C4D	2.64	1.28	1.23
29	e9	201	PEB	OD-C4D	2.64	1.28	1.23
29	NO	202	PEB	OD-C4D	2.64	1.28	1.23
31	C7	1001	CYC	OB-C4B	2.64	1.28	1.23
31	C9	1001	CYC	OB-C4B	2.64	1.28	1.23
31	JP	1001	CYC	C1D-CHD	2.64	1.51	1.41
29	L4	202	PEB	C4A-NA	-2.64	1.31	1.37
29	LD	202	PEB	C4A-NA	-2.64	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gF	203	PEB	OD-C4D	2.64	1.28	1.23
29	gI	203	PEB	OD-C4D	2.64	1.28	1.23
29	UR	201	PEB	C4A-NA	-2.64	1.31	1.37
29	ID	201	PEB	C4A-NA	-2.64	1.31	1.37
29	CD	202	PEB	CHA-C1B	2.64	1.46	1.40
29	B5	201	PEB	OD-C4D	2.64	1.28	1.23
29	I5	202	PEB	OD-C4D	2.64	1.28	1.23
29	I8	202	PEB	OD-C4D	2.64	1.28	1.23
31	iP	1001	CYC	C1B-C2B	2.64	1.49	1.45
29	H4	202	PEB	CHA-C1B	2.64	1.46	1.40
29	FD	202	PEB	CHA-C1B	2.64	1.46	1.40
29	F3	202	PEB	C2A-C1A	-2.64	1.49	1.52
29	IA	201	PEB	C2A-C1A	-2.64	1.49	1.52
29	IG	201	PEB	C2A-C1A	-2.64	1.49	1.52
29	IN	201	PEB	C2A-C1A	-2.64	1.49	1.52
29	FO	202	PEB	C2A-C1A	-2.64	1.49	1.52
29	IQ	201	PEB	C2A-C1A	-2.64	1.49	1.52
29	RF	202	PEB	OD-C4D	2.64	1.28	1.23
29	RI	202	PEB	OD-C4D	2.64	1.28	1.23
29	D4	202	PEB	CHA-C1B	2.64	1.46	1.40
29	JG	201	PEB	OD-C4D	2.64	1.28	1.23
29	JQ	201	PEB	OD-C4D	2.64	1.28	1.23
29	MG	401	PEB	CHA-C1B	2.63	1.46	1.40
29	N3	202	PEB	OD-C4D	2.63	1.28	1.23
29	zJ	501	PEB	OD-C4D	2.63	1.28	1.23
29	L5	201	PEB	OD-C4D	2.63	1.28	1.23
29	BG	201	PEB	OD-C4D	2.63	1.28	1.23
29	BQ	201	PEB	OD-C4D	2.63	1.28	1.23
31	TP	1001	CYC	C1D-CHD	2.63	1.51	1.41
31	IF	1001	CYC	C4C-NC	-2.63	1.31	1.37
31	II	1001	CYC	C4C-NC	-2.63	1.31	1.37
31	cP	1001	CYC	C1D-CHD	2.63	1.51	1.41
31	lP	1001	CYC	C1D-CHD	2.63	1.51	1.41
29	B4	202	PEB	C4A-NA	-2.63	1.31	1.37
29	HC	201	PEB	C4B-C3B	2.63	1.49	1.45
29	HE	201	PEB	C4B-C3B	2.63	1.49	1.45
29	dD	401	PEB	OD-C4D	2.63	1.28	1.23
31	N1	1001	CYC	C1B-C2B	2.63	1.49	1.45
29	BC	202	PEB	OD-C4D	2.63	1.28	1.23
29	BE	202	PEB	OD-C4D	2.63	1.28	1.23
31	K7	1001	CYC	OB-C4B	2.63	1.28	1.23
31	mP	1001	CYC	C1D-CHD	2.63	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GA	201	PEB	C2A-C1A	-2.63	1.49	1.52
29	GN	201	PEB	C2A-C1A	-2.63	1.49	1.52
29	BD	201	PEB	C2C-C3C	2.63	1.45	1.37
31	M1	1001	CYC	OB-C4B	2.63	1.28	1.23
31	MK	1001	CYC	OB-C4B	2.63	1.28	1.23
29	V2	202	PEB	OD-C4D	2.63	1.28	1.23
29	A7	301	PEB	OD-C4D	2.63	1.28	1.23
29	A9	301	PEB	OD-C4D	2.63	1.28	1.23
29	VR	202	PEB	OD-C4D	2.63	1.28	1.23
31	M7	1001	CYC	OB-C4B	2.63	1.28	1.23
29	KD	202	PEB	CHA-C1B	2.63	1.46	1.40
29	M4	201	PEB	OD-C4D	2.63	1.28	1.23
31	M9	1001	CYC	OB-C4B	2.63	1.28	1.23
31	L9	1001	CYC	C3D-C2D	2.63	1.45	1.37
29	G5	201	PEB	OD-C4D	2.63	1.28	1.23
29	ZB	202	PEB	OD-C4D	2.63	1.28	1.23
29	ZM	202	PEB	OD-C4D	2.63	1.28	1.23
31	EP	1001	CYC	C1D-CHD	2.63	1.51	1.41
29	K5	202	PEB	OD-C4D	2.63	1.28	1.23
29	K8	202	PEB	OD-C4D	2.63	1.28	1.23
29	TB	202	PEB	OD-C4D	2.63	1.28	1.23
29	TM	202	PEB	OD-C4D	2.63	1.28	1.23
29	iF	203	PEB	OD-C4D	2.63	1.28	1.23
29	iI	203	PEB	OD-C4D	2.63	1.28	1.23
29	DD	201	PEB	C4A-NA	-2.63	1.31	1.37
31	KP	1001	CYC	C1D-CHD	2.63	1.51	1.41
31	L7	1001	CYC	C3D-C2D	2.63	1.45	1.37
29	ID	202	PEB	CHA-C1B	2.63	1.46	1.40
29	D4	202	PEB	C4A-NA	-2.63	1.31	1.37
29	DD	202	PEB	C4A-NA	-2.63	1.31	1.37
29	m7	201	PEB	OD-C4D	2.63	1.28	1.23
29	m9	201	PEB	OD-C4D	2.63	1.28	1.23
29	RR	201	PEB	OD-C4D	2.62	1.28	1.23
29	DD	201	PEB	CHA-C4A	-2.62	1.31	1.36
29	M2	201	PEB	C4A-NA	-2.62	1.31	1.37
29	mB	202	PEB	OD-C4D	2.62	1.28	1.23
29	mM	202	PEB	OD-C4D	2.62	1.28	1.23
31	K9	1001	CYC	OB-C4B	2.62	1.28	1.23
29	MD	201	PEB	OD-C4D	2.62	1.28	1.23
31	PP	1001	CYC	C1D-CHD	2.62	1.51	1.41
29	QB	202	PEB	OD-C4D	2.62	1.28	1.23
29	QM	202	PEB	OD-C4D	2.62	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	MQ	407	PEB	OD-C4D	2.62	1.28	1.23
29	dD	401	PEB	C4A-NA	-2.62	1.31	1.37
29	BA	202	PEB	OD-C4D	2.62	1.28	1.23
29	BN	202	PEB	OD-C4D	2.62	1.28	1.23
31	iP	1001	CYC	C1D-CHD	2.62	1.51	1.41
29	g7	201	PEB	OD-C4D	2.62	1.28	1.23
29	g9	201	PEB	OD-C4D	2.62	1.28	1.23
31	1P	1002	CYC	OB-C4B	2.62	1.28	1.23
29	wL	301	PEB	C2A-C1A	-2.62	1.49	1.52
31	C1	1001	CYC	C2C-C1C	-2.62	1.49	1.52
29	a7	201	PEB	OD-C4D	2.62	1.28	1.23
29	a9	201	PEB	OD-C4D	2.62	1.28	1.23
29	FD	202	PEB	C4A-NA	-2.62	1.31	1.37
31	C1	1001	CYC	OB-C4B	2.62	1.28	1.23
31	GK	1001	CYC	OB-C4B	2.62	1.28	1.23
29	M4	201	PEB	C4A-NA	-2.62	1.31	1.37
29	WR	201	PEB	C4A-NA	-2.62	1.31	1.37
29	J3	202	PEB	C2A-C1A	-2.62	1.49	1.52
29	JO	202	PEB	C2A-C1A	-2.62	1.49	1.52
29	N2	201	PEB	OD-C4D	2.62	1.28	1.23
29	L3	201	PEB	OD-C4D	2.62	1.28	1.23
29	I4	201	PEB	OD-C4D	2.62	1.28	1.23
29	LO	201	PEB	OD-C4D	2.62	1.28	1.23
31	J1	1001	CYC	C1B-C2B	2.62	1.49	1.45
31	JK	1001	CYC	C1B-C2B	2.62	1.49	1.45
29	B4	202	PEB	CHA-C1B	2.62	1.46	1.40
31	RP	1001	CYC	C1D-CHD	2.62	1.51	1.41
29	G8	201	PEB	OD-C4D	2.62	1.28	1.23
31	tP	1001	CYC	C1D-CHD	2.62	1.51	1.41
31	vP	1001	CYC	C1D-CHD	2.62	1.51	1.41
29	A5	202	PEB	OD-C4D	2.62	1.28	1.23
29	A8	202	PEB	OD-C4D	2.62	1.28	1.23
29	MG	405	PEB	OD-C4D	2.62	1.28	1.23
29	J4	201	PEB	C2C-C3C	2.61	1.45	1.37
29	JD	201	PEB	C2C-C3C	2.61	1.45	1.37
29	LD	201	PEB	C2C-C3C	2.61	1.45	1.37
31	CP	1001	CYC	C1D-CHD	2.61	1.51	1.41
29	AC	203	PEB	OD-C4D	2.61	1.28	1.23
29	AE	203	PEB	OD-C4D	2.61	1.28	1.23
31	pP	1001	CYC	C1D-CHD	2.61	1.51	1.41
29	A1	303	PEB	OD-C4D	2.61	1.28	1.23
29	AK	303	PEB	OD-C4D	2.61	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D4	201	PEB	CHA-C4A	-2.61	1.31	1.36
31	YP	1000	CYC	OB-C4B	2.61	1.28	1.23
29	L4	201	PEB	C4A-NA	-2.61	1.31	1.37
29	FD	201	PEB	C4A-NA	-2.61	1.31	1.37
29	I3	203	PEB	C2A-C1A	-2.61	1.49	1.52
29	IO	203	PEB	C2A-C1A	-2.61	1.49	1.52
31	NP	1001	CYC	C1D-CHD	2.61	1.51	1.41
31	rP	1001	CYC	C1D-CHD	2.61	1.51	1.41
29	L4	201	PEB	C2C-C3C	2.61	1.45	1.37
29	fF	202	PEB	C2A-C1A	-2.61	1.49	1.52
29	fI	202	PEB	C2A-C1A	-2.61	1.49	1.52
30	yJ	302	PUB	OA-C1A	2.61	1.28	1.23
30	yL	302	PUB	OA-C1A	2.61	1.28	1.23
29	B4	201	PEB	CHA-C4A	-2.61	1.31	1.36
31	AP	1001	CYC	C1D-CHD	2.61	1.51	1.41
29	X2	201	PEB	OD-C4D	2.61	1.28	1.23
29	k7	201	PEB	OD-C4D	2.61	1.28	1.23
29	k9	201	PEB	OD-C4D	2.61	1.28	1.23
29	i7	201	PEB	OD-C4D	2.60	1.28	1.23
29	i9	201	PEB	OD-C4D	2.60	1.28	1.23
29	MN	405	PEB	OD-C4D	2.60	1.28	1.23
30	wL	305	PUB	OA-C1A	2.60	1.28	1.23
29	OR	201	PEB	C4A-NA	-2.60	1.31	1.37
29	EG	201	PEB	C2A-C1A	-2.60	1.49	1.52
29	EQ	201	PEB	C2A-C1A	-2.60	1.49	1.52
29	HB	202	PEB	OD-C4D	2.60	1.28	1.23
29	HM	202	PEB	OD-C4D	2.60	1.28	1.23
31	gP	1001	CYC	C1D-CHD	2.60	1.51	1.41
29	B4	201	PEB	C4A-NA	-2.60	1.31	1.37
31	H1	1001	CYC	C1B-C2B	2.60	1.49	1.45
31	NF	1001	CYC	C4B-NB	-2.60	1.32	1.38
31	NI	1001	CYC	C4B-NB	-2.60	1.32	1.38
29	MA	401	PEB	OD-C4D	2.60	1.28	1.23
29	U2	201	PEB	C4A-NA	-2.60	1.31	1.37
29	E4	201	PEB	C4A-NA	-2.60	1.31	1.37
29	K4	201	PEB	OD-C4D	2.60	1.28	1.23
29	KD	201	PEB	OD-C4D	2.60	1.28	1.23
31	FF	1001	CYC	C4B-NB	-2.60	1.32	1.38
31	FI	1001	CYC	C4B-NB	-2.60	1.32	1.38
31	eP	1001	CYC	C1D-CHD	2.60	1.51	1.41
29	yJ	301	PEB	OD-C4D	2.60	1.28	1.23
29	yL	301	PEB	OD-C4D	2.60	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A1	302	PEB	OD-C4D	2.60	1.28	1.23
29	AK	302	PEB	OD-C4D	2.60	1.28	1.23
29	QF	202	PEB	C2A-C1A	-2.60	1.49	1.52
29	QI	202	PEB	C2A-C1A	-2.60	1.49	1.52
29	C4	202	PEB	C4A-NA	-2.60	1.31	1.37
29	R2	201	PEB	OD-C4D	2.60	1.28	1.23
31	KF	1001	CYC	C4C-NC	-2.60	1.31	1.37
29	C4	202	PEB	CHA-C1B	2.60	1.46	1.40
29	R2	203	PEB	OD-C4D	2.60	1.28	1.23
29	RR	203	PEB	OD-C4D	2.60	1.28	1.23
29	FD	201	PEB	CHA-C4A	-2.60	1.31	1.36
29	MD	202	PEB	CHA-C1B	2.60	1.46	1.40
29	I4	201	PEB	C4A-NA	-2.60	1.31	1.37
31	KI	1001	CYC	C4C-NC	-2.60	1.31	1.37
29	aB	203	PEB	OD-C4D	2.60	1.28	1.23
29	aM	203	PEB	OD-C4D	2.60	1.28	1.23
31	GF	1001	CYC	C1B-NB	-2.60	1.33	1.37
31	GI	1001	CYC	C1B-NB	-2.60	1.33	1.37
29	HD	201	PEB	C2C-C3C	2.60	1.45	1.37
29	ED	201	PEB	CHA-C1B	2.60	1.46	1.40
29	BD	201	PEB	C4A-NA	-2.60	1.31	1.37
31	JF	1001	CYC	C4C-NC	-2.60	1.31	1.37
31	JI	1001	CYC	C4C-NC	-2.60	1.31	1.37
31	K1	1001	CYC	OB-C4B	2.60	1.28	1.23
31	KK	1001	CYC	OB-C4B	2.60	1.28	1.23
29	H4	201	PEB	C2C-C3C	2.60	1.45	1.37
31	L9	1001	CYC	C4C-NC	-2.60	1.31	1.37
29	VR	201	PEB	OD-C4D	2.60	1.28	1.23
29	KA	201	PEB	C2A-C1A	-2.60	1.49	1.52
29	KN	201	PEB	C2A-C1A	-2.60	1.49	1.52
29	W2	201	PEB	C4A-NA	-2.60	1.31	1.37
29	C4	201	PEB	OD-C4D	2.60	1.28	1.23
29	CD	201	PEB	OD-C4D	2.60	1.28	1.23
29	FC	201	PEB	C4B-C3B	2.60	1.49	1.45
29	FE	201	PEB	C4B-C3B	2.60	1.49	1.45
29	T7	201	PEB	OD-C4D	2.60	1.28	1.23
29	T9	201	PEB	OD-C4D	2.60	1.28	1.23
29	DA	202	PEB	OD-C4D	2.60	1.28	1.23
29	DN	202	PEB	OD-C4D	2.60	1.28	1.23
29	TR	203	PEB	OD-C4D	2.60	1.28	1.23
31	JF	1001	CYC	C4B-NB	-2.59	1.32	1.38
31	JI	1001	CYC	C4B-NB	-2.59	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V2	203	PEB	OD-C4D	2.59	1.28	1.23
29	KB	203	PEB	OD-C4D	2.59	1.28	1.23
29	KM	203	PEB	OD-C4D	2.59	1.28	1.23
29	VR	203	PEB	OD-C4D	2.59	1.28	1.23
31	D1	1003	CYC	OB-C4B	2.59	1.28	1.23
29	I4	202	PEB	CHA-C1B	2.59	1.46	1.40
30	A1	304	PUB	OA-C1A	2.59	1.28	1.23
30	AK	304	PUB	OA-C1A	2.59	1.28	1.23
29	E4	202	PEB	CHA-C1B	2.59	1.46	1.40
29	F4	201	PEB	C4A-NA	-2.59	1.31	1.37
29	N2	202	PEB	OD-C4D	2.59	1.28	1.23
29	C5	202	PEB	OD-C4D	2.59	1.28	1.23
29	C8	202	PEB	OD-C4D	2.59	1.28	1.23
29	NR	202	PEB	OD-C4D	2.59	1.28	1.23
31	LF	1001	CYC	C4B-NB	-2.59	1.32	1.38
31	LI	1001	CYC	C4B-NB	-2.59	1.32	1.38
31	EF	1001	CYC	C4C-NC	-2.59	1.31	1.37
31	EI	1001	CYC	C4C-NC	-2.59	1.31	1.37
31	D1	1001	CYC	C1B-C2B	2.59	1.49	1.45
31	GF	1001	CYC	C4C-NC	-2.59	1.31	1.37
31	GI	1001	CYC	C4C-NC	-2.59	1.31	1.37
29	BC	201	PEB	C4B-C3B	2.59	1.49	1.45
29	BE	201	PEB	C4B-C3B	2.59	1.49	1.45
29	X2	202	PEB	OD-C4D	2.59	1.28	1.23
29	G4	201	PEB	OD-C4D	2.59	1.28	1.23
29	e2	402	PEB	OD-C4D	2.59	1.28	1.23
29	AG	201	PEB	C2A-C1A	-2.59	1.49	1.52
29	AQ	201	PEB	C2A-C1A	-2.59	1.49	1.52
29	K4	202	PEB	CHA-C1B	2.59	1.46	1.40
29	P2	202	PEB	OD-C4D	2.59	1.28	1.23
29	R7	201	PEB	OD-C4D	2.59	1.28	1.23
29	R9	201	PEB	OD-C4D	2.59	1.28	1.23
29	PR	202	PEB	OD-C4D	2.59	1.28	1.23
29	G4	201	PEB	C4A-NA	-2.59	1.31	1.37
29	GD	201	PEB	C4A-NA	-2.59	1.31	1.37
29	MD	201	PEB	C4A-NA	-2.59	1.31	1.37
29	D4	201	PEB	C2C-C3C	2.59	1.45	1.37
29	DD	201	PEB	C2C-C3C	2.59	1.45	1.37
29	iB	202	PEB	OD-C4D	2.59	1.28	1.23
29	iM	202	PEB	OD-C4D	2.59	1.28	1.23
31	IK	1001	CYC	OB-C4B	2.59	1.28	1.23
29	G4	202	PEB	CHA-C1B	2.59	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GD	202	PEB	CHA-C1B	2.59	1.46	1.40
29	V7	201	PEB	OD-C4D	2.59	1.28	1.23
29	V9	201	PEB	OD-C4D	2.59	1.28	1.23
31	NK	1001	CYC	C1B-C2B	2.59	1.49	1.45
29	KC	201	PEB	OD-C4D	2.59	1.28	1.23
29	KE	201	PEB	OD-C4D	2.59	1.28	1.23
29	O2	201	PEB	C4A-NA	-2.59	1.31	1.37
29	Y7	201	PEB	OD-C4D	2.59	1.28	1.23
29	Y9	201	PEB	OD-C4D	2.59	1.28	1.23
29	JD	201	PEB	CHA-C4A	-2.59	1.31	1.36
29	U1	201	PEB	C2A-C1A	-2.59	1.49	1.52
29	UK	201	PEB	C2A-C1A	-2.59	1.49	1.52
29	XR	203	PEB	OD-C4D	2.59	1.28	1.23
31	HF	1001	CYC	C4B-NB	-2.59	1.32	1.38
31	HI	1001	CYC	C4B-NB	-2.59	1.32	1.38
29	HD	201	PEB	C4A-NA	-2.59	1.31	1.37
29	H4	201	PEB	CHA-C4A	-2.59	1.31	1.36
29	ED	201	PEB	C4A-NA	-2.58	1.31	1.37
29	NR	203	PEB	OD-C4D	2.58	1.28	1.23
29	JD	201	PEB	C4A-NA	-2.58	1.31	1.37
30	wJ	305	PUB	OA-C1A	2.58	1.28	1.23
31	EK	1001	CYC	OB-C4B	2.58	1.28	1.23
29	H3	202	PEB	C2A-C1A	-2.58	1.49	1.52
29	HO	202	PEB	C2A-C1A	-2.58	1.49	1.52
29	K4	202	PEB	C4A-NA	-2.58	1.31	1.37
29	PR	201	PEB	OD-C4D	2.58	1.28	1.23
31	F9	1001	CYC	C4C-NC	-2.58	1.31	1.37
29	T2	203	PEB	OD-C4D	2.58	1.28	1.23
31	LF	1001	CYC	C4C-NC	-2.58	1.31	1.37
31	LI	1001	CYC	C4C-NC	-2.58	1.31	1.37
31	F7	1001	CYC	OB-C4B	2.58	1.28	1.23
29	F4	201	PEB	CHA-C4A	-2.58	1.31	1.36
29	FA	202	PEB	OD-C4D	2.58	1.28	1.23
29	FN	202	PEB	OD-C4D	2.58	1.28	1.23
31	DK	1001	CYC	C1B-C2B	2.58	1.49	1.45
29	P1	202	PEB	C2A-C1A	-2.58	1.49	1.52
29	PK	202	PEB	C2A-C1A	-2.58	1.49	1.52
31	HF	1001	CYC	C4C-NC	-2.58	1.31	1.37
31	HI	1001	CYC	C4C-NC	-2.58	1.31	1.37
31	HK	1001	CYC	C1B-C2B	2.58	1.49	1.45
31	L1	1001	CYC	C1B-C2B	2.58	1.49	1.45
31	LK	1001	CYC	C1B-C2B	2.58	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	xJ	304	PUB	OD-C4D	2.58	1.28	1.23
31	DF	1001	CYC	C4B-NB	-2.58	1.32	1.38
31	DI	1001	CYC	C4B-NB	-2.58	1.32	1.38
31	yP	1001	CYC	C1B-C2B	2.58	1.49	1.45
29	MA	405	PEB	OD-C4D	2.58	1.28	1.23
29	J5	202	PEB	OD-C4D	2.57	1.28	1.23
29	J8	202	PEB	OD-C4D	2.57	1.28	1.23
31	CK	1001	CYC	OB-C4B	2.57	1.28	1.23
31	J9	1001	CYC	OB-C4B	2.57	1.28	1.23
31	F9	1001	CYC	OB-C4B	2.57	1.28	1.23
31	L7	1001	CYC	C4C-NC	-2.57	1.31	1.37
29	EA	201	PEB	C2A-C1A	-2.57	1.49	1.52
29	EN	201	PEB	C2A-C1A	-2.57	1.49	1.52
31	yP	1001	CYC	C4B-NB	-2.57	1.32	1.38
29	wJ	301	PEB	C2A-C1A	-2.57	1.49	1.52
31	F7	1001	CYC	C4C-NC	-2.57	1.31	1.37
31	NF	1001	CYC	C4C-NC	-2.57	1.31	1.37
31	NI	1001	CYC	C4C-NC	-2.57	1.31	1.37
31	E1	1001	CYC	OB-C4B	2.57	1.28	1.23
31	FF	1001	CYC	C4C-NC	-2.57	1.31	1.37
31	FI	1001	CYC	C4C-NC	-2.57	1.31	1.37
30	xL	305	PUB	OA-C1A	2.57	1.28	1.23
31	D7	1001	CYC	OB-C4B	2.57	1.28	1.23
31	D9	1001	CYC	OB-C4B	2.57	1.28	1.23
29	A1	301	PEB	OD-C4D	2.57	1.28	1.23
29	AK	301	PEB	OD-C4D	2.57	1.28	1.23
30	A7	302	PUB	OA-C1A	2.57	1.28	1.23
30	A9	302	PUB	OA-C1A	2.57	1.28	1.23
31	MF	1001	CYC	C4C-NC	-2.57	1.31	1.37
31	MI	1001	CYC	C4C-NC	-2.57	1.31	1.37
29	V2	201	PEB	OD-C4D	2.57	1.28	1.23
31	WP	1001	CYC	C1B-C2B	2.57	1.49	1.45
29	V7	203	PEB	C4B-C3B	2.57	1.49	1.45
29	V9	203	PEB	C4B-C3B	2.57	1.49	1.45
31	J7	1001	CYC	C4C-NC	-2.57	1.32	1.37
29	CJ	201	PEB	OD-C4D	2.57	1.28	1.23
29	CL	201	PEB	OD-C4D	2.57	1.28	1.23
31	M9	1001	CYC	C1B-NB	-2.57	1.33	1.37
29	jF	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	jI	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	T2	202	PEB	OD-C4D	2.56	1.28	1.23
31	CF	1001	CYC	C4C-NC	-2.56	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CI	1001	CYC	C4C-NC	-2.56	1.32	1.37
29	O2	202	PEB	C4B-C3B	2.56	1.49	1.45
31	I7	1001	CYC	C1B-NB	-2.56	1.33	1.37
31	I9	1001	CYC	C1B-NB	-2.56	1.33	1.37
29	G4	202	PEB	C4A-NA	-2.56	1.32	1.37
29	i1	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	WF	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	WI	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	iK	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	KD	203	PEB	OD-C4D	2.56	1.28	1.23
30	wL	304	PUB	OD-C4D	2.56	1.28	1.23
29	H4	201	PEB	C4A-NA	-2.56	1.32	1.37
29	G4	203	PEB	OD-C4D	2.56	1.28	1.23
31	G9	1001	CYC	C1B-NB	-2.56	1.33	1.37
29	gB	201	PEB	OD-C4D	2.56	1.28	1.23
29	gM	201	PEB	OD-C4D	2.56	1.28	1.23
29	TR	202	PEB	OD-C4D	2.56	1.28	1.23
30	xL	304	PUB	OD-C4D	2.56	1.28	1.23
31	MF	1001	CYC	C1B-NB	-2.56	1.33	1.37
31	MI	1001	CYC	C1B-NB	-2.56	1.33	1.37
29	GD	201	PEB	OD-C4D	2.56	1.28	1.23
31	C7	1001	CYC	C1B-NB	-2.56	1.33	1.37
31	C9	1001	CYC	C1B-NB	-2.56	1.33	1.37
29	LA	202	PEB	OD-C4D	2.56	1.28	1.23
29	LN	202	PEB	OD-C4D	2.56	1.28	1.23
29	XR	202	PEB	OD-C4D	2.56	1.28	1.23
29	cB	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	cM	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	JA	202	PEB	OD-C4D	2.56	1.28	1.23
29	JN	202	PEB	OD-C4D	2.56	1.28	1.23
29	XR	201	PEB	OD-C4D	2.56	1.28	1.23
30	wJ	304	PUB	OD-C4D	2.56	1.28	1.23
31	CF	1001	CYC	C1B-NB	-2.56	1.33	1.37
31	CI	1001	CYC	C1B-NB	-2.56	1.33	1.37
31	WP	1001	CYC	C4B-NB	-2.56	1.32	1.38
31	I1	1001	CYC	OB-C4B	2.56	1.28	1.23
29	kJ	201	PEB	OD-C4D	2.56	1.28	1.23
29	kL	201	PEB	OD-C4D	2.56	1.28	1.23
31	H7	1001	CYC	C4C-NC	-2.56	1.32	1.37
31	H9	1001	CYC	C4C-NC	-2.56	1.32	1.37
31	IF	1001	CYC	C1B-NB	-2.55	1.33	1.37
31	II	1001	CYC	C1B-NB	-2.55	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TR	201	PEB	OD-C4D	2.55	1.28	1.23
31	J9	1001	CYC	C4C-NC	-2.55	1.32	1.37
29	I5	201	PEB	C2A-C1A	-2.55	1.49	1.52
29	I8	201	PEB	C2A-C1A	-2.55	1.49	1.52
29	IF	202	PEB	C2A-C1A	-2.55	1.49	1.52
29	II	202	PEB	C2A-C1A	-2.55	1.49	1.52
31	DF	1001	CYC	C4C-NC	-2.55	1.32	1.37
31	DI	1001	CYC	C4C-NC	-2.55	1.32	1.37
29	NR	201	PEB	OD-C4D	2.55	1.28	1.23
29	GD	202	PEB	C4A-NA	-2.55	1.32	1.37
29	HA	202	PEB	OD-C4D	2.55	1.28	1.23
29	qJ	201	PEB	OD-C4D	2.55	1.28	1.23
29	qL	201	PEB	OD-C4D	2.55	1.28	1.23
29	HN	202	PEB	OD-C4D	2.55	1.28	1.23
29	FJ	201	PEB	OD-C4D	2.55	1.28	1.23
29	FL	201	PEB	OD-C4D	2.55	1.28	1.23
29	VB	202	PEB	C2A-C1A	-2.55	1.49	1.52
29	VM	202	PEB	C2A-C1A	-2.55	1.49	1.52
29	K4	203	PEB	OD-C4D	2.55	1.28	1.23
31	G7	1001	CYC	C1B-NB	-2.55	1.33	1.37
31	M7	1001	CYC	C1B-NB	-2.55	1.33	1.37
31	J7	1001	CYC	OB-C4B	2.55	1.28	1.23
31	EF	1001	CYC	OB-C4B	2.55	1.28	1.23
31	EI	1001	CYC	OB-C4B	2.55	1.28	1.23
29	OJ	201	PEB	OD-C4D	2.55	1.28	1.23
29	OL	201	PEB	OD-C4D	2.55	1.28	1.23
31	D7	1001	CYC	C4C-NC	-2.55	1.32	1.37
31	D9	1001	CYC	C4C-NC	-2.55	1.32	1.37
29	CD	202	PEB	C4A-NA	-2.55	1.32	1.37
29	A8	202	PEB	C2A-C1A	-2.55	1.49	1.52
29	bF	202	PEB	C2A-C1A	-2.55	1.49	1.52
29	bI	202	PEB	C2A-C1A	-2.55	1.49	1.52
31	F1	1001	CYC	C1B-C2B	2.55	1.49	1.45
31	FK	1001	CYC	C1B-C2B	2.55	1.49	1.45
31	GF	1001	CYC	OB-C4B	2.54	1.28	1.23
31	GI	1001	CYC	OB-C4B	2.54	1.28	1.23
29	jJ	201	PEB	OD-C4D	2.54	1.28	1.23
29	jL	201	PEB	OD-C4D	2.54	1.28	1.23
31	N7	1001	CYC	OB-C4B	2.54	1.28	1.23
31	N9	1001	CYC	OB-C4B	2.54	1.28	1.23
29	E4	202	PEB	C4A-NA	-2.54	1.32	1.37
29	tJ	201	PEB	OD-C4D	2.54	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	tL	201	PEB	OD-C4D	2.54	1.28	1.23
29	sJ	201	PEB	OD-C4D	2.54	1.28	1.23
29	sL	201	PEB	OD-C4D	2.54	1.28	1.23
29	DJ	201	PEB	OD-C4D	2.54	1.28	1.23
29	DL	201	PEB	OD-C4D	2.54	1.28	1.23
29	V1	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	VK	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	AA	202	PEB	C4B-C3B	2.54	1.49	1.45
29	AN	202	PEB	C4B-C3B	2.54	1.49	1.45
29	K8	201	PEB	C2A-C1A	-2.54	1.49	1.52
29	OF	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	OI	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	RR	202	PEB	OD-C4D	2.54	1.28	1.23
31	CF	1001	CYC	OB-C4B	2.54	1.28	1.23
31	CI	1001	CYC	OB-C4B	2.54	1.28	1.23
31	KI	1001	CYC	C1B-NB	-2.54	1.33	1.37
29	WJ	202	PEB	OD-C4D	2.54	1.28	1.23
29	vJ	201	PEB	OD-C4D	2.54	1.28	1.23
29	WL	202	PEB	OD-C4D	2.54	1.28	1.23
29	vL	201	PEB	OD-C4D	2.54	1.28	1.23
29	M2	202	PEB	C4B-C3B	2.54	1.49	1.45
29	T2	201	PEB	OD-C4D	2.54	1.28	1.23
29	ZJ	201	PEB	OD-C4D	2.54	1.28	1.23
29	ZL	201	PEB	OD-C4D	2.54	1.28	1.23
29	k1	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	kK	202	PEB	C2A-C1A	-2.54	1.49	1.52
31	H7	1001	CYC	OB-C4B	2.54	1.28	1.23
31	H9	1001	CYC	OB-C4B	2.54	1.28	1.23
29	J4	201	PEB	CHA-C4A	-2.54	1.31	1.36
29	HD	201	PEB	CHA-C4A	-2.54	1.31	1.36
29	R2	202	PEB	OD-C4D	2.53	1.28	1.23
29	MD	203	PEB	OD-C4D	2.53	1.28	1.23
29	SJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	SL	201	PEB	OD-C4D	2.53	1.28	1.23
29	c1	202	PEB	C2A-C1A	-2.53	1.49	1.52
29	cK	202	PEB	C2A-C1A	-2.53	1.49	1.52
29	KJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	KL	201	PEB	OD-C4D	2.53	1.28	1.23
29	KD	202	PEB	C4A-NA	-2.53	1.32	1.37
29	E4	203	PEB	OD-C4D	2.53	1.28	1.23
29	MJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	ML	201	PEB	OD-C4D	2.53	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	xJ	302	PEB	C2A-C1A	-2.53	1.49	1.52
29	L4	201	PEB	CHA-C4A	-2.53	1.31	1.36
29	LD	201	PEB	CHA-C4A	-2.53	1.31	1.36
29	C4	203	PEB	OD-C4D	2.53	1.28	1.23
29	J5	201	PEB	OD-C4D	2.53	1.28	1.23
29	J8	201	PEB	OD-C4D	2.53	1.28	1.23
29	ED	202	PEB	OD-C4D	2.53	1.28	1.23
29	LJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	TJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	LL	201	PEB	OD-C4D	2.53	1.28	1.23
29	TL	201	PEB	OD-C4D	2.53	1.28	1.23
29	N2	203	PEB	OD-C4D	2.53	1.28	1.23
31	KF	1001	CYC	OB-C4B	2.53	1.28	1.23
29	GJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	GL	201	PEB	OD-C4D	2.53	1.28	1.23
30	xJ	305	PUB	OA-C1A	2.53	1.28	1.23
29	BJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	hJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	BL	201	PEB	OD-C4D	2.53	1.28	1.23
29	hL	201	PEB	OD-C4D	2.53	1.28	1.23
29	UJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	UL	201	PEB	OD-C4D	2.53	1.28	1.23
29	IJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	IL	201	PEB	OD-C4D	2.53	1.28	1.23
29	aJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	aL	201	PEB	OD-C4D	2.53	1.28	1.23
29	AJ	201	PEB	OD-C4D	2.53	1.28	1.23
29	AL	201	PEB	OD-C4D	2.53	1.28	1.23
29	AF	304	PEB	C4A-NA	-2.53	1.32	1.37
29	AI	304	PEB	C4A-NA	-2.53	1.32	1.37
31	N7	1001	CYC	C4C-NC	-2.52	1.32	1.37
31	N9	1001	CYC	C4C-NC	-2.52	1.32	1.37
29	GD	203	PEB	OD-C4D	2.52	1.28	1.23
30	AF	302	PUB	OA-C1A	2.52	1.28	1.23
30	AI	302	PUB	OA-C1A	2.52	1.28	1.23
29	TB	201	PEB	OD-C4D	2.52	1.28	1.23
29	TM	201	PEB	OD-C4D	2.52	1.28	1.23
29	M4	202	PEB	C4A-NA	-2.52	1.32	1.37
29	iJ	201	PEB	OD-C4D	2.52	1.28	1.23
29	iL	201	PEB	OD-C4D	2.52	1.28	1.23
29	HB	201	PEB	OD-C4D	2.52	1.28	1.23
29	mB	201	PEB	OD-C4D	2.52	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	HM	201	PEB	OD-C4D	2.52	1.28	1.23
29	mM	201	PEB	OD-C4D	2.52	1.28	1.23
29	ZB	201	PEB	OD-C4D	2.52	1.28	1.23
29	ZM	201	PEB	OD-C4D	2.52	1.28	1.23
29	eB	201	PEB	OD-C4D	2.52	1.28	1.23
29	eM	201	PEB	OD-C4D	2.52	1.28	1.23
29	IA	202	PEB	C4B-C3B	2.52	1.49	1.45
29	IN	202	PEB	C4B-C3B	2.52	1.49	1.45
31	K9	1001	CYC	C1B-NB	-2.52	1.33	1.37
29	XB	201	PEB	OD-C4D	2.52	1.28	1.23
29	XM	201	PEB	OD-C4D	2.52	1.28	1.23
29	I4	202	PEB	C4A-NA	-2.52	1.32	1.37
29	ZF	202	PEB	C2A-C1A	-2.52	1.49	1.52
29	ZI	202	PEB	C2A-C1A	-2.52	1.49	1.52
29	WR	202	PEB	C4B-C3B	2.52	1.49	1.45
29	RJ	201	PEB	OD-C4D	2.52	1.28	1.23
29	RL	201	PEB	OD-C4D	2.52	1.28	1.23
29	ID	202	PEB	C4A-NA	-2.52	1.32	1.37
29	QJ	201	PEB	OD-C4D	2.52	1.28	1.23
29	QL	201	PEB	OD-C4D	2.52	1.28	1.23
29	MA	405	PEB	C2A-C1A	-2.52	1.49	1.52
31	L9	1001	CYC	OB-C4B	2.52	1.28	1.23
29	mJ	201	PEB	OD-C4D	2.52	1.28	1.23
29	mL	201	PEB	OD-C4D	2.52	1.28	1.23
31	L7	1001	CYC	OB-C4B	2.52	1.28	1.23
29	EB	202	PEB	C4B-C3B	2.51	1.49	1.45
29	EM	202	PEB	C4B-C3B	2.51	1.49	1.45
29	NJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	NL	201	PEB	OD-C4D	2.51	1.28	1.23
29	iB	201	PEB	OD-C4D	2.51	1.28	1.23
29	iM	201	PEB	OD-C4D	2.51	1.28	1.23
31	KF	1001	CYC	C1B-NB	-2.51	1.33	1.37
29	Y7	203	PEB	C4B-C3B	2.51	1.49	1.45
29	Y9	203	PEB	C4B-C3B	2.51	1.49	1.45
29	UF	203	PEB	C2A-C1A	-2.51	1.49	1.52
29	UI	203	PEB	C2A-C1A	-2.51	1.49	1.52
29	VB	201	PEB	OD-C4D	2.51	1.28	1.23
29	VM	201	PEB	OD-C4D	2.51	1.28	1.23
29	VJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	IJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	nJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	VL	201	PEB	OD-C4D	2.51	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	lL	201	PEB	OD-C4D	2.51	1.28	1.23
29	nL	201	PEB	OD-C4D	2.51	1.28	1.23
29	a7	203	PEB	C4B-C3B	2.51	1.49	1.45
29	a9	203	PEB	C4B-C3B	2.51	1.49	1.45
29	PJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	oJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	PL	201	PEB	OD-C4D	2.51	1.28	1.23
29	oL	201	PEB	OD-C4D	2.51	1.28	1.23
29	ID	203	PEB	OD-C4D	2.51	1.28	1.23
29	FB	201	PEB	OD-C4D	2.51	1.28	1.23
29	FM	201	PEB	OD-C4D	2.51	1.28	1.23
31	MF	1001	CYC	OB-C4B	2.51	1.28	1.23
31	MI	1001	CYC	OB-C4B	2.51	1.28	1.23
29	MD	202	PEB	C4A-NA	-2.51	1.32	1.37
31	E7	1001	CYC	C1B-NB	-2.51	1.33	1.37
31	E9	1001	CYC	C1B-NB	-2.51	1.33	1.37
29	gJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	gL	201	PEB	OD-C4D	2.51	1.28	1.23
29	bJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	bL	201	PEB	OD-C4D	2.51	1.28	1.23
29	C5	202	PEB	C2A-C1A	-2.51	1.49	1.52
29	C8	202	PEB	C2A-C1A	-2.51	1.49	1.52
29	eJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	eL	201	PEB	OD-C4D	2.51	1.28	1.23
29	QR	202	PEB	C4B-C3B	2.51	1.49	1.45
29	JB	201	PEB	OD-C4D	2.51	1.28	1.23
29	cJ	201	PEB	OD-C4D	2.51	1.28	1.23
29	cL	201	PEB	OD-C4D	2.51	1.28	1.23
29	JM	201	PEB	OD-C4D	2.51	1.28	1.23
29	e1	202	PEB	C2A-C1A	-2.51	1.49	1.52
29	g1	202	PEB	C2A-C1A	-2.51	1.49	1.52
29	eK	202	PEB	C2A-C1A	-2.51	1.49	1.52
29	gK	202	PEB	C2A-C1A	-2.51	1.49	1.52
29	R7	203	PEB	C4B-C3B	2.51	1.49	1.45
29	R9	203	PEB	C4B-C3B	2.51	1.49	1.45
29	T7	203	PEB	C4B-C3B	2.50	1.49	1.45
29	T9	203	PEB	C4B-C3B	2.50	1.49	1.45
29	kB	201	PEB	OD-C4D	2.50	1.28	1.23
29	kM	201	PEB	OD-C4D	2.50	1.28	1.23
29	dF	203	PEB	C2A-C1A	-2.50	1.49	1.52
29	dI	203	PEB	C2A-C1A	-2.50	1.49	1.52
29	DB	202	PEB	C2A-C1A	-2.50	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DM	202	PEB	C2A-C1A	-2.50	1.49	1.52
31	KI	1001	CYC	OB-C4B	2.50	1.28	1.23
29	hF	202	PEB	C2A-C1A	-2.50	1.49	1.52
29	hI	202	PEB	C2A-C1A	-2.50	1.49	1.52
29	XJ	201	PEB	OD-C4D	2.50	1.28	1.23
29	dJ	201	PEB	OD-C4D	2.50	1.28	1.23
29	XL	201	PEB	OD-C4D	2.50	1.28	1.23
29	dL	201	PEB	OD-C4D	2.50	1.28	1.23
29	GA	202	PEB	C4B-C3B	2.50	1.49	1.45
29	GN	202	PEB	C4B-C3B	2.50	1.49	1.45
29	JJ	201	PEB	OD-C4D	2.50	1.28	1.23
29	JL	201	PEB	OD-C4D	2.50	1.28	1.23
29	KB	202	PEB	C4B-C3B	2.50	1.49	1.45
29	KM	202	PEB	C4B-C3B	2.50	1.49	1.45
29	AA	201	PEB	C2A-C1A	-2.50	1.49	1.52
29	SF	202	PEB	C2A-C1A	-2.50	1.49	1.52
29	SI	202	PEB	C2A-C1A	-2.50	1.49	1.52
29	AN	201	PEB	C2A-C1A	-2.50	1.49	1.52
31	EF	1001	CYC	C1B-NB	-2.50	1.33	1.37
31	EI	1001	CYC	C1B-NB	-2.50	1.33	1.37
29	RB	201	PEB	OD-C4D	2.50	1.28	1.23
29	iF	201	PEB	OD-C4D	2.50	1.28	1.23
29	iI	201	PEB	OD-C4D	2.50	1.28	1.23
29	RM	201	PEB	OD-C4D	2.50	1.28	1.23
29	DB	201	PEB	OD-C4D	2.49	1.28	1.23
29	YJ	201	PEB	OD-C4D	2.49	1.28	1.23
29	YL	201	PEB	OD-C4D	2.49	1.28	1.23
29	DM	201	PEB	OD-C4D	2.49	1.28	1.23
29	U2	202	PEB	C4B-C3B	2.49	1.49	1.45
29	g7	203	PEB	C4B-C3B	2.49	1.49	1.45
29	g9	203	PEB	C4B-C3B	2.49	1.49	1.45
29	wL	302	PEB	C2A-C1A	-2.49	1.49	1.52
29	BB	301	PEB	OD-C4D	2.49	1.28	1.23
29	BM	301	PEB	OD-C4D	2.49	1.28	1.23
29	xL	302	PEB	C2A-C1A	-2.49	1.49	1.52
29	FD	201	PEB	C4B-NB	-2.49	1.33	1.38
29	PF	201	PEB	OD-C4D	2.49	1.28	1.23
29	PI	201	PEB	OD-C4D	2.49	1.28	1.23
29	EJ	201	PEB	OD-C4D	2.49	1.28	1.23
29	EL	201	PEB	OD-C4D	2.49	1.28	1.23
31	IF	1001	CYC	OB-C4B	2.49	1.28	1.23
31	II	1001	CYC	OB-C4B	2.49	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BB	302	PUB	OA-C1A	2.49	1.28	1.23
30	BM	302	PUB	OA-C1A	2.49	1.28	1.23
29	NB	201	PEB	OD-C4D	2.49	1.28	1.23
29	NM	201	PEB	OD-C4D	2.49	1.28	1.23
29	CD	203	PEB	OD-C4D	2.49	1.28	1.23
29	YF	201	PEB	OD-C4D	2.49	1.28	1.23
29	YI	201	PEB	OD-C4D	2.49	1.28	1.23
29	i7	203	PEB	C4B-C3B	2.49	1.49	1.45
29	i9	203	PEB	C4B-C3B	2.49	1.49	1.45
29	j1	203	PEB	C2A-C1A	-2.49	1.49	1.52
29	jK	203	PEB	C2A-C1A	-2.49	1.49	1.52
29	Q2	202	PEB	C4B-C3B	2.48	1.49	1.45
31	HK	1001	CYC	C4C-NC	-2.48	1.32	1.37
29	a1	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	LB	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	aK	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	LM	202	PEB	C2A-C1A	-2.48	1.49	1.52
31	K7	1001	CYC	C1B-NB	-2.48	1.33	1.37
29	kF	201	PEB	OD-C4D	2.48	1.28	1.23
29	kI	201	PEB	OD-C4D	2.48	1.28	1.23
29	KA	202	PEB	C4B-C3B	2.48	1.49	1.45
29	KN	202	PEB	C4B-C3B	2.48	1.49	1.45
29	PB	201	PEB	OD-C4D	2.48	1.28	1.23
29	PM	201	PEB	OD-C4D	2.48	1.28	1.23
29	e7	203	PEB	C4B-C3B	2.48	1.49	1.45
29	e9	203	PEB	C4B-C3B	2.48	1.49	1.45
29	dB	202	PEB	C4B-C3B	2.48	1.49	1.45
29	dM	202	PEB	C4B-C3B	2.48	1.49	1.45
29	C5	201	PEB	C2A-C1A	-2.48	1.49	1.52
29	C8	201	PEB	C2A-C1A	-2.48	1.49	1.52
29	FB	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	FM	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	c7	203	PEB	C4B-C3B	2.48	1.49	1.45
29	c9	203	PEB	C4B-C3B	2.48	1.49	1.45
29	hB	202	PEB	C4B-C3B	2.48	1.49	1.45
29	hM	202	PEB	C4B-C3B	2.48	1.49	1.45
29	TB	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	TM	202	PEB	C2A-C1A	-2.48	1.49	1.52
29	EA	202	PEB	C4B-C3B	2.48	1.49	1.45
29	EN	202	PEB	C4B-C3B	2.48	1.49	1.45
29	fJ	201	PEB	OD-C4D	2.48	1.28	1.23
29	pJ	201	PEB	OD-C4D	2.48	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fL	201	PEB	OD-C4D	2.48	1.28	1.23
29	pL	201	PEB	OD-C4D	2.48	1.28	1.23
29	W2	202	PEB	C4B-C3B	2.48	1.49	1.45
29	CA	202	PEB	C4B-C3B	2.48	1.49	1.45
29	QB	204	PEB	C4B-C3B	2.48	1.49	1.45
29	QM	204	PEB	C4B-C3B	2.48	1.49	1.45
29	CN	202	PEB	C4B-C3B	2.48	1.49	1.45
29	UB	202	PEB	C4B-C3B	2.48	1.49	1.45
29	MQ	401	PEB	C4B-C3B	2.48	1.49	1.45
29	cB	201	PEB	OD-C4D	2.47	1.28	1.23
29	cM	201	PEB	OD-C4D	2.47	1.28	1.23
29	MA	401	PEB	C4A-NA	-2.47	1.32	1.37
29	rJ	201	PEB	OD-C4D	2.47	1.28	1.23
29	rL	201	PEB	OD-C4D	2.47	1.28	1.23
31	VP	1001	CYC	C4B-NB	-2.47	1.32	1.38
29	P7	203	PEB	C4B-C3B	2.47	1.49	1.45
29	P9	203	PEB	C4B-C3B	2.47	1.49	1.45
31	xP	1001	CYC	C4B-NB	-2.47	1.32	1.38
29	C3	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	CO	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	WB	202	PEB	C4B-C3B	2.47	1.49	1.45
29	WM	202	PEB	C4B-C3B	2.47	1.49	1.45
29	K5	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	HA	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	HN	201	PEB	C2A-C1A	-2.47	1.49	1.52
30	AM	304	PUB	C3C-C4C	2.47	1.51	1.43
29	FJ	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	FL	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	cF	201	PEB	OD-C4D	2.47	1.28	1.23
29	cI	201	PEB	OD-C4D	2.47	1.28	1.23
29	SR	202	PEB	C4B-C3B	2.47	1.49	1.45
29	Z1	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	B5	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	LA	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	ZK	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	LN	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	k7	203	PEB	C4B-C3B	2.47	1.49	1.45
29	k9	203	PEB	C4B-C3B	2.47	1.49	1.45
29	aB	202	PEB	C4B-C3B	2.47	1.49	1.45
29	aM	202	PEB	C4B-C3B	2.47	1.49	1.45
29	aF	201	PEB	OD-C4D	2.47	1.28	1.23
29	aI	201	PEB	OD-C4D	2.47	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QB	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	QM	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	eF	201	PEB	OD-C4D	2.47	1.28	1.23
29	gF	201	PEB	OD-C4D	2.47	1.28	1.23
29	eI	201	PEB	OD-C4D	2.47	1.28	1.23
29	gI	201	PEB	OD-C4D	2.47	1.28	1.23
29	A5	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	A8	201	PEB	C2A-C1A	-2.47	1.49	1.52
29	MN	401	PEB	C4A-NA	-2.47	1.32	1.37
29	LB	201	PEB	OD-C4D	2.47	1.28	1.23
29	VF	201	PEB	OD-C4D	2.47	1.28	1.23
29	VI	201	PEB	OD-C4D	2.47	1.28	1.23
29	LM	201	PEB	OD-C4D	2.47	1.28	1.23
29	a7	202	PEB	C4A-NA	-2.47	1.32	1.37
29	a9	202	PEB	C4A-NA	-2.47	1.32	1.37
29	uJ	202	PEB	OD-C4D	2.47	1.28	1.23
29	uL	202	PEB	OD-C4D	2.47	1.28	1.23
29	JC	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	JE	202	PEB	C2A-C1A	-2.47	1.49	1.52
29	GB	202	PEB	C4B-C3B	2.47	1.49	1.45
29	IB	202	PEB	C4B-C3B	2.47	1.49	1.45
29	GM	202	PEB	C4B-C3B	2.47	1.49	1.45
29	IM	202	PEB	C4B-C3B	2.47	1.49	1.45
29	DD	201	PEB	C4B-NB	-2.47	1.33	1.38
30	AB	304	PUB	C3C-C4C	2.47	1.51	1.43
29	B8	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	HD	201	PEB	OD-C4D	2.46	1.28	1.23
29	F4	201	PEB	OD-C4D	2.46	1.28	1.23
29	FD	201	PEB	OD-C4D	2.46	1.28	1.23
29	G3	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	HB	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	HM	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	GO	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	mF	201	PEB	OD-C4D	2.46	1.28	1.23
29	mI	201	PEB	OD-C4D	2.46	1.28	1.23
29	fB	202	PEB	C4B-C3B	2.46	1.49	1.45
29	fM	202	PEB	C4B-C3B	2.46	1.49	1.45
29	UR	202	PEB	C4B-C3B	2.46	1.49	1.45
29	A5	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	BA	201	PEB	C2A-C1A	-2.46	1.49	1.52
29	BN	201	PEB	C2A-C1A	-2.46	1.49	1.52
29	fF	202	PEB	C4A-NA	-2.46	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fI	202	PEB	C4A-NA	-2.46	1.32	1.37
29	MB	202	PEB	C4B-C3B	2.46	1.49	1.45
29	MM	202	PEB	C4B-C3B	2.46	1.49	1.45
29	KB	203	PEB	C2A-C1A	-2.46	1.49	1.52
29	gB	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	KM	203	PEB	C2A-C1A	-2.46	1.49	1.52
29	gM	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	H8	201	PEB	C4A-NA	-2.46	1.32	1.37
29	MN	404	PEB	C4A-NA	-2.46	1.32	1.37
29	ZB	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	ZM	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	D4	201	PEB	C4B-NB	-2.46	1.33	1.38
29	JB	202	PEB	C2A-C1A	-2.45	1.49	1.52
29	wJ	302	PEB	C2A-C1A	-2.45	1.49	1.52
29	JM	202	PEB	C2A-C1A	-2.45	1.49	1.52
29	uJ	201	PEB	C2A-C1A	-2.45	1.49	1.52
29	uL	201	PEB	C2A-C1A	-2.45	1.49	1.52
29	H4	201	PEB	C4B-NB	-2.45	1.33	1.38
29	BD	201	PEB	C4B-NB	-2.45	1.33	1.38
29	F4	201	PEB	C4B-NB	-2.45	1.33	1.38
29	J5	202	PEB	C4A-NA	-2.45	1.32	1.37
29	AF	301	PEB	C2A-C1A	-2.45	1.49	1.52
29	AI	301	PEB	C2A-C1A	-2.45	1.49	1.52
29	CB	202	PEB	C4B-C3B	2.45	1.49	1.45
29	CM	202	PEB	C4B-C3B	2.45	1.49	1.45
29	eF	201	PEB	C4A-NA	-2.45	1.32	1.37
29	eI	201	PEB	C4A-NA	-2.45	1.32	1.37
31	H1	1001	CYC	C4C-NC	-2.45	1.32	1.37
29	m7	203	PEB	C4B-C3B	2.45	1.49	1.45
29	m9	203	PEB	C4B-C3B	2.45	1.49	1.45
29	jB	202	PEB	C4B-C3B	2.45	1.49	1.45
29	jM	202	PEB	C4B-C3B	2.45	1.49	1.45
29	F5	201	PEB	C4A-NA	-2.45	1.32	1.37
29	F8	201	PEB	C4A-NA	-2.45	1.32	1.37
29	K3	202	PEB	C2A-C1A	-2.45	1.49	1.52
29	KO	202	PEB	C2A-C1A	-2.45	1.49	1.52
29	HD	201	PEB	C4B-NB	-2.45	1.33	1.38
29	Y7	202	PEB	C4A-NA	-2.45	1.32	1.37
29	Y9	202	PEB	C4A-NA	-2.45	1.32	1.37
29	iF	201	PEB	C4A-NA	-2.45	1.32	1.37
29	iI	201	PEB	C4A-NA	-2.45	1.32	1.37
29	LD	201	PEB	OD-C4D	2.45	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V7	202	PEB	C4A-NA	-2.44	1.32	1.37
29	c7	202	PEB	C4A-NA	-2.44	1.32	1.37
29	A9	304	PEB	C4A-NA	-2.44	1.32	1.37
29	V9	202	PEB	C4A-NA	-2.44	1.32	1.37
29	c9	202	PEB	C4A-NA	-2.44	1.32	1.37
29	Z7	201	PEB	C4A-NA	-2.44	1.32	1.37
29	Z9	201	PEB	C4A-NA	-2.44	1.32	1.37
29	kB	202	PEB	C2A-C1A	-2.44	1.49	1.52
29	kM	202	PEB	C2A-C1A	-2.44	1.49	1.52
29	CD	203	PEB	C4A-NA	-2.44	1.32	1.37
29	VF	201	PEB	C4A-NA	-2.44	1.32	1.37
29	VI	201	PEB	C4A-NA	-2.44	1.32	1.37
29	L4	201	PEB	C4B-NB	-2.44	1.33	1.38
29	LD	201	PEB	C4B-NB	-2.44	1.33	1.38
29	YB	201	PEB	C2A-C1A	-2.44	1.49	1.52
29	YM	201	PEB	C2A-C1A	-2.44	1.49	1.52
29	IB	202	PEB	C4B-C3B	2.44	1.49	1.45
29	IM	202	PEB	C4B-C3B	2.44	1.49	1.45
29	SB	202	PEB	C4B-C3B	2.44	1.49	1.45
29	SM	202	PEB	C4B-C3B	2.44	1.49	1.45
29	AJ	203	PEB	C2A-C1A	-2.44	1.49	1.52
29	AL	203	PEB	C2A-C1A	-2.44	1.49	1.52
29	B4	201	PEB	OD-C4D	2.44	1.28	1.23
29	BD	201	PEB	OD-C4D	2.44	1.28	1.23
29	dF	203	PEB	C4A-NA	-2.44	1.32	1.37
29	dI	203	PEB	C4A-NA	-2.44	1.32	1.37
29	RB	202	PEB	C2A-C1A	-2.44	1.49	1.52
29	RM	202	PEB	C2A-C1A	-2.44	1.49	1.52
29	e7	202	PEB	C4A-NA	-2.44	1.32	1.37
29	e9	202	PEB	C4A-NA	-2.44	1.32	1.37
29	O2	201	PEB	OD-C4D	2.44	1.28	1.23
29	MA	404	PEB	C4A-NA	-2.44	1.32	1.37
29	AM	302	PEB	C1A-NA	-2.44	1.34	1.37
29	mB	202	PEB	C2A-C1A	-2.44	1.49	1.52
29	mM	202	PEB	C2A-C1A	-2.44	1.49	1.52
29	B8	201	PEB	C4A-NA	-2.43	1.32	1.37
29	l7	201	PEB	C4A-NA	-2.43	1.32	1.37
29	l9	201	PEB	C4A-NA	-2.43	1.32	1.37
31	J1	1001	CYC	C4C-NC	-2.43	1.32	1.37
31	JK	1001	CYC	C4C-NC	-2.43	1.32	1.37
29	k7	202	PEB	C4A-NA	-2.43	1.32	1.37
29	k9	202	PEB	C4A-NA	-2.43	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TI	201	PEB	C4A-NA	-2.43	1.32	1.37
29	L4	201	PEB	OD-C4D	2.43	1.28	1.23
29	S2	202	PEB	C4B-C3B	2.43	1.49	1.45
29	MG	401	PEB	C2A-C1A	-2.43	1.49	1.52
29	D4	201	PEB	OD-C4D	2.43	1.28	1.23
29	OB	202	PEB	C4B-C3B	2.43	1.49	1.45
29	OM	202	PEB	C4B-C3B	2.43	1.49	1.45
29	J4	201	PEB	OD-C4D	2.43	1.28	1.23
29	AB	302	PEB	C1A-NA	-2.43	1.34	1.37
29	T7	202	PEB	C4A-NA	-2.43	1.32	1.37
29	T9	202	PEB	C4A-NA	-2.43	1.32	1.37
29	AB	303	PEB	C2A-C1A	-2.43	1.49	1.52
29	ZJ	202	PEB	C2A-C1A	-2.43	1.49	1.52
29	ZL	202	PEB	C2A-C1A	-2.43	1.49	1.52
29	RF	201	PEB	OD-C4D	2.43	1.28	1.23
29	RI	201	PEB	OD-C4D	2.43	1.28	1.23
29	A3	202	PEB	C2A-C1A	-2.43	1.49	1.52
29	AO	202	PEB	C2A-C1A	-2.43	1.49	1.52
29	UF	203	PEB	C4A-NA	-2.43	1.32	1.37
29	UI	203	PEB	C4A-NA	-2.43	1.32	1.37
29	H4	201	PEB	OD-C4D	2.43	1.28	1.23
29	e2	401	PEB	C3C-C4C	-2.43	1.38	1.42
29	m7	202	PEB	C4A-NA	-2.43	1.32	1.37
29	m9	202	PEB	C4A-NA	-2.43	1.32	1.37
29	H5	201	PEB	C4A-NA	-2.43	1.32	1.37
29	OF	202	PEB	C4A-NA	-2.43	1.32	1.37
29	OI	202	PEB	C4A-NA	-2.43	1.32	1.37
29	YB	203	PEB	C4B-C3B	2.43	1.49	1.45
29	YM	203	PEB	C4B-C3B	2.43	1.49	1.45
29	E3	201	PEB	OD-C4D	2.42	1.28	1.23
29	EO	201	PEB	OD-C4D	2.42	1.28	1.23
29	OR	201	PEB	OD-C4D	2.42	1.28	1.23
29	J4	201	PEB	C4B-NB	-2.42	1.33	1.38
29	h1	201	PEB	OD-C4D	2.42	1.28	1.23
29	hK	201	PEB	OD-C4D	2.42	1.28	1.23
29	FC	203	PEB	C2A-C1A	-2.42	1.49	1.52
29	FE	203	PEB	C2A-C1A	-2.42	1.49	1.52
29	WJ	201	PEB	C2A-C1A	-2.42	1.49	1.52
29	WL	201	PEB	C2A-C1A	-2.42	1.49	1.52
29	h7	201	PEB	C4A-NA	-2.42	1.32	1.37
29	h9	201	PEB	C4A-NA	-2.42	1.32	1.37
29	JD	201	PEB	C4B-NB	-2.42	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	XJ	202	PEB	C2A-C1A	-2.42	1.49	1.52
29	XL	202	PEB	C2A-C1A	-2.42	1.49	1.52
29	J8	202	PEB	C4A-NA	-2.42	1.32	1.37
29	g7	202	PEB	C4A-NA	-2.42	1.32	1.37
29	g9	202	PEB	C4A-NA	-2.42	1.32	1.37
29	MA	404	PEB	OD-C4D	2.42	1.28	1.23
29	C3	201	PEB	OD-C4D	2.42	1.28	1.23
29	CO	201	PEB	OD-C4D	2.42	1.28	1.23
29	G5	201	PEB	C4A-NA	-2.42	1.32	1.37
29	kF	201	PEB	C4A-NA	-2.42	1.32	1.37
29	kI	201	PEB	C4A-NA	-2.42	1.32	1.37
29	hF	202	PEB	C4A-NA	-2.42	1.32	1.37
29	hI	202	PEB	C4A-NA	-2.42	1.32	1.37
29	wL	301	PEB	OD-C4D	2.42	1.28	1.23
29	QF	202	PEB	C4A-NA	-2.42	1.32	1.37
29	QI	202	PEB	C4A-NA	-2.42	1.32	1.37
29	j1	201	PEB	OD-C4D	2.42	1.28	1.23
29	jK	201	PEB	OD-C4D	2.42	1.28	1.23
29	f7	201	PEB	C4A-NA	-2.42	1.32	1.37
29	f9	201	PEB	C4A-NA	-2.42	1.32	1.37
29	RF	201	PEB	C4A-NA	-2.42	1.32	1.37
29	RI	201	PEB	C4A-NA	-2.42	1.32	1.37
29	DD	201	PEB	OD-C4D	2.42	1.28	1.23
29	rJ	202	PEB	C2A-C1A	-2.42	1.49	1.52
29	rL	202	PEB	C2A-C1A	-2.42	1.49	1.52
29	TI	201	PEB	OD-C4D	2.42	1.28	1.23
29	mF	201	PEB	C4A-NA	-2.41	1.32	1.37
29	mI	201	PEB	C4A-NA	-2.41	1.32	1.37
29	dJ	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	dL	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	AM	303	PEB	C2A-C1A	-2.41	1.49	1.52
29	R7	202	PEB	C4A-NA	-2.41	1.32	1.37
29	R9	202	PEB	C4A-NA	-2.41	1.32	1.37
29	KD	203	PEB	C4A-NA	-2.41	1.32	1.37
29	gF	201	PEB	C4A-NA	-2.41	1.32	1.37
29	gI	201	PEB	C4A-NA	-2.41	1.32	1.37
29	DC	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	DE	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	eR	401	PEB	C3C-C4C	-2.41	1.38	1.42
29	G8	201	PEB	C4A-NA	-2.41	1.32	1.37
29	jF	202	PEB	C4A-NA	-2.41	1.32	1.37
29	FG	203	PEB	C4A-NA	-2.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	jI	202	PEB	C4A-NA	-2.41	1.32	1.37
31	VP	1001	CYC	CBA-CAA	2.41	1.59	1.52
31	DK	1001	CYC	OB-C4B	2.41	1.28	1.23
31	L1	1001	CYC	C4C-NC	-2.41	1.32	1.37
31	LK	1001	CYC	C4C-NC	-2.41	1.32	1.37
31	xP	1001	CYC	CBA-CAA	2.41	1.59	1.52
29	JJ	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	JL	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	B5	201	PEB	C4A-NA	-2.41	1.32	1.37
29	b7	201	PEB	C4A-NA	-2.41	1.32	1.37
29	b9	201	PEB	C4A-NA	-2.41	1.32	1.37
29	Q1	201	PEB	OD-C4D	2.41	1.28	1.23
29	QK	201	PEB	OD-C4D	2.41	1.28	1.23
29	d7	201	PEB	C4A-NA	-2.41	1.32	1.37
29	d9	201	PEB	C4A-NA	-2.41	1.32	1.37
29	aB	203	PEB	C2A-C1A	-2.41	1.49	1.52
29	aM	203	PEB	C2A-C1A	-2.41	1.49	1.52
29	aF	201	PEB	C4A-NA	-2.41	1.32	1.37
29	aI	201	PEB	C4A-NA	-2.41	1.32	1.37
29	ZF	202	PEB	C4A-NA	-2.41	1.32	1.37
29	ZI	202	PEB	C4A-NA	-2.41	1.32	1.37
29	P7	202	PEB	C4A-NA	-2.41	1.32	1.37
29	P9	202	PEB	C4A-NA	-2.41	1.32	1.37
31	VP	1001	CYC	OB-C4B	2.41	1.28	1.23
29	W7	201	PEB	C4A-NA	-2.41	1.32	1.37
29	W9	201	PEB	C4A-NA	-2.41	1.32	1.37
29	wJ	301	PEB	OD-C4D	2.41	1.28	1.23
29	LC	203	PEB	C2A-C1A	-2.40	1.49	1.52
29	LE	203	PEB	C2A-C1A	-2.40	1.49	1.52
29	C4	203	PEB	C4A-NA	-2.40	1.32	1.37
29	PF	201	PEB	C4A-NA	-2.40	1.32	1.37
29	bF	202	PEB	C4A-NA	-2.40	1.32	1.37
29	PI	201	PEB	C4A-NA	-2.40	1.32	1.37
29	bI	202	PEB	C4A-NA	-2.40	1.32	1.37
31	xP	1001	CYC	OB-C4B	2.40	1.28	1.23
29	Q7	201	PEB	C4A-NA	-2.40	1.32	1.37
29	Q9	201	PEB	C4A-NA	-2.40	1.32	1.37
29	F7	1002	PEB	OD-C4D	2.40	1.28	1.23
29	MN	404	PEB	OD-C4D	2.40	1.28	1.23
29	UR	201	PEB	OD-C4D	2.40	1.28	1.23
29	i7	202	PEB	C4A-NA	-2.40	1.32	1.37
29	i9	202	PEB	C4A-NA	-2.40	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	UR	202	PEB	C2A-C1A	-2.40	1.49	1.52
29	W1	201	PEB	OD-C4D	2.40	1.28	1.23
29	WK	201	PEB	OD-C4D	2.40	1.28	1.23
29	YF	201	PEB	C4A-NA	-2.40	1.32	1.37
29	cF	201	PEB	C4A-NA	-2.40	1.32	1.37
29	YI	201	PEB	C4A-NA	-2.40	1.32	1.37
29	cI	201	PEB	C4A-NA	-2.40	1.32	1.37
29	b1	201	PEB	OD-C4D	2.40	1.28	1.23
29	bK	201	PEB	OD-C4D	2.40	1.28	1.23
29	I3	201	PEB	OD-C4D	2.40	1.28	1.23
29	IO	201	PEB	OD-C4D	2.40	1.28	1.23
29	JA	201	PEB	C4A-NA	-2.40	1.32	1.37
29	JN	201	PEB	C4A-NA	-2.40	1.32	1.37
29	U1	202	PEB	OD-C4D	2.40	1.28	1.23
29	UK	202	PEB	OD-C4D	2.40	1.28	1.23
29	B4	201	PEB	C4B-NB	-2.40	1.33	1.38
29	S1	201	PEB	OD-C4D	2.40	1.28	1.23
29	SK	201	PEB	OD-C4D	2.40	1.28	1.23
29	TJ	202	PEB	C2A-C1A	-2.40	1.49	1.52
29	TL	202	PEB	C2A-C1A	-2.40	1.49	1.52
29	M2	201	PEB	OD-C4D	2.40	1.28	1.23
29	MR	201	PEB	OD-C4D	2.40	1.28	1.23
29	SF	202	PEB	C4A-NA	-2.40	1.32	1.37
29	SI	202	PEB	C4A-NA	-2.40	1.32	1.37
29	xL	301	PEB	OD-C4D	2.40	1.28	1.23
29	BA	201	PEB	C4A-NA	-2.40	1.32	1.37
29	BN	201	PEB	C4A-NA	-2.40	1.32	1.37
31	DK	1001	CYC	C4C-NC	-2.40	1.32	1.37
29	I5	202	PEB	C2A-C1A	-2.40	1.50	1.52
29	I8	202	PEB	C2A-C1A	-2.40	1.50	1.52
29	S7	201	PEB	C4A-NA	-2.40	1.32	1.37
29	S9	201	PEB	C4A-NA	-2.40	1.32	1.37
29	F9	1002	PEB	OD-C4D	2.40	1.28	1.23
29	A7	304	PEB	C4A-NA	-2.39	1.32	1.37
29	K3	201	PEB	OD-C4D	2.39	1.28	1.23
29	KO	201	PEB	OD-C4D	2.39	1.28	1.23
31	F1	1001	CYC	OB-C4B	2.39	1.28	1.23
31	FK	1001	CYC	OB-C4B	2.39	1.28	1.23
29	O7	201	PEB	C4A-NA	-2.39	1.32	1.37
29	O9	201	PEB	C4A-NA	-2.39	1.32	1.37
29	WF	202	PEB	C4A-NA	-2.39	1.32	1.37
29	WI	202	PEB	C4A-NA	-2.39	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K5	202	PEB	C2A-C1A	-2.39	1.50	1.52
29	K8	202	PEB	C2A-C1A	-2.39	1.50	1.52
29	BC	203	PEB	C2A-C1A	-2.39	1.50	1.52
29	BE	203	PEB	C2A-C1A	-2.39	1.50	1.52
29	HJ	201	PEB	C2A-C1A	-2.39	1.50	1.52
29	HL	201	PEB	C2A-C1A	-2.39	1.50	1.52
29	U7	201	PEB	C4A-NA	-2.39	1.32	1.37
29	U9	201	PEB	C4A-NA	-2.39	1.32	1.37
29	BG	203	PEB	C4A-NA	-2.39	1.32	1.37
29	W2	201	PEB	OD-C4D	2.39	1.28	1.23
29	WR	201	PEB	OD-C4D	2.39	1.28	1.23
31	G9	1001	CYC	C4C-NC	-2.39	1.32	1.37
29	LQ	202	PEB	C4A-NA	-2.39	1.32	1.37
30	AF	303	PUB	OA-C1A	2.39	1.28	1.23
30	AI	303	PUB	OA-C1A	2.39	1.28	1.23
31	D1	1001	CYC	OB-C4B	2.39	1.28	1.23
29	L5	202	PEB	C2A-C1A	-2.39	1.50	1.52
29	L5	201	PEB	C4A-NA	-2.39	1.32	1.37
31	G7	1001	CYC	C4C-NC	-2.39	1.32	1.37
31	NK	1001	CYC	C4C-NC	-2.39	1.32	1.37
29	d1	201	PEB	OD-C4D	2.39	1.28	1.23
29	dK	201	PEB	OD-C4D	2.39	1.28	1.23
29	G4	203	PEB	C4A-NA	-2.39	1.32	1.37
29	HA	201	PEB	C4A-NA	-2.39	1.32	1.37
29	HN	201	PEB	C4A-NA	-2.39	1.32	1.37
31	G9	1001	CYC	C4B-NB	-2.39	1.32	1.38
29	L8	201	PEB	C4A-NA	-2.39	1.32	1.37
29	JD	201	PEB	OD-C4D	2.39	1.28	1.23
29	B3	201	PEB	C4A-NA	-2.39	1.32	1.37
29	IF	202	PEB	C4A-NA	-2.39	1.32	1.37
29	II	202	PEB	C4A-NA	-2.39	1.32	1.37
29	BO	201	PEB	C4A-NA	-2.39	1.32	1.37
29	l1	201	PEB	OD-C4D	2.39	1.28	1.23
29	lK	201	PEB	OD-C4D	2.39	1.28	1.23
31	FF	1001	CYC	OB-C4B	2.38	1.28	1.23
31	FI	1001	CYC	OB-C4B	2.38	1.28	1.23
31	F1	1001	CYC	C4C-NC	-2.38	1.32	1.37
31	FK	1001	CYC	C4C-NC	-2.38	1.32	1.37
29	O1	201	PEB	OD-C4D	2.38	1.28	1.23
29	OK	201	PEB	OD-C4D	2.38	1.28	1.23
31	M9	1001	CYC	C4B-NB	-2.38	1.32	1.38
29	GD	203	PEB	C4A-NA	-2.38	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	iB	202	PEB	C2A-C1A	-2.38	1.50	1.52
29	iM	202	PEB	C2A-C1A	-2.38	1.50	1.52
31	NF	1001	CYC	OB-C4B	2.38	1.28	1.23
31	NI	1001	CYC	OB-C4B	2.38	1.28	1.23
29	nJ	202	PEB	C2A-C1A	-2.38	1.50	1.52
29	nL	202	PEB	C2A-C1A	-2.38	1.50	1.52
31	N1	1001	CYC	C4C-NC	-2.38	1.32	1.37
29	DA	201	PEB	C4A-NA	-2.38	1.32	1.37
29	DN	201	PEB	C4A-NA	-2.38	1.32	1.37
31	D1	1001	CYC	C4C-NC	-2.38	1.32	1.37
29	LG	203	PEB	C4A-NA	-2.38	1.32	1.37
31	M7	1001	CYC	C4C-NC	-2.38	1.32	1.37
31	HF	1001	CYC	OB-C4B	2.38	1.28	1.23
31	HI	1001	CYC	OB-C4B	2.38	1.28	1.23
29	JQ	203	PEB	C4A-NA	-2.38	1.32	1.37
29	JF	1002	PEB	OD-C4D	2.38	1.28	1.23
29	JI	1002	PEB	OD-C4D	2.38	1.28	1.23
29	L3	201	PEB	C4A-NA	-2.38	1.32	1.37
29	LO	201	PEB	C4A-NA	-2.38	1.32	1.37
29	xL	301	PEB	C2A-C1A	-2.38	1.50	1.52
29	NF	1002	PEB	OD-C4D	2.38	1.28	1.23
29	NI	1002	PEB	OD-C4D	2.38	1.28	1.23
29	G3	201	PEB	OD-C4D	2.38	1.28	1.23
29	GO	201	PEB	OD-C4D	2.38	1.28	1.23
31	eP	1001	CYC	C4B-NB	-2.38	1.32	1.38
29	I3	202	PEB	C2A-C1A	-2.38	1.50	1.52
29	IO	202	PEB	C2A-C1A	-2.38	1.50	1.52
31	E7	1001	CYC	C4B-NB	-2.38	1.32	1.38
31	E9	1001	CYC	C4B-NB	-2.38	1.32	1.38
31	gP	1001	CYC	C4B-NB	-2.37	1.32	1.38
29	J3	201	PEB	C4A-NA	-2.37	1.32	1.37
29	E4	203	PEB	C4A-NA	-2.37	1.32	1.37
29	j7	201	PEB	C4A-NA	-2.37	1.32	1.37
29	j9	201	PEB	C4A-NA	-2.37	1.32	1.37
29	JO	201	PEB	C4A-NA	-2.37	1.32	1.37
31	M7	1001	CYC	C4B-NB	-2.37	1.32	1.38
29	JG	203	PEB	C4A-NA	-2.37	1.32	1.37
29	N7	1002	PEB	OD-C4D	2.37	1.28	1.23
29	N9	1002	PEB	OD-C4D	2.37	1.28	1.23
29	IJ	202	PEB	C2A-C1A	-2.37	1.50	1.52
29	IL	202	PEB	C2A-C1A	-2.37	1.50	1.52
29	QR	201	PEB	OD-C4D	2.37	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K7	1001	CYC	C4C-NC	-2.37	1.32	1.37
29	BC	201	PEB	C2A-C1A	-2.37	1.50	1.52
29	BE	201	PEB	C2A-C1A	-2.37	1.50	1.52
29	Q2	201	PEB	OD-C4D	2.37	1.28	1.23
31	J1	1001	CYC	OB-C4B	2.37	1.28	1.23
31	JK	1001	CYC	OB-C4B	2.37	1.28	1.23
29	hJ	202	PEB	C2A-C1A	-2.37	1.50	1.52
29	hL	202	PEB	C2A-C1A	-2.37	1.50	1.52
29	DF	1002	PEB	OD-C4D	2.37	1.28	1.23
29	DI	1002	PEB	OD-C4D	2.37	1.28	1.23
29	Z1	202	PEB	OD-C4D	2.37	1.28	1.23
29	ZK	202	PEB	OD-C4D	2.37	1.28	1.23
31	I7	1001	CYC	C4B-NB	-2.37	1.33	1.38
31	I9	1001	CYC	C4B-NB	-2.37	1.33	1.38
29	FQ	203	PEB	C4A-NA	-2.37	1.32	1.37
29	A3	201	PEB	OD-C4D	2.37	1.28	1.23
29	xJ	301	PEB	OD-C4D	2.37	1.28	1.23
29	AO	201	PEB	OD-C4D	2.37	1.28	1.23
29	kF	202	PEB	C4A-NA	-2.37	1.32	1.37
29	kI	202	PEB	C4A-NA	-2.37	1.32	1.37
31	K9	1001	CYC	C4C-NC	-2.37	1.32	1.37
31	CK	1001	CYC	C4C-NC	-2.37	1.32	1.37
29	HC	203	PEB	C2A-C1A	-2.37	1.50	1.52
29	HE	203	PEB	C2A-C1A	-2.37	1.50	1.52
29	xJ	301	PEB	C2A-C1A	-2.37	1.50	1.52
31	N1	1001	CYC	C1B-NB	-2.37	1.33	1.37
29	MQ	403	PEB	C4A-NA	-2.37	1.32	1.37
29	IJ	203	PEB	C2A-C1A	-2.36	1.50	1.52
29	jJ	202	PEB	C2A-C1A	-2.36	1.50	1.52
29	IL	203	PEB	C2A-C1A	-2.36	1.50	1.52
29	jL	202	PEB	C2A-C1A	-2.36	1.50	1.52
29	JA	201	PEB	C2A-C1A	-2.36	1.50	1.52
29	JN	201	PEB	C2A-C1A	-2.36	1.50	1.52
29	E3	202	PEB	C2A-C1A	-2.36	1.50	1.52
29	JC	201	PEB	C2A-C1A	-2.36	1.50	1.52
29	JE	201	PEB	C2A-C1A	-2.36	1.50	1.52
29	EO	202	PEB	C2A-C1A	-2.36	1.50	1.52
29	K4	203	PEB	C4A-NA	-2.36	1.32	1.37
31	K7	1001	CYC	C4B-NB	-2.36	1.33	1.38
31	K9	1001	CYC	C4B-NB	-2.36	1.33	1.38
29	L7	1002	PEB	OD-C4D	2.36	1.28	1.23
31	IP	1001	CYC	C4B-NB	-2.36	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	1001	CYC	C4C-NC	-2.36	1.32	1.37
29	U2	201	PEB	OD-C4D	2.36	1.28	1.23
29	D7	1002	PEB	OD-C4D	2.36	1.28	1.23
29	D9	1002	PEB	OD-C4D	2.36	1.28	1.23
29	J9	1002	PEB	OD-C4D	2.36	1.28	1.23
31	LF	1001	CYC	OB-C4B	2.36	1.28	1.23
31	LI	1001	CYC	OB-C4B	2.36	1.28	1.23
29	D3	201	PEB	C4A-NA	-2.36	1.32	1.37
29	H3	201	PEB	C4A-NA	-2.36	1.32	1.37
29	eF	202	PEB	C4A-NA	-2.36	1.32	1.37
29	eI	202	PEB	C4A-NA	-2.36	1.32	1.37
29	DO	201	PEB	C4A-NA	-2.36	1.32	1.37
29	HO	201	PEB	C4A-NA	-2.36	1.32	1.37
31	I7	1001	CYC	C4C-NC	-2.36	1.32	1.37
31	I9	1001	CYC	C4C-NC	-2.36	1.32	1.37
31	N1	1001	CYC	OB-C4B	2.36	1.28	1.23
31	mP	1001	CYC	C4B-NB	-2.36	1.33	1.38
29	NJ	202	PEB	C2A-C1A	-2.36	1.50	1.52
29	NL	202	PEB	C2A-C1A	-2.36	1.50	1.52
29	J7	1002	PEB	OD-C4D	2.36	1.28	1.23
31	L1	1001	CYC	OB-C4B	2.36	1.28	1.23
31	LK	1001	CYC	OB-C4B	2.36	1.28	1.23
29	F3	201	PEB	C4A-NA	-2.36	1.32	1.37
29	FO	201	PEB	C4A-NA	-2.36	1.32	1.37
29	fI	201	PEB	OD-C4D	2.36	1.28	1.23
29	fK	201	PEB	OD-C4D	2.36	1.28	1.23
31	NK	1001	CYC	OB-C4B	2.35	1.28	1.23
29	FA	202	PEB	C4B-C3B	2.35	1.49	1.45
29	FN	202	PEB	C4B-C3B	2.35	1.49	1.45
29	VR	201	PEB	C4B-C3B	2.35	1.49	1.45
29	A7	301	PEB	C2A-C1A	-2.35	1.50	1.52
29	A9	301	PEB	C2A-C1A	-2.35	1.50	1.52
31	HK	1001	CYC	OB-C4B	2.35	1.28	1.23
31	RP	1001	CYC	C4B-NB	-2.35	1.33	1.38
29	VF	202	PEB	C4A-NA	-2.35	1.32	1.37
29	dF	201	PEB	C4A-NA	-2.35	1.32	1.37
29	VI	202	PEB	C4A-NA	-2.35	1.32	1.37
29	dI	201	PEB	C4A-NA	-2.35	1.32	1.37
31	G7	1001	CYC	C4B-NB	-2.35	1.33	1.38
29	FA	201	PEB	C4A-NA	-2.35	1.32	1.37
29	FN	201	PEB	C4A-NA	-2.35	1.32	1.37
31	AP	1001	CYC	C4B-NB	-2.35	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C7	1001	CYC	C4C-NC	-2.35	1.32	1.37
31	C9	1001	CYC	C4C-NC	-2.35	1.32	1.37
29	LC	201	PEB	C2A-C1A	-2.35	1.50	1.52
29	LE	201	PEB	C2A-C1A	-2.35	1.50	1.52
29	pJ	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	pL	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	e7	201	PEB	C4A-NA	-2.35	1.32	1.37
29	e9	201	PEB	C4A-NA	-2.35	1.32	1.37
29	BJ	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	BL	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	HF	1002	PEB	OD-C4D	2.35	1.28	1.23
29	HI	1002	PEB	OD-C4D	2.35	1.28	1.23
29	MQ	403	PEB	OD-C4D	2.35	1.28	1.23
29	JA	202	PEB	C4B-C3B	2.35	1.49	1.45
29	JN	202	PEB	C4B-C3B	2.35	1.49	1.45
29	MD	203	PEB	C4A-NA	-2.35	1.32	1.37
29	h1	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	hK	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	iF	202	PEB	C4A-NA	-2.35	1.32	1.37
29	iI	202	PEB	C4A-NA	-2.35	1.32	1.37
29	fJ	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	fL	202	PEB	C2A-C1A	-2.35	1.50	1.52
29	MN	405	PEB	C2A-C1A	-2.35	1.50	1.52
31	C7	1001	CYC	C4B-NB	-2.35	1.33	1.38
31	C9	1001	CYC	C4B-NB	-2.35	1.33	1.38
31	JP	1001	CYC	C4B-NB	-2.35	1.33	1.38
29	DA	202	PEB	C4B-C3B	2.35	1.49	1.45
29	DN	202	PEB	C4B-C3B	2.35	1.49	1.45
29	N3	203	PEB	C4A-NA	-2.35	1.32	1.37
29	mF	202	PEB	C4A-NA	-2.34	1.32	1.37
29	mI	202	PEB	C4A-NA	-2.34	1.32	1.37
31	E7	1001	CYC	C4C-NC	-2.34	1.32	1.37
31	E9	1001	CYC	C4C-NC	-2.34	1.32	1.37
31	M9	1001	CYC	C4C-NC	-2.34	1.32	1.37
31	KP	1001	CYC	C4B-NB	-2.34	1.33	1.38
29	d1	201	PEB	C4A-NA	-2.34	1.32	1.37
29	dK	201	PEB	C4A-NA	-2.34	1.32	1.37
31	IK	1001	CYC	C4C-NC	-2.34	1.32	1.37
31	tP	1001	CYC	C4B-NB	-2.34	1.33	1.38
29	L9	1002	PEB	OD-C4D	2.34	1.28	1.23
29	ID	203	PEB	C4A-NA	-2.34	1.32	1.37
29	gF	202	PEB	C4A-NA	-2.34	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gI	202	PEB	C4A-NA	-2.34	1.32	1.37
29	H7	1002	PEB	OD-C4D	2.34	1.28	1.23
29	H9	1002	PEB	OD-C4D	2.34	1.28	1.23
29	lI	202	PEB	C2A-C1A	-2.34	1.50	1.52
29	lK	202	PEB	C2A-C1A	-2.34	1.50	1.52
29	YF	202	PEB	C4A-NA	-2.34	1.32	1.37
29	YI	202	PEB	C4A-NA	-2.34	1.32	1.37
29	G8	202	PEB	C2A-C1A	-2.34	1.50	1.52
29	HC	201	PEB	C2A-C1A	-2.34	1.50	1.52
29	HE	201	PEB	C2A-C1A	-2.34	1.50	1.52
29	bJ	202	PEB	C2A-C1A	-2.34	1.50	1.52
29	bL	202	PEB	C2A-C1A	-2.34	1.50	1.52
31	rP	1001	CYC	C4B-NB	-2.34	1.33	1.38
29	M3	203	PEB	C4A-NA	-2.34	1.32	1.37
29	LA	201	PEB	C4A-NA	-2.34	1.32	1.37
29	LN	201	PEB	C4A-NA	-2.34	1.32	1.37
29	MO	203	PEB	C4A-NA	-2.34	1.32	1.37
29	ED	202	PEB	C4A-NA	-2.34	1.32	1.37
29	HG	203	PEB	C4A-NA	-2.34	1.32	1.37
29	V2	201	PEB	C4B-C3B	2.34	1.49	1.45
29	RJ	202	PEB	C2A-C1A	-2.34	1.50	1.52
29	RL	202	PEB	C2A-C1A	-2.34	1.50	1.52
29	PF	202	PEB	C4A-NA	-2.34	1.32	1.37
29	PI	202	PEB	C4A-NA	-2.34	1.32	1.37
29	HQ	203	PEB	C4A-NA	-2.34	1.32	1.37
29	A1	301	PEB	C4A-NA	-2.34	1.32	1.37
29	AK	301	PEB	C4A-NA	-2.34	1.32	1.37
31	M1	1001	CYC	C4C-NC	-2.34	1.32	1.37
31	MK	1001	CYC	C4C-NC	-2.34	1.32	1.37
29	UF	201	PEB	C4A-NA	-2.34	1.32	1.37
29	MG	401	PEB	C4A-NA	-2.34	1.32	1.37
29	UI	201	PEB	C4A-NA	-2.34	1.32	1.37
31	OP	1001	CYC	C4A-C3A	2.34	1.50	1.45
29	HA	202	PEB	C4B-C3B	2.33	1.49	1.45
29	HN	202	PEB	C4B-C3B	2.33	1.49	1.45
29	O1	202	PEB	C2A-C1A	-2.33	1.50	1.52
29	OK	202	PEB	C2A-C1A	-2.33	1.50	1.52
29	ZJ	203	PEB	C4A-NA	-2.33	1.32	1.37
29	ZL	203	PEB	C4A-NA	-2.33	1.32	1.37
31	EK	1001	CYC	C4C-NC	-2.33	1.32	1.37
29	A3	201	PEB	C4A-NA	-2.33	1.32	1.37
29	AO	201	PEB	C4A-NA	-2.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	qP	1001	CYC	C4A-C3A	2.33	1.50	1.45
29	rJ	203	PEB	C4A-NA	-2.33	1.32	1.37
29	rL	203	PEB	C4A-NA	-2.33	1.32	1.37
29	MR	202	PEB	C4B-C3B	2.33	1.49	1.45
31	iP	1001	CYC	C4B-NB	-2.33	1.33	1.38
29	Z1	202	PEB	C4A-NA	-2.33	1.32	1.37
29	ZK	202	PEB	C4A-NA	-2.33	1.32	1.37
31	TP	1001	CYC	C4B-NB	-2.33	1.33	1.38
29	sJ	203	PEB	C2A-C1A	-2.33	1.50	1.52
29	sL	203	PEB	C2A-C1A	-2.33	1.50	1.52
31	GP	1001	CYC	C4B-NB	-2.33	1.33	1.38
29	DC	201	PEB	C2A-C1A	-2.33	1.50	1.52
29	DE	201	PEB	C2A-C1A	-2.33	1.50	1.52
29	FF	1002	PEB	C4A-NA	-2.33	1.32	1.37
29	FI	1002	PEB	C4A-NA	-2.33	1.32	1.37
29	FF	1002	PEB	OD-C4D	2.33	1.28	1.23
29	FI	1002	PEB	OD-C4D	2.33	1.28	1.23
29	j1	201	PEB	C4A-NA	-2.33	1.32	1.37
29	jK	201	PEB	C4A-NA	-2.33	1.32	1.37
31	vP	1001	CYC	C4B-NB	-2.33	1.33	1.38
31	GK	1001	CYC	C4C-NC	-2.33	1.32	1.37
29	U1	202	PEB	C4A-NA	-2.33	1.32	1.37
29	OF	203	PEB	C4A-NA	-2.33	1.32	1.37
29	OI	203	PEB	C4A-NA	-2.33	1.32	1.37
29	UK	202	PEB	C4A-NA	-2.33	1.32	1.37
29	BQ	203	PEB	C4A-NA	-2.33	1.32	1.37
31	DF	1001	CYC	OB-C4B	2.33	1.28	1.23
31	DI	1001	CYC	OB-C4B	2.33	1.28	1.23
31	pP	1001	CYC	C4B-NB	-2.33	1.33	1.38
29	G3	201	PEB	C4A-NA	-2.33	1.32	1.37
29	GO	201	PEB	C4A-NA	-2.33	1.32	1.37
29	Z1	203	PEB	C2A-C1A	-2.33	1.50	1.52
29	ZK	203	PEB	C2A-C1A	-2.33	1.50	1.52
29	MQ	403	PEB	C2A-C1A	-2.33	1.50	1.52
29	W1	201	PEB	C4A-NA	-2.33	1.32	1.37
29	WK	201	PEB	C4A-NA	-2.33	1.32	1.37
31	JF	1001	CYC	OB-C4B	2.33	1.28	1.23
31	JI	1001	CYC	OB-C4B	2.33	1.28	1.23
29	QF	201	PEB	C4A-NA	-2.33	1.32	1.37
29	QI	201	PEB	C4A-NA	-2.33	1.32	1.37
31	cP	1001	CYC	C4B-NB	-2.32	1.33	1.38
31	NP	1001	CYC	C4B-NB	-2.32	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I1	1001	CYC	C4C-NC	-2.32	1.32	1.37
29	S1	201	PEB	C4A-NA	-2.32	1.32	1.37
29	SK	201	PEB	C4A-NA	-2.32	1.32	1.37
29	H5	202	PEB	C2A-C1A	-2.32	1.50	1.52
29	FA	201	PEB	C2A-C1A	-2.32	1.50	1.52
29	FN	201	PEB	C2A-C1A	-2.32	1.50	1.52
29	WF	201	PEB	C4A-NA	-2.32	1.32	1.37
29	WI	201	PEB	C4A-NA	-2.32	1.32	1.37
31	L9	1001	CYC	C1B-NB	-2.32	1.33	1.37
29	W1	202	PEB	C2A-C1A	-2.32	1.50	1.52
29	WK	202	PEB	C2A-C1A	-2.32	1.50	1.52
29	K3	201	PEB	C4A-NA	-2.32	1.32	1.37
29	KO	201	PEB	C4A-NA	-2.32	1.32	1.37
29	IF	201	PEB	C4A-NA	-2.32	1.32	1.37
29	II	201	PEB	C4A-NA	-2.32	1.32	1.37
31	K1	1001	CYC	C4C-NC	-2.32	1.32	1.37
31	KK	1001	CYC	C4C-NC	-2.32	1.32	1.37
29	BA	202	PEB	C4B-C3B	2.32	1.49	1.45
29	BN	202	PEB	C4B-C3B	2.32	1.49	1.45
29	aF	202	PEB	C4A-NA	-2.32	1.32	1.37
29	aI	202	PEB	C4A-NA	-2.32	1.32	1.37
29	fF	201	PEB	C4A-NA	-2.32	1.32	1.37
29	fI	201	PEB	C4A-NA	-2.32	1.32	1.37
29	LF	1002	PEB	OD-C4D	2.32	1.28	1.23
29	LI	1002	PEB	OD-C4D	2.32	1.28	1.23
29	F5	202	PEB	C2A-C1A	-2.32	1.50	1.52
29	F8	202	PEB	C2A-C1A	-2.32	1.50	1.52
29	C3	201	PEB	C4A-NA	-2.32	1.32	1.37
29	CO	201	PEB	C4A-NA	-2.32	1.32	1.37
31	SP	1001	CYC	C4A-C3A	2.32	1.50	1.45
29	DG	203	PEB	C4A-NA	-2.32	1.32	1.37
31	H7	1001	CYC	C1B-NB	-2.32	1.33	1.37
31	H9	1001	CYC	C1B-NB	-2.32	1.33	1.37
29	H8	202	PEB	C2A-C1A	-2.32	1.50	1.52
31	E1	1001	CYC	C4C-NC	-2.32	1.32	1.37
29	f1	201	PEB	C4A-NA	-2.32	1.32	1.37
29	LJ	202	PEB	C4A-NA	-2.32	1.32	1.37
29	IJ	203	PEB	C4A-NA	-2.32	1.32	1.37
29	fK	201	PEB	C4A-NA	-2.32	1.32	1.37
29	LL	202	PEB	C4A-NA	-2.32	1.32	1.37
29	IL	203	PEB	C4A-NA	-2.32	1.32	1.37
31	DP	1001	CYC	C4A-C3A	2.32	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NO	203	PEB	C4A-NA	-2.31	1.32	1.37
29	AC	201	PEB	C2A-C1A	-2.31	1.50	1.52
29	AE	201	PEB	C2A-C1A	-2.31	1.50	1.52
29	JJ	203	PEB	C4A-NA	-2.31	1.32	1.37
29	pJ	202	PEB	C4A-NA	-2.31	1.32	1.37
29	JL	203	PEB	C4A-NA	-2.31	1.32	1.37
29	pL	202	PEB	C4A-NA	-2.31	1.32	1.37
31	NK	1001	CYC	C1B-NB	-2.31	1.33	1.37
29	FJ	203	PEB	C4A-NA	-2.31	1.32	1.37
29	FL	203	PEB	C4A-NA	-2.31	1.32	1.37
31	EP	1001	CYC	C4B-NB	-2.31	1.33	1.38
29	h1	201	PEB	C4A-NA	-2.31	1.32	1.37
29	dF	202	PEB	C4A-NA	-2.31	1.32	1.37
29	jF	201	PEB	C4A-NA	-2.31	1.32	1.37
29	dI	202	PEB	C4A-NA	-2.31	1.32	1.37
29	jI	201	PEB	C4A-NA	-2.31	1.32	1.37
29	hJ	203	PEB	C4A-NA	-2.31	1.32	1.37
29	hK	201	PEB	C4A-NA	-2.31	1.32	1.37
29	hL	203	PEB	C4A-NA	-2.31	1.32	1.37
31	CP	1001	CYC	C4B-NB	-2.31	1.33	1.38
29	b1	201	PEB	C4A-NA	-2.31	1.32	1.37
29	hJ	202	PEB	C4A-NA	-2.31	1.32	1.37
29	bK	201	PEB	C4A-NA	-2.31	1.32	1.37
29	hL	202	PEB	C4A-NA	-2.31	1.32	1.37
31	UP	1001	CYC	C4A-C3A	2.31	1.50	1.45
29	O1	201	PEB	C4A-NA	-2.31	1.32	1.37
29	OK	201	PEB	C4A-NA	-2.31	1.32	1.37
29	DQ	203	PEB	C4A-NA	-2.31	1.32	1.37
29	I3	201	PEB	C4A-NA	-2.31	1.32	1.37
29	IO	201	PEB	C4A-NA	-2.31	1.32	1.37
29	MG	401	PEB	OD-C4D	2.31	1.28	1.23
29	i7	201	PEB	C4A-NA	-2.31	1.32	1.37
29	i9	201	PEB	C4A-NA	-2.31	1.32	1.37
29	dJ	203	PEB	C4A-NA	-2.31	1.32	1.37
29	dL	203	PEB	C4A-NA	-2.31	1.32	1.37
29	PJ	202	PEB	C2A-C1A	-2.31	1.50	1.52
29	PL	202	PEB	C2A-C1A	-2.31	1.50	1.52
29	E3	201	PEB	C4A-NA	-2.31	1.32	1.37
29	NJ	203	PEB	C4A-NA	-2.31	1.32	1.37
29	NL	203	PEB	C4A-NA	-2.31	1.32	1.37
29	EO	201	PEB	C4A-NA	-2.31	1.32	1.37
29	G5	202	PEB	C2A-C1A	-2.31	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L8	202	PEB	C2A-C1A	-2.31	1.50	1.52
29	TF	201	PEB	C2A-C1A	-2.31	1.50	1.52
31	D1	1003	CYC	C4C-NC	-2.31	1.32	1.37
29	U2	202	PEB	C2A-C1A	-2.31	1.50	1.52
31	1P	1001	CYC	C4A-C3A	2.30	1.50	1.45
29	A1	302	PEB	C2A-C1A	-2.30	1.50	1.52
29	AK	302	PEB	C2A-C1A	-2.30	1.50	1.52
29	XR	201	PEB	C4B-C3B	2.30	1.49	1.45
29	KC	202	PEB	C2A-C1A	-2.30	1.50	1.52
29	KE	202	PEB	C2A-C1A	-2.30	1.50	1.52
31	QP	1001	CYC	C4A-C3A	2.30	1.50	1.45
29	Y7	201	PEB	C4A-NA	-2.30	1.32	1.37
29	c7	201	PEB	C4A-NA	-2.30	1.32	1.37
29	Y9	201	PEB	C4A-NA	-2.30	1.32	1.37
29	c9	201	PEB	C4A-NA	-2.30	1.32	1.37
29	ZF	201	PEB	C4A-NA	-2.30	1.32	1.37
29	ZI	201	PEB	C4A-NA	-2.30	1.32	1.37
31	XP	1001	CYC	C4A-C3A	2.30	1.50	1.45
29	P7	201	PEB	C4A-NA	-2.30	1.32	1.37
29	P9	201	PEB	C4A-NA	-2.30	1.32	1.37
29	UF	202	PEB	C4A-NA	-2.30	1.32	1.37
29	UI	202	PEB	C4A-NA	-2.30	1.32	1.37
31	wP	1001	CYC	C4A-C3A	2.30	1.50	1.45
29	LF	1002	PEB	C4A-NA	-2.30	1.32	1.37
29	LI	1002	PEB	C4A-NA	-2.30	1.32	1.37
29	EG	202	PEB	C4B-C3B	2.30	1.49	1.45
29	EQ	202	PEB	C4B-C3B	2.30	1.49	1.45
29	LA	202	PEB	C4B-C3B	2.30	1.49	1.45
29	LN	202	PEB	C4B-C3B	2.30	1.49	1.45
31	L7	1001	CYC	C1B-NB	-2.30	1.34	1.37
29	Q1	201	PEB	C4A-NA	-2.30	1.32	1.37
29	BJ	203	PEB	C4A-NA	-2.30	1.32	1.37
29	HJ	202	PEB	C4A-NA	-2.30	1.32	1.37
29	QK	201	PEB	C4A-NA	-2.30	1.32	1.37
29	BL	203	PEB	C4A-NA	-2.30	1.32	1.37
29	HL	202	PEB	C4A-NA	-2.30	1.32	1.37
31	PP	1001	CYC	C4B-NB	-2.30	1.33	1.38
31	oP	1001	CYC	C4A-C3A	2.30	1.50	1.45
29	R7	201	PEB	C4A-NA	-2.30	1.32	1.37
29	R9	201	PEB	C4A-NA	-2.30	1.32	1.37
29	pJ	203	PEB	C4A-NA	-2.30	1.32	1.37
29	pL	203	PEB	C4A-NA	-2.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	jP	1001	CYC	C4A-C3A	2.30	1.50	1.45
29	k7	201	PEB	C4A-NA	-2.30	1.32	1.37
29	k9	201	PEB	C4A-NA	-2.30	1.32	1.37
29	HF	1002	PEB	C4A-NA	-2.30	1.32	1.37
29	HI	1002	PEB	C4A-NA	-2.30	1.32	1.37
29	BJ	202	PEB	C4A-NA	-2.30	1.32	1.37
29	BL	202	PEB	C4A-NA	-2.30	1.32	1.37
29	GG	202	PEB	C4B-C3B	2.30	1.49	1.45
29	GQ	202	PEB	C4B-C3B	2.30	1.49	1.45
29	d1	202	PEB	C2A-C1A	-2.30	1.50	1.52
29	dK	202	PEB	C2A-C1A	-2.30	1.50	1.52
29	sJ	203	PEB	C4A-NA	-2.30	1.32	1.37
29	sL	203	PEB	C4A-NA	-2.30	1.32	1.37
31	H1	1001	CYC	OB-C4B	2.30	1.28	1.23
31	KI	1001	CYC	C1D-CHD	2.30	1.50	1.41
29	Q1	202	PEB	C2A-C1A	-2.30	1.50	1.52
29	QK	202	PEB	C2A-C1A	-2.30	1.50	1.52
29	OF	201	PEB	C4A-NA	-2.30	1.32	1.37
29	OI	201	PEB	C4A-NA	-2.30	1.32	1.37
29	S7	201	PEB	OD-C4D	2.30	1.28	1.23
29	S9	201	PEB	OD-C4D	2.30	1.28	1.23
29	bJ	203	PEB	C4A-NA	-2.30	1.32	1.37
29	bL	203	PEB	C4A-NA	-2.30	1.32	1.37
29	M2	202	PEB	C4A-NA	-2.30	1.32	1.37
29	TJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	TL	203	PEB	C4A-NA	-2.29	1.32	1.37
31	fP	1001	CYC	C4A-C3A	2.29	1.50	1.45
31	uP	1001	CYC	C4A-C3A	2.29	1.50	1.45
29	HC	202	PEB	C4B-C3B	2.29	1.49	1.45
29	HE	202	PEB	C4B-C3B	2.29	1.49	1.45
31	IF	1001	CYC	C1D-CHD	2.29	1.50	1.41
31	II	1001	CYC	C1D-CHD	2.29	1.50	1.41
31	FP	1001	CYC	C4A-C3A	2.29	1.50	1.45
31	MP	1001	CYC	C4A-C3A	2.29	1.50	1.45
31	D1	1003	CYC	C1B-NB	-2.29	1.34	1.37
31	CF	1001	CYC	C1D-CHD	2.29	1.50	1.41
31	CI	1001	CYC	C1D-CHD	2.29	1.50	1.41
29	l1	201	PEB	C4A-NA	-2.29	1.32	1.37
29	lK	201	PEB	C4A-NA	-2.29	1.32	1.37
31	BP	1001	CYC	C4A-C3A	2.29	1.50	1.45
29	FJ	202	PEB	C4A-NA	-2.29	1.32	1.37
29	dJ	202	PEB	C4A-NA	-2.29	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	fJ	202	PEB	C4A-NA	-2.29	1.32	1.37
29	FL	202	PEB	C4A-NA	-2.29	1.32	1.37
29	dL	202	PEB	C4A-NA	-2.29	1.32	1.37
29	fL	202	PEB	C4A-NA	-2.29	1.32	1.37
29	fJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	jJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	fL	203	PEB	C4A-NA	-2.29	1.32	1.37
29	jL	203	PEB	C4A-NA	-2.29	1.32	1.37
29	RJ	202	PEB	C4A-NA	-2.29	1.32	1.37
29	RL	202	PEB	C4A-NA	-2.29	1.32	1.37
29	nJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	nL	203	PEB	C4A-NA	-2.29	1.32	1.37
29	BB	301	PEB	C3A-C4A	2.29	1.54	1.50
29	BM	301	PEB	C3A-C4A	2.29	1.54	1.50
29	DJ	202	PEB	C4A-NA	-2.29	1.32	1.37
29	XJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	DL	202	PEB	C4A-NA	-2.29	1.32	1.37
29	XL	203	PEB	C4A-NA	-2.29	1.32	1.37
29	H7	1002	PEB	C4A-NA	-2.29	1.32	1.37
29	H9	1002	PEB	C4A-NA	-2.29	1.32	1.37
31	hP	1001	CYC	C4A-C3A	2.29	1.50	1.45
29	g7	201	PEB	C4A-NA	-2.29	1.32	1.37
29	g9	201	PEB	C4A-NA	-2.29	1.32	1.37
29	AJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	IJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	RJ	203	PEB	C4A-NA	-2.29	1.32	1.37
29	AL	203	PEB	C4A-NA	-2.29	1.32	1.37
29	IL	203	PEB	C4A-NA	-2.29	1.32	1.37
29	RL	203	PEB	C4A-NA	-2.29	1.32	1.37
31	KF	1001	CYC	C1D-CHD	2.29	1.50	1.41
29	O7	201	PEB	OD-C4D	2.28	1.27	1.23
29	O9	201	PEB	OD-C4D	2.28	1.27	1.23
29	bF	201	PEB	C4A-NA	-2.28	1.32	1.37
29	hF	201	PEB	C4A-NA	-2.28	1.32	1.37
29	bI	201	PEB	C4A-NA	-2.28	1.32	1.37
29	hI	201	PEB	C4A-NA	-2.28	1.32	1.37
29	TJ	202	PEB	C4A-NA	-2.28	1.32	1.37
29	TL	202	PEB	C4A-NA	-2.28	1.32	1.37
31	MF	1001	CYC	C1D-CHD	2.28	1.50	1.41
31	MI	1001	CYC	C1D-CHD	2.28	1.50	1.41
29	h7	201	PEB	OD-C4D	2.28	1.27	1.23
29	h9	201	PEB	OD-C4D	2.28	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	PJ	203	PEB	C4A-NA	-2.28	1.32	1.37
29	PL	203	PEB	C4A-NA	-2.28	1.32	1.37
29	h7	202	PEB	C2A-C1A	-2.28	1.50	1.52
29	h9	202	PEB	C2A-C1A	-2.28	1.50	1.52
29	DF	1002	PEB	C4A-NA	-2.28	1.32	1.37
29	DI	1002	PEB	C4A-NA	-2.28	1.32	1.37
29	Y1	201	PEB	C4A-NA	-2.28	1.32	1.37
29	a7	201	PEB	C4A-NA	-2.28	1.32	1.37
29	a9	201	PEB	C4A-NA	-2.28	1.32	1.37
29	YK	201	PEB	C4A-NA	-2.28	1.32	1.37
29	EC	201	PEB	C2A-C1A	-2.28	1.50	1.52
29	EE	201	PEB	C2A-C1A	-2.28	1.50	1.52
29	nJ	202	PEB	C4A-NA	-2.28	1.32	1.37
29	nL	202	PEB	C4A-NA	-2.28	1.32	1.37
29	FC	202	PEB	C4B-C3B	2.28	1.49	1.45
29	FE	202	PEB	C4B-C3B	2.28	1.49	1.45
29	tJ	202	PEB	C4A-NA	-2.28	1.32	1.37
29	tL	202	PEB	C4A-NA	-2.28	1.32	1.37
29	m7	201	PEB	C4A-NA	-2.28	1.32	1.37
29	m9	201	PEB	C4A-NA	-2.28	1.32	1.37
29	T1	201	PEB	C4A-NA	-2.28	1.32	1.37
29	TK	201	PEB	C4A-NA	-2.28	1.32	1.37
31	kP	1001	CYC	C4A-C3A	2.28	1.50	1.45
31	GF	1001	CYC	C1D-CHD	2.28	1.49	1.41
31	GI	1001	CYC	C1D-CHD	2.28	1.49	1.41
29	JG	202	PEB	C4A-NA	-2.28	1.32	1.37
29	JQ	202	PEB	C4A-NA	-2.28	1.32	1.37
31	EF	1001	CYC	C1D-CHD	2.28	1.49	1.41
31	EI	1001	CYC	C1D-CHD	2.28	1.49	1.41
31	EK	1001	CYC	C1B-NB	-2.28	1.34	1.37
29	b7	201	PEB	OD-C4D	2.28	1.27	1.23
29	b9	201	PEB	OD-C4D	2.28	1.27	1.23
29	JD	201	PEB	CHA-C1B	2.28	1.45	1.40
29	f7	202	PEB	C2A-C1A	-2.28	1.50	1.52
29	f9	202	PEB	C2A-C1A	-2.28	1.50	1.52
29	WJ	201	PEB	C4A-NA	-2.28	1.32	1.37
29	WL	201	PEB	C4A-NA	-2.28	1.32	1.37
29	IG	202	PEB	C4B-C3B	2.28	1.49	1.45
29	IQ	202	PEB	C4B-C3B	2.28	1.49	1.45
31	N7	1001	CYC	C1B-NB	-2.28	1.34	1.37
31	N9	1001	CYC	C1B-NB	-2.28	1.34	1.37
29	NF	1002	PEB	C4A-NA	-2.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NI	1002	PEB	C4A-NA	-2.28	1.32	1.37
29	uJ	201	PEB	C4A-NA	-2.28	1.32	1.37
29	uL	201	PEB	C4A-NA	-2.28	1.32	1.37
29	Z7	201	PEB	OD-C4D	2.28	1.27	1.23
29	Z9	201	PEB	OD-C4D	2.28	1.27	1.23
29	NJ	202	PEB	C4A-NA	-2.28	1.32	1.37
29	NL	202	PEB	C4A-NA	-2.28	1.32	1.37
31	IP	1001	CYC	C4A-C3A	2.27	1.50	1.45
29	l7	201	PEB	OD-C4D	2.27	1.27	1.23
29	l9	201	PEB	OD-C4D	2.27	1.27	1.23
29	KC	201	PEB	C4B-C3B	2.27	1.49	1.45
29	KE	201	PEB	C4B-C3B	2.27	1.49	1.45
29	H3	202	PEB	C1D-ND	2.27	1.49	1.45
29	HO	202	PEB	C1D-ND	2.27	1.49	1.45
29	V7	201	PEB	C4A-NA	-2.27	1.32	1.37
29	V9	201	PEB	C4A-NA	-2.27	1.32	1.37
29	JJ	202	PEB	C4A-NA	-2.27	1.32	1.37
29	JL	202	PEB	C4A-NA	-2.27	1.32	1.37
31	F7	1001	CYC	C1B-NB	-2.27	1.34	1.37
29	a1	201	PEB	C4A-NA	-2.27	1.32	1.37
29	aK	201	PEB	C4A-NA	-2.27	1.32	1.37
29	DA	201	PEB	C2A-C1A	-2.27	1.50	1.52
29	DN	201	PEB	C2A-C1A	-2.27	1.50	1.52
29	PF	203	PEB	C4A-NA	-2.27	1.32	1.37
29	PI	203	PEB	C4A-NA	-2.27	1.32	1.37
29	yJ	301	PEB	C4A-NA	-2.27	1.32	1.37
29	yL	301	PEB	C4A-NA	-2.27	1.32	1.37
29	WR	202	PEB	C4A-NA	-2.27	1.32	1.37
31	sP	1001	CYC	C4A-C3A	2.27	1.50	1.45
29	vJ	202	PEB	C4A-NA	-2.27	1.32	1.37
29	vL	202	PEB	C4A-NA	-2.27	1.32	1.37
29	UR	202	PEB	C4A-NA	-2.27	1.32	1.37
31	F9	1001	CYC	C1B-NB	-2.27	1.34	1.37
29	J9	1002	PEB	C4A-NA	-2.27	1.32	1.37
29	SF	201	PEB	C4A-NA	-2.27	1.32	1.37
29	SI	201	PEB	C4A-NA	-2.27	1.32	1.37
29	HJ	201	PEB	C4A-NA	-2.27	1.32	1.37
29	HL	201	PEB	C4A-NA	-2.27	1.32	1.37
31	VP	1001	CYC	C4A-C3A	2.27	1.50	1.45
29	kF	201	PEB	C4B-C3B	2.27	1.49	1.45
29	kI	201	PEB	C4B-C3B	2.27	1.49	1.45
29	TF	202	PEB	C4A-NA	-2.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	TI	202	PEB	C4A-NA	-2.27	1.32	1.37
29	VJ	202	PEB	C4A-NA	-2.27	1.32	1.37
29	VL	202	PEB	C4A-NA	-2.27	1.32	1.37
31	HP	1001	CYC	C4A-C3A	2.27	1.50	1.45
29	RR	201	PEB	C4B-C3B	2.27	1.49	1.45
29	HG	202	PEB	C4A-NA	-2.27	1.32	1.37
29	jJ	202	PEB	C4A-NA	-2.27	1.32	1.37
29	jL	202	PEB	C4A-NA	-2.27	1.32	1.37
29	HQ	202	PEB	C4A-NA	-2.27	1.32	1.37
31	F1	1001	CYC	C1B-NB	-2.27	1.34	1.37
31	J7	1001	CYC	C1B-NB	-2.27	1.34	1.37
31	FK	1001	CYC	C1B-NB	-2.27	1.34	1.37
29	JF	1002	PEB	C4A-NA	-2.27	1.32	1.37
29	JI	1002	PEB	C4A-NA	-2.27	1.32	1.37
29	BC	202	PEB	C4B-C3B	2.27	1.49	1.45
29	BE	202	PEB	C4B-C3B	2.27	1.49	1.45
29	CG	202	PEB	C4B-C3B	2.27	1.49	1.45
29	CQ	202	PEB	C4B-C3B	2.27	1.49	1.45
31	mP	1001	CYC	C4D-CHA	2.27	1.49	1.41
29	R2	201	PEB	C4B-C3B	2.27	1.49	1.45
29	CC	202	PEB	C4B-C3B	2.27	1.49	1.45
29	CE	202	PEB	C4B-C3B	2.27	1.49	1.45
29	f7	201	PEB	OD-C4D	2.27	1.27	1.23
29	f9	201	PEB	OD-C4D	2.27	1.27	1.23
31	E1	1001	CYC	C1B-NB	-2.27	1.34	1.37
29	J7	1002	PEB	C4A-NA	-2.27	1.32	1.37
29	T7	201	PEB	C4A-NA	-2.27	1.32	1.37
29	T9	201	PEB	C4A-NA	-2.27	1.32	1.37
29	IJ	202	PEB	C4A-NA	-2.27	1.32	1.37
29	IL	202	PEB	C4A-NA	-2.27	1.32	1.37
29	V2	201	PEB	C4A-NA	-2.27	1.32	1.37
29	rJ	202	PEB	C4A-NA	-2.27	1.32	1.37
29	rL	202	PEB	C4A-NA	-2.27	1.32	1.37
29	P1	201	PEB	C4A-NA	-2.26	1.32	1.37
29	k1	201	PEB	C4A-NA	-2.26	1.32	1.37
29	PK	201	PEB	C4A-NA	-2.26	1.32	1.37
29	kK	201	PEB	C4A-NA	-2.26	1.32	1.37
29	N2	201	PEB	C4A-NA	-2.26	1.32	1.37
29	W2	202	PEB	C4A-NA	-2.26	1.32	1.37
31	RP	1001	CYC	C4D-CHA	2.26	1.49	1.41
31	K1	1001	CYC	C1B-NB	-2.26	1.34	1.37
31	KK	1001	CYC	C1B-NB	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S2	202	PEB	C4A-NA	-2.26	1.32	1.37
29	mF	203	PEB	C4A-NA	-2.26	1.32	1.37
29	mI	203	PEB	C4A-NA	-2.26	1.32	1.37
29	N2	201	PEB	C4B-C3B	2.26	1.49	1.45
29	NR	201	PEB	C4B-C3B	2.26	1.49	1.45
31	PP	1001	CYC	C4D-CHA	2.26	1.49	1.41
31	eP	1001	CYC	C4D-CHA	2.26	1.49	1.41
29	j7	201	PEB	OD-C4D	2.26	1.27	1.23
29	j9	201	PEB	OD-C4D	2.26	1.27	1.23
29	i1	201	PEB	C4A-NA	-2.26	1.32	1.37
29	VB	202	PEB	C4A-NA	-2.26	1.32	1.37
29	iK	201	PEB	C4A-NA	-2.26	1.32	1.37
29	VM	202	PEB	C4A-NA	-2.26	1.32	1.37
31	D7	1001	CYC	C1B-NB	-2.26	1.34	1.37
31	D9	1001	CYC	C1B-NB	-2.26	1.34	1.37
29	V1	201	PEB	C4A-NA	-2.26	1.32	1.37
29	VK	201	PEB	C4A-NA	-2.26	1.32	1.37
31	GK	1001	CYC	C1B-NB	-2.26	1.34	1.37
29	AF	304	PEB	OD-C4D	2.26	1.27	1.23
29	AI	304	PEB	OD-C4D	2.26	1.27	1.23
31	DK	1001	CYC	C1B-NB	-2.26	1.34	1.37
29	Q7	201	PEB	OD-C4D	2.26	1.27	1.23
29	Q9	201	PEB	OD-C4D	2.26	1.27	1.23
29	LG	202	PEB	C4A-NA	-2.26	1.32	1.37
29	LQ	201	PEB	C4A-NA	-2.26	1.32	1.37
31	gP	1001	CYC	C4D-CHA	2.26	1.49	1.41
29	GC	201	PEB	C2A-C1A	-2.26	1.50	1.52
29	GE	201	PEB	C2A-C1A	-2.26	1.50	1.52
31	NP	1001	CYC	C4D-CHA	2.26	1.49	1.41
31	KP	1001	CYC	C4D-CHA	2.26	1.49	1.41
29	b1	202	PEB	C2A-C1A	-2.26	1.50	1.52
29	FC	201	PEB	C2A-C1A	-2.26	1.50	1.52
29	IC	201	PEB	C2A-C1A	-2.26	1.50	1.52
29	FE	201	PEB	C2A-C1A	-2.26	1.50	1.52
29	IE	201	PEB	C2A-C1A	-2.26	1.50	1.52
29	bK	202	PEB	C2A-C1A	-2.26	1.50	1.52
31	1P	1002	CYC	C4B-NB	-2.26	1.33	1.38
29	XJ	202	PEB	C4A-NA	-2.26	1.32	1.37
29	ZJ	202	PEB	C4A-NA	-2.26	1.32	1.37
29	XL	202	PEB	C4A-NA	-2.26	1.32	1.37
29	ZL	202	PEB	C4A-NA	-2.26	1.32	1.37
29	BG	202	PEB	C4A-NA	-2.26	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BQ	202	PEB	C4A-NA	-2.26	1.32	1.37
31	L1	1001	CYC	C1B-NB	-2.26	1.34	1.37
31	M1	1001	CYC	C1B-NB	-2.26	1.34	1.37
31	LK	1001	CYC	C1B-NB	-2.26	1.34	1.37
31	MK	1001	CYC	C1B-NB	-2.26	1.34	1.37
29	AC	203	PEB	C4B-C3B	2.26	1.49	1.45
29	AE	203	PEB	C4B-C3B	2.26	1.49	1.45
29	bJ	202	PEB	C4A-NA	-2.26	1.32	1.37
29	bL	202	PEB	C4A-NA	-2.26	1.32	1.37
29	QR	202	PEB	C4A-NA	-2.26	1.32	1.37
29	TR	201	PEB	C4A-NA	-2.26	1.32	1.37
31	I7	1001	CYC	C1D-CHD	2.26	1.49	1.41
31	I9	1001	CYC	C1D-CHD	2.26	1.49	1.41
29	EG	202	PEB	C4A-NA	-2.25	1.32	1.37
29	EQ	202	PEB	C4A-NA	-2.25	1.32	1.37
29	F3	202	PEB	C1D-ND	2.25	1.49	1.45
29	FO	202	PEB	C1D-ND	2.25	1.49	1.45
29	LC	202	PEB	C4B-C3B	2.25	1.49	1.45
29	LE	202	PEB	C4B-C3B	2.25	1.49	1.45
29	W7	201	PEB	OD-C4D	2.25	1.27	1.23
29	W9	201	PEB	OD-C4D	2.25	1.27	1.23
31	CK	1001	CYC	C1D-CHD	2.25	1.49	1.41
29	d7	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	d9	202	PEB	C2A-C1A	-2.25	1.50	1.52
31	C1	1001	CYC	C1D-CHD	2.25	1.49	1.41
31	rP	1001	CYC	C4D-CHA	2.25	1.49	1.41
29	KG	202	PEB	C4B-C3B	2.25	1.49	1.45
29	KQ	202	PEB	C4B-C3B	2.25	1.49	1.45
29	c1	201	PEB	C4A-NA	-2.25	1.32	1.37
29	cK	201	PEB	C4A-NA	-2.25	1.32	1.37
31	xP	1001	CYC	C4A-C3A	2.25	1.50	1.45
29	S2	201	PEB	C2A-C1A	-2.25	1.50	1.52
29	PJ	202	PEB	C4A-NA	-2.25	1.32	1.37
29	PL	202	PEB	C4A-NA	-2.25	1.32	1.37
31	tP	1001	CYC	C4D-CHA	2.25	1.49	1.41
29	NR	201	PEB	C4A-NA	-2.25	1.32	1.37
31	CP	1001	CYC	C4D-CHA	2.25	1.49	1.41
29	VR	201	PEB	C4A-NA	-2.25	1.32	1.37
31	yP	1001	CYC	C4D-CHA	2.25	1.49	1.41
29	d7	201	PEB	OD-C4D	2.25	1.27	1.23
29	d9	201	PEB	OD-C4D	2.25	1.27	1.23
29	JB	202	PEB	C4A-NA	-2.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JM	202	PEB	C4A-NA	-2.25	1.32	1.37
31	G7	1001	CYC	C1D-CHD	2.25	1.49	1.41
29	I3	203	PEB	C1D-ND	2.25	1.49	1.45
29	IO	203	PEB	C1D-ND	2.25	1.49	1.45
31	CK	1001	CYC	C1B-NB	-2.25	1.34	1.37
31	AP	1001	CYC	C4D-CHA	2.25	1.49	1.41
29	IB	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	IM	202	PEB	C2A-C1A	-2.25	1.50	1.52
31	IP	1001	CYC	C4D-CHA	2.25	1.49	1.41
31	I1	1001	CYC	C1B-NB	-2.25	1.34	1.37
29	N7	1002	PEB	C4A-NA	-2.25	1.32	1.37
29	N9	1002	PEB	C4A-NA	-2.25	1.32	1.37
29	S1	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	SK	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	TR	201	PEB	C4B-C3B	2.25	1.49	1.45
31	I1	1001	CYC	C1D-CHD	2.25	1.49	1.41
31	JP	1001	CYC	C4D-CHA	2.25	1.49	1.41
29	F4	201	PEB	CHA-C1B	2.25	1.45	1.40
29	j1	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	Z7	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	Z9	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	JA	203	PEB	C2A-C1A	-2.25	1.50	1.52
29	jK	202	PEB	C2A-C1A	-2.25	1.50	1.52
29	JN	203	PEB	C2A-C1A	-2.25	1.50	1.52
29	F9	1002	PEB	C4A-NA	-2.25	1.32	1.37
29	BB	301	PEB	C1B-C2B	2.25	1.50	1.45
29	BM	301	PEB	C1B-C2B	2.25	1.50	1.45
31	cP	1001	CYC	C4D-CHA	2.24	1.49	1.41
31	nP	1001	CYC	C4A-C3A	2.24	1.50	1.45
31	IK	1001	CYC	C1B-NB	-2.24	1.34	1.37
29	e2	402	PEB	C4B-C3B	2.24	1.49	1.45
29	iF	203	PEB	C4A-NA	-2.24	1.32	1.37
29	iI	203	PEB	C4A-NA	-2.24	1.32	1.37
31	iP	1001	CYC	C4D-CHA	2.24	1.49	1.41
29	aF	201	PEB	C4B-C3B	2.24	1.49	1.45
29	aI	201	PEB	C4B-C3B	2.24	1.49	1.45
29	U7	201	PEB	OD-C4D	2.24	1.27	1.23
29	U9	201	PEB	OD-C4D	2.24	1.27	1.23
29	B4	201	PEB	CHA-C1B	2.24	1.45	1.40
29	H4	201	PEB	CHA-C1B	2.24	1.45	1.40
31	M1	1001	CYC	C1D-CHD	2.24	1.49	1.41
31	MK	1001	CYC	C1D-CHD	2.24	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YF	201	PEB	C4B-C3B	2.24	1.49	1.45
29	YI	201	PEB	C4B-C3B	2.24	1.49	1.45
29	cB	202	PEB	C4A-NA	-2.24	1.32	1.37
29	cM	202	PEB	C4A-NA	-2.24	1.32	1.37
29	XR	201	PEB	C4A-NA	-2.24	1.32	1.37
29	YF	203	PEB	C4A-NA	-2.24	1.32	1.37
29	YI	203	PEB	C4A-NA	-2.24	1.32	1.37
31	GP	1001	CYC	C4D-CHA	2.24	1.49	1.41
29	VF	201	PEB	C4B-C3B	2.24	1.49	1.45
29	eF	201	PEB	C4B-C3B	2.24	1.49	1.45
29	VI	201	PEB	C4B-C3B	2.24	1.49	1.45
29	eI	201	PEB	C4B-C3B	2.24	1.49	1.45
29	S7	202	PEB	C2A-C1A	-2.24	1.50	1.52
29	S9	202	PEB	C2A-C1A	-2.24	1.50	1.52
29	FA	201	PEB	C4B-C3B	2.24	1.49	1.45
29	FN	201	PEB	C4B-C3B	2.24	1.49	1.45
29	J3	202	PEB	C1D-ND	2.24	1.49	1.45
29	JO	202	PEB	C1D-ND	2.24	1.49	1.45
29	iF	201	PEB	C4B-C3B	2.24	1.49	1.45
29	iI	201	PEB	C4B-C3B	2.24	1.49	1.45
29	TB	202	PEB	C4A-NA	-2.24	1.32	1.37
29	gB	202	PEB	C4A-NA	-2.24	1.32	1.37
29	TM	202	PEB	C4A-NA	-2.24	1.32	1.37
29	gM	202	PEB	C4A-NA	-2.24	1.32	1.37
29	g1	201	PEB	C4A-NA	-2.24	1.32	1.37
29	LB	202	PEB	C4A-NA	-2.24	1.32	1.37
29	gK	201	PEB	C4A-NA	-2.24	1.32	1.37
29	LM	202	PEB	C4A-NA	-2.24	1.32	1.37
31	pP	1001	CYC	C4D-CHA	2.24	1.49	1.41
29	YB	201	PEB	C4A-NA	-2.24	1.32	1.37
29	YM	201	PEB	C4A-NA	-2.24	1.32	1.37
31	E7	1001	CYC	C1D-CHD	2.24	1.49	1.41
31	E9	1001	CYC	C1D-CHD	2.24	1.49	1.41
29	RF	201	PEB	C4B-C3B	2.24	1.49	1.45
29	RI	201	PEB	C4B-C3B	2.24	1.49	1.45
31	C1	1001	CYC	C1B-NB	-2.24	1.34	1.37
29	R2	201	PEB	C4A-NA	-2.24	1.32	1.37
29	A7	301	PEB	C4A-NA	-2.24	1.32	1.37
29	A9	301	PEB	C4A-NA	-2.24	1.32	1.37
29	cF	202	PEB	C4A-NA	-2.24	1.32	1.37
29	cI	202	PEB	C4A-NA	-2.24	1.32	1.37
29	RR	201	PEB	C4A-NA	-2.24	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QB	202	PEB	C4A-NA	-2.24	1.32	1.37
29	QM	202	PEB	C4A-NA	-2.24	1.32	1.37
29	KC	203	PEB	C4B-C3B	2.24	1.49	1.45
29	KE	203	PEB	C4B-C3B	2.24	1.49	1.45
31	K7	1001	CYC	C1D-CHD	2.24	1.49	1.41
29	R1	201	PEB	C4A-NA	-2.24	1.32	1.37
29	RK	201	PEB	C4A-NA	-2.24	1.32	1.37
31	G9	1001	CYC	C1D-CHD	2.24	1.49	1.41
31	HK	1001	CYC	C1B-NB	-2.24	1.34	1.37
29	m1	201	PEB	C4A-NA	-2.24	1.32	1.37
29	kF	203	PEB	C4A-NA	-2.24	1.32	1.37
29	kI	203	PEB	C4A-NA	-2.24	1.32	1.37
29	mK	201	PEB	C4A-NA	-2.24	1.32	1.37
29	UF	202	PEB	OD-C4D	2.24	1.27	1.23
29	UI	202	PEB	OD-C4D	2.24	1.27	1.23
31	E1	1001	CYC	C1D-CHD	2.24	1.49	1.41
29	CG	202	PEB	C4A-NA	-2.24	1.32	1.37
29	CQ	202	PEB	C4A-NA	-2.24	1.32	1.37
31	C7	1001	CYC	C1D-CHD	2.24	1.49	1.41
31	C9	1001	CYC	C1D-CHD	2.24	1.49	1.41
29	A5	201	PEB	C4A-NA	-2.24	1.32	1.37
29	A8	201	PEB	C4A-NA	-2.24	1.32	1.37
31	J1	1001	CYC	C1B-NB	-2.24	1.34	1.37
31	JK	1001	CYC	C1B-NB	-2.24	1.34	1.37
31	EP	1001	CYC	C4D-CHA	2.23	1.49	1.41
31	K9	1001	CYC	C1D-CHD	2.23	1.49	1.41
31	vP	1001	CYC	C4D-CHA	2.23	1.49	1.41
29	BD	201	PEB	CHA-C1B	2.23	1.45	1.40
29	e1	201	PEB	C4A-NA	-2.23	1.32	1.37
29	eK	201	PEB	C4A-NA	-2.23	1.32	1.37
29	ZF	201	PEB	OD-C4D	2.23	1.27	1.23
29	ZI	201	PEB	OD-C4D	2.23	1.27	1.23
31	D1	1001	CYC	C4B-NB	-2.23	1.33	1.38
29	SR	202	PEB	C2A-C1A	-2.23	1.50	1.52
29	FG	202	PEB	C4A-NA	-2.23	1.32	1.37
29	FQ	202	PEB	C4A-NA	-2.23	1.32	1.37
31	H1	1001	CYC	C1B-NB	-2.23	1.34	1.37
31	F1	1001	CYC	C4B-NB	-2.23	1.33	1.38
31	FK	1001	CYC	C4B-NB	-2.23	1.33	1.38
31	WP	1001	CYC	C4D-CHA	2.23	1.49	1.41
29	D7	1002	PEB	C4A-NA	-2.23	1.32	1.37
29	D9	1002	PEB	C4A-NA	-2.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gF	203	PEB	C4A-NA	-2.23	1.32	1.37
29	gI	203	PEB	C4A-NA	-2.23	1.32	1.37
31	DK	1001	CYC	C4B-NB	-2.23	1.33	1.38
31	EK	1001	CYC	C1D-CHD	2.23	1.49	1.41
29	IG	202	PEB	C4A-NA	-2.23	1.32	1.37
29	IQ	202	PEB	C4A-NA	-2.23	1.32	1.37
29	U1	203	PEB	C2A-C1A	-2.23	1.50	1.52
29	UK	203	PEB	C2A-C1A	-2.23	1.50	1.52
31	TP	1001	CYC	C4D-CHA	2.23	1.49	1.41
29	DD	201	PEB	CHA-C1B	2.23	1.45	1.40
29	IC	202	PEB	C4B-C3B	2.23	1.49	1.45
29	IE	202	PEB	C4B-C3B	2.23	1.49	1.45
29	U7	202	PEB	C2A-C1A	-2.23	1.50	1.52
29	U9	202	PEB	C2A-C1A	-2.23	1.50	1.52
31	M7	1001	CYC	C1D-CHD	2.23	1.49	1.41
29	O2	202	PEB	C4A-NA	-2.23	1.32	1.37
29	L7	1002	PEB	C4A-NA	-2.23	1.32	1.37
29	aF	203	PEB	C4A-NA	-2.23	1.32	1.37
29	aI	203	PEB	C4A-NA	-2.23	1.32	1.37
29	V2	203	PEB	C4A-NA	-2.23	1.32	1.37
29	SF	201	PEB	OD-C4D	2.23	1.27	1.23
29	SI	201	PEB	OD-C4D	2.23	1.27	1.23
29	Q2	202	PEB	C4A-NA	-2.23	1.32	1.37
29	VF	203	PEB	C4A-NA	-2.23	1.32	1.37
29	VI	203	PEB	C4A-NA	-2.23	1.32	1.37
29	IB	202	PEB	C2A-C1A	-2.23	1.50	1.52
29	IM	202	PEB	C2A-C1A	-2.23	1.50	1.52
29	HB	202	PEB	C4A-NA	-2.23	1.32	1.37
29	AF	301	PEB	C4A-NA	-2.23	1.32	1.37
29	AI	301	PEB	C4A-NA	-2.23	1.32	1.37
29	HM	202	PEB	C4A-NA	-2.23	1.32	1.37
31	IK	1001	CYC	C1D-CHD	2.23	1.49	1.41
29	UB	202	PEB	C2A-C1A	-2.23	1.50	1.52
29	MQ	401	PEB	C2A-C1A	-2.23	1.50	1.52
31	D1	1003	CYC	C1D-CHD	2.23	1.49	1.41
29	mF	201	PEB	C4B-C3B	2.23	1.49	1.45
29	mI	201	PEB	C4B-C3B	2.23	1.49	1.45
29	X2	202	PEB	C4A-NA	-2.23	1.32	1.37
31	M9	1001	CYC	C1D-CHD	2.23	1.49	1.41
31	J1	1001	CYC	C4B-NB	-2.23	1.33	1.38
31	JK	1001	CYC	C4B-NB	-2.23	1.33	1.38
31	D1	1001	CYC	C1B-NB	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ZB	201	PEB	C4A-NA	-2.22	1.32	1.37
29	eF	203	PEB	C4A-NA	-2.22	1.32	1.37
29	eI	203	PEB	C4A-NA	-2.22	1.32	1.37
29	ZM	201	PEB	C4A-NA	-2.22	1.32	1.37
31	J9	1001	CYC	C1B-NB	-2.22	1.34	1.37
29	cF	201	PEB	C4B-C3B	2.22	1.49	1.45
29	cI	201	PEB	C4B-C3B	2.22	1.49	1.45
29	SR	201	PEB	C4B-C3B	2.22	1.49	1.45
29	GC	202	PEB	C4B-C3B	2.22	1.49	1.45
29	GE	202	PEB	C4B-C3B	2.22	1.49	1.45
29	FD	201	PEB	CHA-C1B	2.22	1.45	1.40
31	GK	1001	CYC	C1D-CHD	2.22	1.49	1.41
29	b7	202	PEB	C2A-C1A	-2.22	1.50	1.52
29	b9	202	PEB	C2A-C1A	-2.22	1.50	1.52
29	DG	202	PEB	C4A-NA	-2.22	1.32	1.37
29	DQ	202	PEB	C4A-NA	-2.22	1.32	1.37
31	KI	1001	CYC	C4B-NB	-2.22	1.33	1.38
29	FB	202	PEB	C4A-NA	-2.22	1.32	1.37
29	FM	202	PEB	C4A-NA	-2.22	1.32	1.37
29	J4	201	PEB	CHA-C1B	2.22	1.45	1.40
29	U2	202	PEB	C4A-NA	-2.22	1.32	1.37
29	S2	202	PEB	C2A-C1A	-2.22	1.50	1.52
29	HA	203	PEB	C2A-C1A	-2.22	1.50	1.52
29	HN	203	PEB	C2A-C1A	-2.22	1.50	1.52
29	kB	202	PEB	C4A-NA	-2.22	1.32	1.37
29	kM	202	PEB	C4A-NA	-2.22	1.32	1.37
29	T2	201	PEB	C4A-NA	-2.22	1.32	1.37
29	KB	203	PEB	C4A-NA	-2.22	1.32	1.37
29	KM	203	PEB	C4A-NA	-2.22	1.32	1.37
29	QF	201	PEB	OD-C4D	2.22	1.27	1.23
29	QI	201	PEB	OD-C4D	2.22	1.27	1.23
31	K1	1001	CYC	C1D-CHD	2.22	1.49	1.41
31	KK	1001	CYC	C1D-CHD	2.22	1.49	1.41
29	C5	201	PEB	C4A-NA	-2.22	1.32	1.37
29	C8	201	PEB	C4A-NA	-2.22	1.32	1.37
29	EB	201	PEB	C4A-NA	-2.22	1.32	1.37
29	EM	201	PEB	C4A-NA	-2.22	1.32	1.37
29	dF	202	PEB	OD-C4D	2.22	1.27	1.23
29	dI	202	PEB	OD-C4D	2.22	1.27	1.23
29	W7	202	PEB	C2A-C1A	-2.22	1.50	1.52
29	j7	202	PEB	C2A-C1A	-2.22	1.50	1.52
29	W9	202	PEB	C2A-C1A	-2.22	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j9	202	PEB	C2A-C1A	-2.22	1.50	1.52
29	F7	1002	PEB	C4A-NA	-2.22	1.32	1.37
29	HA	201	PEB	C4B-C3B	2.22	1.49	1.45
29	HN	201	PEB	C4B-C3B	2.22	1.49	1.45
29	B3	202	PEB	C1D-ND	2.22	1.49	1.45
29	BO	202	PEB	C1D-ND	2.22	1.49	1.45
29	fF	201	PEB	OD-C4D	2.22	1.27	1.23
29	fI	201	PEB	OD-C4D	2.22	1.27	1.23
29	OR	202	PEB	C4B-C3B	2.22	1.49	1.45
29	dB	201	PEB	C4A-NA	-2.22	1.32	1.37
29	dM	201	PEB	C4A-NA	-2.22	1.32	1.37
29	D3	202	PEB	C4B-C3B	2.22	1.49	1.45
29	DO	202	PEB	C4B-C3B	2.22	1.49	1.45
29	AG	202	PEB	C4B-C3B	2.21	1.49	1.45
29	AQ	202	PEB	C4B-C3B	2.21	1.49	1.45
29	L4	201	PEB	CHA-C1B	2.21	1.45	1.40
29	LD	201	PEB	CHA-C1B	2.21	1.45	1.40
29	CB	202	PEB	C2A-C1A	-2.21	1.50	1.52
29	CM	202	PEB	C2A-C1A	-2.21	1.50	1.52
29	JA	201	PEB	C4B-C3B	2.21	1.49	1.45
29	JN	201	PEB	C4B-C3B	2.21	1.49	1.45
31	J9	1001	CYC	C4A-C3A	2.21	1.50	1.45
29	P2	202	PEB	C4A-NA	-2.21	1.32	1.37
29	DB	202	PEB	C4A-NA	-2.21	1.32	1.37
29	DM	202	PEB	C4A-NA	-2.21	1.32	1.37
29	G3	202	PEB	C4B-C3B	2.21	1.49	1.45
29	K3	202	PEB	C4B-C3B	2.21	1.49	1.45
29	GO	202	PEB	C4B-C3B	2.21	1.49	1.45
29	KO	202	PEB	C4B-C3B	2.21	1.49	1.45
29	KG	202	PEB	C4A-NA	-2.21	1.32	1.37
29	MN	405	PEB	C4A-NA	-2.21	1.32	1.37
29	KQ	202	PEB	C4A-NA	-2.21	1.32	1.37
31	J7	1001	CYC	C4A-C3A	2.21	1.50	1.45
29	mB	202	PEB	C4A-NA	-2.21	1.32	1.37
29	RF	202	PEB	C4A-NA	-2.21	1.32	1.37
29	RI	202	PEB	C4A-NA	-2.21	1.32	1.37
29	mM	202	PEB	C4A-NA	-2.21	1.32	1.37
29	C3	202	PEB	C4B-C3B	2.21	1.49	1.45
29	CO	202	PEB	C4B-C3B	2.21	1.49	1.45
29	A5	202	PEB	C4A-NA	-2.21	1.32	1.37
29	MA	405	PEB	C4A-NA	-2.21	1.32	1.37
29	AB	301	PEB	C2A-C1A	-2.21	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	KB	202	PEB	C2A-C1A	-2.21	1.50	1.52
29	KM	202	PEB	C2A-C1A	-2.21	1.50	1.52
31	YP	1000	CYC	C4B-NB	-2.21	1.33	1.38
29	hB	201	PEB	C4A-NA	-2.21	1.32	1.37
29	hM	201	PEB	C4A-NA	-2.21	1.32	1.37
29	a1	201	PEB	OD-C4D	2.21	1.27	1.23
29	aK	201	PEB	OD-C4D	2.21	1.27	1.23
31	EF	1001	CYC	C4B-NB	-2.21	1.33	1.38
31	EI	1001	CYC	C4B-NB	-2.21	1.33	1.38
29	OF	201	PEB	OD-C4D	2.21	1.27	1.23
29	OI	201	PEB	OD-C4D	2.21	1.27	1.23
31	D7	1001	CYC	C4A-C3A	2.21	1.50	1.45
31	D9	1001	CYC	C4A-C3A	2.21	1.50	1.45
31	GF	1001	CYC	C4B-NB	-2.21	1.33	1.38
31	GI	1001	CYC	C4B-NB	-2.21	1.33	1.38
29	T2	201	PEB	C4B-C3B	2.21	1.49	1.45
29	I5	201	PEB	C4A-NA	-2.21	1.32	1.37
29	I8	201	PEB	C4A-NA	-2.21	1.32	1.37
29	PF	201	PEB	C4B-C3B	2.21	1.49	1.45
29	gF	201	PEB	C4B-C3B	2.21	1.49	1.45
29	PI	201	PEB	C4B-C3B	2.21	1.49	1.45
29	gI	201	PEB	C4B-C3B	2.21	1.49	1.45
31	YP	1000	CYC	C4A-C3A	2.21	1.50	1.45
31	1P	1002	CYC	C4A-C3A	2.21	1.50	1.45
29	U7	201	PEB	CHA-C4A	-2.21	1.32	1.36
29	U9	201	PEB	CHA-C4A	-2.21	1.32	1.36
29	e2	402	PEB	C4A-NA	-2.21	1.32	1.37
29	TI	201	PEB	C4B-C3B	2.21	1.49	1.45
29	aB	203	PEB	C4A-NA	-2.20	1.32	1.37
29	aM	203	PEB	C4A-NA	-2.20	1.32	1.37
29	OB	201	PEB	C4A-NA	-2.20	1.32	1.37
29	OM	201	PEB	C4A-NA	-2.20	1.32	1.37
29	VR	203	PEB	C4A-NA	-2.20	1.32	1.37
31	H7	1001	CYC	C4A-C3A	2.20	1.50	1.45
31	H9	1001	CYC	C4A-C3A	2.20	1.50	1.45
29	K5	201	PEB	C4A-NA	-2.20	1.32	1.37
29	K8	201	PEB	C4A-NA	-2.20	1.32	1.37
29	lB	201	PEB	C4A-NA	-2.20	1.32	1.37
29	lM	201	PEB	C4A-NA	-2.20	1.32	1.37
31	N1	1001	CYC	C4B-NB	-2.20	1.33	1.38
31	KF	1001	CYC	C4B-NB	-2.20	1.33	1.38
29	YB	202	PEB	C4A-NA	-2.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	YM	202	PEB	C4A-NA	-2.20	1.32	1.37
29	iB	202	PEB	C4A-NA	-2.20	1.32	1.37
29	iM	202	PEB	C4A-NA	-2.20	1.32	1.37
29	BA	201	PEB	C4B-C3B	2.20	1.49	1.45
29	BN	201	PEB	C4B-C3B	2.20	1.49	1.45
29	DK	1002	PEB	C4A-NA	-2.20	1.32	1.37
29	HD	201	PEB	CHA-C1B	2.20	1.45	1.40
29	l7	202	PEB	C2A-C1A	-2.20	1.50	1.52
29	l9	202	PEB	C2A-C1A	-2.20	1.50	1.52
29	OB	202	PEB	C2A-C1A	-2.20	1.50	1.52
29	OM	202	PEB	C2A-C1A	-2.20	1.50	1.52
29	EC	202	PEB	C4B-C3B	2.20	1.49	1.45
29	EE	202	PEB	C4B-C3B	2.20	1.49	1.45
29	mB	201	PEB	C4A-NA	-2.20	1.32	1.37
29	mM	201	PEB	C4A-NA	-2.20	1.32	1.37
30	MA	403	PUB	C4B-CHB	2.20	1.49	1.41
29	aB	201	PEB	C4A-NA	-2.20	1.32	1.37
29	aM	201	PEB	C4A-NA	-2.20	1.32	1.37
31	mP	1001	CYC	OB-C4B	2.20	1.27	1.23
29	A7	305	PEB	C4A-NA	-2.20	1.32	1.37
29	A9	305	PEB	C4A-NA	-2.20	1.32	1.37
29	c1	201	PEB	OD-C4D	2.20	1.27	1.23
29	cK	201	PEB	OD-C4D	2.20	1.27	1.23
29	A3	202	PEB	C4B-C3B	2.20	1.49	1.45
29	AO	202	PEB	C4B-C3B	2.20	1.49	1.45
29	K5	202	PEB	C4A-NA	-2.20	1.32	1.37
29	K8	202	PEB	C4A-NA	-2.20	1.32	1.37
29	IB	201	PEB	C4A-NA	-2.20	1.32	1.37
29	IM	201	PEB	C4A-NA	-2.20	1.32	1.37
31	VP	1001	CYC	CBA-CGA	2.20	1.55	1.50
29	hF	201	PEB	OD-C4D	2.20	1.27	1.23
29	hI	201	PEB	OD-C4D	2.20	1.27	1.23
29	J1	1002	PEB	C4A-NA	-2.20	1.32	1.37
29	JK	1002	PEB	C4A-NA	-2.20	1.32	1.37
29	SR	202	PEB	C4A-NA	-2.20	1.32	1.37
29	O7	202	PEB	C2A-C1A	-2.20	1.50	1.52
29	O9	202	PEB	C2A-C1A	-2.20	1.50	1.52
29	e1	201	PEB	OD-C4D	2.20	1.27	1.23
29	eK	201	PEB	OD-C4D	2.20	1.27	1.23
29	E3	202	PEB	C4B-C3B	2.20	1.49	1.45
29	EO	202	PEB	C4B-C3B	2.20	1.49	1.45
29	KB	201	PEB	C4A-NA	-2.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	KM	201	PEB	C4A-NA	-2.20	1.32	1.37
31	NK	1001	CYC	C4B-NB	-2.19	1.33	1.38
29	R1	201	PEB	OD-C4D	2.19	1.27	1.23
29	RK	201	PEB	OD-C4D	2.19	1.27	1.23
29	GB	201	PEB	C4A-NA	-2.19	1.32	1.37
29	GM	201	PEB	C4A-NA	-2.19	1.32	1.37
29	C5	202	PEB	C4A-NA	-2.19	1.32	1.37
29	C8	202	PEB	C4A-NA	-2.19	1.32	1.37
29	ZB	202	PEB	C4A-NA	-2.19	1.32	1.37
29	ZM	202	PEB	C4A-NA	-2.19	1.32	1.37
29	kB	201	PEB	C4A-NA	-2.19	1.32	1.37
29	GG	202	PEB	C4A-NA	-2.19	1.32	1.37
29	kM	201	PEB	C4A-NA	-2.19	1.32	1.37
29	GQ	202	PEB	C4A-NA	-2.19	1.32	1.37
32	k6	301	PMS	O3S-S	2.19	1.55	1.47
32	kH	301	PMS	O3S-S	2.19	1.55	1.47
29	oJ	202	PEB	C4A-NA	-2.19	1.32	1.37
29	oL	202	PEB	C4A-NA	-2.19	1.32	1.37
29	A5	203	PEB	C4A-NA	-2.19	1.32	1.37
29	A8	203	PEB	C4A-NA	-2.19	1.32	1.37
29	YJ	202	PEB	C4A-NA	-2.19	1.32	1.37
29	YL	202	PEB	C4A-NA	-2.19	1.32	1.37
29	W2	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	RB	202	PEB	C4A-NA	-2.19	1.32	1.37
29	HK	1002	PEB	C4A-NA	-2.19	1.32	1.37
29	RM	202	PEB	C4A-NA	-2.19	1.32	1.37
29	XB	201	PEB	C4A-NA	-2.19	1.32	1.37
29	XM	201	PEB	C4A-NA	-2.19	1.32	1.37
29	AB	301	PEB	C4B-C3B	2.19	1.49	1.45
30	MN	403	PUB	C1C-C2C	2.19	1.49	1.45
31	MF	1001	CYC	C4B-NB	-2.19	1.33	1.38
31	MI	1001	CYC	C4B-NB	-2.19	1.33	1.38
29	SJ	202	PEB	C4A-NA	-2.19	1.32	1.37
29	SL	202	PEB	C4A-NA	-2.19	1.32	1.37
29	XR	203	PEB	C4A-NA	-2.19	1.32	1.37
31	N7	1001	CYC	C4A-C3A	2.19	1.50	1.45
31	N9	1001	CYC	C4A-C3A	2.19	1.50	1.45
29	gB	203	PEB	C4A-NA	-2.19	1.32	1.37
29	gM	203	PEB	C4A-NA	-2.19	1.32	1.37
29	D4	201	PEB	CHA-C1B	2.19	1.45	1.40
29	WF	201	PEB	OD-C4D	2.19	1.27	1.23
29	WI	201	PEB	OD-C4D	2.19	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L7	1001	CYC	C4A-C3A	2.19	1.50	1.45
29	WB	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	WM	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	jF	201	PEB	OD-C4D	2.19	1.27	1.23
29	lF	201	PEB	OD-C4D	2.19	1.27	1.23
29	jI	201	PEB	OD-C4D	2.19	1.27	1.23
29	lI	201	PEB	OD-C4D	2.19	1.27	1.23
29	j7	201	PEB	CHA-C4A	-2.19	1.32	1.36
29	j9	201	PEB	CHA-C4A	-2.19	1.32	1.36
29	fB	201	PEB	C4A-NA	-2.19	1.32	1.37
29	fM	201	PEB	C4A-NA	-2.19	1.32	1.37
29	L9	1002	PEB	C4A-NA	-2.19	1.32	1.37
29	cB	201	PEB	C4A-NA	-2.19	1.32	1.37
29	AG	202	PEB	C4A-NA	-2.19	1.32	1.37
29	cM	201	PEB	C4A-NA	-2.19	1.32	1.37
29	AQ	202	PEB	C4A-NA	-2.19	1.32	1.37
29	aB	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	aM	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	AJ	202	PEB	C4A-NA	-2.19	1.32	1.37
29	AL	202	PEB	C4A-NA	-2.19	1.32	1.37
29	G8	202	PEB	C4A-NA	-2.19	1.32	1.37
29	EB	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	EM	202	PEB	C2A-C1A	-2.19	1.50	1.52
29	DA	201	PEB	C4B-C3B	2.19	1.49	1.45
29	DN	201	PEB	C4B-C3B	2.19	1.49	1.45
29	L5	202	PEB	C4A-NA	-2.19	1.32	1.37
29	TB	203	PEB	C1B-C2B	2.18	1.50	1.45
29	TM	203	PEB	C1B-C2B	2.18	1.50	1.45
29	F1	1002	PEB	C4A-NA	-2.18	1.32	1.37
29	R2	203	PEB	C4A-NA	-2.18	1.32	1.37
29	FK	1002	PEB	C4A-NA	-2.18	1.32	1.37
29	RR	203	PEB	C4A-NA	-2.18	1.32	1.37
29	L1	1002	PEB	C4A-NA	-2.18	1.32	1.37
29	LK	1002	PEB	C4A-NA	-2.18	1.32	1.37
29	UB	201	PEB	C4A-NA	-2.18	1.32	1.37
29	UM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	WR	202	PEB	C2A-C1A	-2.18	1.50	1.52
29	l7	201	PEB	CHA-C4A	-2.18	1.32	1.36
29	l9	201	PEB	CHA-C4A	-2.18	1.32	1.36
29	D1	1002	PEB	C4A-NA	-2.18	1.32	1.37
29	EA	201	PEB	C4A-NA	-2.18	1.32	1.37
29	SB	201	PEB	C4A-NA	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	EN	201	PEB	C4A-NA	-2.18	1.32	1.37
29	U1	203	PEB	C4A-NA	-2.18	1.32	1.37
29	UK	203	PEB	C4A-NA	-2.18	1.32	1.37
29	LA	201	PEB	C4B-C3B	2.18	1.49	1.45
29	LN	201	PEB	C4B-C3B	2.18	1.49	1.45
29	Q7	202	PEB	C2A-C1A	-2.18	1.50	1.52
29	Q9	202	PEB	C2A-C1A	-2.18	1.50	1.52
29	DA	203	PEB	C2A-C1A	-2.18	1.50	1.52
29	CC	201	PEB	C2A-C1A	-2.18	1.50	1.52
29	CE	201	PEB	C2A-C1A	-2.18	1.50	1.52
29	DN	203	PEB	C2A-C1A	-2.18	1.50	1.52
29	jB	202	PEB	C4A-NA	-2.18	1.32	1.37
29	jM	202	PEB	C4A-NA	-2.18	1.32	1.37
29	O7	201	PEB	CHA-C4A	-2.18	1.32	1.36
29	O9	201	PEB	CHA-C4A	-2.18	1.32	1.36
29	MB	202	PEB	C4A-NA	-2.18	1.32	1.37
29	MM	202	PEB	C4A-NA	-2.18	1.32	1.37
29	O1	202	PEB	C4A-NA	-2.18	1.32	1.37
29	OK	202	PEB	C4A-NA	-2.18	1.32	1.37
29	J5	202	PEB	C2A-C1A	-2.18	1.50	1.52
29	J8	202	PEB	C2A-C1A	-2.18	1.50	1.52
29	FA	203	PEB	C2A-C1A	-2.18	1.50	1.52
29	FN	203	PEB	C2A-C1A	-2.18	1.50	1.52
31	L1	1001	CYC	C4B-NB	-2.18	1.33	1.38
31	LK	1001	CYC	C4B-NB	-2.18	1.33	1.38
29	MB	201	PEB	C4A-NA	-2.18	1.32	1.37
29	QB	203	PEB	C4A-NA	-2.18	1.32	1.37
29	MM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	QM	203	PEB	C4A-NA	-2.18	1.32	1.37
29	P1	201	PEB	OD-C4D	2.18	1.27	1.23
29	PK	201	PEB	OD-C4D	2.18	1.27	1.23
29	gB	201	PEB	C4A-NA	-2.18	1.32	1.37
29	gM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	I8	202	PEB	C4A-NA	-2.18	1.32	1.37
29	I4	203	PEB	C4B-C3B	2.18	1.49	1.45
29	O2	202	PEB	C2A-C1A	-2.18	1.50	1.52
29	I5	202	PEB	C4A-NA	-2.18	1.32	1.37
29	NK	1002	PEB	C4A-NA	-2.18	1.32	1.37
29	WB	201	PEB	C4A-NA	-2.18	1.32	1.37
29	iB	201	PEB	C4A-NA	-2.18	1.32	1.37
29	sJ	202	PEB	C4A-NA	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	sL	202	PEB	C4A-NA	-2.18	1.32	1.37
29	WM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	iM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	T1	201	PEB	OD-C4D	2.18	1.27	1.23
29	TK	201	PEB	OD-C4D	2.18	1.27	1.23
29	LB	201	PEB	C4A-NA	-2.18	1.32	1.37
29	LM	201	PEB	C4A-NA	-2.18	1.32	1.37
29	KA	201	PEB	C4A-NA	-2.18	1.32	1.37
29	lB	202	PEB	C4A-NA	-2.18	1.32	1.37
29	lM	202	PEB	C4A-NA	-2.18	1.32	1.37
29	KN	201	PEB	C4A-NA	-2.18	1.32	1.37
30	MN	403	PUB	C4B-CHB	2.18	1.49	1.41
29	YB	203	PEB	C2A-C1A	-2.18	1.50	1.52
29	AM	301	PEB	C2A-C1A	-2.18	1.50	1.52
29	YM	203	PEB	C2A-C1A	-2.18	1.50	1.52
29	d7	201	PEB	CHA-C4A	-2.18	1.32	1.36
29	d9	201	PEB	CHA-C4A	-2.18	1.32	1.36
29	NR	203	PEB	C4A-NA	-2.18	1.32	1.37
29	bF	201	PEB	OD-C4D	2.18	1.27	1.23
29	bI	201	PEB	OD-C4D	2.18	1.27	1.23
29	C5	203	PEB	C4A-NA	-2.18	1.32	1.37
29	C8	203	PEB	C4A-NA	-2.18	1.32	1.37
29	MA	405	PEB	C1B-C2B	2.18	1.50	1.45
29	eJ	202	PEB	C4A-NA	-2.18	1.32	1.37
29	eL	202	PEB	C4A-NA	-2.18	1.32	1.37
31	CF	1001	CYC	C4B-NB	-2.18	1.33	1.38
31	CI	1001	CYC	C4B-NB	-2.18	1.33	1.38
29	A7	305	PEB	C1B-C2B	2.18	1.50	1.45
29	A9	305	PEB	C1B-C2B	2.18	1.50	1.45
29	i1	201	PEB	OD-C4D	2.17	1.27	1.23
29	iK	201	PEB	OD-C4D	2.17	1.27	1.23
31	TP	1001	CYC	OB-C4B	2.17	1.27	1.23
29	QB	204	PEB	C2A-C1A	-2.17	1.50	1.52
29	QM	204	PEB	C2A-C1A	-2.17	1.50	1.52
29	lB	202	PEB	C4A-NA	-2.17	1.32	1.37
29	TB	201	PEB	C4A-NA	-2.17	1.32	1.37
29	jB	201	PEB	C4A-NA	-2.17	1.32	1.37
29	lM	202	PEB	C4A-NA	-2.17	1.32	1.37
29	TM	201	PEB	C4A-NA	-2.17	1.32	1.37
29	jM	201	PEB	C4A-NA	-2.17	1.32	1.37
29	L8	202	PEB	C4A-NA	-2.17	1.32	1.37
29	JB	201	PEB	C4A-NA	-2.17	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	uJ	203	PEB	C4A-NA	-2.17	1.32	1.37
29	uL	203	PEB	C4A-NA	-2.17	1.32	1.37
29	JM	201	PEB	C4A-NA	-2.17	1.32	1.37
29	W1	202	PEB	C4A-NA	-2.17	1.32	1.37
29	H5	202	PEB	C4A-NA	-2.17	1.32	1.37
29	NB	202	PEB	C4A-NA	-2.17	1.32	1.37
29	WK	202	PEB	C4A-NA	-2.17	1.32	1.37
29	NM	202	PEB	C4A-NA	-2.17	1.32	1.37
29	H1	1002	PEB	C4A-NA	-2.17	1.32	1.37
29	FB	201	PEB	C4A-NA	-2.17	1.32	1.37
29	WJ	203	PEB	C4A-NA	-2.17	1.32	1.37
29	WL	203	PEB	C4A-NA	-2.17	1.32	1.37
29	FM	201	PEB	C4A-NA	-2.17	1.32	1.37
29	cJ	202	PEB	C4A-NA	-2.17	1.32	1.37
29	cL	202	PEB	C4A-NA	-2.17	1.32	1.37
29	C4	202	PEB	C2A-C1A	-2.17	1.50	1.52
29	Z1	203	PEB	C4A-NA	-2.17	1.32	1.37
29	ZK	203	PEB	C4A-NA	-2.17	1.32	1.37
29	KC	203	PEB	C1D-ND	2.17	1.49	1.45
29	KE	203	PEB	C1D-ND	2.17	1.49	1.45
29	B3	201	PEB	C4B-C3B	2.17	1.49	1.45
29	BO	201	PEB	C4B-C3B	2.17	1.49	1.45
29	A8	202	PEB	C4A-NA	-2.17	1.32	1.37
29	RB	201	PEB	C4A-NA	-2.17	1.32	1.37
29	RM	201	PEB	C4A-NA	-2.17	1.32	1.37
29	SR	201	PEB	C2A-C1A	-2.17	1.50	1.52
31	HK	1001	CYC	C4B-NB	-2.17	1.33	1.38
31	BP	1001	CYC	C4B-NB	-2.17	1.33	1.38
29	h7	201	PEB	CHA-C4A	-2.17	1.32	1.36
29	h9	201	PEB	CHA-C4A	-2.17	1.32	1.36
29	T2	203	PEB	C4A-NA	-2.17	1.32	1.37
29	CA	201	PEB	C4A-NA	-2.17	1.32	1.37
29	CN	201	PEB	C4A-NA	-2.17	1.32	1.37
29	TR	203	PEB	C4A-NA	-2.17	1.32	1.37
29	iB	203	PEB	C1B-C2B	2.17	1.50	1.45
29	iM	203	PEB	C1B-C2B	2.17	1.50	1.45
29	M4	203	PEB	C4B-C3B	2.17	1.49	1.45
29	j1	202	PEB	C4A-NA	-2.17	1.32	1.37
29	kB	203	PEB	C4A-NA	-2.17	1.32	1.37
29	jK	202	PEB	C4A-NA	-2.17	1.32	1.37
29	kM	203	PEB	C4A-NA	-2.17	1.32	1.37
29	M2	202	PEB	C1C-CHB	2.17	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	QJ	202	PEB	C2A-C1A	-2.17	1.50	1.52
29	QL	202	PEB	C2A-C1A	-2.17	1.50	1.52
29	HB	203	PEB	C4A-NA	-2.17	1.32	1.37
29	HM	203	PEB	C4A-NA	-2.17	1.32	1.37
31	yP	1001	CYC	C1A-C2A	2.17	1.49	1.45
29	AM	301	PEB	C4B-C3B	2.17	1.49	1.45
29	XB	202	PEB	C4A-NA	-2.17	1.32	1.37
29	kJ	202	PEB	C4A-NA	-2.17	1.32	1.37
29	kL	202	PEB	C4A-NA	-2.17	1.32	1.37
29	XM	202	PEB	C4A-NA	-2.17	1.32	1.37
29	SR	202	PEB	C1C-CHB	2.17	1.49	1.41
29	k1	201	PEB	OD-C4D	2.17	1.27	1.23
29	kK	201	PEB	OD-C4D	2.17	1.27	1.23
29	MJ	202	PEB	C4A-NA	-2.17	1.32	1.37
29	ML	202	PEB	C4A-NA	-2.17	1.32	1.37
29	AC	202	PEB	C4B-C3B	2.17	1.49	1.45
29	AE	202	PEB	C4B-C3B	2.17	1.49	1.45
29	LA	203	PEB	C2A-C1A	-2.17	1.50	1.52
29	LN	203	PEB	C2A-C1A	-2.17	1.50	1.52
31	gP	1001	CYC	OB-C4B	2.16	1.27	1.23
29	A1	301	PEB	C2A-C1A	-2.16	1.50	1.52
29	GB	202	PEB	C2A-C1A	-2.16	1.50	1.52
29	AK	301	PEB	C2A-C1A	-2.16	1.50	1.52
29	GM	202	PEB	C2A-C1A	-2.16	1.50	1.52
29	aJ	202	PEB	C4A-NA	-2.16	1.32	1.37
29	aL	202	PEB	C4A-NA	-2.16	1.32	1.37
29	WR	202	PEB	C1C-CHB	2.16	1.49	1.41
31	L9	1001	CYC	C1A-NA	-2.16	1.33	1.38
29	A1	303	PEB	C4A-NA	-2.16	1.32	1.37
29	aB	202	PEB	C4A-NA	-2.16	1.32	1.37
29	AK	303	PEB	C4A-NA	-2.16	1.32	1.37
29	aM	202	PEB	C4A-NA	-2.16	1.32	1.37
29	PR	202	PEB	C4A-NA	-2.16	1.32	1.37
29	IJ	202	PEB	C4A-NA	-2.16	1.32	1.37
29	IL	202	PEB	C4A-NA	-2.16	1.32	1.37
29	V1	201	PEB	OD-C4D	2.16	1.27	1.23
29	VK	201	PEB	OD-C4D	2.16	1.27	1.23
30	MA	403	PUB	C1C-C2C	2.16	1.49	1.45
29	AA	201	PEB	C4A-NA	-2.16	1.32	1.37
29	AN	201	PEB	C4A-NA	-2.16	1.32	1.37
31	IF	1001	CYC	C4B-NB	-2.16	1.33	1.38
31	II	1001	CYC	C4B-NB	-2.16	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	m1	201	PEB	OD-C4D	2.16	1.27	1.23
29	mK	201	PEB	OD-C4D	2.16	1.27	1.23
29	ZB	203	PEB	C1B-C2B	2.16	1.50	1.45
29	ZM	203	PEB	C1B-C2B	2.16	1.50	1.45
29	AG	201	PEB	C4A-NA	-2.16	1.32	1.37
29	AQ	201	PEB	C4A-NA	-2.16	1.32	1.37
29	f1	202	PEB	C4A-NA	-2.16	1.32	1.37
29	G5	202	PEB	C4A-NA	-2.16	1.32	1.37
29	OB	202	PEB	C4A-NA	-2.16	1.32	1.37
29	fK	202	PEB	C4A-NA	-2.16	1.32	1.37
29	OM	202	PEB	C4A-NA	-2.16	1.32	1.37
29	S7	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	S9	201	PEB	CHA-C4A	-2.16	1.32	1.36
31	sP	1001	CYC	C4B-NB	-2.16	1.33	1.38
29	L3	201	PEB	C4B-C3B	2.16	1.49	1.45
29	LO	201	PEB	C4B-C3B	2.16	1.49	1.45
31	FP	1001	CYC	C4B-NB	-2.16	1.33	1.38
31	L9	1001	CYC	C4A-C3A	2.16	1.50	1.45
29	SB	202	PEB	C4A-NA	-2.16	1.32	1.37
29	eB	202	PEB	C4A-NA	-2.16	1.32	1.37
29	mJ	202	PEB	C4A-NA	-2.16	1.32	1.37
29	mL	202	PEB	C4A-NA	-2.16	1.32	1.37
29	SM	202	PEB	C4A-NA	-2.16	1.32	1.37
29	eM	202	PEB	C4A-NA	-2.16	1.32	1.37
29	B5	202	PEB	C4A-NA	-2.16	1.32	1.37
29	iJ	202	PEB	C4A-NA	-2.16	1.32	1.37
29	iL	202	PEB	C4A-NA	-2.16	1.32	1.37
29	oJ	202	PEB	C2A-C1A	-2.16	1.50	1.52
29	oL	202	PEB	C2A-C1A	-2.16	1.50	1.52
29	Q7	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	Q9	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	kB	203	PEB	C1B-C2B	2.16	1.50	1.45
29	kM	203	PEB	C1B-C2B	2.16	1.50	1.45
29	RB	203	PEB	C4A-NA	-2.16	1.32	1.37
29	RM	203	PEB	C4A-NA	-2.16	1.32	1.37
29	W7	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	W9	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	N1	1002	PEB	C4A-NA	-2.16	1.32	1.37
29	S1	202	PEB	C4A-NA	-2.16	1.32	1.37
29	SK	202	PEB	C4A-NA	-2.16	1.32	1.37
31	H1	1001	CYC	C4B-NB	-2.16	1.33	1.38
29	QB	204	PEB	C4A-NA	-2.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	UJ	202	PEB	C4A-NA	-2.16	1.32	1.37
29	UL	202	PEB	C4A-NA	-2.16	1.32	1.37
29	QM	204	PEB	C4A-NA	-2.16	1.32	1.37
31	H7	1001	CYC	C1B-C2B	2.16	1.49	1.45
31	H9	1001	CYC	C1B-C2B	2.16	1.49	1.45
31	L9	1001	CYC	C1B-C2B	2.16	1.49	1.45
29	b7	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	b9	201	PEB	CHA-C4A	-2.16	1.32	1.36
29	b1	202	PEB	C4A-NA	-2.16	1.32	1.37
29	mB	203	PEB	C4A-NA	-2.16	1.32	1.37
29	bK	202	PEB	C4A-NA	-2.16	1.32	1.37
29	mM	203	PEB	C4A-NA	-2.16	1.32	1.37
31	KP	1001	CYC	OB-C4B	2.16	1.27	1.23
29	d1	202	PEB	C4A-NA	-2.16	1.32	1.37
29	J3	202	PEB	C4A-NA	-2.16	1.32	1.37
29	B8	202	PEB	C4A-NA	-2.16	1.32	1.37
29	dK	202	PEB	C4A-NA	-2.16	1.32	1.37
29	xL	302	PEB	C4A-NA	-2.16	1.32	1.37
29	JO	202	PEB	C4A-NA	-2.16	1.32	1.37
29	f1	202	PEB	C2A-C1A	-2.16	1.50	1.52
29	ID	202	PEB	C2A-C1A	-2.16	1.50	1.52
29	fK	202	PEB	C2A-C1A	-2.16	1.50	1.52
31	oP	1001	CYC	C4B-NB	-2.16	1.33	1.38
29	H8	202	PEB	C4A-NA	-2.16	1.32	1.37
29	GC	202	PEB	C1D-ND	2.16	1.49	1.45
29	GE	202	PEB	C1D-ND	2.16	1.49	1.45
29	MN	405	PEB	C1B-C2B	2.16	1.50	1.45
31	F7	1001	CYC	C4A-C3A	2.15	1.50	1.45
29	I4	202	PEB	C2A-C1A	-2.15	1.50	1.52
29	DB	203	PEB	C4A-NA	-2.15	1.32	1.37
29	PB	201	PEB	C4A-NA	-2.15	1.32	1.37
29	cB	203	PEB	C4A-NA	-2.15	1.32	1.37
29	xJ	302	PEB	C4A-NA	-2.15	1.32	1.37
29	DM	203	PEB	C4A-NA	-2.15	1.32	1.37
29	PM	201	PEB	C4A-NA	-2.15	1.32	1.37
29	cM	203	PEB	C4A-NA	-2.15	1.32	1.37
31	D1	1003	CYC	C4B-NB	-2.15	1.33	1.38
31	F9	1001	CYC	C4A-C3A	2.15	1.50	1.45
29	M2	202	PEB	C2A-C1A	-2.15	1.50	1.52
29	G4	202	PEB	C2A-C1A	-2.15	1.50	1.52
29	K5	203	PEB	C4A-NA	-2.15	1.32	1.37
29	F8	202	PEB	C4A-NA	-2.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K8	203	PEB	C4A-NA	-2.15	1.32	1.37
29	hB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	hM	202	PEB	C4A-NA	-2.15	1.32	1.37
29	QR	202	PEB	C1C-CHB	2.15	1.49	1.41
29	O2	202	PEB	C1C-CHB	2.15	1.49	1.41
29	CC	202	PEB	C1D-ND	2.15	1.49	1.45
29	CE	202	PEB	C1D-ND	2.15	1.49	1.45
29	IA	201	PEB	C4A-NA	-2.15	1.32	1.37
29	eB	201	PEB	C4A-NA	-2.15	1.32	1.37
29	eM	201	PEB	C4A-NA	-2.15	1.32	1.37
29	IN	201	PEB	C4A-NA	-2.15	1.32	1.37
29	NB	202	PEB	C1B-C2B	2.15	1.50	1.45
29	NM	202	PEB	C1B-C2B	2.15	1.50	1.45
31	MP	1001	CYC	C4B-NB	-2.15	1.33	1.38
31	tP	1001	CYC	OB-C4B	2.15	1.27	1.23
29	Z7	201	PEB	CHA-C4A	-2.15	1.32	1.36
29	Z9	201	PEB	CHA-C4A	-2.15	1.32	1.36
29	CB	201	PEB	C4A-NA	-2.15	1.32	1.37
29	CB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	CM	201	PEB	C4A-NA	-2.15	1.32	1.37
29	CM	202	PEB	C4A-NA	-2.15	1.32	1.37
29	fB	202	PEB	C2A-C1A	-2.15	1.50	1.52
29	fM	202	PEB	C2A-C1A	-2.15	1.50	1.52
29	LB	203	PEB	C1B-C2B	2.15	1.50	1.45
29	LM	203	PEB	C1B-C2B	2.15	1.50	1.45
29	DB	201	PEB	C4A-NA	-2.15	1.32	1.37
29	DM	201	PEB	C4A-NA	-2.15	1.32	1.37
29	FB	203	PEB	C4A-NA	-2.15	1.32	1.37
29	FM	203	PEB	C4A-NA	-2.15	1.32	1.37
29	EC	202	PEB	C1D-ND	2.15	1.49	1.45
29	EE	202	PEB	C1D-ND	2.15	1.49	1.45
29	mB	203	PEB	C1B-C2B	2.15	1.50	1.45
29	mM	203	PEB	C1B-C2B	2.15	1.50	1.45
29	HB	201	PEB	C4A-NA	-2.15	1.32	1.37
29	VB	203	PEB	C4A-NA	-2.15	1.32	1.37
29	OJ	202	PEB	C4A-NA	-2.15	1.32	1.37
29	QJ	202	PEB	C4A-NA	-2.15	1.32	1.37
29	OL	202	PEB	C4A-NA	-2.15	1.32	1.37
29	QL	202	PEB	C4A-NA	-2.15	1.32	1.37
29	wL	302	PEB	C4A-NA	-2.15	1.32	1.37
29	HM	201	PEB	C4A-NA	-2.15	1.32	1.37
29	VM	203	PEB	C4A-NA	-2.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l1	202	PEB	C4A-NA	-2.15	1.32	1.37
29	lK	202	PEB	C4A-NA	-2.15	1.32	1.37
29	eB	202	PEB	C1B-C2B	2.15	1.50	1.45
29	eM	202	PEB	C1B-C2B	2.15	1.50	1.45
31	UP	1001	CYC	C4B-NB	-2.15	1.33	1.38
29	H3	202	PEB	C4A-NA	-2.15	1.32	1.37
29	I3	203	PEB	C4A-NA	-2.15	1.32	1.37
29	GB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	fB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	GM	202	PEB	C4A-NA	-2.15	1.32	1.37
29	fM	202	PEB	C4A-NA	-2.15	1.32	1.37
29	HO	202	PEB	C4A-NA	-2.15	1.32	1.37
29	IO	203	PEB	C4A-NA	-2.15	1.32	1.37
29	EB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	JB	203	PEB	C4A-NA	-2.15	1.32	1.37
29	dB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	EM	202	PEB	C4A-NA	-2.15	1.32	1.37
29	JM	203	PEB	C4A-NA	-2.15	1.32	1.37
29	dM	202	PEB	C4A-NA	-2.15	1.32	1.37
31	DP	1001	CYC	C4B-NB	-2.15	1.33	1.38
29	gB	203	PEB	C1B-C2B	2.15	1.50	1.45
29	gM	203	PEB	C1B-C2B	2.15	1.50	1.45
29	WJ	203	PEB	C2A-C1A	-2.15	1.50	1.52
29	WL	203	PEB	C2A-C1A	-2.15	1.50	1.52
31	xP	1001	CYC	CBA-CGA	2.15	1.55	1.50
31	K1	1001	CYC	C4B-NB	-2.15	1.33	1.38
31	KK	1001	CYC	C4B-NB	-2.15	1.33	1.38
31	D7	1001	CYC	C1A-NA	-2.15	1.34	1.38
31	D9	1001	CYC	C1A-NA	-2.15	1.34	1.38
31	pP	1001	CYC	OB-C4B	2.15	1.27	1.23
29	N2	203	PEB	C4A-NA	-2.15	1.32	1.37
29	UB	202	PEB	C4A-NA	-2.15	1.32	1.37
29	MQ	401	PEB	C4A-NA	-2.15	1.32	1.37
29	cB	203	PEB	C1B-C2B	2.14	1.50	1.45
29	cM	203	PEB	C1B-C2B	2.14	1.50	1.45
31	lP	1001	CYC	OB-C4B	2.14	1.27	1.23
31	eP	1001	CYC	OB-C4B	2.14	1.27	1.23
31	F7	1001	CYC	C1B-C2B	2.14	1.49	1.45
29	SJ	202	PEB	C2A-C1A	-2.14	1.50	1.52
29	SL	202	PEB	C2A-C1A	-2.14	1.50	1.52
29	GA	201	PEB	C4A-NA	-2.14	1.32	1.37
29	GN	201	PEB	C4A-NA	-2.14	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q1	202	PEB	C4A-NA	-2.14	1.32	1.37
29	QK	202	PEB	C4A-NA	-2.14	1.32	1.37
31	AP	1001	CYC	OB-C4B	2.14	1.27	1.23
29	xJ	302	PEB	C4B-C3B	2.14	1.49	1.45
29	TB	203	PEB	C4A-NA	-2.14	1.32	1.37
29	TM	203	PEB	C4A-NA	-2.14	1.32	1.37
29	IC	202	PEB	C1D-ND	2.14	1.49	1.45
29	IE	202	PEB	C1D-ND	2.14	1.49	1.45
29	f7	201	PEB	CHA-C4A	-2.14	1.32	1.36
29	f9	201	PEB	CHA-C4A	-2.14	1.32	1.36
29	W2	202	PEB	C1C-CHB	2.14	1.49	1.41
29	IG	201	PEB	C4A-NA	-2.14	1.32	1.37
29	GJ	202	PEB	C4A-NA	-2.14	1.32	1.37
29	GL	202	PEB	C4A-NA	-2.14	1.32	1.37
29	IQ	201	PEB	C4A-NA	-2.14	1.32	1.37
31	iP	1001	CYC	OB-C4B	2.14	1.27	1.23
29	I5	203	PEB	C4A-NA	-2.14	1.32	1.37
29	B8	203	PEB	C4A-NA	-2.14	1.32	1.37
29	I8	203	PEB	C4A-NA	-2.14	1.32	1.37
30	A1	304	PUB	C4B-CHB	2.14	1.49	1.41
30	AK	304	PUB	C4B-CHB	2.14	1.49	1.41
31	fP	1001	CYC	C4B-NB	-2.14	1.33	1.38
29	SB	202	PEB	C2A-C1A	-2.14	1.50	1.52
29	SM	202	PEB	C2A-C1A	-2.14	1.50	1.52
31	J7	1001	CYC	C1B-C2B	2.14	1.49	1.45
29	D3	201	PEB	C4B-C3B	2.14	1.49	1.45
29	DO	201	PEB	C4B-C3B	2.14	1.49	1.45
29	ZB	203	PEB	C4A-NA	-2.14	1.32	1.37
29	ZM	203	PEB	C4A-NA	-2.14	1.32	1.37
29	WB	202	PEB	C4A-NA	-2.14	1.32	1.37
29	WM	202	PEB	C4A-NA	-2.14	1.32	1.37
31	vP	1001	CYC	OB-C4B	2.14	1.27	1.23
31	1P	1001	CYC	C4B-NB	-2.14	1.33	1.38
31	J9	1001	CYC	C1B-C2B	2.14	1.49	1.45
29	S2	202	PEB	C1C-CHB	2.14	1.49	1.41
29	LB	203	PEB	C4A-NA	-2.14	1.32	1.37
29	LM	203	PEB	C4A-NA	-2.14	1.32	1.37
29	VB	201	PEB	C4A-NA	-2.14	1.32	1.37
29	EJ	202	PEB	C4A-NA	-2.14	1.32	1.37
29	EL	202	PEB	C4A-NA	-2.14	1.32	1.37
29	VM	201	PEB	C4A-NA	-2.14	1.32	1.37
31	M1	1001	CYC	C4B-NB	-2.14	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	MK	1001	CYC	C4B-NB	-2.14	1.33	1.38
31	PP	1001	CYC	OB-C4B	2.14	1.27	1.23
29	U2	202	PEB	C1C-CHB	2.14	1.49	1.41
31	GP	1001	CYC	OB-C4B	2.14	1.27	1.23
29	CJ	202	PEB	C4A-NA	-2.14	1.32	1.37
29	CL	202	PEB	C4A-NA	-2.14	1.32	1.37
29	G4	202	PEB	CHA-C4A	-2.14	1.32	1.36
29	UR	202	PEB	C1C-CHB	2.14	1.49	1.41
31	uP	1001	CYC	C4B-NB	-2.14	1.33	1.38
29	I3	202	PEB	C4B-C3B	2.14	1.49	1.45
29	IO	202	PEB	C4B-C3B	2.14	1.49	1.45
29	JB	203	PEB	C1B-C2B	2.14	1.50	1.45
29	JM	203	PEB	C1B-C2B	2.14	1.50	1.45
29	AC	203	PEB	C1C-CHB	2.14	1.49	1.41
29	AE	203	PEB	C1C-CHB	2.14	1.49	1.41
29	h1	202	PEB	C4A-NA	-2.14	1.32	1.37
29	YB	203	PEB	C4A-NA	-2.14	1.32	1.37
29	hK	202	PEB	C4A-NA	-2.14	1.32	1.37
29	YM	203	PEB	C4A-NA	-2.14	1.32	1.37
31	D7	1001	CYC	C4B-NB	-2.14	1.33	1.38
31	D9	1001	CYC	C4B-NB	-2.14	1.33	1.38
29	RB	203	PEB	C1B-C2B	2.14	1.50	1.45
29	RM	203	PEB	C1B-C2B	2.14	1.50	1.45
29	NB	201	PEB	C4A-NA	-2.14	1.32	1.37
29	NM	201	PEB	C4A-NA	-2.14	1.32	1.37
29	FC	202	PEB	C1C-CHB	2.14	1.49	1.41
29	FE	202	PEB	C1C-CHB	2.14	1.49	1.41
29	Q2	202	PEB	C1C-CHB	2.13	1.49	1.41
29	I4	203	PEB	C2A-C1A	-2.13	1.50	1.52
29	XB	202	PEB	C1B-C2B	2.13	1.50	1.45
29	XM	202	PEB	C1B-C2B	2.13	1.50	1.45
29	mJ	202	PEB	C2A-C1A	-2.13	1.50	1.52
29	mL	202	PEB	C2A-C1A	-2.13	1.50	1.52
31	GK	1001	CYC	C4B-NB	-2.13	1.33	1.38
29	Y1	201	PEB	OD-C4D	2.13	1.27	1.23
29	YK	201	PEB	OD-C4D	2.13	1.27	1.23
29	ID	202	PEB	CHA-C4A	-2.13	1.32	1.36
29	F5	202	PEB	C4A-NA	-2.13	1.32	1.37
31	D7	1001	CYC	C1B-C2B	2.13	1.48	1.45
31	D9	1001	CYC	C1B-C2B	2.13	1.48	1.45
31	JF	1001	CYC	C1D-CHD	2.13	1.49	1.41
31	JI	1001	CYC	C1D-CHD	2.13	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	WP	1001	CYC	C1A-C2A	2.13	1.49	1.45
29	AC	202	PEB	C1D-ND	2.13	1.49	1.45
29	AE	202	PEB	C1D-ND	2.13	1.49	1.45
31	LF	1001	CYC	C1D-CHD	2.13	1.49	1.41
31	LI	1001	CYC	C1D-CHD	2.13	1.49	1.41
31	RP	1001	CYC	OB-C4B	2.13	1.27	1.23
31	cP	1001	CYC	OB-C4B	2.13	1.27	1.23
30	AM	304	PUB	C1C-NC	-2.13	1.34	1.38
31	HP	1001	CYC	C4B-NB	-2.13	1.33	1.38
29	E4	202	PEB	CHA-C4A	-2.13	1.32	1.36
31	EP	1001	CYC	OB-C4B	2.13	1.27	1.23
29	ED	201	PEB	CHA-C4A	-2.13	1.32	1.36
31	SP	1001	CYC	C4B-NB	-2.13	1.33	1.38
31	F9	1001	CYC	C4B-NB	-2.13	1.33	1.38
31	hP	1001	CYC	C4B-NB	-2.13	1.33	1.38
29	KB	202	PEB	C4A-NA	-2.13	1.32	1.37
29	KM	202	PEB	C4A-NA	-2.13	1.32	1.37
29	LC	202	PEB	C1C-CHB	2.13	1.49	1.41
29	LE	202	PEB	C1C-CHB	2.13	1.49	1.41
29	GG	201	PEB	C4A-NA	-2.13	1.32	1.37
29	GQ	201	PEB	C4A-NA	-2.13	1.32	1.37
29	TF	201	PEB	C4B-C3B	2.13	1.49	1.45
29	g7	203	PEB	C1C-CHB	2.13	1.49	1.41
29	g9	203	PEB	C1C-CHB	2.13	1.49	1.41
29	B3	202	PEB	C4A-NA	-2.13	1.32	1.37
29	BO	202	PEB	C4A-NA	-2.13	1.32	1.37
31	QP	1001	CYC	C4B-NB	-2.13	1.33	1.38
31	L7	1001	CYC	C1B-C2B	2.13	1.48	1.45
31	HF	1001	CYC	C1D-CHD	2.13	1.49	1.41
31	HI	1001	CYC	C1D-CHD	2.13	1.49	1.41
31	J7	1001	CYC	C1A-NA	-2.13	1.34	1.38
29	PB	202	PEB	C4A-NA	-2.13	1.32	1.37
29	iB	203	PEB	C4A-NA	-2.13	1.32	1.37
29	PM	202	PEB	C4A-NA	-2.13	1.32	1.37
29	iM	203	PEB	C4A-NA	-2.13	1.32	1.37
29	PB	202	PEB	C1B-C2B	2.13	1.50	1.45
29	PM	202	PEB	C1B-C2B	2.13	1.50	1.45
31	FF	1001	CYC	C1D-CHD	2.13	1.49	1.41
31	FI	1001	CYC	C1D-CHD	2.13	1.49	1.41
29	GD	202	PEB	CHA-C4A	-2.13	1.32	1.36
29	k7	203	PEB	C1C-CHB	2.13	1.49	1.41
29	m7	203	PEB	C1C-CHB	2.13	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	k9	203	PEB	C1C-CHB	2.13	1.49	1.41
29	m9	203	PEB	C1C-CHB	2.13	1.49	1.41
29	gJ	202	PEB	C4A-NA	-2.12	1.32	1.37
29	gL	202	PEB	C4A-NA	-2.12	1.32	1.37
31	IP	1001	CYC	C4B-NB	-2.12	1.33	1.38
29	dB	202	PEB	C2A-C1A	-2.12	1.50	1.52
29	dM	202	PEB	C2A-C1A	-2.12	1.50	1.52
31	rP	1001	CYC	OB-C4B	2.12	1.27	1.23
31	nP	1001	CYC	C4B-NB	-2.12	1.33	1.38
29	HC	202	PEB	C1C-CHB	2.12	1.49	1.41
29	HE	202	PEB	C1C-CHB	2.12	1.49	1.41
31	GP	1001	CYC	C4A-C3A	2.12	1.50	1.45
29	wJ	302	PEB	C4A-NA	-2.12	1.32	1.37
29	T7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	T9	203	PEB	C1C-CHB	2.12	1.49	1.41
31	NP	1001	CYC	OB-C4B	2.12	1.27	1.23
29	a7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	a9	203	PEB	C1C-CHB	2.12	1.49	1.41
29	H5	203	PEB	C4A-NA	-2.12	1.32	1.37
29	zL	501	PEB	C4A-NA	-2.12	1.32	1.37
31	XP	1001	CYC	C4B-NB	-2.12	1.33	1.38
29	A1	302	PEB	C4A-NA	-2.12	1.32	1.37
29	AK	302	PEB	C4A-NA	-2.12	1.32	1.37
29	xJ	301	PEB	C4B-C3B	2.12	1.49	1.45
29	DB	203	PEB	C1B-C2B	2.12	1.50	1.45
29	DM	203	PEB	C1B-C2B	2.12	1.50	1.45
29	gI	201	PEB	OD-C4D	2.12	1.27	1.23
29	gK	201	PEB	OD-C4D	2.12	1.27	1.23
31	rP	1001	CYC	C4A-C3A	2.12	1.50	1.45
29	wJ	303	PEB	C1C-CHB	2.12	1.49	1.41
31	qP	1001	CYC	C4B-NB	-2.12	1.33	1.38
29	V7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	V9	203	PEB	C1C-CHB	2.12	1.49	1.41
29	i7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	i9	203	PEB	C1C-CHB	2.12	1.49	1.41
29	FB	203	PEB	C1B-C2B	2.12	1.50	1.45
29	FM	203	PEB	C1B-C2B	2.12	1.50	1.45
29	MB	202	PEB	C2A-C1A	-2.12	1.50	1.52
29	MM	202	PEB	C2A-C1A	-2.12	1.50	1.52
29	R7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	R9	203	PEB	C1C-CHB	2.12	1.49	1.41
29	VB	203	PEB	C1B-C2B	2.12	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	VM	203	PEB	C1B-C2B	2.12	1.50	1.45
29	k7	203	PEB	C4A-NA	-2.12	1.32	1.37
29	k9	203	PEB	C4A-NA	-2.12	1.32	1.37
29	KJ	202	PEB	C4A-NA	-2.12	1.32	1.37
29	KL	202	PEB	C4A-NA	-2.12	1.32	1.37
31	wP	1001	CYC	C4B-NB	-2.12	1.33	1.38
30	AB	304	PUB	C1C-NC	-2.12	1.34	1.38
31	L7	1001	CYC	C1A-NA	-2.12	1.34	1.38
29	qJ	202	PEB	C4A-NA	-2.12	1.32	1.37
29	qL	202	PEB	C4A-NA	-2.12	1.32	1.37
31	J9	1001	CYC	C4B-NB	-2.12	1.33	1.38
31	EP	1001	CYC	C4A-C3A	2.12	1.50	1.45
29	e7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	e9	203	PEB	C1C-CHB	2.12	1.49	1.41
29	P7	203	PEB	C1C-CHB	2.12	1.49	1.41
29	P9	203	PEB	C1C-CHB	2.12	1.49	1.41
30	MG	402	PUB	CMB-C2B	2.12	1.56	1.51
31	J9	1001	CYC	C1A-NA	-2.12	1.34	1.38
29	HB	203	PEB	C1B-C2B	2.12	1.50	1.45
29	HM	203	PEB	C1B-C2B	2.12	1.50	1.45
31	iP	1001	CYC	C4A-C3A	2.12	1.50	1.45
31	NF	1001	CYC	C1D-CHD	2.12	1.49	1.41
31	NI	1001	CYC	C1D-CHD	2.12	1.49	1.41
29	BC	202	PEB	C4A-NA	-2.12	1.32	1.37
29	BE	202	PEB	C4A-NA	-2.12	1.32	1.37
31	kP	1001	CYC	C4B-NB	-2.12	1.33	1.38
29	UJ	202	PEB	C2A-C1A	-2.12	1.50	1.52
29	UL	202	PEB	C2A-C1A	-2.12	1.50	1.52
31	E1	1001	CYC	C4B-NB	-2.12	1.33	1.38
31	DF	1001	CYC	C1D-CHD	2.12	1.49	1.41
31	DI	1001	CYC	C1D-CHD	2.12	1.49	1.41
31	C1	1001	CYC	C4B-NB	-2.11	1.33	1.38
29	i7	203	PEB	C2A-C1A	-2.11	1.50	1.52
29	i9	203	PEB	C2A-C1A	-2.11	1.50	1.52
29	IJ	202	PEB	C2A-C1A	-2.11	1.50	1.52
29	IL	202	PEB	C2A-C1A	-2.11	1.50	1.52
31	jP	1001	CYC	C4B-NB	-2.11	1.33	1.38
29	c7	203	PEB	C1C-CHB	2.11	1.49	1.41
29	c9	203	PEB	C1C-CHB	2.11	1.49	1.41
29	KC	201	PEB	C1C-CHB	2.11	1.49	1.41
29	KE	201	PEB	C1C-CHB	2.11	1.49	1.41
29	g7	203	PEB	O1B-CGB	2.11	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g9	203	PEB	O1B-CGB	2.11	1.29	1.22
29	F3	201	PEB	C4B-C3B	2.11	1.49	1.45
29	FO	201	PEB	C4B-C3B	2.11	1.49	1.45
31	F9	1001	CYC	C1B-C2B	2.11	1.48	1.45
31	H7	1001	CYC	C4B-NB	-2.11	1.33	1.38
31	H9	1001	CYC	C4B-NB	-2.11	1.33	1.38
31	CP	1001	CYC	OB-C4B	2.11	1.27	1.23
29	H8	203	PEB	C4A-NA	-2.11	1.32	1.37
29	k7	203	PEB	O1B-CGB	2.11	1.29	1.22
29	k9	203	PEB	O1B-CGB	2.11	1.29	1.22
29	MA	404	PEB	C4B-NB	-2.11	1.34	1.38
31	OP	1001	CYC	C4B-NB	-2.11	1.33	1.38
29	sJ	202	PEB	C2A-C1A	-2.11	1.50	1.52
29	sL	202	PEB	C2A-C1A	-2.11	1.50	1.52
29	Y7	203	PEB	C1C-CHB	2.11	1.49	1.41
29	Y9	203	PEB	C1C-CHB	2.11	1.49	1.41
31	gP	1001	CYC	C4A-C3A	2.11	1.50	1.45
31	pP	1001	CYC	C4A-C3A	2.11	1.50	1.45
29	AC	203	PEB	C4A-NA	-2.11	1.32	1.37
29	AE	203	PEB	C4A-NA	-2.11	1.32	1.37
29	BC	202	PEB	C1C-CHB	2.11	1.49	1.41
29	BE	202	PEB	C1C-CHB	2.11	1.49	1.41
29	KG	201	PEB	C4A-NA	-2.11	1.32	1.37
29	KQ	201	PEB	C4A-NA	-2.11	1.32	1.37
31	CP	1001	CYC	C4A-C3A	2.11	1.50	1.45
29	R7	203	PEB	O1B-CGB	2.11	1.29	1.22
29	R9	203	PEB	O1B-CGB	2.11	1.29	1.22
29	F5	203	PEB	C4A-NA	-2.11	1.32	1.37
29	F8	203	PEB	C4A-NA	-2.11	1.32	1.37
29	CG	201	PEB	C4A-NA	-2.11	1.32	1.37
29	CQ	201	PEB	C4A-NA	-2.11	1.32	1.37
29	J3	201	PEB	C4B-C3B	2.11	1.49	1.45
29	JO	201	PEB	C4B-C3B	2.11	1.49	1.45
29	xL	303	PEB	C1C-CHB	2.11	1.49	1.41
31	F7	1001	CYC	C4B-NB	-2.11	1.33	1.38
29	AM	301	PEB	C4A-NA	-2.11	1.32	1.37
29	I4	202	PEB	CHA-C4A	-2.11	1.32	1.36
31	JP	1001	CYC	OB-C4B	2.11	1.27	1.23
31	KP	1001	CYC	C4A-C3A	2.11	1.50	1.45
31	tP	1001	CYC	C4A-C3A	2.11	1.50	1.45
29	iJ	202	PEB	C2A-C1A	-2.11	1.50	1.52
29	iL	202	PEB	C2A-C1A	-2.11	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	cP	1001	CYC	C4A-C3A	2.11	1.50	1.45
29	BA	203	PEB	C2A-C1A	-2.10	1.50	1.52
29	BN	203	PEB	C2A-C1A	-2.10	1.50	1.52
31	L7	1001	CYC	C4B-NB	-2.10	1.33	1.38
31	F9	1001	CYC	C1A-NA	-2.10	1.34	1.38
29	Y7	203	PEB	O1B-CGB	2.10	1.29	1.22
29	Y9	203	PEB	O1B-CGB	2.10	1.29	1.22
29	E3	202	PEB	C4A-NA	-2.10	1.32	1.37
29	L5	203	PEB	C4A-NA	-2.10	1.32	1.37
29	EO	202	PEB	C4A-NA	-2.10	1.32	1.37
29	MN	404	PEB	C1B-C2B	2.10	1.50	1.45
31	RP	1001	CYC	C4A-C3A	2.10	1.50	1.45
29	F3	202	PEB	C4A-NA	-2.10	1.32	1.37
29	FO	202	PEB	C4A-NA	-2.10	1.32	1.37
29	M4	202	PEB	CHA-C4A	-2.10	1.32	1.36
31	IK	1001	CYC	C4B-NB	-2.10	1.33	1.38
29	wL	303	PEB	C1C-CHB	2.10	1.49	1.41
31	NP	1001	CYC	C4A-C3A	2.10	1.50	1.45
31	AP	1001	CYC	C4A-C3A	2.10	1.50	1.45
31	mP	1001	CYC	C4A-C3A	2.10	1.50	1.45
29	L4	201	PEB	C3A-C4A	-2.10	1.47	1.50
30	yJ	302	PUB	OD-C4D	2.10	1.27	1.23
30	yL	302	PUB	OD-C4D	2.10	1.27	1.23
29	T7	203	PEB	C4A-NA	-2.10	1.32	1.37
29	T9	203	PEB	C4A-NA	-2.10	1.32	1.37
31	N7	1001	CYC	C1A-NA	-2.10	1.34	1.38
31	N9	1001	CYC	C1A-NA	-2.10	1.34	1.38
29	c7	203	PEB	O1B-CGB	2.10	1.29	1.22
29	c9	203	PEB	O1B-CGB	2.10	1.29	1.22
29	KC	201	PEB	C4A-NA	-2.10	1.32	1.37
29	KE	201	PEB	C4A-NA	-2.10	1.32	1.37
31	N7	1001	CYC	C1B-C2B	2.10	1.48	1.45
31	N9	1001	CYC	C1B-C2B	2.10	1.48	1.45
29	m7	203	PEB	C4A-NA	-2.10	1.32	1.37
29	m9	203	PEB	C4A-NA	-2.10	1.32	1.37
31	TP	1001	CYC	C4A-C3A	2.10	1.50	1.45
31	J7	1001	CYC	C4B-NB	-2.10	1.33	1.38
29	H3	201	PEB	C4B-C3B	2.10	1.49	1.45
29	HO	201	PEB	C4B-C3B	2.10	1.49	1.45
29	hB	202	PEB	C2A-C1A	-2.10	1.50	1.52
29	gJ	202	PEB	C2A-C1A	-2.10	1.50	1.52
29	gL	202	PEB	C2A-C1A	-2.10	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	hM	202	PEB	C2A-C1A	-2.10	1.50	1.52
29	M3	202	PEB	C4A-NA	-2.10	1.32	1.37
29	MO	202	PEB	C4A-NA	-2.10	1.32	1.37
29	a7	203	PEB	O1B-CGB	2.10	1.29	1.22
29	a9	203	PEB	O1B-CGB	2.10	1.29	1.22
31	eP	1001	CYC	C4A-C3A	2.10	1.50	1.45
29	EG	201	PEB	C4A-NA	-2.10	1.32	1.37
29	EQ	201	PEB	C4A-NA	-2.10	1.32	1.37
31	EK	1001	CYC	C4B-NB	-2.10	1.33	1.38
29	i7	203	PEB	O1B-CGB	2.09	1.29	1.22
29	m7	203	PEB	O1B-CGB	2.09	1.29	1.22
29	i9	203	PEB	O1B-CGB	2.09	1.29	1.22
29	m9	203	PEB	O1B-CGB	2.09	1.29	1.22
29	T7	203	PEB	O1B-CGB	2.09	1.29	1.22
29	T9	203	PEB	O1B-CGB	2.09	1.29	1.22
29	P7	203	PEB	O1B-CGB	2.09	1.29	1.22
29	P9	203	PEB	O1B-CGB	2.09	1.29	1.22
29	AB	301	PEB	C4A-NA	-2.09	1.32	1.37
29	wL	302	PEB	C4B-C3B	2.09	1.49	1.45
31	F7	1001	CYC	C1A-NA	-2.09	1.34	1.38
29	C4	202	PEB	CHA-C4A	-2.09	1.32	1.36
29	CD	202	PEB	CHA-C4A	-2.09	1.32	1.36
29	L3	202	PEB	C4A-NA	-2.09	1.33	1.37
29	LO	202	PEB	C4A-NA	-2.09	1.33	1.37
31	N7	1001	CYC	C4B-NB	-2.09	1.33	1.38
31	N9	1001	CYC	C4B-NB	-2.09	1.33	1.38
29	V7	203	PEB	C4A-NA	-2.09	1.33	1.37
29	V9	203	PEB	C4A-NA	-2.09	1.33	1.37
29	jB	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	jM	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	V7	203	PEB	O1B-CGB	2.09	1.29	1.22
29	V9	203	PEB	O1B-CGB	2.09	1.29	1.22
31	L9	1001	CYC	C4B-NB	-2.09	1.33	1.38
29	G5	203	PEB	C4A-NA	-2.09	1.33	1.37
29	B5	203	PEB	C4A-NA	-2.09	1.33	1.37
29	zJ	501	PEB	C4A-NA	-2.09	1.33	1.37
29	NO	202	PEB	C4A-NA	-2.09	1.33	1.37
29	EJ	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	EL	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	F4	201	PEB	C3A-C4A	-2.09	1.47	1.50
29	HG	201	PEB	C4A-NA	-2.09	1.33	1.37
29	HQ	201	PEB	C4A-NA	-2.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q2	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	E4	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	OR	202	PEB	C2A-C1A	-2.09	1.50	1.52
29	S2	201	PEB	C4B-C3B	2.09	1.49	1.45
29	e7	203	PEB	C2A-C1A	-2.08	1.50	1.52
29	g7	203	PEB	C2A-C1A	-2.08	1.50	1.52
29	e9	203	PEB	C2A-C1A	-2.08	1.50	1.52
29	g9	203	PEB	C2A-C1A	-2.08	1.50	1.52
30	MA	403	PUB	C1C-NC	-2.08	1.34	1.38
29	I3	202	PEB	C4A-NA	-2.08	1.33	1.37
29	IO	202	PEB	C4A-NA	-2.08	1.33	1.37
29	MN	404	PEB	C4B-NB	-2.08	1.34	1.38
31	H7	1001	CYC	C1A-NA	-2.08	1.34	1.38
31	H9	1001	CYC	C1A-NA	-2.08	1.34	1.38
29	xL	301	PEB	C4B-C3B	2.08	1.49	1.45
29	xJ	303	PEB	C1C-CHB	2.08	1.49	1.41
29	C3	202	PEB	C4A-NA	-2.08	1.33	1.37
29	CO	202	PEB	C4A-NA	-2.08	1.33	1.37
29	e7	203	PEB	O1B-CGB	2.08	1.29	1.22
29	e9	203	PEB	O1B-CGB	2.08	1.29	1.22
29	EB	201	PEB	OD-C4D	2.08	1.27	1.23
29	EM	201	PEB	OD-C4D	2.08	1.27	1.23
29	FC	202	PEB	C4A-NA	-2.08	1.33	1.37
29	FE	202	PEB	C4A-NA	-2.08	1.33	1.37
29	G3	202	PEB	C1C-CHB	2.08	1.49	1.41
29	GO	202	PEB	C1C-CHB	2.08	1.49	1.41
29	dB	201	PEB	OD-C4D	2.08	1.27	1.23
29	dM	201	PEB	OD-C4D	2.08	1.27	1.23
29	MG	405	PEB	C2A-C1A	-2.08	1.50	1.52
29	KJ	202	PEB	C2A-C1A	-2.08	1.50	1.52
29	KL	202	PEB	C2A-C1A	-2.08	1.50	1.52
29	I3	202	PEB	C1C-CHB	2.08	1.49	1.41
29	IO	202	PEB	C1C-CHB	2.08	1.49	1.41
29	K3	202	PEB	C4A-NA	-2.08	1.33	1.37
29	KO	202	PEB	C4A-NA	-2.08	1.33	1.37
31	PP	1001	CYC	C4A-C3A	2.08	1.50	1.45
31	1P	1002	CYC	C1D-CHD	2.08	1.49	1.41
29	xL	302	PEB	C4B-C3B	2.08	1.49	1.45
29	L8	203	PEB	C4A-NA	-2.08	1.33	1.37
29	k7	203	PEB	C2A-C1A	-2.08	1.50	1.52
29	k9	203	PEB	C2A-C1A	-2.08	1.50	1.52
29	GD	202	PEB	C2A-C1A	-2.08	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	MA	404	PEB	C1B-C2B	2.08	1.50	1.45
29	A3	202	PEB	C4A-NA	-2.08	1.33	1.37
29	AO	202	PEB	C4A-NA	-2.08	1.33	1.37
29	qJ	202	PEB	C2A-C1A	-2.08	1.50	1.52
29	qL	202	PEB	C2A-C1A	-2.08	1.50	1.52
30	MN	403	PUB	C1C-NC	-2.07	1.34	1.38
29	S7	202	PEB	C4A-NA	-2.07	1.33	1.37
29	S9	202	PEB	C4A-NA	-2.07	1.33	1.37
29	j7	202	PEB	C4A-NA	-2.07	1.33	1.37
29	j9	202	PEB	C4A-NA	-2.07	1.33	1.37
31	I1	1001	CYC	C4B-NB	-2.07	1.33	1.38
29	P7	203	PEB	C4A-NA	-2.07	1.33	1.37
29	G8	203	PEB	C4A-NA	-2.07	1.33	1.37
29	P9	203	PEB	C4A-NA	-2.07	1.33	1.37
29	IC	201	PEB	C4A-NA	-2.07	1.33	1.37
29	IE	201	PEB	C4A-NA	-2.07	1.33	1.37
31	JP	1001	CYC	C4A-C3A	2.07	1.50	1.45
29	OB	201	PEB	OD-C4D	2.07	1.27	1.23
29	OM	201	PEB	OD-C4D	2.07	1.27	1.23
29	N3	202	PEB	C4A-NA	-2.07	1.33	1.37
31	IP	1001	CYC	C4A-C3A	2.07	1.50	1.45
29	CC	201	PEB	C4A-NA	-2.07	1.33	1.37
29	CE	201	PEB	C4A-NA	-2.07	1.33	1.37
30	MQ	404	PUB	CMB-C2B	2.07	1.55	1.51
29	aB	201	PEB	OD-C4D	2.07	1.27	1.23
29	aM	201	PEB	OD-C4D	2.07	1.27	1.23
31	CK	1001	CYC	C4B-NB	-2.07	1.33	1.38
29	D3	203	PEB	C4A-NA	-2.07	1.33	1.37
29	DO	203	PEB	C4A-NA	-2.07	1.33	1.37
29	JD	201	PEB	C3A-C4A	-2.07	1.47	1.50
29	wJ	302	PEB	C4B-C3B	2.07	1.49	1.45
30	xL	305	PUB	C4C-NC	2.07	1.38	1.35
29	wJ	301	PEB	C4B-C3B	2.07	1.49	1.45
29	B3	203	PEB	C4A-NA	-2.07	1.33	1.37
29	BO	203	PEB	C4A-NA	-2.07	1.33	1.37
29	g7	203	PEB	C4A-NA	-2.07	1.33	1.37
29	g9	203	PEB	C4A-NA	-2.07	1.33	1.37
29	H4	201	PEB	C3A-C4A	-2.07	1.47	1.50
29	CD	202	PEB	C2A-C1A	-2.07	1.50	1.52
29	K4	202	PEB	CHA-C4A	-2.07	1.32	1.36
29	KD	202	PEB	CHA-C4A	-2.07	1.32	1.36
29	wL	301	PEB	C4B-C3B	2.06	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LC	202	PEB	C4A-NA	-2.06	1.33	1.37
29	LE	202	PEB	C4A-NA	-2.06	1.33	1.37
29	K3	202	PEB	C1C-CHB	2.06	1.49	1.41
29	KO	202	PEB	C1C-CHB	2.06	1.49	1.41
29	T2	201	PEB	C1C-CHB	2.06	1.49	1.41
31	YP	1000	CYC	C1D-CHD	2.06	1.49	1.41
29	H3	203	PEB	C4A-NA	-2.06	1.33	1.37
29	HO	203	PEB	C4A-NA	-2.06	1.33	1.37
29	A3	202	PEB	C1C-CHB	2.06	1.49	1.41
29	AO	202	PEB	C1C-CHB	2.06	1.49	1.41
29	MD	202	PEB	CHA-C4A	-2.06	1.32	1.36
29	C3	202	PEB	C1C-CHB	2.06	1.49	1.41
29	E3	202	PEB	C1C-CHB	2.06	1.49	1.41
29	CO	202	PEB	C1C-CHB	2.06	1.49	1.41
29	EO	202	PEB	C1C-CHB	2.06	1.49	1.41
29	hB	201	PEB	OD-C4D	2.06	1.27	1.23
29	hM	201	PEB	OD-C4D	2.06	1.27	1.23
29	IC	201	PEB	C4B-C3B	2.06	1.49	1.45
29	IE	201	PEB	C4B-C3B	2.06	1.49	1.45
29	KB	201	PEB	OD-C4D	2.06	1.27	1.23
29	KM	201	PEB	OD-C4D	2.06	1.27	1.23
29	J4	201	PEB	C3A-C4A	-2.06	1.47	1.50
29	J3	203	PEB	C4A-NA	-2.06	1.33	1.37
29	JO	203	PEB	C4A-NA	-2.06	1.33	1.37
29	YB	202	PEB	OD-C4D	2.06	1.27	1.23
29	YM	202	PEB	OD-C4D	2.06	1.27	1.23
29	aJ	202	PEB	C2A-C1A	-2.06	1.50	1.52
29	aL	202	PEB	C2A-C1A	-2.06	1.50	1.52
29	jB	201	PEB	OD-C4D	2.06	1.27	1.23
29	jM	201	PEB	OD-C4D	2.06	1.27	1.23
29	wL	303	PEB	C4B-C3B	2.06	1.49	1.45
29	QB	203	PEB	OD-C4D	2.06	1.27	1.23
29	QM	203	PEB	OD-C4D	2.06	1.27	1.23
29	DG	201	PEB	C4A-NA	-2.06	1.33	1.37
29	DQ	201	PEB	C4A-NA	-2.06	1.33	1.37
29	EC	201	PEB	C4A-NA	-2.06	1.33	1.37
29	EE	201	PEB	C4A-NA	-2.06	1.33	1.37
29	QR	202	PEB	C2A-C1A	-2.06	1.50	1.52
31	vP	1001	CYC	C4A-C3A	2.06	1.50	1.45
29	F3	203	PEB	C4A-NA	-2.06	1.33	1.37
29	b7	202	PEB	C4A-NA	-2.06	1.33	1.37
29	b9	202	PEB	C4A-NA	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	FO	203	PEB	C4A-NA	-2.06	1.33	1.37
29	RR	201	PEB	C1C-CHB	2.06	1.49	1.41
29	a7	203	PEB	C2A-C1A	-2.06	1.50	1.52
29	a9	203	PEB	C2A-C1A	-2.06	1.50	1.52
29	YJ	202	PEB	C2A-C1A	-2.06	1.50	1.52
29	YL	202	PEB	C2A-C1A	-2.06	1.50	1.52
29	e7	203	PEB	C4A-NA	-2.06	1.33	1.37
29	e9	203	PEB	C4A-NA	-2.06	1.33	1.37
29	R2	201	PEB	C1C-CHB	2.05	1.49	1.41
29	V2	201	PEB	C1C-CHB	2.05	1.49	1.41
29	VR	201	PEB	C1C-CHB	2.05	1.49	1.41
29	a7	203	PEB	C4A-NA	-2.05	1.33	1.37
29	a9	203	PEB	C4A-NA	-2.05	1.33	1.37
29	TR	201	PEB	C1C-CHB	2.05	1.49	1.41
29	HC	202	PEB	C4A-NA	-2.05	1.33	1.37
29	HE	202	PEB	C4A-NA	-2.05	1.33	1.37
29	KD	202	PEB	C2A-C1A	-2.05	1.50	1.52
29	KC	202	PEB	C4A-NA	-2.05	1.33	1.37
29	KE	202	PEB	C4A-NA	-2.05	1.33	1.37
29	h7	202	PEB	C4A-NA	-2.05	1.33	1.37
29	h9	202	PEB	C4A-NA	-2.05	1.33	1.37
31	DF	1001	CYC	C1B-C2B	2.05	1.48	1.45
31	DI	1001	CYC	C1B-C2B	2.05	1.48	1.45
29	CB	201	PEB	OD-C4D	2.05	1.27	1.23
29	CM	201	PEB	OD-C4D	2.05	1.27	1.23
29	R7	203	PEB	C4A-NA	-2.05	1.33	1.37
29	R9	203	PEB	C4A-NA	-2.05	1.33	1.37
30	AF	302	PUB	C3C-C4C	2.05	1.50	1.43
30	AI	302	PUB	C3C-C4C	2.05	1.50	1.43
29	A9	304	PEB	C2A-C1A	-2.05	1.50	1.52
29	AJ	202	PEB	C2A-C1A	-2.05	1.50	1.52
29	AL	202	PEB	C2A-C1A	-2.05	1.50	1.52
29	BG	201	PEB	C4A-NA	-2.05	1.33	1.37
29	FG	201	PEB	C4A-NA	-2.05	1.33	1.37
29	BQ	201	PEB	C4A-NA	-2.05	1.33	1.37
29	FQ	201	PEB	C4A-NA	-2.05	1.33	1.37
29	FD	201	PEB	C3A-C4A	-2.05	1.47	1.50
31	LF	1001	CYC	C4A-C3A	2.05	1.50	1.45
31	LI	1001	CYC	C4A-C3A	2.05	1.50	1.45
30	MQ	405	PUB	C1C-C2C	2.05	1.49	1.45
29	G3	202	PEB	C4A-NA	-2.05	1.33	1.37
29	GO	202	PEB	C4A-NA	-2.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	JJ	202	PEB	C4B-NB	-2.05	1.34	1.38
29	JL	202	PEB	C4B-NB	-2.05	1.34	1.38
29	UB	201	PEB	OD-C4D	2.04	1.27	1.23
29	UM	201	PEB	OD-C4D	2.04	1.27	1.23
31	AP	1001	CYC	C4C-NC	-2.04	1.33	1.37
29	MQ	403	PEB	CHA-C4A	-2.04	1.32	1.36
29	CJ	202	PEB	C2A-C1A	-2.04	1.50	1.52
29	CL	202	PEB	C2A-C1A	-2.04	1.50	1.52
29	LD	201	PEB	C3A-C4A	-2.04	1.47	1.50
29	MG	404	PEB	C4A-NA	-2.04	1.33	1.37
29	wL	302	PEB	C1B-C2B	2.04	1.50	1.45
29	e2	402	PEB	C1C-CHB	2.04	1.49	1.41
29	XR	201	PEB	C1C-CHB	2.04	1.49	1.41
29	pJ	202	PEB	C4B-NB	-2.04	1.34	1.38
29	pL	202	PEB	C4B-NB	-2.04	1.34	1.38
29	NO	203	PEB	C1B-C2B	2.04	1.50	1.45
29	Y7	203	PEB	C4A-NA	-2.04	1.33	1.37
29	Y9	203	PEB	C4A-NA	-2.04	1.33	1.37
29	SB	201	PEB	OD-C4D	2.04	1.27	1.23
29	SM	201	PEB	OD-C4D	2.04	1.27	1.23
29	OJ	202	PEB	C2A-C1A	-2.04	1.50	1.52
29	OL	202	PEB	C2A-C1A	-2.04	1.50	1.52
29	c7	203	PEB	C4A-NA	-2.04	1.33	1.37
29	c9	203	PEB	C4A-NA	-2.04	1.33	1.37
29	MQ	406	PEB	C4A-NA	-2.04	1.33	1.37
29	N2	201	PEB	C1C-CHB	2.04	1.49	1.41
29	TJ	202	PEB	C4B-NB	-2.04	1.34	1.38
29	TL	202	PEB	C4B-NB	-2.04	1.34	1.38
29	WR	201	PEB	C4B-NB	-2.04	1.34	1.38
29	fB	201	PEB	OD-C4D	2.04	1.27	1.23
29	fM	201	PEB	OD-C4D	2.04	1.27	1.23
29	PJ	202	PEB	C4B-NB	-2.04	1.34	1.38
29	PL	202	PEB	C4B-NB	-2.04	1.34	1.38
31	JF	1001	CYC	C4A-C3A	2.04	1.50	1.45
31	JI	1001	CYC	C4A-C3A	2.04	1.50	1.45
29	SR	201	PEB	C1C-CHB	2.04	1.49	1.41
29	MG	401	PEB	CHA-C4A	-2.04	1.32	1.36
29	Z7	202	PEB	C4A-NA	-2.04	1.33	1.37
29	Z9	202	PEB	C4A-NA	-2.04	1.33	1.37
31	GP	1001	CYC	C4C-NC	-2.04	1.33	1.37
29	M4	202	PEB	C2A-C1A	-2.03	1.50	1.52
29	C3	201	PEB	C1B-C2B	2.03	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	CO	201	PEB	C1B-C2B	2.03	1.50	1.45
29	D4	201	PEB	C1C-CHB	2.03	1.49	1.41
31	HF	1001	CYC	C1B-C2B	2.03	1.48	1.45
31	HI	1001	CYC	C1B-C2B	2.03	1.48	1.45
29	xJ	302	PEB	C1B-C2B	2.03	1.50	1.45
29	cJ	202	PEB	C2A-C1A	-2.03	1.50	1.52
29	cL	202	PEB	C2A-C1A	-2.03	1.50	1.52
31	M7	1001	CYC	C4D-CHA	2.03	1.49	1.41
30	MG	403	PUB	C1C-C2C	2.03	1.48	1.45
29	bJ	202	PEB	C4B-NB	-2.03	1.34	1.38
29	bL	202	PEB	C4B-NB	-2.03	1.34	1.38
29	E3	201	PEB	C1B-C2B	2.03	1.50	1.45
29	G3	201	PEB	C1B-C2B	2.03	1.50	1.45
29	EO	201	PEB	C1B-C2B	2.03	1.50	1.45
29	GO	201	PEB	C1B-C2B	2.03	1.50	1.45
29	i7	203	PEB	C4A-NA	-2.03	1.33	1.37
29	i9	203	PEB	C4A-NA	-2.03	1.33	1.37
31	yP	1001	CYC	C4A-C3A	2.03	1.50	1.45
29	JG	201	PEB	C4A-NA	-2.03	1.33	1.37
29	JQ	201	PEB	C4A-NA	-2.03	1.33	1.37
29	BD	201	PEB	C3A-C4A	-2.03	1.47	1.50
29	AB	303	PEB	C4A-NA	-2.03	1.33	1.37
29	MG	405	PEB	C4A-NA	-2.03	1.33	1.37
31	C7	1001	CYC	C4D-CHA	2.03	1.49	1.41
31	C9	1001	CYC	C4D-CHA	2.03	1.49	1.41
29	R7	203	PEB	C2A-C1A	-2.03	1.50	1.52
29	R9	203	PEB	C2A-C1A	-2.03	1.50	1.52
29	xL	302	PEB	C1B-C2B	2.03	1.50	1.45
29	P7	203	PEB	C2A-C1A	-2.03	1.50	1.52
29	P9	203	PEB	C2A-C1A	-2.03	1.50	1.52
29	MR	202	PEB	C1C-CHB	2.03	1.49	1.41
29	NJ	202	PEB	C4B-NB	-2.03	1.34	1.38
29	NL	202	PEB	C4B-NB	-2.03	1.34	1.38
29	kJ	202	PEB	C2A-C1A	-2.03	1.50	1.52
29	kL	202	PEB	C2A-C1A	-2.03	1.50	1.52
29	GC	201	PEB	C4A-NA	-2.03	1.33	1.37
29	GE	201	PEB	C4A-NA	-2.03	1.33	1.37
29	wJ	303	PEB	C4B-C3B	2.03	1.48	1.45
30	xJ	305	PUB	C4C-NC	2.03	1.38	1.35
29	KA	202	PEB	C4A-NA	-2.03	1.33	1.37
29	KN	202	PEB	C4A-NA	-2.03	1.33	1.37
29	IC	202	PEB	C4A-NA	-2.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	IE	202	PEB	C4A-NA	-2.03	1.33	1.37
29	DC	201	PEB	C4A-NA	-2.03	1.33	1.37
29	DE	201	PEB	C4A-NA	-2.03	1.33	1.37
29	P2	201	PEB	C2A-C1A	-2.03	1.50	1.52
29	T7	203	PEB	C2A-C1A	-2.03	1.50	1.52
29	T9	203	PEB	C2A-C1A	-2.03	1.50	1.52
29	JD	201	PEB	C1C-CHB	2.03	1.49	1.41
29	W2	201	PEB	C4B-NB	-2.03	1.34	1.38
29	DC	201	PEB	C1C-CHB	2.03	1.49	1.41
29	DE	201	PEB	C1C-CHB	2.03	1.49	1.41
29	K4	202	PEB	C2A-C1A	-2.03	1.50	1.52
29	ED	201	PEB	C2A-C1A	-2.03	1.50	1.52
31	1P	1001	CYC	C1B-NB	-2.03	1.34	1.37
30	QB	201	PUB	C3C-C4C	2.03	1.50	1.43
30	QM	201	PUB	C3C-C4C	2.03	1.50	1.43
29	dJ	202	PEB	C4B-NB	-2.03	1.34	1.38
29	dL	202	PEB	C4B-NB	-2.03	1.34	1.38
29	TF	201	PEB	C1C-CHB	2.03	1.49	1.41
29	IB	201	PEB	OD-C4D	2.02	1.27	1.23
29	IM	201	PEB	OD-C4D	2.02	1.27	1.23
29	Q7	202	PEB	C4A-NA	-2.02	1.33	1.37
29	Q9	202	PEB	C4A-NA	-2.02	1.33	1.37
31	cP	1001	CYC	C4C-NC	-2.02	1.33	1.37
29	HC	201	PEB	C4A-NA	-2.02	1.33	1.37
29	HE	201	PEB	C4A-NA	-2.02	1.33	1.37
31	FF	1001	CYC	C4A-C3A	2.02	1.50	1.45
31	FI	1001	CYC	C4A-C3A	2.02	1.50	1.45
31	WP	1001	CYC	C4A-C3A	2.02	1.50	1.45
29	LD	201	PEB	C1C-CHB	2.02	1.49	1.41
29	H3	202	PEB	C1C-CHB	2.02	1.49	1.41
29	FD	201	PEB	C1C-CHB	2.02	1.49	1.41
29	HO	202	PEB	C1C-CHB	2.02	1.49	1.41
31	M9	1001	CYC	C4D-CHA	2.02	1.49	1.41
29	EG	202	PEB	C2A-C1A	-2.02	1.50	1.52
29	EQ	202	PEB	C2A-C1A	-2.02	1.50	1.52
29	MA	405	PEB	C1D-ND	2.02	1.48	1.45
31	E7	1001	CYC	C4D-CHA	2.02	1.49	1.41
31	E9	1001	CYC	C4D-CHA	2.02	1.49	1.41
31	tP	1001	CYC	C4C-NC	-2.02	1.33	1.37
29	NR	201	PEB	C1C-CHB	2.02	1.49	1.41
29	uJ	201	PEB	C4B-NB	-2.02	1.34	1.38
29	uL	201	PEB	C4B-NB	-2.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	GJ	202	PEB	C2A-C1A	-2.02	1.50	1.52
29	GL	202	PEB	C2A-C1A	-2.02	1.50	1.52
29	rJ	202	PEB	C4B-NB	-2.02	1.34	1.38
29	rL	202	PEB	C4B-NB	-2.02	1.34	1.38
29	AM	303	PEB	C4A-NA	-2.02	1.33	1.37
29	a1	202	PEB	C4A-NA	-2.02	1.33	1.37
29	aK	202	PEB	C4A-NA	-2.02	1.33	1.37
29	MQ	407	PEB	C2A-C1A	-2.02	1.50	1.52
29	HC	201	PEB	C1C-CHB	2.02	1.48	1.41
29	HE	201	PEB	C1C-CHB	2.02	1.48	1.41
31	FF	1001	CYC	C1B-C2B	2.02	1.48	1.45
31	FI	1001	CYC	C1B-C2B	2.02	1.48	1.45
29	HD	201	PEB	C3A-C4A	-2.02	1.47	1.50
29	H4	201	PEB	C1C-CHB	2.02	1.48	1.41
29	lB	201	PEB	OD-C4D	2.02	1.27	1.23
29	lM	201	PEB	OD-C4D	2.02	1.27	1.23
29	QR	201	PEB	C4B-NB	-2.02	1.34	1.38
29	WB	201	PEB	OD-C4D	2.02	1.27	1.23
29	WM	201	PEB	OD-C4D	2.02	1.27	1.23
31	NF	1001	CYC	C1B-C2B	2.02	1.48	1.45
31	NI	1001	CYC	C1B-C2B	2.02	1.48	1.45
29	xJ	303	PEB	C4B-C3B	2.02	1.48	1.45
29	LG	201	PEB	C4A-NA	-2.02	1.33	1.37
29	MQ	402	PEB	C4A-NA	-2.02	1.33	1.37
31	NF	1001	CYC	C4A-C3A	2.02	1.50	1.45
31	NI	1001	CYC	C4A-C3A	2.02	1.50	1.45
29	d7	202	PEB	C4A-NA	-2.02	1.33	1.37
29	d9	202	PEB	C4A-NA	-2.02	1.33	1.37
29	GB	201	PEB	OD-C4D	2.02	1.27	1.23
29	GM	201	PEB	OD-C4D	2.02	1.27	1.23
29	W7	202	PEB	C4A-NA	-2.02	1.33	1.37
29	W9	202	PEB	C4A-NA	-2.02	1.33	1.37
31	iP	1001	CYC	C4C-NC	-2.02	1.33	1.37
29	J4	201	PEB	C1C-CHB	2.02	1.48	1.41
29	f7	202	PEB	C4A-NA	-2.02	1.33	1.37
29	f9	202	PEB	C4A-NA	-2.02	1.33	1.37
29	AA	202	PEB	C4A-NA	-2.02	1.33	1.37
29	AN	202	PEB	C4A-NA	-2.02	1.33	1.37
31	I7	1001	CYC	C4D-CHA	2.02	1.48	1.41
31	I9	1001	CYC	C4D-CHA	2.02	1.48	1.41
29	HJ	201	PEB	C4B-NB	-2.02	1.34	1.38
29	HL	201	PEB	C4B-NB	-2.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V1	202	PEB	C4A-NA	-2.02	1.33	1.37
29	VK	202	PEB	C4A-NA	-2.02	1.33	1.37
29	B4	201	PEB	C3A-C4A	-2.02	1.47	1.50
29	U7	202	PEB	C4A-NA	-2.02	1.33	1.37
29	U9	202	PEB	C4A-NA	-2.02	1.33	1.37
31	G7	1001	CYC	C4D-CHA	2.02	1.48	1.41
31	G9	1001	CYC	C4D-CHA	2.02	1.48	1.41
31	RP	1001	CYC	C4C-NC	-2.02	1.33	1.37
29	P1	202	PEB	C4A-NA	-2.01	1.33	1.37
29	PK	202	PEB	C4A-NA	-2.01	1.33	1.37
31	K7	1001	CYC	C4D-CHA	2.01	1.48	1.41
29	R1	202	PEB	C4A-NA	-2.01	1.33	1.37
29	RK	202	PEB	C4A-NA	-2.01	1.33	1.37
29	S2	201	PEB	C1C-CHB	2.01	1.48	1.41
29	DD	201	PEB	C1C-CHB	2.01	1.48	1.41
29	O7	202	PEB	C4A-NA	-2.01	1.33	1.37
29	O9	202	PEB	C4A-NA	-2.01	1.33	1.37
29	KC	202	PEB	C4B-C3B	2.01	1.48	1.45
29	KE	202	PEB	C4B-C3B	2.01	1.48	1.45
29	wJ	302	PEB	C1B-C2B	2.01	1.50	1.45
30	wJ	305	PUB	C4C-NC	2.01	1.38	1.35
31	JP	1001	CYC	C4C-NC	-2.01	1.33	1.37
31	NP	1001	CYC	C4C-NC	-2.01	1.33	1.37
29	FJ	202	PEB	C4B-NB	-2.01	1.34	1.38
29	FL	202	PEB	C4B-NB	-2.01	1.34	1.38
29	DO	202	PEB	C4A-NA	-2.01	1.33	1.37
29	IJ	202	PEB	C4B-NB	-2.01	1.34	1.38
29	IL	202	PEB	C4B-NB	-2.01	1.34	1.38
29	wL	303	PEB	C4A-NA	-2.01	1.33	1.37
29	m7	203	PEB	C2A-C1A	-2.01	1.50	1.52
29	m9	203	PEB	C2A-C1A	-2.01	1.50	1.52
29	EC	202	PEB	C4A-NA	-2.01	1.33	1.37
29	EE	202	PEB	C4A-NA	-2.01	1.33	1.37
29	JC	201	PEB	C1C-CHB	2.01	1.48	1.41
29	JE	201	PEB	C1C-CHB	2.01	1.48	1.41
29	BJ	202	PEB	C4B-NB	-2.01	1.34	1.38
29	BL	202	PEB	C4B-NB	-2.01	1.34	1.38
29	B4	201	PEB	C1C-CHB	2.01	1.48	1.41
31	IK	1001	CYC	C1B-C2B	2.01	1.48	1.45
29	FC	201	PEB	C1C-CHB	2.01	1.48	1.41
29	FE	201	PEB	C1C-CHB	2.01	1.48	1.41
29	CA	202	PEB	C4A-NA	-2.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	CN	202	PEB	C4A-NA	-2.01	1.33	1.37
29	k1	202	PEB	C4A-NA	-2.01	1.33	1.37
29	FC	201	PEB	C4A-NA	-2.01	1.33	1.37
29	FE	201	PEB	C4A-NA	-2.01	1.33	1.37
29	kK	202	PEB	C4A-NA	-2.01	1.33	1.37
30	A1	305	PUB	C1A-NA	2.01	1.37	1.35
30	AK	305	PUB	C1A-NA	2.01	1.37	1.35
29	MQ	403	PEB	C1D-ND	2.01	1.48	1.45
31	LF	1001	CYC	C1B-C2B	2.01	1.48	1.45
31	LI	1001	CYC	C1B-C2B	2.01	1.48	1.45
29	L7	1002	PEB	CMD-C2D	-2.01	1.47	1.50
29	HD	201	PEB	C1C-CHB	2.01	1.48	1.41
29	UR	201	PEB	C4B-NB	-2.01	1.34	1.38
29	MB	201	PEB	OD-C4D	2.01	1.27	1.23
29	MM	201	PEB	OD-C4D	2.01	1.27	1.23
29	LC	201	PEB	C1C-CHB	2.00	1.48	1.41
29	LE	201	PEB	C1C-CHB	2.00	1.48	1.41
29	U1	201	PEB	C4A-NA	-2.00	1.33	1.37
29	UK	201	PEB	C4A-NA	-2.00	1.33	1.37
29	BC	201	PEB	C1C-CHB	2.00	1.48	1.41
29	BE	201	PEB	C1C-CHB	2.00	1.48	1.41
29	rJ	201	PEB	C1C-CHB	2.00	1.48	1.41
29	rL	201	PEB	C1C-CHB	2.00	1.48	1.41
29	e1	202	PEB	C4A-NA	-2.00	1.33	1.37
29	g1	202	PEB	C4A-NA	-2.00	1.33	1.37
29	eK	202	PEB	C4A-NA	-2.00	1.33	1.37
29	gK	202	PEB	C4A-NA	-2.00	1.33	1.37
29	M3	203	PEB	C1B-C2B	2.00	1.50	1.45
29	MO	203	PEB	C1B-C2B	2.00	1.50	1.45
29	BD	201	PEB	C1C-CHB	2.00	1.48	1.41
31	K9	1001	CYC	C4D-CHA	2.00	1.48	1.41
29	sJ	203	PEB	C4B-NB	-2.00	1.34	1.38
29	sL	203	PEB	C4B-NB	-2.00	1.34	1.38
29	JA	203	PEB	C4A-NA	-2.00	1.33	1.37
29	JN	203	PEB	C4A-NA	-2.00	1.33	1.37
29	j1	203	PEB	C4A-NA	-2.00	1.33	1.37
29	jK	203	PEB	C4A-NA	-2.00	1.33	1.37
29	I3	201	PEB	C1B-C2B	2.00	1.50	1.45
29	IO	201	PEB	C1B-C2B	2.00	1.50	1.45
31	HF	1001	CYC	C4A-C3A	2.00	1.50	1.45
31	HI	1001	CYC	C4A-C3A	2.00	1.50	1.45
29	jJ	202	PEB	C4B-NB	-2.00	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	jL	202	PEB	C4B-NB	-2.00	1.34	1.38
29	dJ	201	PEB	C1C-CHB	2.00	1.48	1.41
29	dL	201	PEB	C1C-CHB	2.00	1.48	1.41
31	vP	1001	CYC	C4C-NC	-2.00	1.33	1.37
29	MN	405	PEB	C1D-ND	2.00	1.48	1.45
29	O2	201	PEB	C4B-NB	-2.00	1.34	1.38
29	OR	201	PEB	C4B-NB	-2.00	1.34	1.38
29	wJ	303	PEB	C4A-NA	-2.00	1.33	1.37
29	DO	202	PEB	C1C-CHB	2.00	1.48	1.41

All (23317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A1	305	PUB	CBA-CAA-C3A	-16.33	88.22	112.98
30	AK	305	PUB	CBA-CAA-C3A	-16.33	88.22	112.98
30	A1	305	PUB	C2A-C1A-NA	14.04	119.67	107.21
30	AK	305	PUB	C2A-C1A-NA	14.04	119.67	107.21
30	wL	305	PUB	C2A-C1A-NA	12.40	118.21	107.21
30	xL	305	PUB	C2A-C1A-NA	12.38	118.19	107.21
30	wJ	305	PUB	C2A-C1A-NA	12.33	118.15	107.21
30	xJ	305	PUB	C2A-C1A-NA	12.31	118.13	107.21
29	ZJ	201	PEB	OA-C1A-C2A	-12.23	116.45	126.17
29	ZL	201	PEB	OA-C1A-C2A	-12.23	116.45	126.17
29	hJ	201	PEB	OA-C1A-C2A	-12.20	116.47	126.17
29	hL	201	PEB	OA-C1A-C2A	-12.20	116.47	126.17
29	NJ	201	PEB	OA-C1A-C2A	-12.19	116.48	126.17
29	NL	201	PEB	OA-C1A-C2A	-12.19	116.48	126.17
29	nJ	201	PEB	OA-C1A-C2A	-12.19	116.48	126.17
29	vJ	201	PEB	OA-C1A-C2A	-12.19	116.48	126.17
29	nL	201	PEB	OA-C1A-C2A	-12.19	116.48	126.17
29	vL	201	PEB	OA-C1A-C2A	-12.19	116.48	126.17
29	lJ	201	PEB	OA-C1A-C2A	-12.18	116.48	126.17
29	lL	201	PEB	OA-C1A-C2A	-12.18	116.48	126.17
29	RJ	201	PEB	OA-C1A-C2A	-12.18	116.49	126.17
29	RL	201	PEB	OA-C1A-C2A	-12.18	116.49	126.17
29	VJ	201	PEB	OA-C1A-C2A	-12.18	116.49	126.17
29	VL	201	PEB	OA-C1A-C2A	-12.18	116.49	126.17
29	LJ	201	PEB	OA-C1A-C2A	-12.17	116.50	126.17
29	dJ	201	PEB	OA-C1A-C2A	-12.17	116.50	126.17
29	LL	201	PEB	OA-C1A-C2A	-12.17	116.50	126.17
29	dL	201	PEB	OA-C1A-C2A	-12.17	116.50	126.17
29	BJ	201	PEB	OA-C1A-C2A	-12.16	116.51	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	fJ	201	PEB	OA-C1A-C2A	-12.16	116.51	126.17
29	BL	201	PEB	OA-C1A-C2A	-12.16	116.51	126.17
29	fL	201	PEB	OA-C1A-C2A	-12.16	116.51	126.17
29	TJ	201	PEB	OA-C1A-C2A	-12.15	116.51	126.17
29	TL	201	PEB	OA-C1A-C2A	-12.15	116.51	126.17
29	bJ	201	PEB	OA-C1A-C2A	-12.15	116.51	126.17
29	bL	201	PEB	OA-C1A-C2A	-12.15	116.51	126.17
29	JJ	201	PEB	OA-C1A-C2A	-12.14	116.52	126.17
29	pJ	201	PEB	OA-C1A-C2A	-12.14	116.52	126.17
29	JL	201	PEB	OA-C1A-C2A	-12.14	116.52	126.17
29	pL	201	PEB	OA-C1A-C2A	-12.14	116.52	126.17
29	FJ	201	PEB	OA-C1A-C2A	-12.13	116.53	126.17
29	FL	201	PEB	OA-C1A-C2A	-12.13	116.53	126.17
29	DJ	201	PEB	OA-C1A-C2A	-12.11	116.54	126.17
29	DL	201	PEB	OA-C1A-C2A	-12.11	116.54	126.17
29	rJ	201	PEB	OA-C1A-C2A	-12.11	116.54	126.17
29	rL	201	PEB	OA-C1A-C2A	-12.11	116.54	126.17
29	PJ	201	PEB	OA-C1A-C2A	-12.11	116.55	126.17
29	PL	201	PEB	OA-C1A-C2A	-12.11	116.55	126.17
29	tJ	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
29	tL	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
29	XJ	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
29	jJ	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
29	XL	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
29	jL	201	PEB	OA-C1A-C2A	-12.10	116.55	126.17
29	CA	202	PEB	CHB-C4B-NB	-11.81	112.44	128.83
29	CN	202	PEB	CHB-C4B-NB	-11.81	112.44	128.83
29	KA	202	PEB	CHB-C4B-NB	-11.79	112.48	128.83
29	KN	202	PEB	CHB-C4B-NB	-11.79	112.48	128.83
29	EA	202	PEB	CHB-C4B-NB	-11.79	112.48	128.83
29	EN	202	PEB	CHB-C4B-NB	-11.79	112.48	128.83
29	AA	202	PEB	CHB-C4B-NB	-11.77	112.50	128.83
29	AN	202	PEB	CHB-C4B-NB	-11.77	112.50	128.83
29	IA	202	PEB	CHB-C4B-NB	-11.76	112.52	128.83
29	IN	202	PEB	CHB-C4B-NB	-11.76	112.52	128.83
29	GA	202	PEB	CHB-C4B-NB	-11.73	112.56	128.83
29	GN	202	PEB	CHB-C4B-NB	-11.73	112.56	128.83
31	mP	1001	CYC	C3B-C4B-NB	11.64	116.18	106.78
31	AP	1001	CYC	C3B-C4B-NB	11.62	116.17	106.78
31	gP	1001	CYC	C3B-C4B-NB	11.62	116.16	106.78
31	PP	1001	CYC	C3B-C4B-NB	11.61	116.16	106.78
31	iP	1001	CYC	C3B-C4B-NB	11.61	116.16	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	tP	1001	CYC	C3B-C4B-NB	11.60	116.15	106.78
31	lP	1001	CYC	C3B-C4B-NB	11.60	116.15	106.78
31	JP	1001	CYC	C3B-C4B-NB	11.59	116.14	106.78
31	pP	1001	CYC	C3B-C4B-NB	11.59	116.14	106.78
31	vP	1001	CYC	C3B-C4B-NB	11.58	116.14	106.78
31	TP	1001	CYC	C3B-C4B-NB	11.58	116.13	106.78
31	NP	1001	CYC	C3B-C4B-NB	11.57	116.13	106.78
31	RP	1001	CYC	C3B-C4B-NB	11.57	116.12	106.78
31	KP	1001	CYC	C3B-C4B-NB	11.55	116.11	106.78
31	GP	1001	CYC	C3B-C4B-NB	11.55	116.11	106.78
31	rP	1001	CYC	C3B-C4B-NB	11.55	116.11	106.78
31	CP	1001	CYC	C3B-C4B-NB	11.54	116.11	106.78
31	EP	1001	CYC	C3B-C4B-NB	11.54	116.10	106.78
31	eP	1001	CYC	C3B-C4B-NB	11.52	116.09	106.78
31	cP	1001	CYC	C3B-C4B-NB	11.49	116.06	106.78
30	BB	302	PUB	C2A-C1A-NA	11.40	117.32	107.21
30	BM	302	PUB	C2A-C1A-NA	11.40	117.32	107.21
31	J9	1001	CYC	C3B-C4B-NB	11.22	115.84	106.78
31	N7	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
31	F9	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
31	N9	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
31	D7	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
31	D9	1001	CYC	C3B-C4B-NB	11.21	115.83	106.78
31	nP	1001	CYC	C3B-C4B-NB	11.20	115.83	106.78
31	F7	1001	CYC	C3B-C4B-NB	11.20	115.83	106.78
31	kP	1001	CYC	C3B-C4B-NB	11.19	115.82	106.78
31	H7	1001	CYC	C3B-C4B-NB	11.18	115.81	106.78
31	H9	1001	CYC	C3B-C4B-NB	11.18	115.81	106.78
31	QP	1001	CYC	C3B-C4B-NB	11.18	115.81	106.78
31	J7	1001	CYC	C3B-C4B-NB	11.18	115.81	106.78
31	oP	1001	CYC	C3B-C4B-NB	11.17	115.81	106.78
31	SP	1001	CYC	C3B-C4B-NB	11.17	115.80	106.78
31	lP	1001	CYC	C3B-C4B-NB	11.16	115.80	106.78
31	BP	1001	CYC	C3B-C4B-NB	11.16	115.79	106.78
31	HP	1001	CYC	C3B-C4B-NB	11.15	115.79	106.78
30	MQ	404	PUB	C2A-C1A-NA	11.15	117.10	107.21
31	jP	1001	CYC	C3B-C4B-NB	11.15	115.78	106.78
31	L7	1001	CYC	C3B-C4B-NB	11.14	115.78	106.78
31	hP	1001	CYC	C3B-C4B-NB	11.14	115.78	106.78
31	sP	1001	CYC	C3B-C4B-NB	11.13	115.77	106.78
31	MP	1001	CYC	C3B-C4B-NB	11.13	115.77	106.78
31	uP	1001	CYC	C3B-C4B-NB	11.13	115.77	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DP	1001	CYC	C3B-C4B-NB	11.13	115.77	106.78
31	fP	1001	CYC	C3B-C4B-NB	11.13	115.77	106.78
31	UP	1001	CYC	C3B-C4B-NB	11.12	115.76	106.78
31	FP	1001	CYC	C3B-C4B-NB	11.12	115.76	106.78
31	qP	1001	CYC	C3B-C4B-NB	11.12	115.76	106.78
31	OP	1001	CYC	C3B-C4B-NB	11.12	115.76	106.78
30	MG	402	PUB	C2A-C1A-NA	11.12	117.07	107.21
31	XP	1001	CYC	C3B-C4B-NB	11.11	115.76	106.78
31	L9	1001	CYC	C3B-C4B-NB	11.11	115.75	106.78
31	wP	1001	CYC	C3B-C4B-NB	11.10	115.75	106.78
30	MN	402	PUB	C2A-C1A-NA	11.10	117.06	107.21
31	IP	1001	CYC	C3B-C4B-NB	11.09	115.74	106.78
30	MA	402	PUB	C2A-C1A-NA	11.09	117.05	107.21
30	AF	302	PUB	C2A-C1A-NA	11.09	117.05	107.21
30	AI	302	PUB	C2A-C1A-NA	11.09	117.05	107.21
30	A7	303	PUB	C2A-C1A-NA	11.06	117.02	107.21
30	A9	303	PUB	C2A-C1A-NA	11.06	117.02	107.21
30	A7	302	PUB	C2A-C1A-NA	11.02	116.99	107.21
30	A9	302	PUB	C2A-C1A-NA	11.02	116.99	107.21
31	D1	1001	CYC	C3B-C4B-NB	10.97	115.64	106.78
31	LF	1001	CYC	C3B-C4B-NB	10.94	115.61	106.78
31	LI	1001	CYC	C3B-C4B-NB	10.94	115.61	106.78
31	NF	1001	CYC	C3B-C4B-NB	10.93	115.61	106.78
31	NI	1001	CYC	C3B-C4B-NB	10.93	115.61	106.78
31	FF	1001	CYC	C3B-C4B-NB	10.93	115.61	106.78
31	FI	1001	CYC	C3B-C4B-NB	10.93	115.61	106.78
31	HF	1001	CYC	C3B-C4B-NB	10.92	115.60	106.78
31	HI	1001	CYC	C3B-C4B-NB	10.92	115.60	106.78
30	AF	303	PUB	C2A-C1A-NA	10.92	116.89	107.21
30	AI	303	PUB	C2A-C1A-NA	10.92	116.89	107.21
30	MQ	404	PUB	CBB-CAB-C3B	10.91	131.24	112.62
31	F1	1001	CYC	C3B-C4B-NB	10.89	115.58	106.78
31	FK	1001	CYC	C3B-C4B-NB	10.89	115.58	106.78
31	DK	1001	CYC	C3B-C4B-NB	10.89	115.58	106.78
29	MQ	407	PEB	C1C-CHB-C4B	-10.89	115.81	128.81
31	JF	1001	CYC	C3B-C4B-NB	10.88	115.57	106.78
31	JI	1001	CYC	C3B-C4B-NB	10.88	115.57	106.78
31	NK	1001	CYC	C3B-C4B-NB	10.88	115.57	106.78
30	A1	304	PUB	C2A-C1A-NA	10.88	116.86	107.21
30	AK	304	PUB	C2A-C1A-NA	10.88	116.86	107.21
30	MG	402	PUB	CBB-CAB-C3B	10.87	131.18	112.62
31	J1	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	JK	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78
31	DF	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78
31	DI	1001	CYC	C3B-C4B-NB	10.87	115.56	106.78
31	GK	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
30	QB	201	PUB	C2A-C1A-NA	10.86	116.84	107.21
30	QM	201	PUB	C2A-C1A-NA	10.86	116.84	107.21
31	D1	1003	CYC	C3B-C4B-NB	10.86	115.55	106.78
31	M1	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
31	MK	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
31	L1	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
31	LK	1001	CYC	C3B-C4B-NB	10.86	115.55	106.78
29	MG	405	PEB	C1C-CHB-C4B	-10.85	115.85	128.81
30	xJ	304	PUB	C2A-C1A-NA	10.84	116.83	107.21
31	N1	1001	CYC	C3B-C4B-NB	10.84	115.54	106.78
30	MQ	405	PUB	C2A-C1A-NA	10.84	116.82	107.21
30	wJ	304	PUB	C2A-C1A-NA	10.83	116.81	107.21
31	E1	1001	CYC	C3B-C4B-NB	10.83	115.53	106.78
30	xL	304	PUB	C2A-C1A-NA	10.82	116.81	107.21
30	MG	403	PUB	C2A-C1A-NA	10.82	116.80	107.21
30	wL	304	PUB	C2A-C1A-NA	10.82	116.80	107.21
31	KF	1001	CYC	C3B-C4B-NB	10.81	115.51	106.78
31	HK	1001	CYC	C3B-C4B-NB	10.80	115.51	106.78
31	VP	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
31	EF	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
31	EI	1001	CYC	C3B-C4B-NB	10.80	115.50	106.78
29	MA	401	PEB	CHC-C1D-ND	-10.79	101.41	113.95
31	C1	1001	CYC	C3B-C4B-NB	10.79	115.50	106.78
31	K1	1001	CYC	C3B-C4B-NB	10.79	115.50	106.78
31	KK	1001	CYC	C3B-C4B-NB	10.79	115.50	106.78
31	I1	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
31	H1	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
31	IK	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
31	xP	1001	CYC	C3B-C4B-NB	10.79	115.49	106.78
29	MN	401	PEB	CHC-C1D-ND	-10.78	101.43	113.95
31	CF	1001	CYC	C3B-C4B-NB	10.77	115.48	106.78
31	CI	1001	CYC	C3B-C4B-NB	10.77	115.48	106.78
31	EK	1001	CYC	C3B-C4B-NB	10.77	115.48	106.78
31	CK	1001	CYC	C3B-C4B-NB	10.75	115.46	106.78
31	KI	1001	CYC	C3B-C4B-NB	10.75	115.46	106.78
30	MA	403	PUB	C2A-C1A-NA	10.75	116.74	107.21
31	MF	1001	CYC	C3B-C4B-NB	10.72	115.44	106.78
31	MI	1001	CYC	C3B-C4B-NB	10.72	115.44	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	GF	1001	CYC	C3B-C4B-NB	10.72	115.44	106.78
31	GI	1001	CYC	C3B-C4B-NB	10.72	115.44	106.78
30	MN	403	PUB	C2A-C1A-NA	10.70	116.70	107.21
31	IF	1001	CYC	C3B-C4B-NB	10.69	115.42	106.78
31	II	1001	CYC	C3B-C4B-NB	10.69	115.42	106.78
30	yJ	303	PUB	C2A-C1A-NA	10.66	116.67	107.21
30	yL	303	PUB	C2A-C1A-NA	10.63	116.64	107.21
29	FJ	202	PEB	CHC-C1D-ND	-10.61	101.62	113.95
29	FL	202	PEB	CHC-C1D-ND	-10.61	101.62	113.95
29	IJ	203	PEB	CHC-C1D-ND	-10.60	101.63	113.95
29	IL	203	PEB	CHC-C1D-ND	-10.60	101.63	113.95
29	HJ	201	PEB	CHC-C1D-ND	-10.60	101.64	113.95
29	HL	201	PEB	CHC-C1D-ND	-10.60	101.64	113.95
29	PJ	202	PEB	CHC-C1D-ND	-10.59	101.65	113.95
29	jJ	202	PEB	CHC-C1D-ND	-10.59	101.65	113.95
29	PL	202	PEB	CHC-C1D-ND	-10.59	101.65	113.95
29	jL	202	PEB	CHC-C1D-ND	-10.59	101.65	113.95
29	JJ	202	PEB	CHC-C1D-ND	-10.59	101.65	113.95
29	JL	202	PEB	CHC-C1D-ND	-10.59	101.65	113.95
29	bJ	202	PEB	CHC-C1D-ND	-10.59	101.66	113.95
29	bL	202	PEB	CHC-C1D-ND	-10.59	101.66	113.95
29	BJ	202	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	BL	202	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	lJ	202	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	rJ	202	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	lL	202	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	rL	202	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	AJ	203	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	AL	203	PEB	CHC-C1D-ND	-10.58	101.66	113.95
29	pJ	202	PEB	CHC-C1D-ND	-10.58	101.67	113.95
29	pL	202	PEB	CHC-C1D-ND	-10.58	101.67	113.95
29	TJ	202	PEB	CHC-C1D-ND	-10.58	101.67	113.95
29	TL	202	PEB	CHC-C1D-ND	-10.58	101.67	113.95
29	RJ	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	RL	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	ZJ	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	ZL	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	fJ	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	fL	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	dJ	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	sJ	203	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	dL	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	sL	203	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	NJ	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	NL	202	PEB	CHC-C1D-ND	-10.57	101.67	113.95
29	XJ	202	PEB	CHC-C1D-ND	-10.56	101.68	113.95
29	XL	202	PEB	CHC-C1D-ND	-10.56	101.68	113.95
29	uJ	201	PEB	CHC-C1D-ND	-10.56	101.69	113.95
29	uL	201	PEB	CHC-C1D-ND	-10.56	101.69	113.95
29	hJ	202	PEB	CHC-C1D-ND	-10.55	101.69	113.95
29	hL	202	PEB	CHC-C1D-ND	-10.55	101.69	113.95
29	nJ	202	PEB	CHC-C1D-ND	-10.55	101.69	113.95
29	nL	202	PEB	CHC-C1D-ND	-10.55	101.69	113.95
31	yP	1001	CYC	C3B-C4B-NB	10.55	115.30	106.78
31	WP	1001	CYC	C3B-C4B-NB	10.54	115.29	106.78
29	WJ	201	PEB	CHC-C1D-ND	-10.52	101.73	113.95
29	WL	201	PEB	CHC-C1D-ND	-10.52	101.73	113.95
30	AB	305	PUB	C2A-C1A-NA	10.52	116.54	107.21
29	J5	201	PEB	CMB-C2B-C1B	10.52	141.26	125.06
29	J8	201	PEB	CMB-C2B-C1B	10.52	141.26	125.06
31	1P	1002	CYC	C3B-C4B-NB	10.50	115.26	106.78
30	AM	305	PUB	C2A-C1A-NA	10.48	116.50	107.21
31	YP	1000	CYC	C3B-C4B-NB	10.47	115.24	106.78
31	G7	1001	CYC	C3B-C4B-NB	10.32	115.11	106.78
31	G9	1001	CYC	C3B-C4B-NB	10.32	115.11	106.78
31	M9	1001	CYC	C3B-C4B-NB	10.31	115.11	106.78
31	I7	1001	CYC	C3B-C4B-NB	10.31	115.11	106.78
31	I9	1001	CYC	C3B-C4B-NB	10.31	115.11	106.78
31	E7	1001	CYC	C3B-C4B-NB	10.31	115.11	106.78
31	E9	1001	CYC	C3B-C4B-NB	10.31	115.11	106.78
31	M7	1001	CYC	C3B-C4B-NB	10.30	115.10	106.78
31	K7	1001	CYC	C3B-C4B-NB	10.28	115.08	106.78
31	K9	1001	CYC	C3B-C4B-NB	10.28	115.08	106.78
31	C7	1001	CYC	C3B-C4B-NB	10.24	115.05	106.78
31	C9	1001	CYC	C3B-C4B-NB	10.24	115.05	106.78
30	yJ	302	PUB	C2A-C1A-NA	10.20	116.26	107.21
30	yL	302	PUB	C2A-C1A-NA	10.20	116.26	107.21
30	AB	304	PUB	C2A-C1A-NA	10.17	116.23	107.21
30	AM	304	PUB	C2A-C1A-NA	10.15	116.22	107.21
30	xJ	305	PUB	CBA-CAA-C3A	-9.82	98.08	112.98
30	xL	305	PUB	CBA-CAA-C3A	-9.80	98.11	112.98
30	wJ	305	PUB	CBA-CAA-C3A	-9.79	98.13	112.98
30	BB	302	PUB	CAD-C3D-C4D	9.76	136.80	121.38
30	BM	302	PUB	CAD-C3D-C4D	9.76	136.80	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	wL	305	PUB	CBA-CAA-C3A	-9.76	98.18	112.98
30	yJ	302	PUB	OD-C4D-C3D	-9.56	117.67	128.04
30	yL	302	PUB	OD-C4D-C3D	-9.56	117.67	128.04
30	MG	402	PUB	CHA-C4A-NA	-9.19	103.27	113.95
30	MQ	404	PUB	CHA-C4A-NA	-9.15	103.32	113.95
29	MG	405	PEB	CHB-C4B-NB	-9.00	116.34	128.83
29	MQ	407	PEB	CHB-C4B-NB	-8.98	116.37	128.83
30	MA	403	PUB	CBA-CAA-C3A	-8.78	99.67	112.98
30	MN	403	PUB	CBA-CAA-C3A	-8.78	99.67	112.98
29	F4	201	PEB	CHB-C4B-NB	-8.51	117.03	128.83
29	JD	201	PEB	CHB-C4B-NB	-8.50	117.03	128.83
29	H4	201	PEB	CHB-C4B-NB	-8.49	117.05	128.83
29	L4	201	PEB	CHB-C4B-NB	-8.48	117.06	128.83
29	J4	201	PEB	CHB-C4B-NB	-8.48	117.06	128.83
29	HD	201	PEB	CHB-C4B-NB	-8.46	117.09	128.83
29	DD	201	PEB	CHB-C4B-NB	-8.46	117.09	128.83
29	LD	201	PEB	CHB-C4B-NB	-8.46	117.10	128.83
29	B4	201	PEB	CHB-C4B-NB	-8.45	117.10	128.83
29	BD	201	PEB	CHB-C4B-NB	-8.45	117.10	128.83
29	D4	201	PEB	CHB-C4B-NB	-8.45	117.11	128.83
29	FD	201	PEB	CHB-C4B-NB	-8.44	117.12	128.83
29	b1	202	PEB	CHB-C4B-NB	-8.37	117.22	128.83
29	bK	202	PEB	CHB-C4B-NB	-8.37	117.22	128.83
29	O1	202	PEB	CHB-C4B-NB	-8.37	117.22	128.83
29	l1	202	PEB	CHB-C4B-NB	-8.37	117.22	128.83
29	OK	202	PEB	CHB-C4B-NB	-8.37	117.22	128.83
29	lK	202	PEB	CHB-C4B-NB	-8.37	117.22	128.83
29	d1	202	PEB	CHB-C4B-NB	-8.36	117.23	128.83
29	dK	202	PEB	CHB-C4B-NB	-8.36	117.23	128.83
29	S1	202	PEB	CHB-C4B-NB	-8.36	117.23	128.83
29	SK	202	PEB	CHB-C4B-NB	-8.36	117.23	128.83
29	Z1	203	PEB	CHB-C4B-NB	-8.35	117.24	128.83
29	ZK	203	PEB	CHB-C4B-NB	-8.35	117.24	128.83
29	h1	202	PEB	CHB-C4B-NB	-8.35	117.24	128.83
29	hK	202	PEB	CHB-C4B-NB	-8.35	117.24	128.83
29	U1	203	PEB	CHB-C4B-NB	-8.35	117.25	128.83
29	UK	203	PEB	CHB-C4B-NB	-8.35	117.25	128.83
30	AM	304	PUB	CHC-C1D-ND	-8.35	103.16	113.72
29	j1	202	PEB	CHB-C4B-NB	-8.34	117.26	128.83
29	jK	202	PEB	CHB-C4B-NB	-8.34	117.26	128.83
30	AB	304	PUB	CHC-C1D-ND	-8.33	103.18	113.72
29	f1	202	PEB	CHB-C4B-NB	-8.33	117.27	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	fK	202	PEB	CHB-C4B-NB	-8.33	117.27	128.83
29	Q1	202	PEB	CHB-C4B-NB	-8.33	117.28	128.83
29	QK	202	PEB	CHB-C4B-NB	-8.33	117.28	128.83
29	W1	202	PEB	CHB-C4B-NB	-8.32	117.29	128.83
29	WK	202	PEB	CHB-C4B-NB	-8.32	117.29	128.83
31	xP	1001	CYC	CHD-C4C-NC	8.26	135.02	125.20
30	MN	402	PUB	CHA-C4A-NA	-8.25	104.37	113.95
31	VP	1001	CYC	CHD-C4C-NC	8.25	135.01	125.20
30	MA	402	PUB	CHA-C4A-NA	-8.25	104.37	113.95
29	Q1	202	PEB	C1C-CHB-C4B	-8.19	119.02	128.81
29	U1	203	PEB	C1C-CHB-C4B	-8.19	119.02	128.81
29	QK	202	PEB	C1C-CHB-C4B	-8.19	119.02	128.81
29	UK	203	PEB	C1C-CHB-C4B	-8.19	119.02	128.81
29	W1	202	PEB	C1C-CHB-C4B	-8.18	119.04	128.81
29	WK	202	PEB	C1C-CHB-C4B	-8.18	119.04	128.81
29	f1	202	PEB	C1C-CHB-C4B	-8.18	119.04	128.81
29	fK	202	PEB	C1C-CHB-C4B	-8.18	119.04	128.81
29	d1	202	PEB	C1C-CHB-C4B	-8.17	119.05	128.81
29	dK	202	PEB	C1C-CHB-C4B	-8.17	119.05	128.81
29	j1	202	PEB	C1C-CHB-C4B	-8.17	119.05	128.81
29	jK	202	PEB	C1C-CHB-C4B	-8.17	119.05	128.81
29	S1	202	PEB	C1C-CHB-C4B	-8.16	119.06	128.81
29	l1	202	PEB	C1C-CHB-C4B	-8.16	119.06	128.81
29	SK	202	PEB	C1C-CHB-C4B	-8.16	119.06	128.81
29	lK	202	PEB	C1C-CHB-C4B	-8.16	119.06	128.81
29	b1	202	PEB	C1C-CHB-C4B	-8.16	119.06	128.81
29	bK	202	PEB	C1C-CHB-C4B	-8.16	119.06	128.81
29	Z1	203	PEB	C1C-CHB-C4B	-8.16	119.07	128.81
29	ZK	203	PEB	C1C-CHB-C4B	-8.16	119.07	128.81
29	h1	202	PEB	C1C-CHB-C4B	-8.15	119.07	128.81
29	hK	202	PEB	C1C-CHB-C4B	-8.15	119.07	128.81
29	KD	202	PEB	CHC-C4C-C3C	-8.14	116.45	130.34
29	O1	202	PEB	C1C-CHB-C4B	-8.14	119.09	128.81
29	OK	202	PEB	C1C-CHB-C4B	-8.14	119.09	128.81
29	C4	202	PEB	CHC-C4C-C3C	-8.13	116.47	130.34
29	G4	202	PEB	CHC-C4C-C3C	-8.12	116.48	130.34
29	CD	202	PEB	CHC-C4C-C3C	-8.12	116.48	130.34
29	MD	202	PEB	CHC-C4C-C3C	-8.12	116.49	130.34
29	GD	202	PEB	CHC-C4C-C3C	-8.12	116.49	130.34
29	K4	202	PEB	CHC-C4C-C3C	-8.12	116.49	130.34
29	I4	202	PEB	CHC-C4C-C3C	-8.11	116.51	130.34
29	ED	201	PEB	CHC-C4C-C3C	-8.09	116.55	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ID	202	PEB	CHC-C4C-C3C	-8.08	116.55	130.34
29	M4	202	PEB	CHC-C4C-C3C	-8.08	116.56	130.34
30	MN	403	PUB	CHB-C1C-NC	-8.06	117.65	128.83
29	E4	202	PEB	CHC-C4C-C3C	-8.06	116.60	130.34
30	MA	403	PUB	CHB-C1C-NC	-8.01	117.72	128.83
29	uJ	201	PEB	CHC-C4C-C3C	-7.83	116.99	130.34
29	uL	201	PEB	CHC-C4C-C3C	-7.83	116.99	130.34
29	BJ	202	PEB	CHC-C4C-C3C	-7.82	117.01	130.34
29	BL	202	PEB	CHC-C4C-C3C	-7.82	117.01	130.34
29	pJ	202	PEB	CHC-C4C-C3C	-7.81	117.01	130.34
29	pL	202	PEB	CHC-C4C-C3C	-7.81	117.01	130.34
31	VP	1001	CYC	CHA-C1A-NA	-7.81	117.99	128.83
29	IJ	203	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	PJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	IJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	IL	203	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	PL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	IL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	ZJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	ZL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	AJ	203	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	FJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	JJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	NJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	AL	203	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	FL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	JL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	NL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	fJ	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	fL	202	PEB	CHC-C4C-C3C	-7.81	117.02	130.34
29	nJ	202	PEB	CHC-C4C-C3C	-7.80	117.03	130.34
29	nL	202	PEB	CHC-C4C-C3C	-7.80	117.03	130.34
29	RJ	202	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
29	RL	202	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
29	jJ	202	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
29	jL	202	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
29	rJ	202	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
29	rL	202	PEB	CHC-C4C-C3C	-7.80	117.04	130.34
29	XJ	202	PEB	CHC-C4C-C3C	-7.79	117.05	130.34
29	XL	202	PEB	CHC-C4C-C3C	-7.79	117.05	130.34
30	MA	403	PUB	CAD-C3D-C4D	7.78	133.68	121.38
30	MN	403	PUB	CAD-C3D-C4D	7.78	133.68	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WJ	201	PEB	CHC-C4C-C3C	-7.78	117.06	130.34
29	sJ	203	PEB	CHC-C4C-C3C	-7.78	117.06	130.34
29	WL	201	PEB	CHC-C4C-C3C	-7.78	117.06	130.34
29	sL	203	PEB	CHC-C4C-C3C	-7.78	117.06	130.34
29	bJ	202	PEB	CHC-C4C-C3C	-7.78	117.07	130.34
29	bL	202	PEB	CHC-C4C-C3C	-7.78	117.07	130.34
29	HJ	201	PEB	CHC-C4C-C3C	-7.78	117.07	130.34
29	HL	201	PEB	CHC-C4C-C3C	-7.78	117.07	130.34
29	dJ	202	PEB	CHC-C4C-C3C	-7.78	117.07	130.34
29	dL	202	PEB	CHC-C4C-C3C	-7.78	117.07	130.34
30	wL	304	PUB	CHC-C1D-ND	-7.78	103.88	113.72
29	TJ	202	PEB	CHC-C4C-C3C	-7.77	117.08	130.34
29	TL	202	PEB	CHC-C4C-C3C	-7.77	117.08	130.34
29	hJ	202	PEB	CHC-C4C-C3C	-7.77	117.09	130.34
29	hL	202	PEB	CHC-C4C-C3C	-7.77	117.09	130.34
31	xP	1001	CYC	CHA-C1A-NA	-7.76	118.07	128.83
30	wJ	304	PUB	CHC-C1D-ND	-7.74	103.93	113.72
30	xL	304	PUB	CHC-C1D-ND	-7.73	103.95	113.72
30	xJ	304	PUB	CHC-C1D-ND	-7.71	103.96	113.72
30	xJ	305	PUB	CAD-C3D-C4D	7.70	133.55	121.38
30	wJ	305	PUB	CAD-C3D-C4D	7.69	133.53	121.38
30	xL	305	PUB	CAD-C3D-C4D	7.69	133.52	121.38
30	wL	305	PUB	CAD-C3D-C4D	7.68	133.50	121.38
30	MN	403	PUB	CHC-C1D-ND	-7.66	104.04	113.72
30	MA	403	PUB	CHC-C1D-ND	-7.63	104.07	113.72
30	AB	304	PUB	CHB-C1C-NC	-7.52	118.40	128.83
30	AM	304	PUB	CHB-C1C-NC	-7.52	118.40	128.83
29	SR	201	PEB	CHB-C4B-NB	-7.46	118.47	128.83
29	xL	301	PEB	CHB-C4B-NB	-7.46	118.48	128.83
29	xJ	301	PEB	CHB-C4B-NB	-7.44	118.51	128.83
29	wL	301	PEB	CHB-C4B-NB	-7.43	118.52	128.83
29	wJ	301	PEB	CHB-C4B-NB	-7.42	118.54	128.83
30	AM	304	PUB	C4B-CHB-C1C	-7.35	120.03	128.81
30	MG	403	PUB	CHC-C1D-ND	-7.34	104.43	113.72
30	MQ	405	PUB	CHC-C1D-ND	-7.34	104.44	113.72
30	AB	304	PUB	C4B-CHB-C1C	-7.33	120.05	128.81
31	sP	1001	CYC	CHB-C4A-NA	-7.33	109.59	124.93
29	BB	301	PEB	CHC-C1D-ND	-7.33	105.44	113.95
29	BM	301	PEB	CHC-C1D-ND	-7.33	105.44	113.95
29	dF	201	PEB	CHC-C1D-ND	-7.33	105.44	113.95
29	dI	201	PEB	CHC-C1D-ND	-7.33	105.44	113.95
29	UF	201	PEB	CHC-C1D-ND	-7.33	105.44	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UI	201	PEB	CHC-C1D-ND	-7.33	105.44	113.95
29	VF	202	PEB	CHC-C1D-ND	-7.31	105.45	113.95
29	VI	202	PEB	CHC-C1D-ND	-7.31	105.45	113.95
31	fP	1001	CYC	CHB-C4A-NA	-7.31	109.63	124.93
31	hP	1001	CYC	CHB-C4A-NA	-7.31	109.63	124.93
31	nP	1001	CYC	CHB-C4A-NA	-7.31	109.63	124.93
29	gF	202	PEB	CHC-C1D-ND	-7.31	105.46	113.95
29	gI	202	PEB	CHC-C1D-ND	-7.31	105.46	113.95
31	QP	1001	CYC	CHB-C4A-NA	-7.30	109.65	124.93
31	oP	1001	CYC	CHB-C4A-NA	-7.30	109.66	124.93
29	kF	202	PEB	CHC-C1D-ND	-7.30	105.47	113.95
29	kI	202	PEB	CHC-C1D-ND	-7.30	105.47	113.95
31	HP	1001	CYC	CHB-C4A-NA	-7.30	109.66	124.93
31	lP	1001	CYC	CHB-C4A-NA	-7.30	109.66	124.93
31	DP	1001	CYC	CHB-C4A-NA	-7.30	109.67	124.93
31	IP	1001	CYC	CHB-C4A-NA	-7.29	109.67	124.93
31	XP	1001	CYC	CHB-C4A-NA	-7.29	109.67	124.93
31	MP	1001	CYC	CHB-C4A-NA	-7.29	109.67	124.93
31	SP	1001	CYC	CHB-C4A-NA	-7.29	109.68	124.93
31	jP	1001	CYC	CHB-C4A-NA	-7.29	109.68	124.93
31	BP	1001	CYC	CHB-C4A-NA	-7.29	109.68	124.93
31	wP	1001	CYC	CHB-C4A-NA	-7.29	109.68	124.93
29	aF	202	PEB	CHC-C1D-ND	-7.29	105.48	113.95
29	aI	202	PEB	CHC-C1D-ND	-7.29	105.48	113.95
31	kP	1001	CYC	CHB-C4A-NA	-7.29	109.69	124.93
31	FP	1001	CYC	CHB-C4A-NA	-7.29	109.69	124.93
31	qP	1001	CYC	CHB-C4A-NA	-7.28	109.69	124.93
29	P1	202	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	g1	202	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	OF	203	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	PF	202	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	OI	203	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	PI	202	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	PK	202	PEB	CHC-C1D-ND	-7.28	105.49	113.95
29	gK	202	PEB	CHC-C1D-ND	-7.28	105.49	113.95
31	UP	1001	CYC	CHB-C4A-NA	-7.28	109.70	124.93
31	uP	1001	CYC	CHB-C4A-NA	-7.28	109.71	124.93
29	R1	202	PEB	CHC-C1D-ND	-7.28	105.50	113.95
29	RK	202	PEB	CHC-C1D-ND	-7.28	105.50	113.95
29	eF	202	PEB	CHC-C1D-ND	-7.28	105.50	113.95
29	eI	202	PEB	CHC-C1D-ND	-7.28	105.50	113.95
31	OP	1001	CYC	CHB-C4A-NA	-7.28	109.71	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i1	202	PEB	CHC-C1D-ND	-7.27	105.50	113.95
29	j1	203	PEB	CHC-C1D-ND	-7.27	105.50	113.95
29	iK	202	PEB	CHC-C1D-ND	-7.27	105.50	113.95
29	jK	203	PEB	CHC-C1D-ND	-7.27	105.50	113.95
29	Z1	201	PEB	CHC-C1D-ND	-7.27	105.50	113.95
29	ZK	201	PEB	CHC-C1D-ND	-7.27	105.50	113.95
29	iF	202	PEB	CHC-C1D-ND	-7.27	105.51	113.95
29	iI	202	PEB	CHC-C1D-ND	-7.27	105.51	113.95
29	mF	202	PEB	CHC-C1D-ND	-7.26	105.51	113.95
29	mI	202	PEB	CHC-C1D-ND	-7.26	105.51	113.95
29	k1	202	PEB	CHC-C1D-ND	-7.26	105.52	113.95
29	kK	202	PEB	CHC-C1D-ND	-7.26	105.52	113.95
29	U1	201	PEB	CHC-C1D-ND	-7.26	105.52	113.95
29	UK	201	PEB	CHC-C1D-ND	-7.26	105.52	113.95
29	YF	202	PEB	CHC-C1D-ND	-7.26	105.52	113.95
29	YI	202	PEB	CHC-C1D-ND	-7.26	105.52	113.95
29	a1	202	PEB	CHC-C1D-ND	-7.25	105.53	113.95
29	aK	202	PEB	CHC-C1D-ND	-7.25	105.53	113.95
29	B4	201	PEB	CHC-C4C-C3C	-7.25	117.97	130.34
29	V1	202	PEB	CHC-C1D-ND	-7.25	105.53	113.95
29	VK	202	PEB	CHC-C1D-ND	-7.25	105.53	113.95
29	e1	202	PEB	CHC-C1D-ND	-7.24	105.54	113.95
29	eK	202	PEB	CHC-C1D-ND	-7.24	105.54	113.95
29	BD	201	PEB	CHC-C4C-C3C	-7.23	118.01	130.34
29	F4	201	PEB	CHC-C4C-C3C	-7.23	118.01	130.34
29	JD	201	PEB	CHC-C4C-C3C	-7.23	118.02	130.34
29	LD	201	PEB	CHC-C4C-C3C	-7.22	118.02	130.34
29	H4	201	PEB	CHC-C4C-C3C	-7.22	118.02	130.34
29	FD	201	PEB	CHC-C4C-C3C	-7.22	118.02	130.34
30	MN	402	PUB	CHB-C1C-NC	-7.22	118.81	128.83
29	L4	201	PEB	CHC-C4C-C3C	-7.22	118.03	130.34
29	c1	202	PEB	CHC-C1D-ND	-7.21	105.57	113.95
29	cK	202	PEB	CHC-C1D-ND	-7.21	105.57	113.95
29	DD	201	PEB	CHC-C4C-C3C	-7.21	118.04	130.34
29	HD	201	PEB	CHC-C4C-C3C	-7.20	118.06	130.34
29	D4	201	PEB	CHC-C4C-C3C	-7.20	118.07	130.34
30	MA	402	PUB	CHB-C1C-NC	-7.18	118.86	128.83
29	J4	201	PEB	CHC-C4C-C3C	-7.18	118.09	130.34
30	AB	304	PUB	CAD-C3D-C4D	7.18	132.72	121.38
31	xP	1001	CYC	CHB-C4A-NA	-7.17	109.93	124.93
31	VP	1001	CYC	CHB-C4A-NA	-7.17	109.93	124.93
29	SR	201	PEB	C1C-CHB-C4B	-7.16	120.25	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AM	304	PUB	CAD-C3D-C4D	7.15	132.68	121.38
30	MG	403	PUB	CAD-C3D-C4D	7.13	132.65	121.38
29	MN	401	PEB	C1C-CHB-C4B	-7.13	120.29	128.81
29	MG	401	PEB	C1C-CHB-C4B	-7.13	120.29	128.81
29	MA	401	PEB	C1C-CHB-C4B	-7.13	120.30	128.81
29	N2	201	PEB	CHB-C4B-NB	-7.11	118.96	128.83
30	MQ	405	PUB	CAD-C3D-C4D	7.11	132.61	121.38
29	I4	203	PEB	CHB-C4B-NB	-7.11	118.97	128.83
29	R2	201	PEB	CHB-C4B-NB	-7.08	119.00	128.83
29	NR	201	PEB	CHB-C4B-NB	-7.08	119.01	128.83
29	MN	404	PEB	CHB-C4B-NB	-7.07	119.02	128.83
29	TR	201	PEB	CHB-C4B-NB	-7.07	119.02	128.83
29	MQ	403	PEB	C1C-CHB-C4B	-7.07	120.36	128.81
29	T2	201	PEB	CHB-C4B-NB	-7.07	119.03	128.83
29	e2	402	PEB	CHB-C4B-NB	-7.06	119.03	128.83
31	F9	1001	CYC	CHB-C4A-NA	-7.06	110.17	124.93
31	F7	1001	CYC	CHB-C4A-NA	-7.05	110.17	124.93
31	J9	1001	CYC	CHB-C4A-NA	-7.05	110.18	124.93
31	L7	1001	CYC	CHB-C4A-NA	-7.05	110.19	124.93
31	N7	1001	CYC	CHB-C4A-NA	-7.05	110.19	124.93
31	N9	1001	CYC	CHB-C4A-NA	-7.05	110.19	124.93
29	vJ	201	PEB	CHA-C4A-NA	7.05	133.58	125.20
29	vL	201	PEB	CHA-C4A-NA	7.05	133.58	125.20
30	A1	305	PUB	CHB-C1C-NC	-7.04	119.06	128.83
30	AK	305	PUB	CHB-C1C-NC	-7.04	119.06	128.83
31	L9	1001	CYC	CHB-C4A-NA	-7.04	110.20	124.93
31	J7	1001	CYC	CHB-C4A-NA	-7.04	110.20	124.93
31	D7	1001	CYC	CHB-C4A-NA	-7.04	110.20	124.93
31	D9	1001	CYC	CHB-C4A-NA	-7.04	110.20	124.93
31	H7	1001	CYC	CHB-C4A-NA	-7.04	110.20	124.93
31	H9	1001	CYC	CHB-C4A-NA	-7.04	110.20	124.93
29	RR	201	PEB	CHB-C4B-NB	-7.04	119.06	128.83
29	MA	404	PEB	CHB-C4B-NB	-7.03	119.08	128.83
29	LB	202	PEB	CHC-C4C-C3C	-7.03	118.35	130.34
29	LM	202	PEB	CHC-C4C-C3C	-7.03	118.35	130.34
29	V2	201	PEB	CHB-C4B-NB	-7.03	119.08	128.83
29	aB	203	PEB	CHC-C4C-C3C	-7.03	118.35	130.34
29	aM	203	PEB	CHC-C4C-C3C	-7.03	118.35	130.34
29	mB	202	PEB	CHC-C4C-C3C	-7.03	118.36	130.34
29	mM	202	PEB	CHC-C4C-C3C	-7.03	118.36	130.34
29	VR	201	PEB	CHB-C4B-NB	-7.02	119.09	128.83
29	JB	202	PEB	CHC-C4C-C3C	-7.02	118.36	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JM	202	PEB	CHC-C4C-C3C	-7.02	118.36	130.34
29	HB	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
29	HM	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
29	iB	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
29	iM	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
29	DB	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
29	DM	202	PEB	CHC-C4C-C3C	-7.02	118.37	130.34
29	FB	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	kB	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	FM	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	kM	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	VB	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	VM	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	cB	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	cM	202	PEB	CHC-C4C-C3C	-7.01	118.38	130.34
29	RB	202	PEB	CHC-C4C-C3C	-7.01	118.39	130.34
29	TB	202	PEB	CHC-C4C-C3C	-7.01	118.39	130.34
29	YB	201	PEB	CHC-C4C-C3C	-7.01	118.39	130.34
29	RM	202	PEB	CHC-C4C-C3C	-7.01	118.39	130.34
29	TM	202	PEB	CHC-C4C-C3C	-7.01	118.39	130.34
29	YM	201	PEB	CHC-C4C-C3C	-7.01	118.39	130.34
29	QB	202	PEB	CHC-C4C-C3C	-7.00	118.39	130.34
29	QM	202	PEB	CHC-C4C-C3C	-7.00	118.39	130.34
29	TJ	201	PEB	CHA-C4A-NA	7.00	133.53	125.20
29	TL	201	PEB	CHA-C4A-NA	7.00	133.53	125.20
29	XR	201	PEB	CHB-C4B-NB	-7.00	119.12	128.83
29	nJ	201	PEB	CHA-C4A-NA	7.00	133.52	125.20
29	nL	201	PEB	CHA-C4A-NA	7.00	133.52	125.20
29	XJ	201	PEB	CHA-C4A-NA	6.99	133.52	125.20
29	XL	201	PEB	CHA-C4A-NA	6.99	133.52	125.20
29	KB	203	PEB	CHC-C4C-C3C	-6.99	118.41	130.34
29	KM	203	PEB	CHC-C4C-C3C	-6.99	118.41	130.34
29	FJ	201	PEB	CHA-C4A-NA	6.99	133.52	125.20
29	FL	201	PEB	CHA-C4A-NA	6.99	133.52	125.20
29	tJ	201	PEB	CHA-C4A-NA	6.99	133.51	125.20
29	tL	201	PEB	CHA-C4A-NA	6.99	133.51	125.20
29	PJ	201	PEB	CHA-C4A-NA	6.98	133.51	125.20
29	hJ	201	PEB	CHA-C4A-NA	6.98	133.51	125.20
29	PL	201	PEB	CHA-C4A-NA	6.98	133.51	125.20
29	hL	201	PEB	CHA-C4A-NA	6.98	133.51	125.20
29	gB	202	PEB	CHC-C4C-C3C	-6.98	118.43	130.34
29	gM	202	PEB	CHC-C4C-C3C	-6.98	118.43	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZB	202	PEB	CHC-C4C-C3C	-6.98	118.44	130.34
29	ZM	202	PEB	CHC-C4C-C3C	-6.98	118.44	130.34
29	IJ	201	PEB	CHA-C4A-NA	6.97	133.50	125.20
29	IL	201	PEB	CHA-C4A-NA	6.97	133.50	125.20
29	bJ	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	bL	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	ZJ	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	ZL	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	JJ	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	JL	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	rJ	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	rL	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	LJ	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	LL	201	PEB	CHA-C4A-NA	6.97	133.49	125.20
29	NJ	201	PEB	CHA-C4A-NA	6.96	133.48	125.20
29	NL	201	PEB	CHA-C4A-NA	6.96	133.48	125.20
29	fJ	201	PEB	CHA-C4A-NA	6.96	133.48	125.20
29	fL	201	PEB	CHA-C4A-NA	6.96	133.48	125.20
29	MR	202	PEB	CHB-C4B-NB	-6.96	119.17	128.83
29	RJ	201	PEB	CHA-C4A-NA	6.96	133.48	125.20
29	RL	201	PEB	CHA-C4A-NA	6.96	133.48	125.20
29	VJ	201	PEB	CHA-C4A-NA	6.96	133.47	125.20
29	VL	201	PEB	CHA-C4A-NA	6.96	133.47	125.20
29	OB	202	PEB	CHB-C4B-NB	-6.95	119.18	128.83
29	OM	202	PEB	CHB-C4B-NB	-6.95	119.18	128.83
29	DJ	201	PEB	CHA-C4A-NA	6.95	133.47	125.20
29	DL	201	PEB	CHA-C4A-NA	6.95	133.47	125.20
29	dJ	201	PEB	CHA-C4A-NA	6.95	133.47	125.20
29	jJ	201	PEB	CHA-C4A-NA	6.95	133.47	125.20
29	dL	201	PEB	CHA-C4A-NA	6.95	133.47	125.20
29	jL	201	PEB	CHA-C4A-NA	6.95	133.47	125.20
29	IB	202	PEB	CHB-C4B-NB	-6.95	119.19	128.83
29	IM	202	PEB	CHB-C4B-NB	-6.95	119.19	128.83
29	pJ	201	PEB	CHA-C4A-NA	6.94	133.46	125.20
29	pL	201	PEB	CHA-C4A-NA	6.94	133.46	125.20
29	jB	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	jM	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	SB	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	SM	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	CB	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	CM	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	BJ	201	PEB	CHA-C4A-NA	6.93	133.45	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BL	201	PEB	CHA-C4A-NA	6.93	133.45	125.20
29	hB	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	hM	202	PEB	CHB-C4B-NB	-6.93	119.21	128.83
29	YB	203	PEB	CHB-C4B-NB	-6.93	119.22	128.83
29	YM	203	PEB	CHB-C4B-NB	-6.93	119.22	128.83
29	UB	202	PEB	CHB-C4B-NB	-6.93	119.22	128.83
29	MQ	401	PEB	CHB-C4B-NB	-6.93	119.22	128.83
29	QB	204	PEB	CHB-C4B-NB	-6.93	119.22	128.83
29	QM	204	PEB	CHB-C4B-NB	-6.93	119.22	128.83
29	aB	202	PEB	CHB-C4B-NB	-6.92	119.22	128.83
29	aM	202	PEB	CHB-C4B-NB	-6.92	119.22	128.83
29	WB	202	PEB	CHB-C4B-NB	-6.92	119.23	128.83
29	WM	202	PEB	CHB-C4B-NB	-6.92	119.23	128.83
29	MA	404	PEB	C1C-CHB-C4B	-6.92	120.54	128.81
29	lB	202	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	lM	202	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	xL	303	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	MB	202	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	MM	202	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	KB	202	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	KM	202	PEB	CHB-C4B-NB	-6.91	119.24	128.83
29	MN	404	PEB	C1C-CHB-C4B	-6.91	120.56	128.81
29	fB	202	PEB	CHB-C4B-NB	-6.90	119.25	128.83
29	fM	202	PEB	CHB-C4B-NB	-6.90	119.25	128.83
29	GB	202	PEB	CHB-C4B-NB	-6.90	119.25	128.83
29	GM	202	PEB	CHB-C4B-NB	-6.90	119.25	128.83
29	wJ	303	PEB	CHB-C4B-NB	-6.90	119.25	128.83
29	EB	202	PEB	CHB-C4B-NB	-6.90	119.26	128.83
29	EM	202	PEB	CHB-C4B-NB	-6.90	119.26	128.83
29	dB	202	PEB	CHB-C4B-NB	-6.90	119.26	128.83
29	dM	202	PEB	CHB-C4B-NB	-6.90	119.26	128.83
29	xJ	303	PEB	CHB-C4B-NB	-6.89	119.27	128.83
29	wL	303	PEB	CHB-C4B-NB	-6.86	119.31	128.83
29	eB	202	PEB	CHB-C4B-NB	-6.77	119.43	128.83
29	eM	202	PEB	CHB-C4B-NB	-6.77	119.43	128.83
29	TB	203	PEB	CHB-C4B-NB	-6.77	119.44	128.83
29	TM	203	PEB	CHB-C4B-NB	-6.77	119.44	128.83
31	KF	1001	CYC	CAB-C3B-C4B	6.77	132.07	121.38
29	ZB	203	PEB	CHB-C4B-NB	-6.77	119.44	128.83
29	ZM	203	PEB	CHB-C4B-NB	-6.77	119.44	128.83
31	KI	1001	CYC	CAB-C3B-C4B	6.76	132.05	121.38
31	EF	1001	CYC	CAB-C3B-C4B	6.76	132.05	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	EI	1001	CYC	CAB-C3B-C4B	6.76	132.05	121.38
31	GF	1001	CYC	CAB-C3B-C4B	6.76	132.05	121.38
31	GI	1001	CYC	CAB-C3B-C4B	6.76	132.05	121.38
29	XB	202	PEB	CHB-C4B-NB	-6.75	119.46	128.83
29	XM	202	PEB	CHB-C4B-NB	-6.75	119.46	128.83
29	NB	202	PEB	CHB-C4B-NB	-6.75	119.46	128.83
29	NM	202	PEB	CHB-C4B-NB	-6.75	119.46	128.83
29	DB	203	PEB	CHB-C4B-NB	-6.75	119.47	128.83
29	JB	203	PEB	CHB-C4B-NB	-6.75	119.47	128.83
29	DM	203	PEB	CHB-C4B-NB	-6.75	119.47	128.83
29	JM	203	PEB	CHB-C4B-NB	-6.75	119.47	128.83
31	CF	1001	CYC	CAB-C3B-C4B	6.75	132.03	121.38
31	CI	1001	CYC	CAB-C3B-C4B	6.75	132.03	121.38
29	gB	203	PEB	CHB-C4B-NB	-6.75	119.47	128.83
29	gM	203	PEB	CHB-C4B-NB	-6.75	119.47	128.83
29	PB	202	PEB	CHB-C4B-NB	-6.74	119.47	128.83
29	PM	202	PEB	CHB-C4B-NB	-6.74	119.47	128.83
29	cB	203	PEB	CHB-C4B-NB	-6.74	119.47	128.83
29	cM	203	PEB	CHB-C4B-NB	-6.74	119.47	128.83
29	iB	203	PEB	CHB-C4B-NB	-6.74	119.48	128.83
29	iM	203	PEB	CHB-C4B-NB	-6.74	119.48	128.83
31	IF	1001	CYC	CAB-C3B-C4B	6.74	132.02	121.38
31	MF	1001	CYC	CAB-C3B-C4B	6.74	132.02	121.38
31	II	1001	CYC	CAB-C3B-C4B	6.74	132.02	121.38
31	MI	1001	CYC	CAB-C3B-C4B	6.74	132.02	121.38
29	HB	203	PEB	CHB-C4B-NB	-6.74	119.48	128.83
29	HM	203	PEB	CHB-C4B-NB	-6.74	119.48	128.83
31	yP	1001	CYC	CHD-C4C-NC	6.73	133.21	125.20
29	LB	203	PEB	CHB-C4B-NB	-6.72	119.50	128.83
29	LM	203	PEB	CHB-C4B-NB	-6.72	119.50	128.83
29	VB	203	PEB	CHB-C4B-NB	-6.72	119.50	128.83
29	VM	203	PEB	CHB-C4B-NB	-6.72	119.50	128.83
29	RB	203	PEB	CHB-C4B-NB	-6.72	119.51	128.83
29	RM	203	PEB	CHB-C4B-NB	-6.72	119.51	128.83
31	WP	1001	CYC	CHD-C4C-NC	6.72	133.19	125.20
29	M4	203	PEB	CHB-C4B-NB	-6.72	119.51	128.83
29	kB	203	PEB	CHB-C4B-NB	-6.71	119.51	128.83
29	kM	203	PEB	CHB-C4B-NB	-6.71	119.51	128.83
29	MN	405	PEB	C1C-CHB-C4B	-6.71	120.79	128.81
29	MA	405	PEB	C1C-CHB-C4B	-6.71	120.80	128.81
29	FB	203	PEB	CHB-C4B-NB	-6.71	119.53	128.83
29	FM	203	PEB	CHB-C4B-NB	-6.71	119.53	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mB	203	PEB	CHB-C4B-NB	-6.70	119.54	128.83
29	mM	203	PEB	CHB-C4B-NB	-6.70	119.54	128.83
29	V2	202	PEB	CHC-C4C-C3C	-6.69	118.92	130.34
29	BC	202	PEB	CHC-C4C-C3C	-6.68	118.95	130.34
29	BE	202	PEB	CHC-C4C-C3C	-6.68	118.95	130.34
29	VR	202	PEB	CHC-C4C-C3C	-6.68	118.95	130.34
29	AC	203	PEB	CHC-C4C-C3C	-6.67	118.96	130.34
29	AE	203	PEB	CHC-C4C-C3C	-6.67	118.96	130.34
29	NR	202	PEB	CHC-C4C-C3C	-6.67	118.96	130.34
29	HC	202	PEB	CHC-C4C-C3C	-6.67	118.97	130.34
29	HE	202	PEB	CHC-C4C-C3C	-6.67	118.97	130.34
29	FC	202	PEB	CHC-C4C-C3C	-6.67	118.97	130.34
29	FE	202	PEB	CHC-C4C-C3C	-6.67	118.97	130.34
29	P2	201	PEB	CHC-C4C-C3C	-6.67	118.97	130.34
29	PR	201	PEB	CHC-C4C-C3C	-6.67	118.97	130.34
29	LC	202	PEB	CHC-C4C-C3C	-6.66	118.98	130.34
29	LE	202	PEB	CHC-C4C-C3C	-6.66	118.98	130.34
29	XR	202	PEB	CHC-C4C-C3C	-6.66	118.98	130.34
29	N2	202	PEB	CHC-C4C-C3C	-6.66	118.99	130.34
31	PP	1001	CYC	CHB-C4A-NA	-6.65	111.01	124.93
29	VB	202	PEB	C1C-CHB-C4B	6.65	136.75	128.81
29	VM	202	PEB	C1C-CHB-C4B	6.65	136.75	128.81
31	cP	1001	CYC	CHB-C4A-NA	-6.65	111.03	124.93
31	vP	1001	CYC	CHB-C4A-NA	-6.65	111.03	124.93
29	iB	202	PEB	C1C-CHB-C4B	6.64	136.75	128.81
29	iM	202	PEB	C1C-CHB-C4B	6.64	136.75	128.81
31	GP	1001	CYC	CHB-C4A-NA	-6.64	111.04	124.93
29	RR	202	PEB	CHC-C4C-C3C	-6.64	119.01	130.34
31	AP	1001	CYC	CHB-C4A-NA	-6.64	111.05	124.93
31	JP	1001	CYC	CHB-C4A-NA	-6.64	111.05	124.93
31	mP	1001	CYC	CHB-C4A-NA	-6.64	111.05	124.93
29	TR	202	PEB	CHC-C4C-C3C	-6.64	119.02	130.34
31	CP	1001	CYC	CHB-C4A-NA	-6.63	111.05	124.93
29	T2	202	PEB	CHC-C4C-C3C	-6.63	119.02	130.34
29	X2	201	PEB	CHC-C4C-C3C	-6.63	119.02	130.34
31	pP	1001	CYC	CHB-C4A-NA	-6.63	111.06	124.93
29	KC	201	PEB	CHC-C4C-C3C	-6.63	119.03	130.34
29	KE	201	PEB	CHC-C4C-C3C	-6.63	119.03	130.34
31	tP	1001	CYC	CHB-C4A-NA	-6.63	111.06	124.93
31	eP	1001	CYC	CHB-C4A-NA	-6.63	111.06	124.93
29	aB	203	PEB	C1C-CHB-C4B	6.63	136.73	128.81
29	aM	203	PEB	C1C-CHB-C4B	6.63	136.73	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	TP	1001	CYC	CHB-C4A-NA	-6.63	111.07	124.93
31	KP	1001	CYC	CHB-C4A-NA	-6.63	111.07	124.93
31	lP	1001	CYC	CHB-C4A-NA	-6.63	111.07	124.93
29	R2	202	PEB	CHC-C4C-C3C	-6.62	119.04	130.34
29	HB	202	PEB	C1C-CHB-C4B	6.62	136.72	128.81
29	HM	202	PEB	C1C-CHB-C4B	6.62	136.72	128.81
31	EP	1001	CYC	CHB-C4A-NA	-6.62	111.08	124.93
29	RB	202	PEB	C1C-CHB-C4B	6.62	136.72	128.81
29	RM	202	PEB	C1C-CHB-C4B	6.62	136.72	128.81
31	RP	1001	CYC	CHB-C4A-NA	-6.62	111.08	124.93
31	rP	1001	CYC	CHB-C4A-NA	-6.62	111.08	124.93
31	NP	1001	CYC	CHB-C4A-NA	-6.62	111.09	124.93
31	lP	1002	CYC	CHB-C4A-NA	-6.62	111.09	124.93
31	gP	1001	CYC	CHB-C4A-NA	-6.61	111.09	124.93
31	YP	1000	CYC	CHB-C4A-NA	-6.61	111.11	124.93
29	ZB	202	PEB	C1C-CHB-C4B	6.61	136.70	128.81
29	ZM	202	PEB	C1C-CHB-C4B	6.61	136.70	128.81
31	iP	1001	CYC	CHB-C4A-NA	-6.61	111.11	124.93
29	kB	202	PEB	C1C-CHB-C4B	6.60	136.69	128.81
29	kM	202	PEB	C1C-CHB-C4B	6.60	136.69	128.81
29	FB	202	PEB	C1C-CHB-C4B	6.60	136.69	128.81
29	FM	202	PEB	C1C-CHB-C4B	6.60	136.69	128.81
29	LB	202	PEB	C1C-CHB-C4B	6.59	136.69	128.81
29	LM	202	PEB	C1C-CHB-C4B	6.59	136.69	128.81
29	gB	202	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	gM	202	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	mB	202	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	mM	202	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	YB	201	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	YM	201	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	cB	202	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	cM	202	PEB	C1C-CHB-C4B	6.59	136.68	128.81
29	JB	202	PEB	C1C-CHB-C4B	6.58	136.68	128.81
29	JM	202	PEB	C1C-CHB-C4B	6.58	136.68	128.81
29	DB	202	PEB	C1C-CHB-C4B	6.58	136.67	128.81
29	QB	202	PEB	C1C-CHB-C4B	6.58	136.67	128.81
29	DM	202	PEB	C1C-CHB-C4B	6.58	136.67	128.81
29	QM	202	PEB	C1C-CHB-C4B	6.58	136.67	128.81
29	TB	202	PEB	C1C-CHB-C4B	6.57	136.66	128.81
29	TM	202	PEB	C1C-CHB-C4B	6.57	136.66	128.81
30	MG	402	PUB	CMB-C2B-C3B	6.57	137.33	124.94
29	I8	202	PEB	CHC-C1D-ND	-6.57	106.32	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	MQ	404	PUB	CMB-C2B-C3B	6.57	137.32	124.94
30	yL	303	PUB	CHB-C1C-NC	-6.56	119.72	128.83
29	KB	203	PEB	C1C-CHB-C4B	6.56	136.65	128.81
29	KM	203	PEB	C1C-CHB-C4B	6.56	136.65	128.81
29	C5	202	PEB	CHC-C1D-ND	-6.56	106.33	113.95
29	C8	202	PEB	CHC-C1D-ND	-6.56	106.33	113.95
30	yJ	303	PUB	CHB-C1C-NC	-6.56	119.73	128.83
30	AF	303	PUB	CAD-C3D-C4D	6.55	131.72	121.38
30	AI	303	PUB	CAD-C3D-C4D	6.55	131.72	121.38
29	I5	202	PEB	CHC-C1D-ND	-6.54	106.35	113.95
30	MG	403	PUB	CAC-C2C-C1C	6.52	136.55	125.01
29	K5	202	PEB	CHC-C1D-ND	-6.52	106.38	113.95
30	MQ	405	PUB	CAC-C2C-C1C	6.51	136.53	125.01
29	A5	202	PEB	CHC-C1D-ND	-6.51	106.39	113.95
29	A8	202	PEB	CHC-C1D-ND	-6.51	106.39	113.95
29	MR	201	PEB	CHC-C4C-C3C	-6.50	119.25	130.34
29	O2	201	PEB	CHB-C4B-NB	-6.49	119.82	128.83
29	K8	202	PEB	CHC-C1D-ND	-6.49	106.41	113.95
29	M2	201	PEB	CHC-C4C-C3C	-6.49	119.27	130.34
29	OR	201	PEB	CHB-C4B-NB	-6.48	119.84	128.83
29	O7	201	PEB	CMB-C2B-C1B	6.48	135.04	125.06
29	O9	201	PEB	CMB-C2B-C1B	6.48	135.04	125.06
29	Q2	201	PEB	CHC-C4C-C3C	-6.48	119.29	130.34
29	W2	201	PEB	CHC-C4C-C3C	-6.47	119.30	130.34
29	WR	201	PEB	CHC-C4C-C3C	-6.47	119.30	130.34
29	UR	201	PEB	CHB-C4B-NB	-6.47	119.85	128.83
29	M2	201	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	MR	201	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	Q2	201	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	AC	203	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	KC	201	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	AE	203	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	KE	201	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	WR	201	PEB	CHB-C4B-NB	-6.47	119.86	128.83
29	OR	201	PEB	CHC-C4C-C3C	-6.47	119.31	130.34
29	HC	202	PEB	CHB-C4B-NB	-6.46	119.86	128.83
29	HE	202	PEB	CHB-C4B-NB	-6.46	119.86	128.83
29	U7	201	PEB	CMB-C2B-C1B	6.46	135.01	125.06
29	U9	201	PEB	CMB-C2B-C1B	6.46	135.01	125.06
29	d7	201	PEB	CMB-C2B-C1B	6.46	135.01	125.06
29	d9	201	PEB	CMB-C2B-C1B	6.46	135.01	125.06
29	FC	202	PEB	CHB-C4B-NB	-6.46	119.87	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FE	202	PEB	CHB-C4B-NB	-6.46	119.87	128.83
29	W7	201	PEB	CMB-C2B-C1B	6.45	135.00	125.06
29	W9	201	PEB	CMB-C2B-C1B	6.45	135.00	125.06
29	O2	201	PEB	CHC-C4C-C3C	-6.45	119.33	130.34
29	U2	201	PEB	CHB-C4B-NB	-6.45	119.88	128.83
29	QR	201	PEB	CHC-C4C-C3C	-6.45	119.33	130.34
29	UR	201	PEB	CHC-C4C-C3C	-6.45	119.33	130.34
29	BC	202	PEB	CHB-C4B-NB	-6.45	119.88	128.83
29	LC	202	PEB	CHB-C4B-NB	-6.45	119.88	128.83
29	BE	202	PEB	CHB-C4B-NB	-6.45	119.88	128.83
29	LE	202	PEB	CHB-C4B-NB	-6.45	119.88	128.83
29	U2	201	PEB	CHC-C4C-C3C	-6.45	119.34	130.34
29	W2	201	PEB	CHB-C4B-NB	-6.45	119.89	128.83
29	QR	201	PEB	CHB-C4B-NB	-6.44	119.89	128.83
29	f7	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	f9	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	j7	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	j9	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	Q7	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	Z7	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	Q9	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	Z9	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	S7	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	S9	201	PEB	CMB-C2B-C1B	6.44	134.99	125.06
29	b7	201	PEB	CMB-C2B-C1B	6.44	134.97	125.06
29	l7	201	PEB	CMB-C2B-C1B	6.44	134.97	125.06
29	b9	201	PEB	CMB-C2B-C1B	6.44	134.97	125.06
29	l9	201	PEB	CMB-C2B-C1B	6.44	134.97	125.06
29	h7	201	PEB	CMB-C2B-C1B	6.43	134.97	125.06
29	h9	201	PEB	CMB-C2B-C1B	6.43	134.97	125.06
29	MQ	403	PEB	CHB-C4B-NB	-6.43	119.91	128.83
30	AF	302	PUB	CAD-C3D-C4D	6.43	131.53	121.38
30	AI	302	PUB	CAD-C3D-C4D	6.43	131.53	121.38
29	A9	304	PEB	CHB-C4B-NB	-6.42	119.92	128.83
30	A7	302	PUB	CAD-C3D-C4D	6.42	131.51	121.38
30	A9	302	PUB	CAD-C3D-C4D	6.42	131.51	121.38
29	E4	203	PEB	OA-C1A-C2A	-6.41	121.07	126.17
30	A1	305	PUB	CAD-C3D-C4D	6.41	131.50	121.38
30	AK	305	PUB	CAD-C3D-C4D	6.41	131.50	121.38
30	A1	304	PUB	CAD-C3D-C4D	6.41	131.50	121.38
30	AK	304	PUB	CAD-C3D-C4D	6.41	131.50	121.38
29	E4	203	PEB	CHC-C1D-ND	-6.40	106.51	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MD	203	PEB	CHC-C1D-ND	-6.39	106.52	113.95
29	A7	304	PEB	CHB-C4B-NB	-6.39	119.97	128.83
29	K4	203	PEB	CHC-C1D-ND	-6.38	106.53	113.95
29	MD	203	PEB	OA-C1A-C2A	-6.38	121.10	126.17
29	GD	203	PEB	CHC-C1D-ND	-6.38	106.54	113.95
29	KD	203	PEB	CHC-C1D-ND	-6.37	106.55	113.95
29	MG	401	PEB	CHB-C4B-NB	-6.37	119.99	128.83
29	ED	202	PEB	CHC-C1D-ND	-6.36	106.56	113.95
31	K9	1001	CYC	CAB-C3B-C4B	6.36	131.42	121.38
30	AF	303	PUB	OD-C4D-C3D	-6.35	121.15	128.04
30	AI	303	PUB	OD-C4D-C3D	-6.35	121.15	128.04
29	G4	203	PEB	CHC-C1D-ND	-6.34	106.58	113.95
29	CD	203	PEB	CHC-C1D-ND	-6.34	106.58	113.95
31	I7	1001	CYC	CAB-C3B-C4B	6.34	131.39	121.38
31	I9	1001	CYC	CAB-C3B-C4B	6.34	131.39	121.38
29	KD	203	PEB	OA-C1A-C2A	-6.34	121.13	126.17
30	A7	303	PUB	CAD-C3D-C4D	6.34	131.39	121.38
30	A9	303	PUB	CAD-C3D-C4D	6.34	131.39	121.38
31	G9	1001	CYC	CAB-C3B-C4B	6.34	131.39	121.38
29	C4	203	PEB	CHC-C1D-ND	-6.34	106.59	113.95
29	MA	405	PEB	CHB-C4B-NB	-6.33	120.04	128.83
29	GD	203	PEB	OA-C1A-C2A	-6.33	121.14	126.17
31	G7	1001	CYC	CAB-C3B-C4B	6.33	131.37	121.38
29	MN	401	PEB	CHB-C4B-NB	-6.32	120.06	128.83
31	K7	1001	CYC	CAB-C3B-C4B	6.32	131.36	121.38
29	ID	203	PEB	CHC-C1D-ND	-6.32	106.61	113.95
31	E7	1001	CYC	CAB-C3B-C4B	6.31	131.35	121.38
31	E9	1001	CYC	CAB-C3B-C4B	6.31	131.35	121.38
30	AB	305	PUB	OD-C4D-C3D	-6.31	121.19	128.04
29	hB	202	PEB	CHC-C4C-C3C	-6.31	119.58	130.34
29	hM	202	PEB	CHC-C4C-C3C	-6.31	119.58	130.34
29	HG	202	PEB	C1C-CHB-C4B	6.30	136.34	128.81
29	HQ	202	PEB	C1C-CHB-C4B	6.30	136.34	128.81
29	KB	202	PEB	CHC-C4C-C3C	-6.30	119.59	130.34
29	KM	202	PEB	CHC-C4C-C3C	-6.30	119.59	130.34
31	M7	1001	CYC	CAB-C3B-C4B	6.30	131.33	121.38
31	M9	1001	CYC	CAB-C3B-C4B	6.30	131.33	121.38
29	MA	401	PEB	CHB-C4B-NB	-6.30	120.09	128.83
29	MN	405	PEB	CHB-C4B-NB	-6.30	120.09	128.83
29	GB	202	PEB	CHC-C4C-C3C	-6.30	119.59	130.34
29	GM	202	PEB	CHC-C4C-C3C	-6.30	119.59	130.34
29	fB	202	PEB	CHC-C4C-C3C	-6.30	119.60	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	fM	202	PEB	CHC-C4C-C3C	-6.30	119.60	130.34
29	CB	202	PEB	CHC-C4C-C3C	-6.29	119.60	130.34
29	CM	202	PEB	CHC-C4C-C3C	-6.29	119.60	130.34
29	FG	202	PEB	C1C-CHB-C4B	6.29	136.33	128.81
29	FQ	202	PEB	C1C-CHB-C4B	6.29	136.33	128.81
29	JG	202	PEB	C1C-CHB-C4B	6.29	136.32	128.81
29	JQ	202	PEB	C1C-CHB-C4B	6.29	136.32	128.81
29	K4	203	PEB	OA-C1A-C2A	-6.29	121.17	126.17
30	QB	201	PUB	CAD-C3D-C4D	6.29	131.31	121.38
30	QM	201	PUB	CAD-C3D-C4D	6.29	131.31	121.38
29	jB	202	PEB	CHC-C4C-C3C	-6.29	119.61	130.34
29	jM	202	PEB	CHC-C4C-C3C	-6.29	119.61	130.34
29	ED	202	PEB	OA-C1A-C2A	-6.29	121.17	126.17
29	QB	204	PEB	CHC-C4C-C3C	-6.29	119.61	130.34
29	QM	204	PEB	CHC-C4C-C3C	-6.29	119.61	130.34
29	lB	202	PEB	CHC-C4C-C3C	-6.29	119.62	130.34
29	lM	202	PEB	CHC-C4C-C3C	-6.29	119.62	130.34
29	DG	202	PEB	C1C-CHB-C4B	6.29	136.32	128.81
29	DQ	202	PEB	C1C-CHB-C4B	6.29	136.32	128.81
29	OB	202	PEB	CHC-C4C-C3C	-6.29	119.62	130.34
29	OM	202	PEB	CHC-C4C-C3C	-6.29	119.62	130.34
29	YB	203	PEB	CHC-C4C-C3C	-6.29	119.62	130.34
29	YM	203	PEB	CHC-C4C-C3C	-6.29	119.62	130.34
29	BG	202	PEB	C1C-CHB-C4B	6.28	136.31	128.81
29	BQ	202	PEB	C1C-CHB-C4B	6.28	136.31	128.81
29	ID	203	PEB	OA-C1A-C2A	-6.28	121.18	126.17
29	MB	202	PEB	CHC-C4C-C3C	-6.28	119.63	130.34
29	UB	202	PEB	CHC-C4C-C3C	-6.28	119.63	130.34
29	MM	202	PEB	CHC-C4C-C3C	-6.28	119.63	130.34
29	MQ	401	PEB	CHC-C4C-C3C	-6.28	119.63	130.34
31	C7	1001	CYC	CAB-C3B-C4B	6.28	131.29	121.38
31	C9	1001	CYC	CAB-C3B-C4B	6.28	131.29	121.38
29	EB	202	PEB	CHC-C4C-C3C	-6.28	119.63	130.34
29	EM	202	PEB	CHC-C4C-C3C	-6.28	119.63	130.34
29	WB	202	PEB	CHC-C4C-C3C	-6.27	119.64	130.34
29	WM	202	PEB	CHC-C4C-C3C	-6.27	119.64	130.34
31	RP	1001	CYC	OB-C4B-C3B	-6.27	121.23	128.04
29	SB	202	PEB	CHC-C4C-C3C	-6.27	119.64	130.34
29	SM	202	PEB	CHC-C4C-C3C	-6.27	119.64	130.34
31	gP	1001	CYC	OB-C4B-C3B	-6.27	121.23	128.04
29	dB	202	PEB	CHC-C4C-C3C	-6.27	119.64	130.34
29	dM	202	PEB	CHC-C4C-C3C	-6.27	119.64	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	NP	1001	CYC	OB-C4B-C3B	-6.26	121.24	128.04
29	IB	202	PEB	CHC-C4C-C3C	-6.26	119.65	130.34
29	IM	202	PEB	CHC-C4C-C3C	-6.26	119.65	130.34
29	LG	202	PEB	C1C-CHB-C4B	6.26	136.29	128.81
29	LQ	201	PEB	C1C-CHB-C4B	6.26	136.29	128.81
29	aB	202	PEB	CHC-C4C-C3C	-6.26	119.65	130.34
29	aM	202	PEB	CHC-C4C-C3C	-6.26	119.65	130.34
31	vP	1001	CYC	OB-C4B-C3B	-6.26	121.24	128.04
31	mP	1001	CYC	OB-C4B-C3B	-6.26	121.25	128.04
31	tP	1001	CYC	OB-C4B-C3B	-6.26	121.25	128.04
30	MA	402	PUB	C4B-CHB-C1C	-6.26	121.33	128.81
31	lP	1001	CYC	OB-C4B-C3B	-6.26	121.25	128.04
29	vJ	201	PEB	C2A-C1A-NA	6.25	113.66	108.27
29	vL	201	PEB	C2A-C1A-NA	6.25	113.66	108.27
31	iP	1001	CYC	OB-C4B-C3B	-6.25	121.26	128.04
31	eP	1001	CYC	OB-C4B-C3B	-6.25	121.26	128.04
29	G4	203	PEB	OA-C1A-C2A	-6.25	121.21	126.17
31	AP	1001	CYC	OB-C4B-C3B	-6.24	121.27	128.04
29	C4	203	PEB	OA-C1A-C2A	-6.24	121.21	126.17
30	AM	305	PUB	OD-C4D-C3D	-6.24	121.27	128.04
31	cP	1001	CYC	OB-C4B-C3B	-6.24	121.27	128.04
30	yJ	303	PUB	CAD-C3D-C4D	6.24	131.23	121.38
31	JP	1001	CYC	OB-C4B-C3B	-6.24	121.27	128.04
29	fJ	201	PEB	C2A-C1A-NA	6.24	113.65	108.27
29	fL	201	PEB	C2A-C1A-NA	6.24	113.65	108.27
31	KP	1001	CYC	OB-C4B-C3B	-6.23	121.28	128.04
31	PP	1001	CYC	OB-C4B-C3B	-6.23	121.28	128.04
31	rP	1001	CYC	OB-C4B-C3B	-6.23	121.28	128.04
30	MN	402	PUB	C4B-CHB-C1C	-6.23	121.37	128.81
29	LJ	201	PEB	C2A-C1A-NA	6.23	113.64	108.27
29	LL	201	PEB	C2A-C1A-NA	6.23	113.64	108.27
29	ZJ	201	PEB	C2A-C1A-NA	6.22	113.64	108.27
29	ZL	201	PEB	C2A-C1A-NA	6.22	113.64	108.27
31	TP	1001	CYC	OB-C4B-C3B	-6.22	121.29	128.04
31	pP	1001	CYC	OB-C4B-C3B	-6.22	121.29	128.04
31	EP	1001	CYC	OB-C4B-C3B	-6.22	121.29	128.04
29	lJ	201	PEB	C2A-C1A-NA	6.21	113.63	108.27
29	lL	201	PEB	C2A-C1A-NA	6.21	113.63	108.27
29	aF	202	PEB	C1C-CHB-C4B	6.21	136.23	128.81
29	aI	202	PEB	C1C-CHB-C4B	6.21	136.23	128.81
29	tJ	201	PEB	C2A-C1A-NA	6.21	113.63	108.27
29	tL	201	PEB	C2A-C1A-NA	6.21	113.63	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I4	203	PEB	C1C-CHB-C4B	-6.21	121.39	128.81
30	yL	303	PUB	CAD-C3D-C4D	6.21	131.18	121.38
29	eF	202	PEB	C1C-CHB-C4B	6.20	136.22	128.81
29	eI	202	PEB	C1C-CHB-C4B	6.20	136.22	128.81
29	hJ	201	PEB	C2A-C1A-NA	6.20	113.62	108.27
29	hL	201	PEB	C2A-C1A-NA	6.20	113.62	108.27
29	mF	202	PEB	C1C-CHB-C4B	6.20	136.22	128.81
29	mI	202	PEB	C1C-CHB-C4B	6.20	136.22	128.81
29	RJ	201	PEB	C2A-C1A-NA	6.20	113.62	108.27
29	RL	201	PEB	C2A-C1A-NA	6.20	113.62	108.27
30	AF	302	PUB	CHB-C1C-NC	-6.20	120.23	128.83
30	AI	302	PUB	CHB-C1C-NC	-6.20	120.23	128.83
29	TJ	201	PEB	C2A-C1A-NA	6.20	113.61	108.27
29	TL	201	PEB	C2A-C1A-NA	6.20	113.61	108.27
29	CD	203	PEB	OA-C1A-C2A	-6.19	121.25	126.17
31	GP	1001	CYC	OB-C4B-C3B	-6.19	121.32	128.04
29	YF	202	PEB	C1C-CHB-C4B	6.19	136.21	128.81
29	YI	202	PEB	C1C-CHB-C4B	6.19	136.21	128.81
29	PF	202	PEB	C1C-CHB-C4B	6.19	136.21	128.81
29	PI	202	PEB	C1C-CHB-C4B	6.19	136.21	128.81
29	nJ	201	PEB	C2A-C1A-NA	6.19	113.61	108.27
29	nL	201	PEB	C2A-C1A-NA	6.19	113.61	108.27
29	NJ	201	PEB	C2A-C1A-NA	6.19	113.61	108.27
29	NL	201	PEB	C2A-C1A-NA	6.19	113.61	108.27
29	jJ	201	PEB	C2A-C1A-NA	6.19	113.61	108.27
29	jL	201	PEB	C2A-C1A-NA	6.19	113.61	108.27
29	dF	201	PEB	C1C-CHB-C4B	6.19	136.20	128.81
29	dI	201	PEB	C1C-CHB-C4B	6.19	136.20	128.81
29	VF	202	PEB	C1C-CHB-C4B	6.18	136.20	128.81
29	VI	202	PEB	C1C-CHB-C4B	6.18	136.20	128.81
29	OF	203	PEB	C1C-CHB-C4B	6.18	136.20	128.81
29	OI	203	PEB	C1C-CHB-C4B	6.18	136.20	128.81
29	DJ	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	PJ	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	XJ	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	DL	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	PL	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	XL	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	pJ	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	pL	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	BJ	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	BL	201	PEB	C2A-C1A-NA	6.18	113.60	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MA	405	PEB	CHA-C1B-NB	-6.18	112.01	124.93
29	MN	405	PEB	CHA-C1B-NB	-6.18	112.01	124.93
29	kF	202	PEB	C1C-CHB-C4B	6.18	136.19	128.81
29	kI	202	PEB	C1C-CHB-C4B	6.18	136.19	128.81
29	FJ	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
29	FL	201	PEB	C2A-C1A-NA	6.18	113.60	108.27
31	CP	1001	CYC	OB-C4B-C3B	-6.17	121.34	128.04
29	OR	202	PEB	CHB-C4B-NB	-6.17	120.27	128.83
29	bJ	201	PEB	C2A-C1A-NA	6.17	113.59	108.27
29	bL	201	PEB	C2A-C1A-NA	6.17	113.59	108.27
29	UF	201	PEB	C1C-CHB-C4B	6.17	136.18	128.81
29	UI	201	PEB	C1C-CHB-C4B	6.17	136.18	128.81
29	gF	202	PEB	C1C-CHB-C4B	6.16	136.17	128.81
29	gI	202	PEB	C1C-CHB-C4B	6.16	136.17	128.81
29	dJ	201	PEB	C2A-C1A-NA	6.16	113.58	108.27
29	dL	201	PEB	C2A-C1A-NA	6.16	113.58	108.27
29	VJ	201	PEB	C2A-C1A-NA	6.16	113.58	108.27
29	VL	201	PEB	C2A-C1A-NA	6.16	113.58	108.27
29	JJ	201	PEB	C2A-C1A-NA	6.16	113.58	108.27
29	JL	201	PEB	C2A-C1A-NA	6.16	113.58	108.27
30	MG	402	PUB	CAD-C3D-C4D	6.16	131.11	121.38
29	iF	202	PEB	C1C-CHB-C4B	6.14	136.15	128.81
29	iI	202	PEB	C1C-CHB-C4B	6.14	136.15	128.81
31	UP	1001	CYC	CMA-C3A-C4A	6.14	134.51	125.06
30	MQ	404	PUB	CAD-C3D-C4D	6.13	131.07	121.38
31	jP	1001	CYC	CMA-C3A-C4A	6.13	134.51	125.06
31	MP	1001	CYC	CMA-C3A-C4A	6.13	134.50	125.06
30	AB	305	PUB	CAD-C3D-C4D	6.13	131.06	121.38
29	mB	203	PEB	C1C-CHB-C4B	-6.13	121.49	128.81
29	mM	203	PEB	C1C-CHB-C4B	-6.13	121.49	128.81
29	rJ	201	PEB	C2A-C1A-NA	6.12	113.55	108.27
29	rL	201	PEB	C2A-C1A-NA	6.12	113.55	108.27
31	FP	1001	CYC	CMA-C3A-C4A	6.12	134.49	125.06
31	oP	1001	CYC	CMA-C3A-C4A	6.12	134.49	125.06
31	BP	1001	CYC	CMA-C3A-C4A	6.12	134.49	125.06
31	SP	1001	CYC	CMA-C3A-C4A	6.12	134.49	125.06
31	nP	1001	CYC	CMA-C3A-C4A	6.12	134.49	125.06
31	hP	1001	CYC	CMA-C3A-C4A	6.11	134.48	125.06
31	wP	1001	CYC	CMA-C3A-C4A	6.11	134.47	125.06
29	NB	202	PEB	C1C-CHB-C4B	-6.11	121.51	128.81
29	NM	202	PEB	C1C-CHB-C4B	-6.11	121.51	128.81
31	XP	1001	CYC	CMA-C3A-C4A	6.11	134.47	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	uP	1001	CYC	CMA-C3A-C4A	6.11	134.47	125.06
29	FB	203	PEB	C1C-CHB-C4B	-6.10	121.52	128.81
29	FM	203	PEB	C1C-CHB-C4B	-6.10	121.52	128.81
31	IP	1001	CYC	CMA-C3A-C4A	6.10	134.46	125.06
29	AC	202	PEB	CHB-C4B-NB	-6.10	120.36	128.83
29	AE	202	PEB	CHB-C4B-NB	-6.10	120.36	128.83
29	RB	203	PEB	C1C-CHB-C4B	-6.10	121.53	128.81
29	RM	203	PEB	C1C-CHB-C4B	-6.10	121.53	128.81
29	NR	202	PEB	OA-C1A-C2A	-6.10	121.33	126.17
29	LB	203	PEB	C1C-CHB-C4B	-6.10	121.53	128.81
29	LM	203	PEB	C1C-CHB-C4B	-6.10	121.53	128.81
31	QP	1001	CYC	CMA-C3A-C4A	6.09	134.45	125.06
29	kB	203	PEB	C1C-CHB-C4B	-6.09	121.53	128.81
29	kM	203	PEB	C1C-CHB-C4B	-6.09	121.53	128.81
31	lP	1001	CYC	CMA-C3A-C4A	6.09	134.45	125.06
31	HP	1001	CYC	CMA-C3A-C4A	6.09	134.45	125.06
31	kP	1001	CYC	CMA-C3A-C4A	6.09	134.45	125.06
31	sP	1001	CYC	CMA-C3A-C4A	6.09	134.45	125.06
31	qP	1001	CYC	CMA-C3A-C4A	6.09	134.44	125.06
31	fP	1001	CYC	CMA-C3A-C4A	6.09	134.44	125.06
31	OP	1001	CYC	CMA-C3A-C4A	6.09	134.44	125.06
30	AF	303	PUB	CBA-CAA-C3A	-6.09	103.75	112.98
30	AI	303	PUB	CBA-CAA-C3A	-6.09	103.75	112.98
29	DB	203	PEB	C1C-CHB-C4B	-6.09	121.54	128.81
29	DM	203	PEB	C1C-CHB-C4B	-6.09	121.54	128.81
30	AM	305	PUB	CAD-C3D-C4D	6.08	130.99	121.38
31	DP	1001	CYC	CMA-C3A-C4A	6.08	134.43	125.06
31	VP	1001	CYC	OB-C4B-C3B	-6.08	121.44	128.04
29	GC	202	PEB	CHB-C4B-NB	-6.08	120.40	128.83
29	GE	202	PEB	CHB-C4B-NB	-6.08	120.40	128.83
29	HB	203	PEB	C1C-CHB-C4B	-6.08	121.55	128.81
29	HM	203	PEB	C1C-CHB-C4B	-6.08	121.55	128.81
29	gB	203	PEB	C1C-CHB-C4B	-6.08	121.55	128.81
29	gM	203	PEB	C1C-CHB-C4B	-6.08	121.55	128.81
29	PB	202	PEB	C1C-CHB-C4B	-6.07	121.56	128.81
29	PM	202	PEB	C1C-CHB-C4B	-6.07	121.56	128.81
31	VP	1001	CYC	CAA-C2A-C1A	6.07	135.75	125.01
30	A1	305	PUB	OD-C4D-C3D	-6.07	121.45	128.04
30	AK	305	PUB	OD-C4D-C3D	-6.07	121.45	128.04
29	XB	202	PEB	C1C-CHB-C4B	-6.07	121.56	128.81
29	XM	202	PEB	C1C-CHB-C4B	-6.07	121.56	128.81
29	N2	202	PEB	OA-C1A-C2A	-6.07	121.35	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VB	203	PEB	C1C-CHB-C4B	-6.07	121.56	128.81
29	VM	203	PEB	C1C-CHB-C4B	-6.07	121.56	128.81
29	eB	202	PEB	C1C-CHB-C4B	-6.06	121.56	128.81
29	eM	202	PEB	C1C-CHB-C4B	-6.06	121.56	128.81
29	iB	203	PEB	C1C-CHB-C4B	-6.06	121.57	128.81
29	iM	203	PEB	C1C-CHB-C4B	-6.06	121.57	128.81
29	EC	202	PEB	CHB-C4B-NB	-6.06	120.42	128.83
29	EE	202	PEB	CHB-C4B-NB	-6.06	120.42	128.83
29	X2	201	PEB	OA-C1A-C2A	-6.06	121.36	126.17
29	KC	203	PEB	CHB-C4B-NB	-6.06	120.42	128.83
29	KE	203	PEB	CHB-C4B-NB	-6.06	120.42	128.83
29	ZB	203	PEB	C1C-CHB-C4B	-6.06	121.57	128.81
29	ZM	203	PEB	C1C-CHB-C4B	-6.06	121.57	128.81
30	MA	402	PUB	CAD-C3D-C4D	6.05	130.94	121.38
29	IC	202	PEB	CHB-C4B-NB	-6.05	120.44	128.83
29	IE	202	PEB	CHB-C4B-NB	-6.05	120.44	128.83
29	TB	203	PEB	C1C-CHB-C4B	-6.05	121.59	128.81
29	TM	203	PEB	C1C-CHB-C4B	-6.05	121.59	128.81
31	xP	1001	CYC	CAA-C2A-C1A	6.04	135.71	125.01
30	MN	402	PUB	CAD-C3D-C4D	6.04	130.93	121.38
29	JB	203	PEB	C1C-CHB-C4B	-6.04	121.59	128.81
29	JM	203	PEB	C1C-CHB-C4B	-6.04	121.59	128.81
29	CC	202	PEB	CHB-C4B-NB	-6.04	120.45	128.83
29	CE	202	PEB	CHB-C4B-NB	-6.04	120.45	128.83
29	cB	203	PEB	C1C-CHB-C4B	-6.04	121.59	128.81
29	cM	203	PEB	C1C-CHB-C4B	-6.04	121.59	128.81
29	uJ	202	PEB	CMB-C2B-C1B	6.04	134.36	125.06
29	uL	202	PEB	CMB-C2B-C1B	6.04	134.36	125.06
29	XR	202	PEB	OA-C1A-C2A	-6.04	121.37	126.17
29	PR	201	PEB	OA-C1A-C2A	-6.03	121.38	126.17
29	AJ	201	PEB	CMB-C2B-C1B	6.03	134.35	125.06
29	AL	201	PEB	CMB-C2B-C1B	6.03	134.35	125.06
31	xP	1001	CYC	OB-C4B-C3B	-6.03	121.49	128.04
29	SJ	201	PEB	CMB-C2B-C1B	6.03	134.35	125.06
29	SL	201	PEB	CMB-C2B-C1B	6.03	134.35	125.06
30	A7	303	PUB	OD-C4D-C3D	-6.03	121.50	128.04
30	A9	303	PUB	OD-C4D-C3D	-6.03	121.50	128.04
29	UJ	201	PEB	CMB-C2B-C1B	6.03	134.34	125.06
29	UL	201	PEB	CMB-C2B-C1B	6.03	134.34	125.06
29	YJ	201	PEB	CMB-C2B-C1B	6.03	134.34	125.06
29	YL	201	PEB	CMB-C2B-C1B	6.03	134.34	125.06
29	EJ	201	PEB	CMB-C2B-C1B	6.02	134.34	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EL	201	PEB	CMB-C2B-C1B	6.02	134.34	125.06
29	RR	202	PEB	OA-C1A-C2A	-6.02	121.39	126.17
29	aJ	201	PEB	CMB-C2B-C1B	6.02	134.34	125.06
29	aL	201	PEB	CMB-C2B-C1B	6.02	134.34	125.06
29	eJ	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
29	eL	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
29	oJ	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
29	oL	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
29	KJ	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
29	KL	201	PEB	CMB-C2B-C1B	6.02	134.33	125.06
29	wJ	302	PEB	CHB-C4B-NB	-6.02	120.48	128.83
29	QJ	201	PEB	CMB-C2B-C1B	6.01	134.33	125.06
29	QL	201	PEB	CMB-C2B-C1B	6.01	134.33	125.06
30	MG	402	PUB	OD-C4D-C3D	-6.01	121.51	128.04
30	MQ	404	PUB	OD-C4D-C3D	-6.01	121.52	128.04
29	gJ	201	PEB	CMB-C2B-C1B	6.01	134.32	125.06
29	gL	201	PEB	CMB-C2B-C1B	6.01	134.32	125.06
29	VR	202	PEB	OA-C1A-C2A	-6.01	121.39	126.17
29	TR	202	PEB	OA-C1A-C2A	-6.01	121.40	126.17
29	MJ	201	PEB	CMB-C2B-C1B	6.01	134.32	125.06
29	WJ	202	PEB	CMB-C2B-C1B	6.01	134.32	125.06
29	ML	201	PEB	CMB-C2B-C1B	6.01	134.32	125.06
29	WL	202	PEB	CMB-C2B-C1B	6.01	134.32	125.06
29	GJ	201	PEB	CMB-C2B-C1B	6.01	134.31	125.06
29	GL	201	PEB	CMB-C2B-C1B	6.01	134.31	125.06
29	cJ	201	PEB	CMB-C2B-C1B	6.00	134.31	125.06
29	cL	201	PEB	CMB-C2B-C1B	6.00	134.31	125.06
29	OJ	201	PEB	CMB-C2B-C1B	6.00	134.31	125.06
29	OL	201	PEB	CMB-C2B-C1B	6.00	134.31	125.06
29	sJ	201	PEB	CMB-C2B-C1B	6.00	134.31	125.06
29	sL	201	PEB	CMB-C2B-C1B	6.00	134.31	125.06
29	T2	202	PEB	OA-C1A-C2A	-6.00	121.40	126.17
30	A7	302	PUB	OD-C4D-C3D	-6.00	121.53	128.04
30	A9	302	PUB	OD-C4D-C3D	-6.00	121.53	128.04
29	CJ	201	PEB	CMB-C2B-C1B	6.00	134.30	125.06
29	CL	201	PEB	CMB-C2B-C1B	6.00	134.30	125.06
29	iJ	201	PEB	CMB-C2B-C1B	6.00	134.30	125.06
29	iL	201	PEB	CMB-C2B-C1B	6.00	134.30	125.06
29	kJ	201	PEB	CMB-C2B-C1B	5.99	134.30	125.06
29	kL	201	PEB	CMB-C2B-C1B	5.99	134.30	125.06
29	wL	302	PEB	CHB-C4B-NB	-5.99	120.51	128.83
29	V2	202	PEB	OA-C1A-C2A	-5.99	121.41	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mJ	201	PEB	CMB-C2B-C1B	5.99	134.28	125.06
29	mL	201	PEB	CMB-C2B-C1B	5.99	134.28	125.06
29	IJ	201	PEB	CMB-C2B-C1B	5.99	134.28	125.06
29	IL	201	PEB	CMB-C2B-C1B	5.99	134.28	125.06
29	xL	302	PEB	CHB-C4B-NB	-5.98	120.54	128.83
29	qJ	201	PEB	CMB-C2B-C1B	5.98	134.27	125.06
29	qL	201	PEB	CMB-C2B-C1B	5.98	134.27	125.06
29	O7	201	PEB	C1C-CHB-C4B	5.97	135.94	128.81
29	O9	201	PEB	C1C-CHB-C4B	5.97	135.94	128.81
29	R2	202	PEB	OA-C1A-C2A	-5.97	121.43	126.17
29	P2	201	PEB	OA-C1A-C2A	-5.97	121.43	126.17
31	1P	1002	CYC	CHD-C4C-NC	5.96	132.29	125.20
29	S7	201	PEB	C1C-CHB-C4B	5.95	135.92	128.81
29	S9	201	PEB	C1C-CHB-C4B	5.95	135.92	128.81
29	xJ	302	PEB	CHB-C4B-NB	-5.95	120.58	128.83
29	U7	201	PEB	C1C-CHB-C4B	5.95	135.91	128.81
29	U9	201	PEB	C1C-CHB-C4B	5.95	135.91	128.81
30	wJ	304	PUB	OD-C4D-C3D	-5.94	121.59	128.04
29	d7	201	PEB	C1C-CHB-C4B	5.94	135.90	128.81
29	d9	201	PEB	C1C-CHB-C4B	5.94	135.90	128.81
29	Q7	201	PEB	C1C-CHB-C4B	5.93	135.90	128.81
29	l7	201	PEB	C1C-CHB-C4B	5.93	135.90	128.81
29	Q9	201	PEB	C1C-CHB-C4B	5.93	135.90	128.81
29	l9	201	PEB	C1C-CHB-C4B	5.93	135.90	128.81
29	AM	301	PEB	CHB-C4B-NB	-5.93	120.60	128.83
29	j7	201	PEB	C1C-CHB-C4B	5.93	135.89	128.81
29	j9	201	PEB	C1C-CHB-C4B	5.93	135.89	128.81
29	AB	301	PEB	CHB-C4B-NB	-5.92	120.61	128.83
29	f7	201	PEB	C1C-CHB-C4B	5.92	135.88	128.81
29	f9	201	PEB	C1C-CHB-C4B	5.92	135.88	128.81
29	h7	201	PEB	C1C-CHB-C4B	5.92	135.88	128.81
29	h9	201	PEB	C1C-CHB-C4B	5.92	135.88	128.81
29	b7	201	PEB	C1C-CHB-C4B	5.91	135.87	128.81
29	b9	201	PEB	C1C-CHB-C4B	5.91	135.87	128.81
30	yJ	303	PUB	OD-C4D-C3D	-5.91	121.62	128.04
29	W7	201	PEB	C1C-CHB-C4B	5.91	135.87	128.81
29	W9	201	PEB	C1C-CHB-C4B	5.91	135.87	128.81
30	wL	304	PUB	OD-C4D-C3D	-5.91	121.63	128.04
30	xL	304	PUB	OD-C4D-C3D	-5.90	121.63	128.04
30	yL	303	PUB	OD-C4D-C3D	-5.90	121.64	128.04
31	YP	1000	CYC	CHD-C4C-NC	5.90	132.22	125.20
31	WP	1001	CYC	CHB-C4A-NA	-5.89	112.61	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	yP	1001	CYC	CHB-C4A-NA	-5.89	112.61	124.93
30	xJ	304	PUB	OD-C4D-C3D	-5.89	121.65	128.04
29	Z7	201	PEB	C1C-CHB-C4B	5.88	135.83	128.81
29	Z9	201	PEB	C1C-CHB-C4B	5.88	135.83	128.81
31	D7	1001	CYC	OB-C4B-C3B	-5.86	121.68	128.04
31	D9	1001	CYC	OB-C4B-C3B	-5.86	121.68	128.04
31	F9	1001	CYC	OB-C4B-C3B	-5.86	121.68	128.04
31	LF	1001	CYC	OB-C4B-C3B	-5.84	121.70	128.04
31	LI	1001	CYC	OB-C4B-C3B	-5.84	121.70	128.04
31	AP	1001	CYC	CHD-C4C-NC	5.84	132.15	125.20
31	tP	1001	CYC	CHD-C4C-NC	5.84	132.15	125.20
31	F7	1001	CYC	OB-C4B-C3B	-5.84	121.70	128.04
31	N7	1001	CYC	OB-C4B-C3B	-5.84	121.70	128.04
31	N9	1001	CYC	OB-C4B-C3B	-5.84	121.70	128.04
31	GP	1001	CYC	CHD-C4C-NC	5.84	132.15	125.20
31	FF	1001	CYC	OB-C4B-C3B	-5.84	121.71	128.04
31	FI	1001	CYC	OB-C4B-C3B	-5.84	121.71	128.04
31	L9	1001	CYC	OB-C4B-C3B	-5.83	121.72	128.04
31	mP	1001	CYC	CHD-C4C-NC	5.83	132.13	125.20
31	JP	1001	CYC	CHD-C4C-NC	5.82	132.13	125.20
31	JF	1001	CYC	OB-C4B-C3B	-5.82	121.73	128.04
31	JI	1001	CYC	OB-C4B-C3B	-5.82	121.73	128.04
31	TP	1001	CYC	CHD-C4C-NC	5.82	132.12	125.20
31	DF	1001	CYC	OB-C4B-C3B	-5.81	121.73	128.04
31	DI	1001	CYC	OB-C4B-C3B	-5.81	121.73	128.04
31	PP	1001	CYC	CHD-C4C-NC	5.81	132.12	125.20
31	L7	1001	CYC	OB-C4B-C3B	-5.81	121.73	128.04
31	iP	1001	CYC	CHD-C4C-NC	5.81	132.11	125.20
31	NF	1001	CYC	OB-C4B-C3B	-5.81	121.74	128.04
31	NI	1001	CYC	OB-C4B-C3B	-5.81	121.74	128.04
29	i7	203	PEB	CHB-C4B-NB	-5.81	120.77	128.83
29	i9	203	PEB	CHB-C4B-NB	-5.81	120.77	128.83
31	H7	1001	CYC	OB-C4B-C3B	-5.81	121.74	128.04
31	H9	1001	CYC	OB-C4B-C3B	-5.81	121.74	128.04
31	J7	1001	CYC	OB-C4B-C3B	-5.80	121.74	128.04
31	vP	1001	CYC	CHD-C4C-NC	5.80	132.10	125.20
29	Y7	203	PEB	CHB-C4B-NB	-5.80	120.78	128.83
29	c7	203	PEB	CHB-C4B-NB	-5.80	120.78	128.83
29	Y9	203	PEB	CHB-C4B-NB	-5.80	120.78	128.83
29	c9	203	PEB	CHB-C4B-NB	-5.80	120.78	128.83
29	T7	203	PEB	CHB-C4B-NB	-5.80	120.78	128.83
29	T9	203	PEB	CHB-C4B-NB	-5.80	120.78	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	J9	1001	CYC	OB-C4B-C3B	-5.80	121.75	128.04
29	m7	203	PEB	CHB-C4B-NB	-5.80	120.79	128.83
29	m9	203	PEB	CHB-C4B-NB	-5.80	120.79	128.83
29	ID	203	PEB	CHB-C4B-NB	-5.79	120.79	128.83
29	S2	201	PEB	CHB-C4B-NB	-5.79	120.79	128.83
31	HF	1001	CYC	OB-C4B-C3B	-5.79	121.75	128.04
31	HI	1001	CYC	OB-C4B-C3B	-5.79	121.75	128.04
31	IP	1001	CYC	CHD-C4C-NC	5.79	132.09	125.20
29	P7	203	PEB	CHB-C4B-NB	-5.79	120.80	128.83
29	P9	203	PEB	CHB-C4B-NB	-5.79	120.80	128.83
31	EP	1001	CYC	CHD-C4C-NC	5.79	132.09	125.20
29	e7	203	PEB	CHB-C4B-NB	-5.79	120.80	128.83
29	e9	203	PEB	CHB-C4B-NB	-5.79	120.80	128.83
29	k7	203	PEB	CHB-C4B-NB	-5.79	120.80	128.83
29	k9	203	PEB	CHB-C4B-NB	-5.79	120.80	128.83
29	g7	202	PEB	CHC-C4C-C3C	-5.78	120.47	130.34
29	g9	202	PEB	CHC-C4C-C3C	-5.78	120.47	130.34
29	AF	301	PEB	CHB-C4B-NB	-5.78	120.81	128.83
29	AI	301	PEB	CHB-C4B-NB	-5.78	120.81	128.83
31	RP	1001	CYC	CHD-C4C-NC	5.78	132.08	125.20
29	KD	203	PEB	CHB-C4B-NB	-5.78	120.81	128.83
31	gP	1001	CYC	CHD-C4C-NC	5.78	132.08	125.20
29	MQ	406	PEB	CHB-C4B-NB	-5.78	120.81	128.83
31	pP	1001	CYC	CHD-C4C-NC	5.78	132.08	125.20
29	R7	202	PEB	CHC-C4C-C3C	-5.78	120.48	130.34
29	T7	202	PEB	CHC-C4C-C3C	-5.78	120.48	130.34
29	i7	202	PEB	CHC-C4C-C3C	-5.78	120.48	130.34
29	R9	202	PEB	CHC-C4C-C3C	-5.78	120.48	130.34
29	T9	202	PEB	CHC-C4C-C3C	-5.78	120.48	130.34
29	i9	202	PEB	CHC-C4C-C3C	-5.78	120.48	130.34
31	NP	1001	CYC	CHD-C4C-NC	5.78	132.08	125.20
30	yJ	303	PUB	C4B-CHB-C1C	-5.78	121.91	128.81
29	c7	202	PEB	CHC-C4C-C3C	-5.77	120.49	130.34
29	c9	202	PEB	CHC-C4C-C3C	-5.77	120.49	130.34
29	GD	203	PEB	CHB-C4B-NB	-5.77	120.82	128.83
31	eP	1001	CYC	CHD-C4C-NC	5.77	132.07	125.20
30	yL	303	PUB	C4B-CHB-C1C	-5.77	121.91	128.81
31	KP	1001	CYC	CHD-C4C-NC	5.77	132.06	125.20
29	R7	203	PEB	CHB-C4B-NB	-5.77	120.83	128.83
29	R9	203	PEB	CHB-C4B-NB	-5.77	120.83	128.83
29	K4	203	PEB	CHB-C4B-NB	-5.77	120.83	128.83
29	Y7	202	PEB	CHC-C4C-C3C	-5.77	120.50	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y9	202	PEB	CHC-C4C-C3C	-5.77	120.50	130.34
29	MD	203	PEB	CHB-C4B-NB	-5.77	120.83	128.83
29	k7	202	PEB	CHC-C4C-C3C	-5.76	120.50	130.34
29	k9	202	PEB	CHC-C4C-C3C	-5.76	120.50	130.34
29	a7	203	PEB	CHB-C4B-NB	-5.76	120.83	128.83
29	a9	203	PEB	CHB-C4B-NB	-5.76	120.83	128.83
29	a7	202	PEB	CHC-C4C-C3C	-5.76	120.51	130.34
29	a9	202	PEB	CHC-C4C-C3C	-5.76	120.51	130.34
31	CP	1001	CYC	CHD-C4C-NC	5.76	132.06	125.20
29	m7	202	PEB	CHC-C4C-C3C	-5.76	120.51	130.34
29	m9	202	PEB	CHC-C4C-C3C	-5.76	120.51	130.34
30	MA	402	PUB	OD-C4D-C3D	-5.76	121.79	128.04
31	rP	1001	CYC	CHD-C4C-NC	5.76	132.05	125.20
29	e7	202	PEB	CHC-C4C-C3C	-5.75	120.52	130.34
29	e9	202	PEB	CHC-C4C-C3C	-5.75	120.52	130.34
29	E4	203	PEB	CHB-C4B-NB	-5.75	120.85	128.83
29	g7	203	PEB	CHB-C4B-NB	-5.75	120.85	128.83
29	g9	203	PEB	CHB-C4B-NB	-5.75	120.85	128.83
29	G4	203	PEB	CHB-C4B-NB	-5.75	120.85	128.83
29	V7	202	PEB	CHC-C4C-C3C	-5.75	120.53	130.34
29	V9	202	PEB	CHC-C4C-C3C	-5.75	120.53	130.34
31	cP	1001	CYC	CHD-C4C-NC	5.75	132.04	125.20
29	MG	404	PEB	CHB-C4B-NB	-5.75	120.86	128.83
29	P7	202	PEB	CHC-C4C-C3C	-5.74	120.55	130.34
29	P9	202	PEB	CHC-C4C-C3C	-5.74	120.55	130.34
31	1P	1001	CYC	CHD-C4C-NC	5.74	132.03	125.20
29	C4	203	PEB	CHB-C4B-NB	-5.74	120.87	128.83
29	V7	203	PEB	CHB-C4B-NB	-5.74	120.87	128.83
29	V9	203	PEB	CHB-C4B-NB	-5.74	120.87	128.83
30	MN	402	PUB	OD-C4D-C3D	-5.73	121.82	128.04
31	fP	1001	CYC	CHD-C4C-NC	5.73	132.01	125.20
29	CD	203	PEB	CHB-C4B-NB	-5.73	120.88	128.83
31	wP	1001	CYC	CHD-C4C-NC	5.73	132.01	125.20
31	UP	1001	CYC	CHD-C4C-NC	5.72	132.01	125.20
29	ED	202	PEB	CHB-C4B-NB	-5.72	120.89	128.83
31	jP	1001	CYC	CHD-C4C-NC	5.72	132.00	125.20
31	sP	1001	CYC	CHD-C4C-NC	5.72	132.00	125.20
31	nP	1001	CYC	CHD-C4C-NC	5.71	132.00	125.20
31	HP	1001	CYC	CHD-C4C-NC	5.71	131.99	125.20
29	P7	202	PEB	C1C-CHB-C4B	5.70	135.62	128.81
29	P9	202	PEB	C1C-CHB-C4B	5.70	135.62	128.81
31	qP	1001	CYC	CHD-C4C-NC	5.70	131.98	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	FP	1001	CYC	CHD-C4C-NC	5.70	131.98	125.20
30	MQ	405	PUB	CHA-C4A-NA	-5.70	107.33	113.95
29	KD	202	PEB	C1C-CHB-C4B	5.69	135.61	128.81
31	OP	1001	CYC	CHD-C4C-NC	5.69	131.97	125.20
29	E4	202	PEB	C1C-CHB-C4B	5.69	135.61	128.81
29	M4	202	PEB	C1C-CHB-C4B	5.69	135.61	128.81
31	uP	1001	CYC	CHD-C4C-NC	5.69	131.97	125.20
31	hP	1001	CYC	CHD-C4C-NC	5.69	131.97	125.20
29	GD	202	PEB	C1C-CHB-C4B	5.69	135.60	128.81
31	BP	1001	CYC	CHD-C4C-NC	5.69	131.97	125.20
31	XP	1001	CYC	CHD-C4C-NC	5.69	131.97	125.20
31	DP	1001	CYC	CHD-C4C-NC	5.69	131.97	125.20
31	NK	1001	CYC	CMB-C2B-C1B	5.69	131.27	124.17
29	ED	201	PEB	C1C-CHB-C4B	5.69	135.60	128.81
29	LD	202	PEB	CHC-C1D-ND	-5.68	107.35	113.95
31	MP	1001	CYC	CHD-C4C-NC	5.68	131.96	125.20
29	V7	202	PEB	C1C-CHB-C4B	5.68	135.59	128.81
29	V9	202	PEB	C1C-CHB-C4B	5.68	135.59	128.81
30	MG	403	PUB	CHA-C4A-NA	-5.68	107.35	113.95
29	M3	202	PEB	CHB-C4B-NB	-5.68	120.95	128.83
29	MO	202	PEB	CHB-C4B-NB	-5.68	120.95	128.83
29	CD	202	PEB	C1C-CHB-C4B	5.68	135.59	128.81
31	SP	1001	CYC	CHD-C4C-NC	5.68	131.95	125.20
29	T7	202	PEB	C1C-CHB-C4B	5.67	135.59	128.81
29	T9	202	PEB	C1C-CHB-C4B	5.67	135.59	128.81
29	g7	202	PEB	C1C-CHB-C4B	5.67	135.59	128.81
29	g9	202	PEB	C1C-CHB-C4B	5.67	135.59	128.81
29	Y7	202	PEB	C1C-CHB-C4B	5.67	135.58	128.81
29	Y9	202	PEB	C1C-CHB-C4B	5.67	135.58	128.81
29	NO	202	PEB	CHB-C4B-NB	-5.67	120.96	128.83
29	L4	202	PEB	CHC-C1D-ND	-5.67	107.36	113.95
31	F1	1001	CYC	CMB-C2B-C1B	5.67	131.25	124.17
31	FK	1001	CYC	CMB-C2B-C1B	5.67	131.25	124.17
31	oP	1001	CYC	CHD-C4C-NC	5.67	131.94	125.20
29	K4	202	PEB	C1C-CHB-C4B	5.67	135.58	128.81
29	MG	404	PEB	C1C-CHB-C4B	-5.67	122.04	128.81
29	N3	202	PEB	CHB-C4B-NB	-5.67	120.97	128.83
31	IP	1001	CYC	CHD-C4C-NC	5.66	131.94	125.20
29	c7	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
29	c9	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
31	QP	1001	CYC	CHD-C4C-NC	5.66	131.94	125.20
29	m7	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	m9	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
29	e7	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
29	e9	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
31	HK	1001	CYC	CMB-C2B-C1B	5.66	131.24	124.17
29	i7	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
29	k7	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
29	i9	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
29	k9	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
31	DK	1001	CYC	CMB-C2B-C1B	5.66	131.23	124.17
31	D1	1001	CYC	CMB-C2B-C1B	5.65	131.23	124.17
31	N1	1001	CYC	CMB-C2B-C1B	5.65	131.23	124.17
30	BB	302	PUB	CHB-C1C-NC	-5.65	120.99	128.83
30	BM	302	PUB	CHB-C1C-NC	-5.65	120.99	128.83
31	L1	1001	CYC	CMB-C2B-C1B	5.65	131.22	124.17
31	LK	1001	CYC	CMB-C2B-C1B	5.65	131.22	124.17
31	FF	1001	CYC	CMA-C3A-C4A	5.65	133.76	125.06
31	FI	1001	CYC	CMA-C3A-C4A	5.65	133.76	125.06
29	G4	202	PEB	C1C-CHB-C4B	5.65	135.56	128.81
29	R7	202	PEB	C1C-CHB-C4B	5.65	135.56	128.81
29	R9	202	PEB	C1C-CHB-C4B	5.65	135.56	128.81
31	HF	1001	CYC	CMA-C3A-C4A	5.65	133.76	125.06
31	HI	1001	CYC	CMA-C3A-C4A	5.65	133.76	125.06
29	J4	202	PEB	CHC-C1D-ND	-5.65	107.39	113.95
29	JD	202	PEB	CHC-C1D-ND	-5.65	107.39	113.95
29	dF	201	PEB	CHC-C4C-C3C	-5.64	120.71	130.34
29	dI	201	PEB	CHC-C4C-C3C	-5.64	120.71	130.34
29	C4	202	PEB	C1C-CHB-C4B	5.64	135.55	128.81
31	JF	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
31	JI	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
31	kP	1001	CYC	CHD-C4C-NC	5.64	131.91	125.20
31	NF	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
31	NI	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
29	UF	201	PEB	CHC-C4C-C3C	-5.64	120.72	130.34
29	UI	201	PEB	CHC-C4C-C3C	-5.64	120.72	130.34
29	gF	202	PEB	CHC-C4C-C3C	-5.64	120.72	130.34
29	gI	202	PEB	CHC-C4C-C3C	-5.64	120.72	130.34
29	MQ	406	PEB	C1C-CHB-C4B	-5.64	122.07	128.81
31	DF	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
31	DI	1001	CYC	CMA-C3A-C4A	5.64	133.75	125.06
29	I4	202	PEB	C1C-CHB-C4B	5.64	135.54	128.81
29	IJ	202	PEB	CHB-C4B-NB	-5.64	121.01	128.83
29	IL	202	PEB	CHB-C4B-NB	-5.64	121.01	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GJ	202	PEB	CHB-C4B-NB	-5.63	121.01	128.83
29	iJ	202	PEB	CHB-C4B-NB	-5.63	121.01	128.83
29	GL	202	PEB	CHB-C4B-NB	-5.63	121.01	128.83
29	iL	202	PEB	CHB-C4B-NB	-5.63	121.01	128.83
29	iF	202	PEB	CHC-C4C-C3C	-5.63	120.73	130.34
29	iI	202	PEB	CHC-C4C-C3C	-5.63	120.73	130.34
31	LF	1001	CYC	CMA-C3A-C4A	5.63	133.73	125.06
31	LI	1001	CYC	CMA-C3A-C4A	5.63	133.73	125.06
29	PF	202	PEB	CHC-C4C-C3C	-5.63	120.74	130.34
29	PI	202	PEB	CHC-C4C-C3C	-5.63	120.74	130.34
29	MD	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
29	cJ	202	PEB	CHB-C4B-NB	-5.63	121.02	128.83
29	cL	202	PEB	CHB-C4B-NB	-5.63	121.02	128.83
29	oJ	202	PEB	CHB-C4B-NB	-5.63	121.02	128.83
29	oL	202	PEB	CHB-C4B-NB	-5.63	121.02	128.83
29	JA	201	PEB	CHC-C1D-ND	-5.63	107.41	113.95
29	FD	202	PEB	CHC-C1D-ND	-5.63	107.41	113.95
29	JN	201	PEB	CHC-C1D-ND	-5.63	107.41	113.95
29	eF	202	PEB	CHC-C4C-C3C	-5.63	120.74	130.34
29	eI	202	PEB	CHC-C4C-C3C	-5.63	120.74	130.34
29	H4	202	PEB	CHC-C1D-ND	-5.63	107.42	113.95
29	EJ	202	PEB	CHB-C4B-NB	-5.62	121.03	128.83
29	EL	202	PEB	CHB-C4B-NB	-5.62	121.03	128.83
29	F4	202	PEB	CHC-C1D-ND	-5.62	107.42	113.95
29	gJ	202	PEB	CHB-C4B-NB	-5.62	121.03	128.83
29	gL	202	PEB	CHB-C4B-NB	-5.62	121.03	128.83
29	VF	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	aF	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	VI	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	aI	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	DA	201	PEB	CHC-C1D-ND	-5.62	107.42	113.95
29	DD	202	PEB	CHC-C1D-ND	-5.62	107.42	113.95
29	DN	201	PEB	CHC-C1D-ND	-5.62	107.42	113.95
29	kF	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	kI	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	a7	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
29	a9	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
29	mF	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	mI	202	PEB	CHC-C4C-C3C	-5.62	120.75	130.34
29	OF	203	PEB	CHC-C4C-C3C	-5.62	120.76	130.34
29	OI	203	PEB	CHC-C4C-C3C	-5.62	120.76	130.34
29	HD	202	PEB	CHC-C1D-ND	-5.62	107.42	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FA	201	PEB	CHC-C1D-ND	-5.61	107.43	113.95
29	FN	201	PEB	CHC-C1D-ND	-5.61	107.43	113.95
29	KJ	202	PEB	CHB-C4B-NB	-5.61	121.04	128.83
29	KL	202	PEB	CHB-C4B-NB	-5.61	121.04	128.83
29	YF	202	PEB	CHC-C4C-C3C	-5.61	120.76	130.34
29	YI	202	PEB	CHC-C4C-C3C	-5.61	120.76	130.34
29	kJ	202	PEB	CHB-C4B-NB	-5.61	121.04	128.83
29	kL	202	PEB	CHB-C4B-NB	-5.61	121.04	128.83
29	ID	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
29	mJ	202	PEB	CHB-C4B-NB	-5.61	121.04	128.83
29	mL	202	PEB	CHB-C4B-NB	-5.61	121.04	128.83
29	BD	202	PEB	CHC-C1D-ND	-5.61	107.43	113.95
31	H1	1001	CYC	CMB-C2B-C1B	5.61	131.17	124.17
29	CJ	202	PEB	CHB-C4B-NB	-5.61	121.05	128.83
29	OJ	202	PEB	CHB-C4B-NB	-5.61	121.05	128.83
29	CL	202	PEB	CHB-C4B-NB	-5.61	121.05	128.83
29	OL	202	PEB	CHB-C4B-NB	-5.61	121.05	128.83
29	BA	201	PEB	CHC-C1D-ND	-5.61	107.44	113.95
29	BN	201	PEB	CHC-C1D-ND	-5.61	107.44	113.95
29	YJ	202	PEB	CHB-C4B-NB	-5.61	121.05	128.83
29	YL	202	PEB	CHB-C4B-NB	-5.61	121.05	128.83
29	aJ	202	PEB	CHB-C4B-NB	-5.60	121.05	128.83
29	aL	202	PEB	CHB-C4B-NB	-5.60	121.05	128.83
31	J1	1001	CYC	CMB-C2B-C1B	5.60	131.17	124.17
31	JK	1001	CYC	CMB-C2B-C1B	5.60	131.17	124.17
29	WJ	203	PEB	CHB-C4B-NB	-5.60	121.06	128.83
29	WL	203	PEB	CHB-C4B-NB	-5.60	121.06	128.83
29	D4	202	PEB	CHC-C1D-ND	-5.60	107.45	113.95
29	uJ	203	PEB	CHB-C4B-NB	-5.60	121.06	128.83
29	uL	203	PEB	CHB-C4B-NB	-5.60	121.06	128.83
29	MJ	202	PEB	CHB-C4B-NB	-5.60	121.06	128.83
29	ML	202	PEB	CHB-C4B-NB	-5.60	121.06	128.83
29	B4	202	PEB	CHC-C1D-ND	-5.60	107.45	113.95
30	A1	305	PUB	CHA-C1B-C2B	-5.60	120.79	130.34
30	AK	305	PUB	CHA-C1B-C2B	-5.60	120.79	130.34
29	QJ	202	PEB	CHB-C4B-NB	-5.60	121.07	128.83
29	QL	202	PEB	CHB-C4B-NB	-5.60	121.07	128.83
29	LA	201	PEB	CHC-C1D-ND	-5.60	107.45	113.95
29	LN	201	PEB	CHC-C1D-ND	-5.60	107.45	113.95
29	sJ	202	PEB	CHB-C4B-NB	-5.59	121.07	128.83
29	sL	202	PEB	CHB-C4B-NB	-5.59	121.07	128.83
30	QB	201	PUB	CHC-C1D-ND	-5.59	106.65	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	QM	201	PUB	CHC-C1D-ND	-5.59	106.65	113.72
29	HA	201	PEB	CHC-C1D-ND	-5.59	107.45	113.95
29	HN	201	PEB	CHC-C1D-ND	-5.59	107.45	113.95
29	AJ	202	PEB	CHB-C4B-NB	-5.59	121.07	128.83
29	AL	202	PEB	CHB-C4B-NB	-5.59	121.07	128.83
29	qJ	202	PEB	CHB-C4B-NB	-5.59	121.07	128.83
29	qL	202	PEB	CHB-C4B-NB	-5.59	121.07	128.83
31	J1	1001	CYC	CAB-C3B-C4B	5.58	130.20	121.38
31	JK	1001	CYC	CAB-C3B-C4B	5.58	130.20	121.38
31	F1	1001	CYC	CAB-C3B-C4B	5.58	130.19	121.38
31	FK	1001	CYC	CAB-C3B-C4B	5.58	130.19	121.38
29	UJ	202	PEB	CHB-C4B-NB	-5.58	121.09	128.83
29	UL	202	PEB	CHB-C4B-NB	-5.58	121.09	128.83
29	Z7	201	PEB	CHB-C4B-C3B	-5.58	112.43	125.32
29	Z9	201	PEB	CHB-C4B-C3B	-5.58	112.43	125.32
29	W7	201	PEB	CHB-C4B-C3B	-5.58	112.43	125.32
29	W9	201	PEB	CHB-C4B-C3B	-5.58	112.43	125.32
31	D1	1001	CYC	CAB-C3B-C4B	5.58	130.19	121.38
31	N1	1001	CYC	CAB-C3B-C4B	5.58	130.19	121.38
29	SJ	202	PEB	CHB-C4B-NB	-5.57	121.09	128.83
29	SL	202	PEB	CHB-C4B-NB	-5.57	121.09	128.83
29	U7	201	PEB	CHB-C4B-C3B	-5.57	112.44	125.32
29	U9	201	PEB	CHB-C4B-C3B	-5.57	112.44	125.32
31	NK	1001	CYC	CAB-C3B-C4B	5.57	130.18	121.38
29	h7	201	PEB	CHB-C4B-C3B	-5.57	112.45	125.32
29	h9	201	PEB	CHB-C4B-C3B	-5.57	112.45	125.32
31	HK	1001	CYC	CAB-C3B-C4B	5.57	130.18	121.38
29	b7	201	PEB	CHB-C4B-C3B	-5.57	112.45	125.32
29	b9	201	PEB	CHB-C4B-C3B	-5.57	112.45	125.32
30	A1	304	PUB	OD-C4D-C3D	-5.57	122.00	128.04
30	AK	304	PUB	OD-C4D-C3D	-5.57	122.00	128.04
29	Q7	201	PEB	CHB-C4B-C3B	-5.57	112.46	125.32
29	Q9	201	PEB	CHB-C4B-C3B	-5.57	112.46	125.32
31	L1	1001	CYC	CAB-C3B-C4B	5.57	130.17	121.38
31	LK	1001	CYC	CAB-C3B-C4B	5.57	130.17	121.38
29	eJ	202	PEB	CHB-C4B-NB	-5.56	121.11	128.83
29	eL	202	PEB	CHB-C4B-NB	-5.56	121.11	128.83
30	A1	304	PUB	CHB-C1C-NC	-5.56	121.11	128.83
30	AK	304	PUB	CHB-C1C-NC	-5.56	121.11	128.83
29	j7	201	PEB	CHB-C4B-C3B	-5.56	112.47	125.32
29	j9	201	PEB	CHB-C4B-C3B	-5.56	112.47	125.32
31	H1	1001	CYC	CAB-C3B-C4B	5.56	130.16	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S7	201	PEB	CHB-C4B-C3B	-5.56	112.48	125.32
29	S9	201	PEB	CHB-C4B-C3B	-5.56	112.48	125.32
29	d7	201	PEB	CHB-C4B-C3B	-5.56	112.48	125.32
29	d9	201	PEB	CHB-C4B-C3B	-5.56	112.48	125.32
31	DK	1001	CYC	CAB-C3B-C4B	5.56	130.15	121.38
29	l7	201	PEB	CHB-C4B-C3B	-5.55	112.49	125.32
29	l9	201	PEB	CHB-C4B-C3B	-5.55	112.49	125.32
29	O7	201	PEB	CHB-C4B-C3B	-5.55	112.50	125.32
29	O9	201	PEB	CHB-C4B-C3B	-5.55	112.50	125.32
29	f7	201	PEB	CHB-C4B-C3B	-5.55	112.51	125.32
29	f9	201	PEB	CHB-C4B-C3B	-5.55	112.51	125.32
29	b1	201	PEB	CHB-C4B-NB	-5.54	121.14	128.83
29	bK	201	PEB	CHB-C4B-NB	-5.54	121.14	128.83
29	fB	201	PEB	CHB-C4B-NB	-5.54	121.14	128.83
29	fM	201	PEB	CHB-C4B-NB	-5.54	121.14	128.83
29	IB	201	PEB	CHB-C4B-NB	-5.54	121.15	128.83
29	IM	201	PEB	CHB-C4B-NB	-5.54	121.15	128.83
29	J5	201	PEB	CHC-C1D-ND	-5.53	107.52	113.95
29	W1	201	PEB	CHB-C4B-NB	-5.53	121.16	128.83
29	WK	201	PEB	CHB-C4B-NB	-5.53	121.16	128.83
29	Q1	201	PEB	CHB-C4B-NB	-5.53	121.16	128.83
29	QK	201	PEB	CHB-C4B-NB	-5.53	121.16	128.83
29	U1	202	PEB	CHB-C4B-NB	-5.53	121.16	128.83
29	UK	202	PEB	CHB-C4B-NB	-5.53	121.16	128.83
29	f1	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	fK	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	j1	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	jK	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
30	AF	302	PUB	OD-C4D-C3D	-5.52	122.05	128.04
30	AI	302	PUB	OD-C4D-C3D	-5.52	122.05	128.04
29	aB	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	aM	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	S1	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	SK	201	PEB	CHB-C4B-NB	-5.52	121.17	128.83
29	J8	201	PEB	CHC-C1D-ND	-5.51	107.55	113.95
29	dB	201	PEB	CHB-C4B-NB	-5.51	121.18	128.83
29	dM	201	PEB	CHB-C4B-NB	-5.51	121.18	128.83
29	h1	201	PEB	CHB-C4B-NB	-5.51	121.19	128.83
29	WB	201	PEB	CHB-C4B-NB	-5.51	121.19	128.83
29	hK	201	PEB	CHB-C4B-NB	-5.51	121.19	128.83
29	WM	201	PEB	CHB-C4B-NB	-5.51	121.19	128.83
29	OB	201	PEB	CHB-C4B-NB	-5.51	121.19	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	OM	201	PEB	CHB-C4B-NB	-5.51	121.19	128.83
29	SB	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	SM	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
30	xL	304	PUB	CHB-C1C-NC	-5.50	121.20	128.83
29	O1	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	OK	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
30	xJ	304	PUB	CHB-C1C-NC	-5.50	121.20	128.83
29	Z1	202	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	MB	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	ZK	202	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	MM	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	CB	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	CM	201	PEB	CHB-C4B-NB	-5.50	121.20	128.83
29	l1	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	lK	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	lB	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	lM	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	d1	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	dK	201	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	QB	203	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	QM	203	PEB	CHB-C4B-NB	-5.49	121.21	128.83
29	R1	202	PEB	CHC-C4C-C3C	-5.49	120.98	130.34
29	a1	202	PEB	CHC-C4C-C3C	-5.49	120.98	130.34
29	RK	202	PEB	CHC-C4C-C3C	-5.49	120.98	130.34
29	aK	202	PEB	CHC-C4C-C3C	-5.49	120.98	130.34
29	b1	201	PEB	CHA-C1B-NB	-5.49	113.45	124.93
29	bK	201	PEB	CHA-C1B-NB	-5.49	113.45	124.93
29	EB	201	PEB	CHB-C4B-NB	-5.49	121.22	128.83
29	EM	201	PEB	CHB-C4B-NB	-5.49	121.22	128.83
29	UB	201	PEB	CHB-C4B-NB	-5.48	121.22	128.83
29	UM	201	PEB	CHB-C4B-NB	-5.48	121.22	128.83
31	YP	1000	CYC	CMA-C3A-C4A	5.48	133.51	125.06
31	1P	1002	CYC	CMA-C3A-C4A	5.48	133.51	125.06
29	P1	202	PEB	CHC-C4C-C3C	-5.48	120.99	130.34
29	PK	202	PEB	CHC-C4C-C3C	-5.48	120.99	130.34
29	GB	201	PEB	CHB-C4B-NB	-5.48	121.23	128.83
29	hB	201	PEB	CHB-C4B-NB	-5.48	121.23	128.83
29	GM	201	PEB	CHB-C4B-NB	-5.48	121.23	128.83
29	hM	201	PEB	CHB-C4B-NB	-5.48	121.23	128.83
29	l1	201	PEB	CHA-C1B-NB	-5.48	113.47	124.93
29	lK	201	PEB	CHA-C1B-NB	-5.48	113.47	124.93
29	h1	201	PEB	CHA-C1B-NB	-5.48	113.47	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	hK	201	PEB	CHA-C1B-NB	-5.48	113.47	124.93
29	Z1	201	PEB	CHC-C4C-C3C	-5.48	121.00	130.34
29	ZK	201	PEB	CHC-C4C-C3C	-5.48	121.00	130.34
29	Q1	201	PEB	CHA-C1B-NB	-5.47	113.48	124.93
29	QK	201	PEB	CHA-C1B-NB	-5.47	113.48	124.93
29	W1	201	PEB	CHA-C1B-NB	-5.47	113.48	124.93
29	WK	201	PEB	CHA-C1B-NB	-5.47	113.48	124.93
29	JQ	203	PEB	CHB-C4B-NB	-5.47	121.23	128.83
29	g1	202	PEB	CHC-C4C-C3C	-5.47	121.00	130.34
29	gK	202	PEB	CHC-C4C-C3C	-5.47	121.00	130.34
29	jB	201	PEB	CHB-C4B-NB	-5.47	121.24	128.83
29	jM	201	PEB	CHB-C4B-NB	-5.47	121.24	128.83
31	SP	1001	CYC	OB-C4B-C3B	-5.47	122.10	128.04
29	KB	201	PEB	CHB-C4B-NB	-5.47	121.24	128.83
29	KM	201	PEB	CHB-C4B-NB	-5.47	121.24	128.83
29	O1	201	PEB	CHA-C1B-NB	-5.47	113.49	124.93
29	OK	201	PEB	CHA-C1B-NB	-5.47	113.49	124.93
29	H8	201	PEB	CHB-C4B-NB	-5.47	121.24	128.83
31	1P	1001	CYC	OB-C4B-C3B	-5.47	122.11	128.04
29	c1	202	PEB	CHC-C4C-C3C	-5.47	121.02	130.34
29	cK	202	PEB	CHC-C4C-C3C	-5.47	121.02	130.34
29	B8	201	PEB	CHB-C4B-NB	-5.46	121.25	128.83
31	MP	1001	CYC	OB-C4B-C3B	-5.46	122.11	128.04
29	f1	201	PEB	CHA-C1B-NB	-5.46	113.51	124.93
29	fK	201	PEB	CHA-C1B-NB	-5.46	113.51	124.93
29	YB	202	PEB	CHB-C4B-NB	-5.46	121.25	128.83
29	YM	202	PEB	CHB-C4B-NB	-5.46	121.25	128.83
29	S1	201	PEB	CHA-C1B-NB	-5.46	113.52	124.93
29	U1	202	PEB	CHA-C1B-NB	-5.46	113.52	124.93
29	SK	201	PEB	CHA-C1B-NB	-5.46	113.52	124.93
29	UK	202	PEB	CHA-C1B-NB	-5.46	113.52	124.93
29	i1	202	PEB	CHC-C4C-C3C	-5.46	121.03	130.34
29	iK	202	PEB	CHC-C4C-C3C	-5.46	121.03	130.34
31	QP	1001	CYC	OB-C4B-C3B	-5.46	122.12	128.04
31	BP	1001	CYC	OB-C4B-C3B	-5.46	122.12	128.04
30	wJ	304	PUB	CHB-C1C-NC	-5.46	121.26	128.83
31	HP	1001	CYC	OB-C4B-C3B	-5.46	122.12	128.04
29	j1	201	PEB	CHA-C1B-NB	-5.45	113.52	124.93
29	jK	201	PEB	CHA-C1B-NB	-5.45	113.52	124.93
29	U1	201	PEB	CHC-C4C-C3C	-5.45	121.04	130.34
29	UK	201	PEB	CHC-C4C-C3C	-5.45	121.04	130.34
29	d1	201	PEB	CHA-C1B-NB	-5.45	113.53	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	dK	201	PEB	CHA-C1B-NB	-5.45	113.53	124.93
29	e1	202	PEB	CHC-C4C-C3C	-5.45	121.04	130.34
29	eK	202	PEB	CHC-C4C-C3C	-5.45	121.04	130.34
29	Z1	202	PEB	CHA-C1B-NB	-5.45	113.53	124.93
29	ZK	202	PEB	CHA-C1B-NB	-5.45	113.53	124.93
31	DP	1001	CYC	OB-C4B-C3B	-5.45	122.12	128.04
29	JG	203	PEB	CHB-C4B-NB	-5.45	121.27	128.83
29	F5	201	PEB	CHB-C4B-NB	-5.45	121.27	128.83
29	F8	201	PEB	CHB-C4B-NB	-5.45	121.27	128.83
29	G5	201	PEB	CHB-C4B-NB	-5.45	121.27	128.83
29	DQ	203	PEB	CHB-C4B-NB	-5.45	121.27	128.83
31	kP	1001	CYC	OB-C4B-C3B	-5.44	122.13	128.04
31	fP	1001	CYC	OB-C4B-C3B	-5.44	122.13	128.04
29	TF	201	PEB	CHB-C4B-NB	-5.44	121.28	128.83
29	V1	202	PEB	CHC-C4C-C3C	-5.44	121.05	130.34
29	VK	202	PEB	CHC-C4C-C3C	-5.44	121.05	130.34
29	L5	201	PEB	CHB-C4B-NB	-5.44	121.28	128.83
31	FP	1001	CYC	OB-C4B-C3B	-5.44	122.14	128.04
29	k1	202	PEB	CHC-C4C-C3C	-5.44	121.06	130.34
29	kK	202	PEB	CHC-C4C-C3C	-5.44	121.06	130.34
29	G8	201	PEB	CHB-C4B-NB	-5.44	121.29	128.83
29	j1	203	PEB	CHC-C4C-C3C	-5.43	121.07	130.34
29	jK	203	PEB	CHC-C4C-C3C	-5.43	121.07	130.34
31	nP	1001	CYC	OB-C4B-C3B	-5.43	122.14	128.04
31	wP	1001	CYC	OB-C4B-C3B	-5.43	122.14	128.04
29	H5	201	PEB	CHB-C4B-NB	-5.43	121.29	128.83
31	sP	1001	CYC	OB-C4B-C3B	-5.43	122.15	128.04
29	FG	203	PEB	CHB-C4B-NB	-5.43	121.30	128.83
31	UP	1001	CYC	OB-C4B-C3B	-5.43	122.15	128.04
31	jP	1001	CYC	OB-C4B-C3B	-5.43	122.15	128.04
29	B5	201	PEB	CHB-C4B-NB	-5.42	121.30	128.83
30	wL	304	PUB	CHB-C1C-NC	-5.42	121.31	128.83
29	DG	203	PEB	CHB-C4B-NB	-5.42	121.31	128.83
29	HG	203	PEB	CHB-C4B-NB	-5.42	121.31	128.83
31	qP	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
31	uP	1001	CYC	OB-C4B-C3B	-5.42	122.16	128.04
29	WF	201	PEB	CMB-C2B-C1B	5.42	133.40	125.06
29	WI	201	PEB	CMB-C2B-C1B	5.42	133.40	125.06
29	bF	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06
29	bI	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06
29	SF	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06
29	hF	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SI	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06
29	hI	201	PEB	CMB-C2B-C1B	5.41	133.40	125.06
31	hP	1001	CYC	OB-C4B-C3B	-5.41	122.17	128.04
29	LG	203	PEB	CHB-C4B-NB	-5.41	121.32	128.83
29	HQ	203	PEB	CHB-C4B-NB	-5.41	121.32	128.83
29	ZF	201	PEB	CMB-C2B-C1B	5.41	133.39	125.06
29	ZI	201	PEB	CMB-C2B-C1B	5.41	133.39	125.06
29	FQ	203	PEB	CHB-C4B-NB	-5.41	121.33	128.83
31	oP	1001	CYC	OB-C4B-C3B	-5.41	122.17	128.04
31	XP	1001	CYC	OB-C4B-C3B	-5.41	122.17	128.04
29	BQ	203	PEB	CHB-C4B-NB	-5.40	121.33	128.83
29	fF	201	PEB	CMB-C2B-C1B	5.40	133.38	125.06
29	fI	201	PEB	CMB-C2B-C1B	5.40	133.38	125.06
29	BG	203	PEB	CHB-C4B-NB	-5.40	121.33	128.83
29	QF	201	PEB	CMB-C2B-C1B	5.40	133.38	125.06
29	UF	202	PEB	CMB-C2B-C1B	5.40	133.38	125.06
29	QI	201	PEB	CMB-C2B-C1B	5.40	133.38	125.06
29	UI	202	PEB	CMB-C2B-C1B	5.40	133.38	125.06
29	A1	301	PEB	CHB-C4B-NB	-5.40	121.34	128.83
29	L8	201	PEB	CHB-C4B-NB	-5.40	121.34	128.83
29	AF	304	PEB	CHB-C4B-NB	-5.40	121.34	128.83
29	AI	304	PEB	CHB-C4B-NB	-5.40	121.34	128.83
29	AK	301	PEB	CHB-C4B-NB	-5.40	121.34	128.83
29	D3	202	PEB	CHB-C4B-NB	-5.39	121.34	128.83
29	OF	201	PEB	CMB-C2B-C1B	5.39	133.36	125.06
29	OI	201	PEB	CMB-C2B-C1B	5.39	133.36	125.06
30	A7	302	PUB	CHB-C1C-NC	-5.39	121.35	128.83
30	A9	302	PUB	CHB-C1C-NC	-5.39	121.35	128.83
29	dF	202	PEB	CMB-C2B-C1B	5.39	133.36	125.06
29	dI	202	PEB	CMB-C2B-C1B	5.39	133.36	125.06
29	jF	201	PEB	CMB-C2B-C1B	5.39	133.36	125.06
29	jI	201	PEB	CMB-C2B-C1B	5.39	133.36	125.06
31	OP	1001	CYC	OB-C4B-C3B	-5.39	122.20	128.04
31	IP	1001	CYC	OB-C4B-C3B	-5.38	122.20	128.04
31	H7	1001	CYC	CMA-C3A-C4A	5.37	133.33	125.06
31	H9	1001	CYC	CMA-C3A-C4A	5.37	133.33	125.06
29	lF	201	PEB	CMB-C2B-C1B	5.37	133.33	125.06
29	II	201	PEB	CMB-C2B-C1B	5.37	133.33	125.06
31	F9	1001	CYC	CMA-C3A-C4A	5.36	133.32	125.06
31	J9	1001	CYC	CMA-C3A-C4A	5.36	133.32	125.06
29	LQ	202	PEB	CHB-C4B-NB	-5.35	121.40	128.83
29	AB	303	PEB	CHB-C4B-NB	-5.35	121.40	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A1	305	PUB	C1C-C2C-C3C	-5.35	100.86	106.78
30	AK	305	PUB	C1C-C2C-C3C	-5.35	100.86	106.78
31	J7	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
31	D7	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
31	L7	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
31	D9	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
31	WP	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
31	F7	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
29	A7	305	PEB	CHB-C4B-NB	-5.35	121.41	128.83
29	A9	305	PEB	CHB-C4B-NB	-5.35	121.41	128.83
29	AM	303	PEB	CHB-C4B-NB	-5.35	121.41	128.83
31	N7	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
31	N9	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
29	J5	201	PEB	CHA-C1B-NB	-5.35	113.75	124.93
29	J8	201	PEB	CHA-C1B-NB	-5.35	113.75	124.93
31	yP	1001	CYC	CMA-C3A-C4A	5.35	133.30	125.06
29	dJ	202	PEB	CHB-C4B-NB	-5.33	121.43	128.83
29	dL	202	PEB	CHB-C4B-NB	-5.33	121.43	128.83
29	BC	201	PEB	CHB-C4B-NB	-5.33	121.44	128.83
29	BE	201	PEB	CHB-C4B-NB	-5.33	121.44	128.83
29	nJ	202	PEB	CHB-C4B-NB	-5.33	121.44	128.83
29	nL	202	PEB	CHB-C4B-NB	-5.33	121.44	128.83
31	L9	1001	CYC	CMA-C3A-C4A	5.33	133.27	125.06
31	DF	1001	CYC	CHB-C4A-NA	-5.32	113.80	124.93
31	DI	1001	CYC	CHB-C4A-NA	-5.32	113.80	124.93
31	NF	1001	CYC	CHB-C4A-NA	-5.32	113.80	124.93
31	NI	1001	CYC	CHB-C4A-NA	-5.32	113.80	124.93
29	FC	201	PEB	CHB-C4B-NB	-5.32	121.45	128.83
29	FE	201	PEB	CHB-C4B-NB	-5.32	121.45	128.83
29	H4	201	PEB	CHA-C1B-NB	-5.32	113.81	124.93
31	HF	1001	CYC	CHB-C4A-NA	-5.32	113.81	124.93
31	HI	1001	CYC	CHB-C4A-NA	-5.32	113.81	124.93
31	tP	1001	CYC	C4D-CHA-C1A	5.31	135.16	128.81
30	yJ	302	PUB	CHB-C1C-NC	-5.31	121.46	128.83
30	yL	302	PUB	CHB-C1C-NC	-5.31	121.46	128.83
29	fJ	202	PEB	CHB-C4B-NB	-5.31	121.46	128.83
29	fL	202	PEB	CHB-C4B-NB	-5.31	121.46	128.83
29	WJ	201	PEB	CHB-C4B-NB	-5.31	121.46	128.83
29	WL	201	PEB	CHB-C4B-NB	-5.31	121.46	128.83
29	hJ	202	PEB	CHB-C4B-NB	-5.31	121.46	128.83
29	hL	202	PEB	CHB-C4B-NB	-5.31	121.46	128.83
31	eP	1001	CYC	C4D-CHA-C1A	5.31	135.15	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FD	201	PEB	CHA-C1B-NB	-5.31	113.83	124.93
29	JD	201	PEB	CHA-C1B-NB	-5.31	113.83	124.93
29	F4	201	PEB	CHA-C1B-NB	-5.31	113.83	124.93
29	HD	201	PEB	CHA-C1B-NB	-5.31	113.83	124.93
31	CP	1001	CYC	C4D-CHA-C1A	5.30	135.14	128.81
30	MN	403	PUB	CHA-C1B-C2B	-5.30	121.29	130.34
30	MA	403	PUB	CHA-C1B-C2B	-5.30	121.30	130.34
29	lJ	202	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	sJ	203	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	lL	202	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	sL	203	PEB	CHB-C4B-NB	-5.30	121.47	128.83
31	JF	1001	CYC	CHB-C4A-NA	-5.30	113.84	124.93
31	JI	1001	CYC	CHB-C4A-NA	-5.30	113.84	124.93
29	AJ	203	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	uJ	201	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	AL	203	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	uL	201	PEB	CHB-C4B-NB	-5.30	121.47	128.83
29	BJ	202	PEB	CHB-C4B-NB	-5.30	121.48	128.83
29	PJ	202	PEB	CHB-C4B-NB	-5.30	121.48	128.83
29	BL	202	PEB	CHB-C4B-NB	-5.30	121.48	128.83
29	PL	202	PEB	CHB-C4B-NB	-5.30	121.48	128.83
31	FF	1001	CYC	CHB-C4A-NA	-5.30	113.85	124.93
31	FI	1001	CYC	CHB-C4A-NA	-5.30	113.85	124.93
29	DD	201	PEB	CHA-C1B-NB	-5.30	113.85	124.93
29	BD	201	PEB	CHA-C1B-NB	-5.30	113.85	124.93
29	i7	202	PEB	CHC-C1D-ND	-5.30	107.80	113.95
29	i9	202	PEB	CHC-C1D-ND	-5.30	107.80	113.95
29	J4	201	PEB	CHA-C1B-NB	-5.30	113.85	124.93
29	B4	201	PEB	CHA-C1B-NB	-5.30	113.86	124.93
31	LF	1001	CYC	CHB-C4A-NA	-5.29	113.86	124.93
31	LI	1001	CYC	CHB-C4A-NA	-5.29	113.86	124.93
29	NJ	202	PEB	CHB-C4B-NB	-5.29	121.48	128.83
29	NL	202	PEB	CHB-C4B-NB	-5.29	121.48	128.83
30	QB	201	PUB	OD-C4D-C3D	-5.29	122.30	128.04
30	QM	201	PUB	OD-C4D-C3D	-5.29	122.30	128.04
29	jJ	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	jL	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	ZJ	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	ZL	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	e7	202	PEB	CHC-C1D-ND	-5.29	107.80	113.95
29	e9	202	PEB	CHC-C1D-ND	-5.29	107.80	113.95
29	DO	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	bJ	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	bL	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	D4	201	PEB	CHA-C1B-NB	-5.29	113.87	124.93
29	RJ	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
29	RL	202	PEB	CHB-C4B-NB	-5.29	121.49	128.83
31	IP	1001	CYC	C4D-CHA-C1A	5.29	135.12	128.81
29	HC	201	PEB	CHB-C4B-NB	-5.28	121.50	128.83
29	HE	201	PEB	CHB-C4B-NB	-5.28	121.50	128.83
29	rJ	202	PEB	CHB-C4B-NB	-5.28	121.50	128.83
29	rL	202	PEB	CHB-C4B-NB	-5.28	121.50	128.83
31	KP	1001	CYC	C4D-CHA-C1A	5.28	135.12	128.81
31	PP	1001	CYC	C4D-CHA-C1A	5.28	135.12	128.81
29	LD	201	PEB	CHA-C1B-NB	-5.28	113.88	124.93
29	JC	201	PEB	CHB-C4B-NB	-5.28	121.50	128.83
29	JE	201	PEB	CHB-C4B-NB	-5.28	121.50	128.83
29	L4	201	PEB	CHA-C1B-NB	-5.28	113.89	124.93
29	LC	201	PEB	CHB-C4B-NB	-5.28	121.51	128.83
29	LE	201	PEB	CHB-C4B-NB	-5.28	121.51	128.83
29	FA	202	PEB	CHB-C4B-NB	-5.28	121.51	128.83
29	pJ	202	PEB	CHB-C4B-NB	-5.28	121.51	128.83
29	pL	202	PEB	CHB-C4B-NB	-5.28	121.51	128.83
29	FN	202	PEB	CHB-C4B-NB	-5.28	121.51	128.83
31	AP	1001	CYC	C4D-CHA-C1A	5.28	135.11	128.81
30	MN	403	PUB	C1C-C2C-C3C	-5.27	100.94	106.78
29	g1	202	PEB	CHB-C4B-NB	-5.27	121.51	128.83
29	gK	202	PEB	CHB-C4B-NB	-5.27	121.51	128.83
31	RP	1001	CYC	C4D-CHA-C1A	5.27	135.11	128.81
29	Z1	201	PEB	CHB-C4B-NB	-5.27	121.51	128.83
29	ZK	201	PEB	CHB-C4B-NB	-5.27	121.51	128.83
29	HJ	201	PEB	CHB-C4B-NB	-5.27	121.51	128.83
29	HL	201	PEB	CHB-C4B-NB	-5.27	121.51	128.83
29	P7	202	PEB	CHC-C1D-ND	-5.27	107.83	113.95
29	P9	202	PEB	CHC-C1D-ND	-5.27	107.83	113.95
29	DC	201	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	DE	201	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	IJ	203	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	IL	203	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	JA	202	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	FJ	202	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	FL	202	PEB	CHB-C4B-NB	-5.27	121.52	128.83
29	JN	202	PEB	CHB-C4B-NB	-5.27	121.52	128.83
31	iP	1001	CYC	C4D-CHA-C1A	5.27	135.10	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	mP	1001	CYC	C4D-CHA-C1A	5.27	135.10	128.81
31	TP	1001	CYC	C4D-CHA-C1A	5.27	135.10	128.81
31	EP	1001	CYC	C4D-CHA-C1A	5.26	135.10	128.81
31	rP	1001	CYC	C4D-CHA-C1A	5.26	135.10	128.81
29	V7	202	PEB	CHC-C1D-ND	-5.26	107.84	113.95
29	V9	202	PEB	CHC-C1D-ND	-5.26	107.84	113.95
29	LA	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
29	JJ	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
29	JL	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
29	LN	202	PEB	CHB-C4B-NB	-5.26	121.53	128.83
31	JP	1001	CYC	C4D-CHA-C1A	5.26	135.09	128.81
31	GP	1001	CYC	C4D-CHA-C1A	5.26	135.09	128.81
31	NP	1001	CYC	C4D-CHA-C1A	5.26	135.09	128.81
29	V1	202	PEB	CHB-C4B-NB	-5.26	121.54	128.83
29	VK	202	PEB	CHB-C4B-NB	-5.26	121.54	128.83
29	a7	202	PEB	CHC-C1D-ND	-5.26	107.84	113.95
29	a9	202	PEB	CHC-C1D-ND	-5.26	107.84	113.95
29	TJ	202	PEB	CHB-C4B-NB	-5.26	121.54	128.83
29	TL	202	PEB	CHB-C4B-NB	-5.26	121.54	128.83
29	k7	202	PEB	CHC-C1D-ND	-5.25	107.85	113.95
29	k9	202	PEB	CHC-C1D-ND	-5.25	107.85	113.95
29	HA	202	PEB	CHB-C4B-NB	-5.25	121.54	128.83
29	XJ	202	PEB	CHB-C4B-NB	-5.25	121.54	128.83
29	XL	202	PEB	CHB-C4B-NB	-5.25	121.54	128.83
29	HN	202	PEB	CHB-C4B-NB	-5.25	121.54	128.83
29	zJ	501	PEB	CHB-C4B-NB	-5.25	121.54	128.83
29	c1	202	PEB	CHB-C4B-NB	-5.25	121.55	128.83
29	cK	202	PEB	CHB-C4B-NB	-5.25	121.55	128.83
29	DA	202	PEB	CHB-C4B-NB	-5.25	121.55	128.83
29	DN	202	PEB	CHB-C4B-NB	-5.25	121.55	128.83
29	c7	202	PEB	CHC-C1D-ND	-5.25	107.85	113.95
29	m7	202	PEB	CHC-C1D-ND	-5.25	107.85	113.95
29	c9	202	PEB	CHC-C1D-ND	-5.25	107.85	113.95
29	m9	202	PEB	CHC-C1D-ND	-5.25	107.85	113.95
29	zL	501	PEB	CHB-C4B-NB	-5.24	121.55	128.83
31	RP	1001	CYC	CMA-C3A-C4A	5.24	133.14	125.06
29	P1	202	PEB	CHB-C4B-NB	-5.24	121.56	128.83
29	BA	202	PEB	CHB-C4B-NB	-5.24	121.56	128.83
29	PK	202	PEB	CHB-C4B-NB	-5.24	121.56	128.83
29	BN	202	PEB	CHB-C4B-NB	-5.24	121.56	128.83
31	pP	1001	CYC	C4D-CHA-C1A	5.24	135.07	128.81
29	U1	201	PEB	CHB-C4B-NB	-5.24	121.56	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UK	201	PEB	CHB-C4B-NB	-5.24	121.56	128.83
31	vP	1001	CYC	C4D-CHA-C1A	5.24	135.06	128.81
29	g7	202	PEB	CHC-C1D-ND	-5.23	107.87	113.95
29	g9	202	PEB	CHC-C1D-ND	-5.23	107.87	113.95
29	a1	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	aK	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	i1	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	iK	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
30	MA	403	PUB	C1C-C2C-C3C	-5.23	100.99	106.78
29	j1	203	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	jK	203	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	T7	202	PEB	CHC-C1D-ND	-5.23	107.87	113.95
29	T9	202	PEB	CHC-C1D-ND	-5.23	107.87	113.95
29	Y7	202	PEB	CHC-C1D-ND	-5.23	107.87	113.95
29	Y9	202	PEB	CHC-C1D-ND	-5.23	107.87	113.95
29	e1	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	eK	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	R1	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
29	RK	202	PEB	CHB-C4B-NB	-5.23	121.57	128.83
31	PP	1001	CYC	CMA-C3A-C4A	5.23	133.12	125.06
31	CP	1001	CYC	CMA-C3A-C4A	5.22	133.11	125.06
31	gP	1001	CYC	C4D-CHA-C1A	5.22	135.05	128.81
29	TR	201	PEB	OA-C1A-C2A	-5.22	122.02	126.17
29	AM	302	PEB	CHB-C4B-NB	-5.22	121.59	128.83
29	R7	202	PEB	CHC-C1D-ND	-5.22	107.89	113.95
29	R9	202	PEB	CHC-C1D-ND	-5.22	107.89	113.95
29	JA	201	PEB	C4B-C3B-C2B	-5.22	101.01	106.78
29	JN	201	PEB	C4B-C3B-C2B	-5.22	101.01	106.78
31	KP	1001	CYC	CMA-C3A-C4A	5.22	133.10	125.06
29	MD	203	PEB	C1C-CHB-C4B	-5.22	122.58	128.81
29	AB	302	PEB	CHB-C4B-NB	-5.22	121.59	128.83
29	k1	202	PEB	CHB-C4B-NB	-5.21	121.60	128.83
29	kK	202	PEB	CHB-C4B-NB	-5.21	121.60	128.83
29	ED	202	PEB	C1C-CHB-C4B	-5.21	122.59	128.81
30	BB	302	PUB	CHC-C1D-ND	-5.21	107.13	113.72
30	BM	302	PUB	CHC-C1D-ND	-5.21	107.13	113.72
29	HG	202	PEB	CHC-C4C-C3C	-5.21	121.45	130.34
29	HQ	202	PEB	CHC-C4C-C3C	-5.21	121.45	130.34
31	NP	1001	CYC	CMA-C3A-C4A	5.21	133.08	125.06
29	CD	203	PEB	C1C-CHB-C4B	-5.21	122.59	128.81
29	HA	201	PEB	C4B-C3B-C2B	-5.20	101.02	106.78
29	HN	201	PEB	C4B-C3B-C2B	-5.20	101.02	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	iP	1001	CYC	CMA-C3A-C4A	5.20	133.08	125.06
31	vP	1001	CYC	CMA-C3A-C4A	5.20	133.07	125.06
29	BG	202	PEB	CHC-C4C-C3C	-5.20	121.47	130.34
29	BQ	202	PEB	CHC-C4C-C3C	-5.20	121.47	130.34
31	TP	1001	CYC	CMA-C3A-C4A	5.20	133.07	125.06
29	N2	203	PEB	OA-C1A-C2A	-5.20	122.04	126.17
29	G3	201	PEB	CMB-C2B-C1B	5.20	133.07	125.06
29	GO	201	PEB	CMB-C2B-C1B	5.20	133.07	125.06
29	E3	201	PEB	CMB-C2B-C1B	5.20	133.07	125.06
29	EO	201	PEB	CMB-C2B-C1B	5.20	133.07	125.06
29	I3	203	PEB	CMC-C3C-C2C	-5.19	115.15	124.94
29	IO	203	PEB	CMC-C3C-C2C	-5.19	115.15	124.94
31	eP	1001	CYC	CMA-C3A-C4A	5.19	133.06	125.06
29	A3	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
29	AO	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
29	C4	203	PEB	C1C-CHB-C4B	-5.19	122.61	128.81
31	gP	1001	CYC	CMA-C3A-C4A	5.19	133.06	125.06
31	rP	1001	CYC	CMA-C3A-C4A	5.19	133.06	125.06
31	EP	1001	CYC	CMA-C3A-C4A	5.19	133.06	125.06
29	FG	202	PEB	CHC-C4C-C3C	-5.19	121.48	130.34
29	FQ	202	PEB	CHC-C4C-C3C	-5.19	121.48	130.34
31	lP	1001	CYC	CMA-C3A-C4A	5.19	133.06	125.06
29	I3	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
29	IO	201	PEB	CMB-C2B-C1B	5.19	133.06	125.06
29	R2	201	PEB	OA-C1A-C2A	-5.19	122.05	126.17
29	J3	202	PEB	CMC-C3C-C2C	-5.19	115.16	124.94
29	JO	202	PEB	CMC-C3C-C2C	-5.19	115.16	124.94
29	E4	203	PEB	C1C-CHB-C4B	-5.19	122.61	128.81
29	K4	203	PEB	C1C-CHB-C4B	-5.19	122.61	128.81
31	cP	1001	CYC	CMA-C3A-C4A	5.19	133.05	125.06
29	NR	201	PEB	OA-C1A-C2A	-5.19	122.05	126.17
29	F3	202	PEB	CMC-C3C-C2C	-5.19	115.17	124.94
29	FO	202	PEB	CMC-C3C-C2C	-5.19	115.17	124.94
29	J5	202	PEB	CHB-C4B-NB	-5.18	121.64	128.83
29	RR	203	PEB	OA-C1A-C2A	-5.18	122.05	126.17
29	B3	202	PEB	CMC-C3C-C2C	-5.18	115.17	124.94
29	BO	202	PEB	CMC-C3C-C2C	-5.18	115.17	124.94
31	pP	1001	CYC	CMA-C3A-C4A	5.18	133.05	125.06
29	C3	201	PEB	CMB-C2B-C1B	5.18	133.04	125.06
29	CO	201	PEB	CMB-C2B-C1B	5.18	133.04	125.06
31	mP	1001	CYC	CMA-C3A-C4A	5.18	133.04	125.06
29	LA	201	PEB	C4B-C3B-C2B	-5.18	101.05	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LN	201	PEB	C4B-C3B-C2B	-5.18	101.05	106.78
29	VR	201	PEB	OA-C1A-C2A	-5.18	122.06	126.17
29	DA	201	PEB	C4B-C3B-C2B	-5.18	101.05	106.78
29	DN	201	PEB	C4B-C3B-C2B	-5.18	101.05	106.78
29	K3	201	PEB	CMB-C2B-C1B	5.18	133.04	125.06
29	KO	201	PEB	CMB-C2B-C1B	5.18	133.04	125.06
29	DG	202	PEB	CHC-C4C-C3C	-5.18	121.51	130.34
29	DQ	202	PEB	CHC-C4C-C3C	-5.18	121.51	130.34
31	cP	1001	CYC	C4D-CHA-C1A	5.18	134.99	128.81
29	FA	202	PEB	C1C-CHB-C4B	5.18	134.99	128.81
29	FN	202	PEB	C1C-CHB-C4B	5.18	134.99	128.81
31	tP	1001	CYC	CMA-C3A-C4A	5.18	133.04	125.06
31	JP	1001	CYC	CMA-C3A-C4A	5.17	133.03	125.06
29	G4	203	PEB	C1C-CHB-C4B	-5.17	122.63	128.81
29	XR	201	PEB	OA-C1A-C2A	-5.17	122.06	126.17
29	J8	202	PEB	CHB-C4B-NB	-5.17	121.65	128.83
29	H3	202	PEB	CMC-C3C-C2C	-5.17	115.19	124.94
29	HO	202	PEB	CMC-C3C-C2C	-5.17	115.19	124.94
29	BA	201	PEB	C4B-C3B-C2B	-5.17	101.06	106.78
29	FA	201	PEB	C4B-C3B-C2B	-5.17	101.06	106.78
29	BN	201	PEB	C4B-C3B-C2B	-5.17	101.06	106.78
29	FN	201	PEB	C4B-C3B-C2B	-5.17	101.06	106.78
29	RR	201	PEB	OA-C1A-C2A	-5.17	122.06	126.17
29	GD	203	PEB	C1C-CHB-C4B	-5.17	122.64	128.81
29	P2	202	PEB	OA-C1A-C2A	-5.17	122.06	126.17
29	JG	202	PEB	CHC-C4C-C3C	-5.16	121.53	130.34
29	JQ	202	PEB	CHC-C4C-C3C	-5.16	121.53	130.34
31	AP	1001	CYC	CMA-C3A-C4A	5.16	133.01	125.06
29	VR	203	PEB	OA-C1A-C2A	-5.16	122.07	126.17
29	KD	203	PEB	C1C-CHB-C4B	-5.16	122.65	128.81
29	V2	201	PEB	OA-C1A-C2A	-5.16	122.07	126.17
29	T2	203	PEB	OA-C1A-C2A	-5.16	122.07	126.17
29	LA	202	PEB	C1C-CHB-C4B	5.16	134.97	128.81
29	LN	202	PEB	C1C-CHB-C4B	5.16	134.97	128.81
29	ID	203	PEB	C1C-CHB-C4B	-5.15	122.65	128.81
29	JA	202	PEB	C1C-CHB-C4B	5.15	134.96	128.81
29	JN	202	PEB	C1C-CHB-C4B	5.15	134.96	128.81
29	LG	202	PEB	CHC-C4C-C3C	-5.15	121.55	130.34
29	LQ	201	PEB	CHC-C4C-C3C	-5.15	121.55	130.34
29	HA	202	PEB	C1C-CHB-C4B	5.15	134.96	128.81
29	HN	202	PEB	C1C-CHB-C4B	5.15	134.96	128.81
29	N2	201	PEB	OA-C1A-C2A	-5.15	122.08	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	XR	203	PEB	OA-C1A-C2A	-5.15	122.08	126.17
29	V2	203	PEB	OA-C1A-C2A	-5.15	122.08	126.17
29	T2	201	PEB	OA-C1A-C2A	-5.14	122.08	126.17
31	GP	1001	CYC	CMA-C3A-C4A	5.14	132.98	125.06
29	BA	202	PEB	C1C-CHB-C4B	5.14	134.95	128.81
29	BN	202	PEB	C1C-CHB-C4B	5.14	134.95	128.81
29	NR	203	PEB	OA-C1A-C2A	-5.14	122.09	126.17
29	ZB	201	PEB	C1C-CHB-C4B	-5.13	122.67	128.81
29	ZM	201	PEB	C1C-CHB-C4B	-5.13	122.67	128.81
29	R2	203	PEB	OA-C1A-C2A	-5.13	122.09	126.17
29	DA	202	PEB	C1C-CHB-C4B	5.13	134.93	128.81
29	FB	201	PEB	C1C-CHB-C4B	-5.13	122.68	128.81
29	FM	201	PEB	C1C-CHB-C4B	-5.13	122.68	128.81
29	DN	202	PEB	C1C-CHB-C4B	5.13	134.93	128.81
29	mB	201	PEB	C1C-CHB-C4B	-5.13	122.69	128.81
29	mM	201	PEB	C1C-CHB-C4B	-5.13	122.69	128.81
31	DK	1001	CYC	C4D-CHA-C1A	5.13	134.93	128.81
29	LA	201	PEB	CHB-C4B-NB	-5.12	121.72	128.83
29	LN	201	PEB	CHB-C4B-NB	-5.12	121.72	128.83
29	JA	201	PEB	CHB-C4B-NB	-5.12	121.72	128.83
29	JN	201	PEB	CHB-C4B-NB	-5.12	121.72	128.83
29	PR	202	PEB	OA-C1A-C2A	-5.12	122.10	126.17
31	D1	1001	CYC	C4D-CHA-C1A	5.12	134.92	128.81
29	JB	201	PEB	C1C-CHB-C4B	-5.12	122.70	128.81
29	TB	201	PEB	C1C-CHB-C4B	-5.12	122.70	128.81
29	JM	201	PEB	C1C-CHB-C4B	-5.12	122.70	128.81
29	TM	201	PEB	C1C-CHB-C4B	-5.12	122.70	128.81
31	H1	1001	CYC	C4D-CHA-C1A	5.12	134.92	128.81
29	BA	201	PEB	CHB-C4B-NB	-5.11	121.73	128.83
29	BN	201	PEB	CHB-C4B-NB	-5.11	121.73	128.83
29	XB	201	PEB	C1C-CHB-C4B	-5.11	122.70	128.81
29	XM	201	PEB	C1C-CHB-C4B	-5.11	122.70	128.81
29	DA	201	PEB	CHB-C4B-NB	-5.11	121.73	128.83
29	DN	201	PEB	CHB-C4B-NB	-5.11	121.73	128.83
29	FA	201	PEB	CHB-C4B-NB	-5.11	121.73	128.83
29	FN	201	PEB	CHB-C4B-NB	-5.11	121.73	128.83
29	DB	201	PEB	C1C-CHB-C4B	-5.11	122.70	128.81
29	DM	201	PEB	C1C-CHB-C4B	-5.11	122.70	128.81
29	cB	201	PEB	C1C-CHB-C4B	-5.10	122.71	128.81
29	cM	201	PEB	C1C-CHB-C4B	-5.10	122.71	128.81
29	JA	202	PEB	CHC-C4C-C3C	-5.10	121.63	130.34
29	JN	202	PEB	CHC-C4C-C3C	-5.10	121.63	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LB	201	PEB	C1C-CHB-C4B	-5.10	122.71	128.81
29	LM	201	PEB	C1C-CHB-C4B	-5.10	122.71	128.81
29	TR	203	PEB	OA-C1A-C2A	-5.10	122.12	126.17
31	D1	1003	CYC	CAB-C3B-C4B	5.10	129.44	121.38
29	H1	1002	PEB	C3D-C4D-ND	5.10	117.27	107.26
29	HA	201	PEB	CHB-C4B-NB	-5.10	121.75	128.83
29	HN	201	PEB	CHB-C4B-NB	-5.10	121.75	128.83
29	FA	202	PEB	CHC-C4C-C3C	-5.10	121.64	130.34
29	FN	202	PEB	CHC-C4C-C3C	-5.10	121.64	130.34
31	I1	1001	CYC	CAB-C3B-C4B	5.10	129.43	121.38
29	RB	201	PEB	C1C-CHB-C4B	-5.10	122.72	128.81
29	RM	201	PEB	C1C-CHB-C4B	-5.10	122.72	128.81
31	HK	1001	CYC	C4D-CHA-C1A	5.10	134.90	128.81
29	e2	402	PEB	OA-C1A-C2A	-5.09	122.12	126.17
29	NK	1002	PEB	C3D-C4D-ND	5.09	117.25	107.26
29	L1	1002	PEB	C3D-C4D-ND	5.09	117.25	107.26
29	LK	1002	PEB	C3D-C4D-ND	5.09	117.25	107.26
29	gB	201	PEB	C1C-CHB-C4B	-5.09	122.73	128.81
29	gM	201	PEB	C1C-CHB-C4B	-5.09	122.73	128.81
31	E1	1001	CYC	CAB-C3B-C4B	5.09	129.42	121.38
29	kB	201	PEB	C1C-CHB-C4B	-5.09	122.73	128.81
29	kM	201	PEB	C1C-CHB-C4B	-5.09	122.73	128.81
31	M1	1001	CYC	CAB-C3B-C4B	5.09	129.41	121.38
31	MK	1001	CYC	CAB-C3B-C4B	5.09	129.41	121.38
29	F1	1002	PEB	C3D-C4D-ND	5.09	117.24	107.26
29	FK	1002	PEB	C3D-C4D-ND	5.09	117.24	107.26
31	N1	1001	CYC	C4D-CHA-C1A	5.09	134.89	128.81
29	iB	201	PEB	C1C-CHB-C4B	-5.09	122.73	128.81
29	iM	201	PEB	C1C-CHB-C4B	-5.09	122.73	128.81
29	DK	1002	PEB	C3D-C4D-ND	5.08	117.23	107.26
31	F1	1001	CYC	C4D-CHA-C1A	5.08	134.88	128.81
31	FK	1001	CYC	C4D-CHA-C1A	5.08	134.88	128.81
31	NK	1001	CYC	C4D-CHA-C1A	5.08	134.88	128.81
29	NB	201	PEB	C1C-CHB-C4B	-5.08	122.74	128.81
29	NM	201	PEB	C1C-CHB-C4B	-5.08	122.74	128.81
31	GK	1001	CYC	CAB-C3B-C4B	5.08	129.41	121.38
31	J1	1001	CYC	C4D-CHA-C1A	5.08	134.88	128.81
31	JK	1001	CYC	C4D-CHA-C1A	5.08	134.88	128.81
29	HA	202	PEB	CHC-C4C-C3C	-5.08	121.67	130.34
29	HN	202	PEB	CHC-C4C-C3C	-5.08	121.67	130.34
29	HK	1002	PEB	C3D-C4D-ND	5.08	117.23	107.26
31	K1	1001	CYC	CAB-C3B-C4B	5.08	129.40	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	KK	1001	CYC	CAB-C3B-C4B	5.08	129.40	121.38
29	X2	202	PEB	OA-C1A-C2A	-5.08	122.14	126.17
29	eB	201	PEB	C1C-CHB-C4B	-5.08	122.75	128.81
29	eM	201	PEB	C1C-CHB-C4B	-5.08	122.75	128.81
31	IK	1001	CYC	CAB-C3B-C4B	5.07	129.39	121.38
29	N1	1002	PEB	C3D-C4D-ND	5.07	117.22	107.26
31	L1	1001	CYC	C4D-CHA-C1A	5.07	134.87	128.81
31	LK	1001	CYC	C4D-CHA-C1A	5.07	134.87	128.81
29	BA	202	PEB	CHC-C4C-C3C	-5.07	121.69	130.34
29	BN	202	PEB	CHC-C4C-C3C	-5.07	121.69	130.34
29	VB	201	PEB	C1C-CHB-C4B	-5.07	122.75	128.81
29	VM	201	PEB	C1C-CHB-C4B	-5.07	122.75	128.81
29	D1	1002	PEB	C3D-C4D-ND	5.07	117.21	107.26
29	LA	202	PEB	CHC-C4C-C3C	-5.07	121.69	130.34
29	LN	202	PEB	CHC-C4C-C3C	-5.07	121.69	130.34
29	J1	1002	PEB	C3D-C4D-ND	5.07	117.20	107.26
29	JK	1002	PEB	C3D-C4D-ND	5.07	117.20	107.26
31	EK	1001	CYC	CAB-C3B-C4B	5.07	129.38	121.38
31	CK	1001	CYC	CAB-C3B-C4B	5.07	129.38	121.38
29	DA	202	PEB	CHC-C4C-C3C	-5.06	121.70	130.34
29	DN	202	PEB	CHC-C4C-C3C	-5.06	121.70	130.34
31	C1	1001	CYC	CAB-C3B-C4B	5.06	129.38	121.38
29	HB	201	PEB	C1C-CHB-C4B	-5.06	122.76	128.81
29	HM	201	PEB	C1C-CHB-C4B	-5.06	122.76	128.81
29	PB	201	PEB	C1C-CHB-C4B	-5.06	122.76	128.81
29	PM	201	PEB	C1C-CHB-C4B	-5.06	122.76	128.81
29	J5	202	PEB	CMB-C2B-C1B	5.06	132.86	125.06
29	J8	202	PEB	CMB-C2B-C1B	5.06	132.86	125.06
29	MG	405	PEB	CHA-C1B-NB	-5.06	114.35	124.93
29	ZB	202	PEB	CHC-C1D-ND	-5.06	108.08	113.95
29	ZM	202	PEB	CHC-C1D-ND	-5.06	108.08	113.95
29	MQ	407	PEB	CHA-C1B-NB	-5.06	114.36	124.93
29	MR	202	PEB	C1C-CHB-C4B	-5.05	122.77	128.81
29	U2	201	PEB	CHA-C1B-NB	-5.05	114.37	124.93
31	YP	1000	CYC	CAB-C3B-C4B	5.05	129.35	121.38
31	1P	1002	CYC	CAB-C3B-C4B	5.04	129.35	121.38
29	M2	201	PEB	CHA-C1B-NB	-5.04	114.39	124.93
29	KB	203	PEB	CHC-C1D-ND	-5.04	108.10	113.95
29	KM	203	PEB	CHC-C1D-ND	-5.04	108.10	113.95
31	sP	1001	CYC	CHB-C4A-C3A	5.04	137.86	124.90
29	iB	202	PEB	CHC-C1D-ND	-5.04	108.10	113.95
29	iM	202	PEB	CHC-C1D-ND	-5.04	108.10	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UR	201	PEB	CHA-C1B-NB	-5.04	114.40	124.93
31	QP	1001	CYC	CHB-C4A-C3A	5.04	137.85	124.90
29	JB	202	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	YB	201	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	kB	202	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	JM	202	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	YM	201	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	kM	202	PEB	CHC-C1D-ND	-5.03	108.10	113.95
31	fP	1001	CYC	CHB-C4A-C3A	5.03	137.84	124.90
29	TB	202	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	TM	202	PEB	CHC-C1D-ND	-5.03	108.10	113.95
31	DP	1001	CYC	CHB-C4A-C3A	5.03	137.84	124.90
29	aB	203	PEB	CHC-C1D-ND	-5.03	108.10	113.95
29	aM	203	PEB	CHC-C1D-ND	-5.03	108.10	113.95
31	lP	1001	CYC	CHB-C4A-C3A	5.03	137.84	124.90
31	qP	1001	CYC	CHB-C4A-C3A	5.03	137.83	124.90
29	Q2	201	PEB	CHA-C1B-NB	-5.03	114.41	124.93
29	QB	202	PEB	CHC-C1D-ND	-5.03	108.11	113.95
29	mB	202	PEB	CHC-C1D-ND	-5.03	108.11	113.95
29	QM	202	PEB	CHC-C1D-ND	-5.03	108.11	113.95
29	mM	202	PEB	CHC-C1D-ND	-5.03	108.11	113.95
31	nP	1001	CYC	CHB-C4A-C3A	5.03	137.82	124.90
29	QR	201	PEB	CHA-C1B-NB	-5.02	114.42	124.93
31	wP	1001	CYC	CHB-C4A-C3A	5.02	137.82	124.90
31	XP	1001	CYC	CHB-C4A-C3A	5.02	137.82	124.90
31	hP	1001	CYC	CHB-C4A-C3A	5.02	137.82	124.90
29	HB	202	PEB	CHC-C1D-ND	-5.02	108.11	113.95
29	HM	202	PEB	CHC-C1D-ND	-5.02	108.11	113.95
31	IP	1001	CYC	CHB-C4A-C3A	5.02	137.81	124.90
29	gB	202	PEB	CHC-C1D-ND	-5.02	108.12	113.95
29	gM	202	PEB	CHC-C1D-ND	-5.02	108.12	113.95
31	BP	1001	CYC	CHB-C4A-C3A	5.02	137.81	124.90
29	MR	201	PEB	CHA-C1B-NB	-5.02	114.43	124.93
29	xL	301	PEB	OA-C1A-C2A	-5.02	122.18	126.17
31	HP	1001	CYC	CHB-C4A-C3A	5.02	137.80	124.90
31	oP	1001	CYC	CHB-C4A-C3A	5.02	137.80	124.90
29	FB	202	PEB	CHC-C1D-ND	-5.02	108.12	113.95
29	FM	202	PEB	CHC-C1D-ND	-5.02	108.12	113.95
31	kP	1001	CYC	CHB-C4A-C3A	5.02	137.80	124.90
31	FP	1001	CYC	CHB-C4A-C3A	5.01	137.79	124.90
29	RB	202	PEB	CHC-C1D-ND	-5.01	108.13	113.95
29	RM	202	PEB	CHC-C1D-ND	-5.01	108.13	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DB	202	PEB	CHC-C1D-ND	-5.01	108.13	113.95
29	DM	202	PEB	CHC-C1D-ND	-5.01	108.13	113.95
29	WR	201	PEB	CHA-C1B-NB	-5.01	114.46	124.93
29	O2	201	PEB	CHA-C1B-NB	-5.01	114.46	124.93
29	LB	202	PEB	CHC-C1D-ND	-5.01	108.14	113.95
29	LM	202	PEB	CHC-C1D-ND	-5.01	108.14	113.95
29	C5	203	PEB	OA-C1A-C2A	-5.00	122.19	126.17
31	OP	1001	CYC	CHB-C4A-C3A	5.00	137.77	124.90
31	jP	1001	CYC	CHB-C4A-C3A	5.00	137.77	124.90
31	uP	1001	CYC	CHB-C4A-C3A	5.00	137.77	124.90
31	SP	1001	CYC	CHB-C4A-C3A	5.00	137.77	124.90
29	cB	202	PEB	CHC-C1D-ND	-5.00	108.14	113.95
29	cM	202	PEB	CHC-C1D-ND	-5.00	108.14	113.95
31	MP	1001	CYC	CHB-C4A-C3A	5.00	137.76	124.90
29	VB	202	PEB	CHC-C1D-ND	-5.00	108.14	113.95
29	VM	202	PEB	CHC-C1D-ND	-5.00	108.14	113.95
31	UP	1001	CYC	CHB-C4A-C3A	5.00	137.75	124.90
29	K5	203	PEB	OA-C1A-C2A	-5.00	122.20	126.17
29	K8	203	PEB	OA-C1A-C2A	-5.00	122.20	126.17
29	OR	201	PEB	CHA-C1B-NB	-5.00	114.48	124.93
29	A5	203	PEB	OA-C1A-C2A	-5.00	122.20	126.17
29	A8	203	PEB	OA-C1A-C2A	-5.00	122.20	126.17
29	U7	201	PEB	CMA-C2A-C1A	-5.00	101.64	112.40
29	U9	201	PEB	CMA-C2A-C1A	-5.00	101.64	112.40
29	F1	1002	PEB	CHC-C1D-ND	-4.99	108.15	113.95
29	FK	1002	PEB	CHC-C1D-ND	-4.99	108.15	113.95
29	Z7	201	PEB	CMA-C2A-C1A	-4.99	101.64	112.40
29	Z9	201	PEB	CMA-C2A-C1A	-4.99	101.64	112.40
29	W2	201	PEB	CHA-C1B-NB	-4.99	114.49	124.93
29	f7	201	PEB	CMA-C2A-C1A	-4.99	101.65	112.40
29	f9	201	PEB	CMA-C2A-C1A	-4.99	101.65	112.40
29	M3	201	PEB	CHC-C1D-ND	-4.99	108.16	113.95
29	MO	201	PEB	CHC-C1D-ND	-4.99	108.16	113.95
29	d7	201	PEB	CMA-C2A-C1A	-4.98	101.66	112.40
29	d9	201	PEB	CMA-C2A-C1A	-4.98	101.66	112.40
29	W7	201	PEB	CMA-C2A-C1A	-4.98	101.66	112.40
29	W9	201	PEB	CMA-C2A-C1A	-4.98	101.66	112.40
29	S7	201	PEB	CMA-C2A-C1A	-4.98	101.67	112.40
29	l7	201	PEB	CMA-C2A-C1A	-4.98	101.67	112.40
29	S9	201	PEB	CMA-C2A-C1A	-4.98	101.67	112.40
29	l9	201	PEB	CMA-C2A-C1A	-4.98	101.67	112.40
29	j7	201	PEB	CMA-C2A-C1A	-4.98	101.68	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j9	201	PEB	CMA-C2A-C1A	-4.98	101.68	112.40
29	h7	201	PEB	CMA-C2A-C1A	-4.97	101.68	112.40
29	h9	201	PEB	CMA-C2A-C1A	-4.97	101.68	112.40
29	b7	201	PEB	CMA-C2A-C1A	-4.97	101.68	112.40
29	b9	201	PEB	CMA-C2A-C1A	-4.97	101.68	112.40
29	L1	1002	PEB	CHC-C1D-ND	-4.97	108.17	113.95
29	LK	1002	PEB	CHC-C1D-ND	-4.97	108.17	113.95
29	O7	201	PEB	CMA-C2A-C1A	-4.97	101.69	112.40
29	O9	201	PEB	CMA-C2A-C1A	-4.97	101.69	112.40
29	wL	301	PEB	OA-C1A-C2A	-4.97	122.22	126.17
29	MN	404	PEB	CHA-C1B-NB	-4.97	114.54	124.93
29	MA	404	PEB	CHA-C1B-NB	-4.97	114.54	124.93
30	A7	303	PUB	CHB-C1C-NC	-4.97	121.94	128.83
30	A9	303	PUB	CHB-C1C-NC	-4.97	121.94	128.83
29	xJ	301	PEB	OA-C1A-C2A	-4.96	122.23	126.17
29	Q7	201	PEB	CMA-C2A-C1A	-4.96	101.71	112.40
29	Q9	201	PEB	CMA-C2A-C1A	-4.96	101.71	112.40
29	JB	201	PEB	OA-C1A-C2A	-4.96	122.23	126.17
29	JM	201	PEB	OA-C1A-C2A	-4.96	122.23	126.17
29	M4	203	PEB	C1C-CHB-C4B	-4.96	122.89	128.81
29	AF	305	PEB	CHC-C4C-C3C	-4.96	121.88	130.34
29	AI	305	PEB	CHC-C4C-C3C	-4.96	121.88	130.34
29	HK	1002	PEB	CHC-C1D-ND	-4.95	108.20	113.95
29	NK	1002	PEB	CHC-C1D-ND	-4.95	108.20	113.95
29	I5	203	PEB	OA-C1A-C2A	-4.95	122.24	126.17
29	I8	203	PEB	OA-C1A-C2A	-4.95	122.24	126.17
29	N1	1002	PEB	CHC-C1D-ND	-4.95	108.20	113.95
29	H1	1002	PEB	CHC-C1D-ND	-4.94	108.20	113.95
29	GG	202	PEB	CHC-C1D-ND	-4.94	108.20	113.95
29	GQ	202	PEB	CHC-C1D-ND	-4.94	108.20	113.95
31	DF	1001	CYC	C1B-C2B-C3B	-4.94	102.71	107.87
31	DI	1001	CYC	C1B-C2B-C3B	-4.94	102.71	107.87
29	N3	201	PEB	CHC-C1D-ND	-4.94	108.21	113.95
29	RB	201	PEB	OA-C1A-C2A	-4.94	122.24	126.17
29	gB	201	PEB	OA-C1A-C2A	-4.94	122.24	126.17
29	RM	201	PEB	OA-C1A-C2A	-4.94	122.24	126.17
29	gM	201	PEB	OA-C1A-C2A	-4.94	122.24	126.17
29	IG	202	PEB	CHC-C1D-ND	-4.94	108.21	113.95
29	IQ	202	PEB	CHC-C1D-ND	-4.94	108.21	113.95
30	MG	403	PUB	OD-C4D-ND	-4.94	118.61	125.93
29	J1	1002	PEB	CHC-C1D-ND	-4.94	108.21	113.95
29	JK	1002	PEB	CHC-C1D-ND	-4.94	108.21	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	XB	201	PEB	OA-C1A-C2A	-4.94	122.25	126.17
29	XM	201	PEB	OA-C1A-C2A	-4.94	122.25	126.17
29	wJ	301	PEB	OA-C1A-C2A	-4.94	122.25	126.17
29	cB	201	PEB	OA-C1A-C2A	-4.93	122.25	126.17
29	cM	201	PEB	OA-C1A-C2A	-4.93	122.25	126.17
30	xJ	305	PUB	OD-C4D-C3D	-4.93	122.69	128.04
29	PB	201	PEB	CHB-C4B-NB	-4.93	121.99	128.83
29	PM	201	PEB	CHB-C4B-NB	-4.93	121.99	128.83
29	CG	202	PEB	CHC-C1D-ND	-4.93	108.22	113.95
29	CQ	202	PEB	CHC-C1D-ND	-4.93	108.22	113.95
29	iB	201	PEB	CHB-C4B-NB	-4.93	121.99	128.83
29	iM	201	PEB	CHB-C4B-NB	-4.93	121.99	128.83
29	C8	203	PEB	OA-C1A-C2A	-4.93	122.25	126.17
31	F1	1001	CYC	OB-C4B-C3B	-4.93	122.69	128.04
31	FK	1001	CYC	OB-C4B-C3B	-4.93	122.69	128.04
29	EG	202	PEB	CHC-C1D-ND	-4.93	108.22	113.95
29	EQ	202	PEB	CHC-C1D-ND	-4.93	108.22	113.95
29	NO	201	PEB	CHC-C1D-ND	-4.93	108.23	113.95
29	BB	301	PEB	CHB-C4B-NB	-4.92	122.00	128.83
29	BM	301	PEB	CHB-C4B-NB	-4.92	122.00	128.83
29	KG	202	PEB	CHC-C1D-ND	-4.92	108.23	113.95
29	KQ	202	PEB	CHC-C1D-ND	-4.92	108.23	113.95
29	fI	201	PEB	CHC-C4C-C3C	-4.92	121.94	130.34
29	fK	201	PEB	CHC-C4C-C3C	-4.92	121.94	130.34
29	MN	405	PEB	CMB-C2B-C1B	4.92	132.64	125.06
29	DK	1002	PEB	CHC-C1D-ND	-4.92	108.23	113.95
31	NF	1001	CYC	C1B-C2B-C3B	-4.92	102.74	107.87
31	NI	1001	CYC	C1B-C2B-C3B	-4.92	102.74	107.87
31	J1	1001	CYC	OB-C4B-C3B	-4.92	122.70	128.04
31	JK	1001	CYC	OB-C4B-C3B	-4.92	122.70	128.04
29	TB	201	PEB	OA-C1A-C2A	-4.92	122.26	126.17
29	TM	201	PEB	OA-C1A-C2A	-4.92	122.26	126.17
29	D1	1002	PEB	CHC-C1D-ND	-4.92	108.24	113.95
31	HF	1001	CYC	C1B-C2B-C3B	-4.92	102.74	107.87
31	HI	1001	CYC	C1B-C2B-C3B	-4.92	102.74	107.87
29	Q1	201	PEB	CHC-C4C-C3C	-4.91	121.95	130.34
29	QK	201	PEB	CHC-C4C-C3C	-4.91	121.95	130.34
29	VB	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
29	VM	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
29	HB	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
29	eB	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
29	HM	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	eM	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
31	N1	1001	CYC	OB-C4B-C3B	-4.91	122.71	128.04
31	NK	1001	CYC	OB-C4B-C3B	-4.91	122.71	128.04
29	S1	201	PEB	CHC-C4C-C3C	-4.91	121.96	130.34
29	SK	201	PEB	CHC-C4C-C3C	-4.91	121.96	130.34
29	kB	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	kM	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
31	DK	1001	CYC	OB-C4B-C3B	-4.91	122.71	128.04
29	NB	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	gB	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	NM	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	gM	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	FB	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
29	FM	201	PEB	OA-C1A-C2A	-4.91	122.27	126.17
29	eB	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	eM	201	PEB	CHB-C4B-NB	-4.91	122.02	128.83
29	HG	201	PEB	OA-C1A-C2A	-4.90	122.27	126.17
29	HQ	201	PEB	OA-C1A-C2A	-4.90	122.27	126.17
30	MQ	405	PUB	OD-C4D-ND	-4.90	118.66	125.93
29	AG	202	PEB	CHC-C1D-ND	-4.90	108.25	113.95
29	AQ	202	PEB	CHC-C1D-ND	-4.90	108.25	113.95
30	xL	305	PUB	CHA-C4A-NA	-4.90	108.25	113.95
31	JF	1001	CYC	C1B-C2B-C3B	-4.90	102.75	107.87
31	JI	1001	CYC	C1B-C2B-C3B	-4.90	102.75	107.87
29	XB	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
29	XM	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
29	b1	201	PEB	CHC-C4C-C3C	-4.90	121.98	130.34
29	bK	201	PEB	CHC-C4C-C3C	-4.90	121.98	130.34
29	mB	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
29	mM	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
29	Z1	202	PEB	CHC-C4C-C3C	-4.90	121.98	130.34
29	ZK	202	PEB	CHC-C4C-C3C	-4.90	121.98	130.34
29	HB	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
29	HM	201	PEB	CHB-C4B-NB	-4.90	122.03	128.83
29	iB	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
29	BG	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
29	iM	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
29	BQ	201	PEB	OA-C1A-C2A	-4.90	122.28	126.17
29	IA	201	PEB	CHB-C4B-NB	-4.90	122.04	128.83
29	RB	201	PEB	CHB-C4B-NB	-4.90	122.04	128.83
29	RM	201	PEB	CHB-C4B-NB	-4.90	122.04	128.83
29	IN	201	PEB	CHB-C4B-NB	-4.90	122.04	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MA	405	PEB	CMB-C2B-C1B	4.89	132.60	125.06
29	LB	201	PEB	CHB-C4B-NB	-4.89	122.04	128.83
29	ZB	201	PEB	CHB-C4B-NB	-4.89	122.04	128.83
29	LM	201	PEB	CHB-C4B-NB	-4.89	122.04	128.83
29	ZM	201	PEB	CHB-C4B-NB	-4.89	122.04	128.83
29	JB	201	PEB	CHB-C4B-NB	-4.89	122.04	128.83
29	JM	201	PEB	CHB-C4B-NB	-4.89	122.04	128.83
29	JG	201	PEB	OA-C1A-C2A	-4.89	122.28	126.17
29	JQ	201	PEB	OA-C1A-C2A	-4.89	122.28	126.17
29	W7	201	PEB	C3B-C4B-NB	4.89	117.16	110.05
29	W9	201	PEB	C3B-C4B-NB	4.89	117.16	110.05
31	FF	1001	CYC	C1B-C2B-C3B	-4.89	102.77	107.87
31	FI	1001	CYC	C1B-C2B-C3B	-4.89	102.77	107.87
29	j1	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
29	jK	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
29	O1	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
29	OK	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
29	d1	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
29	dK	201	PEB	CHC-C4C-C3C	-4.89	122.00	130.34
31	D1	1001	CYC	OB-C4B-C3B	-4.89	122.74	128.04
29	DB	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
29	DM	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
31	L1	1001	CYC	OB-C4B-C3B	-4.88	122.74	128.04
31	LK	1001	CYC	OB-C4B-C3B	-4.88	122.74	128.04
30	xJ	305	PUB	CHA-C4A-NA	-4.88	108.28	113.95
31	LF	1001	CYC	C1B-C2B-C3B	-4.88	102.78	107.87
31	LI	1001	CYC	C1B-C2B-C3B	-4.88	102.78	107.87
29	LB	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
29	LG	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
29	LM	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
29	MQ	402	PEB	OA-C1A-C2A	-4.88	122.29	126.17
30	xL	305	PUB	OD-C4D-C3D	-4.88	122.74	128.04
29	CA	201	PEB	CHB-C4B-NB	-4.88	122.06	128.83
29	CN	201	PEB	CHB-C4B-NB	-4.88	122.06	128.83
29	l1	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
29	lK	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
29	NB	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
29	NM	201	PEB	OA-C1A-C2A	-4.88	122.29	126.17
29	hJ	203	PEB	C1C-CHB-C4B	4.88	134.63	128.81
29	hL	203	PEB	C1C-CHB-C4B	4.88	134.63	128.81
29	cB	201	PEB	CHB-C4B-NB	-4.88	122.06	128.83
29	cM	201	PEB	CHB-C4B-NB	-4.88	122.06	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W1	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
29	h1	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
29	WK	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
29	hK	201	PEB	CHC-C4C-C3C	-4.88	122.02	130.34
29	U7	201	PEB	C3B-C4B-NB	4.87	117.14	110.05
29	U9	201	PEB	C3B-C4B-NB	4.87	117.14	110.05
30	wJ	305	PUB	CHA-C4A-NA	-4.87	108.29	113.95
29	VB	201	PEB	CHB-C4B-NB	-4.87	122.07	128.83
29	VM	201	PEB	CHB-C4B-NB	-4.87	122.07	128.83
29	PB	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
29	PM	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
29	DJ	202	PEB	C1C-CHB-C4B	4.87	134.63	128.81
29	bJ	203	PEB	C1C-CHB-C4B	4.87	134.63	128.81
29	DL	202	PEB	C1C-CHB-C4B	4.87	134.63	128.81
29	bL	203	PEB	C1C-CHB-C4B	4.87	134.63	128.81
29	XJ	203	PEB	C1C-CHB-C4B	4.87	134.63	128.81
29	XL	203	PEB	C1C-CHB-C4B	4.87	134.63	128.81
29	ZB	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
29	ZM	201	PEB	OA-C1A-C2A	-4.87	122.30	126.17
29	Q7	201	PEB	C3B-C4B-NB	4.87	117.13	110.05
29	Q9	201	PEB	C3B-C4B-NB	4.87	117.13	110.05
29	U1	202	PEB	CHC-C4C-C3C	-4.87	122.04	130.34
29	UK	202	PEB	CHC-C4C-C3C	-4.87	122.04	130.34
29	Z7	201	PEB	C3B-C4B-NB	4.87	117.13	110.05
29	h7	201	PEB	C3B-C4B-NB	4.87	117.13	110.05
29	Z9	201	PEB	C3B-C4B-NB	4.87	117.13	110.05
29	h9	201	PEB	C3B-C4B-NB	4.87	117.13	110.05
29	kB	201	PEB	OA-C1A-C2A	-4.86	122.31	126.17
29	kM	201	PEB	OA-C1A-C2A	-4.86	122.31	126.17
29	FG	201	PEB	OA-C1A-C2A	-4.86	122.31	126.17
29	FQ	201	PEB	OA-C1A-C2A	-4.86	122.31	126.17
31	1P	1002	CYC	OB-C4B-C3B	-4.86	122.77	128.04
29	TB	201	PEB	CHB-C4B-NB	-4.86	122.09	128.83
29	TM	201	PEB	CHB-C4B-NB	-4.86	122.09	128.83
30	MN	403	PUB	CHA-C4A-NA	-4.86	108.31	113.95
30	wJ	305	PUB	OD-C4D-C3D	-4.86	122.77	128.04
29	rJ	203	PEB	C1C-CHB-C4B	4.86	134.61	128.81
29	rL	203	PEB	C1C-CHB-C4B	4.86	134.61	128.81
29	EA	201	PEB	CHB-C4B-NB	-4.86	122.09	128.83
29	EN	201	PEB	CHB-C4B-NB	-4.86	122.09	128.83
29	S7	201	PEB	C3B-C4B-NB	4.86	117.11	110.05
29	S9	201	PEB	C3B-C4B-NB	4.86	117.11	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	wL	305	PUB	OD-C4D-C3D	-4.85	122.77	128.04
29	fJ	203	PEB	C1C-CHB-C4B	4.85	134.61	128.81
29	fL	203	PEB	C1C-CHB-C4B	4.85	134.61	128.81
29	lJ	203	PEB	C1C-CHB-C4B	4.85	134.61	128.81
29	tJ	202	PEB	C1C-CHB-C4B	4.85	134.61	128.81
29	lL	203	PEB	C1C-CHB-C4B	4.85	134.61	128.81
29	tL	202	PEB	C1C-CHB-C4B	4.85	134.61	128.81
29	PJ	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	PL	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	b7	201	PEB	C3B-C4B-NB	4.85	117.11	110.05
29	f7	201	PEB	C3B-C4B-NB	4.85	117.11	110.05
29	b9	201	PEB	C3B-C4B-NB	4.85	117.11	110.05
29	f9	201	PEB	C3B-C4B-NB	4.85	117.11	110.05
29	AA	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
29	AN	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
29	DB	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
29	DM	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
30	wL	305	PUB	CHA-C4A-NA	-4.85	108.32	113.95
29	VF	201	PEB	CMB-C2B-C1B	4.85	132.53	125.06
29	VI	201	PEB	CMB-C2B-C1B	4.85	132.53	125.06
29	BJ	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	BL	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
31	HK	1001	CYC	OB-C4B-C3B	-4.85	122.78	128.04
29	KA	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
29	KN	201	PEB	CHB-C4B-NB	-4.85	122.10	128.83
29	FB	201	PEB	CHB-C4B-NB	-4.85	122.11	128.83
29	FM	201	PEB	CHB-C4B-NB	-4.85	122.11	128.83
29	RJ	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	TJ	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	RL	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	TL	203	PEB	C1C-CHB-C4B	4.85	134.60	128.81
29	FJ	203	PEB	C1C-CHB-C4B	4.84	134.60	128.81
29	FL	203	PEB	C1C-CHB-C4B	4.84	134.60	128.81
29	l7	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
29	l9	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
29	vJ	202	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	vL	202	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	nJ	203	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	nL	203	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	HJ	202	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	HL	202	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	MA	404	PEB	CMB-C2B-C1B	4.84	132.52	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	O7	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
29	O9	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
29	j7	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
29	j9	201	PEB	C3B-C4B-NB	4.84	117.09	110.05
29	JJ	203	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	JL	203	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	ZJ	203	PEB	C1C-CHB-C4B	4.84	134.59	128.81
29	ZL	203	PEB	C1C-CHB-C4B	4.84	134.59	128.81
31	H1	1001	CYC	OB-C4B-C3B	-4.84	122.79	128.04
29	AB	302	PEB	OA-C1A-C2A	-4.84	122.33	126.17
29	A7	301	PEB	CHB-C4B-NB	-4.83	122.12	128.83
29	A9	301	PEB	CHB-C4B-NB	-4.83	122.12	128.83
30	wJ	304	PUB	CAD-C3D-C4D	4.83	129.01	121.38
29	RF	201	PEB	CMB-C2B-C1B	4.83	132.51	125.06
29	RI	201	PEB	CMB-C2B-C1B	4.83	132.51	125.06
29	dJ	203	PEB	C1C-CHB-C4B	4.83	134.58	128.81
29	dL	203	PEB	C1C-CHB-C4B	4.83	134.58	128.81
29	VJ	202	PEB	C1C-CHB-C4B	4.83	134.58	128.81
29	jJ	203	PEB	C1C-CHB-C4B	4.83	134.58	128.81
29	VL	202	PEB	C1C-CHB-C4B	4.83	134.58	128.81
29	jL	203	PEB	C1C-CHB-C4B	4.83	134.58	128.81
29	kF	201	PEB	CMB-C2B-C1B	4.83	132.50	125.06
29	kI	201	PEB	CMB-C2B-C1B	4.83	132.50	125.06
29	gF	203	PEB	CHB-C4B-NB	-4.83	122.13	128.83
29	gI	203	PEB	CHB-C4B-NB	-4.83	122.13	128.83
29	pJ	203	PEB	C1C-CHB-C4B	4.83	134.57	128.81
29	pL	203	PEB	C1C-CHB-C4B	4.83	134.57	128.81
29	GA	201	PEB	CHB-C4B-NB	-4.83	122.13	128.83
29	GN	201	PEB	CHB-C4B-NB	-4.83	122.13	128.83
30	xL	304	PUB	CAD-C3D-C4D	4.83	129.00	121.38
29	TI	201	PEB	CMB-C2B-C1B	4.83	132.50	125.06
29	mB	201	PEB	OA-C1A-C2A	-4.83	122.34	126.17
29	mM	201	PEB	OA-C1A-C2A	-4.83	122.34	126.17
29	A7	305	PEB	CHC-C4C-C3C	-4.83	122.11	130.34
29	A9	305	PEB	CHC-C4C-C3C	-4.83	122.11	130.34
29	YF	201	PEB	CMB-C2B-C1B	4.82	132.49	125.06
29	YI	201	PEB	CMB-C2B-C1B	4.82	132.49	125.06
29	iF	203	PEB	CHB-C4B-NB	-4.82	122.14	128.83
29	iI	203	PEB	CHB-C4B-NB	-4.82	122.14	128.83
30	MA	403	PUB	CHA-C4A-NA	-4.82	108.35	113.95
29	aF	201	PEB	CMB-C2B-C1B	4.82	132.48	125.06
29	aI	201	PEB	CMB-C2B-C1B	4.82	132.48	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LJ	202	PEB	C1C-CHB-C4B	4.82	134.56	128.81
29	LL	202	PEB	C1C-CHB-C4B	4.82	134.56	128.81
29	YF	203	PEB	CHB-C4B-NB	-4.82	122.15	128.83
29	YI	203	PEB	CHB-C4B-NB	-4.82	122.15	128.83
31	G9	1001	CYC	C2B-C1B-NB	4.82	114.04	106.99
29	eF	201	PEB	CMB-C2B-C1B	4.82	132.48	125.06
29	eI	201	PEB	CMB-C2B-C1B	4.82	132.48	125.06
29	aF	203	PEB	CHB-C4B-NB	-4.82	122.15	128.83
29	aI	203	PEB	CHB-C4B-NB	-4.82	122.15	128.83
29	d7	201	PEB	C3B-C4B-NB	4.81	117.05	110.05
29	d9	201	PEB	C3B-C4B-NB	4.81	117.05	110.05
31	G9	1001	CYC	CHA-C1A-NA	-4.81	122.15	128.83
31	G7	1001	CYC	CHA-C1A-NA	-4.81	122.15	128.83
29	Z1	202	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	mF	201	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	mI	201	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	ZK	202	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	RF	202	PEB	CHB-C4B-NB	-4.81	122.15	128.83
29	cF	202	PEB	CHB-C4B-NB	-4.81	122.15	128.83
29	RI	202	PEB	CHB-C4B-NB	-4.81	122.15	128.83
29	cI	202	PEB	CHB-C4B-NB	-4.81	122.15	128.83
29	VF	203	PEB	CHB-C4B-NB	-4.81	122.16	128.83
29	VI	203	PEB	CHB-C4B-NB	-4.81	122.16	128.83
29	O1	201	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	OK	201	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	NJ	203	PEB	C1C-CHB-C4B	4.81	134.55	128.81
29	NL	203	PEB	C1C-CHB-C4B	4.81	134.55	128.81
29	cF	201	PEB	CMB-C2B-C1B	4.81	132.47	125.06
29	cI	201	PEB	CMB-C2B-C1B	4.81	132.47	125.06
30	wL	304	PUB	CAD-C3D-C4D	4.81	128.97	121.38
29	TR	203	PEB	CHC-C1D-ND	-4.81	108.36	113.95
29	l1	201	PEB	CMB-C2B-C1B	4.81	132.46	125.06
29	lK	201	PEB	CMB-C2B-C1B	4.81	132.46	125.06
29	mF	203	PEB	CHB-C4B-NB	-4.80	122.17	128.83
29	mI	203	PEB	CHB-C4B-NB	-4.80	122.17	128.83
31	K7	1001	CYC	CHA-C1A-NA	-4.80	122.17	128.83
29	LA	201	PEB	C3B-C4B-NB	4.80	117.03	110.05
29	LN	201	PEB	C3B-C4B-NB	4.80	117.03	110.05
29	gF	201	PEB	CMB-C2B-C1B	4.80	132.46	125.06
29	gI	201	PEB	CMB-C2B-C1B	4.80	132.46	125.06
29	HA	201	PEB	C3B-C4B-NB	4.80	117.03	110.05
29	HN	201	PEB	C3B-C4B-NB	4.80	117.03	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DG	201	PEB	OA-C1A-C2A	-4.80	122.36	126.17
29	DQ	201	PEB	OA-C1A-C2A	-4.80	122.36	126.17
29	BA	201	PEB	C3B-C4B-NB	4.80	117.03	110.05
29	BN	201	PEB	C3B-C4B-NB	4.80	117.03	110.05
29	b1	201	PEB	CMB-C2B-C1B	4.80	132.45	125.06
29	bK	201	PEB	CMB-C2B-C1B	4.80	132.45	125.06
29	MN	404	PEB	CMB-C2B-C1B	4.80	132.45	125.06
31	YP	1000	CYC	OB-C4B-C3B	-4.80	122.84	128.04
29	iF	201	PEB	CMB-C2B-C1B	4.79	132.45	125.06
29	iI	201	PEB	CMB-C2B-C1B	4.79	132.45	125.06
31	I7	1001	CYC	CHA-C1A-NA	-4.79	122.18	128.83
31	I9	1001	CYC	CHA-C1A-NA	-4.79	122.18	128.83
29	A1	303	PEB	CHB-C4B-NB	-4.79	122.18	128.83
29	TF	202	PEB	CHB-C4B-NB	-4.79	122.18	128.83
29	TI	202	PEB	CHB-C4B-NB	-4.79	122.18	128.83
29	AK	303	PEB	CHB-C4B-NB	-4.79	122.18	128.83
31	G7	1001	CYC	C2B-C1B-NB	4.79	114.00	106.99
31	D1	1001	CYC	CMA-C3A-C4A	4.79	132.44	125.06
29	eF	203	PEB	CHB-C4B-NB	-4.79	122.18	128.83
29	eI	203	PEB	CHB-C4B-NB	-4.79	122.18	128.83
30	xJ	304	PUB	CAD-C3D-C4D	4.79	128.94	121.38
29	PF	203	PEB	CHB-C4B-NB	-4.79	122.18	128.83
29	PI	203	PEB	CHB-C4B-NB	-4.79	122.18	128.83
29	f1	201	PEB	CMB-C2B-C1B	4.79	132.44	125.06
29	fK	201	PEB	CMB-C2B-C1B	4.79	132.44	125.06
31	E7	1001	CYC	C2B-C1B-NB	4.79	114.00	106.99
31	E9	1001	CYC	C2B-C1B-NB	4.79	114.00	106.99
29	S1	201	PEB	CMB-C2B-C1B	4.79	132.44	125.06
29	SK	201	PEB	CMB-C2B-C1B	4.79	132.44	125.06
31	M7	1001	CYC	CHA-C1A-NA	-4.79	122.19	128.83
31	C7	1001	CYC	CHA-C1A-NA	-4.79	122.19	128.83
31	C9	1001	CYC	CHA-C1A-NA	-4.79	122.19	128.83
29	RR	203	PEB	CHC-C1D-ND	-4.79	108.39	113.95
29	W1	201	PEB	CMB-C2B-C1B	4.79	132.44	125.06
29	WK	201	PEB	CMB-C2B-C1B	4.79	132.44	125.06
29	kF	203	PEB	CHB-C4B-NB	-4.79	122.19	128.83
29	kI	203	PEB	CHB-C4B-NB	-4.79	122.19	128.83
29	PF	201	PEB	CMB-C2B-C1B	4.79	132.43	125.06
29	PI	201	PEB	CMB-C2B-C1B	4.79	132.43	125.06
31	E7	1001	CYC	CHA-C1A-NA	-4.78	122.19	128.83
31	E9	1001	CYC	CHA-C1A-NA	-4.78	122.19	128.83
29	JA	201	PEB	C3B-C4B-NB	4.78	117.01	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JN	201	PEB	C3B-C4B-NB	4.78	117.01	110.05
29	DA	201	PEB	C3B-C4B-NB	4.78	117.01	110.05
29	DN	201	PEB	C3B-C4B-NB	4.78	117.01	110.05
31	M9	1001	CYC	C2B-C1B-NB	4.78	113.99	106.99
29	h1	201	PEB	CMB-C2B-C1B	4.78	132.43	125.06
29	hK	201	PEB	CMB-C2B-C1B	4.78	132.43	125.06
31	C7	1001	CYC	C2B-C1B-NB	4.78	113.99	106.99
31	C9	1001	CYC	C2B-C1B-NB	4.78	113.99	106.99
31	K9	1001	CYC	CHA-C1A-NA	-4.78	122.19	128.83
29	NO	202	PEB	OA-C1A-C2A	-4.78	122.37	126.17
31	F9	1001	CYC	C2B-C1B-NB	4.78	113.98	106.99
29	Q1	201	PEB	CMB-C2B-C1B	4.78	132.42	125.06
29	QK	201	PEB	CMB-C2B-C1B	4.78	132.42	125.06
29	AM	302	PEB	OA-C1A-C2A	-4.77	122.38	126.17
31	DK	1001	CYC	CMA-C3A-C4A	4.77	132.41	125.06
31	N7	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
31	N9	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
31	L9	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
29	DG	203	PEB	C1C-CHB-C4B	-4.77	123.11	128.81
31	I7	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
31	I9	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
29	N2	203	PEB	CHC-C1D-ND	-4.77	108.41	113.95
29	j1	201	PEB	CMB-C2B-C1B	4.77	132.41	125.06
29	jK	201	PEB	CMB-C2B-C1B	4.77	132.41	125.06
29	DQ	203	PEB	C1C-CHB-C4B	-4.77	123.11	128.81
31	L7	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
31	D7	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
31	D9	1001	CYC	C2B-C1B-NB	4.77	113.97	106.99
29	MJ	201	PEB	C4B-C3B-C2B	-4.77	101.51	106.78
29	ML	201	PEB	C4B-C3B-C2B	-4.77	101.51	106.78
29	M3	203	PEB	OA-C1A-C2A	-4.77	122.38	126.17
29	MO	203	PEB	OA-C1A-C2A	-4.77	122.38	126.17
31	K7	1001	CYC	C2B-C1B-NB	4.76	113.96	106.99
29	HD	202	PEB	C1C-CHB-C4B	-4.76	123.12	128.81
31	N1	1001	CYC	CMA-C3A-C4A	4.76	132.40	125.06
31	M9	1001	CYC	CHA-C1A-NA	-4.76	122.22	128.83
29	M3	202	PEB	OA-C1A-C2A	-4.76	122.39	126.17
29	MO	202	PEB	OA-C1A-C2A	-4.76	122.39	126.17
29	UJ	201	PEB	C4B-C3B-C2B	-4.76	101.51	106.78
29	UL	201	PEB	C4B-C3B-C2B	-4.76	101.51	106.78
31	HK	1001	CYC	CMA-C3A-C4A	4.76	132.40	125.06
31	F7	1001	CYC	C2B-C1B-NB	4.76	113.96	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	yP	1001	CYC	C4D-CHA-C1A	4.76	134.50	128.81
31	WP	1001	CYC	C4D-CHA-C1A	4.76	134.49	128.81
29	A8	201	PEB	CHB-C4B-NB	-4.76	122.23	128.83
29	FA	201	PEB	C3B-C4B-NB	4.76	116.97	110.05
29	FN	201	PEB	C3B-C4B-NB	4.76	116.97	110.05
31	J7	1001	CYC	C2B-C1B-NB	4.76	113.95	106.99
31	M7	1001	CYC	C2B-C1B-NB	4.76	113.95	106.99
29	oJ	201	PEB	C4B-C3B-C2B	-4.76	101.52	106.78
29	oL	201	PEB	C4B-C3B-C2B	-4.76	101.52	106.78
31	H7	1001	CYC	C2B-C1B-NB	4.76	113.95	106.99
31	H9	1001	CYC	C2B-C1B-NB	4.76	113.95	106.99
31	K9	1001	CYC	C2B-C1B-NB	4.76	113.95	106.99
29	cJ	201	PEB	C4B-C3B-C2B	-4.76	101.52	106.78
29	cL	201	PEB	C4B-C3B-C2B	-4.76	101.52	106.78
31	NK	1001	CYC	CMA-C3A-C4A	4.76	132.39	125.06
29	U1	202	PEB	CMB-C2B-C1B	4.75	132.39	125.06
29	UK	202	PEB	CMB-C2B-C1B	4.75	132.39	125.06
29	P2	202	PEB	CHC-C1D-ND	-4.75	108.43	113.95
29	PR	202	PEB	CHC-C1D-ND	-4.75	108.43	113.95
31	J9	1001	CYC	C2B-C1B-NB	4.75	113.95	106.99
29	d1	201	PEB	CMB-C2B-C1B	4.75	132.38	125.06
29	dK	201	PEB	CMB-C2B-C1B	4.75	132.38	125.06
29	T2	203	PEB	CHC-C1D-ND	-4.75	108.43	113.95
31	F1	1001	CYC	CMA-C3A-C4A	4.75	132.38	125.06
31	FK	1001	CYC	CMA-C3A-C4A	4.75	132.38	125.06
29	HG	203	PEB	C1C-CHB-C4B	-4.75	123.13	128.81
29	R2	203	PEB	CHC-C1D-ND	-4.75	108.43	113.95
29	V2	203	PEB	CHC-C1D-ND	-4.75	108.43	113.95
29	Y1	202	PEB	OA-C1A-C2A	-4.75	122.40	126.17
29	YK	202	PEB	OA-C1A-C2A	-4.75	122.40	126.17
29	NO	201	PEB	OA-C1A-C2A	-4.75	122.40	126.17
29	LQ	202	PEB	C1C-CHB-C4B	-4.75	123.14	128.81
31	J1	1001	CYC	CMA-C3A-C4A	4.75	132.38	125.06
31	JK	1001	CYC	CMA-C3A-C4A	4.75	132.38	125.06
31	H1	1001	CYC	CMA-C3A-C4A	4.75	132.38	125.06
31	yP	1001	CYC	OB-C4B-C3B	-4.75	122.89	128.04
29	VR	203	PEB	CHC-C1D-ND	-4.75	108.44	113.95
29	A5	201	PEB	CHB-C4B-NB	-4.75	122.24	128.83
29	wJ	301	PEB	CHA-C1B-NB	-4.75	115.00	124.93
30	xJ	305	PUB	C4B-CHB-C1C	4.75	134.48	128.81
29	BD	202	PEB	C1C-CHB-C4B	-4.75	123.14	128.81
29	wL	301	PEB	C1C-CHB-C4B	-4.75	123.14	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KJ	201	PEB	C4B-C3B-C2B	-4.74	101.53	106.78
29	KL	201	PEB	C4B-C3B-C2B	-4.74	101.53	106.78
29	xJ	301	PEB	CHA-C1B-NB	-4.74	115.02	124.93
29	wJ	301	PEB	C1C-CHB-C4B	-4.74	123.15	128.81
29	HQ	203	PEB	C1C-CHB-C4B	-4.74	123.15	128.81
31	L1	1001	CYC	CMA-C3A-C4A	4.74	132.36	125.06
31	LK	1001	CYC	CMA-C3A-C4A	4.74	132.36	125.06
29	LD	202	PEB	C1C-CHB-C4B	-4.74	123.15	128.81
29	IJ	201	PEB	C4B-C3B-C2B	-4.74	101.54	106.78
29	IL	201	PEB	C4B-C3B-C2B	-4.74	101.54	106.78
29	wL	301	PEB	CHA-C1B-NB	-4.74	115.02	124.93
29	BG	203	PEB	C1C-CHB-C4B	-4.74	123.15	128.81
29	MG	404	PEB	CMB-C2B-C1B	4.74	132.36	125.06
29	OJ	201	PEB	C4B-C3B-C2B	-4.73	101.54	106.78
29	OL	201	PEB	C4B-C3B-C2B	-4.73	101.54	106.78
29	qJ	201	PEB	C4B-C3B-C2B	-4.73	101.55	106.78
29	qL	201	PEB	C4B-C3B-C2B	-4.73	101.55	106.78
29	NR	203	PEB	CHC-C1D-ND	-4.73	108.45	113.95
31	VP	1001	CYC	CMB-C2B-C1B	4.73	130.07	124.17
29	WJ	202	PEB	C4B-C3B-C2B	-4.73	101.55	106.78
29	WL	202	PEB	C4B-C3B-C2B	-4.73	101.55	106.78
29	FQ	203	PEB	C1C-CHB-C4B	-4.73	123.16	128.81
29	xL	301	PEB	CHA-C1B-NB	-4.73	115.04	124.93
29	P1	203	PEB	OA-C1A-C2A	-4.73	122.42	126.17
29	PK	203	PEB	OA-C1A-C2A	-4.73	122.42	126.17
29	BQ	203	PEB	C1C-CHB-C4B	-4.72	123.17	128.81
29	D3	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	DO	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	uJ	202	PEB	C4B-C3B-C2B	-4.72	101.56	106.78
29	uL	202	PEB	C4B-C3B-C2B	-4.72	101.56	106.78
29	M3	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	MO	201	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	JG	203	PEB	C1C-CHB-C4B	-4.72	123.17	128.81
29	J3	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	JO	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	k1	203	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	kK	203	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	AJ	201	PEB	C4B-C3B-C2B	-4.72	101.56	106.78
29	AL	201	PEB	C4B-C3B-C2B	-4.72	101.56	106.78
31	xP	1001	CYC	CMB-C2B-C1B	4.72	130.06	124.17
29	SJ	201	PEB	C4B-C3B-C2B	-4.72	101.56	106.78
29	SL	201	PEB	C4B-C3B-C2B	-4.72	101.56	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e1	203	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	eK	203	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	B3	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	K5	201	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	K8	201	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	BO	203	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	F9	1002	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	L3	202	PEB	CHB-C4B-NB	-4.72	122.28	128.83
29	LO	202	PEB	CHB-C4B-NB	-4.72	122.28	128.83
31	J9	1001	CYC	CHA-C1A-NA	-4.72	122.28	128.83
29	NO	203	PEB	OA-C1A-C2A	-4.72	122.42	126.17
29	X2	202	PEB	CHC-C1D-ND	-4.71	108.47	113.95
29	F3	203	PEB	CHB-C4B-NB	-4.71	122.29	128.83
29	FO	203	PEB	CHB-C4B-NB	-4.71	122.29	128.83
29	EJ	201	PEB	C4B-C3B-C2B	-4.71	101.56	106.78
29	EL	201	PEB	C4B-C3B-C2B	-4.71	101.56	106.78
29	H3	203	PEB	CHB-C4B-NB	-4.71	122.29	128.83
29	HO	203	PEB	CHB-C4B-NB	-4.71	122.29	128.83
29	XR	203	PEB	CHC-C1D-ND	-4.71	108.47	113.95
29	xL	301	PEB	C1C-CHB-C4B	-4.71	123.18	128.81
31	1P	1001	CYC	CMB-C2B-C1B	4.71	130.05	124.17
29	mJ	201	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
29	mL	201	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
29	N3	202	PEB	OA-C1A-C2A	-4.71	122.43	126.17
29	JQ	203	PEB	C1C-CHB-C4B	-4.71	123.18	128.81
29	MQ	406	PEB	CMB-C2B-C1B	4.71	132.32	125.06
29	I5	201	PEB	CHB-C4B-NB	-4.71	122.30	128.83
29	I8	201	PEB	CHB-C4B-NB	-4.71	122.30	128.83
29	L4	202	PEB	C1C-CHB-C4B	-4.71	123.18	128.81
29	QJ	201	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
29	QL	201	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
31	J7	1001	CYC	CHA-C1A-NA	-4.71	122.30	128.83
29	JG	202	PEB	OA-C1A-C2A	-4.71	122.43	126.17
29	JQ	202	PEB	OA-C1A-C2A	-4.71	122.43	126.17
29	B4	202	PEB	C1C-CHB-C4B	-4.71	123.19	128.81
29	LG	203	PEB	C1C-CHB-C4B	-4.71	123.19	128.81
29	xJ	301	PEB	C1C-CHB-C4B	-4.71	123.19	128.81
29	C5	201	PEB	CHB-C4B-NB	-4.71	122.30	128.83
29	C8	201	PEB	CHB-C4B-NB	-4.71	122.30	128.83
29	gJ	201	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
29	gL	201	PEB	C4B-C3B-C2B	-4.71	101.57	106.78
29	R1	203	PEB	OA-C1A-C2A	-4.71	122.43	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RK	203	PEB	OA-C1A-C2A	-4.71	122.43	126.17
31	D7	1001	CYC	CHA-C1A-NA	-4.70	122.30	128.83
31	D9	1001	CYC	CHA-C1A-NA	-4.70	122.30	128.83
29	a1	203	PEB	OA-C1A-C2A	-4.70	122.43	126.17
29	aK	203	PEB	OA-C1A-C2A	-4.70	122.43	126.17
31	C1	1001	CYC	OC-C1C-C2C	-4.70	122.43	126.17
29	T1	202	PEB	OA-C1A-C2A	-4.70	122.43	126.17
29	N3	203	PEB	OA-C1A-C2A	-4.70	122.43	126.17
29	DG	202	PEB	OA-C1A-C2A	-4.70	122.43	126.17
29	TK	202	PEB	OA-C1A-C2A	-4.70	122.43	126.17
29	DQ	202	PEB	OA-C1A-C2A	-4.70	122.43	126.17
29	iJ	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	iL	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	FG	202	PEB	OA-C1A-C2A	-4.70	122.44	126.17
29	HG	202	PEB	OA-C1A-C2A	-4.70	122.44	126.17
29	FQ	202	PEB	OA-C1A-C2A	-4.70	122.44	126.17
29	HQ	202	PEB	OA-C1A-C2A	-4.70	122.44	126.17
29	N3	201	PEB	OA-C1A-C2A	-4.70	122.44	126.17
29	CJ	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	sJ	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	CL	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	sL	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	F4	202	PEB	C1C-CHB-C4B	-4.70	123.20	128.81
29	eJ	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	eL	201	PEB	C4B-C3B-C2B	-4.70	101.58	106.78
29	FG	203	PEB	C1C-CHB-C4B	-4.69	123.20	128.81
30	xL	305	PUB	C4B-CHB-C1C	4.69	134.42	128.81
31	WP	1001	CYC	OB-C4B-C3B	-4.69	122.95	128.04
29	DD	202	PEB	C1C-CHB-C4B	-4.69	123.20	128.81
29	YJ	201	PEB	C4B-C3B-C2B	-4.69	101.59	106.78
29	YL	201	PEB	C4B-C3B-C2B	-4.69	101.59	106.78
29	UR	202	PEB	CHB-C4B-NB	-4.69	122.32	128.83
29	D7	1002	PEB	OA-C1A-C2A	-4.69	122.44	126.17
29	D9	1002	PEB	OA-C1A-C2A	-4.69	122.44	126.17
29	BG	202	PEB	CHC-C1D-ND	-4.69	108.50	113.95
29	BQ	202	PEB	CHC-C1D-ND	-4.69	108.50	113.95
29	M2	202	PEB	CHB-C4B-NB	-4.69	122.32	128.83
30	MA	402	PUB	CHA-C1B-C2B	-4.69	122.34	130.34
31	MP	1001	CYC	CMB-C2B-C1B	4.69	130.02	124.17
29	J4	202	PEB	C1C-CHB-C4B	-4.69	123.21	128.81
29	HG	202	PEB	CHC-C1D-ND	-4.68	108.51	113.95
29	HQ	202	PEB	CHC-C1D-ND	-4.68	108.51	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FD	202	PEB	C1C-CHB-C4B	-4.68	123.22	128.81
31	F9	1001	CYC	CHA-C1A-NA	-4.68	122.33	128.83
29	GJ	201	PEB	C4B-C3B-C2B	-4.68	101.60	106.78
29	GL	201	PEB	C4B-C3B-C2B	-4.68	101.60	106.78
31	H7	1001	CYC	CHA-C1A-NA	-4.68	122.33	128.83
31	H9	1001	CYC	CHA-C1A-NA	-4.68	122.33	128.83
29	F7	1002	PEB	OA-C1A-C2A	-4.68	122.45	126.17
31	sP	1001	CYC	CMB-C2B-C1B	4.68	130.01	124.17
31	F7	1001	CYC	CHA-C1A-NA	-4.68	122.34	128.83
30	AB	304	PUB	CHA-C1B-C2B	-4.68	122.36	130.34
30	MN	402	PUB	CHA-C1B-C2B	-4.68	122.36	130.34
29	LG	202	PEB	OA-C1A-C2A	-4.68	122.45	126.17
29	LQ	201	PEB	OA-C1A-C2A	-4.68	122.45	126.17
31	L7	1001	CYC	CHA-C1A-NA	-4.68	122.34	128.83
29	c1	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
29	cK	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
29	kJ	201	PEB	C4B-C3B-C2B	-4.67	101.61	106.78
29	kL	201	PEB	C4B-C3B-C2B	-4.67	101.61	106.78
31	jP	1001	CYC	CMB-C2B-C1B	4.67	130.00	124.17
31	oP	1001	CYC	CMB-C2B-C1B	4.67	130.00	124.17
31	L9	1001	CYC	CHA-C1A-NA	-4.67	122.35	128.83
29	FG	202	PEB	CHC-C1D-ND	-4.67	108.52	113.95
29	FQ	202	PEB	CHC-C1D-ND	-4.67	108.52	113.95
29	V1	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
29	VK	203	PEB	OA-C1A-C2A	-4.67	122.46	126.17
31	L9	1001	CYC	C1B-C2B-C3B	-4.67	103.00	107.87
29	aJ	201	PEB	C4B-C3B-C2B	-4.67	101.61	106.78
29	aL	201	PEB	C4B-C3B-C2B	-4.67	101.61	106.78
29	SR	202	PEB	CHB-C4B-NB	-4.67	122.35	128.83
29	M3	203	PEB	CHC-C1D-ND	-4.67	108.53	113.95
29	MO	203	PEB	CHC-C1D-ND	-4.67	108.53	113.95
29	WR	202	PEB	CHB-C4B-NB	-4.67	122.35	128.83
29	H4	202	PEB	C1C-CHB-C4B	-4.67	123.24	128.81
31	N7	1001	CYC	CHA-C1A-NA	-4.67	122.36	128.83
31	N9	1001	CYC	CHA-C1A-NA	-4.67	122.36	128.83
31	OP	1001	CYC	CMB-C2B-C1B	4.66	129.99	124.17
31	FP	1001	CYC	CMB-C2B-C1B	4.66	129.99	124.17
31	qP	1001	CYC	CMB-C2B-C1B	4.66	129.99	124.17
29	D4	202	PEB	C1C-CHB-C4B	-4.66	123.24	128.81
29	LG	202	PEB	CHC-C1D-ND	-4.66	108.53	113.95
29	LQ	201	PEB	CHC-C1D-ND	-4.66	108.53	113.95
29	S2	202	PEB	CHB-C4B-NB	-4.66	122.36	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W2	202	PEB	CHB-C4B-NB	-4.66	122.36	128.83
30	AM	304	PUB	CHA-C1B-C2B	-4.66	122.39	130.34
31	QP	1001	CYC	CMB-C2B-C1B	4.66	129.99	124.17
31	xP	1001	CYC	CHB-C4A-C3A	4.66	136.88	124.90
30	AF	303	PUB	CHB-C1C-NC	-4.66	122.36	128.83
30	AI	303	PUB	CHB-C1C-NC	-4.66	122.36	128.83
29	JD	202	PEB	C1C-CHB-C4B	-4.66	123.25	128.81
29	BG	202	PEB	OA-C1A-C2A	-4.66	122.47	126.17
29	BQ	202	PEB	OA-C1A-C2A	-4.66	122.47	126.17
31	DP	1001	CYC	CMB-C2B-C1B	4.66	129.98	124.17
29	i1	203	PEB	OA-C1A-C2A	-4.65	122.47	126.17
29	iK	203	PEB	OA-C1A-C2A	-4.65	122.47	126.17
31	YP	1000	CYC	CHB-C4A-C3A	4.65	136.86	124.90
31	BP	1001	CYC	CMB-C2B-C1B	4.65	129.97	124.17
30	wL	305	PUB	C4B-CHB-C1C	4.65	134.36	128.81
31	kP	1001	CYC	CMB-C2B-C1B	4.65	129.97	124.17
31	1P	1002	CYC	CHB-C4A-C3A	4.65	136.85	124.90
29	J9	1002	PEB	OA-C1A-C2A	-4.65	122.48	126.17
31	VP	1001	CYC	CHB-C4A-C3A	4.65	136.85	124.90
30	wJ	305	PUB	C4B-CHB-C1C	4.65	134.36	128.81
31	fP	1001	CYC	CMB-C2B-C1B	4.64	129.96	124.17
31	wP	1001	CYC	CMB-C2B-C1B	4.64	129.96	124.17
29	yJ	301	PEB	CHB-C4B-NB	-4.64	122.39	128.83
29	yL	301	PEB	CHB-C4B-NB	-4.64	122.39	128.83
29	O2	202	PEB	CHB-C4B-NB	-4.64	122.39	128.83
29	DG	202	PEB	CHC-C1D-ND	-4.64	108.56	113.95
29	DQ	202	PEB	CHC-C1D-ND	-4.64	108.56	113.95
29	N7	1002	PEB	OA-C1A-C2A	-4.64	122.48	126.17
29	N9	1002	PEB	OA-C1A-C2A	-4.64	122.48	126.17
31	F7	1001	CYC	C1B-C2B-C3B	-4.64	103.03	107.87
31	SP	1001	CYC	CMB-C2B-C1B	4.64	129.96	124.17
29	JG	202	PEB	CHC-C1D-ND	-4.64	108.56	113.95
29	JQ	202	PEB	CHC-C1D-ND	-4.64	108.56	113.95
29	Q2	202	PEB	CHB-C4B-NB	-4.64	122.40	128.83
31	HP	1001	CYC	CMB-C2B-C1B	4.64	129.96	124.17
29	J7	1002	PEB	OA-C1A-C2A	-4.64	122.49	126.17
31	CK	1001	CYC	OC-C1C-C2C	-4.64	122.49	126.17
31	H7	1001	CYC	C1B-C2B-C3B	-4.64	103.03	107.87
31	L7	1001	CYC	C1B-C2B-C3B	-4.64	103.03	107.87
31	H9	1001	CYC	C1B-C2B-C3B	-4.64	103.03	107.87
29	H7	1002	PEB	OA-C1A-C2A	-4.63	122.49	126.17
29	H9	1002	PEB	OA-C1A-C2A	-4.63	122.49	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	UP	1001	CYC	CMB-C2B-C1B	4.63	129.95	124.17
31	hP	1001	CYC	CMB-C2B-C1B	4.63	129.95	124.17
31	EF	1001	CYC	OC-C1C-C2C	-4.63	122.49	126.17
31	EI	1001	CYC	OC-C1C-C2C	-4.63	122.49	126.17
31	IP	1001	CYC	CMB-C2B-C1B	4.63	129.95	124.17
29	MJ	201	PEB	C3B-C4B-NB	4.63	116.78	110.05
29	ML	201	PEB	C3B-C4B-NB	4.63	116.78	110.05
29	m1	202	PEB	OA-C1A-C2A	-4.63	122.49	126.17
29	mK	202	PEB	OA-C1A-C2A	-4.63	122.49	126.17
31	D7	1001	CYC	C1B-C2B-C3B	-4.63	103.04	107.87
31	D9	1001	CYC	C1B-C2B-C3B	-4.63	103.04	107.87
29	A1	302	PEB	CHB-C4B-NB	-4.63	122.41	128.83
29	AK	302	PEB	CHB-C4B-NB	-4.63	122.41	128.83
29	g1	203	PEB	OA-C1A-C2A	-4.63	122.50	126.17
29	gK	203	PEB	OA-C1A-C2A	-4.63	122.50	126.17
29	U2	202	PEB	CHB-C4B-NB	-4.62	122.41	128.83
31	J7	1001	CYC	C1B-C2B-C3B	-4.62	103.05	107.87
29	E4	202	PEB	CHB-C4B-NB	-4.62	122.41	128.83
31	nP	1001	CYC	CMB-C2B-C1B	4.62	129.94	124.17
31	F9	1001	CYC	C1B-C2B-C3B	-4.62	103.05	107.87
29	g7	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
29	g9	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
29	NO	203	PEB	CHC-C1D-ND	-4.62	108.58	113.95
30	BB	302	PUB	OD-C4D-ND	-4.62	119.08	125.93
30	BM	302	PUB	OD-C4D-ND	-4.62	119.08	125.93
29	J5	201	PEB	CHA-C1B-C2B	4.62	136.78	124.90
29	J8	201	PEB	CHA-C1B-C2B	4.62	136.78	124.90
29	HC	201	PEB	C1C-CHB-C4B	-4.62	123.29	128.81
29	HE	201	PEB	C1C-CHB-C4B	-4.62	123.29	128.81
29	m7	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
29	m9	201	PEB	CMB-C2B-C1B	4.62	132.18	125.06
31	DF	1001	CYC	C2B-C1B-NB	4.62	113.75	106.99
31	DI	1001	CYC	C2B-C1B-NB	4.62	113.75	106.99
29	M4	202	PEB	CHB-C4B-NB	-4.62	122.42	128.83
29	ED	201	PEB	CHB-C4B-NB	-4.62	122.42	128.83
29	U7	202	PEB	CHB-C4B-NB	-4.62	122.42	128.83
29	U9	202	PEB	CHB-C4B-NB	-4.62	122.42	128.83
31	uP	1001	CYC	CMB-C2B-C1B	4.62	129.93	124.17
31	J9	1001	CYC	C1B-C2B-C3B	-4.62	103.06	107.87
29	qJ	201	PEB	C3B-C4B-NB	4.61	116.76	110.05
29	qL	201	PEB	C3B-C4B-NB	4.61	116.76	110.05
29	KD	202	PEB	CHB-C4B-NB	-4.61	122.43	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	XP	1001	CYC	CMB-C2B-C1B	4.61	129.93	124.17
29	UJ	201	PEB	C3B-C4B-NB	4.61	116.76	110.05
29	UL	201	PEB	C3B-C4B-NB	4.61	116.76	110.05
29	P7	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	V7	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	i7	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	P9	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	V9	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	i9	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	N3	203	PEB	CHC-C1D-ND	-4.61	108.59	113.95
29	IJ	201	PEB	C3B-C4B-NB	4.61	116.75	110.05
29	IL	201	PEB	C3B-C4B-NB	4.61	116.75	110.05
29	c7	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	e7	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	c9	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
29	e9	201	PEB	CMB-C2B-C1B	4.61	132.16	125.06
31	HF	1001	CYC	C2B-C1B-NB	4.61	113.73	106.99
31	NF	1001	CYC	C2B-C1B-NB	4.61	113.73	106.99
31	HI	1001	CYC	C2B-C1B-NB	4.61	113.73	106.99
31	NI	1001	CYC	C2B-C1B-NB	4.61	113.73	106.99
29	GD	202	PEB	CHB-C4B-NB	-4.60	122.44	128.83
31	JF	1001	CYC	C2B-C1B-NB	4.60	113.73	106.99
31	JI	1001	CYC	C2B-C1B-NB	4.60	113.73	106.99
29	N3	201	PEB	CAB-CBB-CGB	-4.60	103.70	113.60
29	I4	202	PEB	CHB-C4B-NB	-4.60	122.44	128.83
29	G4	202	PEB	CHB-C4B-NB	-4.60	122.44	128.83
31	FF	1001	CYC	C2B-C1B-NB	4.60	113.72	106.99
31	LF	1001	CYC	C2B-C1B-NB	4.60	113.72	106.99
31	FI	1001	CYC	C2B-C1B-NB	4.60	113.72	106.99
31	LI	1001	CYC	C2B-C1B-NB	4.60	113.72	106.99
29	mJ	201	PEB	C3B-C4B-NB	4.60	116.74	110.05
29	mL	201	PEB	C3B-C4B-NB	4.60	116.74	110.05
29	CD	202	PEB	CHB-C4B-NB	-4.60	122.44	128.83
29	KJ	201	PEB	C3B-C4B-NB	4.60	116.74	110.05
29	KL	201	PEB	C3B-C4B-NB	4.60	116.74	110.05
29	NO	201	PEB	CAB-CBB-CGB	-4.60	103.71	113.60
29	JC	201	PEB	C1C-CHB-C4B	-4.60	123.32	128.81
29	JE	201	PEB	C1C-CHB-C4B	-4.60	123.32	128.81
29	K4	202	PEB	CHB-C4B-NB	-4.60	122.45	128.83
29	QJ	201	PEB	C3B-C4B-NB	4.60	116.74	110.05
29	QL	201	PEB	C3B-C4B-NB	4.60	116.74	110.05
29	a7	201	PEB	CMB-C2B-C1B	4.60	132.14	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a9	201	PEB	CMB-C2B-C1B	4.60	132.14	125.06
29	h7	202	PEB	CHB-C4B-NB	-4.60	122.45	128.83
29	h9	202	PEB	CHB-C4B-NB	-4.60	122.45	128.83
29	T7	201	PEB	CMB-C2B-C1B	4.59	132.14	125.06
29	Y7	201	PEB	CMB-C2B-C1B	4.59	132.14	125.06
29	T9	201	PEB	CMB-C2B-C1B	4.59	132.14	125.06
29	Y9	201	PEB	CMB-C2B-C1B	4.59	132.14	125.06
29	R7	201	PEB	CMB-C2B-C1B	4.59	132.14	125.06
29	R9	201	PEB	CMB-C2B-C1B	4.59	132.14	125.06
29	cJ	201	PEB	C3B-C4B-NB	4.59	116.73	110.05
29	cL	201	PEB	C3B-C4B-NB	4.59	116.73	110.05
29	uJ	202	PEB	C3B-C4B-NB	4.59	116.73	110.05
29	uL	202	PEB	C3B-C4B-NB	4.59	116.73	110.05
30	AF	302	PUB	CHC-C1D-ND	-4.59	107.92	113.72
30	AI	302	PUB	CHC-C1D-ND	-4.59	107.92	113.72
29	QR	202	PEB	CHB-C4B-NB	-4.59	122.46	128.83
29	DC	201	PEB	C1C-CHB-C4B	-4.59	123.33	128.81
29	DE	201	PEB	C1C-CHB-C4B	-4.59	123.33	128.81
29	L7	1002	PEB	OA-C1A-C2A	-4.59	122.53	126.17
29	l7	202	PEB	CHB-C4B-NB	-4.59	122.46	128.83
29	l9	202	PEB	CHB-C4B-NB	-4.59	122.46	128.83
29	OJ	201	PEB	C3B-C4B-NB	4.59	116.72	110.05
29	OL	201	PEB	C3B-C4B-NB	4.59	116.72	110.05
29	MD	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
30	A1	304	PUB	CHA-C4A-NA	-4.58	108.62	113.95
30	AK	304	PUB	CHA-C4A-NA	-4.58	108.62	113.95
29	aJ	201	PEB	C3B-C4B-NB	4.58	116.72	110.05
29	aL	201	PEB	C3B-C4B-NB	4.58	116.72	110.05
29	EJ	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	iJ	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	EL	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	iL	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	H3	203	PEB	OA-C1A-C2A	-4.58	122.53	126.17
29	HO	203	PEB	OA-C1A-C2A	-4.58	122.53	126.17
29	S7	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
29	b7	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
29	S9	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
29	b9	202	PEB	CHB-C4B-NB	-4.58	122.47	128.83
31	N7	1001	CYC	C1B-C2B-C3B	-4.58	103.09	107.87
31	N9	1001	CYC	C1B-C2B-C3B	-4.58	103.09	107.87
31	KF	1001	CYC	OC-C1C-C2C	-4.58	122.53	126.17
29	SJ	201	PEB	C3B-C4B-NB	4.58	116.71	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SL	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	FC	201	PEB	C1C-CHB-C4B	-4.58	123.34	128.81
29	FE	201	PEB	C1C-CHB-C4B	-4.58	123.34	128.81
29	sJ	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	sL	201	PEB	C3B-C4B-NB	4.58	116.71	110.05
29	j7	202	PEB	CHB-C4B-NB	-4.58	122.48	128.83
29	j9	202	PEB	CHB-C4B-NB	-4.58	122.48	128.83
29	M3	201	PEB	CAB-CBB-CGB	-4.58	103.75	113.60
29	MO	201	PEB	CAB-CBB-CGB	-4.58	103.75	113.60
29	BC	201	PEB	C1C-CHB-C4B	-4.58	123.34	128.81
29	BE	201	PEB	C1C-CHB-C4B	-4.58	123.34	128.81
29	L9	1002	PEB	OA-C1A-C2A	-4.58	122.53	126.17
29	d7	202	PEB	CHB-C4B-NB	-4.57	122.48	128.83
29	d9	202	PEB	CHB-C4B-NB	-4.57	122.48	128.83
29	oJ	201	PEB	C3B-C4B-NB	4.57	116.70	110.05
29	oL	201	PEB	C3B-C4B-NB	4.57	116.70	110.05
29	O7	202	PEB	CHB-C4B-NB	-4.57	122.48	128.83
29	O9	202	PEB	CHB-C4B-NB	-4.57	122.48	128.83
29	LC	201	PEB	C1C-CHB-C4B	-4.57	123.35	128.81
29	LE	201	PEB	C1C-CHB-C4B	-4.57	123.35	128.81
29	k7	201	PEB	CMB-C2B-C1B	4.57	132.11	125.06
29	k9	201	PEB	CMB-C2B-C1B	4.57	132.11	125.06
31	VP	1001	CYC	CMA-C3A-C4A	4.57	132.10	125.06
31	xP	1001	CYC	CMA-C3A-C4A	4.57	132.10	125.06
29	AF	305	PEB	CHB-C4B-NB	-4.57	122.49	128.83
29	AI	305	PEB	CHB-C4B-NB	-4.57	122.49	128.83
29	f7	202	PEB	CHB-C4B-NB	-4.57	122.49	128.83
29	f9	202	PEB	CHB-C4B-NB	-4.57	122.49	128.83
29	XR	202	PEB	C2A-C1A-NA	4.57	112.21	108.27
29	W7	202	PEB	CHB-C4B-NB	-4.57	122.49	128.83
29	W9	202	PEB	CHB-C4B-NB	-4.57	122.49	128.83
29	CJ	201	PEB	C3B-C4B-NB	4.57	116.69	110.05
29	CL	201	PEB	C3B-C4B-NB	4.57	116.69	110.05
29	YJ	201	PEB	C3B-C4B-NB	4.57	116.69	110.05
29	YL	201	PEB	C3B-C4B-NB	4.57	116.69	110.05
29	eJ	201	PEB	C3B-C4B-NB	4.56	116.69	110.05
29	eL	201	PEB	C3B-C4B-NB	4.56	116.69	110.05
29	Q7	202	PEB	CHB-C4B-NB	-4.56	122.50	128.83
29	Q9	202	PEB	CHB-C4B-NB	-4.56	122.50	128.83
29	N2	202	PEB	C2A-C1A-NA	4.56	112.21	108.27
29	Z7	202	PEB	CHB-C4B-NB	-4.56	122.50	128.83
29	Z9	202	PEB	CHB-C4B-NB	-4.56	122.50	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WJ	202	PEB	C3B-C4B-NB	4.56	116.69	110.05
29	WL	202	PEB	C3B-C4B-NB	4.56	116.69	110.05
29	NR	202	PEB	C2A-C1A-NA	4.56	112.20	108.27
31	IF	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
31	II	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
31	NF	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
31	NI	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
29	GJ	201	PEB	C3B-C4B-NB	4.56	116.68	110.05
29	GL	201	PEB	C3B-C4B-NB	4.56	116.68	110.05
31	MP	1001	CYC	CAB-C3B-C4B	4.56	128.58	121.38
31	CF	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
31	CI	1001	CYC	OC-C1C-C2C	-4.56	122.55	126.17
29	kJ	201	PEB	C3B-C4B-NB	4.56	116.68	110.05
29	kL	201	PEB	C3B-C4B-NB	4.56	116.68	110.05
31	jP	1001	CYC	CAB-C3B-C4B	4.56	128.57	121.38
29	ID	202	PEB	CHB-C4B-NB	-4.56	122.51	128.83
29	AJ	201	PEB	C3B-C4B-NB	4.56	116.67	110.05
29	AL	201	PEB	C3B-C4B-NB	4.56	116.67	110.05
31	1P	1002	CYC	CMB-C2B-C1B	4.55	129.85	124.17
29	C4	202	PEB	CHB-C4B-NB	-4.55	122.51	128.83
31	SP	1001	CYC	CAB-C3B-C4B	4.55	128.57	121.38
29	gJ	201	PEB	C3B-C4B-NB	4.55	116.67	110.05
29	gL	201	PEB	C3B-C4B-NB	4.55	116.67	110.05
29	TR	202	PEB	C2A-C1A-NA	4.55	112.20	108.27
31	QP	1001	CYC	CAB-C3B-C4B	4.55	128.57	121.38
31	GK	1001	CYC	OC-C1C-C2C	-4.55	122.55	126.17
29	gF	201	PEB	CAB-C3B-C4B	4.55	133.06	125.01
29	gI	201	PEB	CAB-C3B-C4B	4.55	133.06	125.01
31	fP	1001	CYC	CAB-C3B-C4B	4.55	128.56	121.38
29	TI	201	PEB	CAB-C3B-C4B	4.55	133.06	125.01
31	1P	1001	CYC	CAB-C3B-C4B	4.55	128.56	121.38
29	D4	202	PEB	CHB-C4B-NB	-4.54	122.52	128.83
31	kP	1001	CYC	CAB-C3B-C4B	4.54	128.56	121.38
31	I1	1001	CYC	OC-C1C-C2C	-4.54	122.56	126.17
31	KI	1001	CYC	CMA-C3A-C4A	4.54	132.06	125.06
29	L3	202	PEB	OA-C1A-C2A	-4.54	122.56	126.17
29	LO	202	PEB	OA-C1A-C2A	-4.54	122.56	126.17
31	BP	1001	CYC	CAB-C3B-C4B	4.54	128.55	121.38
31	oP	1001	CYC	CAB-C3B-C4B	4.54	128.55	121.38
31	DF	1001	CYC	OC-C1C-C2C	-4.54	122.56	126.17
31	DI	1001	CYC	OC-C1C-C2C	-4.54	122.56	126.17
31	nP	1001	CYC	CAB-C3B-C4B	4.54	128.55	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CF	1001	CYC	CMA-C3A-C4A	4.54	132.05	125.06
31	CI	1001	CYC	CMA-C3A-C4A	4.54	132.05	125.06
29	eF	201	PEB	CAB-C3B-C4B	4.54	133.04	125.01
29	eI	201	PEB	CAB-C3B-C4B	4.54	133.04	125.01
31	hP	1001	CYC	CAB-C3B-C4B	4.54	128.54	121.38
29	VR	202	PEB	C2A-C1A-NA	4.54	112.18	108.27
31	qP	1001	CYC	CAB-C3B-C4B	4.54	128.54	121.38
29	L4	202	PEB	CHB-C4B-NB	-4.54	122.54	128.83
29	aF	201	PEB	CAB-C3B-C4B	4.53	133.03	125.01
29	aI	201	PEB	CAB-C3B-C4B	4.53	133.03	125.01
29	RF	202	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	RI	202	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	ID	203	PEB	C2A-C1A-NA	4.53	112.18	108.27
29	YF	201	PEB	CAB-C3B-C4B	4.53	133.03	125.01
29	YI	201	PEB	CAB-C3B-C4B	4.53	133.03	125.01
29	FD	202	PEB	CHB-C4B-NB	-4.53	122.54	128.83
31	UP	1001	CYC	CAB-C3B-C4B	4.53	128.54	121.38
29	J3	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	JO	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	ED	201	PEB	C3D-C4D-ND	4.53	116.15	107.26
29	F4	202	PEB	CHB-C4B-NB	-4.53	122.54	128.83
29	A7	305	PEB	CHA-C1B-NB	-4.53	115.45	124.93
29	A9	305	PEB	CHA-C1B-NB	-4.53	115.45	124.93
29	cF	201	PEB	CAB-C3B-C4B	4.53	133.03	125.01
29	cI	201	PEB	CAB-C3B-C4B	4.53	133.03	125.01
29	YF	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	YI	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	JD	202	PEB	CHB-C4B-NB	-4.53	122.54	128.83
29	LD	202	PEB	CHB-C4B-NB	-4.53	122.54	128.83
31	KF	1001	CYC	CMA-C3A-C4A	4.53	132.04	125.06
31	DP	1001	CYC	CAB-C3B-C4B	4.53	128.53	121.38
31	M1	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
31	JF	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
31	LF	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
31	JI	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
31	LI	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
31	MK	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
29	kF	201	PEB	CAB-C3B-C4B	4.53	133.02	125.01
29	kI	201	PEB	CAB-C3B-C4B	4.53	133.02	125.01
29	H1	1002	PEB	CHB-C4B-NB	-4.53	122.54	128.83
29	B3	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	BO	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RR	202	PEB	C2A-C1A-NA	4.53	112.18	108.27
31	EK	1001	CYC	OC-C1C-C2C	-4.53	122.57	126.17
31	OP	1001	CYC	CAB-C3B-C4B	4.53	128.53	121.38
29	F3	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	FO	203	PEB	OA-C1A-C2A	-4.53	122.57	126.17
29	VF	201	PEB	CAB-C3B-C4B	4.53	133.02	125.01
29	VI	201	PEB	CAB-C3B-C4B	4.53	133.02	125.01
31	sP	1001	CYC	CAB-C3B-C4B	4.53	128.53	121.38
31	MF	1001	CYC	CMA-C3A-C4A	4.53	132.03	125.06
31	MI	1001	CYC	CMA-C3A-C4A	4.53	132.03	125.06
29	D3	203	PEB	OA-C1A-C2A	-4.53	122.58	126.17
29	DO	203	PEB	OA-C1A-C2A	-4.53	122.58	126.17
29	E4	203	PEB	C2A-C1A-NA	4.53	112.17	108.27
29	E4	202	PEB	C3D-C4D-ND	4.52	116.14	107.26
31	KI	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	wP	1001	CYC	CAB-C3B-C4B	4.52	128.52	121.38
29	PF	201	PEB	CAB-C3B-C4B	4.52	133.01	125.01
29	PI	201	PEB	CAB-C3B-C4B	4.52	133.01	125.01
29	BD	202	PEB	CHB-C4B-NB	-4.52	122.55	128.83
29	HK	1002	PEB	CHB-C4B-NB	-4.52	122.55	128.83
29	NB	201	PEB	CHC-C1D-ND	4.52	119.20	113.95
29	NM	201	PEB	CHC-C1D-ND	4.52	119.20	113.95
31	HP	1001	CYC	CAB-C3B-C4B	4.52	128.52	121.38
31	K1	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	KK	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
29	B4	202	PEB	CHB-C4B-NB	-4.52	122.56	128.83
31	GF	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	GI	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
29	PB	201	PEB	CHC-C1D-ND	4.52	119.20	113.95
29	PM	201	PEB	CHC-C1D-ND	4.52	119.20	113.95
29	X2	201	PEB	C2A-C1A-NA	4.52	112.17	108.27
29	GD	202	PEB	C3D-C4D-ND	4.52	116.13	107.26
29	iF	201	PEB	CAB-C3B-C4B	4.52	133.01	125.01
29	iI	201	PEB	CAB-C3B-C4B	4.52	133.01	125.01
31	FP	1001	CYC	CAB-C3B-C4B	4.52	128.52	121.38
29	ID	202	PEB	C3D-C4D-ND	4.52	116.13	107.26
31	IK	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	EF	1001	CYC	CMA-C3A-C4A	4.52	132.02	125.06
31	EI	1001	CYC	CMA-C3A-C4A	4.52	132.02	125.06
29	V2	202	PEB	C2A-C1A-NA	4.52	112.17	108.27
31	GF	1001	CYC	CMA-C3A-C4A	4.52	132.02	125.06
31	GI	1001	CYC	CMA-C3A-C4A	4.52	132.02	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	PF	203	PEB	OA-C1A-C2A	-4.52	122.58	126.17
29	PI	203	PEB	OA-C1A-C2A	-4.52	122.58	126.17
31	HF	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	MF	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	HI	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
31	MI	1001	CYC	OC-C1C-C2C	-4.52	122.58	126.17
29	F1	1002	PEB	CHB-C4B-NB	-4.52	122.56	128.83
29	FK	1002	PEB	CHB-C4B-NB	-4.52	122.56	128.83
29	RF	201	PEB	CAB-C3B-C4B	4.51	133.00	125.01
29	RI	201	PEB	CAB-C3B-C4B	4.51	133.00	125.01
31	XP	1001	CYC	CAB-C3B-C4B	4.51	128.51	121.38
29	yJ	301	PEB	CMA-C2A-C1A	-4.51	102.67	112.40
29	yL	301	PEB	CMA-C2A-C1A	-4.51	102.67	112.40
29	XB	201	PEB	CHC-C1D-ND	4.51	119.19	113.95
29	XM	201	PEB	CHC-C1D-ND	4.51	119.19	113.95
29	I4	202	PEB	C3D-C4D-ND	4.51	116.11	107.26
29	CD	202	PEB	C3D-C4D-ND	4.51	116.11	107.26
29	NO	202	PEB	CHC-C4C-C3C	-4.51	122.64	130.34
29	EB	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	iF	203	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	iI	203	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	EM	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	U1	201	PEB	OD-C4D-ND	-4.51	119.25	125.93
29	UK	201	PEB	OD-C4D-ND	-4.51	119.25	125.93
29	J4	202	PEB	CHB-C4B-NB	-4.51	122.57	128.83
29	MD	202	PEB	C3D-C4D-ND	4.51	116.11	107.26
29	mF	201	PEB	CAB-C3B-C4B	4.51	132.99	125.01
29	mI	201	PEB	CAB-C3B-C4B	4.51	132.99	125.01
31	E1	1001	CYC	OC-C1C-C2C	-4.51	122.59	126.17
29	M2	201	PEB	C3D-C4D-ND	4.51	116.10	107.26
29	J1	1002	PEB	CHB-C4B-NB	-4.51	122.57	128.83
29	JK	1002	PEB	CHB-C4B-NB	-4.51	122.57	128.83
29	cF	202	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	cI	202	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	GB	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	TF	202	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	TI	202	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	GM	201	PEB	OA-C1A-C2A	-4.51	122.59	126.17
29	DA	203	PEB	CHB-C4B-NB	-4.51	122.58	128.83
29	DN	203	PEB	CHB-C4B-NB	-4.51	122.58	128.83
29	UR	201	PEB	C3D-C4D-ND	4.51	116.10	107.26
29	N3	202	PEB	CHC-C4C-C3C	-4.50	122.66	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R2	202	PEB	C2A-C1A-NA	4.50	112.16	108.27
29	BA	203	PEB	CHB-C4B-NB	-4.50	122.58	128.83
29	BN	203	PEB	CHB-C4B-NB	-4.50	122.58	128.83
31	IF	1001	CYC	CMA-C3A-C4A	4.50	132.00	125.06
31	II	1001	CYC	CMA-C3A-C4A	4.50	132.00	125.06
29	a1	202	PEB	OD-C4D-ND	-4.50	119.26	125.93
29	aK	202	PEB	OD-C4D-ND	-4.50	119.26	125.93
29	LA	203	PEB	CHB-C4B-NB	-4.50	122.58	128.83
29	LN	203	PEB	CHB-C4B-NB	-4.50	122.58	128.83
29	FB	201	PEB	CHC-C1D-ND	4.50	119.17	113.95
29	FM	201	PEB	CHC-C1D-ND	4.50	119.17	113.95
29	H4	202	PEB	CHB-C4B-NB	-4.50	122.58	128.83
29	T2	202	PEB	C2A-C1A-NA	4.50	112.15	108.27
29	KD	202	PEB	C3D-C4D-ND	4.50	116.09	107.26
29	P1	202	PEB	OD-C4D-ND	-4.50	119.27	125.93
29	PK	202	PEB	OD-C4D-ND	-4.50	119.27	125.93
31	IP	1001	CYC	CAB-C3B-C4B	4.50	128.48	121.38
31	YP	1000	CYC	CMB-C2B-C1B	4.50	129.78	124.17
29	C4	202	PEB	C3D-C4D-ND	4.50	116.08	107.26
31	uP	1001	CYC	CAB-C3B-C4B	4.50	128.48	121.38
29	HA	203	PEB	CHB-C4B-NB	-4.50	122.59	128.83
29	HN	203	PEB	CHB-C4B-NB	-4.50	122.59	128.83
29	K4	202	PEB	C3D-C4D-ND	4.50	116.08	107.26
31	J9	1001	CYC	CBD-CAD-C3D	4.50	120.29	112.62
29	j1	203	PEB	OD-C4D-ND	-4.50	119.27	125.93
29	jK	203	PEB	OD-C4D-ND	-4.50	119.27	125.93
29	MR	201	PEB	C3D-C4D-ND	4.50	116.08	107.26
29	DD	202	PEB	CHB-C4B-NB	-4.50	122.59	128.83
29	MG	404	PEB	CHA-C1B-NB	-4.50	115.53	124.93
29	iB	201	PEB	CHC-C1D-ND	4.50	119.17	113.95
29	iM	201	PEB	CHC-C1D-ND	4.50	119.17	113.95
29	P2	201	PEB	C2A-C1A-NA	4.49	112.15	108.27
29	M4	202	PEB	C3D-C4D-ND	4.49	116.08	107.26
31	FF	1001	CYC	OC-C1C-C2C	-4.49	122.60	126.17
31	FI	1001	CYC	OC-C1C-C2C	-4.49	122.60	126.17
30	QB	201	PUB	CHB-C1C-NC	-4.49	122.59	128.83
30	QM	201	PUB	CHB-C1C-NC	-4.49	122.59	128.83
29	Q2	201	PEB	C3D-C4D-ND	4.49	116.07	107.26
29	D1	1002	PEB	CHB-C4B-NB	-4.49	122.59	128.83
29	L1	1002	PEB	CHB-C4B-NB	-4.49	122.59	128.83
29	FA	203	PEB	CHB-C4B-NB	-4.49	122.59	128.83
29	LK	1002	PEB	CHB-C4B-NB	-4.49	122.59	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FN	203	PEB	CHB-C4B-NB	-4.49	122.59	128.83
31	D1	1003	CYC	OC-C1C-C2C	-4.49	122.60	126.17
29	W2	201	PEB	C3D-C4D-ND	4.49	116.07	107.26
29	c1	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
29	cK	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
29	DK	1002	PEB	CHB-C4B-NB	-4.49	122.60	128.83
29	MB	201	PEB	OA-C1A-C2A	-4.49	122.60	126.17
29	SB	201	PEB	OA-C1A-C2A	-4.49	122.60	126.17
29	MM	201	PEB	OA-C1A-C2A	-4.49	122.60	126.17
29	SM	201	PEB	OA-C1A-C2A	-4.49	122.60	126.17
29	cB	201	PEB	CHC-C1D-ND	4.49	119.16	113.95
29	cM	201	PEB	CHC-C1D-ND	4.49	119.16	113.95
29	G4	202	PEB	C3D-C4D-ND	4.49	116.07	107.26
31	J7	1001	CYC	CBD-CAD-C3D	4.49	120.28	112.62
29	i1	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
29	iK	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
29	jB	201	PEB	OA-C1A-C2A	-4.49	122.61	126.17
29	jM	201	PEB	OA-C1A-C2A	-4.49	122.61	126.17
29	V1	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
29	VK	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
31	L7	1001	CYC	CBD-CAD-C3D	4.49	120.28	112.62
29	QR	201	PEB	C3D-C4D-ND	4.49	116.06	107.26
29	R1	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
29	RK	202	PEB	OD-C4D-ND	-4.49	119.28	125.93
31	D7	1001	CYC	CBD-CAD-C3D	4.49	120.27	112.62
31	D9	1001	CYC	CBD-CAD-C3D	4.49	120.27	112.62
31	L9	1001	CYC	CBD-CAD-C3D	4.49	120.27	112.62
29	eF	203	PEB	OA-C1A-C2A	-4.48	122.61	126.17
29	eI	203	PEB	OA-C1A-C2A	-4.48	122.61	126.17
29	g1	202	PEB	OD-C4D-ND	-4.48	119.29	125.93
29	gK	202	PEB	OD-C4D-ND	-4.48	119.29	125.93
29	O2	201	PEB	C3D-C4D-ND	4.48	116.06	107.26
29	OR	201	PEB	C3D-C4D-ND	4.48	116.06	107.26
29	NK	1002	PEB	CHB-C4B-NB	-4.48	122.61	128.83
29	LB	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
29	LM	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
29	JA	203	PEB	CHB-C4B-NB	-4.48	122.61	128.83
29	JN	203	PEB	CHB-C4B-NB	-4.48	122.61	128.83
29	fB	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
29	fM	201	PEB	OA-C1A-C2A	-4.48	122.61	126.17
29	NF	1002	PEB	C3D-C4D-ND	4.48	116.05	107.26
29	NI	1002	PEB	C3D-C4D-ND	4.48	116.05	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HB	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
29	HM	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
29	WR	201	PEB	C3D-C4D-ND	4.48	116.05	107.26
31	H7	1001	CYC	CBD-CAD-C3D	4.48	120.27	112.62
31	H9	1001	CYC	CBD-CAD-C3D	4.48	120.27	112.62
29	MQ	406	PEB	CHA-C1B-NB	-4.48	115.56	124.93
29	RB	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
29	RM	201	PEB	CHC-C1D-ND	4.48	119.15	113.95
29	YB	202	PEB	OA-C1A-C2A	-4.48	122.61	126.17
29	YM	202	PEB	OA-C1A-C2A	-4.48	122.61	126.17
29	U2	201	PEB	C3D-C4D-ND	4.48	116.05	107.26
31	C1	1001	CYC	C2B-C1B-NB	4.48	113.54	106.99
29	JF	1002	PEB	C3D-C4D-ND	4.48	116.05	107.26
29	JI	1002	PEB	C3D-C4D-ND	4.48	116.05	107.26
29	k1	202	PEB	OD-C4D-ND	-4.48	119.30	125.93
29	kK	202	PEB	OD-C4D-ND	-4.48	119.30	125.93
29	M3	202	PEB	CHC-C4C-C3C	-4.48	122.70	130.34
29	MO	202	PEB	CHC-C4C-C3C	-4.48	122.70	130.34
29	kB	201	PEB	CHC-C1D-ND	4.48	119.14	113.95
29	kM	201	PEB	CHC-C1D-ND	4.48	119.14	113.95
29	gB	201	PEB	CHC-C1D-ND	4.47	119.14	113.95
29	gM	201	PEB	CHC-C1D-ND	4.47	119.14	113.95
29	QB	203	PEB	OA-C1A-C2A	-4.47	122.62	126.17
29	QM	203	PEB	OA-C1A-C2A	-4.47	122.62	126.17
29	e1	202	PEB	OD-C4D-ND	-4.47	119.31	125.93
29	eK	202	PEB	OD-C4D-ND	-4.47	119.31	125.93
29	MD	203	PEB	C2A-C1A-NA	4.47	112.13	108.27
29	lB	201	PEB	OA-C1A-C2A	-4.47	122.62	126.17
29	lM	201	PEB	OA-C1A-C2A	-4.47	122.62	126.17
29	HD	202	PEB	CHB-C4B-NB	-4.47	122.63	128.83
30	AF	303	PUB	CHA-C1B-C2B	-4.47	122.72	130.34
30	AI	303	PUB	CHA-C1B-C2B	-4.47	122.72	130.34
31	E1	1001	CYC	C2B-C1B-NB	4.47	113.53	106.99
29	Z1	201	PEB	OD-C4D-ND	-4.46	119.31	125.93
29	ZK	201	PEB	OD-C4D-ND	-4.46	119.31	125.93
29	IB	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
29	IM	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
31	F7	1001	CYC	CBD-CAD-C3D	4.46	120.24	112.62
29	JB	201	PEB	CHC-C1D-ND	4.46	119.13	113.95
29	JM	201	PEB	CHC-C1D-ND	4.46	119.13	113.95
29	dB	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
29	VF	203	PEB	OA-C1A-C2A	-4.46	122.62	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VI	203	PEB	OA-C1A-C2A	-4.46	122.62	126.17
29	dM	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
31	EK	1001	CYC	C2B-C1B-NB	4.46	113.52	106.99
29	UB	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
29	UM	201	PEB	OA-C1A-C2A	-4.46	122.62	126.17
31	I1	1001	CYC	C2B-C1B-NB	4.46	113.52	106.99
31	CK	1001	CYC	C2B-C1B-NB	4.46	113.52	106.99
29	Z1	201	PEB	C1C-CHB-C4B	4.46	134.14	128.81
29	ZK	201	PEB	C1C-CHB-C4B	4.46	134.14	128.81
29	DB	201	PEB	CHC-C1D-ND	4.46	119.12	113.95
29	DM	201	PEB	CHC-C1D-ND	4.46	119.12	113.95
29	VB	201	PEB	CHC-C1D-ND	4.46	119.12	113.95
29	VM	201	PEB	CHC-C1D-ND	4.46	119.12	113.95
31	N7	1001	CYC	CBD-CAD-C3D	4.46	120.23	112.62
31	N9	1001	CYC	CBD-CAD-C3D	4.46	120.23	112.62
29	hB	201	PEB	OA-C1A-C2A	-4.45	122.63	126.17
29	hM	201	PEB	OA-C1A-C2A	-4.45	122.63	126.17
29	GD	203	PEB	C2A-C1A-NA	4.45	112.11	108.27
31	IK	1001	CYC	C2B-C1B-NB	4.45	113.51	106.99
31	F9	1001	CYC	CBD-CAD-C3D	4.45	120.22	112.62
29	gF	203	PEB	OA-C1A-C2A	-4.45	122.63	126.17
29	gI	203	PEB	OA-C1A-C2A	-4.45	122.63	126.17
29	mB	201	PEB	CHC-C1D-ND	4.45	119.11	113.95
29	mM	201	PEB	CHC-C1D-ND	4.45	119.11	113.95
31	K1	1001	CYC	C2B-C1B-NB	4.45	113.50	106.99
31	KK	1001	CYC	C2B-C1B-NB	4.45	113.50	106.99
29	G4	203	PEB	C2A-C1A-NA	4.45	112.11	108.27
29	ED	202	PEB	C2A-C1A-NA	4.45	112.11	108.27
29	LF	1002	PEB	C3D-C4D-ND	4.45	115.99	107.26
29	LI	1002	PEB	C3D-C4D-ND	4.45	115.99	107.26
29	HF	1002	PEB	C3D-C4D-ND	4.45	115.99	107.26
29	HI	1002	PEB	C3D-C4D-ND	4.45	115.99	107.26
29	WB	201	PEB	OA-C1A-C2A	-4.45	122.64	126.17
29	WM	201	PEB	OA-C1A-C2A	-4.45	122.64	126.17
29	c1	202	PEB	C1C-CHB-C4B	4.45	134.12	128.81
29	cK	202	PEB	C1C-CHB-C4B	4.45	134.12	128.81
29	KB	201	PEB	OA-C1A-C2A	-4.45	122.64	126.17
29	KM	201	PEB	OA-C1A-C2A	-4.45	122.64	126.17
29	FF	1002	PEB	C3D-C4D-ND	4.45	115.98	107.26
29	FI	1002	PEB	C3D-C4D-ND	4.45	115.98	107.26
29	DF	1002	PEB	C3D-C4D-ND	4.44	115.98	107.26
29	DI	1002	PEB	C3D-C4D-ND	4.44	115.98	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	KP	1001	CYC	CMB-C2B-C1B	4.44	129.72	124.17
29	mF	203	PEB	OA-C1A-C2A	-4.44	122.64	126.17
29	mI	203	PEB	OA-C1A-C2A	-4.44	122.64	126.17
29	NO	202	PEB	CHC-C1D-ND	-4.44	108.79	113.95
31	D1	1003	CYC	C2B-C1B-NB	4.44	113.49	106.99
31	GK	1001	CYC	C2B-C1B-NB	4.44	113.49	106.99
29	ZB	201	PEB	CHC-C1D-ND	4.44	119.10	113.95
29	ZM	201	PEB	CHC-C1D-ND	4.44	119.10	113.95
30	wL	305	PUB	CMA-C2A-C1A	4.44	131.83	121.39
29	GB	202	PEB	C1C-CHB-C4B	-4.44	123.51	128.81
29	GM	202	PEB	C1C-CHB-C4B	-4.44	123.51	128.81
29	OB	201	PEB	OA-C1A-C2A	-4.44	122.64	126.17
29	OM	201	PEB	OA-C1A-C2A	-4.44	122.64	126.17
29	M3	202	PEB	CHC-C1D-ND	-4.44	108.80	113.95
29	MO	202	PEB	CHC-C1D-ND	-4.44	108.80	113.95
29	QB	204	PEB	C1C-CHB-C4B	-4.44	123.51	128.81
29	QM	204	PEB	C1C-CHB-C4B	-4.44	123.51	128.81
29	TB	201	PEB	CHC-C1D-ND	4.44	119.10	113.95
29	TM	201	PEB	CHC-C1D-ND	4.44	119.10	113.95
31	CF	1001	CYC	C2B-C1B-NB	4.43	113.48	106.99
31	CI	1001	CYC	C2B-C1B-NB	4.43	113.48	106.99
29	N1	1002	PEB	CHB-C4B-NB	-4.43	122.68	128.83
29	V1	203	PEB	CHB-C4B-NB	-4.43	122.68	128.83
29	VK	203	PEB	CHB-C4B-NB	-4.43	122.68	128.83
31	M1	1001	CYC	C2B-C1B-NB	4.43	113.48	106.99
31	MK	1001	CYC	C2B-C1B-NB	4.43	113.48	106.99
29	PR	201	PEB	C2A-C1A-NA	4.43	112.09	108.27
29	kF	203	PEB	OA-C1A-C2A	-4.43	122.65	126.17
29	kI	203	PEB	OA-C1A-C2A	-4.43	122.65	126.17
29	lB	202	PEB	C1C-CHB-C4B	-4.43	123.52	128.81
29	lM	202	PEB	C1C-CHB-C4B	-4.43	123.52	128.81
29	MB	202	PEB	C1C-CHB-C4B	-4.43	123.52	128.81
29	MM	202	PEB	C1C-CHB-C4B	-4.43	123.52	128.81
29	eB	201	PEB	CHC-C1D-ND	4.43	119.09	113.95
29	eM	201	PEB	CHC-C1D-ND	4.43	119.09	113.95
29	N3	202	PEB	CHC-C1D-ND	-4.43	108.81	113.95
29	CB	201	PEB	OA-C1A-C2A	-4.43	122.65	126.17
29	CM	201	PEB	OA-C1A-C2A	-4.43	122.65	126.17
29	GD	202	PEB	OD-C4D-C3D	-4.43	119.43	129.46
31	VP	1001	CYC	C4D-CHA-C1A	4.43	134.10	128.81
29	aF	203	PEB	OA-C1A-C2A	-4.43	122.65	126.17
29	aI	203	PEB	OA-C1A-C2A	-4.43	122.65	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	cP	1001	CYC	CMB-C2B-C1B	4.43	129.69	124.17
29	dB	202	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
29	dM	202	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
29	YB	203	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
29	YM	203	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
31	EP	1001	CYC	CMB-C2B-C1B	4.42	129.69	124.17
29	U1	201	PEB	C1C-CHB-C4B	4.42	134.09	128.81
29	jB	202	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
29	UK	201	PEB	C1C-CHB-C4B	4.42	134.09	128.81
29	jM	202	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
31	AP	1001	CYC	CMB-C2B-C1B	4.42	129.69	124.17
29	g1	202	PEB	C1C-CHB-C4B	4.42	134.09	128.81
29	gK	202	PEB	C1C-CHB-C4B	4.42	134.09	128.81
29	QB	203	PEB	C3D-C4D-ND	4.42	115.93	107.26
29	QM	203	PEB	C3D-C4D-ND	4.42	115.93	107.26
31	IF	1001	CYC	C2B-C1B-NB	4.42	113.45	106.99
31	II	1001	CYC	C2B-C1B-NB	4.42	113.45	106.99
29	WB	202	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
29	WM	202	PEB	C1C-CHB-C4B	-4.42	123.53	128.81
31	KF	1001	CYC	C2B-C1B-NB	4.42	113.45	106.99
29	L5	202	PEB	CHC-C4C-C3C	-4.42	122.81	130.34
31	CP	1001	CYC	CMB-C2B-C1B	4.41	129.68	124.17
31	iP	1001	CYC	CMB-C2B-C1B	4.41	129.68	124.17
29	G8	203	PEB	OA-C1A-C2A	-4.41	122.66	126.17
29	aB	201	PEB	C3D-C4D-ND	4.41	115.92	107.26
29	aM	201	PEB	C3D-C4D-ND	4.41	115.92	107.26
29	KB	202	PEB	C1C-CHB-C4B	-4.41	123.54	128.81
29	fB	202	PEB	C1C-CHB-C4B	-4.41	123.54	128.81
29	KM	202	PEB	C1C-CHB-C4B	-4.41	123.54	128.81
29	fM	202	PEB	C1C-CHB-C4B	-4.41	123.54	128.81
31	KI	1001	CYC	C2B-C1B-NB	4.41	113.45	106.99
29	fB	201	PEB	C3D-C4D-ND	4.41	115.92	107.26
29	fM	201	PEB	C3D-C4D-ND	4.41	115.92	107.26
31	RP	1001	CYC	CMB-C2B-C1B	4.41	129.68	124.17
31	MF	1001	CYC	C2B-C1B-NB	4.41	113.45	106.99
31	MI	1001	CYC	C2B-C1B-NB	4.41	113.45	106.99
30	A1	304	PUB	CHC-C1D-ND	-4.41	108.14	113.72
30	AK	304	PUB	CHC-C1D-ND	-4.41	108.14	113.72
29	a1	202	PEB	C1C-CHB-C4B	4.41	134.08	128.81
29	aK	202	PEB	C1C-CHB-C4B	4.41	134.08	128.81
31	F7	1001	CYC	CHB-C4A-C3A	4.41	136.24	124.90
29	ID	202	PEB	OD-C4D-C3D	-4.41	119.47	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	wJ	305	PUB	CMA-C2A-C1A	4.41	131.76	121.39
29	OB	202	PEB	C1C-CHB-C4B	-4.41	123.54	128.81
29	OM	202	PEB	C1C-CHB-C4B	-4.41	123.54	128.81
29	CB	201	PEB	C3D-C4D-ND	4.41	115.91	107.26
29	CM	201	PEB	C3D-C4D-ND	4.41	115.91	107.26
30	MQ	405	PUB	C1C-C2C-C3C	-4.41	101.91	106.78
29	G4	202	PEB	OD-C4D-C3D	-4.41	119.48	129.46
29	OB	201	PEB	C3D-C4D-ND	4.41	115.90	107.26
29	OM	201	PEB	C3D-C4D-ND	4.41	115.90	107.26
29	K4	203	PEB	C2A-C1A-NA	4.41	112.07	108.27
30	MG	403	PUB	C1C-C2C-C3C	-4.41	101.91	106.78
29	mF	202	PEB	CHB-C4B-NB	-4.41	122.72	128.83
29	mI	202	PEB	CHB-C4B-NB	-4.41	122.72	128.83
29	EB	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
29	EM	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
31	xP	1001	CYC	C4D-CHA-C1A	4.40	134.07	128.81
30	xL	305	PUB	CMA-C2A-C1A	4.40	131.75	121.39
29	UB	201	PEB	C3D-C4D-ND	4.40	115.90	107.26
29	UM	201	PEB	C3D-C4D-ND	4.40	115.90	107.26
29	hB	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
29	hM	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
29	C4	203	PEB	C2A-C1A-NA	4.40	112.07	108.27
29	RR	201	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
31	GP	1001	CYC	CHB-C4A-C3A	4.40	136.22	124.90
31	E7	1001	CYC	C1B-C2B-C3B	-4.40	103.28	107.87
31	E9	1001	CYC	C1B-C2B-C3B	-4.40	103.28	107.87
29	hB	201	PEB	C3D-C4D-ND	4.40	115.90	107.26
29	hM	201	PEB	C3D-C4D-ND	4.40	115.90	107.26
29	T2	201	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
29	TR	201	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
29	i1	202	PEB	C1C-CHB-C4B	4.40	134.07	128.81
29	iK	202	PEB	C1C-CHB-C4B	4.40	134.07	128.81
29	IB	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
29	IM	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
29	F5	202	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
29	F8	202	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
29	G5	203	PEB	OA-C1A-C2A	-4.40	122.67	126.17
31	GP	1001	CYC	CMB-C2B-C1B	4.40	129.66	124.17
31	PP	1001	CYC	CMB-C2B-C1B	4.40	129.66	124.17
31	pP	1001	CYC	CMB-C2B-C1B	4.40	129.66	124.17
29	e2	402	PEB	CHC-C4C-C3C	-4.40	122.83	130.34
29	N2	201	PEB	CHC-C4C-C3C	-4.40	122.83	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KB	201	PEB	C3D-C4D-ND	4.40	115.89	107.26
29	KM	201	PEB	C3D-C4D-ND	4.40	115.89	107.26
29	CB	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
29	CM	202	PEB	C1C-CHB-C4B	-4.40	123.55	128.81
31	JP	1001	CYC	CMB-C2B-C1B	4.40	129.66	124.17
29	KD	203	PEB	C2A-C1A-NA	4.40	112.06	108.27
29	E4	202	PEB	OD-C4D-C3D	-4.40	119.49	129.46
29	XR	201	PEB	CHC-C4C-C3C	-4.40	122.84	130.34
29	jB	201	PEB	C3D-C4D-ND	4.40	115.89	107.26
29	jM	201	PEB	C3D-C4D-ND	4.40	115.89	107.26
29	G8	202	PEB	CHC-C4C-C3C	-4.40	122.84	130.34
29	H8	202	PEB	CHC-C4C-C3C	-4.40	122.84	130.34
29	P1	203	PEB	CHB-C4B-NB	-4.40	122.73	128.83
29	PK	203	PEB	CHB-C4B-NB	-4.40	122.73	128.83
29	MB	201	PEB	C3D-C4D-ND	4.40	115.89	107.26
29	MM	201	PEB	C3D-C4D-ND	4.40	115.89	107.26
29	V1	202	PEB	C1C-CHB-C4B	4.40	134.06	128.81
29	VK	202	PEB	C1C-CHB-C4B	4.40	134.06	128.81
29	I4	202	PEB	OD-C4D-C3D	-4.40	119.50	129.46
29	EB	201	PEB	C3D-C4D-ND	4.40	115.88	107.26
29	dB	201	PEB	C3D-C4D-ND	4.40	115.88	107.26
29	EM	201	PEB	C3D-C4D-ND	4.40	115.88	107.26
29	dM	201	PEB	C3D-C4D-ND	4.40	115.88	107.26
29	P1	202	PEB	C1C-CHB-C4B	4.40	134.06	128.81
29	PK	202	PEB	C1C-CHB-C4B	4.40	134.06	128.81
29	H5	203	PEB	OA-C1A-C2A	-4.40	122.68	126.17
31	rP	1001	CYC	CMB-C2B-C1B	4.39	129.66	124.17
31	L9	1001	CYC	CHB-C4A-C3A	4.39	136.20	124.90
31	F9	1001	CYC	CHB-C4A-C3A	4.39	136.20	124.90
29	I4	201	PEB	C3B-C4B-NB	4.39	116.44	110.05
29	ED	201	PEB	OD-C4D-C3D	-4.39	119.50	129.46
31	GF	1001	CYC	C2B-C1B-NB	4.39	113.42	106.99
31	GI	1001	CYC	C2B-C1B-NB	4.39	113.42	106.99
29	YB	202	PEB	C3D-C4D-ND	4.39	115.88	107.26
29	YM	202	PEB	C3D-C4D-ND	4.39	115.88	107.26
31	IP	1001	CYC	CMB-C2B-C1B	4.39	129.65	124.17
29	k1	203	PEB	CHB-C4B-NB	-4.39	122.73	128.83
29	eF	202	PEB	CHB-C4B-NB	-4.39	122.73	128.83
29	eI	202	PEB	CHB-C4B-NB	-4.39	122.73	128.83
29	kK	203	PEB	CHB-C4B-NB	-4.39	122.73	128.83
29	SB	202	PEB	C1C-CHB-C4B	-4.39	123.56	128.81
29	SM	202	PEB	C1C-CHB-C4B	-4.39	123.56	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N7	1001	CYC	CHB-C4A-C3A	4.39	136.19	124.90
31	N9	1001	CYC	CHB-C4A-C3A	4.39	136.19	124.90
29	H5	202	PEB	CHC-C4C-C3C	-4.39	122.85	130.34
29	F5	203	PEB	OA-C1A-C2A	-4.39	122.68	126.17
29	F8	203	PEB	OA-C1A-C2A	-4.39	122.68	126.17
29	SB	201	PEB	C3D-C4D-ND	4.39	115.87	107.26
29	SM	201	PEB	C3D-C4D-ND	4.39	115.87	107.26
30	AB	304	PUB	CMA-C2A-C1A	4.39	131.72	121.39
31	D7	1001	CYC	CHB-C4A-C3A	4.39	136.19	124.90
31	D9	1001	CYC	CHB-C4A-C3A	4.39	136.19	124.90
29	R1	202	PEB	C1C-CHB-C4B	4.39	134.05	128.81
29	RK	202	PEB	C1C-CHB-C4B	4.39	134.05	128.81
29	L8	202	PEB	CHC-C4C-C3C	-4.39	122.85	130.34
31	EF	1001	CYC	C2B-C1B-NB	4.39	113.41	106.99
31	EI	1001	CYC	C2B-C1B-NB	4.39	113.41	106.99
30	AF	303	PUB	CMA-C2A-C1A	4.39	131.71	121.39
30	AI	303	PUB	CMA-C2A-C1A	4.39	131.71	121.39
29	e1	202	PEB	C1C-CHB-C4B	4.39	134.05	128.81
29	k1	202	PEB	C1C-CHB-C4B	4.39	134.05	128.81
29	eK	202	PEB	C1C-CHB-C4B	4.39	134.05	128.81
29	kK	202	PEB	C1C-CHB-C4B	4.39	134.05	128.81
29	OF	203	PEB	CHB-C4B-NB	-4.39	122.74	128.83
29	OI	203	PEB	CHB-C4B-NB	-4.39	122.74	128.83
31	J7	1001	CYC	CHB-C4A-C3A	4.39	136.19	124.90
29	K4	202	PEB	OD-C4D-C3D	-4.39	119.52	129.46
31	mP	1001	CYC	CHB-C4A-C3A	4.39	136.19	124.90
31	L7	1001	CYC	CHB-C4A-C3A	4.39	136.18	124.90
31	J9	1001	CYC	CHB-C4A-C3A	4.39	136.18	124.90
29	NR	201	PEB	CHC-C4C-C3C	-4.39	122.85	130.34
29	aB	202	PEB	C1C-CHB-C4B	-4.39	123.57	128.81
29	aM	202	PEB	C1C-CHB-C4B	-4.39	123.57	128.81
29	VR	201	PEB	CHC-C4C-C3C	-4.39	122.86	130.34
31	mP	1001	CYC	CMB-C2B-C1B	4.39	129.64	124.17
31	C7	1001	CYC	C1B-C2B-C3B	-4.39	103.29	107.87
31	C9	1001	CYC	C1B-C2B-C3B	-4.39	103.29	107.87
29	B5	202	PEB	CHC-C4C-C3C	-4.38	122.86	130.34
29	IA	201	PEB	C3B-C4B-NB	4.38	116.43	110.05
29	IN	201	PEB	C3B-C4B-NB	4.38	116.43	110.05
29	KA	202	PEB	CAB-C3B-C4B	4.38	132.76	125.01
29	KN	202	PEB	CAB-C3B-C4B	4.38	132.76	125.01
29	CD	202	PEB	OD-C4D-C3D	-4.38	119.53	129.46
29	UB	202	PEB	C1C-CHB-C4B	-4.38	123.57	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MQ	401	PEB	C1C-CHB-C4B	-4.38	123.57	128.81
29	R2	201	PEB	CHC-C4C-C3C	-4.38	122.86	130.34
29	WB	201	PEB	C3D-C4D-ND	4.38	115.86	107.26
29	WM	201	PEB	C3D-C4D-ND	4.38	115.86	107.26
29	B5	203	PEB	OA-C1A-C2A	-4.38	122.69	126.17
29	AF	304	PEB	CHA-C1B-NB	-4.38	115.77	124.93
29	AI	304	PEB	CHA-C1B-NB	-4.38	115.77	124.93
29	B8	202	PEB	CHC-C4C-C3C	-4.38	122.86	130.34
31	tP	1001	CYC	CMB-C2B-C1B	4.38	129.64	124.17
31	vP	1001	CYC	CMB-C2B-C1B	4.38	129.64	124.17
29	IB	201	PEB	C3D-C4D-ND	4.38	115.86	107.26
29	IM	201	PEB	C3D-C4D-ND	4.38	115.86	107.26
30	AM	304	PUB	CMA-C2A-C1A	4.38	131.69	121.39
29	N7	1002	PEB	CMD-C2D-C3D	4.38	136.24	130.06
29	N9	1002	PEB	CMD-C2D-C3D	4.38	136.24	130.06
29	MD	202	PEB	OD-C4D-C3D	-4.38	119.54	129.46
31	AP	1001	CYC	CHB-C4A-C3A	4.38	136.16	124.90
29	G5	202	PEB	CHC-C4C-C3C	-4.38	122.87	130.34
31	G9	1001	CYC	C1B-C2B-C3B	-4.38	103.30	107.87
29	YF	202	PEB	CHB-C4B-NB	-4.38	122.75	128.83
29	YI	202	PEB	CHB-C4B-NB	-4.38	122.75	128.83
31	gP	1001	CYC	CMB-C2B-C1B	4.38	129.63	124.17
31	H7	1001	CYC	CHB-C4A-C3A	4.38	136.16	124.90
31	H9	1001	CYC	CHB-C4A-C3A	4.38	136.16	124.90
29	C4	201	PEB	C3B-C4B-NB	4.38	116.42	110.05
29	lB	201	PEB	C3D-C4D-ND	4.38	115.84	107.26
29	lM	201	PEB	C3D-C4D-ND	4.38	115.84	107.26
31	lP	1001	CYC	CHB-C4A-C3A	4.38	136.15	124.90
29	aB	201	PEB	OA-C1A-C2A	-4.38	122.69	126.17
29	aM	201	PEB	OA-C1A-C2A	-4.38	122.69	126.17
31	G7	1001	CYC	C1B-C2B-C3B	-4.38	103.31	107.87
31	eP	1001	CYC	CHB-C4A-C3A	4.38	136.15	124.90
29	AB	301	PEB	CHA-C1B-NB	-4.37	115.78	124.93
29	V2	201	PEB	CHC-C4C-C3C	-4.37	122.88	130.34
29	g1	203	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	m1	202	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	gK	203	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	mK	202	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	j1	203	PEB	C1C-CHB-C4B	4.37	134.03	128.81
29	jK	203	PEB	C1C-CHB-C4B	4.37	134.03	128.81
29	GB	201	PEB	C3D-C4D-ND	4.37	115.84	107.26
29	GM	201	PEB	C3D-C4D-ND	4.37	115.84	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CA	201	PEB	C3B-C4B-NB	4.37	116.41	110.05
29	CN	201	PEB	C3B-C4B-NB	4.37	116.41	110.05
31	HK	1001	CYC	CHB-C4A-NA	-4.37	115.78	124.93
31	tP	1001	CYC	CHB-C4A-C3A	4.37	136.14	124.90
31	I7	1001	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
31	I9	1001	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
29	AA	201	PEB	C3B-C4B-NB	4.37	116.41	110.05
29	AN	201	PEB	C3B-C4B-NB	4.37	116.41	110.05
30	xJ	305	PUB	CMA-C2A-C1A	4.37	131.67	121.39
31	cP	1001	CYC	CHB-C4A-C3A	4.37	136.14	124.90
29	gF	202	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	kF	202	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	gI	202	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	kI	202	PEB	CHB-C4B-NB	-4.37	122.76	128.83
29	AM	301	PEB	CHA-C1B-NB	-4.37	115.79	124.93
29	c1	203	PEB	CHB-C4B-NB	-4.37	122.77	128.83
29	VF	202	PEB	CHB-C4B-NB	-4.37	122.77	128.83
29	VI	202	PEB	CHB-C4B-NB	-4.37	122.77	128.83
29	cK	203	PEB	CHB-C4B-NB	-4.37	122.77	128.83
31	KP	1001	CYC	CHB-C4A-C3A	4.37	136.14	124.90
31	eP	1001	CYC	CMB-C2B-C1B	4.37	129.62	124.17
29	a1	203	PEB	CHB-C4B-NB	-4.37	122.77	128.83
29	aK	203	PEB	CHB-C4B-NB	-4.37	122.77	128.83
29	C4	202	PEB	OD-C4D-C3D	-4.37	119.56	129.46
29	M4	202	PEB	OD-C4D-C3D	-4.37	119.56	129.46
31	TP	1001	CYC	CHB-C4A-C3A	4.37	136.13	124.90
30	yJ	302	PUB	C1D-CHC-C4C	-4.37	103.87	113.37
30	yL	302	PUB	C1D-CHC-C4C	-4.37	103.87	113.37
29	KA	201	PEB	C3B-C4B-NB	4.37	116.40	110.05
29	KN	201	PEB	C3B-C4B-NB	4.37	116.40	110.05
31	EP	1001	CYC	CHB-C4A-C3A	4.37	136.13	124.90
30	MN	403	PUB	OD-C4D-ND	-4.37	119.46	125.93
31	JP	1001	CYC	CHB-C4A-C3A	4.37	136.13	124.90
29	KD	202	PEB	OD-C4D-C3D	-4.37	119.57	129.46
29	J5	201	PEB	CMB-C2B-C3B	-4.37	114.27	126.12
29	J8	201	PEB	CMB-C2B-C3B	-4.37	114.27	126.12
31	K9	1001	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
29	dD	401	PEB	C3B-C4B-NB	4.37	116.40	110.05
29	i1	203	PEB	CHB-C4B-NB	-4.37	122.77	128.83
29	iK	203	PEB	CHB-C4B-NB	-4.37	122.77	128.83
31	vP	1001	CYC	CHB-C4A-C3A	4.37	136.12	124.90
31	DK	1001	CYC	CHB-C4A-NA	-4.36	115.80	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	E4	201	PEB	C3B-C4B-NB	4.36	116.40	110.05
29	aF	202	PEB	CHB-C4B-NB	-4.36	122.77	128.83
29	aI	202	PEB	CHB-C4B-NB	-4.36	122.77	128.83
31	pP	1001	CYC	CHB-C4A-C3A	4.36	136.12	124.90
29	EC	202	PEB	CHC-C4C-C3C	-4.36	122.89	130.34
29	EE	202	PEB	CHC-C4C-C3C	-4.36	122.89	130.34
29	J9	1002	PEB	CMD-C2D-C3D	4.36	136.22	130.06
30	MA	403	PUB	OD-C4D-ND	-4.36	119.47	125.93
31	rP	1001	CYC	CHB-C4A-C3A	4.36	136.12	124.90
29	RR	202	PEB	C1C-CHB-C4B	4.36	134.02	128.81
31	NP	1001	CYC	CMB-C2B-C1B	4.36	129.61	124.17
31	CP	1001	CYC	CHB-C4A-C3A	4.36	136.12	124.90
29	IC	202	PEB	CHC-C4C-C3C	-4.36	122.90	130.34
29	IE	202	PEB	CHC-C4C-C3C	-4.36	122.90	130.34
31	K7	1001	CYC	C1B-C2B-C3B	-4.36	103.32	107.87
31	L1	1001	CYC	CHB-C4A-NA	-4.36	115.81	124.93
31	LK	1001	CYC	CHB-C4A-NA	-4.36	115.81	124.93
31	gP	1001	CYC	CHB-C4A-C3A	4.36	136.11	124.90
29	Y1	202	PEB	CHB-C4B-NB	-4.36	122.78	128.83
29	YK	202	PEB	CHB-C4B-NB	-4.36	122.78	128.83
29	L7	1002	PEB	CMD-C2D-C3D	4.36	136.21	130.06
29	GA	202	PEB	CAB-C3B-C4B	4.36	132.72	125.01
29	GN	202	PEB	CAB-C3B-C4B	4.36	132.72	125.01
31	NP	1001	CYC	CHB-C4A-C3A	4.36	136.11	124.90
31	PP	1001	CYC	CHB-C4A-C3A	4.36	136.11	124.90
29	e1	203	PEB	CHB-C4B-NB	-4.36	122.78	128.83
29	eK	203	PEB	CHB-C4B-NB	-4.36	122.78	128.83
29	GA	201	PEB	C3B-C4B-NB	4.36	116.39	110.05
29	GN	201	PEB	C3B-C4B-NB	4.36	116.39	110.05
29	XR	202	PEB	C1C-CHB-C4B	4.36	134.01	128.81
29	J7	1002	PEB	CMD-C2D-C3D	4.36	136.21	130.06
29	H7	1002	PEB	CMD-C2D-C3D	4.35	136.20	130.06
29	H9	1002	PEB	CMD-C2D-C3D	4.35	136.20	130.06
29	SR	201	PEB	OA-C1A-C2A	-4.35	122.71	126.17
31	iP	1001	CYC	CHB-C4A-C3A	4.35	136.09	124.90
31	H1	1001	CYC	CHB-C4A-NA	-4.35	115.83	124.93
31	F1	1001	CYC	CHB-C4A-NA	-4.35	115.83	124.93
31	FK	1001	CYC	CHB-C4A-NA	-4.35	115.83	124.93
29	IA	202	PEB	CAB-C3B-C4B	4.35	132.71	125.01
29	IN	202	PEB	CAB-C3B-C4B	4.35	132.71	125.01
29	EA	201	PEB	C3B-C4B-NB	4.35	116.38	110.05
29	EN	201	PEB	C3B-C4B-NB	4.35	116.38	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AG	202	PEB	CHB-C4B-NB	-4.35	122.79	128.83
29	AQ	202	PEB	CHB-C4B-NB	-4.35	122.79	128.83
29	X2	201	PEB	C1C-CHB-C4B	4.35	134.00	128.81
31	TP	1001	CYC	CMB-C2B-C1B	4.35	129.60	124.17
29	CG	202	PEB	CHB-C4B-NB	-4.35	122.79	128.83
29	CQ	202	PEB	CHB-C4B-NB	-4.35	122.79	128.83
31	D1	1001	CYC	CHB-C4A-NA	-4.35	115.84	124.93
29	R1	203	PEB	CHB-C4B-NB	-4.35	122.80	128.83
29	PF	202	PEB	CHB-C4B-NB	-4.35	122.80	128.83
29	PI	202	PEB	CHB-C4B-NB	-4.35	122.80	128.83
29	RK	203	PEB	CHB-C4B-NB	-4.35	122.80	128.83
29	CC	202	PEB	CHC-C4C-C3C	-4.35	122.92	130.34
29	CE	202	PEB	CHC-C4C-C3C	-4.35	122.92	130.34
31	M7	1001	CYC	C1B-C2B-C3B	-4.35	103.33	107.87
29	B8	203	PEB	OA-C1A-C2A	-4.35	122.72	126.17
30	AB	305	PUB	CMA-C2A-C1A	4.35	131.61	121.39
29	G4	201	PEB	C3B-C4B-NB	4.34	116.37	110.05
31	M9	1001	CYC	C1B-C2B-C3B	-4.34	103.34	107.87
31	NK	1001	CYC	CHB-C4A-NA	-4.34	115.85	124.93
29	T1	202	PEB	CHB-C4B-NB	-4.34	122.80	128.83
29	IG	202	PEB	CHB-C4B-NB	-4.34	122.80	128.83
29	TK	202	PEB	CHB-C4B-NB	-4.34	122.80	128.83
29	IQ	202	PEB	CHB-C4B-NB	-4.34	122.80	128.83
29	F7	1002	PEB	CMD-C2D-C3D	4.34	136.19	130.06
29	F9	1002	PEB	CMD-C2D-C3D	4.34	136.19	130.06
29	L8	203	PEB	OA-C1A-C2A	-4.34	122.72	126.17
31	J1	1001	CYC	CHB-C4A-NA	-4.34	115.85	124.93
31	JK	1001	CYC	CHB-C4A-NA	-4.34	115.85	124.93
29	AA	202	PEB	CAB-C3B-C4B	4.34	132.69	125.01
29	AN	202	PEB	CAB-C3B-C4B	4.34	132.69	125.01
31	RP	1001	CYC	CHB-C4A-C3A	4.34	136.06	124.90
29	L9	1002	PEB	CMD-C2D-C3D	4.34	136.18	130.06
29	P2	201	PEB	C1C-CHB-C4B	4.34	133.99	128.81
29	GD	201	PEB	C3B-C4B-NB	4.34	116.36	110.05
29	MD	201	PEB	C3B-C4B-NB	4.34	116.36	110.05
29	dF	201	PEB	CHB-C4B-NB	-4.34	122.81	128.83
29	dI	201	PEB	CHB-C4B-NB	-4.34	122.81	128.83
29	Y7	203	PEB	C4B-C3B-C2B	-4.34	101.98	106.78
29	Y9	203	PEB	C4B-C3B-C2B	-4.34	101.98	106.78
29	M4	201	PEB	C3B-C4B-NB	4.34	116.36	110.05
30	AM	305	PUB	CMA-C2A-C1A	4.34	131.59	121.39
29	KC	203	PEB	CHC-C4C-C3C	-4.34	122.94	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KE	203	PEB	CHC-C4C-C3C	-4.34	122.94	130.34
29	H8	203	PEB	OA-C1A-C2A	-4.34	122.73	126.17
29	EA	202	PEB	CAB-C3B-C4B	4.33	132.68	125.01
29	EN	202	PEB	CAB-C3B-C4B	4.33	132.68	125.01
29	R2	202	PEB	C1C-CHB-C4B	4.33	133.99	128.81
29	NR	202	PEB	C1C-CHB-C4B	4.33	133.99	128.81
29	m7	203	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	m9	203	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	K4	201	PEB	C3B-C4B-NB	4.33	116.35	110.05
29	GC	202	PEB	CHC-C4C-C3C	-4.33	122.95	130.34
29	GE	202	PEB	CHC-C4C-C3C	-4.33	122.95	130.34
29	L5	203	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	KG	202	PEB	CHB-C4B-NB	-4.33	122.82	128.83
29	KQ	202	PEB	CHB-C4B-NB	-4.33	122.82	128.83
29	K4	202	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	KD	202	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	G4	202	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	UF	201	PEB	CHB-C4B-NB	-4.33	122.82	128.83
29	UI	201	PEB	CHB-C4B-NB	-4.33	122.82	128.83
29	D7	1002	PEB	CMD-C2D-C3D	4.33	136.17	130.06
29	D9	1002	PEB	CMD-C2D-C3D	4.33	136.17	130.06
29	k1	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	TF	201	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	kK	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	i7	203	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	i9	203	PEB	C4B-C3B-C2B	-4.33	101.99	106.78
29	CD	203	PEB	C2A-C1A-NA	4.33	112.00	108.27
29	ID	201	PEB	C3B-C4B-NB	4.33	116.34	110.05
30	MA	402	PUB	CHC-C1D-ND	-4.33	108.25	113.72
29	VR	202	PEB	C1C-CHB-C4B	4.33	133.98	128.81
29	iF	202	PEB	CHB-C4B-NB	-4.33	122.83	128.83
29	iI	202	PEB	CHB-C4B-NB	-4.33	122.83	128.83
29	P7	202	PEB	CHB-C4B-NB	-4.33	122.83	128.83
29	P9	202	PEB	CHB-C4B-NB	-4.33	122.83	128.83
29	V1	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	g1	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	VK	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	gK	202	PEB	OA-C1A-C2A	-4.33	122.73	126.17
29	EG	202	PEB	CHB-C4B-NB	-4.32	122.83	128.83
29	EQ	202	PEB	CHB-C4B-NB	-4.32	122.83	128.83
29	T7	203	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
29	T9	203	PEB	C4B-C3B-C2B	-4.32	102.00	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GG	202	PEB	CHB-C4B-NB	-4.32	122.83	128.83
29	GQ	202	PEB	CHB-C4B-NB	-4.32	122.83	128.83
29	M4	202	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
29	CD	201	PEB	C3B-C4B-NB	4.32	116.33	110.05
29	GD	202	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
31	N1	1001	CYC	CHB-C4A-NA	-4.32	115.90	124.93
29	A1	302	PEB	CHC-C1D-ND	-4.32	108.93	113.95
29	AK	302	PEB	CHC-C1D-ND	-4.32	108.93	113.95
29	PR	201	PEB	C1C-CHB-C4B	4.32	133.97	128.81
29	e1	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
29	j1	203	PEB	OA-C1A-C2A	-4.32	122.74	126.17
29	eK	202	PEB	OA-C1A-C2A	-4.32	122.74	126.17
29	jK	203	PEB	OA-C1A-C2A	-4.32	122.74	126.17
29	V7	203	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
29	V9	203	PEB	C4B-C3B-C2B	-4.32	102.00	106.78
29	KD	201	PEB	C3B-C4B-NB	4.31	116.32	110.05
29	AC	202	PEB	CHC-C4C-C3C	-4.31	122.98	130.34
29	AE	202	PEB	CHC-C4C-C3C	-4.31	122.98	130.34
29	N2	202	PEB	C1C-CHB-C4B	4.31	133.96	128.81
30	xL	305	PUB	OA-C1A-NA	-4.31	119.54	125.93
29	T7	202	PEB	CHB-C4B-NB	-4.31	122.85	128.83
29	T9	202	PEB	CHB-C4B-NB	-4.31	122.85	128.83
30	wL	305	PUB	OA-C1A-NA	-4.31	119.55	125.93
29	MG	404	PEB	CHC-C1D-ND	-4.31	108.94	113.95
30	MN	402	PUB	CHC-C1D-ND	-4.31	108.27	113.72
29	g7	203	PEB	C4B-C3B-C2B	-4.31	102.01	106.78
29	g9	203	PEB	C4B-C3B-C2B	-4.31	102.01	106.78
29	CA	202	PEB	CAB-C3B-C4B	4.31	132.63	125.01
29	CN	202	PEB	CAB-C3B-C4B	4.31	132.63	125.01
29	MD	202	PEB	C4B-C3B-C2B	-4.31	102.02	106.78
29	c7	203	PEB	C4B-C3B-C2B	-4.30	102.02	106.78
29	c9	203	PEB	C4B-C3B-C2B	-4.30	102.02	106.78
29	V7	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
29	Y7	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
29	V9	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
29	Y9	202	PEB	CHB-C4B-NB	-4.30	122.86	128.83
30	xL	304	PUB	CHA-C1B-C2B	-4.30	123.00	130.34
29	HK	1002	PEB	CMD-C2D-C3D	4.30	136.13	130.06
29	ID	202	PEB	C4B-C3B-C2B	-4.30	102.02	106.78
29	TR	202	PEB	C1C-CHB-C4B	4.30	133.95	128.81
30	wJ	305	PUB	OA-C1A-NA	-4.30	119.56	125.93
30	wJ	304	PUB	CHA-C1B-C2B	-4.30	123.00	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C4	202	PEB	C4B-C3B-C2B	-4.30	102.02	106.78
30	xJ	305	PUB	OA-C1A-NA	-4.30	119.56	125.93
29	tJ	201	PEB	CHB-C4B-NB	-4.30	122.86	128.83
29	tL	201	PEB	CHB-C4B-NB	-4.30	122.86	128.83
31	E1	1001	CYC	CMA-C3A-C4A	4.30	131.68	125.06
29	a7	203	PEB	C4B-C3B-C2B	-4.30	102.03	106.78
29	a9	203	PEB	C4B-C3B-C2B	-4.30	102.03	106.78
29	k7	202	PEB	CHB-C4B-NB	-4.30	122.87	128.83
29	k9	202	PEB	CHB-C4B-NB	-4.30	122.87	128.83
29	DO	202	PEB	CHC-C1D-ND	-4.30	108.96	113.95
29	i1	202	PEB	OA-C1A-C2A	-4.30	122.76	126.17
29	iK	202	PEB	OA-C1A-C2A	-4.30	122.76	126.17
31	D1	1003	CYC	CMA-C3A-C4A	4.30	131.68	125.06
30	wL	304	PUB	CHA-C1B-C2B	-4.30	123.01	130.34
31	J1	1001	CYC	OC-C1C-C2C	-4.29	122.76	126.17
31	DK	1001	CYC	OC-C1C-C2C	-4.29	122.76	126.17
31	JK	1001	CYC	OC-C1C-C2C	-4.29	122.76	126.17
29	FJ	201	PEB	CHB-C4B-NB	-4.29	122.87	128.83
29	FL	201	PEB	CHB-C4B-NB	-4.29	122.87	128.83
30	MG	403	PUB	CHB-C1C-NC	-4.29	122.87	128.83
29	vJ	201	PEB	CHB-C4B-NB	-4.29	122.87	128.83
29	vL	201	PEB	CHB-C4B-NB	-4.29	122.87	128.83
30	AF	302	PUB	CMA-C2A-C1A	4.29	131.49	121.39
30	AI	302	PUB	CMA-C2A-C1A	4.29	131.49	121.39
29	SF	201	PEB	C3D-C4D-ND	4.29	115.68	107.26
29	SI	201	PEB	C3D-C4D-ND	4.29	115.68	107.26
29	V2	202	PEB	C1C-CHB-C4B	4.29	133.94	128.81
31	D1	1003	CYC	CHB-C4A-NA	-4.29	115.96	124.93
29	m7	202	PEB	OA-C1A-C2A	-4.29	122.76	126.17
29	m9	202	PEB	OA-C1A-C2A	-4.29	122.76	126.17
29	Y1	201	PEB	C3B-C4B-NB	4.29	116.29	110.05
29	YK	201	PEB	C3B-C4B-NB	4.29	116.29	110.05
31	NP	1001	CYC	CAB-C3B-C4B	4.29	128.15	121.38
31	GK	1001	CYC	CMA-C3A-C4A	4.29	131.67	125.06
29	A7	304	PEB	C1C-CHB-C4B	-4.29	123.69	128.81
29	ZF	201	PEB	C3D-C4D-ND	4.29	115.67	107.26
29	ZI	201	PEB	C3D-C4D-ND	4.29	115.67	107.26
29	fJ	201	PEB	CHB-C4B-NB	-4.29	122.88	128.83
29	fL	201	PEB	CHB-C4B-NB	-4.29	122.88	128.83
29	R7	203	PEB	C4B-C3B-C2B	-4.29	102.04	106.78
29	R9	203	PEB	C4B-C3B-C2B	-4.29	102.04	106.78
29	iB	201	PEB	C3D-C4D-ND	4.29	115.67	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	iM	201	PEB	C3D-C4D-ND	4.29	115.67	107.26
29	e7	203	PEB	C4B-C3B-C2B	-4.28	102.04	106.78
29	e9	203	PEB	C4B-C3B-C2B	-4.28	102.04	106.78
29	AJ	203	PEB	OD-C4D-ND	-4.28	119.58	125.93
29	AL	203	PEB	OD-C4D-ND	-4.28	119.58	125.93
29	a7	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	a9	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	RJ	202	PEB	OD-C4D-ND	-4.28	119.58	125.93
29	RL	202	PEB	OD-C4D-ND	-4.28	119.58	125.93
29	mB	201	PEB	C3D-C4D-ND	4.28	115.66	107.26
29	mM	201	PEB	C3D-C4D-ND	4.28	115.66	107.26
30	xJ	304	PUB	CHA-C1B-C2B	-4.28	123.03	130.34
29	a1	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
29	aK	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
29	UF	202	PEB	C3D-C4D-ND	4.28	115.66	107.26
29	UI	202	PEB	C3D-C4D-ND	4.28	115.66	107.26
31	M1	1001	CYC	CMA-C3A-C4A	4.28	131.66	125.06
31	MK	1001	CYC	CMA-C3A-C4A	4.28	131.66	125.06
31	GK	1001	CYC	CHB-C4A-NA	-4.28	115.98	124.93
29	g7	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	g9	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	L8	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
29	R7	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	R9	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	NJ	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	NL	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	H5	202	PEB	OA-C1A-C2A	-4.28	122.77	126.17
31	D1	1001	CYC	OC-C1C-C2C	-4.28	122.77	126.17
31	I1	1001	CYC	CHB-C4A-NA	-4.28	115.98	124.93
31	M1	1001	CYC	CHB-C4A-NA	-4.28	115.98	124.93
31	MK	1001	CYC	CHB-C4A-NA	-4.28	115.98	124.93
29	e7	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	e9	202	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	bJ	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	bL	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	JJ	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	JL	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
31	lP	1001	CYC	CAB-C3B-C4B	4.28	128.14	121.38
29	ED	201	PEB	C4B-C3B-C2B	-4.28	102.05	106.78
29	I4	202	PEB	C4B-C3B-C2B	-4.28	102.05	106.78
29	jJ	202	PEB	OD-C4D-ND	-4.28	119.59	125.93
29	jL	202	PEB	OD-C4D-ND	-4.28	119.59	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BJ	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	BL	201	PEB	CHB-C4B-NB	-4.28	122.89	128.83
29	NJ	202	PEB	OD-C4D-ND	-4.28	119.59	125.93
29	NL	202	PEB	OD-C4D-ND	-4.28	119.59	125.93
30	MN	402	PUB	C1D-CHC-C4C	-4.28	104.06	113.37
29	k7	203	PEB	C4B-C3B-C2B	-4.28	102.05	106.78
29	k9	203	PEB	C4B-C3B-C2B	-4.28	102.05	106.78
29	ZB	201	PEB	C3D-C4D-ND	4.28	115.65	107.26
29	ZM	201	PEB	C3D-C4D-ND	4.28	115.65	107.26
29	jF	201	PEB	C3D-C4D-ND	4.27	115.65	107.26
29	jI	201	PEB	C3D-C4D-ND	4.27	115.65	107.26
31	C1	1001	CYC	CMA-C3A-C4A	4.27	131.65	125.06
31	AP	1001	CYC	CAB-C3B-C4B	4.27	128.13	121.38
29	CD	202	PEB	C4B-C3B-C2B	-4.27	102.05	106.78
29	c7	202	PEB	CHB-C4B-NB	-4.27	122.90	128.83
29	c9	202	PEB	CHB-C4B-NB	-4.27	122.90	128.83
31	JP	1001	CYC	CAB-C3B-C4B	4.27	128.13	121.38
29	HB	201	PEB	C3D-C4D-ND	4.27	115.64	107.26
29	HM	201	PEB	C3D-C4D-ND	4.27	115.64	107.26
31	CK	1001	CYC	CHB-C4A-NA	-4.27	116.00	124.93
31	EK	1001	CYC	CHB-C4A-NA	-4.27	116.00	124.93
31	D1	1003	CYC	OB-C4B-C3B	-4.27	123.40	128.04
31	PP	1001	CYC	CAB-C3B-C4B	4.27	128.13	121.38
29	QF	201	PEB	C3D-C4D-ND	4.27	115.64	107.26
29	QI	201	PEB	C3D-C4D-ND	4.27	115.64	107.26
29	AM	303	PEB	CHC-C1D-ND	-4.27	108.99	113.95
31	iP	1001	CYC	CAB-C3B-C4B	4.27	128.12	121.38
29	dJ	201	PEB	CHB-C4B-NB	-4.27	122.90	128.83
29	dL	201	PEB	CHB-C4B-NB	-4.27	122.90	128.83
29	F1	1002	PEB	CMD-C2D-C3D	4.27	136.09	130.06
29	L1	1002	PEB	CMD-C2D-C3D	4.27	136.09	130.06
29	FK	1002	PEB	CMD-C2D-C3D	4.27	136.09	130.06
29	LK	1002	PEB	CMD-C2D-C3D	4.27	136.09	130.06
29	hF	201	PEB	C3D-C4D-ND	4.27	115.64	107.26
29	hI	201	PEB	C3D-C4D-ND	4.27	115.64	107.26
31	I1	1001	CYC	CMA-C3A-C4A	4.27	131.64	125.06
30	MA	402	PUB	C1D-CHC-C4C	-4.27	104.08	113.37
29	MQ	406	PEB	CHC-C1D-ND	-4.27	108.99	113.95
31	KP	1001	CYC	CAB-C3B-C4B	4.27	128.12	121.38
29	rJ	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
29	rL	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
30	AM	304	PUB	OD-C4D-ND	-4.27	119.61	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i7	202	PEB	CHB-C4B-NB	-4.27	122.91	128.83
29	i9	202	PEB	CHB-C4B-NB	-4.27	122.91	128.83
29	XB	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	XM	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	H1	1002	PEB	CMD-C2D-C3D	4.27	136.08	130.06
29	dF	202	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	dI	202	PEB	C3D-C4D-ND	4.27	115.63	107.26
31	IK	1001	CYC	CHB-C4A-NA	-4.27	116.01	124.93
29	OF	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	OI	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
31	CK	1001	CYC	CMA-C3A-C4A	4.27	131.63	125.06
29	c1	202	PEB	OA-C1A-C2A	-4.27	122.78	126.17
29	cK	202	PEB	OA-C1A-C2A	-4.27	122.78	126.17
29	gB	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	gM	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
31	C1	1001	CYC	CHB-C4A-NA	-4.27	116.01	124.93
31	K1	1001	CYC	CHB-C4A-NA	-4.27	116.01	124.93
31	KK	1001	CYC	CHB-C4A-NA	-4.27	116.01	124.93
30	yJ	302	PUB	C1C-C2C-C3C	-4.27	102.06	106.78
30	yL	302	PUB	C1C-C2C-C3C	-4.27	102.06	106.78
31	tP	1001	CYC	CAB-C3B-C4B	4.27	128.12	121.38
29	hJ	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
29	hL	201	PEB	CHB-C4B-NB	-4.27	122.91	128.83
29	WF	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	WI	201	PEB	C3D-C4D-ND	4.27	115.63	107.26
29	F8	202	PEB	OA-C1A-C2A	-4.26	122.78	126.17
29	nJ	202	PEB	OD-C4D-ND	-4.26	119.61	125.93
29	nL	202	PEB	OD-C4D-ND	-4.26	119.61	125.93
31	E1	1001	CYC	CHB-C4A-NA	-4.26	116.01	124.93
29	U1	201	PEB	OA-C1A-C2A	-4.26	122.78	126.17
29	UK	201	PEB	OA-C1A-C2A	-4.26	122.78	126.17
29	fF	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	fI	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	RJ	201	PEB	CHB-C4B-NB	-4.26	122.91	128.83
29	nJ	201	PEB	CHB-C4B-NB	-4.26	122.91	128.83
29	RL	201	PEB	CHB-C4B-NB	-4.26	122.91	128.83
29	nL	201	PEB	CHB-C4B-NB	-4.26	122.91	128.83
29	P7	203	PEB	C4B-C3B-C2B	-4.26	102.06	106.78
29	P9	203	PEB	C4B-C3B-C2B	-4.26	102.06	106.78
29	ZJ	201	PEB	CHB-C4B-NB	-4.26	122.91	128.83
29	ZL	201	PEB	CHB-C4B-NB	-4.26	122.91	128.83
29	TJ	202	PEB	OD-C4D-ND	-4.26	119.61	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TL	202	PEB	OD-C4D-ND	-4.26	119.61	125.93
31	gP	1001	CYC	CAB-C3B-C4B	4.26	128.11	121.38
29	pJ	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
29	pL	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
31	RP	1001	CYC	CAB-C3B-C4B	4.26	128.11	121.38
31	cP	1001	CYC	CAB-C3B-C4B	4.26	128.11	121.38
29	V1	201	PEB	C3B-C4B-NB	4.26	116.25	110.05
29	e1	201	PEB	C3B-C4B-NB	4.26	116.25	110.05
29	VK	201	PEB	C3B-C4B-NB	4.26	116.25	110.05
29	eK	201	PEB	C3B-C4B-NB	4.26	116.25	110.05
29	HJ	201	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	HL	201	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	XJ	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
29	XL	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
29	PJ	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	PL	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	FB	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	FM	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	RB	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	VB	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	RM	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	VM	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	uJ	201	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	uL	201	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	Z1	201	PEB	OA-C1A-C2A	-4.26	122.79	126.17
29	I4	203	PEB	OA-C1A-C2A	-4.26	122.79	126.17
29	ZK	201	PEB	OA-C1A-C2A	-4.26	122.79	126.17
29	NB	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	cB	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	NM	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
29	cM	201	PEB	C3D-C4D-ND	4.26	115.62	107.26
31	K1	1001	CYC	CMA-C3A-C4A	4.26	131.62	125.06
31	KK	1001	CYC	CMA-C3A-C4A	4.26	131.62	125.06
29	dJ	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	dL	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	jJ	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
29	jL	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
30	MQ	405	PUB	CHB-C1C-NC	-4.26	122.92	128.83
29	bF	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
29	bI	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
31	rP	1001	CYC	CAB-C3B-C4B	4.26	128.10	121.38
29	T2	202	PEB	C1C-CHB-C4B	4.26	133.90	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JB	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
29	JM	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
29	VJ	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
29	VL	201	PEB	CHB-C4B-NB	-4.26	122.92	128.83
29	g1	201	PEB	C3B-C4B-NB	4.26	116.24	110.05
29	gK	201	PEB	C3B-C4B-NB	4.26	116.24	110.05
29	DB	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
29	DM	201	PEB	C3D-C4D-ND	4.26	115.61	107.26
29	DK	1002	PEB	OA-C1A-C2A	-4.26	122.79	126.17
29	rJ	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	rL	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	k1	201	PEB	C3B-C4B-NB	4.26	116.24	110.05
29	kK	201	PEB	C3B-C4B-NB	4.26	116.24	110.05
29	hJ	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	hL	202	PEB	OD-C4D-ND	-4.26	119.62	125.93
29	m7	202	PEB	CHB-C4B-NB	-4.25	122.92	128.83
29	m9	202	PEB	CHB-C4B-NB	-4.25	122.92	128.83
31	I1	1001	CYC	OB-C4B-C3B	-4.25	123.42	128.04
31	K1	1001	CYC	OB-C4B-C3B	-4.25	123.42	128.04
31	KK	1001	CYC	OB-C4B-C3B	-4.25	123.42	128.04
29	FJ	202	PEB	OD-C4D-ND	-4.25	119.63	125.93
29	FL	202	PEB	OD-C4D-ND	-4.25	119.63	125.93
30	AB	304	PUB	OD-C4D-ND	-4.25	119.63	125.93
31	vP	1001	CYC	CAB-C3B-C4B	4.25	128.10	121.38
29	BJ	202	PEB	OD-C4D-ND	-4.25	119.63	125.93
29	BL	202	PEB	OD-C4D-ND	-4.25	119.63	125.93
29	TJ	201	PEB	CHB-C4B-NB	-4.25	122.93	128.83
29	TL	201	PEB	CHB-C4B-NB	-4.25	122.93	128.83
31	E1	1001	CYC	OB-C4B-C3B	-4.25	123.43	128.04
31	mP	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
29	AB	303	PEB	CHC-C1D-ND	-4.25	109.01	113.95
31	eP	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
29	E4	202	PEB	C4B-C3B-C2B	-4.25	102.08	106.78
31	GP	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
29	kB	201	PEB	C3D-C4D-ND	4.25	115.60	107.26
29	kM	201	PEB	C3D-C4D-ND	4.25	115.60	107.26
29	IJ	203	PEB	OD-C4D-ND	-4.25	119.63	125.93
29	IL	203	PEB	OD-C4D-ND	-4.25	119.63	125.93
29	eB	201	PEB	C3D-C4D-ND	4.25	115.60	107.26
29	eM	201	PEB	C3D-C4D-ND	4.25	115.60	107.26
31	EP	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
31	C1	1001	CYC	OB-C4B-C3B	-4.25	123.43	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	GK	1001	CYC	OB-C4B-C3B	-4.25	123.43	128.04
29	D1	1002	PEB	CMD-C2D-C3D	4.25	136.06	130.06
29	KD	203	PEB	C3D-C4D-ND	4.25	115.59	107.26
29	TB	201	PEB	C3D-C4D-ND	4.25	115.59	107.26
29	TM	201	PEB	C3D-C4D-ND	4.25	115.59	107.26
31	IK	1001	CYC	CMA-C3A-C4A	4.25	131.61	125.06
29	LJ	201	PEB	CHB-C4B-NB	-4.25	122.94	128.83
29	LL	201	PEB	CHB-C4B-NB	-4.25	122.94	128.83
29	N1	1002	PEB	CMD-C2D-C3D	4.25	136.05	130.06
29	V7	202	PEB	OA-C1A-C2A	-4.25	122.80	126.17
29	V9	202	PEB	OA-C1A-C2A	-4.25	122.80	126.17
29	CG	201	PEB	OA-C1A-C2A	-4.25	122.80	126.17
29	CQ	201	PEB	OA-C1A-C2A	-4.25	122.80	126.17
29	P1	201	PEB	C3B-C4B-NB	4.25	116.23	110.05
29	a1	201	PEB	C3B-C4B-NB	4.25	116.23	110.05
29	PK	201	PEB	C3B-C4B-NB	4.25	116.23	110.05
29	aK	201	PEB	C3B-C4B-NB	4.25	116.23	110.05
29	DK	1002	PEB	CMD-C2D-C3D	4.25	136.05	130.06
31	pP	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
29	JJ	202	PEB	OD-C4D-ND	-4.25	119.64	125.93
29	JL	202	PEB	OD-C4D-ND	-4.25	119.64	125.93
31	M1	1001	CYC	OB-C4B-C3B	-4.25	123.43	128.04
31	MK	1001	CYC	OB-C4B-C3B	-4.25	123.43	128.04
29	DJ	201	PEB	CHB-C4B-NB	-4.25	122.94	128.83
29	DL	201	PEB	CHB-C4B-NB	-4.25	122.94	128.83
31	TP	1001	CYC	CAB-C3B-C4B	4.25	128.09	121.38
29	NK	1002	PEB	CMD-C2D-C3D	4.25	136.05	130.06
29	PB	201	PEB	C3D-C4D-ND	4.25	115.59	107.26
29	PM	201	PEB	C3D-C4D-ND	4.25	115.59	107.26
29	T1	201	PEB	C3B-C4B-NB	4.24	116.22	110.05
29	TK	201	PEB	C3B-C4B-NB	4.24	116.22	110.05
29	a7	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	a9	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	lF	201	PEB	C3D-C4D-ND	4.24	115.59	107.26
29	lI	201	PEB	C3D-C4D-ND	4.24	115.59	107.26
29	PJ	201	PEB	CHB-C4B-NB	-4.24	122.94	128.83
29	PL	201	PEB	CHB-C4B-NB	-4.24	122.94	128.83
29	T2	203	PEB	C2A-C1A-NA	4.24	111.93	108.27
29	pJ	202	PEB	OD-C4D-ND	-4.24	119.64	125.93
29	pL	202	PEB	OD-C4D-ND	-4.24	119.64	125.93
29	GD	203	PEB	C3D-C4D-ND	4.24	115.58	107.26
29	sJ	203	PEB	OD-C4D-ND	-4.24	119.65	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	sL	203	PEB	OD-C4D-ND	-4.24	119.65	125.93
29	WJ	201	PEB	OD-C4D-ND	-4.24	119.65	125.93
29	WL	201	PEB	OD-C4D-ND	-4.24	119.65	125.93
29	LB	201	PEB	C3D-C4D-ND	4.24	115.58	107.26
29	LM	201	PEB	C3D-C4D-ND	4.24	115.58	107.26
29	P1	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	PK	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	F1	1002	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	FK	1002	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	R1	201	PEB	C3B-C4B-NB	4.24	116.21	110.05
29	RK	201	PEB	C3B-C4B-NB	4.24	116.21	110.05
29	K4	203	PEB	C3D-C4D-ND	4.24	115.57	107.26
29	J1	1002	PEB	CMD-C2D-C3D	4.24	136.04	130.06
29	JK	1002	PEB	CMD-C2D-C3D	4.24	136.04	130.06
29	F5	202	PEB	OA-C1A-C2A	-4.24	122.80	126.17
29	AA	201	PEB	CHC-C1D-ND	-4.24	109.03	113.95
29	AN	201	PEB	CHC-C1D-ND	-4.24	109.03	113.95
29	c1	201	PEB	C3B-C4B-NB	4.24	116.21	110.05
29	cK	201	PEB	C3B-C4B-NB	4.24	116.21	110.05
29	XJ	202	PEB	OD-C4D-ND	-4.24	119.65	125.93
29	XL	202	PEB	OD-C4D-ND	-4.24	119.65	125.93
29	D3	202	PEB	CHC-C1D-ND	-4.24	109.03	113.95
29	GA	201	PEB	CHC-C1D-ND	-4.24	109.03	113.95
29	GN	201	PEB	CHC-C1D-ND	-4.24	109.03	113.95
31	HK	1001	CYC	OC-C1C-C2C	-4.23	122.81	126.17
31	IK	1001	CYC	OB-C4B-C3B	-4.23	123.45	128.04
29	Y7	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
29	B8	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
29	Y9	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
31	EK	1001	CYC	CMA-C3A-C4A	4.23	131.58	125.06
29	G4	203	PEB	C3D-C4D-ND	4.23	115.56	107.26
29	CA	201	PEB	CHC-C1D-ND	-4.23	109.03	113.95
29	CN	201	PEB	CHC-C1D-ND	-4.23	109.03	113.95
29	IJ	201	PEB	CHB-C4B-NB	-4.23	122.96	128.83
29	IL	201	PEB	CHB-C4B-NB	-4.23	122.96	128.83
29	B5	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
29	m1	201	PEB	C3B-C4B-NB	4.23	116.20	110.05
29	mK	201	PEB	C3B-C4B-NB	4.23	116.20	110.05
29	J9	1002	PEB	C3B-C4B-NB	4.23	116.20	110.05
29	EA	201	PEB	CHC-C1D-ND	-4.23	109.03	113.95
29	EN	201	PEB	CHC-C1D-ND	-4.23	109.03	113.95
29	R7	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R9	202	PEB	OA-C1A-C2A	-4.23	122.81	126.17
29	BC	203	PEB	OA-C1A-C2A	-4.23	122.81	126.17
29	BE	203	PEB	OA-C1A-C2A	-4.23	122.81	126.17
31	CP	1001	CYC	CAB-C3B-C4B	4.23	128.06	121.38
29	A9	304	PEB	C1C-CHB-C4B	-4.23	123.76	128.81
29	O7	201	PEB	C3D-C4D-ND	4.23	115.56	107.26
29	O9	201	PEB	C3D-C4D-ND	4.23	115.56	107.26
29	RR	203	PEB	C2A-C1A-NA	4.23	111.92	108.27
29	LJ	202	PEB	CMB-C2B-C1B	4.23	131.57	125.06
29	LL	202	PEB	CMB-C2B-C1B	4.23	131.57	125.06
29	ZJ	202	PEB	OD-C4D-ND	-4.23	119.67	125.93
29	bJ	202	PEB	OD-C4D-ND	-4.23	119.67	125.93
29	ZL	202	PEB	OD-C4D-ND	-4.23	119.67	125.93
29	bL	202	PEB	OD-C4D-ND	-4.23	119.67	125.93
29	NR	203	PEB	C2A-C1A-NA	4.23	111.92	108.27
29	xL	301	PEB	C3D-C4D-ND	4.23	115.55	107.26
29	J7	1002	PEB	C3B-C4B-NB	4.23	116.20	110.05
31	H1	1001	CYC	OC-C1C-C2C	-4.22	122.81	126.17
31	EK	1001	CYC	OB-C4B-C3B	-4.22	123.46	128.04
29	ZJ	203	PEB	CMB-C2B-C1B	4.22	131.57	125.06
29	ZL	203	PEB	CMB-C2B-C1B	4.22	131.57	125.06
29	A7	301	PEB	CHC-C1D-ND	-4.22	109.05	113.95
29	A9	301	PEB	CHC-C1D-ND	-4.22	109.05	113.95
29	MD	203	PEB	C3D-C4D-ND	4.22	115.54	107.26
29	i7	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
29	i9	202	PEB	OA-C1A-C2A	-4.22	122.82	126.17
29	b7	201	PEB	C3D-C4D-ND	4.22	115.54	107.26
29	b9	201	PEB	C3D-C4D-ND	4.22	115.54	107.26
29	N2	203	PEB	C2A-C1A-NA	4.22	111.91	108.27
29	MG	405	PEB	C3D-C4D-ND	4.22	115.54	107.26
29	IJ	202	PEB	OD-C4D-ND	-4.22	119.68	125.93
29	IL	202	PEB	OD-C4D-ND	-4.22	119.68	125.93
29	h7	201	PEB	C3D-C4D-ND	4.22	115.53	107.26
29	h9	201	PEB	C3D-C4D-ND	4.22	115.53	107.26
29	fJ	202	PEB	OD-C4D-ND	-4.22	119.68	125.93
29	fL	202	PEB	OD-C4D-ND	-4.22	119.68	125.93
29	D1	1002	PEB	OA-C1A-C2A	-4.22	122.82	126.17
29	U7	201	PEB	C3D-C4D-ND	4.22	115.53	107.26
29	U9	201	PEB	C3D-C4D-ND	4.22	115.53	107.26
29	MQ	407	PEB	C3D-C4D-ND	4.22	115.53	107.26
29	ID	203	PEB	C3D-C4D-ND	4.21	115.53	107.26
29	L1	1002	PEB	OA-C1A-C2A	-4.21	122.82	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LK	1002	PEB	OA-C1A-C2A	-4.21	122.82	126.17
29	R2	203	PEB	C2A-C1A-NA	4.21	111.91	108.27
29	i1	201	PEB	C3B-C4B-NB	4.21	116.18	110.05
29	iK	201	PEB	C3B-C4B-NB	4.21	116.18	110.05
29	g7	202	PEB	OA-C1A-C2A	-4.21	122.82	126.17
29	g9	202	PEB	OA-C1A-C2A	-4.21	122.82	126.17
31	F1	1001	CYC	OC-C1C-C2C	-4.21	122.83	126.17
31	FK	1001	CYC	OC-C1C-C2C	-4.21	122.83	126.17
29	KA	201	PEB	CHC-C1D-ND	-4.21	109.06	113.95
29	KN	201	PEB	CHC-C1D-ND	-4.21	109.06	113.95
29	f7	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	j7	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	f9	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	j9	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	ED	202	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	VJ	202	PEB	CMB-C2B-C1B	4.21	131.54	125.06
29	VL	202	PEB	CMB-C2B-C1B	4.21	131.54	125.06
29	Z7	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	d7	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	Z9	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	d9	201	PEB	C3D-C4D-ND	4.21	115.52	107.26
29	F7	1002	PEB	C3B-C4B-NB	4.21	116.17	110.05
29	W7	201	PEB	C3D-C4D-ND	4.21	115.51	107.26
29	W9	201	PEB	C3D-C4D-ND	4.21	115.51	107.26
29	P2	202	PEB	C2A-C1A-NA	4.21	111.90	108.27
29	hJ	203	PEB	CMB-C2B-C1B	4.21	131.54	125.06
29	hL	203	PEB	CMB-C2B-C1B	4.21	131.54	125.06
29	L9	1002	PEB	C3B-C4B-NB	4.21	116.17	110.05
29	AG	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
29	AQ	201	PEB	OA-C1A-C2A	-4.21	122.83	126.17
31	N1	1001	CYC	OC-C1C-C2C	-4.21	122.83	126.17
29	L7	1002	PEB	C3B-C4B-NB	4.21	116.17	110.05
29	J1	1002	PEB	OA-C1A-C2A	-4.20	122.83	126.17
29	KG	201	PEB	OA-C1A-C2A	-4.20	122.83	126.17
29	JK	1002	PEB	OA-C1A-C2A	-4.20	122.83	126.17
29	KQ	201	PEB	OA-C1A-C2A	-4.20	122.83	126.17
29	dJ	203	PEB	CMB-C2B-C1B	4.20	131.54	125.06
29	dL	203	PEB	CMB-C2B-C1B	4.20	131.54	125.06
29	HC	203	PEB	OA-C1A-C2A	-4.20	122.83	126.17
29	HE	203	PEB	OA-C1A-C2A	-4.20	122.83	126.17
31	M9	1001	CYC	OC-C1C-C2C	-4.20	122.83	126.17
31	NK	1001	CYC	OC-C1C-C2C	-4.20	122.83	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S7	201	PEB	C3D-C4D-ND	4.20	115.50	107.26
29	S9	201	PEB	C3D-C4D-ND	4.20	115.50	107.26
29	VR	203	PEB	C2A-C1A-NA	4.20	111.89	108.27
29	PJ	203	PEB	CMB-C2B-C1B	4.20	131.53	125.06
29	PL	203	PEB	CMB-C2B-C1B	4.20	131.53	125.06
29	IA	201	PEB	CHC-C1D-ND	-4.20	109.07	113.95
29	IN	201	PEB	CHC-C1D-ND	-4.20	109.07	113.95
29	k7	202	PEB	OA-C1A-C2A	-4.20	122.83	126.17
29	k9	202	PEB	OA-C1A-C2A	-4.20	122.83	126.17
31	L1	1001	CYC	OC-C1C-C2C	-4.20	122.83	126.17
31	LK	1001	CYC	OC-C1C-C2C	-4.20	122.83	126.17
29	MN	404	PEB	C3D-C4D-ND	4.20	115.50	107.26
29	O7	202	PEB	C3D-C4D-ND	4.20	115.49	107.26
29	O9	202	PEB	C3D-C4D-ND	4.20	115.49	107.26
29	Q7	201	PEB	C3D-C4D-ND	4.20	115.49	107.26
29	Q9	201	PEB	C3D-C4D-ND	4.20	115.49	107.26
29	BJ	203	PEB	CMB-C2B-C1B	4.19	131.52	125.06
29	BL	203	PEB	CMB-C2B-C1B	4.19	131.52	125.06
29	E4	203	PEB	C3D-C4D-ND	4.19	115.49	107.26
29	l7	201	PEB	C3D-C4D-ND	4.19	115.49	107.26
29	l9	201	PEB	C3D-C4D-ND	4.19	115.49	107.26
29	R1	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	c7	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	e7	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	c9	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	e9	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	RK	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	xJ	301	PEB	C3D-C4D-ND	4.19	115.49	107.26
29	S7	202	PEB	C3D-C4D-ND	4.19	115.48	107.26
29	S9	202	PEB	C3D-C4D-ND	4.19	115.48	107.26
29	S2	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	G8	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	EG	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	EQ	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	MA	404	PEB	C3D-C4D-ND	4.19	115.48	107.26
29	H7	1002	PEB	C3B-C4B-NB	4.19	116.15	110.05
29	H9	1002	PEB	C3B-C4B-NB	4.19	116.15	110.05
29	tJ	202	PEB	CMB-C2B-C1B	4.19	131.52	125.06
29	tL	202	PEB	CMB-C2B-C1B	4.19	131.52	125.06
29	C4	203	PEB	C3D-C4D-ND	4.19	115.48	107.26
29	IG	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	IQ	201	PEB	OA-C1A-C2A	-4.19	122.84	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V2	203	PEB	C2A-C1A-NA	4.19	111.89	108.27
29	XR	203	PEB	C2A-C1A-NA	4.19	111.89	108.27
29	wJ	301	PEB	C3D-C4D-ND	4.19	115.48	107.26
30	yJ	303	PUB	CMA-C2A-C1A	4.19	131.24	121.39
29	TJ	203	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	TL	203	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	l7	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	l9	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	DC	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	DE	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
31	M7	1001	CYC	OC-C1C-C2C	-4.19	122.84	126.17
29	CD	203	PEB	C3D-C4D-ND	4.19	115.48	107.26
29	NJ	203	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	NL	203	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	Z7	202	PEB	C3D-C4D-ND	4.19	115.47	107.26
29	Z9	202	PEB	C3D-C4D-ND	4.19	115.47	107.26
29	D7	1002	PEB	C3B-C4B-NB	4.19	116.14	110.05
29	N7	1002	PEB	C3B-C4B-NB	4.19	116.14	110.05
29	D9	1002	PEB	C3B-C4B-NB	4.19	116.14	110.05
29	F9	1002	PEB	C3B-C4B-NB	4.19	116.14	110.05
29	N9	1002	PEB	C3B-C4B-NB	4.19	116.14	110.05
29	pJ	203	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	vJ	202	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	pL	203	PEB	CMB-C2B-C1B	4.19	131.51	125.06
29	vL	202	PEB	CMB-C2B-C1B	4.19	131.51	125.06
31	KI	1001	CYC	C4D-CHA-C1A	4.19	133.81	128.81
30	yJ	302	PUB	CHC-C1D-ND	-4.19	108.43	113.72
30	yL	302	PUB	CHC-C1D-ND	-4.19	108.43	113.72
29	G5	202	PEB	OA-C1A-C2A	-4.19	122.84	126.17
29	X2	202	PEB	CAB-CBB-CGB	-4.19	104.60	113.60
29	Q7	202	PEB	C3D-C4D-ND	4.18	115.47	107.26
29	Q9	202	PEB	C3D-C4D-ND	4.18	115.47	107.26
30	yL	303	PUB	CMA-C2A-C1A	4.18	131.23	121.39
29	d7	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
29	d9	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
29	VR	203	PEB	CAB-CBB-CGB	-4.18	104.61	113.60
29	jJ	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	jL	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	D4	202	PEB	C1B-C2B-C3B	-4.18	101.71	106.51
30	wL	305	PUB	C1D-CHC-C4C	-4.18	104.27	113.37
29	U2	202	PEB	C2A-C1A-NA	4.18	111.88	108.27
29	rJ	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	rL	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	L5	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
29	T7	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
29	T9	202	PEB	OA-C1A-C2A	-4.18	122.85	126.17
29	wL	301	PEB	C3D-C4D-ND	4.18	115.46	107.26
29	h7	202	PEB	C3D-C4D-ND	4.18	115.46	107.26
29	h9	202	PEB	C3D-C4D-ND	4.18	115.46	107.26
29	fJ	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	nJ	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	fL	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	nL	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	JF	1002	PEB	CHB-C4B-NB	-4.18	123.03	128.83
29	JI	1002	PEB	CHB-C4B-NB	-4.18	123.03	128.83
29	JJ	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	JL	203	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	j7	202	PEB	C3D-C4D-ND	4.18	115.45	107.26
29	j9	202	PEB	C3D-C4D-ND	4.18	115.45	107.26
31	CK	1001	CYC	OB-C4B-C3B	-4.18	123.51	128.04
29	DJ	202	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	DL	202	PEB	CMB-C2B-C1B	4.18	131.50	125.06
29	HJ	202	PEB	CMB-C2B-C1B	4.18	131.49	125.06
29	bJ	203	PEB	CMB-C2B-C1B	4.18	131.49	125.06
29	HL	202	PEB	CMB-C2B-C1B	4.18	131.49	125.06
29	bL	203	PEB	CMB-C2B-C1B	4.18	131.49	125.06
29	P7	202	PEB	OA-C1A-C2A	-4.17	122.85	126.17
29	P9	202	PEB	OA-C1A-C2A	-4.17	122.85	126.17
29	IJ	203	PEB	CMB-C2B-C1B	4.17	131.49	125.06
29	IL	203	PEB	CMB-C2B-C1B	4.17	131.49	125.06
29	XJ	203	PEB	CMB-C2B-C1B	4.17	131.49	125.06
29	XL	203	PEB	CMB-C2B-C1B	4.17	131.49	125.06
30	xJ	305	PUB	C1D-CHC-C4C	-4.17	104.29	113.37
29	V2	203	PEB	CAB-CBB-CGB	-4.17	104.62	113.60
29	R2	203	PEB	CAB-CBB-CGB	-4.17	104.62	113.60
29	NK	1002	PEB	OA-C1A-C2A	-4.17	122.86	126.17
29	FJ	203	PEB	CMB-C2B-C1B	4.17	131.49	125.06
29	FL	203	PEB	CMB-C2B-C1B	4.17	131.49	125.06
29	PF	202	PEB	OD-C4D-ND	-4.17	119.75	125.93
29	gF	202	PEB	OD-C4D-ND	-4.17	119.75	125.93
29	PI	202	PEB	OD-C4D-ND	-4.17	119.75	125.93
29	gI	202	PEB	OD-C4D-ND	-4.17	119.75	125.93
29	k7	201	PEB	CHC-C1D-ND	-4.17	109.10	113.95
29	k9	201	PEB	CHC-C1D-ND	-4.17	109.10	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	PR	202	PEB	C2A-C1A-NA	4.17	111.87	108.27
29	l7	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
29	l9	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
29	d7	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
29	d9	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
29	XR	203	PEB	CAB-CBB-CGB	-4.17	104.63	113.60
29	DD	202	PEB	C1B-C2B-C3B	-4.17	101.72	106.51
29	xL	302	PEB	CHA-C1B-NB	-4.17	116.21	124.93
29	f7	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
29	f9	202	PEB	C3D-C4D-ND	4.17	115.44	107.26
30	wJ	305	PUB	C1D-CHC-C4C	-4.17	104.30	113.37
29	GG	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17
29	GQ	201	PEB	OA-C1A-C2A	-4.17	122.86	126.17
29	W7	202	PEB	C3D-C4D-ND	4.17	115.43	107.26
29	W9	202	PEB	C3D-C4D-ND	4.17	115.43	107.26
31	J9	1001	CYC	C1B-NB-C4B	-4.17	105.36	110.67
29	RJ	203	PEB	CMB-C2B-C1B	4.17	131.48	125.06
29	RL	203	PEB	CMB-C2B-C1B	4.17	131.48	125.06
29	UR	202	PEB	C2A-C1A-NA	4.16	111.86	108.27
31	K7	1001	CYC	OC-C1C-C2C	-4.16	122.86	126.17
29	L5	202	PEB	CHB-C4B-NB	-4.16	123.05	128.83
31	F9	1001	CYC	C1B-NB-C4B	-4.16	105.37	110.67
29	PR	202	PEB	CAB-CBB-CGB	-4.16	104.65	113.60
29	TR	203	PEB	C2A-C1A-NA	4.16	111.86	108.27
29	Y7	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	c7	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	Y9	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	c9	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	b7	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
29	b9	202	PEB	C3D-C4D-ND	4.16	115.42	107.26
29	UF	201	PEB	OD-C4D-ND	-4.16	119.77	125.93
29	UI	201	PEB	OD-C4D-ND	-4.16	119.77	125.93
29	U7	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	f7	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	U9	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	f9	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	R7	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	R9	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	g7	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	g9	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	h7	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	h9	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	GF	1001	CYC	CHB-C4A-NA	-4.16	116.24	124.93
31	GI	1001	CYC	CHB-C4A-NA	-4.16	116.24	124.93
29	mF	202	PEB	OD-C4D-ND	-4.16	119.77	125.93
29	mI	202	PEB	OD-C4D-ND	-4.16	119.77	125.93
31	CF	1001	CYC	C4D-CHA-C1A	4.16	133.77	128.81
31	CI	1001	CYC	C4D-CHA-C1A	4.16	133.77	128.81
30	xL	305	PUB	C1D-CHC-C4C	-4.16	104.33	113.37
29	O7	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	S7	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	O9	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	S9	202	PEB	OA-C1A-C2A	-4.16	122.87	126.17
29	L8	202	PEB	CHB-C4B-NB	-4.16	123.06	128.83
29	V7	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	V9	201	PEB	CHC-C1D-ND	-4.16	109.12	113.95
29	RR	203	PEB	CAB-CBB-CGB	-4.15	104.66	113.60
29	LF	1002	PEB	CHB-C4B-NB	-4.15	123.06	128.83
29	LI	1002	PEB	CHB-C4B-NB	-4.15	123.06	128.83
29	wJ	302	PEB	CHA-C1B-NB	-4.15	116.24	124.93
29	HD	202	PEB	C1B-C2B-C3B	-4.15	101.74	106.51
29	i7	201	PEB	CHC-C1D-ND	-4.15	109.12	113.95
29	i9	201	PEB	CHC-C1D-ND	-4.15	109.12	113.95
31	F7	1001	CYC	C1B-NB-C4B	-4.15	105.38	110.67
29	U7	202	PEB	C3D-C4D-ND	4.15	115.41	107.26
29	U9	202	PEB	C3D-C4D-ND	4.15	115.41	107.26
29	B8	202	PEB	CHB-C4B-NB	-4.15	123.07	128.83
29	W7	202	PEB	OA-C1A-C2A	-4.15	122.87	126.17
29	W9	202	PEB	OA-C1A-C2A	-4.15	122.87	126.17
31	D7	1001	CYC	C1B-NB-C4B	-4.15	105.38	110.67
31	D9	1001	CYC	C1B-NB-C4B	-4.15	105.38	110.67
29	OF	203	PEB	OD-C4D-ND	-4.15	119.78	125.93
29	OI	203	PEB	OD-C4D-ND	-4.15	119.78	125.93
29	i1	202	PEB	C3D-C4D-ND	4.15	115.40	107.26
29	iK	202	PEB	C3D-C4D-ND	4.15	115.40	107.26
31	N7	1001	CYC	C1B-NB-C4B	-4.15	105.39	110.67
31	N9	1001	CYC	C1B-NB-C4B	-4.15	105.39	110.67
29	B5	202	PEB	CHB-C4B-NB	-4.15	123.07	128.83
30	AB	305	PUB	CHB-C1C-NC	-4.15	123.07	128.83
29	N1	1002	PEB	OA-C1A-C2A	-4.15	122.88	126.17
29	N3	203	PEB	CMB-C2B-C1B	4.15	131.45	125.06
29	Q7	202	PEB	OA-C1A-C2A	-4.15	122.88	126.17
29	Q9	202	PEB	OA-C1A-C2A	-4.15	122.88	126.17
29	AC	203	PEB	CHA-C1B-NB	-4.14	116.26	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AE	203	PEB	CHA-C1B-NB	-4.14	116.26	124.93
31	EF	1001	CYC	C4D-CHA-C1A	4.14	133.76	128.81
31	EI	1001	CYC	C4D-CHA-C1A	4.14	133.76	128.81
29	Z7	202	PEB	OA-C1A-C2A	-4.14	122.88	126.17
29	Z9	202	PEB	OA-C1A-C2A	-4.14	122.88	126.17
29	FF	1002	PEB	CHB-C4B-NB	-4.14	123.08	128.83
29	FI	1002	PEB	CHB-C4B-NB	-4.14	123.08	128.83
29	T7	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
29	T9	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
29	xJ	302	PEB	CHA-C1B-NB	-4.14	116.27	124.93
29	dF	201	PEB	OD-C4D-ND	-4.14	119.80	125.93
29	eF	202	PEB	OD-C4D-ND	-4.14	119.80	125.93
29	dI	201	PEB	OD-C4D-ND	-4.14	119.80	125.93
29	eI	202	PEB	OD-C4D-ND	-4.14	119.80	125.93
31	C7	1001	CYC	OC-C1C-C2C	-4.14	122.88	126.17
31	C9	1001	CYC	OC-C1C-C2C	-4.14	122.88	126.17
30	MN	402	PUB	C1C-C2C-C3C	-4.14	102.20	106.78
29	a1	202	PEB	C3D-C4D-ND	4.14	115.38	107.26
29	aK	202	PEB	C3D-C4D-ND	4.14	115.38	107.26
31	KF	1001	CYC	C4D-CHA-C1A	4.14	133.75	128.81
31	G7	1001	CYC	OC-C1C-C2C	-4.14	122.88	126.17
29	P2	202	PEB	CAB-CBB-CGB	-4.14	104.70	113.60
29	F4	202	PEB	C3B-C4B-NB	4.14	116.07	110.05
29	H1	1002	PEB	OA-C1A-C2A	-4.14	122.88	126.17
29	JC	202	PEB	OA-C1A-C2A	-4.14	122.88	126.17
29	JE	202	PEB	OA-C1A-C2A	-4.14	122.88	126.17
29	JD	202	PEB	C1B-C2B-C3B	-4.14	101.76	106.51
30	MA	402	PUB	C1C-C2C-C3C	-4.14	102.20	106.78
29	G5	202	PEB	CHB-C4B-NB	-4.14	123.09	128.83
29	G8	202	PEB	CHB-C4B-NB	-4.14	123.09	128.83
29	U1	201	PEB	C3D-C4D-ND	4.14	115.38	107.26
29	UK	201	PEB	C3D-C4D-ND	4.14	115.38	107.26
29	a7	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
29	e7	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
29	a9	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
29	e9	201	PEB	CHC-C1D-ND	-4.14	109.14	113.95
29	MA	401	PEB	C4B-C3B-C2B	-4.14	102.20	106.78
29	X2	202	PEB	C2A-C1A-NA	4.14	111.84	108.27
29	TR	203	PEB	CAB-CBB-CGB	-4.14	104.70	113.60
29	MA	401	PEB	C3B-C4B-NB	4.13	116.06	110.05
30	A7	303	PUB	C1C-C2C-C3C	-4.13	102.21	106.78
30	A9	303	PUB	C1C-C2C-C3C	-4.13	102.21	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	OR	202	PEB	C1C-CHB-C4B	-4.13	123.87	128.81
29	B4	202	PEB	C3B-C4B-NB	4.13	116.06	110.05
29	BD	202	PEB	C3B-C4B-NB	4.13	116.06	110.05
29	wL	302	PEB	CHA-C1B-NB	-4.13	116.28	124.93
31	CF	1001	CYC	CHB-C4A-NA	-4.13	116.28	124.93
31	CI	1001	CYC	CHB-C4A-NA	-4.13	116.28	124.93
29	H8	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	FC	203	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	FE	203	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	m7	201	PEB	CHC-C1D-ND	-4.13	109.15	113.95
29	m9	201	PEB	CHC-C1D-ND	-4.13	109.15	113.95
29	N2	203	PEB	CAB-CBB-CGB	-4.13	104.71	113.60
29	NR	203	PEB	CAB-CBB-CGB	-4.13	104.71	113.60
29	LC	202	PEB	CHA-C1B-NB	-4.13	116.29	124.93
29	LE	202	PEB	CHA-C1B-NB	-4.13	116.29	124.93
29	j7	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	j9	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
31	EF	1001	CYC	CHB-C4A-NA	-4.13	116.29	124.93
31	EI	1001	CYC	CHB-C4A-NA	-4.13	116.29	124.93
29	NF	1002	PEB	CHB-C4B-NB	-4.13	123.09	128.83
29	NI	1002	PEB	CHB-C4B-NB	-4.13	123.09	128.83
31	J7	1001	CYC	C1B-NB-C4B	-4.13	105.41	110.67
29	NO	203	PEB	CMB-C2B-C1B	4.13	131.43	125.06
31	H7	1001	CYC	C1B-NB-C4B	-4.13	105.41	110.67
31	H9	1001	CYC	C1B-NB-C4B	-4.13	105.41	110.67
29	YF	202	PEB	OD-C4D-ND	-4.13	119.81	125.93
29	YI	202	PEB	OD-C4D-ND	-4.13	119.81	125.93
29	J4	202	PEB	C1B-C2B-C3B	-4.13	101.77	106.51
29	e1	202	PEB	C3D-C4D-ND	4.13	115.36	107.26
29	eK	202	PEB	C3D-C4D-ND	4.13	115.36	107.26
31	GF	1001	CYC	C4D-CHA-C1A	4.13	133.74	128.81
31	GI	1001	CYC	C4D-CHA-C1A	4.13	133.74	128.81
29	P7	201	PEB	CHC-C1D-ND	-4.13	109.15	113.95
29	P9	201	PEB	CHC-C1D-ND	-4.13	109.15	113.95
31	KF	1001	CYC	CHB-C4A-NA	-4.13	116.30	124.93
29	T2	203	PEB	CAB-CBB-CGB	-4.13	104.72	113.60
29	KC	201	PEB	CHA-C1B-NB	-4.13	116.30	124.93
29	KE	201	PEB	CHA-C1B-NB	-4.13	116.30	124.93
29	b7	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	b9	202	PEB	OA-C1A-C2A	-4.13	122.89	126.17
31	G9	1001	CYC	OC-C1C-C2C	-4.13	122.89	126.17
31	IF	1001	CYC	CHB-C4A-NA	-4.13	116.30	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	II	1001	CYC	CHB-C4A-NA	-4.13	116.30	124.93
29	Y7	201	PEB	C3B-C4B-NB	4.13	116.05	110.05
29	Y9	201	PEB	C3B-C4B-NB	4.13	116.05	110.05
29	Z1	201	PEB	C3D-C4D-ND	4.13	115.35	107.26
29	ZK	201	PEB	C3D-C4D-ND	4.13	115.35	107.26
29	LC	203	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	LE	203	PEB	OA-C1A-C2A	-4.13	122.89	126.17
29	MN	401	PEB	C3B-C4B-NB	4.12	116.05	110.05
29	H4	202	PEB	C1B-C2B-C3B	-4.12	101.77	106.51
29	BD	202	PEB	C1B-C2B-C3B	-4.12	101.77	106.51
29	pJ	203	PEB	C3D-C4D-ND	4.12	115.35	107.26
29	pL	203	PEB	C3D-C4D-ND	4.12	115.35	107.26
29	c7	201	PEB	C3B-C4B-NB	4.12	116.05	110.05
29	c9	201	PEB	C3B-C4B-NB	4.12	116.05	110.05
29	DF	1002	PEB	CHB-C4B-NB	-4.12	123.11	128.83
29	DI	1002	PEB	CHB-C4B-NB	-4.12	123.11	128.83
29	j1	203	PEB	C3D-C4D-ND	4.12	115.35	107.26
29	jK	203	PEB	C3D-C4D-ND	4.12	115.35	107.26
29	B4	202	PEB	C1B-C2B-C3B	-4.12	101.78	106.51
29	HF	1002	PEB	CHB-C4B-NB	-4.12	123.11	128.83
29	HI	1002	PEB	CHB-C4B-NB	-4.12	123.11	128.83
31	L7	1001	CYC	C1B-NB-C4B	-4.12	105.42	110.67
29	WR	202	PEB	C2A-C1A-NA	4.12	111.83	108.27
29	c1	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	cK	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	A1	301	PEB	CHA-C1B-NB	-4.12	116.31	124.93
29	AK	301	PEB	CHA-C1B-NB	-4.12	116.31	124.93
31	MF	1001	CYC	CHB-C4A-NA	-4.12	116.32	124.93
31	MI	1001	CYC	CHB-C4A-NA	-4.12	116.32	124.93
29	L4	202	PEB	C3B-C4B-NB	4.12	116.04	110.05
29	P1	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	PK	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
31	KI	1001	CYC	CHB-C4A-NA	-4.12	116.32	124.93
29	FQ	203	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	R1	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	HJ	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	RK	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	HL	202	PEB	C3D-C4D-ND	4.12	115.34	107.26
29	V7	201	PEB	C3B-C4B-NB	4.12	116.04	110.05
29	V9	201	PEB	C3B-C4B-NB	4.12	116.04	110.05
29	LD	202	PEB	C3B-C4B-NB	4.12	116.04	110.05
29	V1	202	PEB	C3D-C4D-ND	4.12	115.33	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VK	202	PEB	C3D-C4D-ND	4.12	115.33	107.26
29	BC	202	PEB	CHA-C1B-NB	-4.12	116.32	124.93
29	BE	202	PEB	CHA-C1B-NB	-4.12	116.32	124.93
29	H8	202	PEB	CHB-C4B-NB	-4.12	123.12	128.83
29	k7	201	PEB	C3B-C4B-NB	4.12	116.03	110.05
29	k9	201	PEB	C3B-C4B-NB	4.12	116.03	110.05
29	AF	304	PEB	CHC-C1D-ND	-4.11	109.17	113.95
29	AI	304	PEB	CHC-C1D-ND	-4.11	109.17	113.95
29	kF	202	PEB	OD-C4D-ND	-4.11	119.83	125.93
29	kI	202	PEB	OD-C4D-ND	-4.11	119.83	125.93
29	HD	201	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	BJ	203	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	JJ	203	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	BL	203	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	JL	203	PEB	C3D-C4D-ND	4.11	115.33	107.26
31	IF	1001	CYC	C4D-CHA-C1A	4.11	133.72	128.81
31	II	1001	CYC	C4D-CHA-C1A	4.11	133.72	128.81
29	FC	202	PEB	CHA-C1B-NB	-4.11	116.33	124.93
29	FE	202	PEB	CHA-C1B-NB	-4.11	116.33	124.93
29	e7	201	PEB	C3B-C4B-NB	4.11	116.03	110.05
29	e9	201	PEB	C3B-C4B-NB	4.11	116.03	110.05
29	YF	203	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	YI	203	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	FD	202	PEB	C3B-C4B-NB	4.11	116.03	110.05
29	k1	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	XB	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	kK	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	XM	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	B4	201	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	g1	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	gK	202	PEB	C3D-C4D-ND	4.11	115.33	107.26
29	VF	202	PEB	OD-C4D-ND	-4.11	119.84	125.93
29	VI	202	PEB	OD-C4D-ND	-4.11	119.84	125.93
29	bJ	203	PEB	C3D-C4D-ND	4.11	115.32	107.26
29	bL	203	PEB	C3D-C4D-ND	4.11	115.32	107.26
29	iF	202	PEB	OD-C4D-ND	-4.11	119.84	125.93
29	iI	202	PEB	OD-C4D-ND	-4.11	119.84	125.93
30	AM	305	PUB	CHB-C1C-NC	-4.11	123.13	128.83
29	PJ	203	PEB	C3D-C4D-ND	4.11	115.32	107.26
29	PL	203	PEB	C3D-C4D-ND	4.11	115.32	107.26
31	MF	1001	CYC	C4D-CHA-C1A	4.11	133.72	128.81
31	MI	1001	CYC	C4D-CHA-C1A	4.11	133.72	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L4	202	PEB	C1B-C2B-C3B	-4.11	101.79	106.51
29	P7	201	PEB	C3B-C4B-NB	4.11	116.03	110.05
29	P9	201	PEB	C3B-C4B-NB	4.11	116.03	110.05
29	m7	201	PEB	C3B-C4B-NB	4.11	116.02	110.05
29	m9	201	PEB	C3B-C4B-NB	4.11	116.02	110.05
29	H5	202	PEB	CHB-C4B-NB	-4.11	123.13	128.83
29	F5	202	PEB	CHB-C4B-NB	-4.11	123.13	128.83
29	F8	202	PEB	CHB-C4B-NB	-4.11	123.13	128.83
29	R7	201	PEB	C3B-C4B-NB	4.11	116.02	110.05
29	R9	201	PEB	C3B-C4B-NB	4.11	116.02	110.05
29	D4	201	PEB	C3D-C4D-ND	4.11	115.31	107.26
29	F4	201	PEB	C3D-C4D-ND	4.11	115.31	107.26
29	rJ	203	PEB	C3D-C4D-ND	4.11	115.31	107.26
29	rL	203	PEB	C3D-C4D-ND	4.11	115.31	107.26
31	E7	1001	CYC	OC-C1C-C2C	-4.11	122.91	126.17
31	E9	1001	CYC	OC-C1C-C2C	-4.11	122.91	126.17
29	FD	201	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	O2	202	PEB	C2A-C1A-NA	4.10	111.81	108.27
29	kF	201	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	kI	201	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	F4	202	PEB	C1B-C2B-C3B	-4.10	101.80	106.51
29	DJ	202	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	IJ	203	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	DL	202	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	IL	203	PEB	C3D-C4D-ND	4.10	115.31	107.26
29	RJ	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	RL	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	D4	202	PEB	C3B-C4B-NB	4.10	116.01	110.05
29	nJ	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	nL	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	H4	201	PEB	C1B-C2B-C3B	-4.10	101.80	106.51
29	DD	202	PEB	C3B-C4B-NB	4.10	116.01	110.05
29	J4	201	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	FG	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	HC	202	PEB	CHA-C1B-NB	-4.10	116.36	124.93
29	HE	202	PEB	CHA-C1B-NB	-4.10	116.36	124.93
29	xJ	301	PEB	C1B-C2B-C3B	-4.10	101.80	106.51
29	B3	202	PEB	CHB-C4B-NB	-4.10	123.14	128.83
29	BO	202	PEB	CHB-C4B-NB	-4.10	123.14	128.83
29	LJ	202	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	VJ	202	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	LL	202	PEB	C3D-C4D-ND	4.10	115.30	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VL	202	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	FJ	201	PEB	CHC-C4C-C3C	-4.10	123.35	130.34
29	FL	201	PEB	CHC-C4C-C3C	-4.10	123.35	130.34
29	fJ	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	fL	203	PEB	C3D-C4D-ND	4.10	115.30	107.26
29	W2	202	PEB	C2A-C1A-NA	4.10	111.80	108.27
30	A1	304	PUB	CMA-C2A-C1A	4.10	131.02	121.39
30	AK	304	PUB	CMA-C2A-C1A	4.10	131.02	121.39
29	G4	201	PEB	CHB-C4B-NB	-4.10	123.15	128.83
29	H4	201	PEB	C3D-C4D-ND	4.10	115.29	107.26
29	RB	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	eF	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	eI	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	RM	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	PJ	201	PEB	CHC-C4C-C3C	-4.09	123.35	130.34
29	PL	201	PEB	CHC-C4C-C3C	-4.09	123.35	130.34
31	yP	1001	CYC	CAB-C3B-C4B	4.09	127.84	121.38
29	J3	202	PEB	CHB-C4B-NB	-4.09	123.15	128.83
29	JO	202	PEB	CHB-C4B-NB	-4.09	123.15	128.83
29	ZJ	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	ZL	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	BQ	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	NJ	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	NL	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	VJ	201	PEB	OA-C1A-NA	4.09	129.90	124.94
29	VL	201	PEB	OA-C1A-NA	4.09	129.90	124.94
29	B5	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	HK	1002	PEB	OA-C1A-C2A	-4.09	122.92	126.17
29	FD	202	PEB	C1B-C2B-C3B	-4.09	101.81	106.51
29	a7	201	PEB	C3B-C4B-NB	4.09	116.00	110.05
29	a9	201	PEB	C3B-C4B-NB	4.09	116.00	110.05
29	DA	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	BD	201	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	FJ	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	FL	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	DN	203	PEB	C3D-C4D-ND	4.09	115.29	107.26
29	T7	201	PEB	C3B-C4B-NB	4.09	116.00	110.05
29	T9	201	PEB	C3B-C4B-NB	4.09	116.00	110.05
29	RJ	201	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
29	RL	201	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
29	TB	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	DD	201	PEB	C3D-C4D-ND	4.09	115.28	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	TM	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	I3	203	PEB	CHB-C4B-NB	-4.09	123.15	128.83
29	IO	203	PEB	CHB-C4B-NB	-4.09	123.15	128.83
31	I7	1001	CYC	OC-C1C-C2C	-4.09	122.92	126.17
31	I9	1001	CYC	OC-C1C-C2C	-4.09	122.92	126.17
31	L9	1001	CYC	C1B-NB-C4B	-4.09	105.46	110.67
29	H3	202	PEB	CHB-C4B-NB	-4.09	123.15	128.83
29	HO	202	PEB	CHB-C4B-NB	-4.09	123.15	128.83
29	tJ	201	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
29	tL	201	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
29	AM	303	PEB	OA-C1A-C2A	-4.09	122.92	126.17
29	Y7	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	Y9	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	PB	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	TJ	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	TL	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	PM	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	vJ	201	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
29	vL	201	PEB	CHC-C4C-C3C	-4.09	123.36	130.34
29	iB	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	PF	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	PI	201	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	iM	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
30	AB	304	PUB	C1C-C2C-C3C	-4.09	102.26	106.78
29	kB	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	aF	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	aI	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	kM	203	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	JD	202	PEB	C3B-C4B-NB	4.09	116.00	110.05
29	F3	202	PEB	CHB-C4B-NB	-4.09	123.16	128.83
29	FO	202	PEB	CHB-C4B-NB	-4.09	123.16	128.83
29	NB	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	NM	202	PEB	C3D-C4D-ND	4.09	115.28	107.26
29	GD	201	PEB	CHB-C4B-NB	-4.09	123.16	128.83
29	g7	201	PEB	C3B-C4B-NB	4.09	115.99	110.05
29	g9	201	PEB	C3B-C4B-NB	4.09	115.99	110.05
31	K9	1001	CYC	OC-C1C-C2C	-4.08	122.92	126.17
29	ZJ	201	PEB	OA-C1A-NA	4.08	129.89	124.94
29	ZL	201	PEB	OA-C1A-NA	4.08	129.89	124.94
29	HD	201	PEB	C1B-C2B-C3B	-4.08	101.82	106.51
29	aF	202	PEB	OD-C4D-ND	-4.08	119.88	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aI	202	PEB	OD-C4D-ND	-4.08	119.88	125.93
29	hJ	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	hL	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	LD	201	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	dJ	201	PEB	OA-C1A-NA	4.08	129.89	124.94
29	dL	201	PEB	OA-C1A-NA	4.08	129.89	124.94
29	eF	201	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	eI	201	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	tJ	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	tL	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	LD	202	PEB	C1B-C2B-C3B	-4.08	101.82	106.51
29	BA	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	kF	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	kI	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	BN	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	DJ	201	PEB	CHC-C4C-C3C	-4.08	123.37	130.34
29	DL	201	PEB	CHC-C4C-C3C	-4.08	123.37	130.34
29	NJ	201	PEB	OA-C1A-NA	4.08	129.89	124.94
29	NL	201	PEB	OA-C1A-NA	4.08	129.89	124.94
29	mB	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	iF	201	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	iI	201	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	mM	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	FB	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	cB	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	JG	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	vJ	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	vL	202	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	FM	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	cM	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	MN	401	PEB	C4B-C3B-C2B	-4.08	102.27	106.78
29	IJ	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	IL	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	JF	1002	PEB	OA-C1A-C2A	-4.08	122.93	126.17
29	JI	1002	PEB	OA-C1A-C2A	-4.08	122.93	126.17
29	T7	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	T9	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	dJ	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	dL	203	PEB	C3D-C4D-ND	4.08	115.27	107.26
29	L4	201	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	PF	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	PI	203	PEB	C3D-C4D-ND	4.08	115.26	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	fJ	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	fL	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	gF	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	gI	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	JD	201	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	mF	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	mI	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	m7	203	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	m9	203	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	nJ	201	PEB	OA-C1A-NA	4.08	129.88	124.94
29	nL	201	PEB	OA-C1A-NA	4.08	129.88	124.94
29	O7	201	PEB	C1B-C2B-C3B	-4.08	101.83	106.51
29	O9	201	PEB	C1B-C2B-C3B	-4.08	101.83	106.51
29	TF	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	TI	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	i7	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	i9	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	NJ	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	jJ	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	NL	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	jL	201	PEB	CHC-C4C-C3C	-4.08	123.38	130.34
29	hJ	201	PEB	OA-C1A-NA	4.08	129.88	124.94
29	hL	201	PEB	OA-C1A-NA	4.08	129.88	124.94
29	m7	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	m9	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	JB	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	LB	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	JM	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	LM	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	ZB	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	cF	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	cI	202	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	ZM	203	PEB	C3D-C4D-ND	4.08	115.26	107.26
29	gF	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	gI	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	rJ	201	PEB	OA-C1A-NA	4.07	129.88	124.94
29	rL	201	PEB	OA-C1A-NA	4.07	129.88	124.94
29	FF	1002	PEB	OA-C1A-C2A	-4.07	122.93	126.17
29	FI	1002	PEB	OA-C1A-C2A	-4.07	122.93	126.17
30	yJ	302	PUB	CMA-C2A-C1A	4.07	130.97	121.39
30	yL	302	PUB	CMA-C2A-C1A	4.07	130.97	121.39
29	h1	201	PEB	C3D-C4D-ND	4.07	115.25	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a7	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	a9	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	LA	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	hK	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	LN	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	R7	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	R9	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	bJ	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	pJ	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	bL	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	pL	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	yJ	301	PEB	OA-C1A-C2A	-4.07	122.94	126.17
29	yL	301	PEB	OA-C1A-C2A	-4.07	122.94	126.17
29	JA	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	VF	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	YF	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	VI	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	YI	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	XJ	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	XL	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	JN	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	RR	201	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
29	ZJ	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	ZL	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	M3	203	PEB	CMB-C2B-C1B	4.07	131.33	125.06
29	MO	203	PEB	CMB-C2B-C1B	4.07	131.33	125.06
29	DB	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	RF	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	aF	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	LG	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	RI	202	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	aI	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	DM	203	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	bJ	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	bL	201	PEB	OA-C1A-NA	4.07	129.87	124.94
30	AM	304	PUB	C1C-C2C-C3C	-4.07	102.28	106.78
29	VF	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	VI	201	PEB	C3D-C4D-ND	4.07	115.25	107.26
29	TJ	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	TL	201	PEB	CHC-C4C-C3C	-4.07	123.39	130.34
29	b1	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	eB	202	PEB	C3D-C4D-ND	4.07	115.24	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	bK	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	eM	202	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	e7	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	e9	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	NR	202	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	G5	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	B8	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	HA	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	HN	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	FA	202	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
29	FN	202	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
29	TR	201	PEB	C4B-C3B-C2B	-4.07	102.28	106.78
29	K4	201	PEB	CHB-C4B-NB	-4.07	123.18	128.83
29	N3	203	PEB	C1C-CHB-C4B	4.07	133.67	128.81
29	J4	202	PEB	C3B-C4B-NB	4.07	115.97	110.05
29	JJ	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	JL	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	Q1	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	HB	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	gB	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	cF	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	cI	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	QK	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	HM	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	gM	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	KC	201	PEB	OA-C1A-C2A	-4.07	122.94	126.17
29	KE	201	PEB	OA-C1A-C2A	-4.07	122.94	126.17
29	I4	201	PEB	CHB-C4B-NB	-4.07	123.19	128.83
29	E3	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	EO	201	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	xL	301	PEB	C1B-C2B-C3B	-4.07	101.84	106.51
29	GA	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
29	GN	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
29	JJ	201	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
29	JL	201	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
29	RJ	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	RL	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	B4	201	PEB	C1B-C2B-C3B	-4.07	101.84	106.51
29	dJ	201	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
29	dL	201	PEB	CHC-C4C-C3C	-4.07	123.40	130.34
29	L8	201	PEB	OA-C1A-C2A	-4.07	122.94	126.17
29	MN	405	PEB	OA-C1A-C2A	-4.07	122.94	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C4	201	PEB	CHB-C4B-NB	-4.07	123.19	128.83
29	VB	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	VM	203	PEB	C3D-C4D-ND	4.07	115.24	107.26
29	S1	201	PEB	C3D-C4D-ND	4.07	115.23	107.26
29	U1	202	PEB	C3D-C4D-ND	4.07	115.23	107.26
29	SK	201	PEB	C3D-C4D-ND	4.07	115.23	107.26
29	UK	202	PEB	C3D-C4D-ND	4.07	115.23	107.26
29	A3	201	PEB	CHA-C1B-NB	-4.07	116.43	124.93
29	AO	201	PEB	CHA-C1B-NB	-4.07	116.43	124.93
29	BJ	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	BL	201	PEB	OA-C1A-NA	4.07	129.87	124.94
29	i7	201	PEB	C3B-C4B-NB	4.06	115.96	110.05
29	i9	201	PEB	C3B-C4B-NB	4.06	115.96	110.05
29	k7	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	k9	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	FA	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	FN	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	P7	203	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	P9	203	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	hJ	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	hL	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	RF	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	RI	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	jJ	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	jL	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	E4	201	PEB	CHB-C4B-NB	-4.06	123.19	128.83
29	DQ	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	AC	201	PEB	OA-C1A-C2A	-4.06	122.94	126.17
29	AE	201	PEB	OA-C1A-C2A	-4.06	122.94	126.17
30	MA	403	PUB	CMA-C2A-C1A	4.06	130.95	121.39
29	nJ	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	nL	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	O1	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	AF	304	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	AI	304	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	OK	201	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	I3	201	PEB	CHA-C1B-NB	-4.06	116.43	124.93
29	IO	201	PEB	CHA-C1B-NB	-4.06	116.43	124.93
29	H4	202	PEB	C3B-C4B-NB	4.06	115.96	110.05
29	P7	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	P9	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	DG	203	PEB	C3D-C4D-ND	4.06	115.23	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GC	201	PEB	OA-C1A-C2A	-4.06	122.94	126.17
29	GE	201	PEB	OA-C1A-C2A	-4.06	122.94	126.17
29	m1	201	PEB	CHA-C1B-NB	-4.06	116.44	124.93
29	mK	201	PEB	CHA-C1B-NB	-4.06	116.44	124.93
29	BJ	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	BL	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	HG	203	PEB	C3D-C4D-ND	4.06	115.23	107.26
29	Z1	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	BB	301	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	ZK	202	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	BM	301	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	MD	201	PEB	CHB-C4B-NB	-4.06	123.19	128.83
29	AB	303	PEB	OA-C1A-C2A	-4.06	122.94	126.17
31	VP	1001	CYC	C2C-C3C-C4C	4.06	107.42	101.34
29	lJ	201	PEB	OA-C1A-NA	4.06	129.86	124.94
29	lL	201	PEB	OA-C1A-NA	4.06	129.86	124.94
29	d1	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	dK	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	XJ	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	rJ	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	XL	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	rL	201	PEB	CHC-C4C-C3C	-4.06	123.41	130.34
29	V2	201	PEB	C4B-C3B-C2B	-4.06	102.29	106.78
29	A1	303	PEB	OA-C1A-C2A	-4.06	122.95	126.17
29	AK	303	PEB	OA-C1A-C2A	-4.06	122.95	126.17
29	G8	203	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	P1	201	PEB	CHA-C1B-NB	-4.06	116.44	124.93
29	PK	201	PEB	CHA-C1B-NB	-4.06	116.44	124.93
29	XR	201	PEB	C4B-C3B-C2B	-4.06	102.29	106.78
30	MN	403	PUB	CMA-C2A-C1A	4.06	130.94	121.39
29	V7	203	PEB	CHC-C4C-C3C	-4.06	123.42	130.34
29	V9	203	PEB	CHC-C4C-C3C	-4.06	123.42	130.34
29	J4	201	PEB	C1B-C2B-C3B	-4.06	101.85	106.51
29	LJ	201	PEB	CHC-C4C-C3C	-4.06	123.42	130.34
29	LL	201	PEB	CHC-C4C-C3C	-4.06	123.42	130.34
29	TI	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	Y1	201	PEB	CHA-C1B-NB	-4.06	116.45	124.93
29	YK	201	PEB	CHA-C1B-NB	-4.06	116.45	124.93
29	l1	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	lK	201	PEB	C3D-C4D-ND	4.06	115.22	107.26
29	M3	203	PEB	C1C-CHB-C4B	4.06	133.65	128.81
29	MO	203	PEB	C1C-CHB-C4B	4.06	133.65	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HA	202	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	HN	202	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	FD	201	PEB	C1B-C2B-C3B	-4.05	101.85	106.51
29	F5	203	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	F8	203	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	KD	201	PEB	CHB-C4B-NB	-4.05	123.20	128.83
29	W1	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	f1	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	WK	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	fK	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	TJ	201	PEB	OA-C1A-NA	4.05	129.85	124.94
29	TL	201	PEB	OA-C1A-NA	4.05	129.85	124.94
29	DA	202	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	DN	202	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	i1	201	PEB	CHA-C1B-NB	-4.05	116.45	124.93
29	iK	201	PEB	CHA-C1B-NB	-4.05	116.45	124.93
29	Y7	203	PEB	CHC-C4C-C3C	-4.05	123.42	130.34
29	Y9	203	PEB	CHC-C4C-C3C	-4.05	123.42	130.34
29	R7	203	PEB	CHC-C4C-C3C	-4.05	123.42	130.34
29	R9	203	PEB	CHC-C4C-C3C	-4.05	123.42	130.34
29	tJ	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	tL	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	T2	201	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	V7	203	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	V9	203	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	LJ	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	LL	201	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	pJ	201	PEB	OA-C1A-NA	4.05	129.85	124.94
29	pL	201	PEB	OA-C1A-NA	4.05	129.85	124.94
29	c1	201	PEB	CHA-C1B-NB	-4.05	116.46	124.93
29	cK	201	PEB	CHA-C1B-NB	-4.05	116.46	124.93
29	M4	201	PEB	CHB-C4B-NB	-4.05	123.21	128.83
29	F4	201	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
29	YF	202	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	gF	202	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	YI	202	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	gI	202	PEB	C3D-C4D-ND	4.05	115.21	107.26
29	iF	203	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	mF	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	iI	203	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	mI	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	g1	201	PEB	CHA-C1B-NB	-4.05	116.46	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	gK	201	PEB	CHA-C1B-NB	-4.05	116.46	124.93
29	JD	201	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
29	k1	201	PEB	CHA-C1B-NB	-4.05	116.46	124.93
29	kK	201	PEB	CHA-C1B-NB	-4.05	116.46	124.93
29	FJ	201	PEB	OA-C1A-NA	4.05	129.85	124.94
29	FL	201	PEB	OA-C1A-NA	4.05	129.85	124.94
29	I3	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	IO	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	c7	203	PEB	CHC-C4C-C3C	-4.05	123.43	130.34
29	i7	203	PEB	CHC-C4C-C3C	-4.05	123.43	130.34
29	c9	203	PEB	CHC-C4C-C3C	-4.05	123.43	130.34
29	i9	203	PEB	CHC-C4C-C3C	-4.05	123.43	130.34
29	j1	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	jK	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	U7	201	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
29	U9	201	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
29	P2	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	V2	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	c7	203	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	c9	203	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	K5	203	PEB	CHB-C4B-NB	-4.05	123.21	128.83
29	K8	203	PEB	CHB-C4B-NB	-4.05	123.21	128.83
29	jJ	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	jL	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	LF	1002	PEB	OA-C1A-C2A	-4.05	122.95	126.17
29	LI	1002	PEB	OA-C1A-C2A	-4.05	122.95	126.17
29	W7	201	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
29	W9	201	PEB	C1B-C2B-C3B	-4.05	101.86	106.51
29	MQ	403	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	OF	203	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	OI	203	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	N2	201	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	NR	201	PEB	C4B-C3B-C2B	-4.05	102.30	106.78
29	SR	202	PEB	C2A-C1A-NA	4.05	111.76	108.27
29	I5	203	PEB	CHB-C4B-NB	-4.05	123.22	128.83
29	I8	203	PEB	CHB-C4B-NB	-4.05	123.22	128.83
29	VJ	201	PEB	CHC-C4C-C3C	-4.05	123.44	130.34
29	VL	201	PEB	CHC-C4C-C3C	-4.05	123.44	130.34
29	dF	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	eF	202	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	dI	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	eI	202	PEB	C3D-C4D-ND	4.05	115.20	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	lJ	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	lL	201	PEB	C3D-C4D-ND	4.05	115.20	107.26
29	G3	201	PEB	CHA-C1B-NB	-4.05	116.47	124.93
29	GO	201	PEB	CHA-C1B-NB	-4.05	116.47	124.93
29	dD	401	PEB	CHB-C4B-NB	-4.04	123.22	128.83
29	D4	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	Q7	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	b7	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	j7	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	Q9	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	b9	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	j9	201	PEB	C1B-C2B-C3B	-4.04	101.86	106.51
29	g7	203	PEB	CHC-C4C-C3C	-4.04	123.44	130.34
29	g9	203	PEB	CHC-C4C-C3C	-4.04	123.44	130.34
29	mF	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	mI	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	L5	203	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	NJ	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	NL	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	HQ	203	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	N2	202	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	L8	203	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	e7	203	PEB	CHC-C4C-C3C	-4.04	123.44	130.34
29	e9	203	PEB	CHC-C4C-C3C	-4.04	123.44	130.34
31	xP	1001	CYC	C2C-C3C-C4C	4.04	107.39	101.34
29	DJ	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	DL	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	C3	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	CO	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	BA	202	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	BN	202	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	VR	201	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	K3	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	KO	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	R2	201	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	vJ	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	vL	201	PEB	C3D-C4D-ND	4.04	115.19	107.26
29	LD	201	PEB	C1B-C2B-C3B	-4.04	101.87	106.51
29	e1	201	PEB	CHA-C1B-NB	-4.04	116.48	124.93
29	eK	201	PEB	CHA-C1B-NB	-4.04	116.48	124.93
29	e2	402	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	HD	202	PEB	C3B-C4B-NB	4.04	115.92	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T1	201	PEB	CHA-C1B-NB	-4.04	116.49	124.93
29	TK	201	PEB	CHA-C1B-NB	-4.04	116.49	124.93
29	PF	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	PI	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	wL	303	PEB	C1B-C2B-C3B	-4.04	101.87	106.51
29	KA	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
29	KN	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
30	A7	303	PUB	CMA-C2A-C1A	4.04	130.89	121.39
30	A9	303	PUB	CMA-C2A-C1A	4.04	130.89	121.39
29	XR	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	LA	202	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	LN	202	PEB	C4B-C3B-C2B	-4.04	102.31	106.78
29	DJ	201	PEB	OA-C1A-NA	4.04	129.83	124.94
29	LJ	201	PEB	OA-C1A-NA	4.04	129.83	124.94
29	DL	201	PEB	OA-C1A-NA	4.04	129.83	124.94
29	LL	201	PEB	OA-C1A-NA	4.04	129.83	124.94
31	WP	1001	CYC	CAB-C3B-C4B	4.04	127.75	121.38
29	wJ	303	PEB	C1B-C2B-C3B	-4.04	101.87	106.51
29	H5	203	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	UF	201	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	UI	201	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	VR	202	PEB	C3D-C4D-ND	4.04	115.18	107.26
29	C5	203	PEB	CHB-C4B-NB	-4.04	123.23	128.83
29	vJ	201	PEB	OA-C1A-NA	4.04	129.83	124.94
29	vL	201	PEB	OA-C1A-NA	4.04	129.83	124.94
29	R1	201	PEB	CHA-C1B-NB	-4.04	116.49	124.93
29	RK	201	PEB	CHA-C1B-NB	-4.04	116.49	124.93
29	T7	203	PEB	CHC-C4C-C3C	-4.04	123.45	130.34
29	T9	203	PEB	CHC-C4C-C3C	-4.04	123.45	130.34
29	S7	201	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
29	S9	201	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
29	TJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	nJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	TL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	nL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	JA	202	PEB	C4B-C3B-C2B	-4.03	102.32	106.78
29	JN	202	PEB	C4B-C3B-C2B	-4.03	102.32	106.78
29	CD	201	PEB	CHB-C4B-NB	-4.03	123.23	128.83
29	g7	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	g9	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	JJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	bJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	bL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	Q2	202	PEB	C2A-C1A-NA	4.03	111.75	108.27
29	EA	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
29	EN	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
29	M3	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	iF	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	iI	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	RJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	RL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	MO	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	JQ	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	H8	203	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	FJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	FL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	LQ	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	IC	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
29	IE	201	PEB	OA-C1A-C2A	-4.03	122.97	126.17
29	A3	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	AO	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	PJ	201	PEB	OA-C1A-NA	4.03	129.82	124.94
29	PL	201	PEB	OA-C1A-NA	4.03	129.82	124.94
29	V1	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	VK	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	NO	203	PEB	C1C-CHB-C4B	4.03	133.62	128.81
29	h7	201	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
29	h9	201	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
29	VF	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	VI	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	dJ	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	dL	201	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	kF	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	kI	202	PEB	C3D-C4D-ND	4.03	115.17	107.26
29	AA	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
29	AN	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
29	C3	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	K3	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	CO	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	KO	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	DD	201	PEB	C1B-C2B-C3B	-4.03	101.88	106.51
29	a1	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93
29	aK	201	PEB	CHA-C1B-NB	-4.03	116.50	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X2	201	PEB	C3D-C4D-ND	4.03	115.16	107.26
29	M2	202	PEB	CHC-C4C-C3C	-4.03	123.47	130.34
29	LC	202	PEB	OA-C1A-C2A	-4.03	122.97	126.17
29	LE	202	PEB	OA-C1A-C2A	-4.03	122.97	126.17
29	G3	201	PEB	C3D-C4D-ND	4.03	115.16	107.26
29	GO	201	PEB	C3D-C4D-ND	4.03	115.16	107.26
29	G5	201	PEB	CHC-C4C-C3C	-4.03	123.47	130.34
29	a7	203	PEB	CHC-C4C-C3C	-4.03	123.47	130.34
29	a9	203	PEB	CHC-C4C-C3C	-4.03	123.47	130.34
29	XJ	201	PEB	OA-C1A-NA	4.03	129.82	124.94
29	XL	201	PEB	OA-C1A-NA	4.03	129.82	124.94
29	IA	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
29	IN	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
29	fJ	201	PEB	OA-C1A-NA	4.03	129.82	124.94
29	fL	201	PEB	OA-C1A-NA	4.03	129.82	124.94
29	jJ	201	PEB	OA-C1A-NA	4.02	129.82	124.94
29	jL	201	PEB	OA-C1A-NA	4.02	129.82	124.94
29	ZJ	201	PEB	C3D-C4D-ND	4.02	115.16	107.26
29	ZL	201	PEB	C3D-C4D-ND	4.02	115.16	107.26
29	XJ	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	fJ	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	XL	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	fL	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	EC	201	PEB	OA-C1A-C2A	-4.02	122.97	126.17
29	EE	201	PEB	OA-C1A-C2A	-4.02	122.97	126.17
29	pJ	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	pL	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	M2	202	PEB	C2A-C1A-NA	4.02	111.74	108.27
29	l7	201	PEB	C1B-C2B-C3B	-4.02	101.89	106.51
29	l9	201	PEB	C1B-C2B-C3B	-4.02	101.89	106.51
29	BJ	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	BL	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	WF	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	WI	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	L4	201	PEB	C1B-C2B-C3B	-4.02	101.89	106.51
29	hJ	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	rJ	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	hL	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	rL	201	PEB	C3D-C4D-ND	4.02	115.15	107.26
29	jF	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	jI	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	E3	201	PEB	CHA-C1B-NB	-4.02	116.52	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EO	201	PEB	CHA-C1B-NB	-4.02	116.52	124.93
29	Z7	201	PEB	C1B-C2B-C3B	-4.02	101.89	106.51
29	Z9	201	PEB	C1B-C2B-C3B	-4.02	101.89	106.51
29	I5	203	PEB	CHC-C1D-ND	-4.02	109.28	113.95
29	I8	203	PEB	CHC-C1D-ND	-4.02	109.28	113.95
29	KC	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
29	KE	202	PEB	OA-C1A-C2A	-4.02	122.98	126.17
29	DF	1002	PEB	OA-C1A-C2A	-4.02	122.98	126.17
29	DI	1002	PEB	OA-C1A-C2A	-4.02	122.98	126.17
29	SF	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	IF	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	SI	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	II	202	PEB	CHB-C4B-NB	-4.02	123.25	128.83
29	A7	305	PEB	CMB-C2B-C1B	4.02	131.25	125.06
29	A9	305	PEB	CMB-C2B-C1B	4.02	131.25	125.06
29	W2	202	PEB	CHC-C4C-C3C	-4.02	123.48	130.34
29	k7	203	PEB	CHC-C4C-C3C	-4.02	123.48	130.34
29	k9	203	PEB	CHC-C4C-C3C	-4.02	123.48	130.34
29	PR	201	PEB	C3D-C4D-ND	4.02	115.14	107.26
29	FA	203	PEB	CMB-C2B-C1B	4.02	131.25	125.06
29	FN	203	PEB	CMB-C2B-C1B	4.02	131.25	125.06
29	K5	203	PEB	CHC-C1D-ND	-4.02	109.28	113.95
29	H3	203	PEB	C3D-C4D-ND	4.02	115.14	107.26
29	HO	203	PEB	C3D-C4D-ND	4.02	115.14	107.26
29	WR	202	PEB	CHC-C4C-C3C	-4.02	123.49	130.34
30	AF	303	PUB	CHC-C1D-ND	-4.02	108.64	113.72
30	AI	303	PUB	CHC-C1D-ND	-4.02	108.64	113.72
29	O2	202	PEB	CHC-C4C-C3C	-4.02	123.49	130.34
30	BB	302	PUB	CHA-C1B-C2B	-4.02	123.49	130.34
30	BM	302	PUB	CHA-C1B-C2B	-4.02	123.49	130.34
29	wJ	301	PEB	C1B-C2B-C3B	-4.01	101.90	106.51
29	S2	202	PEB	C2A-C1A-NA	4.01	111.73	108.27
29	ID	201	PEB	CHB-C4B-NB	-4.01	123.26	128.83
30	yL	303	PUB	C1C-C2C-C3C	-4.01	102.34	106.78
29	AC	201	PEB	CHC-C1D-ND	-4.01	109.29	113.95
29	AE	201	PEB	CHC-C1D-ND	-4.01	109.29	113.95
29	VJ	201	PEB	C3D-C4D-ND	4.01	115.13	107.26
29	VL	201	PEB	C3D-C4D-ND	4.01	115.13	107.26
29	CC	201	PEB	OA-C1A-C2A	-4.01	122.98	126.17
29	CE	201	PEB	OA-C1A-C2A	-4.01	122.98	126.17
30	A1	305	PUB	CMA-C2A-C1A	4.01	130.83	121.39
30	AK	305	PUB	CMA-C2A-C1A	4.01	130.83	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aF	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
29	MG	401	PEB	C3D-C4D-ND	4.01	115.13	107.26
29	aI	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
29	C5	203	PEB	CHC-C1D-ND	-4.01	109.29	113.95
29	RR	202	PEB	C3D-C4D-ND	4.01	115.13	107.26
29	Q2	202	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
29	tJ	201	PEB	OA-C1A-NA	4.01	129.80	124.94
29	tL	201	PEB	OA-C1A-NA	4.01	129.80	124.94
29	f7	201	PEB	C1B-C2B-C3B	-4.01	101.90	106.51
29	f9	201	PEB	C1B-C2B-C3B	-4.01	101.90	106.51
29	C8	203	PEB	CHB-C4B-NB	-4.01	123.27	128.83
29	TR	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	PJ	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	PL	201	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	fF	202	PEB	CHB-C4B-NB	-4.01	123.27	128.83
29	fI	202	PEB	CHB-C4B-NB	-4.01	123.27	128.83
29	MA	404	PEB	C1B-C2B-C3B	-4.01	101.91	106.51
29	QR	202	PEB	C2A-C1A-NA	4.01	111.73	108.27
31	D7	1001	CYC	C4D-CHA-C1A	4.01	133.59	128.81
31	D9	1001	CYC	C4D-CHA-C1A	4.01	133.59	128.81
29	G8	201	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
29	LC	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	LE	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	B8	201	PEB	CHC-C4C-C3C	-4.01	123.50	130.34
29	T2	202	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	M3	201	PEB	C1B-C2B-C3B	-4.01	101.91	106.51
29	d7	201	PEB	C1B-C2B-C3B	-4.01	101.91	106.51
29	d9	201	PEB	C1B-C2B-C3B	-4.01	101.91	106.51
29	MO	201	PEB	C1B-C2B-C3B	-4.01	101.91	106.51
29	N3	203	PEB	C3D-C4D-ND	4.01	115.12	107.26
29	U2	202	PEB	CHC-C4C-C3C	-4.00	123.51	130.34
29	LC	203	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	LE	203	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	F8	201	PEB	CHC-C4C-C3C	-4.00	123.51	130.34
30	A7	303	PUB	CHA-C1B-C2B	-4.00	123.51	130.34
30	A9	303	PUB	CHA-C1B-C2B	-4.00	123.51	130.34
29	A5	203	PEB	CHC-C1D-ND	-4.00	109.30	113.95
29	xJ	303	PEB	C1B-C2B-C3B	-4.00	101.91	106.51
29	wL	301	PEB	C1B-C2B-C3B	-4.00	101.91	106.51
29	xL	303	PEB	C1B-C2B-C3B	-4.00	101.92	106.51
29	F5	201	PEB	CHC-C4C-C3C	-4.00	123.52	130.34
29	BC	202	PEB	C3D-C4D-ND	4.00	115.11	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BE	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	B5	201	PEB	CHC-C4C-C3C	-4.00	123.52	130.34
29	L3	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	HC	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	HE	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	LO	202	PEB	C3D-C4D-ND	4.00	115.11	107.26
29	OF	202	PEB	CHB-C4B-NB	-4.00	123.28	128.83
29	OI	202	PEB	CHB-C4B-NB	-4.00	123.28	128.83
29	NR	203	PEB	CHB-C4B-NB	-4.00	123.28	128.83
29	FC	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
29	FE	201	PEB	OA-C1A-C2A	-4.00	122.99	126.17
29	JA	203	PEB	CMB-C2B-C1B	4.00	131.22	125.06
29	JN	203	PEB	CMB-C2B-C1B	4.00	131.22	125.06
29	R2	202	PEB	C3D-C4D-ND	4.00	115.10	107.26
29	NF	1002	PEB	OA-C1A-C2A	-4.00	123.00	126.17
29	NI	1002	PEB	OA-C1A-C2A	-4.00	123.00	126.17
29	OF	203	PEB	C4B-C3B-C2B	-4.00	102.36	106.78
29	OI	203	PEB	C4B-C3B-C2B	-4.00	102.36	106.78
30	yJ	303	PUB	C1C-C2C-C3C	-4.00	102.36	106.78
29	bF	202	PEB	CHB-C4B-NB	-4.00	123.28	128.83
29	bI	202	PEB	CHB-C4B-NB	-4.00	123.28	128.83
29	D3	203	PEB	C3D-C4D-ND	4.00	115.10	107.26
29	DO	203	PEB	C3D-C4D-ND	4.00	115.10	107.26
29	JC	202	PEB	C3D-C4D-ND	3.99	115.10	107.26
29	JE	202	PEB	C3D-C4D-ND	3.99	115.10	107.26
29	A8	203	PEB	CHC-C1D-ND	-3.99	109.31	113.95
29	UR	202	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
29	HA	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
29	HN	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
29	NF	1002	PEB	CHC-C1D-ND	3.99	118.58	113.95
29	NI	1002	PEB	CHC-C1D-ND	3.99	118.58	113.95
29	C5	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
29	C8	202	PEB	OA-C1A-C2A	-3.99	123.00	126.17
29	K8	203	PEB	CHC-C1D-ND	-3.99	109.31	113.95
29	A7	301	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
29	A9	301	PEB	CHC-C4C-C3C	-3.99	123.53	130.34
29	T2	203	PEB	CHB-C4B-NB	-3.99	123.29	128.83
29	A5	203	PEB	CHB-C4B-NB	-3.99	123.29	128.83
29	A8	203	PEB	CHB-C4B-NB	-3.99	123.29	128.83
29	TR	203	PEB	CHB-C4B-NB	-3.99	123.29	128.83
31	H7	1001	CYC	C4D-CHA-C1A	3.99	133.58	128.81
31	H9	1001	CYC	C4D-CHA-C1A	3.99	133.58	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KC	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
29	KE	201	PEB	C3D-C4D-ND	3.99	115.09	107.26
29	LA	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
29	LN	203	PEB	CMB-C2B-C1B	3.99	131.21	125.06
29	AC	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
29	AE	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
29	BD	201	PEB	C1B-C2B-C3B	-3.99	101.93	106.51
29	NO	203	PEB	C3D-C4D-ND	3.99	115.09	107.26
29	iF	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
29	iI	201	PEB	OA-C1A-C2A	-3.99	123.00	126.17
29	UF	203	PEB	CHB-C4B-NB	-3.99	123.29	128.83
29	UI	203	PEB	CHB-C4B-NB	-3.99	123.29	128.83
29	A1	301	PEB	C3D-C4D-ND	3.99	115.08	107.26
29	AK	301	PEB	C3D-C4D-ND	3.99	115.08	107.26
31	J7	1001	CYC	C4D-CHA-C1A	3.99	133.57	128.81
29	dF	203	PEB	CHB-C4B-NB	-3.99	123.30	128.83
29	dI	203	PEB	CHB-C4B-NB	-3.99	123.30	128.83
29	S2	202	PEB	CHC-C4C-C3C	-3.99	123.54	130.34
31	J9	1001	CYC	C4D-CHA-C1A	3.99	133.57	128.81
29	H8	201	PEB	CHC-C4C-C3C	-3.99	123.54	130.34
29	LB	203	PEB	C4B-C3B-C2B	-3.98	102.37	106.78
29	LM	203	PEB	C4B-C3B-C2B	-3.98	102.37	106.78
29	CA	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
29	CN	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
29	F3	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	FC	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	FE	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	FO	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	FC	202	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	FE	202	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	DC	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	DE	202	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	BA	203	PEB	CMB-C2B-C1B	3.98	131.20	125.06
29	BN	203	PEB	CMB-C2B-C1B	3.98	131.20	125.06
29	QR	202	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
29	F3	201	PEB	CHC-C1D-ND	-3.98	109.32	113.95
29	FO	201	PEB	CHC-C1D-ND	-3.98	109.32	113.95
29	L5	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	B3	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	BO	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	QF	202	PEB	CHB-C4B-NB	-3.98	123.30	128.83
29	QI	202	PEB	CHB-C4B-NB	-3.98	123.30	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k7	202	PEB	C4B-C3B-C2B	-3.98	102.38	106.78
29	k9	202	PEB	C4B-C3B-C2B	-3.98	102.38	106.78
29	HB	203	PEB	C4B-C3B-C2B	-3.98	102.38	106.78
29	HM	203	PEB	C4B-C3B-C2B	-3.98	102.38	106.78
29	L8	201	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
29	NO	201	PEB	C1B-C2B-C3B	-3.98	101.94	106.51
29	M4	203	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	H5	201	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
29	H3	201	PEB	CHC-C1D-ND	-3.98	109.33	113.95
29	HO	201	PEB	CHC-C1D-ND	-3.98	109.33	113.95
29	J3	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	JO	203	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	VR	201	PEB	C3D-C4D-ND	3.98	115.07	107.26
29	RR	203	PEB	CHB-C4B-NB	-3.98	123.31	128.83
29	CC	201	PEB	CHC-C1D-ND	-3.98	109.33	113.95
29	CE	201	PEB	CHC-C1D-ND	-3.98	109.33	113.95
29	NB	202	PEB	C4B-C3B-C2B	-3.98	102.38	106.78
29	NM	202	PEB	C4B-C3B-C2B	-3.98	102.38	106.78
29	hF	202	PEB	CHB-C4B-NB	-3.98	123.31	128.83
29	hI	202	PEB	CHB-C4B-NB	-3.98	123.31	128.83
29	AF	301	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	AI	301	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	J5	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
29	J8	202	PEB	C3D-C4D-ND	3.98	115.06	107.26
29	L5	201	PEB	CHC-C4C-C3C	-3.98	123.55	130.34
29	N3	201	PEB	C1B-C2B-C3B	-3.98	101.94	106.51
29	JC	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	JE	201	PEB	OA-C1A-C2A	-3.98	123.01	126.17
29	FC	203	PEB	C3D-C4D-ND	3.98	115.06	107.26
29	FE	203	PEB	C3D-C4D-ND	3.98	115.06	107.26
31	F7	1001	CYC	C4D-CHA-C1A	3.98	133.56	128.81
29	TR	203	PEB	C3D-C4D-ND	3.98	115.06	107.26
29	HC	203	PEB	C3D-C4D-ND	3.97	115.06	107.26
29	HE	203	PEB	C3D-C4D-ND	3.97	115.06	107.26
29	N2	201	PEB	C3D-C4D-ND	3.97	115.06	107.26
29	NR	203	PEB	C3D-C4D-ND	3.97	115.06	107.26
29	ZF	202	PEB	CHB-C4B-NB	-3.97	123.32	128.83
29	ZI	202	PEB	CHB-C4B-NB	-3.97	123.32	128.83
29	V2	203	PEB	CHB-C4B-NB	-3.97	123.32	128.83
29	LF	1002	PEB	CHC-C1D-ND	3.97	118.56	113.95
29	LI	1002	PEB	CHC-C1D-ND	3.97	118.56	113.95
29	N2	203	PEB	CHB-C4B-NB	-3.97	123.32	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DA	203	PEB	CMB-C2B-C1B	3.97	131.17	125.06
29	DN	203	PEB	CMB-C2B-C1B	3.97	131.17	125.06
30	AM	305	PUB	CHA-C1B-C2B	-3.97	123.57	130.34
29	JF	1002	PEB	CHC-C1D-ND	3.97	118.55	113.95
29	JI	1002	PEB	CHC-C1D-ND	3.97	118.55	113.95
31	L7	1001	CYC	C4D-CHA-C1A	3.97	133.55	128.81
29	RB	203	PEB	OD-C4D-ND	-3.97	120.05	125.93
29	ZB	203	PEB	OD-C4D-ND	-3.97	120.05	125.93
29	RM	203	PEB	OD-C4D-ND	-3.97	120.05	125.93
29	ZM	203	PEB	OD-C4D-ND	-3.97	120.05	125.93
29	AM	301	PEB	C3D-C4D-ND	3.97	115.04	107.26
29	C8	203	PEB	CHC-C1D-ND	-3.97	109.34	113.95
29	X2	202	PEB	CHB-C4B-NB	-3.96	123.33	128.83
29	XR	203	PEB	CHB-C4B-NB	-3.96	123.33	128.83
29	mB	203	PEB	C4B-C3B-C2B	-3.96	102.39	106.78
29	mM	203	PEB	C4B-C3B-C2B	-3.96	102.39	106.78
29	PB	202	PEB	C4B-C3B-C2B	-3.96	102.40	106.78
29	PM	202	PEB	C4B-C3B-C2B	-3.96	102.40	106.78
29	AC	203	PEB	OA-C1A-C2A	-3.96	123.02	126.17
29	AE	203	PEB	OA-C1A-C2A	-3.96	123.02	126.17
29	VR	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
29	J3	201	PEB	CHC-C1D-ND	-3.96	109.35	113.95
29	HF	1002	PEB	CHC-C1D-ND	3.96	118.55	113.95
29	HI	1002	PEB	CHC-C1D-ND	3.96	118.55	113.95
29	JO	201	PEB	CHC-C1D-ND	-3.96	109.35	113.95
29	T2	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
29	V2	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
29	BC	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
29	BE	202	PEB	OA-C1A-C2A	-3.96	123.02	126.17
29	aF	201	PEB	OA-C1A-C2A	-3.96	123.02	126.17
29	aI	201	PEB	OA-C1A-C2A	-3.96	123.02	126.17
29	MN	404	PEB	C1B-C2B-C3B	-3.96	101.96	106.51
29	DF	1002	PEB	CHC-C1D-ND	3.96	118.55	113.95
29	DI	1002	PEB	CHC-C1D-ND	3.96	118.55	113.95
29	V2	201	PEB	C3D-C4D-ND	3.96	115.03	107.26
29	BC	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
29	BE	203	PEB	C3D-C4D-ND	3.96	115.03	107.26
31	F9	1001	CYC	C4D-CHA-C1A	3.96	133.54	128.81
30	AB	305	PUB	CHA-C1B-C2B	-3.96	123.58	130.34
29	HF	1002	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	VF	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	gF	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HI	1002	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	VI	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	gI	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	VF	202	PEB	C4B-C3B-C2B	-3.96	102.40	106.78
29	VI	202	PEB	C4B-C3B-C2B	-3.96	102.40	106.78
29	N2	203	PEB	C3D-C4D-ND	3.96	115.02	107.26
29	RR	201	PEB	C3D-C4D-ND	3.96	115.02	107.26
29	DC	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	LC	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	DE	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	LE	201	PEB	OA-C1A-C2A	-3.96	123.03	126.17
29	R2	203	PEB	CHB-C4B-NB	-3.96	123.34	128.83
29	NO	201	PEB	CHB-C4B-NB	-3.95	123.34	128.83
29	PR	202	PEB	CHB-C4B-NB	-3.95	123.34	128.83
29	PB	202	PEB	OD-C4D-ND	-3.95	120.07	125.93
29	PM	202	PEB	OD-C4D-ND	-3.95	120.07	125.93
29	gB	203	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	gM	203	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	P2	202	PEB	C3D-C4D-ND	3.95	115.01	107.26
29	XB	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	XM	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
31	L9	1001	CYC	C4D-CHA-C1A	3.95	133.53	128.81
29	FB	203	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	FM	203	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	EC	201	PEB	CHC-C1D-ND	-3.95	109.36	113.95
29	EE	201	PEB	CHC-C1D-ND	-3.95	109.36	113.95
29	VR	203	PEB	CHB-C4B-NB	-3.95	123.35	128.83
29	MA	405	PEB	OA-C1A-C2A	-3.95	123.03	126.17
29	E4	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
29	TF	201	PEB	C3D-C4D-ND	3.95	115.01	107.26
29	A5	202	PEB	OA-C1A-C2A	-3.95	123.03	126.17
29	cF	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
29	cI	201	PEB	OA-C1A-C2A	-3.95	123.03	126.17
29	V7	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	V9	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	VB	203	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	iF	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	iI	202	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	VM	203	PEB	C4B-C3B-C2B	-3.95	102.41	106.78
29	FF	1002	PEB	CHC-C1D-ND	3.95	118.53	113.95
29	FI	1002	PEB	CHC-C1D-ND	3.95	118.53	113.95
29	iB	203	PEB	OD-C4D-ND	-3.95	120.08	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	iM	203	PEB	OD-C4D-ND	-3.95	120.08	125.93
29	c1	203	PEB	C3D-C4D-ND	3.95	115.00	107.26
29	cK	203	PEB	C3D-C4D-ND	3.95	115.00	107.26
29	AB	301	PEB	C3D-C4D-ND	3.95	115.00	107.26
31	sP	1001	CYC	CHA-C1A-NA	-3.95	123.35	128.83
29	e2	402	PEB	C3D-C4D-ND	3.95	115.00	107.26
29	dD	401	PEB	C3D-C4D-ND	3.95	115.00	107.26
29	RR	203	PEB	C3D-C4D-ND	3.95	115.00	107.26
29	a7	202	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
29	a9	202	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
29	DB	203	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
29	DM	203	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
29	IC	201	PEB	CHC-C1D-ND	-3.95	109.36	113.95
29	IE	201	PEB	CHC-C1D-ND	-3.95	109.36	113.95
29	IC	202	PEB	C1C-CHB-C4B	-3.95	124.10	128.81
29	IE	202	PEB	C1C-CHB-C4B	-3.95	124.10	128.81
29	H7	1002	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
29	H9	1002	PEB	C4B-C3B-C2B	-3.95	102.42	106.78
29	J7	1002	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
31	N7	1001	CYC	C4D-CHA-C1A	3.94	133.52	128.81
31	N9	1001	CYC	C4D-CHA-C1A	3.94	133.52	128.81
29	P7	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	P9	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	UJ	201	PEB	CHB-C4B-C3B	-3.94	116.21	125.32
29	UL	201	PEB	CHB-C4B-C3B	-3.94	116.21	125.32
29	EC	202	PEB	C1C-CHB-C4B	-3.94	124.10	128.81
29	EE	202	PEB	C1C-CHB-C4B	-3.94	124.10	128.81
29	D3	201	PEB	CHC-C1D-ND	-3.94	109.37	113.95
29	DO	201	PEB	CHC-C1D-ND	-3.94	109.37	113.95
29	TF	202	PEB	CHC-C4C-C3C	-3.94	123.61	130.34
29	TI	202	PEB	CHC-C4C-C3C	-3.94	123.61	130.34
29	YF	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	YI	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	LA	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
29	LN	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
29	OF	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	OI	203	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	JB	203	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	JM	203	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	I4	201	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	NR	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
29	X2	202	PEB	C3D-C4D-ND	3.94	114.99	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FA	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
29	ID	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
29	FN	201	PEB	C3D-C4D-ND	3.94	114.99	107.26
29	g7	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	g9	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
31	CK	1001	CYC	C1B-C2B-C3B	-3.94	103.76	107.87
29	YF	201	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	YI	201	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	TJ	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	TL	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	aF	203	PEB	CHC-C4C-C3C	-3.94	123.62	130.34
29	aI	203	PEB	CHC-C4C-C3C	-3.94	123.62	130.34
29	iB	203	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	iM	203	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	PF	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	PI	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	HC	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	HE	202	PEB	OA-C1A-C2A	-3.94	123.04	126.17
29	MQ	403	PEB	OA-C1A-C2A	-3.94	123.04	126.17
31	uP	1001	CYC	CHA-C1A-NA	-3.94	123.36	128.83
29	eF	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	eI	202	PEB	C4B-C3B-C2B	-3.94	102.42	106.78
29	GC	201	PEB	CHC-C1D-ND	-3.94	109.38	113.95
29	GE	201	PEB	CHC-C1D-ND	-3.94	109.38	113.95
29	W2	201	PEB	CMB-C2B-C1B	3.94	131.13	125.06
29	uJ	202	PEB	CHB-C4B-C3B	-3.94	116.23	125.32
29	uL	202	PEB	CHB-C4B-C3B	-3.94	116.23	125.32
29	BA	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
29	BN	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
29	CC	202	PEB	C1C-CHB-C4B	-3.94	124.11	128.81
29	CE	202	PEB	C1C-CHB-C4B	-3.94	124.11	128.81
29	eF	203	PEB	CHC-C4C-C3C	-3.94	123.62	130.34
29	eI	203	PEB	CHC-C4C-C3C	-3.94	123.62	130.34
29	R2	201	PEB	C3D-C4D-ND	3.94	114.98	107.26
29	T7	202	PEB	C4B-C3B-C2B	-3.94	102.43	106.78
29	T9	202	PEB	C4B-C3B-C2B	-3.94	102.43	106.78
29	SR	202	PEB	CHC-C4C-C3C	-3.93	123.63	130.34
29	SJ	201	PEB	CHB-C4B-C3B	-3.93	116.23	125.32
29	SL	201	PEB	CHB-C4B-C3B	-3.93	116.23	125.32
29	A7	301	PEB	C3D-C4D-ND	3.93	114.98	107.26
29	A9	301	PEB	C3D-C4D-ND	3.93	114.98	107.26
29	R7	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c7	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	R9	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	c9	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	kB	203	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	kM	203	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	bJ	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	bL	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	TR	201	PEB	C3D-C4D-ND	3.93	114.98	107.26
29	m7	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	m9	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	VB	203	PEB	OD-C4D-ND	-3.93	120.10	125.93
29	eB	202	PEB	OD-C4D-ND	-3.93	120.10	125.93
29	VM	203	PEB	OD-C4D-ND	-3.93	120.10	125.93
29	eM	202	PEB	OD-C4D-ND	-3.93	120.10	125.93
29	VF	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	VI	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	XR	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
29	MJ	201	PEB	CHB-C4B-C3B	-3.93	116.23	125.32
29	ML	201	PEB	CHB-C4B-C3B	-3.93	116.23	125.32
29	N3	201	PEB	CHB-C4B-NB	-3.93	123.37	128.83
29	N7	1002	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	N9	1002	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	cB	203	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	dF	201	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	mF	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	dI	201	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	mI	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	cM	203	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	OJ	201	PEB	CHB-C4B-C3B	-3.93	116.24	125.32
29	OL	201	PEB	CHB-C4B-C3B	-3.93	116.24	125.32
31	FP	1001	CYC	CHA-C1A-NA	-3.93	123.37	128.83
29	kF	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	kI	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	KC	203	PEB	C1C-CHB-C4B	-3.93	124.11	128.81
29	KE	203	PEB	C1C-CHB-C4B	-3.93	124.11	128.81
31	wP	1001	CYC	CHA-C1A-NA	-3.93	123.37	128.83
29	R2	203	PEB	C3D-C4D-ND	3.93	114.97	107.26
29	kF	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	kI	202	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	GC	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	GE	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	eF	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TI	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	eI	201	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	P2	202	PEB	CHB-C4B-NB	-3.93	123.38	128.83
29	L5	201	PEB	C3D-C4D-ND	3.93	114.97	107.26
29	M3	202	PEB	C2A-C1A-NA	3.93	111.66	108.27
29	MO	202	PEB	C2A-C1A-NA	3.93	111.66	108.27
31	SP	1001	CYC	CHA-C1A-NA	-3.93	123.38	128.83
29	J9	1002	PEB	C4B-C3B-C2B	-3.93	102.43	106.78
29	XR	203	PEB	C3D-C4D-ND	3.93	114.97	107.26
29	B3	201	PEB	CHC-C1D-ND	-3.93	109.39	113.95
29	KC	202	PEB	CHC-C1D-ND	-3.93	109.39	113.95
29	KE	202	PEB	CHC-C1D-ND	-3.93	109.39	113.95
29	BO	201	PEB	CHC-C1D-ND	-3.93	109.39	113.95
29	GA	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	GN	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	qJ	201	PEB	CHB-C4B-C3B	-3.93	116.25	125.32
29	qL	201	PEB	CHB-C4B-C3B	-3.93	116.25	125.32
29	YF	203	PEB	CHC-C4C-C3C	-3.93	123.64	130.34
29	YI	203	PEB	CHC-C4C-C3C	-3.93	123.64	130.34
29	JA	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
29	JN	201	PEB	C3D-C4D-ND	3.93	114.96	107.26
29	L7	1002	PEB	C4B-C3B-C2B	-3.93	102.44	106.78
29	hJ	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	hL	202	PEB	OA-C1A-C2A	-3.93	123.05	126.17
29	JB	203	PEB	OD-C4D-ND	-3.93	120.11	125.93
29	LB	203	PEB	OD-C4D-ND	-3.93	120.11	125.93
29	JM	203	PEB	OD-C4D-ND	-3.93	120.11	125.93
29	LM	203	PEB	OD-C4D-ND	-3.93	120.11	125.93
31	OP	1001	CYC	CHA-C1A-NA	-3.93	123.38	128.83
29	AF	304	PEB	CHC-C4C-C3C	-3.93	123.64	130.34
29	AI	304	PEB	CHC-C4C-C3C	-3.93	123.64	130.34
31	XP	1001	CYC	CHA-C1A-NA	-3.93	123.38	128.83
29	D7	1002	PEB	C4B-C3B-C2B	-3.93	102.44	106.78
29	D9	1002	PEB	C4B-C3B-C2B	-3.93	102.44	106.78
29	KJ	201	PEB	CHB-C4B-C3B	-3.92	116.25	125.32
29	KL	201	PEB	CHB-C4B-C3B	-3.92	116.25	125.32
29	TB	203	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	aF	202	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	aI	202	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	TM	203	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
31	IK	1001	CYC	C1B-C2B-C3B	-3.92	103.78	107.87
29	T2	201	PEB	C3D-C4D-ND	3.92	114.96	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H5	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
29	HA	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
29	HN	201	PEB	C3D-C4D-ND	3.92	114.96	107.26
29	cJ	201	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	cL	201	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	gF	202	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	gI	202	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	cB	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
29	cM	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
29	DA	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	DN	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	PR	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	HB	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
29	HM	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
29	k1	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	kK	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	SR	201	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	EJ	201	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	EL	201	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	R1	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	RK	203	PEB	C3D-C4D-ND	3.92	114.95	107.26
31	oP	1001	CYC	CHA-C1A-NA	-3.92	123.39	128.83
29	ZB	203	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	ZM	203	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	sJ	201	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	sL	201	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	M3	201	PEB	CHB-C4B-NB	-3.92	123.39	128.83
29	MO	201	PEB	CHB-C4B-NB	-3.92	123.39	128.83
29	I5	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
29	I8	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
30	A7	302	PUB	CMA-C2A-C1A	3.92	130.61	121.39
30	A9	302	PUB	CMA-C2A-C1A	3.92	130.61	121.39
29	WJ	202	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	WL	202	PEB	CHB-C4B-C3B	-3.92	116.26	125.32
29	dD	401	PEB	C4B-C3B-C2B	-3.92	102.44	106.78
29	AJ	201	PEB	CHB-C4B-C3B	-3.92	116.27	125.32
29	oJ	201	PEB	CHB-C4B-C3B	-3.92	116.27	125.32
29	AL	201	PEB	CHB-C4B-C3B	-3.92	116.27	125.32
29	oL	201	PEB	CHB-C4B-C3B	-3.92	116.27	125.32
31	QP	1001	CYC	CHA-C1A-NA	-3.92	123.39	128.83
29	Y1	202	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	YK	202	PEB	C3D-C4D-ND	3.92	114.95	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	1001	CYC	C1B-C2B-C3B	-3.92	103.78	107.87
29	kB	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
29	kM	203	PEB	OD-C4D-ND	-3.92	120.12	125.93
29	yJ	301	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	yL	301	PEB	C3D-C4D-ND	3.92	114.95	107.26
29	NR	201	PEB	C2A-C1A-NA	3.92	111.65	108.27
29	IJ	201	PEB	CHB-C4B-C3B	-3.92	116.27	125.32
29	IL	201	PEB	CHB-C4B-C3B	-3.92	116.27	125.32
29	L3	201	PEB	CHC-C1D-ND	-3.92	109.40	113.95
29	LO	201	PEB	CHC-C1D-ND	-3.92	109.40	113.95
31	DP	1001	CYC	CHA-C1A-NA	-3.92	123.39	128.83
29	H8	201	PEB	C3D-C4D-ND	3.92	114.94	107.26
29	HC	203	PEB	CHB-C4B-NB	-3.92	123.39	128.83
29	HE	203	PEB	CHB-C4B-NB	-3.92	123.39	128.83
29	H3	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
29	FJ	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
29	FL	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
29	HO	202	PEB	OA-C1A-C2A	-3.92	123.06	126.17
29	L8	201	PEB	C3D-C4D-ND	3.92	114.94	107.26
29	eB	202	PEB	C4B-C3B-C2B	-3.92	102.45	106.78
29	UF	201	PEB	C4B-C3B-C2B	-3.92	102.45	106.78
29	UI	201	PEB	C4B-C3B-C2B	-3.92	102.45	106.78
29	eM	202	PEB	C4B-C3B-C2B	-3.92	102.45	106.78
29	e1	203	PEB	C3D-C4D-ND	3.92	114.94	107.26
29	eK	203	PEB	C3D-C4D-ND	3.92	114.94	107.26
29	GC	202	PEB	C1C-CHB-C4B	-3.92	124.13	128.81
29	GE	202	PEB	C1C-CHB-C4B	-3.92	124.13	128.81
29	I4	201	PEB	C3D-C4D-ND	3.91	114.94	107.26
31	nP	1001	CYC	CHA-C1A-NA	-3.91	123.40	128.83
29	wJ	303	PEB	C1C-CHB-C4B	-3.91	124.13	128.81
29	i7	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	L9	1002	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	i9	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	DB	203	PEB	OD-C4D-ND	-3.91	120.13	125.93
29	XB	202	PEB	OD-C4D-ND	-3.91	120.13	125.93
29	DM	203	PEB	OD-C4D-ND	-3.91	120.13	125.93
29	XM	202	PEB	OD-C4D-ND	-3.91	120.13	125.93
29	PF	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	PI	201	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	TB	203	PEB	OD-C4D-ND	-3.91	120.13	125.93
29	TM	203	PEB	OD-C4D-ND	-3.91	120.13	125.93
31	WP	1001	CYC	CHB-C4A-C3A	3.91	134.96	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e7	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	e9	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	cF	202	PEB	CHC-C4C-C3C	-3.91	123.66	130.34
29	cI	202	PEB	CHC-C4C-C3C	-3.91	123.66	130.34
29	WR	201	PEB	CMB-C2B-C1B	3.91	131.09	125.06
29	BC	203	PEB	CHB-C4B-NB	-3.91	123.40	128.83
29	BE	203	PEB	CHB-C4B-NB	-3.91	123.40	128.83
29	RB	203	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	RM	203	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	CJ	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	GJ	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	CL	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	GL	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	KD	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	YJ	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	YL	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	YF	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	YI	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	PJ	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	PL	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	zL	501	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	NB	202	PEB	OD-C4D-ND	-3.91	120.14	125.93
29	NM	202	PEB	OD-C4D-ND	-3.91	120.14	125.93
29	gJ	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	gL	201	PEB	CHB-C4B-C3B	-3.91	116.28	125.32
29	OR	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	mF	203	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
29	mI	203	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
31	yP	1001	CYC	CHB-C4A-C3A	3.91	134.96	124.90
29	eF	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	eI	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	Y7	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	Y9	202	PEB	C4B-C3B-C2B	-3.91	102.45	106.78
29	F5	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	F8	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	kJ	201	PEB	CHB-C4B-C3B	-3.91	116.29	125.32
29	kL	201	PEB	CHB-C4B-C3B	-3.91	116.29	125.32
29	kF	203	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
29	kI	203	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
29	E4	201	PEB	C4B-C3B-C2B	-3.91	102.46	106.78
31	M7	1001	CYC	CHB-C4A-NA	-3.91	116.76	124.93
29	J3	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JO	202	PEB	OA-C1A-C2A	-3.91	123.06	126.17
29	V1	202	PEB	C3B-C4B-NB	3.91	115.73	110.05
29	VK	202	PEB	C3B-C4B-NB	3.91	115.73	110.05
31	K1	1001	CYC	C1B-C2B-C3B	-3.91	103.79	107.87
31	KK	1001	CYC	C1B-C2B-C3B	-3.91	103.79	107.87
29	K4	201	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	HB	203	PEB	CMB-C2B-C1B	3.91	131.08	125.06
29	HM	203	PEB	CMB-C2B-C1B	3.91	131.08	125.06
29	T1	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	g1	203	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	TK	202	PEB	C3D-C4D-ND	3.91	114.93	107.26
29	gK	203	PEB	C3D-C4D-ND	3.91	114.93	107.26
31	K7	1001	CYC	CHB-C4A-NA	-3.91	116.76	124.93
29	jJ	202	PEB	OA-C1A-C2A	-3.91	123.07	126.17
29	jL	202	PEB	OA-C1A-C2A	-3.91	123.07	126.17
29	mB	203	PEB	OD-C4D-ND	-3.91	120.14	125.93
29	mM	203	PEB	OD-C4D-ND	-3.91	120.14	125.93
29	i1	202	PEB	C3B-C4B-NB	3.91	115.73	110.05
29	iK	202	PEB	C3B-C4B-NB	3.91	115.73	110.05
29	eJ	201	PEB	CHB-C4B-C3B	-3.91	116.29	125.32
29	iJ	201	PEB	CHB-C4B-C3B	-3.91	116.29	125.32
29	eL	201	PEB	CHB-C4B-C3B	-3.91	116.29	125.32
29	iL	201	PEB	CHB-C4B-C3B	-3.91	116.29	125.32
31	I7	1001	CYC	CHB-C4A-NA	-3.91	116.76	124.93
31	I9	1001	CYC	CHB-C4A-NA	-3.91	116.76	124.93
29	AC	202	PEB	C1C-CHB-C4B	-3.91	124.14	128.81
29	AE	202	PEB	C1C-CHB-C4B	-3.91	124.14	128.81
29	iF	203	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
29	iI	203	PEB	CHC-C4C-C3C	-3.91	123.67	130.34
29	I5	203	PEB	C3D-C4D-ND	3.91	114.92	107.26
29	I8	203	PEB	C3D-C4D-ND	3.91	114.92	107.26
29	zJ	501	PEB	C3D-C4D-ND	3.91	114.92	107.26
29	gB	203	PEB	OD-C4D-ND	-3.91	120.14	125.93
29	gM	203	PEB	OD-C4D-ND	-3.91	120.14	125.93
29	LC	203	PEB	CHB-C4B-NB	-3.91	123.41	128.83
29	LE	203	PEB	CHB-C4B-NB	-3.91	123.41	128.83
31	I1	1001	CYC	C1B-C2B-C3B	-3.90	103.80	107.87
29	mJ	201	PEB	CHB-C4B-C3B	-3.90	116.30	125.32
29	mL	201	PEB	CHB-C4B-C3B	-3.90	116.30	125.32
30	MQ	404	PUB	CAB-C3B-C2B	3.90	138.47	127.25
29	C4	201	PEB	C4B-C3B-C2B	-3.90	102.46	106.78
29	MD	201	PEB	C4B-C3B-C2B	-3.90	102.46	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aJ	201	PEB	CHB-C4B-C3B	-3.90	116.30	125.32
29	aL	201	PEB	CHB-C4B-C3B	-3.90	116.30	125.32
29	K5	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	K8	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	AC	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	AE	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	RJ	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	RL	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	F9	1002	PEB	C4B-C3B-C2B	-3.90	102.46	106.78
29	QJ	201	PEB	CHB-C4B-C3B	-3.90	116.30	125.32
29	QL	201	PEB	CHB-C4B-C3B	-3.90	116.30	125.32
31	qP	1001	CYC	CHA-C1A-NA	-3.90	123.41	128.83
31	G9	1001	CYC	CHB-C4A-NA	-3.90	116.77	124.93
29	TB	203	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	TM	203	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	a1	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
29	G5	201	PEB	C3D-C4D-ND	3.90	114.92	107.26
29	aK	203	PEB	C3D-C4D-ND	3.90	114.92	107.26
29	IJ	203	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	IL	203	PEB	OA-C1A-C2A	-3.90	123.07	126.17
31	hP	1001	CYC	CHA-C1A-NA	-3.90	123.41	128.83
29	U2	201	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	gF	203	PEB	CHC-C4C-C3C	-3.90	123.68	130.34
29	gI	203	PEB	CHC-C4C-C3C	-3.90	123.68	130.34
29	NO	202	PEB	C2A-C1A-NA	3.90	111.64	108.27
29	B5	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
29	BJ	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	sJ	203	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	BL	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	sL	203	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	C5	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
29	C8	203	PEB	C3D-C4D-ND	3.90	114.91	107.26
29	JC	202	PEB	CHB-C4B-NB	-3.90	123.42	128.83
29	JE	202	PEB	CHB-C4B-NB	-3.90	123.42	128.83
29	F1	1002	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
29	J1	1002	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
29	FK	1002	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
29	JK	1002	PEB	C4B-C3B-C2B	-3.90	102.47	106.78
29	g1	202	PEB	C3B-C4B-NB	3.90	115.72	110.05
29	gK	202	PEB	C3B-C4B-NB	3.90	115.72	110.05
31	C7	1001	CYC	CHB-C4A-NA	-3.90	116.78	124.93
31	C9	1001	CYC	CHB-C4A-NA	-3.90	116.78	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	jP	1001	CYC	CHA-C1A-NA	-3.90	123.42	128.83
29	RF	202	PEB	CHC-C4C-C3C	-3.90	123.69	130.34
29	RI	202	PEB	CHC-C4C-C3C	-3.90	123.69	130.34
29	M2	201	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	XB	202	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	XM	202	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	QR	201	PEB	CMB-C2B-C1B	3.90	131.07	125.06
29	G8	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
31	GK	1001	CYC	C1B-C2B-C3B	-3.90	103.80	107.87
29	B8	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
31	IP	1001	CYC	CHA-C1A-NA	-3.90	123.42	128.83
31	MP	1001	CYC	CHA-C1A-NA	-3.90	123.42	128.83
29	B3	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	HJ	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	HL	201	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	BO	202	PEB	OA-C1A-C2A	-3.90	123.07	126.17
29	FB	203	PEB	OD-C4D-ND	-3.90	120.16	125.93
29	FM	203	PEB	OD-C4D-ND	-3.90	120.16	125.93
29	PF	203	PEB	CHC-C4C-C3C	-3.90	123.69	130.34
29	PI	203	PEB	CHC-C4C-C3C	-3.90	123.69	130.34
29	CD	201	PEB	C3D-C4D-ND	3.90	114.91	107.26
29	S2	201	PEB	C3D-C4D-ND	3.90	114.90	107.26
29	AA	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	BC	201	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	BE	201	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	AN	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	OR	201	PEB	CMB-C2B-C1B	3.90	131.06	125.06
29	F3	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	IA	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	IN	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
29	FO	202	PEB	OA-C1A-C2A	-3.90	123.08	126.17
31	BP	1001	CYC	CHA-C1A-NA	-3.89	123.42	128.83
29	VF	203	PEB	CHC-C4C-C3C	-3.89	123.69	130.34
29	VI	203	PEB	CHC-C4C-C3C	-3.89	123.69	130.34
29	RB	203	PEB	CMB-C2B-C1B	3.89	131.06	125.06
29	RM	203	PEB	CMB-C2B-C1B	3.89	131.06	125.06
29	B5	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	HC	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	HE	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
31	fP	1001	CYC	CHA-C1A-NA	-3.89	123.43	128.83
29	C4	201	PEB	C3D-C4D-ND	3.89	114.90	107.26
31	E7	1001	CYC	CHB-C4A-NA	-3.89	116.79	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	E9	1001	CYC	CHB-C4A-NA	-3.89	116.79	124.93
29	U1	201	PEB	C3B-C4B-NB	3.89	115.71	110.05
29	UK	201	PEB	C3B-C4B-NB	3.89	115.71	110.05
31	kP	1001	CYC	CHA-C1A-NA	-3.89	123.43	128.83
29	V1	203	PEB	C3D-C4D-ND	3.89	114.90	107.26
29	F3	201	PEB	C3D-C4D-ND	3.89	114.90	107.26
29	VK	203	PEB	C3D-C4D-ND	3.89	114.90	107.26
29	FO	201	PEB	C3D-C4D-ND	3.89	114.90	107.26
31	D1	1003	CYC	C1B-C2B-C3B	-3.89	103.81	107.87
29	RF	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	RI	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	P1	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	i1	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	m1	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	A9	304	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	PK	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	iK	203	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	mK	202	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	LB	203	PEB	CMB-C2B-C1B	3.89	131.06	125.06
29	LM	203	PEB	CMB-C2B-C1B	3.89	131.06	125.06
29	P1	202	PEB	C3B-C4B-NB	3.89	115.71	110.05
29	PK	202	PEB	C3B-C4B-NB	3.89	115.71	110.05
29	aF	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	mF	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	aI	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	mI	201	PEB	OA-C1A-C2A	-3.89	123.08	126.17
31	G7	1001	CYC	CHB-C4A-NA	-3.89	116.80	124.93
31	M9	1001	CYC	CHB-C4A-NA	-3.89	116.80	124.93
31	EK	1001	CYC	C1B-C2B-C3B	-3.89	103.81	107.87
29	a1	202	PEB	C3B-C4B-NB	3.89	115.71	110.05
29	aK	202	PEB	C3B-C4B-NB	3.89	115.71	110.05
30	MG	402	PUB	CAB-C3B-C2B	3.89	138.42	127.25
31	K9	1001	CYC	CHB-C4A-NA	-3.89	116.80	124.93
29	fJ	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	fL	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	I4	201	PEB	CHC-C4C-C3C	-3.89	123.70	130.34
29	mJ	201	PEB	C1C-CHB-C4B	3.89	133.45	128.81
29	mL	201	PEB	C1C-CHB-C4B	3.89	133.45	128.81
29	NJ	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	NL	202	PEB	OA-C1A-C2A	-3.89	123.08	126.17
29	Z1	201	PEB	C3B-C4B-NB	3.89	115.70	110.05
29	ZK	201	PEB	C3B-C4B-NB	3.89	115.70	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N2	201	PEB	C2A-C1A-NA	3.89	111.62	108.27
29	G4	201	PEB	C3D-C4D-ND	3.89	114.89	107.26
29	eB	202	PEB	CMB-C2B-C1B	3.89	131.05	125.06
29	eM	202	PEB	CMB-C2B-C1B	3.89	131.05	125.06
29	dD	401	PEB	CHC-C4C-C3C	-3.89	123.71	130.34
29	N3	202	PEB	C2A-C1A-NA	3.89	111.62	108.27
29	FB	203	PEB	CMB-C2B-C1B	3.89	131.05	125.06
29	FM	203	PEB	CMB-C2B-C1B	3.89	131.05	125.06
29	F7	1002	PEB	C4B-C3B-C2B	-3.89	102.48	106.78
29	wL	303	PEB	C1C-CHB-C4B	-3.89	124.17	128.81
29	ID	201	PEB	CHC-C4C-C3C	-3.88	123.71	130.34
29	GD	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	AF	305	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	AI	305	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	ZB	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	cB	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	ZM	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	cM	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	K5	203	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	K8	203	PEB	C3D-C4D-ND	3.88	114.88	107.26
31	1P	1001	CYC	CHA-C1A-NA	-3.88	123.44	128.83
29	MD	201	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	kB	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	kM	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
31	E1	1001	CYC	C1B-C2B-C3B	-3.88	103.82	107.87
29	A5	203	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	AM	302	PEB	C3D-C4D-ND	3.88	114.88	107.26
29	iB	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	iM	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	KA	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	KN	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
31	UP	1001	CYC	CHA-C1A-NA	-3.88	123.44	128.83
29	e1	202	PEB	C3B-C4B-NB	3.88	115.70	110.05
29	eK	202	PEB	C3B-C4B-NB	3.88	115.70	110.05
29	PB	202	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	PM	202	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	NO	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
29	ID	201	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
29	HK	1002	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
29	Q2	201	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	MD	201	PEB	CHC-C4C-C3C	-3.88	123.72	130.34
29	R2	201	PEB	C2A-C1A-NA	3.88	111.62	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T2	201	PEB	C2A-C1A-NA	3.88	111.62	108.27
29	QJ	201	PEB	C1C-CHB-C4B	3.88	133.44	128.81
29	QL	201	PEB	C1C-CHB-C4B	3.88	133.44	128.81
29	j1	203	PEB	C3B-C4B-NB	3.88	115.69	110.05
29	jK	203	PEB	C3B-C4B-NB	3.88	115.69	110.05
29	UR	201	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	J3	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
29	JO	201	PEB	C3D-C4D-ND	3.88	114.87	107.26
29	M4	201	PEB	C4B-C3B-C2B	-3.88	102.49	106.78
29	dF	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	iF	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	dI	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	iI	202	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	L9	1002	PEB	C3D-C4D-ND	3.88	114.87	107.26
29	MR	202	PEB	C3D-C4D-ND	3.88	114.87	107.26
29	JB	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	JM	203	PEB	CMB-C2B-C1B	3.88	131.04	125.06
29	HC	202	PEB	CHC-C1D-ND	-3.88	109.44	113.95
29	HE	202	PEB	CHC-C1D-ND	-3.88	109.44	113.95
29	c1	202	PEB	C3B-C4B-NB	3.88	115.69	110.05
29	cK	202	PEB	C3B-C4B-NB	3.88	115.69	110.05
29	O2	201	PEB	CMB-C2B-C1B	3.88	131.03	125.06
31	M1	1001	CYC	C1B-C2B-C3B	-3.88	103.83	107.87
31	MK	1001	CYC	C1B-C2B-C3B	-3.88	103.83	107.87
31	HP	1001	CYC	CHA-C1A-NA	-3.88	123.45	128.83
29	F5	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	H5	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	F8	201	PEB	OA-C1A-C2A	-3.88	123.09	126.17
29	dJ	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	dL	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	VB	203	PEB	CMB-C2B-C1B	3.87	131.03	125.06
29	VM	203	PEB	CMB-C2B-C1B	3.87	131.03	125.06
29	A1	303	PEB	C3D-C4D-ND	3.87	114.86	107.26
29	AK	303	PEB	C3D-C4D-ND	3.87	114.86	107.26
29	M3	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
29	MO	201	PEB	C3D-C4D-ND	3.87	114.86	107.26
29	yJ	301	PEB	CMB-C2B-C1B	3.87	131.03	125.06
29	yL	301	PEB	CMB-C2B-C1B	3.87	131.03	125.06
29	FC	203	PEB	CHB-C4B-NB	-3.87	123.45	128.83
29	FE	203	PEB	CHB-C4B-NB	-3.87	123.45	128.83
29	N3	202	PEB	C3D-C4D-ND	3.87	114.86	107.26
29	UF	201	PEB	OA-C1A-C2A	-3.87	123.09	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UI	201	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	MR	201	PEB	CMB-C2B-C1B	3.87	131.03	125.06
30	wL	304	PUB	C1C-C2C-C3C	-3.87	102.50	106.78
29	I3	203	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	EA	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	uJ	201	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	uL	201	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	EN	202	PEB	OA-C1A-C2A	-3.87	123.09	126.17
29	IO	203	PEB	OA-C1A-C2A	-3.87	123.09	126.17
30	xL	304	PUB	CMA-C2A-C1A	3.87	130.50	121.39
29	GD	201	PEB	CHC-C4C-C3C	-3.87	123.73	130.34
29	K4	201	PEB	CHC-C4C-C3C	-3.87	123.74	130.34
29	CC	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	CE	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	IJ	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	rJ	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	IL	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	rL	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	L1	1002	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
29	LK	1002	PEB	C4B-C3B-C2B	-3.87	102.50	106.78
29	DC	202	PEB	CHB-C4B-NB	-3.87	123.46	128.83
29	DE	202	PEB	CHB-C4B-NB	-3.87	123.46	128.83
29	L8	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
29	CA	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	CN	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	E4	201	PEB	CMB-C2B-C1B	3.87	131.02	125.06
29	dD	401	PEB	CMB-C2B-C1B	3.87	131.02	125.06
29	T1	202	PEB	CHC-C1D-ND	-3.87	109.46	113.95
29	TK	202	PEB	CHC-C1D-ND	-3.87	109.46	113.95
29	eJ	201	PEB	C1C-CHB-C4B	3.87	133.43	128.81
29	eL	201	PEB	C1C-CHB-C4B	3.87	133.43	128.81
29	M3	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
29	N3	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
29	kJ	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
29	kL	201	PEB	C3D-C4D-ND	3.87	114.85	107.26
29	MO	202	PEB	C3D-C4D-ND	3.87	114.85	107.26
29	A8	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	OB	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	OM	202	PEB	OA-C1A-C2A	-3.87	123.10	126.17
29	A7	304	PEB	C3D-C4D-ND	3.87	114.84	107.26
29	M4	201	PEB	C3D-C4D-ND	3.87	114.84	107.26
29	AB	302	PEB	C3D-C4D-ND	3.87	114.84	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NB	202	PEB	CMB-C2B-C1B	3.87	131.02	125.06
29	NM	202	PEB	CMB-C2B-C1B	3.87	131.02	125.06
29	FC	202	PEB	CHC-C1D-ND	-3.87	109.46	113.95
29	FE	202	PEB	CHC-C1D-ND	-3.87	109.46	113.95
29	oJ	201	PEB	C1C-CHB-C4B	3.86	133.43	128.81
29	sJ	201	PEB	C1C-CHB-C4B	3.86	133.43	128.81
29	oL	201	PEB	C1C-CHB-C4B	3.86	133.43	128.81
29	sL	201	PEB	C1C-CHB-C4B	3.86	133.43	128.81
29	A8	203	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	pJ	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	pL	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	M4	201	PEB	CHC-C4C-C3C	-3.86	123.75	130.34
29	KJ	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	KL	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	D1	1002	PEB	C2A-C1A-NA	3.86	111.60	108.27
29	A1	302	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	AK	302	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	wL	302	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	gB	203	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	gM	203	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	DB	203	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	mB	203	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	DM	203	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	mM	203	PEB	CMB-C2B-C1B	3.86	131.01	125.06
30	wL	304	PUB	CMA-C2A-C1A	3.86	130.48	121.39
29	KC	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	KE	202	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	C4	201	PEB	CHC-C4C-C3C	-3.86	123.75	130.34
29	XJ	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	XL	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	D3	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	DO	201	PEB	C3D-C4D-ND	3.86	114.84	107.26
29	MG	401	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	NO	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	ID	201	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	IC	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	IE	202	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	WJ	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	WL	201	PEB	OA-C1A-C2A	-3.86	123.10	126.17
29	C8	201	PEB	CMB-C2B-C1B	3.86	131.01	125.06
29	QJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	wJ	302	PEB	C3D-C4D-ND	3.86	114.83	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	QL	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	RR	201	PEB	C2A-C1A-NA	3.86	111.60	108.27
29	NK	1002	PEB	C4B-C3B-C2B	-3.86	102.51	106.78
29	R1	202	PEB	C3B-C4B-NB	3.86	115.66	110.05
29	RK	202	PEB	C3B-C4B-NB	3.86	115.66	110.05
29	KJ	201	PEB	C1C-CHB-C4B	3.86	133.42	128.81
29	WJ	202	PEB	C1C-CHB-C4B	3.86	133.42	128.81
29	KL	201	PEB	C1C-CHB-C4B	3.86	133.42	128.81
29	WL	202	PEB	C1C-CHB-C4B	3.86	133.42	128.81
29	N7	1002	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	N9	1002	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	E4	201	PEB	CHC-C4C-C3C	-3.86	123.76	130.34
29	I4	203	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	GJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	GL	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	gJ	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	gL	201	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	J9	1002	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	cJ	201	PEB	C1C-CHB-C4B	3.86	133.42	128.81
29	cL	201	PEB	C1C-CHB-C4B	3.86	133.42	128.81
30	AF	303	PUB	C1C-C2C-C3C	-3.86	102.51	106.78
30	AI	303	PUB	C1C-C2C-C3C	-3.86	102.51	106.78
29	BC	202	PEB	CHC-C1D-ND	-3.86	109.47	113.95
29	BE	202	PEB	CHC-C1D-ND	-3.86	109.47	113.95
29	L7	1002	PEB	C3D-C4D-ND	3.86	114.83	107.26
29	IJ	201	PEB	C1C-CHB-C4B	3.86	133.41	128.81
29	IL	201	PEB	C1C-CHB-C4B	3.86	133.41	128.81
29	B3	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
29	BO	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
29	CD	201	PEB	C4B-C3B-C2B	-3.86	102.52	106.78
30	wJ	304	PUB	C1C-C2C-C3C	-3.86	102.52	106.78
29	IC	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
29	IE	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
29	AJ	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
29	AL	201	PEB	C3D-C4D-ND	3.86	114.82	107.26
29	k1	202	PEB	C3B-C4B-NB	3.86	115.66	110.05
29	kK	202	PEB	C3B-C4B-NB	3.86	115.66	110.05
30	wJ	304	PUB	CMA-C2A-C1A	3.85	130.46	121.39
29	G5	201	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	B8	201	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	nJ	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	nL	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H1	1002	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
29	k1	201	PEB	CHC-C4C-C3C	-3.85	123.76	130.34
29	kK	201	PEB	CHC-C4C-C3C	-3.85	123.76	130.34
29	gJ	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	gL	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	KD	201	PEB	CHC-C4C-C3C	-3.85	123.76	130.34
29	N1	1002	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
29	H3	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	HO	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	MJ	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	ML	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	MQ	403	PEB	CHC-C4C-C3C	-3.85	123.77	130.34
30	xJ	304	PUB	CMA-C2A-C1A	3.85	130.45	121.39
29	m7	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	m9	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	CD	201	PEB	CHC-C4C-C3C	-3.85	123.77	130.34
29	CC	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	GC	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	CE	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	GE	201	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	A8	201	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	DO	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	GA	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	GN	202	PEB	C3D-C4D-ND	3.85	114.82	107.26
29	A5	201	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	PF	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	PI	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	GJ	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	GL	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	F7	1002	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	G8	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	CJ	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	CL	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	Y1	202	PEB	CHC-C1D-ND	-3.85	109.48	113.95
29	LC	202	PEB	CHC-C1D-ND	-3.85	109.48	113.95
29	LE	202	PEB	CHC-C1D-ND	-3.85	109.48	113.95
29	YK	202	PEB	CHC-C1D-ND	-3.85	109.48	113.95
29	DJ	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
29	DL	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
29	kJ	202	PEB	CHA-C1B-NB	-3.85	116.88	124.93
29	kL	202	PEB	CHA-C1B-NB	-3.85	116.88	124.93
29	G5	202	PEB	C3D-C4D-ND	3.85	114.81	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CA	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	CN	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
30	A7	302	PUB	C1C-C2C-C3C	-3.85	102.52	106.78
30	A9	302	PUB	C1C-C2C-C3C	-3.85	102.52	106.78
29	G4	201	PEB	CHC-C4C-C3C	-3.85	123.77	130.34
29	J7	1002	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	e7	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	e9	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	xL	302	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	AJ	203	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	AL	203	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	tJ	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
29	tL	201	PEB	C4B-C3B-C2B	-3.85	102.52	106.78
29	MJ	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	UJ	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	ML	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	UL	201	PEB	C1C-CHB-C4B	3.85	133.41	128.81
29	NO	201	PEB	CHA-C1B-NB	-3.85	116.88	124.93
29	c7	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	c9	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	MG	404	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	mJ	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	mL	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	BB	301	PEB	CHA-C4A-NA	-3.85	120.63	125.20
29	BM	301	PEB	CHA-C4A-NA	-3.85	120.63	125.20
29	eR	401	PEB	CHC-C1D-ND	-3.85	109.48	113.95
29	UJ	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	UL	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	KC	203	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	KE	203	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	kF	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	kI	202	PEB	OA-C1A-C2A	-3.85	123.11	126.17
29	L3	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	LO	201	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	IA	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	IN	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	B5	202	PEB	C3D-C4D-ND	3.85	114.81	107.26
29	M3	201	PEB	CHA-C1B-NB	-3.85	116.89	124.93
29	MO	201	PEB	CHA-C1B-NB	-3.85	116.89	124.93
29	CJ	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	SJ	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	aJ	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	qJ	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	CL	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	SL	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	aL	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	qL	201	PEB	C1C-CHB-C4B	3.85	133.40	128.81
29	PJ	201	PEB	C4B-C3B-C2B	-3.85	102.53	106.78
29	PL	201	PEB	C4B-C3B-C2B	-3.85	102.53	106.78
29	H8	202	PEB	C3D-C4D-ND	3.85	114.80	107.26
29	EJ	201	PEB	C3D-C4D-ND	3.85	114.80	107.26
29	xJ	302	PEB	C3D-C4D-ND	3.85	114.80	107.26
29	EL	201	PEB	C3D-C4D-ND	3.85	114.80	107.26
29	a7	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	F9	1002	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	a9	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	KA	202	PEB	CHA-C4A-NA	-3.84	120.63	125.20
29	KN	202	PEB	CHA-C4A-NA	-3.84	120.63	125.20
29	OJ	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	OL	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	xJ	303	PEB	C1C-CHB-C4B	-3.84	124.22	128.81
29	IJ	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	WJ	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	IL	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	WL	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	SR	201	PEB	CHA-C1B-NB	-3.84	116.89	124.93
29	MD	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
29	L5	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	D7	1002	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	D9	1002	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	YJ	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	YL	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	DG	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	DQ	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	C4	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
29	uJ	203	PEB	CHA-C1B-NB	-3.84	116.89	124.93
29	uL	203	PEB	CHA-C1B-NB	-3.84	116.89	124.93
29	H5	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	k7	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	k9	201	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	AJ	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	AL	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	JJ	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
29	JL	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c1	201	PEB	CHC-C4C-C3C	-3.84	123.78	130.34
29	cK	201	PEB	CHC-C4C-C3C	-3.84	123.78	130.34
29	DK	1002	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
29	N1	1002	PEB	C2A-C1A-NA	3.84	111.58	108.27
29	iJ	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	iL	201	PEB	C1C-CHB-C4B	3.84	133.40	128.81
29	SJ	202	PEB	CHA-C1B-NB	-3.84	116.90	124.93
29	mJ	202	PEB	CHA-C1B-NB	-3.84	116.90	124.93
29	SL	202	PEB	CHA-C1B-NB	-3.84	116.90	124.93
29	mL	202	PEB	CHA-C1B-NB	-3.84	116.90	124.93
29	D1	1002	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
29	K4	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
29	MB	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	MM	202	PEB	C3D-C4D-ND	3.84	114.80	107.26
29	C5	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
29	P1	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	PK	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	MQ	406	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	xL	303	PEB	C1C-CHB-C4B	-3.84	124.22	128.81
29	M4	201	PEB	CMB-C2B-C1B	3.84	130.98	125.06
29	c1	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	cK	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	vJ	201	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
29	vL	201	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
29	qJ	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	qL	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	G4	201	PEB	C4B-C3B-C2B	-3.84	102.53	106.78
31	C1	1001	CYC	C1B-NB-C4B	-3.84	105.78	110.67
29	m1	202	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	QF	201	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	QI	201	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	mK	202	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	MG	401	PEB	CHC-C4C-C3C	-3.84	123.79	130.34
29	AC	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	AE	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	aJ	202	PEB	CHA-C1B-NB	-3.84	116.91	124.93
29	aL	202	PEB	CHA-C1B-NB	-3.84	116.91	124.93
29	J5	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	EC	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	EE	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	GD	201	PEB	C4B-C3B-C2B	-3.84	102.54	106.78
29	R1	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RK	203	PEB	CHC-C1D-ND	-3.84	109.49	113.95
29	P7	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	T7	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	P9	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	T9	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
29	R1	201	PEB	CHC-C4C-C3C	-3.84	123.79	130.34
29	RK	201	PEB	CHC-C4C-C3C	-3.84	123.79	130.34
29	gF	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
29	gI	202	PEB	OA-C1A-C2A	-3.84	123.12	126.17
29	CJ	202	PEB	CHA-C1B-NB	-3.84	116.91	124.93
29	QJ	202	PEB	CHA-C1B-NB	-3.84	116.91	124.93
29	CL	202	PEB	CHA-C1B-NB	-3.84	116.91	124.93
29	QL	202	PEB	CHA-C1B-NB	-3.84	116.91	124.93
29	I4	202	PEB	C3B-C4B-NB	3.84	115.63	110.05
30	xJ	304	PUB	C1C-C2C-C3C	-3.83	102.54	106.78
29	WR	201	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
29	BG	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	BQ	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	P1	201	PEB	CHC-C4C-C3C	-3.83	123.80	130.34
29	PK	201	PEB	CHC-C4C-C3C	-3.83	123.80	130.34
29	G4	202	PEB	C3B-C4B-NB	3.83	115.62	110.05
29	GD	202	PEB	C3B-C4B-NB	3.83	115.62	110.05
29	M4	202	PEB	C3B-C4B-NB	3.83	115.62	110.05
29	MJ	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	ML	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	M2	201	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
29	N3	201	PEB	CHA-C1B-NB	-3.83	116.92	124.93
29	K4	202	PEB	C3B-C4B-NB	3.83	115.62	110.05
29	V7	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	V9	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	cJ	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	cL	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	LG	202	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	YJ	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	iJ	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	YL	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	iL	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	LQ	201	PEB	C3D-C4D-ND	3.83	114.78	107.26
29	JJ	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
29	ZJ	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
29	JL	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
29	ZL	201	PEB	C4B-C3B-C2B	-3.83	102.54	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CD	201	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	ZJ	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	ZL	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	LQ	202	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
29	Q2	201	PEB	C1B-C2B-C3B	-3.83	102.11	106.51
29	sJ	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	sL	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	IJ	202	PEB	CHA-C1B-NB	-3.83	116.92	124.93
29	KJ	202	PEB	CHA-C1B-NB	-3.83	116.92	124.93
29	IL	202	PEB	CHA-C1B-NB	-3.83	116.92	124.93
29	KL	202	PEB	CHA-C1B-NB	-3.83	116.92	124.93
29	AA	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	EA	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	EB	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	EM	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	AN	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	EN	202	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	EC	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	EE	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	D3	203	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	DO	203	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	SJ	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	SL	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	NK	1002	PEB	C2A-C1A-NA	3.83	111.57	108.27
29	TR	201	PEB	C2A-C1A-NA	3.83	111.57	108.27
29	kJ	201	PEB	C1C-CHB-C4B	3.83	133.38	128.81
29	kL	201	PEB	C1C-CHB-C4B	3.83	133.38	128.81
29	AC	203	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	AE	203	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	OF	201	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	OI	201	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	OJ	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	OL	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	LG	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	MQ	402	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	EJ	201	PEB	C1C-CHB-C4B	3.83	133.38	128.81
29	EL	201	PEB	C1C-CHB-C4B	3.83	133.38	128.81
29	I4	201	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	a1	201	PEB	CHC-C4C-C3C	-3.83	123.81	130.34
29	aK	201	PEB	CHC-C4C-C3C	-3.83	123.81	130.34
29	i7	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	i9	201	PEB	C3D-C4D-ND	3.83	114.77	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mF	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	mI	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	aJ	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	aL	202	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	AF	304	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	AI	304	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	AA	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	AN	201	PEB	C3D-C4D-ND	3.83	114.77	107.26
29	bJ	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	rJ	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	bL	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	rL	203	PEB	OA-C1A-C2A	-3.83	123.13	126.17
29	K4	201	PEB	C4B-C3B-C2B	-3.83	102.55	106.78
29	F1	1002	PEB	C2A-C1A-NA	3.83	111.57	108.27
29	DK	1002	PEB	C2A-C1A-NA	3.83	111.57	108.27
29	FK	1002	PEB	C2A-C1A-NA	3.83	111.57	108.27
29	KD	202	PEB	C3B-C4B-NB	3.83	115.61	110.05
29	F3	203	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	FO	203	PEB	CMB-C2B-C1B	3.83	130.96	125.06
29	a1	203	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	UF	202	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	UI	202	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	aK	203	PEB	CHC-C1D-ND	-3.83	109.50	113.95
29	GA	201	PEB	C3D-C4D-ND	3.83	114.76	107.26
29	GN	201	PEB	C3D-C4D-ND	3.83	114.76	107.26
29	MR	201	PEB	C1B-C2B-C3B	-3.83	102.12	106.51
29	BD	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	MJ	202	PEB	CHA-C1B-NB	-3.82	116.93	124.93
29	ML	202	PEB	CHA-C1B-NB	-3.82	116.93	124.93
29	DO	202	PEB	OA-C1A-C2A	-3.82	123.13	126.17
29	D3	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	e2	402	PEB	C2A-C1A-NA	3.82	111.57	108.27
30	MQ	405	PUB	C1D-CHC-C4C	-3.82	105.05	113.37
29	cJ	202	PEB	CHA-C1B-NB	-3.82	116.93	124.93
29	cL	202	PEB	CHA-C1B-NB	-3.82	116.93	124.93
29	J8	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	HC	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	HE	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	B3	203	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	A5	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	A8	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	JG	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BO	203	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	JQ	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	IA	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	IN	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	KD	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	OJ	202	PEB	OA-C1A-C2A	-3.82	123.13	126.17
29	OL	202	PEB	OA-C1A-C2A	-3.82	123.13	126.17
29	jJ	202	PEB	CHA-C1B-NB	-3.82	116.94	124.93
29	jL	202	PEB	CHA-C1B-NB	-3.82	116.94	124.93
29	FD	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	lJ	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	lL	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
31	GK	1001	CYC	C1B-NB-C4B	-3.82	105.80	110.67
29	IA	202	PEB	CHA-C4A-NA	-3.82	120.66	125.20
29	IN	202	PEB	CHA-C4A-NA	-3.82	120.66	125.20
30	yJ	302	PUB	CMD-C2D-C3D	3.82	133.51	127.77
30	yL	302	PUB	CMD-C2D-C3D	3.82	133.51	127.77
29	LJ	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	fJ	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	LL	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	fL	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	ED	201	PEB	C3B-C4B-NB	3.82	115.61	110.05
29	i1	201	PEB	CHC-C4C-C3C	-3.82	123.82	130.34
29	iK	201	PEB	CHC-C4C-C3C	-3.82	123.82	130.34
29	g7	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	g9	201	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	i1	203	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	iK	203	PEB	CHC-C1D-ND	-3.82	109.51	113.95
31	CF	1001	CYC	C1B-NB-C4B	-3.82	105.80	110.67
31	CI	1001	CYC	C1B-NB-C4B	-3.82	105.80	110.67
29	F5	202	PEB	C3D-C4D-ND	3.82	114.76	107.26
29	E4	202	PEB	C3B-C4B-NB	3.82	115.61	110.05
29	CD	202	PEB	C3B-C4B-NB	3.82	115.61	110.05
29	J3	203	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	JO	203	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	YJ	202	PEB	CHA-C1B-NB	-3.82	116.94	124.93
29	YL	202	PEB	CHA-C1B-NB	-3.82	116.94	124.93
29	G8	201	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	DG	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	DQ	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	hJ	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78
29	hL	201	PEB	C4B-C3B-C2B	-3.82	102.55	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M4	203	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	I5	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	I8	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	KA	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	KN	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	U2	201	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
29	UR	201	PEB	C1B-C2B-C3B	-3.82	102.12	106.51
29	dJ	203	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	gJ	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	dL	203	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	gL	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	GD	201	PEB	CMB-C2B-C1B	3.82	130.95	125.06
29	IF	201	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	II	201	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	EA	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	BC	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	BE	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	FG	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	EN	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	FQ	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	MD	202	PEB	C3B-C4B-NB	3.82	115.60	110.05
29	L1	1002	PEB	C2A-C1A-NA	3.82	111.56	108.27
29	LK	1002	PEB	C2A-C1A-NA	3.82	111.56	108.27
29	EJ	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	EL	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	H3	203	PEB	CMB-C2B-C1B	3.82	130.94	125.06
29	HO	203	PEB	CMB-C2B-C1B	3.82	130.94	125.06
29	qJ	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	qL	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	SB	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	WB	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	SM	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	WM	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	SF	201	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	fF	201	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	SI	201	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	fI	201	PEB	CHC-C1D-ND	-3.82	109.51	113.95
29	m1	201	PEB	CHC-C4C-C3C	-3.82	123.83	130.34
29	mK	201	PEB	CHC-C4C-C3C	-3.82	123.83	130.34
29	e1	201	PEB	CHC-C4C-C3C	-3.82	123.83	130.34
29	eK	201	PEB	CHC-C4C-C3C	-3.82	123.83	130.34
29	XJ	201	PEB	C4B-C3B-C2B	-3.82	102.56	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	XL	201	PEB	C4B-C3B-C2B	-3.82	102.56	106.78
29	B8	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	lB	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	aJ	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	aL	201	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	lM	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	V2	201	PEB	C2A-C1A-NA	3.82	111.56	108.27
29	LG	201	PEB	C2A-C1A-NA	3.82	111.56	108.27
29	MQ	402	PEB	C2A-C1A-NA	3.82	111.56	108.27
29	UJ	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	oJ	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	UL	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	oL	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	U2	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	CB	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	CM	202	PEB	OA-C1A-C2A	-3.82	123.14	126.17
29	T1	201	PEB	CHC-C4C-C3C	-3.82	123.83	130.34
29	TK	201	PEB	CHC-C4C-C3C	-3.82	123.83	130.34
29	WJ	203	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	WL	203	PEB	CHA-C1B-NB	-3.82	116.95	124.93
31	M1	1001	CYC	C1B-NB-C4B	-3.82	105.81	110.67
31	MK	1001	CYC	C1B-NB-C4B	-3.82	105.81	110.67
29	lB	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	lM	202	PEB	C3D-C4D-ND	3.82	114.75	107.26
29	OJ	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	gJ	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	OL	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	gL	202	PEB	CHA-C1B-NB	-3.82	116.95	124.93
29	KC	201	PEB	CHC-C1D-ND	-3.82	109.52	113.95
29	KE	201	PEB	CHC-C1D-ND	-3.82	109.52	113.95
29	R7	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	R9	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	oJ	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	oL	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	sJ	202	PEB	CHA-C1B-NB	-3.81	116.95	124.93
29	sL	202	PEB	CHA-C1B-NB	-3.81	116.95	124.93
29	KA	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	KN	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	GC	201	PEB	CHB-C4B-NB	-3.81	123.54	128.83
29	GE	201	PEB	CHB-C4B-NB	-3.81	123.54	128.83
29	Y7	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	Y9	201	PEB	C3D-C4D-ND	3.81	114.74	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HG	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	JG	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	HQ	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	JQ	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	k1	203	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	WF	201	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	WI	201	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	kK	203	PEB	CHC-C1D-ND	-3.81	109.52	113.95
30	MQ	405	PUB	CAC-CBC-CGC	-3.81	105.40	113.60
31	KF	1001	CYC	C1B-NB-C4B	-3.81	105.81	110.67
29	KD	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
29	DG	203	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
30	xL	304	PUB	C1C-C2C-C3C	-3.81	102.56	106.78
29	W7	201	PEB	C4B-NB-C1B	-3.81	99.33	106.51
29	W9	201	PEB	C4B-NB-C1B	-3.81	99.33	106.51
29	BG	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
29	BQ	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
29	L3	202	PEB	CMB-C2B-C1B	3.81	130.94	125.06
29	LO	202	PEB	CMB-C2B-C1B	3.81	130.94	125.06
29	KB	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	KM	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
30	MG	403	PUB	CAC-CBC-CGC	-3.81	105.40	113.60
29	NJ	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
29	NL	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
29	OR	201	PEB	C1B-C2B-C3B	-3.81	102.13	106.51
29	AJ	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
29	AL	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
29	DC	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	DE	201	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	AA	202	PEB	CHA-C4A-NA	-3.81	120.67	125.20
29	AN	202	PEB	CHA-C4A-NA	-3.81	120.67	125.20
29	g1	203	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	L5	202	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	gK	203	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	GJ	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
29	GL	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
29	F4	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
29	jB	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	jM	202	PEB	C3D-C4D-ND	3.81	114.74	107.26
29	ID	202	PEB	C3B-C4B-NB	3.81	115.59	110.05
31	EK	1001	CYC	C1B-NB-C4B	-3.81	105.82	110.67
29	ZJ	203	PEB	OA-C1A-C2A	-3.81	123.14	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZL	203	PEB	OA-C1A-C2A	-3.81	123.14	126.17
29	dF	202	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	dI	202	PEB	CHC-C1D-ND	-3.81	109.52	113.95
29	XR	201	PEB	C2A-C1A-NA	3.81	111.56	108.27
29	FJ	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
29	FL	201	PEB	C4B-C3B-C2B	-3.81	102.56	106.78
29	H7	1002	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	H9	1002	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	CA	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	CB	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	OB	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	DG	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	CM	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	OM	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	CN	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	DQ	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	GA	202	PEB	CHA-C4A-NA	-3.81	120.67	125.20
29	GN	202	PEB	CHA-C4A-NA	-3.81	120.67	125.20
29	eJ	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	eL	201	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	nJ	201	PEB	C4B-C3B-C2B	-3.81	102.57	106.78
29	nL	201	PEB	C4B-C3B-C2B	-3.81	102.57	106.78
29	fJ	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
29	fL	202	PEB	CHA-C1B-NB	-3.81	116.96	124.93
29	J1	1002	PEB	C2A-C1A-NA	3.81	111.56	108.27
29	JK	1002	PEB	C2A-C1A-NA	3.81	111.56	108.27
29	hB	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	uJ	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	uL	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	hM	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	iJ	202	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	iL	202	PEB	CHA-C1B-NB	-3.81	116.97	124.93
31	D1	1003	CYC	C1B-NB-C4B	-3.81	105.82	110.67
29	YB	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	YM	203	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	f7	201	PEB	C4B-NB-C1B	-3.81	99.34	106.51
29	f9	201	PEB	C4B-NB-C1B	-3.81	99.34	106.51
29	HG	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
29	HQ	202	PEB	C3D-C4D-ND	3.81	114.73	107.26
31	CK	1001	CYC	C1B-NB-C4B	-3.81	105.82	110.67
29	dJ	201	PEB	C4B-C3B-C2B	-3.81	102.57	106.78
29	dL	201	PEB	C4B-C3B-C2B	-3.81	102.57	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WB	201	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	WM	201	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	XJ	202	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	XL	202	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	HJ	201	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	HL	201	PEB	CHA-C1B-NB	-3.81	116.97	124.93
29	SF	202	PEB	CHC-C1D-ND	-3.81	109.53	113.95
29	SI	202	PEB	CHC-C1D-ND	-3.81	109.53	113.95
29	V1	201	PEB	CHC-C4C-C3C	-3.81	123.85	130.34
29	VK	201	PEB	CHC-C4C-C3C	-3.81	123.85	130.34
29	dB	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	dM	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	WJ	201	PEB	CHA-C1B-NB	-3.80	116.97	124.93
29	WL	201	PEB	CHA-C1B-NB	-3.80	116.97	124.93
29	uJ	202	PEB	C1C-CHB-C4B	3.80	133.35	128.81
29	uL	202	PEB	C1C-CHB-C4B	3.80	133.35	128.81
29	uJ	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	uL	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	ZJ	202	PEB	CHA-C1B-NB	-3.80	116.97	124.93
29	ZL	202	PEB	CHA-C1B-NB	-3.80	116.97	124.93
29	A8	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	FG	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	FQ	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	bJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	sJ	203	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	bL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	sL	203	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	fB	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	fM	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	eJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	pJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	eL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	pL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	DQ	203	PEB	C4B-C3B-C2B	-3.80	102.57	106.78
29	NJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	NL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	LC	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	LE	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	EC	201	PEB	CHB-C4B-NB	-3.80	123.55	128.83
29	EE	201	PEB	CHB-C4B-NB	-3.80	123.55	128.83
29	YF	203	PEB	C2A-C1A-NA	3.80	111.55	108.27
29	YI	203	PEB	C2A-C1A-NA	3.80	111.55	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	pJ	201	PEB	C4B-C3B-C2B	-3.80	102.57	106.78
29	pL	201	PEB	C4B-C3B-C2B	-3.80	102.57	106.78
29	JJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	JL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	F8	202	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	Q7	201	PEB	C4B-NB-C1B	-3.80	99.35	106.51
29	Q9	201	PEB	C4B-NB-C1B	-3.80	99.35	106.51
29	e1	203	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	bF	201	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	bI	201	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	eK	203	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	QB	204	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	GJ	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	IJ	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	GL	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	IL	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	QM	204	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	IJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	IL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	HQ	203	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	WF	202	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	WI	202	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	M4	203	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	A7	305	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	A9	305	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	QB	204	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	FC	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	FE	201	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	QM	204	PEB	C3D-C4D-ND	3.80	114.72	107.26
29	SB	201	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	SM	201	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	SB	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	FJ	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	FL	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	SM	202	PEB	OA-C1A-C2A	-3.80	123.15	126.17
31	E1	1001	CYC	C1B-NB-C4B	-3.80	105.83	110.67
29	BQ	203	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	EJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	PJ	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	EL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	PL	202	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	jF	202	PEB	CHC-C1D-ND	-3.80	109.53	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	jI	202	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	ZF	201	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	ZI	201	PEB	CHC-C1D-ND	-3.80	109.53	113.95
29	K5	201	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	AJ	203	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	AL	203	PEB	CHA-C1B-NB	-3.80	116.98	124.93
29	g1	201	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
29	gK	201	PEB	CHC-C4C-C3C	-3.80	123.86	130.34
31	K1	1001	CYC	C1B-NB-C4B	-3.80	105.83	110.67
31	KK	1001	CYC	C1B-NB-C4B	-3.80	105.83	110.67
29	TJ	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	TL	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	TJ	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	TL	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	U7	201	PEB	C4B-NB-C1B	-3.80	99.35	106.51
29	U9	201	PEB	C4B-NB-C1B	-3.80	99.35	106.51
29	MA	405	PEB	CHA-C1B-C2B	3.80	134.67	124.90
29	AC	201	PEB	CHB-C4B-NB	-3.80	123.56	128.83
29	AE	201	PEB	CHB-C4B-NB	-3.80	123.56	128.83
29	YB	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	YM	203	PEB	OA-C1A-C2A	-3.80	123.15	126.17
29	A1	302	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	UB	201	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	AK	302	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	UM	201	PEB	CHA-C1B-NB	-3.80	116.99	124.93
30	BB	302	PUB	CMA-C2A-C1A	3.80	130.32	121.39
30	BM	302	PUB	CMA-C2A-C1A	3.80	130.32	121.39
29	L4	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	uJ	201	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	uL	201	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	G4	201	PEB	CMB-C2B-C1B	3.80	130.91	125.06
29	GB	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
29	GM	202	PEB	C3D-C4D-ND	3.80	114.71	107.26
29	LD	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	nJ	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	nL	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	QR	201	PEB	C1B-C2B-C3B	-3.80	102.15	106.51
29	D4	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	VJ	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	VL	201	PEB	C4B-C3B-C2B	-3.80	102.58	106.78
29	O7	201	PEB	C4B-NB-C1B	-3.80	99.36	106.51
29	O9	201	PEB	C4B-NB-C1B	-3.80	99.36	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RJ	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
29	RL	202	PEB	CHA-C1B-NB	-3.80	116.99	124.93
31	I1	1001	CYC	C1B-NB-C4B	-3.80	105.84	110.67
31	IK	1001	CYC	C1B-NB-C4B	-3.80	105.84	110.67
29	h7	201	PEB	C4B-NB-C1B	-3.80	99.36	106.51
29	h9	201	PEB	C4B-NB-C1B	-3.80	99.36	106.51
29	EA	202	PEB	CHA-C4A-NA	-3.79	120.69	125.20
29	EN	202	PEB	CHA-C4A-NA	-3.79	120.69	125.20
29	F5	202	PEB	CHC-C1D-ND	-3.79	109.54	113.95
29	F8	202	PEB	CHC-C1D-ND	-3.79	109.54	113.95
29	RJ	201	PEB	C4B-C3B-C2B	-3.79	102.58	106.78
29	jJ	201	PEB	C4B-C3B-C2B	-3.79	102.58	106.78
29	RL	201	PEB	C4B-C3B-C2B	-3.79	102.58	106.78
29	jL	201	PEB	C4B-C3B-C2B	-3.79	102.58	106.78
29	QB	203	PEB	CHA-C1B-NB	-3.79	117.00	124.93
29	QM	203	PEB	CHA-C1B-NB	-3.79	117.00	124.93
29	aB	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
29	aM	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
29	V1	203	PEB	CHC-C1D-ND	-3.79	109.54	113.95
29	hF	201	PEB	CHC-C1D-ND	-3.79	109.54	113.95
29	hI	201	PEB	CHC-C1D-ND	-3.79	109.54	113.95
29	VK	203	PEB	CHC-C1D-ND	-3.79	109.54	113.95
29	CC	201	PEB	CHB-C4B-NB	-3.79	123.56	128.83
29	CE	201	PEB	CHB-C4B-NB	-3.79	123.56	128.83
29	CB	201	PEB	CHA-C1B-NB	-3.79	117.00	124.93
29	CM	201	PEB	CHA-C1B-NB	-3.79	117.00	124.93
29	H8	201	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	DJ	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	DL	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	JG	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
29	JQ	201	PEB	C3D-C4D-ND	3.79	114.70	107.26
29	UB	202	PEB	C3D-C4D-ND	3.79	114.70	107.26
29	MQ	401	PEB	C3D-C4D-ND	3.79	114.70	107.26
29	CA	202	PEB	CHA-C4A-NA	-3.79	120.70	125.20
29	CN	202	PEB	CHA-C4A-NA	-3.79	120.70	125.20
29	AG	201	PEB	CMB-C2B-C1B	3.79	130.90	125.06
29	AQ	201	PEB	CMB-C2B-C1B	3.79	130.90	125.06
29	Z7	201	PEB	C4B-NB-C1B	-3.79	99.37	106.51
29	Z9	201	PEB	C4B-NB-C1B	-3.79	99.37	106.51
29	QJ	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	QL	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	FJ	202	PEB	CHA-C1B-NB	-3.79	117.00	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FL	202	PEB	CHA-C1B-NB	-3.79	117.00	124.93
29	TJ	203	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	TL	203	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	W2	201	PEB	C1B-C2B-C3B	-3.79	102.16	106.51
29	LG	203	PEB	C2A-C1A-NA	3.79	111.54	108.27
29	JQ	203	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	K5	201	PEB	CMB-C2B-C1B	3.79	130.90	125.06
31	EF	1001	CYC	C1B-NB-C4B	-3.79	105.84	110.67
31	EI	1001	CYC	C1B-NB-C4B	-3.79	105.84	110.67
29	dJ	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
29	dL	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
29	UB	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	CJ	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	LJ	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	CL	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	LL	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	MQ	401	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	lF	202	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	lI	202	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	MB	201	PEB	CHA-C1B-NB	-3.79	117.01	124.93
29	MM	201	PEB	CHA-C1B-NB	-3.79	117.01	124.93
29	rJ	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	rL	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	hJ	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
29	hL	202	PEB	CHA-C1B-NB	-3.79	117.01	124.93
29	DD	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	BG	203	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	MN	405	PEB	CHA-C1B-C2B	3.79	134.64	124.90
29	jF	201	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	jI	201	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	l7	201	PEB	C4B-NB-C1B	-3.79	99.37	106.51
29	l9	201	PEB	C4B-NB-C1B	-3.79	99.37	106.51
29	K5	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
29	K8	202	PEB	C3D-C4D-ND	3.79	114.69	107.26
29	H8	203	PEB	CHB-C4B-NB	-3.79	123.57	128.83
29	e7	203	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	e9	203	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	BJ	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	BL	201	PEB	C4B-C3B-C2B	-3.79	102.59	106.78
29	AF	301	PEB	C3D-C4D-ND	3.79	114.69	107.26
29	AI	301	PEB	C3D-C4D-ND	3.79	114.69	107.26
29	bF	202	PEB	CHC-C1D-ND	-3.79	109.55	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	bI	202	PEB	CHC-C1D-ND	-3.79	109.55	113.95
29	fB	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	fM	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	OR	202	PEB	OA-C1A-C2A	-3.79	123.16	126.17
29	JC	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
29	JE	201	PEB	C3D-C4D-ND	3.79	114.69	107.26
29	FG	201	PEB	CMB-C2B-C1B	3.79	130.89	125.06
29	FQ	201	PEB	CMB-C2B-C1B	3.79	130.89	125.06
29	hB	201	PEB	CHA-C1B-NB	-3.79	117.02	124.93
29	hM	201	PEB	CHA-C1B-NB	-3.79	117.02	124.93
29	rJ	202	PEB	C1B-C2B-C3B	-3.78	102.16	106.51
29	rL	202	PEB	C1B-C2B-C3B	-3.78	102.16	106.51
29	L8	202	PEB	CHC-C1D-ND	-3.78	109.55	113.95
30	MG	403	PUB	C1D-CHC-C4C	-3.78	105.13	113.37
29	dB	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	dM	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	S7	201	PEB	C4B-NB-C1B	-3.78	99.38	106.51
29	S9	201	PEB	C4B-NB-C1B	-3.78	99.38	106.51
29	C4	202	PEB	C3B-C4B-NB	3.78	115.55	110.05
29	GB	202	PEB	OA-C1A-C2A	-3.78	123.16	126.17
29	GM	202	PEB	OA-C1A-C2A	-3.78	123.16	126.17
29	A5	202	PEB	C3D-C4D-ND	3.78	114.68	107.26
29	Y1	201	PEB	CHC-C4C-C3C	-3.78	123.88	130.34
29	YK	201	PEB	CHC-C4C-C3C	-3.78	123.88	130.34
29	H4	201	PEB	C4B-C3B-C2B	-3.78	102.59	106.78
29	O2	201	PEB	C1B-C2B-C3B	-3.78	102.16	106.51
29	fB	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	fM	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	vJ	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	vL	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	OB	202	PEB	C2A-C1A-NA	3.78	111.53	108.27
29	OM	202	PEB	C2A-C1A-NA	3.78	111.53	108.27
29	VR	201	PEB	C2A-C1A-NA	3.78	111.53	108.27
29	BG	201	PEB	CMB-C2B-C1B	3.78	130.89	125.06
29	BQ	201	PEB	CMB-C2B-C1B	3.78	130.89	125.06
29	C5	201	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	C8	201	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	mJ	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	mL	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	JG	203	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
29	bJ	201	PEB	C4B-C3B-C2B	-3.78	102.60	106.78
29	bL	201	PEB	C4B-C3B-C2B	-3.78	102.60	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	IB	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	aB	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	IM	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	aM	201	PEB	CHA-C1B-NB	-3.78	117.02	124.93
29	HG	201	PEB	CMB-C2B-C1B	3.78	130.89	125.06
29	HQ	201	PEB	CMB-C2B-C1B	3.78	130.89	125.06
29	dF	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	dI	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	e2	401	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	GG	201	PEB	CMB-C2B-C1B	3.78	130.88	125.06
29	GQ	201	PEB	CMB-C2B-C1B	3.78	130.88	125.06
31	F1	1001	CYC	CAD-CBD-CGD	-3.78	103.16	113.76
31	FK	1001	CYC	CAD-CBD-CGD	-3.78	103.16	113.76
31	HK	1001	CYC	CAD-CBD-CGD	-3.78	103.16	113.76
29	dB	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	dM	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	IJ	203	PEB	CHA-C1B-NB	-3.78	117.03	124.93
29	IL	203	PEB	CHA-C1B-NB	-3.78	117.03	124.93
29	G8	202	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	hF	202	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	hI	202	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	BG	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
29	BQ	201	PEB	C3D-C4D-ND	3.78	114.67	107.26
29	iJ	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	pJ	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	iL	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	pL	203	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	ZJ	202	PEB	C1B-C2B-C3B	-3.78	102.17	106.51
29	ZL	202	PEB	C1B-C2B-C3B	-3.78	102.17	106.51
29	j7	201	PEB	C4B-NB-C1B	-3.78	99.39	106.51
29	j9	201	PEB	C4B-NB-C1B	-3.78	99.39	106.51
29	K8	201	PEB	CMB-C2B-C1B	3.78	130.88	125.06
29	B8	202	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	fF	202	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	fI	202	PEB	CHC-C1D-ND	-3.78	109.56	113.95
29	OB	201	PEB	CHA-C1B-NB	-3.78	117.03	124.93
29	OM	201	PEB	CHA-C1B-NB	-3.78	117.03	124.93
31	NK	1001	CYC	CAD-CBD-CGD	-3.78	103.17	113.76
29	MB	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	RB	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	MM	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17
29	RM	202	PEB	OA-C1A-C2A	-3.78	123.17	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	H1	1001	CYC	CAD-CBD-CGD	-3.78	103.17	113.76
30	BB	302	PUB	C1C-C2C-C3C	-3.78	102.60	106.78
30	BM	302	PUB	C1C-C2C-C3C	-3.78	102.60	106.78
29	b7	201	PEB	C4B-NB-C1B	-3.78	99.40	106.51
29	b9	201	PEB	C4B-NB-C1B	-3.78	99.40	106.51
29	GB	201	PEB	CHA-C1B-NB	-3.78	117.04	124.93
29	GM	201	PEB	CHA-C1B-NB	-3.78	117.04	124.93
29	LG	201	PEB	CMB-C2B-C1B	3.77	130.88	125.06
29	MQ	402	PEB	CMB-C2B-C1B	3.77	130.88	125.06
31	C7	1001	CYC	CMA-C3A-C4A	3.77	130.88	125.06
31	C9	1001	CYC	CMA-C3A-C4A	3.77	130.88	125.06
29	A1	302	PEB	CHC-C4C-C3C	-3.77	123.90	130.34
29	AK	302	PEB	CHC-C4C-C3C	-3.77	123.90	130.34
29	K8	201	PEB	OA-C1A-C2A	-3.77	123.17	126.17
29	BJ	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	BL	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	MN	401	PEB	CHA-C1B-NB	-3.77	117.04	124.93
31	D1	1001	CYC	CAD-CBD-CGD	-3.77	103.18	113.76
31	KI	1001	CYC	C1B-NB-C4B	-3.77	105.86	110.67
29	rJ	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	rL	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	EG	201	PEB	CMB-C2B-C1B	3.77	130.88	125.06
29	EQ	201	PEB	CMB-C2B-C1B	3.77	130.88	125.06
30	wJ	305	PUB	CHB-C1C-C2C	-3.77	116.60	125.32
29	YB	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	YM	202	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	KC	202	PEB	CHB-C4B-NB	-3.77	123.59	128.83
29	KE	202	PEB	CHB-C4B-NB	-3.77	123.59	128.83
31	N1	1001	CYC	CAD-CBD-CGD	-3.77	103.18	113.76
29	I5	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
29	C5	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
29	I8	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
29	W2	202	PEB	OA-C1A-C2A	-3.77	123.17	126.17
29	KB	201	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	KM	201	PEB	CHA-C1B-NB	-3.77	117.04	124.93
29	DA	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
29	DN	202	PEB	C3D-C4D-ND	3.77	114.66	107.26
29	KG	201	PEB	CMB-C2B-C1B	3.77	130.87	125.06
29	KQ	201	PEB	CMB-C2B-C1B	3.77	130.87	125.06
29	WB	202	PEB	OA-C1A-C2A	-3.77	123.17	126.17
29	WM	202	PEB	OA-C1A-C2A	-3.77	123.17	126.17
29	ZF	202	PEB	CHC-C1D-ND	-3.77	109.57	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZI	202	PEB	CHC-C1D-ND	-3.77	109.57	113.95
29	AB	301	PEB	CHA-C4A-NA	-3.77	120.72	125.20
29	T7	203	PEB	CHC-C1D-ND	-3.77	109.57	113.95
29	T9	203	PEB	CHC-C1D-ND	-3.77	109.57	113.95
29	QF	202	PEB	CHC-C1D-ND	-3.77	109.57	113.95
29	QI	202	PEB	CHC-C1D-ND	-3.77	109.57	113.95
29	DB	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	kJ	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	kL	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	DM	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	BA	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
29	BN	202	PEB	C3D-C4D-ND	3.77	114.65	107.26
29	B4	201	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
29	LQ	202	PEB	C2A-C1A-NA	3.77	111.52	108.27
31	IF	1001	CYC	C1B-NB-C4B	-3.77	105.87	110.67
31	II	1001	CYC	C1B-NB-C4B	-3.77	105.87	110.67
29	IF	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	II	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	EB	201	PEB	CHA-C1B-NB	-3.77	117.05	124.93
29	EM	201	PEB	CHA-C1B-NB	-3.77	117.05	124.93
31	DK	1001	CYC	CAD-CBD-CGD	-3.77	103.20	113.76
31	L1	1001	CYC	CHB-C1B-NB	-3.77	117.97	126.06
31	LK	1001	CYC	CHB-C1B-NB	-3.77	117.97	126.06
29	sJ	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
29	sL	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
29	FQ	203	PEB	C4B-C3B-C2B	-3.77	102.61	106.78
29	h7	202	PEB	CHC-C4C-C3C	-3.77	123.91	130.34
29	h9	202	PEB	CHC-C4C-C3C	-3.77	123.91	130.34
29	TB	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	TM	202	PEB	OA-C1A-C2A	-3.77	123.18	126.17
29	HG	203	PEB	C2A-C1A-NA	3.77	111.52	108.27
29	FQ	203	PEB	C2A-C1A-NA	3.77	111.52	108.27
29	G5	202	PEB	CHC-C1D-ND	-3.77	109.57	113.95
31	LF	1001	CYC	CHA-C1A-NA	-3.77	123.60	128.83
31	LI	1001	CYC	CHA-C1A-NA	-3.77	123.60	128.83
29	d7	201	PEB	C4B-NB-C1B	-3.77	99.41	106.51
29	d9	201	PEB	C4B-NB-C1B	-3.77	99.41	106.51
29	FG	201	PEB	C2A-C1A-NA	3.77	111.52	108.27
29	FQ	201	PEB	C2A-C1A-NA	3.77	111.52	108.27
29	CG	201	PEB	CMB-C2B-C1B	3.77	130.86	125.06
29	CQ	201	PEB	CMB-C2B-C1B	3.77	130.86	125.06
29	G3	202	PEB	C3D-C4D-ND	3.76	114.65	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GO	202	PEB	C3D-C4D-ND	3.76	114.65	107.26
29	LA	203	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	IJ	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	IL	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	LN	203	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	H8	202	PEB	CHC-C1D-ND	-3.76	109.58	113.95
29	MA	401	PEB	CHA-C1B-NB	-3.76	117.06	124.93
29	IJ	203	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	IL	203	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	F5	203	PEB	CHB-C4B-NB	-3.76	123.61	128.83
29	i1	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	iK	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
31	K7	1001	CYC	CMA-C3A-C4A	3.76	130.86	125.06
29	FB	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	FM	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	QR	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	C8	202	PEB	C3D-C4D-ND	3.76	114.64	107.26
29	UF	203	PEB	CHC-C1D-ND	-3.76	109.58	113.95
29	dF	203	PEB	CHC-C1D-ND	-3.76	109.58	113.95
29	UI	203	PEB	CHC-C1D-ND	-3.76	109.58	113.95
29	dI	203	PEB	CHC-C1D-ND	-3.76	109.58	113.95
29	WJ	201	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	bJ	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	lJ	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	sJ	203	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	WL	201	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	bL	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	lL	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	sL	203	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	UB	202	PEB	C2A-C1A-NA	3.76	111.52	108.27
29	MQ	401	PEB	C2A-C1A-NA	3.76	111.52	108.27
31	I7	1001	CYC	CMA-C3A-C4A	3.76	130.86	125.06
31	I9	1001	CYC	CMA-C3A-C4A	3.76	130.86	125.06
29	qJ	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	qL	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	xL	302	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	jJ	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	jL	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	jB	201	PEB	CHA-C1B-NB	-3.76	117.06	124.93
29	jM	201	PEB	CHA-C1B-NB	-3.76	117.06	124.93
29	g7	203	PEB	CHC-C1D-ND	-3.76	109.58	113.95
29	g9	203	PEB	CHC-C1D-ND	-3.76	109.58	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	MF	1001	CYC	C1B-NB-C4B	-3.76	105.88	110.67
31	MI	1001	CYC	C1B-NB-C4B	-3.76	105.88	110.67
29	lB	201	PEB	CHA-C1B-NB	-3.76	117.07	124.93
29	lM	201	PEB	CHA-C1B-NB	-3.76	117.07	124.93
29	eF	203	PEB	C2A-C1A-NA	3.76	111.52	108.27
29	eI	203	PEB	C2A-C1A-NA	3.76	111.52	108.27
30	wL	305	PUB	CHB-C1C-C2C	-3.76	116.63	125.32
31	G7	1001	CYC	C1B-NB-C4B	-3.76	105.88	110.67
29	tJ	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	tL	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	J4	202	PEB	CHA-C4A-NA	-3.76	120.73	125.20
31	J1	1001	CYC	CAD-CBD-CGD	-3.76	103.22	113.76
31	JK	1001	CYC	CAD-CBD-CGD	-3.76	103.22	113.76
31	G7	1001	CYC	CMA-C3A-C4A	3.76	130.85	125.06
29	hJ	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	hL	202	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	DG	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
29	DQ	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
29	U7	202	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
29	W7	202	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
29	U9	202	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
29	W9	202	PEB	CHC-C4C-C3C	-3.76	123.92	130.34
29	IB	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	JJ	203	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	JL	203	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	IM	202	PEB	OA-C1A-C2A	-3.76	123.18	126.17
29	BB	301	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	BM	301	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	Q7	202	PEB	CHC-C4C-C3C	-3.76	123.93	130.34
29	b7	202	PEB	CHC-C4C-C3C	-3.76	123.93	130.34
29	Q9	202	PEB	CHC-C4C-C3C	-3.76	123.93	130.34
29	b9	202	PEB	CHC-C4C-C3C	-3.76	123.93	130.34
31	L1	1001	CYC	CAD-CBD-CGD	-3.76	103.22	113.76
31	LK	1001	CYC	CAD-CBD-CGD	-3.76	103.22	113.76
31	FF	1001	CYC	CHA-C1A-NA	-3.76	123.61	128.83
31	FI	1001	CYC	CHA-C1A-NA	-3.76	123.61	128.83
29	RJ	203	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	YJ	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	RL	203	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	YL	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
31	G9	1001	CYC	C1B-NB-C4B	-3.76	105.89	110.67
29	H1	1002	PEB	C2A-C1A-NA	3.76	111.51	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JG	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
29	JQ	201	PEB	C2A-C1A-NA	3.76	111.51	108.27
29	dJ	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	dL	202	PEB	C4B-C3B-C2B	-3.76	102.62	106.78
29	OF	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	QF	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	OI	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	QI	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	j7	202	PEB	CHC-C4C-C3C	-3.76	123.93	130.34
29	j9	202	PEB	CHC-C4C-C3C	-3.76	123.93	130.34
29	EA	201	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	EN	201	PEB	C1B-C2B-C3B	-3.76	102.19	106.51
29	H5	203	PEB	CHB-C4B-NB	-3.76	123.62	128.83
31	F1	1001	CYC	CHB-C1B-NB	-3.76	118.00	126.06
31	FK	1001	CYC	CHB-C1B-NB	-3.76	118.00	126.06
29	eJ	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	jJ	203	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	eL	202	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	jL	203	PEB	OA-C1A-C2A	-3.76	123.19	126.17
29	LA	202	PEB	C3D-C4D-ND	3.76	114.63	107.26
29	LN	202	PEB	C3D-C4D-ND	3.76	114.63	107.26
29	iF	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	iI	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	PJ	202	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
29	PL	202	PEB	C1B-C2B-C3B	-3.75	102.20	106.51
29	KJ	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	KL	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	PF	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	PI	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	HD	201	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
29	G8	203	PEB	CHB-C4B-NB	-3.75	123.62	128.83
29	SF	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	SI	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	HJ	201	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
29	HL	201	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
31	E7	1001	CYC	CMA-C3A-C4A	3.75	130.84	125.06
31	E9	1001	CYC	CMA-C3A-C4A	3.75	130.84	125.06
29	DQ	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	B8	203	PEB	CHB-C4B-NB	-3.75	123.62	128.83
29	R7	203	PEB	CHC-C1D-ND	-3.75	109.59	113.95
29	R9	203	PEB	CHC-C1D-ND	-3.75	109.59	113.95
29	MQ	407	PEB	C1B-C2B-C3B	-3.75	102.20	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l7	202	PEB	CHC-C4C-C3C	-3.75	123.94	130.34
29	l9	202	PEB	CHC-C4C-C3C	-3.75	123.94	130.34
29	lB	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	cJ	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	oJ	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	cL	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	oL	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	lM	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	kF	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	kI	203	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	CA	201	PEB	CMB-C2B-C1B	3.75	130.84	125.06
29	IG	201	PEB	CMB-C2B-C1B	3.75	130.84	125.06
29	CN	201	PEB	CMB-C2B-C1B	3.75	130.84	125.06
29	IQ	201	PEB	CMB-C2B-C1B	3.75	130.84	125.06
29	pJ	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
29	pL	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
29	G5	203	PEB	CHB-C4B-NB	-3.75	123.62	128.83
29	HB	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	hB	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	AJ	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	AL	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	HM	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	hM	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	SB	202	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	SM	202	PEB	C2A-C1A-NA	3.75	111.51	108.27
29	FA	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
29	FN	202	PEB	C3D-C4D-ND	3.75	114.62	107.26
29	B5	202	PEB	CHC-C1D-ND	-3.75	109.59	113.95
29	f7	202	PEB	CHC-C4C-C3C	-3.75	123.94	130.34
29	f9	202	PEB	CHC-C4C-C3C	-3.75	123.94	130.34
30	xL	305	PUB	CHB-C1C-C2C	-3.75	116.66	125.32
29	GG	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	GQ	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	I5	201	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	AM	301	PEB	CHA-C4A-NA	-3.75	120.75	125.20
29	PJ	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
29	PL	202	PEB	C4B-C3B-C2B	-3.75	102.63	106.78
29	FA	203	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	FN	203	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	c7	203	PEB	CHC-C1D-ND	-3.75	109.59	113.95
29	c9	203	PEB	CHC-C1D-ND	-3.75	109.59	113.95
29	HA	202	PEB	C3D-C4D-ND	3.75	114.61	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HN	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	MN	405	PEB	C3D-C4D-ND	3.75	114.61	107.26
31	M7	1001	CYC	CMA-C3A-C4A	3.75	130.84	125.06
29	JJ	202	PEB	C4B-C3B-C2B	-3.75	102.64	106.78
29	JL	202	PEB	C4B-C3B-C2B	-3.75	102.64	106.78
29	C3	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	CO	202	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	VF	203	PEB	C2A-C1A-NA	3.75	111.50	108.27
29	VI	203	PEB	C2A-C1A-NA	3.75	111.50	108.27
31	HF	1001	CYC	CHA-C1A-NA	-3.75	123.63	128.83
31	HI	1001	CYC	CHA-C1A-NA	-3.75	123.63	128.83
29	FJ	202	PEB	C4B-C3B-C2B	-3.75	102.64	106.78
29	FL	202	PEB	C4B-C3B-C2B	-3.75	102.64	106.78
29	d7	202	PEB	CHC-C4C-C3C	-3.75	123.95	130.34
29	d9	202	PEB	CHC-C4C-C3C	-3.75	123.95	130.34
29	MG	405	PEB	C1B-C2B-C3B	-3.75	102.21	106.51
29	nJ	202	PEB	C1B-C2B-C3B	-3.75	102.21	106.51
29	nL	202	PEB	C1B-C2B-C3B	-3.75	102.21	106.51
29	MA	405	PEB	C3D-C4D-ND	3.75	114.61	107.26
29	HJ	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	HL	202	PEB	OA-C1A-C2A	-3.75	123.19	126.17
29	A3	202	PEB	C3D-C4D-ND	3.74	114.61	107.26
29	AO	202	PEB	C3D-C4D-ND	3.74	114.61	107.26
29	fB	202	PEB	C2A-C1A-NA	3.74	111.50	108.27
29	fM	202	PEB	C2A-C1A-NA	3.74	111.50	108.27
29	m7	203	PEB	CHC-C1D-ND	-3.74	109.60	113.95
29	m9	203	PEB	CHC-C1D-ND	-3.74	109.60	113.95
29	L5	203	PEB	CHB-C4B-NB	-3.74	123.63	128.83
31	G9	1001	CYC	CMA-C3A-C4A	3.74	130.83	125.06
29	CA	201	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	CN	201	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	J4	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
29	JD	201	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
29	E3	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
29	EO	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
29	H5	201	PEB	CMB-C2B-C1B	3.74	130.83	125.06
29	F4	202	PEB	CHA-C4A-NA	-3.74	120.75	125.20
29	HJ	201	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	HL	201	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	OF	202	PEB	CHC-C1D-ND	-3.74	109.60	113.95
29	OI	202	PEB	CHC-C1D-ND	-3.74	109.60	113.95
29	TJ	202	PEB	C4B-C3B-C2B	-3.74	102.64	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TL	202	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
31	E7	1001	CYC	C1B-NB-C4B	-3.74	105.91	110.67
31	E9	1001	CYC	C1B-NB-C4B	-3.74	105.91	110.67
29	QB	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	QM	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	K3	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
29	KO	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
29	AJ	203	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	AL	203	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
31	NF	1001	CYC	CHA-C1A-NA	-3.74	123.64	128.83
31	NI	1001	CYC	CHA-C1A-NA	-3.74	123.64	128.83
29	JA	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
29	JN	202	PEB	C3D-C4D-ND	3.74	114.60	107.26
29	hF	201	PEB	C3B-C4B-NB	3.74	115.49	110.05
29	hI	201	PEB	C3B-C4B-NB	3.74	115.49	110.05
29	EA	201	PEB	CMB-C2B-C1B	3.74	130.82	125.06
29	EN	201	PEB	CMB-C2B-C1B	3.74	130.82	125.06
31	DK	1001	CYC	CHB-C1B-NB	-3.74	118.03	126.06
29	DG	203	PEB	C2A-C1A-NA	3.74	111.50	108.27
29	pJ	202	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	pL	202	PEB	C1B-C2B-C3B	-3.74	102.21	106.51
29	O7	202	PEB	CHC-C4C-C3C	-3.74	123.96	130.34
29	O9	202	PEB	CHC-C4C-C3C	-3.74	123.96	130.34
29	Y7	203	PEB	CHC-C1D-ND	-3.74	109.61	113.95
29	Y9	203	PEB	CHC-C1D-ND	-3.74	109.61	113.95
29	F8	203	PEB	CHB-C4B-NB	-3.74	123.64	128.83
29	LG	203	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
29	I5	201	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	I8	201	PEB	OA-C1A-C2A	-3.74	123.20	126.17
31	K9	1001	CYC	CMA-C3A-C4A	3.74	130.82	125.06
29	FJ	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	fJ	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	FL	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	fL	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
31	M9	1001	CYC	C1B-NB-C4B	-3.74	105.91	110.67
29	RJ	202	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
29	RL	202	PEB	C4B-C3B-C2B	-3.74	102.64	106.78
29	GA	201	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	uJ	201	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	uL	201	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	GN	201	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	aB	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SJ	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	nJ	203	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	SL	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	nL	203	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	aM	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	FG	201	PEB	C3B-C4B-NB	3.74	115.49	110.05
29	FQ	201	PEB	C3B-C4B-NB	3.74	115.49	110.05
29	i7	203	PEB	CHC-C1D-ND	-3.74	109.61	113.95
29	i9	203	PEB	CHC-C1D-ND	-3.74	109.61	113.95
29	HK	1002	PEB	C2A-C1A-NA	3.74	111.50	108.27
29	bJ	202	PEB	C4B-C3B-C2B	-3.74	102.65	106.78
29	lJ	202	PEB	C4B-C3B-C2B	-3.74	102.65	106.78
29	bL	202	PEB	C4B-C3B-C2B	-3.74	102.65	106.78
29	lL	202	PEB	C4B-C3B-C2B	-3.74	102.65	106.78
31	HK	1001	CYC	CHB-C1B-NB	-3.74	118.03	126.06
29	BJ	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	BL	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	EB	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	EM	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	aB	202	PEB	C2A-C1A-NA	3.74	111.49	108.27
29	aM	202	PEB	C2A-C1A-NA	3.74	111.49	108.27
29	P2	201	PEB	C3B-C4B-NB	3.74	115.48	110.05
29	H8	203	PEB	CMB-C2B-C1B	3.74	130.82	125.06
29	IC	201	PEB	CHB-C4B-NB	-3.74	123.64	128.83
29	IE	201	PEB	CHB-C4B-NB	-3.74	123.64	128.83
29	iB	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	ZF	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	ZI	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	iM	202	PEB	OA-C1A-C2A	-3.74	123.20	126.17
29	NJ	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	TJ	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	NL	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	TL	202	PEB	C1B-C2B-C3B	-3.74	102.22	106.51
29	LD	202	PEB	CHA-C4A-NA	-3.74	120.76	125.20
29	HB	202	PEB	CHB-C4B-NB	-3.73	123.65	128.83
29	HM	202	PEB	CHB-C4B-NB	-3.73	123.65	128.83
30	AF	302	PUB	CHA-C1B-C2B	-3.73	123.97	130.34
30	AI	302	PUB	CHA-C1B-C2B	-3.73	123.97	130.34
31	K7	1001	CYC	C1B-NB-C4B	-3.73	105.91	110.67
29	S7	202	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
29	S9	202	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
29	XR	202	PEB	C3B-C4B-NB	3.73	115.48	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BA	203	PEB	OA-C1A-C2A	-3.73	123.20	126.17
29	BJ	203	PEB	OA-C1A-C2A	-3.73	123.20	126.17
29	BL	203	PEB	OA-C1A-C2A	-3.73	123.20	126.17
29	BN	203	PEB	OA-C1A-C2A	-3.73	123.20	126.17
29	WB	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	WM	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	AM	302	PEB	CHC-C4C-C3C	-3.73	123.97	130.34
29	V7	203	PEB	CHC-C1D-ND	-3.73	109.61	113.95
29	V9	203	PEB	CHC-C1D-ND	-3.73	109.61	113.95
31	M9	1001	CYC	CMA-C3A-C4A	3.73	130.81	125.06
29	I3	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
29	IO	202	PEB	C3D-C4D-ND	3.73	114.58	107.26
29	Q2	202	PEB	OA-C1A-C2A	-3.73	123.20	126.17
31	NK	1001	CYC	CHB-C1B-NB	-3.73	118.05	126.06
29	k7	203	PEB	CHC-C1D-ND	-3.73	109.61	113.95
29	k9	203	PEB	CHC-C1D-ND	-3.73	109.61	113.95
29	K5	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
29	K8	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
29	DG	201	PEB	C3B-C4B-NB	3.73	115.48	110.05
29	DQ	201	PEB	C3B-C4B-NB	3.73	115.48	110.05
29	PR	201	PEB	C3B-C4B-NB	3.73	115.48	110.05
29	F8	201	PEB	CMB-C2B-C1B	3.73	130.81	125.06
29	IG	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
29	IQ	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
31	N1	1001	CYC	CHB-C1B-NB	-3.73	118.05	126.06
29	HG	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	HQ	201	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	C8	201	PEB	C3D-C4D-ND	3.73	114.58	107.26
29	G5	201	PEB	CMB-C2B-C1B	3.73	130.81	125.06
31	J1	1001	CYC	CHB-C1B-NB	-3.73	118.05	126.06
31	JK	1001	CYC	CHB-C1B-NB	-3.73	118.05	126.06
29	MB	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	cF	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	cI	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	MM	202	PEB	C2A-C1A-NA	3.73	111.49	108.27
29	JJ	202	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
29	JL	202	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
29	KB	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	mB	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	hF	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	hI	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	KM	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mM	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
31	D1	1001	CYC	CHB-C1B-NB	-3.73	118.05	126.06
29	B5	203	PEB	CHB-C4B-NB	-3.73	123.66	128.83
29	XJ	202	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
29	XL	202	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
29	I8	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
29	IA	201	PEB	CMB-C2B-C1B	3.73	130.81	125.06
29	IN	201	PEB	CMB-C2B-C1B	3.73	130.81	125.06
29	aB	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	aM	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	TR	202	PEB	C3B-C4B-NB	3.73	115.47	110.05
29	AB	301	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
29	AB	302	PEB	CHC-C4C-C3C	-3.73	123.98	130.34
29	XJ	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	XL	203	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	H5	202	PEB	CHC-C1D-ND	-3.73	109.62	113.95
29	bF	201	PEB	CHA-C1B-NB	-3.73	117.14	124.93
29	bI	201	PEB	CHA-C1B-NB	-3.73	117.14	124.93
29	CB	202	PEB	C2A-C1A-NA	3.73	111.48	108.27
29	YB	203	PEB	C2A-C1A-NA	3.73	111.48	108.27
29	CM	202	PEB	C2A-C1A-NA	3.73	111.48	108.27
29	YM	203	PEB	C2A-C1A-NA	3.73	111.48	108.27
29	L4	202	PEB	CHA-C4A-NA	-3.73	120.78	125.20
29	XJ	202	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
29	XL	202	PEB	C1B-C2B-C3B	-3.73	102.23	106.51
29	FG	203	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
29	IJ	203	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
29	IL	203	PEB	C4B-C3B-C2B	-3.73	102.66	106.78
29	D3	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	JB	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	JM	202	PEB	OA-C1A-C2A	-3.73	123.21	126.17
29	A5	201	PEB	C3D-C4D-ND	3.73	114.57	107.26
31	M7	1001	CYC	C1B-NB-C4B	-3.73	105.93	110.67
29	AM	301	PEB	C1B-C2B-C3B	-3.72	102.23	106.51
29	gF	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	gI	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	KA	201	PEB	CMB-C2B-C1B	3.72	130.80	125.06
29	KN	201	PEB	CMB-C2B-C1B	3.72	130.80	125.06
29	V1	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
29	VK	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
31	GF	1001	CYC	C1B-NB-C4B	-3.72	105.93	110.67
31	GI	1001	CYC	C1B-NB-C4B	-3.72	105.93	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KB	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
29	KM	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
30	xJ	305	PUB	CHB-C1C-C2C	-3.72	116.72	125.32
29	H4	201	PEB	C3B-C4B-NB	3.72	115.47	110.05
29	HG	203	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
29	CG	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	CQ	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	hJ	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
29	hL	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
29	B5	201	PEB	CMB-C2B-C1B	3.72	130.80	125.06
29	A8	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	IG	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	IQ	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	lB	202	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	lM	202	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	JQ	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	KA	201	PEB	C1B-C2B-C3B	-3.72	102.23	106.51
29	KN	201	PEB	C1B-C2B-C3B	-3.72	102.23	106.51
29	A9	304	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
29	C5	201	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	ZB	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
29	kB	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
29	ZM	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
29	kM	202	PEB	OA-C1A-C2A	-3.72	123.21	126.17
31	C7	1001	CYC	C1B-NB-C4B	-3.72	105.93	110.67
31	C9	1001	CYC	C1B-NB-C4B	-3.72	105.93	110.67
29	VB	202	PEB	CHB-C4B-NB	-3.72	123.67	128.83
29	VM	202	PEB	CHB-C4B-NB	-3.72	123.67	128.83
31	JF	1001	CYC	CHA-C1A-NA	-3.72	123.67	128.83
31	JI	1001	CYC	CHA-C1A-NA	-3.72	123.67	128.83
29	NJ	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
29	NL	202	PEB	C4B-C3B-C2B	-3.72	102.66	106.78
29	L5	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	GA	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	GN	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	hF	201	PEB	CHA-C1B-NB	-3.72	117.15	124.93
29	hI	201	PEB	CHA-C1B-NB	-3.72	117.15	124.93
29	T2	202	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	V2	202	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	WF	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	WI	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	A7	304	PEB	OA-C1A-C2A	-3.72	123.22	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	hJ	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	hL	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	P1	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	PK	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	Z7	202	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
29	Z9	202	PEB	CHC-C4C-C3C	-3.72	123.99	130.34
29	GG	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	GQ	202	PEB	C3D-C4D-ND	3.72	114.56	107.26
29	QB	204	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	QM	204	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	bF	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	bI	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	WF	201	PEB	CHA-C1B-NB	-3.72	117.15	124.93
29	WI	201	PEB	CHA-C1B-NB	-3.72	117.15	124.93
31	H1	1001	CYC	CHB-C1B-NB	-3.72	118.07	126.06
29	S2	202	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	jJ	202	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	jL	202	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	SF	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	BG	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	SI	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	BQ	201	PEB	C3B-C4B-NB	3.72	115.46	110.05
29	a1	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	fJ	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	aK	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	fL	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	NJ	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	NL	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	F5	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	L8	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	AA	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	AN	201	PEB	CMB-C2B-C1B	3.72	130.79	125.06
29	c1	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
29	cK	202	PEB	C4B-C3B-C2B	-3.72	102.67	106.78
31	I7	1001	CYC	C1B-NB-C4B	-3.72	105.94	110.67
31	I9	1001	CYC	C1B-NB-C4B	-3.72	105.94	110.67
29	EG	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
29	EQ	201	PEB	C3D-C4D-ND	3.72	114.55	107.26
29	AA	201	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	IA	201	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	AN	201	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	IN	201	PEB	C1B-C2B-C3B	-3.72	102.24	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L8	203	PEB	CHB-C4B-NB	-3.72	123.67	128.83
29	KB	202	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	aF	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	aI	203	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	KM	202	PEB	C2A-C1A-NA	3.72	111.48	108.27
29	YB	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	jB	202	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	PJ	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	WJ	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	PL	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	WL	203	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	YM	201	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	jM	202	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	wL	302	PEB	CHA-C4A-NA	-3.72	120.79	125.20
29	X2	201	PEB	C3B-C4B-NB	3.72	115.45	110.05
29	UF	202	PEB	C3B-C4B-NB	3.72	115.45	110.05
29	UI	202	PEB	C3B-C4B-NB	3.72	115.45	110.05
29	dJ	202	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	dL	202	PEB	C1B-C2B-C3B	-3.72	102.24	106.51
29	UR	202	PEB	OA-C1A-C2A	-3.72	123.22	126.17
29	QB	203	PEB	OD-C4D-ND	-3.72	120.43	125.93
29	QM	203	PEB	OD-C4D-ND	-3.72	120.43	125.93
29	a7	203	PEB	CHC-C1D-ND	-3.72	109.63	113.95
29	a9	203	PEB	CHC-C1D-ND	-3.72	109.63	113.95
29	F5	203	PEB	CMB-C2B-C1B	3.72	130.78	125.06
29	fF	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	fI	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	U1	201	PEB	C4B-C3B-C2B	-3.71	102.67	106.78
29	UK	201	PEB	C4B-C3B-C2B	-3.71	102.67	106.78
29	KG	201	PEB	C3D-C4D-ND	3.71	114.55	107.26
29	KG	202	PEB	C3D-C4D-ND	3.71	114.55	107.26
29	KQ	201	PEB	C3D-C4D-ND	3.71	114.55	107.26
29	KQ	202	PEB	C3D-C4D-ND	3.71	114.55	107.26
29	OF	201	PEB	CHA-C1B-NB	-3.71	117.16	124.93
29	dF	202	PEB	CHA-C1B-NB	-3.71	117.16	124.93
29	fF	201	PEB	CHA-C1B-NB	-3.71	117.16	124.93
29	OI	201	PEB	CHA-C1B-NB	-3.71	117.16	124.93
29	dI	202	PEB	CHA-C1B-NB	-3.71	117.16	124.93
29	fI	201	PEB	CHA-C1B-NB	-3.71	117.16	124.93
29	G8	201	PEB	CMB-C2B-C1B	3.71	130.78	125.06
29	JG	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	JQ	201	PEB	C3B-C4B-NB	3.71	115.45	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DF	1001	CYC	CHA-C1A-NA	-3.71	123.67	128.83
31	DI	1001	CYC	CHA-C1A-NA	-3.71	123.67	128.83
29	cB	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	UJ	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	sJ	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	UL	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	sL	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	cM	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	MN	404	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	CG	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
29	CQ	201	PEB	C3D-C4D-ND	3.71	114.54	107.26
29	VR	202	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	R1	202	PEB	C4B-C3B-C2B	-3.71	102.67	106.78
29	RK	202	PEB	C4B-C3B-C2B	-3.71	102.67	106.78
29	HQ	203	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	HG	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	HQ	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	AB	303	PEB	C3D-C4D-ND	3.71	114.54	107.26
29	EB	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	EM	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	L8	203	PEB	CMB-C2B-C1B	3.71	130.78	125.06
29	Z1	201	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	ZK	201	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	F4	201	PEB	C3B-C4B-NB	3.71	115.45	110.05
29	RF	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	RI	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	SF	201	PEB	CHA-C1B-NB	-3.71	117.17	124.93
29	SI	201	PEB	CHA-C1B-NB	-3.71	117.17	124.93
29	BJ	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	BL	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	WR	202	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	LG	201	PEB	C3B-C4B-NB	3.71	115.44	110.05
29	MQ	402	PEB	C3B-C4B-NB	3.71	115.44	110.05
29	e1	202	PEB	C1B-C2B-C3B	-3.71	102.25	106.51
29	eK	202	PEB	C1B-C2B-C3B	-3.71	102.25	106.51
29	dF	202	PEB	C3B-C4B-NB	3.71	115.44	110.05
29	dI	202	PEB	C3B-C4B-NB	3.71	115.44	110.05
29	e7	201	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	e9	201	PEB	OA-C1A-C2A	-3.71	123.22	126.17
29	uJ	201	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	uL	201	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	C5	203	PEB	C2A-C1A-NA	3.71	111.47	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	hB	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	hM	202	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	F8	203	PEB	CMB-C2B-C1B	3.71	130.77	125.06
31	K9	1001	CYC	C1B-NB-C4B	-3.71	105.95	110.67
29	OB	201	PEB	OD-C4D-ND	-3.71	120.44	125.93
29	OM	201	PEB	OD-C4D-ND	-3.71	120.44	125.93
29	AG	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
29	AQ	201	PEB	C3D-C4D-ND	3.71	114.53	107.26
29	k1	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	kK	202	PEB	C4B-C3B-C2B	-3.71	102.68	106.78
29	gB	202	PEB	OA-C1A-C2A	-3.71	123.23	126.17
29	gM	202	PEB	OA-C1A-C2A	-3.71	123.23	126.17
29	FD	201	PEB	C3B-C4B-NB	3.71	115.44	110.05
29	L5	203	PEB	CMB-C2B-C1B	3.71	130.77	125.06
29	HA	203	PEB	OA-C1A-C2A	-3.71	123.23	126.17
29	HN	203	PEB	OA-C1A-C2A	-3.71	123.23	126.17
29	I5	203	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	I8	203	PEB	C2A-C1A-NA	3.71	111.47	108.27
29	e1	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
29	eK	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
29	P7	203	PEB	CHC-C1D-ND	-3.70	109.64	113.95
29	P9	203	PEB	CHC-C1D-ND	-3.70	109.64	113.95
29	j1	203	PEB	C4B-C3B-C2B	-3.70	102.68	106.78
29	AJ	203	PEB	C4B-C3B-C2B	-3.70	102.68	106.78
29	jK	203	PEB	C4B-C3B-C2B	-3.70	102.68	106.78
29	AL	203	PEB	C4B-C3B-C2B	-3.70	102.68	106.78
29	RR	202	PEB	C3B-C4B-NB	3.70	115.44	110.05
29	QF	201	PEB	CHA-C1B-NB	-3.70	117.18	124.93
29	QI	201	PEB	CHA-C1B-NB	-3.70	117.18	124.93
29	c1	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
29	cK	201	PEB	C3D-C4D-ND	3.70	114.53	107.26
29	F3	201	PEB	CMB-C2B-C1B	3.70	130.77	125.06
29	FO	201	PEB	CMB-C2B-C1B	3.70	130.77	125.06
29	RJ	202	PEB	C1B-C2B-C3B	-3.70	102.25	106.51
29	RL	202	PEB	C1B-C2B-C3B	-3.70	102.25	106.51
29	bF	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	bI	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	VB	201	PEB	C2A-C1A-NA	3.70	111.47	108.27
29	VM	201	PEB	C2A-C1A-NA	3.70	111.47	108.27
29	iB	202	PEB	CHB-C4B-NB	-3.70	123.69	128.83
29	iM	202	PEB	CHB-C4B-NB	-3.70	123.69	128.83
30	wL	305	PUB	OD-C4D-ND	-3.70	120.44	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1F	201	PEB	CHA-C1B-NB	-3.70	117.19	124.93
29	1I	201	PEB	CHA-C1B-NB	-3.70	117.19	124.93
29	EG	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
29	EQ	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
29	GB	202	PEB	C2A-C1A-NA	3.70	111.47	108.27
29	FG	203	PEB	C2A-C1A-NA	3.70	111.47	108.27
29	GM	202	PEB	C2A-C1A-NA	3.70	111.47	108.27
29	B8	203	PEB	CMB-C2B-C1B	3.70	130.77	125.06
29	M2	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	fJ	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	fL	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	QF	201	PEB	C3B-C4B-NB	3.70	115.44	110.05
29	QI	201	PEB	C3B-C4B-NB	3.70	115.44	110.05
29	X2	201	PEB	CHB-C4B-NB	-3.70	123.69	128.83
29	e1	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
29	eK	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
29	H8	201	PEB	CMB-C2B-C1B	3.70	130.76	125.06
29	AG	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
29	AQ	202	PEB	C3D-C4D-ND	3.70	114.52	107.26
29	rJ	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
29	rL	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
29	m7	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	m9	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	xL	303	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	FD	202	PEB	CHA-C4A-NA	-3.70	120.81	125.20
29	UF	202	PEB	CHA-C1B-NB	-3.70	117.19	124.93
29	UI	202	PEB	CHA-C1B-NB	-3.70	117.19	124.93
29	R2	202	PEB	C3B-C4B-NB	3.70	115.43	110.05
29	NR	202	PEB	C3B-C4B-NB	3.70	115.43	110.05
29	nJ	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
29	nL	202	PEB	C4B-C3B-C2B	-3.70	102.69	106.78
29	jF	201	PEB	C3B-C4B-NB	3.70	115.43	110.05
29	jI	201	PEB	C3B-C4B-NB	3.70	115.43	110.05
29	U1	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	VJ	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	UK	203	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	VL	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	B8	201	PEB	CMB-C2B-C1B	3.70	130.76	125.06
29	N2	202	PEB	C3B-C4B-NB	3.70	115.43	110.05
29	MA	404	PEB	C3B-C4B-NB	3.70	115.43	110.05
29	V7	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	V9	201	PEB	OA-C1A-C2A	-3.70	123.23	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VB	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	fF	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	jF	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	fI	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	jI	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	VM	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	BG	203	PEB	C2A-C1A-NA	3.70	111.46	108.27
29	a1	201	PEB	C3D-C4D-ND	3.70	114.51	107.26
29	aK	201	PEB	C3D-C4D-ND	3.70	114.51	107.26
29	MB	201	PEB	OD-C4D-ND	-3.70	120.45	125.93
29	MM	201	PEB	OD-C4D-ND	-3.70	120.45	125.93
29	LB	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
29	LM	202	PEB	OA-C1A-C2A	-3.70	123.23	126.17
30	wJ	305	PUB	OD-C4D-ND	-3.69	120.46	125.93
29	MB	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	MM	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	g1	202	PEB	C4B-C3B-C2B	-3.69	102.69	106.78
29	WJ	201	PEB	C4B-C3B-C2B	-3.69	102.69	106.78
29	gK	202	PEB	C4B-C3B-C2B	-3.69	102.69	106.78
29	WL	201	PEB	C4B-C3B-C2B	-3.69	102.69	106.78
29	F3	202	PEB	C2A-C1A-NA	3.69	111.46	108.27
29	FO	202	PEB	C2A-C1A-NA	3.69	111.46	108.27
29	P7	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	P9	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	WF	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	WI	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	jF	201	PEB	CHA-C1B-NB	-3.69	117.21	124.93
29	jI	201	PEB	CHA-C1B-NB	-3.69	117.21	124.93
29	AM	303	PEB	C3D-C4D-ND	3.69	114.51	107.26
29	K5	203	PEB	C2A-C1A-NA	3.69	111.46	108.27
29	K8	203	PEB	C2A-C1A-NA	3.69	111.46	108.27
29	M3	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	B5	203	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	MO	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	A7	304	PEB	CHC-C4C-C3C	-3.69	124.04	130.34
29	wJ	302	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	H5	203	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	BD	201	PEB	C3B-C4B-NB	3.69	115.42	110.05
29	BQ	203	PEB	C2A-C1A-NA	3.69	111.46	108.27
29	wJ	302	PEB	CHA-C4A-NA	-3.69	120.81	125.20
29	SR	201	PEB	CHC-C4C-C3C	-3.69	124.04	130.34
29	C5	201	PEB	CHC-C4C-C3C	-3.69	124.04	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	xJ	302	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	YB	201	PEB	CHB-C4B-NB	-3.69	123.71	128.83
29	YM	201	PEB	CHB-C4B-NB	-3.69	123.71	128.83
29	RR	202	PEB	CHB-C4B-NB	-3.69	123.71	128.83
29	U1	201	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
29	Z1	201	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
29	UK	201	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
29	ZK	201	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
29	R1	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
29	RK	201	PEB	C3D-C4D-ND	3.69	114.50	107.26
29	ZJ	202	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
29	ZL	202	PEB	C4B-C3B-C2B	-3.69	102.70	106.78
31	I1	1001	CYC	C4D-CHA-C1A	3.69	133.22	128.81
31	HF	1001	CYC	C4A-C3A-C2A	-3.69	102.27	106.51
31	HI	1001	CYC	C4A-C3A-C2A	-3.69	102.27	106.51
29	A5	201	PEB	CHC-C4C-C3C	-3.69	124.05	130.34
29	A8	201	PEB	CHC-C4C-C3C	-3.69	124.05	130.34
29	J3	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	wL	302	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	JO	201	PEB	CMB-C2B-C1B	3.69	130.75	125.06
29	O2	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	a7	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	a9	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	XR	202	PEB	CHB-C4B-NB	-3.69	123.71	128.83
29	IB	201	PEB	CMB-C2B-C1B	3.69	130.74	125.06
29	IM	201	PEB	CMB-C2B-C1B	3.69	130.74	125.06
29	l1	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	lK	202	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	h1	202	PEB	C3D-C4D-ND	3.69	114.49	107.26
29	hK	202	PEB	C3D-C4D-ND	3.69	114.49	107.26
29	g1	202	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
29	gK	202	PEB	C1B-C2B-C3B	-3.69	102.27	106.51
29	R7	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	R9	201	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	DA	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	DN	203	PEB	OA-C1A-C2A	-3.69	123.24	126.17
29	ZB	202	PEB	CHB-C4B-NB	-3.69	123.71	128.83
29	ZM	202	PEB	CHB-C4B-NB	-3.69	123.71	128.83
29	G4	202	PEB	CBC-CAC-C2C	-3.69	106.33	112.62
29	I4	202	PEB	CBC-CAC-C2C	-3.69	106.33	112.62
29	HD	201	PEB	C3B-C4B-NB	3.69	115.41	110.05
29	lF	201	PEB	C3B-C4B-NB	3.69	115.41	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	II	201	PEB	C3B-C4B-NB	3.69	115.41	110.05
29	dB	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
29	TF	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
29	TI	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
29	dM	202	PEB	C2A-C1A-NA	3.69	111.45	108.27
29	W1	202	PEB	C3D-C4D-ND	3.68	114.49	107.26
29	WK	202	PEB	C3D-C4D-ND	3.68	114.49	107.26
29	D4	201	PEB	C3B-C4B-NB	3.68	115.41	110.05
29	DD	201	PEB	C3B-C4B-NB	3.68	115.41	110.05
29	KB	201	PEB	CMB-C2B-C1B	3.68	130.74	125.06
29	wJ	302	PEB	CMB-C2B-C1B	3.68	130.74	125.06
29	KM	201	PEB	CMB-C2B-C1B	3.68	130.74	125.06
29	ZF	201	PEB	CHA-C1B-NB	-3.68	117.23	124.93
29	ZI	201	PEB	CHA-C1B-NB	-3.68	117.23	124.93
29	IB	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	IM	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	C4	202	PEB	CBC-CAC-C2C	-3.68	106.33	112.62
31	LF	1001	CYC	C4A-C3A-C2A	-3.68	102.28	106.51
31	LI	1001	CYC	C4A-C3A-C2A	-3.68	102.28	106.51
29	RB	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
29	RM	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
31	HF	1001	CYC	C1B-NB-C4B	-3.68	105.98	110.67
31	HI	1001	CYC	C1B-NB-C4B	-3.68	105.98	110.67
29	A1	301	PEB	CMB-C2B-C1B	3.68	130.74	125.06
29	AK	301	PEB	CMB-C2B-C1B	3.68	130.74	125.06
31	NF	1001	CYC	C4A-C3A-C2A	-3.68	102.28	106.51
31	NI	1001	CYC	C4A-C3A-C2A	-3.68	102.28	106.51
29	J3	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	jB	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	mF	203	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	mI	203	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	jM	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	JO	202	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	Z1	203	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	j1	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	ZK	203	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	jK	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	MN	401	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	K5	201	PEB	CHC-C4C-C3C	-3.68	124.06	130.34
29	K8	201	PEB	CHC-C4C-C3C	-3.68	124.06	130.34
29	D3	201	PEB	CMB-C2B-C1B	3.68	130.74	125.06
29	DO	201	PEB	CMB-C2B-C1B	3.68	130.74	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j1	202	PEB	OA-C1A-C2A	-3.68	123.25	126.17
29	jK	202	PEB	OA-C1A-C2A	-3.68	123.25	126.17
29	CC	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	CE	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	c1	202	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
29	cK	202	PEB	C1B-C2B-C3B	-3.68	102.28	106.51
29	xJ	303	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	G8	203	PEB	CMB-C2B-C1B	3.68	130.73	125.06
29	P2	201	PEB	CHB-C4B-NB	-3.68	123.72	128.83
29	mB	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
29	mM	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
31	JF	1001	CYC	C4A-C3A-C2A	-3.68	102.28	106.51
31	JI	1001	CYC	C4A-C3A-C2A	-3.68	102.28	106.51
29	QB	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
29	QM	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
29	FB	201	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	FM	201	PEB	C2A-C1A-NA	3.68	111.45	108.27
29	HC	201	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
29	HE	201	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
31	LF	1001	CYC	C1B-NB-C4B	-3.68	105.98	110.67
31	LI	1001	CYC	C1B-NB-C4B	-3.68	105.98	110.67
29	E4	202	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
29	UF	203	PEB	OA-C1A-C2A	-3.68	123.25	126.17
29	UI	203	PEB	OA-C1A-C2A	-3.68	123.25	126.17
29	l1	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	lK	202	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	F7	1002	PEB	C2A-C1A-NA	3.68	111.44	108.27
29	LC	201	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
29	LE	201	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
29	R2	202	PEB	CHB-C4B-NB	-3.68	123.72	128.83
29	xL	303	PEB	C3D-C4D-ND	3.68	114.48	107.26
31	NF	1001	CYC	C1B-NB-C4B	-3.68	105.98	110.67
31	NI	1001	CYC	C1B-NB-C4B	-3.68	105.98	110.67
29	MD	202	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
29	IB	201	PEB	OD-C4D-ND	-3.68	120.48	125.93
29	IM	201	PEB	OD-C4D-ND	-3.68	120.48	125.93
29	JF	1002	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
29	JI	1002	PEB	C4B-C3B-C2B	-3.68	102.71	106.78
29	j1	202	PEB	CHC-C4C-C3C	-3.68	124.06	130.34
29	jK	202	PEB	CHC-C4C-C3C	-3.68	124.06	130.34
29	I4	203	PEB	C2A-C1A-NA	3.68	111.44	108.27
29	T1	201	PEB	C3D-C4D-ND	3.68	114.48	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TK	201	PEB	C3D-C4D-ND	3.68	114.48	107.26
29	k1	201	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	AC	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	AE	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	kK	201	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	MA	401	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	T2	202	PEB	CHB-C4B-NB	-3.68	123.73	128.83
29	ID	202	PEB	CBC-CAC-C2C	-3.68	106.34	112.62
29	fB	201	PEB	OD-C4D-ND	-3.68	120.48	125.93
29	hB	201	PEB	OD-C4D-ND	-3.68	120.48	125.93
29	fM	201	PEB	OD-C4D-ND	-3.68	120.48	125.93
29	hM	201	PEB	OD-C4D-ND	-3.68	120.48	125.93
29	OF	201	PEB	C3B-C4B-NB	3.68	115.40	110.05
29	OI	201	PEB	C3B-C4B-NB	3.68	115.40	110.05
29	U1	203	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	GC	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	GE	202	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	UK	203	PEB	C3D-C4D-ND	3.68	114.47	107.26
29	gB	202	PEB	CHB-C4B-NB	-3.68	123.73	128.83
29	gM	202	PEB	CHB-C4B-NB	-3.68	123.73	128.83
31	DF	1001	CYC	C4A-C3A-C2A	-3.68	102.29	106.51
31	DI	1001	CYC	C4A-C3A-C2A	-3.68	102.29	106.51
29	T7	201	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	T9	201	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	xJ	302	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	CB	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	CM	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	BC	201	PEB	CBC-CAC-C2C	-3.67	106.35	112.62
29	BE	201	PEB	CBC-CAC-C2C	-3.67	106.35	112.62
29	QB	203	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	IB	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	QM	203	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	IM	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	L4	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
29	LD	201	PEB	C3B-C4B-NB	3.67	115.39	110.05
29	CD	202	PEB	CBC-CAC-C2C	-3.67	106.35	112.62
29	aB	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	aM	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	ED	201	PEB	CBC-CAC-C2C	-3.67	106.35	112.62
29	V1	201	PEB	C3D-C4D-ND	3.67	114.47	107.26
29	VK	201	PEB	C3D-C4D-ND	3.67	114.47	107.26
29	C8	203	PEB	C2A-C1A-NA	3.67	111.44	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L9	1002	PEB	C2A-C1A-NA	3.67	111.44	108.27
29	FA	202	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	FN	202	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	b1	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	bK	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	DC	201	PEB	CBC-CAC-C2C	-3.67	106.35	112.62
29	DE	201	PEB	CBC-CAC-C2C	-3.67	106.35	112.62
29	F9	1002	PEB	C2A-C1A-NA	3.67	111.44	108.27
29	Q1	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	S1	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	QK	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	SK	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	k7	201	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	k9	201	PEB	OA-C1A-C2A	-3.67	123.25	126.17
29	UB	201	PEB	OD-C4D-ND	-3.67	120.49	125.93
29	UM	201	PEB	OD-C4D-ND	-3.67	120.49	125.93
29	eB	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
29	eM	201	PEB	C2A-C1A-NA	3.67	111.44	108.27
29	dJ	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	dL	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	aB	203	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	aM	203	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	j1	203	PEB	C1B-C2B-C3B	-3.67	102.29	106.51
29	jK	203	PEB	C1B-C2B-C3B	-3.67	102.29	106.51
29	EB	201	PEB	OD-C4D-ND	-3.67	120.49	125.93
29	EM	201	PEB	OD-C4D-ND	-3.67	120.49	125.93
29	OB	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	OM	201	PEB	CMB-C2B-C1B	3.67	130.72	125.06
29	HD	202	PEB	CHA-C4A-NA	-3.67	120.84	125.20
29	LC	203	PEB	CHC-C1D-ND	-3.67	109.69	113.95
29	LE	203	PEB	CHC-C1D-ND	-3.67	109.69	113.95
29	m1	201	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	mK	201	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	d1	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	dK	202	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	P1	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
29	V1	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
29	a1	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
29	PK	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
29	VK	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
29	aK	202	PEB	C1B-C2B-C3B	-3.67	102.30	106.51
29	KC	203	PEB	C3D-C4D-ND	3.67	114.46	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KE	203	PEB	C3D-C4D-ND	3.67	114.46	107.26
29	aB	201	PEB	OD-C4D-ND	-3.67	120.50	125.93
29	aM	201	PEB	OD-C4D-ND	-3.67	120.50	125.93
29	K4	202	PEB	CBC-CAC-C2C	-3.67	106.36	112.62
29	JC	201	PEB	CBC-CAC-C2C	-3.67	106.36	112.62
29	JE	201	PEB	CBC-CAC-C2C	-3.67	106.36	112.62
29	TR	202	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	M4	202	PEB	CBC-CAC-C2C	-3.67	106.36	112.62
29	ZF	201	PEB	C3B-C4B-NB	3.67	115.38	110.05
29	ZI	201	PEB	C3B-C4B-NB	3.67	115.38	110.05
29	GB	201	PEB	OD-C4D-ND	-3.67	120.50	125.93
29	GM	201	PEB	OD-C4D-ND	-3.67	120.50	125.93
30	MA	402	PUB	CBA-CAA-C3A	-3.67	107.42	112.98
29	FB	202	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	KB	203	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	FM	202	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	KM	203	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	PR	201	PEB	CHB-C4B-NB	-3.67	123.74	128.83
29	xL	302	PEB	CMB-C2B-C1B	3.67	130.71	125.06
31	FF	1001	CYC	C4A-C3A-C2A	-3.67	102.30	106.51
31	FI	1001	CYC	C4A-C3A-C2A	-3.67	102.30	106.51
29	RJ	202	PEB	C3D-C4D-ND	3.67	114.45	107.26
29	RL	202	PEB	C3D-C4D-ND	3.67	114.45	107.26
31	FF	1001	CYC	C1B-NB-C4B	-3.67	106.00	110.67
31	FI	1001	CYC	C1B-NB-C4B	-3.67	106.00	110.67
29	GD	202	PEB	CBC-CAC-C2C	-3.67	106.36	112.62
30	AF	302	PUB	C1C-C2C-C3C	-3.67	102.73	106.78
30	AI	302	PUB	C1C-C2C-C3C	-3.67	102.73	106.78
29	H3	201	PEB	CMB-C2B-C1B	3.67	130.71	125.06
29	HO	201	PEB	CMB-C2B-C1B	3.67	130.71	125.06
29	wL	302	PEB	OA-C1A-C2A	-3.66	123.26	126.17
29	dB	201	PEB	OD-C4D-ND	-3.66	120.50	125.93
29	dM	201	PEB	OD-C4D-ND	-3.66	120.50	125.93
29	C8	201	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	GB	201	PEB	CMB-C2B-C1B	3.66	130.71	125.06
29	GM	201	PEB	CMB-C2B-C1B	3.66	130.71	125.06
29	TB	202	PEB	CHB-C4B-NB	-3.66	123.74	128.83
29	TM	202	PEB	CHB-C4B-NB	-3.66	123.74	128.83
29	MQ	407	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
29	Q1	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	QK	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	O1	202	PEB	C3D-C4D-ND	3.66	114.45	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HJ	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
29	OK	202	PEB	C3D-C4D-ND	3.66	114.45	107.26
29	HL	201	PEB	C3D-C4D-ND	3.66	114.45	107.26
29	DB	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	DM	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	BC	203	PEB	CHC-C1D-ND	-3.66	109.69	113.95
29	BE	203	PEB	CHC-C1D-ND	-3.66	109.69	113.95
29	FC	201	PEB	CBC-CAC-C2C	-3.66	106.37	112.62
29	FE	201	PEB	CBC-CAC-C2C	-3.66	106.37	112.62
29	L3	201	PEB	CMB-C2B-C1B	3.66	130.70	125.06
29	UB	201	PEB	CMB-C2B-C1B	3.66	130.70	125.06
29	UM	201	PEB	CMB-C2B-C1B	3.66	130.70	125.06
29	LO	201	PEB	CMB-C2B-C1B	3.66	130.70	125.06
29	f1	202	PEB	OA-C1A-C2A	-3.66	123.26	126.17
29	fK	202	PEB	OA-C1A-C2A	-3.66	123.26	126.17
29	wL	303	PEB	OA-C1A-C2A	-3.66	123.26	126.17
29	AF	301	PEB	C1C-CHB-C4B	-3.66	124.44	128.81
29	AI	301	PEB	C1C-CHB-C4B	-3.66	124.44	128.81
29	b1	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	bK	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	HF	1002	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
29	HI	1002	PEB	C4B-C3B-C2B	-3.66	102.73	106.78
29	EC	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	EE	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	jJ	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	jL	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	f1	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	l1	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	fK	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	lK	202	PEB	CHC-C4C-C3C	-3.66	124.09	130.34
29	P1	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	i1	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	PK	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	iK	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
31	JF	1001	CYC	C1B-NB-C4B	-3.66	106.01	110.67
31	JI	1001	CYC	C1B-NB-C4B	-3.66	106.01	110.67
29	JD	201	PEB	C3B-C4B-NB	3.66	115.37	110.05
29	IJ	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	IL	203	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	NR	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	Y1	201	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	YK	201	PEB	C3D-C4D-ND	3.66	114.44	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	E7	1001	CYC	CBD-CAD-C3D	-3.66	106.38	112.62
31	E9	1001	CYC	CBD-CAD-C3D	-3.66	106.38	112.62
31	D7	1001	CYC	C2A-C1A-NA	3.66	115.37	110.05
31	D9	1001	CYC	C2A-C1A-NA	3.66	115.37	110.05
29	Z1	203	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	cF	201	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	cI	201	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	ZK	203	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	f1	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
29	fK	202	PEB	C3D-C4D-ND	3.66	114.44	107.26
31	LF	1001	CYC	CHB-C1B-NB	-3.66	118.20	126.06
31	LI	1001	CYC	CHB-C1B-NB	-3.66	118.20	126.06
29	LB	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	cB	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	LM	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	cM	202	PEB	CHB-C4B-NB	-3.66	123.75	128.83
29	i7	201	PEB	OA-C1A-C2A	-3.66	123.27	126.17
29	i9	201	PEB	OA-C1A-C2A	-3.66	123.27	126.17
29	fJ	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	fL	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	AM	301	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	J7	1002	PEB	C2A-C1A-NA	3.66	111.42	108.27
29	I8	201	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	JD	202	PEB	CHA-C4A-NA	-3.66	120.86	125.20
29	hB	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
29	hM	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
29	WJ	201	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	nJ	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	WL	201	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	nL	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	lB	201	PEB	OD-C4D-ND	-3.66	120.51	125.93
29	lM	201	PEB	OD-C4D-ND	-3.66	120.51	125.93
29	VR	202	PEB	CHB-C4B-NB	-3.66	123.76	128.83
29	pJ	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	pL	202	PEB	C3D-C4D-ND	3.66	114.43	107.26
29	fB	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
29	fM	201	PEB	CMB-C2B-C1B	3.66	130.69	125.06
29	TB	201	PEB	C2A-C1A-NA	3.66	111.42	108.27
29	TM	201	PEB	C2A-C1A-NA	3.66	111.42	108.27
29	W1	202	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	WK	202	PEB	CHC-C4C-C3C	-3.66	124.10	130.34
29	O1	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	OK	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
29	jB	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	jM	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	J4	201	PEB	C3B-C4B-NB	3.65	115.36	110.05
29	xL	302	PEB	CHA-C4A-NA	-3.65	120.86	125.20
29	sJ	203	PEB	C3D-C4D-ND	3.65	114.43	107.26
29	sL	203	PEB	C3D-C4D-ND	3.65	114.43	107.26
29	DF	1002	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
29	DI	1002	PEB	C4B-C3B-C2B	-3.65	102.74	106.78
31	E1	1001	CYC	C4D-CHA-C1A	3.65	133.17	128.81
29	B3	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	dB	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	dM	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	BO	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	S1	202	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
29	SK	202	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
29	XJ	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
29	XL	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
29	CB	201	PEB	OD-C4D-ND	-3.65	120.52	125.93
29	CM	201	PEB	OD-C4D-ND	-3.65	120.52	125.93
29	h1	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
29	hK	202	PEB	OA-C1A-C2A	-3.65	123.27	126.17
29	NO	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	hJ	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
29	hL	202	PEB	C3D-C4D-ND	3.65	114.43	107.26
29	JB	202	PEB	CHB-C4B-NB	-3.65	123.76	128.83
29	JM	202	PEB	CHB-C4B-NB	-3.65	123.76	128.83
29	ZJ	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	ZL	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	EB	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	YB	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	EM	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	YM	202	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	xJ	302	PEB	CHA-C4A-NA	-3.65	120.86	125.20
29	OF	203	PEB	C3B-C4B-NB	3.65	115.36	110.05
29	OI	203	PEB	C3B-C4B-NB	3.65	115.36	110.05
29	K8	201	PEB	CHA-C1B-NB	-3.65	117.30	124.93
31	C7	1001	CYC	CBD-CAD-C3D	-3.65	106.39	112.62
31	C9	1001	CYC	CBD-CAD-C3D	-3.65	106.39	112.62
29	JG	203	PEB	C2A-C1A-NA	3.65	111.42	108.27
31	NF	1001	CYC	C2C-C1C-NC	3.65	111.42	108.27
31	NI	1001	CYC	C2C-C1C-NC	3.65	111.42	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WB	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	WM	201	PEB	CMB-C2B-C1B	3.65	130.69	125.06
29	JJ	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	wJ	303	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	JL	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
31	K7	1001	CYC	CBD-CAD-C3D	-3.65	106.39	112.62
29	A5	203	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	A8	203	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	JB	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	cB	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	JM	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	cM	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	N2	202	PEB	CHB-C4B-NB	-3.65	123.77	128.83
29	i1	202	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
29	iK	202	PEB	C1B-C2B-C3B	-3.65	102.32	106.51
29	B4	201	PEB	C3B-C4B-NB	3.65	115.36	110.05
31	G7	1001	CYC	CBD-CAD-C3D	-3.65	106.39	112.62
29	IC	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	IE	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	D4	202	PEB	CHA-C4A-NA	-3.65	120.87	125.20
29	WB	201	PEB	OD-C4D-ND	-3.65	120.53	125.93
29	WM	201	PEB	OD-C4D-ND	-3.65	120.53	125.93
29	FJ	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	FL	202	PEB	C3D-C4D-ND	3.65	114.42	107.26
29	LC	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	LE	201	PEB	C2A-C1A-NA	3.65	111.42	108.27
31	FF	1001	CYC	CHB-C1B-NB	-3.65	118.23	126.06
31	FI	1001	CYC	CHB-C1B-NB	-3.65	118.23	126.06
29	I5	201	PEB	CHC-C4C-C3C	-3.65	124.11	130.34
30	MN	402	PUB	CBA-CAA-C3A	-3.65	107.45	112.98
29	SB	201	PEB	OD-C4D-ND	-3.65	120.53	125.93
29	SM	201	PEB	OD-C4D-ND	-3.65	120.53	125.93
29	G5	203	PEB	CMB-C2B-C1B	3.65	130.68	125.06
29	h1	202	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	AB	301	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	hK	202	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
30	xL	305	PUB	OD-C4D-ND	-3.65	120.53	125.93
29	D7	1002	PEB	C2A-C1A-NA	3.65	111.42	108.27
29	D9	1002	PEB	C2A-C1A-NA	3.65	111.42	108.27
31	LF	1001	CYC	C2C-C1C-NC	3.65	111.42	108.27
31	LI	1001	CYC	C2C-C1C-NC	3.65	111.42	108.27
29	PJ	202	PEB	C3D-C4D-ND	3.65	114.41	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	PL	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
29	U1	203	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	d1	202	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	UK	203	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	dK	202	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
31	NF	1001	CYC	CHB-C1B-NB	-3.65	118.23	126.06
31	NI	1001	CYC	CHB-C1B-NB	-3.65	118.23	126.06
29	rJ	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
29	rL	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
29	KB	201	PEB	OD-C4D-ND	-3.65	120.53	125.93
29	KM	201	PEB	OD-C4D-ND	-3.65	120.53	125.93
29	SB	201	PEB	CMB-C2B-C1B	3.65	130.68	125.06
29	SM	201	PEB	CMB-C2B-C1B	3.65	130.68	125.06
31	J7	1001	CYC	C2A-C1A-NA	3.65	115.35	110.05
31	JF	1001	CYC	CHB-C1B-NB	-3.65	118.23	126.06
31	JI	1001	CYC	CHB-C1B-NB	-3.65	118.23	126.06
29	TJ	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
29	TL	202	PEB	C3D-C4D-ND	3.65	114.41	107.26
29	YF	201	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	YI	201	PEB	CHC-C4C-C3C	-3.65	124.12	130.34
29	KD	202	PEB	CBC-CAC-C2C	-3.64	106.40	112.62
29	I5	202	PEB	CHB-C4B-NB	-3.64	123.77	128.83
29	I8	202	PEB	CHB-C4B-NB	-3.64	123.77	128.83
29	kB	202	PEB	CHB-C4B-NB	-3.64	123.77	128.83
29	kM	202	PEB	CHB-C4B-NB	-3.64	123.77	128.83
31	DF	1001	CYC	C2C-C1C-NC	3.64	111.42	108.27
31	DI	1001	CYC	C2C-C1C-NC	3.64	111.42	108.27
29	NJ	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	NL	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
31	K9	1001	CYC	CBD-CAD-C3D	-3.64	106.40	112.62
29	bJ	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	bL	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
31	D1	1003	CYC	C4D-CHA-C1A	3.64	133.16	128.81
29	YB	201	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	YM	201	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	H3	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	J9	1002	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	NB	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	NM	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	HO	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	b1	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17
29	bK	202	PEB	OA-C1A-C2A	-3.64	123.28	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k1	202	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
29	kK	202	PEB	C1B-C2B-C3B	-3.64	102.33	106.51
29	g1	201	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	lJ	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	gK	201	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	lL	202	PEB	C3D-C4D-ND	3.64	114.41	107.26
29	wL	303	PEB	C3D-C4D-ND	3.64	114.41	107.26
30	AM	305	PUB	C1C-C2C-C3C	-3.64	102.75	106.78
29	N7	1002	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	N9	1002	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	JC	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	JE	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	FB	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
29	FM	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
29	FF	1002	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
29	FI	1002	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
29	eF	202	PEB	C3B-C4B-NB	3.64	115.35	110.05
29	eI	202	PEB	C3B-C4B-NB	3.64	115.35	110.05
29	C5	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	C8	202	PEB	C2A-C1A-NA	3.64	111.41	108.27
31	HF	1001	CYC	CHB-C1B-NB	-3.64	118.24	126.06
31	HI	1001	CYC	CHB-C1B-NB	-3.64	118.24	126.06
29	BJ	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
29	BL	202	PEB	C3D-C4D-ND	3.64	114.40	107.26
29	J3	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
29	JO	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
31	J9	1001	CYC	C2A-C1A-NA	3.64	115.34	110.05
29	uJ	201	PEB	C3D-C4D-ND	3.64	114.40	107.26
29	uL	201	PEB	C3D-C4D-ND	3.64	114.40	107.26
29	TI	201	PEB	CHC-C4C-C3C	-3.64	124.13	130.34
29	g7	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
29	g9	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
30	xJ	305	PUB	OD-C4D-ND	-3.64	120.54	125.93
29	AJ	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
29	AL	203	PEB	C3D-C4D-ND	3.64	114.40	107.26
29	kB	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	kM	201	PEB	C2A-C1A-NA	3.64	111.41	108.27
29	LF	1002	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
29	LI	1002	PEB	C4B-C3B-C2B	-3.64	102.75	106.78
29	mF	202	PEB	C3B-C4B-NB	3.64	115.34	110.05
29	mI	202	PEB	C3B-C4B-NB	3.64	115.34	110.05
31	F7	1001	CYC	C2A-C1A-NA	3.64	115.34	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B4	202	PEB	CHA-C4A-NA	-3.64	120.88	125.20
29	mB	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
29	mM	201	PEB	CMB-C2B-C1B	3.64	130.67	125.06
31	EK	1001	CYC	C4D-CHA-C1A	3.64	133.16	128.81
29	DC	202	PEB	CHC-C1D-ND	-3.64	109.72	113.95
29	DE	202	PEB	CHC-C1D-ND	-3.64	109.72	113.95
29	gF	201	PEB	CHC-C4C-C3C	-3.64	124.13	130.34
29	gI	201	PEB	CHC-C4C-C3C	-3.64	124.13	130.34
29	Y7	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
29	Y9	201	PEB	OA-C1A-C2A	-3.64	123.28	126.17
31	G9	1001	CYC	CBD-CAD-C3D	-3.64	106.41	112.62
29	JC	202	PEB	CHC-C1D-ND	-3.64	109.72	113.95
29	JE	202	PEB	CHC-C1D-ND	-3.64	109.72	113.95
31	F9	1001	CYC	C2A-C1A-NA	3.64	115.34	110.05
29	NB	201	PEB	CMB-C2B-C1B	3.64	130.66	125.06
29	NM	201	PEB	CMB-C2B-C1B	3.64	130.66	125.06
29	xJ	301	PEB	CHC-C4C-C3C	-3.64	124.14	130.34
29	YB	202	PEB	OD-C4D-ND	-3.64	120.54	125.93
29	jB	201	PEB	OD-C4D-ND	-3.64	120.54	125.93
29	YM	202	PEB	OD-C4D-ND	-3.64	120.54	125.93
29	jM	201	PEB	OD-C4D-ND	-3.64	120.54	125.93
29	cB	202	PEB	C3D-C4D-ND	3.64	114.39	107.26
29	cM	202	PEB	C3D-C4D-ND	3.64	114.39	107.26
29	A9	304	PEB	OA-C1A-C2A	-3.64	123.28	126.17
31	CK	1001	CYC	C4D-CHA-C1A	3.64	133.15	128.81
29	RF	201	PEB	CHC-C4C-C3C	-3.64	124.14	130.34
29	RI	201	PEB	CHC-C4C-C3C	-3.64	124.14	130.34
29	I5	201	PEB	CHA-C1B-NB	-3.64	117.33	124.93
29	K5	201	PEB	CHA-C1B-NB	-3.64	117.33	124.93
29	I8	201	PEB	CHA-C1B-NB	-3.64	117.33	124.93
31	M9	1001	CYC	CBD-CAD-C3D	-3.63	106.42	112.62
29	JA	202	PEB	OA-C1A-C2A	-3.63	123.28	126.17
29	JA	203	PEB	OA-C1A-C2A	-3.63	123.28	126.17
29	JN	202	PEB	OA-C1A-C2A	-3.63	123.28	126.17
29	JN	203	PEB	OA-C1A-C2A	-3.63	123.28	126.17
29	C8	201	PEB	CHA-C1B-NB	-3.63	117.33	124.93
29	VF	201	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
29	VI	201	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
29	MR	202	PEB	OA-C1A-C2A	-3.63	123.28	126.17
31	DF	1001	CYC	C1B-NB-C4B	-3.63	106.04	110.67
31	DI	1001	CYC	C1B-NB-C4B	-3.63	106.04	110.67
29	C8	201	PEB	C2A-C1A-NA	3.63	111.41	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	GK	1001	CYC	C4D-CHA-C1A	3.63	133.15	128.81
31	IK	1001	CYC	C4D-CHA-C1A	3.63	133.15	128.81
31	DF	1001	CYC	CHB-C1B-NB	-3.63	118.26	126.06
31	DI	1001	CYC	CHB-C1B-NB	-3.63	118.26	126.06
29	ZB	201	PEB	CMB-C2B-C1B	3.63	130.66	125.06
29	ZM	201	PEB	CMB-C2B-C1B	3.63	130.66	125.06
29	A8	202	PEB	CHB-C4B-NB	-3.63	123.79	128.83
29	A5	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	A8	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	R1	202	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
29	RK	202	PEB	C1B-C2B-C3B	-3.63	102.34	106.51
29	JB	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	JM	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	MG	401	PEB	CBC-CAC-C2C	-3.63	106.42	112.62
29	O1	202	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
29	OK	202	PEB	CHC-C4C-C3C	-3.63	124.14	130.34
29	S1	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	d1	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	SK	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	dK	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	FA	203	PEB	CHC-C1D-ND	-3.63	109.73	113.95
29	FN	203	PEB	CHC-C1D-ND	-3.63	109.73	113.95
30	AB	305	PUB	C1C-C2C-C3C	-3.63	102.76	106.78
29	HB	201	PEB	CMB-C2B-C1B	3.63	130.66	125.06
29	HM	201	PEB	CMB-C2B-C1B	3.63	130.66	125.06
29	H4	202	PEB	CHA-C4A-NA	-3.63	120.89	125.20
29	ZB	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	ZM	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	FB	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	RB	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	FM	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	RM	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	AB	303	PEB	CMB-C2B-C1B	3.63	130.65	125.06
29	eF	202	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	eI	202	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	B3	201	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	BA	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	BN	202	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	BO	201	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	K8	202	PEB	CHB-C4B-NB	-3.63	123.79	128.83
29	TB	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	TM	202	PEB	C3D-C4D-ND	3.63	114.38	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BC	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	BE	201	PEB	C2A-C1A-NA	3.63	111.40	108.27
29	C5	201	PEB	CHA-C1B-NB	-3.63	117.35	124.93
29	gB	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	gM	202	PEB	C3D-C4D-ND	3.63	114.38	107.26
29	V1	203	PEB	CMB-C2B-C1B	3.63	130.65	125.06
29	PB	201	PEB	CMB-C2B-C1B	3.63	130.65	125.06
29	VK	203	PEB	CMB-C2B-C1B	3.63	130.65	125.06
29	PM	201	PEB	CMB-C2B-C1B	3.63	130.65	125.06
29	AF	304	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	AI	304	PEB	OA-C1A-C2A	-3.63	123.29	126.17
29	BD	202	PEB	CHA-C4A-NA	-3.63	120.89	125.20
29	DD	202	PEB	CHA-C4A-NA	-3.63	120.89	125.20
29	A5	201	PEB	CHA-C1B-NB	-3.63	117.35	124.93
29	A8	201	PEB	CHA-C1B-NB	-3.63	117.35	124.93
29	kB	202	PEB	C3D-C4D-ND	3.63	114.37	107.26
29	mB	202	PEB	C3D-C4D-ND	3.63	114.37	107.26
29	kM	202	PEB	C3D-C4D-ND	3.63	114.37	107.26
29	mM	202	PEB	C3D-C4D-ND	3.63	114.37	107.26
29	N3	201	PEB	CMB-C2B-C1B	3.62	130.65	125.06
29	JB	201	PEB	CMB-C2B-C1B	3.62	130.65	125.06
29	JM	201	PEB	CMB-C2B-C1B	3.62	130.65	125.06
29	HC	203	PEB	CHC-C1D-ND	-3.62	109.74	113.95
29	HE	203	PEB	CHC-C1D-ND	-3.62	109.74	113.95
29	MG	405	PEB	C4B-C3B-C2B	-3.62	102.77	106.78
30	MQ	405	PUB	CMA-C2A-C1A	3.62	129.92	121.39
29	MQ	403	PEB	CBC-CAC-C2C	-3.62	106.44	112.62
31	M7	1001	CYC	CBD-CAD-C3D	-3.62	106.44	112.62
29	iB	201	PEB	CMB-C2B-C1B	3.62	130.65	125.06
29	iM	201	PEB	CMB-C2B-C1B	3.62	130.65	125.06
29	aF	201	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	aI	201	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	B3	202	PEB	C2A-C1A-NA	3.62	111.40	108.27
29	BO	202	PEB	C2A-C1A-NA	3.62	111.40	108.27
29	Q1	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
29	QK	202	PEB	OA-C1A-C2A	-3.62	123.29	126.17
29	A5	202	PEB	CHB-C4B-NB	-3.62	123.80	128.83
29	BJ	203	PEB	C3B-C4B-NB	3.62	115.32	110.05
29	BL	203	PEB	C3B-C4B-NB	3.62	115.32	110.05
29	I5	201	PEB	C2A-C1A-NA	3.62	111.40	108.27
31	M1	1001	CYC	C4D-CHA-C1A	3.62	133.14	128.81
31	MK	1001	CYC	C4D-CHA-C1A	3.62	133.14	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	iI	203	PEB	CMB-C2B-C1B	3.62	130.64	125.06
29	iK	203	PEB	CMB-C2B-C1B	3.62	130.64	125.06
29	MQ	407	PEB	C3B-C4B-NB	3.62	115.32	110.05
29	DA	203	PEB	CHC-C1D-ND	-3.62	109.74	113.95
29	DN	203	PEB	CHC-C1D-ND	-3.62	109.74	113.95
29	DB	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
29	DM	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
29	iF	201	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	iI	201	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	wL	301	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	XJ	203	PEB	C3B-C4B-NB	3.62	115.32	110.05
29	XL	203	PEB	C3B-C4B-NB	3.62	115.32	110.05
29	kF	201	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	kI	201	PEB	CHC-C4C-C3C	-3.62	124.16	130.34
29	I3	203	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	gB	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	gM	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	IO	203	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	YF	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	gF	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	YI	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	gI	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	C5	202	PEB	CHB-C4B-NB	-3.62	123.81	128.83
29	C8	202	PEB	CHB-C4B-NB	-3.62	123.81	128.83
29	HB	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	iB	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	HM	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	iM	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	SR	201	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	Y1	202	PEB	CMB-C2B-C1B	3.62	130.64	125.06
29	YK	202	PEB	CMB-C2B-C1B	3.62	130.64	125.06
31	C1	1001	CYC	C4D-CHA-C1A	3.62	133.13	128.81
29	VF	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	VI	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	xL	301	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
29	LA	203	PEB	CHC-C1D-ND	-3.62	109.75	113.95
29	LN	203	PEB	CHC-C1D-ND	-3.62	109.75	113.95
29	VB	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
29	VM	202	PEB	C3D-C4D-ND	3.62	114.36	107.26
29	Z1	203	PEB	OA-C1A-C2A	-3.62	123.30	126.17
29	ZK	203	PEB	OA-C1A-C2A	-3.62	123.30	126.17
29	CC	202	PEB	C2A-C1A-NA	3.62	111.39	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CE	202	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	tJ	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	tL	202	PEB	C3B-C4B-NB	3.62	115.31	110.05
29	PF	201	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
29	PI	201	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
29	MQ	403	PEB	C2A-C1A-NA	3.62	111.39	108.27
29	xL	301	PEB	CHC-C1D-ND	-3.62	109.75	113.95
29	l7	201	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
29	l9	201	PEB	CHC-C4C-C3C	-3.62	124.17	130.34
29	wJ	303	PEB	OA-C1A-C2A	-3.61	123.30	126.17
29	T1	202	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	eB	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	TK	202	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	eM	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	mB	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
29	mM	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
31	N7	1001	CYC	C2A-C1A-NA	3.61	115.31	110.05
31	N9	1001	CYC	C2A-C1A-NA	3.61	115.31	110.05
29	aB	203	PEB	C3D-C4D-ND	3.61	114.35	107.26
29	aM	203	PEB	C3D-C4D-ND	3.61	114.35	107.26
29	DB	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	DM	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	NJ	203	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	NL	203	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	RB	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	RM	201	PEB	CMB-C2B-C1B	3.61	130.63	125.06
29	W1	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
29	WK	202	PEB	OA-C1A-C2A	-3.61	123.30	126.17
29	FC	203	PEB	CHC-C1D-ND	-3.61	109.75	113.95
29	FE	203	PEB	CHC-C1D-ND	-3.61	109.75	113.95
29	V2	202	PEB	CHB-C4B-NB	-3.61	123.82	128.83
31	K1	1001	CYC	C4D-CHA-C1A	3.61	133.12	128.81
31	KK	1001	CYC	C4D-CHA-C1A	3.61	133.12	128.81
29	QB	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
29	QM	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
29	BD	202	PEB	C3D-C4D-ND	3.61	114.34	107.26
29	PF	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	PI	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
31	H7	1001	CYC	C2A-C1A-NA	3.61	115.30	110.05
31	H9	1001	CYC	C2A-C1A-NA	3.61	115.30	110.05
31	L9	1001	CYC	C2A-C1A-NA	3.61	115.30	110.05
29	cB	201	PEB	CMB-C2B-C1B	3.61	130.62	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	cM	201	PEB	CMB-C2B-C1B	3.61	130.62	125.06
29	NF	1002	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
29	NI	1002	PEB	C4B-C3B-C2B	-3.61	102.79	106.78
29	RB	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
29	RM	201	PEB	C2A-C1A-NA	3.61	111.39	108.27
29	AM	303	PEB	CMB-C2B-C1B	3.61	130.62	125.06
29	aF	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	aI	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	AB	303	PEB	CHA-C1B-NB	-3.61	117.38	124.93
30	MG	403	PUB	CMA-C2A-C1A	3.61	129.88	121.39
29	TJ	203	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	TL	203	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	I4	203	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
29	wJ	301	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
29	kF	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	kI	202	PEB	C3B-C4B-NB	3.61	115.30	110.05
29	K5	202	PEB	CHB-C4B-NB	-3.61	123.82	128.83
29	DB	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
29	DM	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
29	mF	201	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
29	mI	201	PEB	CHC-C4C-C3C	-3.61	124.18	130.34
29	c7	201	PEB	OA-C1A-C2A	-3.61	123.31	126.17
29	c9	201	PEB	OA-C1A-C2A	-3.61	123.31	126.17
29	HA	202	PEB	OA-C1A-C2A	-3.61	123.31	126.17
29	HN	202	PEB	OA-C1A-C2A	-3.61	123.31	126.17
29	LB	202	PEB	C3D-C4D-ND	3.61	114.33	107.26
29	LM	202	PEB	C3D-C4D-ND	3.61	114.33	107.26
29	DC	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
29	DE	201	PEB	C2A-C1A-NA	3.61	111.38	108.27
31	I7	1001	CYC	CBD-CAD-C3D	-3.61	106.47	112.62
31	I9	1001	CYC	CBD-CAD-C3D	-3.61	106.47	112.62
29	MQ	406	PEB	C3B-C4B-NB	3.60	115.29	110.05
31	L7	1001	CYC	C2A-C1A-NA	3.60	115.29	110.05
31	xP	1001	CYC	OC-C1C-C2C	-3.60	123.31	126.17
29	LB	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	LM	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	VB	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	VM	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	dF	201	PEB	C3B-C4B-NB	3.60	115.29	110.05
29	MG	404	PEB	C3B-C4B-NB	3.60	115.29	110.05
29	dI	201	PEB	C3B-C4B-NB	3.60	115.29	110.05
29	eF	201	PEB	CHC-C4C-C3C	-3.60	124.19	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	eI	201	PEB	CHC-C4C-C3C	-3.60	124.19	130.34
29	ZB	202	PEB	C3D-C4D-ND	3.60	114.33	107.26
29	ZM	202	PEB	C3D-C4D-ND	3.60	114.33	107.26
31	VP	1001	CYC	OC-C1C-C2C	-3.60	123.31	126.17
29	A5	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	L7	1002	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	A8	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	iB	202	PEB	C3D-C4D-ND	3.60	114.33	107.26
29	iM	202	PEB	C3D-C4D-ND	3.60	114.33	107.26
29	FC	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
29	FE	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
29	MG	405	PEB	C3B-C4B-NB	3.60	115.29	110.05
29	PJ	203	PEB	C3B-C4B-NB	3.60	115.29	110.05
29	PL	203	PEB	C3B-C4B-NB	3.60	115.29	110.05
29	a1	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	k1	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	aK	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	kK	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	VF	201	PEB	CBC-CAC-C2C	3.60	118.77	112.62
29	VI	201	PEB	CBC-CAC-C2C	3.60	118.77	112.62
29	kB	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	kM	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	D4	202	PEB	C3D-C4D-ND	3.60	114.33	107.26
29	H4	202	PEB	C3D-C4D-ND	3.60	114.32	107.26
29	OR	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
29	c1	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	cK	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
30	QB	201	PUB	CHA-C1B-C2B	-3.60	124.20	130.34
30	QM	201	PUB	CHA-C1B-C2B	-3.60	124.20	130.34
29	AF	304	PEB	OD-C4D-ND	-3.60	120.60	125.93
29	AI	304	PEB	OD-C4D-ND	-3.60	120.60	125.93
29	PB	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	PM	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
31	HF	1001	CYC	C2C-C1C-NC	3.60	111.38	108.27
31	HI	1001	CYC	C2C-C1C-NC	3.60	111.38	108.27
29	e1	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	XB	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	eK	203	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	XM	201	PEB	CMB-C2B-C1B	3.60	130.61	125.06
29	HA	203	PEB	CHC-C1D-ND	-3.60	109.77	113.95
29	HN	203	PEB	CHC-C1D-ND	-3.60	109.77	113.95
29	DJ	202	PEB	C3B-C4B-NB	3.60	115.28	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DL	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	K5	201	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	PF	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	VF	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	PI	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	VI	202	PEB	C2A-C1A-NA	3.60	111.38	108.27
29	M2	201	PEB	OA-C1A-C2A	-3.60	123.31	126.17
29	HC	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
29	HE	202	PEB	C4B-C3B-C2B	-3.60	102.80	106.78
29	iF	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	iI	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	vJ	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	vL	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
31	L1	1001	CYC	C2B-C1B-NB	3.60	112.25	106.99
31	LK	1001	CYC	C2B-C1B-NB	3.60	112.25	106.99
29	J4	202	PEB	C3D-C4D-ND	3.60	114.32	107.26
29	b7	201	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
29	b9	201	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
29	BA	203	PEB	CHC-C1D-ND	-3.60	109.77	113.95
29	BN	203	PEB	CHC-C1D-ND	-3.60	109.77	113.95
29	UF	201	PEB	C2A-C1A-NA	3.60	111.37	108.27
29	UI	201	PEB	C2A-C1A-NA	3.60	111.37	108.27
29	LB	201	PEB	CMB-C2B-C1B	3.60	130.60	125.06
29	LM	201	PEB	CMB-C2B-C1B	3.60	130.60	125.06
29	VJ	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	VL	202	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	IJ	203	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	IL	203	PEB	C3B-C4B-NB	3.60	115.28	110.05
29	MG	401	PEB	C2A-C1A-NA	3.60	111.37	108.27
29	AM	303	PEB	CHA-C1B-NB	-3.60	117.41	124.93
29	CG	202	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
29	CQ	202	PEB	CHC-C4C-C3C	-3.60	124.20	130.34
29	R1	203	PEB	CMB-C2B-C1B	3.60	130.60	125.06
29	RK	203	PEB	CMB-C2B-C1B	3.60	130.60	125.06
31	F7	1001	CYC	C1A-C2A-C3A	-3.60	102.80	106.78
31	FF	1001	CYC	C2C-C1C-NC	3.59	111.37	108.27
31	FI	1001	CYC	C2C-C1C-NC	3.59	111.37	108.27
29	B4	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
29	HJ	202	PEB	C3B-C4B-NB	3.59	115.28	110.05
29	HL	202	PEB	C3B-C4B-NB	3.59	115.28	110.05
29	Q1	202	PEB	CHA-C1B-NB	-3.59	117.41	124.93
29	QK	202	PEB	CHA-C1B-NB	-3.59	117.41	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HB	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
29	HM	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
29	FJ	203	PEB	C3B-C4B-NB	3.59	115.28	110.05
29	FL	203	PEB	C3B-C4B-NB	3.59	115.28	110.05
29	C5	201	PEB	C2A-C1A-NA	3.59	111.37	108.27
29	KB	203	PEB	C3D-C4D-ND	3.59	114.31	107.26
29	KM	203	PEB	C3D-C4D-ND	3.59	114.31	107.26
29	K8	201	PEB	C2A-C1A-NA	3.59	111.37	108.27
29	GG	201	PEB	C1B-C2B-C3B	-3.59	102.38	106.51
29	GQ	201	PEB	C1B-C2B-C3B	-3.59	102.38	106.51
29	EG	202	PEB	CHC-C4C-C3C	-3.59	124.21	130.34
29	EQ	202	PEB	CHC-C4C-C3C	-3.59	124.21	130.34
29	P1	203	PEB	CMB-C2B-C1B	3.59	130.60	125.06
29	TB	201	PEB	CMB-C2B-C1B	3.59	130.60	125.06
29	PK	203	PEB	CMB-C2B-C1B	3.59	130.60	125.06
29	TM	201	PEB	CMB-C2B-C1B	3.59	130.60	125.06
29	F4	202	PEB	C3D-C4D-ND	3.59	114.31	107.26
29	I8	201	PEB	C2A-C1A-NA	3.59	111.37	108.27
29	aF	202	PEB	C2A-C1A-NA	3.59	111.37	108.27
29	aI	202	PEB	C2A-C1A-NA	3.59	111.37	108.27
29	xL	301	PEB	C3B-C4B-NB	3.59	115.27	110.05
31	xP	1001	CYC	CAA-CBA-CGA	3.59	121.33	113.60
29	ZJ	203	PEB	C3B-C4B-NB	3.59	115.27	110.05
29	ZL	203	PEB	C3B-C4B-NB	3.59	115.27	110.05
29	LD	202	PEB	C3D-C4D-ND	3.59	114.30	107.26
29	Q7	201	PEB	CHC-C4C-C3C	-3.59	124.22	130.34
29	Q9	201	PEB	CHC-C4C-C3C	-3.59	124.22	130.34
29	A1	302	PEB	OA-C1A-C2A	-3.59	123.32	126.17
29	AK	302	PEB	OA-C1A-C2A	-3.59	123.32	126.17
31	F1	1001	CYC	C2B-C1B-NB	3.59	112.24	106.99
31	FK	1001	CYC	C2B-C1B-NB	3.59	112.24	106.99
31	NK	1001	CYC	C2B-C1B-NB	3.59	112.24	106.99
29	iF	201	PEB	CBC-CAC-C2C	3.59	118.74	112.62
29	iI	201	PEB	CBC-CAC-C2C	3.59	118.74	112.62
29	AA	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
29	AN	201	PEB	C4B-C3B-C2B	-3.59	102.81	106.78
29	RJ	203	PEB	C3B-C4B-NB	3.59	115.27	110.05
29	RL	203	PEB	C3B-C4B-NB	3.59	115.27	110.05
29	L4	202	PEB	C3D-C4D-ND	3.59	114.30	107.26
29	m1	202	PEB	CMB-C2B-C1B	3.59	130.59	125.06
29	gB	201	PEB	CMB-C2B-C1B	3.59	130.59	125.06
29	mK	202	PEB	CMB-C2B-C1B	3.59	130.59	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	gM	201	PEB	CMB-C2B-C1B	3.59	130.59	125.06
29	L3	201	PEB	OA-C1A-C2A	-3.59	123.32	126.17
29	LO	201	PEB	OA-C1A-C2A	-3.59	123.32	126.17
31	JF	1001	CYC	C2C-C1C-NC	3.59	111.36	108.27
31	JI	1001	CYC	C2C-C1C-NC	3.59	111.36	108.27
29	JD	202	PEB	C3D-C4D-ND	3.59	114.30	107.26
29	YF	201	PEB	C3B-C4B-NB	3.59	115.27	110.05
29	YI	201	PEB	C3B-C4B-NB	3.59	115.27	110.05
31	N1	1001	CYC	C2B-C1B-NB	3.59	112.24	106.99
29	OF	203	PEB	C2A-C1A-NA	3.59	111.36	108.27
29	OI	203	PEB	C2A-C1A-NA	3.59	111.36	108.27
29	fF	202	PEB	C3D-C4D-ND	3.59	114.29	107.26
29	fI	202	PEB	C3D-C4D-ND	3.59	114.29	107.26
29	dJ	202	PEB	C3B-C4B-NB	3.59	115.26	110.05
29	dL	202	PEB	C3B-C4B-NB	3.59	115.26	110.05
29	fF	201	PEB	C1B-C2B-C3B	-3.58	102.39	106.51
29	fI	201	PEB	C1B-C2B-C3B	-3.58	102.39	106.51
29	HA	202	PEB	CAB-C3B-C4B	3.58	131.35	125.01
29	HN	202	PEB	CAB-C3B-C4B	3.58	131.35	125.01
29	fI	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	fK	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	jJ	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
29	jL	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
29	FF	1002	PEB	OD-C4D-C3D	-3.58	121.34	129.46
29	FI	1002	PEB	OD-C4D-C3D	-3.58	121.34	129.46
29	mF	201	PEB	CBC-CAC-C2C	3.58	118.74	112.62
29	mI	201	PEB	CBC-CAC-C2C	3.58	118.74	112.62
29	T2	201	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	dJ	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
29	dL	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
30	AF	303	PUB	CHA-C4A-NA	-3.58	109.79	113.95
30	AI	303	PUB	CHA-C4A-NA	-3.58	109.79	113.95
29	cF	201	PEB	CBC-CAC-C2C	3.58	118.73	112.62
29	cI	201	PEB	CBC-CAC-C2C	3.58	118.73	112.62
29	H7	1002	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	H9	1002	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	F3	201	PEB	OA-C1A-C2A	-3.58	123.32	126.17
29	FO	201	PEB	OA-C1A-C2A	-3.58	123.32	126.17
29	b1	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	bK	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	CA	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
29	CN	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JA	203	PEB	CHC-C1D-ND	-3.58	109.79	113.95
29	JN	203	PEB	CHC-C1D-ND	-3.58	109.79	113.95
29	xJ	301	PEB	C3B-C4B-NB	3.58	115.26	110.05
29	FD	202	PEB	C3D-C4D-ND	3.58	114.29	107.26
29	HD	202	PEB	C3D-C4D-ND	3.58	114.29	107.26
29	O7	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	O9	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	BG	201	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
29	BQ	201	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
29	JF	1002	PEB	OD-C4D-C3D	-3.58	121.35	129.46
29	JI	1002	PEB	OD-C4D-C3D	-3.58	121.35	129.46
29	S7	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	S9	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
30	MQ	404	PUB	C1C-C2C-C3C	-3.58	102.82	106.78
29	j7	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	j9	201	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	IG	202	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	IQ	202	PEB	CHC-C4C-C3C	-3.58	124.23	130.34
29	AC	202	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	AE	202	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	O1	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	OK	202	PEB	CHA-C1B-NB	-3.58	117.44	124.93
29	nJ	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
29	nL	203	PEB	C3B-C4B-NB	3.58	115.26	110.05
29	g1	203	PEB	CMB-C2B-C1B	3.58	130.58	125.06
29	gK	203	PEB	CMB-C2B-C1B	3.58	130.58	125.06
29	Z1	203	PEB	CHA-C1B-NB	-3.58	117.45	124.93
29	ZK	203	PEB	CHA-C1B-NB	-3.58	117.45	124.93
29	A1	303	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	CG	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	AK	303	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	CQ	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	jF	201	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
29	jI	201	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
29	TI	201	PEB	C3B-C4B-NB	3.58	115.25	110.05
29	YF	202	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	YI	202	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	KG	202	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
29	KQ	202	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
29	MG	404	PEB	C1B-C2B-C3B	-3.58	102.40	106.51
29	bJ	203	PEB	C3B-C4B-NB	3.58	115.25	110.05
29	bL	203	PEB	C3B-C4B-NB	3.58	115.25	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KA	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
29	KN	201	PEB	C4B-C3B-C2B	-3.58	102.82	106.78
29	XB	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	XM	201	PEB	C2A-C1A-NA	3.58	111.36	108.27
29	GA	201	PEB	C4B-C3B-C2B	-3.58	102.83	106.78
29	GN	201	PEB	C4B-C3B-C2B	-3.58	102.83	106.78
29	NF	1002	PEB	OD-C4D-C3D	-3.58	121.36	129.46
29	NI	1002	PEB	OD-C4D-C3D	-3.58	121.36	129.46
29	JJ	203	PEB	C3B-C4B-NB	3.58	115.25	110.05
29	JL	203	PEB	C3B-C4B-NB	3.58	115.25	110.05
29	Z7	201	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
29	Z9	201	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
29	MQ	407	PEB	CHC-C4C-C3C	-3.58	124.24	130.34
30	MG	402	PUB	C1C-C2C-C3C	-3.57	102.83	106.78
29	W7	201	PEB	CHC-C4C-C3C	-3.57	124.24	130.34
29	W9	201	PEB	CHC-C4C-C3C	-3.57	124.24	130.34
29	S2	201	PEB	CHA-C1B-NB	-3.57	117.46	124.93
29	wL	301	PEB	C3B-C4B-NB	3.57	115.25	110.05
29	iF	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
29	iI	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
29	eF	201	PEB	CBC-CAC-C2C	3.57	118.72	112.62
29	eI	201	PEB	CBC-CAC-C2C	3.57	118.72	112.62
29	h1	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
29	hK	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
29	AG	202	PEB	CHC-C4C-C3C	-3.57	124.24	130.34
29	AQ	202	PEB	CHC-C4C-C3C	-3.57	124.24	130.34
29	aF	201	PEB	C3B-C4B-NB	3.57	115.25	110.05
29	aI	201	PEB	C3B-C4B-NB	3.57	115.25	110.05
29	rJ	203	PEB	C3B-C4B-NB	3.57	115.25	110.05
29	rL	203	PEB	C3B-C4B-NB	3.57	115.25	110.05
29	DD	202	PEB	C3D-C4D-ND	3.57	114.27	107.26
29	dF	202	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	dI	202	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	hF	202	PEB	C3D-C4D-ND	3.57	114.27	107.26
29	hI	202	PEB	C3D-C4D-ND	3.57	114.27	107.26
29	GG	202	PEB	CHC-C4C-C3C	-3.57	124.25	130.34
29	GQ	202	PEB	CHC-C4C-C3C	-3.57	124.25	130.34
29	d1	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
29	dK	202	PEB	CHA-C1B-NB	-3.57	117.46	124.93
29	ZF	201	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	ZI	201	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	HF	1002	PEB	OD-C4D-C3D	-3.57	121.37	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LF	1002	PEB	OD-C4D-C3D	-3.57	121.37	129.46
29	HI	1002	PEB	OD-C4D-C3D	-3.57	121.37	129.46
29	LI	1002	PEB	OD-C4D-C3D	-3.57	121.37	129.46
29	UF	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	gF	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	mF	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	UI	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	gI	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	mI	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
31	F9	1001	CYC	C1A-C2A-C3A	-3.57	102.83	106.78
29	sJ	203	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	sL	203	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	ZF	202	PEB	C3D-C4D-ND	3.57	114.26	107.26
29	ZI	202	PEB	C3D-C4D-ND	3.57	114.26	107.26
29	l1	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	lK	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	NB	202	PEB	CAB-C3B-C4B	3.57	131.32	125.01
29	NM	202	PEB	CAB-C3B-C4B	3.57	131.32	125.01
29	IA	201	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
29	IN	201	PEB	C4B-C3B-C2B	-3.57	102.83	106.78
29	xJ	303	PEB	OA-C1A-C2A	-3.57	123.33	126.17
29	VF	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	VI	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	hJ	203	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	hL	203	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	U1	203	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	UK	203	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	h7	201	PEB	CHC-C4C-C3C	-3.57	124.25	130.34
29	h9	201	PEB	CHC-C4C-C3C	-3.57	124.25	130.34
29	LB	203	PEB	CAB-C3B-C4B	3.57	131.32	125.01
29	LM	203	PEB	CAB-C3B-C4B	3.57	131.32	125.01
29	j1	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	jK	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	kF	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	kI	201	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	S1	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	SK	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	RF	201	PEB	CBC-CAC-C2C	3.57	118.71	112.62
29	RI	201	PEB	CBC-CAC-C2C	3.57	118.71	112.62
29	TR	201	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	I5	202	PEB	C2A-C1A-NA	3.57	111.35	108.27
29	I8	202	PEB	C2A-C1A-NA	3.57	111.35	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DG	201	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	DQ	201	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	W1	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	WK	202	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	LJ	202	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	LL	202	PEB	C3B-C4B-NB	3.57	115.24	110.05
29	NR	201	PEB	CHA-C1B-NB	-3.57	117.47	124.93
29	LG	201	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	MQ	402	PEB	C1B-C2B-C3B	-3.57	102.41	106.51
29	HB	203	PEB	CAB-C3B-C4B	3.57	131.32	125.01
29	HM	203	PEB	CAB-C3B-C4B	3.57	131.32	125.01
29	YF	201	PEB	CBC-CAC-C2C	3.57	118.70	112.62
29	YI	201	PEB	CBC-CAC-C2C	3.57	118.70	112.62
29	DF	1002	PEB	OD-C4D-C3D	-3.56	121.38	129.46
29	DI	1002	PEB	OD-C4D-C3D	-3.56	121.38	129.46
29	TI	201	PEB	CBC-CAC-C2C	3.56	118.70	112.62
29	AB	301	PEB	CBA-CAA-C3A	3.56	121.40	113.47
29	bJ	202	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	fJ	203	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	bL	202	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	fL	203	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	gF	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	gI	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	UR	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	QF	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	QI	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
31	VP	1001	CYC	CAB-C3B-C4B	3.56	127.00	121.38
31	HK	1001	CYC	C2B-C1B-NB	3.56	112.20	106.99
29	GC	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	GE	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	PF	201	PEB	CBC-CAC-C2C	3.56	118.70	112.62
29	PI	201	PEB	CBC-CAC-C2C	3.56	118.70	112.62
29	SF	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	SI	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	D3	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	DO	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	iF	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	iI	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	wJ	301	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	HC	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	HE	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	kF	201	PEB	CBC-CAC-C2C	3.56	118.70	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	kI	201	PEB	CBC-CAC-C2C	3.56	118.70	112.62
29	BA	202	PEB	CAB-C3B-C4B	3.56	131.31	125.01
29	BN	202	PEB	CAB-C3B-C4B	3.56	131.31	125.01
29	eF	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	eI	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	hF	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	lF	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	AG	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	hI	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	II	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	AQ	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	K5	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	K8	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	dF	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	dI	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	LA	202	PEB	CAB-C3B-C4B	3.56	131.31	125.01
29	LN	202	PEB	CAB-C3B-C4B	3.56	131.31	125.01
29	WR	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
29	U2	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	UR	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	cF	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	cI	201	PEB	C3B-C4B-NB	3.56	115.23	110.05
29	d7	201	PEB	CHC-C4C-C3C	-3.56	124.27	130.34
29	d9	201	PEB	CHC-C4C-C3C	-3.56	124.27	130.34
29	FC	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	FE	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	EC	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	EE	202	PEB	C2A-C1A-NA	3.56	111.34	108.27
29	XR	201	PEB	CHA-C1B-NB	-3.56	117.49	124.93
29	AC	203	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
29	AE	203	PEB	C4B-C3B-C2B	-3.56	102.84	106.78
29	PJ	202	PEB	C3B-C4B-NB	3.56	115.22	110.05
29	PL	202	PEB	C3B-C4B-NB	3.56	115.22	110.05
29	lF	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
29	II	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
31	xP	1001	CYC	CAA-C2A-C3A	-3.56	121.25	127.88
29	OF	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
29	OI	202	PEB	C3D-C4D-ND	3.56	114.24	107.26
31	D1	1001	CYC	C2B-C1B-NB	3.56	112.19	106.99
29	JG	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	JQ	201	PEB	C1B-C2B-C3B	-3.56	102.42	106.51
29	H3	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LA	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	LN	202	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	HO	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
29	NJ	202	PEB	C3B-C4B-NB	3.56	115.22	110.05
29	NL	202	PEB	C3B-C4B-NB	3.56	115.22	110.05
31	VP	1001	CYC	CAA-C2A-C3A	-3.56	121.26	127.88
29	jF	202	PEB	C3D-C4D-ND	3.56	114.23	107.26
29	jI	202	PEB	C3D-C4D-ND	3.56	114.23	107.26
29	pJ	203	PEB	C3B-C4B-NB	3.56	115.22	110.05
29	pL	203	PEB	C3B-C4B-NB	3.56	115.22	110.05
31	VP	1001	CYC	CAA-CBA-CGA	3.55	121.25	113.60
29	U7	201	PEB	CHC-C4C-C3C	-3.55	124.27	130.34
29	U9	201	PEB	CHC-C4C-C3C	-3.55	124.27	130.34
29	aF	201	PEB	CBC-CAC-C2C	3.55	118.69	112.62
29	aI	201	PEB	CBC-CAC-C2C	3.55	118.69	112.62
29	f7	201	PEB	CHC-C4C-C3C	-3.55	124.28	130.34
29	f9	201	PEB	CHC-C4C-C3C	-3.55	124.28	130.34
29	QF	202	PEB	C3D-C4D-ND	3.55	114.23	107.26
29	QI	202	PEB	C3D-C4D-ND	3.55	114.23	107.26
29	gF	201	PEB	CBC-CAC-C2C	3.55	118.68	112.62
29	gI	201	PEB	CBC-CAC-C2C	3.55	118.68	112.62
29	AF	301	PEB	C3B-C4B-NB	3.55	115.22	110.05
29	AI	301	PEB	C3B-C4B-NB	3.55	115.22	110.05
31	D7	1001	CYC	C1A-C2A-C3A	-3.55	102.85	106.78
31	D9	1001	CYC	C1A-C2A-C3A	-3.55	102.85	106.78
29	mF	202	PEB	C2A-C1A-NA	3.55	111.33	108.27
29	mI	202	PEB	C2A-C1A-NA	3.55	111.33	108.27
29	N2	201	PEB	CHA-C1B-NB	-3.55	117.50	124.93
29	HJ	201	PEB	C3B-C4B-NB	3.55	115.22	110.05
29	HL	201	PEB	C3B-C4B-NB	3.55	115.22	110.05
29	LC	202	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
29	LE	202	PEB	C4B-C3B-C2B	-3.55	102.85	106.78
29	HG	201	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
29	HQ	201	PEB	C1B-C2B-C3B	-3.55	102.43	106.51
29	F1	1002	PEB	OD-C4D-ND	-3.55	120.67	125.93
29	FK	1002	PEB	OD-C4D-ND	-3.55	120.67	125.93
29	FJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	FL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	RR	201	PEB	CHA-C1B-NB	-3.55	117.51	124.93
29	bF	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
29	bI	202	PEB	C3D-C4D-ND	3.55	114.22	107.26
29	FA	202	PEB	CAB-C3B-C4B	3.55	131.29	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FN	202	PEB	CAB-C3B-C4B	3.55	131.29	125.01
29	DA	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
29	DN	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
29	MR	201	PEB	OA-C1A-C2A	-3.55	123.35	126.17
29	SR	202	PEB	OA-C1A-C2A	-3.55	123.35	126.17
29	jJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	nJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	pJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	jL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	nL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	pL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	iB	203	PEB	CAB-C3B-C4B	3.55	131.29	125.01
29	iM	203	PEB	CAB-C3B-C4B	3.55	131.29	125.01
29	PB	202	PEB	CAB-C3B-C4B	3.55	131.28	125.01
29	PM	202	PEB	CAB-C3B-C4B	3.55	131.28	125.01
29	xL	301	PEB	C2A-C1A-NA	3.55	111.33	108.27
29	MG	405	PEB	CHC-C4C-C3C	-3.55	124.29	130.34
29	A7	304	PEB	CMB-C2B-C1B	3.55	130.53	125.06
29	PF	201	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	PI	201	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	TJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	IJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	TL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	IL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	MQ	406	PEB	C1B-C2B-C3B	-3.55	102.44	106.51
29	L1	1002	PEB	OD-C4D-ND	-3.55	120.68	125.93
29	LK	1002	PEB	OD-C4D-ND	-3.55	120.68	125.93
31	KI	1001	CYC	C4A-C3A-C2A	-3.55	102.44	106.51
29	hJ	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	hL	202	PEB	C3B-C4B-NB	3.55	115.21	110.05
29	AM	301	PEB	CBA-CAA-C3A	3.55	121.36	113.47
29	KG	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	KQ	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	l1	202	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
29	lK	202	PEB	C4B-C3B-C2B	-3.54	102.86	106.78
31	xP	1001	CYC	CAB-C3B-C4B	3.54	126.98	121.38
31	J1	1001	CYC	C2B-C1B-NB	3.54	112.18	106.99
31	JK	1001	CYC	C2B-C1B-NB	3.54	112.18	106.99
29	DA	202	PEB	CAB-C3B-C4B	3.54	131.28	125.01
29	cB	203	PEB	CAB-C3B-C4B	3.54	131.28	125.01
29	cM	203	PEB	CAB-C3B-C4B	3.54	131.28	125.01
29	DN	202	PEB	CAB-C3B-C4B	3.54	131.28	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	rJ	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	rL	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	k7	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	k9	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	R2	201	PEB	CHA-C1B-NB	-3.54	117.52	124.93
29	xJ	301	PEB	CHC-C1D-ND	-3.54	109.83	113.95
29	U2	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	LC	202	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	LE	202	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	GG	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	GQ	201	PEB	C2A-C1A-NA	3.54	111.33	108.27
29	AG	201	PEB	CHC-C4C-C3C	-3.54	124.30	130.34
29	AQ	201	PEB	CHC-C4C-C3C	-3.54	124.30	130.34
31	N7	1001	CYC	C1A-C2A-C3A	-3.54	102.86	106.78
31	N9	1001	CYC	C1A-C2A-C3A	-3.54	102.86	106.78
29	M2	202	PEB	C3D-C4D-ND	3.54	114.21	107.26
29	RF	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	RI	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	SF	202	PEB	C3D-C4D-ND	3.54	114.21	107.26
29	SI	202	PEB	C3D-C4D-ND	3.54	114.21	107.26
29	DB	203	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	DM	203	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	DG	202	PEB	OD-C4D-ND	-3.54	120.69	125.93
29	DQ	202	PEB	OD-C4D-ND	-3.54	120.69	125.93
29	WJ	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	WL	201	PEB	C3B-C4B-NB	3.54	115.20	110.05
31	KI	1001	CYC	CHA-C1A-NA	-3.54	123.92	128.83
29	CG	201	PEB	C1B-C2B-C3B	-3.54	102.44	106.51
29	CQ	201	PEB	C1B-C2B-C3B	-3.54	102.44	106.51
29	WF	202	PEB	C3D-C4D-ND	3.54	114.20	107.26
29	WI	202	PEB	C3D-C4D-ND	3.54	114.20	107.26
29	fJ	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	fL	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	e2	402	PEB	CHA-C1B-NB	-3.54	117.53	124.93
29	wJ	301	PEB	C2A-C1A-NA	3.54	111.32	108.27
29	qJ	202	PEB	CMB-C2B-C1B	3.54	130.51	125.06
29	qL	202	PEB	CMB-C2B-C1B	3.54	130.51	125.06
29	V7	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	V9	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	RJ	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	RL	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	UF	203	PEB	C3D-C4D-ND	3.54	114.20	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UI	203	PEB	C3D-C4D-ND	3.54	114.20	107.26
29	U1	203	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
29	UK	203	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
29	FG	201	PEB	C1B-C2B-C3B	-3.54	102.44	106.51
29	FQ	201	PEB	C1B-C2B-C3B	-3.54	102.44	106.51
29	eB	202	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	eM	202	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	T7	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	T9	202	PEB	C3B-C4B-NB	3.54	115.20	110.05
29	VB	203	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	kB	203	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	VM	203	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	kM	203	PEB	CAB-C3B-C4B	3.54	131.27	125.01
29	KC	201	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
29	KE	201	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
29	BG	202	PEB	OD-C4D-ND	-3.54	120.69	125.93
29	BQ	202	PEB	OD-C4D-ND	-3.54	120.69	125.93
29	WF	201	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
29	WI	201	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
29	P7	202	PEB	C3B-C4B-NB	3.54	115.19	110.05
29	P9	202	PEB	C3B-C4B-NB	3.54	115.19	110.05
31	DK	1001	CYC	C2B-C1B-NB	3.54	112.17	106.99
29	EG	201	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
29	EQ	201	PEB	C1B-C2B-C3B	-3.54	102.45	106.51
29	QR	201	PEB	OA-C1A-C2A	-3.54	123.36	126.17
29	gB	203	PEB	CAB-C3B-C4B	3.54	131.26	125.01
29	gM	203	PEB	CAB-C3B-C4B	3.54	131.26	125.01
31	KF	1001	CYC	C4A-C3A-C2A	-3.54	102.45	106.51
29	G3	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
29	GO	202	PEB	OA-C1A-C2A	-3.54	123.36	126.17
29	AF	301	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
29	AI	301	PEB	C4B-C3B-C2B	-3.54	102.87	106.78
29	JJ	202	PEB	C3B-C4B-NB	3.53	115.19	110.05
29	JL	202	PEB	C3B-C4B-NB	3.53	115.19	110.05
29	QR	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	GG	201	PEB	CHC-C4C-C3C	-3.53	124.31	130.34
29	GQ	201	PEB	CHC-C4C-C3C	-3.53	124.31	130.34
29	bF	201	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	bI	201	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
31	MF	1001	CYC	C4A-C3A-C2A	-3.53	102.45	106.51
31	MI	1001	CYC	C4A-C3A-C2A	-3.53	102.45	106.51
29	JB	203	PEB	CAB-C3B-C4B	3.53	131.26	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JM	203	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	IJ	203	PEB	C3B-C4B-NB	3.53	115.19	110.05
29	IL	203	PEB	C3B-C4B-NB	3.53	115.19	110.05
29	kJ	202	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	kL	202	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	fI	202	PEB	C4B-C3B-C2B	-3.53	102.87	106.78
29	fK	202	PEB	C4B-C3B-C2B	-3.53	102.87	106.78
29	FB	203	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	FM	203	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	L8	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	EG	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	EQ	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	BB	301	PEB	C3B-C4B-NB	3.53	115.19	110.05
29	BM	301	PEB	C3B-C4B-NB	3.53	115.19	110.05
29	RB	203	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	RM	203	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	cJ	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
29	cL	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
29	kF	202	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	kI	202	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	JA	202	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	JN	202	PEB	CAB-C3B-C4B	3.53	131.26	125.01
29	KG	201	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	KQ	201	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	a7	202	PEB	C3B-C4B-NB	3.53	115.18	110.05
29	a9	202	PEB	C3B-C4B-NB	3.53	115.18	110.05
29	EJ	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
29	eJ	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
29	EL	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
29	eL	202	PEB	CMB-C2B-C1B	3.53	130.50	125.06
29	AG	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	AQ	201	PEB	C2A-C1A-NA	3.53	111.32	108.27
29	ZB	203	PEB	CAB-C3B-C4B	3.53	131.25	125.01
29	ZM	203	PEB	CAB-C3B-C4B	3.53	131.25	125.01
29	UF	202	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	UI	202	PEB	C1B-C2B-C3B	-3.53	102.45	106.51
29	BC	202	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
29	BE	202	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
29	UR	202	PEB	C3D-C4D-ND	3.53	114.18	107.26
29	OR	202	PEB	CHC-C4C-C3C	-3.53	124.32	130.34
31	FF	1001	CYC	CAB-C3B-C2B	3.53	133.56	127.53
31	FI	1001	CYC	CAB-C3B-C2B	3.53	133.56	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	dF	203	PEB	C3D-C4D-ND	3.53	114.18	107.26
29	dI	203	PEB	C3D-C4D-ND	3.53	114.18	107.26
29	CG	201	PEB	CHC-C4C-C3C	-3.53	124.32	130.34
29	CQ	201	PEB	CHC-C4C-C3C	-3.53	124.32	130.34
31	LF	1001	CYC	CAB-C3B-C2B	3.53	133.56	127.53
31	LI	1001	CYC	CAB-C3B-C2B	3.53	133.56	127.53
29	KC	203	PEB	C2A-C1A-NA	3.53	111.31	108.27
29	KE	203	PEB	C2A-C1A-NA	3.53	111.31	108.27
29	AJ	203	PEB	C3B-C4B-NB	3.53	115.18	110.05
29	AL	203	PEB	C3B-C4B-NB	3.53	115.18	110.05
31	EF	1001	CYC	C4A-C3A-C2A	-3.53	102.46	106.51
31	EI	1001	CYC	C4A-C3A-C2A	-3.53	102.46	106.51
29	EJ	202	PEB	C1B-C2B-C3B	-3.53	102.46	106.51
29	EL	202	PEB	C1B-C2B-C3B	-3.53	102.46	106.51
30	AF	303	PUB	OA-C1A-NA	-3.53	120.71	125.93
30	AI	303	PUB	OA-C1A-NA	-3.53	120.71	125.93
29	ZJ	202	PEB	C3B-C4B-NB	3.53	115.18	110.05
29	ZL	202	PEB	C3B-C4B-NB	3.53	115.18	110.05
29	EA	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
29	EN	201	PEB	C4B-C3B-C2B	-3.53	102.88	106.78
29	LG	202	PEB	OD-C4D-ND	-3.52	120.71	125.93
29	LQ	201	PEB	OD-C4D-ND	-3.52	120.71	125.93
29	mB	203	PEB	CAB-C3B-C4B	3.52	131.25	125.01
29	mM	203	PEB	CAB-C3B-C4B	3.52	131.25	125.01
31	yP	1001	CYC	CMB-C2B-C1B	3.52	128.57	124.17
31	CF	1001	CYC	C4A-C3A-C2A	-3.52	102.46	106.51
31	CI	1001	CYC	C4A-C3A-C2A	-3.52	102.46	106.51
29	uJ	201	PEB	C3B-C4B-NB	3.52	115.18	110.05
29	uL	201	PEB	C3B-C4B-NB	3.52	115.18	110.05
29	sJ	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
29	sL	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
29	UJ	202	PEB	C1B-C2B-C3B	-3.52	102.46	106.51
29	UL	202	PEB	C1B-C2B-C3B	-3.52	102.46	106.51
31	MF	1001	CYC	CHA-C1A-NA	-3.52	123.94	128.83
31	MI	1001	CYC	CHA-C1A-NA	-3.52	123.94	128.83
29	wL	301	PEB	C2A-C1A-NA	3.52	111.31	108.27
29	IG	201	PEB	C1B-C2B-C3B	-3.52	102.46	106.51
29	IQ	201	PEB	C1B-C2B-C3B	-3.52	102.46	106.51
31	KF	1001	CYC	CHA-C1A-NA	-3.52	123.94	128.83
31	H1	1001	CYC	C2B-C1B-NB	3.52	112.14	106.99
29	U2	202	PEB	C3D-C4D-ND	3.52	114.17	107.26
29	a1	201	PEB	OA-C1A-C2A	-3.52	123.37	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aK	201	PEB	OA-C1A-C2A	-3.52	123.37	126.17
29	MQ	407	PEB	OA-C1A-C2A	-3.52	123.37	126.17
29	d1	202	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
29	dK	202	PEB	C4B-C3B-C2B	-3.52	102.89	106.78
31	H7	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
31	H9	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
31	L9	1001	CYC	C1A-C2A-C3A	-3.52	102.89	106.78
29	I5	201	PEB	CHC-C1D-ND	-3.52	109.86	113.95
31	JF	1001	CYC	CAB-C3B-C2B	3.52	133.55	127.53
31	JI	1001	CYC	CAB-C3B-C2B	3.52	133.55	127.53
29	LQ	202	PEB	CHA-C4A-NA	-3.52	121.02	125.20
29	XB	202	PEB	CAB-C3B-C4B	3.52	131.24	125.01
29	XM	202	PEB	CAB-C3B-C4B	3.52	131.24	125.01
29	iJ	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
29	iL	202	PEB	CMB-C2B-C1B	3.52	130.49	125.06
29	C5	201	PEB	CHC-C1D-ND	-3.52	109.86	113.95
29	sJ	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
29	sL	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
31	FF	1001	CYC	C4D-CHA-C1A	3.52	133.01	128.81
31	FI	1001	CYC	C4D-CHA-C1A	3.52	133.01	128.81
29	XJ	202	PEB	C3B-C4B-NB	3.52	115.17	110.05
29	XL	202	PEB	C3B-C4B-NB	3.52	115.17	110.05
29	m1	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
29	mK	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
29	I8	201	PEB	CHC-C1D-ND	-3.52	109.86	113.95
29	KJ	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
29	KL	202	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
31	HF	1001	CYC	CAB-C3B-C2B	3.52	133.55	127.53
31	HI	1001	CYC	CAB-C3B-C2B	3.52	133.55	127.53
29	N3	203	PEB	C3B-C4B-NB	3.52	115.17	110.05
29	WR	201	PEB	C2A-C1A-NA	3.52	111.31	108.27
29	TB	203	PEB	CAB-C3B-C4B	3.52	131.23	125.01
29	TM	203	PEB	CAB-C3B-C4B	3.52	131.23	125.01
31	NF	1001	CYC	CAB-C3B-C2B	3.52	133.55	127.53
31	NI	1001	CYC	CAB-C3B-C2B	3.52	133.55	127.53
29	WJ	203	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
29	WL	203	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
29	xJ	301	PEB	C2A-C1A-NA	3.52	111.31	108.27
29	OF	201	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
29	OI	201	PEB	C1B-C2B-C3B	-3.52	102.47	106.51
29	cJ	201	PEB	CBC-CAC-C2C	-3.52	106.62	112.62
29	cL	201	PEB	CBC-CAC-C2C	-3.52	106.62	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
29	gK	201	PEB	OA-C1A-C2A	-3.52	123.38	126.17
29	BJ	202	PEB	C3B-C4B-NB	3.52	115.16	110.05
29	BL	202	PEB	C3B-C4B-NB	3.52	115.16	110.05
29	M2	201	PEB	C2A-C1A-NA	3.52	111.30	108.27
29	DK	1002	PEB	OD-C4D-ND	-3.52	120.72	125.93
29	AB	303	PEB	C2A-C1A-NA	3.51	111.30	108.27
29	oJ	201	PEB	CBC-CAC-C2C	-3.51	106.62	112.62
29	uJ	202	PEB	CBC-CAC-C2C	-3.51	106.62	112.62
29	oL	201	PEB	CBC-CAC-C2C	-3.51	106.62	112.62
29	uL	202	PEB	CBC-CAC-C2C	-3.51	106.62	112.62
29	W1	202	PEB	C4B-C3B-C2B	-3.51	102.89	106.78
29	WK	202	PEB	C4B-C3B-C2B	-3.51	102.89	106.78
29	iJ	202	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
29	iL	202	PEB	C1B-C2B-C3B	-3.51	102.47	106.51
29	IC	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
29	IE	202	PEB	C2A-C1A-NA	3.51	111.30	108.27
29	KJ	201	PEB	CBC-CAC-C2C	-3.51	106.62	112.62
29	KL	201	PEB	CBC-CAC-C2C	-3.51	106.62	112.62
29	O2	201	PEB	C2A-C1A-NA	3.51	111.30	108.27
29	WJ	203	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	kJ	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	WL	203	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	kL	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	Y7	202	PEB	C3B-C4B-NB	3.51	115.16	110.05
29	Y9	202	PEB	C3B-C4B-NB	3.51	115.16	110.05
29	KG	201	PEB	CHC-C4C-C3C	-3.51	124.35	130.34
29	KQ	201	PEB	CHC-C4C-C3C	-3.51	124.35	130.34
29	eJ	201	PEB	CBC-CAC-C2C	-3.51	106.63	112.62
29	eL	201	PEB	CBC-CAC-C2C	-3.51	106.63	112.62
29	h1	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
29	hK	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
29	YJ	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	cJ	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	YL	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	cL	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	MG	405	PEB	OA-C1A-C2A	-3.51	123.38	126.17
31	CF	1001	CYC	CHA-C1A-NA	-3.51	123.96	128.83
31	CI	1001	CYC	CHA-C1A-NA	-3.51	123.96	128.83
29	m7	202	PEB	C3B-C4B-NB	3.51	115.16	110.05
29	m9	202	PEB	C3B-C4B-NB	3.51	115.16	110.05
29	V2	201	PEB	CHA-C1B-NB	-3.51	117.59	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GJ	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	mJ	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	GL	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	mL	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	R7	202	PEB	C3B-C4B-NB	3.51	115.15	110.05
29	R9	202	PEB	C3B-C4B-NB	3.51	115.15	110.05
29	H1	1002	PEB	OD-C4D-ND	-3.51	120.73	125.93
29	VR	201	PEB	CHA-C1B-NB	-3.51	117.59	124.93
29	oJ	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	oL	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	OR	201	PEB	C2A-C1A-NA	3.51	111.30	108.27
29	c1	201	PEB	OA-C1A-C2A	-3.51	123.38	126.17
29	cK	201	PEB	OA-C1A-C2A	-3.51	123.38	126.17
29	YJ	201	PEB	CBC-CAC-C2C	-3.51	106.63	112.62
29	YL	201	PEB	CBC-CAC-C2C	-3.51	106.63	112.62
29	AJ	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	AL	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
31	EF	1001	CYC	CHA-C1A-NA	-3.51	123.96	128.83
31	EI	1001	CYC	CHA-C1A-NA	-3.51	123.96	128.83
29	wL	301	PEB	CHC-C1D-ND	-3.51	109.87	113.95
31	L7	1001	CYC	C1A-C2A-C3A	-3.51	102.90	106.78
29	AJ	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	AL	202	PEB	CMB-C2B-C1B	3.51	130.47	125.06
29	A1	301	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	eJ	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	AK	301	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	eL	202	PEB	C1B-C2B-C3B	-3.51	102.48	106.51
29	Q1	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
29	S1	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
29	QK	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
29	SK	202	PEB	C4B-C3B-C2B	-3.51	102.90	106.78
29	AJ	201	PEB	CBC-CAC-C2C	-3.51	106.64	112.62
29	AL	201	PEB	CBC-CAC-C2C	-3.51	106.64	112.62
29	IG	201	PEB	CHC-C4C-C3C	-3.51	124.36	130.34
29	IQ	201	PEB	CHC-C4C-C3C	-3.51	124.36	130.34
30	A1	304	PUB	CHA-C1B-C2B	-3.51	124.36	130.34
30	AK	304	PUB	CHA-C1B-C2B	-3.51	124.36	130.34
29	g7	202	PEB	C3B-C4B-NB	3.51	115.15	110.05
29	g9	202	PEB	C3B-C4B-NB	3.51	115.15	110.05
29	NO	203	PEB	C3B-C4B-NB	3.51	115.15	110.05
29	C8	201	PEB	CHC-C1D-ND	-3.51	109.88	113.95
29	WJ	202	PEB	CBC-CAC-C2C	-3.50	106.64	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WL	202	PEB	CBC-CAC-C2C	-3.50	106.64	112.62
29	e7	202	PEB	C3B-C4B-NB	3.50	115.15	110.05
29	e9	202	PEB	C3B-C4B-NB	3.50	115.15	110.05
29	W2	202	PEB	C3D-C4D-ND	3.50	114.14	107.26
29	IG	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
29	AM	303	PEB	C2A-C1A-NA	3.50	111.29	108.27
29	IQ	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
29	EG	201	PEB	CHC-C4C-C3C	-3.50	124.36	130.34
29	EQ	201	PEB	CHC-C4C-C3C	-3.50	124.36	130.34
31	J7	1001	CYC	C1A-C2A-C3A	-3.50	102.90	106.78
29	UJ	202	PEB	CMB-C2B-C1B	3.50	130.46	125.06
29	UL	202	PEB	CMB-C2B-C1B	3.50	130.46	125.06
29	KA	202	PEB	C3B-C4B-NB	3.50	115.15	110.05
29	KN	202	PEB	C3B-C4B-NB	3.50	115.15	110.05
29	L5	201	PEB	C2A-C1A-NA	3.50	111.29	108.27
29	SJ	202	PEB	CMB-C2B-C1B	3.50	130.46	125.06
29	SL	202	PEB	CMB-C2B-C1B	3.50	130.46	125.06
29	O2	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
29	C3	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	I3	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	c7	202	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	c9	202	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	CO	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	IO	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
31	WP	1001	CYC	CMB-C2B-C1B	3.50	128.54	124.17
31	GF	1001	CYC	CHA-C1A-NA	-3.50	123.97	128.83
31	GI	1001	CYC	CHA-C1A-NA	-3.50	123.97	128.83
29	QR	202	PEB	C3D-C4D-ND	3.50	114.13	107.26
31	DF	1001	CYC	CAB-C3B-C2B	3.50	133.52	127.53
31	DI	1001	CYC	CAB-C3B-C2B	3.50	133.52	127.53
29	gJ	201	PEB	CBC-CAC-C2C	-3.50	106.64	112.62
29	gL	201	PEB	CBC-CAC-C2C	-3.50	106.64	112.62
29	M3	203	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	MO	203	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	O2	202	PEB	C3D-C4D-ND	3.50	114.13	107.26
29	K5	201	PEB	CHC-C1D-ND	-3.50	109.88	113.95
29	K8	201	PEB	CHC-C1D-ND	-3.50	109.88	113.95
29	wJ	301	PEB	CHC-C1D-ND	-3.50	109.88	113.95
29	sJ	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	sL	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	D1	1002	PEB	OD-C4D-ND	-3.50	120.74	125.93
29	NK	1002	PEB	OD-C4D-ND	-3.50	120.74	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	oJ	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
29	oL	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
29	b1	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
29	bK	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
29	UJ	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	UL	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	Q2	202	PEB	C3D-C4D-ND	3.50	114.12	107.26
29	CA	202	PEB	OD-C4D-ND	-3.50	120.75	125.93
29	CN	202	PEB	OD-C4D-ND	-3.50	120.75	125.93
29	IJ	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	iJ	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	kJ	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	IL	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	iL	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	kL	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	MJ	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	ML	201	PEB	CBC-CAC-C2C	-3.50	106.65	112.62
29	j1	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
29	N3	203	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
29	jK	202	PEB	C4B-C3B-C2B	-3.50	102.91	106.78
29	HG	202	PEB	OD-C4D-ND	-3.50	120.75	125.93
29	HQ	202	PEB	OD-C4D-ND	-3.50	120.75	125.93
29	WR	201	PEB	OA-C1A-C2A	-3.50	123.39	126.17
29	SJ	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
29	SL	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
31	GF	1001	CYC	C4A-C3A-C2A	-3.50	102.49	106.51
31	GI	1001	CYC	C4A-C3A-C2A	-3.50	102.49	106.51
31	LF	1001	CYC	C4D-CHA-C1A	3.50	132.99	128.81
31	LI	1001	CYC	C4D-CHA-C1A	3.50	132.99	128.81
29	K3	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
29	KO	201	PEB	C3B-C4B-NB	3.50	115.14	110.05
31	IF	1001	CYC	C4A-C3A-C2A	-3.50	102.49	106.51
31	II	1001	CYC	C4A-C3A-C2A	-3.50	102.49	106.51
29	GA	202	PEB	CHA-C1B-NB	-3.50	117.62	124.93
29	GN	202	PEB	CHA-C1B-NB	-3.50	117.62	124.93
29	OJ	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
29	OL	202	PEB	C1B-C2B-C3B	-3.50	102.49	106.51
29	U1	203	PEB	C3B-C4B-NB	3.50	115.13	110.05
29	UK	203	PEB	C3B-C4B-NB	3.50	115.13	110.05
29	J3	203	PEB	CHC-C1D-ND	-3.50	109.89	113.95
29	JO	203	PEB	CHC-C1D-ND	-3.50	109.89	113.95
29	CJ	202	PEB	CMB-C2B-C1B	3.50	130.45	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aJ	202	PEB	CMB-C2B-C1B	3.50	130.45	125.06
29	CL	202	PEB	CMB-C2B-C1B	3.50	130.45	125.06
29	aL	202	PEB	CMB-C2B-C1B	3.50	130.45	125.06
29	SJ	202	PEB	C3D-C4D-ND	3.49	114.12	107.26
29	SL	202	PEB	C3D-C4D-ND	3.49	114.12	107.26
29	IA	202	PEB	CHA-C1B-NB	-3.49	117.62	124.93
29	IN	202	PEB	CHA-C1B-NB	-3.49	117.62	124.93
29	qJ	201	PEB	CBC-CAC-C2C	-3.49	106.66	112.62
29	qL	201	PEB	CBC-CAC-C2C	-3.49	106.66	112.62
29	mJ	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	uJ	203	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	mL	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	uL	203	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	W2	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	aJ	202	PEB	C3D-C4D-ND	3.49	114.11	107.26
29	aL	202	PEB	C3D-C4D-ND	3.49	114.11	107.26
29	OJ	201	PEB	CBC-CAC-C2C	-3.49	106.66	112.62
29	OL	201	PEB	CBC-CAC-C2C	-3.49	106.66	112.62
29	qJ	202	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	qL	202	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	CJ	201	PEB	CBC-CAC-C2C	-3.49	106.66	112.62
29	CL	201	PEB	CBC-CAC-C2C	-3.49	106.66	112.62
29	G3	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	GO	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	SR	202	PEB	C3D-C4D-ND	3.49	114.11	107.26
29	JG	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
29	JQ	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
29	CA	202	PEB	CHA-C1B-NB	-3.49	117.63	124.93
29	CN	202	PEB	CHA-C1B-NB	-3.49	117.63	124.93
29	KJ	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	MJ	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	KL	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	ML	202	PEB	CMB-C2B-C1B	3.49	130.44	125.06
29	i7	202	PEB	C3B-C4B-NB	3.49	115.13	110.05
29	i9	202	PEB	C3B-C4B-NB	3.49	115.13	110.05
29	g7	202	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	g9	202	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	HC	202	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	HE	202	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	JG	203	PEB	CHA-C4A-NA	-3.49	121.06	125.20
31	N1	1001	CYC	C1B-C2B-C3B	-3.49	104.23	107.87
29	KA	202	PEB	CHA-C1B-NB	-3.49	117.63	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KN	202	PEB	CHA-C1B-NB	-3.49	117.63	124.93
29	e1	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	eK	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	FG	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
29	FQ	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
29	SF	201	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	lF	201	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	SI	201	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	lI	201	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	c1	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	cK	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	fF	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	fI	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	S2	202	PEB	C3D-C4D-ND	3.49	114.10	107.26
29	I3	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	IO	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	MQ	403	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	QJ	201	PEB	CBC-CAC-C2C	-3.49	106.67	112.62
29	QL	201	PEB	CBC-CAC-C2C	-3.49	106.67	112.62
29	SJ	201	PEB	CBC-CAC-C2C	-3.49	106.67	112.62
29	aJ	201	PEB	CBC-CAC-C2C	-3.49	106.67	112.62
29	SL	201	PEB	CBC-CAC-C2C	-3.49	106.67	112.62
29	aL	201	PEB	CBC-CAC-C2C	-3.49	106.67	112.62
29	IA	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
29	IN	202	PEB	OD-C4D-ND	-3.49	120.76	125.93
29	A9	304	PEB	CMB-C2B-C1B	3.49	130.43	125.06
29	GJ	202	PEB	CMB-C2B-C1B	3.49	130.43	125.06
29	GL	202	PEB	CMB-C2B-C1B	3.49	130.43	125.06
29	Y1	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	YK	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	V1	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	VK	201	PEB	C1B-C2B-C3B	-3.49	102.50	106.51
29	M4	203	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	hF	201	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	hI	201	PEB	CHC-C4C-C3C	-3.49	124.39	130.34
29	Q2	201	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	AC	203	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	AE	203	PEB	C2A-C1A-NA	3.49	111.28	108.27
29	J1	1002	PEB	OD-C4D-ND	-3.49	120.77	125.93
29	JK	1002	PEB	OD-C4D-ND	-3.49	120.77	125.93
29	JQ	203	PEB	CHA-C4A-NA	-3.49	121.06	125.20
29	T1	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i1	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	TK	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	iK	201	PEB	OA-C1A-C2A	-3.49	123.40	126.17
29	GJ	201	PEB	CBC-CAC-C2C	-3.48	106.67	112.62
29	GL	201	PEB	CBC-CAC-C2C	-3.48	106.67	112.62
29	UJ	202	PEB	C3D-C4D-ND	3.48	114.10	107.26
29	UL	202	PEB	C3D-C4D-ND	3.48	114.10	107.26
29	A5	201	PEB	CHC-C1D-ND	-3.48	109.90	113.95
29	A8	201	PEB	CHC-C1D-ND	-3.48	109.90	113.95
29	mJ	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	mL	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	mJ	201	PEB	CBC-CAC-C2C	-3.48	106.67	112.62
29	mL	201	PEB	CBC-CAC-C2C	-3.48	106.67	112.62
29	aJ	202	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
29	aL	202	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
29	gJ	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
29	gL	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
29	KJ	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	KL	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	B3	203	PEB	CHC-C1D-ND	-3.48	109.90	113.95
29	BO	203	PEB	CHC-C1D-ND	-3.48	109.90	113.95
29	KC	201	PEB	C2A-C1A-NA	3.48	111.28	108.27
29	KE	201	PEB	C2A-C1A-NA	3.48	111.28	108.27
29	c1	203	PEB	OD-C4D-ND	-3.48	120.77	125.93
29	cK	203	PEB	OD-C4D-ND	-3.48	120.77	125.93
29	QJ	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
29	QL	202	PEB	CMB-C2B-C1B	3.48	130.43	125.06
29	l1	202	PEB	C3B-C4B-NB	3.48	115.11	110.05
29	lK	202	PEB	C3B-C4B-NB	3.48	115.11	110.05
29	EA	202	PEB	CHA-C1B-NB	-3.48	117.65	124.93
29	EN	202	PEB	CHA-C1B-NB	-3.48	117.65	124.93
29	qJ	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	qL	202	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	HK	1002	PEB	OD-C4D-ND	-3.48	120.77	125.93
29	g1	201	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
29	IJ	202	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
29	gK	201	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
29	IL	202	PEB	C1B-C2B-C3B	-3.48	102.51	106.51
29	UF	202	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
29	UI	202	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
29	WJ	203	PEB	C3D-C4D-ND	3.48	114.09	107.26
29	WL	203	PEB	C3D-C4D-ND	3.48	114.09	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CF	1001	CYC	C1B-C2B-C3B	-3.48	104.24	107.87
31	CI	1001	CYC	C1B-C2B-C3B	-3.48	104.24	107.87
31	IF	1001	CYC	CHA-C1A-NA	-3.48	124.00	128.83
31	II	1001	CYC	CHA-C1A-NA	-3.48	124.00	128.83
29	a1	203	PEB	OD-C4D-ND	-3.48	120.77	125.93
29	aK	203	PEB	OD-C4D-ND	-3.48	120.77	125.93
29	A3	202	PEB	OA-C1A-C2A	-3.48	123.41	126.17
29	AO	202	PEB	OA-C1A-C2A	-3.48	123.41	126.17
31	I1	1001	CYC	C2C-C1C-NC	3.48	111.27	108.27
31	NF	1001	CYC	C4D-CHA-C1A	3.48	132.97	128.81
31	NI	1001	CYC	C4D-CHA-C1A	3.48	132.97	128.81
29	IJ	202	PEB	CMB-C2B-C1B	3.48	130.42	125.06
29	IL	202	PEB	CMB-C2B-C1B	3.48	130.42	125.06
31	CK	1001	CYC	C2C-C1C-NC	3.48	111.27	108.27
29	YJ	202	PEB	CMB-C2B-C1B	3.48	130.42	125.06
29	YL	202	PEB	CMB-C2B-C1B	3.48	130.42	125.06
29	bF	201	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
29	bI	201	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
29	AA	202	PEB	CHA-C1B-NB	-3.48	117.66	124.93
29	AN	202	PEB	CHA-C1B-NB	-3.48	117.66	124.93
29	GA	202	PEB	OD-C4D-ND	-3.48	120.78	125.93
29	GN	202	PEB	OD-C4D-ND	-3.48	120.78	125.93
29	gJ	202	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
29	gL	202	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
29	QJ	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	eJ	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	QL	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	eL	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	cJ	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	cL	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	V1	201	PEB	OA-C1A-C2A	-3.48	123.41	126.17
29	VK	201	PEB	OA-C1A-C2A	-3.48	123.41	126.17
29	EJ	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	EL	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	P2	201	PEB	C1B-C2B-C3B	-3.48	102.52	106.51
29	wJ	302	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
29	AJ	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	AL	202	PEB	C3D-C4D-ND	3.48	114.08	107.26
29	A1	301	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
29	AK	301	PEB	CHC-C4C-C3C	-3.48	124.41	130.34
29	e1	203	PEB	OD-C4D-ND	-3.47	120.78	125.93
29	eK	203	PEB	OD-C4D-ND	-3.47	120.78	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MR	202	PEB	C2A-C1A-NA	3.47	111.27	108.27
29	gJ	202	PEB	C3D-C4D-ND	3.47	114.08	107.26
29	gL	202	PEB	C3D-C4D-ND	3.47	114.08	107.26
29	d1	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	dK	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	uJ	203	PEB	C3D-C4D-ND	3.47	114.07	107.26
29	uL	203	PEB	C3D-C4D-ND	3.47	114.07	107.26
29	D3	203	PEB	CHC-C1D-ND	-3.47	109.91	113.95
29	DO	203	PEB	CHC-C1D-ND	-3.47	109.91	113.95
29	DQ	203	PEB	CHA-C4A-NA	-3.47	121.08	125.20
29	M3	203	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
29	MO	203	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
29	IJ	202	PEB	C3D-C4D-ND	3.47	114.07	107.26
29	IL	202	PEB	C3D-C4D-ND	3.47	114.07	107.26
29	F3	203	PEB	CHC-C1D-ND	-3.47	109.92	113.95
29	FO	203	PEB	CHC-C1D-ND	-3.47	109.92	113.95
29	E3	201	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	EO	201	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	oJ	202	PEB	C3D-C4D-ND	3.47	114.07	107.26
29	oL	202	PEB	C3D-C4D-ND	3.47	114.07	107.26
29	MR	201	PEB	C2A-C1A-NA	3.47	111.27	108.27
31	VP	1001	CYC	C1A-C2A-C3A	-3.47	102.94	106.78
29	b1	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	IA	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	bK	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	IN	202	PEB	C3B-C4B-NB	3.47	115.10	110.05
29	OJ	202	PEB	CMB-C2B-C1B	3.47	130.41	125.06
29	OL	202	PEB	CMB-C2B-C1B	3.47	130.41	125.06
29	EJ	201	PEB	CBC-CAC-C2C	-3.47	106.70	112.62
29	EL	201	PEB	CBC-CAC-C2C	-3.47	106.70	112.62
31	JF	1001	CYC	C4D-CHA-C1A	3.47	132.96	128.81
31	JI	1001	CYC	C4D-CHA-C1A	3.47	132.96	128.81
31	J9	1001	CYC	C1A-C2A-C3A	-3.47	102.94	106.78
31	F1	1001	CYC	C1B-C2B-C3B	-3.47	104.25	107.87
31	FK	1001	CYC	C1B-C2B-C3B	-3.47	104.25	107.87
29	E3	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
29	EO	201	PEB	C1B-C2B-C3B	-3.47	102.52	106.51
29	f1	202	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	fK	202	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	uJ	203	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
29	uL	203	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
29	ZF	201	PEB	OA-C1A-C2A	-3.47	123.42	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZI	201	PEB	OA-C1A-C2A	-3.47	123.42	126.17
29	zJ	501	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
30	MG	402	PUB	CHC-C1D-ND	-3.47	109.34	113.72
29	zL	501	PEB	CHC-C4C-C3C	-3.47	124.42	130.34
29	a1	201	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
29	aK	201	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
29	iJ	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
29	iL	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
29	EA	202	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	EN	202	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	PR	201	PEB	C4B-C3B-C2B	-3.47	102.94	106.78
29	DO	202	PEB	C2A-C1A-NA	3.47	111.26	108.27
29	R1	203	PEB	OD-C4D-ND	-3.47	120.79	125.93
29	RK	203	PEB	OD-C4D-ND	-3.47	120.79	125.93
29	BQ	203	PEB	CHA-C4A-NA	-3.47	121.08	125.20
29	h1	202	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	A3	201	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	hK	202	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	AO	201	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	W1	202	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
29	WK	202	PEB	C1B-C2B-C3B	-3.47	102.53	106.51
31	IK	1001	CYC	C2C-C1C-NC	3.47	111.26	108.27
29	DG	203	PEB	CHA-C4A-NA	-3.47	121.08	125.20
29	OJ	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
29	OL	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
29	G3	201	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	GO	201	PEB	C3B-C4B-NB	3.47	115.09	110.05
29	CJ	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
29	CL	202	PEB	C3D-C4D-ND	3.47	114.06	107.26
29	BG	203	PEB	CHA-C4A-NA	-3.47	121.08	125.20
29	B5	201	PEB	C2A-C1A-NA	3.46	111.26	108.27
29	MJ	202	PEB	C3D-C4D-ND	3.46	114.06	107.26
29	ML	202	PEB	C3D-C4D-ND	3.46	114.06	107.26
29	C3	201	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
29	CO	201	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
29	MQ	403	PEB	CHA-C1B-NB	-3.46	117.69	124.93
31	L1	1001	CYC	C1B-C2B-C3B	-3.46	104.26	107.87
31	LK	1001	CYC	C1B-C2B-C3B	-3.46	104.26	107.87
31	NK	1001	CYC	C1B-C2B-C3B	-3.46	104.26	107.87
29	Y1	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
29	YK	201	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
29	BB	301	PEB	CBC-CAC-C2C	3.46	118.53	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BM	301	PEB	CBC-CAC-C2C	3.46	118.53	112.62
29	sJ	202	PEB	C3D-C4D-ND	3.46	114.05	107.26
29	sL	202	PEB	C3D-C4D-ND	3.46	114.05	107.26
29	N1	1002	PEB	OD-C4D-ND	-3.46	120.80	125.93
29	CA	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
29	CN	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
29	QJ	202	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
29	QL	202	PEB	C1B-C2B-C3B	-3.46	102.53	106.51
29	ZF	201	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
29	ZI	201	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
29	xJ	302	PEB	CHC-C4C-C3C	-3.46	124.43	130.34
29	A1	303	PEB	CMB-C2B-C1B	3.46	130.39	125.06
29	AK	303	PEB	CMB-C2B-C1B	3.46	130.39	125.06
29	EA	202	PEB	OD-C4D-ND	-3.46	120.80	125.93
29	EN	202	PEB	OD-C4D-ND	-3.46	120.80	125.93
29	L3	202	PEB	CHC-C1D-ND	-3.46	109.93	113.95
29	LO	202	PEB	CHC-C1D-ND	-3.46	109.93	113.95
29	MG	401	PEB	CHA-C1B-NB	-3.46	117.69	124.93
31	HK	1001	CYC	C1B-C2B-C3B	-3.46	104.26	107.87
29	V2	202	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
29	RR	202	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
29	O1	202	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
29	OK	202	PEB	C4B-C3B-C2B	-3.46	102.95	106.78
31	HF	1001	CYC	C4D-CHA-C1A	3.46	132.94	128.81
31	HI	1001	CYC	C4D-CHA-C1A	3.46	132.94	128.81
29	T1	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
29	TK	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
29	R7	202	PEB	C2A-C1A-NA	3.46	111.25	108.27
29	R9	202	PEB	C2A-C1A-NA	3.46	111.25	108.27
31	C1	1001	CYC	C2C-C1C-NC	3.46	111.25	108.27
29	YJ	202	PEB	C3D-C4D-ND	3.46	114.04	107.26
29	YL	202	PEB	C3D-C4D-ND	3.46	114.04	107.26
29	P1	201	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
29	CJ	202	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
29	PK	201	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
29	CL	202	PEB	C1B-C2B-C3B	-3.46	102.54	106.51
29	MB	201	PEB	C2A-C1A-NA	3.46	111.25	108.27
29	MM	201	PEB	C2A-C1A-NA	3.46	111.25	108.27
31	I1	1001	CYC	CHA-C1A-NA	-3.46	124.03	128.83
31	EK	1001	CYC	CHA-C1A-NA	-3.46	124.03	128.83
29	GJ	202	PEB	C3D-C4D-ND	3.46	114.04	107.26
29	GL	202	PEB	C3D-C4D-ND	3.46	114.04	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AA	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
29	AN	202	PEB	C3B-C4B-NB	3.46	115.08	110.05
29	m1	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
29	mK	202	PEB	OD-C4D-ND	-3.46	120.81	125.93
29	i1	203	PEB	OD-C4D-ND	-3.46	120.81	125.93
29	iK	203	PEB	OD-C4D-ND	-3.46	120.81	125.93
29	fF	201	PEB	CHC-C4C-C3C	-3.46	124.44	130.34
29	fI	201	PEB	CHC-C4C-C3C	-3.46	124.44	130.34
29	LG	203	PEB	CHA-C4A-NA	-3.46	121.10	125.20
29	Q1	202	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
29	j1	202	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
29	QK	202	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
29	jK	202	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
29	Y1	202	PEB	OD-C4D-ND	-3.45	120.81	125.93
29	YK	202	PEB	OD-C4D-ND	-3.45	120.81	125.93
29	Z1	203	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
29	ZK	203	PEB	C1B-C2B-C3B	-3.45	102.54	106.51
29	Q1	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
29	QK	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
29	H3	203	PEB	CHC-C1D-ND	-3.45	109.94	113.95
29	HO	203	PEB	CHC-C1D-ND	-3.45	109.94	113.95
29	HK	1002	PEB	C3B-C4B-NB	3.45	115.07	110.05
29	Z1	203	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
29	ZK	203	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
29	AA	202	PEB	OD-C4D-ND	-3.45	120.81	125.93
29	AN	202	PEB	OD-C4D-ND	-3.45	120.81	125.93
31	IF	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
31	II	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
29	W2	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
31	YP	1000	CYC	OC-C1C-C2C	-3.45	123.43	126.17
29	a1	201	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
29	aK	201	PEB	C4B-C3B-C2B	-3.45	102.96	106.78
29	jF	201	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
29	jI	201	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
29	K3	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	KO	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
30	MN	403	PUB	OD-C4D-C3D	-3.45	124.30	128.04
29	FC	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
29	FE	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
29	GA	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
29	GN	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
29	P1	203	PEB	OD-C4D-ND	-3.45	120.82	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	PK	203	PEB	OD-C4D-ND	-3.45	120.82	125.93
29	QF	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
29	QI	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
29	i7	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
29	i9	202	PEB	C2A-C1A-NA	3.45	111.25	108.27
29	k1	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	kK	201	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	S1	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
29	SK	202	PEB	C3B-C4B-NB	3.45	115.07	110.05
31	J1	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
31	JK	1001	CYC	C1B-C2B-C3B	-3.45	104.27	107.87
29	WF	201	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
29	WI	201	PEB	CHC-C4C-C3C	-3.45	124.45	130.34
29	k1	201	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
29	kK	201	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
29	MJ	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	ML	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	MN	405	PEB	C2A-C1A-NA	3.45	111.25	108.27
29	e1	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
29	Q2	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
29	eK	201	PEB	OA-C1A-C2A	-3.45	123.43	126.17
29	k1	203	PEB	OD-C4D-ND	-3.45	120.82	125.93
29	kK	203	PEB	OD-C4D-ND	-3.45	120.82	125.93
29	O1	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	OK	202	PEB	C1B-C2B-C3B	-3.45	102.55	106.51
29	dF	202	PEB	CHC-C4C-C3C	-3.45	124.46	130.34
29	dI	202	PEB	CHC-C4C-C3C	-3.45	124.46	130.34
29	A7	304	PEB	CHA-C1B-NB	-3.45	117.72	124.93
31	CF	1001	CYC	C2C-C1C-NC	3.45	111.24	108.27
31	CI	1001	CYC	C2C-C1C-NC	3.45	111.24	108.27
29	I4	203	PEB	C4B-C3B-C2B	-3.45	102.97	106.78
30	A1	304	PUB	C1C-C2C-C3C	-3.45	102.97	106.78
30	AK	304	PUB	C1C-C2C-C3C	-3.45	102.97	106.78
29	JC	202	PEB	CMB-C2B-C1B	3.45	130.37	125.06
29	JE	202	PEB	CMB-C2B-C1B	3.45	130.37	125.06
29	KA	202	PEB	OD-C4D-ND	-3.45	120.83	125.93
29	KN	202	PEB	OD-C4D-ND	-3.45	120.83	125.93
29	kJ	202	PEB	C3D-C4D-ND	3.44	114.02	107.26
29	kL	202	PEB	C3D-C4D-ND	3.44	114.02	107.26
29	b1	202	PEB	C1B-C2B-C3B	-3.44	102.55	106.51
29	bK	202	PEB	C1B-C2B-C3B	-3.44	102.55	106.51
29	a7	202	PEB	C2A-C1A-NA	3.44	111.24	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a9	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	A9	304	PEB	CHA-C1B-NB	-3.44	117.73	124.93
29	R2	202	PEB	C1B-C2B-C3B	-3.44	102.55	106.51
29	VR	202	PEB	C4B-C3B-C2B	-3.44	102.97	106.78
29	SB	201	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	SM	201	PEB	C2A-C1A-NA	3.44	111.24	108.27
30	MQ	404	PUB	CHC-C1D-ND	-3.44	109.37	113.72
31	KF	1001	CYC	C1B-C2B-C3B	-3.44	104.28	107.87
29	J1	1002	PEB	C3B-C4B-NB	3.44	115.06	110.05
29	j1	202	PEB	C3B-C4B-NB	3.44	115.06	110.05
29	JK	1002	PEB	C3B-C4B-NB	3.44	115.06	110.05
29	jK	202	PEB	C3B-C4B-NB	3.44	115.06	110.05
29	MG	401	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	MA	405	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	OF	201	PEB	CHC-C4C-C3C	-3.44	124.47	130.34
29	OI	201	PEB	CHC-C4C-C3C	-3.44	124.47	130.34
29	A7	301	PEB	CBC-CAC-C2C	-3.44	106.75	112.62
29	A9	301	PEB	CBC-CAC-C2C	-3.44	106.75	112.62
31	E1	1001	CYC	CHA-C1A-NA	-3.44	124.05	128.83
29	O1	202	PEB	C3B-C4B-NB	3.44	115.06	110.05
29	OK	202	PEB	C3B-C4B-NB	3.44	115.06	110.05
29	V7	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	V9	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	X2	201	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	A3	201	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	AO	201	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	TR	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	XR	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	xL	302	PEB	CHC-C4C-C3C	-3.44	124.47	130.34
29	NO	203	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
29	S1	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	SK	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
31	DF	1001	CYC	C4D-CHA-C1A	3.44	132.92	128.81
31	DI	1001	CYC	C4D-CHA-C1A	3.44	132.92	128.81
29	U1	203	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	UK	203	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
31	MF	1001	CYC	C1B-C2B-C3B	-3.44	104.28	107.87
31	MI	1001	CYC	C1B-C2B-C3B	-3.44	104.28	107.87
29	W1	202	PEB	C3B-C4B-NB	3.44	115.05	110.05
29	WK	202	PEB	C3B-C4B-NB	3.44	115.05	110.05
29	E3	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17
29	EO	202	PEB	OA-C1A-C2A	-3.44	123.44	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V1	203	PEB	OD-C4D-ND	-3.44	120.84	125.93
29	VK	203	PEB	OD-C4D-ND	-3.44	120.84	125.93
29	P7	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	P9	202	PEB	C2A-C1A-NA	3.44	111.24	108.27
29	SR	201	PEB	CHC-C1D-ND	-3.44	109.96	113.95
31	D1	1001	CYC	C1B-C2B-C3B	-3.44	104.28	107.87
31	KI	1001	CYC	C1B-C2B-C3B	-3.44	104.28	107.87
29	wJ	303	PEB	CHC-C4C-C3C	-3.44	124.48	130.34
29	J5	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	J8	202	PEB	C1B-C2B-C3B	-3.44	102.56	106.51
29	V2	202	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
29	NR	202	PEB	C4B-C3B-C2B	-3.44	102.98	106.78
29	N2	202	PEB	C1B-C2B-C3B	-3.43	102.56	106.51
29	R1	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	RK	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	wL	302	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
29	F5	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	F8	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	QF	201	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
29	QI	201	PEB	CHC-C4C-C3C	-3.43	124.48	130.34
29	d1	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	dK	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	P1	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	MG	401	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	PK	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	e7	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	e9	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	IB	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	IM	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	EG	201	PEB	C3B-C4B-NB	3.43	115.04	110.05
29	EQ	201	PEB	C3B-C4B-NB	3.43	115.04	110.05
29	R1	201	PEB	OA-C1A-C2A	-3.43	123.44	126.17
29	RK	201	PEB	OA-C1A-C2A	-3.43	123.44	126.17
29	m1	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	mK	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	yJ	301	PEB	OD-C4D-ND	-3.43	120.85	125.93
29	yL	301	PEB	OD-C4D-ND	-3.43	120.85	125.93
31	GF	1001	CYC	C1B-C2B-C3B	-3.43	104.29	107.87
31	GI	1001	CYC	C1B-C2B-C3B	-3.43	104.29	107.87
29	H5	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	T1	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78
29	TK	201	PEB	C4B-C3B-C2B	-3.43	102.98	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	xP	1001	CYC	C1A-C2A-C3A	-3.43	102.98	106.78
29	P1	201	PEB	OA-C1A-C2A	-3.43	123.44	126.17
29	PK	201	PEB	OA-C1A-C2A	-3.43	123.44	126.17
29	Y1	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	YK	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	D3	202	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	lF	201	PEB	OA-C1A-C2A	-3.43	123.45	126.17
29	lI	201	PEB	OA-C1A-C2A	-3.43	123.45	126.17
29	R1	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	l1	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	RK	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	lK	202	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	k1	201	PEB	OA-C1A-C2A	-3.43	123.45	126.17
29	kK	201	PEB	OA-C1A-C2A	-3.43	123.45	126.17
29	V1	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
29	i1	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
29	VK	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
29	iK	201	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
29	g1	203	PEB	OD-C4D-ND	-3.43	120.85	125.93
29	gK	203	PEB	OD-C4D-ND	-3.43	120.85	125.93
29	DC	202	PEB	CMB-C2B-C1B	3.43	130.34	125.06
29	DE	202	PEB	CMB-C2B-C1B	3.43	130.34	125.06
31	GK	1001	CYC	C2C-C1C-NC	3.43	111.23	108.27
29	XR	202	PEB	C4B-C3B-C2B	-3.43	102.99	106.78
29	H1	1002	PEB	C3B-C4B-NB	3.43	115.03	110.05
31	EF	1001	CYC	C1B-C2B-C3B	-3.43	104.30	107.87
31	EI	1001	CYC	C1B-C2B-C3B	-3.43	104.30	107.87
29	fB	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	fM	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
31	KF	1001	CYC	C2C-C1C-NC	3.43	111.23	108.27
29	AG	201	PEB	C3B-C4B-NB	3.43	115.03	110.05
29	CG	201	PEB	C3B-C4B-NB	3.43	115.03	110.05
29	AQ	201	PEB	C3B-C4B-NB	3.43	115.03	110.05
29	CQ	201	PEB	C3B-C4B-NB	3.43	115.03	110.05
29	T1	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	TK	201	PEB	C1B-C2B-C3B	-3.43	102.57	106.51
29	I3	202	PEB	OA-C1A-C2A	-3.43	123.45	126.17
29	IO	202	PEB	OA-C1A-C2A	-3.43	123.45	126.17
29	F3	201	PEB	C3B-C4B-NB	3.43	115.03	110.05
29	FO	201	PEB	C3B-C4B-NB	3.43	115.03	110.05
29	KB	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	WB	201	PEB	C2A-C1A-NA	3.43	111.23	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KM	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	WM	201	PEB	C2A-C1A-NA	3.43	111.23	108.27
29	BC	203	PEB	CMB-C2B-C1B	3.43	130.34	125.06
29	BE	203	PEB	CMB-C2B-C1B	3.43	130.34	125.06
29	MA	401	PEB	OD-C4D-ND	-3.43	120.86	125.93
29	kF	201	PEB	OD-C4D-ND	-3.43	120.86	125.93
29	kI	201	PEB	OD-C4D-ND	-3.43	120.86	125.93
29	HQ	203	PEB	CHA-C4A-NA	-3.42	121.13	125.20
30	MA	403	PUB	OD-C4D-C3D	-3.42	124.32	128.04
29	G5	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	Y7	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	Y9	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	UB	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	UM	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	Z1	203	PEB	C3B-C4B-NB	3.42	115.03	110.05
29	ZK	203	PEB	C3B-C4B-NB	3.42	115.03	110.05
31	IK	1001	CYC	CHA-C1A-NA	-3.42	124.08	128.83
29	K3	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	KO	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	wL	303	PEB	CHC-C4C-C3C	-3.42	124.50	130.34
29	f1	201	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	fK	201	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	EB	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	EM	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
31	D1	1003	CYC	C2C-C1C-NC	3.42	111.22	108.27
29	LC	202	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
29	LE	202	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
29	e1	201	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
29	eK	201	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
29	MN	401	PEB	OD-C4D-ND	-3.42	120.86	125.93
29	i1	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
29	iK	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
29	EG	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	GG	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	EQ	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	GQ	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	LC	203	PEB	CMB-C2B-C1B	3.42	130.33	125.06
29	LE	203	PEB	CMB-C2B-C1B	3.42	130.33	125.06
31	H1	1001	CYC	C1B-C2B-C3B	-3.42	104.30	107.87
29	S2	201	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	BC	202	PEB	C2A-C1A-NA	3.42	111.22	108.27
29	BE	202	PEB	C2A-C1A-NA	3.42	111.22	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AG	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	AQ	202	PEB	OA-C1A-C2A	-3.42	123.45	126.17
29	I3	202	PEB	OD-C4D-ND	-3.42	120.86	125.93
29	IO	202	PEB	OD-C4D-ND	-3.42	120.86	125.93
29	KC	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
29	KE	201	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
30	MG	403	PUB	CAC-C2C-C3C	-3.42	121.51	127.88
29	FG	203	PEB	CHA-C4A-NA	-3.42	121.14	125.20
29	KG	201	PEB	C3B-C4B-NB	3.42	115.02	110.05
29	KQ	201	PEB	C3B-C4B-NB	3.42	115.02	110.05
29	VR	202	PEB	C1B-C2B-C3B	-3.42	102.58	106.51
31	K1	1001	CYC	C2C-C1C-NC	3.42	111.22	108.27
31	EF	1001	CYC	C2C-C1C-NC	3.42	111.22	108.27
31	EI	1001	CYC	C2C-C1C-NC	3.42	111.22	108.27
31	KK	1001	CYC	C2C-C1C-NC	3.42	111.22	108.27
29	C3	202	PEB	OA-C1A-C2A	-3.42	123.46	126.17
29	CO	202	PEB	OA-C1A-C2A	-3.42	123.46	126.17
29	F1	1002	PEB	C3B-C4B-NB	3.42	115.02	110.05
29	FK	1002	PEB	C3B-C4B-NB	3.42	115.02	110.05
29	FC	203	PEB	CMB-C2B-C1B	3.42	130.32	125.06
29	FE	203	PEB	CMB-C2B-C1B	3.42	130.32	125.06
31	D1	1003	CYC	CHA-C1A-NA	-3.42	124.09	128.83
29	P2	201	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
29	T2	202	PEB	C4B-C3B-C2B	-3.42	103.00	106.78
29	A3	202	PEB	OD-C4D-ND	-3.42	120.87	125.93
29	AO	202	PEB	OD-C4D-ND	-3.42	120.87	125.93
29	N2	202	PEB	C4B-C3B-C2B	-3.41	103.00	106.78
29	NR	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
30	QB	201	PUB	CHA-C4A-NA	-3.41	109.98	113.95
30	QM	201	PUB	CHA-C4A-NA	-3.41	109.98	113.95
29	T7	202	PEB	C2A-C1A-NA	3.41	111.22	108.27
29	T9	202	PEB	C2A-C1A-NA	3.41	111.22	108.27
29	J3	201	PEB	C3B-C4B-NB	3.41	115.02	110.05
29	JO	201	PEB	C3B-C4B-NB	3.41	115.02	110.05
29	I8	203	PEB	CHC-C4C-C3C	-3.41	124.52	130.34
29	m7	202	PEB	C2A-C1A-NA	3.41	111.22	108.27
29	m9	202	PEB	C2A-C1A-NA	3.41	111.22	108.27
29	CB	201	PEB	C2A-C1A-NA	3.41	111.22	108.27
29	CM	201	PEB	C2A-C1A-NA	3.41	111.22	108.27
31	CK	1001	CYC	CHA-C1A-NA	-3.41	124.09	128.83
29	m1	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
29	mK	201	PEB	C1B-C2B-C3B	-3.41	102.59	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HG	203	PEB	CHA-C4A-NA	-3.41	121.15	125.20
29	T7	202	PEB	C3D-C4D-ND	3.41	113.95	107.26
29	T9	202	PEB	C3D-C4D-ND	3.41	113.95	107.26
29	E3	202	PEB	OD-C4D-ND	-3.41	120.88	125.93
29	EO	202	PEB	OD-C4D-ND	-3.41	120.88	125.93
29	yJ	301	PEB	CBA-CAA-C3A	-3.41	105.88	113.47
29	yL	301	PEB	CBA-CAA-C3A	-3.41	105.88	113.47
29	GG	201	PEB	C3B-C4B-NB	3.41	115.01	110.05
29	GQ	201	PEB	C3B-C4B-NB	3.41	115.01	110.05
29	hF	201	PEB	OA-C1A-C2A	-3.41	123.46	126.17
29	hI	201	PEB	OA-C1A-C2A	-3.41	123.46	126.17
29	c1	201	PEB	CHC-C1D-ND	-3.41	109.99	113.95
29	cK	201	PEB	CHC-C1D-ND	-3.41	109.99	113.95
29	jB	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
29	jM	201	PEB	C2A-C1A-NA	3.41	111.21	108.27
29	IG	201	PEB	C3B-C4B-NB	3.41	115.01	110.05
29	IQ	201	PEB	C3B-C4B-NB	3.41	115.01	110.05
29	CG	202	PEB	OA-C1A-C2A	-3.41	123.46	126.17
29	CQ	202	PEB	OA-C1A-C2A	-3.41	123.46	126.17
29	FQ	203	PEB	CHA-C4A-NA	-3.41	121.15	125.20
29	h1	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
29	hK	202	PEB	C1B-C2B-C3B	-3.41	102.59	106.51
29	yJ	301	PEB	CHC-C1D-ND	-3.41	109.99	113.95
29	yL	301	PEB	CHC-C1D-ND	-3.41	109.99	113.95
29	a7	202	PEB	C3D-C4D-ND	3.41	113.94	107.26
29	a9	202	PEB	C3D-C4D-ND	3.41	113.94	107.26
29	PR	201	PEB	C1B-C2B-C3B	-3.41	102.60	106.51
31	M1	1001	CYC	C2C-C1C-NC	3.41	111.21	108.27
31	MK	1001	CYC	C2C-C1C-NC	3.41	111.21	108.27
30	MQ	405	PUB	CAC-C2C-C3C	-3.41	121.53	127.88
29	c7	202	PEB	C3D-C4D-ND	3.41	113.94	107.26
29	c9	202	PEB	C3D-C4D-ND	3.41	113.94	107.26
29	MA	404	PEB	OA-C1A-C2A	-3.41	123.47	126.17
29	C3	202	PEB	OD-C4D-ND	-3.41	120.89	125.93
29	CO	202	PEB	OD-C4D-ND	-3.41	120.89	125.93
29	RF	201	PEB	OD-C4D-ND	-3.40	120.89	125.93
29	RI	201	PEB	OD-C4D-ND	-3.40	120.89	125.93
29	bF	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	bI	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	xL	303	PEB	CHC-C4C-C3C	-3.40	124.53	130.34
31	WP	1001	CYC	OC-C1C-C2C	-3.40	123.47	126.17
29	DK	1002	PEB	C3B-C4B-NB	3.40	115.00	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f1	202	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
29	fK	202	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
29	G8	201	PEB	C2A-C1A-NA	3.40	111.21	108.27
29	g1	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
29	X2	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
29	gK	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
29	dF	202	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	dI	202	PEB	OA-C1A-C2A	-3.40	123.47	126.17
31	K1	1001	CYC	CHA-C1A-NA	-3.40	124.11	128.83
31	KK	1001	CYC	CHA-C1A-NA	-3.40	124.11	128.83
29	T2	202	PEB	C1B-C2B-C3B	-3.40	102.60	106.51
29	g1	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
29	gK	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
31	M1	1001	CYC	CHA-C1A-NA	-3.40	124.11	128.83
31	MK	1001	CYC	CHA-C1A-NA	-3.40	124.11	128.83
29	D1	1002	PEB	C3B-C4B-NB	3.40	115.00	110.05
29	P7	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	k7	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	P9	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	k9	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	S1	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	SK	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	g7	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	g9	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	eJ	202	PEB	CHC-C4C-C3C	-3.40	124.54	130.34
29	eL	202	PEB	CHC-C4C-C3C	-3.40	124.54	130.34
29	G3	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
29	iF	201	PEB	OD-C4D-ND	-3.40	120.89	125.93
29	iI	201	PEB	OD-C4D-ND	-3.40	120.89	125.93
29	GO	202	PEB	OD-C4D-ND	-3.40	120.89	125.93
29	BC	202	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
29	BE	202	PEB	C1B-C2B-C3B	-3.40	102.61	106.51
31	C1	1001	CYC	CHA-C1A-NA	-3.40	124.11	128.83
29	HC	203	PEB	CMB-C2B-C1B	3.40	130.30	125.06
29	HE	203	PEB	CMB-C2B-C1B	3.40	130.30	125.06
29	WF	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	WI	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
31	1P	1002	CYC	OC-C1C-C2C	-3.40	123.47	126.17
29	K5	203	PEB	CHC-C4C-C3C	-3.40	124.54	130.34
29	K8	203	PEB	CHC-C4C-C3C	-3.40	124.54	130.34
29	R7	202	PEB	C3D-C4D-ND	3.40	113.93	107.26
29	R9	202	PEB	C3D-C4D-ND	3.40	113.93	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B3	202	PEB	CMD-C2D-C3D	-3.40	125.27	130.06
29	BO	202	PEB	CMD-C2D-C3D	-3.40	125.27	130.06
31	GK	1001	CYC	CHA-C1A-NA	-3.40	124.11	128.83
29	B3	201	PEB	C3B-C4B-NB	3.40	114.99	110.05
29	BO	201	PEB	C3B-C4B-NB	3.40	114.99	110.05
29	j1	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	jK	201	PEB	OA-C1A-C2A	-3.40	123.47	126.17
29	c1	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
29	cK	201	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
31	MF	1001	CYC	C2C-C1C-NC	3.40	111.20	108.27
31	MI	1001	CYC	C2C-C1C-NC	3.40	111.20	108.27
29	TR	202	PEB	C4B-C3B-C2B	-3.40	103.02	106.78
29	T1	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
29	m1	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
29	TK	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
29	mK	201	PEB	CHC-C1D-ND	-3.40	110.00	113.95
29	e7	202	PEB	C3D-C4D-ND	3.40	113.92	107.26
29	e9	202	PEB	C3D-C4D-ND	3.40	113.92	107.26
29	LC	203	PEB	OD-C4D-ND	-3.40	120.90	125.93
29	LE	203	PEB	OD-C4D-ND	-3.40	120.90	125.93
29	L1	1002	PEB	C3B-C4B-NB	3.40	114.99	110.05
29	LK	1002	PEB	C3B-C4B-NB	3.40	114.99	110.05
29	fB	202	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
29	fM	202	PEB	C1B-C2B-C3B	-3.39	102.61	106.51
29	DB	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	GB	201	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	YB	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	DM	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	GM	201	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	YM	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	V1	201	PEB	CHC-C1D-ND	-3.39	110.01	113.95
29	VK	201	PEB	CHC-C1D-ND	-3.39	110.01	113.95
29	A1	302	PEB	CMB-C2B-C1B	3.39	130.29	125.06
29	AK	302	PEB	CMB-C2B-C1B	3.39	130.29	125.06
29	K3	202	PEB	OD-C4D-ND	-3.39	120.90	125.93
29	KO	202	PEB	OD-C4D-ND	-3.39	120.90	125.93
29	H3	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
29	HO	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
31	D1	1001	CYC	C1B-NB-C4B	-3.39	106.35	110.67
29	17	202	PEB	C3B-C4B-NB	3.39	114.98	110.05
29	19	202	PEB	C3B-C4B-NB	3.39	114.98	110.05
29	NK	1002	PEB	C3B-C4B-NB	3.39	114.98	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	xJ	303	PEB	CHC-C4C-C3C	-3.39	124.55	130.34
29	c7	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	c9	202	PEB	C2A-C1A-NA	3.39	111.20	108.27
29	M4	203	PEB	CHA-C1B-NB	-3.39	117.84	124.93
29	Y7	202	PEB	C3D-C4D-ND	3.39	113.91	107.26
29	Y9	202	PEB	C3D-C4D-ND	3.39	113.91	107.26
29	PF	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
29	PI	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
29	D3	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
29	DO	201	PEB	C3B-C4B-NB	3.39	114.98	110.05
29	UR	202	PEB	CBB-CAB-C3B	-3.39	103.21	112.63
29	kF	201	PEB	CAB-CBB-CGB	-3.39	106.31	113.60
29	kI	201	PEB	CAB-CBB-CGB	-3.39	106.31	113.60
29	OB	201	PEB	C2A-C1A-NA	3.39	111.19	108.27
29	OM	201	PEB	C2A-C1A-NA	3.39	111.19	108.27
31	DK	1001	CYC	C1B-C2B-C3B	-3.39	104.33	107.87
29	M2	202	PEB	CBB-CAB-C3B	-3.39	103.21	112.63
29	c7	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
29	c9	201	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
29	RR	202	PEB	C4B-C3B-C2B	-3.39	103.03	106.78
29	OB	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	OM	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	H3	202	PEB	CHC-C4C-C3C	3.39	136.11	130.34
29	HO	202	PEB	CHC-C4C-C3C	3.39	136.11	130.34
29	SF	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
29	UF	202	PEB	OA-C1A-C2A	-3.39	123.48	126.17
29	jF	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
29	SI	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
29	UI	202	PEB	OA-C1A-C2A	-3.39	123.48	126.17
29	jI	201	PEB	OA-C1A-C2A	-3.39	123.48	126.17
29	A5	203	PEB	CHC-C4C-C3C	-3.39	124.56	130.34
29	A8	203	PEB	CHC-C4C-C3C	-3.39	124.56	130.34
29	UJ	202	PEB	CHC-C4C-C3C	-3.39	124.56	130.34
29	UL	202	PEB	CHC-C4C-C3C	-3.39	124.56	130.34
29	m7	202	PEB	C3D-C4D-ND	3.39	113.91	107.26
29	m9	202	PEB	C3D-C4D-ND	3.39	113.91	107.26
29	TB	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
29	TM	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
31	IF	1001	CYC	C2C-C1C-NC	3.39	111.19	108.27
31	II	1001	CYC	C2C-C1C-NC	3.39	111.19	108.27
29	SB	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	SM	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MQ	403	PEB	OD-C4D-C3D	-3.39	121.79	129.46
29	O2	202	PEB	CBB-CAB-C3B	-3.39	103.22	112.63
29	FC	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	HC	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	FE	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	HE	202	PEB	C1B-C2B-C3B	-3.39	102.62	106.51
29	k7	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
29	k9	202	PEB	C2A-C1A-NA	3.39	111.19	108.27
29	QB	203	PEB	C2A-C1A-NA	3.39	111.19	108.27
29	QM	203	PEB	C2A-C1A-NA	3.39	111.19	108.27
29	eF	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
29	eI	201	PEB	OD-C4D-ND	-3.39	120.91	125.93
29	C5	203	PEB	CHC-C4C-C3C	-3.39	124.56	130.34
29	AC	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
29	AE	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
29	gJ	202	PEB	CHC-C4C-C3C	-3.38	124.56	130.34
29	gL	202	PEB	CHC-C4C-C3C	-3.38	124.56	130.34
29	P7	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
29	V7	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
29	P9	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
29	V9	201	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
31	KI	1001	CYC	C2C-C1C-NC	3.38	111.19	108.27
29	IJ	202	PEB	CHC-C1D-ND	-3.38	110.02	113.95
29	IL	202	PEB	CHC-C1D-ND	-3.38	110.02	113.95
29	R2	202	PEB	C4B-C3B-C2B	-3.38	103.04	106.78
29	KC	202	PEB	CMB-C2B-C1B	3.38	130.27	125.06
29	KE	202	PEB	CMB-C2B-C1B	3.38	130.27	125.06
29	a1	201	PEB	CHC-C1D-ND	-3.38	110.02	113.95
29	aK	201	PEB	CHC-C1D-ND	-3.38	110.02	113.95
29	aF	201	PEB	OD-C4D-ND	-3.38	120.92	125.93
29	aI	201	PEB	OD-C4D-ND	-3.38	120.92	125.93
29	C3	201	PEB	CHC-C1D-ND	-3.38	110.02	113.95
29	CO	201	PEB	CHC-C1D-ND	-3.38	110.02	113.95
29	YF	201	PEB	OD-C4D-ND	-3.38	120.92	125.93
29	YI	201	PEB	OD-C4D-ND	-3.38	120.92	125.93
29	IB	202	PEB	C1B-C2B-C3B	-3.38	102.62	106.51
29	IM	202	PEB	C1B-C2B-C3B	-3.38	102.62	106.51
29	I5	203	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
29	i7	202	PEB	C3D-C4D-ND	3.38	113.89	107.26
29	i9	202	PEB	C3D-C4D-ND	3.38	113.89	107.26
29	MG	404	PEB	OA-C1A-C2A	-3.38	123.48	126.17
29	E3	202	PEB	CHC-C4C-C3C	-3.38	124.57	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EO	202	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
29	J3	202	PEB	CMD-C2D-C3D	-3.38	125.30	130.06
29	JO	202	PEB	CMD-C2D-C3D	-3.38	125.30	130.06
29	I5	202	PEB	C3B-C4B-NB	3.38	114.97	110.05
29	I8	202	PEB	C3B-C4B-NB	3.38	114.97	110.05
29	GB	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	GM	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	CJ	202	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
29	CL	202	PEB	CHC-C4C-C3C	-3.38	124.57	130.34
29	U7	202	PEB	C3B-C4B-NB	3.38	114.96	110.05
29	U9	202	PEB	C3B-C4B-NB	3.38	114.96	110.05
29	cJ	202	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
29	cL	202	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
29	AC	203	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	AE	203	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	B8	201	PEB	C2A-C1A-NA	3.38	111.19	108.27
29	RF	201	PEB	CAB-CBB-CGB	-3.38	106.33	113.60
29	RI	201	PEB	CAB-CBB-CGB	-3.38	106.33	113.60
29	cF	201	PEB	OD-C4D-ND	-3.38	120.93	125.93
29	cI	201	PEB	OD-C4D-ND	-3.38	120.93	125.93
29	N1	1002	PEB	C3B-C4B-NB	3.38	114.96	110.05
29	S2	201	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
29	MG	401	PEB	OD-C4D-C3D	-3.38	121.81	129.46
29	MQ	406	PEB	OA-C1A-C2A	-3.38	123.49	126.17
29	P1	201	PEB	CHC-C1D-ND	-3.38	110.03	113.95
29	UJ	202	PEB	CHC-C1D-ND	-3.38	110.03	113.95
29	PK	201	PEB	CHC-C1D-ND	-3.38	110.03	113.95
29	UL	202	PEB	CHC-C1D-ND	-3.38	110.03	113.95
29	H3	202	PEB	CMD-C2D-C3D	-3.38	125.30	130.06
29	HO	202	PEB	CMD-C2D-C3D	-3.38	125.30	130.06
29	oJ	202	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
29	oL	202	PEB	CHC-C4C-C3C	-3.38	124.58	130.34
29	Y7	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
29	Y9	201	PEB	C4B-C3B-C2B	-3.38	103.05	106.78
29	IC	201	PEB	CMB-C2B-C1B	3.38	130.26	125.06
29	IE	201	PEB	CMB-C2B-C1B	3.38	130.26	125.06
29	mB	203	PEB	OA-C1A-C2A	-3.38	123.49	126.17
29	mM	203	PEB	OA-C1A-C2A	-3.38	123.49	126.17
29	MB	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	FG	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	MM	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51
29	FQ	202	PEB	C1B-C2B-C3B	-3.38	102.63	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k1	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
29	kK	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
31	L1	1001	CYC	C1B-NB-C4B	-3.37	106.37	110.67
31	LK	1001	CYC	C1B-NB-C4B	-3.37	106.37	110.67
29	Q2	201	PEB	OD-C4D-C3D	-3.37	121.81	129.46
29	MR	202	PEB	CHC-C4C-C3C	-3.37	124.58	130.34
29	d7	202	PEB	C3B-C4B-NB	3.37	114.96	110.05
29	d9	202	PEB	C3B-C4B-NB	3.37	114.96	110.05
29	KJ	202	PEB	CHC-C4C-C3C	-3.37	124.58	130.34
29	KL	202	PEB	CHC-C4C-C3C	-3.37	124.58	130.34
29	i1	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
29	iK	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
29	WB	202	PEB	C1B-C2B-C3B	-3.37	102.63	106.51
29	WM	202	PEB	C1B-C2B-C3B	-3.37	102.63	106.51
29	SJ	202	PEB	CHC-C4C-C3C	-3.37	124.58	130.34
29	SL	202	PEB	CHC-C4C-C3C	-3.37	124.58	130.34
29	MN	401	PEB	CMB-C2B-C1B	3.37	130.26	125.06
29	MG	401	PEB	C3B-C4B-NB	3.37	114.96	110.05
29	FB	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
29	FM	202	PEB	C2A-C1A-NA	3.37	111.18	108.27
29	Q2	202	PEB	CBB-CAB-C3B	-3.37	103.25	112.63
29	OF	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
29	OI	201	PEB	OA-C1A-C2A	-3.37	123.49	126.17
29	PF	201	PEB	CAB-CBB-CGB	-3.37	106.34	113.60
29	PI	201	PEB	CAB-CBB-CGB	-3.37	106.34	113.60
29	V7	202	PEB	C3D-C4D-ND	3.37	113.88	107.26
29	V9	202	PEB	C3D-C4D-ND	3.37	113.88	107.26
29	sJ	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	sL	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	TI	201	PEB	CAB-CBB-CGB	-3.37	106.35	113.60
29	WR	202	PEB	CBB-CAB-C3B	-3.37	103.26	112.63
29	A7	301	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
29	A9	301	PEB	C4B-C3B-C2B	-3.37	103.05	106.78
29	gF	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
29	gI	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
29	hB	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
29	hM	201	PEB	C2A-C1A-NA	3.37	111.18	108.27
31	GF	1001	CYC	C2C-C1C-NC	3.37	111.18	108.27
31	GI	1001	CYC	C2C-C1C-NC	3.37	111.18	108.27
29	R1	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
29	RK	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
29	jB	202	PEB	C1B-C2B-C3B	-3.37	102.64	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	jM	202	PEB	C1B-C2B-C3B	-3.37	102.64	106.51
29	S2	202	PEB	CBB-CAB-C3B	-3.37	103.26	112.63
29	C3	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	GJ	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	GL	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	CO	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	B3	202	PEB	CHC-C4C-C3C	3.37	136.08	130.34
29	BO	202	PEB	CHC-C4C-C3C	3.37	136.08	130.34
29	VF	201	PEB	CAB-CBB-CGB	-3.37	106.35	113.60
29	VI	201	PEB	CAB-CBB-CGB	-3.37	106.35	113.60
29	TI	201	PEB	OD-C4D-ND	-3.37	120.94	125.93
29	E3	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
29	EO	201	PEB	CHC-C1D-ND	-3.37	110.03	113.95
31	D1	1003	CYC	C4A-C3A-C2A	-3.37	102.64	106.51
29	mJ	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	mL	202	PEB	CHC-C4C-C3C	-3.37	124.59	130.34
29	I3	201	PEB	CHC-C1D-ND	-3.37	110.04	113.95
29	IO	201	PEB	CHC-C1D-ND	-3.37	110.04	113.95
29	F3	202	PEB	CMD-C2D-C3D	-3.37	125.31	130.06
29	FO	202	PEB	CMD-C2D-C3D	-3.37	125.31	130.06
29	mJ	202	PEB	CHC-C1D-ND	-3.37	110.04	113.95
29	sJ	202	PEB	CHC-C1D-ND	-3.37	110.04	113.95
29	mL	202	PEB	CHC-C1D-ND	-3.37	110.04	113.95
29	sL	202	PEB	CHC-C1D-ND	-3.37	110.04	113.95
29	MQ	403	PEB	C4B-C3B-C2B	-3.37	103.06	106.78
29	JG	202	PEB	CBA-CAA-C3A	-3.37	105.97	113.47
29	JQ	202	PEB	CBA-CAA-C3A	-3.37	105.97	113.47
29	S7	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
29	S9	202	PEB	C3B-C4B-NB	3.37	114.95	110.05
29	mF	201	PEB	CAB-CBB-CGB	-3.37	106.36	113.60
29	mI	201	PEB	CAB-CBB-CGB	-3.37	106.36	113.60
29	C8	203	PEB	CHC-C4C-C3C	-3.37	124.60	130.34
29	MQ	403	PEB	C3B-C4B-NB	3.37	114.94	110.05
29	zJ	501	PEB	C2A-C1A-NA	3.37	111.17	108.27
29	xL	301	PEB	OD-C4D-C3D	-3.37	121.83	129.46
29	B8	201	PEB	CHA-C1B-NB	-3.36	117.89	124.93
29	jF	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
29	jI	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
29	kJ	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	kL	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	F3	202	PEB	CHC-C4C-C3C	3.36	136.07	130.34
29	FO	202	PEB	CHC-C4C-C3C	3.36	136.07	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	cJ	202	PEB	CHC-C1D-ND	-3.36	110.04	113.95
29	cL	202	PEB	CHC-C1D-ND	-3.36	110.04	113.95
29	iJ	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	iL	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	F8	201	PEB	CHA-C1B-NB	-3.36	117.90	124.93
29	V1	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	VK	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	AJ	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	AL	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	h7	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
29	h9	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
29	GJ	202	PEB	CHC-C1D-ND	-3.36	110.04	113.95
29	GL	202	PEB	CHC-C1D-ND	-3.36	110.04	113.95
29	VF	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
29	VI	201	PEB	OD-C4D-ND	-3.36	120.95	125.93
29	IA	202	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
29	IN	202	PEB	C4B-C3B-C2B	-3.36	103.06	106.78
29	gF	201	PEB	CAB-CBB-CGB	-3.36	106.37	113.60
29	iF	201	PEB	CAB-CBB-CGB	-3.36	106.37	113.60
29	gI	201	PEB	CAB-CBB-CGB	-3.36	106.37	113.60
29	iI	201	PEB	CAB-CBB-CGB	-3.36	106.37	113.60
29	OJ	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
29	OL	202	PEB	CHC-C4C-C3C	-3.36	124.60	130.34
31	E1	1001	CYC	C4A-C3A-C2A	-3.36	102.65	106.51
29	B8	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	LB	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	LM	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
31	F1	1001	CYC	C1B-NB-C4B	-3.36	106.39	110.67
31	FK	1001	CYC	C1B-NB-C4B	-3.36	106.39	110.67
29	P1	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	PK	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	SR	202	PEB	CBB-CAB-C3B	-3.36	103.29	112.63
29	RB	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	RM	202	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	CC	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	CE	201	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	JC	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
29	JE	202	PEB	OD-C4D-ND	-3.36	120.95	125.93
29	QJ	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	QL	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	O7	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
29	W7	202	PEB	C3B-C4B-NB	3.36	114.94	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	O9	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
29	W9	202	PEB	C3B-C4B-NB	3.36	114.94	110.05
29	MJ	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	ML	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	lB	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	lM	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	I3	203	PEB	CMD-C2D-C3D	-3.36	125.33	130.06
29	IO	203	PEB	CMD-C2D-C3D	-3.36	125.33	130.06
29	K3	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	IJ	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	IL	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	KO	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	H8	201	PEB	CHA-C1B-NB	-3.36	117.91	124.93
29	CA	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
29	CN	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
29	H8	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	dB	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
29	dM	201	PEB	C2A-C1A-NA	3.36	111.17	108.27
31	EK	1001	CYC	C2C-C1C-NC	3.36	111.17	108.27
29	f7	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	f9	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	a7	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	m7	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	a9	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	m9	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	KA	202	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	KN	202	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	MA	401	PEB	CMB-C2B-C1B	3.36	130.24	125.06
29	F5	201	PEB	CHA-C1B-NB	-3.36	117.91	124.93
29	M2	201	PEB	OD-C4D-C3D	-3.36	121.85	129.46
29	MR	201	PEB	OD-C4D-C3D	-3.36	121.85	129.46
29	L3	201	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	LO	201	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	cF	201	PEB	CAB-CBB-CGB	-3.36	106.38	113.60
29	cI	201	PEB	CAB-CBB-CGB	-3.36	106.38	113.60
29	U2	202	PEB	CBB-CAB-C3B	-3.36	103.30	112.63
29	FC	203	PEB	OD-C4D-ND	-3.36	120.96	125.93
29	FE	203	PEB	OD-C4D-ND	-3.36	120.96	125.93
29	A5	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	A8	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	C8	202	PEB	C3B-C4B-NB	3.36	114.93	110.05
29	aJ	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aL	202	PEB	CHC-C4C-C3C	-3.36	124.61	130.34
29	g1	201	PEB	CMB-C2B-C1B	3.36	130.23	125.06
29	gK	201	PEB	CMB-C2B-C1B	3.36	130.23	125.06
29	DG	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
29	DQ	202	PEB	C1B-C2B-C3B	-3.36	102.65	106.51
29	HC	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	HE	201	PEB	C4B-C3B-C2B	-3.36	103.07	106.78
29	QJ	202	PEB	CHC-C1D-ND	-3.36	110.05	113.95
29	QL	202	PEB	CHC-C1D-ND	-3.36	110.05	113.95
29	UR	201	PEB	OD-C4D-C3D	-3.36	121.86	129.46
29	W1	201	PEB	OA-C1A-C2A	-3.36	123.50	126.17
29	WK	201	PEB	OA-C1A-C2A	-3.36	123.50	126.17
31	yP	1001	CYC	OC-C1C-C2C	-3.36	123.50	126.17
29	AC	201	PEB	CMB-C2B-C1B	3.36	130.23	125.06
29	AE	201	PEB	CMB-C2B-C1B	3.36	130.23	125.06
29	I3	202	PEB	CHC-C4C-C3C	-3.35	124.61	130.34
29	IO	202	PEB	CHC-C4C-C3C	-3.35	124.61	130.34
29	J3	202	PEB	CHC-C4C-C3C	3.35	136.06	130.34
29	JO	202	PEB	CHC-C4C-C3C	3.35	136.06	130.34
29	j7	202	PEB	C3B-C4B-NB	3.35	114.93	110.05
29	j9	202	PEB	C3B-C4B-NB	3.35	114.93	110.05
29	GA	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	GN	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	QR	202	PEB	CBB-CAB-C3B	-3.35	103.31	112.63
29	WJ	203	PEB	CHC-C1D-ND	-3.35	110.05	113.95
29	WL	203	PEB	CHC-C1D-ND	-3.35	110.05	113.95
29	KG	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
29	KQ	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
31	NK	1001	CYC	C1B-NB-C4B	-3.35	106.40	110.67
29	gJ	202	PEB	CHC-C1D-ND	-3.35	110.05	113.95
29	gL	202	PEB	CHC-C1D-ND	-3.35	110.05	113.95
29	QR	201	PEB	OD-C4D-C3D	-3.35	121.86	129.46
29	W2	202	PEB	CBB-CAB-C3B	-3.35	103.31	112.63
29	G3	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	GO	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	eF	201	PEB	CAB-CBB-CGB	-3.35	106.39	113.60
29	eI	201	PEB	CAB-CBB-CGB	-3.35	106.39	113.60
29	R1	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
29	RK	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
29	A3	202	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
29	AO	202	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
29	O2	201	PEB	OD-C4D-C3D	-3.35	121.86	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K3	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	LG	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	KO	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	LQ	201	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	c1	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
29	cK	201	PEB	CMB-C2B-C1B	3.35	130.23	125.06
29	uJ	203	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
29	uL	203	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
29	MN	404	PEB	OA-C1A-C2A	-3.35	123.51	126.17
29	e7	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
29	e9	201	PEB	C4B-C3B-C2B	-3.35	103.07	106.78
29	S1	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	SK	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	e1	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
29	eK	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
29	I3	203	PEB	CHC-C4C-C3C	3.35	136.05	130.34
29	IO	203	PEB	CHC-C4C-C3C	3.35	136.05	130.34
30	A7	303	PUB	CHC-C1D-ND	-3.35	109.48	113.72
30	A9	303	PUB	CHC-C1D-ND	-3.35	109.48	113.72
29	LG	202	PEB	CBA-CAA-C3A	-3.35	106.01	113.47
29	LQ	201	PEB	CBA-CAA-C3A	-3.35	106.01	113.47
29	W2	201	PEB	OD-C4D-C3D	-3.35	121.87	129.46
29	WR	201	PEB	OD-C4D-C3D	-3.35	121.87	129.46
29	h7	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	h9	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	aB	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	aM	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	OF	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	OI	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	KC	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	KE	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	TF	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
30	yL	303	PUB	CHA-C1B-C2B	-3.35	124.62	130.34
29	AC	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	AE	202	PEB	C1B-C2B-C3B	-3.35	102.66	106.51
29	HC	203	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	HE	203	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	U1	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
29	l1	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
29	UK	202	PEB	OA-C1A-C2A	-3.35	123.51	126.17
29	IK	201	PEB	OA-C1A-C2A	-3.35	123.51	126.17
29	OJ	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SJ	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	OL	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	SL	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	YF	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	YI	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	qJ	202	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
29	qL	202	PEB	CHC-C4C-C3C	-3.35	124.62	130.34
29	VB	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	EC	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	EE	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	VM	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	a1	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
29	aK	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
29	A3	201	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	AO	201	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	O1	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	OK	201	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	BC	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	BE	201	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	DG	202	PEB	CBA-CAA-C3A	-3.35	106.01	113.47
29	DQ	202	PEB	CBA-CAA-C3A	-3.35	106.01	113.47
29	GC	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	GE	201	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	EC	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
29	EE	201	PEB	CMB-C2B-C1B	3.35	130.22	125.06
29	e1	201	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	eK	201	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	dF	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	dI	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	kB	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	kM	202	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	hB	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
29	hM	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
31	CK	1001	CYC	C4A-C3A-C2A	-3.35	102.67	106.51
29	U2	201	PEB	OD-C4D-C3D	-3.35	121.88	129.46
29	HG	202	PEB	CBA-CAA-C3A	-3.35	106.02	113.47
29	HQ	202	PEB	CBA-CAA-C3A	-3.35	106.02	113.47
29	aJ	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	eJ	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	aL	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	eL	202	PEB	CHC-C1D-ND	-3.35	110.06	113.95
29	KB	203	PEB	C4B-C3B-C2B	-3.35	103.08	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KM	203	PEB	C4B-C3B-C2B	-3.35	103.08	106.78
29	DC	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	DE	202	PEB	OD-C4D-ND	-3.35	120.97	125.93
29	cB	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
29	cM	202	PEB	C2A-C1A-NA	3.35	111.16	108.27
30	wJ	305	PUB	C1C-C2C-C3C	-3.35	103.08	106.78
29	N1	1002	PEB	OD-C4D-C3D	-3.35	121.88	129.46
29	CB	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
29	HG	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
29	CM	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
29	HQ	202	PEB	C1B-C2B-C3B	-3.35	102.67	106.51
29	Q7	202	PEB	C3B-C4B-NB	3.35	114.92	110.05
29	Q9	202	PEB	C3B-C4B-NB	3.35	114.92	110.05
29	B5	201	PEB	CHA-C1B-NB	-3.34	117.94	124.93
29	B5	202	PEB	C2A-C1A-NA	3.34	111.16	108.27
31	E1	1001	CYC	C2C-C1C-NC	3.34	111.16	108.27
29	YJ	202	PEB	CHC-C4C-C3C	-3.34	124.63	130.34
29	YL	202	PEB	CHC-C4C-C3C	-3.34	124.63	130.34
31	L9	1001	CYC	O2A-CGA-CBA	3.34	124.77	114.03
29	YB	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	YM	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
31	GK	1001	CYC	C4A-C3A-C2A	-3.34	102.67	106.51
29	HB	202	PEB	C2A-C1A-NA	3.34	111.16	108.27
29	aB	201	PEB	C2A-C1A-NA	3.34	111.16	108.27
29	HM	202	PEB	C2A-C1A-NA	3.34	111.16	108.27
29	aM	201	PEB	C2A-C1A-NA	3.34	111.16	108.27
29	OR	201	PEB	OD-C4D-C3D	-3.34	121.89	129.46
29	YF	201	PEB	CAB-CBB-CGB	-3.34	106.41	113.60
29	YI	201	PEB	CAB-CBB-CGB	-3.34	106.41	113.60
29	T7	201	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
29	T9	201	PEB	C4B-C3B-C2B	-3.34	103.08	106.78
29	QB	204	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	QM	204	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
31	M1	1001	CYC	C4A-C3A-C2A	-3.34	102.67	106.51
31	MK	1001	CYC	C4A-C3A-C2A	-3.34	102.67	106.51
29	aF	201	PEB	CAB-CBB-CGB	-3.34	106.41	113.60
29	aI	201	PEB	CAB-CBB-CGB	-3.34	106.41	113.60
29	m7	203	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	m9	203	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	EB	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	dB	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	EM	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	dM	202	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	C5	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	Z7	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	Z9	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	HB	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	HM	202	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	GC	201	PEB	CMB-C2B-C1B	3.34	130.21	125.06
29	GE	201	PEB	CMB-C2B-C1B	3.34	130.21	125.06
29	xJ	301	PEB	OD-C4D-C3D	-3.34	121.89	129.46
29	G3	202	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
29	EJ	202	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
29	EL	202	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
29	GO	202	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
29	iB	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
29	ZF	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
29	ZI	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
29	iM	201	PEB	OD-C4D-ND	-3.34	120.98	125.93
29	DC	201	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
29	DE	201	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
29	KC	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	KE	203	PEB	C1B-C2B-C3B	-3.34	102.67	106.51
29	CJ	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	CL	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	k1	201	PEB	CMB-C2B-C1B	3.34	130.21	125.06
29	kK	201	PEB	CMB-C2B-C1B	3.34	130.21	125.06
29	FG	202	PEB	CBA-CAA-C3A	-3.34	106.03	113.47
29	FQ	202	PEB	CBA-CAA-C3A	-3.34	106.03	113.47
29	JB	202	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
29	JM	202	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
29	BG	202	PEB	CBA-CAA-C3A	-3.34	106.03	113.47
29	BQ	202	PEB	CBA-CAA-C3A	-3.34	106.03	113.47
29	A7	301	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	A9	301	PEB	C3B-C4B-NB	3.34	114.91	110.05
29	K3	201	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	EJ	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	oJ	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	EL	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	oL	202	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	KO	201	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	IG	202	PEB	OA-C1A-C2A	-3.34	123.52	126.17
29	IQ	202	PEB	OA-C1A-C2A	-3.34	123.52	126.17
29	K5	202	PEB	C3B-C4B-NB	3.34	114.90	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K8	202	PEB	C3B-C4B-NB	3.34	114.90	110.05
29	uJ	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
29	uL	201	PEB	C2A-C1A-NA	3.34	111.15	108.27
29	Q1	201	PEB	OD-C4D-ND	-3.34	120.99	125.93
29	QK	201	PEB	OD-C4D-ND	-3.34	120.99	125.93
29	WJ	203	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
29	WL	203	PEB	CHC-C4C-C3C	-3.34	124.64	130.34
29	cB	202	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
29	cM	202	PEB	C4B-C3B-C2B	-3.34	103.09	106.78
31	HK	1001	CYC	C1B-NB-C4B	-3.34	106.42	110.67
31	DK	1001	CYC	C1B-NB-C4B	-3.34	106.42	110.67
29	MA	405	PEB	CHC-C1D-ND	-3.34	110.07	113.95
29	HK	1002	PEB	OD-C4D-C3D	-3.34	121.90	129.46
31	J1	1001	CYC	C1B-NB-C4B	-3.34	106.42	110.67
31	JK	1001	CYC	C1B-NB-C4B	-3.34	106.42	110.67
29	NK	1002	PEB	OD-C4D-C3D	-3.34	121.90	129.46
29	W1	201	PEB	OD-C4D-ND	-3.34	120.99	125.93
29	WK	201	PEB	OD-C4D-ND	-3.34	120.99	125.93
29	QB	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	kB	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	IC	201	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	IE	201	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	QM	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	kM	202	PEB	C2A-C1A-NA	3.33	111.15	108.27
30	yJ	303	PUB	CHA-C1B-C2B	-3.33	124.65	130.34
29	L8	201	PEB	CHA-C1B-NB	-3.33	117.96	124.93
29	J5	201	PEB	CAA-C3A-C4A	-3.33	104.11	112.67
29	H1	1002	PEB	OD-C4D-C3D	-3.33	121.91	129.46
29	R7	201	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
29	R9	201	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
29	aB	203	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
29	aM	203	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
29	mF	201	PEB	OD-C4D-ND	-3.33	120.99	125.93
29	mI	201	PEB	OD-C4D-ND	-3.33	120.99	125.93
29	i1	201	PEB	CMB-C2B-C1B	3.33	130.20	125.06
29	iK	201	PEB	CMB-C2B-C1B	3.33	130.20	125.06
29	W7	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
29	W9	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
29	JG	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
29	JQ	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
31	C1	1001	CYC	C4A-C3A-C2A	-3.33	102.68	106.51
29	YJ	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	YL	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	CC	201	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	CE	201	PEB	C2A-C1A-NA	3.33	111.15	108.27
29	G5	201	PEB	CHA-C1B-NB	-3.33	117.96	124.93
29	H5	201	PEB	CHA-C1B-NB	-3.33	117.96	124.93
29	gB	202	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
29	gM	202	PEB	C4B-C3B-C2B	-3.33	103.09	106.78
29	lB	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
29	lM	202	PEB	C1B-C2B-C3B	-3.33	102.68	106.51
29	f1	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	lF	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	lI	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	fK	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	i7	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	i9	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
31	N1	1001	CYC	C1B-NB-C4B	-3.33	106.43	110.67
29	F5	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	YB	201	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	YM	201	PEB	C2A-C1A-NA	3.33	111.14	108.27
31	D7	1001	CYC	O2A-CGA-CBA	3.33	124.73	114.03
31	D9	1001	CYC	O2A-CGA-CBA	3.33	124.73	114.03
29	G3	201	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	MJ	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	iJ	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	ML	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	iL	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	GO	201	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	g7	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	k7	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	g9	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	k9	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
31	H7	1001	CYC	O2A-CGA-CBA	3.33	124.73	114.03
31	L7	1001	CYC	O2A-CGA-CBA	3.33	124.73	114.03
31	H9	1001	CYC	O2A-CGA-CBA	3.33	124.73	114.03
29	A3	202	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
29	AO	202	PEB	C1B-C2B-C3B	-3.33	102.69	106.51
29	AJ	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
29	AL	202	PEB	CHC-C1D-ND	-3.33	110.08	113.95
30	xL	305	PUB	C1C-C2C-C3C	-3.33	103.10	106.78
29	KB	203	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	KM	203	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	h1	201	PEB	OD-C4D-ND	-3.33	121.00	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	YF	203	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	YI	203	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	hK	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	LB	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	eF	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	kF	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	mF	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	eI	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	kI	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	mI	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	LM	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	JB	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	JM	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	d1	201	PEB	OA-C1A-C2A	-3.33	123.53	126.17
29	h1	201	PEB	OA-C1A-C2A	-3.33	123.53	126.17
29	dK	201	PEB	OA-C1A-C2A	-3.33	123.53	126.17
29	hK	201	PEB	OA-C1A-C2A	-3.33	123.53	126.17
32	k6	302	PMS	O3S-S-O2S	3.33	119.40	111.27
32	kH	302	PMS	O3S-S-O2S	3.33	119.40	111.27
29	U1	202	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	WF	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	WI	201	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	UK	202	PEB	OD-C4D-ND	-3.33	121.00	125.93
29	AA	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	FC	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	FE	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	AN	202	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	b7	202	PEB	C3B-C4B-NB	3.33	114.89	110.05
29	b9	202	PEB	C3B-C4B-NB	3.33	114.89	110.05
29	FJ	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	gJ	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	FL	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	gL	202	PEB	C2A-C1A-NA	3.33	111.14	108.27
29	TI	201	PEB	C4B-C3B-C2B	-3.33	103.10	106.78
29	FJ	203	PEB	CHB-C4B-C3B	-3.33	117.64	125.32
29	FL	203	PEB	CHB-C4B-C3B	-3.33	117.64	125.32
31	DK	1001	CYC	C4A-C3A-C2A	-3.33	102.69	106.51
29	QF	201	PEB	OD-C4D-ND	-3.32	121.00	125.93
29	SF	201	PEB	OD-C4D-ND	-3.32	121.00	125.93
29	QI	201	PEB	OD-C4D-ND	-3.32	121.00	125.93
29	SI	201	PEB	OD-C4D-ND	-3.32	121.00	125.93
29	KA	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KN	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
31	IK	1001	CYC	C4A-C3A-C2A	-3.32	102.69	106.51
29	J8	201	PEB	CAA-C3A-C4A	-3.32	104.14	112.67
29	m1	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
29	mK	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
29	J1	1002	PEB	OD-C4D-C3D	-3.32	121.93	129.46
29	JK	1002	PEB	OD-C4D-C3D	-3.32	121.93	129.46
29	l1	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
29	lK	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
29	rJ	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
29	rL	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
29	EB	202	PEB	CHA-C1B-NB	-3.32	117.98	124.93
29	EM	202	PEB	CHA-C1B-NB	-3.32	117.98	124.93
29	VJ	202	PEB	CHB-C4B-C3B	-3.32	117.64	125.32
29	VL	202	PEB	CHB-C4B-C3B	-3.32	117.64	125.32
29	PB	202	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	PM	202	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	UB	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
29	MQ	401	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
30	A7	302	PUB	CHA-C4A-NA	-3.32	110.09	113.95
30	A9	302	PUB	CHA-C4A-NA	-3.32	110.09	113.95
29	gB	202	PEB	C3B-C4B-NB	3.32	114.88	110.05
29	gM	202	PEB	C3B-C4B-NB	3.32	114.88	110.05
29	BB	301	PEB	CAA-C3A-C4A	3.32	121.20	112.67
29	BM	301	PEB	CAA-C3A-C4A	3.32	121.20	112.67
31	E7	1001	CYC	CMB-C2B-C1B	3.32	128.31	124.17
31	E9	1001	CYC	CMB-C2B-C1B	3.32	128.31	124.17
29	DK	1002	PEB	OD-C4D-C3D	-3.32	121.94	129.46
29	EA	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
29	EN	202	PEB	C1B-C2B-C3B	-3.32	102.69	106.51
29	vJ	202	PEB	CHB-C4B-C3B	-3.32	117.65	125.32
29	vL	202	PEB	CHB-C4B-C3B	-3.32	117.65	125.32
29	Z1	202	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	FB	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	kB	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	ZK	202	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	FM	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	kM	203	PEB	OA-C1A-C2A	-3.32	123.53	126.17
29	TJ	203	PEB	CHB-C4B-C3B	-3.32	117.65	125.32
29	TL	203	PEB	CHB-C4B-C3B	-3.32	117.65	125.32
31	F9	1001	CYC	O2A-CGA-CBA	3.32	124.70	114.03
29	ZJ	202	PEB	C2A-C1A-NA	3.32	111.14	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZL	202	PEB	C2A-C1A-NA	3.32	111.14	108.27
29	l1	201	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	BG	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	lK	201	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	BQ	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	KJ	202	PEB	CHC-C1D-ND	-3.32	110.09	113.95
29	kJ	202	PEB	CHC-C1D-ND	-3.32	110.09	113.95
29	KL	202	PEB	CHC-C1D-ND	-3.32	110.09	113.95
29	kL	202	PEB	CHC-C1D-ND	-3.32	110.09	113.95
29	HB	202	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
29	cF	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
29	cI	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
29	HM	202	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
29	c7	203	PEB	C3B-C4B-NB	3.32	114.88	110.05
29	c9	203	PEB	C3B-C4B-NB	3.32	114.88	110.05
29	T1	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
29	Y1	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
29	TK	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
29	YK	201	PEB	CMB-C2B-C1B	3.32	130.18	125.06
29	fF	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
29	fI	201	PEB	OD-C4D-ND	-3.32	121.01	125.93
29	lJ	203	PEB	CHB-C4B-C3B	-3.32	117.65	125.32
29	lL	203	PEB	CHB-C4B-C3B	-3.32	117.65	125.32
29	wL	301	PEB	OD-C4D-C3D	-3.32	121.94	129.46
29	KB	203	PEB	C3B-C4B-NB	3.32	114.88	110.05
29	KM	203	PEB	C3B-C4B-NB	3.32	114.88	110.05
29	C3	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	I3	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	f7	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	f9	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	CO	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	IO	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	UB	202	PEB	CHA-C1B-NB	-3.32	117.99	124.93
29	MQ	401	PEB	CHA-C1B-NB	-3.32	117.99	124.93
29	nJ	203	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	tJ	202	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	nL	203	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	tL	202	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	D1	1002	PEB	OD-C4D-C3D	-3.32	121.94	129.46
29	UF	202	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	UI	202	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	TJ	202	PEB	C2A-C1A-NA	3.32	111.13	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TL	202	PEB	C2A-C1A-NA	3.32	111.13	108.27
29	XJ	203	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	jJ	203	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	XL	203	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	jL	203	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	JC	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
29	JE	201	PEB	C4B-C3B-C2B	-3.32	103.11	106.78
31	N7	1001	CYC	O2A-CGA-CBA	3.32	124.69	114.03
31	N9	1001	CYC	O2A-CGA-CBA	3.32	124.69	114.03
29	Y7	203	PEB	C3B-C4B-NB	3.32	114.87	110.05
29	Y9	203	PEB	C3B-C4B-NB	3.32	114.87	110.05
29	A3	201	PEB	CHC-C4C-C3C	-3.32	124.68	130.34
29	AO	201	PEB	CHC-C4C-C3C	-3.32	124.68	130.34
29	S7	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	S9	202	PEB	C1B-C2B-C3B	-3.32	102.70	106.51
29	HB	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	BC	203	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	BE	203	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	HM	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	DJ	202	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	DL	202	PEB	CHB-C4B-C3B	-3.32	117.66	125.32
29	wJ	301	PEB	OD-C4D-C3D	-3.32	121.95	129.46
29	b1	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	MG	405	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	bK	201	PEB	OD-C4D-ND	-3.32	121.02	125.93
29	K3	201	PEB	CHC-C4C-C3C	-3.31	124.68	130.34
29	KO	201	PEB	CHC-C4C-C3C	-3.31	124.68	130.34
29	JB	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	JM	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	Z7	202	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
29	Z9	202	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
29	LC	201	PEB	C4B-C3B-C2B	-3.31	103.11	106.78
29	LE	201	PEB	C4B-C3B-C2B	-3.31	103.11	106.78
31	H1	1001	CYC	C1B-NB-C4B	-3.31	106.45	110.67
29	H5	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
31	F7	1001	CYC	O2A-CGA-CBA	3.31	124.68	114.03
29	HB	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	HM	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	KB	202	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
29	KM	202	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
29	MN	405	PEB	C1B-C2B-C3B	-3.31	102.70	106.51
31	I1	1001	CYC	C4A-C3A-C2A	-3.31	102.70	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d1	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
29	dK	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
29	i7	203	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	i9	203	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	YB	201	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	YM	201	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	LJ	202	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	LL	202	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	EJ	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	OJ	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	EL	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	OL	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	ZB	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	ZM	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	NJ	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	NL	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	j1	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
29	jK	201	PEB	OD-C4D-ND	-3.31	121.02	125.93
29	BJ	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	BL	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	Y1	201	PEB	CHC-C1D-ND	-3.31	110.10	113.95
29	YK	201	PEB	CHC-C1D-ND	-3.31	110.10	113.95
31	EK	1001	CYC	C4A-C3A-C2A	-3.31	102.70	106.51
29	EA	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
29	EN	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
29	G8	201	PEB	CHA-C1B-NB	-3.31	118.00	124.93
29	JJ	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	JL	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	lB	202	PEB	CHA-C1B-NB	-3.31	118.01	124.93
29	lM	202	PEB	CHA-C1B-NB	-3.31	118.01	124.93
29	VB	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	VM	202	PEB	C3B-C4B-NB	3.31	114.87	110.05
29	hF	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
29	hI	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
31	J9	1001	CYC	O2A-CGA-CBA	3.31	124.67	114.03
29	mB	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	BJ	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	JJ	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	BL	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	JL	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	mM	202	PEB	C2A-C1A-NA	3.31	111.13	108.27
29	RJ	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RL	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	RB	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
29	RM	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
29	HJ	202	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	pJ	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	HL	202	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	pL	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	CB	202	PEB	CHA-C1B-NB	-3.31	118.01	124.93
29	CM	202	PEB	CHA-C1B-NB	-3.31	118.01	124.93
29	EC	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
29	EE	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
29	PJ	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	PL	203	PEB	CHB-C4B-C3B	-3.31	117.67	125.32
29	E3	201	PEB	CHC-C4C-C3C	-3.31	124.69	130.34
29	EO	201	PEB	CHC-C4C-C3C	-3.31	124.69	130.34
29	E3	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
29	EO	202	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
29	GA	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
29	GN	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
30	A7	302	PUB	C4B-CHB-C1C	-3.31	124.86	128.81
30	A9	302	PUB	C4B-CHB-C1C	-3.31	124.86	128.81
29	G5	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
29	iB	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
29	aJ	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
29	aL	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
29	iM	202	PEB	C2A-C1A-NA	3.31	111.12	108.27
29	KB	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	KM	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	Z1	202	PEB	OD-C4D-ND	-3.31	121.03	125.93
29	ZK	202	PEB	OD-C4D-ND	-3.31	121.03	125.93
29	L1	1002	PEB	OD-C4D-C3D	-3.31	121.97	129.46
29	LK	1002	PEB	OD-C4D-C3D	-3.31	121.97	129.46
29	AF	304	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
29	AI	304	PEB	C1B-C2B-C3B	-3.31	102.71	106.51
29	b1	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	JB	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	gB	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	bK	201	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	JM	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	gM	203	PEB	OA-C1A-C2A	-3.31	123.54	126.17
29	mF	203	PEB	OD-C4D-ND	-3.31	121.03	125.93
29	mI	203	PEB	OD-C4D-ND	-3.31	121.03	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MB	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	aB	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	MM	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	aM	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
31	J7	1001	CYC	O2A-CGA-CBA	3.31	124.65	114.03
29	MD	201	PEB	C2A-C1A-NA	3.31	111.12	108.27
29	HA	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
29	HN	202	PEB	C3B-C4B-NB	3.31	114.86	110.05
29	bF	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
29	bI	201	PEB	OD-C4D-ND	-3.31	121.03	125.93
29	fB	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	fM	202	PEB	CHA-C1B-NB	-3.31	118.02	124.93
29	I3	201	PEB	CHC-C4C-C3C	-3.30	124.70	130.34
29	IO	201	PEB	CHC-C4C-C3C	-3.30	124.70	130.34
29	aB	203	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	aM	203	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	T7	203	PEB	C3B-C4B-NB	3.30	114.86	110.05
29	T9	203	PEB	C3B-C4B-NB	3.30	114.86	110.05
29	cB	202	PEB	C3B-C4B-NB	3.30	114.86	110.05
29	cM	202	PEB	C3B-C4B-NB	3.30	114.86	110.05
29	rJ	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
29	rL	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
29	NB	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	VB	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	NM	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	VM	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	gB	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	gM	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	ZJ	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
29	ZL	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
29	L5	201	PEB	CHA-C1B-NB	-3.30	118.02	124.93
29	FA	202	PEB	C3B-C4B-NB	3.30	114.85	110.05
29	FN	202	PEB	C3B-C4B-NB	3.30	114.85	110.05
29	DB	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	DM	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	O1	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	XB	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	cB	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	OK	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	XM	202	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	cM	203	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	MN	405	PEB	CHC-C1D-ND	-3.30	110.11	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AF	301	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	AI	301	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	dJ	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
29	dL	203	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
29	P7	203	PEB	OD-C4D-ND	-3.30	121.04	125.93
29	P9	203	PEB	OD-C4D-ND	-3.30	121.04	125.93
31	G9	1001	CYC	CMB-C2B-C1B	3.30	128.29	124.17
29	EB	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	EM	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	uJ	203	PEB	CHC-C1D-ND	-3.30	110.11	113.95
29	uL	203	PEB	CHC-C1D-ND	-3.30	110.11	113.95
29	ZB	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
29	ZM	201	PEB	OD-C4D-ND	-3.30	121.04	125.93
29	MQ	407	PEB	OD-C4D-ND	-3.30	121.04	125.93
29	SB	202	PEB	CHA-C1B-NB	-3.30	118.03	124.93
29	hB	202	PEB	CHA-C1B-NB	-3.30	118.03	124.93
29	SM	202	PEB	CHA-C1B-NB	-3.30	118.03	124.93
29	hM	202	PEB	CHA-C1B-NB	-3.30	118.03	124.93
29	AJ	203	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	AL	203	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	QB	204	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	QM	204	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
30	wL	305	PUB	C1C-C2C-C3C	-3.30	103.13	106.78
29	eF	203	PEB	OD-C4D-ND	-3.30	121.04	125.93
29	eI	203	PEB	OD-C4D-ND	-3.30	121.04	125.93
29	F8	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	iF	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	iI	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	qJ	202	PEB	CHC-C1D-ND	-3.30	110.11	113.95
29	qL	202	PEB	CHC-C1D-ND	-3.30	110.11	113.95
29	OB	202	PEB	CHA-C1B-NB	-3.30	118.03	124.93
29	OM	202	PEB	CHA-C1B-NB	-3.30	118.03	124.93
29	b7	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
29	b9	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
29	C3	201	PEB	CHC-C4C-C3C	-3.30	124.71	130.34
29	CO	201	PEB	CHC-C4C-C3C	-3.30	124.71	130.34
29	aF	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	aI	201	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	OR	202	PEB	C2A-C1A-NA	3.30	111.12	108.27
29	hJ	203	PEB	CHB-C4B-C3B	-3.30	117.70	125.32
29	hL	203	PEB	CHB-C4B-C3B	-3.30	117.70	125.32
29	g7	203	PEB	C3B-C4B-NB	3.30	114.85	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g9	203	PEB	C3B-C4B-NB	3.30	114.85	110.05
29	AA	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
29	AN	202	PEB	C1B-C2B-C3B	-3.30	102.72	106.51
31	K1	1001	CYC	C4A-C3A-C2A	-3.30	102.72	106.51
31	KK	1001	CYC	C4A-C3A-C2A	-3.30	102.72	106.51
29	e1	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
29	eK	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
29	bJ	203	PEB	CHB-C4B-C3B	-3.30	117.70	125.32
29	bL	203	PEB	CHB-C4B-C3B	-3.30	117.70	125.32
29	VB	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	VM	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	T7	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
29	T9	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
29	F1	1002	PEB	OD-C4D-C3D	-3.30	121.99	129.46
29	FK	1002	PEB	OD-C4D-C3D	-3.30	121.99	129.46
29	ZB	202	PEB	C2A-C1A-NA	3.30	111.11	108.27
29	ZM	202	PEB	C2A-C1A-NA	3.30	111.11	108.27
29	QB	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	QM	202	PEB	C4B-C3B-C2B	-3.30	103.13	106.78
29	FG	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
29	FQ	202	PEB	CMB-C2B-C1B	3.30	130.14	125.06
29	m7	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
29	m9	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
29	pJ	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
29	pL	203	PEB	OD-C4D-ND	-3.30	121.05	125.93
29	HJ	201	PEB	C2A-C1A-NA	3.30	111.11	108.27
29	IJ	203	PEB	C2A-C1A-NA	3.30	111.11	108.27
29	HL	201	PEB	C2A-C1A-NA	3.30	111.11	108.27
29	IL	203	PEB	C2A-C1A-NA	3.30	111.11	108.27
29	Q1	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	QK	201	PEB	OA-C1A-C2A	-3.30	123.55	126.17
29	gF	203	PEB	OD-C4D-ND	-3.29	121.05	125.93
29	gI	203	PEB	OD-C4D-ND	-3.29	121.05	125.93
29	WB	202	PEB	CHA-C1B-NB	-3.29	118.04	124.93
29	WM	202	PEB	CHA-C1B-NB	-3.29	118.04	124.93
29	qJ	201	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
29	qL	201	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
29	PJ	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	bJ	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	PL	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	bL	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	zL	501	PEB	C2A-C1A-NA	3.29	111.11	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TB	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	YB	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	VF	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	VI	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	zJ	501	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	TM	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	YM	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	IA	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	MA	405	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	IN	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
31	F1	1001	CYC	C4A-C3A-C2A	-3.29	102.73	106.51
31	FK	1001	CYC	C4A-C3A-C2A	-3.29	102.73	106.51
29	QB	204	PEB	CHA-C1B-NB	-3.29	118.04	124.93
29	QM	204	PEB	CHA-C1B-NB	-3.29	118.04	124.93
29	fJ	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	fL	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	IC	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	IE	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	ZB	202	PEB	C3B-C4B-NB	3.29	114.84	110.05
29	iB	202	PEB	C3B-C4B-NB	3.29	114.84	110.05
29	ZM	202	PEB	C3B-C4B-NB	3.29	114.84	110.05
29	iM	202	PEB	C3B-C4B-NB	3.29	114.84	110.05
29	fJ	203	PEB	CHB-C4B-C3B	-3.29	117.71	125.32
29	fL	203	PEB	CHB-C4B-C3B	-3.29	117.71	125.32
29	e7	201	PEB	OD-C4D-ND	-3.29	121.05	125.93
29	e9	201	PEB	OD-C4D-ND	-3.29	121.05	125.93
29	cJ	201	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
29	cL	201	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
30	yL	303	PUB	CHC-C1D-ND	-3.29	109.56	113.72
29	JJ	203	PEB	OD-C4D-ND	-3.29	121.05	125.93
29	JL	203	PEB	OD-C4D-ND	-3.29	121.05	125.93
29	AF	305	PEB	OA-C1A-C2A	-3.29	123.56	126.17
29	AI	305	PEB	OA-C1A-C2A	-3.29	123.56	126.17
29	WJ	201	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	WL	201	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	WJ	202	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
29	WL	202	PEB	CHC-C4C-C3C	-3.29	124.72	130.34
29	GB	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
29	jB	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
29	GM	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
29	jM	202	PEB	CHA-C1B-NB	-3.29	118.05	124.93
29	LG	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LQ	201	PEB	CMB-C2B-C1B	3.29	130.13	125.06
29	O7	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	U7	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	O9	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	U9	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	ZB	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	gF	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	gI	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	ZM	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	LB	203	PEB	OA-C1A-C2A	-3.29	123.56	126.17
29	LM	203	PEB	OA-C1A-C2A	-3.29	123.56	126.17
30	A7	302	PUB	CHC-C1D-ND	-3.29	109.56	113.72
30	A9	302	PUB	CHC-C1D-ND	-3.29	109.56	113.72
29	QB	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	kB	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	QM	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	kM	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	O1	201	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	OK	201	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
31	N1	1001	CYC	C4A-C3A-C2A	-3.29	102.73	106.51
29	e7	203	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	k7	203	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	e9	203	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	k9	203	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	YB	203	PEB	CHA-C1B-NB	-3.29	118.05	124.93
29	YM	203	PEB	CHA-C1B-NB	-3.29	118.05	124.93
29	iB	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	RF	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	RI	201	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	iM	202	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
30	xJ	305	PUB	C1C-C2C-C3C	-3.29	103.14	106.78
29	c1	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06
29	cK	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06
29	FB	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	FM	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	M4	203	PEB	C4B-C3B-C2B	-3.29	103.14	106.78
29	MJ	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	hJ	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	ML	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	hL	202	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	JA	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	JN	202	PEB	C3B-C4B-NB	3.29	114.83	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T7	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
29	T9	201	PEB	OD-C4D-ND	-3.29	121.06	125.93
29	HG	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06
29	HQ	202	PEB	CMB-C2B-C1B	3.29	130.13	125.06
29	d7	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	d9	202	PEB	C1B-C2B-C3B	-3.29	102.73	106.51
29	sJ	203	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	sL	203	PEB	C2A-C1A-NA	3.29	111.11	108.27
29	G3	201	PEB	CHC-C4C-C3C	-3.29	124.73	130.34
29	GO	201	PEB	CHC-C4C-C3C	-3.29	124.73	130.34
29	FB	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	FM	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	IB	202	PEB	CHA-C1B-NB	-3.29	118.06	124.93
29	dB	202	PEB	CHA-C1B-NB	-3.29	118.06	124.93
29	IM	202	PEB	CHA-C1B-NB	-3.29	118.06	124.93
29	dM	202	PEB	CHA-C1B-NB	-3.29	118.06	124.93
29	mB	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
29	mM	202	PEB	C3B-C4B-NB	3.29	114.83	110.05
31	D1	1001	CYC	C4A-C3A-C2A	-3.29	102.74	106.51
30	A7	302	PUB	CHA-C1B-C2B	-3.29	124.73	130.34
30	A9	302	PUB	CHA-C1B-C2B	-3.29	124.73	130.34
29	wJ	303	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	RB	202	PEB	C3B-C4B-NB	3.28	114.83	110.05
29	RM	202	PEB	C3B-C4B-NB	3.28	114.83	110.05
29	OJ	201	PEB	CHC-C4C-C3C	-3.28	124.73	130.34
29	OL	201	PEB	CHC-C4C-C3C	-3.28	124.73	130.34
29	dJ	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	dL	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	a7	203	PEB	C3B-C4B-NB	3.28	114.83	110.05
29	a9	203	PEB	C3B-C4B-NB	3.28	114.83	110.05
29	Z1	201	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	ZK	201	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	A7	305	PEB	OA-C1A-C2A	-3.28	123.56	126.17
29	A9	305	PEB	OA-C1A-C2A	-3.28	123.56	126.17
29	mB	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	mM	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	KJ	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	KL	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	XJ	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	XL	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	DG	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	DQ	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	IA	201	PEB	CHA-C1B-NB	-3.28	118.07	124.93
29	IN	201	PEB	CHA-C1B-NB	-3.28	118.07	124.93
29	KB	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	hB	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	KM	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	hM	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	iJ	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	iL	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	eF	201	PEB	CHC-C1D-ND	-3.28	110.14	113.95
29	eI	201	PEB	CHC-C1D-ND	-3.28	110.14	113.95
29	kB	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	cF	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	cI	202	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	kM	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	TB	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	aB	203	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	TM	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	aM	203	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	Q7	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
29	Q9	202	PEB	C1B-C2B-C3B	-3.28	102.74	106.51
29	TB	203	PEB	OA-C1A-C2A	-3.28	123.56	126.17
29	TM	203	PEB	OA-C1A-C2A	-3.28	123.56	126.17
29	a7	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	a9	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	j1	203	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	jK	203	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	C4	203	PEB	CMA-C2A-C1A	-3.28	105.33	112.40
29	J3	201	PEB	CHB-C4B-NB	-3.28	124.28	128.83
29	JO	201	PEB	CHB-C4B-NB	-3.28	124.28	128.83
29	U1	201	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	UK	201	PEB	CMB-C2B-C1B	3.28	130.12	125.06
31	I7	1001	CYC	CMB-C2B-C1B	3.28	128.26	124.17
31	I9	1001	CYC	CMB-C2B-C1B	3.28	128.26	124.17
29	LB	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	LM	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	L5	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	G8	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	jJ	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	jL	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	g1	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	BB	301	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	gK	202	PEB	CMB-C2B-C1B	3.28	130.12	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BM	301	PEB	CMB-C2B-C1B	3.28	130.12	125.06
29	XB	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	XM	201	PEB	OD-C4D-ND	-3.28	121.07	125.93
31	NK	1001	CYC	C4A-C3A-C2A	-3.28	102.74	106.51
29	TF	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	PF	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	PI	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	SJ	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	SL	201	PEB	CHC-C4C-C3C	-3.28	124.74	130.34
29	LA	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	LN	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	mB	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	mM	202	PEB	C4B-C3B-C2B	-3.28	103.15	106.78
29	DA	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	DN	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	mJ	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	mL	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	AJ	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	MJ	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	AL	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	ML	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	VF	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	VI	203	PEB	OD-C4D-ND	-3.28	121.07	125.93
29	DB	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	DM	202	PEB	C3B-C4B-NB	3.28	114.82	110.05
29	eB	202	PEB	OA-C1A-C2A	-3.28	123.57	126.17
29	eM	202	PEB	OA-C1A-C2A	-3.28	123.57	126.17
29	sJ	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	sL	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	AF	301	PEB	C1B-C2B-C3B	-3.28	102.75	106.51
29	AI	301	PEB	C1B-C2B-C3B	-3.28	102.75	106.51
29	gB	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	TJ	203	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	TL	203	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	gM	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	nJ	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	nL	202	PEB	C2A-C1A-NA	3.28	111.10	108.27
29	YJ	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	YL	201	PEB	CHC-C4C-C3C	-3.28	124.75	130.34
29	P7	203	PEB	C3B-C4B-NB	3.28	114.81	110.05
29	P9	203	PEB	C3B-C4B-NB	3.28	114.81	110.05
29	cB	201	PEB	OD-C4D-ND	-3.28	121.08	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	cM	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
30	yJ	303	PUB	CHC-C1D-ND	-3.28	109.58	113.72
29	EA	201	PEB	CHA-C1B-NB	-3.28	118.08	124.93
29	EN	201	PEB	CHA-C1B-NB	-3.28	118.08	124.93
29	i1	202	PEB	CMB-C2B-C1B	3.28	130.11	125.06
29	iK	202	PEB	CMB-C2B-C1B	3.28	130.11	125.06
29	i7	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	i9	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	FB	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	FM	201	PEB	OD-C4D-ND	-3.28	121.08	125.93
29	CA	201	PEB	CHA-C1B-NB	-3.28	118.08	124.93
29	CN	201	PEB	CHA-C1B-NB	-3.28	118.08	124.93
29	BA	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
29	BN	202	PEB	C3B-C4B-NB	3.27	114.81	110.05
29	B3	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	UB	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	BO	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	MQ	401	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	P1	202	PEB	CMB-C2B-C1B	3.27	130.11	125.06
29	PK	202	PEB	CMB-C2B-C1B	3.27	130.11	125.06
29	M4	203	PEB	C2A-C1A-NA	3.27	111.10	108.27
29	pJ	202	PEB	C2A-C1A-NA	3.27	111.10	108.27
29	pL	202	PEB	C2A-C1A-NA	3.27	111.10	108.27
29	JG	202	PEB	CMB-C2B-C1B	3.27	130.11	125.06
29	JQ	202	PEB	CMB-C2B-C1B	3.27	130.11	125.06
29	c7	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	c7	203	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	c9	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	c9	203	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	JB	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	JM	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	D3	202	PEB	OD-C4D-C3D	-3.27	122.04	129.46
31	J9	1001	CYC	C4A-C3A-C2A	-3.27	102.75	106.51
29	uJ	202	PEB	CHC-C4C-C3C	-3.27	124.75	130.34
29	uL	202	PEB	CHC-C4C-C3C	-3.27	124.75	130.34
29	F3	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
29	FO	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
29	m7	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	m9	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	b1	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
29	bK	201	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
29	YF	201	PEB	CHC-C1D-ND	-3.27	110.15	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	YI	201	PEB	CHC-C1D-ND	-3.27	110.15	113.95
29	RB	203	PEB	OA-C1A-C2A	-3.27	123.57	126.17
29	RM	203	PEB	OA-C1A-C2A	-3.27	123.57	126.17
29	bJ	203	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	bL	203	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	TF	202	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	TI	202	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	AA	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
29	AN	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
29	CA	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	CN	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	iB	203	PEB	OA-C1A-C2A	-3.27	123.57	126.17
29	iM	203	PEB	OA-C1A-C2A	-3.27	123.57	126.17
29	PB	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	VB	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	PM	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	VM	201	PEB	OD-C4D-ND	-3.27	121.08	125.93
29	gF	201	PEB	CHC-C1D-ND	-3.27	110.15	113.95
29	gI	201	PEB	CHC-C1D-ND	-3.27	110.15	113.95
29	PF	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	PI	201	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	GA	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
29	GN	201	PEB	CHA-C1B-NB	-3.27	118.09	124.93
29	aB	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
29	aM	202	PEB	C4B-C3B-C2B	-3.27	103.16	106.78
31	G7	1001	CYC	CMB-C2B-C1B	3.27	128.25	124.17
30	A1	304	PUB	OD-C4D-ND	-3.27	121.09	125.93
30	AK	304	PUB	OD-C4D-ND	-3.27	121.09	125.93
29	LA	203	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	iJ	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	iL	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	LN	203	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	wL	303	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
29	Z1	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
29	ZK	202	PEB	C1B-C2B-C3B	-3.27	102.75	106.51
29	eB	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	DJ	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	DL	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	eM	201	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	F3	201	PEB	CHB-C4B-NB	-3.27	124.29	128.83
29	FO	201	PEB	CHB-C4B-NB	-3.27	124.29	128.83
29	oJ	201	PEB	CHC-C4C-C3C	-3.27	124.76	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	oL	201	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
29	RF	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	RI	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
31	K9	1001	CYC	CMB-C2B-C1B	3.27	128.25	124.17
29	k1	202	PEB	CMB-C2B-C1B	3.27	130.10	125.06
29	kK	202	PEB	CMB-C2B-C1B	3.27	130.10	125.06
29	IJ	201	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
29	IL	201	PEB	CHC-C4C-C3C	-3.27	124.76	130.34
29	i7	203	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	i9	203	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	EJ	201	PEB	CHC-C4C-C3C	-3.27	124.77	130.34
29	EL	201	PEB	CHC-C4C-C3C	-3.27	124.77	130.34
29	FB	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
29	FM	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
29	GC	202	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
29	GE	202	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
29	E4	201	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	GD	203	PEB	CMA-C2A-C1A	-3.27	105.36	112.40
29	AB	301	PEB	OA-C1A-C2A	-3.27	123.58	126.17
29	CB	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
29	CM	202	PEB	C4B-C3B-C2B	-3.27	103.17	106.78
29	XJ	203	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	XL	203	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	kJ	201	PEB	CHC-C4C-C3C	-3.27	124.77	130.34
29	kL	201	PEB	CHC-C4C-C3C	-3.27	124.77	130.34
29	B3	201	PEB	CHA-C1B-NB	-3.27	118.10	124.93
29	BO	201	PEB	CHA-C1B-NB	-3.27	118.10	124.93
29	dD	401	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	QJ	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	QL	202	PEB	C2A-C1A-NA	3.27	111.09	108.27
29	H3	201	PEB	CHA-C1B-NB	-3.27	118.10	124.93
29	HO	201	PEB	CHA-C1B-NB	-3.27	118.10	124.93
29	HJ	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	HL	202	PEB	OD-C4D-ND	-3.27	121.09	125.93
29	j7	202	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
29	j9	202	PEB	C1B-C2B-C3B	-3.27	102.76	106.51
29	CD	203	PEB	CMA-C2A-C1A	-3.26	105.37	112.40
29	RJ	202	PEB	C2A-C1A-NA	3.26	111.09	108.27
29	qJ	202	PEB	C2A-C1A-NA	3.26	111.09	108.27
29	RL	202	PEB	C2A-C1A-NA	3.26	111.09	108.27
29	qL	202	PEB	C2A-C1A-NA	3.26	111.09	108.27
29	ED	202	PEB	CMA-C2A-C1A	-3.26	105.37	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CJ	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	eJ	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	mJ	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	CL	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	eL	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	mL	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	K4	203	PEB	CMA-C2A-C1A	-3.26	105.37	112.40
29	fI	201	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
29	fK	201	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
29	NJ	202	PEB	C2A-C1A-NA	3.26	111.09	108.27
29	NL	202	PEB	C2A-C1A-NA	3.26	111.09	108.27
29	P7	201	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	P9	201	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	nJ	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	nL	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	S2	201	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
29	S2	201	PEB	CHC-C1D-ND	-3.26	110.16	113.95
31	1P	1001	CYC	C1B-C2B-C3B	-3.26	104.47	107.87
30	AF	302	PUB	CMD-C2D-C3D	3.26	132.66	127.77
30	AI	302	PUB	CMD-C2D-C3D	3.26	132.66	127.77
29	R7	203	PEB	C3B-C4B-NB	3.26	114.79	110.05
29	R9	203	PEB	C3B-C4B-NB	3.26	114.79	110.05
29	D3	201	PEB	CHB-C4B-NB	-3.26	124.30	128.83
29	DO	201	PEB	CHB-C4B-NB	-3.26	124.30	128.83
29	gJ	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	gL	201	PEB	CHC-C4C-C3C	-3.26	124.77	130.34
29	A7	301	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
29	A9	301	PEB	C1B-C2B-C3B	-3.26	102.76	106.51
29	mB	201	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	mM	201	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	DB	203	PEB	OA-C1A-C2A	-3.26	123.58	126.17
29	DM	203	PEB	OA-C1A-C2A	-3.26	123.58	126.17
29	GJ	201	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
29	UJ	201	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
29	GL	201	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
29	UL	201	PEB	CHC-C4C-C3C	-3.26	124.78	130.34
29	KD	203	PEB	CMA-C2A-C1A	-3.26	105.37	112.40
29	CJ	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
29	CL	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
29	V7	203	PEB	C3B-C4B-NB	3.26	114.79	110.05
29	V9	203	PEB	C3B-C4B-NB	3.26	114.79	110.05
29	GC	201	PEB	C3B-C4B-NB	3.26	114.79	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GE	201	PEB	C3B-C4B-NB	3.26	114.79	110.05
29	AM	301	PEB	CAA-C3A-C4A	3.26	121.05	112.67
29	R7	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	k7	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	R9	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	k9	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	DB	201	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	RJ	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	RL	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	DM	201	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	lF	202	PEB	CBA-CAA-C3A	-3.26	106.21	113.47
29	II	202	PEB	CBA-CAA-C3A	-3.26	106.21	113.47
29	h1	201	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	YB	201	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	hK	201	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	YM	201	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	aF	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	kF	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	aI	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	kI	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	JA	202	PEB	CHC-C1D-ND	-3.26	110.16	113.95
29	iF	201	PEB	CHC-C1D-ND	-3.26	110.16	113.95
29	iI	201	PEB	CHC-C1D-ND	-3.26	110.16	113.95
29	JN	202	PEB	CHC-C1D-ND	-3.26	110.16	113.95
29	IB	202	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	OB	202	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	YB	203	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	zL	501	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	IM	202	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	OM	202	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	YM	203	PEB	C4B-C3B-C2B	-3.26	103.17	106.78
29	UF	203	PEB	CBA-CAA-C3A	-3.26	106.21	113.47
29	UI	203	PEB	CBA-CAA-C3A	-3.26	106.21	113.47
31	M9	1001	CYC	CMB-C2B-C1B	3.26	128.24	124.17
29	KA	201	PEB	CHA-C1B-NB	-3.26	118.12	124.93
29	KN	201	PEB	CHA-C1B-NB	-3.26	118.12	124.93
29	e7	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	e9	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	BJ	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
29	BL	203	PEB	OD-C4D-ND	-3.26	121.10	125.93
31	C7	1001	CYC	CMB-C2B-C1B	3.26	128.24	124.17
31	C9	1001	CYC	CMB-C2B-C1B	3.26	128.24	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L1	1001	CYC	C4A-C3A-C2A	-3.26	102.77	106.51
31	LK	1001	CYC	C4A-C3A-C2A	-3.26	102.77	106.51
29	AB	301	PEB	CAA-C3A-C4A	3.26	121.04	112.67
29	jB	202	PEB	C4B-C3B-C2B	-3.26	103.18	106.78
29	jM	202	PEB	C4B-C3B-C2B	-3.26	103.18	106.78
29	DO	202	PEB	OD-C4D-C3D	-3.26	122.08	129.46
29	I5	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
29	I8	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
31	M7	1001	CYC	CMB-C2B-C1B	3.26	128.23	124.17
29	JB	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	JM	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	Y7	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	Y9	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	ZJ	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	ZL	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	l7	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
29	l9	202	PEB	C2A-C1A-NA	3.26	111.08	108.27
29	g7	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	g9	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	FJ	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	vJ	202	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	FL	203	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	vL	202	PEB	OD-C4D-ND	-3.26	121.11	125.93
29	l7	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	l9	202	PEB	C1B-C2B-C3B	-3.26	102.77	106.51
29	TI	201	PEB	CHC-C1D-ND	-3.26	110.17	113.95
29	A5	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
29	A8	203	PEB	CMB-C2B-C1B	3.26	130.08	125.06
31	K1	1001	CYC	C2A-C1A-NA	3.26	114.78	110.05
31	KK	1001	CYC	C2A-C1A-NA	3.26	114.78	110.05
29	G4	203	PEB	CMA-C2A-C1A	-3.25	105.39	112.40
29	LJ	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	LL	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	MB	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
29	MM	202	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
29	NB	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	NM	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	K5	203	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	K8	203	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	R7	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	R9	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	RB	201	PEB	OD-C4D-ND	-3.25	121.11	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RM	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	PF	201	PEB	CHC-C1D-ND	-3.25	110.17	113.95
29	PI	201	PEB	CHC-C1D-ND	-3.25	110.17	113.95
29	J3	201	PEB	CHA-C1B-NB	-3.25	118.13	124.93
29	JO	201	PEB	CHA-C1B-NB	-3.25	118.13	124.93
29	KJ	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
29	oJ	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
29	KL	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
29	oL	202	PEB	C2A-C1A-NA	3.25	111.08	108.27
29	H3	201	PEB	CHB-C4B-NB	-3.25	124.31	128.83
29	HO	201	PEB	CHB-C4B-NB	-3.25	124.31	128.83
29	YF	203	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
29	YI	203	PEB	C4B-C3B-C2B	-3.25	103.18	106.78
29	a1	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	BG	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	aK	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	BQ	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	S1	201	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
29	SK	201	PEB	C1B-C2B-C3B	-3.25	102.77	106.51
29	D3	201	PEB	CHA-C1B-NB	-3.25	118.13	124.93
29	DO	201	PEB	CHA-C1B-NB	-3.25	118.13	124.93
29	VJ	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	VL	202	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	M4	201	PEB	C2A-C1A-NA	3.25	111.08	108.27
31	K7	1001	CYC	CMB-C2B-C1B	3.25	128.23	124.17
29	k7	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	k9	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	lB	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	lM	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	QJ	201	PEB	CHC-C4C-C3C	-3.25	124.79	130.34
29	QL	201	PEB	CHC-C4C-C3C	-3.25	124.79	130.34
29	V7	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	V9	201	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	iF	203	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	iI	203	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	fJ	203	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	fL	203	PEB	OD-C4D-ND	-3.25	121.11	125.93
29	V1	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	VK	202	PEB	CMB-C2B-C1B	3.25	130.07	125.06
29	ZF	202	PEB	CBA-CAA-C3A	-3.25	106.23	113.47
29	ZI	202	PEB	CBA-CAA-C3A	-3.25	106.23	113.47
29	CC	202	PEB	C1B-C2B-C3B	-3.25	102.78	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CE	202	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
29	FA	202	PEB	CHC-C1D-ND	-3.25	110.17	113.95
29	VF	201	PEB	CHC-C1D-ND	-3.25	110.17	113.95
29	VI	201	PEB	CHC-C1D-ND	-3.25	110.17	113.95
29	FN	202	PEB	CHC-C1D-ND	-3.25	110.17	113.95
29	PJ	203	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	PL	203	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	DB	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	dB	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	DM	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	dM	202	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	aJ	201	PEB	CHC-C4C-C3C	-3.25	124.80	130.34
29	aL	201	PEB	CHC-C4C-C3C	-3.25	124.80	130.34
29	aF	201	PEB	CHA-C1B-NB	-3.25	118.14	124.93
29	aI	201	PEB	CHA-C1B-NB	-3.25	118.14	124.93
29	uJ	203	PEB	C2A-C1A-NA	3.25	111.07	108.27
29	uL	203	PEB	C2A-C1A-NA	3.25	111.07	108.27
31	J1	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
31	JK	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
29	R1	202	PEB	CMB-C2B-C1B	3.25	130.06	125.06
29	RK	202	PEB	CMB-C2B-C1B	3.25	130.06	125.06
29	a7	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	a9	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
31	HK	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
29	N2	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
29	AC	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
29	AE	201	PEB	C3B-C4B-NB	3.25	114.77	110.05
29	W1	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
29	WK	201	PEB	C1B-C2B-C3B	-3.25	102.78	106.51
31	J7	1001	CYC	C4A-C3A-C2A	-3.25	102.78	106.51
29	AM	303	PEB	CHC-C4C-C3C	-3.25	124.80	130.34
29	kJ	202	PEB	C2A-C1A-NA	3.25	111.07	108.27
29	kL	202	PEB	C2A-C1A-NA	3.25	111.07	108.27
29	bF	202	PEB	CBA-CAA-C3A	-3.25	106.24	113.47
29	bI	202	PEB	CBA-CAA-C3A	-3.25	106.24	113.47
29	LB	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	TB	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	LM	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	TM	201	PEB	OD-C4D-ND	-3.25	121.12	125.93
29	F3	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	FO	201	PEB	C4B-C3B-C2B	-3.25	103.19	106.78
29	L8	202	PEB	C2A-C1A-NA	3.24	111.07	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I1	1001	CYC	C2A-C1A-NA	3.24	114.77	110.05
29	jF	202	PEB	CBA-CAA-C3A	-3.24	106.25	113.47
29	jI	202	PEB	CBA-CAA-C3A	-3.24	106.25	113.47
29	NB	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	RB	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	NM	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	RM	201	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	d1	201	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
29	dK	201	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
29	QR	202	PEB	C1B-C2B-C3B	-3.24	102.78	106.51
29	cF	202	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	cI	202	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	ID	203	PEB	CMA-C2A-C1A	-3.24	105.41	112.40
29	HA	203	PEB	C2A-C1A-NA	3.24	111.07	108.27
29	HN	203	PEB	C2A-C1A-NA	3.24	111.07	108.27
29	V7	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	V9	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	HB	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	VB	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	HM	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	VM	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	GB	202	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	yJ	301	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	yL	301	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	GM	202	PEB	C4B-C3B-C2B	-3.24	103.19	106.78
29	RF	201	PEB	CHA-C1B-NB	-3.24	118.15	124.93
29	RI	201	PEB	CHA-C1B-NB	-3.24	118.15	124.93
29	DA	203	PEB	C2A-C1A-NA	3.24	111.07	108.27
29	DN	203	PEB	C2A-C1A-NA	3.24	111.07	108.27
29	E4	203	PEB	CMA-C2A-C1A	-3.24	105.42	112.40
29	dJ	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	dL	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	I5	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	I8	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	C5	203	PEB	CMB-C2B-C1B	3.24	130.05	125.06
29	C8	203	PEB	CMB-C2B-C1B	3.24	130.05	125.06
29	lJ	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	lL	203	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	aF	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	cF	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	aI	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	cI	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mB	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	mM	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
31	L7	1001	CYC	C4A-C3A-C2A	-3.24	102.79	106.51
29	eB	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	eM	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	IC	202	PEB	CHA-C1B-NB	-3.24	118.16	124.93
29	IE	202	PEB	CHA-C1B-NB	-3.24	118.16	124.93
29	Q1	201	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	QK	201	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
31	H1	1001	CYC	C4A-C3A-C2A	-3.24	102.79	106.51
29	GJ	202	PEB	C2A-C1A-NA	3.24	111.06	108.27
29	GL	202	PEB	C2A-C1A-NA	3.24	111.06	108.27
29	EC	201	PEB	C3B-C4B-NB	3.24	114.76	110.05
29	EE	201	PEB	C3B-C4B-NB	3.24	114.76	110.05
29	tJ	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	tL	202	PEB	OD-C4D-ND	-3.24	121.13	125.93
29	A7	305	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	A9	305	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	TB	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	TM	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	MA	405	PEB	C3B-C4B-NB	3.24	114.76	110.05
29	L3	201	PEB	CHA-C1B-NB	-3.24	118.16	124.93
29	LO	201	PEB	CHA-C1B-NB	-3.24	118.16	124.93
29	mF	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	mI	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	yJ	301	PEB	C3B-C4B-NB	3.24	114.76	110.05
29	yL	301	PEB	C3B-C4B-NB	3.24	114.76	110.05
29	iB	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	iM	202	PEB	C1B-C2B-C3B	-3.24	102.79	106.51
29	WB	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	WM	202	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
31	IK	1001	CYC	C2A-C1A-NA	3.24	114.76	110.05
29	RF	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	RI	201	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	WF	202	PEB	CBA-CAA-C3A	-3.24	106.26	113.47
29	WI	202	PEB	CBA-CAA-C3A	-3.24	106.26	113.47
29	XB	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	XM	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	eF	201	PEB	CHA-C1B-NB	-3.24	118.16	124.93
29	eI	201	PEB	CHA-C1B-NB	-3.24	118.16	124.93
29	LA	202	PEB	CHC-C1D-ND	-3.24	110.19	113.95
29	LN	202	PEB	CHC-C1D-ND	-3.24	110.19	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y7	201	PEB	OD-C4D-ND	-3.24	121.14	125.93
29	Y9	201	PEB	OD-C4D-ND	-3.24	121.14	125.93
29	QF	202	PEB	CBA-CAA-C3A	-3.24	106.26	113.47
29	SF	202	PEB	CBA-CAA-C3A	-3.24	106.26	113.47
29	QI	202	PEB	CBA-CAA-C3A	-3.24	106.26	113.47
29	SI	202	PEB	CBA-CAA-C3A	-3.24	106.26	113.47
29	D3	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
29	DO	201	PEB	C4B-C3B-C2B	-3.24	103.20	106.78
31	H7	1001	CYC	C4A-C3A-C2A	-3.23	102.79	106.51
31	H9	1001	CYC	C4A-C3A-C2A	-3.23	102.79	106.51
29	FB	201	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
29	FM	201	PEB	C4B-C3B-C2B	-3.23	103.20	106.78
29	WJ	203	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	IJ	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	WL	203	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	IL	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	VF	201	PEB	CHA-C1B-NB	-3.23	118.17	124.93
29	VI	201	PEB	CHA-C1B-NB	-3.23	118.17	124.93
29	L3	201	PEB	CHB-C4B-NB	-3.23	124.34	128.83
29	LO	201	PEB	CHB-C4B-NB	-3.23	124.34	128.83
29	HA	202	PEB	CHC-C1D-ND	-3.23	110.19	113.95
29	HN	202	PEB	CHC-C1D-ND	-3.23	110.19	113.95
29	AB	303	PEB	CHC-C4C-C3C	-3.23	124.82	130.34
29	UR	202	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
29	I4	203	PEB	CHA-C1B-NB	-3.23	118.17	124.93
29	NJ	203	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	rJ	203	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	NL	203	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	rL	203	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	NO	201	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	QJ	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	mJ	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	QL	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	mL	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	SB	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	fB	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	xL	303	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	SM	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	fM	202	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	g7	201	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	g9	201	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	BA	202	PEB	CHC-C1D-ND	-3.23	110.19	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BN	202	PEB	CHC-C1D-ND	-3.23	110.19	113.95
29	T2	201	PEB	C3B-C4B-NB	3.23	114.75	110.05
29	CC	201	PEB	C3B-C4B-NB	3.23	114.75	110.05
29	CE	201	PEB	C3B-C4B-NB	3.23	114.75	110.05
29	B3	201	PEB	CHB-C4B-NB	-3.23	124.34	128.83
29	BO	201	PEB	CHB-C4B-NB	-3.23	124.34	128.83
29	gF	203	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	gI	203	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	H8	202	PEB	OD-C4D-ND	-3.23	121.14	125.93
29	AM	301	PEB	OA-C1A-C2A	-3.23	123.61	126.17
29	cF	201	PEB	CHA-C1B-NB	-3.23	118.18	124.93
29	cI	201	PEB	CHA-C1B-NB	-3.23	118.18	124.93
29	AJ	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	SJ	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	AL	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	SL	202	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	fF	202	PEB	CBA-CAA-C3A	-3.23	106.28	113.47
29	fI	202	PEB	CBA-CAA-C3A	-3.23	106.28	113.47
30	wJ	305	PUB	C2C-C1C-NC	3.23	114.75	110.05
29	hF	202	PEB	CBA-CAA-C3A	-3.23	106.28	113.47
29	hI	202	PEB	CBA-CAA-C3A	-3.23	106.28	113.47
29	FA	203	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	FN	203	PEB	C2A-C1A-NA	3.23	111.06	108.27
29	J3	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	JO	201	PEB	C4B-C3B-C2B	-3.23	103.21	106.78
29	j1	201	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
29	jK	201	PEB	C1B-C2B-C3B	-3.23	102.80	106.51
29	SJ	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	SL	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	AB	302	PEB	CHA-C1B-NB	-3.23	118.18	124.93
29	N3	201	PEB	OD-C4D-ND	-3.23	121.15	125.93
29	aJ	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	aL	201	PEB	C2A-C1A-NA	-3.23	105.49	108.27
29	TI	201	PEB	CHA-C1B-NB	-3.23	118.19	124.93
29	MD	203	PEB	CMA-C2A-C1A	-3.23	105.45	112.40
29	dF	203	PEB	CBA-CAA-C3A	-3.22	106.29	113.47
29	dI	203	PEB	CBA-CAA-C3A	-3.22	106.29	113.47
29	f7	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	f9	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	ID	201	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	sJ	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	sL	202	PEB	C2A-C1A-NA	3.22	111.05	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	gF	201	PEB	CHA-C1B-NB	-3.22	118.19	124.93
29	gI	201	PEB	CHA-C1B-NB	-3.22	118.19	124.93
29	OF	202	PEB	CBA-CAA-C3A	-3.22	106.29	113.47
29	OI	202	PEB	CBA-CAA-C3A	-3.22	106.29	113.47
30	QB	201	PUB	CMA-C2A-C1A	3.22	128.97	121.39
30	QM	201	PUB	CMA-C2A-C1A	3.22	128.97	121.39
31	E1	1001	CYC	C2A-C1A-NA	3.22	114.74	110.05
31	EK	1001	CYC	C2A-C1A-NA	3.22	114.74	110.05
29	kF	201	PEB	CHC-C1D-ND	-3.22	110.20	113.95
29	kI	201	PEB	CHC-C1D-ND	-3.22	110.20	113.95
29	eF	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	eI	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
31	L9	1001	CYC	C4A-C3A-C2A	-3.22	102.81	106.51
31	C1	1001	CYC	C2A-C1A-NA	3.22	114.73	110.05
29	iF	201	PEB	CHA-C1B-NB	-3.22	118.19	124.93
29	iI	201	PEB	CHA-C1B-NB	-3.22	118.19	124.93
29	jJ	203	PEB	OD-C4D-ND	-3.22	121.16	125.93
29	jL	203	PEB	OD-C4D-ND	-3.22	121.16	125.93
29	H8	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	YJ	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	YL	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	G4	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	kF	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	kI	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	DA	202	PEB	CHC-C1D-ND	-3.22	110.21	113.95
29	DN	202	PEB	CHC-C1D-ND	-3.22	110.21	113.95
29	l7	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	l9	202	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	W2	202	PEB	C1B-C2B-C3B	-3.22	102.81	106.51
29	CC	202	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	CE	202	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	UJ	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	eJ	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	UL	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	eL	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	kJ	201	PEB	C2A-C1A-NA	-3.22	105.50	108.27
29	kL	201	PEB	C2A-C1A-NA	-3.22	105.50	108.27
29	G5	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
31	M1	1001	CYC	C2A-C1A-NA	3.22	114.73	110.05
31	MK	1001	CYC	C2A-C1A-NA	3.22	114.73	110.05
29	LB	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	PB	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	iF	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	iI	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	LM	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	PM	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
31	D7	1001	CYC	C4A-C3A-C2A	-3.22	102.81	106.51
31	D9	1001	CYC	C4A-C3A-C2A	-3.22	102.81	106.51
29	IJ	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	IL	202	PEB	C2A-C1A-NA	3.22	111.05	108.27
29	GD	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	ID	201	PEB	CHA-C1B-NB	-3.22	118.20	124.93
31	D1	1003	CYC	C2A-C1A-NA	3.22	114.73	110.05
29	zJ	501	PEB	OA-C1A-C2A	-3.22	123.61	126.17
29	dD	401	PEB	CHA-C1B-NB	-3.22	118.20	124.93
29	UJ	201	PEB	C2A-C1A-NA	-3.22	105.50	108.27
29	UL	201	PEB	C2A-C1A-NA	-3.22	105.50	108.27
29	HB	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	iB	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	kF	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	kI	203	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	xJ	303	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	HM	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	iM	201	PEB	C4B-C3B-C2B	-3.22	103.22	106.78
29	TR	201	PEB	C3B-C4B-NB	3.22	114.73	110.05
29	IC	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	IE	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
31	GK	1001	CYC	C2A-C1A-NA	3.21	114.72	110.05
29	KC	203	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	KE	203	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	PF	201	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	PI	201	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	H3	201	PEB	C4B-C3B-C2B	-3.21	103.22	106.78
29	AM	301	PEB	C4B-C3B-C2B	-3.21	103.22	106.78
29	HO	201	PEB	C4B-C3B-C2B	-3.21	103.22	106.78
29	GD	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
29	AM	302	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	R2	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	hJ	203	PEB	OD-C4D-ND	-3.21	121.17	125.93
29	hL	203	PEB	OD-C4D-ND	-3.21	121.17	125.93
29	DB	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
29	DM	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
29	A1	303	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	AK	303	PEB	CHA-C1B-NB	-3.21	118.21	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	IJ	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	IL	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	ZB	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
29	ZM	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
29	PF	203	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	PI	203	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	NR	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	CD	201	PEB	C2A-C1A-NA	3.21	111.04	108.27
29	YF	201	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	YI	201	PEB	CHA-C1B-NB	-3.21	118.21	124.93
29	A7	301	PEB	OD-C4D-ND	-3.21	121.17	125.93
29	A9	301	PEB	OD-C4D-ND	-3.21	121.17	125.93
29	e2	402	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	RR	201	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	h7	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
29	h9	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
29	A5	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	A8	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	Z7	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
29	Z9	202	PEB	C2A-C1A-NA	3.21	111.04	108.27
29	AC	202	PEB	CHA-C1B-NB	-3.21	118.22	124.93
29	AE	202	PEB	CHA-C1B-NB	-3.21	118.22	124.93
29	Q2	202	PEB	C1B-C2B-C3B	-3.21	102.82	106.51
29	cJ	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	cL	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	KA	202	PEB	CMB-C2B-C1B	3.21	130.00	125.06
29	KN	202	PEB	CMB-C2B-C1B	3.21	130.00	125.06
29	kJ	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	kL	202	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	MN	405	PEB	C3B-C4B-NB	3.21	114.72	110.05
29	KJ	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	KL	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	mF	201	PEB	CHA-C1B-NB	-3.21	118.22	124.93
29	mI	201	PEB	CHA-C1B-NB	-3.21	118.22	124.93
29	TB	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	TM	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	uJ	203	PEB	C3B-C4B-NB	3.21	114.71	110.05
29	uL	203	PEB	C3B-C4B-NB	3.21	114.71	110.05
29	U1	202	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
29	UK	202	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
31	N7	1001	CYC	C4A-C3A-C2A	-3.21	102.83	106.51
31	N9	1001	CYC	C4A-C3A-C2A	-3.21	102.83	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K5	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	K8	202	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	AJ	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	AL	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	O7	201	PEB	C2B-C1B-NB	3.21	117.37	110.53
29	O9	201	PEB	C2B-C1B-NB	3.21	117.37	110.53
29	gB	202	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
29	gM	202	PEB	C1B-C2B-C3B	-3.21	102.83	106.51
29	AF	301	PEB	OD-C4D-C3D	-3.21	122.20	129.46
29	AI	301	PEB	OD-C4D-C3D	-3.21	122.20	129.46
29	ZB	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	ZM	201	PEB	C4B-C3B-C2B	-3.21	103.23	106.78
29	YJ	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	iJ	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	YL	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	iL	201	PEB	C2A-C1A-NA	-3.21	105.51	108.27
29	AG	201	PEB	CHB-C4B-NB	-3.20	124.38	128.83
29	AQ	201	PEB	CHB-C4B-NB	-3.20	124.38	128.83
29	cB	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
29	cM	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
29	BA	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
29	BN	203	PEB	C2A-C1A-NA	3.20	111.03	108.27
29	KC	202	PEB	C3B-C4B-NB	3.20	114.71	110.05
29	KE	202	PEB	C3B-C4B-NB	3.20	114.71	110.05
30	xL	305	PUB	C2C-C1C-NC	3.20	114.71	110.05
29	uJ	202	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	uL	202	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	J5	202	PEB	CHC-C1D-ND	-3.20	110.23	113.95
29	J8	202	PEB	CHC-C1D-ND	-3.20	110.23	113.95
29	j7	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	C8	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	j9	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
31	UP	1001	CYC	C1B-C2B-C3B	-3.20	104.53	107.87
29	kB	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
29	kM	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
29	gB	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	kB	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	RF	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	RI	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	gM	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	kM	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
31	MP	1001	CYC	C1B-C2B-C3B	-3.20	104.53	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GJ	201	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	qJ	201	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	GL	201	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	qL	201	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	J9	1002	PEB	CHB-C4B-NB	-3.20	124.39	128.83
29	L8	202	PEB	OD-C4D-ND	-3.20	121.19	125.93
29	L1	1002	PEB	CHC-C4C-C3C	-3.20	124.88	130.34
29	LK	1002	PEB	CHC-C4C-C3C	-3.20	124.88	130.34
29	C4	201	PEB	CHA-C1B-NB	-3.20	118.24	124.93
29	I4	201	PEB	C2A-C1A-NA	3.20	111.03	108.27
29	d7	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
29	d9	202	PEB	C2A-C1A-NA	3.20	111.03	108.27
29	oJ	201	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	oL	201	PEB	C2A-C1A-NA	-3.20	105.51	108.27
29	CA	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
29	CN	202	PEB	CMB-C2B-C1B	3.20	129.99	125.06
29	K8	202	PEB	CHC-C4C-C3C	-3.20	124.88	130.34
29	L3	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	LO	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	U2	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
29	SR	202	PEB	C1B-C2B-C3B	-3.20	102.83	106.51
31	CK	1001	CYC	C2A-C1A-NA	3.20	114.70	110.05
29	W7	201	PEB	C2B-C1B-NB	3.20	117.36	110.53
29	W9	201	PEB	C2B-C1B-NB	3.20	117.36	110.53
29	cB	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	mF	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	mI	203	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	cM	201	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
31	iP	1001	CYC	C4A-C3A-C2A	-3.20	102.83	106.51
31	FP	1001	CYC	C1B-C2B-C3B	-3.20	104.53	107.87
31	oP	1001	CYC	C1B-C2B-C3B	-3.20	104.53	107.87
29	M3	201	PEB	OD-C4D-ND	-3.20	121.19	125.93
29	MO	201	PEB	OD-C4D-ND	-3.20	121.19	125.93
29	d7	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	d9	202	PEB	C4B-C3B-C2B	-3.20	103.24	106.78
29	RB	202	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
29	RM	202	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
31	RP	1001	CYC	C4A-C3A-C2A	-3.20	102.84	106.51
29	GC	202	PEB	CHA-C1B-NB	-3.20	118.24	124.93
29	GE	202	PEB	CHA-C1B-NB	-3.20	118.24	124.93
29	oJ	202	PEB	C3B-C4B-NB	3.20	114.70	110.05
29	oL	202	PEB	C3B-C4B-NB	3.20	114.70	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sP	1001	CYC	C1A-C2A-C3A	-3.20	103.24	106.78
29	CJ	201	PEB	C2A-C1A-NA	-3.20	105.52	108.27
29	CL	201	PEB	C2A-C1A-NA	-3.20	105.52	108.27
29	OR	202	PEB	C1B-C2B-C3B	-3.20	102.84	106.51
31	DP	1001	CYC	C1B-C2B-C3B	-3.20	104.54	107.87
29	E4	201	PEB	CHA-C1B-NB	-3.20	118.25	124.93
29	U7	201	PEB	C2B-C1B-NB	3.20	117.35	110.53
29	U9	201	PEB	C2B-C1B-NB	3.20	117.35	110.53
29	V2	201	PEB	C3B-C4B-NB	3.20	114.70	110.05
29	MJ	201	PEB	C2A-C1A-NA	-3.19	105.52	108.27
29	ML	201	PEB	C2A-C1A-NA	-3.19	105.52	108.27
29	VB	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	VM	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	LB	202	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
29	LM	202	PEB	C1B-C2B-C3B	-3.19	102.84	106.51
29	H5	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
29	C5	202	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
29	C8	202	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
31	QP	1001	CYC	C1B-C2B-C3B	-3.19	104.54	107.87
31	hP	1001	CYC	C1B-C2B-C3B	-3.19	104.54	107.87
29	xL	301	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	L5	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
29	OR	202	PEB	OD-C4D-C3D	-3.19	122.22	129.46
29	U7	202	PEB	C2A-C1A-NA	3.19	111.03	108.27
29	U9	202	PEB	C2A-C1A-NA	3.19	111.03	108.27
29	cJ	202	PEB	C2A-C1A-NA	3.19	111.03	108.27
29	cL	202	PEB	C2A-C1A-NA	3.19	111.03	108.27
29	K5	202	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
29	G8	201	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
30	wL	305	PUB	C2C-C1C-NC	3.19	114.69	110.05
29	sJ	201	PEB	C2A-C1A-NA	-3.19	105.52	108.27
29	sL	201	PEB	C2A-C1A-NA	-3.19	105.52	108.27
31	jP	1001	CYC	C1B-C2B-C3B	-3.19	104.54	107.87
29	A7	304	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	yJ	301	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
29	yL	301	PEB	CHC-C4C-C3C	-3.19	124.89	130.34
30	AM	304	PUB	C2C-C1C-NC	3.19	114.69	110.05
29	I4	201	PEB	CHA-C1B-NB	-3.19	118.26	124.93
29	TF	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	TI	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	B5	202	PEB	OD-C4D-ND	-3.19	121.20	125.93
29	NO	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EJ	201	PEB	C2A-C1A-NA	-3.19	105.52	108.27
29	EL	201	PEB	C2A-C1A-NA	-3.19	105.52	108.27
29	VR	201	PEB	C3B-C4B-NB	3.19	114.69	110.05
29	ED	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	S7	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	S9	202	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	AB	301	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
29	wL	301	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
31	1P	1001	CYC	C1B-NB-C4B	-3.19	106.61	110.67
29	Q7	201	PEB	C2B-C1B-NB	3.19	117.33	110.53
29	Q9	201	PEB	C2B-C1B-NB	3.19	117.33	110.53
29	AJ	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
29	CJ	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
29	AL	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
29	CL	202	PEB	C3B-C4B-NB	3.19	114.69	110.05
30	AB	304	PUB	C2C-C1C-NC	3.19	114.69	110.05
29	G4	201	PEB	C2A-C1A-NA	3.19	111.02	108.27
29	J3	203	PEB	CHA-C1B-NB	-3.19	118.27	124.93
29	JO	203	PEB	CHA-C1B-NB	-3.19	118.27	124.93
29	MQ	406	PEB	C4B-C3B-C2B	-3.19	103.25	106.78
31	kP	1001	CYC	C1B-NB-C4B	-3.19	106.61	110.67
29	AA	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	IA	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	AN	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	IN	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06
30	xJ	305	PUB	C2C-C1C-NC	3.19	114.69	110.05
29	F5	202	PEB	OD-C4D-ND	-3.19	121.21	125.93
31	K7	1001	CYC	C2C-C1C-NC	3.19	111.02	108.27
29	MG	404	PEB	C4B-C3B-C2B	-3.19	103.26	106.78
29	YJ	202	PEB	C3B-C4B-NB	3.19	114.68	110.05
29	YL	202	PEB	C3B-C4B-NB	3.19	114.68	110.05
29	EC	202	PEB	CHA-C1B-NB	-3.19	118.27	124.93
29	EE	202	PEB	CHA-C1B-NB	-3.19	118.27	124.93
29	EA	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	EN	202	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	QB	202	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
29	QM	202	PEB	C1B-C2B-C3B	-3.19	102.85	106.51
31	F9	1001	CYC	C4A-C3A-C2A	-3.19	102.85	106.51
29	Q7	202	PEB	C4B-C3B-C2B	-3.19	103.26	106.78
29	Q9	202	PEB	C4B-C3B-C2B	-3.19	103.26	106.78
29	h1	202	PEB	C2A-C1A-NA	3.19	111.02	108.27
29	hK	202	PEB	C2A-C1A-NA	3.19	111.02	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	xL	302	PEB	CAA-C3A-C4A	3.19	120.85	112.67
29	AF	305	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	AI	305	PEB	CMB-C2B-C1B	3.19	129.97	125.06
29	h7	201	PEB	C2B-C1B-NB	3.18	117.33	110.53
29	h9	201	PEB	C2B-C1B-NB	3.18	117.33	110.53
29	GA	202	PEB	CMB-C2B-C1B	3.18	129.97	125.06
29	GN	202	PEB	CMB-C2B-C1B	3.18	129.97	125.06
29	JA	203	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	JN	203	PEB	C2A-C1A-NA	3.18	111.02	108.27
31	pP	1001	CYC	C1B-NB-C4B	-3.18	106.61	110.67
31	wP	1001	CYC	C1B-C2B-C3B	-3.18	104.55	107.87
29	LC	202	PEB	OD-C4D-C3D	-3.18	122.25	129.46
29	LE	202	PEB	OD-C4D-C3D	-3.18	122.25	129.46
31	pP	1001	CYC	C4A-C3A-C2A	-3.18	102.85	106.51
31	lP	1002	CYC	C4A-C3A-C2A	-3.18	102.85	106.51
29	WJ	202	PEB	C2A-C1A-NA	-3.18	105.53	108.27
29	WL	202	PEB	C2A-C1A-NA	-3.18	105.53	108.27
31	M7	1001	CYC	C2C-C1C-NC	3.18	111.02	108.27
30	yL	303	PUB	CHA-C4A-NA	-3.18	110.25	113.95
29	B8	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
30	MA	402	PUB	CAC-CBC-CGC	-3.18	106.75	113.60
29	j7	201	PEB	C2B-C1B-NB	3.18	117.32	110.53
29	j9	201	PEB	C2B-C1B-NB	3.18	117.32	110.53
31	PP	1001	CYC	C4A-C3A-C2A	-3.18	102.85	106.51
29	iJ	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	mJ	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	iL	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	mL	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	AM	301	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	l1	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	S7	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	S9	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	lK	202	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	C5	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
29	D1	1002	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
31	QP	1001	CYC	C1B-NB-C4B	-3.18	106.62	110.67
29	AF	305	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	AI	305	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	cJ	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	cL	202	PEB	C3B-C4B-NB	3.18	114.68	110.05
29	TF	201	PEB	OD-C4D-C3D	-3.18	122.25	129.46
29	Z7	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Z9	202	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
29	xJ	301	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
29	U1	203	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	UK	203	PEB	C2A-C1A-NA	3.18	111.02	108.27
29	aB	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
29	aM	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
29	I5	202	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
29	I8	202	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
29	wJ	301	PEB	C4B-C3B-C2B	-3.18	103.26	106.78
29	KD	201	PEB	CHA-C1B-NB	-3.18	118.28	124.93
29	GD	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
29	KD	203	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
29	O7	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
29	O9	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
29	CD	201	PEB	CHA-C1B-NB	-3.18	118.28	124.93
29	J1	1002	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
29	JK	1002	PEB	CHC-C4C-C3C	-3.18	124.91	130.34
31	CP	1001	CYC	C1B-NB-C4B	-3.18	106.62	110.67
29	D3	203	PEB	CHA-C1B-NB	-3.18	118.28	124.93
29	DO	203	PEB	CHA-C1B-NB	-3.18	118.28	124.93
29	G8	202	PEB	OD-C4D-ND	-3.18	121.22	125.93
31	qP	1001	CYC	C1B-C2B-C3B	-3.18	104.55	107.87
29	f7	201	PEB	C2B-C1B-NB	3.18	117.31	110.53
29	f9	201	PEB	C2B-C1B-NB	3.18	117.31	110.53
29	EA	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
29	EN	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
29	EG	202	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
29	IG	202	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
29	EQ	202	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
29	IQ	202	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
29	M2	202	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
30	yJ	302	PUB	CHA-C1B-C2B	-3.18	124.92	130.34
30	yL	302	PUB	CHA-C1B-C2B	-3.18	124.92	130.34
29	S2	201	PEB	C1C-CHB-C4B	-3.18	125.01	128.81
29	K4	201	PEB	CHA-C1B-NB	-3.18	118.29	124.93
29	OJ	202	PEB	C3B-C4B-NB	3.18	114.67	110.05
29	OL	202	PEB	C3B-C4B-NB	3.18	114.67	110.05
31	I7	1001	CYC	C1A-C2A-C3A	-3.18	103.27	106.78
31	I9	1001	CYC	C1A-C2A-C3A	-3.18	103.27	106.78
29	S2	202	PEB	C1B-C2B-C3B	-3.18	102.86	106.51
31	HP	1001	CYC	C1B-C2B-C3B	-3.18	104.56	107.87
29	xJ	302	PEB	CAA-C3A-C4A	3.18	120.83	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A5	202	PEB	CHC-C4C-C3C	-3.18	124.92	130.34
29	A8	202	PEB	CHC-C4C-C3C	-3.18	124.92	130.34
29	DK	1002	PEB	CHC-C4C-C3C	-3.18	124.92	130.34
30	QB	201	PUB	C1C-C2C-C3C	-3.18	103.27	106.78
30	QM	201	PUB	C1C-C2C-C3C	-3.18	103.27	106.78
31	cP	1001	CYC	C4A-C3A-C2A	-3.18	102.86	106.51
29	W7	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
29	W9	202	PEB	C2A-C1A-NA	3.18	111.01	108.27
30	AF	302	PUB	OD-C4D-ND	-3.18	121.22	125.93
30	AI	302	PUB	OD-C4D-ND	-3.18	121.22	125.93
29	Y7	201	PEB	CHB-C4B-C3B	-3.18	117.98	125.32
29	Y9	201	PEB	CHB-C4B-C3B	-3.18	117.98	125.32
29	m7	203	PEB	OA-C1A-C2A	-3.18	123.65	126.17
29	m9	203	PEB	OA-C1A-C2A	-3.18	123.65	126.17
29	l7	201	PEB	C2B-C1B-NB	3.18	117.31	110.53
29	l9	201	PEB	C2B-C1B-NB	3.18	117.31	110.53
29	JB	201	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
29	JM	201	PEB	C4B-C3B-C2B	-3.18	103.27	106.78
29	AC	203	PEB	OD-C4D-C3D	-3.18	122.27	129.46
29	AE	203	PEB	OD-C4D-C3D	-3.18	122.27	129.46
31	M9	1001	CYC	C4A-C3A-C2A	-3.18	102.86	106.51
29	Z7	201	PEB	C2B-C1B-NB	3.18	117.31	110.53
29	Z9	201	PEB	C2B-C1B-NB	3.18	117.31	110.53
29	N1	1002	PEB	CHC-C4C-C3C	-3.17	124.92	130.34
29	XR	201	PEB	C3B-C4B-NB	3.17	114.67	110.05
31	AP	1001	CYC	C1B-NB-C4B	-3.17	106.63	110.67
31	OP	1001	CYC	C1B-C2B-C3B	-3.17	104.56	107.87
29	B3	203	PEB	CHA-C1B-NB	-3.17	118.29	124.93
29	BO	203	PEB	CHA-C1B-NB	-3.17	118.29	124.93
29	S7	201	PEB	C2B-C1B-NB	3.17	117.30	110.53
29	d7	201	PEB	C2B-C1B-NB	3.17	117.30	110.53
29	S9	201	PEB	C2B-C1B-NB	3.17	117.30	110.53
29	d9	201	PEB	C2B-C1B-NB	3.17	117.30	110.53
29	O7	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	O9	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	wJ	302	PEB	CAA-C3A-C4A	3.17	120.82	112.67
29	sJ	202	PEB	C3B-C4B-NB	3.17	114.67	110.05
29	sL	202	PEB	C3B-C4B-NB	3.17	114.67	110.05
29	P7	201	PEB	CHB-C4B-C3B	-3.17	117.99	125.32
29	P9	201	PEB	CHB-C4B-C3B	-3.17	117.99	125.32
29	VF	203	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	VI	203	PEB	C4B-C3B-C2B	-3.17	103.27	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	wL	302	PEB	CAA-C3A-C4A	3.17	120.82	112.67
31	NP	1001	CYC	C4A-C3A-C2A	-3.17	102.86	106.51
31	gP	1001	CYC	C4A-C3A-C2A	-3.17	102.86	106.51
31	vP	1001	CYC	C1B-NB-C4B	-3.17	106.63	110.67
29	MR	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
31	fP	1001	CYC	C1B-C2B-C3B	-3.17	104.56	107.87
31	EP	1001	CYC	C4A-C3A-C2A	-3.17	102.87	106.51
29	J7	1002	PEB	CHB-C4B-NB	-3.17	124.43	128.83
29	gJ	201	PEB	C2A-C1A-NA	-3.17	105.54	108.27
29	gL	201	PEB	C2A-C1A-NA	-3.17	105.54	108.27
29	M4	201	PEB	CHA-C1B-NB	-3.17	118.30	124.93
29	gJ	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
29	gL	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
29	f7	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	f9	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	E4	203	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
31	XP	1001	CYC	C1B-C2B-C3B	-3.17	104.56	107.87
29	b7	201	PEB	C2B-C1B-NB	3.17	117.30	110.53
29	b9	201	PEB	C2B-C1B-NB	3.17	117.30	110.53
29	L3	202	PEB	CHA-C1B-NB	-3.17	118.30	124.93
29	LO	202	PEB	CHA-C1B-NB	-3.17	118.30	124.93
29	V7	201	PEB	CHB-C4B-C3B	-3.17	118.00	125.32
29	V9	201	PEB	CHB-C4B-C3B	-3.17	118.00	125.32
29	C4	201	PEB	C2A-C1A-NA	3.17	111.01	108.27
29	U7	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	U9	202	PEB	C4B-C3B-C2B	-3.17	103.27	106.78
29	KB	203	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
29	KM	203	PEB	C1B-C2B-C3B	-3.17	102.87	106.51
31	CP	1001	CYC	C4A-C3A-C2A	-3.17	102.87	106.51
31	PP	1001	CYC	C1B-NB-C4B	-3.17	106.63	110.67
29	W7	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
29	W9	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
31	kP	1001	CYC	C1A-C2A-C3A	-3.17	103.28	106.78
31	KP	1001	CYC	C4A-C3A-C2A	-3.17	102.87	106.51
29	KJ	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
29	KL	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
31	EP	1001	CYC	C1B-NB-C4B	-3.17	106.63	110.67
31	iP	1001	CYC	C1B-NB-C4B	-3.17	106.63	110.67
29	AF	301	PEB	CHA-C1B-NB	-3.17	118.31	124.93
29	AI	301	PEB	CHA-C1B-NB	-3.17	118.31	124.93
29	BC	202	PEB	OD-C4D-C3D	-3.17	122.28	129.46
29	BE	202	PEB	OD-C4D-C3D	-3.17	122.28	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aF	203	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
29	aI	203	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
31	lP	1001	CYC	C1B-NB-C4B	-3.17	106.64	110.67
29	Y7	203	PEB	OA-C1A-C2A	-3.17	123.65	126.17
29	Y9	203	PEB	OA-C1A-C2A	-3.17	123.65	126.17
31	E7	1001	CYC	C2C-C1C-NC	3.17	111.00	108.27
31	E9	1001	CYC	C2C-C1C-NC	3.17	111.00	108.27
31	G9	1001	CYC	C2C-C1C-NC	3.17	111.00	108.27
29	CD	203	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
29	F1	1002	PEB	CHC-C4C-C3C	-3.17	124.94	130.34
29	FK	1002	PEB	CHC-C4C-C3C	-3.17	124.94	130.34
29	GJ	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
29	GL	202	PEB	C3B-C4B-NB	3.17	114.66	110.05
29	AF	301	PEB	CHC-C4C-C3C	-3.17	124.94	130.34
29	AI	301	PEB	CHC-C4C-C3C	-3.17	124.94	130.34
31	mP	1001	CYC	C1B-NB-C4B	-3.17	106.64	110.67
29	G5	202	PEB	OD-C4D-ND	-3.17	121.24	125.93
29	U1	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
29	F8	201	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
29	UK	202	PEB	C4B-C3B-C2B	-3.17	103.28	106.78
29	a7	201	PEB	CHB-C4B-C3B	-3.17	118.01	125.32
29	a9	201	PEB	CHB-C4B-C3B	-3.17	118.01	125.32
29	NK	1002	PEB	CHC-C4C-C3C	-3.17	124.94	130.34
29	c7	201	PEB	CHB-C4B-C3B	-3.17	118.01	125.32
29	c9	201	PEB	CHB-C4B-C3B	-3.17	118.01	125.32
29	EJ	202	PEB	C3B-C4B-NB	3.17	114.65	110.05
29	EL	202	PEB	C3B-C4B-NB	3.17	114.65	110.05
31	G9	1001	CYC	C4A-C3A-C2A	-3.16	102.87	106.51
29	MD	203	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
29	d1	202	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	V7	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	V9	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	dK	202	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	G4	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
29	aJ	202	PEB	C3B-C4B-NB	3.16	114.65	110.05
29	aL	202	PEB	C3B-C4B-NB	3.16	114.65	110.05
31	nP	1001	CYC	C1B-NB-C4B	-3.16	106.64	110.67
29	P7	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	P9	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	MD	201	PEB	CHA-C1B-NB	-3.16	118.32	124.93
31	M7	1001	CYC	C4A-C3A-C2A	-3.16	102.88	106.51
29	HK	1002	PEB	CHC-C4C-C3C	-3.16	124.94	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D3	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
29	DO	201	PEB	OD-C4D-ND	-3.16	121.25	125.93
31	C7	1001	CYC	C2C-C1C-NC	3.16	111.00	108.27
31	C9	1001	CYC	C2C-C1C-NC	3.16	111.00	108.27
29	wL	302	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
29	K4	203	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
29	F8	202	PEB	OD-C4D-ND	-3.16	121.25	125.93
31	K7	1001	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
31	G7	1001	CYC	C2C-C1C-NC	3.16	111.00	108.27
29	IJ	201	PEB	C2A-C1A-NA	-3.16	105.55	108.27
29	IL	201	PEB	C2A-C1A-NA	-3.16	105.55	108.27
29	C4	203	PEB	C4B-C3B-C2B	-3.16	103.28	106.78
31	HP	1001	CYC	C1A-C2A-C3A	-3.16	103.28	106.78
29	H3	203	PEB	CHA-C1B-NB	-3.16	118.32	124.93
29	HO	203	PEB	CHA-C1B-NB	-3.16	118.32	124.93
29	K4	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	KD	201	PEB	C2A-C1A-NA	3.16	111.00	108.27
29	IG	201	PEB	CHB-C4B-NB	-3.16	124.44	128.83
29	IQ	201	PEB	CHB-C4B-NB	-3.16	124.44	128.83
29	m7	201	PEB	CHB-C4B-C3B	-3.16	118.02	125.32
29	m9	201	PEB	CHB-C4B-C3B	-3.16	118.02	125.32
29	EG	201	PEB	CHB-C4B-NB	-3.16	124.44	128.83
29	EQ	201	PEB	CHB-C4B-NB	-3.16	124.44	128.83
31	SP	1001	CYC	C1B-C2B-C3B	-3.16	104.58	107.87
29	N3	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
29	A9	304	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
29	SR	201	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
31	TP	1001	CYC	C4A-C3A-C2A	-3.16	102.88	106.51
29	k7	201	PEB	CHB-C4B-C3B	-3.16	118.03	125.32
29	k9	201	PEB	CHB-C4B-C3B	-3.16	118.03	125.32
31	IP	1001	CYC	C1B-C2B-C3B	-3.16	104.58	107.87
31	E7	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
31	E9	1001	CYC	C1A-C2A-C3A	-3.16	103.29	106.78
29	QJ	202	PEB	C3B-C4B-NB	3.16	114.64	110.05
29	QL	202	PEB	C3B-C4B-NB	3.16	114.64	110.05
31	TP	1001	CYC	C1B-NB-C4B	-3.16	106.65	110.67
29	AF	305	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
29	AI	305	PEB	C1B-C2B-C3B	-3.16	102.88	106.51
31	G7	1001	CYC	C4A-C3A-C2A	-3.16	102.88	106.51
31	rP	1001	CYC	C4A-C3A-C2A	-3.16	102.88	106.51
29	b7	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78
29	b9	202	PEB	C4B-C3B-C2B	-3.16	103.29	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T7	201	PEB	CHB-C4B-C3B	-3.16	118.03	125.32
29	T9	201	PEB	CHB-C4B-C3B	-3.16	118.03	125.32
29	F3	203	PEB	CHA-C1B-NB	-3.16	118.33	124.93
29	FO	203	PEB	CHA-C1B-NB	-3.16	118.33	124.93
29	WJ	203	PEB	C3B-C4B-NB	3.16	114.64	110.05
29	WL	203	PEB	C3B-C4B-NB	3.16	114.64	110.05
31	tP	1001	CYC	C4A-C3A-C2A	-3.16	102.89	106.51
31	F7	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
31	YP	1000	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
29	R7	201	PEB	CHB-C4B-C3B	-3.15	118.03	125.32
29	R9	201	PEB	CHB-C4B-C3B	-3.15	118.03	125.32
29	zL	501	PEB	OA-C1A-C2A	-3.15	123.67	126.17
31	SP	1001	CYC	C1B-NB-C4B	-3.15	106.65	110.67
29	eJ	202	PEB	C3B-C4B-NB	3.15	114.64	110.05
29	eL	202	PEB	C3B-C4B-NB	3.15	114.64	110.05
31	MP	1001	CYC	C1A-C2A-C3A	-3.15	103.29	106.78
29	GG	201	PEB	CHB-C4B-NB	-3.15	124.45	128.83
29	GQ	201	PEB	CHB-C4B-NB	-3.15	124.45	128.83
31	sP	1001	CYC	C1B-C2B-C3B	-3.15	104.58	107.87
31	C7	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
31	C9	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
31	eP	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
29	KC	201	PEB	OD-C4D-C3D	-3.15	122.31	129.46
29	KE	201	PEB	OD-C4D-C3D	-3.15	122.31	129.46
29	e7	201	PEB	CHB-C4B-C3B	-3.15	118.04	125.32
29	e9	201	PEB	CHB-C4B-C3B	-3.15	118.04	125.32
29	wJ	302	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
31	G7	1001	CYC	C1A-C2A-C3A	-3.15	103.29	106.78
30	yJ	303	PUB	CHA-C4A-NA	-3.15	110.29	113.95
29	C4	201	PEB	CAB-C3B-C4B	3.15	130.59	125.01
29	UF	203	PEB	OD-C4D-ND	-3.15	121.26	125.93
29	UI	203	PEB	OD-C4D-ND	-3.15	121.26	125.93
29	AG	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
29	KG	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
29	AQ	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
29	KQ	202	PEB	C4B-C3B-C2B	-3.15	103.29	106.78
31	C7	1001	CYC	C1A-C2A-C3A	-3.15	103.29	106.78
31	C9	1001	CYC	C1A-C2A-C3A	-3.15	103.29	106.78
29	I4	201	PEB	CAB-C3B-C4B	3.15	130.59	125.01
31	E7	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
31	E9	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
31	gP	1001	CYC	C1B-NB-C4B	-3.15	106.66	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g7	201	PEB	C2A-C1A-NA	3.15	110.99	108.27
29	g9	201	PEB	C2A-C1A-NA	3.15	110.99	108.27
31	M9	1001	CYC	C2C-C1C-NC	3.15	110.99	108.27
29	KG	201	PEB	CHB-C4B-NB	-3.15	124.45	128.83
29	KQ	201	PEB	CHB-C4B-NB	-3.15	124.45	128.83
29	UJ	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	UL	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	B8	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
29	L7	1002	PEB	CHB-C4B-NB	-3.15	124.46	128.83
29	qJ	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	qL	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	O1	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
29	OK	202	PEB	C2A-C1A-NA	3.15	110.99	108.27
29	eJ	201	PEB	C2A-C1A-NA	-3.15	105.56	108.27
29	eL	201	PEB	C2A-C1A-NA	-3.15	105.56	108.27
30	MN	402	PUB	CAC-CBC-CGC	-3.15	106.82	113.60
31	K7	1001	CYC	C4A-C3A-C2A	-3.15	102.89	106.51
29	AB	301	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	SJ	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	SL	202	PEB	C3B-C4B-NB	3.15	114.63	110.05
29	xL	302	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
29	J3	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
29	JO	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
31	M9	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
29	WR	202	PEB	C1B-C2B-C3B	-3.15	102.89	106.51
31	nP	1001	CYC	C1B-C2B-C3B	-3.15	104.59	107.87
31	uP	1001	CYC	C1B-C2B-C3B	-3.15	104.59	107.87
31	fP	1001	CYC	C1B-NB-C4B	-3.15	106.66	110.67
29	HC	202	PEB	OD-C4D-C3D	-3.15	122.33	129.46
29	HE	202	PEB	OD-C4D-C3D	-3.15	122.33	129.46
29	h7	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
29	h9	202	PEB	C4B-C3B-C2B	-3.15	103.30	106.78
31	jP	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
31	KI	1001	CYC	C2A-C1A-NA	3.15	114.63	110.05
29	k7	201	PEB	C2A-C1A-NA	3.15	110.99	108.27
29	k9	201	PEB	C2A-C1A-NA	3.15	110.99	108.27
31	K9	1001	CYC	C2C-C1C-NC	3.15	110.99	108.27
29	J3	201	PEB	OD-C4D-ND	-3.15	121.27	125.93
29	JO	201	PEB	OD-C4D-ND	-3.15	121.27	125.93
29	T7	203	PEB	OA-C1A-C2A	-3.15	123.67	126.17
29	T9	203	PEB	OA-C1A-C2A	-3.15	123.67	126.17
29	F5	201	PEB	C4B-C3B-C2B	-3.15	103.30	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZF	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
29	fF	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
29	ZI	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
29	fI	202	PEB	OD-C4D-ND	-3.15	121.27	125.93
31	kP	1001	CYC	C1B-C2B-C3B	-3.15	104.59	107.87
29	Z1	203	PEB	C2A-C1A-NA	3.15	110.98	108.27
29	T7	201	PEB	C2A-C1A-NA	3.15	110.98	108.27
29	T9	201	PEB	C2A-C1A-NA	3.15	110.98	108.27
29	ZK	203	PEB	C2A-C1A-NA	3.15	110.98	108.27
31	DK	1001	CYC	C2C-C1C-NC	3.15	110.98	108.27
31	UP	1001	CYC	C1A-C2A-C3A	-3.15	103.30	106.78
29	MA	401	PEB	OA-C1A-C2A	-3.15	123.67	126.17
31	JP	1001	CYC	C1B-NB-C4B	-3.15	106.66	110.67
31	BP	1001	CYC	C1B-C2B-C3B	-3.15	104.59	107.87
31	M7	1001	CYC	C1A-C2A-C3A	-3.14	103.30	106.78
31	QP	1001	CYC	C1A-C2A-C3A	-3.14	103.30	106.78
31	vP	1001	CYC	C4A-C3A-C2A	-3.14	102.90	106.51
29	i7	201	PEB	CHB-C4B-C3B	-3.14	118.06	125.32
29	i9	201	PEB	CHB-C4B-C3B	-3.14	118.06	125.32
29	OJ	201	PEB	C2A-C1A-NA	-3.14	105.56	108.27
29	OL	201	PEB	C2A-C1A-NA	-3.14	105.56	108.27
31	JP	1001	CYC	C4A-C3A-C2A	-3.14	102.90	106.51
31	tP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
29	i7	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	j7	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	i9	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	j9	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	BC	203	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	LC	203	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	BE	203	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	LE	203	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	QF	202	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	QI	202	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	g7	201	PEB	CHB-C4B-C3B	-3.14	118.06	125.32
29	g9	201	PEB	CHB-C4B-C3B	-3.14	118.06	125.32
29	xJ	302	PEB	C4B-C3B-C2B	-3.14	103.30	106.78
31	XP	1001	CYC	C1A-C2A-C3A	-3.14	103.30	106.78
31	HP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
31	oP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
29	CG	201	PEB	CHB-C4B-NB	-3.14	124.47	128.83
29	CQ	201	PEB	CHB-C4B-NB	-3.14	124.47	128.83
29	O2	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ED	202	PEB	C3B-C4B-NB	3.14	114.62	110.05
31	DP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
31	K9	1001	CYC	C4A-C3A-C2A	-3.14	102.90	106.51
29	W1	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	WK	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	FC	202	PEB	OD-C4D-C3D	-3.14	122.34	129.46
29	FE	202	PEB	OD-C4D-C3D	-3.14	122.34	129.46
31	nP	1001	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
29	KB	201	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	KM	201	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	j1	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	Q7	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	Q9	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	jK	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
31	jP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
29	C5	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
29	C8	202	PEB	C1B-C2B-C3B	-3.14	102.90	106.51
31	rP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
31	G7	1001	CYC	CHB-C1B-NB	-3.14	119.32	126.06
31	G9	1001	CYC	CHB-C1B-NB	-3.14	119.32	126.06
29	B5	203	PEB	OD-C4D-ND	-3.14	121.28	125.93
29	F7	1002	PEB	CHB-C4B-NB	-3.14	124.47	128.83
31	wP	1001	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
29	jF	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
29	jI	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
29	hF	202	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	hI	202	PEB	CHC-C4C-C3C	-3.14	124.98	130.34
29	W1	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
29	WK	201	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
29	MD	201	PEB	CAB-C3B-C4B	3.14	130.56	125.01
29	hF	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
29	hI	202	PEB	OD-C4D-ND	-3.14	121.28	125.93
31	XP	1001	CYC	C1B-NB-C4B	-3.14	106.67	110.67
29	B5	202	PEB	C4B-C3B-C2B	-3.14	103.31	106.78
31	BP	1001	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
31	OP	1001	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
31	oP	1001	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
29	KA	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	KN	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
31	I7	1001	CYC	C2C-C1C-NC	3.14	110.98	108.27
31	I9	1001	CYC	C2C-C1C-NC	3.14	110.98	108.27
29	H3	201	PEB	OD-C4D-ND	-3.14	121.28	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HO	201	PEB	OD-C4D-ND	-3.14	121.28	125.93
29	A5	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
29	A8	202	PEB	C1B-C2B-C3B	-3.14	102.91	106.51
31	DP	1001	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
29	IF	202	PEB	CHC-C4C-C3C	-3.14	124.99	130.34
29	II	202	PEB	CHC-C4C-C3C	-3.14	124.99	130.34
29	dD	401	PEB	CAB-C3B-C4B	3.14	130.56	125.01
29	fI	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	fK	202	PEB	C2A-C1A-NA	3.14	110.98	108.27
29	B8	201	PEB	OD-C4D-ND	-3.13	121.29	125.93
31	MP	1001	CYC	C1B-NB-C4B	-3.13	106.68	110.67
29	D3	203	PEB	C2A-C1A-NA	3.13	110.97	108.27
29	DO	203	PEB	C2A-C1A-NA	3.13	110.97	108.27
29	GD	203	PEB	C3B-C4B-NB	3.13	114.61	110.05
31	KF	1001	CYC	C2A-C1A-NA	3.13	114.61	110.05
31	IP	1001	CYC	C1A-C2A-C3A	-3.13	103.31	106.78
31	KP	1001	CYC	C1B-NB-C4B	-3.13	106.68	110.67
31	qP	1001	CYC	C1B-NB-C4B	-3.13	106.68	110.67
29	H7	1002	PEB	CHB-C4B-NB	-3.13	124.48	128.83
29	H9	1002	PEB	CHB-C4B-NB	-3.13	124.48	128.83
29	MJ	202	PEB	C3B-C4B-NB	3.13	114.61	110.05
29	ML	202	PEB	C3B-C4B-NB	3.13	114.61	110.05
29	H1	1002	PEB	CHC-C4C-C3C	-3.13	124.99	130.34
29	M3	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	MO	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
31	BP	1001	CYC	C1B-NB-C4B	-3.13	106.68	110.67
29	L9	1002	PEB	CHB-C4B-NB	-3.13	124.48	128.83
29	GG	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	GQ	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
31	K9	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
29	fI	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	fK	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	c7	203	PEB	OA-C1A-C2A	-3.13	123.68	126.17
29	c9	203	PEB	OA-C1A-C2A	-3.13	123.68	126.17
31	NP	1001	CYC	C1B-NB-C4B	-3.13	106.68	110.67
29	Q1	202	PEB	C2A-C1A-NA	3.13	110.97	108.27
29	b1	202	PEB	C2A-C1A-NA	3.13	110.97	108.27
29	QK	202	PEB	C2A-C1A-NA	3.13	110.97	108.27
29	bK	202	PEB	C2A-C1A-NA	3.13	110.97	108.27
29	B5	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	B8	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	G8	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CD	201	PEB	CAB-C3B-C4B	3.13	130.54	125.01
31	K7	1001	CYC	CHB-C1B-NB	-3.13	119.34	126.06
29	R7	203	PEB	OA-C1A-C2A	-3.13	123.69	126.17
29	R9	203	PEB	OA-C1A-C2A	-3.13	123.69	126.17
31	fP	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
29	RR	203	PEB	CHC-C4C-C3C	-3.13	125.00	130.34
29	F9	1002	PEB	CHB-C4B-NB	-3.13	124.49	128.83
31	uP	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
31	uP	1001	CYC	C1B-NB-C4B	-3.13	106.69	110.67
31	lP	1001	CYC	C4A-C3A-C2A	-3.13	102.92	106.51
29	j1	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	G5	202	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	GD	203	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
29	jK	201	PEB	C4B-C3B-C2B	-3.13	103.32	106.78
31	FP	1001	CYC	C1A-C2A-C3A	-3.13	103.32	106.78
29	A1	303	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
29	AK	303	PEB	C1B-C2B-C3B	-3.13	102.92	106.51
31	GP	1001	CYC	C1B-NB-C4B	-3.13	106.69	110.67
31	UP	1001	CYC	C1B-NB-C4B	-3.13	106.69	110.67
31	hP	1001	CYC	C1A-C2A-C3A	-3.12	103.32	106.78
29	MD	203	PEB	C1B-C2B-C3B	-3.12	102.92	106.51
29	bF	202	PEB	CHC-C4C-C3C	-3.12	125.01	130.34
29	bI	202	PEB	CHC-C4C-C3C	-3.12	125.01	130.34
29	R1	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	CG	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	RK	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	CQ	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	H5	201	PEB	OD-C4D-ND	-3.12	121.30	125.93
29	H8	201	PEB	OD-C4D-ND	-3.12	121.30	125.93
29	ID	203	PEB	C3B-C4B-NB	3.12	114.59	110.05
31	hP	1001	CYC	C1B-NB-C4B	-3.12	106.69	110.67
31	wP	1001	CYC	C1B-NB-C4B	-3.12	106.69	110.67
29	uJ	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	uL	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
31	AP	1001	CYC	C4A-C3A-C2A	-3.12	102.92	106.51
31	MF	1001	CYC	C2A-C1A-NA	3.12	114.59	110.05
31	MI	1001	CYC	C2A-C1A-NA	3.12	114.59	110.05
29	bF	202	PEB	OD-C4D-ND	-3.12	121.30	125.93
29	bI	202	PEB	OD-C4D-ND	-3.12	121.30	125.93
29	mF	201	PEB	C1C-CHB-C4B	3.12	132.54	128.81
29	mI	201	PEB	C1C-CHB-C4B	3.12	132.54	128.81
29	k7	203	PEB	OA-C1A-C2A	-3.12	123.69	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k9	203	PEB	OA-C1A-C2A	-3.12	123.69	126.17
29	R7	201	PEB	C2A-C1A-NA	3.12	110.96	108.27
29	R9	201	PEB	C2A-C1A-NA	3.12	110.96	108.27
29	c1	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	L8	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	ID	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	cK	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
31	1P	1001	CYC	C1A-C2A-C3A	-3.12	103.33	106.78
31	mP	1001	CYC	C4A-C3A-C2A	-3.12	102.92	106.51
29	MD	203	PEB	C3B-C4B-NB	3.12	114.59	110.05
29	WF	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	WI	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	M3	201	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
29	MO	201	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
29	KD	203	PEB	C3B-C4B-NB	3.12	114.59	110.05
29	S1	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	SK	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
31	RP	1001	CYC	C1B-NB-C4B	-3.12	106.70	110.67
29	F5	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	F8	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	BB	301	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	BM	301	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	M4	201	PEB	CAB-C3B-C4B	3.12	130.53	125.01
29	g1	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	H5	201	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	gK	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	B3	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	SF	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	SI	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	BO	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	E4	203	PEB	C3B-C4B-NB	3.12	114.58	110.05
29	ID	203	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	CD	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
29	K4	203	PEB	C3B-C4B-NB	3.12	114.58	110.05
30	A1	305	PUB	CAC-C2C-C1C	3.12	130.52	125.01
30	AK	305	PUB	CAC-C2C-C1C	3.12	130.52	125.01
29	L8	201	PEB	OD-C4D-ND	-3.12	121.31	125.93
31	SP	1001	CYC	C1A-C2A-C3A	-3.12	103.33	106.78
29	fF	202	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
29	fI	202	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
29	lF	202	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	II	202	PEB	OD-C4D-ND	-3.12	121.31	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	xJ	303	PEB	O1B-CGB-CBB	-3.12	113.07	123.08
31	IP	1001	CYC	C1B-NB-C4B	-3.12	106.70	110.67
29	SB	201	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	SM	201	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	Z1	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	K4	203	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	ZK	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	A1	302	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	AK	302	PEB	OD-C4D-ND	-3.12	121.31	125.93
31	K9	1001	CYC	CHB-C1B-NB	-3.12	119.37	126.06
29	TR	203	PEB	CHC-C4C-C3C	-3.12	125.02	130.34
29	wJ	303	PEB	O1B-CGB-CBB	-3.12	113.07	123.08
29	H3	203	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	HO	203	PEB	OD-C4D-ND	-3.12	121.31	125.93
29	H3	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	I3	203	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	HO	202	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	IO	203	PEB	C1B-C2B-C3B	-3.12	102.93	106.51
29	CJ	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	CL	202	PEB	C4B-C3B-C2B	-3.12	103.33	106.78
29	U1	202	PEB	C3B-C4B-NB	3.11	114.58	110.05
29	UK	202	PEB	C3B-C4B-NB	3.11	114.58	110.05
31	C7	1001	CYC	CHB-C1B-NB	-3.11	119.37	126.06
31	C9	1001	CYC	CHB-C1B-NB	-3.11	119.37	126.06
29	JF	1002	PEB	C2A-C1A-NA	3.11	110.96	108.27
29	JI	1002	PEB	C2A-C1A-NA	3.11	110.96	108.27
30	xL	304	PUB	CBD-CAD-C3D	-3.11	103.84	112.43
29	WB	201	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
29	WM	201	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
31	GP	1001	CYC	C4A-C3A-C2A	-3.11	102.93	106.51
29	a7	203	PEB	OA-C1A-C2A	-3.11	123.70	126.17
29	a9	203	PEB	OA-C1A-C2A	-3.11	123.70	126.17
29	E4	201	PEB	CAB-C3B-C4B	3.11	130.52	125.01
29	B5	201	PEB	OD-C4D-ND	-3.11	121.32	125.93
31	I7	1001	CYC	CHB-C1B-NB	-3.11	119.37	126.06
31	I9	1001	CYC	CHB-C1B-NB	-3.11	119.37	126.06
29	FC	203	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
29	FE	203	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
29	C4	203	PEB	C3B-C4B-NB	3.11	114.58	110.05
29	VR	203	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
29	MR	202	PEB	C1B-C2B-C3B	-3.11	102.93	106.51
31	OP	1001	CYC	C1B-NB-C4B	-3.11	106.71	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e1	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	eK	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	ID	201	PEB	CAB-C3B-C4B	3.11	130.51	125.01
29	JF	1002	PEB	C3B-C4B-NB	3.11	114.58	110.05
29	JI	1002	PEB	C3B-C4B-NB	3.11	114.58	110.05
29	CA	202	PEB	CAB-CBB-CGB	-3.11	106.91	113.60
29	CN	202	PEB	CAB-CBB-CGB	-3.11	106.91	113.60
29	I5	202	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	I8	202	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
31	E7	1001	CYC	CHB-C1B-NB	-3.11	119.38	126.06
31	E9	1001	CYC	CHB-C1B-NB	-3.11	119.38	126.06
31	M9	1001	CYC	CHB-C1B-NB	-3.11	119.38	126.06
29	JC	202	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
29	JE	202	PEB	CHC-C4C-C3C	-3.11	125.03	130.34
31	qP	1001	CYC	C1A-C2A-C3A	-3.11	103.34	106.78
29	e7	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	e9	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
31	G9	1001	CYC	C1A-C2A-C3A	-3.11	103.34	106.78
29	GD	203	PEB	CMB-C2B-C1B	3.11	129.85	125.06
29	KB	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	KM	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	JB	202	PEB	CMB-C2B-C1B	3.11	129.85	125.06
29	JM	202	PEB	CMB-C2B-C1B	3.11	129.85	125.06
29	D7	1002	PEB	CHB-C4B-NB	-3.11	124.51	128.83
29	D9	1002	PEB	CHB-C4B-NB	-3.11	124.51	128.83
29	zJ	501	PEB	CHC-C1D-ND	-3.11	110.34	113.95
31	sP	1001	CYC	C1B-NB-C4B	-3.11	106.71	110.67
29	EC	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	EE	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	MA	404	PEB	OD-C4D-C3D	-3.11	122.42	129.46
30	MA	403	PUB	C1D-CHC-C4C	-3.11	106.60	113.37
31	GF	1001	CYC	C2A-C1A-NA	3.11	114.57	110.05
31	GI	1001	CYC	C2A-C1A-NA	3.11	114.57	110.05
29	MB	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	MM	201	PEB	C1B-C2B-C3B	-3.11	102.94	106.51
29	j1	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
29	jK	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
29	fB	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	fM	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	QF	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	QI	202	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	Y1	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AB	302	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	YK	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	OR	202	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	GA	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	IA	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	gF	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	gI	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	GN	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	IN	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
31	D1	1001	CYC	C2C-C1C-NC	3.11	110.95	108.27
29	OB	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	DC	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	DE	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	OF	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	SF	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	OI	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	SI	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	OM	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	TB	202	PEB	CMB-C2B-C1B	3.11	129.85	125.06
29	TM	202	PEB	CMB-C2B-C1B	3.11	129.85	125.06
29	F3	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	FO	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	Q1	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	QK	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	AM	303	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	eF	201	PEB	C1C-CHB-C4B	3.11	132.52	128.81
29	eI	201	PEB	C1C-CHB-C4B	3.11	132.52	128.81
31	I7	1001	CYC	C4A-C3A-C2A	-3.11	102.94	106.51
31	I9	1001	CYC	C4A-C3A-C2A	-3.11	102.94	106.51
29	Y7	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	c7	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	Y9	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	c9	201	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	yJ	301	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	yL	301	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	I5	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	H8	203	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	GB	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	WF	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	WI	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	GM	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	h1	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J3	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	hK	201	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	JO	203	PEB	C4B-C3B-C2B	-3.11	103.34	106.78
29	W1	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
29	WK	201	PEB	C3B-C4B-NB	3.11	114.57	110.05
29	X2	202	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	XR	203	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	A3	202	PEB	CHB-C4B-NB	-3.11	124.52	128.83
29	N7	1002	PEB	CHB-C4B-NB	-3.11	124.52	128.83
29	N9	1002	PEB	CHB-C4B-NB	-3.11	124.52	128.83
29	AO	202	PEB	CHB-C4B-NB	-3.11	124.52	128.83
29	b7	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	b9	202	PEB	C2A-C1A-NA	3.11	110.95	108.27
29	L3	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	H5	203	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	L5	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	LO	201	PEB	OD-C4D-ND	-3.11	121.33	125.93
29	jB	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
29	jM	201	PEB	CHC-C4C-C3C	-3.11	125.04	130.34
30	wJ	304	PUB	CBD-CAD-C3D	-3.10	103.87	112.43
29	jB	201	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
29	jM	201	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
29	F3	203	PEB	OD-C4D-ND	-3.10	121.33	125.93
29	FO	203	PEB	OD-C4D-ND	-3.10	121.33	125.93
29	P1	203	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	d1	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	PK	203	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	dK	201	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	AA	202	PEB	C2A-C1A-NA	3.10	110.95	108.27
29	AN	202	PEB	C2A-C1A-NA	3.10	110.95	108.27
29	V7	203	PEB	OA-C1A-C2A	-3.10	123.70	126.17
29	V9	203	PEB	OA-C1A-C2A	-3.10	123.70	126.17
29	CB	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	IB	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	MB	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	dB	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	CM	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	IM	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	MM	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	dM	201	PEB	CHC-C4C-C3C	-3.10	125.04	130.34
29	f1	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
29	fK	201	PEB	C3B-C4B-NB	3.10	114.56	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	cP	1001	CYC	C1B-NB-C4B	-3.10	106.72	110.67
29	E4	203	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	b1	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
29	bK	201	PEB	C3B-C4B-NB	3.10	114.56	110.05
29	K5	202	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
29	K8	202	PEB	C1B-C2B-C3B	-3.10	102.94	106.51
29	F3	203	PEB	C2A-C1A-NA	3.10	110.95	108.27
29	FO	203	PEB	C2A-C1A-NA	3.10	110.95	108.27
29	AF	301	PEB	CMB-C2B-C1B	3.10	129.84	125.06
29	AI	301	PEB	CMB-C2B-C1B	3.10	129.84	125.06
29	OF	202	PEB	OD-C4D-ND	-3.10	121.33	125.93
29	OI	202	PEB	OD-C4D-ND	-3.10	121.33	125.93
31	M7	1001	CYC	CHB-C1B-NB	-3.10	119.40	126.06
29	B3	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	IB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	GC	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	GE	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	IM	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	BO	202	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	HC	203	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	HE	203	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	MD	203	PEB	CMB-C2B-C1B	3.10	129.84	125.06
29	P2	202	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	PR	202	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	GB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	TF	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	yJ	301	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	yL	301	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	GM	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	DF	1002	PEB	C3B-C4B-NB	3.10	114.56	110.05
29	DI	1002	PEB	C3B-C4B-NB	3.10	114.56	110.05
31	EF	1001	CYC	C2A-C1A-NA	3.10	114.56	110.05
31	EI	1001	CYC	C2A-C1A-NA	3.10	114.56	110.05
30	xJ	304	PUB	CBD-CAD-C3D	-3.10	103.88	112.43
29	K4	201	PEB	CAB-C3B-C4B	3.10	130.49	125.01
29	G4	203	PEB	C3B-C4B-NB	3.10	114.56	110.05
29	ZF	202	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	ZI	202	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	xL	303	PEB	O1B-CGB-CBB	-3.10	113.12	123.08
31	FP	1001	CYC	C1B-NB-C4B	-3.10	106.72	110.67
29	N3	201	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	F5	203	PEB	OD-C4D-ND	-3.10	121.34	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F8	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	G8	201	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	QB	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	UB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	QM	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	UM	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	OB	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
29	OM	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
29	hB	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
29	hM	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
29	G4	201	PEB	CAB-C3B-C4B	3.10	130.49	125.01
29	EB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	EM	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	EB	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
29	EM	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
30	A1	305	PUB	OA-C1A-NA	-3.10	121.34	125.93
30	AK	305	PUB	OA-C1A-NA	-3.10	121.34	125.93
29	H3	203	PEB	C2A-C1A-NA	3.10	110.94	108.27
29	HO	203	PEB	C2A-C1A-NA	3.10	110.94	108.27
29	H8	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	oJ	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	oL	202	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
29	C4	203	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	OB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	OM	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	wL	303	PEB	O1B-CGB-CBB	-3.10	113.13	123.08
29	dF	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	dI	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	UB	201	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	UM	201	PEB	CHC-C4C-C3C	-3.10	125.05	130.34
29	MR	202	PEB	OD-C4D-C3D	-3.10	122.44	129.46
29	AF	305	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
29	AI	305	PEB	C4B-C3B-C2B	-3.10	103.36	106.78
29	Q1	201	PEB	C3B-C4B-NB	3.10	114.55	110.05
29	QK	201	PEB	C3B-C4B-NB	3.10	114.55	110.05
29	R2	203	PEB	CHC-C4C-C3C	-3.10	125.06	130.34
29	B3	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	BO	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	CD	203	PEB	C3B-C4B-NB	3.10	114.55	110.05
29	B8	203	PEB	OD-C4D-ND	-3.10	121.34	125.93
29	I3	202	PEB	CHB-C4B-NB	-3.10	124.53	128.83
29	IO	202	PEB	CHB-C4B-NB	-3.10	124.53	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	lB	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	CC	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	CE	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	lM	201	PEB	C1B-C2B-C3B	-3.10	102.95	106.51
29	J5	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	J8	202	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	LF	1002	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	LI	1002	PEB	C3B-C4B-NB	3.09	114.55	110.05
31	J1	1001	CYC	C2C-C1C-NC	3.09	110.94	108.27
31	JK	1001	CYC	C2C-C1C-NC	3.09	110.94	108.27
29	KD	203	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	SR	201	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	IC	201	PEB	C1B-C2B-C3B	-3.09	102.95	106.51
29	IE	201	PEB	C1B-C2B-C3B	-3.09	102.95	106.51
29	a1	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	aK	203	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	IB	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	IM	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	HF	1002	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	HI	1002	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	SB	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
29	SM	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
29	fB	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	fM	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	S1	202	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	TI	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	SK	202	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	UF	203	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
29	UI	203	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
29	gF	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	iF	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	gI	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	iI	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
30	MN	403	PUB	C1D-CHC-C4C	-3.09	106.64	113.37
29	I5	203	PEB	OD-C4D-ND	-3.09	121.35	125.93
29	I8	203	PEB	OD-C4D-ND	-3.09	121.35	125.93
31	eP	1001	CYC	C1B-NB-C4B	-3.09	106.73	110.67
29	lB	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
29	lM	201	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
30	wL	304	PUB	CBD-CAD-C3D	-3.09	103.91	112.43
29	J3	203	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	JO	203	PEB	C2A-C1A-NA	3.09	110.94	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	201	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	D3	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	bK	201	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	G5	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
29	T2	203	PEB	CHC-C4C-C3C	-3.09	125.06	130.34
29	YB	201	PEB	CMB-C2B-C1B	3.09	129.82	125.06
29	YM	201	PEB	CMB-C2B-C1B	3.09	129.82	125.06
29	L3	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
29	LO	202	PEB	OD-C4D-ND	-3.09	121.35	125.93
29	XR	202	PEB	OD-C4D-C3D	-3.09	122.45	129.46
29	IJ	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	IL	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	PF	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	PI	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	dD	401	PEB	OA-C1A-C2A	-3.09	123.72	126.17
29	m7	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	m9	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	J3	202	PEB	C3D-C4D-ND	3.09	113.32	107.26
29	JO	202	PEB	C3D-C4D-ND	3.09	113.32	107.26
29	QR	201	PEB	CHC-C1D-ND	3.09	117.54	113.95
29	S1	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	SK	201	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	DQ	203	PEB	C3B-C4B-NB	3.09	114.55	110.05
29	lB	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	lM	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	QJ	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	QL	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	YB	202	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	YM	202	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	NO	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	A5	201	PEB	OD-C4D-ND	-3.09	121.35	125.93
29	JQ	203	PEB	C3B-C4B-NB	3.09	114.54	110.05
29	QB	204	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	UB	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	QM	204	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	MQ	401	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	L5	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	FB	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
29	FM	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
29	dB	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	dM	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	WB	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KC	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
29	KE	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
29	WM	201	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
29	iF	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	iI	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	T1	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	TK	202	PEB	C4B-C3B-C2B	-3.09	103.36	106.78
29	D3	203	PEB	OD-C4D-ND	-3.09	121.36	125.93
29	DO	203	PEB	OD-C4D-ND	-3.09	121.36	125.93
29	dF	203	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	dI	203	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	NR	203	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	H3	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
29	HO	201	PEB	C2A-C1A-NA	3.09	110.94	108.27
31	N1	1001	CYC	C2C-C1C-NC	3.09	110.94	108.27
29	IA	202	PEB	CAB-CBB-CGB	-3.09	106.96	113.60
29	IN	202	PEB	CAB-CBB-CGB	-3.09	106.96	113.60
29	CB	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	CM	202	PEB	OD-C4D-C3D	-3.09	122.46	129.46
29	DO	202	PEB	C1B-C2B-C3B	-3.09	102.96	106.51
29	W2	201	PEB	CHC-C1D-ND	3.09	117.53	113.95
29	DG	203	PEB	C3B-C4B-NB	3.09	114.54	110.05
29	YF	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	YI	201	PEB	C1C-CHB-C4B	3.09	132.50	128.81
29	iI	203	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
29	F5	202	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
29	iK	203	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
29	hB	201	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	hM	201	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	LF	1002	PEB	C2A-C1A-NA	3.09	110.93	108.27
29	LI	1002	PEB	C2A-C1A-NA	3.09	110.93	108.27
29	MD	202	PEB	CHA-C4A-NA	-3.09	121.53	125.20
29	jF	202	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	jI	202	PEB	CHC-C4C-C3C	-3.09	125.07	130.34
29	L5	201	PEB	C4B-C3B-C2B	-3.09	103.37	106.78
29	h1	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
29	hK	201	PEB	C3B-C4B-NB	3.09	114.54	110.05
29	HB	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
29	HM	202	PEB	CMB-C2B-C1B	3.09	129.82	125.06
29	WB	202	PEB	OD-C4D-C3D	-3.09	122.47	129.46
29	WM	202	PEB	OD-C4D-C3D	-3.09	122.47	129.46
29	MN	404	PEB	OD-C4D-C3D	-3.09	122.47	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DB	202	PEB	CMB-C2B-C1B	3.09	129.81	125.06
29	DM	202	PEB	CMB-C2B-C1B	3.09	129.81	125.06
29	MB	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	SB	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	MM	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	SM	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	KA	202	PEB	CAB-CBB-CGB	-3.08	106.97	113.60
29	KN	202	PEB	CAB-CBB-CGB	-3.08	106.97	113.60
29	S2	201	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	K4	203	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	A3	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	CA	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	CN	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	AO	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
31	IF	1001	CYC	C2A-C1A-NA	3.08	114.53	110.05
31	II	1001	CYC	C2A-C1A-NA	3.08	114.53	110.05
29	hB	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	hM	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	GB	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	GM	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	a7	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	a9	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	KB	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	KM	202	PEB	OD-C4D-C3D	-3.08	122.47	129.46
29	K5	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
29	G8	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
29	K8	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
29	A8	201	PEB	OD-C4D-ND	-3.08	121.36	125.93
29	L8	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	AB	303	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	AJ	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	AL	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	AA	202	PEB	CAB-CBB-CGB	-3.08	106.97	113.60
29	AN	202	PEB	CAB-CBB-CGB	-3.08	106.97	113.60
29	L5	203	PEB	OD-C4D-ND	-3.08	121.36	125.93
29	H8	201	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	CB	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	dB	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	AC	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	AE	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	CM	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	dM	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FC	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	FE	202	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	kF	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	kI	201	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	MA	404	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	qJ	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	qL	202	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	AM	302	PEB	C4B-C3B-C2B	-3.08	103.37	106.78
29	KD	201	PEB	CAB-C3B-C4B	3.08	130.46	125.01
29	A1	303	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	AK	303	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	D3	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	QB	203	PEB	CHC-C4C-C3C	-3.08	125.08	130.34
29	QM	203	PEB	CHC-C4C-C3C	-3.08	125.08	130.34
29	CA	201	PEB	OA-C1A-C2A	-3.08	123.72	126.17
29	CN	201	PEB	OA-C1A-C2A	-3.08	123.72	126.17
29	I3	203	PEB	C3D-C4D-ND	3.08	113.30	107.26
29	IO	203	PEB	C3D-C4D-ND	3.08	113.30	107.26
29	G3	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	GO	202	PEB	C2A-C1A-NA	3.08	110.93	108.27
29	RF	201	PEB	C1C-CHB-C4B	3.08	132.49	128.81
29	RI	201	PEB	C1C-CHB-C4B	3.08	132.49	128.81
29	MD	203	PEB	OD-C4D-C3D	-3.08	122.48	129.46
29	O2	201	PEB	CHC-C1D-ND	3.08	117.52	113.95
29	G3	202	PEB	CHB-C4B-NB	-3.08	124.56	128.83
29	GO	202	PEB	CHB-C4B-NB	-3.08	124.56	128.83
29	I8	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
29	GD	201	PEB	CAB-C3B-C4B	3.08	130.46	125.01
29	TF	201	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	aB	202	PEB	OD-C4D-C3D	-3.08	122.48	129.46
29	aM	202	PEB	OD-C4D-C3D	-3.08	122.48	129.46
29	ED	202	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	f7	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
29	f9	202	PEB	CMB-C2B-C1B	3.08	129.81	125.06
29	NO	201	PEB	CHC-C4C-C3C	-3.08	125.09	130.34
29	H3	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	GC	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	GE	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	sJ	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	sL	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	HO	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	aB	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aM	201	PEB	C1B-C2B-C3B	-3.08	102.97	106.51
29	A1	301	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	FF	1002	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	FI	1002	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	AK	301	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	HQ	203	PEB	C3B-C4B-NB	3.08	114.53	110.05
29	g7	203	PEB	OA-C1A-C2A	-3.08	123.73	126.17
29	g9	203	PEB	OA-C1A-C2A	-3.08	123.73	126.17
29	M3	202	PEB	OD-C4D-C3D	-3.08	122.49	129.46
29	MO	202	PEB	OD-C4D-C3D	-3.08	122.49	129.46
29	F3	202	PEB	C3D-C4D-ND	3.08	113.30	107.26
29	FO	202	PEB	C3D-C4D-ND	3.08	113.30	107.26
29	VB	202	PEB	CMB-C2B-C1B	3.08	129.80	125.06
29	VM	202	PEB	CMB-C2B-C1B	3.08	129.80	125.06
29	K5	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
29	K8	202	PEB	OD-C4D-ND	-3.08	121.37	125.93
29	B5	202	PEB	C3B-C4B-NB	3.08	114.52	110.05
29	B3	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	eJ	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	eL	202	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	BO	203	PEB	C4B-C3B-C2B	-3.08	103.38	106.78
29	B3	202	PEB	C3D-C4D-ND	3.08	113.29	107.26
29	BO	202	PEB	C3D-C4D-ND	3.08	113.29	107.26
29	EA	202	PEB	CAB-CBB-CGB	-3.08	106.98	113.60
29	GA	202	PEB	CAB-CBB-CGB	-3.08	106.98	113.60
29	EN	202	PEB	CAB-CBB-CGB	-3.08	106.98	113.60
29	GN	202	PEB	CAB-CBB-CGB	-3.08	106.98	113.60
29	V2	203	PEB	CHC-C4C-C3C	-3.08	125.09	130.34
29	wJ	303	PEB	C3B-C4B-NB	3.08	114.52	110.05
29	K5	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
29	K8	201	PEB	OD-C4D-ND	-3.08	121.37	125.93
29	V2	202	PEB	OD-C4D-C3D	-3.08	122.49	129.46
29	NR	202	PEB	OD-C4D-C3D	-3.08	122.49	129.46
29	VR	202	PEB	OD-C4D-C3D	-3.08	122.49	129.46
29	Z1	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	ZK	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	H3	202	PEB	C3D-C4D-ND	3.07	113.29	107.26
29	HO	202	PEB	C3D-C4D-ND	3.07	113.29	107.26
29	H5	202	PEB	CMB-C2B-C1B	3.07	129.80	125.06
29	mB	202	PEB	CMB-C2B-C1B	3.07	129.80	125.06
29	mM	202	PEB	CMB-C2B-C1B	3.07	129.80	125.06
29	C3	202	PEB	CHB-C4B-NB	-3.07	124.56	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CO	202	PEB	CHB-C4B-NB	-3.07	124.56	128.83
31	CF	1001	CYC	C2A-C1A-NA	3.07	114.52	110.05
31	CI	1001	CYC	C2A-C1A-NA	3.07	114.52	110.05
29	MN	401	PEB	OA-C1A-C2A	-3.07	123.73	126.17
29	K4	203	PEB	CMB-C2B-C1B	3.07	129.80	125.06
29	AB	303	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
29	fB	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
29	fM	201	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
29	YB	203	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	jB	202	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	YM	203	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	jM	202	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	d1	201	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	dK	201	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	B3	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
29	BO	203	PEB	C2A-C1A-NA	3.07	110.92	108.27
29	cJ	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	cL	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	F3	202	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
29	FO	202	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
29	e7	203	PEB	OA-C1A-C2A	-3.07	123.73	126.17
29	e9	203	PEB	OA-C1A-C2A	-3.07	123.73	126.17
29	I4	202	PEB	CHA-C4A-NA	-3.07	121.55	125.20
29	N2	203	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
29	N3	202	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	G4	203	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	IC	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	IE	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	MJ	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	ML	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	SR	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	YB	202	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
29	YM	202	PEB	C1B-C2B-C3B	-3.07	102.98	106.51
31	F1	1001	CYC	C2C-C1C-NC	3.07	110.92	108.27
31	FK	1001	CYC	C2C-C1C-NC	3.07	110.92	108.27
29	EB	201	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
29	aB	201	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
29	EM	201	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
29	aM	201	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
29	L5	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	h7	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	h9	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HC	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	HE	202	PEB	C3B-C4B-NB	3.07	114.52	110.05
29	O1	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	MA	405	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	gJ	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	OK	201	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	gL	202	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	MN	404	PEB	C4B-C3B-C2B	-3.07	103.38	106.78
29	B3	201	PEB	C2A-C1A-NA	3.07	110.92	108.27
29	BO	201	PEB	C2A-C1A-NA	3.07	110.92	108.27
29	X2	201	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	G4	203	PEB	OD-C4D-C3D	-3.07	122.50	129.46
29	W7	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	Z7	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	W9	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	Z9	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	L3	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	LO	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
31	NK	1001	CYC	C2C-C1C-NC	3.07	110.92	108.27
31	1P	1001	CYC	C2B-C1B-NB	3.07	111.48	106.99
29	A1	303	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	F4	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	AK	303	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	A7	304	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	AC	203	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	AE	203	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	E3	202	PEB	CHB-C4B-NB	-3.07	124.57	128.83
29	EO	202	PEB	CHB-C4B-NB	-3.07	124.57	128.83
29	MQ	406	PEB	CHC-C4C-C3C	-3.07	125.10	130.34
29	L5	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	V1	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	l1	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	VK	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	IK	201	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	LC	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	LE	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	K3	202	PEB	CHB-C4B-NB	-3.07	124.57	128.83
29	KO	202	PEB	CHB-C4B-NB	-3.07	124.57	128.83
29	LB	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	cB	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	LM	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	cM	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i7	203	PEB	OA-C1A-C2A	-3.07	123.73	126.17
29	i9	203	PEB	OA-C1A-C2A	-3.07	123.73	126.17
29	B8	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	G8	202	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	kF	201	PEB	C1C-CHB-C4B	3.07	132.47	128.81
29	kI	201	PEB	C1C-CHB-C4B	3.07	132.47	128.81
29	m1	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	CC	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	KD	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	CE	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	mK	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	MN	405	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	XB	202	PEB	CHC-C4C-C3C	-3.07	125.11	130.34
29	XM	202	PEB	CHC-C4C-C3C	-3.07	125.11	130.34
29	JG	203	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	G8	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	RB	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	iB	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	RM	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	iM	202	PEB	CMB-C2B-C1B	3.07	129.79	125.06
29	B4	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	A9	304	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	F3	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	aJ	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	aL	202	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	FO	203	PEB	C4B-C3B-C2B	-3.07	103.39	106.78
29	l1	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	lK	201	PEB	C3B-C4B-NB	3.07	114.51	110.05
29	C5	203	PEB	OD-C4D-ND	-3.07	121.39	125.93
29	C8	203	PEB	OD-C4D-ND	-3.07	121.39	125.93
29	RR	202	PEB	OD-C4D-C3D	-3.07	122.52	129.46
29	CD	203	PEB	C1B-C2B-C3B	-3.06	102.99	106.51
29	zJ	501	PEB	OD-C4D-C3D	-3.06	122.52	129.46
29	J3	203	PEB	OD-C4D-ND	-3.06	121.39	125.93
29	JO	203	PEB	OD-C4D-ND	-3.06	121.39	125.93
29	JB	203	PEB	CHC-C4C-C3C	-3.06	125.11	130.34
29	JM	203	PEB	CHC-C4C-C3C	-3.06	125.11	130.34
29	L4	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	BD	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	L8	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
29	aF	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	aI	201	PEB	C2A-C1A-NA	3.06	110.91	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KC	201	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	KE	201	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	hB	201	PEB	CHC-C1D-ND	-3.06	110.39	113.95
29	hM	201	PEB	CHC-C1D-ND	-3.06	110.39	113.95
29	A1	303	PEB	CHC-C4C-C3C	-3.06	125.11	130.34
29	AK	303	PEB	CHC-C4C-C3C	-3.06	125.11	130.34
29	mJ	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	mL	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	C5	201	PEB	OD-C4D-ND	-3.06	121.39	125.93
29	C8	201	PEB	OD-C4D-ND	-3.06	121.39	125.93
29	C3	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	CO	202	PEB	C2A-C1A-NA	3.06	110.91	108.27
31	L1	1001	CYC	C2C-C1C-NC	3.06	110.91	108.27
31	LK	1001	CYC	C2C-C1C-NC	3.06	110.91	108.27
29	A5	203	PEB	OD-C4D-ND	-3.06	121.39	125.93
29	D3	203	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	kJ	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	kL	202	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	DO	203	PEB	C4B-C3B-C2B	-3.06	103.39	106.78
29	cB	203	PEB	CHC-C4C-C3C	-3.06	125.11	130.34
29	cM	203	PEB	CHC-C4C-C3C	-3.06	125.11	130.34
29	O1	201	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	OK	201	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	G5	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
29	S7	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
29	S9	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
29	gB	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
29	gM	202	PEB	CMB-C2B-C1B	3.06	129.78	125.06
29	L3	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	VF	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	VI	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	LO	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	X2	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	FB	203	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
29	FM	203	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
29	NF	1002	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	NI	1002	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	N2	202	PEB	OD-C4D-C3D	-3.06	122.53	129.46
29	zL	501	PEB	OD-C4D-C3D	-3.06	122.53	129.46
29	G5	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	YJ	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	YL	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DB	203	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
29	DM	203	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
29	k1	203	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	LD	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	kK	203	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	D3	202	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
31	sP	1001	CYC	CAA-C2A-C1A	3.06	130.42	125.01
29	IB	201	PEB	CHC-C1D-ND	-3.06	110.40	113.95
29	IM	201	PEB	CHC-C1D-ND	-3.06	110.40	113.95
29	TI	201	PEB	C1C-CHB-C4B	3.06	132.46	128.81
29	WF	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	WI	202	PEB	C3B-C4B-NB	3.06	114.50	110.05
29	kB	203	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
29	kM	203	PEB	CHC-C4C-C3C	-3.06	125.12	130.34
29	SJ	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	iJ	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	SL	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	iL	202	PEB	C4B-C3B-C2B	-3.06	103.40	106.78
29	F5	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	F8	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	A8	202	PEB	OD-C4D-ND	-3.06	121.40	125.93
29	LG	201	PEB	CHB-C4B-NB	-3.06	124.59	128.83
29	MQ	402	PEB	CHB-C4B-NB	-3.06	124.59	128.83
29	DA	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
29	DN	201	PEB	OD-C4D-ND	-3.06	121.40	125.93
29	aF	201	PEB	C1C-CHB-C4B	3.06	132.46	128.81
29	aI	201	PEB	C1C-CHB-C4B	3.06	132.46	128.81
29	KA	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
29	KN	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
29	kB	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	kM	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	P2	201	PEB	OD-C4D-C3D	-3.06	122.54	129.46
29	J3	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	JO	201	PEB	C2A-C1A-NA	3.06	110.91	108.27
29	E4	203	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	b7	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	b9	202	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	CD	203	PEB	CMB-C2B-C1B	3.06	129.77	125.06
29	G5	203	PEB	OD-C4D-ND	-3.06	121.40	125.93
29	M3	203	PEB	C2A-C1A-NA	3.05	110.91	108.27
29	YF	201	PEB	C2A-C1A-NA	3.05	110.91	108.27
29	YI	201	PEB	C2A-C1A-NA	3.05	110.91	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MO	203	PEB	C2A-C1A-NA	3.05	110.91	108.27
29	RB	203	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
29	RM	203	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
29	KB	203	PEB	CMB-C2B-C1B	3.05	129.77	125.06
29	KM	203	PEB	CMB-C2B-C1B	3.05	129.77	125.06
29	cF	201	PEB	C1C-CHB-C4B	3.05	132.46	128.81
29	cI	201	PEB	C1C-CHB-C4B	3.05	132.46	128.81
29	OR	201	PEB	CHC-C1D-ND	3.05	117.49	113.95
29	H5	202	PEB	C4B-C3B-C2B	-3.05	103.40	106.78
29	AA	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
29	AN	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
29	F8	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
29	WJ	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
29	WL	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
29	BA	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
29	BN	201	PEB	OD-C4D-ND	-3.05	121.41	125.93
29	M2	201	PEB	CHC-C1D-ND	3.05	117.49	113.95
29	MR	201	PEB	CHC-C1D-ND	3.05	117.49	113.95
29	PB	202	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
29	PM	202	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
29	FG	201	PEB	CHB-C4B-NB	-3.05	124.59	128.83
29	FQ	201	PEB	CHB-C4B-NB	-3.05	124.59	128.83
29	CD	202	PEB	CHA-C4A-NA	-3.05	121.58	125.20
29	HB	203	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
29	HM	203	PEB	CHC-C4C-C3C	-3.05	125.13	130.34
29	L8	202	PEB	C3B-C4B-NB	3.05	114.49	110.05
29	KD	203	PEB	CMB-C2B-C1B	3.05	129.76	125.06
29	P7	203	PEB	OA-C1A-C2A	-3.05	123.75	126.17
29	P9	203	PEB	OA-C1A-C2A	-3.05	123.75	126.17
29	IA	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
29	IN	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
29	L3	202	PEB	C2A-C1A-NA	3.05	110.90	108.27
29	FF	1002	PEB	C2A-C1A-NA	3.05	110.90	108.27
29	FI	1002	PEB	C2A-C1A-NA	3.05	110.90	108.27
29	LO	202	PEB	C2A-C1A-NA	3.05	110.90	108.27
29	G4	203	PEB	CMB-C2B-C1B	3.05	129.76	125.06
29	mF	201	PEB	CHB-C4B-NB	-3.05	124.60	128.83
29	mI	201	PEB	CHB-C4B-NB	-3.05	124.60	128.83
29	XR	203	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
29	FQ	203	PEB	C3B-C4B-NB	3.05	114.48	110.05
29	C4	203	PEB	OD-C4D-C3D	-3.05	122.55	129.46
29	GD	203	PEB	OD-C4D-C3D	-3.05	122.55	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	OB	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
29	OM	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
29	L8	203	PEB	OD-C4D-ND	-3.05	121.41	125.93
29	T2	202	PEB	OD-C4D-C3D	-3.05	122.55	129.46
29	ED	202	PEB	OD-C4D-C3D	-3.05	122.55	129.46
29	ID	203	PEB	OD-C4D-C3D	-3.05	122.55	129.46
29	CA	202	PEB	CHB-C4B-C3B	3.05	132.36	125.32
29	CN	202	PEB	CHB-C4B-C3B	3.05	132.36	125.32
29	R7	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
29	R9	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
29	VF	201	PEB	C1C-CHB-C4B	3.05	132.45	128.81
29	VI	201	PEB	C1C-CHB-C4B	3.05	132.45	128.81
29	MG	404	PEB	CHC-C4C-C3C	-3.05	125.14	130.34
29	DO	202	PEB	C4B-C3B-C2B	-3.05	103.41	106.78
29	J5	202	PEB	CMC-C3C-C2C	-3.05	119.20	124.94
29	J8	202	PEB	CMC-C3C-C2C	-3.05	119.20	124.94
29	JA	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
29	JN	201	PEB	OD-C4D-ND	-3.05	121.42	125.93
29	GB	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
29	GM	201	PEB	CHC-C1D-ND	-3.05	110.41	113.95
29	O7	202	PEB	CMB-C2B-C1B	3.05	129.76	125.06
29	O9	202	PEB	CMB-C2B-C1B	3.05	129.76	125.06
29	a7	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
29	a9	201	PEB	CHA-C1B-NB	-3.05	118.56	124.93
29	bF	202	PEB	CAA-C3A-C2A	-3.05	106.65	114.26
29	bI	202	PEB	CAA-C3A-C2A	-3.05	106.65	114.26
29	d7	202	PEB	CMB-C2B-C1B	3.05	129.75	125.06
29	d9	202	PEB	CMB-C2B-C1B	3.05	129.75	125.06
29	WF	202	PEB	CAA-C3A-C2A	-3.04	106.65	114.26
29	WI	202	PEB	CAA-C3A-C2A	-3.04	106.65	114.26
29	NR	203	PEB	C4B-C3B-C2B	-3.04	103.41	106.78
29	H8	202	PEB	CMB-C2B-C1B	3.04	129.75	125.06
29	D3	201	PEB	C2A-C1A-NA	3.04	110.90	108.27
29	DO	201	PEB	C2A-C1A-NA	3.04	110.90	108.27
29	K4	201	PEB	OA-C1A-C2A	-3.04	123.75	126.17
31	AP	1001	CYC	OC-C1C-C2C	-3.04	123.75	126.17
29	UR	201	PEB	CHC-C1D-ND	3.04	117.48	113.95
30	MN	403	PUB	C2C-C1C-NC	3.04	114.48	110.05
31	M9	1001	CYC	C2A-C1A-NA	3.04	114.48	110.05
29	OF	203	PEB	CHA-C1B-NB	-3.04	118.57	124.93
29	OI	203	PEB	CHA-C1B-NB	-3.04	118.57	124.93
29	I5	201	PEB	C1B-C2B-C3B	-3.04	103.01	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I8	201	PEB	C1B-C2B-C3B	-3.04	103.01	106.51
29	mB	203	PEB	CHC-C4C-C3C	-3.04	125.15	130.34
29	mM	203	PEB	CHC-C4C-C3C	-3.04	125.15	130.34
29	EJ	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	EL	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	YF	201	PEB	CHB-C4B-NB	-3.04	124.61	128.83
29	YI	201	PEB	CHB-C4B-NB	-3.04	124.61	128.83
29	HG	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	LQ	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	J4	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	KJ	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	OJ	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	KL	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	OL	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	ZB	203	PEB	CHC-C4C-C3C	-3.04	125.15	130.34
29	ZM	203	PEB	CHC-C4C-C3C	-3.04	125.15	130.34
29	LA	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
29	LN	201	PEB	OD-C4D-ND	-3.04	121.42	125.93
29	I8	202	PEB	CMB-C2B-C1B	3.04	129.75	125.06
29	A8	202	PEB	CMB-C2B-C1B	3.04	129.75	125.06
29	U2	201	PEB	CHC-C1D-ND	3.04	117.48	113.95
29	BG	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	CD	203	PEB	OD-C4D-C3D	-3.04	122.57	129.46
29	TR	202	PEB	OD-C4D-C3D	-3.04	122.57	129.46
29	mF	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	mI	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	U7	202	PEB	CMB-C2B-C1B	3.04	129.75	125.06
29	U9	202	PEB	CMB-C2B-C1B	3.04	129.75	125.06
29	R2	202	PEB	OD-C4D-C3D	-3.04	122.57	129.46
29	N3	203	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	RF	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	RI	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	hF	202	PEB	CAA-C3A-C2A	-3.04	106.67	114.26
29	hI	202	PEB	CAA-C3A-C2A	-3.04	106.67	114.26
29	dF	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	dI	203	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	I5	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
29	I8	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
29	A8	203	PEB	OD-C4D-ND	-3.04	121.43	125.93
29	YB	202	PEB	CHC-C1D-ND	-3.04	110.42	113.95
29	YM	202	PEB	CHC-C1D-ND	-3.04	110.42	113.95
29	VF	202	PEB	CHA-C1B-NB	-3.04	118.58	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VI	202	PEB	CHA-C1B-NB	-3.04	118.58	124.93
31	M7	1001	CYC	C2A-C1A-NA	3.04	114.47	110.05
31	MP	1001	CYC	CAA-C2A-C1A	3.04	130.38	125.01
29	BC	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	BE	202	PEB	C3B-C4B-NB	3.04	114.47	110.05
29	aB	203	PEB	CMB-C2B-C1B	3.04	129.74	125.06
29	aM	203	PEB	CMB-C2B-C1B	3.04	129.74	125.06
29	C4	202	PEB	CHA-C4A-NA	-3.04	121.59	125.20
29	C5	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
29	C8	202	PEB	OD-C4D-ND	-3.04	121.43	125.93
29	cF	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	cI	201	PEB	C2A-C1A-NA	3.04	110.89	108.27
29	i7	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
29	i9	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
29	kF	202	PEB	CHA-C1B-NB	-3.04	118.58	124.93
29	kI	202	PEB	CHA-C1B-NB	-3.04	118.58	124.93
29	gB	203	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
29	gM	203	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
29	k7	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
29	k9	201	PEB	CHA-C1B-NB	-3.04	118.58	124.93
29	FD	202	PEB	C4B-C3B-C2B	-3.04	103.42	106.78
29	iB	203	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
29	iM	203	PEB	CHC-C4C-C3C	-3.04	125.16	130.34
29	NB	202	PEB	C3B-C4B-NB	3.04	114.46	110.05
29	NM	202	PEB	C3B-C4B-NB	3.04	114.46	110.05
29	KB	201	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	fB	201	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	KM	201	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	fM	201	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	ID	201	PEB	OA-C1A-C2A	-3.03	123.76	126.17
31	HP	1001	CYC	CAA-C2A-C1A	3.03	130.38	125.01
29	YF	202	PEB	CHA-C1B-NB	-3.03	118.59	124.93
29	YI	202	PEB	CHA-C1B-NB	-3.03	118.59	124.93
31	GF	1001	CYC	OB-C4B-C3B	-3.03	124.75	128.04
31	GI	1001	CYC	OB-C4B-C3B	-3.03	124.75	128.04
29	j7	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
29	j9	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
31	IP	1001	CYC	CAA-C2A-C1A	3.03	130.38	125.01
29	KB	201	PEB	C4B-C3B-C2B	-3.03	103.42	106.78
29	KM	201	PEB	C4B-C3B-C2B	-3.03	103.42	106.78
29	c7	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
29	c9	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	wL	303	PEB	C3B-C4B-NB	3.03	114.46	110.05
29	BQ	203	PEB	C3B-C4B-NB	3.03	114.46	110.05
29	PF	201	PEB	C2A-C1A-NA	3.03	110.89	108.27
29	PI	201	PEB	C2A-C1A-NA	3.03	110.89	108.27
29	QB	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
29	SF	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
29	SI	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
29	QM	202	PEB	CMB-C2B-C1B	3.03	129.74	125.06
29	C3	202	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	G3	202	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	K3	202	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	CO	202	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	GO	202	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	KO	202	PEB	CHC-C1D-ND	-3.03	110.42	113.95
29	H8	202	PEB	C3B-C4B-NB	3.03	114.46	110.05
29	iF	201	PEB	CHB-C4B-NB	-3.03	124.62	128.83
29	DG	201	PEB	CHB-C4B-NB	-3.03	124.62	128.83
29	HG	201	PEB	CHB-C4B-NB	-3.03	124.62	128.83
29	iI	201	PEB	CHB-C4B-NB	-3.03	124.62	128.83
29	DQ	201	PEB	CHB-C4B-NB	-3.03	124.62	128.83
29	HQ	201	PEB	CHB-C4B-NB	-3.03	124.62	128.83
29	SF	202	PEB	CAA-C3A-C2A	-3.03	106.68	114.26
29	lF	202	PEB	CAA-C3A-C2A	-3.03	106.68	114.26
29	SI	202	PEB	CAA-C3A-C2A	-3.03	106.68	114.26
29	II	202	PEB	CAA-C3A-C2A	-3.03	106.68	114.26
29	FG	203	PEB	C3B-C4B-NB	3.03	114.46	110.05
29	WB	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	WM	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	PR	201	PEB	OD-C4D-C3D	-3.03	122.59	129.46
29	aF	202	PEB	CHA-C1B-NB	-3.03	118.59	124.93
29	aI	202	PEB	CHA-C1B-NB	-3.03	118.59	124.93
29	UF	203	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	UI	203	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	L3	202	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	TB	203	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	TM	203	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	LO	202	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	C4	203	PEB	CMB-C2B-C1B	3.03	129.73	125.06
31	kP	1001	CYC	CAA-C2A-C1A	3.03	130.37	125.01
29	m7	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
29	m9	201	PEB	CHA-C1B-NB	-3.03	118.59	124.93
29	dF	203	PEB	CAA-C3A-C2A	-3.03	106.69	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	dI	203	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	A5	202	PEB	OD-C4D-ND	-3.03	121.44	125.93
29	aB	201	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	aM	201	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
31	H1	1001	CYC	C2C-C1C-NC	3.03	110.89	108.27
29	A1	302	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
29	AK	302	PEB	C1B-C2B-C3B	-3.03	103.03	106.51
29	E4	203	PEB	OD-C4D-C3D	-3.03	122.59	129.46
29	I3	202	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	IO	202	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	ZB	202	PEB	CMB-C2B-C1B	3.03	129.73	125.06
29	ZM	202	PEB	CMB-C2B-C1B	3.03	129.73	125.06
29	T7	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	T9	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	NB	202	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	NM	202	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	HF	1002	PEB	C2A-C1A-NA	3.03	110.88	108.27
29	HI	1002	PEB	C2A-C1A-NA	3.03	110.88	108.27
30	yJ	302	PUB	CBA-CAA-C3A	-3.03	108.39	112.98
30	yL	302	PUB	CBA-CAA-C3A	-3.03	108.39	112.98
31	FP	1001	CYC	CAA-C2A-C1A	3.03	130.37	125.01
29	ID	203	PEB	CMB-C2B-C1B	3.03	129.73	125.06
29	AA	202	PEB	CHB-C4B-C3B	3.03	132.32	125.32
29	AN	202	PEB	CHB-C4B-C3B	3.03	132.32	125.32
29	P2	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
31	QP	1001	CYC	C2B-C1B-NB	3.03	111.42	106.99
29	gF	201	PEB	CHB-C4B-NB	-3.03	124.63	128.83
29	gI	201	PEB	CHB-C4B-NB	-3.03	124.63	128.83
29	ZF	202	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	ZI	202	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	bF	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
29	bI	202	PEB	C3B-C4B-NB	3.03	114.45	110.05
29	EA	202	PEB	CHB-C4B-C3B	3.03	132.32	125.32
29	EN	202	PEB	CHB-C4B-C3B	3.03	132.32	125.32
29	N2	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	KC	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	KE	203	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	WF	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	WI	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	fF	202	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	fI	202	PEB	CAA-C3A-C2A	-3.03	106.69	114.26
29	E4	201	PEB	OA-C1A-C2A	-3.03	123.77	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MD	201	PEB	OA-C1A-C2A	-3.03	123.77	126.17
29	e7	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	e9	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
31	DP	1001	CYC	CAA-C2A-C1A	3.03	130.36	125.01
31	fP	1001	CYC	CAA-C2A-C1A	3.03	130.36	125.01
29	J3	203	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	MA	405	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	JO	203	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	GD	202	PEB	CHA-C4A-NA	-3.03	121.61	125.20
29	Y7	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	Y9	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	GJ	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	GL	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	VB	203	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
29	VM	203	PEB	CHC-C4C-C3C	-3.03	125.17	130.34
31	L9	1001	CYC	CAD-CBD-CGD	-3.03	105.28	113.76
29	UB	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	jB	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	UM	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	jM	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
31	mP	1001	CYC	CHA-C1A-NA	-3.03	124.63	128.83
29	dF	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	dI	201	PEB	CHA-C1B-NB	-3.03	118.60	124.93
29	GA	201	PEB	OA-C1A-C2A	-3.03	123.77	126.17
29	GN	201	PEB	OA-C1A-C2A	-3.03	123.77	126.17
29	eB	202	PEB	CHC-C4C-C3C	-3.03	125.18	130.34
29	eM	202	PEB	CHC-C4C-C3C	-3.03	125.18	130.34
29	EC	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
29	EE	202	PEB	C4B-C3B-C2B	-3.03	103.43	106.78
31	MP	1001	CYC	C2B-C1B-NB	3.03	111.42	106.99
29	SB	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	SM	201	PEB	CHC-C1D-ND	-3.03	110.43	113.95
29	NF	1002	PEB	C2A-C1A-NA	3.03	110.88	108.27
29	eF	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
29	NI	1002	PEB	C2A-C1A-NA	3.03	110.88	108.27
29	eI	201	PEB	C2A-C1A-NA	3.03	110.88	108.27
30	MA	403	PUB	C2C-C1C-NC	3.02	114.45	110.05
31	uP	1001	CYC	CAA-C2A-C1A	3.02	130.36	125.01
29	jF	202	PEB	CAA-C3A-C2A	-3.02	106.70	114.26
29	jI	202	PEB	CAA-C3A-C2A	-3.02	106.70	114.26
29	UF	203	PEB	CMB-C2B-C1B	3.02	129.72	125.06
29	UI	203	PEB	CMB-C2B-C1B	3.02	129.72	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MB	201	PEB	CHC-C1D-ND	-3.02	110.44	113.95
29	MM	201	PEB	CHC-C1D-ND	-3.02	110.44	113.95
29	FA	201	PEB	OD-C4D-ND	-3.02	121.45	125.93
29	FN	201	PEB	OD-C4D-ND	-3.02	121.45	125.93
29	Q7	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
29	Q9	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
29	fF	202	PEB	C3B-C4B-NB	3.02	114.45	110.05
29	fI	202	PEB	C3B-C4B-NB	3.02	114.45	110.05
29	xL	303	PEB	C3B-C4B-NB	3.02	114.45	110.05
29	TI	201	PEB	CHB-C4B-NB	-3.02	124.63	128.83
31	J9	1001	CYC	CAD-CBD-CGD	-3.02	105.28	113.76
31	UP	1001	CYC	CAA-C2A-C1A	3.02	130.36	125.01
31	wP	1001	CYC	CAA-C2A-C1A	3.02	130.36	125.01
29	K3	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
29	KO	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
29	F7	1002	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
29	fB	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	fM	201	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	BG	201	PEB	CHB-C4B-NB	-3.02	124.63	128.83
29	BQ	201	PEB	CHB-C4B-NB	-3.02	124.63	128.83
31	oP	1001	CYC	CAA-C2A-C1A	3.02	130.36	125.01
31	L7	1001	CYC	CAD-CBD-CGD	-3.02	105.29	113.76
29	I4	201	PEB	OA-C1A-C2A	-3.02	123.77	126.17
29	A7	301	PEB	OA-C1A-C2A	-3.02	123.77	126.17
29	A9	301	PEB	OA-C1A-C2A	-3.02	123.77	126.17
29	UJ	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	UL	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	g7	201	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	g9	201	PEB	CHA-C1B-NB	-3.02	118.61	124.93
31	J7	1001	CYC	CAD-CBD-CGD	-3.02	105.29	113.76
29	OF	202	PEB	CAA-C3A-C2A	-3.02	106.71	114.26
29	OI	202	PEB	CAA-C3A-C2A	-3.02	106.71	114.26
29	hF	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	hI	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	B3	203	PEB	CHC-C4C-C3C	-3.02	125.18	130.34
29	BO	203	PEB	CHC-C4C-C3C	-3.02	125.18	130.34
29	I5	202	PEB	CMB-C2B-C1B	3.02	129.72	125.06
29	P7	201	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	P9	201	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	mF	202	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	mI	202	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	LB	203	PEB	CHC-C4C-C3C	-3.02	125.19	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LM	203	PEB	CHC-C4C-C3C	-3.02	125.19	130.34
29	JG	201	PEB	CHB-C4B-NB	-3.02	124.64	128.83
29	JQ	201	PEB	CHB-C4B-NB	-3.02	124.64	128.83
29	iF	202	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	iI	202	PEB	CHA-C1B-NB	-3.02	118.61	124.93
29	ID	202	PEB	CHA-C4A-NA	-3.02	121.61	125.20
29	J5	202	PEB	CAB-CBB-CGB	-3.02	107.10	113.60
29	J8	202	PEB	CAB-CBB-CGB	-3.02	107.10	113.60
29	PF	202	PEB	CHA-C1B-NB	-3.02	118.62	124.93
29	PI	202	PEB	CHA-C1B-NB	-3.02	118.62	124.93
29	C5	202	PEB	CMB-C2B-C1B	3.02	129.71	125.06
29	C8	202	PEB	CMB-C2B-C1B	3.02	129.71	125.06
31	OP	1001	CYC	CAA-C2A-C1A	3.02	130.35	125.01
31	QP	1001	CYC	CAA-C2A-C1A	3.02	130.35	125.01
29	UF	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	UI	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	KD	201	PEB	OA-C1A-C2A	-3.02	123.77	126.17
29	FD	202	PEB	C2A-C1A-NA	3.02	110.88	108.27
29	G3	202	PEB	CMB-C2B-C1B	3.02	129.71	125.06
29	GO	202	PEB	CMB-C2B-C1B	3.02	129.71	125.06
29	F5	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	A5	201	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
29	A8	201	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
29	A5	202	PEB	CMB-C2B-C1B	3.02	129.71	125.06
29	RF	201	PEB	CHB-C4B-NB	-3.02	124.64	128.83
29	RI	201	PEB	CHB-C4B-NB	-3.02	124.64	128.83
29	LA	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	LN	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
31	G7	1001	CYC	C2A-C1A-NA	3.02	114.44	110.05
29	C4	201	PEB	OA-C1A-C2A	-3.02	123.77	126.17
29	AM	303	PEB	C1B-C2B-C3B	-3.02	103.04	106.51
29	AC	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	AE	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	bF	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	bI	202	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
29	lF	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	lI	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
30	A1	305	PUB	C2C-C1C-NC	3.02	114.44	110.05
30	AK	305	PUB	C2C-C1C-NC	3.02	114.44	110.05
29	Q1	201	PEB	CHA-C1B-C2B	3.02	132.66	124.90
29	U1	202	PEB	CHA-C1B-C2B	3.02	132.66	124.90
29	QK	201	PEB	CHA-C1B-C2B	3.02	132.66	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UK	202	PEB	CHA-C1B-C2B	3.02	132.66	124.90
30	xL	304	PUB	CMD-C2D-C3D	3.02	132.29	127.77
29	UF	201	PEB	CHA-C1B-NB	-3.02	118.62	124.93
29	eF	202	PEB	CHA-C1B-NB	-3.02	118.62	124.93
29	UI	201	PEB	CHA-C1B-NB	-3.02	118.62	124.93
29	eI	202	PEB	CHA-C1B-NB	-3.02	118.62	124.93
29	G4	202	PEB	CHA-C4A-NA	-3.02	121.62	125.20
31	vP	1001	CYC	OC-C1C-C2C	-3.02	123.78	126.17
29	Q2	201	PEB	CHC-C1D-ND	3.02	117.45	113.95
29	H5	203	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	F8	202	PEB	C3B-C4B-NB	3.02	114.44	110.05
29	l7	202	PEB	CMB-C2B-C1B	3.01	129.71	125.06
29	l9	202	PEB	CMB-C2B-C1B	3.01	129.71	125.06
29	QB	203	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	QM	203	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	V7	201	PEB	CHA-C1B-NB	-3.01	118.63	124.93
29	V9	201	PEB	CHA-C1B-NB	-3.01	118.63	124.93
31	K7	1001	CYC	C2A-C1A-NA	3.01	114.43	110.05
29	K4	202	PEB	CHA-C4A-NA	-3.01	121.62	125.20
29	QF	202	PEB	CMB-C2B-C1B	3.01	129.71	125.06
29	QI	202	PEB	CMB-C2B-C1B	3.01	129.71	125.06
29	HA	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
29	KC	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
29	KE	202	PEB	OD-C4D-ND	-3.01	121.47	125.93
29	HN	201	PEB	OD-C4D-ND	-3.01	121.47	125.93
29	JD	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
31	D7	1001	CYC	CAD-CBD-CGD	-3.01	105.31	113.76
31	D9	1001	CYC	CAD-CBD-CGD	-3.01	105.31	113.76
29	LG	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	D3	203	PEB	CHC-C4C-C3C	-3.01	125.20	130.34
29	DO	203	PEB	CHC-C4C-C3C	-3.01	125.20	130.34
29	KD	202	PEB	CHA-C4A-NA	-3.01	121.62	125.20
29	VF	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
29	VI	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
30	MA	402	PUB	CMD-C2D-C3D	3.01	132.29	127.77
29	QF	202	PEB	CAA-C3A-C2A	-3.01	106.73	114.26
29	QI	202	PEB	CAA-C3A-C2A	-3.01	106.73	114.26
29	aF	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
29	aI	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
29	A3	202	PEB	CHC-C1D-ND	-3.01	110.45	113.95
29	AO	202	PEB	CHC-C1D-ND	-3.01	110.45	113.95
29	HA	203	PEB	C3B-C4B-NB	3.01	114.43	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SF	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	SI	202	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	HN	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	UB	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	QF	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	QI	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	UM	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
31	H7	1001	CYC	CAD-CBD-CGD	-3.01	105.31	113.76
31	H9	1001	CYC	CAD-CBD-CGD	-3.01	105.31	113.76
31	kP	1001	CYC	C2B-C1B-NB	3.01	111.40	106.99
29	DO	202	PEB	CHC-C4C-C3C	-3.01	125.20	130.34
29	ZF	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
29	ZI	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
29	PF	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
29	PI	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
31	CP	1001	CYC	CHA-C1A-NA	-3.01	124.65	128.83
29	dB	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	dM	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	IA	202	PEB	CHB-C4B-C3B	3.01	132.28	125.32
29	IN	202	PEB	CHB-C4B-C3B	3.01	132.28	125.32
29	B8	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
31	BP	1001	CYC	CAA-C2A-C1A	3.01	130.34	125.01
29	xJ	303	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	d1	201	PEB	CHA-C1B-C2B	3.01	132.64	124.90
29	dK	201	PEB	CHA-C1B-C2B	3.01	132.64	124.90
29	B8	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
29	jF	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
29	jI	202	PEB	CMB-C2B-C1B	3.01	129.70	125.06
29	H8	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	LB	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	LM	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
31	G9	1001	CYC	C2A-C1A-NA	3.01	114.43	110.05
29	DF	1002	PEB	C2A-C1A-NA	3.01	110.87	108.27
29	DI	1002	PEB	C2A-C1A-NA	3.01	110.87	108.27
29	NO	203	PEB	C2A-C1A-NA	3.01	110.87	108.27
29	E3	202	PEB	CHC-C1D-ND	-3.01	110.45	113.95
29	QB	203	PEB	CHC-C1D-ND	-3.01	110.45	113.95
29	QM	203	PEB	CHC-C1D-ND	-3.01	110.45	113.95
29	EO	202	PEB	CHC-C1D-ND	-3.01	110.45	113.95
29	WR	201	PEB	CHC-C1D-ND	3.01	117.44	113.95
29	CG	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51
29	CQ	202	PEB	C1B-C2B-C3B	-3.01	103.05	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BA	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
29	BN	203	PEB	C3B-C4B-NB	3.01	114.43	110.05
31	C7	1001	CYC	C2A-C1A-NA	3.01	114.43	110.05
31	C9	1001	CYC	C2A-C1A-NA	3.01	114.43	110.05
31	qP	1001	CYC	CAA-C2A-C1A	3.01	130.33	125.01
29	YB	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	YM	202	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	M4	202	PEB	CHA-C4A-NA	-3.01	121.63	125.20
29	NO	201	PEB	C3B-C4B-NB	3.01	114.42	110.05
29	kF	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
29	kI	201	PEB	CHB-C4B-NB	-3.01	124.65	128.83
31	HK	1001	CYC	C2C-C1C-NC	3.01	110.87	108.27
31	fP	1001	CYC	C2B-C1B-NB	3.01	111.39	106.99
31	SP	1001	CYC	CAA-C2A-C1A	3.01	130.33	125.01
29	WB	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
29	WM	201	PEB	C4B-C3B-C2B	-3.01	103.45	106.78
31	F9	1001	CYC	CAD-CBD-CGD	-3.01	105.33	113.76
29	KA	202	PEB	CHB-C4B-C3B	3.01	132.27	125.32
29	KN	202	PEB	CHB-C4B-C3B	3.01	132.27	125.32
29	eF	201	PEB	CHB-C4B-NB	-3.01	124.66	128.83
29	eI	201	PEB	CHB-C4B-NB	-3.01	124.66	128.83
31	XP	1001	CYC	CAA-C2A-C1A	3.01	130.33	125.01
29	C8	201	PEB	C1B-C2B-C3B	-3.01	103.06	106.51
29	GA	202	PEB	CHB-C4B-C3B	3.01	132.27	125.32
29	GN	202	PEB	CHB-C4B-C3B	3.01	132.27	125.32
31	DP	1001	CYC	C2B-C1B-NB	3.01	111.39	106.99
29	hB	201	PEB	C4B-C3B-C2B	-3.01	103.46	106.78
29	jB	201	PEB	C4B-C3B-C2B	-3.01	103.46	106.78
29	hM	201	PEB	C4B-C3B-C2B	-3.01	103.46	106.78
29	jM	201	PEB	C4B-C3B-C2B	-3.01	103.46	106.78
29	b1	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	bK	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	OF	202	PEB	C3B-C4B-NB	3.01	114.42	110.05
29	OI	202	PEB	C3B-C4B-NB	3.01	114.42	110.05
31	lP	1001	CYC	CHA-C1A-NA	-3.01	124.66	128.83
29	S1	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	h1	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	j1	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	SK	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	hK	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	jK	201	PEB	CHA-C1B-C2B	3.01	132.63	124.90
29	hF	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	hI	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	DB	203	PEB	C3B-C4B-NB	3.00	114.42	110.05
29	DM	203	PEB	C3B-C4B-NB	3.00	114.42	110.05
29	KG	202	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
29	KQ	202	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
29	IB	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	IM	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	lB	201	PEB	CHC-C1D-ND	-3.00	110.46	113.95
29	lM	201	PEB	CHC-C1D-ND	-3.00	110.46	113.95
30	A1	305	PUB	CHC-C1D-ND	-3.00	109.92	113.72
30	AK	305	PUB	CHC-C1D-ND	-3.00	109.92	113.72
31	yP	1001	CYC	C2C-C3C-C4C	3.00	105.84	101.34
29	gF	202	PEB	CHA-C1B-NB	-3.00	118.65	124.93
29	gI	202	PEB	CHA-C1B-NB	-3.00	118.65	124.93
29	G5	203	PEB	C3B-C4B-NB	3.00	114.42	110.05
29	H5	202	PEB	C3B-C4B-NB	3.00	114.42	110.05
31	E7	1001	CYC	C2A-C1A-NA	3.00	114.42	110.05
31	E9	1001	CYC	C2A-C1A-NA	3.00	114.42	110.05
29	I3	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
29	IO	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
29	fF	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	fI	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	CC	202	PEB	OD-C4D-C3D	-3.00	122.66	129.46
29	CE	202	PEB	OD-C4D-C3D	-3.00	122.66	129.46
29	OF	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	OI	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
31	PP	1001	CYC	OC-C1C-C2C	-3.00	123.79	126.17
29	ED	202	PEB	CMB-C2B-C1B	3.00	129.69	125.06
31	N7	1001	CYC	CAD-CBD-CGD	-3.00	105.34	113.76
31	N9	1001	CYC	CAD-CBD-CGD	-3.00	105.34	113.76
29	K3	201	PEB	CHB-C4B-NB	-3.00	124.66	128.83
29	KO	201	PEB	CHB-C4B-NB	-3.00	124.66	128.83
29	F3	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
29	FO	201	PEB	C2A-C1A-NA	3.00	110.86	108.27
29	lF	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	lI	202	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
31	jP	1001	CYC	C2B-C1B-NB	3.00	111.38	106.99
29	QF	202	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	QI	202	PEB	C3B-C4B-NB	3.00	114.41	110.05
31	GP	1001	CYC	OC-C1C-C2C	-3.00	123.79	126.17
29	GC	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
29	GE	201	PEB	OD-C4D-ND	-3.00	121.49	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZB	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	ZM	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	C4	201	PEB	C1B-C2B-C3B	-3.00	103.06	106.51
29	CB	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	GB	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	MB	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	CM	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	GM	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	MM	201	PEB	C4B-C3B-C2B	-3.00	103.46	106.78
29	MN	405	PEB	CHC-C4C-C3C	-3.00	125.22	130.34
31	tP	1001	CYC	CHA-C1A-NA	-3.00	124.67	128.83
31	I7	1001	CYC	C2A-C1A-NA	3.00	114.41	110.05
31	I9	1001	CYC	C2A-C1A-NA	3.00	114.41	110.05
29	CB	201	PEB	CHC-C1D-ND	-3.00	110.47	113.95
29	CM	201	PEB	CHC-C1D-ND	-3.00	110.47	113.95
29	GC	202	PEB	OD-C4D-C3D	-3.00	122.67	129.46
29	GE	202	PEB	OD-C4D-C3D	-3.00	122.67	129.46
29	H4	202	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
31	oP	1001	CYC	C2B-C1B-NB	3.00	111.38	106.99
29	DA	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	HB	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	HM	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	DN	203	PEB	C3B-C4B-NB	3.00	114.41	110.05
29	IC	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
29	IE	201	PEB	OD-C4D-ND	-3.00	121.49	125.93
29	G3	201	PEB	OA-C1A-C2A	-3.00	123.79	126.17
29	GO	201	PEB	OA-C1A-C2A	-3.00	123.79	126.17
29	AG	202	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
29	AQ	202	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
29	H5	203	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
29	OB	201	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
29	OM	201	PEB	C4B-C3B-C2B	-3.00	103.47	106.78
29	O1	201	PEB	CHA-C1B-C2B	3.00	132.61	124.90
29	OK	201	PEB	CHA-C1B-C2B	3.00	132.61	124.90
31	vP	1001	CYC	CHA-C1A-NA	-3.00	124.67	128.83
29	HD	202	PEB	C2A-C1A-NA	3.00	110.86	108.27
30	xJ	304	PUB	CMD-C2D-C3D	3.00	132.26	127.77
29	CD	201	PEB	C1B-C2B-C3B	-3.00	103.07	106.51
29	MA	405	PEB	OD-C4D-C3D	-3.00	122.67	129.46
29	W1	201	PEB	CHA-C1B-C2B	3.00	132.60	124.90
29	WK	201	PEB	CHA-C1B-C2B	3.00	132.60	124.90
29	OF	202	PEB	CMB-C2B-C1B	3.00	129.68	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	OI	202	PEB	CMB-C2B-C1B	3.00	129.68	125.06
29	AM	302	PEB	OD-C4D-C3D	-3.00	122.67	129.46
29	IB	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	IM	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
31	XP	1001	CYC	C2B-C1B-NB	2.99	111.37	106.99
31	pP	1001	CYC	OC-C1C-C2C	-2.99	123.79	126.17
29	AC	202	PEB	OD-C4D-C3D	-2.99	122.67	129.46
29	AE	202	PEB	OD-C4D-C3D	-2.99	122.67	129.46
31	eP	1001	CYC	CHA-C1A-NA	-2.99	124.67	128.83
29	WF	202	PEB	CMB-C2B-C1B	2.99	129.68	125.06
29	WI	202	PEB	CMB-C2B-C1B	2.99	129.68	125.06
29	HB	203	PEB	CHA-C4A-NA	-2.99	121.64	125.20
29	HM	203	PEB	CHA-C4A-NA	-2.99	121.64	125.20
29	SF	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	SI	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	EC	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
29	EE	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
31	qP	1001	CYC	C2B-C1B-NB	2.99	111.37	106.99
31	jP	1001	CYC	CAA-C2A-C1A	2.99	130.30	125.01
29	AC	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
29	AE	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
29	cF	201	PEB	CHB-C4B-NB	-2.99	124.67	128.83
29	cI	201	PEB	CHB-C4B-NB	-2.99	124.67	128.83
31	PP	1001	CYC	CHA-C1A-NA	-2.99	124.67	128.83
29	fI	201	PEB	CHA-C1B-C2B	2.99	132.60	124.90
29	fK	201	PEB	CHA-C1B-C2B	2.99	132.60	124.90
29	dB	201	PEB	CHC-C1D-ND	-2.99	110.47	113.95
29	dM	201	PEB	CHC-C1D-ND	-2.99	110.47	113.95
29	EC	202	PEB	OD-C4D-C3D	-2.99	122.68	129.46
29	EE	202	PEB	OD-C4D-C3D	-2.99	122.68	129.46
29	EB	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	EM	201	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
31	SP	1001	CYC	C2B-C1B-NB	2.99	111.37	106.99
31	JP	1001	CYC	OC-C1C-C2C	-2.99	123.79	126.17
29	BD	201	PEB	C1C-CHB-C4B	-2.99	125.23	128.81
29	F3	203	PEB	CHC-C4C-C3C	-2.99	125.23	130.34
29	FO	203	PEB	CHC-C4C-C3C	-2.99	125.23	130.34
29	TB	203	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	iB	203	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	TM	203	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	iM	203	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	f7	201	PEB	OD-C4D-C3D	-2.99	122.68	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f9	201	PEB	OD-C4D-C3D	-2.99	122.68	129.46
31	F7	1001	CYC	CAD-CBD-CGD	-2.99	105.37	113.76
29	PR	202	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	jF	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	jI	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
30	A1	304	PUB	OA-C1A-NA	-2.99	121.50	125.93
30	AK	304	PUB	OA-C1A-NA	-2.99	121.50	125.93
29	E3	202	PEB	CMB-C2B-C1B	2.99	129.67	125.06
29	EO	202	PEB	CMB-C2B-C1B	2.99	129.67	125.06
29	aB	201	PEB	CHC-C1D-ND	-2.99	110.47	113.95
29	aM	201	PEB	CHC-C1D-ND	-2.99	110.47	113.95
29	ZB	203	PEB	CHA-C4A-NA	-2.99	121.65	125.20
29	ZM	203	PEB	CHA-C4A-NA	-2.99	121.65	125.20
29	E3	201	PEB	OA-C1A-C2A	-2.99	123.80	126.17
29	EO	201	PEB	OA-C1A-C2A	-2.99	123.80	126.17
31	RP	1001	CYC	OC-C1C-C2C	-2.99	123.80	126.17
31	TP	1001	CYC	OC-C1C-C2C	-2.99	123.80	126.17
29	UF	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	dF	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	UI	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	dI	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
29	K4	201	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
29	K5	201	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
29	K8	201	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
29	KD	201	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
29	ZF	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	ZI	202	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	E3	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
29	EO	202	PEB	C2A-C1A-NA	2.99	110.85	108.27
29	gB	203	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	gM	203	PEB	C3B-C4B-NB	2.99	114.40	110.05
29	L8	203	PEB	C4B-C3B-C2B	-2.99	103.47	106.78
31	K9	1001	CYC	C2A-C1A-NA	2.99	114.40	110.05
29	k1	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	kK	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	M4	203	PEB	C1B-C2B-C3B	-2.99	103.08	106.51
31	nP	1001	CYC	CAA-C2A-C1A	2.99	130.29	125.01
29	L5	203	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
29	c1	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
29	cK	201	PEB	OD-C4D-ND	-2.99	121.50	125.93
29	MN	405	PEB	OD-C4D-C3D	-2.99	122.69	129.46
29	a1	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aK	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	EA	201	PEB	OA-C1A-C2A	-2.99	123.80	126.17
29	EN	201	PEB	OA-C1A-C2A	-2.99	123.80	126.17
31	cP	1001	CYC	OC-C1C-C2C	-2.99	123.80	126.17
29	JA	203	PEB	C3B-C4B-NB	2.99	114.39	110.05
29	eB	202	PEB	C3B-C4B-NB	2.99	114.39	110.05
29	eM	202	PEB	C3B-C4B-NB	2.99	114.39	110.05
29	JN	203	PEB	C3B-C4B-NB	2.99	114.39	110.05
30	wJ	304	PUB	CMD-C2D-C3D	2.99	132.25	127.77
29	Z1	202	PEB	CHA-C1B-C2B	2.99	132.58	124.90
29	ZK	202	PEB	CHA-C1B-C2B	2.99	132.58	124.90
29	AB	302	PEB	OD-C4D-C3D	-2.99	122.69	129.46
29	H3	203	PEB	CHC-C4C-C3C	-2.99	125.24	130.34
29	HO	203	PEB	CHC-C4C-C3C	-2.99	125.24	130.34
31	TP	1001	CYC	CHA-C1A-NA	-2.99	124.68	128.83
29	P1	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	PK	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	FD	201	PEB	C1C-CHB-C4B	-2.99	125.24	128.81
31	HP	1001	CYC	C2B-C1B-NB	2.99	111.36	106.99
31	nP	1001	CYC	C2B-C1B-NB	2.99	111.36	106.99
31	wP	1001	CYC	C2B-C1B-NB	2.99	111.36	106.99
29	DD	202	PEB	C4B-C3B-C2B	-2.99	103.48	106.78
29	E3	201	PEB	CHB-C4B-NB	-2.99	124.69	128.83
29	EO	201	PEB	CHB-C4B-NB	-2.99	124.69	128.83
29	IF	202	PEB	CMB-C2B-C1B	2.99	129.66	125.06
29	II	202	PEB	CMB-C2B-C1B	2.99	129.66	125.06
29	EB	201	PEB	CHC-C1D-ND	-2.99	110.48	113.95
29	EM	201	PEB	CHC-C1D-ND	-2.99	110.48	113.95
29	Q7	201	PEB	OD-C4D-C3D	-2.99	122.69	129.46
29	Q9	201	PEB	OD-C4D-C3D	-2.99	122.69	129.46
29	AM	301	PEB	CMB-C2B-C1B	2.99	129.66	125.06
29	e1	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	eK	201	PEB	CHB-C4B-C3B	-2.99	118.42	125.32
29	J5	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
29	J8	201	PEB	OD-C4D-ND	-2.98	121.51	125.93
29	H8	203	PEB	C4B-C3B-C2B	-2.98	103.48	106.78
29	N3	201	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	zJ	501	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	IC	202	PEB	OD-C4D-C3D	-2.98	122.70	129.46
29	IE	202	PEB	OD-C4D-C3D	-2.98	122.70	129.46
29	ID	201	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
31	lP	1001	CYC	OC-C1C-C2C	-2.98	123.80	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I3	201	PEB	CHB-C4B-NB	-2.98	124.69	128.83
29	IO	201	PEB	CHB-C4B-NB	-2.98	124.69	128.83
31	iP	1001	CYC	CHA-C1A-NA	-2.98	124.69	128.83
29	L5	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	l1	201	PEB	CHA-C1B-C2B	2.98	132.57	124.90
29	lK	201	PEB	CHA-C1B-C2B	2.98	132.57	124.90
31	hP	1001	CYC	CAA-C2A-C1A	2.98	130.29	125.01
31	UP	1001	CYC	C2B-C1B-NB	2.98	111.36	106.99
29	A3	202	PEB	CMB-C2B-C1B	2.98	129.66	125.06
29	fF	202	PEB	CMB-C2B-C1B	2.98	129.66	125.06
29	fI	202	PEB	CMB-C2B-C1B	2.98	129.66	125.06
29	AO	202	PEB	CMB-C2B-C1B	2.98	129.66	125.06
29	PB	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	PM	202	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	hF	202	PEB	CMB-C2B-C1B	2.98	129.66	125.06
29	hI	202	PEB	CMB-C2B-C1B	2.98	129.66	125.06
29	IG	202	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
29	IQ	202	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
29	G8	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	FA	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	cB	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	cM	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
29	FN	203	PEB	C3B-C4B-NB	2.98	114.39	110.05
31	FP	1001	CYC	C2B-C1B-NB	2.98	111.35	106.99
31	OP	1001	CYC	C2B-C1B-NB	2.98	111.35	106.99
29	I4	203	PEB	C1B-C2B-C3B	-2.98	103.08	106.51
29	AB	301	PEB	CMB-C2B-C1B	2.98	129.66	125.06
31	hP	1001	CYC	C2B-C1B-NB	2.98	111.35	106.99
29	J5	202	PEB	CHA-C1B-NB	-2.98	118.70	124.93
29	J8	202	PEB	CHA-C1B-NB	-2.98	118.70	124.93
31	1P	1001	CYC	CAA-C2A-C1A	2.98	130.28	125.01
31	MF	1001	CYC	OB-C4B-C3B	-2.98	124.81	128.04
31	MI	1001	CYC	OB-C4B-C3B	-2.98	124.81	128.04
29	T1	201	PEB	OD-C4D-ND	-2.98	121.52	125.93
29	TK	201	PEB	OD-C4D-ND	-2.98	121.52	125.93
29	E4	202	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
29	IA	201	PEB	CHC-C4C-C3C	-2.98	125.25	130.34
29	IN	201	PEB	CHC-C4C-C3C	-2.98	125.25	130.34
29	V1	201	PEB	CHB-C4B-C3B	-2.98	118.44	125.32
29	Y1	201	PEB	CHB-C4B-C3B	-2.98	118.44	125.32
29	VK	201	PEB	CHB-C4B-C3B	-2.98	118.44	125.32
29	YK	201	PEB	CHB-C4B-C3B	-2.98	118.44	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	wL	304	PUB	CMD-C2D-C3D	2.98	132.24	127.77
29	K3	201	PEB	OA-C1A-C2A	-2.98	123.80	126.17
29	M4	201	PEB	OA-C1A-C2A	-2.98	123.80	126.17
29	KO	201	PEB	OA-C1A-C2A	-2.98	123.80	126.17
29	C5	201	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
29	j1	203	PEB	C2A-C1A-NA	2.98	110.84	108.27
29	jK	203	PEB	C2A-C1A-NA	2.98	110.84	108.27
29	F8	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
29	SB	201	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
29	SM	201	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
29	J1	1002	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	I3	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	JK	1002	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	IO	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
31	WP	1001	CYC	C2C-C3C-C4C	2.98	105.80	101.34
29	F5	203	PEB	C3B-C4B-NB	2.98	114.38	110.05
29	XB	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
29	XM	202	PEB	C3B-C4B-NB	2.98	114.38	110.05
29	B5	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	OB	202	PEB	CHC-C1D-ND	-2.98	110.49	113.95
29	OM	202	PEB	CHC-C1D-ND	-2.98	110.49	113.95
31	rP	1001	CYC	CHA-C1A-NA	-2.98	124.70	128.83
29	G5	203	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
29	CD	202	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
29	AM	302	PEB	C1B-C2B-C3B	-2.98	103.09	106.51
29	C3	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	dF	203	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	dI	203	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	CO	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	gB	201	PEB	CAB-CBB-CGB	-2.98	107.20	113.60
29	gM	201	PEB	CAB-CBB-CGB	-2.98	107.20	113.60
29	C3	201	PEB	CHB-C4B-NB	-2.98	124.70	128.83
29	CO	201	PEB	CHB-C4B-NB	-2.98	124.70	128.83
29	KC	203	PEB	OD-C4D-C3D	-2.98	122.72	129.46
29	KE	203	PEB	OD-C4D-C3D	-2.98	122.72	129.46
29	VR	203	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
31	EP	1001	CYC	CHA-C1A-NA	-2.98	124.70	128.83
29	K3	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	KO	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
30	AM	305	PUB	CBA-CAA-C3A	-2.98	108.47	112.98
29	uJ	201	PEB	C1C-CHB-C4B	2.98	132.36	128.81
29	uL	201	PEB	C1C-CHB-C4B	2.98	132.36	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R2	203	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
29	RR	203	PEB	C4B-C3B-C2B	-2.98	103.49	106.78
30	AB	304	PUB	CAC-CBC-CGC	-2.98	107.20	113.60
31	EF	1001	CYC	OB-C4B-C3B	-2.98	124.81	128.04
31	KF	1001	CYC	OB-C4B-C3B	-2.98	124.81	128.04
31	EI	1001	CYC	OB-C4B-C3B	-2.98	124.81	128.04
31	RP	1001	CYC	CHA-C1A-NA	-2.98	124.70	128.83
29	zL	501	PEB	CHC-C1D-ND	-2.98	110.49	113.95
29	K5	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	K8	202	PEB	CMB-C2B-C1B	2.98	129.65	125.06
29	T1	201	PEB	CHB-C4B-C3B	-2.98	118.45	125.32
29	TK	201	PEB	CHB-C4B-C3B	-2.98	118.45	125.32
29	i1	201	PEB	CHB-C4B-C3B	-2.97	118.45	125.32
29	iK	201	PEB	CHB-C4B-C3B	-2.97	118.45	125.32
29	G3	201	PEB	CHB-C4B-NB	-2.97	124.70	128.83
29	GO	201	PEB	CHB-C4B-NB	-2.97	124.70	128.83
29	A7	304	PEB	C2A-C1A-NA	2.97	110.84	108.27
29	XB	202	PEB	CHA-C4A-NA	-2.97	121.67	125.20
29	XM	202	PEB	CHA-C4A-NA	-2.97	121.67	125.20
29	b7	201	PEB	OD-C4D-C3D	-2.97	122.72	129.46
29	b9	201	PEB	OD-C4D-C3D	-2.97	122.72	129.46
29	B8	203	PEB	C4B-C3B-C2B	-2.97	103.49	106.78
29	FB	203	PEB	C3B-C4B-NB	2.97	114.37	110.05
29	FM	203	PEB	C3B-C4B-NB	2.97	114.37	110.05
29	k1	202	PEB	C2A-C1A-NA	2.97	110.84	108.27
29	kK	202	PEB	C2A-C1A-NA	2.97	110.84	108.27
29	MJ	201	PEB	CAB-C3B-C4B	2.97	130.27	125.01
29	ML	201	PEB	CAB-C3B-C4B	2.97	130.27	125.01
31	K7	1001	CYC	C4D-CHA-C1A	2.97	132.36	128.81
29	TB	201	PEB	CHA-C1B-NB	-2.97	118.72	124.93
29	TM	201	PEB	CHA-C1B-NB	-2.97	118.72	124.93
29	I3	203	PEB	CAC-CBC-CGC	-2.97	105.43	113.76
29	IO	203	PEB	CAC-CBC-CGC	-2.97	105.43	113.76
30	yJ	302	PUB	CAB-CBB-CGB	-2.97	105.43	113.76
30	yL	302	PUB	CAB-CBB-CGB	-2.97	105.43	113.76
29	F9	1002	PEB	C1B-C2B-C3B	-2.97	103.09	106.51
30	MN	402	PUB	CMD-C2D-C3D	2.97	132.23	127.77
29	CC	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
29	CE	201	PEB	OD-C4D-ND	-2.97	121.53	125.93
29	bF	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
29	bI	202	PEB	CMB-C2B-C1B	2.97	129.64	125.06
29	NK	1002	PEB	CMB-C2B-C1B	2.97	129.64	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AP	1001	CYC	CHA-C1A-NA	-2.97	124.70	128.83
31	iP	1001	CYC	OC-C1C-C2C	-2.97	123.81	126.17
29	jF	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
29	jI	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
29	M3	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
29	MO	201	PEB	C3B-C4B-NB	2.97	114.37	110.05
31	pP	1001	CYC	CHA-C1A-NA	-2.97	124.71	128.83
29	d7	201	PEB	OD-C4D-C3D	-2.97	122.73	129.46
29	d9	201	PEB	OD-C4D-C3D	-2.97	122.73	129.46
29	E4	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
29	ZF	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
29	ZI	202	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
29	AA	201	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
29	AN	201	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
29	G4	201	PEB	OA-C1A-C2A	-2.97	123.81	126.17
29	GD	201	PEB	OA-C1A-C2A	-2.97	123.81	126.17
29	kB	203	PEB	C3B-C4B-NB	2.97	114.37	110.05
29	kM	203	PEB	C3B-C4B-NB	2.97	114.37	110.05
29	L7	1002	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
30	AM	304	PUB	CAC-CBC-CGC	-2.97	107.21	113.60
31	IP	1001	CYC	C2B-C1B-NB	2.97	111.33	106.99
29	TR	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
29	KB	202	PEB	CHC-C1D-ND	-2.97	110.50	113.95
29	KM	202	PEB	CHC-C1D-ND	-2.97	110.50	113.95
29	KA	201	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
29	KN	201	PEB	CHC-C4C-C3C	-2.97	125.27	130.34
29	SJ	201	PEB	CAB-C3B-C4B	2.97	130.26	125.01
29	SL	201	PEB	CAB-C3B-C4B	2.97	130.26	125.01
29	RB	201	PEB	CHA-C1B-NB	-2.97	118.72	124.93
29	RM	201	PEB	CHA-C1B-NB	-2.97	118.72	124.93
29	GG	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
29	GQ	202	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
29	LB	201	PEB	CAB-CBB-CGB	-2.97	107.22	113.60
29	LM	201	PEB	CAB-CBB-CGB	-2.97	107.22	113.60
31	VP	1001	CYC	C1B-C2B-C3B	-2.97	104.77	107.87
29	g1	201	PEB	CHB-C4B-C3B	-2.97	118.47	125.32
29	gK	201	PEB	CHB-C4B-C3B	-2.97	118.47	125.32
29	j7	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
29	l7	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
29	j9	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
29	l9	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
29	RB	203	PEB	C3B-C4B-NB	2.97	114.36	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	RM	203	PEB	C3B-C4B-NB	2.97	114.36	110.05
29	mJ	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
29	mL	202	PEB	OD-C4D-ND	-2.97	121.53	125.93
29	E4	202	PEB	CHA-C4A-NA	-2.97	121.68	125.20
29	JB	203	PEB	C3B-C4B-NB	2.97	114.36	110.05
29	JM	203	PEB	C3B-C4B-NB	2.97	114.36	110.05
29	GD	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
29	c1	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	e1	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	i1	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	AF	304	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	AI	304	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	cK	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	eK	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	iK	202	PEB	C2A-C1A-NA	2.97	110.83	108.27
29	A1	303	PEB	OD-C4D-ND	-2.97	121.54	125.93
29	AK	303	PEB	OD-C4D-ND	-2.97	121.54	125.93
31	KI	1001	CYC	OB-C4B-C3B	-2.97	124.82	128.04
29	PB	201	PEB	CAB-CBB-CGB	-2.97	107.22	113.60
29	PM	201	PEB	CAB-CBB-CGB	-2.97	107.22	113.60
29	N1	1002	PEB	CMB-C2B-C1B	2.97	129.63	125.06
31	L7	1001	CYC	OC-C1C-C2C	-2.97	123.81	126.17
29	G4	201	PEB	C1B-C2B-C3B	-2.97	103.10	106.51
29	Z7	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
29	Z9	201	PEB	OD-C4D-C3D	-2.97	122.74	129.46
29	V2	203	PEB	C4B-C3B-C2B	-2.97	103.50	106.78
29	W7	201	PEB	OD-C4D-C3D	-2.96	122.74	129.46
29	W9	201	PEB	OD-C4D-C3D	-2.96	122.74	129.46
29	mB	203	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	mM	203	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	RB	203	PEB	CHA-C4A-NA	-2.96	121.68	125.20
29	RM	203	PEB	CHA-C4A-NA	-2.96	121.68	125.20
29	mB	201	PEB	CAB-CBB-CGB	-2.96	107.22	113.60
29	mM	201	PEB	CAB-CBB-CGB	-2.96	107.22	113.60
29	O7	201	PEB	OD-C4D-C3D	-2.96	122.74	129.46
29	O9	201	PEB	OD-C4D-C3D	-2.96	122.74	129.46
29	NJ	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	vJ	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	NL	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	vL	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	B4	201	PEB	C1C-CHB-C4B	-2.96	125.27	128.81
31	KP	1001	CYC	CHA-C1A-NA	-2.96	124.72	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NB	201	PEB	CHA-C1B-NB	-2.96	118.73	124.93
29	NM	201	PEB	CHA-C1B-NB	-2.96	118.73	124.93
29	xL	303	PEB	C2A-C1A-NA	2.96	110.83	108.27
29	LB	201	PEB	CHA-C1B-NB	-2.96	118.73	124.93
29	LM	201	PEB	CHA-C1B-NB	-2.96	118.73	124.93
30	AB	305	PUB	CBA-CAA-C3A	-2.96	108.48	112.98
29	BJ	202	PEB	C1C-CHB-C4B	2.96	132.35	128.81
29	BL	202	PEB	C1C-CHB-C4B	2.96	132.35	128.81
29	i1	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
29	iK	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
29	NB	201	PEB	CAB-CBB-CGB	-2.96	107.23	113.60
29	NM	201	PEB	CAB-CBB-CGB	-2.96	107.23	113.60
29	FJ	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
29	FL	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
29	h7	201	PEB	OD-C4D-C3D	-2.96	122.75	129.46
29	h9	201	PEB	OD-C4D-C3D	-2.96	122.75	129.46
29	UJ	201	PEB	CAB-C3B-C4B	2.96	130.25	125.01
29	UL	201	PEB	CAB-C3B-C4B	2.96	130.25	125.01
29	P7	201	PEB	CHC-C4C-C3C	-2.96	125.28	130.34
29	P9	201	PEB	CHC-C4C-C3C	-2.96	125.28	130.34
29	m1	201	PEB	CHB-C4B-C3B	-2.96	118.47	125.32
29	mK	201	PEB	CHB-C4B-C3B	-2.96	118.47	125.32
29	tJ	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	tL	201	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	L9	1002	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
31	BP	1001	CYC	C2B-C1B-NB	2.96	111.33	106.99
29	R7	201	PEB	CHC-C4C-C3C	-2.96	125.28	130.34
29	R9	201	PEB	CHC-C4C-C3C	-2.96	125.28	130.34
29	F5	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
29	F8	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
31	uP	1001	CYC	C2B-C1B-NB	2.96	111.32	106.99
29	PB	201	PEB	CHA-C1B-NB	-2.96	118.74	124.93
29	PM	201	PEB	CHA-C1B-NB	-2.96	118.74	124.93
29	DD	201	PEB	C1C-CHB-C4B	-2.96	125.27	128.81
29	XJ	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
29	XL	203	PEB	C4B-C3B-C2B	-2.96	103.50	106.78
29	U7	201	PEB	OD-C4D-C3D	-2.96	122.75	129.46
29	U9	201	PEB	OD-C4D-C3D	-2.96	122.75	129.46
29	F1	1002	PEB	CMB-C2B-C1B	2.96	129.62	125.06
29	FK	1002	PEB	CMB-C2B-C1B	2.96	129.62	125.06
29	VB	203	PEB	C3B-C4B-NB	2.96	114.36	110.05
29	VM	203	PEB	C3B-C4B-NB	2.96	114.36	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MB	202	PEB	CHC-C1D-ND	-2.96	110.51	113.95
29	MM	202	PEB	CHC-C1D-ND	-2.96	110.51	113.95
29	B3	202	PEB	CAC-CBC-CGC	-2.96	105.46	113.76
29	BO	202	PEB	CAC-CBC-CGC	-2.96	105.46	113.76
29	k1	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
29	kK	201	PEB	OD-C4D-ND	-2.96	121.54	125.93
29	eB	201	PEB	CHA-C1B-NB	-2.96	118.74	124.93
29	eM	201	PEB	CHA-C1B-NB	-2.96	118.74	124.93
29	N3	202	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	D7	1002	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	D9	1002	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	EG	202	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	EQ	202	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	dJ	202	PEB	C1C-CHB-C4B	2.96	132.34	128.81
29	dL	202	PEB	C1C-CHB-C4B	2.96	132.34	128.81
29	R1	201	PEB	CHB-C4B-C3B	-2.96	118.48	125.32
29	RK	201	PEB	CHB-C4B-C3B	-2.96	118.48	125.32
29	ED	201	PEB	CHA-C4A-NA	-2.96	121.69	125.20
29	L8	203	PEB	C3B-C4B-NB	2.96	114.35	110.05
29	QJ	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
29	QL	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
29	J7	1002	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	dD	401	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
29	M4	201	PEB	C1B-C2B-C3B	-2.96	103.11	106.51
31	JP	1001	CYC	CHA-C1A-NA	-2.96	124.72	128.83
29	wL	303	PEB	C2A-C1A-NA	2.96	110.82	108.27
29	HB	201	PEB	CAB-CBB-CGB	-2.96	107.24	113.60
29	HM	201	PEB	CAB-CBB-CGB	-2.96	107.24	113.60
31	GP	1001	CYC	CHA-C1A-NA	-2.96	124.72	128.83
29	J3	202	PEB	CAC-CBC-CGC	-2.96	105.47	113.76
29	JO	202	PEB	CAC-CBC-CGC	-2.96	105.47	113.76
29	HD	201	PEB	C1C-CHB-C4B	-2.96	125.28	128.81
29	SJ	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
29	SL	202	PEB	OD-C4D-ND	-2.96	121.55	125.93
29	B3	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
29	BO	202	PEB	CMB-C2B-C1B	2.96	129.62	125.06
29	IJ	201	PEB	CAB-C3B-C4B	2.96	130.24	125.01
29	IL	201	PEB	CAB-C3B-C4B	2.96	130.24	125.01
29	c1	201	PEB	CHB-C4B-C3B	-2.96	118.49	125.32
29	cK	201	PEB	CHB-C4B-C3B	-2.96	118.49	125.32
29	DJ	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
29	DL	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	kB	201	PEB	CHA-C1B-NB	-2.96	118.75	124.93
29	kM	201	PEB	CHA-C1B-NB	-2.96	118.75	124.93
30	yJ	302	PUB	CHA-C4A-NA	-2.96	110.52	113.95
30	yL	302	PUB	CHA-C4A-NA	-2.96	110.52	113.95
31	EP	1001	CYC	OC-C1C-C2C	-2.96	123.82	126.17
31	sP	1001	CYC	C2B-C1B-NB	2.96	111.31	106.99
29	D4	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
29	HD	202	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
31	G9	1001	CYC	C4D-CHA-C1A	2.96	132.34	128.81
29	wJ	302	PEB	C1B-C2B-C3B	-2.95	103.11	106.51
29	iB	201	PEB	CAB-CBB-CGB	-2.95	107.24	113.60
29	iM	201	PEB	CAB-CBB-CGB	-2.95	107.24	113.60
29	BC	201	PEB	C3B-C4B-NB	2.95	114.35	110.05
29	BE	201	PEB	C3B-C4B-NB	2.95	114.35	110.05
29	V1	201	PEB	OD-C4D-ND	-2.95	121.55	125.93
29	VK	201	PEB	OD-C4D-ND	-2.95	121.55	125.93
29	U1	201	PEB	C2A-C1A-NA	2.95	110.82	108.27
29	UK	201	PEB	C2A-C1A-NA	2.95	110.82	108.27
29	c7	201	PEB	CHC-C4C-C3C	-2.95	125.30	130.34
29	c9	201	PEB	CHC-C4C-C3C	-2.95	125.30	130.34
29	T2	203	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
31	K1	1001	CYC	C1A-C2A-C3A	-2.95	103.51	106.78
31	KK	1001	CYC	C1A-C2A-C3A	-2.95	103.51	106.78
31	K9	1001	CYC	C4D-CHA-C1A	2.95	132.34	128.81
29	SB	202	PEB	CHC-C1D-ND	-2.95	110.52	113.95
29	SM	202	PEB	CHC-C1D-ND	-2.95	110.52	113.95
29	RB	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	VB	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	RM	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	VM	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	G8	203	PEB	C4B-C3B-C2B	-2.95	103.51	106.78
29	R1	202	PEB	C2A-C1A-NA	2.95	110.82	108.27
29	RK	202	PEB	C2A-C1A-NA	2.95	110.82	108.27
29	ZJ	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
29	ZL	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
29	L5	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	J9	1002	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	MD	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	uJ	202	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	uL	202	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	fB	202	PEB	CHC-C1D-ND	-2.95	110.52	113.95
29	fM	202	PEB	CHC-C1D-ND	-2.95	110.52	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JB	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	JM	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	cB	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	cM	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	D4	201	PEB	C1C-CHB-C4B	-2.95	125.28	128.81
29	oJ	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	sJ	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	oL	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	sL	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	N7	1002	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	N9	1002	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	S7	201	PEB	OD-C4D-C3D	-2.95	122.77	129.46
29	S9	201	PEB	OD-C4D-C3D	-2.95	122.77	129.46
29	kB	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	kM	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	J3	202	PEB	CMB-C2B-C1B	2.95	129.61	125.06
29	JO	202	PEB	CMB-C2B-C1B	2.95	129.61	125.06
29	gB	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	iB	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	gM	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	iM	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	AJ	203	PEB	C1C-CHB-C4B	2.95	132.34	128.81
29	AL	203	PEB	C1C-CHB-C4B	2.95	132.34	128.81
30	MA	402	PUB	CBB-CAB-C3B	-2.95	107.58	112.62
29	OJ	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	OL	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	B5	203	PEB	C3B-C4B-NB	2.95	114.34	110.05
29	FC	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
29	FE	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
31	NP	1001	CYC	CHA-C1A-NA	-2.95	124.73	128.83
31	cP	1001	CYC	CHA-C1A-NA	-2.95	124.73	128.83
29	HB	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	VB	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	HM	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	VM	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	PJ	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	PL	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	cB	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	cM	201	PEB	CHA-C1B-NB	-2.95	118.76	124.93
31	L9	1001	CYC	OC-C1C-C2C	-2.95	123.83	126.17
31	xP	1001	CYC	C1B-C2B-C3B	-2.95	104.79	107.87
29	EA	201	PEB	CHC-C4C-C3C	-2.95	125.31	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EN	201	PEB	CHC-C4C-C3C	-2.95	125.31	130.34
29	QJ	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	QL	201	PEB	CAB-C3B-C4B	2.95	130.23	125.01
29	cB	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	cM	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	XB	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	XM	201	PEB	CAB-CBB-CGB	-2.95	107.25	113.60
29	JJ	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
29	JL	201	PEB	C3B-C4B-NB	2.95	114.34	110.05
29	L8	202	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	xJ	302	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	wL	302	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	QR	202	PEB	CHA-C1B-NB	-2.95	118.76	124.93
29	GA	201	PEB	CHC-C4C-C3C	-2.95	125.31	130.34
29	GN	201	PEB	CHC-C4C-C3C	-2.95	125.31	130.34
29	AC	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
29	IC	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
29	AE	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
29	IE	201	PEB	C4B-C3B-C2B	-2.95	103.52	106.78
29	P1	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
29	g1	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
29	PK	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
29	gK	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
29	FB	201	PEB	CHA-C1B-NB	-2.95	118.77	124.93
29	FM	201	PEB	CHA-C1B-NB	-2.95	118.77	124.93
29	nJ	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	nL	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	ED	201	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	V1	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
29	VK	202	PEB	C2A-C1A-NA	2.95	110.81	108.27
29	pJ	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	pL	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	gB	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	gM	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	AB	302	PEB	C1B-C2B-C3B	-2.95	103.12	106.51
29	DB	201	PEB	CAB-CBB-CGB	-2.95	107.26	113.60
29	FB	201	PEB	CAB-CBB-CGB	-2.95	107.26	113.60
29	DM	201	PEB	CAB-CBB-CGB	-2.95	107.26	113.60
29	FM	201	PEB	CAB-CBB-CGB	-2.95	107.26	113.60
29	CJ	201	PEB	CAB-C3B-C4B	2.95	130.22	125.01
29	cJ	201	PEB	CAB-C3B-C4B	2.95	130.22	125.01
29	CL	201	PEB	CAB-C3B-C4B	2.95	130.22	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	cL	201	PEB	CAB-C3B-C4B	2.95	130.22	125.01
31	mP	1001	CYC	OC-C1C-C2C	-2.95	123.83	126.17
31	rP	1001	CYC	OC-C1C-C2C	-2.95	123.83	126.17
29	fJ	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	fL	202	PEB	C1C-CHB-C4B	2.95	132.33	128.81
29	H4	201	PEB	C1C-CHB-C4B	-2.95	125.29	128.81
29	m1	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	aJ	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	mK	201	PEB	OD-C4D-ND	-2.95	121.56	125.93
29	aL	202	PEB	OD-C4D-ND	-2.95	121.56	125.93
30	MG	402	PUB	OA-C1A-NA	-2.95	121.56	125.93
31	N7	1001	CYC	CAA-CBA-CGA	2.95	119.94	113.60
31	N9	1001	CYC	CAA-CBA-CGA	2.95	119.94	113.60
29	H3	202	PEB	CAC-CBC-CGC	-2.95	105.50	113.76
29	HO	202	PEB	CAC-CBC-CGC	-2.95	105.50	113.76
30	A7	303	PUB	OD-C4D-ND	-2.95	121.57	125.93
30	A9	303	PUB	OD-C4D-ND	-2.95	121.57	125.93
29	mB	201	PEB	CHA-C1B-NB	-2.95	118.77	124.93
29	mM	201	PEB	CHA-C1B-NB	-2.95	118.77	124.93
29	TJ	201	PEB	C3B-C4B-NB	2.95	114.33	110.05
29	TL	201	PEB	C3B-C4B-NB	2.95	114.33	110.05
29	F8	202	PEB	C1B-C2B-C3B	-2.95	103.13	106.51
29	iB	203	PEB	CHA-C4A-NA	-2.95	121.70	125.20
29	iM	203	PEB	CHA-C4A-NA	-2.95	121.70	125.20
29	cJ	202	PEB	OD-C4D-ND	-2.95	121.57	125.93
29	iJ	202	PEB	OD-C4D-ND	-2.95	121.57	125.93
29	cL	202	PEB	OD-C4D-ND	-2.95	121.57	125.93
29	iL	202	PEB	OD-C4D-ND	-2.95	121.57	125.93
29	D1	1002	PEB	CMB-C2B-C1B	2.94	129.60	125.06
29	XB	201	PEB	CHA-C1B-NB	-2.94	118.77	124.93
29	XM	201	PEB	CHA-C1B-NB	-2.94	118.77	124.93
29	B4	201	PEB	OD-C4D-C3D	-2.94	122.79	129.46
29	qJ	201	PEB	CAB-C3B-C4B	2.94	130.22	125.01
29	qL	201	PEB	CAB-C3B-C4B	2.94	130.22	125.01
29	JC	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	JE	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	sJ	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	sL	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
30	A7	302	PUB	OD-C4D-ND	-2.94	121.57	125.93
30	A9	302	PUB	OD-C4D-ND	-2.94	121.57	125.93
29	BJ	203	PEB	C4B-C3B-C2B	-2.94	103.52	106.78
29	vJ	202	PEB	C4B-C3B-C2B	-2.94	103.52	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BL	203	PEB	C4B-C3B-C2B	-2.94	103.52	106.78
29	vL	202	PEB	C4B-C3B-C2B	-2.94	103.52	106.78
29	eB	201	PEB	CAB-CBB-CGB	-2.94	107.27	113.60
29	eM	201	PEB	CAB-CBB-CGB	-2.94	107.27	113.60
29	ID	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	lB	202	PEB	CHC-C1D-ND	-2.94	110.53	113.95
29	lM	202	PEB	CHC-C1D-ND	-2.94	110.53	113.95
30	MN	402	PUB	CBB-CAB-C3B	-2.94	107.60	112.62
29	FB	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	UJ	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	UL	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	FM	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	ZB	201	PEB	CHA-C1B-NB	-2.94	118.78	124.93
29	ZM	201	PEB	CHA-C1B-NB	-2.94	118.78	124.93
29	TB	201	PEB	CAB-CBB-CGB	-2.94	107.27	113.60
29	TM	201	PEB	CAB-CBB-CGB	-2.94	107.27	113.60
29	MD	201	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	hJ	202	PEB	C1C-CHB-C4B	2.94	132.32	128.81
29	hL	202	PEB	C1C-CHB-C4B	2.94	132.32	128.81
31	I7	1001	CYC	C4D-CHA-C1A	2.94	132.32	128.81
31	I9	1001	CYC	C4D-CHA-C1A	2.94	132.32	128.81
29	LB	203	PEB	CHA-C4A-NA	-2.94	121.71	125.20
29	LM	203	PEB	CHA-C4A-NA	-2.94	121.71	125.20
29	g7	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	g9	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	M3	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	C4	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	I4	201	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	MO	202	PEB	C1B-C2B-C3B	-2.94	103.13	106.51
29	A3	201	PEB	CHB-C4B-NB	-2.94	124.75	128.83
29	AO	201	PEB	CHB-C4B-NB	-2.94	124.75	128.83
29	ZJ	202	PEB	C1C-CHB-C4B	2.94	132.32	128.81
29	sJ	203	PEB	C1C-CHB-C4B	2.94	132.32	128.81
29	ZL	202	PEB	C1C-CHB-C4B	2.94	132.32	128.81
29	sL	203	PEB	C1C-CHB-C4B	2.94	132.32	128.81
29	HC	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	HE	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	ZB	201	PEB	CAB-CBB-CGB	-2.94	107.27	113.60
29	ZM	201	PEB	CAB-CBB-CGB	-2.94	107.27	113.60
29	a7	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	a9	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	CA	202	PEB	CMD-C2D-C3D	2.94	134.21	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CN	202	PEB	CMD-C2D-C3D	2.94	134.21	130.06
29	KJ	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
29	KL	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
29	qJ	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	qL	202	PEB	OD-C4D-ND	-2.94	121.57	125.93
29	k7	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	k9	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	jJ	202	PEB	C1C-CHB-C4B	2.94	132.32	128.81
29	jL	202	PEB	C1C-CHB-C4B	2.94	132.32	128.81
31	G7	1001	CYC	C4D-CHA-C1A	2.94	132.32	128.81
29	I8	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
29	B4	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
29	BD	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
29	aJ	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
29	aL	201	PEB	CAB-C3B-C4B	2.94	130.21	125.01
29	H7	1002	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
29	H9	1002	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
31	gP	1001	CYC	OC-C1C-C2C	-2.94	123.83	126.17
30	MG	402	PUB	OD-C4D-ND	-2.94	121.57	125.93
29	dJ	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	fJ	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	dL	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	fL	201	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	zL	501	PEB	C3B-C4B-NB	2.94	114.33	110.05
29	JB	201	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
29	JM	201	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
29	YB	203	PEB	CHC-C1D-ND	-2.94	110.53	113.95
29	YM	203	PEB	CHC-C1D-ND	-2.94	110.53	113.95
29	J5	202	PEB	CBC-CAC-C2C	2.94	117.64	112.62
29	J8	202	PEB	CBC-CAC-C2C	2.94	117.64	112.62
31	IF	1001	CYC	OB-C4B-C3B	-2.94	124.85	128.04
31	II	1001	CYC	OB-C4B-C3B	-2.94	124.85	128.04
29	Z7	202	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	Z9	202	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	H3	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
29	HO	201	PEB	CHC-C4C-C3C	-2.94	125.32	130.34
31	D1	1001	CYC	C2A-C1A-NA	2.94	114.33	110.05
29	TB	203	PEB	CHA-C4A-NA	-2.94	121.71	125.20
29	TM	203	PEB	CHA-C4A-NA	-2.94	121.71	125.20
29	H4	202	PEB	C2A-C1A-NA	2.94	110.81	108.27
29	F3	202	PEB	CAC-CBC-CGC	-2.94	105.52	113.76
29	FO	202	PEB	CAC-CBC-CGC	-2.94	105.52	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BJ	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
29	BL	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
31	DK	1001	CYC	C2A-C1A-NA	2.94	114.32	110.05
29	J9	1002	PEB	CAB-CBB-CGB	-2.94	107.28	113.60
29	P1	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	e1	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	uJ	203	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	PK	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	eK	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	uL	203	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	DQ	203	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	FQ	203	PEB	OD-C4D-ND	-2.94	121.58	125.93
30	MQ	404	PUB	OD-C4D-ND	-2.94	121.58	125.93
29	F3	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
29	FO	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
31	L9	1001	CYC	CAA-CBA-CGA	2.94	119.92	113.60
29	H3	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
29	VF	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
29	VI	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
29	HO	202	PEB	CMB-C2B-C1B	2.94	129.59	125.06
29	NO	203	PEB	CHB-C4B-NB	-2.94	124.75	128.83
29	DJ	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
29	DL	201	PEB	C3B-C4B-NB	2.94	114.32	110.05
29	A5	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
29	A8	203	PEB	C4B-C3B-C2B	-2.94	103.53	106.78
29	dB	202	PEB	CHC-C1D-ND	-2.94	110.54	113.95
29	dM	202	PEB	CHC-C1D-ND	-2.94	110.54	113.95
29	QB	204	PEB	CHC-C1D-ND	-2.94	110.54	113.95
29	QM	204	PEB	CHC-C1D-ND	-2.94	110.54	113.95
29	YB	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	YM	201	PEB	OD-C4D-ND	-2.94	121.58	125.93
29	J7	1002	PEB	CAB-CBB-CGB	-2.94	107.29	113.60
29	BD	201	PEB	OD-C4D-C3D	-2.94	122.81	129.46
29	IG	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
29	IQ	202	PEB	C3B-C4B-NB	2.94	114.32	110.05
31	DF	1001	CYC	CHB-C4A-C3A	2.94	132.45	124.90
31	DI	1001	CYC	CHB-C4A-C3A	2.94	132.45	124.90
29	dF	201	PEB	CMB-C2B-C1B	2.94	129.58	125.06
29	dI	201	PEB	CMB-C2B-C1B	2.94	129.58	125.06
29	H5	202	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
29	NO	202	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
29	LD	201	PEB	C1C-CHB-C4B	-2.93	125.30	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	kJ	201	PEB	CAB-C3B-C4B	2.93	130.20	125.01
29	kL	201	PEB	CAB-C3B-C4B	2.93	130.20	125.01
29	PJ	201	PEB	C3B-C4B-NB	2.93	114.32	110.05
29	PL	201	PEB	C3B-C4B-NB	2.93	114.32	110.05
29	LD	201	PEB	OD-C4D-C3D	-2.93	122.81	129.46
29	jJ	203	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
29	jL	203	PEB	C4B-C3B-C2B	-2.93	103.53	106.78
29	CJ	202	PEB	OD-C4D-ND	-2.93	121.58	125.93
29	CL	202	PEB	OD-C4D-ND	-2.93	121.58	125.93
29	U1	202	PEB	CMA-C2A-C1A	-2.93	106.08	112.40
29	UK	202	PEB	CMA-C2A-C1A	-2.93	106.08	112.40
31	NP	1001	CYC	OC-C1C-C2C	-2.93	123.84	126.17
29	xJ	303	PEB	C2A-C1A-NA	2.93	110.80	108.27
29	VB	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	VM	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	LA	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	LN	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	RJ	201	PEB	C3B-C4B-NB	2.93	114.32	110.05
29	RL	201	PEB	C3B-C4B-NB	2.93	114.32	110.05
29	zL	501	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
29	WB	202	PEB	CHC-C1D-ND	-2.93	110.54	113.95
29	WM	202	PEB	CHC-C1D-ND	-2.93	110.54	113.95
29	a1	201	PEB	OD-C4D-ND	-2.93	121.58	125.93
29	aK	201	PEB	OD-C4D-ND	-2.93	121.58	125.93
29	lJ	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
29	lL	201	PEB	C3B-C4B-NB	2.93	114.31	110.05
29	GC	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	GE	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	h7	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	h9	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	TB	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	TM	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	xL	302	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
29	K8	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	VJ	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	ZJ	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	VL	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	ZL	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	lJ	202	PEB	C1C-CHB-C4B	2.93	132.31	128.81
29	lL	202	PEB	C1C-CHB-C4B	2.93	132.31	128.81
31	CF	1001	CYC	OB-C4B-C3B	-2.93	124.86	128.04
31	CI	1001	CYC	OB-C4B-C3B	-2.93	124.86	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EJ	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	EL	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	GB	202	PEB	CHC-C1D-ND	-2.93	110.54	113.95
29	FC	201	PEB	CHC-C1D-ND	-2.93	110.54	113.95
29	FE	201	PEB	CHC-C1D-ND	-2.93	110.54	113.95
29	GM	202	PEB	CHC-C1D-ND	-2.93	110.54	113.95
29	H7	1002	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
29	H9	1002	PEB	C1B-C2B-C3B	-2.93	103.14	106.51
29	Q2	202	PEB	CHA-C1B-NB	-2.93	118.80	124.93
31	D7	1001	CYC	CAA-CBA-CGA	2.93	119.91	113.60
31	D9	1001	CYC	CAA-CBA-CGA	2.93	119.91	113.60
29	DK	1002	PEB	CMB-C2B-C1B	2.93	129.58	125.06
29	JB	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	JM	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	JG	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	JQ	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
31	L7	1001	CYC	CAA-CBA-CGA	2.93	119.91	113.60
29	gJ	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	gL	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	N3	203	PEB	CHB-C4B-NB	-2.93	124.76	128.83
29	eB	202	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	eM	202	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	DB	201	PEB	CHA-C1B-NB	-2.93	118.80	124.93
29	DM	201	PEB	CHA-C1B-NB	-2.93	118.80	124.93
29	WJ	201	PEB	C1C-CHB-C4B	2.93	132.31	128.81
29	WL	201	PEB	C1C-CHB-C4B	2.93	132.31	128.81
29	AJ	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	AL	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	IB	202	PEB	CHC-C1D-ND	-2.93	110.55	113.95
29	IM	202	PEB	CHC-C1D-ND	-2.93	110.55	113.95
29	CA	201	PEB	CHC-C4C-C3C	-2.93	125.34	130.34
29	CN	201	PEB	CHC-C4C-C3C	-2.93	125.34	130.34
29	SR	202	PEB	CHA-C1B-NB	-2.93	118.81	124.93
31	WP	1001	CYC	C2C-C1C-NC	2.93	110.80	108.27
29	NJ	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	NL	203	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	KJ	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	KL	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	eR	401	PEB	CHB-C4B-NB	-2.93	124.76	128.83
29	AB	303	PEB	C3B-C4B-NB	2.93	114.31	110.05
31	F7	1001	CYC	CAA-CBA-CGA	2.93	119.91	113.60
29	iB	202	PEB	OD-C4D-ND	-2.93	121.59	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	iM	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	DG	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	DQ	201	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
31	HF	1001	CYC	CHB-C4A-C3A	2.93	132.43	124.90
31	HI	1001	CYC	CHB-C4A-C3A	2.93	132.43	124.90
29	gB	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	gM	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	R1	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	RK	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
31	F9	1001	CYC	CAA-CBA-CGA	2.93	119.90	113.60
29	KC	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	KE	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	K4	202	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
29	KD	202	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
29	mJ	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	mL	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	GG	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	JG	203	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	GQ	201	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	mB	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	mM	203	PEB	CHA-C4A-NA	-2.93	121.72	125.20
29	b1	201	PEB	CMA-C2A-C1A	-2.93	106.09	112.40
29	bK	201	PEB	CMA-C2A-C1A	-2.93	106.09	112.40
31	J9	1001	CYC	OC-C1C-C2C	-2.93	123.85	126.17
29	I4	203	PEB	C3B-C4B-NB	2.93	114.31	110.05
29	GJ	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	GL	201	PEB	CAB-C3B-C4B	2.93	130.19	125.01
29	CB	202	PEB	CHC-C1D-ND	-2.93	110.55	113.95
29	CM	202	PEB	CHC-C1D-ND	-2.93	110.55	113.95
29	LJ	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	LL	202	PEB	C4B-C3B-C2B	-2.93	103.54	106.78
29	AJ	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
29	AL	202	PEB	OD-C4D-ND	-2.93	121.59	125.93
30	BB	302	PUB	OA-C1A-NA	-2.93	121.59	125.93
30	BM	302	PUB	OA-C1A-NA	-2.93	121.59	125.93
29	I4	202	PEB	C1B-C2B-C3B	-2.93	103.15	106.51
31	gP	1001	CYC	CHA-C1A-NA	-2.93	124.77	128.83
29	F4	201	PEB	C1C-CHB-C4B	-2.93	125.31	128.81
29	N7	1002	PEB	CAB-CBB-CGB	-2.93	107.31	113.60
29	L9	1002	PEB	CAB-CBB-CGB	-2.93	107.31	113.60
29	N9	1002	PEB	CAB-CBB-CGB	-2.93	107.31	113.60
29	D7	1002	PEB	CAB-CBB-CGB	-2.93	107.31	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D9	1002	PEB	CAB-CBB-CGB	-2.93	107.31	113.60
31	NK	1001	CYC	C2A-C1A-NA	2.93	114.30	110.05
29	Y7	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	Y9	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	QB	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	IJ	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	IL	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	QM	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	L1	1002	PEB	CMB-C2B-C1B	2.92	129.57	125.06
29	LK	1002	PEB	CMB-C2B-C1B	2.92	129.57	125.06
31	LF	1001	CYC	CHB-C4A-C3A	2.92	132.42	124.90
31	LI	1001	CYC	CHB-C4A-C3A	2.92	132.42	124.90
29	UB	202	PEB	CHC-C1D-ND	-2.92	110.55	113.95
29	jB	202	PEB	CHC-C1D-ND	-2.92	110.55	113.95
29	jM	202	PEB	CHC-C1D-ND	-2.92	110.55	113.95
29	MQ	401	PEB	CHC-C1D-ND	-2.92	110.55	113.95
29	M4	202	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
29	C5	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	C8	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	i7	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	i9	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	FJ	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	jJ	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	FL	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	jL	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	a1	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
29	aK	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
31	H7	1001	CYC	OC-C1C-C2C	-2.92	123.85	126.17
31	H9	1001	CYC	OC-C1C-C2C	-2.92	123.85	126.17
31	J7	1001	CYC	CAA-CBA-CGA	2.92	119.89	113.60
29	V7	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	m7	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	V9	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	m9	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	pJ	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	pL	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
31	J1	1001	CYC	C2A-C1A-NA	2.92	114.30	110.05
31	JK	1001	CYC	C2A-C1A-NA	2.92	114.30	110.05
29	WJ	202	PEB	CAB-C3B-C4B	2.92	130.18	125.01
29	WL	202	PEB	CAB-C3B-C4B	2.92	130.18	125.01
29	Y1	201	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	YK	201	PEB	OD-C4D-ND	-2.92	121.60	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FG	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	FQ	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	J3	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	JO	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	DC	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
29	DD	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
29	DE	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
31	NF	1001	CYC	CHB-C4A-C3A	2.92	132.42	124.90
31	NI	1001	CYC	CHB-C4A-C3A	2.92	132.42	124.90
29	mB	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	mM	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
31	J9	1001	CYC	CAA-CBA-CGA	2.92	119.89	113.60
29	I3	201	PEB	OA-C1A-C2A	-2.92	123.85	126.17
29	IO	201	PEB	OA-C1A-C2A	-2.92	123.85	126.17
29	LC	203	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
29	LE	203	PEB	C1B-C2B-C3B	-2.92	103.15	106.51
29	tJ	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	tL	202	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	e7	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	e9	201	PEB	CHC-C4C-C3C	-2.92	125.35	130.34
29	O7	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	O9	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	I3	203	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	IO	203	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	F4	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
29	DC	201	PEB	CHC-C1D-ND	-2.92	110.55	113.95
29	DE	201	PEB	CHC-C1D-ND	-2.92	110.55	113.95
29	bJ	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	bL	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	JJ	202	PEB	C1C-CHB-C4B	2.92	132.30	128.81
29	RJ	202	PEB	C1C-CHB-C4B	2.92	132.30	128.81
29	JL	202	PEB	C1C-CHB-C4B	2.92	132.30	128.81
29	RL	202	PEB	C1C-CHB-C4B	2.92	132.30	128.81
29	JB	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	JM	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	F4	201	PEB	OD-C4D-C3D	-2.92	122.84	129.46
29	DB	203	PEB	CHA-C4A-NA	-2.92	121.73	125.20
29	DM	203	PEB	CHA-C4A-NA	-2.92	121.73	125.20
29	KG	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	hJ	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	hL	201	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	KQ	202	PEB	C3B-C4B-NB	2.92	114.30	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LD	202	PEB	C2A-C1A-NA	2.92	110.79	108.27
29	eJ	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	eL	202	PEB	OD-C4D-ND	-2.92	121.60	125.93
29	EC	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	EE	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	UF	201	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	UI	201	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	aB	202	PEB	CHC-C1D-ND	-2.92	110.56	113.95
29	aM	202	PEB	CHC-C1D-ND	-2.92	110.56	113.95
29	EG	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	EQ	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	FC	203	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
29	FE	203	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
29	YJ	201	PEB	CAB-C3B-C4B	2.92	130.17	125.01
29	YL	201	PEB	CAB-C3B-C4B	2.92	130.17	125.01
31	L1	1001	CYC	C2A-C1A-NA	2.92	114.30	110.05
31	LK	1001	CYC	C2A-C1A-NA	2.92	114.30	110.05
29	I4	203	PEB	OD-C4D-C3D	-2.92	122.84	129.46
29	iF	202	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	iI	202	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	S2	202	PEB	CHA-C1B-NB	-2.92	118.83	124.93
29	M3	203	PEB	CHB-C4B-NB	-2.92	124.78	128.83
29	MO	203	PEB	CHB-C4B-NB	-2.92	124.78	128.83
29	HC	201	PEB	CHC-C1D-ND	-2.92	110.56	113.95
29	HE	201	PEB	CHC-C1D-ND	-2.92	110.56	113.95
31	eP	1001	CYC	OC-C1C-C2C	-2.92	123.85	126.17
29	CC	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	CE	201	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
29	XJ	202	PEB	C1C-CHB-C4B	2.92	132.30	128.81
29	XL	202	PEB	C1C-CHB-C4B	2.92	132.30	128.81
29	AG	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	AQ	202	PEB	C3B-C4B-NB	2.92	114.30	110.05
29	HD	201	PEB	OD-C4D-C3D	-2.92	122.85	129.46
29	cB	203	PEB	CHA-C4A-NA	-2.92	121.73	125.20
29	cM	203	PEB	CHA-C4A-NA	-2.92	121.73	125.20
29	F7	1002	PEB	CAB-CBB-CGB	-2.92	107.32	113.60
29	aF	202	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	aI	202	PEB	CMB-C2B-C1B	2.92	129.56	125.06
29	nJ	201	PEB	C3B-C4B-NB	2.92	114.29	110.05
29	nL	201	PEB	C3B-C4B-NB	2.92	114.29	110.05
31	F1	1001	CYC	C2A-C1A-NA	2.92	114.29	110.05
31	FK	1001	CYC	C2A-C1A-NA	2.92	114.29	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J4	201	PEB	C1C-CHB-C4B	-2.92	125.32	128.81
29	K5	203	PEB	C4B-C3B-C2B	-2.92	103.55	106.78
31	FF	1001	CYC	CHB-C4A-C3A	2.92	132.40	124.90
31	FI	1001	CYC	CHB-C4A-C3A	2.92	132.40	124.90
29	wJ	302	PEB	OD-C4D-C3D	-2.92	122.85	129.46
29	ZB	201	PEB	CBC-CAC-C2C	-2.92	107.64	112.62
29	ZM	201	PEB	CBC-CAC-C2C	-2.92	107.64	112.62
29	O2	202	PEB	CHA-C1B-NB	-2.92	118.83	124.93
29	AM	303	PEB	C3B-C4B-NB	2.92	114.29	110.05
29	RB	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	KG	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	YJ	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	YL	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	RM	202	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	KQ	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
30	MQ	404	PUB	OA-C1A-NA	-2.92	121.61	125.93
29	wJ	303	PEB	C2A-C1A-NA	2.92	110.79	108.27
31	E7	1001	CYC	C4D-CHA-C1A	2.92	132.29	128.81
31	E9	1001	CYC	C4D-CHA-C1A	2.92	132.29	128.81
29	IC	201	PEB	C1C-CHB-C4B	-2.92	125.33	128.81
29	IE	201	PEB	C1C-CHB-C4B	-2.92	125.33	128.81
31	H7	1001	CYC	CAA-CBA-CGA	2.92	119.88	113.60
31	H9	1001	CYC	CAA-CBA-CGA	2.92	119.88	113.60
29	EB	202	PEB	CHC-C1D-ND	-2.92	110.56	113.95
29	EM	202	PEB	CHC-C1D-ND	-2.92	110.56	113.95
29	F9	1002	PEB	CAB-CBB-CGB	-2.92	107.33	113.60
29	MN	401	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
29	g1	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	gK	201	PEB	OD-C4D-ND	-2.92	121.61	125.93
29	HJ	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
29	HL	202	PEB	C4B-C3B-C2B	-2.92	103.56	106.78
29	FB	203	PEB	CHA-C4A-NA	-2.92	121.74	125.20
29	FM	203	PEB	CHA-C4A-NA	-2.92	121.74	125.20
29	T7	201	PEB	CHC-C4C-C3C	-2.92	125.36	130.34
29	T9	201	PEB	CHC-C4C-C3C	-2.92	125.36	130.34
31	WP	1001	CYC	C4A-C3A-C2A	-2.91	103.16	106.51
29	oJ	202	PEB	OD-C4D-ND	-2.91	121.61	125.93
29	oL	202	PEB	OD-C4D-ND	-2.91	121.61	125.93
29	W1	201	PEB	CMA-C2A-C1A	-2.91	106.12	112.40
29	WK	201	PEB	CMA-C2A-C1A	-2.91	106.12	112.40
29	J4	201	PEB	OD-C4D-C3D	-2.91	122.86	129.46
31	I1	1001	CYC	C1A-C2A-C3A	-2.91	103.56	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	JF	1001	CYC	CHB-C4A-C3A	2.91	132.39	124.90
31	JI	1001	CYC	CHB-C4A-C3A	2.91	132.39	124.90
29	MJ	202	PEB	OD-C4D-ND	-2.91	121.61	125.93
29	ML	202	PEB	OD-C4D-ND	-2.91	121.61	125.93
31	CP	1001	CYC	OC-C1C-C2C	-2.91	123.86	126.17
29	F5	202	PEB	C1B-C2B-C3B	-2.91	103.16	106.51
29	eJ	201	PEB	CAB-C3B-C4B	2.91	130.16	125.01
29	eL	201	PEB	CAB-C3B-C4B	2.91	130.16	125.01
29	Z1	202	PEB	CMA-C2A-C1A	-2.91	106.12	112.40
29	ZK	202	PEB	CMA-C2A-C1A	-2.91	106.12	112.40
29	M4	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
29	FA	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
29	FN	203	PEB	OD-C4D-C3D	-2.91	122.86	129.46
29	F3	201	PEB	CHC-C4C-C3C	-2.91	125.37	130.34
29	FO	201	PEB	CHC-C4C-C3C	-2.91	125.37	130.34
29	wL	302	PEB	OD-C4D-C3D	-2.91	122.86	129.46
29	PB	202	PEB	CHA-C4A-NA	-2.91	121.74	125.20
29	kB	203	PEB	CHA-C4A-NA	-2.91	121.74	125.20
29	PM	202	PEB	CHA-C4A-NA	-2.91	121.74	125.20
29	kM	203	PEB	CHA-C4A-NA	-2.91	121.74	125.20
29	H8	202	PEB	C1B-C2B-C3B	-2.91	103.16	106.51
29	OJ	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	OL	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	iB	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	XJ	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	XL	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	iM	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	JJ	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	JL	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	iJ	201	PEB	CAB-C3B-C4B	2.91	130.16	125.01
29	iL	201	PEB	CAB-C3B-C4B	2.91	130.16	125.01
29	PF	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	YF	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	eF	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	PI	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	YI	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	eI	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	lI	201	PEB	CMA-C2A-C1A	-2.91	106.13	112.40
29	lK	201	PEB	CMA-C2A-C1A	-2.91	106.13	112.40
29	rJ	202	PEB	C1C-CHB-C4B	2.91	132.29	128.81
29	rL	202	PEB	C1C-CHB-C4B	2.91	132.29	128.81
29	O2	201	PEB	C3B-C4B-NB	2.91	114.28	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	XB	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	XM	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	kF	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	kI	202	PEB	CMB-C2B-C1B	2.91	129.55	125.06
29	EJ	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	EL	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	bJ	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	bL	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
31	HK	1001	CYC	C2A-C1A-NA	2.91	114.28	110.05
29	I5	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	AF	304	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	AI	304	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	PJ	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	nJ	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	PL	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	nL	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	XB	201	PEB	CBC-CAC-C2C	-2.91	107.65	112.62
29	XM	201	PEB	CBC-CAC-C2C	-2.91	107.65	112.62
29	LJ	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	LL	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	TF	201	PEB	CHC-C1D-ND	-2.91	110.57	113.95
29	gF	202	PEB	CMB-C2B-C1B	2.91	129.54	125.06
29	gI	202	PEB	CMB-C2B-C1B	2.91	129.54	125.06
29	D3	201	PEB	CHC-C4C-C3C	-2.91	125.38	130.34
29	DO	201	PEB	CHC-C4C-C3C	-2.91	125.38	130.34
29	hB	202	PEB	CHC-C1D-ND	-2.91	110.57	113.95
29	hM	202	PEB	CHC-C1D-ND	-2.91	110.57	113.95
29	D4	201	PEB	OD-C4D-C3D	-2.91	122.87	129.46
29	BQ	203	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	IA	202	PEB	CMD-C2D-C3D	2.91	134.17	130.06
29	IN	202	PEB	CMD-C2D-C3D	2.91	134.17	130.06
29	kB	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	kM	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	mF	202	PEB	CMB-C2B-C1B	2.91	129.54	125.06
29	mI	202	PEB	CMB-C2B-C1B	2.91	129.54	125.06
29	L7	1002	PEB	CAB-CBB-CGB	-2.91	107.34	113.60
29	S1	201	PEB	CMA-C2A-C1A	-2.91	106.13	112.40
29	SK	201	PEB	CMA-C2A-C1A	-2.91	106.13	112.40
29	RJ	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	RL	203	PEB	C4B-C3B-C2B	-2.91	103.56	106.78
29	W2	202	PEB	CHA-C1B-NB	-2.91	118.85	124.93
29	B3	201	PEB	CHC-C4C-C3C	-2.91	125.38	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BO	201	PEB	CHC-C4C-C3C	-2.91	125.38	130.34
29	DC	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	DE	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
31	tP	1001	CYC	OC-C1C-C2C	-2.91	123.86	126.17
29	O1	201	PEB	CMA-C2A-C1A	-2.91	106.14	112.40
29	OK	201	PEB	CMA-C2A-C1A	-2.91	106.14	112.40
29	gJ	201	PEB	CAB-C3B-C4B	2.91	130.15	125.01
29	gL	201	PEB	CAB-C3B-C4B	2.91	130.15	125.01
29	PB	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	PM	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	G4	202	PEB	C1B-C2B-C3B	-2.91	103.17	106.51
29	UR	202	PEB	CHA-C1B-NB	-2.91	118.85	124.93
29	Z1	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
29	ZK	201	PEB	C2A-C1A-NA	2.91	110.78	108.27
29	BA	203	PEB	OD-C4D-C3D	-2.91	122.87	129.46
29	BN	203	PEB	OD-C4D-C3D	-2.91	122.87	129.46
29	j7	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	j9	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	mB	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	kJ	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	kL	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	mM	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	OB	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	WB	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	OM	202	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	WM	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	J5	202	PEB	OA-C1A-C2A	-2.91	123.86	126.17
29	J8	202	PEB	OA-C1A-C2A	-2.91	123.86	126.17
29	BA	201	PEB	OA-C1A-C2A	-2.91	123.86	126.17
29	BN	201	PEB	OA-C1A-C2A	-2.91	123.86	126.17
31	N7	1001	CYC	OC-C1C-C2C	-2.91	123.86	126.17
31	N9	1001	CYC	OC-C1C-C2C	-2.91	123.86	126.17
29	LC	201	PEB	CHC-C1D-ND	-2.91	110.57	113.95
29	LE	201	PEB	CHC-C1D-ND	-2.91	110.57	113.95
29	TJ	203	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
29	TL	203	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
29	JA	203	PEB	OD-C4D-C3D	-2.91	122.88	129.46
29	JN	203	PEB	OD-C4D-C3D	-2.91	122.88	129.46
29	S7	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	S9	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	kB	202	PEB	OD-C4D-ND	-2.91	121.62	125.93
29	kM	202	PEB	OD-C4D-ND	-2.91	121.62	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	rJ	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	rL	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	lJ	203	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
29	lL	203	PEB	C4B-C3B-C2B	-2.91	103.57	106.78
29	JD	201	PEB	OD-C4D-C3D	-2.91	122.88	129.46
29	Q7	202	PEB	OD-C4D-ND	-2.91	121.63	125.93
29	Q9	202	PEB	OD-C4D-ND	-2.91	121.63	125.93
29	GJ	202	PEB	OD-C4D-ND	-2.91	121.63	125.93
29	GL	202	PEB	OD-C4D-ND	-2.91	121.63	125.93
31	yP	1001	CYC	C4A-C3A-C2A	-2.91	103.17	106.51
31	KP	1001	CYC	OC-C1C-C2C	-2.91	123.86	126.17
29	fB	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	fM	201	PEB	C3B-C4B-NB	2.91	114.28	110.05
29	h1	201	PEB	CMA-C2A-C1A	-2.91	106.14	112.40
29	hK	201	PEB	CMA-C2A-C1A	-2.91	106.14	112.40
31	C7	1001	CYC	C4D-CHA-C1A	2.90	132.28	128.81
31	C9	1001	CYC	C4D-CHA-C1A	2.90	132.28	128.81
29	U2	202	PEB	CHA-C1B-NB	-2.90	118.86	124.93
29	FG	203	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	rJ	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
29	rL	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
29	H4	201	PEB	OD-C4D-C3D	-2.90	122.88	129.46
29	BC	203	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
29	BE	203	PEB	C1B-C2B-C3B	-2.90	103.17	106.51
29	CG	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	CQ	202	PEB	C3B-C4B-NB	2.90	114.27	110.05
31	N1	1001	CYC	C2A-C1A-NA	2.90	114.27	110.05
29	S7	202	PEB	OD-C4D-C3D	-2.90	122.88	129.46
29	S9	202	PEB	OD-C4D-C3D	-2.90	122.88	129.46
29	NJ	202	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	bJ	202	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	NL	202	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	bL	202	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	fF	201	PEB	CHB-C4B-C3B	-2.90	118.61	125.32
29	fI	201	PEB	CHB-C4B-C3B	-2.90	118.61	125.32
29	Q1	201	PEB	CMA-C2A-C1A	-2.90	106.14	112.40
29	QK	201	PEB	CMA-C2A-C1A	-2.90	106.14	112.40
29	A9	304	PEB	C2A-C1A-NA	2.90	110.78	108.27
29	l7	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	l9	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	HJ	201	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	HL	201	PEB	C1C-CHB-C4B	2.90	132.28	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KB	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	KM	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	KB	203	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	KM	203	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	hF	201	PEB	CHB-C4B-C3B	-2.90	118.61	125.32
29	hI	201	PEB	CHB-C4B-C3B	-2.90	118.61	125.32
29	UB	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	UM	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	HK	1002	PEB	CMB-C2B-C1B	2.90	129.53	125.06
29	WJ	203	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	WL	203	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	B5	203	PEB	C4B-C3B-C2B	-2.90	103.57	106.78
29	kB	201	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
29	kM	201	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
29	JC	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	JE	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	FJ	202	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	FL	202	PEB	C1C-CHB-C4B	2.90	132.28	128.81
29	FD	201	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	d7	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	d9	202	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	D4	202	PEB	C2A-C1A-NA	2.90	110.77	108.27
29	KA	202	PEB	CMD-C2D-C3D	2.90	134.16	130.06
29	KN	202	PEB	CMD-C2D-C3D	2.90	134.16	130.06
29	OF	203	PEB	CMB-C2B-C1B	2.90	129.53	125.06
29	OI	203	PEB	CMB-C2B-C1B	2.90	129.53	125.06
29	CG	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	CQ	201	PEB	OD-C4D-ND	-2.90	121.63	125.93
29	A7	305	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	A9	305	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	IB	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	IM	201	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	bF	201	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
29	bI	201	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
29	L4	201	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	DA	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	DN	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	iB	201	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
29	iM	201	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
29	d1	201	PEB	CMA-C2A-C1A	-2.90	106.15	112.40
29	dK	201	PEB	CMA-C2A-C1A	-2.90	106.15	112.40
29	L4	201	PEB	C1C-CHB-C4B	-2.90	125.34	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	QB	203	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	QB	204	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	QM	203	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	QM	204	PEB	C3B-C4B-NB	2.90	114.27	110.05
29	JC	201	PEB	CHC-C1D-ND	-2.90	110.58	113.95
29	JE	201	PEB	CHC-C1D-ND	-2.90	110.58	113.95
29	H4	201	PEB	CMB-C2B-C1B	2.90	129.53	125.06
29	DC	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
29	DE	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
29	UF	202	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
29	UI	202	PEB	CHB-C4B-C3B	-2.90	118.62	125.32
29	LA	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	LN	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	WR	202	PEB	CHA-C1B-NB	-2.90	118.87	124.93
29	Q7	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	b7	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	Q9	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	b9	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	DB	201	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
29	DM	201	PEB	CBC-CAC-C2C	-2.90	107.67	112.62
29	dB	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
29	VJ	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
29	VL	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
29	dM	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
29	M2	202	PEB	CHA-C1B-NB	-2.90	118.87	124.93
29	M3	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	O7	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	O9	202	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	MO	203	PEB	OD-C4D-C3D	-2.90	122.89	129.46
29	FD	201	PEB	CMB-C2B-C1B	2.90	129.53	125.06
29	A1	301	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
29	AK	301	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
29	EG	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
29	EQ	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
30	wL	304	PUB	CAC-CBC-CGC	-2.90	107.37	113.60
29	H1	1002	PEB	CMB-C2B-C1B	2.90	129.53	125.06
29	GD	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
29	BC	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
29	BE	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
29	F3	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
29	FO	202	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
29	e2	401	PEB	CHB-C4B-NB	-2.90	124.81	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aB	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
29	aM	201	PEB	C3B-C4B-NB	2.90	114.26	110.05
29	V2	201	PEB	OD-C4D-C3D	-2.90	122.90	129.46
29	f7	202	PEB	OD-C4D-C3D	-2.90	122.90	129.46
29	f9	202	PEB	OD-C4D-C3D	-2.90	122.90	129.46
29	HA	203	PEB	OD-C4D-C3D	-2.90	122.90	129.46
29	HN	203	PEB	OD-C4D-C3D	-2.90	122.90	129.46
29	G5	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
29	G8	202	PEB	C1B-C2B-C3B	-2.90	103.18	106.51
29	dJ	203	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
29	dL	203	PEB	C4B-C3B-C2B	-2.90	103.58	106.78
31	yP	1001	CYC	C2C-C1C-NC	2.90	110.77	108.27
29	f1	201	PEB	CMA-C2A-C1A	-2.90	106.16	112.40
29	fK	201	PEB	CMA-C2A-C1A	-2.90	106.16	112.40
29	HC	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
29	HE	201	PEB	OD-C4D-ND	-2.90	121.64	125.93
29	HA	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	HG	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	HN	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	HQ	201	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	L3	201	PEB	CHC-C4C-C3C	-2.89	125.40	130.34
29	LO	201	PEB	CHC-C4C-C3C	-2.89	125.40	130.34
30	xL	304	PUB	CAC-CBC-CGC	-2.89	107.38	113.60
29	A3	201	PEB	OA-C1A-C2A	-2.89	123.87	126.17
29	DA	201	PEB	OA-C1A-C2A	-2.89	123.87	126.17
29	DN	201	PEB	OA-C1A-C2A	-2.89	123.87	126.17
29	AO	201	PEB	OA-C1A-C2A	-2.89	123.87	126.17
29	HA	203	PEB	C1C-CHB-C4B	-2.89	125.35	128.81
29	HN	203	PEB	C1C-CHB-C4B	-2.89	125.35	128.81
29	AA	202	PEB	CMD-C2D-C3D	2.89	134.15	130.06
29	AN	202	PEB	CMD-C2D-C3D	2.89	134.15	130.06
29	TB	201	PEB	CBC-CAC-C2C	-2.89	107.68	112.62
29	TM	201	PEB	CBC-CAC-C2C	-2.89	107.68	112.62
29	gB	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
29	gM	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
29	E3	201	PEB	OD-C4D-ND	-2.89	121.64	125.93
29	W7	202	PEB	OD-C4D-ND	-2.89	121.64	125.93
29	W9	202	PEB	OD-C4D-ND	-2.89	121.64	125.93
29	DG	203	PEB	OD-C4D-ND	-2.89	121.64	125.93
29	EO	201	PEB	OD-C4D-ND	-2.89	121.64	125.93
29	JD	201	PEB	C1C-CHB-C4B	-2.89	125.35	128.81
29	TJ	202	PEB	C1C-CHB-C4B	2.89	132.26	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TL	202	PEB	C1C-CHB-C4B	2.89	132.26	128.81
29	J4	202	PEB	C2A-C1A-NA	2.89	110.77	108.27
29	mB	201	PEB	CBC-CAC-C2C	-2.89	107.68	112.62
29	mM	201	PEB	CBC-CAC-C2C	-2.89	107.68	112.62
29	hJ	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	hL	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	NB	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
29	ZB	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
29	NM	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
29	ZM	201	PEB	C3B-C4B-NB	2.89	114.26	110.05
31	H1	1001	CYC	C2A-C1A-NA	2.89	114.26	110.05
29	QF	201	PEB	CHB-C4B-C3B	-2.89	118.64	125.32
29	QI	201	PEB	CHB-C4B-C3B	-2.89	118.64	125.32
29	NB	202	PEB	CHA-C4A-NA	-2.89	121.77	125.20
29	NM	202	PEB	CHA-C4A-NA	-2.89	121.77	125.20
29	HC	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
29	HE	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
29	xJ	302	PEB	OD-C4D-C3D	-2.89	122.91	129.46
29	C3	201	PEB	OA-C1A-C2A	-2.89	123.87	126.17
29	CO	201	PEB	OA-C1A-C2A	-2.89	123.87	126.17
31	F9	1001	CYC	OC-C1C-C2C	-2.89	123.87	126.17
29	IB	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	IM	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	RB	201	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
29	RM	201	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
29	FA	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	fJ	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	fL	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	FN	203	PEB	C4B-C3B-C2B	-2.89	103.58	106.78
29	aB	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	aM	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	U7	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
29	U9	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
31	GK	1001	CYC	C1A-C2A-C3A	-2.89	103.58	106.78
29	cB	201	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
29	cM	201	PEB	CBC-CAC-C2C	-2.89	107.69	112.62
29	IJ	203	PEB	C1C-CHB-C4B	2.89	132.26	128.81
29	IL	203	PEB	C1C-CHB-C4B	2.89	132.26	128.81
29	TJ	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
29	TL	203	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
29	j7	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
29	j9	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SB	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	jB	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	SM	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	jM	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	OR	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	AG	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	kJ	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	kL	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	AQ	201	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	W7	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
29	W9	202	PEB	OD-C4D-C3D	-2.89	122.91	129.46
29	xL	302	PEB	OD-C4D-C3D	-2.89	122.91	129.46
30	xJ	304	PUB	CAC-CBC-CGC	-2.89	107.39	113.60
29	N3	203	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	jB	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	GG	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	jM	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	GQ	202	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	LG	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	j1	201	PEB	CMA-C2A-C1A	-2.89	106.18	112.40
29	jK	201	PEB	CMA-C2A-C1A	-2.89	106.18	112.40
29	EB	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	eB	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	LC	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	LE	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	EM	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	eM	201	PEB	C3B-C4B-NB	2.89	114.25	110.05
29	MA	401	PEB	C1B-C2B-C3B	-2.89	103.19	106.51
30	QB	201	PUB	OD-C4D-ND	-2.89	121.65	125.93
30	QM	201	PUB	OD-C4D-ND	-2.89	121.65	125.93
29	NR	203	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	DA	203	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
29	pJ	203	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
29	pL	203	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
29	DN	203	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
29	d7	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	l7	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	d9	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	l9	202	PEB	OD-C4D-C3D	-2.89	122.92	129.46
31	IK	1001	CYC	C1A-C2A-C3A	-2.89	103.59	106.78
29	L9	1002	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	f7	202	PEB	OD-C4D-ND	-2.89	121.65	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f9	202	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	BG	203	PEB	OD-C4D-ND	-2.89	121.65	125.93
29	jF	201	PEB	CHB-C4B-C3B	-2.89	118.65	125.32
29	jI	201	PEB	CHB-C4B-C3B	-2.89	118.65	125.32
29	HA	201	PEB	OA-C1A-C2A	-2.89	123.88	126.17
29	HN	201	PEB	OA-C1A-C2A	-2.89	123.88	126.17
29	IF	202	PEB	C2A-C1A-NA	2.89	110.76	108.27
29	II	202	PEB	C2A-C1A-NA	2.89	110.76	108.27
29	L7	1002	PEB	OD-C4D-C3D	-2.89	122.92	129.46
29	A1	302	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
29	AK	302	PEB	C4B-C3B-C2B	-2.89	103.59	106.78
31	M1	1001	CYC	C1A-C2A-C3A	-2.88	103.59	106.78
31	MK	1001	CYC	C1A-C2A-C3A	-2.88	103.59	106.78
29	N2	203	PEB	OD-C4D-C3D	-2.88	122.92	129.46
31	M7	1001	CYC	C4D-CHA-C1A	2.88	132.25	128.81
31	C1	1001	CYC	C1A-C2A-C3A	-2.88	103.59	106.78
29	VB	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	VM	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	VB	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	VM	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	LB	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	hB	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	LM	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	hM	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	JB	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	JM	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	W2	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	A9	304	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	IG	201	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	IQ	201	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	IJ	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	IL	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	pJ	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
29	pL	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
29	MB	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	MM	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	A7	304	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	DB	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	LB	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	DM	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	LM	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	ZB	202	PEB	OD-C4D-ND	-2.88	121.66	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZM	202	PEB	OD-C4D-ND	-2.88	121.66	125.93
29	FB	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	RJ	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	RL	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	FM	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	M2	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	UB	202	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	MQ	401	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	MR	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	S2	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
29	BG	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
29	BQ	201	PEB	C4B-C3B-C2B	-2.88	103.59	106.78
30	wJ	304	PUB	CAC-CBC-CGC	-2.88	107.41	113.60
29	gB	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	gM	201	PEB	CBC-CAC-C2C	-2.88	107.70	112.62
29	BD	201	PEB	OA-C1A-C2A	-2.88	123.88	126.17
31	J7	1001	CYC	OC-C1C-C2C	-2.88	123.88	126.17
29	VR	201	PEB	OD-C4D-C3D	-2.88	122.94	129.46
29	TB	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	TM	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	GA	202	PEB	CMD-C2D-C3D	2.88	134.12	130.06
29	GN	202	PEB	CMD-C2D-C3D	2.88	134.12	130.06
29	C5	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
29	C8	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
29	F4	201	PEB	CMB-C2B-C1B	2.88	129.50	125.06
29	L4	202	PEB	C2A-C1A-NA	2.88	110.75	108.27
29	BC	203	PEB	C2A-C1A-NA	2.88	110.75	108.27
29	BE	203	PEB	C2A-C1A-NA	2.88	110.75	108.27
29	T2	203	PEB	OD-C4D-C3D	-2.88	122.94	129.46
29	EA	202	PEB	CMD-C2D-C3D	2.88	134.12	130.06
29	EN	202	PEB	CMD-C2D-C3D	2.88	134.12	130.06
29	EC	201	PEB	C1C-CHB-C4B	-2.88	125.37	128.81
29	EE	201	PEB	C1C-CHB-C4B	-2.88	125.37	128.81
29	LG	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
29	MQ	402	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
29	VJ	201	PEB	CBC-CAC-C2C	-2.88	107.71	112.62
29	VL	201	PEB	CBC-CAC-C2C	-2.88	107.71	112.62
29	KJ	201	PEB	OD-C4D-ND	-2.88	121.67	125.93
29	KL	201	PEB	OD-C4D-ND	-2.88	121.67	125.93
30	MN	402	PUB	OD-C4D-ND	-2.88	121.67	125.93
29	RB	201	PEB	C3B-C4B-NB	2.88	114.24	110.05
29	RM	201	PEB	C3B-C4B-NB	2.88	114.24	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DD	201	PEB	OD-C4D-C3D	-2.88	122.94	129.46
29	QF	202	PEB	C2A-C1A-NA	2.88	110.75	108.27
29	QI	202	PEB	C2A-C1A-NA	2.88	110.75	108.27
29	lB	201	PEB	C3B-C4B-NB	2.88	114.23	110.05
29	lM	201	PEB	C3B-C4B-NB	2.88	114.23	110.05
31	NF	1001	CYC	C2A-C1A-NA	2.88	114.23	110.05
31	NI	1001	CYC	C2A-C1A-NA	2.88	114.23	110.05
29	hJ	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
29	hL	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
29	B4	201	PEB	CMB-C2B-C1B	2.88	129.50	125.06
29	WF	201	PEB	CHB-C4B-C3B	-2.88	118.67	125.32
29	WI	201	PEB	CHB-C4B-C3B	-2.88	118.67	125.32
29	Z7	202	PEB	OD-C4D-C3D	-2.88	122.94	129.46
29	Z9	202	PEB	OD-C4D-C3D	-2.88	122.94	129.46
29	gJ	201	PEB	OD-C4D-ND	-2.88	121.67	125.93
29	gL	201	PEB	OD-C4D-ND	-2.88	121.67	125.93
29	CB	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
29	CM	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
31	HF	1001	CYC	C2A-C1A-NA	2.88	114.23	110.05
31	HI	1001	CYC	C2A-C1A-NA	2.88	114.23	110.05
29	dJ	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
29	dL	203	PEB	C1B-C2B-C3B	-2.88	103.20	106.51
29	O2	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
29	W2	201	PEB	C4B-C3B-C2B	-2.88	103.60	106.78
29	AM	301	PEB	OD-C4D-ND	-2.88	121.67	125.93
29	YB	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
29	hB	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
29	YM	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
29	hM	202	PEB	C3B-C4B-NB	2.88	114.23	110.05
29	dF	202	PEB	CHB-C4B-C3B	-2.88	118.68	125.32
29	dI	202	PEB	CHB-C4B-C3B	-2.88	118.68	125.32
29	h7	202	PEB	OD-C4D-C3D	-2.87	122.95	129.46
29	h9	202	PEB	OD-C4D-C3D	-2.87	122.95	129.46
29	NO	203	PEB	OD-C4D-C3D	-2.87	122.95	129.46
30	A1	305	PUB	OD-C4D-ND	-2.87	121.67	125.93
30	AK	305	PUB	OD-C4D-ND	-2.87	121.67	125.93
30	MG	403	PUB	OA-C1A-NA	-2.87	121.67	125.93
29	D7	1002	PEB	CAB-C3B-C2B	2.87	133.23	127.88
29	D9	1002	PEB	CAB-C3B-C2B	2.87	133.23	127.88
29	MB	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	OB	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	YB	203	PEB	C3B-C4B-NB	2.87	114.23	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MM	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	OM	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	YM	203	PEB	C3B-C4B-NB	2.87	114.23	110.05
31	LF	1001	CYC	C2A-C1A-NA	2.87	114.23	110.05
31	LI	1001	CYC	C2A-C1A-NA	2.87	114.23	110.05
29	HD	201	PEB	CMB-C2B-C1B	2.87	129.49	125.06
29	IJ	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	IL	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	SF	201	PEB	CHB-C4B-C3B	-2.87	118.68	125.32
29	SI	201	PEB	CHB-C4B-C3B	-2.87	118.68	125.32
29	J9	1002	PEB	CAB-C3B-C2B	2.87	133.23	127.88
29	e2	402	PEB	OD-C4D-C3D	-2.87	122.95	129.46
29	VR	203	PEB	OD-C4D-C3D	-2.87	122.95	129.46
29	DC	201	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	FC	201	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	DE	201	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	FE	201	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	WJ	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	WL	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	cB	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	cM	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	U7	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	U9	202	PEB	OD-C4D-ND	-2.87	121.67	125.93
29	PB	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	PM	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	nJ	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	nL	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	JA	203	PEB	C1C-CHB-C4B	-2.87	125.38	128.81
29	JN	203	PEB	C1C-CHB-C4B	-2.87	125.38	128.81
29	GB	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	GM	201	PEB	C3B-C4B-NB	2.87	114.23	110.05
31	DF	1001	CYC	C2A-C1A-NA	2.87	114.23	110.05
31	DI	1001	CYC	C2A-C1A-NA	2.87	114.23	110.05
29	KB	202	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	KM	202	PEB	C3B-C4B-NB	2.87	114.23	110.05
29	A7	304	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	zJ	501	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	HC	203	PEB	C2A-C1A-NA	2.87	110.75	108.27
29	HE	203	PEB	C2A-C1A-NA	2.87	110.75	108.27
29	bF	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
29	bI	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
29	EB	202	PEB	C3B-C4B-NB	2.87	114.22	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	EM	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	eB	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	eM	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	PJ	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	PL	203	PEB	C1B-C2B-C3B	-2.87	103.21	106.51
29	b7	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	b9	202	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	J4	201	PEB	CMB-C2B-C1B	2.87	129.48	125.06
29	JB	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	JM	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	UR	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	V2	203	PEB	OD-C4D-C3D	-2.87	122.96	129.46
29	NB	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	NM	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	CJ	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	CL	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	LC	203	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	LE	203	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	LB	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	fJ	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	fL	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	LM	201	PEB	CBC-CAC-C2C	-2.87	107.72	112.62
29	A3	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	AO	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	R2	201	PEB	OD-C4D-C3D	-2.87	122.96	129.46
29	J7	1002	PEB	CAB-C3B-C2B	2.87	133.22	127.88
29	GJ	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	QJ	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	GL	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	QL	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	FB	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	FM	201	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	IJ	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	IL	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	JC	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
29	JE	202	PEB	C2A-C1A-NA	2.87	110.75	108.27
29	X2	202	PEB	OD-C4D-C3D	-2.87	122.96	129.46
29	N7	1002	PEB	CAB-C3B-C2B	2.87	133.22	127.88
29	N9	1002	PEB	CAB-C3B-C2B	2.87	133.22	127.88
29	HB	201	PEB	CBC-CAC-C2C	-2.87	107.73	112.62
29	HM	201	PEB	CBC-CAC-C2C	-2.87	107.73	112.62
29	JJ	203	PEB	C1B-C2B-C3B	-2.87	103.22	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LJ	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	tJ	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	JL	203	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	LL	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	tL	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	ZF	201	PEB	CHB-C4B-C3B	-2.87	118.70	125.32
29	ZI	201	PEB	CHB-C4B-C3B	-2.87	118.70	125.32
29	mJ	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	mL	201	PEB	OD-C4D-ND	-2.87	121.68	125.93
29	H3	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
29	HO	202	PEB	C4B-C3B-C2B	-2.87	103.61	106.78
29	lB	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
29	lM	202	PEB	C3B-C4B-NB	2.87	114.22	110.05
31	DF	1001	CYC	CAD-CBD-CGD	-2.87	105.72	113.76
31	DI	1001	CYC	CAD-CBD-CGD	-2.87	105.72	113.76
29	CC	201	PEB	C1C-CHB-C4B	-2.87	125.39	128.81
29	CE	201	PEB	C1C-CHB-C4B	-2.87	125.39	128.81
29	AM	303	PEB	OD-C4D-C3D	-2.87	122.97	129.46
29	T2	201	PEB	OD-C4D-C3D	-2.87	122.97	129.46
29	H7	1002	PEB	CAB-C3B-C2B	2.87	133.22	127.88
29	H9	1002	PEB	CAB-C3B-C2B	2.87	133.22	127.88
29	VJ	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	VL	202	PEB	C1B-C2B-C3B	-2.87	103.22	106.51
29	AB	303	PEB	C1C-CHB-C4B	-2.86	125.39	128.81
29	fB	202	PEB	C3B-C4B-NB	2.86	114.22	110.05
29	fM	202	PEB	C3B-C4B-NB	2.86	114.22	110.05
29	DJ	201	PEB	CBC-CAC-C2C	-2.86	107.73	112.62
29	DL	201	PEB	CBC-CAC-C2C	-2.86	107.73	112.62
31	JF	1001	CYC	CAD-CBD-CGD	-2.86	105.73	113.76
31	JI	1001	CYC	CAD-CBD-CGD	-2.86	105.73	113.76
29	BA	203	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	BN	203	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	SB	202	PEB	C3B-C4B-NB	2.86	114.22	110.05
29	SM	202	PEB	C3B-C4B-NB	2.86	114.22	110.05
29	WR	201	PEB	C3B-C4B-NB	2.86	114.22	110.05
31	F7	1001	CYC	OC-C1C-C2C	-2.86	123.90	126.17
29	nJ	201	PEB	CBC-CAC-C2C	-2.86	107.73	112.62
29	nL	201	PEB	CBC-CAC-C2C	-2.86	107.73	112.62
29	g7	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
29	g9	201	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
29	RR	203	PEB	OD-C4D-C3D	-2.86	122.97	129.46
29	TR	201	PEB	OD-C4D-C3D	-2.86	122.97	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A3	202	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	LC	203	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	LE	203	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	AO	202	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
31	D1	1003	CYC	C1A-C2A-C3A	-2.86	103.61	106.78
29	FC	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
29	FE	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
29	aB	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	aM	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
31	NF	1001	CYC	CAD-CBD-CGD	-2.86	105.73	113.76
31	NI	1001	CYC	CAD-CBD-CGD	-2.86	105.73	113.76
29	R2	203	PEB	OD-C4D-C3D	-2.86	122.97	129.46
29	AB	303	PEB	OD-C4D-C3D	-2.86	122.97	129.46
29	K5	201	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	K8	201	PEB	C4B-C3B-C2B	-2.86	103.61	106.78
29	AC	201	PEB	C1C-CHB-C4B	-2.86	125.39	128.81
29	AE	201	PEB	C1C-CHB-C4B	-2.86	125.39	128.81
29	B8	202	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
29	HJ	202	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
29	HL	202	PEB	C1B-C2B-C3B	-2.86	103.22	106.51
29	BC	201	PEB	CHC-C1D-ND	-2.86	110.62	113.95
29	BE	201	PEB	CHC-C1D-ND	-2.86	110.62	113.95
29	vJ	201	PEB	CBC-CAC-C2C	-2.86	107.74	112.62
29	vL	201	PEB	CBC-CAC-C2C	-2.86	107.74	112.62
29	AF	305	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	AI	305	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	IF	201	PEB	CHB-C4B-C3B	-2.86	118.71	125.32
29	II	201	PEB	CHB-C4B-C3B	-2.86	118.71	125.32
29	FA	203	PEB	C1C-CHB-C4B	-2.86	125.39	128.81
29	FN	203	PEB	C1C-CHB-C4B	-2.86	125.39	128.81
29	I3	203	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
29	IO	203	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
31	E1	1001	CYC	C1A-C2A-C3A	-2.86	103.62	106.78
29	MJ	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
29	ML	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
29	WB	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	WM	202	PEB	C3B-C4B-NB	2.86	114.21	110.05
31	LF	1001	CYC	CAD-CBD-CGD	-2.86	105.74	113.76
31	LI	1001	CYC	CAD-CBD-CGD	-2.86	105.74	113.76
29	J9	1002	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	TR	203	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	pJ	201	PEB	CBC-CAC-C2C	-2.86	107.74	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	pL	201	PEB	CBC-CAC-C2C	-2.86	107.74	112.62
29	HB	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
29	HM	202	PEB	OD-C4D-ND	-2.86	121.69	125.93
29	RR	201	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	JD	201	PEB	CMB-C2B-C1B	2.86	129.47	125.06
29	N2	201	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	LC	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
29	LE	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
31	VP	1001	CYC	C2C-C1C-NC	2.86	110.74	108.27
29	J4	202	PEB	CMB-C2B-C1B	2.86	129.47	125.06
29	cJ	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
29	cL	201	PEB	OD-C4D-ND	-2.86	121.69	125.93
29	JQ	203	PEB	OD-C4D-ND	-2.86	121.69	125.93
30	MQ	405	PUB	OA-C1A-NA	-2.86	121.69	125.93
29	CB	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	CM	201	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	A9	304	PEB	C1B-C2B-C3B	-2.86	103.23	106.51
29	J7	1002	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	O7	201	PEB	OD-C4D-ND	-2.86	121.70	125.93
29	O9	201	PEB	OD-C4D-ND	-2.86	121.70	125.93
29	LQ	202	PEB	OD-C4D-ND	-2.86	121.70	125.93
29	OF	201	PEB	CHB-C4B-C3B	-2.86	118.72	125.32
29	OI	201	PEB	CHB-C4B-C3B	-2.86	118.72	125.32
29	bJ	201	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	bL	201	PEB	OD-C4D-C3D	-2.86	122.98	129.46
29	BC	203	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	HC	203	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	BE	203	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	HE	203	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	AF	304	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	AI	304	PEB	C3B-C4B-NB	2.86	114.21	110.05
29	B3	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
29	E3	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
29	BO	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
29	EO	202	PEB	C4B-C3B-C2B	-2.86	103.62	106.78
29	A1	301	PEB	OD-C4D-ND	-2.86	121.70	125.93
29	AK	301	PEB	OD-C4D-ND	-2.86	121.70	125.93
30	MQ	404	PUB	C4B-CHB-C1C	-2.86	125.40	128.81
31	xP	1001	CYC	C2C-C1C-NC	2.86	110.74	108.27
29	dB	202	PEB	C3B-C4B-NB	2.86	114.20	110.05
29	dM	202	PEB	C3B-C4B-NB	2.86	114.20	110.05
29	AJ	201	PEB	OD-C4D-ND	-2.86	121.70	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AL	201	PEB	OD-C4D-ND	-2.86	121.70	125.93
29	N7	1002	PEB	OD-C4D-C3D	-2.86	122.99	129.46
29	N9	1002	PEB	OD-C4D-C3D	-2.86	122.99	129.46
29	LA	203	PEB	C1C-CHB-C4B	-2.86	125.40	128.81
29	LN	203	PEB	C1C-CHB-C4B	-2.86	125.40	128.81
30	yL	303	PUB	OD-C4D-ND	-2.86	121.70	125.93
29	JD	202	PEB	C2A-C1A-NA	2.86	110.73	108.27
30	MN	402	PUB	C2C-C1C-NC	2.85	114.20	110.05
29	NJ	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	fJ	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	NL	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	fL	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	dF	203	PEB	C2A-C1A-NA	2.85	110.73	108.27
29	jF	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
29	dI	203	PEB	C2A-C1A-NA	2.85	110.73	108.27
29	jI	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
29	HG	203	PEB	OD-C4D-ND	-2.85	121.70	125.93
29	qJ	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
29	qL	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
29	FJ	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	FL	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	F7	1002	PEB	OD-C4D-C3D	-2.85	122.99	129.46
29	XR	201	PEB	OD-C4D-C3D	-2.85	122.99	129.46
29	C3	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
29	CO	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
29	JA	203	PEB	C4B-C3B-C2B	-2.85	103.62	106.78
29	JN	203	PEB	C4B-C3B-C2B	-2.85	103.62	106.78
29	tJ	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	tL	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	KC	202	PEB	C1C-CHB-C4B	-2.85	125.40	128.81
29	KE	202	PEB	C1C-CHB-C4B	-2.85	125.40	128.81
29	iJ	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
29	iL	201	PEB	OD-C4D-ND	-2.85	121.70	125.93
30	MA	402	PUB	OD-C4D-ND	-2.85	121.70	125.93
29	ZJ	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	ZL	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	K5	203	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	K8	203	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	GB	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	GM	202	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	FG	203	PEB	CHC-C4C-C3C	-2.85	125.47	130.34
29	JQ	203	PEB	CHC-C4C-C3C	-2.85	125.47	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L7	1002	PEB	CAB-C3B-C2B	2.85	133.19	127.88
29	vJ	202	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	vL	202	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
31	EK	1001	CYC	C1A-C2A-C3A	-2.85	103.63	106.78
31	I1	1001	CYC	CHB-C1B-NB	-2.85	119.94	126.06
29	BA	203	PEB	C1C-CHB-C4B	-2.85	125.40	128.81
29	BN	203	PEB	C1C-CHB-C4B	-2.85	125.40	128.81
29	eF	201	PEB	CBB-CAB-C3B	2.85	120.55	112.63
29	eI	201	PEB	CBB-CAB-C3B	2.85	120.55	112.63
31	JF	1001	CYC	C2A-C1A-NA	2.85	114.20	110.05
31	JI	1001	CYC	C2A-C1A-NA	2.85	114.20	110.05
29	LJ	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	LL	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	AB	301	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	HQ	203	PEB	OD-C4D-ND	-2.85	121.71	125.93
30	yJ	302	PUB	OA-C1A-NA	-2.85	121.71	125.93
30	yJ	303	PUB	OA-C1A-NA	-2.85	121.71	125.93
30	yL	302	PUB	OA-C1A-NA	-2.85	121.71	125.93
29	RF	202	PEB	CMB-C2B-C1B	2.85	129.46	125.06
29	RI	202	PEB	CMB-C2B-C1B	2.85	129.46	125.06
29	RJ	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	ZJ	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	RL	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	ZL	203	PEB	C1B-C2B-C3B	-2.85	103.23	106.51
29	BC	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	BE	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	F9	1002	PEB	OD-C4D-C3D	-2.85	123.00	129.46
29	DB	201	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	HB	201	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	DM	201	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	HM	201	PEB	C3B-C4B-NB	2.85	114.20	110.05
29	hJ	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
29	hL	201	PEB	CBC-CAC-C2C	-2.85	107.75	112.62
31	FF	1001	CYC	CAD-CBD-CGD	-2.85	105.77	113.76
31	FI	1001	CYC	CAD-CBD-CGD	-2.85	105.77	113.76
29	P2	202	PEB	OD-C4D-C3D	-2.85	123.00	129.46
29	HC	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	HE	203	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	JJ	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	JL	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	C3	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	CO	202	PEB	C4B-C3B-C2B	-2.85	103.63	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	QR	201	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	TF	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
29	eF	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06
29	TI	202	PEB	CMB-C2B-C1B	2.85	129.45	125.06
29	eI	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06
29	I3	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	K3	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	LC	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	LE	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	IO	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	KO	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	TJ	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	TL	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	FJ	201	PEB	OD-C4D-C3D	-2.85	123.00	129.46
29	FL	201	PEB	OD-C4D-C3D	-2.85	123.00	129.46
29	PR	202	PEB	OD-C4D-C3D	-2.85	123.00	129.46
30	MQ	404	PUB	C2C-C1C-NC	2.85	114.19	110.05
29	aF	201	PEB	CBB-CAB-C3B	2.85	120.54	112.63
29	aI	201	PEB	CBB-CAB-C3B	2.85	120.54	112.63
29	BJ	203	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
29	BL	203	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
29	EJ	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	EL	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	TJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	TL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	NR	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	bJ	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	bL	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	vJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	vL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	R7	201	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
29	R9	201	PEB	C1B-C2B-C3B	-2.85	103.24	106.51
29	SF	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
29	SI	202	PEB	C2A-C1A-NA	2.85	110.73	108.27
29	OR	201	PEB	C4B-C3B-C2B	-2.85	103.63	106.78
29	PJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	IJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	PL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	IL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
30	MQ	404	PUB	CAB-CBB-CGB	-2.85	105.78	113.76
29	PF	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06
29	PI	203	PEB	CMB-C2B-C1B	2.85	129.45	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	301	PEB	OA-C1A-C2A	-2.85	123.91	126.17
29	AK	301	PEB	OA-C1A-C2A	-2.85	123.91	126.17
29	RJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	hJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	RL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	hL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	QR	201	PEB	C3B-C4B-NB	2.85	114.19	110.05
29	U7	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	h7	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	U9	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	h9	201	PEB	OD-C4D-ND	-2.85	121.71	125.93
29	iF	201	PEB	CBB-CAB-C3B	2.85	120.53	112.63
29	iI	201	PEB	CBB-CAB-C3B	2.85	120.53	112.63
29	jJ	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	jL	201	PEB	CBC-CAC-C2C	-2.85	107.76	112.62
29	tJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	tL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	ZJ	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
29	ZL	201	PEB	OD-C4D-C3D	-2.85	123.01	129.46
31	M9	1001	CYC	C4D-CHA-C1A	2.85	132.21	128.81
31	CK	1001	CYC	C1A-C2A-C3A	-2.84	103.63	106.78
29	cF	201	PEB	CBB-CAB-C3B	2.84	120.53	112.63
29	cI	201	PEB	CBB-CAB-C3B	2.84	120.53	112.63
30	MG	402	PUB	CAB-CBB-CGB	-2.84	105.78	113.76
29	VB	201	PEB	C3B-C4B-NB	2.84	114.19	110.05
29	VM	201	PEB	C3B-C4B-NB	2.84	114.19	110.05
31	FF	1001	CYC	C2A-C1A-NA	2.84	114.19	110.05
31	FI	1001	CYC	C2A-C1A-NA	2.84	114.19	110.05
29	K5	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
29	rJ	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
29	rL	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
29	PR	202	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
29	HG	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	HQ	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
31	K1	1001	CYC	CHB-C1B-NB	-2.84	119.95	126.06
31	KK	1001	CYC	CHB-C1B-NB	-2.84	119.95	126.06
29	F9	1002	PEB	CAB-C3B-C2B	2.84	133.17	127.88
29	cF	202	PEB	CMB-C2B-C1B	2.84	129.44	125.06
29	cI	202	PEB	CMB-C2B-C1B	2.84	129.44	125.06
29	bJ	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
29	bL	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51
29	VR	203	PEB	C1B-C2B-C3B	-2.84	103.24	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	xP	1001	CYC	CBB-CAB-C3B	-2.84	104.59	112.43
29	JJ	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	JL	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
31	EK	1001	CYC	CHB-C1B-NB	-2.84	119.95	126.06
30	MG	402	PUB	C2C-C1C-NC	2.84	114.18	110.05
29	VJ	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	VL	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	MQ	406	PEB	OD-C4D-C3D	-2.84	123.02	129.46
31	C1	1001	CYC	CHB-C1B-NB	-2.84	119.96	126.06
29	L9	1002	PEB	CHC-C1D-ND	2.84	117.25	113.95
29	nJ	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	nL	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
31	N7	1001	CYC	CAB-C3B-C2B	2.84	132.39	127.53
31	N9	1001	CYC	CAB-C3B-C2B	2.84	132.39	127.53
29	S7	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
29	S9	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
29	OJ	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
29	OL	201	PEB	OD-C4D-ND	-2.84	121.72	125.93
30	yJ	303	PUB	OD-C4D-ND	-2.84	121.72	125.93
31	FP	1001	CYC	OC-C1C-C2C	-2.84	123.91	126.17
29	B5	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
29	PJ	201	PEB	CBC-CAC-C2C	-2.84	107.77	112.62
29	PL	201	PEB	CBC-CAC-C2C	-2.84	107.77	112.62
29	UF	203	PEB	C2A-C1A-NA	2.84	110.72	108.27
29	UI	203	PEB	C2A-C1A-NA	2.84	110.72	108.27
29	LJ	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	LL	201	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	XR	203	PEB	OD-C4D-C3D	-2.84	123.02	129.46
29	A7	305	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	A9	305	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	mF	201	PEB	CBB-CAB-C3B	2.84	120.52	112.63
29	mI	201	PEB	CBB-CAB-C3B	2.84	120.52	112.63
29	dJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	dL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	kF	203	PEB	CMB-C2B-C1B	2.84	129.44	125.06
29	kI	203	PEB	CMB-C2B-C1B	2.84	129.44	125.06
30	MG	402	PUB	C4B-CHB-C1C	-2.84	125.42	128.81
29	LD	202	PEB	CMB-C2B-C1B	2.84	129.44	125.06
29	pJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	pL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	I3	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	IO	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	IK	1001	CYC	CHB-C1B-NB	-2.84	119.96	126.06
29	jJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	jL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	A5	203	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
29	A8	203	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
29	JC	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
29	JE	202	PEB	C3B-C4B-NB	2.84	114.18	110.05
29	LG	203	PEB	CMB-C2B-C1B	2.84	129.43	125.06
29	NJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	NL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	V2	203	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
29	PF	201	PEB	CBB-CAB-C3B	2.84	120.51	112.63
29	YF	201	PEB	CBB-CAB-C3B	2.84	120.51	112.63
29	PI	201	PEB	CBB-CAB-C3B	2.84	120.51	112.63
29	YI	201	PEB	CBB-CAB-C3B	2.84	120.51	112.63
29	F7	1002	PEB	CAB-C3B-C2B	2.84	133.16	127.88
29	L9	1002	PEB	CAB-C3B-C2B	2.84	133.16	127.88
29	MG	404	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	DJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	DL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
31	N7	1001	CYC	CAB-C3B-C4B	2.84	125.86	121.38
31	N9	1001	CYC	CAB-C3B-C4B	2.84	125.86	121.38
29	FQ	203	PEB	CHC-C4C-C3C	-2.84	125.50	130.34
29	DC	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	DE	202	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	BJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	rJ	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	BL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
29	rL	201	PEB	OD-C4D-C3D	-2.84	123.03	129.46
31	HF	1001	CYC	CAD-CBD-CGD	-2.84	105.81	113.76
31	HI	1001	CYC	CAD-CBD-CGD	-2.84	105.81	113.76
29	DJ	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
29	DL	202	PEB	C1B-C2B-C3B	-2.84	103.25	106.51
29	DD	201	PEB	OA-C1A-C2A	-2.84	123.92	126.17
29	I5	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	I8	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	UR	201	PEB	C4B-C3B-C2B	-2.84	103.64	106.78
29	LD	201	PEB	CMB-C2B-C1B	2.84	129.43	125.06
29	b7	201	PEB	OD-C4D-ND	-2.84	121.73	125.93
29	b9	201	PEB	OD-C4D-ND	-2.84	121.73	125.93
29	YF	203	PEB	CMB-C2B-C1B	2.84	129.43	125.06
29	YI	203	PEB	CMB-C2B-C1B	2.84	129.43	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VF	201	PEB	CBB-CAB-C3B	2.84	120.50	112.63
29	VI	201	PEB	CBB-CAB-C3B	2.84	120.50	112.63
29	fF	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
29	fI	202	PEB	C2A-C1A-NA	2.84	110.72	108.27
29	XJ	201	PEB	CBC-CAC-C2C	-2.84	107.78	112.62
29	XL	201	PEB	CBC-CAC-C2C	-2.84	107.78	112.62
29	H7	1002	PEB	OD-C4D-C3D	-2.83	123.04	129.46
29	H9	1002	PEB	OD-C4D-C3D	-2.83	123.04	129.46
29	H5	201	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
29	L5	201	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
29	VF	203	PEB	CMB-C2B-C1B	2.83	129.43	125.06
29	VI	203	PEB	CMB-C2B-C1B	2.83	129.43	125.06
29	DG	203	PEB	CHC-C4C-C3C	-2.83	125.50	130.34
29	H8	201	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
29	J5	202	PEB	OD-C4D-ND	-2.83	121.73	125.93
29	J8	202	PEB	OD-C4D-ND	-2.83	121.73	125.93
29	oJ	201	PEB	OD-C4D-ND	-2.83	121.73	125.93
29	oL	201	PEB	OD-C4D-ND	-2.83	121.73	125.93
29	HQ	203	PEB	CHC-C4C-C3C	-2.83	125.50	130.34
29	N7	1002	PEB	CHC-C1D-ND	2.83	117.24	113.95
29	N9	1002	PEB	CHC-C1D-ND	2.83	117.24	113.95
29	I5	203	PEB	C1B-C2B-C3B	-2.83	103.25	106.51
31	VP	1001	CYC	C1B-CHB-C4A	2.83	135.00	128.08
29	D7	1002	PEB	OD-C4D-C3D	-2.83	123.04	129.46
29	D9	1002	PEB	OD-C4D-C3D	-2.83	123.04	129.46
31	H7	1001	CYC	CAB-C3B-C4B	2.83	125.85	121.38
31	H9	1001	CYC	CAB-C3B-C4B	2.83	125.85	121.38
29	N2	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	m7	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	K8	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	m9	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
30	A1	304	PUB	C1D-CHC-C4C	-2.83	107.21	113.37
30	AK	304	PUB	C1D-CHC-C4C	-2.83	107.21	113.37
29	RF	201	PEB	CBB-CAB-C3B	2.83	120.50	112.63
29	RI	201	PEB	CBB-CAB-C3B	2.83	120.50	112.63
29	W7	201	PEB	OD-C4D-ND	-2.83	121.73	125.93
29	W9	201	PEB	OD-C4D-ND	-2.83	121.73	125.93
29	D4	201	PEB	CMB-C2B-C1B	2.83	129.42	125.06
29	BG	203	PEB	CMB-C2B-C1B	2.83	129.42	125.06
29	UJ	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	UL	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	J4	201	PEB	OA-C1A-C2A	-2.83	123.92	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	xP	1001	CYC	C1B-CHB-C4A	2.83	135.00	128.08
29	Z7	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	Z9	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	SJ	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	SL	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	ZF	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
29	ZI	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
29	DA	203	PEB	C1C-CHB-C4B	-2.83	125.43	128.81
29	AM	303	PEB	C1C-CHB-C4B	-2.83	125.43	128.81
29	DN	203	PEB	C1C-CHB-C4B	-2.83	125.43	128.81
31	J7	1001	CYC	CAB-C3B-C4B	2.83	125.85	121.38
29	gF	201	PEB	CBB-CAB-C3B	2.83	120.49	112.63
29	gI	201	PEB	CBB-CAB-C3B	2.83	120.49	112.63
29	j7	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	j9	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	aJ	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	sJ	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	aL	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	sL	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	rJ	201	PEB	CBC-CAC-C2C	-2.83	107.79	112.62
29	rL	201	PEB	CBC-CAC-C2C	-2.83	107.79	112.62
31	E1	1001	CYC	CHB-C1B-NB	-2.83	119.98	126.06
29	M2	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
29	J3	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
29	JO	202	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
29	MR	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
29	F3	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	FO	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	DG	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
29	DQ	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
29	JC	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	JE	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	eJ	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	eL	201	PEB	OD-C4D-ND	-2.83	121.74	125.93
29	I5	203	PEB	C3B-C4B-NB	2.83	114.16	110.05
29	I8	203	PEB	C3B-C4B-NB	2.83	114.16	110.05
29	A5	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
29	GC	201	PEB	C1C-CHB-C4B	-2.83	125.43	128.81
29	GE	201	PEB	C1C-CHB-C4B	-2.83	125.43	128.81
29	BD	202	PEB	CMB-C2B-C1B	2.83	129.42	125.06
29	FA	201	PEB	OA-C1A-C2A	-2.83	123.92	126.17
29	FN	201	PEB	OA-C1A-C2A	-2.83	123.92	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	IC	202	PEB	C3B-C4B-NB	2.83	114.16	110.05
29	IE	202	PEB	C3B-C4B-NB	2.83	114.16	110.05
29	hF	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
29	hI	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
29	NJ	201	PEB	CBC-CAC-C2C	-2.83	107.79	112.62
29	NL	201	PEB	CBC-CAC-C2C	-2.83	107.79	112.62
29	HG	203	PEB	CMB-C2B-C1B	2.83	129.42	125.06
29	k7	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	k9	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	A8	201	PEB	C4B-C3B-C2B	-2.83	103.65	106.78
29	fJ	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
29	fL	201	PEB	OD-C4D-C3D	-2.83	123.05	129.46
29	BQ	203	PEB	CHC-C4C-C3C	-2.83	125.51	130.34
29	U2	201	PEB	C3B-C4B-NB	2.83	114.16	110.05
29	dJ	201	PEB	CBC-CAC-C2C	-2.83	107.80	112.62
29	dL	201	PEB	CBC-CAC-C2C	-2.83	107.80	112.62
30	A7	303	PUB	OA-C1A-NA	-2.83	121.74	125.93
30	A9	303	PUB	OA-C1A-NA	-2.83	121.74	125.93
29	BA	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	BN	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	BG	203	PEB	OD-C4D-C3D	-2.83	123.06	129.46
29	BJ	201	PEB	CBC-CAC-C2C	-2.83	107.80	112.62
29	BL	201	PEB	CBC-CAC-C2C	-2.83	107.80	112.62
31	VP	1001	CYC	CBB-CAB-C3B	-2.83	104.64	112.43
29	L3	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	LO	201	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	D4	201	PEB	OA-C1A-C2A	-2.83	123.93	126.17
31	D7	1001	CYC	OC-C1C-C2C	-2.83	123.93	126.17
31	D9	1001	CYC	OC-C1C-C2C	-2.83	123.93	126.17
29	FG	201	PEB	OD-C4D-C3D	-2.83	123.06	129.46
29	FQ	201	PEB	OD-C4D-C3D	-2.83	123.06	129.46
29	G3	202	PEB	C4B-C3B-C2B	-2.83	103.66	106.78
29	GO	202	PEB	C4B-C3B-C2B	-2.83	103.66	106.78
31	M1	1001	CYC	CHB-C1B-NB	-2.83	119.99	126.06
31	MK	1001	CYC	CHB-C1B-NB	-2.83	119.99	126.06
29	AC	202	PEB	C3B-C4B-NB	2.83	114.16	110.05
29	AE	202	PEB	C3B-C4B-NB	2.83	114.16	110.05
30	MA	402	PUB	C2C-C1C-NC	2.83	114.16	110.05
29	jJ	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	jL	203	PEB	C1B-C2B-C3B	-2.83	103.26	106.51
29	B4	201	PEB	OA-C1A-C2A	-2.82	123.93	126.17
29	J5	201	PEB	CHC-C4C-C3C	-2.82	125.52	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J8	201	PEB	CHC-C4C-C3C	-2.82	125.52	130.34
29	L4	202	PEB	CMB-C2B-C1B	2.82	129.41	125.06
31	F9	1001	CYC	CAB-C3B-C2B	2.82	132.36	127.53
31	D7	1001	CYC	CAB-C3B-C4B	2.82	125.84	121.38
31	D9	1001	CYC	CAB-C3B-C4B	2.82	125.84	121.38
29	d7	201	PEB	OD-C4D-ND	-2.82	121.75	125.93
29	d9	201	PEB	OD-C4D-ND	-2.82	121.75	125.93
29	uJ	202	PEB	OD-C4D-ND	-2.82	121.75	125.93
29	uL	202	PEB	OD-C4D-ND	-2.82	121.75	125.93
29	e7	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	e9	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	Q2	201	PEB	C3B-C4B-NB	2.82	114.16	110.05
29	A5	203	PEB	C3B-C4B-NB	2.82	114.16	110.05
29	A8	203	PEB	C3B-C4B-NB	2.82	114.16	110.05
31	CK	1001	CYC	CHB-C1B-NB	-2.82	120.00	126.06
31	F9	1001	CYC	CAB-C3B-C4B	2.82	125.84	121.38
29	FJ	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	FL	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	FG	203	PEB	OD-C4D-C3D	-2.82	123.06	129.46
31	L9	1001	CYC	CAB-C3B-C4B	2.82	125.84	121.38
29	WF	202	PEB	C2A-C1A-NA	2.82	110.71	108.27
29	WI	202	PEB	C2A-C1A-NA	2.82	110.71	108.27
31	MP	1001	CYC	OC-C1C-C2C	-2.82	123.93	126.17
29	DD	201	PEB	CMB-C2B-C1B	2.82	129.41	125.06
29	XJ	201	PEB	OD-C4D-C3D	-2.82	123.07	129.46
29	XL	201	PEB	OD-C4D-C3D	-2.82	123.07	129.46
29	J5	202	PEB	CAB-C3B-C4B	2.82	130.00	125.01
29	J8	202	PEB	CAB-C3B-C4B	2.82	130.00	125.01
29	HG	203	PEB	OD-C4D-C3D	-2.82	123.07	129.46
30	yL	303	PUB	OA-C1A-NA	-2.82	121.75	125.93
29	B5	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	L4	201	PEB	CMB-C2B-C1B	2.82	129.41	125.06
29	kF	201	PEB	CBB-CAB-C3B	2.82	120.46	112.63
29	kI	201	PEB	CBB-CAB-C3B	2.82	120.46	112.63
29	iF	203	PEB	CMB-C2B-C1B	2.82	129.41	125.06
29	iI	203	PEB	CMB-C2B-C1B	2.82	129.41	125.06
29	c7	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	i7	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	c9	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	i9	201	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	JA	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	XJ	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	XL	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	JN	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	D3	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
29	JA	201	PEB	OA-C1A-C2A	-2.82	123.93	126.17
29	JN	201	PEB	OA-C1A-C2A	-2.82	123.93	126.17
29	CG	201	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
29	EG	201	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
29	CQ	201	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
29	EQ	201	PEB	C4B-C3B-C2B	-2.82	103.66	106.78
29	gF	203	PEB	CMB-C2B-C1B	2.82	129.41	125.06
29	gI	203	PEB	CMB-C2B-C1B	2.82	129.41	125.06
29	A1	302	PEB	CAA-C3A-C4A	2.82	119.91	112.67
29	AK	302	PEB	CAA-C3A-C4A	2.82	119.91	112.67
29	J9	1002	PEB	CHC-C1D-ND	2.82	117.22	113.95
29	TR	203	PEB	C1B-C2B-C3B	-2.82	103.27	106.51
29	HD	202	PEB	CMB-C2B-C1B	2.82	129.40	125.06
29	DG	203	PEB	CMB-C2B-C1B	2.82	129.40	125.06
29	TI	201	PEB	CBB-CAB-C3B	2.82	120.46	112.63
29	DA	201	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
29	DN	201	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
29	FQ	203	PEB	OD-C4D-C3D	-2.82	123.08	129.46
29	P1	203	PEB	C2A-C1A-NA	2.82	110.70	108.27
29	PK	203	PEB	C2A-C1A-NA	2.82	110.70	108.27
29	G3	201	PEB	OD-C4D-ND	-2.82	121.76	125.93
29	GO	201	PEB	OD-C4D-ND	-2.82	121.76	125.93
29	B4	202	PEB	CMB-C2B-C1B	2.82	129.40	125.06
31	D7	1001	CYC	CAB-C3B-C2B	2.82	132.35	127.53
31	D9	1001	CYC	CAB-C3B-C2B	2.82	132.35	127.53
29	JD	201	PEB	OA-C1A-C2A	-2.82	123.93	126.17
29	FC	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
29	GC	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
29	FE	203	PEB	C3B-C4B-NB	2.82	114.15	110.05
29	GE	202	PEB	C3B-C4B-NB	2.82	114.15	110.05
29	JC	202	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
29	JE	202	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
29	aF	203	PEB	CMB-C2B-C1B	2.82	129.40	125.06
29	aI	203	PEB	CMB-C2B-C1B	2.82	129.40	125.06
29	LQ	202	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
29	OF	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
29	OI	202	PEB	C2A-C1A-NA	2.82	110.70	108.27
29	G3	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
29	LG	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GO	201	PEB	OD-C4D-C3D	-2.82	123.08	129.46
29	MQ	402	PEB	OD-C4D-C3D	-2.82	123.08	129.46
29	HQ	203	PEB	CMB-C2B-C1B	2.82	129.40	125.06
29	BQ	203	PEB	OD-C4D-C3D	-2.82	123.08	129.46
31	D1	1003	CYC	CHB-C1B-NB	-2.82	120.01	126.06
29	F4	202	PEB	CMB-C2B-C1B	2.82	129.40	125.06
29	P2	202	PEB	C1B-C2B-C3B	-2.82	103.28	106.51
31	L7	1001	CYC	CAB-C3B-C4B	2.82	125.83	121.38
31	J9	1001	CYC	CAB-C3B-C4B	2.82	125.83	121.38
29	JA	201	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
29	JN	201	PEB	CHC-C4C-C3C	-2.82	125.53	130.34
29	FC	203	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
29	FE	203	PEB	C4B-C3B-C2B	-2.82	103.67	106.78
29	BD	201	PEB	CMB-C2B-C1B	2.81	129.40	125.06
29	CG	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
29	CQ	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
29	Y7	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	Y9	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	JG	203	PEB	CHC-C4C-C3C	-2.81	125.54	130.34
29	LG	203	PEB	CHC-C4C-C3C	-2.81	125.54	130.34
31	J9	1001	CYC	CAB-C3B-C2B	2.81	132.34	127.53
29	DC	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
29	DE	202	PEB	C3B-C4B-NB	2.81	114.14	110.05
29	H7	1002	PEB	CHC-C1D-ND	2.81	117.22	113.95
29	H9	1002	PEB	CHC-C1D-ND	2.81	117.22	113.95
31	GK	1001	CYC	CHB-C1B-NB	-2.81	120.02	126.06
29	I3	201	PEB	OD-C4D-C3D	-2.81	123.08	129.46
29	IO	201	PEB	OD-C4D-C3D	-2.81	123.08	129.46
29	P7	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	P9	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	RR	203	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	BG	203	PEB	CHC-C4C-C3C	-2.81	125.54	130.34
31	F7	1001	CYC	CAB-C3B-C2B	2.81	132.34	127.53
29	J3	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	T7	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	T9	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	JO	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	DA	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
29	YJ	201	PEB	OD-C4D-ND	-2.81	121.76	125.93
29	YL	201	PEB	OD-C4D-ND	-2.81	121.76	125.93
29	DN	202	PEB	OD-C4D-ND	-2.81	121.76	125.93
31	L7	1001	CYC	CAB-C3B-C2B	2.81	132.34	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LA	201	PEB	OA-C1A-C2A	-2.81	123.94	126.17
29	LN	201	PEB	OA-C1A-C2A	-2.81	123.94	126.17
29	H3	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	HO	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	HG	203	PEB	CHC-C4C-C3C	-2.81	125.54	130.34
29	GG	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	GQ	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	J7	1002	PEB	CHC-C1D-ND	2.81	117.21	113.95
31	F7	1001	CYC	CAB-C3B-C4B	2.81	125.82	121.38
29	dF	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	dI	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	G4	203	PEB	CBC-CAC-C2C	-2.81	107.82	112.62
29	IG	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
29	KG	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
29	IQ	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
29	KQ	201	PEB	C4B-C3B-C2B	-2.81	103.67	106.78
31	nP	1001	CYC	OC-C1C-C2C	-2.81	123.94	126.17
29	a7	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	a9	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	LJ	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	LL	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	wJ	303	PEB	CAB-C3B-C2B	2.81	133.11	127.88
29	LG	203	PEB	OD-C4D-C3D	-2.81	123.09	129.46
29	HA	201	PEB	CHC-C4C-C3C	-2.81	125.55	130.34
29	HN	201	PEB	CHC-C4C-C3C	-2.81	125.55	130.34
29	l7	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	l9	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	E4	201	PEB	OD-C4D-C3D	-2.81	123.10	129.46
29	R2	203	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	V7	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	V9	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	H4	202	PEB	CMB-C2B-C1B	2.81	129.39	125.06
29	HQ	203	PEB	OD-C4D-C3D	-2.81	123.10	129.46
29	jJ	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	jL	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	JG	202	PEB	CHA-C1B-NB	-2.81	119.06	124.93
29	JQ	202	PEB	CHA-C1B-NB	-2.81	119.06	124.93
29	e2	402	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	K3	201	PEB	OD-C4D-C3D	-2.81	123.10	129.46
29	KO	201	PEB	OD-C4D-C3D	-2.81	123.10	129.46
29	DQ	203	PEB	CHC-C4C-C3C	-2.81	125.55	130.34
29	D3	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DO	201	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	NR	203	PEB	C1B-C2B-C3B	-2.81	103.28	106.51
29	wJ	302	PEB	C3B-C4B-NB	2.81	114.13	110.05
29	BA	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	BN	202	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	FG	202	PEB	CHA-C1B-NB	-2.81	119.06	124.93
29	FQ	202	PEB	CHA-C1B-NB	-2.81	119.06	124.93
29	T1	202	PEB	C2A-C1A-NA	2.81	110.69	108.27
29	TK	202	PEB	C2A-C1A-NA	2.81	110.69	108.27
29	mF	203	PEB	CMB-C2B-C1B	2.81	129.38	125.06
29	mI	203	PEB	CMB-C2B-C1B	2.81	129.38	125.06
31	J7	1001	CYC	CAB-C3B-C2B	2.81	132.33	127.53
29	DD	201	PEB	OD-C4D-ND	-2.81	121.77	125.93
29	K3	202	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
29	KO	202	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
29	WR	201	PEB	C4B-C3B-C2B	-2.81	103.68	106.78
29	AG	202	PEB	CAB-CBB-CGB	-2.80	107.57	113.60
29	AQ	202	PEB	CAB-CBB-CGB	-2.80	107.57	113.60
29	D4	202	PEB	CMB-C2B-C1B	2.80	129.38	125.06
29	C3	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
29	CO	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
29	T2	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
31	YP	1000	CYC	C1B-CHB-C4A	2.80	134.93	128.08
29	OR	202	PEB	C3B-C4B-NB	2.80	114.13	110.05
29	D7	1002	PEB	CHC-C1D-ND	2.80	117.20	113.95
29	D9	1002	PEB	CHC-C1D-ND	2.80	117.20	113.95
29	wL	303	PEB	CAB-C3B-C2B	2.80	133.10	127.88
29	a1	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
29	aK	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
29	I8	203	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
29	NJ	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	tJ	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	NL	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	tL	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	YF	203	PEB	C3B-C4B-NB	2.80	114.13	110.05
29	YI	203	PEB	C3B-C4B-NB	2.80	114.13	110.05
29	JD	202	PEB	CMB-C2B-C1B	2.80	129.38	125.06
29	DJ	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	DL	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	BQ	203	PEB	CMB-C2B-C1B	2.80	129.38	125.06
29	BG	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
29	BQ	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L8	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
29	GG	202	PEB	CAB-CBB-CGB	-2.80	107.57	113.60
29	GQ	202	PEB	CAB-CBB-CGB	-2.80	107.57	113.60
31	DP	1001	CYC	OC-C1C-C2C	-2.80	123.94	126.17
30	xJ	304	PUB	OA-C1A-NA	-2.80	121.78	125.93
29	DG	202	PEB	CHA-C1B-NB	-2.80	119.07	124.93
29	DQ	202	PEB	CHA-C1B-NB	-2.80	119.07	124.93
29	XJ	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	XL	201	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	KC	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
29	KE	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
29	E3	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
29	EO	201	PEB	OD-C4D-C3D	-2.80	123.11	129.46
29	F4	201	PEB	OA-C1A-C2A	-2.80	123.95	126.17
29	B8	203	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
29	aF	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
29	aI	202	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
29	AG	201	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
29	AQ	201	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
29	R1	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
29	RK	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
29	IG	202	PEB	CAB-CBB-CGB	-2.80	107.58	113.60
29	IQ	202	PEB	CAB-CBB-CGB	-2.80	107.58	113.60
31	KP	1001	CYC	C1B-C2B-C3B	-2.80	104.95	107.87
29	gF	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
29	gI	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
29	U2	201	PEB	C4B-C3B-C2B	-2.80	103.68	106.78
30	MG	402	PUB	CHB-C1C-NC	-2.80	124.94	128.83
29	ID	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
29	dF	203	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
29	dI	203	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
31	H7	1001	CYC	CAB-C3B-C2B	2.80	132.32	127.53
31	H9	1001	CYC	CAB-C3B-C2B	2.80	132.32	127.53
29	FA	202	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	FN	202	PEB	OD-C4D-ND	-2.80	121.78	125.93
29	C5	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
29	C8	203	PEB	C3B-C4B-NB	2.80	114.12	110.05
29	xJ	303	PEB	CAB-C3B-C2B	2.80	133.09	127.88
29	T2	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	C5	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	C8	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	VR	201	PEB	C1B-C2B-C3B	-2.80	103.30	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LG	202	PEB	CHA-C1B-NB	-2.80	119.08	124.93
29	LQ	201	PEB	CHA-C1B-NB	-2.80	119.08	124.93
29	i7	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
29	i9	203	PEB	C2A-C1A-NA	2.80	110.69	108.27
29	DG	203	PEB	OD-C4D-C3D	-2.80	123.12	129.46
29	JG	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
29	JQ	201	PEB	OD-C4D-C3D	-2.80	123.12	129.46
29	F8	201	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	UF	201	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	UI	201	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	LQ	202	PEB	OD-C4D-C3D	-2.80	123.12	129.46
29	LQ	202	PEB	CMB-C2B-C1B	2.80	129.37	125.06
29	LA	202	PEB	OD-C4D-ND	-2.80	121.79	125.93
29	LN	202	PEB	OD-C4D-ND	-2.80	121.79	125.93
29	BA	201	PEB	CHC-C4C-C3C	-2.80	125.57	130.34
29	BN	201	PEB	CHC-C4C-C3C	-2.80	125.57	130.34
29	DA	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	gF	202	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	gI	202	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	DN	203	PEB	C1B-C2B-C3B	-2.80	103.30	106.51
29	Y1	202	PEB	C2A-C1A-NA	2.80	110.68	108.27
29	YK	202	PEB	C2A-C1A-NA	2.80	110.68	108.27
29	JQ	203	PEB	OD-C4D-C3D	-2.80	123.13	129.46
29	JG	203	PEB	CMB-C2B-C1B	2.80	129.37	125.06
29	HA	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
29	HN	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
29	UF	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
29	UI	203	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
31	L9	1001	CYC	CAB-C3B-C2B	2.79	132.31	127.53
29	GD	203	PEB	CBC-CAC-C2C	-2.79	107.85	112.62
29	JG	203	PEB	OD-C4D-C3D	-2.79	123.13	129.46
29	f7	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
29	f9	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
29	a1	201	PEB	C2A-C1A-NA	2.79	110.68	108.27
29	aK	201	PEB	C2A-C1A-NA	2.79	110.68	108.27
29	L4	201	PEB	OA-C1A-C2A	-2.79	123.95	126.17
31	XP	1001	CYC	OC-C1C-C2C	-2.79	123.95	126.17
29	IG	202	PEB	OD-C4D-ND	-2.79	121.79	125.93
29	fJ	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
29	fL	201	PEB	OD-C4D-ND	-2.79	121.79	125.93
29	IQ	202	PEB	OD-C4D-ND	-2.79	121.79	125.93
29	LA	201	PEB	CHC-C4C-C3C	-2.79	125.58	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LN	201	PEB	CHC-C4C-C3C	-2.79	125.58	130.34
29	dD	401	PEB	OD-C4D-C3D	-2.79	123.14	129.46
29	ZF	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
29	ZI	202	PEB	C1B-C2B-C3B	-2.79	103.30	106.51
29	L7	1002	PEB	CHC-C1D-ND	2.79	117.19	113.95
29	kF	203	PEB	C1C-CHB-C4B	-2.79	125.47	128.81
29	kI	203	PEB	C1C-CHB-C4B	-2.79	125.47	128.81
29	lJ	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
29	lL	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
29	wL	302	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	EG	202	PEB	OD-C4D-ND	-2.79	121.80	125.93
29	EQ	202	PEB	OD-C4D-ND	-2.79	121.80	125.93
31	UP	1001	CYC	OC-C1C-C2C	-2.79	123.95	126.17
29	HG	202	PEB	CHA-C1B-NB	-2.79	119.10	124.93
29	HQ	202	PEB	CHA-C1B-NB	-2.79	119.10	124.93
29	CG	202	PEB	CAB-CBB-CGB	-2.79	107.60	113.60
29	CQ	202	PEB	CAB-CBB-CGB	-2.79	107.60	113.60
29	cF	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	iF	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	cI	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	iI	203	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	F9	1002	PEB	CHC-C1D-ND	2.79	117.19	113.95
29	JQ	203	PEB	CMB-C2B-C1B	2.79	129.36	125.06
29	CC	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	CE	202	PEB	C3B-C4B-NB	2.79	114.11	110.05
29	FD	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
29	G8	203	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
29	SF	202	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
29	SI	202	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
29	m7	203	PEB	C2A-C1A-NA	2.79	110.68	108.27
29	m9	203	PEB	C2A-C1A-NA	2.79	110.68	108.27
29	kF	203	PEB	C3B-C4B-NB	2.79	114.10	110.05
29	kI	203	PEB	C3B-C4B-NB	2.79	114.10	110.05
29	F5	201	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
29	A3	201	PEB	OD-C4D-C3D	-2.79	123.15	129.46
29	AO	201	PEB	OD-C4D-C3D	-2.79	123.15	129.46
31	1P	1002	CYC	C1B-CHB-C4A	2.79	134.89	128.08
29	EC	202	PEB	C3B-C4B-NB	2.79	114.10	110.05
29	EE	202	PEB	C3B-C4B-NB	2.79	114.10	110.05
29	nJ	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
29	nL	201	PEB	OD-C4D-ND	-2.79	121.80	125.93
29	I4	201	PEB	OD-C4D-C3D	-2.79	123.15	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K4	203	PEB	CBC-CAC-C2C	-2.79	107.87	112.62
29	A3	202	PEB	C3B-C4B-NB	2.79	114.10	110.05
29	AO	202	PEB	C3B-C4B-NB	2.79	114.10	110.05
29	CD	203	PEB	CBC-CAC-C2C	-2.79	107.87	112.62
29	B5	201	PEB	C1B-C2B-C3B	-2.79	103.31	106.51
29	F7	1002	PEB	CHC-C1D-ND	2.79	117.18	113.95
29	dJ	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	dL	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	FQ	203	PEB	CMB-C2B-C1B	2.78	129.35	125.06
29	F5	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	FA	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	PF	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	PI	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	FN	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	ED	202	PEB	CBC-CAC-C2C	-2.78	107.87	112.62
29	k1	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	kK	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	vJ	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	vL	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	VF	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	VI	202	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	MD	201	PEB	OD-C4D-C3D	-2.78	123.15	129.46
29	DD	202	PEB	CMB-C2B-C1B	2.78	129.35	125.06
29	BA	203	PEB	CHC-C4C-C3C	-2.78	125.59	130.34
29	BN	203	PEB	CHC-C4C-C3C	-2.78	125.59	130.34
29	EG	202	PEB	CAB-CBB-CGB	-2.78	107.61	113.60
29	EQ	202	PEB	CAB-CBB-CGB	-2.78	107.61	113.60
29	e7	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	e9	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	Q7	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	Q9	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
31	EP	1001	CYC	C2B-C1B-NB	2.78	111.06	106.99
29	xL	303	PEB	CAB-C3B-C2B	2.78	133.06	127.88
29	OR	202	PEB	CHA-C1B-NB	-2.78	119.11	124.93
29	JJ	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	JL	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	BG	202	PEB	CHA-C1B-NB	-2.78	119.11	124.93
29	BQ	202	PEB	CHA-C1B-NB	-2.78	119.11	124.93
30	MQ	404	PUB	CHB-C1C-NC	-2.78	124.97	128.83
29	R1	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	RK	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	H8	203	PEB	C1B-C2B-C3B	-2.78	103.31	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G5	201	PEB	C3B-C4B-NB	2.78	114.09	110.05
29	N2	201	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
29	R2	201	PEB	C1B-C2B-C3B	-2.78	103.31	106.51
31	uP	1001	CYC	OC-C1C-C2C	-2.78	123.96	126.17
29	T7	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	T9	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
31	GP	1001	CYC	C1B-C2B-C3B	-2.78	104.97	107.87
29	jF	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	jI	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
31	IP	1001	CYC	OC-C1C-C2C	-2.78	123.96	126.17
29	g7	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	g9	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	DO	202	PEB	C3B-C4B-NB	2.78	114.09	110.05
30	xL	304	PUB	OA-C1A-NA	-2.78	121.81	125.93
29	YF	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	YI	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	KG	202	PEB	CAB-CBB-CGB	-2.78	107.62	113.60
29	KQ	202	PEB	CAB-CBB-CGB	-2.78	107.62	113.60
29	KD	201	PEB	OD-C4D-C3D	-2.78	123.17	129.46
29	X2	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	XR	203	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	D4	201	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	AG	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
29	AQ	202	PEB	OD-C4D-ND	-2.78	121.81	125.93
31	iP	1001	CYC	C2B-C1B-NB	2.78	111.05	106.99
29	BJ	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	BL	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	a7	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	a9	203	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	LA	203	PEB	CHC-C4C-C3C	-2.78	125.60	130.34
29	LN	203	PEB	CHC-C4C-C3C	-2.78	125.60	130.34
29	TF	201	PEB	C3B-C4B-NB	2.78	114.09	110.05
29	L5	203	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	eF	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	eI	202	PEB	C1B-C2B-C3B	-2.78	103.32	106.51
29	V1	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	VK	201	PEB	C2A-C1A-NA	2.78	110.67	108.27
29	RJ	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	RL	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	GD	201	PEB	OD-C4D-C3D	-2.78	123.17	129.46
29	DA	203	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	HD	201	PEB	OD-C4D-ND	-2.78	121.82	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TJ	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	rJ	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	TL	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	rL	201	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	DN	203	PEB	OD-C4D-ND	-2.78	121.82	125.93
29	F8	203	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
29	lF	202	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
29	lI	202	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
31	hP	1001	CYC	OC-C1C-C2C	-2.77	123.97	126.17
29	pJ	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
29	pL	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
29	RF	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	RI	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	FD	202	PEB	CMB-C2B-C1B	2.77	129.34	125.06
31	EP	1001	CYC	C1B-C2B-C3B	-2.77	104.98	107.87
29	LA	203	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
29	LN	203	PEB	C1B-C2B-C3B	-2.77	103.32	106.51
30	MQ	404	PUB	CBA-CAA-C3A	-2.77	108.77	112.98
31	pP	1001	CYC	C2B-C1B-NB	2.77	111.05	106.99
29	TF	202	PEB	C1C-CHB-C4B	-2.77	125.50	128.81
29	TI	202	PEB	C1C-CHB-C4B	-2.77	125.50	128.81
29	F8	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	FJ	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
29	FL	201	PEB	OD-C4D-ND	-2.77	121.82	125.93
30	A7	302	PUB	OA-C1A-NA	-2.77	121.82	125.93
30	A9	302	PUB	OA-C1A-NA	-2.77	121.82	125.93
30	AM	305	PUB	OD-C4D-ND	-2.77	121.82	125.93
29	MD	203	PEB	CBC-CAC-C2C	-2.77	107.89	112.62
31	CP	1001	CYC	C2B-C1B-NB	2.77	111.05	106.99
29	B8	201	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	Q2	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
29	P1	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	PK	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	xJ	301	PEB	CMB-C2B-C1B	2.77	129.33	125.06
29	L8	203	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	QF	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	mF	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	QI	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	mI	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	KG	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	KQ	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	G4	201	PEB	OD-C4D-C3D	-2.77	123.18	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C4	203	PEB	CBC-CAC-C2C	-2.77	107.89	112.62
29	TF	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	TI	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
31	IP	1001	CYC	C1B-C2B-C3B	-2.77	104.98	107.87
29	H4	201	PEB	OD-C4D-ND	-2.77	121.83	125.93
31	KP	1001	CYC	C2B-C1B-NB	2.77	111.04	106.99
29	JA	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	JN	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	DQ	203	PEB	OD-C4D-C3D	-2.77	123.19	129.46
29	iF	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	iI	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	XR	201	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
31	AP	1001	CYC	C1B-C2B-C3B	-2.77	104.98	107.87
29	ID	203	PEB	CBC-CAC-C2C	-2.77	107.89	112.62
29	GG	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
29	GQ	201	PEB	C4B-C3B-C2B	-2.77	103.72	106.78
29	C4	201	PEB	OD-C4D-C3D	-2.77	123.19	129.46
29	PF	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	mF	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	PI	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	mI	203	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	FA	201	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
29	FN	201	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
29	KD	203	PEB	CBC-CAC-C2C	-2.77	107.89	112.62
29	MG	404	PEB	CMA-C2A-C1A	-2.77	106.44	112.40
29	HF	1002	PEB	CAA-C3A-C2A	-2.77	107.34	114.26
29	HI	1002	PEB	CAA-C3A-C2A	-2.77	107.34	114.26
29	BD	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	C3	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	CO	202	PEB	C3B-C4B-NB	2.77	114.08	110.05
31	OP	1001	CYC	OC-C1C-C2C	-2.77	123.97	126.17
29	NF	1002	PEB	CAA-C3A-C2A	-2.77	107.34	114.26
29	NI	1002	PEB	CAA-C3A-C2A	-2.77	107.34	114.26
29	G8	201	PEB	C3B-C4B-NB	2.77	114.08	110.05
29	FG	203	PEB	CMB-C2B-C1B	2.77	129.33	125.06
29	PF	203	PEB	C1C-CHB-C4B	-2.77	125.50	128.81
29	PI	203	PEB	C1C-CHB-C4B	-2.77	125.50	128.81
31	tP	1001	CYC	C1B-C2B-C3B	-2.77	104.98	107.87
29	HA	202	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	ZJ	201	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	ZL	201	PEB	OD-C4D-ND	-2.77	121.83	125.93
29	HN	202	PEB	OD-C4D-ND	-2.77	121.83	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	wJ	304	PUB	OA-C1A-NA	-2.77	121.83	125.93
29	i1	201	PEB	C2A-C1A-NA	2.77	110.66	108.27
29	R7	203	PEB	C2A-C1A-NA	2.77	110.66	108.27
29	c7	203	PEB	C2A-C1A-NA	2.77	110.66	108.27
29	R9	203	PEB	C2A-C1A-NA	2.77	110.66	108.27
29	c9	203	PEB	C2A-C1A-NA	2.77	110.66	108.27
29	iK	201	PEB	C2A-C1A-NA	2.77	110.66	108.27
29	aF	203	PEB	C3B-C4B-NB	2.77	114.07	110.05
29	aI	203	PEB	C3B-C4B-NB	2.77	114.07	110.05
29	hF	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	hI	202	PEB	C1B-C2B-C3B	-2.77	103.33	106.51
29	M4	203	PEB	C3B-C4B-NB	2.76	114.07	110.05
29	MR	202	PEB	C3B-C4B-NB	2.76	114.07	110.05
29	m1	201	PEB	C2A-C1A-NA	2.76	110.66	108.27
29	mK	201	PEB	C2A-C1A-NA	2.76	110.66	108.27
29	eF	203	PEB	C3B-C4B-NB	2.76	114.07	110.05
29	eI	203	PEB	C3B-C4B-NB	2.76	114.07	110.05
29	HG	202	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
29	HQ	202	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
29	kF	202	PEB	C1B-C2B-C3B	-2.76	103.33	106.51
29	kI	202	PEB	C1B-C2B-C3B	-2.76	103.33	106.51
31	fP	1001	CYC	OC-C1C-C2C	-2.76	123.98	126.17
29	Y7	203	PEB	C2A-C1A-NA	2.76	110.66	108.27
29	Y9	203	PEB	C2A-C1A-NA	2.76	110.66	108.27
29	VF	203	PEB	C3B-C4B-NB	2.76	114.07	110.05
29	VI	203	PEB	C3B-C4B-NB	2.76	114.07	110.05
31	lP	1001	CYC	C2B-C1B-NB	2.76	111.03	106.99
29	gF	203	PEB	C1C-CHB-C4B	-2.76	125.51	128.81
29	gI	203	PEB	C1C-CHB-C4B	-2.76	125.51	128.81
31	pP	1001	CYC	C1B-C2B-C3B	-2.76	104.99	107.87
29	DG	202	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
29	DQ	202	PEB	CAB-CBB-CGB	-2.76	107.66	113.60
29	RR	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	FA	203	PEB	CHC-C4C-C3C	-2.76	125.63	130.34
29	FN	203	PEB	CHC-C4C-C3C	-2.76	125.63	130.34
29	K4	201	PEB	OD-C4D-C3D	-2.76	123.20	129.46
29	J5	202	PEB	OD-C4D-C3D	-2.76	123.20	129.46
29	J8	202	PEB	OD-C4D-C3D	-2.76	123.20	129.46
29	TR	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	Z1	203	PEB	OD-C4D-ND	-2.76	121.84	125.93
29	hJ	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
29	ZK	203	PEB	OD-C4D-ND	-2.76	121.84	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	hL	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
31	GF	1001	CYC	C1A-C2A-C3A	-2.76	103.73	106.78
31	GI	1001	CYC	C1A-C2A-C3A	-2.76	103.73	106.78
29	V2	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	G8	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	WF	202	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	WI	202	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	F4	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
29	J4	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
29	bJ	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
29	bL	201	PEB	OD-C4D-ND	-2.76	121.84	125.93
29	G5	203	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	eF	203	PEB	C1C-CHB-C4B	-2.76	125.51	128.81
29	eI	203	PEB	C1C-CHB-C4B	-2.76	125.51	128.81
29	OF	202	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	OI	202	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
31	UP	1001	CYC	C4A-C3A-C2A	-2.76	103.34	106.51
29	HD	202	PEB	OA-C1A-C2A	-2.76	123.98	126.17
29	NO	201	PEB	CAA-C3A-C2A	-2.76	107.37	114.26
29	E3	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
29	EO	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
29	DA	203	PEB	CHC-C4C-C3C	-2.76	125.63	130.34
29	DN	203	PEB	CHC-C4C-C3C	-2.76	125.63	130.34
29	xL	301	PEB	CMB-C2B-C1B	2.76	129.31	125.06
29	E4	203	PEB	CBC-CAC-C2C	-2.76	107.91	112.62
29	BB	301	PEB	C2A-C1A-NA	2.76	110.65	108.27
29	BM	301	PEB	C2A-C1A-NA	2.76	110.65	108.27
31	iP	1001	CYC	C1B-C2B-C3B	-2.76	104.99	107.87
29	U1	203	PEB	OD-C4D-ND	-2.76	121.85	125.93
29	L4	201	PEB	OD-C4D-ND	-2.76	121.85	125.93
29	UK	203	PEB	OD-C4D-ND	-2.76	121.85	125.93
29	I3	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
29	xL	302	PEB	C3B-C4B-NB	2.76	114.06	110.05
29	IO	202	PEB	C3B-C4B-NB	2.76	114.06	110.05
31	AP	1001	CYC	C2B-C1B-NB	2.76	111.02	106.99
31	KI	1001	CYC	C1A-C2A-C3A	-2.76	103.73	106.78
29	NR	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
31	CP	1001	CYC	C1B-C2B-C3B	-2.76	105.00	107.87
31	NP	1001	CYC	C1B-C2B-C3B	-2.76	105.00	107.87
31	eP	1001	CYC	C1B-C2B-C3B	-2.76	105.00	107.87
31	gP	1001	CYC	C1B-C2B-C3B	-2.76	105.00	107.87
29	B3	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BO	201	PEB	C1B-C2B-C3B	-2.76	103.34	106.51
29	DF	1002	PEB	CAA-C3A-C2A	-2.76	107.38	114.26
29	DI	1002	PEB	CAA-C3A-C2A	-2.76	107.38	114.26
31	mP	1001	CYC	C1B-C2B-C3B	-2.76	105.00	107.87
29	mF	203	PEB	C1C-CHB-C4B	-2.75	125.52	128.81
29	mI	203	PEB	C1C-CHB-C4B	-2.75	125.52	128.81
29	VJ	201	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	VL	201	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	fF	202	PEB	C1B-C2B-C3B	-2.75	103.34	106.51
29	fI	202	PEB	C1B-C2B-C3B	-2.75	103.34	106.51
29	A1	301	PEB	OD-C4D-C3D	-2.75	123.22	129.46
29	AK	301	PEB	OD-C4D-C3D	-2.75	123.22	129.46
31	BP	1001	CYC	OC-C1C-C2C	-2.75	123.98	126.17
31	1P	1001	CYC	OC-C1C-C2C	-2.75	123.98	126.17
29	B8	201	PEB	C3B-C4B-NB	2.75	114.06	110.05
31	GP	1001	CYC	C2B-C1B-NB	2.75	111.02	106.99
29	BG	202	PEB	CAB-CBB-CGB	-2.75	107.68	113.60
29	BQ	202	PEB	CAB-CBB-CGB	-2.75	107.68	113.60
29	JA	203	PEB	CHC-C4C-C3C	-2.75	125.64	130.34
29	JN	203	PEB	CHC-C4C-C3C	-2.75	125.64	130.34
29	CD	201	PEB	OD-C4D-C3D	-2.75	123.22	129.46
29	H4	202	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	LA	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	LN	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	LF	1002	PEB	CAA-C3A-C2A	-2.75	107.38	114.26
29	LI	1002	PEB	CAA-C3A-C2A	-2.75	107.38	114.26
29	HA	203	PEB	CHC-C4C-C3C	-2.75	125.64	130.34
29	HN	203	PEB	CHC-C4C-C3C	-2.75	125.64	130.34
29	MQ	406	PEB	CMA-C2A-C1A	-2.75	106.47	112.40
29	BA	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	BN	203	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	JF	1002	PEB	CAA-C3A-C2A	-2.75	107.38	114.26
29	JI	1002	PEB	CAA-C3A-C2A	-2.75	107.38	114.26
31	rP	1001	CYC	C2B-C1B-NB	2.75	111.02	106.99
29	FG	202	PEB	CAB-CBB-CGB	-2.75	107.68	113.60
29	FQ	202	PEB	CAB-CBB-CGB	-2.75	107.68	113.60
31	cP	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
29	A7	305	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	A9	305	PEB	OD-C4D-ND	-2.75	121.85	125.93
29	G5	201	PEB	C1B-C2B-C3B	-2.75	103.35	106.51
31	qP	1001	CYC	OC-C1C-C2C	-2.75	123.98	126.17
29	H5	203	PEB	C1B-C2B-C3B	-2.75	103.35	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DQ	203	PEB	CMB-C2B-C1B	2.75	129.30	125.06
31	PP	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
29	HA	203	PEB	OD-C4D-ND	-2.75	121.86	125.93
29	HN	203	PEB	OD-C4D-ND	-2.75	121.86	125.93
29	F5	201	PEB	C3B-C4B-NB	2.75	114.05	110.05
31	SP	1001	CYC	C4A-C3A-C2A	-2.75	103.35	106.51
31	TP	1001	CYC	C1B-C2B-C3B	-2.75	105.00	107.87
31	sP	1001	CYC	OC-C1C-C2C	-2.75	123.99	126.17
29	M4	201	PEB	OD-C4D-C3D	-2.75	123.23	129.46
29	LG	202	PEB	CAB-CBB-CGB	-2.75	107.69	113.60
29	LQ	201	PEB	CAB-CBB-CGB	-2.75	107.69	113.60
31	RP	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
31	vP	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
29	M3	201	PEB	CAA-C3A-C2A	-2.75	107.39	114.26
29	MO	201	PEB	CAA-C3A-C2A	-2.75	107.39	114.26
29	m1	202	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	mK	202	PEB	C2A-C1A-NA	2.75	110.64	108.27
31	oP	1001	CYC	C4A-C3A-C2A	-2.75	103.35	106.51
29	JD	201	PEB	OD-C4D-ND	-2.75	121.86	125.93
29	CA	201	PEB	OD-C4D-C3D	-2.75	123.24	129.46
29	CN	201	PEB	OD-C4D-C3D	-2.75	123.24	129.46
29	T1	201	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	c1	203	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	g1	201	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	g1	203	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	TK	201	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	cK	203	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	gK	201	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	gK	203	PEB	C2A-C1A-NA	2.75	110.64	108.27
29	G3	202	PEB	C3B-C4B-NB	2.75	114.04	110.05
29	GO	202	PEB	C3B-C4B-NB	2.75	114.04	110.05
31	JP	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
31	mP	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
31	kP	1001	CYC	OC-C1C-C2C	-2.75	123.99	126.17
31	RP	1001	CYC	C1B-C2B-C3B	-2.75	105.01	107.87
29	J4	202	PEB	OD-C4D-ND	-2.75	121.86	125.93
29	dD	401	PEB	OD-C4D-ND	-2.75	121.86	125.93
30	wL	304	PUB	OA-C1A-NA	-2.75	121.86	125.93
29	GD	203	PEB	OD-C4D-ND	-2.74	121.86	125.93
29	V1	203	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	c1	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	e1	201	PEB	C2A-C1A-NA	2.74	110.64	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e1	203	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	VK	203	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	cK	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	eK	201	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	eK	203	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	LD	201	PEB	OA-C1A-C2A	-2.74	123.99	126.17
29	bF	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
29	bI	202	PEB	C1B-C2B-C3B	-2.74	103.36	106.51
31	FP	1001	CYC	C4A-C3A-C2A	-2.74	103.36	106.51
29	FF	1002	PEB	CAA-C3A-C2A	-2.74	107.40	114.26
29	FI	1002	PEB	CAA-C3A-C2A	-2.74	107.40	114.26
29	g1	203	PEB	C3B-C4B-NB	2.74	114.04	110.05
29	gK	203	PEB	C3B-C4B-NB	2.74	114.04	110.05
29	JG	202	PEB	CAB-CBB-CGB	-2.74	107.70	113.60
29	JQ	202	PEB	CAB-CBB-CGB	-2.74	107.70	113.60
29	AA	201	PEB	OD-C4D-C3D	-2.74	123.24	129.46
29	AN	201	PEB	OD-C4D-C3D	-2.74	123.24	129.46
30	MG	402	PUB	CBA-CAA-C3A	-2.74	108.82	112.98
29	N3	201	PEB	CAA-C3A-C2A	-2.74	107.41	114.26
29	K4	201	PEB	OD-C4D-ND	-2.74	121.87	125.93
29	iF	203	PEB	C1C-CHB-C4B	-2.74	125.53	128.81
29	iI	203	PEB	C1C-CHB-C4B	-2.74	125.53	128.81
29	I4	202	PEB	C2A-C1A-NA	2.74	110.64	108.27
29	B4	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
31	PP	1001	CYC	C1B-C2B-C3B	-2.74	105.01	107.87
31	MP	1001	CYC	C4A-C3A-C2A	-2.74	103.36	106.51
29	xJ	302	PEB	C3B-C4B-NB	2.74	114.04	110.05
31	gP	1001	CYC	C2B-C1B-NB	2.74	111.00	106.99
31	tP	1001	CYC	C2B-C1B-NB	2.74	111.00	106.99
31	KF	1001	CYC	C1A-C2A-C3A	-2.74	103.75	106.78
29	PJ	201	PEB	OD-C4D-ND	-2.74	121.87	125.93
29	PL	201	PEB	OD-C4D-ND	-2.74	121.87	125.93
29	GA	201	PEB	OD-C4D-C3D	-2.74	123.25	129.46
29	GN	201	PEB	OD-C4D-C3D	-2.74	123.25	129.46
31	cP	1001	CYC	C2B-C1B-NB	2.74	111.00	106.99
29	J5	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	J8	201	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	JA	203	PEB	OD-C4D-ND	-2.74	121.87	125.93
29	JN	203	PEB	OD-C4D-ND	-2.74	121.87	125.93
31	rP	1001	CYC	C1B-C2B-C3B	-2.74	105.01	107.87
29	h1	202	PEB	OD-C4D-ND	-2.74	121.87	125.93
29	hK	202	PEB	OD-C4D-ND	-2.74	121.87	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	uP	1001	CYC	C4A-C3A-C2A	-2.74	103.36	106.51
29	CD	201	PEB	OD-C4D-ND	-2.74	121.87	125.93
29	H3	202	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	K3	202	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	HO	202	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	KO	202	PEB	C3B-C4B-NB	2.74	114.03	110.05
31	NP	1001	CYC	C2B-C1B-NB	2.74	110.99	106.99
29	O1	202	PEB	OD-C4D-ND	-2.74	121.88	125.93
29	OK	202	PEB	OD-C4D-ND	-2.74	121.88	125.93
29	VF	203	PEB	C1C-CHB-C4B	-2.74	125.54	128.81
29	VI	203	PEB	C1C-CHB-C4B	-2.74	125.54	128.81
31	OP	1001	CYC	C4A-C3A-C2A	-2.74	103.37	106.51
29	V1	203	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	VK	203	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	DO	202	PEB	CBC-CAC-C2C	-2.74	107.95	112.62
29	HD	202	PEB	OD-C4D-ND	-2.74	121.88	125.93
31	vP	1001	CYC	C1B-C2B-C3B	-2.74	105.02	107.87
31	QP	1001	CYC	OC-C1C-C2C	-2.74	124.00	126.17
31	wP	1001	CYC	OC-C1C-C2C	-2.74	124.00	126.17
29	I3	203	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	IO	203	PEB	C3B-C4B-NB	2.74	114.03	110.05
29	k7	203	PEB	C2A-C1A-NA	2.74	110.63	108.27
29	k9	203	PEB	C2A-C1A-NA	2.74	110.63	108.27
29	IA	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
29	IN	201	PEB	OD-C4D-C3D	-2.74	123.26	129.46
29	aF	203	PEB	C1C-CHB-C4B	-2.73	125.54	128.81
29	cF	202	PEB	C1C-CHB-C4B	-2.73	125.54	128.81
29	aI	203	PEB	C1C-CHB-C4B	-2.73	125.54	128.81
29	cI	202	PEB	C1C-CHB-C4B	-2.73	125.54	128.81
29	R1	203	PEB	C3B-C4B-NB	2.73	114.03	110.05
29	RK	203	PEB	C3B-C4B-NB	2.73	114.03	110.05
29	j1	202	PEB	OD-C4D-ND	-2.73	121.88	125.93
29	jK	202	PEB	OD-C4D-ND	-2.73	121.88	125.93
31	SP	1001	CYC	OC-C1C-C2C	-2.73	124.00	126.17
29	i1	203	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	V7	203	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	V9	203	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	ID	202	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	iK	203	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	J4	201	PEB	CAB-CBB-CGB	-2.73	107.72	113.60
29	H8	201	PEB	C3B-C4B-NB	2.73	114.03	110.05
31	BP	1001	CYC	C4A-C3A-C2A	-2.73	103.37	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	302	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	AK	302	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	f1	202	PEB	OD-C4D-ND	-2.73	121.88	125.93
29	fK	202	PEB	OD-C4D-ND	-2.73	121.88	125.93
29	YF	203	PEB	C1C-CHB-C4B	-2.73	125.55	128.81
29	YI	203	PEB	C1C-CHB-C4B	-2.73	125.55	128.81
29	OF	203	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
29	OI	203	PEB	C1B-C2B-C3B	-2.73	103.37	106.51
29	Y1	201	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	HA	202	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	YK	201	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	HN	202	PEB	C2A-C1A-NA	2.73	110.63	108.27
29	mB	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	mM	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	e1	203	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	K5	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	K8	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	eK	203	PEB	C3B-C4B-NB	2.73	114.02	110.05
31	IF	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
31	II	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
29	RB	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	RM	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	KA	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	KN	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	B4	201	PEB	OD-C4D-ND	-2.73	121.89	125.93
31	jP	1001	CYC	OC-C1C-C2C	-2.73	124.00	126.17
29	NB	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
29	NM	201	PEB	OD-C4D-C3D	-2.73	123.27	129.46
31	wP	1001	CYC	C4A-C3A-C2A	-2.73	103.37	106.51
30	MQ	404	PUB	CBC-CAC-C2C	-2.73	105.04	112.63
29	L4	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
29	JD	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
29	wJ	301	PEB	CMB-C2B-C1B	2.73	129.27	125.06
31	HP	1001	CYC	OC-C1C-C2C	-2.73	124.00	126.17
29	Y1	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	m1	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	YK	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	mK	202	PEB	C3B-C4B-NB	2.73	114.02	110.05
30	xL	305	PUB	CHA-C1B-C2B	-2.73	125.68	130.34
29	MR	201	PEB	O1C-CGC-CBC	-2.73	114.31	123.08
29	d1	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
29	dK	202	PEB	OD-C4D-ND	-2.73	121.89	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H5	201	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	P7	203	PEB	C2A-C1A-NA	2.73	110.62	108.27
29	P9	203	PEB	C2A-C1A-NA	2.73	110.62	108.27
29	c1	203	PEB	C3B-C4B-NB	2.73	114.02	110.05
29	cK	203	PEB	C3B-C4B-NB	2.73	114.02	110.05
31	MF	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
31	MI	1001	CYC	C1A-C2A-C3A	-2.73	103.76	106.78
29	RF	202	PEB	C1C-CHB-C4B	-2.73	125.55	128.81
29	RI	202	PEB	C1C-CHB-C4B	-2.73	125.55	128.81
30	MA	403	PUB	CAC-C2C-C1C	2.73	129.83	125.01
29	P1	201	PEB	C2A-C1A-NA	2.73	110.62	108.27
29	PK	201	PEB	C2A-C1A-NA	2.73	110.62	108.27
31	IP	1001	CYC	C4A-C3A-C2A	-2.73	103.38	106.51
31	jP	1001	CYC	C4A-C3A-C2A	-2.73	103.38	106.51
29	TB	201	PEB	OD-C4D-C3D	-2.73	123.28	129.46
29	TM	201	PEB	OD-C4D-C3D	-2.73	123.28	129.46
29	ID	201	PEB	OD-C4D-ND	-2.73	121.89	125.93
31	TP	1001	CYC	C2B-C1B-NB	2.73	110.98	106.99
30	MG	402	PUB	CBC-CAC-C2C	-2.73	105.06	112.63
29	b1	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
29	bK	202	PEB	OD-C4D-ND	-2.73	121.89	125.93
29	DB	201	PEB	OD-C4D-C3D	-2.72	123.29	129.46
29	DM	201	PEB	OD-C4D-C3D	-2.72	123.29	129.46
29	F4	202	PEB	OD-C4D-ND	-2.72	121.89	125.93
29	FD	202	PEB	OD-C4D-ND	-2.72	121.89	125.93
30	AB	305	PUB	OD-C4D-ND	-2.72	121.89	125.93
30	wJ	305	PUB	CHA-C1B-C2B	-2.72	125.69	130.34
31	DP	1001	CYC	C4A-C3A-C2A	-2.72	103.38	106.51
30	xJ	305	PUB	CAC-CBC-CGC	-2.72	107.74	113.60
29	E4	201	PEB	OD-C4D-ND	-2.72	121.89	125.93
29	AB	301	PEB	OD-C4D-C3D	-2.72	123.29	129.46
29	B5	201	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	wL	302	PEB	C1C-CHB-C4B	-2.72	125.56	128.81
29	F4	202	PEB	OA-C1A-C2A	-2.72	124.01	126.17
31	oP	1001	CYC	OC-C1C-C2C	-2.72	124.01	126.17
29	AM	301	PEB	OD-C4D-C3D	-2.72	123.29	129.46
29	S1	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
29	LD	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
29	SK	202	PEB	OD-C4D-ND	-2.72	121.90	125.93
29	U1	202	PEB	CBC-CAC-C2C	-2.72	107.97	112.62
29	UK	202	PEB	CBC-CAC-C2C	-2.72	107.97	112.62
29	a1	203	PEB	C3B-C4B-NB	2.72	114.01	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k1	203	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	aK	203	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	kK	203	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	FA	202	PEB	C2A-C1A-NA	2.72	110.62	108.27
29	FN	202	PEB	C2A-C1A-NA	2.72	110.62	108.27
29	B3	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	F3	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	BO	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	FO	202	PEB	C3B-C4B-NB	2.72	114.01	110.05
29	XB	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	XM	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	KD	201	PEB	OD-C4D-ND	-2.72	121.90	125.93
30	MN	403	PUB	OA-C1A-NA	-2.72	121.90	125.93
29	gB	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	gM	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
30	AM	304	PUB	CBA-CAA-C3A	-2.72	108.85	112.98
31	fP	1001	CYC	C4A-C3A-C2A	-2.72	103.39	106.51
31	qP	1001	CYC	C4A-C3A-C2A	-2.72	103.39	106.51
29	wJ	302	PEB	C1C-CHB-C4B	-2.72	125.56	128.81
30	wL	305	PUB	CHA-C1B-C2B	-2.72	125.70	130.34
30	AM	305	PUB	CMD-C2D-C3D	2.72	131.85	127.77
29	VB	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	VM	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	OR	201	PEB	O1C-CGC-CBC	-2.72	114.34	123.08
31	hP	1001	CYC	C4A-C3A-C2A	-2.72	103.39	106.51
29	EA	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	EN	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	JD	201	PEB	CAB-CBB-CGB	-2.72	107.75	113.60
29	FA	203	PEB	OD-C4D-ND	-2.72	121.90	125.93
29	BD	201	PEB	OD-C4D-ND	-2.72	121.90	125.93
29	FN	203	PEB	OD-C4D-ND	-2.72	121.90	125.93
29	LB	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	LM	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
31	XP	1001	CYC	C4A-C3A-C2A	-2.72	103.39	106.51
29	W2	201	PEB	O1C-CGC-CBC	-2.72	114.35	123.08
29	W1	201	PEB	CBC-CAC-C2C	-2.72	107.98	112.62
29	WK	201	PEB	CBC-CAC-C2C	-2.72	107.98	112.62
29	J3	202	PEB	C3B-C4B-NB	2.72	114.00	110.05
29	JO	202	PEB	C3B-C4B-NB	2.72	114.00	110.05
30	xJ	305	PUB	CHA-C1B-C2B	-2.72	125.70	130.34
29	FB	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46
29	FM	201	PEB	OD-C4D-C3D	-2.72	123.30	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Q1	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
29	QK	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
29	FD	201	PEB	OA-C1A-C2A	-2.72	124.01	126.17
29	W1	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
29	WK	202	PEB	OD-C4D-ND	-2.72	121.91	125.93
29	JB	201	PEB	OD-C4D-C3D	-2.72	123.31	129.46
29	cB	201	PEB	OD-C4D-C3D	-2.72	123.31	129.46
29	JM	201	PEB	OD-C4D-C3D	-2.72	123.31	129.46
29	cM	201	PEB	OD-C4D-C3D	-2.72	123.31	129.46
29	I5	201	PEB	C3B-C4B-NB	2.72	114.00	110.05
29	I8	201	PEB	C3B-C4B-NB	2.72	114.00	110.05
31	JP	1001	CYC	C1B-C2B-C3B	-2.72	105.04	107.87
29	f7	201	PEB	CHA-C1B-NB	-2.72	119.25	124.93
29	f9	201	PEB	CHA-C1B-NB	-2.72	119.25	124.93
31	F1	1001	CYC	CAC-C3C-C2C	-2.72	107.47	114.26
31	FK	1001	CYC	CAC-C3C-C2C	-2.72	107.47	114.26
29	O2	201	PEB	O1C-CGC-CBC	-2.72	114.36	123.08
29	S1	201	PEB	CBC-CAC-C2C	-2.71	107.99	112.62
29	SK	201	PEB	CBC-CAC-C2C	-2.71	107.99	112.62
29	SF	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
29	SI	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
29	S2	201	PEB	CMB-C2B-C1B	2.71	129.24	125.06
30	wL	305	PUB	CAC-CBC-CGC	-2.71	107.76	113.60
31	EF	1001	CYC	C1A-C2A-C3A	-2.71	103.78	106.78
31	EI	1001	CYC	C1A-C2A-C3A	-2.71	103.78	106.78
29	AF	304	PEB	C1C-CHB-C4B	-2.71	125.57	128.81
29	AI	304	PEB	C1C-CHB-C4B	-2.71	125.57	128.81
29	k1	201	PEB	C2A-C1A-NA	2.71	110.61	108.27
29	kK	201	PEB	C2A-C1A-NA	2.71	110.61	108.27
29	Z1	202	PEB	CBC-CAC-C2C	-2.71	107.99	112.62
29	ZK	202	PEB	CBC-CAC-C2C	-2.71	107.99	112.62
29	QR	201	PEB	O1C-CGC-CBC	-2.71	114.36	123.08
29	A8	201	PEB	C3B-C4B-NB	2.71	114.00	110.05
29	ZB	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
29	ZM	201	PEB	OD-C4D-C3D	-2.71	123.31	129.46
29	M2	201	PEB	O1C-CGC-CBC	-2.71	114.37	123.08
29	I4	201	PEB	OD-C4D-ND	-2.71	121.91	125.93
31	HP	1001	CYC	C4A-C3A-C2A	-2.71	103.39	106.51
29	eB	201	PEB	OD-C4D-C3D	-2.71	123.32	129.46
29	eM	201	PEB	OD-C4D-C3D	-2.71	123.32	129.46
29	UF	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46
29	UI	202	PEB	OD-C4D-C3D	-2.71	123.32	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T1	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
29	TK	202	PEB	C3B-C4B-NB	2.71	113.99	110.05
31	nP	1001	CYC	C4A-C3A-C2A	-2.71	103.39	106.51
29	U2	201	PEB	O1C-CGC-CBC	-2.71	114.37	123.08
29	UR	201	PEB	O1C-CGC-CBC	-2.71	114.37	123.08
29	K8	201	PEB	CAB-CBB-CGB	-2.71	107.77	113.60
29	C4	201	PEB	OD-C4D-ND	-2.71	121.92	125.93
29	D4	202	PEB	OD-C4D-ND	-2.71	121.92	125.93
29	O1	201	PEB	CBC-CAC-C2C	-2.71	108.00	112.62
29	OK	201	PEB	CBC-CAC-C2C	-2.71	108.00	112.62
31	eP	1001	CYC	C2B-C1B-NB	2.71	110.95	106.99
29	L5	201	PEB	C3B-C4B-NB	2.71	113.99	110.05
29	KD	202	PEB	C2A-C1A-NA	2.71	110.61	108.27
31	YP	1000	CYC	C2C-C1C-NC	2.71	110.61	108.27
29	h7	201	PEB	CHA-C1B-NB	-2.71	119.27	124.93
29	h9	201	PEB	CHA-C1B-NB	-2.71	119.27	124.93
29	E4	203	PEB	OD-C4D-ND	-2.71	121.92	125.93
31	QP	1001	CYC	C4A-C3A-C2A	-2.71	103.40	106.51
29	j1	201	PEB	CBC-CAC-C2C	-2.71	108.00	112.62
29	jK	201	PEB	CBC-CAC-C2C	-2.71	108.00	112.62
29	ID	203	PEB	OD-C4D-ND	-2.71	121.92	125.93
29	LD	201	PEB	OD-C4D-ND	-2.71	121.92	125.93
29	JA	202	PEB	C2A-C1A-NA	2.71	110.61	108.27
29	JN	202	PEB	C2A-C1A-NA	2.71	110.61	108.27
29	Q7	201	PEB	CHA-C1B-NB	-2.71	119.27	124.93
29	Q9	201	PEB	CHA-C1B-NB	-2.71	119.27	124.93
29	WR	201	PEB	O1C-CGC-CBC	-2.71	114.38	123.08
30	AB	304	PUB	CBA-CAA-C3A	-2.71	108.87	112.98
29	TF	201	PEB	CAB-CBB-CGB	-2.71	107.78	113.60
29	PB	201	PEB	OD-C4D-C3D	-2.71	123.33	129.46
29	PM	201	PEB	OD-C4D-C3D	-2.71	123.33	129.46
29	xJ	302	PEB	C1C-CHB-C4B	-2.71	125.58	128.81
29	xL	302	PEB	C1C-CHB-C4B	-2.71	125.58	128.81
30	xL	305	PUB	CAC-CBC-CGC	-2.71	107.78	113.60
30	AB	305	PUB	CMD-C2D-C3D	2.71	131.83	127.77
31	1P	1001	CYC	C2C-C3C-C4C	2.71	105.39	101.34
31	kP	1001	CYC	C4A-C3A-C2A	-2.71	103.40	106.51
29	D4	201	PEB	CAB-CBB-CGB	-2.71	107.78	113.60
29	hF	201	PEB	OD-C4D-C3D	-2.71	123.33	129.46
29	hI	201	PEB	OD-C4D-C3D	-2.71	123.33	129.46
29	l1	202	PEB	OD-C4D-ND	-2.71	121.92	125.93
29	lK	202	PEB	OD-C4D-ND	-2.71	121.92	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T1	202	PEB	CHC-C4C-C3C	-2.71	125.72	130.34
29	TK	202	PEB	CHC-C4C-C3C	-2.71	125.72	130.34
29	l1	201	PEB	CBC-CAC-C2C	-2.70	108.00	112.62
29	lK	201	PEB	CBC-CAC-C2C	-2.70	108.00	112.62
29	M4	201	PEB	OD-C4D-ND	-2.70	121.92	125.93
29	MJ	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
29	ML	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
29	kB	201	PEB	OD-C4D-C3D	-2.70	123.33	129.46
29	kM	201	PEB	OD-C4D-C3D	-2.70	123.33	129.46
29	Q2	201	PEB	O1C-CGC-CBC	-2.70	114.40	123.08
31	1P	1001	CYC	C4A-C3A-C2A	-2.70	103.40	106.51
31	CF	1001	CYC	C1A-C2A-C3A	-2.70	103.79	106.78
31	CI	1001	CYC	C1A-C2A-C3A	-2.70	103.79	106.78
29	H4	201	PEB	OA-C1A-C2A	-2.70	124.02	126.17
29	HD	201	PEB	OA-C1A-C2A	-2.70	124.02	126.17
29	d1	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	f1	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	dK	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	fK	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
31	BP	1001	CYC	C2C-C3C-C4C	2.70	105.39	101.34
29	A5	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
29	C5	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
29	C8	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
29	ED	202	PEB	OD-C4D-ND	-2.70	121.93	125.93
29	FD	202	PEB	OA-C1A-C2A	-2.70	124.03	126.17
30	wJ	305	PUB	CAC-CBC-CGC	-2.70	107.79	113.60
31	N1	1001	CYC	CAC-C3C-C2C	-2.70	107.51	114.26
29	b7	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
29	b9	201	PEB	CHA-C1B-NB	-2.70	119.28	124.93
29	Q1	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	QK	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
31	hP	1001	CYC	C2C-C3C-C4C	2.70	105.38	101.34
31	kP	1001	CYC	C2C-C3C-C4C	2.70	105.38	101.34
31	L1	1001	CYC	CAC-C3C-C2C	-2.70	107.51	114.26
31	LK	1001	CYC	CAC-C3C-C2C	-2.70	107.51	114.26
29	H4	201	PEB	CAB-CBB-CGB	-2.70	107.79	113.60
29	HB	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
29	HM	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
29	L8	201	PEB	C3B-C4B-NB	2.70	113.98	110.05
29	h1	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	hK	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
30	MA	403	PUB	OA-C1A-NA	-2.70	121.93	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AC	202	PEB	CMB-C2B-C1B	2.70	129.22	125.06
29	AE	202	PEB	CMB-C2B-C1B	2.70	129.22	125.06
29	ZF	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
29	ZI	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
29	TF	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	AM	302	PEB	C3B-C4B-NB	2.70	113.98	110.05
29	wL	301	PEB	CMB-C2B-C1B	2.70	129.22	125.06
29	b1	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	bK	201	PEB	CBC-CAC-C2C	-2.70	108.01	112.62
29	bF	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
29	bI	201	PEB	OD-C4D-C3D	-2.70	123.34	129.46
29	M3	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
29	G4	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
29	MO	203	PEB	OD-C4D-ND	-2.70	121.93	125.93
31	NK	1001	CYC	CAC-C3C-C2C	-2.70	107.52	114.26
29	Z7	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	Z9	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	G4	201	PEB	OD-C4D-ND	-2.70	121.93	125.93
29	QF	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
29	QI	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
31	H1	1001	CYC	CAC-C3C-C2C	-2.70	107.52	114.26
31	J1	1001	CYC	CAC-C3C-C2C	-2.70	107.52	114.26
31	JK	1001	CYC	CAC-C3C-C2C	-2.70	107.52	114.26
31	FP	1001	CYC	C2C-C3C-C4C	2.70	105.38	101.34
29	eJ	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	eL	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	F4	201	PEB	CAB-CBB-CGB	-2.70	107.80	113.60
29	D3	202	PEB	CBC-CAC-C2C	-2.70	108.02	112.62
31	DK	1001	CYC	CAC-C3C-C2C	-2.70	107.52	114.26
29	U7	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	U9	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
30	MN	403	PUB	CAC-C2C-C1C	2.70	129.78	125.01
29	KC	203	PEB	CMB-C2B-C1B	2.70	129.22	125.06
29	KE	203	PEB	CMB-C2B-C1B	2.70	129.22	125.06
29	iB	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
29	iM	201	PEB	OD-C4D-C3D	-2.70	123.35	129.46
29	O7	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	O9	201	PEB	CHA-C1B-NB	-2.70	119.29	124.93
29	K5	201	PEB	CAB-CBB-CGB	-2.70	107.80	113.60
29	DD	201	PEB	CAB-CBB-CGB	-2.70	107.80	113.60
29	HD	201	PEB	CAB-CBB-CGB	-2.70	107.80	113.60
29	W7	201	PEB	CHA-C1B-NB	-2.70	119.30	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W9	201	PEB	CHA-C1B-NB	-2.70	119.30	124.93
29	G5	203	PEB	OD-C4D-C3D	-2.70	123.35	129.46
30	MN	403	PUB	CMD-C2D-C3D	2.69	131.81	127.77
29	fF	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
29	fI	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
29	iI	203	PEB	C3B-C4B-NB	2.69	113.97	110.05
29	iK	203	PEB	C3B-C4B-NB	2.69	113.97	110.05
29	qJ	201	PEB	CHA-C1B-NB	-2.69	119.30	124.93
29	qL	201	PEB	CHA-C1B-NB	-2.69	119.30	124.93
29	WJ	202	PEB	CHA-C1B-NB	-2.69	119.30	124.93
29	WL	202	PEB	CHA-C1B-NB	-2.69	119.30	124.93
29	NR	203	PEB	C3B-C4B-NB	2.69	113.97	110.05
29	R1	203	PEB	CHC-C4C-C3C	-2.69	125.74	130.34
29	RK	203	PEB	CHC-C4C-C3C	-2.69	125.74	130.34
29	H4	202	PEB	OA-C1A-C2A	-2.69	124.03	126.17
29	AB	302	PEB	C3B-C4B-NB	2.69	113.97	110.05
31	XP	1001	CYC	C2C-C3C-C4C	2.69	105.37	101.34
31	nP	1001	CYC	C2C-C3C-C4C	2.69	105.37	101.34
29	g1	203	PEB	CHC-C4C-C3C	-2.69	125.75	130.34
29	gK	203	PEB	CHC-C4C-C3C	-2.69	125.75	130.34
31	jP	1001	CYC	C2C-C3C-C4C	2.69	105.37	101.34
29	WF	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
29	WI	201	PEB	OD-C4D-C3D	-2.69	123.36	129.46
29	SJ	201	PEB	CHA-C1B-NB	-2.69	119.30	124.93
29	SL	201	PEB	CHA-C1B-NB	-2.69	119.30	124.93
29	N2	203	PEB	C3B-C4B-NB	2.69	113.96	110.05
31	DP	1001	CYC	C2C-C3C-C4C	2.69	105.37	101.34
31	IP	1001	CYC	C2C-C3C-C4C	2.69	105.37	101.34
29	j7	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
29	j9	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
29	LA	202	PEB	C2A-C1A-NA	2.69	110.59	108.27
29	LN	202	PEB	C2A-C1A-NA	2.69	110.59	108.27
30	MG	403	PUB	CBA-CAA-C3A	-2.69	108.90	112.98
31	sP	1001	CYC	C4A-C3A-C2A	-2.69	103.42	106.51
31	D1	1001	CYC	CAC-C3C-C2C	-2.69	107.54	114.26
29	GD	201	PEB	OD-C4D-ND	-2.69	121.95	125.93
31	oP	1001	CYC	C2C-C3C-C4C	2.69	105.37	101.34
29	JC	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
29	JE	201	PEB	C1B-C2B-C3B	-2.69	103.42	106.51
29	IC	202	PEB	CMB-C2B-C1B	2.69	129.20	125.06
29	IE	202	PEB	CMB-C2B-C1B	2.69	129.20	125.06
29	d7	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d9	201	PEB	CHA-C1B-NB	-2.69	119.31	124.93
29	EA	201	PEB	OD-C4D-ND	-2.69	121.95	125.93
29	EN	201	PEB	OD-C4D-ND	-2.69	121.95	125.93
29	M3	202	PEB	CHA-C1B-NB	-2.69	119.31	124.93
29	MO	202	PEB	CHA-C1B-NB	-2.69	119.31	124.93
31	HK	1001	CYC	CAC-C3C-C2C	-2.69	107.54	114.26
29	j1	203	PEB	CHA-C1B-NB	-2.69	119.31	124.93
29	jK	203	PEB	CHA-C1B-NB	-2.69	119.31	124.93
29	FD	201	PEB	CAB-CBB-CGB	-2.69	107.82	113.60
29	X2	202	PEB	C3B-C4B-NB	2.69	113.96	110.05
29	BD	201	PEB	CAB-CBB-CGB	-2.69	107.82	113.60
29	CD	203	PEB	OD-C4D-ND	-2.69	121.95	125.93
29	mJ	201	PEB	CHA-C1B-NB	-2.69	119.32	124.93
29	mL	201	PEB	CHA-C1B-NB	-2.69	119.32	124.93
31	QP	1001	CYC	C2C-C3C-C4C	2.69	105.36	101.34
29	aJ	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	aL	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	JA	201	PEB	O2B-CGB-CBB	2.68	122.66	114.03
29	JN	201	PEB	O2B-CGB-CBB	2.68	122.66	114.03
30	MQ	405	PUB	CBA-CAA-C3A	-2.68	108.91	112.98
29	P1	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	R1	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	PK	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	RK	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	A7	305	PEB	CAA-C3A-C4A	2.68	119.56	112.67
29	A9	305	PEB	CAA-C3A-C4A	2.68	119.56	112.67
29	K4	203	PEB	OD-C4D-ND	-2.68	121.95	125.93
29	DA	201	PEB	O2B-CGB-CBB	2.68	122.65	114.03
29	DN	201	PEB	O2B-CGB-CBB	2.68	122.65	114.03
29	FD	202	PEB	CMD-C2D-C3D	2.68	133.85	130.06
29	AA	202	PEB	CBC-CAC-C2C	-2.68	108.04	112.62
29	AN	202	PEB	CBC-CAC-C2C	-2.68	108.04	112.62
29	KD	203	PEB	OD-C4D-ND	-2.68	121.95	125.93
29	JG	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	uJ	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	uL	202	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	JQ	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	CJ	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	kJ	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	CL	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	kL	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	FA	201	PEB	O2B-CGB-CBB	2.68	122.65	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FN	201	PEB	O2B-CGB-CBB	2.68	122.65	114.03
29	P1	203	PEB	CHC-C4C-C3C	-2.68	125.76	130.34
29	PK	203	PEB	CHC-C4C-C3C	-2.68	125.76	130.34
29	FC	201	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
29	FE	201	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
29	YJ	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	YL	201	PEB	CHA-C1B-NB	-2.68	119.32	124.93
29	wL	303	PEB	OD-C4D-C3D	-2.68	123.39	129.46
29	BG	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	AJ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	QJ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	gJ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	AL	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	QL	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	gL	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	BQ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
31	sP	1001	CYC	C2A-C1A-NA	2.68	113.95	110.05
29	BA	201	PEB	O2B-CGB-CBB	2.68	122.64	114.03
29	BN	201	PEB	O2B-CGB-CBB	2.68	122.64	114.03
29	wL	303	PEB	CHC-C1D-ND	-2.68	110.83	113.95
29	HC	201	PEB	CAB-C3B-C4B	2.68	129.75	125.01
29	HE	201	PEB	CAB-C3B-C4B	2.68	129.75	125.01
29	dF	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
29	dI	202	PEB	OD-C4D-C3D	-2.68	123.39	129.46
29	l7	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	l9	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	NO	202	PEB	C3B-C4B-NB	2.68	113.95	110.05
29	TR	203	PEB	OD-C4D-ND	-2.68	121.96	125.93
29	P2	202	PEB	C3B-C4B-NB	2.68	113.94	110.05
29	NO	202	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	DC	201	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
29	DE	201	PEB	C1B-C2B-C3B	-2.68	103.43	106.51
29	J5	202	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
29	J8	202	PEB	C4B-C3B-C2B	-2.68	103.82	106.78
29	EJ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	UJ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	EL	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	UL	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	XR	203	PEB	C3B-C4B-NB	2.68	113.94	110.05
29	FG	201	PEB	CHC-C4C-C3C	-2.68	125.77	130.34
29	FQ	201	PEB	CHC-C4C-C3C	-2.68	125.77	130.34
29	L8	203	PEB	OD-C4D-C3D	-2.68	123.39	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N2	201	PEB	OD-C4D-ND	-2.68	121.96	125.93
29	HA	201	PEB	O2B-CGB-CBB	2.68	122.63	114.03
29	HN	201	PEB	O2B-CGB-CBB	2.68	122.63	114.03
29	B4	201	PEB	CAB-CBB-CGB	-2.68	107.84	113.60
29	C4	203	PEB	OD-C4D-ND	-2.68	121.97	125.93
29	OF	201	PEB	OD-C4D-C3D	-2.68	123.40	129.46
29	OI	201	PEB	OD-C4D-C3D	-2.68	123.40	129.46
29	KJ	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	KL	201	PEB	CHA-C1B-NB	-2.68	119.33	124.93
29	NO	203	PEB	OD-C4D-ND	-2.68	121.97	125.93
29	S7	201	PEB	CHA-C1B-NB	-2.68	119.34	124.93
29	S9	201	PEB	CHA-C1B-NB	-2.68	119.34	124.93
29	cJ	201	PEB	CHA-C1B-NB	-2.68	119.34	124.93
29	cL	201	PEB	CHA-C1B-NB	-2.68	119.34	124.93
29	N3	203	PEB	OD-C4D-ND	-2.68	121.97	125.93
29	MD	201	PEB	OD-C4D-ND	-2.68	121.97	125.93
29	OJ	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	OL	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	B4	202	PEB	CMD-C2D-C3D	2.67	133.84	130.06
31	qP	1001	CYC	C2C-C3C-C4C	2.67	105.34	101.34
29	JA	202	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
29	JN	202	PEB	C1B-C2B-C3B	-2.67	103.44	106.51
29	U1	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	HG	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	UK	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	HQ	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	jF	201	PEB	OD-C4D-C3D	-2.67	123.40	129.46
29	jI	201	PEB	OD-C4D-C3D	-2.67	123.40	129.46
29	V7	203	PEB	CBB-CAB-C3B	2.67	120.06	112.63
29	V9	203	PEB	CBB-CAB-C3B	2.67	120.06	112.63
29	DD	202	PEB	OD-C4D-ND	-2.67	121.97	125.93
29	BD	202	PEB	OA-C1A-C2A	-2.67	124.05	126.17
29	N3	202	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	xL	302	PEB	C2A-C1A-NA	2.67	110.58	108.27
29	m1	202	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
29	mK	202	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
29	FC	201	PEB	CAB-C3B-C4B	2.67	129.74	125.01
29	FE	201	PEB	CAB-C3B-C4B	2.67	129.74	125.01
29	sJ	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	sL	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
31	xP	1001	CYC	C1B-NB-C4B	-2.67	107.27	110.67
31	fP	1001	CYC	C2C-C3C-C4C	2.67	105.34	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	202	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	IJ	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	gK	202	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	IL	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	Y1	202	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
29	YK	202	PEB	CHC-C4C-C3C	-2.67	125.78	130.34
29	C5	201	PEB	CAB-CBB-CGB	-2.67	107.85	113.60
29	C8	201	PEB	CAB-CBB-CGB	-2.67	107.85	113.60
31	UP	1001	CYC	C2C-C3C-C4C	2.67	105.34	101.34
29	F4	202	PEB	CMD-C2D-C3D	2.67	133.83	130.06
29	CD	202	PEB	C2A-C1A-NA	2.67	110.58	108.27
29	GJ	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
29	GL	201	PEB	CHA-C1B-NB	-2.67	119.34	124.93
31	OP	1001	CYC	C2C-C3C-C4C	2.67	105.34	101.34
29	lF	201	PEB	OD-C4D-C3D	-2.67	123.41	129.46
29	lI	201	PEB	OD-C4D-C3D	-2.67	123.41	129.46
29	wJ	303	PEB	OD-C4D-C3D	-2.67	123.41	129.46
29	xL	303	PEB	OD-C4D-C3D	-2.67	123.41	129.46
29	IA	202	PEB	CBC-CAC-C2C	-2.67	108.06	112.62
29	IN	202	PEB	CBC-CAC-C2C	-2.67	108.06	112.62
29	g7	203	PEB	CBB-CAB-C3B	2.67	120.05	112.63
29	g9	203	PEB	CBB-CAB-C3B	2.67	120.05	112.63
29	oJ	201	PEB	CHA-C1B-NB	-2.67	119.35	124.93
29	oL	201	PEB	CHA-C1B-NB	-2.67	119.35	124.93
31	HP	1001	CYC	C2C-C3C-C4C	2.67	105.34	101.34
31	uP	1001	CYC	C2C-C3C-C4C	2.67	105.34	101.34
31	VP	1001	CYC	C1B-NB-C4B	-2.67	107.27	110.67
29	IA	201	PEB	OD-C4D-ND	-2.67	121.98	125.93
29	MD	203	PEB	OD-C4D-ND	-2.67	121.98	125.93
29	IN	201	PEB	OD-C4D-ND	-2.67	121.98	125.93
29	iJ	201	PEB	CHA-C1B-NB	-2.67	119.35	124.93
29	iL	201	PEB	CHA-C1B-NB	-2.67	119.35	124.93
29	B8	203	PEB	OD-C4D-C3D	-2.67	123.41	129.46
29	L4	201	PEB	CAB-CBB-CGB	-2.67	107.86	113.60
29	G8	203	PEB	OD-C4D-C3D	-2.67	123.42	129.46
29	WR	202	PEB	OD-C4D-C3D	-2.67	123.42	129.46
29	GA	202	PEB	CBC-CAC-C2C	-2.67	108.07	112.62
29	GN	202	PEB	CBC-CAC-C2C	-2.67	108.07	112.62
31	MP	1001	CYC	C2C-C3C-C4C	2.67	105.33	101.34
29	BC	201	PEB	CAB-C3B-C4B	2.67	129.73	125.01
29	BE	201	PEB	CAB-C3B-C4B	2.67	129.73	125.01
29	e1	202	PEB	CHA-C1B-NB	-2.67	119.35	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	eK	202	PEB	CHA-C1B-NB	-2.67	119.35	124.93
29	i1	203	PEB	CHC-C4C-C3C	-2.67	125.79	130.34
29	iK	203	PEB	CHC-C4C-C3C	-2.67	125.79	130.34
29	EC	202	PEB	CMB-C2B-C1B	2.67	129.17	125.06
29	GC	202	PEB	CMB-C2B-C1B	2.67	129.17	125.06
29	EE	202	PEB	CMB-C2B-C1B	2.67	129.17	125.06
29	GE	202	PEB	CMB-C2B-C1B	2.67	129.17	125.06
29	BA	202	PEB	C2A-C1A-NA	2.67	110.57	108.27
29	BN	202	PEB	C2A-C1A-NA	2.67	110.57	108.27
29	BA	202	PEB	C1B-C2B-C3B	-2.67	103.45	106.51
29	BC	201	PEB	C1B-C2B-C3B	-2.67	103.45	106.51
29	BE	201	PEB	C1B-C2B-C3B	-2.67	103.45	106.51
29	BN	202	PEB	C1B-C2B-C3B	-2.67	103.45	106.51
29	P7	203	PEB	CBB-CAB-C3B	2.67	120.04	112.63
29	P9	203	PEB	CBB-CAB-C3B	2.67	120.04	112.63
29	d7	201	PEB	OA-C1A-C2A	-2.67	124.05	126.17
29	d9	201	PEB	OA-C1A-C2A	-2.67	124.05	126.17
29	N3	202	PEB	C3B-C4B-NB	2.67	113.93	110.05
31	1P	1002	CYC	C2C-C1C-NC	2.67	110.57	108.27
29	m7	203	PEB	CBB-CAB-C3B	2.67	120.03	112.63
29	m9	203	PEB	CBB-CAB-C3B	2.67	120.03	112.63
29	J4	202	PEB	CMD-C2D-C3D	2.67	133.82	130.06
29	LA	201	PEB	O2B-CGB-CBB	2.67	122.59	114.03
29	LN	201	PEB	O2B-CGB-CBB	2.67	122.59	114.03
30	AF	303	PUB	OD-C4D-ND	-2.67	121.98	125.93
30	AI	303	PUB	OD-C4D-ND	-2.67	121.98	125.93
29	EA	202	PEB	CBC-CAC-C2C	-2.67	108.07	112.62
29	EN	202	PEB	CBC-CAC-C2C	-2.67	108.07	112.62
29	J5	201	PEB	OA-C1A-C2A	-2.67	124.05	126.17
29	J8	201	PEB	OA-C1A-C2A	-2.67	124.05	126.17
29	LA	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	LN	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	LC	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	LE	201	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	L4	202	PEB	CMD-C2D-C3D	2.66	133.82	130.06
29	P2	202	PEB	OD-C4D-ND	-2.66	121.98	125.93
29	KA	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
29	KN	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
29	A1	302	PEB	C2A-C1A-NA	2.66	110.57	108.27
29	E4	202	PEB	C2A-C1A-NA	2.66	110.57	108.27
29	K4	202	PEB	C2A-C1A-NA	2.66	110.57	108.27
29	AK	302	PEB	C2A-C1A-NA	2.66	110.57	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D4	202	PEB	CMD-C2D-C3D	2.66	133.82	130.06
29	GA	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
29	GN	201	PEB	OD-C4D-ND	-2.66	121.98	125.93
29	FG	201	PEB	CHA-C1B-NB	-2.66	119.36	124.93
29	FQ	201	PEB	CHA-C1B-NB	-2.66	119.36	124.93
29	KA	202	PEB	CBC-CAC-C2C	-2.66	108.08	112.62
29	KN	202	PEB	CBC-CAC-C2C	-2.66	108.08	112.62
29	BD	202	PEB	CMD-C2D-C3D	2.66	133.82	130.06
29	DD	202	PEB	CMD-C2D-C3D	2.66	133.82	130.06
31	IP	1001	CYC	C2C-C3C-C4C	2.66	105.33	101.34
29	HA	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	HN	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	LG	201	PEB	CHA-C1B-NB	-2.66	119.36	124.93
29	MQ	402	PEB	CHA-C1B-NB	-2.66	119.36	124.93
29	i7	203	PEB	CBB-CAB-C3B	2.66	120.02	112.63
29	i9	203	PEB	CBB-CAB-C3B	2.66	120.02	112.63
29	a7	203	PEB	CBB-CAB-C3B	2.66	120.02	112.63
29	a9	203	PEB	CBB-CAB-C3B	2.66	120.02	112.63
29	A7	305	PEB	OD-C4D-C3D	-2.66	123.43	129.46
29	A9	305	PEB	OD-C4D-C3D	-2.66	123.43	129.46
29	k1	202	PEB	CHA-C1B-NB	-2.66	119.36	124.93
29	kK	202	PEB	CHA-C1B-NB	-2.66	119.36	124.93
29	DC	201	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
29	DE	201	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
29	MQ	407	PEB	OD-C4D-C3D	-2.66	123.43	129.46
31	wP	1001	CYC	C2C-C3C-C4C	2.66	105.33	101.34
29	AA	201	PEB	OD-C4D-ND	-2.66	121.99	125.93
29	AN	201	PEB	OD-C4D-ND	-2.66	121.99	125.93
29	M4	202	PEB	C2A-C1A-NA	2.66	110.57	108.27
29	B5	203	PEB	OD-C4D-C3D	-2.66	123.43	129.46
29	FA	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	FN	202	PEB	C1B-C2B-C3B	-2.66	103.45	106.51
29	xJ	303	PEB	OD-C4D-C3D	-2.66	123.43	129.46
29	e1	203	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
29	eK	203	PEB	CHC-C4C-C3C	-2.66	125.80	130.34
30	MA	403	PUB	CMD-C2D-C3D	2.66	131.76	127.77
29	V1	202	PEB	CHA-C1B-NB	-2.66	119.37	124.93
29	VK	202	PEB	CHA-C1B-NB	-2.66	119.37	124.93
30	AB	304	PUB	OA-C1A-NA	-2.66	121.99	125.93
29	c1	202	PEB	CHA-C1B-NB	-2.66	119.37	124.93
29	cK	202	PEB	CHA-C1B-NB	-2.66	119.37	124.93
29	I5	201	PEB	CAB-CBB-CGB	-2.66	107.88	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I8	201	PEB	CAB-CBB-CGB	-2.66	107.88	113.60
29	k7	203	PEB	CBB-CAB-C3B	2.66	120.01	112.63
29	k9	203	PEB	CBB-CAB-C3B	2.66	120.01	112.63
29	UJ	201	PEB	OD-C4D-C3D	-2.66	123.44	129.46
29	UL	201	PEB	OD-C4D-C3D	-2.66	123.44	129.46
29	JG	201	PEB	CHC-C4C-C3C	-2.66	125.81	130.34
29	JQ	201	PEB	CHC-C4C-C3C	-2.66	125.81	130.34
29	a1	202	PEB	CHA-C1B-NB	-2.66	119.38	124.93
29	aK	202	PEB	CHA-C1B-NB	-2.66	119.38	124.93
31	SP	1001	CYC	C2C-C3C-C4C	2.66	105.32	101.34
31	TP	1001	CYC	C2C-C3C-C4C	2.66	105.32	101.34
29	DA	202	PEB	C2A-C1A-NA	2.66	110.56	108.27
29	DN	202	PEB	C2A-C1A-NA	2.66	110.56	108.27
29	B4	202	PEB	OA-C1A-C2A	-2.66	124.06	126.17
29	h7	201	PEB	OA-C1A-C2A	-2.66	124.06	126.17
29	h9	201	PEB	OA-C1A-C2A	-2.66	124.06	126.17
29	LD	201	PEB	CAB-CBB-CGB	-2.66	107.89	113.60
29	ZB	202	PEB	CHA-C1B-NB	-2.66	119.38	124.93
29	ZM	202	PEB	CHA-C1B-NB	-2.66	119.38	124.93
30	BB	302	PUB	OD-C4D-C3D	-2.66	125.16	128.04
30	BM	302	PUB	OD-C4D-C3D	-2.66	125.16	128.04
29	wJ	303	PEB	CHC-C1D-ND	-2.66	110.86	113.95
29	a1	203	PEB	CHC-C4C-C3C	-2.66	125.81	130.34
29	aK	203	PEB	CHC-C4C-C3C	-2.66	125.81	130.34
29	L5	203	PEB	OD-C4D-C3D	-2.66	123.44	129.46
29	VR	201	PEB	OD-C4D-ND	-2.66	122.00	125.93
29	L3	202	PEB	C3B-C4B-NB	2.66	113.91	110.05
29	LO	202	PEB	C3B-C4B-NB	2.66	113.91	110.05
29	TR	203	PEB	C3B-C4B-NB	2.66	113.91	110.05
29	e7	203	PEB	CBB-CAB-C3B	2.66	120.00	112.63
29	e9	203	PEB	CBB-CAB-C3B	2.66	120.00	112.63
29	RR	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
29	F3	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
29	FO	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
29	MG	405	PEB	OD-C4D-C3D	-2.65	123.44	129.46
29	YJ	201	PEB	OD-C4D-C3D	-2.65	123.44	129.46
29	YL	201	PEB	OD-C4D-C3D	-2.65	123.44	129.46
29	V1	203	PEB	CHC-C4C-C3C	-2.65	125.81	130.34
29	VK	203	PEB	CHC-C4C-C3C	-2.65	125.81	130.34
31	VP	1001	CYC	CAD-CBD-CGD	-2.65	106.32	113.76
29	Y7	203	PEB	CBB-CAB-C3B	2.65	120.00	112.63
29	Y9	203	PEB	CBB-CAB-C3B	2.65	120.00	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i1	202	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	YB	201	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	DG	201	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	iK	202	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	YM	201	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	DQ	201	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	G4	202	PEB	C2A-C1A-NA	2.65	110.56	108.27
29	A9	304	PEB	OD-C4D-C3D	-2.65	123.45	129.46
29	T2	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
29	F5	203	PEB	OD-C4D-C3D	-2.65	123.45	129.46
29	F8	203	PEB	OD-C4D-C3D	-2.65	123.45	129.46
31	xP	1001	CYC	CAD-CBD-CGD	-2.65	106.32	113.76
29	HB	202	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	HM	202	PEB	CHA-C1B-NB	-2.65	119.38	124.93
29	FC	201	PEB	CHC-C4C-C3C	-2.65	125.81	130.34
29	FE	201	PEB	CHC-C4C-C3C	-2.65	125.81	130.34
29	CA	202	PEB	CBC-CAC-C2C	-2.65	108.09	112.62
29	CN	202	PEB	CBC-CAC-C2C	-2.65	108.09	112.62
29	A5	201	PEB	CAB-CBB-CGB	-2.65	107.90	113.60
29	A8	201	PEB	CAB-CBB-CGB	-2.65	107.90	113.60
29	NR	201	PEB	OD-C4D-ND	-2.65	122.00	125.93
29	Z1	201	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	JB	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	TB	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	ZK	201	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	JM	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	TM	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	R2	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
29	RR	203	PEB	C3B-C4B-NB	2.65	113.91	110.05
29	DC	201	PEB	CAB-C3B-C4B	2.65	129.70	125.01
29	DE	201	PEB	CAB-C3B-C4B	2.65	129.70	125.01
29	JC	201	PEB	CHC-C4C-C3C	-2.65	125.82	130.34
29	JE	201	PEB	CHC-C4C-C3C	-2.65	125.82	130.34
29	D3	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	DO	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	LD	202	PEB	OA-C1A-C2A	-2.65	124.07	126.17
29	xL	303	PEB	CHC-C1D-ND	-2.65	110.87	113.95
29	HD	202	PEB	CMD-C2D-C3D	2.65	133.80	130.06
29	JD	202	PEB	CMD-C2D-C3D	2.65	133.80	130.06
29	IA	201	PEB	C2A-C1A-NA	2.65	110.56	108.27
29	IN	201	PEB	C2A-C1A-NA	2.65	110.56	108.27
31	sP	1001	CYC	C2C-C3C-C4C	2.65	105.31	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mB	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	mM	202	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	T7	203	PEB	CBB-CAB-C3B	2.65	119.98	112.63
29	T9	203	PEB	CBB-CAB-C3B	2.65	119.98	112.63
29	GD	202	PEB	C2A-C1A-NA	2.65	110.56	108.27
29	BC	203	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	BE	203	PEB	CHA-C1B-NB	-2.65	119.39	124.93
29	XR	203	PEB	OD-C4D-ND	-2.65	122.01	125.93
29	DD	202	PEB	OA-C1A-C2A	-2.65	124.07	126.17
29	R7	203	PEB	CBB-CAB-C3B	2.65	119.98	112.63
29	R9	203	PEB	CBB-CAB-C3B	2.65	119.98	112.63
31	1P	1002	CYC	C1B-C2B-C3B	-2.65	105.11	107.87
29	VR	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	RB	202	PEB	CHA-C1B-NB	-2.65	119.40	124.93
29	RM	202	PEB	CHA-C1B-NB	-2.65	119.40	124.93
29	c7	203	PEB	CBB-CAB-C3B	2.65	119.98	112.63
29	c9	203	PEB	CBB-CAB-C3B	2.65	119.98	112.63
29	AJ	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
29	AL	201	PEB	OD-C4D-C3D	-2.65	123.46	129.46
29	V2	203	PEB	OD-C4D-ND	-2.65	122.01	125.93
29	BB	301	PEB	OD-C4D-C3D	-2.65	123.47	129.46
29	BM	301	PEB	OD-C4D-C3D	-2.65	123.47	129.46
29	H3	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	HO	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	PR	202	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	DG	202	PEB	C2A-C1A-NA	2.65	110.55	108.27
29	DQ	202	PEB	C2A-C1A-NA	2.65	110.55	108.27
29	HG	201	PEB	CHC-C4C-C3C	-2.65	125.82	130.34
29	HQ	201	PEB	CHC-C4C-C3C	-2.65	125.82	130.34
29	QR	202	PEB	OD-C4D-C3D	-2.65	123.47	129.46
29	B3	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	BO	203	PEB	C3B-C4B-NB	2.65	113.90	110.05
29	xJ	302	PEB	C2A-C1A-NA	2.64	110.55	108.27
29	BC	201	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
29	BE	201	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
29	DG	201	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
29	DQ	201	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
29	JD	202	PEB	OA-C1A-C2A	-2.64	124.07	126.17
29	QJ	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
29	sJ	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
29	QL	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
29	sL	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	eP	1001	CYC	C2C-C3C-C4C	2.64	105.30	101.34
29	EJ	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
29	EL	201	PEB	OD-C4D-C3D	-2.64	123.47	129.46
29	W2	202	PEB	OD-C4D-C3D	-2.64	123.47	129.46
29	FG	202	PEB	C2A-C1A-NA	2.64	110.55	108.27
29	FQ	202	PEB	C2A-C1A-NA	2.64	110.55	108.27
29	J3	203	PEB	C3B-C4B-NB	2.64	113.89	110.05
29	JO	203	PEB	C3B-C4B-NB	2.64	113.89	110.05
29	VR	203	PEB	OD-C4D-ND	-2.64	122.02	125.93
29	VB	202	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	DC	202	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	DE	202	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	VM	202	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	MD	202	PEB	C2A-C1A-NA	2.64	110.55	108.27
29	SJ	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
29	SL	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
31	wP	1001	CYC	C2A-C1A-NA	2.64	113.89	110.05
29	CC	202	PEB	CMB-C2B-C1B	2.64	129.13	125.06
29	CE	202	PEB	CMB-C2B-C1B	2.64	129.13	125.06
29	GJ	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
29	KJ	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
29	GL	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
29	KL	201	PEB	OD-C4D-C3D	-2.64	123.48	129.46
29	k1	203	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
29	kK	203	PEB	CHC-C4C-C3C	-2.64	125.83	130.34
31	XP	1001	CYC	C2A-C1A-NA	2.64	113.89	110.05
29	E4	203	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	MN	404	PEB	OD-C4D-ND	-2.64	122.02	125.93
29	H4	202	PEB	CMD-C2D-C3D	2.64	133.79	130.06
29	Q2	202	PEB	OD-C4D-C3D	-2.64	123.48	129.46
29	W7	201	PEB	OA-C1A-C2A	-2.64	124.08	126.17
29	W9	201	PEB	OA-C1A-C2A	-2.64	124.08	126.17
29	DB	202	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	DM	202	PEB	CHA-C1B-NB	-2.64	119.41	124.93
29	c1	203	PEB	CHC-C4C-C3C	-2.64	125.84	130.34
29	cK	203	PEB	CHC-C4C-C3C	-2.64	125.84	130.34
29	DA	202	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
29	DN	202	PEB	C1B-C2B-C3B	-2.64	103.48	106.51
31	oP	1001	CYC	C2A-C1A-NA	2.64	113.89	110.05
29	aB	203	PEB	CHA-C1B-NB	-2.64	119.42	124.93
29	aM	203	PEB	CHA-C1B-NB	-2.64	119.42	124.93
29	LC	201	PEB	CHC-C4C-C3C	-2.64	125.84	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LE	201	PEB	CHC-C4C-C3C	-2.64	125.84	130.34
29	M3	202	PEB	C3B-C4B-NB	2.64	113.89	110.05
29	MO	202	PEB	C3B-C4B-NB	2.64	113.89	110.05
29	KB	203	PEB	CHA-C1B-NB	-2.64	119.42	124.93
29	KM	203	PEB	CHA-C1B-NB	-2.64	119.42	124.93
29	xJ	303	PEB	CHC-C1D-ND	-2.64	110.89	113.95
29	kJ	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
29	kL	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
29	RR	203	PEB	OD-C4D-ND	-2.64	122.03	125.93
30	AM	304	PUB	OA-C1A-NA	-2.64	122.03	125.93
29	A7	301	PEB	C2A-C1A-NA	2.64	110.55	108.27
29	A9	301	PEB	C2A-C1A-NA	2.64	110.55	108.27
29	CA	201	PEB	OD-C4D-ND	-2.64	122.03	125.93
29	CN	201	PEB	OD-C4D-ND	-2.64	122.03	125.93
29	CJ	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
29	CL	201	PEB	OD-C4D-C3D	-2.64	123.49	129.46
29	LC	201	PEB	CAB-C3B-C4B	2.63	129.67	125.01
29	LE	201	PEB	CAB-C3B-C4B	2.63	129.67	125.01
29	NR	203	PEB	OD-C4D-ND	-2.63	122.03	125.93
30	AB	304	PUB	CMD-C2D-C3D	2.63	131.72	127.77
29	OJ	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
29	OL	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
29	BB	301	PEB	CHA-C1B-NB	-2.63	119.42	124.93
29	BM	301	PEB	CHA-C1B-NB	-2.63	119.42	124.93
29	gJ	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
29	gL	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
30	MQ	405	PUB	CMD-C2D-C3D	2.63	131.72	127.77
29	H5	203	PEB	OD-C4D-C3D	-2.63	123.49	129.46
29	mJ	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
29	mL	201	PEB	OD-C4D-C3D	-2.63	123.49	129.46
31	QP	1001	CYC	C2A-C1A-NA	2.63	113.88	110.05
29	A7	305	PEB	C1C-CHB-C4B	-2.63	125.66	128.81
29	A9	305	PEB	C1C-CHB-C4B	-2.63	125.66	128.81
31	yP	1001	CYC	C1B-C2B-C3B	-2.63	105.12	107.87
29	JC	201	PEB	CAB-C3B-C4B	2.63	129.67	125.01
29	JE	201	PEB	CAB-C3B-C4B	2.63	129.67	125.01
29	C4	202	PEB	C2A-C1A-NA	2.63	110.54	108.27
29	A7	304	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	HC	201	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
29	HE	201	PEB	C1B-C2B-C3B	-2.63	103.48	106.51
29	T2	203	PEB	OD-C4D-ND	-2.63	122.03	125.93
29	qJ	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	qL	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	QB	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
29	QM	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
29	V2	203	PEB	C3B-C4B-NB	2.63	113.88	110.05
29	XR	201	PEB	OD-C4D-ND	-2.63	122.03	125.93
31	AP	1001	CYC	C2C-C3C-C4C	2.63	105.28	101.34
31	rP	1001	CYC	C2C-C3C-C4C	2.63	105.28	101.34
29	aJ	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	aL	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	ED	201	PEB	C2A-C1A-NA	2.63	110.54	108.27
29	FB	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
29	FM	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
29	H8	203	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	IJ	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	IL	201	PEB	OD-C4D-C3D	-2.63	123.50	129.46
29	HC	201	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
29	HE	201	PEB	CHC-C4C-C3C	-2.63	125.85	130.34
31	DP	1001	CYC	C2A-C1A-NA	2.63	113.87	110.05
29	kB	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
29	kM	202	PEB	CHA-C1B-NB	-2.63	119.43	124.93
31	CP	1001	CYC	C2C-C3C-C4C	2.63	105.28	101.34
29	M2	202	PEB	OD-C4D-C3D	-2.63	123.50	129.46
31	IP	1001	CYC	C2A-C1A-NA	2.63	113.87	110.05
31	OP	1001	CYC	C2A-C1A-NA	2.63	113.87	110.05
29	iJ	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	uJ	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	iL	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	uL	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	LG	201	PEB	CHC-C4C-C3C	-2.63	125.86	130.34
29	MQ	402	PEB	CHC-C4C-C3C	-2.63	125.86	130.34
29	gB	202	PEB	CHA-C1B-NB	-2.63	119.44	124.93
29	gM	202	PEB	CHA-C1B-NB	-2.63	119.44	124.93
31	kP	1001	CYC	C2A-C1A-NA	2.63	113.87	110.05
29	Z7	201	PEB	OA-C1A-C2A	-2.63	124.08	126.17
29	Z9	201	PEB	OA-C1A-C2A	-2.63	124.08	126.17
29	oJ	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	oL	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	MR	202	PEB	CHA-C1B-NB	-2.63	119.44	124.93
29	UR	201	PEB	OD-C4D-ND	-2.63	122.04	125.93
31	GP	1001	CYC	C2C-C3C-C4C	2.63	105.27	101.34
29	A1	301	PEB	C1C-CHB-C4B	-2.63	125.67	128.81
29	AK	301	PEB	C1C-CHB-C4B	-2.63	125.67	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M2	201	PEB	OD-C4D-ND	-2.63	122.04	125.93
29	PR	202	PEB	OD-C4D-ND	-2.63	122.04	125.93
30	wL	304	PUB	OD-C4D-ND	-2.63	122.04	125.93
29	WJ	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	eJ	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	WL	202	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	eL	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	MJ	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	cJ	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	ML	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	cL	201	PEB	OD-C4D-C3D	-2.63	123.51	129.46
29	CA	201	PEB	C2B-C1B-NB	2.63	116.13	110.53
29	CN	201	PEB	C2B-C1B-NB	2.63	116.13	110.53
31	FP	1001	CYC	C2A-C1A-NA	2.62	113.87	110.05
29	J3	202	PEB	OD-C4D-C3D	-2.62	123.51	129.46
29	JO	202	PEB	OD-C4D-C3D	-2.62	123.51	129.46
29	iB	202	PEB	CHA-C1B-NB	-2.62	119.44	124.93
29	iM	202	PEB	CHA-C1B-NB	-2.62	119.44	124.93
30	AM	304	PUB	CMD-C2D-C3D	2.62	131.71	127.77
29	C4	203	PEB	CHA-C1B-NB	-2.62	119.45	124.93
29	MG	405	PEB	C2A-C1A-NA	2.62	110.53	108.27
29	O2	202	PEB	OD-C4D-C3D	-2.62	123.52	129.46
29	l7	201	PEB	OA-C1A-C2A	-2.62	124.09	126.17
29	l9	201	PEB	OA-C1A-C2A	-2.62	124.09	126.17
29	MQ	407	PEB	CMB-C2B-C1B	2.62	129.10	125.06
30	MG	403	PUB	CMD-C2D-C3D	2.62	131.70	127.77
29	JA	201	PEB	CAA-C3A-C2A	-2.62	107.71	114.26
29	JN	201	PEB	CAA-C3A-C2A	-2.62	107.71	114.26
31	uP	1001	CYC	C2A-C1A-NA	2.62	113.86	110.05
29	X2	202	PEB	OD-C4D-ND	-2.62	122.05	125.93
29	K3	201	PEB	CMA-C2A-C1A	-2.62	106.75	112.40
29	KO	201	PEB	CMA-C2A-C1A	-2.62	106.75	112.40
29	A3	201	PEB	CMA-C2A-C1A	-2.62	106.75	112.40
29	AO	201	PEB	CMA-C2A-C1A	-2.62	106.75	112.40
29	BG	201	PEB	CHC-C4C-C3C	-2.62	125.87	130.34
29	BQ	201	PEB	CHC-C4C-C3C	-2.62	125.87	130.34
31	MP	1001	CYC	C2A-C1A-NA	2.62	113.86	110.05
29	e2	402	PEB	OD-C4D-ND	-2.62	122.05	125.93
29	LB	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
29	ED	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
29	LM	202	PEB	CHA-C1B-NB	-2.62	119.45	124.93
29	N2	203	PEB	OD-C4D-ND	-2.62	122.05	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TR	201	PEB	OD-C4D-ND	-2.62	122.05	125.93
29	MG	405	PEB	CMB-C2B-C1B	2.62	129.10	125.06
29	MQ	407	PEB	C2A-C1A-NA	2.62	110.53	108.27
29	cB	202	PEB	CHA-C1B-NB	-2.62	119.46	124.93
29	cM	202	PEB	CHA-C1B-NB	-2.62	119.46	124.93
31	SP	1001	CYC	C2A-C1A-NA	2.62	113.86	110.05
29	W2	201	PEB	OD-C4D-ND	-2.62	122.05	125.93
29	L4	202	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	GA	201	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	IA	201	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	GN	201	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	IN	201	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	R2	203	PEB	OD-C4D-ND	-2.62	122.05	125.93
31	BP	1001	CYC	C2A-C1A-NA	2.62	113.86	110.05
29	J4	202	PEB	C2B-C1B-NB	2.62	116.11	110.53
31	NP	1001	CYC	C2C-C3C-C4C	2.62	105.26	101.34
29	FA	201	PEB	CAA-C3A-C2A	-2.62	107.72	114.26
29	FN	201	PEB	CAA-C3A-C2A	-2.62	107.72	114.26
29	aF	201	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
29	aI	201	PEB	C1B-C2B-C3B	-2.62	103.50	106.51
29	EA	201	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	EN	201	PEB	C2B-C1B-NB	2.62	116.11	110.53
29	OR	201	PEB	OD-C4D-ND	-2.62	122.06	125.93
30	xJ	304	PUB	OD-C4D-ND	-2.62	122.06	125.93
29	LD	202	PEB	CMD-C2D-C3D	2.62	133.75	130.06
29	JC	202	PEB	CHA-C1B-NB	-2.61	119.46	124.93
29	JE	202	PEB	CHA-C1B-NB	-2.61	119.46	124.93
29	B3	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	BO	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	E3	201	PEB	CMA-C2A-C1A	-2.61	106.77	112.40
29	EO	201	PEB	CMA-C2A-C1A	-2.61	106.77	112.40
29	FC	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
29	HC	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
29	FE	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
29	HE	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
31	EP	1001	CYC	C2C-C3C-C4C	2.61	105.25	101.34
29	S2	201	PEB	C3B-C4B-NB	2.61	113.85	110.05
29	VF	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
29	VI	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
29	MD	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93
29	MQ	403	PEB	CMB-C2B-C1B	2.61	129.09	125.06
29	KD	203	PEB	CHA-C1B-NB	-2.61	119.47	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J3	203	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	JO	203	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	R2	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
31	HP	1001	CYC	C2A-C1A-NA	2.61	113.85	110.05
29	rJ	203	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	rL	203	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	SR	202	PEB	OD-C4D-C3D	-2.61	123.54	129.46
29	AA	201	PEB	C2B-C1B-NB	2.61	116.10	110.53
29	AN	201	PEB	C2B-C1B-NB	2.61	116.10	110.53
29	H3	203	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	L3	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	HO	203	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	LO	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	D3	203	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	DO	203	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	UR	201	PEB	CMA-C2A-C1A	-2.61	106.78	112.40
29	F3	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	FO	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	MR	201	PEB	OD-C4D-ND	-2.61	122.06	125.93
30	A1	304	PUB	C4B-CHB-C1C	-2.61	125.69	128.81
30	AK	304	PUB	C4B-CHB-C1C	-2.61	125.69	128.81
29	gF	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
29	gI	201	PEB	C1B-C2B-C3B	-2.61	103.51	106.51
29	DD	202	PEB	C2B-C1B-NB	2.61	116.10	110.53
31	vP	1001	CYC	C2C-C3C-C4C	2.61	105.25	101.34
30	xL	304	PUB	OD-C4D-ND	-2.61	122.07	125.93
29	V7	202	PEB	CAB-C3B-C4B	2.61	129.62	125.01
29	V9	202	PEB	CAB-C3B-C4B	2.61	129.62	125.01
29	FA	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	FN	201	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	J4	202	PEB	OA-C1A-C2A	-2.61	124.10	126.17
29	ID	203	PEB	CHA-C1B-NB	-2.61	119.48	124.93
29	U2	202	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	I3	203	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	IO	203	PEB	OD-C4D-C3D	-2.61	123.55	129.46
29	RF	201	PEB	C1B-C2B-C3B	-2.61	103.52	106.51
29	RI	201	PEB	C1B-C2B-C3B	-2.61	103.52	106.51
31	iP	1001	CYC	C2C-C3C-C4C	2.61	105.24	101.34
31	pP	1001	CYC	C2C-C3C-C4C	2.61	105.24	101.34
29	gB	203	PEB	O2B-CGB-CBB	2.61	122.40	114.03
29	gM	203	PEB	O2B-CGB-CBB	2.61	122.40	114.03
31	UP	1001	CYC	C2A-C1A-NA	2.61	113.84	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	fP	1001	CYC	C2A-C1A-NA	2.61	113.84	110.05
31	hP	1001	CYC	C2A-C1A-NA	2.61	113.84	110.05
31	nP	1001	CYC	C2A-C1A-NA	2.61	113.84	110.05
29	HA	201	PEB	CAA-C3A-C2A	-2.61	107.75	114.26
29	HN	201	PEB	CAA-C3A-C2A	-2.61	107.75	114.26
29	LC	203	PEB	CHA-C1B-NB	-2.61	119.48	124.93
29	LE	203	PEB	CHA-C1B-NB	-2.61	119.48	124.93
29	L4	202	PEB	OA-C1A-C2A	-2.61	124.10	126.17
29	U2	201	PEB	OD-C4D-ND	-2.61	122.07	125.93
29	HA	202	PEB	OD-C4D-C3D	-2.61	123.56	129.46
29	hJ	203	PEB	OD-C4D-C3D	-2.61	123.56	129.46
29	hL	203	PEB	OD-C4D-C3D	-2.61	123.56	129.46
29	HN	202	PEB	OD-C4D-C3D	-2.61	123.56	129.46
29	wJ	302	PEB	C2A-C1A-NA	2.61	110.52	108.27
31	KP	1001	CYC	C2C-C3C-C4C	2.61	105.24	101.34
31	RP	1001	CYC	C2C-C3C-C4C	2.61	105.24	101.34
29	LD	202	PEB	C2B-C1B-NB	2.60	116.09	110.53
29	RB	203	PEB	O2B-CGB-CBB	2.60	122.40	114.03
29	RM	203	PEB	O2B-CGB-CBB	2.60	122.40	114.03
31	WP	1001	CYC	C1B-C2B-C3B	-2.60	105.15	107.87
29	PJ	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	PL	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	D4	202	PEB	C2B-C1B-NB	2.60	116.09	110.53
29	wJ	303	PEB	CHA-C1B-NB	-2.60	119.49	124.93
29	QR	201	PEB	OD-C4D-ND	-2.60	122.07	125.93
29	IJ	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	IL	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
31	JP	1001	CYC	C2C-C3C-C4C	2.60	105.24	101.34
29	VB	203	PEB	O2B-CGB-CBB	2.60	122.39	114.03
29	VM	203	PEB	O2B-CGB-CBB	2.60	122.39	114.03
29	jB	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	jM	201	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	V2	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
29	WR	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
29	HD	202	PEB	C2B-C1B-NB	2.60	116.08	110.53
29	kB	203	PEB	O2B-CGB-CBB	2.60	122.39	114.03
29	kM	203	PEB	O2B-CGB-CBB	2.60	122.39	114.03
31	qP	1001	CYC	C2A-C1A-NA	2.60	113.83	110.05
29	BJ	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	BL	203	PEB	OD-C4D-C3D	-2.60	123.56	129.46
29	LA	201	PEB	CAA-C3A-C2A	-2.60	107.76	114.26
29	LN	201	PEB	CAA-C3A-C2A	-2.60	107.76	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NJ	203	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	NL	203	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	cB	203	PEB	O2B-CGB-CBB	2.60	122.39	114.03
29	cM	203	PEB	O2B-CGB-CBB	2.60	122.39	114.03
31	cP	1001	CYC	C2C-C3C-C4C	2.60	105.23	101.34
29	O2	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
29	T2	201	PEB	OD-C4D-ND	-2.60	122.08	125.93
29	KA	201	PEB	C2B-C1B-NB	2.60	116.08	110.53
29	KN	201	PEB	C2B-C1B-NB	2.60	116.08	110.53
29	MR	201	PEB	CMA-C2A-C1A	-2.60	106.80	112.40
29	DF	1002	PEB	CBC-CAC-C2C	-2.60	108.18	112.62
29	DI	1002	PEB	CBC-CAC-C2C	-2.60	108.18	112.62
29	U2	201	PEB	CMA-C2A-C1A	-2.60	106.80	112.40
29	LC	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	LE	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	HJ	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	HL	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	H3	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	HO	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	UB	201	PEB	C1C-CHB-C4B	-2.60	125.70	128.81
29	UM	201	PEB	C1C-CHB-C4B	-2.60	125.70	128.81
29	HA	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	CB	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	CM	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	HN	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	FB	203	PEB	O2B-CGB-CBB	2.60	122.38	114.03
29	FM	203	PEB	O2B-CGB-CBB	2.60	122.38	114.03
29	wL	302	PEB	C2A-C1A-NA	2.60	110.51	108.27
29	BA	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	JA	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	JC	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	JE	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	BN	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	JN	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	UR	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	S7	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
29	j7	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
29	S9	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
29	j9	201	PEB	OA-C1A-C2A	-2.60	124.11	126.17
29	BA	201	PEB	CAA-C3A-C2A	-2.60	107.77	114.26
29	BN	201	PEB	CAA-C3A-C2A	-2.60	107.77	114.26
29	KB	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	YB	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	KM	201	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	YM	202	PEB	OD-C4D-C3D	-2.60	123.57	129.46
29	DB	203	PEB	O2B-CGB-CBB	2.60	122.38	114.03
29	TB	203	PEB	O2B-CGB-CBB	2.60	122.38	114.03
29	DM	203	PEB	O2B-CGB-CBB	2.60	122.38	114.03
29	TM	203	PEB	O2B-CGB-CBB	2.60	122.38	114.03
29	HF	1002	PEB	CBC-CAC-C2C	-2.60	108.19	112.62
29	HI	1002	PEB	CBC-CAC-C2C	-2.60	108.19	112.62
29	MA	404	PEB	OD-C4D-ND	-2.60	122.08	125.93
29	KB	201	PEB	C1C-CHB-C4B	-2.60	125.71	128.81
29	KM	201	PEB	C1C-CHB-C4B	-2.60	125.71	128.81
29	BD	202	PEB	C2B-C1B-NB	2.60	116.07	110.53
30	A7	303	PUB	C2C-C1C-NC	2.60	113.83	110.05
30	A9	303	PUB	C2C-C1C-NC	2.60	113.83	110.05
31	mP	1001	CYC	C2C-C3C-C4C	2.60	105.23	101.34
29	LA	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	LN	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	DA	202	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	DN	202	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	F4	202	PEB	C2B-C1B-NB	2.60	116.07	110.53
31	PP	1001	CYC	C2C-C3C-C4C	2.60	105.23	101.34
29	xJ	303	PEB	OD-C4D-ND	-2.60	122.08	125.93
29	S2	202	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	aB	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	aM	201	PEB	OD-C4D-C3D	-2.60	123.58	129.46
29	DA	201	PEB	CAA-C3A-C2A	-2.60	107.77	114.26
29	DN	201	PEB	CAA-C3A-C2A	-2.60	107.77	114.26
29	FF	1002	PEB	CBC-CAC-C2C	-2.60	108.19	112.62
29	FI	1002	PEB	CBC-CAC-C2C	-2.60	108.19	112.62
29	D4	202	PEB	OA-C1A-C2A	-2.60	124.11	126.17
31	jP	1001	CYC	C2A-C1A-NA	2.60	113.82	110.05
31	tP	1001	CYC	C2C-C3C-C4C	2.60	105.23	101.34
29	YB	202	PEB	C1C-CHB-C4B	-2.60	125.71	128.81
29	YM	202	PEB	C1C-CHB-C4B	-2.60	125.71	128.81
29	CA	201	PEB	C2A-C1A-NA	2.59	110.51	108.27
29	CN	201	PEB	C2A-C1A-NA	2.59	110.51	108.27
29	MG	401	PEB	CMB-C2B-C1B	2.59	129.06	125.06
29	k7	202	PEB	CAB-C3B-C4B	2.59	129.60	125.01
29	k9	202	PEB	CAB-C3B-C4B	2.59	129.60	125.01
29	Q2	201	PEB	CMA-C2A-C1A	-2.59	106.81	112.40
29	ZB	203	PEB	C2A-C1A-NA	2.59	110.51	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZM	203	PEB	C2A-C1A-NA	2.59	110.51	108.27
29	LA	202	PEB	OD-C4D-C3D	-2.59	123.58	129.46
29	LN	202	PEB	OD-C4D-C3D	-2.59	123.58	129.46
29	G3	201	PEB	CMA-C2A-C1A	-2.59	106.81	112.40
29	GO	201	PEB	CMA-C2A-C1A	-2.59	106.81	112.40
29	JD	202	PEB	C2B-C1B-NB	2.59	116.06	110.53
29	B3	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	BO	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
31	gP	1001	CYC	C2C-C3C-C4C	2.59	105.22	101.34
29	M2	201	PEB	CMA-C2A-C1A	-2.59	106.81	112.40
29	ZB	203	PEB	O2B-CGB-CBB	2.59	122.36	114.03
29	ZM	203	PEB	O2B-CGB-CBB	2.59	122.36	114.03
29	DC	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	DE	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	fJ	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	fL	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	W2	201	PEB	CMA-C2A-C1A	-2.59	106.82	112.40
29	VJ	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	VL	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	hB	201	PEB	C1C-CHB-C4B	-2.59	125.71	128.81
29	hM	201	PEB	C1C-CHB-C4B	-2.59	125.71	128.81
29	B4	202	PEB	C2B-C1B-NB	2.59	116.06	110.53
29	N7	1002	PEB	CHB-C4B-C3B	-2.59	119.34	125.32
29	N9	1002	PEB	CHB-C4B-C3B	-2.59	119.34	125.32
30	wJ	304	PUB	OD-C4D-ND	-2.59	122.09	125.93
29	LJ	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	bJ	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	LL	202	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	bL	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	iB	203	PEB	O2B-CGB-CBB	2.59	122.35	114.03
29	iM	203	PEB	O2B-CGB-CBB	2.59	122.35	114.03
29	fB	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	fM	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
31	YP	1000	CYC	C1B-C2B-C3B	-2.59	105.17	107.87
29	Y1	201	PEB	CHB-C4B-NB	-2.59	125.23	128.83
29	YK	201	PEB	CHB-C4B-NB	-2.59	125.23	128.83
29	RJ	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	RL	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	F3	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	SB	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	HC	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	HE	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SM	201	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	FO	203	PEB	OD-C4D-C3D	-2.59	123.59	129.46
29	HB	203	PEB	O2B-CGB-CBB	2.59	122.35	114.03
29	PB	202	PEB	O2B-CGB-CBB	2.59	122.35	114.03
29	HM	203	PEB	O2B-CGB-CBB	2.59	122.35	114.03
29	PM	202	PEB	O2B-CGB-CBB	2.59	122.35	114.03
29	EB	201	PEB	C1C-CHB-C4B	-2.59	125.72	128.81
29	EM	201	PEB	C1C-CHB-C4B	-2.59	125.72	128.81
29	C3	201	PEB	CMA-C2A-C1A	-2.59	106.82	112.40
29	CO	201	PEB	CMA-C2A-C1A	-2.59	106.82	112.40
29	QR	201	PEB	CMA-C2A-C1A	-2.59	106.82	112.40
29	NB	202	PEB	O2B-CGB-CBB	2.59	122.34	114.03
29	NM	202	PEB	O2B-CGB-CBB	2.59	122.34	114.03
29	m7	202	PEB	CAB-C3B-C4B	2.59	129.59	125.01
29	m9	202	PEB	CAB-C3B-C4B	2.59	129.59	125.01
29	tJ	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	tL	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	D7	1002	PEB	CHB-C4B-C3B	-2.59	119.34	125.32
29	D9	1002	PEB	CHB-C4B-C3B	-2.59	119.34	125.32
29	XB	202	PEB	O2B-CGB-CBB	2.59	122.34	114.03
29	XM	202	PEB	O2B-CGB-CBB	2.59	122.34	114.03
29	l1	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	FA	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	lK	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	FN	202	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	L9	1002	PEB	CHB-C4B-C3B	-2.59	119.34	125.32
29	FB	203	PEB	C2A-C1A-NA	2.59	110.50	108.27
29	FM	203	PEB	C2A-C1A-NA	2.59	110.50	108.27
29	ZJ	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	ZL	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	NF	1002	PEB	CAA-C3A-C4A	-2.59	106.03	112.67
29	NI	1002	PEB	CAA-C3A-C4A	-2.59	106.03	112.67
29	SR	202	PEB	CHA-C4A-NA	-2.59	122.13	125.20
29	nJ	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	nL	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	dB	201	PEB	C1C-CHB-C4B	-2.59	125.72	128.81
29	dM	201	PEB	C1C-CHB-C4B	-2.59	125.72	128.81
29	UB	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	UM	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	A1	303	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	BA	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	pJ	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AK	303	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	pL	203	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	BN	201	PEB	OD-C4D-C3D	-2.59	123.60	129.46
29	QB	203	PEB	C1C-CHB-C4B	-2.59	125.72	128.81
29	QM	203	PEB	C1C-CHB-C4B	-2.59	125.72	128.81
29	LB	203	PEB	O2B-CGB-CBB	2.58	122.33	114.03
29	LM	203	PEB	O2B-CGB-CBB	2.58	122.33	114.03
29	I3	201	PEB	CMA-C2A-C1A	-2.58	106.83	112.40
29	IO	201	PEB	CMA-C2A-C1A	-2.58	106.83	112.40
31	1P	1001	CYC	C2A-C1A-NA	2.58	113.81	110.05
29	dJ	203	PEB	OD-C4D-C3D	-2.58	123.60	129.46
29	dL	203	PEB	OD-C4D-C3D	-2.58	123.60	129.46
29	a7	202	PEB	CAB-C3B-C4B	2.58	129.58	125.01
29	a9	202	PEB	CAB-C3B-C4B	2.58	129.58	125.01
29	F7	1002	PEB	CHB-C4B-C3B	-2.58	119.35	125.32
29	W1	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	FJ	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	WK	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	FL	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	PF	201	PEB	C1B-C2B-C3B	-2.58	103.54	106.51
29	PI	201	PEB	C1B-C2B-C3B	-2.58	103.54	106.51
29	DJ	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	DL	202	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	BC	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	BE	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	jJ	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	jL	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
31	pP	1001	CYC	C2C-C1C-NC	2.58	110.50	108.27
29	A3	201	PEB	C4B-C3B-C2B	-2.58	103.92	106.78
29	AO	201	PEB	C4B-C3B-C2B	-2.58	103.92	106.78
29	FC	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	FE	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	JF	1002	PEB	CBC-CAC-C2C	-2.58	108.21	112.62
29	JI	1002	PEB	CBC-CAC-C2C	-2.58	108.21	112.62
29	JG	202	PEB	C2A-C1A-NA	2.58	110.50	108.27
29	JQ	202	PEB	C2A-C1A-NA	2.58	110.50	108.27
29	dB	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	dM	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	H4	202	PEB	C2B-C1B-NB	2.58	116.04	110.53
29	Y7	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	Y9	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	LF	1002	PEB	CBC-CAC-C2C	-2.58	108.22	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NF	1002	PEB	CBC-CAC-C2C	-2.58	108.22	112.62
29	LI	1002	PEB	CBC-CAC-C2C	-2.58	108.22	112.62
29	NI	1002	PEB	CBC-CAC-C2C	-2.58	108.22	112.62
29	HG	202	PEB	C2A-C1A-NA	2.58	110.50	108.27
29	HQ	202	PEB	C2A-C1A-NA	2.58	110.50	108.27
29	DF	1002	PEB	CAA-C3A-C4A	-2.58	106.05	112.67
29	DI	1002	PEB	CAA-C3A-C4A	-2.58	106.05	112.67
29	JA	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	WB	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	WM	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	JN	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	CD	203	PEB	CHA-C1B-NB	-2.58	119.53	124.93
29	cF	201	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
29	cI	201	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
29	hB	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	JJ	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	JL	203	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	hM	201	PEB	OD-C4D-C3D	-2.58	123.61	129.46
29	xL	303	PEB	CHA-C1B-NB	-2.58	119.54	124.93
29	Q2	201	PEB	OD-C4D-ND	-2.58	122.11	125.93
29	FD	202	PEB	C2B-C1B-NB	2.58	116.03	110.53
29	P7	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
29	P9	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
29	g7	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	g9	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	EB	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	EM	201	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	TI	201	PEB	C1B-C2B-C3B	-2.58	103.55	106.51
29	wL	303	PEB	CHA-C1B-NB	-2.58	119.54	124.93
29	R7	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	c7	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	R9	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	c9	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	eB	202	PEB	O2B-CGB-CBB	2.58	122.31	114.03
29	eM	202	PEB	O2B-CGB-CBB	2.58	122.31	114.03
29	g1	201	PEB	CHB-C4B-NB	-2.58	125.25	128.83
29	gK	201	PEB	CHB-C4B-NB	-2.58	125.25	128.83
29	lB	201	PEB	C1C-CHB-C4B	-2.58	125.73	128.81
29	lM	201	PEB	C1C-CHB-C4B	-2.58	125.73	128.81
29	U7	201	PEB	OA-C1A-C2A	-2.58	124.12	126.17
29	U9	201	PEB	OA-C1A-C2A	-2.58	124.12	126.17
29	aF	203	PEB	OD-C4D-C3D	-2.58	123.62	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	aI	203	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	F9	1002	PEB	CHB-C4B-C3B	-2.58	119.37	125.32
29	K4	203	PEB	CHA-C1B-NB	-2.58	119.54	124.93
29	H7	1002	PEB	CHB-C4B-C3B	-2.58	119.37	125.32
29	H9	1002	PEB	CHB-C4B-C3B	-2.58	119.37	125.32
29	i7	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
29	i9	202	PEB	CAB-C3B-C4B	2.58	129.57	125.01
29	xL	303	PEB	OD-C4D-ND	-2.58	122.11	125.93
29	GD	203	PEB	CHA-C1B-NB	-2.58	119.54	124.93
29	vJ	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	vL	202	PEB	OD-C4D-C3D	-2.58	123.62	129.46
29	XB	202	PEB	C2A-C1A-NA	2.58	110.49	108.27
29	XM	202	PEB	C2A-C1A-NA	2.58	110.49	108.27
31	RP	1001	CYC	C2C-C1C-NC	2.58	110.49	108.27
29	J7	1002	PEB	CHB-C4B-C3B	-2.57	119.37	125.32
29	L7	1002	PEB	CHB-C4B-C3B	-2.57	119.37	125.32
29	c1	201	PEB	CHB-C4B-NB	-2.57	125.25	128.83
29	cK	201	PEB	CHB-C4B-NB	-2.57	125.25	128.83
29	TF	202	PEB	C1B-C2B-C3B	-2.57	103.55	106.51
29	TI	202	PEB	C1B-C2B-C3B	-2.57	103.55	106.51
29	B4	202	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
29	WR	201	PEB	CMA-C2A-C1A	-2.57	106.85	112.40
29	KG	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	KQ	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	mB	203	PEB	O2B-CGB-CBB	2.57	122.30	114.03
29	mM	203	PEB	O2B-CGB-CBB	2.57	122.30	114.03
29	NO	201	PEB	C4B-C3B-C2B	-2.57	103.93	106.78
29	G5	203	PEB	C2A-C1A-NA	2.57	110.49	108.27
29	e7	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	e9	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	kF	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	kI	203	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	g7	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	g9	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	SB	201	PEB	C1C-CHB-C4B	-2.57	125.73	128.81
29	SM	201	PEB	C1C-CHB-C4B	-2.57	125.73	128.81
29	N3	201	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
31	TP	1001	CYC	C2C-C1C-NC	2.57	110.49	108.27
29	JB	203	PEB	O2B-CGB-CBB	2.57	122.30	114.03
29	JM	203	PEB	O2B-CGB-CBB	2.57	122.30	114.03
29	T7	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	T9	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	kF	201	PEB	C1B-C2B-C3B	-2.57	103.55	106.51
29	kI	201	PEB	C1B-C2B-C3B	-2.57	103.55	106.51
29	jB	201	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
29	jM	201	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
29	Q1	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	QK	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	h1	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	hK	202	PEB	OD-C4D-C3D	-2.57	123.63	129.46
29	DG	202	PEB	C3B-C4B-NB	2.57	113.79	110.05
29	DQ	202	PEB	C3B-C4B-NB	2.57	113.79	110.05
29	B5	203	PEB	C2A-C1A-NA	2.57	110.49	108.27
29	R1	201	PEB	CHB-C4B-NB	-2.57	125.26	128.83
29	RK	201	PEB	CHB-C4B-NB	-2.57	125.26	128.83
29	JF	1002	PEB	CAA-C3A-C4A	-2.57	106.07	112.67
29	JI	1002	PEB	CAA-C3A-C4A	-2.57	106.07	112.67
29	j1	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	lB	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	jK	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	lM	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	lB	203	PEB	C2A-C1A-NA	2.57	110.49	108.27
29	lM	203	PEB	C2A-C1A-NA	2.57	110.49	108.27
29	R7	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	e7	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	R9	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	e9	202	PEB	CAB-C3B-C4B	2.57	129.56	125.01
29	HD	202	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
29	DA	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	DN	201	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	AM	301	PEB	C2A-C3A-C4A	-2.57	97.49	101.34
29	c7	202	PEB	CAB-C3B-C4B	2.57	129.55	125.01
29	c9	202	PEB	CAB-C3B-C4B	2.57	129.55	125.01
29	Y7	202	PEB	CAB-C3B-C4B	2.57	129.55	125.01
29	Y9	202	PEB	CAB-C3B-C4B	2.57	129.55	125.01
29	S1	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	SK	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	C3	201	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
29	CO	201	PEB	C4B-C3B-C2B	-2.57	103.94	106.78
29	QB	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	QM	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	LF	1002	PEB	CAA-C3A-C4A	-2.57	106.08	112.67
29	LI	1002	PEB	CAA-C3A-C4A	-2.57	106.08	112.67
29	vJ	202	PEB	C2A-C1A-NA	2.57	110.49	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	vL	202	PEB	C2A-C1A-NA	2.57	110.49	108.27
29	IG	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	TJ	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	TL	203	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	IQ	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	b1	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	bK	202	PEB	OD-C4D-C3D	-2.57	123.64	129.46
29	MB	201	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
29	MM	201	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
29	xJ	303	PEB	CHA-C1B-NB	-2.57	119.56	124.93
29	P7	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
29	R7	203	PEB	OD-C4D-C3D	-2.57	123.65	129.46
29	P9	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
29	R9	203	PEB	OD-C4D-C3D	-2.57	123.65	129.46
29	WR	202	PEB	CHA-C4A-NA	-2.57	122.15	125.20
29	GB	201	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
29	GM	201	PEB	C1C-CHB-C4B	-2.57	125.74	128.81
29	f7	201	PEB	OA-C1A-C2A	-2.57	124.13	126.17
29	f9	201	PEB	OA-C1A-C2A	-2.57	124.13	126.17
29	a7	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
29	a9	202	PEB	OD-C4D-C3D	-2.57	123.65	129.46
29	A1	302	PEB	CHA-C4A-NA	-2.57	122.16	125.20
29	AK	302	PEB	CHA-C4A-NA	-2.57	122.16	125.20
29	OR	201	PEB	CMA-C2A-C1A	-2.56	106.87	112.40
29	mF	201	PEB	C1B-C2B-C3B	-2.56	103.56	106.51
29	mI	201	PEB	C1B-C2B-C3B	-2.56	103.56	106.51
29	O2	201	PEB	CMA-C2A-C1A	-2.56	106.88	112.40
29	T7	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	i7	203	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	T9	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	i9	203	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	DD	202	PEB	CHC-C4C-C3C	-2.56	125.96	130.34
29	Y7	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	e7	203	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	Y9	202	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	e9	203	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	GA	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	GN	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	CC	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	CE	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	V1	201	PEB	CHB-C4B-NB	-2.56	125.27	128.83
29	VK	201	PEB	CHB-C4B-NB	-2.56	125.27	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M3	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
29	MO	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
29	AB	301	PEB	C2A-C3A-C4A	-2.56	97.50	101.34
29	OB	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	OM	201	PEB	OD-C4D-C3D	-2.56	123.65	129.46
29	HF	1002	PEB	CAA-C3A-C4A	-2.56	106.09	112.67
29	HI	1002	PEB	CAA-C3A-C4A	-2.56	106.09	112.67
29	KA	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	BG	202	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	KN	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	BQ	202	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	TF	201	PEB	CMB-C2B-C1B	2.56	129.01	125.06
29	d1	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	GB	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	MB	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	dK	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	GM	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	MM	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	XJ	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	XL	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	TF	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	TI	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
30	yJ	302	PUB	C2C-C1C-NC	2.56	113.77	110.05
30	yL	302	PUB	C2C-C1C-NC	2.56	113.77	110.05
29	J9	1002	PEB	CHB-C4B-C3B	-2.56	119.41	125.32
29	iF	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
29	iI	201	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
29	IB	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	IM	201	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	U2	202	PEB	CHA-C4A-NA	-2.56	122.16	125.20
29	EA	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	kB	203	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	LG	202	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	kM	203	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	EN	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	LQ	201	PEB	C2A-C1A-NA	2.56	110.48	108.27
29	k7	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	k9	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	b7	201	PEB	OA-C1A-C2A	-2.56	124.14	126.17
29	b9	201	PEB	OA-C1A-C2A	-2.56	124.14	126.17
29	FG	202	PEB	C3B-C4B-NB	2.56	113.77	110.05
29	FQ	202	PEB	C3B-C4B-NB	2.56	113.77	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V7	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	V9	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	J4	202	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
29	m1	201	PEB	CHB-C4B-NB	-2.56	125.28	128.83
29	mK	201	PEB	CHB-C4B-NB	-2.56	125.28	128.83
29	k7	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	k9	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	PF	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	AG	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	PI	203	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	AQ	202	PEB	OD-C4D-C3D	-2.56	123.66	129.46
29	H4	202	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
29	RF	202	PEB	OD-C4D-C3D	-2.56	123.67	129.46
29	RI	202	PEB	OD-C4D-C3D	-2.56	123.67	129.46
29	AF	305	PEB	OD-C4D-ND	-2.56	122.14	125.93
29	AI	305	PEB	OD-C4D-ND	-2.56	122.14	125.93
29	M2	202	PEB	CHA-C4A-NA	-2.56	122.16	125.20
29	aF	203	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
29	aI	203	PEB	C1B-C2B-C3B	-2.56	103.57	106.51
29	m7	202	PEB	OD-C4D-C3D	-2.56	123.67	129.46
29	m9	202	PEB	OD-C4D-C3D	-2.56	123.67	129.46
29	eF	203	PEB	OD-C4D-C3D	-2.56	123.67	129.46
29	eI	203	PEB	OD-C4D-C3D	-2.56	123.67	129.46
29	S2	202	PEB	CHA-C4A-NA	-2.56	122.17	125.20
29	P2	201	PEB	CMB-C2B-C1B	2.56	129.00	125.06
29	K3	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
29	KO	201	PEB	C4B-C3B-C2B	-2.56	103.95	106.78
29	G4	203	PEB	CHA-C1B-NB	-2.56	119.59	124.93
29	i7	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	i9	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	YF	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	YI	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	RR	202	PEB	CMB-C2B-C1B	2.55	129.00	125.06
29	VB	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	VM	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	FF	1002	PEB	CAA-C3A-C4A	-2.55	106.11	112.67
29	FI	1002	PEB	CAA-C3A-C4A	-2.55	106.11	112.67
29	Z1	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	CG	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	ZK	203	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	CQ	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	cF	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GG	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	cI	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	GQ	202	PEB	OD-C4D-C3D	-2.55	123.67	129.46
29	VF	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	VI	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	O1	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	a7	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	a9	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	OK	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	G8	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	JB	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	JM	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	Q2	202	PEB	CHA-C4A-NA	-2.55	122.17	125.20
29	UR	202	PEB	CHA-C4A-NA	-2.55	122.17	125.20
29	eF	201	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
29	eI	201	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
29	e1	201	PEB	CHB-C4B-NB	-2.55	125.29	128.83
29	eK	201	PEB	CHB-C4B-NB	-2.55	125.29	128.83
29	LG	201	PEB	OD-C4D-ND	-2.55	122.15	125.93
29	MQ	402	PEB	OD-C4D-ND	-2.55	122.15	125.93
29	EG	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	EQ	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	I3	201	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
29	IO	201	PEB	C4B-C3B-C2B	-2.55	103.96	106.78
29	iF	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	iI	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	T1	201	PEB	CHB-C4B-NB	-2.55	125.29	128.83
29	TK	201	PEB	CHB-C4B-NB	-2.55	125.29	128.83
29	U1	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	f1	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	UK	203	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	fK	202	PEB	OD-C4D-C3D	-2.55	123.68	129.46
29	BD	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
29	MG	404	PEB	CBC-CAC-C2C	-2.55	108.27	112.62
29	WB	201	PEB	C1C-CHB-C4B	-2.55	125.76	128.81
29	WM	201	PEB	C1C-CHB-C4B	-2.55	125.76	128.81
29	HB	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	HM	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	CB	201	PEB	C1C-CHB-C4B	-2.55	125.76	128.81
29	CM	201	PEB	C1C-CHB-C4B	-2.55	125.76	128.81
29	IC	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	IE	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V2	202	PEB	CMB-C2B-C1B	2.55	128.99	125.06
29	MA	401	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	mB	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	mM	203	PEB	C2A-C1A-NA	2.55	110.47	108.27
31	lP	1001	CYC	C2C-C1C-NC	2.55	110.47	108.27
29	T7	203	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	T9	203	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	gF	203	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	gI	203	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	D7	1002	PEB	OD-C4D-ND	-2.55	122.16	125.93
29	D9	1002	PEB	OD-C4D-ND	-2.55	122.16	125.93
29	MG	404	PEB	OD-C4D-ND	-2.55	122.16	125.93
29	ID	201	PEB	C2B-C1B-NB	2.55	115.97	110.53
29	PB	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	PM	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
29	RF	202	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
29	RI	202	PEB	C1B-C2B-C3B	-2.55	103.58	106.51
29	GC	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	GE	201	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	m7	203	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	m9	203	PEB	OD-C4D-C3D	-2.55	123.69	129.46
29	YF	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
29	YI	201	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
29	C5	203	PEB	OD-C4D-C3D	-2.54	123.69	129.46
29	V7	202	PEB	OD-C4D-C3D	-2.54	123.69	129.46
29	C8	203	PEB	OD-C4D-C3D	-2.54	123.69	129.46
29	V9	202	PEB	OD-C4D-C3D	-2.54	123.69	129.46
29	KC	202	PEB	OD-C4D-C3D	-2.54	123.70	129.46
29	KE	202	PEB	OD-C4D-C3D	-2.54	123.70	129.46
29	k1	201	PEB	CHB-C4B-NB	-2.54	125.30	128.83
29	kK	201	PEB	CHB-C4B-NB	-2.54	125.30	128.83
29	QR	202	PEB	CBC-CAC-C2C	-2.54	108.28	112.62
29	VR	202	PEB	CMB-C2B-C1B	2.54	128.98	125.06
29	MQ	406	PEB	CBC-CAC-C2C	-2.54	108.28	112.62
29	kF	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
29	kI	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
29	RB	203	PEB	C2A-C1A-NA	2.54	110.47	108.27
29	DJ	202	PEB	C2A-C1A-NA	2.54	110.47	108.27
29	DL	202	PEB	C2A-C1A-NA	2.54	110.47	108.27
29	RM	203	PEB	C2A-C1A-NA	2.54	110.47	108.27
29	eF	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51
29	eI	203	PEB	C1B-C2B-C3B	-2.54	103.59	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
29	J5	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
29	L5	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
29	bK	201	PEB	OD-C4D-C3D	-2.54	123.70	129.46
29	LD	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
29	SR	201	PEB	C3B-C4B-NB	2.54	113.75	110.05
29	O7	201	PEB	OA-C1A-C2A	-2.54	124.15	126.17
29	O9	201	PEB	OA-C1A-C2A	-2.54	124.15	126.17
29	cB	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	cM	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	MN	401	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	JD	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
29	mF	203	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	mI	203	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	F4	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
29	Z1	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	h1	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	ZK	202	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	hK	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	E3	201	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
29	EO	201	PEB	C4B-C3B-C2B	-2.54	103.97	106.78
29	GD	203	PEB	CMD-C2D-C3D	2.54	133.64	130.06
29	X2	201	PEB	CMB-C2B-C1B	2.54	128.97	125.06
29	wJ	303	PEB	OD-C4D-ND	-2.54	122.17	125.93
29	tJ	202	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	tL	202	PEB	C2A-C1A-NA	2.54	110.46	108.27
31	vP	1001	CYC	C2C-C1C-NC	2.54	110.46	108.27
29	Q7	201	PEB	OA-C1A-C2A	-2.54	124.16	126.17
29	Q9	201	PEB	OA-C1A-C2A	-2.54	124.16	126.17
31	yP	1001	CYC	CHB-C1B-C2B	-2.54	121.92	126.95
29	P1	201	PEB	CHB-C4B-NB	-2.54	125.31	128.83
29	PK	201	PEB	CHB-C4B-NB	-2.54	125.31	128.83
29	pJ	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	pL	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	MR	202	PEB	CBC-CAC-C2C	-2.54	108.29	112.62
29	IB	201	PEB	C1C-CHB-C4B	-2.54	125.78	128.81
29	IM	201	PEB	C1C-CHB-C4B	-2.54	125.78	128.81
30	AB	305	PUB	OA-C1A-NA	-2.54	122.17	125.93
29	AC	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	AE	201	PEB	OD-C4D-C3D	-2.54	123.71	129.46
29	PF	203	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
29	PI	203	PEB	C1B-C2B-C3B	-2.54	103.60	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	FJ	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	FL	203	PEB	C2A-C1A-NA	2.54	110.46	108.27
29	EC	201	PEB	OD-C4D-C3D	-2.54	123.72	129.46
29	EE	201	PEB	OD-C4D-C3D	-2.54	123.72	129.46
29	aB	201	PEB	C1C-CHB-C4B	-2.54	125.78	128.81
29	aM	201	PEB	C1C-CHB-C4B	-2.54	125.78	128.81
29	VF	203	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
29	VI	203	PEB	C1B-C2B-C3B	-2.54	103.60	106.51
29	a1	201	PEB	CHB-C4B-NB	-2.54	125.31	128.83
29	aK	201	PEB	CHB-C4B-NB	-2.54	125.31	128.83
29	c7	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	c9	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	JG	201	PEB	OD-C4D-ND	-2.53	122.17	125.93
29	JQ	201	PEB	OD-C4D-ND	-2.53	122.17	125.93
29	AA	201	PEB	C2A-C1A-NA	2.53	110.46	108.27
29	AN	201	PEB	C2A-C1A-NA	2.53	110.46	108.27
29	g7	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	g9	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	d1	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	dK	201	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	C4	201	PEB	C2B-C1B-NB	2.53	115.94	110.53
29	LC	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	LE	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	B8	203	PEB	C2A-C1A-NA	2.53	110.46	108.27
31	DK	1001	CYC	CHA-C1A-NA	-2.53	125.31	128.83
29	U1	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	UK	202	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	D4	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
29	I5	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	A5	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	I8	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	A8	203	PEB	OD-C4D-C3D	-2.53	123.72	129.46
29	F5	203	PEB	C2A-C1A-NA	2.53	110.45	108.27
29	F8	203	PEB	C2A-C1A-NA	2.53	110.45	108.27
29	N2	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	FC	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	FE	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	JG	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
29	JQ	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
29	J8	201	PEB	OD-C4D-C3D	-2.53	123.73	129.46
29	MD	201	PEB	CAC-CBC-CGC	-2.53	106.67	113.76
29	J5	201	PEB	CMA-C2A-C1A	-2.53	106.95	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J8	201	PEB	CMA-C2A-C1A	-2.53	106.95	112.40
29	E4	201	PEB	C2B-C1B-NB	2.53	115.93	110.53
29	dD	401	PEB	C2B-C1B-NB	2.53	115.93	110.53
29	N7	1002	PEB	OD-C4D-ND	-2.53	122.18	125.93
29	N9	1002	PEB	OD-C4D-ND	-2.53	122.18	125.93
29	HC	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	HE	202	PEB	CMB-C2B-C1B	2.53	128.96	125.06
29	LG	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
29	LQ	201	PEB	C3B-C4B-NB	2.53	113.73	110.05
29	iB	203	PEB	C2A-C1A-NA	2.53	110.45	108.27
29	iM	203	PEB	C2A-C1A-NA	2.53	110.45	108.27
31	PP	1001	CYC	C2C-C1C-NC	2.53	110.45	108.27
29	P7	203	PEB	OD-C4D-C3D	-2.53	123.73	129.46
29	P9	203	PEB	OD-C4D-C3D	-2.53	123.73	129.46
29	HG	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
29	HQ	202	PEB	C3B-C4B-NB	2.53	113.73	110.05
30	xJ	304	PUB	C2C-C1C-NC	2.53	113.73	110.05
29	l7	201	PEB	OA-C1A-NA	2.53	128.00	124.94
29	l9	201	PEB	OA-C1A-NA	2.53	128.00	124.94
29	MQ	406	PEB	OD-C4D-ND	-2.53	122.19	125.93
29	O2	202	PEB	CHA-C4A-NA	-2.53	122.20	125.20
29	G5	201	PEB	OD-C4D-C3D	-2.53	123.73	129.46
29	M4	201	PEB	CAC-CBC-CGC	-2.53	106.67	113.76
29	Q1	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
29	QK	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
31	iP	1001	CYC	C2C-C1C-NC	2.53	110.45	108.27
29	b7	202	PEB	CHA-C1B-NB	-2.53	119.65	124.93
29	b9	202	PEB	CHA-C1B-NB	-2.53	119.65	124.93
29	j1	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
29	jK	201	PEB	OD-C4D-C3D	-2.53	123.74	129.46
29	CD	201	PEB	C2B-C1B-NB	2.52	115.92	110.53
29	H5	201	PEB	OD-C4D-C3D	-2.52	123.74	129.46
29	NR	202	PEB	CMB-C2B-C1B	2.52	128.95	125.06
29	l1	201	PEB	OD-C4D-C3D	-2.52	123.74	129.46
29	lK	201	PEB	OD-C4D-C3D	-2.52	123.74	129.46
29	W7	201	PEB	OA-C1A-NA	2.52	128.00	124.94
29	W9	201	PEB	OA-C1A-NA	2.52	128.00	124.94
29	F7	1002	PEB	OD-C4D-ND	-2.52	122.19	125.93
29	OB	201	PEB	C1C-CHB-C4B	-2.52	125.80	128.81
29	OM	201	PEB	C1C-CHB-C4B	-2.52	125.80	128.81
29	KC	201	PEB	CMB-C2B-C1B	2.52	128.95	125.06
29	KE	201	PEB	CMB-C2B-C1B	2.52	128.95	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L8	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	U2	202	PEB	CHC-C1D-ND	-2.52	111.02	113.95
30	AM	305	PUB	CAC-CBC-CGC	-2.52	108.17	113.60
31	WP	1001	CYC	CHB-C1B-C2B	-2.52	121.95	126.95
29	bJ	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	bL	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	RB	203	PEB	CHC-C1D-ND	-2.52	111.02	113.95
29	RM	203	PEB	CHC-C1D-ND	-2.52	111.02	113.95
29	J9	1002	PEB	OD-C4D-ND	-2.52	122.19	125.93
29	FD	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
29	K4	201	PEB	CAC-CBC-CGC	-2.52	106.69	113.76
29	iI	201	PEB	CHB-C4B-NB	-2.52	125.33	128.83
29	iK	201	PEB	CHB-C4B-NB	-2.52	125.33	128.83
29	NB	202	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	ZJ	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	rJ	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	ZL	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	rL	203	PEB	C2A-C1A-NA	2.52	110.45	108.27
29	NM	202	PEB	C2A-C1A-NA	2.52	110.45	108.27
31	gP	1001	CYC	C2C-C1C-NC	2.52	110.45	108.27
29	XR	202	PEB	CMB-C2B-C1B	2.52	128.94	125.06
29	F9	1002	PEB	OD-C4D-ND	-2.52	122.20	125.93
29	mF	203	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
29	mI	203	PEB	C1B-C2B-C3B	-2.52	103.61	106.51
31	GP	1001	CYC	C2C-C1C-NC	2.52	110.44	108.27
31	VP	1001	CYC	C2B-C1B-NB	2.52	110.68	106.99
29	GD	201	PEB	CAC-CBC-CGC	-2.52	106.70	113.76
30	MA	402	PUB	OA-C1A-NA	-2.52	122.20	125.93
29	fI	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	G8	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	H8	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	fK	201	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	G4	201	PEB	C2B-C1B-NB	2.52	115.91	110.53
29	GD	201	PEB	C2B-C1B-NB	2.52	115.91	110.53
29	iF	203	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
29	iI	203	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
29	WR	202	PEB	CBC-CAC-C2C	-2.52	108.32	112.62
29	K5	203	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	K8	203	PEB	OD-C4D-C3D	-2.52	123.75	129.46
29	TB	203	PEB	C2A-C1A-NA	2.52	110.44	108.27
29	LJ	202	PEB	C2A-C1A-NA	2.52	110.44	108.27
29	LL	202	PEB	C2A-C1A-NA	2.52	110.44	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TM	203	PEB	C2A-C1A-NA	2.52	110.44	108.27
31	tP	1001	CYC	C2C-C1C-NC	2.52	110.44	108.27
30	AB	305	PUB	CAC-CBC-CGC	-2.52	108.18	113.60
29	cF	202	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
29	cI	202	PEB	C1B-C2B-C3B	-2.52	103.62	106.51
29	PR	201	PEB	CMB-C2B-C1B	2.52	128.94	125.06
29	W1	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	IG	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	WK	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	IQ	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	D4	202	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	DD	202	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	C4	201	PEB	CAC-CBC-CGC	-2.52	106.70	113.76
29	Z7	202	PEB	CHA-C1B-NB	-2.52	119.67	124.93
29	Z9	202	PEB	CHA-C1B-NB	-2.52	119.67	124.93
29	S1	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	F5	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	F8	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	SK	201	PEB	OD-C4D-C3D	-2.52	123.76	129.46
29	G3	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
29	GO	201	PEB	C4B-C3B-C2B	-2.52	104.00	106.78
29	J7	1002	PEB	OD-C4D-ND	-2.52	122.20	125.93
29	L4	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
31	KP	1001	CYC	C2C-C1C-NC	2.51	110.44	108.27
29	BG	202	PEB	C3B-C4B-NB	2.51	113.71	110.05
29	BQ	202	PEB	C3B-C4B-NB	2.51	113.71	110.05
29	O1	201	PEB	OD-C4D-C3D	-2.51	123.76	129.46
29	OK	201	PEB	OD-C4D-C3D	-2.51	123.76	129.46
29	G4	201	PEB	CAC-CBC-CGC	-2.51	106.71	113.76
29	A1	303	PEB	CBC-CAC-C2C	-2.51	108.33	112.62
29	AK	303	PEB	CBC-CAC-C2C	-2.51	108.33	112.62
29	eB	202	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	eM	202	PEB	C2A-C1A-NA	2.51	110.44	108.27
31	eP	1001	CYC	C2C-C1C-NC	2.51	110.44	108.27
29	Q1	202	PEB	CMB-C2B-C1B	2.51	128.94	125.06
29	W1	202	PEB	CMB-C2B-C1B	2.51	128.94	125.06
29	QK	202	PEB	CMB-C2B-C1B	2.51	128.94	125.06
29	WK	202	PEB	CMB-C2B-C1B	2.51	128.94	125.06
29	d7	202	PEB	CHA-C1B-NB	-2.51	119.68	124.93
29	d9	202	PEB	CHA-C1B-NB	-2.51	119.68	124.93
29	Z7	201	PEB	OA-C1A-NA	2.51	127.98	124.94
29	Z9	201	PEB	OA-C1A-NA	2.51	127.98	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BJ	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	BL	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	wL	303	PEB	OD-C4D-ND	-2.51	122.21	125.93
30	AM	305	PUB	OA-C1A-NA	-2.51	122.21	125.93
29	h7	201	PEB	OA-C1A-NA	2.51	127.98	124.94
29	h9	201	PEB	OA-C1A-NA	2.51	127.98	124.94
29	l1	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
29	lK	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
29	TR	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
29	B5	201	PEB	OD-C4D-C3D	-2.51	123.77	129.46
29	TJ	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	TL	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
31	EP	1001	CYC	C2C-C1C-NC	2.51	110.44	108.27
29	fB	201	PEB	C1C-CHB-C4B	-2.51	125.81	128.81
29	fM	201	PEB	C1C-CHB-C4B	-2.51	125.81	128.81
29	L9	1002	PEB	OD-C4D-ND	-2.51	122.21	125.93
29	R2	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
29	K4	203	PEB	CMD-C2D-C3D	2.51	133.60	130.06
29	U7	202	PEB	CHA-C1B-NB	-2.51	119.68	124.93
29	U9	202	PEB	CHA-C1B-NB	-2.51	119.68	124.93
29	LQ	202	PEB	CHA-C1B-NB	-2.51	119.68	124.93
31	D1	1001	CYC	CHA-C1A-NA	-2.51	125.35	128.83
29	T2	202	PEB	CMB-C2B-C1B	2.51	128.93	125.06
29	HJ	202	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	HL	202	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	ID	201	PEB	CAC-CBC-CGC	-2.51	106.72	113.76
29	F3	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
29	FO	201	PEB	OD-C4D-C3D	-2.51	123.78	129.46
29	PB	202	PEB	CHC-C1D-ND	-2.51	111.03	113.95
29	PM	202	PEB	CHC-C1D-ND	-2.51	111.03	113.95
30	MN	402	PUB	OA-C1A-NA	-2.51	122.21	125.93
30	xL	304	PUB	CBA-CAA-C3A	-2.51	109.17	112.98
29	dJ	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
29	dL	203	PEB	C2A-C1A-NA	2.51	110.44	108.27
30	wL	304	PUB	CBA-CAA-C3A	-2.51	109.17	112.98
29	TB	203	PEB	CHC-C1D-ND	-2.51	111.03	113.95
29	TM	203	PEB	CHC-C1D-ND	-2.51	111.03	113.95
31	YP	1000	CYC	C1B-NB-C4B	-2.51	107.48	110.67
29	I4	201	PEB	C2B-C1B-NB	2.51	115.88	110.53
30	A1	304	PUB	CAC-C2C-C1C	2.51	129.44	125.01
30	AK	304	PUB	CAC-C2C-C1C	2.51	129.44	125.01
29	BG	201	PEB	OD-C4D-ND	-2.51	122.22	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DG	201	PEB	OD-C4D-ND	-2.51	122.22	125.93
29	BQ	201	PEB	OD-C4D-ND	-2.51	122.22	125.93
29	DQ	201	PEB	OD-C4D-ND	-2.51	122.22	125.93
29	gB	203	PEB	C2A-C1A-NA	2.51	110.43	108.27
29	gM	203	PEB	C2A-C1A-NA	2.51	110.43	108.27
29	KD	201	PEB	CAC-CBC-CGC	-2.51	106.73	113.76
30	xL	304	PUB	C2C-C1C-NC	2.51	113.69	110.05
29	A1	301	PEB	C2A-C1A-NA	2.51	110.43	108.27
29	AK	301	PEB	C2A-C1A-NA	2.51	110.43	108.27
31	AP	1001	CYC	C2C-C1C-NC	2.51	110.43	108.27
31	CP	1001	CYC	C2C-C1C-NC	2.51	110.43	108.27
29	FG	201	PEB	OD-C4D-ND	-2.51	122.22	125.93
29	FQ	201	PEB	OD-C4D-ND	-2.51	122.22	125.93
29	YF	203	PEB	C1B-C2B-C3B	-2.50	103.63	106.51
29	YI	203	PEB	C1B-C2B-C3B	-2.50	103.63	106.51
31	1P	1002	CYC	C2B-C1B-NB	2.50	110.65	106.99
29	XB	202	PEB	CHC-C1D-ND	-2.50	111.04	113.95
29	XM	202	PEB	CHC-C1D-ND	-2.50	111.04	113.95
29	MD	201	PEB	C2B-C1B-NB	2.50	115.87	110.53
29	BC	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
29	BE	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
29	BB	301	PEB	C2A-C3A-C4A	-2.50	97.59	101.34
29	BM	301	PEB	C2A-C3A-C4A	-2.50	97.59	101.34
29	S1	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
29	SK	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
30	AF	302	PUB	C1D-CHC-C4C	-2.50	107.92	113.37
30	AI	302	PUB	C1D-CHC-C4C	-2.50	107.92	113.37
29	M2	202	PEB	CBC-CAC-C2C	-2.50	108.35	112.62
29	GG	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
29	GQ	201	PEB	OD-C4D-C3D	-2.50	123.79	129.46
29	b1	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
29	bK	202	PEB	CMB-C2B-C1B	2.50	128.92	125.06
29	CD	201	PEB	CAC-CBC-CGC	-2.50	106.74	113.76
29	h7	202	PEB	CHA-C1B-NB	-2.50	119.70	124.93
29	h9	202	PEB	CHA-C1B-NB	-2.50	119.70	124.93
29	RJ	203	PEB	C2A-C1A-NA	2.50	110.43	108.27
29	RL	203	PEB	C2A-C1A-NA	2.50	110.43	108.27
29	M4	201	PEB	C2B-C1B-NB	2.50	115.87	110.53
29	O7	202	PEB	CHA-C1B-NB	-2.50	119.70	124.93
29	O9	202	PEB	CHA-C1B-NB	-2.50	119.70	124.93
29	DB	203	PEB	C2A-C1A-NA	2.50	110.43	108.27
29	DM	203	PEB	C2A-C1A-NA	2.50	110.43	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1P	1002	CYC	C1B-NB-C4B	-2.50	107.48	110.67
29	I4	201	PEB	CAC-CBC-CGC	-2.50	106.75	113.76
29	IJ	203	PEB	C2A-C1A-NA	2.50	110.43	108.27
29	IL	203	PEB	C2A-C1A-NA	2.50	110.43	108.27
29	H7	1002	PEB	OD-C4D-ND	-2.50	122.23	125.93
29	H9	1002	PEB	OD-C4D-ND	-2.50	122.23	125.93
29	F4	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
29	F3	202	PEB	CHC-C1D-ND	-2.50	111.05	113.95
29	FO	202	PEB	CHC-C1D-ND	-2.50	111.05	113.95
31	xP	1001	CYC	C2B-C1B-NB	2.50	110.65	106.99
29	l7	202	PEB	CHA-C1B-NB	-2.50	119.71	124.93
29	l9	202	PEB	CHA-C1B-NB	-2.50	119.71	124.93
29	K4	201	PEB	C2B-C1B-NB	2.50	115.86	110.53
29	FB	203	PEB	CHC-C1D-ND	-2.50	111.05	113.95
29	FM	203	PEB	CHC-C1D-ND	-2.50	111.05	113.95
29	LD	202	PEB	OD-C4D-C3D	-2.50	123.80	129.46
30	wJ	304	PUB	CBA-CAA-C3A	-2.50	109.19	112.98
29	gF	203	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
29	gI	203	PEB	C1B-C2B-C3B	-2.50	103.64	106.51
31	cP	1001	CYC	C2C-C1C-NC	2.50	110.43	108.27
29	U1	203	PEB	CMB-C2B-C1B	2.50	128.91	125.06
29	UK	203	PEB	CMB-C2B-C1B	2.50	128.91	125.06
29	gB	203	PEB	CHC-C1D-ND	-2.50	111.05	113.95
29	gM	203	PEB	CHC-C1D-ND	-2.50	111.05	113.95
29	mF	201	PEB	OD-C4D-C3D	-2.50	123.80	129.46
29	mI	201	PEB	OD-C4D-C3D	-2.50	123.80	129.46
29	UR	202	PEB	CHC-C1D-ND	-2.50	111.05	113.95
29	VF	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
29	VI	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
29	B8	201	PEB	OD-C4D-C3D	-2.50	123.81	129.46
29	mB	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	mM	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	gF	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	gI	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	ZB	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	ZM	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
31	iP	1001	CYC	C1B-CHB-C4A	2.49	134.17	128.08
29	EG	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	EQ	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	j1	202	PEB	CMB-C2B-C1B	2.49	128.90	125.06
29	jK	202	PEB	CMB-C2B-C1B	2.49	128.90	125.06
29	S7	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j7	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
29	S9	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
29	j9	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
29	PF	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	PI	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	NB	202	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	VB	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	NM	202	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	VM	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	Q2	202	PEB	CBC-CAC-C2C	-2.49	108.37	112.62
29	SR	202	PEB	CBC-CAC-C2C	-2.49	108.37	112.62
29	W7	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
29	W9	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
29	d7	201	PEB	OA-C1A-NA	2.49	127.96	124.94
29	d9	201	PEB	OA-C1A-NA	2.49	127.96	124.94
29	E4	201	PEB	CAC-CBC-CGC	-2.49	106.77	113.76
29	HG	203	PEB	CHA-C1B-NB	-2.49	119.72	124.93
31	rP	1001	CYC	C2C-C1C-NC	2.49	110.42	108.27
29	L4	202	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	eF	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	eI	201	PEB	OD-C4D-C3D	-2.49	123.81	129.46
29	B3	202	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	b7	201	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	b9	201	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	JB	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	JM	203	PEB	CHC-C1D-ND	-2.49	111.05	113.95
29	BO	202	PEB	CHC-C1D-ND	-2.49	111.05	113.95
30	wJ	304	PUB	C2C-C1C-NC	2.49	113.67	110.05
29	J4	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	P2	202	PEB	CAC-CBC-CGC	-2.49	106.78	113.76
29	JD	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	AG	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	AQ	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	JJ	203	PEB	C2A-C1A-NA	2.49	110.42	108.27
29	JL	203	PEB	C2A-C1A-NA	2.49	110.42	108.27
29	NR	203	PEB	CAC-CBC-CGC	-2.49	106.78	113.76
29	B4	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	f7	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
29	f9	202	PEB	CHA-C1B-NB	-2.49	119.72	124.93
30	yL	303	PUB	CBA-CAA-C3A	-2.49	109.20	112.98
29	L7	1002	PEB	CAA-C3A-C2A	-2.49	108.04	114.26
29	FD	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HG	201	PEB	OD-C4D-ND	-2.49	122.24	125.93
29	HQ	201	PEB	OD-C4D-ND	-2.49	122.24	125.93
29	S7	201	PEB	OA-C1A-NA	2.49	127.96	124.94
29	S9	201	PEB	OA-C1A-NA	2.49	127.96	124.94
29	N7	1002	PEB	CAA-C3A-C2A	-2.49	108.04	114.26
29	N9	1002	PEB	CAA-C3A-C2A	-2.49	108.04	114.26
29	fJ	203	PEB	C2A-C1A-NA	2.49	110.42	108.27
29	fL	203	PEB	C2A-C1A-NA	2.49	110.42	108.27
29	H4	202	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	CG	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
29	CQ	201	PEB	OD-C4D-C3D	-2.49	123.82	129.46
30	xJ	304	PUB	CBA-CAA-C3A	-2.49	109.20	112.98
29	HB	203	PEB	CHC-C1D-ND	-2.49	111.06	113.95
29	HM	203	PEB	CHC-C1D-ND	-2.49	111.06	113.95
29	UR	202	PEB	OD-C4D-ND	-2.49	122.25	125.93
29	S2	202	PEB	CBC-CAC-C2C	-2.49	108.38	112.62
29	FG	203	PEB	CHA-C1B-NB	-2.49	119.73	124.93
29	cB	203	PEB	CHC-C1D-ND	-2.49	111.06	113.95
29	cM	203	PEB	CHC-C1D-ND	-2.49	111.06	113.95
29	O2	202	PEB	CBC-CAC-C2C	-2.49	108.38	112.62
29	U2	202	PEB	CBC-CAC-C2C	-2.49	108.38	112.62
29	dD	401	PEB	CAC-CBC-CGC	-2.49	106.79	113.76
31	H1	1001	CYC	CHA-C1A-NA	-2.49	125.38	128.83
29	BD	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
29	C4	203	PEB	CMD-C2D-C3D	2.49	133.57	130.06
29	KD	201	PEB	C2B-C1B-NB	2.49	115.84	110.53
31	GF	1001	CYC	CBD-CAD-C3D	-2.49	108.38	112.62
31	GI	1001	CYC	CBD-CAD-C3D	-2.49	108.38	112.62
30	QB	201	PUB	OA-C1A-NA	-2.49	122.25	125.93
30	QM	201	PUB	OA-C1A-NA	-2.49	122.25	125.93
29	H5	203	PEB	C2A-C1A-NA	2.49	110.42	108.27
29	PR	202	PEB	CAC-CBC-CGC	-2.49	106.79	113.76
29	Q7	201	PEB	OA-C1A-NA	2.49	127.95	124.94
29	Q9	201	PEB	OA-C1A-NA	2.49	127.95	124.94
29	DB	203	PEB	CHC-C1D-ND	-2.49	111.06	113.95
29	DM	203	PEB	CHC-C1D-ND	-2.49	111.06	113.95
29	A5	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
29	A8	202	PEB	OD-C4D-C3D	-2.49	123.83	129.46
29	YF	201	PEB	OD-C4D-C3D	-2.49	123.83	129.46
29	YI	201	PEB	OD-C4D-C3D	-2.49	123.83	129.46
29	L9	1002	PEB	CAA-C3A-C2A	-2.48	108.05	114.26
31	J1	1001	CYC	C1A-C2A-C3A	-2.48	104.03	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	JK	1001	CYC	C1A-C2A-C3A	-2.48	104.03	106.78
29	cF	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
29	cI	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
31	IF	1001	CYC	CBD-CAD-C3D	-2.48	108.38	112.62
31	II	1001	CYC	CBD-CAD-C3D	-2.48	108.38	112.62
31	RP	1001	CYC	C1B-CHB-C4A	2.48	134.15	128.08
29	aF	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
29	aI	201	PEB	OD-C4D-C3D	-2.48	123.83	129.46
29	O7	201	PEB	OA-C1A-NA	2.48	127.95	124.94
29	U7	201	PEB	OA-C1A-NA	2.48	127.95	124.94
29	O9	201	PEB	OA-C1A-NA	2.48	127.95	124.94
29	U9	201	PEB	OA-C1A-NA	2.48	127.95	124.94
29	HD	202	PEB	OD-C4D-C3D	-2.48	123.83	129.46
29	RR	203	PEB	CAC-CBC-CGC	-2.48	106.80	113.76
29	XJ	203	PEB	C2A-C1A-NA	2.48	110.41	108.27
29	XL	203	PEB	C2A-C1A-NA	2.48	110.41	108.27
31	mP	1001	CYC	C2C-C1C-NC	2.48	110.41	108.27
29	D7	1002	PEB	CAA-C3A-C2A	-2.48	108.06	114.26
29	D9	1002	PEB	CAA-C3A-C2A	-2.48	108.06	114.26
29	L7	1002	PEB	OD-C4D-ND	-2.48	122.25	125.93
29	HQ	203	PEB	CHA-C1B-NB	-2.48	119.74	124.93
31	JP	1001	CYC	C1B-CHB-C4A	2.48	134.15	128.08
29	iF	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
29	kF	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
29	iI	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
29	kI	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
29	J7	1002	PEB	CAA-C3A-C2A	-2.48	108.06	114.26
29	Z1	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06
29	AC	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06
29	AE	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06
29	ZK	203	PEB	CMB-C2B-C1B	2.48	128.89	125.06
31	NK	1001	CYC	CHA-C1A-NA	-2.48	125.38	128.83
29	iF	203	PEB	CHA-C1B-NB	-2.48	119.74	124.93
29	iI	203	PEB	CHA-C1B-NB	-2.48	119.74	124.93
31	YP	1000	CYC	C2B-C1B-NB	2.48	110.62	106.99
29	V2	203	PEB	CAC-CBC-CGC	-2.48	106.80	113.76
29	gF	203	PEB	CHA-C1B-NB	-2.48	119.74	124.93
29	gI	203	PEB	CHA-C1B-NB	-2.48	119.74	124.93
31	HK	1001	CYC	C1A-C2A-C3A	-2.48	104.04	106.78
31	AP	1001	CYC	C1B-CHB-C4A	2.48	134.14	128.08
31	pP	1001	CYC	C1B-CHB-C4A	2.48	134.14	128.08
31	gP	1001	CYC	C1B-CHB-C4A	2.48	134.14	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NJ	203	PEB	C2A-C1A-NA	2.48	110.41	108.27
29	NL	203	PEB	C2A-C1A-NA	2.48	110.41	108.27
31	CF	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
31	CI	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
31	KI	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
29	E4	203	PEB	CMD-C2D-C3D	2.48	133.56	130.06
29	f7	201	PEB	OA-C1A-NA	2.48	127.94	124.94
29	f9	201	PEB	OA-C1A-NA	2.48	127.94	124.94
31	F1	1001	CYC	CHA-C1A-NA	-2.48	125.39	128.83
31	FK	1001	CYC	CHA-C1A-NA	-2.48	125.39	128.83
29	iB	203	PEB	CHC-C1D-ND	-2.48	111.07	113.95
29	iM	203	PEB	CHC-C1D-ND	-2.48	111.07	113.95
31	EF	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
31	EI	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
29	mF	203	PEB	CHA-C1B-NB	-2.48	119.75	124.93
29	BG	203	PEB	CHA-C1B-NB	-2.48	119.75	124.93
29	mI	203	PEB	CHA-C1B-NB	-2.48	119.75	124.93
29	FQ	203	PEB	CHA-C1B-NB	-2.48	119.75	124.93
29	KG	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
29	KQ	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
29	TI	201	PEB	OD-C4D-C3D	-2.48	123.84	129.46
31	KF	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
29	N2	203	PEB	CAC-CBC-CGC	-2.48	106.81	113.76
31	JP	1001	CYC	C2C-C1C-NC	2.48	110.41	108.27
29	W2	202	PEB	CHA-C4A-NA	-2.48	122.26	125.20
29	H3	202	PEB	CHC-C1D-ND	-2.48	111.07	113.95
29	LB	203	PEB	CHC-C1D-ND	-2.48	111.07	113.95
29	LM	203	PEB	CHC-C1D-ND	-2.48	111.07	113.95
29	HO	202	PEB	CHC-C1D-ND	-2.48	111.07	113.95
29	A1	302	PEB	OD-C4D-C3D	-2.48	123.85	129.46
29	AK	302	PEB	OD-C4D-C3D	-2.48	123.85	129.46
31	N1	1001	CYC	CHA-C1A-NA	-2.48	125.39	128.83
29	B5	203	PEB	CHA-C1B-NB	-2.48	119.75	124.93
31	MF	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
31	MI	1001	CYC	CBD-CAD-C3D	-2.48	108.39	112.62
29	Q7	202	PEB	CHA-C1B-NB	-2.48	119.75	124.93
29	Q9	202	PEB	CHA-C1B-NB	-2.48	119.75	124.93
29	P2	201	PEB	OD-C4D-ND	-2.48	122.26	125.93
29	F7	1002	PEB	CAA-C3A-C2A	-2.48	108.07	114.26
29	P2	201	PEB	C2B-C1B-NB	2.48	115.81	110.53
31	D1	1001	CYC	C1A-C2A-C3A	-2.48	104.04	106.78
29	F9	1002	PEB	CAA-C3A-C2A	-2.48	108.07	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A7	301	PEB	OD-C4D-C3D	-2.48	123.85	129.46
29	A9	301	PEB	OD-C4D-C3D	-2.48	123.85	129.46
29	NR	202	PEB	OD-C4D-ND	-2.48	122.26	125.93
29	O1	202	PEB	CMB-C2B-C1B	2.48	128.88	125.06
29	OK	202	PEB	CMB-C2B-C1B	2.48	128.88	125.06
29	aF	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
29	aI	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
31	HK	1001	CYC	CHA-C1A-NA	-2.47	125.39	128.83
29	VF	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
29	VI	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
29	R2	203	PEB	CAC-CBC-CGC	-2.47	106.82	113.76
29	cF	202	PEB	CHA-C1B-NB	-2.47	119.76	124.93
29	cI	202	PEB	CHA-C1B-NB	-2.47	119.76	124.93
29	PR	201	PEB	OD-C4D-ND	-2.47	122.27	125.93
31	cP	1001	CYC	C1B-CHB-C4A	2.47	134.12	128.08
31	1P	1002	CYC	O2A-CGA-CBA	2.47	121.97	114.03
31	CP	1001	CYC	C1B-CHB-C4A	2.47	134.12	128.08
31	J1	1001	CYC	CHA-C1A-NA	-2.47	125.40	128.83
31	L1	1001	CYC	CHA-C1A-NA	-2.47	125.40	128.83
31	JK	1001	CYC	CHA-C1A-NA	-2.47	125.40	128.83
31	LK	1001	CYC	CHA-C1A-NA	-2.47	125.40	128.83
29	DQ	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
31	NP	1001	CYC	C2C-C1C-NC	2.47	110.40	108.27
29	J3	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	JO	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	IB	202	PEB	CMB-C2B-C1B	2.47	128.87	125.06
29	IM	202	PEB	CMB-C2B-C1B	2.47	128.87	125.06
30	A7	302	PUB	C1D-CHC-C4C	-2.47	107.99	113.37
30	A9	302	PUB	C1D-CHC-C4C	-2.47	107.99	113.37
29	L3	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	LO	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	XR	203	PEB	CAC-CBC-CGC	-2.47	106.83	113.76
29	LG	203	PEB	CHA-C1B-NB	-2.47	119.76	124.93
29	C5	202	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	BQ	203	PEB	CHA-C1B-NB	-2.47	119.77	124.93
29	B3	203	PEB	CAC-CBC-CGC	-2.47	106.83	113.76
29	BO	203	PEB	CAC-CBC-CGC	-2.47	106.83	113.76
29	B3	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	BO	201	PEB	OD-C4D-C3D	-2.47	123.86	129.46
29	PJ	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
29	PL	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
30	yL	303	PUB	CMD-C2D-C3D	2.47	131.47	127.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	NP	1001	CYC	C1B-CHB-C4A	2.47	134.11	128.08
29	MQ	407	PEB	CBC-CAC-C2C	-2.47	108.41	112.62
29	W2	202	PEB	CBC-CAC-C2C	-2.47	108.41	112.62
29	VR	203	PEB	CAC-CBC-CGC	-2.47	106.84	113.76
29	I5	202	PEB	OD-C4D-C3D	-2.47	123.87	129.46
29	I8	202	PEB	OD-C4D-C3D	-2.47	123.87	129.46
29	nJ	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
29	nL	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
31	NK	1001	CYC	C1A-C2A-C3A	-2.47	104.05	106.78
29	XR	202	PEB	CMD-C2D-C3D	2.47	133.54	130.06
29	M2	202	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	T2	203	PEB	CAC-CBC-CGC	-2.47	106.84	113.76
31	lP	1001	CYC	C1B-CHB-C4A	2.47	134.11	128.08
31	rP	1001	CYC	C1B-CHB-C4A	2.47	134.11	128.08
29	L8	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
29	jJ	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
29	jL	203	PEB	C2A-C1A-NA	2.47	110.40	108.27
29	l7	201	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	l9	201	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	G4	203	PEB	CMD-C2D-C3D	2.47	133.54	130.06
31	KP	1001	CYC	C1B-CHB-C4A	2.47	134.11	128.08
29	U2	202	PEB	OD-C4D-ND	-2.47	122.28	125.93
29	xL	302	PEB	OD-C4D-ND	-2.47	122.28	125.93
29	TR	202	PEB	CMD-C2D-C3D	2.47	133.54	130.06
29	YF	203	PEB	CHA-C1B-NB	-2.47	119.78	124.93
29	DG	203	PEB	CHA-C1B-NB	-2.47	119.78	124.93
29	YI	203	PEB	CHA-C1B-NB	-2.47	119.78	124.93
29	H7	1002	PEB	CAA-C3A-C2A	-2.47	108.10	114.26
29	H9	1002	PEB	CAA-C3A-C2A	-2.47	108.10	114.26
29	Z7	201	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	Z9	201	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	kB	203	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	kM	203	PEB	CHC-C1D-ND	-2.47	111.08	113.95
29	KD	203	PEB	CMD-C2D-C3D	2.47	133.54	130.06
29	N2	202	PEB	OD-C4D-ND	-2.47	122.28	125.93
29	d1	202	PEB	CMB-C2B-C1B	2.46	128.86	125.06
29	A7	301	PEB	CMB-C2B-C1B	2.46	128.86	125.06
29	A9	301	PEB	CMB-C2B-C1B	2.46	128.86	125.06
29	dK	202	PEB	CMB-C2B-C1B	2.46	128.86	125.06
29	eF	203	PEB	CHA-C1B-NB	-2.46	119.78	124.93
29	eI	203	PEB	CHA-C1B-NB	-2.46	119.78	124.93
29	j7	201	PEB	OA-C1A-NA	2.46	127.93	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j9	201	PEB	OA-C1A-NA	2.46	127.93	124.94
29	bF	201	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
29	bI	201	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
29	J5	201	PEB	CHB-C4B-C3B	-2.46	119.63	125.32
29	J8	201	PEB	CHB-C4B-C3B	-2.46	119.63	125.32
29	J9	1002	PEB	CAA-C3A-C2A	-2.46	108.10	114.26
29	F3	203	PEB	CAC-CBC-CGC	-2.46	106.85	113.76
29	FO	203	PEB	CAC-CBC-CGC	-2.46	106.85	113.76
29	CD	203	PEB	CMD-C2D-C3D	2.46	133.54	130.06
29	TF	202	PEB	CHA-C1B-NB	-2.46	119.78	124.93
29	TI	202	PEB	CHA-C1B-NB	-2.46	119.78	124.93
29	RF	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
29	RI	201	PEB	OD-C4D-C3D	-2.46	123.88	129.46
29	VJ	202	PEB	C2A-C1A-NA	2.46	110.40	108.27
29	hJ	203	PEB	C2A-C1A-NA	2.46	110.40	108.27
29	VL	202	PEB	C2A-C1A-NA	2.46	110.40	108.27
29	hL	203	PEB	C2A-C1A-NA	2.46	110.40	108.27
29	QR	202	PEB	CHA-C4A-NA	-2.46	122.28	125.20
29	F4	201	PEB	C2B-C1B-NB	2.46	115.78	110.53
31	GP	1001	CYC	CHB-C1B-C2B	-2.46	122.07	126.95
31	TP	1001	CYC	C1B-CHB-C4A	2.46	134.10	128.08
29	C8	202	PEB	OD-C4D-C3D	-2.46	123.88	129.46
31	vP	1001	CYC	C1B-CHB-C4A	2.46	134.09	128.08
29	b7	201	PEB	OA-C1A-NA	2.46	127.92	124.94
29	b9	201	PEB	OA-C1A-NA	2.46	127.92	124.94
31	EP	1001	CYC	C1B-CHB-C4A	2.46	134.09	128.08
31	PP	1001	CYC	C1B-CHB-C4A	2.46	134.09	128.08
31	L1	1001	CYC	C1A-C2A-C3A	-2.46	104.06	106.78
31	LK	1001	CYC	C1A-C2A-C3A	-2.46	104.06	106.78
31	tP	1001	CYC	C1B-CHB-C4A	2.46	134.09	128.08
29	VR	202	PEB	C2B-C1B-NB	2.46	115.78	110.53
29	M2	202	PEB	OD-C4D-ND	-2.46	122.28	125.93
31	xP	1001	CYC	CBD-CAD-C3D	2.46	116.82	112.62
29	h1	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
29	hK	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
29	MD	203	PEB	CMD-C2D-C3D	2.46	133.53	130.06
29	V2	202	PEB	C2B-C1B-NB	2.46	115.78	110.53
29	PR	201	PEB	C2B-C1B-NB	2.46	115.78	110.53
29	OR	202	PEB	CMB-C2B-C1B	2.46	128.85	125.06
29	PF	203	PEB	CHA-C1B-NB	-2.46	119.79	124.93
29	JG	203	PEB	CHA-C1B-NB	-2.46	119.79	124.93
29	PI	203	PEB	CHA-C1B-NB	-2.46	119.79	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	GD	203	PEB	CHC-C4C-C3C	-2.46	126.14	130.34
31	M7	1001	CYC	OB-C4B-NB	-2.46	119.36	125.08
29	BA	201	PEB	CAA-C3A-C4A	-2.46	106.36	112.67
29	BN	201	PEB	CAA-C3A-C4A	-2.46	106.36	112.67
29	J3	202	PEB	CHC-C1D-ND	-2.46	111.09	113.95
29	JO	202	PEB	CHC-C1D-ND	-2.46	111.09	113.95
29	xJ	302	PEB	OD-C4D-ND	-2.46	122.29	125.93
29	WF	201	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
29	WI	201	PEB	C4B-C3B-C2B	-2.46	104.06	106.78
29	D3	203	PEB	CAC-CBC-CGC	-2.46	106.87	113.76
29	DO	203	PEB	CAC-CBC-CGC	-2.46	106.87	113.76
29	JQ	203	PEB	CHA-C1B-NB	-2.46	119.79	124.93
29	e1	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
29	K5	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46
29	K8	202	PEB	OD-C4D-C3D	-2.46	123.89	129.46
29	eK	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
29	UR	202	PEB	CBC-CAC-C2C	-2.46	108.43	112.62
29	Q2	202	PEB	CHC-C1D-ND	-2.46	111.09	113.95
29	IJ	201	PEB	CHA-C1B-NB	-2.46	119.79	124.93
29	IL	201	PEB	CHA-C1B-NB	-2.46	119.79	124.93
29	H3	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
29	HO	201	PEB	OD-C4D-C3D	-2.46	123.89	129.46
29	RR	202	PEB	CMD-C2D-C3D	2.46	133.53	130.06
29	MG	405	PEB	CBC-CAC-C2C	-2.46	108.43	112.62
29	L3	202	PEB	CAC-CBC-CGC	-2.46	106.88	113.76
29	LO	202	PEB	CAC-CBC-CGC	-2.46	106.88	113.76
29	H4	201	PEB	C2B-C1B-NB	2.46	115.77	110.53
31	F1	1001	CYC	C1A-C2A-C3A	-2.45	104.07	106.78
31	FK	1001	CYC	C1A-C2A-C3A	-2.45	104.07	106.78
29	RF	202	PEB	CHA-C1B-NB	-2.45	119.80	124.93
29	RI	202	PEB	CHA-C1B-NB	-2.45	119.80	124.93
29	TR	203	PEB	CAC-CBC-CGC	-2.45	106.88	113.76
29	kF	203	PEB	CHA-C1B-NB	-2.45	119.80	124.93
29	kI	203	PEB	CHA-C1B-NB	-2.45	119.80	124.93
29	UF	202	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
29	UI	202	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
29	D3	203	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
29	DO	203	PEB	C1B-C2B-C3B	-2.45	103.69	106.51
31	mP	1001	CYC	C1B-CHB-C4A	2.45	134.07	128.08
29	G4	203	PEB	CHC-C4C-C3C	-2.45	126.15	130.34
31	E7	1001	CYC	OB-C4B-NB	-2.45	119.38	125.08
31	G7	1001	CYC	OB-C4B-NB	-2.45	119.38	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	E9	1001	CYC	OB-C4B-NB	-2.45	119.38	125.08
29	a1	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46
29	aK	201	PEB	OD-C4D-C3D	-2.45	123.90	129.46
29	N2	202	PEB	C2B-C1B-NB	2.45	115.76	110.53
29	NR	202	PEB	C2B-C1B-NB	2.45	115.76	110.53
31	H1	1001	CYC	C1A-C2A-C3A	-2.45	104.07	106.78
29	R2	202	PEB	CMD-C2D-C3D	2.45	133.52	130.06
29	X2	202	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
29	H3	203	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
29	HO	203	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
30	QB	201	PUB	O2B-CGB-CBB	2.45	121.91	114.03
30	QM	201	PUB	O2B-CGB-CBB	2.45	121.91	114.03
31	KP	1001	CYC	CHB-C1B-C2B	-2.45	122.09	126.95
29	ED	202	PEB	CHC-C4C-C3C	-2.45	126.16	130.34
29	O7	201	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	O9	201	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	R1	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
29	RK	201	PEB	OD-C4D-C3D	-2.45	123.91	129.46
29	G8	203	PEB	CHA-C1B-NB	-2.45	119.81	124.93
29	wL	302	PEB	OD-C4D-ND	-2.45	122.30	125.93
30	MG	402	PUB	CMA-C2A-C3A	2.45	134.71	129.67
29	hF	201	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
29	hI	201	PEB	C4B-C3B-C2B	-2.45	104.07	106.78
31	eP	1001	CYC	C1B-CHB-C4A	2.45	134.07	128.08
29	ED	202	PEB	CMD-C2D-C3D	2.45	133.52	130.06
31	YP	1000	CYC	O2A-CGA-CBA	2.45	121.90	114.03
29	J3	203	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
29	JO	203	PEB	CAC-CBC-CGC	-2.45	106.89	113.76
29	TR	202	PEB	OD-C4D-ND	-2.45	122.30	125.93
29	AA	202	PEB	CAA-C3A-C2A	-2.45	108.14	114.26
29	AN	202	PEB	CAA-C3A-C2A	-2.45	108.14	114.26
29	f1	202	PEB	CMB-C2B-C1B	2.45	128.84	125.06
29	fK	202	PEB	CMB-C2B-C1B	2.45	128.84	125.06
30	wL	304	PUB	C2C-C1C-NC	2.45	113.61	110.05
31	eP	1001	CYC	CHB-C1B-C2B	-2.45	122.09	126.95
29	I3	203	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	IO	203	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	LJ	201	PEB	CHA-C1B-NB	-2.45	119.81	124.93
29	LL	201	PEB	CHA-C1B-NB	-2.45	119.81	124.93
29	A7	305	PEB	C2A-C1A-NA	2.45	110.38	108.27
29	A9	305	PEB	C2A-C1A-NA	2.45	110.38	108.27
31	K7	1001	CYC	OB-C4B-NB	-2.45	119.39	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	eB	202	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	eM	202	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	LQ	202	PEB	CHC-C1D-ND	-2.45	111.10	113.95
29	L3	202	PEB	C1B-C2B-C3B	-2.45	103.70	106.51
29	LO	202	PEB	C1B-C2B-C3B	-2.45	103.70	106.51
29	T2	202	PEB	CMD-C2D-C3D	2.45	133.52	130.06
29	JD	201	PEB	C2B-C1B-NB	2.45	115.75	110.53
30	yJ	303	PUB	CMD-C2D-C3D	2.45	131.44	127.77
29	Q7	201	PEB	CHC-C1D-ND	-2.45	111.11	113.95
29	Q9	201	PEB	CHC-C1D-ND	-2.45	111.11	113.95
29	EB	202	PEB	CMB-C2B-C1B	2.45	128.83	125.06
29	EM	202	PEB	CMB-C2B-C1B	2.45	128.83	125.06
29	V2	202	PEB	OD-C4D-ND	-2.45	122.31	125.93
31	VP	1001	CYC	CBD-CAD-C3D	2.45	116.80	112.62
31	G9	1001	CYC	OB-C4B-NB	-2.45	119.39	125.08
29	B8	203	PEB	CHA-C1B-NB	-2.45	119.81	124.93
29	ID	203	PEB	CHC-C4C-C3C	-2.45	126.16	130.34
31	EP	1001	CYC	CHB-C1B-C2B	-2.45	122.10	126.95
29	NJ	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	XJ	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	ZJ	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	pJ	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	NL	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	XL	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	ZL	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	pL	201	PEB	CHA-C1B-NB	-2.45	119.82	124.93
29	D3	201	PEB	OD-C4D-C3D	-2.45	123.92	129.46
29	DO	201	PEB	OD-C4D-C3D	-2.45	123.92	129.46
31	N1	1001	CYC	C1A-C2A-C3A	-2.45	104.08	106.78
29	BB	301	PEB	C1B-C2B-C3B	-2.45	103.70	106.51
29	BM	301	PEB	C1B-C2B-C3B	-2.45	103.70	106.51
29	FD	201	PEB	C2B-C1B-NB	2.45	115.75	110.53
29	XR	201	PEB	C1C-CHB-C4B	-2.45	125.89	128.81
29	B4	201	PEB	C2B-C1B-NB	2.44	115.75	110.53
29	XR	202	PEB	C2B-C1B-NB	2.44	115.75	110.53
29	OR	202	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	TJ	201	PEB	CHA-C1B-NB	-2.44	119.82	124.93
29	TL	201	PEB	CHA-C1B-NB	-2.44	119.82	124.93
29	RR	202	PEB	C2B-C1B-NB	2.44	115.75	110.53
31	PP	1001	CYC	CHB-C1B-C2B	-2.44	122.11	126.95
29	hB	202	PEB	CMB-C2B-C1B	2.44	128.83	125.06
29	hM	202	PEB	CMB-C2B-C1B	2.44	128.83	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	VR	202	PEB	CMD-C2D-C3D	2.44	133.51	130.06
31	M9	1001	CYC	OB-C4B-NB	-2.44	119.40	125.08
29	SR	202	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	QF	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
29	QI	201	PEB	C4B-C3B-C2B	-2.44	104.08	106.78
29	SB	202	PEB	CMB-C2B-C1B	2.44	128.83	125.06
29	SM	202	PEB	CMB-C2B-C1B	2.44	128.83	125.06
29	X2	201	PEB	CMD-C2D-C3D	2.44	133.51	130.06
29	HG	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	HQ	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	GA	202	PEB	CAA-C3A-C2A	-2.44	108.16	114.26
29	IA	202	PEB	CAA-C3A-C2A	-2.44	108.16	114.26
29	GN	202	PEB	CAA-C3A-C2A	-2.44	108.16	114.26
29	IN	202	PEB	CAA-C3A-C2A	-2.44	108.16	114.26
29	WB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	WM	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	P2	201	PEB	CMD-C2D-C3D	2.44	133.51	130.06
30	AF	303	PUB	C2C-C1C-NC	2.44	113.60	110.05
30	AI	303	PUB	C2C-C1C-NC	2.44	113.60	110.05
29	zL	501	PEB	CHA-C1B-NB	-2.44	119.83	124.93
29	JJ	201	PEB	CHA-C1B-NB	-2.44	119.83	124.93
29	JL	201	PEB	CHA-C1B-NB	-2.44	119.83	124.93
29	GB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	GM	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
31	tP	1001	CYC	CHB-C1B-C2B	-2.44	122.11	126.95
29	K4	203	PEB	CHC-C4C-C3C	-2.44	126.17	130.34
29	J4	201	PEB	C2B-C1B-NB	2.44	115.74	110.53
29	W7	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	W9	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	LG	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	MQ	402	PEB	CHC-C1D-ND	-2.44	111.11	113.95
31	C7	1001	CYC	OB-C4B-NB	-2.44	119.41	125.08
31	C9	1001	CYC	OB-C4B-NB	-2.44	119.41	125.08
31	GP	1001	CYC	C1B-CHB-C4A	2.44	134.04	128.08
29	fB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	fM	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	E4	203	PEB	CHC-C4C-C3C	-2.44	126.17	130.34
29	W2	202	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	MB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	jB	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	MM	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06
29	jM	202	PEB	CMB-C2B-C1B	2.44	128.82	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TR	203	PEB	CBC-CAC-C2C	-2.44	108.46	112.62
29	S2	202	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	f7	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	f9	201	PEB	CHC-C1D-ND	-2.44	111.11	113.95
29	S2	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
29	wJ	302	PEB	OD-C4D-ND	-2.44	122.32	125.93
31	RP	1001	CYC	CHB-C1B-C2B	-2.44	122.12	126.95
31	mP	1001	CYC	CHB-C1B-C2B	-2.44	122.12	126.95
31	rP	1001	CYC	CHB-C1B-C2B	-2.44	122.12	126.95
29	VJ	201	PEB	CHA-C1B-NB	-2.44	119.83	124.93
29	VL	201	PEB	CHA-C1B-NB	-2.44	119.83	124.93
31	vP	1001	CYC	CHB-C1B-C2B	-2.44	122.12	126.95
29	WR	202	PEB	CHC-C1D-ND	-2.44	111.12	113.95
29	FA	201	PEB	CAA-C3A-C4A	-2.44	106.42	112.67
29	FN	201	PEB	CAA-C3A-C4A	-2.44	106.42	112.67
31	xP	1001	CYC	C4A-C3A-C2A	-2.44	103.71	106.51
31	K9	1001	CYC	OB-C4B-NB	-2.44	119.42	125.08
29	R2	202	PEB	OD-C4D-ND	-2.44	122.32	125.93
29	HD	201	PEB	C2B-C1B-NB	2.44	115.73	110.53
29	DJ	201	PEB	CHA-C1B-NB	-2.44	119.84	124.93
29	DL	201	PEB	CHA-C1B-NB	-2.44	119.84	124.93
29	ID	203	PEB	CMD-C2D-C3D	2.44	133.50	130.06
29	PJ	201	PEB	CHA-C1B-NB	-2.44	119.84	124.93
29	PL	201	PEB	CHA-C1B-NB	-2.44	119.84	124.93
29	NO	201	PEB	C2A-C1A-NA	2.43	110.37	108.27
29	FD	201	PEB	CBC-CAC-C2C	-2.43	108.47	112.62
29	M3	201	PEB	OD-C4D-C3D	-2.43	123.94	129.46
29	MO	201	PEB	OD-C4D-C3D	-2.43	123.94	129.46
29	dJ	201	PEB	CHA-C1B-NB	-2.43	119.84	124.93
29	rJ	201	PEB	CHA-C1B-NB	-2.43	119.84	124.93
29	dL	201	PEB	CHA-C1B-NB	-2.43	119.84	124.93
29	rL	201	PEB	CHA-C1B-NB	-2.43	119.84	124.93
29	JA	201	PEB	CAA-C3A-C4A	-2.43	106.42	112.67
29	JN	201	PEB	CAA-C3A-C4A	-2.43	106.42	112.67
29	CA	202	PEB	CAA-C3A-C2A	-2.43	108.18	114.26
29	CN	202	PEB	CAA-C3A-C2A	-2.43	108.18	114.26
29	BG	201	PEB	CHC-C1D-ND	-2.43	111.12	113.95
29	FG	201	PEB	CHC-C1D-ND	-2.43	111.12	113.95
29	BQ	201	PEB	CHC-C1D-ND	-2.43	111.12	113.95
29	FQ	201	PEB	CHC-C1D-ND	-2.43	111.12	113.95
31	CP	1001	CYC	CHB-C1B-C2B	-2.43	122.13	126.95
29	T2	202	PEB	OD-C4D-ND	-2.43	122.33	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G5	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
30	AB	305	PUB	CHC-C1D-ND	-2.43	110.65	113.72
29	QB	204	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	QM	204	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	JC	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
29	JE	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
29	O2	202	PEB	CHC-C1D-ND	-2.43	111.12	113.95
29	HA	201	PEB	CAA-C3A-C4A	-2.43	106.43	112.67
29	HN	201	PEB	CAA-C3A-C4A	-2.43	106.43	112.67
29	P7	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	V7	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	P9	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	V9	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	aB	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	aM	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	I4	203	PEB	OD-C4D-ND	-2.43	122.33	125.93
31	DK	1001	CYC	C1A-C2A-C3A	-2.43	104.09	106.78
29	OB	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	OM	202	PEB	CMB-C2B-C1B	2.43	128.81	125.06
29	e2	402	PEB	CBC-CAC-C2C	-2.43	108.47	112.62
29	XR	201	PEB	CBC-CAC-C2C	-2.43	108.47	112.62
29	DC	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
29	DE	202	PEB	OD-C4D-C3D	-2.43	123.95	129.46
29	VR	202	PEB	OD-C4D-ND	-2.43	122.33	125.93
31	VP	1001	CYC	C4A-C3A-C2A	-2.43	103.72	106.51
29	FJ	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	tJ	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	FL	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	tL	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	X2	201	PEB	C2B-C1B-NB	2.43	115.72	110.53
31	NP	1001	CYC	CHB-C1B-C2B	-2.43	122.13	126.95
29	hJ	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	hL	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	X2	201	PEB	OD-C4D-ND	-2.43	122.33	125.93
29	BC	203	PEB	OD-C4D-C3D	-2.43	123.95	129.46
29	BE	203	PEB	OD-C4D-C3D	-2.43	123.95	129.46
31	lP	1001	CYC	CHB-C1B-C2B	-2.43	122.13	126.95
31	I7	1001	CYC	OB-C4B-NB	-2.43	119.43	125.08
31	I9	1001	CYC	OB-C4B-NB	-2.43	119.43	125.08
29	EA	202	PEB	CAA-C3A-C2A	-2.43	108.19	114.26
29	EN	202	PEB	CAA-C3A-C2A	-2.43	108.19	114.26
31	AP	1001	CYC	CHB-C1B-C2B	-2.43	122.13	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	iP	1001	CYC	CHB-C1B-C2B	-2.43	122.13	126.95
29	L8	203	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	L4	201	PEB	CMA-C2A-C1A	-2.43	107.17	112.40
29	LA	201	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
29	LN	201	PEB	CAA-C3A-C4A	-2.43	106.44	112.67
29	C4	203	PEB	CHC-C4C-C3C	-2.43	126.19	130.34
30	AF	302	PUB	C2C-C1C-NC	2.43	113.58	110.05
30	AI	302	PUB	C2C-C1C-NC	2.43	113.58	110.05
29	L5	203	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	nJ	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	nL	201	PEB	CHA-C1B-NB	-2.43	119.85	124.93
29	d7	201	PEB	CHC-C1D-ND	-2.43	111.13	113.95
29	d9	201	PEB	CHC-C1D-ND	-2.43	111.13	113.95
30	AM	305	PUB	CHC-C1D-ND	-2.43	110.65	113.72
30	A7	303	PUB	CBA-CAA-C3A	-2.43	109.30	112.98
30	A9	303	PUB	CBA-CAA-C3A	-2.43	109.30	112.98
29	T2	202	PEB	C2B-C1B-NB	2.43	115.71	110.53
29	TR	202	PEB	C2B-C1B-NB	2.43	115.71	110.53
29	H8	203	PEB	C2A-C1A-NA	2.43	110.37	108.27
29	TR	201	PEB	CBC-CAC-C2C	-2.43	108.48	112.62
29	h7	201	PEB	CHC-C1D-ND	-2.43	111.13	113.95
29	j7	201	PEB	CHC-C1D-ND	-2.43	111.13	113.95
29	h9	201	PEB	CHC-C1D-ND	-2.43	111.13	113.95
29	j9	201	PEB	CHC-C1D-ND	-2.43	111.13	113.95
29	Y1	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
29	YK	201	PEB	OD-C4D-C3D	-2.43	123.96	129.46
29	PR	201	PEB	CMD-C2D-C3D	2.43	133.49	130.06
29	F5	203	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	F8	203	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	jJ	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	jL	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
31	TP	1001	CYC	CHB-C1B-C2B	-2.43	122.14	126.95
31	gP	1001	CYC	CHB-C1B-C2B	-2.43	122.14	126.95
29	CD	203	PEB	CHC-C4C-C3C	-2.43	126.20	130.34
29	V2	201	PEB	C1C-CHB-C4B	-2.43	125.91	128.81
29	VR	201	PEB	C1C-CHB-C4B	-2.43	125.91	128.81
29	L8	202	PEB	OD-C4D-C3D	-2.43	123.96	129.46
29	bJ	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	bL	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	B3	203	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
29	BO	203	PEB	C1B-C2B-C3B	-2.43	103.72	106.51
31	pP	1001	CYC	CHB-C1B-C2B	-2.43	122.14	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R2	202	PEB	C2B-C1B-NB	2.43	115.71	110.53
29	fF	201	PEB	C4B-C3B-C2B	-2.43	104.10	106.78
29	fI	201	PEB	C4B-C3B-C2B	-2.43	104.10	106.78
29	G8	202	PEB	OD-C4D-C3D	-2.43	123.96	129.46
31	HF	1001	CYC	CAC-C3C-C2C	-2.43	108.20	114.26
31	HI	1001	CYC	CAC-C3C-C2C	-2.43	108.20	114.26
29	fJ	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	fL	201	PEB	CHA-C1B-NB	-2.43	119.86	124.93
29	N2	202	PEB	CMD-C2D-C3D	2.43	133.48	130.06
29	c1	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
29	cK	201	PEB	OD-C4D-C3D	-2.42	123.97	129.46
29	N3	201	PEB	C2A-C1A-NA	2.42	110.36	108.27
31	yP	1001	CYC	C1B-CHB-C4A	2.42	134.00	128.08
29	vJ	201	PEB	CHA-C1B-NB	-2.42	119.86	124.93
29	vL	201	PEB	CHA-C1B-NB	-2.42	119.86	124.93
29	DA	201	PEB	CAA-C3A-C4A	-2.42	106.45	112.67
29	DN	201	PEB	CAA-C3A-C4A	-2.42	106.45	112.67
29	WR	202	PEB	OD-C4D-ND	-2.42	122.34	125.93
29	CB	202	PEB	CMB-C2B-C1B	2.42	128.80	125.06
29	CM	202	PEB	CMB-C2B-C1B	2.42	128.80	125.06
29	N2	201	PEB	CBC-CAC-C2C	-2.42	108.48	112.62
29	F4	201	PEB	CBC-CAC-C2C	-2.42	108.48	112.62
29	F3	203	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
29	FO	203	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
29	DB	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
29	DM	202	PEB	OD-C4D-C3D	-2.42	123.97	129.46
29	RR	201	PEB	C1C-CHB-C4B	-2.42	125.92	128.81
29	DD	201	PEB	CBC-CAC-C2C	-2.42	108.49	112.62
29	RJ	201	PEB	CHA-C1B-NB	-2.42	119.87	124.93
29	RL	201	PEB	CHA-C1B-NB	-2.42	119.87	124.93
29	HC	203	PEB	OD-C4D-C3D	-2.42	123.97	129.46
29	HE	203	PEB	OD-C4D-C3D	-2.42	123.97	129.46
29	G5	203	PEB	CHA-C1B-NB	-2.42	119.87	124.93
29	UR	201	PEB	CHA-C1B-C2B	2.42	131.13	124.90
29	KA	202	PEB	CAA-C3A-C2A	-2.42	108.21	114.26
29	KN	202	PEB	CAA-C3A-C2A	-2.42	108.21	114.26
31	FF	1001	CYC	CAC-C3C-C2C	-2.42	108.21	114.26
31	FI	1001	CYC	CAC-C3C-C2C	-2.42	108.21	114.26
29	H8	203	PEB	CHA-C1B-NB	-2.42	119.87	124.93
29	BJ	201	PEB	CHA-C1B-NB	-2.42	119.87	124.93
29	BL	201	PEB	CHA-C1B-NB	-2.42	119.87	124.93
29	dB	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	dM	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
31	WP	1001	CYC	C1B-CHB-C4A	2.42	134.00	128.08
29	m1	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	mK	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	BD	201	PEB	CBC-CAC-C2C	-2.42	108.49	112.62
29	NR	202	PEB	CMD-C2D-C3D	2.42	133.48	130.06
29	NR	203	PEB	CBC-CAC-C2C	-2.42	108.49	112.62
29	k1	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	kK	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	SR	202	PEB	OD-C4D-ND	-2.42	122.35	125.93
31	cP	1001	CYC	CHB-C1B-C2B	-2.42	122.16	126.95
29	V1	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	VB	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	FC	203	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	FE	203	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	VK	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	VM	202	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	U2	201	PEB	CHA-C1B-C2B	2.42	131.12	124.90
29	KD	203	PEB	CHC-C4C-C3C	-2.42	126.21	130.34
29	a7	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
29	a9	202	PEB	CMB-C2B-C1B	2.42	128.79	125.06
31	JP	1001	CYC	CHB-C1B-C2B	-2.42	122.16	126.95
29	P1	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	g1	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	PK	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	gK	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	R2	201	PEB	CBC-CAC-C2C	-2.42	108.49	112.62
29	MA	401	PEB	CBC-CAC-C2C	-2.42	108.49	112.62
29	SF	201	PEB	C4B-C3B-C2B	-2.42	104.11	106.78
29	SI	201	PEB	C4B-C3B-C2B	-2.42	104.11	106.78
29	MR	201	PEB	CHA-C1B-C2B	2.42	131.12	124.90
29	T1	202	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
29	TK	202	PEB	C1B-C2B-C3B	-2.42	103.73	106.51
29	LC	203	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	LE	203	PEB	OD-C4D-C3D	-2.42	123.98	129.46
29	T2	203	PEB	CBC-CAC-C2C	-2.42	108.50	112.62
29	S7	201	PEB	CHC-C1D-ND	-2.42	111.14	113.95
29	S9	201	PEB	CHC-C1D-ND	-2.42	111.14	113.95
29	Q2	201	PEB	CHA-C1B-C2B	2.42	131.11	124.90
29	g7	202	PEB	CMB-C2B-C1B	2.42	128.78	125.06
29	g9	202	PEB	CMB-C2B-C1B	2.42	128.78	125.06
29	MN	401	PEB	CBC-CAC-C2C	-2.42	108.50	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	LF	1001	CYC	CAC-C3C-C2C	-2.42	108.22	114.26
31	LI	1001	CYC	CAC-C3C-C2C	-2.42	108.22	114.26
29	WR	201	PEB	CHA-C1B-C2B	2.41	131.11	124.90
29	QR	201	PEB	CHA-C1B-C2B	2.41	131.11	124.90
29	B5	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
29	O2	202	PEB	OD-C4D-ND	-2.41	122.35	125.93
29	HB	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
29	HM	202	PEB	OD-C4D-C3D	-2.41	123.99	129.46
29	L5	203	PEB	C2A-C1A-NA	2.41	110.35	108.27
29	LD	201	PEB	C2B-C1B-NB	2.41	115.68	110.53
29	M2	201	PEB	CHA-C1B-C2B	2.41	131.11	124.90
29	D4	201	PEB	C2B-C1B-NB	2.41	115.68	110.53
31	uP	1001	CYC	C4D-CHA-C1A	2.41	131.69	128.81
29	RR	202	PEB	OD-C4D-ND	-2.41	122.36	125.93
29	V2	202	PEB	CMD-C2D-C3D	2.41	133.47	130.06
29	TR	201	PEB	C1C-CHB-C4B	-2.41	125.93	128.81
29	DD	201	PEB	C2B-C1B-NB	2.41	115.68	110.53
29	UB	202	PEB	CMB-C2B-C1B	2.41	128.78	125.06
29	MQ	401	PEB	CMB-C2B-C1B	2.41	128.78	125.06
30	A7	302	PUB	C2C-C1C-NC	2.41	113.56	110.05
30	A9	302	PUB	C2C-C1C-NC	2.41	113.56	110.05
29	P2	202	PEB	CBC-CAC-C2C	-2.41	108.50	112.62
29	PR	202	PEB	CBC-CAC-C2C	-2.41	108.50	112.62
29	RR	201	PEB	CBC-CAC-C2C	-2.41	108.50	112.62
29	B4	201	PEB	CMA-C2A-C1A	-2.41	107.20	112.40
29	OR	202	PEB	CAB-CBB-CGB	-2.41	108.41	113.60
30	MQ	404	PUB	CMA-C2A-C3A	2.41	134.62	129.67
29	MG	404	PEB	CMD-C2D-C3D	2.41	133.46	130.06
29	N3	201	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	kB	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	kM	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	RR	203	PEB	CBC-CAC-C2C	-2.41	108.51	112.62
29	MD	203	PEB	CHC-C4C-C3C	-2.41	126.22	130.34
29	aB	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	mB	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	aM	203	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	mM	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	T2	201	PEB	CBC-CAC-C2C	-2.41	108.51	112.62
29	HD	201	PEB	CBC-CAC-C2C	-2.41	108.51	112.62
29	L5	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	LB	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	LM	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DG	201	PEB	CHC-C1D-ND	-2.41	111.15	113.95
29	DQ	201	PEB	CHC-C1D-ND	-2.41	111.15	113.95
29	JD	201	PEB	CMA-C2A-C1A	-2.41	107.21	112.40
29	BD	201	PEB	C2A-C1A-NA	2.41	110.35	108.27
29	H5	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	D4	201	PEB	CMA-C2A-C1A	-2.41	107.21	112.40
31	DF	1001	CYC	CAC-C3C-C2C	-2.41	108.24	114.26
31	DI	1001	CYC	CAC-C3C-C2C	-2.41	108.24	114.26
29	m1	202	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
29	NF	1002	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
29	NI	1002	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
29	mK	202	PEB	C1B-C2B-C3B	-2.41	103.74	106.51
29	O2	201	PEB	CHA-C1B-C2B	2.41	131.09	124.90
29	XR	202	PEB	OD-C4D-ND	-2.41	122.36	125.93
29	e2	402	PEB	C1C-CHB-C4B	-2.41	125.93	128.81
29	ZB	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	ZM	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	H5	203	PEB	CHA-C1B-NB	-2.41	119.90	124.93
29	i7	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	i9	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	YB	203	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	YM	203	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	N2	203	PEB	CBC-CAC-C2C	-2.41	108.51	112.62
29	RB	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	RM	202	PEB	OD-C4D-C3D	-2.41	124.00	129.46
29	AG	201	PEB	C1C-CHB-C4B	2.41	131.69	128.81
29	AQ	201	PEB	C1C-CHB-C4B	2.41	131.69	128.81
29	YB	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
29	YM	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
29	J4	201	PEB	CMA-C2A-C1A	-2.41	107.21	112.40
29	T7	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	T9	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
31	JF	1001	CYC	CAC-C3C-C2C	-2.41	108.25	114.26
31	JI	1001	CYC	CAC-C3C-C2C	-2.41	108.25	114.26
29	OF	201	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
29	OI	201	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
29	e1	202	PEB	C2B-C1B-NB	2.41	115.67	110.53
29	eK	202	PEB	C2B-C1B-NB	2.41	115.67	110.53
29	T1	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
29	TK	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
29	U7	201	PEB	CHC-C1D-ND	-2.41	111.15	113.95
29	U9	201	PEB	CHC-C1D-ND	-2.41	111.15	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HQ	203	PEB	CHC-C1D-ND	-2.41	111.15	113.95
29	J5	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
29	JB	202	PEB	OD-C4D-C3D	-2.41	124.01	129.46
29	JM	202	PEB	OD-C4D-C3D	-2.41	124.01	129.46
29	k7	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	k9	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	U1	201	PEB	C2B-C1B-NB	2.41	115.66	110.53
29	UK	201	PEB	C2B-C1B-NB	2.41	115.66	110.53
29	Y1	202	PEB	C1B-C2B-C3B	-2.41	103.75	106.51
29	YK	202	PEB	C1B-C2B-C3B	-2.41	103.75	106.51
29	KB	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	AM	302	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	KM	202	PEB	CMB-C2B-C1B	2.41	128.77	125.06
29	jF	201	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
29	jI	201	PEB	C4B-C3B-C2B	-2.41	104.12	106.78
29	M3	201	PEB	C2A-C1A-NA	2.40	110.35	108.27
29	MO	201	PEB	C2A-C1A-NA	2.40	110.35	108.27
29	V1	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
29	H3	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
29	VK	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
29	HO	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
29	F4	201	PEB	CMA-C2A-C1A	-2.40	107.22	112.40
31	SP	1001	CYC	C4D-CHA-C1A	2.40	131.68	128.81
29	j1	203	PEB	C2B-C1B-NB	2.40	115.66	110.53
29	jK	203	PEB	C2B-C1B-NB	2.40	115.66	110.53
29	Y7	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	Y9	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	P1	202	PEB	C2B-C1B-NB	2.40	115.66	110.53
29	PK	202	PEB	C2B-C1B-NB	2.40	115.66	110.53
29	i1	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
29	iK	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
29	NO	201	PEB	OD-C4D-C3D	-2.40	124.02	129.46
29	NR	201	PEB	CBC-CAC-C2C	-2.40	108.52	112.62
29	AB	302	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	lB	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	lM	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	BG	203	PEB	CHC-C1D-ND	-2.40	111.16	113.95
31	sP	1001	CYC	C4D-CHA-C1A	2.40	131.68	128.81
29	BD	201	PEB	C2B-C1B-NB	2.40	115.65	110.53
29	L4	201	PEB	C2B-C1B-NB	2.40	115.65	110.53
29	H4	201	PEB	CBC-CAC-C2C	-2.40	108.52	112.62
29	G4	201	PEB	C4B-NB-C1B	-2.40	101.99	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JG	203	PEB	CHC-C1D-ND	-2.40	111.16	113.95
29	g1	202	PEB	C2B-C1B-NB	2.40	115.65	110.53
29	gK	202	PEB	C2B-C1B-NB	2.40	115.65	110.53
29	DD	201	PEB	CMA-C2A-C1A	-2.40	107.23	112.40
29	D1	1002	PEB	CBA-CAA-C3A	-2.40	108.12	113.47
29	W2	201	PEB	CHA-C1B-C2B	2.40	131.07	124.90
29	A7	305	PEB	CHA-C1B-C2B	2.40	131.07	124.90
29	A9	305	PEB	CHA-C1B-C2B	2.40	131.07	124.90
30	yJ	303	PUB	CBA-CAA-C3A	-2.40	109.34	112.98
29	e7	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	e9	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	k1	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
29	kK	203	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
31	DP	1001	CYC	C4D-CHA-C1A	2.40	131.68	128.81
31	FP	1001	CYC	C4D-CHA-C1A	2.40	131.68	128.81
29	L4	201	PEB	C2A-C1A-NA	2.40	110.34	108.27
29	dF	202	PEB	C4B-C3B-C2B	-2.40	104.13	106.78
29	dI	202	PEB	C4B-C3B-C2B	-2.40	104.13	106.78
29	HF	1002	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
29	HI	1002	PEB	C1B-C2B-C3B	-2.40	103.75	106.51
31	jP	1001	CYC	C4D-CHA-C1A	2.40	131.67	128.81
29	c7	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	c9	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	c1	202	PEB	C2B-C1B-NB	2.40	115.65	110.53
29	cK	202	PEB	C2B-C1B-NB	2.40	115.65	110.53
29	m7	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	m9	202	PEB	CMB-C2B-C1B	2.40	128.76	125.06
29	C8	201	PEB	OD-C4D-C3D	-2.40	124.03	129.46
29	R7	202	PEB	CMB-C2B-C1B	2.40	128.75	125.06
29	R9	202	PEB	CMB-C2B-C1B	2.40	128.75	125.06
29	R2	203	PEB	CBC-CAC-C2C	-2.40	108.53	112.62
29	dF	201	PEB	CAB-C3B-C4B	2.40	129.25	125.01
29	dI	201	PEB	CAB-C3B-C4B	2.40	129.25	125.01
29	GD	201	PEB	C4B-NB-C1B	-2.40	102.00	106.51
29	TB	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
29	TM	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
31	nP	1001	CYC	C4D-CHA-C1A	2.40	131.67	128.81
29	JG	201	PEB	CHC-C1D-ND	-2.40	111.17	113.95
29	JQ	201	PEB	CHC-C1D-ND	-2.40	111.17	113.95
29	VR	203	PEB	CBC-CAC-C2C	-2.40	108.53	112.62
31	NF	1001	CYC	CAC-C3C-C2C	-2.40	108.28	114.26
31	NI	1001	CYC	CAC-C3C-C2C	-2.40	108.28	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F5	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
29	F8	202	PEB	OD-C4D-C3D	-2.40	124.03	129.46
29	J8	201	PEB	CBB-CAB-C3B	-2.39	105.97	112.63
29	Z1	201	PEB	C2B-C1B-NB	2.39	115.64	110.53
29	ZK	201	PEB	C2B-C1B-NB	2.39	115.64	110.53
30	AF	302	PUB	OA-C1A-NA	-2.39	122.38	125.93
30	AI	302	PUB	OA-C1A-NA	-2.39	122.38	125.93
29	J4	201	PEB	CBC-CAC-C2C	-2.39	108.53	112.62
29	JD	201	PEB	CBC-CAC-C2C	-2.39	108.53	112.62
29	XR	203	PEB	CBC-CAC-C2C	-2.39	108.53	112.62
29	FD	201	PEB	CMA-C2A-C1A	-2.39	107.24	112.40
29	PF	202	PEB	CAB-C3B-C4B	2.39	129.24	125.01
29	PI	202	PEB	CAB-C3B-C4B	2.39	129.24	125.01
29	B8	202	PEB	OD-C4D-C3D	-2.39	124.04	129.46
29	HG	203	PEB	CHC-C1D-ND	-2.39	111.17	113.95
30	MQ	404	PUB	CMA-C2A-C1A	2.39	127.02	121.39
29	VR	201	PEB	CBC-CAC-C2C	-2.39	108.54	112.62
29	BD	201	PEB	CMA-C2A-C1A	-2.39	107.25	112.40
29	P1	203	PEB	C1B-C2B-C3B	-2.39	103.76	106.51
29	PK	203	PEB	C1B-C2B-C3B	-2.39	103.76	106.51
29	K5	201	PEB	OD-C4D-C3D	-2.39	124.04	129.46
29	K8	201	PEB	OD-C4D-C3D	-2.39	124.04	129.46
29	cB	202	PEB	OD-C4D-C3D	-2.39	124.04	129.46
29	cM	202	PEB	OD-C4D-C3D	-2.39	124.04	129.46
29	N1	1002	PEB	CBA-CAA-C3A	-2.39	108.14	113.47
29	LD	201	PEB	CMA-C2A-C1A	-2.39	107.25	112.40
29	A1	301	PEB	CAA-C3A-C4A	2.39	118.81	112.67
29	AK	301	PEB	CAA-C3A-C4A	2.39	118.81	112.67
29	R1	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
29	RK	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
29	F1	1002	PEB	CBA-CAA-C3A	-2.39	108.14	113.47
29	FK	1002	PEB	CBA-CAA-C3A	-2.39	108.14	113.47
29	B4	201	PEB	CBC-CAC-C2C	-2.39	108.54	112.62
29	C5	201	PEB	OD-C4D-C3D	-2.39	124.05	129.46
29	FB	202	PEB	OD-C4D-C3D	-2.39	124.05	129.46
29	FM	202	PEB	OD-C4D-C3D	-2.39	124.05	129.46
29	V1	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
29	VK	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
29	i1	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
29	iK	202	PEB	C2B-C1B-NB	2.39	115.63	110.53
29	V2	201	PEB	CBC-CAC-C2C	-2.39	108.54	112.62
29	L4	201	PEB	CBC-CAC-C2C	-2.39	108.54	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LD	201	PEB	CBC-CAC-C2C	-2.39	108.54	112.62
29	J3	203	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
29	DF	1002	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
29	DI	1002	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
29	JO	203	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
29	OR	201	PEB	CHA-C1B-C2B	2.39	131.04	124.90
29	DD	201	PEB	C2A-C1A-NA	2.39	110.33	108.27
29	W2	202	PEB	OD-C4D-ND	-2.39	122.39	125.93
29	zL	501	PEB	CMB-C2B-C1B	2.39	128.74	125.06
29	OF	203	PEB	CAB-C3B-C4B	2.39	129.23	125.01
29	mF	202	PEB	CAB-C3B-C4B	2.39	129.23	125.01
29	OI	203	PEB	CAB-C3B-C4B	2.39	129.23	125.01
29	mI	202	PEB	CAB-C3B-C4B	2.39	129.23	125.01
31	OP	1001	CYC	C4D-CHA-C1A	2.39	131.66	128.81
31	UP	1001	CYC	C4D-CHA-C1A	2.39	131.66	128.81
29	dD	401	PEB	C4B-NB-C1B	-2.39	102.01	106.51
29	V2	203	PEB	CBC-CAC-C2C	-2.39	108.55	112.62
29	D4	201	PEB	CBC-CAC-C2C	-2.39	108.55	112.62
29	MN	404	PEB	C2A-C1A-NA	2.39	110.33	108.27
29	R1	203	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
29	RK	203	PEB	C1B-C2B-C3B	-2.39	103.77	106.51
31	I7	1001	CYC	OB-C4B-C3B	-2.39	125.45	128.04
31	I9	1001	CYC	OB-C4B-C3B	-2.39	125.45	128.04
29	Q2	202	PEB	OD-C4D-ND	-2.39	122.39	125.93
29	H8	202	PEB	OD-C4D-C3D	-2.39	124.05	129.46
29	U2	201	PEB	CAB-CBB-CGB	-2.39	108.47	113.60
29	DK	1002	PEB	CBA-CAA-C3A	-2.39	108.16	113.47
29	NK	1002	PEB	CBA-CAA-C3A	-2.39	108.16	113.47
29	QB	202	PEB	OD-C4D-C3D	-2.39	124.06	129.46
29	QM	202	PEB	OD-C4D-C3D	-2.39	124.06	129.46
30	A7	302	PUB	CMD-C2D-C3D	2.39	131.35	127.77
30	A9	302	PUB	CMD-C2D-C3D	2.39	131.35	127.77
29	E4	201	PEB	C4B-NB-C1B	-2.39	102.02	106.51
29	wL	301	PEB	CAA-C3A-C2A	2.39	120.22	114.26
29	IG	201	PEB	C1C-CHB-C4B	2.38	131.66	128.81
29	IQ	201	PEB	C1C-CHB-C4B	2.38	131.66	128.81
31	MP	1001	CYC	C4D-CHA-C1A	2.38	131.66	128.81
31	oP	1001	CYC	C4D-CHA-C1A	2.38	131.66	128.81
29	I5	201	PEB	OD-C4D-C3D	-2.38	124.06	129.46
29	I8	201	PEB	OD-C4D-C3D	-2.38	124.06	129.46
29	KB	203	PEB	OD-C4D-C3D	-2.38	124.06	129.46
29	gB	202	PEB	OD-C4D-C3D	-2.38	124.06	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KM	203	PEB	OD-C4D-C3D	-2.38	124.06	129.46
29	gM	202	PEB	OD-C4D-C3D	-2.38	124.06	129.46
29	H4	201	PEB	CMA-C2A-C1A	-2.38	107.26	112.40
29	T7	202	PEB	OD-C4D-ND	-2.38	122.40	125.93
29	T9	202	PEB	OD-C4D-ND	-2.38	122.40	125.93
31	fP	1001	CYC	C4D-CHA-C1A	2.38	131.66	128.81
29	T2	201	PEB	C1C-CHB-C4B	-2.38	125.96	128.81
29	VF	202	PEB	CAB-C3B-C4B	2.38	129.23	125.01
29	VI	202	PEB	CAB-C3B-C4B	2.38	129.23	125.01
29	ZF	201	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
29	ZI	201	PEB	C4B-C3B-C2B	-2.38	104.14	106.78
29	HD	201	PEB	CMA-C2A-C1A	-2.38	107.27	112.40
31	kP	1001	CYC	C4D-CHA-C1A	2.38	131.66	128.81
31	wP	1001	CYC	C4D-CHA-C1A	2.38	131.66	128.81
29	gF	202	PEB	CAB-C3B-C4B	2.38	129.22	125.01
29	gI	202	PEB	CAB-C3B-C4B	2.38	129.22	125.01
29	I4	201	PEB	CAA-C3A-C4A	-2.38	106.56	112.67
29	ID	201	PEB	C4B-NB-C1B	-2.38	102.02	106.51
29	GG	202	PEB	C2A-C1A-NA	2.38	110.33	108.27
29	GQ	202	PEB	C2A-C1A-NA	2.38	110.33	108.27
29	c1	201	PEB	C2B-C1B-NB	2.38	115.61	110.53
29	cK	201	PEB	C2B-C1B-NB	2.38	115.61	110.53
29	QR	202	PEB	OD-C4D-ND	-2.38	122.40	125.93
29	C4	201	PEB	C4B-NB-C1B	-2.38	102.03	106.51
29	JQ	203	PEB	CHC-C1D-ND	-2.38	111.18	113.95
29	F4	201	PEB	C2A-C1A-NA	2.38	110.33	108.27
29	J1	1002	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
29	JK	1002	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
29	CA	202	PEB	C2B-C1B-NB	2.38	115.61	110.53
29	CN	202	PEB	C2B-C1B-NB	2.38	115.61	110.53
29	I4	201	PEB	C4B-NB-C1B	-2.38	102.03	106.51
29	e1	203	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
29	LF	1002	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
29	LI	1002	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
29	eK	203	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
31	BP	1001	CYC	C4D-CHA-C1A	2.38	131.65	128.81
29	a7	202	PEB	OD-C4D-ND	-2.38	122.41	125.93
29	a9	202	PEB	OD-C4D-ND	-2.38	122.41	125.93
29	HK	1002	PEB	CBA-CAA-C3A	-2.38	108.17	113.47
29	H4	201	PEB	C2A-C1A-NA	2.38	110.32	108.27
29	zJ	501	PEB	CMB-C2B-C1B	2.38	128.73	125.06
29	g1	201	PEB	C2B-C1B-NB	2.38	115.60	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	gK	201	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	A8	201	PEB	OD-C4D-C3D	-2.38	124.07	129.46
29	k7	202	PEB	OD-C4D-ND	-2.38	122.41	125.93
29	k9	202	PEB	OD-C4D-ND	-2.38	122.41	125.93
29	i1	203	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
29	iK	203	PEB	C1B-C2B-C3B	-2.38	103.78	106.51
29	G4	201	PEB	CAA-C3A-C4A	-2.38	106.57	112.67
29	R2	201	PEB	C1C-CHB-C4B	-2.38	125.97	128.81
29	a1	202	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	aK	202	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	SR	201	PEB	CMB-C2B-C1B	2.38	128.72	125.06
29	iB	202	PEB	OD-C4D-C3D	-2.38	124.08	129.46
29	iM	202	PEB	OD-C4D-C3D	-2.38	124.08	129.46
29	xJ	301	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	MQ	406	PEB	CMD-C2D-C3D	2.38	133.42	130.06
29	X2	202	PEB	CBC-CAC-C2C	-2.38	108.56	112.62
29	a7	201	PEB	OD-C4D-C3D	-2.38	124.08	129.46
29	a9	201	PEB	OD-C4D-C3D	-2.38	124.08	129.46
29	A5	201	PEB	OD-C4D-C3D	-2.38	124.08	129.46
29	P1	201	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	k1	202	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	PK	201	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	kK	202	PEB	C2B-C1B-NB	2.38	115.60	110.53
29	i7	201	PEB	CAB-CBB-CGB	-2.38	108.49	113.60
29	i9	201	PEB	CAB-CBB-CGB	-2.38	108.49	113.60
29	V1	201	PEB	C2B-C1B-NB	2.37	115.60	110.53
29	VK	201	PEB	C2B-C1B-NB	2.37	115.60	110.53
29	EG	201	PEB	C1C-CHB-C4B	2.37	131.65	128.81
29	EQ	201	PEB	C1C-CHB-C4B	2.37	131.65	128.81
31	1P	1001	CYC	C4D-CHA-C1A	2.37	131.65	128.81
29	B4	201	PEB	C2A-C1A-NA	2.37	110.32	108.27
31	IP	1001	CYC	C4D-CHA-C1A	2.37	131.64	128.81
31	hP	1001	CYC	C4D-CHA-C1A	2.37	131.64	128.81
29	oJ	201	PEB	CMB-C2B-C3B	-2.37	119.67	126.12
29	oL	201	PEB	CMB-C2B-C3B	-2.37	119.67	126.12
29	aF	202	PEB	CAB-C3B-C4B	2.37	129.21	125.01
29	aI	202	PEB	CAB-C3B-C4B	2.37	129.21	125.01
29	wJ	301	PEB	CAA-C3A-C2A	2.37	120.19	114.26
29	A1	303	PEB	CAC-CBC-CGC	-2.37	107.11	113.76
29	AK	303	PEB	CAC-CBC-CGC	-2.37	107.11	113.76
29	L1	1002	PEB	CBA-CAA-C3A	-2.37	108.19	113.47
29	LK	1002	PEB	CBA-CAA-C3A	-2.37	108.19	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	cJ	201	PEB	CMB-C2B-C3B	-2.37	119.68	126.12
29	cL	201	PEB	CMB-C2B-C3B	-2.37	119.68	126.12
29	M3	203	PEB	CHA-C1B-NB	-2.37	119.97	124.93
29	MO	203	PEB	CHA-C1B-NB	-2.37	119.97	124.93
29	UJ	201	PEB	CMB-C2B-C3B	-2.37	119.68	126.12
29	UL	201	PEB	CMB-C2B-C3B	-2.37	119.68	126.12
29	lF	201	PEB	C4B-C3B-C2B	-2.37	104.16	106.78
29	lI	201	PEB	C4B-C3B-C2B	-2.37	104.16	106.78
29	a1	203	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
29	aK	203	PEB	C1B-C2B-C3B	-2.37	103.78	106.51
29	KA	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
29	KN	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
29	k7	201	PEB	OD-C4D-C3D	-2.37	124.09	129.46
29	k9	201	PEB	OD-C4D-C3D	-2.37	124.09	129.46
29	k7	201	PEB	CAB-CBB-CGB	-2.37	108.50	113.60
29	k9	201	PEB	CAB-CBB-CGB	-2.37	108.50	113.60
29	N3	203	PEB	CHA-C1B-NB	-2.37	119.97	124.93
29	GA	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
29	GN	202	PEB	C2B-C1B-NB	2.37	115.59	110.53
29	k1	203	PEB	CHA-C1B-NB	-2.37	119.97	124.93
29	kK	203	PEB	CHA-C1B-NB	-2.37	119.97	124.93
29	l4	203	PEB	CHC-C1D-ND	-2.37	111.19	113.95
29	QR	202	PEB	CHC-C1D-ND	-2.37	111.19	113.95
29	eF	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
29	eI	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
29	MD	201	PEB	CAA-C3A-C4A	-2.37	106.59	112.67
29	iF	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
29	iI	202	PEB	CAB-C3B-C4B	2.37	129.20	125.01
29	P7	202	PEB	OD-C4D-ND	-2.37	122.42	125.93
29	P9	202	PEB	OD-C4D-ND	-2.37	122.42	125.93
29	g1	203	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
29	FF	1002	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
29	FI	1002	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
29	gK	203	PEB	C1B-C2B-C3B	-2.37	103.79	106.51
29	xL	301	PEB	CAA-C3A-C2A	2.37	120.17	114.26
29	DQ	203	PEB	CHC-C1D-ND	-2.37	111.20	113.95
30	MG	403	PUB	OD-C4D-C3D	-2.37	125.47	128.04
29	M4	203	PEB	OD-C4D-ND	-2.37	122.42	125.93
29	K4	201	PEB	CAA-C3A-C4A	-2.37	106.60	112.67
29	AJ	201	PEB	CMB-C2B-C3B	-2.37	119.69	126.12
29	AL	201	PEB	CMB-C2B-C3B	-2.37	119.69	126.12
29	D4	201	PEB	C2A-C1A-NA	2.37	110.31	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AB	302	PEB	C2A-C1A-NA	2.37	110.31	108.27
29	g7	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
29	m7	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
29	g9	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
29	m9	201	PEB	OD-C4D-C3D	-2.37	124.10	129.46
29	e1	201	PEB	C2B-C1B-NB	2.37	115.58	110.53
29	k1	201	PEB	C2B-C1B-NB	2.37	115.58	110.53
29	eK	201	PEB	C2B-C1B-NB	2.37	115.58	110.53
29	kK	201	PEB	C2B-C1B-NB	2.37	115.58	110.53
31	F7	1001	CYC	CAD-C3D-C2D	-2.37	120.45	127.25
29	WJ	202	PEB	CMB-C2B-C3B	-2.37	119.69	126.12
29	WL	202	PEB	CMB-C2B-C3B	-2.37	119.69	126.12
29	LG	203	PEB	CHC-C1D-ND	-2.37	111.20	113.95
29	ID	201	PEB	CAA-C3A-C4A	-2.37	106.60	112.67
29	a1	201	PEB	C2B-C1B-NB	2.37	115.58	110.53
29	aK	201	PEB	C2B-C1B-NB	2.37	115.58	110.53
29	OR	201	PEB	CAB-CBB-CGB	-2.36	108.51	113.60
29	Y1	201	PEB	C2B-C1B-NB	2.36	115.58	110.53
29	YK	201	PEB	C2B-C1B-NB	2.36	115.58	110.53
29	H1	1002	PEB	CBA-CAA-C3A	-2.36	108.20	113.47
29	KJ	201	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	gJ	201	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	KL	201	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	gL	201	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	m7	202	PEB	OD-C4D-ND	-2.36	122.43	125.93
29	m9	202	PEB	OD-C4D-ND	-2.36	122.43	125.93
29	KD	201	PEB	CAA-C3A-C4A	-2.36	106.60	112.67
29	V7	202	PEB	OD-C4D-ND	-2.36	122.43	125.93
29	V9	202	PEB	OD-C4D-ND	-2.36	122.43	125.93
29	uJ	202	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	uL	202	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	R7	201	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	R9	201	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	MJ	201	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	ML	201	PEB	CMB-C2B-C3B	-2.36	119.70	126.12
29	YF	202	PEB	CAB-C3B-C4B	2.36	129.19	125.01
29	YI	202	PEB	CAB-C3B-C4B	2.36	129.19	125.01
29	V7	201	PEB	OD-C4D-C3D	-2.36	124.11	129.46
29	V9	201	PEB	OD-C4D-C3D	-2.36	124.11	129.46
31	qP	1001	CYC	C4D-CHA-C1A	2.36	131.63	128.81
29	GD	201	PEB	CAA-C3A-C4A	-2.36	106.61	112.67
31	M9	1001	CYC	OB-C4B-C3B	-2.36	125.48	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	xJ	301	PEB	CAA-C3A-C2A	2.36	120.16	114.26
31	NF	1001	CYC	C1A-C2A-C3A	-2.36	104.17	106.78
31	NI	1001	CYC	C1A-C2A-C3A	-2.36	104.17	106.78
29	eJ	201	PEB	CMB-C2B-C3B	-2.36	119.71	126.12
29	eL	201	PEB	CMB-C2B-C3B	-2.36	119.71	126.12
29	Y7	201	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	Y9	201	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	c7	201	PEB	OD-C4D-C3D	-2.36	124.11	129.46
29	c9	201	PEB	OD-C4D-C3D	-2.36	124.11	129.46
31	QP	1001	CYC	C4D-CHA-C1A	2.36	131.63	128.81
29	T7	201	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	T9	201	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	MA	404	PEB	C2A-C1A-NA	2.36	110.31	108.27
29	MG	404	PEB	CAB-CBB-CGB	-2.36	108.52	113.60
29	c1	203	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
29	cK	203	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
29	yJ	301	PEB	CAB-C3B-C4B	2.36	129.18	125.01
29	yL	301	PEB	CAB-C3B-C4B	2.36	129.18	125.01
29	iJ	201	PEB	CMB-C2B-C3B	-2.36	119.71	126.12
29	iL	201	PEB	CMB-C2B-C3B	-2.36	119.71	126.12
30	A7	303	PUB	CMD-C2D-C3D	2.36	131.31	127.77
30	A9	303	PUB	CMD-C2D-C3D	2.36	131.31	127.77
29	i7	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
29	i9	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
29	g7	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	g9	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
31	HP	1001	CYC	C4D-CHA-C1A	2.36	131.63	128.81
29	m7	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	m9	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	Y7	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
29	Y9	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
29	YJ	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	YL	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	JD	201	PEB	C2A-C1A-NA	2.36	110.31	108.27
29	xL	301	PEB	C2B-C1B-NB	2.36	115.56	110.53
29	P7	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
29	P9	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
29	EJ	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	EL	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	g1	203	PEB	CHA-C1B-NB	-2.36	120.00	124.93
29	gK	203	PEB	CHA-C1B-NB	-2.36	120.00	124.93
29	CD	201	PEB	C4B-NB-C1B	-2.36	102.07	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K4	201	PEB	C4B-NB-C1B	-2.36	102.07	106.51
29	CJ	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	CL	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	R1	201	PEB	C2B-C1B-NB	2.36	115.56	110.53
29	RK	201	PEB	C2B-C1B-NB	2.36	115.56	110.53
29	Y7	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
29	Y9	201	PEB	OD-C4D-C3D	-2.36	124.12	129.46
29	NO	202	PEB	CMB-C2B-C1B	2.36	128.69	125.06
29	W2	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	MQ	406	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	UR	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	m1	202	PEB	CHA-C1B-NB	-2.36	120.00	124.93
29	mK	202	PEB	CHA-C1B-NB	-2.36	120.00	124.93
29	EA	202	PEB	C2B-C1B-NB	2.36	115.56	110.53
29	EN	202	PEB	C2B-C1B-NB	2.36	115.56	110.53
29	c7	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
29	c9	202	PEB	OD-C4D-ND	-2.36	122.44	125.93
29	HD	201	PEB	C2A-C1A-NA	2.36	110.30	108.27
29	M3	202	PEB	CMB-C2B-C1B	2.36	128.69	125.06
29	MO	202	PEB	CMB-C2B-C1B	2.36	128.69	125.06
29	JF	1002	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
29	JI	1002	PEB	C1B-C2B-C3B	-2.36	103.80	106.51
29	M4	201	PEB	CAA-C3A-C4A	-2.36	106.62	112.67
29	M4	201	PEB	C4B-NB-C1B	-2.36	102.07	106.51
29	MD	201	PEB	C4B-NB-C1B	-2.36	102.07	106.51
29	V7	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	e7	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	V9	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	e9	201	PEB	CAB-CBB-CGB	-2.36	108.53	113.60
29	DG	201	PEB	CHB-C4B-C3B	-2.36	119.88	125.32
29	DQ	201	PEB	CHB-C4B-C3B	-2.36	119.88	125.32
29	UF	201	PEB	CAB-C3B-C4B	2.36	129.18	125.01
29	UI	201	PEB	CAB-C3B-C4B	2.36	129.18	125.01
29	OJ	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	OL	201	PEB	CMB-C2B-C3B	-2.36	119.72	126.12
29	IA	202	PEB	C2B-C1B-NB	2.35	115.56	110.53
29	IN	202	PEB	C2B-C1B-NB	2.35	115.56	110.53
31	G9	1001	CYC	OB-C4B-C3B	-2.35	125.48	128.04
31	DF	1001	CYC	C1A-C2A-C3A	-2.35	104.18	106.78
31	DI	1001	CYC	C1A-C2A-C3A	-2.35	104.18	106.78
31	F9	1001	CYC	CAD-C3D-C2D	-2.35	120.48	127.25
29	AA	202	PEB	C2B-C1B-NB	2.35	115.55	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AN	202	PEB	C2B-C1B-NB	2.35	115.55	110.53
31	XP	1001	CYC	C4D-CHA-C1A	2.35	131.62	128.81
31	K9	1001	CYC	OB-C4B-C3B	-2.35	125.49	128.04
29	IJ	201	PEB	CMB-C2B-C3B	-2.35	119.73	126.12
29	IL	201	PEB	CMB-C2B-C3B	-2.35	119.73	126.12
29	xJ	303	PEB	CMB-C2B-C3B	2.35	132.51	126.12
29	m1	201	PEB	C2B-C1B-NB	2.35	115.55	110.53
29	mK	201	PEB	C2B-C1B-NB	2.35	115.55	110.53
29	QJ	201	PEB	CMB-C2B-C3B	-2.35	119.73	126.12
29	QL	201	PEB	CMB-C2B-C3B	-2.35	119.73	126.12
29	GG	201	PEB	C1C-CHB-C4B	2.35	131.62	128.81
29	GQ	201	PEB	C1C-CHB-C4B	2.35	131.62	128.81
29	EB	202	PEB	CMC-C3C-C2C	2.35	129.38	124.94
29	EM	202	PEB	CMC-C3C-C2C	2.35	129.38	124.94
29	BG	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
29	JG	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
29	BQ	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
29	JQ	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
29	T1	202	PEB	CHA-C1B-NB	-2.35	120.01	124.93
29	V1	203	PEB	CHA-C1B-NB	-2.35	120.01	124.93
29	TK	202	PEB	CHA-C1B-NB	-2.35	120.01	124.93
29	VK	203	PEB	CHA-C1B-NB	-2.35	120.01	124.93
29	NR	201	PEB	C1C-CHB-C4B	-2.35	126.00	128.81
29	fB	202	PEB	CMC-C3C-C2C	2.35	129.38	124.94
29	fM	202	PEB	CMC-C3C-C2C	2.35	129.38	124.94
29	e1	203	PEB	CHA-C1B-NB	-2.35	120.02	124.93
29	eK	203	PEB	CHA-C1B-NB	-2.35	120.02	124.93
29	dD	401	PEB	CAA-C3A-C4A	-2.35	106.64	112.67
29	AM	302	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	mJ	201	PEB	CMB-C2B-C3B	-2.35	119.74	126.12
29	mL	201	PEB	CMB-C2B-C3B	-2.35	119.74	126.12
30	MG	402	PUB	CMA-C2A-C1A	2.35	126.92	121.39
29	e7	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
29	e9	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
29	e7	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	e9	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	zJ	501	PEB	CHA-C1B-NB	-2.35	120.02	124.93
29	MR	202	PEB	CAB-C3B-C4B	2.35	129.16	125.01
29	c7	201	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
29	c9	201	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
29	c1	203	PEB	CHA-C1B-NB	-2.35	120.02	124.93
29	cK	203	PEB	CHA-C1B-NB	-2.35	120.02	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SJ	201	PEB	CMB-C2B-C3B	-2.35	119.74	126.12
29	SL	201	PEB	CMB-C2B-C3B	-2.35	119.74	126.12
29	BQ	203	PEB	CHC-C1D-ND	-2.35	111.22	113.95
29	FG	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
29	FQ	201	PEB	CHB-C4B-C3B	-2.35	119.89	125.32
30	MQ	405	PUB	OD-C4D-C3D	-2.35	125.49	128.04
31	N7	1001	CYC	CAD-C3D-C2D	-2.35	120.50	127.25
31	N9	1001	CYC	CAD-C3D-C2D	-2.35	120.50	127.25
29	ZB	201	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
29	ZM	201	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
29	a7	201	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
29	a9	201	PEB	CAB-CBB-CGB	-2.35	108.55	113.60
29	g7	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	g9	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	aJ	201	PEB	CMB-C2B-C3B	-2.35	119.75	126.12
29	aL	201	PEB	CMB-C2B-C3B	-2.35	119.75	126.12
29	R7	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
29	R9	201	PEB	OD-C4D-C3D	-2.35	124.14	129.46
29	i1	201	PEB	C2B-C1B-NB	2.35	115.54	110.53
29	iK	201	PEB	C2B-C1B-NB	2.35	115.54	110.53
29	R7	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	R9	202	PEB	OD-C4D-ND	-2.35	122.45	125.93
29	T1	201	PEB	C2B-C1B-NB	2.35	115.53	110.53
29	TK	201	PEB	C2B-C1B-NB	2.35	115.53	110.53
31	HF	1001	CYC	C1A-C2A-C3A	-2.35	104.19	106.78
31	HI	1001	CYC	C1A-C2A-C3A	-2.35	104.19	106.78
29	PB	201	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
29	PM	201	PEB	C1B-C2B-C3B	-2.35	103.81	106.51
29	kF	202	PEB	CAB-C3B-C4B	2.35	129.16	125.01
29	kI	202	PEB	CAB-C3B-C4B	2.35	129.16	125.01
29	R2	203	PEB	CHA-C1B-NB	-2.34	120.03	124.93
31	G7	1001	CYC	OB-C4B-C3B	-2.34	125.50	128.04
29	GB	202	PEB	CMC-C3C-C2C	2.34	129.36	124.94
29	GM	202	PEB	CMC-C3C-C2C	2.34	129.36	124.94
29	MR	201	PEB	CAB-CBB-CGB	-2.34	108.56	113.60
29	jB	202	PEB	CMC-C3C-C2C	2.34	129.36	124.94
29	jM	202	PEB	CMC-C3C-C2C	2.34	129.36	124.94
31	JF	1001	CYC	C1A-C2A-C3A	-2.34	104.19	106.78
31	JI	1001	CYC	C1A-C2A-C3A	-2.34	104.19	106.78
29	kJ	201	PEB	CMB-C2B-C3B	-2.34	119.75	126.12
29	kL	201	PEB	CMB-C2B-C3B	-2.34	119.75	126.12
29	xL	303	PEB	CMB-C2B-C3B	2.34	132.48	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P7	201	PEB	CAB-CBB-CGB	-2.34	108.56	113.60
29	P9	201	PEB	CAB-CBB-CGB	-2.34	108.56	113.60
29	K4	202	PEB	CAB-C3B-C4B	2.34	129.15	125.01
29	CD	201	PEB	CAA-C3A-C4A	-2.34	106.66	112.67
29	qJ	201	PEB	CMB-C2B-C3B	-2.34	119.76	126.12
29	qL	201	PEB	CMB-C2B-C3B	-2.34	119.76	126.12
29	HG	201	PEB	CHB-C4B-C3B	-2.34	119.91	125.32
29	HQ	201	PEB	CHB-C4B-C3B	-2.34	119.91	125.32
29	DA	201	PEB	CBC-CAC-C2C	-2.34	108.62	112.62
29	DN	201	PEB	CBC-CAC-C2C	-2.34	108.62	112.62
29	T7	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
29	T9	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
29	E4	201	PEB	CAA-C3A-C4A	-2.34	106.66	112.67
29	NO	203	PEB	CHA-C1B-NB	-2.34	120.03	124.93
29	i7	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
29	i9	201	PEB	OD-C4D-C3D	-2.34	124.15	129.46
29	cB	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	iB	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	cM	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	iM	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	O2	201	PEB	CAB-CBB-CGB	-2.34	108.56	113.60
29	GJ	201	PEB	CMB-C2B-C3B	-2.34	119.76	126.12
29	GL	201	PEB	CMB-C2B-C3B	-2.34	119.76	126.12
29	AB	302	PEB	OD-C4D-ND	-2.34	122.46	125.93
29	kB	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	kM	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
31	DF	1001	CYC	CMB-C2B-C1B	2.34	127.09	124.17
31	DI	1001	CYC	CMB-C2B-C1B	2.34	127.09	124.17
29	i1	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	iK	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	M2	201	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
29	P2	202	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	WR	201	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
29	X2	202	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	DG	203	PEB	CHC-C1D-ND	-2.34	111.23	113.95
29	CG	201	PEB	C1C-CHB-C4B	2.34	131.60	128.81
29	CQ	201	PEB	C1C-CHB-C4B	2.34	131.60	128.81
29	a1	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	aK	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	FD	201	PEB	C2A-C1A-NA	2.34	110.29	108.27
29	JB	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	JM	201	PEB	C1B-C2B-C3B	-2.34	103.82	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NO	203	PEB	C1B-C2B-C3B	-2.34	103.82	106.51
29	Y1	202	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	N2	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	YK	202	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	NR	203	PEB	CHA-C1B-NB	-2.34	120.04	124.93
29	KG	201	PEB	C1C-CHB-C4B	2.34	131.60	128.81
29	KQ	201	PEB	C1C-CHB-C4B	2.34	131.60	128.81
29	sJ	201	PEB	CMB-C2B-C3B	-2.34	119.77	126.12
29	sL	201	PEB	CMB-C2B-C3B	-2.34	119.77	126.12
29	Q2	201	PEB	CAB-CBB-CGB	-2.34	108.57	113.60
29	MQ	407	PEB	CAA-C3A-C2A	-2.34	108.42	114.26
29	GD	202	PEB	CAB-C3B-C4B	2.34	129.14	125.01
29	aB	202	PEB	CMC-C3C-C2C	2.34	129.35	124.94
29	aM	202	PEB	CMC-C3C-C2C	2.34	129.35	124.94
30	MN	402	PUB	CMA-C2A-C1A	2.34	126.89	121.39
29	BA	201	PEB	CBC-CAC-C2C	-2.34	108.63	112.62
29	BN	201	PEB	CBC-CAC-C2C	-2.34	108.63	112.62
29	XR	203	PEB	CHA-C1B-NB	-2.34	120.05	124.93
29	wL	303	PEB	CMB-C2B-C3B	2.34	132.46	126.12
29	KD	202	PEB	C2B-C1B-NB	2.34	115.51	110.53
31	E7	1001	CYC	OB-C4B-C3B	-2.34	125.51	128.04
31	E9	1001	CYC	OB-C4B-C3B	-2.34	125.51	128.04
29	KD	201	PEB	C4B-NB-C1B	-2.34	102.11	106.51
29	FB	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
29	FM	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
31	FF	1001	CYC	C1A-C2A-C3A	-2.33	104.20	106.78
31	FI	1001	CYC	C1A-C2A-C3A	-2.33	104.20	106.78
29	M4	202	PEB	CAB-C3B-C4B	2.33	129.14	125.01
29	UB	202	PEB	CMC-C3C-C2C	2.33	129.34	124.94
29	MQ	401	PEB	CMC-C3C-C2C	2.33	129.34	124.94
29	KD	202	PEB	CAB-C3B-C4B	2.33	129.14	125.01
29	AF	304	PEB	OD-C4D-C3D	-2.33	124.17	129.46
29	AI	304	PEB	OD-C4D-C3D	-2.33	124.17	129.46
29	R1	203	PEB	CHA-C1B-NB	-2.33	120.05	124.93
29	RK	203	PEB	CHA-C1B-NB	-2.33	120.05	124.93
31	D7	1001	CYC	CAD-C3D-C2D	-2.33	120.54	127.25
31	D9	1001	CYC	CAD-C3D-C2D	-2.33	120.54	127.25
29	GC	201	PEB	CHA-C1B-NB	-2.33	120.05	124.93
29	GE	201	PEB	CHA-C1B-NB	-2.33	120.05	124.93
31	CF	1001	CYC	OB-C4B-NB	-2.33	119.66	125.08
31	CI	1001	CYC	OB-C4B-NB	-2.33	119.66	125.08
29	TB	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TM	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
29	ID	202	PEB	CAB-C3B-C4B	2.33	129.13	125.01
29	FQ	203	PEB	CHC-C1D-ND	-2.33	111.24	113.95
29	EG	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
29	EQ	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
29	mB	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
29	mM	201	PEB	C1B-C2B-C3B	-2.33	103.83	106.51
29	T2	203	PEB	CHA-C1B-NB	-2.33	120.06	124.93
29	AG	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
29	AQ	202	PEB	C2A-C1A-NA	2.33	110.28	108.27
29	C4	201	PEB	CAA-C3A-C4A	-2.33	106.69	112.67
29	FA	201	PEB	CBC-CAC-C2C	-2.33	108.64	112.62
29	FN	201	PEB	CBC-CAC-C2C	-2.33	108.64	112.62
30	MA	402	PUB	CMA-C2A-C1A	2.33	126.87	121.39
29	VR	203	PEB	CHA-C1B-NB	-2.33	120.06	124.93
29	L3	202	PEB	CAB-C3B-C4B	2.33	129.13	125.01
29	LO	202	PEB	CAB-C3B-C4B	2.33	129.13	125.01
29	AM	302	PEB	C2A-C1A-NA	2.33	110.28	108.27
29	wJ	301	PEB	C2B-C1B-NB	2.33	115.50	110.53
31	K7	1001	CYC	OB-C4B-C3B	-2.33	125.51	128.04
29	MB	202	PEB	CMC-C3C-C2C	2.33	129.33	124.94
29	MM	202	PEB	CMC-C3C-C2C	2.33	129.33	124.94
31	L7	1001	CYC	CAD-C3D-C2D	-2.33	120.56	127.25
31	KF	1001	CYC	OB-C4B-NB	-2.33	119.67	125.08
29	MD	202	PEB	C2B-C1B-NB	2.33	115.50	110.53
31	L9	1001	CYC	CAD-C3D-C2D	-2.33	120.56	127.25
29	IB	202	PEB	CMC-C3C-C2C	2.33	129.33	124.94
29	IM	202	PEB	CMC-C3C-C2C	2.33	129.33	124.94
29	AB	303	PEB	OD-C4D-ND	-2.33	122.48	125.93
29	LG	201	PEB	CHB-C4B-C3B	-2.33	119.95	125.32
29	MQ	402	PEB	CHB-C4B-C3B	-2.33	119.95	125.32
29	MD	202	PEB	CAB-C3B-C4B	2.33	129.12	125.01
29	E4	202	PEB	C2B-C1B-NB	2.33	115.49	110.53
29	MG	405	PEB	CAA-C3A-C2A	-2.33	108.45	114.26
29	PR	202	PEB	CHA-C1B-NB	-2.33	120.07	124.93
31	H7	1001	CYC	CAD-C3D-C2D	-2.33	120.56	127.25
31	H9	1001	CYC	CAD-C3D-C2D	-2.33	120.56	127.25
29	hB	202	PEB	CMC-C3C-C2C	2.33	129.33	124.94
29	hM	202	PEB	CMC-C3C-C2C	2.33	129.33	124.94
29	NB	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
29	NM	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
29	P1	203	PEB	CHA-C1B-NB	-2.32	120.07	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	PK	203	PEB	CHA-C1B-NB	-2.32	120.07	124.93
29	CB	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	CM	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	KB	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	SB	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	KM	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	SM	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	QR	201	PEB	CAB-CBB-CGB	-2.32	108.60	113.60
31	LF	1001	CYC	C1A-C2A-C3A	-2.32	104.21	106.78
31	LI	1001	CYC	C1A-C2A-C3A	-2.32	104.21	106.78
31	J7	1001	CYC	CAD-C3D-C2D	-2.32	120.57	127.25
29	MN	404	PEB	CHA-C1B-C2B	2.32	130.87	124.90
29	E4	202	PEB	CAB-C3B-C4B	2.32	129.12	125.01
29	D3	203	PEB	CAB-C3B-C4B	2.32	129.12	125.01
29	DO	203	PEB	CAB-C3B-C4B	2.32	129.12	125.01
31	EF	1001	CYC	OB-C4B-NB	-2.32	119.68	125.08
31	EI	1001	CYC	OB-C4B-NB	-2.32	119.68	125.08
29	SF	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
29	SI	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
29	HA	201	PEB	CBC-CAC-C2C	-2.32	108.66	112.62
29	HN	201	PEB	CBC-CAC-C2C	-2.32	108.66	112.62
29	YB	203	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	YM	203	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	LB	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
29	LM	201	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
29	PF	203	PEB	CHC-C1D-ND	-2.32	111.25	113.95
29	PI	203	PEB	CHC-C1D-ND	-2.32	111.25	113.95
29	G4	202	PEB	CAB-C3B-C4B	2.32	129.11	125.01
29	AC	201	PEB	CHA-C1B-NB	-2.32	120.08	124.93
29	AE	201	PEB	CHA-C1B-NB	-2.32	120.08	124.93
29	OB	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	OM	202	PEB	CMC-C3C-C2C	2.32	129.32	124.94
29	yJ	301	PEB	OD-C4D-C3D	-2.32	124.20	129.46
29	yL	301	PEB	OD-C4D-C3D	-2.32	124.20	129.46
29	LD	201	PEB	C2A-C1A-NA	2.32	110.27	108.27
31	M7	1001	CYC	OB-C4B-C3B	-2.32	125.52	128.04
29	wL	301	PEB	C2B-C1B-NB	2.32	115.48	110.53
29	N3	202	PEB	CMB-C2B-C1B	2.32	128.64	125.06
29	M4	202	PEB	C2B-C1B-NB	2.32	115.48	110.53
30	xL	304	PUB	C1D-CHC-C4C	-2.32	108.32	113.37
29	wJ	303	PEB	CMB-C2B-C3B	2.32	132.41	126.12
29	FG	203	PEB	CHC-C1D-ND	-2.32	111.25	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CD	202	PEB	C2B-C1B-NB	2.32	115.48	110.53
29	WF	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
29	WI	201	PEB	C2B-C1B-NB	2.32	115.48	110.53
29	gB	201	PEB	C1B-C2B-C3B	-2.32	103.85	106.51
29	gM	201	PEB	C1B-C2B-C3B	-2.32	103.85	106.51
29	J4	201	PEB	C2A-C1A-NA	2.32	110.27	108.27
29	T7	202	PEB	CAA-C3A-C4A	-2.32	106.72	112.67
29	T9	202	PEB	CAA-C3A-C4A	-2.32	106.72	112.67
29	I4	202	PEB	CAB-C3B-C4B	2.32	129.11	125.01
29	DG	203	PEB	CAC-CBC-CGC	-2.32	107.26	113.76
29	H3	203	PEB	CAB-C3B-C4B	2.32	129.11	125.01
29	HO	203	PEB	CAB-C3B-C4B	2.32	129.11	125.01
29	L1	1002	PEB	CHA-C1B-NB	-2.32	120.09	124.93
29	LK	1002	PEB	CHA-C1B-NB	-2.32	120.09	124.93
31	HF	1001	CYC	CMB-C2B-C1B	2.32	127.06	124.17
31	HI	1001	CYC	CMB-C2B-C1B	2.32	127.06	124.17
29	EC	201	PEB	CHA-C1B-NB	-2.32	120.09	124.93
29	EE	201	PEB	CHA-C1B-NB	-2.32	120.09	124.93
29	HG	203	PEB	CAC-CBC-CGC	-2.32	107.27	113.76
29	fF	201	PEB	C2B-C1B-NB	2.32	115.47	110.53
29	fI	201	PEB	C2B-C1B-NB	2.32	115.47	110.53
29	dF	202	PEB	C2B-C1B-NB	2.32	115.47	110.53
29	dI	202	PEB	C2B-C1B-NB	2.32	115.47	110.53
31	NF	1001	CYC	CMB-C2B-C1B	2.32	127.06	124.17
31	NI	1001	CYC	CMB-C2B-C1B	2.32	127.06	124.17
29	RR	203	PEB	CHA-C1B-NB	-2.31	120.09	124.93
29	K4	202	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	TR	203	PEB	CHA-C1B-NB	-2.31	120.09	124.93
29	g1	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
29	gK	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
29	hF	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	hI	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	ED	201	PEB	CAB-C3B-C4B	2.31	129.10	125.01
29	g7	202	PEB	CAA-C3A-C4A	-2.31	106.73	112.67
29	g9	202	PEB	CAA-C3A-C4A	-2.31	106.73	112.67
29	C4	202	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	bF	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	bI	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
31	JF	1001	CYC	CMB-C2B-C1B	2.31	127.06	124.17
31	JI	1001	CYC	CMB-C2B-C1B	2.31	127.06	124.17
29	c1	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
29	cK	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	eB	201	PEB	C1B-C2B-C3B	-2.31	103.85	106.51
29	eM	201	PEB	C1B-C2B-C3B	-2.31	103.85	106.51
29	J5	202	PEB	C2A-C1A-NA	2.31	110.27	108.27
29	J8	202	PEB	C2A-C1A-NA	2.31	110.27	108.27
29	IG	202	PEB	C2A-C1A-NA	2.31	110.27	108.27
29	IQ	202	PEB	C2A-C1A-NA	2.31	110.27	108.27
29	k1	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
29	kK	203	PEB	OD-C4D-C3D	-2.31	124.22	129.46
29	DA	203	PEB	CHA-C1B-NB	-2.31	120.09	124.93
29	DN	203	PEB	CHA-C1B-NB	-2.31	120.09	124.93
29	JG	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	JQ	201	PEB	C2B-C1B-NB	2.31	115.47	110.53
29	JA	201	PEB	CBC-CAC-C2C	-2.31	108.67	112.62
29	JN	201	PEB	CBC-CAC-C2C	-2.31	108.67	112.62
29	H1	1002	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	F3	203	PEB	CAB-C3B-C4B	2.31	129.10	125.01
29	FO	203	PEB	CAB-C3B-C4B	2.31	129.10	125.01
29	FA	203	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	FN	203	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	QF	201	PEB	C2B-C1B-NB	2.31	115.46	110.53
29	QI	201	PEB	C2B-C1B-NB	2.31	115.46	110.53
29	N2	201	PEB	C1C-CHB-C4B	-2.31	126.05	128.81
31	J9	1001	CYC	CAD-C3D-C2D	-2.31	120.61	127.25
29	J1	1002	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	JK	1002	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	L4	201	PEB	CMD-C2D-C3D	2.31	133.32	130.06
31	C7	1001	CYC	OB-C4B-C3B	-2.31	125.53	128.04
31	C9	1001	CYC	OB-C4B-C3B	-2.31	125.53	128.04
29	IC	201	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	IE	201	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	cF	201	PEB	CHB-C4B-C3B	-2.31	119.98	125.32
29	cI	201	PEB	CHB-C4B-C3B	-2.31	119.98	125.32
29	VB	201	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
29	VM	201	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
31	FF	1001	CYC	CMB-C2B-C1B	2.31	127.05	124.17
31	FI	1001	CYC	CMB-C2B-C1B	2.31	127.05	124.17
29	lF	201	PEB	CMA-C2A-C1A	-2.31	107.42	112.40
29	II	201	PEB	CMA-C2A-C1A	-2.31	107.42	112.40
31	KI	1001	CYC	OB-C4B-NB	-2.31	119.71	125.08
29	B3	203	PEB	CAB-C3B-C4B	2.31	129.09	125.01
29	CD	202	PEB	CAB-C3B-C4B	2.31	129.09	125.01
29	BO	203	PEB	CAB-C3B-C4B	2.31	129.09	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	MQ	405	PUB	CHA-C1B-C2B	-2.31	126.40	130.34
29	KC	202	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	KE	202	PEB	CHA-C1B-NB	-2.31	120.10	124.93
29	P7	202	PEB	CAA-C3A-C4A	-2.31	106.75	112.67
29	P9	202	PEB	CAA-C3A-C4A	-2.31	106.75	112.67
29	HQ	203	PEB	CAC-CBC-CGC	-2.31	107.29	113.76
29	Y1	202	PEB	OD-C4D-C3D	-2.31	124.23	129.46
29	YK	202	PEB	OD-C4D-C3D	-2.31	124.23	129.46
29	e7	202	PEB	CAA-C3A-C4A	-2.31	106.75	112.67
29	e9	202	PEB	CAA-C3A-C4A	-2.31	106.75	112.67
29	J3	203	PEB	CAB-C3B-C4B	2.31	129.09	125.01
29	JO	203	PEB	CAB-C3B-C4B	2.31	129.09	125.01
31	HF	1001	CYC	CBD-CAD-C3D	2.31	116.56	112.62
31	HI	1001	CYC	CBD-CAD-C3D	2.31	116.56	112.62
29	MA	405	PEB	CHA-C4A-NA	2.31	127.95	125.20
29	N3	203	PEB	C1B-C2B-C3B	-2.31	103.86	106.51
29	C4	202	PEB	CAB-C3B-C4B	2.31	129.09	125.01
29	c7	202	PEB	CAA-C3A-C4A	-2.31	106.75	112.67
29	c9	202	PEB	CAA-C3A-C4A	-2.31	106.75	112.67
29	VF	201	PEB	CHB-C4B-C3B	-2.31	119.99	125.32
29	VI	201	PEB	CHB-C4B-C3B	-2.31	119.99	125.32
29	aF	201	PEB	CHB-C4B-C3B	-2.31	120.00	125.32
29	aI	201	PEB	CHB-C4B-C3B	-2.31	120.00	125.32
29	LQ	202	PEB	CAC-CBC-CGC	-2.30	107.30	113.76
29	ZF	201	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
29	ZI	201	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
29	XB	201	PEB	C1B-C2B-C3B	-2.30	103.86	106.51
29	XM	201	PEB	C1B-C2B-C3B	-2.30	103.86	106.51
29	kF	201	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
29	TI	201	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
29	kI	201	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
29	k7	202	PEB	CAA-C3A-C4A	-2.30	106.76	112.67
29	k9	202	PEB	CAA-C3A-C4A	-2.30	106.76	112.67
29	CG	202	PEB	C2A-C1A-NA	2.30	110.26	108.27
29	CQ	202	PEB	C2A-C1A-NA	2.30	110.26	108.27
29	C3	201	PEB	CBC-CAC-C2C	-2.30	108.69	112.62
29	CO	201	PEB	CBC-CAC-C2C	-2.30	108.69	112.62
29	YF	203	PEB	CHC-C1D-ND	-2.30	111.27	113.95
29	YI	203	PEB	CHC-C1D-ND	-2.30	111.27	113.95
29	QB	204	PEB	CMC-C3C-C2C	2.30	129.28	124.94
29	dB	202	PEB	CMC-C3C-C2C	2.30	129.28	124.94
29	QM	204	PEB	CMC-C3C-C2C	2.30	129.28	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	dM	202	PEB	CMC-C3C-C2C	2.30	129.28	124.94
31	LF	1001	CYC	CMB-C2B-C1B	2.30	127.04	124.17
31	LI	1001	CYC	CMB-C2B-C1B	2.30	127.04	124.17
29	ED	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
29	D4	201	PEB	CMD-C2D-C3D	2.30	133.31	130.06
30	A7	303	PUB	CBC-CAC-C2C	-2.30	106.23	112.63
30	A9	303	PUB	CBC-CAC-C2C	-2.30	106.23	112.63
31	IF	1001	CYC	OB-C4B-NB	-2.30	119.73	125.08
31	II	1001	CYC	OB-C4B-NB	-2.30	119.73	125.08
29	HK	1002	PEB	CHA-C1B-NB	-2.30	120.12	124.93
29	eF	201	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
29	eI	201	PEB	CHB-C4B-C3B	-2.30	120.00	125.32
29	LA	201	PEB	CBC-CAC-C2C	-2.30	108.69	112.62
29	LN	201	PEB	CBC-CAC-C2C	-2.30	108.69	112.62
29	G4	202	PEB	C2B-C1B-NB	2.30	115.44	110.53
29	DK	1002	PEB	CHA-C1B-NB	-2.30	120.12	124.93
30	yJ	303	PUB	C2C-C1C-NC	2.30	113.40	110.05
31	M7	1001	CYC	CAA-CBA-CGA	-2.30	108.65	113.60
29	jF	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
29	BG	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
29	jI	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
29	BQ	201	PEB	C2B-C1B-NB	2.30	115.44	110.53
29	R1	203	PEB	OD-C4D-C3D	-2.30	124.25	129.46
29	RK	203	PEB	OD-C4D-C3D	-2.30	124.25	129.46
29	dF	202	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
29	dI	202	PEB	CMA-C2A-C1A	-2.30	107.44	112.40
29	lB	202	PEB	CMC-C3C-C2C	2.30	129.28	124.94
29	lM	202	PEB	CMC-C3C-C2C	2.30	129.28	124.94
29	e7	203	PEB	CAC-CBC-CGC	-2.30	107.31	113.76
29	e9	203	PEB	CAC-CBC-CGC	-2.30	107.31	113.76
29	WB	202	PEB	CMC-C3C-C2C	2.30	129.28	124.94
29	WM	202	PEB	CMC-C3C-C2C	2.30	129.28	124.94
30	yJ	302	PUB	CAD-C3D-C4D	2.30	125.01	121.38
30	yL	302	PUB	CAD-C3D-C4D	2.30	125.01	121.38
29	i7	202	PEB	CAA-C3A-C4A	-2.30	106.77	112.67
29	i9	202	PEB	CAA-C3A-C4A	-2.30	106.77	112.67
29	LD	201	PEB	CMD-C2D-C3D	2.30	133.31	130.06
29	F1	1002	PEB	CHA-C1B-NB	-2.30	120.12	124.93
29	FK	1002	PEB	CHA-C1B-NB	-2.30	120.12	124.93
29	CC	201	PEB	CHA-C1B-NB	-2.30	120.12	124.93
29	CE	201	PEB	CHA-C1B-NB	-2.30	120.12	124.93
29	P7	203	PEB	CAC-CBC-CGC	-2.30	107.31	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P9	203	PEB	CAC-CBC-CGC	-2.30	107.31	113.76
29	lB	202	PEB	CBC-CAC-C2C	-2.30	108.70	112.62
29	lM	202	PEB	CBC-CAC-C2C	-2.30	108.70	112.62
31	G7	1001	CYC	CAA-CBA-CGA	-2.30	108.66	113.60
29	DG	202	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
29	DQ	202	PEB	C4B-C3B-C2B	-2.30	104.24	106.78
29	TF	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	cF	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	TI	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	cI	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	m7	202	PEB	CAA-C3A-C4A	-2.30	106.77	112.67
29	m9	202	PEB	CAA-C3A-C4A	-2.30	106.77	112.67
29	Y7	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
29	Y9	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
29	JQ	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
29	DQ	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
29	DG	201	PEB	C2B-C1B-NB	2.30	115.43	110.53
29	DQ	201	PEB	C2B-C1B-NB	2.30	115.43	110.53
29	bF	201	PEB	CMA-C2A-C1A	-2.30	107.45	112.40
29	bI	201	PEB	CMA-C2A-C1A	-2.30	107.45	112.40
29	JA	203	PEB	CHA-C1B-NB	-2.30	120.13	124.93
29	JN	203	PEB	CHA-C1B-NB	-2.30	120.13	124.93
29	LG	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
29	gF	201	PEB	CHB-C4B-C3B	-2.30	120.01	125.32
29	gI	201	PEB	CHB-C4B-C3B	-2.30	120.01	125.32
31	L9	1001	CYC	O2A-CGA-O1A	-2.30	117.57	123.30
30	wL	304	PUB	C1D-CHC-C4C	-2.30	108.37	113.37
29	AM	303	PEB	OD-C4D-ND	-2.30	122.53	125.93
29	HB	201	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
29	HM	201	PEB	C1B-C2B-C3B	-2.30	103.87	106.51
31	G9	1001	CYC	CAA-CBA-CGA	-2.30	108.66	113.60
29	OF	201	PEB	C2B-C1B-NB	2.30	115.43	110.53
29	OI	201	PEB	C2B-C1B-NB	2.30	115.43	110.53
29	BA	203	PEB	CHA-C1B-NB	-2.30	120.13	124.93
29	BN	203	PEB	CHA-C1B-NB	-2.30	120.13	124.93
29	a7	202	PEB	CAA-C3A-C4A	-2.30	106.78	112.67
29	a9	202	PEB	CAA-C3A-C4A	-2.30	106.78	112.67
31	WP	1001	CYC	CAA-C2A-C1A	2.30	129.07	125.01
29	V7	202	PEB	CAA-C3A-C4A	-2.30	106.78	112.67
29	V9	202	PEB	CAA-C3A-C4A	-2.30	106.78	112.67
29	c7	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76
29	c9	203	PEB	CAC-CBC-CGC	-2.30	107.32	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	YF	201	PEB	CHB-C4B-C3B	-2.30	120.02	125.32
29	YI	201	PEB	CHB-C4B-C3B	-2.30	120.02	125.32
29	VF	203	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	VI	203	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	ZF	201	PEB	C2B-C1B-NB	2.29	115.43	110.53
29	ZI	201	PEB	C2B-C1B-NB	2.29	115.43	110.53
29	Y7	202	PEB	CAA-C3A-C4A	-2.29	106.78	112.67
29	Y9	202	PEB	CAA-C3A-C4A	-2.29	106.78	112.67
29	T1	202	PEB	OD-C4D-C3D	-2.29	124.26	129.46
29	TK	202	PEB	OD-C4D-C3D	-2.29	124.26	129.46
29	RB	201	PEB	C1B-C2B-C3B	-2.29	103.87	106.51
29	RM	201	PEB	C1B-C2B-C3B	-2.29	103.87	106.51
29	a7	203	PEB	CAC-CBC-CGC	-2.29	107.33	113.76
29	a9	203	PEB	CAC-CBC-CGC	-2.29	107.33	113.76
29	R7	202	PEB	CAA-C3A-C4A	-2.29	106.78	112.67
29	R9	202	PEB	CAA-C3A-C4A	-2.29	106.78	112.67
29	HG	201	PEB	C2B-C1B-NB	2.29	115.43	110.53
29	HQ	201	PEB	C2B-C1B-NB	2.29	115.43	110.53
30	wJ	304	PUB	C1D-CHC-C4C	-2.29	108.38	113.37
29	V1	203	PEB	OD-C4D-C3D	-2.29	124.26	129.46
29	VK	203	PEB	OD-C4D-C3D	-2.29	124.26	129.46
29	I3	201	PEB	CBC-CAC-C2C	-2.29	108.70	112.62
29	IO	201	PEB	CBC-CAC-C2C	-2.29	108.70	112.62
29	BQ	203	PEB	CAC-CBC-CGC	-2.29	107.33	113.76
29	i7	203	PEB	CAC-CBC-CGC	-2.29	107.33	113.76
29	i9	203	PEB	CAC-CBC-CGC	-2.29	107.33	113.76
29	MR	202	PEB	CMB-C2B-C1B	2.29	128.60	125.06
31	H1	1001	CYC	CBC-CAC-C3C	-2.29	108.36	113.47
29	ID	202	PEB	C2B-C1B-NB	2.29	115.42	110.53
29	MA	404	PEB	CHA-C1B-C2B	2.29	130.79	124.90
29	LA	203	PEB	CHA-C1B-NB	-2.29	120.14	124.93
29	LN	203	PEB	CHA-C1B-NB	-2.29	120.14	124.93
29	FG	202	PEB	C4B-C3B-C2B	-2.29	104.25	106.78
29	FQ	202	PEB	C4B-C3B-C2B	-2.29	104.25	106.78
31	MF	1001	CYC	OB-C4B-NB	-2.29	119.75	125.08
31	MI	1001	CYC	OB-C4B-NB	-2.29	119.75	125.08
29	NK	1002	PEB	CHA-C1B-NB	-2.29	120.14	124.93
31	K9	1001	CYC	CAA-CBA-CGA	-2.29	108.67	113.60
29	eF	203	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	eI	203	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	e1	203	PEB	OD-C4D-C3D	-2.29	124.27	129.46
29	eK	203	PEB	OD-C4D-C3D	-2.29	124.27	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I4	202	PEB	C2B-C1B-NB	2.29	115.42	110.53
31	VP	1001	CYC	CAC-C3C-C2C	-2.29	108.54	114.26
29	DB	201	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
29	DM	201	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
29	k7	203	PEB	CAC-CBC-CGC	-2.29	107.34	113.76
29	k9	203	PEB	CAC-CBC-CGC	-2.29	107.34	113.76
29	PF	201	PEB	CHB-C4B-C3B	-2.29	120.03	125.32
29	PI	201	PEB	CHB-C4B-C3B	-2.29	120.03	125.32
30	A1	305	PUB	C1D-CHC-C4C	-2.29	108.39	113.37
30	AK	305	PUB	C1D-CHC-C4C	-2.29	108.39	113.37
29	lF	201	PEB	C2B-C1B-NB	2.29	115.42	110.53
29	lI	201	PEB	C2B-C1B-NB	2.29	115.42	110.53
29	DO	202	PEB	CMB-C2B-C1B	2.29	128.59	125.06
29	zL	501	PEB	OD-C4D-ND	-2.29	122.54	125.93
29	GD	202	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	FG	201	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	FQ	201	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	FD	201	PEB	CMD-C2D-C3D	2.29	133.29	130.06
31	xP	1001	CYC	CAC-C3C-C2C	-2.29	108.54	114.26
29	UF	202	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	UI	202	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	iF	201	PEB	CHB-C4B-C3B	-2.29	120.03	125.32
29	iI	201	PEB	CHB-C4B-C3B	-2.29	120.03	125.32
29	SF	201	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
29	SI	201	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
29	KG	202	PEB	C2A-C1A-NA	2.29	110.25	108.27
29	KQ	202	PEB	C2A-C1A-NA	2.29	110.25	108.27
29	k1	201	PEB	CAB-CBB-CGB	-2.29	108.68	113.60
29	kK	201	PEB	CAB-CBB-CGB	-2.29	108.68	113.60
31	HK	1001	CYC	CBC-CAC-C3C	-2.29	108.38	113.47
29	P7	202	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
29	m7	202	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
29	P9	202	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
29	m9	202	PEB	C1B-C2B-C3B	-2.29	103.88	106.51
29	JG	203	PEB	CAC-CBC-CGC	-2.29	107.35	113.76
29	jF	201	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
29	jI	201	PEB	CMA-C2A-C1A	-2.29	107.47	112.40
29	LG	201	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	MQ	402	PEB	C2B-C1B-NB	2.29	115.41	110.53
29	WJ	203	PEB	OD-C4D-C3D	-2.29	124.28	129.46
29	WL	203	PEB	OD-C4D-C3D	-2.29	124.28	129.46
29	kF	203	PEB	CHC-C1D-ND	-2.29	111.29	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	kI	203	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	D1	1002	PEB	CHA-C1B-NB	-2.29	120.15	124.93
31	F1	1001	CYC	CBC-CAC-C3C	-2.29	108.38	113.47
31	FK	1001	CYC	CBC-CAC-C3C	-2.29	108.38	113.47
29	RF	201	PEB	CHB-C4B-C3B	-2.29	120.04	125.32
29	RI	201	PEB	CHB-C4B-C3B	-2.29	120.04	125.32
29	hF	201	PEB	CMA-C2A-C1A	-2.29	107.48	112.40
29	hI	201	PEB	CMA-C2A-C1A	-2.29	107.48	112.40
31	H7	1001	CYC	O2A-CGA-O1A	-2.29	117.60	123.30
31	H9	1001	CYC	O2A-CGA-O1A	-2.29	117.60	123.30
29	RF	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	aF	203	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	RI	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	aI	203	PEB	CHC-C1D-ND	-2.29	111.29	113.95
29	SB	202	PEB	CBC-CAC-C2C	-2.29	108.72	112.62
29	SM	202	PEB	CBC-CAC-C2C	-2.29	108.72	112.62
29	P1	203	PEB	OD-C4D-C3D	-2.29	124.28	129.46
29	PK	203	PEB	OD-C4D-C3D	-2.29	124.28	129.46
29	O1	201	PEB	CHA-C4A-NA	2.29	127.92	125.20
29	OK	201	PEB	CHA-C4A-NA	2.29	127.92	125.20
29	MN	405	PEB	CHA-C4A-NA	2.29	127.92	125.20
29	g7	203	PEB	CAC-CBC-CGC	-2.29	107.35	113.76
29	g9	203	PEB	CAC-CBC-CGC	-2.29	107.35	113.76
29	V2	203	PEB	CHA-C1B-NB	-2.28	120.15	124.93
29	HA	203	PEB	CHA-C1B-NB	-2.28	120.15	124.93
29	HN	203	PEB	CHA-C1B-NB	-2.28	120.15	124.93
31	L7	1001	CYC	O2A-CGA-O1A	-2.28	117.61	123.30
29	cF	202	PEB	CMC-C3C-C2C	2.28	129.25	124.94
29	cI	202	PEB	CMC-C3C-C2C	2.28	129.25	124.94
30	xJ	304	PUB	C1D-CHC-C4C	-2.28	108.40	113.37
29	A7	305	PEB	CHA-C4A-NA	-2.28	122.49	125.20
29	A9	305	PEB	CHA-C4A-NA	-2.28	122.49	125.20
29	T7	203	PEB	CAC-CBC-CGC	-2.28	107.36	113.76
29	T9	203	PEB	CAC-CBC-CGC	-2.28	107.36	113.76
29	e1	201	PEB	CAB-CBB-CGB	-2.28	108.69	113.60
29	eK	201	PEB	CAB-CBB-CGB	-2.28	108.69	113.60
29	kF	203	PEB	CMC-C3C-C2C	2.28	129.25	124.94
29	kI	203	PEB	CMC-C3C-C2C	2.28	129.25	124.94
29	F4	201	PEB	CMD-C2D-C3D	2.28	133.28	130.06
29	Y1	201	PEB	CAB-CBB-CGB	-2.28	108.69	113.60
29	YK	201	PEB	CAB-CBB-CGB	-2.28	108.69	113.60
29	WF	201	PEB	CMA-C2A-C1A	-2.28	107.48	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WI	201	PEB	CMA-C2A-C1A	-2.28	107.48	112.40
31	IP	1001	CYC	C2C-C1C-NC	2.28	110.24	108.27
29	V7	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	V9	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	mF	201	PEB	CHB-C4B-C3B	-2.28	120.05	125.32
29	mI	201	PEB	CHB-C4B-C3B	-2.28	120.05	125.32
31	M9	1001	CYC	CAA-CBA-CGA	-2.28	108.69	113.60
29	R7	203	PEB	CAC-CBC-CGC	-2.28	107.36	113.76
29	R9	203	PEB	CAC-CBC-CGC	-2.28	107.36	113.76
31	FF	1001	CYC	CBD-CAD-C3D	2.28	116.52	112.62
31	FI	1001	CYC	CBD-CAD-C3D	2.28	116.52	112.62
30	AB	305	PUB	C2C-C1C-NC	2.28	113.37	110.05
29	i1	203	PEB	OD-C4D-C3D	-2.28	124.29	129.46
29	iK	203	PEB	OD-C4D-C3D	-2.28	124.29	129.46
29	V1	202	PEB	CAB-C3B-C4B	2.28	129.04	125.01
29	VK	202	PEB	CAB-C3B-C4B	2.28	129.04	125.01
29	M3	203	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	MO	203	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	D3	202	PEB	CMB-C2B-C1B	2.28	128.58	125.06
29	m1	202	PEB	OD-C4D-C3D	-2.28	124.29	129.46
29	mK	202	PEB	OD-C4D-C3D	-2.28	124.29	129.46
29	FG	203	PEB	CAC-CBC-CGC	-2.28	107.36	113.76
29	H3	201	PEB	CAB-C3B-C4B	2.28	129.04	125.01
29	HO	201	PEB	CAB-C3B-C4B	2.28	129.04	125.01
29	J4	201	PEB	CMD-C2D-C3D	2.28	133.28	130.06
31	F9	1001	CYC	O2A-CGA-O1A	-2.28	117.62	123.30
29	JG	202	PEB	C4B-C3B-C2B	-2.28	104.26	106.78
29	JQ	202	PEB	C4B-C3B-C2B	-2.28	104.26	106.78
30	AB	305	PUB	C1D-CHC-C4C	-2.28	108.41	113.37
29	V7	203	PEB	CAC-CBC-CGC	-2.28	107.37	113.76
29	V9	203	PEB	CAC-CBC-CGC	-2.28	107.37	113.76
30	yL	303	PUB	C2C-C1C-NC	2.28	113.36	110.05
29	DG	202	PEB	CHB-C4B-C3B	-2.28	120.06	125.32
29	DQ	202	PEB	CHB-C4B-C3B	-2.28	120.06	125.32
29	g7	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	g9	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	ff	201	PEB	CMA-C2A-C1A	-2.28	107.49	112.40
29	fl	201	PEB	CMA-C2A-C1A	-2.28	107.49	112.40
31	D7	1001	CYC	O2A-CGA-O1A	-2.28	117.62	123.30
31	D9	1001	CYC	O2A-CGA-O1A	-2.28	117.62	123.30
31	J1	1001	CYC	CBC-CAC-C3C	-2.28	108.39	113.47
31	JK	1001	CYC	CBC-CAC-C3C	-2.28	108.39	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	K7	1001	CYC	CAA-CBA-CGA	-2.28	108.70	113.60
29	FQ	203	PEB	CAC-CBC-CGC	-2.28	107.37	113.76
29	mF	203	PEB	CMC-C3C-C2C	2.28	129.24	124.94
29	mI	203	PEB	CMC-C3C-C2C	2.28	129.24	124.94
29	T7	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	T9	202	PEB	C1B-C2B-C3B	-2.28	103.89	106.51
29	M2	202	PEB	CMB-C2B-C1B	2.28	128.57	125.06
29	EJ	202	PEB	OD-C4D-C3D	-2.28	124.30	129.46
29	EL	202	PEB	OD-C4D-C3D	-2.28	124.30	129.46
30	MG	403	PUB	CHA-C1B-C2B	-2.28	126.45	130.34
29	A1	301	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	AK	301	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	OF	201	PEB	CMA-C2A-C1A	-2.28	107.50	112.40
29	OI	201	PEB	CMA-C2A-C1A	-2.28	107.50	112.40
29	DD	201	PEB	CMD-C2D-C3D	2.28	133.28	130.06
29	BG	203	PEB	CAC-CBC-CGC	-2.28	107.38	113.76
29	FG	202	PEB	CHB-C4B-C3B	-2.28	120.06	125.32
29	FQ	202	PEB	CHB-C4B-C3B	-2.28	120.06	125.32
29	mF	203	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	mI	203	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	c1	201	PEB	CAB-CBB-CGB	-2.28	108.70	113.60
29	cK	201	PEB	CAB-CBB-CGB	-2.28	108.70	113.60
31	qP	1001	CYC	C2C-C1C-NC	2.28	110.23	108.27
29	JG	201	PEB	CAB-CBB-CGB	-2.28	108.71	113.60
29	JQ	201	PEB	CAB-CBB-CGB	-2.28	108.71	113.60
29	a1	203	PEB	OD-C4D-C3D	-2.28	124.31	129.46
29	aK	203	PEB	OD-C4D-C3D	-2.28	124.31	129.46
29	m7	203	PEB	CAC-CBC-CGC	-2.28	107.38	113.76
29	m9	203	PEB	CAC-CBC-CGC	-2.28	107.38	113.76
31	E7	1001	CYC	CAA-CBA-CGA	-2.28	108.71	113.60
31	E9	1001	CYC	CAA-CBA-CGA	-2.28	108.71	113.60
29	UF	202	PEB	CMA-C2A-C1A	-2.28	107.50	112.40
29	UI	202	PEB	CMA-C2A-C1A	-2.28	107.50	112.40
29	gF	201	PEB	CAB-C3B-C2B	-2.27	123.64	127.88
29	gI	201	PEB	CAB-C3B-C2B	-2.27	123.64	127.88
29	P1	201	PEB	CAB-CBB-CGB	-2.27	108.71	113.60
29	PK	201	PEB	CAB-CBB-CGB	-2.27	108.71	113.60
31	C7	1001	CYC	CAA-CBA-CGA	-2.27	108.71	113.60
31	C9	1001	CYC	CAA-CBA-CGA	-2.27	108.71	113.60
29	C8	203	PEB	CAC-CBC-CGC	-2.27	107.38	113.76
29	F3	201	PEB	CAB-C3B-C4B	2.27	129.03	125.01
29	FO	201	PEB	CAB-C3B-C4B	2.27	129.03	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	zJ	501	PEB	OD-C4D-ND	-2.27	122.56	125.93
29	QF	201	PEB	CMA-C2A-C1A	-2.27	107.50	112.40
29	QI	201	PEB	CMA-C2A-C1A	-2.27	107.50	112.40
31	N1	1001	CYC	CBC-CAC-C3C	-2.27	108.41	113.47
29	G3	201	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
29	GO	201	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
29	N3	203	PEB	CHB-C4B-C3B	-2.27	120.07	125.32
29	QB	204	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
29	jB	202	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
29	QM	204	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
29	jM	202	PEB	CBC-CAC-C2C	-2.27	108.74	112.62
30	AM	305	PUB	C2C-C1C-NC	2.27	113.35	110.05
29	LD	202	PEB	CMA-C2A-C1A	-2.27	107.51	112.40
29	LG	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
29	MQ	402	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
29	I3	203	PEB	CHA-C1B-NB	-2.27	120.18	124.93
29	IO	203	PEB	CHA-C1B-NB	-2.27	120.18	124.93
29	i1	202	PEB	CAB-C3B-C4B	2.27	129.03	125.01
29	iK	202	PEB	CAB-C3B-C4B	2.27	129.03	125.01
31	WP	1001	CYC	C1B-NB-C4B	-2.27	107.78	110.67
29	KJ	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
29	eJ	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
29	KL	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
29	eL	202	PEB	OD-C4D-C3D	-2.27	124.31	129.46
29	N1	1002	PEB	CHA-C1B-NB	-2.27	120.18	124.93
29	A3	201	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	AO	201	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	oJ	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
29	oL	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
29	MG	404	PEB	CAC-CBC-CGC	-2.27	107.39	113.76
29	MQ	406	PEB	CAC-CBC-CGC	-2.27	107.39	113.76
29	J3	201	PEB	CAB-C3B-C4B	2.27	129.02	125.01
29	JO	201	PEB	CAB-C3B-C4B	2.27	129.02	125.01
31	L1	1001	CYC	CBC-CAC-C3C	-2.27	108.41	113.47
31	LK	1001	CYC	CBC-CAC-C3C	-2.27	108.41	113.47
29	HC	202	PEB	OD-C4D-ND	-2.27	122.57	125.93
29	HE	202	PEB	OD-C4D-ND	-2.27	122.57	125.93
29	c7	202	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
29	c9	202	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
29	fB	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	fM	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
31	NK	1001	CYC	CBC-CAC-C3C	-2.27	108.41	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L4	202	PEB	CMA-C2A-C1A	-2.27	107.51	112.40
29	l1	201	PEB	CBB-CAB-C3B	-2.27	106.32	112.63
29	lK	201	PEB	CBB-CAB-C3B	-2.27	106.32	112.63
30	MA	402	PUB	CMA-C2A-C3A	2.27	134.33	129.67
29	aJ	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
29	aL	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
31	J9	1001	CYC	O2A-CGA-O1A	-2.27	117.64	123.30
29	Y7	202	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
29	Y9	202	PEB	C1B-C2B-C3B	-2.27	103.90	106.51
29	HG	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
29	HQ	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
29	C5	203	PEB	CAC-CBC-CGC	-2.27	107.40	113.76
29	M3	203	PEB	CHB-C4B-C3B	-2.27	120.08	125.32
29	MO	203	PEB	CHB-C4B-C3B	-2.27	120.08	125.32
29	NF	1002	PEB	OD-C4D-ND	-2.27	122.57	125.93
29	NI	1002	PEB	OD-C4D-ND	-2.27	122.57	125.93
29	BG	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
29	BQ	201	PEB	CAB-CBB-CGB	-2.27	108.72	113.60
29	W1	201	PEB	CBB-CAB-C3B	-2.27	106.33	112.63
29	WK	201	PEB	CBB-CAB-C3B	-2.27	106.33	112.63
29	JD	201	PEB	CMD-C2D-C3D	2.27	133.26	130.06
31	DK	1001	CYC	CBC-CAC-C3C	-2.27	108.42	113.47
29	IB	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	IM	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	I5	203	PEB	CAC-CBC-CGC	-2.27	107.40	113.76
29	I8	203	PEB	CAC-CBC-CGC	-2.27	107.40	113.76
29	OJ	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
29	OL	202	PEB	OD-C4D-C3D	-2.27	124.32	129.46
29	R7	202	PEB	C1B-C2B-C3B	-2.27	103.91	106.51
29	R9	202	PEB	C1B-C2B-C3B	-2.27	103.91	106.51
31	GF	1001	CYC	OB-C4B-NB	-2.27	119.81	125.08
31	GI	1001	CYC	OB-C4B-NB	-2.27	119.81	125.08
31	kP	1001	CYC	C2C-C1C-NC	2.27	110.23	108.27
29	YB	203	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	YM	203	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	J3	202	PEB	CHA-C1B-NB	-2.27	120.19	124.93
29	JO	202	PEB	CHA-C1B-NB	-2.27	120.19	124.93
29	K8	203	PEB	CAC-CBC-CGC	-2.27	107.41	113.76
29	wJ	301	PEB	OD-C4D-ND	-2.27	122.57	125.93
29	AJ	202	PEB	OD-C4D-C3D	-2.27	124.33	129.46
29	AL	202	PEB	OD-C4D-C3D	-2.27	124.33	129.46
29	LG	202	PEB	C4B-C3B-C2B	-2.27	104.28	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LQ	201	PEB	C4B-C3B-C2B	-2.27	104.28	106.78
31	F7	1001	CYC	O2A-CGA-O1A	-2.27	117.65	123.30
29	aB	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	aM	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	WB	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	WM	202	PEB	CBC-CAC-C2C	-2.27	108.75	112.62
29	W2	202	PEB	CMB-C2B-C1B	2.26	128.55	125.06
29	MJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	ML	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	J4	202	PEB	CMA-C2A-C1A	-2.26	107.52	112.40
29	a1	202	PEB	CAB-C3B-C4B	2.26	129.01	125.01
29	B3	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
29	aK	202	PEB	CAB-C3B-C4B	2.26	129.01	125.01
29	BO	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
29	iF	203	PEB	CHC-C1D-ND	-2.26	111.32	113.95
29	iI	203	PEB	CHC-C1D-ND	-2.26	111.32	113.95
29	IJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	IL	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	GJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	GL	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	g1	201	PEB	CAB-CBB-CGB	-2.26	108.73	113.60
29	gK	201	PEB	CAB-CBB-CGB	-2.26	108.73	113.60
29	W7	201	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
29	W9	201	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
31	N7	1001	CYC	O2A-CGA-O1A	-2.26	117.66	123.30
31	N9	1001	CYC	O2A-CGA-O1A	-2.26	117.66	123.30
29	BG	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
29	JG	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
29	BQ	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
29	JQ	202	PEB	CHB-C4B-C3B	-2.26	120.09	125.32
29	UJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	UL	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	VF	203	PEB	CMC-C3C-C2C	2.26	129.21	124.94
29	VI	203	PEB	CMC-C3C-C2C	2.26	129.21	124.94
29	SJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	SL	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	K3	201	PEB	CBC-CAC-C2C	-2.26	108.76	112.62
29	KO	201	PEB	CBC-CAC-C2C	-2.26	108.76	112.62
31	JF	1001	CYC	CBD-CAD-C3D	2.26	116.48	112.62
31	JI	1001	CYC	CBD-CAD-C3D	2.26	116.48	112.62
29	gJ	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46
29	gL	202	PEB	OD-C4D-C3D	-2.26	124.33	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KB	202	PEB	CBC-CAC-C2C	-2.26	108.76	112.62
29	KM	202	PEB	CBC-CAC-C2C	-2.26	108.76	112.62
29	sJ	203	PEB	C2B-C1B-NB	2.26	115.36	110.53
29	sL	203	PEB	C2B-C1B-NB	2.26	115.36	110.53
29	j1	201	PEB	CBB-CAB-C3B	-2.26	106.34	112.63
29	jK	201	PEB	CBB-CAB-C3B	-2.26	106.34	112.63
29	qJ	202	PEB	OD-C4D-C3D	-2.26	124.34	129.46
29	qL	202	PEB	OD-C4D-C3D	-2.26	124.34	129.46
29	FD	202	PEB	CMA-C2A-C1A	-2.26	107.53	112.40
29	e7	202	PEB	C1B-C2B-C3B	-2.26	103.91	106.51
29	e9	202	PEB	C1B-C2B-C3B	-2.26	103.91	106.51
29	FC	202	PEB	OD-C4D-ND	-2.26	122.58	125.93
29	FE	202	PEB	OD-C4D-ND	-2.26	122.58	125.93
31	FP	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
29	UB	202	PEB	CBC-CAC-C2C	-2.26	108.76	112.62
29	MQ	401	PEB	CBC-CAC-C2C	-2.26	108.76	112.62
29	R1	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
29	RK	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
29	U7	201	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
29	U9	201	PEB	C4B-C3B-C2B	-2.26	104.28	106.78
30	MN	402	PUB	CMA-C2A-C3A	2.26	134.32	129.67
29	U1	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
29	UK	201	PEB	CAB-C3B-C4B	2.26	129.01	125.01
29	A1	302	PEB	C1C-CHB-C4B	-2.26	126.11	128.81
29	AK	302	PEB	C1C-CHB-C4B	-2.26	126.11	128.81
29	NO	203	PEB	CHB-C4B-C3B	-2.26	120.10	125.32
29	a7	202	PEB	C1B-C2B-C3B	-2.26	103.91	106.51
29	a9	202	PEB	C1B-C2B-C3B	-2.26	103.91	106.51
29	PF	201	PEB	CAB-C3B-C2B	-2.26	123.67	127.88
29	PI	201	PEB	CAB-C3B-C2B	-2.26	123.67	127.88
29	Q1	201	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
29	QK	201	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
31	nP	1001	CYC	C2C-C1C-NC	2.26	110.22	108.27
31	J7	1001	CYC	O2A-CGA-O1A	-2.26	117.67	123.30
29	Z1	202	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
29	ZK	202	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
29	TF	202	PEB	CMC-C3C-C2C	2.26	129.20	124.94
29	TI	202	PEB	CMC-C3C-C2C	2.26	129.20	124.94
31	I7	1001	CYC	CAA-CBA-CGA	-2.26	108.74	113.60
31	I9	1001	CYC	CAA-CBA-CGA	-2.26	108.74	113.60
29	eF	203	PEB	CMC-C3C-C2C	2.26	129.20	124.94
29	eI	203	PEB	CMC-C3C-C2C	2.26	129.20	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CG	202	PEB	C2A-C3A-C4A	-2.26	97.96	101.34
29	CQ	202	PEB	C2A-C3A-C4A	-2.26	97.96	101.34
29	i1	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
29	m1	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
29	iK	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
29	mK	201	PEB	CAB-CBB-CGB	-2.26	108.74	113.60
29	B3	202	PEB	CHA-C1B-NB	-2.26	120.21	124.93
29	BO	202	PEB	CHA-C1B-NB	-2.26	120.21	124.93
29	KG	202	PEB	C2A-C3A-C4A	-2.26	97.96	101.34
29	KQ	202	PEB	C2A-C3A-C4A	-2.26	97.96	101.34
29	d1	201	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
29	dK	201	PEB	CBB-CAB-C3B	-2.26	106.35	112.63
29	HD	201	PEB	CMD-C2D-C3D	2.26	133.25	130.06
30	AM	305	PUB	C1D-CHC-C4C	-2.26	108.45	113.37
29	MG	404	PEB	C2A-C1A-NA	2.26	110.22	108.27
29	dB	202	PEB	CBC-CAC-C2C	-2.26	108.77	112.62
29	dM	202	PEB	CBC-CAC-C2C	-2.26	108.77	112.62
29	NR	203	PEB	CMB-C2B-C1B	2.26	128.54	125.06
29	gF	203	PEB	CHC-C1D-ND	-2.26	111.33	113.95
29	gI	203	PEB	CHC-C1D-ND	-2.26	111.33	113.95
29	FG	201	PEB	CAB-CBB-CGB	-2.26	108.75	113.60
29	FQ	201	PEB	CAB-CBB-CGB	-2.26	108.75	113.60
29	uJ	203	PEB	OD-C4D-C3D	-2.26	124.35	129.46
29	uL	203	PEB	OD-C4D-C3D	-2.26	124.35	129.46
29	YF	203	PEB	CMC-C3C-C2C	2.26	129.20	124.94
29	YI	203	PEB	CMC-C3C-C2C	2.26	129.20	124.94
31	LF	1001	CYC	CBD-CAD-C3D	2.26	116.47	112.62
31	LI	1001	CYC	CBD-CAD-C3D	2.26	116.47	112.62
29	YJ	202	PEB	OD-C4D-C3D	-2.26	124.35	129.46
29	YL	202	PEB	OD-C4D-C3D	-2.26	124.35	129.46
29	G4	203	PEB	CAC-CBC-CGC	-2.26	107.43	113.76
29	C4	203	PEB	CAC-CBC-CGC	-2.26	107.43	113.76
31	D1	1001	CYC	CBC-CAC-C3C	-2.26	108.44	113.47
29	GG	202	PEB	C2A-C3A-C4A	-2.26	97.96	101.34
29	GQ	202	PEB	C2A-C3A-C4A	-2.26	97.96	101.34
29	JD	202	PEB	CMA-C2A-C1A	-2.26	107.54	112.40
29	K5	203	PEB	CAC-CBC-CGC	-2.26	107.44	113.76
29	O1	201	PEB	CBB-CAB-C3B	-2.25	106.36	112.63
29	OK	201	PEB	CBB-CAB-C3B	-2.25	106.36	112.63
29	OB	202	PEB	CBC-CAC-C2C	-2.25	108.77	112.62
29	OM	202	PEB	CBC-CAC-C2C	-2.25	108.77	112.62
29	Z1	202	PEB	CHA-C4A-NA	2.25	127.89	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZK	202	PEB	CHA-C4A-NA	2.25	127.89	125.20
29	JF	1002	PEB	OD-C4D-ND	-2.25	122.59	125.93
29	JI	1002	PEB	OD-C4D-ND	-2.25	122.59	125.93
29	wJ	303	PEB	C2B-C1B-NB	2.25	115.34	110.53
31	yP	1001	CYC	C2B-C1B-NB	2.25	110.29	106.99
31	KF	1001	CYC	CHB-C1B-NB	-2.25	121.22	126.06
29	BG	202	PEB	C4B-C3B-C2B	-2.25	104.29	106.78
29	BQ	202	PEB	C4B-C3B-C2B	-2.25	104.29	106.78
29	cJ	202	PEB	OD-C4D-C3D	-2.25	124.35	129.46
29	cL	202	PEB	OD-C4D-C3D	-2.25	124.35	129.46
29	AG	201	PEB	C2B-C1B-NB	2.25	115.34	110.53
29	bJ	202	PEB	C2B-C1B-NB	2.25	115.34	110.53
29	bL	202	PEB	C2B-C1B-NB	2.25	115.34	110.53
29	AQ	201	PEB	C2B-C1B-NB	2.25	115.34	110.53
29	B4	201	PEB	CMD-C2D-C3D	2.25	133.24	130.06
29	i7	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
29	i9	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
31	XP	1001	CYC	C2C-C1C-NC	2.25	110.22	108.27
29	B5	201	PEB	CHC-C1D-ND	-2.25	111.33	113.95
29	E3	201	PEB	CBC-CAC-C2C	-2.25	108.77	112.62
29	EO	201	PEB	CBC-CAC-C2C	-2.25	108.77	112.62
31	DF	1001	CYC	CBD-CAD-C3D	2.25	116.47	112.62
31	DI	1001	CYC	CBD-CAD-C3D	2.25	116.47	112.62
29	D4	202	PEB	CMA-C2A-C1A	-2.25	107.55	112.40
29	RF	202	PEB	CMC-C3C-C2C	2.25	129.19	124.94
29	RI	202	PEB	CMC-C3C-C2C	2.25	129.19	124.94
29	TI	201	PEB	CAB-C3B-C2B	-2.25	123.68	127.88
30	MQ	405	PUB	CBC-CAC-C2C	2.25	118.89	112.63
29	W1	201	PEB	CHA-C4A-NA	2.25	127.88	125.20
29	WK	201	PEB	CHA-C4A-NA	2.25	127.88	125.20
29	EB	202	PEB	CBC-CAC-C2C	-2.25	108.78	112.62
29	EM	202	PEB	CBC-CAC-C2C	-2.25	108.78	112.62
30	A7	302	PUB	CAC-C2C-C1C	2.25	128.99	125.01
30	A9	302	PUB	CAC-C2C-C1C	2.25	128.99	125.01
31	UP	1001	CYC	C2C-C1C-NC	2.25	110.22	108.27
29	kJ	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
29	kL	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
29	aF	201	PEB	CAB-C3B-C2B	-2.25	123.68	127.88
29	aI	201	PEB	CAB-C3B-C2B	-2.25	123.68	127.88
29	e1	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	eK	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	CJ	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CL	202	PEB	OD-C4D-C3D	-2.25	124.36	129.46
29	c1	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	cK	202	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	HG	202	PEB	C4B-C3B-C2B	-2.25	104.29	106.78
29	HQ	202	PEB	C4B-C3B-C2B	-2.25	104.29	106.78
29	ZJ	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	ZL	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	H4	201	PEB	CMD-C2D-C3D	2.25	133.24	130.06
31	yP	1001	CYC	CAA-C2A-C1A	2.25	128.99	125.01
29	b1	201	PEB	CBB-CAB-C3B	-2.25	106.37	112.63
29	bK	201	PEB	CBB-CAB-C3B	-2.25	106.37	112.63
31	IF	1001	CYC	CHB-C1B-NB	-2.25	121.22	126.06
31	II	1001	CYC	CHB-C1B-NB	-2.25	121.22	126.06
29	H3	202	PEB	CHA-C1B-NB	-2.25	120.22	124.93
29	HO	202	PEB	CHA-C1B-NB	-2.25	120.22	124.93
29	KC	201	PEB	OD-C4D-ND	-2.25	122.60	125.93
29	KE	201	PEB	OD-C4D-ND	-2.25	122.60	125.93
29	h7	201	PEB	C4B-C3B-C2B	-2.25	104.29	106.78
29	h9	201	PEB	C4B-C3B-C2B	-2.25	104.29	106.78
29	lJ	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	lL	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	gF	203	PEB	CMC-C3C-C2C	2.25	129.19	124.94
29	gI	203	PEB	CMC-C3C-C2C	2.25	129.19	124.94
29	k7	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
29	k9	202	PEB	C1B-C2B-C3B	-2.25	103.92	106.51
31	CF	1001	CYC	CHB-C1B-NB	-2.25	121.23	126.06
31	CI	1001	CYC	CHB-C1B-NB	-2.25	121.23	126.06
29	HJ	201	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	pJ	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	HL	201	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	pL	202	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	DD	202	PEB	CMA-C2A-C1A	-2.25	107.55	112.40
29	U1	202	PEB	CHA-C4A-NA	2.25	127.88	125.20
29	UK	202	PEB	CHA-C4A-NA	2.25	127.88	125.20
29	VF	201	PEB	CAB-C3B-C2B	-2.25	123.69	127.88
29	VI	201	PEB	CAB-C3B-C2B	-2.25	123.69	127.88
29	D3	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	DO	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	AF	301	PEB	CBC-CAC-C2C	-2.25	108.78	112.62
29	AI	301	PEB	CBC-CAC-C2C	-2.25	108.78	112.62
29	MD	203	PEB	CAC-CBC-CGC	-2.25	107.45	113.76
29	L3	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	LO	201	PEB	CAB-C3B-C4B	2.25	128.99	125.01
29	K4	203	PEB	CAC-CBC-CGC	-2.25	107.45	113.76
29	iF	203	PEB	CMC-C3C-C2C	2.25	129.18	124.94
29	iI	203	PEB	CMC-C3C-C2C	2.25	129.18	124.94
29	LG	202	PEB	CHB-C4B-C3B	-2.25	120.12	125.32
29	LQ	201	PEB	CHB-C4B-C3B	-2.25	120.12	125.32
29	U1	202	PEB	CBB-CAB-C3B	-2.25	106.38	112.63
29	UK	202	PEB	CBB-CAB-C3B	-2.25	106.38	112.63
29	SR	201	PEB	OD-C4D-ND	-2.25	122.60	125.93
29	GG	201	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	GQ	201	PEB	C2B-C1B-NB	2.25	115.33	110.53
29	MB	202	PEB	CBC-CAC-C2C	-2.25	108.78	112.62
29	MM	202	PEB	CBC-CAC-C2C	-2.25	108.78	112.62
29	fI	201	PEB	CBB-CAB-C3B	-2.25	106.38	112.63
29	fK	201	PEB	CBB-CAB-C3B	-2.25	106.38	112.63
31	WP	1001	CYC	C2B-C1B-NB	2.25	110.28	106.99
29	T1	201	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
29	TK	201	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
29	S1	201	PEB	CHA-C4A-NA	2.25	127.88	125.20
29	SK	201	PEB	CHA-C4A-NA	2.25	127.88	125.20
29	H4	202	PEB	CMA-C2A-C1A	-2.25	107.56	112.40
31	OP	1001	CYC	C2C-C1C-NC	2.25	110.21	108.27
29	IG	202	PEB	C2A-C3A-C4A	-2.25	97.97	101.34
29	IQ	202	PEB	C2A-C3A-C4A	-2.25	97.97	101.34
29	wL	301	PEB	OD-C4D-ND	-2.25	122.60	125.93
29	A5	203	PEB	CAC-CBC-CGC	-2.25	107.46	113.76
29	A8	203	PEB	CAC-CBC-CGC	-2.25	107.46	113.76
29	V1	201	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
29	VK	201	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
29	iJ	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
29	iL	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
29	H5	201	PEB	CHC-C1D-ND	-2.25	111.34	113.95
29	GD	203	PEB	CAC-CBC-CGC	-2.25	107.46	113.76
29	Z1	201	PEB	CAB-C3B-C4B	2.25	128.98	125.01
29	ZK	201	PEB	CAB-C3B-C4B	2.25	128.98	125.01
29	mJ	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
29	mL	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
29	CB	202	PEB	CBC-CAC-C2C	-2.25	108.79	112.62
29	CM	202	PEB	CBC-CAC-C2C	-2.25	108.79	112.62
29	Z7	201	PEB	C4B-C3B-C2B	-2.25	104.30	106.78
29	Z9	201	PEB	C4B-C3B-C2B	-2.25	104.30	106.78
29	QJ	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	QL	202	PEB	OD-C4D-C3D	-2.25	124.37	129.46
29	a1	201	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
29	aK	201	PEB	CAB-CBB-CGB	-2.25	108.77	113.60
29	MQ	406	PEB	C2A-C1A-NA	2.25	110.21	108.27
31	NF	1001	CYC	CBD-CAD-C3D	2.25	116.45	112.62
31	NI	1001	CYC	CBD-CAD-C3D	2.25	116.45	112.62
29	hB	202	PEB	CBC-CAC-C2C	-2.24	108.79	112.62
29	hM	202	PEB	CBC-CAC-C2C	-2.24	108.79	112.62
29	h1	201	PEB	CBB-CAB-C3B	-2.24	106.39	112.63
29	hK	201	PEB	CBB-CAB-C3B	-2.24	106.39	112.63
31	EF	1001	CYC	CHB-C1B-NB	-2.24	121.24	126.06
31	EI	1001	CYC	CHB-C1B-NB	-2.24	121.24	126.06
29	S1	201	PEB	CBB-CAB-C3B	-2.24	106.39	112.63
29	SK	201	PEB	CBB-CAB-C3B	-2.24	106.39	112.63
29	B4	202	PEB	CMA-C2A-C1A	-2.24	107.57	112.40
29	N2	203	PEB	CMB-C2B-C1B	2.24	128.52	125.06
29	IJ	203	PEB	C2B-C1B-NB	2.24	115.32	110.53
29	PJ	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
29	IL	203	PEB	C2B-C1B-NB	2.24	115.32	110.53
29	PL	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
29	wL	303	PEB	C2B-C1B-NB	2.24	115.32	110.53
31	DP	1001	CYC	C2C-C1C-NC	2.24	110.21	108.27
29	G8	201	PEB	CHC-C1D-ND	-2.24	111.34	113.95
29	GB	202	PEB	CBC-CAC-C2C	-2.24	108.79	112.62
29	GM	202	PEB	CBC-CAC-C2C	-2.24	108.79	112.62
29	jJ	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
29	jL	202	PEB	C2B-C1B-NB	2.24	115.32	110.53
29	HD	202	PEB	CMA-C2A-C1A	-2.24	107.57	112.40
29	sJ	202	PEB	OD-C4D-C3D	-2.24	124.38	129.46
29	sL	202	PEB	OD-C4D-C3D	-2.24	124.38	129.46
31	KI	1001	CYC	CHB-C1B-NB	-2.24	121.24	126.06
29	RF	201	PEB	CAB-C3B-C2B	-2.24	123.70	127.88
29	RI	201	PEB	CAB-C3B-C2B	-2.24	123.70	127.88
29	AG	202	PEB	C2A-C3A-C4A	-2.24	97.98	101.34
29	AQ	202	PEB	C2A-C3A-C4A	-2.24	97.98	101.34
29	hJ	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	hL	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	aF	203	PEB	CMC-C3C-C2C	2.24	129.17	124.94
29	aI	203	PEB	CMC-C3C-C2C	2.24	129.17	124.94
29	PF	203	PEB	CMC-C3C-C2C	2.24	129.17	124.94
29	PI	203	PEB	CMC-C3C-C2C	2.24	129.17	124.94
29	WJ	201	PEB	C2B-C1B-NB	2.24	115.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WL	201	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	CG	201	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	CQ	201	PEB	C2B-C1B-NB	2.24	115.31	110.53
30	MG	403	PUB	CBC-CAC-C2C	2.24	118.85	112.63
29	F3	202	PEB	CHA-C1B-NB	-2.24	120.25	124.93
29	FO	202	PEB	CHA-C1B-NB	-2.24	120.25	124.93
29	NR	201	PEB	CAC-CBC-CGC	-2.24	107.48	113.76
29	l1	201	PEB	CHA-C4A-NA	2.24	127.87	125.20
29	lK	201	PEB	CHA-C4A-NA	2.24	127.87	125.20
31	H1	1001	CYC	C1B-CHB-C4A	-2.24	122.61	128.08
29	EG	202	PEB	C2A-C3A-C4A	-2.24	97.98	101.34
29	EQ	202	PEB	C2A-C3A-C4A	-2.24	97.98	101.34
31	BP	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
29	BC	202	PEB	OD-C4D-ND	-2.24	122.61	125.93
29	BE	202	PEB	OD-C4D-ND	-2.24	122.61	125.93
29	xL	301	PEB	OD-C4D-ND	-2.24	122.61	125.93
29	HG	202	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
29	HQ	202	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
29	U2	202	PEB	CMB-C2B-C1B	2.24	128.51	125.06
29	iF	201	PEB	CAB-C3B-C2B	-2.24	123.71	127.88
29	iI	201	PEB	CAB-C3B-C2B	-2.24	123.71	127.88
30	A7	302	PUB	CBA-CAA-C3A	-2.24	109.58	112.98
30	A9	302	PUB	CBA-CAA-C3A	-2.24	109.58	112.98
29	C3	201	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
29	CO	201	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
29	HA	201	PEB	C1C-CHB-C4B	-2.24	126.13	128.81
29	HN	201	PEB	C1C-CHB-C4B	-2.24	126.13	128.81
29	cF	201	PEB	CAB-C3B-C2B	-2.24	123.71	127.88
29	cI	201	PEB	CAB-C3B-C2B	-2.24	123.71	127.88
29	rJ	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	rL	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
31	MP	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
31	HK	1001	CYC	C1B-CHB-C4A	-2.24	122.61	128.08
29	O2	202	PEB	CMB-C2B-C1B	2.24	128.51	125.06
29	nJ	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	nL	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
31	yP	1001	CYC	C1B-NB-C4B	-2.24	107.82	110.67
29	A3	201	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
29	AO	201	PEB	CHB-C4B-C3B	-2.24	120.15	125.32
29	d7	201	PEB	C4B-C3B-C2B	-2.24	104.31	106.78
29	d9	201	PEB	C4B-C3B-C2B	-2.24	104.31	106.78
29	eF	201	PEB	CAB-C3B-C2B	-2.24	123.71	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	eI	201	PEB	CAB-C3B-C2B	-2.24	123.71	127.88
29	NJ	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
29	NL	202	PEB	C2B-C1B-NB	2.24	115.31	110.53
31	H7	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
31	H9	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
29	ED	202	PEB	CAC-CBC-CGC	-2.24	107.49	113.76
29	B4	201	PEB	CAA-C3A-C4A	-2.24	106.93	112.67
30	A1	304	PUB	CMD-C2D-C3D	2.24	131.12	127.77
30	AK	304	PUB	CMD-C2D-C3D	2.24	131.12	127.77
29	PR	202	PEB	CMB-C2B-C1B	2.24	128.51	125.06
29	A9	304	PEB	CAA-C3A-C4A	2.24	118.42	112.67
29	e2	402	PEB	CAC-CBC-CGC	-2.24	107.49	113.76
29	KD	203	PEB	CAC-CBC-CGC	-2.24	107.49	113.76
29	XR	201	PEB	CAC-CBC-CGC	-2.24	107.49	113.76
31	N7	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
31	N9	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
31	hP	1001	CYC	C2C-C1C-NC	2.24	110.20	108.27
29	j1	201	PEB	CHA-C4A-NA	2.24	127.86	125.20
29	jK	201	PEB	CHA-C4A-NA	2.24	127.86	125.20
29	DA	201	PEB	C1C-CHB-C4B	-2.24	126.14	128.81
29	DN	201	PEB	C1C-CHB-C4B	-2.24	126.14	128.81
29	I3	201	PEB	CHB-C4B-C3B	-2.24	120.16	125.32
29	IO	201	PEB	CHB-C4B-C3B	-2.24	120.16	125.32
29	DF	1002	PEB	OD-C4D-ND	-2.24	122.62	125.93
29	DI	1002	PEB	OD-C4D-ND	-2.24	122.62	125.93
29	HA	201	PEB	C2B-C1B-NB	2.24	115.30	110.53
29	EG	201	PEB	C2B-C1B-NB	2.24	115.30	110.53
29	fJ	202	PEB	C2B-C1B-NB	2.24	115.30	110.53
29	fL	202	PEB	C2B-C1B-NB	2.24	115.30	110.53
29	HN	201	PEB	C2B-C1B-NB	2.24	115.30	110.53
29	EQ	201	PEB	C2B-C1B-NB	2.24	115.30	110.53
29	ID	203	PEB	CAC-CBC-CGC	-2.23	107.49	113.76
29	DG	201	PEB	CAB-CBB-CGB	-2.23	108.79	113.60
29	DQ	201	PEB	CAB-CBB-CGB	-2.23	108.79	113.60
29	WR	202	PEB	CMB-C2B-C1B	2.23	128.50	125.06
31	MF	1001	CYC	CHB-C1B-NB	-2.23	121.26	126.06
31	MI	1001	CYC	CHB-C1B-NB	-2.23	121.26	126.06
29	k1	202	PEB	CAB-C3B-C4B	2.23	128.96	125.01
29	kK	202	PEB	CAB-C3B-C4B	2.23	128.96	125.01
31	J7	1001	CYC	C2C-C1C-NC	2.23	110.20	108.27
31	L7	1001	CYC	C2C-C1C-NC	2.23	110.20	108.27
31	jP	1001	CYC	C2C-C1C-NC	2.23	110.20	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KG	201	PEB	C2B-C1B-NB	2.23	115.30	110.53
29	KQ	201	PEB	C2B-C1B-NB	2.23	115.30	110.53
29	b1	201	PEB	CHA-C4A-NA	2.23	127.86	125.20
29	bK	201	PEB	CHA-C4A-NA	2.23	127.86	125.20
29	g1	202	PEB	CAB-C3B-C4B	2.23	128.96	125.01
29	gK	202	PEB	CAB-C3B-C4B	2.23	128.96	125.01
29	LA	201	PEB	C1C-CHB-C4B	-2.23	126.14	128.81
29	LN	201	PEB	C1C-CHB-C4B	-2.23	126.14	128.81
29	MQ	407	PEB	C2B-C1B-NB	2.23	115.30	110.53
29	N2	201	PEB	CAC-CBC-CGC	-2.23	107.50	113.76
29	Q7	201	PEB	C4B-C3B-C2B	-2.23	104.31	106.78
29	Q9	201	PEB	C4B-C3B-C2B	-2.23	104.31	106.78
29	kF	201	PEB	CAB-C3B-C2B	-2.23	123.72	127.88
29	kI	201	PEB	CAB-C3B-C2B	-2.23	123.72	127.88
29	HF	1002	PEB	OD-C4D-ND	-2.23	122.62	125.93
29	LF	1002	PEB	OD-C4D-ND	-2.23	122.62	125.93
29	HI	1002	PEB	OD-C4D-ND	-2.23	122.62	125.93
29	LI	1002	PEB	OD-C4D-ND	-2.23	122.62	125.93
29	j1	203	PEB	CAB-C3B-C4B	2.23	128.96	125.01
29	jK	203	PEB	CAB-C3B-C4B	2.23	128.96	125.01
29	UR	202	PEB	CMB-C2B-C1B	2.23	128.50	125.06
29	CD	203	PEB	CAC-CBC-CGC	-2.23	107.50	113.76
29	S2	201	PEB	OD-C4D-ND	-2.23	122.62	125.93
29	xJ	301	PEB	OD-C4D-ND	-2.23	122.62	125.93
29	S7	201	PEB	C4B-C3B-C2B	-2.23	104.31	106.78
29	S9	201	PEB	C4B-C3B-C2B	-2.23	104.31	106.78
29	G5	201	PEB	CAB-C3B-C4B	2.23	128.96	125.01
29	GA	202	PEB	OD-C4D-C3D	-2.23	124.41	129.46
29	GN	202	PEB	OD-C4D-C3D	-2.23	124.41	129.46
29	I3	202	PEB	C1C-CHB-C4B	2.23	131.47	128.81
29	BA	201	PEB	C1C-CHB-C4B	-2.23	126.14	128.81
29	BN	201	PEB	C1C-CHB-C4B	-2.23	126.14	128.81
29	IO	202	PEB	C1C-CHB-C4B	2.23	131.47	128.81
29	G3	202	PEB	C2B-C1B-NB	2.23	115.29	110.53
29	GO	202	PEB	C2B-C1B-NB	2.23	115.29	110.53
29	R2	201	PEB	CAC-CBC-CGC	-2.23	107.50	113.76
29	F4	202	PEB	CMA-C2A-C1A	-2.23	107.59	112.40
29	d1	201	PEB	CHA-C4A-NA	2.23	127.86	125.20
29	dK	201	PEB	CHA-C4A-NA	2.23	127.86	125.20
31	D1	1001	CYC	C1B-CHB-C4A	-2.23	122.63	128.08
29	TR	201	PEB	CAC-CBC-CGC	-2.23	107.51	113.76
29	G5	201	PEB	CHC-C1D-ND	-2.23	111.36	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BD	202	PEB	CMA-C2A-C1A	-2.23	107.60	112.40
29	FJ	202	PEB	C2B-C1B-NB	2.23	115.29	110.53
29	FL	202	PEB	C2B-C1B-NB	2.23	115.29	110.53
29	I5	203	PEB	CAB-CBB-CGB	-2.23	108.81	113.60
29	I8	203	PEB	CAB-CBB-CGB	-2.23	108.81	113.60
29	A8	203	PEB	CAB-CBB-CGB	-2.23	108.81	113.60
29	P1	202	PEB	CAB-C3B-C4B	2.23	128.95	125.01
29	PK	202	PEB	CAB-C3B-C4B	2.23	128.95	125.01
29	AA	202	PEB	OD-C4D-C3D	-2.23	124.41	129.46
29	AN	202	PEB	OD-C4D-C3D	-2.23	124.41	129.46
29	DA	201	PEB	C2B-C1B-NB	2.23	115.28	110.53
29	xL	303	PEB	C2B-C1B-NB	2.23	115.28	110.53
29	DN	201	PEB	C2B-C1B-NB	2.23	115.28	110.53
31	uP	1001	CYC	C2C-C1C-NC	2.23	110.19	108.27
29	K3	202	PEB	C1C-CHB-C4B	2.23	131.47	128.81
29	KO	202	PEB	C1C-CHB-C4B	2.23	131.47	128.81
29	S2	202	PEB	CMB-C2B-C1B	2.23	128.49	125.06
29	j7	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
29	j9	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
31	HP	1001	CYC	C2C-C1C-NC	2.23	110.19	108.27
29	N1	1002	PEB	C1B-C2B-C3B	-2.23	103.95	106.51
31	VP	1001	CYC	CHB-C1B-C2B	-2.23	122.54	126.95
29	VR	203	PEB	CMB-C2B-C1B	2.23	128.49	125.06
29	FA	201	PEB	C2B-C1B-NB	2.23	115.28	110.53
29	FN	201	PEB	C2B-C1B-NB	2.23	115.28	110.53
29	Q2	202	PEB	CMB-C2B-C1B	2.23	128.49	125.06
29	R1	202	PEB	CAB-C3B-C4B	2.23	128.95	125.01
29	RK	202	PEB	CAB-C3B-C4B	2.23	128.95	125.01
29	l7	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
29	l9	201	PEB	C4B-C3B-C2B	-2.23	104.32	106.78
29	P2	202	PEB	CMB-C2B-C1B	2.23	128.49	125.06
29	QR	202	PEB	CMB-C2B-C1B	2.23	128.49	125.06
29	LC	202	PEB	OD-C4D-ND	-2.23	122.63	125.93
29	LE	202	PEB	OD-C4D-ND	-2.23	122.63	125.93
29	LD	201	PEB	CAA-C3A-C4A	-2.22	106.96	112.67
29	AJ	203	PEB	C2B-C1B-NB	2.22	115.28	110.53
29	XJ	202	PEB	C2B-C1B-NB	2.22	115.28	110.53
29	AL	203	PEB	C2B-C1B-NB	2.22	115.28	110.53
29	XL	202	PEB	C2B-C1B-NB	2.22	115.28	110.53
29	KA	202	PEB	OD-C4D-C3D	-2.22	124.42	129.46
29	KN	202	PEB	OD-C4D-C3D	-2.22	124.42	129.46
31	NK	1001	CYC	C1B-CHB-C4A	-2.22	122.65	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	YF	201	PEB	CAB-C3B-C2B	-2.22	123.73	127.88
29	YI	201	PEB	CAB-C3B-C2B	-2.22	123.73	127.88
29	N3	202	PEB	OD-C4D-ND	-2.22	122.64	125.93
29	T2	201	PEB	CAC-CBC-CGC	-2.22	107.52	113.76
29	E4	203	PEB	CAC-CBC-CGC	-2.22	107.52	113.76
29	yJ	301	PEB	CHA-C1B-NB	-2.22	120.28	124.93
29	yL	301	PEB	CHA-C1B-NB	-2.22	120.28	124.93
29	V2	201	PEB	CAC-CBC-CGC	-2.22	107.52	113.76
31	J1	1001	CYC	C1B-CHB-C4A	-2.22	122.65	128.08
31	JK	1001	CYC	C1B-CHB-C4A	-2.22	122.65	128.08
30	MQ	404	PUB	C1D-CHC-C4C	-2.22	108.53	113.37
29	b7	201	PEB	C4B-C3B-C2B	-2.22	104.32	106.78
29	b9	201	PEB	C4B-C3B-C2B	-2.22	104.32	106.78
29	EA	202	PEB	OD-C4D-C3D	-2.22	124.42	129.46
29	EN	202	PEB	OD-C4D-C3D	-2.22	124.42	129.46
29	FA	201	PEB	C1C-CHB-C4B	-2.22	126.15	128.81
29	FN	201	PEB	C1C-CHB-C4B	-2.22	126.15	128.81
29	TJ	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	TL	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	RR	201	PEB	CAC-CBC-CGC	-2.22	107.53	113.76
31	SP	1001	CYC	C2C-C1C-NC	2.22	110.19	108.27
29	VR	201	PEB	CAC-CBC-CGC	-2.22	107.53	113.76
29	XR	203	PEB	CMB-C2B-C1B	2.22	128.49	125.06
31	H1	1001	CYC	CHB-C4A-C3A	2.22	130.61	124.90
29	A3	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	JJ	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	JL	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	AO	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	K3	201	PEB	CHB-C4B-C3B	-2.22	120.19	125.32
29	KO	201	PEB	CHB-C4B-C3B	-2.22	120.19	125.32
31	J9	1001	CYC	C2C-C1C-NC	2.22	110.19	108.27
29	IA	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
29	OF	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
29	OI	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
29	IN	202	PEB	OD-C4D-C3D	-2.22	124.43	129.46
29	F5	201	PEB	CHC-C1D-ND	-2.22	111.37	113.95
29	F8	201	PEB	CHC-C1D-ND	-2.22	111.37	113.95
29	BD	201	PEB	CAA-C3A-C4A	-2.22	106.97	112.67
29	f7	201	PEB	C4B-C3B-C2B	-2.22	104.33	106.78
29	f9	201	PEB	C4B-C3B-C2B	-2.22	104.33	106.78
29	fF	202	PEB	CBC-CAC-C2C	-2.22	108.83	112.62
29	fI	202	PEB	CBC-CAC-C2C	-2.22	108.83	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f1	201	PEB	CHA-C4A-NA	2.22	127.84	125.20
29	fK	201	PEB	CHA-C4A-NA	2.22	127.84	125.20
29	G8	201	PEB	CAB-C3B-C4B	2.22	128.94	125.01
29	AB	301	PEB	C2A-C1A-NA	2.22	110.19	108.27
29	SR	202	PEB	CMB-C2B-C1B	2.22	128.48	125.06
29	J1	1002	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
29	JK	1002	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
29	A5	203	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
29	G5	201	PEB	CAB-CBB-CGB	-2.22	108.83	113.60
29	A3	202	PEB	C1C-CHB-C4B	2.22	131.46	128.81
29	AO	202	PEB	C1C-CHB-C4B	2.22	131.46	128.81
29	JA	201	PEB	C1C-CHB-C4B	-2.22	126.16	128.81
29	JN	201	PEB	C1C-CHB-C4B	-2.22	126.16	128.81
29	BJ	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	uJ	201	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	BL	202	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	uL	201	PEB	C2B-C1B-NB	2.22	115.27	110.53
29	X2	202	PEB	CMB-C2B-C1B	2.22	128.48	125.06
29	BD	201	PEB	CMD-C2D-C3D	2.22	133.19	130.06
29	MG	405	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	H4	201	PEB	CAA-C3A-C4A	-2.22	106.98	112.67
29	RJ	202	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	RL	202	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	G3	201	PEB	CHB-C4B-C3B	-2.22	120.20	125.32
29	GO	201	PEB	CHB-C4B-C3B	-2.22	120.20	125.32
29	dJ	202	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	dL	202	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	AC	203	PEB	OD-C4D-ND	-2.22	122.65	125.93
29	AE	203	PEB	OD-C4D-ND	-2.22	122.65	125.93
29	xJ	303	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	fF	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
29	fI	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
30	MG	402	PUB	C1D-CHC-C4C	-2.22	108.54	113.37
31	DK	1001	CYC	C1B-CHB-C4A	-2.22	122.67	128.08
31	J1	1001	CYC	CHB-C4A-C3A	2.22	130.60	124.90
31	JK	1001	CYC	CHB-C4A-C3A	2.22	130.60	124.90
31	N1	1001	CYC	C1B-CHB-C4A	-2.22	122.67	128.08
29	CA	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
29	CN	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
29	K3	202	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	KO	202	PEB	C2B-C1B-NB	2.22	115.26	110.53
31	GF	1001	CYC	CHB-C1B-NB	-2.22	121.30	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	GI	1001	CYC	CHB-C1B-NB	-2.22	121.30	126.06
31	HK	1001	CYC	CHB-C4A-C3A	2.22	130.60	124.90
29	V2	203	PEB	CMB-C2B-C1B	2.22	128.48	125.06
31	L1	1001	CYC	C1B-CHB-C4A	-2.22	122.67	128.08
31	LK	1001	CYC	C1B-CHB-C4A	-2.22	122.67	128.08
29	LG	203	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
29	NK	1002	PEB	C1B-C2B-C3B	-2.22	103.96	106.51
29	BA	201	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	BN	201	PEB	C2B-C1B-NB	2.22	115.26	110.53
29	K5	203	PEB	CAB-CBB-CGB	-2.22	108.84	113.60
29	K8	203	PEB	CAB-CBB-CGB	-2.22	108.84	113.60
29	E3	201	PEB	CHB-C4B-C3B	-2.22	120.20	125.32
29	EO	201	PEB	CHB-C4B-C3B	-2.22	120.20	125.32
29	QF	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
29	QI	202	PEB	OD-C4D-C3D	-2.22	124.44	129.46
31	vP	1001	CYC	C1A-C2A-C3A	-2.21	104.33	106.78
29	mF	201	PEB	CAB-C3B-C2B	-2.21	123.75	127.88
29	mI	201	PEB	CAB-C3B-C2B	-2.21	123.75	127.88
29	JD	201	PEB	CAA-C3A-C4A	-2.21	106.99	112.67
29	xJ	303	PEB	O2B-CGB-CBB	2.21	121.14	114.03
29	L4	201	PEB	CAA-C3A-C4A	-2.21	106.99	112.67
31	L1	1001	CYC	CHB-C4A-C3A	2.21	130.59	124.90
31	LK	1001	CYC	CHB-C4A-C3A	2.21	130.59	124.90
29	C5	203	PEB	CAB-CBB-CGB	-2.21	108.84	113.60
29	C8	203	PEB	CAB-CBB-CGB	-2.21	108.84	113.60
30	AF	302	PUB	CBB-CAB-C3B	-2.21	108.84	112.62
30	AI	302	PUB	CBB-CAB-C3B	-2.21	108.84	112.62
31	F7	1001	CYC	C2C-C1C-NC	2.21	110.18	108.27
29	IA	201	PEB	C4B-NB-C1B	-2.21	102.34	106.51
29	IN	201	PEB	C4B-NB-C1B	-2.21	102.34	106.51
29	J5	201	PEB	C4B-C3B-C2B	-2.21	104.33	106.78
29	J8	201	PEB	C4B-C3B-C2B	-2.21	104.33	106.78
29	F4	201	PEB	CAA-C3A-C4A	-2.21	106.99	112.67
29	H8	201	PEB	CHC-C1D-ND	-2.21	111.38	113.95
30	BB	302	PUB	C2C-C1C-NC	2.21	113.27	110.05
30	BM	302	PUB	C2C-C1C-NC	2.21	113.27	110.05
29	IG	201	PEB	C2B-C1B-NB	2.21	115.25	110.53
29	IQ	201	PEB	C2B-C1B-NB	2.21	115.25	110.53
31	D7	1001	CYC	C2C-C1C-NC	2.21	110.18	108.27
31	D9	1001	CYC	C2C-C1C-NC	2.21	110.18	108.27
29	HG	203	PEB	C1B-C2B-C3B	-2.21	103.97	106.51
29	HD	201	PEB	CBA-CAA-C3A	-2.21	108.54	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A7	304	PEB	CAA-C3A-C4A	2.21	118.35	112.67
29	lF	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
29	lI	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
29	wJ	303	PEB	O2B-CGB-CBB	2.21	121.14	114.03
29	wL	303	PEB	O2B-CGB-CBB	2.21	121.14	114.03
29	JD	201	PEB	CBA-CAA-C3A	-2.21	108.54	113.47
29	wJ	302	PEB	CHC-C1D-ND	-2.21	111.38	113.95
29	hF	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
29	hI	202	PEB	OD-C4D-C3D	-2.21	124.45	129.46
29	J4	201	PEB	CAA-C3A-C4A	-2.21	107.00	112.67
29	B8	201	PEB	CHC-C1D-ND	-2.21	111.38	113.95
29	HD	201	PEB	CAA-C3A-C4A	-2.21	107.00	112.67
29	O7	201	PEB	C4B-C3B-C2B	-2.21	104.34	106.78
29	O9	201	PEB	C4B-C3B-C2B	-2.21	104.34	106.78
31	L9	1001	CYC	C2C-C1C-NC	2.21	110.18	108.27
29	TR	203	PEB	CMB-C2B-C1B	2.21	128.47	125.06
29	J1	1002	PEB	O1C-CGC-CBC	-2.21	115.98	123.08
29	JK	1002	PEB	O1C-CGC-CBC	-2.21	115.98	123.08
29	MR	202	PEB	CHC-C1D-ND	-2.21	111.38	113.95
31	xP	1001	CYC	CHB-C1B-C2B	-2.21	122.57	126.95
29	M3	202	PEB	OD-C4D-ND	-2.21	122.66	125.93
29	MO	202	PEB	OD-C4D-ND	-2.21	122.66	125.93
29	xJ	302	PEB	CHC-C1D-ND	-2.21	111.38	113.95
29	G8	201	PEB	CAB-CBB-CGB	-2.21	108.85	113.60
29	G3	202	PEB	OD-C4D-C3D	-2.21	124.46	129.46
29	GO	202	PEB	OD-C4D-C3D	-2.21	124.46	129.46
29	DD	201	PEB	CAA-C3A-C4A	-2.21	107.00	112.67
29	H5	203	PEB	CAB-C3B-C4B	2.21	128.91	125.01
29	LA	201	PEB	C2B-C1B-NB	2.21	115.24	110.53
29	LN	201	PEB	C2B-C1B-NB	2.21	115.24	110.53
29	N1	1002	PEB	O1C-CGC-CBC	-2.21	115.99	123.08
29	FF	1002	PEB	OD-C4D-ND	-2.21	122.66	125.93
29	FI	1002	PEB	OD-C4D-ND	-2.21	122.66	125.93
29	NO	202	PEB	OD-C4D-ND	-2.21	122.66	125.93
31	YP	1000	CYC	C4D-CHA-C1A	2.21	131.44	128.81
31	F1	1001	CYC	C1B-CHB-C4A	-2.21	122.69	128.08
31	FK	1001	CYC	C1B-CHB-C4A	-2.21	122.69	128.08
29	F5	201	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
29	H5	201	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
29	F8	201	PEB	CAB-CBB-CGB	-2.21	108.86	113.60
31	fP	1001	CYC	C2C-C1C-NC	2.21	110.17	108.27
31	oP	1001	CYC	C2C-C1C-NC	2.21	110.17	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZF	202	PEB	CBC-CAC-C2C	-2.21	108.86	112.62
29	ZI	202	PEB	CBC-CAC-C2C	-2.21	108.86	112.62
29	F8	201	PEB	CAB-C3B-C4B	2.21	128.91	125.01
29	D1	1002	PEB	O1C-CGC-CBC	-2.21	116.00	123.08
29	I4	203	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	Q1	201	PEB	CHA-C4A-NA	2.20	127.83	125.20
29	QK	201	PEB	CHA-C4A-NA	2.20	127.83	125.20
29	D1	1002	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
31	NK	1001	CYC	CHB-C4A-C3A	2.20	130.57	124.90
29	ZF	202	PEB	OD-C4D-C3D	-2.20	124.47	129.46
29	ZI	202	PEB	OD-C4D-C3D	-2.20	124.47	129.46
29	J4	201	PEB	CBA-CAA-C3A	-2.20	108.56	113.47
29	L1	1002	PEB	O1C-CGC-CBC	-2.20	116.00	123.08
29	LK	1002	PEB	O1C-CGC-CBC	-2.20	116.00	123.08
29	FG	203	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
29	DK	1002	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
29	FC	202	PEB	CAB-C3B-C4B	2.20	128.91	125.01
29	FE	202	PEB	CAB-C3B-C4B	2.20	128.91	125.01
29	E3	202	PEB	C2B-C1B-NB	2.20	115.23	110.53
29	EO	202	PEB	C2B-C1B-NB	2.20	115.23	110.53
29	bF	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	dF	203	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	bI	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	dI	203	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	AM	302	PEB	CHA-C4A-NA	2.20	127.82	125.20
29	bF	202	PEB	OD-C4D-C3D	-2.20	124.47	129.46
29	bI	202	PEB	OD-C4D-C3D	-2.20	124.47	129.46
30	A7	302	PUB	CAC-CBC-CGC	-2.20	108.86	113.60
30	A9	302	PUB	CAC-CBC-CGC	-2.20	108.86	113.60
29	A3	202	PEB	CHA-C1B-NB	-2.20	120.33	124.93
29	AO	202	PEB	CHA-C1B-NB	-2.20	120.33	124.93
30	AB	304	PUB	CMC-C3C-C4C	2.20	132.97	126.37
29	SF	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	SI	202	PEB	CBC-CAC-C2C	-2.20	108.86	112.62
29	JA	201	PEB	C2B-C1B-NB	2.20	115.23	110.53
29	JN	201	PEB	C2B-C1B-NB	2.20	115.23	110.53
31	E1	1001	CYC	CMB-C2B-C1B	2.20	126.91	124.17
29	C3	202	PEB	C2B-C1B-NB	2.20	115.22	110.53
29	CO	202	PEB	C2B-C1B-NB	2.20	115.22	110.53
29	dF	203	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	dI	203	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	H1	1002	PEB	C1B-C2B-C3B	-2.20	103.98	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B8	201	PEB	CAB-CBB-CGB	-2.20	108.87	113.60
29	hF	202	PEB	CBC-CAC-C2C	-2.20	108.87	112.62
29	hI	202	PEB	CBC-CAC-C2C	-2.20	108.87	112.62
29	I3	202	PEB	C2B-C1B-NB	2.20	115.22	110.53
29	IO	202	PEB	C2B-C1B-NB	2.20	115.22	110.53
29	HK	1002	PEB	C1B-C2B-C3B	-2.20	103.98	106.51
29	H4	201	PEB	CBA-CAA-C3A	-2.20	108.57	113.47
29	G4	202	PEB	CMD-C2D-C3D	2.20	133.16	130.06
29	SF	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	FG	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	SI	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	FQ	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	ED	201	PEB	CMD-C2D-C3D	2.20	133.16	130.06
29	jF	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	jI	202	PEB	OD-C4D-C3D	-2.20	124.48	129.46
29	L8	201	PEB	CAB-CBB-CGB	-2.20	108.88	113.60
29	F1	1002	PEB	O1C-CGC-CBC	-2.20	116.03	123.08
29	FK	1002	PEB	O1C-CGC-CBC	-2.20	116.03	123.08
31	QP	1001	CYC	C2C-C1C-NC	2.20	110.17	108.27
29	LA	203	PEB	CAB-C3B-C4B	2.20	128.89	125.01
29	LN	203	PEB	CAB-C3B-C4B	2.20	128.89	125.01
29	ID	202	PEB	CMD-C2D-C3D	2.20	133.16	130.06
29	WF	202	PEB	OD-C4D-C3D	-2.20	124.49	129.46
29	WI	202	PEB	OD-C4D-C3D	-2.20	124.49	129.46
31	F1	1001	CYC	CHB-C4A-C3A	2.20	130.54	124.90
31	FK	1001	CYC	CHB-C4A-C3A	2.20	130.54	124.90
29	DD	201	PEB	CBA-CAA-C3A	-2.19	108.58	113.47
29	E3	202	PEB	CHA-C1B-NB	-2.19	120.34	124.93
29	EO	202	PEB	CHA-C1B-NB	-2.19	120.34	124.93
29	HC	202	PEB	CAB-C3B-C4B	2.19	128.89	125.01
29	HE	202	PEB	CAB-C3B-C4B	2.19	128.89	125.01
29	F1	1002	PEB	C1B-C2B-C3B	-2.19	103.99	106.51
29	FK	1002	PEB	C1B-C2B-C3B	-2.19	103.99	106.51
29	E4	202	PEB	CMD-C2D-C3D	2.19	133.16	130.06
29	OF	202	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
29	OI	202	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
30	AM	304	PUB	CMC-C3C-C4C	2.19	132.95	126.37
29	aF	201	PEB	C2B-C1B-NB	2.19	115.21	110.53
29	aI	201	PEB	C2B-C1B-NB	2.19	115.21	110.53
31	F9	1001	CYC	C2C-C1C-NC	2.19	110.16	108.27
31	DK	1001	CYC	CHB-C4A-C3A	2.19	130.54	124.90
31	rP	1001	CYC	C1A-C2A-C3A	-2.19	104.36	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	NK	1002	PEB	O1C-CGC-CBC	-2.19	116.04	123.08
31	wP	1001	CYC	C2C-C1C-NC	2.19	110.16	108.27
31	1P	1001	CYC	C2C-C1C-NC	2.19	110.16	108.27
29	L5	203	PEB	CAB-C3B-C4B	2.19	128.89	125.01
29	AC	203	PEB	CAB-C3B-C4B	2.19	128.89	125.01
29	AE	203	PEB	CAB-C3B-C4B	2.19	128.89	125.01
29	AA	201	PEB	CMA-C2A-C1A	-2.19	107.68	112.40
29	AN	201	PEB	CMA-C2A-C1A	-2.19	107.68	112.40
29	M4	202	PEB	CMD-C2D-C3D	2.19	133.16	130.06
29	K3	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
29	KO	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
29	H8	201	PEB	CAB-CBB-CGB	-2.19	108.89	113.60
29	JG	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
29	JQ	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
29	B5	201	PEB	C1C-CHB-C4B	-2.19	126.19	128.81
31	N1	1001	CYC	CHB-C4A-C3A	2.19	130.53	124.90
29	jF	202	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
29	jI	202	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
29	DK	1002	PEB	O1C-CGC-CBC	-2.19	116.04	123.08
29	AB	302	PEB	CHA-C4A-NA	2.19	127.81	125.20
30	AB	304	PUB	CBB-CAB-C3B	-2.19	108.88	112.62
29	RR	203	PEB	CMB-C2B-C1B	2.19	128.44	125.06
31	mP	1001	CYC	C1A-C2A-C3A	-2.19	104.36	106.78
29	WF	202	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
29	WI	202	PEB	CBC-CAC-C2C	-2.19	108.88	112.62
29	FQ	203	PEB	C1B-C2B-C3B	-2.19	104.00	106.51
29	D4	201	PEB	CAA-C3A-C4A	-2.19	107.05	112.67
29	BD	201	PEB	CBA-CAA-C3A	-2.19	108.59	113.47
29	C3	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
29	CO	202	PEB	OD-C4D-C3D	-2.19	124.50	129.46
29	AM	301	PEB	CHC-C1D-ND	-2.19	111.41	113.95
29	MR	202	PEB	OD-C4D-ND	-2.19	122.69	125.93
29	K3	202	PEB	CHA-C1B-NB	-2.19	120.36	124.93
29	KO	202	PEB	CHA-C1B-NB	-2.19	120.36	124.93
31	CK	1001	CYC	CMB-C2B-C1B	2.19	126.90	124.17
29	F5	201	PEB	CAB-C3B-C4B	2.19	128.88	125.01
29	L4	201	PEB	CBA-CAA-C3A	-2.19	108.60	113.47
29	L5	201	PEB	CAB-CBB-CGB	-2.19	108.90	113.60
29	CA	201	PEB	C4B-NB-C1B	-2.19	102.39	106.51
29	CN	201	PEB	C4B-NB-C1B	-2.19	102.39	106.51
29	FD	201	PEB	CAA-C3A-C4A	-2.19	107.06	112.67
29	L5	201	PEB	CHC-C1D-ND	-2.19	111.41	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L9	1002	PEB	CAA-C3A-C4A	-2.19	107.06	112.67
29	AA	201	PEB	C4B-NB-C1B	-2.19	102.39	106.51
29	AN	201	PEB	C4B-NB-C1B	-2.19	102.39	106.51
29	m1	202	PEB	CMA-C2A-C1A	-2.19	107.69	112.40
29	mK	202	PEB	CMA-C2A-C1A	-2.19	107.69	112.40
31	sP	1001	CYC	C2C-C1C-NC	2.19	110.16	108.27
29	G5	203	PEB	CAB-C3B-C4B	2.19	128.87	125.01
29	B8	203	PEB	CAB-C3B-C4B	2.19	128.87	125.01
29	EA	201	PEB	C4B-NB-C1B	-2.19	102.39	106.51
29	EN	201	PEB	C4B-NB-C1B	-2.19	102.39	106.51
29	R2	203	PEB	CMB-C2B-C1B	2.19	128.43	125.06
29	DG	202	PEB	OD-C4D-C3D	-2.19	124.51	129.46
29	LG	202	PEB	OD-C4D-C3D	-2.19	124.51	129.46
29	DQ	202	PEB	OD-C4D-C3D	-2.19	124.51	129.46
29	LQ	201	PEB	OD-C4D-C3D	-2.19	124.51	129.46
29	xL	303	PEB	O2B-CGB-CBB	2.18	121.05	114.03
29	IF	202	PEB	CBC-CAC-C2C	-2.18	108.89	112.62
29	II	202	PEB	CBC-CAC-C2C	-2.18	108.89	112.62
31	D1	1001	CYC	CHB-C4A-C3A	2.18	130.52	124.90
29	EA	201	PEB	CMA-C2A-C1A	-2.18	107.69	112.40
29	EN	201	PEB	CMA-C2A-C1A	-2.18	107.69	112.40
29	KC	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
29	KE	201	PEB	CAB-C3B-C4B	2.18	128.87	125.01
29	UF	203	PEB	CBC-CAC-C2C	-2.18	108.89	112.62
29	UI	203	PEB	CBC-CAC-C2C	-2.18	108.89	112.62
29	B4	201	PEB	CBA-CAA-C3A	-2.18	108.61	113.47
29	RF	201	PEB	C2B-C1B-NB	2.18	115.19	110.53
29	RI	201	PEB	C2B-C1B-NB	2.18	115.19	110.53
29	H1	1002	PEB	O1C-CGC-CBC	-2.18	116.07	123.08
30	AM	304	PUB	CBB-CAB-C3B	-2.18	108.89	112.62
29	MN	405	PEB	OD-C4D-ND	-2.18	122.70	125.93
29	h1	201	PEB	CHA-C4A-NA	2.18	127.80	125.20
29	hK	201	PEB	CHA-C4A-NA	2.18	127.80	125.20
29	LC	202	PEB	CAB-C3B-C4B	2.18	128.87	125.01
29	LE	202	PEB	CAB-C3B-C4B	2.18	128.87	125.01
29	I3	202	PEB	CHA-C1B-NB	-2.18	120.37	124.93
29	IO	202	PEB	CHA-C1B-NB	-2.18	120.37	124.93
29	E3	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	EO	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	HG	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	HQ	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
31	I1	1001	CYC	CMB-C2B-C1B	2.18	126.89	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CP	1001	CYC	C1A-C2A-C3A	-2.18	104.37	106.78
31	NP	1001	CYC	C1A-C2A-C3A	-2.18	104.37	106.78
29	DG	203	PEB	C1B-C2B-C3B	-2.18	104.00	106.51
29	E3	202	PEB	C1C-CHB-C4B	2.18	131.41	128.81
29	EO	202	PEB	C1C-CHB-C4B	2.18	131.41	128.81
29	H5	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	HA	203	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	HN	203	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	e1	203	PEB	CMA-C2A-C1A	-2.18	107.70	112.40
29	eK	203	PEB	CMA-C2A-C1A	-2.18	107.70	112.40
29	B5	201	PEB	CAB-CBB-CGB	-2.18	108.91	113.60
29	A3	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	BG	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	AO	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	BQ	202	PEB	OD-C4D-C3D	-2.18	124.52	129.46
29	g1	203	PEB	CMA-C2A-C1A	-2.18	107.71	112.40
29	gK	203	PEB	CMA-C2A-C1A	-2.18	107.71	112.40
30	yL	303	PUB	CAC-C2C-C1C	2.18	128.86	125.01
29	xL	302	PEB	CHC-C1D-ND	-2.18	111.42	113.95
29	G3	202	PEB	CHA-C1B-NB	-2.18	120.38	124.93
29	GO	202	PEB	CHA-C1B-NB	-2.18	120.38	124.93
29	C4	202	PEB	CMD-C2D-C3D	2.18	133.13	130.06
29	P2	201	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	C3	202	PEB	CHA-C1B-NB	-2.18	120.38	124.93
29	CO	202	PEB	CHA-C1B-NB	-2.18	120.38	124.93
29	H5	201	PEB	C1C-CHB-C4B	-2.18	126.21	128.81
29	BG	203	PEB	C1B-C2B-C3B	-2.18	104.01	106.51
29	I4	201	PEB	CHB-C4B-C3B	-2.18	120.29	125.32
29	BB	301	PEB	O2C-CGC-CBC	2.18	121.02	114.03
29	BM	301	PEB	O2C-CGC-CBC	2.18	121.02	114.03
31	AP	1001	CYC	C1A-C2A-C3A	-2.18	104.38	106.78
29	BA	203	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	BN	203	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	D4	201	PEB	CBA-CAA-C3A	-2.18	108.62	113.47
29	F4	201	PEB	CBA-CAA-C3A	-2.18	108.62	113.47
29	G8	203	PEB	CAB-C3B-C4B	2.18	128.86	125.01
29	cF	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
29	cI	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
29	QF	202	PEB	CBC-CAC-C2C	-2.17	108.91	112.62
29	QI	202	PEB	CBC-CAC-C2C	-2.17	108.91	112.62
29	i1	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	IA	201	PEB	CMA-C2A-C1A	-2.17	107.72	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	iK	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	IN	201	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	J9	1002	PEB	CAA-C3A-C4A	-2.17	107.09	112.67
29	VF	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
29	VI	201	PEB	C2B-C1B-NB	2.17	115.17	110.53
29	GA	201	PEB	C4B-NB-C1B	-2.17	102.42	106.51
29	GN	201	PEB	C4B-NB-C1B	-2.17	102.42	106.51
29	V1	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	VK	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	A1	303	PEB	CBA-CAA-C3A	-2.17	108.63	113.47
29	AK	303	PEB	CBA-CAA-C3A	-2.17	108.63	113.47
29	dD	401	PEB	CHB-C4B-C3B	-2.17	120.30	125.32
31	J1	1001	CYC	CHA-C1A-C2A	-2.17	120.30	125.32
31	JK	1001	CYC	CHA-C1A-C2A	-2.17	120.30	125.32
31	eP	1001	CYC	C1A-C2A-C3A	-2.17	104.38	106.78
29	KA	201	PEB	C4B-NB-C1B	-2.17	102.42	106.51
29	KN	201	PEB	C4B-NB-C1B	-2.17	102.42	106.51
29	UF	203	PEB	OD-C4D-C3D	-2.17	124.54	129.46
29	UI	203	PEB	OD-C4D-C3D	-2.17	124.54	129.46
29	FD	201	PEB	CBA-CAA-C3A	-2.17	108.63	113.47
29	C3	202	PEB	C1C-CHB-C4B	2.17	131.40	128.81
29	F5	201	PEB	C1C-CHB-C4B	-2.17	126.21	128.81
29	F8	201	PEB	C1C-CHB-C4B	-2.17	126.21	128.81
29	CO	202	PEB	C1C-CHB-C4B	2.17	131.40	128.81
29	L8	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
29	R1	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	RK	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	L1	1002	PEB	C1B-C2B-C3B	-2.17	104.01	106.51
29	LK	1002	PEB	C1B-C2B-C3B	-2.17	104.01	106.51
29	MD	202	PEB	CMD-C2D-C3D	2.17	133.13	130.06
29	DA	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
29	DN	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
29	LD	201	PEB	CBA-CAA-C3A	-2.17	108.63	113.47
29	BC	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
29	JC	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
29	BE	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
29	JE	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
31	RP	1001	CYC	C1A-C2A-C3A	-2.17	104.38	106.78
29	P1	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	PK	203	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	L7	1002	PEB	CAA-C3A-C4A	-2.17	107.10	112.67
29	XB	202	PEB	OD-C4D-C3D	-2.17	124.54	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	XM	202	PEB	OD-C4D-C3D	-2.17	124.54	129.46
29	HK	1002	PEB	O1C-CGC-CBC	-2.17	116.11	123.08
31	L1	1001	CYC	CHA-C1A-C2A	-2.17	120.31	125.32
31	LK	1001	CYC	CHA-C1A-C2A	-2.17	120.31	125.32
29	HQ	203	PEB	C1B-C2B-C3B	-2.17	104.02	106.51
30	MG	403	PUB	C2C-C1C-NC	2.17	113.21	110.05
29	GA	201	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	GN	201	PEB	CMA-C2A-C1A	-2.17	107.72	112.40
29	G3	202	PEB	C1C-CHB-C4B	2.17	131.40	128.81
29	GO	202	PEB	C1C-CHB-C4B	2.17	131.40	128.81
29	U2	202	PEB	CAA-C3A-C4A	2.17	118.24	112.67
29	F5	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
29	F8	203	PEB	CAB-C3B-C4B	2.17	128.85	125.01
29	L8	201	PEB	CHC-C1D-ND	-2.17	111.43	113.95
29	AB	301	PEB	CHC-C1D-ND	-2.17	111.43	113.95
31	NK	1001	CYC	CHA-C1A-C2A	-2.17	120.31	125.32
29	c1	203	PEB	CMA-C2A-C1A	-2.17	107.73	112.40
29	cK	203	PEB	CMA-C2A-C1A	-2.17	107.73	112.40
29	CG	201	PEB	CHA-C1B-NB	-2.17	120.40	124.93
29	CQ	201	PEB	CHA-C1B-NB	-2.17	120.40	124.93
29	MA	405	PEB	OD-C4D-ND	-2.17	122.72	125.93
29	B5	203	PEB	CAB-C3B-C4B	2.17	128.84	125.01
29	ID	201	PEB	CHB-C4B-C3B	-2.17	120.31	125.32
29	I3	202	PEB	OD-C4D-C3D	-2.17	124.55	129.46
29	IO	202	PEB	OD-C4D-C3D	-2.17	124.55	129.46
29	H8	203	PEB	CAB-C3B-C4B	2.17	128.84	125.01
29	TI	201	PEB	C2B-C1B-NB	2.17	115.15	110.53
29	a1	203	PEB	CMA-C2A-C1A	-2.17	107.73	112.40
29	aK	203	PEB	CMA-C2A-C1A	-2.17	107.73	112.40
29	C4	201	PEB	CHB-C4B-C3B	-2.17	120.32	125.32
29	AM	301	PEB	C2A-C1A-NA	2.17	110.14	108.27
29	kF	201	PEB	C2B-C1B-NB	2.17	115.15	110.53
29	kI	201	PEB	C2B-C1B-NB	2.17	115.15	110.53
29	J7	1002	PEB	CAA-C3A-C4A	-2.17	107.11	112.67
31	F1	1001	CYC	CHA-C1A-C2A	-2.16	120.32	125.32
31	FK	1001	CYC	CHA-C1A-C2A	-2.16	120.32	125.32
29	SF	201	PEB	CAB-CBB-CGB	-2.16	108.94	113.60
29	SI	201	PEB	CAB-CBB-CGB	-2.16	108.94	113.60
29	D7	1002	PEB	CAA-C3A-C4A	-2.16	107.12	112.67
29	D9	1002	PEB	CAA-C3A-C4A	-2.16	107.12	112.67
30	AM	304	PUB	CAC-C2C-C1C	2.16	128.84	125.01
29	SF	201	PEB	C4B-NB-C1B	-2.16	102.43	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SI	201	PEB	C4B-NB-C1B	-2.16	102.43	106.51
29	AF	304	PEB	CHA-C1B-C2B	2.16	130.46	124.90
29	AI	304	PEB	CHA-C1B-C2B	2.16	130.46	124.90
31	HK	1001	CYC	CHA-C1A-C2A	-2.16	120.32	125.32
31	IK	1001	CYC	CMB-C2B-C1B	2.16	126.87	124.17
29	JG	203	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
29	Y1	202	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
29	YK	202	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
31	M1	1001	CYC	CMB-C2B-C1B	2.16	126.87	124.17
31	MK	1001	CYC	CMB-C2B-C1B	2.16	126.87	124.17
29	V2	202	PEB	CAB-C3B-C4B	2.16	128.83	125.01
29	H8	201	PEB	CAB-C3B-C4B	2.16	128.83	125.01
29	gF	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
29	gI	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
29	I4	202	PEB	CMD-C2D-C3D	2.16	133.11	130.06
29	JQ	203	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
29	YF	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
29	YI	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
31	JP	1001	CYC	C1A-C2A-C3A	-2.16	104.39	106.78
29	H7	1002	PEB	CAA-C3A-C4A	-2.16	107.12	112.67
29	H9	1002	PEB	CAA-C3A-C4A	-2.16	107.12	112.67
29	BC	202	PEB	CAB-C3B-C4B	2.16	128.83	125.01
29	BE	202	PEB	CAB-C3B-C4B	2.16	128.83	125.01
31	D1	1001	CYC	CHA-C1A-C2A	-2.16	120.33	125.32
29	E4	201	PEB	CHB-C4B-C3B	-2.16	120.33	125.32
29	c7	203	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
29	c9	203	PEB	C1B-C2B-C3B	-2.16	104.03	106.51
29	mF	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
29	mI	201	PEB	C2B-C1B-NB	2.16	115.14	110.53
29	SF	201	PEB	CHB-C4B-NB	-2.16	125.83	128.83
29	SI	201	PEB	CHB-C4B-NB	-2.16	125.83	128.83
29	LC	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
29	LE	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
29	H8	201	PEB	C1C-CHB-C4B	-2.16	126.23	128.81
29	TR	202	PEB	CAB-C3B-C4B	2.16	128.83	125.01
31	N1	1001	CYC	CHA-C1A-C2A	-2.16	120.33	125.32
29	B8	201	PEB	C1C-CHB-C4B	-2.16	126.23	128.81
29	BD	201	PEB	CHA-C1B-C2B	2.16	130.45	124.90
29	k1	203	PEB	CMA-C2A-C1A	-2.16	107.75	112.40
29	kK	203	PEB	CMA-C2A-C1A	-2.16	107.75	112.40
29	T2	203	PEB	CMB-C2B-C1B	2.16	128.39	125.06
31	F9	1001	CYC	CHB-C1B-NB	-2.16	121.43	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MB	202	PEB	OD-C4D-ND	-2.16	122.73	125.93
29	MM	202	PEB	OD-C4D-ND	-2.16	122.73	125.93
29	WF	201	PEB	CHB-C4B-NB	-2.16	125.83	128.83
29	WI	201	PEB	CHB-C4B-NB	-2.16	125.83	128.83
31	1P	1002	CYC	C4D-CHA-C1A	2.16	131.38	128.81
29	h7	201	PEB	CAB-C3B-C4B	2.16	128.82	125.01
29	B8	201	PEB	CAB-C3B-C4B	2.16	128.82	125.01
29	h9	201	PEB	CAB-C3B-C4B	2.16	128.82	125.01
31	PP	1001	CYC	C1A-C2A-C3A	-2.16	104.40	106.78
31	TP	1001	CYC	C1A-C2A-C3A	-2.16	104.40	106.78
29	JA	203	PEB	CAB-C3B-C4B	2.16	128.82	125.01
29	JN	203	PEB	CAB-C3B-C4B	2.16	128.82	125.01
30	MQ	405	PUB	C2C-C1C-NC	2.16	113.19	110.05
29	CD	202	PEB	CMD-C2D-C3D	2.16	133.10	130.06
29	dF	202	PEB	C4B-NB-C1B	-2.16	102.45	106.51
29	hF	201	PEB	C4B-NB-C1B	-2.16	102.45	106.51
29	dI	202	PEB	C4B-NB-C1B	-2.16	102.45	106.51
29	hI	201	PEB	C4B-NB-C1B	-2.16	102.45	106.51
29	FB	203	PEB	OD-C4D-C3D	-2.16	124.58	129.46
29	FM	203	PEB	OD-C4D-C3D	-2.16	124.58	129.46
29	N7	1002	PEB	CAA-C3A-C4A	-2.16	107.14	112.67
29	N9	1002	PEB	CAA-C3A-C4A	-2.16	107.14	112.67
30	AB	304	PUB	CAC-C2C-C1C	2.15	128.82	125.01
29	PF	201	PEB	C2B-C1B-NB	2.15	115.13	110.53
29	PI	201	PEB	C2B-C1B-NB	2.15	115.13	110.53
29	T1	202	PEB	CMA-C2A-C1A	-2.15	107.76	112.40
29	TK	202	PEB	CMA-C2A-C1A	-2.15	107.76	112.40
29	WF	201	PEB	C4B-NB-C1B	-2.15	102.45	106.51
29	WI	201	PEB	C4B-NB-C1B	-2.15	102.45	106.51
29	iF	201	PEB	C2B-C1B-NB	2.15	115.12	110.53
29	iI	201	PEB	C2B-C1B-NB	2.15	115.12	110.53
29	PR	201	PEB	CAB-C3B-C4B	2.15	128.82	125.01
29	TF	201	PEB	OD-C4D-ND	-2.15	122.74	125.93
31	1P	1001	CYC	C1A-C2A-C3A	-2.15	104.40	106.78
29	FA	203	PEB	CAB-C3B-C4B	2.15	128.82	125.01
29	FN	203	PEB	CAB-C3B-C4B	2.15	128.82	125.01
29	TB	203	PEB	OD-C4D-C3D	-2.15	124.58	129.46
29	TM	203	PEB	OD-C4D-C3D	-2.15	124.58	129.46
29	EG	201	PEB	CHA-C1B-NB	-2.15	120.43	124.93
29	EQ	201	PEB	CHA-C1B-NB	-2.15	120.43	124.93
29	GG	201	PEB	CHA-C1B-NB	-2.15	120.43	124.93
29	GQ	201	PEB	CHA-C1B-NB	-2.15	120.43	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	KA	201	PEB	CMA-C2A-C1A	-2.15	107.76	112.40
29	KN	201	PEB	CMA-C2A-C1A	-2.15	107.76	112.40
29	NB	202	PEB	OD-C4D-C3D	-2.15	124.59	129.46
29	NM	202	PEB	OD-C4D-C3D	-2.15	124.59	129.46
29	L8	201	PEB	C1C-CHB-C4B	-2.15	126.24	128.81
31	C1	1001	CYC	CMB-C2B-C1B	2.15	126.85	124.17
29	K5	203	PEB	CHA-C1B-NB	-2.15	120.43	124.93
29	KG	201	PEB	CHA-C1B-NB	-2.15	120.43	124.93
29	KQ	201	PEB	CHA-C1B-NB	-2.15	120.43	124.93
29	bF	201	PEB	C4B-NB-C1B	-2.15	102.46	106.51
29	bI	201	PEB	C4B-NB-C1B	-2.15	102.46	106.51
29	K4	202	PEB	CMD-C2D-C3D	2.15	133.10	130.06
29	GD	202	PEB	CMD-C2D-C3D	2.15	133.10	130.06
29	AG	201	PEB	CHA-C1B-NB	-2.15	120.44	124.93
29	AQ	201	PEB	CHA-C1B-NB	-2.15	120.44	124.93
29	g7	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
29	g9	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
29	CD	201	PEB	CHB-C4B-C3B	-2.15	120.35	125.32
29	hF	201	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
29	hI	201	PEB	CAB-CBB-CGB	-2.15	108.98	113.60
29	M4	201	PEB	CHB-C4B-C3B	-2.15	120.36	125.32
29	CA	201	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
29	CN	201	PEB	CMA-C2A-C1A	-2.15	107.77	112.40
29	mB	203	PEB	OD-C4D-C3D	-2.15	124.59	129.46
29	mM	203	PEB	OD-C4D-C3D	-2.15	124.59	129.46
29	DA	201	PEB	C4B-NB-C1B	-2.15	102.46	106.51
29	DN	201	PEB	C4B-NB-C1B	-2.15	102.46	106.51
31	cP	1001	CYC	C1A-C2A-C3A	-2.15	104.41	106.78
29	DD	201	PEB	CHA-C1B-C2B	2.15	130.43	124.90
29	dF	202	PEB	CHB-C4B-NB	-2.15	125.85	128.83
29	dI	202	PEB	CHB-C4B-NB	-2.15	125.85	128.83
29	a7	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
29	e7	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
29	a9	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
29	e9	203	PEB	C1B-C2B-C3B	-2.15	104.04	106.51
29	MD	201	PEB	CHB-C4B-C3B	-2.15	120.36	125.32
29	I5	203	PEB	CHA-C1B-NB	-2.15	120.44	124.93
29	FF	1002	PEB	CBD-CAD-C3D	-2.15	116.94	127.62
29	FI	1002	PEB	CBD-CAD-C3D	-2.15	116.94	127.62
29	eF	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
29	eI	201	PEB	C2B-C1B-NB	2.15	115.11	110.53
29	BA	201	PEB	C4B-NB-C1B	-2.15	102.46	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BN	201	PEB	C4B-NB-C1B	-2.15	102.46	106.51
29	IF	201	PEB	CHB-C4B-NB	-2.15	125.85	128.83
29	II	201	PEB	CHB-C4B-NB	-2.15	125.85	128.83
29	FA	201	PEB	C4B-NB-C1B	-2.15	102.47	106.51
29	FN	201	PEB	C4B-NB-C1B	-2.15	102.47	106.51
29	L5	201	PEB	CAB-C3B-C4B	2.15	128.81	125.01
31	DK	1001	CYC	CHA-C1A-C2A	-2.15	120.36	125.32
29	kB	203	PEB	OD-C4D-C3D	-2.15	124.60	129.46
29	kM	203	PEB	OD-C4D-C3D	-2.15	124.60	129.46
29	XR	202	PEB	CAB-C3B-C4B	2.15	128.81	125.01
29	W7	201	PEB	CAB-C3B-C4B	2.15	128.80	125.01
29	W9	201	PEB	CAB-C3B-C4B	2.15	128.80	125.01
29	VR	202	PEB	CAB-C3B-C4B	2.15	128.80	125.01
31	tP	1001	CYC	C1A-C2A-C3A	-2.15	104.41	106.78
29	W2	202	PEB	CAA-C3A-C4A	2.15	118.18	112.67
29	IF	201	PEB	CAB-CBB-CGB	-2.15	108.99	113.60
29	II	201	PEB	CAB-CBB-CGB	-2.15	108.99	113.60
31	F7	1001	CYC	CHB-C1B-NB	-2.14	121.45	126.06
29	DC	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
29	DE	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
29	G5	201	PEB	C1C-CHB-C4B	-2.14	126.25	128.81
29	L5	201	PEB	C1C-CHB-C4B	-2.14	126.25	128.81
31	H1	1001	CYC	CHA-C1A-C2A	-2.14	120.37	125.32
29	A7	305	PEB	CMC-C3C-C2C	2.14	128.99	124.94
29	A9	305	PEB	CMC-C3C-C2C	2.14	128.99	124.94
29	HA	201	PEB	C4B-NB-C1B	-2.14	102.47	106.51
29	HN	201	PEB	C4B-NB-C1B	-2.14	102.47	106.51
29	AF	305	PEB	CHA-C1B-NB	-2.14	120.45	124.93
29	AI	305	PEB	CHA-C1B-NB	-2.14	120.45	124.93
31	KP	1001	CYC	C1A-C2A-C3A	-2.14	104.41	106.78
29	LF	1002	PEB	CMC-C3C-C2C	-2.14	120.90	124.94
29	LI	1002	PEB	CMC-C3C-C2C	-2.14	120.90	124.94
29	OF	201	PEB	CHB-C4B-NB	-2.14	125.85	128.83
29	OI	201	PEB	CHB-C4B-NB	-2.14	125.85	128.83
29	B5	201	PEB	CAB-C3B-C4B	2.14	128.80	125.01
29	K8	203	PEB	CHA-C1B-NB	-2.14	120.45	124.93
31	iP	1001	CYC	C1A-C2A-C3A	-2.14	104.41	106.78
29	L4	201	PEB	CHA-C1B-C2B	2.14	130.41	124.90
29	DF	1002	PEB	CMC-C3C-C2C	-2.14	120.90	124.94
29	DI	1002	PEB	CMC-C3C-C2C	-2.14	120.90	124.94
31	GK	1001	CYC	CMB-C2B-C1B	2.14	126.84	124.17
31	N7	1001	CYC	CHB-C1B-NB	-2.14	121.46	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	J9	1001	CYC	CHB-C1B-NB	-2.14	121.46	126.06
31	N9	1001	CYC	CHB-C1B-NB	-2.14	121.46	126.06
29	QF	201	PEB	CAB-CBB-CGB	-2.14	108.99	113.60
29	QI	201	PEB	CAB-CBB-CGB	-2.14	108.99	113.60
29	Z7	201	PEB	CAB-C3B-C4B	2.14	128.80	125.01
29	Z9	201	PEB	CAB-C3B-C4B	2.14	128.80	125.01
29	I4	203	PEB	CMB-C2B-C1B	2.14	128.36	125.06
31	EP	1001	CYC	C1A-C2A-C3A	-2.14	104.41	106.78
31	gP	1001	CYC	C1A-C2A-C3A	-2.14	104.41	106.78
29	F9	1002	PEB	CAA-C3A-C4A	-2.14	107.17	112.67
29	UR	202	PEB	CAA-C3A-C4A	2.14	118.17	112.67
29	D4	201	PEB	CHA-C1B-C2B	2.14	130.41	124.90
29	AB	301	PEB	C2B-C1B-NB	2.14	115.10	110.53
29	S2	202	PEB	CAA-C3A-C4A	2.14	118.17	112.67
29	DF	1002	PEB	CBD-CAD-C3D	-2.14	116.97	127.62
29	DI	1002	PEB	CBD-CAD-C3D	-2.14	116.97	127.62
29	QR	202	PEB	CAA-C3A-C4A	2.14	118.17	112.67
29	U7	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
29	U9	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
29	O2	202	PEB	CAA-C3A-C4A	2.14	118.17	112.67
31	xP	1001	CYC	CAB-C3B-C2B	2.14	131.19	127.53
29	LQ	202	PEB	C1B-C2B-C3B	-2.14	104.05	106.51
29	cB	203	PEB	OD-C4D-C3D	-2.14	124.61	129.46
29	cM	203	PEB	OD-C4D-C3D	-2.14	124.61	129.46
29	wL	302	PEB	CHC-C1D-ND	-2.14	111.46	113.95
29	AM	301	PEB	C2B-C1B-NB	2.14	115.09	110.53
31	EK	1001	CYC	CMB-C2B-C1B	2.14	126.84	124.17
29	gB	203	PEB	OD-C4D-C3D	-2.14	124.61	129.46
29	gM	203	PEB	OD-C4D-C3D	-2.14	124.61	129.46
31	VP	1001	CYC	CAB-C3B-C2B	2.14	131.19	127.53
29	OF	201	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
29	OI	201	PEB	CAB-CBB-CGB	-2.14	109.00	113.60
29	C5	203	PEB	CHA-C1B-NB	-2.14	120.46	124.93
29	C8	203	PEB	CHA-C1B-NB	-2.14	120.46	124.93
31	D1	1003	CYC	CMB-C2B-C1B	2.14	126.84	124.17
29	LF	1002	PEB	CBD-CAD-C3D	-2.14	116.98	127.62
29	NF	1002	PEB	CBD-CAD-C3D	-2.14	116.98	127.62
29	LI	1002	PEB	CBD-CAD-C3D	-2.14	116.98	127.62
29	NI	1002	PEB	CBD-CAD-C3D	-2.14	116.98	127.62
29	G8	201	PEB	C1C-CHB-C4B	-2.14	126.25	128.81
29	OF	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51
29	OI	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	HC	201	PEB	CAC-CBC-CGC	-2.14	107.77	113.76
29	HE	201	PEB	CAC-CBC-CGC	-2.14	107.77	113.76
29	fF	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51
29	fI	201	PEB	C4B-NB-C1B	-2.14	102.48	106.51
29	HD	201	PEB	CHA-C1B-C2B	2.14	130.40	124.90
29	SR	202	PEB	CAA-C3A-C4A	2.14	118.16	112.67
29	b7	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
29	b9	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
31	D7	1001	CYC	CHB-C1B-NB	-2.14	121.47	126.06
31	D9	1001	CYC	CHB-C1B-NB	-2.14	121.47	126.06
29	FC	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
29	FE	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
29	m7	203	PEB	C1B-C2B-C3B	-2.14	104.06	106.51
29	m9	203	PEB	C1B-C2B-C3B	-2.14	104.06	106.51
29	fF	201	PEB	CAB-CBB-CGB	-2.14	109.01	113.60
29	fI	201	PEB	CAB-CBB-CGB	-2.14	109.01	113.60
29	jB	202	PEB	OD-C4D-ND	-2.14	122.77	125.93
29	jM	202	PEB	OD-C4D-ND	-2.14	122.77	125.93
29	OR	202	PEB	CBC-CAC-C2C	-2.14	108.97	112.62
29	DC	201	PEB	CAC-CBC-CGC	-2.14	107.77	113.76
29	DE	201	PEB	CAC-CBC-CGC	-2.14	107.77	113.76
29	L8	201	PEB	CAB-C3B-C4B	2.14	128.79	125.01
29	LD	201	PEB	CHA-C1B-C2B	2.14	130.39	124.90
29	F7	1002	PEB	CAA-C3A-C4A	-2.14	107.19	112.67
31	J7	1001	CYC	CHB-C1B-NB	-2.14	121.47	126.06
31	L7	1001	CYC	CHB-C1B-NB	-2.14	121.47	126.06
29	DB	203	PEB	OD-C4D-C3D	-2.14	124.62	129.46
29	DM	203	PEB	OD-C4D-C3D	-2.14	124.62	129.46
29	IG	201	PEB	CHA-C1B-NB	-2.13	120.47	124.93
29	IQ	201	PEB	CHA-C1B-NB	-2.13	120.47	124.93
29	LA	201	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	LN	201	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	BQ	203	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	CC	201	PEB	CHC-C4C-C3C	-2.13	126.70	130.34
29	CE	201	PEB	CHC-C4C-C3C	-2.13	126.70	130.34
29	FF	1002	PEB	CMC-C3C-C2C	-2.13	120.92	124.94
29	FI	1002	PEB	CMC-C3C-C2C	-2.13	120.92	124.94
29	WF	201	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
29	WI	201	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
29	hF	201	PEB	CHB-C4B-NB	-2.13	125.87	128.83
29	hI	201	PEB	CHB-C4B-NB	-2.13	125.87	128.83
31	GP	1001	CYC	C1A-C2A-C3A	-2.13	104.42	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K4	201	PEB	CHB-C4B-C3B	-2.13	120.39	125.32
29	A5	203	PEB	CHA-C1B-NB	-2.13	120.47	124.93
29	I8	203	PEB	CHA-C1B-NB	-2.13	120.47	124.93
29	A8	203	PEB	CHA-C1B-NB	-2.13	120.47	124.93
29	BC	201	PEB	CAC-CBC-CGC	-2.13	107.78	113.76
29	BE	201	PEB	CAC-CBC-CGC	-2.13	107.78	113.76
29	Q2	202	PEB	CAA-C3A-C4A	2.13	118.15	112.67
29	WR	202	PEB	CAA-C3A-C4A	2.13	118.15	112.67
29	HA	201	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	HN	201	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	WF	202	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	WI	202	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	k7	203	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	k9	203	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	Q7	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	Q9	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	dF	203	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	dI	203	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	HF	1002	PEB	CBD-CAD-C3D	-2.13	117.01	127.62
29	HI	1002	PEB	CBD-CAD-C3D	-2.13	117.01	127.62
29	bF	201	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
29	bI	201	PEB	CAB-CBB-CGB	-2.13	109.01	113.60
29	JC	201	PEB	CAC-CBC-CGC	-2.13	107.78	113.76
29	JE	201	PEB	CAC-CBC-CGC	-2.13	107.78	113.76
29	JB	203	PEB	OD-C4D-C3D	-2.13	124.63	129.46
29	LB	203	PEB	OD-C4D-C3D	-2.13	124.63	129.46
29	JM	203	PEB	OD-C4D-C3D	-2.13	124.63	129.46
29	LM	203	PEB	OD-C4D-C3D	-2.13	124.63	129.46
29	JF	1002	PEB	CBD-CAD-C3D	-2.13	117.02	127.62
29	JI	1002	PEB	CBD-CAD-C3D	-2.13	117.02	127.62
29	YB	203	PEB	OD-C4D-ND	-2.13	122.77	125.93
29	YM	203	PEB	OD-C4D-ND	-2.13	122.77	125.93
29	lF	201	PEB	C4B-NB-C1B	-2.13	102.50	106.51
29	lI	201	PEB	C4B-NB-C1B	-2.13	102.50	106.51
29	H4	201	PEB	CHA-C1B-C2B	2.13	130.38	124.90
29	X2	201	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	MG	405	PEB	CHA-C1B-C2B	2.13	130.38	124.90
31	K1	1001	CYC	CMB-C2B-C1B	2.13	126.83	124.17
31	KK	1001	CYC	CMB-C2B-C1B	2.13	126.83	124.17
31	L9	1001	CYC	CHB-C1B-NB	-2.13	121.48	126.06
29	dJ	203	PEB	CHA-C1B-NB	-2.13	120.48	124.93
29	dL	203	PEB	CHA-C1B-NB	-2.13	120.48	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T2	202	PEB	CAB-C3B-C4B	2.13	128.78	125.01
29	KD	201	PEB	CHB-C4B-C3B	-2.13	120.40	125.32
29	FD	201	PEB	CHA-C1B-C2B	2.13	130.38	124.90
29	M2	202	PEB	CAA-C3A-C4A	2.13	118.14	112.67
29	GD	201	PEB	CHB-C4B-C3B	-2.13	120.40	125.32
29	JA	202	PEB	C2B-C1B-NB	2.13	115.07	110.53
29	JN	202	PEB	C2B-C1B-NB	2.13	115.07	110.53
29	HC	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
29	HE	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
29	G4	201	PEB	CHB-C4B-C3B	-2.13	120.40	125.32
29	R7	203	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	R9	203	PEB	C1B-C2B-C3B	-2.13	104.06	106.51
29	PJ	203	PEB	CHA-C1B-NB	-2.13	120.48	124.93
29	PL	203	PEB	CHA-C1B-NB	-2.13	120.48	124.93
29	LA	201	PEB	C4B-NB-C1B	-2.13	102.50	106.51
29	LN	201	PEB	C4B-NB-C1B	-2.13	102.50	106.51
29	LC	201	PEB	CAC-CBC-CGC	-2.13	107.79	113.76
29	LE	201	PEB	CAC-CBC-CGC	-2.13	107.79	113.76
29	S7	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
29	S9	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
29	iB	203	PEB	OD-C4D-C3D	-2.13	124.64	129.46
29	iM	203	PEB	OD-C4D-C3D	-2.13	124.64	129.46
29	kF	203	PEB	CAC-CBC-CGC	-2.13	107.79	113.76
29	kI	203	PEB	CAC-CBC-CGC	-2.13	107.79	113.76
29	KD	202	PEB	CMD-C2D-C3D	2.13	133.06	130.06
29	JD	201	PEB	CHA-C1B-C2B	2.13	130.37	124.90
29	UF	202	PEB	CAB-CBB-CGB	-2.13	109.02	113.60
29	UI	202	PEB	CAB-CBB-CGB	-2.13	109.02	113.60
29	HB	203	PEB	OD-C4D-C3D	-2.13	124.64	129.46
29	HM	203	PEB	OD-C4D-C3D	-2.13	124.64	129.46
29	ZF	201	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
29	ZI	201	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
29	SB	202	PEB	OD-C4D-ND	-2.13	122.78	125.93
29	SM	202	PEB	OD-C4D-ND	-2.13	122.78	125.93
30	yJ	303	PUB	CAC-C2C-C1C	2.13	128.77	125.01
29	P7	203	PEB	C1B-C2B-C3B	-2.13	104.07	106.51
29	P9	203	PEB	C1B-C2B-C3B	-2.13	104.07	106.51
29	TJ	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
29	TL	201	PEB	CAB-C3B-C4B	2.13	128.77	125.01
29	jF	201	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
29	jI	201	PEB	CAB-CBB-CGB	-2.13	109.03	113.60
29	MN	401	PEB	OD-C4D-C3D	-2.13	124.64	129.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	WB	202	PEB	OD-C4D-ND	-2.13	122.78	125.93
29	WM	202	PEB	OD-C4D-ND	-2.13	122.78	125.93
31	H7	1001	CYC	CHB-C1B-NB	-2.13	121.50	126.06
31	H9	1001	CYC	CHB-C1B-NB	-2.13	121.50	126.06
29	QF	201	PEB	C4B-NB-C1B	-2.13	102.51	106.51
29	QI	201	PEB	C4B-NB-C1B	-2.13	102.51	106.51
29	DO	202	PEB	CHA-C1B-NB	-2.13	120.49	124.93
29	PB	202	PEB	OD-C4D-C3D	-2.13	124.65	129.46
29	PM	202	PEB	OD-C4D-C3D	-2.13	124.65	129.46
29	ZJ	203	PEB	CHA-C1B-NB	-2.12	120.49	124.93
29	ZL	203	PEB	CHA-C1B-NB	-2.12	120.49	124.93
29	JF	1002	PEB	CMC-C3C-C2C	-2.12	120.94	124.94
29	JI	1002	PEB	CMC-C3C-C2C	-2.12	120.94	124.94
29	j7	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	j9	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	ZJ	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	ZL	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	jF	201	PEB	C4B-NB-C1B	-2.12	102.51	106.51
29	jI	201	PEB	C4B-NB-C1B	-2.12	102.51	106.51
31	vP	1001	CYC	C2A-C1A-NA	2.12	113.14	110.05
29	J4	201	PEB	CHA-C1B-C2B	2.12	130.36	124.90
29	RB	203	PEB	OD-C4D-C3D	-2.12	124.65	129.46
29	RM	203	PEB	OD-C4D-C3D	-2.12	124.65	129.46
29	FC	201	PEB	CAC-CBC-CGC	-2.12	107.81	113.76
29	FE	201	PEB	CAC-CBC-CGC	-2.12	107.81	113.76
29	eB	202	PEB	OD-C4D-C3D	-2.12	124.65	129.46
29	eM	202	PEB	OD-C4D-C3D	-2.12	124.65	129.46
29	KB	202	PEB	OD-C4D-ND	-2.12	122.79	125.93
29	KM	202	PEB	OD-C4D-ND	-2.12	122.79	125.93
29	IJ	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	IL	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	cF	202	PEB	CAC-CBC-CGC	-2.12	107.81	113.76
29	cI	202	PEB	CAC-CBC-CGC	-2.12	107.81	113.76
31	pP	1001	CYC	C1A-C2A-C3A	-2.12	104.44	106.78
29	BA	201	PEB	C1B-C2B-C3B	-2.12	104.07	106.51
29	BN	201	PEB	C1B-C2B-C3B	-2.12	104.07	106.51
29	JA	201	PEB	C4B-NB-C1B	-2.12	102.51	106.51
29	JN	201	PEB	C4B-NB-C1B	-2.12	102.51	106.51
29	IJ	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
29	IL	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
29	EB	202	PEB	OD-C4D-ND	-2.12	122.79	125.93
29	EM	202	PEB	OD-C4D-ND	-2.12	122.79	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UF	202	PEB	C4B-NB-C1B	-2.12	102.51	106.51
29	UI	202	PEB	C4B-NB-C1B	-2.12	102.51	106.51
29	TF	202	PEB	CAC-CBC-CGC	-2.12	107.81	113.76
29	TI	202	PEB	CAC-CBC-CGC	-2.12	107.81	113.76
29	Z7	202	PEB	C2B-C1B-NB	2.12	115.06	110.53
29	Z9	202	PEB	C2B-C1B-NB	2.12	115.06	110.53
29	O7	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	O9	201	PEB	CAB-C3B-C4B	2.12	128.76	125.01
31	mP	1001	CYC	C2A-C1A-NA	2.12	113.13	110.05
29	B4	201	PEB	CHA-C1B-C2B	2.12	130.35	124.90
29	lF	202	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	lI	202	PEB	CAB-C3B-C4B	2.12	128.76	125.01
29	iF	203	PEB	CAC-CBC-CGC	-2.12	107.82	113.76
29	iI	203	PEB	CAC-CBC-CGC	-2.12	107.82	113.76
29	bF	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	jF	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	bI	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	jI	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	dF	202	PEB	CAB-CBB-CGB	-2.12	109.04	113.60
29	dI	202	PEB	CAB-CBB-CGB	-2.12	109.04	113.60
29	FJ	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	FL	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	IJ	203	PEB	CMB-C2B-C1B	2.12	128.33	125.06
29	IL	203	PEB	CMB-C2B-C1B	2.12	128.33	125.06
29	MA	401	PEB	OD-C4D-C3D	-2.12	124.66	129.46
29	VB	203	PEB	OD-C4D-C3D	-2.12	124.66	129.46
29	VM	203	PEB	OD-C4D-C3D	-2.12	124.66	129.46
29	RJ	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	RL	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	AC	201	PEB	CHC-C4C-C3C	-2.12	126.72	130.34
29	AE	201	PEB	CHC-C4C-C3C	-2.12	126.72	130.34
29	FA	202	PEB	C2B-C1B-NB	2.12	115.05	110.53
29	FN	202	PEB	C2B-C1B-NB	2.12	115.05	110.53
29	N2	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	l7	201	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	l9	201	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	DF	1002	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	DI	1002	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	NR	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	JA	202	PEB	CHA-C4A-NA	-2.12	122.69	125.20
29	JN	202	PEB	CHA-C4A-NA	-2.12	122.69	125.20
29	ZF	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZI	201	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	eJ	201	PEB	CHC-C1D-ND	-2.12	111.49	113.95
29	eL	201	PEB	CHC-C1D-ND	-2.12	111.49	113.95
29	JJ	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	JL	203	PEB	CHA-C1B-NB	-2.12	120.50	124.93
29	hF	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	hI	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	MQ	407	PEB	CHA-C1B-C2B	2.12	130.34	124.90
29	DA	201	PEB	C1B-C2B-C3B	-2.12	104.08	106.51
29	DN	201	PEB	C1B-C2B-C3B	-2.12	104.08	106.51
29	HF	1002	PEB	CMC-C3C-C2C	-2.12	120.95	124.94
29	HI	1002	PEB	CMC-C3C-C2C	-2.12	120.95	124.94
29	mF	203	PEB	CAC-CBC-CGC	-2.12	107.83	113.76
29	mI	203	PEB	CAC-CBC-CGC	-2.12	107.83	113.76
29	RR	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	lB	202	PEB	OD-C4D-ND	-2.12	122.80	125.93
29	lM	202	PEB	OD-C4D-ND	-2.12	122.80	125.93
29	UF	202	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	UI	202	PEB	CHB-C4B-NB	-2.12	125.89	128.83
29	i7	203	PEB	C1B-C2B-C3B	-2.12	104.08	106.51
29	i9	203	PEB	C1B-C2B-C3B	-2.12	104.08	106.51
29	TF	201	PEB	C1C-CHB-C4B	-2.12	126.28	128.81
29	R2	202	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	HK	1002	PEB	CAB-C3B-C4B	2.12	128.75	125.01
29	VF	203	PEB	CAC-CBC-CGC	-2.11	107.83	113.76
29	VI	203	PEB	CAC-CBC-CGC	-2.11	107.83	113.76
29	DJ	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	DL	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	xL	302	PEB	CHA-C1B-C2B	2.11	130.34	124.90
29	bJ	203	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	rJ	203	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	vJ	202	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	bL	203	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	rL	203	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	vL	202	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	PJ	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	tJ	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	PL	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	tL	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	aF	203	PEB	CAC-CBC-CGC	-2.11	107.83	113.76
29	aI	203	PEB	CAC-CBC-CGC	-2.11	107.83	113.76
29	rJ	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	rL	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
29	D3	202	PEB	CHA-C1B-NB	-2.11	120.51	124.93
29	d7	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	d9	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	lJ	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	lL	201	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	DA	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
29	DN	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
29	RF	202	PEB	CAC-CBC-CGC	-2.11	107.83	113.76
29	RI	202	PEB	CAC-CBC-CGC	-2.11	107.83	113.76
29	CB	202	PEB	OD-C4D-ND	-2.11	122.80	125.93
29	CM	202	PEB	OD-C4D-ND	-2.11	122.80	125.93
29	gB	202	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	gM	202	PEB	CAB-C3B-C4B	2.11	128.75	125.01
29	F4	201	PEB	CHA-C1B-C2B	2.11	130.33	124.90
29	M4	203	PEB	CMB-C2B-C1B	2.11	128.32	125.06
29	ZF	201	PEB	C2A-C1A-NA	2.11	110.09	108.27
29	ZI	201	PEB	C2A-C1A-NA	2.11	110.09	108.27
29	TJ	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	TL	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	HA	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
29	HN	202	PEB	C2B-C1B-NB	2.11	115.04	110.53
29	hJ	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	hL	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	kJ	201	PEB	CHC-C1D-ND	-2.11	111.50	113.95
29	kL	201	PEB	CHC-C1D-ND	-2.11	111.50	113.95
29	XJ	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	XL	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	JB	202	PEB	CAB-C3B-C4B	2.11	128.74	125.01
29	JM	202	PEB	CAB-C3B-C4B	2.11	128.74	125.01
29	QF	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
29	QI	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
29	HJ	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
29	HL	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
29	NF	1002	PEB	CMC-C3C-C2C	-2.11	120.96	124.94
29	NI	1002	PEB	CMC-C3C-C2C	-2.11	120.96	124.94
29	eF	203	PEB	CAC-CBC-CGC	-2.11	107.84	113.76
29	eI	203	PEB	CAC-CBC-CGC	-2.11	107.84	113.76
29	nJ	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	nL	203	PEB	CHA-C1B-NB	-2.11	120.52	124.93
29	BA	202	PEB	CHA-C4A-NA	-2.11	122.70	125.20
29	BN	202	PEB	CHA-C4A-NA	-2.11	122.70	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DQ	203	PEB	C1B-C2B-C3B	-2.11	104.08	106.51
29	T7	203	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
29	T9	203	PEB	C1B-C2B-C3B	-2.11	104.09	106.51
29	IB	202	PEB	OD-C4D-ND	-2.11	122.81	125.93
29	IM	202	PEB	OD-C4D-ND	-2.11	122.81	125.93
29	S7	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
29	S9	202	PEB	C2B-C1B-NB	2.11	115.03	110.53
29	bJ	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
29	bL	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
29	e7	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
29	e9	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
29	ZF	201	PEB	C4B-NB-C1B	-2.11	102.54	106.51
29	ZI	201	PEB	C4B-NB-C1B	-2.11	102.54	106.51
29	kB	202	PEB	CAB-C3B-C4B	2.11	128.74	125.01
29	kM	202	PEB	CAB-C3B-C4B	2.11	128.74	125.01
29	fF	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
29	fI	201	PEB	CHB-C4B-NB	-2.11	125.90	128.83
29	CD	202	PEB	CAC-CBC-CGC	-2.11	107.85	113.76
29	E4	202	PEB	CAC-CBC-CGC	-2.11	107.85	113.76
29	LA	202	PEB	CHA-C4A-NA	-2.11	122.70	125.20
29	LN	202	PEB	CHA-C4A-NA	-2.11	122.70	125.20
29	YB	201	PEB	CAB-C3B-C4B	2.11	128.74	125.01
29	YM	201	PEB	CAB-C3B-C4B	2.11	128.74	125.01
29	Y1	201	PEB	C4B-NB-C1B	-2.11	102.54	106.51
29	YK	201	PEB	C4B-NB-C1B	-2.11	102.54	106.51
29	bF	201	PEB	C2A-C1A-NA	2.11	110.09	108.27
29	bI	201	PEB	C2A-C1A-NA	2.11	110.09	108.27
29	G5	202	PEB	CHA-C1B-NB	-2.11	120.53	124.93
29	V2	202	PEB	CAC-CBC-CGC	-2.11	107.85	113.76
29	HC	202	PEB	C1C-CHB-C4B	2.11	131.32	128.81
29	HE	202	PEB	C1C-CHB-C4B	2.11	131.32	128.81
29	jJ	201	PEB	CAB-C3B-C4B	2.11	128.73	125.01
29	jL	201	PEB	CAB-C3B-C4B	2.11	128.73	125.01
29	ZB	203	PEB	OD-C4D-C3D	-2.11	124.69	129.46
29	ZM	203	PEB	OD-C4D-C3D	-2.11	124.69	129.46
29	JJ	201	PEB	CAB-C3B-C4B	2.11	128.73	125.01
29	JL	201	PEB	CAB-C3B-C4B	2.11	128.73	125.01
29	tJ	202	PEB	CHA-C1B-NB	-2.11	120.53	124.93
29	tL	202	PEB	CHA-C1B-NB	-2.11	120.53	124.93
29	f7	202	PEB	C2B-C1B-NB	2.11	115.02	110.53
29	f9	202	PEB	C2B-C1B-NB	2.11	115.02	110.53
29	UF	203	PEB	CAB-C3B-C4B	2.11	128.73	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UI	203	PEB	CAB-C3B-C4B	2.11	128.73	125.01
29	h7	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
29	h9	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
29	PF	203	PEB	CAC-CBC-CGC	-2.10	107.86	113.76
29	PI	203	PEB	CAC-CBC-CGC	-2.10	107.86	113.76
29	bF	202	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	bI	202	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	b7	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
29	b9	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
29	NJ	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	NL	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	aB	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
29	aM	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
29	f7	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	f9	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	cB	202	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	iB	202	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	cM	202	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	iM	202	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	VJ	202	PEB	CHA-C1B-NB	-2.10	120.53	124.93
29	VL	202	PEB	CHA-C1B-NB	-2.10	120.53	124.93
29	QF	201	PEB	C2A-C1A-NA	2.10	110.09	108.27
29	QI	201	PEB	C2A-C1A-NA	2.10	110.09	108.27
29	dB	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
29	dM	202	PEB	OD-C4D-ND	-2.10	122.81	125.93
29	ED	201	PEB	CAC-CBC-CGC	-2.10	107.86	113.76
29	RR	202	PEB	CHA-C4A-NA	2.10	127.70	125.20
29	ZJ	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
29	ZL	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
29	W7	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
29	W9	202	PEB	C2B-C1B-NB	2.10	115.02	110.53
29	a7	203	PEB	CBC-CAC-C2C	-2.10	109.03	112.62
29	a9	203	PEB	CBC-CAC-C2C	-2.10	109.03	112.62
29	EC	201	PEB	CHC-C4C-C3C	-2.10	126.75	130.34
29	EE	201	PEB	CHC-C4C-C3C	-2.10	126.75	130.34
29	vJ	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	vL	201	PEB	CAB-C3B-C4B	2.10	128.73	125.01
29	BJ	203	PEB	CHA-C1B-NB	-2.10	120.54	124.93
29	BL	203	PEB	CHA-C1B-NB	-2.10	120.54	124.93
29	AC	203	PEB	C1C-CHB-C4B	2.10	131.32	128.81
29	AE	203	PEB	C1C-CHB-C4B	2.10	131.32	128.81
29	k7	203	PEB	CBC-CAC-C2C	-2.10	109.03	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k9	203	PEB	CBC-CAC-C2C	-2.10	109.03	112.62
29	DA	202	PEB	CHA-C4A-NA	-2.10	122.71	125.20
29	DN	202	PEB	CHA-C4A-NA	-2.10	122.71	125.20
29	k7	201	PEB	CHB-C4B-NB	-2.10	125.91	128.83
29	k9	201	PEB	CHB-C4B-NB	-2.10	125.91	128.83
29	GB	202	PEB	OD-C4D-ND	-2.10	122.82	125.93
29	GM	202	PEB	OD-C4D-ND	-2.10	122.82	125.93
29	g1	201	PEB	C4B-NB-C1B	-2.10	102.55	106.51
29	gK	201	PEB	C4B-NB-C1B	-2.10	102.55	106.51
29	I4	202	PEB	CAC-CBC-CGC	-2.10	107.87	113.76
29	fF	202	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	fI	202	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	HA	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	fF	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	fI	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	HN	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	LA	202	PEB	C2B-C1B-NB	2.10	115.01	110.53
29	LN	202	PEB	C2B-C1B-NB	2.10	115.01	110.53
29	KD	202	PEB	CAC-CBC-CGC	-2.10	107.87	113.76
29	GC	201	PEB	CHC-C4C-C3C	-2.10	126.75	130.34
29	GE	201	PEB	CHC-C4C-C3C	-2.10	126.75	130.34
29	DJ	202	PEB	CHA-C1B-NB	-2.10	120.54	124.93
29	DL	202	PEB	CHA-C1B-NB	-2.10	120.54	124.93
29	X2	201	PEB	CAC-CBC-CGC	-2.10	107.87	113.76
29	c7	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
29	c9	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
29	qJ	201	PEB	CHC-C1D-ND	-2.10	111.51	113.95
29	qL	201	PEB	CHC-C1D-ND	-2.10	111.51	113.95
29	BA	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	hF	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	hI	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	BN	201	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	Y7	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	Y9	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	R7	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
29	R9	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
29	sJ	203	PEB	CMB-C2B-C1B	2.10	128.29	125.06
29	sL	203	PEB	CMB-C2B-C1B	2.10	128.29	125.06
31	rP	1001	CYC	C2A-C1A-NA	2.10	113.10	110.05
29	U7	201	PEB	CAB-CBB-CGB	-2.10	109.09	113.60
29	b7	201	PEB	CAB-CBB-CGB	-2.10	109.09	113.60
29	U9	201	PEB	CAB-CBB-CGB	-2.10	109.09	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b9	201	PEB	CAB-CBB-CGB	-2.10	109.09	113.60
29	YF	203	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
29	YI	203	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
29	e7	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	e9	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	fJ	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	fL	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	R2	202	PEB	CHA-C4A-NA	2.10	127.70	125.20
29	pJ	202	PEB	CMB-C2B-C1B	2.10	128.29	125.06
29	pL	202	PEB	CMB-C2B-C1B	2.10	128.29	125.06
29	jJ	203	PEB	CHA-C1B-NB	-2.10	120.55	124.93
29	pJ	203	PEB	CHA-C1B-NB	-2.10	120.55	124.93
29	jL	203	PEB	CHA-C1B-NB	-2.10	120.55	124.93
29	pL	203	PEB	CHA-C1B-NB	-2.10	120.55	124.93
29	UF	202	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	UI	202	PEB	C2A-C1A-NA	2.10	110.08	108.27
29	KJ	201	PEB	CHC-C1D-ND	-2.10	111.51	113.95
29	KL	201	PEB	CHC-C1D-ND	-2.10	111.51	113.95
29	LJ	202	PEB	CHA-C1B-NB	-2.10	120.55	124.93
29	LL	202	PEB	CHA-C1B-NB	-2.10	120.55	124.93
29	QB	204	PEB	OD-C4D-ND	-2.10	122.82	125.93
29	QM	204	PEB	OD-C4D-ND	-2.10	122.82	125.93
31	CP	1001	CYC	C2A-C1A-NA	2.10	113.10	110.05
29	gF	203	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
29	gI	203	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
29	VJ	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	VL	201	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	c7	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	c9	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	g7	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
29	g9	201	PEB	CHB-C4B-NB	-2.10	125.92	128.83
29	ZF	202	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	ZI	202	PEB	CAB-C3B-C4B	2.10	128.72	125.01
29	KC	202	PEB	CHC-C4C-C3C	-2.10	126.76	130.34
29	KE	202	PEB	CHC-C4C-C3C	-2.10	126.76	130.34
29	C4	202	PEB	CAC-CBC-CGC	-2.10	107.88	113.76
29	d7	202	PEB	C2B-C1B-NB	2.10	115.00	110.53
29	d9	202	PEB	C2B-C1B-NB	2.10	115.00	110.53
29	i7	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	i9	203	PEB	CBC-CAC-C2C	-2.10	109.04	112.62
29	wJ	302	PEB	CHA-C1B-C2B	2.10	130.29	124.90
29	hJ	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	hL	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	Z7	201	PEB	CAB-CBB-CGB	-2.09	109.09	113.60
29	Z9	201	PEB	CAB-CBB-CGB	-2.09	109.09	113.60
29	BA	202	PEB	C2B-C1B-NB	2.09	115.00	110.53
29	BN	202	PEB	C2B-C1B-NB	2.09	115.00	110.53
29	m7	201	PEB	CHB-C4B-NB	-2.09	125.92	128.83
29	m9	201	PEB	CHB-C4B-NB	-2.09	125.92	128.83
29	OF	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	OI	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	RJ	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	RL	201	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	OB	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	OM	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	WF	201	PEB	C2A-C1A-NA	2.09	110.08	108.27
29	WI	201	PEB	C2A-C1A-NA	2.09	110.08	108.27
29	KB	203	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	ZB	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	KM	203	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	ZM	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	xJ	302	PEB	CHA-C1B-C2B	2.09	130.28	124.90
29	FA	201	PEB	C1B-C2B-C3B	-2.09	104.10	106.51
29	FN	201	PEB	C1B-C2B-C3B	-2.09	104.10	106.51
29	DD	202	PEB	CHA-C1B-NB	-2.09	120.55	124.93
29	fB	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	hB	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	KC	203	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	KE	203	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	fM	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	hM	202	PEB	OD-C4D-ND	-2.09	122.83	125.93
29	S7	201	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
29	S9	201	PEB	CAB-CBB-CGB	-2.09	109.10	113.60
29	wL	302	PEB	CHA-C1B-C2B	2.09	130.28	124.90
29	HB	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	aB	203	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	HM	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	aM	203	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	IC	201	PEB	CHC-C4C-C3C	-2.09	126.77	130.34
29	IE	201	PEB	CHC-C4C-C3C	-2.09	126.77	130.34
29	KC	201	PEB	C1C-CHB-C4B	2.09	131.31	128.81
29	KE	201	PEB	C1C-CHB-C4B	2.09	131.31	128.81
29	SF	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01
29	SI	202	PEB	CAB-C3B-C4B	2.09	128.71	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	kP	1001	CYC	C1B-CHB-C4A	2.09	133.19	128.08
29	HJ	202	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	HL	202	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	M4	202	PEB	CAC-CBC-CGC	-2.09	107.90	113.76
29	G8	202	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	NJ	203	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	NL	203	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	P1	201	PEB	C4B-NB-C1B	-2.09	102.57	106.51
29	PK	201	PEB	C4B-NB-C1B	-2.09	102.57	106.51
29	U7	202	PEB	C2B-C1B-NB	2.09	114.99	110.53
29	U9	202	PEB	C2B-C1B-NB	2.09	114.99	110.53
29	HF	1002	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	QF	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	HI	1002	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	QI	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	BJ	201	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	BL	201	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	XR	202	PEB	CHA-C4A-NA	2.09	127.69	125.20
31	eP	1001	CYC	C2A-C1A-NA	2.09	113.09	110.05
29	c1	201	PEB	C4B-NB-C1B	-2.09	102.57	106.51
29	cK	201	PEB	C4B-NB-C1B	-2.09	102.57	106.51
29	FA	201	PEB	CBB-CAB-C3B	2.09	118.43	112.63
29	FN	201	PEB	CBB-CAB-C3B	2.09	118.43	112.63
30	A1	305	PUB	CMA-C2A-C3A	2.09	133.96	129.67
30	AK	305	PUB	CMA-C2A-C3A	2.09	133.96	129.67
29	fJ	203	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	fL	203	PEB	CHA-C1B-NB	-2.09	120.56	124.93
29	ID	202	PEB	CAC-CBC-CGC	-2.09	107.90	113.76
29	Y7	203	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
29	Y9	203	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
29	CJ	201	PEB	CHC-C1D-ND	-2.09	111.52	113.95
29	CL	201	PEB	CHC-C1D-ND	-2.09	111.52	113.95
30	A1	305	PUB	OA-C1A-C2A	-2.09	118.99	128.48
30	AK	305	PUB	OA-C1A-C2A	-2.09	118.99	128.48
29	RB	203	PEB	CAB-CBB-CGB	2.09	118.10	113.60
29	RM	203	PEB	CAB-CBB-CGB	2.09	118.10	113.60
31	uP	1001	CYC	C1B-CHB-C4A	2.09	133.18	128.08
29	H5	202	PEB	CHA-C1B-NB	-2.09	120.56	124.93
31	yP	1001	CYC	CHA-C1A-NA	-2.09	125.93	128.83
31	HP	1001	CYC	C1B-CHB-C4A	2.09	133.18	128.08
29	P7	203	PEB	CBC-CAC-C2C	-2.09	109.06	112.62
29	P9	203	PEB	CBC-CAC-C2C	-2.09	109.06	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	JF	1002	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	JI	1002	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	CG	201	PEB	CHB-C4B-C3B	-2.09	120.50	125.32
29	CQ	201	PEB	CHB-C4B-C3B	-2.09	120.50	125.32
29	GD	202	PEB	CAC-CBC-CGC	-2.09	107.91	113.76
29	L4	202	PEB	CHA-C1B-NB	-2.09	120.57	124.93
29	HA	201	PEB	CBB-CAB-C3B	2.09	118.43	112.63
29	HN	201	PEB	CBB-CAB-C3B	2.09	118.43	112.63
31	MP	1001	CYC	C1B-CHB-C4A	2.09	133.18	128.08
29	G4	202	PEB	CAC-CBC-CGC	-2.09	107.91	113.76
29	AF	305	PEB	CMC-C3C-C2C	2.09	128.88	124.94
29	AI	305	PEB	CMC-C3C-C2C	2.09	128.88	124.94
30	BB	302	PUB	CBA-CAA-C3A	-2.09	109.81	112.98
30	BM	302	PUB	CBA-CAA-C3A	-2.09	109.81	112.98
29	g7	203	PEB	CBC-CAC-C2C	-2.09	109.06	112.62
29	g9	203	PEB	CBC-CAC-C2C	-2.09	109.06	112.62
29	Y7	201	PEB	CHB-C4B-NB	-2.09	125.93	128.83
29	Y9	201	PEB	CHB-C4B-NB	-2.09	125.93	128.83
29	D4	202	PEB	CHA-C1B-NB	-2.09	120.57	124.93
29	V7	203	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
29	V9	203	PEB	C1B-C2B-C3B	-2.09	104.11	106.51
29	RB	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	wL	302	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	RM	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	sJ	201	PEB	CHC-C1D-ND	-2.09	111.53	113.95
29	sL	201	PEB	CHC-C1D-ND	-2.09	111.53	113.95
29	N2	202	PEB	CAC-CBC-CGC	-2.09	107.91	113.76
31	OP	1001	CYC	C1B-CHB-C4A	2.09	133.18	128.08
29	UB	202	PEB	OD-C4D-ND	-2.09	122.84	125.93
29	MQ	401	PEB	OD-C4D-ND	-2.09	122.84	125.93
29	FB	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	dJ	201	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	dL	201	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	FM	202	PEB	CAB-C3B-C4B	2.09	128.70	125.01
29	cF	202	PEB	CAB-CBB-CGB	-2.09	109.12	113.60
29	cI	202	PEB	CAB-CBB-CGB	-2.09	109.12	113.60
29	X2	201	PEB	CHA-C4A-NA	2.08	127.68	125.20
31	SP	1001	CYC	C1B-CHB-C4A	2.08	133.17	128.08
29	Q7	201	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
29	Q9	201	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
29	VR	202	PEB	CAC-CBC-CGC	-2.08	107.92	113.76
29	AJ	203	PEB	CMB-C2B-C1B	2.08	128.27	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BJ	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	PJ	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	AL	203	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	BL	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	PL	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
31	PP	1001	CYC	C2A-C1A-NA	2.08	113.08	110.05
29	j7	202	PEB	C2B-C1B-NB	2.08	114.98	110.53
29	j9	202	PEB	C2B-C1B-NB	2.08	114.98	110.53
29	TR	202	PEB	CHA-C4A-NA	2.08	127.68	125.20
29	l7	201	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
29	l9	201	PEB	CAB-CBB-CGB	-2.08	109.12	113.60
29	nJ	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	pJ	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	nL	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	pL	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	uJ	202	PEB	CHC-C1D-ND	-2.08	111.53	113.95
29	uL	202	PEB	CHC-C1D-ND	-2.08	111.53	113.95
29	OR	202	PEB	OD-C4D-ND	-2.08	122.84	125.93
29	B5	202	PEB	CHA-C1B-NB	-2.08	120.57	124.93
29	V1	201	PEB	C4B-NB-C1B	-2.08	102.58	106.51
29	VK	201	PEB	C4B-NB-C1B	-2.08	102.58	106.51
29	V7	201	PEB	CHB-C4B-NB	-2.08	125.94	128.83
29	V9	201	PEB	CHB-C4B-NB	-2.08	125.94	128.83
31	RP	1001	CYC	C2A-C1A-NA	2.08	113.08	110.05
29	bJ	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	bL	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	jF	201	PEB	C2A-C1A-NA	2.08	110.07	108.27
29	lF	201	PEB	C2A-C1A-NA	2.08	110.07	108.27
29	jI	201	PEB	C2A-C1A-NA	2.08	110.07	108.27
29	lI	201	PEB	C2A-C1A-NA	2.08	110.07	108.27
29	W1	202	PEB	CHA-C4A-NA	-2.08	122.73	125.20
29	WK	202	PEB	CHA-C4A-NA	-2.08	122.73	125.20
29	XJ	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	XL	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
31	iP	1001	CYC	C2A-C1A-NA	2.08	113.08	110.05
30	MQ	404	PUB	CMD-C2D-C3D	2.08	130.89	127.77
30	AF	303	PUB	C1D-CHC-C4C	-2.08	108.84	113.37
30	AI	303	PUB	C1D-CHC-C4C	-2.08	108.84	113.37
29	LJ	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	wJ	302	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	LL	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	TB	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	TM	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60
29	B8	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
29	JA	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
29	JN	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
29	T2	202	PEB	CAC-CBC-CGC	-2.08	107.92	113.76
29	QB	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	QM	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
31	WP	1001	CYC	CHA-C1A-NA	-2.08	125.94	128.83
30	MG	402	PUB	CMD-C2D-C3D	2.08	130.89	127.77
29	EG	201	PEB	CHB-C4B-C3B	-2.08	120.51	125.32
29	EQ	201	PEB	CHB-C4B-C3B	-2.08	120.51	125.32
29	ZB	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60
29	ZM	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60
29	m1	201	PEB	C4B-NB-C1B	-2.08	102.59	106.51
29	mK	201	PEB	C4B-NB-C1B	-2.08	102.59	106.51
29	h7	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	h9	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	TF	202	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	TI	202	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	E4	202	PEB	OA-C1A-C2A	-2.08	124.52	126.17
29	T7	201	PEB	CHB-C4B-NB	-2.08	125.94	128.83
29	T9	201	PEB	CHB-C4B-NB	-2.08	125.94	128.83
29	f1	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	LF	1002	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	LI	1002	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	fK	201	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	k1	201	PEB	C4B-NB-C1B	-2.08	102.59	106.51
29	kK	201	PEB	C4B-NB-C1B	-2.08	102.59	106.51
29	hJ	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	uJ	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	hL	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	uL	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	OF	201	PEB	C2A-C1A-NA	2.08	110.07	108.27
29	OI	201	PEB	C2A-C1A-NA	2.08	110.07	108.27
29	LD	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
29	mB	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	NF	1002	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	NI	1002	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	mM	202	PEB	CAB-C3B-C4B	2.08	128.69	125.01
31	cP	1001	CYC	C2A-C1A-NA	2.08	113.07	110.05
29	kB	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60
29	kM	203	PEB	CAB-CBB-CGB	2.08	118.08	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f7	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	f9	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	AC	202	PEB	OD-C4D-ND	-2.08	122.85	125.93
29	AE	202	PEB	OD-C4D-ND	-2.08	122.85	125.93
29	nJ	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	nL	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	XR	202	PEB	CAC-CBC-CGC	-2.08	107.93	113.76
29	xL	302	PEB	CAB-C3B-C4B	2.08	128.69	125.01
29	F8	202	PEB	CHA-C1B-NB	-2.08	120.58	124.93
29	O7	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	O9	201	PEB	CAB-CBB-CGB	-2.08	109.13	113.60
29	O7	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
29	O9	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
31	NP	1001	CYC	C2A-C1A-NA	2.08	113.07	110.05
29	NR	202	PEB	CAC-CBC-CGC	-2.08	107.93	113.76
29	FA	201	PEB	O1B-CGB-CBB	-2.08	116.41	123.08
29	FN	201	PEB	O1B-CGB-CBB	-2.08	116.41	123.08
29	DB	203	PEB	CAB-CBB-CGB	2.08	118.07	113.60
29	DM	203	PEB	CAB-CBB-CGB	2.08	118.07	113.60
29	SF	201	PEB	C2A-C1A-NA	2.08	110.06	108.27
29	SI	201	PEB	C2A-C1A-NA	2.08	110.06	108.27
29	KG	201	PEB	CHB-C4B-C3B	-2.08	120.52	125.32
29	KQ	201	PEB	CHB-C4B-C3B	-2.08	120.52	125.32
29	HA	202	PEB	CHA-C1B-NB	-2.08	120.59	124.93
29	HN	202	PEB	CHA-C1B-NB	-2.08	120.59	124.93
31	AP	1001	CYC	C2A-C1A-NA	2.08	113.07	110.05
29	rJ	201	PEB	CAB-C3B-C4B	2.08	128.68	125.01
29	rL	201	PEB	CAB-C3B-C4B	2.08	128.68	125.01
29	HA	202	PEB	CHA-C4A-NA	-2.08	122.74	125.20
29	HN	202	PEB	CHA-C4A-NA	-2.08	122.74	125.20
29	R1	201	PEB	C4B-NB-C1B	-2.08	102.60	106.51
29	RK	201	PEB	C4B-NB-C1B	-2.08	102.60	106.51
29	l7	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
29	l9	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
29	aF	203	PEB	CAB-CBB-CGB	-2.08	109.14	113.60
29	aI	203	PEB	CAB-CBB-CGB	-2.08	109.14	113.60
29	FA	202	PEB	CHA-C1B-NB	-2.08	120.59	124.93
29	FN	202	PEB	CHA-C1B-NB	-2.08	120.59	124.93
29	W7	201	PEB	CAB-CBB-CGB	-2.08	109.14	113.60
29	W9	201	PEB	CAB-CBB-CGB	-2.08	109.14	113.60
29	H1	1002	PEB	CAB-C3B-C4B	2.08	128.68	125.01
29	K4	202	PEB	CAC-CBC-CGC	-2.08	107.94	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Q7	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
29	Q9	202	PEB	C2B-C1B-NB	2.08	114.96	110.53
29	HD	202	PEB	CHA-C1B-NB	-2.08	120.59	124.93
29	dJ	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
29	dL	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
29	P2	201	PEB	CAC-CBC-CGC	-2.08	107.94	113.76
29	MD	202	PEB	CAC-CBC-CGC	-2.07	107.94	113.76
29	TR	202	PEB	CAC-CBC-CGC	-2.07	107.94	113.76
29	RF	202	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
29	RI	202	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
31	IP	1001	CYC	C1B-CHB-C4A	2.07	133.15	128.08
30	AF	302	PUB	CAC-C2C-C3C	2.07	131.74	127.88
30	AI	302	PUB	CAC-C2C-C3C	2.07	131.74	127.88
29	jJ	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
29	jL	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
29	IJ	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	cJ	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	IL	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	cL	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
31	1P	1002	CYC	O1A-CGA-CBA	-2.07	116.42	123.08
29	e1	201	PEB	C4B-NB-C1B	-2.07	102.60	106.51
29	eK	201	PEB	C4B-NB-C1B	-2.07	102.60	106.51
29	NJ	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
29	NL	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
29	VB	202	PEB	CAB-C3B-C4B	2.07	128.68	125.01
29	VM	202	PEB	CAB-C3B-C4B	2.07	128.68	125.01
29	T7	203	PEB	CBC-CAC-C2C	-2.07	109.08	112.62
29	T9	203	PEB	CBC-CAC-C2C	-2.07	109.08	112.62
29	JA	201	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
29	JN	201	PEB	C1B-C2B-C3B	-2.07	104.13	106.51
29	XB	202	PEB	CAB-CBB-CGB	2.07	118.06	113.60
29	XM	202	PEB	CAB-CBB-CGB	2.07	118.06	113.60
29	WJ	201	PEB	CMB-C2B-C1B	2.07	128.26	125.06
29	WL	201	PEB	CMB-C2B-C1B	2.07	128.26	125.06
31	hP	1001	CYC	C1B-CHB-C4A	2.07	133.15	128.08
29	HA	201	PEB	O1B-CGB-CBB	-2.07	116.42	123.08
29	HN	201	PEB	O1B-CGB-CBB	-2.07	116.42	123.08
31	UP	1001	CYC	C1B-CHB-C4A	2.07	133.15	128.08
29	A7	301	PEB	C2B-C1B-NB	2.07	114.95	110.53
29	A9	301	PEB	C2B-C1B-NB	2.07	114.95	110.53
29	CC	202	PEB	OD-C4D-ND	-2.07	122.86	125.93
29	GC	202	PEB	OD-C4D-ND	-2.07	122.86	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	CE	202	PEB	OD-C4D-ND	-2.07	122.86	125.93
29	GE	202	PEB	OD-C4D-ND	-2.07	122.86	125.93
29	b1	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	bK	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	j7	201	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
29	j9	201	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
29	BA	201	PEB	CBB-CAB-C3B	2.07	118.38	112.63
29	BN	201	PEB	CBB-CAB-C3B	2.07	118.38	112.63
29	EJ	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	UJ	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	gJ	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	EL	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	UL	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	gL	201	PEB	CHC-C1D-ND	-2.07	111.54	113.95
29	FF	1002	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	FI	1002	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	FB	203	PEB	CAB-CBB-CGB	2.07	118.06	113.60
29	FM	203	PEB	CAB-CBB-CGB	2.07	118.06	113.60
31	jP	1001	CYC	C1B-CHB-C4A	2.07	133.14	128.08
29	i7	201	PEB	CHB-C4B-NB	-2.07	125.95	128.83
29	i9	201	PEB	CHB-C4B-NB	-2.07	125.95	128.83
29	LA	201	PEB	O1B-CGB-CBB	-2.07	116.43	123.08
29	LN	201	PEB	O1B-CGB-CBB	-2.07	116.43	123.08
29	R7	203	PEB	CBC-CAC-C2C	-2.07	109.08	112.62
29	R9	203	PEB	CBC-CAC-C2C	-2.07	109.08	112.62
29	jF	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	jI	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	T1	201	PEB	C4B-NB-C1B	-2.07	102.61	106.51
29	TK	201	PEB	C4B-NB-C1B	-2.07	102.61	106.51
29	P7	201	PEB	CHB-C4B-NB	-2.07	125.95	128.83
29	P9	201	PEB	CHB-C4B-NB	-2.07	125.95	128.83
29	FD	202	PEB	CAA-C3A-C4A	-2.07	107.36	112.67
29	V7	203	PEB	CBC-CAC-C2C	-2.07	109.09	112.62
29	m7	203	PEB	CBC-CAC-C2C	-2.07	109.09	112.62
29	V9	203	PEB	CBC-CAC-C2C	-2.07	109.09	112.62
29	m9	203	PEB	CBC-CAC-C2C	-2.07	109.09	112.62
29	GG	201	PEB	CHB-C4B-C3B	-2.07	120.54	125.32
29	GQ	201	PEB	CHB-C4B-C3B	-2.07	120.54	125.32
31	fP	1001	CYC	C1B-CHB-C4A	2.07	133.14	128.08
31	qP	1001	CYC	C1B-CHB-C4A	2.07	133.14	128.08
29	eF	203	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
29	eI	203	PEB	CAB-CBB-CGB	-2.07	109.15	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	gB	203	PEB	CAB-CBB-CGB	2.07	118.06	113.60
29	gM	203	PEB	CAB-CBB-CGB	2.07	118.06	113.60
29	S1	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	SK	201	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	iF	203	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
29	iI	203	PEB	CAB-CBB-CGB	-2.07	109.15	113.60
29	DA	202	PEB	CHA-C1B-NB	-2.07	120.61	124.93
29	DN	202	PEB	CHA-C1B-NB	-2.07	120.61	124.93
29	LD	202	PEB	CAA-C3A-C4A	-2.07	107.36	112.67
29	LB	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	LM	202	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	LA	201	PEB	C2A-C1A-NA	2.07	110.06	108.27
29	AF	305	PEB	C2A-C1A-NA	2.07	110.06	108.27
29	AI	305	PEB	C2A-C1A-NA	2.07	110.06	108.27
29	LN	201	PEB	C2A-C1A-NA	2.07	110.06	108.27
29	fJ	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
29	fL	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
31	lP	1001	CYC	C2A-C1A-NA	2.07	113.06	110.05
29	xJ	302	PEB	CAB-C3B-C4B	2.07	128.67	125.01
29	FJ	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
29	FL	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
29	a7	201	PEB	CHB-C4B-NB	-2.07	125.96	128.83
29	a9	201	PEB	CHB-C4B-NB	-2.07	125.96	128.83
29	d1	201	PEB	CAB-C3B-C4B	2.07	128.66	125.01
29	TB	202	PEB	CAB-C3B-C4B	2.07	128.66	125.01
29	dK	201	PEB	CAB-C3B-C4B	2.07	128.66	125.01
29	TM	202	PEB	CAB-C3B-C4B	2.07	128.66	125.01
29	R2	202	PEB	CAC-CBC-CGC	-2.07	107.96	113.76
29	RR	202	PEB	CAC-CBC-CGC	-2.07	107.96	113.76
31	FP	1001	CYC	C1B-CHB-C4A	2.07	133.13	128.08
31	XP	1001	CYC	C1B-CHB-C4A	2.07	133.13	128.08
29	D4	202	PEB	CAA-C3A-C4A	-2.07	107.37	112.67
29	DA	201	PEB	O1B-CGB-CBB	-2.07	116.44	123.08
29	DN	201	PEB	O1B-CGB-CBB	-2.07	116.44	123.08
29	PB	202	PEB	CAB-CBB-CGB	2.07	118.05	113.60
29	PM	202	PEB	CAB-CBB-CGB	2.07	118.05	113.60
29	FA	202	PEB	CHA-C4A-NA	-2.07	122.75	125.20
29	FN	202	PEB	CHA-C4A-NA	-2.07	122.75	125.20
29	JJ	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
29	JL	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
29	SJ	201	PEB	CHC-C1D-ND	-2.07	111.55	113.95
29	YJ	201	PEB	CHC-C1D-ND	-2.07	111.55	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SL	201	PEB	CHC-C1D-ND	-2.07	111.55	113.95
29	YL	201	PEB	CHC-C1D-ND	-2.07	111.55	113.95
29	IG	201	PEB	CHB-C4B-C3B	-2.07	120.55	125.32
29	IQ	201	PEB	CHB-C4B-C3B	-2.07	120.55	125.32
31	QP	1001	CYC	C1B-CHB-C4A	2.07	133.13	128.08
31	TP	1001	CYC	C2A-C1A-NA	2.07	113.05	110.05
29	U1	202	PEB	CAB-C3B-C4B	2.07	128.66	125.01
29	UK	202	PEB	CAB-C3B-C4B	2.07	128.66	125.01
29	BC	202	PEB	C1C-CHB-C4B	2.07	131.28	128.81
29	BE	202	PEB	C1C-CHB-C4B	2.07	131.28	128.81
29	d1	202	PEB	CHA-C4A-NA	-2.06	122.75	125.20
29	dK	202	PEB	CHA-C4A-NA	-2.06	122.75	125.20
29	BA	201	PEB	O1B-CGB-CBB	-2.06	116.45	123.08
29	BN	201	PEB	O1B-CGB-CBB	-2.06	116.45	123.08
29	VB	203	PEB	CAB-CBB-CGB	2.06	118.05	113.60
29	VM	203	PEB	CAB-CBB-CGB	2.06	118.05	113.60
29	DB	202	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	DM	202	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	GJ	201	PEB	CHC-C1D-ND	-2.06	111.55	113.95
29	GL	201	PEB	CHC-C1D-ND	-2.06	111.55	113.95
29	h1	201	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	hK	201	PEB	CAB-C3B-C4B	2.06	128.66	125.01
31	wP	1001	CYC	C1B-CHB-C4A	2.06	133.12	128.08
31	1P	1001	CYC	C1B-CHB-C4A	2.06	133.12	128.08
29	zL	501	PEB	CBC-CAC-C2C	-2.06	109.10	112.62
29	F4	202	PEB	CAA-C3A-C4A	-2.06	107.38	112.67
29	BB	301	PEB	CBA-CAA-C3A	2.06	118.06	113.47
29	BM	301	PEB	CBA-CAA-C3A	2.06	118.06	113.47
29	JA	201	PEB	CBB-CAB-C3B	2.06	118.36	112.63
29	JN	201	PEB	CBB-CAB-C3B	2.06	118.36	112.63
29	J1	1002	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	JK	1002	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	OJ	201	PEB	CHC-C1D-ND	-2.06	111.55	113.95
29	OL	201	PEB	CHC-C1D-ND	-2.06	111.55	113.95
29	PR	201	PEB	CAC-CBC-CGC	-2.06	107.98	113.76
29	LA	201	PEB	CBB-CAB-C3B	2.06	118.36	112.63
29	LN	201	PEB	CBB-CAB-C3B	2.06	118.36	112.63
29	mF	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	mI	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	HQ	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
31	nP	1001	CYC	C1B-CHB-C4A	2.06	133.12	128.08
29	HD	202	PEB	CAA-C3A-C4A	-2.06	107.38	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G4	201	PEB	CMA-C2A-C1A	-2.06	107.96	112.40
29	Z1	202	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	ZK	202	PEB	CAB-C3B-C4B	2.06	128.66	125.01
29	F4	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
31	tP	1001	CYC	C2A-C1A-NA	2.06	113.05	110.05
29	FJ	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
29	FL	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
29	eB	202	PEB	CAB-CBB-CGB	2.06	118.04	113.60
29	eM	202	PEB	CAB-CBB-CGB	2.06	118.04	113.60
29	JD	202	PEB	CAA-C3A-C4A	-2.06	107.38	112.67
29	H8	202	PEB	CHA-C1B-NB	-2.06	120.62	124.93
29	HB	203	PEB	CAB-CBB-CGB	2.06	118.04	113.60
29	HM	203	PEB	CAB-CBB-CGB	2.06	118.04	113.60
29	EC	202	PEB	OD-C4D-ND	-2.06	122.88	125.93
29	EE	202	PEB	OD-C4D-ND	-2.06	122.88	125.93
29	j1	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
29	jK	201	PEB	CAB-C3B-C4B	2.06	128.65	125.01
29	MJ	201	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	WJ	202	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	oJ	201	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	ML	201	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	WL	202	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	oL	201	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	T2	202	PEB	CHA-C4A-NA	2.06	127.65	125.20
29	d7	201	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	d9	201	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	VF	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	VI	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	MQ	403	PEB	C2B-C1B-NB	2.06	114.92	110.53
29	a1	201	PEB	C4B-NB-C1B	-2.06	102.63	106.51
29	aK	201	PEB	C4B-NB-C1B	-2.06	102.63	106.51
29	RJ	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
29	RL	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
29	PF	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	PI	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	JA	201	PEB	O1B-CGB-CBB	-2.06	116.47	123.08
29	JN	201	PEB	O1B-CGB-CBB	-2.06	116.47	123.08
29	ED	201	PEB	OA-C1A-C2A	-2.06	124.54	126.17
29	KD	202	PEB	OA-C1A-C2A	-2.06	124.54	126.17
31	vP	1001	CYC	CBD-CAD-C3D	-2.06	109.11	112.62
29	DA	201	PEB	CBB-CAB-C3B	2.06	118.35	112.63
29	DN	201	PEB	CBB-CAB-C3B	2.06	118.35	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	mJ	201	PEB	CHC-C1D-ND	-2.06	111.56	113.95
29	mL	201	PEB	CHC-C1D-ND	-2.06	111.56	113.95
31	pP	1001	CYC	C2A-C1A-NA	2.06	113.04	110.05
29	gF	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
29	gI	203	PEB	CAB-CBB-CGB	-2.06	109.17	113.60
31	YP	1000	CYC	O1A-CGA-CBA	-2.06	116.47	123.08
29	U2	201	PEB	O2C-CGC-CBC	2.06	120.64	114.03
29	UR	201	PEB	O2C-CGC-CBC	2.06	120.64	114.03
31	oP	1001	CYC	C1B-CHB-C4A	2.06	133.11	128.08
29	TJ	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
29	TL	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
29	iB	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
29	iM	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
29	K4	202	PEB	OA-C1A-C2A	-2.06	124.54	126.17
29	N2	202	PEB	CHA-C4A-NA	2.06	127.65	125.20
29	F5	202	PEB	CHA-C1B-NB	-2.06	120.63	124.93
29	cB	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
29	cM	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
29	I4	201	PEB	CBA-CAA-C3A	-2.06	108.89	113.47
30	AB	304	PUB	C1D-CHC-C4C	-2.06	108.89	113.37
29	dF	202	PEB	C2A-C1A-NA	2.06	110.05	108.27
29	dI	202	PEB	C2A-C1A-NA	2.06	110.05	108.27
31	BP	1001	CYC	C1B-CHB-C4A	2.06	133.10	128.08
29	kF	203	PEB	CAB-CBB-CGB	-2.06	109.18	113.60
29	kI	203	PEB	CAB-CBB-CGB	-2.06	109.18	113.60
29	FC	202	PEB	C1C-CHB-C4B	2.06	131.26	128.81
29	FE	202	PEB	C1C-CHB-C4B	2.06	131.26	128.81
29	mB	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
29	mM	203	PEB	CAB-CBB-CGB	2.06	118.03	113.60
29	B4	202	PEB	CHA-C1B-NB	-2.06	120.63	124.93
29	L5	202	PEB	CHA-C1B-NB	-2.06	120.63	124.93
29	IC	202	PEB	OD-C4D-ND	-2.06	122.89	125.93
29	IE	202	PEB	OD-C4D-ND	-2.06	122.89	125.93
31	sP	1001	CYC	C1B-CHB-C4A	2.06	133.10	128.08
31	EP	1001	CYC	C2A-C1A-NA	2.06	113.04	110.05
29	DD	202	PEB	CAA-C3A-C4A	-2.06	107.40	112.67
29	O1	202	PEB	CHA-C4A-NA	-2.05	122.76	125.20
29	OK	202	PEB	CHA-C4A-NA	-2.05	122.76	125.20
29	J4	202	PEB	CAA-C3A-C4A	-2.05	107.40	112.67
29	NB	202	PEB	CAB-CBB-CGB	2.05	118.02	113.60
29	NM	202	PEB	CAB-CBB-CGB	2.05	118.02	113.60
29	B4	202	PEB	CAA-C3A-C4A	-2.05	107.40	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	O1	201	PEB	CAB-C3B-C4B	2.05	128.64	125.01
29	OK	201	PEB	CAB-C3B-C4B	2.05	128.64	125.01
29	JB	203	PEB	CAB-CBB-CGB	2.05	118.02	113.60
29	JM	203	PEB	CAB-CBB-CGB	2.05	118.02	113.60
29	H4	202	PEB	CAA-C3A-C4A	-2.05	107.40	112.67
29	L4	202	PEB	CAA-C3A-C4A	-2.05	107.40	112.67
31	JP	1001	CYC	C2A-C1A-NA	2.05	113.04	110.05
29	O2	201	PEB	O2C-CGC-CBC	2.05	120.63	114.03
29	W1	201	PEB	CAB-C3B-C4B	2.05	128.64	125.01
29	WK	201	PEB	CAB-C3B-C4B	2.05	128.64	125.01
29	i1	201	PEB	C4B-NB-C1B	-2.05	102.64	106.51
29	iK	201	PEB	C4B-NB-C1B	-2.05	102.64	106.51
29	YF	203	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
29	YI	203	PEB	CAB-CBB-CGB	-2.05	109.19	113.60
29	LA	202	PEB	CHA-C1B-NB	-2.05	120.64	124.93
29	BD	202	PEB	CHA-C1B-NB	-2.05	120.64	124.93
29	LN	202	PEB	CHA-C1B-NB	-2.05	120.64	124.93
29	F1	1002	PEB	CAB-C3B-C4B	2.05	128.64	125.01
29	FK	1002	PEB	CAB-C3B-C4B	2.05	128.64	125.01
31	DP	1001	CYC	C1B-CHB-C4A	2.05	133.09	128.08
29	LC	202	PEB	C1C-CHB-C4B	2.05	131.26	128.81
29	LE	202	PEB	C1C-CHB-C4B	2.05	131.26	128.81
29	N1	1002	PEB	CAB-C3B-C4B	2.05	128.64	125.01
31	M9	1001	CYC	CAA-C2A-C1A	2.05	128.64	125.01
29	M2	201	PEB	O2C-CGC-CBC	2.05	120.62	114.03
31	E7	1001	CYC	CAA-C2A-C1A	2.05	128.64	125.01
31	E9	1001	CYC	CAA-C2A-C1A	2.05	128.64	125.01
29	LB	203	PEB	CAB-CBB-CGB	2.05	118.02	113.60
29	LM	203	PEB	CAB-CBB-CGB	2.05	118.02	113.60
29	QJ	201	PEB	CHC-C1D-ND	-2.05	111.57	113.95
29	QL	201	PEB	CHC-C1D-ND	-2.05	111.57	113.95
29	AG	201	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
29	AQ	201	PEB	CHB-C4B-C3B	-2.05	120.58	125.32
29	Q1	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
29	QK	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
29	S1	202	PEB	CHA-C4A-NA	-2.05	122.77	125.20
29	U1	203	PEB	CHA-C4A-NA	-2.05	122.77	125.20
29	V2	202	PEB	CHA-C4A-NA	2.05	127.64	125.20
29	SK	202	PEB	CHA-C4A-NA	-2.05	122.77	125.20
29	UK	203	PEB	CHA-C4A-NA	-2.05	122.77	125.20
31	H7	1001	CYC	CAC-C3C-C4C	-2.05	107.41	112.67
31	H9	1001	CYC	CAC-C3C-C4C	-2.05	107.41	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K4	201	PEB	CMA-C2A-C1A	-2.05	107.98	112.40
30	AM	304	PUB	C1D-CHC-C4C	-2.05	108.91	113.37
31	NP	1001	CYC	CBD-CAD-C3D	-2.05	109.12	112.62
29	TJ	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	TL	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	Z1	203	PEB	CHA-C4A-NA	-2.05	122.77	125.20
29	ZK	203	PEB	CHA-C4A-NA	-2.05	122.77	125.20
29	DK	1002	PEB	CAB-C3B-C4B	2.05	128.63	125.01
31	GP	1001	CYC	C2A-C1A-NA	2.05	113.03	110.05
31	KP	1001	CYC	C2A-C1A-NA	2.05	113.03	110.05
31	gP	1001	CYC	C2A-C1A-NA	2.05	113.03	110.05
29	LD	202	PEB	C4B-NB-C1B	-2.05	102.65	106.51
29	XJ	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
29	XL	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
29	GD	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	KD	201	PEB	CBA-CAA-C3A	-2.05	108.91	113.47
29	L8	202	PEB	CHA-C1B-NB	-2.05	120.65	124.93
29	BA	202	PEB	CHA-C1B-NB	-2.05	120.65	124.93
29	FD	202	PEB	CHA-C1B-NB	-2.05	120.65	124.93
29	BN	202	PEB	CHA-C1B-NB	-2.05	120.65	124.93
29	IC	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
29	IE	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
29	NJ	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	NL	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	GC	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
29	GE	201	PEB	C2B-C1B-NB	2.05	114.90	110.53
29	DJ	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	DL	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
29	J4	202	PEB	CHA-C1B-NB	-2.05	120.65	124.93
29	AJ	201	PEB	CHC-C1D-ND	-2.05	111.57	113.95
29	iJ	201	PEB	CHC-C1D-ND	-2.05	111.57	113.95
29	AL	201	PEB	CHC-C1D-ND	-2.05	111.57	113.95
29	iL	201	PEB	CHC-C1D-ND	-2.05	111.57	113.95
29	ID	201	PEB	CBA-CAA-C3A	-2.05	108.91	113.47
31	J9	1001	CYC	CAC-C3C-C4C	-2.05	107.42	112.67
29	l1	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
29	lK	201	PEB	CAB-C3B-C4B	2.05	128.63	125.01
29	FG	203	PEB	CAB-CBB-CGB	-2.05	109.20	113.60
29	PR	201	PEB	CHA-C4A-NA	2.05	127.64	125.20
29	C4	201	PEB	CMA-C2A-C1A	-2.05	107.99	112.40
31	GK	1001	CYC	C1B-CHB-C4A	-2.05	123.08	128.08
31	DK	1001	CYC	CBA-CAA-C2A	-2.05	106.94	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G4	201	PEB	CBA-CAA-C3A	-2.04	108.91	113.47
29	BD	202	PEB	CAA-C3A-C4A	-2.04	107.42	112.67
29	wL	301	PEB	CAC-CBC-CGC	-2.04	108.03	113.76
29	LG	203	PEB	CAB-CBB-CGB	-2.04	109.20	113.60
31	D7	1001	CYC	CAC-C3C-C4C	-2.04	107.42	112.67
31	D9	1001	CYC	CAC-C3C-C4C	-2.04	107.42	112.67
29	L4	202	PEB	C4B-NB-C1B	-2.04	102.66	106.51
29	e7	201	PEB	C4B-NB-C1B	-2.04	102.66	106.51
29	e9	201	PEB	C4B-NB-C1B	-2.04	102.66	106.51
29	MG	401	PEB	C2B-C1B-NB	2.04	114.89	110.53
29	NK	1002	PEB	CAB-C3B-C4B	2.04	128.62	125.01
31	D1	1003	CYC	C1B-CHB-C4A	-2.04	123.09	128.08
29	dD	401	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
29	FA	201	PEB	C2A-C1A-NA	2.04	110.03	108.27
29	FN	201	PEB	C2A-C1A-NA	2.04	110.03	108.27
31	pP	1001	CYC	CBD-CAD-C3D	-2.04	109.13	112.62
29	M4	201	PEB	CBA-CAA-C3A	-2.04	108.92	113.47
29	E4	201	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
29	W2	201	PEB	O2C-CGC-CBC	2.04	120.59	114.03
29	D1	1002	PEB	CAB-C3B-C4B	2.04	128.62	125.01
29	EC	201	PEB	C2B-C1B-NB	2.04	114.89	110.53
29	EE	201	PEB	C2B-C1B-NB	2.04	114.89	110.53
30	QB	201	PUB	CMB-C2B-C3B	2.04	128.79	124.94
30	QM	201	PUB	CMB-C2B-C3B	2.04	128.79	124.94
31	D1	1001	CYC	CBA-CAA-C2A	-2.04	106.95	112.63
31	L9	1001	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
31	EP	1001	CYC	CBD-CAD-C3D	-2.04	109.14	112.62
29	K4	201	PEB	CBA-CAA-C3A	-2.04	108.92	113.47
29	bJ	201	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
29	bL	201	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
29	DQ	203	PEB	CAB-CBB-CGB	-2.04	109.21	113.60
29	KC	202	PEB	C2B-C1B-NB	2.04	114.88	110.53
29	KE	202	PEB	C2B-C1B-NB	2.04	114.88	110.53
29	JJ	201	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
29	JL	201	PEB	CMA-C2A-C1A	-2.04	108.00	112.40
31	M1	1001	CYC	C1B-CHB-C4A	-2.04	123.10	128.08
31	MK	1001	CYC	C1B-CHB-C4A	-2.04	123.10	128.08
31	N7	1001	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
31	N9	1001	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
29	VJ	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
29	VL	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
31	rP	1001	CYC	CBD-CAD-C3D	-2.04	109.14	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	tP	1001	CYC	CBD-CAD-C3D	-2.04	109.14	112.62
31	EK	1001	CYC	C1B-CHB-C4A	-2.04	123.10	128.08
29	KD	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
31	CK	1001	CYC	C1B-CHB-C4A	-2.04	123.10	128.08
29	jF	201	PEB	CAA-C3A-C2A	-2.04	109.17	114.26
29	jI	201	PEB	CAA-C3A-C2A	-2.04	109.17	114.26
29	F4	202	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	R7	201	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	R9	201	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	JD	202	PEB	CHA-C1B-NB	-2.04	120.67	124.93
29	c7	201	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	c9	201	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	MR	201	PEB	O2C-CGC-CBC	2.04	120.58	114.03
29	OR	201	PEB	O2C-CGC-CBC	2.04	120.58	114.03
29	MD	201	PEB	CBA-CAA-C3A	-2.04	108.93	113.47
29	tJ	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
29	tL	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
29	wJ	301	PEB	CAC-CBC-CGC	-2.04	108.05	113.76
31	L1	1001	CYC	CBA-CAA-C2A	-2.04	106.97	112.63
31	LK	1001	CYC	CBA-CAA-C2A	-2.04	106.97	112.63
31	J7	1001	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
29	ZJ	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
29	ZL	201	PEB	CMA-C2A-C1A	-2.04	108.01	112.40
31	H1	1001	CYC	CBA-CAA-C2A	-2.04	106.97	112.63
29	L1	1002	PEB	CAB-C3B-C4B	2.04	128.61	125.01
29	LK	1002	PEB	CAB-C3B-C4B	2.04	128.61	125.01
29	k7	201	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	k9	201	PEB	C4B-NB-C1B	-2.04	102.67	106.51
29	dD	401	PEB	CBA-CAA-C3A	-2.04	108.94	113.47
29	I4	202	PEB	OA-C1A-C2A	-2.03	124.56	126.17
29	D4	202	PEB	C4B-NB-C1B	-2.03	102.68	106.51
31	C1	1001	CYC	C1B-CHB-C4A	-2.03	123.11	128.08
31	E1	1001	CYC	C1B-CHB-C4A	-2.03	123.11	128.08
31	C7	1001	CYC	CAA-C2A-C1A	2.03	128.61	125.01
31	C9	1001	CYC	CAA-C2A-C1A	2.03	128.61	125.01
29	PJ	201	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
29	PL	201	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
29	hF	201	PEB	CAA-C3A-C2A	-2.03	109.18	114.26
29	hI	201	PEB	CAA-C3A-C2A	-2.03	109.18	114.26
31	J1	1001	CYC	CBA-CAA-C2A	-2.03	106.98	112.63
31	JK	1001	CYC	CBA-CAA-C2A	-2.03	106.98	112.63
29	F7	1002	PEB	CMC-C3C-C2C	-2.03	121.11	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	MD	201	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
29	l1	202	PEB	CHA-C4A-NA	-2.03	122.79	125.20
29	lK	202	PEB	CHA-C4A-NA	-2.03	122.79	125.20
31	F7	1001	CYC	CAC-C3C-C4C	-2.03	107.45	112.67
29	gB	203	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
29	gM	203	PEB	CMA-C2A-C1A	-2.03	108.02	112.40
31	AP	1001	CYC	CBD-CAD-C3D	-2.03	109.15	112.62
31	CP	1001	CYC	CBD-CAD-C3D	-2.03	109.15	112.62
29	Q1	202	PEB	CHA-C4A-NA	-2.03	122.79	125.20
29	P2	201	PEB	CHA-C4A-NA	2.03	127.62	125.20
29	QK	202	PEB	CHA-C4A-NA	-2.03	122.79	125.20
29	CD	201	PEB	CBA-CAA-C3A	-2.03	108.94	113.47
29	FQ	203	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
29	JQ	203	PEB	CAB-CBB-CGB	-2.03	109.23	113.60
31	RP	1001	CYC	CBD-CAD-C3D	-2.03	109.15	112.62
31	iP	1001	CYC	CBD-CAD-C3D	-2.03	109.15	112.62
29	NR	202	PEB	CHA-C4A-NA	2.03	127.62	125.20
31	G7	1001	CYC	CAA-C2A-C1A	2.03	128.60	125.01
29	H4	202	PEB	CHA-C1B-NB	-2.03	120.69	124.93
29	iB	203	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
29	iM	203	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
31	cP	1001	CYC	CBD-CAD-C3D	-2.03	109.16	112.62
29	c1	203	PEB	CAB-C3B-C4B	2.03	128.60	125.01
29	cK	203	PEB	CAB-C3B-C4B	2.03	128.60	125.01
29	m7	201	PEB	C4B-NB-C1B	-2.03	102.69	106.51
29	m9	201	PEB	C4B-NB-C1B	-2.03	102.69	106.51
29	dJ	201	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
29	dL	201	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
30	QB	201	PUB	O1B-CGB-CBB	-2.03	116.56	123.08
30	QM	201	PUB	O1B-CGB-CBB	-2.03	116.56	123.08
29	AC	201	PEB	C2B-C1B-NB	2.03	114.86	110.53
29	AE	201	PEB	C2B-C1B-NB	2.03	114.86	110.53
31	L7	1001	CYC	CAC-C3C-C4C	-2.03	107.46	112.67
31	HF	1001	CYC	CMC-C2C-C1C	-2.03	108.03	112.40
31	HI	1001	CYC	CMC-C2C-C1C	-2.03	108.03	112.40
31	NK	1001	CYC	CBA-CAA-C2A	-2.03	106.99	112.63
29	HG	203	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
31	PP	1001	CYC	CBD-CAD-C3D	-2.03	109.16	112.62
31	gP	1001	CYC	CBD-CAD-C3D	-2.03	109.16	112.62
29	a7	201	PEB	C4B-NB-C1B	-2.03	102.69	106.51
29	a9	201	PEB	C4B-NB-C1B	-2.03	102.69	106.51
29	UF	202	PEB	CAA-C3A-C2A	-2.03	109.19	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	UI	202	PEB	CAA-C3A-C2A	-2.03	109.19	114.26
29	E4	201	PEB	CBA-CAA-C3A	-2.03	108.95	113.47
29	DD	202	PEB	C4B-NB-C1B	-2.03	102.69	106.51
31	eP	1001	CYC	CBD-CAD-C3D	-2.03	109.16	112.62
31	K7	1001	CYC	CAA-C2A-C1A	2.03	128.59	125.01
31	KP	1001	CYC	CBD-CAD-C3D	-2.03	109.16	112.62
29	C4	201	PEB	CBA-CAA-C3A	-2.03	108.95	113.47
29	G4	202	PEB	OA-C1A-C2A	-2.03	124.56	126.17
29	jJ	201	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
29	rJ	201	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
29	jL	201	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
29	rL	201	PEB	CMA-C2A-C1A	-2.03	108.03	112.40
29	DG	203	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
29	VR	202	PEB	CHA-C4A-NA	2.03	127.61	125.20
29	D7	1002	PEB	CMC-C3C-C2C	-2.03	121.12	124.94
29	D9	1002	PEB	CMC-C3C-C2C	-2.03	121.12	124.94
31	M7	1001	CYC	CAA-C2A-C1A	2.03	128.59	125.01
29	CC	201	PEB	C2B-C1B-NB	2.03	114.85	110.53
29	CE	201	PEB	C2B-C1B-NB	2.03	114.85	110.53
29	ID	202	PEB	OA-C1A-C2A	-2.03	124.56	126.17
29	DB	203	PEB	CMA-C2A-C1A	-2.03	108.04	112.40
29	DM	203	PEB	CMA-C2A-C1A	-2.03	108.04	112.40
29	NR	202	PEB	CAB-CBB-CGB	-2.03	109.24	113.60
29	FJ	201	PEB	CMA-C2A-C1A	-2.03	108.04	112.40
29	FL	201	PEB	CMA-C2A-C1A	-2.03	108.04	112.40
29	BD	202	PEB	C4B-NB-C1B	-2.03	102.69	106.51
29	QR	201	PEB	O2C-CGC-CBC	2.03	120.54	114.03
29	DA	201	PEB	C2A-C1A-NA	2.03	110.02	108.27
29	DN	201	PEB	C2A-C1A-NA	2.03	110.02	108.27
29	T1	202	PEB	CAB-C3B-C4B	2.03	128.59	125.01
29	TK	202	PEB	CAB-C3B-C4B	2.03	128.59	125.01
29	B3	201	PEB	CHB-C4B-C3B	-2.03	120.64	125.32
29	BO	201	PEB	CHB-C4B-C3B	-2.03	120.64	125.32
29	XJ	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	XL	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	V7	201	PEB	C4B-NB-C1B	-2.02	102.69	106.51
29	V9	201	PEB	C4B-NB-C1B	-2.02	102.69	106.51
31	HK	1001	CYC	CBA-CAA-C2A	-2.02	107.00	112.63
29	LQ	202	PEB	CAB-CBB-CGB	-2.02	109.25	113.60
29	pJ	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	pL	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	f1	202	PEB	CBC-CAC-C2C	-2.02	109.17	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	fK	202	PEB	CBC-CAC-C2C	-2.02	109.17	112.62
31	lP	1001	CYC	CBD-CAD-C3D	-2.02	109.17	112.62
29	GD	201	PEB	CBA-CAA-C3A	-2.02	108.96	113.47
29	aJ	201	PEB	CHC-C1D-ND	-2.02	111.60	113.95
29	aL	201	PEB	CHC-C1D-ND	-2.02	111.60	113.95
31	mP	1001	CYC	CBD-CAD-C3D	-2.02	109.17	112.62
29	nJ	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	nL	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	BG	203	PEB	CAB-CBB-CGB	-2.02	109.25	113.60
29	Y7	201	PEB	C4B-NB-C1B	-2.02	102.70	106.51
29	Y9	201	PEB	C4B-NB-C1B	-2.02	102.70	106.51
29	FD	202	PEB	C4B-NB-C1B	-2.02	102.70	106.51
29	CD	201	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	WR	201	PEB	O2C-CGC-CBC	2.02	120.53	114.03
29	I3	201	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
29	IO	201	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
31	GP	1001	CYC	CBD-CAD-C3D	-2.02	109.17	112.62
31	YP	1000	CYC	CBD-CAD-C3D	-2.02	109.17	112.62
29	ZB	203	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	ZM	203	PEB	CMA-C2A-C1A	-2.02	108.04	112.40
29	bF	201	PEB	CAA-C3A-C2A	-2.02	109.21	114.26
29	bI	201	PEB	CAA-C3A-C2A	-2.02	109.21	114.26
31	K1	1001	CYC	C1B-CHB-C4A	-2.02	123.14	128.08
31	KK	1001	CYC	C1B-CHB-C4A	-2.02	123.14	128.08
29	P1	203	PEB	CAB-C3B-C4B	2.02	128.59	125.01
29	PK	203	PEB	CAB-C3B-C4B	2.02	128.59	125.01
31	G9	1001	CYC	CAA-C2A-C1A	2.02	128.59	125.01
29	b1	202	PEB	CHA-C4A-NA	-2.02	122.80	125.20
29	bK	202	PEB	CHA-C4A-NA	-2.02	122.80	125.20
29	I3	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	IO	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	R1	203	PEB	CAB-C3B-C4B	2.02	128.58	125.01
29	RK	203	PEB	CAB-C3B-C4B	2.02	128.58	125.01
29	E3	201	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
29	EO	201	PEB	CBB-CAB-C3B	-2.02	107.01	112.63
29	F3	201	PEB	CHB-C4B-C3B	-2.02	120.65	125.32
29	FO	201	PEB	CHB-C4B-C3B	-2.02	120.65	125.32
29	CD	202	PEB	OA-C1A-C2A	-2.02	124.57	126.17
31	JP	1001	CYC	CBD-CAD-C3D	-2.02	109.17	112.62
31	IK	1001	CYC	C1B-CHB-C4A	-2.02	123.14	128.08
29	T7	201	PEB	C4B-NB-C1B	-2.02	102.70	106.51
29	T9	201	PEB	C4B-NB-C1B	-2.02	102.70	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ID	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
29	vJ	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
29	vL	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
29	A5	203	PEB	CAB-C3B-C4B	2.02	128.58	125.01
29	A8	203	PEB	CAB-C3B-C4B	2.02	128.58	125.01
31	F9	1001	CYC	CAC-C3C-C4C	-2.02	107.49	112.67
29	GD	202	PEB	OA-C1A-C2A	-2.02	124.57	126.17
29	A3	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	AO	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
31	N7	1001	CYC	CAC-C3C-C2C	-2.02	109.21	114.26
31	N9	1001	CYC	CAC-C3C-C2C	-2.02	109.21	114.26
31	FF	1001	CYC	CMC-C2C-C1C	-2.02	108.05	112.40
31	FI	1001	CYC	CMC-C2C-C1C	-2.02	108.05	112.40
31	K9	1001	CYC	CAA-C2A-C1A	2.02	128.58	125.01
31	N1	1001	CYC	CBA-CAA-C2A	-2.02	107.02	112.63
29	N2	202	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
29	lF	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	lI	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	c7	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	c9	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	m1	202	PEB	CAB-C3B-C4B	2.02	128.58	125.01
29	mK	202	PEB	CAB-C3B-C4B	2.02	128.58	125.01
29	i7	201	PEB	C4B-NB-C1B	-2.02	102.71	106.51
29	i9	201	PEB	C4B-NB-C1B	-2.02	102.71	106.51
29	g7	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	g9	201	PEB	C2B-C1B-NB	2.02	114.84	110.53
29	C3	201	PEB	CBB-CAB-C3B	-2.02	107.02	112.63
29	CO	201	PEB	CBB-CAB-C3B	-2.02	107.02	112.63
29	fJ	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
29	fL	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
29	dF	202	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	dI	202	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	R7	201	PEB	C2B-C1B-NB	2.02	114.83	110.53
29	R9	201	PEB	C2B-C1B-NB	2.02	114.83	110.53
29	BQ	203	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
29	hJ	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
29	hL	201	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
31	I7	1001	CYC	CAA-C2A-C1A	2.02	128.58	125.01
31	I9	1001	CYC	CAA-C2A-C1A	2.02	128.58	125.01
29	A5	203	PEB	CMD-C2D-C3D	2.02	132.91	130.06
29	A8	203	PEB	CMD-C2D-C3D	2.02	132.91	130.06
29	M4	202	PEB	OA-C1A-C2A	-2.02	124.57	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	ZF	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	ZI	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	RJ	201	PEB	CMA-C2A-C1A	-2.02	108.06	112.40
29	RL	201	PEB	CMA-C2A-C1A	-2.02	108.06	112.40
29	xL	301	PEB	CAC-CBC-CGC	-2.02	108.10	113.76
29	B4	202	PEB	C4B-NB-C1B	-2.02	102.71	106.51
29	P7	201	PEB	C4B-NB-C1B	-2.02	102.71	106.51
29	P9	201	PEB	C4B-NB-C1B	-2.02	102.71	106.51
29	Q2	201	PEB	O2C-CGC-CBC	2.02	120.51	114.03
29	g7	201	PEB	C4B-NB-C1B	-2.02	102.71	106.51
29	g9	201	PEB	C4B-NB-C1B	-2.02	102.71	106.51
31	L9	1001	CYC	CAC-C3C-C2C	-2.02	109.22	114.26
29	JG	203	PEB	CAB-CBB-CGB	-2.02	109.26	113.60
29	A3	201	PEB	CBB-CAB-C3B	-2.02	107.03	112.63
29	AO	201	PEB	CBB-CAB-C3B	-2.02	107.03	112.63
29	Y1	202	PEB	CAB-C3B-C4B	2.02	128.57	125.01
29	YK	202	PEB	CAB-C3B-C4B	2.02	128.57	125.01
29	OF	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
29	OI	201	PEB	CAA-C3A-C2A	-2.02	109.22	114.26
31	F1	1001	CYC	CBA-CAA-C2A	-2.02	107.03	112.63
31	FK	1001	CYC	CBA-CAA-C2A	-2.02	107.03	112.63
29	F9	1002	PEB	CMC-C3C-C2C	-2.02	121.14	124.94
29	I4	201	PEB	CMA-C2A-C1A	-2.02	108.06	112.40
29	SF	201	PEB	CAA-C3A-C2A	-2.01	109.22	114.26
29	SI	201	PEB	CAA-C3A-C2A	-2.01	109.22	114.26
29	IJ	201	PEB	CMA-C2A-C1A	-2.01	108.06	112.40
29	IL	201	PEB	CMA-C2A-C1A	-2.01	108.06	112.40
29	I5	203	PEB	CAB-C3B-C4B	2.01	128.57	125.01
29	I8	203	PEB	CAB-C3B-C4B	2.01	128.57	125.01
29	e7	201	PEB	C2B-C1B-NB	2.01	114.83	110.53
29	e9	201	PEB	C2B-C1B-NB	2.01	114.83	110.53
29	QF	201	PEB	CAA-C3A-C2A	-2.01	109.23	114.26
29	QI	201	PEB	CAA-C3A-C2A	-2.01	109.23	114.26
29	MQ	406	PEB	CAB-C3B-C4B	2.01	128.57	125.01
31	TP	1001	CYC	CBD-CAD-C3D	-2.01	109.18	112.62
29	PR	201	PEB	CAB-CBB-CGB	-2.01	109.27	113.60
29	G3	201	PEB	CBB-CAB-C3B	-2.01	107.03	112.63
29	GO	201	PEB	CBB-CAB-C3B	-2.01	107.03	112.63
31	H7	1001	CYC	CAC-C3C-C2C	-2.01	109.23	114.26
31	H9	1001	CYC	CAC-C3C-C2C	-2.01	109.23	114.26
29	K3	201	PEB	CBB-CAB-C3B	-2.01	107.03	112.63
29	KO	201	PEB	CBB-CAB-C3B	-2.01	107.03	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j1	202	PEB	CHA-C4A-NA	-2.01	122.81	125.20
29	jK	202	PEB	CHA-C4A-NA	-2.01	122.81	125.20
29	g1	203	PEB	CAB-C3B-C4B	2.01	128.57	125.01
29	gK	203	PEB	CAB-C3B-C4B	2.01	128.57	125.01
29	BJ	201	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	BL	201	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	i7	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
29	i9	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
29	xJ	301	PEB	CAC-CBC-CGC	-2.01	108.12	113.76
29	WF	201	PEB	CAA-C3A-C2A	-2.01	109.23	114.26
29	WI	201	PEB	CAA-C3A-C2A	-2.01	109.23	114.26
31	D7	1001	CYC	CAC-C3C-C2C	-2.01	109.23	114.26
31	D9	1001	CYC	CAC-C3C-C2C	-2.01	109.23	114.26
30	A1	304	PUB	CAC-CBC-CGC	-2.01	109.28	113.60
30	AK	304	PUB	CAC-CBC-CGC	-2.01	109.28	113.60
29	NB	202	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	NM	202	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	a7	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
29	m7	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
29	a9	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
29	m9	201	PEB	C2B-C1B-NB	2.01	114.82	110.53
29	J7	1002	PEB	CMC-C3C-C2C	-2.01	121.15	124.94
29	RB	203	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	RM	203	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	MG	404	PEB	CAB-C3B-C4B	2.01	128.56	125.01
29	H7	1002	PEB	CMC-C3C-C2C	-2.01	121.15	124.94
29	H9	1002	PEB	CMC-C3C-C2C	-2.01	121.15	124.94
31	I1	1001	CYC	C1B-CHB-C4A	-2.01	123.17	128.08
29	JA	201	PEB	C2A-C1A-NA	2.01	110.00	108.27
29	JN	201	PEB	C2A-C1A-NA	2.01	110.00	108.27
29	H3	201	PEB	CHB-C4B-C3B	-2.01	120.68	125.32
29	HO	201	PEB	CHB-C4B-C3B	-2.01	120.68	125.32
29	LC	202	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	LE	202	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	JB	203	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	JM	203	PEB	CMA-C2A-C1A	-2.01	108.07	112.40
29	xJ	302	PEB	CAC-CBC-CGC	-2.01	108.13	113.76
29	xL	302	PEB	CAC-CBC-CGC	-2.01	108.13	113.76
29	F3	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	FO	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	V2	202	PEB	CAB-CBB-CGB	-2.01	109.28	113.60
29	cB	203	PEB	CMA-C2A-C1A	-2.01	108.08	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	cM	203	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	bF	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
29	bI	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
29	NJ	201	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
29	NL	201	PEB	C1B-C2B-C3B	-2.01	104.20	106.51
29	eB	202	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	mB	203	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	eM	202	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	mM	203	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	KG	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
29	KQ	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
29	G3	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	P7	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	P9	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	GO	201	PEB	C2B-C1B-NB	2.01	114.81	110.53
29	zJ	501	PEB	CBC-CAC-C2C	-2.01	109.19	112.62
29	fI	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
29	hI	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
29	fK	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
29	hK	202	PEB	CHA-C4A-NA	-2.01	122.82	125.20
29	FB	203	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	FM	203	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	fF	201	PEB	CAA-C3A-C2A	-2.01	109.25	114.26
29	fI	201	PEB	CAA-C3A-C2A	-2.01	109.25	114.26
29	J3	201	PEB	CHB-C4B-C3B	-2.01	120.69	125.32
29	JO	201	PEB	CHB-C4B-C3B	-2.01	120.69	125.32
31	L7	1001	CYC	CAC-C3C-C2C	-2.01	109.25	114.26
29	LJ	201	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	LL	201	PEB	CMA-C2A-C1A	-2.01	108.08	112.40
29	N1	1002	PEB	C1C-CHB-C4B	-2.01	126.41	128.81
29	AM	301	PEB	C1C-CHB-C4B	-2.01	126.41	128.81
29	CG	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
29	CQ	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
29	eI	203	PEB	CAB-C3B-C4B	2.01	128.56	125.01
29	eK	203	PEB	CAB-C3B-C4B	2.01	128.56	125.01
29	AB	301	PEB	C1C-CHB-C4B	-2.00	126.41	128.81
29	wJ	302	PEB	CAC-CBC-CGC	-2.00	108.14	113.76
29	L7	1002	PEB	CMC-C3C-C2C	-2.00	121.16	124.94
29	JD	202	PEB	C4B-NB-C1B	-2.00	102.73	106.51
29	Q1	202	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
29	QK	202	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
29	V7	201	PEB	C2B-C1B-NB	2.00	114.80	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V9	201	PEB	C2B-C1B-NB	2.00	114.80	110.53
29	wL	302	PEB	CAC-CBC-CGC	-2.00	108.14	113.76
29	J4	202	PEB	C4B-NB-C1B	-2.00	102.74	106.51
31	J7	1001	CYC	CAC-C3C-C2C	-2.00	109.26	114.26
29	FC	202	PEB	C2B-C1B-NB	2.00	114.80	110.53
29	FE	202	PEB	C2B-C1B-NB	2.00	114.80	110.53
31	F7	1001	CYC	CAC-C3C-C2C	-2.00	109.26	114.26
29	I5	203	PEB	CMD-C2D-C3D	2.00	132.89	130.06
29	I8	203	PEB	CMD-C2D-C3D	2.00	132.89	130.06
29	I1	202	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
29	IK	202	PEB	CBC-CAC-C2C	-2.00	109.20	112.62
29	HD	202	PEB	C4B-NB-C1B	-2.00	102.74	106.51
29	PB	202	PEB	CMA-C2A-C1A	-2.00	108.09	112.40
29	PM	202	PEB	CMA-C2A-C1A	-2.00	108.09	112.40
31	1P	1002	CYC	CBD-CAD-C3D	-2.00	109.20	112.62
29	GA	202	PEB	CAB-C3B-C2B	-2.00	124.15	127.88
29	GN	202	PEB	CAB-C3B-C2B	-2.00	124.15	127.88
29	M4	201	PEB	CMA-C2A-C1A	-2.00	108.09	112.40
29	D3	201	PEB	CHB-C4B-C3B	-2.00	120.70	125.32
29	DO	201	PEB	CHB-C4B-C3B	-2.00	120.70	125.32

There are no chirality outliers.

All (12797) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A1	301	PEB	NB-C1B-CHA-C4A
29	A1	301	PEB	C2B-C1B-CHA-C4A
29	A1	302	PEB	ND-C1D-CHC-C4C
29	A1	302	PEB	NB-C1B-CHA-C4A
29	A1	302	PEB	C2B-C1B-CHA-C4A
29	A1	303	PEB	C4A-C3A-CAA-CBA
29	A1	303	PEB	NB-C1B-CHA-C4A
29	A1	303	PEB	C2B-C1B-CHA-C4A
29	D1	1002	PEB	C2A-C3A-CAA-CBA
29	D1	1002	PEB	C4A-C3A-CAA-CBA
29	D1	1002	PEB	NB-C1B-CHA-C4A
29	D1	1002	PEB	C2B-C1B-CHA-C4A
29	F1	1002	PEB	C2A-C3A-CAA-CBA
29	F1	1002	PEB	C4A-C3A-CAA-CBA
29	F1	1002	PEB	NB-C1B-CHA-C4A
29	F1	1002	PEB	C2B-C1B-CHA-C4A
29	H1	1002	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	H1	1002	PEB	C4A-C3A-CAA-CBA
29	H1	1002	PEB	NB-C1B-CHA-C4A
29	H1	1002	PEB	C2B-C1B-CHA-C4A
29	J1	1002	PEB	C2A-C3A-CAA-CBA
29	J1	1002	PEB	C4A-C3A-CAA-CBA
29	J1	1002	PEB	NB-C1B-CHA-C4A
29	J1	1002	PEB	C2B-C1B-CHA-C4A
29	L1	1002	PEB	C2A-C3A-CAA-CBA
29	L1	1002	PEB	C4A-C3A-CAA-CBA
29	L1	1002	PEB	NB-C1B-CHA-C4A
29	L1	1002	PEB	C2B-C1B-CHA-C4A
29	N1	1002	PEB	C2A-C3A-CAA-CBA
29	N1	1002	PEB	C4A-C3A-CAA-CBA
29	N1	1002	PEB	NB-C1B-CHA-C4A
29	N1	1002	PEB	C2B-C1B-CHA-C4A
29	O1	201	PEB	ND-C1D-CHC-C4C
29	O1	201	PEB	NB-C1B-CHA-C4A
29	O1	201	PEB	C2B-C1B-CHA-C4A
29	O1	202	PEB	NB-C1B-CHA-C4A
29	O1	202	PEB	C2B-C1B-CHA-C4A
29	P1	201	PEB	NB-C1B-CHA-C4A
29	P1	201	PEB	C2B-C1B-CHA-C4A
29	P1	202	PEB	NB-C1B-CHA-C4A
29	P1	202	PEB	C2B-C1B-CHA-C4A
29	P1	203	PEB	NB-C1B-CHA-C4A
29	P1	203	PEB	C2B-C1B-CHA-C4A
29	Q1	201	PEB	ND-C1D-CHC-C4C
29	Q1	201	PEB	NB-C1B-CHA-C4A
29	Q1	201	PEB	C2B-C1B-CHA-C4A
29	Q1	202	PEB	NB-C1B-CHA-C4A
29	Q1	202	PEB	C2B-C1B-CHA-C4A
29	R1	201	PEB	NB-C1B-CHA-C4A
29	R1	201	PEB	C2B-C1B-CHA-C4A
29	R1	202	PEB	NB-C1B-CHA-C4A
29	R1	202	PEB	C2B-C1B-CHA-C4A
29	R1	203	PEB	NB-C1B-CHA-C4A
29	R1	203	PEB	C2B-C1B-CHA-C4A
29	S1	201	PEB	ND-C1D-CHC-C4C
29	S1	201	PEB	NB-C1B-CHA-C4A
29	S1	201	PEB	C2B-C1B-CHA-C4A
29	S1	202	PEB	NB-C1B-CHA-C4A
29	S1	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	T1	201	PEB	NB-C1B-CHA-C4A
29	T1	201	PEB	C2B-C1B-CHA-C4A
29	T1	202	PEB	NB-C1B-CHA-C4A
29	T1	202	PEB	C2B-C1B-CHA-C4A
29	U1	201	PEB	NB-C1B-CHA-C4A
29	U1	201	PEB	C2B-C1B-CHA-C4A
29	U1	202	PEB	ND-C1D-CHC-C4C
29	U1	202	PEB	NB-C1B-CHA-C4A
29	U1	202	PEB	C2B-C1B-CHA-C4A
29	U1	203	PEB	NB-C1B-CHA-C4A
29	U1	203	PEB	C2B-C1B-CHA-C4A
29	V1	201	PEB	NB-C1B-CHA-C4A
29	V1	201	PEB	C2B-C1B-CHA-C4A
29	V1	202	PEB	NB-C1B-CHA-C4A
29	V1	202	PEB	C2B-C1B-CHA-C4A
29	V1	203	PEB	NB-C1B-CHA-C4A
29	V1	203	PEB	C2B-C1B-CHA-C4A
29	W1	201	PEB	ND-C1D-CHC-C4C
29	W1	201	PEB	NB-C1B-CHA-C4A
29	W1	201	PEB	C2B-C1B-CHA-C4A
29	W1	202	PEB	NB-C1B-CHA-C4A
29	W1	202	PEB	C2B-C1B-CHA-C4A
29	Y1	201	PEB	NB-C1B-CHA-C4A
29	Y1	201	PEB	C2B-C1B-CHA-C4A
29	Y1	202	PEB	NB-C1B-CHA-C4A
29	Y1	202	PEB	C2B-C1B-CHA-C4A
29	Z1	201	PEB	NB-C1B-CHA-C4A
29	Z1	201	PEB	C2B-C1B-CHA-C4A
29	Z1	202	PEB	ND-C1D-CHC-C4C
29	Z1	202	PEB	NB-C1B-CHA-C4A
29	Z1	202	PEB	C2B-C1B-CHA-C4A
29	Z1	203	PEB	NB-C1B-CHA-C4A
29	Z1	203	PEB	C2B-C1B-CHA-C4A
29	a1	201	PEB	NB-C1B-CHA-C4A
29	a1	201	PEB	C2B-C1B-CHA-C4A
29	a1	202	PEB	NB-C1B-CHA-C4A
29	a1	202	PEB	C2B-C1B-CHA-C4A
29	a1	203	PEB	NB-C1B-CHA-C4A
29	a1	203	PEB	C2B-C1B-CHA-C4A
29	b1	201	PEB	ND-C1D-CHC-C4C
29	b1	201	PEB	NB-C1B-CHA-C4A
29	b1	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	b1	202	PEB	NB-C1B-CHA-C4A
29	b1	202	PEB	C2B-C1B-CHA-C4A
29	c1	201	PEB	NB-C1B-CHA-C4A
29	c1	201	PEB	C2B-C1B-CHA-C4A
29	c1	202	PEB	NB-C1B-CHA-C4A
29	c1	202	PEB	C2B-C1B-CHA-C4A
29	c1	203	PEB	NB-C1B-CHA-C4A
29	c1	203	PEB	C2B-C1B-CHA-C4A
29	d1	201	PEB	ND-C1D-CHC-C4C
29	d1	201	PEB	NB-C1B-CHA-C4A
29	d1	201	PEB	C2B-C1B-CHA-C4A
29	d1	202	PEB	NB-C1B-CHA-C4A
29	d1	202	PEB	C2B-C1B-CHA-C4A
29	e1	201	PEB	NB-C1B-CHA-C4A
29	e1	201	PEB	C2B-C1B-CHA-C4A
29	e1	202	PEB	NB-C1B-CHA-C4A
29	e1	202	PEB	C2B-C1B-CHA-C4A
29	e1	203	PEB	NB-C1B-CHA-C4A
29	e1	203	PEB	C2B-C1B-CHA-C4A
29	f1	201	PEB	ND-C1D-CHC-C4C
29	f1	201	PEB	NB-C1B-CHA-C4A
29	f1	201	PEB	C2B-C1B-CHA-C4A
29	f1	202	PEB	NB-C1B-CHA-C4A
29	f1	202	PEB	C2B-C1B-CHA-C4A
29	g1	201	PEB	NB-C1B-CHA-C4A
29	g1	201	PEB	C2B-C1B-CHA-C4A
29	g1	202	PEB	NB-C1B-CHA-C4A
29	g1	202	PEB	C2B-C1B-CHA-C4A
29	g1	203	PEB	NB-C1B-CHA-C4A
29	g1	203	PEB	C2B-C1B-CHA-C4A
29	h1	201	PEB	ND-C1D-CHC-C4C
29	h1	201	PEB	NB-C1B-CHA-C4A
29	h1	201	PEB	C2B-C1B-CHA-C4A
29	h1	202	PEB	NB-C1B-CHA-C4A
29	h1	202	PEB	C2B-C1B-CHA-C4A
29	i1	201	PEB	NB-C1B-CHA-C4A
29	i1	201	PEB	C2B-C1B-CHA-C4A
29	i1	202	PEB	NB-C1B-CHA-C4A
29	i1	202	PEB	C2B-C1B-CHA-C4A
29	i1	203	PEB	NB-C1B-CHA-C4A
29	i1	203	PEB	C2B-C1B-CHA-C4A
29	j1	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	j1	201	PEB	NB-C1B-CHA-C4A
29	j1	201	PEB	C2B-C1B-CHA-C4A
29	j1	202	PEB	NB-C1B-CHA-C4A
29	j1	202	PEB	C2B-C1B-CHA-C4A
29	j1	203	PEB	NB-C1B-CHA-C4A
29	j1	203	PEB	C2B-C1B-CHA-C4A
29	k1	201	PEB	NB-C1B-CHA-C4A
29	k1	201	PEB	C2B-C1B-CHA-C4A
29	k1	202	PEB	NB-C1B-CHA-C4A
29	k1	202	PEB	C2B-C1B-CHA-C4A
29	k1	203	PEB	NB-C1B-CHA-C4A
29	k1	203	PEB	C2B-C1B-CHA-C4A
29	l1	201	PEB	ND-C1D-CHC-C4C
29	l1	201	PEB	NB-C1B-CHA-C4A
29	l1	201	PEB	C2B-C1B-CHA-C4A
29	l1	202	PEB	NB-C1B-CHA-C4A
29	l1	202	PEB	C2B-C1B-CHA-C4A
29	m1	201	PEB	NB-C1B-CHA-C4A
29	m1	201	PEB	C2B-C1B-CHA-C4A
29	m1	202	PEB	NB-C1B-CHA-C4A
29	m1	202	PEB	C2B-C1B-CHA-C4A
29	e2	401	PEB	C1C-C2C-CAC-CBC
29	e2	401	PEB	C3C-C2C-CAC-CBC
29	e2	401	PEB	C2C-CAC-CBC-CGC
29	e2	401	PEB	C4A-C3A-CAA-CBA
29	e2	401	PEB	NB-C1B-CHA-C4A
29	e2	401	PEB	C2B-C1B-CHA-C4A
29	e2	402	PEB	NB-C1B-CHA-C4A
29	e2	402	PEB	C2B-C1B-CHA-C4A
29	e2	402	PEB	C2B-C3B-CAB-CBB
29	e2	402	PEB	C4B-C3B-CAB-CBB
29	M2	201	PEB	C2A-C3A-CAA-CBA
29	M2	201	PEB	C4A-C3A-CAA-CBA
29	M2	201	PEB	NB-C1B-CHA-C4A
29	M2	201	PEB	C2B-C1B-CHA-C4A
29	M2	202	PEB	NB-C1B-CHA-C4A
29	M2	202	PEB	C2B-C1B-CHA-C4A
29	N2	201	PEB	NB-C1B-CHA-C4A
29	N2	201	PEB	C2B-C1B-CHA-C4A
29	N2	201	PEB	C2B-C3B-CAB-CBB
29	N2	201	PEB	C4B-C3B-CAB-CBB
29	N2	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	N2	202	PEB	C4A-C3A-CAA-CBA
29	N2	202	PEB	NB-C1B-CHA-C4A
29	N2	202	PEB	C2B-C1B-CHA-C4A
29	N2	203	PEB	ND-C1D-CHC-C4C
29	N2	203	PEB	C2D-C1D-CHC-C4C
29	N2	203	PEB	NC-C1C-CHB-C4B
29	N2	203	PEB	C2C-C1C-CHB-C4B
29	N2	203	PEB	C2A-C3A-CAA-CBA
29	N2	203	PEB	NB-C1B-CHA-C4A
29	N2	203	PEB	C2B-C1B-CHA-C4A
29	O2	201	PEB	C2A-C3A-CAA-CBA
29	O2	201	PEB	C4A-C3A-CAA-CBA
29	O2	201	PEB	NB-C1B-CHA-C4A
29	O2	201	PEB	C2B-C1B-CHA-C4A
29	O2	202	PEB	NC-C1C-CHB-C4B
29	O2	202	PEB	NB-C1B-CHA-C4A
29	O2	202	PEB	C2B-C1B-CHA-C4A
29	P2	201	PEB	C2A-C3A-CAA-CBA
29	P2	201	PEB	C4A-C3A-CAA-CBA
29	P2	201	PEB	NB-C1B-CHA-C4A
29	P2	201	PEB	C2B-C1B-CHA-C4A
29	P2	202	PEB	ND-C1D-CHC-C4C
29	P2	202	PEB	C2D-C1D-CHC-C4C
29	P2	202	PEB	NC-C1C-CHB-C4B
29	P2	202	PEB	C2C-C1C-CHB-C4B
29	P2	202	PEB	C2A-C3A-CAA-CBA
29	P2	202	PEB	NB-C1B-CHA-C4A
29	P2	202	PEB	C2B-C1B-CHA-C4A
29	Q2	201	PEB	C2A-C3A-CAA-CBA
29	Q2	201	PEB	C4A-C3A-CAA-CBA
29	Q2	201	PEB	NB-C1B-CHA-C4A
29	Q2	201	PEB	C2B-C1B-CHA-C4A
29	Q2	202	PEB	NC-C1C-CHB-C4B
29	Q2	202	PEB	NB-C1B-CHA-C4A
29	Q2	202	PEB	C2B-C1B-CHA-C4A
29	R2	201	PEB	NB-C1B-CHA-C4A
29	R2	201	PEB	C2B-C1B-CHA-C4A
29	R2	201	PEB	C2B-C3B-CAB-CBB
29	R2	201	PEB	C4B-C3B-CAB-CBB
29	R2	202	PEB	C2A-C3A-CAA-CBA
29	R2	202	PEB	C4A-C3A-CAA-CBA
29	R2	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	R2	202	PEB	C2B-C1B-CHA-C4A
29	R2	203	PEB	ND-C1D-CHC-C4C
29	R2	203	PEB	C2D-C1D-CHC-C4C
29	R2	203	PEB	NC-C1C-CHB-C4B
29	R2	203	PEB	C2C-C1C-CHB-C4B
29	R2	203	PEB	C2A-C3A-CAA-CBA
29	R2	203	PEB	NB-C1B-CHA-C4A
29	R2	203	PEB	C2B-C1B-CHA-C4A
29	S2	201	PEB	NB-C1B-CHA-C4A
29	S2	201	PEB	C2B-C1B-CHA-C4A
29	S2	202	PEB	NB-C1B-CHA-C4A
29	S2	202	PEB	C2B-C1B-CHA-C4A
29	T2	201	PEB	NB-C1B-CHA-C4A
29	T2	201	PEB	C2B-C1B-CHA-C4A
29	T2	201	PEB	C2B-C3B-CAB-CBB
29	T2	201	PEB	C4B-C3B-CAB-CBB
29	T2	202	PEB	C2A-C3A-CAA-CBA
29	T2	202	PEB	C4A-C3A-CAA-CBA
29	T2	202	PEB	NB-C1B-CHA-C4A
29	T2	202	PEB	C2B-C1B-CHA-C4A
29	T2	203	PEB	ND-C1D-CHC-C4C
29	T2	203	PEB	C2D-C1D-CHC-C4C
29	T2	203	PEB	NC-C1C-CHB-C4B
29	T2	203	PEB	C2C-C1C-CHB-C4B
29	T2	203	PEB	C2A-C3A-CAA-CBA
29	T2	203	PEB	NB-C1B-CHA-C4A
29	T2	203	PEB	C2B-C1B-CHA-C4A
29	U2	201	PEB	C2A-C3A-CAA-CBA
29	U2	201	PEB	C4A-C3A-CAA-CBA
29	U2	201	PEB	NB-C1B-CHA-C4A
29	U2	201	PEB	C2B-C1B-CHA-C4A
29	U2	202	PEB	NB-C1B-CHA-C4A
29	U2	202	PEB	C2B-C1B-CHA-C4A
29	V2	201	PEB	NB-C1B-CHA-C4A
29	V2	201	PEB	C2B-C1B-CHA-C4A
29	V2	201	PEB	C2B-C3B-CAB-CBB
29	V2	201	PEB	C4B-C3B-CAB-CBB
29	V2	202	PEB	C2A-C3A-CAA-CBA
29	V2	202	PEB	C4A-C3A-CAA-CBA
29	V2	202	PEB	NB-C1B-CHA-C4A
29	V2	202	PEB	C2B-C1B-CHA-C4A
29	V2	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	V2	203	PEB	C2D-C1D-CHC-C4C
29	V2	203	PEB	NC-C1C-CHB-C4B
29	V2	203	PEB	C2C-C1C-CHB-C4B
29	V2	203	PEB	C2A-C3A-CAA-CBA
29	V2	203	PEB	NB-C1B-CHA-C4A
29	V2	203	PEB	C2B-C1B-CHA-C4A
29	W2	201	PEB	C2A-C3A-CAA-CBA
29	W2	201	PEB	C4A-C3A-CAA-CBA
29	W2	201	PEB	NB-C1B-CHA-C4A
29	W2	201	PEB	C2B-C1B-CHA-C4A
29	W2	202	PEB	NB-C1B-CHA-C4A
29	W2	202	PEB	C2B-C1B-CHA-C4A
29	X2	201	PEB	C2A-C3A-CAA-CBA
29	X2	201	PEB	C4A-C3A-CAA-CBA
29	X2	201	PEB	NB-C1B-CHA-C4A
29	X2	201	PEB	C2B-C1B-CHA-C4A
29	X2	202	PEB	ND-C1D-CHC-C4C
29	X2	202	PEB	C2D-C1D-CHC-C4C
29	X2	202	PEB	NC-C1C-CHB-C4B
29	X2	202	PEB	C2C-C1C-CHB-C4B
29	X2	202	PEB	C2A-C3A-CAA-CBA
29	X2	202	PEB	NB-C1B-CHA-C4A
29	X2	202	PEB	C2B-C1B-CHA-C4A
29	A3	201	PEB	NB-C1B-CHA-C4A
29	A3	201	PEB	C2B-C1B-CHA-C4A
29	A3	202	PEB	C2C-CAC-CBC-CGC
29	A3	202	PEB	C2A-C3A-CAA-CBA
29	A3	202	PEB	C4A-C3A-CAA-CBA
29	A3	202	PEB	NB-C1B-CHA-C4A
29	A3	202	PEB	C2B-C1B-CHA-C4A
29	B3	201	PEB	NB-C1B-CHA-C4A
29	B3	201	PEB	C2B-C1B-CHA-C4A
29	B3	202	PEB	C2C-CAC-CBC-CGC
29	B3	202	PEB	C2A-C3A-CAA-CBA
29	B3	202	PEB	C4A-C3A-CAA-CBA
29	B3	202	PEB	NB-C1B-CHA-C4A
29	B3	202	PEB	C2B-C1B-CHA-C4A
29	B3	203	PEB	ND-C1D-CHC-C4C
29	B3	203	PEB	C2D-C1D-CHC-C4C
29	B3	203	PEB	NC-C1C-CHB-C4B
29	B3	203	PEB	C2C-C1C-CHB-C4B
29	B3	203	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	B3	203	PEB	C4A-C3A-CAA-CBA
29	B3	203	PEB	NB-C1B-CHA-C4A
29	B3	203	PEB	C2B-C1B-CHA-C4A
29	C3	201	PEB	NB-C1B-CHA-C4A
29	C3	201	PEB	C2B-C1B-CHA-C4A
29	C3	202	PEB	C2C-CAC-CBC-CGC
29	C3	202	PEB	C2A-C3A-CAA-CBA
29	C3	202	PEB	C4A-C3A-CAA-CBA
29	C3	202	PEB	NB-C1B-CHA-C4A
29	C3	202	PEB	C2B-C1B-CHA-C4A
29	D3	201	PEB	NB-C1B-CHA-C4A
29	D3	201	PEB	C2B-C1B-CHA-C4A
29	D3	202	PEB	C2A-C3A-CAA-CBA
29	D3	202	PEB	C4A-C3A-CAA-CBA
29	D3	202	PEB	NB-C1B-CHA-C4A
29	D3	202	PEB	C2B-C1B-CHA-C4A
29	D3	203	PEB	ND-C1D-CHC-C4C
29	D3	203	PEB	C2D-C1D-CHC-C4C
29	D3	203	PEB	NC-C1C-CHB-C4B
29	D3	203	PEB	C2C-C1C-CHB-C4B
29	D3	203	PEB	C2A-C3A-CAA-CBA
29	D3	203	PEB	C4A-C3A-CAA-CBA
29	D3	203	PEB	NB-C1B-CHA-C4A
29	D3	203	PEB	C2B-C1B-CHA-C4A
29	E3	201	PEB	NB-C1B-CHA-C4A
29	E3	201	PEB	C2B-C1B-CHA-C4A
29	E3	202	PEB	C2C-CAC-CBC-CGC
29	E3	202	PEB	C2A-C3A-CAA-CBA
29	E3	202	PEB	C4A-C3A-CAA-CBA
29	E3	202	PEB	NB-C1B-CHA-C4A
29	E3	202	PEB	C2B-C1B-CHA-C4A
29	F3	201	PEB	NB-C1B-CHA-C4A
29	F3	201	PEB	C2B-C1B-CHA-C4A
29	F3	202	PEB	C2C-CAC-CBC-CGC
29	F3	202	PEB	C2A-C3A-CAA-CBA
29	F3	202	PEB	C4A-C3A-CAA-CBA
29	F3	202	PEB	NB-C1B-CHA-C4A
29	F3	202	PEB	C2B-C1B-CHA-C4A
29	F3	203	PEB	ND-C1D-CHC-C4C
29	F3	203	PEB	C2D-C1D-CHC-C4C
29	F3	203	PEB	NC-C1C-CHB-C4B
29	F3	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	F3	203	PEB	C2A-C3A-CAA-CBA
29	F3	203	PEB	C4A-C3A-CAA-CBA
29	F3	203	PEB	NB-C1B-CHA-C4A
29	F3	203	PEB	C2B-C1B-CHA-C4A
29	G3	201	PEB	NB-C1B-CHA-C4A
29	G3	201	PEB	C2B-C1B-CHA-C4A
29	G3	202	PEB	C2C-CAC-CBC-CGC
29	G3	202	PEB	C2A-C3A-CAA-CBA
29	G3	202	PEB	C4A-C3A-CAA-CBA
29	G3	202	PEB	NB-C1B-CHA-C4A
29	G3	202	PEB	C2B-C1B-CHA-C4A
29	H3	201	PEB	NB-C1B-CHA-C4A
29	H3	201	PEB	C2B-C1B-CHA-C4A
29	H3	202	PEB	C2C-CAC-CBC-CGC
29	H3	202	PEB	C2A-C3A-CAA-CBA
29	H3	202	PEB	C4A-C3A-CAA-CBA
29	H3	202	PEB	NB-C1B-CHA-C4A
29	H3	202	PEB	C2B-C1B-CHA-C4A
29	H3	203	PEB	ND-C1D-CHC-C4C
29	H3	203	PEB	C2D-C1D-CHC-C4C
29	H3	203	PEB	NC-C1C-CHB-C4B
29	H3	203	PEB	C2C-C1C-CHB-C4B
29	H3	203	PEB	C2A-C3A-CAA-CBA
29	H3	203	PEB	C4A-C3A-CAA-CBA
29	H3	203	PEB	NB-C1B-CHA-C4A
29	H3	203	PEB	C2B-C1B-CHA-C4A
29	I3	201	PEB	NB-C1B-CHA-C4A
29	I3	201	PEB	C2B-C1B-CHA-C4A
29	I3	202	PEB	C2C-CAC-CBC-CGC
29	I3	202	PEB	C2A-C3A-CAA-CBA
29	I3	202	PEB	C4A-C3A-CAA-CBA
29	I3	202	PEB	NB-C1B-CHA-C4A
29	I3	202	PEB	C2B-C1B-CHA-C4A
29	I3	203	PEB	C2C-CAC-CBC-CGC
29	I3	203	PEB	C2A-C3A-CAA-CBA
29	I3	203	PEB	C4A-C3A-CAA-CBA
29	I3	203	PEB	NB-C1B-CHA-C4A
29	I3	203	PEB	C2B-C1B-CHA-C4A
29	J3	201	PEB	NB-C1B-CHA-C4A
29	J3	201	PEB	C2B-C1B-CHA-C4A
29	J3	202	PEB	C2C-CAC-CBC-CGC
29	J3	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	J3	202	PEB	C4A-C3A-CAA-CBA
29	J3	202	PEB	NB-C1B-CHA-C4A
29	J3	202	PEB	C2B-C1B-CHA-C4A
29	J3	203	PEB	ND-C1D-CHC-C4C
29	J3	203	PEB	C2D-C1D-CHC-C4C
29	J3	203	PEB	NC-C1C-CHB-C4B
29	J3	203	PEB	C2C-C1C-CHB-C4B
29	J3	203	PEB	C2A-C3A-CAA-CBA
29	J3	203	PEB	C4A-C3A-CAA-CBA
29	J3	203	PEB	NB-C1B-CHA-C4A
29	J3	203	PEB	C2B-C1B-CHA-C4A
29	K3	201	PEB	NB-C1B-CHA-C4A
29	K3	201	PEB	C2B-C1B-CHA-C4A
29	K3	202	PEB	C2C-CAC-CBC-CGC
29	K3	202	PEB	C2A-C3A-CAA-CBA
29	K3	202	PEB	C4A-C3A-CAA-CBA
29	K3	202	PEB	NB-C1B-CHA-C4A
29	K3	202	PEB	C2B-C1B-CHA-C4A
29	L3	201	PEB	NB-C1B-CHA-C4A
29	L3	201	PEB	C2B-C1B-CHA-C4A
29	L3	202	PEB	ND-C1D-CHC-C4C
29	L3	202	PEB	C2D-C1D-CHC-C4C
29	L3	202	PEB	NC-C1C-CHB-C4B
29	L3	202	PEB	C2C-C1C-CHB-C4B
29	L3	202	PEB	C2A-C3A-CAA-CBA
29	L3	202	PEB	C4A-C3A-CAA-CBA
29	L3	202	PEB	NB-C1B-CHA-C4A
29	L3	202	PEB	C2B-C1B-CHA-C4A
29	M3	201	PEB	NB-C1B-CHA-C4A
29	M3	201	PEB	C2B-C1B-CHA-C4A
29	M3	202	PEB	NB-C1B-CHA-C4A
29	M3	202	PEB	C2B-C1B-CHA-C4A
29	M3	203	PEB	ND-C1D-CHC-C4C
29	M3	203	PEB	C2D-C1D-CHC-C4C
29	M3	203	PEB	NC-C1C-CHB-C4B
29	M3	203	PEB	C2C-C1C-CHB-C4B
29	M3	203	PEB	NB-C1B-CHA-C4A
29	M3	203	PEB	C2B-C1B-CHA-C4A
29	N3	201	PEB	NB-C1B-CHA-C4A
29	N3	201	PEB	C2B-C1B-CHA-C4A
29	N3	202	PEB	NB-C1B-CHA-C4A
29	N3	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	N3	203	PEB	ND-C1D-CHC-C4C
29	N3	203	PEB	C2D-C1D-CHC-C4C
29	N3	203	PEB	NC-C1C-CHB-C4B
29	N3	203	PEB	C2C-C1C-CHB-C4B
29	N3	203	PEB	NB-C1B-CHA-C4A
29	N3	203	PEB	C2B-C1B-CHA-C4A
29	B4	201	PEB	ND-C1D-CHC-C4C
29	B4	201	PEB	C2D-C1D-CHC-C4C
29	B4	201	PEB	NC-C1C-CHB-C4B
29	B4	201	PEB	NB-C1B-CHA-C4A
29	B4	201	PEB	C2B-C1B-CHA-C4A
29	B4	202	PEB	NC-C1C-CHB-C4B
29	B4	202	PEB	C2C-C1C-CHB-C4B
29	B4	202	PEB	NB-C1B-CHA-C4A
29	B4	202	PEB	C2B-C1B-CHA-C4A
29	C4	201	PEB	NB-C1B-CHA-C4A
29	C4	201	PEB	C2B-C1B-CHA-C4A
29	C4	202	PEB	NC-C1C-CHB-C4B
29	C4	202	PEB	C2C-CAC-CBC-CGC
29	C4	202	PEB	C4A-C3A-CAA-CBA
29	C4	202	PEB	NB-C1B-CHA-C4A
29	C4	202	PEB	C2B-C1B-CHA-C4A
29	C4	203	PEB	NC-C1C-CHB-C4B
29	C4	203	PEB	C2C-C1C-CHB-C4B
29	C4	203	PEB	NB-C1B-CHA-C4A
29	C4	203	PEB	C2B-C1B-CHA-C4A
29	C4	203	PEB	C3B-CAB-CBB-CGB
29	D4	201	PEB	ND-C1D-CHC-C4C
29	D4	201	PEB	C2D-C1D-CHC-C4C
29	D4	201	PEB	NC-C1C-CHB-C4B
29	D4	201	PEB	NB-C1B-CHA-C4A
29	D4	201	PEB	C2B-C1B-CHA-C4A
29	D4	202	PEB	NC-C1C-CHB-C4B
29	D4	202	PEB	C2C-C1C-CHB-C4B
29	D4	202	PEB	NB-C1B-CHA-C4A
29	D4	202	PEB	C2B-C1B-CHA-C4A
29	E4	201	PEB	NB-C1B-CHA-C4A
29	E4	201	PEB	C2B-C1B-CHA-C4A
29	E4	202	PEB	NC-C1C-CHB-C4B
29	E4	202	PEB	C2C-CAC-CBC-CGC
29	E4	202	PEB	C4A-C3A-CAA-CBA
29	E4	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	E4	202	PEB	C2B-C1B-CHA-C4A
29	E4	203	PEB	NC-C1C-CHB-C4B
29	E4	203	PEB	C2C-C1C-CHB-C4B
29	E4	203	PEB	NB-C1B-CHA-C4A
29	E4	203	PEB	C2B-C1B-CHA-C4A
29	E4	203	PEB	C3B-CAB-CBB-CGB
29	F4	201	PEB	ND-C1D-CHC-C4C
29	F4	201	PEB	C2D-C1D-CHC-C4C
29	F4	201	PEB	NB-C1B-CHA-C4A
29	F4	201	PEB	C2B-C1B-CHA-C4A
29	F4	202	PEB	NC-C1C-CHB-C4B
29	F4	202	PEB	C2C-C1C-CHB-C4B
29	F4	202	PEB	NB-C1B-CHA-C4A
29	F4	202	PEB	C2B-C1B-CHA-C4A
29	G4	201	PEB	NB-C1B-CHA-C4A
29	G4	201	PEB	C2B-C1B-CHA-C4A
29	G4	202	PEB	NC-C1C-CHB-C4B
29	G4	202	PEB	C2C-CAC-CBC-CGC
29	G4	202	PEB	C4A-C3A-CAA-CBA
29	G4	202	PEB	NB-C1B-CHA-C4A
29	G4	202	PEB	C2B-C1B-CHA-C4A
29	G4	203	PEB	NC-C1C-CHB-C4B
29	G4	203	PEB	C2C-C1C-CHB-C4B
29	G4	203	PEB	NB-C1B-CHA-C4A
29	G4	203	PEB	C2B-C1B-CHA-C4A
29	G4	203	PEB	C3B-CAB-CBB-CGB
29	H4	201	PEB	ND-C1D-CHC-C4C
29	H4	201	PEB	C2D-C1D-CHC-C4C
29	H4	201	PEB	NC-C1C-CHB-C4B
29	H4	201	PEB	NB-C1B-CHA-C4A
29	H4	201	PEB	C2B-C1B-CHA-C4A
29	H4	202	PEB	NC-C1C-CHB-C4B
29	H4	202	PEB	C2C-C1C-CHB-C4B
29	H4	202	PEB	NB-C1B-CHA-C4A
29	H4	202	PEB	C2B-C1B-CHA-C4A
29	I4	201	PEB	NB-C1B-CHA-C4A
29	I4	201	PEB	C2B-C1B-CHA-C4A
29	I4	202	PEB	NC-C1C-CHB-C4B
29	I4	202	PEB	C2C-CAC-CBC-CGC
29	I4	202	PEB	C4A-C3A-CAA-CBA
29	I4	202	PEB	NB-C1B-CHA-C4A
29	I4	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	I4	203	PEB	ND-C1D-CHC-C4C
29	I4	203	PEB	C2D-C1D-CHC-C4C
29	I4	203	PEB	NB-C1B-CHA-C4A
29	I4	203	PEB	C2B-C1B-CHA-C4A
29	J4	201	PEB	ND-C1D-CHC-C4C
29	J4	201	PEB	C2D-C1D-CHC-C4C
29	J4	201	PEB	NC-C1C-CHB-C4B
29	J4	201	PEB	NB-C1B-CHA-C4A
29	J4	201	PEB	C2B-C1B-CHA-C4A
29	J4	202	PEB	NC-C1C-CHB-C4B
29	J4	202	PEB	C2C-C1C-CHB-C4B
29	J4	202	PEB	NB-C1B-CHA-C4A
29	J4	202	PEB	C2B-C1B-CHA-C4A
29	K4	201	PEB	NB-C1B-CHA-C4A
29	K4	201	PEB	C2B-C1B-CHA-C4A
29	K4	202	PEB	NC-C1C-CHB-C4B
29	K4	202	PEB	C2C-CAC-CBC-CGC
29	K4	202	PEB	C4A-C3A-CAA-CBA
29	K4	202	PEB	NB-C1B-CHA-C4A
29	K4	202	PEB	C2B-C1B-CHA-C4A
29	K4	203	PEB	NC-C1C-CHB-C4B
29	K4	203	PEB	C2C-C1C-CHB-C4B
29	K4	203	PEB	NB-C1B-CHA-C4A
29	K4	203	PEB	C2B-C1B-CHA-C4A
29	K4	203	PEB	C3B-CAB-CBB-CGB
29	L4	201	PEB	ND-C1D-CHC-C4C
29	L4	201	PEB	C2D-C1D-CHC-C4C
29	L4	201	PEB	NC-C1C-CHB-C4B
29	L4	201	PEB	NB-C1B-CHA-C4A
29	L4	201	PEB	C2B-C1B-CHA-C4A
29	L4	202	PEB	NC-C1C-CHB-C4B
29	L4	202	PEB	C2C-C1C-CHB-C4B
29	L4	202	PEB	NB-C1B-CHA-C4A
29	L4	202	PEB	C2B-C1B-CHA-C4A
29	M4	201	PEB	NB-C1B-CHA-C4A
29	M4	201	PEB	C2B-C1B-CHA-C4A
29	M4	202	PEB	NC-C1C-CHB-C4B
29	M4	202	PEB	C2C-CAC-CBC-CGC
29	M4	202	PEB	C4A-C3A-CAA-CBA
29	M4	202	PEB	NB-C1B-CHA-C4A
29	M4	202	PEB	C2B-C1B-CHA-C4A
29	M4	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	M4	203	PEB	C2C-C1C-CHB-C4B
29	M4	203	PEB	C2A-C3A-CAA-CBA
29	M4	203	PEB	NB-C1B-CHA-C4A
29	M4	203	PEB	C2B-C1B-CHA-C4A
29	B5	201	PEB	NB-C1B-CHA-C4A
29	B5	201	PEB	C2B-C1B-CHA-C4A
29	B5	202	PEB	C2C-CAC-CBC-CGC
29	B5	202	PEB	C2A-C3A-CAA-CBA
29	B5	202	PEB	C4A-C3A-CAA-CBA
29	B5	202	PEB	NB-C1B-CHA-C4A
29	B5	202	PEB	C2B-C1B-CHA-C4A
29	B5	203	PEB	ND-C1D-CHC-C4C
29	B5	203	PEB	C2D-C1D-CHC-C4C
29	B5	203	PEB	NC-C1C-CHB-C4B
29	B5	203	PEB	C2C-C1C-CHB-C4B
29	B5	203	PEB	NB-C1B-CHA-C4A
29	B5	203	PEB	C2B-C1B-CHA-C4A
29	F5	201	PEB	NB-C1B-CHA-C4A
29	F5	201	PEB	C2B-C1B-CHA-C4A
29	F5	202	PEB	C2C-CAC-CBC-CGC
29	F5	202	PEB	C2A-C3A-CAA-CBA
29	F5	202	PEB	C4A-C3A-CAA-CBA
29	F5	202	PEB	NB-C1B-CHA-C4A
29	F5	202	PEB	C2B-C1B-CHA-C4A
29	F5	203	PEB	ND-C1D-CHC-C4C
29	F5	203	PEB	C2D-C1D-CHC-C4C
29	F5	203	PEB	NC-C1C-CHB-C4B
29	F5	203	PEB	C2C-C1C-CHB-C4B
29	F5	203	PEB	NB-C1B-CHA-C4A
29	F5	203	PEB	C2B-C1B-CHA-C4A
29	G5	201	PEB	NB-C1B-CHA-C4A
29	G5	201	PEB	C2B-C1B-CHA-C4A
29	G5	202	PEB	C2C-CAC-CBC-CGC
29	G5	202	PEB	C2A-C3A-CAA-CBA
29	G5	202	PEB	C4A-C3A-CAA-CBA
29	G5	202	PEB	NB-C1B-CHA-C4A
29	G5	202	PEB	C2B-C1B-CHA-C4A
29	G5	203	PEB	ND-C1D-CHC-C4C
29	G5	203	PEB	C2D-C1D-CHC-C4C
29	G5	203	PEB	NC-C1C-CHB-C4B
29	G5	203	PEB	C2C-C1C-CHB-C4B
29	G5	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	G5	203	PEB	C2B-C1B-CHA-C4A
29	H5	201	PEB	NB-C1B-CHA-C4A
29	H5	201	PEB	C2B-C1B-CHA-C4A
29	H5	202	PEB	C2C-CAC-CBC-CGC
29	H5	202	PEB	C2A-C3A-CAA-CBA
29	H5	202	PEB	C4A-C3A-CAA-CBA
29	H5	202	PEB	NB-C1B-CHA-C4A
29	H5	202	PEB	C2B-C1B-CHA-C4A
29	H5	203	PEB	ND-C1D-CHC-C4C
29	H5	203	PEB	C2D-C1D-CHC-C4C
29	H5	203	PEB	NC-C1C-CHB-C4B
29	H5	203	PEB	C2C-C1C-CHB-C4B
29	H5	203	PEB	NB-C1B-CHA-C4A
29	H5	203	PEB	C2B-C1B-CHA-C4A
29	I5	201	PEB	NB-C1B-CHA-C4A
29	I5	201	PEB	C2B-C1B-CHA-C4A
29	I5	202	PEB	C4A-C3A-CAA-CBA
29	I5	202	PEB	NB-C1B-CHA-C4A
29	I5	202	PEB	C2B-C1B-CHA-C4A
29	I5	203	PEB	NC-C1C-CHB-C4B
29	I5	203	PEB	C2C-C1C-CHB-C4B
29	I5	203	PEB	NB-C1B-CHA-C4A
29	I5	203	PEB	C2B-C1B-CHA-C4A
29	J5	201	PEB	C2B-C1B-CHA-C4A
29	J5	202	PEB	C1C-C2C-CAC-CBC
29	J5	202	PEB	C3C-C2C-CAC-CBC
29	J5	202	PEB	C2A-C3A-CAA-CBA
29	J5	202	PEB	NB-C1B-CHA-C4A
29	J5	202	PEB	C2B-C1B-CHA-C4A
29	K5	201	PEB	NB-C1B-CHA-C4A
29	K5	201	PEB	C2B-C1B-CHA-C4A
29	K5	202	PEB	C4A-C3A-CAA-CBA
29	K5	202	PEB	NB-C1B-CHA-C4A
29	K5	202	PEB	C2B-C1B-CHA-C4A
29	K5	203	PEB	NC-C1C-CHB-C4B
29	K5	203	PEB	C2C-C1C-CHB-C4B
29	K5	203	PEB	NB-C1B-CHA-C4A
29	K5	203	PEB	C2B-C1B-CHA-C4A
29	L5	201	PEB	NB-C1B-CHA-C4A
29	L5	201	PEB	C2B-C1B-CHA-C4A
29	L5	202	PEB	C2C-CAC-CBC-CGC
29	L5	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	L5	202	PEB	C4A-C3A-CAA-CBA
29	L5	202	PEB	NB-C1B-CHA-C4A
29	L5	202	PEB	C2B-C1B-CHA-C4A
29	L5	203	PEB	ND-C1D-CHC-C4C
29	L5	203	PEB	C2D-C1D-CHC-C4C
29	L5	203	PEB	NC-C1C-CHB-C4B
29	L5	203	PEB	C2C-C1C-CHB-C4B
29	L5	203	PEB	NB-C1B-CHA-C4A
29	L5	203	PEB	C2B-C1B-CHA-C4A
29	A5	201	PEB	NB-C1B-CHA-C4A
29	A5	201	PEB	C2B-C1B-CHA-C4A
29	A5	202	PEB	C4A-C3A-CAA-CBA
29	A5	202	PEB	NB-C1B-CHA-C4A
29	A5	202	PEB	C2B-C1B-CHA-C4A
29	A5	203	PEB	NC-C1C-CHB-C4B
29	A5	203	PEB	C2C-C1C-CHB-C4B
29	A5	203	PEB	NB-C1B-CHA-C4A
29	A5	203	PEB	C2B-C1B-CHA-C4A
29	C5	201	PEB	NB-C1B-CHA-C4A
29	C5	201	PEB	C2B-C1B-CHA-C4A
29	C5	202	PEB	C4A-C3A-CAA-CBA
29	C5	202	PEB	NB-C1B-CHA-C4A
29	C5	202	PEB	C2B-C1B-CHA-C4A
29	C5	203	PEB	NC-C1C-CHB-C4B
29	C5	203	PEB	C2C-C1C-CHB-C4B
29	C5	203	PEB	NB-C1B-CHA-C4A
29	C5	203	PEB	C2B-C1B-CHA-C4A
29	A7	301	PEB	C2C-CAC-CBC-CGC
29	A7	301	PEB	C4A-C3A-CAA-CBA
29	A7	301	PEB	NB-C1B-CHA-C4A
29	A7	301	PEB	C2B-C1B-CHA-C4A
29	A7	304	PEB	NB-C1B-CHA-C4A
29	A7	304	PEB	C2B-C1B-CHA-C4A
29	A7	305	PEB	NB-C1B-CHA-C4A
29	A7	305	PEB	C2B-C1B-CHA-C4A
29	D7	1002	PEB	NC-C1C-CHB-C4B
29	D7	1002	PEB	C2A-C3A-CAA-CBA
29	D7	1002	PEB	C4A-C3A-CAA-CBA
29	D7	1002	PEB	NB-C1B-CHA-C4A
29	D7	1002	PEB	C2B-C1B-CHA-C4A
29	F7	1002	PEB	NC-C1C-CHB-C4B
29	F7	1002	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	F7	1002	PEB	C4A-C3A-CAA-CBA
29	F7	1002	PEB	NB-C1B-CHA-C4A
29	F7	1002	PEB	C2B-C1B-CHA-C4A
29	H7	1002	PEB	NC-C1C-CHB-C4B
29	H7	1002	PEB	C2A-C3A-CAA-CBA
29	H7	1002	PEB	C4A-C3A-CAA-CBA
29	H7	1002	PEB	NB-C1B-CHA-C4A
29	H7	1002	PEB	C2B-C1B-CHA-C4A
29	J7	1002	PEB	NC-C1C-CHB-C4B
29	J7	1002	PEB	C2A-C3A-CAA-CBA
29	J7	1002	PEB	C4A-C3A-CAA-CBA
29	J7	1002	PEB	NB-C1B-CHA-C4A
29	J7	1002	PEB	C2B-C1B-CHA-C4A
29	L7	1002	PEB	NC-C1C-CHB-C4B
29	L7	1002	PEB	C2A-C3A-CAA-CBA
29	L7	1002	PEB	C4A-C3A-CAA-CBA
29	L7	1002	PEB	NB-C1B-CHA-C4A
29	L7	1002	PEB	C2B-C1B-CHA-C4A
29	N7	1002	PEB	NC-C1C-CHB-C4B
29	N7	1002	PEB	C2A-C3A-CAA-CBA
29	N7	1002	PEB	C4A-C3A-CAA-CBA
29	N7	1002	PEB	NB-C1B-CHA-C4A
29	N7	1002	PEB	C2B-C1B-CHA-C4A
29	O7	201	PEB	C4A-C3A-CAA-CBA
29	O7	201	PEB	NB-C1B-CHA-C4A
29	O7	201	PEB	C2B-C1B-CHA-C4A
29	O7	202	PEB	ND-C1D-CHC-C4C
29	O7	202	PEB	C2D-C1D-CHC-C4C
29	O7	202	PEB	NB-C1B-CHA-C4A
29	O7	202	PEB	C2B-C1B-CHA-C4A
29	P7	201	PEB	NB-C1B-CHA-C4A
29	P7	201	PEB	C2B-C1B-CHA-C4A
29	P7	202	PEB	ND-C1D-CHC-C4C
29	P7	202	PEB	C2D-C1D-CHC-C4C
29	P7	202	PEB	NB-C1B-CHA-C4A
29	P7	202	PEB	C2B-C1B-CHA-C4A
29	P7	203	PEB	NC-C1C-CHB-C4B
29	P7	203	PEB	C2C-C1C-CHB-C4B
29	P7	203	PEB	NB-C1B-CHA-C4A
29	P7	203	PEB	C2B-C1B-CHA-C4A
29	P7	203	PEB	C2B-C3B-CAB-CBB
29	P7	203	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	Q7	201	PEB	C4A-C3A-CAA-CBA
29	Q7	201	PEB	NB-C1B-CHA-C4A
29	Q7	201	PEB	C2B-C1B-CHA-C4A
29	Q7	202	PEB	ND-C1D-CHC-C4C
29	Q7	202	PEB	C2D-C1D-CHC-C4C
29	Q7	202	PEB	NB-C1B-CHA-C4A
29	Q7	202	PEB	C2B-C1B-CHA-C4A
29	R7	201	PEB	NB-C1B-CHA-C4A
29	R7	201	PEB	C2B-C1B-CHA-C4A
29	R7	202	PEB	ND-C1D-CHC-C4C
29	R7	202	PEB	C2D-C1D-CHC-C4C
29	R7	202	PEB	NB-C1B-CHA-C4A
29	R7	202	PEB	C2B-C1B-CHA-C4A
29	R7	203	PEB	NC-C1C-CHB-C4B
29	R7	203	PEB	C2C-C1C-CHB-C4B
29	R7	203	PEB	NB-C1B-CHA-C4A
29	R7	203	PEB	C2B-C1B-CHA-C4A
29	R7	203	PEB	C2B-C3B-CAB-CBB
29	R7	203	PEB	C4B-C3B-CAB-CBB
29	S7	201	PEB	C4A-C3A-CAA-CBA
29	S7	201	PEB	NB-C1B-CHA-C4A
29	S7	201	PEB	C2B-C1B-CHA-C4A
29	S7	202	PEB	ND-C1D-CHC-C4C
29	S7	202	PEB	C2D-C1D-CHC-C4C
29	S7	202	PEB	NB-C1B-CHA-C4A
29	S7	202	PEB	C2B-C1B-CHA-C4A
29	T7	201	PEB	NB-C1B-CHA-C4A
29	T7	201	PEB	C2B-C1B-CHA-C4A
29	T7	202	PEB	ND-C1D-CHC-C4C
29	T7	202	PEB	C2D-C1D-CHC-C4C
29	T7	202	PEB	NB-C1B-CHA-C4A
29	T7	202	PEB	C2B-C1B-CHA-C4A
29	T7	203	PEB	NC-C1C-CHB-C4B
29	T7	203	PEB	C2C-C1C-CHB-C4B
29	T7	203	PEB	NB-C1B-CHA-C4A
29	T7	203	PEB	C2B-C1B-CHA-C4A
29	T7	203	PEB	C2B-C3B-CAB-CBB
29	T7	203	PEB	C4B-C3B-CAB-CBB
29	U7	201	PEB	C4A-C3A-CAA-CBA
29	U7	201	PEB	NB-C1B-CHA-C4A
29	U7	201	PEB	C2B-C1B-CHA-C4A
29	U7	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	U7	202	PEB	C2D-C1D-CHC-C4C
29	U7	202	PEB	NB-C1B-CHA-C4A
29	U7	202	PEB	C2B-C1B-CHA-C4A
29	V7	201	PEB	NB-C1B-CHA-C4A
29	V7	201	PEB	C2B-C1B-CHA-C4A
29	V7	202	PEB	ND-C1D-CHC-C4C
29	V7	202	PEB	C2D-C1D-CHC-C4C
29	V7	202	PEB	NB-C1B-CHA-C4A
29	V7	202	PEB	C2B-C1B-CHA-C4A
29	V7	203	PEB	NC-C1C-CHB-C4B
29	V7	203	PEB	C2C-C1C-CHB-C4B
29	V7	203	PEB	NB-C1B-CHA-C4A
29	V7	203	PEB	C2B-C1B-CHA-C4A
29	V7	203	PEB	C2B-C3B-CAB-CBB
29	V7	203	PEB	C4B-C3B-CAB-CBB
29	W7	201	PEB	C4A-C3A-CAA-CBA
29	W7	201	PEB	NB-C1B-CHA-C4A
29	W7	201	PEB	C2B-C1B-CHA-C4A
29	W7	202	PEB	ND-C1D-CHC-C4C
29	W7	202	PEB	C2D-C1D-CHC-C4C
29	W7	202	PEB	NB-C1B-CHA-C4A
29	W7	202	PEB	C2B-C1B-CHA-C4A
29	Y7	201	PEB	NB-C1B-CHA-C4A
29	Y7	201	PEB	C2B-C1B-CHA-C4A
29	Y7	202	PEB	ND-C1D-CHC-C4C
29	Y7	202	PEB	C2D-C1D-CHC-C4C
29	Y7	202	PEB	NB-C1B-CHA-C4A
29	Y7	202	PEB	C2B-C1B-CHA-C4A
29	Y7	203	PEB	NC-C1C-CHB-C4B
29	Y7	203	PEB	C2C-C1C-CHB-C4B
29	Y7	203	PEB	NB-C1B-CHA-C4A
29	Y7	203	PEB	C2B-C1B-CHA-C4A
29	Y7	203	PEB	C2B-C3B-CAB-CBB
29	Y7	203	PEB	C4B-C3B-CAB-CBB
29	Z7	201	PEB	C4A-C3A-CAA-CBA
29	Z7	201	PEB	NB-C1B-CHA-C4A
29	Z7	201	PEB	C2B-C1B-CHA-C4A
29	Z7	202	PEB	ND-C1D-CHC-C4C
29	Z7	202	PEB	C2D-C1D-CHC-C4C
29	Z7	202	PEB	NB-C1B-CHA-C4A
29	Z7	202	PEB	C2B-C1B-CHA-C4A
29	a7	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	a7	201	PEB	C2B-C1B-CHA-C4A
29	a7	202	PEB	ND-C1D-CHC-C4C
29	a7	202	PEB	C2D-C1D-CHC-C4C
29	a7	202	PEB	NB-C1B-CHA-C4A
29	a7	202	PEB	C2B-C1B-CHA-C4A
29	a7	203	PEB	NC-C1C-CHB-C4B
29	a7	203	PEB	C2C-C1C-CHB-C4B
29	a7	203	PEB	NB-C1B-CHA-C4A
29	a7	203	PEB	C2B-C1B-CHA-C4A
29	a7	203	PEB	C2B-C3B-CAB-CBB
29	a7	203	PEB	C4B-C3B-CAB-CBB
29	b7	201	PEB	C4A-C3A-CAA-CBA
29	b7	201	PEB	NB-C1B-CHA-C4A
29	b7	201	PEB	C2B-C1B-CHA-C4A
29	b7	202	PEB	ND-C1D-CHC-C4C
29	b7	202	PEB	C2D-C1D-CHC-C4C
29	b7	202	PEB	NB-C1B-CHA-C4A
29	b7	202	PEB	C2B-C1B-CHA-C4A
29	c7	201	PEB	NB-C1B-CHA-C4A
29	c7	201	PEB	C2B-C1B-CHA-C4A
29	c7	202	PEB	ND-C1D-CHC-C4C
29	c7	202	PEB	C2D-C1D-CHC-C4C
29	c7	202	PEB	NB-C1B-CHA-C4A
29	c7	202	PEB	C2B-C1B-CHA-C4A
29	c7	203	PEB	NC-C1C-CHB-C4B
29	c7	203	PEB	C2C-C1C-CHB-C4B
29	c7	203	PEB	NB-C1B-CHA-C4A
29	c7	203	PEB	C2B-C1B-CHA-C4A
29	c7	203	PEB	C2B-C3B-CAB-CBB
29	c7	203	PEB	C4B-C3B-CAB-CBB
29	d7	201	PEB	C4A-C3A-CAA-CBA
29	d7	201	PEB	NB-C1B-CHA-C4A
29	d7	201	PEB	C2B-C1B-CHA-C4A
29	d7	202	PEB	ND-C1D-CHC-C4C
29	d7	202	PEB	C2D-C1D-CHC-C4C
29	d7	202	PEB	NB-C1B-CHA-C4A
29	d7	202	PEB	C2B-C1B-CHA-C4A
29	e7	201	PEB	NB-C1B-CHA-C4A
29	e7	201	PEB	C2B-C1B-CHA-C4A
29	e7	202	PEB	ND-C1D-CHC-C4C
29	e7	202	PEB	C2D-C1D-CHC-C4C
29	e7	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	e7	202	PEB	C2B-C1B-CHA-C4A
29	e7	203	PEB	NC-C1C-CHB-C4B
29	e7	203	PEB	C2C-C1C-CHB-C4B
29	e7	203	PEB	NB-C1B-CHA-C4A
29	e7	203	PEB	C2B-C1B-CHA-C4A
29	e7	203	PEB	C2B-C3B-CAB-CBB
29	e7	203	PEB	C4B-C3B-CAB-CBB
29	f7	201	PEB	C4A-C3A-CAA-CBA
29	f7	201	PEB	NB-C1B-CHA-C4A
29	f7	201	PEB	C2B-C1B-CHA-C4A
29	f7	202	PEB	ND-C1D-CHC-C4C
29	f7	202	PEB	C2D-C1D-CHC-C4C
29	f7	202	PEB	NB-C1B-CHA-C4A
29	f7	202	PEB	C2B-C1B-CHA-C4A
29	g7	201	PEB	NB-C1B-CHA-C4A
29	g7	201	PEB	C2B-C1B-CHA-C4A
29	g7	202	PEB	ND-C1D-CHC-C4C
29	g7	202	PEB	C2D-C1D-CHC-C4C
29	g7	202	PEB	NB-C1B-CHA-C4A
29	g7	202	PEB	C2B-C1B-CHA-C4A
29	g7	203	PEB	NC-C1C-CHB-C4B
29	g7	203	PEB	C2C-C1C-CHB-C4B
29	g7	203	PEB	NB-C1B-CHA-C4A
29	g7	203	PEB	C2B-C1B-CHA-C4A
29	g7	203	PEB	C2B-C3B-CAB-CBB
29	g7	203	PEB	C4B-C3B-CAB-CBB
29	h7	201	PEB	C4A-C3A-CAA-CBA
29	h7	201	PEB	NB-C1B-CHA-C4A
29	h7	201	PEB	C2B-C1B-CHA-C4A
29	h7	202	PEB	ND-C1D-CHC-C4C
29	h7	202	PEB	C2D-C1D-CHC-C4C
29	h7	202	PEB	NB-C1B-CHA-C4A
29	h7	202	PEB	C2B-C1B-CHA-C4A
29	i7	201	PEB	NB-C1B-CHA-C4A
29	i7	201	PEB	C2B-C1B-CHA-C4A
29	i7	202	PEB	ND-C1D-CHC-C4C
29	i7	202	PEB	C2D-C1D-CHC-C4C
29	i7	202	PEB	NB-C1B-CHA-C4A
29	i7	202	PEB	C2B-C1B-CHA-C4A
29	i7	203	PEB	NC-C1C-CHB-C4B
29	i7	203	PEB	C2C-C1C-CHB-C4B
29	i7	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	i7	203	PEB	C2B-C1B-CHA-C4A
29	i7	203	PEB	C2B-C3B-CAB-CBB
29	i7	203	PEB	C4B-C3B-CAB-CBB
29	j7	201	PEB	C4A-C3A-CAA-CBA
29	j7	201	PEB	NB-C1B-CHA-C4A
29	j7	201	PEB	C2B-C1B-CHA-C4A
29	j7	202	PEB	ND-C1D-CHC-C4C
29	j7	202	PEB	C2D-C1D-CHC-C4C
29	j7	202	PEB	NB-C1B-CHA-C4A
29	j7	202	PEB	C2B-C1B-CHA-C4A
29	k7	201	PEB	NB-C1B-CHA-C4A
29	k7	201	PEB	C2B-C1B-CHA-C4A
29	k7	202	PEB	ND-C1D-CHC-C4C
29	k7	202	PEB	C2D-C1D-CHC-C4C
29	k7	202	PEB	NB-C1B-CHA-C4A
29	k7	202	PEB	C2B-C1B-CHA-C4A
29	k7	203	PEB	NC-C1C-CHB-C4B
29	k7	203	PEB	C2C-C1C-CHB-C4B
29	k7	203	PEB	NB-C1B-CHA-C4A
29	k7	203	PEB	C2B-C1B-CHA-C4A
29	k7	203	PEB	C2B-C3B-CAB-CBB
29	k7	203	PEB	C4B-C3B-CAB-CBB
29	l7	201	PEB	C4A-C3A-CAA-CBA
29	l7	201	PEB	NB-C1B-CHA-C4A
29	l7	201	PEB	C2B-C1B-CHA-C4A
29	l7	202	PEB	ND-C1D-CHC-C4C
29	l7	202	PEB	C2D-C1D-CHC-C4C
29	l7	202	PEB	NB-C1B-CHA-C4A
29	l7	202	PEB	C2B-C1B-CHA-C4A
29	m7	201	PEB	NB-C1B-CHA-C4A
29	m7	201	PEB	C2B-C1B-CHA-C4A
29	m7	202	PEB	ND-C1D-CHC-C4C
29	m7	202	PEB	C2D-C1D-CHC-C4C
29	m7	202	PEB	NB-C1B-CHA-C4A
29	m7	202	PEB	C2B-C1B-CHA-C4A
29	m7	203	PEB	NC-C1C-CHB-C4B
29	m7	203	PEB	C2C-C1C-CHB-C4B
29	m7	203	PEB	NB-C1B-CHA-C4A
29	m7	203	PEB	C2B-C1B-CHA-C4A
29	m7	203	PEB	C2B-C3B-CAB-CBB
29	m7	203	PEB	C4B-C3B-CAB-CBB
29	B8	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	B8	201	PEB	C2B-C1B-CHA-C4A
29	B8	202	PEB	C2C-CAC-CBC-CGC
29	B8	202	PEB	C2A-C3A-CAA-CBA
29	B8	202	PEB	C4A-C3A-CAA-CBA
29	B8	202	PEB	NB-C1B-CHA-C4A
29	B8	202	PEB	C2B-C1B-CHA-C4A
29	B8	203	PEB	ND-C1D-CHC-C4C
29	B8	203	PEB	C2D-C1D-CHC-C4C
29	B8	203	PEB	NC-C1C-CHB-C4B
29	B8	203	PEB	C2C-C1C-CHB-C4B
29	B8	203	PEB	NB-C1B-CHA-C4A
29	B8	203	PEB	C2B-C1B-CHA-C4A
29	F8	201	PEB	NB-C1B-CHA-C4A
29	F8	201	PEB	C2B-C1B-CHA-C4A
29	F8	202	PEB	C2C-CAC-CBC-CGC
29	F8	202	PEB	C2A-C3A-CAA-CBA
29	F8	202	PEB	C4A-C3A-CAA-CBA
29	F8	202	PEB	NB-C1B-CHA-C4A
29	F8	202	PEB	C2B-C1B-CHA-C4A
29	F8	203	PEB	ND-C1D-CHC-C4C
29	F8	203	PEB	C2D-C1D-CHC-C4C
29	F8	203	PEB	NC-C1C-CHB-C4B
29	F8	203	PEB	C2C-C1C-CHB-C4B
29	F8	203	PEB	NB-C1B-CHA-C4A
29	F8	203	PEB	C2B-C1B-CHA-C4A
29	G8	201	PEB	NB-C1B-CHA-C4A
29	G8	201	PEB	C2B-C1B-CHA-C4A
29	G8	202	PEB	C2C-CAC-CBC-CGC
29	G8	202	PEB	C2A-C3A-CAA-CBA
29	G8	202	PEB	C4A-C3A-CAA-CBA
29	G8	202	PEB	NB-C1B-CHA-C4A
29	G8	202	PEB	C2B-C1B-CHA-C4A
29	G8	203	PEB	ND-C1D-CHC-C4C
29	G8	203	PEB	C2D-C1D-CHC-C4C
29	G8	203	PEB	NC-C1C-CHB-C4B
29	G8	203	PEB	C2C-C1C-CHB-C4B
29	G8	203	PEB	NB-C1B-CHA-C4A
29	G8	203	PEB	C2B-C1B-CHA-C4A
29	H8	201	PEB	NB-C1B-CHA-C4A
29	H8	201	PEB	C2B-C1B-CHA-C4A
29	H8	202	PEB	C2C-CAC-CBC-CGC
29	H8	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	H8	202	PEB	C4A-C3A-CAA-CBA
29	H8	202	PEB	NB-C1B-CHA-C4A
29	H8	202	PEB	C2B-C1B-CHA-C4A
29	H8	203	PEB	ND-C1D-CHC-C4C
29	H8	203	PEB	C2D-C1D-CHC-C4C
29	H8	203	PEB	NC-C1C-CHB-C4B
29	H8	203	PEB	C2C-C1C-CHB-C4B
29	H8	203	PEB	NB-C1B-CHA-C4A
29	H8	203	PEB	C2B-C1B-CHA-C4A
29	I8	201	PEB	NB-C1B-CHA-C4A
29	I8	201	PEB	C2B-C1B-CHA-C4A
29	I8	202	PEB	C4A-C3A-CAA-CBA
29	I8	202	PEB	NB-C1B-CHA-C4A
29	I8	202	PEB	C2B-C1B-CHA-C4A
29	I8	203	PEB	NC-C1C-CHB-C4B
29	I8	203	PEB	C2C-C1C-CHB-C4B
29	I8	203	PEB	NB-C1B-CHA-C4A
29	I8	203	PEB	C2B-C1B-CHA-C4A
29	J8	201	PEB	C2B-C1B-CHA-C4A
29	J8	202	PEB	C1C-C2C-CAC-CBC
29	J8	202	PEB	C3C-C2C-CAC-CBC
29	J8	202	PEB	C2A-C3A-CAA-CBA
29	J8	202	PEB	NB-C1B-CHA-C4A
29	J8	202	PEB	C2B-C1B-CHA-C4A
29	K8	201	PEB	NB-C1B-CHA-C4A
29	K8	201	PEB	C2B-C1B-CHA-C4A
29	K8	202	PEB	C4A-C3A-CAA-CBA
29	K8	202	PEB	NB-C1B-CHA-C4A
29	K8	202	PEB	C2B-C1B-CHA-C4A
29	K8	203	PEB	NC-C1C-CHB-C4B
29	K8	203	PEB	C2C-C1C-CHB-C4B
29	K8	203	PEB	NB-C1B-CHA-C4A
29	K8	203	PEB	C2B-C1B-CHA-C4A
29	L8	201	PEB	NB-C1B-CHA-C4A
29	L8	201	PEB	C2B-C1B-CHA-C4A
29	L8	202	PEB	C2C-CAC-CBC-CGC
29	L8	202	PEB	C2A-C3A-CAA-CBA
29	L8	202	PEB	C4A-C3A-CAA-CBA
29	L8	202	PEB	NB-C1B-CHA-C4A
29	L8	202	PEB	C2B-C1B-CHA-C4A
29	L8	203	PEB	ND-C1D-CHC-C4C
29	L8	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	L8	203	PEB	NC-C1C-CHB-C4B
29	L8	203	PEB	C2C-C1C-CHB-C4B
29	L8	203	PEB	NB-C1B-CHA-C4A
29	L8	203	PEB	C2B-C1B-CHA-C4A
29	A8	201	PEB	NB-C1B-CHA-C4A
29	A8	201	PEB	C2B-C1B-CHA-C4A
29	A8	202	PEB	C4A-C3A-CAA-CBA
29	A8	202	PEB	NB-C1B-CHA-C4A
29	A8	202	PEB	C2B-C1B-CHA-C4A
29	A8	203	PEB	NC-C1C-CHB-C4B
29	A8	203	PEB	C2C-C1C-CHB-C4B
29	A8	203	PEB	NB-C1B-CHA-C4A
29	A8	203	PEB	C2B-C1B-CHA-C4A
29	C8	201	PEB	NB-C1B-CHA-C4A
29	C8	201	PEB	C2B-C1B-CHA-C4A
29	C8	202	PEB	C4A-C3A-CAA-CBA
29	C8	202	PEB	NB-C1B-CHA-C4A
29	C8	202	PEB	C2B-C1B-CHA-C4A
29	C8	203	PEB	NC-C1C-CHB-C4B
29	C8	203	PEB	C2C-C1C-CHB-C4B
29	C8	203	PEB	NB-C1B-CHA-C4A
29	C8	203	PEB	C2B-C1B-CHA-C4A
29	A9	301	PEB	C2C-CAC-CBC-CGC
29	A9	301	PEB	C4A-C3A-CAA-CBA
29	A9	301	PEB	NB-C1B-CHA-C4A
29	A9	301	PEB	C2B-C1B-CHA-C4A
29	A9	304	PEB	NB-C1B-CHA-C4A
29	A9	304	PEB	C2B-C1B-CHA-C4A
29	A9	305	PEB	NB-C1B-CHA-C4A
29	A9	305	PEB	C2B-C1B-CHA-C4A
29	D9	1002	PEB	NC-C1C-CHB-C4B
29	D9	1002	PEB	C2A-C3A-CAA-CBA
29	D9	1002	PEB	C4A-C3A-CAA-CBA
29	D9	1002	PEB	NB-C1B-CHA-C4A
29	D9	1002	PEB	C2B-C1B-CHA-C4A
29	F9	1002	PEB	NC-C1C-CHB-C4B
29	F9	1002	PEB	C2A-C3A-CAA-CBA
29	F9	1002	PEB	C4A-C3A-CAA-CBA
29	F9	1002	PEB	NB-C1B-CHA-C4A
29	F9	1002	PEB	C2B-C1B-CHA-C4A
29	H9	1002	PEB	NC-C1C-CHB-C4B
29	H9	1002	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	H9	1002	PEB	C4A-C3A-CAA-CBA
29	H9	1002	PEB	NB-C1B-CHA-C4A
29	H9	1002	PEB	C2B-C1B-CHA-C4A
29	J9	1002	PEB	NC-C1C-CHB-C4B
29	J9	1002	PEB	C2A-C3A-CAA-CBA
29	J9	1002	PEB	C4A-C3A-CAA-CBA
29	J9	1002	PEB	NB-C1B-CHA-C4A
29	J9	1002	PEB	C2B-C1B-CHA-C4A
29	L9	1002	PEB	NC-C1C-CHB-C4B
29	L9	1002	PEB	C2A-C3A-CAA-CBA
29	L9	1002	PEB	C4A-C3A-CAA-CBA
29	L9	1002	PEB	NB-C1B-CHA-C4A
29	L9	1002	PEB	C2B-C1B-CHA-C4A
29	N9	1002	PEB	NC-C1C-CHB-C4B
29	N9	1002	PEB	C2A-C3A-CAA-CBA
29	N9	1002	PEB	C4A-C3A-CAA-CBA
29	N9	1002	PEB	NB-C1B-CHA-C4A
29	N9	1002	PEB	C2B-C1B-CHA-C4A
29	O9	201	PEB	C4A-C3A-CAA-CBA
29	O9	201	PEB	NB-C1B-CHA-C4A
29	O9	201	PEB	C2B-C1B-CHA-C4A
29	O9	202	PEB	ND-C1D-CHC-C4C
29	O9	202	PEB	C2D-C1D-CHC-C4C
29	O9	202	PEB	NB-C1B-CHA-C4A
29	O9	202	PEB	C2B-C1B-CHA-C4A
29	P9	201	PEB	NB-C1B-CHA-C4A
29	P9	201	PEB	C2B-C1B-CHA-C4A
29	P9	202	PEB	ND-C1D-CHC-C4C
29	P9	202	PEB	C2D-C1D-CHC-C4C
29	P9	202	PEB	NB-C1B-CHA-C4A
29	P9	202	PEB	C2B-C1B-CHA-C4A
29	P9	203	PEB	NC-C1C-CHB-C4B
29	P9	203	PEB	C2C-C1C-CHB-C4B
29	P9	203	PEB	NB-C1B-CHA-C4A
29	P9	203	PEB	C2B-C1B-CHA-C4A
29	P9	203	PEB	C2B-C3B-CAB-CBB
29	P9	203	PEB	C4B-C3B-CAB-CBB
29	Q9	201	PEB	C4A-C3A-CAA-CBA
29	Q9	201	PEB	NB-C1B-CHA-C4A
29	Q9	201	PEB	C2B-C1B-CHA-C4A
29	Q9	202	PEB	ND-C1D-CHC-C4C
29	Q9	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	Q9	202	PEB	NB-C1B-CHA-C4A
29	Q9	202	PEB	C2B-C1B-CHA-C4A
29	R9	201	PEB	NB-C1B-CHA-C4A
29	R9	201	PEB	C2B-C1B-CHA-C4A
29	R9	202	PEB	ND-C1D-CHC-C4C
29	R9	202	PEB	C2D-C1D-CHC-C4C
29	R9	202	PEB	NB-C1B-CHA-C4A
29	R9	202	PEB	C2B-C1B-CHA-C4A
29	R9	203	PEB	NC-C1C-CHB-C4B
29	R9	203	PEB	C2C-C1C-CHB-C4B
29	R9	203	PEB	NB-C1B-CHA-C4A
29	R9	203	PEB	C2B-C1B-CHA-C4A
29	R9	203	PEB	C2B-C3B-CAB-CBB
29	R9	203	PEB	C4B-C3B-CAB-CBB
29	S9	201	PEB	C4A-C3A-CAA-CBA
29	S9	201	PEB	NB-C1B-CHA-C4A
29	S9	201	PEB	C2B-C1B-CHA-C4A
29	S9	202	PEB	ND-C1D-CHC-C4C
29	S9	202	PEB	C2D-C1D-CHC-C4C
29	S9	202	PEB	NB-C1B-CHA-C4A
29	S9	202	PEB	C2B-C1B-CHA-C4A
29	T9	201	PEB	NB-C1B-CHA-C4A
29	T9	201	PEB	C2B-C1B-CHA-C4A
29	T9	202	PEB	ND-C1D-CHC-C4C
29	T9	202	PEB	C2D-C1D-CHC-C4C
29	T9	202	PEB	NB-C1B-CHA-C4A
29	T9	202	PEB	C2B-C1B-CHA-C4A
29	T9	203	PEB	NC-C1C-CHB-C4B
29	T9	203	PEB	C2C-C1C-CHB-C4B
29	T9	203	PEB	NB-C1B-CHA-C4A
29	T9	203	PEB	C2B-C1B-CHA-C4A
29	T9	203	PEB	C2B-C3B-CAB-CBB
29	T9	203	PEB	C4B-C3B-CAB-CBB
29	U9	201	PEB	C4A-C3A-CAA-CBA
29	U9	201	PEB	NB-C1B-CHA-C4A
29	U9	201	PEB	C2B-C1B-CHA-C4A
29	U9	202	PEB	ND-C1D-CHC-C4C
29	U9	202	PEB	C2D-C1D-CHC-C4C
29	U9	202	PEB	NB-C1B-CHA-C4A
29	U9	202	PEB	C2B-C1B-CHA-C4A
29	V9	201	PEB	NB-C1B-CHA-C4A
29	V9	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	V9	202	PEB	ND-C1D-CHC-C4C
29	V9	202	PEB	C2D-C1D-CHC-C4C
29	V9	202	PEB	NB-C1B-CHA-C4A
29	V9	202	PEB	C2B-C1B-CHA-C4A
29	V9	203	PEB	NC-C1C-CHB-C4B
29	V9	203	PEB	C2C-C1C-CHB-C4B
29	V9	203	PEB	NB-C1B-CHA-C4A
29	V9	203	PEB	C2B-C1B-CHA-C4A
29	V9	203	PEB	C2B-C3B-CAB-CBB
29	V9	203	PEB	C4B-C3B-CAB-CBB
29	W9	201	PEB	C4A-C3A-CAA-CBA
29	W9	201	PEB	NB-C1B-CHA-C4A
29	W9	201	PEB	C2B-C1B-CHA-C4A
29	W9	202	PEB	ND-C1D-CHC-C4C
29	W9	202	PEB	C2D-C1D-CHC-C4C
29	W9	202	PEB	NB-C1B-CHA-C4A
29	W9	202	PEB	C2B-C1B-CHA-C4A
29	Y9	201	PEB	NB-C1B-CHA-C4A
29	Y9	201	PEB	C2B-C1B-CHA-C4A
29	Y9	202	PEB	ND-C1D-CHC-C4C
29	Y9	202	PEB	C2D-C1D-CHC-C4C
29	Y9	202	PEB	NB-C1B-CHA-C4A
29	Y9	202	PEB	C2B-C1B-CHA-C4A
29	Y9	203	PEB	NC-C1C-CHB-C4B
29	Y9	203	PEB	C2C-C1C-CHB-C4B
29	Y9	203	PEB	NB-C1B-CHA-C4A
29	Y9	203	PEB	C2B-C1B-CHA-C4A
29	Y9	203	PEB	C2B-C3B-CAB-CBB
29	Y9	203	PEB	C4B-C3B-CAB-CBB
29	Z9	201	PEB	C4A-C3A-CAA-CBA
29	Z9	201	PEB	NB-C1B-CHA-C4A
29	Z9	201	PEB	C2B-C1B-CHA-C4A
29	Z9	202	PEB	ND-C1D-CHC-C4C
29	Z9	202	PEB	C2D-C1D-CHC-C4C
29	Z9	202	PEB	NB-C1B-CHA-C4A
29	Z9	202	PEB	C2B-C1B-CHA-C4A
29	a9	201	PEB	NB-C1B-CHA-C4A
29	a9	201	PEB	C2B-C1B-CHA-C4A
29	a9	202	PEB	ND-C1D-CHC-C4C
29	a9	202	PEB	C2D-C1D-CHC-C4C
29	a9	202	PEB	NB-C1B-CHA-C4A
29	a9	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	a9	203	PEB	NC-C1C-CHB-C4B
29	a9	203	PEB	C2C-C1C-CHB-C4B
29	a9	203	PEB	NB-C1B-CHA-C4A
29	a9	203	PEB	C2B-C1B-CHA-C4A
29	a9	203	PEB	C2B-C3B-CAB-CBB
29	a9	203	PEB	C4B-C3B-CAB-CBB
29	b9	201	PEB	C4A-C3A-CAA-CBA
29	b9	201	PEB	NB-C1B-CHA-C4A
29	b9	201	PEB	C2B-C1B-CHA-C4A
29	b9	202	PEB	ND-C1D-CHC-C4C
29	b9	202	PEB	C2D-C1D-CHC-C4C
29	b9	202	PEB	NB-C1B-CHA-C4A
29	b9	202	PEB	C2B-C1B-CHA-C4A
29	c9	201	PEB	NB-C1B-CHA-C4A
29	c9	201	PEB	C2B-C1B-CHA-C4A
29	c9	202	PEB	ND-C1D-CHC-C4C
29	c9	202	PEB	C2D-C1D-CHC-C4C
29	c9	202	PEB	NB-C1B-CHA-C4A
29	c9	202	PEB	C2B-C1B-CHA-C4A
29	c9	203	PEB	NC-C1C-CHB-C4B
29	c9	203	PEB	C2C-C1C-CHB-C4B
29	c9	203	PEB	NB-C1B-CHA-C4A
29	c9	203	PEB	C2B-C1B-CHA-C4A
29	c9	203	PEB	C2B-C3B-CAB-CBB
29	c9	203	PEB	C4B-C3B-CAB-CBB
29	d9	201	PEB	C4A-C3A-CAA-CBA
29	d9	201	PEB	NB-C1B-CHA-C4A
29	d9	201	PEB	C2B-C1B-CHA-C4A
29	d9	202	PEB	ND-C1D-CHC-C4C
29	d9	202	PEB	C2D-C1D-CHC-C4C
29	d9	202	PEB	NB-C1B-CHA-C4A
29	d9	202	PEB	C2B-C1B-CHA-C4A
29	e9	201	PEB	NB-C1B-CHA-C4A
29	e9	201	PEB	C2B-C1B-CHA-C4A
29	e9	202	PEB	ND-C1D-CHC-C4C
29	e9	202	PEB	C2D-C1D-CHC-C4C
29	e9	202	PEB	NB-C1B-CHA-C4A
29	e9	202	PEB	C2B-C1B-CHA-C4A
29	e9	203	PEB	NC-C1C-CHB-C4B
29	e9	203	PEB	C2C-C1C-CHB-C4B
29	e9	203	PEB	NB-C1B-CHA-C4A
29	e9	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	e9	203	PEB	C2B-C3B-CAB-CBB
29	e9	203	PEB	C4B-C3B-CAB-CBB
29	f9	201	PEB	C4A-C3A-CAA-CBA
29	f9	201	PEB	NB-C1B-CHA-C4A
29	f9	201	PEB	C2B-C1B-CHA-C4A
29	f9	202	PEB	ND-C1D-CHC-C4C
29	f9	202	PEB	C2D-C1D-CHC-C4C
29	f9	202	PEB	NB-C1B-CHA-C4A
29	f9	202	PEB	C2B-C1B-CHA-C4A
29	g9	201	PEB	NB-C1B-CHA-C4A
29	g9	201	PEB	C2B-C1B-CHA-C4A
29	g9	202	PEB	ND-C1D-CHC-C4C
29	g9	202	PEB	C2D-C1D-CHC-C4C
29	g9	202	PEB	NB-C1B-CHA-C4A
29	g9	202	PEB	C2B-C1B-CHA-C4A
29	g9	203	PEB	NC-C1C-CHB-C4B
29	g9	203	PEB	C2C-C1C-CHB-C4B
29	g9	203	PEB	NB-C1B-CHA-C4A
29	g9	203	PEB	C2B-C1B-CHA-C4A
29	g9	203	PEB	C2B-C3B-CAB-CBB
29	g9	203	PEB	C4B-C3B-CAB-CBB
29	h9	201	PEB	C4A-C3A-CAA-CBA
29	h9	201	PEB	NB-C1B-CHA-C4A
29	h9	201	PEB	C2B-C1B-CHA-C4A
29	h9	202	PEB	ND-C1D-CHC-C4C
29	h9	202	PEB	C2D-C1D-CHC-C4C
29	h9	202	PEB	NB-C1B-CHA-C4A
29	h9	202	PEB	C2B-C1B-CHA-C4A
29	i9	201	PEB	NB-C1B-CHA-C4A
29	i9	201	PEB	C2B-C1B-CHA-C4A
29	i9	202	PEB	ND-C1D-CHC-C4C
29	i9	202	PEB	C2D-C1D-CHC-C4C
29	i9	202	PEB	NB-C1B-CHA-C4A
29	i9	202	PEB	C2B-C1B-CHA-C4A
29	i9	203	PEB	NC-C1C-CHB-C4B
29	i9	203	PEB	C2C-C1C-CHB-C4B
29	i9	203	PEB	NB-C1B-CHA-C4A
29	i9	203	PEB	C2B-C1B-CHA-C4A
29	i9	203	PEB	C2B-C3B-CAB-CBB
29	i9	203	PEB	C4B-C3B-CAB-CBB
29	j9	201	PEB	C4A-C3A-CAA-CBA
29	j9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	j9	201	PEB	C2B-C1B-CHA-C4A
29	j9	202	PEB	ND-C1D-CHC-C4C
29	j9	202	PEB	C2D-C1D-CHC-C4C
29	j9	202	PEB	NB-C1B-CHA-C4A
29	j9	202	PEB	C2B-C1B-CHA-C4A
29	k9	201	PEB	NB-C1B-CHA-C4A
29	k9	201	PEB	C2B-C1B-CHA-C4A
29	k9	202	PEB	ND-C1D-CHC-C4C
29	k9	202	PEB	C2D-C1D-CHC-C4C
29	k9	202	PEB	NB-C1B-CHA-C4A
29	k9	202	PEB	C2B-C1B-CHA-C4A
29	k9	203	PEB	NC-C1C-CHB-C4B
29	k9	203	PEB	C2C-C1C-CHB-C4B
29	k9	203	PEB	NB-C1B-CHA-C4A
29	k9	203	PEB	C2B-C1B-CHA-C4A
29	k9	203	PEB	C2B-C3B-CAB-CBB
29	k9	203	PEB	C4B-C3B-CAB-CBB
29	l9	201	PEB	C4A-C3A-CAA-CBA
29	l9	201	PEB	NB-C1B-CHA-C4A
29	l9	201	PEB	C2B-C1B-CHA-C4A
29	l9	202	PEB	ND-C1D-CHC-C4C
29	l9	202	PEB	C2D-C1D-CHC-C4C
29	l9	202	PEB	NB-C1B-CHA-C4A
29	l9	202	PEB	C2B-C1B-CHA-C4A
29	m9	201	PEB	NB-C1B-CHA-C4A
29	m9	201	PEB	C2B-C1B-CHA-C4A
29	m9	202	PEB	ND-C1D-CHC-C4C
29	m9	202	PEB	C2D-C1D-CHC-C4C
29	m9	202	PEB	NB-C1B-CHA-C4A
29	m9	202	PEB	C2B-C1B-CHA-C4A
29	m9	203	PEB	NC-C1C-CHB-C4B
29	m9	203	PEB	C2C-C1C-CHB-C4B
29	m9	203	PEB	NB-C1B-CHA-C4A
29	m9	203	PEB	C2B-C1B-CHA-C4A
29	m9	203	PEB	C2B-C3B-CAB-CBB
29	m9	203	PEB	C4B-C3B-CAB-CBB
29	AA	201	PEB	ND-C1D-CHC-C4C
29	AA	201	PEB	C4A-C3A-CAA-CBA
29	AA	201	PEB	NB-C1B-CHA-C4A
29	AA	201	PEB	C2B-C1B-CHA-C4A
29	AA	202	PEB	ND-C1D-CHC-C4C
29	AA	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	AA	202	PEB	NC-C1C-CHB-C4B
29	AA	202	PEB	C2C-C1C-CHB-C4B
29	AA	202	PEB	C4A-C3A-CAA-CBA
29	AA	202	PEB	NB-C1B-CHA-C4A
29	AA	202	PEB	C2B-C1B-CHA-C4A
29	AA	202	PEB	C3B-C4B-CHB-C1C
29	BA	201	PEB	ND-C1D-CHC-C4C
29	BA	201	PEB	C2D-C1D-CHC-C4C
29	BA	201	PEB	C2C-CAC-CBC-CGC
29	BA	201	PEB	NB-C1B-CHA-C4A
29	BA	201	PEB	C2B-C1B-CHA-C4A
29	BA	202	PEB	NC-C1C-CHB-C4B
29	BA	202	PEB	C2C-C1C-CHB-C4B
29	BA	202	PEB	C2A-C3A-CAA-CBA
29	BA	202	PEB	C4A-C3A-CAA-CBA
29	BA	202	PEB	NB-C1B-CHA-C4A
29	BA	202	PEB	C2B-C1B-CHA-C4A
29	BA	203	PEB	NC-C1C-CHB-C4B
29	BA	203	PEB	C2C-C1C-CHB-C4B
29	BA	203	PEB	C2A-C3A-CAA-CBA
29	BA	203	PEB	NB-C1B-CHA-C4A
29	BA	203	PEB	C2B-C1B-CHA-C4A
29	CA	201	PEB	ND-C1D-CHC-C4C
29	CA	201	PEB	C4A-C3A-CAA-CBA
29	CA	201	PEB	NB-C1B-CHA-C4A
29	CA	201	PEB	C2B-C1B-CHA-C4A
29	CA	202	PEB	ND-C1D-CHC-C4C
29	CA	202	PEB	C2D-C1D-CHC-C4C
29	CA	202	PEB	NC-C1C-CHB-C4B
29	CA	202	PEB	C2C-C1C-CHB-C4B
29	CA	202	PEB	C4A-C3A-CAA-CBA
29	CA	202	PEB	NB-C1B-CHA-C4A
29	CA	202	PEB	C2B-C1B-CHA-C4A
29	CA	202	PEB	C3B-C4B-CHB-C1C
29	DA	201	PEB	ND-C1D-CHC-C4C
29	DA	201	PEB	C2D-C1D-CHC-C4C
29	DA	201	PEB	C2C-CAC-CBC-CGC
29	DA	201	PEB	NB-C1B-CHA-C4A
29	DA	201	PEB	C2B-C1B-CHA-C4A
29	DA	202	PEB	NC-C1C-CHB-C4B
29	DA	202	PEB	C2C-C1C-CHB-C4B
29	DA	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	DA	202	PEB	C4A-C3A-CAA-CBA
29	DA	202	PEB	NB-C1B-CHA-C4A
29	DA	202	PEB	C2B-C1B-CHA-C4A
29	DA	203	PEB	NC-C1C-CHB-C4B
29	DA	203	PEB	C2C-C1C-CHB-C4B
29	DA	203	PEB	C2A-C3A-CAA-CBA
29	DA	203	PEB	NB-C1B-CHA-C4A
29	DA	203	PEB	C2B-C1B-CHA-C4A
29	EA	201	PEB	ND-C1D-CHC-C4C
29	EA	201	PEB	C4A-C3A-CAA-CBA
29	EA	201	PEB	NB-C1B-CHA-C4A
29	EA	201	PEB	C2B-C1B-CHA-C4A
29	EA	202	PEB	ND-C1D-CHC-C4C
29	EA	202	PEB	C2D-C1D-CHC-C4C
29	EA	202	PEB	NC-C1C-CHB-C4B
29	EA	202	PEB	C2C-C1C-CHB-C4B
29	EA	202	PEB	C4A-C3A-CAA-CBA
29	EA	202	PEB	NB-C1B-CHA-C4A
29	EA	202	PEB	C2B-C1B-CHA-C4A
29	EA	202	PEB	C3B-C4B-CHB-C1C
29	FA	201	PEB	ND-C1D-CHC-C4C
29	FA	201	PEB	C2D-C1D-CHC-C4C
29	FA	201	PEB	C2C-CAC-CBC-CGC
29	FA	201	PEB	NB-C1B-CHA-C4A
29	FA	201	PEB	C2B-C1B-CHA-C4A
29	FA	202	PEB	NC-C1C-CHB-C4B
29	FA	202	PEB	C2C-C1C-CHB-C4B
29	FA	202	PEB	C2A-C3A-CAA-CBA
29	FA	202	PEB	C4A-C3A-CAA-CBA
29	FA	202	PEB	NB-C1B-CHA-C4A
29	FA	202	PEB	C2B-C1B-CHA-C4A
29	FA	203	PEB	NC-C1C-CHB-C4B
29	FA	203	PEB	C2C-C1C-CHB-C4B
29	FA	203	PEB	C2A-C3A-CAA-CBA
29	FA	203	PEB	NB-C1B-CHA-C4A
29	FA	203	PEB	C2B-C1B-CHA-C4A
29	GA	201	PEB	ND-C1D-CHC-C4C
29	GA	201	PEB	C4A-C3A-CAA-CBA
29	GA	201	PEB	NB-C1B-CHA-C4A
29	GA	201	PEB	C2B-C1B-CHA-C4A
29	GA	202	PEB	ND-C1D-CHC-C4C
29	GA	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	GA	202	PEB	NC-C1C-CHB-C4B
29	GA	202	PEB	C2C-C1C-CHB-C4B
29	GA	202	PEB	C4A-C3A-CAA-CBA
29	GA	202	PEB	NB-C1B-CHA-C4A
29	GA	202	PEB	C2B-C1B-CHA-C4A
29	GA	202	PEB	C3B-C4B-CHB-C1C
29	HA	201	PEB	ND-C1D-CHC-C4C
29	HA	201	PEB	C2D-C1D-CHC-C4C
29	HA	201	PEB	C2C-CAC-CBC-CGC
29	HA	201	PEB	NB-C1B-CHA-C4A
29	HA	201	PEB	C2B-C1B-CHA-C4A
29	HA	202	PEB	NC-C1C-CHB-C4B
29	HA	202	PEB	C2C-C1C-CHB-C4B
29	HA	202	PEB	C2A-C3A-CAA-CBA
29	HA	202	PEB	C4A-C3A-CAA-CBA
29	HA	202	PEB	NB-C1B-CHA-C4A
29	HA	202	PEB	C2B-C1B-CHA-C4A
29	HA	203	PEB	NC-C1C-CHB-C4B
29	HA	203	PEB	C2C-C1C-CHB-C4B
29	HA	203	PEB	C2A-C3A-CAA-CBA
29	HA	203	PEB	NB-C1B-CHA-C4A
29	HA	203	PEB	C2B-C1B-CHA-C4A
29	IA	201	PEB	ND-C1D-CHC-C4C
29	IA	201	PEB	C4A-C3A-CAA-CBA
29	IA	201	PEB	NB-C1B-CHA-C4A
29	IA	201	PEB	C2B-C1B-CHA-C4A
29	IA	202	PEB	ND-C1D-CHC-C4C
29	IA	202	PEB	C2D-C1D-CHC-C4C
29	IA	202	PEB	NC-C1C-CHB-C4B
29	IA	202	PEB	C2C-C1C-CHB-C4B
29	IA	202	PEB	C4A-C3A-CAA-CBA
29	IA	202	PEB	NB-C1B-CHA-C4A
29	IA	202	PEB	C2B-C1B-CHA-C4A
29	IA	202	PEB	C3B-C4B-CHB-C1C
29	JA	201	PEB	ND-C1D-CHC-C4C
29	JA	201	PEB	C2D-C1D-CHC-C4C
29	JA	201	PEB	C2C-CAC-CBC-CGC
29	JA	201	PEB	NB-C1B-CHA-C4A
29	JA	201	PEB	C2B-C1B-CHA-C4A
29	JA	202	PEB	NC-C1C-CHB-C4B
29	JA	202	PEB	C2C-C1C-CHB-C4B
29	JA	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	JA	202	PEB	C4A-C3A-CAA-CBA
29	JA	202	PEB	NB-C1B-CHA-C4A
29	JA	202	PEB	C2B-C1B-CHA-C4A
29	JA	203	PEB	NC-C1C-CHB-C4B
29	JA	203	PEB	C2C-C1C-CHB-C4B
29	JA	203	PEB	C2A-C3A-CAA-CBA
29	JA	203	PEB	NB-C1B-CHA-C4A
29	JA	203	PEB	C2B-C1B-CHA-C4A
29	KA	201	PEB	ND-C1D-CHC-C4C
29	KA	201	PEB	C4A-C3A-CAA-CBA
29	KA	201	PEB	NB-C1B-CHA-C4A
29	KA	201	PEB	C2B-C1B-CHA-C4A
29	KA	202	PEB	ND-C1D-CHC-C4C
29	KA	202	PEB	C2D-C1D-CHC-C4C
29	KA	202	PEB	NC-C1C-CHB-C4B
29	KA	202	PEB	C2C-C1C-CHB-C4B
29	KA	202	PEB	C4A-C3A-CAA-CBA
29	KA	202	PEB	NB-C1B-CHA-C4A
29	KA	202	PEB	C2B-C1B-CHA-C4A
29	KA	202	PEB	C3B-C4B-CHB-C1C
29	LA	201	PEB	ND-C1D-CHC-C4C
29	LA	201	PEB	C2D-C1D-CHC-C4C
29	LA	201	PEB	C2C-CAC-CBC-CGC
29	LA	201	PEB	NB-C1B-CHA-C4A
29	LA	201	PEB	C2B-C1B-CHA-C4A
29	LA	202	PEB	NC-C1C-CHB-C4B
29	LA	202	PEB	C2C-C1C-CHB-C4B
29	LA	202	PEB	C2A-C3A-CAA-CBA
29	LA	202	PEB	C4A-C3A-CAA-CBA
29	LA	202	PEB	NB-C1B-CHA-C4A
29	LA	202	PEB	C2B-C1B-CHA-C4A
29	LA	203	PEB	NC-C1C-CHB-C4B
29	LA	203	PEB	C2C-C1C-CHB-C4B
29	LA	203	PEB	C2A-C3A-CAA-CBA
29	LA	203	PEB	NB-C1B-CHA-C4A
29	LA	203	PEB	C2B-C1B-CHA-C4A
29	MA	401	PEB	ND-C1D-CHC-C4C
29	MA	401	PEB	NC-C1C-CHB-C4B
29	MA	401	PEB	C2C-C1C-CHB-C4B
29	MA	401	PEB	C4A-C3A-CAA-CBA
29	MA	401	PEB	NB-C1B-CHA-C4A
29	MA	401	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	MA	404	PEB	ND-C1D-CHC-C4C
29	MA	404	PEB	C2D-C1D-CHC-C4C
29	MA	404	PEB	NC-C1C-CHB-C4B
29	MA	404	PEB	C2C-C1C-CHB-C4B
29	MA	404	PEB	NB-C1B-CHA-C4A
29	MA	404	PEB	C2B-C1B-CHA-C4A
29	MA	405	PEB	ND-C1D-CHC-C4C
29	MA	405	PEB	C2D-C1D-CHC-C4C
29	MA	405	PEB	C2C-CAC-CBC-CGC
29	AB	301	PEB	ND-C1D-CHC-C4C
29	AB	301	PEB	C2D-C1D-CHC-C4C
29	AB	301	PEB	NB-C1B-CHA-C4A
29	AB	301	PEB	C2B-C1B-CHA-C4A
29	AB	302	PEB	C2A-C3A-CAA-CBA
29	AB	302	PEB	C4A-C3A-CAA-CBA
29	AB	302	PEB	NB-C1B-CHA-C4A
29	AB	302	PEB	C2B-C1B-CHA-C4A
29	AB	303	PEB	NC-C1C-CHB-C4B
29	AB	303	PEB	C2C-C1C-CHB-C4B
29	AB	303	PEB	C4A-C3A-CAA-CBA
29	AB	303	PEB	NB-C1B-CHA-C4A
29	AB	303	PEB	C2B-C1B-CHA-C4A
29	BB	301	PEB	NC-C1C-CHB-C4B
29	BB	301	PEB	C1C-C2C-CAC-CBC
29	BB	301	PEB	C3C-C2C-CAC-CBC
29	BB	301	PEB	C4A-C3A-CAA-CBA
29	BB	301	PEB	NB-C1B-CHA-C4A
29	BB	301	PEB	C2B-C1B-CHA-C4A
29	CB	201	PEB	NB-C1B-CHA-C4A
29	CB	201	PEB	C2B-C1B-CHA-C4A
29	CB	202	PEB	NC-C1C-CHB-C4B
29	CB	202	PEB	C2C-C1C-CHB-C4B
29	CB	202	PEB	NB-C1B-CHA-C4A
29	CB	202	PEB	C2B-C1B-CHA-C4A
29	DB	201	PEB	ND-C1D-CHC-C4C
29	DB	201	PEB	C2D-C1D-CHC-C4C
29	DB	201	PEB	NB-C1B-CHA-C4A
29	DB	201	PEB	C2B-C1B-CHA-C4A
29	DB	202	PEB	C4A-C3A-CAA-CBA
29	DB	202	PEB	NB-C1B-CHA-C4A
29	DB	202	PEB	C2B-C1B-CHA-C4A
29	DB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	DB	203	PEB	C2D-C1D-CHC-C4C
29	DB	203	PEB	NC-C1C-CHB-C4B
29	DB	203	PEB	C2C-C1C-CHB-C4B
29	DB	203	PEB	C2A-C3A-CAA-CBA
29	DB	203	PEB	C4A-C3A-CAA-CBA
29	DB	203	PEB	NB-C1B-CHA-C4A
29	DB	203	PEB	C2B-C1B-CHA-C4A
29	EB	201	PEB	NB-C1B-CHA-C4A
29	EB	201	PEB	C2B-C1B-CHA-C4A
29	EB	202	PEB	NC-C1C-CHB-C4B
29	EB	202	PEB	C2C-C1C-CHB-C4B
29	EB	202	PEB	NB-C1B-CHA-C4A
29	EB	202	PEB	C2B-C1B-CHA-C4A
29	FB	201	PEB	ND-C1D-CHC-C4C
29	FB	201	PEB	C2D-C1D-CHC-C4C
29	FB	201	PEB	NB-C1B-CHA-C4A
29	FB	201	PEB	C2B-C1B-CHA-C4A
29	FB	202	PEB	C4A-C3A-CAA-CBA
29	FB	202	PEB	NB-C1B-CHA-C4A
29	FB	202	PEB	C2B-C1B-CHA-C4A
29	FB	203	PEB	ND-C1D-CHC-C4C
29	FB	203	PEB	C2D-C1D-CHC-C4C
29	FB	203	PEB	NC-C1C-CHB-C4B
29	FB	203	PEB	C2C-C1C-CHB-C4B
29	FB	203	PEB	C2A-C3A-CAA-CBA
29	FB	203	PEB	C4A-C3A-CAA-CBA
29	FB	203	PEB	NB-C1B-CHA-C4A
29	FB	203	PEB	C2B-C1B-CHA-C4A
29	GB	201	PEB	NB-C1B-CHA-C4A
29	GB	201	PEB	C2B-C1B-CHA-C4A
29	GB	202	PEB	NC-C1C-CHB-C4B
29	GB	202	PEB	C2C-C1C-CHB-C4B
29	GB	202	PEB	NB-C1B-CHA-C4A
29	GB	202	PEB	C2B-C1B-CHA-C4A
29	HB	201	PEB	ND-C1D-CHC-C4C
29	HB	201	PEB	C2D-C1D-CHC-C4C
29	HB	201	PEB	NB-C1B-CHA-C4A
29	HB	201	PEB	C2B-C1B-CHA-C4A
29	HB	202	PEB	C4A-C3A-CAA-CBA
29	HB	202	PEB	NB-C1B-CHA-C4A
29	HB	202	PEB	C2B-C1B-CHA-C4A
29	HB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	HB	203	PEB	C2D-C1D-CHC-C4C
29	HB	203	PEB	NC-C1C-CHB-C4B
29	HB	203	PEB	C2C-C1C-CHB-C4B
29	HB	203	PEB	C2A-C3A-CAA-CBA
29	HB	203	PEB	C4A-C3A-CAA-CBA
29	HB	203	PEB	NB-C1B-CHA-C4A
29	HB	203	PEB	C2B-C1B-CHA-C4A
29	IB	201	PEB	NB-C1B-CHA-C4A
29	IB	201	PEB	C2B-C1B-CHA-C4A
29	IB	202	PEB	NC-C1C-CHB-C4B
29	IB	202	PEB	C2C-C1C-CHB-C4B
29	IB	202	PEB	NB-C1B-CHA-C4A
29	IB	202	PEB	C2B-C1B-CHA-C4A
29	JB	201	PEB	ND-C1D-CHC-C4C
29	JB	201	PEB	C2D-C1D-CHC-C4C
29	JB	201	PEB	NB-C1B-CHA-C4A
29	JB	201	PEB	C2B-C1B-CHA-C4A
29	JB	202	PEB	C4A-C3A-CAA-CBA
29	JB	202	PEB	NB-C1B-CHA-C4A
29	JB	202	PEB	C2B-C1B-CHA-C4A
29	JB	203	PEB	ND-C1D-CHC-C4C
29	JB	203	PEB	C2D-C1D-CHC-C4C
29	JB	203	PEB	NC-C1C-CHB-C4B
29	JB	203	PEB	C2C-C1C-CHB-C4B
29	JB	203	PEB	C2A-C3A-CAA-CBA
29	JB	203	PEB	C4A-C3A-CAA-CBA
29	JB	203	PEB	NB-C1B-CHA-C4A
29	JB	203	PEB	C2B-C1B-CHA-C4A
29	KB	201	PEB	NB-C1B-CHA-C4A
29	KB	201	PEB	C2B-C1B-CHA-C4A
29	KB	202	PEB	NC-C1C-CHB-C4B
29	KB	202	PEB	C2C-C1C-CHB-C4B
29	KB	202	PEB	NB-C1B-CHA-C4A
29	KB	202	PEB	C2B-C1B-CHA-C4A
29	KB	203	PEB	C4A-C3A-CAA-CBA
29	KB	203	PEB	NB-C1B-CHA-C4A
29	KB	203	PEB	C2B-C1B-CHA-C4A
29	LB	201	PEB	ND-C1D-CHC-C4C
29	LB	201	PEB	C2D-C1D-CHC-C4C
29	LB	201	PEB	NB-C1B-CHA-C4A
29	LB	201	PEB	C2B-C1B-CHA-C4A
29	LB	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	LB	202	PEB	NB-C1B-CHA-C4A
29	LB	202	PEB	C2B-C1B-CHA-C4A
29	LB	203	PEB	ND-C1D-CHC-C4C
29	LB	203	PEB	C2D-C1D-CHC-C4C
29	LB	203	PEB	NC-C1C-CHB-C4B
29	LB	203	PEB	C2C-C1C-CHB-C4B
29	LB	203	PEB	C2A-C3A-CAA-CBA
29	LB	203	PEB	C4A-C3A-CAA-CBA
29	LB	203	PEB	NB-C1B-CHA-C4A
29	LB	203	PEB	C2B-C1B-CHA-C4A
29	MB	201	PEB	NB-C1B-CHA-C4A
29	MB	201	PEB	C2B-C1B-CHA-C4A
29	MB	202	PEB	NC-C1C-CHB-C4B
29	MB	202	PEB	C2C-C1C-CHB-C4B
29	MB	202	PEB	NB-C1B-CHA-C4A
29	MB	202	PEB	C2B-C1B-CHA-C4A
29	NB	201	PEB	ND-C1D-CHC-C4C
29	NB	201	PEB	C2D-C1D-CHC-C4C
29	NB	201	PEB	NB-C1B-CHA-C4A
29	NB	201	PEB	C2B-C1B-CHA-C4A
29	NB	202	PEB	ND-C1D-CHC-C4C
29	NB	202	PEB	C2D-C1D-CHC-C4C
29	NB	202	PEB	NC-C1C-CHB-C4B
29	NB	202	PEB	C2C-C1C-CHB-C4B
29	NB	202	PEB	C2A-C3A-CAA-CBA
29	NB	202	PEB	C4A-C3A-CAA-CBA
29	NB	202	PEB	NB-C1B-CHA-C4A
29	NB	202	PEB	C2B-C1B-CHA-C4A
29	OB	201	PEB	NB-C1B-CHA-C4A
29	OB	201	PEB	C2B-C1B-CHA-C4A
29	OB	202	PEB	NC-C1C-CHB-C4B
29	OB	202	PEB	C2C-C1C-CHB-C4B
29	OB	202	PEB	NB-C1B-CHA-C4A
29	OB	202	PEB	C2B-C1B-CHA-C4A
29	PB	201	PEB	ND-C1D-CHC-C4C
29	PB	201	PEB	C2D-C1D-CHC-C4C
29	PB	201	PEB	NB-C1B-CHA-C4A
29	PB	201	PEB	C2B-C1B-CHA-C4A
29	PB	202	PEB	ND-C1D-CHC-C4C
29	PB	202	PEB	C2D-C1D-CHC-C4C
29	PB	202	PEB	NC-C1C-CHB-C4B
29	PB	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	PB	202	PEB	C2A-C3A-CAA-CBA
29	PB	202	PEB	C4A-C3A-CAA-CBA
29	PB	202	PEB	NB-C1B-CHA-C4A
29	PB	202	PEB	C2B-C1B-CHA-C4A
29	QB	202	PEB	C4A-C3A-CAA-CBA
29	QB	202	PEB	NB-C1B-CHA-C4A
29	QB	202	PEB	C2B-C1B-CHA-C4A
29	QB	203	PEB	NB-C1B-CHA-C4A
29	QB	203	PEB	C2B-C1B-CHA-C4A
29	QB	204	PEB	NC-C1C-CHB-C4B
29	QB	204	PEB	C2C-C1C-CHB-C4B
29	QB	204	PEB	NB-C1B-CHA-C4A
29	QB	204	PEB	C2B-C1B-CHA-C4A
29	RB	201	PEB	ND-C1D-CHC-C4C
29	RB	201	PEB	C2D-C1D-CHC-C4C
29	RB	201	PEB	NB-C1B-CHA-C4A
29	RB	201	PEB	C2B-C1B-CHA-C4A
29	RB	202	PEB	C4A-C3A-CAA-CBA
29	RB	202	PEB	NB-C1B-CHA-C4A
29	RB	202	PEB	C2B-C1B-CHA-C4A
29	RB	203	PEB	ND-C1D-CHC-C4C
29	RB	203	PEB	C2D-C1D-CHC-C4C
29	RB	203	PEB	NC-C1C-CHB-C4B
29	RB	203	PEB	C2C-C1C-CHB-C4B
29	RB	203	PEB	C2A-C3A-CAA-CBA
29	RB	203	PEB	C4A-C3A-CAA-CBA
29	RB	203	PEB	NB-C1B-CHA-C4A
29	RB	203	PEB	C2B-C1B-CHA-C4A
29	SB	201	PEB	NB-C1B-CHA-C4A
29	SB	201	PEB	C2B-C1B-CHA-C4A
29	SB	202	PEB	NC-C1C-CHB-C4B
29	SB	202	PEB	C2C-C1C-CHB-C4B
29	SB	202	PEB	NB-C1B-CHA-C4A
29	SB	202	PEB	C2B-C1B-CHA-C4A
29	TB	201	PEB	ND-C1D-CHC-C4C
29	TB	201	PEB	C2D-C1D-CHC-C4C
29	TB	201	PEB	NB-C1B-CHA-C4A
29	TB	201	PEB	C2B-C1B-CHA-C4A
29	TB	202	PEB	C4A-C3A-CAA-CBA
29	TB	202	PEB	NB-C1B-CHA-C4A
29	TB	202	PEB	C2B-C1B-CHA-C4A
29	TB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	TB	203	PEB	C2D-C1D-CHC-C4C
29	TB	203	PEB	NC-C1C-CHB-C4B
29	TB	203	PEB	C2C-C1C-CHB-C4B
29	TB	203	PEB	C2A-C3A-CAA-CBA
29	TB	203	PEB	C4A-C3A-CAA-CBA
29	TB	203	PEB	NB-C1B-CHA-C4A
29	TB	203	PEB	C2B-C1B-CHA-C4A
29	UB	201	PEB	NB-C1B-CHA-C4A
29	UB	201	PEB	C2B-C1B-CHA-C4A
29	UB	202	PEB	NC-C1C-CHB-C4B
29	UB	202	PEB	C2C-C1C-CHB-C4B
29	UB	202	PEB	NB-C1B-CHA-C4A
29	UB	202	PEB	C2B-C1B-CHA-C4A
29	VB	201	PEB	ND-C1D-CHC-C4C
29	VB	201	PEB	C2D-C1D-CHC-C4C
29	VB	201	PEB	NB-C1B-CHA-C4A
29	VB	201	PEB	C2B-C1B-CHA-C4A
29	VB	202	PEB	C4A-C3A-CAA-CBA
29	VB	202	PEB	NB-C1B-CHA-C4A
29	VB	202	PEB	C2B-C1B-CHA-C4A
29	VB	203	PEB	ND-C1D-CHC-C4C
29	VB	203	PEB	C2D-C1D-CHC-C4C
29	VB	203	PEB	NC-C1C-CHB-C4B
29	VB	203	PEB	C2C-C1C-CHB-C4B
29	VB	203	PEB	C2A-C3A-CAA-CBA
29	VB	203	PEB	C4A-C3A-CAA-CBA
29	VB	203	PEB	NB-C1B-CHA-C4A
29	VB	203	PEB	C2B-C1B-CHA-C4A
29	WB	201	PEB	NB-C1B-CHA-C4A
29	WB	201	PEB	C2B-C1B-CHA-C4A
29	WB	202	PEB	NC-C1C-CHB-C4B
29	WB	202	PEB	C2C-C1C-CHB-C4B
29	WB	202	PEB	NB-C1B-CHA-C4A
29	WB	202	PEB	C2B-C1B-CHA-C4A
29	XB	201	PEB	ND-C1D-CHC-C4C
29	XB	201	PEB	C2D-C1D-CHC-C4C
29	XB	201	PEB	NB-C1B-CHA-C4A
29	XB	201	PEB	C2B-C1B-CHA-C4A
29	XB	202	PEB	ND-C1D-CHC-C4C
29	XB	202	PEB	C2D-C1D-CHC-C4C
29	XB	202	PEB	NC-C1C-CHB-C4B
29	XB	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	XB	202	PEB	C2A-C3A-CAA-CBA
29	XB	202	PEB	C4A-C3A-CAA-CBA
29	XB	202	PEB	NB-C1B-CHA-C4A
29	XB	202	PEB	C2B-C1B-CHA-C4A
29	YB	201	PEB	C4A-C3A-CAA-CBA
29	YB	201	PEB	NB-C1B-CHA-C4A
29	YB	201	PEB	C2B-C1B-CHA-C4A
29	YB	202	PEB	NB-C1B-CHA-C4A
29	YB	202	PEB	C2B-C1B-CHA-C4A
29	YB	203	PEB	NC-C1C-CHB-C4B
29	YB	203	PEB	C2C-C1C-CHB-C4B
29	YB	203	PEB	NB-C1B-CHA-C4A
29	YB	203	PEB	C2B-C1B-CHA-C4A
29	ZB	201	PEB	ND-C1D-CHC-C4C
29	ZB	201	PEB	C2D-C1D-CHC-C4C
29	ZB	201	PEB	NB-C1B-CHA-C4A
29	ZB	201	PEB	C2B-C1B-CHA-C4A
29	ZB	202	PEB	C4A-C3A-CAA-CBA
29	ZB	202	PEB	NB-C1B-CHA-C4A
29	ZB	202	PEB	C2B-C1B-CHA-C4A
29	ZB	203	PEB	ND-C1D-CHC-C4C
29	ZB	203	PEB	C2D-C1D-CHC-C4C
29	ZB	203	PEB	NC-C1C-CHB-C4B
29	ZB	203	PEB	C2C-C1C-CHB-C4B
29	ZB	203	PEB	C2A-C3A-CAA-CBA
29	ZB	203	PEB	C4A-C3A-CAA-CBA
29	ZB	203	PEB	NB-C1B-CHA-C4A
29	ZB	203	PEB	C2B-C1B-CHA-C4A
29	aB	201	PEB	NB-C1B-CHA-C4A
29	aB	201	PEB	C2B-C1B-CHA-C4A
29	aB	202	PEB	NC-C1C-CHB-C4B
29	aB	202	PEB	C2C-C1C-CHB-C4B
29	aB	202	PEB	NB-C1B-CHA-C4A
29	aB	202	PEB	C2B-C1B-CHA-C4A
29	aB	203	PEB	C4A-C3A-CAA-CBA
29	aB	203	PEB	NB-C1B-CHA-C4A
29	aB	203	PEB	C2B-C1B-CHA-C4A
29	cB	201	PEB	ND-C1D-CHC-C4C
29	cB	201	PEB	C2D-C1D-CHC-C4C
29	cB	201	PEB	NB-C1B-CHA-C4A
29	cB	201	PEB	C2B-C1B-CHA-C4A
29	cB	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	cB	202	PEB	NB-C1B-CHA-C4A
29	cB	202	PEB	C2B-C1B-CHA-C4A
29	cB	203	PEB	ND-C1D-CHC-C4C
29	cB	203	PEB	C2D-C1D-CHC-C4C
29	cB	203	PEB	NC-C1C-CHB-C4B
29	cB	203	PEB	C2C-C1C-CHB-C4B
29	cB	203	PEB	C2A-C3A-CAA-CBA
29	cB	203	PEB	C4A-C3A-CAA-CBA
29	cB	203	PEB	NB-C1B-CHA-C4A
29	cB	203	PEB	C2B-C1B-CHA-C4A
29	dB	201	PEB	NB-C1B-CHA-C4A
29	dB	201	PEB	C2B-C1B-CHA-C4A
29	dB	202	PEB	NC-C1C-CHB-C4B
29	dB	202	PEB	C2C-C1C-CHB-C4B
29	dB	202	PEB	NB-C1B-CHA-C4A
29	dB	202	PEB	C2B-C1B-CHA-C4A
29	eB	201	PEB	ND-C1D-CHC-C4C
29	eB	201	PEB	C2D-C1D-CHC-C4C
29	eB	201	PEB	NB-C1B-CHA-C4A
29	eB	201	PEB	C2B-C1B-CHA-C4A
29	eB	202	PEB	ND-C1D-CHC-C4C
29	eB	202	PEB	C2D-C1D-CHC-C4C
29	eB	202	PEB	NC-C1C-CHB-C4B
29	eB	202	PEB	C2C-C1C-CHB-C4B
29	eB	202	PEB	C2A-C3A-CAA-CBA
29	eB	202	PEB	C4A-C3A-CAA-CBA
29	eB	202	PEB	NB-C1B-CHA-C4A
29	eB	202	PEB	C2B-C1B-CHA-C4A
29	fB	201	PEB	NB-C1B-CHA-C4A
29	fB	201	PEB	C2B-C1B-CHA-C4A
29	fB	202	PEB	NC-C1C-CHB-C4B
29	fB	202	PEB	C2C-C1C-CHB-C4B
29	fB	202	PEB	NB-C1B-CHA-C4A
29	fB	202	PEB	C2B-C1B-CHA-C4A
29	gB	201	PEB	ND-C1D-CHC-C4C
29	gB	201	PEB	C2D-C1D-CHC-C4C
29	gB	201	PEB	NB-C1B-CHA-C4A
29	gB	201	PEB	C2B-C1B-CHA-C4A
29	gB	202	PEB	C4A-C3A-CAA-CBA
29	gB	202	PEB	NB-C1B-CHA-C4A
29	gB	202	PEB	C2B-C1B-CHA-C4A
29	gB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	gB	203	PEB	C2D-C1D-CHC-C4C
29	gB	203	PEB	NC-C1C-CHB-C4B
29	gB	203	PEB	C2C-C1C-CHB-C4B
29	gB	203	PEB	C2A-C3A-CAA-CBA
29	gB	203	PEB	C4A-C3A-CAA-CBA
29	gB	203	PEB	NB-C1B-CHA-C4A
29	gB	203	PEB	C2B-C1B-CHA-C4A
29	hB	201	PEB	NB-C1B-CHA-C4A
29	hB	201	PEB	C2B-C1B-CHA-C4A
29	hB	202	PEB	NC-C1C-CHB-C4B
29	hB	202	PEB	C2C-C1C-CHB-C4B
29	hB	202	PEB	NB-C1B-CHA-C4A
29	hB	202	PEB	C2B-C1B-CHA-C4A
29	iB	201	PEB	ND-C1D-CHC-C4C
29	iB	201	PEB	C2D-C1D-CHC-C4C
29	iB	201	PEB	NB-C1B-CHA-C4A
29	iB	201	PEB	C2B-C1B-CHA-C4A
29	iB	202	PEB	C4A-C3A-CAA-CBA
29	iB	202	PEB	NB-C1B-CHA-C4A
29	iB	202	PEB	C2B-C1B-CHA-C4A
29	iB	203	PEB	ND-C1D-CHC-C4C
29	iB	203	PEB	C2D-C1D-CHC-C4C
29	iB	203	PEB	NC-C1C-CHB-C4B
29	iB	203	PEB	C2C-C1C-CHB-C4B
29	iB	203	PEB	C2A-C3A-CAA-CBA
29	iB	203	PEB	C4A-C3A-CAA-CBA
29	iB	203	PEB	NB-C1B-CHA-C4A
29	iB	203	PEB	C2B-C1B-CHA-C4A
29	jB	201	PEB	NB-C1B-CHA-C4A
29	jB	201	PEB	C2B-C1B-CHA-C4A
29	jB	202	PEB	NC-C1C-CHB-C4B
29	jB	202	PEB	C2C-C1C-CHB-C4B
29	jB	202	PEB	NB-C1B-CHA-C4A
29	jB	202	PEB	C2B-C1B-CHA-C4A
29	kB	201	PEB	ND-C1D-CHC-C4C
29	kB	201	PEB	C2D-C1D-CHC-C4C
29	kB	201	PEB	NB-C1B-CHA-C4A
29	kB	201	PEB	C2B-C1B-CHA-C4A
29	kB	202	PEB	C4A-C3A-CAA-CBA
29	kB	202	PEB	NB-C1B-CHA-C4A
29	kB	202	PEB	C2B-C1B-CHA-C4A
29	kB	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	kB	203	PEB	C2D-C1D-CHC-C4C
29	kB	203	PEB	NC-C1C-CHB-C4B
29	kB	203	PEB	C2C-C1C-CHB-C4B
29	kB	203	PEB	C2A-C3A-CAA-CBA
29	kB	203	PEB	C4A-C3A-CAA-CBA
29	kB	203	PEB	NB-C1B-CHA-C4A
29	kB	203	PEB	C2B-C1B-CHA-C4A
29	lB	201	PEB	NB-C1B-CHA-C4A
29	lB	201	PEB	C2B-C1B-CHA-C4A
29	lB	202	PEB	NC-C1C-CHB-C4B
29	lB	202	PEB	C2C-C1C-CHB-C4B
29	lB	202	PEB	NB-C1B-CHA-C4A
29	lB	202	PEB	C2B-C1B-CHA-C4A
29	mB	201	PEB	ND-C1D-CHC-C4C
29	mB	201	PEB	C2D-C1D-CHC-C4C
29	mB	201	PEB	NB-C1B-CHA-C4A
29	mB	201	PEB	C2B-C1B-CHA-C4A
29	mB	202	PEB	C4A-C3A-CAA-CBA
29	mB	202	PEB	NB-C1B-CHA-C4A
29	mB	202	PEB	C2B-C1B-CHA-C4A
29	mB	203	PEB	ND-C1D-CHC-C4C
29	mB	203	PEB	C2D-C1D-CHC-C4C
29	mB	203	PEB	NC-C1C-CHB-C4B
29	mB	203	PEB	C2C-C1C-CHB-C4B
29	mB	203	PEB	C2A-C3A-CAA-CBA
29	mB	203	PEB	C4A-C3A-CAA-CBA
29	mB	203	PEB	NB-C1B-CHA-C4A
29	mB	203	PEB	C2B-C1B-CHA-C4A
29	AC	201	PEB	NB-C1B-CHA-C4A
29	AC	201	PEB	C2B-C1B-CHA-C4A
29	AC	202	PEB	NB-C1B-CHA-C4A
29	AC	202	PEB	C2B-C1B-CHA-C4A
29	AC	203	PEB	NC-C1C-CHB-C4B
29	AC	203	PEB	C2C-C1C-CHB-C4B
29	AC	203	PEB	C2A-C3A-CAA-CBA
29	AC	203	PEB	C4A-C3A-CAA-CBA
29	AC	203	PEB	NB-C1B-CHA-C4A
29	AC	203	PEB	C2B-C1B-CHA-C4A
29	BC	201	PEB	ND-C1D-CHC-C4C
29	BC	201	PEB	C2D-C1D-CHC-C4C
29	BC	201	PEB	NB-C1B-CHA-C4A
29	BC	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	BC	202	PEB	NC-C1C-CHB-C4B
29	BC	202	PEB	C2C-C1C-CHB-C4B
29	BC	202	PEB	C2A-C3A-CAA-CBA
29	BC	202	PEB	C4A-C3A-CAA-CBA
29	BC	202	PEB	NB-C1B-CHA-C4A
29	BC	202	PEB	C2B-C1B-CHA-C4A
29	BC	203	PEB	NC-C1C-CHB-C4B
29	BC	203	PEB	C2C-C1C-CHB-C4B
29	BC	203	PEB	NB-C1B-CHA-C4A
29	BC	203	PEB	C2B-C1B-CHA-C4A
29	CC	201	PEB	NB-C1B-CHA-C4A
29	CC	201	PEB	C2B-C1B-CHA-C4A
29	CC	202	PEB	NB-C1B-CHA-C4A
29	CC	202	PEB	C2B-C1B-CHA-C4A
29	DC	201	PEB	ND-C1D-CHC-C4C
29	DC	201	PEB	C2D-C1D-CHC-C4C
29	DC	201	PEB	NB-C1B-CHA-C4A
29	DC	201	PEB	C2B-C1B-CHA-C4A
29	DC	202	PEB	NC-C1C-CHB-C4B
29	DC	202	PEB	C2C-C1C-CHB-C4B
29	DC	202	PEB	NB-C1B-CHA-C4A
29	DC	202	PEB	C2B-C1B-CHA-C4A
29	EC	201	PEB	NB-C1B-CHA-C4A
29	EC	201	PEB	C2B-C1B-CHA-C4A
29	EC	202	PEB	NB-C1B-CHA-C4A
29	EC	202	PEB	C2B-C1B-CHA-C4A
29	FC	201	PEB	ND-C1D-CHC-C4C
29	FC	201	PEB	C2D-C1D-CHC-C4C
29	FC	201	PEB	NB-C1B-CHA-C4A
29	FC	201	PEB	C2B-C1B-CHA-C4A
29	FC	202	PEB	NC-C1C-CHB-C4B
29	FC	202	PEB	C2C-C1C-CHB-C4B
29	FC	202	PEB	C2A-C3A-CAA-CBA
29	FC	202	PEB	C4A-C3A-CAA-CBA
29	FC	202	PEB	NB-C1B-CHA-C4A
29	FC	202	PEB	C2B-C1B-CHA-C4A
29	FC	203	PEB	NC-C1C-CHB-C4B
29	FC	203	PEB	C2C-C1C-CHB-C4B
29	FC	203	PEB	NB-C1B-CHA-C4A
29	FC	203	PEB	C2B-C1B-CHA-C4A
29	GC	201	PEB	NB-C1B-CHA-C4A
29	GC	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	GC	202	PEB	NB-C1B-CHA-C4A
29	GC	202	PEB	C2B-C1B-CHA-C4A
29	HC	201	PEB	ND-C1D-CHC-C4C
29	HC	201	PEB	C2D-C1D-CHC-C4C
29	HC	201	PEB	NB-C1B-CHA-C4A
29	HC	201	PEB	C2B-C1B-CHA-C4A
29	HC	202	PEB	NC-C1C-CHB-C4B
29	HC	202	PEB	C2C-C1C-CHB-C4B
29	HC	202	PEB	C2A-C3A-CAA-CBA
29	HC	202	PEB	C4A-C3A-CAA-CBA
29	HC	202	PEB	NB-C1B-CHA-C4A
29	HC	202	PEB	C2B-C1B-CHA-C4A
29	HC	203	PEB	NC-C1C-CHB-C4B
29	HC	203	PEB	C2C-C1C-CHB-C4B
29	HC	203	PEB	NB-C1B-CHA-C4A
29	HC	203	PEB	C2B-C1B-CHA-C4A
29	IC	201	PEB	NB-C1B-CHA-C4A
29	IC	201	PEB	C2B-C1B-CHA-C4A
29	IC	202	PEB	NB-C1B-CHA-C4A
29	IC	202	PEB	C2B-C1B-CHA-C4A
29	JC	201	PEB	ND-C1D-CHC-C4C
29	JC	201	PEB	C2D-C1D-CHC-C4C
29	JC	201	PEB	NB-C1B-CHA-C4A
29	JC	201	PEB	C2B-C1B-CHA-C4A
29	JC	202	PEB	NC-C1C-CHB-C4B
29	JC	202	PEB	C2C-C1C-CHB-C4B
29	JC	202	PEB	NB-C1B-CHA-C4A
29	JC	202	PEB	C2B-C1B-CHA-C4A
29	KC	201	PEB	NC-C1C-CHB-C4B
29	KC	201	PEB	C2C-C1C-CHB-C4B
29	KC	201	PEB	C2A-C3A-CAA-CBA
29	KC	201	PEB	C4A-C3A-CAA-CBA
29	KC	201	PEB	NB-C1B-CHA-C4A
29	KC	201	PEB	C2B-C1B-CHA-C4A
29	KC	202	PEB	NB-C1B-CHA-C4A
29	KC	202	PEB	C2B-C1B-CHA-C4A
29	KC	203	PEB	NB-C1B-CHA-C4A
29	KC	203	PEB	C2B-C1B-CHA-C4A
29	LC	201	PEB	ND-C1D-CHC-C4C
29	LC	201	PEB	C2D-C1D-CHC-C4C
29	LC	201	PEB	NB-C1B-CHA-C4A
29	LC	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	LC	202	PEB	NC-C1C-CHB-C4B
29	LC	202	PEB	C2C-C1C-CHB-C4B
29	LC	202	PEB	C2A-C3A-CAA-CBA
29	LC	202	PEB	C4A-C3A-CAA-CBA
29	LC	202	PEB	NB-C1B-CHA-C4A
29	LC	202	PEB	C2B-C1B-CHA-C4A
29	LC	203	PEB	NC-C1C-CHB-C4B
29	LC	203	PEB	C2C-C1C-CHB-C4B
29	LC	203	PEB	NB-C1B-CHA-C4A
29	LC	203	PEB	C2B-C1B-CHA-C4A
29	dD	401	PEB	NB-C1B-CHA-C4A
29	dD	401	PEB	C2B-C1B-CHA-C4A
29	BD	201	PEB	ND-C1D-CHC-C4C
29	BD	201	PEB	C2D-C1D-CHC-C4C
29	BD	201	PEB	NC-C1C-CHB-C4B
29	BD	201	PEB	NB-C1B-CHA-C4A
29	BD	201	PEB	C2B-C1B-CHA-C4A
29	BD	202	PEB	NC-C1C-CHB-C4B
29	BD	202	PEB	C2C-C1C-CHB-C4B
29	BD	202	PEB	NB-C1B-CHA-C4A
29	BD	202	PEB	C2B-C1B-CHA-C4A
29	CD	201	PEB	NB-C1B-CHA-C4A
29	CD	201	PEB	C2B-C1B-CHA-C4A
29	CD	202	PEB	NC-C1C-CHB-C4B
29	CD	202	PEB	C2C-CAC-CBC-CGC
29	CD	202	PEB	C4A-C3A-CAA-CBA
29	CD	202	PEB	NB-C1B-CHA-C4A
29	CD	202	PEB	C2B-C1B-CHA-C4A
29	CD	203	PEB	NC-C1C-CHB-C4B
29	CD	203	PEB	C2C-C1C-CHB-C4B
29	CD	203	PEB	NB-C1B-CHA-C4A
29	CD	203	PEB	C2B-C1B-CHA-C4A
29	CD	203	PEB	C3B-CAB-CBB-CGB
29	DD	201	PEB	ND-C1D-CHC-C4C
29	DD	201	PEB	C2D-C1D-CHC-C4C
29	DD	201	PEB	NC-C1C-CHB-C4B
29	DD	201	PEB	NB-C1B-CHA-C4A
29	DD	201	PEB	C2B-C1B-CHA-C4A
29	DD	202	PEB	NC-C1C-CHB-C4B
29	DD	202	PEB	C2C-C1C-CHB-C4B
29	DD	202	PEB	NB-C1B-CHA-C4A
29	DD	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	ED	201	PEB	NC-C1C-CHB-C4B
29	ED	201	PEB	C2C-CAC-CBC-CGC
29	ED	201	PEB	C4A-C3A-CAA-CBA
29	ED	201	PEB	NB-C1B-CHA-C4A
29	ED	201	PEB	C2B-C1B-CHA-C4A
29	ED	202	PEB	NC-C1C-CHB-C4B
29	ED	202	PEB	C2C-C1C-CHB-C4B
29	ED	202	PEB	NB-C1B-CHA-C4A
29	ED	202	PEB	C2B-C1B-CHA-C4A
29	ED	202	PEB	C3B-CAB-CBB-CGB
29	FD	201	PEB	ND-C1D-CHC-C4C
29	FD	201	PEB	C2D-C1D-CHC-C4C
29	FD	201	PEB	NC-C1C-CHB-C4B
29	FD	201	PEB	NB-C1B-CHA-C4A
29	FD	201	PEB	C2B-C1B-CHA-C4A
29	FD	202	PEB	NC-C1C-CHB-C4B
29	FD	202	PEB	C2C-C1C-CHB-C4B
29	FD	202	PEB	NB-C1B-CHA-C4A
29	FD	202	PEB	C2B-C1B-CHA-C4A
29	GD	201	PEB	NB-C1B-CHA-C4A
29	GD	201	PEB	C2B-C1B-CHA-C4A
29	GD	202	PEB	NC-C1C-CHB-C4B
29	GD	202	PEB	C2C-CAC-CBC-CGC
29	GD	202	PEB	C4A-C3A-CAA-CBA
29	GD	202	PEB	NB-C1B-CHA-C4A
29	GD	202	PEB	C2B-C1B-CHA-C4A
29	GD	203	PEB	NC-C1C-CHB-C4B
29	GD	203	PEB	C2C-C1C-CHB-C4B
29	GD	203	PEB	NB-C1B-CHA-C4A
29	GD	203	PEB	C2B-C1B-CHA-C4A
29	GD	203	PEB	C3B-CAB-CBB-CGB
29	HD	201	PEB	ND-C1D-CHC-C4C
29	HD	201	PEB	C2D-C1D-CHC-C4C
29	HD	201	PEB	NC-C1C-CHB-C4B
29	HD	201	PEB	NB-C1B-CHA-C4A
29	HD	201	PEB	C2B-C1B-CHA-C4A
29	HD	202	PEB	NC-C1C-CHB-C4B
29	HD	202	PEB	C2C-C1C-CHB-C4B
29	HD	202	PEB	NB-C1B-CHA-C4A
29	HD	202	PEB	C2B-C1B-CHA-C4A
29	ID	201	PEB	NB-C1B-CHA-C4A
29	ID	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	ID	202	PEB	NC-C1C-CHB-C4B
29	ID	202	PEB	C2C-CAC-CBC-CGC
29	ID	202	PEB	C4A-C3A-CAA-CBA
29	ID	202	PEB	NB-C1B-CHA-C4A
29	ID	202	PEB	C2B-C1B-CHA-C4A
29	ID	203	PEB	NC-C1C-CHB-C4B
29	ID	203	PEB	C2C-C1C-CHB-C4B
29	ID	203	PEB	NB-C1B-CHA-C4A
29	ID	203	PEB	C2B-C1B-CHA-C4A
29	ID	203	PEB	C3B-CAB-CBB-CGB
29	JD	201	PEB	ND-C1D-CHC-C4C
29	JD	201	PEB	C2D-C1D-CHC-C4C
29	JD	201	PEB	NC-C1C-CHB-C4B
29	JD	201	PEB	NB-C1B-CHA-C4A
29	JD	201	PEB	C2B-C1B-CHA-C4A
29	JD	202	PEB	NC-C1C-CHB-C4B
29	JD	202	PEB	C2C-C1C-CHB-C4B
29	JD	202	PEB	NB-C1B-CHA-C4A
29	JD	202	PEB	C2B-C1B-CHA-C4A
29	KD	201	PEB	NB-C1B-CHA-C4A
29	KD	201	PEB	C2B-C1B-CHA-C4A
29	KD	202	PEB	NC-C1C-CHB-C4B
29	KD	202	PEB	C2C-CAC-CBC-CGC
29	KD	202	PEB	C4A-C3A-CAA-CBA
29	KD	202	PEB	NB-C1B-CHA-C4A
29	KD	202	PEB	C2B-C1B-CHA-C4A
29	KD	203	PEB	NC-C1C-CHB-C4B
29	KD	203	PEB	C2C-C1C-CHB-C4B
29	KD	203	PEB	NB-C1B-CHA-C4A
29	KD	203	PEB	C2B-C1B-CHA-C4A
29	KD	203	PEB	C3B-CAB-CBB-CGB
29	LD	201	PEB	ND-C1D-CHC-C4C
29	LD	201	PEB	C2D-C1D-CHC-C4C
29	LD	201	PEB	NC-C1C-CHB-C4B
29	LD	201	PEB	NB-C1B-CHA-C4A
29	LD	201	PEB	C2B-C1B-CHA-C4A
29	LD	202	PEB	NC-C1C-CHB-C4B
29	LD	202	PEB	C2C-C1C-CHB-C4B
29	LD	202	PEB	NB-C1B-CHA-C4A
29	LD	202	PEB	C2B-C1B-CHA-C4A
29	MD	201	PEB	NB-C1B-CHA-C4A
29	MD	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	MD	202	PEB	NC-C1C-CHB-C4B
29	MD	202	PEB	C2C-CAC-CBC-CGC
29	MD	202	PEB	C4A-C3A-CAA-CBA
29	MD	202	PEB	NB-C1B-CHA-C4A
29	MD	202	PEB	C2B-C1B-CHA-C4A
29	MD	203	PEB	NC-C1C-CHB-C4B
29	MD	203	PEB	C2C-C1C-CHB-C4B
29	MD	203	PEB	NB-C1B-CHA-C4A
29	MD	203	PEB	C2B-C1B-CHA-C4A
29	MD	203	PEB	C3B-CAB-CBB-CGB
29	AE	201	PEB	NB-C1B-CHA-C4A
29	AE	201	PEB	C2B-C1B-CHA-C4A
29	AE	202	PEB	NB-C1B-CHA-C4A
29	AE	202	PEB	C2B-C1B-CHA-C4A
29	AE	203	PEB	NC-C1C-CHB-C4B
29	AE	203	PEB	C2C-C1C-CHB-C4B
29	AE	203	PEB	C2A-C3A-CAA-CBA
29	AE	203	PEB	C4A-C3A-CAA-CBA
29	AE	203	PEB	NB-C1B-CHA-C4A
29	AE	203	PEB	C2B-C1B-CHA-C4A
29	BE	201	PEB	ND-C1D-CHC-C4C
29	BE	201	PEB	C2D-C1D-CHC-C4C
29	BE	201	PEB	NB-C1B-CHA-C4A
29	BE	201	PEB	C2B-C1B-CHA-C4A
29	BE	202	PEB	NC-C1C-CHB-C4B
29	BE	202	PEB	C2C-C1C-CHB-C4B
29	BE	202	PEB	C2A-C3A-CAA-CBA
29	BE	202	PEB	C4A-C3A-CAA-CBA
29	BE	202	PEB	NB-C1B-CHA-C4A
29	BE	202	PEB	C2B-C1B-CHA-C4A
29	BE	203	PEB	NC-C1C-CHB-C4B
29	BE	203	PEB	C2C-C1C-CHB-C4B
29	BE	203	PEB	NB-C1B-CHA-C4A
29	BE	203	PEB	C2B-C1B-CHA-C4A
29	CE	201	PEB	NB-C1B-CHA-C4A
29	CE	201	PEB	C2B-C1B-CHA-C4A
29	CE	202	PEB	NB-C1B-CHA-C4A
29	CE	202	PEB	C2B-C1B-CHA-C4A
29	DE	201	PEB	ND-C1D-CHC-C4C
29	DE	201	PEB	C2D-C1D-CHC-C4C
29	DE	201	PEB	NB-C1B-CHA-C4A
29	DE	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	DE	202	PEB	NC-C1C-CHB-C4B
29	DE	202	PEB	C2C-C1C-CHB-C4B
29	DE	202	PEB	NB-C1B-CHA-C4A
29	DE	202	PEB	C2B-C1B-CHA-C4A
29	EE	201	PEB	NB-C1B-CHA-C4A
29	EE	201	PEB	C2B-C1B-CHA-C4A
29	EE	202	PEB	NB-C1B-CHA-C4A
29	EE	202	PEB	C2B-C1B-CHA-C4A
29	FE	201	PEB	ND-C1D-CHC-C4C
29	FE	201	PEB	C2D-C1D-CHC-C4C
29	FE	201	PEB	NB-C1B-CHA-C4A
29	FE	201	PEB	C2B-C1B-CHA-C4A
29	FE	202	PEB	NC-C1C-CHB-C4B
29	FE	202	PEB	C2C-C1C-CHB-C4B
29	FE	202	PEB	C2A-C3A-CAA-CBA
29	FE	202	PEB	C4A-C3A-CAA-CBA
29	FE	202	PEB	NB-C1B-CHA-C4A
29	FE	202	PEB	C2B-C1B-CHA-C4A
29	FE	203	PEB	NC-C1C-CHB-C4B
29	FE	203	PEB	C2C-C1C-CHB-C4B
29	FE	203	PEB	NB-C1B-CHA-C4A
29	FE	203	PEB	C2B-C1B-CHA-C4A
29	GE	201	PEB	NB-C1B-CHA-C4A
29	GE	201	PEB	C2B-C1B-CHA-C4A
29	GE	202	PEB	NB-C1B-CHA-C4A
29	GE	202	PEB	C2B-C1B-CHA-C4A
29	HE	201	PEB	ND-C1D-CHC-C4C
29	HE	201	PEB	C2D-C1D-CHC-C4C
29	HE	201	PEB	NB-C1B-CHA-C4A
29	HE	201	PEB	C2B-C1B-CHA-C4A
29	HE	202	PEB	NC-C1C-CHB-C4B
29	HE	202	PEB	C2C-C1C-CHB-C4B
29	HE	202	PEB	C2A-C3A-CAA-CBA
29	HE	202	PEB	C4A-C3A-CAA-CBA
29	HE	202	PEB	NB-C1B-CHA-C4A
29	HE	202	PEB	C2B-C1B-CHA-C4A
29	HE	203	PEB	NC-C1C-CHB-C4B
29	HE	203	PEB	C2C-C1C-CHB-C4B
29	HE	203	PEB	NB-C1B-CHA-C4A
29	HE	203	PEB	C2B-C1B-CHA-C4A
29	IE	201	PEB	NB-C1B-CHA-C4A
29	IE	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	IE	202	PEB	NB-C1B-CHA-C4A
29	IE	202	PEB	C2B-C1B-CHA-C4A
29	JE	201	PEB	ND-C1D-CHC-C4C
29	JE	201	PEB	C2D-C1D-CHC-C4C
29	JE	201	PEB	NB-C1B-CHA-C4A
29	JE	201	PEB	C2B-C1B-CHA-C4A
29	JE	202	PEB	NC-C1C-CHB-C4B
29	JE	202	PEB	C2C-C1C-CHB-C4B
29	JE	202	PEB	NB-C1B-CHA-C4A
29	JE	202	PEB	C2B-C1B-CHA-C4A
29	KE	201	PEB	NC-C1C-CHB-C4B
29	KE	201	PEB	C2C-C1C-CHB-C4B
29	KE	201	PEB	C2A-C3A-CAA-CBA
29	KE	201	PEB	C4A-C3A-CAA-CBA
29	KE	201	PEB	NB-C1B-CHA-C4A
29	KE	201	PEB	C2B-C1B-CHA-C4A
29	KE	202	PEB	NB-C1B-CHA-C4A
29	KE	202	PEB	C2B-C1B-CHA-C4A
29	KE	203	PEB	NB-C1B-CHA-C4A
29	KE	203	PEB	C2B-C1B-CHA-C4A
29	LE	201	PEB	ND-C1D-CHC-C4C
29	LE	201	PEB	C2D-C1D-CHC-C4C
29	LE	201	PEB	NB-C1B-CHA-C4A
29	LE	201	PEB	C2B-C1B-CHA-C4A
29	LE	202	PEB	NC-C1C-CHB-C4B
29	LE	202	PEB	C2C-C1C-CHB-C4B
29	LE	202	PEB	C2A-C3A-CAA-CBA
29	LE	202	PEB	C4A-C3A-CAA-CBA
29	LE	202	PEB	NB-C1B-CHA-C4A
29	LE	202	PEB	C2B-C1B-CHA-C4A
29	LE	203	PEB	NC-C1C-CHB-C4B
29	LE	203	PEB	C2C-C1C-CHB-C4B
29	LE	203	PEB	NB-C1B-CHA-C4A
29	LE	203	PEB	C2B-C1B-CHA-C4A
29	AF	301	PEB	NC-C1C-CHB-C4B
29	AF	301	PEB	C2C-C1C-CHB-C4B
29	AF	301	PEB	NB-C1B-CHA-C4A
29	AF	301	PEB	C2B-C1B-CHA-C4A
29	AF	304	PEB	C2A-C3A-CAA-CBA
29	AF	304	PEB	NB-C1B-CHA-C4A
29	AF	304	PEB	C2B-C1B-CHA-C4A
29	AF	305	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	AF	305	PEB	C2B-C1B-CHA-C4A
29	DF	1002	PEB	ND-C1D-CHC-C4C
29	DF	1002	PEB	C2D-C3D-CAD-CBD
29	DF	1002	PEB	C4D-C3D-CAD-CBD
29	DF	1002	PEB	C4A-C3A-CAA-CBA
29	DF	1002	PEB	NB-C1B-CHA-C4A
29	DF	1002	PEB	C2B-C1B-CHA-C4A
29	FF	1002	PEB	ND-C1D-CHC-C4C
29	FF	1002	PEB	C2D-C3D-CAD-CBD
29	FF	1002	PEB	C4D-C3D-CAD-CBD
29	FF	1002	PEB	C4A-C3A-CAA-CBA
29	FF	1002	PEB	NB-C1B-CHA-C4A
29	FF	1002	PEB	C2B-C1B-CHA-C4A
29	HF	1002	PEB	ND-C1D-CHC-C4C
29	HF	1002	PEB	C2D-C3D-CAD-CBD
29	HF	1002	PEB	C4D-C3D-CAD-CBD
29	HF	1002	PEB	C4A-C3A-CAA-CBA
29	HF	1002	PEB	NB-C1B-CHA-C4A
29	HF	1002	PEB	C2B-C1B-CHA-C4A
29	JF	1002	PEB	ND-C1D-CHC-C4C
29	JF	1002	PEB	C2D-C3D-CAD-CBD
29	JF	1002	PEB	C4D-C3D-CAD-CBD
29	JF	1002	PEB	C4A-C3A-CAA-CBA
29	JF	1002	PEB	NB-C1B-CHA-C4A
29	JF	1002	PEB	C2B-C1B-CHA-C4A
29	LF	1002	PEB	ND-C1D-CHC-C4C
29	LF	1002	PEB	C2D-C3D-CAD-CBD
29	LF	1002	PEB	C4D-C3D-CAD-CBD
29	LF	1002	PEB	C4A-C3A-CAA-CBA
29	LF	1002	PEB	NB-C1B-CHA-C4A
29	LF	1002	PEB	C2B-C1B-CHA-C4A
29	NF	1002	PEB	ND-C1D-CHC-C4C
29	NF	1002	PEB	C2D-C3D-CAD-CBD
29	NF	1002	PEB	C4D-C3D-CAD-CBD
29	NF	1002	PEB	C4A-C3A-CAA-CBA
29	NF	1002	PEB	NB-C1B-CHA-C4A
29	NF	1002	PEB	C2B-C1B-CHA-C4A
29	OF	201	PEB	NB-C1B-CHA-C4A
29	OF	201	PEB	C2B-C1B-CHA-C4A
29	OF	202	PEB	NB-C1B-CHA-C4A
29	OF	202	PEB	C2B-C1B-CHA-C4A
29	OF	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	OF	203	PEB	C4A-C3A-CAA-CBA
29	OF	203	PEB	NB-C1B-CHA-C4A
29	OF	203	PEB	C2B-C1B-CHA-C4A
29	PF	201	PEB	C1C-C2C-CAC-CBC
29	PF	201	PEB	C3C-C2C-CAC-CBC
29	PF	201	PEB	NB-C1B-CHA-C4A
29	PF	201	PEB	C2B-C1B-CHA-C4A
29	PF	202	PEB	C4A-C3A-CAA-CBA
29	PF	202	PEB	NB-C1B-CHA-C4A
29	PF	202	PEB	C2B-C1B-CHA-C4A
29	PF	203	PEB	ND-C1D-CHC-C4C
29	PF	203	PEB	NC-C1C-CHB-C4B
29	PF	203	PEB	C2C-C1C-CHB-C4B
29	PF	203	PEB	NB-C1B-CHA-C4A
29	PF	203	PEB	C2B-C1B-CHA-C4A
29	QF	201	PEB	NB-C1B-CHA-C4A
29	QF	201	PEB	C2B-C1B-CHA-C4A
29	QF	202	PEB	NB-C1B-CHA-C4A
29	QF	202	PEB	C2B-C1B-CHA-C4A
29	QF	202	PEB	C3B-CAB-CBB-CGB
29	RF	201	PEB	C1C-C2C-CAC-CBC
29	RF	201	PEB	C3C-C2C-CAC-CBC
29	RF	201	PEB	NB-C1B-CHA-C4A
29	RF	201	PEB	C2B-C1B-CHA-C4A
29	RF	202	PEB	ND-C1D-CHC-C4C
29	RF	202	PEB	NC-C1C-CHB-C4B
29	RF	202	PEB	C2C-C1C-CHB-C4B
29	RF	202	PEB	NB-C1B-CHA-C4A
29	RF	202	PEB	C2B-C1B-CHA-C4A
29	SF	201	PEB	NB-C1B-CHA-C4A
29	SF	201	PEB	C2B-C1B-CHA-C4A
29	SF	202	PEB	NB-C1B-CHA-C4A
29	SF	202	PEB	C2B-C1B-CHA-C4A
29	SF	202	PEB	C3B-CAB-CBB-CGB
29	TF	201	PEB	NB-C1B-CHA-C4A
29	TF	201	PEB	C2B-C1B-CHA-C4A
29	TF	202	PEB	ND-C1D-CHC-C4C
29	TF	202	PEB	NC-C1C-CHB-C4B
29	TF	202	PEB	C2C-C1C-CHB-C4B
29	TF	202	PEB	NB-C1B-CHA-C4A
29	TF	202	PEB	C2B-C1B-CHA-C4A
29	UF	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	UF	201	PEB	NB-C1B-CHA-C4A
29	UF	201	PEB	C2B-C1B-CHA-C4A
29	UF	202	PEB	NB-C1B-CHA-C4A
29	UF	202	PEB	C2B-C1B-CHA-C4A
29	UF	203	PEB	NB-C1B-CHA-C4A
29	UF	203	PEB	C2B-C1B-CHA-C4A
29	UF	203	PEB	C3B-CAB-CBB-CGB
29	VF	201	PEB	C1C-C2C-CAC-CBC
29	VF	201	PEB	C3C-C2C-CAC-CBC
29	VF	201	PEB	NB-C1B-CHA-C4A
29	VF	201	PEB	C2B-C1B-CHA-C4A
29	VF	202	PEB	C4A-C3A-CAA-CBA
29	VF	202	PEB	NB-C1B-CHA-C4A
29	VF	202	PEB	C2B-C1B-CHA-C4A
29	VF	203	PEB	ND-C1D-CHC-C4C
29	VF	203	PEB	NC-C1C-CHB-C4B
29	VF	203	PEB	C2C-C1C-CHB-C4B
29	VF	203	PEB	NB-C1B-CHA-C4A
29	VF	203	PEB	C2B-C1B-CHA-C4A
29	WF	201	PEB	NB-C1B-CHA-C4A
29	WF	201	PEB	C2B-C1B-CHA-C4A
29	WF	202	PEB	NB-C1B-CHA-C4A
29	WF	202	PEB	C2B-C1B-CHA-C4A
29	WF	202	PEB	C3B-CAB-CBB-CGB
29	YF	201	PEB	C1C-C2C-CAC-CBC
29	YF	201	PEB	C3C-C2C-CAC-CBC
29	YF	201	PEB	NB-C1B-CHA-C4A
29	YF	201	PEB	C2B-C1B-CHA-C4A
29	YF	202	PEB	C4A-C3A-CAA-CBA
29	YF	202	PEB	NB-C1B-CHA-C4A
29	YF	202	PEB	C2B-C1B-CHA-C4A
29	YF	203	PEB	ND-C1D-CHC-C4C
29	YF	203	PEB	NC-C1C-CHB-C4B
29	YF	203	PEB	C2C-C1C-CHB-C4B
29	YF	203	PEB	NB-C1B-CHA-C4A
29	YF	203	PEB	C2B-C1B-CHA-C4A
29	ZF	201	PEB	NB-C1B-CHA-C4A
29	ZF	201	PEB	C2B-C1B-CHA-C4A
29	ZF	202	PEB	NB-C1B-CHA-C4A
29	ZF	202	PEB	C2B-C1B-CHA-C4A
29	ZF	202	PEB	C3B-CAB-CBB-CGB
29	aF	201	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	aF	201	PEB	C3C-C2C-CAC-CBC
29	aF	201	PEB	NB-C1B-CHA-C4A
29	aF	201	PEB	C2B-C1B-CHA-C4A
29	aF	202	PEB	C4A-C3A-CAA-CBA
29	aF	202	PEB	NB-C1B-CHA-C4A
29	aF	202	PEB	C2B-C1B-CHA-C4A
29	aF	203	PEB	ND-C1D-CHC-C4C
29	aF	203	PEB	NC-C1C-CHB-C4B
29	aF	203	PEB	C2C-C1C-CHB-C4B
29	aF	203	PEB	NB-C1B-CHA-C4A
29	aF	203	PEB	C2B-C1B-CHA-C4A
29	bF	201	PEB	NB-C1B-CHA-C4A
29	bF	201	PEB	C2B-C1B-CHA-C4A
29	bF	202	PEB	NB-C1B-CHA-C4A
29	bF	202	PEB	C2B-C1B-CHA-C4A
29	bF	202	PEB	C3B-CAB-CBB-CGB
29	cF	201	PEB	C1C-C2C-CAC-CBC
29	cF	201	PEB	C3C-C2C-CAC-CBC
29	cF	201	PEB	NB-C1B-CHA-C4A
29	cF	201	PEB	C2B-C1B-CHA-C4A
29	cF	202	PEB	ND-C1D-CHC-C4C
29	cF	202	PEB	NC-C1C-CHB-C4B
29	cF	202	PEB	C2C-C1C-CHB-C4B
29	cF	202	PEB	NB-C1B-CHA-C4A
29	cF	202	PEB	C2B-C1B-CHA-C4A
29	dF	201	PEB	C4A-C3A-CAA-CBA
29	dF	201	PEB	NB-C1B-CHA-C4A
29	dF	201	PEB	C2B-C1B-CHA-C4A
29	dF	202	PEB	NB-C1B-CHA-C4A
29	dF	202	PEB	C2B-C1B-CHA-C4A
29	dF	203	PEB	NB-C1B-CHA-C4A
29	dF	203	PEB	C2B-C1B-CHA-C4A
29	dF	203	PEB	C3B-CAB-CBB-CGB
29	eF	201	PEB	C1C-C2C-CAC-CBC
29	eF	201	PEB	C3C-C2C-CAC-CBC
29	eF	201	PEB	NB-C1B-CHA-C4A
29	eF	201	PEB	C2B-C1B-CHA-C4A
29	eF	202	PEB	C4A-C3A-CAA-CBA
29	eF	202	PEB	NB-C1B-CHA-C4A
29	eF	202	PEB	C2B-C1B-CHA-C4A
29	eF	203	PEB	ND-C1D-CHC-C4C
29	eF	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	eF	203	PEB	C2C-C1C-CHB-C4B
29	eF	203	PEB	NB-C1B-CHA-C4A
29	eF	203	PEB	C2B-C1B-CHA-C4A
29	fF	201	PEB	NB-C1B-CHA-C4A
29	fF	201	PEB	C2B-C1B-CHA-C4A
29	fF	202	PEB	NB-C1B-CHA-C4A
29	fF	202	PEB	C2B-C1B-CHA-C4A
29	fF	202	PEB	C3B-CAB-CBB-CGB
29	gF	201	PEB	C1C-C2C-CAC-CBC
29	gF	201	PEB	C3C-C2C-CAC-CBC
29	gF	201	PEB	NB-C1B-CHA-C4A
29	gF	201	PEB	C2B-C1B-CHA-C4A
29	gF	202	PEB	C4A-C3A-CAA-CBA
29	gF	202	PEB	NB-C1B-CHA-C4A
29	gF	202	PEB	C2B-C1B-CHA-C4A
29	gF	203	PEB	ND-C1D-CHC-C4C
29	gF	203	PEB	NC-C1C-CHB-C4B
29	gF	203	PEB	C2C-C1C-CHB-C4B
29	gF	203	PEB	NB-C1B-CHA-C4A
29	gF	203	PEB	C2B-C1B-CHA-C4A
29	hF	201	PEB	NB-C1B-CHA-C4A
29	hF	201	PEB	C2B-C1B-CHA-C4A
29	hF	202	PEB	NB-C1B-CHA-C4A
29	hF	202	PEB	C2B-C1B-CHA-C4A
29	hF	202	PEB	C3B-CAB-CBB-CGB
29	iF	201	PEB	C1C-C2C-CAC-CBC
29	iF	201	PEB	C3C-C2C-CAC-CBC
29	iF	201	PEB	NB-C1B-CHA-C4A
29	iF	201	PEB	C2B-C1B-CHA-C4A
29	iF	202	PEB	C4A-C3A-CAA-CBA
29	iF	202	PEB	NB-C1B-CHA-C4A
29	iF	202	PEB	C2B-C1B-CHA-C4A
29	iF	203	PEB	ND-C1D-CHC-C4C
29	iF	203	PEB	NC-C1C-CHB-C4B
29	iF	203	PEB	C2C-C1C-CHB-C4B
29	iF	203	PEB	NB-C1B-CHA-C4A
29	iF	203	PEB	C2B-C1B-CHA-C4A
29	jF	201	PEB	NB-C1B-CHA-C4A
29	jF	201	PEB	C2B-C1B-CHA-C4A
29	jF	202	PEB	NB-C1B-CHA-C4A
29	jF	202	PEB	C2B-C1B-CHA-C4A
29	jF	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	kF	201	PEB	C1C-C2C-CAC-CBC
29	kF	201	PEB	C3C-C2C-CAC-CBC
29	kF	201	PEB	NB-C1B-CHA-C4A
29	kF	201	PEB	C2B-C1B-CHA-C4A
29	kF	202	PEB	C4A-C3A-CAA-CBA
29	kF	202	PEB	NB-C1B-CHA-C4A
29	kF	202	PEB	C2B-C1B-CHA-C4A
29	kF	203	PEB	ND-C1D-CHC-C4C
29	kF	203	PEB	NC-C1C-CHB-C4B
29	kF	203	PEB	C2C-C1C-CHB-C4B
29	kF	203	PEB	NB-C1B-CHA-C4A
29	kF	203	PEB	C2B-C1B-CHA-C4A
29	lF	201	PEB	NB-C1B-CHA-C4A
29	lF	201	PEB	C2B-C1B-CHA-C4A
29	lF	202	PEB	NB-C1B-CHA-C4A
29	lF	202	PEB	C2B-C1B-CHA-C4A
29	lF	202	PEB	C3B-CAB-CBB-CGB
29	mF	201	PEB	C1C-C2C-CAC-CBC
29	mF	201	PEB	C3C-C2C-CAC-CBC
29	mF	201	PEB	NB-C1B-CHA-C4A
29	mF	201	PEB	C2B-C1B-CHA-C4A
29	mF	202	PEB	C4A-C3A-CAA-CBA
29	mF	202	PEB	NB-C1B-CHA-C4A
29	mF	202	PEB	C2B-C1B-CHA-C4A
29	mF	203	PEB	ND-C1D-CHC-C4C
29	mF	203	PEB	NC-C1C-CHB-C4B
29	mF	203	PEB	C2C-C1C-CHB-C4B
29	mF	203	PEB	NB-C1B-CHA-C4A
29	mF	203	PEB	C2B-C1B-CHA-C4A
29	AG	201	PEB	NB-C1B-CHA-C4A
29	AG	201	PEB	C2B-C1B-CHA-C4A
29	AG	202	PEB	NC-C1C-CHB-C4B
29	AG	202	PEB	C2C-C1C-CHB-C4B
29	AG	202	PEB	C2C-CAC-CBC-CGC
29	AG	202	PEB	C4A-C3A-CAA-CBA
29	AG	202	PEB	NB-C1B-CHA-C4A
29	AG	202	PEB	C2B-C1B-CHA-C4A
29	BG	201	PEB	ND-C1D-CHC-C4C
29	BG	201	PEB	C2C-CAC-CBC-CGC
29	BG	201	PEB	NB-C1B-CHA-C4A
29	BG	201	PEB	C2B-C1B-CHA-C4A
29	BG	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	BG	202	PEB	C4A-C3A-CAA-CBA
29	BG	202	PEB	NB-C1B-CHA-C4A
29	BG	202	PEB	C2B-C1B-CHA-C4A
29	BG	203	PEB	ND-C1D-CHC-C4C
29	BG	203	PEB	C2D-C1D-CHC-C4C
29	BG	203	PEB	NC-C1C-CHB-C4B
29	BG	203	PEB	C2C-C1C-CHB-C4B
29	BG	203	PEB	NB-C1B-CHA-C4A
29	BG	203	PEB	C2B-C1B-CHA-C4A
29	CG	201	PEB	NB-C1B-CHA-C4A
29	CG	201	PEB	C2B-C1B-CHA-C4A
29	CG	202	PEB	NC-C1C-CHB-C4B
29	CG	202	PEB	C2C-C1C-CHB-C4B
29	CG	202	PEB	C2C-CAC-CBC-CGC
29	CG	202	PEB	C4A-C3A-CAA-CBA
29	CG	202	PEB	NB-C1B-CHA-C4A
29	CG	202	PEB	C2B-C1B-CHA-C4A
29	DG	201	PEB	ND-C1D-CHC-C4C
29	DG	201	PEB	C2C-CAC-CBC-CGC
29	DG	201	PEB	NB-C1B-CHA-C4A
29	DG	201	PEB	C2B-C1B-CHA-C4A
29	DG	202	PEB	C2A-C3A-CAA-CBA
29	DG	202	PEB	C4A-C3A-CAA-CBA
29	DG	202	PEB	NB-C1B-CHA-C4A
29	DG	202	PEB	C2B-C1B-CHA-C4A
29	DG	203	PEB	ND-C1D-CHC-C4C
29	DG	203	PEB	C2D-C1D-CHC-C4C
29	DG	203	PEB	NC-C1C-CHB-C4B
29	DG	203	PEB	C2C-C1C-CHB-C4B
29	DG	203	PEB	NB-C1B-CHA-C4A
29	DG	203	PEB	C2B-C1B-CHA-C4A
29	EG	201	PEB	NB-C1B-CHA-C4A
29	EG	201	PEB	C2B-C1B-CHA-C4A
29	EG	202	PEB	NC-C1C-CHB-C4B
29	EG	202	PEB	C2C-C1C-CHB-C4B
29	EG	202	PEB	C2C-CAC-CBC-CGC
29	EG	202	PEB	C4A-C3A-CAA-CBA
29	EG	202	PEB	NB-C1B-CHA-C4A
29	EG	202	PEB	C2B-C1B-CHA-C4A
29	FG	201	PEB	ND-C1D-CHC-C4C
29	FG	201	PEB	C2C-CAC-CBC-CGC
29	FG	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	FG	201	PEB	C2B-C1B-CHA-C4A
29	FG	202	PEB	C2A-C3A-CAA-CBA
29	FG	202	PEB	C4A-C3A-CAA-CBA
29	FG	202	PEB	NB-C1B-CHA-C4A
29	FG	202	PEB	C2B-C1B-CHA-C4A
29	FG	203	PEB	ND-C1D-CHC-C4C
29	FG	203	PEB	C2D-C1D-CHC-C4C
29	FG	203	PEB	NC-C1C-CHB-C4B
29	FG	203	PEB	C2C-C1C-CHB-C4B
29	FG	203	PEB	NB-C1B-CHA-C4A
29	FG	203	PEB	C2B-C1B-CHA-C4A
29	GG	201	PEB	NB-C1B-CHA-C4A
29	GG	201	PEB	C2B-C1B-CHA-C4A
29	GG	202	PEB	NC-C1C-CHB-C4B
29	GG	202	PEB	C2C-C1C-CHB-C4B
29	GG	202	PEB	C2C-CAC-CBC-CGC
29	GG	202	PEB	C4A-C3A-CAA-CBA
29	GG	202	PEB	NB-C1B-CHA-C4A
29	GG	202	PEB	C2B-C1B-CHA-C4A
29	HG	201	PEB	ND-C1D-CHC-C4C
29	HG	201	PEB	C2C-CAC-CBC-CGC
29	HG	201	PEB	NB-C1B-CHA-C4A
29	HG	201	PEB	C2B-C1B-CHA-C4A
29	HG	202	PEB	C2A-C3A-CAA-CBA
29	HG	202	PEB	C4A-C3A-CAA-CBA
29	HG	202	PEB	NB-C1B-CHA-C4A
29	HG	202	PEB	C2B-C1B-CHA-C4A
29	HG	203	PEB	ND-C1D-CHC-C4C
29	HG	203	PEB	C2D-C1D-CHC-C4C
29	HG	203	PEB	NC-C1C-CHB-C4B
29	HG	203	PEB	C2C-C1C-CHB-C4B
29	HG	203	PEB	NB-C1B-CHA-C4A
29	HG	203	PEB	C2B-C1B-CHA-C4A
29	IG	201	PEB	NB-C1B-CHA-C4A
29	IG	201	PEB	C2B-C1B-CHA-C4A
29	IG	202	PEB	NC-C1C-CHB-C4B
29	IG	202	PEB	C2C-C1C-CHB-C4B
29	IG	202	PEB	C2C-CAC-CBC-CGC
29	IG	202	PEB	C4A-C3A-CAA-CBA
29	IG	202	PEB	NB-C1B-CHA-C4A
29	IG	202	PEB	C2B-C1B-CHA-C4A
29	JG	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	JG	201	PEB	C2C-CAC-CBC-CGC
29	JG	201	PEB	NB-C1B-CHA-C4A
29	JG	201	PEB	C2B-C1B-CHA-C4A
29	JG	202	PEB	C2A-C3A-CAA-CBA
29	JG	202	PEB	C4A-C3A-CAA-CBA
29	JG	202	PEB	NB-C1B-CHA-C4A
29	JG	202	PEB	C2B-C1B-CHA-C4A
29	JG	203	PEB	ND-C1D-CHC-C4C
29	JG	203	PEB	C2D-C1D-CHC-C4C
29	JG	203	PEB	NC-C1C-CHB-C4B
29	JG	203	PEB	C2C-C1C-CHB-C4B
29	JG	203	PEB	NB-C1B-CHA-C4A
29	JG	203	PEB	C2B-C1B-CHA-C4A
29	KG	201	PEB	NB-C1B-CHA-C4A
29	KG	201	PEB	C2B-C1B-CHA-C4A
29	KG	202	PEB	NC-C1C-CHB-C4B
29	KG	202	PEB	C2C-C1C-CHB-C4B
29	KG	202	PEB	C2C-CAC-CBC-CGC
29	KG	202	PEB	C4A-C3A-CAA-CBA
29	KG	202	PEB	NB-C1B-CHA-C4A
29	KG	202	PEB	C2B-C1B-CHA-C4A
29	LG	201	PEB	ND-C1D-CHC-C4C
29	LG	201	PEB	C2C-CAC-CBC-CGC
29	LG	201	PEB	NB-C1B-CHA-C4A
29	LG	201	PEB	C2B-C1B-CHA-C4A
29	LG	202	PEB	C2A-C3A-CAA-CBA
29	LG	202	PEB	C4A-C3A-CAA-CBA
29	LG	202	PEB	NB-C1B-CHA-C4A
29	LG	202	PEB	C2B-C1B-CHA-C4A
29	LG	203	PEB	ND-C1D-CHC-C4C
29	LG	203	PEB	C2D-C1D-CHC-C4C
29	LG	203	PEB	NC-C1C-CHB-C4B
29	LG	203	PEB	C2C-C1C-CHB-C4B
29	LG	203	PEB	NB-C1B-CHA-C4A
29	LG	203	PEB	C2B-C1B-CHA-C4A
29	MG	401	PEB	C2A-C3A-CAA-CBA
29	MG	401	PEB	C4A-C3A-CAA-CBA
29	MG	401	PEB	NB-C1B-CHA-C4A
29	MG	401	PEB	C2B-C1B-CHA-C4A
29	MG	404	PEB	ND-C1D-CHC-C4C
29	MG	404	PEB	NC-C1C-CHB-C4B
29	MG	404	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	MG	404	PEB	NB-C1B-CHA-C4A
29	MG	404	PEB	C2B-C1B-CHA-C4A
29	MG	405	PEB	NC-C1C-CHB-C4B
29	MG	405	PEB	C2C-C1C-CHB-C4B
29	MG	405	PEB	NB-C1B-CHA-C4A
29	MG	405	PEB	C2B-C1B-CHA-C4A
29	AI	301	PEB	NC-C1C-CHB-C4B
29	AI	301	PEB	C2C-C1C-CHB-C4B
29	AI	301	PEB	NB-C1B-CHA-C4A
29	AI	301	PEB	C2B-C1B-CHA-C4A
29	AI	304	PEB	C2A-C3A-CAA-CBA
29	AI	304	PEB	NB-C1B-CHA-C4A
29	AI	304	PEB	C2B-C1B-CHA-C4A
29	AI	305	PEB	NB-C1B-CHA-C4A
29	AI	305	PEB	C2B-C1B-CHA-C4A
29	DI	1002	PEB	ND-C1D-CHC-C4C
29	DI	1002	PEB	C2D-C3D-CAD-CBD
29	DI	1002	PEB	C4D-C3D-CAD-CBD
29	DI	1002	PEB	C4A-C3A-CAA-CBA
29	DI	1002	PEB	NB-C1B-CHA-C4A
29	DI	1002	PEB	C2B-C1B-CHA-C4A
29	FI	1002	PEB	ND-C1D-CHC-C4C
29	FI	1002	PEB	C2D-C3D-CAD-CBD
29	FI	1002	PEB	C4D-C3D-CAD-CBD
29	FI	1002	PEB	C4A-C3A-CAA-CBA
29	FI	1002	PEB	NB-C1B-CHA-C4A
29	FI	1002	PEB	C2B-C1B-CHA-C4A
29	HI	1002	PEB	ND-C1D-CHC-C4C
29	HI	1002	PEB	C2D-C3D-CAD-CBD
29	HI	1002	PEB	C4D-C3D-CAD-CBD
29	HI	1002	PEB	C4A-C3A-CAA-CBA
29	HI	1002	PEB	NB-C1B-CHA-C4A
29	HI	1002	PEB	C2B-C1B-CHA-C4A
29	JI	1002	PEB	ND-C1D-CHC-C4C
29	JI	1002	PEB	C2D-C3D-CAD-CBD
29	JI	1002	PEB	C4D-C3D-CAD-CBD
29	JI	1002	PEB	C4A-C3A-CAA-CBA
29	JI	1002	PEB	NB-C1B-CHA-C4A
29	JI	1002	PEB	C2B-C1B-CHA-C4A
29	LI	1002	PEB	ND-C1D-CHC-C4C
29	LI	1002	PEB	C2D-C3D-CAD-CBD
29	LI	1002	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
29	LI	1002	PEB	C4A-C3A-CAA-CBA
29	LI	1002	PEB	NB-C1B-CHA-C4A
29	LI	1002	PEB	C2B-C1B-CHA-C4A
29	NI	1002	PEB	ND-C1D-CHC-C4C
29	NI	1002	PEB	C2D-C3D-CAD-CBD
29	NI	1002	PEB	C4D-C3D-CAD-CBD
29	NI	1002	PEB	C4A-C3A-CAA-CBA
29	NI	1002	PEB	NB-C1B-CHA-C4A
29	NI	1002	PEB	C2B-C1B-CHA-C4A
29	OI	201	PEB	NB-C1B-CHA-C4A
29	OI	201	PEB	C2B-C1B-CHA-C4A
29	OI	202	PEB	NB-C1B-CHA-C4A
29	OI	202	PEB	C2B-C1B-CHA-C4A
29	OI	202	PEB	C3B-CAB-CBB-CGB
29	OI	203	PEB	C4A-C3A-CAA-CBA
29	OI	203	PEB	NB-C1B-CHA-C4A
29	OI	203	PEB	C2B-C1B-CHA-C4A
29	PI	201	PEB	C1C-C2C-CAC-CBC
29	PI	201	PEB	C3C-C2C-CAC-CBC
29	PI	201	PEB	NB-C1B-CHA-C4A
29	PI	201	PEB	C2B-C1B-CHA-C4A
29	PI	202	PEB	C4A-C3A-CAA-CBA
29	PI	202	PEB	NB-C1B-CHA-C4A
29	PI	202	PEB	C2B-C1B-CHA-C4A
29	PI	203	PEB	ND-C1D-CHC-C4C
29	PI	203	PEB	NC-C1C-CHB-C4B
29	PI	203	PEB	C2C-C1C-CHB-C4B
29	PI	203	PEB	NB-C1B-CHA-C4A
29	PI	203	PEB	C2B-C1B-CHA-C4A
29	QI	201	PEB	NB-C1B-CHA-C4A
29	QI	201	PEB	C2B-C1B-CHA-C4A
29	QI	202	PEB	NB-C1B-CHA-C4A
29	QI	202	PEB	C2B-C1B-CHA-C4A
29	QI	202	PEB	C3B-CAB-CBB-CGB
29	RI	201	PEB	C1C-C2C-CAC-CBC
29	RI	201	PEB	C3C-C2C-CAC-CBC
29	RI	201	PEB	NB-C1B-CHA-C4A
29	RI	201	PEB	C2B-C1B-CHA-C4A
29	RI	202	PEB	ND-C1D-CHC-C4C
29	RI	202	PEB	NC-C1C-CHB-C4B
29	RI	202	PEB	C2C-C1C-CHB-C4B
29	RI	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	RI	202	PEB	C2B-C1B-CHA-C4A
29	SI	201	PEB	NB-C1B-CHA-C4A
29	SI	201	PEB	C2B-C1B-CHA-C4A
29	SI	202	PEB	NB-C1B-CHA-C4A
29	SI	202	PEB	C2B-C1B-CHA-C4A
29	SI	202	PEB	C3B-CAB-CBB-CGB
29	TI	201	PEB	C1C-C2C-CAC-CBC
29	TI	201	PEB	C3C-C2C-CAC-CBC
29	TI	201	PEB	NB-C1B-CHA-C4A
29	TI	201	PEB	C2B-C1B-CHA-C4A
29	TI	202	PEB	ND-C1D-CHC-C4C
29	TI	202	PEB	NC-C1C-CHB-C4B
29	TI	202	PEB	C2C-C1C-CHB-C4B
29	TI	202	PEB	NB-C1B-CHA-C4A
29	TI	202	PEB	C2B-C1B-CHA-C4A
29	UI	201	PEB	C4A-C3A-CAA-CBA
29	UI	201	PEB	NB-C1B-CHA-C4A
29	UI	201	PEB	C2B-C1B-CHA-C4A
29	UI	202	PEB	NB-C1B-CHA-C4A
29	UI	202	PEB	C2B-C1B-CHA-C4A
29	UI	203	PEB	NB-C1B-CHA-C4A
29	UI	203	PEB	C2B-C1B-CHA-C4A
29	UI	203	PEB	C3B-CAB-CBB-CGB
29	VI	201	PEB	C1C-C2C-CAC-CBC
29	VI	201	PEB	C3C-C2C-CAC-CBC
29	VI	201	PEB	NB-C1B-CHA-C4A
29	VI	201	PEB	C2B-C1B-CHA-C4A
29	VI	202	PEB	C4A-C3A-CAA-CBA
29	VI	202	PEB	NB-C1B-CHA-C4A
29	VI	202	PEB	C2B-C1B-CHA-C4A
29	VI	203	PEB	ND-C1D-CHC-C4C
29	VI	203	PEB	NC-C1C-CHB-C4B
29	VI	203	PEB	C2C-C1C-CHB-C4B
29	VI	203	PEB	NB-C1B-CHA-C4A
29	VI	203	PEB	C2B-C1B-CHA-C4A
29	WI	201	PEB	NB-C1B-CHA-C4A
29	WI	201	PEB	C2B-C1B-CHA-C4A
29	WI	202	PEB	NB-C1B-CHA-C4A
29	WI	202	PEB	C2B-C1B-CHA-C4A
29	WI	202	PEB	C3B-CAB-CBB-CGB
29	YI	201	PEB	C1C-C2C-CAC-CBC
29	YI	201	PEB	C3C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	YI	201	PEB	NB-C1B-CHA-C4A
29	YI	201	PEB	C2B-C1B-CHA-C4A
29	YI	202	PEB	C4A-C3A-CAA-CBA
29	YI	202	PEB	NB-C1B-CHA-C4A
29	YI	202	PEB	C2B-C1B-CHA-C4A
29	YI	203	PEB	ND-C1D-CHC-C4C
29	YI	203	PEB	NC-C1C-CHB-C4B
29	YI	203	PEB	C2C-C1C-CHB-C4B
29	YI	203	PEB	NB-C1B-CHA-C4A
29	YI	203	PEB	C2B-C1B-CHA-C4A
29	ZI	201	PEB	NB-C1B-CHA-C4A
29	ZI	201	PEB	C2B-C1B-CHA-C4A
29	ZI	202	PEB	NB-C1B-CHA-C4A
29	ZI	202	PEB	C2B-C1B-CHA-C4A
29	ZI	202	PEB	C3B-CAB-CBB-CGB
29	aI	201	PEB	C1C-C2C-CAC-CBC
29	aI	201	PEB	C3C-C2C-CAC-CBC
29	aI	201	PEB	NB-C1B-CHA-C4A
29	aI	201	PEB	C2B-C1B-CHA-C4A
29	aI	202	PEB	C4A-C3A-CAA-CBA
29	aI	202	PEB	NB-C1B-CHA-C4A
29	aI	202	PEB	C2B-C1B-CHA-C4A
29	aI	203	PEB	ND-C1D-CHC-C4C
29	aI	203	PEB	NC-C1C-CHB-C4B
29	aI	203	PEB	C2C-C1C-CHB-C4B
29	aI	203	PEB	NB-C1B-CHA-C4A
29	aI	203	PEB	C2B-C1B-CHA-C4A
29	bI	201	PEB	NB-C1B-CHA-C4A
29	bI	201	PEB	C2B-C1B-CHA-C4A
29	bI	202	PEB	NB-C1B-CHA-C4A
29	bI	202	PEB	C2B-C1B-CHA-C4A
29	bI	202	PEB	C3B-CAB-CBB-CGB
29	cI	201	PEB	C1C-C2C-CAC-CBC
29	cI	201	PEB	C3C-C2C-CAC-CBC
29	cI	201	PEB	NB-C1B-CHA-C4A
29	cI	201	PEB	C2B-C1B-CHA-C4A
29	cI	202	PEB	ND-C1D-CHC-C4C
29	cI	202	PEB	NC-C1C-CHB-C4B
29	cI	202	PEB	C2C-C1C-CHB-C4B
29	cI	202	PEB	NB-C1B-CHA-C4A
29	cI	202	PEB	C2B-C1B-CHA-C4A
29	dI	201	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	dI	201	PEB	NB-C1B-CHA-C4A
29	dI	201	PEB	C2B-C1B-CHA-C4A
29	dI	202	PEB	NB-C1B-CHA-C4A
29	dI	202	PEB	C2B-C1B-CHA-C4A
29	dI	203	PEB	NB-C1B-CHA-C4A
29	dI	203	PEB	C2B-C1B-CHA-C4A
29	dI	203	PEB	C3B-CAB-CBB-CGB
29	eI	201	PEB	C1C-C2C-CAC-CBC
29	eI	201	PEB	C3C-C2C-CAC-CBC
29	eI	201	PEB	NB-C1B-CHA-C4A
29	eI	201	PEB	C2B-C1B-CHA-C4A
29	eI	202	PEB	C4A-C3A-CAA-CBA
29	eI	202	PEB	NB-C1B-CHA-C4A
29	eI	202	PEB	C2B-C1B-CHA-C4A
29	eI	203	PEB	ND-C1D-CHC-C4C
29	eI	203	PEB	NC-C1C-CHB-C4B
29	eI	203	PEB	C2C-C1C-CHB-C4B
29	eI	203	PEB	NB-C1B-CHA-C4A
29	eI	203	PEB	C2B-C1B-CHA-C4A
29	fI	201	PEB	NB-C1B-CHA-C4A
29	fI	201	PEB	C2B-C1B-CHA-C4A
29	fI	202	PEB	NB-C1B-CHA-C4A
29	fI	202	PEB	C2B-C1B-CHA-C4A
29	fI	202	PEB	C3B-CAB-CBB-CGB
29	gI	201	PEB	C1C-C2C-CAC-CBC
29	gI	201	PEB	C3C-C2C-CAC-CBC
29	gI	201	PEB	NB-C1B-CHA-C4A
29	gI	201	PEB	C2B-C1B-CHA-C4A
29	gI	202	PEB	C4A-C3A-CAA-CBA
29	gI	202	PEB	NB-C1B-CHA-C4A
29	gI	202	PEB	C2B-C1B-CHA-C4A
29	gI	203	PEB	ND-C1D-CHC-C4C
29	gI	203	PEB	NC-C1C-CHB-C4B
29	gI	203	PEB	C2C-C1C-CHB-C4B
29	gI	203	PEB	NB-C1B-CHA-C4A
29	gI	203	PEB	C2B-C1B-CHA-C4A
29	hI	201	PEB	NB-C1B-CHA-C4A
29	hI	201	PEB	C2B-C1B-CHA-C4A
29	hI	202	PEB	NB-C1B-CHA-C4A
29	hI	202	PEB	C2B-C1B-CHA-C4A
29	hI	202	PEB	C3B-CAB-CBB-CGB
29	iI	201	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	iI	201	PEB	C3C-C2C-CAC-CBC
29	iI	201	PEB	NB-C1B-CHA-C4A
29	iI	201	PEB	C2B-C1B-CHA-C4A
29	iI	202	PEB	C4A-C3A-CAA-CBA
29	iI	202	PEB	NB-C1B-CHA-C4A
29	iI	202	PEB	C2B-C1B-CHA-C4A
29	iI	203	PEB	ND-C1D-CHC-C4C
29	iI	203	PEB	NC-C1C-CHB-C4B
29	iI	203	PEB	C2C-C1C-CHB-C4B
29	iI	203	PEB	NB-C1B-CHA-C4A
29	iI	203	PEB	C2B-C1B-CHA-C4A
29	jI	201	PEB	NB-C1B-CHA-C4A
29	jI	201	PEB	C2B-C1B-CHA-C4A
29	jI	202	PEB	NB-C1B-CHA-C4A
29	jI	202	PEB	C2B-C1B-CHA-C4A
29	jI	202	PEB	C3B-CAB-CBB-CGB
29	kI	201	PEB	C1C-C2C-CAC-CBC
29	kI	201	PEB	C3C-C2C-CAC-CBC
29	kI	201	PEB	NB-C1B-CHA-C4A
29	kI	201	PEB	C2B-C1B-CHA-C4A
29	kI	202	PEB	C4A-C3A-CAA-CBA
29	kI	202	PEB	NB-C1B-CHA-C4A
29	kI	202	PEB	C2B-C1B-CHA-C4A
29	kI	203	PEB	ND-C1D-CHC-C4C
29	kI	203	PEB	NC-C1C-CHB-C4B
29	kI	203	PEB	C2C-C1C-CHB-C4B
29	kI	203	PEB	NB-C1B-CHA-C4A
29	kI	203	PEB	C2B-C1B-CHA-C4A
29	lI	201	PEB	NB-C1B-CHA-C4A
29	lI	201	PEB	C2B-C1B-CHA-C4A
29	lI	202	PEB	NB-C1B-CHA-C4A
29	lI	202	PEB	C2B-C1B-CHA-C4A
29	lI	202	PEB	C3B-CAB-CBB-CGB
29	mI	201	PEB	C1C-C2C-CAC-CBC
29	mI	201	PEB	C3C-C2C-CAC-CBC
29	mI	201	PEB	NB-C1B-CHA-C4A
29	mI	201	PEB	C2B-C1B-CHA-C4A
29	mI	202	PEB	C4A-C3A-CAA-CBA
29	mI	202	PEB	NB-C1B-CHA-C4A
29	mI	202	PEB	C2B-C1B-CHA-C4A
29	mI	203	PEB	ND-C1D-CHC-C4C
29	mI	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	mI	203	PEB	C2C-C1C-CHB-C4B
29	mI	203	PEB	NB-C1B-CHA-C4A
29	mI	203	PEB	C2B-C1B-CHA-C4A
29	AJ	201	PEB	C4A-C3A-CAA-CBA
29	AJ	201	PEB	NB-C1B-CHA-C4A
29	AJ	201	PEB	C2B-C1B-CHA-C4A
29	AJ	202	PEB	NC-C1C-CHB-C4B
29	AJ	202	PEB	C2C-C1C-CHB-C4B
29	AJ	202	PEB	C2C-CAC-CBC-CGC
29	AJ	202	PEB	C2A-C3A-CAA-CBA
29	AJ	202	PEB	NB-C1B-CHA-C4A
29	AJ	202	PEB	C2B-C1B-CHA-C4A
29	AJ	203	PEB	C2D-C3D-CAD-CBD
29	AJ	203	PEB	C4D-C3D-CAD-CBD
29	AJ	203	PEB	C4A-C3A-CAA-CBA
29	AJ	203	PEB	NB-C1B-CHA-C4A
29	AJ	203	PEB	C2B-C1B-CHA-C4A
29	BJ	201	PEB	NB-C1B-CHA-C4A
29	BJ	201	PEB	C2B-C1B-CHA-C4A
29	BJ	202	PEB	C2D-C3D-CAD-CBD
29	BJ	202	PEB	C4D-C3D-CAD-CBD
29	BJ	202	PEB	C4A-C3A-CAA-CBA
29	BJ	202	PEB	NB-C1B-CHA-C4A
29	BJ	202	PEB	C2B-C1B-CHA-C4A
29	BJ	203	PEB	ND-C1D-CHC-C4C
29	BJ	203	PEB	C2D-C1D-CHC-C4C
29	BJ	203	PEB	NC-C1C-CHB-C4B
29	BJ	203	PEB	C2C-C1C-CHB-C4B
29	BJ	203	PEB	C2A-C3A-CAA-CBA
29	BJ	203	PEB	C4A-C3A-CAA-CBA
29	BJ	203	PEB	NB-C1B-CHA-C4A
29	BJ	203	PEB	C2B-C1B-CHA-C4A
29	CJ	201	PEB	C4A-C3A-CAA-CBA
29	CJ	201	PEB	NB-C1B-CHA-C4A
29	CJ	201	PEB	C2B-C1B-CHA-C4A
29	CJ	202	PEB	NC-C1C-CHB-C4B
29	CJ	202	PEB	C2C-C1C-CHB-C4B
29	CJ	202	PEB	C2C-CAC-CBC-CGC
29	CJ	202	PEB	C2A-C3A-CAA-CBA
29	CJ	202	PEB	NB-C1B-CHA-C4A
29	CJ	202	PEB	C2B-C1B-CHA-C4A
29	DJ	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	DJ	201	PEB	C2B-C1B-CHA-C4A
29	DJ	202	PEB	ND-C1D-CHC-C4C
29	DJ	202	PEB	C2D-C1D-CHC-C4C
29	DJ	202	PEB	NC-C1C-CHB-C4B
29	DJ	202	PEB	C2C-C1C-CHB-C4B
29	DJ	202	PEB	C2A-C3A-CAA-CBA
29	DJ	202	PEB	C4A-C3A-CAA-CBA
29	DJ	202	PEB	NB-C1B-CHA-C4A
29	DJ	202	PEB	C2B-C1B-CHA-C4A
29	EJ	201	PEB	C4A-C3A-CAA-CBA
29	EJ	201	PEB	NB-C1B-CHA-C4A
29	EJ	201	PEB	C2B-C1B-CHA-C4A
29	EJ	202	PEB	NC-C1C-CHB-C4B
29	EJ	202	PEB	C2C-C1C-CHB-C4B
29	EJ	202	PEB	C2C-CAC-CBC-CGC
29	EJ	202	PEB	C2A-C3A-CAA-CBA
29	EJ	202	PEB	NB-C1B-CHA-C4A
29	EJ	202	PEB	C2B-C1B-CHA-C4A
29	FJ	201	PEB	NB-C1B-CHA-C4A
29	FJ	201	PEB	C2B-C1B-CHA-C4A
29	FJ	202	PEB	C2D-C3D-CAD-CBD
29	FJ	202	PEB	C4D-C3D-CAD-CBD
29	FJ	202	PEB	C4A-C3A-CAA-CBA
29	FJ	202	PEB	NB-C1B-CHA-C4A
29	FJ	202	PEB	C2B-C1B-CHA-C4A
29	FJ	203	PEB	ND-C1D-CHC-C4C
29	FJ	203	PEB	C2D-C1D-CHC-C4C
29	FJ	203	PEB	NC-C1C-CHB-C4B
29	FJ	203	PEB	C2C-C1C-CHB-C4B
29	FJ	203	PEB	C2A-C3A-CAA-CBA
29	FJ	203	PEB	C4A-C3A-CAA-CBA
29	FJ	203	PEB	NB-C1B-CHA-C4A
29	FJ	203	PEB	C2B-C1B-CHA-C4A
29	GJ	201	PEB	C4A-C3A-CAA-CBA
29	GJ	201	PEB	NB-C1B-CHA-C4A
29	GJ	201	PEB	C2B-C1B-CHA-C4A
29	GJ	202	PEB	NC-C1C-CHB-C4B
29	GJ	202	PEB	C2C-C1C-CHB-C4B
29	GJ	202	PEB	C2C-CAC-CBC-CGC
29	GJ	202	PEB	C2A-C3A-CAA-CBA
29	GJ	202	PEB	NB-C1B-CHA-C4A
29	GJ	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	HJ	201	PEB	C2D-C3D-CAD-CBD
29	HJ	201	PEB	C4D-C3D-CAD-CBD
29	HJ	201	PEB	C4A-C3A-CAA-CBA
29	HJ	201	PEB	NB-C1B-CHA-C4A
29	HJ	201	PEB	C2B-C1B-CHA-C4A
29	HJ	202	PEB	ND-C1D-CHC-C4C
29	HJ	202	PEB	C2D-C1D-CHC-C4C
29	HJ	202	PEB	NC-C1C-CHB-C4B
29	HJ	202	PEB	C2C-C1C-CHB-C4B
29	HJ	202	PEB	C2A-C3A-CAA-CBA
29	HJ	202	PEB	C4A-C3A-CAA-CBA
29	HJ	202	PEB	NB-C1B-CHA-C4A
29	HJ	202	PEB	C2B-C1B-CHA-C4A
29	IJ	201	PEB	C4A-C3A-CAA-CBA
29	IJ	201	PEB	NB-C1B-CHA-C4A
29	IJ	201	PEB	C2B-C1B-CHA-C4A
29	IJ	202	PEB	NC-C1C-CHB-C4B
29	IJ	202	PEB	C2C-C1C-CHB-C4B
29	IJ	202	PEB	C2C-CAC-CBC-CGC
29	IJ	202	PEB	C2A-C3A-CAA-CBA
29	IJ	202	PEB	NB-C1B-CHA-C4A
29	IJ	202	PEB	C2B-C1B-CHA-C4A
29	IJ	203	PEB	C2D-C3D-CAD-CBD
29	IJ	203	PEB	C4D-C3D-CAD-CBD
29	IJ	203	PEB	C4A-C3A-CAA-CBA
29	IJ	203	PEB	NB-C1B-CHA-C4A
29	IJ	203	PEB	C2B-C1B-CHA-C4A
29	JJ	201	PEB	NB-C1B-CHA-C4A
29	JJ	201	PEB	C2B-C1B-CHA-C4A
29	JJ	202	PEB	C2D-C3D-CAD-CBD
29	JJ	202	PEB	C4D-C3D-CAD-CBD
29	JJ	202	PEB	C4A-C3A-CAA-CBA
29	JJ	202	PEB	NB-C1B-CHA-C4A
29	JJ	202	PEB	C2B-C1B-CHA-C4A
29	JJ	203	PEB	ND-C1D-CHC-C4C
29	JJ	203	PEB	C2D-C1D-CHC-C4C
29	JJ	203	PEB	NC-C1C-CHB-C4B
29	JJ	203	PEB	C2C-C1C-CHB-C4B
29	JJ	203	PEB	C2A-C3A-CAA-CBA
29	JJ	203	PEB	C4A-C3A-CAA-CBA
29	JJ	203	PEB	NB-C1B-CHA-C4A
29	JJ	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	KJ	201	PEB	C4A-C3A-CAA-CBA
29	KJ	201	PEB	NB-C1B-CHA-C4A
29	KJ	201	PEB	C2B-C1B-CHA-C4A
29	KJ	202	PEB	NC-C1C-CHB-C4B
29	KJ	202	PEB	C2C-C1C-CHB-C4B
29	KJ	202	PEB	C2C-CAC-CBC-CGC
29	KJ	202	PEB	C2A-C3A-CAA-CBA
29	KJ	202	PEB	NB-C1B-CHA-C4A
29	KJ	202	PEB	C2B-C1B-CHA-C4A
29	LJ	201	PEB	NB-C1B-CHA-C4A
29	LJ	201	PEB	C2B-C1B-CHA-C4A
29	LJ	202	PEB	ND-C1D-CHC-C4C
29	LJ	202	PEB	C2D-C1D-CHC-C4C
29	LJ	202	PEB	NC-C1C-CHB-C4B
29	LJ	202	PEB	C2C-C1C-CHB-C4B
29	LJ	202	PEB	C2A-C3A-CAA-CBA
29	LJ	202	PEB	C4A-C3A-CAA-CBA
29	LJ	202	PEB	NB-C1B-CHA-C4A
29	LJ	202	PEB	C2B-C1B-CHA-C4A
29	MJ	201	PEB	C4A-C3A-CAA-CBA
29	MJ	201	PEB	NB-C1B-CHA-C4A
29	MJ	201	PEB	C2B-C1B-CHA-C4A
29	MJ	202	PEB	NC-C1C-CHB-C4B
29	MJ	202	PEB	C2C-C1C-CHB-C4B
29	MJ	202	PEB	C2C-CAC-CBC-CGC
29	MJ	202	PEB	C2A-C3A-CAA-CBA
29	MJ	202	PEB	NB-C1B-CHA-C4A
29	MJ	202	PEB	C2B-C1B-CHA-C4A
29	NJ	201	PEB	NB-C1B-CHA-C4A
29	NJ	201	PEB	C2B-C1B-CHA-C4A
29	NJ	202	PEB	C2D-C3D-CAD-CBD
29	NJ	202	PEB	C4D-C3D-CAD-CBD
29	NJ	202	PEB	C4A-C3A-CAA-CBA
29	NJ	202	PEB	NB-C1B-CHA-C4A
29	NJ	202	PEB	C2B-C1B-CHA-C4A
29	NJ	203	PEB	ND-C1D-CHC-C4C
29	NJ	203	PEB	C2D-C1D-CHC-C4C
29	NJ	203	PEB	NC-C1C-CHB-C4B
29	NJ	203	PEB	C2C-C1C-CHB-C4B
29	NJ	203	PEB	C2A-C3A-CAA-CBA
29	NJ	203	PEB	C4A-C3A-CAA-CBA
29	NJ	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	NJ	203	PEB	C2B-C1B-CHA-C4A
29	OJ	201	PEB	C4A-C3A-CAA-CBA
29	OJ	201	PEB	NB-C1B-CHA-C4A
29	OJ	201	PEB	C2B-C1B-CHA-C4A
29	OJ	202	PEB	NC-C1C-CHB-C4B
29	OJ	202	PEB	C2C-C1C-CHB-C4B
29	OJ	202	PEB	C2C-CAC-CBC-CGC
29	OJ	202	PEB	C2A-C3A-CAA-CBA
29	OJ	202	PEB	NB-C1B-CHA-C4A
29	OJ	202	PEB	C2B-C1B-CHA-C4A
29	PJ	201	PEB	NB-C1B-CHA-C4A
29	PJ	201	PEB	C2B-C1B-CHA-C4A
29	PJ	202	PEB	C2D-C3D-CAD-CBD
29	PJ	202	PEB	C4D-C3D-CAD-CBD
29	PJ	202	PEB	C4A-C3A-CAA-CBA
29	PJ	202	PEB	NB-C1B-CHA-C4A
29	PJ	202	PEB	C2B-C1B-CHA-C4A
29	PJ	203	PEB	ND-C1D-CHC-C4C
29	PJ	203	PEB	C2D-C1D-CHC-C4C
29	PJ	203	PEB	NC-C1C-CHB-C4B
29	PJ	203	PEB	C2C-C1C-CHB-C4B
29	PJ	203	PEB	C2A-C3A-CAA-CBA
29	PJ	203	PEB	C4A-C3A-CAA-CBA
29	PJ	203	PEB	NB-C1B-CHA-C4A
29	PJ	203	PEB	C2B-C1B-CHA-C4A
29	QJ	201	PEB	C4A-C3A-CAA-CBA
29	QJ	201	PEB	NB-C1B-CHA-C4A
29	QJ	201	PEB	C2B-C1B-CHA-C4A
29	QJ	202	PEB	NC-C1C-CHB-C4B
29	QJ	202	PEB	C2C-C1C-CHB-C4B
29	QJ	202	PEB	C2C-CAC-CBC-CGC
29	QJ	202	PEB	C2A-C3A-CAA-CBA
29	QJ	202	PEB	NB-C1B-CHA-C4A
29	QJ	202	PEB	C2B-C1B-CHA-C4A
29	RJ	201	PEB	NB-C1B-CHA-C4A
29	RJ	201	PEB	C2B-C1B-CHA-C4A
29	RJ	202	PEB	C2D-C3D-CAD-CBD
29	RJ	202	PEB	C4D-C3D-CAD-CBD
29	RJ	202	PEB	C4A-C3A-CAA-CBA
29	RJ	202	PEB	NB-C1B-CHA-C4A
29	RJ	202	PEB	C2B-C1B-CHA-C4A
29	RJ	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	RJ	203	PEB	C2D-C1D-CHC-C4C
29	RJ	203	PEB	NC-C1C-CHB-C4B
29	RJ	203	PEB	C2C-C1C-CHB-C4B
29	RJ	203	PEB	C2A-C3A-CAA-CBA
29	RJ	203	PEB	C4A-C3A-CAA-CBA
29	RJ	203	PEB	NB-C1B-CHA-C4A
29	RJ	203	PEB	C2B-C1B-CHA-C4A
29	SJ	201	PEB	C4A-C3A-CAA-CBA
29	SJ	201	PEB	NB-C1B-CHA-C4A
29	SJ	201	PEB	C2B-C1B-CHA-C4A
29	SJ	202	PEB	NC-C1C-CHB-C4B
29	SJ	202	PEB	C2C-C1C-CHB-C4B
29	SJ	202	PEB	C2C-CAC-CBC-CGC
29	SJ	202	PEB	C2A-C3A-CAA-CBA
29	SJ	202	PEB	NB-C1B-CHA-C4A
29	SJ	202	PEB	C2B-C1B-CHA-C4A
29	TJ	201	PEB	NB-C1B-CHA-C4A
29	TJ	201	PEB	C2B-C1B-CHA-C4A
29	TJ	202	PEB	C2D-C3D-CAD-CBD
29	TJ	202	PEB	C4D-C3D-CAD-CBD
29	TJ	202	PEB	C4A-C3A-CAA-CBA
29	TJ	202	PEB	NB-C1B-CHA-C4A
29	TJ	202	PEB	C2B-C1B-CHA-C4A
29	TJ	203	PEB	ND-C1D-CHC-C4C
29	TJ	203	PEB	C2D-C1D-CHC-C4C
29	TJ	203	PEB	NC-C1C-CHB-C4B
29	TJ	203	PEB	C2C-C1C-CHB-C4B
29	TJ	203	PEB	C2A-C3A-CAA-CBA
29	TJ	203	PEB	C4A-C3A-CAA-CBA
29	TJ	203	PEB	NB-C1B-CHA-C4A
29	TJ	203	PEB	C2B-C1B-CHA-C4A
29	UJ	201	PEB	C4A-C3A-CAA-CBA
29	UJ	201	PEB	NB-C1B-CHA-C4A
29	UJ	201	PEB	C2B-C1B-CHA-C4A
29	UJ	202	PEB	NC-C1C-CHB-C4B
29	UJ	202	PEB	C2C-C1C-CHB-C4B
29	UJ	202	PEB	C2C-CAC-CBC-CGC
29	UJ	202	PEB	C2A-C3A-CAA-CBA
29	UJ	202	PEB	NB-C1B-CHA-C4A
29	UJ	202	PEB	C2B-C1B-CHA-C4A
29	VJ	201	PEB	NB-C1B-CHA-C4A
29	VJ	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	VJ	202	PEB	ND-C1D-CHC-C4C
29	VJ	202	PEB	C2D-C1D-CHC-C4C
29	VJ	202	PEB	NC-C1C-CHB-C4B
29	VJ	202	PEB	C2C-C1C-CHB-C4B
29	VJ	202	PEB	C2A-C3A-CAA-CBA
29	VJ	202	PEB	C4A-C3A-CAA-CBA
29	VJ	202	PEB	NB-C1B-CHA-C4A
29	VJ	202	PEB	C2B-C1B-CHA-C4A
29	WJ	201	PEB	C2D-C3D-CAD-CBD
29	WJ	201	PEB	C4D-C3D-CAD-CBD
29	WJ	201	PEB	C4A-C3A-CAA-CBA
29	WJ	201	PEB	NB-C1B-CHA-C4A
29	WJ	201	PEB	C2B-C1B-CHA-C4A
29	WJ	202	PEB	C4A-C3A-CAA-CBA
29	WJ	202	PEB	NB-C1B-CHA-C4A
29	WJ	202	PEB	C2B-C1B-CHA-C4A
29	WJ	203	PEB	NC-C1C-CHB-C4B
29	WJ	203	PEB	C2C-C1C-CHB-C4B
29	WJ	203	PEB	C2C-CAC-CBC-CGC
29	WJ	203	PEB	C2A-C3A-CAA-CBA
29	WJ	203	PEB	NB-C1B-CHA-C4A
29	WJ	203	PEB	C2B-C1B-CHA-C4A
29	XJ	201	PEB	NB-C1B-CHA-C4A
29	XJ	201	PEB	C2B-C1B-CHA-C4A
29	XJ	202	PEB	C2D-C3D-CAD-CBD
29	XJ	202	PEB	C4D-C3D-CAD-CBD
29	XJ	202	PEB	C4A-C3A-CAA-CBA
29	XJ	202	PEB	NB-C1B-CHA-C4A
29	XJ	202	PEB	C2B-C1B-CHA-C4A
29	XJ	203	PEB	ND-C1D-CHC-C4C
29	XJ	203	PEB	C2D-C1D-CHC-C4C
29	XJ	203	PEB	NC-C1C-CHB-C4B
29	XJ	203	PEB	C2C-C1C-CHB-C4B
29	XJ	203	PEB	C2A-C3A-CAA-CBA
29	XJ	203	PEB	C4A-C3A-CAA-CBA
29	XJ	203	PEB	NB-C1B-CHA-C4A
29	XJ	203	PEB	C2B-C1B-CHA-C4A
29	YJ	201	PEB	C4A-C3A-CAA-CBA
29	YJ	201	PEB	NB-C1B-CHA-C4A
29	YJ	201	PEB	C2B-C1B-CHA-C4A
29	YJ	202	PEB	NC-C1C-CHB-C4B
29	YJ	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	YJ	202	PEB	C2C-CAC-CBC-CGC
29	YJ	202	PEB	C2A-C3A-CAA-CBA
29	YJ	202	PEB	NB-C1B-CHA-C4A
29	YJ	202	PEB	C2B-C1B-CHA-C4A
29	ZJ	201	PEB	NB-C1B-CHA-C4A
29	ZJ	201	PEB	C2B-C1B-CHA-C4A
29	ZJ	202	PEB	C2D-C3D-CAD-CBD
29	ZJ	202	PEB	C4D-C3D-CAD-CBD
29	ZJ	202	PEB	C4A-C3A-CAA-CBA
29	ZJ	202	PEB	NB-C1B-CHA-C4A
29	ZJ	202	PEB	C2B-C1B-CHA-C4A
29	ZJ	203	PEB	ND-C1D-CHC-C4C
29	ZJ	203	PEB	C2D-C1D-CHC-C4C
29	ZJ	203	PEB	NC-C1C-CHB-C4B
29	ZJ	203	PEB	C2C-C1C-CHB-C4B
29	ZJ	203	PEB	C2A-C3A-CAA-CBA
29	ZJ	203	PEB	C4A-C3A-CAA-CBA
29	ZJ	203	PEB	NB-C1B-CHA-C4A
29	ZJ	203	PEB	C2B-C1B-CHA-C4A
29	aJ	201	PEB	C4A-C3A-CAA-CBA
29	aJ	201	PEB	NB-C1B-CHA-C4A
29	aJ	201	PEB	C2B-C1B-CHA-C4A
29	aJ	202	PEB	NC-C1C-CHB-C4B
29	aJ	202	PEB	C2C-C1C-CHB-C4B
29	aJ	202	PEB	C2C-CAC-CBC-CGC
29	aJ	202	PEB	C2A-C3A-CAA-CBA
29	aJ	202	PEB	NB-C1B-CHA-C4A
29	aJ	202	PEB	C2B-C1B-CHA-C4A
29	bJ	201	PEB	NB-C1B-CHA-C4A
29	bJ	201	PEB	C2B-C1B-CHA-C4A
29	bJ	202	PEB	C2D-C3D-CAD-CBD
29	bJ	202	PEB	C4D-C3D-CAD-CBD
29	bJ	202	PEB	C4A-C3A-CAA-CBA
29	bJ	202	PEB	NB-C1B-CHA-C4A
29	bJ	202	PEB	C2B-C1B-CHA-C4A
29	bJ	203	PEB	ND-C1D-CHC-C4C
29	bJ	203	PEB	C2D-C1D-CHC-C4C
29	bJ	203	PEB	NC-C1C-CHB-C4B
29	bJ	203	PEB	C2C-C1C-CHB-C4B
29	bJ	203	PEB	C2A-C3A-CAA-CBA
29	bJ	203	PEB	C4A-C3A-CAA-CBA
29	bJ	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	bJ	203	PEB	C2B-C1B-CHA-C4A
29	cJ	201	PEB	C4A-C3A-CAA-CBA
29	cJ	201	PEB	NB-C1B-CHA-C4A
29	cJ	201	PEB	C2B-C1B-CHA-C4A
29	cJ	202	PEB	NC-C1C-CHB-C4B
29	cJ	202	PEB	C2C-C1C-CHB-C4B
29	cJ	202	PEB	C2C-CAC-CBC-CGC
29	cJ	202	PEB	C2A-C3A-CAA-CBA
29	cJ	202	PEB	NB-C1B-CHA-C4A
29	cJ	202	PEB	C2B-C1B-CHA-C4A
29	dJ	201	PEB	NB-C1B-CHA-C4A
29	dJ	201	PEB	C2B-C1B-CHA-C4A
29	dJ	202	PEB	C2D-C3D-CAD-CBD
29	dJ	202	PEB	C4D-C3D-CAD-CBD
29	dJ	202	PEB	C4A-C3A-CAA-CBA
29	dJ	202	PEB	NB-C1B-CHA-C4A
29	dJ	202	PEB	C2B-C1B-CHA-C4A
29	dJ	203	PEB	ND-C1D-CHC-C4C
29	dJ	203	PEB	C2D-C1D-CHC-C4C
29	dJ	203	PEB	NC-C1C-CHB-C4B
29	dJ	203	PEB	C2C-C1C-CHB-C4B
29	dJ	203	PEB	C2A-C3A-CAA-CBA
29	dJ	203	PEB	C4A-C3A-CAA-CBA
29	dJ	203	PEB	NB-C1B-CHA-C4A
29	dJ	203	PEB	C2B-C1B-CHA-C4A
29	eJ	201	PEB	C4A-C3A-CAA-CBA
29	eJ	201	PEB	NB-C1B-CHA-C4A
29	eJ	201	PEB	C2B-C1B-CHA-C4A
29	eJ	202	PEB	NC-C1C-CHB-C4B
29	eJ	202	PEB	C2C-C1C-CHB-C4B
29	eJ	202	PEB	C2C-CAC-CBC-CGC
29	eJ	202	PEB	C2A-C3A-CAA-CBA
29	eJ	202	PEB	NB-C1B-CHA-C4A
29	eJ	202	PEB	C2B-C1B-CHA-C4A
29	fJ	201	PEB	NB-C1B-CHA-C4A
29	fJ	201	PEB	C2B-C1B-CHA-C4A
29	fJ	202	PEB	C2D-C3D-CAD-CBD
29	fJ	202	PEB	C4D-C3D-CAD-CBD
29	fJ	202	PEB	C4A-C3A-CAA-CBA
29	fJ	202	PEB	NB-C1B-CHA-C4A
29	fJ	202	PEB	C2B-C1B-CHA-C4A
29	fJ	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	fJ	203	PEB	C2D-C1D-CHC-C4C
29	fJ	203	PEB	NC-C1C-CHB-C4B
29	fJ	203	PEB	C2C-C1C-CHB-C4B
29	fJ	203	PEB	C2A-C3A-CAA-CBA
29	fJ	203	PEB	C4A-C3A-CAA-CBA
29	fJ	203	PEB	NB-C1B-CHA-C4A
29	fJ	203	PEB	C2B-C1B-CHA-C4A
29	gJ	201	PEB	C4A-C3A-CAA-CBA
29	gJ	201	PEB	NB-C1B-CHA-C4A
29	gJ	201	PEB	C2B-C1B-CHA-C4A
29	gJ	202	PEB	NC-C1C-CHB-C4B
29	gJ	202	PEB	C2C-C1C-CHB-C4B
29	gJ	202	PEB	C2C-CAC-CBC-CGC
29	gJ	202	PEB	C2A-C3A-CAA-CBA
29	gJ	202	PEB	NB-C1B-CHA-C4A
29	gJ	202	PEB	C2B-C1B-CHA-C4A
29	hJ	201	PEB	NB-C1B-CHA-C4A
29	hJ	201	PEB	C2B-C1B-CHA-C4A
29	hJ	202	PEB	C2D-C3D-CAD-CBD
29	hJ	202	PEB	C4D-C3D-CAD-CBD
29	hJ	202	PEB	C4A-C3A-CAA-CBA
29	hJ	202	PEB	NB-C1B-CHA-C4A
29	hJ	202	PEB	C2B-C1B-CHA-C4A
29	hJ	203	PEB	ND-C1D-CHC-C4C
29	hJ	203	PEB	C2D-C1D-CHC-C4C
29	hJ	203	PEB	NC-C1C-CHB-C4B
29	hJ	203	PEB	C2C-C1C-CHB-C4B
29	hJ	203	PEB	C2A-C3A-CAA-CBA
29	hJ	203	PEB	C4A-C3A-CAA-CBA
29	hJ	203	PEB	NB-C1B-CHA-C4A
29	hJ	203	PEB	C2B-C1B-CHA-C4A
29	iJ	201	PEB	C4A-C3A-CAA-CBA
29	iJ	201	PEB	NB-C1B-CHA-C4A
29	iJ	201	PEB	C2B-C1B-CHA-C4A
29	iJ	202	PEB	NC-C1C-CHB-C4B
29	iJ	202	PEB	C2C-C1C-CHB-C4B
29	iJ	202	PEB	C2C-CAC-CBC-CGC
29	iJ	202	PEB	C2A-C3A-CAA-CBA
29	iJ	202	PEB	NB-C1B-CHA-C4A
29	iJ	202	PEB	C2B-C1B-CHA-C4A
29	jJ	201	PEB	NB-C1B-CHA-C4A
29	jJ	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	jJ	202	PEB	C2D-C3D-CAD-CBD
29	jJ	202	PEB	C4D-C3D-CAD-CBD
29	jJ	202	PEB	C4A-C3A-CAA-CBA
29	jJ	202	PEB	NB-C1B-CHA-C4A
29	jJ	202	PEB	C2B-C1B-CHA-C4A
29	jJ	203	PEB	ND-C1D-CHC-C4C
29	jJ	203	PEB	C2D-C1D-CHC-C4C
29	jJ	203	PEB	NC-C1C-CHB-C4B
29	jJ	203	PEB	C2C-C1C-CHB-C4B
29	jJ	203	PEB	C2A-C3A-CAA-CBA
29	jJ	203	PEB	C4A-C3A-CAA-CBA
29	jJ	203	PEB	NB-C1B-CHA-C4A
29	jJ	203	PEB	C2B-C1B-CHA-C4A
29	kJ	201	PEB	C4A-C3A-CAA-CBA
29	kJ	201	PEB	NB-C1B-CHA-C4A
29	kJ	201	PEB	C2B-C1B-CHA-C4A
29	kJ	202	PEB	NC-C1C-CHB-C4B
29	kJ	202	PEB	C2C-C1C-CHB-C4B
29	kJ	202	PEB	C2C-CAC-CBC-CGC
29	kJ	202	PEB	C2A-C3A-CAA-CBA
29	kJ	202	PEB	NB-C1B-CHA-C4A
29	kJ	202	PEB	C2B-C1B-CHA-C4A
29	lJ	201	PEB	NB-C1B-CHA-C4A
29	lJ	201	PEB	C2B-C1B-CHA-C4A
29	lJ	202	PEB	C2D-C3D-CAD-CBD
29	lJ	202	PEB	C4D-C3D-CAD-CBD
29	lJ	202	PEB	C4A-C3A-CAA-CBA
29	lJ	202	PEB	NB-C1B-CHA-C4A
29	lJ	202	PEB	C2B-C1B-CHA-C4A
29	lJ	203	PEB	ND-C1D-CHC-C4C
29	lJ	203	PEB	C2D-C1D-CHC-C4C
29	lJ	203	PEB	NC-C1C-CHB-C4B
29	lJ	203	PEB	C2C-C1C-CHB-C4B
29	lJ	203	PEB	C2A-C3A-CAA-CBA
29	lJ	203	PEB	C4A-C3A-CAA-CBA
29	lJ	203	PEB	NB-C1B-CHA-C4A
29	lJ	203	PEB	C2B-C1B-CHA-C4A
29	mJ	201	PEB	C4A-C3A-CAA-CBA
29	mJ	201	PEB	NB-C1B-CHA-C4A
29	mJ	201	PEB	C2B-C1B-CHA-C4A
29	mJ	202	PEB	NC-C1C-CHB-C4B
29	mJ	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	mJ	202	PEB	C2C-CAC-CBC-CGC
29	mJ	202	PEB	C2A-C3A-CAA-CBA
29	mJ	202	PEB	NB-C1B-CHA-C4A
29	mJ	202	PEB	C2B-C1B-CHA-C4A
29	nJ	201	PEB	NB-C1B-CHA-C4A
29	nJ	201	PEB	C2B-C1B-CHA-C4A
29	nJ	202	PEB	C2D-C3D-CAD-CBD
29	nJ	202	PEB	C4D-C3D-CAD-CBD
29	nJ	202	PEB	C4A-C3A-CAA-CBA
29	nJ	202	PEB	NB-C1B-CHA-C4A
29	nJ	202	PEB	C2B-C1B-CHA-C4A
29	nJ	203	PEB	ND-C1D-CHC-C4C
29	nJ	203	PEB	C2D-C1D-CHC-C4C
29	nJ	203	PEB	NC-C1C-CHB-C4B
29	nJ	203	PEB	C2C-C1C-CHB-C4B
29	nJ	203	PEB	C2A-C3A-CAA-CBA
29	nJ	203	PEB	C4A-C3A-CAA-CBA
29	nJ	203	PEB	NB-C1B-CHA-C4A
29	nJ	203	PEB	C2B-C1B-CHA-C4A
29	oJ	201	PEB	C4A-C3A-CAA-CBA
29	oJ	201	PEB	NB-C1B-CHA-C4A
29	oJ	201	PEB	C2B-C1B-CHA-C4A
29	oJ	202	PEB	NC-C1C-CHB-C4B
29	oJ	202	PEB	C2C-C1C-CHB-C4B
29	oJ	202	PEB	C2C-CAC-CBC-CGC
29	oJ	202	PEB	C2A-C3A-CAA-CBA
29	oJ	202	PEB	NB-C1B-CHA-C4A
29	oJ	202	PEB	C2B-C1B-CHA-C4A
29	pJ	201	PEB	NB-C1B-CHA-C4A
29	pJ	201	PEB	C2B-C1B-CHA-C4A
29	pJ	202	PEB	C2D-C3D-CAD-CBD
29	pJ	202	PEB	C4D-C3D-CAD-CBD
29	pJ	202	PEB	C4A-C3A-CAA-CBA
29	pJ	202	PEB	NB-C1B-CHA-C4A
29	pJ	202	PEB	C2B-C1B-CHA-C4A
29	pJ	203	PEB	ND-C1D-CHC-C4C
29	pJ	203	PEB	C2D-C1D-CHC-C4C
29	pJ	203	PEB	NC-C1C-CHB-C4B
29	pJ	203	PEB	C2C-C1C-CHB-C4B
29	pJ	203	PEB	C2A-C3A-CAA-CBA
29	pJ	203	PEB	C4A-C3A-CAA-CBA
29	pJ	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	pJ	203	PEB	C2B-C1B-CHA-C4A
29	qJ	201	PEB	C4A-C3A-CAA-CBA
29	qJ	201	PEB	NB-C1B-CHA-C4A
29	qJ	201	PEB	C2B-C1B-CHA-C4A
29	qJ	202	PEB	NC-C1C-CHB-C4B
29	qJ	202	PEB	C2C-C1C-CHB-C4B
29	qJ	202	PEB	C2C-CAC-CBC-CGC
29	qJ	202	PEB	C2A-C3A-CAA-CBA
29	qJ	202	PEB	NB-C1B-CHA-C4A
29	qJ	202	PEB	C2B-C1B-CHA-C4A
29	rJ	201	PEB	NB-C1B-CHA-C4A
29	rJ	201	PEB	C2B-C1B-CHA-C4A
29	rJ	202	PEB	C2D-C3D-CAD-CBD
29	rJ	202	PEB	C4D-C3D-CAD-CBD
29	rJ	202	PEB	C4A-C3A-CAA-CBA
29	rJ	202	PEB	NB-C1B-CHA-C4A
29	rJ	202	PEB	C2B-C1B-CHA-C4A
29	rJ	203	PEB	ND-C1D-CHC-C4C
29	rJ	203	PEB	C2D-C1D-CHC-C4C
29	rJ	203	PEB	NC-C1C-CHB-C4B
29	rJ	203	PEB	C2C-C1C-CHB-C4B
29	rJ	203	PEB	C2A-C3A-CAA-CBA
29	rJ	203	PEB	C4A-C3A-CAA-CBA
29	rJ	203	PEB	NB-C1B-CHA-C4A
29	rJ	203	PEB	C2B-C1B-CHA-C4A
29	sJ	201	PEB	C4A-C3A-CAA-CBA
29	sJ	201	PEB	NB-C1B-CHA-C4A
29	sJ	201	PEB	C2B-C1B-CHA-C4A
29	sJ	202	PEB	NC-C1C-CHB-C4B
29	sJ	202	PEB	C2C-C1C-CHB-C4B
29	sJ	202	PEB	C2C-CAC-CBC-CGC
29	sJ	202	PEB	C2A-C3A-CAA-CBA
29	sJ	202	PEB	NB-C1B-CHA-C4A
29	sJ	202	PEB	C2B-C1B-CHA-C4A
29	sJ	203	PEB	C2D-C3D-CAD-CBD
29	sJ	203	PEB	C4D-C3D-CAD-CBD
29	sJ	203	PEB	C4A-C3A-CAA-CBA
29	sJ	203	PEB	NB-C1B-CHA-C4A
29	sJ	203	PEB	C2B-C1B-CHA-C4A
29	tJ	201	PEB	NB-C1B-CHA-C4A
29	tJ	201	PEB	C2B-C1B-CHA-C4A
29	tJ	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	tJ	202	PEB	C2D-C1D-CHC-C4C
29	tJ	202	PEB	NC-C1C-CHB-C4B
29	tJ	202	PEB	C2C-C1C-CHB-C4B
29	tJ	202	PEB	C2A-C3A-CAA-CBA
29	tJ	202	PEB	C4A-C3A-CAA-CBA
29	tJ	202	PEB	NB-C1B-CHA-C4A
29	tJ	202	PEB	C2B-C1B-CHA-C4A
29	uJ	201	PEB	C2D-C3D-CAD-CBD
29	uJ	201	PEB	C4D-C3D-CAD-CBD
29	uJ	201	PEB	C4A-C3A-CAA-CBA
29	uJ	201	PEB	NB-C1B-CHA-C4A
29	uJ	201	PEB	C2B-C1B-CHA-C4A
29	uJ	202	PEB	C4A-C3A-CAA-CBA
29	uJ	202	PEB	NB-C1B-CHA-C4A
29	uJ	202	PEB	C2B-C1B-CHA-C4A
29	uJ	203	PEB	NC-C1C-CHB-C4B
29	uJ	203	PEB	C2C-C1C-CHB-C4B
29	uJ	203	PEB	C2C-CAC-CBC-CGC
29	uJ	203	PEB	C2A-C3A-CAA-CBA
29	uJ	203	PEB	NB-C1B-CHA-C4A
29	uJ	203	PEB	C2B-C1B-CHA-C4A
29	vJ	201	PEB	NB-C1B-CHA-C4A
29	vJ	201	PEB	C2B-C1B-CHA-C4A
29	vJ	202	PEB	ND-C1D-CHC-C4C
29	vJ	202	PEB	C2D-C1D-CHC-C4C
29	vJ	202	PEB	NC-C1C-CHB-C4B
29	vJ	202	PEB	C2C-C1C-CHB-C4B
29	vJ	202	PEB	C2A-C3A-CAA-CBA
29	vJ	202	PEB	C4A-C3A-CAA-CBA
29	vJ	202	PEB	NB-C1B-CHA-C4A
29	vJ	202	PEB	C2B-C1B-CHA-C4A
29	wJ	301	PEB	ND-C1D-CHC-C4C
29	wJ	301	PEB	C2C-CAC-CBC-CGC
29	wJ	301	PEB	C2A-C3A-CAA-CBA
29	wJ	301	PEB	C4A-C3A-CAA-CBA
29	wJ	301	PEB	NB-C1B-CHA-C4A
29	wJ	301	PEB	C2B-C1B-CHA-C4A
29	wJ	302	PEB	NB-C1B-CHA-C4A
29	wJ	302	PEB	C2B-C1B-CHA-C4A
29	wJ	303	PEB	NC-C1C-CHB-C4B
29	wJ	303	PEB	C2C-C1C-CHB-C4B
29	wJ	303	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	wJ	303	PEB	C2A-C3A-CAA-CBA
29	wJ	303	PEB	C4A-C3A-CAA-CBA
29	wJ	303	PEB	NB-C1B-CHA-C4A
29	wJ	303	PEB	C2B-C1B-CHA-C4A
29	wJ	303	PEB	C4B-C3B-CAB-CBB
29	xJ	301	PEB	ND-C1D-CHC-C4C
29	xJ	301	PEB	C2C-CAC-CBC-CGC
29	xJ	301	PEB	C2A-C3A-CAA-CBA
29	xJ	301	PEB	C4A-C3A-CAA-CBA
29	xJ	301	PEB	NB-C1B-CHA-C4A
29	xJ	301	PEB	C2B-C1B-CHA-C4A
29	xJ	302	PEB	NB-C1B-CHA-C4A
29	xJ	302	PEB	C2B-C1B-CHA-C4A
29	xJ	303	PEB	NC-C1C-CHB-C4B
29	xJ	303	PEB	C2C-C1C-CHB-C4B
29	xJ	303	PEB	C2C-CAC-CBC-CGC
29	xJ	303	PEB	C2A-C3A-CAA-CBA
29	xJ	303	PEB	C4A-C3A-CAA-CBA
29	xJ	303	PEB	NB-C1B-CHA-C4A
29	xJ	303	PEB	C2B-C1B-CHA-C4A
29	xJ	303	PEB	C4B-C3B-CAB-CBB
29	yJ	301	PEB	C2A-C3A-CAA-CBA
29	yJ	301	PEB	C4A-C3A-CAA-CBA
29	yJ	301	PEB	NB-C1B-CHA-C4A
29	yJ	301	PEB	C2B-C1B-CHA-C4A
29	zJ	501	PEB	C4A-C3A-CAA-CBA
29	zJ	501	PEB	NB-C1B-CHA-C4A
29	zJ	501	PEB	C2B-C1B-CHA-C4A
29	AK	301	PEB	NB-C1B-CHA-C4A
29	AK	301	PEB	C2B-C1B-CHA-C4A
29	AK	302	PEB	ND-C1D-CHC-C4C
29	AK	302	PEB	NB-C1B-CHA-C4A
29	AK	302	PEB	C2B-C1B-CHA-C4A
29	AK	303	PEB	C4A-C3A-CAA-CBA
29	AK	303	PEB	NB-C1B-CHA-C4A
29	AK	303	PEB	C2B-C1B-CHA-C4A
29	DK	1002	PEB	C2A-C3A-CAA-CBA
29	DK	1002	PEB	C4A-C3A-CAA-CBA
29	DK	1002	PEB	NB-C1B-CHA-C4A
29	DK	1002	PEB	C2B-C1B-CHA-C4A
29	FK	1002	PEB	C2A-C3A-CAA-CBA
29	FK	1002	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	FK	1002	PEB	NB-C1B-CHA-C4A
29	FK	1002	PEB	C2B-C1B-CHA-C4A
29	HK	1002	PEB	C2A-C3A-CAA-CBA
29	HK	1002	PEB	C4A-C3A-CAA-CBA
29	HK	1002	PEB	NB-C1B-CHA-C4A
29	HK	1002	PEB	C2B-C1B-CHA-C4A
29	JK	1002	PEB	C2A-C3A-CAA-CBA
29	JK	1002	PEB	C4A-C3A-CAA-CBA
29	JK	1002	PEB	NB-C1B-CHA-C4A
29	JK	1002	PEB	C2B-C1B-CHA-C4A
29	LK	1002	PEB	C2A-C3A-CAA-CBA
29	LK	1002	PEB	C4A-C3A-CAA-CBA
29	LK	1002	PEB	NB-C1B-CHA-C4A
29	LK	1002	PEB	C2B-C1B-CHA-C4A
29	NK	1002	PEB	C2A-C3A-CAA-CBA
29	NK	1002	PEB	C4A-C3A-CAA-CBA
29	NK	1002	PEB	NB-C1B-CHA-C4A
29	NK	1002	PEB	C2B-C1B-CHA-C4A
29	OK	201	PEB	ND-C1D-CHC-C4C
29	OK	201	PEB	NB-C1B-CHA-C4A
29	OK	201	PEB	C2B-C1B-CHA-C4A
29	OK	202	PEB	NB-C1B-CHA-C4A
29	OK	202	PEB	C2B-C1B-CHA-C4A
29	PK	201	PEB	NB-C1B-CHA-C4A
29	PK	201	PEB	C2B-C1B-CHA-C4A
29	PK	202	PEB	NB-C1B-CHA-C4A
29	PK	202	PEB	C2B-C1B-CHA-C4A
29	PK	203	PEB	NB-C1B-CHA-C4A
29	PK	203	PEB	C2B-C1B-CHA-C4A
29	QK	201	PEB	ND-C1D-CHC-C4C
29	QK	201	PEB	NB-C1B-CHA-C4A
29	QK	201	PEB	C2B-C1B-CHA-C4A
29	QK	202	PEB	NB-C1B-CHA-C4A
29	QK	202	PEB	C2B-C1B-CHA-C4A
29	RK	201	PEB	NB-C1B-CHA-C4A
29	RK	201	PEB	C2B-C1B-CHA-C4A
29	RK	202	PEB	NB-C1B-CHA-C4A
29	RK	202	PEB	C2B-C1B-CHA-C4A
29	RK	203	PEB	NB-C1B-CHA-C4A
29	RK	203	PEB	C2B-C1B-CHA-C4A
29	SK	201	PEB	ND-C1D-CHC-C4C
29	SK	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	SK	201	PEB	C2B-C1B-CHA-C4A
29	SK	202	PEB	NB-C1B-CHA-C4A
29	SK	202	PEB	C2B-C1B-CHA-C4A
29	TK	201	PEB	NB-C1B-CHA-C4A
29	TK	201	PEB	C2B-C1B-CHA-C4A
29	TK	202	PEB	NB-C1B-CHA-C4A
29	TK	202	PEB	C2B-C1B-CHA-C4A
29	UK	201	PEB	NB-C1B-CHA-C4A
29	UK	201	PEB	C2B-C1B-CHA-C4A
29	UK	202	PEB	ND-C1D-CHC-C4C
29	UK	202	PEB	NB-C1B-CHA-C4A
29	UK	202	PEB	C2B-C1B-CHA-C4A
29	UK	203	PEB	NB-C1B-CHA-C4A
29	UK	203	PEB	C2B-C1B-CHA-C4A
29	VK	201	PEB	NB-C1B-CHA-C4A
29	VK	201	PEB	C2B-C1B-CHA-C4A
29	VK	202	PEB	NB-C1B-CHA-C4A
29	VK	202	PEB	C2B-C1B-CHA-C4A
29	VK	203	PEB	NB-C1B-CHA-C4A
29	VK	203	PEB	C2B-C1B-CHA-C4A
29	WK	201	PEB	ND-C1D-CHC-C4C
29	WK	201	PEB	NB-C1B-CHA-C4A
29	WK	201	PEB	C2B-C1B-CHA-C4A
29	WK	202	PEB	NB-C1B-CHA-C4A
29	WK	202	PEB	C2B-C1B-CHA-C4A
29	YK	201	PEB	NB-C1B-CHA-C4A
29	YK	201	PEB	C2B-C1B-CHA-C4A
29	YK	202	PEB	NB-C1B-CHA-C4A
29	YK	202	PEB	C2B-C1B-CHA-C4A
29	ZK	201	PEB	NB-C1B-CHA-C4A
29	ZK	201	PEB	C2B-C1B-CHA-C4A
29	ZK	202	PEB	ND-C1D-CHC-C4C
29	ZK	202	PEB	NB-C1B-CHA-C4A
29	ZK	202	PEB	C2B-C1B-CHA-C4A
29	ZK	203	PEB	NB-C1B-CHA-C4A
29	ZK	203	PEB	C2B-C1B-CHA-C4A
29	aK	201	PEB	NB-C1B-CHA-C4A
29	aK	201	PEB	C2B-C1B-CHA-C4A
29	aK	202	PEB	NB-C1B-CHA-C4A
29	aK	202	PEB	C2B-C1B-CHA-C4A
29	aK	203	PEB	NB-C1B-CHA-C4A
29	aK	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	bK	201	PEB	ND-C1D-CHC-C4C
29	bK	201	PEB	NB-C1B-CHA-C4A
29	bK	201	PEB	C2B-C1B-CHA-C4A
29	bK	202	PEB	NB-C1B-CHA-C4A
29	bK	202	PEB	C2B-C1B-CHA-C4A
29	cK	201	PEB	NB-C1B-CHA-C4A
29	cK	201	PEB	C2B-C1B-CHA-C4A
29	cK	202	PEB	NB-C1B-CHA-C4A
29	cK	202	PEB	C2B-C1B-CHA-C4A
29	cK	203	PEB	NB-C1B-CHA-C4A
29	cK	203	PEB	C2B-C1B-CHA-C4A
29	dK	201	PEB	ND-C1D-CHC-C4C
29	dK	201	PEB	NB-C1B-CHA-C4A
29	dK	201	PEB	C2B-C1B-CHA-C4A
29	dK	202	PEB	NB-C1B-CHA-C4A
29	dK	202	PEB	C2B-C1B-CHA-C4A
29	eK	201	PEB	NB-C1B-CHA-C4A
29	eK	201	PEB	C2B-C1B-CHA-C4A
29	eK	202	PEB	NB-C1B-CHA-C4A
29	eK	202	PEB	C2B-C1B-CHA-C4A
29	eK	203	PEB	NB-C1B-CHA-C4A
29	eK	203	PEB	C2B-C1B-CHA-C4A
29	fK	201	PEB	ND-C1D-CHC-C4C
29	fK	201	PEB	NB-C1B-CHA-C4A
29	fK	201	PEB	C2B-C1B-CHA-C4A
29	fK	202	PEB	NB-C1B-CHA-C4A
29	fK	202	PEB	C2B-C1B-CHA-C4A
29	gK	201	PEB	NB-C1B-CHA-C4A
29	gK	201	PEB	C2B-C1B-CHA-C4A
29	gK	202	PEB	NB-C1B-CHA-C4A
29	gK	202	PEB	C2B-C1B-CHA-C4A
29	gK	203	PEB	NB-C1B-CHA-C4A
29	gK	203	PEB	C2B-C1B-CHA-C4A
29	hK	201	PEB	ND-C1D-CHC-C4C
29	hK	201	PEB	NB-C1B-CHA-C4A
29	hK	201	PEB	C2B-C1B-CHA-C4A
29	hK	202	PEB	NB-C1B-CHA-C4A
29	hK	202	PEB	C2B-C1B-CHA-C4A
29	iK	201	PEB	NB-C1B-CHA-C4A
29	iK	201	PEB	C2B-C1B-CHA-C4A
29	iK	202	PEB	NB-C1B-CHA-C4A
29	iK	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	iK	203	PEB	NB-C1B-CHA-C4A
29	iK	203	PEB	C2B-C1B-CHA-C4A
29	jK	201	PEB	ND-C1D-CHC-C4C
29	jK	201	PEB	NB-C1B-CHA-C4A
29	jK	201	PEB	C2B-C1B-CHA-C4A
29	jK	202	PEB	NB-C1B-CHA-C4A
29	jK	202	PEB	C2B-C1B-CHA-C4A
29	jK	203	PEB	NB-C1B-CHA-C4A
29	jK	203	PEB	C2B-C1B-CHA-C4A
29	kK	201	PEB	NB-C1B-CHA-C4A
29	kK	201	PEB	C2B-C1B-CHA-C4A
29	kK	202	PEB	NB-C1B-CHA-C4A
29	kK	202	PEB	C2B-C1B-CHA-C4A
29	kK	203	PEB	NB-C1B-CHA-C4A
29	kK	203	PEB	C2B-C1B-CHA-C4A
29	lK	201	PEB	ND-C1D-CHC-C4C
29	lK	201	PEB	NB-C1B-CHA-C4A
29	lK	201	PEB	C2B-C1B-CHA-C4A
29	lK	202	PEB	NB-C1B-CHA-C4A
29	lK	202	PEB	C2B-C1B-CHA-C4A
29	mK	201	PEB	NB-C1B-CHA-C4A
29	mK	201	PEB	C2B-C1B-CHA-C4A
29	mK	202	PEB	NB-C1B-CHA-C4A
29	mK	202	PEB	C2B-C1B-CHA-C4A
29	AL	201	PEB	C4A-C3A-CAA-CBA
29	AL	201	PEB	NB-C1B-CHA-C4A
29	AL	201	PEB	C2B-C1B-CHA-C4A
29	AL	202	PEB	NC-C1C-CHB-C4B
29	AL	202	PEB	C2C-C1C-CHB-C4B
29	AL	202	PEB	C2C-CAC-CBC-CGC
29	AL	202	PEB	C2A-C3A-CAA-CBA
29	AL	202	PEB	NB-C1B-CHA-C4A
29	AL	202	PEB	C2B-C1B-CHA-C4A
29	AL	203	PEB	C2D-C3D-CAD-CBD
29	AL	203	PEB	C4D-C3D-CAD-CBD
29	AL	203	PEB	C4A-C3A-CAA-CBA
29	AL	203	PEB	NB-C1B-CHA-C4A
29	AL	203	PEB	C2B-C1B-CHA-C4A
29	BL	201	PEB	NB-C1B-CHA-C4A
29	BL	201	PEB	C2B-C1B-CHA-C4A
29	BL	202	PEB	C2D-C3D-CAD-CBD
29	BL	202	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
29	BL	202	PEB	C4A-C3A-CAA-CBA
29	BL	202	PEB	NB-C1B-CHA-C4A
29	BL	202	PEB	C2B-C1B-CHA-C4A
29	BL	203	PEB	ND-C1D-CHC-C4C
29	BL	203	PEB	C2D-C1D-CHC-C4C
29	BL	203	PEB	NC-C1C-CHB-C4B
29	BL	203	PEB	C2C-C1C-CHB-C4B
29	BL	203	PEB	C2A-C3A-CAA-CBA
29	BL	203	PEB	C4A-C3A-CAA-CBA
29	BL	203	PEB	NB-C1B-CHA-C4A
29	BL	203	PEB	C2B-C1B-CHA-C4A
29	CL	201	PEB	C4A-C3A-CAA-CBA
29	CL	201	PEB	NB-C1B-CHA-C4A
29	CL	201	PEB	C2B-C1B-CHA-C4A
29	CL	202	PEB	NC-C1C-CHB-C4B
29	CL	202	PEB	C2C-C1C-CHB-C4B
29	CL	202	PEB	C2C-CAC-CBC-CGC
29	CL	202	PEB	C2A-C3A-CAA-CBA
29	CL	202	PEB	NB-C1B-CHA-C4A
29	CL	202	PEB	C2B-C1B-CHA-C4A
29	DL	201	PEB	NB-C1B-CHA-C4A
29	DL	201	PEB	C2B-C1B-CHA-C4A
29	DL	202	PEB	ND-C1D-CHC-C4C
29	DL	202	PEB	C2D-C1D-CHC-C4C
29	DL	202	PEB	NC-C1C-CHB-C4B
29	DL	202	PEB	C2C-C1C-CHB-C4B
29	DL	202	PEB	C2A-C3A-CAA-CBA
29	DL	202	PEB	C4A-C3A-CAA-CBA
29	DL	202	PEB	NB-C1B-CHA-C4A
29	DL	202	PEB	C2B-C1B-CHA-C4A
29	EL	201	PEB	C4A-C3A-CAA-CBA
29	EL	201	PEB	NB-C1B-CHA-C4A
29	EL	201	PEB	C2B-C1B-CHA-C4A
29	EL	202	PEB	NC-C1C-CHB-C4B
29	EL	202	PEB	C2C-C1C-CHB-C4B
29	EL	202	PEB	C2C-CAC-CBC-CGC
29	EL	202	PEB	C2A-C3A-CAA-CBA
29	EL	202	PEB	NB-C1B-CHA-C4A
29	EL	202	PEB	C2B-C1B-CHA-C4A
29	FL	201	PEB	NB-C1B-CHA-C4A
29	FL	201	PEB	C2B-C1B-CHA-C4A
29	FL	202	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
29	FL	202	PEB	C4D-C3D-CAD-CBD
29	FL	202	PEB	C4A-C3A-CAA-CBA
29	FL	202	PEB	NB-C1B-CHA-C4A
29	FL	202	PEB	C2B-C1B-CHA-C4A
29	FL	203	PEB	ND-C1D-CHC-C4C
29	FL	203	PEB	C2D-C1D-CHC-C4C
29	FL	203	PEB	NC-C1C-CHB-C4B
29	FL	203	PEB	C2C-C1C-CHB-C4B
29	FL	203	PEB	C2A-C3A-CAA-CBA
29	FL	203	PEB	C4A-C3A-CAA-CBA
29	FL	203	PEB	NB-C1B-CHA-C4A
29	FL	203	PEB	C2B-C1B-CHA-C4A
29	GL	201	PEB	C4A-C3A-CAA-CBA
29	GL	201	PEB	NB-C1B-CHA-C4A
29	GL	201	PEB	C2B-C1B-CHA-C4A
29	GL	202	PEB	NC-C1C-CHB-C4B
29	GL	202	PEB	C2C-C1C-CHB-C4B
29	GL	202	PEB	C2C-CAC-CBC-CGC
29	GL	202	PEB	C2A-C3A-CAA-CBA
29	GL	202	PEB	NB-C1B-CHA-C4A
29	GL	202	PEB	C2B-C1B-CHA-C4A
29	HL	201	PEB	C2D-C3D-CAD-CBD
29	HL	201	PEB	C4D-C3D-CAD-CBD
29	HL	201	PEB	C4A-C3A-CAA-CBA
29	HL	201	PEB	NB-C1B-CHA-C4A
29	HL	201	PEB	C2B-C1B-CHA-C4A
29	HL	202	PEB	ND-C1D-CHC-C4C
29	HL	202	PEB	C2D-C1D-CHC-C4C
29	HL	202	PEB	NC-C1C-CHB-C4B
29	HL	202	PEB	C2C-C1C-CHB-C4B
29	HL	202	PEB	C2A-C3A-CAA-CBA
29	HL	202	PEB	C4A-C3A-CAA-CBA
29	HL	202	PEB	NB-C1B-CHA-C4A
29	HL	202	PEB	C2B-C1B-CHA-C4A
29	IL	201	PEB	C4A-C3A-CAA-CBA
29	IL	201	PEB	NB-C1B-CHA-C4A
29	IL	201	PEB	C2B-C1B-CHA-C4A
29	IL	202	PEB	NC-C1C-CHB-C4B
29	IL	202	PEB	C2C-C1C-CHB-C4B
29	IL	202	PEB	C2C-CAC-CBC-CGC
29	IL	202	PEB	C2A-C3A-CAA-CBA
29	IL	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	IL	202	PEB	C2B-C1B-CHA-C4A
29	IL	203	PEB	C2D-C3D-CAD-CBD
29	IL	203	PEB	C4D-C3D-CAD-CBD
29	IL	203	PEB	C4A-C3A-CAA-CBA
29	IL	203	PEB	NB-C1B-CHA-C4A
29	IL	203	PEB	C2B-C1B-CHA-C4A
29	JL	201	PEB	NB-C1B-CHA-C4A
29	JL	201	PEB	C2B-C1B-CHA-C4A
29	JL	202	PEB	C2D-C3D-CAD-CBD
29	JL	202	PEB	C4D-C3D-CAD-CBD
29	JL	202	PEB	C4A-C3A-CAA-CBA
29	JL	202	PEB	NB-C1B-CHA-C4A
29	JL	202	PEB	C2B-C1B-CHA-C4A
29	JL	203	PEB	ND-C1D-CHC-C4C
29	JL	203	PEB	C2D-C1D-CHC-C4C
29	JL	203	PEB	NC-C1C-CHB-C4B
29	JL	203	PEB	C2C-C1C-CHB-C4B
29	JL	203	PEB	C2A-C3A-CAA-CBA
29	JL	203	PEB	C4A-C3A-CAA-CBA
29	JL	203	PEB	NB-C1B-CHA-C4A
29	JL	203	PEB	C2B-C1B-CHA-C4A
29	KL	201	PEB	C4A-C3A-CAA-CBA
29	KL	201	PEB	NB-C1B-CHA-C4A
29	KL	201	PEB	C2B-C1B-CHA-C4A
29	KL	202	PEB	NC-C1C-CHB-C4B
29	KL	202	PEB	C2C-C1C-CHB-C4B
29	KL	202	PEB	C2C-CAC-CBC-CGC
29	KL	202	PEB	C2A-C3A-CAA-CBA
29	KL	202	PEB	NB-C1B-CHA-C4A
29	KL	202	PEB	C2B-C1B-CHA-C4A
29	LL	201	PEB	NB-C1B-CHA-C4A
29	LL	201	PEB	C2B-C1B-CHA-C4A
29	LL	202	PEB	ND-C1D-CHC-C4C
29	LL	202	PEB	C2D-C1D-CHC-C4C
29	LL	202	PEB	NC-C1C-CHB-C4B
29	LL	202	PEB	C2C-C1C-CHB-C4B
29	LL	202	PEB	C2A-C3A-CAA-CBA
29	LL	202	PEB	C4A-C3A-CAA-CBA
29	LL	202	PEB	NB-C1B-CHA-C4A
29	LL	202	PEB	C2B-C1B-CHA-C4A
29	ML	201	PEB	C4A-C3A-CAA-CBA
29	ML	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	ML	201	PEB	C2B-C1B-CHA-C4A
29	ML	202	PEB	NC-C1C-CHB-C4B
29	ML	202	PEB	C2C-C1C-CHB-C4B
29	ML	202	PEB	C2C-CAC-CBC-CGC
29	ML	202	PEB	C2A-C3A-CAA-CBA
29	ML	202	PEB	NB-C1B-CHA-C4A
29	ML	202	PEB	C2B-C1B-CHA-C4A
29	NL	201	PEB	NB-C1B-CHA-C4A
29	NL	201	PEB	C2B-C1B-CHA-C4A
29	NL	202	PEB	C2D-C3D-CAD-CBD
29	NL	202	PEB	C4D-C3D-CAD-CBD
29	NL	202	PEB	C4A-C3A-CAA-CBA
29	NL	202	PEB	NB-C1B-CHA-C4A
29	NL	202	PEB	C2B-C1B-CHA-C4A
29	NL	203	PEB	ND-C1D-CHC-C4C
29	NL	203	PEB	C2D-C1D-CHC-C4C
29	NL	203	PEB	NC-C1C-CHB-C4B
29	NL	203	PEB	C2C-C1C-CHB-C4B
29	NL	203	PEB	C2A-C3A-CAA-CBA
29	NL	203	PEB	C4A-C3A-CAA-CBA
29	NL	203	PEB	NB-C1B-CHA-C4A
29	NL	203	PEB	C2B-C1B-CHA-C4A
29	OL	201	PEB	C4A-C3A-CAA-CBA
29	OL	201	PEB	NB-C1B-CHA-C4A
29	OL	201	PEB	C2B-C1B-CHA-C4A
29	OL	202	PEB	NC-C1C-CHB-C4B
29	OL	202	PEB	C2C-C1C-CHB-C4B
29	OL	202	PEB	C2C-CAC-CBC-CGC
29	OL	202	PEB	C2A-C3A-CAA-CBA
29	OL	202	PEB	NB-C1B-CHA-C4A
29	OL	202	PEB	C2B-C1B-CHA-C4A
29	PL	201	PEB	NB-C1B-CHA-C4A
29	PL	201	PEB	C2B-C1B-CHA-C4A
29	PL	202	PEB	C2D-C3D-CAD-CBD
29	PL	202	PEB	C4D-C3D-CAD-CBD
29	PL	202	PEB	C4A-C3A-CAA-CBA
29	PL	202	PEB	NB-C1B-CHA-C4A
29	PL	202	PEB	C2B-C1B-CHA-C4A
29	PL	203	PEB	ND-C1D-CHC-C4C
29	PL	203	PEB	C2D-C1D-CHC-C4C
29	PL	203	PEB	NC-C1C-CHB-C4B
29	PL	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	PL	203	PEB	C2A-C3A-CAA-CBA
29	PL	203	PEB	C4A-C3A-CAA-CBA
29	PL	203	PEB	NB-C1B-CHA-C4A
29	PL	203	PEB	C2B-C1B-CHA-C4A
29	QL	201	PEB	C4A-C3A-CAA-CBA
29	QL	201	PEB	NB-C1B-CHA-C4A
29	QL	201	PEB	C2B-C1B-CHA-C4A
29	QL	202	PEB	NC-C1C-CHB-C4B
29	QL	202	PEB	C2C-C1C-CHB-C4B
29	QL	202	PEB	C2C-CAC-CBC-CGC
29	QL	202	PEB	C2A-C3A-CAA-CBA
29	QL	202	PEB	NB-C1B-CHA-C4A
29	QL	202	PEB	C2B-C1B-CHA-C4A
29	RL	201	PEB	NB-C1B-CHA-C4A
29	RL	201	PEB	C2B-C1B-CHA-C4A
29	RL	202	PEB	C2D-C3D-CAD-CBD
29	RL	202	PEB	C4D-C3D-CAD-CBD
29	RL	202	PEB	C4A-C3A-CAA-CBA
29	RL	202	PEB	NB-C1B-CHA-C4A
29	RL	202	PEB	C2B-C1B-CHA-C4A
29	RL	203	PEB	ND-C1D-CHC-C4C
29	RL	203	PEB	C2D-C1D-CHC-C4C
29	RL	203	PEB	NC-C1C-CHB-C4B
29	RL	203	PEB	C2C-C1C-CHB-C4B
29	RL	203	PEB	C2A-C3A-CAA-CBA
29	RL	203	PEB	C4A-C3A-CAA-CBA
29	RL	203	PEB	NB-C1B-CHA-C4A
29	RL	203	PEB	C2B-C1B-CHA-C4A
29	SL	201	PEB	C4A-C3A-CAA-CBA
29	SL	201	PEB	NB-C1B-CHA-C4A
29	SL	201	PEB	C2B-C1B-CHA-C4A
29	SL	202	PEB	NC-C1C-CHB-C4B
29	SL	202	PEB	C2C-C1C-CHB-C4B
29	SL	202	PEB	C2C-CAC-CBC-CGC
29	SL	202	PEB	C2A-C3A-CAA-CBA
29	SL	202	PEB	NB-C1B-CHA-C4A
29	SL	202	PEB	C2B-C1B-CHA-C4A
29	TL	201	PEB	NB-C1B-CHA-C4A
29	TL	201	PEB	C2B-C1B-CHA-C4A
29	TL	202	PEB	C2D-C3D-CAD-CBD
29	TL	202	PEB	C4D-C3D-CAD-CBD
29	TL	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	TL	202	PEB	NB-C1B-CHA-C4A
29	TL	202	PEB	C2B-C1B-CHA-C4A
29	TL	203	PEB	ND-C1D-CHC-C4C
29	TL	203	PEB	C2D-C1D-CHC-C4C
29	TL	203	PEB	NC-C1C-CHB-C4B
29	TL	203	PEB	C2C-C1C-CHB-C4B
29	TL	203	PEB	C2A-C3A-CAA-CBA
29	TL	203	PEB	C4A-C3A-CAA-CBA
29	TL	203	PEB	NB-C1B-CHA-C4A
29	TL	203	PEB	C2B-C1B-CHA-C4A
29	UL	201	PEB	C4A-C3A-CAA-CBA
29	UL	201	PEB	NB-C1B-CHA-C4A
29	UL	201	PEB	C2B-C1B-CHA-C4A
29	UL	202	PEB	NC-C1C-CHB-C4B
29	UL	202	PEB	C2C-C1C-CHB-C4B
29	UL	202	PEB	C2C-CAC-CBC-CGC
29	UL	202	PEB	C2A-C3A-CAA-CBA
29	UL	202	PEB	NB-C1B-CHA-C4A
29	UL	202	PEB	C2B-C1B-CHA-C4A
29	VL	201	PEB	NB-C1B-CHA-C4A
29	VL	201	PEB	C2B-C1B-CHA-C4A
29	VL	202	PEB	ND-C1D-CHC-C4C
29	VL	202	PEB	C2D-C1D-CHC-C4C
29	VL	202	PEB	NC-C1C-CHB-C4B
29	VL	202	PEB	C2C-C1C-CHB-C4B
29	VL	202	PEB	C2A-C3A-CAA-CBA
29	VL	202	PEB	C4A-C3A-CAA-CBA
29	VL	202	PEB	NB-C1B-CHA-C4A
29	VL	202	PEB	C2B-C1B-CHA-C4A
29	WL	201	PEB	C2D-C3D-CAD-CBD
29	WL	201	PEB	C4D-C3D-CAD-CBD
29	WL	201	PEB	C4A-C3A-CAA-CBA
29	WL	201	PEB	NB-C1B-CHA-C4A
29	WL	201	PEB	C2B-C1B-CHA-C4A
29	WL	202	PEB	C4A-C3A-CAA-CBA
29	WL	202	PEB	NB-C1B-CHA-C4A
29	WL	202	PEB	C2B-C1B-CHA-C4A
29	WL	203	PEB	NC-C1C-CHB-C4B
29	WL	203	PEB	C2C-C1C-CHB-C4B
29	WL	203	PEB	C2C-CAC-CBC-CGC
29	WL	203	PEB	C2A-C3A-CAA-CBA
29	WL	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	WL	203	PEB	C2B-C1B-CHA-C4A
29	XL	201	PEB	NB-C1B-CHA-C4A
29	XL	201	PEB	C2B-C1B-CHA-C4A
29	XL	202	PEB	C2D-C3D-CAD-CBD
29	XL	202	PEB	C4D-C3D-CAD-CBD
29	XL	202	PEB	C4A-C3A-CAA-CBA
29	XL	202	PEB	NB-C1B-CHA-C4A
29	XL	202	PEB	C2B-C1B-CHA-C4A
29	XL	203	PEB	ND-C1D-CHC-C4C
29	XL	203	PEB	C2D-C1D-CHC-C4C
29	XL	203	PEB	NC-C1C-CHB-C4B
29	XL	203	PEB	C2C-C1C-CHB-C4B
29	XL	203	PEB	C2A-C3A-CAA-CBA
29	XL	203	PEB	C4A-C3A-CAA-CBA
29	XL	203	PEB	NB-C1B-CHA-C4A
29	XL	203	PEB	C2B-C1B-CHA-C4A
29	YL	201	PEB	C4A-C3A-CAA-CBA
29	YL	201	PEB	NB-C1B-CHA-C4A
29	YL	201	PEB	C2B-C1B-CHA-C4A
29	YL	202	PEB	NC-C1C-CHB-C4B
29	YL	202	PEB	C2C-C1C-CHB-C4B
29	YL	202	PEB	C2C-CAC-CBC-CGC
29	YL	202	PEB	C2A-C3A-CAA-CBA
29	YL	202	PEB	NB-C1B-CHA-C4A
29	YL	202	PEB	C2B-C1B-CHA-C4A
29	ZL	201	PEB	NB-C1B-CHA-C4A
29	ZL	201	PEB	C2B-C1B-CHA-C4A
29	ZL	202	PEB	C2D-C3D-CAD-CBD
29	ZL	202	PEB	C4D-C3D-CAD-CBD
29	ZL	202	PEB	C4A-C3A-CAA-CBA
29	ZL	202	PEB	NB-C1B-CHA-C4A
29	ZL	202	PEB	C2B-C1B-CHA-C4A
29	ZL	203	PEB	ND-C1D-CHC-C4C
29	ZL	203	PEB	C2D-C1D-CHC-C4C
29	ZL	203	PEB	NC-C1C-CHB-C4B
29	ZL	203	PEB	C2C-C1C-CHB-C4B
29	ZL	203	PEB	C2A-C3A-CAA-CBA
29	ZL	203	PEB	C4A-C3A-CAA-CBA
29	ZL	203	PEB	NB-C1B-CHA-C4A
29	ZL	203	PEB	C2B-C1B-CHA-C4A
29	aL	201	PEB	C4A-C3A-CAA-CBA
29	aL	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	aL	201	PEB	C2B-C1B-CHA-C4A
29	aL	202	PEB	NC-C1C-CHB-C4B
29	aL	202	PEB	C2C-C1C-CHB-C4B
29	aL	202	PEB	C2C-CAC-CBC-CGC
29	aL	202	PEB	C2A-C3A-CAA-CBA
29	aL	202	PEB	NB-C1B-CHA-C4A
29	aL	202	PEB	C2B-C1B-CHA-C4A
29	bL	201	PEB	NB-C1B-CHA-C4A
29	bL	201	PEB	C2B-C1B-CHA-C4A
29	bL	202	PEB	C2D-C3D-CAD-CBD
29	bL	202	PEB	C4D-C3D-CAD-CBD
29	bL	202	PEB	C4A-C3A-CAA-CBA
29	bL	202	PEB	NB-C1B-CHA-C4A
29	bL	202	PEB	C2B-C1B-CHA-C4A
29	bL	203	PEB	ND-C1D-CHC-C4C
29	bL	203	PEB	C2D-C1D-CHC-C4C
29	bL	203	PEB	NC-C1C-CHB-C4B
29	bL	203	PEB	C2C-C1C-CHB-C4B
29	bL	203	PEB	C2A-C3A-CAA-CBA
29	bL	203	PEB	C4A-C3A-CAA-CBA
29	bL	203	PEB	NB-C1B-CHA-C4A
29	bL	203	PEB	C2B-C1B-CHA-C4A
29	cL	201	PEB	C4A-C3A-CAA-CBA
29	cL	201	PEB	NB-C1B-CHA-C4A
29	cL	201	PEB	C2B-C1B-CHA-C4A
29	cL	202	PEB	NC-C1C-CHB-C4B
29	cL	202	PEB	C2C-C1C-CHB-C4B
29	cL	202	PEB	C2C-CAC-CBC-CGC
29	cL	202	PEB	C2A-C3A-CAA-CBA
29	cL	202	PEB	NB-C1B-CHA-C4A
29	cL	202	PEB	C2B-C1B-CHA-C4A
29	dL	201	PEB	NB-C1B-CHA-C4A
29	dL	201	PEB	C2B-C1B-CHA-C4A
29	dL	202	PEB	C2D-C3D-CAD-CBD
29	dL	202	PEB	C4D-C3D-CAD-CBD
29	dL	202	PEB	C4A-C3A-CAA-CBA
29	dL	202	PEB	NB-C1B-CHA-C4A
29	dL	202	PEB	C2B-C1B-CHA-C4A
29	dL	203	PEB	ND-C1D-CHC-C4C
29	dL	203	PEB	C2D-C1D-CHC-C4C
29	dL	203	PEB	NC-C1C-CHB-C4B
29	dL	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	dL	203	PEB	C2A-C3A-CAA-CBA
29	dL	203	PEB	C4A-C3A-CAA-CBA
29	dL	203	PEB	NB-C1B-CHA-C4A
29	dL	203	PEB	C2B-C1B-CHA-C4A
29	eL	201	PEB	C4A-C3A-CAA-CBA
29	eL	201	PEB	NB-C1B-CHA-C4A
29	eL	201	PEB	C2B-C1B-CHA-C4A
29	eL	202	PEB	NC-C1C-CHB-C4B
29	eL	202	PEB	C2C-C1C-CHB-C4B
29	eL	202	PEB	C2C-CAC-CBC-CGC
29	eL	202	PEB	C2A-C3A-CAA-CBA
29	eL	202	PEB	NB-C1B-CHA-C4A
29	eL	202	PEB	C2B-C1B-CHA-C4A
29	fL	201	PEB	NB-C1B-CHA-C4A
29	fL	201	PEB	C2B-C1B-CHA-C4A
29	fL	202	PEB	C2D-C3D-CAD-CBD
29	fL	202	PEB	C4D-C3D-CAD-CBD
29	fL	202	PEB	C4A-C3A-CAA-CBA
29	fL	202	PEB	NB-C1B-CHA-C4A
29	fL	202	PEB	C2B-C1B-CHA-C4A
29	fL	203	PEB	ND-C1D-CHC-C4C
29	fL	203	PEB	C2D-C1D-CHC-C4C
29	fL	203	PEB	NC-C1C-CHB-C4B
29	fL	203	PEB	C2C-C1C-CHB-C4B
29	fL	203	PEB	C2A-C3A-CAA-CBA
29	fL	203	PEB	C4A-C3A-CAA-CBA
29	fL	203	PEB	NB-C1B-CHA-C4A
29	fL	203	PEB	C2B-C1B-CHA-C4A
29	gL	201	PEB	C4A-C3A-CAA-CBA
29	gL	201	PEB	NB-C1B-CHA-C4A
29	gL	201	PEB	C2B-C1B-CHA-C4A
29	gL	202	PEB	NC-C1C-CHB-C4B
29	gL	202	PEB	C2C-C1C-CHB-C4B
29	gL	202	PEB	C2C-CAC-CBC-CGC
29	gL	202	PEB	C2A-C3A-CAA-CBA
29	gL	202	PEB	NB-C1B-CHA-C4A
29	gL	202	PEB	C2B-C1B-CHA-C4A
29	hL	201	PEB	NB-C1B-CHA-C4A
29	hL	201	PEB	C2B-C1B-CHA-C4A
29	hL	202	PEB	C2D-C3D-CAD-CBD
29	hL	202	PEB	C4D-C3D-CAD-CBD
29	hL	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	hL	202	PEB	NB-C1B-CHA-C4A
29	hL	202	PEB	C2B-C1B-CHA-C4A
29	hL	203	PEB	ND-C1D-CHC-C4C
29	hL	203	PEB	C2D-C1D-CHC-C4C
29	hL	203	PEB	NC-C1C-CHB-C4B
29	hL	203	PEB	C2C-C1C-CHB-C4B
29	hL	203	PEB	C2A-C3A-CAA-CBA
29	hL	203	PEB	C4A-C3A-CAA-CBA
29	hL	203	PEB	NB-C1B-CHA-C4A
29	hL	203	PEB	C2B-C1B-CHA-C4A
29	iL	201	PEB	C4A-C3A-CAA-CBA
29	iL	201	PEB	NB-C1B-CHA-C4A
29	iL	201	PEB	C2B-C1B-CHA-C4A
29	iL	202	PEB	NC-C1C-CHB-C4B
29	iL	202	PEB	C2C-C1C-CHB-C4B
29	iL	202	PEB	C2C-CAC-CBC-CGC
29	iL	202	PEB	C2A-C3A-CAA-CBA
29	iL	202	PEB	NB-C1B-CHA-C4A
29	iL	202	PEB	C2B-C1B-CHA-C4A
29	jL	201	PEB	NB-C1B-CHA-C4A
29	jL	201	PEB	C2B-C1B-CHA-C4A
29	jL	202	PEB	C2D-C3D-CAD-CBD
29	jL	202	PEB	C4D-C3D-CAD-CBD
29	jL	202	PEB	C4A-C3A-CAA-CBA
29	jL	202	PEB	NB-C1B-CHA-C4A
29	jL	202	PEB	C2B-C1B-CHA-C4A
29	jL	203	PEB	ND-C1D-CHC-C4C
29	jL	203	PEB	C2D-C1D-CHC-C4C
29	jL	203	PEB	NC-C1C-CHB-C4B
29	jL	203	PEB	C2C-C1C-CHB-C4B
29	jL	203	PEB	C2A-C3A-CAA-CBA
29	jL	203	PEB	C4A-C3A-CAA-CBA
29	jL	203	PEB	NB-C1B-CHA-C4A
29	jL	203	PEB	C2B-C1B-CHA-C4A
29	kL	201	PEB	C4A-C3A-CAA-CBA
29	kL	201	PEB	NB-C1B-CHA-C4A
29	kL	201	PEB	C2B-C1B-CHA-C4A
29	kL	202	PEB	NC-C1C-CHB-C4B
29	kL	202	PEB	C2C-C1C-CHB-C4B
29	kL	202	PEB	C2C-CAC-CBC-CGC
29	kL	202	PEB	C2A-C3A-CAA-CBA
29	kL	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	kL	202	PEB	C2B-C1B-CHA-C4A
29	lL	201	PEB	NB-C1B-CHA-C4A
29	lL	201	PEB	C2B-C1B-CHA-C4A
29	lL	202	PEB	C2D-C3D-CAD-CBD
29	lL	202	PEB	C4D-C3D-CAD-CBD
29	lL	202	PEB	C4A-C3A-CAA-CBA
29	lL	202	PEB	NB-C1B-CHA-C4A
29	lL	202	PEB	C2B-C1B-CHA-C4A
29	lL	203	PEB	ND-C1D-CHC-C4C
29	lL	203	PEB	C2D-C1D-CHC-C4C
29	lL	203	PEB	NC-C1C-CHB-C4B
29	lL	203	PEB	C2C-C1C-CHB-C4B
29	lL	203	PEB	C2A-C3A-CAA-CBA
29	lL	203	PEB	C4A-C3A-CAA-CBA
29	lL	203	PEB	NB-C1B-CHA-C4A
29	lL	203	PEB	C2B-C1B-CHA-C4A
29	mL	201	PEB	C4A-C3A-CAA-CBA
29	mL	201	PEB	NB-C1B-CHA-C4A
29	mL	201	PEB	C2B-C1B-CHA-C4A
29	mL	202	PEB	NC-C1C-CHB-C4B
29	mL	202	PEB	C2C-C1C-CHB-C4B
29	mL	202	PEB	C2C-CAC-CBC-CGC
29	mL	202	PEB	C2A-C3A-CAA-CBA
29	mL	202	PEB	NB-C1B-CHA-C4A
29	mL	202	PEB	C2B-C1B-CHA-C4A
29	nL	201	PEB	NB-C1B-CHA-C4A
29	nL	201	PEB	C2B-C1B-CHA-C4A
29	nL	202	PEB	C2D-C3D-CAD-CBD
29	nL	202	PEB	C4D-C3D-CAD-CBD
29	nL	202	PEB	C4A-C3A-CAA-CBA
29	nL	202	PEB	NB-C1B-CHA-C4A
29	nL	202	PEB	C2B-C1B-CHA-C4A
29	nL	203	PEB	ND-C1D-CHC-C4C
29	nL	203	PEB	C2D-C1D-CHC-C4C
29	nL	203	PEB	NC-C1C-CHB-C4B
29	nL	203	PEB	C2C-C1C-CHB-C4B
29	nL	203	PEB	C2A-C3A-CAA-CBA
29	nL	203	PEB	C4A-C3A-CAA-CBA
29	nL	203	PEB	NB-C1B-CHA-C4A
29	nL	203	PEB	C2B-C1B-CHA-C4A
29	oL	201	PEB	C4A-C3A-CAA-CBA
29	oL	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	oL	201	PEB	C2B-C1B-CHA-C4A
29	oL	202	PEB	NC-C1C-CHB-C4B
29	oL	202	PEB	C2C-C1C-CHB-C4B
29	oL	202	PEB	C2C-CAC-CBC-CGC
29	oL	202	PEB	C2A-C3A-CAA-CBA
29	oL	202	PEB	NB-C1B-CHA-C4A
29	oL	202	PEB	C2B-C1B-CHA-C4A
29	pL	201	PEB	NB-C1B-CHA-C4A
29	pL	201	PEB	C2B-C1B-CHA-C4A
29	pL	202	PEB	C2D-C3D-CAD-CBD
29	pL	202	PEB	C4D-C3D-CAD-CBD
29	pL	202	PEB	C4A-C3A-CAA-CBA
29	pL	202	PEB	NB-C1B-CHA-C4A
29	pL	202	PEB	C2B-C1B-CHA-C4A
29	pL	203	PEB	ND-C1D-CHC-C4C
29	pL	203	PEB	C2D-C1D-CHC-C4C
29	pL	203	PEB	NC-C1C-CHB-C4B
29	pL	203	PEB	C2C-C1C-CHB-C4B
29	pL	203	PEB	C2A-C3A-CAA-CBA
29	pL	203	PEB	C4A-C3A-CAA-CBA
29	pL	203	PEB	NB-C1B-CHA-C4A
29	pL	203	PEB	C2B-C1B-CHA-C4A
29	qL	201	PEB	C4A-C3A-CAA-CBA
29	qL	201	PEB	NB-C1B-CHA-C4A
29	qL	201	PEB	C2B-C1B-CHA-C4A
29	qL	202	PEB	NC-C1C-CHB-C4B
29	qL	202	PEB	C2C-C1C-CHB-C4B
29	qL	202	PEB	C2C-CAC-CBC-CGC
29	qL	202	PEB	C2A-C3A-CAA-CBA
29	qL	202	PEB	NB-C1B-CHA-C4A
29	qL	202	PEB	C2B-C1B-CHA-C4A
29	rL	201	PEB	NB-C1B-CHA-C4A
29	rL	201	PEB	C2B-C1B-CHA-C4A
29	rL	202	PEB	C2D-C3D-CAD-CBD
29	rL	202	PEB	C4D-C3D-CAD-CBD
29	rL	202	PEB	C4A-C3A-CAA-CBA
29	rL	202	PEB	NB-C1B-CHA-C4A
29	rL	202	PEB	C2B-C1B-CHA-C4A
29	rL	203	PEB	ND-C1D-CHC-C4C
29	rL	203	PEB	C2D-C1D-CHC-C4C
29	rL	203	PEB	NC-C1C-CHB-C4B
29	rL	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	rL	203	PEB	C2A-C3A-CAA-CBA
29	rL	203	PEB	C4A-C3A-CAA-CBA
29	rL	203	PEB	NB-C1B-CHA-C4A
29	rL	203	PEB	C2B-C1B-CHA-C4A
29	sL	201	PEB	C4A-C3A-CAA-CBA
29	sL	201	PEB	NB-C1B-CHA-C4A
29	sL	201	PEB	C2B-C1B-CHA-C4A
29	sL	202	PEB	NC-C1C-CHB-C4B
29	sL	202	PEB	C2C-C1C-CHB-C4B
29	sL	202	PEB	C2C-CAC-CBC-CGC
29	sL	202	PEB	C2A-C3A-CAA-CBA
29	sL	202	PEB	NB-C1B-CHA-C4A
29	sL	202	PEB	C2B-C1B-CHA-C4A
29	sL	203	PEB	C2D-C3D-CAD-CBD
29	sL	203	PEB	C4D-C3D-CAD-CBD
29	sL	203	PEB	C4A-C3A-CAA-CBA
29	sL	203	PEB	NB-C1B-CHA-C4A
29	sL	203	PEB	C2B-C1B-CHA-C4A
29	tL	201	PEB	NB-C1B-CHA-C4A
29	tL	201	PEB	C2B-C1B-CHA-C4A
29	tL	202	PEB	ND-C1D-CHC-C4C
29	tL	202	PEB	C2D-C1D-CHC-C4C
29	tL	202	PEB	NC-C1C-CHB-C4B
29	tL	202	PEB	C2C-C1C-CHB-C4B
29	tL	202	PEB	C2A-C3A-CAA-CBA
29	tL	202	PEB	C4A-C3A-CAA-CBA
29	tL	202	PEB	NB-C1B-CHA-C4A
29	tL	202	PEB	C2B-C1B-CHA-C4A
29	uL	201	PEB	C2D-C3D-CAD-CBD
29	uL	201	PEB	C4D-C3D-CAD-CBD
29	uL	201	PEB	C4A-C3A-CAA-CBA
29	uL	201	PEB	NB-C1B-CHA-C4A
29	uL	201	PEB	C2B-C1B-CHA-C4A
29	uL	202	PEB	C4A-C3A-CAA-CBA
29	uL	202	PEB	NB-C1B-CHA-C4A
29	uL	202	PEB	C2B-C1B-CHA-C4A
29	uL	203	PEB	NC-C1C-CHB-C4B
29	uL	203	PEB	C2C-C1C-CHB-C4B
29	uL	203	PEB	C2C-CAC-CBC-CGC
29	uL	203	PEB	C2A-C3A-CAA-CBA
29	uL	203	PEB	NB-C1B-CHA-C4A
29	uL	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	vL	201	PEB	NB-C1B-CHA-C4A
29	vL	201	PEB	C2B-C1B-CHA-C4A
29	vL	202	PEB	ND-C1D-CHC-C4C
29	vL	202	PEB	C2D-C1D-CHC-C4C
29	vL	202	PEB	NC-C1C-CHB-C4B
29	vL	202	PEB	C2C-C1C-CHB-C4B
29	vL	202	PEB	C2A-C3A-CAA-CBA
29	vL	202	PEB	C4A-C3A-CAA-CBA
29	vL	202	PEB	NB-C1B-CHA-C4A
29	vL	202	PEB	C2B-C1B-CHA-C4A
29	wL	301	PEB	ND-C1D-CHC-C4C
29	wL	301	PEB	C2C-CAC-CBC-CGC
29	wL	301	PEB	C2A-C3A-CAA-CBA
29	wL	301	PEB	C4A-C3A-CAA-CBA
29	wL	301	PEB	NB-C1B-CHA-C4A
29	wL	301	PEB	C2B-C1B-CHA-C4A
29	wL	302	PEB	NB-C1B-CHA-C4A
29	wL	302	PEB	C2B-C1B-CHA-C4A
29	wL	303	PEB	NC-C1C-CHB-C4B
29	wL	303	PEB	C2C-C1C-CHB-C4B
29	wL	303	PEB	C2C-CAC-CBC-CGC
29	wL	303	PEB	C2A-C3A-CAA-CBA
29	wL	303	PEB	C4A-C3A-CAA-CBA
29	wL	303	PEB	NB-C1B-CHA-C4A
29	wL	303	PEB	C2B-C1B-CHA-C4A
29	wL	303	PEB	C4B-C3B-CAB-CBB
29	xL	301	PEB	ND-C1D-CHC-C4C
29	xL	301	PEB	C2C-CAC-CBC-CGC
29	xL	301	PEB	C2A-C3A-CAA-CBA
29	xL	301	PEB	C4A-C3A-CAA-CBA
29	xL	301	PEB	NB-C1B-CHA-C4A
29	xL	301	PEB	C2B-C1B-CHA-C4A
29	xL	302	PEB	NB-C1B-CHA-C4A
29	xL	302	PEB	C2B-C1B-CHA-C4A
29	xL	303	PEB	NC-C1C-CHB-C4B
29	xL	303	PEB	C2C-C1C-CHB-C4B
29	xL	303	PEB	C2C-CAC-CBC-CGC
29	xL	303	PEB	C2A-C3A-CAA-CBA
29	xL	303	PEB	C4A-C3A-CAA-CBA
29	xL	303	PEB	NB-C1B-CHA-C4A
29	xL	303	PEB	C2B-C1B-CHA-C4A
29	xL	303	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	yL	301	PEB	C2A-C3A-CAA-CBA
29	yL	301	PEB	C4A-C3A-CAA-CBA
29	yL	301	PEB	NB-C1B-CHA-C4A
29	yL	301	PEB	C2B-C1B-CHA-C4A
29	zL	501	PEB	C4A-C3A-CAA-CBA
29	zL	501	PEB	NB-C1B-CHA-C4A
29	zL	501	PEB	C2B-C1B-CHA-C4A
29	AM	301	PEB	ND-C1D-CHC-C4C
29	AM	301	PEB	C2D-C1D-CHC-C4C
29	AM	301	PEB	NB-C1B-CHA-C4A
29	AM	301	PEB	C2B-C1B-CHA-C4A
29	AM	302	PEB	C2A-C3A-CAA-CBA
29	AM	302	PEB	C4A-C3A-CAA-CBA
29	AM	302	PEB	NB-C1B-CHA-C4A
29	AM	302	PEB	C2B-C1B-CHA-C4A
29	AM	303	PEB	NC-C1C-CHB-C4B
29	AM	303	PEB	C2C-C1C-CHB-C4B
29	AM	303	PEB	C4A-C3A-CAA-CBA
29	AM	303	PEB	NB-C1B-CHA-C4A
29	AM	303	PEB	C2B-C1B-CHA-C4A
29	BM	301	PEB	NC-C1C-CHB-C4B
29	BM	301	PEB	C1C-C2C-CAC-CBC
29	BM	301	PEB	C3C-C2C-CAC-CBC
29	BM	301	PEB	C4A-C3A-CAA-CBA
29	BM	301	PEB	NB-C1B-CHA-C4A
29	BM	301	PEB	C2B-C1B-CHA-C4A
29	CM	201	PEB	NB-C1B-CHA-C4A
29	CM	201	PEB	C2B-C1B-CHA-C4A
29	CM	202	PEB	NC-C1C-CHB-C4B
29	CM	202	PEB	C2C-C1C-CHB-C4B
29	CM	202	PEB	NB-C1B-CHA-C4A
29	CM	202	PEB	C2B-C1B-CHA-C4A
29	DM	201	PEB	ND-C1D-CHC-C4C
29	DM	201	PEB	C2D-C1D-CHC-C4C
29	DM	201	PEB	NB-C1B-CHA-C4A
29	DM	201	PEB	C2B-C1B-CHA-C4A
29	DM	202	PEB	C4A-C3A-CAA-CBA
29	DM	202	PEB	NB-C1B-CHA-C4A
29	DM	202	PEB	C2B-C1B-CHA-C4A
29	DM	203	PEB	ND-C1D-CHC-C4C
29	DM	203	PEB	C2D-C1D-CHC-C4C
29	DM	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	DM	203	PEB	C2C-C1C-CHB-C4B
29	DM	203	PEB	C2A-C3A-CAA-CBA
29	DM	203	PEB	C4A-C3A-CAA-CBA
29	DM	203	PEB	NB-C1B-CHA-C4A
29	DM	203	PEB	C2B-C1B-CHA-C4A
29	EM	201	PEB	NB-C1B-CHA-C4A
29	EM	201	PEB	C2B-C1B-CHA-C4A
29	EM	202	PEB	NC-C1C-CHB-C4B
29	EM	202	PEB	C2C-C1C-CHB-C4B
29	EM	202	PEB	NB-C1B-CHA-C4A
29	EM	202	PEB	C2B-C1B-CHA-C4A
29	FM	201	PEB	ND-C1D-CHC-C4C
29	FM	201	PEB	C2D-C1D-CHC-C4C
29	FM	201	PEB	NB-C1B-CHA-C4A
29	FM	201	PEB	C2B-C1B-CHA-C4A
29	FM	202	PEB	C4A-C3A-CAA-CBA
29	FM	202	PEB	NB-C1B-CHA-C4A
29	FM	202	PEB	C2B-C1B-CHA-C4A
29	FM	203	PEB	ND-C1D-CHC-C4C
29	FM	203	PEB	C2D-C1D-CHC-C4C
29	FM	203	PEB	NC-C1C-CHB-C4B
29	FM	203	PEB	C2C-C1C-CHB-C4B
29	FM	203	PEB	C2A-C3A-CAA-CBA
29	FM	203	PEB	C4A-C3A-CAA-CBA
29	FM	203	PEB	NB-C1B-CHA-C4A
29	FM	203	PEB	C2B-C1B-CHA-C4A
29	GM	201	PEB	NB-C1B-CHA-C4A
29	GM	201	PEB	C2B-C1B-CHA-C4A
29	GM	202	PEB	NC-C1C-CHB-C4B
29	GM	202	PEB	C2C-C1C-CHB-C4B
29	GM	202	PEB	NB-C1B-CHA-C4A
29	GM	202	PEB	C2B-C1B-CHA-C4A
29	HM	201	PEB	ND-C1D-CHC-C4C
29	HM	201	PEB	C2D-C1D-CHC-C4C
29	HM	201	PEB	NB-C1B-CHA-C4A
29	HM	201	PEB	C2B-C1B-CHA-C4A
29	HM	202	PEB	C4A-C3A-CAA-CBA
29	HM	202	PEB	NB-C1B-CHA-C4A
29	HM	202	PEB	C2B-C1B-CHA-C4A
29	HM	203	PEB	ND-C1D-CHC-C4C
29	HM	203	PEB	C2D-C1D-CHC-C4C
29	HM	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	HM	203	PEB	C2C-C1C-CHB-C4B
29	HM	203	PEB	C2A-C3A-CAA-CBA
29	HM	203	PEB	C4A-C3A-CAA-CBA
29	HM	203	PEB	NB-C1B-CHA-C4A
29	HM	203	PEB	C2B-C1B-CHA-C4A
29	IM	201	PEB	NB-C1B-CHA-C4A
29	IM	201	PEB	C2B-C1B-CHA-C4A
29	IM	202	PEB	NC-C1C-CHB-C4B
29	IM	202	PEB	C2C-C1C-CHB-C4B
29	IM	202	PEB	NB-C1B-CHA-C4A
29	IM	202	PEB	C2B-C1B-CHA-C4A
29	JM	201	PEB	ND-C1D-CHC-C4C
29	JM	201	PEB	C2D-C1D-CHC-C4C
29	JM	201	PEB	NB-C1B-CHA-C4A
29	JM	201	PEB	C2B-C1B-CHA-C4A
29	JM	202	PEB	C4A-C3A-CAA-CBA
29	JM	202	PEB	NB-C1B-CHA-C4A
29	JM	202	PEB	C2B-C1B-CHA-C4A
29	JM	203	PEB	ND-C1D-CHC-C4C
29	JM	203	PEB	C2D-C1D-CHC-C4C
29	JM	203	PEB	NC-C1C-CHB-C4B
29	JM	203	PEB	C2C-C1C-CHB-C4B
29	JM	203	PEB	C2A-C3A-CAA-CBA
29	JM	203	PEB	C4A-C3A-CAA-CBA
29	JM	203	PEB	NB-C1B-CHA-C4A
29	JM	203	PEB	C2B-C1B-CHA-C4A
29	KM	201	PEB	NB-C1B-CHA-C4A
29	KM	201	PEB	C2B-C1B-CHA-C4A
29	KM	202	PEB	NC-C1C-CHB-C4B
29	KM	202	PEB	C2C-C1C-CHB-C4B
29	KM	202	PEB	NB-C1B-CHA-C4A
29	KM	202	PEB	C2B-C1B-CHA-C4A
29	KM	203	PEB	C4A-C3A-CAA-CBA
29	KM	203	PEB	NB-C1B-CHA-C4A
29	KM	203	PEB	C2B-C1B-CHA-C4A
29	LM	201	PEB	ND-C1D-CHC-C4C
29	LM	201	PEB	C2D-C1D-CHC-C4C
29	LM	201	PEB	NB-C1B-CHA-C4A
29	LM	201	PEB	C2B-C1B-CHA-C4A
29	LM	202	PEB	C4A-C3A-CAA-CBA
29	LM	202	PEB	NB-C1B-CHA-C4A
29	LM	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	LM	203	PEB	ND-C1D-CHC-C4C
29	LM	203	PEB	C2D-C1D-CHC-C4C
29	LM	203	PEB	NC-C1C-CHB-C4B
29	LM	203	PEB	C2C-C1C-CHB-C4B
29	LM	203	PEB	C2A-C3A-CAA-CBA
29	LM	203	PEB	C4A-C3A-CAA-CBA
29	LM	203	PEB	NB-C1B-CHA-C4A
29	LM	203	PEB	C2B-C1B-CHA-C4A
29	MM	201	PEB	NB-C1B-CHA-C4A
29	MM	201	PEB	C2B-C1B-CHA-C4A
29	MM	202	PEB	NC-C1C-CHB-C4B
29	MM	202	PEB	C2C-C1C-CHB-C4B
29	MM	202	PEB	NB-C1B-CHA-C4A
29	MM	202	PEB	C2B-C1B-CHA-C4A
29	NM	201	PEB	ND-C1D-CHC-C4C
29	NM	201	PEB	C2D-C1D-CHC-C4C
29	NM	201	PEB	NB-C1B-CHA-C4A
29	NM	201	PEB	C2B-C1B-CHA-C4A
29	NM	202	PEB	ND-C1D-CHC-C4C
29	NM	202	PEB	C2D-C1D-CHC-C4C
29	NM	202	PEB	NC-C1C-CHB-C4B
29	NM	202	PEB	C2C-C1C-CHB-C4B
29	NM	202	PEB	C2A-C3A-CAA-CBA
29	NM	202	PEB	C4A-C3A-CAA-CBA
29	NM	202	PEB	NB-C1B-CHA-C4A
29	NM	202	PEB	C2B-C1B-CHA-C4A
29	OM	201	PEB	NB-C1B-CHA-C4A
29	OM	201	PEB	C2B-C1B-CHA-C4A
29	OM	202	PEB	NC-C1C-CHB-C4B
29	OM	202	PEB	C2C-C1C-CHB-C4B
29	OM	202	PEB	NB-C1B-CHA-C4A
29	OM	202	PEB	C2B-C1B-CHA-C4A
29	PM	201	PEB	ND-C1D-CHC-C4C
29	PM	201	PEB	C2D-C1D-CHC-C4C
29	PM	201	PEB	NB-C1B-CHA-C4A
29	PM	201	PEB	C2B-C1B-CHA-C4A
29	PM	202	PEB	ND-C1D-CHC-C4C
29	PM	202	PEB	C2D-C1D-CHC-C4C
29	PM	202	PEB	NC-C1C-CHB-C4B
29	PM	202	PEB	C2C-C1C-CHB-C4B
29	PM	202	PEB	C2A-C3A-CAA-CBA
29	PM	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	PM	202	PEB	NB-C1B-CHA-C4A
29	PM	202	PEB	C2B-C1B-CHA-C4A
29	QM	202	PEB	C4A-C3A-CAA-CBA
29	QM	202	PEB	NB-C1B-CHA-C4A
29	QM	202	PEB	C2B-C1B-CHA-C4A
29	QM	203	PEB	NB-C1B-CHA-C4A
29	QM	203	PEB	C2B-C1B-CHA-C4A
29	QM	204	PEB	NC-C1C-CHB-C4B
29	QM	204	PEB	C2C-C1C-CHB-C4B
29	QM	204	PEB	NB-C1B-CHA-C4A
29	QM	204	PEB	C2B-C1B-CHA-C4A
29	RM	201	PEB	ND-C1D-CHC-C4C
29	RM	201	PEB	C2D-C1D-CHC-C4C
29	RM	201	PEB	NB-C1B-CHA-C4A
29	RM	201	PEB	C2B-C1B-CHA-C4A
29	RM	202	PEB	C4A-C3A-CAA-CBA
29	RM	202	PEB	NB-C1B-CHA-C4A
29	RM	202	PEB	C2B-C1B-CHA-C4A
29	RM	203	PEB	ND-C1D-CHC-C4C
29	RM	203	PEB	C2D-C1D-CHC-C4C
29	RM	203	PEB	NC-C1C-CHB-C4B
29	RM	203	PEB	C2C-C1C-CHB-C4B
29	RM	203	PEB	C2A-C3A-CAA-CBA
29	RM	203	PEB	C4A-C3A-CAA-CBA
29	RM	203	PEB	NB-C1B-CHA-C4A
29	RM	203	PEB	C2B-C1B-CHA-C4A
29	SM	201	PEB	NB-C1B-CHA-C4A
29	SM	201	PEB	C2B-C1B-CHA-C4A
29	SM	202	PEB	NC-C1C-CHB-C4B
29	SM	202	PEB	C2C-C1C-CHB-C4B
29	SM	202	PEB	NB-C1B-CHA-C4A
29	SM	202	PEB	C2B-C1B-CHA-C4A
29	TM	201	PEB	ND-C1D-CHC-C4C
29	TM	201	PEB	C2D-C1D-CHC-C4C
29	TM	201	PEB	NB-C1B-CHA-C4A
29	TM	201	PEB	C2B-C1B-CHA-C4A
29	TM	202	PEB	C4A-C3A-CAA-CBA
29	TM	202	PEB	NB-C1B-CHA-C4A
29	TM	202	PEB	C2B-C1B-CHA-C4A
29	TM	203	PEB	ND-C1D-CHC-C4C
29	TM	203	PEB	C2D-C1D-CHC-C4C
29	TM	203	PEB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	TM	203	PEB	C2C-C1C-CHB-C4B
29	TM	203	PEB	C2A-C3A-CAA-CBA
29	TM	203	PEB	C4A-C3A-CAA-CBA
29	TM	203	PEB	NB-C1B-CHA-C4A
29	TM	203	PEB	C2B-C1B-CHA-C4A
29	UM	201	PEB	NB-C1B-CHA-C4A
29	UM	201	PEB	C2B-C1B-CHA-C4A
29	VM	201	PEB	ND-C1D-CHC-C4C
29	VM	201	PEB	C2D-C1D-CHC-C4C
29	VM	201	PEB	NB-C1B-CHA-C4A
29	VM	201	PEB	C2B-C1B-CHA-C4A
29	VM	202	PEB	C4A-C3A-CAA-CBA
29	VM	202	PEB	NB-C1B-CHA-C4A
29	VM	202	PEB	C2B-C1B-CHA-C4A
29	VM	203	PEB	ND-C1D-CHC-C4C
29	VM	203	PEB	C2D-C1D-CHC-C4C
29	VM	203	PEB	NC-C1C-CHB-C4B
29	VM	203	PEB	C2C-C1C-CHB-C4B
29	VM	203	PEB	C2A-C3A-CAA-CBA
29	VM	203	PEB	C4A-C3A-CAA-CBA
29	VM	203	PEB	NB-C1B-CHA-C4A
29	VM	203	PEB	C2B-C1B-CHA-C4A
29	WM	201	PEB	NB-C1B-CHA-C4A
29	WM	201	PEB	C2B-C1B-CHA-C4A
29	WM	202	PEB	NC-C1C-CHB-C4B
29	WM	202	PEB	C2C-C1C-CHB-C4B
29	WM	202	PEB	NB-C1B-CHA-C4A
29	WM	202	PEB	C2B-C1B-CHA-C4A
29	XM	201	PEB	ND-C1D-CHC-C4C
29	XM	201	PEB	C2D-C1D-CHC-C4C
29	XM	201	PEB	NB-C1B-CHA-C4A
29	XM	201	PEB	C2B-C1B-CHA-C4A
29	XM	202	PEB	ND-C1D-CHC-C4C
29	XM	202	PEB	C2D-C1D-CHC-C4C
29	XM	202	PEB	NC-C1C-CHB-C4B
29	XM	202	PEB	C2C-C1C-CHB-C4B
29	XM	202	PEB	C2A-C3A-CAA-CBA
29	XM	202	PEB	C4A-C3A-CAA-CBA
29	XM	202	PEB	NB-C1B-CHA-C4A
29	XM	202	PEB	C2B-C1B-CHA-C4A
29	YM	201	PEB	C4A-C3A-CAA-CBA
29	YM	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	YM	201	PEB	C2B-C1B-CHA-C4A
29	YM	202	PEB	NB-C1B-CHA-C4A
29	YM	202	PEB	C2B-C1B-CHA-C4A
29	YM	203	PEB	NC-C1C-CHB-C4B
29	YM	203	PEB	C2C-C1C-CHB-C4B
29	YM	203	PEB	NB-C1B-CHA-C4A
29	YM	203	PEB	C2B-C1B-CHA-C4A
29	ZM	201	PEB	ND-C1D-CHC-C4C
29	ZM	201	PEB	C2D-C1D-CHC-C4C
29	ZM	201	PEB	NB-C1B-CHA-C4A
29	ZM	201	PEB	C2B-C1B-CHA-C4A
29	ZM	202	PEB	C4A-C3A-CAA-CBA
29	ZM	202	PEB	NB-C1B-CHA-C4A
29	ZM	202	PEB	C2B-C1B-CHA-C4A
29	ZM	203	PEB	ND-C1D-CHC-C4C
29	ZM	203	PEB	C2D-C1D-CHC-C4C
29	ZM	203	PEB	NC-C1C-CHB-C4B
29	ZM	203	PEB	C2C-C1C-CHB-C4B
29	ZM	203	PEB	C2A-C3A-CAA-CBA
29	ZM	203	PEB	C4A-C3A-CAA-CBA
29	ZM	203	PEB	NB-C1B-CHA-C4A
29	ZM	203	PEB	C2B-C1B-CHA-C4A
29	aM	201	PEB	NB-C1B-CHA-C4A
29	aM	201	PEB	C2B-C1B-CHA-C4A
29	aM	202	PEB	NC-C1C-CHB-C4B
29	aM	202	PEB	C2C-C1C-CHB-C4B
29	aM	202	PEB	NB-C1B-CHA-C4A
29	aM	202	PEB	C2B-C1B-CHA-C4A
29	aM	203	PEB	C4A-C3A-CAA-CBA
29	aM	203	PEB	NB-C1B-CHA-C4A
29	aM	203	PEB	C2B-C1B-CHA-C4A
29	cM	201	PEB	ND-C1D-CHC-C4C
29	cM	201	PEB	C2D-C1D-CHC-C4C
29	cM	201	PEB	NB-C1B-CHA-C4A
29	cM	201	PEB	C2B-C1B-CHA-C4A
29	cM	202	PEB	C4A-C3A-CAA-CBA
29	cM	202	PEB	NB-C1B-CHA-C4A
29	cM	202	PEB	C2B-C1B-CHA-C4A
29	cM	203	PEB	ND-C1D-CHC-C4C
29	cM	203	PEB	C2D-C1D-CHC-C4C
29	cM	203	PEB	NC-C1C-CHB-C4B
29	cM	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	cM	203	PEB	C2A-C3A-CAA-CBA
29	cM	203	PEB	C4A-C3A-CAA-CBA
29	cM	203	PEB	NB-C1B-CHA-C4A
29	cM	203	PEB	C2B-C1B-CHA-C4A
29	dM	201	PEB	NB-C1B-CHA-C4A
29	dM	201	PEB	C2B-C1B-CHA-C4A
29	dM	202	PEB	NC-C1C-CHB-C4B
29	dM	202	PEB	C2C-C1C-CHB-C4B
29	dM	202	PEB	NB-C1B-CHA-C4A
29	dM	202	PEB	C2B-C1B-CHA-C4A
29	eM	201	PEB	ND-C1D-CHC-C4C
29	eM	201	PEB	C2D-C1D-CHC-C4C
29	eM	201	PEB	NB-C1B-CHA-C4A
29	eM	201	PEB	C2B-C1B-CHA-C4A
29	eM	202	PEB	ND-C1D-CHC-C4C
29	eM	202	PEB	C2D-C1D-CHC-C4C
29	eM	202	PEB	NC-C1C-CHB-C4B
29	eM	202	PEB	C2C-C1C-CHB-C4B
29	eM	202	PEB	C2A-C3A-CAA-CBA
29	eM	202	PEB	C4A-C3A-CAA-CBA
29	eM	202	PEB	NB-C1B-CHA-C4A
29	eM	202	PEB	C2B-C1B-CHA-C4A
29	fM	201	PEB	NB-C1B-CHA-C4A
29	fM	201	PEB	C2B-C1B-CHA-C4A
29	fM	202	PEB	NC-C1C-CHB-C4B
29	fM	202	PEB	C2C-C1C-CHB-C4B
29	fM	202	PEB	NB-C1B-CHA-C4A
29	fM	202	PEB	C2B-C1B-CHA-C4A
29	gM	201	PEB	ND-C1D-CHC-C4C
29	gM	201	PEB	C2D-C1D-CHC-C4C
29	gM	201	PEB	NB-C1B-CHA-C4A
29	gM	201	PEB	C2B-C1B-CHA-C4A
29	gM	202	PEB	C4A-C3A-CAA-CBA
29	gM	202	PEB	NB-C1B-CHA-C4A
29	gM	202	PEB	C2B-C1B-CHA-C4A
29	gM	203	PEB	ND-C1D-CHC-C4C
29	gM	203	PEB	C2D-C1D-CHC-C4C
29	gM	203	PEB	NC-C1C-CHB-C4B
29	gM	203	PEB	C2C-C1C-CHB-C4B
29	gM	203	PEB	C2A-C3A-CAA-CBA
29	gM	203	PEB	C4A-C3A-CAA-CBA
29	gM	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	gM	203	PEB	C2B-C1B-CHA-C4A
29	hM	201	PEB	NB-C1B-CHA-C4A
29	hM	201	PEB	C2B-C1B-CHA-C4A
29	hM	202	PEB	NC-C1C-CHB-C4B
29	hM	202	PEB	C2C-C1C-CHB-C4B
29	hM	202	PEB	NB-C1B-CHA-C4A
29	hM	202	PEB	C2B-C1B-CHA-C4A
29	iM	201	PEB	ND-C1D-CHC-C4C
29	iM	201	PEB	C2D-C1D-CHC-C4C
29	iM	201	PEB	NB-C1B-CHA-C4A
29	iM	201	PEB	C2B-C1B-CHA-C4A
29	iM	202	PEB	C4A-C3A-CAA-CBA
29	iM	202	PEB	NB-C1B-CHA-C4A
29	iM	202	PEB	C2B-C1B-CHA-C4A
29	iM	203	PEB	ND-C1D-CHC-C4C
29	iM	203	PEB	C2D-C1D-CHC-C4C
29	iM	203	PEB	NC-C1C-CHB-C4B
29	iM	203	PEB	C2C-C1C-CHB-C4B
29	iM	203	PEB	C2A-C3A-CAA-CBA
29	iM	203	PEB	C4A-C3A-CAA-CBA
29	iM	203	PEB	NB-C1B-CHA-C4A
29	iM	203	PEB	C2B-C1B-CHA-C4A
29	jM	201	PEB	NB-C1B-CHA-C4A
29	jM	201	PEB	C2B-C1B-CHA-C4A
29	jM	202	PEB	NC-C1C-CHB-C4B
29	jM	202	PEB	C2C-C1C-CHB-C4B
29	jM	202	PEB	NB-C1B-CHA-C4A
29	jM	202	PEB	C2B-C1B-CHA-C4A
29	kM	201	PEB	ND-C1D-CHC-C4C
29	kM	201	PEB	C2D-C1D-CHC-C4C
29	kM	201	PEB	NB-C1B-CHA-C4A
29	kM	201	PEB	C2B-C1B-CHA-C4A
29	kM	202	PEB	C4A-C3A-CAA-CBA
29	kM	202	PEB	NB-C1B-CHA-C4A
29	kM	202	PEB	C2B-C1B-CHA-C4A
29	kM	203	PEB	ND-C1D-CHC-C4C
29	kM	203	PEB	C2D-C1D-CHC-C4C
29	kM	203	PEB	NC-C1C-CHB-C4B
29	kM	203	PEB	C2C-C1C-CHB-C4B
29	kM	203	PEB	C2A-C3A-CAA-CBA
29	kM	203	PEB	C4A-C3A-CAA-CBA
29	kM	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	kM	203	PEB	C2B-C1B-CHA-C4A
29	lM	201	PEB	NB-C1B-CHA-C4A
29	lM	201	PEB	C2B-C1B-CHA-C4A
29	lM	202	PEB	NC-C1C-CHB-C4B
29	lM	202	PEB	C2C-C1C-CHB-C4B
29	lM	202	PEB	NB-C1B-CHA-C4A
29	lM	202	PEB	C2B-C1B-CHA-C4A
29	mM	201	PEB	ND-C1D-CHC-C4C
29	mM	201	PEB	C2D-C1D-CHC-C4C
29	mM	201	PEB	NB-C1B-CHA-C4A
29	mM	201	PEB	C2B-C1B-CHA-C4A
29	mM	202	PEB	C4A-C3A-CAA-CBA
29	mM	202	PEB	NB-C1B-CHA-C4A
29	mM	202	PEB	C2B-C1B-CHA-C4A
29	mM	203	PEB	ND-C1D-CHC-C4C
29	mM	203	PEB	C2D-C1D-CHC-C4C
29	mM	203	PEB	NC-C1C-CHB-C4B
29	mM	203	PEB	C2C-C1C-CHB-C4B
29	mM	203	PEB	C2A-C3A-CAA-CBA
29	mM	203	PEB	C4A-C3A-CAA-CBA
29	mM	203	PEB	NB-C1B-CHA-C4A
29	mM	203	PEB	C2B-C1B-CHA-C4A
29	AN	201	PEB	ND-C1D-CHC-C4C
29	AN	201	PEB	C4A-C3A-CAA-CBA
29	AN	201	PEB	NB-C1B-CHA-C4A
29	AN	201	PEB	C2B-C1B-CHA-C4A
29	AN	202	PEB	ND-C1D-CHC-C4C
29	AN	202	PEB	C2D-C1D-CHC-C4C
29	AN	202	PEB	NC-C1C-CHB-C4B
29	AN	202	PEB	C2C-C1C-CHB-C4B
29	AN	202	PEB	C4A-C3A-CAA-CBA
29	AN	202	PEB	NB-C1B-CHA-C4A
29	AN	202	PEB	C2B-C1B-CHA-C4A
29	AN	202	PEB	C3B-C4B-CHB-C1C
29	BN	201	PEB	ND-C1D-CHC-C4C
29	BN	201	PEB	C2D-C1D-CHC-C4C
29	BN	201	PEB	C2C-CAC-CBC-CGC
29	BN	201	PEB	NB-C1B-CHA-C4A
29	BN	201	PEB	C2B-C1B-CHA-C4A
29	BN	202	PEB	NC-C1C-CHB-C4B
29	BN	202	PEB	C2C-C1C-CHB-C4B
29	BN	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	BN	202	PEB	C4A-C3A-CAA-CBA
29	BN	202	PEB	NB-C1B-CHA-C4A
29	BN	202	PEB	C2B-C1B-CHA-C4A
29	BN	203	PEB	NC-C1C-CHB-C4B
29	BN	203	PEB	C2C-C1C-CHB-C4B
29	BN	203	PEB	C2A-C3A-CAA-CBA
29	BN	203	PEB	NB-C1B-CHA-C4A
29	BN	203	PEB	C2B-C1B-CHA-C4A
29	CN	201	PEB	ND-C1D-CHC-C4C
29	CN	201	PEB	C4A-C3A-CAA-CBA
29	CN	201	PEB	NB-C1B-CHA-C4A
29	CN	201	PEB	C2B-C1B-CHA-C4A
29	CN	202	PEB	ND-C1D-CHC-C4C
29	CN	202	PEB	C2D-C1D-CHC-C4C
29	CN	202	PEB	NC-C1C-CHB-C4B
29	CN	202	PEB	C2C-C1C-CHB-C4B
29	CN	202	PEB	C4A-C3A-CAA-CBA
29	CN	202	PEB	NB-C1B-CHA-C4A
29	CN	202	PEB	C2B-C1B-CHA-C4A
29	CN	202	PEB	C3B-C4B-CHB-C1C
29	DN	201	PEB	ND-C1D-CHC-C4C
29	DN	201	PEB	C2D-C1D-CHC-C4C
29	DN	201	PEB	C2C-CAC-CBC-CGC
29	DN	201	PEB	NB-C1B-CHA-C4A
29	DN	201	PEB	C2B-C1B-CHA-C4A
29	DN	202	PEB	NC-C1C-CHB-C4B
29	DN	202	PEB	C2C-C1C-CHB-C4B
29	DN	202	PEB	C2A-C3A-CAA-CBA
29	DN	202	PEB	C4A-C3A-CAA-CBA
29	DN	202	PEB	NB-C1B-CHA-C4A
29	DN	202	PEB	C2B-C1B-CHA-C4A
29	DN	203	PEB	NC-C1C-CHB-C4B
29	DN	203	PEB	C2C-C1C-CHB-C4B
29	DN	203	PEB	C2A-C3A-CAA-CBA
29	DN	203	PEB	NB-C1B-CHA-C4A
29	DN	203	PEB	C2B-C1B-CHA-C4A
29	EN	201	PEB	ND-C1D-CHC-C4C
29	EN	201	PEB	C4A-C3A-CAA-CBA
29	EN	201	PEB	NB-C1B-CHA-C4A
29	EN	201	PEB	C2B-C1B-CHA-C4A
29	EN	202	PEB	ND-C1D-CHC-C4C
29	EN	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	EN	202	PEB	NC-C1C-CHB-C4B
29	EN	202	PEB	C2C-C1C-CHB-C4B
29	EN	202	PEB	C4A-C3A-CAA-CBA
29	EN	202	PEB	NB-C1B-CHA-C4A
29	EN	202	PEB	C2B-C1B-CHA-C4A
29	EN	202	PEB	C3B-C4B-CHB-C1C
29	FN	201	PEB	ND-C1D-CHC-C4C
29	FN	201	PEB	C2D-C1D-CHC-C4C
29	FN	201	PEB	C2C-CAC-CBC-CGC
29	FN	201	PEB	NB-C1B-CHA-C4A
29	FN	201	PEB	C2B-C1B-CHA-C4A
29	FN	202	PEB	NC-C1C-CHB-C4B
29	FN	202	PEB	C2C-C1C-CHB-C4B
29	FN	202	PEB	C2A-C3A-CAA-CBA
29	FN	202	PEB	C4A-C3A-CAA-CBA
29	FN	202	PEB	NB-C1B-CHA-C4A
29	FN	202	PEB	C2B-C1B-CHA-C4A
29	FN	203	PEB	NC-C1C-CHB-C4B
29	FN	203	PEB	C2C-C1C-CHB-C4B
29	FN	203	PEB	C2A-C3A-CAA-CBA
29	FN	203	PEB	NB-C1B-CHA-C4A
29	FN	203	PEB	C2B-C1B-CHA-C4A
29	GN	201	PEB	ND-C1D-CHC-C4C
29	GN	201	PEB	C4A-C3A-CAA-CBA
29	GN	201	PEB	NB-C1B-CHA-C4A
29	GN	201	PEB	C2B-C1B-CHA-C4A
29	GN	202	PEB	ND-C1D-CHC-C4C
29	GN	202	PEB	C2D-C1D-CHC-C4C
29	GN	202	PEB	NC-C1C-CHB-C4B
29	GN	202	PEB	C2C-C1C-CHB-C4B
29	GN	202	PEB	C4A-C3A-CAA-CBA
29	GN	202	PEB	NB-C1B-CHA-C4A
29	GN	202	PEB	C2B-C1B-CHA-C4A
29	GN	202	PEB	C3B-C4B-CHB-C1C
29	HN	201	PEB	ND-C1D-CHC-C4C
29	HN	201	PEB	C2D-C1D-CHC-C4C
29	HN	201	PEB	C2C-CAC-CBC-CGC
29	HN	201	PEB	NB-C1B-CHA-C4A
29	HN	201	PEB	C2B-C1B-CHA-C4A
29	HN	202	PEB	NC-C1C-CHB-C4B
29	HN	202	PEB	C2C-C1C-CHB-C4B
29	HN	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	HN	202	PEB	C4A-C3A-CAA-CBA
29	HN	202	PEB	NB-C1B-CHA-C4A
29	HN	202	PEB	C2B-C1B-CHA-C4A
29	HN	203	PEB	NC-C1C-CHB-C4B
29	HN	203	PEB	C2C-C1C-CHB-C4B
29	HN	203	PEB	C2A-C3A-CAA-CBA
29	HN	203	PEB	NB-C1B-CHA-C4A
29	HN	203	PEB	C2B-C1B-CHA-C4A
29	IN	201	PEB	ND-C1D-CHC-C4C
29	IN	201	PEB	C4A-C3A-CAA-CBA
29	IN	201	PEB	NB-C1B-CHA-C4A
29	IN	201	PEB	C2B-C1B-CHA-C4A
29	IN	202	PEB	ND-C1D-CHC-C4C
29	IN	202	PEB	C2D-C1D-CHC-C4C
29	IN	202	PEB	NC-C1C-CHB-C4B
29	IN	202	PEB	C2C-C1C-CHB-C4B
29	IN	202	PEB	C4A-C3A-CAA-CBA
29	IN	202	PEB	NB-C1B-CHA-C4A
29	IN	202	PEB	C2B-C1B-CHA-C4A
29	IN	202	PEB	C3B-C4B-CHB-C1C
29	JN	201	PEB	ND-C1D-CHC-C4C
29	JN	201	PEB	C2D-C1D-CHC-C4C
29	JN	201	PEB	C2C-CAC-CBC-CGC
29	JN	201	PEB	NB-C1B-CHA-C4A
29	JN	201	PEB	C2B-C1B-CHA-C4A
29	JN	202	PEB	NC-C1C-CHB-C4B
29	JN	202	PEB	C2C-C1C-CHB-C4B
29	JN	202	PEB	C2A-C3A-CAA-CBA
29	JN	202	PEB	C4A-C3A-CAA-CBA
29	JN	202	PEB	NB-C1B-CHA-C4A
29	JN	202	PEB	C2B-C1B-CHA-C4A
29	JN	203	PEB	NC-C1C-CHB-C4B
29	JN	203	PEB	C2C-C1C-CHB-C4B
29	JN	203	PEB	C2A-C3A-CAA-CBA
29	JN	203	PEB	NB-C1B-CHA-C4A
29	JN	203	PEB	C2B-C1B-CHA-C4A
29	KN	201	PEB	ND-C1D-CHC-C4C
29	KN	201	PEB	C4A-C3A-CAA-CBA
29	KN	201	PEB	NB-C1B-CHA-C4A
29	KN	201	PEB	C2B-C1B-CHA-C4A
29	KN	202	PEB	ND-C1D-CHC-C4C
29	KN	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	KN	202	PEB	NC-C1C-CHB-C4B
29	KN	202	PEB	C2C-C1C-CHB-C4B
29	KN	202	PEB	C4A-C3A-CAA-CBA
29	KN	202	PEB	NB-C1B-CHA-C4A
29	KN	202	PEB	C2B-C1B-CHA-C4A
29	KN	202	PEB	C3B-C4B-CHB-C1C
29	LN	201	PEB	ND-C1D-CHC-C4C
29	LN	201	PEB	C2D-C1D-CHC-C4C
29	LN	201	PEB	C2C-CAC-CBC-CGC
29	LN	201	PEB	NB-C1B-CHA-C4A
29	LN	201	PEB	C2B-C1B-CHA-C4A
29	LN	202	PEB	NC-C1C-CHB-C4B
29	LN	202	PEB	C2C-C1C-CHB-C4B
29	LN	202	PEB	C2A-C3A-CAA-CBA
29	LN	202	PEB	C4A-C3A-CAA-CBA
29	LN	202	PEB	NB-C1B-CHA-C4A
29	LN	202	PEB	C2B-C1B-CHA-C4A
29	LN	203	PEB	NC-C1C-CHB-C4B
29	LN	203	PEB	C2C-C1C-CHB-C4B
29	LN	203	PEB	C2A-C3A-CAA-CBA
29	LN	203	PEB	NB-C1B-CHA-C4A
29	LN	203	PEB	C2B-C1B-CHA-C4A
29	MN	401	PEB	ND-C1D-CHC-C4C
29	MN	401	PEB	NC-C1C-CHB-C4B
29	MN	401	PEB	C2C-C1C-CHB-C4B
29	MN	401	PEB	C4A-C3A-CAA-CBA
29	MN	401	PEB	NB-C1B-CHA-C4A
29	MN	401	PEB	C2B-C1B-CHA-C4A
29	MN	404	PEB	ND-C1D-CHC-C4C
29	MN	404	PEB	C2D-C1D-CHC-C4C
29	MN	404	PEB	NC-C1C-CHB-C4B
29	MN	404	PEB	C2C-C1C-CHB-C4B
29	MN	404	PEB	NB-C1B-CHA-C4A
29	MN	404	PEB	C2B-C1B-CHA-C4A
29	MN	405	PEB	ND-C1D-CHC-C4C
29	MN	405	PEB	C2D-C1D-CHC-C4C
29	MN	405	PEB	C2C-CAC-CBC-CGC
29	AO	201	PEB	NB-C1B-CHA-C4A
29	AO	201	PEB	C2B-C1B-CHA-C4A
29	AO	202	PEB	C2C-CAC-CBC-CGC
29	AO	202	PEB	C2A-C3A-CAA-CBA
29	AO	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	AO	202	PEB	NB-C1B-CHA-C4A
29	AO	202	PEB	C2B-C1B-CHA-C4A
29	BO	201	PEB	NB-C1B-CHA-C4A
29	BO	201	PEB	C2B-C1B-CHA-C4A
29	BO	202	PEB	C2C-CAC-CBC-CGC
29	BO	202	PEB	C2A-C3A-CAA-CBA
29	BO	202	PEB	C4A-C3A-CAA-CBA
29	BO	202	PEB	NB-C1B-CHA-C4A
29	BO	202	PEB	C2B-C1B-CHA-C4A
29	BO	203	PEB	ND-C1D-CHC-C4C
29	BO	203	PEB	C2D-C1D-CHC-C4C
29	BO	203	PEB	NC-C1C-CHB-C4B
29	BO	203	PEB	C2C-C1C-CHB-C4B
29	BO	203	PEB	C2A-C3A-CAA-CBA
29	BO	203	PEB	C4A-C3A-CAA-CBA
29	BO	203	PEB	NB-C1B-CHA-C4A
29	BO	203	PEB	C2B-C1B-CHA-C4A
29	CO	201	PEB	NB-C1B-CHA-C4A
29	CO	201	PEB	C2B-C1B-CHA-C4A
29	CO	202	PEB	C2C-CAC-CBC-CGC
29	CO	202	PEB	C2A-C3A-CAA-CBA
29	CO	202	PEB	C4A-C3A-CAA-CBA
29	CO	202	PEB	NB-C1B-CHA-C4A
29	CO	202	PEB	C2B-C1B-CHA-C4A
29	DO	201	PEB	NB-C1B-CHA-C4A
29	DO	201	PEB	C2B-C1B-CHA-C4A
29	DO	202	PEB	C2A-C3A-CAA-CBA
29	DO	202	PEB	C4A-C3A-CAA-CBA
29	DO	202	PEB	NB-C1B-CHA-C4A
29	DO	202	PEB	C2B-C1B-CHA-C4A
29	DO	203	PEB	ND-C1D-CHC-C4C
29	DO	203	PEB	C2D-C1D-CHC-C4C
29	DO	203	PEB	NC-C1C-CHB-C4B
29	DO	203	PEB	C2C-C1C-CHB-C4B
29	DO	203	PEB	C2A-C3A-CAA-CBA
29	DO	203	PEB	C4A-C3A-CAA-CBA
29	DO	203	PEB	NB-C1B-CHA-C4A
29	DO	203	PEB	C2B-C1B-CHA-C4A
29	EO	201	PEB	NB-C1B-CHA-C4A
29	EO	201	PEB	C2B-C1B-CHA-C4A
29	EO	202	PEB	C2C-CAC-CBC-CGC
29	EO	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	EO	202	PEB	C4A-C3A-CAA-CBA
29	EO	202	PEB	NB-C1B-CHA-C4A
29	EO	202	PEB	C2B-C1B-CHA-C4A
29	FO	201	PEB	NB-C1B-CHA-C4A
29	FO	201	PEB	C2B-C1B-CHA-C4A
29	FO	202	PEB	C2C-CAC-CBC-CGC
29	FO	202	PEB	C2A-C3A-CAA-CBA
29	FO	202	PEB	C4A-C3A-CAA-CBA
29	FO	202	PEB	NB-C1B-CHA-C4A
29	FO	202	PEB	C2B-C1B-CHA-C4A
29	FO	203	PEB	ND-C1D-CHC-C4C
29	FO	203	PEB	C2D-C1D-CHC-C4C
29	FO	203	PEB	NC-C1C-CHB-C4B
29	FO	203	PEB	C2C-C1C-CHB-C4B
29	FO	203	PEB	C2A-C3A-CAA-CBA
29	FO	203	PEB	C4A-C3A-CAA-CBA
29	FO	203	PEB	NB-C1B-CHA-C4A
29	FO	203	PEB	C2B-C1B-CHA-C4A
29	GO	201	PEB	NB-C1B-CHA-C4A
29	GO	201	PEB	C2B-C1B-CHA-C4A
29	GO	202	PEB	C2C-CAC-CBC-CGC
29	GO	202	PEB	C2A-C3A-CAA-CBA
29	GO	202	PEB	C4A-C3A-CAA-CBA
29	GO	202	PEB	NB-C1B-CHA-C4A
29	GO	202	PEB	C2B-C1B-CHA-C4A
29	HO	201	PEB	NB-C1B-CHA-C4A
29	HO	201	PEB	C2B-C1B-CHA-C4A
29	HO	202	PEB	C2C-CAC-CBC-CGC
29	HO	202	PEB	C2A-C3A-CAA-CBA
29	HO	202	PEB	C4A-C3A-CAA-CBA
29	HO	202	PEB	NB-C1B-CHA-C4A
29	HO	202	PEB	C2B-C1B-CHA-C4A
29	HO	203	PEB	ND-C1D-CHC-C4C
29	HO	203	PEB	C2D-C1D-CHC-C4C
29	HO	203	PEB	NC-C1C-CHB-C4B
29	HO	203	PEB	C2C-C1C-CHB-C4B
29	HO	203	PEB	C2A-C3A-CAA-CBA
29	HO	203	PEB	C4A-C3A-CAA-CBA
29	HO	203	PEB	NB-C1B-CHA-C4A
29	HO	203	PEB	C2B-C1B-CHA-C4A
29	IO	201	PEB	NB-C1B-CHA-C4A
29	IO	201	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	IO	202	PEB	C2C-CAC-CBC-CGC
29	IO	202	PEB	C2A-C3A-CAA-CBA
29	IO	202	PEB	C4A-C3A-CAA-CBA
29	IO	202	PEB	NB-C1B-CHA-C4A
29	IO	202	PEB	C2B-C1B-CHA-C4A
29	IO	203	PEB	C2C-CAC-CBC-CGC
29	IO	203	PEB	C2A-C3A-CAA-CBA
29	IO	203	PEB	C4A-C3A-CAA-CBA
29	IO	203	PEB	NB-C1B-CHA-C4A
29	IO	203	PEB	C2B-C1B-CHA-C4A
29	JO	201	PEB	NB-C1B-CHA-C4A
29	JO	201	PEB	C2B-C1B-CHA-C4A
29	JO	202	PEB	C2C-CAC-CBC-CGC
29	JO	202	PEB	C2A-C3A-CAA-CBA
29	JO	202	PEB	C4A-C3A-CAA-CBA
29	JO	202	PEB	NB-C1B-CHA-C4A
29	JO	202	PEB	C2B-C1B-CHA-C4A
29	JO	203	PEB	ND-C1D-CHC-C4C
29	JO	203	PEB	C2D-C1D-CHC-C4C
29	JO	203	PEB	NC-C1C-CHB-C4B
29	JO	203	PEB	C2C-C1C-CHB-C4B
29	JO	203	PEB	C2A-C3A-CAA-CBA
29	JO	203	PEB	C4A-C3A-CAA-CBA
29	JO	203	PEB	NB-C1B-CHA-C4A
29	JO	203	PEB	C2B-C1B-CHA-C4A
29	KO	201	PEB	NB-C1B-CHA-C4A
29	KO	201	PEB	C2B-C1B-CHA-C4A
29	KO	202	PEB	C2C-CAC-CBC-CGC
29	KO	202	PEB	C2A-C3A-CAA-CBA
29	KO	202	PEB	C4A-C3A-CAA-CBA
29	KO	202	PEB	NB-C1B-CHA-C4A
29	KO	202	PEB	C2B-C1B-CHA-C4A
29	LO	201	PEB	NB-C1B-CHA-C4A
29	LO	201	PEB	C2B-C1B-CHA-C4A
29	LO	202	PEB	ND-C1D-CHC-C4C
29	LO	202	PEB	C2D-C1D-CHC-C4C
29	LO	202	PEB	NC-C1C-CHB-C4B
29	LO	202	PEB	C2C-C1C-CHB-C4B
29	LO	202	PEB	C2A-C3A-CAA-CBA
29	LO	202	PEB	C4A-C3A-CAA-CBA
29	LO	202	PEB	NB-C1B-CHA-C4A
29	LO	202	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	MO	201	PEB	NB-C1B-CHA-C4A
29	MO	201	PEB	C2B-C1B-CHA-C4A
29	MO	202	PEB	NB-C1B-CHA-C4A
29	MO	202	PEB	C2B-C1B-CHA-C4A
29	MO	203	PEB	ND-C1D-CHC-C4C
29	MO	203	PEB	C2D-C1D-CHC-C4C
29	MO	203	PEB	NC-C1C-CHB-C4B
29	MO	203	PEB	C2C-C1C-CHB-C4B
29	MO	203	PEB	NB-C1B-CHA-C4A
29	MO	203	PEB	C2B-C1B-CHA-C4A
29	NO	201	PEB	NB-C1B-CHA-C4A
29	NO	201	PEB	C2B-C1B-CHA-C4A
29	NO	202	PEB	NB-C1B-CHA-C4A
29	NO	202	PEB	C2B-C1B-CHA-C4A
29	NO	203	PEB	ND-C1D-CHC-C4C
29	NO	203	PEB	C2D-C1D-CHC-C4C
29	NO	203	PEB	NC-C1C-CHB-C4B
29	NO	203	PEB	C2C-C1C-CHB-C4B
29	NO	203	PEB	NB-C1B-CHA-C4A
29	NO	203	PEB	C2B-C1B-CHA-C4A
29	AQ	201	PEB	NB-C1B-CHA-C4A
29	AQ	201	PEB	C2B-C1B-CHA-C4A
29	AQ	202	PEB	NC-C1C-CHB-C4B
29	AQ	202	PEB	C2C-C1C-CHB-C4B
29	AQ	202	PEB	C2C-CAC-CBC-CGC
29	AQ	202	PEB	C4A-C3A-CAA-CBA
29	AQ	202	PEB	NB-C1B-CHA-C4A
29	AQ	202	PEB	C2B-C1B-CHA-C4A
29	BQ	201	PEB	ND-C1D-CHC-C4C
29	BQ	201	PEB	C2C-CAC-CBC-CGC
29	BQ	201	PEB	NB-C1B-CHA-C4A
29	BQ	201	PEB	C2B-C1B-CHA-C4A
29	BQ	202	PEB	C2A-C3A-CAA-CBA
29	BQ	202	PEB	C4A-C3A-CAA-CBA
29	BQ	202	PEB	NB-C1B-CHA-C4A
29	BQ	202	PEB	C2B-C1B-CHA-C4A
29	BQ	203	PEB	ND-C1D-CHC-C4C
29	BQ	203	PEB	C2D-C1D-CHC-C4C
29	BQ	203	PEB	NC-C1C-CHB-C4B
29	BQ	203	PEB	C2C-C1C-CHB-C4B
29	BQ	203	PEB	NB-C1B-CHA-C4A
29	BQ	203	PEB	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	CQ	201	PEB	NB-C1B-CHA-C4A
29	CQ	201	PEB	C2B-C1B-CHA-C4A
29	CQ	202	PEB	NC-C1C-CHB-C4B
29	CQ	202	PEB	C2C-C1C-CHB-C4B
29	CQ	202	PEB	C2C-CAC-CBC-CGC
29	CQ	202	PEB	C4A-C3A-CAA-CBA
29	CQ	202	PEB	NB-C1B-CHA-C4A
29	CQ	202	PEB	C2B-C1B-CHA-C4A
29	DQ	201	PEB	ND-C1D-CHC-C4C
29	DQ	201	PEB	C2C-CAC-CBC-CGC
29	DQ	201	PEB	NB-C1B-CHA-C4A
29	DQ	201	PEB	C2B-C1B-CHA-C4A
29	DQ	202	PEB	C2A-C3A-CAA-CBA
29	DQ	202	PEB	C4A-C3A-CAA-CBA
29	DQ	202	PEB	NB-C1B-CHA-C4A
29	DQ	202	PEB	C2B-C1B-CHA-C4A
29	DQ	203	PEB	ND-C1D-CHC-C4C
29	DQ	203	PEB	C2D-C1D-CHC-C4C
29	DQ	203	PEB	NC-C1C-CHB-C4B
29	DQ	203	PEB	C2C-C1C-CHB-C4B
29	DQ	203	PEB	NB-C1B-CHA-C4A
29	DQ	203	PEB	C2B-C1B-CHA-C4A
29	EQ	201	PEB	NB-C1B-CHA-C4A
29	EQ	201	PEB	C2B-C1B-CHA-C4A
29	EQ	202	PEB	NC-C1C-CHB-C4B
29	EQ	202	PEB	C2C-C1C-CHB-C4B
29	EQ	202	PEB	C2C-CAC-CBC-CGC
29	EQ	202	PEB	C4A-C3A-CAA-CBA
29	EQ	202	PEB	NB-C1B-CHA-C4A
29	EQ	202	PEB	C2B-C1B-CHA-C4A
29	FQ	201	PEB	ND-C1D-CHC-C4C
29	FQ	201	PEB	C2C-CAC-CBC-CGC
29	FQ	201	PEB	NB-C1B-CHA-C4A
29	FQ	201	PEB	C2B-C1B-CHA-C4A
29	FQ	202	PEB	C2A-C3A-CAA-CBA
29	FQ	202	PEB	C4A-C3A-CAA-CBA
29	FQ	202	PEB	NB-C1B-CHA-C4A
29	FQ	202	PEB	C2B-C1B-CHA-C4A
29	FQ	203	PEB	ND-C1D-CHC-C4C
29	FQ	203	PEB	C2D-C1D-CHC-C4C
29	FQ	203	PEB	NC-C1C-CHB-C4B
29	FQ	203	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	FQ	203	PEB	NB-C1B-CHA-C4A
29	FQ	203	PEB	C2B-C1B-CHA-C4A
29	GQ	201	PEB	NB-C1B-CHA-C4A
29	GQ	201	PEB	C2B-C1B-CHA-C4A
29	GQ	202	PEB	NC-C1C-CHB-C4B
29	GQ	202	PEB	C2C-C1C-CHB-C4B
29	GQ	202	PEB	C2C-CAC-CBC-CGC
29	GQ	202	PEB	C4A-C3A-CAA-CBA
29	GQ	202	PEB	NB-C1B-CHA-C4A
29	GQ	202	PEB	C2B-C1B-CHA-C4A
29	HQ	201	PEB	ND-C1D-CHC-C4C
29	HQ	201	PEB	C2C-CAC-CBC-CGC
29	HQ	201	PEB	NB-C1B-CHA-C4A
29	HQ	201	PEB	C2B-C1B-CHA-C4A
29	HQ	202	PEB	C2A-C3A-CAA-CBA
29	HQ	202	PEB	C4A-C3A-CAA-CBA
29	HQ	202	PEB	NB-C1B-CHA-C4A
29	HQ	202	PEB	C2B-C1B-CHA-C4A
29	HQ	203	PEB	ND-C1D-CHC-C4C
29	HQ	203	PEB	C2D-C1D-CHC-C4C
29	HQ	203	PEB	NC-C1C-CHB-C4B
29	HQ	203	PEB	C2C-C1C-CHB-C4B
29	HQ	203	PEB	NB-C1B-CHA-C4A
29	HQ	203	PEB	C2B-C1B-CHA-C4A
29	IQ	201	PEB	NB-C1B-CHA-C4A
29	IQ	201	PEB	C2B-C1B-CHA-C4A
29	IQ	202	PEB	NC-C1C-CHB-C4B
29	IQ	202	PEB	C2C-C1C-CHB-C4B
29	IQ	202	PEB	C2C-CAC-CBC-CGC
29	IQ	202	PEB	C4A-C3A-CAA-CBA
29	IQ	202	PEB	NB-C1B-CHA-C4A
29	IQ	202	PEB	C2B-C1B-CHA-C4A
29	JQ	201	PEB	ND-C1D-CHC-C4C
29	JQ	201	PEB	C2C-CAC-CBC-CGC
29	JQ	201	PEB	NB-C1B-CHA-C4A
29	JQ	201	PEB	C2B-C1B-CHA-C4A
29	JQ	202	PEB	C2A-C3A-CAA-CBA
29	JQ	202	PEB	C4A-C3A-CAA-CBA
29	JQ	202	PEB	NB-C1B-CHA-C4A
29	JQ	202	PEB	C2B-C1B-CHA-C4A
29	JQ	203	PEB	ND-C1D-CHC-C4C
29	JQ	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	JQ	203	PEB	NC-C1C-CHB-C4B
29	JQ	203	PEB	C2C-C1C-CHB-C4B
29	JQ	203	PEB	NB-C1B-CHA-C4A
29	JQ	203	PEB	C2B-C1B-CHA-C4A
29	KQ	201	PEB	NB-C1B-CHA-C4A
29	KQ	201	PEB	C2B-C1B-CHA-C4A
29	KQ	202	PEB	NC-C1C-CHB-C4B
29	KQ	202	PEB	C2C-C1C-CHB-C4B
29	KQ	202	PEB	C2C-CAC-CBC-CGC
29	KQ	202	PEB	C4A-C3A-CAA-CBA
29	KQ	202	PEB	NB-C1B-CHA-C4A
29	KQ	202	PEB	C2B-C1B-CHA-C4A
29	LQ	201	PEB	C2A-C3A-CAA-CBA
29	LQ	201	PEB	C4A-C3A-CAA-CBA
29	LQ	201	PEB	NB-C1B-CHA-C4A
29	LQ	201	PEB	C2B-C1B-CHA-C4A
29	LQ	202	PEB	ND-C1D-CHC-C4C
29	LQ	202	PEB	C2D-C1D-CHC-C4C
29	LQ	202	PEB	NC-C1C-CHB-C4B
29	LQ	202	PEB	C2C-C1C-CHB-C4B
29	LQ	202	PEB	NB-C1B-CHA-C4A
29	LQ	202	PEB	C2B-C1B-CHA-C4A
29	MQ	401	PEB	NC-C1C-CHB-C4B
29	MQ	401	PEB	C2C-C1C-CHB-C4B
29	MQ	401	PEB	NB-C1B-CHA-C4A
29	MQ	401	PEB	C2B-C1B-CHA-C4A
29	MQ	402	PEB	ND-C1D-CHC-C4C
29	MQ	402	PEB	C2C-CAC-CBC-CGC
29	MQ	402	PEB	NB-C1B-CHA-C4A
29	MQ	402	PEB	C2B-C1B-CHA-C4A
29	MQ	403	PEB	C2A-C3A-CAA-CBA
29	MQ	403	PEB	C4A-C3A-CAA-CBA
29	MQ	403	PEB	NB-C1B-CHA-C4A
29	MQ	403	PEB	C2B-C1B-CHA-C4A
29	MQ	406	PEB	ND-C1D-CHC-C4C
29	MQ	406	PEB	NC-C1C-CHB-C4B
29	MQ	406	PEB	C2C-C1C-CHB-C4B
29	MQ	406	PEB	NB-C1B-CHA-C4A
29	MQ	406	PEB	C2B-C1B-CHA-C4A
29	MQ	407	PEB	NC-C1C-CHB-C4B
29	MQ	407	PEB	C2C-C1C-CHB-C4B
29	MQ	407	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	MQ	407	PEB	C2B-C1B-CHA-C4A
29	eR	401	PEB	C1C-C2C-CAC-CBC
29	eR	401	PEB	C3C-C2C-CAC-CBC
29	eR	401	PEB	C2C-CAC-CBC-CGC
29	eR	401	PEB	C4A-C3A-CAA-CBA
29	eR	401	PEB	NB-C1B-CHA-C4A
29	eR	401	PEB	C2B-C1B-CHA-C4A
29	MR	201	PEB	C2A-C3A-CAA-CBA
29	MR	201	PEB	C4A-C3A-CAA-CBA
29	MR	201	PEB	NB-C1B-CHA-C4A
29	MR	201	PEB	C2B-C1B-CHA-C4A
29	MR	202	PEB	NB-C1B-CHA-C4A
29	MR	202	PEB	C2B-C1B-CHA-C4A
29	NR	201	PEB	NB-C1B-CHA-C4A
29	NR	201	PEB	C2B-C1B-CHA-C4A
29	NR	201	PEB	C2B-C3B-CAB-CBB
29	NR	201	PEB	C4B-C3B-CAB-CBB
29	NR	202	PEB	C2A-C3A-CAA-CBA
29	NR	202	PEB	C4A-C3A-CAA-CBA
29	NR	202	PEB	NB-C1B-CHA-C4A
29	NR	202	PEB	C2B-C1B-CHA-C4A
29	NR	203	PEB	ND-C1D-CHC-C4C
29	NR	203	PEB	C2D-C1D-CHC-C4C
29	NR	203	PEB	NC-C1C-CHB-C4B
29	NR	203	PEB	C2C-C1C-CHB-C4B
29	NR	203	PEB	C2A-C3A-CAA-CBA
29	NR	203	PEB	NB-C1B-CHA-C4A
29	NR	203	PEB	C2B-C1B-CHA-C4A
29	OR	201	PEB	C2A-C3A-CAA-CBA
29	OR	201	PEB	C4A-C3A-CAA-CBA
29	OR	201	PEB	NB-C1B-CHA-C4A
29	OR	201	PEB	C2B-C1B-CHA-C4A
29	OR	202	PEB	NB-C1B-CHA-C4A
29	OR	202	PEB	C2B-C1B-CHA-C4A
29	PR	201	PEB	C2A-C3A-CAA-CBA
29	PR	201	PEB	C4A-C3A-CAA-CBA
29	PR	201	PEB	NB-C1B-CHA-C4A
29	PR	201	PEB	C2B-C1B-CHA-C4A
29	PR	202	PEB	ND-C1D-CHC-C4C
29	PR	202	PEB	C2D-C1D-CHC-C4C
29	PR	202	PEB	NC-C1C-CHB-C4B
29	PR	202	PEB	C2C-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
29	PR	202	PEB	C2A-C3A-CAA-CBA
29	PR	202	PEB	NB-C1B-CHA-C4A
29	PR	202	PEB	C2B-C1B-CHA-C4A
29	QR	201	PEB	C2A-C3A-CAA-CBA
29	QR	201	PEB	C4A-C3A-CAA-CBA
29	QR	201	PEB	NB-C1B-CHA-C4A
29	QR	201	PEB	C2B-C1B-CHA-C4A
29	QR	202	PEB	NB-C1B-CHA-C4A
29	QR	202	PEB	C2B-C1B-CHA-C4A
29	RR	201	PEB	NB-C1B-CHA-C4A
29	RR	201	PEB	C2B-C1B-CHA-C4A
29	RR	201	PEB	C2B-C3B-CAB-CBB
29	RR	201	PEB	C4B-C3B-CAB-CBB
29	RR	202	PEB	C2A-C3A-CAA-CBA
29	RR	202	PEB	C4A-C3A-CAA-CBA
29	RR	202	PEB	NB-C1B-CHA-C4A
29	RR	202	PEB	C2B-C1B-CHA-C4A
29	RR	203	PEB	ND-C1D-CHC-C4C
29	RR	203	PEB	C2D-C1D-CHC-C4C
29	RR	203	PEB	NC-C1C-CHB-C4B
29	RR	203	PEB	C2C-C1C-CHB-C4B
29	RR	203	PEB	C2A-C3A-CAA-CBA
29	RR	203	PEB	NB-C1B-CHA-C4A
29	RR	203	PEB	C2B-C1B-CHA-C4A
29	SR	201	PEB	NB-C1B-CHA-C4A
29	SR	201	PEB	C2B-C1B-CHA-C4A
29	SR	202	PEB	NB-C1B-CHA-C4A
29	SR	202	PEB	C2B-C1B-CHA-C4A
29	TR	201	PEB	NB-C1B-CHA-C4A
29	TR	201	PEB	C2B-C1B-CHA-C4A
29	TR	201	PEB	C2B-C3B-CAB-CBB
29	TR	201	PEB	C4B-C3B-CAB-CBB
29	TR	202	PEB	C2A-C3A-CAA-CBA
29	TR	202	PEB	C4A-C3A-CAA-CBA
29	TR	202	PEB	NB-C1B-CHA-C4A
29	TR	202	PEB	C2B-C1B-CHA-C4A
29	TR	203	PEB	ND-C1D-CHC-C4C
29	TR	203	PEB	C2D-C1D-CHC-C4C
29	TR	203	PEB	NC-C1C-CHB-C4B
29	TR	203	PEB	C2C-C1C-CHB-C4B
29	TR	203	PEB	C2A-C3A-CAA-CBA
29	TR	203	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
29	TR	203	PEB	C2B-C1B-CHA-C4A
29	UR	201	PEB	C2A-C3A-CAA-CBA
29	UR	201	PEB	C4A-C3A-CAA-CBA
29	UR	201	PEB	NB-C1B-CHA-C4A
29	UR	201	PEB	C2B-C1B-CHA-C4A
29	UR	202	PEB	NC-C1C-CHB-C4B
29	UR	202	PEB	NB-C1B-CHA-C4A
29	UR	202	PEB	C2B-C1B-CHA-C4A
29	VR	201	PEB	NB-C1B-CHA-C4A
29	VR	201	PEB	C2B-C1B-CHA-C4A
29	VR	201	PEB	C2B-C3B-CAB-CBB
29	VR	201	PEB	C4B-C3B-CAB-CBB
29	VR	202	PEB	C2A-C3A-CAA-CBA
29	VR	202	PEB	C4A-C3A-CAA-CBA
29	VR	202	PEB	NB-C1B-CHA-C4A
29	VR	202	PEB	C2B-C1B-CHA-C4A
29	VR	203	PEB	ND-C1D-CHC-C4C
29	VR	203	PEB	C2D-C1D-CHC-C4C
29	VR	203	PEB	NC-C1C-CHB-C4B
29	VR	203	PEB	C2C-C1C-CHB-C4B
29	VR	203	PEB	C2A-C3A-CAA-CBA
29	VR	203	PEB	NB-C1B-CHA-C4A
29	VR	203	PEB	C2B-C1B-CHA-C4A
29	WR	201	PEB	C2A-C3A-CAA-CBA
29	WR	201	PEB	C4A-C3A-CAA-CBA
29	WR	201	PEB	NB-C1B-CHA-C4A
29	WR	201	PEB	C2B-C1B-CHA-C4A
29	WR	202	PEB	NB-C1B-CHA-C4A
29	WR	202	PEB	C2B-C1B-CHA-C4A
29	XR	201	PEB	NB-C1B-CHA-C4A
29	XR	201	PEB	C2B-C1B-CHA-C4A
29	XR	201	PEB	C2B-C3B-CAB-CBB
29	XR	201	PEB	C4B-C3B-CAB-CBB
29	XR	202	PEB	C2A-C3A-CAA-CBA
29	XR	202	PEB	C4A-C3A-CAA-CBA
29	XR	202	PEB	NB-C1B-CHA-C4A
29	XR	202	PEB	C2B-C1B-CHA-C4A
29	XR	203	PEB	ND-C1D-CHC-C4C
29	XR	203	PEB	C2D-C1D-CHC-C4C
29	XR	203	PEB	NC-C1C-CHB-C4B
29	XR	203	PEB	C2C-C1C-CHB-C4B
29	XR	203	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	XR	203	PEB	NB-C1B-CHA-C4A
29	XR	203	PEB	C2B-C1B-CHA-C4A
30	A1	305	PUB	C3C-C4C-CHC-C1D
30	A1	305	PUB	ND-C1D-CHC-C4C
30	A1	305	PUB	NA-C4A-CHA-C1B
30	A1	305	PUB	C3A-C4A-CHA-C1B
30	A7	303	PUB	C3C-C4C-CHC-C1D
30	A9	303	PUB	C3C-C4C-CHC-C1D
30	MA	402	PUB	NC-C4C-CHC-C1D
30	MA	402	PUB	NA-C4A-CHA-C1B
30	MA	403	PUB	NC-C4C-CHC-C1D
30	MA	403	PUB	ND-C1D-CHC-C4C
30	MA	403	PUB	NA-C4A-CHA-C1B
30	MA	403	PUB	NB-C4B-CHB-C1C
30	MA	403	PUB	C3B-C4B-CHB-C1C
30	AB	304	PUB	NC-C4C-CHC-C1D
30	AB	304	PUB	C3C-C4C-CHC-C1D
30	AB	304	PUB	ND-C1D-CHC-C4C
30	AB	304	PUB	NA-C4A-CHA-C1B
30	AB	304	PUB	C3A-C4A-CHA-C1B
30	AB	304	PUB	NB-C4B-CHB-C1C
30	AB	304	PUB	C3B-C4B-CHB-C1C
30	AB	304	PUB	C3B-CAB-CBB-CGB
30	AB	305	PUB	NA-C4A-CHA-C1B
30	AB	305	PUB	C3A-C4A-CHA-C1B
30	BB	302	PUB	NC-C4C-CHC-C1D
30	BB	302	PUB	C2D-C3D-CAD-CBD
30	QB	201	PUB	NC-C4C-CHC-C1D
30	QB	201	PUB	NA-C4A-CHA-C1B
30	QB	201	PUB	C3A-C4A-CHA-C1B
30	QB	201	PUB	NB-C4B-CHB-C1C
30	AF	302	PUB	C3C-C4C-CHC-C1D
30	AF	302	PUB	NA-C4A-CHA-C1B
30	AF	302	PUB	C3A-C4A-CHA-C1B
30	AF	303	PUB	NC-C4C-CHC-C1D
30	MG	402	PUB	C3C-C4C-CHC-C1D
30	MG	402	PUB	ND-C1D-CHC-C4C
30	MG	402	PUB	C2D-C1D-CHC-C4C
30	MG	402	PUB	NA-C4A-CHA-C1B
30	MG	402	PUB	C3A-C4A-CHA-C1B
30	MG	402	PUB	C2B-C3B-CAB-CBB
30	MG	402	PUB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	MG	403	PUB	C3C-C2C-CAC-CBC
30	MG	403	PUB	NB-C4B-CHB-C1C
30	MG	403	PUB	C3B-C4B-CHB-C1C
30	AI	302	PUB	C3C-C4C-CHC-C1D
30	AI	302	PUB	NA-C4A-CHA-C1B
30	AI	302	PUB	C3A-C4A-CHA-C1B
30	AI	303	PUB	NC-C4C-CHC-C1D
30	wJ	304	PUB	NC-C4C-CHC-C1D
30	wJ	304	PUB	ND-C1D-CHC-C4C
30	wJ	304	PUB	C2D-C1D-CHC-C4C
30	wJ	304	PUB	NB-C4B-CHB-C1C
30	wJ	304	PUB	C3B-C4B-CHB-C1C
30	wJ	304	PUB	C3B-CAB-CBB-CGB
30	xJ	304	PUB	NC-C4C-CHC-C1D
30	xJ	304	PUB	ND-C1D-CHC-C4C
30	xJ	304	PUB	C2D-C1D-CHC-C4C
30	xJ	304	PUB	NB-C4B-CHB-C1C
30	xJ	304	PUB	C3B-C4B-CHB-C1C
30	xJ	304	PUB	C3B-CAB-CBB-CGB
30	yJ	302	PUB	C4D-C3D-CAD-CBD
30	yJ	302	PUB	NB-C4B-CHB-C1C
30	yJ	303	PUB	C3C-C4C-CHC-C1D
30	AK	305	PUB	C3C-C4C-CHC-C1D
30	AK	305	PUB	ND-C1D-CHC-C4C
30	AK	305	PUB	NA-C4A-CHA-C1B
30	AK	305	PUB	C3A-C4A-CHA-C1B
30	wL	304	PUB	NC-C4C-CHC-C1D
30	wL	304	PUB	ND-C1D-CHC-C4C
30	wL	304	PUB	C2D-C1D-CHC-C4C
30	wL	304	PUB	NB-C4B-CHB-C1C
30	wL	304	PUB	C3B-C4B-CHB-C1C
30	wL	304	PUB	C3B-CAB-CBB-CGB
30	xL	304	PUB	NC-C4C-CHC-C1D
30	xL	304	PUB	ND-C1D-CHC-C4C
30	xL	304	PUB	C2D-C1D-CHC-C4C
30	xL	304	PUB	NB-C4B-CHB-C1C
30	xL	304	PUB	C3B-C4B-CHB-C1C
30	xL	304	PUB	C3B-CAB-CBB-CGB
30	yL	302	PUB	C4D-C3D-CAD-CBD
30	yL	302	PUB	NB-C4B-CHB-C1C
30	yL	303	PUB	C3C-C4C-CHC-C1D
30	yL	303	PUB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
30	AM	304	PUB	NC-C4C-CHC-C1D
30	AM	304	PUB	C3C-C4C-CHC-C1D
30	AM	304	PUB	ND-C1D-CHC-C4C
30	AM	304	PUB	NA-C4A-CHA-C1B
30	AM	304	PUB	C3A-C4A-CHA-C1B
30	AM	304	PUB	NB-C4B-CHB-C1C
30	AM	304	PUB	C3B-C4B-CHB-C1C
30	AM	304	PUB	C3B-CAB-CBB-CGB
30	AM	305	PUB	NA-C4A-CHA-C1B
30	AM	305	PUB	C3A-C4A-CHA-C1B
30	BM	302	PUB	NC-C4C-CHC-C1D
30	BM	302	PUB	C2D-C3D-CAD-CBD
30	QM	201	PUB	NC-C4C-CHC-C1D
30	QM	201	PUB	NA-C4A-CHA-C1B
30	QM	201	PUB	C3A-C4A-CHA-C1B
30	QM	201	PUB	NB-C4B-CHB-C1C
30	MN	402	PUB	NC-C4C-CHC-C1D
30	MN	402	PUB	NA-C4A-CHA-C1B
30	MN	403	PUB	NC-C4C-CHC-C1D
30	MN	403	PUB	ND-C1D-CHC-C4C
30	MN	403	PUB	NA-C4A-CHA-C1B
30	MN	403	PUB	NB-C4B-CHB-C1C
30	MN	403	PUB	C3B-C4B-CHB-C1C
30	MQ	404	PUB	C3C-C4C-CHC-C1D
30	MQ	404	PUB	ND-C1D-CHC-C4C
30	MQ	404	PUB	C2D-C1D-CHC-C4C
30	MQ	404	PUB	NA-C4A-CHA-C1B
30	MQ	404	PUB	C3A-C4A-CHA-C1B
30	MQ	404	PUB	C2B-C3B-CAB-CBB
30	MQ	404	PUB	C4B-C3B-CAB-CBB
30	MQ	405	PUB	C3C-C2C-CAC-CBC
30	MQ	405	PUB	NB-C4B-CHB-C1C
30	MQ	405	PUB	C3B-C4B-CHB-C1C
31	C1	1001	CYC	NA-C4A-CHB-C1B
31	C1	1001	CYC	C3A-C4A-CHB-C1B
31	D1	1001	CYC	NA-C4A-CHB-C1B
31	D1	1001	CYC	C3A-C4A-CHB-C1B
31	D1	1003	CYC	NA-C4A-CHB-C1B
31	D1	1003	CYC	C3A-C4A-CHB-C1B
31	E1	1001	CYC	NA-C4A-CHB-C1B
31	E1	1001	CYC	C3A-C4A-CHB-C1B
31	F1	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
31	F1	1001	CYC	C3A-C4A-CHB-C1B
31	H1	1001	CYC	NA-C4A-CHB-C1B
31	H1	1001	CYC	C3A-C4A-CHB-C1B
31	I1	1001	CYC	NA-C4A-CHB-C1B
31	I1	1001	CYC	C3A-C4A-CHB-C1B
31	J1	1001	CYC	NA-C4A-CHB-C1B
31	J1	1001	CYC	C3A-C4A-CHB-C1B
31	K1	1001	CYC	NA-C4A-CHB-C1B
31	K1	1001	CYC	C3A-C4A-CHB-C1B
31	L1	1001	CYC	NA-C4A-CHB-C1B
31	L1	1001	CYC	C3A-C4A-CHB-C1B
31	M1	1001	CYC	NA-C4A-CHB-C1B
31	M1	1001	CYC	C3A-C4A-CHB-C1B
31	N1	1001	CYC	NA-C4A-CHB-C1B
31	N1	1001	CYC	C3A-C4A-CHB-C1B
31	C7	1001	CYC	NA-C4A-CHB-C1B
31	C7	1001	CYC	C3A-C4A-CHB-C1B
31	D7	1001	CYC	NA-C4A-CHB-C1B
31	D7	1001	CYC	C4B-C3B-CAB-CBB
31	D7	1001	CYC	C2D-C3D-CAD-CBD
31	D7	1001	CYC	C4D-C3D-CAD-CBD
31	D7	1001	CYC	C3D-CAD-CBD-CGD
31	E7	1001	CYC	NA-C4A-CHB-C1B
31	E7	1001	CYC	C3A-C4A-CHB-C1B
31	F7	1001	CYC	NA-C4A-CHB-C1B
31	F7	1001	CYC	C4B-C3B-CAB-CBB
31	F7	1001	CYC	C2D-C3D-CAD-CBD
31	F7	1001	CYC	C4D-C3D-CAD-CBD
31	F7	1001	CYC	C3D-CAD-CBD-CGD
31	G7	1001	CYC	NA-C4A-CHB-C1B
31	G7	1001	CYC	C3A-C4A-CHB-C1B
31	H7	1001	CYC	NA-C4A-CHB-C1B
31	H7	1001	CYC	C4B-C3B-CAB-CBB
31	H7	1001	CYC	C2D-C3D-CAD-CBD
31	H7	1001	CYC	C4D-C3D-CAD-CBD
31	H7	1001	CYC	C3D-CAD-CBD-CGD
31	I7	1001	CYC	NA-C4A-CHB-C1B
31	I7	1001	CYC	C3A-C4A-CHB-C1B
31	J7	1001	CYC	NA-C4A-CHB-C1B
31	J7	1001	CYC	C4B-C3B-CAB-CBB
31	J7	1001	CYC	C2D-C3D-CAD-CBD
31	J7	1001	CYC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
31	J7	1001	CYC	C3D-CAD-CBD-CGD
31	K7	1001	CYC	NA-C4A-CHB-C1B
31	K7	1001	CYC	C3A-C4A-CHB-C1B
31	L7	1001	CYC	NA-C4A-CHB-C1B
31	L7	1001	CYC	C4B-C3B-CAB-CBB
31	L7	1001	CYC	C2D-C3D-CAD-CBD
31	L7	1001	CYC	C4D-C3D-CAD-CBD
31	L7	1001	CYC	C3D-CAD-CBD-CGD
31	M7	1001	CYC	NA-C4A-CHB-C1B
31	M7	1001	CYC	C3A-C4A-CHB-C1B
31	N7	1001	CYC	NA-C4A-CHB-C1B
31	N7	1001	CYC	C4B-C3B-CAB-CBB
31	N7	1001	CYC	C2D-C3D-CAD-CBD
31	N7	1001	CYC	C4D-C3D-CAD-CBD
31	N7	1001	CYC	C3D-CAD-CBD-CGD
31	C9	1001	CYC	NA-C4A-CHB-C1B
31	C9	1001	CYC	C3A-C4A-CHB-C1B
31	D9	1001	CYC	NA-C4A-CHB-C1B
31	D9	1001	CYC	C4B-C3B-CAB-CBB
31	D9	1001	CYC	C2D-C3D-CAD-CBD
31	D9	1001	CYC	C4D-C3D-CAD-CBD
31	D9	1001	CYC	C3D-CAD-CBD-CGD
31	E9	1001	CYC	NA-C4A-CHB-C1B
31	E9	1001	CYC	C3A-C4A-CHB-C1B
31	F9	1001	CYC	NA-C4A-CHB-C1B
31	F9	1001	CYC	C4B-C3B-CAB-CBB
31	F9	1001	CYC	C2D-C3D-CAD-CBD
31	F9	1001	CYC	C4D-C3D-CAD-CBD
31	F9	1001	CYC	C3D-CAD-CBD-CGD
31	G9	1001	CYC	NA-C4A-CHB-C1B
31	G9	1001	CYC	C3A-C4A-CHB-C1B
31	H9	1001	CYC	NA-C4A-CHB-C1B
31	H9	1001	CYC	C4B-C3B-CAB-CBB
31	H9	1001	CYC	C2D-C3D-CAD-CBD
31	H9	1001	CYC	C4D-C3D-CAD-CBD
31	H9	1001	CYC	C3D-CAD-CBD-CGD
31	I9	1001	CYC	NA-C4A-CHB-C1B
31	I9	1001	CYC	C3A-C4A-CHB-C1B
31	J9	1001	CYC	NA-C4A-CHB-C1B
31	J9	1001	CYC	C4B-C3B-CAB-CBB
31	J9	1001	CYC	C2D-C3D-CAD-CBD
31	J9	1001	CYC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
31	J9	1001	CYC	C3D-CAD-CBD-CGD
31	K9	1001	CYC	NA-C4A-CHB-C1B
31	K9	1001	CYC	C3A-C4A-CHB-C1B
31	L9	1001	CYC	NA-C4A-CHB-C1B
31	L9	1001	CYC	C4B-C3B-CAB-CBB
31	L9	1001	CYC	C2D-C3D-CAD-CBD
31	L9	1001	CYC	C4D-C3D-CAD-CBD
31	L9	1001	CYC	C3D-CAD-CBD-CGD
31	M9	1001	CYC	NA-C4A-CHB-C1B
31	M9	1001	CYC	C3A-C4A-CHB-C1B
31	N9	1001	CYC	NA-C4A-CHB-C1B
31	N9	1001	CYC	C4B-C3B-CAB-CBB
31	N9	1001	CYC	C2D-C3D-CAD-CBD
31	N9	1001	CYC	C4D-C3D-CAD-CBD
31	N9	1001	CYC	C3D-CAD-CBD-CGD
31	CF	1001	CYC	NA-C4A-CHB-C1B
31	CF	1001	CYC	C3A-C4A-CHB-C1B
31	CF	1001	CYC	C4B-C3B-CAB-CBB
31	CF	1001	CYC	C2C-C3C-CAC-CBC
31	CF	1001	CYC	C4C-C3C-CAC-CBC
31	DF	1001	CYC	NA-C4A-CHB-C1B
31	DF	1001	CYC	C3A-C4A-CHB-C1B
31	DF	1001	CYC	C4B-C3B-CAB-CBB
31	EF	1001	CYC	NA-C4A-CHB-C1B
31	EF	1001	CYC	C3A-C4A-CHB-C1B
31	EF	1001	CYC	C4B-C3B-CAB-CBB
31	EF	1001	CYC	C2C-C3C-CAC-CBC
31	EF	1001	CYC	C4C-C3C-CAC-CBC
31	FF	1001	CYC	NA-C4A-CHB-C1B
31	FF	1001	CYC	C3A-C4A-CHB-C1B
31	FF	1001	CYC	C4B-C3B-CAB-CBB
31	GF	1001	CYC	NA-C4A-CHB-C1B
31	GF	1001	CYC	C3A-C4A-CHB-C1B
31	GF	1001	CYC	C4B-C3B-CAB-CBB
31	GF	1001	CYC	C2C-C3C-CAC-CBC
31	GF	1001	CYC	C4C-C3C-CAC-CBC
31	HF	1001	CYC	NA-C4A-CHB-C1B
31	HF	1001	CYC	C3A-C4A-CHB-C1B
31	HF	1001	CYC	C4B-C3B-CAB-CBB
31	IF	1001	CYC	NA-C4A-CHB-C1B
31	IF	1001	CYC	C3A-C4A-CHB-C1B
31	IF	1001	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	IF	1001	CYC	C2C-C3C-CAC-CBC
31	IF	1001	CYC	C4C-C3C-CAC-CBC
31	JF	1001	CYC	NA-C4A-CHB-C1B
31	JF	1001	CYC	C3A-C4A-CHB-C1B
31	JF	1001	CYC	C4B-C3B-CAB-CBB
31	KF	1001	CYC	NA-C4A-CHB-C1B
31	KF	1001	CYC	C3A-C4A-CHB-C1B
31	KF	1001	CYC	C4B-C3B-CAB-CBB
31	KF	1001	CYC	C2C-C3C-CAC-CBC
31	KF	1001	CYC	C4C-C3C-CAC-CBC
31	LF	1001	CYC	NA-C4A-CHB-C1B
31	LF	1001	CYC	C3A-C4A-CHB-C1B
31	LF	1001	CYC	C4B-C3B-CAB-CBB
31	MF	1001	CYC	NA-C4A-CHB-C1B
31	MF	1001	CYC	C3A-C4A-CHB-C1B
31	MF	1001	CYC	C4B-C3B-CAB-CBB
31	MF	1001	CYC	C2C-C3C-CAC-CBC
31	MF	1001	CYC	C4C-C3C-CAC-CBC
31	NF	1001	CYC	NA-C4A-CHB-C1B
31	NF	1001	CYC	C3A-C4A-CHB-C1B
31	NF	1001	CYC	C4B-C3B-CAB-CBB
31	CI	1001	CYC	NA-C4A-CHB-C1B
31	CI	1001	CYC	C3A-C4A-CHB-C1B
31	CI	1001	CYC	C4B-C3B-CAB-CBB
31	CI	1001	CYC	C2C-C3C-CAC-CBC
31	CI	1001	CYC	C4C-C3C-CAC-CBC
31	DI	1001	CYC	NA-C4A-CHB-C1B
31	DI	1001	CYC	C3A-C4A-CHB-C1B
31	DI	1001	CYC	C4B-C3B-CAB-CBB
31	EI	1001	CYC	NA-C4A-CHB-C1B
31	EI	1001	CYC	C3A-C4A-CHB-C1B
31	EI	1001	CYC	C4B-C3B-CAB-CBB
31	EI	1001	CYC	C2C-C3C-CAC-CBC
31	EI	1001	CYC	C4C-C3C-CAC-CBC
31	FI	1001	CYC	NA-C4A-CHB-C1B
31	FI	1001	CYC	C3A-C4A-CHB-C1B
31	FI	1001	CYC	C4B-C3B-CAB-CBB
31	GI	1001	CYC	NA-C4A-CHB-C1B
31	GI	1001	CYC	C3A-C4A-CHB-C1B
31	GI	1001	CYC	C4B-C3B-CAB-CBB
31	GI	1001	CYC	C2C-C3C-CAC-CBC
31	GI	1001	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
31	HI	1001	CYC	NA-C4A-CHB-C1B
31	HI	1001	CYC	C3A-C4A-CHB-C1B
31	HI	1001	CYC	C4B-C3B-CAB-CBB
31	II	1001	CYC	NA-C4A-CHB-C1B
31	II	1001	CYC	C3A-C4A-CHB-C1B
31	II	1001	CYC	C4B-C3B-CAB-CBB
31	II	1001	CYC	C2C-C3C-CAC-CBC
31	II	1001	CYC	C4C-C3C-CAC-CBC
31	JI	1001	CYC	NA-C4A-CHB-C1B
31	JI	1001	CYC	C3A-C4A-CHB-C1B
31	JI	1001	CYC	C4B-C3B-CAB-CBB
31	KI	1001	CYC	NA-C4A-CHB-C1B
31	KI	1001	CYC	C3A-C4A-CHB-C1B
31	KI	1001	CYC	C4B-C3B-CAB-CBB
31	KI	1001	CYC	C2C-C3C-CAC-CBC
31	KI	1001	CYC	C4C-C3C-CAC-CBC
31	LI	1001	CYC	NA-C4A-CHB-C1B
31	LI	1001	CYC	C3A-C4A-CHB-C1B
31	LI	1001	CYC	C4B-C3B-CAB-CBB
31	MI	1001	CYC	NA-C4A-CHB-C1B
31	MI	1001	CYC	C3A-C4A-CHB-C1B
31	MI	1001	CYC	C4B-C3B-CAB-CBB
31	MI	1001	CYC	C2C-C3C-CAC-CBC
31	MI	1001	CYC	C4C-C3C-CAC-CBC
31	NI	1001	CYC	NA-C4A-CHB-C1B
31	NI	1001	CYC	C3A-C4A-CHB-C1B
31	NI	1001	CYC	C4B-C3B-CAB-CBB
31	CK	1001	CYC	NA-C4A-CHB-C1B
31	CK	1001	CYC	C3A-C4A-CHB-C1B
31	DK	1001	CYC	NA-C4A-CHB-C1B
31	DK	1001	CYC	C3A-C4A-CHB-C1B
31	EK	1001	CYC	NA-C4A-CHB-C1B
31	EK	1001	CYC	C3A-C4A-CHB-C1B
31	FK	1001	CYC	NA-C4A-CHB-C1B
31	FK	1001	CYC	C3A-C4A-CHB-C1B
31	GK	1001	CYC	NA-C4A-CHB-C1B
31	GK	1001	CYC	C3A-C4A-CHB-C1B
31	HK	1001	CYC	NA-C4A-CHB-C1B
31	HK	1001	CYC	C3A-C4A-CHB-C1B
31	IK	1001	CYC	NA-C4A-CHB-C1B
31	IK	1001	CYC	C3A-C4A-CHB-C1B
31	JK	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
31	JK	1001	CYC	C3A-C4A-CHB-C1B
31	KK	1001	CYC	NA-C4A-CHB-C1B
31	KK	1001	CYC	C3A-C4A-CHB-C1B
31	LK	1001	CYC	NA-C4A-CHB-C1B
31	LK	1001	CYC	C3A-C4A-CHB-C1B
31	MK	1001	CYC	NA-C4A-CHB-C1B
31	MK	1001	CYC	C3A-C4A-CHB-C1B
31	NK	1001	CYC	NA-C4A-CHB-C1B
31	NK	1001	CYC	C3A-C4A-CHB-C1B
31	AP	1001	CYC	ND-C1D-CHD-C4C
31	AP	1001	CYC	C2D-C1D-CHD-C4C
31	DP	1001	CYC	ND-C1D-CHD-C4C
31	DP	1001	CYC	C2D-C1D-CHD-C4C
31	CP	1001	CYC	ND-C1D-CHD-C4C
31	CP	1001	CYC	C2D-C1D-CHD-C4C
31	FP	1001	CYC	ND-C1D-CHD-C4C
31	FP	1001	CYC	C2D-C1D-CHD-C4C
31	EP	1001	CYC	ND-C1D-CHD-C4C
31	EP	1001	CYC	C2D-C1D-CHD-C4C
31	BP	1001	CYC	ND-C1D-CHD-C4C
31	BP	1001	CYC	C2D-C1D-CHD-C4C
31	GP	1001	CYC	ND-C1D-CHD-C4C
31	GP	1001	CYC	C2D-C1D-CHD-C4C
31	HP	1001	CYC	ND-C1D-CHD-C4C
31	HP	1001	CYC	C2D-C1D-CHD-C4C
31	IP	1001	CYC	ND-C1D-CHD-C4C
31	IP	1001	CYC	C2D-C1D-CHD-C4C
31	JP	1001	CYC	ND-C1D-CHD-C4C
31	JP	1001	CYC	C2D-C1D-CHD-C4C
31	KP	1001	CYC	ND-C1D-CHD-C4C
31	KP	1001	CYC	C2D-C1D-CHD-C4C
31	MP	1001	CYC	ND-C1D-CHD-C4C
31	MP	1001	CYC	C2D-C1D-CHD-C4C
31	NP	1001	CYC	ND-C1D-CHD-C4C
31	NP	1001	CYC	C2D-C1D-CHD-C4C
31	OP	1001	CYC	ND-C1D-CHD-C4C
31	OP	1001	CYC	C2D-C1D-CHD-C4C
31	PP	1001	CYC	ND-C1D-CHD-C4C
31	PP	1001	CYC	C2D-C1D-CHD-C4C
31	QP	1001	CYC	ND-C1D-CHD-C4C
31	QP	1001	CYC	C2D-C1D-CHD-C4C
31	RP	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
31	RP	1001	CYC	C2D-C1D-CHD-C4C
31	SP	1001	CYC	ND-C1D-CHD-C4C
31	SP	1001	CYC	C2D-C1D-CHD-C4C
31	TP	1001	CYC	ND-C1D-CHD-C4C
31	TP	1001	CYC	C2D-C1D-CHD-C4C
31	UP	1001	CYC	ND-C1D-CHD-C4C
31	UP	1001	CYC	C2D-C1D-CHD-C4C
31	VP	1001	CYC	ND-C4D-CHA-C1A
31	VP	1001	CYC	C3D-C4D-CHA-C1A
31	VP	1001	CYC	C3A-C4A-CHB-C1B
31	VP	1001	CYC	ND-C1D-CHD-C4C
31	VP	1001	CYC	C2D-C1D-CHD-C4C
31	WP	1001	CYC	ND-C1D-CHD-C4C
31	WP	1001	CYC	C2D-C1D-CHD-C4C
31	XP	1001	CYC	ND-C1D-CHD-C4C
31	XP	1001	CYC	C2D-C1D-CHD-C4C
31	YP	1000	CYC	NA-C4A-CHB-C1B
31	YP	1000	CYC	C3A-C4A-CHB-C1B
31	YP	1000	CYC	C3D-CAD-CBD-CGD
31	eP	1001	CYC	ND-C1D-CHD-C4C
31	eP	1001	CYC	C2D-C1D-CHD-C4C
31	eP	1001	CYC	ND-C1D-CHD-C4C
31	eP	1001	CYC	C2D-C1D-CHD-C4C
31	fP	1001	CYC	ND-C1D-CHD-C4C
31	fP	1001	CYC	C2D-C1D-CHD-C4C
31	gP	1001	CYC	ND-C1D-CHD-C4C
31	gP	1001	CYC	C2D-C1D-CHD-C4C
31	hP	1001	CYC	ND-C1D-CHD-C4C
31	hP	1001	CYC	C2D-C1D-CHD-C4C
31	iP	1001	CYC	ND-C1D-CHD-C4C
31	iP	1001	CYC	C2D-C1D-CHD-C4C
31	jP	1001	CYC	ND-C1D-CHD-C4C
31	jP	1001	CYC	C2D-C1D-CHD-C4C
31	kP	1001	CYC	ND-C1D-CHD-C4C
31	kP	1001	CYC	C2D-C1D-CHD-C4C
31	lP	1001	CYC	ND-C1D-CHD-C4C
31	lP	1001	CYC	C2D-C1D-CHD-C4C
31	mP	1001	CYC	ND-C1D-CHD-C4C
31	mP	1001	CYC	C2D-C1D-CHD-C4C
31	nP	1001	CYC	ND-C1D-CHD-C4C
31	nP	1001	CYC	C2D-C1D-CHD-C4C
31	oP	1001	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
31	oP	1001	CYC	C2D-C1D-CHD-C4C
31	pP	1001	CYC	ND-C1D-CHD-C4C
31	pP	1001	CYC	C2D-C1D-CHD-C4C
31	qP	1001	CYC	ND-C1D-CHD-C4C
31	qP	1001	CYC	C2D-C1D-CHD-C4C
31	rP	1001	CYC	ND-C1D-CHD-C4C
31	rP	1001	CYC	C2D-C1D-CHD-C4C
31	sP	1001	CYC	ND-C1D-CHD-C4C
31	sP	1001	CYC	C2D-C1D-CHD-C4C
31	tP	1001	CYC	ND-C1D-CHD-C4C
31	tP	1001	CYC	C2D-C1D-CHD-C4C
31	uP	1001	CYC	ND-C1D-CHD-C4C
31	uP	1001	CYC	C2D-C1D-CHD-C4C
31	vP	1001	CYC	ND-C1D-CHD-C4C
31	vP	1001	CYC	C2D-C1D-CHD-C4C
31	wP	1001	CYC	ND-C1D-CHD-C4C
31	wP	1001	CYC	C2D-C1D-CHD-C4C
31	xP	1001	CYC	ND-C4D-CHA-C1A
31	xP	1001	CYC	C3D-C4D-CHA-C1A
31	xP	1001	CYC	C3A-C4A-CHB-C1B
31	xP	1001	CYC	ND-C1D-CHD-C4C
31	xP	1001	CYC	C2D-C1D-CHD-C4C
31	yP	1001	CYC	ND-C1D-CHD-C4C
31	yP	1001	CYC	C2D-C1D-CHD-C4C
31	1P	1001	CYC	ND-C1D-CHD-C4C
31	1P	1001	CYC	C2D-C1D-CHD-C4C
31	1P	1002	CYC	NA-C4A-CHB-C1B
31	1P	1002	CYC	C3A-C4A-CHB-C1B
31	1P	1002	CYC	C3D-CAD-CBD-CGD
32	k6	301	PMS	S-C-C1-C2
32	k6	301	PMS	S-C-C1-C6
32	kH	301	PMS	S-C-C1-C2
32	kH	301	PMS	S-C-C1-C6
31	CF	1001	CYC	C2B-C3B-CAB-CBB
31	EF	1001	CYC	C2B-C3B-CAB-CBB
31	GF	1001	CYC	C2B-C3B-CAB-CBB
31	IF	1001	CYC	C2B-C3B-CAB-CBB
31	KF	1001	CYC	C2B-C3B-CAB-CBB
31	MF	1001	CYC	C2B-C3B-CAB-CBB
31	CI	1001	CYC	C2B-C3B-CAB-CBB
31	EI	1001	CYC	C2B-C3B-CAB-CBB
31	GI	1001	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	II	1001	CYC	C2B-C3B-CAB-CBB
31	KI	1001	CYC	C2B-C3B-CAB-CBB
31	MI	1001	CYC	C2B-C3B-CAB-CBB
30	yJ	302	PUB	C2D-C3D-CAD-CBD
30	yL	302	PUB	C2D-C3D-CAD-CBD
31	C7	1001	CYC	C2B-C3B-CAB-CBB
31	E7	1001	CYC	C2B-C3B-CAB-CBB
31	G7	1001	CYC	C2B-C3B-CAB-CBB
31	I7	1001	CYC	C2B-C3B-CAB-CBB
31	K7	1001	CYC	C2B-C3B-CAB-CBB
31	M7	1001	CYC	C2B-C3B-CAB-CBB
31	C9	1001	CYC	C2B-C3B-CAB-CBB
31	E9	1001	CYC	C2B-C3B-CAB-CBB
31	G9	1001	CYC	C2B-C3B-CAB-CBB
31	I9	1001	CYC	C2B-C3B-CAB-CBB
31	K9	1001	CYC	C2B-C3B-CAB-CBB
31	M9	1001	CYC	C2B-C3B-CAB-CBB
29	wJ	303	PEB	C2B-C3B-CAB-CBB
29	xJ	303	PEB	C2B-C3B-CAB-CBB
29	wL	303	PEB	C2B-C3B-CAB-CBB
29	xL	303	PEB	C2B-C3B-CAB-CBB
30	MG	403	PUB	C1C-C2C-CAC-CBC
30	MQ	405	PUB	C1C-C2C-CAC-CBC
30	wJ	305	PUB	C2D-C3D-CAD-CBD
30	xJ	305	PUB	C2D-C3D-CAD-CBD
30	wL	305	PUB	C2D-C3D-CAD-CBD
30	xL	305	PUB	C2D-C3D-CAD-CBD
29	P1	203	PEB	C3B-CAB-CBB-CGB
29	R1	203	PEB	C3B-CAB-CBB-CGB
29	T1	202	PEB	C3B-CAB-CBB-CGB
29	V1	203	PEB	C3B-CAB-CBB-CGB
29	Y1	202	PEB	C3B-CAB-CBB-CGB
29	a1	203	PEB	C3B-CAB-CBB-CGB
29	c1	203	PEB	C3B-CAB-CBB-CGB
29	e1	203	PEB	C3B-CAB-CBB-CGB
29	g1	203	PEB	C3B-CAB-CBB-CGB
29	i1	203	PEB	C3B-CAB-CBB-CGB
29	k1	203	PEB	C3B-CAB-CBB-CGB
29	m1	202	PEB	C3B-CAB-CBB-CGB
29	M2	201	PEB	C3B-CAB-CBB-CGB
29	O2	201	PEB	C3B-CAB-CBB-CGB
29	Q2	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	U2	201	PEB	C3B-CAB-CBB-CGB
29	W2	201	PEB	C3B-CAB-CBB-CGB
29	D3	202	PEB	C3B-CAB-CBB-CGB
29	M4	203	PEB	C3B-CAB-CBB-CGB
29	D7	1002	PEB	C3B-CAB-CBB-CGB
29	F7	1002	PEB	C3B-CAB-CBB-CGB
29	H7	1002	PEB	C3B-CAB-CBB-CGB
29	J7	1002	PEB	C3B-CAB-CBB-CGB
29	L7	1002	PEB	C3B-CAB-CBB-CGB
29	N7	1002	PEB	C3B-CAB-CBB-CGB
29	P7	203	PEB	C3B-CAB-CBB-CGB
29	R7	203	PEB	C3B-CAB-CBB-CGB
29	T7	203	PEB	C3B-CAB-CBB-CGB
29	V7	203	PEB	C3B-CAB-CBB-CGB
29	Y7	203	PEB	C3B-CAB-CBB-CGB
29	a7	203	PEB	C3B-CAB-CBB-CGB
29	c7	203	PEB	C3B-CAB-CBB-CGB
29	e7	203	PEB	C3B-CAB-CBB-CGB
29	g7	203	PEB	C3B-CAB-CBB-CGB
29	i7	203	PEB	C3B-CAB-CBB-CGB
29	k7	203	PEB	C3B-CAB-CBB-CGB
29	m7	203	PEB	C3B-CAB-CBB-CGB
29	D9	1002	PEB	C3B-CAB-CBB-CGB
29	F9	1002	PEB	C3B-CAB-CBB-CGB
29	H9	1002	PEB	C3B-CAB-CBB-CGB
29	J9	1002	PEB	C3B-CAB-CBB-CGB
29	L9	1002	PEB	C3B-CAB-CBB-CGB
29	N9	1002	PEB	C3B-CAB-CBB-CGB
29	P9	203	PEB	C3B-CAB-CBB-CGB
29	R9	203	PEB	C3B-CAB-CBB-CGB
29	T9	203	PEB	C3B-CAB-CBB-CGB
29	V9	203	PEB	C3B-CAB-CBB-CGB
29	Y9	203	PEB	C3B-CAB-CBB-CGB
29	a9	203	PEB	C3B-CAB-CBB-CGB
29	c9	203	PEB	C3B-CAB-CBB-CGB
29	e9	203	PEB	C3B-CAB-CBB-CGB
29	g9	203	PEB	C3B-CAB-CBB-CGB
29	i9	203	PEB	C3B-CAB-CBB-CGB
29	k9	203	PEB	C3B-CAB-CBB-CGB
29	m9	203	PEB	C3B-CAB-CBB-CGB
29	BA	201	PEB	C3B-CAB-CBB-CGB
29	BA	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	BA	203	PEB	C3B-CAB-CBB-CGB
29	DA	201	PEB	C3B-CAB-CBB-CGB
29	DA	202	PEB	C3B-CAB-CBB-CGB
29	DA	203	PEB	C3B-CAB-CBB-CGB
29	FA	201	PEB	C3B-CAB-CBB-CGB
29	FA	202	PEB	C3B-CAB-CBB-CGB
29	FA	203	PEB	C3B-CAB-CBB-CGB
29	HA	201	PEB	C3B-CAB-CBB-CGB
29	HA	202	PEB	C3B-CAB-CBB-CGB
29	HA	203	PEB	C3B-CAB-CBB-CGB
29	JA	201	PEB	C3B-CAB-CBB-CGB
29	JA	202	PEB	C3B-CAB-CBB-CGB
29	JA	203	PEB	C3B-CAB-CBB-CGB
29	LA	201	PEB	C3B-CAB-CBB-CGB
29	LA	202	PEB	C3B-CAB-CBB-CGB
29	LA	203	PEB	C3B-CAB-CBB-CGB
29	CB	202	PEB	C3B-CAB-CBB-CGB
29	EB	202	PEB	C3B-CAB-CBB-CGB
29	GB	202	PEB	C3B-CAB-CBB-CGB
29	IB	202	PEB	C3B-CAB-CBB-CGB
29	KB	202	PEB	C3B-CAB-CBB-CGB
29	MB	202	PEB	C3B-CAB-CBB-CGB
29	OB	202	PEB	C3B-CAB-CBB-CGB
29	QB	204	PEB	C3B-CAB-CBB-CGB
29	SB	202	PEB	C3B-CAB-CBB-CGB
29	UB	202	PEB	C3B-CAB-CBB-CGB
29	WB	202	PEB	C3B-CAB-CBB-CGB
29	YB	203	PEB	C3B-CAB-CBB-CGB
29	aB	202	PEB	C3B-CAB-CBB-CGB
29	dB	202	PEB	C3B-CAB-CBB-CGB
29	fB	202	PEB	C3B-CAB-CBB-CGB
29	hB	202	PEB	C3B-CAB-CBB-CGB
29	jB	202	PEB	C3B-CAB-CBB-CGB
29	lB	202	PEB	C3B-CAB-CBB-CGB
29	AF	301	PEB	C3B-CAB-CBB-CGB
29	BG	202	PEB	C3B-CAB-CBB-CGB
29	DG	202	PEB	C3B-CAB-CBB-CGB
29	FG	202	PEB	C3B-CAB-CBB-CGB
29	HG	202	PEB	C3B-CAB-CBB-CGB
29	JG	202	PEB	C3B-CAB-CBB-CGB
29	LG	202	PEB	C3B-CAB-CBB-CGB
29	MG	401	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	AI	301	PEB	C3B-CAB-CBB-CGB
29	wJ	302	PEB	C3B-CAB-CBB-CGB
29	wJ	303	PEB	C3B-CAB-CBB-CGB
29	xJ	302	PEB	C3B-CAB-CBB-CGB
29	xJ	303	PEB	C3B-CAB-CBB-CGB
29	PK	203	PEB	C3B-CAB-CBB-CGB
29	RK	203	PEB	C3B-CAB-CBB-CGB
29	TK	202	PEB	C3B-CAB-CBB-CGB
29	VK	203	PEB	C3B-CAB-CBB-CGB
29	YK	202	PEB	C3B-CAB-CBB-CGB
29	aK	203	PEB	C3B-CAB-CBB-CGB
29	cK	203	PEB	C3B-CAB-CBB-CGB
29	eK	203	PEB	C3B-CAB-CBB-CGB
29	gK	203	PEB	C3B-CAB-CBB-CGB
29	iK	203	PEB	C3B-CAB-CBB-CGB
29	kK	203	PEB	C3B-CAB-CBB-CGB
29	mK	202	PEB	C3B-CAB-CBB-CGB
29	wL	302	PEB	C3B-CAB-CBB-CGB
29	wL	303	PEB	C3B-CAB-CBB-CGB
29	xL	302	PEB	C3B-CAB-CBB-CGB
29	xL	303	PEB	C3B-CAB-CBB-CGB
29	CM	202	PEB	C3B-CAB-CBB-CGB
29	EM	202	PEB	C3B-CAB-CBB-CGB
29	GM	202	PEB	C3B-CAB-CBB-CGB
29	IM	202	PEB	C3B-CAB-CBB-CGB
29	KM	202	PEB	C3B-CAB-CBB-CGB
29	MM	202	PEB	C3B-CAB-CBB-CGB
29	OM	202	PEB	C3B-CAB-CBB-CGB
29	QM	204	PEB	C3B-CAB-CBB-CGB
29	SM	202	PEB	C3B-CAB-CBB-CGB
29	WM	202	PEB	C3B-CAB-CBB-CGB
29	YM	203	PEB	C3B-CAB-CBB-CGB
29	aM	202	PEB	C3B-CAB-CBB-CGB
29	dM	202	PEB	C3B-CAB-CBB-CGB
29	fM	202	PEB	C3B-CAB-CBB-CGB
29	hM	202	PEB	C3B-CAB-CBB-CGB
29	jM	202	PEB	C3B-CAB-CBB-CGB
29	lM	202	PEB	C3B-CAB-CBB-CGB
29	BN	201	PEB	C3B-CAB-CBB-CGB
29	BN	202	PEB	C3B-CAB-CBB-CGB
29	BN	203	PEB	C3B-CAB-CBB-CGB
29	DN	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	DN	202	PEB	C3B-CAB-CBB-CGB
29	DN	203	PEB	C3B-CAB-CBB-CGB
29	FN	201	PEB	C3B-CAB-CBB-CGB
29	FN	202	PEB	C3B-CAB-CBB-CGB
29	FN	203	PEB	C3B-CAB-CBB-CGB
29	HN	201	PEB	C3B-CAB-CBB-CGB
29	HN	202	PEB	C3B-CAB-CBB-CGB
29	HN	203	PEB	C3B-CAB-CBB-CGB
29	JN	201	PEB	C3B-CAB-CBB-CGB
29	JN	202	PEB	C3B-CAB-CBB-CGB
29	JN	203	PEB	C3B-CAB-CBB-CGB
29	LN	201	PEB	C3B-CAB-CBB-CGB
29	LN	202	PEB	C3B-CAB-CBB-CGB
29	LN	203	PEB	C3B-CAB-CBB-CGB
29	DO	202	PEB	C3B-CAB-CBB-CGB
29	BQ	202	PEB	C3B-CAB-CBB-CGB
29	DQ	202	PEB	C3B-CAB-CBB-CGB
29	FQ	202	PEB	C3B-CAB-CBB-CGB
29	HQ	202	PEB	C3B-CAB-CBB-CGB
29	JQ	202	PEB	C3B-CAB-CBB-CGB
29	LQ	201	PEB	C3B-CAB-CBB-CGB
29	MQ	401	PEB	C3B-CAB-CBB-CGB
29	MQ	403	PEB	C3B-CAB-CBB-CGB
29	MR	201	PEB	C3B-CAB-CBB-CGB
29	OR	201	PEB	C3B-CAB-CBB-CGB
29	QR	201	PEB	C3B-CAB-CBB-CGB
29	UR	201	PEB	C3B-CAB-CBB-CGB
29	WR	201	PEB	C3B-CAB-CBB-CGB
30	A7	302	PUB	C2C-CAC-CBC-CGC
30	A9	302	PUB	C2C-CAC-CBC-CGC
30	MG	402	PUB	C2C-CAC-CBC-CGC
30	MQ	404	PUB	C2C-CAC-CBC-CGC
29	BA	201	PEB	C4B-C3B-CAB-CBB
29	DA	201	PEB	C4B-C3B-CAB-CBB
29	FA	201	PEB	C4B-C3B-CAB-CBB
29	HA	201	PEB	C4B-C3B-CAB-CBB
29	JA	201	PEB	C4B-C3B-CAB-CBB
29	LA	201	PEB	C4B-C3B-CAB-CBB
29	BN	201	PEB	C4B-C3B-CAB-CBB
29	DN	201	PEB	C4B-C3B-CAB-CBB
29	FN	201	PEB	C4B-C3B-CAB-CBB
29	HN	201	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	JN	201	PEB	C4B-C3B-CAB-CBB
29	LN	201	PEB	C4B-C3B-CAB-CBB
29	A1	302	PEB	C2C-CAC-CBC-CGC
29	A1	303	PEB	C2C-CAC-CBC-CGC
29	O1	202	PEB	C2C-CAC-CBC-CGC
29	P1	201	PEB	C2C-CAC-CBC-CGC
29	Q1	202	PEB	C2C-CAC-CBC-CGC
29	R1	201	PEB	C2C-CAC-CBC-CGC
29	S1	202	PEB	C2C-CAC-CBC-CGC
29	T1	201	PEB	C2C-CAC-CBC-CGC
29	U1	203	PEB	C2C-CAC-CBC-CGC
29	V1	201	PEB	C2C-CAC-CBC-CGC
29	W1	202	PEB	C2C-CAC-CBC-CGC
29	Y1	201	PEB	C2C-CAC-CBC-CGC
29	Z1	203	PEB	C2C-CAC-CBC-CGC
29	a1	201	PEB	C2C-CAC-CBC-CGC
29	b1	202	PEB	C2C-CAC-CBC-CGC
29	c1	201	PEB	C2C-CAC-CBC-CGC
29	d1	202	PEB	C2C-CAC-CBC-CGC
29	e1	201	PEB	C2C-CAC-CBC-CGC
29	f1	202	PEB	C2C-CAC-CBC-CGC
29	g1	201	PEB	C2C-CAC-CBC-CGC
29	h1	202	PEB	C2C-CAC-CBC-CGC
29	i1	201	PEB	C2C-CAC-CBC-CGC
29	j1	202	PEB	C2C-CAC-CBC-CGC
29	k1	201	PEB	C2C-CAC-CBC-CGC
29	l1	202	PEB	C2C-CAC-CBC-CGC
29	m1	201	PEB	C2C-CAC-CBC-CGC
29	M2	202	PEB	C2C-CAC-CBC-CGC
29	N2	202	PEB	C2C-CAC-CBC-CGC
29	N2	203	PEB	C2C-CAC-CBC-CGC
29	O2	202	PEB	C2C-CAC-CBC-CGC
29	P2	201	PEB	C2C-CAC-CBC-CGC
29	P2	202	PEB	C2C-CAC-CBC-CGC
29	Q2	202	PEB	C2C-CAC-CBC-CGC
29	R2	202	PEB	C2C-CAC-CBC-CGC
29	R2	203	PEB	C2C-CAC-CBC-CGC
29	S2	202	PEB	C2C-CAC-CBC-CGC
29	T2	202	PEB	C2C-CAC-CBC-CGC
29	T2	203	PEB	C2C-CAC-CBC-CGC
29	U2	202	PEB	C2C-CAC-CBC-CGC
29	V2	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	V2	203	PEB	C2C-CAC-CBC-CGC
29	W2	202	PEB	C2C-CAC-CBC-CGC
29	X2	201	PEB	C2C-CAC-CBC-CGC
29	X2	202	PEB	C2C-CAC-CBC-CGC
29	D3	202	PEB	C2C-CAC-CBC-CGC
29	B5	203	PEB	C2C-CAC-CBC-CGC
29	F5	203	PEB	C2C-CAC-CBC-CGC
29	G5	203	PEB	C2C-CAC-CBC-CGC
29	H5	203	PEB	C2C-CAC-CBC-CGC
29	I5	202	PEB	C2C-CAC-CBC-CGC
29	K5	202	PEB	C2C-CAC-CBC-CGC
29	L5	203	PEB	C2C-CAC-CBC-CGC
29	A5	202	PEB	C2C-CAC-CBC-CGC
29	C5	202	PEB	C2C-CAC-CBC-CGC
29	A7	304	PEB	C2C-CAC-CBC-CGC
29	B8	203	PEB	C2C-CAC-CBC-CGC
29	F8	203	PEB	C2C-CAC-CBC-CGC
29	G8	203	PEB	C2C-CAC-CBC-CGC
29	H8	203	PEB	C2C-CAC-CBC-CGC
29	I8	202	PEB	C2C-CAC-CBC-CGC
29	K8	202	PEB	C2C-CAC-CBC-CGC
29	L8	203	PEB	C2C-CAC-CBC-CGC
29	A8	202	PEB	C2C-CAC-CBC-CGC
29	C8	202	PEB	C2C-CAC-CBC-CGC
29	A9	304	PEB	C2C-CAC-CBC-CGC
29	AA	202	PEB	C2C-CAC-CBC-CGC
29	CA	202	PEB	C2C-CAC-CBC-CGC
29	EA	202	PEB	C2C-CAC-CBC-CGC
29	GA	202	PEB	C2C-CAC-CBC-CGC
29	IA	202	PEB	C2C-CAC-CBC-CGC
29	KA	202	PEB	C2C-CAC-CBC-CGC
29	DB	203	PEB	C2C-CAC-CBC-CGC
29	FB	203	PEB	C2C-CAC-CBC-CGC
29	HB	203	PEB	C2C-CAC-CBC-CGC
29	JB	203	PEB	C2C-CAC-CBC-CGC
29	LB	203	PEB	C2C-CAC-CBC-CGC
29	NB	202	PEB	C2C-CAC-CBC-CGC
29	PB	202	PEB	C2C-CAC-CBC-CGC
29	RB	203	PEB	C2C-CAC-CBC-CGC
29	TB	203	PEB	C2C-CAC-CBC-CGC
29	VB	203	PEB	C2C-CAC-CBC-CGC
29	XB	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	ZB	203	PEB	C2C-CAC-CBC-CGC
29	cB	203	PEB	C2C-CAC-CBC-CGC
29	eB	202	PEB	C2C-CAC-CBC-CGC
29	gB	203	PEB	C2C-CAC-CBC-CGC
29	iB	203	PEB	C2C-CAC-CBC-CGC
29	kB	203	PEB	C2C-CAC-CBC-CGC
29	mB	203	PEB	C2C-CAC-CBC-CGC
29	AC	201	PEB	C2C-CAC-CBC-CGC
29	AC	202	PEB	C2C-CAC-CBC-CGC
29	BC	203	PEB	C2C-CAC-CBC-CGC
29	CC	201	PEB	C2C-CAC-CBC-CGC
29	CC	202	PEB	C2C-CAC-CBC-CGC
29	DC	202	PEB	C2C-CAC-CBC-CGC
29	EC	201	PEB	C2C-CAC-CBC-CGC
29	EC	202	PEB	C2C-CAC-CBC-CGC
29	FC	203	PEB	C2C-CAC-CBC-CGC
29	GC	201	PEB	C2C-CAC-CBC-CGC
29	GC	202	PEB	C2C-CAC-CBC-CGC
29	HC	203	PEB	C2C-CAC-CBC-CGC
29	IC	201	PEB	C2C-CAC-CBC-CGC
29	IC	202	PEB	C2C-CAC-CBC-CGC
29	JC	202	PEB	C2C-CAC-CBC-CGC
29	KC	202	PEB	C2C-CAC-CBC-CGC
29	KC	203	PEB	C2C-CAC-CBC-CGC
29	LC	203	PEB	C2C-CAC-CBC-CGC
29	AE	201	PEB	C2C-CAC-CBC-CGC
29	AE	202	PEB	C2C-CAC-CBC-CGC
29	BE	203	PEB	C2C-CAC-CBC-CGC
29	CE	201	PEB	C2C-CAC-CBC-CGC
29	CE	202	PEB	C2C-CAC-CBC-CGC
29	DE	202	PEB	C2C-CAC-CBC-CGC
29	EE	201	PEB	C2C-CAC-CBC-CGC
29	EE	202	PEB	C2C-CAC-CBC-CGC
29	FE	203	PEB	C2C-CAC-CBC-CGC
29	GE	201	PEB	C2C-CAC-CBC-CGC
29	GE	202	PEB	C2C-CAC-CBC-CGC
29	HE	203	PEB	C2C-CAC-CBC-CGC
29	IE	201	PEB	C2C-CAC-CBC-CGC
29	IE	202	PEB	C2C-CAC-CBC-CGC
29	JE	202	PEB	C2C-CAC-CBC-CGC
29	KE	202	PEB	C2C-CAC-CBC-CGC
29	KE	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	LE	203	PEB	C2C-CAC-CBC-CGC
29	AG	201	PEB	C2C-CAC-CBC-CGC
29	BG	202	PEB	C2C-CAC-CBC-CGC
29	BG	203	PEB	C2C-CAC-CBC-CGC
29	CG	201	PEB	C2C-CAC-CBC-CGC
29	DG	202	PEB	C2C-CAC-CBC-CGC
29	DG	203	PEB	C2C-CAC-CBC-CGC
29	EG	201	PEB	C2C-CAC-CBC-CGC
29	FG	202	PEB	C2C-CAC-CBC-CGC
29	FG	203	PEB	C2C-CAC-CBC-CGC
29	GG	201	PEB	C2C-CAC-CBC-CGC
29	HG	202	PEB	C2C-CAC-CBC-CGC
29	HG	203	PEB	C2C-CAC-CBC-CGC
29	IG	201	PEB	C2C-CAC-CBC-CGC
29	JG	202	PEB	C2C-CAC-CBC-CGC
29	JG	203	PEB	C2C-CAC-CBC-CGC
29	KG	201	PEB	C2C-CAC-CBC-CGC
29	LG	202	PEB	C2C-CAC-CBC-CGC
29	LG	203	PEB	C2C-CAC-CBC-CGC
29	BJ	203	PEB	C2C-CAC-CBC-CGC
29	DJ	202	PEB	C2C-CAC-CBC-CGC
29	FJ	203	PEB	C2C-CAC-CBC-CGC
29	HJ	202	PEB	C2C-CAC-CBC-CGC
29	JJ	203	PEB	C2C-CAC-CBC-CGC
29	LJ	202	PEB	C2C-CAC-CBC-CGC
29	NJ	203	PEB	C2C-CAC-CBC-CGC
29	PJ	203	PEB	C2C-CAC-CBC-CGC
29	RJ	203	PEB	C2C-CAC-CBC-CGC
29	TJ	203	PEB	C2C-CAC-CBC-CGC
29	VJ	202	PEB	C2C-CAC-CBC-CGC
29	XJ	203	PEB	C2C-CAC-CBC-CGC
29	ZJ	203	PEB	C2C-CAC-CBC-CGC
29	bJ	203	PEB	C2C-CAC-CBC-CGC
29	dJ	203	PEB	C2C-CAC-CBC-CGC
29	fJ	203	PEB	C2C-CAC-CBC-CGC
29	hJ	203	PEB	C2C-CAC-CBC-CGC
29	jJ	203	PEB	C2C-CAC-CBC-CGC
29	lJ	203	PEB	C2C-CAC-CBC-CGC
29	nJ	203	PEB	C2C-CAC-CBC-CGC
29	pJ	203	PEB	C2C-CAC-CBC-CGC
29	rJ	203	PEB	C2C-CAC-CBC-CGC
29	tJ	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	vJ	202	PEB	C2C-CAC-CBC-CGC
29	AK	302	PEB	C2C-CAC-CBC-CGC
29	AK	303	PEB	C2C-CAC-CBC-CGC
29	OK	202	PEB	C2C-CAC-CBC-CGC
29	PK	201	PEB	C2C-CAC-CBC-CGC
29	QK	202	PEB	C2C-CAC-CBC-CGC
29	RK	201	PEB	C2C-CAC-CBC-CGC
29	SK	202	PEB	C2C-CAC-CBC-CGC
29	TK	201	PEB	C2C-CAC-CBC-CGC
29	UK	203	PEB	C2C-CAC-CBC-CGC
29	VK	201	PEB	C2C-CAC-CBC-CGC
29	WK	202	PEB	C2C-CAC-CBC-CGC
29	YK	201	PEB	C2C-CAC-CBC-CGC
29	ZK	203	PEB	C2C-CAC-CBC-CGC
29	aK	201	PEB	C2C-CAC-CBC-CGC
29	bK	202	PEB	C2C-CAC-CBC-CGC
29	cK	201	PEB	C2C-CAC-CBC-CGC
29	dK	202	PEB	C2C-CAC-CBC-CGC
29	eK	201	PEB	C2C-CAC-CBC-CGC
29	fK	202	PEB	C2C-CAC-CBC-CGC
29	gK	201	PEB	C2C-CAC-CBC-CGC
29	hK	202	PEB	C2C-CAC-CBC-CGC
29	iK	201	PEB	C2C-CAC-CBC-CGC
29	jK	202	PEB	C2C-CAC-CBC-CGC
29	kK	201	PEB	C2C-CAC-CBC-CGC
29	lK	202	PEB	C2C-CAC-CBC-CGC
29	mK	201	PEB	C2C-CAC-CBC-CGC
29	BL	203	PEB	C2C-CAC-CBC-CGC
29	DL	202	PEB	C2C-CAC-CBC-CGC
29	FL	203	PEB	C2C-CAC-CBC-CGC
29	HL	202	PEB	C2C-CAC-CBC-CGC
29	JL	203	PEB	C2C-CAC-CBC-CGC
29	LL	202	PEB	C2C-CAC-CBC-CGC
29	NL	203	PEB	C2C-CAC-CBC-CGC
29	PL	203	PEB	C2C-CAC-CBC-CGC
29	RL	203	PEB	C2C-CAC-CBC-CGC
29	TL	203	PEB	C2C-CAC-CBC-CGC
29	VL	202	PEB	C2C-CAC-CBC-CGC
29	XL	203	PEB	C2C-CAC-CBC-CGC
29	ZL	203	PEB	C2C-CAC-CBC-CGC
29	bL	203	PEB	C2C-CAC-CBC-CGC
29	dL	203	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	fL	203	PEB	C2C-CAC-CBC-CGC
29	hL	203	PEB	C2C-CAC-CBC-CGC
29	jL	203	PEB	C2C-CAC-CBC-CGC
29	lL	203	PEB	C2C-CAC-CBC-CGC
29	nL	203	PEB	C2C-CAC-CBC-CGC
29	pL	203	PEB	C2C-CAC-CBC-CGC
29	rL	203	PEB	C2C-CAC-CBC-CGC
29	tL	202	PEB	C2C-CAC-CBC-CGC
29	vL	202	PEB	C2C-CAC-CBC-CGC
29	DM	203	PEB	C2C-CAC-CBC-CGC
29	FM	203	PEB	C2C-CAC-CBC-CGC
29	HM	203	PEB	C2C-CAC-CBC-CGC
29	JM	203	PEB	C2C-CAC-CBC-CGC
29	LM	203	PEB	C2C-CAC-CBC-CGC
29	NM	202	PEB	C2C-CAC-CBC-CGC
29	PM	202	PEB	C2C-CAC-CBC-CGC
29	RM	203	PEB	C2C-CAC-CBC-CGC
29	TM	203	PEB	C2C-CAC-CBC-CGC
29	VM	203	PEB	C2C-CAC-CBC-CGC
29	XM	202	PEB	C2C-CAC-CBC-CGC
29	ZM	203	PEB	C2C-CAC-CBC-CGC
29	cM	203	PEB	C2C-CAC-CBC-CGC
29	eM	202	PEB	C2C-CAC-CBC-CGC
29	gM	203	PEB	C2C-CAC-CBC-CGC
29	iM	203	PEB	C2C-CAC-CBC-CGC
29	kM	203	PEB	C2C-CAC-CBC-CGC
29	mM	203	PEB	C2C-CAC-CBC-CGC
29	AN	202	PEB	C2C-CAC-CBC-CGC
29	CN	202	PEB	C2C-CAC-CBC-CGC
29	EN	202	PEB	C2C-CAC-CBC-CGC
29	GN	202	PEB	C2C-CAC-CBC-CGC
29	IN	202	PEB	C2C-CAC-CBC-CGC
29	KN	202	PEB	C2C-CAC-CBC-CGC
29	DO	202	PEB	C2C-CAC-CBC-CGC
29	AQ	201	PEB	C2C-CAC-CBC-CGC
29	BQ	202	PEB	C2C-CAC-CBC-CGC
29	BQ	203	PEB	C2C-CAC-CBC-CGC
29	CQ	201	PEB	C2C-CAC-CBC-CGC
29	DQ	202	PEB	C2C-CAC-CBC-CGC
29	DQ	203	PEB	C2C-CAC-CBC-CGC
29	EQ	201	PEB	C2C-CAC-CBC-CGC
29	FQ	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	FQ	203	PEB	C2C-CAC-CBC-CGC
29	GQ	201	PEB	C2C-CAC-CBC-CGC
29	HQ	202	PEB	C2C-CAC-CBC-CGC
29	HQ	203	PEB	C2C-CAC-CBC-CGC
29	IQ	201	PEB	C2C-CAC-CBC-CGC
29	JQ	202	PEB	C2C-CAC-CBC-CGC
29	JQ	203	PEB	C2C-CAC-CBC-CGC
29	KQ	201	PEB	C2C-CAC-CBC-CGC
29	LQ	201	PEB	C2C-CAC-CBC-CGC
29	LQ	202	PEB	C2C-CAC-CBC-CGC
29	NR	202	PEB	C2C-CAC-CBC-CGC
29	NR	203	PEB	C2C-CAC-CBC-CGC
29	PR	201	PEB	C2C-CAC-CBC-CGC
29	PR	202	PEB	C2C-CAC-CBC-CGC
29	QR	202	PEB	C2C-CAC-CBC-CGC
29	RR	202	PEB	C2C-CAC-CBC-CGC
29	RR	203	PEB	C2C-CAC-CBC-CGC
29	SR	202	PEB	C2C-CAC-CBC-CGC
29	TR	202	PEB	C2C-CAC-CBC-CGC
29	TR	203	PEB	C2C-CAC-CBC-CGC
29	UR	202	PEB	C2C-CAC-CBC-CGC
29	VR	202	PEB	C2C-CAC-CBC-CGC
29	VR	203	PEB	C2C-CAC-CBC-CGC
29	WR	202	PEB	C2C-CAC-CBC-CGC
29	XR	202	PEB	C2C-CAC-CBC-CGC
29	XR	203	PEB	C2C-CAC-CBC-CGC
30	A7	303	PUB	C3B-CAB-CBB-CGB
30	A9	303	PUB	C3B-CAB-CBB-CGB
30	MG	402	PUB	C3B-CAB-CBB-CGB
30	MQ	404	PUB	C3B-CAB-CBB-CGB
30	BB	302	PUB	C4D-C3D-CAD-CBD
30	wJ	305	PUB	C4D-C3D-CAD-CBD
30	xJ	305	PUB	C4D-C3D-CAD-CBD
30	wL	305	PUB	C4D-C3D-CAD-CBD
30	xL	305	PUB	C4D-C3D-CAD-CBD
30	BM	302	PUB	C4D-C3D-CAD-CBD
31	C7	1001	CYC	C4B-C3B-CAB-CBB
31	E7	1001	CYC	C4B-C3B-CAB-CBB
31	G7	1001	CYC	C4B-C3B-CAB-CBB
31	I7	1001	CYC	C4B-C3B-CAB-CBB
31	K7	1001	CYC	C4B-C3B-CAB-CBB
31	M7	1001	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	C9	1001	CYC	C4B-C3B-CAB-CBB
31	E9	1001	CYC	C4B-C3B-CAB-CBB
31	G9	1001	CYC	C4B-C3B-CAB-CBB
31	I9	1001	CYC	C4B-C3B-CAB-CBB
31	K9	1001	CYC	C4B-C3B-CAB-CBB
31	M9	1001	CYC	C4B-C3B-CAB-CBB
29	BA	201	PEB	C2B-C3B-CAB-CBB
29	DA	201	PEB	C2B-C3B-CAB-CBB
29	FA	201	PEB	C2B-C3B-CAB-CBB
29	HA	201	PEB	C2B-C3B-CAB-CBB
29	JA	201	PEB	C2B-C3B-CAB-CBB
29	LA	201	PEB	C2B-C3B-CAB-CBB
29	BN	201	PEB	C2B-C3B-CAB-CBB
29	DN	201	PEB	C2B-C3B-CAB-CBB
29	FN	201	PEB	C2B-C3B-CAB-CBB
29	HN	201	PEB	C2B-C3B-CAB-CBB
29	JN	201	PEB	C2B-C3B-CAB-CBB
29	LN	201	PEB	C2B-C3B-CAB-CBB
31	FF	1001	CYC	C2B-C3B-CAB-CBB
31	FI	1001	CYC	C2B-C3B-CAB-CBB
31	DF	1001	CYC	C2B-C3B-CAB-CBB
31	HF	1001	CYC	C2B-C3B-CAB-CBB
31	JF	1001	CYC	C2B-C3B-CAB-CBB
31	NF	1001	CYC	C2B-C3B-CAB-CBB
31	DI	1001	CYC	C2B-C3B-CAB-CBB
31	HI	1001	CYC	C2B-C3B-CAB-CBB
31	JI	1001	CYC	C2B-C3B-CAB-CBB
31	NI	1001	CYC	C2B-C3B-CAB-CBB
29	A1	301	PEB	C3B-CAB-CBB-CGB
29	W1	202	PEB	C3B-CAB-CBB-CGB
29	Z1	203	PEB	C3B-CAB-CBB-CGB
29	f1	202	PEB	C3B-CAB-CBB-CGB
29	h1	202	PEB	C3B-CAB-CBB-CGB
29	A7	305	PEB	C3B-CAB-CBB-CGB
29	A9	305	PEB	C3B-CAB-CBB-CGB
29	AB	301	PEB	C3B-CAB-CBB-CGB
29	AC	202	PEB	C3B-CAB-CBB-CGB
29	CC	202	PEB	C3B-CAB-CBB-CGB
29	EC	202	PEB	C3B-CAB-CBB-CGB
29	GC	202	PEB	C3B-CAB-CBB-CGB
29	IC	202	PEB	C3B-CAB-CBB-CGB
29	KC	203	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	AE	202	PEB	C3B-CAB-CBB-CGB
29	CE	202	PEB	C3B-CAB-CBB-CGB
29	EE	202	PEB	C3B-CAB-CBB-CGB
29	GE	202	PEB	C3B-CAB-CBB-CGB
29	IE	202	PEB	C3B-CAB-CBB-CGB
29	KE	203	PEB	C3B-CAB-CBB-CGB
29	BG	203	PEB	C3B-CAB-CBB-CGB
29	DG	203	PEB	C3B-CAB-CBB-CGB
29	FG	203	PEB	C3B-CAB-CBB-CGB
29	HG	203	PEB	C3B-CAB-CBB-CGB
29	JG	203	PEB	C3B-CAB-CBB-CGB
29	LG	203	PEB	C3B-CAB-CBB-CGB
29	wJ	301	PEB	C3B-CAB-CBB-CGB
29	xJ	301	PEB	C3B-CAB-CBB-CGB
29	yJ	301	PEB	C3B-CAB-CBB-CGB
29	AK	301	PEB	C3B-CAB-CBB-CGB
29	WK	202	PEB	C3B-CAB-CBB-CGB
29	ZK	203	PEB	C3B-CAB-CBB-CGB
29	fK	202	PEB	C3B-CAB-CBB-CGB
29	hK	202	PEB	C3B-CAB-CBB-CGB
29	wL	301	PEB	C3B-CAB-CBB-CGB
29	xL	301	PEB	C3B-CAB-CBB-CGB
29	yL	301	PEB	C3B-CAB-CBB-CGB
29	AM	301	PEB	C3B-CAB-CBB-CGB
29	BQ	203	PEB	C3B-CAB-CBB-CGB
29	DQ	203	PEB	C3B-CAB-CBB-CGB
29	FQ	203	PEB	C3B-CAB-CBB-CGB
29	HQ	203	PEB	C3B-CAB-CBB-CGB
29	JQ	203	PEB	C3B-CAB-CBB-CGB
29	LQ	202	PEB	C3B-CAB-CBB-CGB
29	OR	202	PEB	C3B-CAB-CBB-CGB
31	AP	1001	CYC	C2A-CAA-CBA-CGA
31	CP	1001	CYC	C2A-CAA-CBA-CGA
31	EP	1001	CYC	C2A-CAA-CBA-CGA
31	GP	1001	CYC	C2A-CAA-CBA-CGA
31	JP	1001	CYC	C2A-CAA-CBA-CGA
31	KP	1001	CYC	C2A-CAA-CBA-CGA
31	NP	1001	CYC	C2A-CAA-CBA-CGA
31	PP	1001	CYC	C2A-CAA-CBA-CGA
31	RP	1001	CYC	C2A-CAA-CBA-CGA
31	TP	1001	CYC	C2A-CAA-CBA-CGA
31	VP	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
31	cP	1001	CYC	C2A-CAA-CBA-CGA
31	eP	1001	CYC	C2A-CAA-CBA-CGA
31	gP	1001	CYC	C2A-CAA-CBA-CGA
31	iP	1001	CYC	C2A-CAA-CBA-CGA
31	lP	1001	CYC	C2A-CAA-CBA-CGA
31	mP	1001	CYC	C2A-CAA-CBA-CGA
31	pP	1001	CYC	C2A-CAA-CBA-CGA
31	rP	1001	CYC	C2A-CAA-CBA-CGA
31	tP	1001	CYC	C2A-CAA-CBA-CGA
31	vP	1001	CYC	C2A-CAA-CBA-CGA
31	xP	1001	CYC	NA-C4A-CHB-C1B
31	LF	1001	CYC	C2B-C3B-CAB-CBB
31	LI	1001	CYC	C2B-C3B-CAB-CBB
30	MG	402	PUB	C4A-C3A-CAA-CBA
30	MQ	404	PUB	C4A-C3A-CAA-CBA
31	D1	1003	CYC	C2B-C3B-CAB-CBB
31	IK	1001	CYC	C2B-C3B-CAB-CBB
31	D7	1001	CYC	C2B-C3B-CAB-CBB
31	F7	1001	CYC	C2B-C3B-CAB-CBB
31	N7	1001	CYC	C2B-C3B-CAB-CBB
31	D9	1001	CYC	C2B-C3B-CAB-CBB
31	F9	1001	CYC	C2B-C3B-CAB-CBB
31	N9	1001	CYC	C2B-C3B-CAB-CBB
29	O1	202	PEB	C3B-CAB-CBB-CGB
29	Q1	202	PEB	C3B-CAB-CBB-CGB
29	S1	202	PEB	C3B-CAB-CBB-CGB
29	U1	203	PEB	C3B-CAB-CBB-CGB
29	b1	202	PEB	C3B-CAB-CBB-CGB
29	d1	202	PEB	C3B-CAB-CBB-CGB
29	j1	202	PEB	C3B-CAB-CBB-CGB
29	l1	202	PEB	C3B-CAB-CBB-CGB
29	J5	201	PEB	NB-C1B-CHA-C4A
29	J8	201	PEB	NB-C1B-CHA-C4A
29	MA	405	PEB	NB-C1B-CHA-C4A
29	AF	304	PEB	C3B-CAB-CBB-CGB
29	DF	1002	PEB	C3B-CAB-CBB-CGB
29	FF	1002	PEB	C3B-CAB-CBB-CGB
29	HF	1002	PEB	C3B-CAB-CBB-CGB
29	JF	1002	PEB	C3B-CAB-CBB-CGB
29	LF	1002	PEB	C3B-CAB-CBB-CGB
29	NF	1002	PEB	C3B-CAB-CBB-CGB
29	AG	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	CG	201	PEB	C3B-CAB-CBB-CGB
29	EG	201	PEB	C3B-CAB-CBB-CGB
29	GG	201	PEB	C3B-CAB-CBB-CGB
29	IG	201	PEB	C3B-CAB-CBB-CGB
29	KG	201	PEB	C3B-CAB-CBB-CGB
29	AI	304	PEB	C3B-CAB-CBB-CGB
29	DI	1002	PEB	C3B-CAB-CBB-CGB
29	FI	1002	PEB	C3B-CAB-CBB-CGB
29	HI	1002	PEB	C3B-CAB-CBB-CGB
29	JI	1002	PEB	C3B-CAB-CBB-CGB
29	LI	1002	PEB	C3B-CAB-CBB-CGB
29	NI	1002	PEB	C3B-CAB-CBB-CGB
29	OK	202	PEB	C3B-CAB-CBB-CGB
29	QK	202	PEB	C3B-CAB-CBB-CGB
29	SK	202	PEB	C3B-CAB-CBB-CGB
29	UK	203	PEB	C3B-CAB-CBB-CGB
29	bK	202	PEB	C3B-CAB-CBB-CGB
29	dK	202	PEB	C3B-CAB-CBB-CGB
29	jK	202	PEB	C3B-CAB-CBB-CGB
29	lK	202	PEB	C3B-CAB-CBB-CGB
29	MN	405	PEB	NB-C1B-CHA-C4A
29	AQ	201	PEB	C3B-CAB-CBB-CGB
29	CQ	201	PEB	C3B-CAB-CBB-CGB
29	EQ	201	PEB	C3B-CAB-CBB-CGB
29	GQ	201	PEB	C3B-CAB-CBB-CGB
29	IQ	201	PEB	C3B-CAB-CBB-CGB
29	KQ	201	PEB	C3B-CAB-CBB-CGB
31	AP	1001	CYC	NA-C4A-CHB-C1B
31	DP	1001	CYC	NA-C4A-CHB-C1B
31	DP	1001	CYC	C2A-CAA-CBA-CGA
31	CP	1001	CYC	NA-C4A-CHB-C1B
31	FP	1001	CYC	NA-C4A-CHB-C1B
31	FP	1001	CYC	C2A-CAA-CBA-CGA
31	EP	1001	CYC	NA-C4A-CHB-C1B
31	BP	1001	CYC	NA-C4A-CHB-C1B
31	BP	1001	CYC	C2A-CAA-CBA-CGA
31	GP	1001	CYC	NA-C4A-CHB-C1B
31	HP	1001	CYC	NA-C4A-CHB-C1B
31	HP	1001	CYC	C2A-CAA-CBA-CGA
31	IP	1001	CYC	NA-C4A-CHB-C1B
31	IP	1001	CYC	C2A-CAA-CBA-CGA
31	JP	1001	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
31	KP	1001	CYC	NA-C4A-CHB-C1B
31	MP	1001	CYC	NA-C4A-CHB-C1B
31	MP	1001	CYC	C2A-CAA-CBA-CGA
31	NP	1001	CYC	NA-C4A-CHB-C1B
31	OP	1001	CYC	NA-C4A-CHB-C1B
31	OP	1001	CYC	C2A-CAA-CBA-CGA
31	PP	1001	CYC	NA-C4A-CHB-C1B
31	QP	1001	CYC	NA-C4A-CHB-C1B
31	QP	1001	CYC	C2A-CAA-CBA-CGA
31	RP	1001	CYC	NA-C4A-CHB-C1B
31	SP	1001	CYC	NA-C4A-CHB-C1B
31	SP	1001	CYC	C2A-CAA-CBA-CGA
31	TP	1001	CYC	NA-C4A-CHB-C1B
31	UP	1001	CYC	NA-C4A-CHB-C1B
31	UP	1001	CYC	C2A-CAA-CBA-CGA
31	WP	1001	CYC	NA-C4A-CHB-C1B
31	XP	1001	CYC	NA-C4A-CHB-C1B
31	XP	1001	CYC	C2A-CAA-CBA-CGA
31	cP	1001	CYC	NA-C4A-CHB-C1B
31	eP	1001	CYC	NA-C4A-CHB-C1B
31	fP	1001	CYC	NA-C4A-CHB-C1B
31	fP	1001	CYC	C2A-CAA-CBA-CGA
31	gP	1001	CYC	NA-C4A-CHB-C1B
31	hP	1001	CYC	NA-C4A-CHB-C1B
31	hP	1001	CYC	C2A-CAA-CBA-CGA
31	iP	1001	CYC	NA-C4A-CHB-C1B
31	jP	1001	CYC	NA-C4A-CHB-C1B
31	jP	1001	CYC	C2A-CAA-CBA-CGA
31	kP	1001	CYC	NA-C4A-CHB-C1B
31	kP	1001	CYC	C2A-CAA-CBA-CGA
31	lP	1001	CYC	NA-C4A-CHB-C1B
31	mP	1001	CYC	NA-C4A-CHB-C1B
31	nP	1001	CYC	NA-C4A-CHB-C1B
31	nP	1001	CYC	C2A-CAA-CBA-CGA
31	oP	1001	CYC	NA-C4A-CHB-C1B
31	oP	1001	CYC	C2A-CAA-CBA-CGA
31	pP	1001	CYC	NA-C4A-CHB-C1B
31	qP	1001	CYC	NA-C4A-CHB-C1B
31	qP	1001	CYC	C2A-CAA-CBA-CGA
31	rP	1001	CYC	NA-C4A-CHB-C1B
31	sP	1001	CYC	NA-C4A-CHB-C1B
31	sP	1001	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	tP	1001	CYC	NA-C4A-CHB-C1B
31	uP	1001	CYC	NA-C4A-CHB-C1B
31	uP	1001	CYC	C2A-CAA-CBA-CGA
31	vP	1001	CYC	NA-C4A-CHB-C1B
31	wP	1001	CYC	NA-C4A-CHB-C1B
31	wP	1001	CYC	C2A-CAA-CBA-CGA
31	yP	1001	CYC	NA-C4A-CHB-C1B
31	1P	1001	CYC	NA-C4A-CHB-C1B
31	1P	1001	CYC	C2A-CAA-CBA-CGA
31	C1	1001	CYC	C2B-C3B-CAB-CBB
31	I1	1001	CYC	C2B-C3B-CAB-CBB
31	K1	1001	CYC	C2B-C3B-CAB-CBB
31	M1	1001	CYC	C2B-C3B-CAB-CBB
31	H7	1001	CYC	C2B-C3B-CAB-CBB
31	J7	1001	CYC	C2B-C3B-CAB-CBB
31	L7	1001	CYC	C2B-C3B-CAB-CBB
31	H9	1001	CYC	C2B-C3B-CAB-CBB
31	J9	1001	CYC	C2B-C3B-CAB-CBB
31	L9	1001	CYC	C2B-C3B-CAB-CBB
31	CK	1001	CYC	C2B-C3B-CAB-CBB
31	EK	1001	CYC	C2B-C3B-CAB-CBB
31	GK	1001	CYC	C2B-C3B-CAB-CBB
31	KK	1001	CYC	C2B-C3B-CAB-CBB
31	MK	1001	CYC	C2B-C3B-CAB-CBB
31	E1	1001	CYC	C2B-C3B-CAB-CBB
29	MA	405	PEB	C2B-C1B-CHA-C4A
29	MN	405	PEB	C2B-C1B-CHA-C4A
31	D7	1001	CYC	C3A-C4A-CHB-C1B
31	F7	1001	CYC	C3A-C4A-CHB-C1B
31	H7	1001	CYC	C3A-C4A-CHB-C1B
31	J7	1001	CYC	C3A-C4A-CHB-C1B
31	L7	1001	CYC	C3A-C4A-CHB-C1B
31	N7	1001	CYC	C3A-C4A-CHB-C1B
31	D9	1001	CYC	C3A-C4A-CHB-C1B
31	F9	1001	CYC	C3A-C4A-CHB-C1B
31	H9	1001	CYC	C3A-C4A-CHB-C1B
31	J9	1001	CYC	C3A-C4A-CHB-C1B
31	L9	1001	CYC	C3A-C4A-CHB-C1B
31	N9	1001	CYC	C3A-C4A-CHB-C1B
31	AP	1001	CYC	C3A-C4A-CHB-C1B
31	DP	1001	CYC	C3A-C4A-CHB-C1B
31	CP	1001	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
31	FP	1001	CYC	C3A-C4A-CHB-C1B
31	EP	1001	CYC	C3A-C4A-CHB-C1B
31	BP	1001	CYC	C3A-C4A-CHB-C1B
31	GP	1001	CYC	C3A-C4A-CHB-C1B
31	HP	1001	CYC	C3A-C4A-CHB-C1B
31	IP	1001	CYC	C3A-C4A-CHB-C1B
31	JP	1001	CYC	C3A-C4A-CHB-C1B
31	KP	1001	CYC	C3A-C4A-CHB-C1B
31	MP	1001	CYC	C3A-C4A-CHB-C1B
31	NP	1001	CYC	C3A-C4A-CHB-C1B
31	OP	1001	CYC	C3A-C4A-CHB-C1B
31	PP	1001	CYC	C3A-C4A-CHB-C1B
31	QP	1001	CYC	C3A-C4A-CHB-C1B
31	RP	1001	CYC	C3A-C4A-CHB-C1B
31	SP	1001	CYC	C3A-C4A-CHB-C1B
31	TP	1001	CYC	C3A-C4A-CHB-C1B
31	UP	1001	CYC	C3A-C4A-CHB-C1B
31	WP	1001	CYC	C3A-C4A-CHB-C1B
31	XP	1001	CYC	C3A-C4A-CHB-C1B
31	eP	1001	CYC	C3A-C4A-CHB-C1B
31	eP	1001	CYC	C3A-C4A-CHB-C1B
31	fP	1001	CYC	C3A-C4A-CHB-C1B
31	gP	1001	CYC	C3A-C4A-CHB-C1B
31	hP	1001	CYC	C3A-C4A-CHB-C1B
31	iP	1001	CYC	C3A-C4A-CHB-C1B
31	jP	1001	CYC	C3A-C4A-CHB-C1B
31	kP	1001	CYC	C3A-C4A-CHB-C1B
31	lP	1001	CYC	C3A-C4A-CHB-C1B
31	mP	1001	CYC	C3A-C4A-CHB-C1B
31	nP	1001	CYC	C3A-C4A-CHB-C1B
31	oP	1001	CYC	C3A-C4A-CHB-C1B
31	pP	1001	CYC	C3A-C4A-CHB-C1B
31	qP	1001	CYC	C3A-C4A-CHB-C1B
31	rP	1001	CYC	C3A-C4A-CHB-C1B
31	sP	1001	CYC	C3A-C4A-CHB-C1B
31	tP	1001	CYC	C3A-C4A-CHB-C1B
31	uP	1001	CYC	C3A-C4A-CHB-C1B
31	vP	1001	CYC	C3A-C4A-CHB-C1B
31	wP	1001	CYC	C3A-C4A-CHB-C1B
31	yP	1001	CYC	C3A-C4A-CHB-C1B
31	1P	1001	CYC	C3A-C4A-CHB-C1B
29	B3	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	D3	201	PEB	C2C-CAC-CBC-CGC
29	F3	201	PEB	C2C-CAC-CBC-CGC
29	H3	201	PEB	C2C-CAC-CBC-CGC
29	J3	201	PEB	C2C-CAC-CBC-CGC
29	L3	201	PEB	C2C-CAC-CBC-CGC
29	M3	202	PEB	C2C-CAC-CBC-CGC
29	N3	202	PEB	C2C-CAC-CBC-CGC
29	BO	201	PEB	C2C-CAC-CBC-CGC
29	DO	201	PEB	C2C-CAC-CBC-CGC
29	FO	201	PEB	C2C-CAC-CBC-CGC
29	HO	201	PEB	C2C-CAC-CBC-CGC
29	JO	201	PEB	C2C-CAC-CBC-CGC
29	LO	201	PEB	C2C-CAC-CBC-CGC
29	MO	202	PEB	C2C-CAC-CBC-CGC
29	NO	202	PEB	C2C-CAC-CBC-CGC
29	SR	201	PEB	C2C-CAC-CBC-CGC
30	yJ	302	PUB	C3B-CAB-CBB-CGB
30	yL	302	PUB	C3B-CAB-CBB-CGB
29	D7	1002	PEB	C4B-C3B-CAB-CBB
29	F7	1002	PEB	C4B-C3B-CAB-CBB
29	H7	1002	PEB	C4B-C3B-CAB-CBB
29	J7	1002	PEB	C4B-C3B-CAB-CBB
29	L7	1002	PEB	C4B-C3B-CAB-CBB
29	N7	1002	PEB	C4B-C3B-CAB-CBB
29	D9	1002	PEB	C4B-C3B-CAB-CBB
29	F9	1002	PEB	C4B-C3B-CAB-CBB
29	H9	1002	PEB	C4B-C3B-CAB-CBB
29	J9	1002	PEB	C4B-C3B-CAB-CBB
29	L9	1002	PEB	C4B-C3B-CAB-CBB
29	N9	1002	PEB	C4B-C3B-CAB-CBB
32	k6	302	PMS	S-C-C1-C2
32	k6	302	PMS	S-C-C1-C6
32	kH	302	PMS	S-C-C1-C2
32	kH	302	PMS	S-C-C1-C6
29	C4	201	PEB	C4D-C3D-CAD-CBD
29	E4	201	PEB	C4D-C3D-CAD-CBD
29	G4	201	PEB	C4D-C3D-CAD-CBD
29	I4	201	PEB	C4D-C3D-CAD-CBD
29	K4	201	PEB	C4D-C3D-CAD-CBD
29	M4	201	PEB	C4D-C3D-CAD-CBD
29	dD	401	PEB	C4D-C3D-CAD-CBD
29	CD	201	PEB	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
29	GD	201	PEB	C4D-C3D-CAD-CBD
29	ID	201	PEB	C4D-C3D-CAD-CBD
29	KD	201	PEB	C4D-C3D-CAD-CBD
29	MD	201	PEB	C4D-C3D-CAD-CBD
29	BG	201	PEB	C4D-C3D-CAD-CBD
29	DG	201	PEB	C4D-C3D-CAD-CBD
29	FG	201	PEB	C4D-C3D-CAD-CBD
29	HG	201	PEB	C4D-C3D-CAD-CBD
29	JG	201	PEB	C4D-C3D-CAD-CBD
29	LG	201	PEB	C4D-C3D-CAD-CBD
29	BQ	201	PEB	C4D-C3D-CAD-CBD
29	DQ	201	PEB	C4D-C3D-CAD-CBD
29	FQ	201	PEB	C4D-C3D-CAD-CBD
29	HQ	201	PEB	C4D-C3D-CAD-CBD
29	JQ	201	PEB	C4D-C3D-CAD-CBD
29	MQ	402	PEB	C4D-C3D-CAD-CBD
29	J5	202	PEB	C3B-CAB-CBB-CGB
29	J8	202	PEB	C3B-CAB-CBB-CGB
29	AJ	201	PEB	C3B-CAB-CBB-CGB
29	CJ	201	PEB	C3B-CAB-CBB-CGB
29	EJ	201	PEB	C3B-CAB-CBB-CGB
29	GJ	201	PEB	C3B-CAB-CBB-CGB
29	IJ	201	PEB	C3B-CAB-CBB-CGB
29	KJ	201	PEB	C3B-CAB-CBB-CGB
29	MJ	201	PEB	C3B-CAB-CBB-CGB
29	OJ	201	PEB	C3B-CAB-CBB-CGB
29	QJ	201	PEB	C3B-CAB-CBB-CGB
29	SJ	201	PEB	C3B-CAB-CBB-CGB
29	UJ	201	PEB	C3B-CAB-CBB-CGB
29	WJ	202	PEB	C3B-CAB-CBB-CGB
29	YJ	201	PEB	C3B-CAB-CBB-CGB
29	aJ	201	PEB	C3B-CAB-CBB-CGB
29	cJ	201	PEB	C3B-CAB-CBB-CGB
29	eJ	201	PEB	C3B-CAB-CBB-CGB
29	gJ	201	PEB	C3B-CAB-CBB-CGB
29	iJ	201	PEB	C3B-CAB-CBB-CGB
29	kJ	201	PEB	C3B-CAB-CBB-CGB
29	mJ	201	PEB	C3B-CAB-CBB-CGB
29	oJ	201	PEB	C3B-CAB-CBB-CGB
29	qJ	201	PEB	C3B-CAB-CBB-CGB
29	sJ	201	PEB	C3B-CAB-CBB-CGB
29	uJ	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	AL	201	PEB	C3B-CAB-CBB-CGB
29	CL	201	PEB	C3B-CAB-CBB-CGB
29	EL	201	PEB	C3B-CAB-CBB-CGB
29	GL	201	PEB	C3B-CAB-CBB-CGB
29	IL	201	PEB	C3B-CAB-CBB-CGB
29	KL	201	PEB	C3B-CAB-CBB-CGB
29	ML	201	PEB	C3B-CAB-CBB-CGB
29	OL	201	PEB	C3B-CAB-CBB-CGB
29	QL	201	PEB	C3B-CAB-CBB-CGB
29	SL	201	PEB	C3B-CAB-CBB-CGB
29	UL	201	PEB	C3B-CAB-CBB-CGB
29	WL	202	PEB	C3B-CAB-CBB-CGB
29	YL	201	PEB	C3B-CAB-CBB-CGB
29	aL	201	PEB	C3B-CAB-CBB-CGB
29	cL	201	PEB	C3B-CAB-CBB-CGB
29	eL	201	PEB	C3B-CAB-CBB-CGB
29	gL	201	PEB	C3B-CAB-CBB-CGB
29	iL	201	PEB	C3B-CAB-CBB-CGB
29	kL	201	PEB	C3B-CAB-CBB-CGB
29	mL	201	PEB	C3B-CAB-CBB-CGB
29	oL	201	PEB	C3B-CAB-CBB-CGB
29	qL	201	PEB	C3B-CAB-CBB-CGB
29	sL	201	PEB	C3B-CAB-CBB-CGB
29	uL	202	PEB	C3B-CAB-CBB-CGB
30	AF	302	PUB	C2C-CAC-CBC-CGC
30	AI	302	PUB	C2C-CAC-CBC-CGC
29	M3	202	PEB	C2D-C3D-CAD-CBD
29	N3	202	PEB	C2D-C3D-CAD-CBD
29	C4	201	PEB	C2D-C3D-CAD-CBD
29	E4	201	PEB	C2D-C3D-CAD-CBD
29	G4	201	PEB	C2D-C3D-CAD-CBD
29	I4	201	PEB	C2D-C3D-CAD-CBD
29	K4	201	PEB	C2D-C3D-CAD-CBD
29	M4	201	PEB	C2D-C3D-CAD-CBD
29	dD	401	PEB	C2D-C3D-CAD-CBD
29	CD	201	PEB	C2D-C3D-CAD-CBD
29	GD	201	PEB	C2D-C3D-CAD-CBD
29	ID	201	PEB	C2D-C3D-CAD-CBD
29	KD	201	PEB	C2D-C3D-CAD-CBD
29	MD	201	PEB	C2D-C3D-CAD-CBD
29	BG	201	PEB	C2D-C3D-CAD-CBD
29	DG	201	PEB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
29	FG	201	PEB	C2D-C3D-CAD-CBD
29	HG	201	PEB	C2D-C3D-CAD-CBD
29	JG	201	PEB	C2D-C3D-CAD-CBD
29	LG	201	PEB	C2D-C3D-CAD-CBD
29	MO	202	PEB	C2D-C3D-CAD-CBD
29	NO	202	PEB	C2D-C3D-CAD-CBD
29	BQ	201	PEB	C2D-C3D-CAD-CBD
29	DQ	201	PEB	C2D-C3D-CAD-CBD
29	FQ	201	PEB	C2D-C3D-CAD-CBD
29	HQ	201	PEB	C2D-C3D-CAD-CBD
29	JQ	201	PEB	C2D-C3D-CAD-CBD
29	MQ	402	PEB	C2D-C3D-CAD-CBD
30	MA	402	PUB	C4A-C3A-CAA-CBA
30	MN	402	PUB	C4A-C3A-CAA-CBA
29	B5	203	PEB	C3B-CAB-CBB-CGB
29	F5	203	PEB	C3B-CAB-CBB-CGB
29	G5	203	PEB	C3B-CAB-CBB-CGB
29	H5	203	PEB	C3B-CAB-CBB-CGB
29	L5	203	PEB	C3B-CAB-CBB-CGB
29	B8	203	PEB	C3B-CAB-CBB-CGB
29	F8	203	PEB	C3B-CAB-CBB-CGB
29	G8	203	PEB	C3B-CAB-CBB-CGB
29	H8	203	PEB	C3B-CAB-CBB-CGB
29	L8	203	PEB	C3B-CAB-CBB-CGB
29	A1	303	PEB	C2A-C3A-CAA-CBA
29	O1	202	PEB	C2A-C3A-CAA-CBA
29	Q1	202	PEB	C2A-C3A-CAA-CBA
29	S1	202	PEB	C2A-C3A-CAA-CBA
29	U1	203	PEB	C2A-C3A-CAA-CBA
29	W1	202	PEB	C2A-C3A-CAA-CBA
29	Z1	203	PEB	C2A-C3A-CAA-CBA
29	b1	202	PEB	C2A-C3A-CAA-CBA
29	d1	202	PEB	C2A-C3A-CAA-CBA
29	f1	202	PEB	C2A-C3A-CAA-CBA
29	h1	202	PEB	C2A-C3A-CAA-CBA
29	j1	202	PEB	C2A-C3A-CAA-CBA
29	l1	202	PEB	C2A-C3A-CAA-CBA
29	e2	402	PEB	C2C-CAC-CBC-CGC
29	M2	202	PEB	C2A-C3A-CAA-CBA
29	N2	201	PEB	C2C-CAC-CBC-CGC
29	O2	202	PEB	C2A-C3A-CAA-CBA
29	Q2	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	R2	201	PEB	C2C-CAC-CBC-CGC
29	S2	202	PEB	C2A-C3A-CAA-CBA
29	T2	201	PEB	C2C-CAC-CBC-CGC
29	U2	202	PEB	C2A-C3A-CAA-CBA
29	V2	201	PEB	C2C-CAC-CBC-CGC
29	W2	202	PEB	C2A-C3A-CAA-CBA
29	C4	202	PEB	C2A-C3A-CAA-CBA
29	E4	202	PEB	C2A-C3A-CAA-CBA
29	G4	202	PEB	C2A-C3A-CAA-CBA
29	I4	202	PEB	C2A-C3A-CAA-CBA
29	K4	202	PEB	C2A-C3A-CAA-CBA
29	M4	202	PEB	C2A-C3A-CAA-CBA
29	I5	202	PEB	C2A-C3A-CAA-CBA
29	K5	202	PEB	C2A-C3A-CAA-CBA
29	A5	202	PEB	C2A-C3A-CAA-CBA
29	C5	202	PEB	C2A-C3A-CAA-CBA
29	O7	201	PEB	C2A-C3A-CAA-CBA
29	Q7	201	PEB	C2A-C3A-CAA-CBA
29	S7	201	PEB	C2A-C3A-CAA-CBA
29	U7	201	PEB	C2A-C3A-CAA-CBA
29	W7	201	PEB	C2A-C3A-CAA-CBA
29	Z7	201	PEB	C2A-C3A-CAA-CBA
29	b7	201	PEB	C2A-C3A-CAA-CBA
29	d7	201	PEB	C2A-C3A-CAA-CBA
29	f7	201	PEB	C2A-C3A-CAA-CBA
29	h7	201	PEB	C2A-C3A-CAA-CBA
29	j7	201	PEB	C2A-C3A-CAA-CBA
29	l7	201	PEB	C2A-C3A-CAA-CBA
29	I8	202	PEB	C2A-C3A-CAA-CBA
29	K8	202	PEB	C2A-C3A-CAA-CBA
29	A8	202	PEB	C2A-C3A-CAA-CBA
29	C8	202	PEB	C2A-C3A-CAA-CBA
29	O9	201	PEB	C2A-C3A-CAA-CBA
29	Q9	201	PEB	C2A-C3A-CAA-CBA
29	S9	201	PEB	C2A-C3A-CAA-CBA
29	U9	201	PEB	C2A-C3A-CAA-CBA
29	W9	201	PEB	C2A-C3A-CAA-CBA
29	Z9	201	PEB	C2A-C3A-CAA-CBA
29	b9	201	PEB	C2A-C3A-CAA-CBA
29	d9	201	PEB	C2A-C3A-CAA-CBA
29	f9	201	PEB	C2A-C3A-CAA-CBA
29	h9	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	j9	201	PEB	C2A-C3A-CAA-CBA
29	l9	201	PEB	C2A-C3A-CAA-CBA
29	AA	201	PEB	C2A-C3A-CAA-CBA
29	AA	202	PEB	C2A-C3A-CAA-CBA
29	CA	201	PEB	C2A-C3A-CAA-CBA
29	CA	202	PEB	C2A-C3A-CAA-CBA
29	EA	201	PEB	C2A-C3A-CAA-CBA
29	EA	202	PEB	C2A-C3A-CAA-CBA
29	GA	201	PEB	C2A-C3A-CAA-CBA
29	GA	202	PEB	C2A-C3A-CAA-CBA
29	IA	201	PEB	C2A-C3A-CAA-CBA
29	IA	202	PEB	C2A-C3A-CAA-CBA
29	KA	201	PEB	C2A-C3A-CAA-CBA
29	KA	202	PEB	C2A-C3A-CAA-CBA
29	MA	401	PEB	C2A-C3A-CAA-CBA
29	AB	303	PEB	C2A-C3A-CAA-CBA
29	BB	301	PEB	C2A-C3A-CAA-CBA
29	DB	202	PEB	C2A-C3A-CAA-CBA
29	FB	202	PEB	C2A-C3A-CAA-CBA
29	HB	202	PEB	C2A-C3A-CAA-CBA
29	JB	202	PEB	C2A-C3A-CAA-CBA
29	KB	203	PEB	C2A-C3A-CAA-CBA
29	LB	202	PEB	C2A-C3A-CAA-CBA
29	QB	202	PEB	C2A-C3A-CAA-CBA
29	RB	202	PEB	C2A-C3A-CAA-CBA
29	TB	202	PEB	C2A-C3A-CAA-CBA
29	VB	202	PEB	C2A-C3A-CAA-CBA
29	YB	201	PEB	C2A-C3A-CAA-CBA
29	ZB	202	PEB	C2A-C3A-CAA-CBA
29	aB	203	PEB	C2A-C3A-CAA-CBA
29	cB	202	PEB	C2A-C3A-CAA-CBA
29	gB	202	PEB	C2A-C3A-CAA-CBA
29	iB	202	PEB	C2A-C3A-CAA-CBA
29	kB	202	PEB	C2A-C3A-CAA-CBA
29	mB	202	PEB	C2A-C3A-CAA-CBA
29	CD	202	PEB	C2A-C3A-CAA-CBA
29	ED	201	PEB	C2A-C3A-CAA-CBA
29	GD	202	PEB	C2A-C3A-CAA-CBA
29	ID	202	PEB	C2A-C3A-CAA-CBA
29	KD	202	PEB	C2A-C3A-CAA-CBA
29	MD	202	PEB	C2A-C3A-CAA-CBA
29	DF	1002	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	FF	1002	PEB	C2A-C3A-CAA-CBA
29	HF	1002	PEB	C2A-C3A-CAA-CBA
29	JF	1002	PEB	C2A-C3A-CAA-CBA
29	LF	1002	PEB	C2A-C3A-CAA-CBA
29	NF	1002	PEB	C2A-C3A-CAA-CBA
29	OF	203	PEB	C2C-CAC-CBC-CGC
29	OF	203	PEB	C2A-C3A-CAA-CBA
29	PF	202	PEB	C2C-CAC-CBC-CGC
29	PF	202	PEB	C2A-C3A-CAA-CBA
29	UF	201	PEB	C2A-C3A-CAA-CBA
29	VF	202	PEB	C2A-C3A-CAA-CBA
29	YF	202	PEB	C2C-CAC-CBC-CGC
29	YF	202	PEB	C2A-C3A-CAA-CBA
29	aF	202	PEB	C2C-CAC-CBC-CGC
29	aF	202	PEB	C2A-C3A-CAA-CBA
29	dF	201	PEB	C2C-CAC-CBC-CGC
29	dF	201	PEB	C2A-C3A-CAA-CBA
29	eF	202	PEB	C2C-CAC-CBC-CGC
29	eF	202	PEB	C2A-C3A-CAA-CBA
29	gF	202	PEB	C2C-CAC-CBC-CGC
29	gF	202	PEB	C2A-C3A-CAA-CBA
29	iF	202	PEB	C2C-CAC-CBC-CGC
29	iF	202	PEB	C2A-C3A-CAA-CBA
29	kF	202	PEB	C2C-CAC-CBC-CGC
29	kF	202	PEB	C2A-C3A-CAA-CBA
29	mF	202	PEB	C2C-CAC-CBC-CGC
29	mF	202	PEB	C2A-C3A-CAA-CBA
29	AG	202	PEB	C2A-C3A-CAA-CBA
29	CG	202	PEB	C2A-C3A-CAA-CBA
29	EG	202	PEB	C2A-C3A-CAA-CBA
29	GG	202	PEB	C2A-C3A-CAA-CBA
29	IG	202	PEB	C2A-C3A-CAA-CBA
29	KG	202	PEB	C2A-C3A-CAA-CBA
29	DI	1002	PEB	C2A-C3A-CAA-CBA
29	FI	1002	PEB	C2A-C3A-CAA-CBA
29	HI	1002	PEB	C2A-C3A-CAA-CBA
29	JI	1002	PEB	C2A-C3A-CAA-CBA
29	LI	1002	PEB	C2A-C3A-CAA-CBA
29	NI	1002	PEB	C2A-C3A-CAA-CBA
29	OI	203	PEB	C2C-CAC-CBC-CGC
29	OI	203	PEB	C2A-C3A-CAA-CBA
29	PI	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	PI	202	PEB	C2A-C3A-CAA-CBA
29	UI	201	PEB	C2A-C3A-CAA-CBA
29	VI	202	PEB	C2A-C3A-CAA-CBA
29	YI	202	PEB	C2C-CAC-CBC-CGC
29	YI	202	PEB	C2A-C3A-CAA-CBA
29	aI	202	PEB	C2C-CAC-CBC-CGC
29	aI	202	PEB	C2A-C3A-CAA-CBA
29	dI	201	PEB	C2C-CAC-CBC-CGC
29	dI	201	PEB	C2A-C3A-CAA-CBA
29	eI	202	PEB	C2C-CAC-CBC-CGC
29	eI	202	PEB	C2A-C3A-CAA-CBA
29	gI	202	PEB	C2C-CAC-CBC-CGC
29	gI	202	PEB	C2A-C3A-CAA-CBA
29	iI	202	PEB	C2C-CAC-CBC-CGC
29	iI	202	PEB	C2A-C3A-CAA-CBA
29	kI	202	PEB	C2C-CAC-CBC-CGC
29	kI	202	PEB	C2A-C3A-CAA-CBA
29	mI	202	PEB	C2C-CAC-CBC-CGC
29	mI	202	PEB	C2A-C3A-CAA-CBA
29	AJ	201	PEB	C2A-C3A-CAA-CBA
29	AJ	203	PEB	C2A-C3A-CAA-CBA
29	BJ	202	PEB	C2A-C3A-CAA-CBA
29	CJ	201	PEB	C2A-C3A-CAA-CBA
29	EJ	201	PEB	C2A-C3A-CAA-CBA
29	FJ	202	PEB	C2A-C3A-CAA-CBA
29	GJ	201	PEB	C2A-C3A-CAA-CBA
29	HJ	201	PEB	C2A-C3A-CAA-CBA
29	IJ	201	PEB	C2A-C3A-CAA-CBA
29	IJ	203	PEB	C2A-C3A-CAA-CBA
29	JJ	202	PEB	C2A-C3A-CAA-CBA
29	KJ	201	PEB	C2A-C3A-CAA-CBA
29	MJ	201	PEB	C2A-C3A-CAA-CBA
29	NJ	202	PEB	C2A-C3A-CAA-CBA
29	OJ	201	PEB	C2A-C3A-CAA-CBA
29	PJ	202	PEB	C2A-C3A-CAA-CBA
29	QJ	201	PEB	C2A-C3A-CAA-CBA
29	RJ	202	PEB	C2A-C3A-CAA-CBA
29	SJ	201	PEB	C2A-C3A-CAA-CBA
29	TJ	202	PEB	C2A-C3A-CAA-CBA
29	UJ	201	PEB	C2A-C3A-CAA-CBA
29	WJ	201	PEB	C2A-C3A-CAA-CBA
29	WJ	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	XJ	202	PEB	C2A-C3A-CAA-CBA
29	YJ	201	PEB	C2A-C3A-CAA-CBA
29	ZJ	202	PEB	C2A-C3A-CAA-CBA
29	aJ	201	PEB	C2A-C3A-CAA-CBA
29	bJ	202	PEB	C2A-C3A-CAA-CBA
29	cJ	201	PEB	C2A-C3A-CAA-CBA
29	dJ	202	PEB	C2A-C3A-CAA-CBA
29	eJ	201	PEB	C2A-C3A-CAA-CBA
29	fJ	202	PEB	C2A-C3A-CAA-CBA
29	gJ	201	PEB	C2A-C3A-CAA-CBA
29	hJ	202	PEB	C2A-C3A-CAA-CBA
29	iJ	201	PEB	C2A-C3A-CAA-CBA
29	jJ	202	PEB	C2A-C3A-CAA-CBA
29	kJ	201	PEB	C2A-C3A-CAA-CBA
29	lJ	202	PEB	C2A-C3A-CAA-CBA
29	mJ	201	PEB	C2A-C3A-CAA-CBA
29	nJ	202	PEB	C2A-C3A-CAA-CBA
29	oJ	201	PEB	C2A-C3A-CAA-CBA
29	pJ	202	PEB	C2A-C3A-CAA-CBA
29	qJ	201	PEB	C2A-C3A-CAA-CBA
29	rJ	202	PEB	C2A-C3A-CAA-CBA
29	sJ	201	PEB	C2A-C3A-CAA-CBA
29	sJ	203	PEB	C2A-C3A-CAA-CBA
29	uJ	201	PEB	C2A-C3A-CAA-CBA
29	uJ	202	PEB	C2A-C3A-CAA-CBA
29	zJ	501	PEB	C2A-C3A-CAA-CBA
29	AK	303	PEB	C2A-C3A-CAA-CBA
29	OK	202	PEB	C2A-C3A-CAA-CBA
29	QK	202	PEB	C2A-C3A-CAA-CBA
29	SK	202	PEB	C2A-C3A-CAA-CBA
29	UK	203	PEB	C2A-C3A-CAA-CBA
29	WK	202	PEB	C2A-C3A-CAA-CBA
29	ZK	203	PEB	C2A-C3A-CAA-CBA
29	bK	202	PEB	C2A-C3A-CAA-CBA
29	dK	202	PEB	C2A-C3A-CAA-CBA
29	fK	202	PEB	C2A-C3A-CAA-CBA
29	hK	202	PEB	C2A-C3A-CAA-CBA
29	jK	202	PEB	C2A-C3A-CAA-CBA
29	lK	202	PEB	C2A-C3A-CAA-CBA
29	AL	201	PEB	C2A-C3A-CAA-CBA
29	AL	203	PEB	C2A-C3A-CAA-CBA
29	BL	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	CL	201	PEB	C2A-C3A-CAA-CBA
29	EL	201	PEB	C2A-C3A-CAA-CBA
29	FL	202	PEB	C2A-C3A-CAA-CBA
29	GL	201	PEB	C2A-C3A-CAA-CBA
29	HL	201	PEB	C2A-C3A-CAA-CBA
29	IL	201	PEB	C2A-C3A-CAA-CBA
29	IL	203	PEB	C2A-C3A-CAA-CBA
29	JL	202	PEB	C2A-C3A-CAA-CBA
29	KL	201	PEB	C2A-C3A-CAA-CBA
29	ML	201	PEB	C2A-C3A-CAA-CBA
29	NL	202	PEB	C2A-C3A-CAA-CBA
29	OL	201	PEB	C2A-C3A-CAA-CBA
29	PL	202	PEB	C2A-C3A-CAA-CBA
29	QL	201	PEB	C2A-C3A-CAA-CBA
29	RL	202	PEB	C2A-C3A-CAA-CBA
29	SL	201	PEB	C2A-C3A-CAA-CBA
29	TL	202	PEB	C2A-C3A-CAA-CBA
29	UL	201	PEB	C2A-C3A-CAA-CBA
29	WL	201	PEB	C2A-C3A-CAA-CBA
29	WL	202	PEB	C2A-C3A-CAA-CBA
29	XL	202	PEB	C2A-C3A-CAA-CBA
29	YL	201	PEB	C2A-C3A-CAA-CBA
29	ZL	202	PEB	C2A-C3A-CAA-CBA
29	aL	201	PEB	C2A-C3A-CAA-CBA
29	bL	202	PEB	C2A-C3A-CAA-CBA
29	cL	201	PEB	C2A-C3A-CAA-CBA
29	dL	202	PEB	C2A-C3A-CAA-CBA
29	eL	201	PEB	C2A-C3A-CAA-CBA
29	fL	202	PEB	C2A-C3A-CAA-CBA
29	gL	201	PEB	C2A-C3A-CAA-CBA
29	hL	202	PEB	C2A-C3A-CAA-CBA
29	iL	201	PEB	C2A-C3A-CAA-CBA
29	jL	202	PEB	C2A-C3A-CAA-CBA
29	kL	201	PEB	C2A-C3A-CAA-CBA
29	lL	202	PEB	C2A-C3A-CAA-CBA
29	mL	201	PEB	C2A-C3A-CAA-CBA
29	nL	202	PEB	C2A-C3A-CAA-CBA
29	oL	201	PEB	C2A-C3A-CAA-CBA
29	pL	202	PEB	C2A-C3A-CAA-CBA
29	qL	201	PEB	C2A-C3A-CAA-CBA
29	rL	202	PEB	C2A-C3A-CAA-CBA
29	sL	201	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	sL	203	PEB	C2A-C3A-CAA-CBA
29	uL	201	PEB	C2A-C3A-CAA-CBA
29	uL	202	PEB	C2A-C3A-CAA-CBA
29	zL	501	PEB	C2A-C3A-CAA-CBA
29	AM	303	PEB	C2A-C3A-CAA-CBA
29	BM	301	PEB	C2A-C3A-CAA-CBA
29	DM	202	PEB	C2A-C3A-CAA-CBA
29	FM	202	PEB	C2A-C3A-CAA-CBA
29	HM	202	PEB	C2A-C3A-CAA-CBA
29	JM	202	PEB	C2A-C3A-CAA-CBA
29	KM	203	PEB	C2A-C3A-CAA-CBA
29	LM	202	PEB	C2A-C3A-CAA-CBA
29	QM	202	PEB	C2A-C3A-CAA-CBA
29	RM	202	PEB	C2A-C3A-CAA-CBA
29	TM	202	PEB	C2A-C3A-CAA-CBA
29	VM	202	PEB	C2A-C3A-CAA-CBA
29	YM	201	PEB	C2A-C3A-CAA-CBA
29	ZM	202	PEB	C2A-C3A-CAA-CBA
29	aM	203	PEB	C2A-C3A-CAA-CBA
29	cM	202	PEB	C2A-C3A-CAA-CBA
29	gM	202	PEB	C2A-C3A-CAA-CBA
29	iM	202	PEB	C2A-C3A-CAA-CBA
29	kM	202	PEB	C2A-C3A-CAA-CBA
29	mM	202	PEB	C2A-C3A-CAA-CBA
29	AN	201	PEB	C2A-C3A-CAA-CBA
29	AN	202	PEB	C2A-C3A-CAA-CBA
29	CN	201	PEB	C2A-C3A-CAA-CBA
29	CN	202	PEB	C2A-C3A-CAA-CBA
29	EN	201	PEB	C2A-C3A-CAA-CBA
29	EN	202	PEB	C2A-C3A-CAA-CBA
29	GN	201	PEB	C2A-C3A-CAA-CBA
29	GN	202	PEB	C2A-C3A-CAA-CBA
29	IN	201	PEB	C2A-C3A-CAA-CBA
29	IN	202	PEB	C2A-C3A-CAA-CBA
29	KN	201	PEB	C2A-C3A-CAA-CBA
29	KN	202	PEB	C2A-C3A-CAA-CBA
29	MN	401	PEB	C2A-C3A-CAA-CBA
29	AQ	202	PEB	C2A-C3A-CAA-CBA
29	CQ	202	PEB	C2A-C3A-CAA-CBA
29	EQ	202	PEB	C2A-C3A-CAA-CBA
29	GQ	202	PEB	C2A-C3A-CAA-CBA
29	IQ	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	KQ	202	PEB	C2A-C3A-CAA-CBA
29	NR	201	PEB	C2C-CAC-CBC-CGC
29	QR	202	PEB	C2A-C3A-CAA-CBA
29	RR	201	PEB	C2C-CAC-CBC-CGC
29	SR	202	PEB	C2A-C3A-CAA-CBA
29	TR	201	PEB	C2C-CAC-CBC-CGC
29	UR	202	PEB	C2A-C3A-CAA-CBA
29	VR	201	PEB	C2C-CAC-CBC-CGC
29	WR	202	PEB	C2A-C3A-CAA-CBA
29	XR	201	PEB	C2C-CAC-CBC-CGC
31	C1	1001	CYC	C2C-C3C-CAC-CBC
31	D1	1003	CYC	C2C-C3C-CAC-CBC
31	E1	1001	CYC	C2C-C3C-CAC-CBC
31	I1	1001	CYC	C2C-C3C-CAC-CBC
31	K1	1001	CYC	C2C-C3C-CAC-CBC
31	M1	1001	CYC	C2C-C3C-CAC-CBC
31	CK	1001	CYC	C2C-C3C-CAC-CBC
31	EK	1001	CYC	C2C-C3C-CAC-CBC
31	GK	1001	CYC	C2C-C3C-CAC-CBC
31	IK	1001	CYC	C2C-C3C-CAC-CBC
31	KK	1001	CYC	C2C-C3C-CAC-CBC
31	MK	1001	CYC	C2C-C3C-CAC-CBC
31	D1	1001	CYC	C2B-C3B-CAB-CBB
31	L1	1001	CYC	C2B-C3B-CAB-CBB
31	HK	1001	CYC	C2B-C3B-CAB-CBB
31	LK	1001	CYC	C2B-C3B-CAB-CBB
30	QB	201	PUB	C4A-C3A-CAA-CBA
30	QM	201	PUB	C4A-C3A-CAA-CBA
29	D7	1002	PEB	C2B-C3B-CAB-CBB
29	D9	1002	PEB	C2B-C3B-CAB-CBB
31	F1	1001	CYC	C2B-C3B-CAB-CBB
31	N1	1001	CYC	C2B-C3B-CAB-CBB
31	DK	1001	CYC	C2B-C3B-CAB-CBB
31	FK	1001	CYC	C2B-C3B-CAB-CBB
31	H1	1001	CYC	C2B-C3B-CAB-CBB
31	J1	1001	CYC	C2B-C3B-CAB-CBB
31	JK	1001	CYC	C2B-C3B-CAB-CBB
31	NK	1001	CYC	C2B-C3B-CAB-CBB
29	F7	1002	PEB	C2B-C3B-CAB-CBB
29	H7	1002	PEB	C2B-C3B-CAB-CBB
29	J7	1002	PEB	C2B-C3B-CAB-CBB
29	L7	1002	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	N7	1002	PEB	C2B-C3B-CAB-CBB
29	F9	1002	PEB	C2B-C3B-CAB-CBB
29	H9	1002	PEB	C2B-C3B-CAB-CBB
29	J9	1002	PEB	C2B-C3B-CAB-CBB
29	L9	1002	PEB	C2B-C3B-CAB-CBB
29	N9	1002	PEB	C2B-C3B-CAB-CBB
30	MA	402	PUB	C2A-C3A-CAA-CBA
30	QB	201	PUB	C2A-C3A-CAA-CBA
30	MG	402	PUB	C2A-C3A-CAA-CBA
30	QM	201	PUB	C2A-C3A-CAA-CBA
30	MN	402	PUB	C2A-C3A-CAA-CBA
30	MQ	404	PUB	C2A-C3A-CAA-CBA
29	P1	201	PEB	C4B-C3B-CAB-CBB
29	R1	201	PEB	C4B-C3B-CAB-CBB
29	T1	201	PEB	C4B-C3B-CAB-CBB
29	V1	201	PEB	C4B-C3B-CAB-CBB
29	Y1	201	PEB	C4B-C3B-CAB-CBB
29	a1	201	PEB	C4B-C3B-CAB-CBB
29	c1	201	PEB	C4B-C3B-CAB-CBB
29	e1	201	PEB	C4B-C3B-CAB-CBB
29	g1	201	PEB	C4B-C3B-CAB-CBB
29	i1	201	PEB	C4B-C3B-CAB-CBB
29	k1	201	PEB	C4B-C3B-CAB-CBB
29	m1	201	PEB	C4B-C3B-CAB-CBB
29	PK	201	PEB	C4B-C3B-CAB-CBB
29	RK	201	PEB	C4B-C3B-CAB-CBB
29	TK	201	PEB	C4B-C3B-CAB-CBB
29	VK	201	PEB	C4B-C3B-CAB-CBB
29	YK	201	PEB	C4B-C3B-CAB-CBB
29	aK	201	PEB	C4B-C3B-CAB-CBB
29	cK	201	PEB	C4B-C3B-CAB-CBB
29	eK	201	PEB	C4B-C3B-CAB-CBB
29	gK	201	PEB	C4B-C3B-CAB-CBB
29	iK	201	PEB	C4B-C3B-CAB-CBB
29	kK	201	PEB	C4B-C3B-CAB-CBB
29	mK	201	PEB	C4B-C3B-CAB-CBB
31	DP	1001	CYC	C2B-C3B-CAB-CBB
31	FP	1001	CYC	C2B-C3B-CAB-CBB
31	BP	1001	CYC	C2B-C3B-CAB-CBB
31	HP	1001	CYC	C2B-C3B-CAB-CBB
31	IP	1001	CYC	C2B-C3B-CAB-CBB
31	MP	1001	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	OP	1001	CYC	C2B-C3B-CAB-CBB
31	QP	1001	CYC	C2B-C3B-CAB-CBB
31	SP	1001	CYC	C2B-C3B-CAB-CBB
31	UP	1001	CYC	C2B-C3B-CAB-CBB
31	XP	1001	CYC	C2B-C3B-CAB-CBB
31	fP	1001	CYC	C2B-C3B-CAB-CBB
31	hP	1001	CYC	C2B-C3B-CAB-CBB
31	jP	1001	CYC	C2B-C3B-CAB-CBB
31	kP	1001	CYC	C2B-C3B-CAB-CBB
31	nP	1001	CYC	C2B-C3B-CAB-CBB
31	oP	1001	CYC	C2B-C3B-CAB-CBB
31	qP	1001	CYC	C2B-C3B-CAB-CBB
31	sP	1001	CYC	C2B-C3B-CAB-CBB
31	wP	1001	CYC	C2B-C3B-CAB-CBB
31	lP	1001	CYC	C2B-C3B-CAB-CBB
31	uP	1001	CYC	C2B-C3B-CAB-CBB
29	AA	202	PEB	NA-C4A-CHA-C1B
29	CA	202	PEB	NA-C4A-CHA-C1B
29	EA	202	PEB	NA-C4A-CHA-C1B
29	GA	202	PEB	NA-C4A-CHA-C1B
29	IA	202	PEB	NA-C4A-CHA-C1B
29	KA	202	PEB	NA-C4A-CHA-C1B
29	AG	202	PEB	NA-C4A-CHA-C1B
29	CG	202	PEB	NA-C4A-CHA-C1B
29	EG	202	PEB	NA-C4A-CHA-C1B
29	GG	202	PEB	NA-C4A-CHA-C1B
29	IG	202	PEB	NA-C4A-CHA-C1B
29	KG	202	PEB	NA-C4A-CHA-C1B
29	AN	202	PEB	NA-C4A-CHA-C1B
29	CN	202	PEB	NA-C4A-CHA-C1B
29	EN	202	PEB	NA-C4A-CHA-C1B
29	GN	202	PEB	NA-C4A-CHA-C1B
29	IN	202	PEB	NA-C4A-CHA-C1B
29	KN	202	PEB	NA-C4A-CHA-C1B
29	AQ	202	PEB	NA-C4A-CHA-C1B
29	CQ	202	PEB	NA-C4A-CHA-C1B
29	EQ	202	PEB	NA-C4A-CHA-C1B
29	GQ	202	PEB	NA-C4A-CHA-C1B
29	IQ	202	PEB	NA-C4A-CHA-C1B
29	KQ	202	PEB	NA-C4A-CHA-C1B
29	A1	302	PEB	C2D-C1D-CHC-C4C
29	O1	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	P1	203	PEB	C2D-C1D-CHC-C4C
29	Q1	201	PEB	C2D-C1D-CHC-C4C
29	R1	203	PEB	C2D-C1D-CHC-C4C
29	S1	201	PEB	C2D-C1D-CHC-C4C
29	T1	202	PEB	C2D-C1D-CHC-C4C
29	U1	202	PEB	C2D-C1D-CHC-C4C
29	V1	203	PEB	C2D-C1D-CHC-C4C
29	W1	201	PEB	C2D-C1D-CHC-C4C
29	Y1	202	PEB	C2D-C1D-CHC-C4C
29	Z1	202	PEB	C2D-C1D-CHC-C4C
29	a1	203	PEB	C2D-C1D-CHC-C4C
29	b1	201	PEB	C2D-C1D-CHC-C4C
29	c1	203	PEB	C2D-C1D-CHC-C4C
29	d1	201	PEB	C2D-C1D-CHC-C4C
29	e1	203	PEB	C2D-C1D-CHC-C4C
29	f1	201	PEB	C2D-C1D-CHC-C4C
29	g1	203	PEB	C2D-C1D-CHC-C4C
29	h1	201	PEB	C2D-C1D-CHC-C4C
29	i1	203	PEB	C2D-C1D-CHC-C4C
29	j1	201	PEB	C2D-C1D-CHC-C4C
29	k1	203	PEB	C2D-C1D-CHC-C4C
29	l1	201	PEB	C2D-C1D-CHC-C4C
29	m1	202	PEB	C2D-C1D-CHC-C4C
29	M3	202	PEB	C2D-C1D-CHC-C4C
29	N3	202	PEB	C2D-C1D-CHC-C4C
29	C4	203	PEB	C2D-C1D-CHC-C4C
29	E4	203	PEB	C2D-C1D-CHC-C4C
29	G4	203	PEB	C2D-C1D-CHC-C4C
29	K4	203	PEB	C2D-C1D-CHC-C4C
29	M4	203	PEB	C2D-C1D-CHC-C4C
29	I5	203	PEB	C2D-C1D-CHC-C4C
29	K5	203	PEB	C2D-C1D-CHC-C4C
29	A5	203	PEB	C2D-C1D-CHC-C4C
29	C5	203	PEB	C2D-C1D-CHC-C4C
29	A7	304	PEB	C2D-C1D-CHC-C4C
29	A7	305	PEB	C2D-C1D-CHC-C4C
29	P7	203	PEB	C2D-C1D-CHC-C4C
29	R7	203	PEB	C2D-C1D-CHC-C4C
29	T7	203	PEB	C2D-C1D-CHC-C4C
29	V7	203	PEB	C2D-C1D-CHC-C4C
29	Y7	203	PEB	C2D-C1D-CHC-C4C
29	a7	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	c7	203	PEB	C2D-C1D-CHC-C4C
29	e7	203	PEB	C2D-C1D-CHC-C4C
29	g7	203	PEB	C2D-C1D-CHC-C4C
29	i7	203	PEB	C2D-C1D-CHC-C4C
29	k7	203	PEB	C2D-C1D-CHC-C4C
29	m7	203	PEB	C2D-C1D-CHC-C4C
29	I8	203	PEB	C2D-C1D-CHC-C4C
29	K8	203	PEB	C2D-C1D-CHC-C4C
29	A8	203	PEB	C2D-C1D-CHC-C4C
29	C8	203	PEB	C2D-C1D-CHC-C4C
29	A9	304	PEB	C2D-C1D-CHC-C4C
29	A9	305	PEB	C2D-C1D-CHC-C4C
29	P9	203	PEB	C2D-C1D-CHC-C4C
29	R9	203	PEB	C2D-C1D-CHC-C4C
29	T9	203	PEB	C2D-C1D-CHC-C4C
29	V9	203	PEB	C2D-C1D-CHC-C4C
29	Y9	203	PEB	C2D-C1D-CHC-C4C
29	a9	203	PEB	C2D-C1D-CHC-C4C
29	c9	203	PEB	C2D-C1D-CHC-C4C
29	e9	203	PEB	C2D-C1D-CHC-C4C
29	g9	203	PEB	C2D-C1D-CHC-C4C
29	i9	203	PEB	C2D-C1D-CHC-C4C
29	k9	203	PEB	C2D-C1D-CHC-C4C
29	m9	203	PEB	C2D-C1D-CHC-C4C
29	AA	201	PEB	C2D-C1D-CHC-C4C
29	BA	203	PEB	C2D-C1D-CHC-C4C
29	CA	201	PEB	C2D-C1D-CHC-C4C
29	DA	203	PEB	C2D-C1D-CHC-C4C
29	EA	201	PEB	C2D-C1D-CHC-C4C
29	FA	203	PEB	C2D-C1D-CHC-C4C
29	GA	201	PEB	C2D-C1D-CHC-C4C
29	HA	203	PEB	C2D-C1D-CHC-C4C
29	IA	201	PEB	C2D-C1D-CHC-C4C
29	JA	203	PEB	C2D-C1D-CHC-C4C
29	KA	201	PEB	C2D-C1D-CHC-C4C
29	LA	203	PEB	C2D-C1D-CHC-C4C
29	MA	401	PEB	C2D-C1D-CHC-C4C
29	AC	201	PEB	C2D-C1D-CHC-C4C
29	BC	203	PEB	C2D-C1D-CHC-C4C
29	CC	201	PEB	C2D-C1D-CHC-C4C
29	DC	202	PEB	C2D-C1D-CHC-C4C
29	EC	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	FC	203	PEB	C2D-C1D-CHC-C4C
29	GC	201	PEB	C2D-C1D-CHC-C4C
29	HC	203	PEB	C2D-C1D-CHC-C4C
29	IC	201	PEB	C2D-C1D-CHC-C4C
29	JC	202	PEB	C2D-C1D-CHC-C4C
29	KC	202	PEB	C2D-C1D-CHC-C4C
29	LC	203	PEB	C2D-C1D-CHC-C4C
29	CD	203	PEB	C2D-C1D-CHC-C4C
29	ED	202	PEB	C2D-C1D-CHC-C4C
29	GD	203	PEB	C2D-C1D-CHC-C4C
29	ID	203	PEB	C2D-C1D-CHC-C4C
29	KD	203	PEB	C2D-C1D-CHC-C4C
29	MD	203	PEB	C2D-C1D-CHC-C4C
29	AE	201	PEB	C2D-C1D-CHC-C4C
29	BE	203	PEB	C2D-C1D-CHC-C4C
29	CE	201	PEB	C2D-C1D-CHC-C4C
29	DE	202	PEB	C2D-C1D-CHC-C4C
29	EE	201	PEB	C2D-C1D-CHC-C4C
29	FE	203	PEB	C2D-C1D-CHC-C4C
29	GE	201	PEB	C2D-C1D-CHC-C4C
29	HE	203	PEB	C2D-C1D-CHC-C4C
29	IE	201	PEB	C2D-C1D-CHC-C4C
29	JE	202	PEB	C2D-C1D-CHC-C4C
29	KE	202	PEB	C2D-C1D-CHC-C4C
29	LE	203	PEB	C2D-C1D-CHC-C4C
29	AF	301	PEB	C2D-C1D-CHC-C4C
29	AF	304	PEB	C2D-C1D-CHC-C4C
29	DF	1002	PEB	C2D-C1D-CHC-C4C
29	FF	1002	PEB	C2D-C1D-CHC-C4C
29	HF	1002	PEB	C2D-C1D-CHC-C4C
29	JF	1002	PEB	C2D-C1D-CHC-C4C
29	LF	1002	PEB	C2D-C1D-CHC-C4C
29	NF	1002	PEB	C2D-C1D-CHC-C4C
29	PF	203	PEB	C2D-C1D-CHC-C4C
29	RF	202	PEB	C2D-C1D-CHC-C4C
29	TF	202	PEB	C2D-C1D-CHC-C4C
29	VF	203	PEB	C2D-C1D-CHC-C4C
29	YF	203	PEB	C2D-C1D-CHC-C4C
29	aF	203	PEB	C2D-C1D-CHC-C4C
29	cF	202	PEB	C2D-C1D-CHC-C4C
29	eF	203	PEB	C2D-C1D-CHC-C4C
29	gF	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	iF	203	PEB	C2D-C1D-CHC-C4C
29	kF	203	PEB	C2D-C1D-CHC-C4C
29	mF	203	PEB	C2D-C1D-CHC-C4C
29	AG	201	PEB	C2D-C1D-CHC-C4C
29	BG	201	PEB	C2D-C1D-CHC-C4C
29	CG	201	PEB	C2D-C1D-CHC-C4C
29	DG	201	PEB	C2D-C1D-CHC-C4C
29	EG	201	PEB	C2D-C1D-CHC-C4C
29	FG	201	PEB	C2D-C1D-CHC-C4C
29	GG	201	PEB	C2D-C1D-CHC-C4C
29	HG	201	PEB	C2D-C1D-CHC-C4C
29	IG	201	PEB	C2D-C1D-CHC-C4C
29	JG	201	PEB	C2D-C1D-CHC-C4C
29	KG	201	PEB	C2D-C1D-CHC-C4C
29	LG	201	PEB	C2D-C1D-CHC-C4C
29	MG	404	PEB	C2D-C1D-CHC-C4C
29	MG	405	PEB	C2D-C1D-CHC-C4C
29	AI	301	PEB	C2D-C1D-CHC-C4C
29	AI	304	PEB	C2D-C1D-CHC-C4C
29	DI	1002	PEB	C2D-C1D-CHC-C4C
29	FI	1002	PEB	C2D-C1D-CHC-C4C
29	HI	1002	PEB	C2D-C1D-CHC-C4C
29	JI	1002	PEB	C2D-C1D-CHC-C4C
29	LI	1002	PEB	C2D-C1D-CHC-C4C
29	NI	1002	PEB	C2D-C1D-CHC-C4C
29	PI	203	PEB	C2D-C1D-CHC-C4C
29	RI	202	PEB	C2D-C1D-CHC-C4C
29	TI	202	PEB	C2D-C1D-CHC-C4C
29	VI	203	PEB	C2D-C1D-CHC-C4C
29	YI	203	PEB	C2D-C1D-CHC-C4C
29	aI	203	PEB	C2D-C1D-CHC-C4C
29	cI	202	PEB	C2D-C1D-CHC-C4C
29	eI	203	PEB	C2D-C1D-CHC-C4C
29	gI	203	PEB	C2D-C1D-CHC-C4C
29	iI	203	PEB	C2D-C1D-CHC-C4C
29	kI	203	PEB	C2D-C1D-CHC-C4C
29	mI	203	PEB	C2D-C1D-CHC-C4C
29	AJ	201	PEB	C2D-C1D-CHC-C4C
29	CJ	201	PEB	C2D-C1D-CHC-C4C
29	EJ	201	PEB	C2D-C1D-CHC-C4C
29	GJ	201	PEB	C2D-C1D-CHC-C4C
29	IJ	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	KJ	201	PEB	C2D-C1D-CHC-C4C
29	MJ	201	PEB	C2D-C1D-CHC-C4C
29	OJ	201	PEB	C2D-C1D-CHC-C4C
29	QJ	201	PEB	C2D-C1D-CHC-C4C
29	SJ	201	PEB	C2D-C1D-CHC-C4C
29	UJ	201	PEB	C2D-C1D-CHC-C4C
29	WJ	202	PEB	C2D-C1D-CHC-C4C
29	YJ	201	PEB	C2D-C1D-CHC-C4C
29	aJ	201	PEB	C2D-C1D-CHC-C4C
29	cJ	201	PEB	C2D-C1D-CHC-C4C
29	eJ	201	PEB	C2D-C1D-CHC-C4C
29	gJ	201	PEB	C2D-C1D-CHC-C4C
29	iJ	201	PEB	C2D-C1D-CHC-C4C
29	kJ	201	PEB	C2D-C1D-CHC-C4C
29	mJ	201	PEB	C2D-C1D-CHC-C4C
29	oJ	201	PEB	C2D-C1D-CHC-C4C
29	qJ	201	PEB	C2D-C1D-CHC-C4C
29	sJ	201	PEB	C2D-C1D-CHC-C4C
29	uJ	202	PEB	C2D-C1D-CHC-C4C
29	wJ	301	PEB	C2D-C1D-CHC-C4C
29	xJ	301	PEB	C2D-C1D-CHC-C4C
29	AK	302	PEB	C2D-C1D-CHC-C4C
29	OK	201	PEB	C2D-C1D-CHC-C4C
29	PK	203	PEB	C2D-C1D-CHC-C4C
29	QK	201	PEB	C2D-C1D-CHC-C4C
29	RK	203	PEB	C2D-C1D-CHC-C4C
29	SK	201	PEB	C2D-C1D-CHC-C4C
29	TK	202	PEB	C2D-C1D-CHC-C4C
29	UK	202	PEB	C2D-C1D-CHC-C4C
29	VK	203	PEB	C2D-C1D-CHC-C4C
29	WK	201	PEB	C2D-C1D-CHC-C4C
29	YK	202	PEB	C2D-C1D-CHC-C4C
29	ZK	202	PEB	C2D-C1D-CHC-C4C
29	aK	203	PEB	C2D-C1D-CHC-C4C
29	bK	201	PEB	C2D-C1D-CHC-C4C
29	cK	203	PEB	C2D-C1D-CHC-C4C
29	dK	201	PEB	C2D-C1D-CHC-C4C
29	eK	203	PEB	C2D-C1D-CHC-C4C
29	fK	201	PEB	C2D-C1D-CHC-C4C
29	gK	203	PEB	C2D-C1D-CHC-C4C
29	hK	201	PEB	C2D-C1D-CHC-C4C
29	iK	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	jK	201	PEB	C2D-C1D-CHC-C4C
29	kK	203	PEB	C2D-C1D-CHC-C4C
29	lK	201	PEB	C2D-C1D-CHC-C4C
29	mK	202	PEB	C2D-C1D-CHC-C4C
29	AL	201	PEB	C2D-C1D-CHC-C4C
29	CL	201	PEB	C2D-C1D-CHC-C4C
29	EL	201	PEB	C2D-C1D-CHC-C4C
29	GL	201	PEB	C2D-C1D-CHC-C4C
29	IL	201	PEB	C2D-C1D-CHC-C4C
29	KL	201	PEB	C2D-C1D-CHC-C4C
29	ML	201	PEB	C2D-C1D-CHC-C4C
29	OL	201	PEB	C2D-C1D-CHC-C4C
29	QL	201	PEB	C2D-C1D-CHC-C4C
29	SL	201	PEB	C2D-C1D-CHC-C4C
29	UL	201	PEB	C2D-C1D-CHC-C4C
29	WL	202	PEB	C2D-C1D-CHC-C4C
29	YL	201	PEB	C2D-C1D-CHC-C4C
29	aL	201	PEB	C2D-C1D-CHC-C4C
29	cL	201	PEB	C2D-C1D-CHC-C4C
29	eL	201	PEB	C2D-C1D-CHC-C4C
29	gL	201	PEB	C2D-C1D-CHC-C4C
29	iL	201	PEB	C2D-C1D-CHC-C4C
29	kL	201	PEB	C2D-C1D-CHC-C4C
29	mL	201	PEB	C2D-C1D-CHC-C4C
29	oL	201	PEB	C2D-C1D-CHC-C4C
29	qL	201	PEB	C2D-C1D-CHC-C4C
29	sL	201	PEB	C2D-C1D-CHC-C4C
29	uL	202	PEB	C2D-C1D-CHC-C4C
29	wL	301	PEB	C2D-C1D-CHC-C4C
29	xL	301	PEB	C2D-C1D-CHC-C4C
29	AN	201	PEB	C2D-C1D-CHC-C4C
29	BN	203	PEB	C2D-C1D-CHC-C4C
29	CN	201	PEB	C2D-C1D-CHC-C4C
29	DN	203	PEB	C2D-C1D-CHC-C4C
29	EN	201	PEB	C2D-C1D-CHC-C4C
29	FN	203	PEB	C2D-C1D-CHC-C4C
29	GN	201	PEB	C2D-C1D-CHC-C4C
29	HN	203	PEB	C2D-C1D-CHC-C4C
29	IN	201	PEB	C2D-C1D-CHC-C4C
29	JN	203	PEB	C2D-C1D-CHC-C4C
29	KN	201	PEB	C2D-C1D-CHC-C4C
29	LN	203	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	MN	401	PEB	C2D-C1D-CHC-C4C
29	MO	202	PEB	C2D-C1D-CHC-C4C
29	NO	202	PEB	C2D-C1D-CHC-C4C
29	AQ	201	PEB	C2D-C1D-CHC-C4C
29	BQ	201	PEB	C2D-C1D-CHC-C4C
29	CQ	201	PEB	C2D-C1D-CHC-C4C
29	DQ	201	PEB	C2D-C1D-CHC-C4C
29	EQ	201	PEB	C2D-C1D-CHC-C4C
29	FQ	201	PEB	C2D-C1D-CHC-C4C
29	GQ	201	PEB	C2D-C1D-CHC-C4C
29	HQ	201	PEB	C2D-C1D-CHC-C4C
29	IQ	201	PEB	C2D-C1D-CHC-C4C
29	JQ	201	PEB	C2D-C1D-CHC-C4C
29	KQ	201	PEB	C2D-C1D-CHC-C4C
29	MQ	402	PEB	C2D-C1D-CHC-C4C
29	MQ	406	PEB	C2D-C1D-CHC-C4C
29	MQ	407	PEB	C2D-C1D-CHC-C4C
29	OR	202	PEB	C2D-C1D-CHC-C4C
29	SR	201	PEB	C2D-C1D-CHC-C4C
30	A1	304	PUB	C3A-C4A-CHA-C1B
30	A7	302	PUB	C3A-C4A-CHA-C1B
30	A7	303	PUB	C3A-C4A-CHA-C1B
30	A9	302	PUB	C3A-C4A-CHA-C1B
30	A9	303	PUB	C3A-C4A-CHA-C1B
30	MA	402	PUB	C3A-C4A-CHA-C1B
30	MA	403	PUB	C3A-C4A-CHA-C1B
30	AF	303	PUB	C3A-C4A-CHA-C1B
30	AI	303	PUB	C3A-C4A-CHA-C1B
30	wJ	304	PUB	C3A-C4A-CHA-C1B
30	wJ	305	PUB	C3A-C4A-CHA-C1B
30	xJ	304	PUB	C3A-C4A-CHA-C1B
30	xJ	305	PUB	C3A-C4A-CHA-C1B
30	yJ	302	PUB	C3A-C4A-CHA-C1B
30	yJ	303	PUB	C3A-C4A-CHA-C1B
30	AK	304	PUB	C3A-C4A-CHA-C1B
30	wL	304	PUB	C3A-C4A-CHA-C1B
30	wL	305	PUB	C3A-C4A-CHA-C1B
30	xL	304	PUB	C3A-C4A-CHA-C1B
30	xL	305	PUB	C3A-C4A-CHA-C1B
30	yL	302	PUB	C3A-C4A-CHA-C1B
30	yL	303	PUB	C3A-C4A-CHA-C1B
30	MN	402	PUB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
30	MN	403	PUB	C3A-C4A-CHA-C1B
29	AB	301	PEB	C2C-CAC-CBC-CGC
29	AB	303	PEB	C2C-CAC-CBC-CGC
29	UF	201	PEB	C2C-CAC-CBC-CGC
29	VF	202	PEB	C2C-CAC-CBC-CGC
29	UI	201	PEB	C2C-CAC-CBC-CGC
29	VI	202	PEB	C2C-CAC-CBC-CGC
29	AM	301	PEB	C2C-CAC-CBC-CGC
29	AM	303	PEB	C2C-CAC-CBC-CGC
30	AF	302	PUB	C3B-CAB-CBB-CGB
30	AI	302	PUB	C3B-CAB-CBB-CGB
31	rP	1001	CYC	C2B-C3B-CAB-CBB
29	P1	202	PEB	C3B-CAB-CBB-CGB
29	R1	202	PEB	C3B-CAB-CBB-CGB
29	Z1	201	PEB	C3B-CAB-CBB-CGB
29	e1	202	PEB	C3B-CAB-CBB-CGB
29	i1	202	PEB	C3B-CAB-CBB-CGB
29	j1	203	PEB	C3B-CAB-CBB-CGB
29	k1	202	PEB	C3B-CAB-CBB-CGB
29	PK	202	PEB	C3B-CAB-CBB-CGB
29	RK	202	PEB	C3B-CAB-CBB-CGB
29	ZK	201	PEB	C3B-CAB-CBB-CGB
29	eK	202	PEB	C3B-CAB-CBB-CGB
29	iK	202	PEB	C3B-CAB-CBB-CGB
29	jK	203	PEB	C3B-CAB-CBB-CGB
29	kK	202	PEB	C3B-CAB-CBB-CGB
30	MG	403	PUB	C2C-CAC-CBC-CGC
30	MQ	405	PUB	C2C-CAC-CBC-CGC
31	DF	1001	CYC	C2A-CAA-CBA-CGA
31	FF	1001	CYC	C2A-CAA-CBA-CGA
31	HF	1001	CYC	C2A-CAA-CBA-CGA
31	LF	1001	CYC	C2A-CAA-CBA-CGA
31	DI	1001	CYC	C2A-CAA-CBA-CGA
31	FI	1001	CYC	C2A-CAA-CBA-CGA
31	HI	1001	CYC	C2A-CAA-CBA-CGA
31	LI	1001	CYC	C2A-CAA-CBA-CGA
29	AA	202	PEB	NB-C4B-CHB-C1C
29	CA	202	PEB	NB-C4B-CHB-C1C
29	EA	202	PEB	NB-C4B-CHB-C1C
29	GA	202	PEB	NB-C4B-CHB-C1C
29	IA	202	PEB	NB-C4B-CHB-C1C
29	KA	202	PEB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
29	AN	202	PEB	NB-C4B-CHB-C1C
29	CN	202	PEB	NB-C4B-CHB-C1C
29	EN	202	PEB	NB-C4B-CHB-C1C
29	GN	202	PEB	NB-C4B-CHB-C1C
29	IN	202	PEB	NB-C4B-CHB-C1C
29	KN	202	PEB	NB-C4B-CHB-C1C
31	AP	1001	CYC	C2B-C3B-CAB-CBB
31	CP	1001	CYC	C2B-C3B-CAB-CBB
31	EP	1001	CYC	C2B-C3B-CAB-CBB
31	JP	1001	CYC	C2B-C3B-CAB-CBB
31	KP	1001	CYC	C2B-C3B-CAB-CBB
31	NP	1001	CYC	C2B-C3B-CAB-CBB
31	PP	1001	CYC	C2B-C3B-CAB-CBB
31	RP	1001	CYC	C2B-C3B-CAB-CBB
31	TP	1001	CYC	C2B-C3B-CAB-CBB
31	iP	1001	CYC	C2B-C3B-CAB-CBB
31	tP	1001	CYC	C2B-C3B-CAB-CBB
31	vP	1001	CYC	C2B-C3B-CAB-CBB
31	cP	1001	CYC	C2B-C3B-CAB-CBB
31	lP	1001	CYC	C2B-C3B-CAB-CBB
31	mP	1001	CYC	C2B-C3B-CAB-CBB
31	GP	1001	CYC	C2B-C3B-CAB-CBB
31	eP	1001	CYC	C2B-C3B-CAB-CBB
31	gP	1001	CYC	C2B-C3B-CAB-CBB
31	pP	1001	CYC	C2B-C3B-CAB-CBB
29	M3	202	PEB	C4D-C3D-CAD-CBD
29	N3	202	PEB	C4D-C3D-CAD-CBD
29	MO	202	PEB	C4D-C3D-CAD-CBD
29	NO	202	PEB	C4D-C3D-CAD-CBD
29	M2	202	PEB	C4A-C3A-CAA-CBA
29	O2	202	PEB	C4A-C3A-CAA-CBA
29	Q2	202	PEB	C4A-C3A-CAA-CBA
29	S2	202	PEB	C4A-C3A-CAA-CBA
29	U2	202	PEB	C4A-C3A-CAA-CBA
29	W2	202	PEB	C4A-C3A-CAA-CBA
29	J5	202	PEB	C4A-C3A-CAA-CBA
29	J8	202	PEB	C4A-C3A-CAA-CBA
29	MA	404	PEB	C4A-C3A-CAA-CBA
29	AF	304	PEB	C4A-C3A-CAA-CBA
29	MG	405	PEB	C4A-C3A-CAA-CBA
29	AI	304	PEB	C4A-C3A-CAA-CBA
29	MN	404	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	MQ	407	PEB	C4A-C3A-CAA-CBA
29	QR	202	PEB	C4A-C3A-CAA-CBA
29	SR	202	PEB	C4A-C3A-CAA-CBA
29	UR	202	PEB	C4A-C3A-CAA-CBA
29	WR	202	PEB	C4A-C3A-CAA-CBA
31	C1	1001	CYC	C4C-C3C-CAC-CBC
31	D1	1003	CYC	C4C-C3C-CAC-CBC
31	E1	1001	CYC	C4C-C3C-CAC-CBC
31	I1	1001	CYC	C4C-C3C-CAC-CBC
31	K1	1001	CYC	C4C-C3C-CAC-CBC
31	M1	1001	CYC	C4C-C3C-CAC-CBC
31	CK	1001	CYC	C4C-C3C-CAC-CBC
31	EK	1001	CYC	C4C-C3C-CAC-CBC
31	GK	1001	CYC	C4C-C3C-CAC-CBC
31	IK	1001	CYC	C4C-C3C-CAC-CBC
31	KK	1001	CYC	C4C-C3C-CAC-CBC
31	MK	1001	CYC	C4C-C3C-CAC-CBC
29	U1	201	PEB	C3B-CAB-CBB-CGB
29	V1	202	PEB	C3B-CAB-CBB-CGB
29	a1	202	PEB	C3B-CAB-CBB-CGB
29	c1	202	PEB	C3B-CAB-CBB-CGB
29	g1	202	PEB	C3B-CAB-CBB-CGB
29	UK	201	PEB	C3B-CAB-CBB-CGB
29	VK	202	PEB	C3B-CAB-CBB-CGB
29	aK	202	PEB	C3B-CAB-CBB-CGB
29	cK	202	PEB	C3B-CAB-CBB-CGB
29	gK	202	PEB	C3B-CAB-CBB-CGB
31	JF	1001	CYC	C2A-CAA-CBA-CGA
31	NF	1001	CYC	C2A-CAA-CBA-CGA
31	JI	1001	CYC	C2A-CAA-CBA-CGA
31	NI	1001	CYC	C2A-CAA-CBA-CGA
29	PF	201	PEB	C2B-C3B-CAB-CBB
29	RF	201	PEB	C2B-C3B-CAB-CBB
29	VF	201	PEB	C2B-C3B-CAB-CBB
29	YF	201	PEB	C2B-C3B-CAB-CBB
29	aF	201	PEB	C2B-C3B-CAB-CBB
29	cF	201	PEB	C2B-C3B-CAB-CBB
29	eF	201	PEB	C2B-C3B-CAB-CBB
29	gF	201	PEB	C2B-C3B-CAB-CBB
29	iF	201	PEB	C2B-C3B-CAB-CBB
29	kF	201	PEB	C2B-C3B-CAB-CBB
29	mF	201	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	PI	201	PEB	C2B-C3B-CAB-CBB
29	RI	201	PEB	C2B-C3B-CAB-CBB
29	TI	201	PEB	C2B-C3B-CAB-CBB
29	VI	201	PEB	C2B-C3B-CAB-CBB
29	YI	201	PEB	C2B-C3B-CAB-CBB
29	aI	201	PEB	C2B-C3B-CAB-CBB
29	cI	201	PEB	C2B-C3B-CAB-CBB
29	eI	201	PEB	C2B-C3B-CAB-CBB
29	gI	201	PEB	C2B-C3B-CAB-CBB
29	iI	201	PEB	C2B-C3B-CAB-CBB
29	kI	201	PEB	C2B-C3B-CAB-CBB
29	mI	201	PEB	C2B-C3B-CAB-CBB
30	A1	305	PUB	C2D-C1D-CHC-C4C
30	AB	304	PUB	C2D-C1D-CHC-C4C
30	AK	305	PUB	C2D-C1D-CHC-C4C
30	AM	304	PUB	C2D-C1D-CHC-C4C
29	A1	301	PEB	C2C-CAC-CBC-CGC
29	PF	203	PEB	C2C-CAC-CBC-CGC
29	RF	202	PEB	C2C-CAC-CBC-CGC
29	TF	202	PEB	C2C-CAC-CBC-CGC
29	VF	203	PEB	C2C-CAC-CBC-CGC
29	YF	203	PEB	C2C-CAC-CBC-CGC
29	aF	203	PEB	C2C-CAC-CBC-CGC
29	cF	202	PEB	C2C-CAC-CBC-CGC
29	eF	203	PEB	C2C-CAC-CBC-CGC
29	gF	203	PEB	C2C-CAC-CBC-CGC
29	iF	203	PEB	C2C-CAC-CBC-CGC
29	kF	203	PEB	C2C-CAC-CBC-CGC
29	mF	203	PEB	C2C-CAC-CBC-CGC
29	PI	203	PEB	C2C-CAC-CBC-CGC
29	RI	202	PEB	C2C-CAC-CBC-CGC
29	TI	202	PEB	C2C-CAC-CBC-CGC
29	VI	203	PEB	C2C-CAC-CBC-CGC
29	YI	203	PEB	C2C-CAC-CBC-CGC
29	aI	203	PEB	C2C-CAC-CBC-CGC
29	cI	202	PEB	C2C-CAC-CBC-CGC
29	eI	203	PEB	C2C-CAC-CBC-CGC
29	gI	203	PEB	C2C-CAC-CBC-CGC
29	iI	203	PEB	C2C-CAC-CBC-CGC
29	kI	203	PEB	C2C-CAC-CBC-CGC
29	mI	203	PEB	C2C-CAC-CBC-CGC
29	AK	301	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	AF	301	PEB	C2D-C3D-CAD-CBD
29	AI	301	PEB	C2D-C3D-CAD-CBD
29	BG	201	PEB	C3B-CAB-CBB-CGB
29	DG	201	PEB	C3B-CAB-CBB-CGB
29	FG	201	PEB	C3B-CAB-CBB-CGB
29	HG	201	PEB	C3B-CAB-CBB-CGB
29	JG	201	PEB	C3B-CAB-CBB-CGB
29	LG	201	PEB	C3B-CAB-CBB-CGB
29	BQ	201	PEB	C3B-CAB-CBB-CGB
29	DQ	201	PEB	C3B-CAB-CBB-CGB
29	FQ	201	PEB	C3B-CAB-CBB-CGB
29	HQ	201	PEB	C3B-CAB-CBB-CGB
29	JQ	201	PEB	C3B-CAB-CBB-CGB
29	MQ	402	PEB	C3B-CAB-CBB-CGB
29	P1	201	PEB	C2B-C3B-CAB-CBB
29	R1	201	PEB	C2B-C3B-CAB-CBB
29	T1	201	PEB	C2B-C3B-CAB-CBB
29	V1	201	PEB	C2B-C3B-CAB-CBB
29	Y1	201	PEB	C2B-C3B-CAB-CBB
29	a1	201	PEB	C2B-C3B-CAB-CBB
29	c1	201	PEB	C2B-C3B-CAB-CBB
29	e1	201	PEB	C2B-C3B-CAB-CBB
29	g1	201	PEB	C2B-C3B-CAB-CBB
29	i1	201	PEB	C2B-C3B-CAB-CBB
29	k1	201	PEB	C2B-C3B-CAB-CBB
29	m1	201	PEB	C2B-C3B-CAB-CBB
29	PK	201	PEB	C2B-C3B-CAB-CBB
29	RK	201	PEB	C2B-C3B-CAB-CBB
29	TK	201	PEB	C2B-C3B-CAB-CBB
29	VK	201	PEB	C2B-C3B-CAB-CBB
29	YK	201	PEB	C2B-C3B-CAB-CBB
29	aK	201	PEB	C2B-C3B-CAB-CBB
29	cK	201	PEB	C2B-C3B-CAB-CBB
29	eK	201	PEB	C2B-C3B-CAB-CBB
29	gK	201	PEB	C2B-C3B-CAB-CBB
29	iK	201	PEB	C2B-C3B-CAB-CBB
29	kK	201	PEB	C2B-C3B-CAB-CBB
29	mK	201	PEB	C2B-C3B-CAB-CBB
30	A1	305	PUB	C2D-C3D-CAD-CBD
30	AK	305	PUB	C2D-C3D-CAD-CBD
29	e2	401	PEB	C2A-C3A-CAA-CBA
29	D3	202	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	B4	202	PEB	ND-C1D-CHC-C4C
29	D4	202	PEB	ND-C1D-CHC-C4C
29	F4	202	PEB	ND-C1D-CHC-C4C
29	H4	202	PEB	ND-C1D-CHC-C4C
29	J4	202	PEB	ND-C1D-CHC-C4C
29	L4	202	PEB	ND-C1D-CHC-C4C
29	M4	203	PEB	ND-C1D-CHC-C4C
29	J5	202	PEB	ND-C1D-CHC-C4C
29	A7	301	PEB	C2A-C3A-CAA-CBA
29	D7	1002	PEB	ND-C1D-CHC-C4C
29	F7	1002	PEB	ND-C1D-CHC-C4C
29	H7	1002	PEB	ND-C1D-CHC-C4C
29	J7	1002	PEB	ND-C1D-CHC-C4C
29	L7	1002	PEB	ND-C1D-CHC-C4C
29	N7	1002	PEB	ND-C1D-CHC-C4C
29	J8	202	PEB	ND-C1D-CHC-C4C
29	A9	301	PEB	C2A-C3A-CAA-CBA
29	D9	1002	PEB	ND-C1D-CHC-C4C
29	F9	1002	PEB	ND-C1D-CHC-C4C
29	H9	1002	PEB	ND-C1D-CHC-C4C
29	J9	1002	PEB	ND-C1D-CHC-C4C
29	L9	1002	PEB	ND-C1D-CHC-C4C
29	N9	1002	PEB	ND-C1D-CHC-C4C
29	AB	303	PEB	ND-C1D-CHC-C4C
29	BB	301	PEB	ND-C1D-CHC-C4C
29	BD	202	PEB	ND-C1D-CHC-C4C
29	DD	202	PEB	ND-C1D-CHC-C4C
29	FD	202	PEB	ND-C1D-CHC-C4C
29	HD	202	PEB	ND-C1D-CHC-C4C
29	JD	202	PEB	ND-C1D-CHC-C4C
29	LD	202	PEB	ND-C1D-CHC-C4C
29	AF	301	PEB	ND-C1D-CHC-C4C
29	AI	301	PEB	ND-C1D-CHC-C4C
29	AJ	201	PEB	ND-C1D-CHC-C4C
29	AJ	203	PEB	C2C-CAC-CBC-CGC
29	BJ	202	PEB	C2C-CAC-CBC-CGC
29	CJ	201	PEB	ND-C1D-CHC-C4C
29	EJ	201	PEB	ND-C1D-CHC-C4C
29	FJ	202	PEB	C2C-CAC-CBC-CGC
29	GJ	201	PEB	ND-C1D-CHC-C4C
29	HJ	201	PEB	C2C-CAC-CBC-CGC
29	IJ	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	IJ	203	PEB	C2C-CAC-CBC-CGC
29	JJ	202	PEB	C2C-CAC-CBC-CGC
29	KJ	201	PEB	ND-C1D-CHC-C4C
29	MJ	201	PEB	ND-C1D-CHC-C4C
29	NJ	202	PEB	C2C-CAC-CBC-CGC
29	OJ	201	PEB	ND-C1D-CHC-C4C
29	PJ	202	PEB	C2C-CAC-CBC-CGC
29	QJ	201	PEB	ND-C1D-CHC-C4C
29	SJ	201	PEB	ND-C1D-CHC-C4C
29	TJ	202	PEB	C2C-CAC-CBC-CGC
29	UJ	201	PEB	ND-C1D-CHC-C4C
29	WJ	201	PEB	C2C-CAC-CBC-CGC
29	WJ	202	PEB	ND-C1D-CHC-C4C
29	XJ	202	PEB	C2C-CAC-CBC-CGC
29	YJ	201	PEB	ND-C1D-CHC-C4C
29	ZJ	202	PEB	C2C-CAC-CBC-CGC
29	aJ	201	PEB	ND-C1D-CHC-C4C
29	bJ	202	PEB	C2C-CAC-CBC-CGC
29	cJ	201	PEB	ND-C1D-CHC-C4C
29	dJ	202	PEB	C2C-CAC-CBC-CGC
29	eJ	201	PEB	ND-C1D-CHC-C4C
29	fJ	202	PEB	C2C-CAC-CBC-CGC
29	gJ	201	PEB	ND-C1D-CHC-C4C
29	hJ	202	PEB	C2C-CAC-CBC-CGC
29	iJ	201	PEB	ND-C1D-CHC-C4C
29	jJ	202	PEB	C2C-CAC-CBC-CGC
29	kJ	201	PEB	ND-C1D-CHC-C4C
29	lJ	202	PEB	C2C-CAC-CBC-CGC
29	mJ	201	PEB	ND-C1D-CHC-C4C
29	nJ	202	PEB	C2C-CAC-CBC-CGC
29	oJ	201	PEB	ND-C1D-CHC-C4C
29	pJ	202	PEB	C2C-CAC-CBC-CGC
29	qJ	201	PEB	ND-C1D-CHC-C4C
29	rJ	202	PEB	C2C-CAC-CBC-CGC
29	sJ	201	PEB	ND-C1D-CHC-C4C
29	sJ	203	PEB	C2C-CAC-CBC-CGC
29	uJ	201	PEB	C2C-CAC-CBC-CGC
29	uJ	202	PEB	ND-C1D-CHC-C4C
29	AL	201	PEB	ND-C1D-CHC-C4C
29	AL	203	PEB	C2C-CAC-CBC-CGC
29	BL	202	PEB	C2C-CAC-CBC-CGC
29	CL	201	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	EL	201	PEB	ND-C1D-CHC-C4C
29	FL	202	PEB	C2C-CAC-CBC-CGC
29	GL	201	PEB	ND-C1D-CHC-C4C
29	HL	201	PEB	C2C-CAC-CBC-CGC
29	IL	201	PEB	ND-C1D-CHC-C4C
29	IL	203	PEB	C2C-CAC-CBC-CGC
29	JL	202	PEB	C2C-CAC-CBC-CGC
29	KL	201	PEB	ND-C1D-CHC-C4C
29	ML	201	PEB	ND-C1D-CHC-C4C
29	NL	202	PEB	C2C-CAC-CBC-CGC
29	OL	201	PEB	ND-C1D-CHC-C4C
29	PL	202	PEB	C2C-CAC-CBC-CGC
29	QL	201	PEB	ND-C1D-CHC-C4C
29	SL	201	PEB	ND-C1D-CHC-C4C
29	TL	202	PEB	C2C-CAC-CBC-CGC
29	UL	201	PEB	ND-C1D-CHC-C4C
29	WL	201	PEB	C2C-CAC-CBC-CGC
29	WL	202	PEB	ND-C1D-CHC-C4C
29	XL	202	PEB	C2C-CAC-CBC-CGC
29	YL	201	PEB	ND-C1D-CHC-C4C
29	ZL	202	PEB	C2C-CAC-CBC-CGC
29	aL	201	PEB	ND-C1D-CHC-C4C
29	bL	202	PEB	C2C-CAC-CBC-CGC
29	cL	201	PEB	ND-C1D-CHC-C4C
29	dL	202	PEB	C2C-CAC-CBC-CGC
29	eL	201	PEB	ND-C1D-CHC-C4C
29	fL	202	PEB	C2C-CAC-CBC-CGC
29	gL	201	PEB	ND-C1D-CHC-C4C
29	hL	202	PEB	C2C-CAC-CBC-CGC
29	iL	201	PEB	ND-C1D-CHC-C4C
29	jL	202	PEB	C2C-CAC-CBC-CGC
29	kL	201	PEB	ND-C1D-CHC-C4C
29	lL	202	PEB	C2C-CAC-CBC-CGC
29	mL	201	PEB	ND-C1D-CHC-C4C
29	nL	202	PEB	C2C-CAC-CBC-CGC
29	oL	201	PEB	ND-C1D-CHC-C4C
29	pL	202	PEB	C2C-CAC-CBC-CGC
29	qL	201	PEB	ND-C1D-CHC-C4C
29	rL	202	PEB	C2C-CAC-CBC-CGC
29	sL	201	PEB	ND-C1D-CHC-C4C
29	sL	203	PEB	C2C-CAC-CBC-CGC
29	uL	201	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	uL	202	PEB	ND-C1D-CHC-C4C
29	AM	303	PEB	ND-C1D-CHC-C4C
29	BM	301	PEB	ND-C1D-CHC-C4C
29	DO	202	PEB	ND-C1D-CHC-C4C
29	eR	401	PEB	C2A-C3A-CAA-CBA
29	SR	201	PEB	ND-C1D-CHC-C4C
30	A1	304	PUB	NA-C4A-CHA-C1B
30	AF	303	PUB	NA-C4A-CHA-C1B
30	AI	303	PUB	NA-C4A-CHA-C1B
30	wJ	304	PUB	NA-C4A-CHA-C1B
30	xJ	304	PUB	NA-C4A-CHA-C1B
30	yJ	303	PUB	NA-C4A-CHA-C1B
30	AK	304	PUB	NA-C4A-CHA-C1B
30	wL	304	PUB	NA-C4A-CHA-C1B
30	xL	304	PUB	NA-C4A-CHA-C1B
29	PF	203	PEB	C1C-C2C-CAC-CBC
29	PF	203	PEB	C3C-C2C-CAC-CBC
29	RF	202	PEB	C1C-C2C-CAC-CBC
29	RF	202	PEB	C3C-C2C-CAC-CBC
29	TF	202	PEB	C1C-C2C-CAC-CBC
29	TF	202	PEB	C3C-C2C-CAC-CBC
29	VF	203	PEB	C1C-C2C-CAC-CBC
29	VF	203	PEB	C3C-C2C-CAC-CBC
29	YF	203	PEB	C1C-C2C-CAC-CBC
29	YF	203	PEB	C3C-C2C-CAC-CBC
29	aF	203	PEB	C1C-C2C-CAC-CBC
29	aF	203	PEB	C3C-C2C-CAC-CBC
29	cF	202	PEB	C1C-C2C-CAC-CBC
29	cF	202	PEB	C3C-C2C-CAC-CBC
29	eF	203	PEB	C1C-C2C-CAC-CBC
29	eF	203	PEB	C3C-C2C-CAC-CBC
29	gF	203	PEB	C1C-C2C-CAC-CBC
29	gF	203	PEB	C3C-C2C-CAC-CBC
29	iF	203	PEB	C1C-C2C-CAC-CBC
29	iF	203	PEB	C3C-C2C-CAC-CBC
29	kF	203	PEB	C1C-C2C-CAC-CBC
29	kF	203	PEB	C3C-C2C-CAC-CBC
29	mF	203	PEB	C1C-C2C-CAC-CBC
29	mF	203	PEB	C3C-C2C-CAC-CBC
29	PI	203	PEB	C1C-C2C-CAC-CBC
29	PI	203	PEB	C3C-C2C-CAC-CBC
29	RI	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	RI	202	PEB	C3C-C2C-CAC-CBC
29	TI	202	PEB	C1C-C2C-CAC-CBC
29	TI	202	PEB	C3C-C2C-CAC-CBC
29	VI	203	PEB	C1C-C2C-CAC-CBC
29	VI	203	PEB	C3C-C2C-CAC-CBC
29	YI	203	PEB	C1C-C2C-CAC-CBC
29	YI	203	PEB	C3C-C2C-CAC-CBC
29	aI	203	PEB	C1C-C2C-CAC-CBC
29	aI	203	PEB	C3C-C2C-CAC-CBC
29	cI	202	PEB	C1C-C2C-CAC-CBC
29	cI	202	PEB	C3C-C2C-CAC-CBC
29	eI	203	PEB	C1C-C2C-CAC-CBC
29	eI	203	PEB	C3C-C2C-CAC-CBC
29	gI	203	PEB	C1C-C2C-CAC-CBC
29	gI	203	PEB	C3C-C2C-CAC-CBC
29	iI	203	PEB	C1C-C2C-CAC-CBC
29	iI	203	PEB	C3C-C2C-CAC-CBC
29	kI	203	PEB	C1C-C2C-CAC-CBC
29	kI	203	PEB	C3C-C2C-CAC-CBC
29	mI	203	PEB	C1C-C2C-CAC-CBC
29	mI	203	PEB	C3C-C2C-CAC-CBC
30	MA	402	PUB	ND-C1D-CHC-C4C
30	MN	402	PUB	ND-C1D-CHC-C4C
31	VP	1001	CYC	C2D-C3D-CAD-CBD
31	xP	1001	CYC	C2D-C3D-CAD-CBD
29	BJ	201	PEB	C3B-CAB-CBB-CGB
29	DJ	201	PEB	C3B-CAB-CBB-CGB
29	FJ	201	PEB	C3B-CAB-CBB-CGB
29	JJ	201	PEB	C3B-CAB-CBB-CGB
29	LJ	201	PEB	C3B-CAB-CBB-CGB
29	NJ	201	PEB	C3B-CAB-CBB-CGB
29	PJ	201	PEB	C3B-CAB-CBB-CGB
29	RJ	201	PEB	C3B-CAB-CBB-CGB
29	TJ	201	PEB	C3B-CAB-CBB-CGB
29	VJ	201	PEB	C3B-CAB-CBB-CGB
29	XJ	201	PEB	C3B-CAB-CBB-CGB
29	ZJ	201	PEB	C3B-CAB-CBB-CGB
29	bJ	201	PEB	C3B-CAB-CBB-CGB
29	dJ	201	PEB	C3B-CAB-CBB-CGB
29	fJ	201	PEB	C3B-CAB-CBB-CGB
29	hJ	201	PEB	C3B-CAB-CBB-CGB
29	jJ	201	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	lJ	201	PEB	C3B-CAB-CBB-CGB
29	nJ	201	PEB	C3B-CAB-CBB-CGB
29	pJ	201	PEB	C3B-CAB-CBB-CGB
29	rJ	201	PEB	C3B-CAB-CBB-CGB
29	tJ	201	PEB	C3B-CAB-CBB-CGB
29	vJ	201	PEB	C3B-CAB-CBB-CGB
29	BL	201	PEB	C3B-CAB-CBB-CGB
29	DL	201	PEB	C3B-CAB-CBB-CGB
29	FL	201	PEB	C3B-CAB-CBB-CGB
29	JL	201	PEB	C3B-CAB-CBB-CGB
29	LL	201	PEB	C3B-CAB-CBB-CGB
29	NL	201	PEB	C3B-CAB-CBB-CGB
29	PL	201	PEB	C3B-CAB-CBB-CGB
29	RL	201	PEB	C3B-CAB-CBB-CGB
29	TL	201	PEB	C3B-CAB-CBB-CGB
29	VL	201	PEB	C3B-CAB-CBB-CGB
29	XL	201	PEB	C3B-CAB-CBB-CGB
29	ZL	201	PEB	C3B-CAB-CBB-CGB
29	bL	201	PEB	C3B-CAB-CBB-CGB
29	dL	201	PEB	C3B-CAB-CBB-CGB
29	fL	201	PEB	C3B-CAB-CBB-CGB
29	hL	201	PEB	C3B-CAB-CBB-CGB
29	jL	201	PEB	C3B-CAB-CBB-CGB
29	lL	201	PEB	C3B-CAB-CBB-CGB
29	nL	201	PEB	C3B-CAB-CBB-CGB
29	pL	201	PEB	C3B-CAB-CBB-CGB
29	rL	201	PEB	C3B-CAB-CBB-CGB
29	tL	201	PEB	C3B-CAB-CBB-CGB
29	vL	201	PEB	C3B-CAB-CBB-CGB
29	AF	304	PEB	C2C-CAC-CBC-CGC
29	AI	304	PEB	C2C-CAC-CBC-CGC
29	RJ	202	PEB	C2C-CAC-CBC-CGC
29	RL	202	PEB	C2C-CAC-CBC-CGC
29	I4	203	PEB	CAB-CBB-CGB-O1B
29	EA	201	PEB	CAB-CBB-CGB-O1B
29	IA	201	PEB	CAB-CBB-CGB-O1B
29	EN	201	PEB	CAB-CBB-CGB-O1B
29	IN	201	PEB	CAB-CBB-CGB-O1B
29	AA	201	PEB	CAB-CBB-CGB-O1B
29	CA	201	PEB	CAB-CBB-CGB-O1B
29	GA	201	PEB	CAB-CBB-CGB-O1B
29	KA	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	AN	201	PEB	CAB-CBB-CGB-O1B
29	CN	201	PEB	CAB-CBB-CGB-O1B
29	GN	201	PEB	CAB-CBB-CGB-O1B
29	KN	201	PEB	CAB-CBB-CGB-O1B
29	C4	202	PEB	C2D-C3D-CAD-CBD
29	E4	202	PEB	C2D-C3D-CAD-CBD
29	G4	202	PEB	C2D-C3D-CAD-CBD
29	I4	202	PEB	C2D-C3D-CAD-CBD
29	K4	202	PEB	C2D-C3D-CAD-CBD
29	M4	202	PEB	C2D-C3D-CAD-CBD
29	CD	202	PEB	C2D-C3D-CAD-CBD
29	ED	201	PEB	C2D-C3D-CAD-CBD
29	GD	202	PEB	C2D-C3D-CAD-CBD
29	ID	202	PEB	C2D-C3D-CAD-CBD
29	KD	202	PEB	C2D-C3D-CAD-CBD
29	MD	202	PEB	C2D-C3D-CAD-CBD
29	MR	202	PEB	C3B-CAB-CBB-CGB
30	A1	305	PUB	C2C-CAC-CBC-CGC
30	AK	305	PUB	C2C-CAC-CBC-CGC
29	O2	202	PEB	CAB-CBB-CGB-O2B
29	U2	202	PEB	CAB-CBB-CGB-O2B
29	J5	201	PEB	CAC-CBC-CGC-O2C
29	P7	201	PEB	CAC-CBC-CGC-O2C
29	R7	201	PEB	CAC-CBC-CGC-O2C
29	T7	201	PEB	CAC-CBC-CGC-O2C
29	V7	201	PEB	CAC-CBC-CGC-O2C
29	Y7	201	PEB	CAC-CBC-CGC-O2C
29	a7	201	PEB	CAC-CBC-CGC-O2C
29	c7	201	PEB	CAC-CBC-CGC-O2C
29	e7	201	PEB	CAC-CBC-CGC-O2C
29	g7	201	PEB	CAC-CBC-CGC-O2C
29	i7	201	PEB	CAC-CBC-CGC-O2C
29	k7	201	PEB	CAC-CBC-CGC-O2C
29	m7	201	PEB	CAC-CBC-CGC-O2C
29	J8	201	PEB	CAC-CBC-CGC-O2C
29	P9	201	PEB	CAC-CBC-CGC-O2C
29	R9	201	PEB	CAC-CBC-CGC-O2C
29	T9	201	PEB	CAC-CBC-CGC-O2C
29	V9	201	PEB	CAC-CBC-CGC-O2C
29	Y9	201	PEB	CAC-CBC-CGC-O2C
29	a9	201	PEB	CAC-CBC-CGC-O2C
29	c9	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	e9	201	PEB	CAC-CBC-CGC-O2C
29	g9	201	PEB	CAC-CBC-CGC-O2C
29	i9	201	PEB	CAC-CBC-CGC-O2C
29	k9	201	PEB	CAC-CBC-CGC-O2C
29	m9	201	PEB	CAC-CBC-CGC-O2C
29	AA	201	PEB	CAC-CBC-CGC-O2C
29	CA	201	PEB	CAC-CBC-CGC-O2C
29	EA	201	PEB	CAC-CBC-CGC-O2C
29	GA	201	PEB	CAC-CBC-CGC-O2C
29	IA	201	PEB	CAC-CBC-CGC-O2C
29	KA	201	PEB	CAC-CBC-CGC-O2C
29	AC	201	PEB	CAB-CBB-CGB-O2B
29	CC	201	PEB	CAB-CBB-CGB-O2B
29	EC	201	PEB	CAB-CBB-CGB-O2B
29	GC	201	PEB	CAB-CBB-CGB-O2B
29	IC	201	PEB	CAB-CBB-CGB-O2B
29	KC	202	PEB	CAB-CBB-CGB-O2B
29	AE	201	PEB	CAB-CBB-CGB-O2B
29	CE	201	PEB	CAB-CBB-CGB-O2B
29	EE	201	PEB	CAB-CBB-CGB-O2B
29	GE	201	PEB	CAB-CBB-CGB-O2B
29	IE	201	PEB	CAB-CBB-CGB-O2B
29	KE	202	PEB	CAB-CBB-CGB-O2B
29	PF	203	PEB	CAB-CBB-CGB-O2B
29	QF	202	PEB	CAB-CBB-CGB-O2B
29	RF	202	PEB	CAB-CBB-CGB-O2B
29	TF	201	PEB	CAB-CBB-CGB-O1B
29	TF	202	PEB	CAB-CBB-CGB-O2B
29	UF	203	PEB	CAB-CBB-CGB-O2B
29	VF	203	PEB	CAB-CBB-CGB-O2B
29	YF	203	PEB	CAB-CBB-CGB-O2B
29	aF	203	PEB	CAB-CBB-CGB-O2B
29	bF	202	PEB	CAB-CBB-CGB-O2B
29	cF	202	PEB	CAB-CBB-CGB-O2B
29	dF	203	PEB	CAB-CBB-CGB-O2B
29	fF	202	PEB	CAB-CBB-CGB-O2B
29	gF	203	PEB	CAB-CBB-CGB-O2B
29	jF	202	PEB	CAB-CBB-CGB-O2B
29	kF	203	PEB	CAB-CBB-CGB-O2B
29	mF	203	PEB	CAB-CBB-CGB-O2B
29	PI	203	PEB	CAB-CBB-CGB-O2B
29	QI	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	RI	202	PEB	CAB-CBB-CGB-O2B
29	TI	202	PEB	CAB-CBB-CGB-O2B
29	UI	203	PEB	CAB-CBB-CGB-O2B
29	VI	203	PEB	CAB-CBB-CGB-O2B
29	YI	203	PEB	CAB-CBB-CGB-O2B
29	aI	203	PEB	CAB-CBB-CGB-O2B
29	bI	202	PEB	CAB-CBB-CGB-O2B
29	cI	202	PEB	CAB-CBB-CGB-O2B
29	dI	203	PEB	CAB-CBB-CGB-O2B
29	fI	202	PEB	CAB-CBB-CGB-O2B
29	gI	203	PEB	CAB-CBB-CGB-O2B
29	jI	202	PEB	CAB-CBB-CGB-O2B
29	kI	203	PEB	CAB-CBB-CGB-O2B
29	mI	203	PEB	CAB-CBB-CGB-O2B
29	AJ	201	PEB	CAC-CBC-CGC-O2C
29	CJ	201	PEB	CAC-CBC-CGC-O2C
29	GJ	201	PEB	CAC-CBC-CGC-O2C
29	IJ	201	PEB	CAC-CBC-CGC-O2C
29	KJ	201	PEB	CAC-CBC-CGC-O2C
29	MJ	201	PEB	CAC-CBC-CGC-O2C
29	OJ	201	PEB	CAC-CBC-CGC-O2C
29	WJ	202	PEB	CAC-CBC-CGC-O2C
29	YJ	201	PEB	CAC-CBC-CGC-O2C
29	aJ	201	PEB	CAC-CBC-CGC-O2C
29	cJ	201	PEB	CAC-CBC-CGC-O2C
29	gJ	201	PEB	CAC-CBC-CGC-O2C
29	iJ	201	PEB	CAC-CBC-CGC-O2C
29	kJ	201	PEB	CAC-CBC-CGC-O2C
29	oJ	201	PEB	CAC-CBC-CGC-O2C
29	sJ	201	PEB	CAC-CBC-CGC-O2C
29	uJ	202	PEB	CAC-CBC-CGC-O2C
29	AL	201	PEB	CAC-CBC-CGC-O2C
29	CL	201	PEB	CAC-CBC-CGC-O2C
29	GL	201	PEB	CAC-CBC-CGC-O2C
29	IL	201	PEB	CAC-CBC-CGC-O2C
29	KL	201	PEB	CAC-CBC-CGC-O2C
29	ML	201	PEB	CAC-CBC-CGC-O2C
29	OL	201	PEB	CAC-CBC-CGC-O2C
29	WL	202	PEB	CAC-CBC-CGC-O2C
29	YL	201	PEB	CAC-CBC-CGC-O2C
29	aL	201	PEB	CAC-CBC-CGC-O2C
29	cL	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	gL	201	PEB	CAC-CBC-CGC-O2C
29	iL	201	PEB	CAC-CBC-CGC-O2C
29	kL	201	PEB	CAC-CBC-CGC-O2C
29	oL	201	PEB	CAC-CBC-CGC-O2C
29	sL	201	PEB	CAC-CBC-CGC-O2C
29	uL	202	PEB	CAC-CBC-CGC-O2C
29	AN	201	PEB	CAC-CBC-CGC-O2C
29	CN	201	PEB	CAC-CBC-CGC-O2C
29	EN	201	PEB	CAC-CBC-CGC-O2C
29	GN	201	PEB	CAC-CBC-CGC-O2C
29	IN	201	PEB	CAC-CBC-CGC-O2C
29	KN	201	PEB	CAC-CBC-CGC-O2C
30	AB	305	PUB	CAC-CBC-CGC-O2C
30	AM	305	PUB	CAC-CBC-CGC-O2C
29	A1	301	PEB	C2D-C1D-CHC-C4C
29	M2	202	PEB	C2D-C1D-CHC-C4C
29	O2	202	PEB	C2D-C1D-CHC-C4C
29	Q2	202	PEB	C2D-C1D-CHC-C4C
29	S2	202	PEB	C2D-C1D-CHC-C4C
29	U2	202	PEB	C2D-C1D-CHC-C4C
29	W2	202	PEB	C2D-C1D-CHC-C4C
29	B4	202	PEB	C2D-C1D-CHC-C4C
29	D4	202	PEB	C2D-C1D-CHC-C4C
29	F4	202	PEB	C2D-C1D-CHC-C4C
29	H4	202	PEB	C2D-C1D-CHC-C4C
29	J4	202	PEB	C2D-C1D-CHC-C4C
29	L4	202	PEB	C2D-C1D-CHC-C4C
29	L5	202	PEB	C2D-C1D-CHC-C4C
29	B8	202	PEB	C2D-C1D-CHC-C4C
29	F8	202	PEB	C2D-C1D-CHC-C4C
29	L8	202	PEB	C2D-C1D-CHC-C4C
29	BD	202	PEB	C2D-C1D-CHC-C4C
29	DD	202	PEB	C2D-C1D-CHC-C4C
29	FD	202	PEB	C2D-C1D-CHC-C4C
29	HD	202	PEB	C2D-C1D-CHC-C4C
29	JD	202	PEB	C2D-C1D-CHC-C4C
29	LD	202	PEB	C2D-C1D-CHC-C4C
29	AK	301	PEB	C2D-C1D-CHC-C4C
29	QR	202	PEB	C2D-C1D-CHC-C4C
29	SR	202	PEB	C2D-C1D-CHC-C4C
29	UR	202	PEB	C2D-C1D-CHC-C4C
29	WR	202	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	Q2	202	PEB	CAB-CBB-CGB-O2B
29	S2	202	PEB	CAB-CBB-CGB-O2B
29	W2	202	PEB	CAB-CBB-CGB-O2B
29	K8	202	PEB	CAB-CBB-CGB-O2B
29	C8	202	PEB	CAB-CBB-CGB-O2B
29	DF	1002	PEB	CAC-CBC-CGC-O2C
29	HF	1002	PEB	CAC-CBC-CGC-O2C
29	JF	1002	PEB	CAC-CBC-CGC-O2C
29	LF	1002	PEB	CAC-CBC-CGC-O2C
29	NF	1002	PEB	CAC-CBC-CGC-O2C
29	eF	203	PEB	CAB-CBB-CGB-O2B
29	iF	203	PEB	CAB-CBB-CGB-O2B
29	DI	1002	PEB	CAC-CBC-CGC-O2C
29	HI	1002	PEB	CAC-CBC-CGC-O2C
29	JI	1002	PEB	CAC-CBC-CGC-O2C
29	LI	1002	PEB	CAC-CBC-CGC-O2C
29	NI	1002	PEB	CAC-CBC-CGC-O2C
29	eI	203	PEB	CAB-CBB-CGB-O2B
29	iI	203	PEB	CAB-CBB-CGB-O2B
29	QJ	201	PEB	CAC-CBC-CGC-O2C
29	eJ	201	PEB	CAC-CBC-CGC-O2C
29	qJ	201	PEB	CAC-CBC-CGC-O2C
29	wJ	301	PEB	CAB-CBB-CGB-O2B
29	xJ	301	PEB	CAB-CBB-CGB-O2B
29	QL	201	PEB	CAC-CBC-CGC-O2C
29	eL	201	PEB	CAC-CBC-CGC-O2C
29	qL	201	PEB	CAC-CBC-CGC-O2C
29	wL	301	PEB	CAB-CBB-CGB-O2B
29	xL	301	PEB	CAB-CBB-CGB-O2B
29	MQ	407	PEB	CAB-CBB-CGB-O2B
29	QR	202	PEB	CAB-CBB-CGB-O2B
29	SR	202	PEB	CAB-CBB-CGB-O2B
29	UR	202	PEB	CAB-CBB-CGB-O2B
29	WR	202	PEB	CAB-CBB-CGB-O2B
29	A3	202	PEB	CAC-CBC-CGC-O2C
29	C3	202	PEB	CAC-CBC-CGC-O2C
29	I3	202	PEB	CAC-CBC-CGC-O2C
29	M4	203	PEB	CAC-CBC-CGC-O1C
29	I5	202	PEB	CAB-CBB-CGB-O2B
29	K5	202	PEB	CAB-CBB-CGB-O2B
29	A5	202	PEB	CAB-CBB-CGB-O2B
29	C5	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	I8	202	PEB	CAB-CBB-CGB-O2B
29	MA	404	PEB	CAB-CBB-CGB-O2B
29	FF	1002	PEB	CAC-CBC-CGC-O2C
29	SF	202	PEB	CAB-CBB-CGB-O2B
29	TF	201	PEB	CAC-CBC-CGC-O1C
29	WF	202	PEB	CAB-CBB-CGB-O2B
29	ZF	202	PEB	CAB-CBB-CGB-O2B
29	hF	202	PEB	CAB-CBB-CGB-O2B
29	lF	202	PEB	CAB-CBB-CGB-O2B
29	MG	405	PEB	CAB-CBB-CGB-O2B
29	FI	1002	PEB	CAC-CBC-CGC-O2C
29	SI	202	PEB	CAB-CBB-CGB-O2B
29	WI	202	PEB	CAB-CBB-CGB-O2B
29	ZI	202	PEB	CAB-CBB-CGB-O2B
29	hI	202	PEB	CAB-CBB-CGB-O2B
29	lI	202	PEB	CAB-CBB-CGB-O2B
29	SJ	201	PEB	CAC-CBC-CGC-O2C
29	mJ	201	PEB	CAC-CBC-CGC-O2C
29	SL	201	PEB	CAC-CBC-CGC-O2C
29	mL	201	PEB	CAC-CBC-CGC-O2C
29	AO	202	PEB	CAC-CBC-CGC-O2C
29	CO	202	PEB	CAC-CBC-CGC-O2C
29	IO	202	PEB	CAC-CBC-CGC-O2C
30	MG	403	PUB	C4A-C3A-CAA-CBA
29	e2	402	PEB	CAB-CBB-CGB-O1B
29	M2	202	PEB	CAB-CBB-CGB-O2B
29	N2	201	PEB	CAB-CBB-CGB-O1B
29	E3	202	PEB	CAC-CBC-CGC-O2C
29	G3	202	PEB	CAC-CBC-CGC-O2C
29	K3	202	PEB	CAC-CBC-CGC-O2C
29	B4	202	PEB	CAC-CBC-CGC-O1C
29	D4	202	PEB	CAC-CBC-CGC-O1C
29	F4	202	PEB	CAC-CBC-CGC-O1C
29	H4	202	PEB	CAC-CBC-CGC-O1C
29	J4	202	PEB	CAC-CBC-CGC-O1C
29	L4	202	PEB	CAC-CBC-CGC-O1C
29	A7	301	PEB	CAB-CBB-CGB-O2B
29	A8	202	PEB	CAB-CBB-CGB-O2B
29	A9	301	PEB	CAB-CBB-CGB-O2B
29	MA	405	PEB	CAB-CBB-CGB-O1B
29	AB	303	PEB	CAC-CBC-CGC-O2C
29	CB	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	EB	201	PEB	CAC-CBC-CGC-O1C
29	GB	201	PEB	CAC-CBC-CGC-O1C
29	IB	201	PEB	CAC-CBC-CGC-O1C
29	KB	201	PEB	CAC-CBC-CGC-O1C
29	MB	201	PEB	CAC-CBC-CGC-O1C
29	OB	201	PEB	CAC-CBC-CGC-O1C
29	QB	203	PEB	CAC-CBC-CGC-O1C
29	SB	201	PEB	CAC-CBC-CGC-O1C
29	UB	201	PEB	CAC-CBC-CGC-O1C
29	WB	201	PEB	CAC-CBC-CGC-O1C
29	YB	202	PEB	CAC-CBC-CGC-O1C
29	aB	201	PEB	CAC-CBC-CGC-O1C
29	dB	201	PEB	CAC-CBC-CGC-O1C
29	fB	201	PEB	CAC-CBC-CGC-O1C
29	hB	201	PEB	CAC-CBC-CGC-O1C
29	jB	201	PEB	CAC-CBC-CGC-O1C
29	lB	201	PEB	CAC-CBC-CGC-O1C
29	BD	202	PEB	CAC-CBC-CGC-O1C
29	DD	202	PEB	CAC-CBC-CGC-O1C
29	FD	202	PEB	CAC-CBC-CGC-O1C
29	HD	202	PEB	CAC-CBC-CGC-O1C
29	JD	202	PEB	CAC-CBC-CGC-O1C
29	LD	202	PEB	CAC-CBC-CGC-O1C
29	OF	202	PEB	CAB-CBB-CGB-O2B
29	OI	202	PEB	CAB-CBB-CGB-O2B
29	EJ	201	PEB	CAC-CBC-CGC-O2C
29	UJ	201	PEB	CAC-CBC-CGC-O2C
29	EL	201	PEB	CAC-CBC-CGC-O2C
29	UL	201	PEB	CAC-CBC-CGC-O2C
29	AM	303	PEB	CAC-CBC-CGC-O2C
29	CM	201	PEB	CAC-CBC-CGC-O1C
29	EM	201	PEB	CAC-CBC-CGC-O1C
29	GM	201	PEB	CAC-CBC-CGC-O1C
29	IM	201	PEB	CAC-CBC-CGC-O1C
29	KM	201	PEB	CAC-CBC-CGC-O1C
29	MM	201	PEB	CAC-CBC-CGC-O1C
29	OM	201	PEB	CAC-CBC-CGC-O1C
29	QM	203	PEB	CAC-CBC-CGC-O1C
29	SM	201	PEB	CAC-CBC-CGC-O1C
29	UM	201	PEB	CAC-CBC-CGC-O1C
29	WM	201	PEB	CAC-CBC-CGC-O1C
29	YM	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	aM	201	PEB	CAC-CBC-CGC-O1C
29	dM	201	PEB	CAC-CBC-CGC-O1C
29	fM	201	PEB	CAC-CBC-CGC-O1C
29	hM	201	PEB	CAC-CBC-CGC-O1C
29	jM	201	PEB	CAC-CBC-CGC-O1C
29	lM	201	PEB	CAC-CBC-CGC-O1C
29	MN	404	PEB	CAB-CBB-CGB-O2B
29	EO	202	PEB	CAC-CBC-CGC-O2C
29	GO	202	PEB	CAC-CBC-CGC-O2C
29	KO	202	PEB	CAC-CBC-CGC-O2C
30	MG	402	PUB	CAC-CBC-CGC-O2C
30	MQ	404	PUB	CAC-CBC-CGC-O2C
31	E7	1001	CYC	CAA-CBA-CGA-O1A
31	I7	1001	CYC	CAA-CBA-CGA-O1A
31	K7	1001	CYC	CAA-CBA-CGA-O1A
31	M7	1001	CYC	CAA-CBA-CGA-O1A
31	E9	1001	CYC	CAA-CBA-CGA-O1A
31	I9	1001	CYC	CAA-CBA-CGA-O1A
31	M9	1001	CYC	CAA-CBA-CGA-O1A
31	DF	1001	CYC	CAA-CBA-CGA-O1A
31	FF	1001	CYC	CAA-CBA-CGA-O1A
31	HF	1001	CYC	CAA-CBA-CGA-O1A
31	JF	1001	CYC	CAA-CBA-CGA-O1A
31	LF	1001	CYC	CAA-CBA-CGA-O1A
31	NF	1001	CYC	CAA-CBA-CGA-O1A
31	DI	1001	CYC	CAA-CBA-CGA-O1A
31	FI	1001	CYC	CAA-CBA-CGA-O1A
31	HI	1001	CYC	CAA-CBA-CGA-O1A
31	JI	1001	CYC	CAA-CBA-CGA-O1A
31	LI	1001	CYC	CAA-CBA-CGA-O1A
31	NI	1001	CYC	CAA-CBA-CGA-O1A
30	MQ	405	PUB	C4A-C3A-CAA-CBA
29	A1	302	PEB	CAC-CBC-CGC-O1C
29	S1	202	PEB	CAC-CBC-CGC-O2C
29	W1	202	PEB	CAC-CBC-CGC-O2C
29	c1	202	PEB	CAC-CBC-CGC-O2C
29	d1	202	PEB	CAC-CBC-CGC-O2C
29	g1	202	PEB	CAC-CBC-CGC-O2C
29	h1	202	PEB	CAC-CBC-CGC-O2C
29	i1	202	PEB	CAC-CBC-CGC-O2C
29	e2	402	PEB	CAC-CBC-CGC-O1C
29	N2	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	R2	201	PEB	CAC-CBC-CGC-O1C
29	T2	201	PEB	CAC-CBC-CGC-O1C
29	V2	201	PEB	CAC-CBC-CGC-O1C
29	N3	202	PEB	CAC-CBC-CGC-O2C
29	B5	203	PEB	CAC-CBC-CGC-O1C
29	F5	203	PEB	CAC-CBC-CGC-O1C
29	G5	203	PEB	CAC-CBC-CGC-O1C
29	H5	203	PEB	CAC-CBC-CGC-O1C
29	L5	203	PEB	CAC-CBC-CGC-O1C
29	B8	203	PEB	CAC-CBC-CGC-O1C
29	F8	203	PEB	CAC-CBC-CGC-O1C
29	G8	203	PEB	CAC-CBC-CGC-O1C
29	H8	203	PEB	CAC-CBC-CGC-O1C
29	L8	203	PEB	CAC-CBC-CGC-O1C
29	MA	401	PEB	CAC-CBC-CGC-O1C
29	MA	404	PEB	CAB-CBB-CGB-O1B
29	MA	405	PEB	CAC-CBC-CGC-O1C
29	BC	202	PEB	CAC-CBC-CGC-O1C
29	FC	202	PEB	CAC-CBC-CGC-O1C
29	HC	202	PEB	CAC-CBC-CGC-O1C
29	KC	201	PEB	CAC-CBC-CGC-O1C
29	BE	202	PEB	CAC-CBC-CGC-O1C
29	FE	202	PEB	CAC-CBC-CGC-O1C
29	HE	202	PEB	CAC-CBC-CGC-O1C
29	KE	201	PEB	CAC-CBC-CGC-O1C
29	AF	301	PEB	CAB-CBB-CGB-O1B
29	HF	1002	PEB	CAC-CBC-CGC-O1C
29	AI	301	PEB	CAB-CBB-CGB-O1B
29	HI	1002	PEB	CAC-CBC-CGC-O1C
29	AJ	203	PEB	CAC-CBC-CGC-O1C
29	BJ	202	PEB	CAC-CBC-CGC-O1C
29	HJ	201	PEB	CAC-CBC-CGC-O1C
29	IJ	203	PEB	CAC-CBC-CGC-O1C
29	JJ	202	PEB	CAC-CBC-CGC-O1C
29	NJ	202	PEB	CAC-CBC-CGC-O1C
29	RJ	202	PEB	CAC-CBC-CGC-O1C
29	XJ	202	PEB	CAC-CBC-CGC-O1C
29	ZJ	202	PEB	CAC-CBC-CGC-O1C
29	bJ	202	PEB	CAC-CBC-CGC-O1C
29	dJ	202	PEB	CAC-CBC-CGC-O1C
29	jJ	202	PEB	CAC-CBC-CGC-O1C
29	lJ	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	nJ	202	PEB	CAC-CBC-CGC-O1C
29	pJ	202	PEB	CAC-CBC-CGC-O1C
29	rJ	202	PEB	CAC-CBC-CGC-O1C
29	wJ	303	PEB	CAB-CBB-CGB-O1B
29	xJ	303	PEB	CAB-CBB-CGB-O1B
29	yJ	301	PEB	CAC-CBC-CGC-O1C
29	yJ	301	PEB	CAB-CBB-CGB-O1B
29	AK	302	PEB	CAC-CBC-CGC-O1C
29	SK	202	PEB	CAC-CBC-CGC-O2C
29	WK	202	PEB	CAC-CBC-CGC-O2C
29	cK	202	PEB	CAC-CBC-CGC-O2C
29	dK	202	PEB	CAC-CBC-CGC-O2C
29	gK	202	PEB	CAC-CBC-CGC-O2C
29	hK	202	PEB	CAC-CBC-CGC-O2C
29	iK	202	PEB	CAC-CBC-CGC-O2C
29	AL	203	PEB	CAC-CBC-CGC-O1C
29	BL	202	PEB	CAC-CBC-CGC-O1C
29	HL	201	PEB	CAC-CBC-CGC-O1C
29	IL	203	PEB	CAC-CBC-CGC-O1C
29	JL	202	PEB	CAC-CBC-CGC-O1C
29	NL	202	PEB	CAC-CBC-CGC-O1C
29	RL	202	PEB	CAC-CBC-CGC-O1C
29	XL	202	PEB	CAC-CBC-CGC-O1C
29	ZL	202	PEB	CAC-CBC-CGC-O1C
29	bL	202	PEB	CAC-CBC-CGC-O1C
29	dL	202	PEB	CAC-CBC-CGC-O1C
29	jL	202	PEB	CAC-CBC-CGC-O1C
29	lL	202	PEB	CAC-CBC-CGC-O1C
29	nL	202	PEB	CAC-CBC-CGC-O1C
29	pL	202	PEB	CAC-CBC-CGC-O1C
29	rL	202	PEB	CAC-CBC-CGC-O1C
29	wL	303	PEB	CAB-CBB-CGB-O1B
29	xL	303	PEB	CAB-CBB-CGB-O1B
29	yL	301	PEB	CAC-CBC-CGC-O1C
29	yL	301	PEB	CAB-CBB-CGB-O1B
29	MN	401	PEB	CAC-CBC-CGC-O1C
29	MN	404	PEB	CAB-CBB-CGB-O1B
29	MN	405	PEB	CAC-CBC-CGC-O1C
29	MN	405	PEB	CAB-CBB-CGB-O1B
29	NR	201	PEB	CAC-CBC-CGC-O1C
29	RR	201	PEB	CAC-CBC-CGC-O1C
29	RR	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	TR	201	PEB	CAC-CBC-CGC-O1C
29	VR	201	PEB	CAC-CBC-CGC-O1C
29	VR	201	PEB	CAB-CBB-CGB-O1B
29	XR	201	PEB	CAC-CBC-CGC-O1C
29	XR	201	PEB	CAB-CBB-CGB-O1B
30	A1	305	PUB	CAC-CBC-CGC-O1C
30	AB	305	PUB	CAC-CBC-CGC-O1C
30	AK	305	PUB	CAC-CBC-CGC-O1C
31	C7	1001	CYC	CAA-CBA-CGA-O1A
31	G7	1001	CYC	CAA-CBA-CGA-O1A
31	C9	1001	CYC	CAA-CBA-CGA-O1A
31	G9	1001	CYC	CAA-CBA-CGA-O1A
31	K9	1001	CYC	CAA-CBA-CGA-O1A
29	A1	301	PEB	CAC-CBC-CGC-O1C
29	A1	301	PEB	CAB-CBB-CGB-O2B
29	D1	1002	PEB	CAB-CBB-CGB-O1B
29	F1	1002	PEB	CAB-CBB-CGB-O1B
29	H1	1002	PEB	CAB-CBB-CGB-O1B
29	J1	1002	PEB	CAB-CBB-CGB-O1B
29	L1	1002	PEB	CAB-CBB-CGB-O1B
29	N1	1002	PEB	CAB-CBB-CGB-O1B
29	O1	202	PEB	CAC-CBC-CGC-O2C
29	P1	202	PEB	CAC-CBC-CGC-O1C
29	P1	202	PEB	CAC-CBC-CGC-O2C
29	Q1	202	PEB	CAC-CBC-CGC-O2C
29	R1	202	PEB	CAC-CBC-CGC-O2C
29	U1	201	PEB	CAC-CBC-CGC-O2C
29	U1	203	PEB	CAC-CBC-CGC-O2C
29	V1	202	PEB	CAC-CBC-CGC-O2C
29	Z1	201	PEB	CAC-CBC-CGC-O1C
29	Z1	201	PEB	CAC-CBC-CGC-O2C
29	Z1	203	PEB	CAC-CBC-CGC-O2C
29	a1	202	PEB	CAC-CBC-CGC-O2C
29	b1	202	PEB	CAC-CBC-CGC-O2C
29	c1	202	PEB	CAC-CBC-CGC-O1C
29	e1	202	PEB	CAC-CBC-CGC-O1C
29	e1	202	PEB	CAC-CBC-CGC-O2C
29	f1	202	PEB	CAC-CBC-CGC-O2C
29	g1	202	PEB	CAC-CBC-CGC-O1C
29	i1	202	PEB	CAC-CBC-CGC-O1C
29	j1	202	PEB	CAC-CBC-CGC-O2C
29	j1	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	j1	203	PEB	CAC-CBC-CGC-O2C
29	k1	202	PEB	CAC-CBC-CGC-O2C
29	l1	202	PEB	CAC-CBC-CGC-O2C
29	M2	202	PEB	CAC-CBC-CGC-O2C
29	O2	202	PEB	CAC-CBC-CGC-O2C
29	Q2	202	PEB	CAC-CBC-CGC-O2C
29	R2	201	PEB	CAB-CBB-CGB-O1B
29	S2	202	PEB	CAC-CBC-CGC-O2C
29	T2	201	PEB	CAB-CBB-CGB-O1B
29	U2	202	PEB	CAC-CBC-CGC-O2C
29	V2	201	PEB	CAB-CBB-CGB-O1B
29	W2	202	PEB	CAC-CBC-CGC-O2C
29	B3	202	PEB	CAB-CBB-CGB-O1B
29	D3	202	PEB	CAC-CBC-CGC-O1C
29	F3	202	PEB	CAB-CBB-CGB-O1B
29	H3	202	PEB	CAB-CBB-CGB-O1B
29	I3	203	PEB	CAB-CBB-CGB-O1B
29	J3	202	PEB	CAB-CBB-CGB-O1B
29	M3	202	PEB	CAC-CBC-CGC-O2C
29	A7	301	PEB	CAC-CBC-CGC-O1C
29	A9	301	PEB	CAC-CBC-CGC-O1C
29	BA	201	PEB	CAC-CBC-CGC-O2C
29	DA	201	PEB	CAC-CBC-CGC-O2C
29	HA	201	PEB	CAC-CBC-CGC-O2C
29	JA	201	PEB	CAC-CBC-CGC-O2C
29	LA	201	PEB	CAC-CBC-CGC-O2C
29	DB	203	PEB	CAC-CBC-CGC-O1C
29	FB	203	PEB	CAC-CBC-CGC-O1C
29	HB	203	PEB	CAC-CBC-CGC-O1C
29	LB	203	PEB	CAC-CBC-CGC-O1C
29	NB	202	PEB	CAC-CBC-CGC-O1C
29	PB	202	PEB	CAC-CBC-CGC-O1C
29	RB	203	PEB	CAC-CBC-CGC-O1C
29	TB	203	PEB	CAC-CBC-CGC-O1C
29	VB	203	PEB	CAC-CBC-CGC-O1C
29	XB	202	PEB	CAC-CBC-CGC-O1C
29	ZB	203	PEB	CAC-CBC-CGC-O1C
29	eB	202	PEB	CAC-CBC-CGC-O1C
29	gB	203	PEB	CAC-CBC-CGC-O1C
29	iB	203	PEB	CAC-CBC-CGC-O1C
29	kB	203	PEB	CAC-CBC-CGC-O1C
29	mB	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	AC	203	PEB	CAC-CBC-CGC-O1C
29	LC	202	PEB	CAC-CBC-CGC-O1C
29	AE	203	PEB	CAC-CBC-CGC-O1C
29	LE	202	PEB	CAC-CBC-CGC-O1C
29	AF	304	PEB	CAB-CBB-CGB-O2B
29	DF	1002	PEB	CAC-CBC-CGC-O1C
29	FF	1002	PEB	CAC-CBC-CGC-O1C
29	JF	1002	PEB	CAC-CBC-CGC-O1C
29	LF	1002	PEB	CAC-CBC-CGC-O1C
29	NF	1002	PEB	CAC-CBC-CGC-O1C
29	QF	202	PEB	CAB-CBB-CGB-O1B
29	bF	202	PEB	CAB-CBB-CGB-O1B
29	hF	202	PEB	CAB-CBB-CGB-O1B
29	jF	202	PEB	CAB-CBB-CGB-O1B
29	AG	201	PEB	CAB-CBB-CGB-O1B
29	CG	201	PEB	CAB-CBB-CGB-O1B
29	EG	201	PEB	CAB-CBB-CGB-O1B
29	GG	201	PEB	CAB-CBB-CGB-O1B
29	IG	201	PEB	CAB-CBB-CGB-O1B
29	KG	201	PEB	CAB-CBB-CGB-O1B
29	MG	401	PEB	CAB-CBB-CGB-O1B
29	AI	304	PEB	CAB-CBB-CGB-O2B
29	DI	1002	PEB	CAC-CBC-CGC-O1C
29	FI	1002	PEB	CAC-CBC-CGC-O1C
29	JI	1002	PEB	CAC-CBC-CGC-O1C
29	LI	1002	PEB	CAC-CBC-CGC-O1C
29	NI	1002	PEB	CAC-CBC-CGC-O1C
29	QI	202	PEB	CAB-CBB-CGB-O1B
29	bI	202	PEB	CAB-CBB-CGB-O1B
29	hI	202	PEB	CAB-CBB-CGB-O1B
29	jI	202	PEB	CAB-CBB-CGB-O1B
29	FJ	202	PEB	CAC-CBC-CGC-O1C
29	FJ	203	PEB	CAB-CBB-CGB-O2B
29	PJ	202	PEB	CAC-CBC-CGC-O1C
29	TJ	202	PEB	CAC-CBC-CGC-O1C
29	WJ	201	PEB	CAC-CBC-CGC-O1C
29	fJ	202	PEB	CAC-CBC-CGC-O1C
29	hJ	202	PEB	CAC-CBC-CGC-O1C
29	sJ	203	PEB	CAC-CBC-CGC-O1C
29	uJ	201	PEB	CAC-CBC-CGC-O1C
29	wJ	303	PEB	CAC-CBC-CGC-O2C
29	xJ	303	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	AK	301	PEB	CAC-CBC-CGC-O1C
29	AK	301	PEB	CAB-CBB-CGB-O2B
29	DK	1002	PEB	CAB-CBB-CGB-O1B
29	FK	1002	PEB	CAB-CBB-CGB-O1B
29	HK	1002	PEB	CAB-CBB-CGB-O1B
29	JK	1002	PEB	CAB-CBB-CGB-O1B
29	LK	1002	PEB	CAB-CBB-CGB-O1B
29	NK	1002	PEB	CAB-CBB-CGB-O1B
29	OK	202	PEB	CAC-CBC-CGC-O2C
29	PK	202	PEB	CAC-CBC-CGC-O1C
29	PK	202	PEB	CAC-CBC-CGC-O2C
29	QK	202	PEB	CAC-CBC-CGC-O2C
29	RK	202	PEB	CAC-CBC-CGC-O2C
29	UK	201	PEB	CAC-CBC-CGC-O2C
29	UK	203	PEB	CAC-CBC-CGC-O2C
29	VK	202	PEB	CAC-CBC-CGC-O2C
29	ZK	201	PEB	CAC-CBC-CGC-O1C
29	ZK	201	PEB	CAC-CBC-CGC-O2C
29	ZK	203	PEB	CAC-CBC-CGC-O2C
29	aK	202	PEB	CAC-CBC-CGC-O2C
29	bK	202	PEB	CAC-CBC-CGC-O2C
29	cK	202	PEB	CAC-CBC-CGC-O1C
29	eK	202	PEB	CAC-CBC-CGC-O1C
29	eK	202	PEB	CAC-CBC-CGC-O2C
29	fK	202	PEB	CAC-CBC-CGC-O2C
29	gK	202	PEB	CAC-CBC-CGC-O1C
29	iK	202	PEB	CAC-CBC-CGC-O1C
29	jK	202	PEB	CAC-CBC-CGC-O2C
29	jK	203	PEB	CAC-CBC-CGC-O1C
29	jK	203	PEB	CAC-CBC-CGC-O2C
29	kK	202	PEB	CAC-CBC-CGC-O2C
29	lK	202	PEB	CAC-CBC-CGC-O2C
29	FL	202	PEB	CAC-CBC-CGC-O1C
29	FL	203	PEB	CAB-CBB-CGB-O2B
29	PL	202	PEB	CAC-CBC-CGC-O1C
29	TL	202	PEB	CAC-CBC-CGC-O1C
29	WL	201	PEB	CAC-CBC-CGC-O1C
29	fL	202	PEB	CAC-CBC-CGC-O1C
29	hL	202	PEB	CAC-CBC-CGC-O1C
29	sL	203	PEB	CAC-CBC-CGC-O1C
29	uL	201	PEB	CAC-CBC-CGC-O1C
29	wL	303	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	xL	303	PEB	CAC-CBC-CGC-O2C
29	DM	203	PEB	CAC-CBC-CGC-O1C
29	FM	203	PEB	CAC-CBC-CGC-O1C
29	HM	203	PEB	CAC-CBC-CGC-O1C
29	LM	203	PEB	CAC-CBC-CGC-O1C
29	NM	202	PEB	CAC-CBC-CGC-O1C
29	PM	202	PEB	CAC-CBC-CGC-O1C
29	RM	203	PEB	CAC-CBC-CGC-O1C
29	TM	203	PEB	CAC-CBC-CGC-O1C
29	VM	203	PEB	CAC-CBC-CGC-O1C
29	XM	202	PEB	CAC-CBC-CGC-O1C
29	ZM	203	PEB	CAC-CBC-CGC-O1C
29	eM	202	PEB	CAC-CBC-CGC-O1C
29	gM	203	PEB	CAC-CBC-CGC-O1C
29	iM	203	PEB	CAC-CBC-CGC-O1C
29	kM	203	PEB	CAC-CBC-CGC-O1C
29	mM	203	PEB	CAC-CBC-CGC-O1C
29	BN	201	PEB	CAC-CBC-CGC-O2C
29	DN	201	PEB	CAC-CBC-CGC-O2C
29	HN	201	PEB	CAC-CBC-CGC-O2C
29	JN	201	PEB	CAC-CBC-CGC-O2C
29	LN	201	PEB	CAC-CBC-CGC-O2C
29	BO	202	PEB	CAB-CBB-CGB-O1B
29	DO	202	PEB	CAC-CBC-CGC-O1C
29	FO	202	PEB	CAB-CBB-CGB-O1B
29	HO	202	PEB	CAB-CBB-CGB-O1B
29	IO	203	PEB	CAB-CBB-CGB-O1B
29	JO	202	PEB	CAB-CBB-CGB-O1B
29	MO	202	PEB	CAC-CBC-CGC-O2C
29	AQ	201	PEB	CAB-CBB-CGB-O1B
29	CQ	201	PEB	CAB-CBB-CGB-O1B
29	EQ	201	PEB	CAB-CBB-CGB-O1B
29	GQ	201	PEB	CAB-CBB-CGB-O1B
29	IQ	201	PEB	CAB-CBB-CGB-O1B
29	KQ	201	PEB	CAB-CBB-CGB-O1B
29	NR	201	PEB	CAB-CBB-CGB-O1B
29	OR	202	PEB	CAC-CBC-CGC-O2C
29	QR	202	PEB	CAC-CBC-CGC-O2C
29	SR	202	PEB	CAC-CBC-CGC-O2C
29	TR	201	PEB	CAB-CBB-CGB-O1B
29	UR	202	PEB	CAC-CBC-CGC-O2C
29	WR	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
30	AM	305	PUB	CAC-CBC-CGC-O1C
31	F1	1001	CYC	CAA-CBA-CGA-O2A
31	H1	1001	CYC	CAA-CBA-CGA-O2A
31	N1	1001	CYC	CAA-CBA-CGA-O2A
31	FK	1001	CYC	CAA-CBA-CGA-O2A
31	HK	1001	CYC	CAA-CBA-CGA-O2A
31	NK	1001	CYC	CAA-CBA-CGA-O2A
29	A1	303	PEB	CAC-CBC-CGC-O1C
29	O1	202	PEB	CAB-CBB-CGB-O1B
29	R1	202	PEB	CAC-CBC-CGC-O1C
29	U1	201	PEB	CAC-CBC-CGC-O1C
29	a1	202	PEB	CAC-CBC-CGC-O1C
29	k1	202	PEB	CAC-CBC-CGC-O1C
29	P2	201	PEB	CAC-CBC-CGC-O2C
29	A3	202	PEB	CAB-CBB-CGB-O2B
29	B3	203	PEB	CAB-CBB-CGB-O1B
29	C3	202	PEB	CAB-CBB-CGB-O2B
29	D3	203	PEB	CAB-CBB-CGB-O1B
29	E3	202	PEB	CAB-CBB-CGB-O2B
29	F3	202	PEB	CAC-CBC-CGC-O1C
29	F3	203	PEB	CAB-CBB-CGB-O1B
29	G3	202	PEB	CAB-CBB-CGB-O2B
29	H3	203	PEB	CAB-CBB-CGB-O1B
29	I3	202	PEB	CAB-CBB-CGB-O2B
29	J3	203	PEB	CAB-CBB-CGB-O1B
29	K3	202	PEB	CAB-CBB-CGB-O2B
29	L3	202	PEB	CAB-CBB-CGB-O1B
29	M3	202	PEB	CAC-CBC-CGC-O1C
29	N3	202	PEB	CAC-CBC-CGC-O1C
29	B5	202	PEB	CAB-CBB-CGB-O1B
29	F5	202	PEB	CAB-CBB-CGB-O1B
29	G5	202	PEB	CAB-CBB-CGB-O1B
29	H5	202	PEB	CAB-CBB-CGB-O1B
29	K5	202	PEB	CAC-CBC-CGC-O2C
29	L5	202	PEB	CAB-CBB-CGB-O1B
29	A5	202	PEB	CAC-CBC-CGC-O2C
29	C5	202	PEB	CAC-CBC-CGC-O2C
29	A7	304	PEB	CAB-CBB-CGB-O2B
29	P7	202	PEB	CAC-CBC-CGC-O1C
29	R7	202	PEB	CAC-CBC-CGC-O1C
29	T7	202	PEB	CAC-CBC-CGC-O1C
29	V7	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	Y7	202	PEB	CAC-CBC-CGC-O1C
29	a7	202	PEB	CAC-CBC-CGC-O1C
29	c7	202	PEB	CAC-CBC-CGC-O1C
29	e7	202	PEB	CAC-CBC-CGC-O1C
29	g7	202	PEB	CAC-CBC-CGC-O1C
29	i7	202	PEB	CAC-CBC-CGC-O1C
29	k7	202	PEB	CAC-CBC-CGC-O1C
29	m7	202	PEB	CAC-CBC-CGC-O1C
29	B8	202	PEB	CAB-CBB-CGB-O1B
29	F8	202	PEB	CAB-CBB-CGB-O1B
29	G8	202	PEB	CAB-CBB-CGB-O1B
29	H8	202	PEB	CAB-CBB-CGB-O1B
29	K8	202	PEB	CAC-CBC-CGC-O2C
29	L8	202	PEB	CAB-CBB-CGB-O1B
29	A8	202	PEB	CAC-CBC-CGC-O2C
29	C8	202	PEB	CAC-CBC-CGC-O2C
29	A9	304	PEB	CAB-CBB-CGB-O2B
29	P9	202	PEB	CAC-CBC-CGC-O1C
29	R9	202	PEB	CAC-CBC-CGC-O1C
29	T9	202	PEB	CAC-CBC-CGC-O1C
29	V9	202	PEB	CAC-CBC-CGC-O1C
29	Y9	202	PEB	CAC-CBC-CGC-O1C
29	a9	202	PEB	CAC-CBC-CGC-O1C
29	c9	202	PEB	CAC-CBC-CGC-O1C
29	e9	202	PEB	CAC-CBC-CGC-O1C
29	g9	202	PEB	CAC-CBC-CGC-O1C
29	i9	202	PEB	CAC-CBC-CGC-O1C
29	k9	202	PEB	CAC-CBC-CGC-O1C
29	m9	202	PEB	CAC-CBC-CGC-O1C
29	BA	201	PEB	CAC-CBC-CGC-O1C
29	DA	201	PEB	CAC-CBC-CGC-O1C
29	EA	201	PEB	CAC-CBC-CGC-O1C
29	FA	201	PEB	CAC-CBC-CGC-O1C
29	FA	201	PEB	CAC-CBC-CGC-O2C
29	HA	201	PEB	CAC-CBC-CGC-O1C
29	JA	201	PEB	CAC-CBC-CGC-O1C
29	LA	201	PEB	CAC-CBC-CGC-O1C
29	MA	404	PEB	CAC-CBC-CGC-O2C
29	CB	202	PEB	CAC-CBC-CGC-O2C
29	EB	202	PEB	CAC-CBC-CGC-O2C
29	GB	202	PEB	CAC-CBC-CGC-O2C
29	IB	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	JB	203	PEB	CAC-CBC-CGC-O1C
29	MB	202	PEB	CAC-CBC-CGC-O2C
29	SB	202	PEB	CAC-CBC-CGC-O2C
29	UB	202	PEB	CAC-CBC-CGC-O2C
29	YB	203	PEB	CAC-CBC-CGC-O2C
29	aB	202	PEB	CAC-CBC-CGC-O2C
29	cB	203	PEB	CAC-CBC-CGC-O1C
29	dB	202	PEB	CAC-CBC-CGC-O2C
29	fB	202	PEB	CAC-CBC-CGC-O2C
29	hB	202	PEB	CAC-CBC-CGC-O2C
29	jB	202	PEB	CAC-CBC-CGC-O2C
29	DC	201	PEB	CAC-CBC-CGC-O2C
29	DE	201	PEB	CAC-CBC-CGC-O2C
29	OF	202	PEB	CAB-CBB-CGB-O1B
29	SF	202	PEB	CAB-CBB-CGB-O1B
29	UF	203	PEB	CAB-CBB-CGB-O1B
29	WF	202	PEB	CAB-CBB-CGB-O1B
29	ZF	202	PEB	CAB-CBB-CGB-O1B
29	dF	203	PEB	CAB-CBB-CGB-O1B
29	fF	202	PEB	CAB-CBB-CGB-O1B
29	lF	202	PEB	CAB-CBB-CGB-O1B
29	OI	202	PEB	CAB-CBB-CGB-O1B
29	SI	202	PEB	CAB-CBB-CGB-O1B
29	UI	203	PEB	CAB-CBB-CGB-O1B
29	WI	202	PEB	CAB-CBB-CGB-O1B
29	ZI	202	PEB	CAB-CBB-CGB-O1B
29	dI	203	PEB	CAB-CBB-CGB-O1B
29	fI	202	PEB	CAB-CBB-CGB-O1B
29	II	202	PEB	CAB-CBB-CGB-O1B
29	DJ	202	PEB	CAB-CBB-CGB-O2B
29	HJ	202	PEB	CAB-CBB-CGB-O2B
29	LJ	202	PEB	CAB-CBB-CGB-O2B
29	NJ	203	PEB	CAB-CBB-CGB-O2B
29	PJ	203	PEB	CAB-CBB-CGB-O2B
29	RJ	203	PEB	CAB-CBB-CGB-O2B
29	TJ	203	PEB	CAB-CBB-CGB-O2B
29	VJ	202	PEB	CAB-CBB-CGB-O2B
29	XJ	203	PEB	CAB-CBB-CGB-O2B
29	ZJ	203	PEB	CAB-CBB-CGB-O2B
29	bJ	203	PEB	CAB-CBB-CGB-O2B
29	dJ	203	PEB	CAB-CBB-CGB-O2B
29	fJ	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	hJ	203	PEB	CAB-CBB-CGB-O2B
29	jJ	203	PEB	CAB-CBB-CGB-O2B
29	nJ	203	PEB	CAB-CBB-CGB-O2B
29	pJ	203	PEB	CAB-CBB-CGB-O2B
29	rJ	203	PEB	CAB-CBB-CGB-O2B
29	tJ	202	PEB	CAB-CBB-CGB-O2B
29	vJ	202	PEB	CAB-CBB-CGB-O2B
29	AK	303	PEB	CAC-CBC-CGC-O1C
29	OK	202	PEB	CAB-CBB-CGB-O1B
29	RK	202	PEB	CAC-CBC-CGC-O1C
29	UK	201	PEB	CAC-CBC-CGC-O1C
29	aK	202	PEB	CAC-CBC-CGC-O1C
29	kK	202	PEB	CAC-CBC-CGC-O1C
29	DL	202	PEB	CAB-CBB-CGB-O2B
29	HL	202	PEB	CAB-CBB-CGB-O2B
29	LL	202	PEB	CAB-CBB-CGB-O2B
29	NL	203	PEB	CAB-CBB-CGB-O2B
29	PL	203	PEB	CAB-CBB-CGB-O2B
29	RL	203	PEB	CAB-CBB-CGB-O2B
29	TL	203	PEB	CAB-CBB-CGB-O2B
29	VL	202	PEB	CAB-CBB-CGB-O2B
29	XL	203	PEB	CAB-CBB-CGB-O2B
29	ZL	203	PEB	CAB-CBB-CGB-O2B
29	bL	203	PEB	CAB-CBB-CGB-O2B
29	dL	203	PEB	CAB-CBB-CGB-O2B
29	fL	203	PEB	CAB-CBB-CGB-O2B
29	hL	203	PEB	CAB-CBB-CGB-O2B
29	jL	203	PEB	CAB-CBB-CGB-O2B
29	nL	203	PEB	CAB-CBB-CGB-O2B
29	pL	203	PEB	CAB-CBB-CGB-O2B
29	rL	203	PEB	CAB-CBB-CGB-O2B
29	tL	202	PEB	CAB-CBB-CGB-O2B
29	vL	202	PEB	CAB-CBB-CGB-O2B
29	zL	501	PEB	CAC-CBC-CGC-O1C
29	CM	202	PEB	CAC-CBC-CGC-O2C
29	EM	202	PEB	CAC-CBC-CGC-O2C
29	GM	202	PEB	CAC-CBC-CGC-O2C
29	IM	202	PEB	CAC-CBC-CGC-O2C
29	JM	203	PEB	CAC-CBC-CGC-O1C
29	MM	202	PEB	CAC-CBC-CGC-O2C
29	SM	202	PEB	CAC-CBC-CGC-O2C
29	YM	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	aM	202	PEB	CAC-CBC-CGC-O2C
29	cM	203	PEB	CAC-CBC-CGC-O1C
29	dM	202	PEB	CAC-CBC-CGC-O2C
29	fM	202	PEB	CAC-CBC-CGC-O2C
29	hM	202	PEB	CAC-CBC-CGC-O2C
29	jM	202	PEB	CAC-CBC-CGC-O2C
29	BN	201	PEB	CAC-CBC-CGC-O1C
29	DN	201	PEB	CAC-CBC-CGC-O1C
29	EN	201	PEB	CAC-CBC-CGC-O1C
29	FN	201	PEB	CAC-CBC-CGC-O1C
29	FN	201	PEB	CAC-CBC-CGC-O2C
29	HN	201	PEB	CAC-CBC-CGC-O1C
29	JN	201	PEB	CAC-CBC-CGC-O1C
29	LN	201	PEB	CAC-CBC-CGC-O1C
29	MN	404	PEB	CAC-CBC-CGC-O2C
29	AO	202	PEB	CAB-CBB-CGB-O2B
29	BO	203	PEB	CAB-CBB-CGB-O1B
29	CO	202	PEB	CAB-CBB-CGB-O2B
29	DO	203	PEB	CAB-CBB-CGB-O1B
29	EO	202	PEB	CAB-CBB-CGB-O2B
29	FO	202	PEB	CAC-CBC-CGC-O1C
29	FO	203	PEB	CAB-CBB-CGB-O1B
29	GO	202	PEB	CAB-CBB-CGB-O2B
29	HO	203	PEB	CAB-CBB-CGB-O1B
29	IO	202	PEB	CAB-CBB-CGB-O2B
29	JO	203	PEB	CAB-CBB-CGB-O1B
29	KO	202	PEB	CAB-CBB-CGB-O2B
29	LO	202	PEB	CAB-CBB-CGB-O1B
29	MO	202	PEB	CAC-CBC-CGC-O1C
29	NO	202	PEB	CAC-CBC-CGC-O1C
29	NO	202	PEB	CAC-CBC-CGC-O2C
29	MQ	401	PEB	CAC-CBC-CGC-O2C
29	MQ	403	PEB	CAB-CBB-CGB-O1B
29	SR	201	PEB	CAC-CBC-CGC-O1C
30	MG	403	PUB	CAB-CBB-CGB-O2B
30	yJ	303	PUB	CAB-CBB-CGB-O1B
30	yL	303	PUB	CAB-CBB-CGB-O1B
31	D1	1001	CYC	CAA-CBA-CGA-O2A
31	J1	1001	CYC	CAA-CBA-CGA-O2A
31	L1	1001	CYC	CAA-CBA-CGA-O2A
31	DK	1001	CYC	CAA-CBA-CGA-O2A
31	JK	1001	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	LK	1001	CYC	CAA-CBA-CGA-O2A
29	A1	302	PEB	CAB-CBB-CGB-O1B
29	S1	202	PEB	CAB-CBB-CGB-O1B
29	U1	203	PEB	CAB-CBB-CGB-O1B
29	V1	202	PEB	CAC-CBC-CGC-O1C
29	W1	202	PEB	CAB-CBB-CGB-O1B
29	Z1	203	PEB	CAB-CBB-CGB-O1B
29	Z1	203	PEB	CAB-CBB-CGB-O2B
29	b1	202	PEB	CAB-CBB-CGB-O1B
29	d1	202	PEB	CAB-CBB-CGB-O1B
29	f1	202	PEB	CAB-CBB-CGB-O1B
29	h1	202	PEB	CAB-CBB-CGB-O1B
29	j1	202	PEB	CAB-CBB-CGB-O1B
29	j1	202	PEB	CAB-CBB-CGB-O2B
29	l1	202	PEB	CAB-CBB-CGB-O1B
29	e2	402	PEB	CAC-CBC-CGC-O2C
29	N2	201	PEB	CAC-CBC-CGC-O2C
29	N2	202	PEB	CAC-CBC-CGC-O2C
29	R2	201	PEB	CAC-CBC-CGC-O2C
29	R2	202	PEB	CAC-CBC-CGC-O2C
29	T2	201	PEB	CAC-CBC-CGC-O2C
29	T2	202	PEB	CAC-CBC-CGC-O2C
29	V2	201	PEB	CAC-CBC-CGC-O2C
29	V2	202	PEB	CAC-CBC-CGC-O2C
29	X2	201	PEB	CAC-CBC-CGC-O2C
29	B3	202	PEB	CAC-CBC-CGC-O1C
29	H3	202	PEB	CAC-CBC-CGC-O1C
29	I3	203	PEB	CAC-CBC-CGC-O1C
29	J3	202	PEB	CAC-CBC-CGC-O1C
29	I5	201	PEB	CAC-CBC-CGC-O1C
29	I5	202	PEB	CAC-CBC-CGC-O2C
29	K5	201	PEB	CAC-CBC-CGC-O1C
29	A5	201	PEB	CAC-CBC-CGC-O1C
29	A7	305	PEB	CAB-CBB-CGB-O2B
29	P7	203	PEB	CAC-CBC-CGC-O1C
29	R7	203	PEB	CAC-CBC-CGC-O1C
29	T7	203	PEB	CAC-CBC-CGC-O1C
29	V7	203	PEB	CAC-CBC-CGC-O1C
29	Y7	203	PEB	CAC-CBC-CGC-O1C
29	a7	203	PEB	CAC-CBC-CGC-O1C
29	c7	203	PEB	CAC-CBC-CGC-O1C
29	e7	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	g7	203	PEB	CAC-CBC-CGC-O1C
29	k7	203	PEB	CAC-CBC-CGC-O1C
29	m7	203	PEB	CAC-CBC-CGC-O1C
29	I8	201	PEB	CAC-CBC-CGC-O1C
29	I8	202	PEB	CAC-CBC-CGC-O2C
29	A8	201	PEB	CAC-CBC-CGC-O1C
29	A9	305	PEB	CAB-CBB-CGB-O2B
29	P9	203	PEB	CAC-CBC-CGC-O1C
29	R9	203	PEB	CAC-CBC-CGC-O1C
29	T9	203	PEB	CAC-CBC-CGC-O1C
29	V9	203	PEB	CAC-CBC-CGC-O1C
29	Y9	203	PEB	CAC-CBC-CGC-O1C
29	a9	203	PEB	CAC-CBC-CGC-O1C
29	c9	203	PEB	CAC-CBC-CGC-O1C
29	e9	203	PEB	CAC-CBC-CGC-O1C
29	g9	203	PEB	CAC-CBC-CGC-O1C
29	k9	203	PEB	CAC-CBC-CGC-O1C
29	m9	203	PEB	CAC-CBC-CGC-O1C
29	AA	201	PEB	CAC-CBC-CGC-O1C
29	CA	201	PEB	CAC-CBC-CGC-O1C
29	GA	201	PEB	CAC-CBC-CGC-O1C
29	IA	201	PEB	CAC-CBC-CGC-O1C
29	KA	201	PEB	CAC-CBC-CGC-O1C
29	AB	301	PEB	CAB-CBB-CGB-O2B
29	KB	202	PEB	CAC-CBC-CGC-O2C
29	OB	202	PEB	CAC-CBC-CGC-O2C
29	QB	204	PEB	CAC-CBC-CGC-O2C
29	WB	202	PEB	CAC-CBC-CGC-O2C
29	IB	202	PEB	CAC-CBC-CGC-O2C
29	BC	201	PEB	CAC-CBC-CGC-O2C
29	FC	201	PEB	CAC-CBC-CGC-O2C
29	HC	201	PEB	CAC-CBC-CGC-O2C
29	JC	201	PEB	CAC-CBC-CGC-O2C
29	LC	201	PEB	CAC-CBC-CGC-O2C
29	BE	201	PEB	CAC-CBC-CGC-O2C
29	FE	201	PEB	CAC-CBC-CGC-O2C
29	HE	201	PEB	CAC-CBC-CGC-O2C
29	JE	201	PEB	CAC-CBC-CGC-O2C
29	LE	201	PEB	CAC-CBC-CGC-O2C
29	AF	305	PEB	CAB-CBB-CGB-O1B
29	OF	201	PEB	CAB-CBB-CGB-O1B
29	PF	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	QF	201	PEB	CAB-CBB-CGB-O1B
29	RF	202	PEB	CAB-CBB-CGB-O1B
29	SF	201	PEB	CAB-CBB-CGB-O1B
29	TF	202	PEB	CAB-CBB-CGB-O1B
29	WF	201	PEB	CAB-CBB-CGB-O1B
29	YF	203	PEB	CAB-CBB-CGB-O1B
29	ZF	201	PEB	CAB-CBB-CGB-O1B
29	aF	203	PEB	CAB-CBB-CGB-O1B
29	bF	201	PEB	CAB-CBB-CGB-O1B
29	cF	202	PEB	CAB-CBB-CGB-O1B
29	dF	202	PEB	CAB-CBB-CGB-O1B
29	eF	203	PEB	CAB-CBB-CGB-O1B
29	fF	201	PEB	CAB-CBB-CGB-O1B
29	gF	203	PEB	CAB-CBB-CGB-O1B
29	hF	201	PEB	CAB-CBB-CGB-O1B
29	iF	203	PEB	CAB-CBB-CGB-O1B
29	jF	201	PEB	CAB-CBB-CGB-O1B
29	kF	203	PEB	CAB-CBB-CGB-O1B
29	AI	305	PEB	CAB-CBB-CGB-O1B
29	OI	201	PEB	CAB-CBB-CGB-O1B
29	PI	203	PEB	CAB-CBB-CGB-O1B
29	QI	201	PEB	CAB-CBB-CGB-O1B
29	RI	202	PEB	CAB-CBB-CGB-O1B
29	SI	201	PEB	CAB-CBB-CGB-O1B
29	TI	202	PEB	CAB-CBB-CGB-O1B
29	WI	201	PEB	CAB-CBB-CGB-O1B
29	YI	203	PEB	CAB-CBB-CGB-O1B
29	ZI	201	PEB	CAB-CBB-CGB-O1B
29	aI	203	PEB	CAB-CBB-CGB-O1B
29	bI	201	PEB	CAB-CBB-CGB-O1B
29	cI	202	PEB	CAB-CBB-CGB-O1B
29	dI	202	PEB	CAB-CBB-CGB-O1B
29	eI	203	PEB	CAB-CBB-CGB-O1B
29	fI	201	PEB	CAB-CBB-CGB-O1B
29	gI	203	PEB	CAB-CBB-CGB-O1B
29	hI	201	PEB	CAB-CBB-CGB-O1B
29	iI	203	PEB	CAB-CBB-CGB-O1B
29	jI	201	PEB	CAB-CBB-CGB-O1B
29	kI	203	PEB	CAB-CBB-CGB-O1B
29	AJ	202	PEB	CAC-CBC-CGC-O1C
29	BJ	203	PEB	CAB-CBB-CGB-O2B
29	GJ	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	IJ	202	PEB	CAC-CBC-CGC-O1C
29	JJ	203	PEB	CAB-CBB-CGB-O2B
29	SJ	202	PEB	CAC-CBC-CGC-O1C
29	aJ	202	PEB	CAC-CBC-CGC-O1C
29	kJ	202	PEB	CAC-CBC-CGC-O1C
29	kJ	202	PEB	CAB-CBB-CGB-O2B
29	lJ	203	PEB	CAB-CBB-CGB-O2B
29	mJ	202	PEB	CAC-CBC-CGC-O1C
29	wJ	301	PEB	CAB-CBB-CGB-O1B
29	wJ	302	PEB	CAC-CBC-CGC-O1C
29	wJ	303	PEB	CAC-CBC-CGC-O1C
29	xJ	301	PEB	CAB-CBB-CGB-O1B
29	xJ	302	PEB	CAC-CBC-CGC-O1C
29	xJ	303	PEB	CAC-CBC-CGC-O1C
29	AK	302	PEB	CAB-CBB-CGB-O1B
29	SK	202	PEB	CAB-CBB-CGB-O1B
29	UK	203	PEB	CAB-CBB-CGB-O1B
29	VK	202	PEB	CAC-CBC-CGC-O1C
29	WK	202	PEB	CAB-CBB-CGB-O1B
29	ZK	203	PEB	CAB-CBB-CGB-O1B
29	ZK	203	PEB	CAB-CBB-CGB-O2B
29	bK	202	PEB	CAB-CBB-CGB-O1B
29	dK	202	PEB	CAB-CBB-CGB-O1B
29	fK	202	PEB	CAB-CBB-CGB-O1B
29	hK	202	PEB	CAB-CBB-CGB-O1B
29	jK	202	PEB	CAB-CBB-CGB-O1B
29	jK	202	PEB	CAB-CBB-CGB-O2B
29	lK	202	PEB	CAB-CBB-CGB-O1B
29	AL	202	PEB	CAC-CBC-CGC-O1C
29	BL	203	PEB	CAB-CBB-CGB-O2B
29	GL	202	PEB	CAB-CBB-CGB-O2B
29	IL	202	PEB	CAC-CBC-CGC-O1C
29	JL	203	PEB	CAB-CBB-CGB-O2B
29	SL	202	PEB	CAC-CBC-CGC-O1C
29	aL	202	PEB	CAC-CBC-CGC-O1C
29	kL	202	PEB	CAC-CBC-CGC-O1C
29	kL	202	PEB	CAB-CBB-CGB-O2B
29	lL	203	PEB	CAB-CBB-CGB-O2B
29	mL	202	PEB	CAC-CBC-CGC-O1C
29	wL	301	PEB	CAB-CBB-CGB-O1B
29	wL	302	PEB	CAC-CBC-CGC-O1C
29	wL	303	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	xL	301	PEB	CAB-CBB-CGB-O1B
29	xL	302	PEB	CAC-CBC-CGC-O1C
29	xL	303	PEB	CAC-CBC-CGC-O1C
29	AM	301	PEB	CAB-CBB-CGB-O2B
29	KM	202	PEB	CAC-CBC-CGC-O2C
29	OM	202	PEB	CAC-CBC-CGC-O2C
29	QM	204	PEB	CAC-CBC-CGC-O2C
29	WM	202	PEB	CAC-CBC-CGC-O2C
29	IM	202	PEB	CAC-CBC-CGC-O2C
29	AN	201	PEB	CAC-CBC-CGC-O1C
29	CN	201	PEB	CAC-CBC-CGC-O1C
29	GN	201	PEB	CAC-CBC-CGC-O1C
29	IN	201	PEB	CAC-CBC-CGC-O1C
29	KN	201	PEB	CAC-CBC-CGC-O1C
29	BO	202	PEB	CAC-CBC-CGC-O1C
29	HO	202	PEB	CAC-CBC-CGC-O1C
29	IO	203	PEB	CAC-CBC-CGC-O1C
29	JO	202	PEB	CAC-CBC-CGC-O1C
29	NR	201	PEB	CAC-CBC-CGC-O2C
29	NR	202	PEB	CAC-CBC-CGC-O2C
29	PR	201	PEB	CAC-CBC-CGC-O2C
29	RR	201	PEB	CAC-CBC-CGC-O2C
29	RR	202	PEB	CAC-CBC-CGC-O2C
29	TR	201	PEB	CAC-CBC-CGC-O2C
29	TR	202	PEB	CAC-CBC-CGC-O2C
29	VR	201	PEB	CAC-CBC-CGC-O2C
29	VR	202	PEB	CAC-CBC-CGC-O2C
29	XR	201	PEB	CAC-CBC-CGC-O2C
29	XR	202	PEB	CAC-CBC-CGC-O2C
30	A1	305	PUB	CAB-CBB-CGB-O2B
30	AB	305	PUB	CAB-CBB-CGB-O2B
30	BB	302	PUB	CAB-CBB-CGB-O2B
30	AF	302	PUB	CAC-CBC-CGC-O1C
30	AI	302	PUB	CAC-CBC-CGC-O1C
30	AK	305	PUB	CAB-CBB-CGB-O2B
30	AM	305	PUB	CAB-CBB-CGB-O2B
30	BM	302	PUB	CAB-CBB-CGB-O2B
30	MQ	405	PUB	CAB-CBB-CGB-O2B
29	PF	203	PEB	C3B-CAB-CBB-CGB
29	RF	202	PEB	C3B-CAB-CBB-CGB
29	TF	202	PEB	C3B-CAB-CBB-CGB
29	VF	203	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
29	YF	203	PEB	C3B-CAB-CBB-CGB
29	aF	203	PEB	C3B-CAB-CBB-CGB
29	cF	202	PEB	C3B-CAB-CBB-CGB
29	eF	203	PEB	C3B-CAB-CBB-CGB
29	gF	203	PEB	C3B-CAB-CBB-CGB
29	iF	203	PEB	C3B-CAB-CBB-CGB
29	kF	203	PEB	C3B-CAB-CBB-CGB
29	mF	203	PEB	C3B-CAB-CBB-CGB
29	PI	203	PEB	C3B-CAB-CBB-CGB
29	RI	202	PEB	C3B-CAB-CBB-CGB
29	TI	202	PEB	C3B-CAB-CBB-CGB
29	VI	203	PEB	C3B-CAB-CBB-CGB
29	YI	203	PEB	C3B-CAB-CBB-CGB
29	aI	203	PEB	C3B-CAB-CBB-CGB
29	cI	202	PEB	C3B-CAB-CBB-CGB
29	eI	203	PEB	C3B-CAB-CBB-CGB
29	gI	203	PEB	C3B-CAB-CBB-CGB
29	iI	203	PEB	C3B-CAB-CBB-CGB
29	kI	203	PEB	C3B-CAB-CBB-CGB
29	mI	203	PEB	C3B-CAB-CBB-CGB
29	A1	303	PEB	CAB-CBB-CGB-O1B
29	H1	1002	PEB	CAC-CBC-CGC-O2C
29	O1	202	PEB	CAB-CBB-CGB-O2B
29	Q1	202	PEB	CAB-CBB-CGB-O2B
29	S1	202	PEB	CAB-CBB-CGB-O2B
29	U1	203	PEB	CAB-CBB-CGB-O2B
29	W1	202	PEB	CAB-CBB-CGB-O2B
29	b1	202	PEB	CAB-CBB-CGB-O2B
29	d1	202	PEB	CAB-CBB-CGB-O2B
29	f1	202	PEB	CAB-CBB-CGB-O2B
29	h1	202	PEB	CAB-CBB-CGB-O2B
29	l1	202	PEB	CAB-CBB-CGB-O2B
29	M2	202	PEB	CAC-CBC-CGC-O1C
29	S2	202	PEB	CAC-CBC-CGC-O1C
29	W2	202	PEB	CAC-CBC-CGC-O1C
29	A3	202	PEB	CAB-CBB-CGB-O1B
29	C3	202	PEB	CAB-CBB-CGB-O1B
29	E3	202	PEB	CAB-CBB-CGB-O1B
29	G3	202	PEB	CAB-CBB-CGB-O1B
29	I3	202	PEB	CAB-CBB-CGB-O1B
29	K3	202	PEB	CAB-CBB-CGB-O1B
29	B5	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	B5	203	PEB	CAB-CBB-CGB-01B
29	F5	203	PEB	CAC-CBC-CGC-02C
29	F5	203	PEB	CAB-CBB-CGB-01B
29	G5	203	PEB	CAB-CBB-CGB-01B
29	H5	203	PEB	CAB-CBB-CGB-01B
29	I5	202	PEB	CAB-CBB-CGB-01B
29	I5	203	PEB	CAB-CBB-CGB-01B
29	J5	201	PEB	CAC-CBC-CGC-01C
29	K5	202	PEB	CAC-CBC-CGC-01C
29	K5	202	PEB	CAB-CBB-CGB-01B
29	K5	203	PEB	CAB-CBB-CGB-01B
29	L5	203	PEB	CAB-CBB-CGB-01B
29	A5	202	PEB	CAB-CBB-CGB-01B
29	A5	203	PEB	CAB-CBB-CGB-01B
29	C5	201	PEB	CAC-CBC-CGC-01C
29	C5	202	PEB	CAB-CBB-CGB-01B
29	C5	203	PEB	CAB-CBB-CGB-01B
29	i7	203	PEB	CAC-CBC-CGC-01C
29	B8	203	PEB	CAC-CBC-CGC-02C
29	B8	203	PEB	CAB-CBB-CGB-01B
29	F8	203	PEB	CAC-CBC-CGC-02C
29	F8	203	PEB	CAB-CBB-CGB-01B
29	G8	203	PEB	CAC-CBC-CGC-02C
29	G8	203	PEB	CAB-CBB-CGB-01B
29	H8	203	PEB	CAC-CBC-CGC-02C
29	H8	203	PEB	CAB-CBB-CGB-01B
29	I8	202	PEB	CAB-CBB-CGB-01B
29	I8	203	PEB	CAB-CBB-CGB-01B
29	J8	201	PEB	CAC-CBC-CGC-01C
29	K8	201	PEB	CAC-CBC-CGC-01C
29	K8	202	PEB	CAC-CBC-CGC-01C
29	K8	202	PEB	CAB-CBB-CGB-01B
29	K8	203	PEB	CAB-CBB-CGB-01B
29	L8	203	PEB	CAB-CBB-CGB-01B
29	A8	202	PEB	CAB-CBB-CGB-01B
29	A8	203	PEB	CAB-CBB-CGB-01B
29	C8	201	PEB	CAC-CBC-CGC-01C
29	C8	202	PEB	CAC-CBC-CGC-01C
29	C8	202	PEB	CAB-CBB-CGB-01B
29	C8	203	PEB	CAB-CBB-CGB-01B
29	i9	203	PEB	CAC-CBC-CGC-01C
29	AA	202	PEB	CAC-CBC-CGC-01C

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Mol	Chain	Res	Type	Atoms
29	CA	202	PEB	CAC-CBC-CGC-O1C
29	EA	202	PEB	CAC-CBC-CGC-O1C
29	GA	202	PEB	CAC-CBC-CGC-O1C
29	IA	202	PEB	CAC-CBC-CGC-O1C
29	KA	202	PEB	CAC-CBC-CGC-O1C
29	MA	401	PEB	CAC-CBC-CGC-O2C
29	MA	405	PEB	CAC-CBC-CGC-O2C
29	MA	405	PEB	CAB-CBB-CGB-O2B
29	FB	203	PEB	CAC-CBC-CGC-O2C
29	HB	203	PEB	CAC-CBC-CGC-O2C
29	LB	203	PEB	CAC-CBC-CGC-O2C
29	eB	202	PEB	CAC-CBC-CGC-O2C
29	iB	203	PEB	CAC-CBC-CGC-O2C
29	kB	203	PEB	CAC-CBC-CGC-O2C
29	mB	203	PEB	CAC-CBC-CGC-O2C
29	AC	202	PEB	CAC-CBC-CGC-O1C
29	EC	202	PEB	CAC-CBC-CGC-O1C
29	GC	202	PEB	CAC-CBC-CGC-O1C
29	IC	202	PEB	CAC-CBC-CGC-O1C
29	KC	203	PEB	CAC-CBC-CGC-O1C
29	AE	202	PEB	CAC-CBC-CGC-O1C
29	EE	202	PEB	CAC-CBC-CGC-O1C
29	GE	202	PEB	CAC-CBC-CGC-O1C
29	IE	202	PEB	CAC-CBC-CGC-O1C
29	KE	203	PEB	CAC-CBC-CGC-O1C
29	UF	202	PEB	CAB-CBB-CGB-O1B
29	VF	203	PEB	CAB-CBB-CGB-O1B
29	lF	201	PEB	CAB-CBB-CGB-O1B
29	mF	203	PEB	CAB-CBB-CGB-O1B
29	CG	201	PEB	CAB-CBB-CGB-O2B
29	IG	201	PEB	CAB-CBB-CGB-O2B
29	MG	405	PEB	CAB-CBB-CGB-O1B
29	UI	202	PEB	CAB-CBB-CGB-O1B
29	VI	203	PEB	CAB-CBB-CGB-O1B
29	lI	201	PEB	CAB-CBB-CGB-O1B
29	mI	203	PEB	CAB-CBB-CGB-O1B
29	AJ	202	PEB	CAB-CBB-CGB-O2B
29	CJ	202	PEB	CAC-CBC-CGC-O1C
29	CJ	202	PEB	CAB-CBB-CGB-O2B
29	EJ	202	PEB	CAC-CBC-CGC-O1C
29	EJ	202	PEB	CAB-CBB-CGB-O2B
29	GJ	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	IJ	202	PEB	CAB-CBB-CGB-O2B
29	KJ	202	PEB	CAC-CBC-CGC-O1C
29	KJ	202	PEB	CAB-CBB-CGB-O2B
29	MJ	202	PEB	CAB-CBB-CGB-O2B
29	OJ	202	PEB	CAC-CBC-CGC-O1C
29	OJ	202	PEB	CAB-CBB-CGB-O2B
29	QJ	202	PEB	CAC-CBC-CGC-O1C
29	QJ	202	PEB	CAB-CBB-CGB-O2B
29	SJ	202	PEB	CAB-CBB-CGB-O2B
29	UJ	202	PEB	CAC-CBC-CGC-O1C
29	UJ	202	PEB	CAB-CBB-CGB-O2B
29	WJ	203	PEB	CAB-CBB-CGB-O2B
29	YJ	202	PEB	CAB-CBB-CGB-O2B
29	aJ	202	PEB	CAB-CBB-CGB-O2B
29	cJ	202	PEB	CAC-CBC-CGC-O1C
29	cJ	202	PEB	CAB-CBB-CGB-O2B
29	eJ	202	PEB	CAC-CBC-CGC-O1C
29	eJ	202	PEB	CAB-CBB-CGB-O2B
29	gJ	202	PEB	CAB-CBB-CGB-O2B
29	iJ	202	PEB	CAB-CBB-CGB-O2B
29	mJ	202	PEB	CAB-CBB-CGB-O2B
29	oJ	202	PEB	CAC-CBC-CGC-O1C
29	oJ	202	PEB	CAB-CBB-CGB-O2B
29	qJ	202	PEB	CAB-CBB-CGB-O2B
29	sJ	202	PEB	CAB-CBB-CGB-O2B
29	uJ	203	PEB	CAB-CBB-CGB-O2B
29	yJ	301	PEB	CAB-CBB-CGB-O2B
29	AK	303	PEB	CAB-CBB-CGB-O1B
29	HK	1002	PEB	CAC-CBC-CGC-O2C
29	NK	1002	PEB	CAC-CBC-CGC-O2C
29	OK	202	PEB	CAB-CBB-CGB-O2B
29	QK	202	PEB	CAB-CBB-CGB-O2B
29	SK	202	PEB	CAB-CBB-CGB-O2B
29	UK	203	PEB	CAB-CBB-CGB-O2B
29	WK	202	PEB	CAB-CBB-CGB-O2B
29	bK	202	PEB	CAB-CBB-CGB-O2B
29	dK	202	PEB	CAB-CBB-CGB-O2B
29	fK	202	PEB	CAB-CBB-CGB-O2B
29	hK	202	PEB	CAB-CBB-CGB-O2B
29	lK	202	PEB	CAB-CBB-CGB-O2B
29	AL	202	PEB	CAB-CBB-CGB-O2B
29	CL	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	CL	202	PEB	CAB-CBB-CGB-O2B
29	EL	202	PEB	CAC-CBC-CGC-O1C
29	EL	202	PEB	CAB-CBB-CGB-O2B
29	GL	202	PEB	CAC-CBC-CGC-O1C
29	IL	202	PEB	CAB-CBB-CGB-O2B
29	KL	202	PEB	CAC-CBC-CGC-O1C
29	KL	202	PEB	CAB-CBB-CGB-O2B
29	ML	202	PEB	CAB-CBB-CGB-O2B
29	OL	202	PEB	CAC-CBC-CGC-O1C
29	OL	202	PEB	CAB-CBB-CGB-O2B
29	QL	202	PEB	CAC-CBC-CGC-O1C
29	QL	202	PEB	CAB-CBB-CGB-O2B
29	SL	202	PEB	CAB-CBB-CGB-O2B
29	UL	202	PEB	CAC-CBC-CGC-O1C
29	UL	202	PEB	CAB-CBB-CGB-O2B
29	WL	203	PEB	CAB-CBB-CGB-O2B
29	YL	202	PEB	CAB-CBB-CGB-O2B
29	aL	202	PEB	CAB-CBB-CGB-O2B
29	cL	202	PEB	CAC-CBC-CGC-O1C
29	cL	202	PEB	CAB-CBB-CGB-O2B
29	eL	202	PEB	CAC-CBC-CGC-O1C
29	eL	202	PEB	CAB-CBB-CGB-O2B
29	gL	202	PEB	CAB-CBB-CGB-O2B
29	iL	202	PEB	CAB-CBB-CGB-O2B
29	mL	202	PEB	CAB-CBB-CGB-O2B
29	oL	202	PEB	CAC-CBC-CGC-O1C
29	oL	202	PEB	CAB-CBB-CGB-O2B
29	qL	202	PEB	CAB-CBB-CGB-O2B
29	sL	202	PEB	CAB-CBB-CGB-O2B
29	uL	203	PEB	CAB-CBB-CGB-O2B
29	yL	301	PEB	CAB-CBB-CGB-O2B
29	FM	203	PEB	CAC-CBC-CGC-O2C
29	HM	203	PEB	CAC-CBC-CGC-O2C
29	LM	203	PEB	CAC-CBC-CGC-O2C
29	eM	202	PEB	CAC-CBC-CGC-O2C
29	iM	203	PEB	CAC-CBC-CGC-O2C
29	kM	203	PEB	CAC-CBC-CGC-O2C
29	mM	203	PEB	CAC-CBC-CGC-O2C
29	AN	202	PEB	CAC-CBC-CGC-O1C
29	CN	202	PEB	CAC-CBC-CGC-O1C
29	EN	202	PEB	CAC-CBC-CGC-O1C
29	GN	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	IN	202	PEB	CAC-CBC-CGC-O1C
29	KN	202	PEB	CAC-CBC-CGC-O1C
29	MN	401	PEB	CAC-CBC-CGC-O2C
29	MN	405	PEB	CAC-CBC-CGC-O2C
29	MN	405	PEB	CAB-CBB-CGB-O2B
29	AO	202	PEB	CAB-CBB-CGB-O1B
29	CO	202	PEB	CAB-CBB-CGB-O1B
29	EO	202	PEB	CAB-CBB-CGB-O1B
29	GO	202	PEB	CAB-CBB-CGB-O1B
29	IO	202	PEB	CAB-CBB-CGB-O1B
29	KO	202	PEB	CAB-CBB-CGB-O1B
29	CQ	201	PEB	CAB-CBB-CGB-O2B
29	IQ	201	PEB	CAB-CBB-CGB-O2B
29	MQ	407	PEB	CAB-CBB-CGB-O1B
29	SR	202	PEB	CAC-CBC-CGC-O1C
29	UR	202	PEB	CAC-CBC-CGC-O1C
30	MA	403	PUB	CAC-CBC-CGC-O1C
30	MN	403	PUB	CAC-CBC-CGC-O1C
31	D1	1001	CYC	CAD-CBD-CGD-O1D
31	VP	1001	CYC	CAD-CBD-CGD-O1D
31	xP	1001	CYC	CAD-CBD-CGD-O1D
29	A1	301	PEB	CAC-CBC-CGC-O2C
29	A1	302	PEB	CAB-CBB-CGB-O2B
29	D1	1002	PEB	CAC-CBC-CGC-O2C
29	F1	1002	PEB	CAC-CBC-CGC-O2C
29	J1	1002	PEB	CAC-CBC-CGC-O2C
29	Q1	201	PEB	CAC-CBC-CGC-O1C
29	Q1	202	PEB	CAB-CBB-CGB-O1B
29	d1	202	PEB	CAC-CBC-CGC-O1C
29	O2	202	PEB	CAC-CBC-CGC-O1C
29	P2	201	PEB	CAC-CBC-CGC-O1C
29	Q2	202	PEB	CAC-CBC-CGC-O1C
29	T2	202	PEB	CAC-CBC-CGC-O1C
29	U2	202	PEB	CAC-CBC-CGC-O1C
29	A3	201	PEB	CAC-CBC-CGC-O2C
29	B3	203	PEB	CAB-CBB-CGB-O2B
29	C3	201	PEB	CAC-CBC-CGC-O2C
29	D3	203	PEB	CAB-CBB-CGB-O2B
29	F3	203	PEB	CAB-CBB-CGB-O2B
29	G3	201	PEB	CAC-CBC-CGC-O2C
29	H3	203	PEB	CAB-CBB-CGB-O2B
29	I3	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	J3	203	PEB	CAB-CBB-CGB-O2B
29	K3	201	PEB	CAC-CBC-CGC-O2C
29	L3	202	PEB	CAB-CBB-CGB-O2B
29	M3	202	PEB	CAB-CBB-CGB-O2B
29	N3	202	PEB	CAB-CBB-CGB-O2B
29	C4	203	PEB	CAC-CBC-CGC-O2C
29	E4	203	PEB	CAC-CBC-CGC-O2C
29	G4	203	PEB	CAC-CBC-CGC-O2C
29	K4	203	PEB	CAC-CBC-CGC-O2C
29	G5	203	PEB	CAC-CBC-CGC-O2C
29	H5	203	PEB	CAC-CBC-CGC-O2C
29	I5	202	PEB	CAC-CBC-CGC-O1C
29	L5	203	PEB	CAC-CBC-CGC-O2C
29	A5	202	PEB	CAC-CBC-CGC-O1C
29	C5	202	PEB	CAC-CBC-CGC-O1C
29	A7	305	PEB	CAC-CBC-CGC-O1C
29	I8	202	PEB	CAC-CBC-CGC-O1C
29	L8	203	PEB	CAC-CBC-CGC-O2C
29	A8	202	PEB	CAC-CBC-CGC-O1C
29	A9	305	PEB	CAC-CBC-CGC-O1C
29	AA	202	PEB	CAC-CBC-CGC-O2C
29	CA	202	PEB	CAC-CBC-CGC-O2C
29	GA	202	PEB	CAC-CBC-CGC-O2C
29	IA	202	PEB	CAC-CBC-CGC-O2C
29	KA	202	PEB	CAC-CBC-CGC-O2C
29	MA	404	PEB	CAC-CBC-CGC-O1C
29	AB	301	PEB	CAC-CBC-CGC-O2C
29	PB	202	PEB	CAC-CBC-CGC-O2C
29	VB	203	PEB	CAC-CBC-CGC-O2C
29	XB	202	PEB	CAC-CBC-CGC-O2C
29	YB	203	PEB	CAC-CBC-CGC-O1C
29	ZB	203	PEB	CAC-CBC-CGC-O2C
29	cB	203	PEB	CAC-CBC-CGC-O2C
29	hB	202	PEB	CAC-CBC-CGC-O1C
29	AC	202	PEB	CAB-CBB-CGB-O1B
29	CC	202	PEB	CAC-CBC-CGC-O1C
29	CC	202	PEB	CAB-CBB-CGB-O1B
29	CD	203	PEB	CAC-CBC-CGC-O2C
29	ED	202	PEB	CAC-CBC-CGC-O2C
29	GD	203	PEB	CAC-CBC-CGC-O2C
29	ID	203	PEB	CAC-CBC-CGC-O2C
29	KD	203	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	MD	203	PEB	CAC-CBC-CGC-O2C
29	AE	202	PEB	CAB-CBB-CGB-O1B
29	CE	202	PEB	CAC-CBC-CGC-O1C
29	CE	202	PEB	CAB-CBB-CGB-O1B
29	AF	304	PEB	CAB-CBB-CGB-O1B
29	AG	201	PEB	CAB-CBB-CGB-O2B
29	GG	201	PEB	CAB-CBB-CGB-O2B
29	AI	304	PEB	CAB-CBB-CGB-O1B
29	AJ	202	PEB	CAB-CBB-CGB-O1B
29	CJ	202	PEB	CAB-CBB-CGB-O1B
29	EJ	202	PEB	CAB-CBB-CGB-O1B
29	FJ	203	PEB	CAB-CBB-CGB-O1B
29	GJ	202	PEB	CAB-CBB-CGB-O1B
29	IJ	202	PEB	CAB-CBB-CGB-O1B
29	KJ	202	PEB	CAB-CBB-CGB-O1B
29	MJ	202	PEB	CAC-CBC-CGC-O1C
29	MJ	202	PEB	CAB-CBB-CGB-O1B
29	NJ	203	PEB	CAB-CBB-CGB-O1B
29	OJ	202	PEB	CAB-CBB-CGB-O1B
29	QJ	202	PEB	CAB-CBB-CGB-O1B
29	SJ	202	PEB	CAB-CBB-CGB-O1B
29	UJ	202	PEB	CAB-CBB-CGB-O1B
29	WJ	203	PEB	CAC-CBC-CGC-O1C
29	WJ	203	PEB	CAB-CBB-CGB-O1B
29	YJ	202	PEB	CAC-CBC-CGC-O1C
29	YJ	202	PEB	CAB-CBB-CGB-O1B
29	aJ	202	PEB	CAB-CBB-CGB-O1B
29	cJ	202	PEB	CAB-CBB-CGB-O1B
29	eJ	202	PEB	CAB-CBB-CGB-O1B
29	gJ	202	PEB	CAC-CBC-CGC-O1C
29	gJ	202	PEB	CAB-CBB-CGB-O1B
29	iJ	202	PEB	CAC-CBC-CGC-O1C
29	iJ	202	PEB	CAB-CBB-CGB-O1B
29	kJ	202	PEB	CAB-CBB-CGB-O1B
29	mJ	202	PEB	CAB-CBB-CGB-O1B
29	oJ	202	PEB	CAB-CBB-CGB-O1B
29	qJ	202	PEB	CAC-CBC-CGC-O1C
29	qJ	202	PEB	CAB-CBB-CGB-O1B
29	sJ	202	PEB	CAC-CBC-CGC-O1C
29	sJ	202	PEB	CAB-CBB-CGB-O1B
29	uJ	203	PEB	CAC-CBC-CGC-O1C
29	uJ	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	AK	301	PEB	CAC-CBC-CGC-O2C
29	AK	302	PEB	CAB-CBB-CGB-O2B
29	FK	1002	PEB	CAC-CBC-CGC-O2C
29	JK	1002	PEB	CAC-CBC-CGC-O2C
29	QK	201	PEB	CAC-CBC-CGC-O1C
29	QK	202	PEB	CAB-CBB-CGB-O1B
29	dK	202	PEB	CAC-CBC-CGC-O1C
29	AL	202	PEB	CAB-CBB-CGB-O1B
29	CL	202	PEB	CAB-CBB-CGB-O1B
29	EL	202	PEB	CAB-CBB-CGB-O1B
29	FL	203	PEB	CAB-CBB-CGB-O1B
29	GL	202	PEB	CAB-CBB-CGB-O1B
29	IL	202	PEB	CAB-CBB-CGB-O1B
29	KL	202	PEB	CAB-CBB-CGB-O1B
29	ML	202	PEB	CAC-CBC-CGC-O1C
29	ML	202	PEB	CAB-CBB-CGB-O1B
29	NL	203	PEB	CAB-CBB-CGB-O1B
29	OL	202	PEB	CAB-CBB-CGB-O1B
29	QL	202	PEB	CAB-CBB-CGB-O1B
29	SL	202	PEB	CAB-CBB-CGB-O1B
29	UL	202	PEB	CAB-CBB-CGB-O1B
29	WL	203	PEB	CAC-CBC-CGC-O1C
29	WL	203	PEB	CAB-CBB-CGB-O1B
29	YL	202	PEB	CAC-CBC-CGC-O1C
29	YL	202	PEB	CAB-CBB-CGB-O1B
29	aL	202	PEB	CAB-CBB-CGB-O1B
29	cL	202	PEB	CAB-CBB-CGB-O1B
29	eL	202	PEB	CAB-CBB-CGB-O1B
29	gL	202	PEB	CAC-CBC-CGC-O1C
29	gL	202	PEB	CAB-CBB-CGB-O1B
29	iL	202	PEB	CAC-CBC-CGC-O1C
29	iL	202	PEB	CAB-CBB-CGB-O1B
29	kL	202	PEB	CAB-CBB-CGB-O1B
29	mL	202	PEB	CAB-CBB-CGB-O1B
29	oL	202	PEB	CAB-CBB-CGB-O1B
29	qL	202	PEB	CAC-CBC-CGC-O1C
29	qL	202	PEB	CAB-CBB-CGB-O1B
29	sL	202	PEB	CAC-CBC-CGC-O1C
29	sL	202	PEB	CAB-CBB-CGB-O1B
29	uL	203	PEB	CAC-CBC-CGC-O1C
29	uL	203	PEB	CAB-CBB-CGB-O1B
29	AM	301	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	PM	202	PEB	CAC-CBC-CGC-O2C
29	VM	203	PEB	CAC-CBC-CGC-O2C
29	XM	202	PEB	CAC-CBC-CGC-O2C
29	YM	203	PEB	CAC-CBC-CGC-O1C
29	ZM	203	PEB	CAC-CBC-CGC-O2C
29	cM	203	PEB	CAC-CBC-CGC-O2C
29	hM	202	PEB	CAC-CBC-CGC-O1C
29	AN	202	PEB	CAC-CBC-CGC-O2C
29	CN	202	PEB	CAC-CBC-CGC-O2C
29	GN	202	PEB	CAC-CBC-CGC-O2C
29	IN	202	PEB	CAC-CBC-CGC-O2C
29	KN	202	PEB	CAC-CBC-CGC-O2C
29	AO	201	PEB	CAC-CBC-CGC-O2C
29	BO	203	PEB	CAB-CBB-CGB-O2B
29	CO	201	PEB	CAC-CBC-CGC-O2C
29	DO	203	PEB	CAB-CBB-CGB-O2B
29	FO	203	PEB	CAB-CBB-CGB-O2B
29	GO	201	PEB	CAC-CBC-CGC-O2C
29	HO	203	PEB	CAB-CBB-CGB-O2B
29	IO	201	PEB	CAC-CBC-CGC-O2C
29	JO	203	PEB	CAB-CBB-CGB-O2B
29	KO	201	PEB	CAC-CBC-CGC-O2C
29	LO	202	PEB	CAB-CBB-CGB-O2B
29	MO	202	PEB	CAB-CBB-CGB-O2B
29	NO	202	PEB	CAB-CBB-CGB-O2B
29	AQ	201	PEB	CAB-CBB-CGB-O2B
29	GQ	201	PEB	CAB-CBB-CGB-O2B
29	MR	202	PEB	CAC-CBC-CGC-O1C
29	MR	202	PEB	CAC-CBC-CGC-O2C
29	NR	202	PEB	CAC-CBC-CGC-O1C
29	OR	202	PEB	CAC-CBC-CGC-O1C
29	PR	201	PEB	CAC-CBC-CGC-O1C
29	QR	202	PEB	CAC-CBC-CGC-O1C
29	RR	202	PEB	CAC-CBC-CGC-O1C
29	TR	202	PEB	CAC-CBC-CGC-O1C
31	F1	1001	CYC	CAD-CBD-CGD-O1D
31	H1	1001	CYC	CAD-CBD-CGD-O1D
31	L1	1001	CYC	CAD-CBD-CGD-O1D
31	FK	1001	CYC	CAD-CBD-CGD-O1D
31	HK	1001	CYC	CAD-CBD-CGD-O1D
31	LK	1001	CYC	CAD-CBD-CGD-O1D
31	NK	1001	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	WP	1001	CYC	CAD-CBD-CGD-O1D
31	yP	1001	CYC	CAD-CBD-CGD-O1D
29	A1	301	PEB	CAB-CBB-CGB-O1B
29	O1	201	PEB	CAC-CBC-CGC-O1C
29	O1	202	PEB	CAC-CBC-CGC-O1C
29	Q1	202	PEB	CAC-CBC-CGC-O1C
29	S1	201	PEB	CAC-CBC-CGC-O1C
29	S1	202	PEB	CAC-CBC-CGC-O1C
29	U1	202	PEB	CAC-CBC-CGC-O1C
29	U1	203	PEB	CAC-CBC-CGC-O1C
29	W1	201	PEB	CAC-CBC-CGC-O1C
29	W1	202	PEB	CAC-CBC-CGC-O1C
29	Z1	202	PEB	CAC-CBC-CGC-O1C
29	Z1	203	PEB	CAC-CBC-CGC-O1C
29	b1	201	PEB	CAC-CBC-CGC-O1C
29	b1	202	PEB	CAC-CBC-CGC-O1C
29	d1	201	PEB	CAC-CBC-CGC-O1C
29	f1	201	PEB	CAC-CBC-CGC-O1C
29	f1	202	PEB	CAC-CBC-CGC-O1C
29	h1	201	PEB	CAC-CBC-CGC-O1C
29	h1	202	PEB	CAC-CBC-CGC-O1C
29	j1	201	PEB	CAC-CBC-CGC-O1C
29	j1	202	PEB	CAC-CBC-CGC-O1C
29	l1	201	PEB	CAC-CBC-CGC-O1C
29	l1	202	PEB	CAC-CBC-CGC-O1C
29	N2	202	PEB	CAC-CBC-CGC-O1C
29	R2	202	PEB	CAC-CBC-CGC-O1C
29	V2	202	PEB	CAC-CBC-CGC-O1C
29	X2	201	PEB	CAC-CBC-CGC-O1C
29	E3	201	PEB	CAC-CBC-CGC-O2C
29	B4	202	PEB	CAC-CBC-CGC-O2C
29	D4	202	PEB	CAC-CBC-CGC-O2C
29	F4	202	PEB	CAC-CBC-CGC-O2C
29	H4	202	PEB	CAC-CBC-CGC-O2C
29	J4	202	PEB	CAC-CBC-CGC-O2C
29	L4	202	PEB	CAC-CBC-CGC-O2C
29	G5	201	PEB	CAC-CBC-CGC-O1C
29	A7	304	PEB	CAB-CBB-CGB-O1B
29	A7	305	PEB	CAB-CBB-CGB-O1B
29	A9	304	PEB	CAB-CBB-CGB-O1B
29	A9	305	PEB	CAB-CBB-CGB-O1B
29	EA	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	HA	203	PEB	CAB-CBB-CGB-O1B
29	MA	401	PEB	CAB-CBB-CGB-O2B
29	CB	201	PEB	CAC-CBC-CGC-O2C
29	CB	202	PEB	CAC-CBC-CGC-O1C
29	DB	203	PEB	CAC-CBC-CGC-O2C
29	EB	201	PEB	CAC-CBC-CGC-O2C
29	GB	201	PEB	CAC-CBC-CGC-O2C
29	IB	201	PEB	CAC-CBC-CGC-O2C
29	JB	203	PEB	CAC-CBC-CGC-O2C
29	KB	201	PEB	CAC-CBC-CGC-O2C
29	KB	202	PEB	CAC-CBC-CGC-O1C
29	MB	201	PEB	CAC-CBC-CGC-O2C
29	NB	202	PEB	CAC-CBC-CGC-O2C
29	OB	201	PEB	CAC-CBC-CGC-O2C
29	OB	202	PEB	CAC-CBC-CGC-O1C
29	QB	203	PEB	CAC-CBC-CGC-O2C
29	RB	203	PEB	CAC-CBC-CGC-O2C
29	SB	201	PEB	CAC-CBC-CGC-O2C
29	TB	203	PEB	CAC-CBC-CGC-O2C
29	UB	201	PEB	CAC-CBC-CGC-O2C
29	WB	201	PEB	CAC-CBC-CGC-O2C
29	YB	202	PEB	CAC-CBC-CGC-O2C
29	aB	201	PEB	CAC-CBC-CGC-O2C
29	dB	201	PEB	CAC-CBC-CGC-O2C
29	dB	202	PEB	CAC-CBC-CGC-O1C
29	fB	201	PEB	CAC-CBC-CGC-O2C
29	fB	202	PEB	CAC-CBC-CGC-O1C
29	gB	203	PEB	CAC-CBC-CGC-O2C
29	hB	201	PEB	CAC-CBC-CGC-O2C
29	jB	201	PEB	CAC-CBC-CGC-O2C
29	lB	201	PEB	CAC-CBC-CGC-O2C
29	BC	201	PEB	CAC-CBC-CGC-O1C
29	DC	201	PEB	CAC-CBC-CGC-O1C
29	FC	201	PEB	CAC-CBC-CGC-O1C
29	HC	201	PEB	CAC-CBC-CGC-O1C
29	JC	201	PEB	CAC-CBC-CGC-O1C
29	LC	201	PEB	CAC-CBC-CGC-O1C
29	BD	202	PEB	CAC-CBC-CGC-O2C
29	DD	202	PEB	CAC-CBC-CGC-O2C
29	FD	202	PEB	CAC-CBC-CGC-O2C
29	HD	202	PEB	CAC-CBC-CGC-O2C
29	JD	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	LD	202	PEB	CAC-CBC-CGC-O2C
29	BE	201	PEB	CAC-CBC-CGC-O1C
29	DE	201	PEB	CAC-CBC-CGC-O1C
29	FE	201	PEB	CAC-CBC-CGC-O1C
29	HE	201	PEB	CAC-CBC-CGC-O1C
29	JE	201	PEB	CAC-CBC-CGC-O1C
29	LE	201	PEB	CAC-CBC-CGC-O1C
29	QF	201	PEB	CAC-CBC-CGC-O2C
29	SF	201	PEB	CAC-CBC-CGC-O2C
29	WF	201	PEB	CAC-CBC-CGC-O2C
29	AG	202	PEB	CAB-CBB-CGB-O1B
29	CG	202	PEB	CAB-CBB-CGB-O1B
29	EG	201	PEB	CAB-CBB-CGB-O2B
29	GG	202	PEB	CAB-CBB-CGB-O1B
29	IG	202	PEB	CAB-CBB-CGB-O1B
29	KG	201	PEB	CAB-CBB-CGB-O2B
29	KG	202	PEB	CAB-CBB-CGB-O1B
29	QI	201	PEB	CAC-CBC-CGC-O2C
29	SI	201	PEB	CAC-CBC-CGC-O2C
29	WI	201	PEB	CAC-CBC-CGC-O2C
29	BJ	203	PEB	CAB-CBB-CGB-O1B
29	DJ	202	PEB	CAB-CBB-CGB-O1B
29	HJ	202	PEB	CAB-CBB-CGB-O1B
29	JJ	203	PEB	CAB-CBB-CGB-O1B
29	LJ	202	PEB	CAB-CBB-CGB-O1B
29	PJ	203	PEB	CAB-CBB-CGB-O1B
29	RJ	203	PEB	CAB-CBB-CGB-O1B
29	TJ	203	PEB	CAB-CBB-CGB-O1B
29	VJ	202	PEB	CAB-CBB-CGB-O1B
29	XJ	203	PEB	CAB-CBB-CGB-O1B
29	ZJ	203	PEB	CAB-CBB-CGB-O1B
29	bJ	203	PEB	CAB-CBB-CGB-O1B
29	dJ	203	PEB	CAB-CBB-CGB-O1B
29	fJ	203	PEB	CAB-CBB-CGB-O1B
29	hJ	203	PEB	CAB-CBB-CGB-O1B
29	jJ	203	PEB	CAB-CBB-CGB-O1B
29	lJ	203	PEB	CAB-CBB-CGB-O1B
29	nJ	203	PEB	CAB-CBB-CGB-O1B
29	pJ	203	PEB	CAB-CBB-CGB-O1B
29	rJ	203	PEB	CAB-CBB-CGB-O1B
29	tJ	202	PEB	CAB-CBB-CGB-O1B
29	vJ	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	AK	301	PEB	CAB-CBB-CGB-01B
29	DK	1002	PEB	CAC-CBC-CGC-02C
29	OK	201	PEB	CAC-CBC-CGC-01C
29	OK	202	PEB	CAC-CBC-CGC-01C
29	QK	202	PEB	CAC-CBC-CGC-01C
29	SK	201	PEB	CAC-CBC-CGC-01C
29	SK	202	PEB	CAC-CBC-CGC-01C
29	UK	202	PEB	CAC-CBC-CGC-01C
29	UK	203	PEB	CAC-CBC-CGC-01C
29	WK	201	PEB	CAC-CBC-CGC-01C
29	WK	202	PEB	CAC-CBC-CGC-01C
29	ZK	202	PEB	CAC-CBC-CGC-01C
29	ZK	203	PEB	CAC-CBC-CGC-01C
29	bK	201	PEB	CAC-CBC-CGC-01C
29	bK	202	PEB	CAC-CBC-CGC-01C
29	dK	201	PEB	CAC-CBC-CGC-01C
29	fK	201	PEB	CAC-CBC-CGC-01C
29	fK	202	PEB	CAC-CBC-CGC-01C
29	hK	201	PEB	CAC-CBC-CGC-01C
29	hK	202	PEB	CAC-CBC-CGC-01C
29	jK	201	PEB	CAC-CBC-CGC-01C
29	jK	202	PEB	CAC-CBC-CGC-01C
29	lK	201	PEB	CAC-CBC-CGC-01C
29	lK	202	PEB	CAC-CBC-CGC-01C
29	BL	203	PEB	CAB-CBB-CGB-01B
29	DL	202	PEB	CAB-CBB-CGB-01B
29	HL	202	PEB	CAB-CBB-CGB-01B
29	JL	203	PEB	CAB-CBB-CGB-01B
29	LL	202	PEB	CAB-CBB-CGB-01B
29	PL	203	PEB	CAB-CBB-CGB-01B
29	RL	203	PEB	CAB-CBB-CGB-01B
29	TL	203	PEB	CAB-CBB-CGB-01B
29	VL	202	PEB	CAB-CBB-CGB-01B
29	XL	203	PEB	CAB-CBB-CGB-01B
29	ZL	203	PEB	CAB-CBB-CGB-01B
29	bL	203	PEB	CAB-CBB-CGB-01B
29	dL	203	PEB	CAB-CBB-CGB-01B
29	fL	203	PEB	CAB-CBB-CGB-01B
29	hL	203	PEB	CAB-CBB-CGB-01B
29	jL	203	PEB	CAB-CBB-CGB-01B
29	lL	203	PEB	CAB-CBB-CGB-01B
29	nL	203	PEB	CAB-CBB-CGB-01B

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Mol	Chain	Res	Type	Atoms
29	pL	203	PEB	CAB-CBB-CGB-01B
29	rL	203	PEB	CAB-CBB-CGB-01B
29	tL	202	PEB	CAB-CBB-CGB-01B
29	vL	202	PEB	CAB-CBB-CGB-01B
29	CM	201	PEB	CAC-CBC-CGC-02C
29	CM	202	PEB	CAC-CBC-CGC-01C
29	DM	203	PEB	CAC-CBC-CGC-02C
29	EM	201	PEB	CAC-CBC-CGC-02C
29	GM	201	PEB	CAC-CBC-CGC-02C
29	IM	201	PEB	CAC-CBC-CGC-02C
29	JM	203	PEB	CAC-CBC-CGC-02C
29	KM	201	PEB	CAC-CBC-CGC-02C
29	KM	202	PEB	CAC-CBC-CGC-01C
29	MM	201	PEB	CAC-CBC-CGC-02C
29	NM	202	PEB	CAC-CBC-CGC-02C
29	OM	201	PEB	CAC-CBC-CGC-02C
29	OM	202	PEB	CAC-CBC-CGC-01C
29	QM	203	PEB	CAC-CBC-CGC-02C
29	RM	203	PEB	CAC-CBC-CGC-02C
29	SM	201	PEB	CAC-CBC-CGC-02C
29	TM	203	PEB	CAC-CBC-CGC-02C
29	UM	201	PEB	CAC-CBC-CGC-02C
29	WM	201	PEB	CAC-CBC-CGC-02C
29	YM	202	PEB	CAC-CBC-CGC-02C
29	aM	201	PEB	CAC-CBC-CGC-02C
29	dM	201	PEB	CAC-CBC-CGC-02C
29	dM	202	PEB	CAC-CBC-CGC-01C
29	fM	201	PEB	CAC-CBC-CGC-02C
29	fM	202	PEB	CAC-CBC-CGC-01C
29	gM	203	PEB	CAC-CBC-CGC-02C
29	hM	201	PEB	CAC-CBC-CGC-02C
29	jM	201	PEB	CAC-CBC-CGC-02C
29	lM	201	PEB	CAC-CBC-CGC-02C
29	EN	202	PEB	CAC-CBC-CGC-02C
29	HN	203	PEB	CAB-CBB-CGB-01B
29	MN	404	PEB	CAC-CBC-CGC-01C
29	EO	201	PEB	CAC-CBC-CGC-02C
29	AQ	202	PEB	CAB-CBB-CGB-01B
29	CQ	202	PEB	CAB-CBB-CGB-01B
29	EQ	201	PEB	CAB-CBB-CGB-02B
29	GQ	202	PEB	CAB-CBB-CGB-01B
29	IQ	202	PEB	CAB-CBB-CGB-01B

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Mol	Chain	Res	Type	Atoms
29	KQ	201	PEB	CAB-CBB-CGB-O2B
29	KQ	202	PEB	CAB-CBB-CGB-O1B
29	VR	202	PEB	CAC-CBC-CGC-O1C
29	WR	202	PEB	CAC-CBC-CGC-O1C
29	XR	202	PEB	CAC-CBC-CGC-O1C
30	A1	305	PUB	CAB-CBB-CGB-O1B
30	A7	302	PUB	CAB-CBB-CGB-O2B
30	A9	302	PUB	CAB-CBB-CGB-O2B
30	MG	403	PUB	CAB-CBB-CGB-O1B
30	AK	305	PUB	CAB-CBB-CGB-O1B
30	MQ	405	PUB	CAB-CBB-CGB-O1B
31	J1	1001	CYC	CAD-CBD-CGD-O1D
31	N1	1001	CYC	CAD-CBD-CGD-O1D
31	DF	1001	CYC	CAA-CBA-CGA-O2A
31	FF	1001	CYC	CAA-CBA-CGA-O2A
31	HF	1001	CYC	CAA-CBA-CGA-O2A
31	JF	1001	CYC	CAA-CBA-CGA-O2A
31	LF	1001	CYC	CAA-CBA-CGA-O2A
31	NF	1001	CYC	CAA-CBA-CGA-O2A
31	DI	1001	CYC	CAA-CBA-CGA-O2A
31	FI	1001	CYC	CAA-CBA-CGA-O2A
31	HI	1001	CYC	CAA-CBA-CGA-O2A
31	JI	1001	CYC	CAA-CBA-CGA-O2A
31	LI	1001	CYC	CAA-CBA-CGA-O2A
31	NI	1001	CYC	CAA-CBA-CGA-O2A
31	DK	1001	CYC	CAD-CBD-CGD-O1D
31	JK	1001	CYC	CAD-CBD-CGD-O1D
29	C4	201	PEB	C2B-C3B-CAB-CBB
29	E4	201	PEB	C2B-C3B-CAB-CBB
29	G4	201	PEB	C2B-C3B-CAB-CBB
29	I4	201	PEB	C2B-C3B-CAB-CBB
29	K4	201	PEB	C2B-C3B-CAB-CBB
29	M4	201	PEB	C2B-C3B-CAB-CBB
29	dD	401	PEB	C2B-C3B-CAB-CBB
29	CD	201	PEB	C2B-C3B-CAB-CBB
29	ID	201	PEB	C2B-C3B-CAB-CBB
29	KD	201	PEB	C2B-C3B-CAB-CBB
29	MD	201	PEB	C2B-C3B-CAB-CBB
30	A1	305	PUB	C3C-C2C-CAC-CBC
30	AK	305	PUB	C3C-C2C-CAC-CBC
29	L1	1002	PEB	CAC-CBC-CGC-O2C
29	N1	1002	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	N2	201	PEB	CAB-CBB-CGB-O2B
29	S2	201	PEB	CAC-CBC-CGC-O2C
29	T2	201	PEB	CAB-CBB-CGB-O2B
29	B4	202	PEB	CAB-CBB-CGB-O2B
29	D4	202	PEB	CAB-CBB-CGB-O2B
29	F4	202	PEB	CAB-CBB-CGB-O2B
29	H4	202	PEB	CAB-CBB-CGB-O2B
29	J4	202	PEB	CAB-CBB-CGB-O2B
29	L4	202	PEB	CAB-CBB-CGB-O2B
29	B5	201	PEB	CAB-CBB-CGB-O2B
29	F5	201	PEB	CAC-CBC-CGC-O1C
29	F5	201	PEB	CAB-CBB-CGB-O2B
29	G5	201	PEB	CAB-CBB-CGB-O2B
29	H5	201	PEB	CAC-CBC-CGC-O1C
29	H5	201	PEB	CAB-CBB-CGB-O2B
29	L5	201	PEB	CAB-CBB-CGB-O2B
29	A7	301	PEB	CAC-CBC-CGC-O2C
29	A7	304	PEB	CAC-CBC-CGC-O2C
29	P7	202	PEB	CAC-CBC-CGC-O2C
29	R7	202	PEB	CAC-CBC-CGC-O2C
29	T7	202	PEB	CAC-CBC-CGC-O2C
29	V7	202	PEB	CAC-CBC-CGC-O2C
29	Y7	202	PEB	CAC-CBC-CGC-O2C
29	g7	202	PEB	CAC-CBC-CGC-O2C
29	B8	201	PEB	CAB-CBB-CGB-O2B
29	F8	201	PEB	CAC-CBC-CGC-O1C
29	F8	201	PEB	CAB-CBB-CGB-O2B
29	G8	201	PEB	CAB-CBB-CGB-O2B
29	H8	201	PEB	CAB-CBB-CGB-O2B
29	L8	201	PEB	CAB-CBB-CGB-O2B
29	A9	301	PEB	CAC-CBC-CGC-O2C
29	A9	304	PEB	CAC-CBC-CGC-O2C
29	P9	202	PEB	CAC-CBC-CGC-O2C
29	R9	202	PEB	CAC-CBC-CGC-O2C
29	T9	202	PEB	CAC-CBC-CGC-O2C
29	V9	202	PEB	CAC-CBC-CGC-O2C
29	Y9	202	PEB	CAC-CBC-CGC-O2C
29	g9	202	PEB	CAC-CBC-CGC-O2C
29	BA	201	PEB	CAB-CBB-CGB-O2B
29	BA	203	PEB	CAB-CBB-CGB-O1B
29	DA	201	PEB	CAB-CBB-CGB-O2B
29	DA	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	FA	201	PEB	CAB-CBB-CGB-O2B
29	FA	203	PEB	CAB-CBB-CGB-O1B
29	HA	201	PEB	CAB-CBB-CGB-O2B
29	JA	201	PEB	CAB-CBB-CGB-O2B
29	JA	203	PEB	CAB-CBB-CGB-O1B
29	LA	201	PEB	CAB-CBB-CGB-O2B
29	LA	203	PEB	CAB-CBB-CGB-O1B
29	AB	301	PEB	CAB-CBB-CGB-O1B
29	AB	302	PEB	CAC-CBC-CGC-O1C
29	EB	202	PEB	CAC-CBC-CGC-O1C
29	GB	202	PEB	CAC-CBC-CGC-O1C
29	IB	202	PEB	CAC-CBC-CGC-O1C
29	MB	202	PEB	CAC-CBC-CGC-O1C
29	QB	204	PEB	CAC-CBC-CGC-O1C
29	SB	202	PEB	CAC-CBC-CGC-O1C
29	UB	202	PEB	CAC-CBC-CGC-O1C
29	WB	202	PEB	CAC-CBC-CGC-O1C
29	aB	202	PEB	CAC-CBC-CGC-O1C
29	jB	202	PEB	CAC-CBC-CGC-O1C
29	lB	202	PEB	CAC-CBC-CGC-O1C
29	GC	202	PEB	CAB-CBB-CGB-O1B
29	BD	202	PEB	CAB-CBB-CGB-O2B
29	DD	202	PEB	CAB-CBB-CGB-O2B
29	FD	202	PEB	CAB-CBB-CGB-O2B
29	HD	202	PEB	CAB-CBB-CGB-O2B
29	JD	202	PEB	CAB-CBB-CGB-O2B
29	LD	202	PEB	CAB-CBB-CGB-O2B
29	GE	202	PEB	CAB-CBB-CGB-O1B
29	OF	201	PEB	CAC-CBC-CGC-O2C
29	QF	201	PEB	CAC-CBC-CGC-O1C
29	SF	201	PEB	CAC-CBC-CGC-O1C
29	UF	202	PEB	CAC-CBC-CGC-O2C
29	WF	201	PEB	CAC-CBC-CGC-O1C
29	ZF	201	PEB	CAC-CBC-CGC-O1C
29	ZF	201	PEB	CAC-CBC-CGC-O2C
29	bF	201	PEB	CAC-CBC-CGC-O1C
29	bF	201	PEB	CAC-CBC-CGC-O2C
29	dF	202	PEB	CAC-CBC-CGC-O1C
29	dF	202	PEB	CAC-CBC-CGC-O2C
29	fF	201	PEB	CAC-CBC-CGC-O1C
29	fF	201	PEB	CAC-CBC-CGC-O2C
29	hF	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	hF	201	PEB	CAC-CBC-CGC-O2C
29	jF	201	PEB	CAC-CBC-CGC-O1C
29	jF	201	PEB	CAC-CBC-CGC-O2C
29	lF	201	PEB	CAC-CBC-CGC-O1C
29	lF	201	PEB	CAC-CBC-CGC-O2C
29	EG	202	PEB	CAB-CBB-CGB-O1B
29	OI	201	PEB	CAC-CBC-CGC-O2C
29	QI	201	PEB	CAC-CBC-CGC-O1C
29	SI	201	PEB	CAC-CBC-CGC-O1C
29	UI	202	PEB	CAC-CBC-CGC-O2C
29	WI	201	PEB	CAC-CBC-CGC-O1C
29	ZI	201	PEB	CAC-CBC-CGC-O1C
29	ZI	201	PEB	CAC-CBC-CGC-O2C
29	bI	201	PEB	CAC-CBC-CGC-O1C
29	bI	201	PEB	CAC-CBC-CGC-O2C
29	dI	202	PEB	CAC-CBC-CGC-O1C
29	dI	202	PEB	CAC-CBC-CGC-O2C
29	fI	201	PEB	CAC-CBC-CGC-O1C
29	fI	201	PEB	CAC-CBC-CGC-O2C
29	hI	201	PEB	CAC-CBC-CGC-O1C
29	hI	201	PEB	CAC-CBC-CGC-O2C
29	jI	201	PEB	CAC-CBC-CGC-O1C
29	jI	201	PEB	CAC-CBC-CGC-O2C
29	lI	201	PEB	CAC-CBC-CGC-O1C
29	lI	201	PEB	CAC-CBC-CGC-O2C
29	zJ	501	PEB	CAC-CBC-CGC-O2C
29	LK	1002	PEB	CAC-CBC-CGC-O2C
29	AM	301	PEB	CAB-CBB-CGB-O1B
29	EM	202	PEB	CAC-CBC-CGC-O1C
29	GM	202	PEB	CAC-CBC-CGC-O1C
29	IM	202	PEB	CAC-CBC-CGC-O1C
29	MM	202	PEB	CAC-CBC-CGC-O1C
29	QM	204	PEB	CAC-CBC-CGC-O1C
29	SM	202	PEB	CAC-CBC-CGC-O1C
29	WM	202	PEB	CAC-CBC-CGC-O1C
29	aM	202	PEB	CAC-CBC-CGC-O1C
29	jM	202	PEB	CAC-CBC-CGC-O1C
29	lM	202	PEB	CAC-CBC-CGC-O1C
29	BN	201	PEB	CAB-CBB-CGB-O2B
29	BN	203	PEB	CAB-CBB-CGB-O1B
29	DN	201	PEB	CAB-CBB-CGB-O2B
29	DN	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	FN	201	PEB	CAB-CBB-CGB-O2B
29	FN	203	PEB	CAB-CBB-CGB-O1B
29	HN	201	PEB	CAB-CBB-CGB-O2B
29	JN	201	PEB	CAB-CBB-CGB-O2B
29	JN	203	PEB	CAB-CBB-CGB-O1B
29	LN	201	PEB	CAB-CBB-CGB-O2B
29	LN	203	PEB	CAB-CBB-CGB-O1B
29	MN	401	PEB	CAB-CBB-CGB-O2B
29	EQ	202	PEB	CAB-CBB-CGB-O1B
29	MQ	401	PEB	CAC-CBC-CGC-O1C
29	RR	201	PEB	CAB-CBB-CGB-O2B
30	AB	305	PUB	CAB-CBB-CGB-O1B
30	BB	302	PUB	CAB-CBB-CGB-O1B
30	AM	305	PUB	CAB-CBB-CGB-O1B
30	BM	302	PUB	CAB-CBB-CGB-O1B
31	C7	1001	CYC	CAA-CBA-CGA-O2A
31	E7	1001	CYC	CAA-CBA-CGA-O2A
31	G7	1001	CYC	CAA-CBA-CGA-O2A
31	I7	1001	CYC	CAA-CBA-CGA-O2A
31	K7	1001	CYC	CAA-CBA-CGA-O2A
31	M7	1001	CYC	CAA-CBA-CGA-O2A
31	C9	1001	CYC	CAA-CBA-CGA-O2A
31	E9	1001	CYC	CAA-CBA-CGA-O2A
31	G9	1001	CYC	CAA-CBA-CGA-O2A
31	I9	1001	CYC	CAA-CBA-CGA-O2A
31	M9	1001	CYC	CAA-CBA-CGA-O2A
29	R2	201	PEB	CAB-CBB-CGB-O2B
29	B3	202	PEB	CAC-CBC-CGC-O2C
29	B3	202	PEB	CAB-CBB-CGB-O2B
29	F3	202	PEB	CAC-CBC-CGC-O2C
29	F3	202	PEB	CAB-CBB-CGB-O2B
29	H3	202	PEB	CAC-CBC-CGC-O2C
29	H3	202	PEB	CAB-CBB-CGB-O2B
29	I3	203	PEB	CAC-CBC-CGC-O2C
29	I3	203	PEB	CAB-CBB-CGB-O2B
29	J3	202	PEB	CAC-CBC-CGC-O2C
29	J3	202	PEB	CAB-CBB-CGB-O2B
29	N3	203	PEB	CAB-CBB-CGB-O1B
29	C4	202	PEB	CAC-CBC-CGC-O2C
29	E4	202	PEB	CAC-CBC-CGC-O2C
29	G4	202	PEB	CAC-CBC-CGC-O2C
29	I4	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	M4	202	PEB	CAC-CBC-CGC-O2C
29	B5	201	PEB	CAC-CBC-CGC-O1C
29	B5	202	PEB	CAB-CBB-CGB-O2B
29	F5	202	PEB	CAB-CBB-CGB-O2B
29	H5	202	PEB	CAB-CBB-CGB-O2B
29	I5	201	PEB	CAC-CBC-CGC-O2C
29	K5	201	PEB	CAC-CBC-CGC-O2C
29	L5	201	PEB	CAC-CBC-CGC-O1C
29	L5	202	PEB	CAB-CBB-CGB-O2B
29	A5	201	PEB	CAC-CBC-CGC-O2C
29	C5	201	PEB	CAC-CBC-CGC-O2C
29	A7	304	PEB	CAC-CBC-CGC-O1C
29	a7	202	PEB	CAC-CBC-CGC-O2C
29	c7	202	PEB	CAC-CBC-CGC-O2C
29	e7	202	PEB	CAC-CBC-CGC-O2C
29	i7	202	PEB	CAC-CBC-CGC-O2C
29	k7	202	PEB	CAC-CBC-CGC-O2C
29	m7	202	PEB	CAC-CBC-CGC-O2C
29	B8	201	PEB	CAC-CBC-CGC-O1C
29	F8	202	PEB	CAB-CBB-CGB-O2B
29	G8	201	PEB	CAC-CBC-CGC-O1C
29	H8	201	PEB	CAC-CBC-CGC-O1C
29	H8	202	PEB	CAB-CBB-CGB-O2B
29	I8	201	PEB	CAC-CBC-CGC-O2C
29	K8	201	PEB	CAC-CBC-CGC-O2C
29	L8	202	PEB	CAB-CBB-CGB-O2B
29	A8	201	PEB	CAC-CBC-CGC-O2C
29	C8	201	PEB	CAC-CBC-CGC-O2C
29	a9	202	PEB	CAC-CBC-CGC-O2C
29	c9	202	PEB	CAC-CBC-CGC-O2C
29	e9	202	PEB	CAC-CBC-CGC-O2C
29	i9	202	PEB	CAC-CBC-CGC-O2C
29	k9	202	PEB	CAC-CBC-CGC-O2C
29	m9	202	PEB	CAC-CBC-CGC-O2C
29	AB	302	PEB	CAB-CBB-CGB-O1B
29	CB	202	PEB	CAB-CBB-CGB-O1B
29	EB	202	PEB	CAB-CBB-CGB-O1B
29	GB	202	PEB	CAB-CBB-CGB-O1B
29	IB	202	PEB	CAB-CBB-CGB-O1B
29	KB	202	PEB	CAB-CBB-CGB-O1B
29	MB	202	PEB	CAB-CBB-CGB-O1B
29	OB	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	QB	204	PEB	CAB-CBB-CGB-01B
29	SB	202	PEB	CAB-CBB-CGB-01B
29	UB	202	PEB	CAB-CBB-CGB-01B
29	WB	202	PEB	CAB-CBB-CGB-01B
29	YB	203	PEB	CAB-CBB-CGB-01B
29	aB	202	PEB	CAB-CBB-CGB-01B
29	dB	202	PEB	CAB-CBB-CGB-01B
29	fB	202	PEB	CAB-CBB-CGB-01B
29	hB	202	PEB	CAB-CBB-CGB-01B
29	jB	202	PEB	CAB-CBB-CGB-01B
29	lB	202	PEB	CAB-CBB-CGB-01B
29	EC	202	PEB	CAB-CBB-CGB-01B
29	IC	202	PEB	CAB-CBB-CGB-01B
29	KC	203	PEB	CAB-CBB-CGB-01B
29	CD	202	PEB	CAC-CBC-CGC-02C
29	ED	201	PEB	CAC-CBC-CGC-02C
29	GD	202	PEB	CAC-CBC-CGC-02C
29	ID	202	PEB	CAC-CBC-CGC-02C
29	KD	202	PEB	CAC-CBC-CGC-02C
29	EE	202	PEB	CAB-CBB-CGB-01B
29	IE	202	PEB	CAB-CBB-CGB-01B
29	KE	203	PEB	CAB-CBB-CGB-01B
29	AF	301	PEB	CAC-CBC-CGC-01C
29	AF	301	PEB	CAC-CBC-CGC-02C
29	AF	301	PEB	CAB-CBB-CGB-02B
29	AF	305	PEB	CAB-CBB-CGB-02B
29	OF	201	PEB	CAC-CBC-CGC-01C
29	OF	202	PEB	CAC-CBC-CGC-01C
29	OF	202	PEB	CAC-CBC-CGC-02C
29	QF	202	PEB	CAC-CBC-CGC-01C
29	QF	202	PEB	CAC-CBC-CGC-02C
29	SF	202	PEB	CAC-CBC-CGC-01C
29	SF	202	PEB	CAC-CBC-CGC-02C
29	UF	202	PEB	CAC-CBC-CGC-01C
29	UF	203	PEB	CAC-CBC-CGC-01C
29	UF	203	PEB	CAC-CBC-CGC-02C
29	WF	202	PEB	CAC-CBC-CGC-01C
29	WF	202	PEB	CAC-CBC-CGC-02C
29	ZF	202	PEB	CAC-CBC-CGC-01C
29	ZF	202	PEB	CAC-CBC-CGC-02C
29	bF	202	PEB	CAC-CBC-CGC-01C
29	bF	202	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
29	dF	203	PEB	CAC-CBC-CGC-O1C
29	dF	203	PEB	CAC-CBC-CGC-O2C
29	fF	202	PEB	CAC-CBC-CGC-O1C
29	fF	202	PEB	CAC-CBC-CGC-O2C
29	hF	202	PEB	CAC-CBC-CGC-O1C
29	hF	202	PEB	CAC-CBC-CGC-O2C
29	jF	202	PEB	CAC-CBC-CGC-O1C
29	jF	202	PEB	CAC-CBC-CGC-O2C
29	lF	202	PEB	CAC-CBC-CGC-O1C
29	lF	202	PEB	CAC-CBC-CGC-O2C
29	JG	203	PEB	CAB-CBB-CGB-O2B
29	AI	301	PEB	CAC-CBC-CGC-O1C
29	AI	301	PEB	CAC-CBC-CGC-O2C
29	AI	301	PEB	CAB-CBB-CGB-O2B
29	AI	305	PEB	CAB-CBB-CGB-O2B
29	OI	201	PEB	CAC-CBC-CGC-O1C
29	OI	202	PEB	CAC-CBC-CGC-O1C
29	OI	202	PEB	CAC-CBC-CGC-O2C
29	QI	202	PEB	CAC-CBC-CGC-O1C
29	QI	202	PEB	CAC-CBC-CGC-O2C
29	SI	202	PEB	CAC-CBC-CGC-O1C
29	SI	202	PEB	CAC-CBC-CGC-O2C
29	UI	202	PEB	CAC-CBC-CGC-O1C
29	UI	203	PEB	CAC-CBC-CGC-O1C
29	UI	203	PEB	CAC-CBC-CGC-O2C
29	WI	202	PEB	CAC-CBC-CGC-O1C
29	WI	202	PEB	CAC-CBC-CGC-O2C
29	ZI	202	PEB	CAC-CBC-CGC-O1C
29	ZI	202	PEB	CAC-CBC-CGC-O2C
29	bI	202	PEB	CAC-CBC-CGC-O1C
29	bI	202	PEB	CAC-CBC-CGC-O2C
29	dI	203	PEB	CAC-CBC-CGC-O1C
29	dI	203	PEB	CAC-CBC-CGC-O2C
29	fI	202	PEB	CAC-CBC-CGC-O1C
29	fI	202	PEB	CAC-CBC-CGC-O2C
29	hI	202	PEB	CAC-CBC-CGC-O1C
29	hI	202	PEB	CAC-CBC-CGC-O2C
29	jI	202	PEB	CAC-CBC-CGC-O1C
29	jI	202	PEB	CAC-CBC-CGC-O2C
29	lI	202	PEB	CAC-CBC-CGC-O1C
29	lI	202	PEB	CAC-CBC-CGC-O2C
29	AJ	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	CJ	202	PEB	CAC-CBC-CGC-O2C
29	EJ	202	PEB	CAC-CBC-CGC-O2C
29	GJ	202	PEB	CAC-CBC-CGC-O2C
29	IJ	202	PEB	CAC-CBC-CGC-O2C
29	KJ	202	PEB	CAC-CBC-CGC-O2C
29	MJ	202	PEB	CAC-CBC-CGC-O2C
29	OJ	202	PEB	CAC-CBC-CGC-O2C
29	WJ	203	PEB	CAC-CBC-CGC-O2C
29	YJ	202	PEB	CAC-CBC-CGC-O2C
29	aJ	202	PEB	CAC-CBC-CGC-O2C
29	eJ	202	PEB	CAC-CBC-CGC-O2C
29	gJ	202	PEB	CAC-CBC-CGC-O2C
29	iJ	202	PEB	CAC-CBC-CGC-O2C
29	kJ	202	PEB	CAC-CBC-CGC-O2C
29	mJ	202	PEB	CAC-CBC-CGC-O2C
29	oJ	202	PEB	CAC-CBC-CGC-O2C
29	sJ	202	PEB	CAC-CBC-CGC-O2C
29	wJ	302	PEB	CAC-CBC-CGC-O2C
29	zJ	501	PEB	CAC-CBC-CGC-O1C
29	AL	202	PEB	CAC-CBC-CGC-O2C
29	CL	202	PEB	CAC-CBC-CGC-O2C
29	EL	202	PEB	CAC-CBC-CGC-O2C
29	GL	202	PEB	CAC-CBC-CGC-O2C
29	IL	202	PEB	CAC-CBC-CGC-O2C
29	KL	202	PEB	CAC-CBC-CGC-O2C
29	ML	202	PEB	CAC-CBC-CGC-O2C
29	OL	202	PEB	CAC-CBC-CGC-O2C
29	WL	203	PEB	CAC-CBC-CGC-O2C
29	YL	202	PEB	CAC-CBC-CGC-O2C
29	aL	202	PEB	CAC-CBC-CGC-O2C
29	eL	202	PEB	CAC-CBC-CGC-O2C
29	gL	202	PEB	CAC-CBC-CGC-O2C
29	iL	202	PEB	CAC-CBC-CGC-O2C
29	kL	202	PEB	CAC-CBC-CGC-O2C
29	mL	202	PEB	CAC-CBC-CGC-O2C
29	oL	202	PEB	CAC-CBC-CGC-O2C
29	sL	202	PEB	CAC-CBC-CGC-O2C
29	wL	302	PEB	CAC-CBC-CGC-O2C
29	xL	302	PEB	CAC-CBC-CGC-O2C
29	AM	302	PEB	CAC-CBC-CGC-O1C
29	AM	302	PEB	CAB-CBB-CGB-O1B
29	CM	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	EM	202	PEB	CAB-CBB-CGB-01B
29	GM	202	PEB	CAB-CBB-CGB-01B
29	IM	202	PEB	CAB-CBB-CGB-01B
29	KM	202	PEB	CAB-CBB-CGB-01B
29	MM	202	PEB	CAB-CBB-CGB-01B
29	OM	202	PEB	CAB-CBB-CGB-01B
29	QM	204	PEB	CAB-CBB-CGB-01B
29	SM	202	PEB	CAB-CBB-CGB-01B
29	WM	202	PEB	CAB-CBB-CGB-01B
29	YM	203	PEB	CAB-CBB-CGB-01B
29	aM	202	PEB	CAB-CBB-CGB-01B
29	dM	202	PEB	CAB-CBB-CGB-01B
29	fM	202	PEB	CAB-CBB-CGB-01B
29	hM	202	PEB	CAB-CBB-CGB-01B
29	jM	202	PEB	CAB-CBB-CGB-01B
29	lM	202	PEB	CAB-CBB-CGB-01B
29	MN	401	PEB	CAB-CBB-CGB-01B
29	BO	202	PEB	CAC-CBC-CGC-02C
29	BO	202	PEB	CAB-CBB-CGB-02B
29	FO	202	PEB	CAC-CBC-CGC-02C
29	FO	202	PEB	CAB-CBB-CGB-02B
29	HO	202	PEB	CAC-CBC-CGC-02C
29	HO	202	PEB	CAB-CBB-CGB-02B
29	IO	203	PEB	CAC-CBC-CGC-02C
29	IO	203	PEB	CAB-CBB-CGB-02B
29	JO	202	PEB	CAC-CBC-CGC-02C
29	JO	202	PEB	CAB-CBB-CGB-02B
29	BQ	203	PEB	CAB-CBB-CGB-02B
29	FQ	203	PEB	CAB-CBB-CGB-02B
29	LQ	202	PEB	CAB-CBB-CGB-02B
29	MQ	401	PEB	CAB-CBB-CGB-01B
30	MA	402	PUB	CAB-CBB-CGB-01B
30	AF	302	PUB	CAC-CBC-CGC-02C
30	AI	302	PUB	CAC-CBC-CGC-02C
31	K9	1001	CYC	CAA-CBA-CGA-02A
29	O1	201	PEB	CAC-CBC-CGC-02C
29	Q1	201	PEB	CAC-CBC-CGC-02C
29	S1	201	PEB	CAC-CBC-CGC-02C
29	U1	202	PEB	CAC-CBC-CGC-02C
29	W1	201	PEB	CAC-CBC-CGC-02C
29	Z1	202	PEB	CAC-CBC-CGC-02C
29	b1	201	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
29	d1	201	PEB	CAC-CBC-CGC-O2C
29	f1	201	PEB	CAC-CBC-CGC-O2C
29	h1	201	PEB	CAC-CBC-CGC-O2C
29	j1	201	PEB	CAC-CBC-CGC-O2C
29	l1	201	PEB	CAC-CBC-CGC-O2C
29	e2	401	PEB	CAB-CBB-CGB-O2B
29	e2	402	PEB	CAB-CBB-CGB-O2B
29	V2	201	PEB	CAB-CBB-CGB-O2B
29	A3	201	PEB	CAC-CBC-CGC-O1C
29	G3	201	PEB	CAC-CBC-CGC-O1C
29	I3	201	PEB	CAC-CBC-CGC-O1C
29	K3	201	PEB	CAC-CBC-CGC-O1C
29	M3	203	PEB	CAB-CBB-CGB-O1B
29	C4	202	PEB	CAC-CBC-CGC-O1C
29	E4	202	PEB	CAC-CBC-CGC-O1C
29	K4	202	PEB	CAC-CBC-CGC-O2C
29	G5	202	PEB	CAB-CBB-CGB-O2B
29	I5	201	PEB	CAB-CBB-CGB-O1B
29	K5	201	PEB	CAB-CBB-CGB-O1B
29	A5	201	PEB	CAB-CBB-CGB-O1B
29	C5	201	PEB	CAB-CBB-CGB-O1B
29	B8	202	PEB	CAB-CBB-CGB-O2B
29	G8	202	PEB	CAB-CBB-CGB-O2B
29	I8	201	PEB	CAB-CBB-CGB-O1B
29	K8	201	PEB	CAB-CBB-CGB-O1B
29	L8	201	PEB	CAC-CBC-CGC-O1C
29	A8	201	PEB	CAB-CBB-CGB-O1B
29	C8	201	PEB	CAB-CBB-CGB-O1B
29	A9	304	PEB	CAC-CBC-CGC-O1C
29	BA	201	PEB	CAB-CBB-CGB-O1B
29	DA	201	PEB	CAB-CBB-CGB-O1B
29	FA	201	PEB	CAB-CBB-CGB-O1B
29	HA	201	PEB	CAB-CBB-CGB-O1B
29	JA	201	PEB	CAB-CBB-CGB-O1B
29	LA	201	PEB	CAB-CBB-CGB-O1B
29	MA	401	PEB	CAB-CBB-CGB-O1B
29	MD	202	PEB	CAC-CBC-CGC-O2C
29	LG	203	PEB	CAB-CBB-CGB-O2B
29	MG	401	PEB	CAB-CBB-CGB-O2B
29	MG	404	PEB	CAB-CBB-CGB-O1B
29	UJ	202	PEB	CAC-CBC-CGC-O2C
29	cJ	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	xJ	302	PEB	CAC-CBC-CGC-O2C
29	yJ	301	PEB	CAC-CBC-CGC-O2C
29	OK	201	PEB	CAC-CBC-CGC-O2C
29	QK	201	PEB	CAC-CBC-CGC-O2C
29	SK	201	PEB	CAC-CBC-CGC-O2C
29	UK	202	PEB	CAC-CBC-CGC-O2C
29	WK	201	PEB	CAC-CBC-CGC-O2C
29	ZK	202	PEB	CAC-CBC-CGC-O2C
29	bK	201	PEB	CAC-CBC-CGC-O2C
29	dK	201	PEB	CAC-CBC-CGC-O2C
29	fK	201	PEB	CAC-CBC-CGC-O2C
29	hK	201	PEB	CAC-CBC-CGC-O2C
29	jK	201	PEB	CAC-CBC-CGC-O2C
29	lK	201	PEB	CAC-CBC-CGC-O2C
29	UL	202	PEB	CAC-CBC-CGC-O2C
29	cL	202	PEB	CAC-CBC-CGC-O2C
29	yL	301	PEB	CAC-CBC-CGC-O2C
29	BN	201	PEB	CAB-CBB-CGB-O1B
29	DN	201	PEB	CAB-CBB-CGB-O1B
29	FN	201	PEB	CAB-CBB-CGB-O1B
29	HN	201	PEB	CAB-CBB-CGB-O1B
29	JN	201	PEB	CAB-CBB-CGB-O1B
29	LN	201	PEB	CAB-CBB-CGB-O1B
29	AO	201	PEB	CAC-CBC-CGC-O1C
29	GO	201	PEB	CAC-CBC-CGC-O1C
29	IO	201	PEB	CAC-CBC-CGC-O1C
29	KO	201	PEB	CAC-CBC-CGC-O1C
29	MO	203	PEB	CAB-CBB-CGB-O1B
29	NO	203	PEB	CAB-CBB-CGB-O1B
29	JQ	203	PEB	CAB-CBB-CGB-O2B
29	MQ	403	PEB	CAB-CBB-CGB-O2B
29	MQ	406	PEB	CAB-CBB-CGB-O1B
29	MQ	406	PEB	CAB-CBB-CGB-O2B
29	eR	401	PEB	CAB-CBB-CGB-O2B
29	NR	201	PEB	CAB-CBB-CGB-O2B
29	TR	201	PEB	CAB-CBB-CGB-O2B
29	VR	201	PEB	CAB-CBB-CGB-O2B
30	yJ	302	PUB	CAB-CBB-CGB-O1B
30	yL	302	PUB	CAB-CBB-CGB-O1B
30	MN	402	PUB	CAB-CBB-CGB-O1B
31	D1	1001	CYC	CAA-CBA-CGA-O1A
31	F1	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	H1	1001	CYC	CAA-CBA-CGA-O1A
31	J1	1001	CYC	CAA-CBA-CGA-O1A
31	L1	1001	CYC	CAA-CBA-CGA-O1A
31	N1	1001	CYC	CAA-CBA-CGA-O1A
31	DK	1001	CYC	CAA-CBA-CGA-O1A
31	FK	1001	CYC	CAA-CBA-CGA-O1A
31	HK	1001	CYC	CAA-CBA-CGA-O1A
31	JK	1001	CYC	CAA-CBA-CGA-O1A
31	LK	1001	CYC	CAA-CBA-CGA-O1A
31	NK	1001	CYC	CAA-CBA-CGA-O1A
29	D1	1002	PEB	CAB-CBB-CGB-O2B
29	F1	1002	PEB	CAB-CBB-CGB-O2B
29	H1	1002	PEB	CAB-CBB-CGB-O2B
29	J1	1002	PEB	CAB-CBB-CGB-O2B
29	L1	1002	PEB	CAB-CBB-CGB-O2B
29	N1	1002	PEB	CAB-CBB-CGB-O2B
29	C3	201	PEB	CAC-CBC-CGC-O1C
29	D3	202	PEB	CAC-CBC-CGC-O2C
29	E3	201	PEB	CAC-CBC-CGC-O1C
29	B4	202	PEB	CAB-CBB-CGB-O1B
29	C4	203	PEB	CAC-CBC-CGC-O1C
29	E4	203	PEB	CAC-CBC-CGC-O1C
29	F4	202	PEB	CAB-CBB-CGB-O1B
29	G4	202	PEB	CAC-CBC-CGC-O1C
29	G4	203	PEB	CAC-CBC-CGC-O1C
29	I4	202	PEB	CAC-CBC-CGC-O1C
29	J4	202	PEB	CAB-CBB-CGB-O1B
29	K4	202	PEB	CAC-CBC-CGC-O1C
29	K4	203	PEB	CAC-CBC-CGC-O1C
29	M4	202	PEB	CAC-CBC-CGC-O1C
29	B5	201	PEB	CAC-CBC-CGC-O2C
29	B5	202	PEB	CAC-CBC-CGC-O1C
29	B5	203	PEB	CAB-CBB-CGB-O2B
29	F5	201	PEB	CAC-CBC-CGC-O2C
29	F5	202	PEB	CAC-CBC-CGC-O1C
29	F5	203	PEB	CAB-CBB-CGB-O2B
29	G5	201	PEB	CAC-CBC-CGC-O2C
29	G5	202	PEB	CAC-CBC-CGC-O1C
29	G5	203	PEB	CAB-CBB-CGB-O2B
29	H5	201	PEB	CAC-CBC-CGC-O2C
29	H5	202	PEB	CAC-CBC-CGC-O1C
29	K5	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	L5	201	PEB	CAC-CBC-CGC-O2C
29	L5	202	PEB	CAC-CBC-CGC-O1C
29	L5	203	PEB	CAB-CBB-CGB-O2B
29	A5	203	PEB	CAB-CBB-CGB-O2B
29	R7	201	PEB	CAC-CBC-CGC-O1C
29	m7	201	PEB	CAC-CBC-CGC-O1C
29	B8	201	PEB	CAC-CBC-CGC-O2C
29	B8	202	PEB	CAC-CBC-CGC-O1C
29	B8	203	PEB	CAB-CBB-CGB-O2B
29	F8	201	PEB	CAC-CBC-CGC-O2C
29	F8	202	PEB	CAC-CBC-CGC-O1C
29	F8	203	PEB	CAB-CBB-CGB-O2B
29	G8	201	PEB	CAC-CBC-CGC-O2C
29	G8	202	PEB	CAC-CBC-CGC-O1C
29	G8	203	PEB	CAB-CBB-CGB-O2B
29	H8	202	PEB	CAC-CBC-CGC-O1C
29	K8	203	PEB	CAB-CBB-CGB-O2B
29	L8	201	PEB	CAC-CBC-CGC-O2C
29	L8	202	PEB	CAC-CBC-CGC-O1C
29	L8	203	PEB	CAB-CBB-CGB-O2B
29	A8	203	PEB	CAB-CBB-CGB-O2B
29	C8	203	PEB	CAB-CBB-CGB-O2B
29	R9	201	PEB	CAC-CBC-CGC-O1C
29	m9	201	PEB	CAC-CBC-CGC-O1C
29	BA	202	PEB	CAC-CBC-CGC-O1C
29	DA	202	PEB	CAC-CBC-CGC-O1C
29	FA	202	PEB	CAC-CBC-CGC-O1C
29	HA	202	PEB	CAC-CBC-CGC-O1C
29	JA	202	PEB	CAC-CBC-CGC-O1C
29	LA	202	PEB	CAC-CBC-CGC-O1C
29	AB	303	PEB	CAC-CBC-CGC-O1C
29	CD	202	PEB	CAC-CBC-CGC-O1C
29	CD	203	PEB	CAC-CBC-CGC-O1C
29	ED	201	PEB	CAC-CBC-CGC-O1C
29	ED	202	PEB	CAC-CBC-CGC-O1C
29	FD	202	PEB	CAB-CBB-CGB-O1B
29	GD	202	PEB	CAC-CBC-CGC-O1C
29	GD	203	PEB	CAC-CBC-CGC-O1C
29	ID	202	PEB	CAC-CBC-CGC-O1C
29	ID	203	PEB	CAC-CBC-CGC-O1C
29	JD	202	PEB	CAB-CBB-CGB-O1B
29	KD	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	KD	203	PEB	CAC-CBC-CGC-O1C
29	MD	202	PEB	CAC-CBC-CGC-O1C
29	MD	203	PEB	CAC-CBC-CGC-O1C
29	AG	202	PEB	CAC-CBC-CGC-O1C
29	BG	203	PEB	CAB-CBB-CGB-O2B
29	CG	202	PEB	CAC-CBC-CGC-O1C
29	DG	203	PEB	CAB-CBB-CGB-O2B
29	EG	202	PEB	CAC-CBC-CGC-O1C
29	FG	203	PEB	CAB-CBB-CGB-O2B
29	GG	202	PEB	CAC-CBC-CGC-O1C
29	HG	203	PEB	CAB-CBB-CGB-O2B
29	IG	202	PEB	CAC-CBC-CGC-O1C
29	KG	202	PEB	CAC-CBC-CGC-O1C
29	MG	404	PEB	CAB-CBB-CGB-O2B
29	QJ	202	PEB	CAC-CBC-CGC-O2C
29	SJ	202	PEB	CAC-CBC-CGC-O2C
29	qJ	202	PEB	CAC-CBC-CGC-O2C
29	uJ	203	PEB	CAC-CBC-CGC-O2C
29	DK	1002	PEB	CAC-CBC-CGC-O1C
29	FK	1002	PEB	CAB-CBB-CGB-O2B
29	HK	1002	PEB	CAB-CBB-CGB-O2B
29	JK	1002	PEB	CAB-CBB-CGB-O2B
29	LK	1002	PEB	CAB-CBB-CGB-O2B
29	NK	1002	PEB	CAB-CBB-CGB-O2B
29	QL	202	PEB	CAC-CBC-CGC-O2C
29	SL	202	PEB	CAC-CBC-CGC-O2C
29	qL	202	PEB	CAC-CBC-CGC-O2C
29	uL	203	PEB	CAC-CBC-CGC-O2C
29	zL	501	PEB	CAC-CBC-CGC-O2C
29	AM	303	PEB	CAC-CBC-CGC-O1C
29	BN	202	PEB	CAC-CBC-CGC-O1C
29	DN	202	PEB	CAC-CBC-CGC-O1C
29	FN	202	PEB	CAC-CBC-CGC-O1C
29	HN	202	PEB	CAC-CBC-CGC-O1C
29	JN	202	PEB	CAC-CBC-CGC-O1C
29	LN	202	PEB	CAC-CBC-CGC-O1C
29	CO	201	PEB	CAC-CBC-CGC-O1C
29	EO	201	PEB	CAC-CBC-CGC-O1C
29	AQ	202	PEB	CAC-CBC-CGC-O1C
29	CQ	202	PEB	CAC-CBC-CGC-O1C
29	DQ	203	PEB	CAB-CBB-CGB-O2B
29	EQ	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	GQ	202	PEB	CAC-CBC-CGC-O1C
29	HQ	203	PEB	CAB-CBB-CGB-O2B
29	IQ	202	PEB	CAC-CBC-CGC-O1C
29	KQ	202	PEB	CAC-CBC-CGC-O1C
29	XR	201	PEB	CAB-CBB-CGB-O2B
30	yJ	302	PUB	CAB-CBB-CGB-O2B
30	yJ	303	PUB	CAB-CBB-CGB-O2B
30	yL	302	PUB	CAB-CBB-CGB-O2B
29	GD	201	PEB	C2B-C3B-CAB-CBB
29	D1	1002	PEB	CAC-CBC-CGC-O1C
29	P1	203	PEB	CAB-CBB-CGB-O1B
29	R1	203	PEB	CAB-CBB-CGB-O1B
29	T1	202	PEB	CAB-CBB-CGB-O1B
29	Y1	202	PEB	CAB-CBB-CGB-O1B
29	a1	203	PEB	CAB-CBB-CGB-O1B
29	m1	202	PEB	CAB-CBB-CGB-O1B
29	S2	201	PEB	CAC-CBC-CGC-O1C
29	B3	201	PEB	CAB-CBB-CGB-O2B
29	D3	201	PEB	CAB-CBB-CGB-O2B
29	F3	201	PEB	CAB-CBB-CGB-O2B
29	H3	201	PEB	CAB-CBB-CGB-O2B
29	J3	201	PEB	CAB-CBB-CGB-O2B
29	L3	201	PEB	CAB-CBB-CGB-O2B
29	M3	203	PEB	CAC-CBC-CGC-O2C
29	D4	202	PEB	CAB-CBB-CGB-O1B
29	I4	203	PEB	CAB-CBB-CGB-O2B
29	L4	202	PEB	CAB-CBB-CGB-O1B
29	B5	201	PEB	CAB-CBB-CGB-O1B
29	F5	201	PEB	CAB-CBB-CGB-O1B
29	H5	203	PEB	CAB-CBB-CGB-O2B
29	I5	203	PEB	CAB-CBB-CGB-O2B
29	L5	201	PEB	CAB-CBB-CGB-O1B
29	C5	203	PEB	CAB-CBB-CGB-O2B
29	A7	305	PEB	CAC-CBC-CGC-O2C
29	P7	201	PEB	CAC-CBC-CGC-O1C
29	P7	203	PEB	CAC-CBC-CGC-O2C
29	R7	203	PEB	CAC-CBC-CGC-O2C
29	T7	201	PEB	CAC-CBC-CGC-O1C
29	T7	203	PEB	CAC-CBC-CGC-O2C
29	V7	201	PEB	CAC-CBC-CGC-O1C
29	V7	203	PEB	CAC-CBC-CGC-O2C
29	Y7	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	Y7	203	PEB	CAC-CBC-CGC-O2C
29	a7	201	PEB	CAC-CBC-CGC-O1C
29	a7	203	PEB	CAC-CBC-CGC-O2C
29	c7	201	PEB	CAC-CBC-CGC-O1C
29	c7	203	PEB	CAC-CBC-CGC-O2C
29	e7	201	PEB	CAC-CBC-CGC-O1C
29	e7	203	PEB	CAC-CBC-CGC-O2C
29	g7	201	PEB	CAC-CBC-CGC-O1C
29	g7	203	PEB	CAC-CBC-CGC-O2C
29	i7	201	PEB	CAC-CBC-CGC-O1C
29	i7	203	PEB	CAC-CBC-CGC-O2C
29	k7	201	PEB	CAC-CBC-CGC-O1C
29	k7	203	PEB	CAC-CBC-CGC-O2C
29	m7	203	PEB	CAC-CBC-CGC-O2C
29	B8	201	PEB	CAB-CBB-CGB-O1B
29	F8	201	PEB	CAB-CBB-CGB-O1B
29	H8	201	PEB	CAC-CBC-CGC-O2C
29	H8	201	PEB	CAB-CBB-CGB-O1B
29	H8	203	PEB	CAB-CBB-CGB-O2B
29	I8	203	PEB	CAB-CBB-CGB-O2B
29	L8	201	PEB	CAB-CBB-CGB-O1B
29	A9	305	PEB	CAC-CBC-CGC-O2C
29	P9	201	PEB	CAC-CBC-CGC-O1C
29	P9	203	PEB	CAC-CBC-CGC-O2C
29	R9	203	PEB	CAC-CBC-CGC-O2C
29	T9	201	PEB	CAC-CBC-CGC-O1C
29	T9	203	PEB	CAC-CBC-CGC-O2C
29	V9	201	PEB	CAC-CBC-CGC-O1C
29	V9	203	PEB	CAC-CBC-CGC-O2C
29	Y9	201	PEB	CAC-CBC-CGC-O1C
29	Y9	203	PEB	CAC-CBC-CGC-O2C
29	a9	201	PEB	CAC-CBC-CGC-O1C
29	a9	203	PEB	CAC-CBC-CGC-O2C
29	c9	201	PEB	CAC-CBC-CGC-O1C
29	c9	203	PEB	CAC-CBC-CGC-O2C
29	e9	201	PEB	CAC-CBC-CGC-O1C
29	e9	203	PEB	CAC-CBC-CGC-O2C
29	g9	201	PEB	CAC-CBC-CGC-O1C
29	g9	203	PEB	CAC-CBC-CGC-O2C
29	i9	201	PEB	CAC-CBC-CGC-O1C
29	i9	203	PEB	CAC-CBC-CGC-O2C
29	k9	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	k9	203	PEB	CAC-CBC-CGC-O2C
29	m9	203	PEB	CAC-CBC-CGC-O2C
29	AA	201	PEB	CAB-CBB-CGB-O2B
29	CA	201	PEB	CAB-CBB-CGB-O2B
29	EA	201	PEB	CAB-CBB-CGB-O2B
29	GA	201	PEB	CAB-CBB-CGB-O2B
29	IA	201	PEB	CAB-CBB-CGB-O2B
29	KA	201	PEB	CAB-CBB-CGB-O2B
29	AB	301	PEB	CAC-CBC-CGC-O1C
29	AC	201	PEB	CAB-CBB-CGB-O1B
29	CC	201	PEB	CAB-CBB-CGB-O1B
29	EC	201	PEB	CAB-CBB-CGB-O1B
29	KC	202	PEB	CAB-CBB-CGB-O1B
29	BD	202	PEB	CAB-CBB-CGB-O1B
29	DD	202	PEB	CAB-CBB-CGB-O1B
29	HD	202	PEB	CAB-CBB-CGB-O1B
29	LD	202	PEB	CAB-CBB-CGB-O1B
29	AE	201	PEB	CAB-CBB-CGB-O1B
29	CE	201	PEB	CAB-CBB-CGB-O1B
29	EE	201	PEB	CAB-CBB-CGB-O1B
29	KE	202	PEB	CAB-CBB-CGB-O1B
29	QF	201	PEB	CAB-CBB-CGB-O2B
29	SF	201	PEB	CAB-CBB-CGB-O2B
29	UF	202	PEB	CAB-CBB-CGB-O2B
29	WF	201	PEB	CAB-CBB-CGB-O2B
29	ZF	201	PEB	CAB-CBB-CGB-O2B
29	bF	201	PEB	CAB-CBB-CGB-O2B
29	dF	202	PEB	CAB-CBB-CGB-O2B
29	fF	201	PEB	CAB-CBB-CGB-O2B
29	hF	201	PEB	CAB-CBB-CGB-O2B
29	jF	201	PEB	CAB-CBB-CGB-O2B
29	lF	201	PEB	CAB-CBB-CGB-O2B
29	DG	201	PEB	CAC-CBC-CGC-O2C
29	HG	203	PEB	CAB-CBB-CGB-O1B
29	QI	201	PEB	CAB-CBB-CGB-O2B
29	SI	201	PEB	CAB-CBB-CGB-O2B
29	UI	202	PEB	CAB-CBB-CGB-O2B
29	WI	201	PEB	CAB-CBB-CGB-O2B
29	ZI	201	PEB	CAB-CBB-CGB-O2B
29	bI	201	PEB	CAB-CBB-CGB-O2B
29	dI	202	PEB	CAB-CBB-CGB-O2B
29	fI	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	hI	201	PEB	CAB-CBB-CGB-O2B
29	jI	201	PEB	CAB-CBB-CGB-O2B
29	lI	201	PEB	CAB-CBB-CGB-O2B
29	AJ	201	PEB	CAC-CBC-CGC-O1C
29	CJ	201	PEB	CAC-CBC-CGC-O1C
29	EJ	201	PEB	CAC-CBC-CGC-O1C
29	KJ	201	PEB	CAC-CBC-CGC-O1C
29	MJ	201	PEB	CAC-CBC-CGC-O1C
29	OJ	201	PEB	CAC-CBC-CGC-O1C
29	QJ	201	PEB	CAC-CBC-CGC-O1C
29	SJ	201	PEB	CAC-CBC-CGC-O1C
29	UJ	201	PEB	CAC-CBC-CGC-O1C
29	WJ	202	PEB	CAC-CBC-CGC-O1C
29	YJ	201	PEB	CAC-CBC-CGC-O1C
29	aJ	201	PEB	CAC-CBC-CGC-O1C
29	cJ	201	PEB	CAC-CBC-CGC-O1C
29	eJ	201	PEB	CAC-CBC-CGC-O1C
29	gJ	201	PEB	CAC-CBC-CGC-O1C
29	iJ	201	PEB	CAC-CBC-CGC-O1C
29	kJ	201	PEB	CAC-CBC-CGC-O1C
29	mJ	201	PEB	CAC-CBC-CGC-O1C
29	oJ	201	PEB	CAC-CBC-CGC-O1C
29	qJ	201	PEB	CAC-CBC-CGC-O1C
29	sJ	201	PEB	CAC-CBC-CGC-O1C
29	uJ	202	PEB	CAC-CBC-CGC-O1C
29	wJ	303	PEB	CAB-CBB-CGB-O2B
29	xJ	303	PEB	CAB-CBB-CGB-O2B
29	DK	1002	PEB	CAB-CBB-CGB-O2B
29	HK	1002	PEB	CAC-CBC-CGC-O1C
29	PK	203	PEB	CAB-CBB-CGB-O1B
29	RK	203	PEB	CAB-CBB-CGB-O1B
29	TK	202	PEB	CAB-CBB-CGB-O1B
29	YK	202	PEB	CAB-CBB-CGB-O1B
29	aK	203	PEB	CAB-CBB-CGB-O1B
29	mK	202	PEB	CAB-CBB-CGB-O1B
29	AL	201	PEB	CAC-CBC-CGC-O1C
29	CL	201	PEB	CAC-CBC-CGC-O1C
29	EL	201	PEB	CAC-CBC-CGC-O1C
29	KL	201	PEB	CAC-CBC-CGC-O1C
29	ML	201	PEB	CAC-CBC-CGC-O1C
29	OL	201	PEB	CAC-CBC-CGC-O1C
29	QL	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	SL	201	PEB	CAC-CBC-CGC-O1C
29	UL	201	PEB	CAC-CBC-CGC-O1C
29	WL	202	PEB	CAC-CBC-CGC-O1C
29	YL	201	PEB	CAC-CBC-CGC-O1C
29	aL	201	PEB	CAC-CBC-CGC-O1C
29	cL	201	PEB	CAC-CBC-CGC-O1C
29	eL	201	PEB	CAC-CBC-CGC-O1C
29	gL	201	PEB	CAC-CBC-CGC-O1C
29	iL	201	PEB	CAC-CBC-CGC-O1C
29	kL	201	PEB	CAC-CBC-CGC-O1C
29	mL	201	PEB	CAC-CBC-CGC-O1C
29	oL	201	PEB	CAC-CBC-CGC-O1C
29	qL	201	PEB	CAC-CBC-CGC-O1C
29	sL	201	PEB	CAC-CBC-CGC-O1C
29	uL	202	PEB	CAC-CBC-CGC-O1C
29	wL	303	PEB	CAB-CBB-CGB-O2B
29	xL	303	PEB	CAB-CBB-CGB-O2B
29	AM	301	PEB	CAC-CBC-CGC-O1C
29	AN	201	PEB	CAB-CBB-CGB-O2B
29	CN	201	PEB	CAB-CBB-CGB-O2B
29	EN	201	PEB	CAB-CBB-CGB-O2B
29	GN	201	PEB	CAB-CBB-CGB-O2B
29	IN	201	PEB	CAB-CBB-CGB-O2B
29	KN	201	PEB	CAB-CBB-CGB-O2B
29	BO	201	PEB	CAB-CBB-CGB-O2B
29	DO	201	PEB	CAB-CBB-CGB-O2B
29	DO	202	PEB	CAC-CBC-CGC-O2C
29	FO	201	PEB	CAB-CBB-CGB-O2B
29	HO	201	PEB	CAB-CBB-CGB-O2B
29	JO	201	PEB	CAB-CBB-CGB-O2B
29	LO	201	PEB	CAB-CBB-CGB-O2B
29	MO	203	PEB	CAC-CBC-CGC-O2C
29	NO	203	PEB	CAC-CBC-CGC-O2C
29	DQ	201	PEB	CAC-CBC-CGC-O2C
29	SR	201	PEB	CAC-CBC-CGC-O2C
30	yL	303	PUB	CAB-CBB-CGB-O2B
31	VP	1001	CYC	C2A-CAA-CBA-CGA
31	xP	1001	CYC	C2A-CAA-CBA-CGA
29	F1	1002	PEB	CAC-CBC-CGC-O1C
29	H1	1002	PEB	CAC-CBC-CGC-O1C
29	J1	1002	PEB	CAC-CBC-CGC-O1C
29	L1	1002	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	N1	1002	PEB	CAC-CBC-CGC-O1C
29	V1	203	PEB	CAB-CBB-CGB-O1B
29	c1	203	PEB	CAB-CBB-CGB-O1B
29	e1	203	PEB	CAB-CBB-CGB-O1B
29	g1	203	PEB	CAB-CBB-CGB-O1B
29	i1	203	PEB	CAB-CBB-CGB-O1B
29	k1	203	PEB	CAB-CBB-CGB-O1B
29	e2	401	PEB	CAB-CBB-CGB-O1B
29	M2	201	PEB	CAC-CBC-CGC-O1C
29	M2	201	PEB	CAC-CBC-CGC-O2C
29	O2	201	PEB	CAC-CBC-CGC-O1C
29	Q2	201	PEB	CAC-CBC-CGC-O1C
29	Q2	201	PEB	CAC-CBC-CGC-O2C
29	U2	201	PEB	CAC-CBC-CGC-O1C
29	W2	201	PEB	CAC-CBC-CGC-O1C
29	W2	201	PEB	CAC-CBC-CGC-O2C
29	M3	202	PEB	CAB-CBB-CGB-O1B
29	N3	202	PEB	CAB-CBB-CGB-O1B
29	N3	203	PEB	CAC-CBC-CGC-O2C
29	H4	202	PEB	CAB-CBB-CGB-O1B
29	G5	201	PEB	CAB-CBB-CGB-O1B
29	H5	201	PEB	CAB-CBB-CGB-O1B
29	G8	201	PEB	CAB-CBB-CGB-O1B
29	GC	201	PEB	CAB-CBB-CGB-O1B
29	IC	201	PEB	CAB-CBB-CGB-O1B
29	GE	201	PEB	CAB-CBB-CGB-O1B
29	IE	201	PEB	CAB-CBB-CGB-O1B
29	OF	201	PEB	CAB-CBB-CGB-O2B
29	PF	203	PEB	CAC-CBC-CGC-O1C
29	PF	203	PEB	CAC-CBC-CGC-O2C
29	RF	202	PEB	CAC-CBC-CGC-O1C
29	TF	201	PEB	CAB-CBB-CGB-O2B
29	TF	202	PEB	CAC-CBC-CGC-O1C
29	TF	202	PEB	CAC-CBC-CGC-O2C
29	VF	203	PEB	CAC-CBC-CGC-O1C
29	VF	203	PEB	CAC-CBC-CGC-O2C
29	YF	203	PEB	CAC-CBC-CGC-O1C
29	aF	203	PEB	CAC-CBC-CGC-O1C
29	aF	203	PEB	CAC-CBC-CGC-O2C
29	cF	202	PEB	CAC-CBC-CGC-O1C
29	cF	202	PEB	CAC-CBC-CGC-O2C
29	eF	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	eF	203	PEB	CAC-CBC-CGC-O2C
29	gF	203	PEB	CAC-CBC-CGC-O1C
29	iF	203	PEB	CAC-CBC-CGC-O1C
29	iF	203	PEB	CAC-CBC-CGC-O2C
29	kF	203	PEB	CAC-CBC-CGC-O1C
29	kF	203	PEB	CAC-CBC-CGC-O2C
29	mF	203	PEB	CAC-CBC-CGC-O1C
29	mF	203	PEB	CAC-CBC-CGC-O2C
29	BG	201	PEB	CAC-CBC-CGC-O2C
29	BG	203	PEB	CAB-CBB-CGB-O1B
29	DG	203	PEB	CAB-CBB-CGB-O1B
29	FG	201	PEB	CAC-CBC-CGC-O2C
29	FG	203	PEB	CAB-CBB-CGB-O1B
29	HG	201	PEB	CAC-CBC-CGC-O2C
29	JG	201	PEB	CAC-CBC-CGC-O2C
29	JG	203	PEB	CAB-CBB-CGB-O1B
29	LG	201	PEB	CAC-CBC-CGC-O2C
29	LG	203	PEB	CAB-CBB-CGB-O1B
29	OI	201	PEB	CAB-CBB-CGB-O2B
29	PI	203	PEB	CAC-CBC-CGC-O1C
29	PI	203	PEB	CAC-CBC-CGC-O2C
29	RI	202	PEB	CAC-CBC-CGC-O1C
29	TI	202	PEB	CAC-CBC-CGC-O1C
29	TI	202	PEB	CAC-CBC-CGC-O2C
29	VI	203	PEB	CAC-CBC-CGC-O1C
29	VI	203	PEB	CAC-CBC-CGC-O2C
29	YI	203	PEB	CAC-CBC-CGC-O1C
29	aI	203	PEB	CAC-CBC-CGC-O1C
29	aI	203	PEB	CAC-CBC-CGC-O2C
29	cI	202	PEB	CAC-CBC-CGC-O1C
29	cI	202	PEB	CAC-CBC-CGC-O2C
29	eI	203	PEB	CAC-CBC-CGC-O1C
29	eI	203	PEB	CAC-CBC-CGC-O2C
29	gI	203	PEB	CAC-CBC-CGC-O1C
29	iI	203	PEB	CAC-CBC-CGC-O1C
29	iI	203	PEB	CAC-CBC-CGC-O2C
29	kI	203	PEB	CAC-CBC-CGC-O1C
29	kI	203	PEB	CAC-CBC-CGC-O2C
29	mI	203	PEB	CAC-CBC-CGC-O1C
29	mI	203	PEB	CAC-CBC-CGC-O2C
29	GJ	201	PEB	CAC-CBC-CGC-O1C
29	IJ	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	FK	1002	PEB	CAC-CBC-CGC-O1C
29	JK	1002	PEB	CAC-CBC-CGC-O1C
29	LK	1002	PEB	CAC-CBC-CGC-O1C
29	NK	1002	PEB	CAC-CBC-CGC-O1C
29	VK	203	PEB	CAB-CBB-CGB-O1B
29	cK	203	PEB	CAB-CBB-CGB-O1B
29	eK	203	PEB	CAB-CBB-CGB-O1B
29	gK	203	PEB	CAB-CBB-CGB-O1B
29	iK	203	PEB	CAB-CBB-CGB-O1B
29	kK	203	PEB	CAB-CBB-CGB-O1B
29	GL	201	PEB	CAC-CBC-CGC-O1C
29	IL	201	PEB	CAC-CBC-CGC-O1C
29	MO	202	PEB	CAB-CBB-CGB-O1B
29	NO	202	PEB	CAB-CBB-CGB-O1B
29	BQ	201	PEB	CAC-CBC-CGC-O2C
29	BQ	203	PEB	CAB-CBB-CGB-O1B
29	DQ	203	PEB	CAB-CBB-CGB-O1B
29	FQ	201	PEB	CAC-CBC-CGC-O2C
29	FQ	203	PEB	CAB-CBB-CGB-O1B
29	HQ	201	PEB	CAC-CBC-CGC-O2C
29	HQ	203	PEB	CAB-CBB-CGB-O1B
29	JQ	201	PEB	CAC-CBC-CGC-O2C
29	JQ	203	PEB	CAB-CBB-CGB-O1B
29	LQ	202	PEB	CAB-CBB-CGB-O1B
29	MQ	402	PEB	CAC-CBC-CGC-O2C
29	eR	401	PEB	CAB-CBB-CGB-O1B
29	MR	201	PEB	CAC-CBC-CGC-O1C
29	OR	201	PEB	CAC-CBC-CGC-O1C
29	QR	201	PEB	CAC-CBC-CGC-O1C
29	UR	201	PEB	CAC-CBC-CGC-O1C
29	WR	201	PEB	CAC-CBC-CGC-O1C
30	A1	305	PUB	CAC-CBC-CGC-O2C
30	AK	305	PUB	CAC-CBC-CGC-O2C
29	O2	201	PEB	CAC-CBC-CGC-O2C
29	U2	201	PEB	CAC-CBC-CGC-O2C
29	B3	201	PEB	CAB-CBB-CGB-O1B
29	D3	201	PEB	CAB-CBB-CGB-O1B
29	F3	201	PEB	CAB-CBB-CGB-O1B
29	H3	201	PEB	CAB-CBB-CGB-O1B
29	J3	201	PEB	CAB-CBB-CGB-O1B
29	L3	201	PEB	CAB-CBB-CGB-O1B
29	KC	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	KE	201	PEB	CAC-CBC-CGC-O2C
29	RF	202	PEB	CAC-CBC-CGC-O2C
29	YF	203	PEB	CAC-CBC-CGC-O2C
29	gF	203	PEB	CAC-CBC-CGC-O2C
29	MG	401	PEB	CAC-CBC-CGC-O2C
29	RI	202	PEB	CAC-CBC-CGC-O2C
29	YI	203	PEB	CAC-CBC-CGC-O2C
29	gI	203	PEB	CAC-CBC-CGC-O2C
29	BO	201	PEB	CAB-CBB-CGB-O1B
29	DO	201	PEB	CAB-CBB-CGB-O1B
29	FO	201	PEB	CAB-CBB-CGB-O1B
29	HO	201	PEB	CAB-CBB-CGB-O1B
29	JO	201	PEB	CAB-CBB-CGB-O1B
29	LO	201	PEB	CAB-CBB-CGB-O1B
29	MQ	403	PEB	CAC-CBC-CGC-O2C
29	MR	201	PEB	CAC-CBC-CGC-O2C
29	OR	201	PEB	CAC-CBC-CGC-O2C
29	QR	201	PEB	CAC-CBC-CGC-O2C
29	UR	201	PEB	CAC-CBC-CGC-O2C
29	WR	201	PEB	CAC-CBC-CGC-O2C
31	YP	1000	CYC	CAA-CBA-CGA-O1A
31	1P	1002	CYC	CAA-CBA-CGA-O1A
29	M4	203	PEB	CAC-CBC-CGC-O2C
29	AC	203	PEB	CAC-CBC-CGC-O2C
29	BC	202	PEB	CAC-CBC-CGC-O2C
29	HC	202	PEB	CAC-CBC-CGC-O2C
29	AE	203	PEB	CAC-CBC-CGC-O2C
29	BE	202	PEB	CAC-CBC-CGC-O2C
29	HE	202	PEB	CAC-CBC-CGC-O2C
29	wL	302	PEB	CAB-CBB-CGB-O1B
30	MG	402	PUB	CAC-CBC-CGC-O1C
30	MQ	404	PUB	CAC-CBC-CGC-O1C
31	WP	1001	CYC	CAA-CBA-CGA-O1A
31	yP	1001	CYC	CAA-CBA-CGA-O1A
29	A1	302	PEB	CAC-CBC-CGC-O2C
29	N2	203	PEB	CAC-CBC-CGC-O2C
29	P2	202	PEB	CAC-CBC-CGC-O2C
29	R2	203	PEB	CAC-CBC-CGC-O2C
29	T2	203	PEB	CAC-CBC-CGC-O2C
29	V2	203	PEB	CAC-CBC-CGC-O2C
29	X2	202	PEB	CAC-CBC-CGC-O2C
29	CC	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	FC	202	PEB	CAC-CBC-CGC-O2C
29	LC	202	PEB	CAC-CBC-CGC-O2C
29	CE	202	PEB	CAB-CBB-CGB-O2B
29	FE	202	PEB	CAC-CBC-CGC-O2C
29	LE	202	PEB	CAC-CBC-CGC-O2C
29	AJ	203	PEB	CAC-CBC-CGC-O2C
29	BJ	202	PEB	CAC-CBC-CGC-O2C
29	FJ	202	PEB	CAC-CBC-CGC-O2C
29	HJ	201	PEB	CAC-CBC-CGC-O2C
29	IJ	203	PEB	CAC-CBC-CGC-O2C
29	JJ	202	PEB	CAC-CBC-CGC-O2C
29	NJ	202	PEB	CAC-CBC-CGC-O2C
29	PJ	202	PEB	CAC-CBC-CGC-O2C
29	RJ	202	PEB	CAC-CBC-CGC-O2C
29	TJ	202	PEB	CAC-CBC-CGC-O2C
29	WJ	201	PEB	CAC-CBC-CGC-O2C
29	XJ	202	PEB	CAC-CBC-CGC-O2C
29	ZJ	202	PEB	CAC-CBC-CGC-O2C
29	bJ	202	PEB	CAC-CBC-CGC-O2C
29	dJ	202	PEB	CAC-CBC-CGC-O2C
29	fJ	202	PEB	CAC-CBC-CGC-O2C
29	hJ	202	PEB	CAC-CBC-CGC-O2C
29	jJ	202	PEB	CAC-CBC-CGC-O2C
29	nJ	202	PEB	CAC-CBC-CGC-O2C
29	rJ	202	PEB	CAC-CBC-CGC-O2C
29	sJ	203	PEB	CAC-CBC-CGC-O2C
29	uJ	201	PEB	CAC-CBC-CGC-O2C
29	wJ	302	PEB	CAB-CBB-CGB-O1B
29	xJ	302	PEB	CAB-CBB-CGB-O1B
29	AK	302	PEB	CAC-CBC-CGC-O2C
29	AL	203	PEB	CAC-CBC-CGC-O2C
29	BL	202	PEB	CAC-CBC-CGC-O2C
29	FL	202	PEB	CAC-CBC-CGC-O2C
29	HL	201	PEB	CAC-CBC-CGC-O2C
29	IL	203	PEB	CAC-CBC-CGC-O2C
29	JL	202	PEB	CAC-CBC-CGC-O2C
29	NL	202	PEB	CAC-CBC-CGC-O2C
29	PL	202	PEB	CAC-CBC-CGC-O2C
29	RL	202	PEB	CAC-CBC-CGC-O2C
29	TL	202	PEB	CAC-CBC-CGC-O2C
29	WL	201	PEB	CAC-CBC-CGC-O2C
29	XL	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	ZL	202	PEB	CAC-CBC-CGC-O2C
29	bL	202	PEB	CAC-CBC-CGC-O2C
29	dL	202	PEB	CAC-CBC-CGC-O2C
29	fL	202	PEB	CAC-CBC-CGC-O2C
29	hL	202	PEB	CAC-CBC-CGC-O2C
29	jL	202	PEB	CAC-CBC-CGC-O2C
29	nL	202	PEB	CAC-CBC-CGC-O2C
29	rL	202	PEB	CAC-CBC-CGC-O2C
29	sL	203	PEB	CAC-CBC-CGC-O2C
29	uL	201	PEB	CAC-CBC-CGC-O2C
29	xL	302	PEB	CAB-CBB-CGB-O1B
29	NR	203	PEB	CAC-CBC-CGC-O2C
29	PR	202	PEB	CAC-CBC-CGC-O2C
29	RR	203	PEB	CAC-CBC-CGC-O2C
29	TR	203	PEB	CAC-CBC-CGC-O2C
29	VR	203	PEB	CAC-CBC-CGC-O2C
29	XR	203	PEB	CAC-CBC-CGC-O2C
30	A1	305	PUB	C1C-C2C-CAC-CBC
30	AK	305	PUB	C1C-C2C-CAC-CBC
29	OF	202	PEB	C2A-C3A-CAA-CBA
29	QF	202	PEB	C2A-C3A-CAA-CBA
29	SF	202	PEB	C2A-C3A-CAA-CBA
29	UF	203	PEB	C2A-C3A-CAA-CBA
29	WF	202	PEB	C2A-C3A-CAA-CBA
29	ZF	202	PEB	C2A-C3A-CAA-CBA
29	bF	202	PEB	C2A-C3A-CAA-CBA
29	dF	203	PEB	C2A-C3A-CAA-CBA
29	fF	202	PEB	C2A-C3A-CAA-CBA
29	hF	202	PEB	C2A-C3A-CAA-CBA
29	jF	202	PEB	C2A-C3A-CAA-CBA
29	lF	202	PEB	C2A-C3A-CAA-CBA
29	OI	202	PEB	C2A-C3A-CAA-CBA
29	QI	202	PEB	C2A-C3A-CAA-CBA
29	SI	202	PEB	C2A-C3A-CAA-CBA
29	UI	203	PEB	C2A-C3A-CAA-CBA
29	WI	202	PEB	C2A-C3A-CAA-CBA
29	ZI	202	PEB	C2A-C3A-CAA-CBA
29	bI	202	PEB	C2A-C3A-CAA-CBA
29	dI	203	PEB	C2A-C3A-CAA-CBA
29	fI	202	PEB	C2A-C3A-CAA-CBA
29	hI	202	PEB	C2A-C3A-CAA-CBA
29	jI	202	PEB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	I1	202	PEB	C2A-C3A-CAA-CBA
31	C7	1001	CYC	C2C-C3C-CAC-CBC
31	E7	1001	CYC	C2C-C3C-CAC-CBC
31	G7	1001	CYC	C2C-C3C-CAC-CBC
31	I7	1001	CYC	C2C-C3C-CAC-CBC
31	K7	1001	CYC	C2C-C3C-CAC-CBC
31	M7	1001	CYC	C2C-C3C-CAC-CBC
31	C9	1001	CYC	C2C-C3C-CAC-CBC
31	E9	1001	CYC	C2C-C3C-CAC-CBC
31	G9	1001	CYC	C2C-C3C-CAC-CBC
31	I9	1001	CYC	C2C-C3C-CAC-CBC
31	K9	1001	CYC	C2C-C3C-CAC-CBC
31	M9	1001	CYC	C2C-C3C-CAC-CBC
29	O1	201	PEB	CAB-CBB-CGB-O2B
29	Q1	201	PEB	CAB-CBB-CGB-O2B
29	S1	201	PEB	CAB-CBB-CGB-O2B
29	U1	202	PEB	CAB-CBB-CGB-O2B
29	W1	201	PEB	CAB-CBB-CGB-O2B
29	Z1	202	PEB	CAB-CBB-CGB-O2B
29	b1	201	PEB	CAB-CBB-CGB-O2B
29	d1	201	PEB	CAB-CBB-CGB-O2B
29	f1	201	PEB	CAB-CBB-CGB-O2B
29	h1	201	PEB	CAB-CBB-CGB-O2B
29	j1	201	PEB	CAB-CBB-CGB-O2B
29	l1	201	PEB	CAB-CBB-CGB-O2B
29	M2	202	PEB	CAB-CBB-CGB-O1B
29	O2	202	PEB	CAB-CBB-CGB-O1B
29	Q2	202	PEB	CAB-CBB-CGB-O1B
29	U2	202	PEB	CAB-CBB-CGB-O1B
29	W2	202	PEB	CAB-CBB-CGB-O1B
29	A3	202	PEB	CAC-CBC-CGC-O1C
29	C3	202	PEB	CAC-CBC-CGC-O1C
29	E3	202	PEB	CAC-CBC-CGC-O1C
29	G3	202	PEB	CAC-CBC-CGC-O1C
29	I3	202	PEB	CAC-CBC-CGC-O1C
29	K3	202	PEB	CAC-CBC-CGC-O1C
29	B4	201	PEB	CAB-CBB-CGB-O2B
29	D4	201	PEB	CAB-CBB-CGB-O2B
29	F4	201	PEB	CAB-CBB-CGB-O2B
29	H4	201	PEB	CAB-CBB-CGB-O2B
29	J4	201	PEB	CAB-CBB-CGB-O2B
29	L4	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	I5	201	PEB	CAB-CBB-CGB-O2B
29	K5	201	PEB	CAB-CBB-CGB-O2B
29	A5	201	PEB	CAB-CBB-CGB-O2B
29	C5	201	PEB	CAB-CBB-CGB-O2B
29	I8	201	PEB	CAB-CBB-CGB-O2B
29	K8	201	PEB	CAB-CBB-CGB-O2B
29	A8	201	PEB	CAB-CBB-CGB-O2B
29	C8	201	PEB	CAB-CBB-CGB-O2B
29	BA	203	PEB	CAB-CBB-CGB-O2B
29	DA	203	PEB	CAB-CBB-CGB-O2B
29	HA	203	PEB	CAB-CBB-CGB-O2B
29	JA	203	PEB	CAB-CBB-CGB-O2B
29	AB	302	PEB	CAC-CBC-CGC-O2C
29	SB	202	PEB	CAB-CBB-CGB-O2B
29	IC	202	PEB	CAB-CBB-CGB-O2B
29	BD	201	PEB	CAB-CBB-CGB-O2B
29	DD	201	PEB	CAB-CBB-CGB-O2B
29	FD	201	PEB	CAB-CBB-CGB-O2B
29	HD	201	PEB	CAB-CBB-CGB-O2B
29	JD	201	PEB	CAB-CBB-CGB-O2B
29	LD	201	PEB	CAB-CBB-CGB-O2B
29	IE	202	PEB	CAB-CBB-CGB-O2B
29	TF	201	PEB	CAC-CBC-CGC-O2C
29	AG	202	PEB	CAB-CBB-CGB-O2B
29	EG	202	PEB	CAB-CBB-CGB-O2B
29	GG	202	PEB	CAB-CBB-CGB-O2B
29	IG	202	PEB	CAB-CBB-CGB-O2B
29	IJ	202	PEB	CAC-CBC-CGC-O2C
29	pJ	202	PEB	CAC-CBC-CGC-O2C
29	OK	201	PEB	CAB-CBB-CGB-O2B
29	QK	201	PEB	CAB-CBB-CGB-O2B
29	SK	201	PEB	CAB-CBB-CGB-O2B
29	UK	202	PEB	CAB-CBB-CGB-O2B
29	WK	201	PEB	CAB-CBB-CGB-O2B
29	ZK	202	PEB	CAB-CBB-CGB-O2B
29	bK	201	PEB	CAB-CBB-CGB-O2B
29	dK	201	PEB	CAB-CBB-CGB-O2B
29	fK	201	PEB	CAB-CBB-CGB-O2B
29	hK	201	PEB	CAB-CBB-CGB-O2B
29	jK	201	PEB	CAB-CBB-CGB-O2B
29	lK	201	PEB	CAB-CBB-CGB-O2B
29	lL	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	pL	202	PEB	CAC-CBC-CGC-O2C
29	AM	302	PEB	CAC-CBC-CGC-O2C
29	SM	202	PEB	CAB-CBB-CGB-O2B
29	BN	203	PEB	CAB-CBB-CGB-O2B
29	DN	203	PEB	CAB-CBB-CGB-O2B
29	HN	203	PEB	CAB-CBB-CGB-O2B
29	JN	203	PEB	CAB-CBB-CGB-O2B
29	AO	202	PEB	CAC-CBC-CGC-O1C
29	CO	202	PEB	CAC-CBC-CGC-O1C
29	EO	202	PEB	CAC-CBC-CGC-O1C
29	GO	202	PEB	CAC-CBC-CGC-O1C
29	IO	202	PEB	CAC-CBC-CGC-O1C
29	KO	202	PEB	CAC-CBC-CGC-O1C
29	AQ	202	PEB	CAB-CBB-CGB-O2B
29	EQ	202	PEB	CAB-CBB-CGB-O2B
29	GQ	202	PEB	CAB-CBB-CGB-O2B
29	IQ	202	PEB	CAB-CBB-CGB-O2B
29	UR	202	PEB	CAB-CBB-CGB-O1B
31	AP	1001	CYC	CAA-CBA-CGA-O2A
31	CP	1001	CYC	CAA-CBA-CGA-O2A
31	EP	1001	CYC	CAA-CBA-CGA-O2A
31	GP	1001	CYC	CAA-CBA-CGA-O2A
31	JP	1001	CYC	CAA-CBA-CGA-O2A
31	KP	1001	CYC	CAA-CBA-CGA-O2A
31	NP	1001	CYC	CAA-CBA-CGA-O2A
31	PP	1001	CYC	CAA-CBA-CGA-O2A
31	RP	1001	CYC	CAA-CBA-CGA-O2A
31	TP	1001	CYC	CAA-CBA-CGA-O2A
31	cP	1001	CYC	CAA-CBA-CGA-O2A
31	eP	1001	CYC	CAA-CBA-CGA-O2A
31	gP	1001	CYC	CAA-CBA-CGA-O2A
31	iP	1001	CYC	CAA-CBA-CGA-O2A
31	lP	1001	CYC	CAA-CBA-CGA-O2A
31	pP	1001	CYC	CAA-CBA-CGA-O2A
31	rP	1001	CYC	CAA-CBA-CGA-O2A
31	tP	1001	CYC	CAA-CBA-CGA-O2A
29	A1	303	PEB	CAB-CBB-CGB-O2B
29	R1	203	PEB	CAB-CBB-CGB-O2B
29	Y1	202	PEB	CAB-CBB-CGB-O2B
29	a1	203	PEB	CAB-CBB-CGB-O2B
29	c1	203	PEB	CAB-CBB-CGB-O2B
29	i1	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	S2	202	PEB	CAB-CBB-CGB-O1B
29	M3	203	PEB	CAC-CBC-CGC-O1C
29	N3	203	PEB	CAC-CBC-CGC-O1C
29	N3	203	PEB	CAB-CBB-CGB-O2B
29	A7	301	PEB	CAB-CBB-CGB-O1B
29	A9	301	PEB	CAB-CBB-CGB-O1B
29	GB	202	PEB	CAB-CBB-CGB-O2B
29	IB	202	PEB	CAB-CBB-CGB-O2B
29	OB	202	PEB	CAB-CBB-CGB-O2B
29	QB	204	PEB	CAB-CBB-CGB-O2B
29	dB	202	PEB	CAB-CBB-CGB-O2B
29	fB	202	PEB	CAB-CBB-CGB-O2B
29	hB	202	PEB	CAB-CBB-CGB-O2B
29	lB	202	PEB	CAB-CBB-CGB-O2B
29	AC	202	PEB	CAC-CBC-CGC-O2C
29	AC	202	PEB	CAB-CBB-CGB-O2B
29	CC	202	PEB	CAC-CBC-CGC-O2C
29	EC	202	PEB	CAC-CBC-CGC-O2C
29	EC	202	PEB	CAB-CBB-CGB-O2B
29	GC	202	PEB	CAC-CBC-CGC-O2C
29	IC	202	PEB	CAC-CBC-CGC-O2C
29	KC	203	PEB	CAC-CBC-CGC-O2C
29	KC	203	PEB	CAB-CBB-CGB-O2B
29	AE	202	PEB	CAC-CBC-CGC-O2C
29	AE	202	PEB	CAB-CBB-CGB-O2B
29	CE	202	PEB	CAC-CBC-CGC-O2C
29	EE	202	PEB	CAC-CBC-CGC-O2C
29	EE	202	PEB	CAB-CBB-CGB-O2B
29	GE	202	PEB	CAC-CBC-CGC-O2C
29	IE	202	PEB	CAC-CBC-CGC-O2C
29	KE	203	PEB	CAC-CBC-CGC-O2C
29	KE	203	PEB	CAB-CBB-CGB-O2B
29	CG	202	PEB	CAB-CBB-CGB-O2B
29	KG	202	PEB	CAB-CBB-CGB-O2B
29	AK	303	PEB	CAB-CBB-CGB-O2B
29	RK	203	PEB	CAB-CBB-CGB-O2B
29	YK	202	PEB	CAB-CBB-CGB-O2B
29	aK	203	PEB	CAB-CBB-CGB-O2B
29	cK	203	PEB	CAB-CBB-CGB-O2B
29	iK	203	PEB	CAB-CBB-CGB-O2B
29	GM	202	PEB	CAB-CBB-CGB-O2B
29	IM	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	OM	202	PEB	CAB-CBB-CGB-O2B
29	QM	204	PEB	CAB-CBB-CGB-O2B
29	dM	202	PEB	CAB-CBB-CGB-O2B
29	fM	202	PEB	CAB-CBB-CGB-O2B
29	hM	202	PEB	CAB-CBB-CGB-O2B
29	lM	202	PEB	CAB-CBB-CGB-O2B
29	MO	203	PEB	CAC-CBC-CGC-O1C
29	NO	203	PEB	CAC-CBC-CGC-O1C
29	CQ	202	PEB	CAB-CBB-CGB-O2B
29	KQ	202	PEB	CAB-CBB-CGB-O2B
30	MA	402	PUB	CAB-CBB-CGB-O2B
30	MN	402	PUB	CAB-CBB-CGB-O2B
31	WP	1001	CYC	CAA-CBA-CGA-O2A
31	mP	1001	CYC	CAA-CBA-CGA-O2A
31	vP	1001	CYC	CAA-CBA-CGA-O2A
29	V1	203	PEB	CAB-CBB-CGB-O2B
29	e1	203	PEB	CAB-CBB-CGB-O2B
29	k1	203	PEB	CAB-CBB-CGB-O2B
29	m1	202	PEB	CAB-CBB-CGB-O2B
29	M3	203	PEB	CAB-CBB-CGB-O2B
29	C4	201	PEB	CAB-CBB-CGB-O1B
29	E4	201	PEB	CAB-CBB-CGB-O1B
29	G4	201	PEB	CAB-CBB-CGB-O1B
29	I4	201	PEB	CAB-CBB-CGB-O1B
29	K4	201	PEB	CAB-CBB-CGB-O1B
29	M4	201	PEB	CAB-CBB-CGB-O1B
29	O7	201	PEB	CAC-CBC-CGC-O1C
29	O7	201	PEB	CAB-CBB-CGB-O1B
29	P7	202	PEB	CAB-CBB-CGB-O1B
29	Q7	201	PEB	CAC-CBC-CGC-O1C
29	R7	202	PEB	CAB-CBB-CGB-O1B
29	S7	201	PEB	CAC-CBC-CGC-O1C
29	S7	201	PEB	CAB-CBB-CGB-O1B
29	T7	202	PEB	CAB-CBB-CGB-O1B
29	U7	201	PEB	CAC-CBC-CGC-O1C
29	V7	202	PEB	CAB-CBB-CGB-O1B
29	W7	201	PEB	CAC-CBC-CGC-O1C
29	Y7	202	PEB	CAB-CBB-CGB-O1B
29	Z7	201	PEB	CAC-CBC-CGC-O1C
29	a7	202	PEB	CAB-CBB-CGB-O1B
29	b7	201	PEB	CAC-CBC-CGC-O1C
29	c7	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	d7	201	PEB	CAC-CBC-CGC-O1C
29	e7	202	PEB	CAB-CBB-CGB-O1B
29	f7	201	PEB	CAC-CBC-CGC-O1C
29	g7	202	PEB	CAB-CBB-CGB-O1B
29	h7	201	PEB	CAC-CBC-CGC-O1C
29	i7	202	PEB	CAB-CBB-CGB-O1B
29	j7	201	PEB	CAC-CBC-CGC-O1C
29	j7	201	PEB	CAB-CBB-CGB-O1B
29	k7	202	PEB	CAB-CBB-CGB-O1B
29	l7	201	PEB	CAC-CBC-CGC-O1C
29	l7	201	PEB	CAB-CBB-CGB-O1B
29	m7	202	PEB	CAB-CBB-CGB-O1B
29	O9	201	PEB	CAC-CBC-CGC-O1C
29	O9	201	PEB	CAB-CBB-CGB-O1B
29	P9	202	PEB	CAB-CBB-CGB-O1B
29	Q9	201	PEB	CAC-CBC-CGC-O1C
29	R9	202	PEB	CAB-CBB-CGB-O1B
29	S9	201	PEB	CAC-CBC-CGC-O1C
29	S9	201	PEB	CAB-CBB-CGB-O1B
29	T9	202	PEB	CAB-CBB-CGB-O1B
29	U9	201	PEB	CAC-CBC-CGC-O1C
29	V9	202	PEB	CAB-CBB-CGB-O1B
29	W9	201	PEB	CAC-CBC-CGC-O1C
29	Y9	202	PEB	CAB-CBB-CGB-O1B
29	Z9	201	PEB	CAC-CBC-CGC-O1C
29	a9	202	PEB	CAB-CBB-CGB-O1B
29	b9	201	PEB	CAC-CBC-CGC-O1C
29	c9	202	PEB	CAB-CBB-CGB-O1B
29	d9	201	PEB	CAC-CBC-CGC-O1C
29	e9	202	PEB	CAB-CBB-CGB-O1B
29	f9	201	PEB	CAC-CBC-CGC-O1C
29	g9	202	PEB	CAB-CBB-CGB-O1B
29	h9	201	PEB	CAC-CBC-CGC-O1C
29	i9	202	PEB	CAB-CBB-CGB-O1B
29	j9	201	PEB	CAC-CBC-CGC-O1C
29	j9	201	PEB	CAB-CBB-CGB-O1B
29	k9	202	PEB	CAB-CBB-CGB-O1B
29	l9	201	PEB	CAC-CBC-CGC-O1C
29	l9	201	PEB	CAB-CBB-CGB-O1B
29	m9	202	PEB	CAB-CBB-CGB-O1B
29	FA	203	PEB	CAB-CBB-CGB-O2B
29	LA	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	CB	202	PEB	CAB-CBB-CGB-O2B
29	EB	202	PEB	CAB-CBB-CGB-O2B
29	KB	202	PEB	CAB-CBB-CGB-O2B
29	MB	202	PEB	CAB-CBB-CGB-O2B
29	UB	202	PEB	CAB-CBB-CGB-O2B
29	WB	202	PEB	CAB-CBB-CGB-O2B
29	YB	203	PEB	CAB-CBB-CGB-O2B
29	aB	202	PEB	CAB-CBB-CGB-O2B
29	jB	202	PEB	CAB-CBB-CGB-O2B
29	GC	202	PEB	CAB-CBB-CGB-O2B
29	dD	401	PEB	CAB-CBB-CGB-O1B
29	CD	201	PEB	CAB-CBB-CGB-O1B
29	GD	201	PEB	CAB-CBB-CGB-O1B
29	ID	201	PEB	CAB-CBB-CGB-O1B
29	KD	201	PEB	CAB-CBB-CGB-O1B
29	MD	201	PEB	CAB-CBB-CGB-O1B
29	GE	202	PEB	CAB-CBB-CGB-O2B
29	PF	201	PEB	CAB-CBB-CGB-O1B
29	RF	201	PEB	CAB-CBB-CGB-O1B
29	VF	201	PEB	CAB-CBB-CGB-O1B
29	YF	201	PEB	CAB-CBB-CGB-O1B
29	aF	201	PEB	CAB-CBB-CGB-O1B
29	cF	201	PEB	CAB-CBB-CGB-O1B
29	eF	201	PEB	CAB-CBB-CGB-O1B
29	gF	201	PEB	CAB-CBB-CGB-O1B
29	iF	201	PEB	CAB-CBB-CGB-O1B
29	kF	201	PEB	CAB-CBB-CGB-O1B
29	mF	201	PEB	CAB-CBB-CGB-O1B
29	CG	202	PEB	CAC-CBC-CGC-O2C
29	PI	201	PEB	CAB-CBB-CGB-O1B
29	RI	201	PEB	CAB-CBB-CGB-O1B
29	TI	201	PEB	CAB-CBB-CGB-O1B
29	VI	201	PEB	CAB-CBB-CGB-O1B
29	YI	201	PEB	CAB-CBB-CGB-O1B
29	aI	201	PEB	CAB-CBB-CGB-O1B
29	cI	201	PEB	CAB-CBB-CGB-O1B
29	eI	201	PEB	CAB-CBB-CGB-O1B
29	gI	201	PEB	CAB-CBB-CGB-O1B
29	iI	201	PEB	CAB-CBB-CGB-O1B
29	kI	201	PEB	CAB-CBB-CGB-O1B
29	mI	201	PEB	CAB-CBB-CGB-O1B
29	VK	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	eK	203	PEB	CAB-CBB-CGB-O2B
29	kK	203	PEB	CAB-CBB-CGB-O2B
29	mK	202	PEB	CAB-CBB-CGB-O2B
29	CM	202	PEB	CAB-CBB-CGB-O2B
29	EM	202	PEB	CAB-CBB-CGB-O2B
29	KM	202	PEB	CAB-CBB-CGB-O2B
29	MM	202	PEB	CAB-CBB-CGB-O2B
29	WM	202	PEB	CAB-CBB-CGB-O2B
29	YM	203	PEB	CAB-CBB-CGB-O2B
29	aM	202	PEB	CAB-CBB-CGB-O2B
29	jM	202	PEB	CAB-CBB-CGB-O2B
29	FN	203	PEB	CAB-CBB-CGB-O2B
29	LN	203	PEB	CAB-CBB-CGB-O2B
29	MO	203	PEB	CAB-CBB-CGB-O2B
29	NO	203	PEB	CAB-CBB-CGB-O2B
29	CQ	202	PEB	CAC-CBC-CGC-O2C
29	MQ	401	PEB	CAB-CBB-CGB-O2B
29	QR	202	PEB	CAB-CBB-CGB-O1B
29	SR	202	PEB	CAB-CBB-CGB-O1B
29	WR	202	PEB	CAB-CBB-CGB-O1B
31	AP	1001	CYC	CAA-CBA-CGA-O1A
31	EP	1001	CYC	CAA-CBA-CGA-O1A
31	GP	1001	CYC	CAA-CBA-CGA-O1A
31	JP	1001	CYC	CAA-CBA-CGA-O1A
31	KP	1001	CYC	CAA-CBA-CGA-O1A
31	PP	1001	CYC	CAA-CBA-CGA-O1A
31	TP	1001	CYC	CAA-CBA-CGA-O1A
31	WP	1001	CYC	CAD-CBD-CGD-O2D
31	cP	1001	CYC	CAA-CBA-CGA-O1A
31	eP	1001	CYC	CAA-CBA-CGA-O1A
31	mP	1001	CYC	CAA-CBA-CGA-O1A
31	pP	1001	CYC	CAA-CBA-CGA-O1A
31	yP	1001	CYC	CAA-CBA-CGA-O2A
31	yP	1001	CYC	CAD-CBD-CGD-O2D
29	P1	203	PEB	CAB-CBB-CGB-O2B
29	T1	202	PEB	CAB-CBB-CGB-O2B
29	g1	203	PEB	CAB-CBB-CGB-O2B
29	Q7	201	PEB	CAB-CBB-CGB-O1B
29	U7	201	PEB	CAB-CBB-CGB-O1B
29	W7	201	PEB	CAB-CBB-CGB-O1B
29	Z7	201	PEB	CAB-CBB-CGB-O1B
29	b7	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	d7	201	PEB	CAB-CBB-CGB-O1B
29	f7	201	PEB	CAB-CBB-CGB-O1B
29	h7	201	PEB	CAB-CBB-CGB-O1B
29	Q9	201	PEB	CAB-CBB-CGB-O1B
29	U9	201	PEB	CAB-CBB-CGB-O1B
29	W9	201	PEB	CAB-CBB-CGB-O1B
29	Z9	201	PEB	CAB-CBB-CGB-O1B
29	b9	201	PEB	CAB-CBB-CGB-O1B
29	d9	201	PEB	CAB-CBB-CGB-O1B
29	f9	201	PEB	CAB-CBB-CGB-O1B
29	h9	201	PEB	CAB-CBB-CGB-O1B
29	AG	202	PEB	CAC-CBC-CGC-O2C
29	EG	202	PEB	CAC-CBC-CGC-O2C
29	GG	202	PEB	CAC-CBC-CGC-O2C
29	KG	202	PEB	CAC-CBC-CGC-O2C
29	MG	404	PEB	CAC-CBC-CGC-O2C
29	BJ	201	PEB	CAB-CBB-CGB-O2B
29	DJ	201	PEB	CAB-CBB-CGB-O2B
29	FJ	201	PEB	CAB-CBB-CGB-O2B
29	JJ	201	PEB	CAB-CBB-CGB-O2B
29	LJ	201	PEB	CAB-CBB-CGB-O2B
29	NJ	201	PEB	CAB-CBB-CGB-O2B
29	RJ	201	PEB	CAB-CBB-CGB-O2B
29	TJ	201	PEB	CAB-CBB-CGB-O2B
29	VJ	201	PEB	CAB-CBB-CGB-O2B
29	XJ	201	PEB	CAB-CBB-CGB-O2B
29	ZJ	201	PEB	CAB-CBB-CGB-O2B
29	bJ	201	PEB	CAB-CBB-CGB-O2B
29	dJ	201	PEB	CAB-CBB-CGB-O2B
29	fJ	201	PEB	CAB-CBB-CGB-O2B
29	hJ	201	PEB	CAB-CBB-CGB-O2B
29	jJ	201	PEB	CAB-CBB-CGB-O2B
29	lJ	201	PEB	CAB-CBB-CGB-O2B
29	nJ	201	PEB	CAB-CBB-CGB-O2B
29	pJ	201	PEB	CAB-CBB-CGB-O2B
29	rJ	201	PEB	CAB-CBB-CGB-O2B
29	tJ	201	PEB	CAB-CBB-CGB-O2B
29	vJ	201	PEB	CAB-CBB-CGB-O2B
29	wJ	302	PEB	CAB-CBB-CGB-O2B
29	xJ	302	PEB	CAB-CBB-CGB-O2B
29	PK	203	PEB	CAB-CBB-CGB-O2B
29	TK	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	gK	203	PEB	CAB-CBB-CGB-O2B
29	BL	201	PEB	CAB-CBB-CGB-O2B
29	DL	201	PEB	CAB-CBB-CGB-O2B
29	FL	201	PEB	CAB-CBB-CGB-O2B
29	JL	201	PEB	CAB-CBB-CGB-O2B
29	LL	201	PEB	CAB-CBB-CGB-O2B
29	NL	201	PEB	CAB-CBB-CGB-O2B
29	RL	201	PEB	CAB-CBB-CGB-O2B
29	TL	201	PEB	CAB-CBB-CGB-O2B
29	VL	201	PEB	CAB-CBB-CGB-O2B
29	XL	201	PEB	CAB-CBB-CGB-O2B
29	ZL	201	PEB	CAB-CBB-CGB-O2B
29	bL	201	PEB	CAB-CBB-CGB-O2B
29	dL	201	PEB	CAB-CBB-CGB-O2B
29	fL	201	PEB	CAB-CBB-CGB-O2B
29	hL	201	PEB	CAB-CBB-CGB-O2B
29	jL	201	PEB	CAB-CBB-CGB-O2B
29	lL	201	PEB	CAB-CBB-CGB-O2B
29	nL	201	PEB	CAB-CBB-CGB-O2B
29	pL	201	PEB	CAB-CBB-CGB-O2B
29	rL	201	PEB	CAB-CBB-CGB-O2B
29	tL	201	PEB	CAB-CBB-CGB-O2B
29	vL	201	PEB	CAB-CBB-CGB-O2B
29	zL	501	PEB	CAB-CBB-CGB-O1B
29	AQ	202	PEB	CAC-CBC-CGC-O2C
29	EQ	202	PEB	CAC-CBC-CGC-O2C
29	GQ	202	PEB	CAC-CBC-CGC-O2C
29	KQ	202	PEB	CAC-CBC-CGC-O2C
31	CP	1001	CYC	CAA-CBA-CGA-O1A
29	A1	301	PEB	C4A-C3A-CAA-CBA
29	A7	305	PEB	C4A-C3A-CAA-CBA
29	A9	305	PEB	C4A-C3A-CAA-CBA
29	AK	301	PEB	C4A-C3A-CAA-CBA
29	BB	301	PEB	C3B-CAB-CBB-CGB
29	BM	301	PEB	C3B-CAB-CBB-CGB
29	IG	202	PEB	CAC-CBC-CGC-O2C
29	PJ	201	PEB	CAB-CBB-CGB-O2B
29	PL	201	PEB	CAB-CBB-CGB-O2B
29	IQ	202	PEB	CAC-CBC-CGC-O2C
29	MQ	406	PEB	CAC-CBC-CGC-O2C
30	A7	302	PUB	CAB-CBB-CGB-O1B
30	A9	302	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
31	D7	1001	CYC	CAA-CBA-CGA-O2A
31	F7	1001	CYC	CAA-CBA-CGA-O2A
31	H7	1001	CYC	CAA-CBA-CGA-O2A
31	J7	1001	CYC	CAA-CBA-CGA-O2A
31	L7	1001	CYC	CAA-CBA-CGA-O2A
31	N7	1001	CYC	CAA-CBA-CGA-O2A
31	D9	1001	CYC	CAA-CBA-CGA-O2A
31	F9	1001	CYC	CAA-CBA-CGA-O2A
31	H9	1001	CYC	CAA-CBA-CGA-O2A
31	J9	1001	CYC	CAA-CBA-CGA-O2A
31	L9	1001	CYC	CAA-CBA-CGA-O2A
31	N9	1001	CYC	CAA-CBA-CGA-O2A
31	NP	1001	CYC	CAA-CBA-CGA-O1A
31	RP	1001	CYC	CAA-CBA-CGA-O1A
31	YP	1000	CYC	CAA-CBA-CGA-O2A
31	gP	1001	CYC	CAA-CBA-CGA-O1A
31	iP	1001	CYC	CAA-CBA-CGA-O1A
31	lP	1001	CYC	CAA-CBA-CGA-O1A
31	rP	1001	CYC	CAA-CBA-CGA-O1A
31	tP	1001	CYC	CAA-CBA-CGA-O1A
31	vP	1001	CYC	CAA-CBA-CGA-O1A
29	A1	303	PEB	CAC-CBC-CGC-O2C
29	B5	202	PEB	CAC-CBC-CGC-O2C
29	F5	202	PEB	CAC-CBC-CGC-O2C
29	L5	202	PEB	CAC-CBC-CGC-O2C
29	O7	201	PEB	CAC-CBC-CGC-O2C
29	Q7	201	PEB	CAC-CBC-CGC-O2C
29	S7	201	PEB	CAC-CBC-CGC-O2C
29	U7	201	PEB	CAC-CBC-CGC-O2C
29	W7	201	PEB	CAC-CBC-CGC-O2C
29	Z7	201	PEB	CAC-CBC-CGC-O2C
29	b7	201	PEB	CAC-CBC-CGC-O2C
29	d7	201	PEB	CAC-CBC-CGC-O2C
29	f7	201	PEB	CAC-CBC-CGC-O2C
29	h7	201	PEB	CAC-CBC-CGC-O2C
29	l7	201	PEB	CAC-CBC-CGC-O2C
29	B8	202	PEB	CAC-CBC-CGC-O2C
29	F8	202	PEB	CAC-CBC-CGC-O2C
29	O9	201	PEB	CAC-CBC-CGC-O2C
29	Q9	201	PEB	CAC-CBC-CGC-O2C
29	S9	201	PEB	CAC-CBC-CGC-O2C
29	U9	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	W9	201	PEB	CAC-CBC-CGC-O2C
29	Z9	201	PEB	CAC-CBC-CGC-O2C
29	b9	201	PEB	CAC-CBC-CGC-O2C
29	d9	201	PEB	CAC-CBC-CGC-O2C
29	f9	201	PEB	CAC-CBC-CGC-O2C
29	h9	201	PEB	CAC-CBC-CGC-O2C
29	l9	201	PEB	CAC-CBC-CGC-O2C
29	BA	202	PEB	CAC-CBC-CGC-O2C
29	DA	202	PEB	CAC-CBC-CGC-O2C
29	FA	202	PEB	CAC-CBC-CGC-O2C
29	HA	202	PEB	CAC-CBC-CGC-O2C
29	JA	202	PEB	CAC-CBC-CGC-O2C
29	LA	202	PEB	CAC-CBC-CGC-O2C
29	DF	1002	PEB	CAB-CBB-CGB-O2B
29	FF	1002	PEB	CAB-CBB-CGB-O2B
29	HF	1002	PEB	CAB-CBB-CGB-O2B
29	JF	1002	PEB	CAB-CBB-CGB-O2B
29	LF	1002	PEB	CAB-CBB-CGB-O2B
29	NF	1002	PEB	CAB-CBB-CGB-O2B
29	DG	201	PEB	CAC-CBC-CGC-O1C
29	DI	1002	PEB	CAB-CBB-CGB-O2B
29	FI	1002	PEB	CAB-CBB-CGB-O2B
29	HI	1002	PEB	CAB-CBB-CGB-O2B
29	JI	1002	PEB	CAB-CBB-CGB-O2B
29	LI	1002	PEB	CAB-CBB-CGB-O2B
29	NI	1002	PEB	CAB-CBB-CGB-O2B
29	wJ	301	PEB	CAC-CBC-CGC-O1C
29	AK	303	PEB	CAC-CBC-CGC-O2C
29	wL	302	PEB	CAB-CBB-CGB-O2B
29	xL	301	PEB	CAC-CBC-CGC-O1C
29	xL	302	PEB	CAB-CBB-CGB-O2B
29	BN	202	PEB	CAC-CBC-CGC-O2C
29	DN	202	PEB	CAC-CBC-CGC-O2C
29	FN	202	PEB	CAC-CBC-CGC-O2C
29	HN	202	PEB	CAC-CBC-CGC-O2C
29	JN	202	PEB	CAC-CBC-CGC-O2C
29	LN	202	PEB	CAC-CBC-CGC-O2C
29	DQ	201	PEB	CAC-CBC-CGC-O1C
30	A7	303	PUB	CAB-CBB-CGB-O2B
30	A9	303	PUB	CAB-CBB-CGB-O2B
31	CF	1001	CYC	CAA-CBA-CGA-O2A
31	EF	1001	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	IF	1001	CYC	CAA-CBA-CGA-O2A
31	MF	1001	CYC	CAA-CBA-CGA-O2A
31	CI	1001	CYC	CAA-CBA-CGA-O2A
31	EI	1001	CYC	CAA-CBA-CGA-O2A
31	II	1001	CYC	CAA-CBA-CGA-O2A
31	MI	1001	CYC	CAA-CBA-CGA-O2A
31	1P	1002	CYC	CAA-CBA-CGA-O2A
29	V2	203	PEB	CAC-CBC-CGC-O1C
29	C4	202	PEB	CAB-CBB-CGB-O2B
29	E4	202	PEB	CAB-CBB-CGB-O2B
29	j7	201	PEB	CAC-CBC-CGC-O2C
29	L8	202	PEB	CAC-CBC-CGC-O2C
29	j9	201	PEB	CAC-CBC-CGC-O2C
29	ED	201	PEB	CAB-CBB-CGB-O2B
29	DF	1002	PEB	CAB-CBB-CGB-O1B
29	FF	1002	PEB	CAB-CBB-CGB-O1B
29	JF	1002	PEB	CAB-CBB-CGB-O1B
29	JG	201	PEB	CAC-CBC-CGC-O1C
29	DI	1002	PEB	CAB-CBB-CGB-O1B
29	FI	1002	PEB	CAB-CBB-CGB-O1B
29	JI	1002	PEB	CAB-CBB-CGB-O1B
29	BJ	201	PEB	CAC-CBC-CGC-O2C
29	DJ	201	PEB	CAC-CBC-CGC-O2C
29	FJ	201	PEB	CAC-CBC-CGC-O2C
29	JJ	201	PEB	CAC-CBC-CGC-O2C
29	LJ	201	PEB	CAC-CBC-CGC-O2C
29	NJ	201	PEB	CAC-CBC-CGC-O2C
29	PJ	201	PEB	CAC-CBC-CGC-O2C
29	RJ	201	PEB	CAC-CBC-CGC-O2C
29	TJ	201	PEB	CAC-CBC-CGC-O2C
29	VJ	201	PEB	CAC-CBC-CGC-O2C
29	ZJ	201	PEB	CAC-CBC-CGC-O2C
29	bJ	201	PEB	CAC-CBC-CGC-O2C
29	dJ	201	PEB	CAC-CBC-CGC-O2C
29	fJ	201	PEB	CAC-CBC-CGC-O2C
29	hJ	201	PEB	CAC-CBC-CGC-O2C
29	jJ	201	PEB	CAC-CBC-CGC-O2C
29	lJ	201	PEB	CAC-CBC-CGC-O2C
29	nJ	201	PEB	CAC-CBC-CGC-O2C
29	pJ	201	PEB	CAC-CBC-CGC-O2C
29	rJ	201	PEB	CAC-CBC-CGC-O2C
29	tJ	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	vJ	201	PEB	CAC-CBC-CGC-O2C
29	xJ	301	PEB	CAC-CBC-CGC-O1C
29	BL	201	PEB	CAC-CBC-CGC-O2C
29	DL	201	PEB	CAC-CBC-CGC-O2C
29	FL	201	PEB	CAC-CBC-CGC-O2C
29	JL	201	PEB	CAC-CBC-CGC-O2C
29	LL	201	PEB	CAC-CBC-CGC-O2C
29	NL	201	PEB	CAC-CBC-CGC-O2C
29	PL	201	PEB	CAC-CBC-CGC-O2C
29	RL	201	PEB	CAC-CBC-CGC-O2C
29	TL	201	PEB	CAC-CBC-CGC-O2C
29	VL	201	PEB	CAC-CBC-CGC-O2C
29	ZL	201	PEB	CAC-CBC-CGC-O2C
29	bL	201	PEB	CAC-CBC-CGC-O2C
29	dL	201	PEB	CAC-CBC-CGC-O2C
29	fL	201	PEB	CAC-CBC-CGC-O2C
29	hL	201	PEB	CAC-CBC-CGC-O2C
29	jL	201	PEB	CAC-CBC-CGC-O2C
29	lL	201	PEB	CAC-CBC-CGC-O2C
29	nL	201	PEB	CAC-CBC-CGC-O2C
29	pL	201	PEB	CAC-CBC-CGC-O2C
29	rL	201	PEB	CAC-CBC-CGC-O2C
29	tL	201	PEB	CAC-CBC-CGC-O2C
29	vL	201	PEB	CAC-CBC-CGC-O2C
29	JQ	201	PEB	CAC-CBC-CGC-O1C
30	MA	403	PUB	CAB-CBB-CGB-O2B
30	AF	303	PUB	CAB-CBB-CGB-O2B
30	AI	303	PUB	CAB-CBB-CGB-O2B
30	MN	403	PUB	CAB-CBB-CGB-O2B
31	KF	1001	CYC	CAA-CBA-CGA-O2A
31	KI	1001	CYC	CAA-CBA-CGA-O2A
31	DP	1001	CYC	CAA-CBA-CGA-O1A
31	FP	1001	CYC	CAA-CBA-CGA-O1A
31	MP	1001	CYC	CAA-CBA-CGA-O1A
31	UP	1001	CYC	CAA-CBA-CGA-O1A
31	fP	1001	CYC	CAA-CBA-CGA-O1A
31	jP	1001	CYC	CAA-CBA-CGA-O1A
31	kP	1001	CYC	CAA-CBA-CGA-O1A
31	nP	1001	CYC	CAA-CBA-CGA-O1A
31	qP	1001	CYC	CAA-CBA-CGA-O1A
31	uP	1001	CYC	CAA-CBA-CGA-O1A
31	wP	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	1P	1001	CYC	CAA-CBA-CGA-O1A
30	A7	302	PUB	C2D-C1D-CHC-C4C
30	A9	302	PUB	C2D-C1D-CHC-C4C
29	E4	201	PEB	CAC-CBC-CGC-O1C
29	G5	202	PEB	CAC-CBC-CGC-O2C
29	H5	202	PEB	CAC-CBC-CGC-O2C
29	G8	202	PEB	CAC-CBC-CGC-O2C
29	H8	202	PEB	CAC-CBC-CGC-O2C
29	DC	202	PEB	CAB-CBB-CGB-O2B
29	HC	203	PEB	CAB-CBB-CGB-O2B
29	LC	203	PEB	CAB-CBB-CGB-O2B
29	CD	202	PEB	CAB-CBB-CGB-O2B
29	GD	202	PEB	CAB-CBB-CGB-O2B
29	DE	202	PEB	CAB-CBB-CGB-O2B
29	HE	203	PEB	CAB-CBB-CGB-O2B
29	LE	203	PEB	CAB-CBB-CGB-O2B
29	HF	1002	PEB	CAB-CBB-CGB-O1B
29	LF	1002	PEB	CAB-CBB-CGB-O1B
29	NF	1002	PEB	CAB-CBB-CGB-O1B
29	OF	203	PEB	CAC-CBC-CGC-O1C
29	aF	202	PEB	CAC-CBC-CGC-O1C
29	eF	202	PEB	CAC-CBC-CGC-O1C
29	iF	202	PEB	CAC-CBC-CGC-O1C
29	BG	201	PEB	CAC-CBC-CGC-O1C
29	FG	201	PEB	CAC-CBC-CGC-O1C
29	HG	201	PEB	CAC-CBC-CGC-O1C
29	LG	201	PEB	CAC-CBC-CGC-O1C
29	MG	405	PEB	CAC-CBC-CGC-O1C
29	HI	1002	PEB	CAB-CBB-CGB-O1B
29	LI	1002	PEB	CAB-CBB-CGB-O1B
29	NI	1002	PEB	CAB-CBB-CGB-O1B
29	OI	203	PEB	CAC-CBC-CGC-O1C
29	aI	202	PEB	CAC-CBC-CGC-O1C
29	eI	202	PEB	CAC-CBC-CGC-O1C
29	iI	202	PEB	CAC-CBC-CGC-O1C
29	XJ	201	PEB	CAC-CBC-CGC-O2C
29	zJ	501	PEB	CAB-CBB-CGB-O1B
29	XL	201	PEB	CAC-CBC-CGC-O2C
29	wL	301	PEB	CAC-CBC-CGC-O1C
29	BQ	201	PEB	CAC-CBC-CGC-O1C
29	FQ	201	PEB	CAC-CBC-CGC-O1C
29	HQ	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	MQ	402	PEB	CAC-CBC-CGC-O1C
29	MQ	407	PEB	CAC-CBC-CGC-O1C
29	VR	203	PEB	CAC-CBC-CGC-O1C
30	A1	304	PUB	CAB-CBB-CGB-O1B
30	AF	303	PUB	CAB-CBB-CGB-O1B
30	AI	303	PUB	CAB-CBB-CGB-O1B
30	AK	304	PUB	CAB-CBB-CGB-O1B
31	CF	1001	CYC	CAA-CBA-CGA-O1A
31	EF	1001	CYC	CAA-CBA-CGA-O1A
31	GF	1001	CYC	CAA-CBA-CGA-O2A
31	KF	1001	CYC	CAA-CBA-CGA-O1A
31	CI	1001	CYC	CAA-CBA-CGA-O1A
31	EI	1001	CYC	CAA-CBA-CGA-O1A
31	GI	1001	CYC	CAA-CBA-CGA-O2A
31	KI	1001	CYC	CAA-CBA-CGA-O1A
31	BP	1001	CYC	CAA-CBA-CGA-O1A
31	HP	1001	CYC	CAA-CBA-CGA-O1A
31	IP	1001	CYC	CAA-CBA-CGA-O1A
31	OP	1001	CYC	CAA-CBA-CGA-O1A
31	QP	1001	CYC	CAA-CBA-CGA-O1A
31	SP	1001	CYC	CAA-CBA-CGA-O1A
31	XP	1001	CYC	CAA-CBA-CGA-O1A
31	hP	1001	CYC	CAA-CBA-CGA-O1A
31	oP	1001	CYC	CAA-CBA-CGA-O1A
31	qP	1001	CYC	CAA-CBA-CGA-O2A
31	sP	1001	CYC	CAA-CBA-CGA-O1A
29	N2	203	PEB	CAC-CBC-CGC-O1C
29	P2	202	PEB	CAC-CBC-CGC-O1C
29	R2	203	PEB	CAC-CBC-CGC-O1C
29	T2	203	PEB	CAC-CBC-CGC-O1C
29	X2	202	PEB	CAC-CBC-CGC-O1C
29	M3	201	PEB	CAB-CBB-CGB-O2B
29	C4	201	PEB	CAC-CBC-CGC-O1C
29	G4	201	PEB	CAC-CBC-CGC-O1C
29	G4	202	PEB	CAB-CBB-CGB-O2B
29	I4	201	PEB	CAC-CBC-CGC-O1C
29	I4	202	PEB	CAB-CBB-CGB-O2B
29	K4	201	PEB	CAC-CBC-CGC-O1C
29	K4	202	PEB	CAB-CBB-CGB-O2B
29	M4	201	PEB	CAC-CBC-CGC-O1C
29	M4	202	PEB	CAB-CBB-CGB-O2B
29	F7	1002	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	H7	1002	PEB	CAC-CBC-CGC-O1C
29	J7	1002	PEB	CAC-CBC-CGC-O1C
29	L7	1002	PEB	CAC-CBC-CGC-O1C
29	N7	1002	PEB	CAC-CBC-CGC-O1C
29	O7	202	PEB	CAC-CBC-CGC-O1C
29	Q7	202	PEB	CAC-CBC-CGC-O1C
29	S7	202	PEB	CAC-CBC-CGC-O1C
29	U7	202	PEB	CAC-CBC-CGC-O1C
29	W7	202	PEB	CAC-CBC-CGC-O1C
29	Z7	202	PEB	CAC-CBC-CGC-O1C
29	b7	202	PEB	CAC-CBC-CGC-O1C
29	d7	202	PEB	CAC-CBC-CGC-O1C
29	f7	202	PEB	CAC-CBC-CGC-O1C
29	h7	202	PEB	CAC-CBC-CGC-O1C
29	j7	202	PEB	CAC-CBC-CGC-O1C
29	l7	202	PEB	CAC-CBC-CGC-O1C
29	F9	1002	PEB	CAC-CBC-CGC-O1C
29	H9	1002	PEB	CAC-CBC-CGC-O1C
29	J9	1002	PEB	CAC-CBC-CGC-O1C
29	N9	1002	PEB	CAC-CBC-CGC-O1C
29	O9	202	PEB	CAC-CBC-CGC-O1C
29	Q9	202	PEB	CAC-CBC-CGC-O1C
29	S9	202	PEB	CAC-CBC-CGC-O1C
29	U9	202	PEB	CAC-CBC-CGC-O1C
29	W9	202	PEB	CAC-CBC-CGC-O1C
29	Z9	202	PEB	CAC-CBC-CGC-O1C
29	b9	202	PEB	CAC-CBC-CGC-O1C
29	d9	202	PEB	CAC-CBC-CGC-O1C
29	f9	202	PEB	CAC-CBC-CGC-O1C
29	h9	202	PEB	CAC-CBC-CGC-O1C
29	j9	202	PEB	CAC-CBC-CGC-O1C
29	l9	202	PEB	CAC-CBC-CGC-O1C
29	BC	203	PEB	CAB-CBB-CGB-O2B
29	DC	202	PEB	CAB-CBB-CGB-O1B
29	FC	203	PEB	CAB-CBB-CGB-O1B
29	FC	203	PEB	CAB-CBB-CGB-O2B
29	HC	203	PEB	CAB-CBB-CGB-O1B
29	JC	202	PEB	CAB-CBB-CGB-O1B
29	JC	202	PEB	CAB-CBB-CGB-O2B
29	dD	401	PEB	CAC-CBC-CGC-O1C
29	CD	201	PEB	CAC-CBC-CGC-O1C
29	ID	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	ID	202	PEB	CAB-CBB-CGB-O2B
29	KD	201	PEB	CAC-CBC-CGC-O1C
29	KD	202	PEB	CAB-CBB-CGB-O2B
29	MD	201	PEB	CAC-CBC-CGC-O1C
29	MD	202	PEB	CAB-CBB-CGB-O2B
29	BE	203	PEB	CAB-CBB-CGB-O2B
29	DE	202	PEB	CAB-CBB-CGB-O1B
29	FE	203	PEB	CAB-CBB-CGB-O1B
29	FE	203	PEB	CAB-CBB-CGB-O2B
29	HE	203	PEB	CAB-CBB-CGB-O1B
29	JE	202	PEB	CAB-CBB-CGB-O1B
29	JE	202	PEB	CAB-CBB-CGB-O2B
29	PF	202	PEB	CAC-CBC-CGC-O1C
29	UF	201	PEB	CAC-CBC-CGC-O1C
29	VF	202	PEB	CAC-CBC-CGC-O1C
29	YF	202	PEB	CAC-CBC-CGC-O1C
29	dF	201	PEB	CAC-CBC-CGC-O1C
29	gF	202	PEB	CAC-CBC-CGC-O1C
29	kF	202	PEB	CAC-CBC-CGC-O1C
29	mF	202	PEB	CAC-CBC-CGC-O1C
29	PI	202	PEB	CAC-CBC-CGC-O1C
29	UI	201	PEB	CAC-CBC-CGC-O1C
29	VI	202	PEB	CAC-CBC-CGC-O1C
29	YI	202	PEB	CAC-CBC-CGC-O1C
29	dI	201	PEB	CAC-CBC-CGC-O1C
29	gI	202	PEB	CAC-CBC-CGC-O1C
29	kI	202	PEB	CAC-CBC-CGC-O1C
29	mI	202	PEB	CAC-CBC-CGC-O1C
29	MO	201	PEB	CAB-CBB-CGB-O2B
29	NR	203	PEB	CAC-CBC-CGC-O1C
29	PR	202	PEB	CAC-CBC-CGC-O1C
29	RR	203	PEB	CAC-CBC-CGC-O1C
29	TR	203	PEB	CAC-CBC-CGC-O1C
29	XR	203	PEB	CAC-CBC-CGC-O1C
30	AF	302	PUB	CAB-CBB-CGB-O2B
30	MG	402	PUB	CAB-CBB-CGB-O2B
30	AI	302	PUB	CAB-CBB-CGB-O2B
30	MQ	404	PUB	CAB-CBB-CGB-O2B
31	GF	1001	CYC	CAA-CBA-CGA-O1A
31	IF	1001	CYC	CAA-CBA-CGA-O1A
31	MF	1001	CYC	CAA-CBA-CGA-O1A
31	GI	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	II	1001	CYC	CAA-CBA-CGA-O1A
31	MI	1001	CYC	CAA-CBA-CGA-O1A
31	DP	1001	CYC	CAA-CBA-CGA-O2A
31	FP	1001	CYC	CAA-CBA-CGA-O2A
31	BP	1001	CYC	CAA-CBA-CGA-O2A
31	HP	1001	CYC	CAA-CBA-CGA-O2A
31	IP	1001	CYC	CAA-CBA-CGA-O2A
31	MP	1001	CYC	CAA-CBA-CGA-O2A
31	OP	1001	CYC	CAA-CBA-CGA-O2A
31	QP	1001	CYC	CAA-CBA-CGA-O2A
31	SP	1001	CYC	CAA-CBA-CGA-O2A
31	UP	1001	CYC	CAA-CBA-CGA-O2A
31	XP	1001	CYC	CAA-CBA-CGA-O2A
31	fP	1001	CYC	CAA-CBA-CGA-O2A
31	hP	1001	CYC	CAA-CBA-CGA-O2A
31	jP	1001	CYC	CAA-CBA-CGA-O2A
31	kP	1001	CYC	CAA-CBA-CGA-O2A
31	nP	1001	CYC	CAA-CBA-CGA-O2A
31	oP	1001	CYC	CAA-CBA-CGA-O2A
31	sP	1001	CYC	CAA-CBA-CGA-O2A
31	uP	1001	CYC	CAA-CBA-CGA-O2A
31	wP	1001	CYC	CAA-CBA-CGA-O2A
31	lP	1001	CYC	CAA-CBA-CGA-O2A
29	N3	201	PEB	CAB-CBB-CGB-O2B
29	K4	201	PEB	CAC-CBC-CGC-O2C
29	U7	202	PEB	CAC-CBC-CGC-O2C
29	L9	1002	PEB	CAC-CBC-CGC-O1C
29	U9	202	PEB	CAC-CBC-CGC-O2C
29	BC	203	PEB	CAB-CBB-CGB-O1B
29	LC	203	PEB	CAB-CBB-CGB-O1B
29	GD	201	PEB	CAC-CBC-CGC-O1C
29	KD	201	PEB	CAC-CBC-CGC-O2C
29	BE	203	PEB	CAB-CBB-CGB-O1B
29	LE	203	PEB	CAB-CBB-CGB-O1B
29	mF	202	PEB	CAC-CBC-CGC-O2C
29	mI	202	PEB	CAC-CBC-CGC-O2C
30	A1	304	PUB	CAB-CBB-CGB-O2B
30	AB	304	PUB	CAB-CBB-CGB-O1B
30	AK	304	PUB	CAB-CBB-CGB-O2B
30	AM	304	PUB	CAB-CBB-CGB-O1B
31	C1	1001	CYC	CAA-CBA-CGA-O2A
31	D1	1003	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	E1	1001	CYC	CAA-CBA-CGA-O2A
31	I1	1001	CYC	CAA-CBA-CGA-O2A
31	K1	1001	CYC	CAA-CBA-CGA-O2A
31	M1	1001	CYC	CAA-CBA-CGA-O2A
31	CK	1001	CYC	CAA-CBA-CGA-O2A
31	EK	1001	CYC	CAA-CBA-CGA-O2A
31	GK	1001	CYC	CAA-CBA-CGA-O2A
31	IK	1001	CYC	CAA-CBA-CGA-O2A
31	KK	1001	CYC	CAA-CBA-CGA-O2A
31	MK	1001	CYC	CAA-CBA-CGA-O2A
29	C4	201	PEB	CAC-CBC-CGC-O2C
29	E4	201	PEB	CAC-CBC-CGC-O2C
29	G4	201	PEB	CAC-CBC-CGC-O2C
29	I4	201	PEB	CAC-CBC-CGC-O2C
29	I4	203	PEB	CAC-CBC-CGC-O1C
29	M4	201	PEB	CAC-CBC-CGC-O2C
29	D7	1002	PEB	CAC-CBC-CGC-O1C
29	O7	202	PEB	CAC-CBC-CGC-O2C
29	Q7	202	PEB	CAC-CBC-CGC-O2C
29	S7	202	PEB	CAC-CBC-CGC-O2C
29	W7	202	PEB	CAC-CBC-CGC-O2C
29	Z7	202	PEB	CAC-CBC-CGC-O2C
29	b7	202	PEB	CAC-CBC-CGC-O2C
29	d7	202	PEB	CAC-CBC-CGC-O2C
29	f7	202	PEB	CAC-CBC-CGC-O2C
29	h7	202	PEB	CAC-CBC-CGC-O2C
29	j7	202	PEB	CAC-CBC-CGC-O2C
29	l7	202	PEB	CAC-CBC-CGC-O2C
29	D9	1002	PEB	CAC-CBC-CGC-O1C
29	O9	202	PEB	CAC-CBC-CGC-O2C
29	Q9	202	PEB	CAC-CBC-CGC-O2C
29	S9	202	PEB	CAC-CBC-CGC-O2C
29	W9	202	PEB	CAC-CBC-CGC-O2C
29	Z9	202	PEB	CAC-CBC-CGC-O2C
29	b9	202	PEB	CAC-CBC-CGC-O2C
29	d9	202	PEB	CAC-CBC-CGC-O2C
29	f9	202	PEB	CAC-CBC-CGC-O2C
29	h9	202	PEB	CAC-CBC-CGC-O2C
29	j9	202	PEB	CAC-CBC-CGC-O2C
29	l9	202	PEB	CAC-CBC-CGC-O2C
29	dD	401	PEB	CAC-CBC-CGC-O2C
29	CD	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	GD	201	PEB	CAC-CBC-CGC-O2C
29	ID	201	PEB	CAC-CBC-CGC-O2C
29	MD	201	PEB	CAC-CBC-CGC-O2C
29	VF	202	PEB	CAC-CBC-CGC-O2C
29	VI	202	PEB	CAC-CBC-CGC-O2C
29	NO	201	PEB	CAB-CBB-CGB-O2B
30	A7	303	PUB	CAB-CBB-CGB-O1B
30	A9	303	PUB	CAB-CBB-CGB-O1B
29	N2	203	PEB	CAB-CBB-CGB-O1B
29	R2	203	PEB	CAB-CBB-CGB-O1B
29	V2	203	PEB	CAB-CBB-CGB-O1B
29	X2	202	PEB	CAB-CBB-CGB-O1B
29	OF	203	PEB	CAC-CBC-CGC-O2C
29	PF	202	PEB	CAC-CBC-CGC-O2C
29	UF	201	PEB	CAC-CBC-CGC-O2C
29	YF	202	PEB	CAC-CBC-CGC-O2C
29	aF	202	PEB	CAC-CBC-CGC-O2C
29	dF	201	PEB	CAC-CBC-CGC-O2C
29	eF	202	PEB	CAC-CBC-CGC-O2C
29	gF	202	PEB	CAC-CBC-CGC-O2C
29	iF	202	PEB	CAC-CBC-CGC-O2C
29	kF	202	PEB	CAC-CBC-CGC-O2C
29	MG	401	PEB	CAC-CBC-CGC-O1C
29	MG	405	PEB	CAC-CBC-CGC-O2C
29	OI	203	PEB	CAC-CBC-CGC-O2C
29	PI	202	PEB	CAC-CBC-CGC-O2C
29	UI	201	PEB	CAC-CBC-CGC-O2C
29	YI	202	PEB	CAC-CBC-CGC-O2C
29	aI	202	PEB	CAC-CBC-CGC-O2C
29	dI	201	PEB	CAC-CBC-CGC-O2C
29	eI	202	PEB	CAC-CBC-CGC-O2C
29	gI	202	PEB	CAC-CBC-CGC-O2C
29	iI	202	PEB	CAC-CBC-CGC-O2C
29	kI	202	PEB	CAC-CBC-CGC-O2C
29	MQ	403	PEB	CAC-CBC-CGC-O1C
29	MQ	407	PEB	CAC-CBC-CGC-O2C
29	PR	202	PEB	CAB-CBB-CGB-O1B
29	RR	203	PEB	CAB-CBB-CGB-O1B
29	TR	203	PEB	CAB-CBB-CGB-O1B
29	VR	203	PEB	CAB-CBB-CGB-O1B
29	XR	203	PEB	CAB-CBB-CGB-O1B
30	AF	302	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
30	AI	302	PUB	CAB-CBB-CGB-O1B
29	P2	202	PEB	CAB-CBB-CGB-O1B
29	T2	203	PEB	CAB-CBB-CGB-O1B
29	D4	201	PEB	CAC-CBC-CGC-O1C
29	O7	202	PEB	CAB-CBB-CGB-O1B
29	O7	202	PEB	CAB-CBB-CGB-O2B
29	Q7	202	PEB	CAB-CBB-CGB-O1B
29	S7	202	PEB	CAB-CBB-CGB-O1B
29	S7	202	PEB	CAB-CBB-CGB-O2B
29	U7	202	PEB	CAB-CBB-CGB-O1B
29	U7	202	PEB	CAB-CBB-CGB-O2B
29	W7	202	PEB	CAB-CBB-CGB-O1B
29	W7	202	PEB	CAB-CBB-CGB-O2B
29	Z7	202	PEB	CAB-CBB-CGB-O1B
29	b7	202	PEB	CAB-CBB-CGB-O1B
29	b7	202	PEB	CAB-CBB-CGB-O2B
29	d7	202	PEB	CAB-CBB-CGB-O1B
29	f7	202	PEB	CAB-CBB-CGB-O1B
29	h7	202	PEB	CAB-CBB-CGB-O1B
29	j7	202	PEB	CAB-CBB-CGB-O1B
29	j7	202	PEB	CAB-CBB-CGB-O2B
29	l7	202	PEB	CAB-CBB-CGB-O1B
29	O9	202	PEB	CAB-CBB-CGB-O1B
29	O9	202	PEB	CAB-CBB-CGB-O2B
29	Q9	202	PEB	CAB-CBB-CGB-O1B
29	S9	202	PEB	CAB-CBB-CGB-O1B
29	S9	202	PEB	CAB-CBB-CGB-O2B
29	U9	202	PEB	CAB-CBB-CGB-O1B
29	U9	202	PEB	CAB-CBB-CGB-O2B
29	W9	202	PEB	CAB-CBB-CGB-O1B
29	W9	202	PEB	CAB-CBB-CGB-O2B
29	Z9	202	PEB	CAB-CBB-CGB-O1B
29	b9	202	PEB	CAB-CBB-CGB-O1B
29	b9	202	PEB	CAB-CBB-CGB-O2B
29	d9	202	PEB	CAB-CBB-CGB-O1B
29	f9	202	PEB	CAB-CBB-CGB-O1B
29	h9	202	PEB	CAB-CBB-CGB-O1B
29	j9	202	PEB	CAB-CBB-CGB-O1B
29	j9	202	PEB	CAB-CBB-CGB-O2B
29	l9	202	PEB	CAB-CBB-CGB-O1B
29	AB	303	PEB	CAB-CBB-CGB-O2B
29	NR	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	O1	201	PEB	CAB-CBB-CGB-01B
29	S1	201	PEB	CAB-CBB-CGB-01B
29	U1	202	PEB	CAB-CBB-CGB-01B
29	W1	201	PEB	CAB-CBB-CGB-01B
29	Z1	202	PEB	CAB-CBB-CGB-01B
29	b1	201	PEB	CAB-CBB-CGB-01B
29	f1	201	PEB	CAB-CBB-CGB-01B
29	h1	201	PEB	CAB-CBB-CGB-01B
29	j1	201	PEB	CAB-CBB-CGB-01B
29	l1	201	PEB	CAB-CBB-CGB-01B
29	F4	201	PEB	CAC-CBC-CGC-01C
29	H4	201	PEB	CAC-CBC-CGC-01C
29	J4	201	PEB	CAC-CBC-CGC-01C
29	Q7	202	PEB	CAB-CBB-CGB-02B
29	Z7	202	PEB	CAB-CBB-CGB-02B
29	d7	202	PEB	CAB-CBB-CGB-02B
29	f7	202	PEB	CAB-CBB-CGB-02B
29	h7	202	PEB	CAB-CBB-CGB-02B
29	l7	202	PEB	CAB-CBB-CGB-02B
29	Q9	202	PEB	CAB-CBB-CGB-02B
29	Z9	202	PEB	CAB-CBB-CGB-02B
29	d9	202	PEB	CAB-CBB-CGB-02B
29	f9	202	PEB	CAB-CBB-CGB-02B
29	h9	202	PEB	CAB-CBB-CGB-02B
29	l9	202	PEB	CAB-CBB-CGB-02B
29	AB	302	PEB	CAB-CBB-CGB-02B
29	HB	201	PEB	CAC-CBC-CGC-02C
29	NB	201	PEB	CAC-CBC-CGC-02C
29	VB	201	PEB	CAC-CBC-CGC-02C
29	ZB	201	PEB	CAC-CBC-CGC-02C
29	cB	201	PEB	CAC-CBC-CGC-02C
29	gB	203	PEB	CAB-CBB-CGB-01B
29	iB	201	PEB	CAC-CBC-CGC-02C
29	kB	201	PEB	CAC-CBC-CGC-02C
29	mB	203	PEB	CAB-CBB-CGB-01B
29	DD	201	PEB	CAC-CBC-CGC-01C
29	FD	201	PEB	CAC-CBC-CGC-01C
29	HD	201	PEB	CAC-CBC-CGC-01C
29	ID	202	PEB	CAB-CBB-CGB-01B
29	LD	201	PEB	CAC-CBC-CGC-01C
29	BJ	203	PEB	CAC-CBC-CGC-02C
29	DJ	202	PEB	CAC-CBC-CGC-02C

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Mol	Chain	Res	Type	Atoms
29	FJ	203	PEB	CAC-CBC-CGC-O2C
29	HJ	202	PEB	CAC-CBC-CGC-O2C
29	JJ	203	PEB	CAC-CBC-CGC-O2C
29	LJ	202	PEB	CAC-CBC-CGC-O2C
29	NJ	203	PEB	CAC-CBC-CGC-O2C
29	PJ	203	PEB	CAC-CBC-CGC-O2C
29	RJ	203	PEB	CAC-CBC-CGC-O2C
29	TJ	203	PEB	CAC-CBC-CGC-O2C
29	VJ	202	PEB	CAC-CBC-CGC-O2C
29	XJ	203	PEB	CAC-CBC-CGC-O2C
29	ZJ	203	PEB	CAC-CBC-CGC-O2C
29	dJ	203	PEB	CAC-CBC-CGC-O2C
29	fJ	203	PEB	CAC-CBC-CGC-O2C
29	hJ	203	PEB	CAC-CBC-CGC-O2C
29	jJ	203	PEB	CAC-CBC-CGC-O2C
29	lJ	203	PEB	CAC-CBC-CGC-O2C
29	nJ	203	PEB	CAC-CBC-CGC-O2C
29	pJ	203	PEB	CAC-CBC-CGC-O2C
29	rJ	203	PEB	CAC-CBC-CGC-O2C
29	tJ	202	PEB	CAC-CBC-CGC-O2C
29	vJ	202	PEB	CAC-CBC-CGC-O2C
29	OK	201	PEB	CAB-CBB-CGB-O1B
29	SK	201	PEB	CAB-CBB-CGB-O1B
29	UK	202	PEB	CAB-CBB-CGB-O1B
29	WK	201	PEB	CAB-CBB-CGB-O1B
29	ZK	202	PEB	CAB-CBB-CGB-O1B
29	bK	201	PEB	CAB-CBB-CGB-O1B
29	fK	201	PEB	CAB-CBB-CGB-O1B
29	hK	201	PEB	CAB-CBB-CGB-O1B
29	jK	201	PEB	CAB-CBB-CGB-O1B
29	lK	201	PEB	CAB-CBB-CGB-O1B
29	BL	203	PEB	CAC-CBC-CGC-O2C
29	DL	202	PEB	CAC-CBC-CGC-O2C
29	FL	203	PEB	CAC-CBC-CGC-O2C
29	HL	202	PEB	CAC-CBC-CGC-O2C
29	JL	203	PEB	CAC-CBC-CGC-O2C
29	LL	202	PEB	CAC-CBC-CGC-O2C
29	NL	203	PEB	CAC-CBC-CGC-O2C
29	PL	203	PEB	CAC-CBC-CGC-O2C
29	RL	203	PEB	CAC-CBC-CGC-O2C
29	TL	203	PEB	CAC-CBC-CGC-O2C
29	VL	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	XL	203	PEB	CAC-CBC-CGC-O2C
29	ZL	203	PEB	CAC-CBC-CGC-O2C
29	dL	203	PEB	CAC-CBC-CGC-O2C
29	fL	203	PEB	CAC-CBC-CGC-O2C
29	hL	203	PEB	CAC-CBC-CGC-O2C
29	jL	203	PEB	CAC-CBC-CGC-O2C
29	lL	203	PEB	CAC-CBC-CGC-O2C
29	nL	203	PEB	CAC-CBC-CGC-O2C
29	pL	203	PEB	CAC-CBC-CGC-O2C
29	rL	203	PEB	CAC-CBC-CGC-O2C
29	tL	202	PEB	CAC-CBC-CGC-O2C
29	vL	202	PEB	CAC-CBC-CGC-O2C
29	AM	302	PEB	CAB-CBB-CGB-O2B
29	AM	303	PEB	CAB-CBB-CGB-O2B
29	HM	201	PEB	CAC-CBC-CGC-O2C
29	NM	201	PEB	CAC-CBC-CGC-O2C
29	VM	201	PEB	CAC-CBC-CGC-O2C
29	ZM	201	PEB	CAC-CBC-CGC-O2C
29	cM	201	PEB	CAC-CBC-CGC-O2C
29	gM	203	PEB	CAB-CBB-CGB-O1B
29	iM	201	PEB	CAC-CBC-CGC-O2C
29	kM	201	PEB	CAC-CBC-CGC-O2C
29	mM	203	PEB	CAB-CBB-CGB-O1B
30	MQ	404	PUB	CAB-CBB-CGB-O1B
29	Q1	201	PEB	CAB-CBB-CGB-O1B
29	d1	201	PEB	CAB-CBB-CGB-O1B
29	D3	202	PEB	CAB-CBB-CGB-O1B
29	B4	201	PEB	CAC-CBC-CGC-O1C
29	I4	202	PEB	CAB-CBB-CGB-O1B
29	DB	201	PEB	CAC-CBC-CGC-O2C
29	FB	201	PEB	CAC-CBC-CGC-O2C
29	HB	203	PEB	CAB-CBB-CGB-O1B
29	JB	201	PEB	CAC-CBC-CGC-O2C
29	LB	201	PEB	CAC-CBC-CGC-O2C
29	PB	201	PEB	CAC-CBC-CGC-O2C
29	PB	202	PEB	CAB-CBB-CGB-O1B
29	RB	201	PEB	CAC-CBC-CGC-O2C
29	TB	201	PEB	CAC-CBC-CGC-O2C
29	TB	203	PEB	CAB-CBB-CGB-O1B
29	XB	201	PEB	CAC-CBC-CGC-O2C
29	cB	203	PEB	CAB-CBB-CGB-O1B
29	eB	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	eB	202	PEB	CAB-CBB-CGB-O1B
29	gB	201	PEB	CAC-CBC-CGC-O2C
29	mB	201	PEB	CAC-CBC-CGC-O2C
29	KD	202	PEB	CAB-CBB-CGB-O1B
29	AF	305	PEB	CAC-CBC-CGC-O1C
29	AI	305	PEB	CAC-CBC-CGC-O1C
29	TJ	201	PEB	CAC-CBC-CGC-O1C
29	bJ	203	PEB	CAC-CBC-CGC-O2C
29	QK	201	PEB	CAB-CBB-CGB-O1B
29	dK	201	PEB	CAB-CBB-CGB-O1B
29	TL	201	PEB	CAC-CBC-CGC-O1C
29	bL	203	PEB	CAC-CBC-CGC-O2C
29	DM	201	PEB	CAC-CBC-CGC-O2C
29	FM	201	PEB	CAC-CBC-CGC-O2C
29	HM	203	PEB	CAB-CBB-CGB-O1B
29	JM	201	PEB	CAC-CBC-CGC-O2C
29	LM	201	PEB	CAC-CBC-CGC-O2C
29	PM	201	PEB	CAC-CBC-CGC-O2C
29	PM	202	PEB	CAB-CBB-CGB-O1B
29	RM	201	PEB	CAC-CBC-CGC-O2C
29	TM	201	PEB	CAC-CBC-CGC-O2C
29	TM	203	PEB	CAB-CBB-CGB-O1B
29	XM	201	PEB	CAC-CBC-CGC-O2C
29	cM	203	PEB	CAB-CBB-CGB-O1B
29	eM	201	PEB	CAC-CBC-CGC-O2C
29	eM	202	PEB	CAB-CBB-CGB-O1B
29	gM	201	PEB	CAC-CBC-CGC-O2C
29	mM	201	PEB	CAC-CBC-CGC-O2C
30	MG	402	PUB	CAB-CBB-CGB-O1B
31	VP	1001	CYC	CAD-CBD-CGD-O2D
29	C4	202	PEB	CAB-CBB-CGB-O1B
29	E4	202	PEB	CAB-CBB-CGB-O1B
29	G4	202	PEB	CAB-CBB-CGB-O1B
29	K4	202	PEB	CAB-CBB-CGB-O1B
29	L4	201	PEB	CAC-CBC-CGC-O1C
29	M4	202	PEB	CAB-CBB-CGB-O1B
29	BD	201	PEB	CAC-CBC-CGC-O1C
29	CD	202	PEB	CAB-CBB-CGB-O1B
29	ED	201	PEB	CAB-CBB-CGB-O1B
29	GD	202	PEB	CAB-CBB-CGB-O1B
29	JD	201	PEB	CAC-CBC-CGC-O1C
29	MD	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	DJ	201	PEB	CAB-CBB-CGB-O1B
29	DL	201	PEB	CAB-CBB-CGB-O1B
29	DO	202	PEB	CAB-CBB-CGB-O1B
30	MA	403	PUB	CAC-CBC-CGC-O2C
30	MN	403	PUB	CAC-CBC-CGC-O2C
31	C1	1001	CYC	CAA-CBA-CGA-O1A
31	D1	1003	CYC	CAA-CBA-CGA-O1A
31	E1	1001	CYC	CAA-CBA-CGA-O1A
31	I1	1001	CYC	CAA-CBA-CGA-O1A
31	K1	1001	CYC	CAA-CBA-CGA-O1A
31	M1	1001	CYC	CAA-CBA-CGA-O1A
31	EK	1001	CYC	CAA-CBA-CGA-O1A
31	GK	1001	CYC	CAA-CBA-CGA-O1A
31	IK	1001	CYC	CAA-CBA-CGA-O1A
31	KK	1001	CYC	CAA-CBA-CGA-O1A
31	MK	1001	CYC	CAA-CBA-CGA-O1A
31	xP	1001	CYC	CAD-CBD-CGD-O2D
29	I5	203	PEB	CAC-CBC-CGC-O2C
29	A5	203	PEB	CAC-CBC-CGC-O2C
29	C5	203	PEB	CAC-CBC-CGC-O2C
29	I8	203	PEB	CAC-CBC-CGC-O2C
29	A8	203	PEB	CAC-CBC-CGC-O2C
29	C8	203	PEB	CAC-CBC-CGC-O2C
29	AA	202	PEB	CAB-CBB-CGB-O2B
29	CA	202	PEB	CAB-CBB-CGB-O2B
29	EA	202	PEB	CAB-CBB-CGB-O2B
29	GA	202	PEB	CAB-CBB-CGB-O2B
29	IA	202	PEB	CAB-CBB-CGB-O2B
29	KA	202	PEB	CAB-CBB-CGB-O2B
29	AB	303	PEB	CAB-CBB-CGB-O1B
29	DB	203	PEB	CAB-CBB-CGB-O1B
29	DB	203	PEB	CAB-CBB-CGB-O2B
29	FB	203	PEB	CAB-CBB-CGB-O1B
29	FB	203	PEB	CAB-CBB-CGB-O2B
29	JB	203	PEB	CAB-CBB-CGB-O1B
29	LB	203	PEB	CAB-CBB-CGB-O1B
29	LB	203	PEB	CAB-CBB-CGB-O2B
29	NB	202	PEB	CAB-CBB-CGB-O1B
29	NB	202	PEB	CAB-CBB-CGB-O2B
29	RB	203	PEB	CAB-CBB-CGB-O1B
29	VB	203	PEB	CAB-CBB-CGB-O1B
29	VB	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	XB	202	PEB	CAB-CBB-CGB-O1B
29	ZB	203	PEB	CAB-CBB-CGB-O1B
29	eB	202	PEB	CAB-CBB-CGB-O2B
29	gB	203	PEB	CAB-CBB-CGB-O2B
29	iB	203	PEB	CAB-CBB-CGB-O1B
29	iB	203	PEB	CAB-CBB-CGB-O2B
29	kB	203	PEB	CAB-CBB-CGB-O1B
29	mB	203	PEB	CAB-CBB-CGB-O2B
29	AF	305	PEB	CAC-CBC-CGC-O2C
29	AI	305	PEB	CAC-CBC-CGC-O2C
29	BJ	201	PEB	CAB-CBB-CGB-O1B
29	DJ	201	PEB	CAC-CBC-CGC-O1C
29	FJ	201	PEB	CAC-CBC-CGC-O1C
29	FJ	201	PEB	CAB-CBB-CGB-O1B
29	JJ	201	PEB	CAC-CBC-CGC-O1C
29	JJ	201	PEB	CAB-CBB-CGB-O1B
29	LJ	201	PEB	CAC-CBC-CGC-O1C
29	LJ	201	PEB	CAB-CBB-CGB-O1B
29	NJ	201	PEB	CAC-CBC-CGC-O1C
29	NJ	201	PEB	CAB-CBB-CGB-O1B
29	PJ	201	PEB	CAC-CBC-CGC-O1C
29	PJ	201	PEB	CAB-CBB-CGB-O1B
29	RJ	201	PEB	CAC-CBC-CGC-O1C
29	RJ	201	PEB	CAB-CBB-CGB-O1B
29	TJ	201	PEB	CAB-CBB-CGB-O1B
29	VJ	201	PEB	CAC-CBC-CGC-O1C
29	VJ	201	PEB	CAB-CBB-CGB-O1B
29	XJ	201	PEB	CAC-CBC-CGC-O1C
29	XJ	201	PEB	CAB-CBB-CGB-O1B
29	ZJ	201	PEB	CAC-CBC-CGC-O1C
29	ZJ	201	PEB	CAB-CBB-CGB-O1B
29	bJ	201	PEB	CAC-CBC-CGC-O1C
29	bJ	201	PEB	CAB-CBB-CGB-O1B
29	dJ	201	PEB	CAC-CBC-CGC-O1C
29	dJ	201	PEB	CAB-CBB-CGB-O1B
29	fJ	201	PEB	CAC-CBC-CGC-O1C
29	fJ	201	PEB	CAB-CBB-CGB-O1B
29	hJ	201	PEB	CAC-CBC-CGC-O1C
29	hJ	201	PEB	CAB-CBB-CGB-O1B
29	jJ	201	PEB	CAC-CBC-CGC-O1C
29	jJ	201	PEB	CAB-CBB-CGB-O1B
29	lJ	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	lJ	201	PEB	CAB-CBB-CGB-O1B
29	nJ	201	PEB	CAC-CBC-CGC-O1C
29	nJ	201	PEB	CAB-CBB-CGB-O1B
29	pJ	201	PEB	CAC-CBC-CGC-O1C
29	pJ	201	PEB	CAB-CBB-CGB-O1B
29	rJ	201	PEB	CAC-CBC-CGC-O1C
29	rJ	201	PEB	CAB-CBB-CGB-O1B
29	tJ	201	PEB	CAC-CBC-CGC-O1C
29	tJ	201	PEB	CAB-CBB-CGB-O1B
29	vJ	201	PEB	CAC-CBC-CGC-O1C
29	vJ	201	PEB	CAB-CBB-CGB-O1B
29	BL	201	PEB	CAB-CBB-CGB-O1B
29	DL	201	PEB	CAC-CBC-CGC-O1C
29	FL	201	PEB	CAC-CBC-CGC-O1C
29	FL	201	PEB	CAB-CBB-CGB-O1B
29	JL	201	PEB	CAC-CBC-CGC-O1C
29	JL	201	PEB	CAB-CBB-CGB-O1B
29	LL	201	PEB	CAC-CBC-CGC-O1C
29	LL	201	PEB	CAB-CBB-CGB-O1B
29	NL	201	PEB	CAC-CBC-CGC-O1C
29	NL	201	PEB	CAB-CBB-CGB-O1B
29	PL	201	PEB	CAC-CBC-CGC-O1C
29	PL	201	PEB	CAB-CBB-CGB-O1B
29	RL	201	PEB	CAC-CBC-CGC-O1C
29	RL	201	PEB	CAB-CBB-CGB-O1B
29	TL	201	PEB	CAB-CBB-CGB-O1B
29	VL	201	PEB	CAC-CBC-CGC-O1C
29	VL	201	PEB	CAB-CBB-CGB-O1B
29	XL	201	PEB	CAC-CBC-CGC-O1C
29	XL	201	PEB	CAB-CBB-CGB-O1B
29	ZL	201	PEB	CAC-CBC-CGC-O1C
29	ZL	201	PEB	CAB-CBB-CGB-O1B
29	bL	201	PEB	CAC-CBC-CGC-O1C
29	bL	201	PEB	CAB-CBB-CGB-O1B
29	dL	201	PEB	CAC-CBC-CGC-O1C
29	dL	201	PEB	CAB-CBB-CGB-O1B
29	fL	201	PEB	CAC-CBC-CGC-O1C
29	fL	201	PEB	CAB-CBB-CGB-O1B
29	hL	201	PEB	CAC-CBC-CGC-O1C
29	hL	201	PEB	CAB-CBB-CGB-O1B
29	jL	201	PEB	CAC-CBC-CGC-O1C
29	jL	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	lL	201	PEB	CAC-CBC-CGC-O1C
29	lL	201	PEB	CAB-CBB-CGB-O1B
29	nL	201	PEB	CAC-CBC-CGC-O1C
29	nL	201	PEB	CAB-CBB-CGB-O1B
29	pL	201	PEB	CAC-CBC-CGC-O1C
29	pL	201	PEB	CAB-CBB-CGB-O1B
29	rL	201	PEB	CAC-CBC-CGC-O1C
29	rL	201	PEB	CAB-CBB-CGB-O1B
29	tL	201	PEB	CAC-CBC-CGC-O1C
29	tL	201	PEB	CAB-CBB-CGB-O1B
29	vL	201	PEB	CAC-CBC-CGC-O1C
29	vL	201	PEB	CAB-CBB-CGB-O1B
29	DM	203	PEB	CAB-CBB-CGB-O1B
29	DM	203	PEB	CAB-CBB-CGB-O2B
29	FM	203	PEB	CAB-CBB-CGB-O1B
29	FM	203	PEB	CAB-CBB-CGB-O2B
29	JM	203	PEB	CAB-CBB-CGB-O1B
29	LM	203	PEB	CAB-CBB-CGB-O1B
29	LM	203	PEB	CAB-CBB-CGB-O2B
29	NM	202	PEB	CAB-CBB-CGB-O1B
29	NM	202	PEB	CAB-CBB-CGB-O2B
29	RM	203	PEB	CAB-CBB-CGB-O1B
29	VM	203	PEB	CAB-CBB-CGB-O1B
29	VM	203	PEB	CAB-CBB-CGB-O2B
29	XM	202	PEB	CAB-CBB-CGB-O1B
29	ZM	203	PEB	CAB-CBB-CGB-O1B
29	eM	202	PEB	CAB-CBB-CGB-O2B
29	gM	203	PEB	CAB-CBB-CGB-O2B
29	iM	203	PEB	CAB-CBB-CGB-O1B
29	iM	203	PEB	CAB-CBB-CGB-O2B
29	kM	203	PEB	CAB-CBB-CGB-O1B
29	mM	203	PEB	CAB-CBB-CGB-O2B
29	AN	202	PEB	CAB-CBB-CGB-O2B
29	CN	202	PEB	CAB-CBB-CGB-O2B
29	EN	202	PEB	CAB-CBB-CGB-O2B
29	GN	202	PEB	CAB-CBB-CGB-O2B
29	IN	202	PEB	CAB-CBB-CGB-O2B
29	KN	202	PEB	CAB-CBB-CGB-O2B
30	wL	305	PUB	CAB-CBB-CGB-O2B
31	CK	1001	CYC	CAA-CBA-CGA-O1A
31	YP	1000	CYC	CAD-CBD-CGD-O2D
31	1P	1002	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	K4	203	PEB	CAB-CBB-CGB-01B
29	K5	203	PEB	CAC-CBC-CGC-01C
29	K5	203	PEB	CAC-CBC-CGC-02C
29	K8	203	PEB	CAC-CBC-CGC-01C
29	K8	203	PEB	CAC-CBC-CGC-02C
29	AA	202	PEB	CAB-CBB-CGB-01B
29	CA	202	PEB	CAB-CBB-CGB-01B
29	EA	202	PEB	CAB-CBB-CGB-01B
29	IA	202	PEB	CAB-CBB-CGB-01B
29	KA	202	PEB	CAB-CBB-CGB-01B
29	DB	202	PEB	CAC-CBC-CGC-01C
29	FB	202	PEB	CAC-CBC-CGC-01C
29	HB	202	PEB	CAC-CBC-CGC-01C
29	JB	202	PEB	CAC-CBC-CGC-01C
29	KB	203	PEB	CAC-CBC-CGC-01C
29	XB	202	PEB	CAB-CBB-CGB-02B
29	ZB	202	PEB	CAC-CBC-CGC-01C
29	kB	202	PEB	CAC-CBC-CGC-01C
29	ED	202	PEB	CAB-CBB-CGB-01B
29	MD	203	PEB	CAB-CBB-CGB-01B
29	MG	404	PEB	CAC-CBC-CGC-01C
29	BJ	201	PEB	CAC-CBC-CGC-01C
29	BL	201	PEB	CAC-CBC-CGC-01C
29	AM	303	PEB	CAB-CBB-CGB-01B
29	DM	202	PEB	CAC-CBC-CGC-01C
29	FM	202	PEB	CAC-CBC-CGC-01C
29	HM	202	PEB	CAC-CBC-CGC-01C
29	JM	202	PEB	CAC-CBC-CGC-01C
29	KM	203	PEB	CAC-CBC-CGC-01C
29	XM	202	PEB	CAB-CBB-CGB-02B
29	ZM	202	PEB	CAC-CBC-CGC-01C
29	kM	202	PEB	CAC-CBC-CGC-01C
29	AN	202	PEB	CAB-CBB-CGB-01B
29	CN	202	PEB	CAB-CBB-CGB-01B
29	EN	202	PEB	CAB-CBB-CGB-01B
29	IN	202	PEB	CAB-CBB-CGB-01B
29	KN	202	PEB	CAB-CBB-CGB-01B
29	MQ	406	PEB	CAC-CBC-CGC-01C
29	OR	202	PEB	CAB-CBB-CGB-02B
30	wJ	305	PUB	CAB-CBB-CGB-01B
30	wJ	305	PUB	CAB-CBB-CGB-02B
30	xJ	305	PUB	CAB-CBB-CGB-02B

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Mol	Chain	Res	Type	Atoms
30	xL	305	PUB	CAB-CBB-CGB-O2B
31	1P	1002	CYC	CAD-CBD-CGD-O1D
29	M3	201	PEB	CAB-CBB-CGB-O1B
29	N3	201	PEB	CAB-CBB-CGB-O1B
29	C4	203	PEB	CAB-CBB-CGB-O1B
29	E4	203	PEB	CAB-CBB-CGB-O1B
29	G4	203	PEB	CAB-CBB-CGB-O1B
29	M4	203	PEB	CAB-CBB-CGB-O2B
29	I5	203	PEB	CAC-CBC-CGC-O1C
29	A5	203	PEB	CAC-CBC-CGC-O1C
29	C5	203	PEB	CAC-CBC-CGC-O1C
29	R7	202	PEB	CAB-CBB-CGB-O2B
29	T7	202	PEB	CAB-CBB-CGB-O2B
29	V7	202	PEB	CAB-CBB-CGB-O2B
29	a7	202	PEB	CAB-CBB-CGB-O2B
29	c7	202	PEB	CAB-CBB-CGB-O2B
29	e7	202	PEB	CAB-CBB-CGB-O2B
29	g7	202	PEB	CAB-CBB-CGB-O2B
29	k7	202	PEB	CAB-CBB-CGB-O2B
29	m7	202	PEB	CAB-CBB-CGB-O2B
29	I8	203	PEB	CAC-CBC-CGC-O1C
29	A8	203	PEB	CAC-CBC-CGC-O1C
29	C8	203	PEB	CAC-CBC-CGC-O1C
29	R9	202	PEB	CAB-CBB-CGB-O2B
29	T9	202	PEB	CAB-CBB-CGB-O2B
29	V9	202	PEB	CAB-CBB-CGB-O2B
29	a9	202	PEB	CAB-CBB-CGB-O2B
29	c9	202	PEB	CAB-CBB-CGB-O2B
29	e9	202	PEB	CAB-CBB-CGB-O2B
29	g9	202	PEB	CAB-CBB-CGB-O2B
29	k9	202	PEB	CAB-CBB-CGB-O2B
29	m9	202	PEB	CAB-CBB-CGB-O2B
29	GA	202	PEB	CAB-CBB-CGB-O1B
29	DB	201	PEB	CAC-CBC-CGC-O1C
29	FB	201	PEB	CAC-CBC-CGC-O1C
29	HB	202	PEB	CAC-CBC-CGC-O2C
29	HB	203	PEB	CAB-CBB-CGB-O2B
29	JB	203	PEB	CAB-CBB-CGB-O2B
29	KB	203	PEB	CAC-CBC-CGC-O2C
29	LB	202	PEB	CAC-CBC-CGC-O1C
29	LB	202	PEB	CAC-CBC-CGC-O2C
29	PB	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	QB	202	PEB	CAC-CBC-CGC-O1C
29	RB	202	PEB	CAC-CBC-CGC-O1C
29	RB	203	PEB	CAB-CBB-CGB-O2B
29	TB	202	PEB	CAC-CBC-CGC-O1C
29	TB	203	PEB	CAB-CBB-CGB-O2B
29	VB	202	PEB	CAC-CBC-CGC-O1C
29	YB	201	PEB	CAC-CBC-CGC-O1C
29	ZB	202	PEB	CAC-CBC-CGC-O2C
29	ZB	203	PEB	CAB-CBB-CGB-O2B
29	aB	203	PEB	CAC-CBC-CGC-O1C
29	cB	202	PEB	CAC-CBC-CGC-O1C
29	cB	202	PEB	CAC-CBC-CGC-O2C
29	cB	203	PEB	CAB-CBB-CGB-O2B
29	gB	202	PEB	CAC-CBC-CGC-O1C
29	iB	202	PEB	CAC-CBC-CGC-O1C
29	iB	202	PEB	CAC-CBC-CGC-O2C
29	kB	201	PEB	CAC-CBC-CGC-O1C
29	kB	203	PEB	CAB-CBB-CGB-O2B
29	mB	202	PEB	CAC-CBC-CGC-O1C
29	CD	203	PEB	CAB-CBB-CGB-O1B
29	GD	203	PEB	CAB-CBB-CGB-O1B
29	ID	203	PEB	CAB-CBB-CGB-O1B
29	KD	203	PEB	CAB-CBB-CGB-O1B
29	KD	203	PEB	CAB-CBB-CGB-O2B
29	FG	203	PEB	CAC-CBC-CGC-O1C
29	HG	203	PEB	CAC-CBC-CGC-O1C
29	BJ	203	PEB	CAC-CBC-CGC-O1C
29	DJ	202	PEB	CAC-CBC-CGC-O1C
29	FJ	203	PEB	CAC-CBC-CGC-O1C
29	HJ	202	PEB	CAC-CBC-CGC-O1C
29	JJ	203	PEB	CAC-CBC-CGC-O1C
29	LJ	202	PEB	CAC-CBC-CGC-O1C
29	NJ	203	PEB	CAC-CBC-CGC-O1C
29	PJ	203	PEB	CAC-CBC-CGC-O1C
29	RJ	203	PEB	CAC-CBC-CGC-O1C
29	TJ	203	PEB	CAC-CBC-CGC-O1C
29	XJ	203	PEB	CAC-CBC-CGC-O1C
29	ZJ	203	PEB	CAC-CBC-CGC-O1C
29	bJ	203	PEB	CAC-CBC-CGC-O1C
29	dJ	203	PEB	CAC-CBC-CGC-O1C
29	fJ	203	PEB	CAC-CBC-CGC-O1C
29	hJ	203	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	jJ	203	PEB	CAC-CBC-CGC-O1C
29	lJ	203	PEB	CAC-CBC-CGC-O1C
29	nJ	203	PEB	CAC-CBC-CGC-O1C
29	pJ	203	PEB	CAC-CBC-CGC-O1C
29	rJ	203	PEB	CAC-CBC-CGC-O1C
29	tJ	202	PEB	CAC-CBC-CGC-O1C
29	vJ	202	PEB	CAC-CBC-CGC-O1C
29	BL	203	PEB	CAC-CBC-CGC-O1C
29	DL	202	PEB	CAC-CBC-CGC-O1C
29	FL	203	PEB	CAC-CBC-CGC-O1C
29	HL	202	PEB	CAC-CBC-CGC-O1C
29	JL	203	PEB	CAC-CBC-CGC-O1C
29	LL	202	PEB	CAC-CBC-CGC-O1C
29	NL	203	PEB	CAC-CBC-CGC-O1C
29	PL	203	PEB	CAC-CBC-CGC-O1C
29	RL	203	PEB	CAC-CBC-CGC-O1C
29	TL	203	PEB	CAC-CBC-CGC-O1C
29	XL	203	PEB	CAC-CBC-CGC-O1C
29	ZL	203	PEB	CAC-CBC-CGC-O1C
29	bL	203	PEB	CAC-CBC-CGC-O1C
29	dL	203	PEB	CAC-CBC-CGC-O1C
29	fL	203	PEB	CAC-CBC-CGC-O1C
29	hL	203	PEB	CAC-CBC-CGC-O1C
29	jL	203	PEB	CAC-CBC-CGC-O1C
29	lL	203	PEB	CAC-CBC-CGC-O1C
29	nL	203	PEB	CAC-CBC-CGC-O1C
29	pL	203	PEB	CAC-CBC-CGC-O1C
29	rL	203	PEB	CAC-CBC-CGC-O1C
29	tL	202	PEB	CAC-CBC-CGC-O1C
29	vL	202	PEB	CAC-CBC-CGC-O1C
29	DM	201	PEB	CAC-CBC-CGC-O1C
29	FM	201	PEB	CAC-CBC-CGC-O1C
29	HM	202	PEB	CAC-CBC-CGC-O2C
29	HM	203	PEB	CAB-CBB-CGB-O2B
29	JM	203	PEB	CAB-CBB-CGB-O2B
29	KM	203	PEB	CAC-CBC-CGC-O2C
29	LM	202	PEB	CAC-CBC-CGC-O1C
29	LM	202	PEB	CAC-CBC-CGC-O2C
29	PM	202	PEB	CAB-CBB-CGB-O2B
29	QM	202	PEB	CAC-CBC-CGC-O1C
29	RM	202	PEB	CAC-CBC-CGC-O1C
29	RM	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	TM	202	PEB	CAC-CBC-CGC-O1C
29	TM	203	PEB	CAB-CBB-CGB-O2B
29	VM	202	PEB	CAC-CBC-CGC-O1C
29	YM	201	PEB	CAC-CBC-CGC-O1C
29	ZM	202	PEB	CAC-CBC-CGC-O2C
29	ZM	203	PEB	CAB-CBB-CGB-O2B
29	aM	203	PEB	CAC-CBC-CGC-O1C
29	cM	202	PEB	CAC-CBC-CGC-O1C
29	cM	202	PEB	CAC-CBC-CGC-O2C
29	cM	203	PEB	CAB-CBB-CGB-O2B
29	gM	202	PEB	CAC-CBC-CGC-O1C
29	iM	202	PEB	CAC-CBC-CGC-O1C
29	iM	202	PEB	CAC-CBC-CGC-O2C
29	kM	201	PEB	CAC-CBC-CGC-O1C
29	kM	203	PEB	CAB-CBB-CGB-O2B
29	mM	202	PEB	CAC-CBC-CGC-O1C
29	GN	202	PEB	CAB-CBB-CGB-O1B
29	MO	201	PEB	CAB-CBB-CGB-O1B
29	NO	201	PEB	CAB-CBB-CGB-O1B
29	FQ	203	PEB	CAC-CBC-CGC-O1C
29	HQ	203	PEB	CAC-CBC-CGC-O1C
29	OR	202	PEB	CAB-CBB-CGB-O1B
30	MA	403	PUB	CAB-CBB-CGB-O1B
30	xJ	305	PUB	CAB-CBB-CGB-O1B
30	wL	305	PUB	CAB-CBB-CGB-O1B
30	xL	305	PUB	CAB-CBB-CGB-O1B
30	MN	403	PUB	CAB-CBB-CGB-O1B
31	D7	1001	CYC	CAA-CBA-CGA-O1A
31	F7	1001	CYC	CAA-CBA-CGA-O1A
31	H7	1001	CYC	CAA-CBA-CGA-O1A
31	J7	1001	CYC	CAA-CBA-CGA-O1A
31	L7	1001	CYC	CAA-CBA-CGA-O1A
31	N7	1001	CYC	CAA-CBA-CGA-O1A
31	D9	1001	CYC	CAA-CBA-CGA-O1A
31	H9	1001	CYC	CAA-CBA-CGA-O1A
31	J9	1001	CYC	CAA-CBA-CGA-O1A
31	L9	1001	CYC	CAA-CBA-CGA-O1A
31	N9	1001	CYC	CAA-CBA-CGA-O1A
29	B4	201	PEB	CAB-CBB-CGB-O1B
29	D4	201	PEB	CAB-CBB-CGB-O1B
29	E4	203	PEB	CAB-CBB-CGB-O2B
29	F4	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	G4	203	PEB	CAB-CBB-CGB-O2B
29	J4	201	PEB	CAB-CBB-CGB-O1B
29	K4	203	PEB	CAB-CBB-CGB-O2B
29	L4	201	PEB	CAB-CBB-CGB-O1B
29	M4	203	PEB	CAB-CBB-CGB-O1B
29	P7	202	PEB	CAB-CBB-CGB-O2B
29	Y7	202	PEB	CAB-CBB-CGB-O2B
29	i7	202	PEB	CAB-CBB-CGB-O2B
29	P9	202	PEB	CAB-CBB-CGB-O2B
29	Y9	202	PEB	CAB-CBB-CGB-O2B
29	i9	202	PEB	CAB-CBB-CGB-O2B
29	DB	202	PEB	CAC-CBC-CGC-O2C
29	FB	202	PEB	CAC-CBC-CGC-O2C
29	HB	201	PEB	CAC-CBC-CGC-O1C
29	JB	201	PEB	CAC-CBC-CGC-O1C
29	JB	202	PEB	CAC-CBC-CGC-O2C
29	LB	201	PEB	CAC-CBC-CGC-O1C
29	NB	201	PEB	CAC-CBC-CGC-O1C
29	PB	201	PEB	CAC-CBC-CGC-O1C
29	QB	202	PEB	CAC-CBC-CGC-O2C
29	RB	201	PEB	CAC-CBC-CGC-O1C
29	RB	202	PEB	CAC-CBC-CGC-O2C
29	TB	201	PEB	CAC-CBC-CGC-O1C
29	TB	202	PEB	CAC-CBC-CGC-O2C
29	VB	201	PEB	CAC-CBC-CGC-O1C
29	VB	202	PEB	CAC-CBC-CGC-O2C
29	XB	201	PEB	CAC-CBC-CGC-O1C
29	YB	201	PEB	CAC-CBC-CGC-O2C
29	ZB	201	PEB	CAC-CBC-CGC-O1C
29	aB	203	PEB	CAC-CBC-CGC-O2C
29	cB	201	PEB	CAC-CBC-CGC-O1C
29	eB	201	PEB	CAC-CBC-CGC-O1C
29	gB	201	PEB	CAC-CBC-CGC-O1C
29	gB	202	PEB	CAC-CBC-CGC-O2C
29	iB	201	PEB	CAC-CBC-CGC-O1C
29	kB	202	PEB	CAC-CBC-CGC-O2C
29	mB	201	PEB	CAC-CBC-CGC-O1C
29	mB	202	PEB	CAC-CBC-CGC-O2C
29	CD	203	PEB	CAB-CBB-CGB-O2B
29	DD	201	PEB	CAB-CBB-CGB-O1B
29	ED	202	PEB	CAB-CBB-CGB-O2B
29	FD	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
29	HD	201	PEB	CAB-CBB-CGB-O1B
29	LD	201	PEB	CAB-CBB-CGB-O1B
29	MD	203	PEB	CAB-CBB-CGB-O2B
29	BG	203	PEB	CAC-CBC-CGC-O1C
29	DG	203	PEB	CAC-CBC-CGC-O1C
29	JG	203	PEB	CAC-CBC-CGC-O1C
29	LG	203	PEB	CAC-CBC-CGC-O1C
29	VJ	202	PEB	CAC-CBC-CGC-O1C
29	VL	202	PEB	CAC-CBC-CGC-O1C
29	DM	202	PEB	CAC-CBC-CGC-O2C
29	FM	202	PEB	CAC-CBC-CGC-O2C
29	HM	201	PEB	CAC-CBC-CGC-O1C
29	JM	201	PEB	CAC-CBC-CGC-O1C
29	JM	202	PEB	CAC-CBC-CGC-O2C
29	LM	201	PEB	CAC-CBC-CGC-O1C
29	NM	201	PEB	CAC-CBC-CGC-O1C
29	PM	201	PEB	CAC-CBC-CGC-O1C
29	QM	202	PEB	CAC-CBC-CGC-O2C
29	RM	201	PEB	CAC-CBC-CGC-O1C
29	RM	202	PEB	CAC-CBC-CGC-O2C
29	TM	201	PEB	CAC-CBC-CGC-O1C
29	TM	202	PEB	CAC-CBC-CGC-O2C
29	VM	201	PEB	CAC-CBC-CGC-O1C
29	VM	202	PEB	CAC-CBC-CGC-O2C
29	XM	201	PEB	CAC-CBC-CGC-O1C
29	YM	201	PEB	CAC-CBC-CGC-O2C
29	ZM	201	PEB	CAC-CBC-CGC-O1C
29	aM	203	PEB	CAC-CBC-CGC-O2C
29	cM	201	PEB	CAC-CBC-CGC-O1C
29	eM	201	PEB	CAC-CBC-CGC-O1C
29	gM	201	PEB	CAC-CBC-CGC-O1C
29	gM	202	PEB	CAC-CBC-CGC-O2C
29	iM	201	PEB	CAC-CBC-CGC-O1C
29	kM	202	PEB	CAC-CBC-CGC-O2C
29	mM	201	PEB	CAC-CBC-CGC-O1C
29	mM	202	PEB	CAC-CBC-CGC-O2C
29	BQ	203	PEB	CAC-CBC-CGC-O1C
29	DQ	203	PEB	CAC-CBC-CGC-O1C
29	JQ	203	PEB	CAC-CBC-CGC-O1C
29	LQ	202	PEB	CAC-CBC-CGC-O1C
31	I1	1001	CYC	CAD-CBD-CGD-O2D
31	F9	1001	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	EK	1001	CYC	CAD-CBD-CGD-O2D
31	YP	1000	CYC	CAD-CBD-CGD-O1D
29	C4	203	PEB	CAB-CBB-CGB-O2B
29	H4	201	PEB	CAC-CBC-CGC-O2C
29	H4	201	PEB	CAB-CBB-CGB-O1B
29	BD	201	PEB	CAB-CBB-CGB-O1B
29	GD	203	PEB	CAB-CBB-CGB-O2B
29	ID	203	PEB	CAB-CBB-CGB-O2B
29	JD	201	PEB	CAB-CBB-CGB-O1B
31	C1	1001	CYC	CAD-CBD-CGD-O2D
31	D1	1003	CYC	CAD-CBD-CGD-O2D
31	E1	1001	CYC	CAD-CBD-CGD-O2D
31	K1	1001	CYC	CAD-CBD-CGD-O2D
31	M1	1001	CYC	CAD-CBD-CGD-O2D
31	CK	1001	CYC	CAD-CBD-CGD-O2D
31	GK	1001	CYC	CAD-CBD-CGD-O2D
31	IK	1001	CYC	CAD-CBD-CGD-O2D
31	KK	1001	CYC	CAD-CBD-CGD-O2D
31	MK	1001	CYC	CAD-CBD-CGD-O2D
29	B4	201	PEB	CAC-CBC-CGC-O2C
29	D4	201	PEB	CAC-CBC-CGC-O2C
29	F4	201	PEB	CAC-CBC-CGC-O2C
29	J4	201	PEB	CAC-CBC-CGC-O2C
29	L4	201	PEB	CAC-CBC-CGC-O2C
29	BD	201	PEB	CAC-CBC-CGC-O2C
29	HD	201	PEB	CAC-CBC-CGC-O2C
29	JD	201	PEB	CAC-CBC-CGC-O2C
29	LD	201	PEB	CAC-CBC-CGC-O2C
29	PF	201	PEB	CAC-CBC-CGC-O1C
29	RF	201	PEB	CAC-CBC-CGC-O1C
29	VF	201	PEB	CAC-CBC-CGC-O1C
29	YF	201	PEB	CAC-CBC-CGC-O1C
29	aF	201	PEB	CAC-CBC-CGC-O1C
29	cF	201	PEB	CAC-CBC-CGC-O1C
29	eF	201	PEB	CAC-CBC-CGC-O1C
29	gF	201	PEB	CAC-CBC-CGC-O1C
29	iF	201	PEB	CAC-CBC-CGC-O1C
29	kF	201	PEB	CAC-CBC-CGC-O1C
29	mF	201	PEB	CAC-CBC-CGC-O1C
29	PI	201	PEB	CAC-CBC-CGC-O1C
29	RI	201	PEB	CAC-CBC-CGC-O1C
29	TI	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
29	VI	201	PEB	CAC-CBC-CGC-O1C
29	YI	201	PEB	CAC-CBC-CGC-O1C
29	aI	201	PEB	CAC-CBC-CGC-O1C
29	cI	201	PEB	CAC-CBC-CGC-O1C
29	eI	201	PEB	CAC-CBC-CGC-O1C
29	gI	201	PEB	CAC-CBC-CGC-O1C
29	iI	201	PEB	CAC-CBC-CGC-O1C
29	kI	201	PEB	CAC-CBC-CGC-O1C
29	mI	201	PEB	CAC-CBC-CGC-O1C
29	DD	201	PEB	CAC-CBC-CGC-O2C
29	FD	201	PEB	CAC-CBC-CGC-O2C
29	DO	202	PEB	CAB-CBB-CGB-O2B
29	D3	202	PEB	CAB-CBB-CGB-O2B
29	BG	203	PEB	CAC-CBC-CGC-O2C
29	DG	203	PEB	CAC-CBC-CGC-O2C
29	FG	203	PEB	CAC-CBC-CGC-O2C
29	HG	203	PEB	CAC-CBC-CGC-O2C
29	JG	203	PEB	CAC-CBC-CGC-O2C
29	LG	203	PEB	CAC-CBC-CGC-O2C
29	zL	501	PEB	CAB-CBB-CGB-O2B
29	BQ	203	PEB	CAC-CBC-CGC-O2C
29	DQ	203	PEB	CAC-CBC-CGC-O2C
29	FQ	203	PEB	CAC-CBC-CGC-O2C
29	HQ	203	PEB	CAC-CBC-CGC-O2C
29	JQ	203	PEB	CAC-CBC-CGC-O2C
29	LQ	202	PEB	CAC-CBC-CGC-O2C
30	AB	304	PUB	CAC-CBC-CGC-O2C
30	AM	304	PUB	CAC-CBC-CGC-O2C
29	PF	201	PEB	C4B-C3B-CAB-CBB
29	RF	201	PEB	C4B-C3B-CAB-CBB
29	VF	201	PEB	C4B-C3B-CAB-CBB
29	YF	201	PEB	C4B-C3B-CAB-CBB
29	aF	201	PEB	C4B-C3B-CAB-CBB
29	cF	201	PEB	C4B-C3B-CAB-CBB
29	eF	201	PEB	C4B-C3B-CAB-CBB
29	gF	201	PEB	C4B-C3B-CAB-CBB
29	iF	201	PEB	C4B-C3B-CAB-CBB
29	kF	201	PEB	C4B-C3B-CAB-CBB
29	mF	201	PEB	C4B-C3B-CAB-CBB
29	PI	201	PEB	C4B-C3B-CAB-CBB
29	RI	201	PEB	C4B-C3B-CAB-CBB
29	TI	201	PEB	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	VI	201	PEB	C4B-C3B-CAB-CBB
29	YI	201	PEB	C4B-C3B-CAB-CBB
29	aI	201	PEB	C4B-C3B-CAB-CBB
29	cI	201	PEB	C4B-C3B-CAB-CBB
29	eI	201	PEB	C4B-C3B-CAB-CBB
29	gI	201	PEB	C4B-C3B-CAB-CBB
29	iI	201	PEB	C4B-C3B-CAB-CBB
29	kI	201	PEB	C4B-C3B-CAB-CBB
29	mI	201	PEB	C4B-C3B-CAB-CBB
29	iF	201	PEB	CAB-CBB-CGB-O2B
29	kF	201	PEB	CAB-CBB-CGB-O2B
29	iI	201	PEB	CAB-CBB-CGB-O2B
29	kI	201	PEB	CAB-CBB-CGB-O2B
29	DA	202	PEB	C2B-C3B-CAB-CBB
29	JA	202	PEB	C2B-C3B-CAB-CBB
29	LA	202	PEB	C2B-C3B-CAB-CBB
29	DN	202	PEB	C2B-C3B-CAB-CBB
29	JN	202	PEB	C2B-C3B-CAB-CBB
29	LN	202	PEB	C2B-C3B-CAB-CBB
29	O7	201	PEB	CAB-CBB-CGB-O2B
29	h7	201	PEB	CAB-CBB-CGB-O2B
29	O9	201	PEB	CAB-CBB-CGB-O2B
29	h9	201	PEB	CAB-CBB-CGB-O2B
29	N2	203	PEB	CAB-CBB-CGB-O2B
29	P2	202	PEB	CAB-CBB-CGB-O2B
29	R2	203	PEB	CAB-CBB-CGB-O2B
29	T2	203	PEB	CAB-CBB-CGB-O2B
29	V2	203	PEB	CAB-CBB-CGB-O2B
29	X2	202	PEB	CAB-CBB-CGB-O2B
29	Q7	201	PEB	CAB-CBB-CGB-O2B
29	S7	201	PEB	CAB-CBB-CGB-O2B
29	U7	201	PEB	CAB-CBB-CGB-O2B
29	W7	201	PEB	CAB-CBB-CGB-O2B
29	Z7	201	PEB	CAB-CBB-CGB-O2B
29	b7	201	PEB	CAB-CBB-CGB-O2B
29	d7	201	PEB	CAB-CBB-CGB-O2B
29	f7	201	PEB	CAB-CBB-CGB-O2B
29	j7	201	PEB	CAB-CBB-CGB-O2B
29	l7	201	PEB	CAB-CBB-CGB-O2B
29	Q9	201	PEB	CAB-CBB-CGB-O2B
29	S9	201	PEB	CAB-CBB-CGB-O2B
29	U9	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
29	W9	201	PEB	CAB-CBB-CGB-O2B
29	Z9	201	PEB	CAB-CBB-CGB-O2B
29	b9	201	PEB	CAB-CBB-CGB-O2B
29	d9	201	PEB	CAB-CBB-CGB-O2B
29	f9	201	PEB	CAB-CBB-CGB-O2B
29	j9	201	PEB	CAB-CBB-CGB-O2B
29	l9	201	PEB	CAB-CBB-CGB-O2B
29	PF	201	PEB	CAB-CBB-CGB-O2B
29	RF	201	PEB	CAB-CBB-CGB-O2B
29	VF	201	PEB	CAB-CBB-CGB-O2B
29	YF	201	PEB	CAB-CBB-CGB-O2B
29	aF	201	PEB	CAB-CBB-CGB-O2B
29	cF	201	PEB	CAB-CBB-CGB-O2B
29	eF	201	PEB	CAB-CBB-CGB-O2B
29	gF	201	PEB	CAB-CBB-CGB-O2B
29	mF	201	PEB	CAB-CBB-CGB-O2B
29	PI	201	PEB	CAB-CBB-CGB-O2B
29	RI	201	PEB	CAB-CBB-CGB-O2B
29	TI	201	PEB	CAB-CBB-CGB-O2B
29	VI	201	PEB	CAB-CBB-CGB-O2B
29	YI	201	PEB	CAB-CBB-CGB-O2B
29	aI	201	PEB	CAB-CBB-CGB-O2B
29	cI	201	PEB	CAB-CBB-CGB-O2B
29	eI	201	PEB	CAB-CBB-CGB-O2B
29	gI	201	PEB	CAB-CBB-CGB-O2B
29	mI	201	PEB	CAB-CBB-CGB-O2B
29	zJ	501	PEB	CAB-CBB-CGB-O2B
29	NR	203	PEB	CAB-CBB-CGB-O2B
29	PR	202	PEB	CAB-CBB-CGB-O2B
29	RR	203	PEB	CAB-CBB-CGB-O2B
29	TR	203	PEB	CAB-CBB-CGB-O2B
29	VR	203	PEB	CAB-CBB-CGB-O2B
29	XR	203	PEB	CAB-CBB-CGB-O2B
30	AM	304	PUB	CAB-CBB-CGB-O2B
29	C4	201	PEB	CAB-CBB-CGB-O2B
30	AB	304	PUB	CAB-CBB-CGB-O2B
29	P7	202	PEB	C2C-CAC-CBC-CGC
29	R7	202	PEB	C2C-CAC-CBC-CGC
29	T7	202	PEB	C2C-CAC-CBC-CGC
29	V7	202	PEB	C2C-CAC-CBC-CGC
29	Y7	202	PEB	C2C-CAC-CBC-CGC
29	a7	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	c7	202	PEB	C2C-CAC-CBC-CGC
29	e7	202	PEB	C2C-CAC-CBC-CGC
29	g7	202	PEB	C2C-CAC-CBC-CGC
29	i7	202	PEB	C2C-CAC-CBC-CGC
29	k7	202	PEB	C2C-CAC-CBC-CGC
29	m7	202	PEB	C2C-CAC-CBC-CGC
29	P9	202	PEB	C2C-CAC-CBC-CGC
29	R9	202	PEB	C2C-CAC-CBC-CGC
29	T9	202	PEB	C2C-CAC-CBC-CGC
29	V9	202	PEB	C2C-CAC-CBC-CGC
29	Y9	202	PEB	C2C-CAC-CBC-CGC
29	a9	202	PEB	C2C-CAC-CBC-CGC
29	c9	202	PEB	C2C-CAC-CBC-CGC
29	e9	202	PEB	C2C-CAC-CBC-CGC
29	g9	202	PEB	C2C-CAC-CBC-CGC
29	i9	202	PEB	C2C-CAC-CBC-CGC
29	k9	202	PEB	C2C-CAC-CBC-CGC
29	m9	202	PEB	C2C-CAC-CBC-CGC
29	VF	201	PEB	C2C-CAC-CBC-CGC
29	VI	201	PEB	C2C-CAC-CBC-CGC
30	AB	305	PUB	C3B-CAB-CBB-CGB
30	BB	302	PUB	C3B-CAB-CBB-CGB
30	AM	305	PUB	C3B-CAB-CBB-CGB
30	BM	302	PUB	C3B-CAB-CBB-CGB
29	A7	304	PEB	C3B-CAB-CBB-CGB
29	A9	304	PEB	C3B-CAB-CBB-CGB
29	D7	1002	PEB	CAC-CBC-CGC-O2C
29	F7	1002	PEB	CAC-CBC-CGC-O2C
29	H7	1002	PEB	CAC-CBC-CGC-O2C
29	J7	1002	PEB	CAC-CBC-CGC-O2C
29	L7	1002	PEB	CAC-CBC-CGC-O2C
29	N7	1002	PEB	CAC-CBC-CGC-O2C
29	D9	1002	PEB	CAC-CBC-CGC-O2C
29	F9	1002	PEB	CAC-CBC-CGC-O2C
29	H9	1002	PEB	CAC-CBC-CGC-O2C
29	J9	1002	PEB	CAC-CBC-CGC-O2C
29	L9	1002	PEB	CAC-CBC-CGC-O2C
29	N9	1002	PEB	CAC-CBC-CGC-O2C
29	MD	201	PEB	CAB-CBB-CGB-O2B
29	xL	301	PEB	CAC-CBC-CGC-O2C
31	NK	1001	CYC	CAD-CBD-CGD-O2D
29	BA	202	PEB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	FA	202	PEB	C2B-C3B-CAB-CBB
29	HA	202	PEB	C2B-C3B-CAB-CBB
29	BN	202	PEB	C2B-C3B-CAB-CBB
29	FN	202	PEB	C2B-C3B-CAB-CBB
29	HN	202	PEB	C2B-C3B-CAB-CBB
29	E4	201	PEB	CAB-CBB-CGB-O2B
29	G4	201	PEB	CAB-CBB-CGB-O2B
29	I4	201	PEB	CAB-CBB-CGB-O2B
29	K4	201	PEB	CAB-CBB-CGB-O2B
29	M4	201	PEB	CAB-CBB-CGB-O2B
29	dD	401	PEB	CAB-CBB-CGB-O2B
29	CD	201	PEB	CAB-CBB-CGB-O2B
29	GD	201	PEB	CAB-CBB-CGB-O2B
29	ID	201	PEB	CAB-CBB-CGB-O2B
29	KD	201	PEB	CAB-CBB-CGB-O2B
29	wJ	301	PEB	CAC-CBC-CGC-O2C
29	xJ	301	PEB	CAC-CBC-CGC-O2C
29	wL	301	PEB	CAC-CBC-CGC-O2C
31	D1	1001	CYC	CAD-CBD-CGD-O2D
31	F1	1001	CYC	CAD-CBD-CGD-O2D
31	H1	1001	CYC	CAD-CBD-CGD-O2D
31	J1	1001	CYC	CAD-CBD-CGD-O2D
31	L1	1001	CYC	CAD-CBD-CGD-O2D
31	N1	1001	CYC	CAD-CBD-CGD-O2D
31	DK	1001	CYC	CAD-CBD-CGD-O2D
31	FK	1001	CYC	CAD-CBD-CGD-O2D
31	HK	1001	CYC	CAD-CBD-CGD-O2D
31	JK	1001	CYC	CAD-CBD-CGD-O2D
31	LK	1001	CYC	CAD-CBD-CGD-O2D
29	I4	203	PEB	CAC-CBC-CGC-O2C
30	A7	303	PUB	CAC-CBC-CGC-O2C
30	A9	303	PUB	CAC-CBC-CGC-O2C
30	AF	303	PUB	CAC-CBC-CGC-O2C
30	AI	303	PUB	CAC-CBC-CGC-O2C
29	D3	202	PEB	C2D-C1D-CHC-C4C
29	B5	201	PEB	C2D-C1D-CHC-C4C
29	B5	202	PEB	C2D-C1D-CHC-C4C
29	F5	201	PEB	C2D-C1D-CHC-C4C
29	F5	202	PEB	C2D-C1D-CHC-C4C
29	G5	201	PEB	C2D-C1D-CHC-C4C
29	G5	202	PEB	C2D-C1D-CHC-C4C
29	H5	201	PEB	C2D-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	H5	202	PEB	C2D-C1D-CHC-C4C
29	L5	201	PEB	C2D-C1D-CHC-C4C
29	D7	1002	PEB	C2D-C1D-CHC-C4C
29	F7	1002	PEB	C2D-C1D-CHC-C4C
29	H7	1002	PEB	C2D-C1D-CHC-C4C
29	J7	1002	PEB	C2D-C1D-CHC-C4C
29	L7	1002	PEB	C2D-C1D-CHC-C4C
29	N7	1002	PEB	C2D-C1D-CHC-C4C
29	B8	201	PEB	C2D-C1D-CHC-C4C
29	F8	201	PEB	C2D-C1D-CHC-C4C
29	G8	201	PEB	C2D-C1D-CHC-C4C
29	G8	202	PEB	C2D-C1D-CHC-C4C
29	H8	201	PEB	C2D-C1D-CHC-C4C
29	H8	202	PEB	C2D-C1D-CHC-C4C
29	L8	201	PEB	C2D-C1D-CHC-C4C
29	D9	1002	PEB	C2D-C1D-CHC-C4C
29	F9	1002	PEB	C2D-C1D-CHC-C4C
29	H9	1002	PEB	C2D-C1D-CHC-C4C
29	J9	1002	PEB	C2D-C1D-CHC-C4C
29	L9	1002	PEB	C2D-C1D-CHC-C4C
29	N9	1002	PEB	C2D-C1D-CHC-C4C
29	AB	303	PEB	C2D-C1D-CHC-C4C
29	BB	301	PEB	C2D-C1D-CHC-C4C
29	AF	305	PEB	C2D-C1D-CHC-C4C
29	AI	305	PEB	C2D-C1D-CHC-C4C
29	AM	303	PEB	C2D-C1D-CHC-C4C
29	BM	301	PEB	C2D-C1D-CHC-C4C
29	DO	202	PEB	C2D-C1D-CHC-C4C
30	BB	302	PUB	C3A-C4A-CHA-C1B
30	BM	302	PUB	C3A-C4A-CHA-C1B
29	BB	301	PEB	CAC-CBC-CGC-O2C
29	BM	301	PEB	CAC-CBC-CGC-O2C
29	BB	301	PEB	CAB-CBB-CGB-O2B
29	BM	301	PEB	CAB-CBB-CGB-O2B
31	C1	1001	CYC	CAD-CBD-CGD-O1D
31	D1	1003	CYC	CAD-CBD-CGD-O1D
31	E1	1001	CYC	CAD-CBD-CGD-O1D
31	I1	1001	CYC	CAD-CBD-CGD-O1D
31	K1	1001	CYC	CAD-CBD-CGD-O1D
31	M1	1001	CYC	CAD-CBD-CGD-O1D
31	CK	1001	CYC	CAD-CBD-CGD-O1D
31	EK	1001	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	GK	1001	CYC	CAD-CBD-CGD-O1D
31	IK	1001	CYC	CAD-CBD-CGD-O1D
31	KK	1001	CYC	CAD-CBD-CGD-O1D
31	MK	1001	CYC	CAD-CBD-CGD-O1D
29	M3	201	PEB	CAC-CBC-CGC-O2C
29	N3	201	PEB	CAC-CBC-CGC-O2C
29	MO	201	PEB	CAC-CBC-CGC-O2C
30	MG	403	PUB	CAC-CBC-CGC-O2C
30	MQ	405	PUB	CAC-CBC-CGC-O2C
29	NO	201	PEB	CAC-CBC-CGC-O2C
30	A7	303	PUB	CAC-CBC-CGC-O1C
30	A9	303	PUB	CAC-CBC-CGC-O1C
29	P1	201	PEB	CAB-CBB-CGB-O2B
29	R1	201	PEB	CAB-CBB-CGB-O2B
29	T1	201	PEB	CAB-CBB-CGB-O2B
29	V1	201	PEB	CAB-CBB-CGB-O2B
29	Y1	201	PEB	CAB-CBB-CGB-O2B
29	a1	201	PEB	CAB-CBB-CGB-O2B
29	c1	201	PEB	CAB-CBB-CGB-O2B
29	e1	201	PEB	CAB-CBB-CGB-O2B
29	g1	201	PEB	CAB-CBB-CGB-O2B
29	i1	201	PEB	CAB-CBB-CGB-O2B
29	k1	201	PEB	CAB-CBB-CGB-O2B
29	m1	201	PEB	CAB-CBB-CGB-O2B
29	V7	203	PEB	CAB-CBB-CGB-O2B
29	i7	203	PEB	CAB-CBB-CGB-O2B
29	V9	203	PEB	CAB-CBB-CGB-O2B
29	i9	203	PEB	CAB-CBB-CGB-O2B
29	PF	201	PEB	CAC-CBC-CGC-O2C
29	RF	201	PEB	CAC-CBC-CGC-O2C
29	YF	201	PEB	CAC-CBC-CGC-O2C
29	aF	201	PEB	CAC-CBC-CGC-O2C
29	cF	201	PEB	CAC-CBC-CGC-O2C
29	gF	201	PEB	CAC-CBC-CGC-O2C
29	iF	201	PEB	CAC-CBC-CGC-O2C
29	mF	201	PEB	CAC-CBC-CGC-O2C
29	PI	201	PEB	CAC-CBC-CGC-O2C
29	RI	201	PEB	CAC-CBC-CGC-O2C
29	YI	201	PEB	CAC-CBC-CGC-O2C
29	aI	201	PEB	CAC-CBC-CGC-O2C
29	cI	201	PEB	CAC-CBC-CGC-O2C
29	gI	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
29	iI	201	PEB	CAC-CBC-CGC-O2C
29	mI	201	PEB	CAC-CBC-CGC-O2C
29	PK	201	PEB	CAB-CBB-CGB-O2B
29	RK	201	PEB	CAB-CBB-CGB-O2B
29	TK	201	PEB	CAB-CBB-CGB-O2B
29	VK	201	PEB	CAB-CBB-CGB-O2B
29	YK	201	PEB	CAB-CBB-CGB-O2B
29	aK	201	PEB	CAB-CBB-CGB-O2B
29	cK	201	PEB	CAB-CBB-CGB-O2B
29	eK	201	PEB	CAB-CBB-CGB-O2B
29	gK	201	PEB	CAB-CBB-CGB-O2B
29	iK	201	PEB	CAB-CBB-CGB-O2B
29	kK	201	PEB	CAB-CBB-CGB-O2B
29	mK	201	PEB	CAB-CBB-CGB-O2B
29	P7	203	PEB	CAB-CBB-CGB-O2B
29	R7	203	PEB	CAB-CBB-CGB-O2B
29	T7	203	PEB	CAB-CBB-CGB-O2B
29	Y7	203	PEB	CAB-CBB-CGB-O2B
29	a7	203	PEB	CAB-CBB-CGB-O2B
29	c7	203	PEB	CAB-CBB-CGB-O2B
29	e7	203	PEB	CAB-CBB-CGB-O2B
29	g7	203	PEB	CAB-CBB-CGB-O2B
29	k7	203	PEB	CAB-CBB-CGB-O2B
29	m7	203	PEB	CAB-CBB-CGB-O2B
29	P9	203	PEB	CAB-CBB-CGB-O2B
29	R9	203	PEB	CAB-CBB-CGB-O2B
29	T9	203	PEB	CAB-CBB-CGB-O2B
29	Y9	203	PEB	CAB-CBB-CGB-O2B
29	a9	203	PEB	CAB-CBB-CGB-O2B
29	c9	203	PEB	CAB-CBB-CGB-O2B
29	e9	203	PEB	CAB-CBB-CGB-O2B
29	g9	203	PEB	CAB-CBB-CGB-O2B
29	k9	203	PEB	CAB-CBB-CGB-O2B
29	m9	203	PEB	CAB-CBB-CGB-O2B
29	VF	201	PEB	CAC-CBC-CGC-O2C
29	eF	201	PEB	CAC-CBC-CGC-O2C
29	kF	201	PEB	CAC-CBC-CGC-O2C
29	TI	201	PEB	CAC-CBC-CGC-O2C
29	VI	201	PEB	CAC-CBC-CGC-O2C
29	eI	201	PEB	CAC-CBC-CGC-O2C
29	kI	201	PEB	CAC-CBC-CGC-O2C
30	AB	304	PUB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
30	AM	304	PUB	CAC-CBC-CGC-O1C
29	J8	201	PEB	CAB-CBB-CGB-O2B
29	BB	301	PEB	CAC-CBC-CGC-O1C
29	BM	301	PEB	CAC-CBC-CGC-O1C
30	MG	403	PUB	CAC-CBC-CGC-O1C
30	MQ	405	PUB	CAC-CBC-CGC-O1C
29	P1	202	PEB	C2C-CAC-CBC-CGC
29	R1	202	PEB	C2C-CAC-CBC-CGC
29	U1	201	PEB	C2C-CAC-CBC-CGC
29	V1	202	PEB	C2C-CAC-CBC-CGC
29	Z1	201	PEB	C2C-CAC-CBC-CGC
29	a1	202	PEB	C2C-CAC-CBC-CGC
29	c1	202	PEB	C2C-CAC-CBC-CGC
29	e1	202	PEB	C2C-CAC-CBC-CGC
29	g1	202	PEB	C2C-CAC-CBC-CGC
29	i1	202	PEB	C2C-CAC-CBC-CGC
29	j1	203	PEB	C2C-CAC-CBC-CGC
29	k1	202	PEB	C2C-CAC-CBC-CGC
29	C4	202	PEB	ND-C1D-CHC-C4C
29	C4	203	PEB	ND-C1D-CHC-C4C
29	E4	202	PEB	ND-C1D-CHC-C4C
29	E4	203	PEB	ND-C1D-CHC-C4C
29	G4	202	PEB	ND-C1D-CHC-C4C
29	G4	203	PEB	ND-C1D-CHC-C4C
29	I4	202	PEB	ND-C1D-CHC-C4C
29	K4	202	PEB	ND-C1D-CHC-C4C
29	K4	203	PEB	ND-C1D-CHC-C4C
29	M4	202	PEB	ND-C1D-CHC-C4C
29	A7	304	PEB	ND-C1D-CHC-C4C
29	A7	305	PEB	ND-C1D-CHC-C4C
29	A9	304	PEB	ND-C1D-CHC-C4C
29	A9	305	PEB	ND-C1D-CHC-C4C
29	CB	201	PEB	C2C-CAC-CBC-CGC
29	CB	202	PEB	C2C-CAC-CBC-CGC
29	EB	201	PEB	C2C-CAC-CBC-CGC
29	EB	202	PEB	C2C-CAC-CBC-CGC
29	GB	201	PEB	C2C-CAC-CBC-CGC
29	GB	202	PEB	C2C-CAC-CBC-CGC
29	IB	201	PEB	C2C-CAC-CBC-CGC
29	IB	202	PEB	C2C-CAC-CBC-CGC
29	KB	201	PEB	C2C-CAC-CBC-CGC
29	KB	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	MB	201	PEB	C2C-CAC-CBC-CGC
29	MB	202	PEB	C2C-CAC-CBC-CGC
29	OB	201	PEB	C2C-CAC-CBC-CGC
29	OB	202	PEB	C2C-CAC-CBC-CGC
29	QB	203	PEB	C2C-CAC-CBC-CGC
29	QB	204	PEB	C2C-CAC-CBC-CGC
29	SB	201	PEB	C2C-CAC-CBC-CGC
29	SB	202	PEB	C2C-CAC-CBC-CGC
29	UB	201	PEB	C2C-CAC-CBC-CGC
29	UB	202	PEB	C2C-CAC-CBC-CGC
29	WB	201	PEB	C2C-CAC-CBC-CGC
29	WB	202	PEB	C2C-CAC-CBC-CGC
29	YB	202	PEB	C2C-CAC-CBC-CGC
29	YB	203	PEB	C2C-CAC-CBC-CGC
29	aB	201	PEB	C2C-CAC-CBC-CGC
29	aB	202	PEB	C2C-CAC-CBC-CGC
29	dB	201	PEB	C2C-CAC-CBC-CGC
29	dB	202	PEB	C2C-CAC-CBC-CGC
29	fB	201	PEB	C2C-CAC-CBC-CGC
29	fB	202	PEB	C2C-CAC-CBC-CGC
29	hB	201	PEB	C2C-CAC-CBC-CGC
29	hB	202	PEB	C2C-CAC-CBC-CGC
29	jB	201	PEB	C2C-CAC-CBC-CGC
29	jB	202	PEB	C2C-CAC-CBC-CGC
29	lB	201	PEB	C2C-CAC-CBC-CGC
29	lB	202	PEB	C2C-CAC-CBC-CGC
29	BC	203	PEB	ND-C1D-CHC-C4C
29	DC	202	PEB	ND-C1D-CHC-C4C
29	FC	203	PEB	ND-C1D-CHC-C4C
29	HC	203	PEB	ND-C1D-CHC-C4C
29	JC	202	PEB	ND-C1D-CHC-C4C
29	LC	203	PEB	ND-C1D-CHC-C4C
29	CD	202	PEB	ND-C1D-CHC-C4C
29	CD	203	PEB	ND-C1D-CHC-C4C
29	ED	201	PEB	ND-C1D-CHC-C4C
29	ED	202	PEB	ND-C1D-CHC-C4C
29	GD	202	PEB	ND-C1D-CHC-C4C
29	GD	203	PEB	ND-C1D-CHC-C4C
29	ID	202	PEB	ND-C1D-CHC-C4C
29	ID	203	PEB	ND-C1D-CHC-C4C
29	KD	202	PEB	ND-C1D-CHC-C4C
29	KD	203	PEB	ND-C1D-CHC-C4C

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Mol	Chain	Res	Type	Atoms
29	MD	202	PEB	ND-C1D-CHC-C4C
29	MD	203	PEB	ND-C1D-CHC-C4C
29	BE	203	PEB	ND-C1D-CHC-C4C
29	DE	202	PEB	ND-C1D-CHC-C4C
29	FE	203	PEB	ND-C1D-CHC-C4C
29	HE	203	PEB	ND-C1D-CHC-C4C
29	JE	202	PEB	ND-C1D-CHC-C4C
29	LE	203	PEB	ND-C1D-CHC-C4C
29	PF	201	PEB	C2C-CAC-CBC-CGC
29	RF	201	PEB	C2C-CAC-CBC-CGC
29	YF	201	PEB	C2C-CAC-CBC-CGC
29	aF	201	PEB	C2C-CAC-CBC-CGC
29	cF	201	PEB	C2C-CAC-CBC-CGC
29	eF	201	PEB	C2C-CAC-CBC-CGC
29	gF	201	PEB	C2C-CAC-CBC-CGC
29	iF	201	PEB	C2C-CAC-CBC-CGC
29	kF	201	PEB	C2C-CAC-CBC-CGC
29	mF	201	PEB	C2C-CAC-CBC-CGC
29	MG	405	PEB	ND-C1D-CHC-C4C
29	PI	201	PEB	C2C-CAC-CBC-CGC
29	RI	201	PEB	C2C-CAC-CBC-CGC
29	TI	201	PEB	C2C-CAC-CBC-CGC
29	YI	201	PEB	C2C-CAC-CBC-CGC
29	aI	201	PEB	C2C-CAC-CBC-CGC
29	cI	201	PEB	C2C-CAC-CBC-CGC
29	eI	201	PEB	C2C-CAC-CBC-CGC
29	gI	201	PEB	C2C-CAC-CBC-CGC
29	iI	201	PEB	C2C-CAC-CBC-CGC
29	kI	201	PEB	C2C-CAC-CBC-CGC
29	mI	201	PEB	C2C-CAC-CBC-CGC
29	PK	202	PEB	C2C-CAC-CBC-CGC
29	RK	202	PEB	C2C-CAC-CBC-CGC
29	UK	201	PEB	C2C-CAC-CBC-CGC
29	VK	202	PEB	C2C-CAC-CBC-CGC
29	ZK	201	PEB	C2C-CAC-CBC-CGC
29	aK	202	PEB	C2C-CAC-CBC-CGC
29	cK	202	PEB	C2C-CAC-CBC-CGC
29	eK	202	PEB	C2C-CAC-CBC-CGC
29	gK	202	PEB	C2C-CAC-CBC-CGC
29	iK	202	PEB	C2C-CAC-CBC-CGC
29	jK	203	PEB	C2C-CAC-CBC-CGC
29	kK	202	PEB	C2C-CAC-CBC-CGC

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Mol	Chain	Res	Type	Atoms
29	CM	201	PEB	C2C-CAC-CBC-CGC
29	CM	202	PEB	C2C-CAC-CBC-CGC
29	EM	201	PEB	C2C-CAC-CBC-CGC
29	EM	202	PEB	C2C-CAC-CBC-CGC
29	GM	201	PEB	C2C-CAC-CBC-CGC
29	GM	202	PEB	C2C-CAC-CBC-CGC
29	IM	201	PEB	C2C-CAC-CBC-CGC
29	IM	202	PEB	C2C-CAC-CBC-CGC
29	KM	201	PEB	C2C-CAC-CBC-CGC
29	KM	202	PEB	C2C-CAC-CBC-CGC
29	MM	201	PEB	C2C-CAC-CBC-CGC
29	MM	202	PEB	C2C-CAC-CBC-CGC
29	OM	201	PEB	C2C-CAC-CBC-CGC
29	OM	202	PEB	C2C-CAC-CBC-CGC
29	QM	203	PEB	C2C-CAC-CBC-CGC
29	QM	204	PEB	C2C-CAC-CBC-CGC
29	SM	201	PEB	C2C-CAC-CBC-CGC
29	SM	202	PEB	C2C-CAC-CBC-CGC
29	UM	201	PEB	C2C-CAC-CBC-CGC
29	WM	201	PEB	C2C-CAC-CBC-CGC
29	WM	202	PEB	C2C-CAC-CBC-CGC
29	YM	202	PEB	C2C-CAC-CBC-CGC
29	YM	203	PEB	C2C-CAC-CBC-CGC
29	aM	201	PEB	C2C-CAC-CBC-CGC
29	aM	202	PEB	C2C-CAC-CBC-CGC
29	dM	201	PEB	C2C-CAC-CBC-CGC
29	dM	202	PEB	C2C-CAC-CBC-CGC
29	fM	201	PEB	C2C-CAC-CBC-CGC
29	fM	202	PEB	C2C-CAC-CBC-CGC
29	hM	201	PEB	C2C-CAC-CBC-CGC
29	hM	202	PEB	C2C-CAC-CBC-CGC
29	jM	201	PEB	C2C-CAC-CBC-CGC
29	jM	202	PEB	C2C-CAC-CBC-CGC
29	lM	201	PEB	C2C-CAC-CBC-CGC
29	lM	202	PEB	C2C-CAC-CBC-CGC
29	MQ	401	PEB	C2C-CAC-CBC-CGC
29	MQ	407	PEB	ND-C1D-CHC-C4C
30	A7	303	PUB	NA-C4A-CHA-C1B
30	A9	303	PUB	NA-C4A-CHA-C1B
29	J5	201	PEB	CAB-CBB-CGB-O2B
30	wJ	304	PUB	CAB-CBB-CGB-O2B
30	xJ	304	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
30	wL	304	PUB	CAB-CBB-CGB-O2B
30	xL	304	PUB	CAB-CBB-CGB-O2B
29	P7	203	PEB	CAB-CBB-CGB-O1B
29	R7	203	PEB	CAB-CBB-CGB-O1B
29	T7	203	PEB	CAB-CBB-CGB-O1B
29	V7	203	PEB	CAB-CBB-CGB-O1B
29	Y7	203	PEB	CAB-CBB-CGB-O1B
29	a7	203	PEB	CAB-CBB-CGB-O1B
29	c7	203	PEB	CAB-CBB-CGB-O1B
29	e7	203	PEB	CAB-CBB-CGB-O1B
29	g7	203	PEB	CAB-CBB-CGB-O1B
29	i7	203	PEB	CAB-CBB-CGB-O1B
29	k7	203	PEB	CAB-CBB-CGB-O1B
29	m7	203	PEB	CAB-CBB-CGB-O1B
29	P9	203	PEB	CAB-CBB-CGB-O1B
29	R9	203	PEB	CAB-CBB-CGB-O1B
29	T9	203	PEB	CAB-CBB-CGB-O1B
29	V9	203	PEB	CAB-CBB-CGB-O1B
29	Y9	203	PEB	CAB-CBB-CGB-O1B
29	a9	203	PEB	CAB-CBB-CGB-O1B
29	c9	203	PEB	CAB-CBB-CGB-O1B
29	e9	203	PEB	CAB-CBB-CGB-O1B
29	g9	203	PEB	CAB-CBB-CGB-O1B
29	i9	203	PEB	CAB-CBB-CGB-O1B
29	k9	203	PEB	CAB-CBB-CGB-O1B
29	m9	203	PEB	CAB-CBB-CGB-O1B
29	BA	202	PEB	C4B-C3B-CAB-CBB
29	DA	202	PEB	C4B-C3B-CAB-CBB
29	FA	202	PEB	C4B-C3B-CAB-CBB
29	HA	202	PEB	C4B-C3B-CAB-CBB
29	JA	202	PEB	C4B-C3B-CAB-CBB
29	LA	202	PEB	C4B-C3B-CAB-CBB
29	BN	202	PEB	C4B-C3B-CAB-CBB
29	DN	202	PEB	C4B-C3B-CAB-CBB
29	FN	202	PEB	C4B-C3B-CAB-CBB
29	HN	202	PEB	C4B-C3B-CAB-CBB
29	JN	202	PEB	C4B-C3B-CAB-CBB
29	LN	202	PEB	C4B-C3B-CAB-CBB
29	B4	202	PEB	C3B-CAB-CBB-CGB
29	D4	202	PEB	C3B-CAB-CBB-CGB
29	F4	202	PEB	C3B-CAB-CBB-CGB
29	H4	202	PEB	C3B-CAB-CBB-CGB

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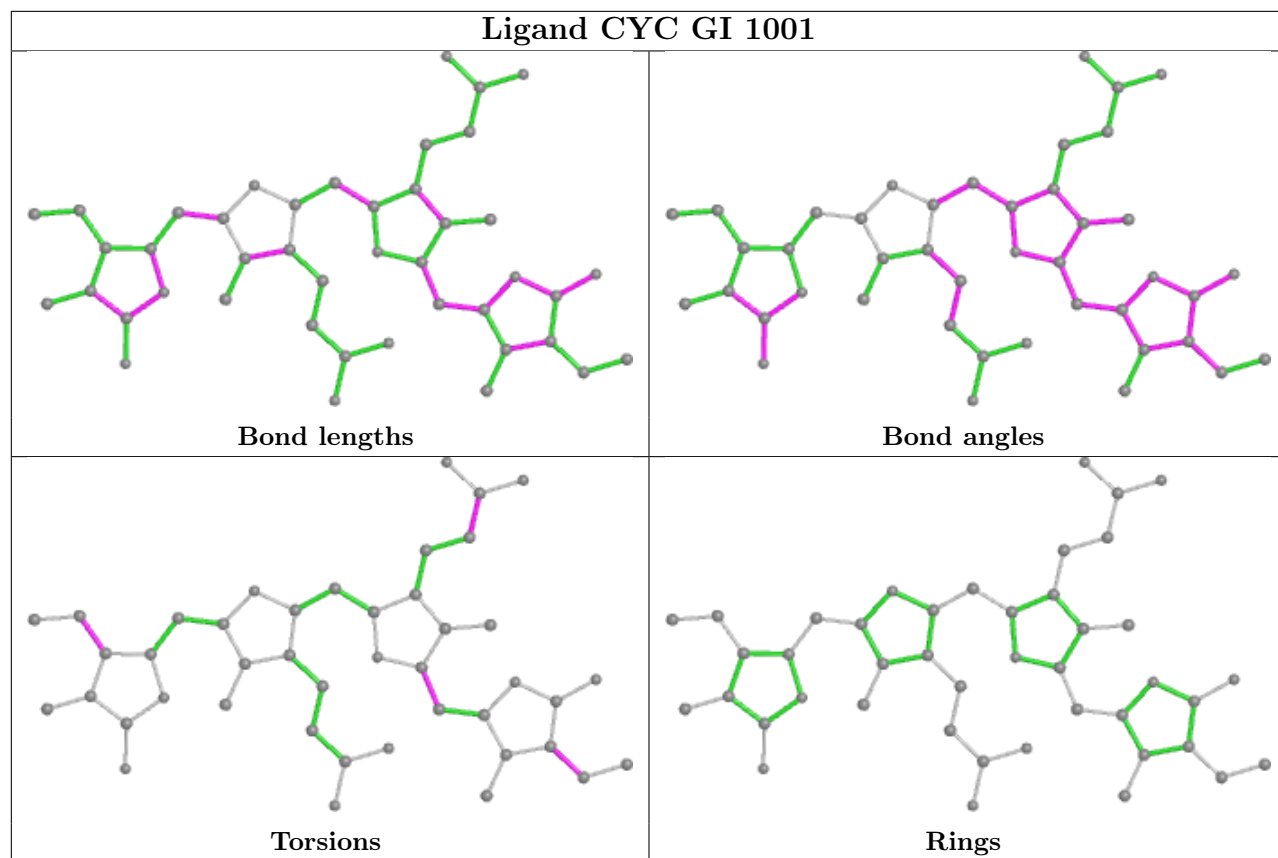
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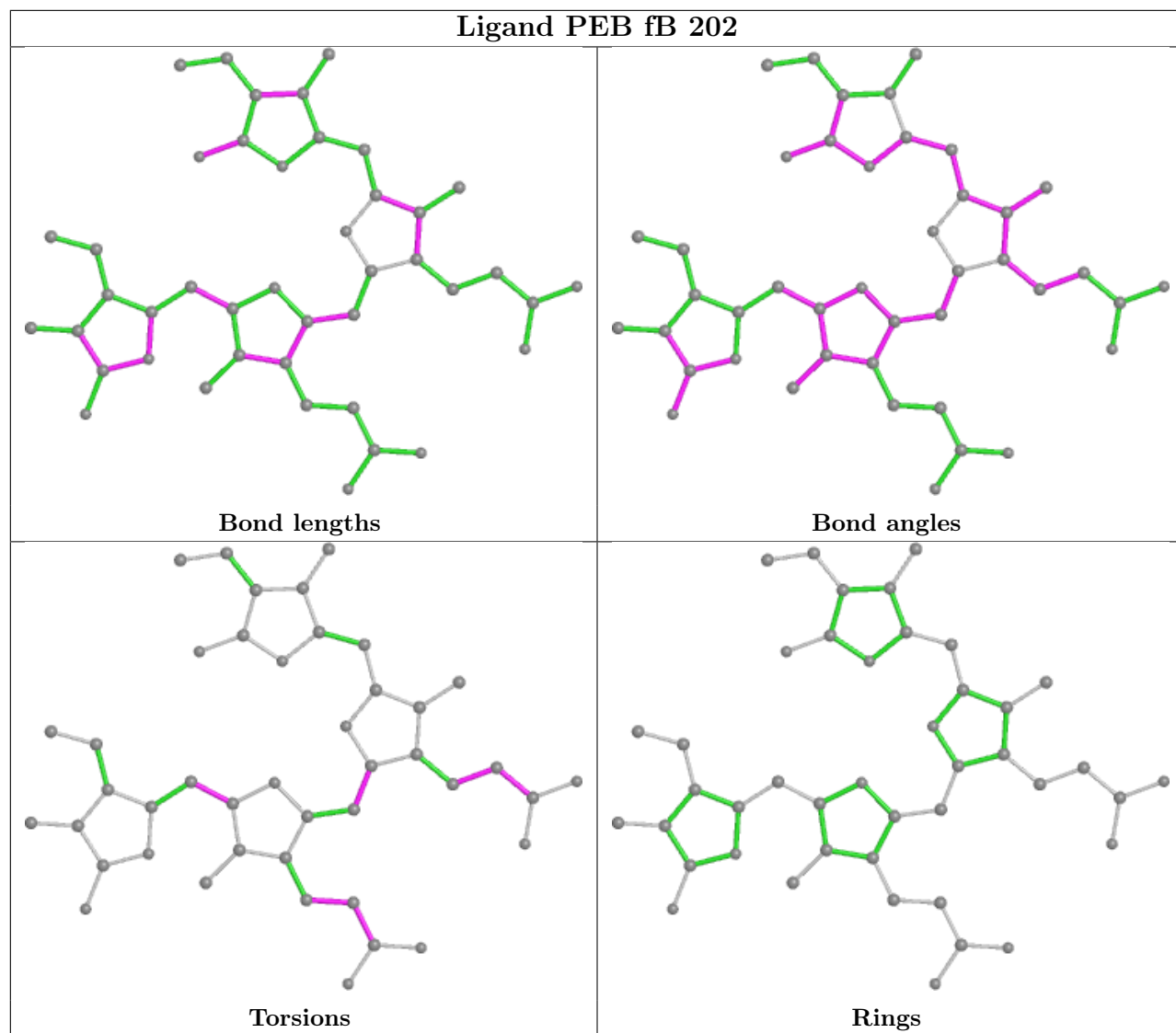
Mol	Chain	Res	Type	Atoms
29	J4	202	PEB	C3B-CAB-CBB-CGB
29	L4	202	PEB	C3B-CAB-CBB-CGB
29	BD	202	PEB	C3B-CAB-CBB-CGB
29	DD	202	PEB	C3B-CAB-CBB-CGB
29	FD	202	PEB	C3B-CAB-CBB-CGB
29	HD	202	PEB	C3B-CAB-CBB-CGB
29	JD	202	PEB	C3B-CAB-CBB-CGB
29	LD	202	PEB	C3B-CAB-CBB-CGB
29	M3	201	PEB	CAC-CBC-CGC-O1C
29	N3	201	PEB	CAC-CBC-CGC-O1C
29	MO	201	PEB	CAC-CBC-CGC-O1C
29	NO	201	PEB	CAC-CBC-CGC-O1C

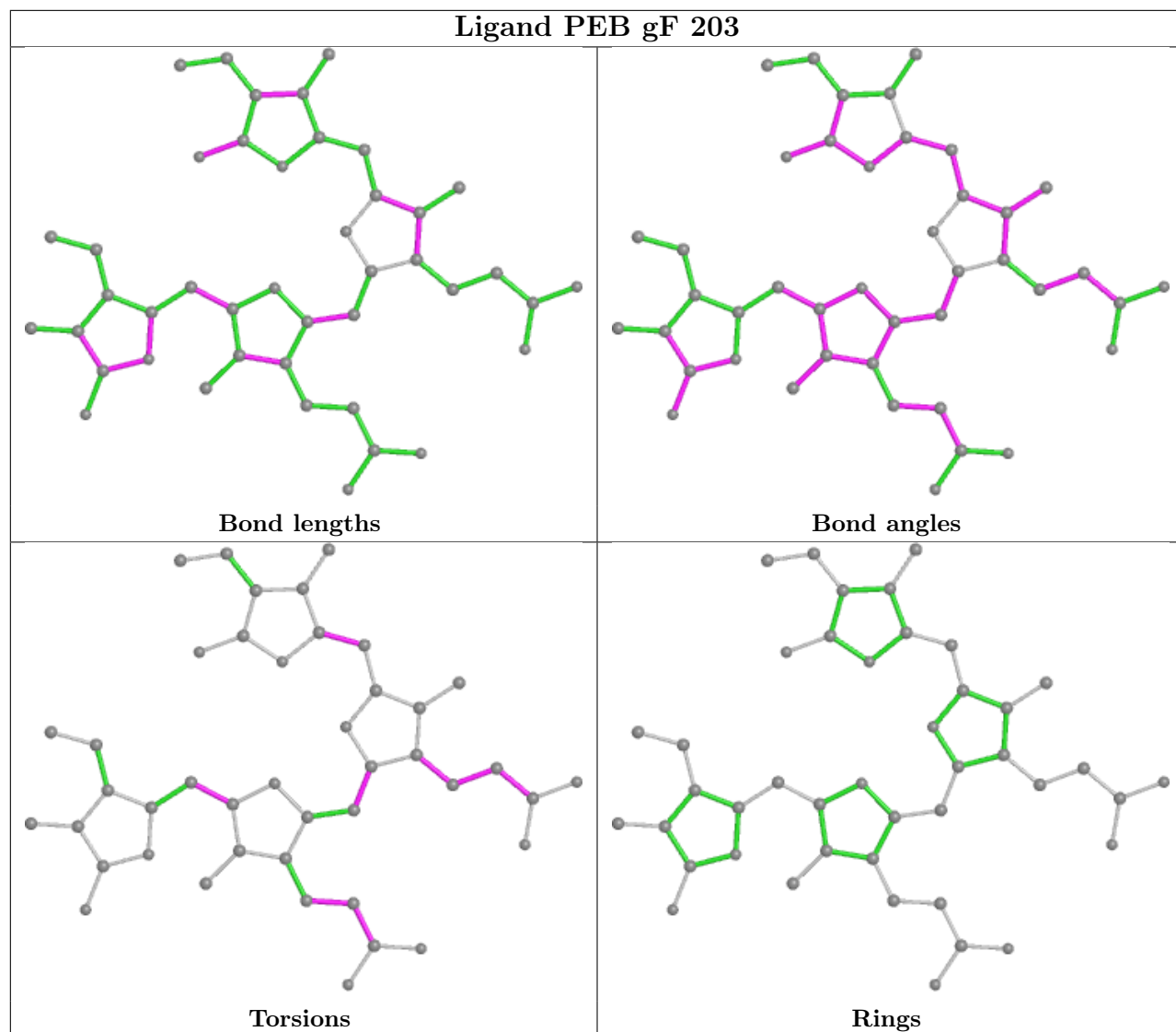
There are no ring outliers.

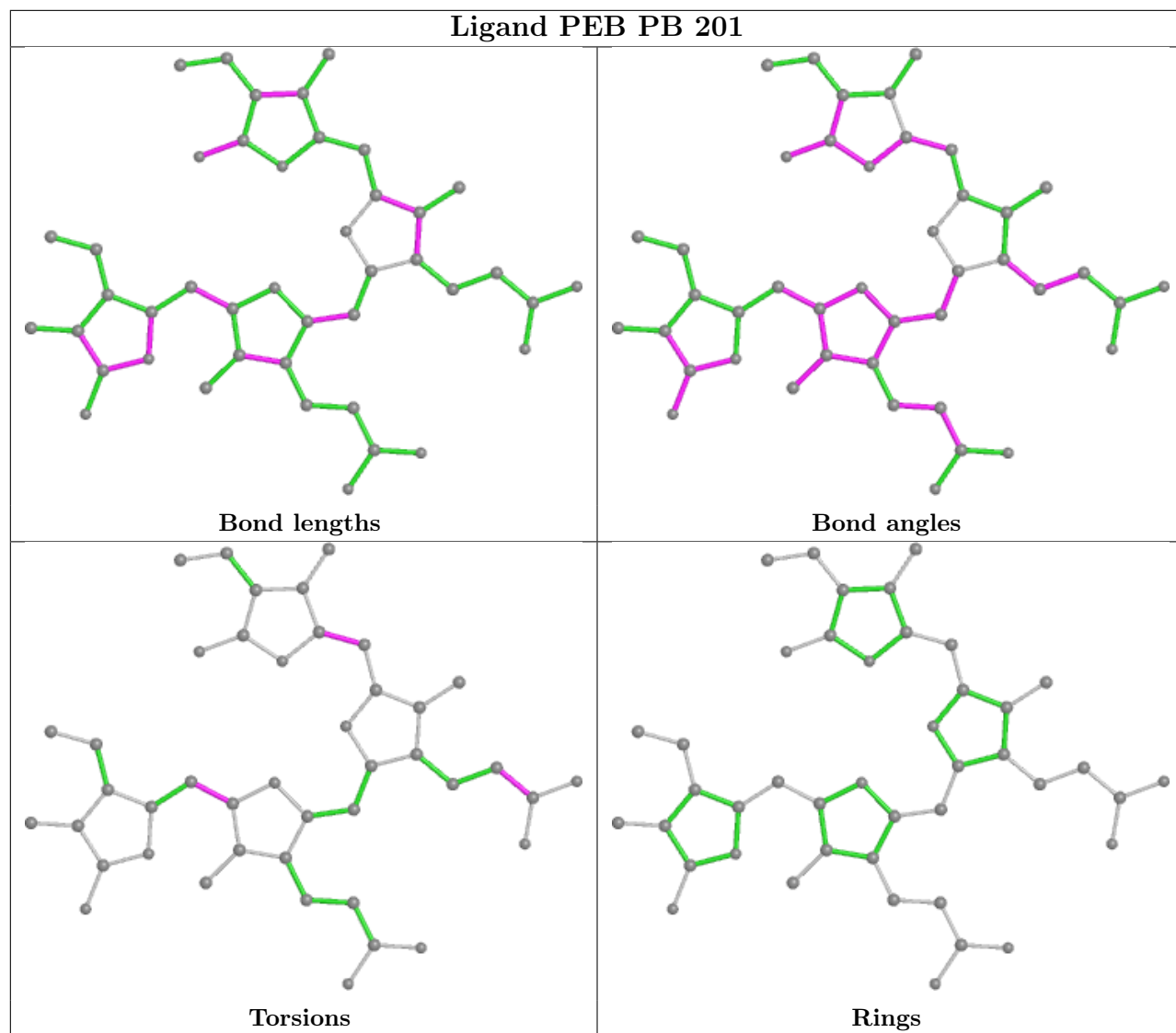
No monomer is involved in short contacts.

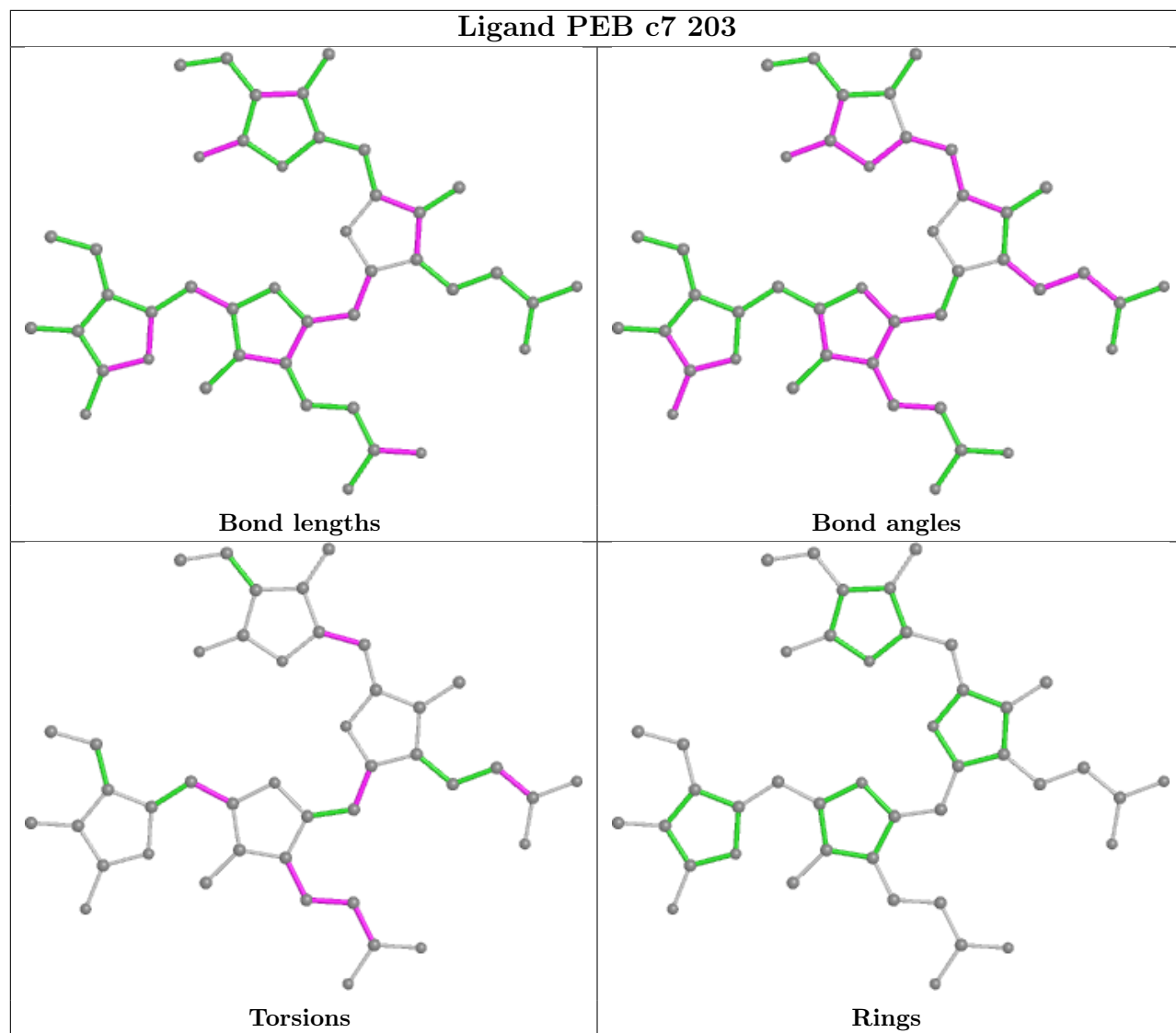
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

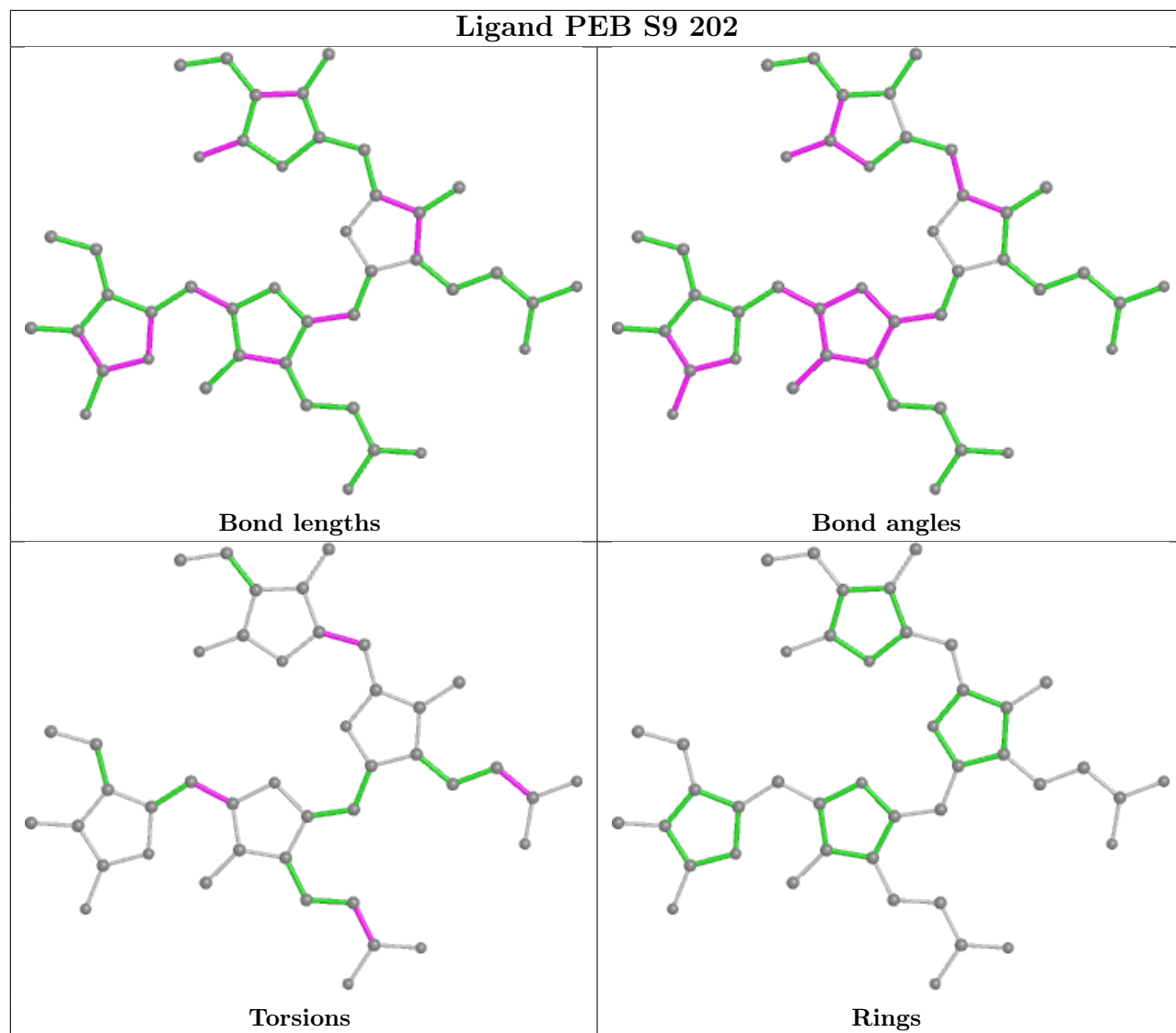


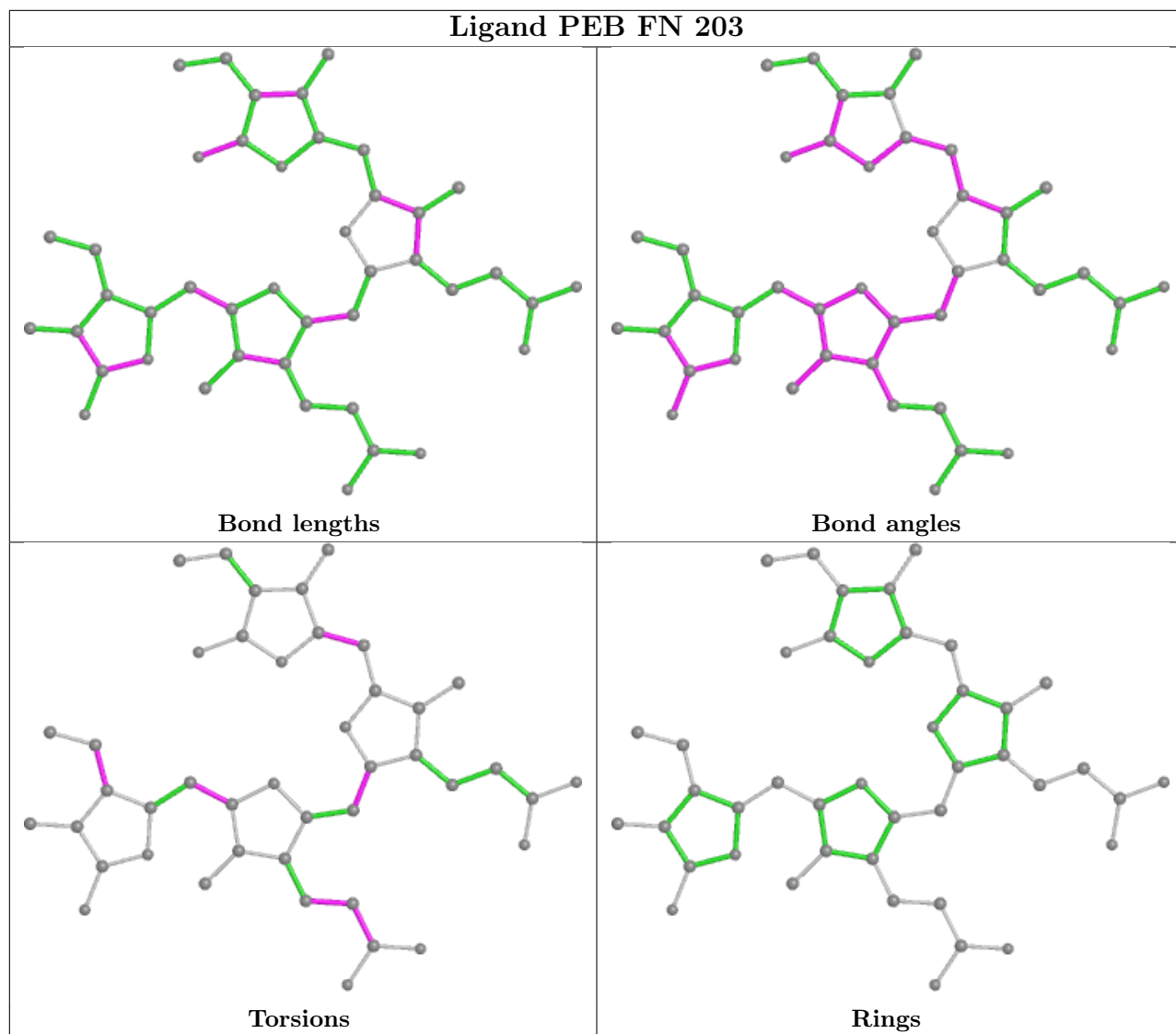


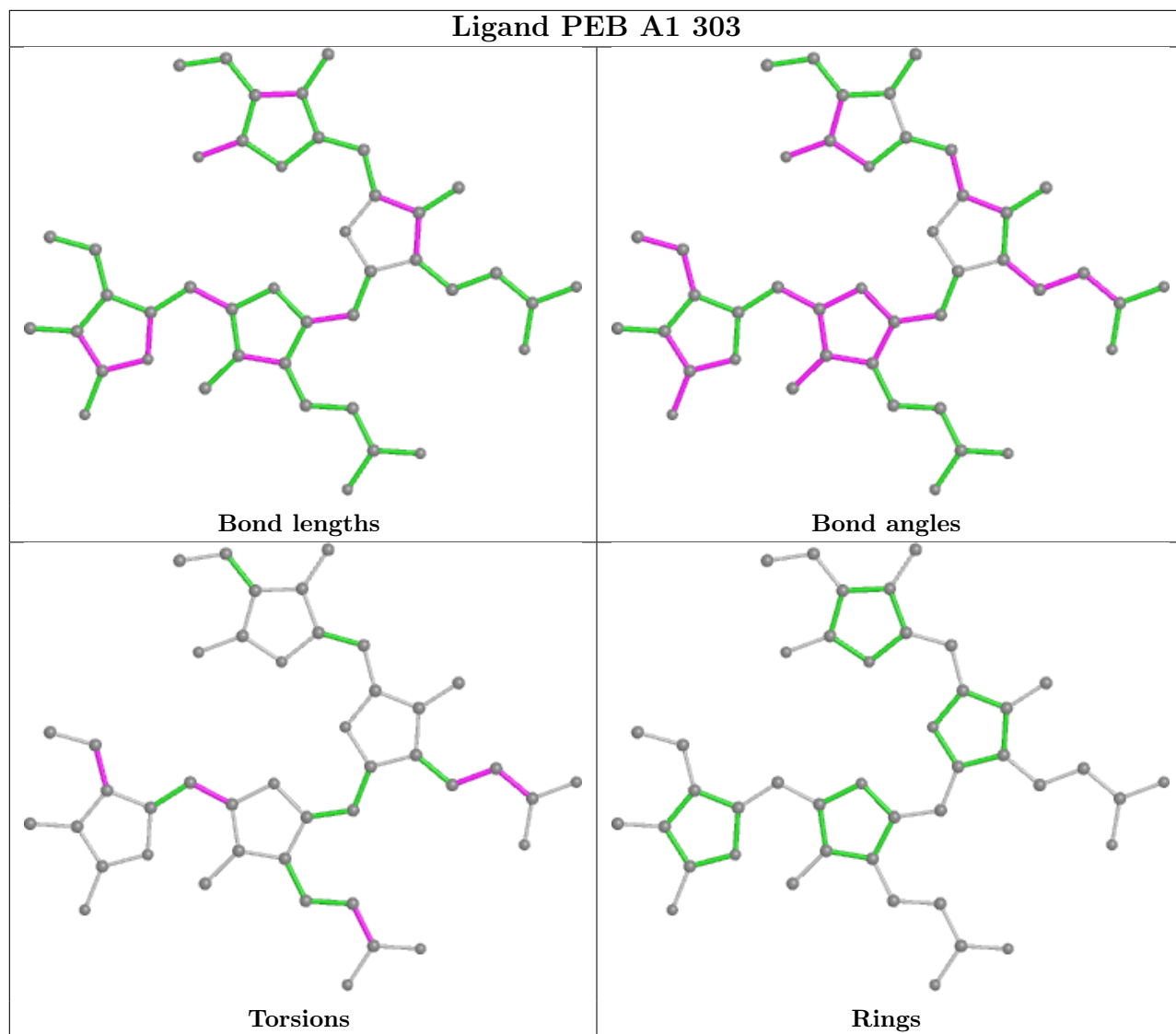


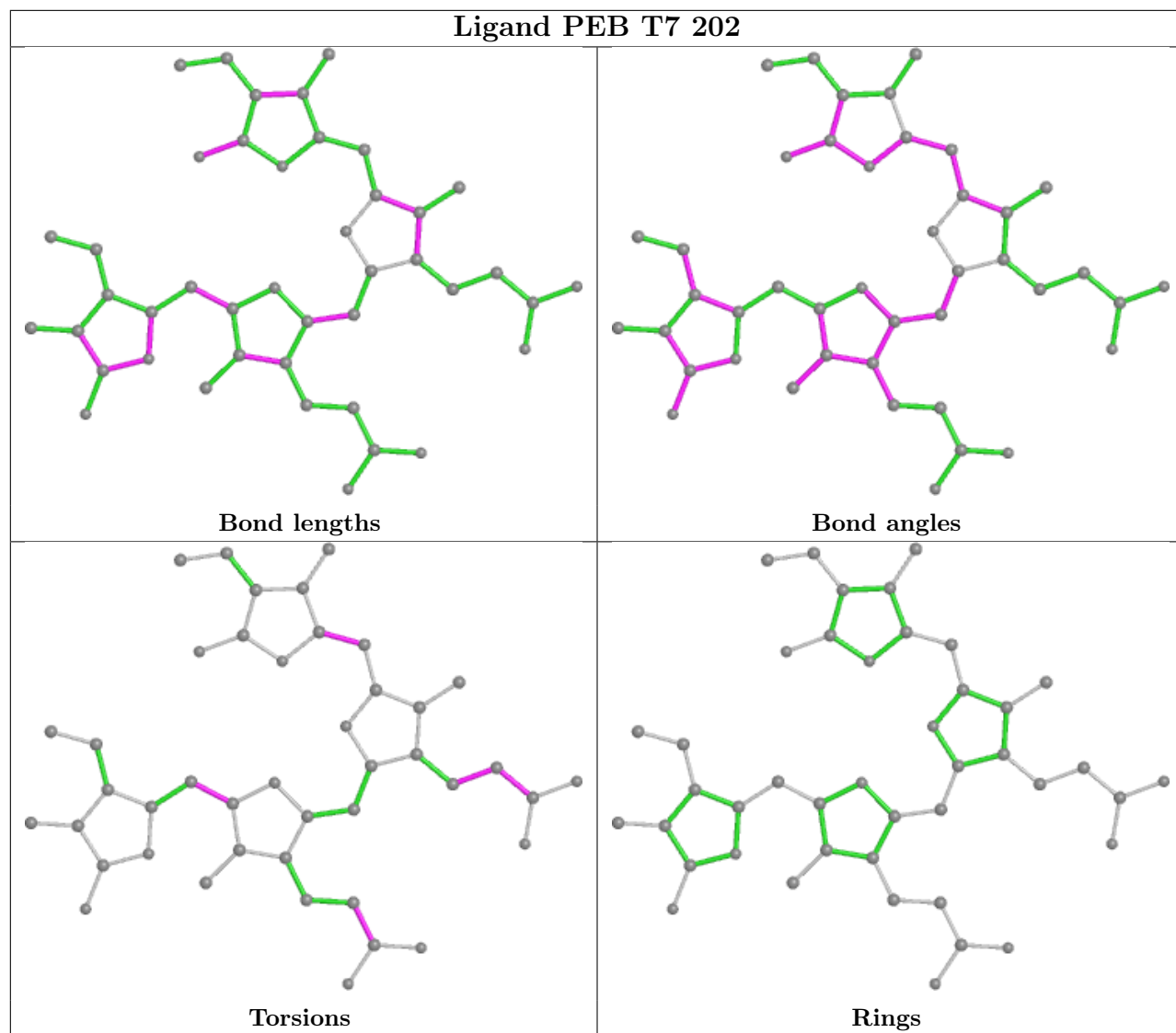


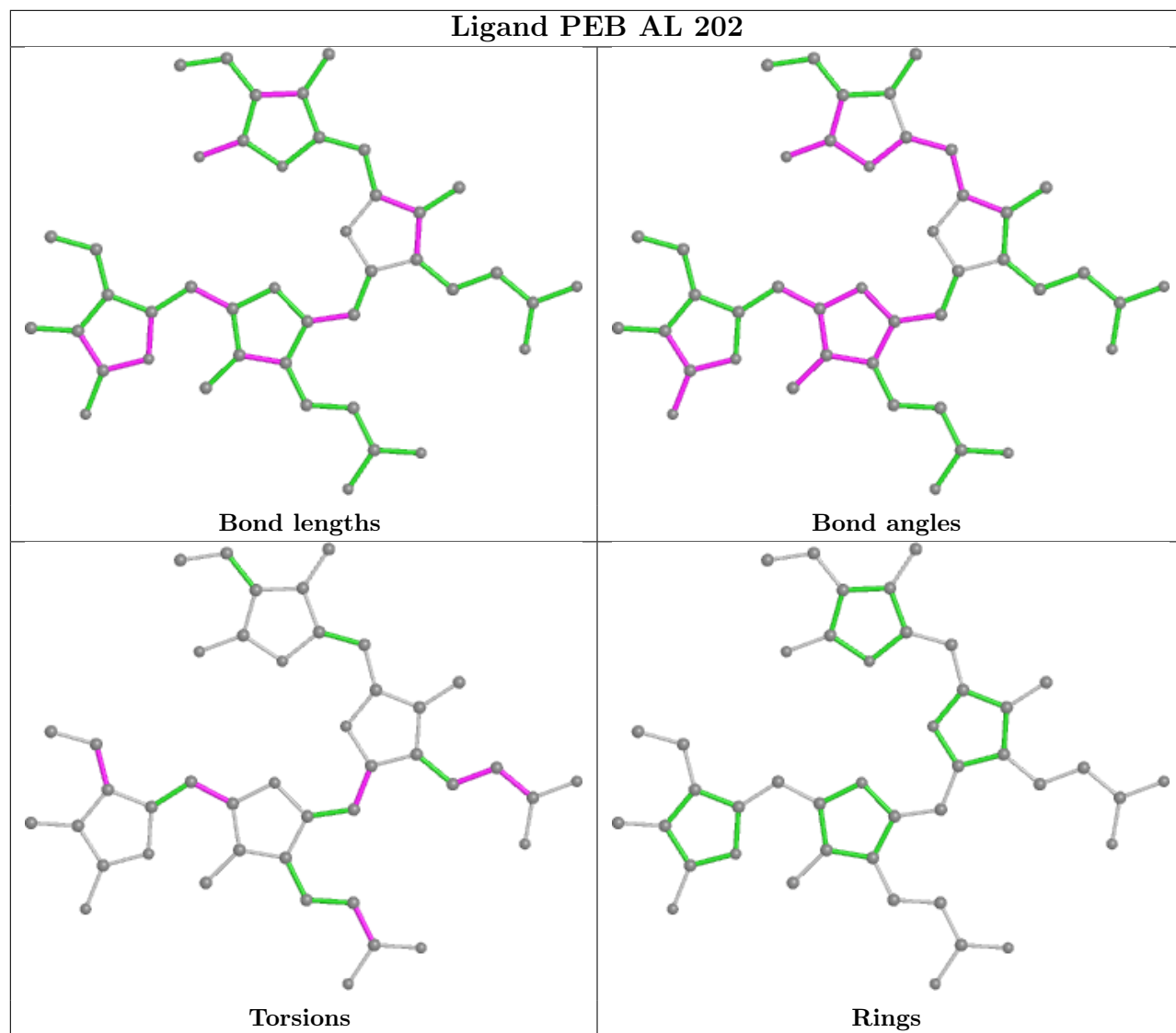


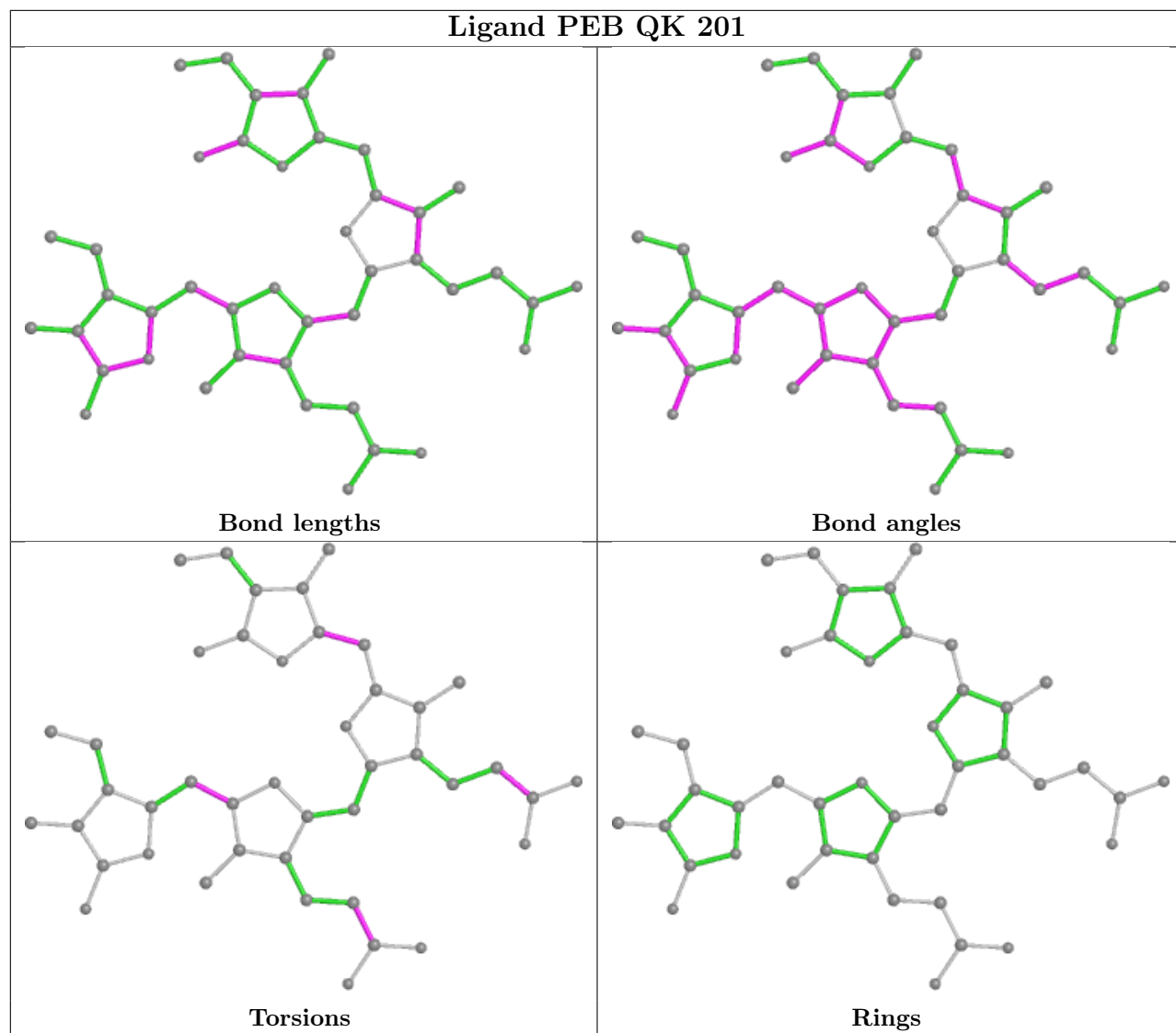


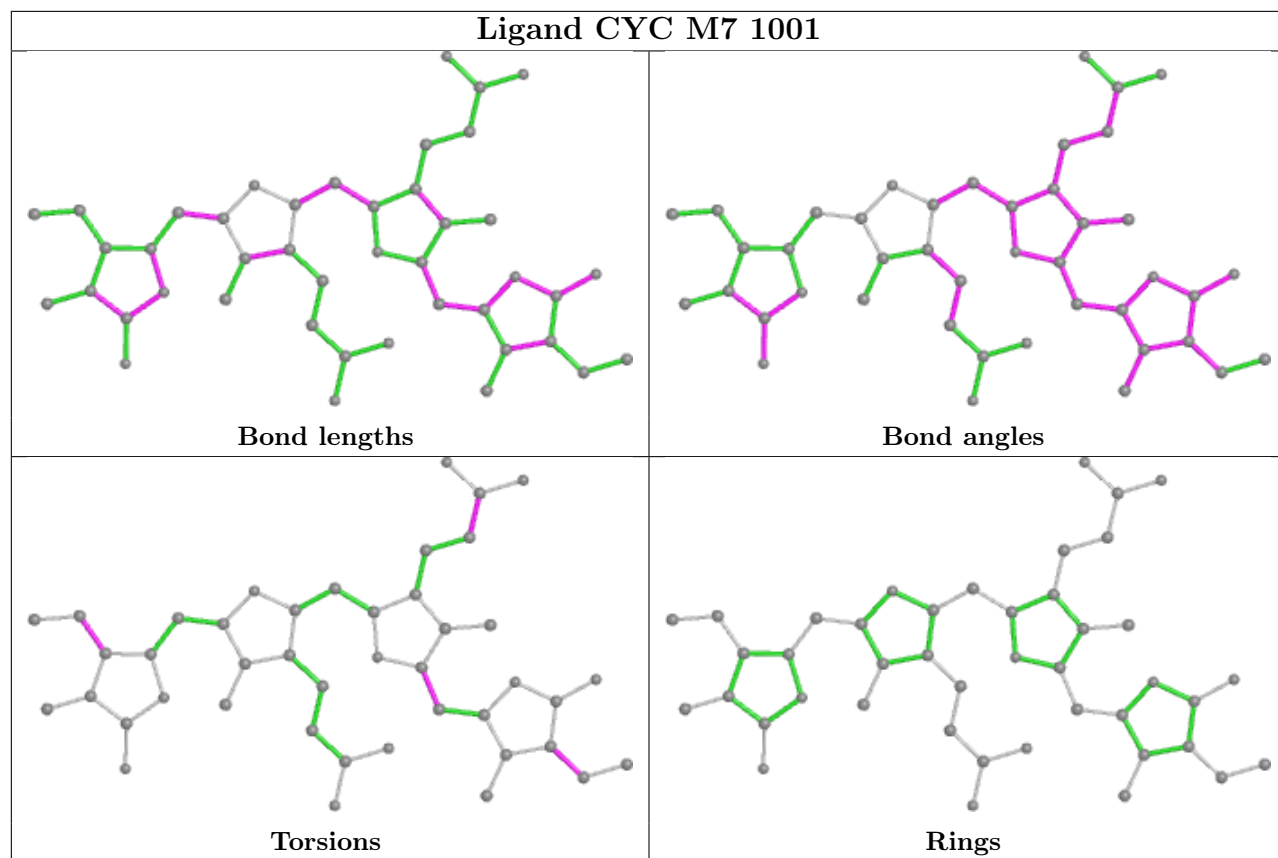


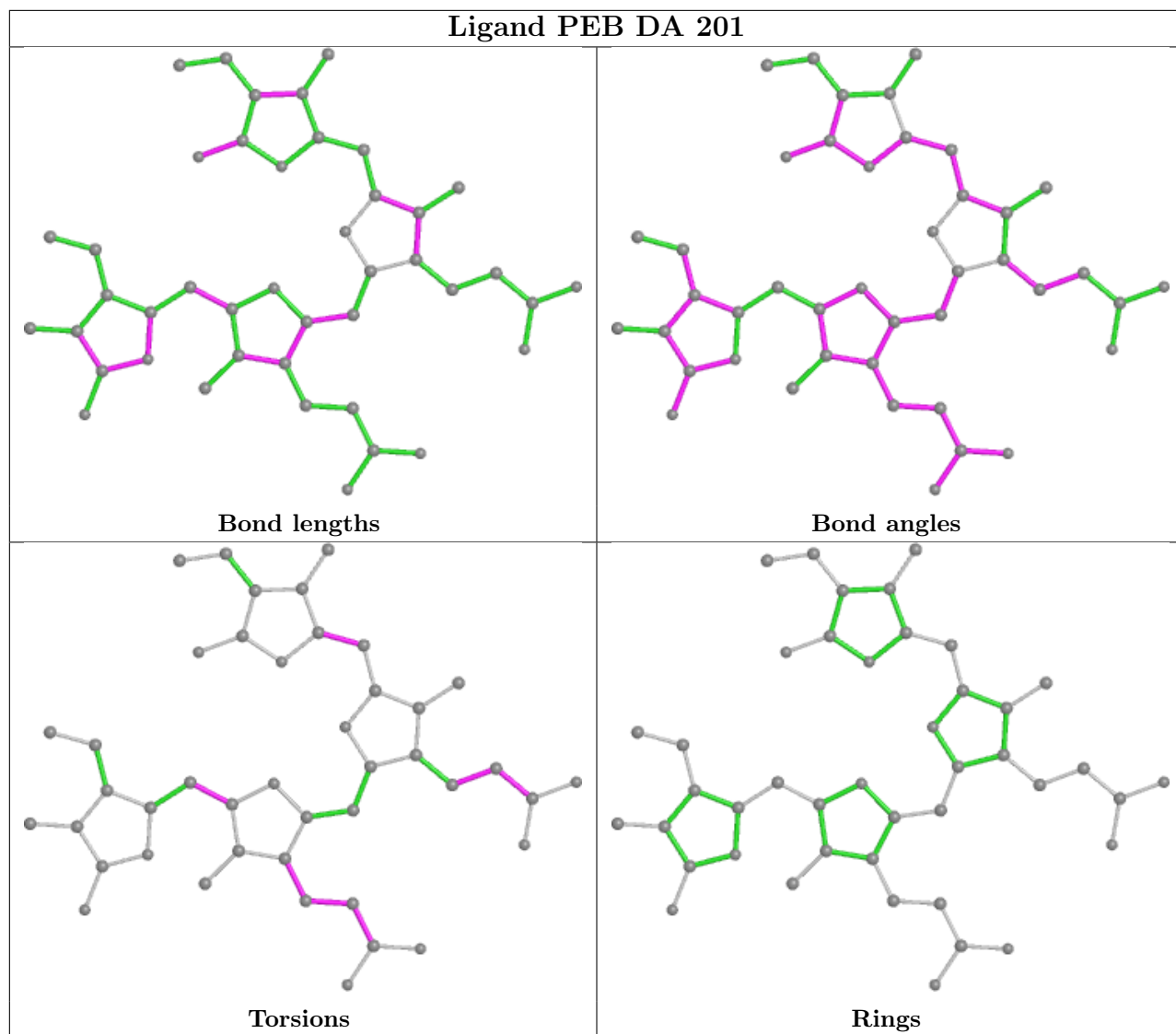


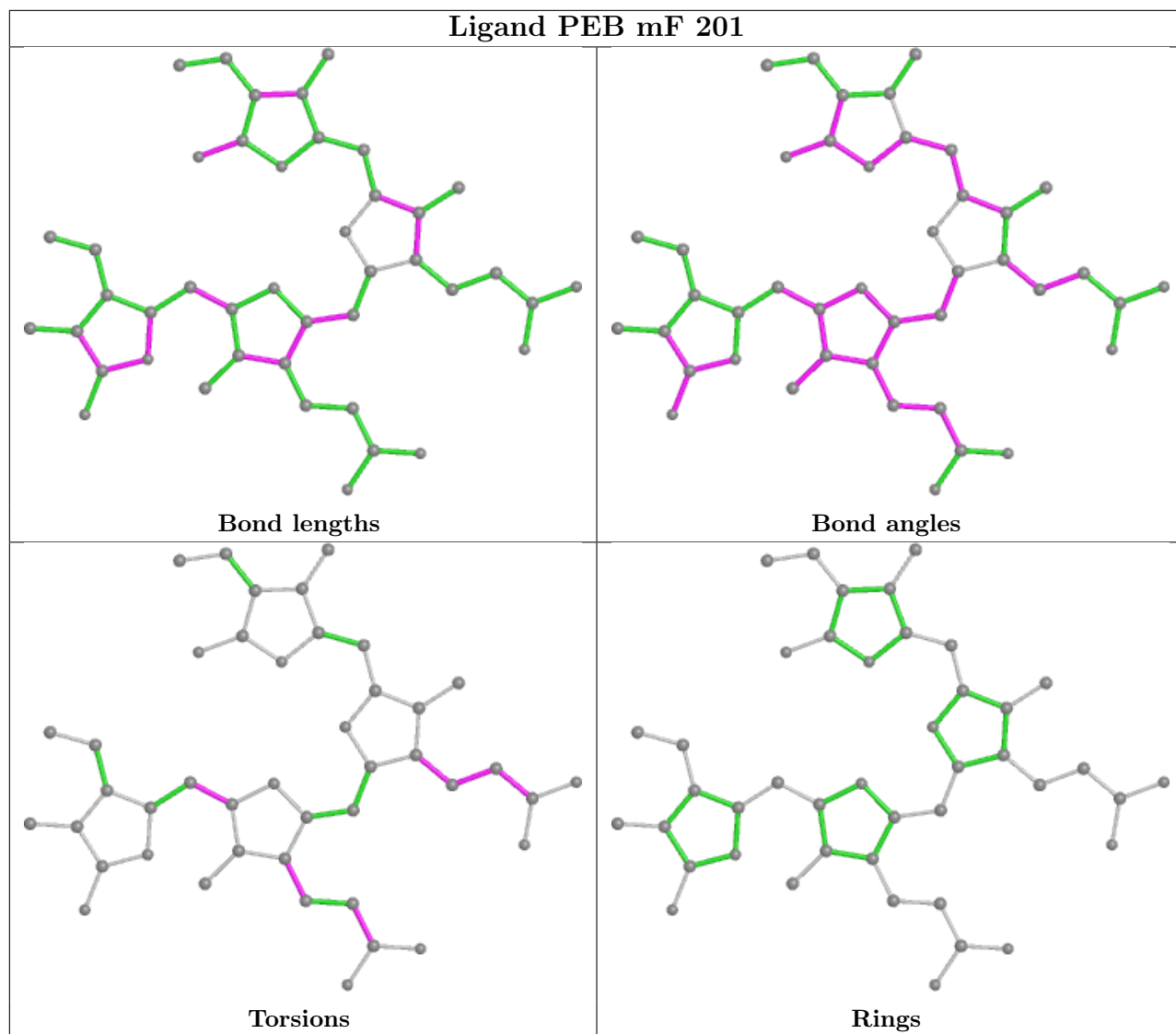


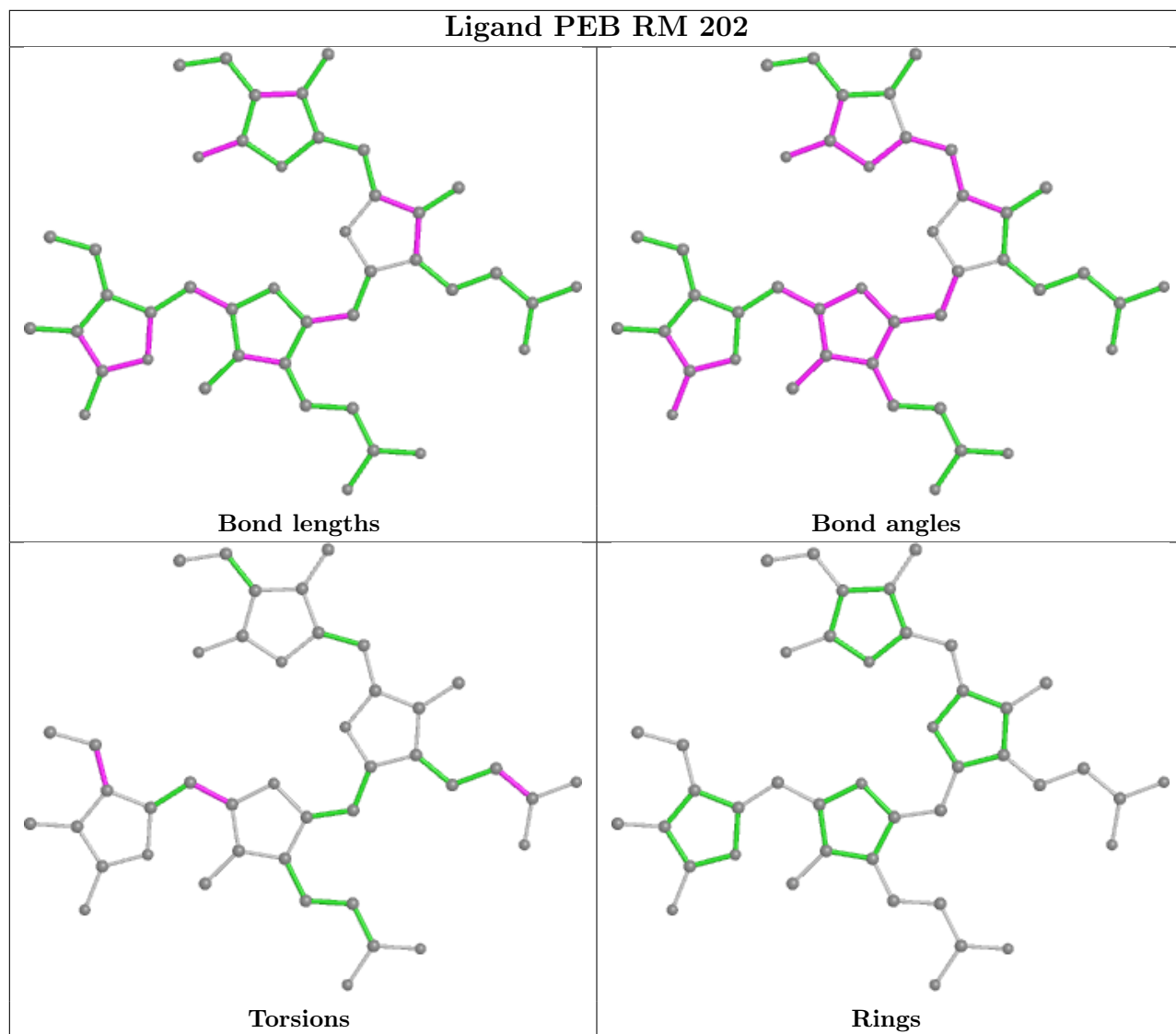


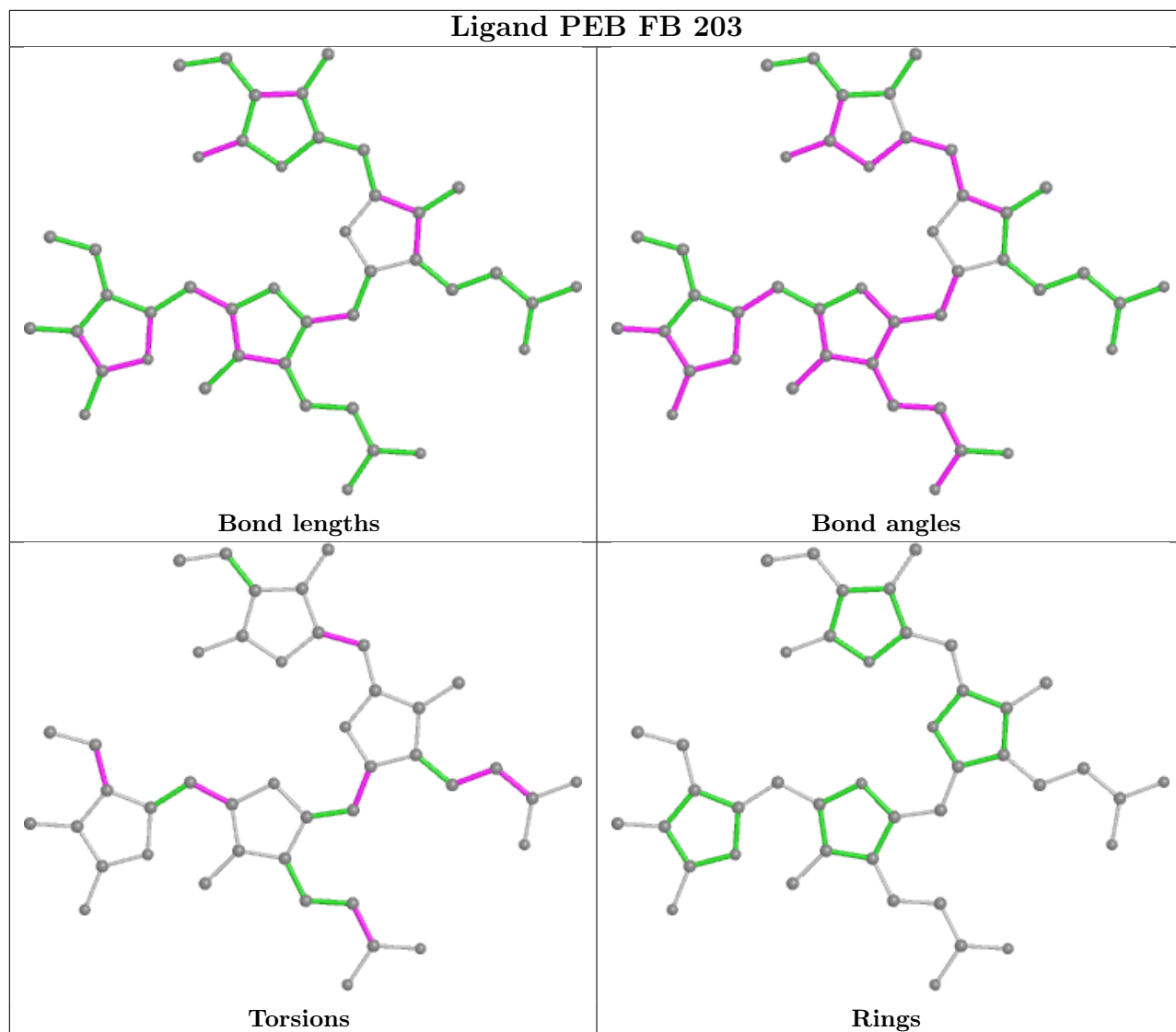


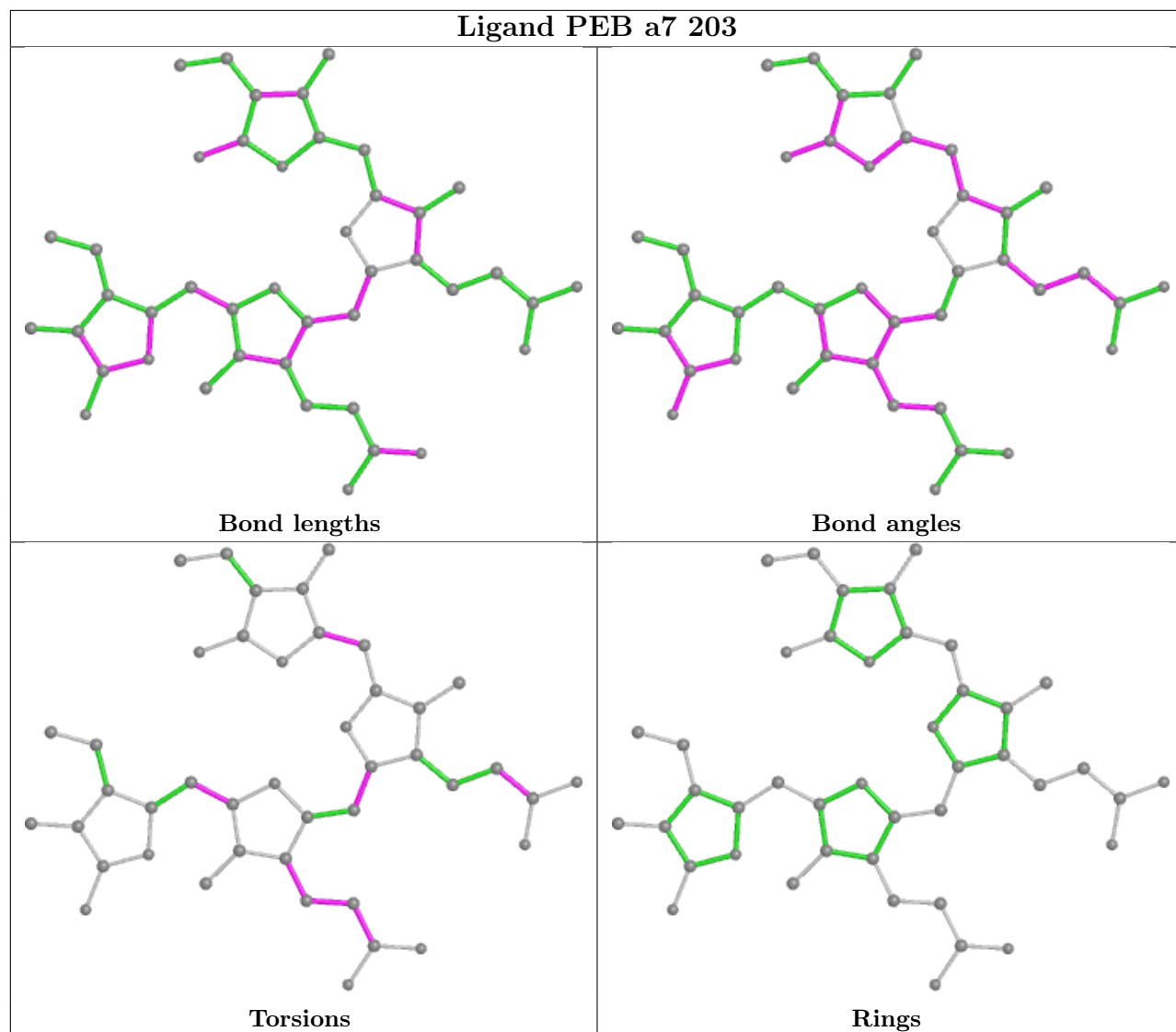


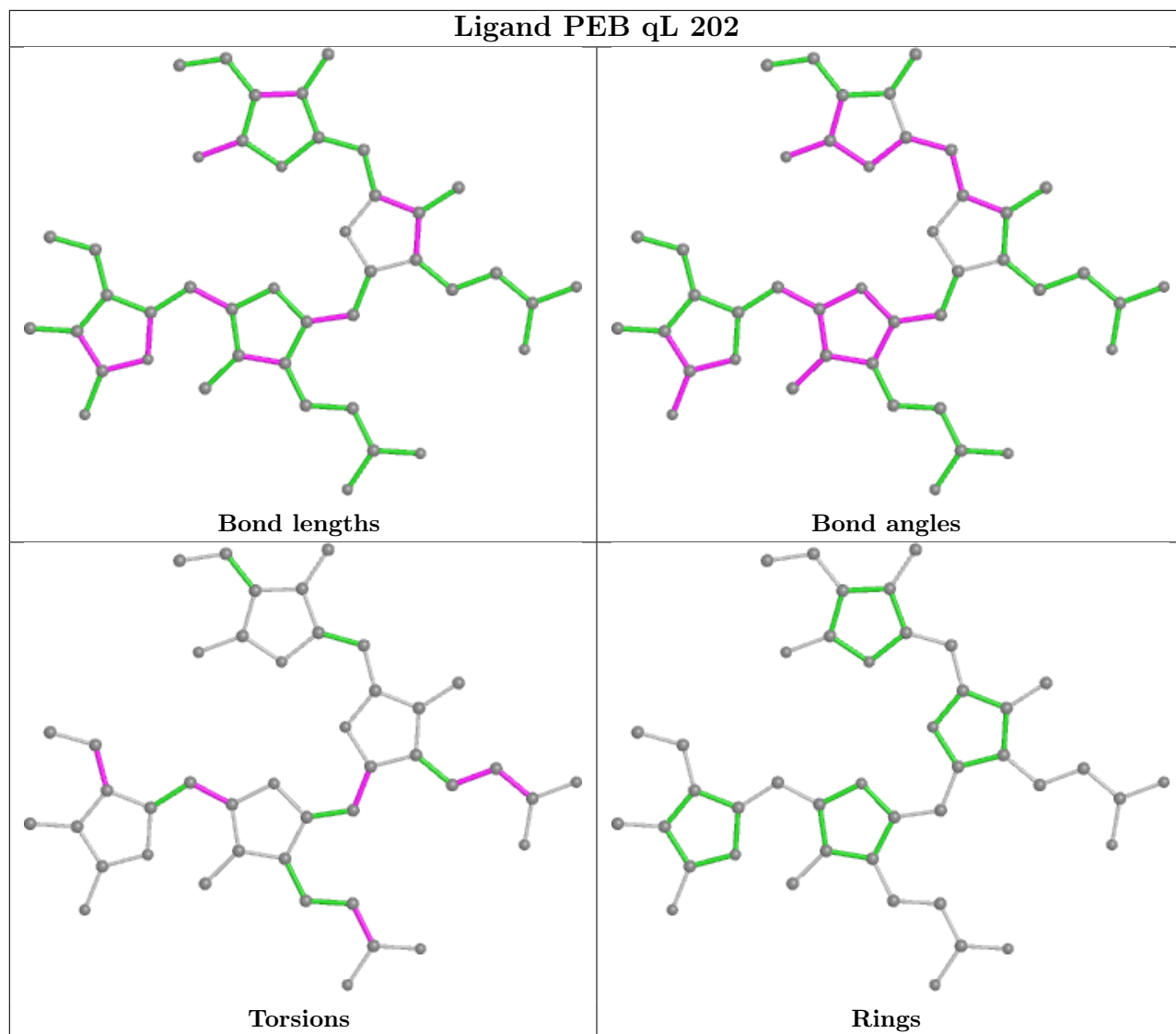


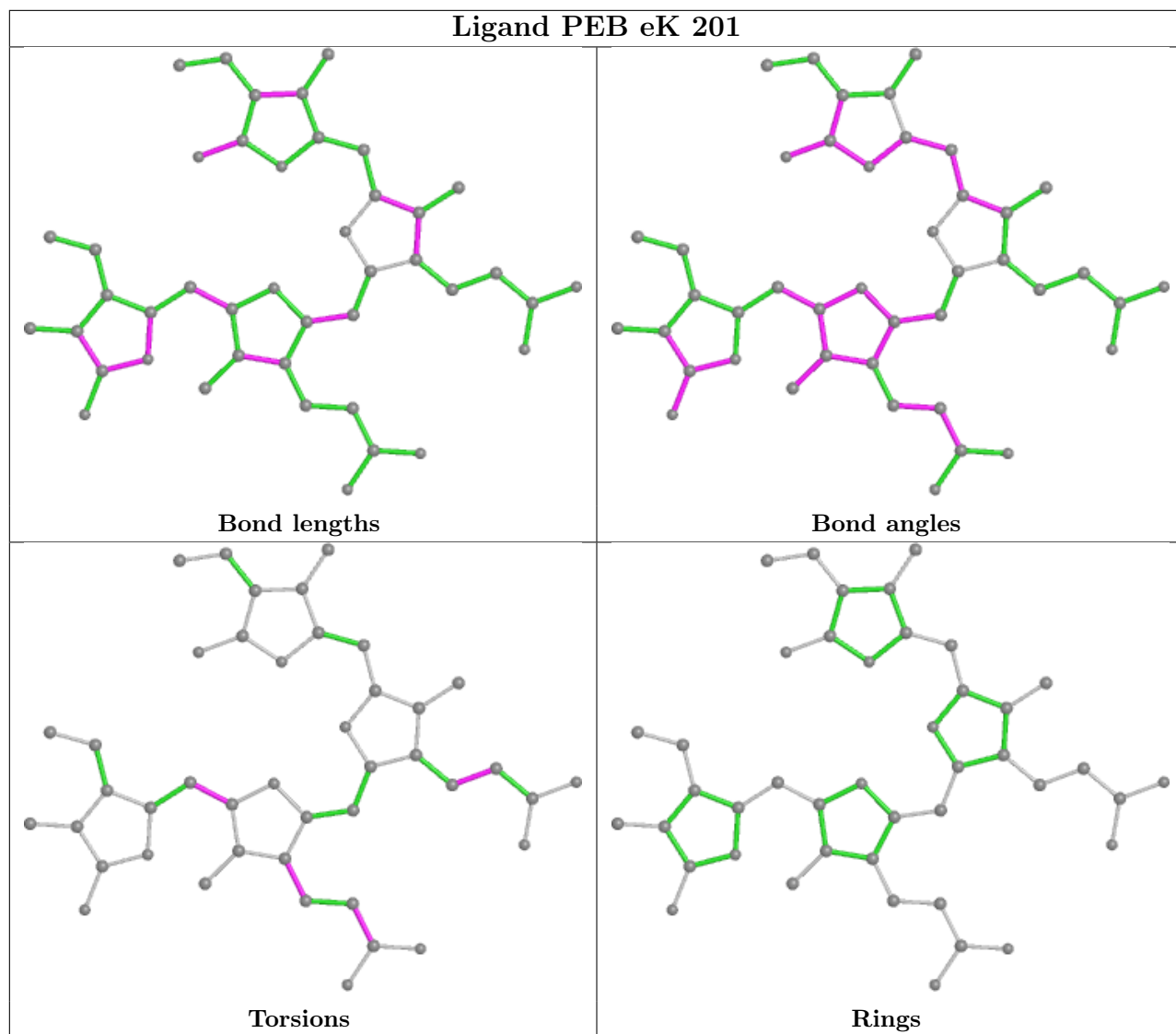


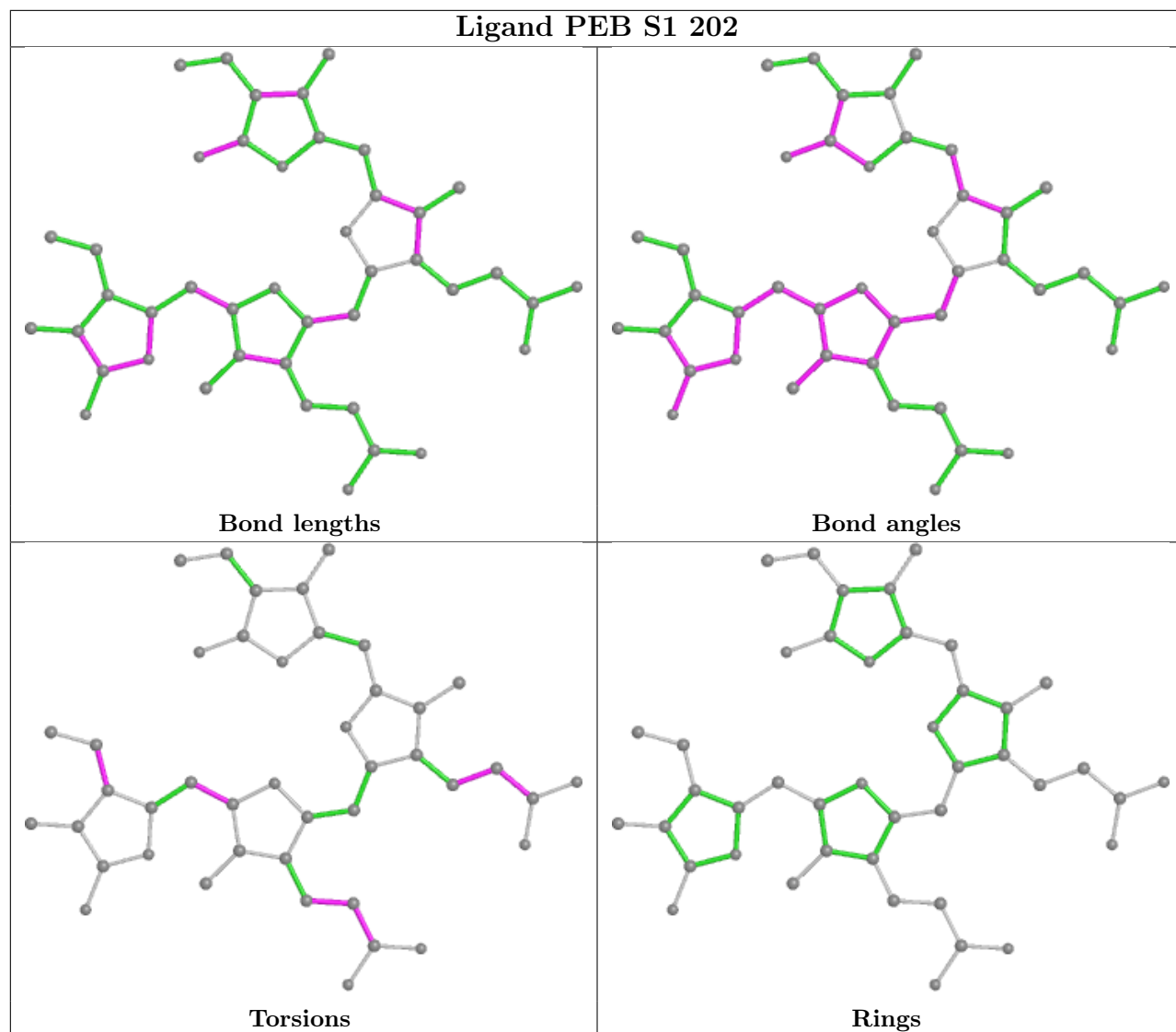


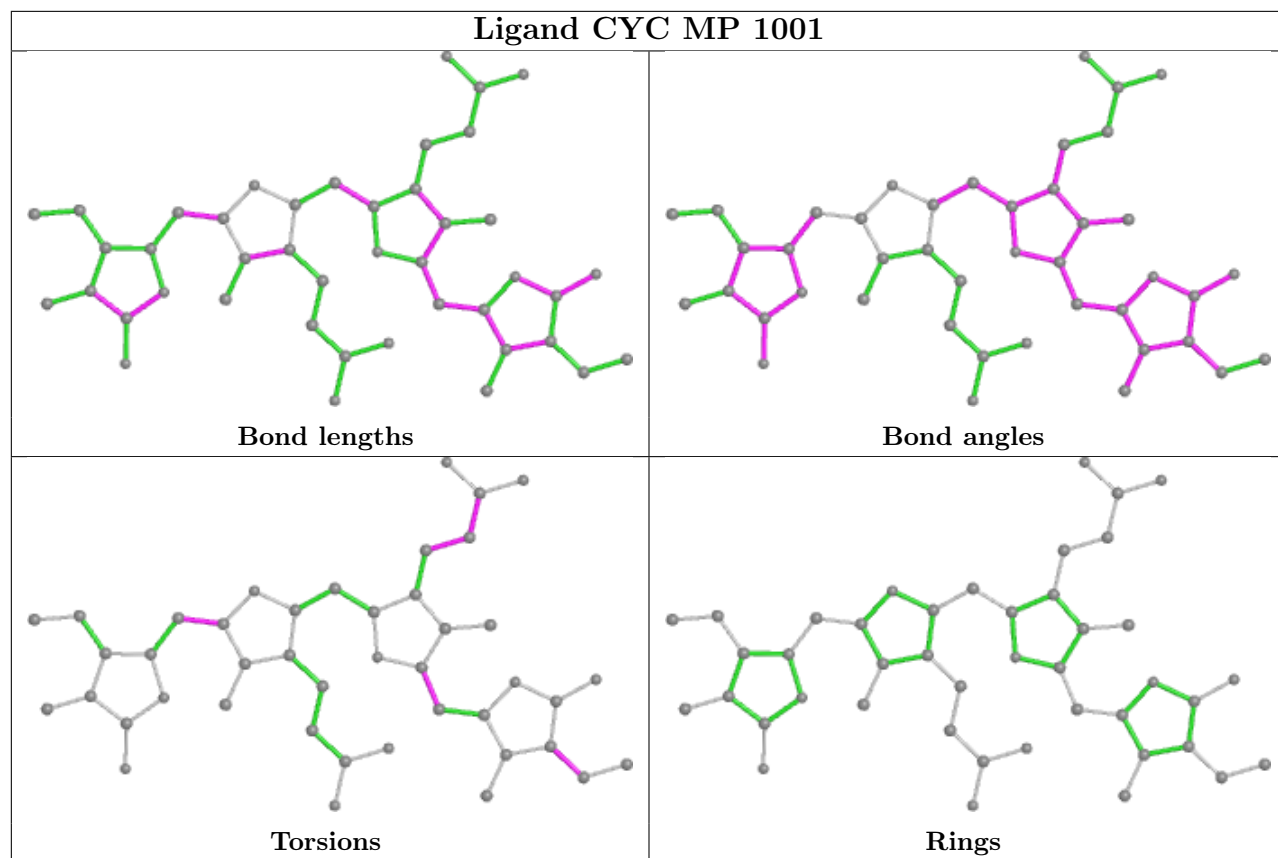


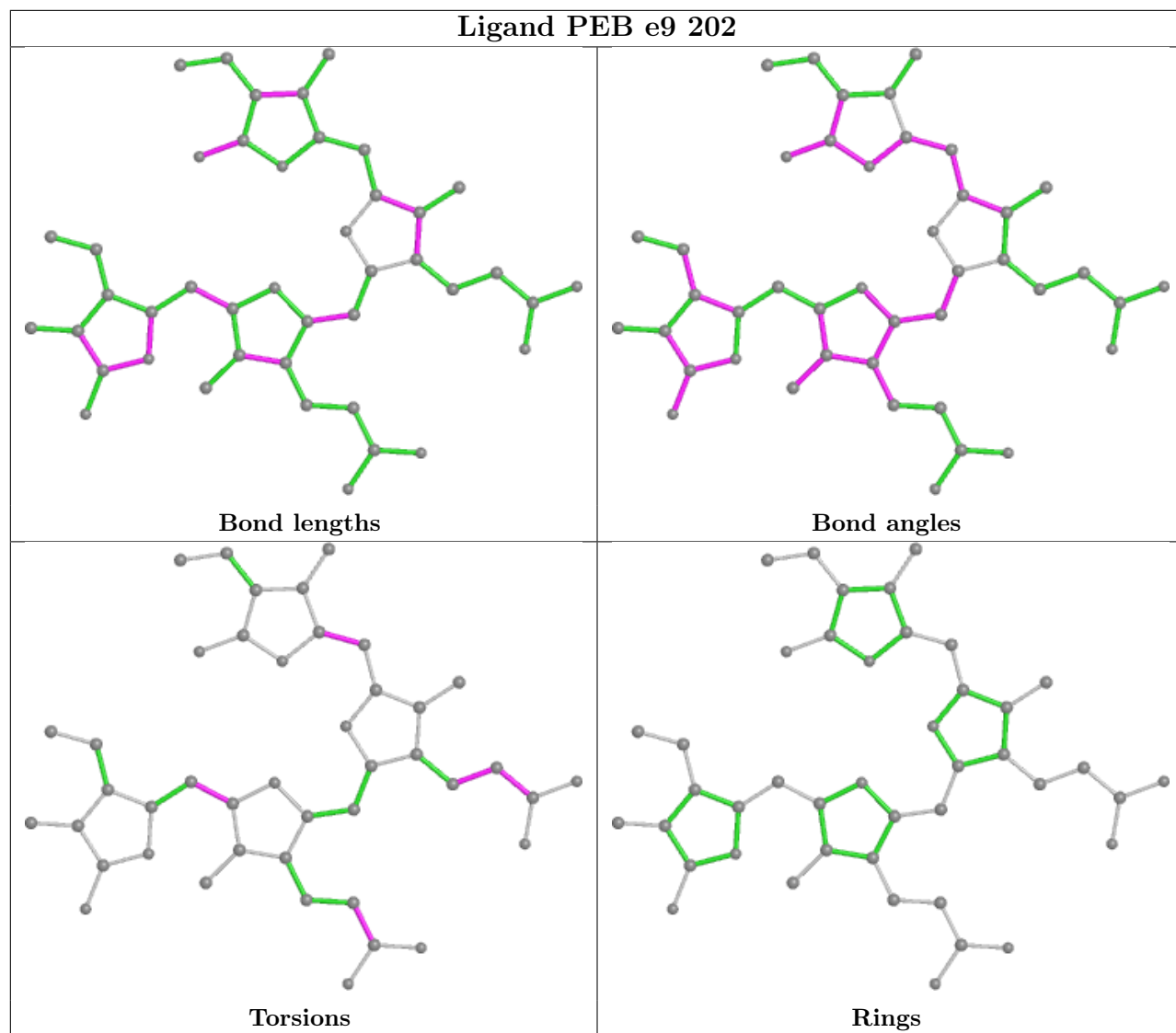


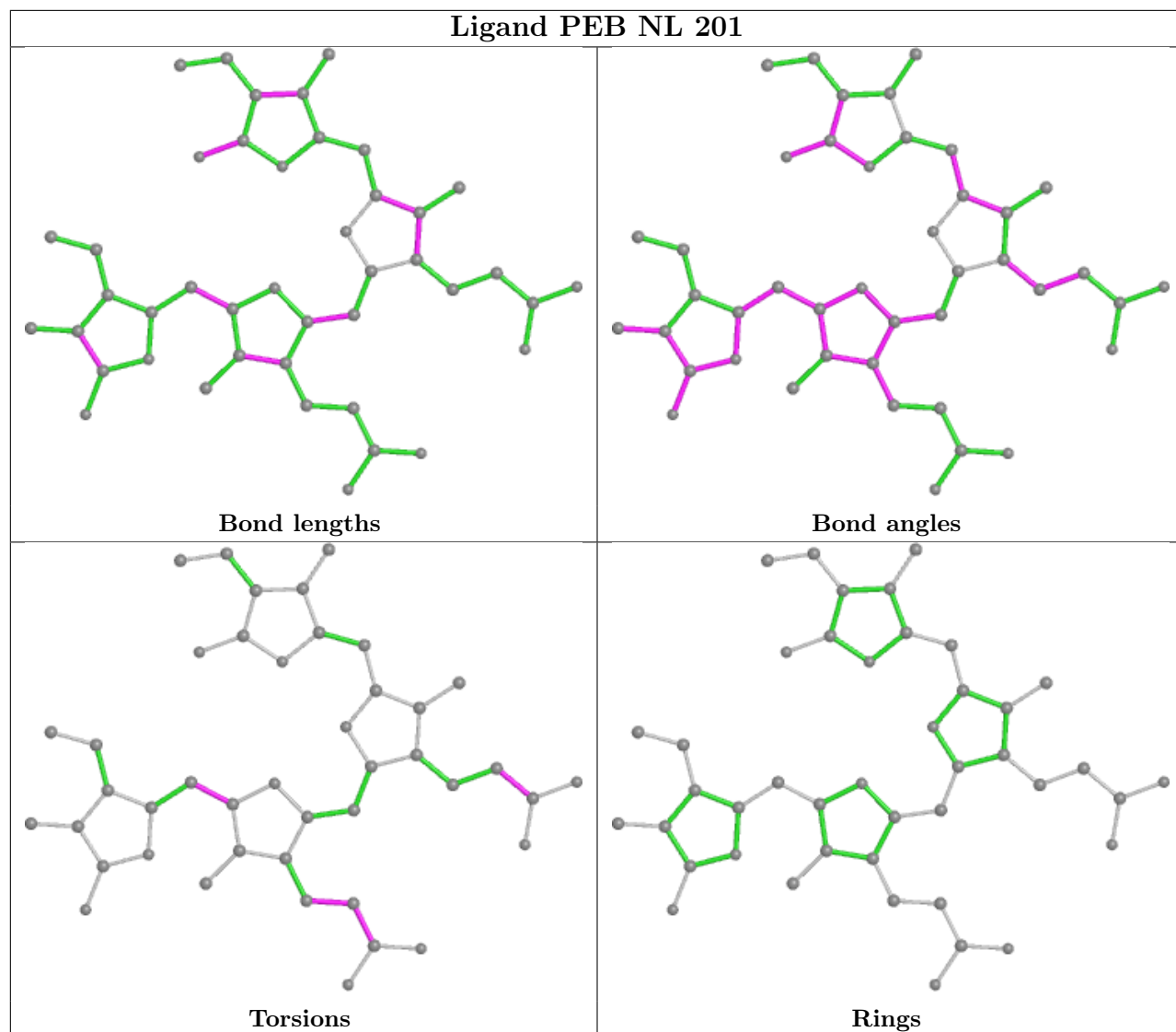


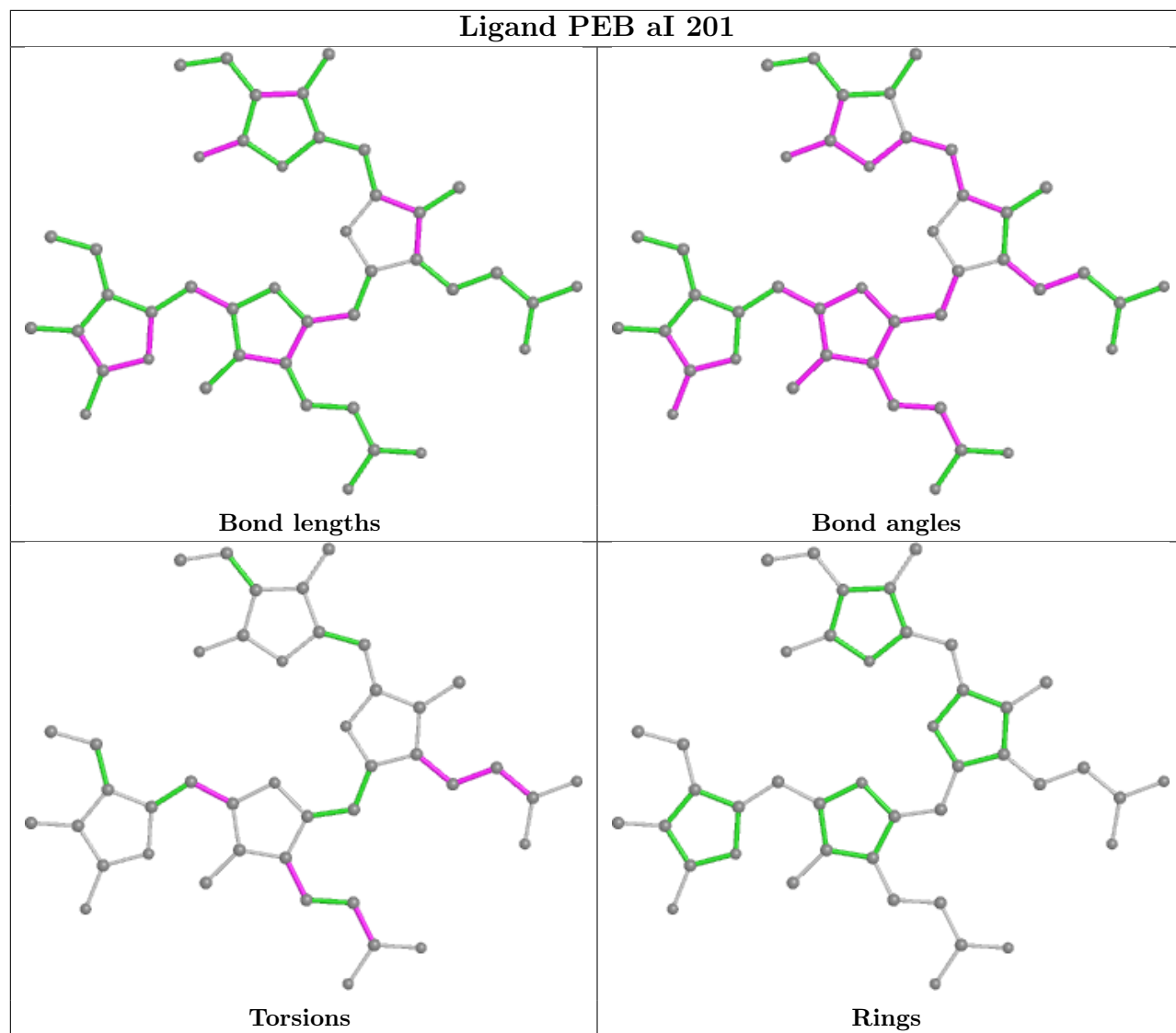


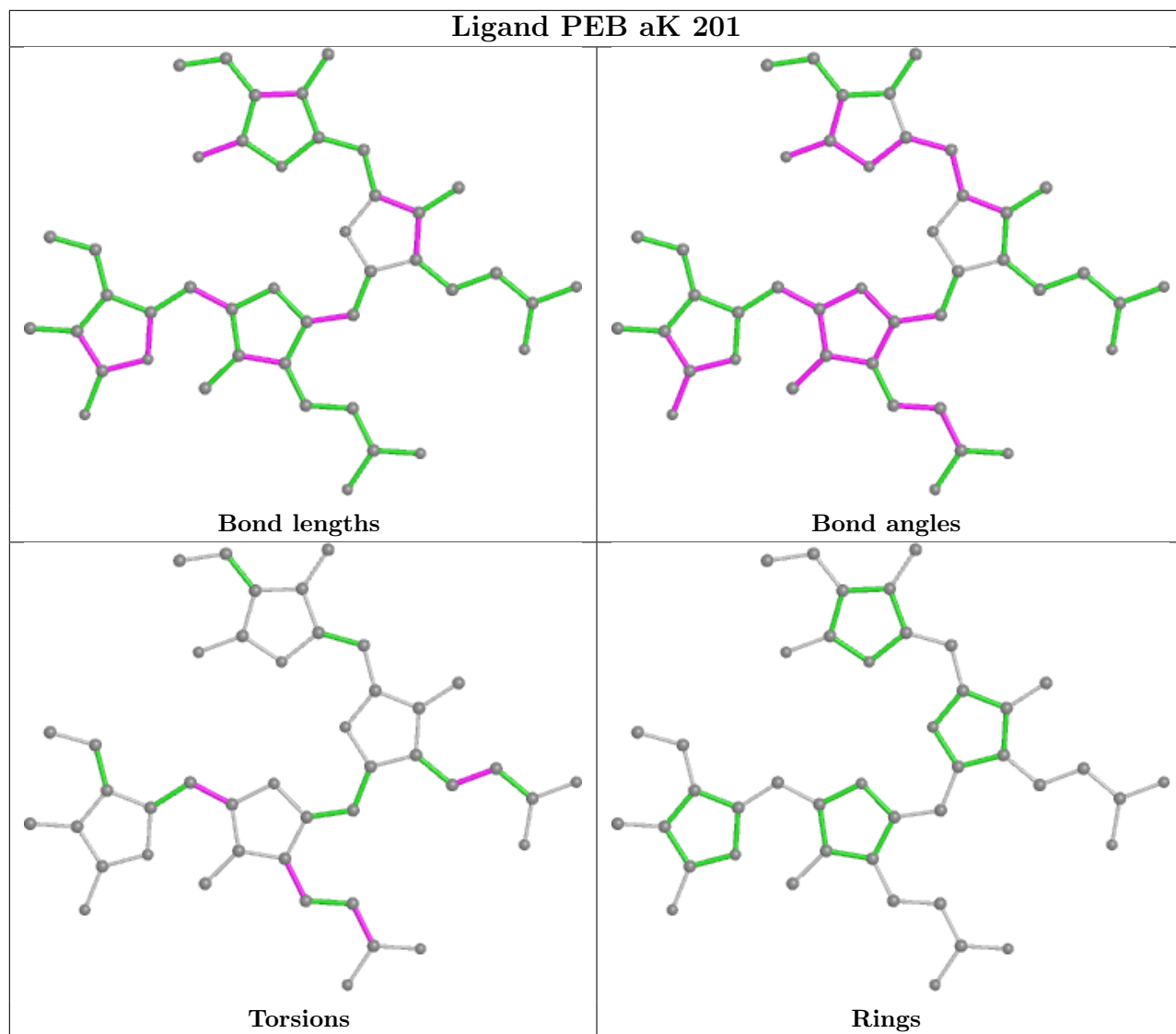


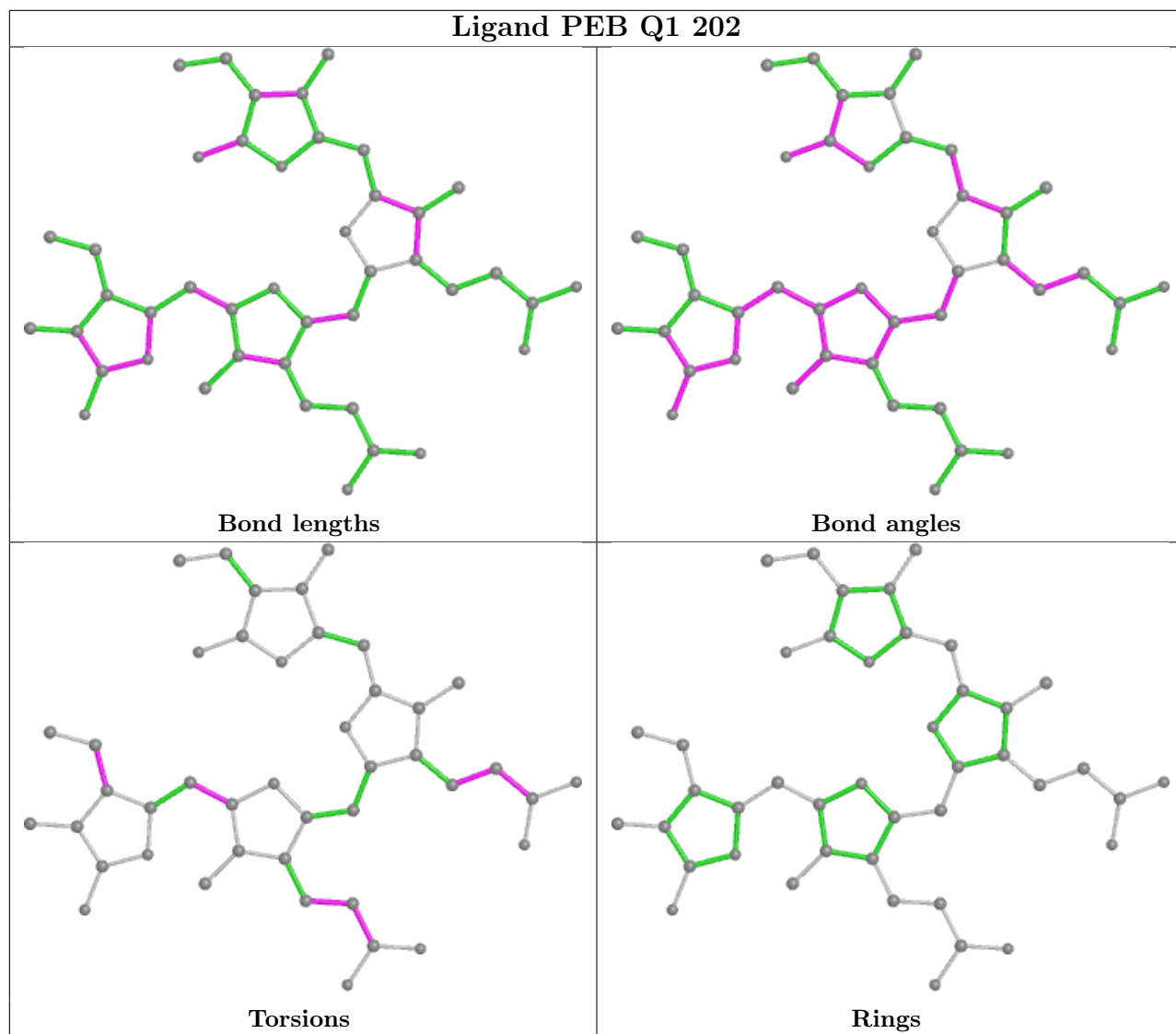


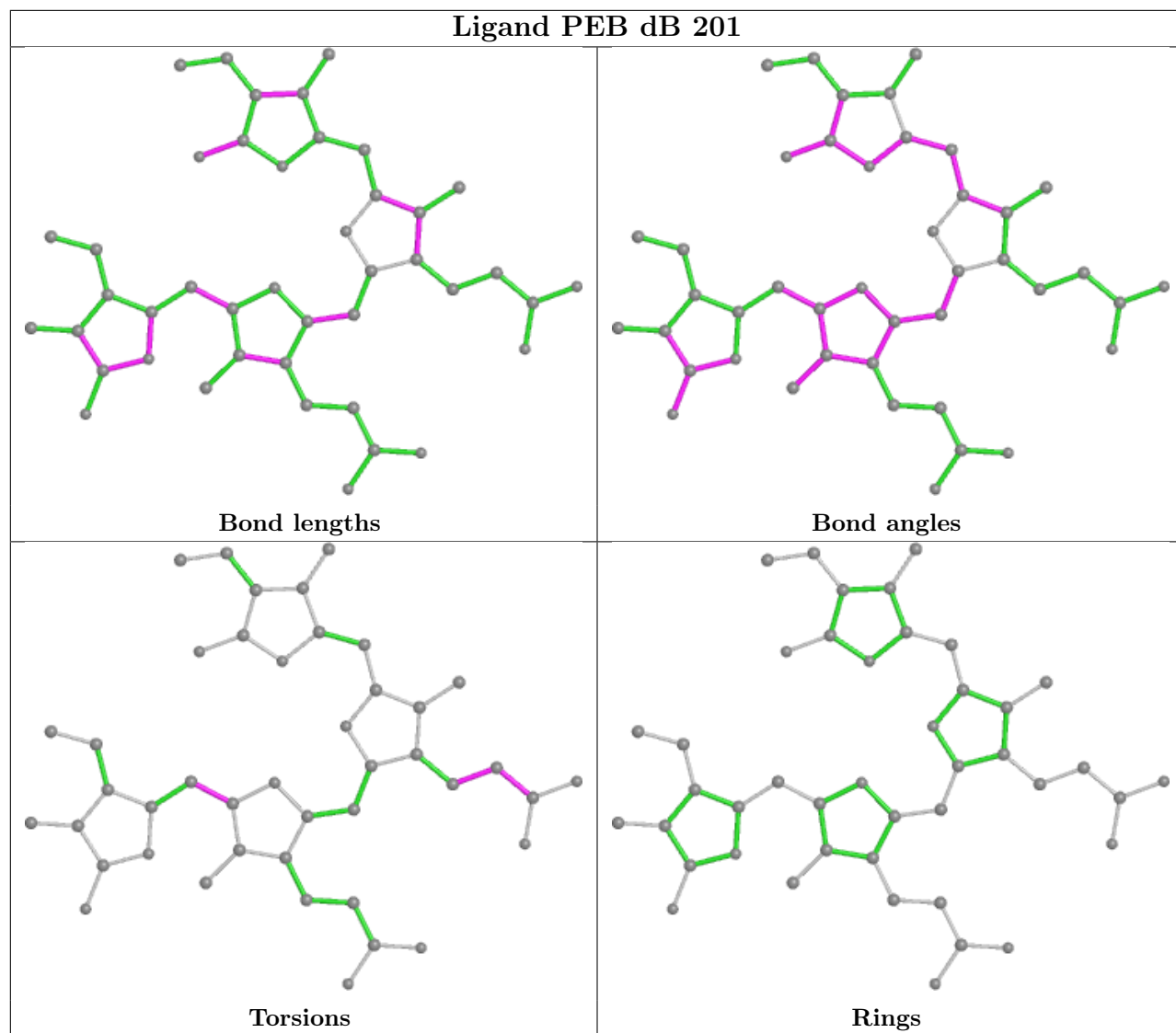


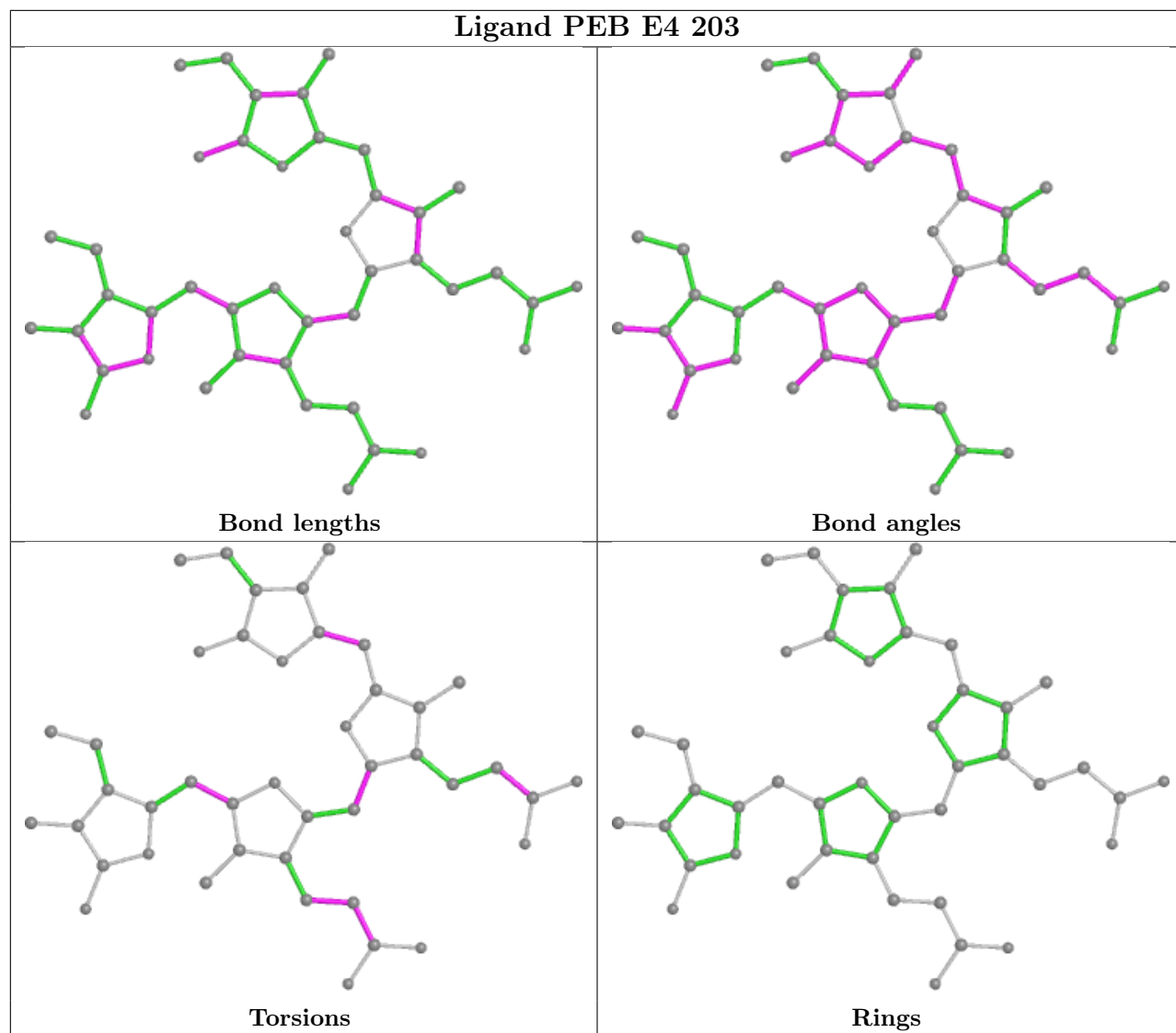


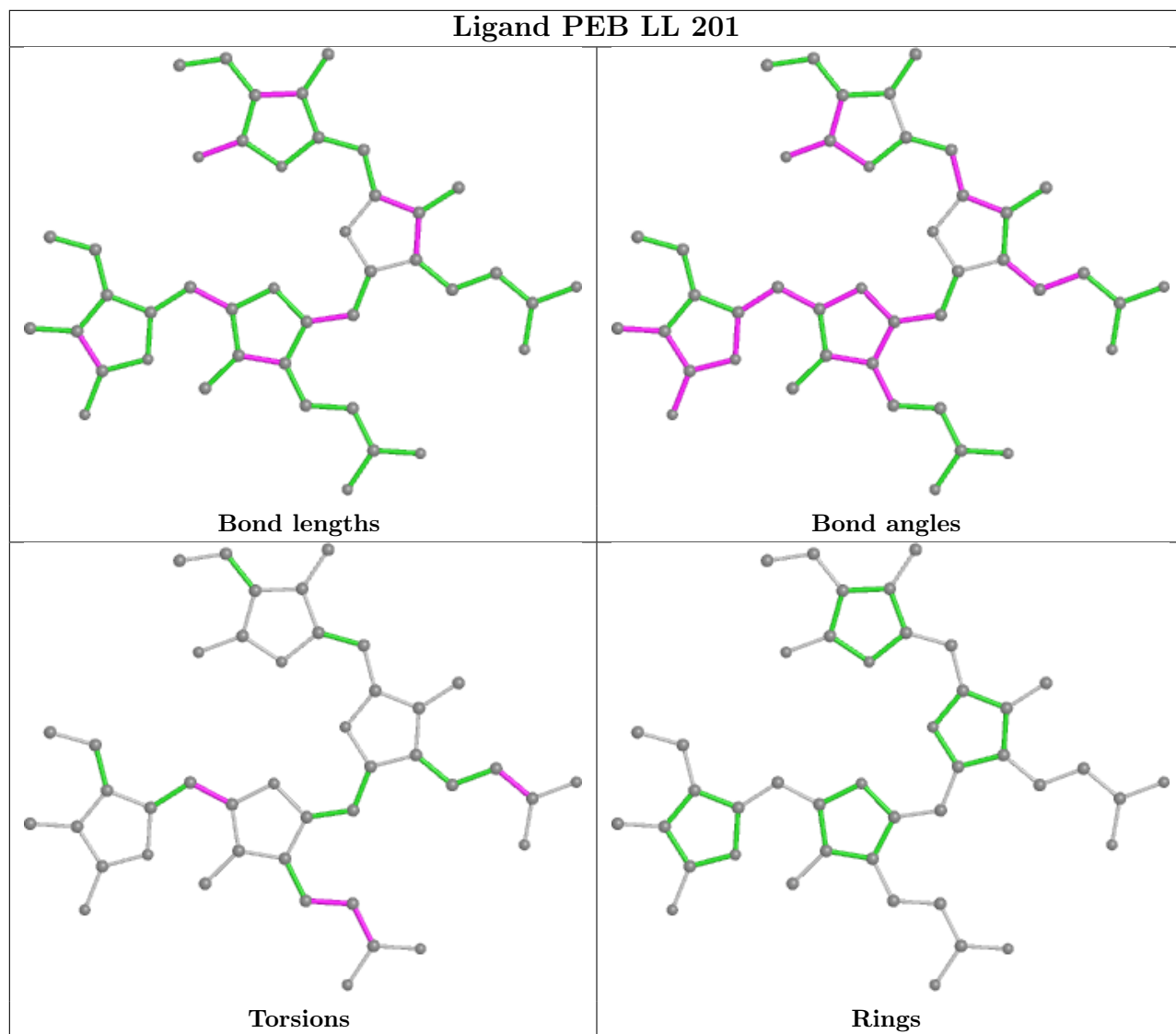


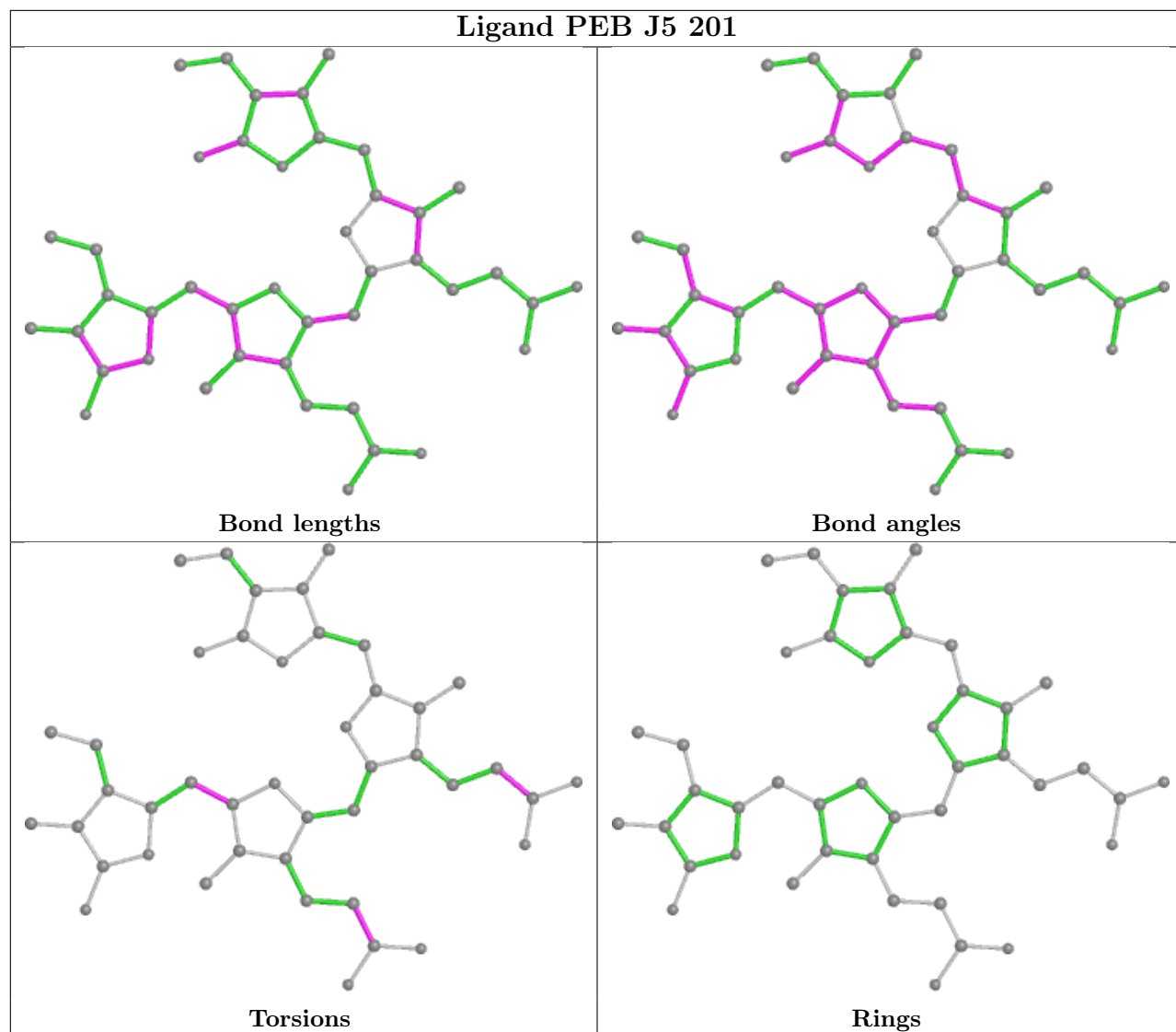


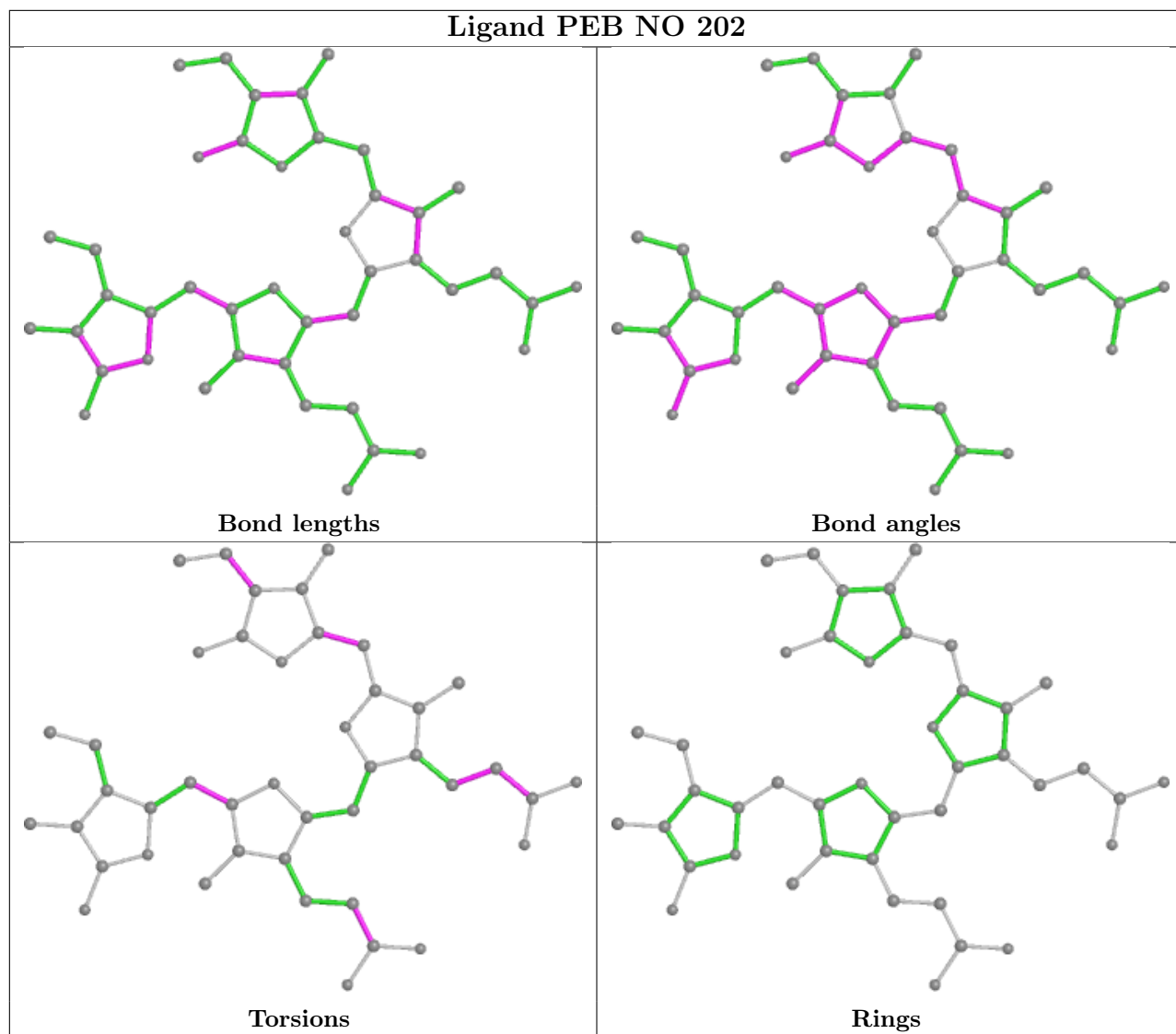


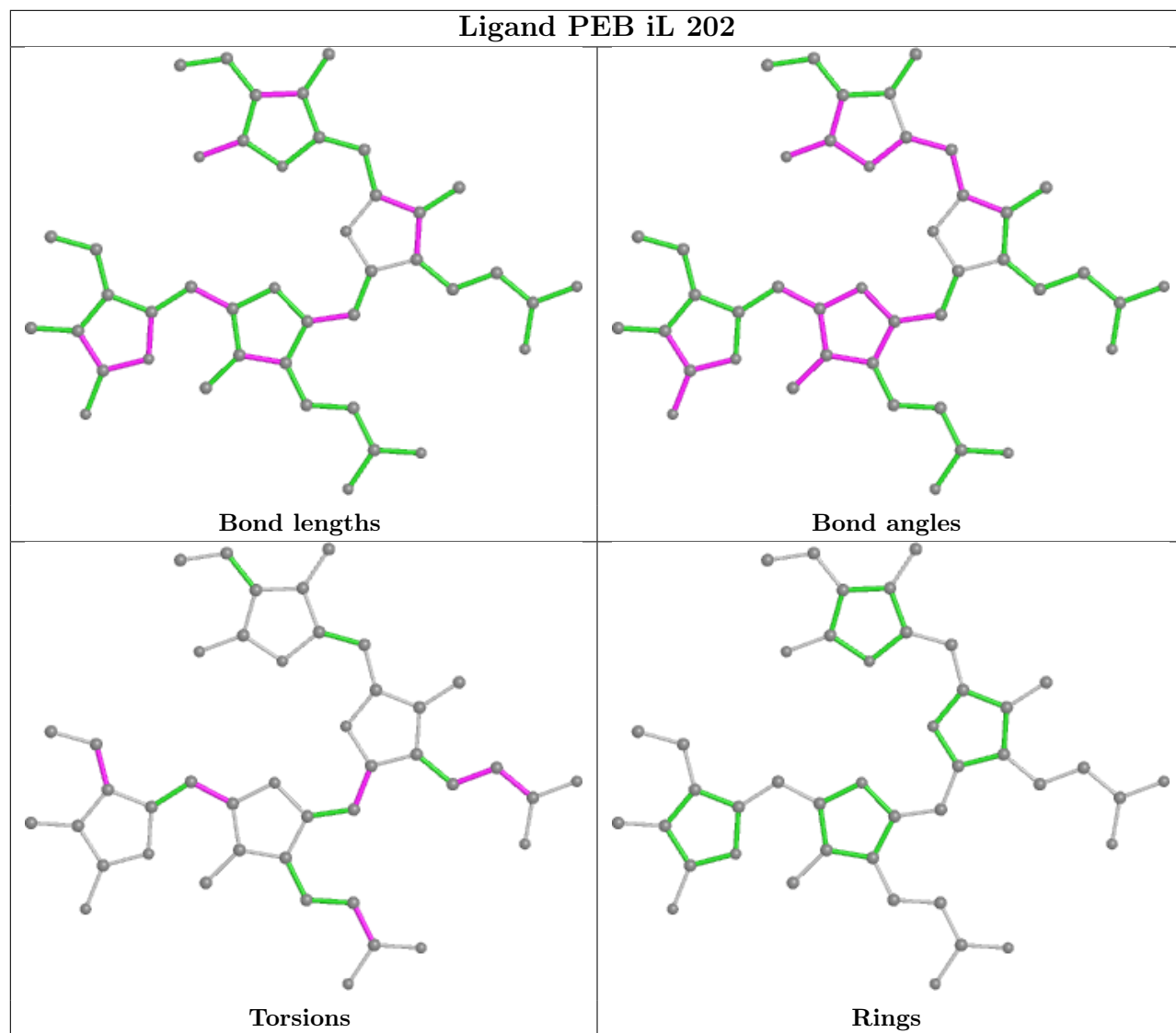


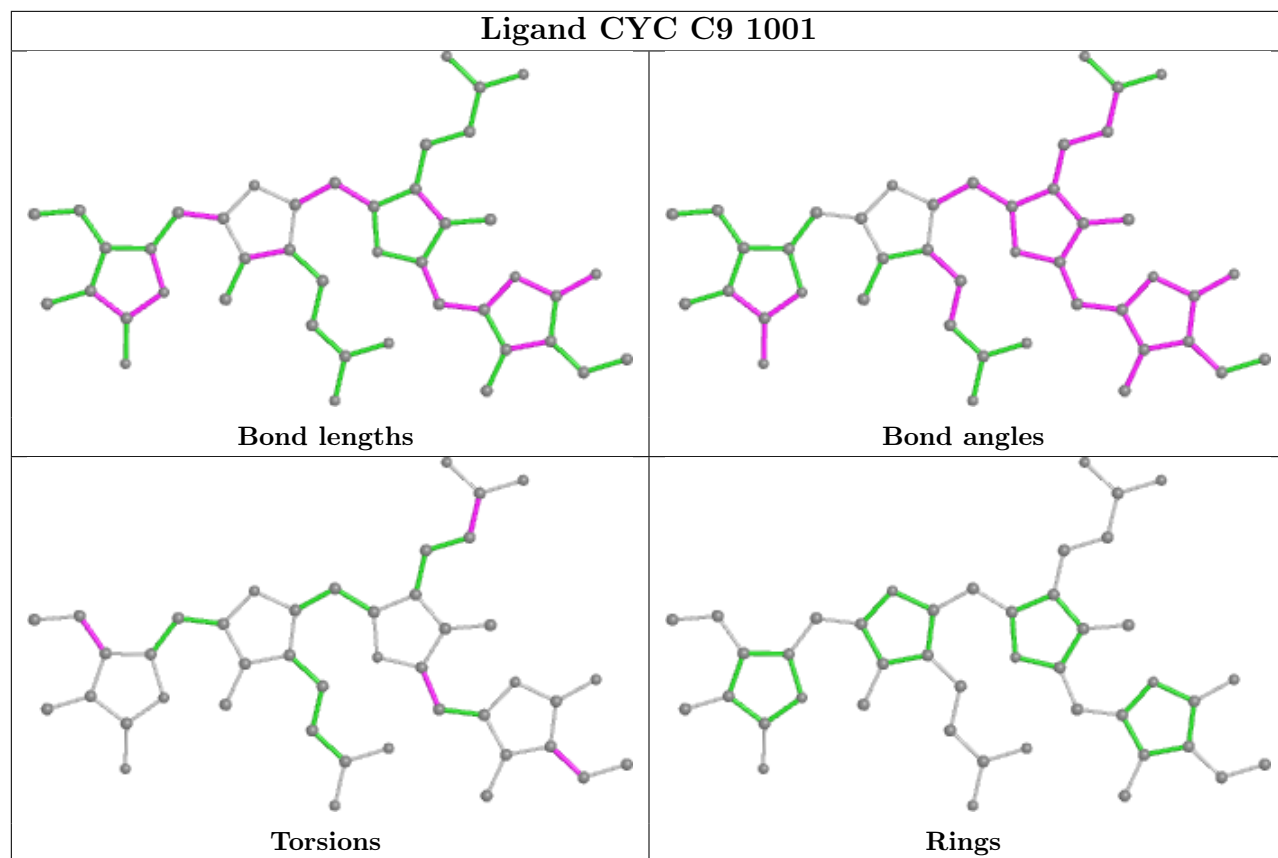


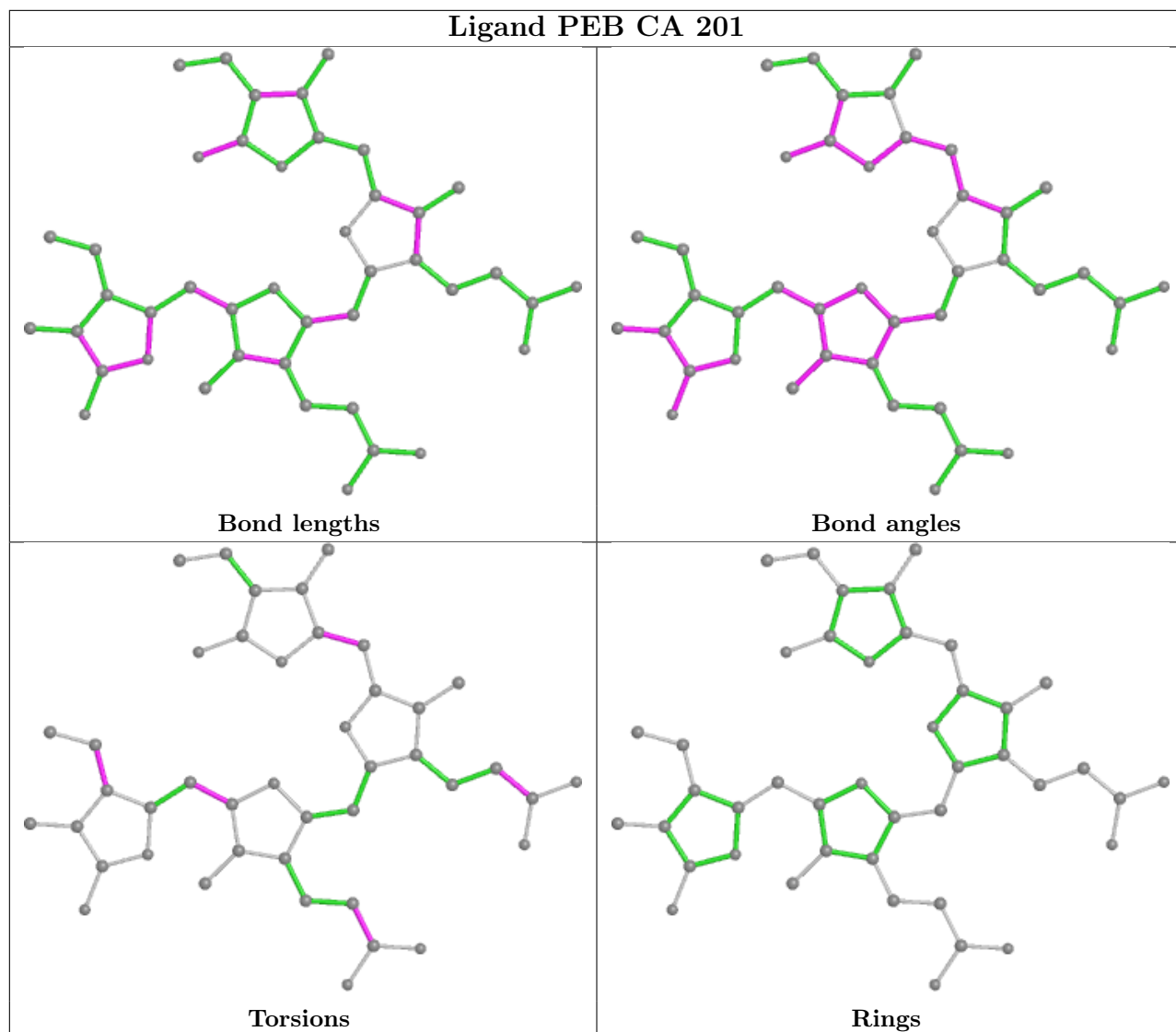


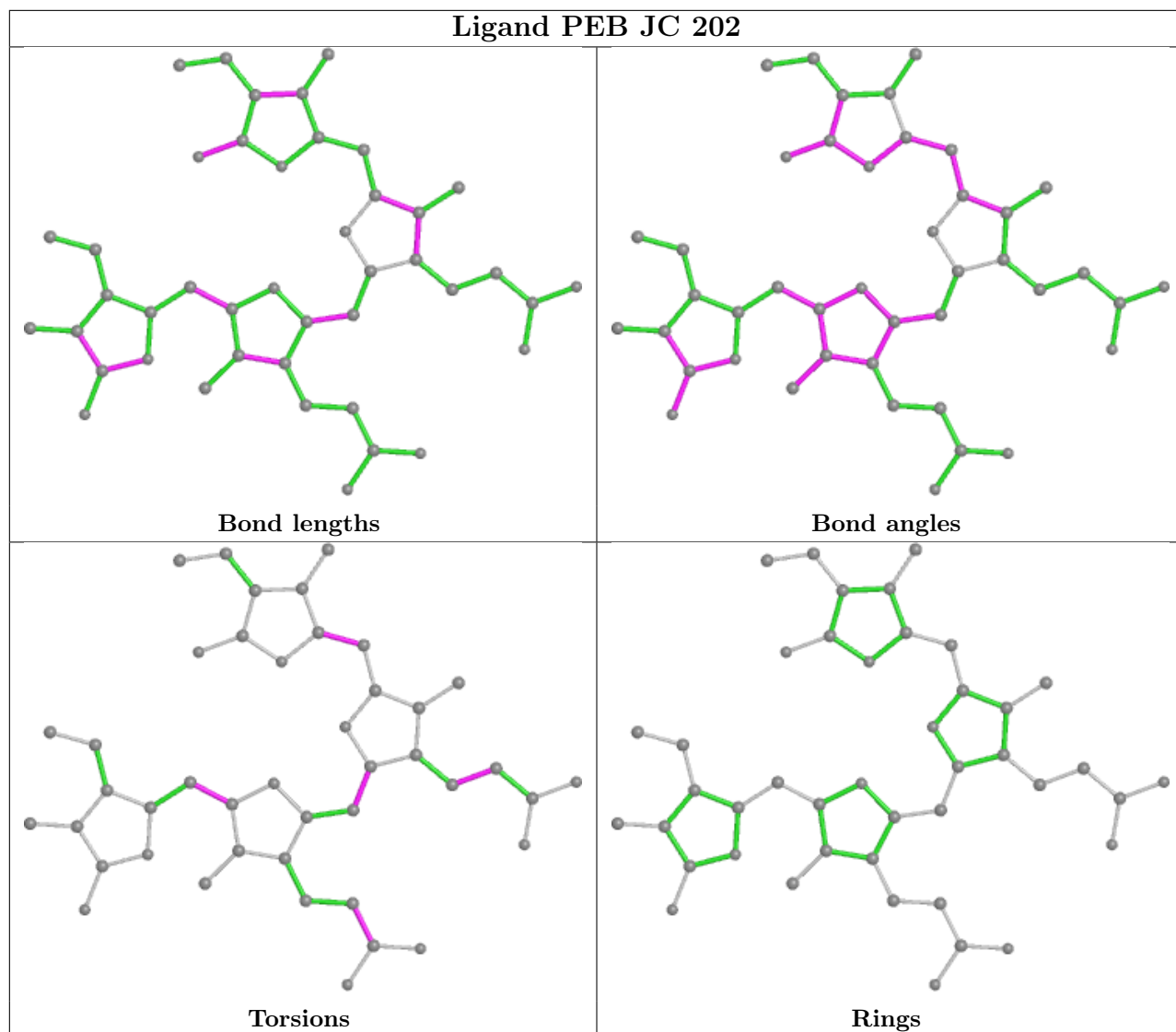


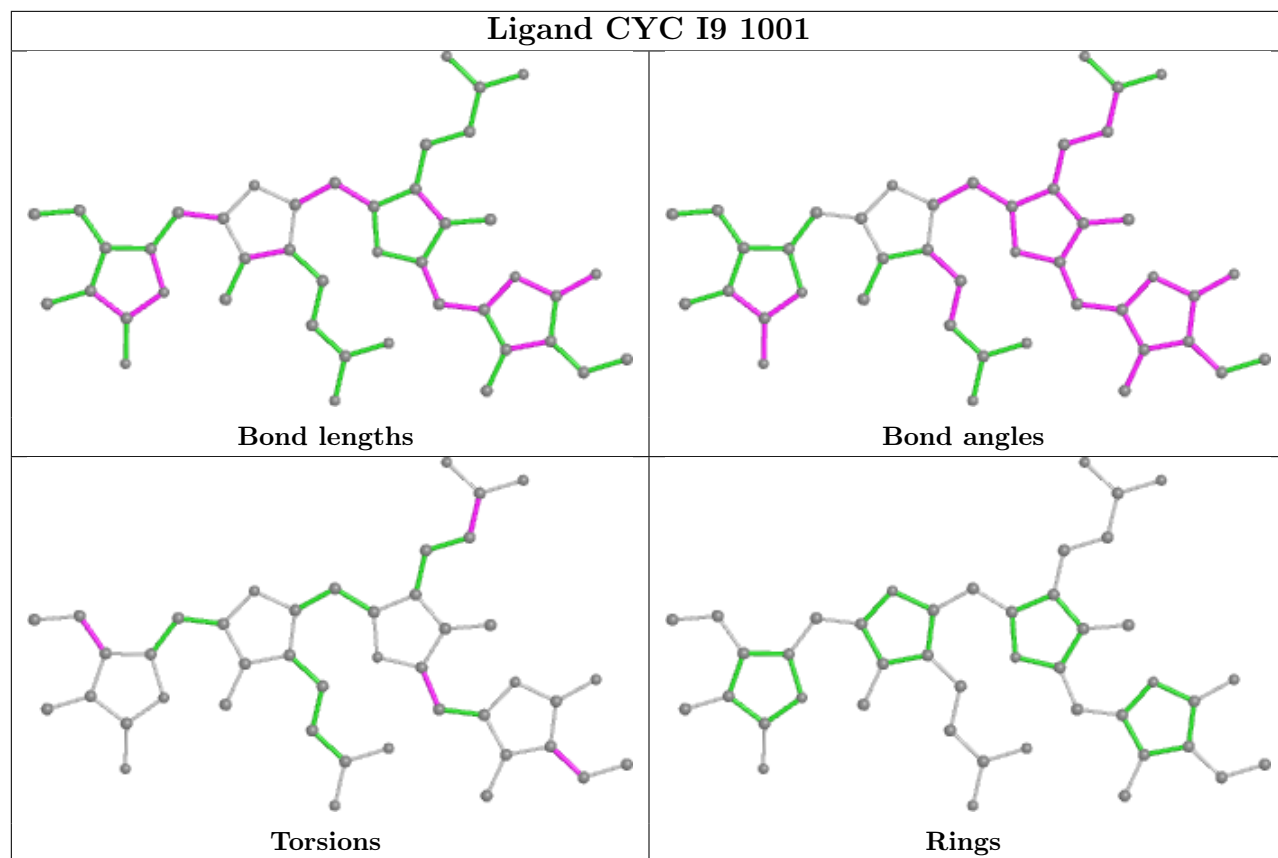


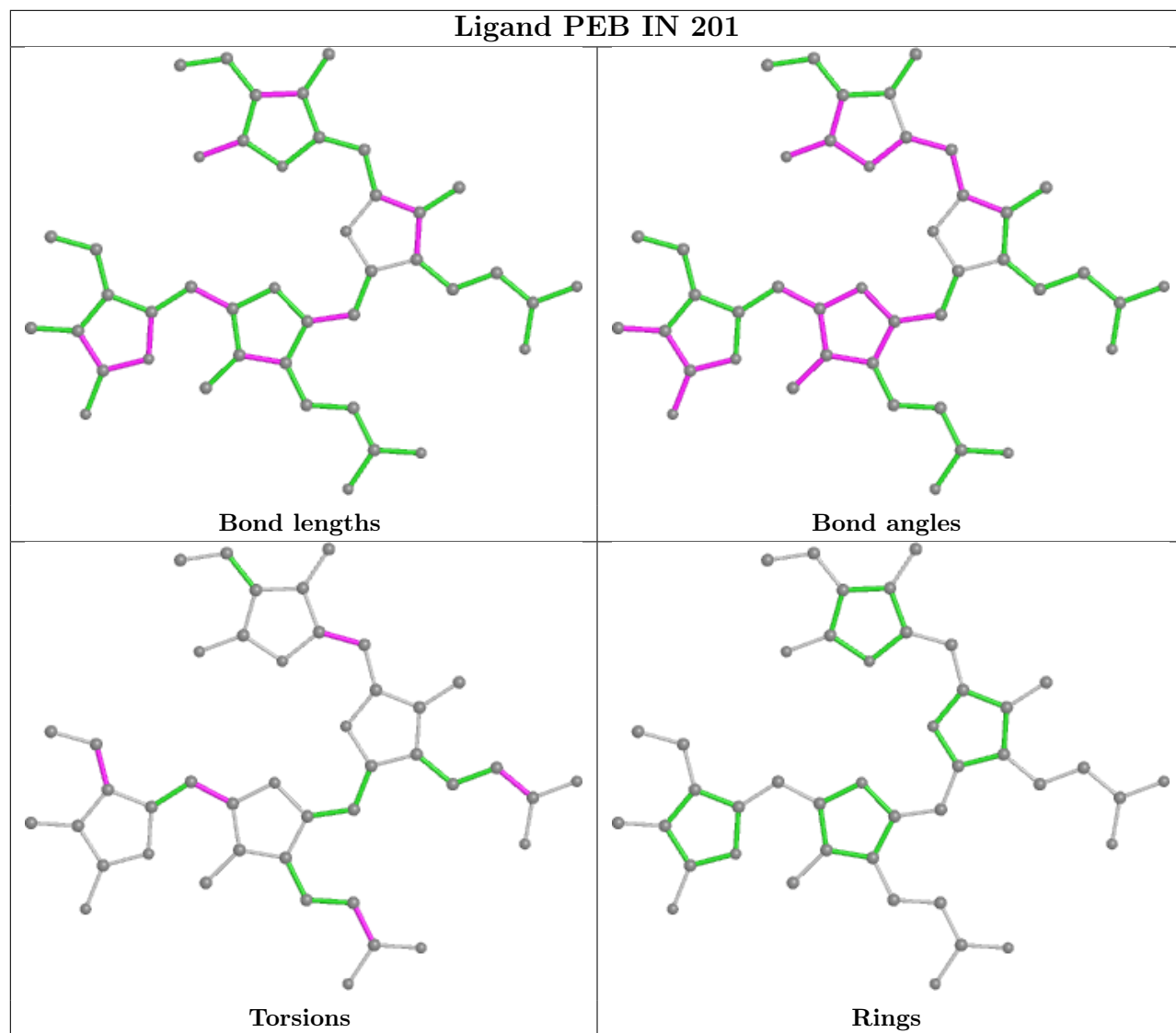


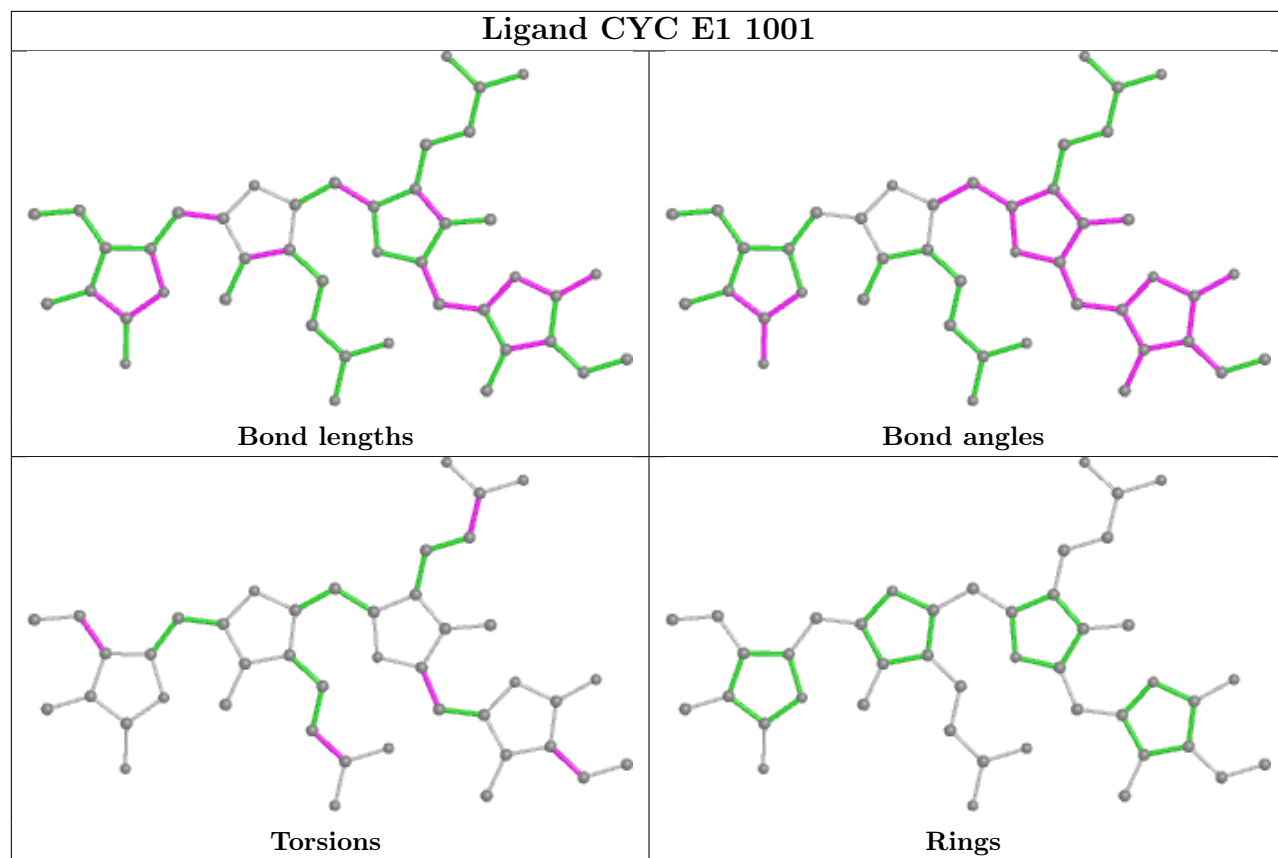


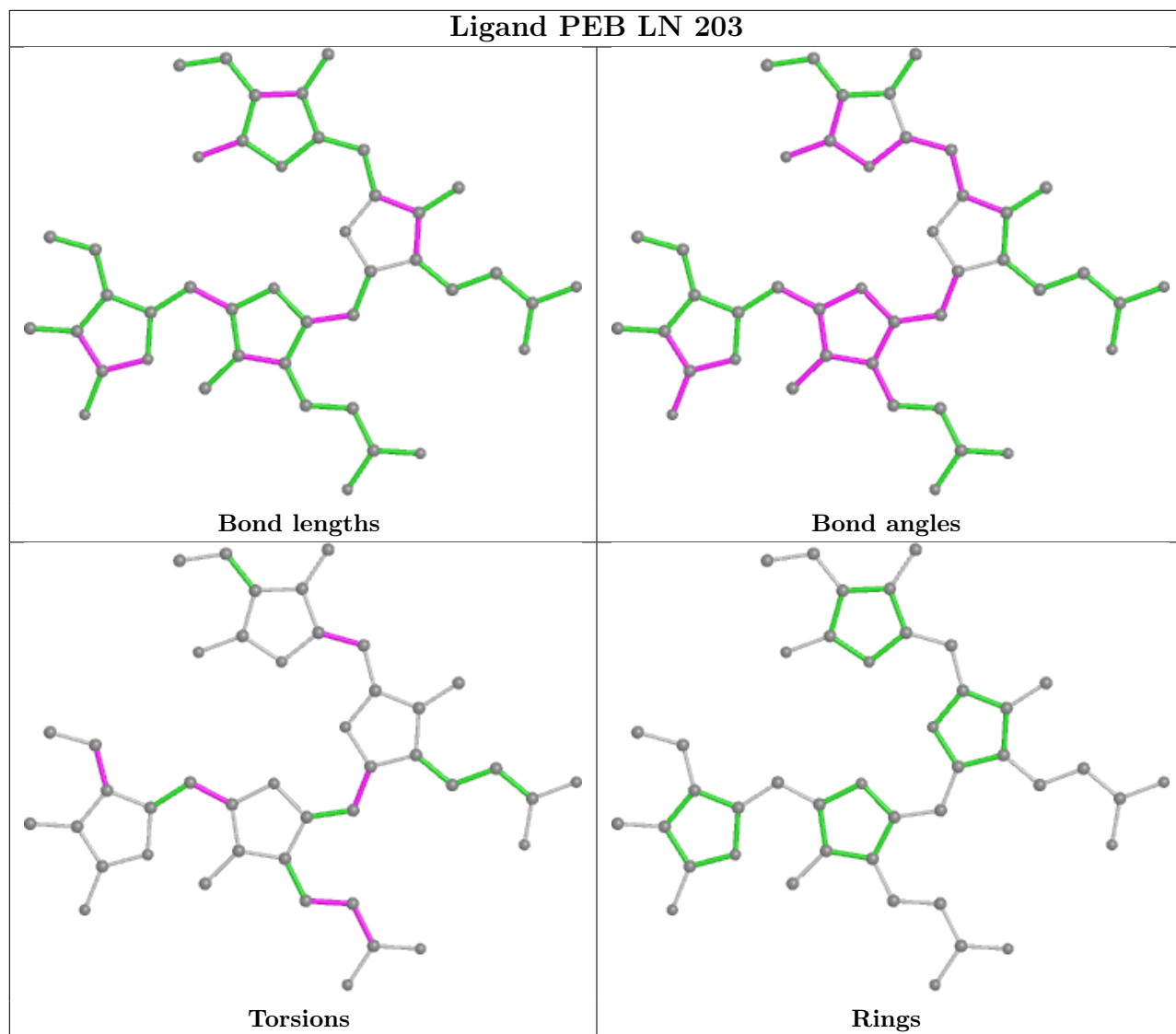


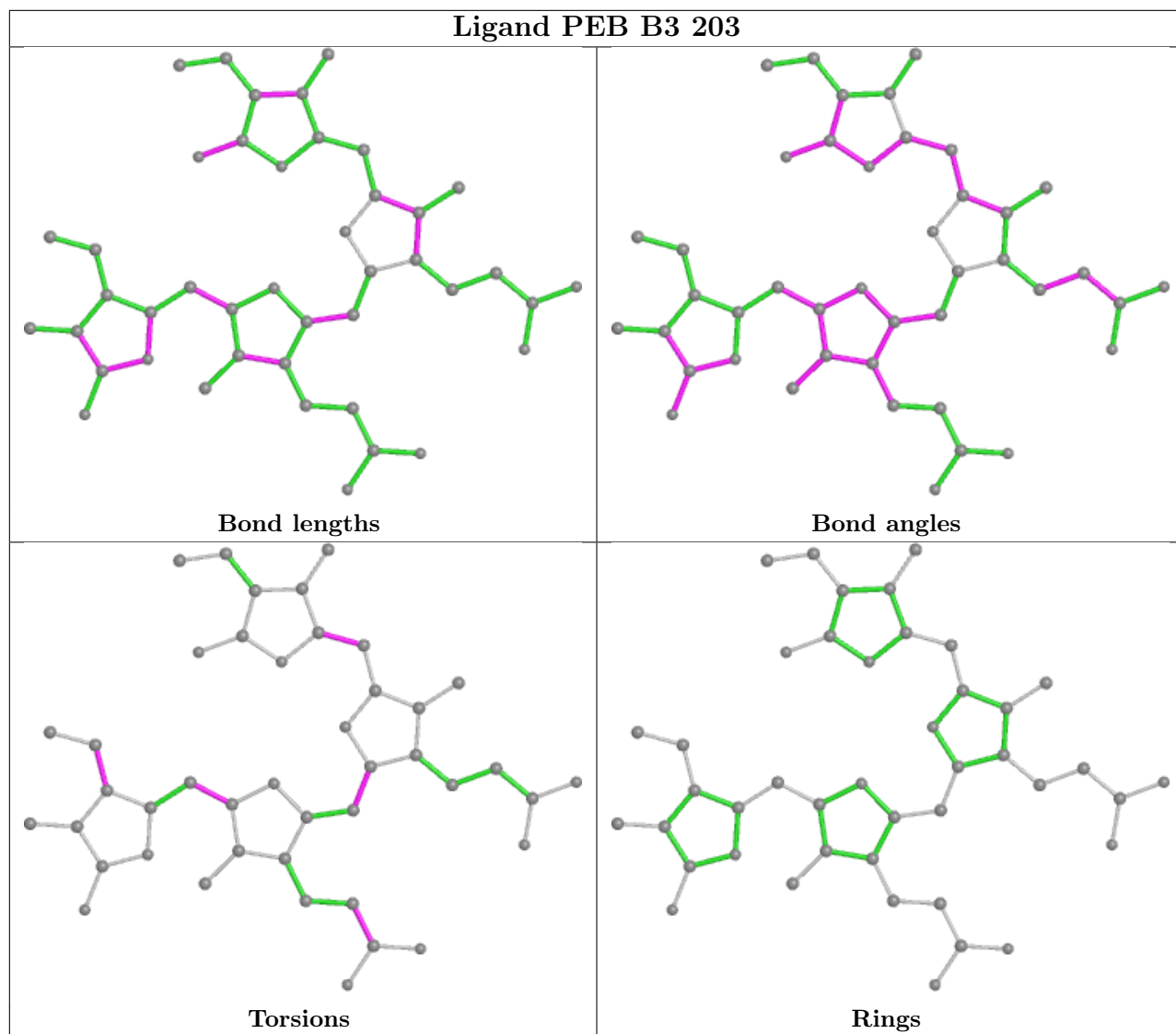


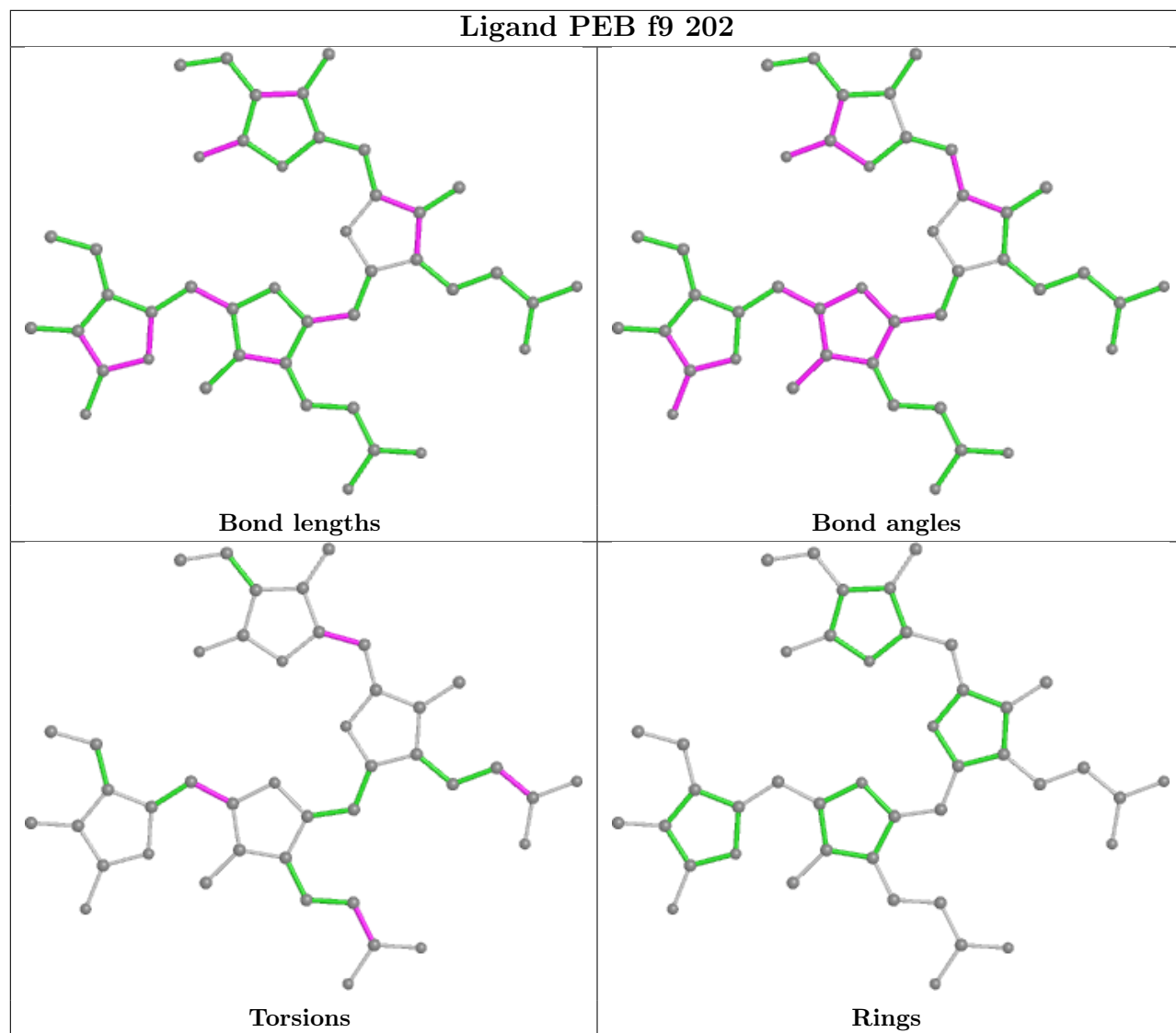


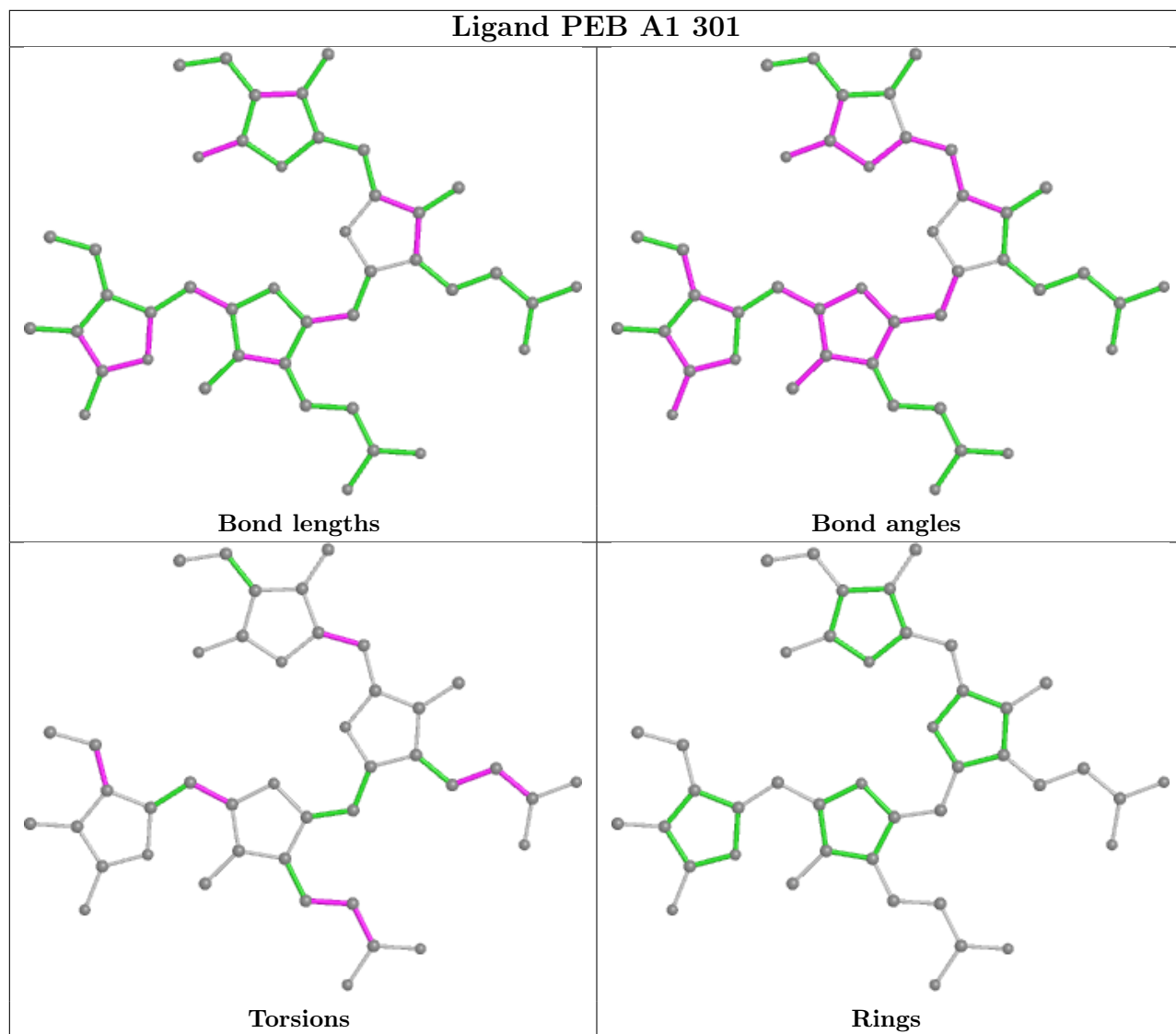


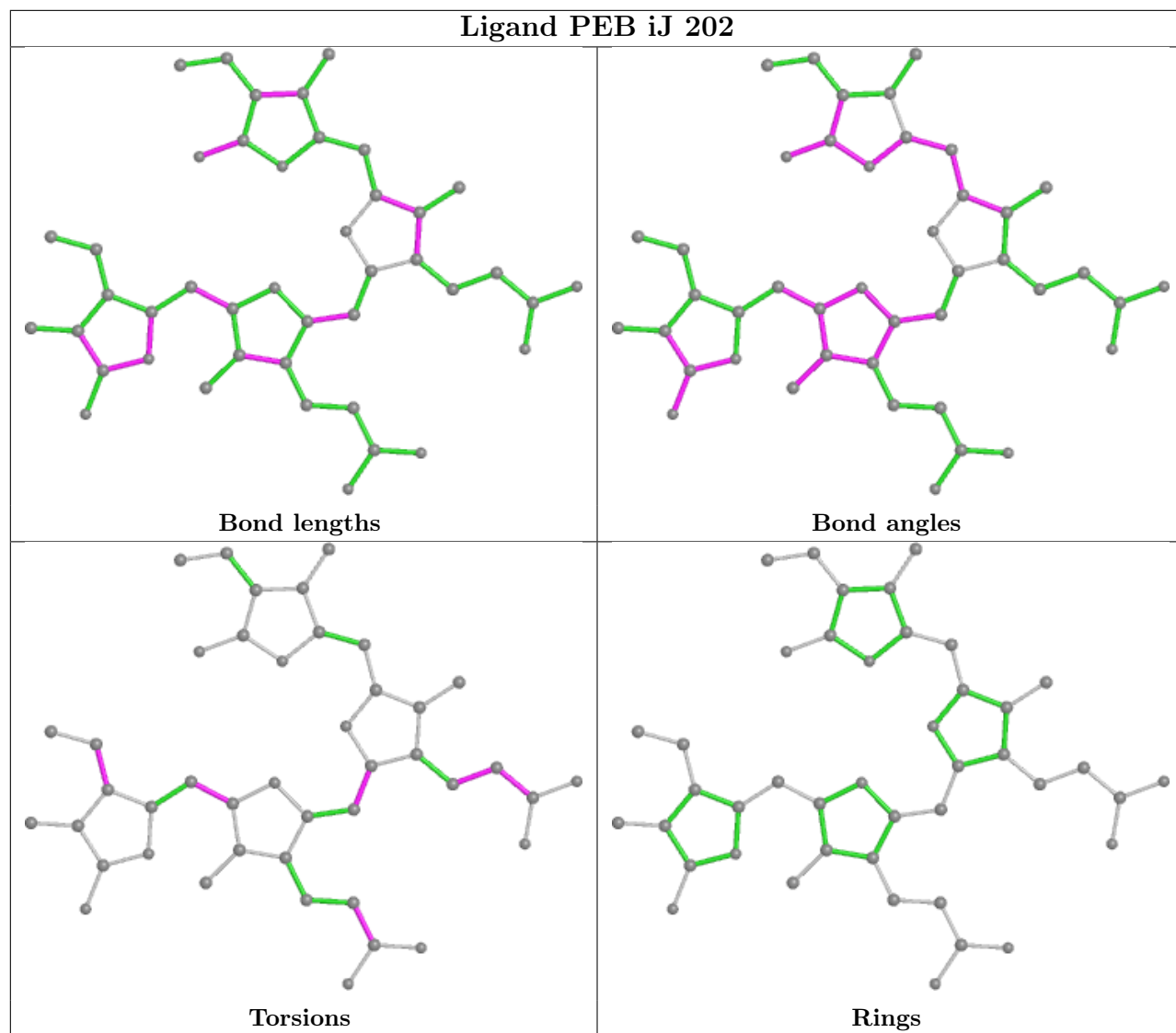


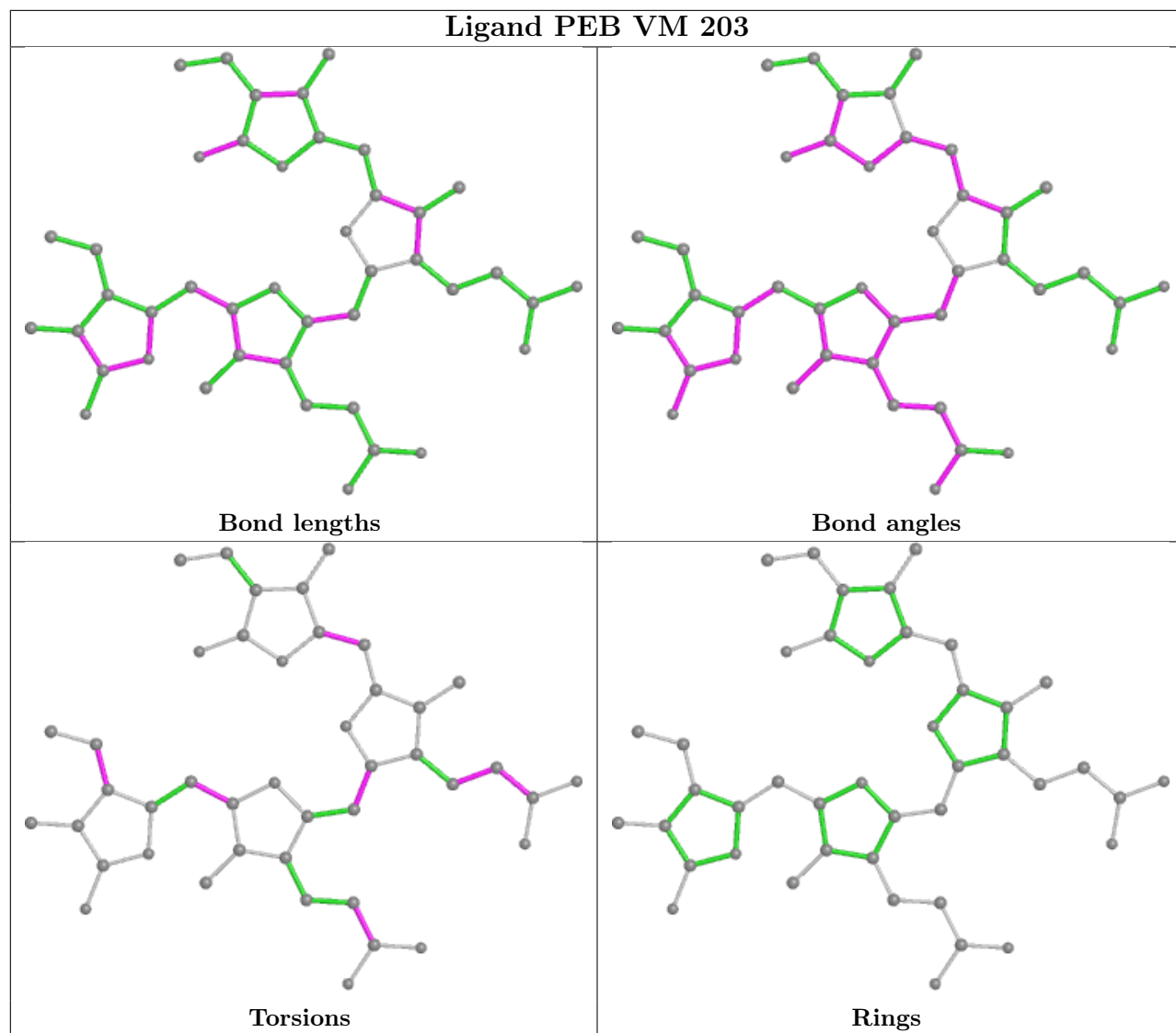


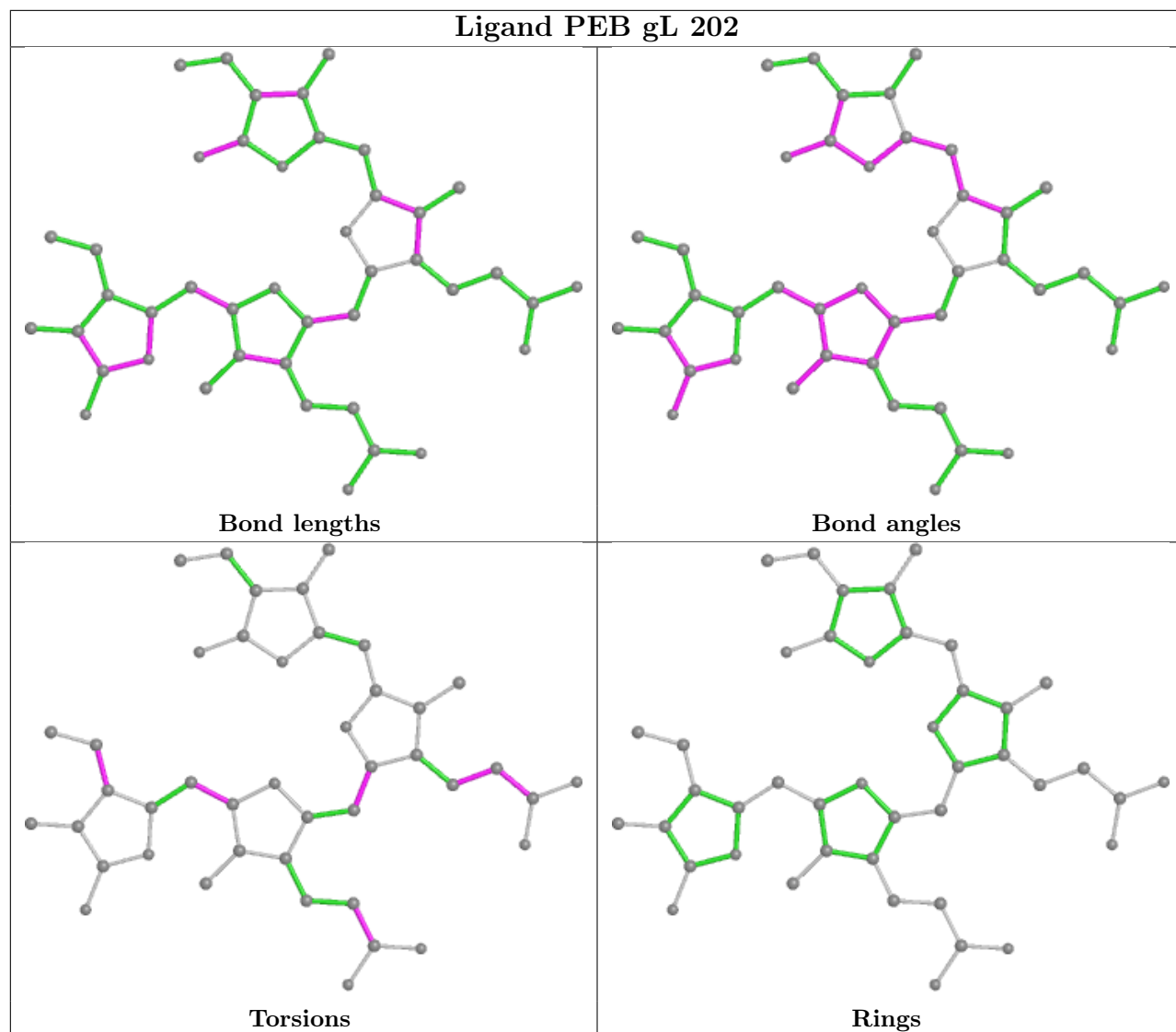


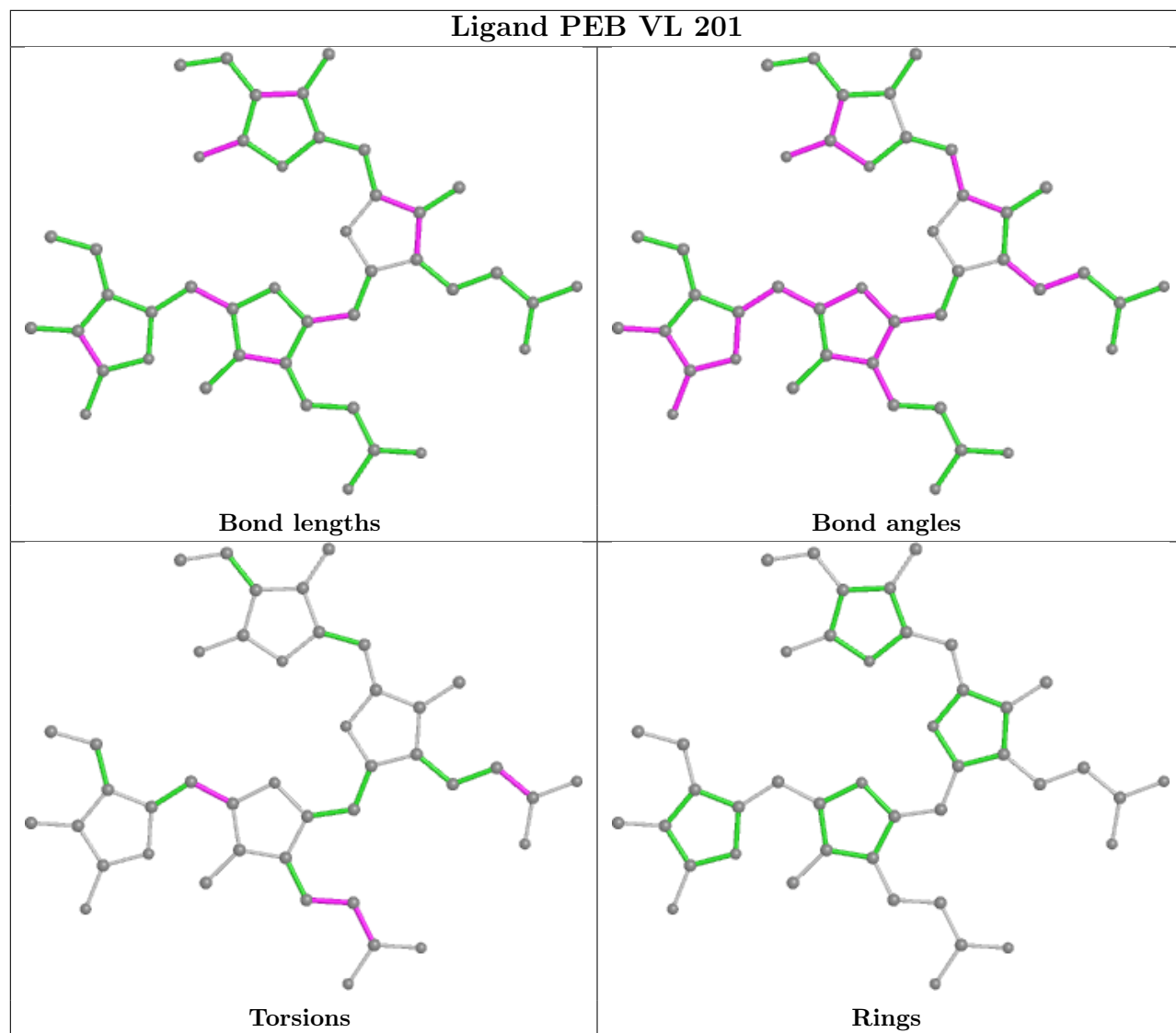


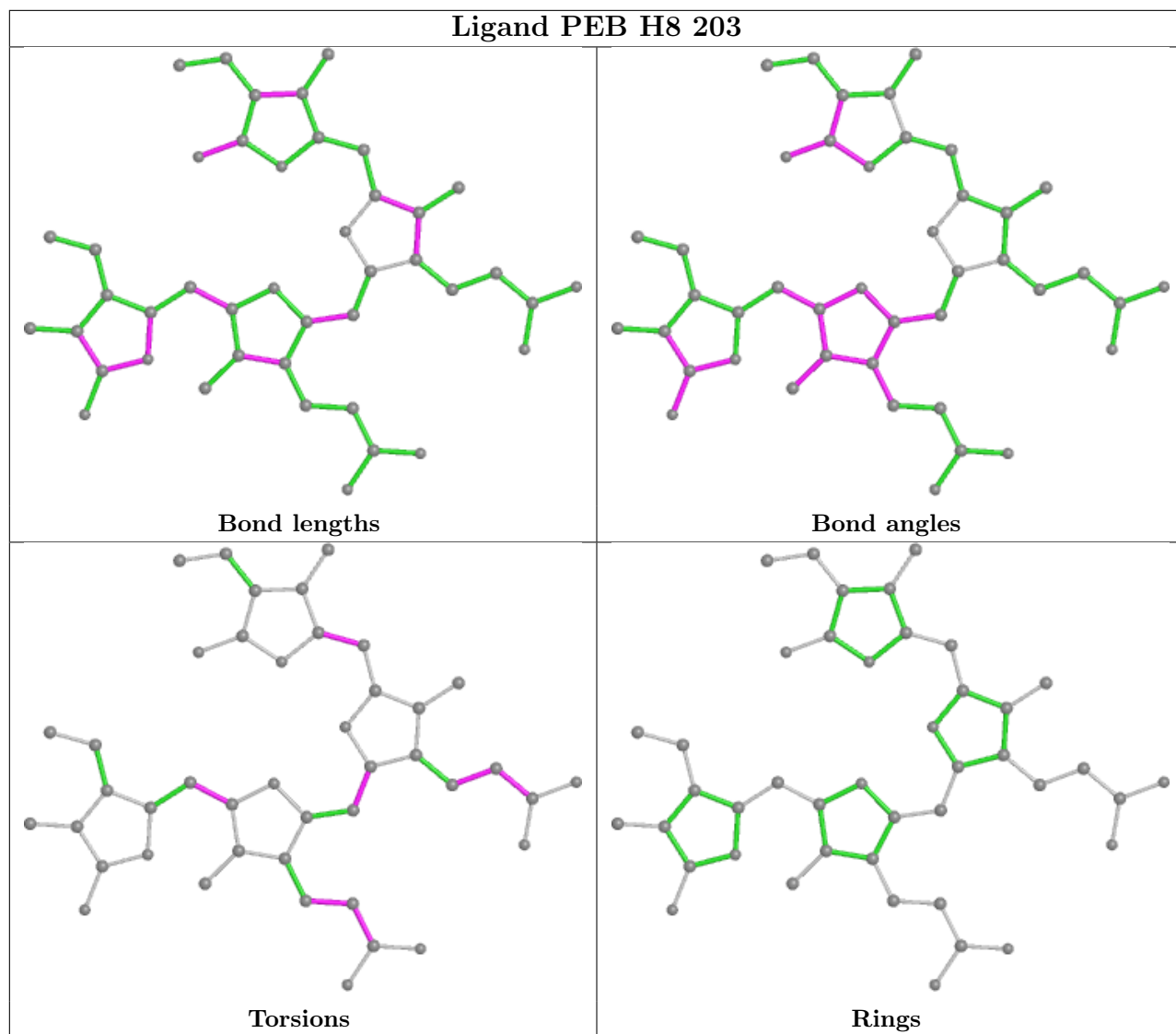


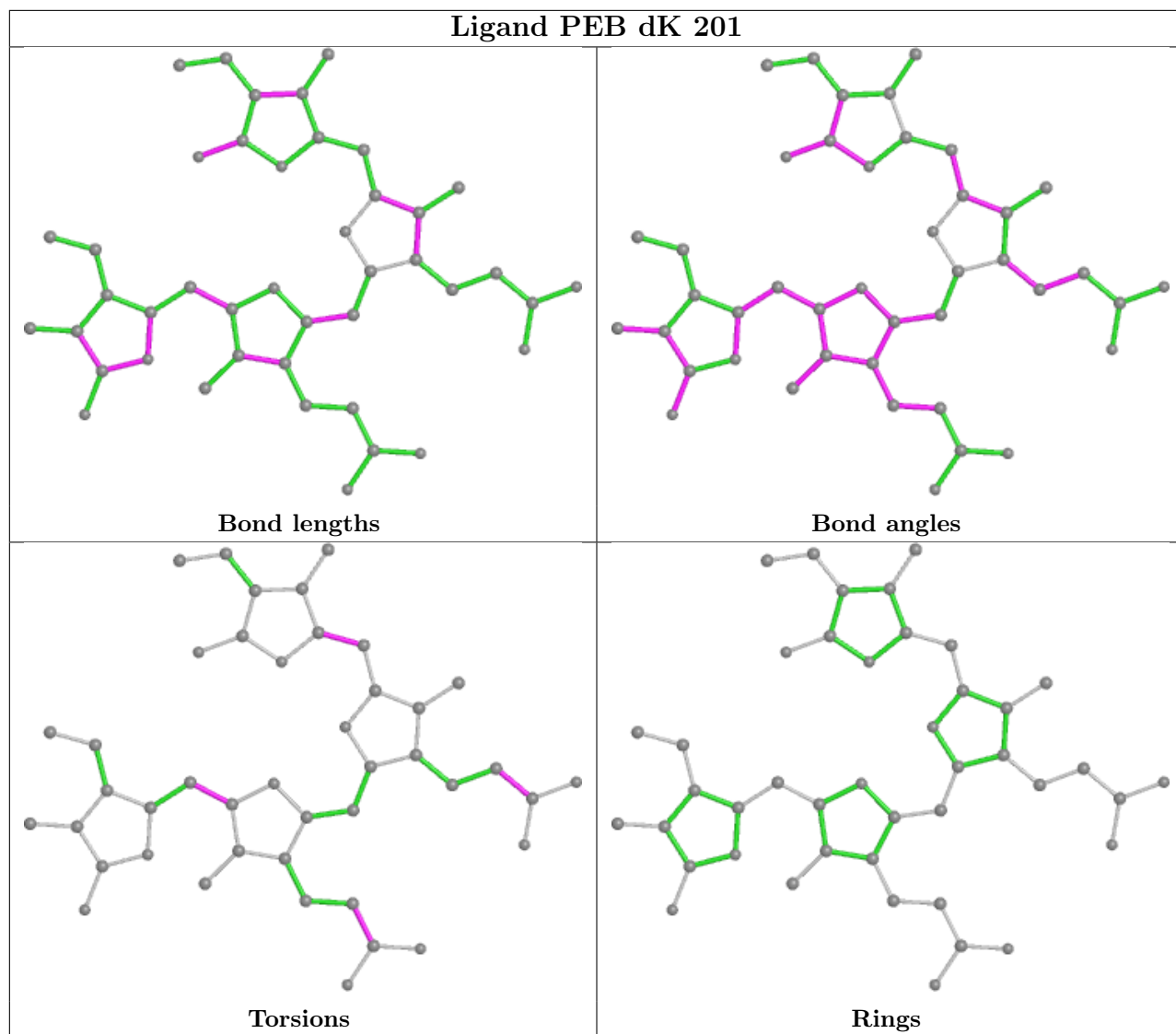


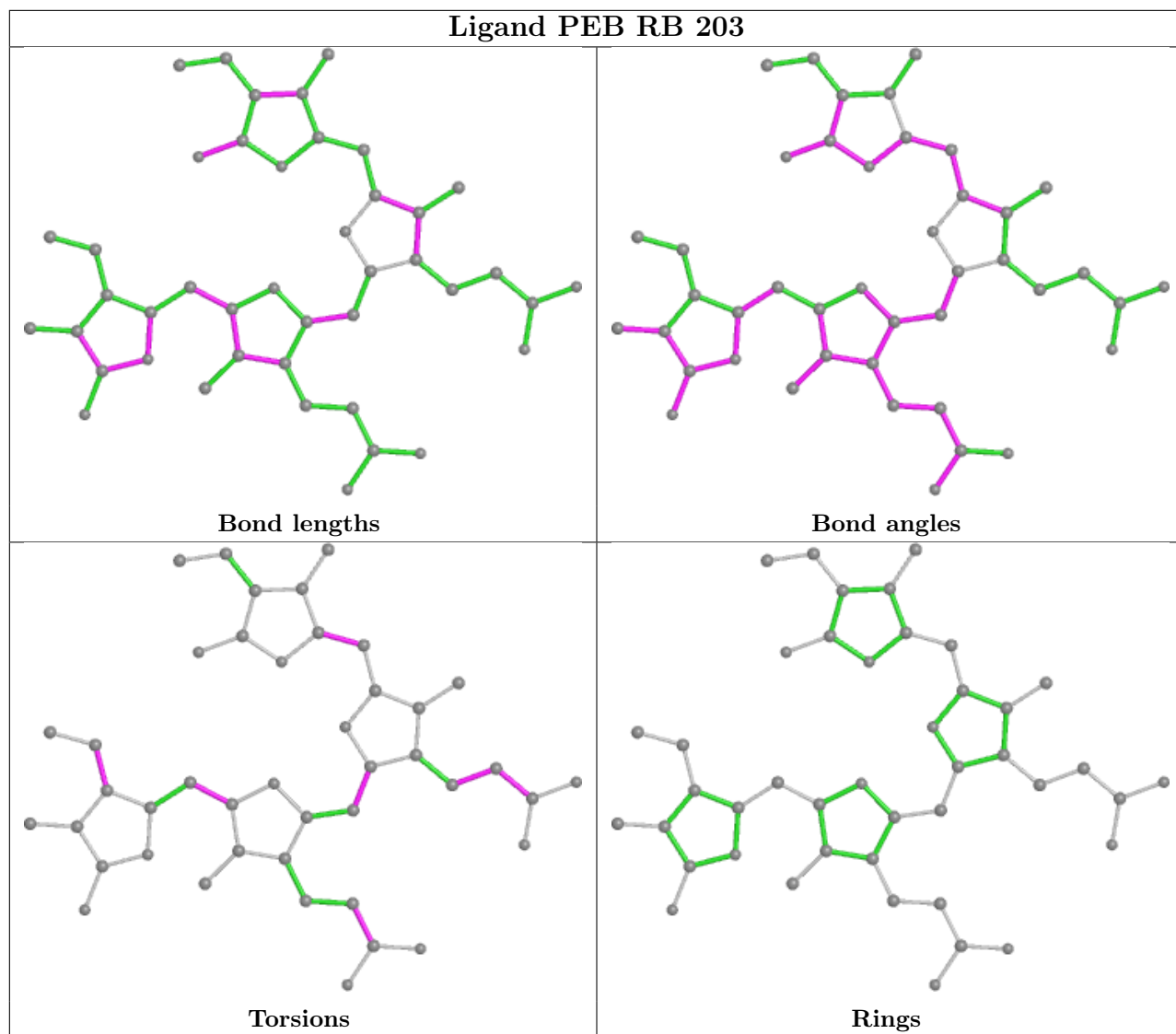


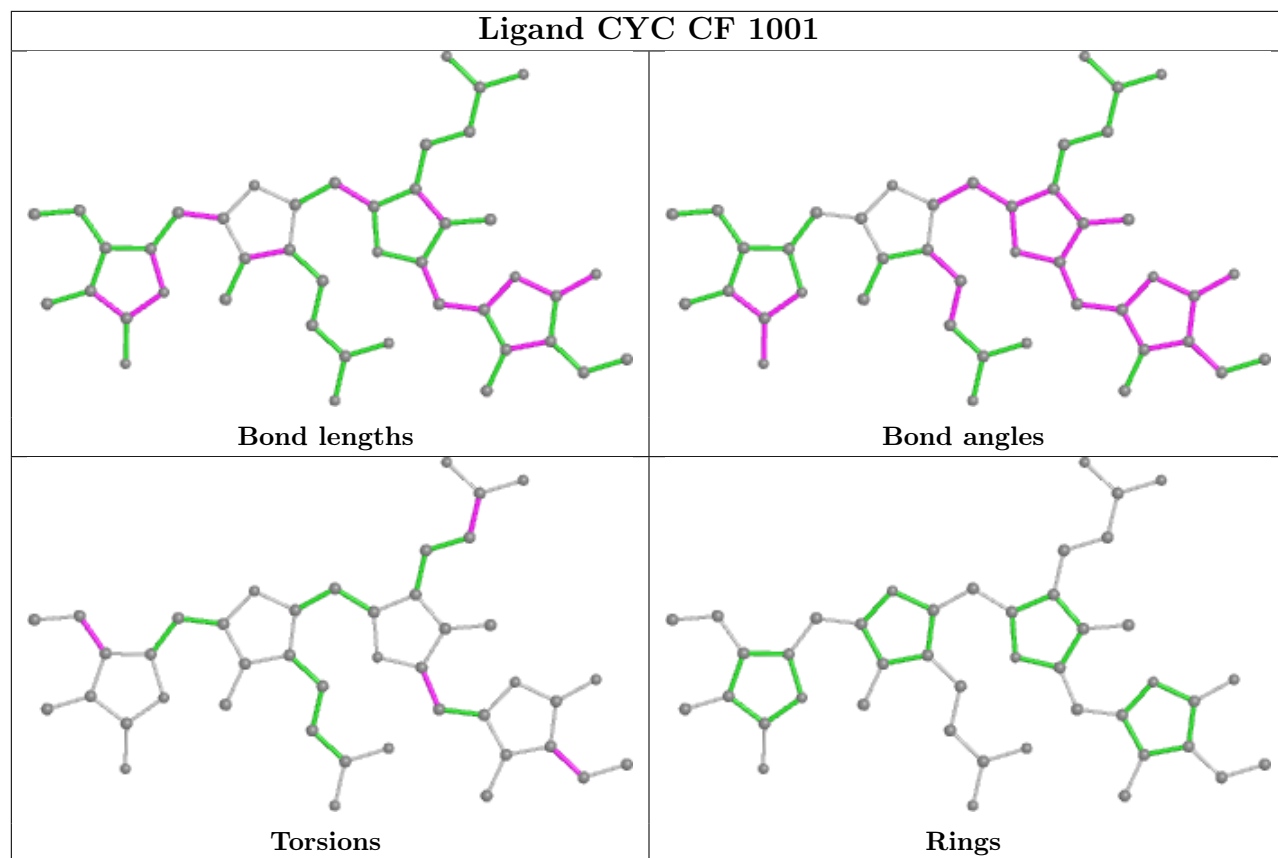


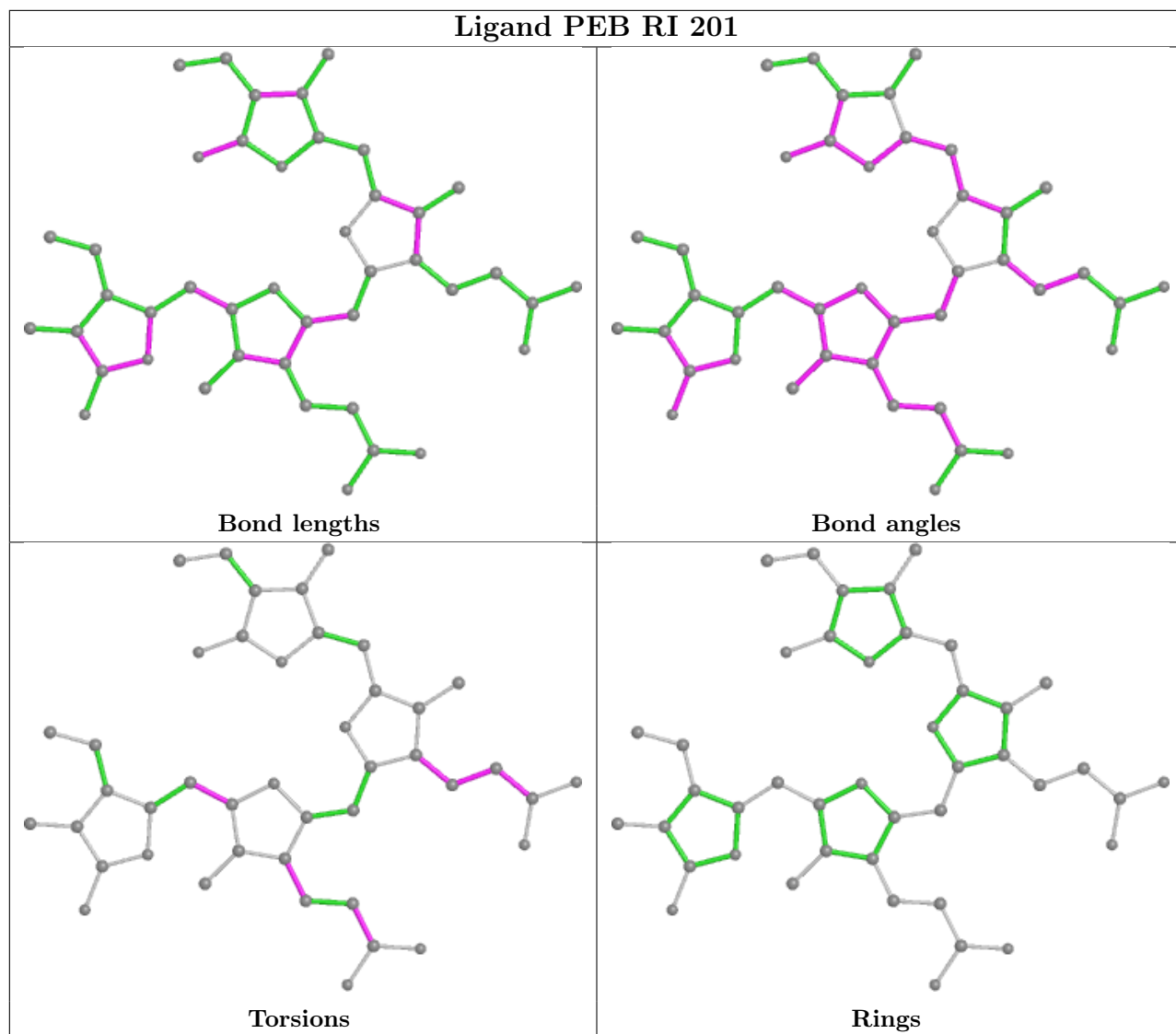


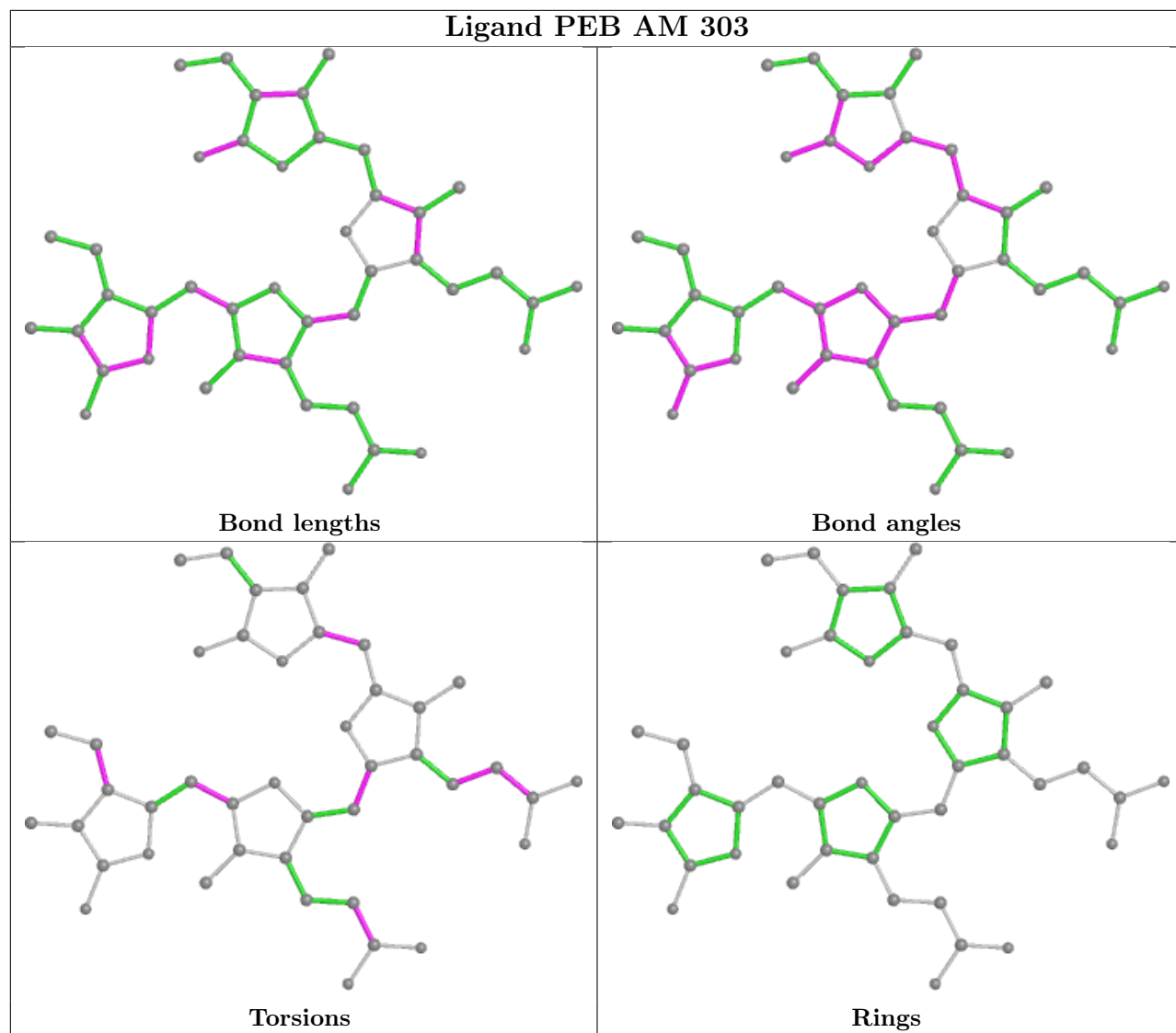


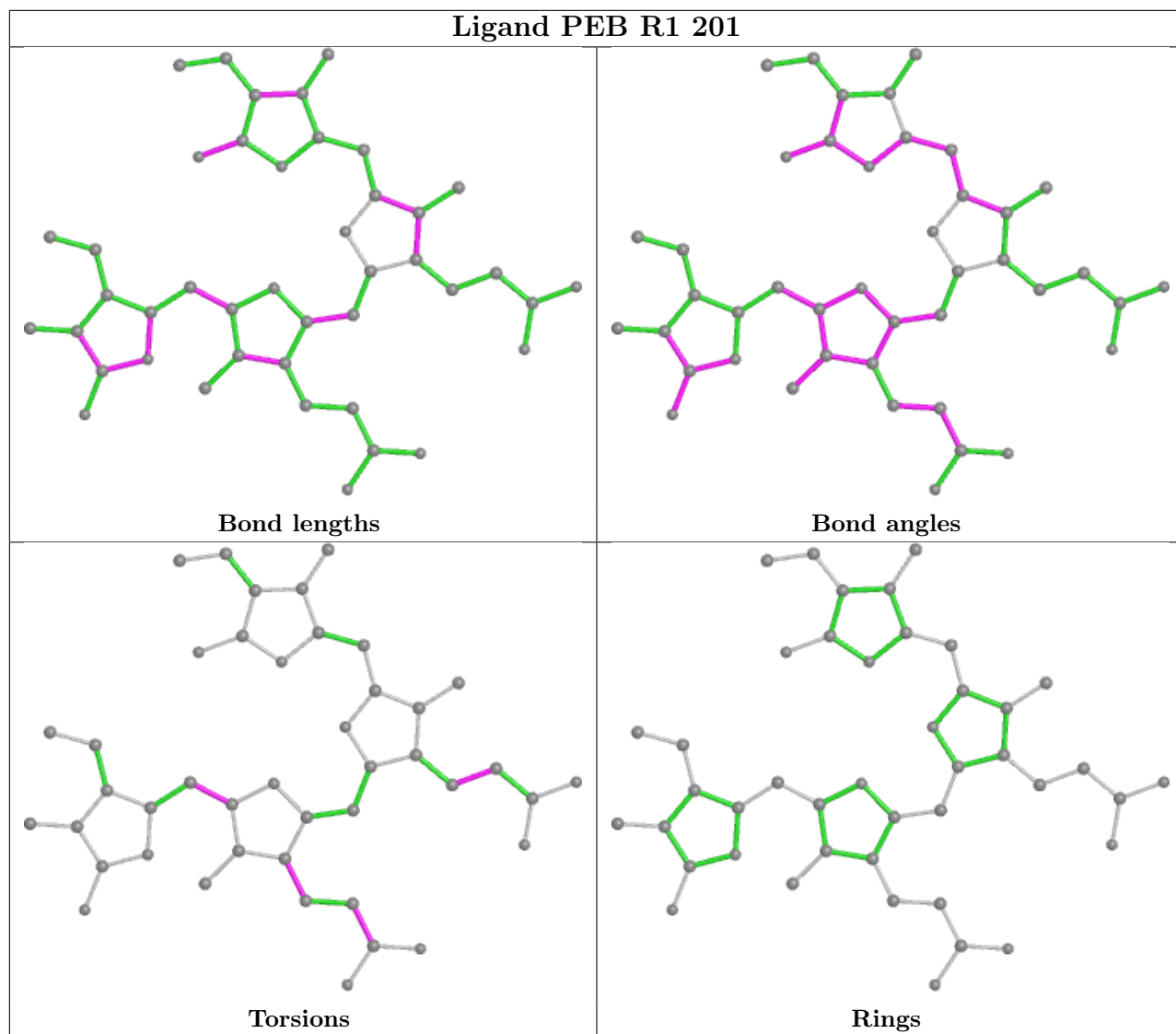


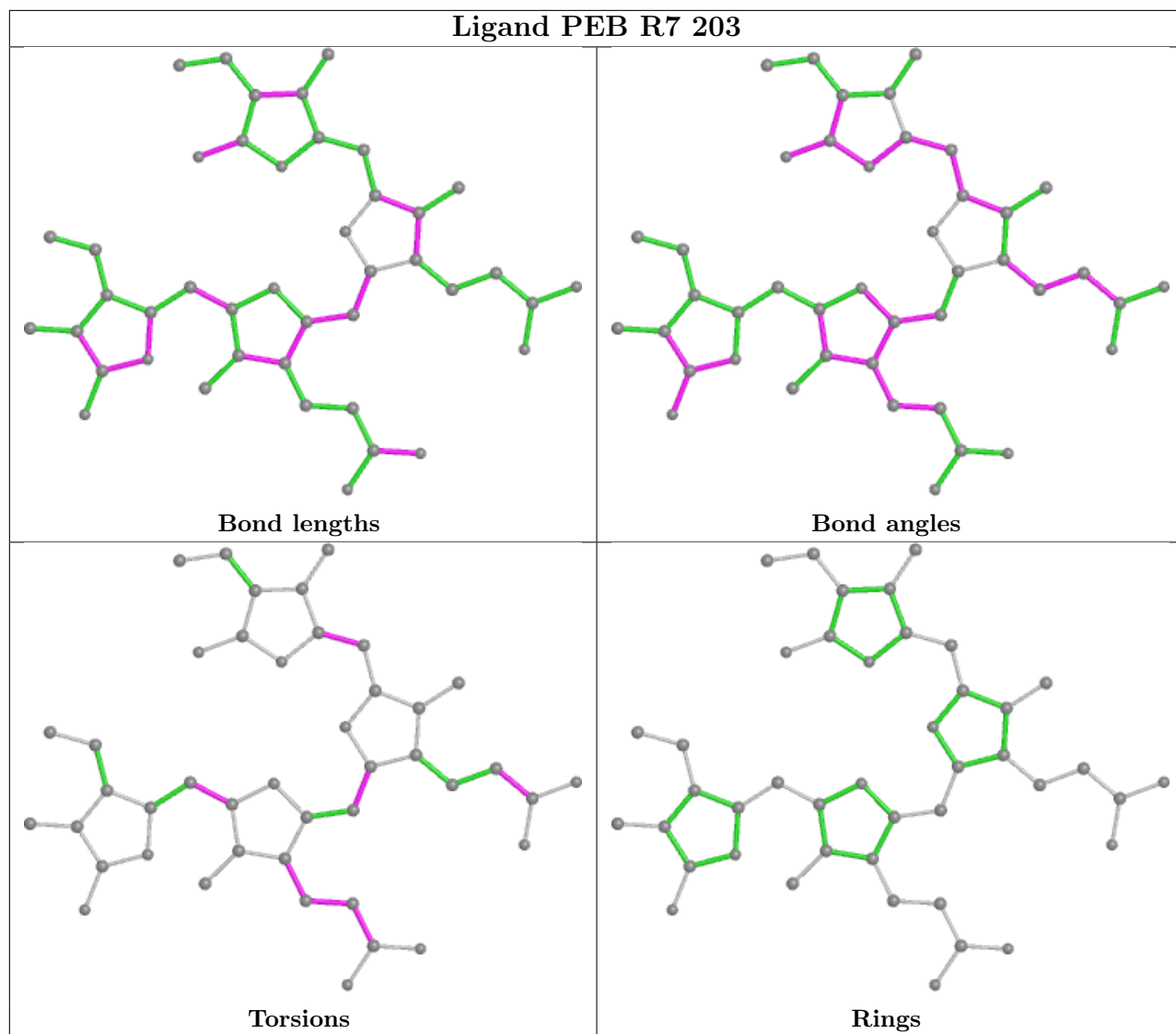


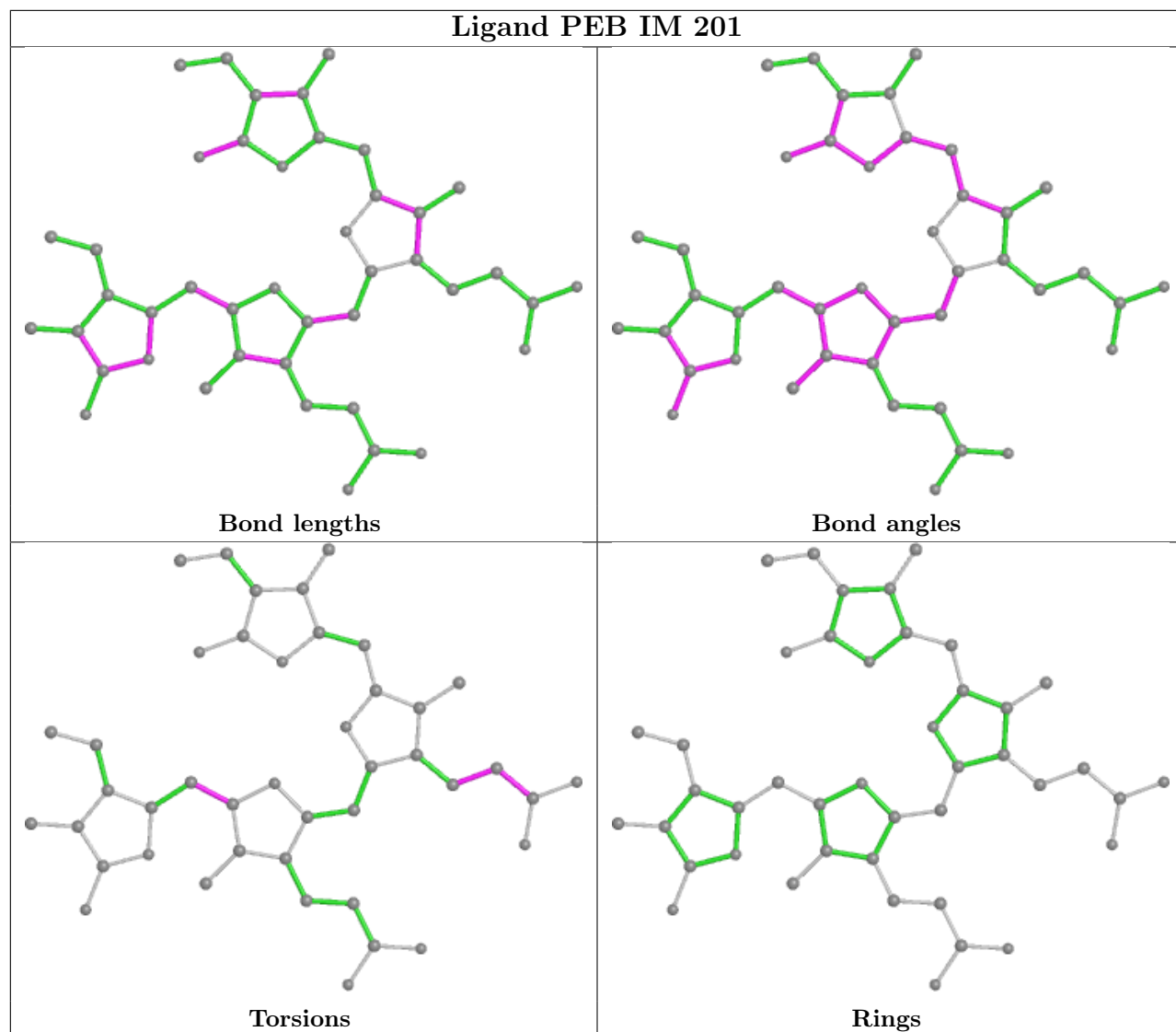


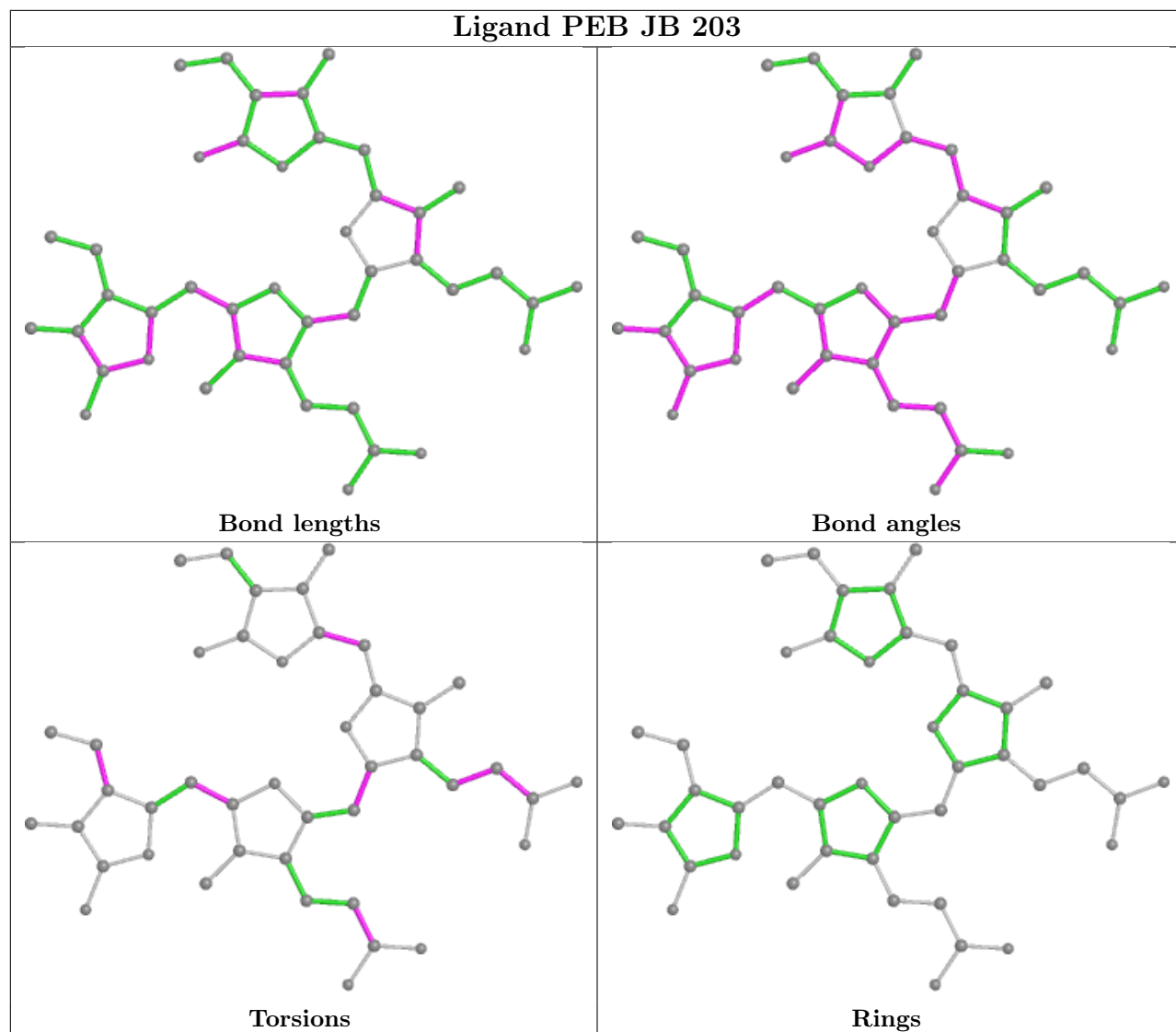


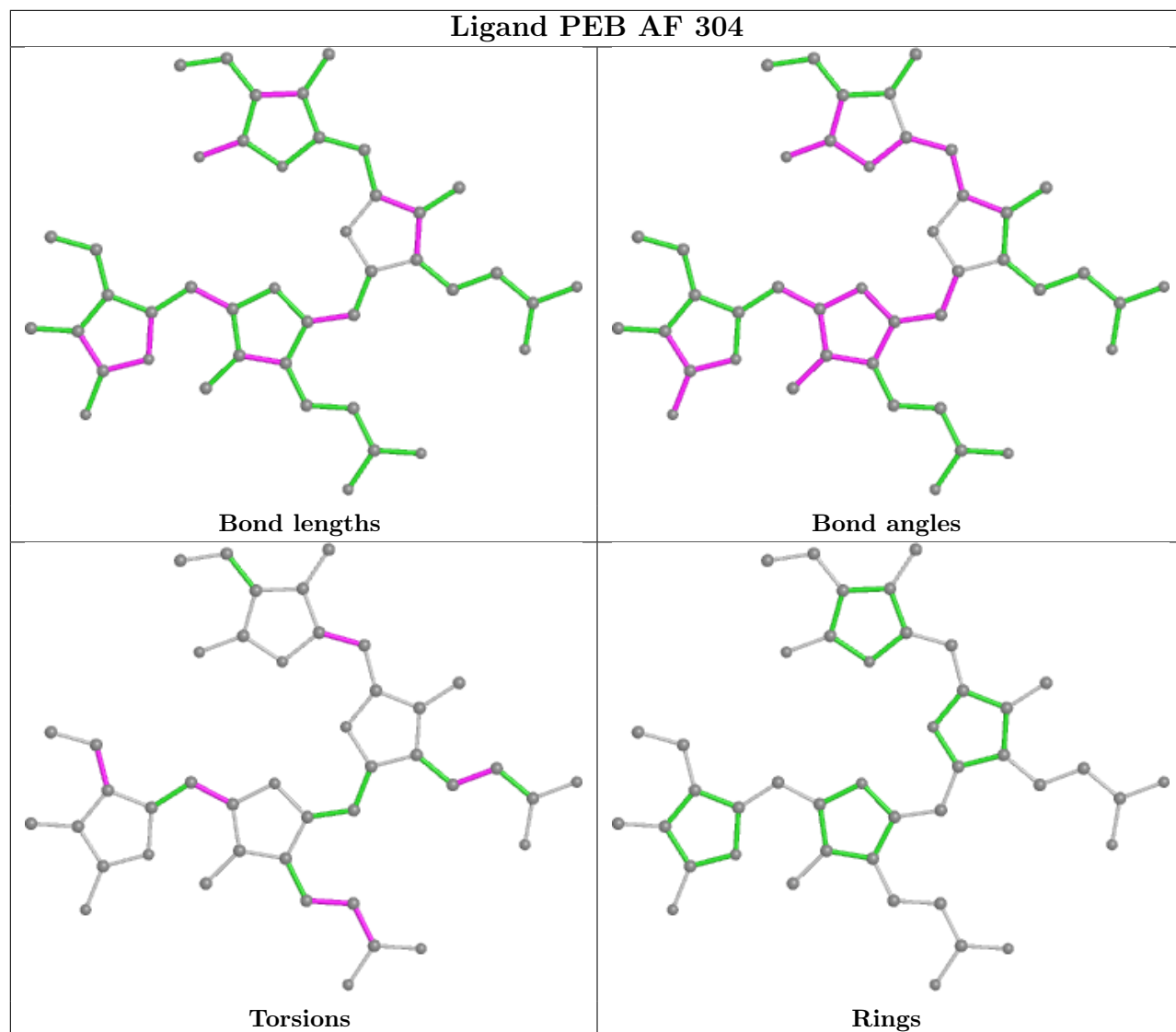


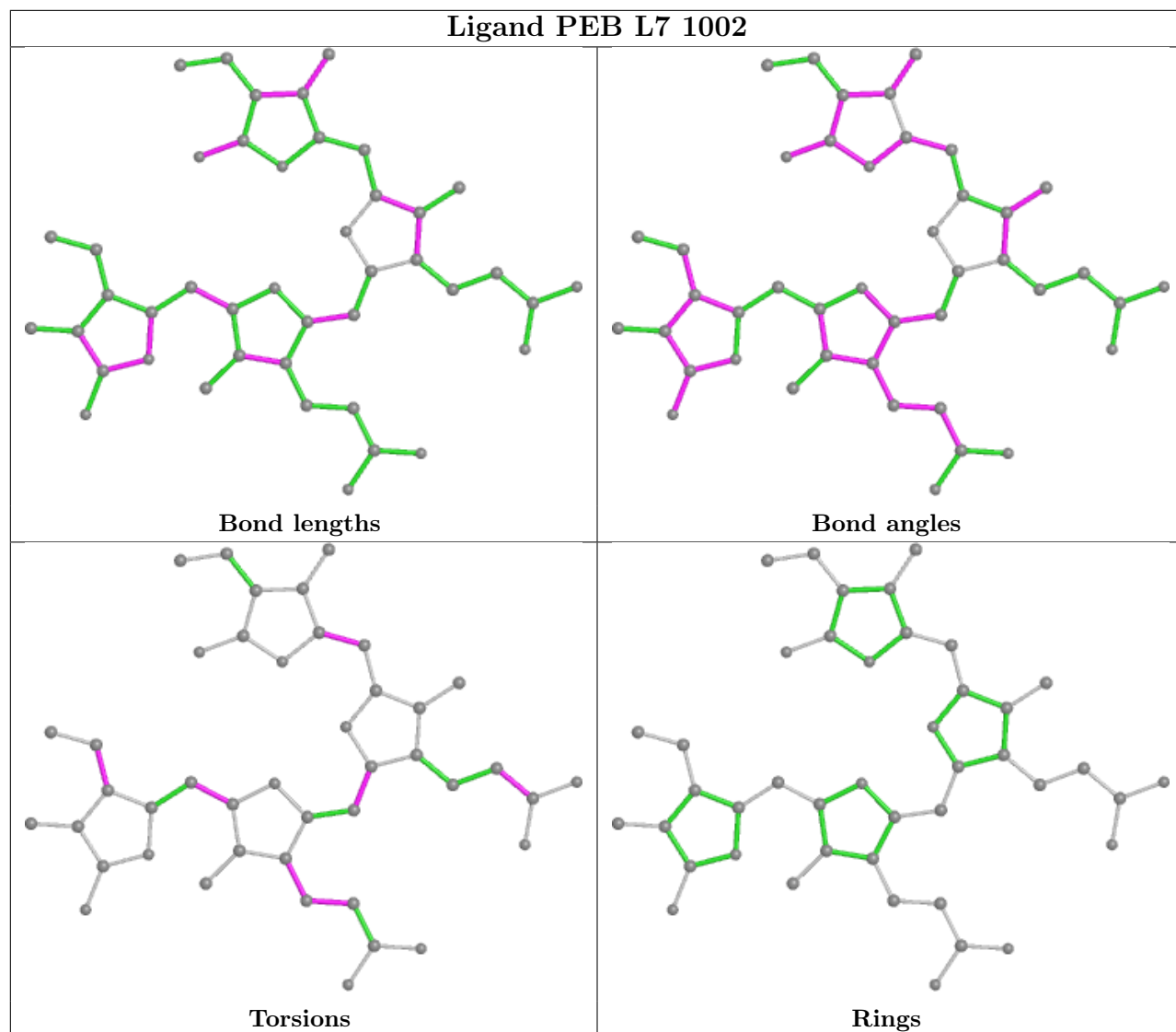


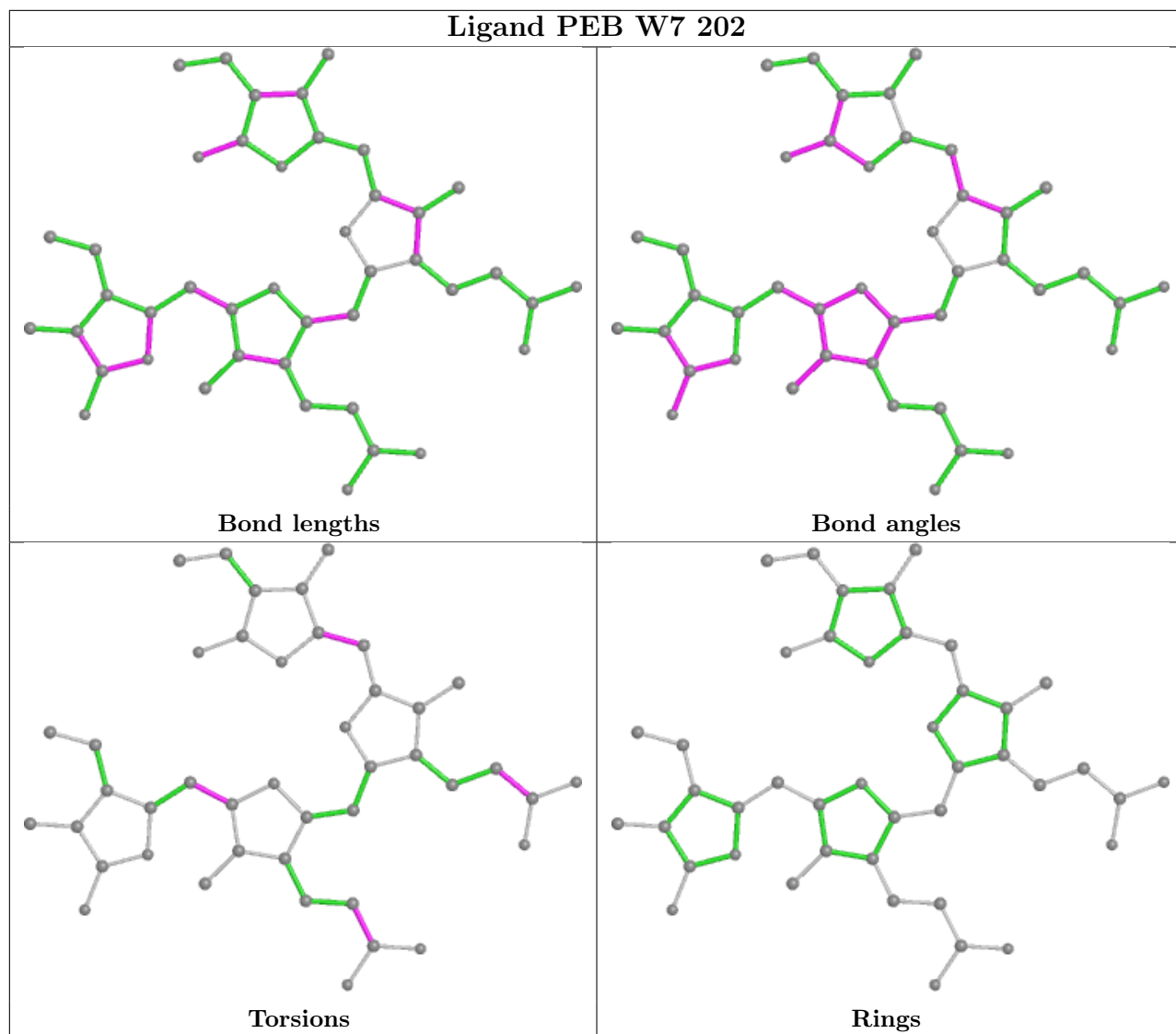


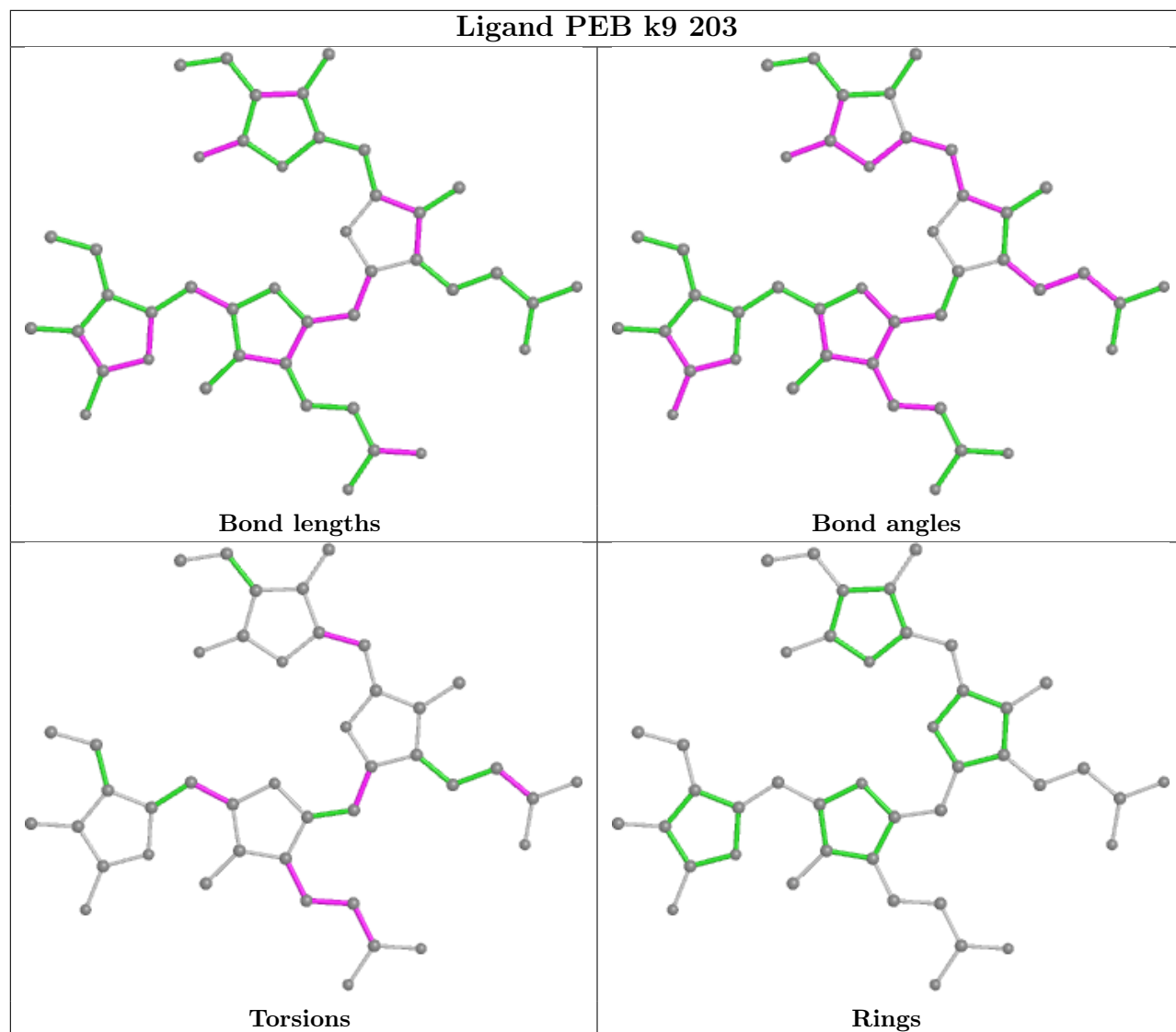


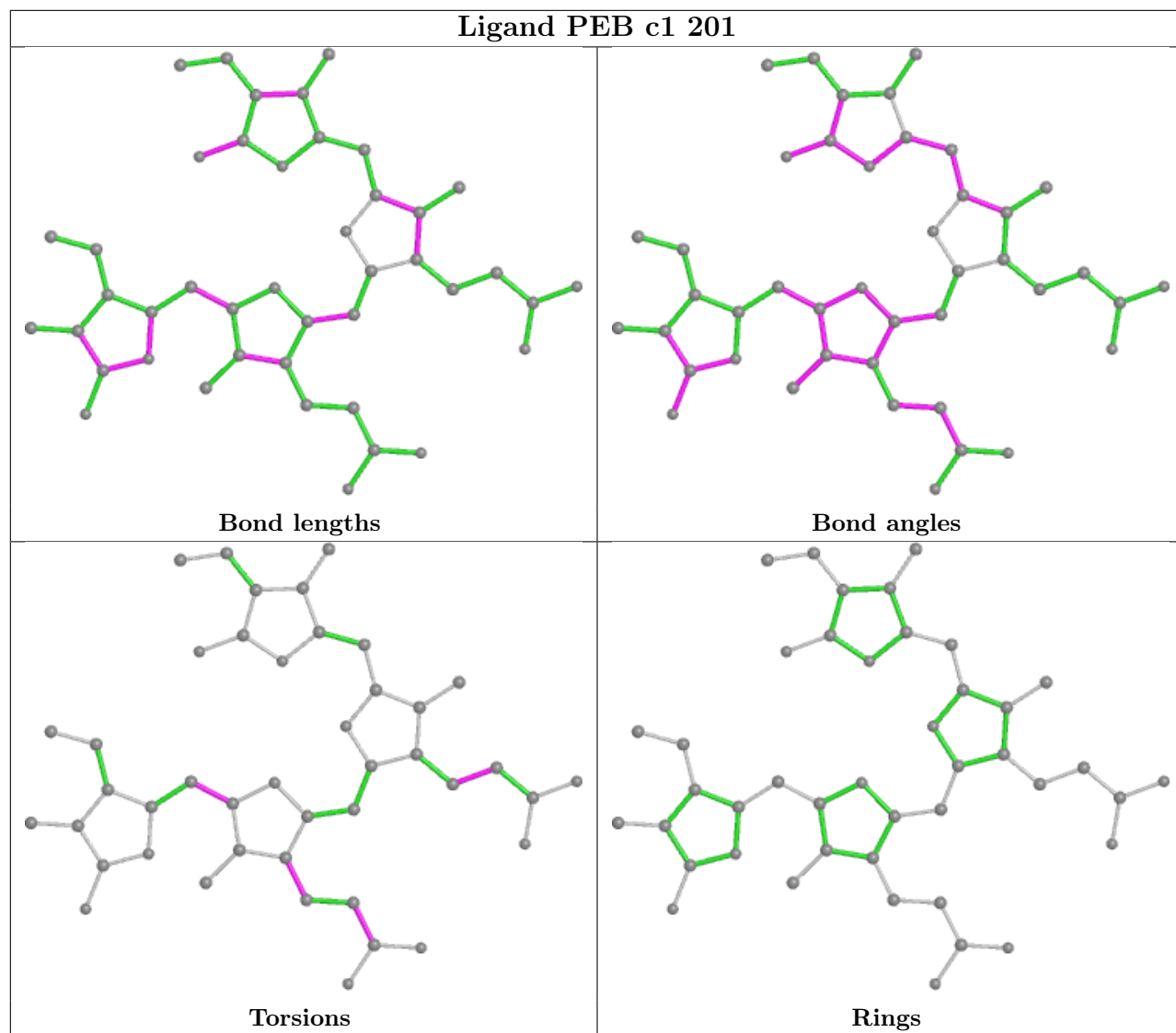


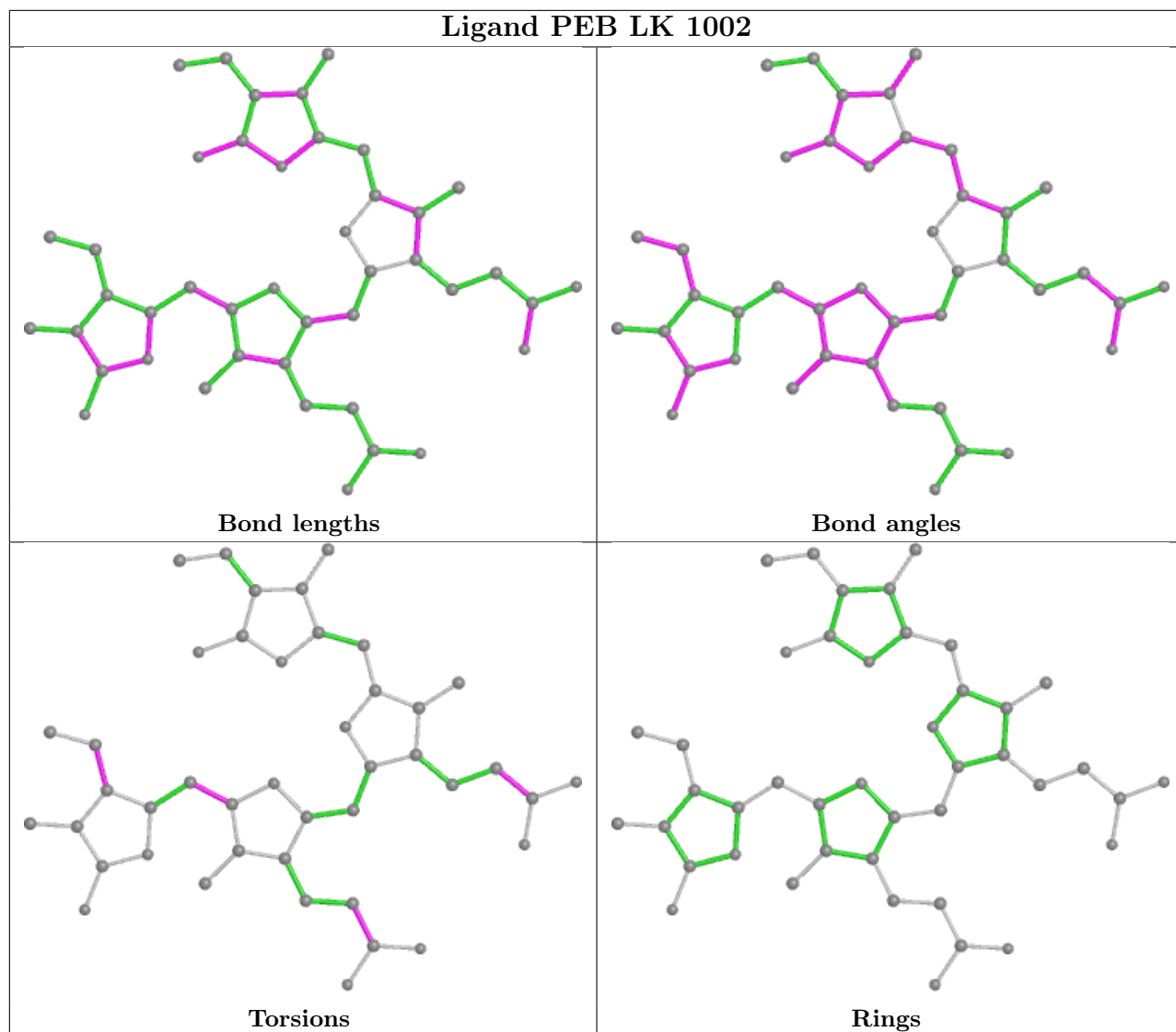


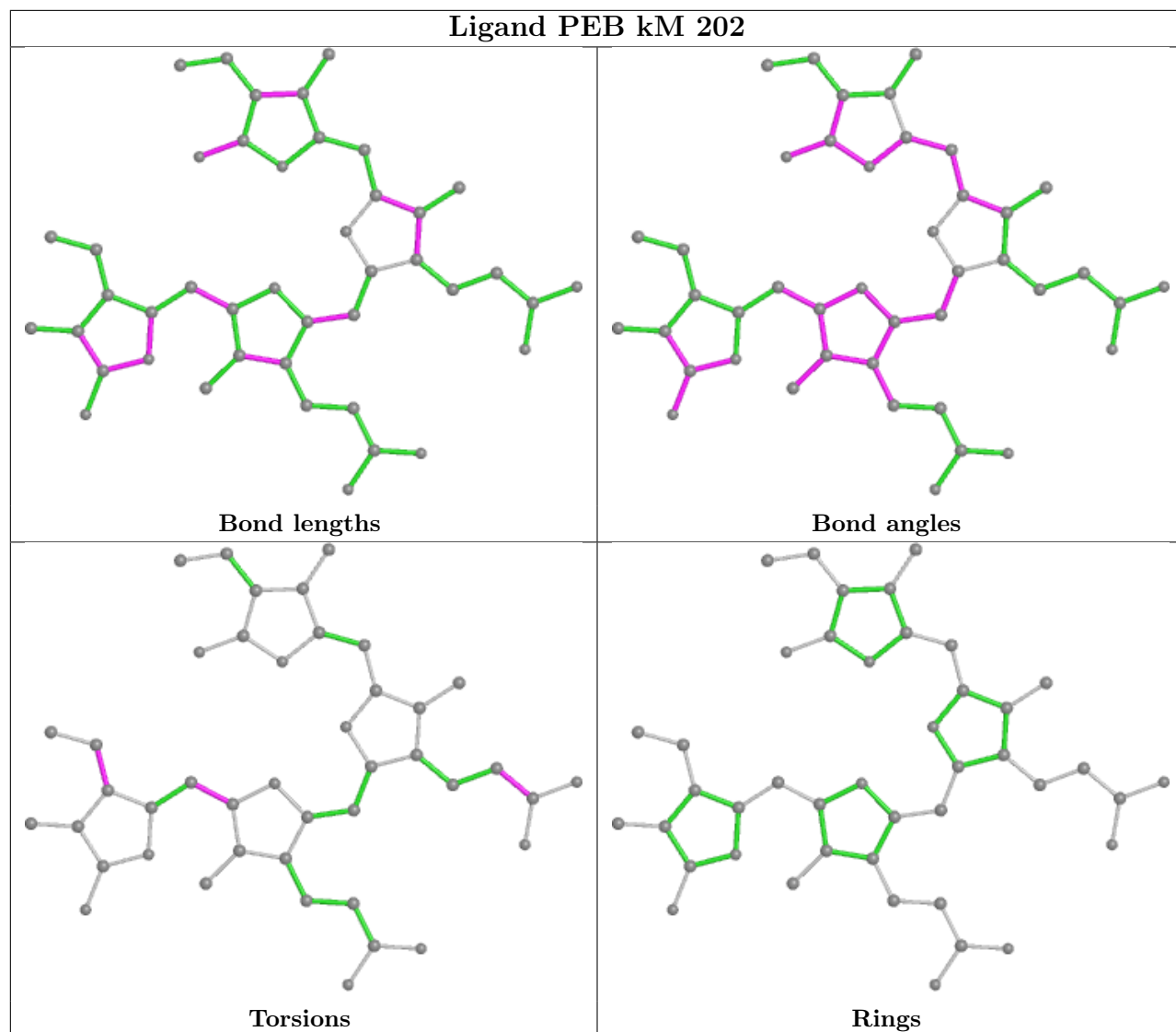


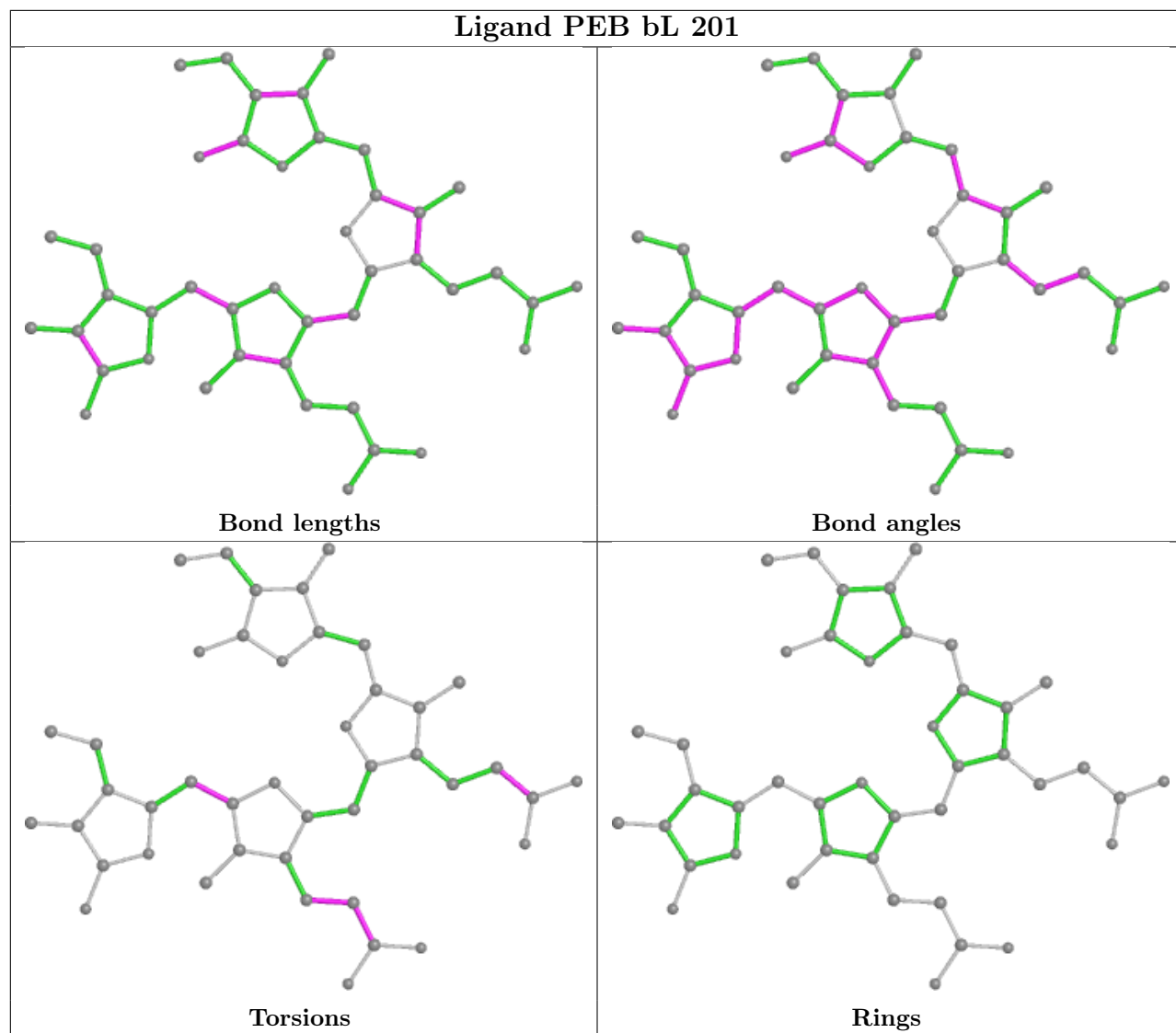


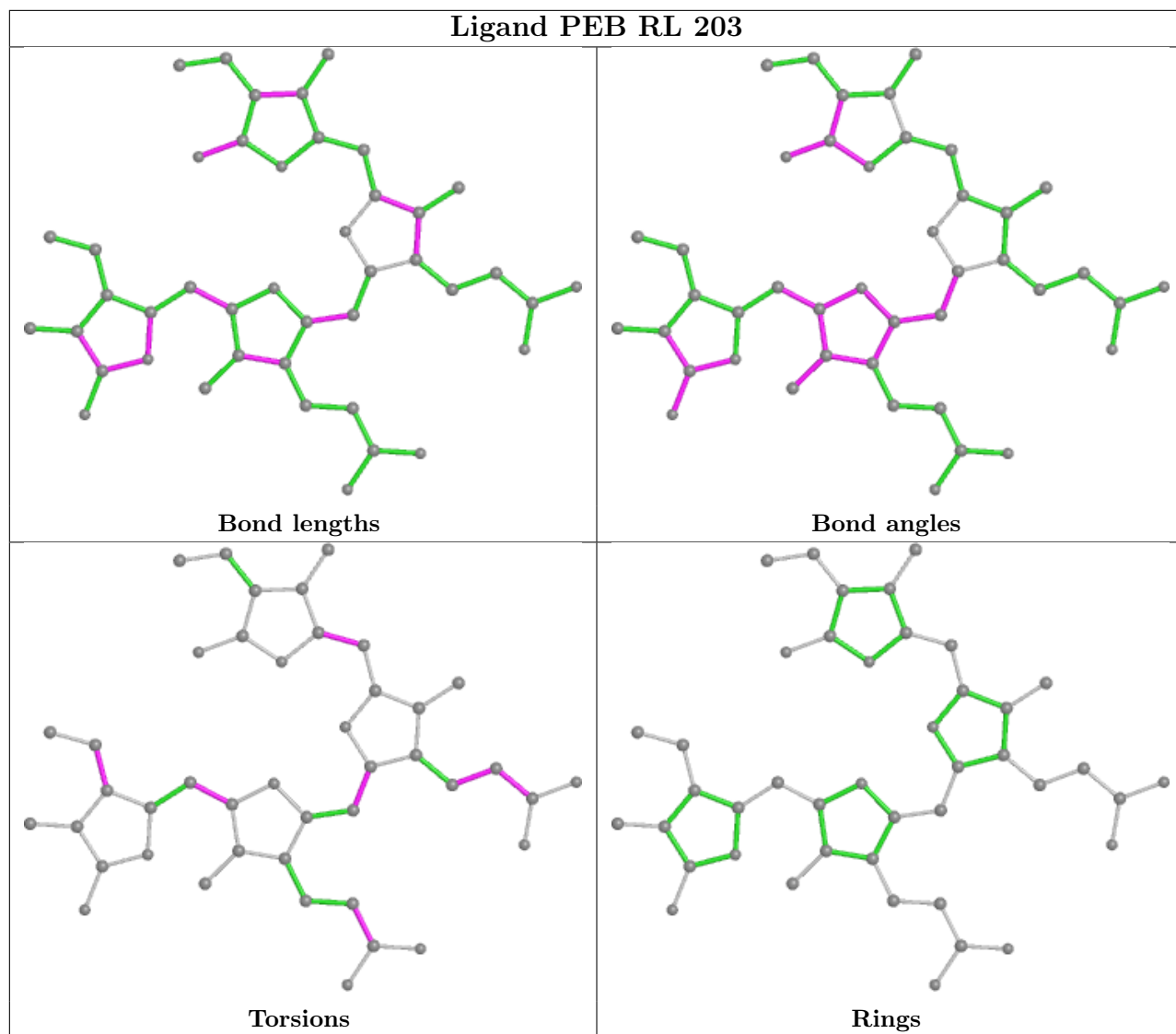


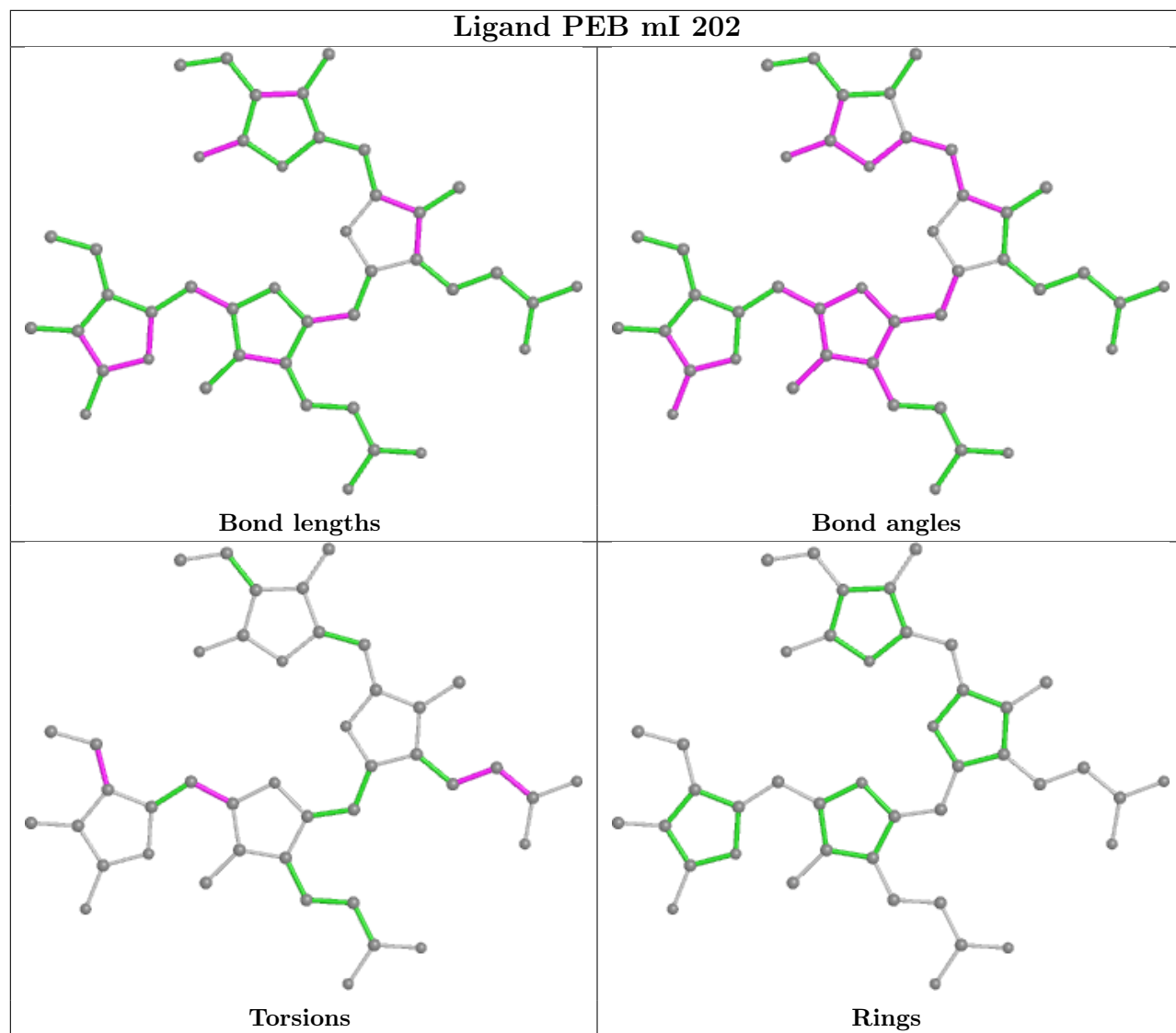


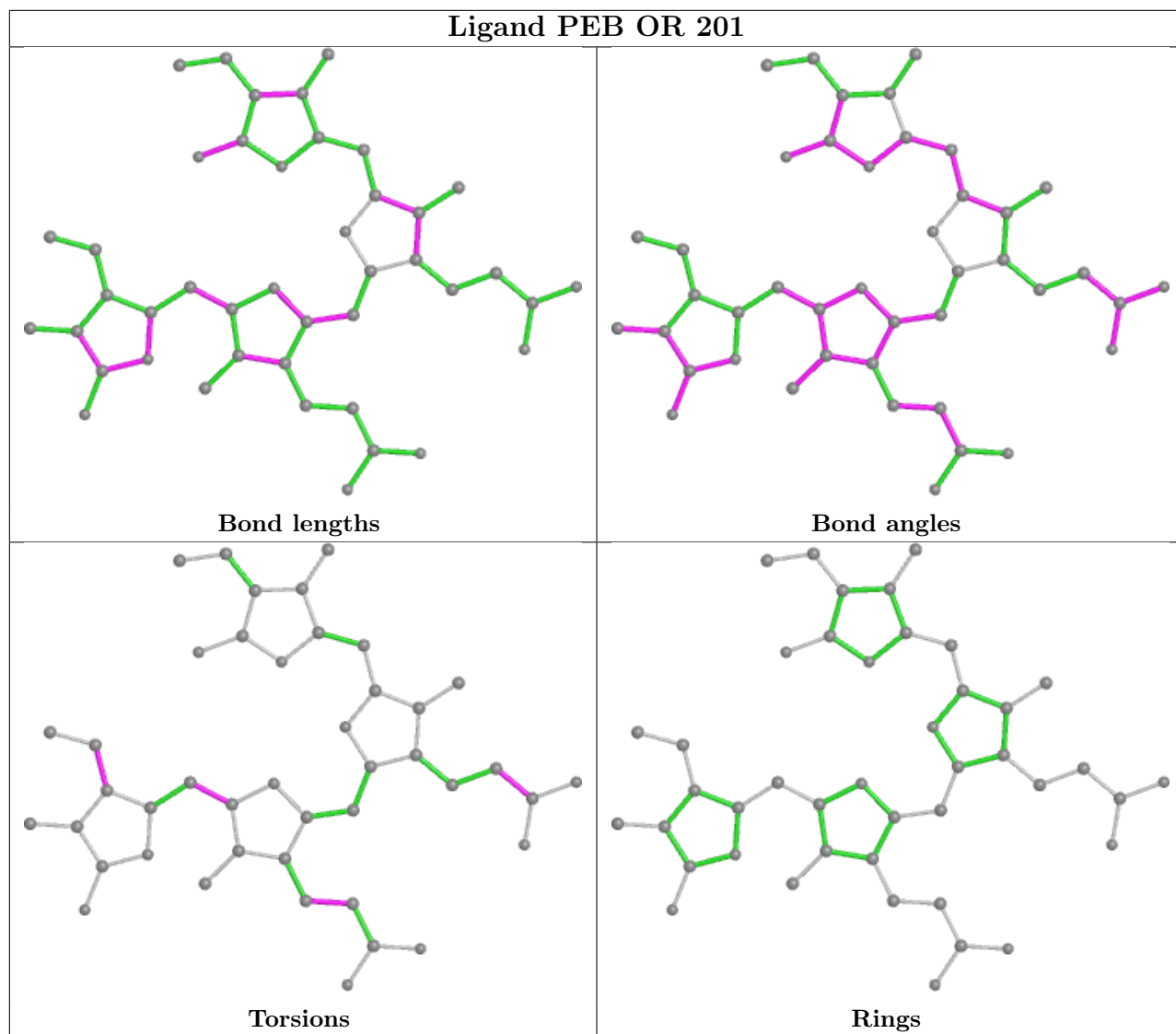


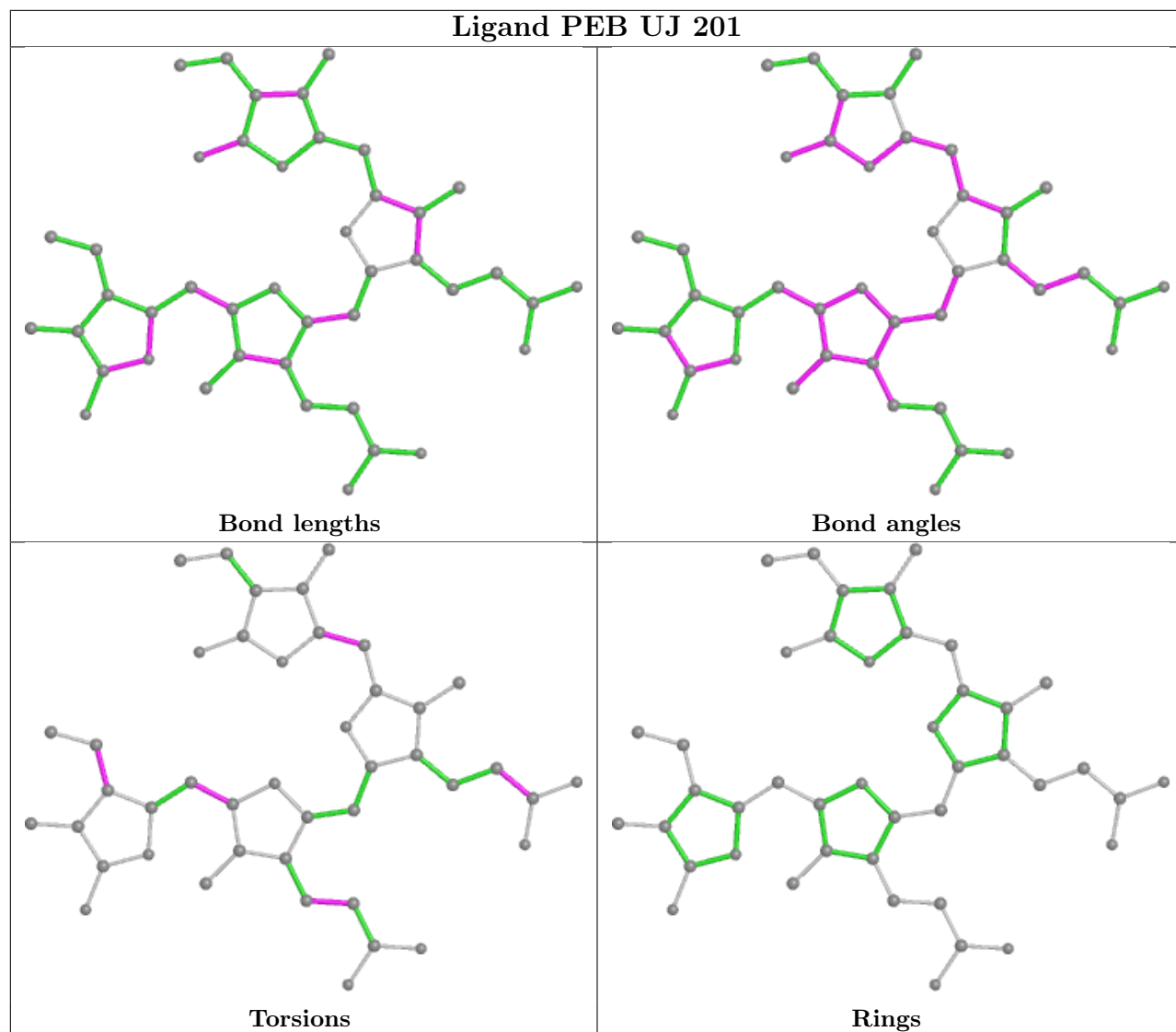


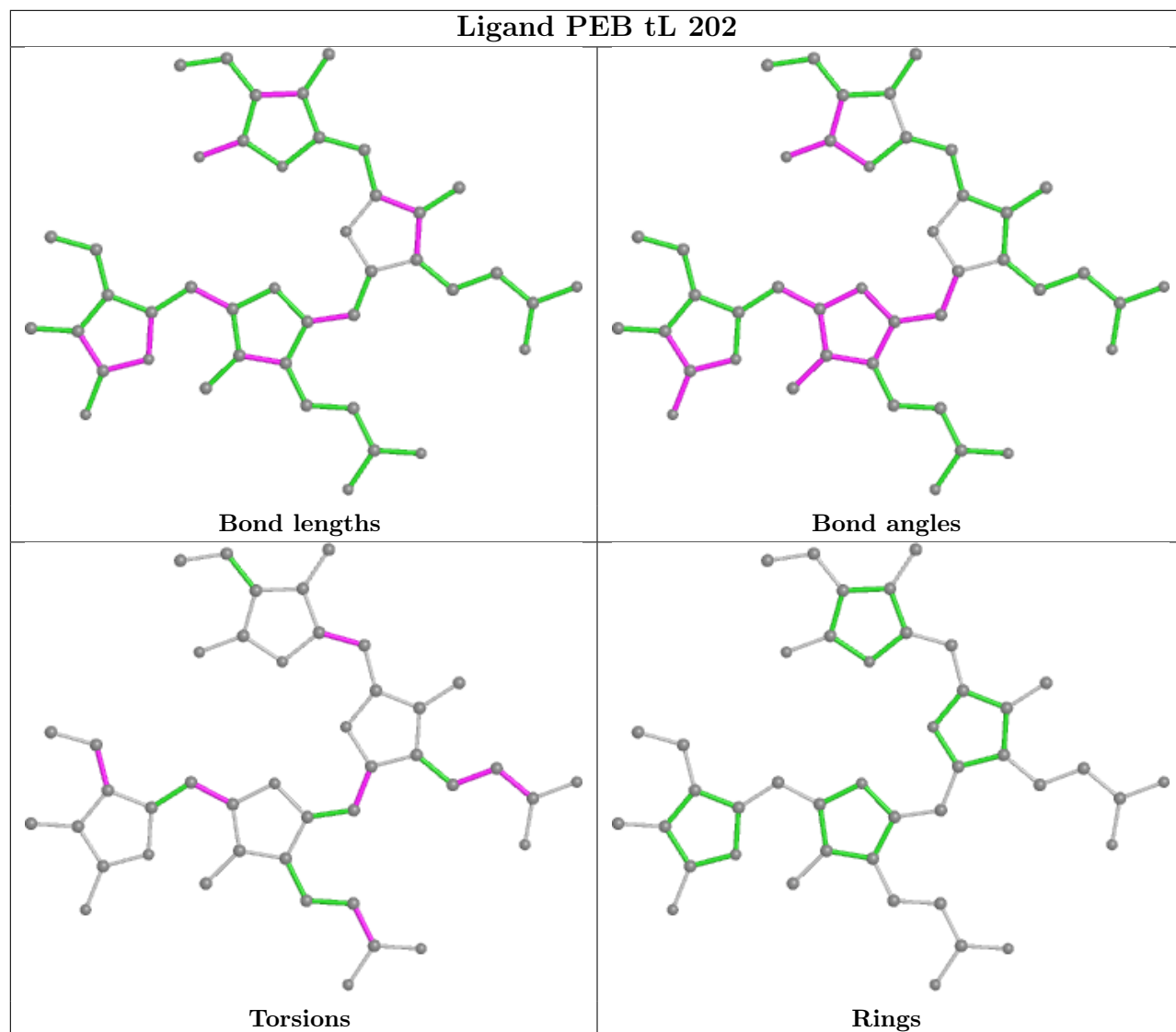


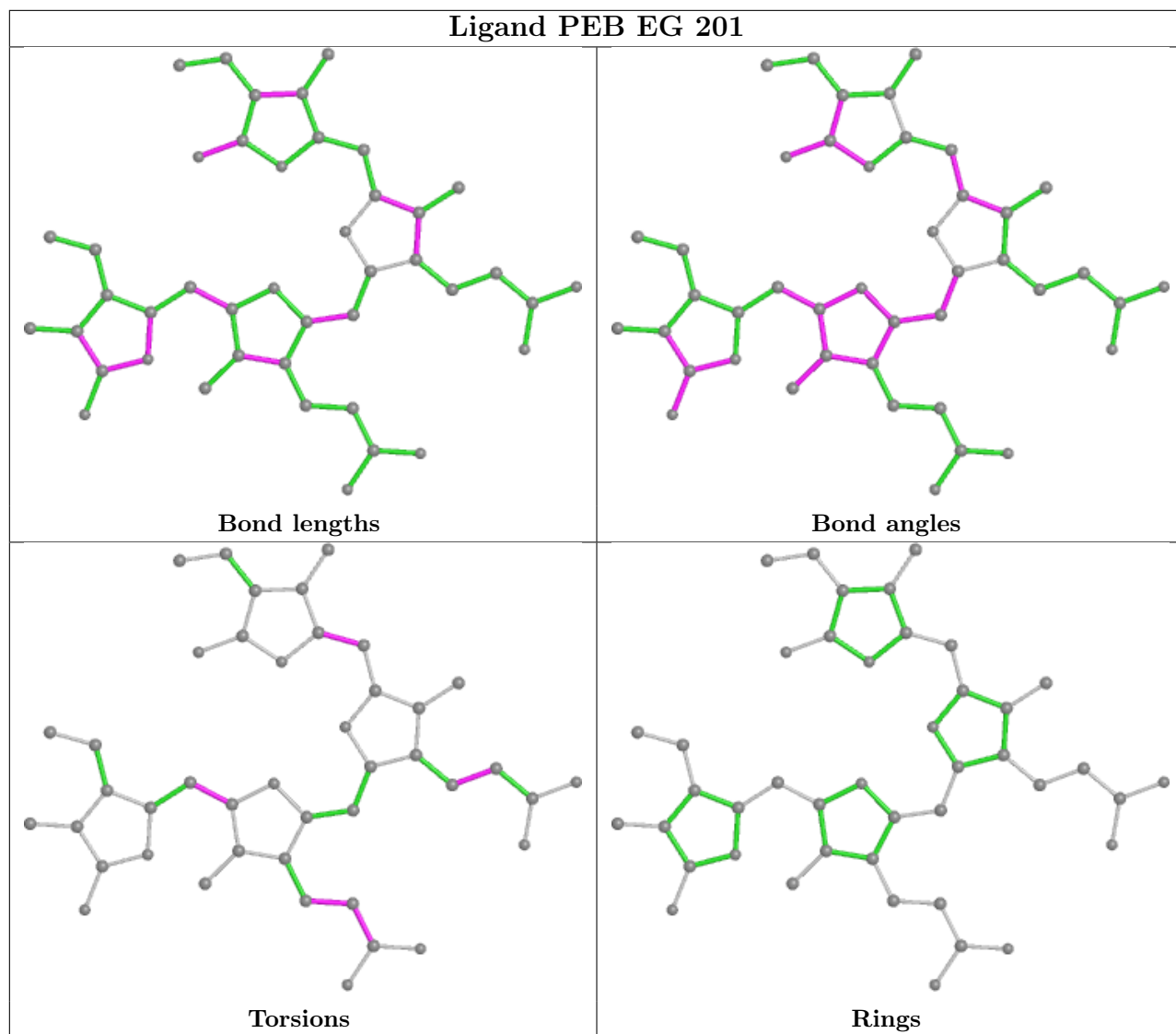


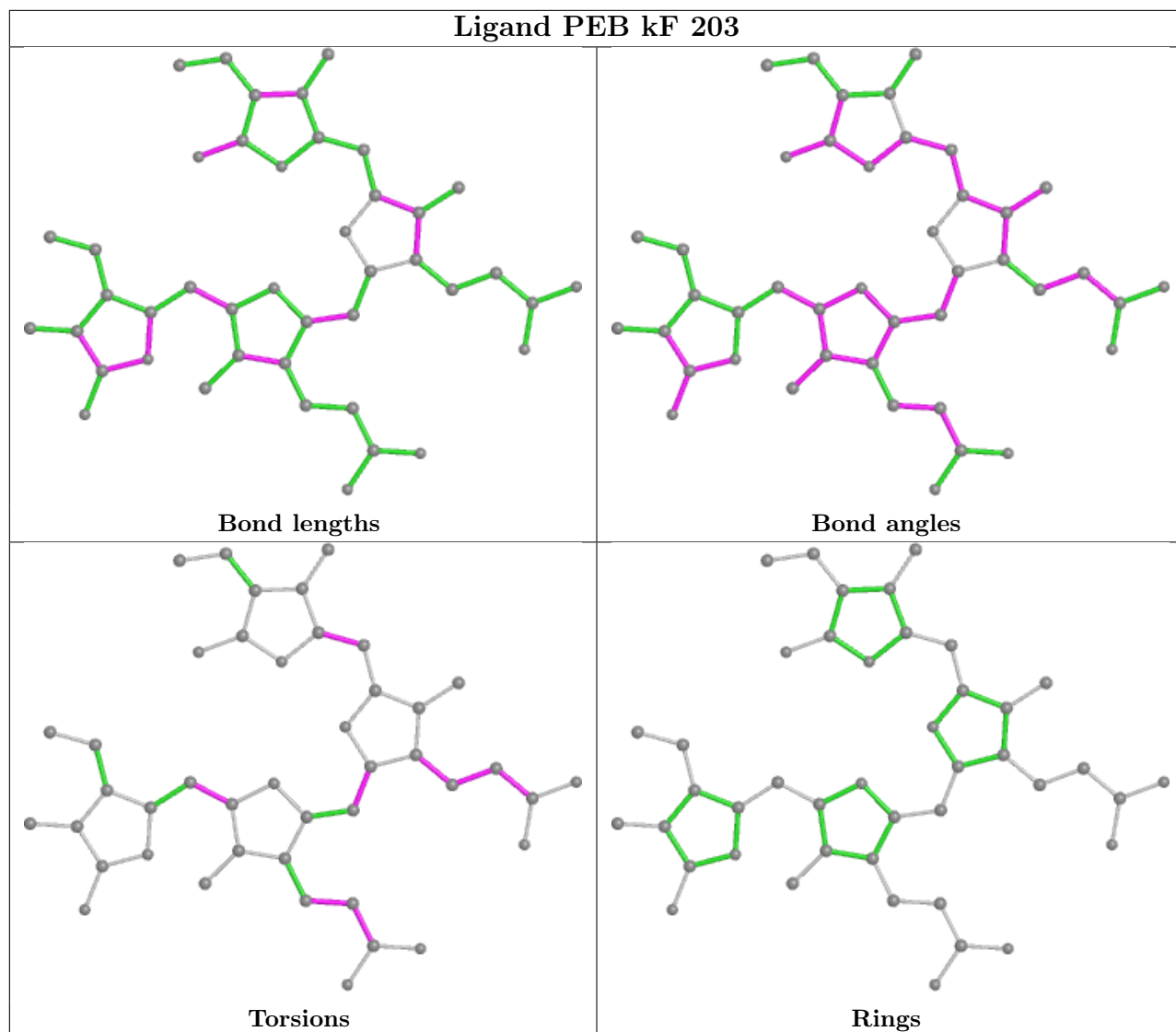


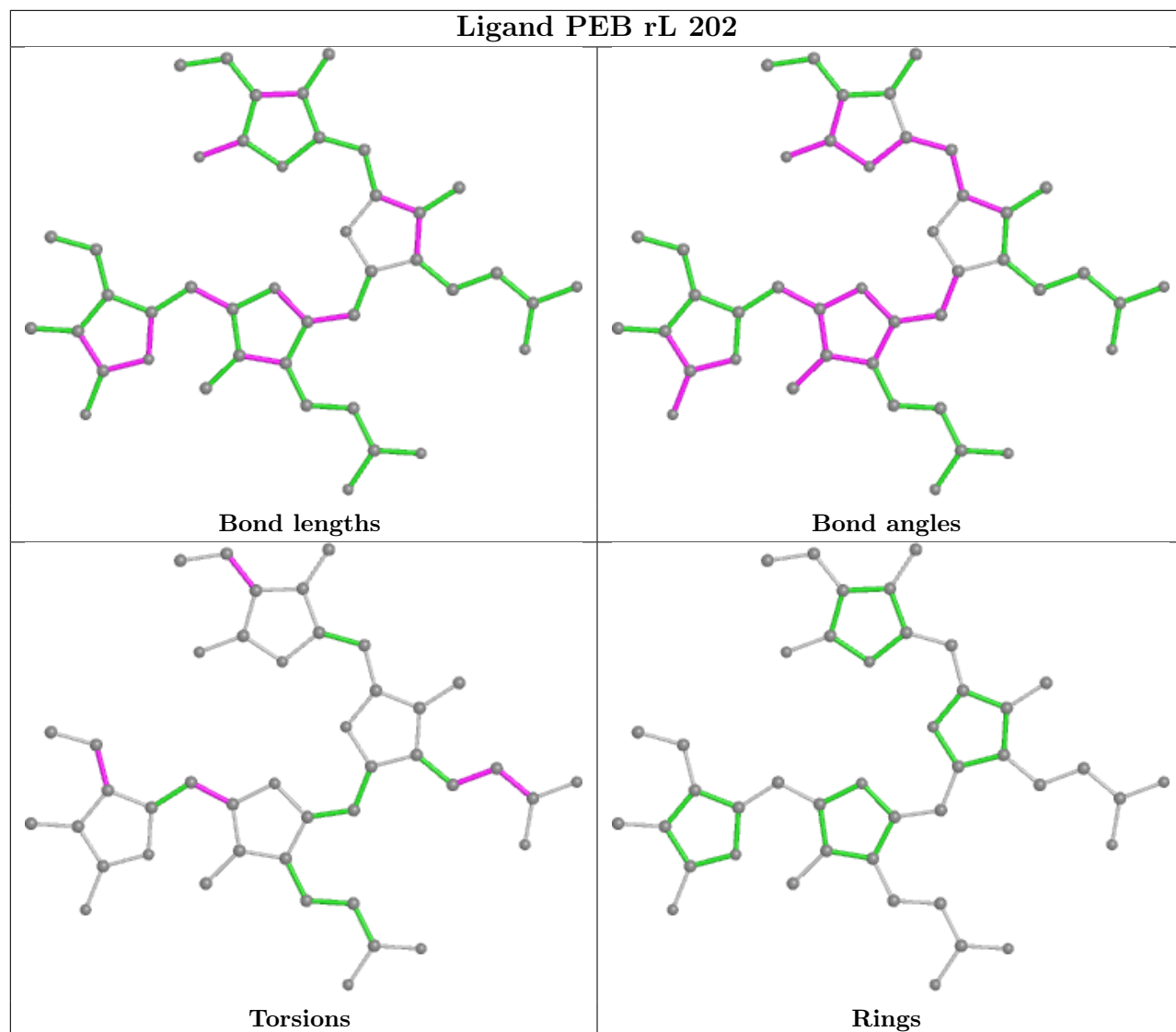


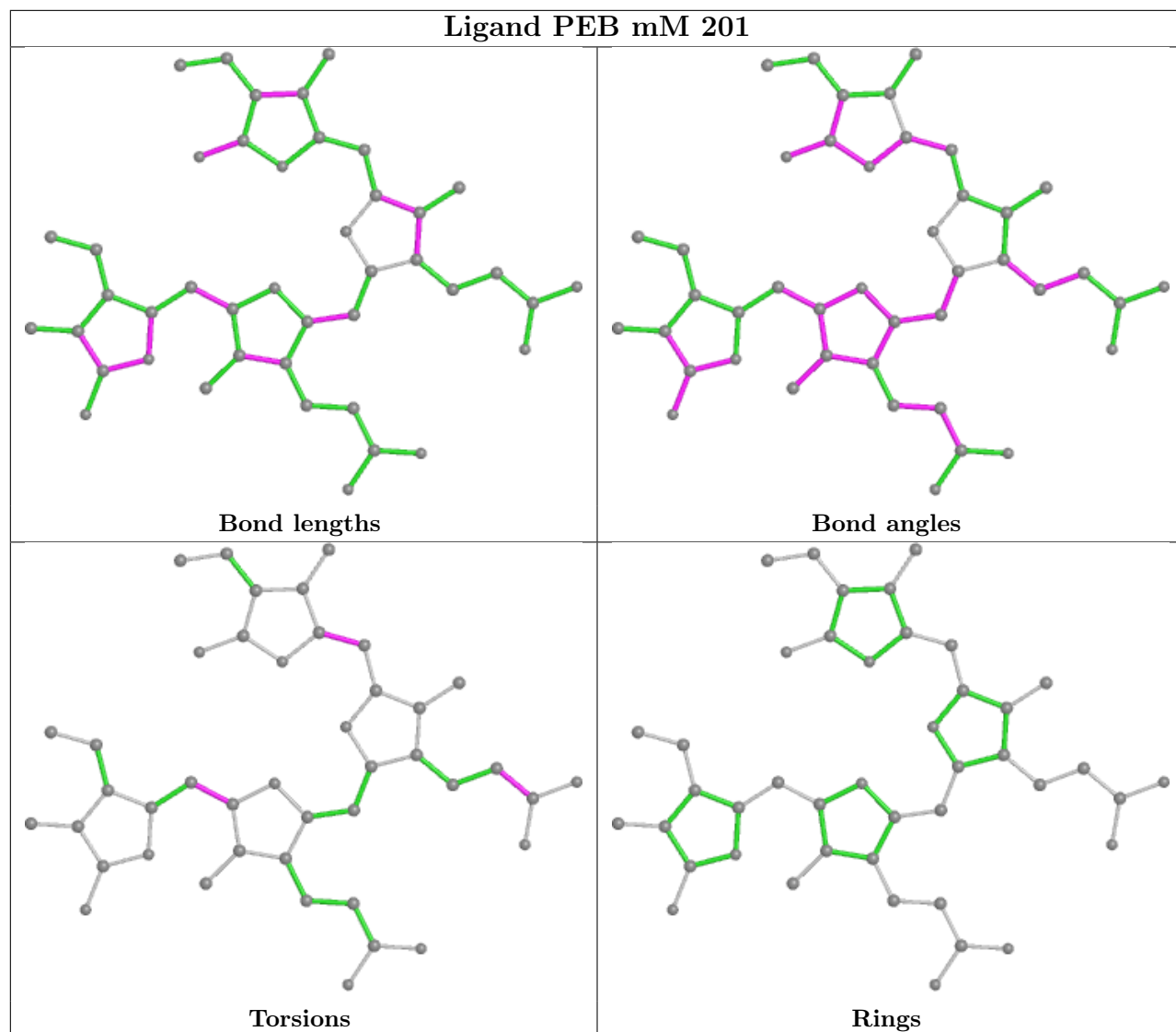


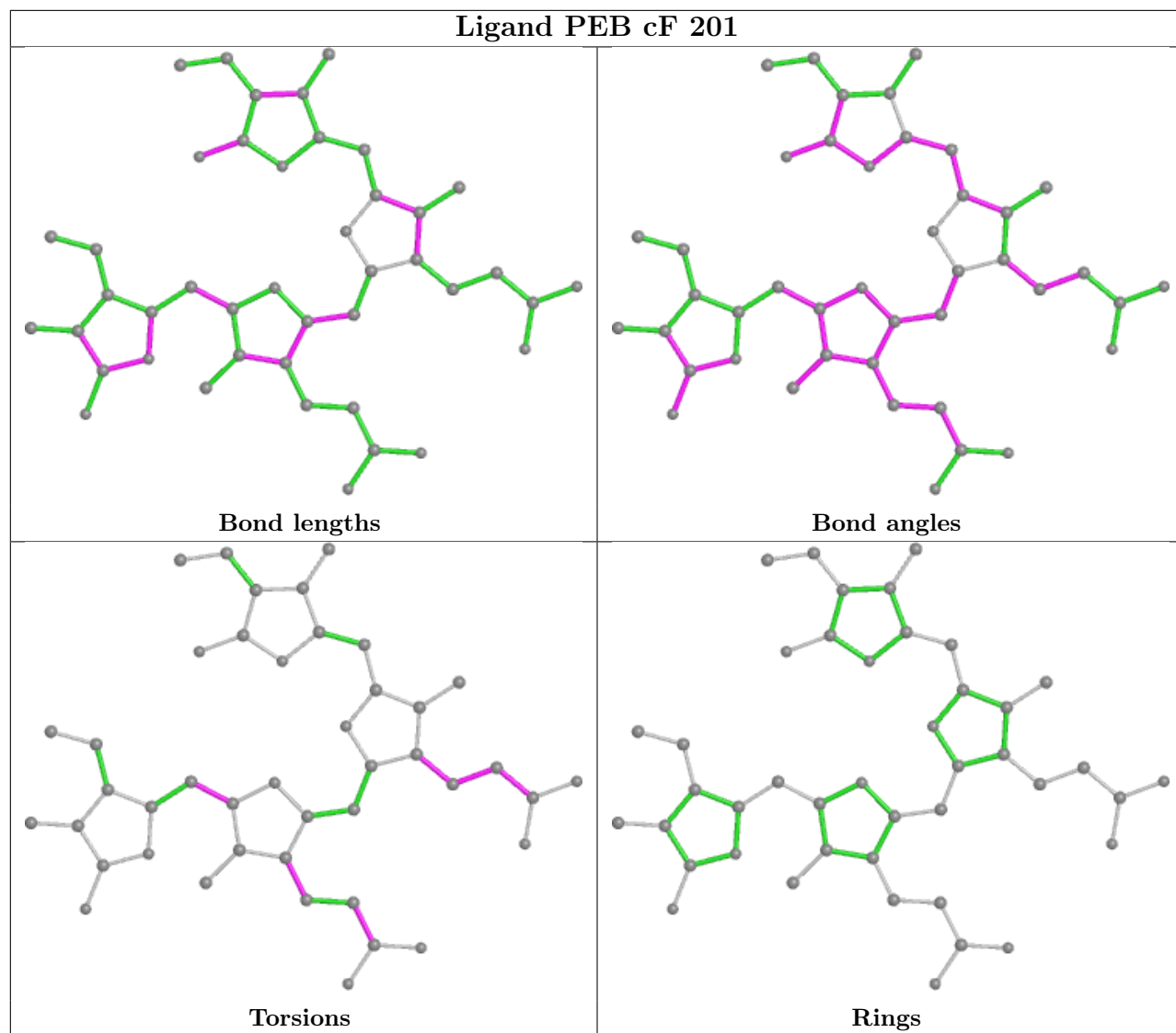


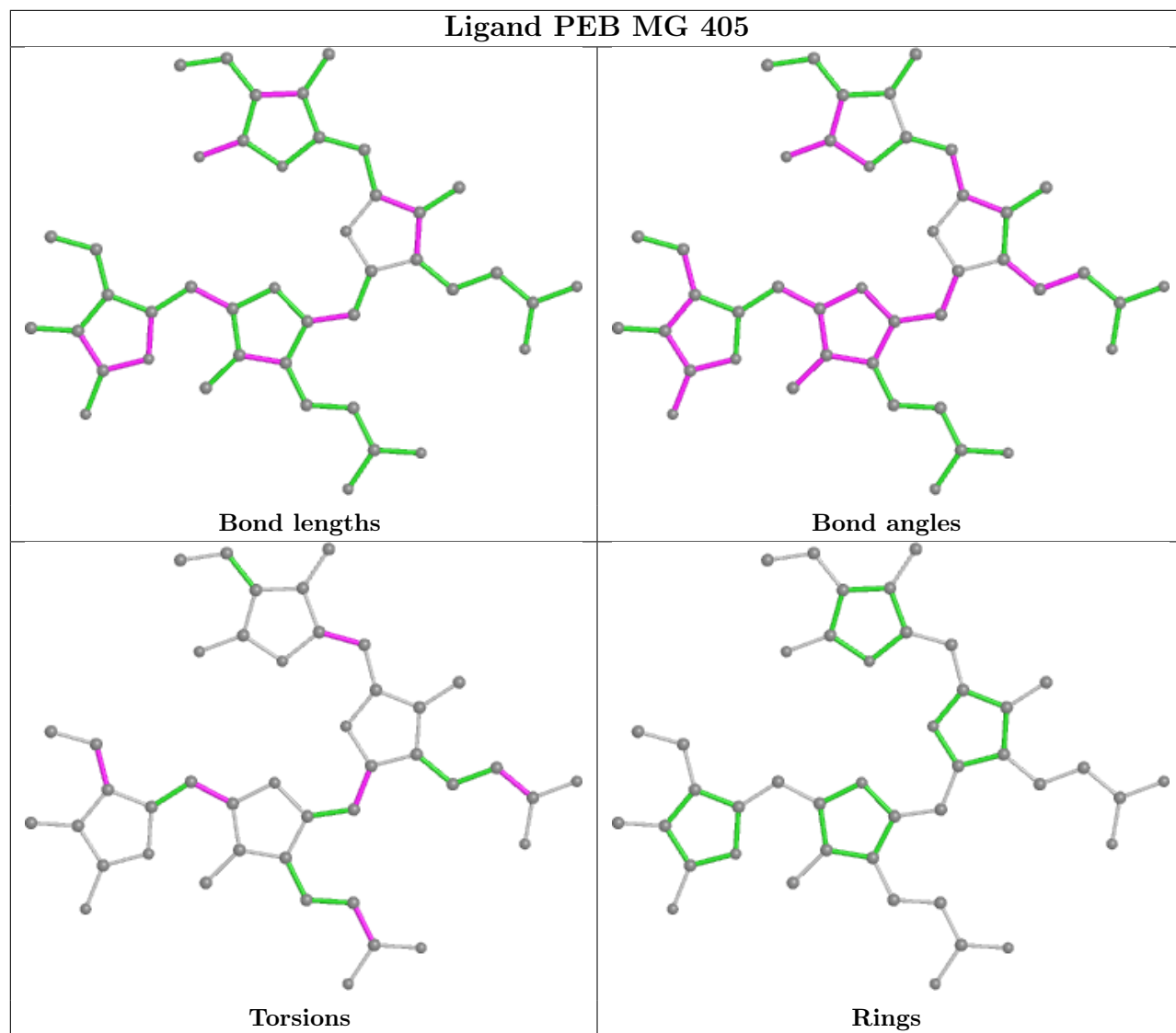


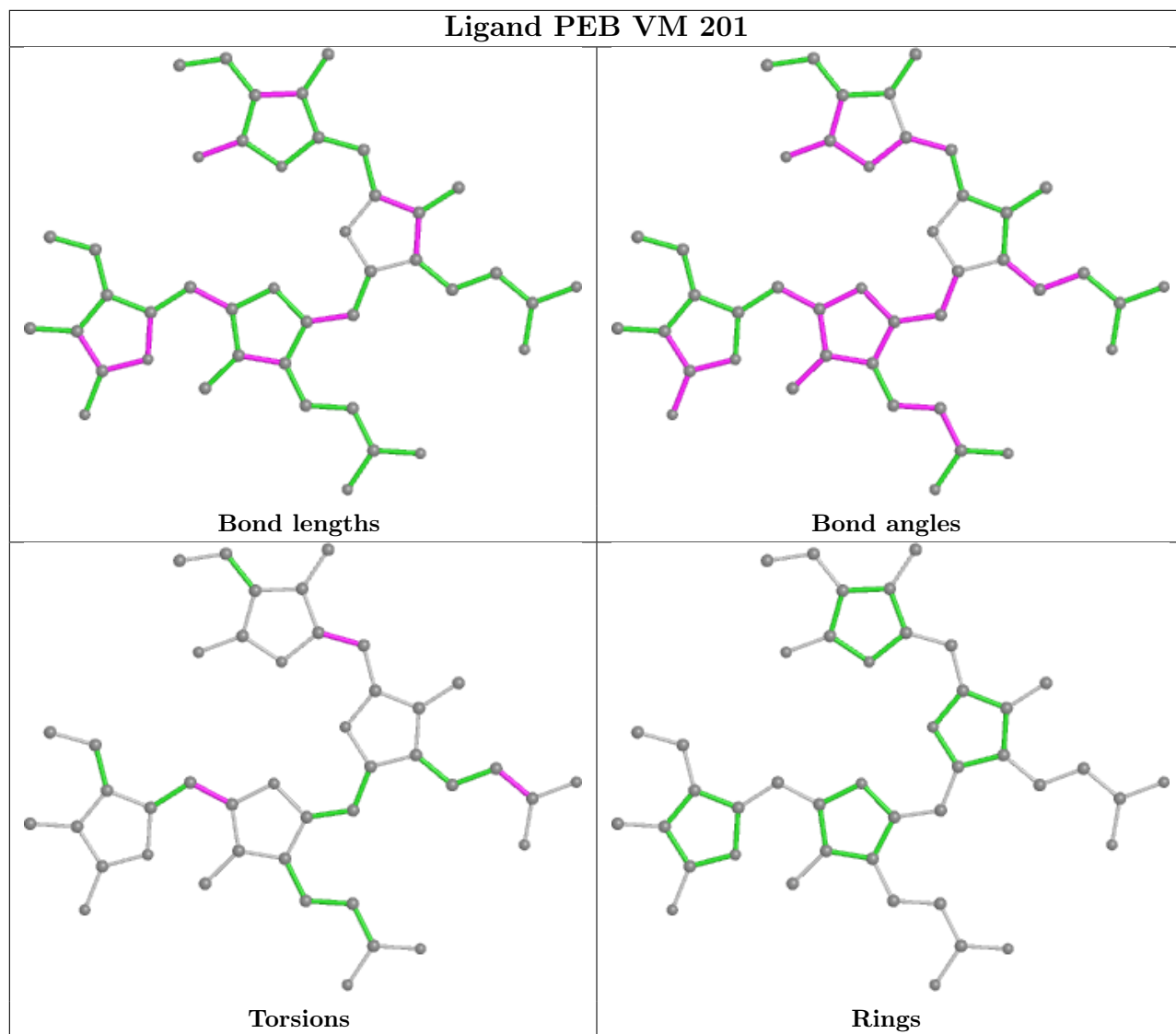


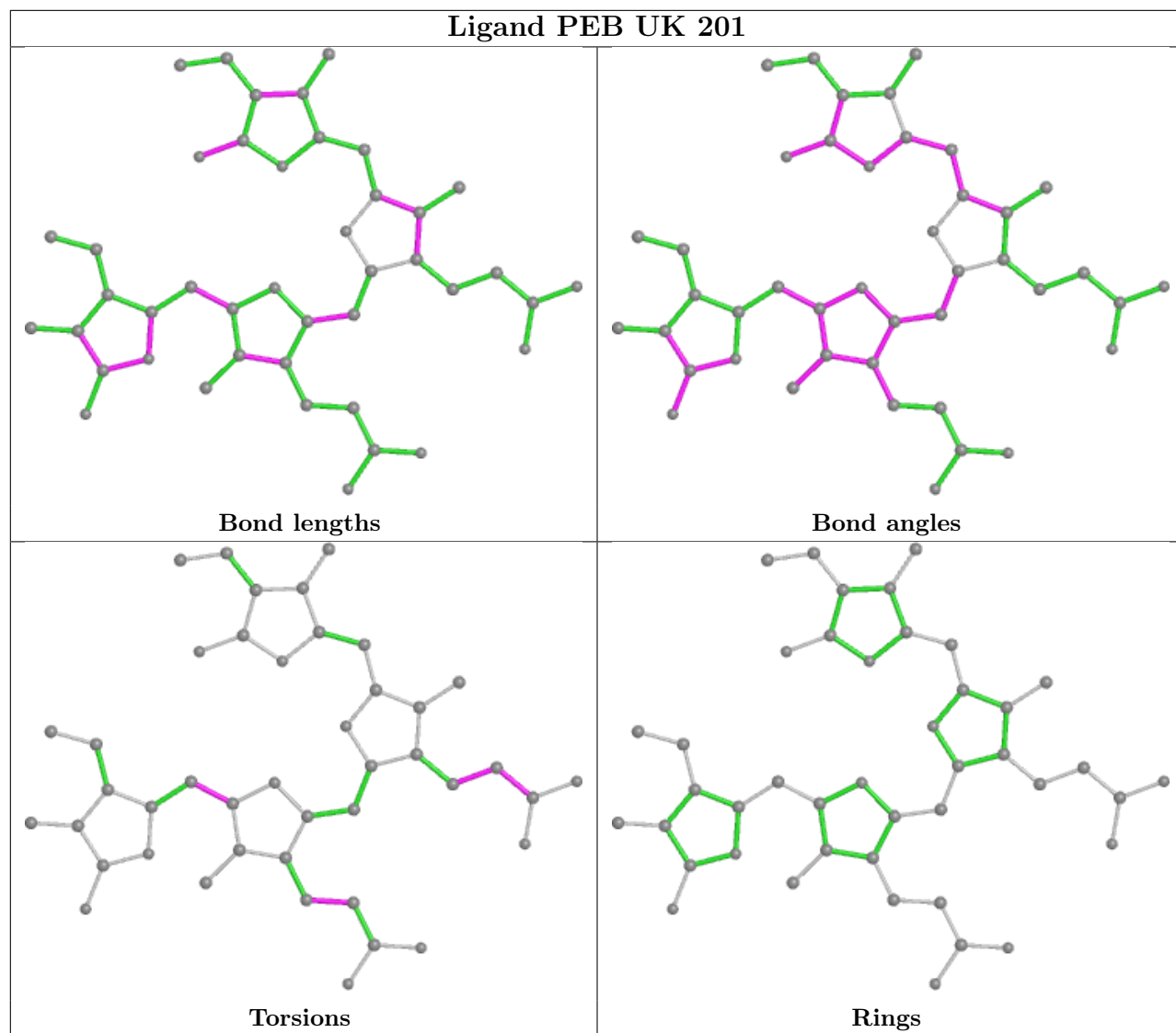


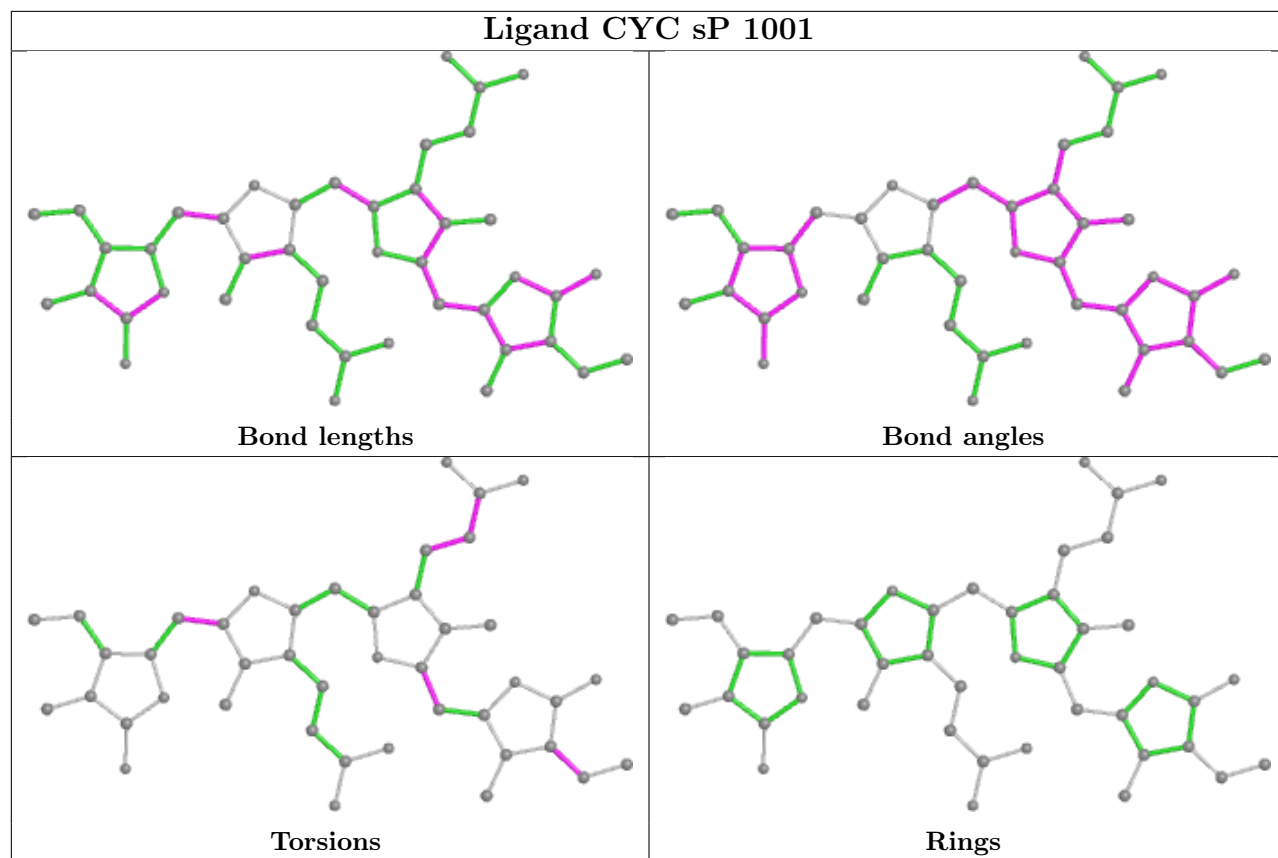


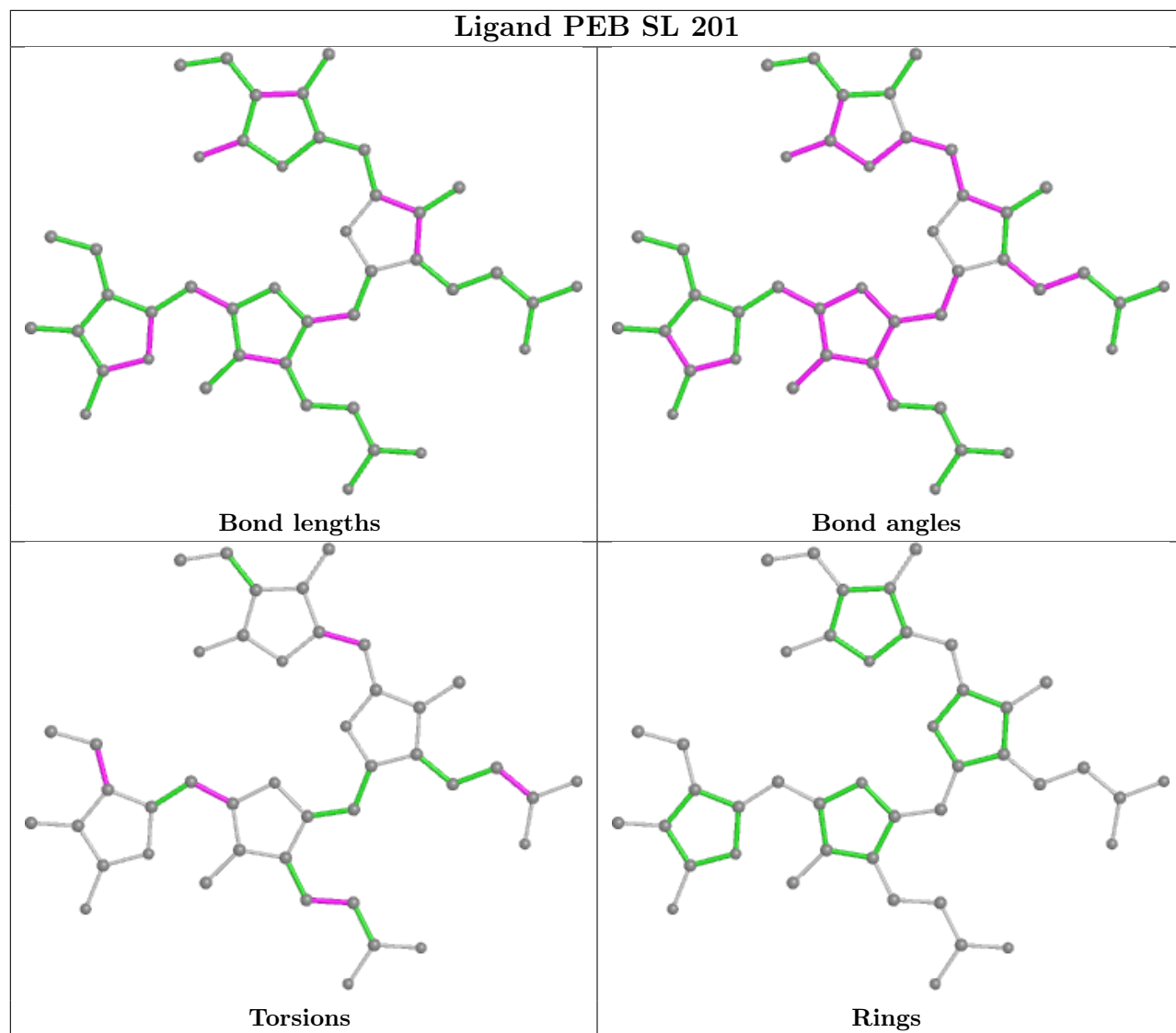


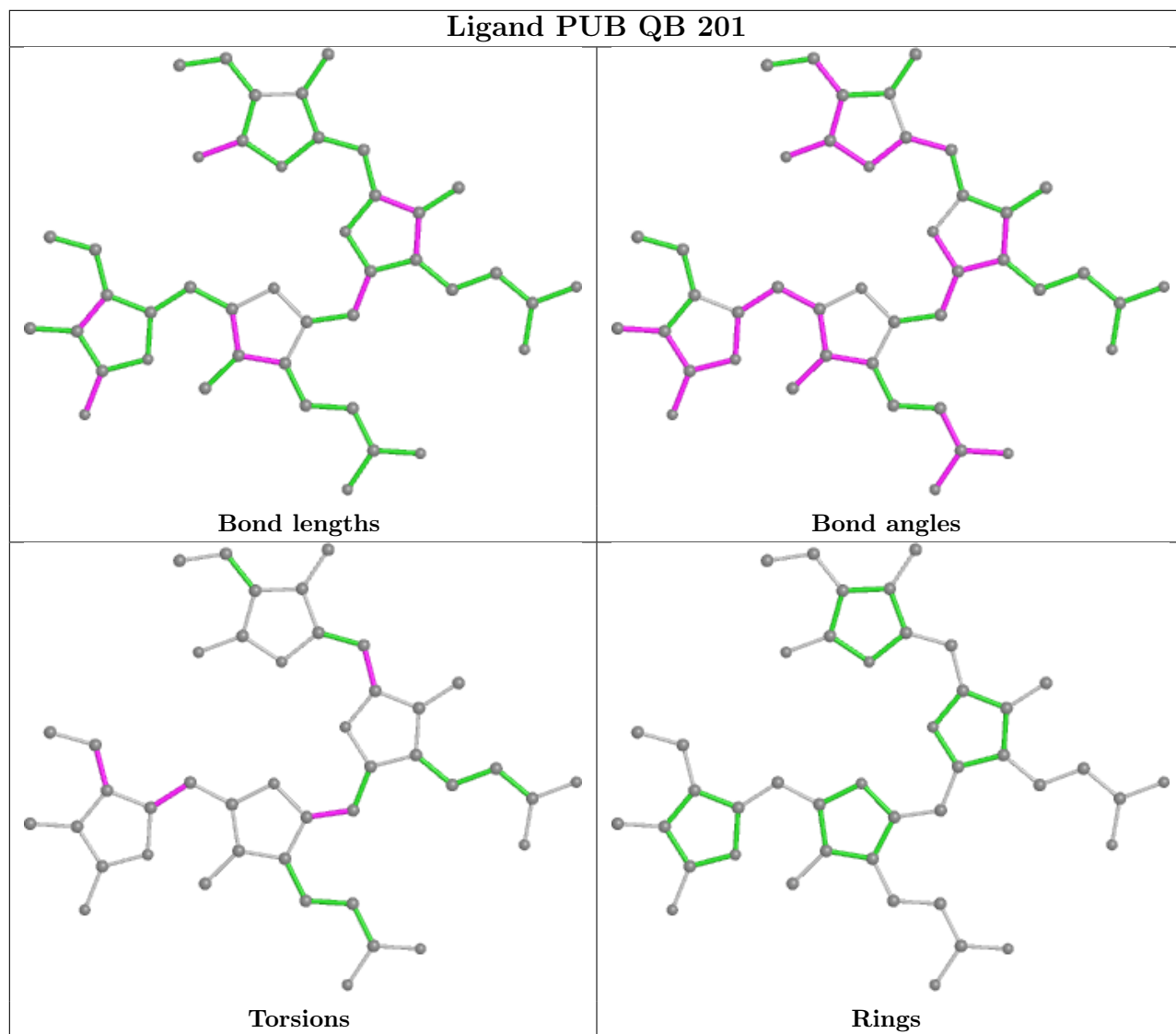


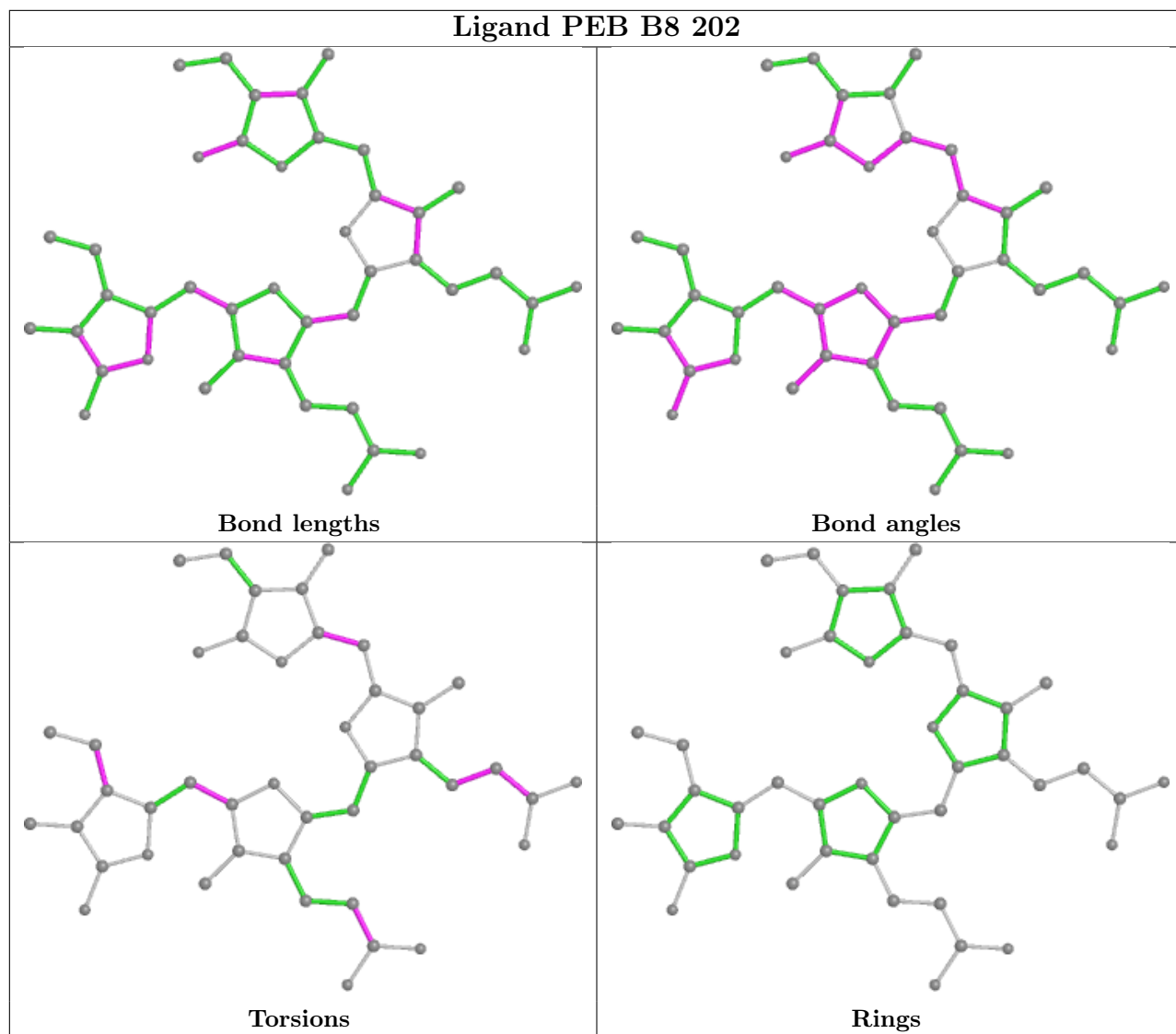


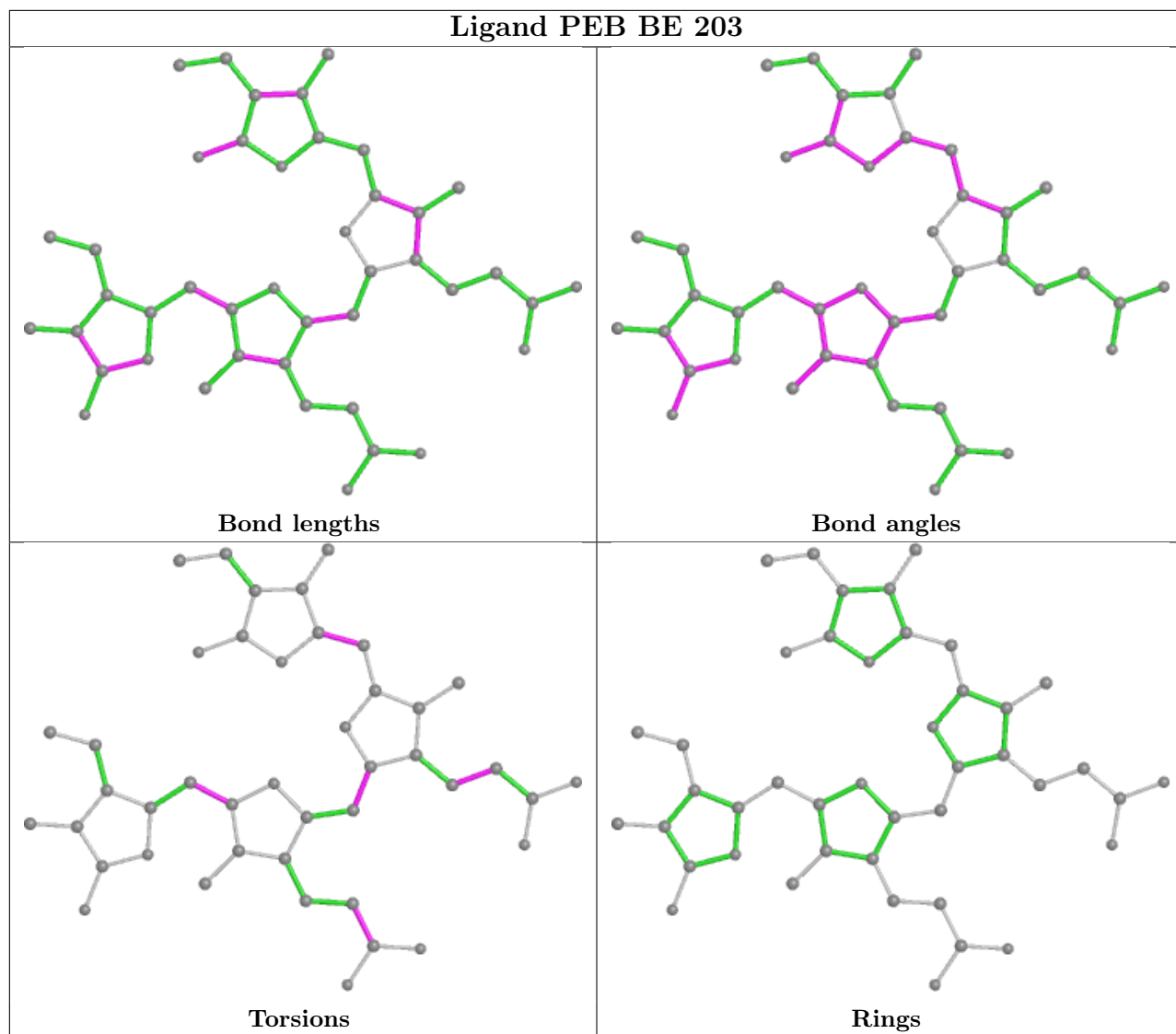


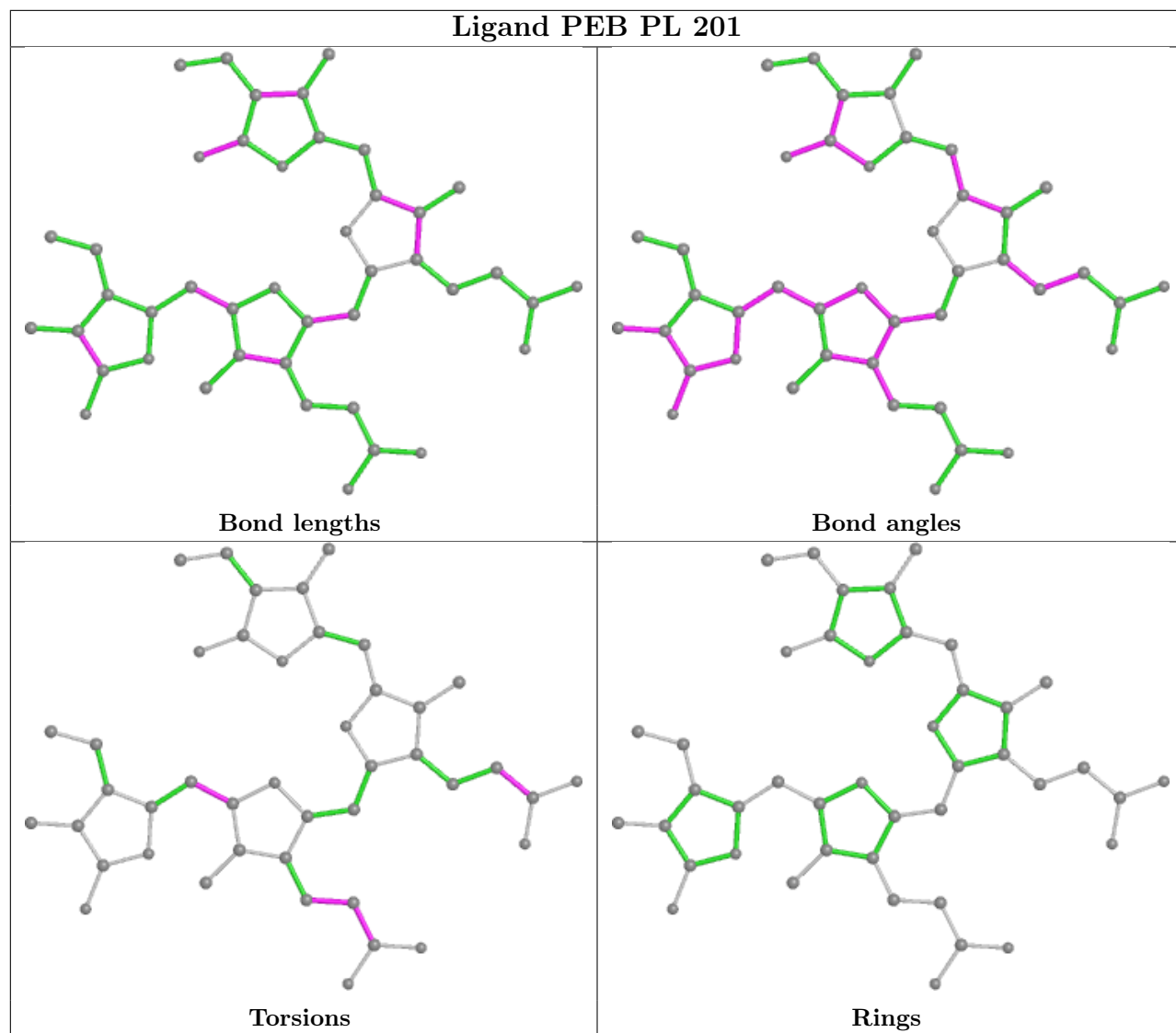


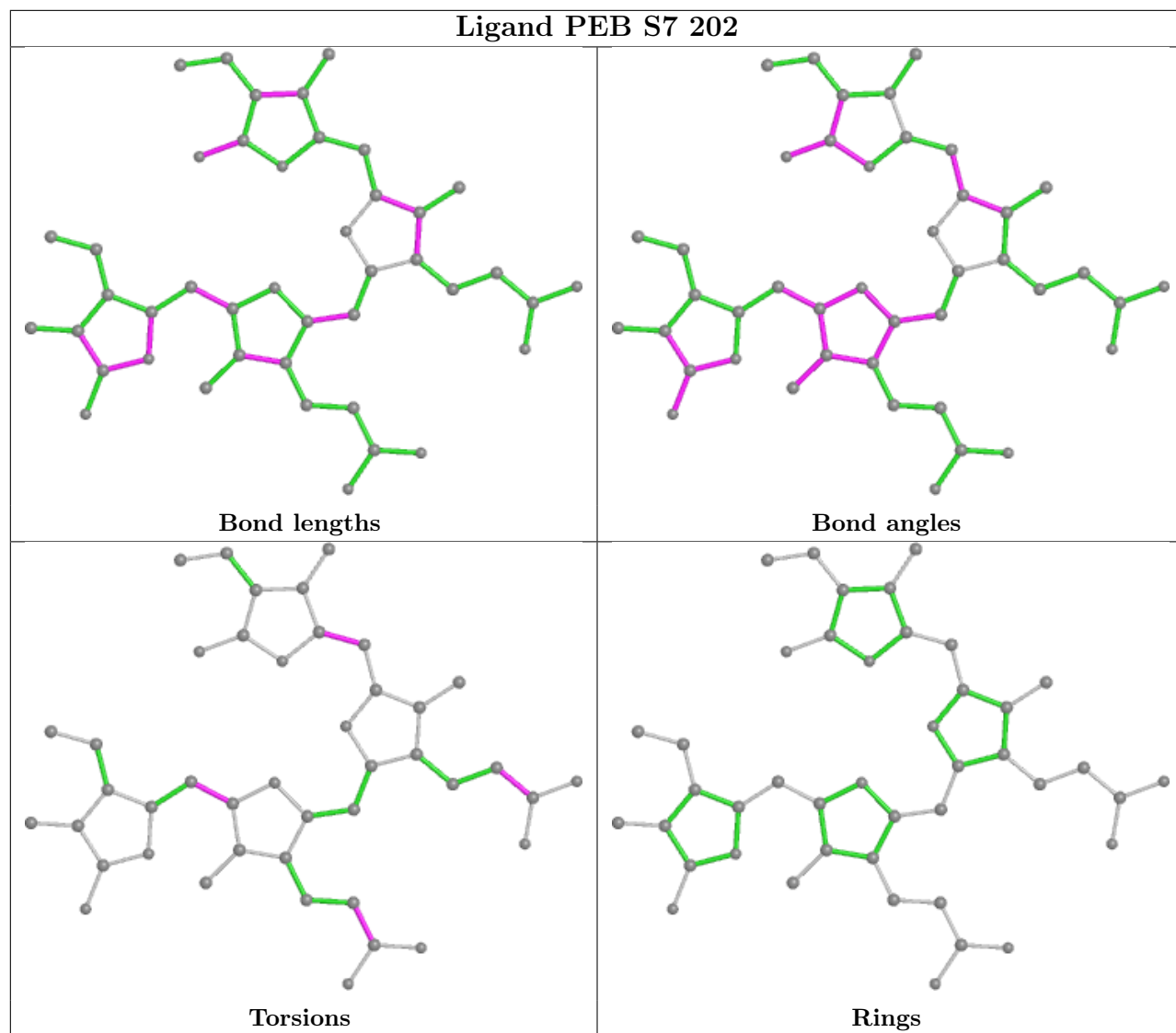


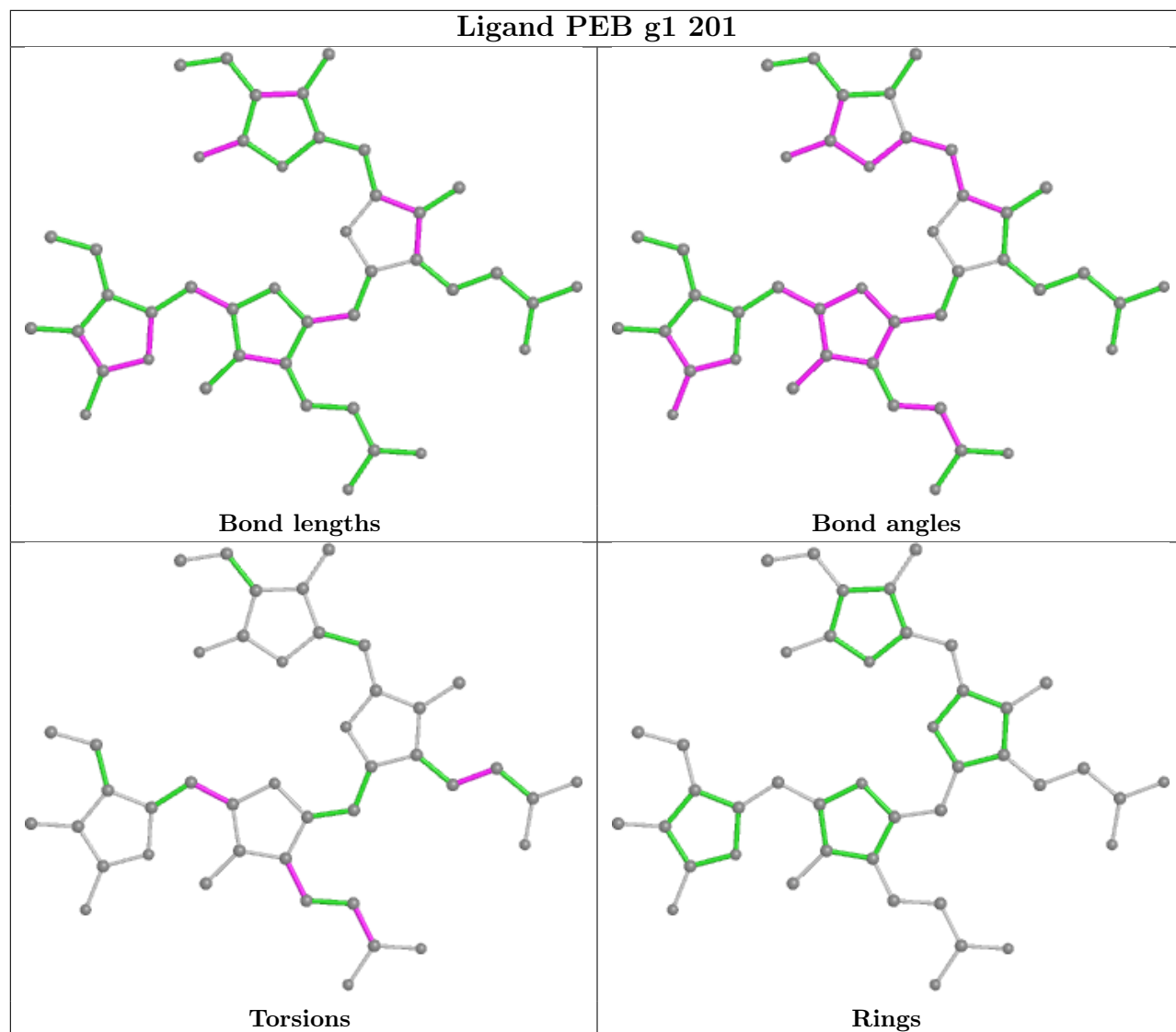


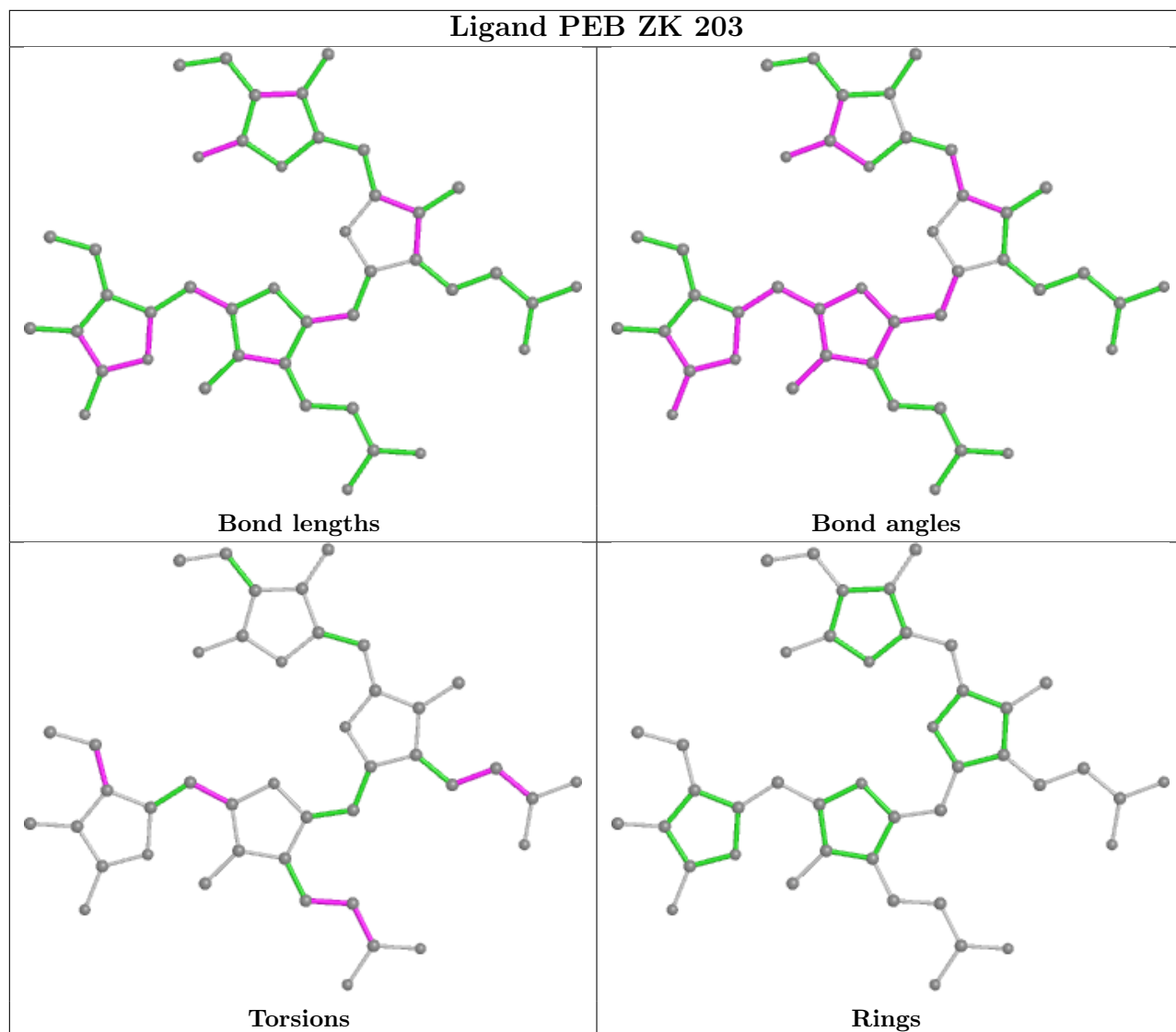


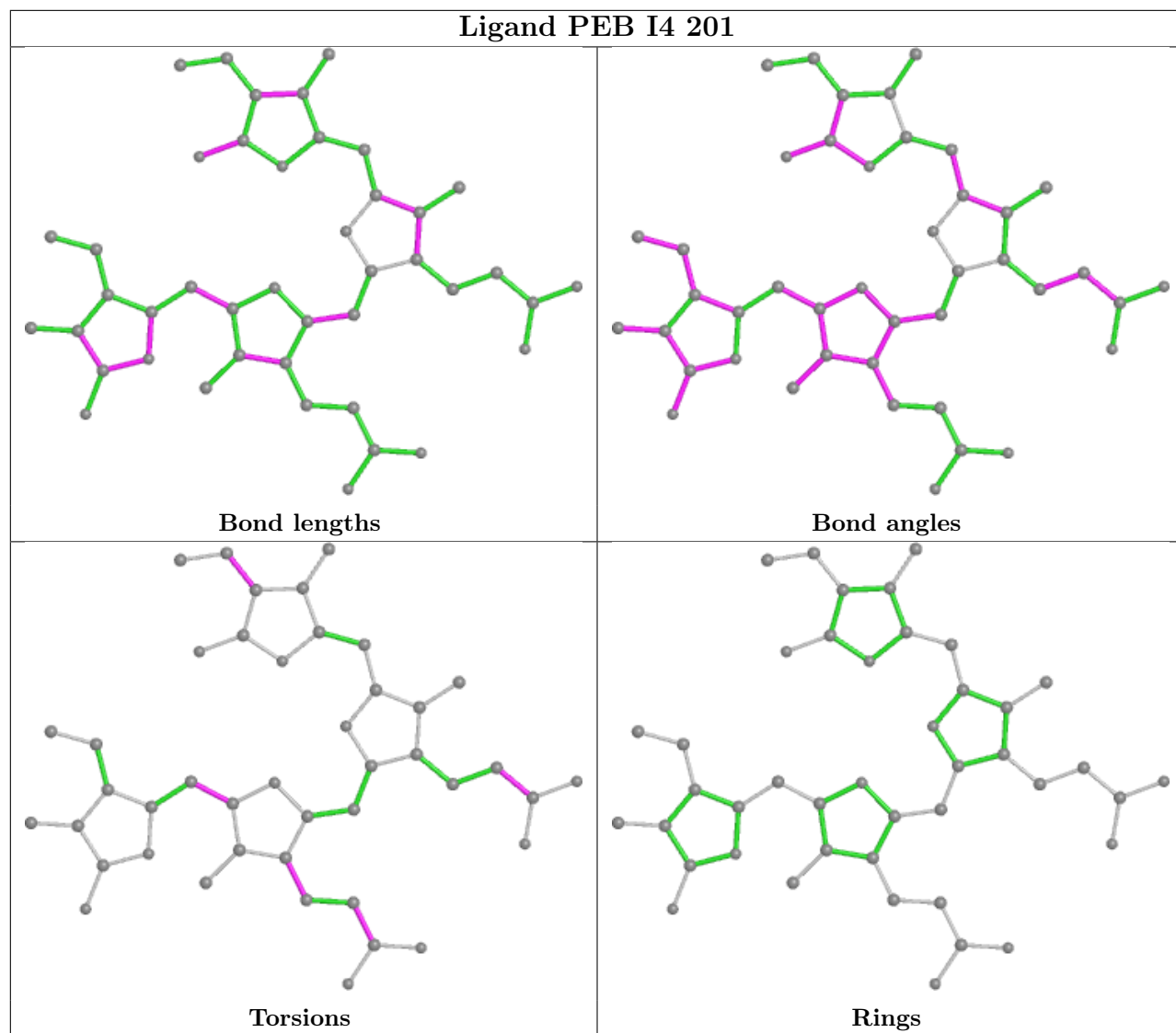


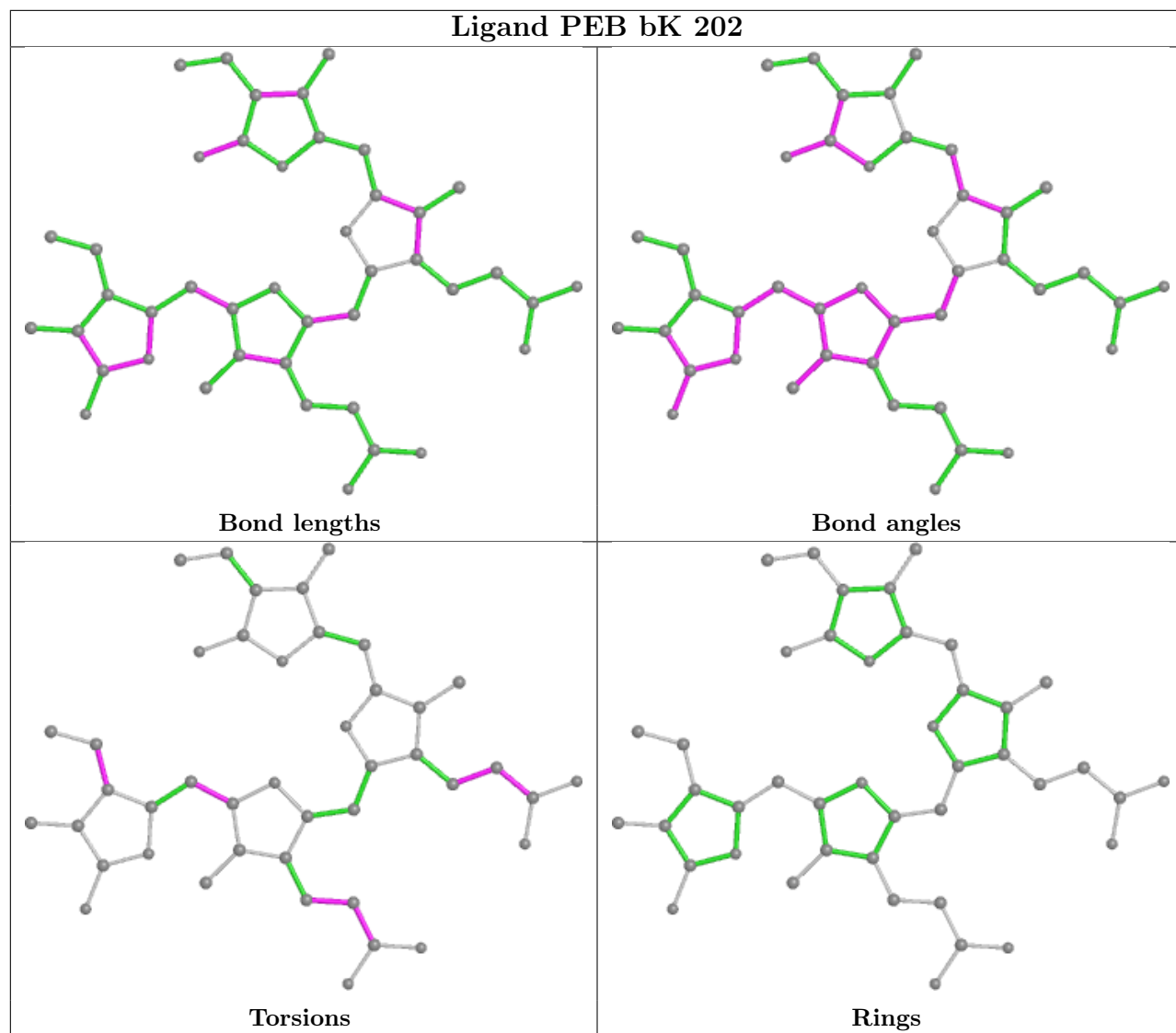


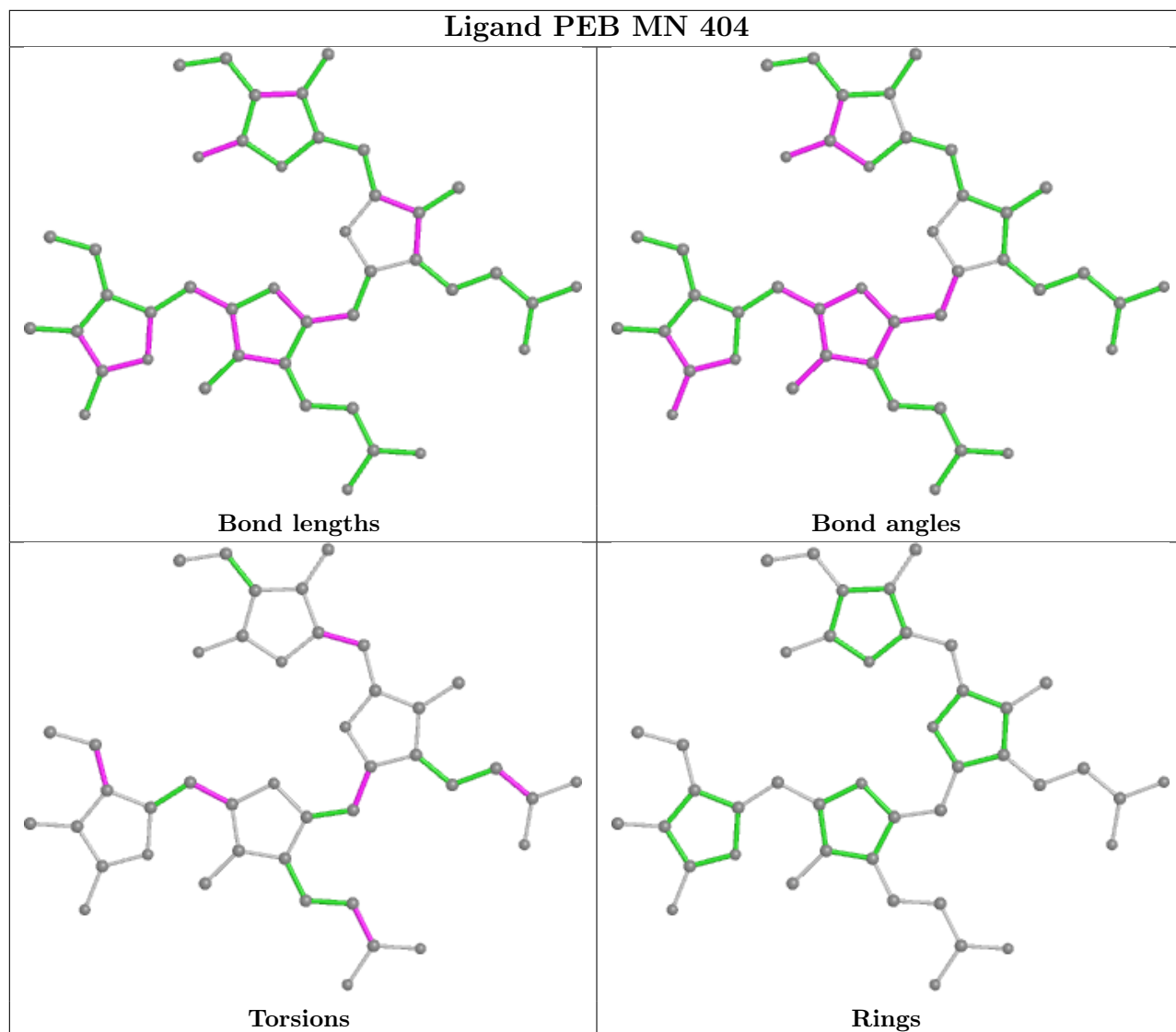


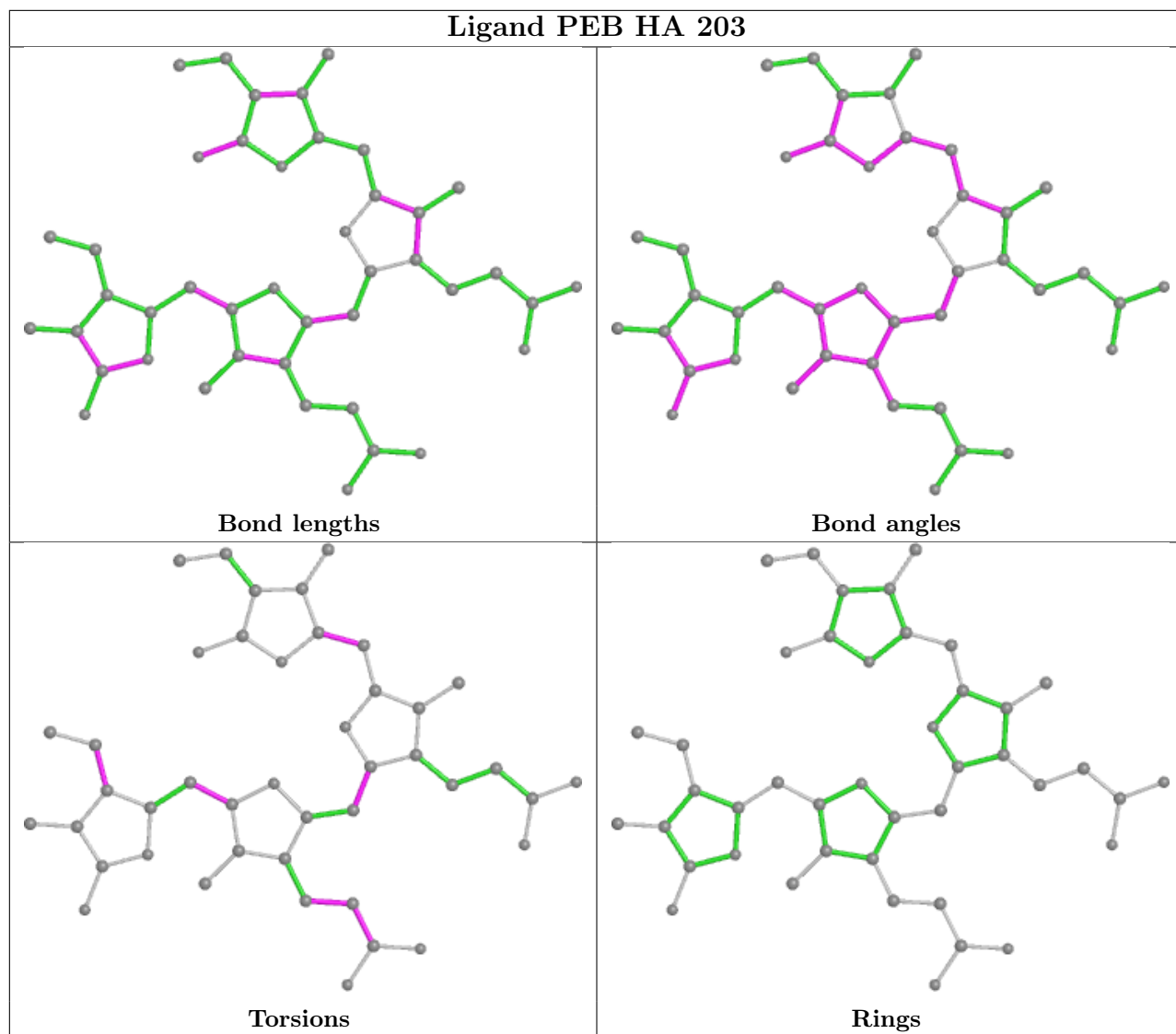


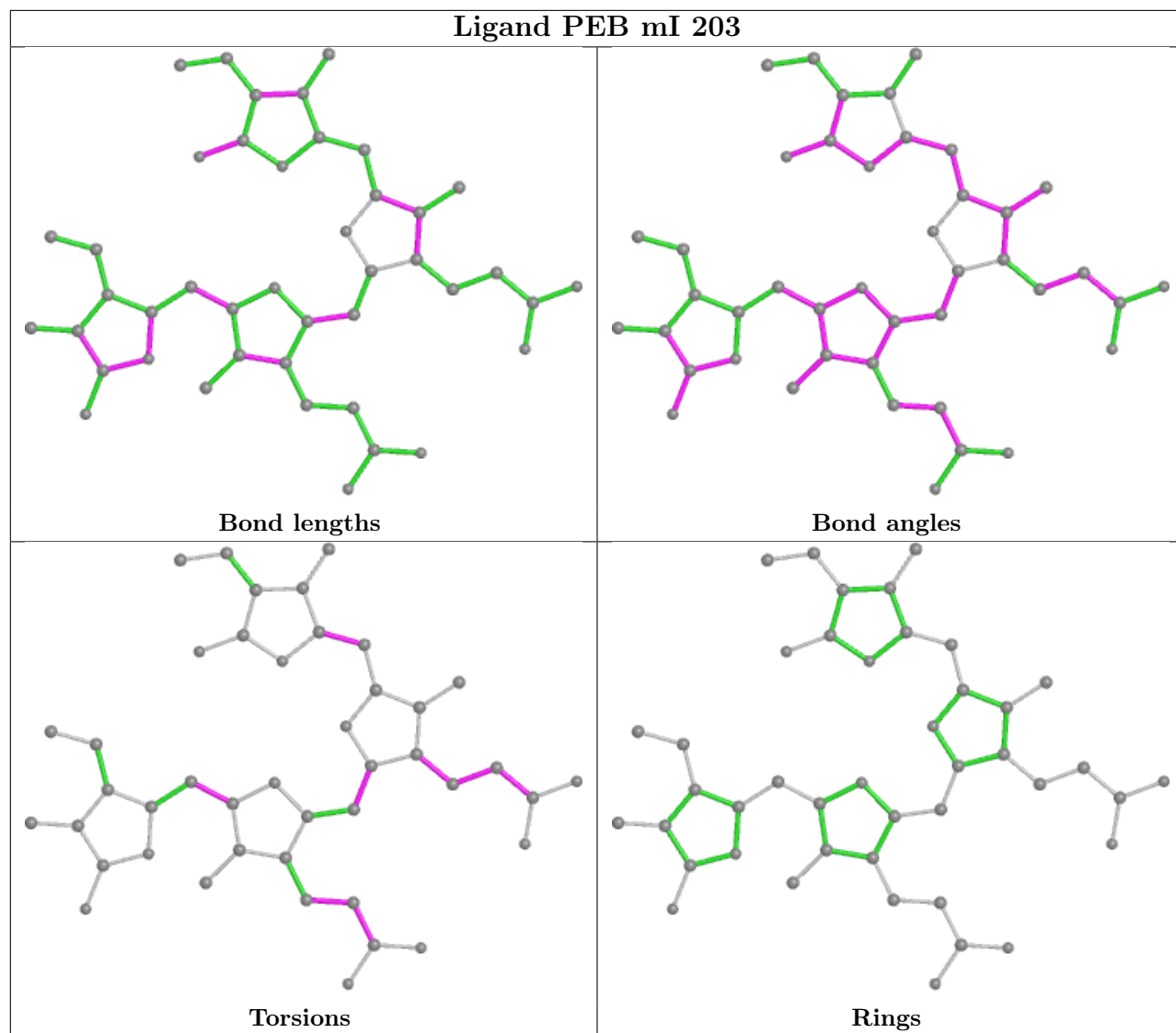


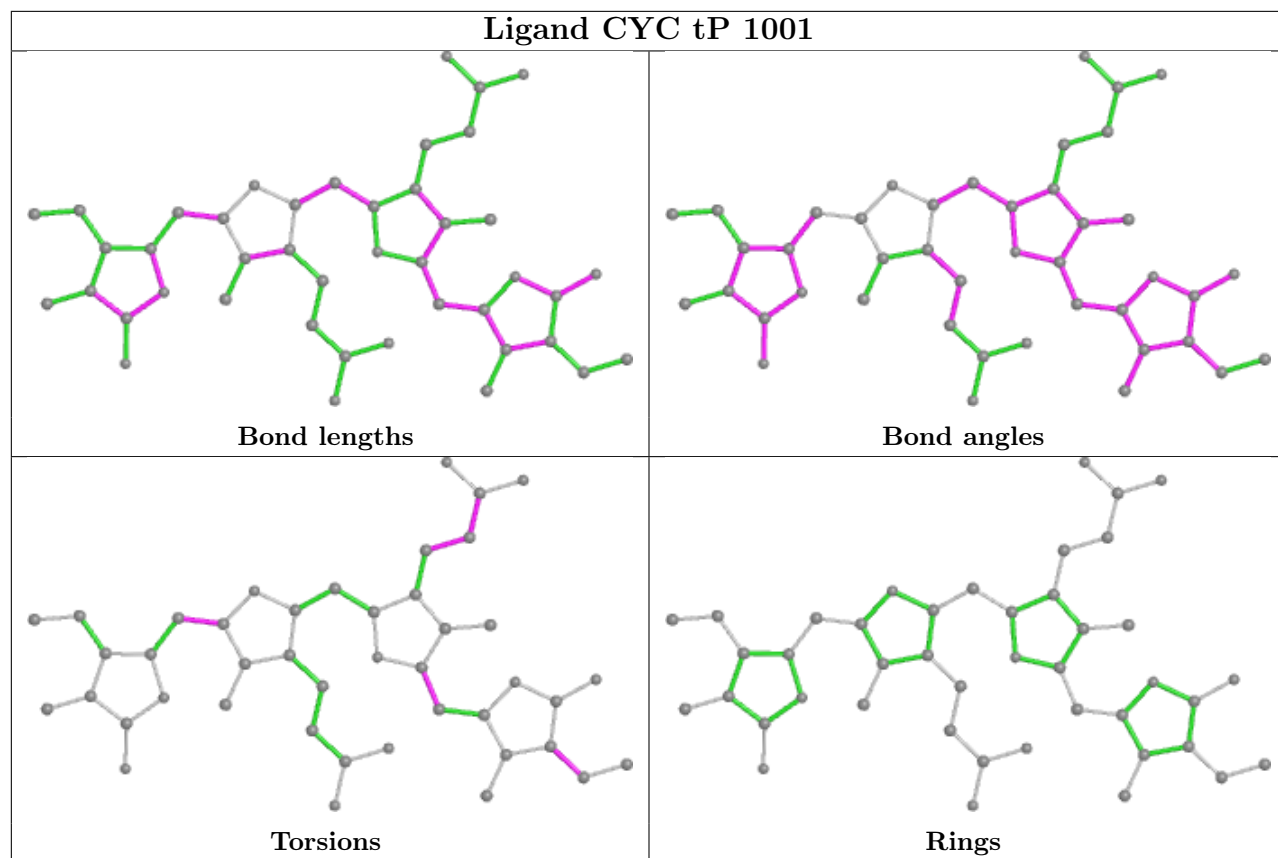


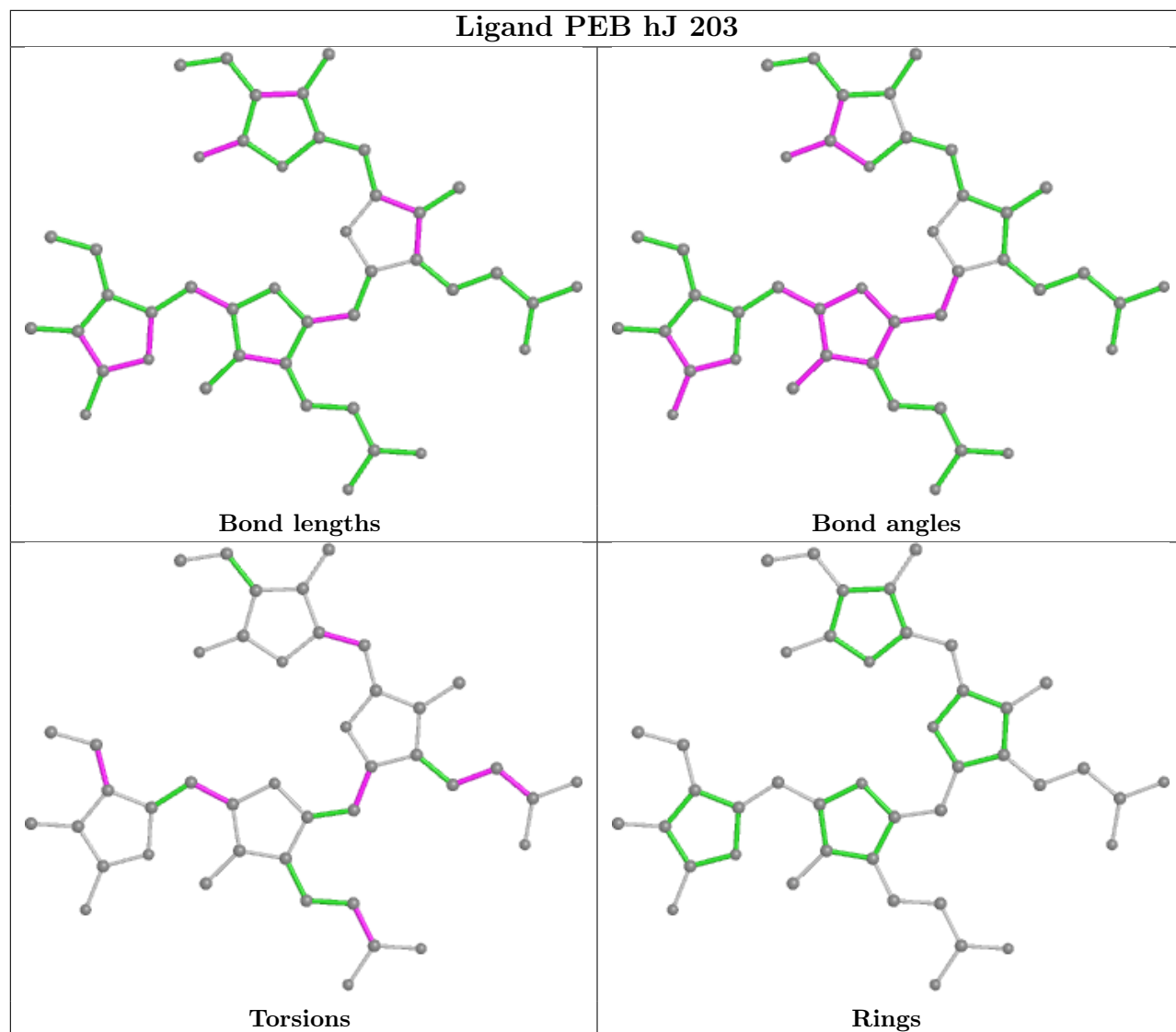


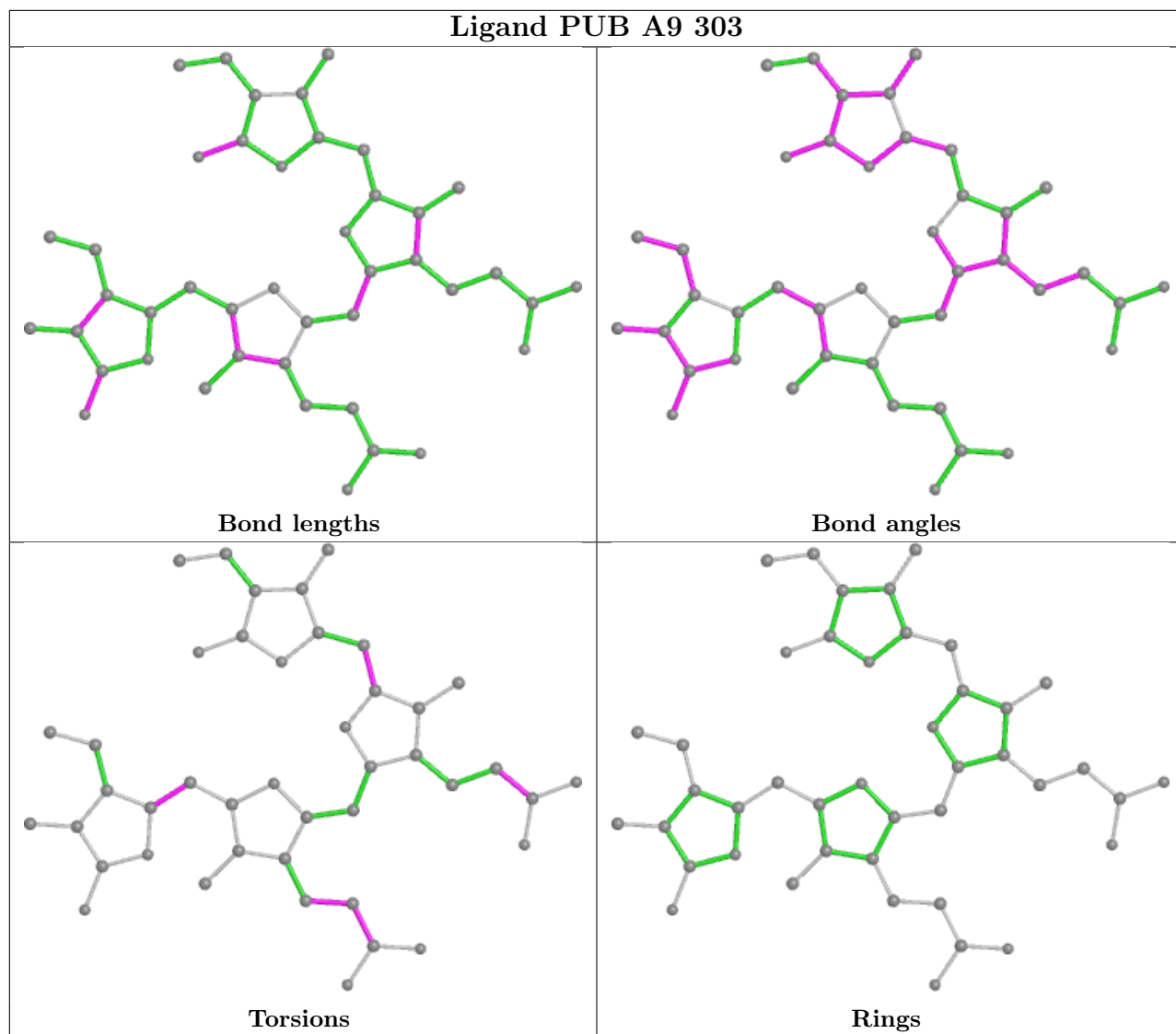


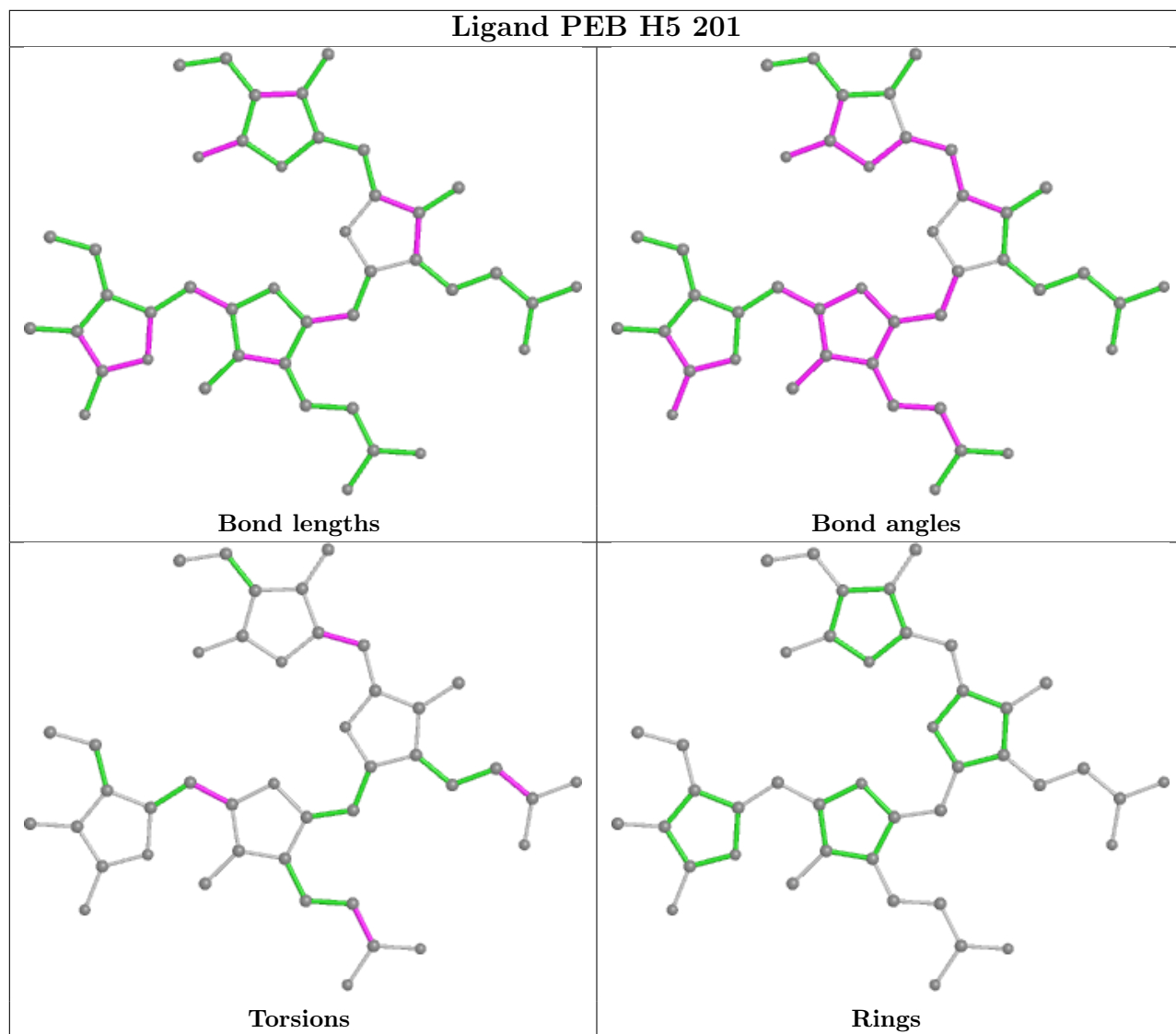


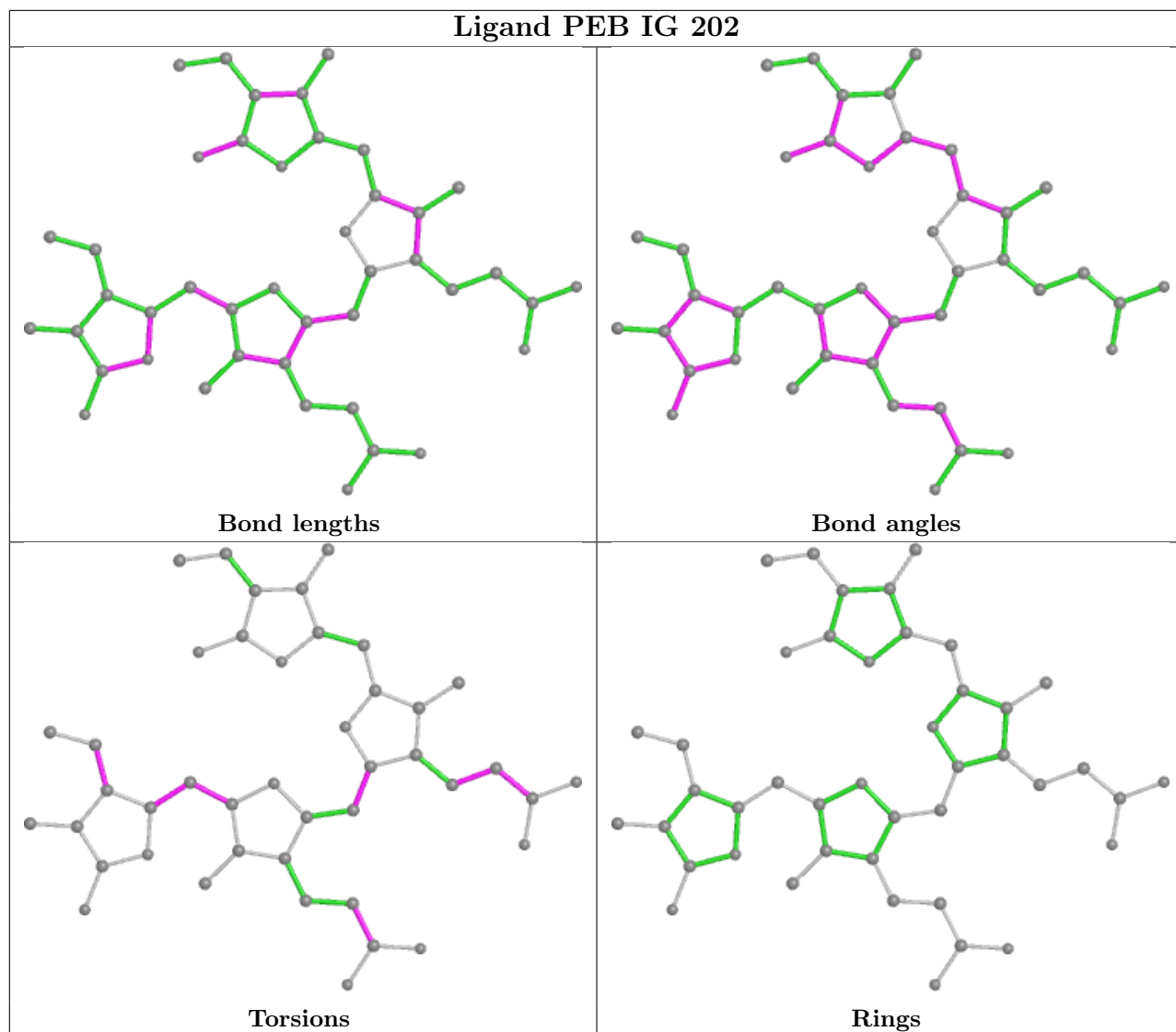


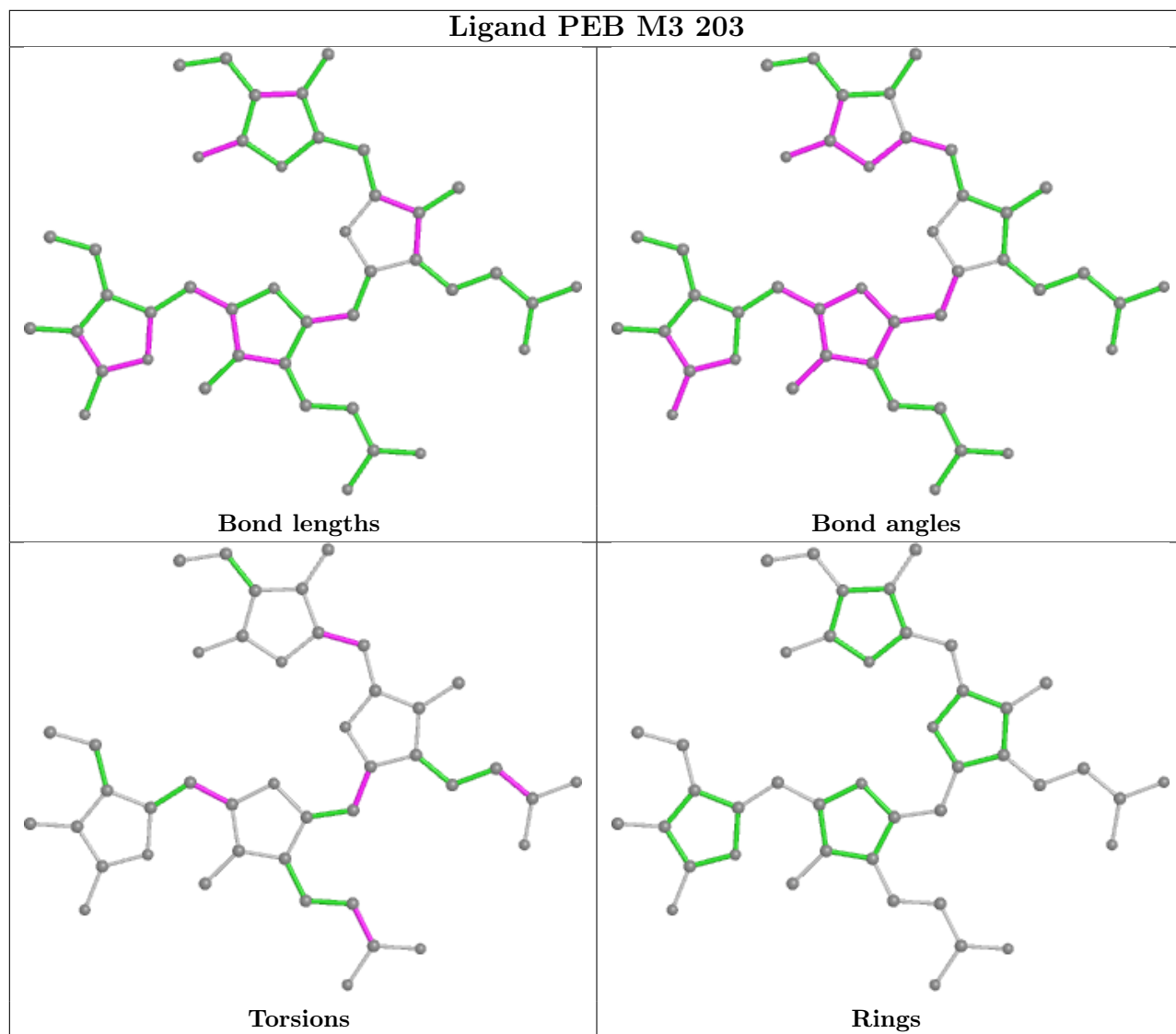


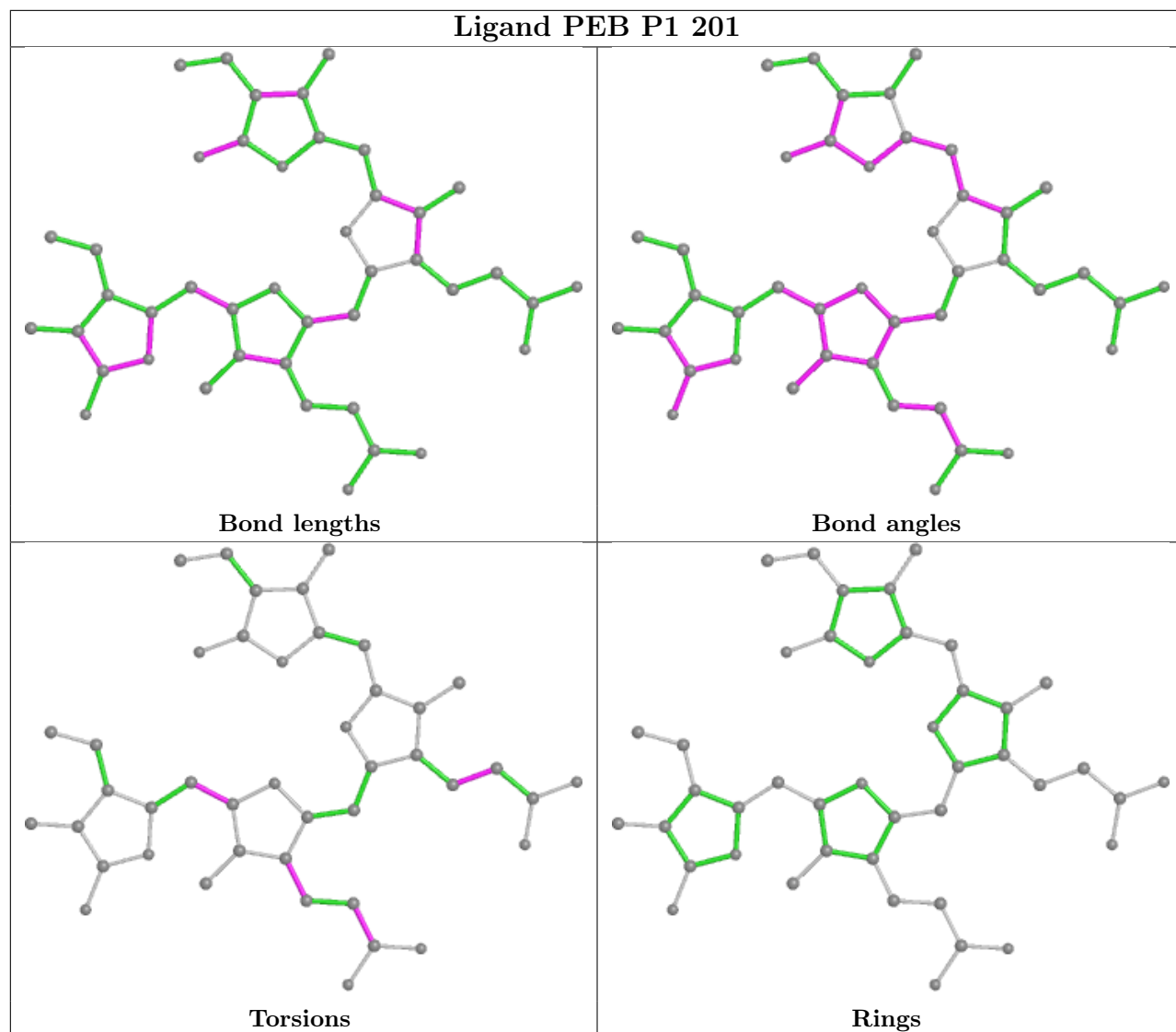


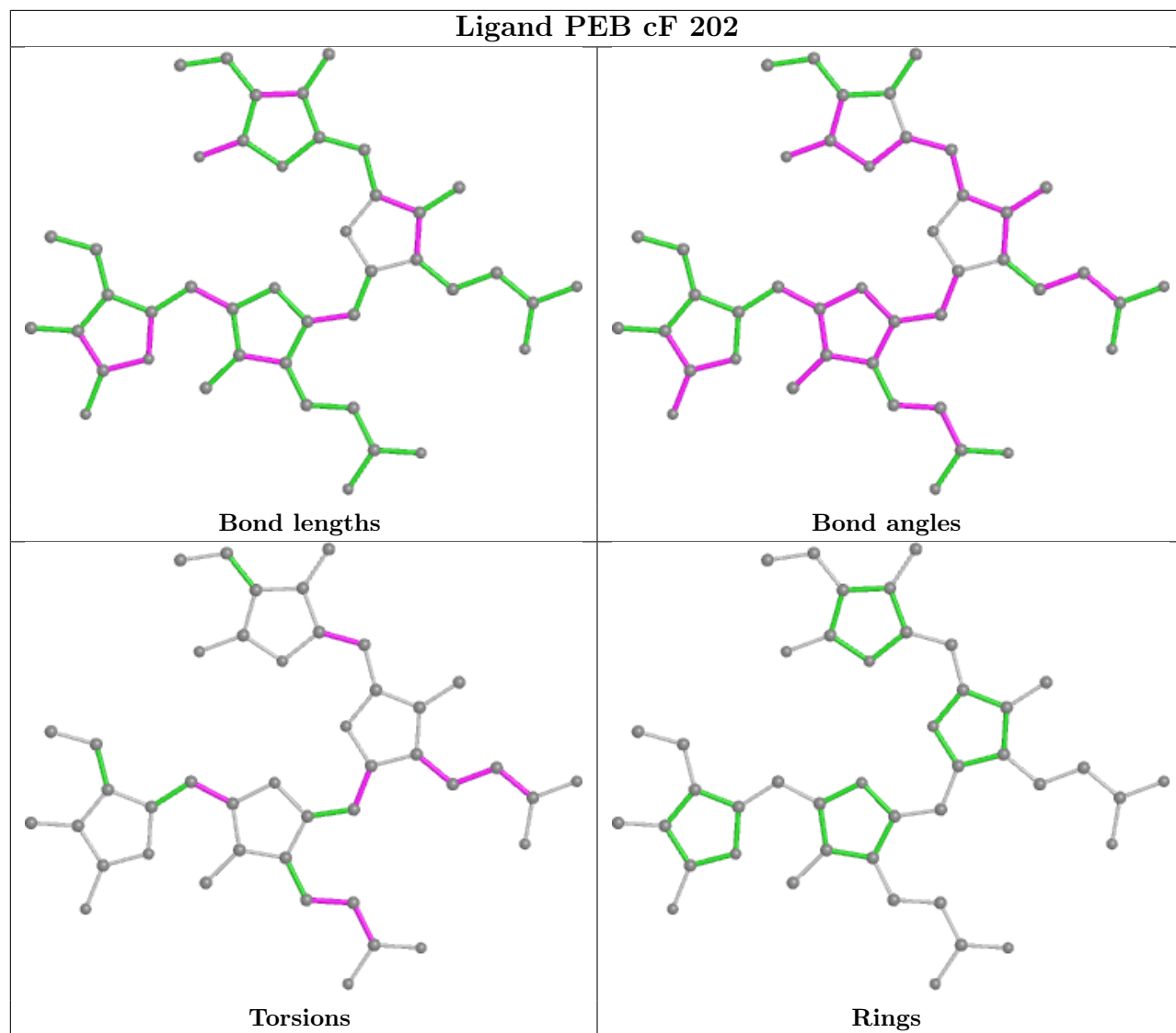


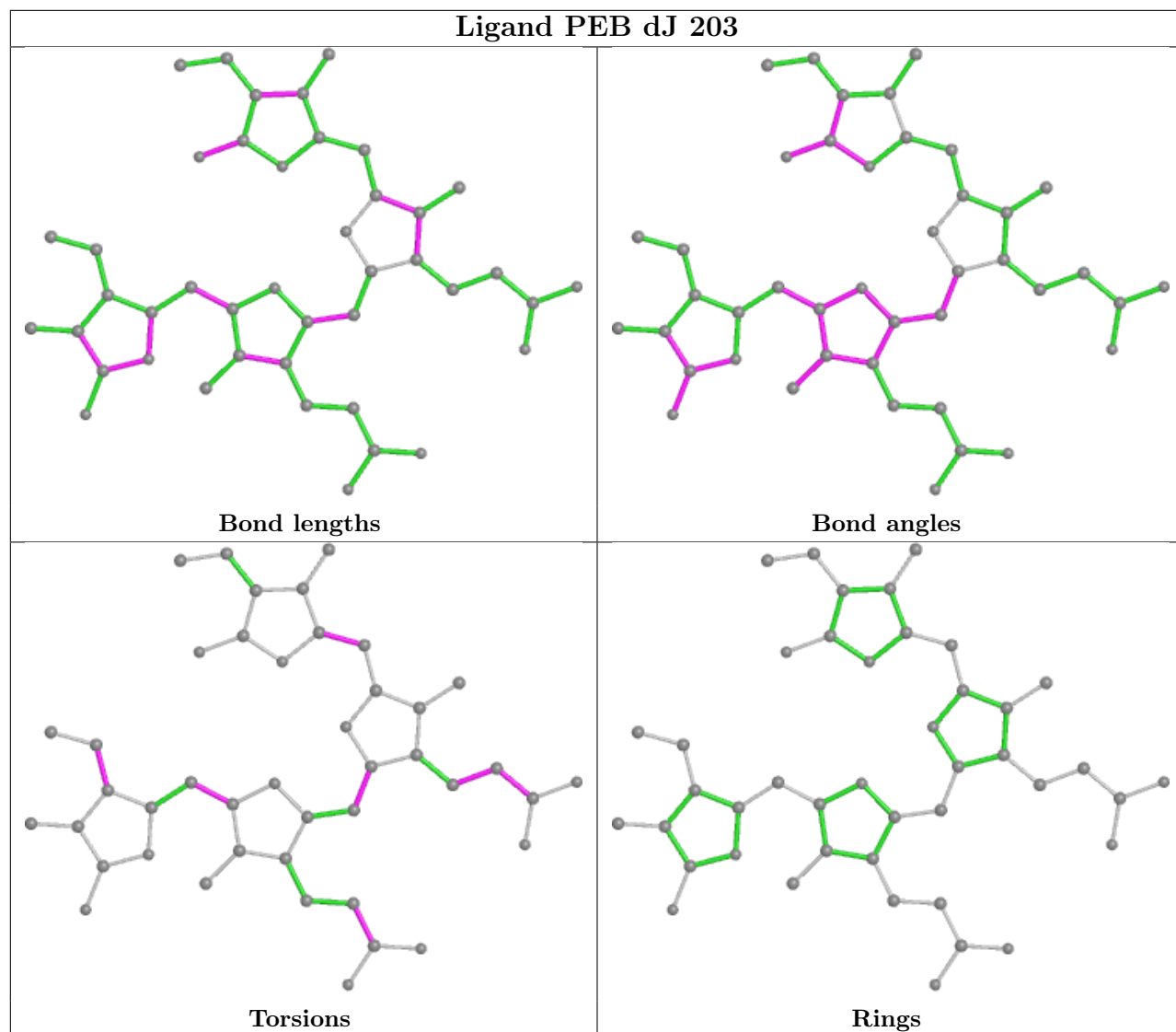


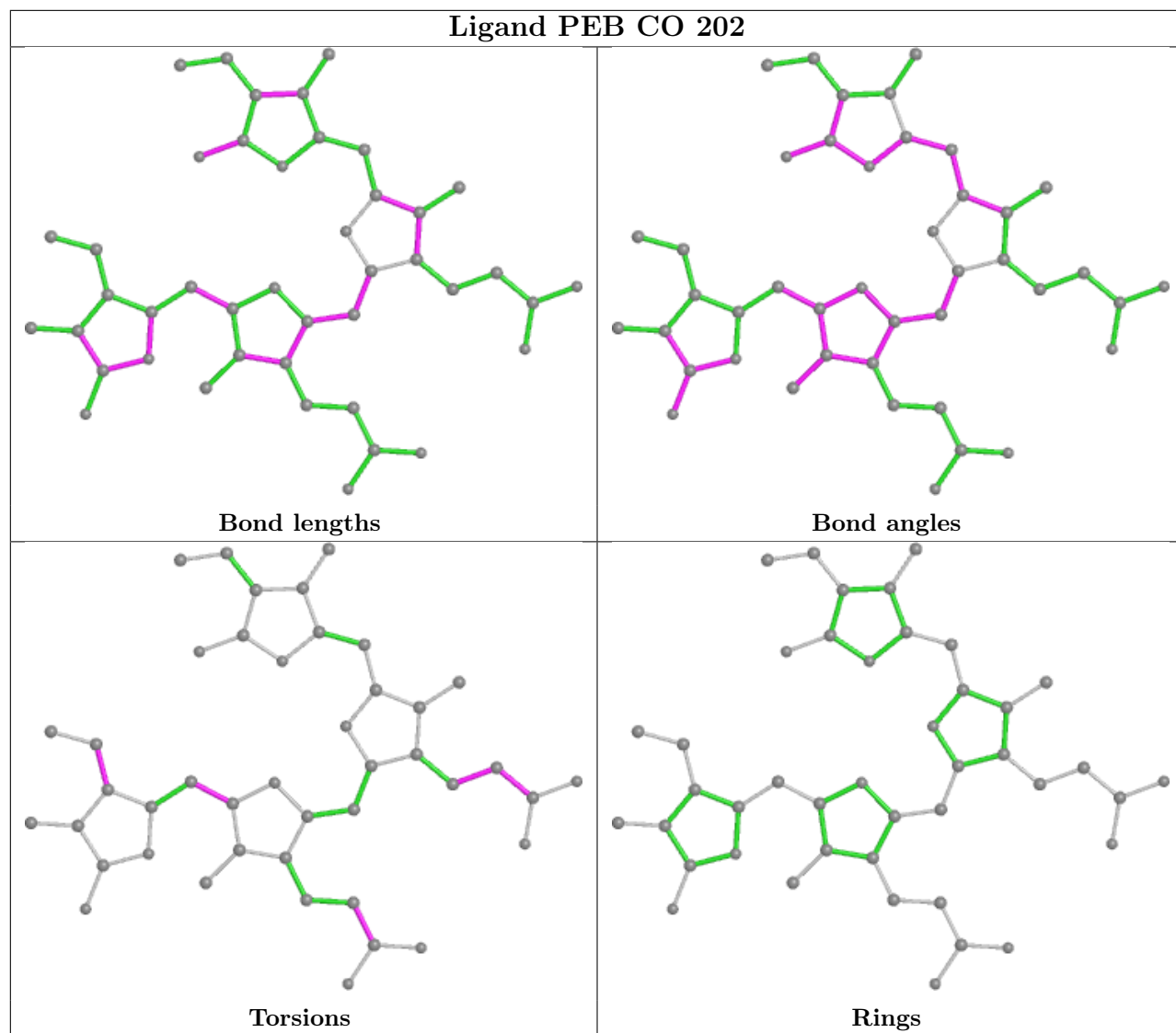


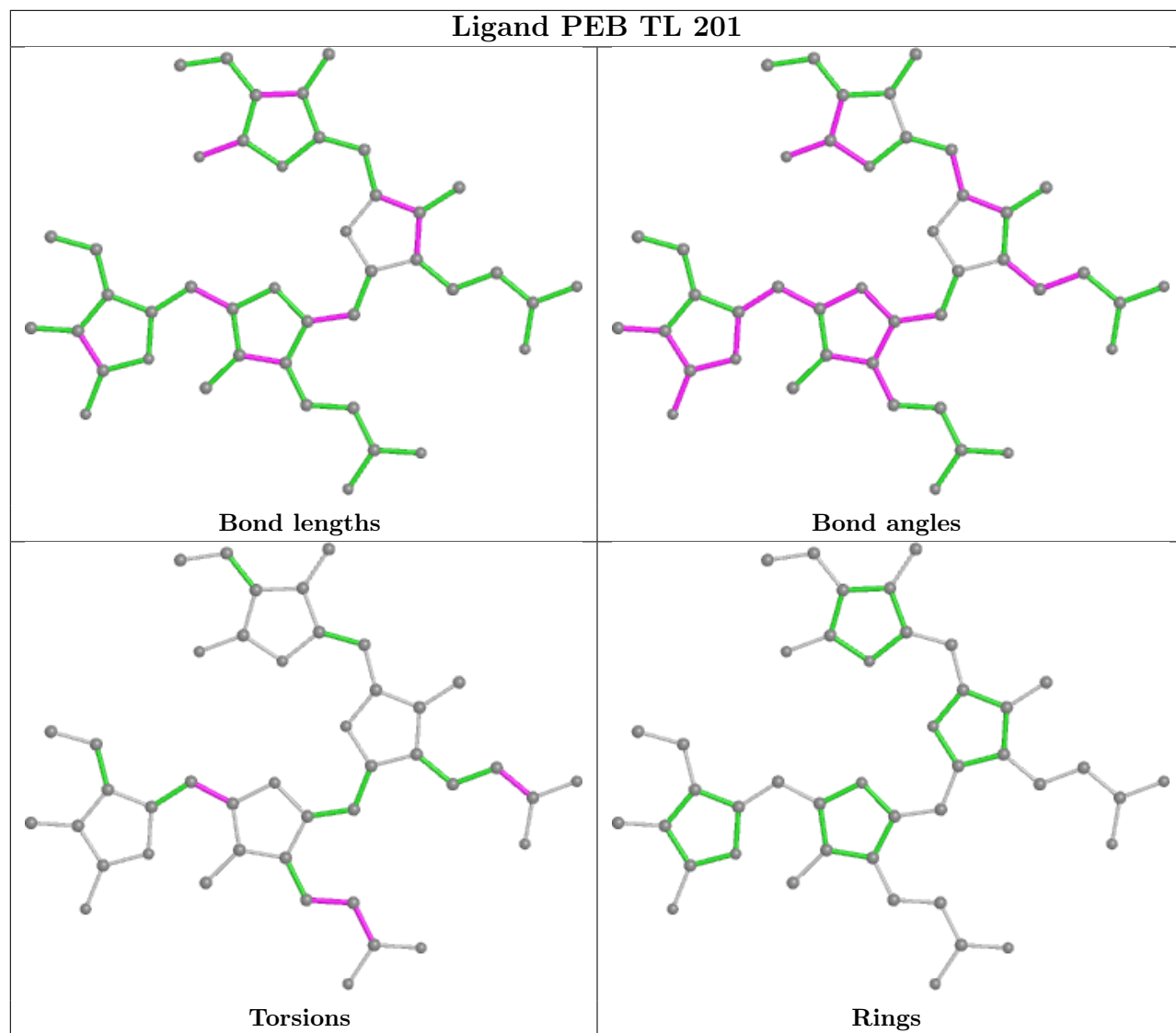


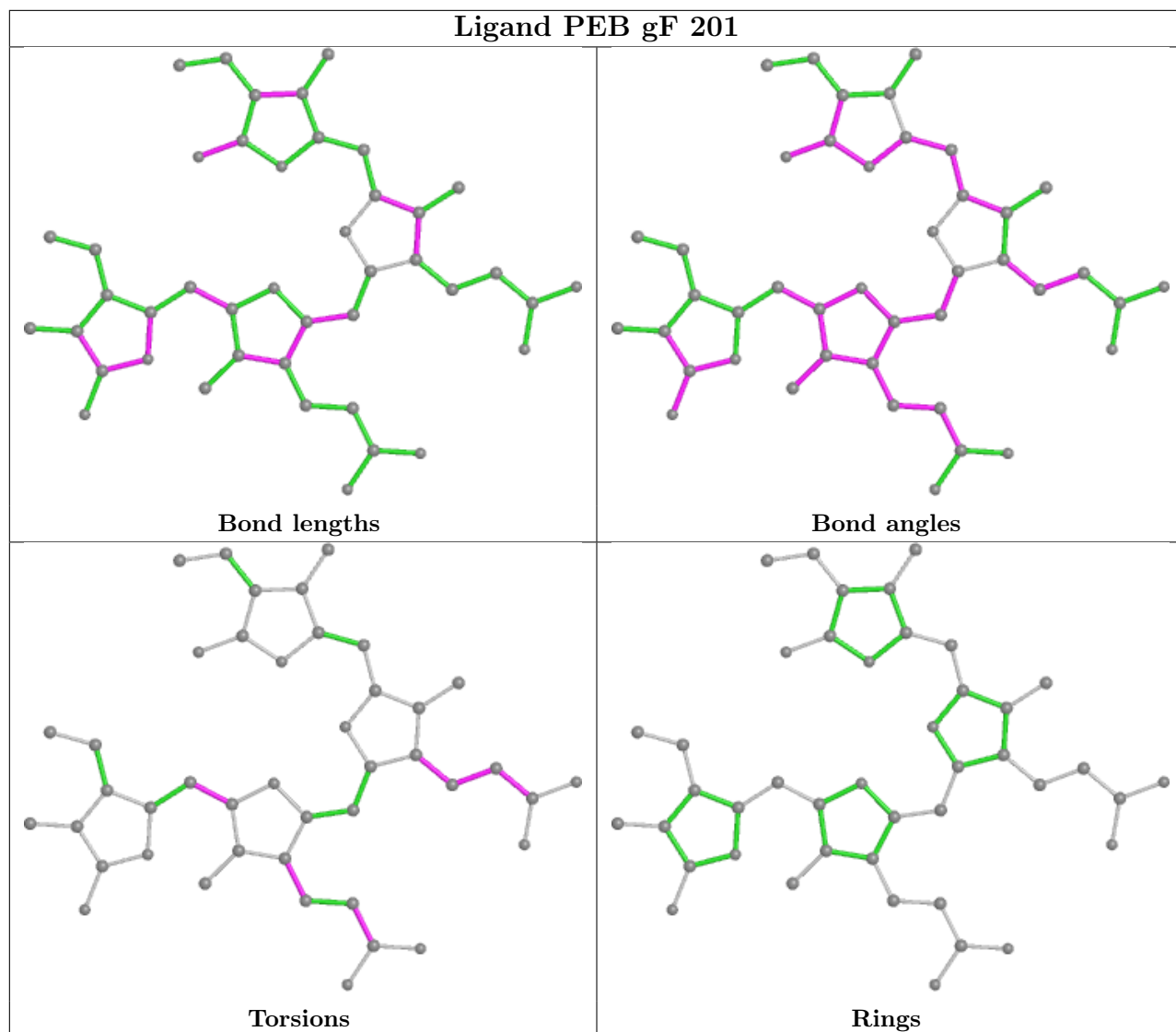


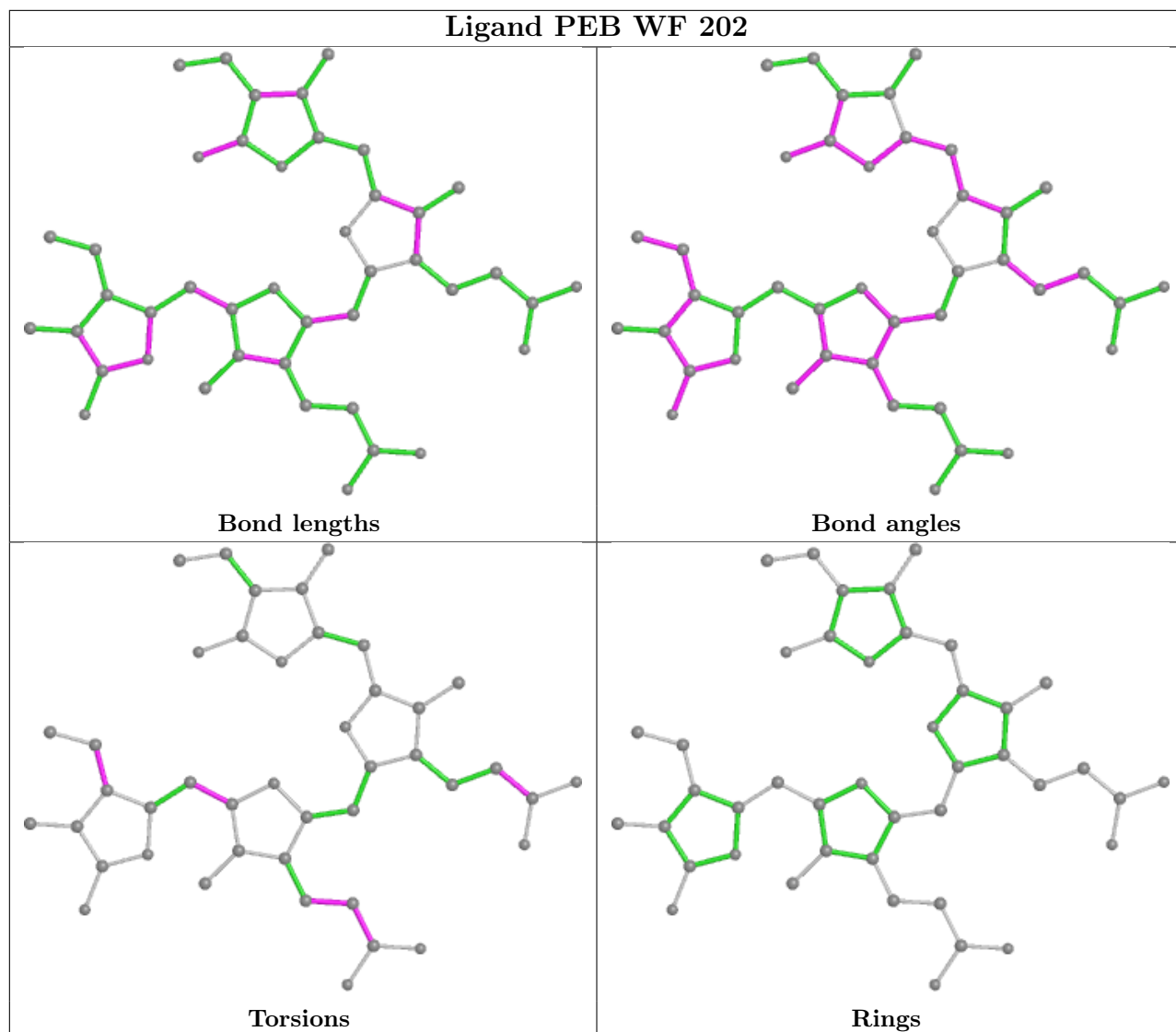


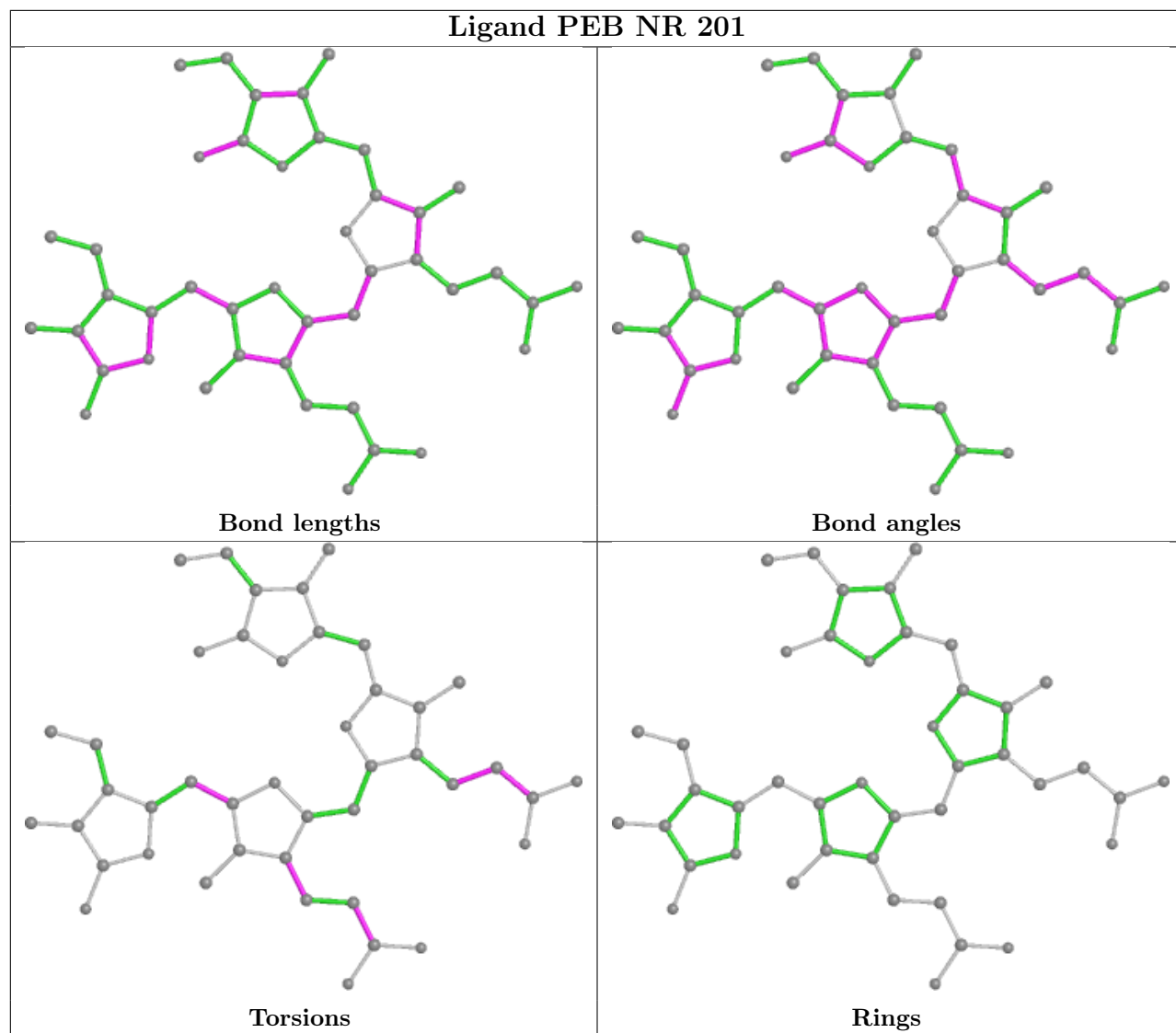


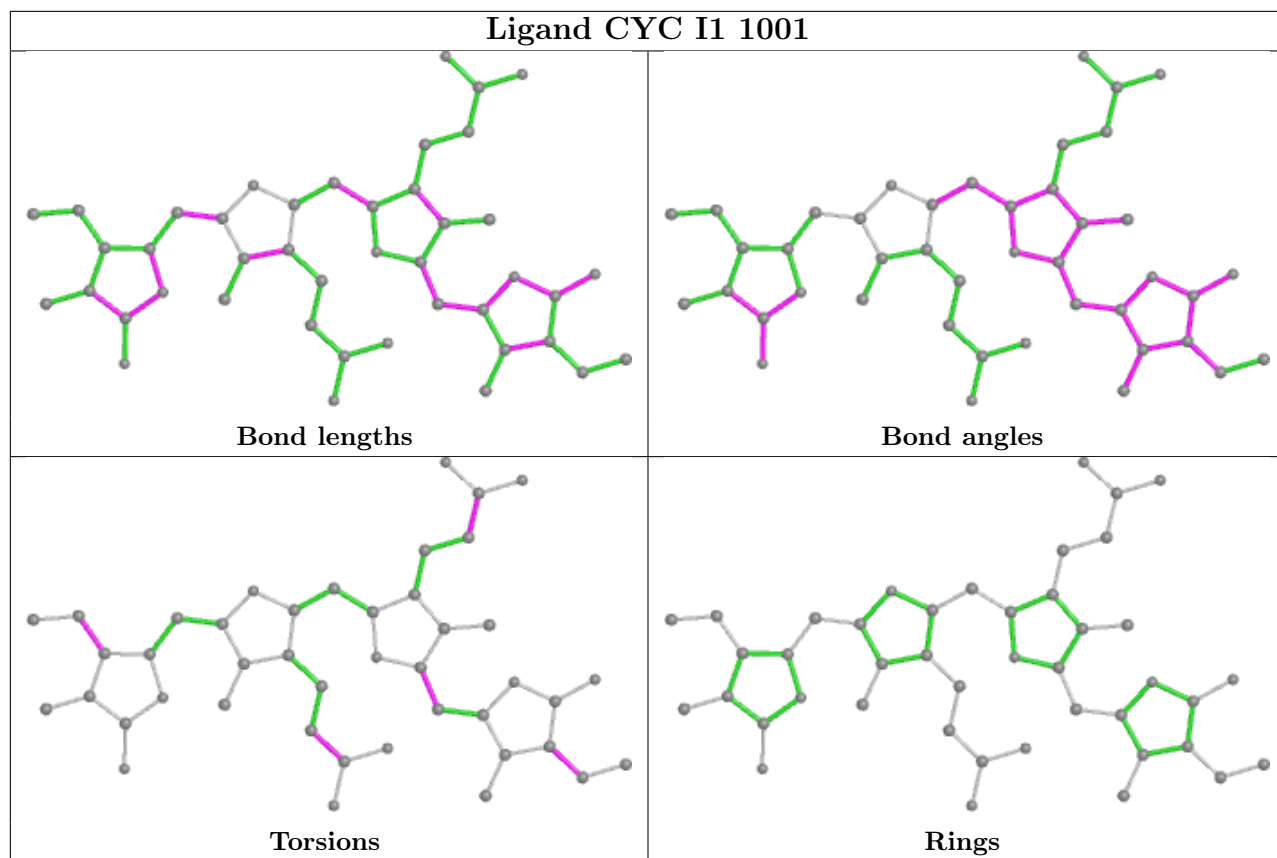


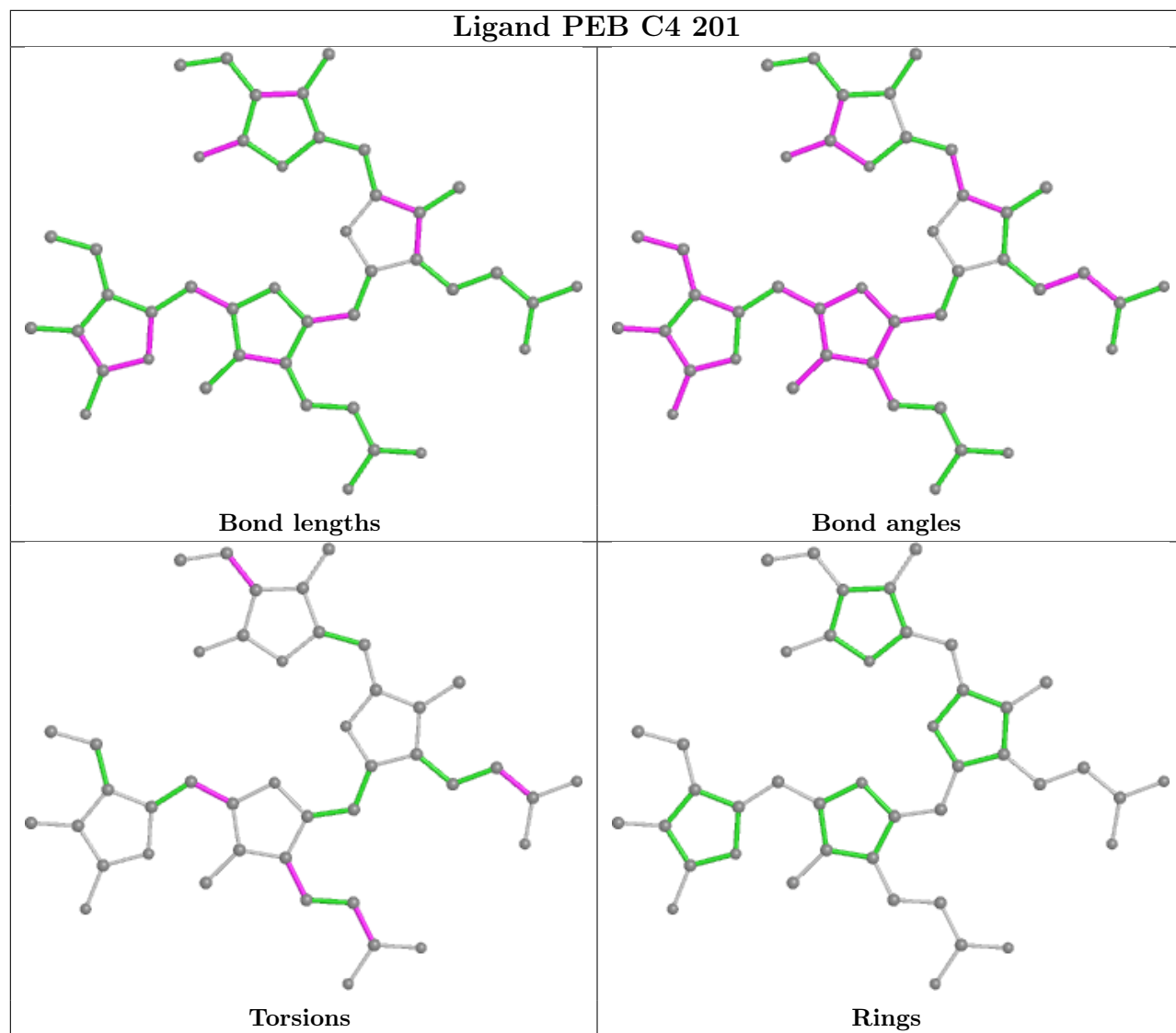


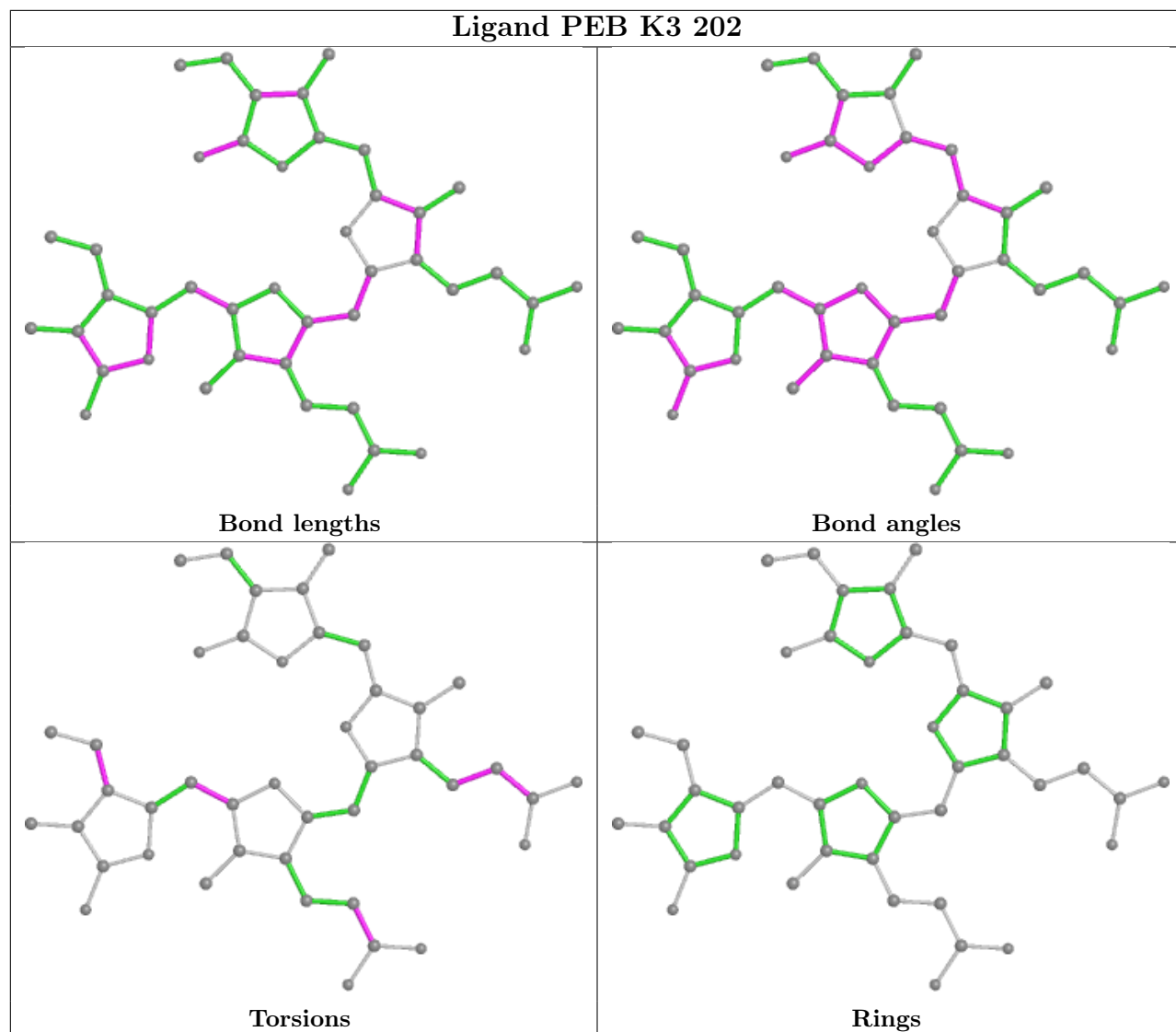


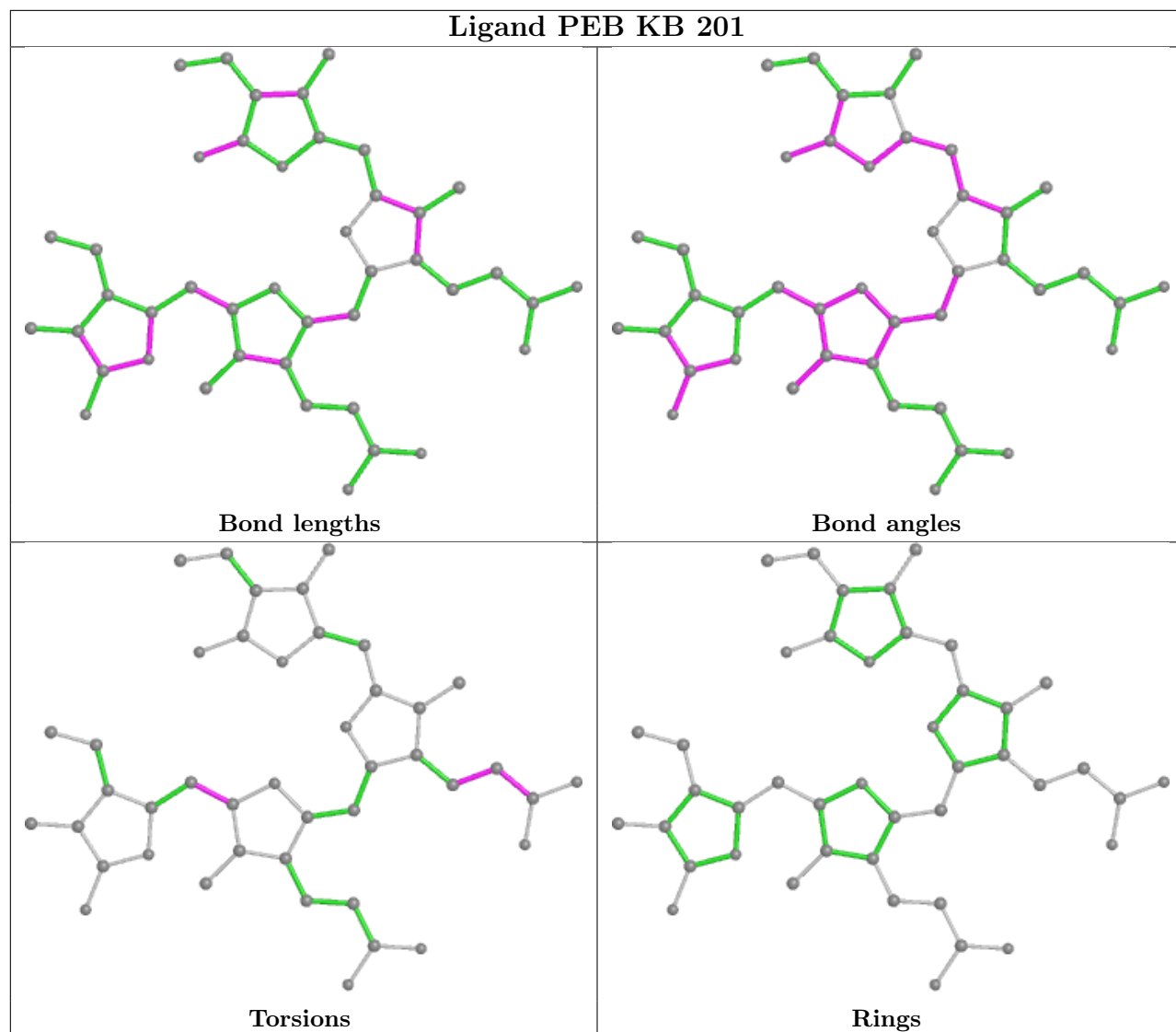


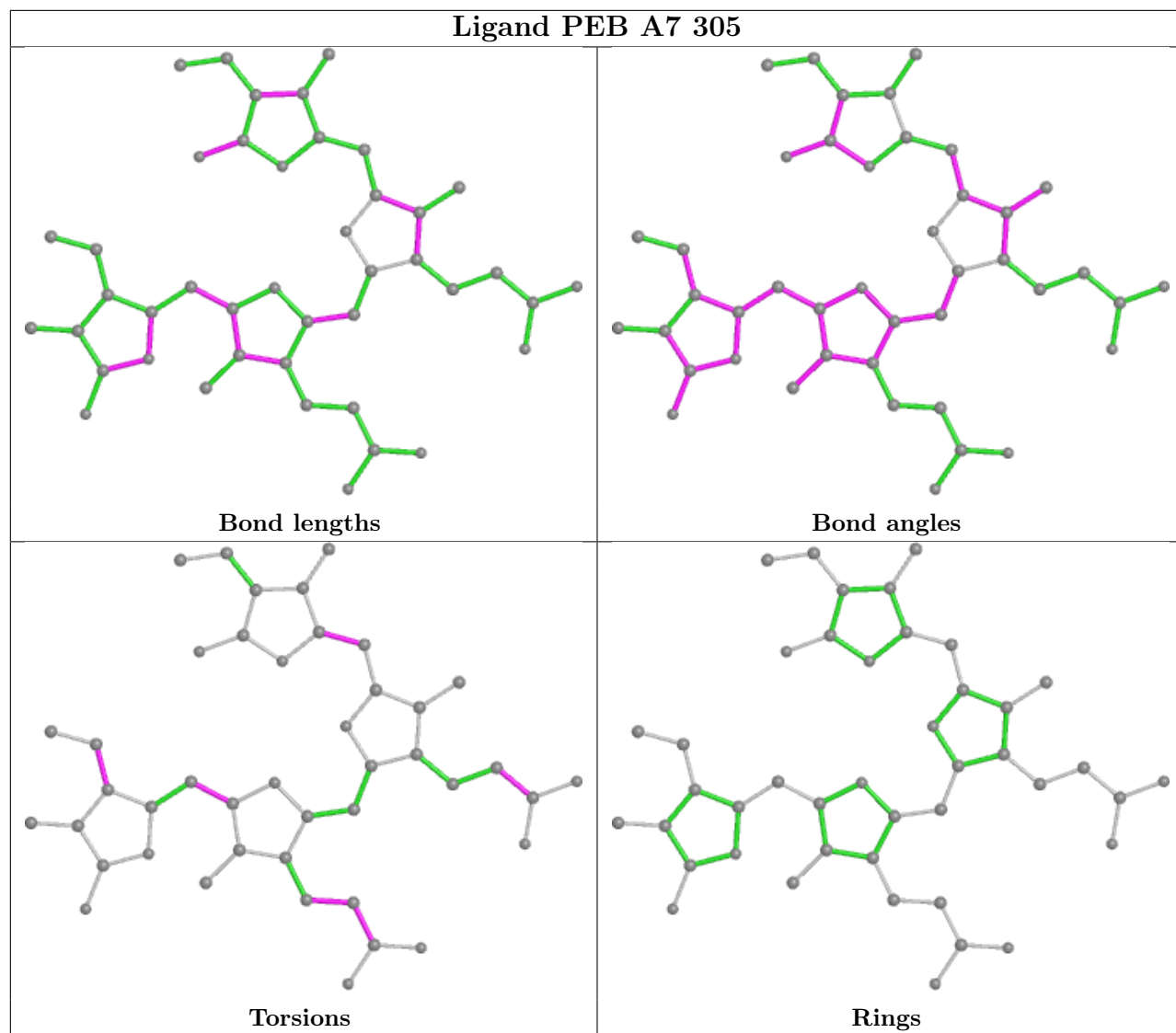


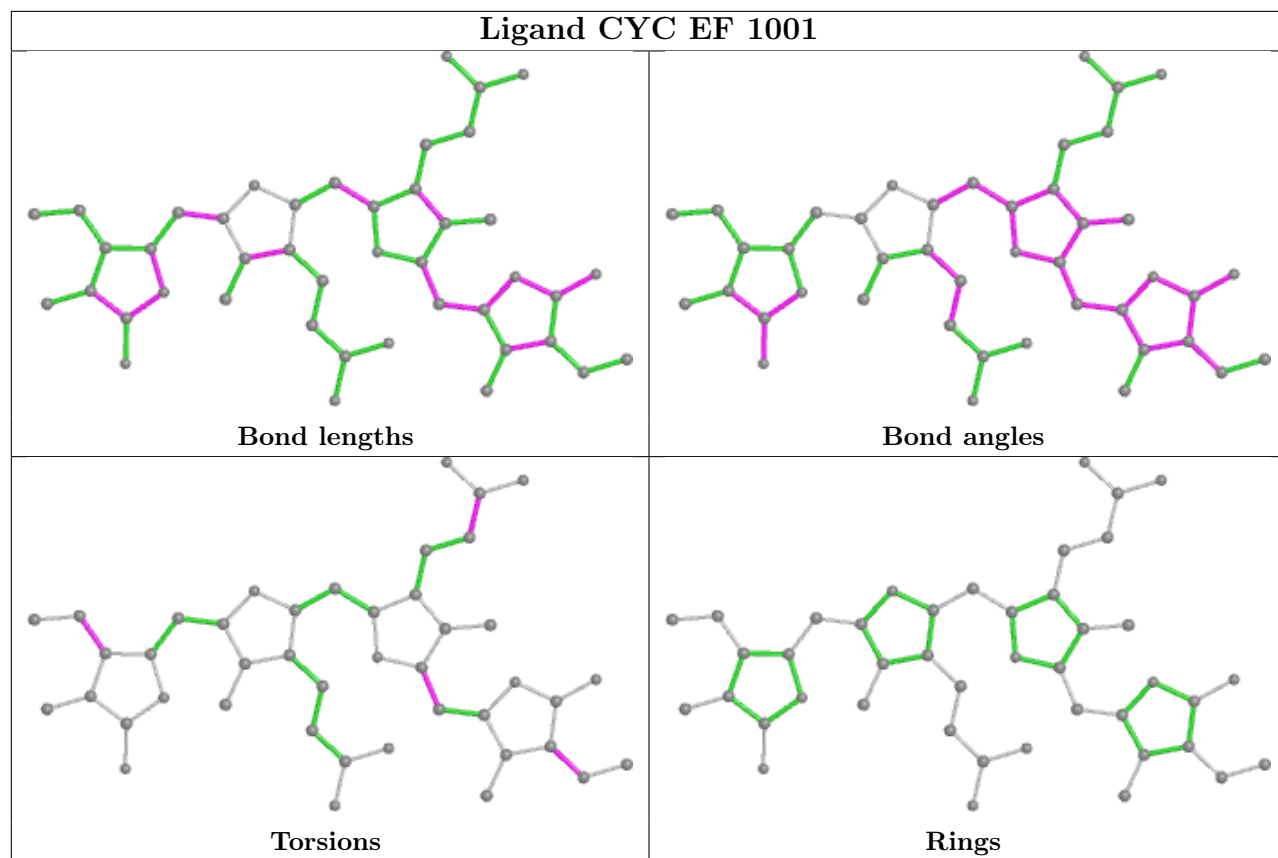


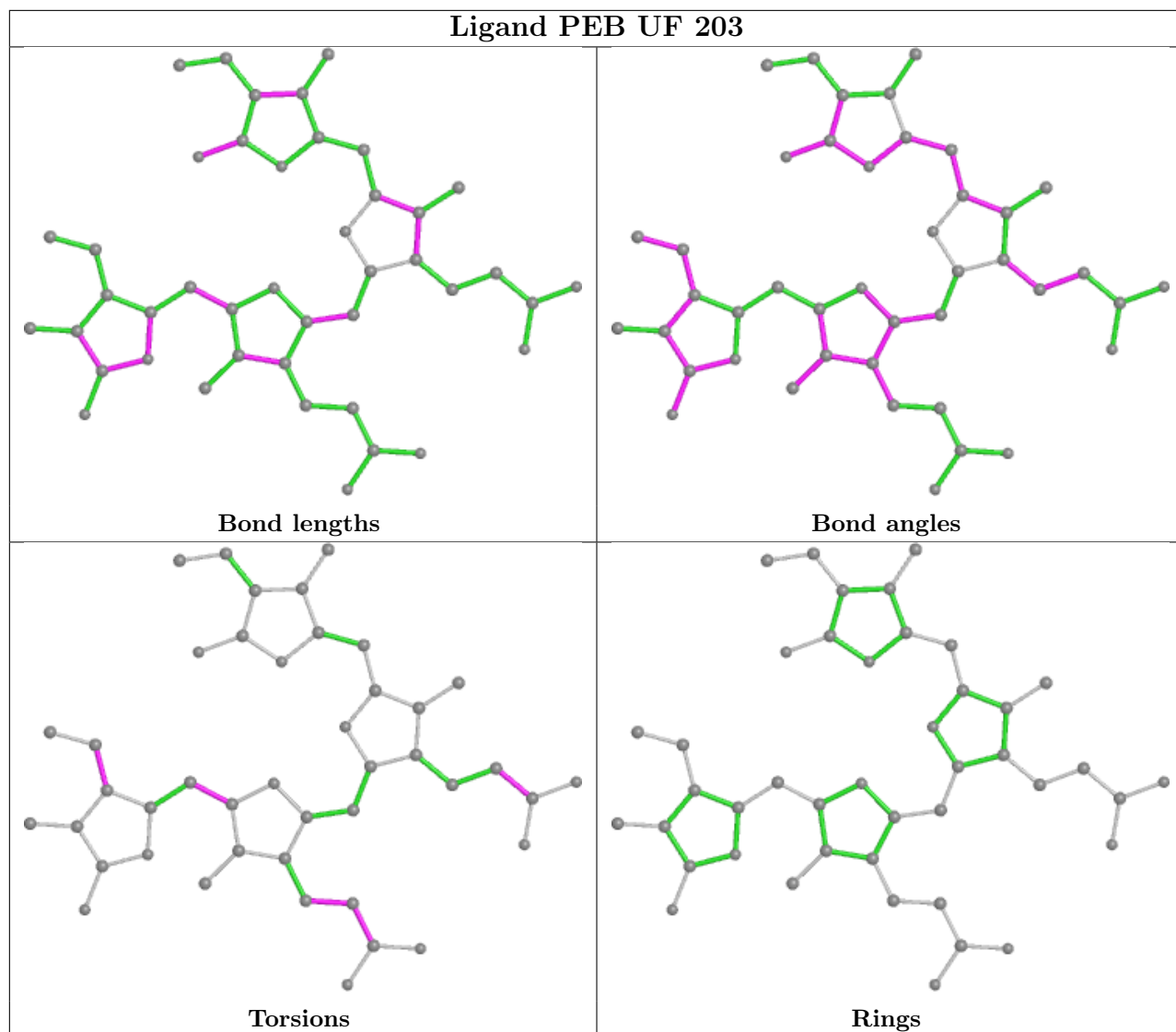


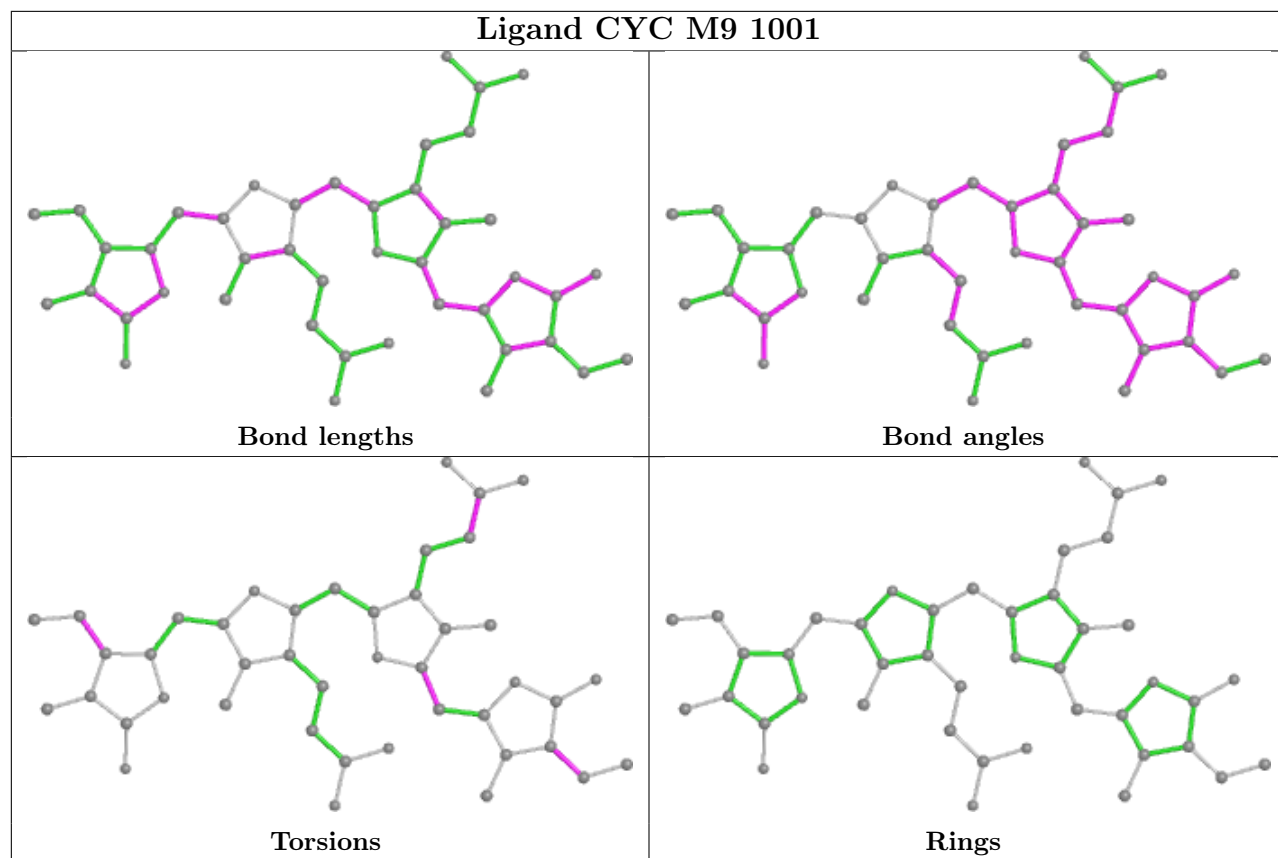


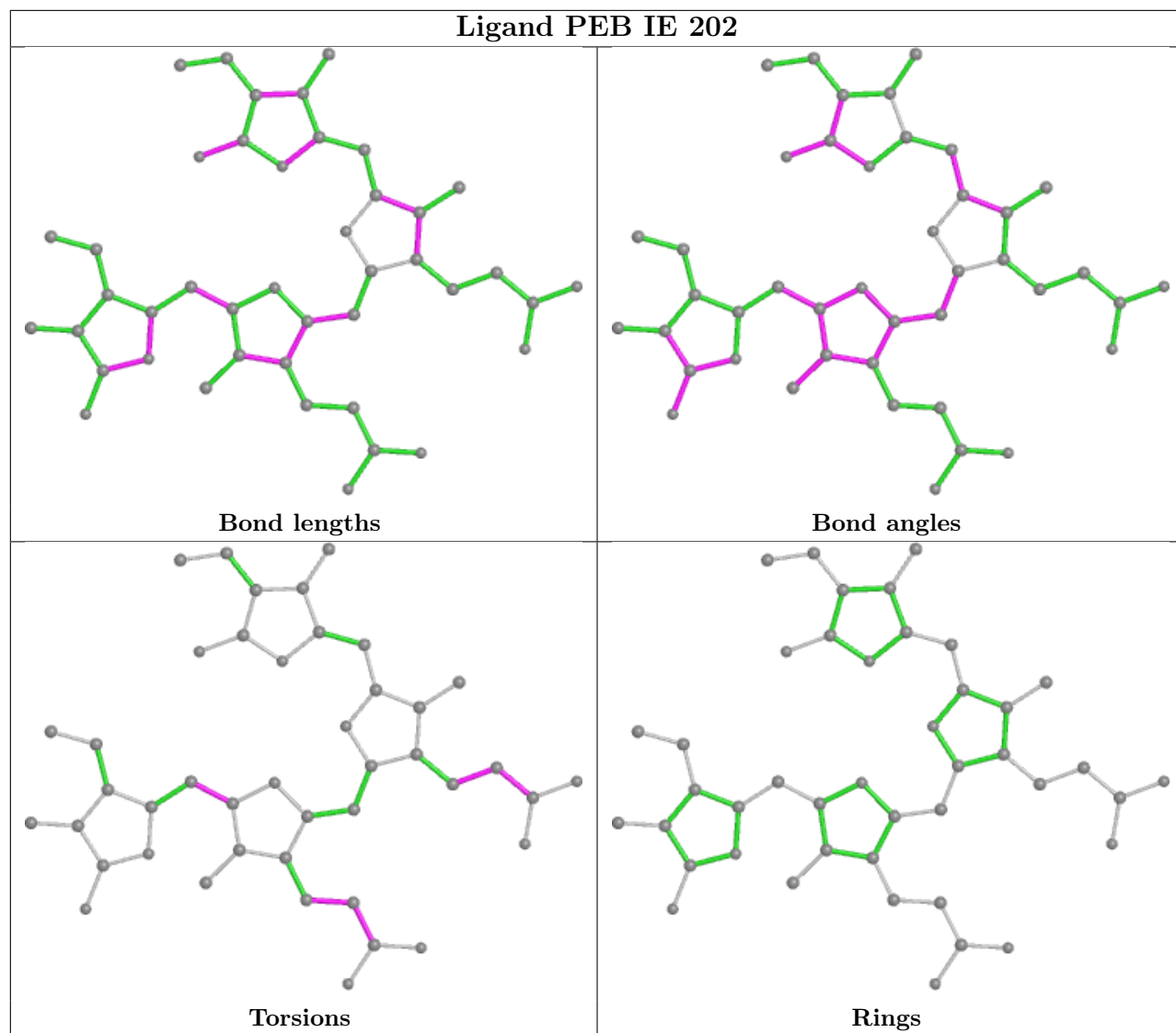


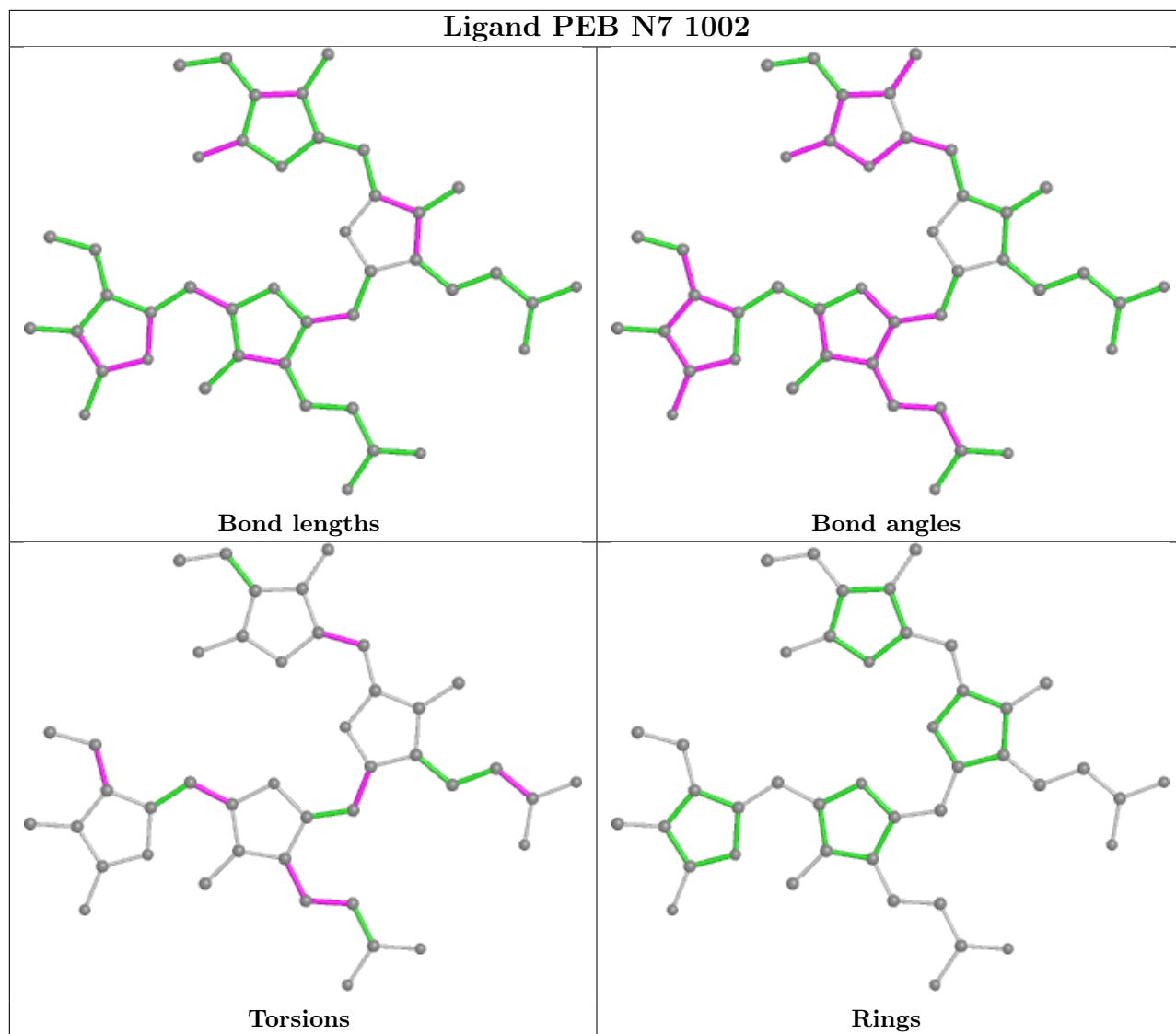


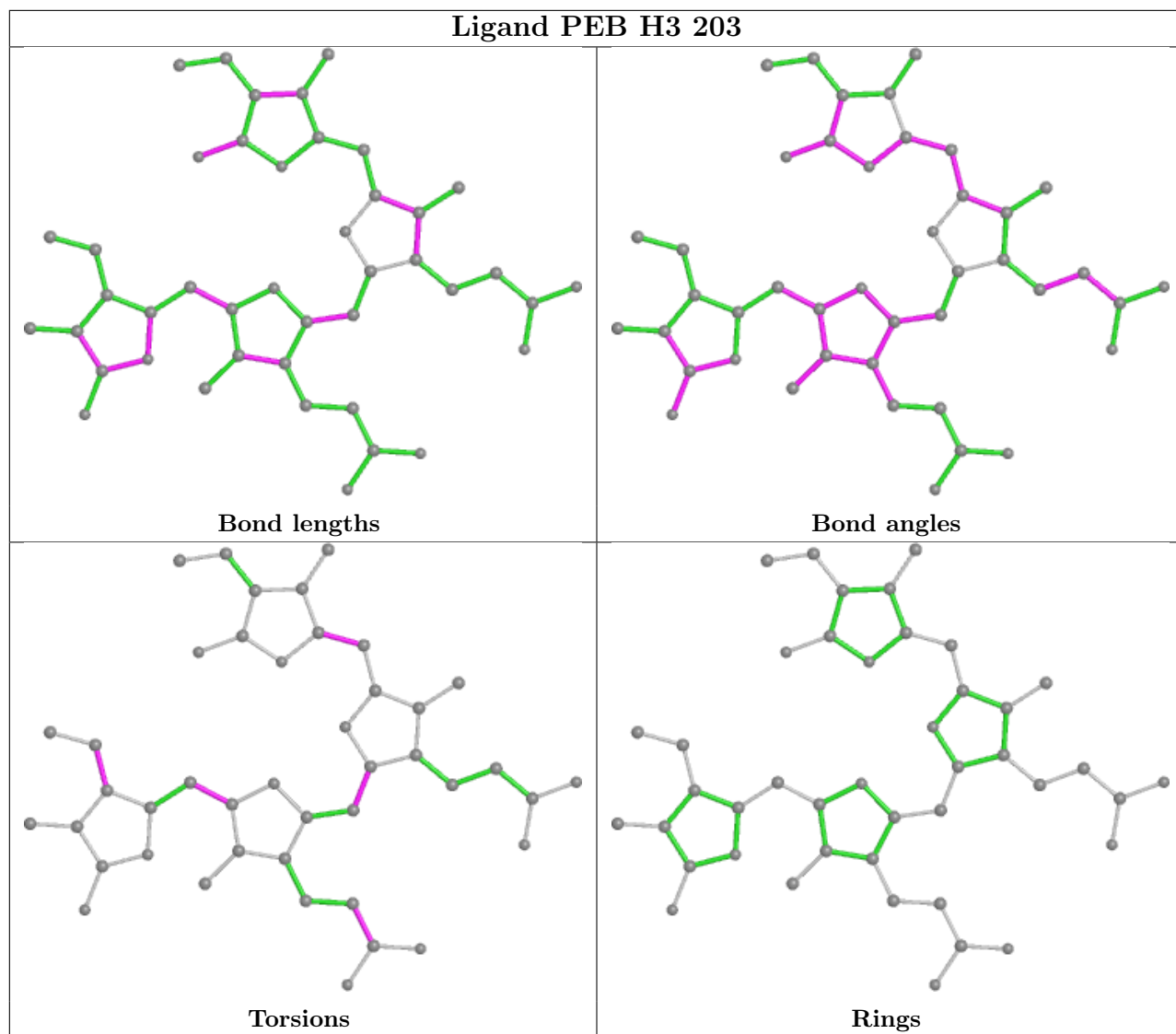


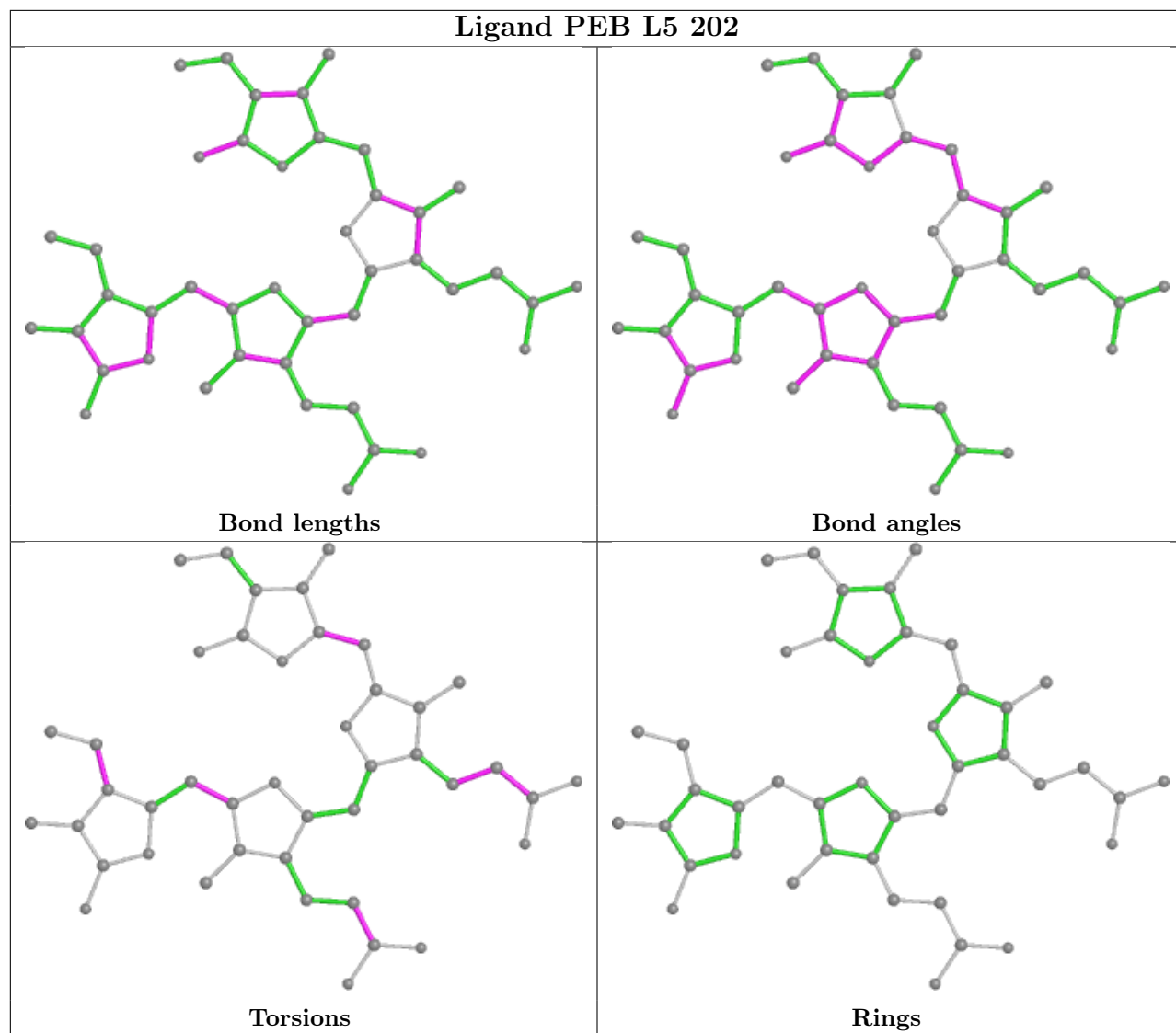


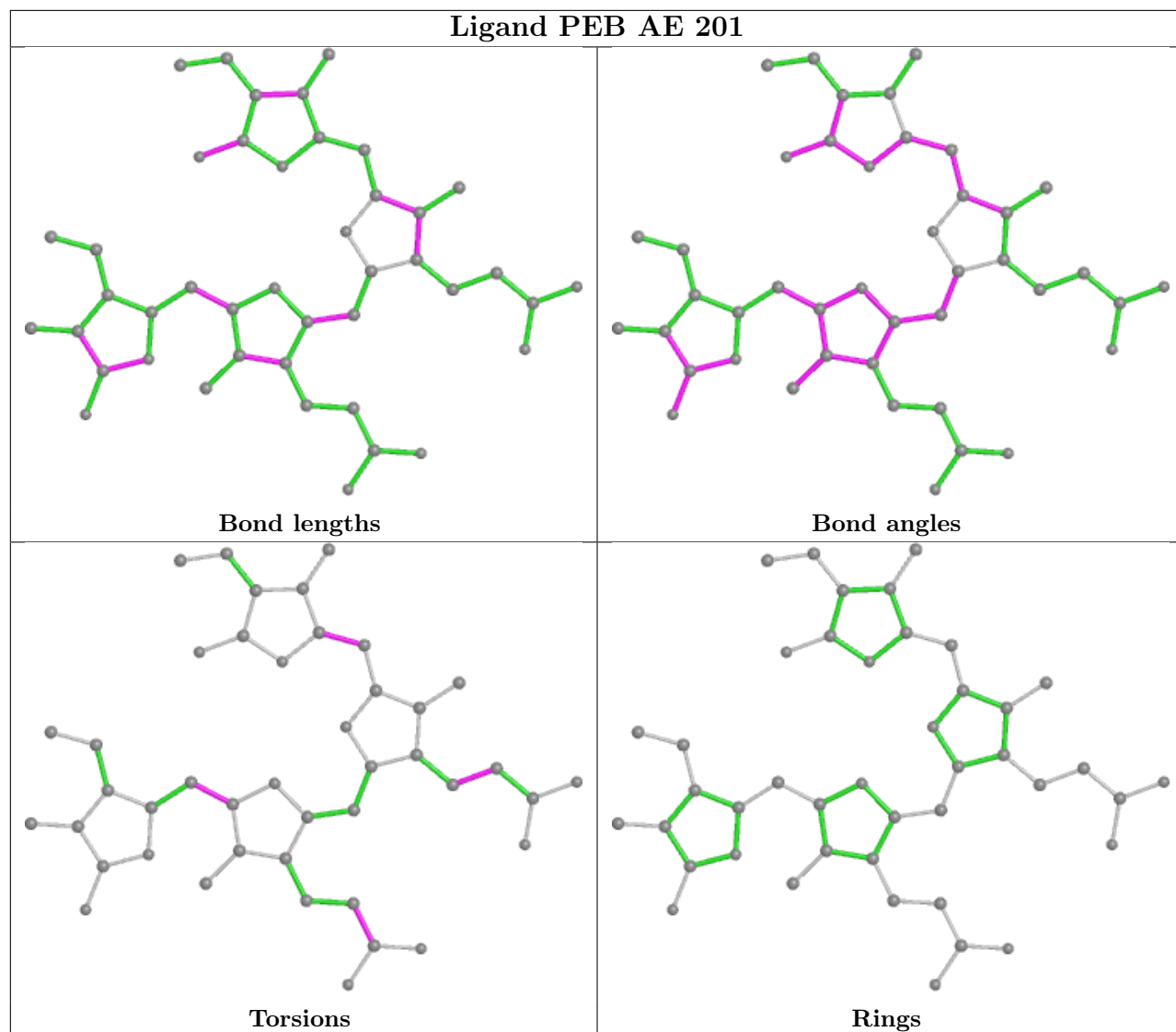


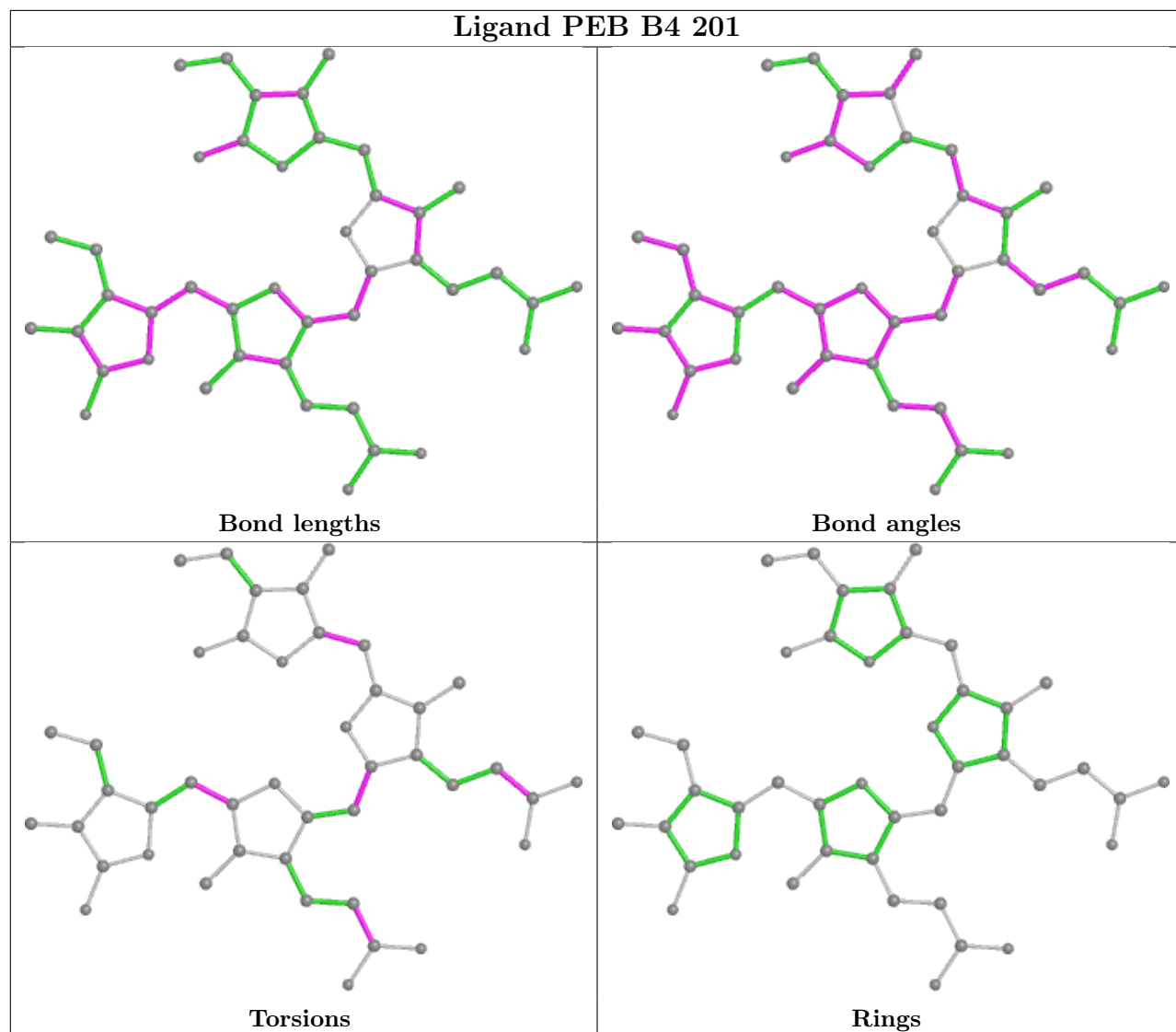


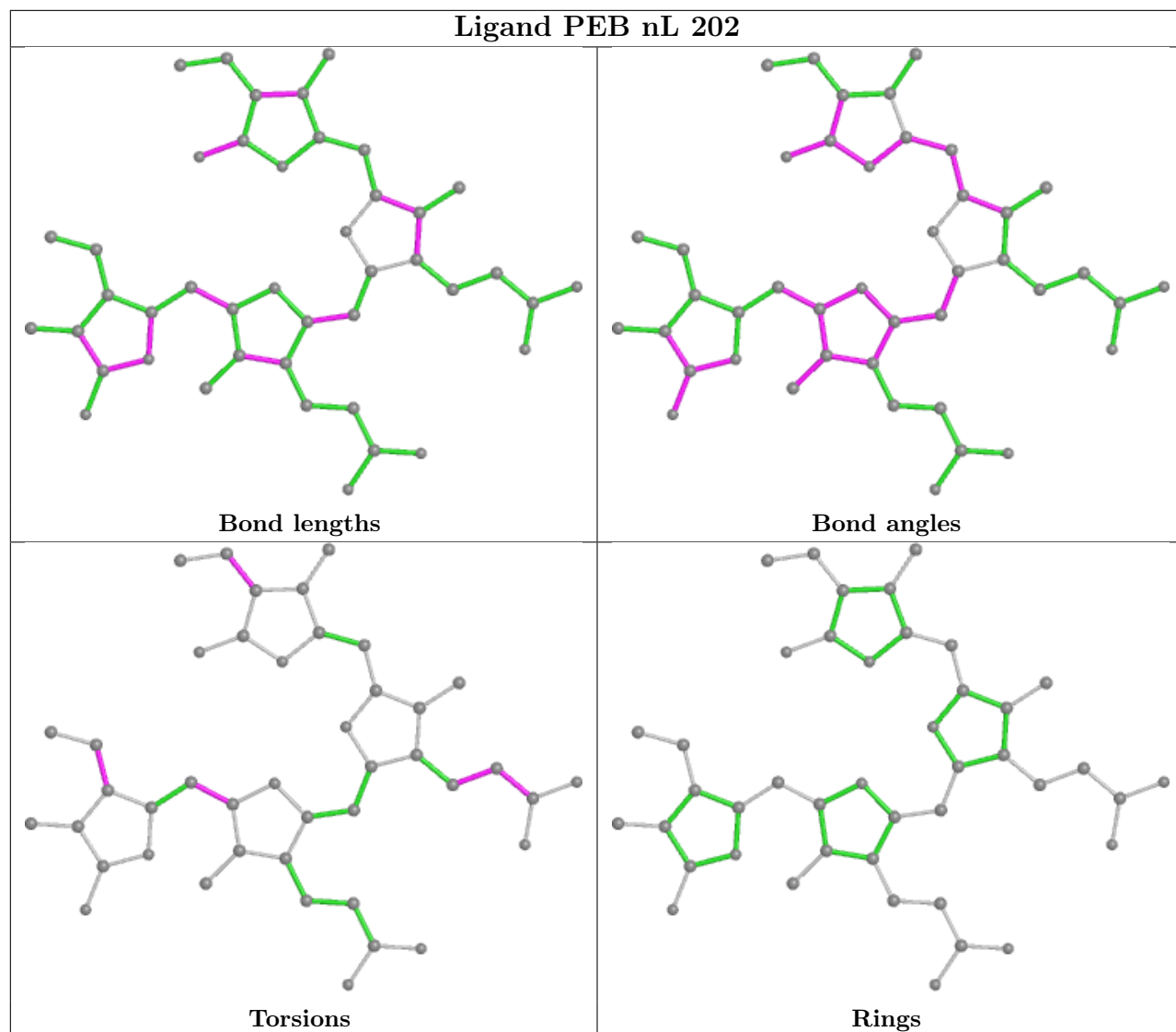


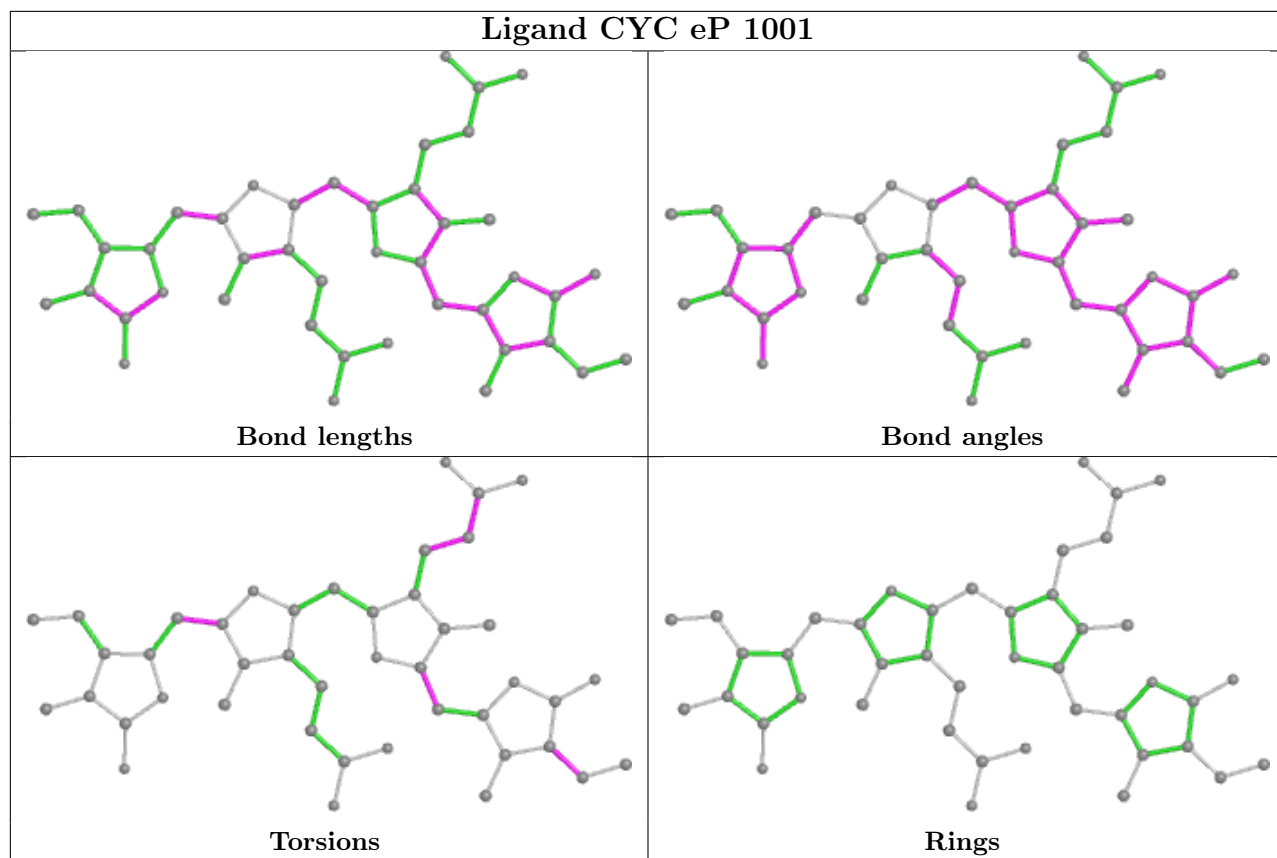


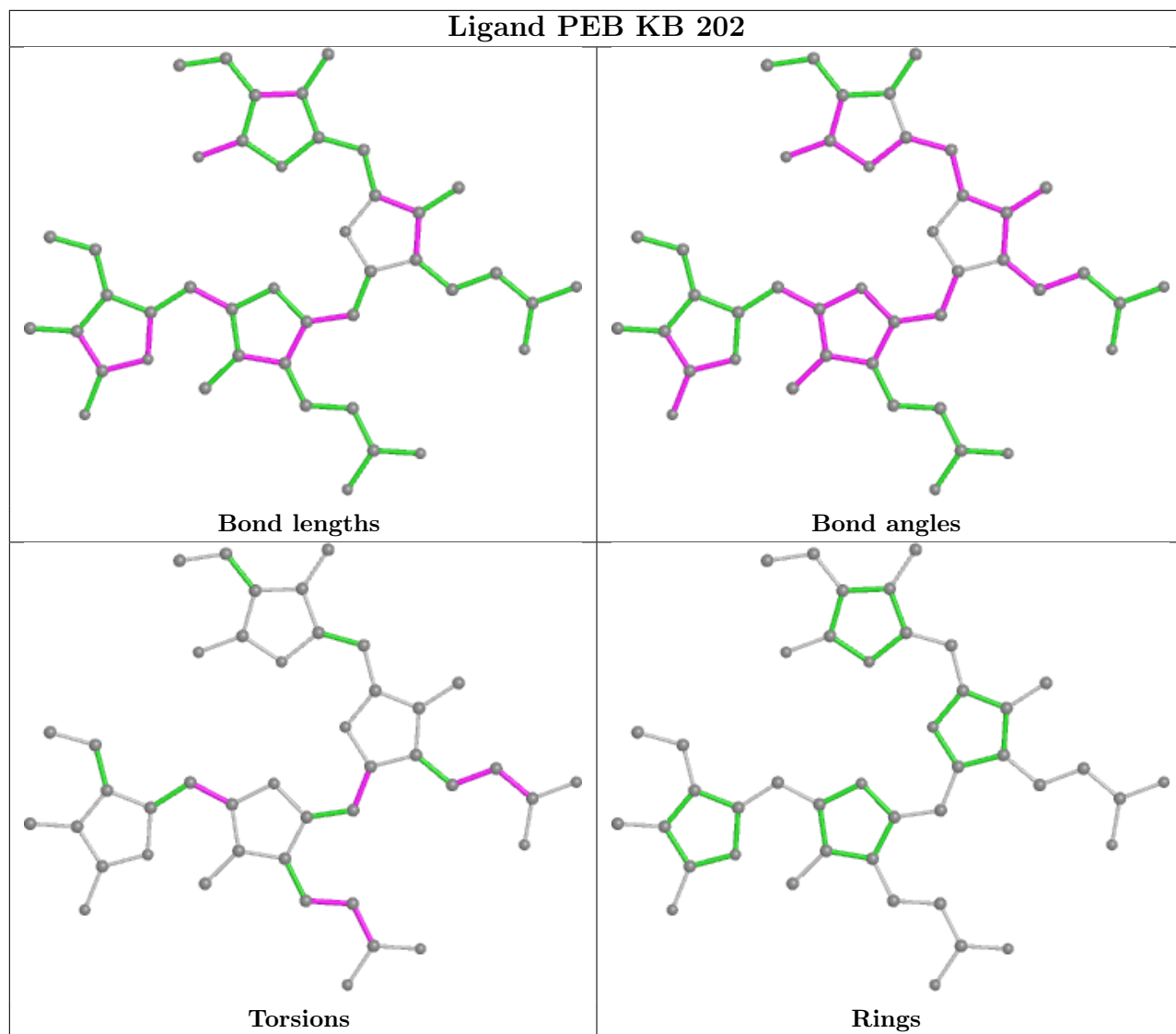


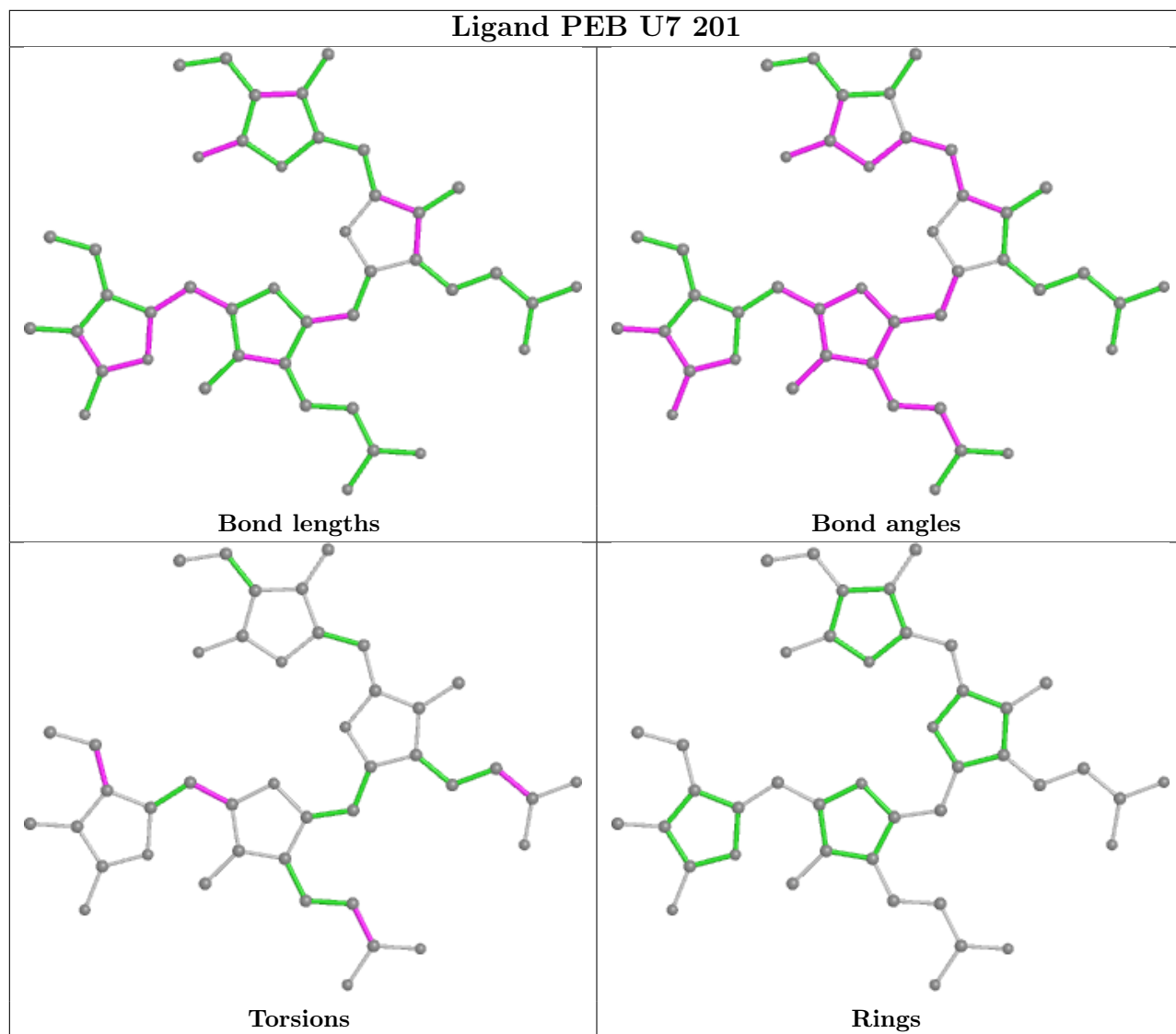


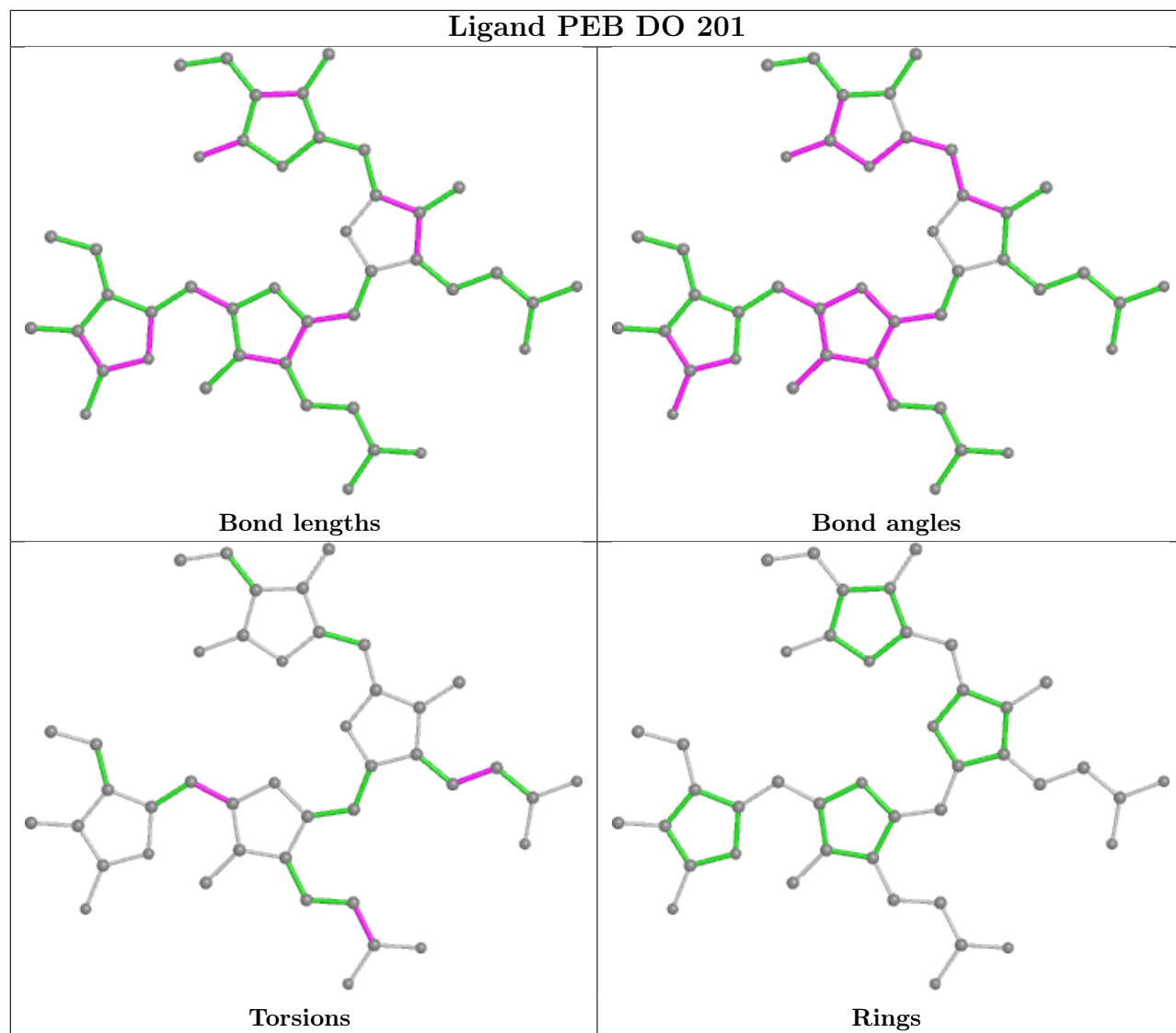


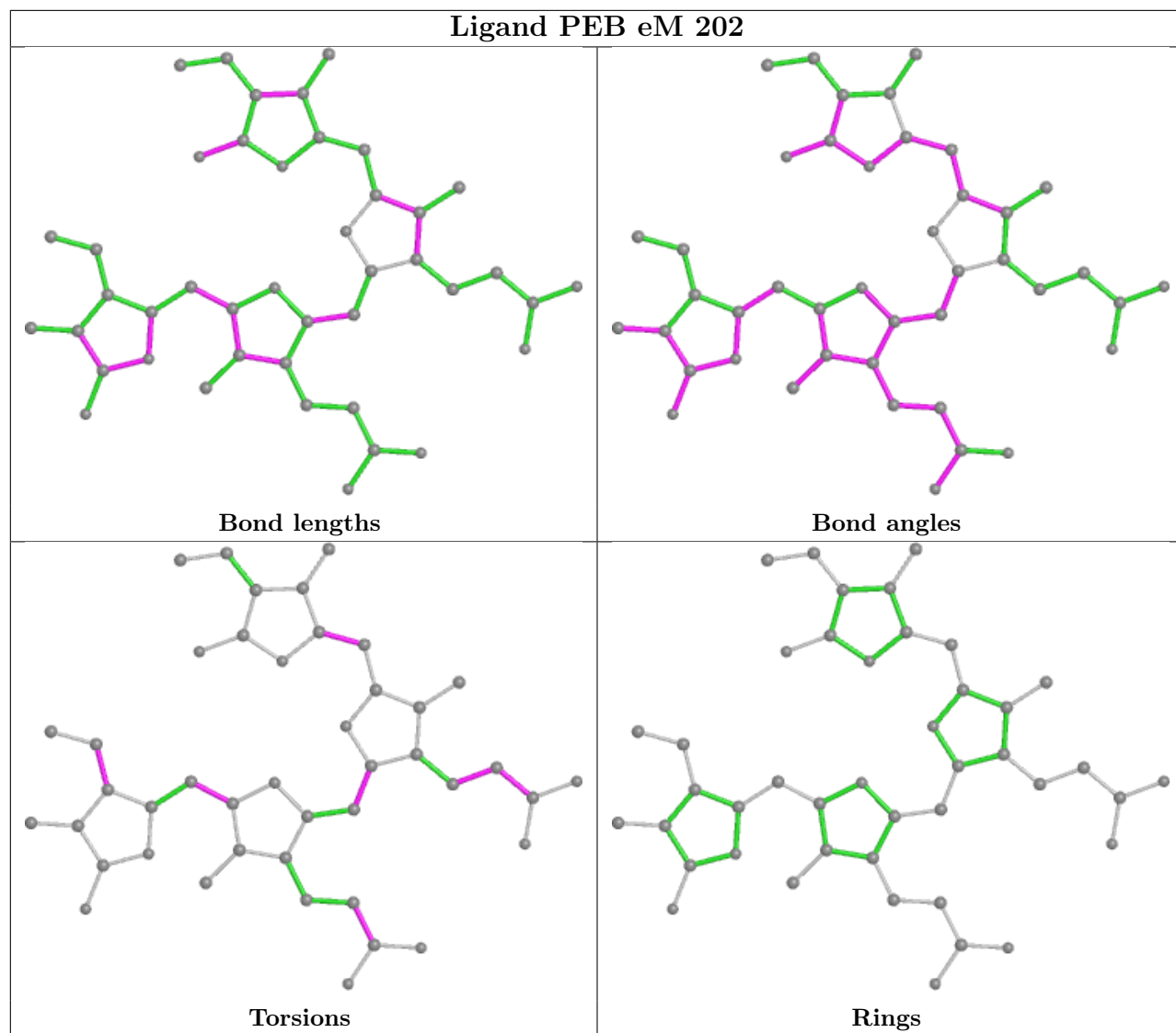


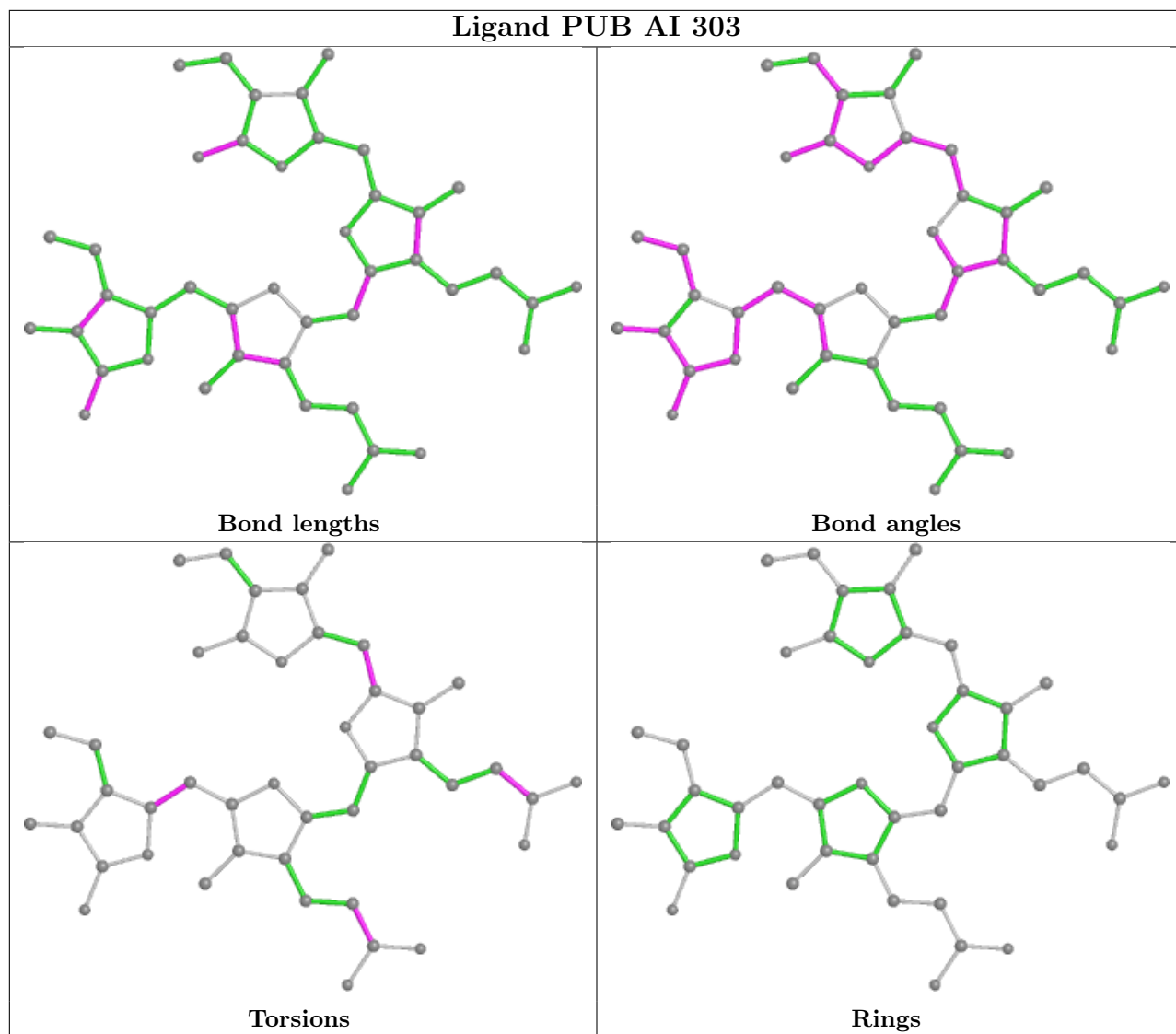


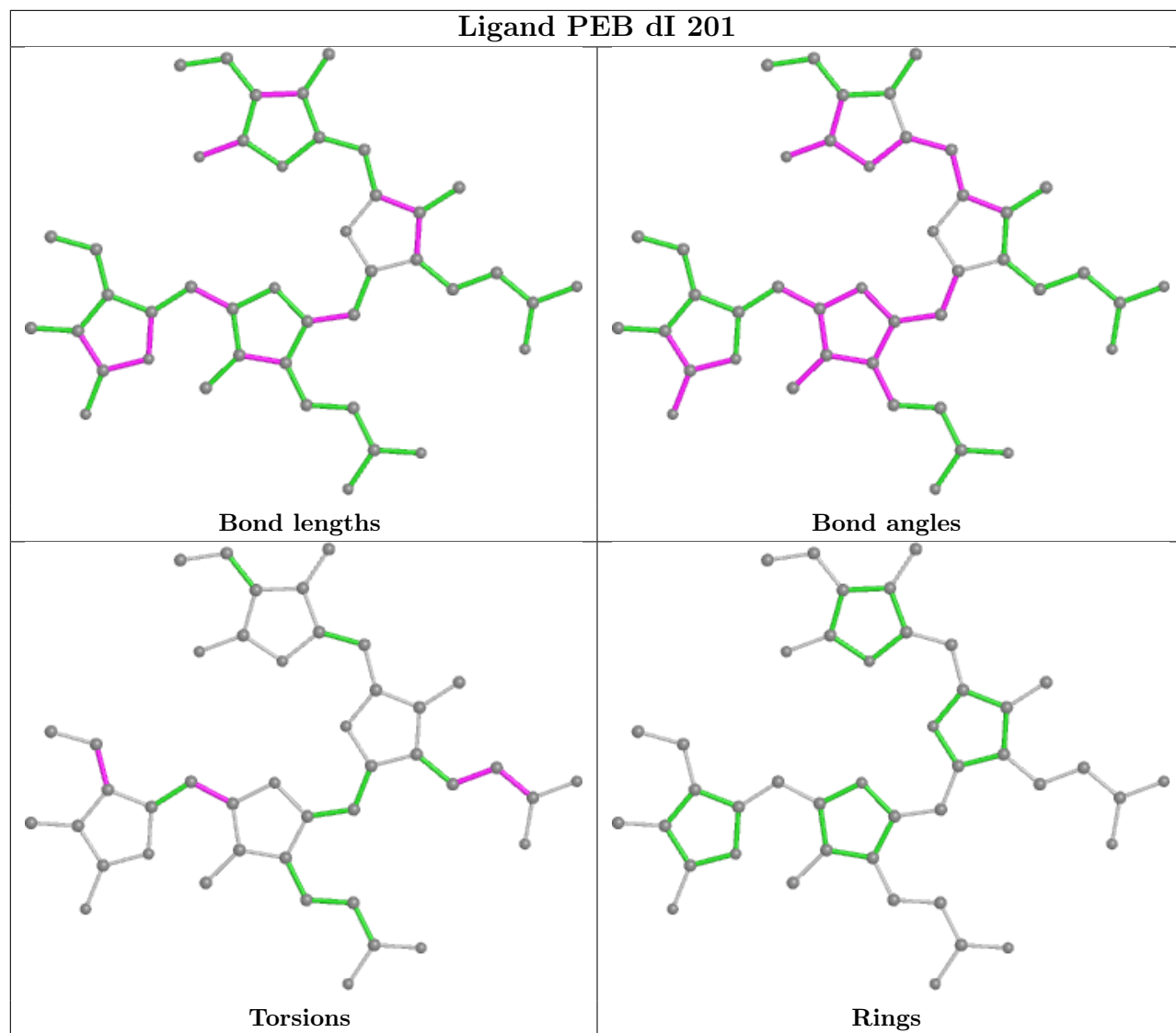


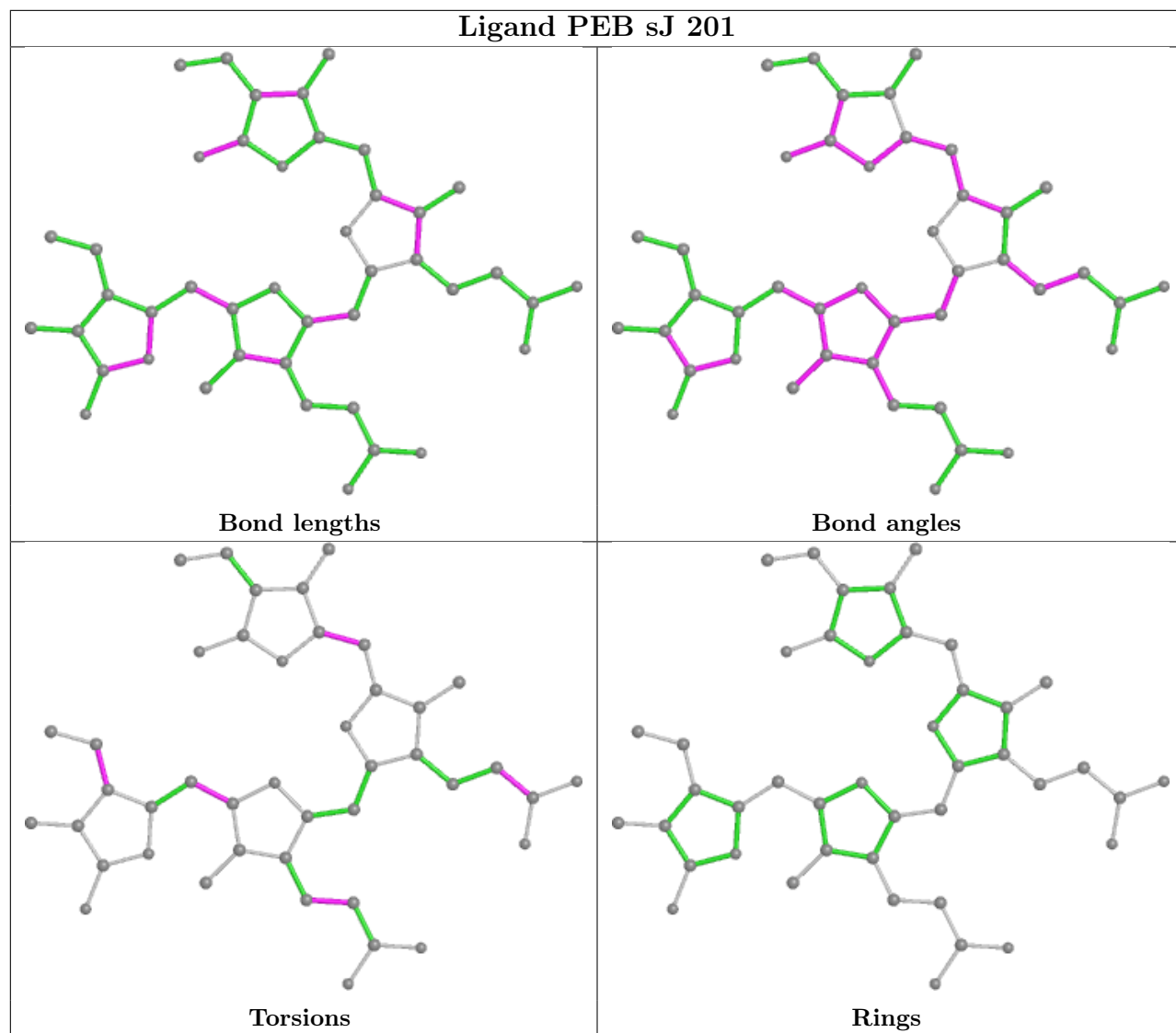


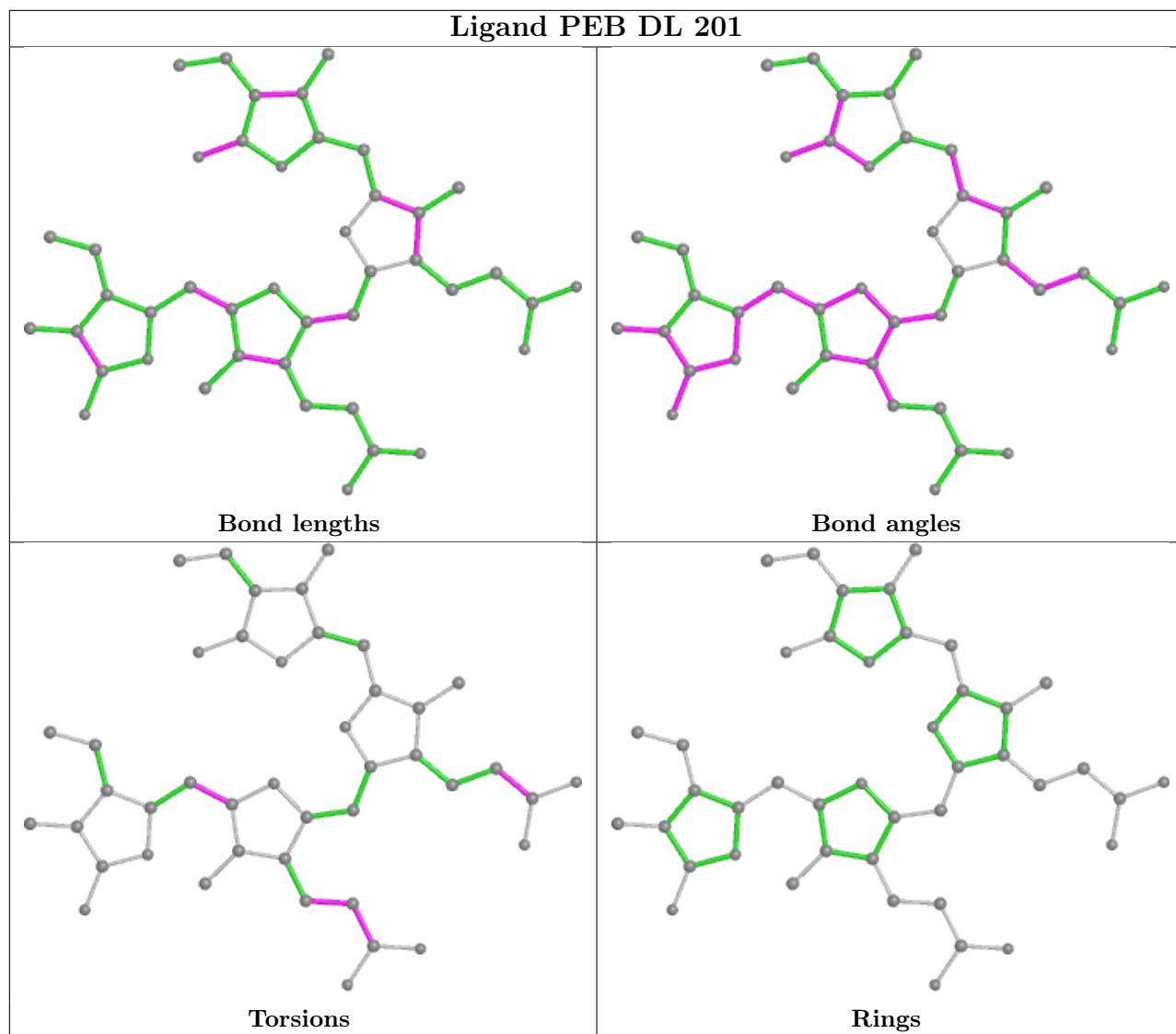


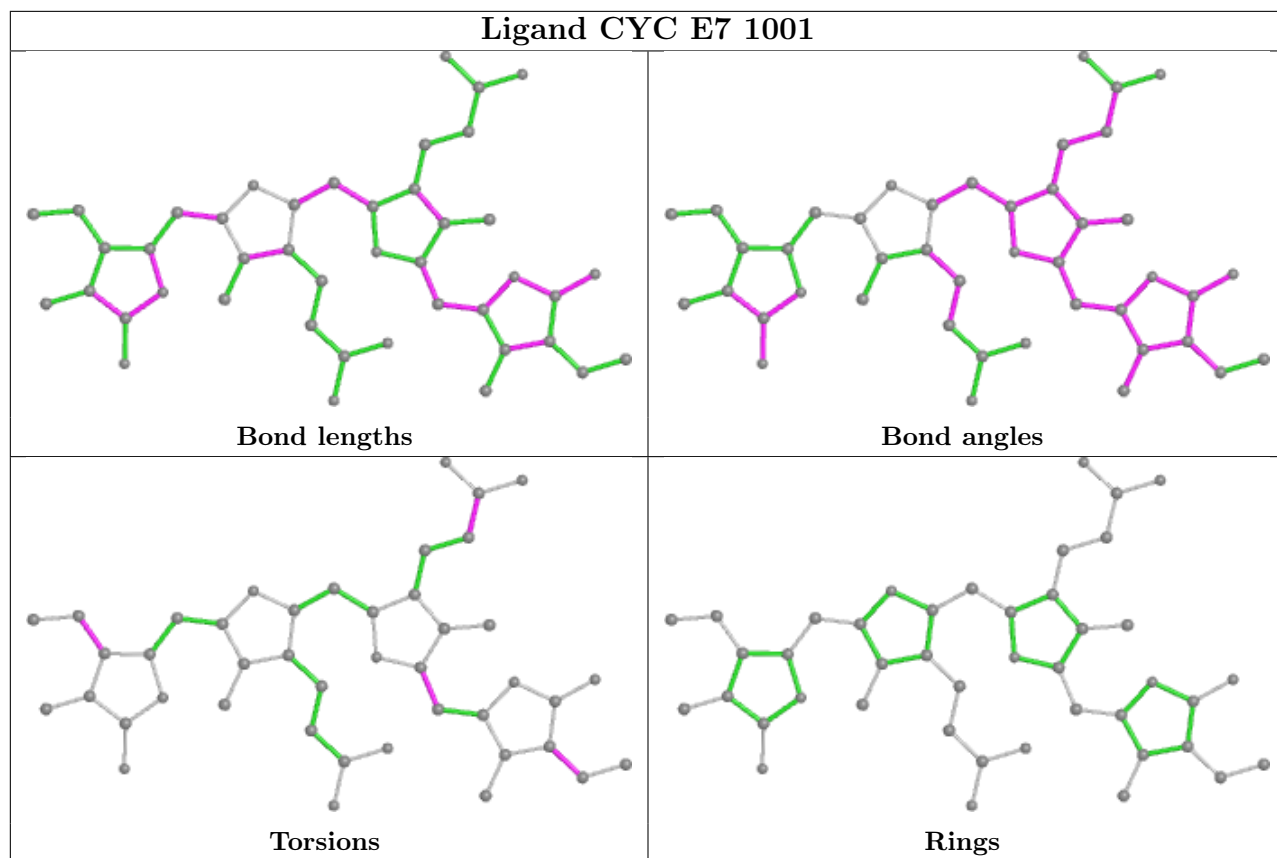


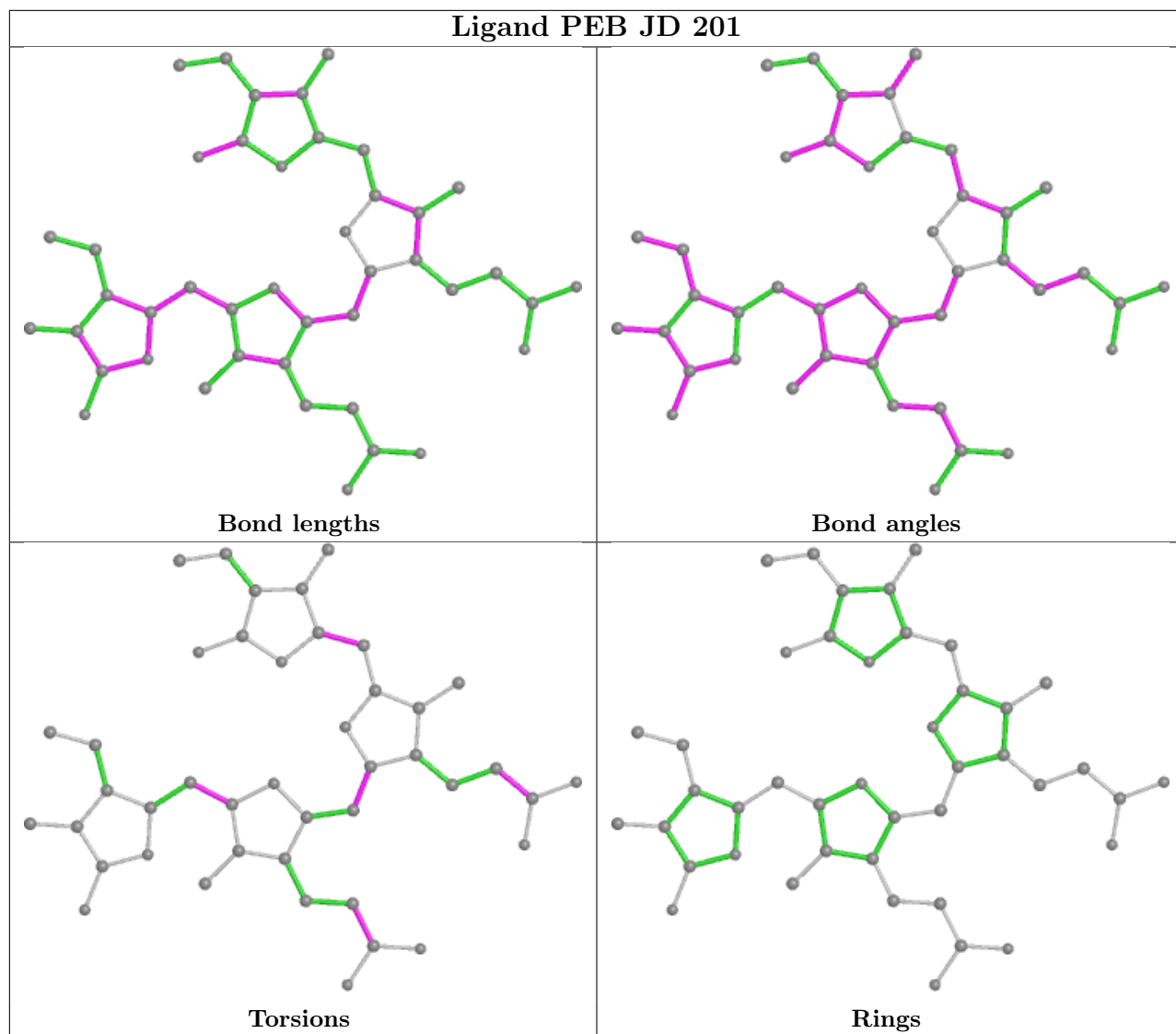


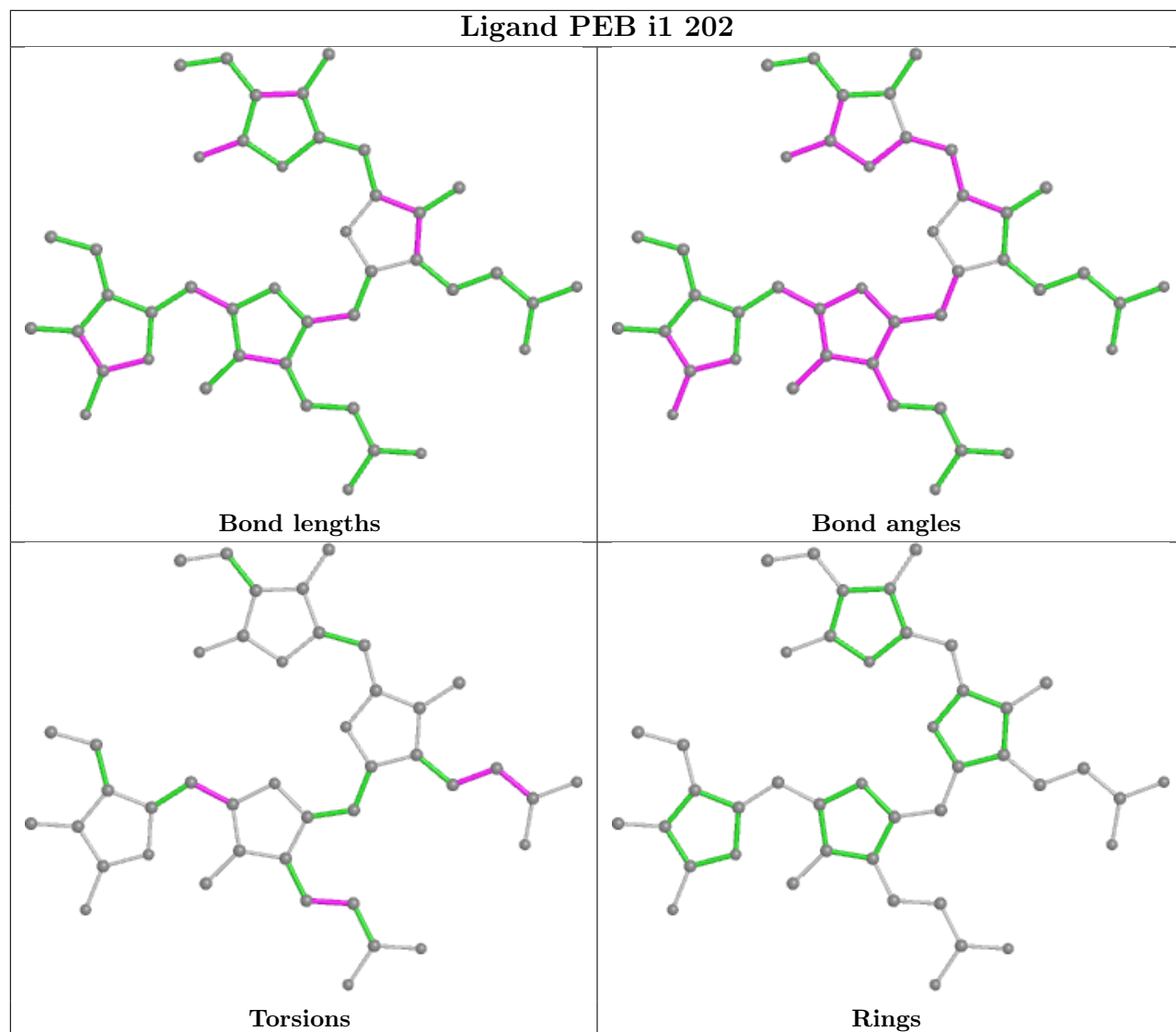


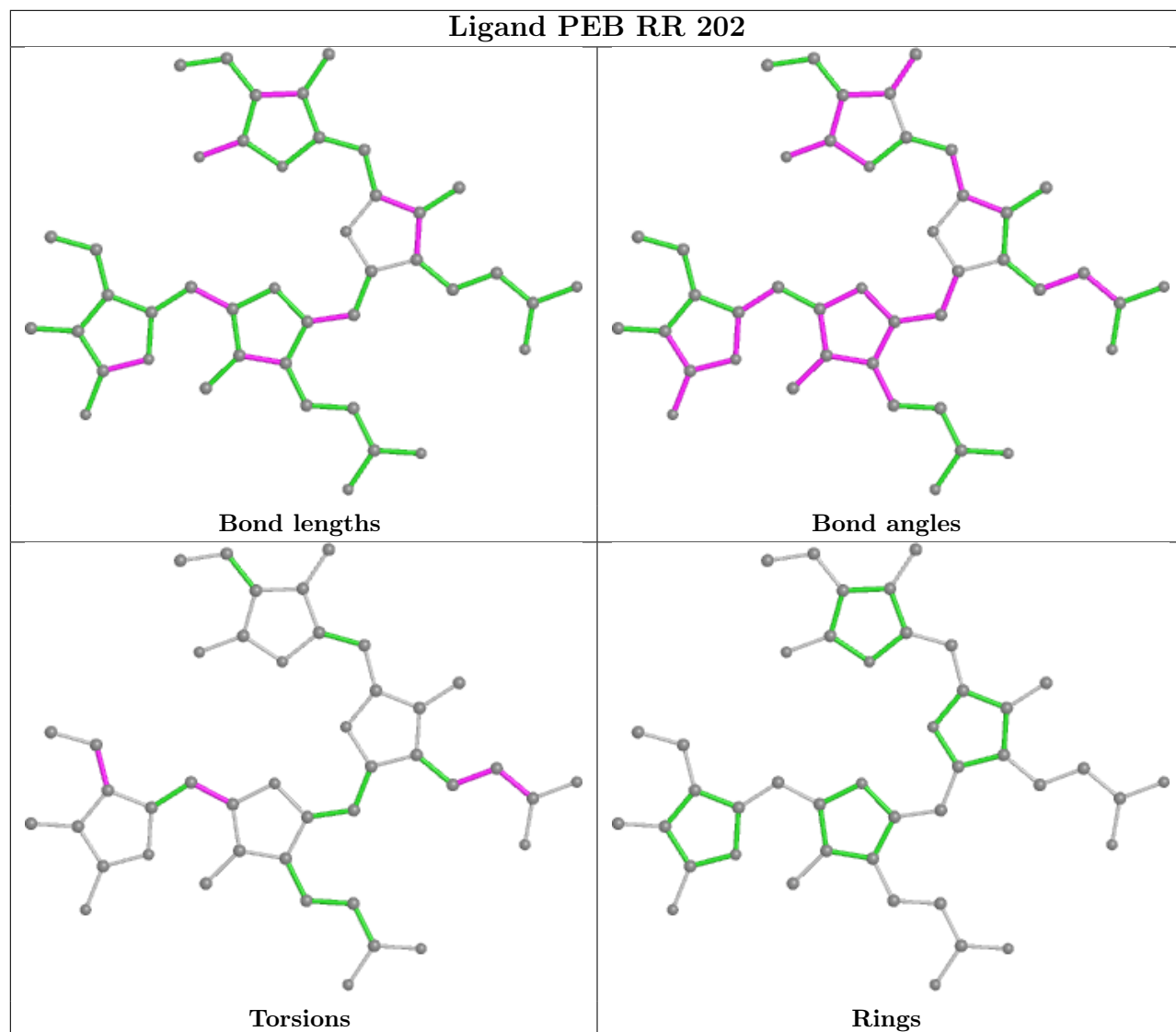


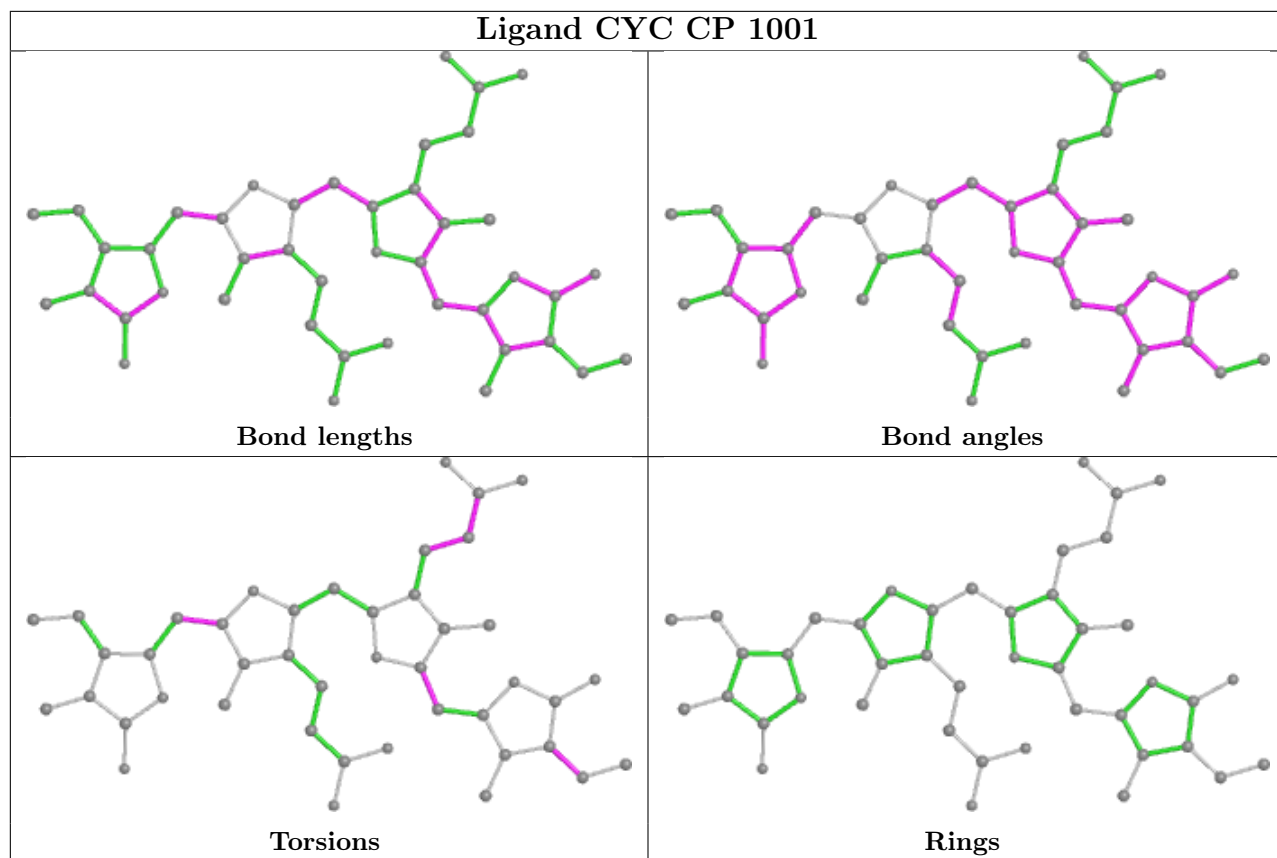


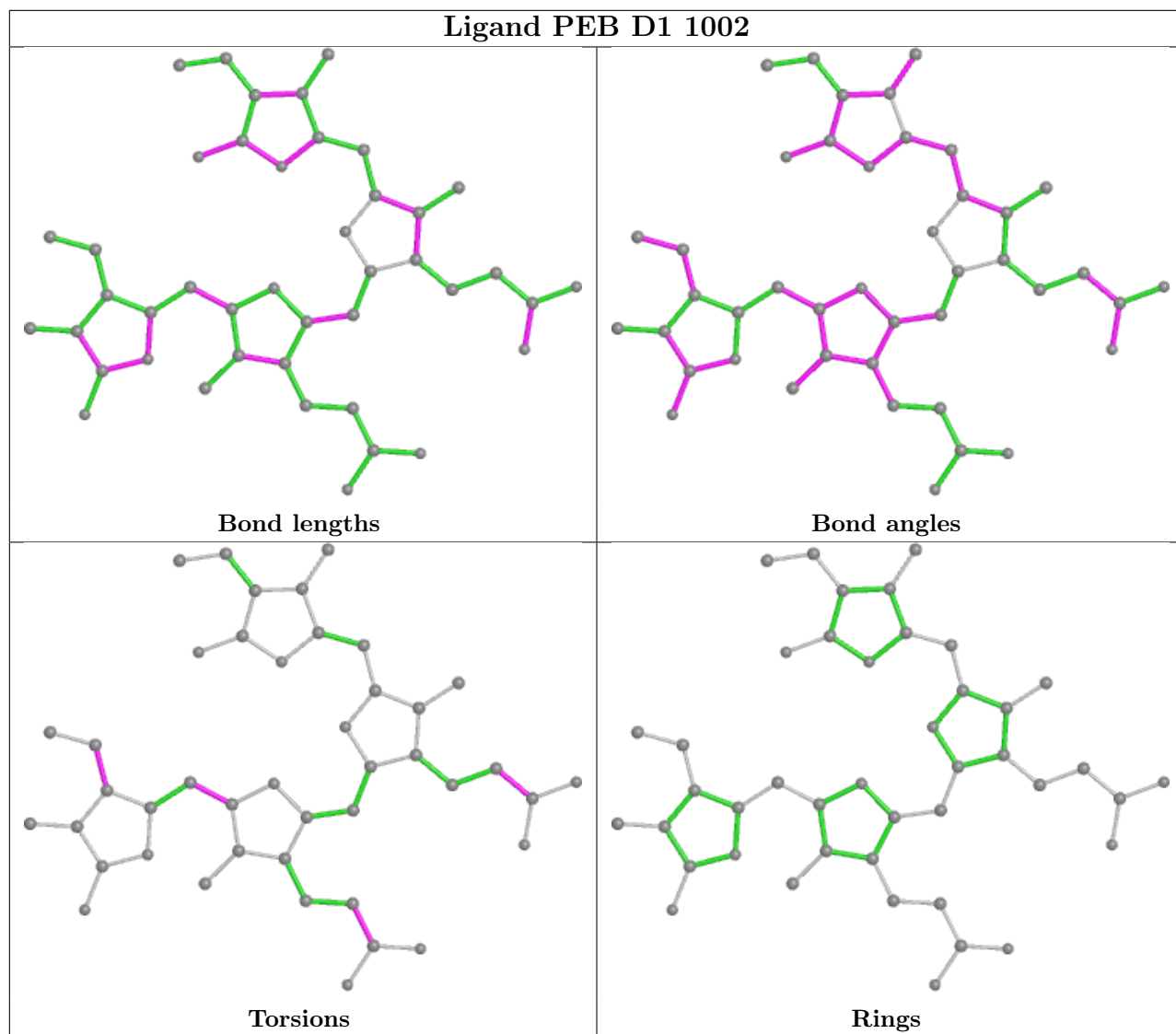


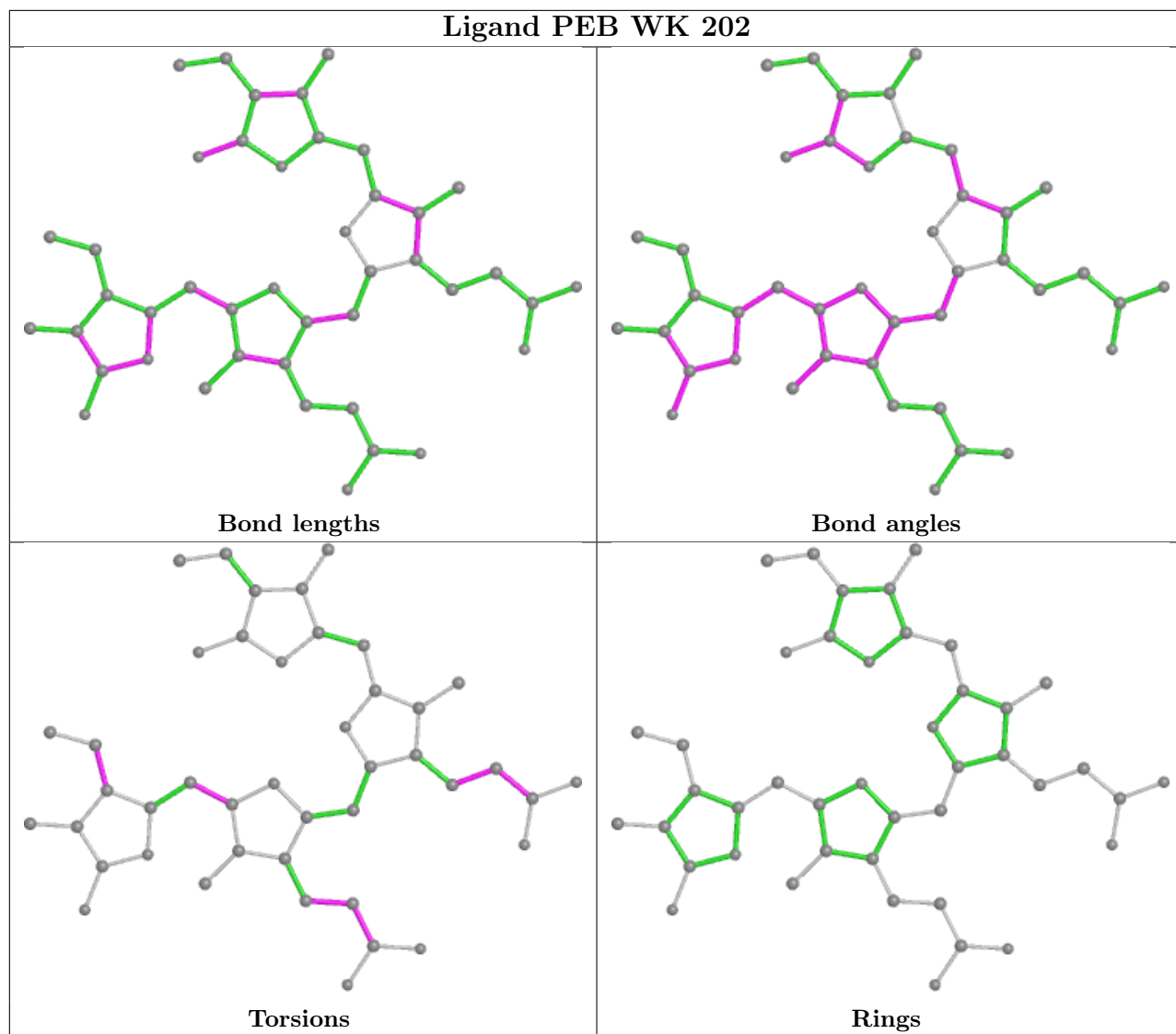


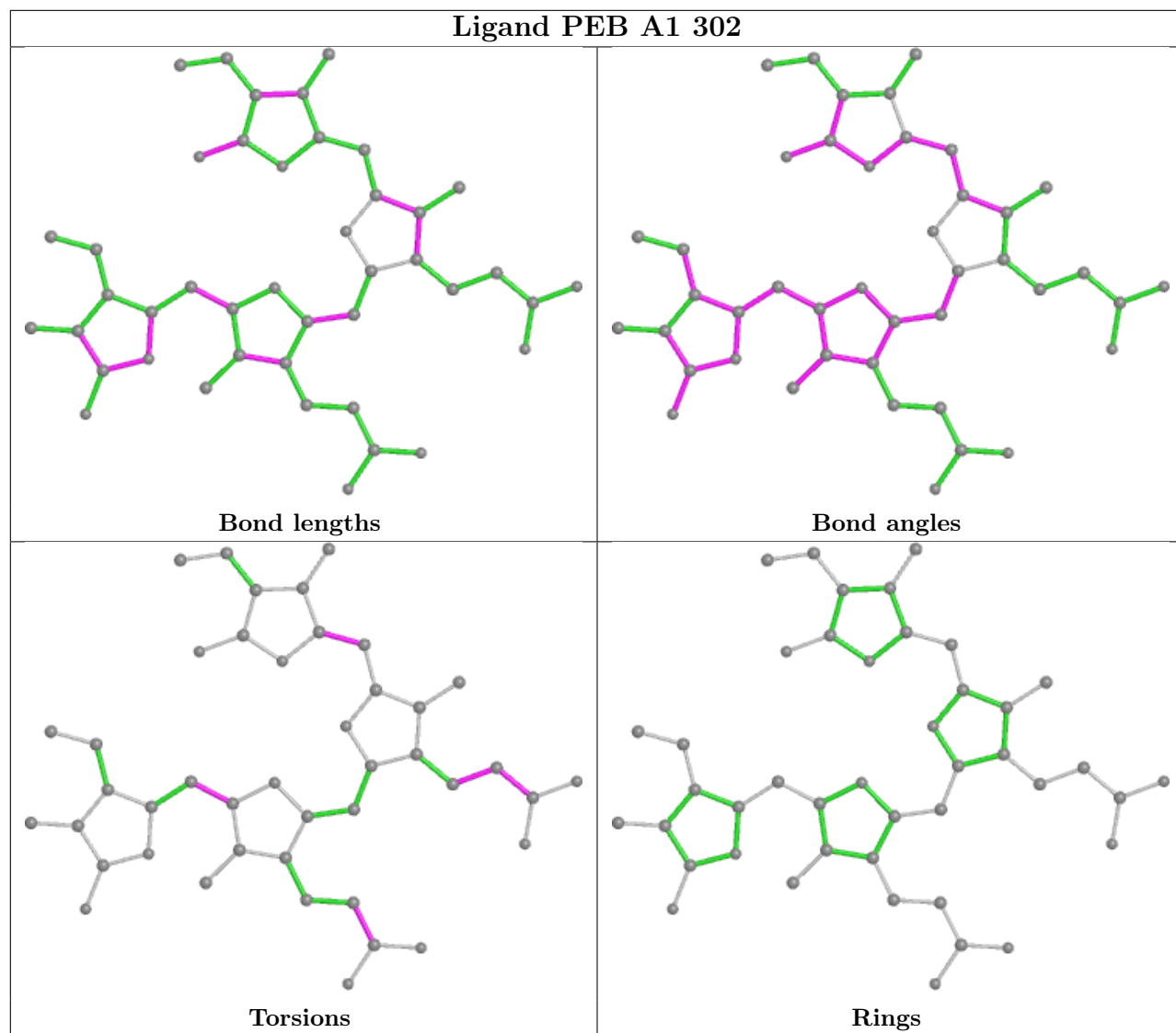


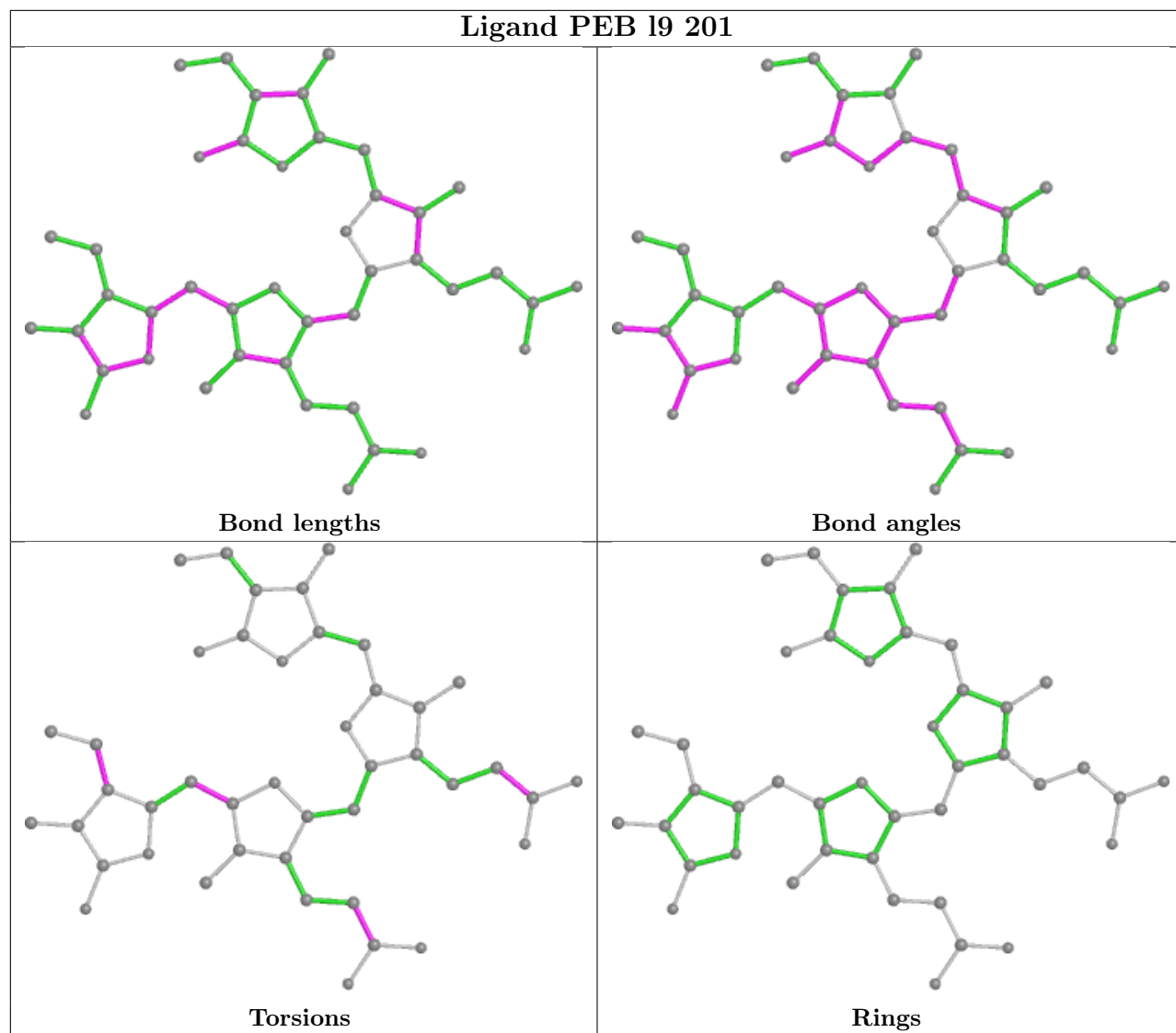


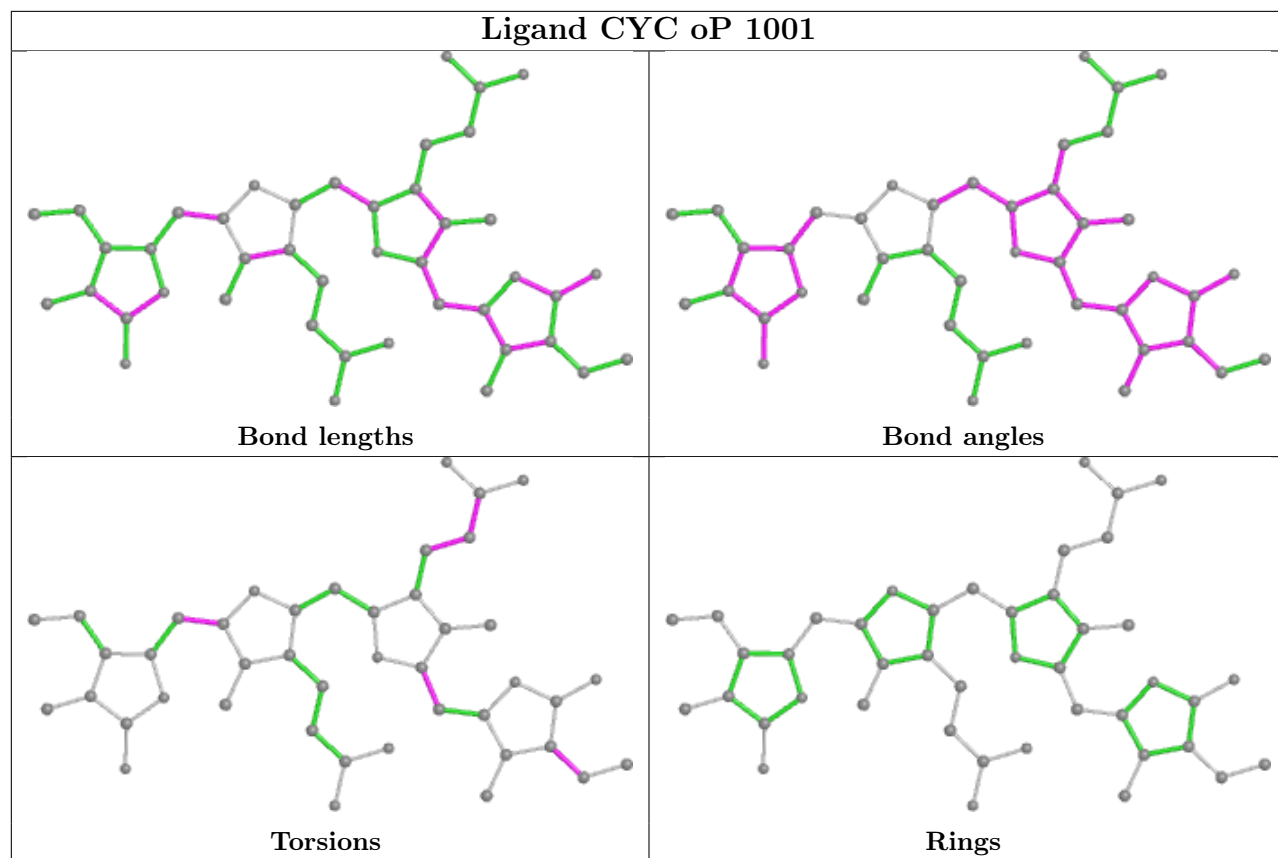


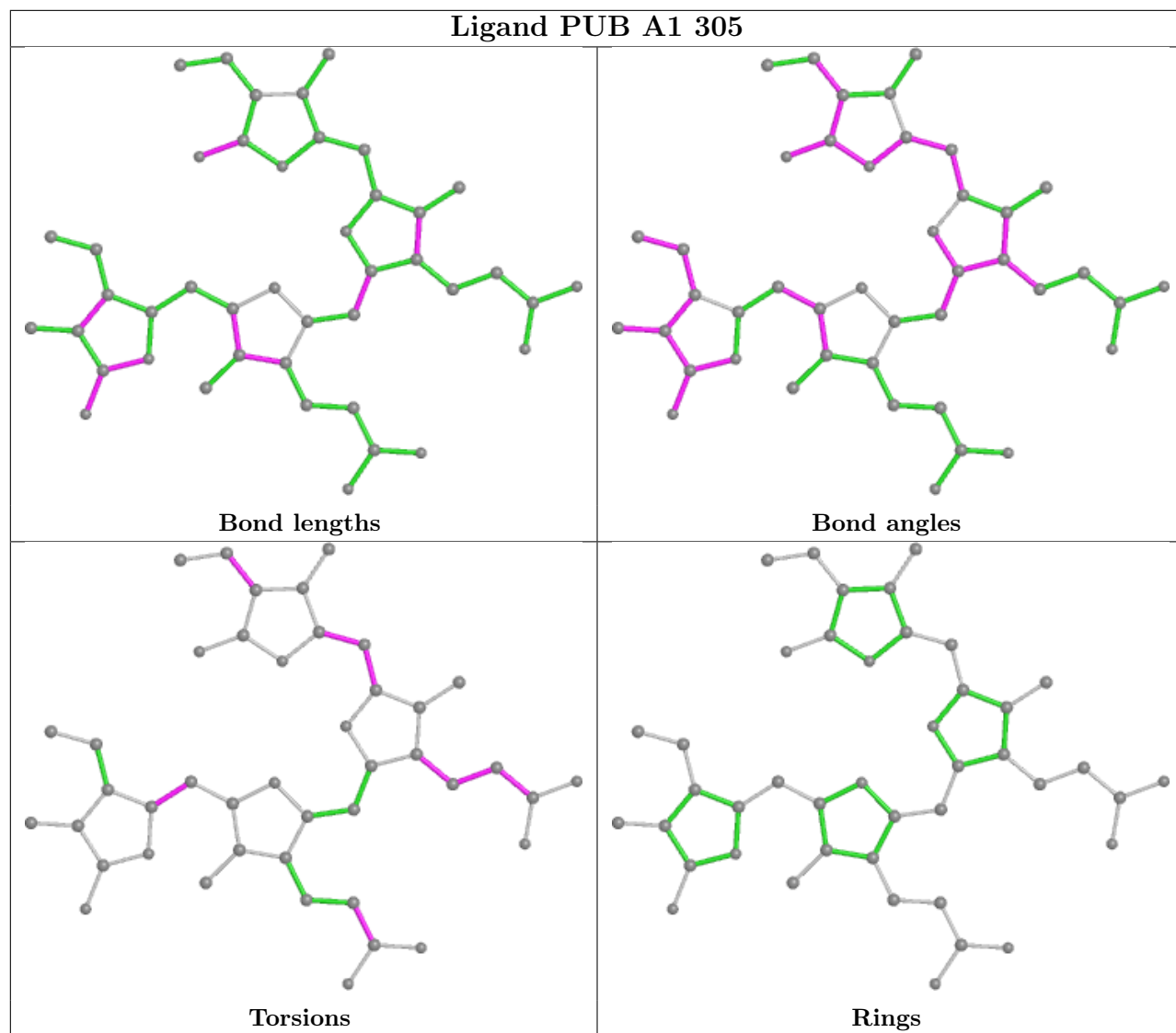


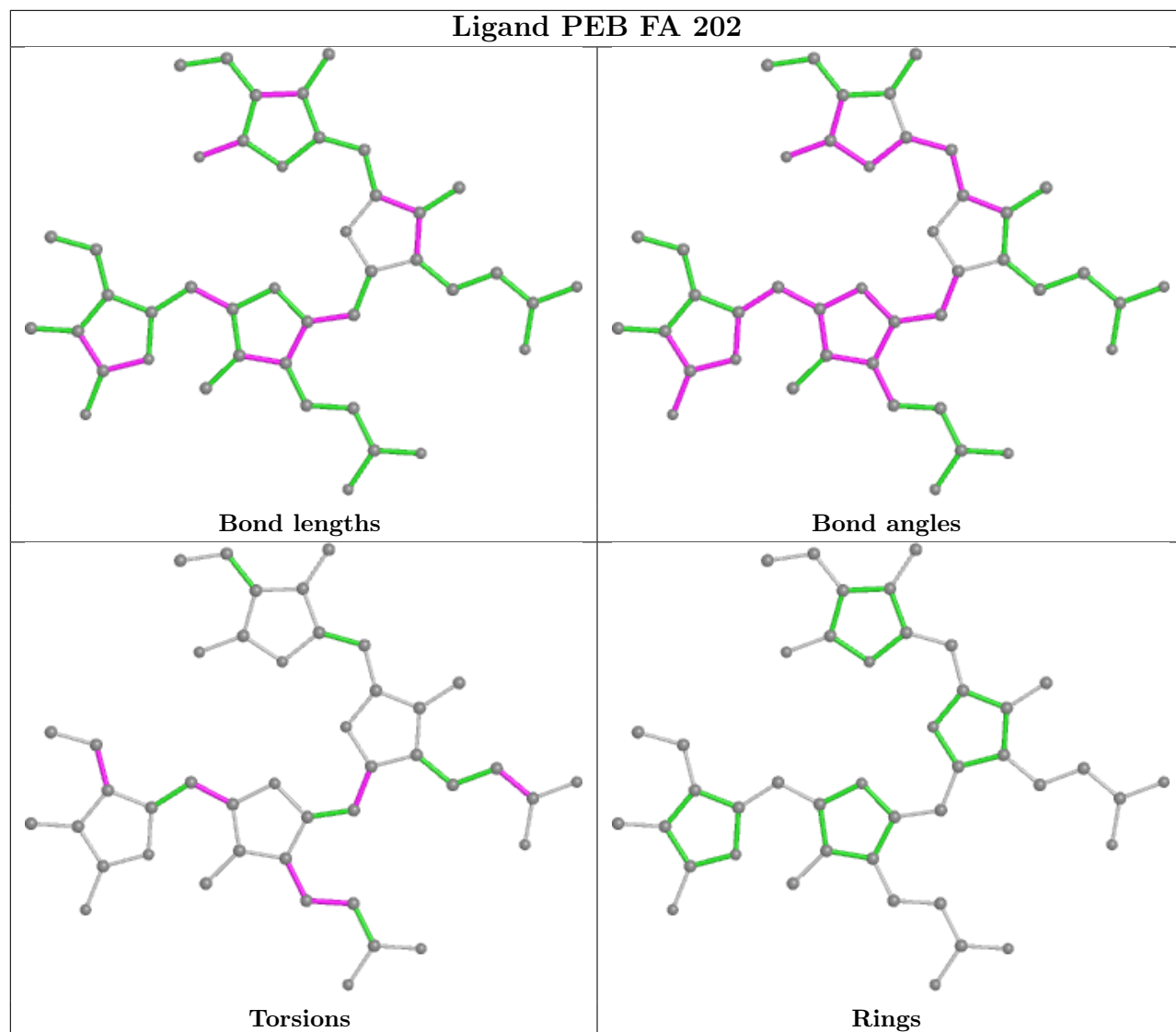


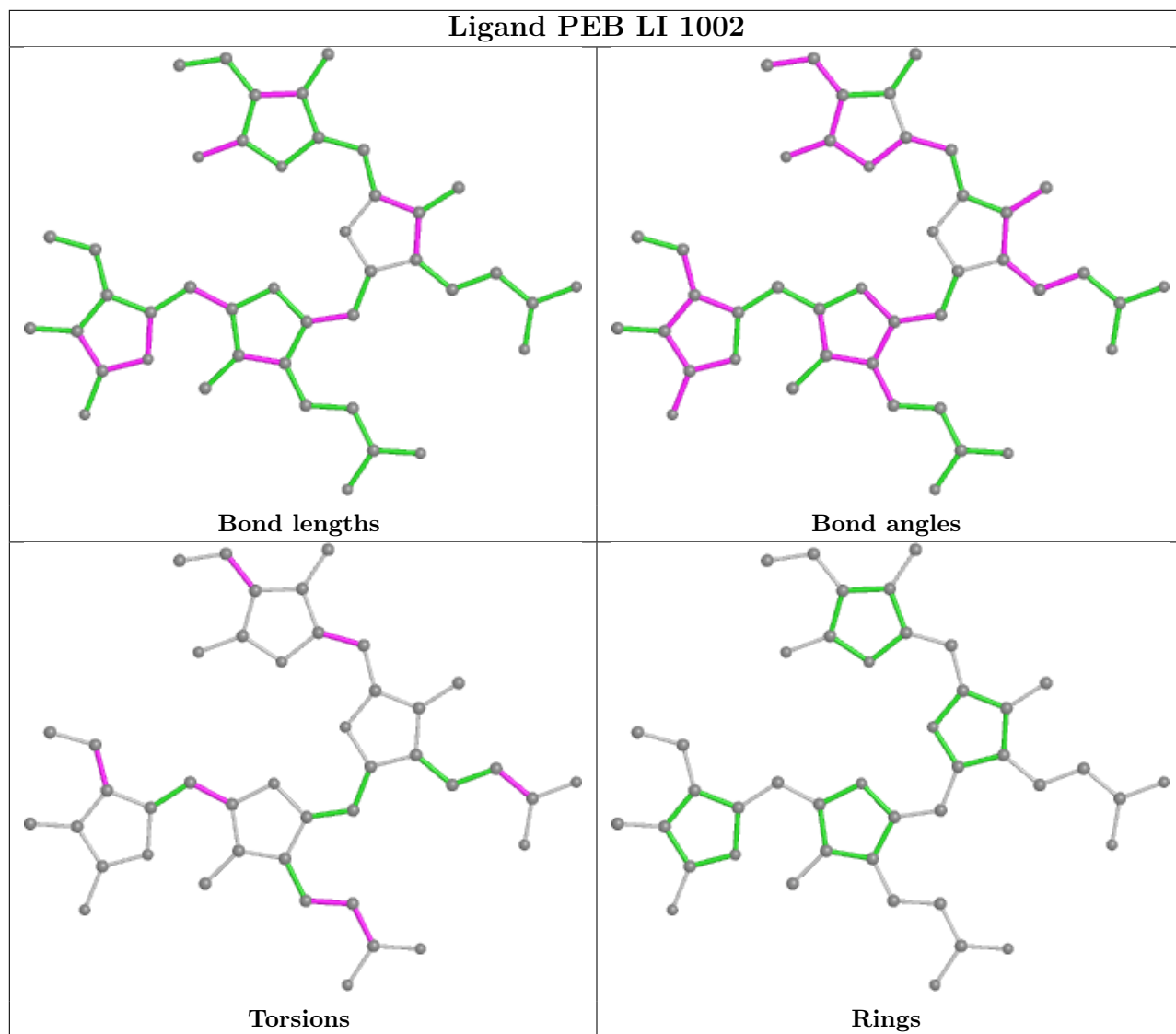


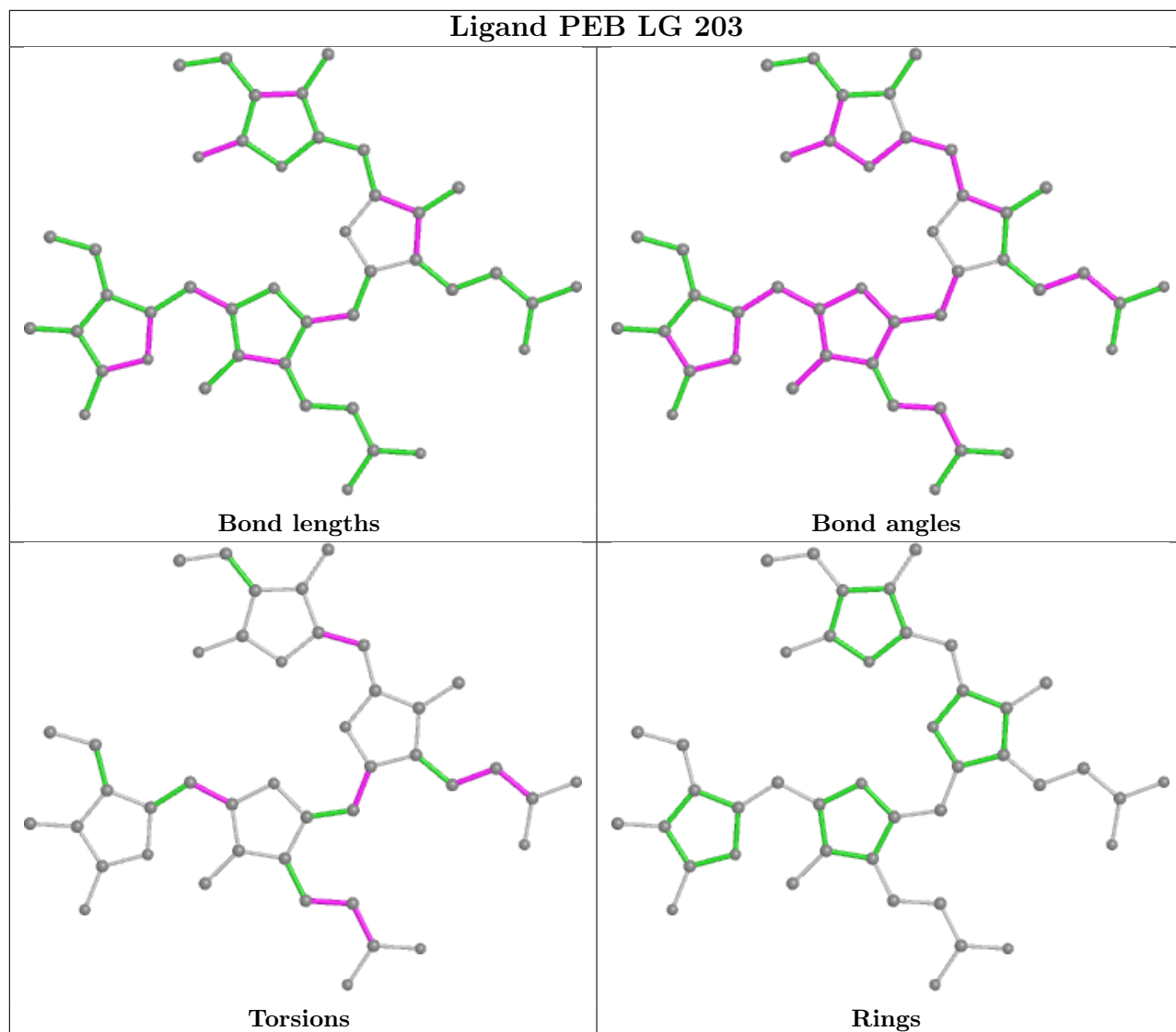


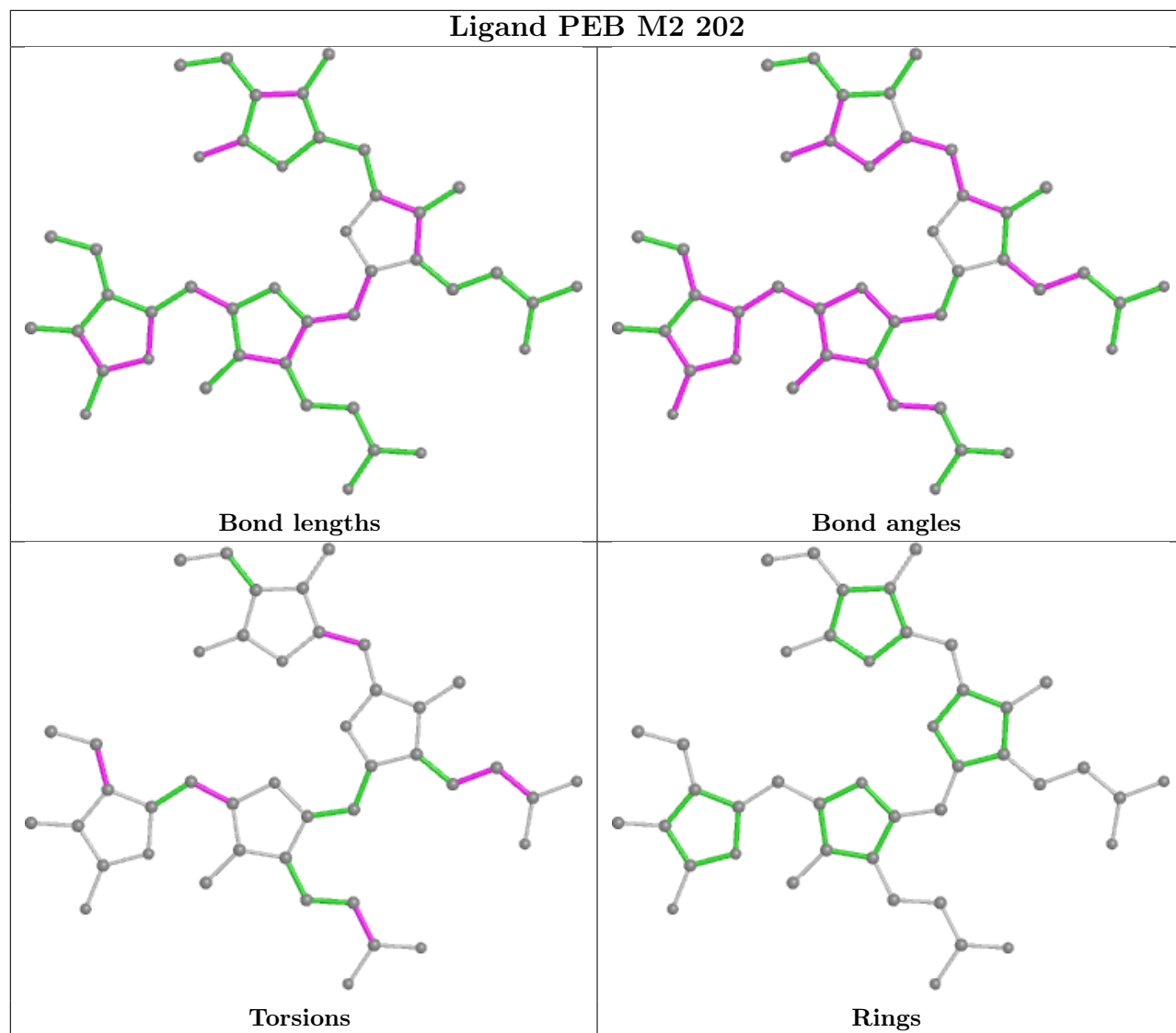


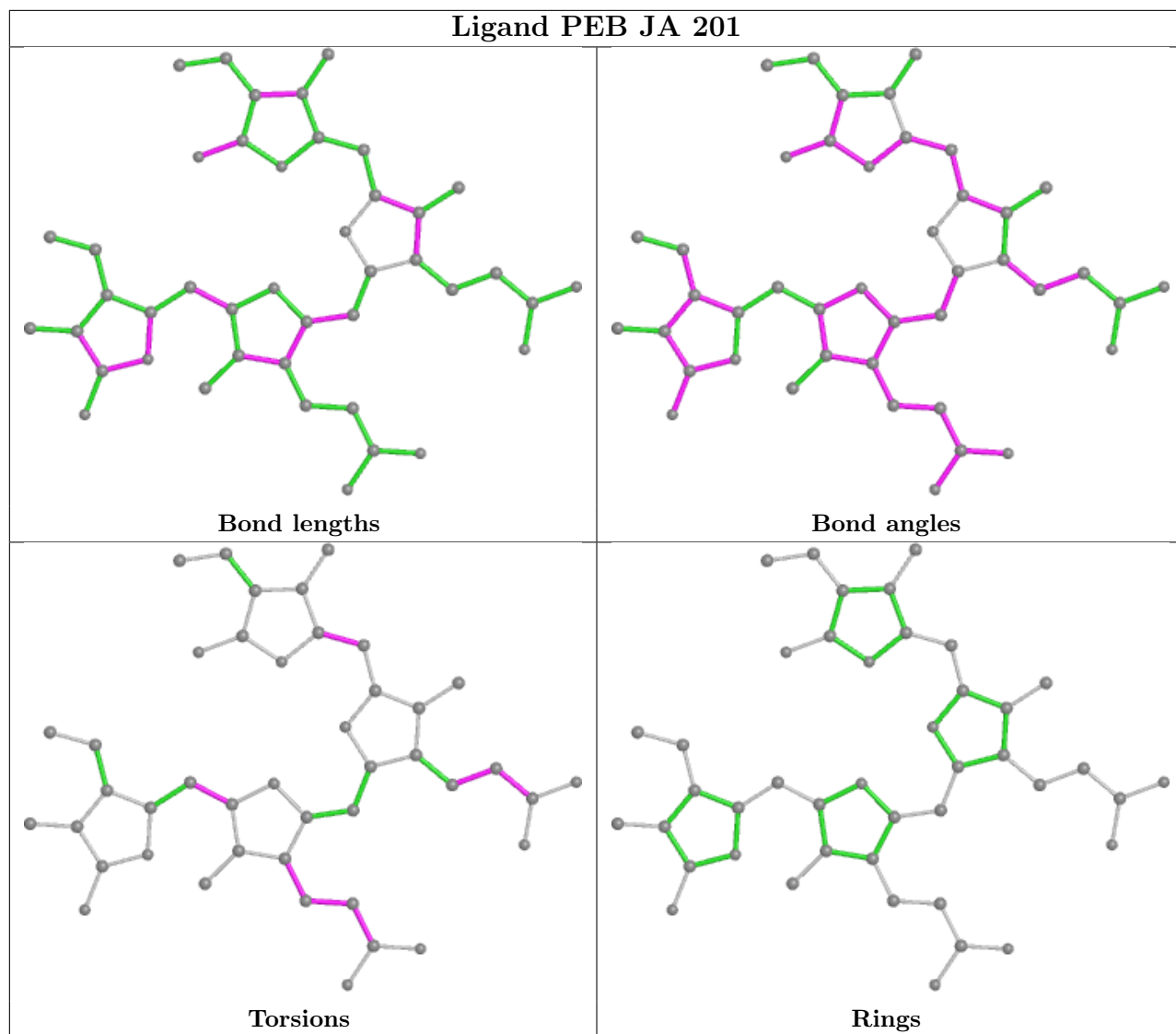


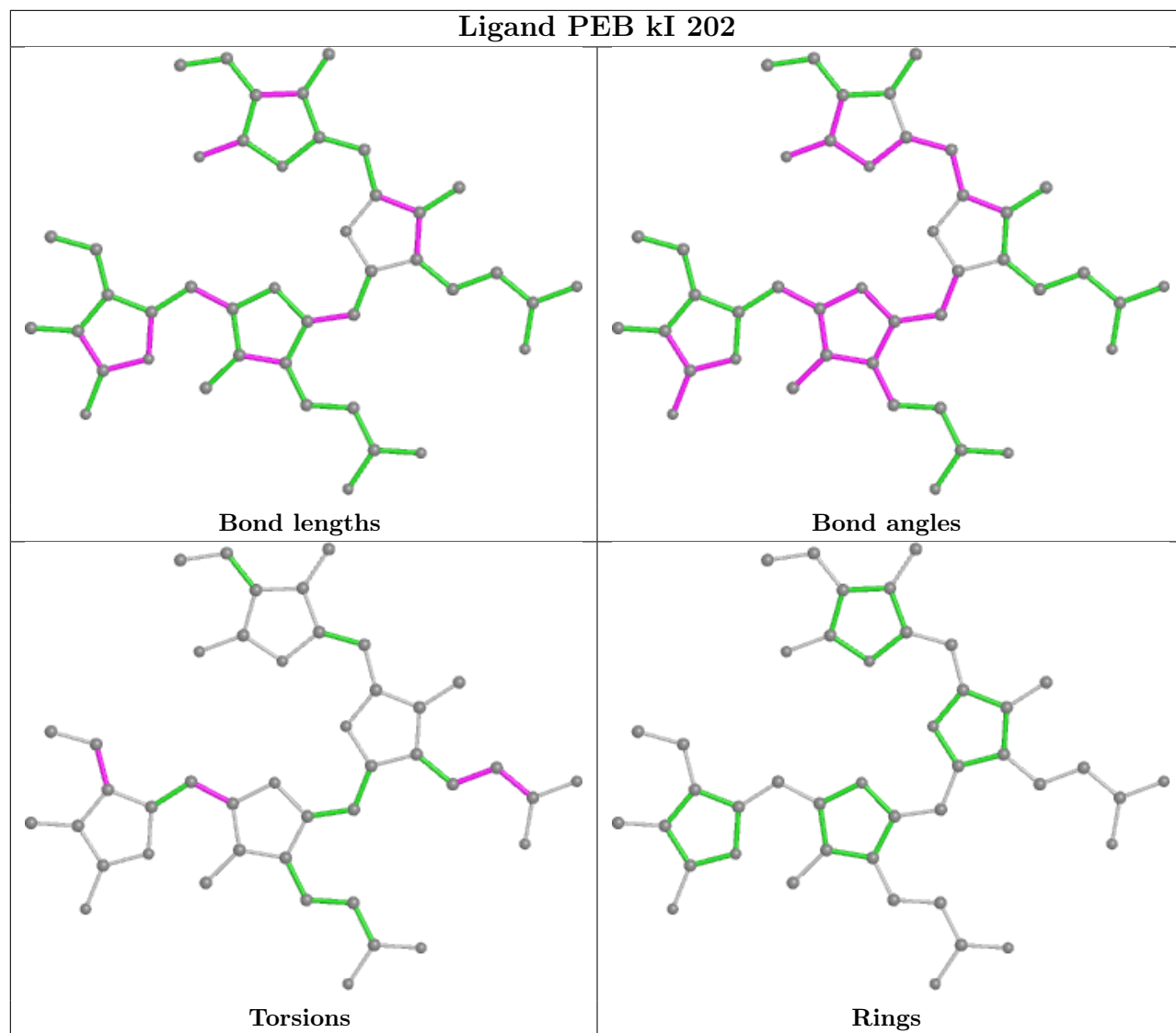


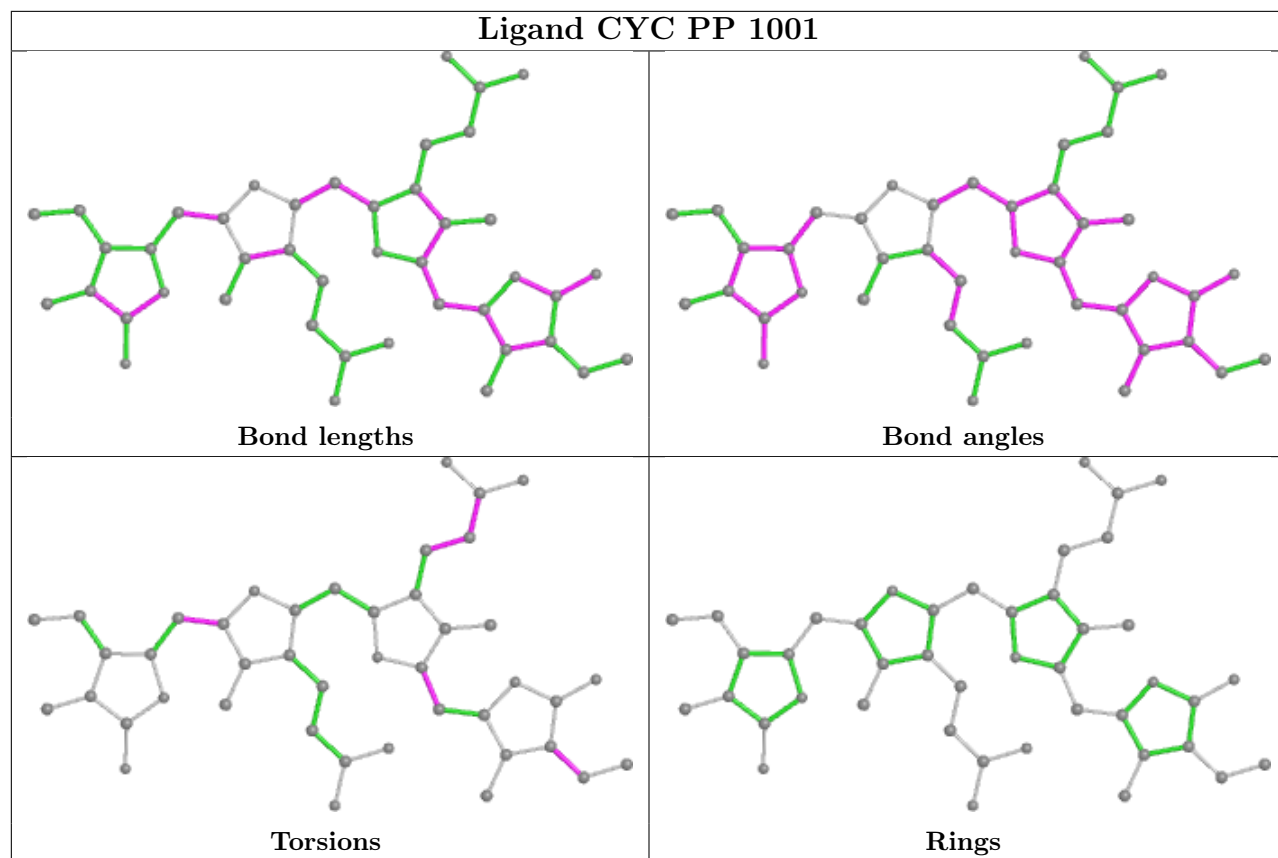


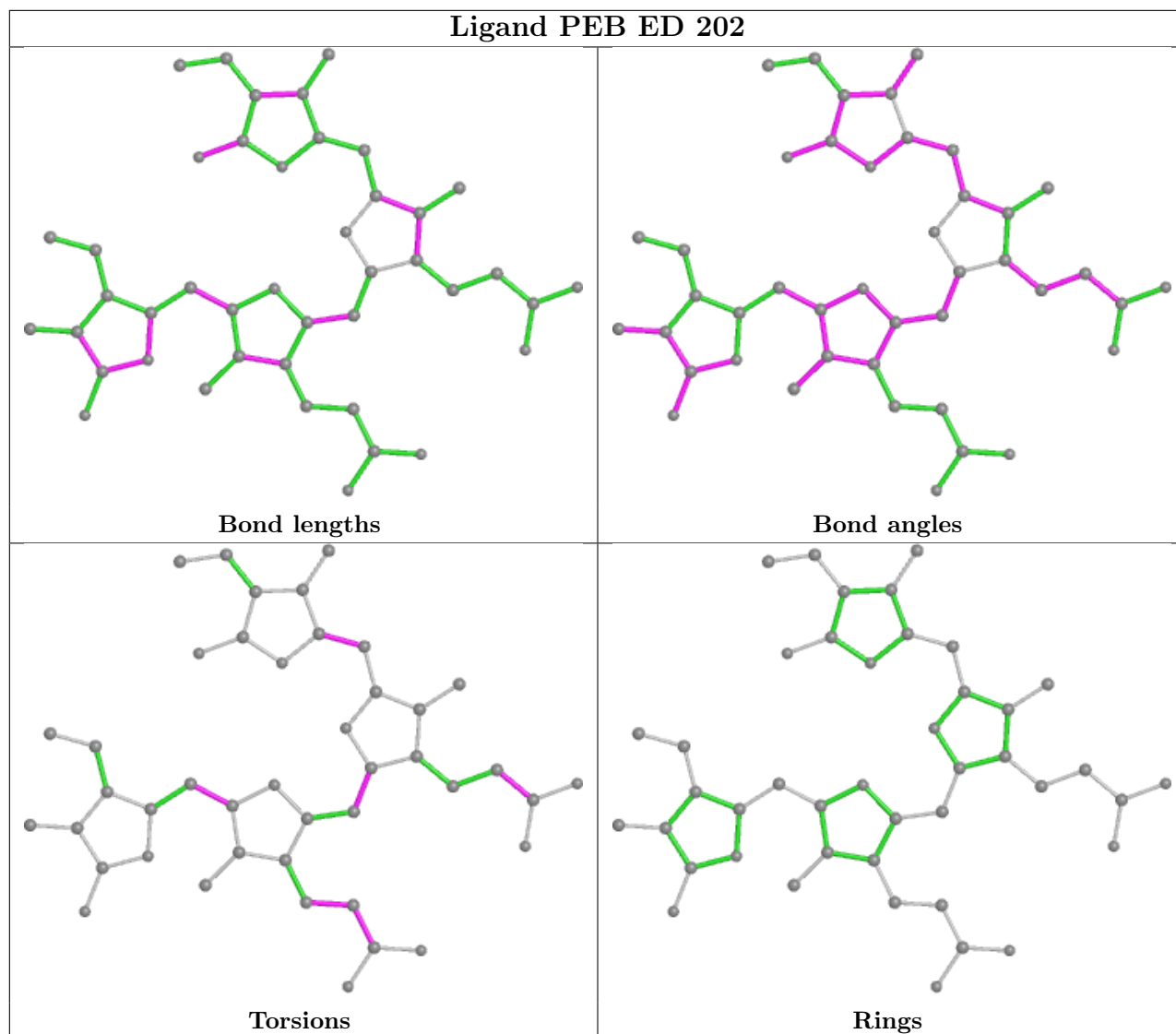


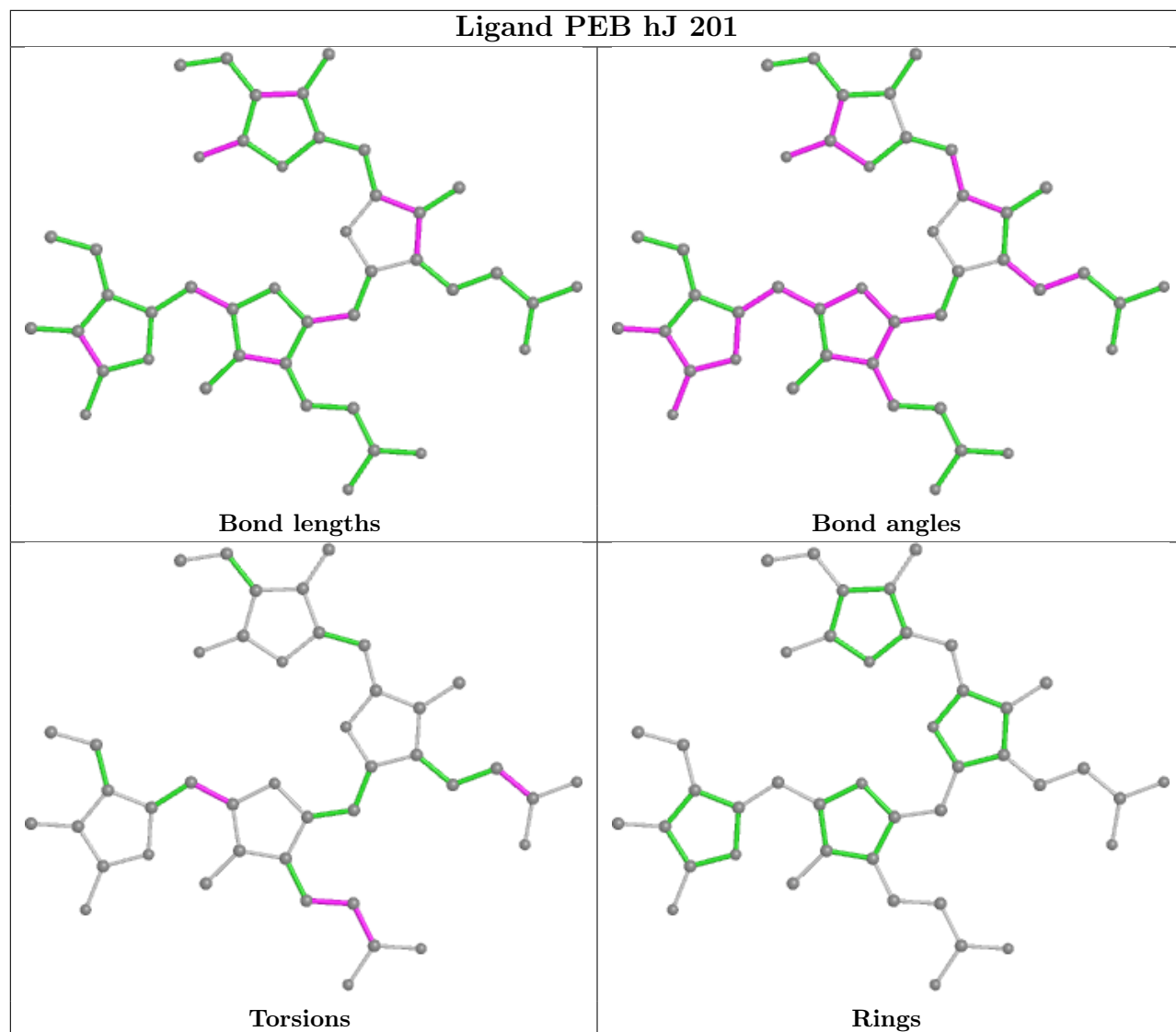


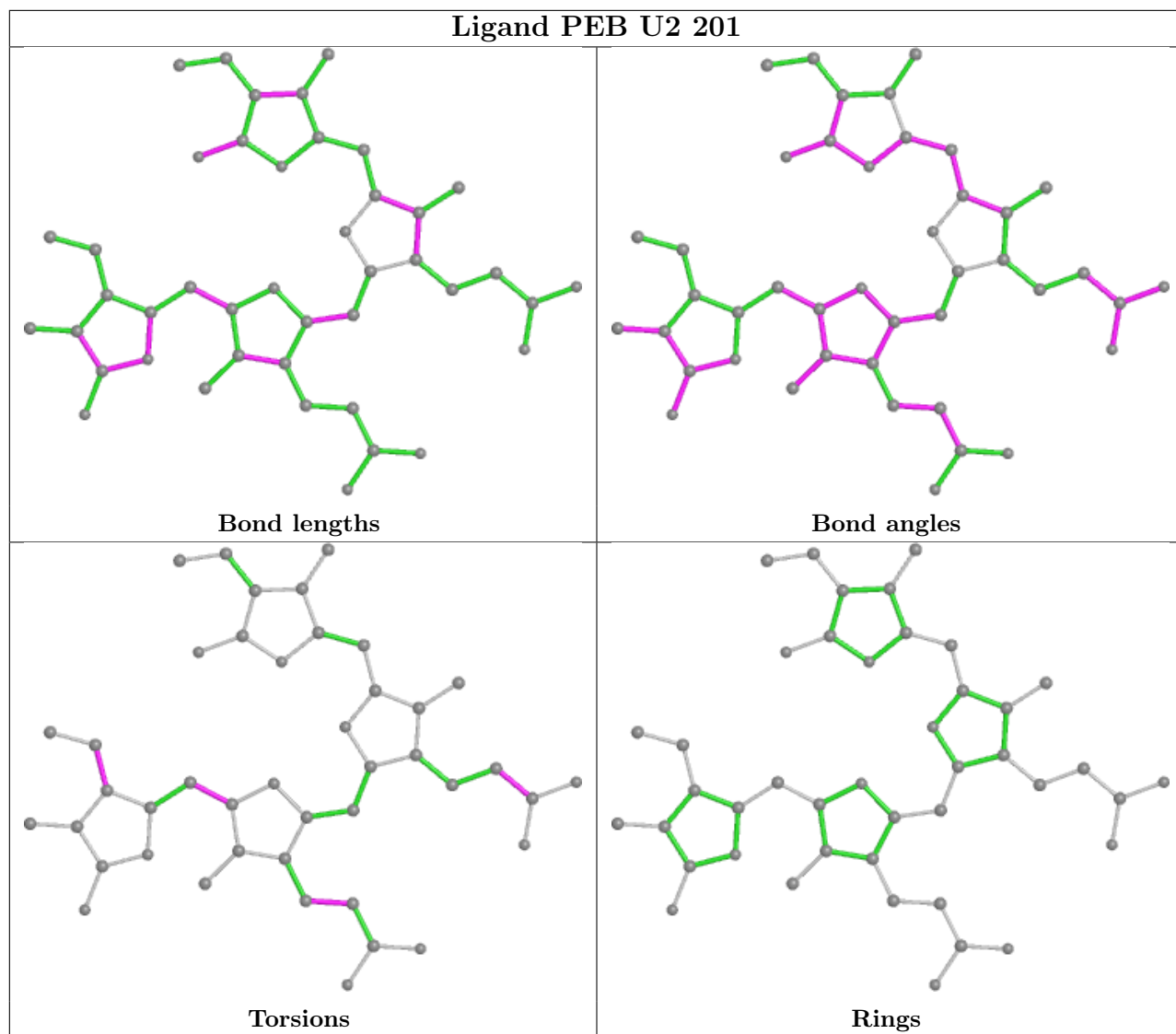


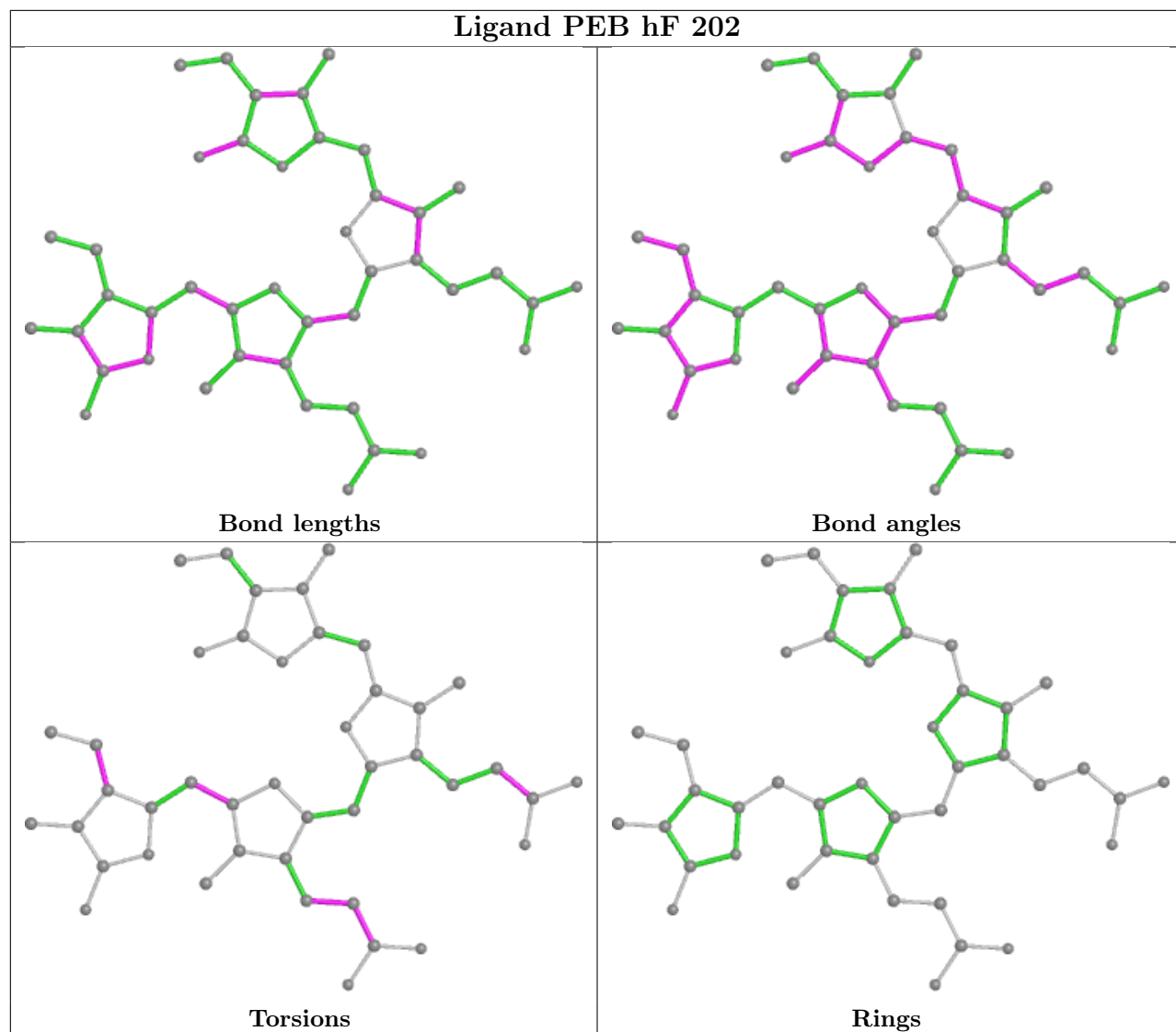


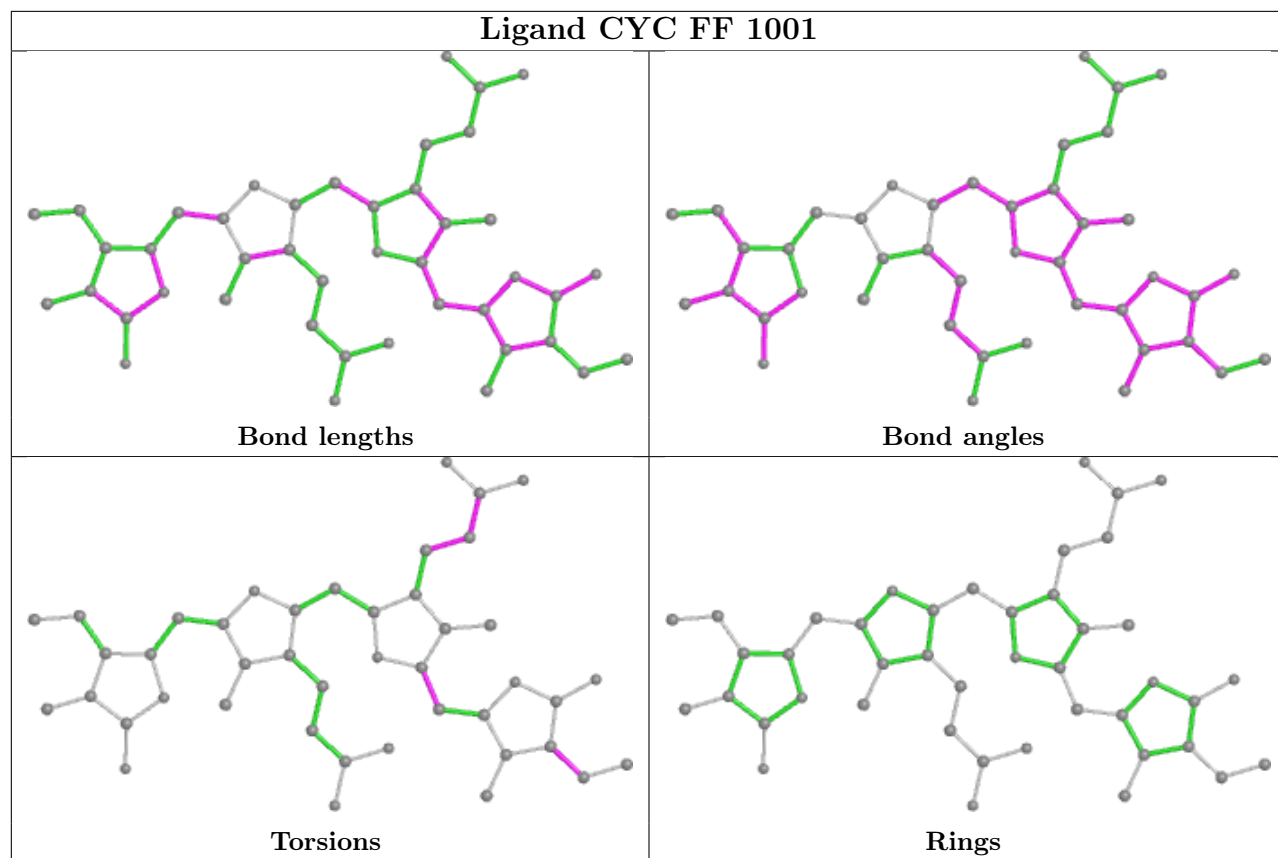


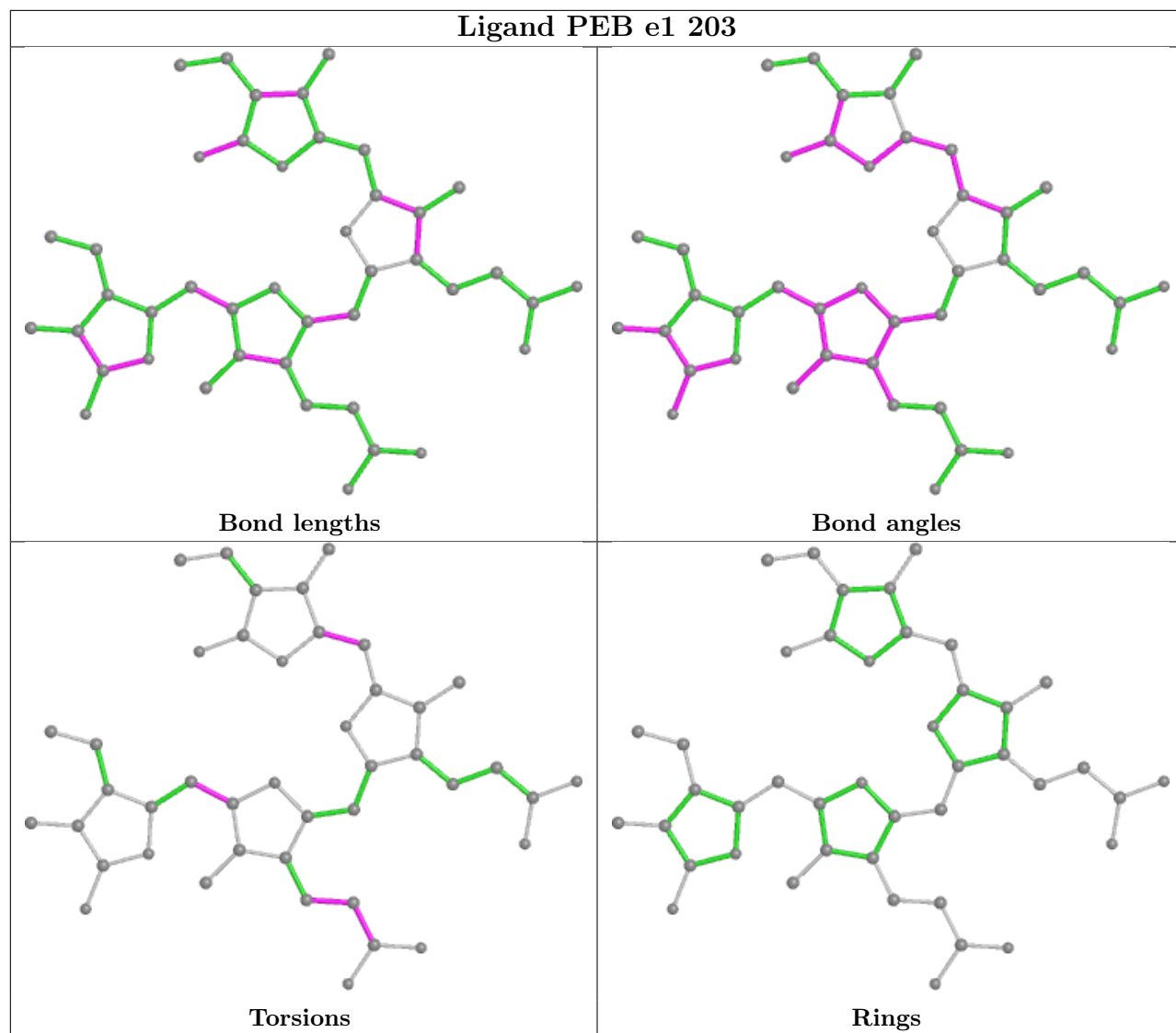


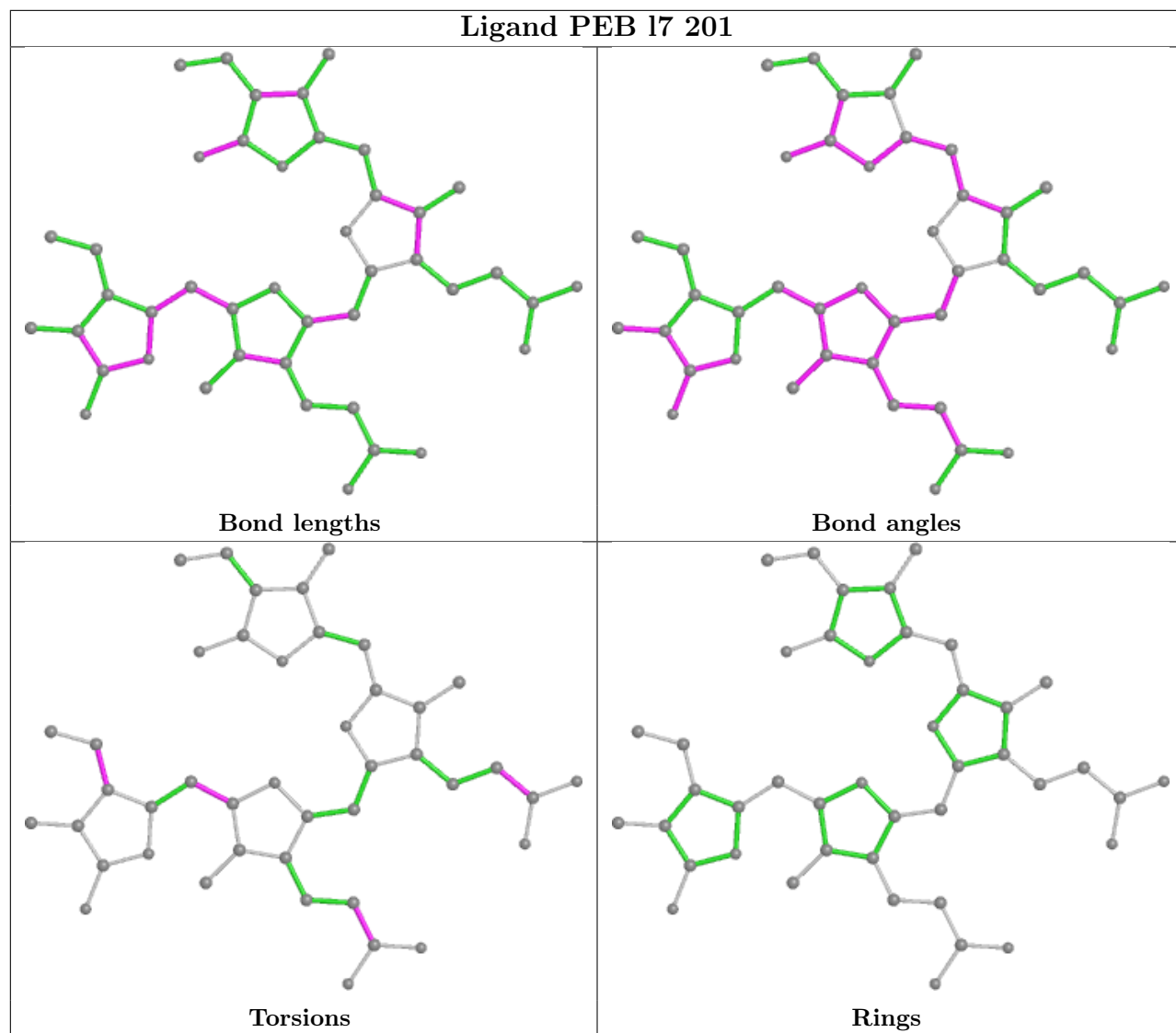


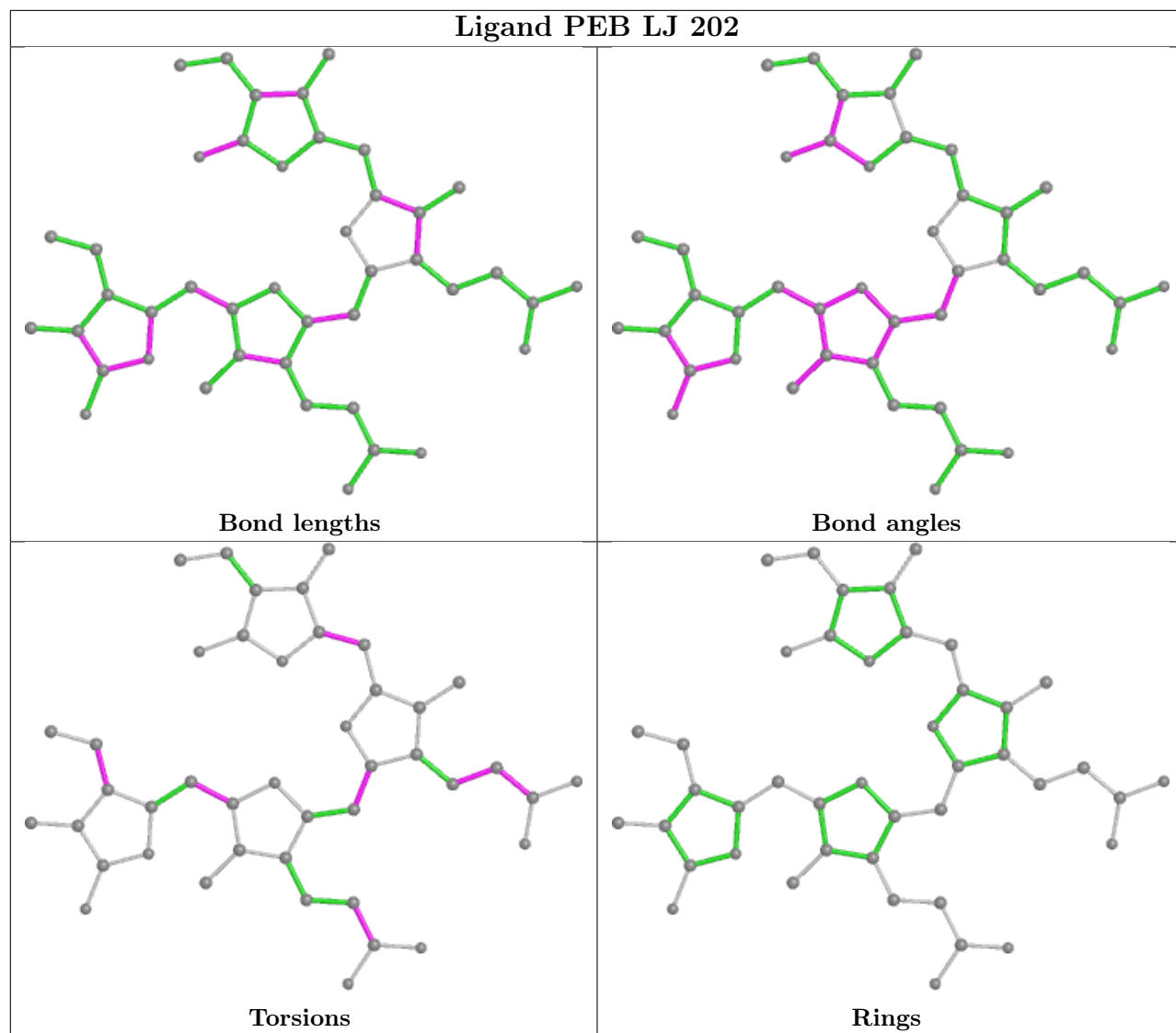


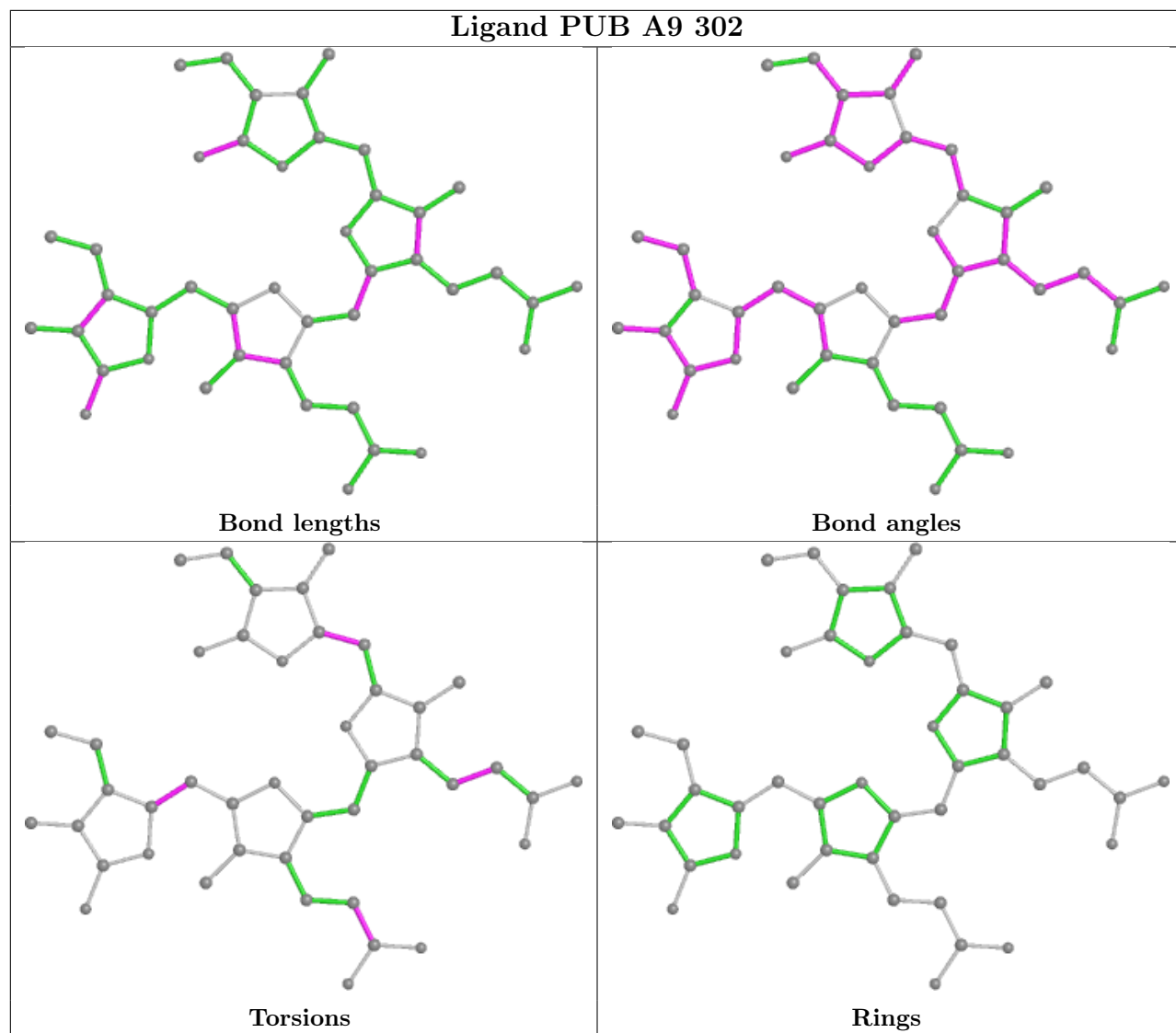


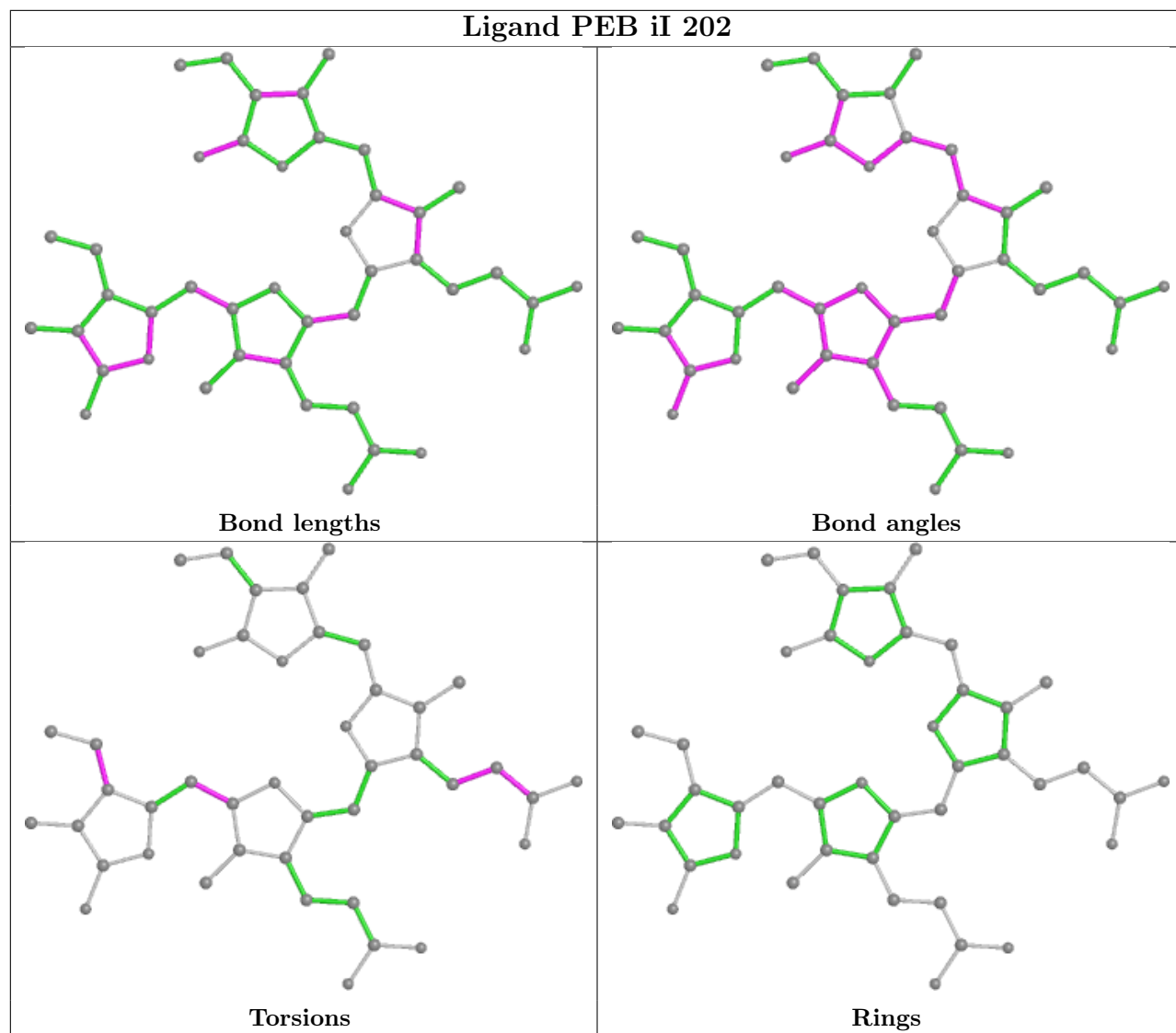


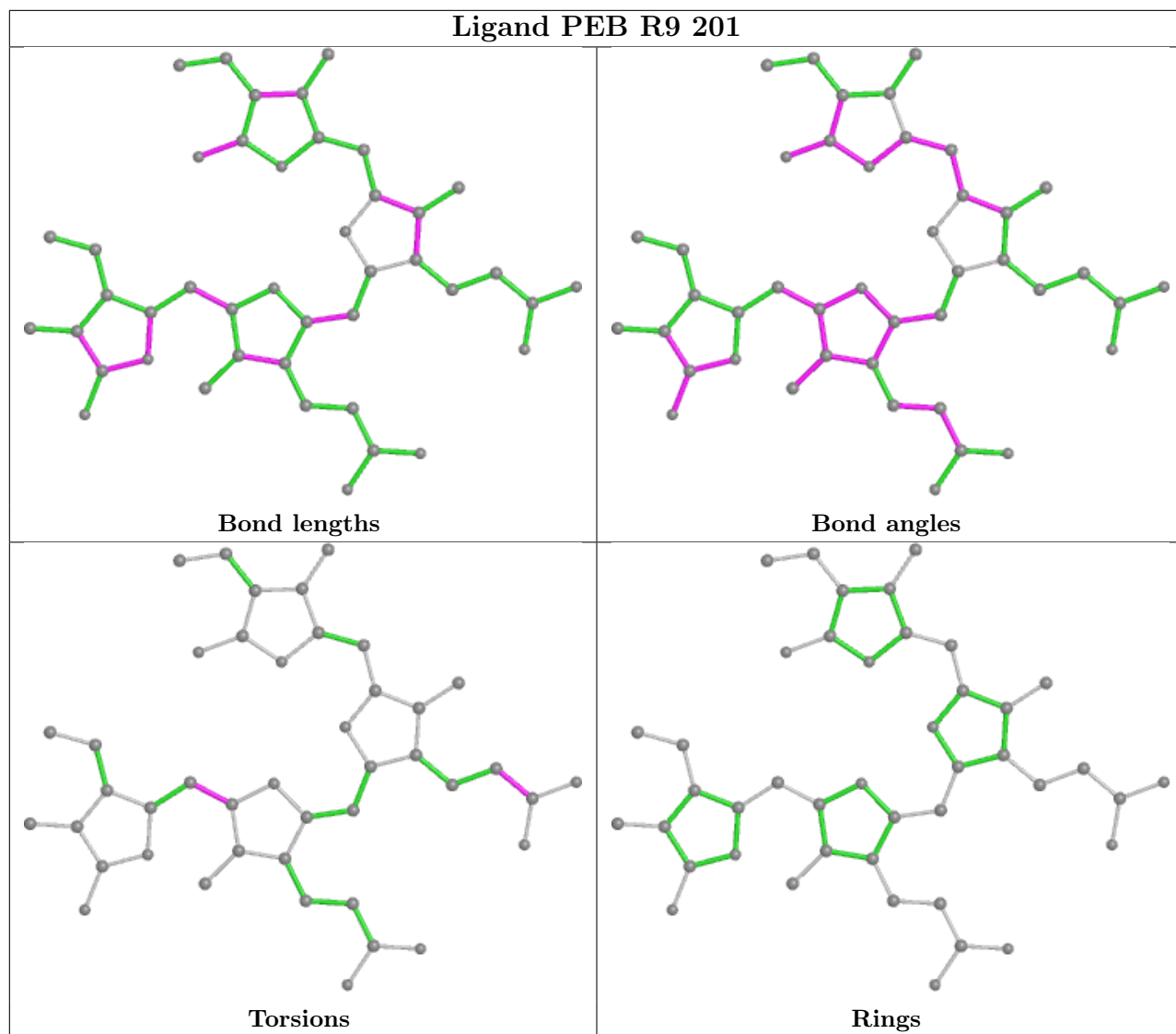


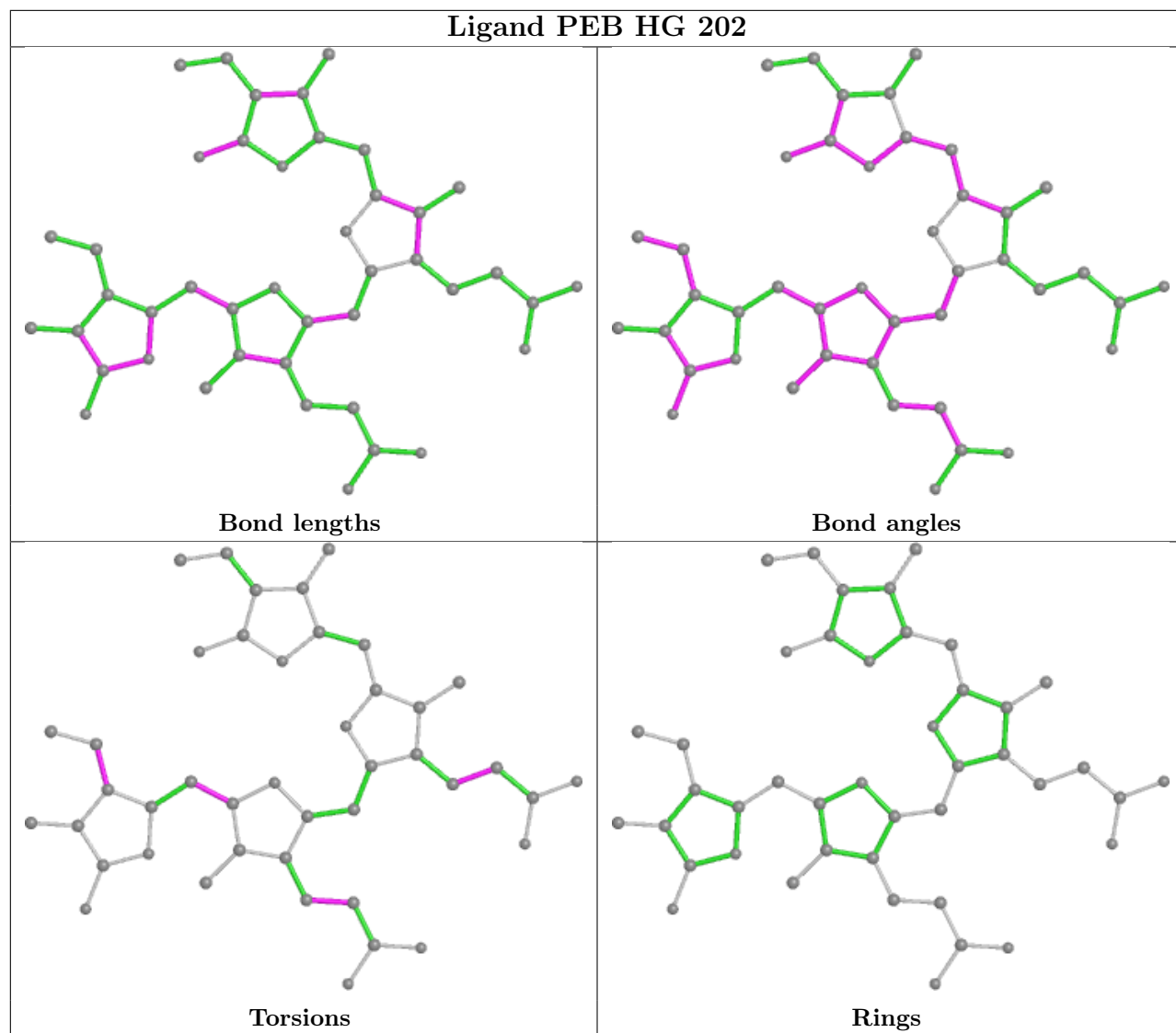


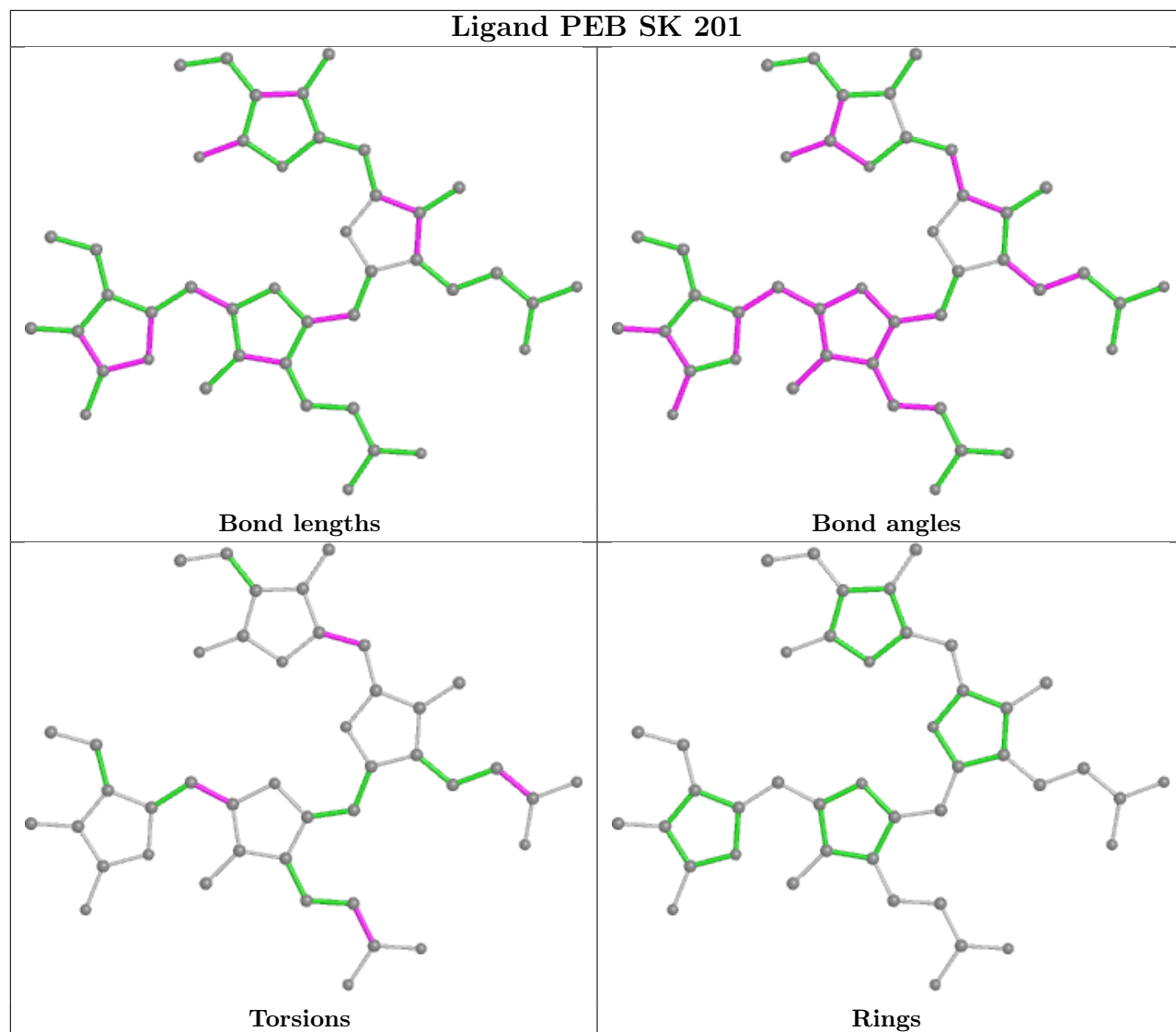


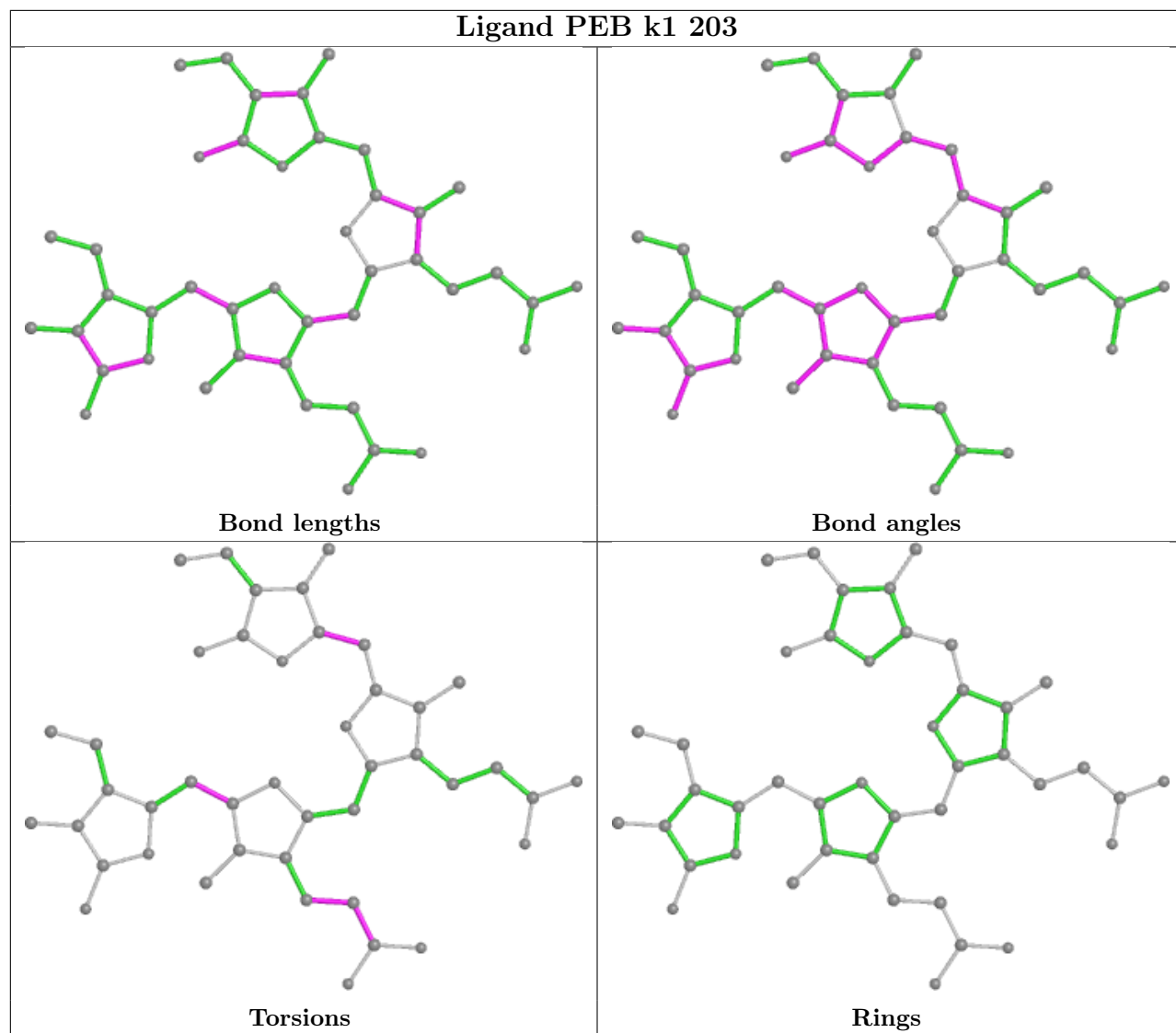


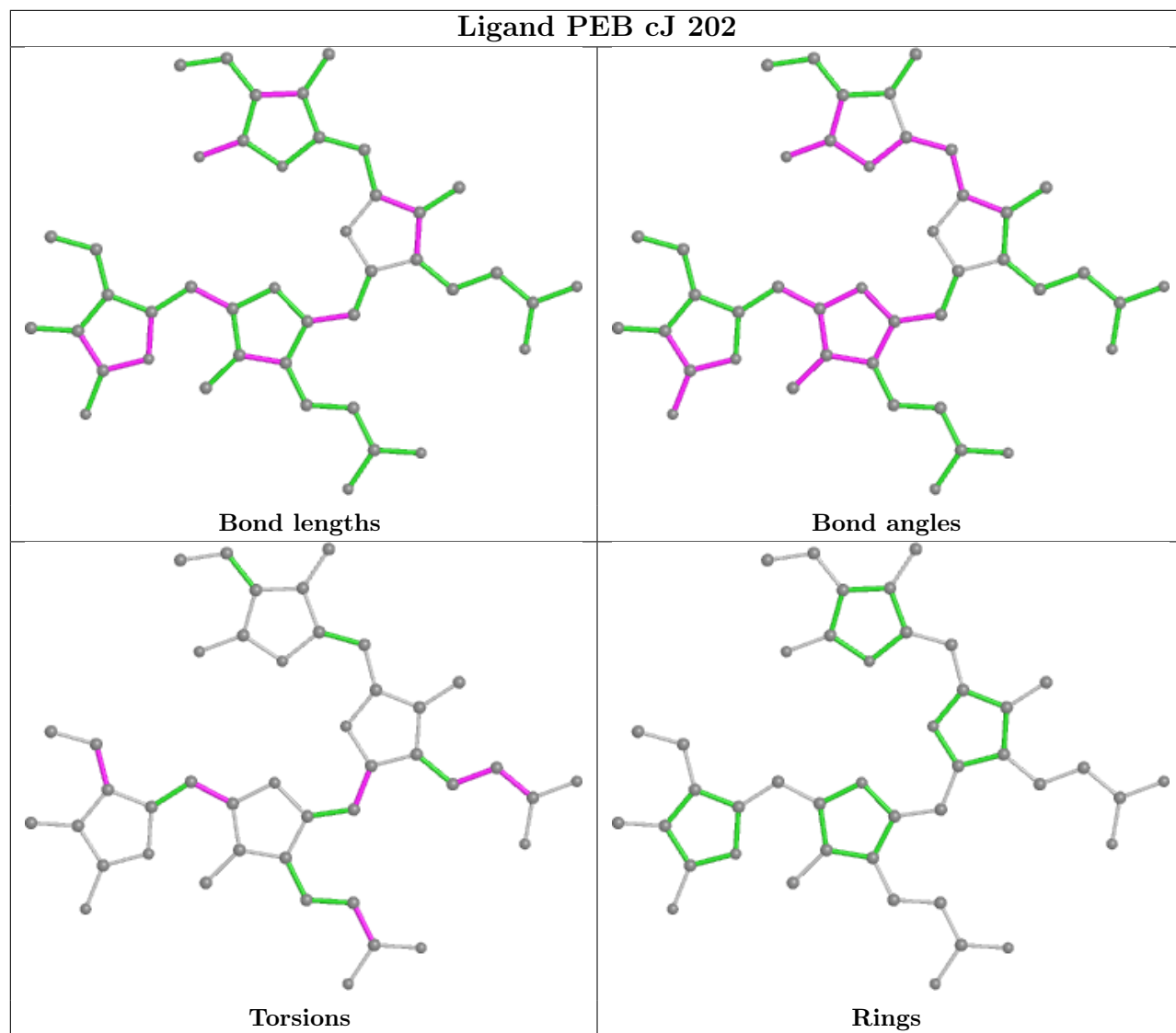


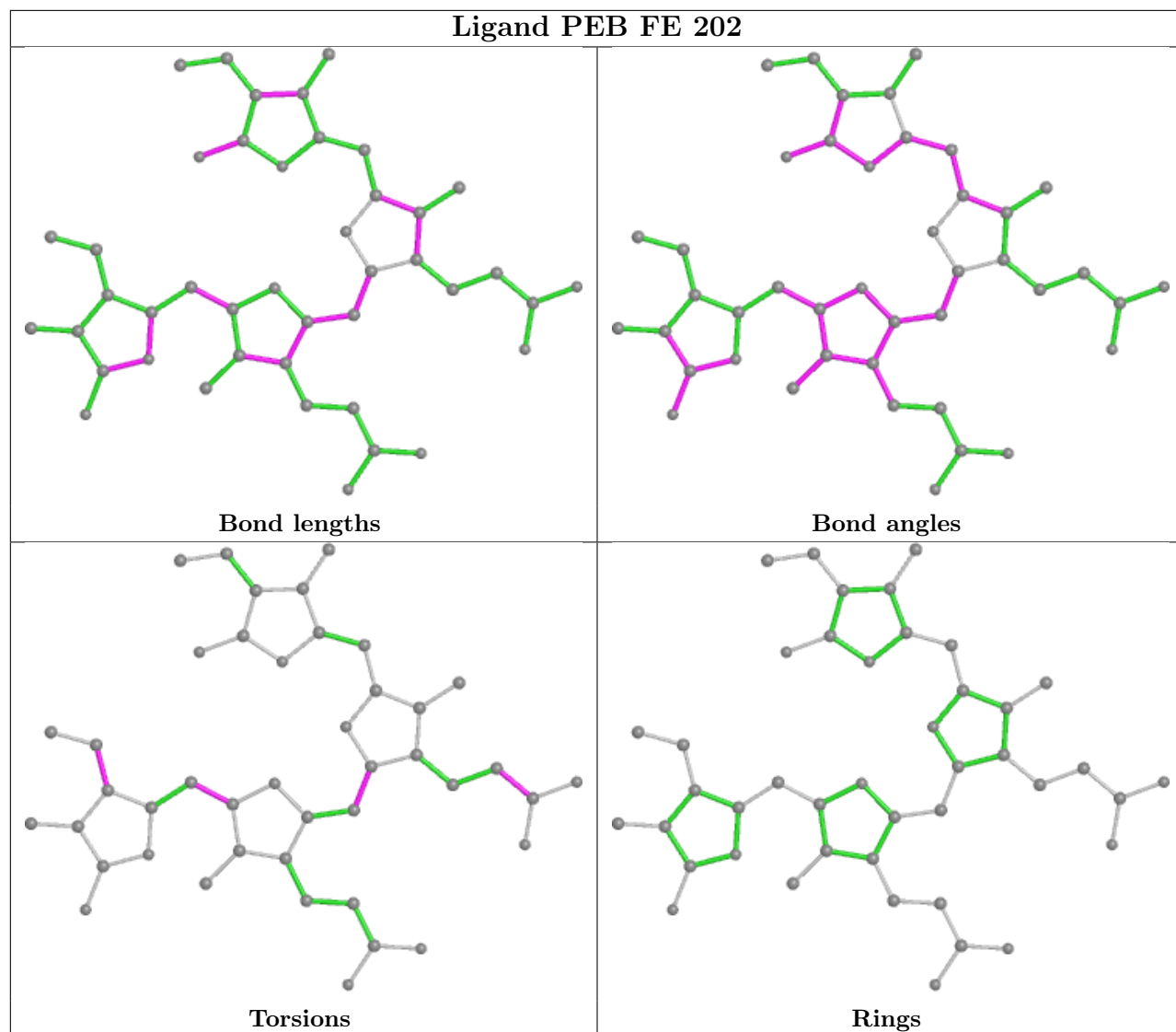


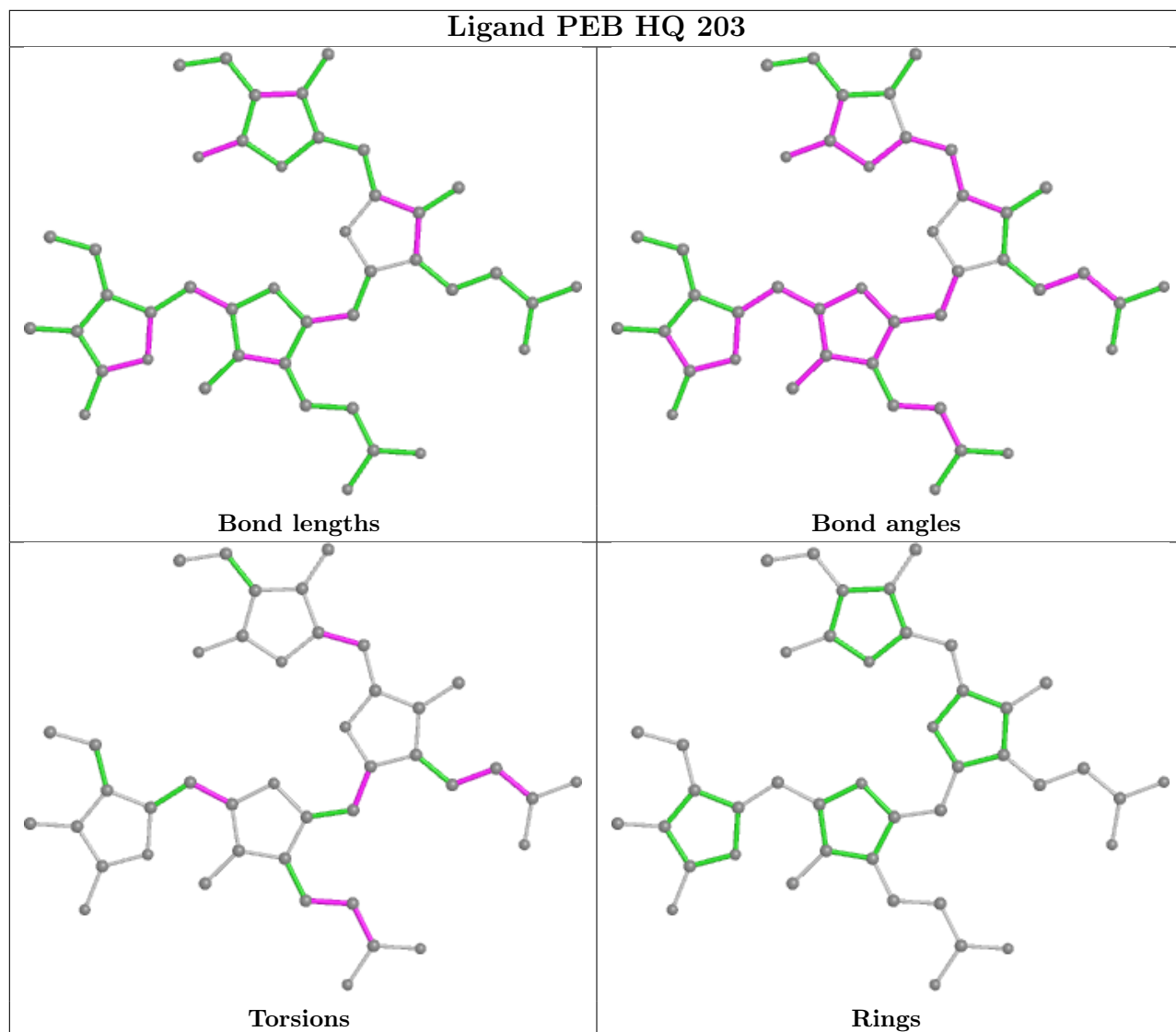


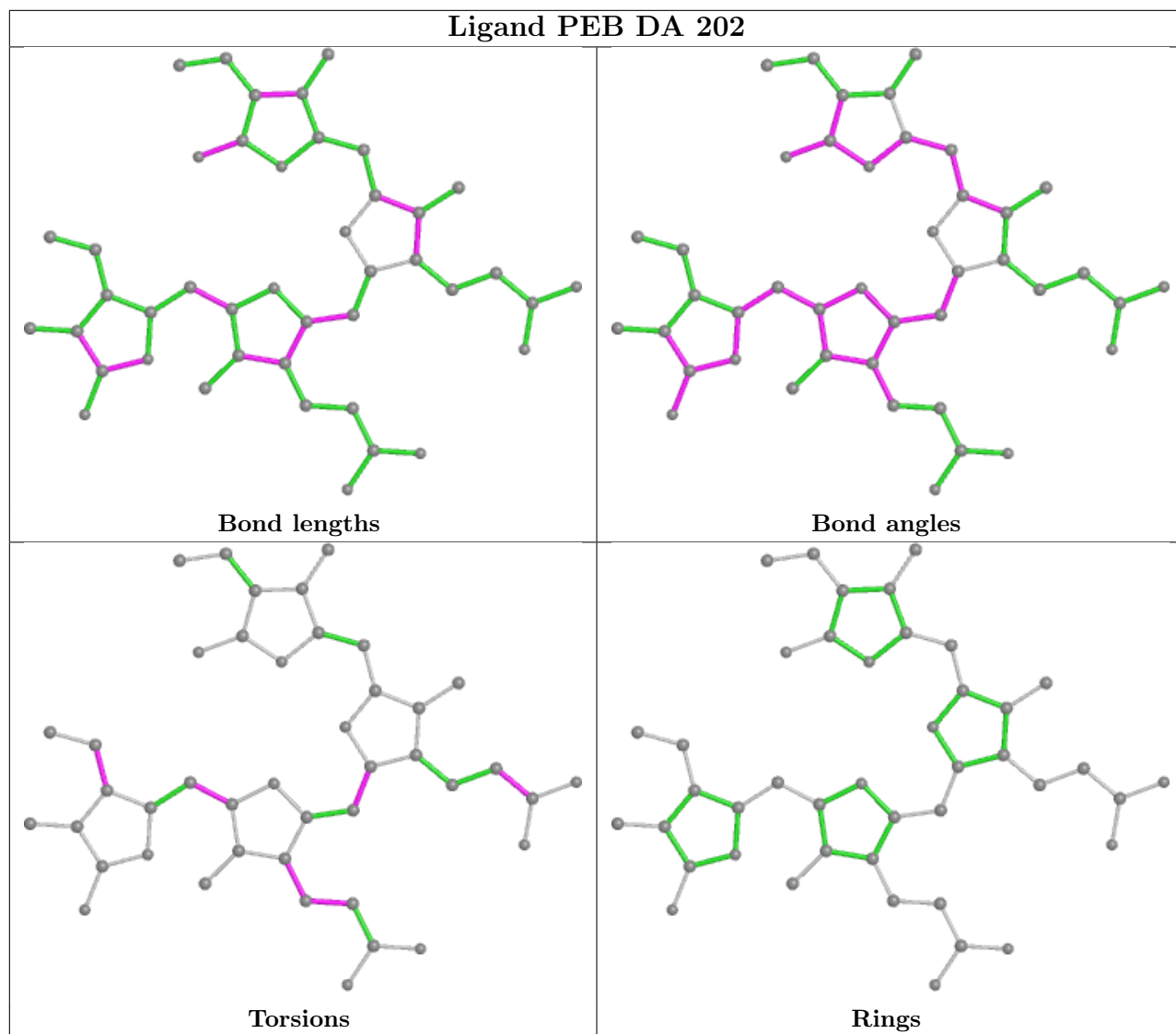


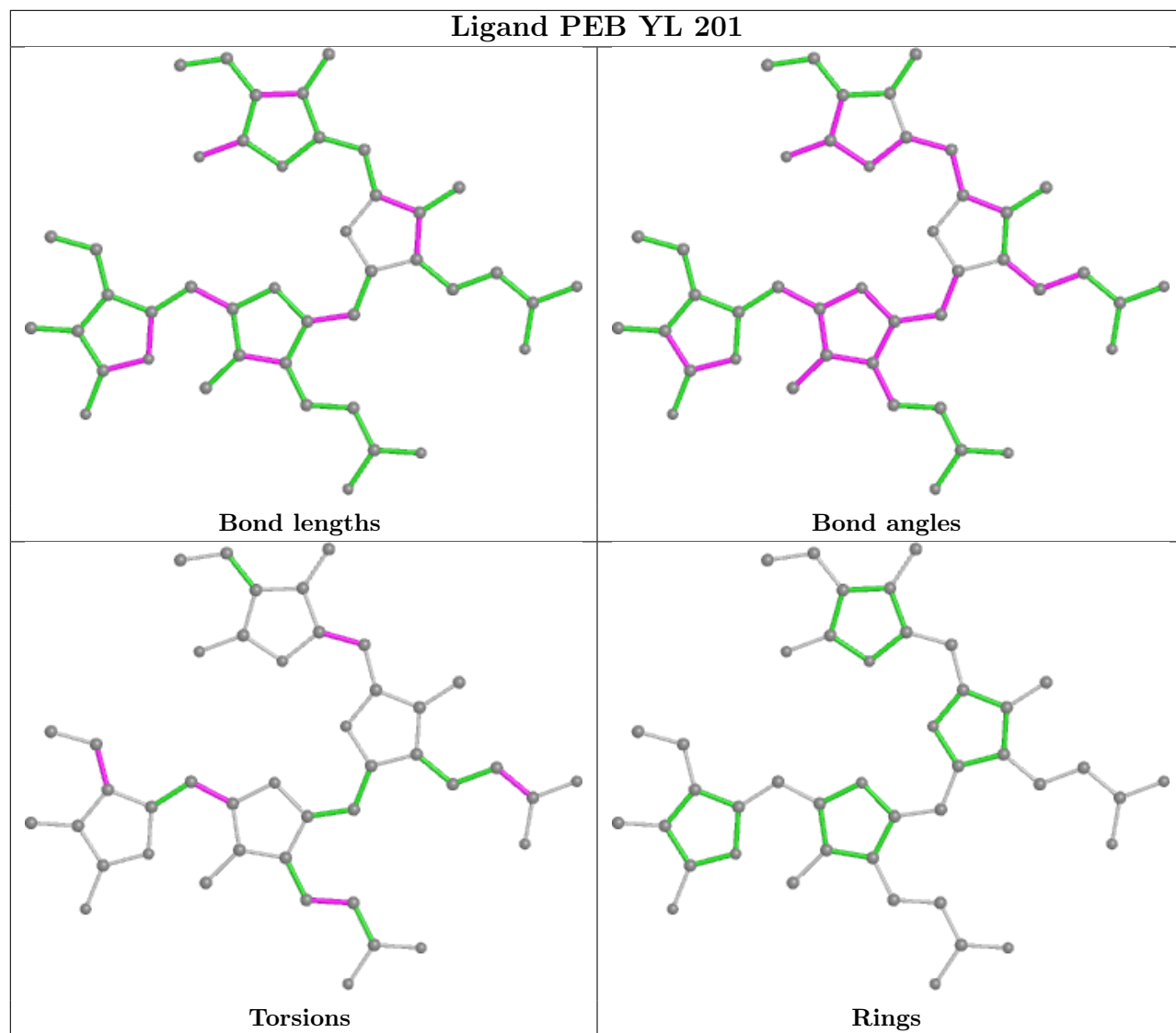


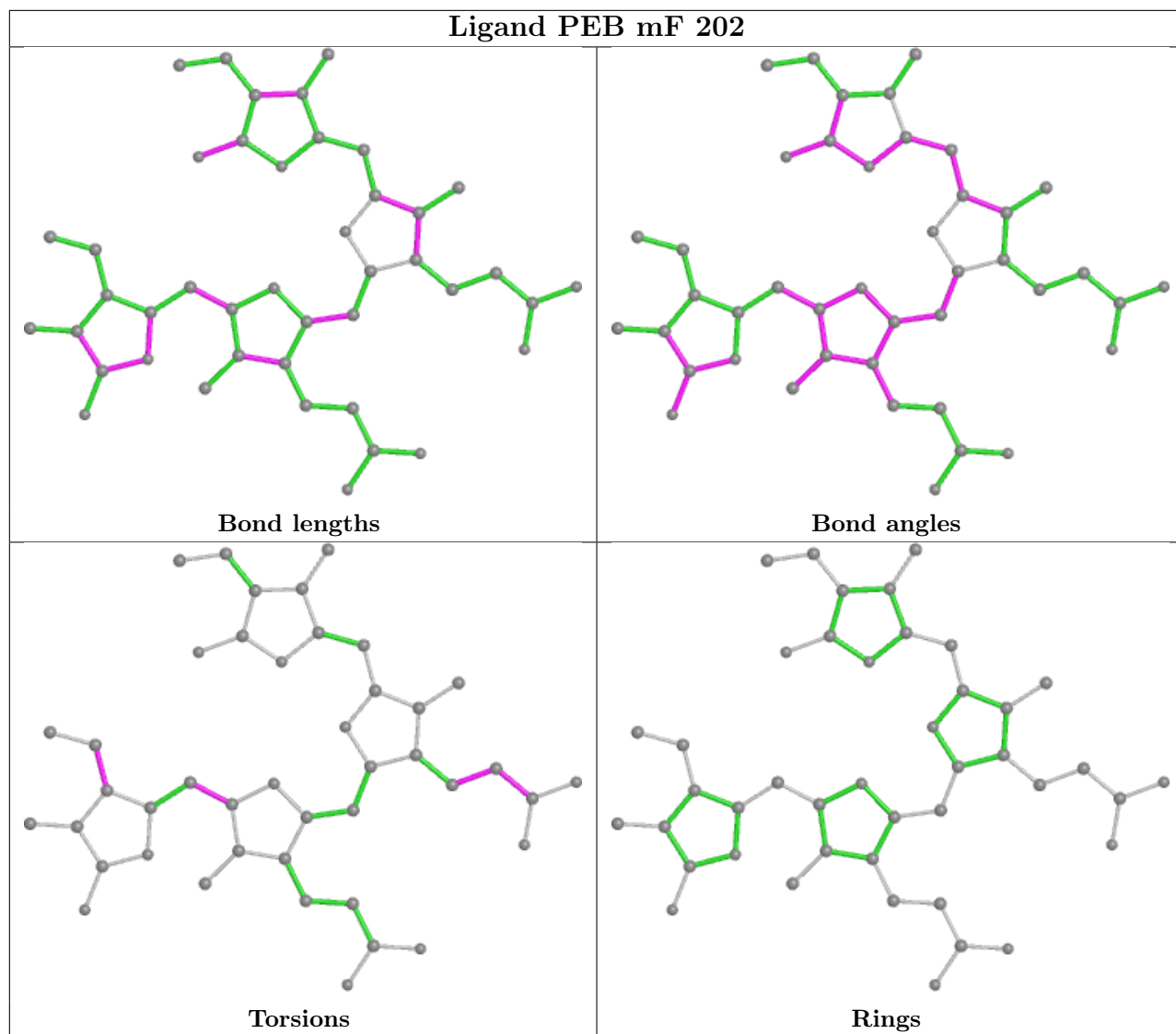


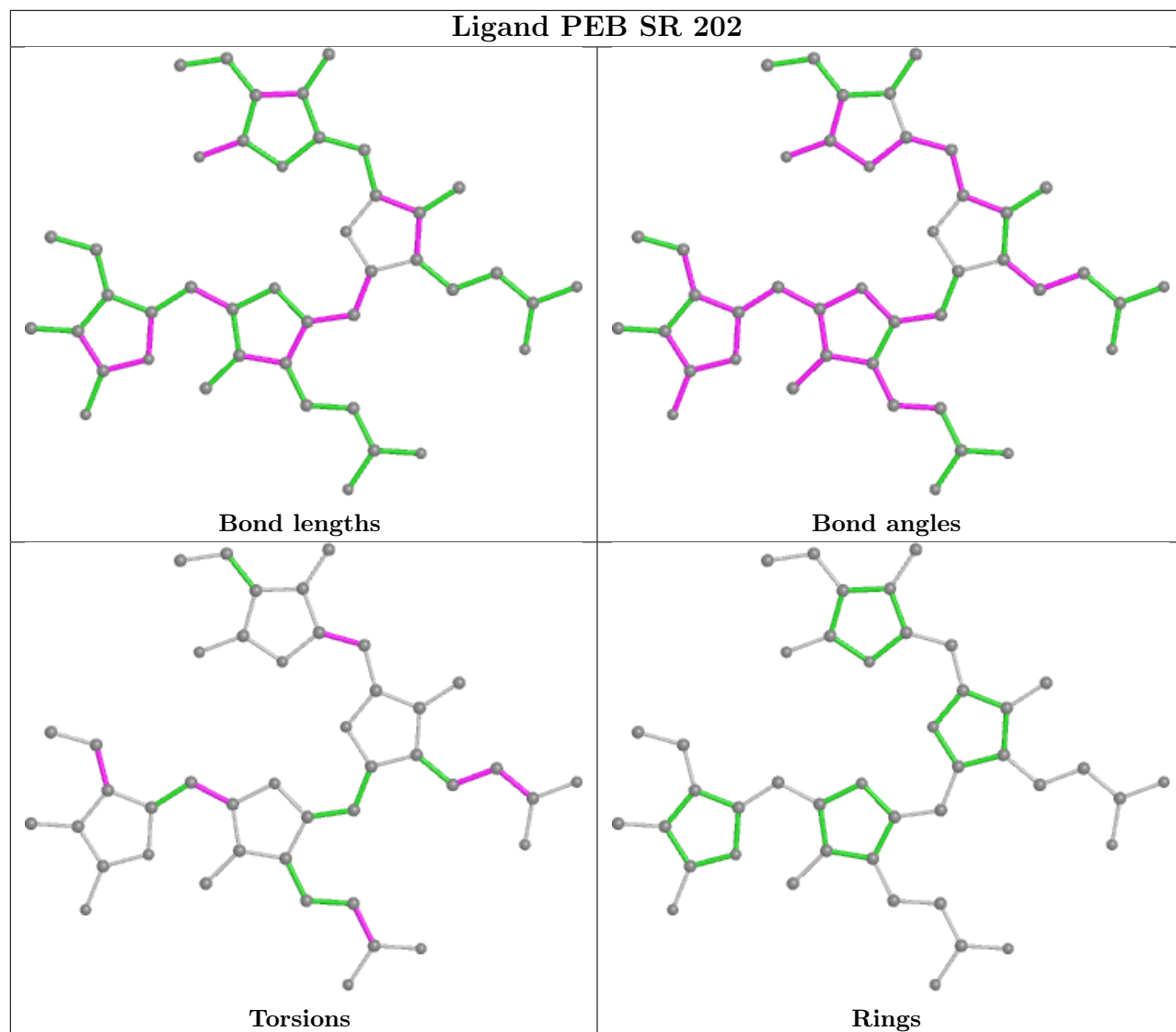


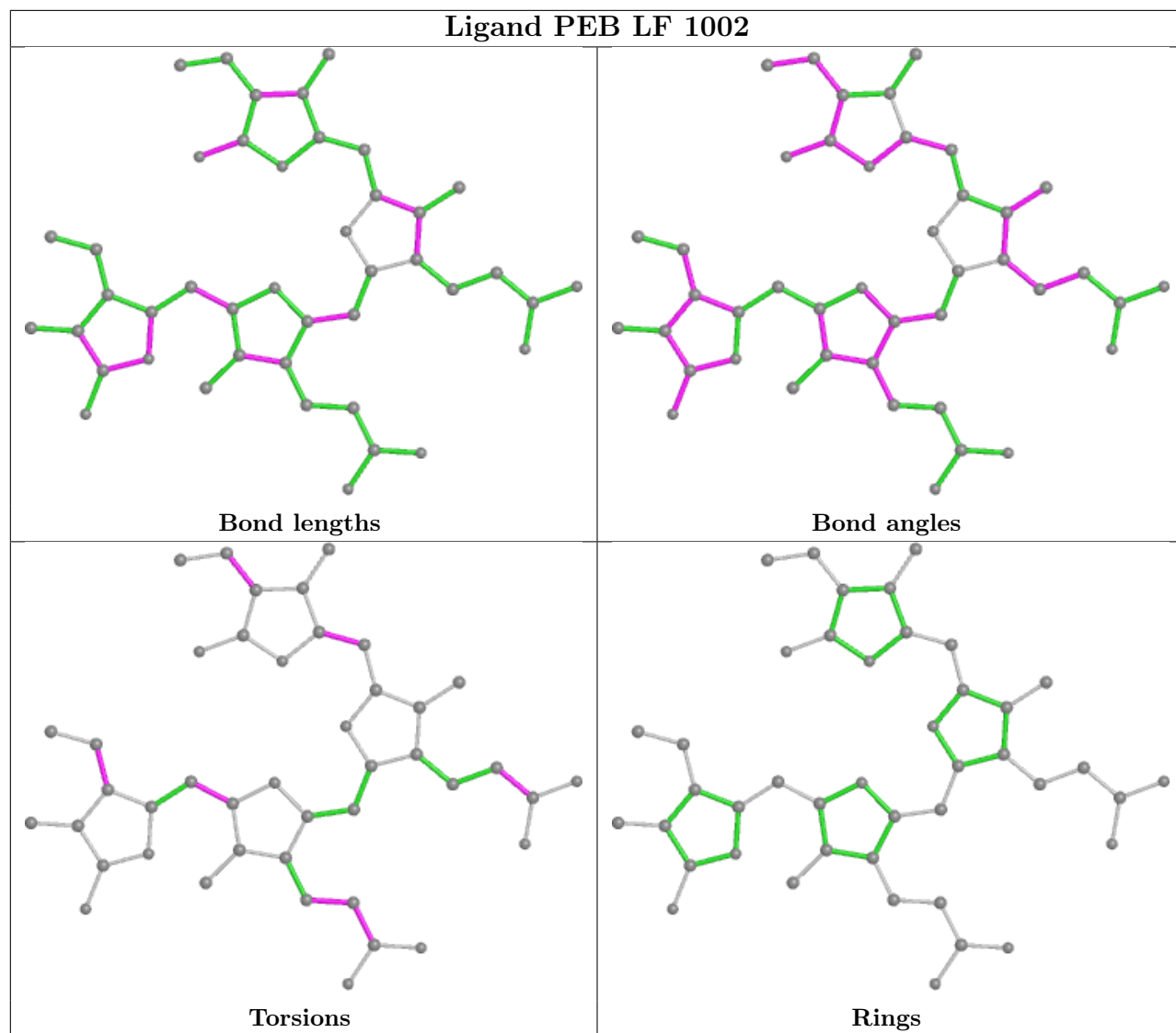


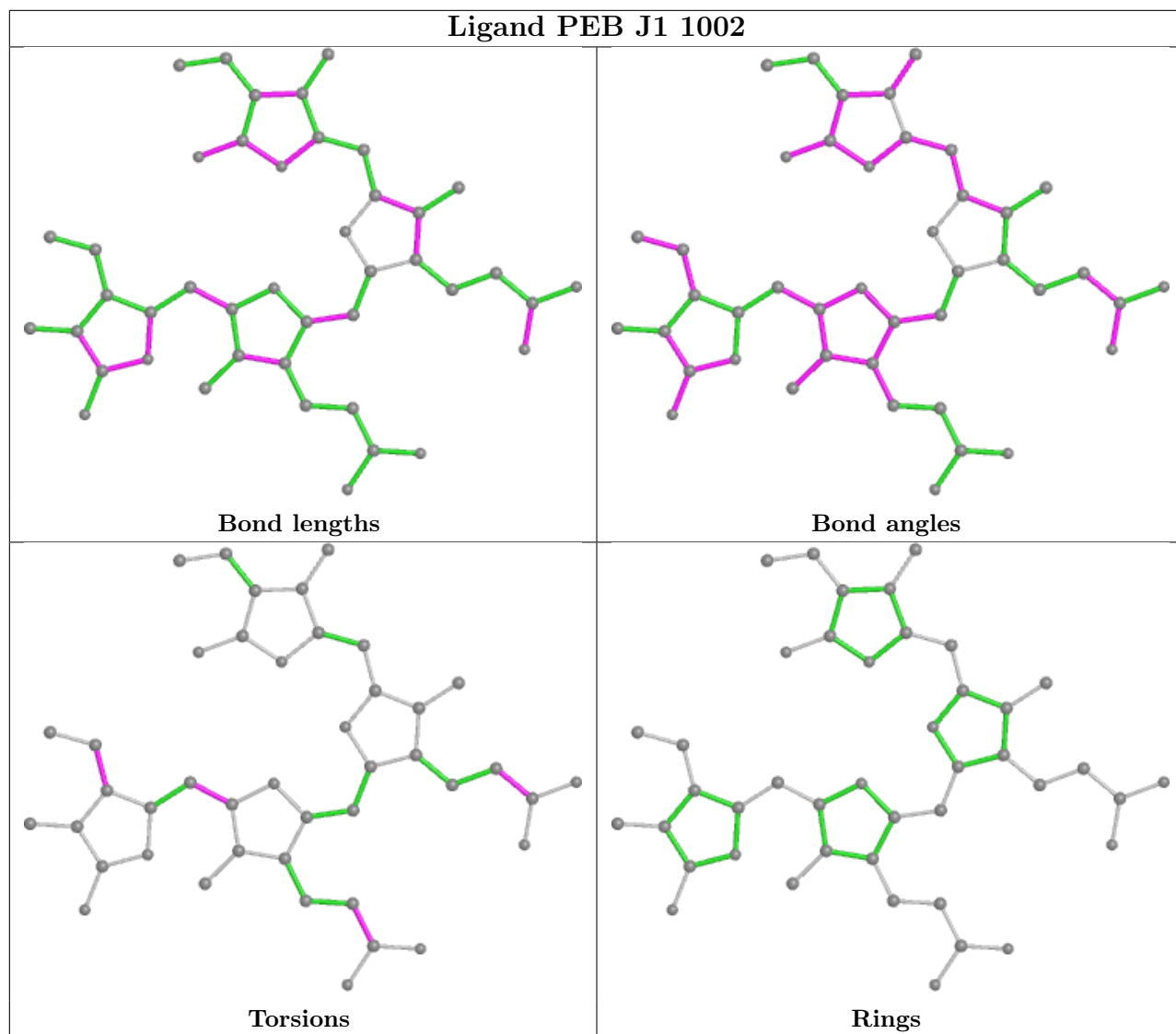


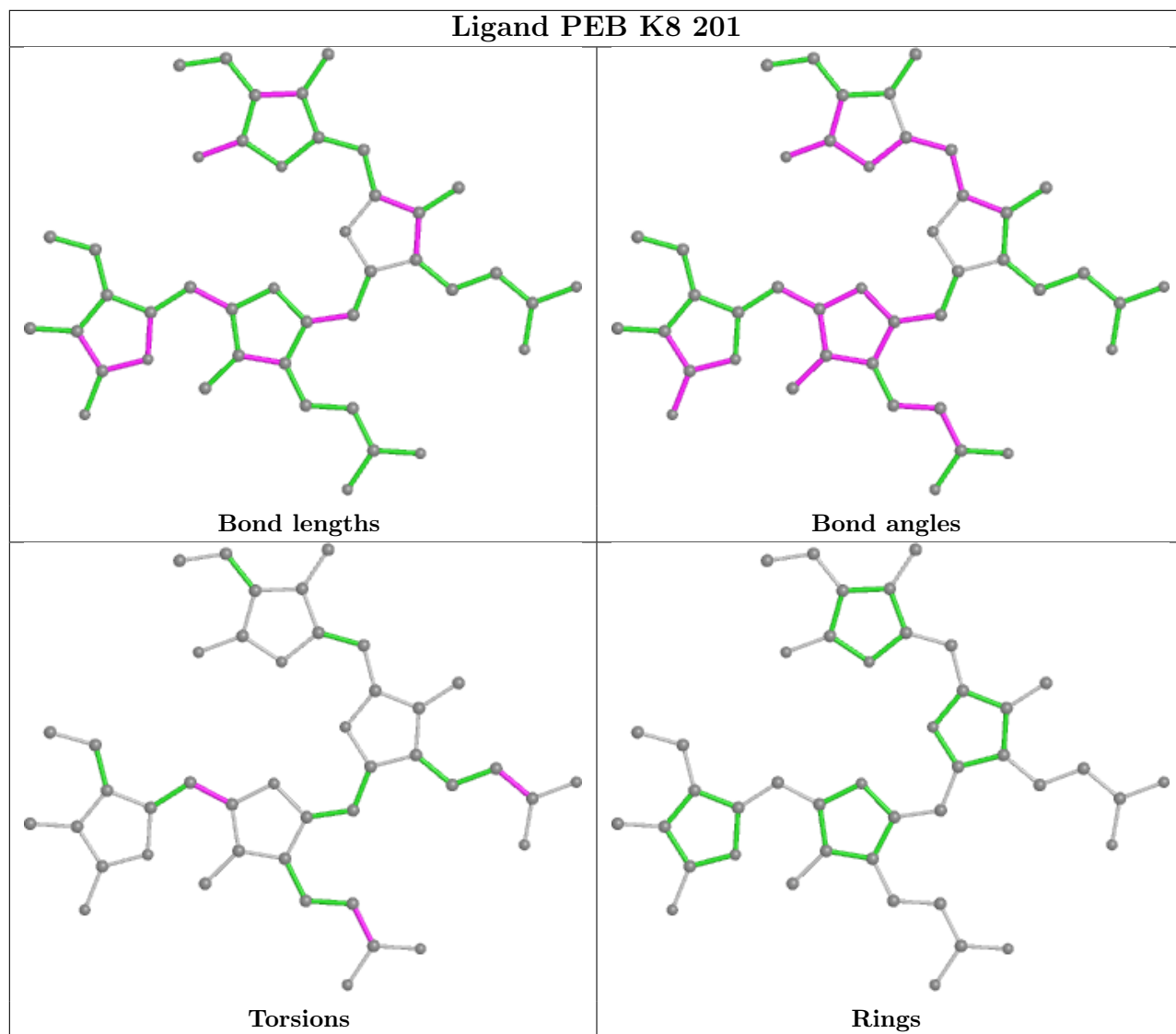


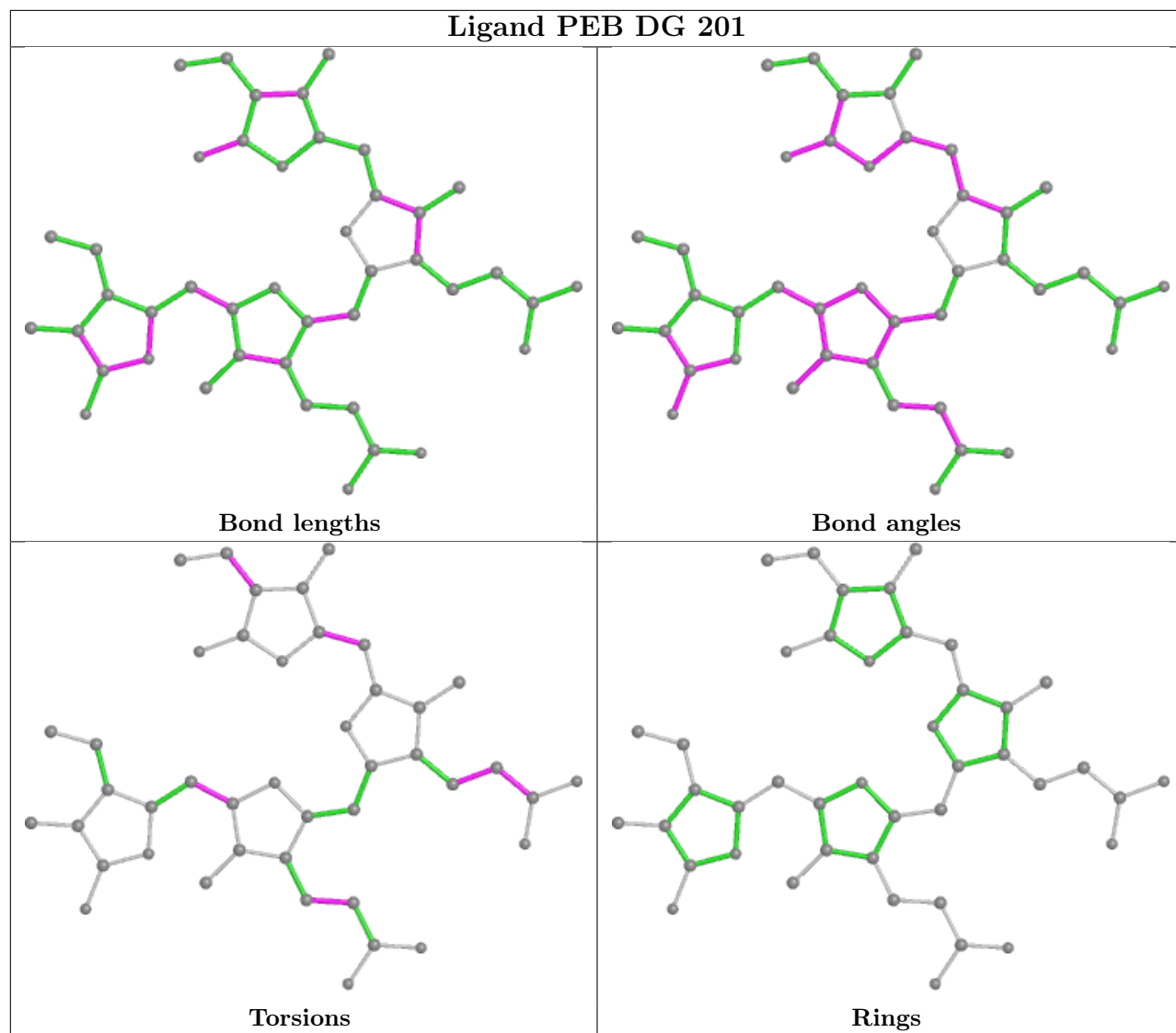


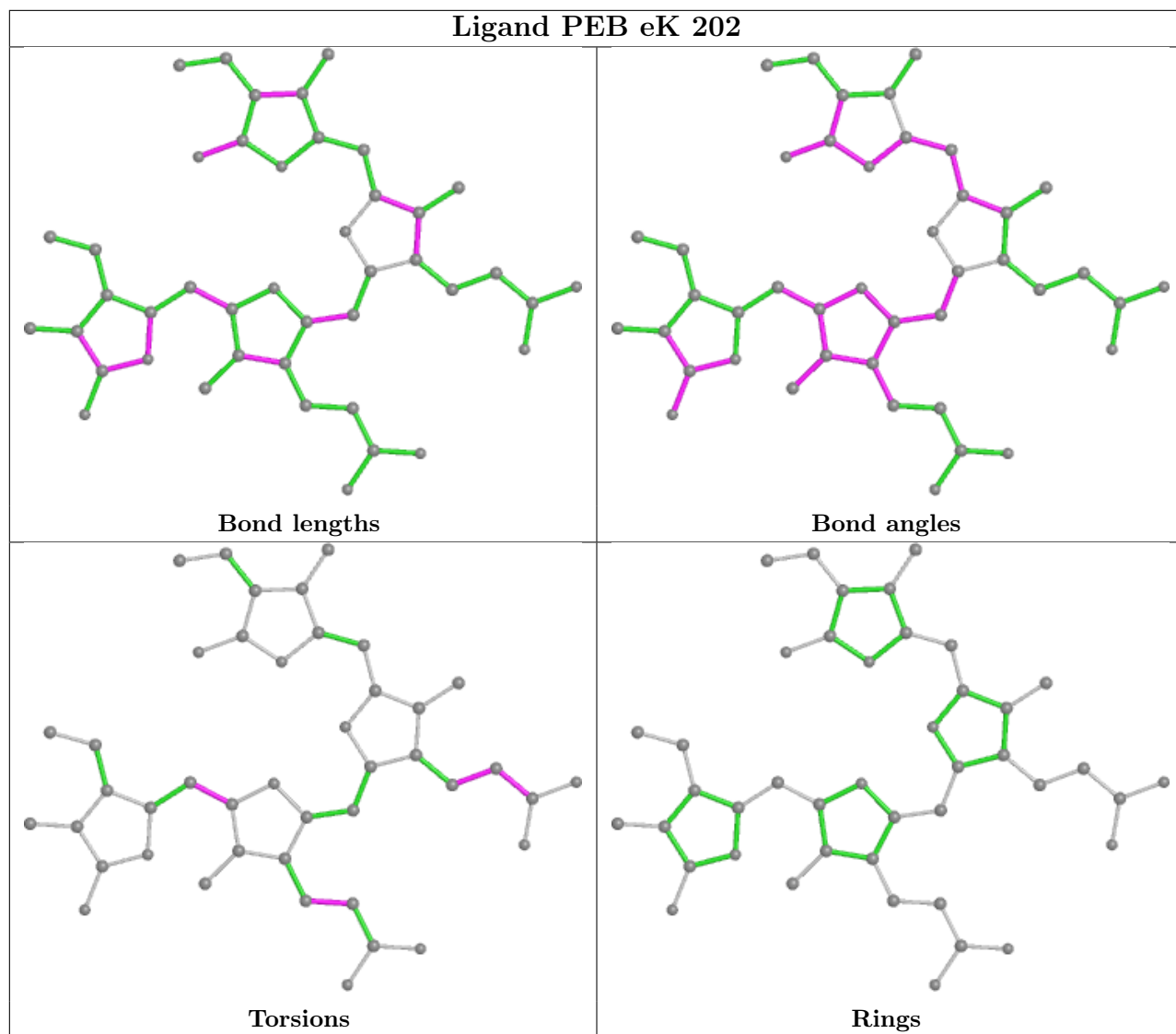


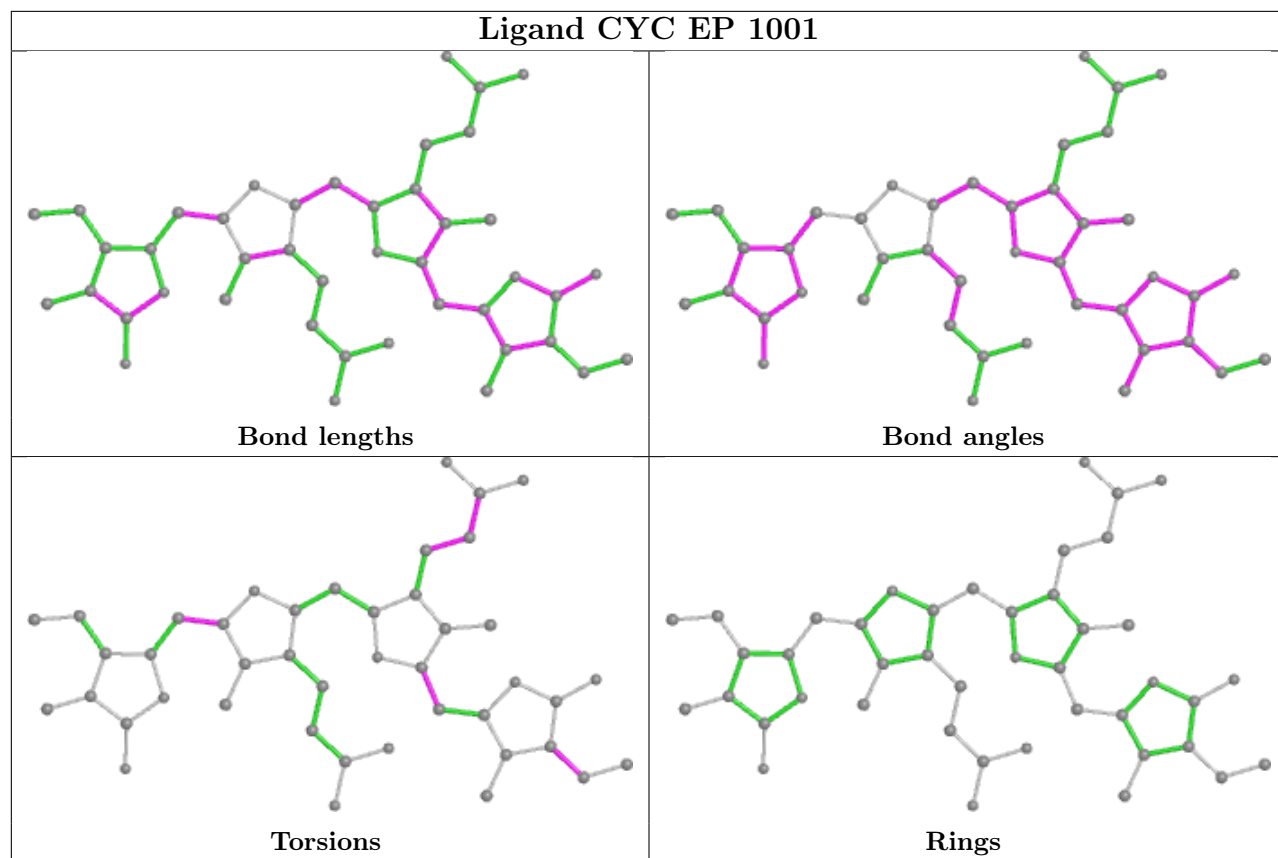


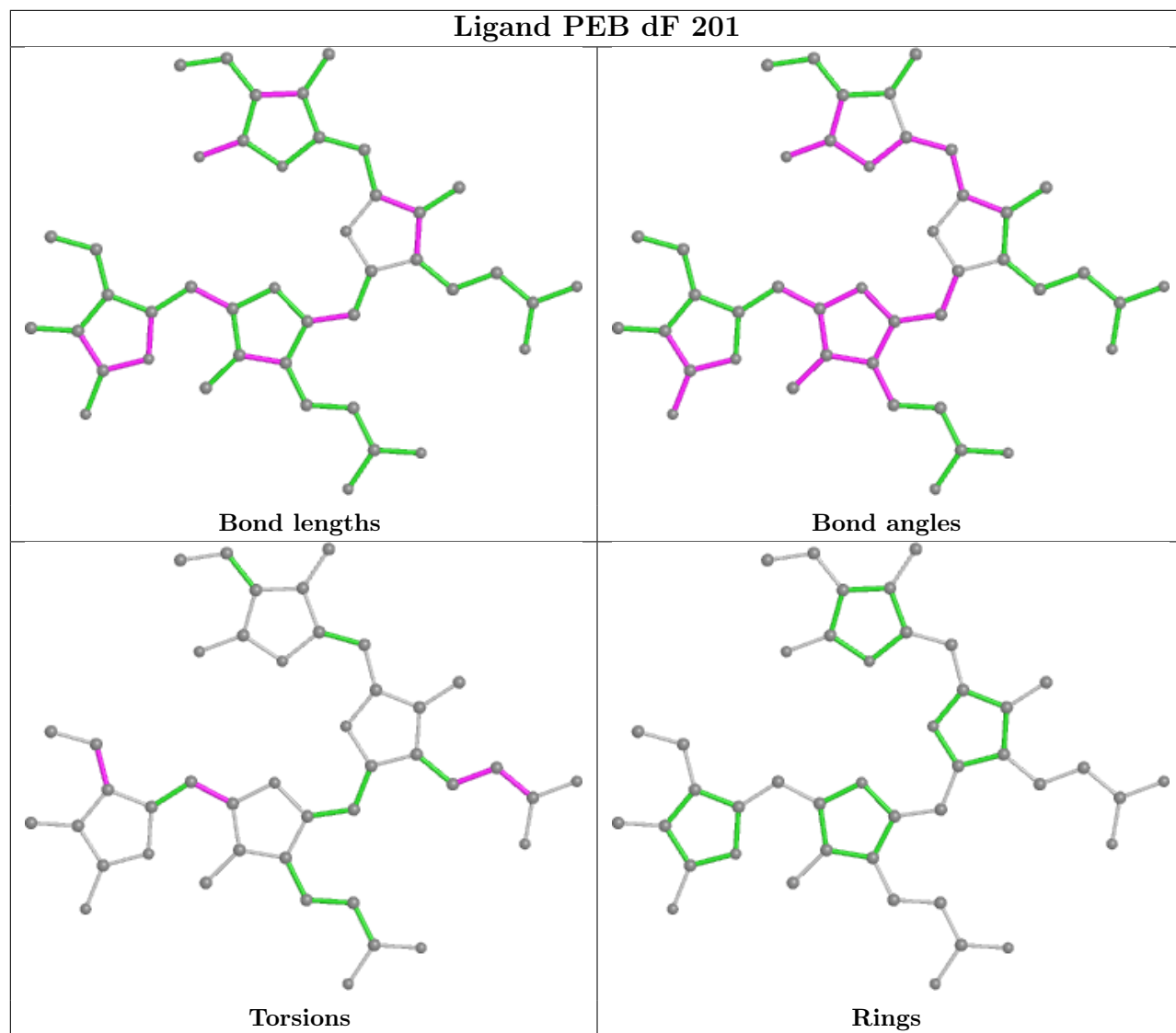


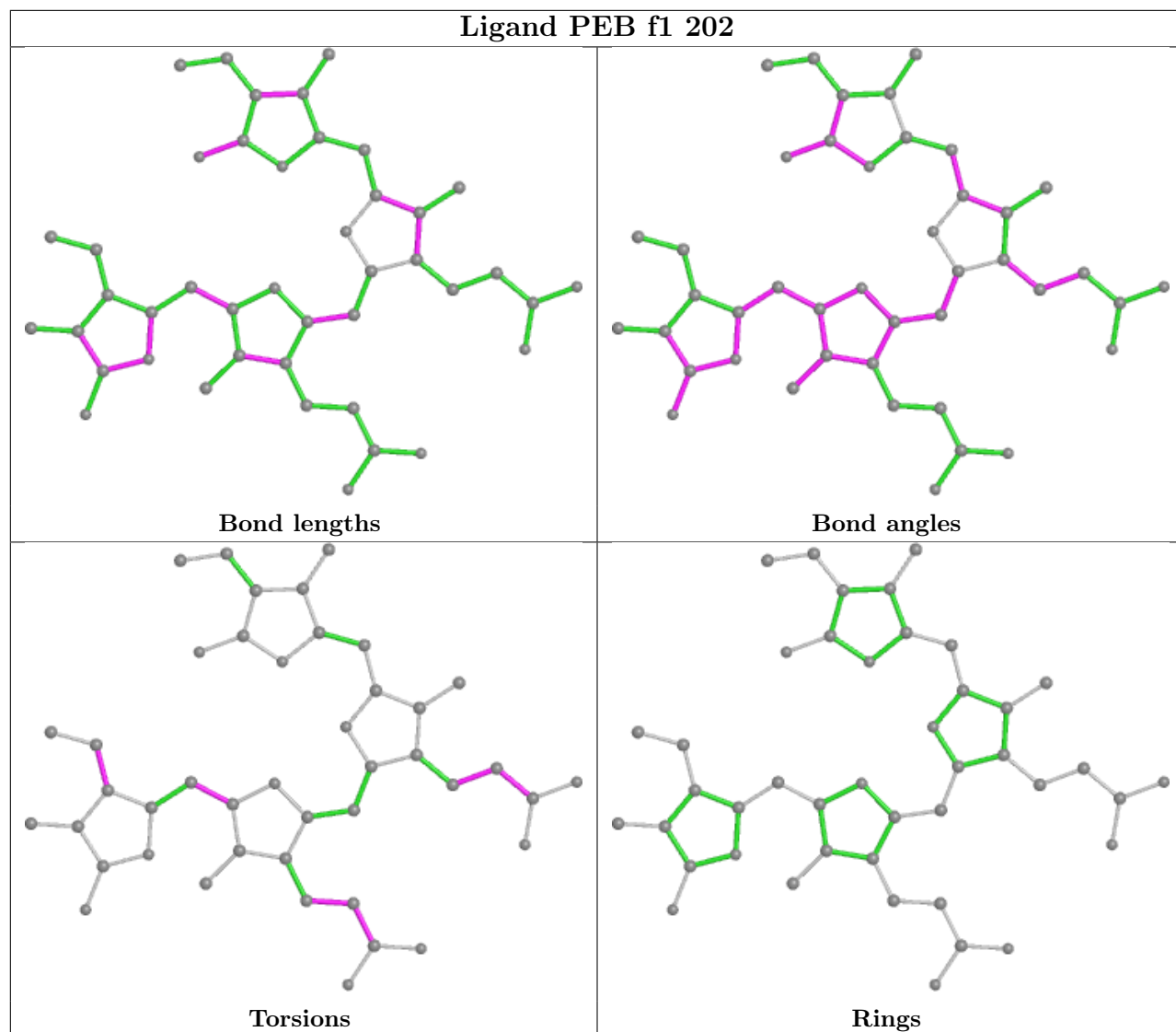


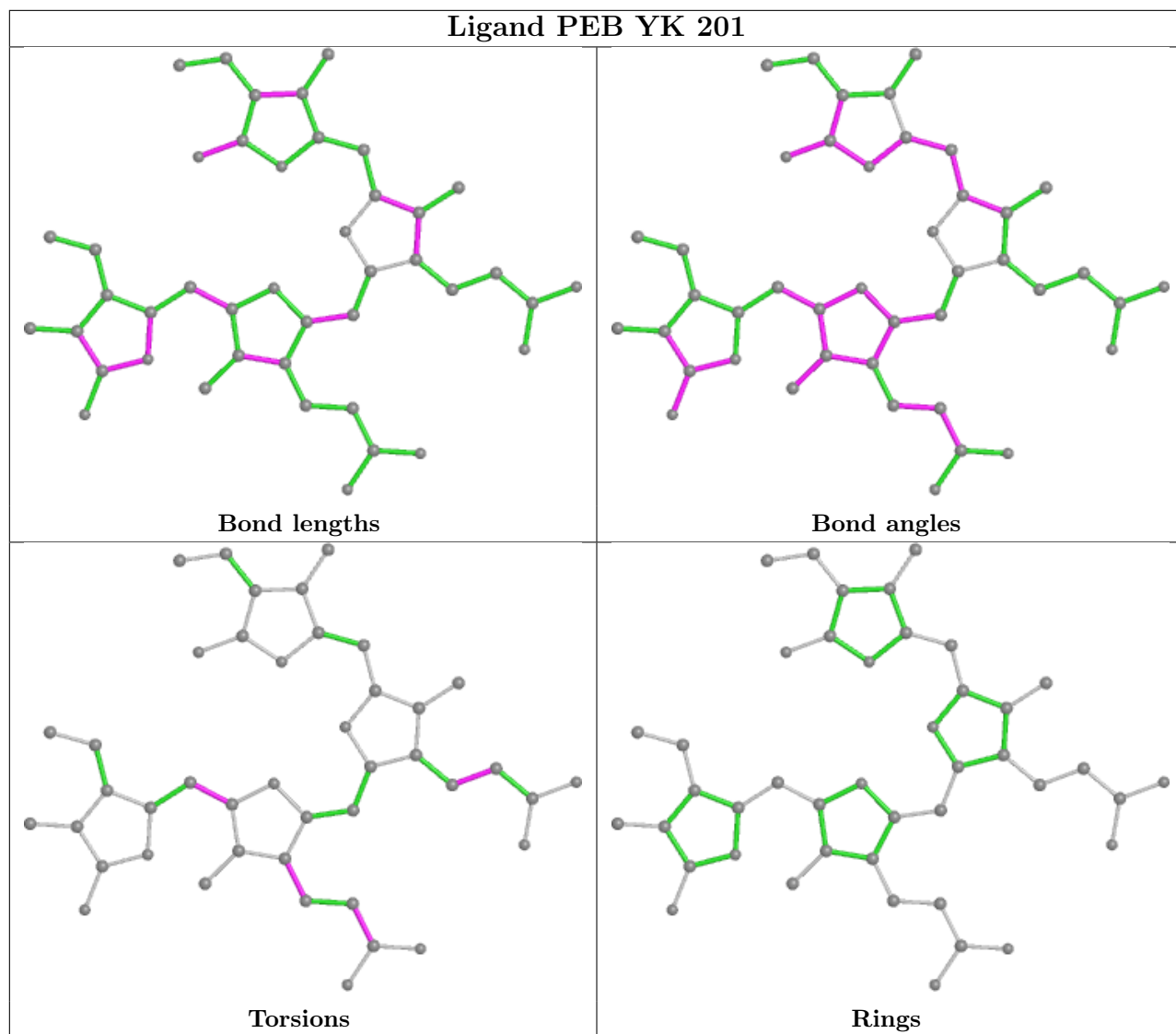


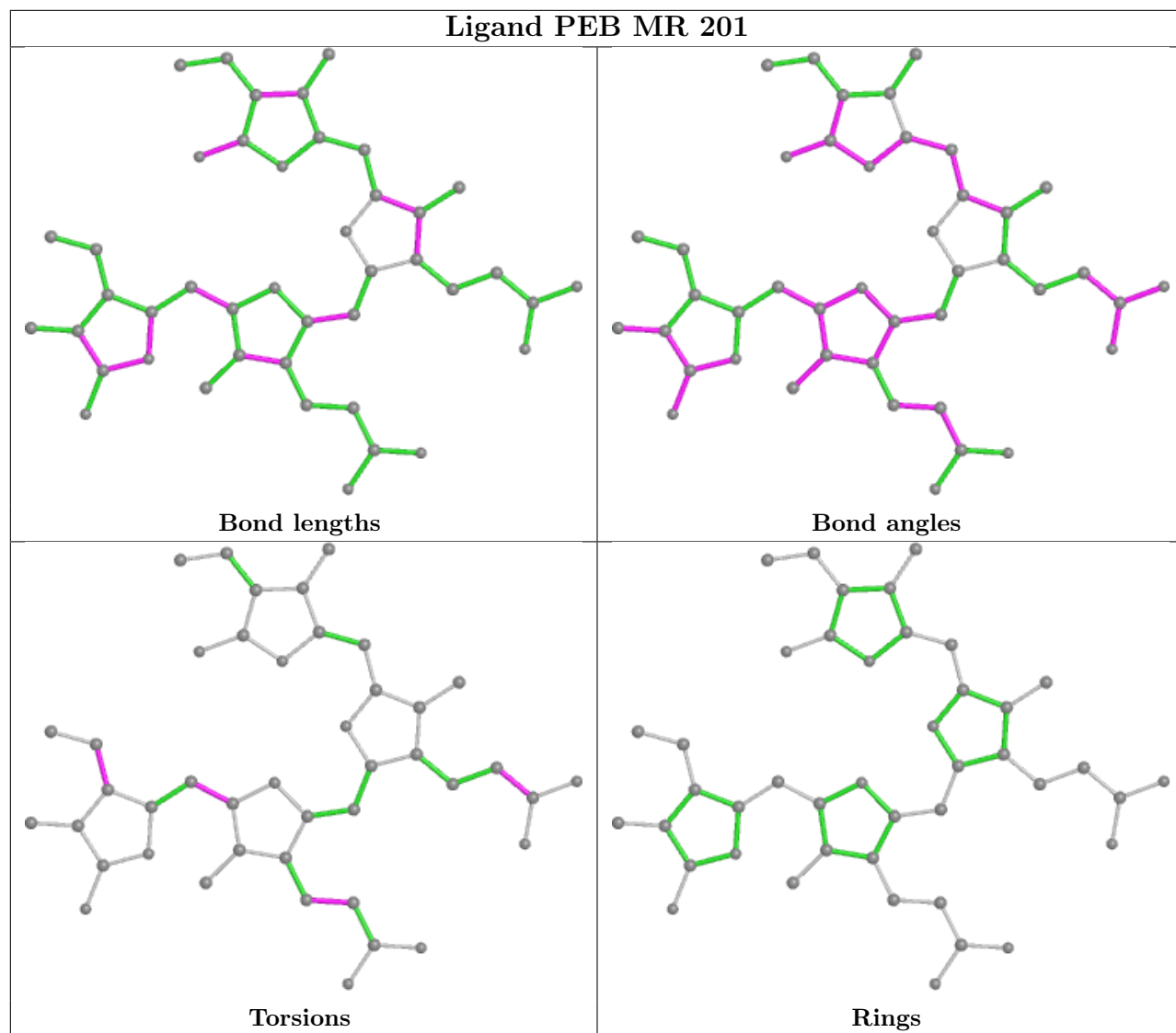


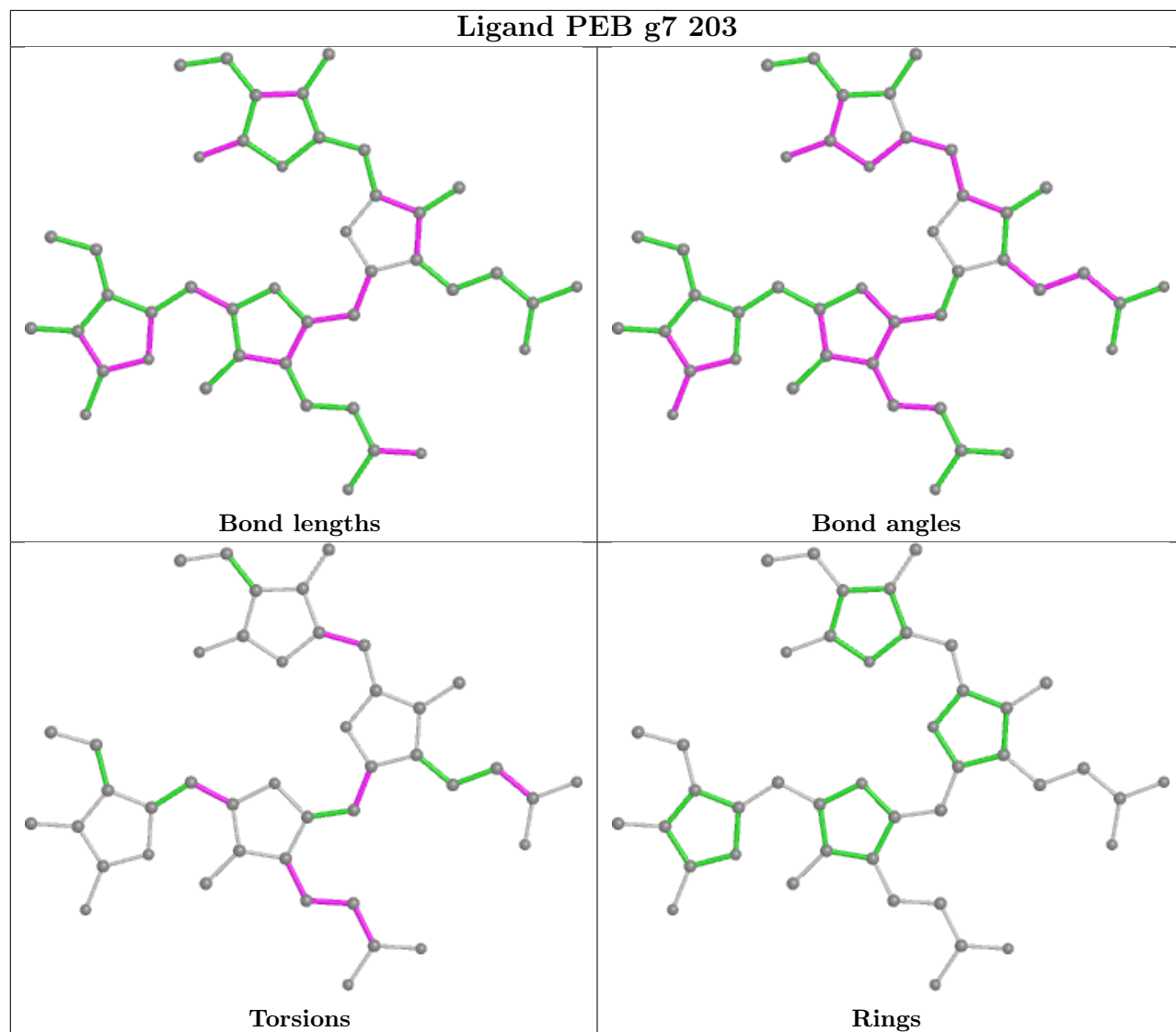


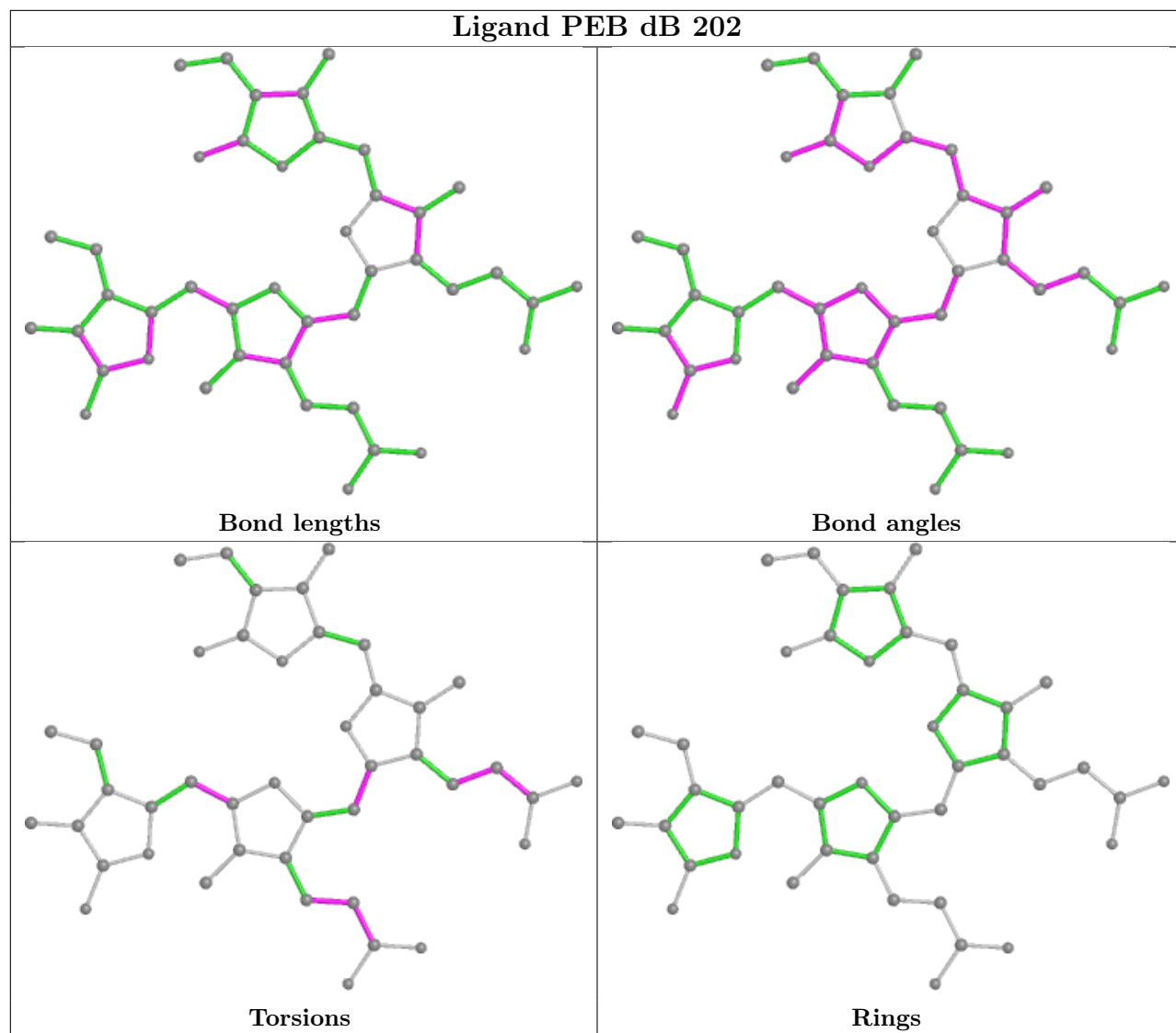


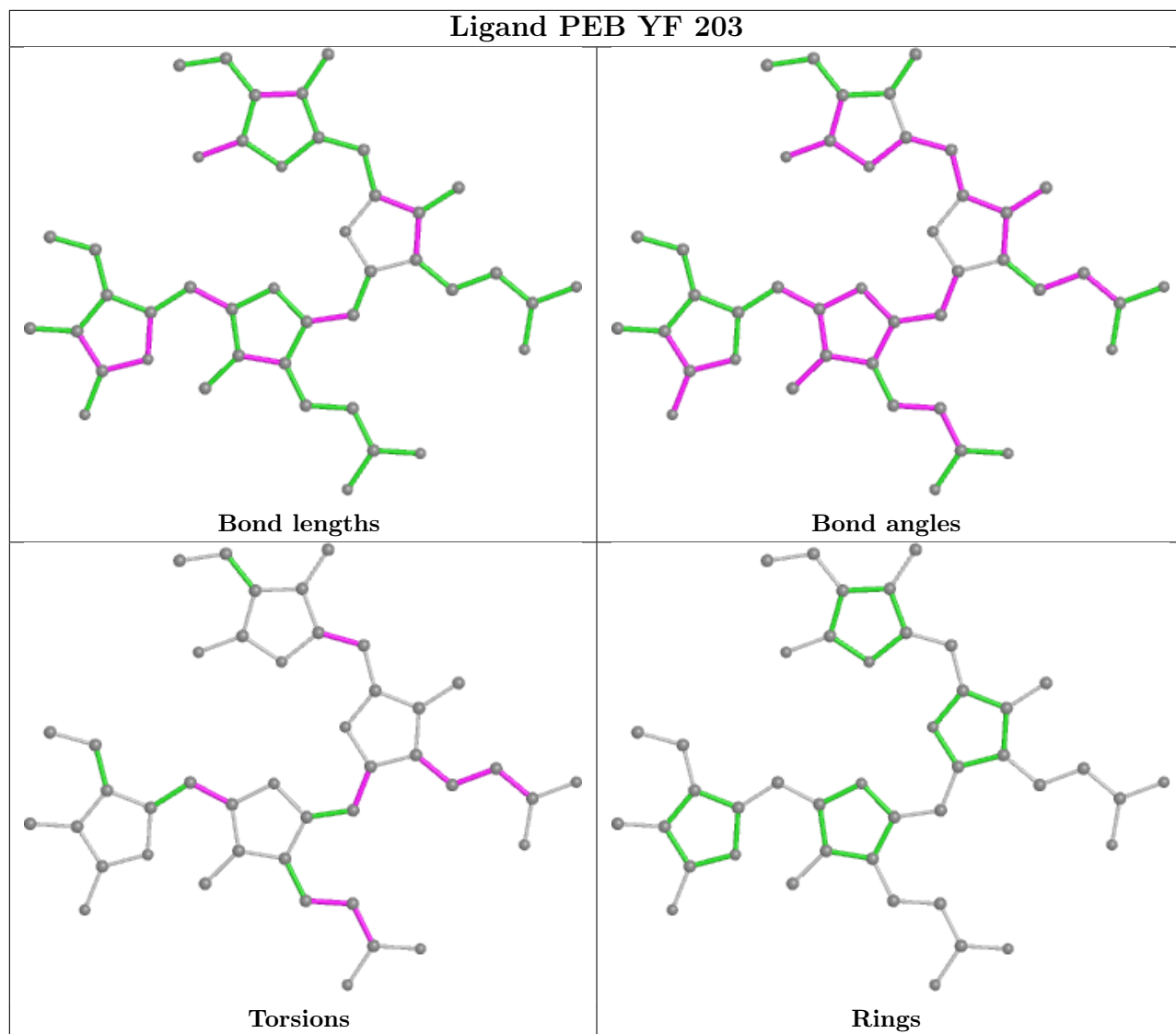


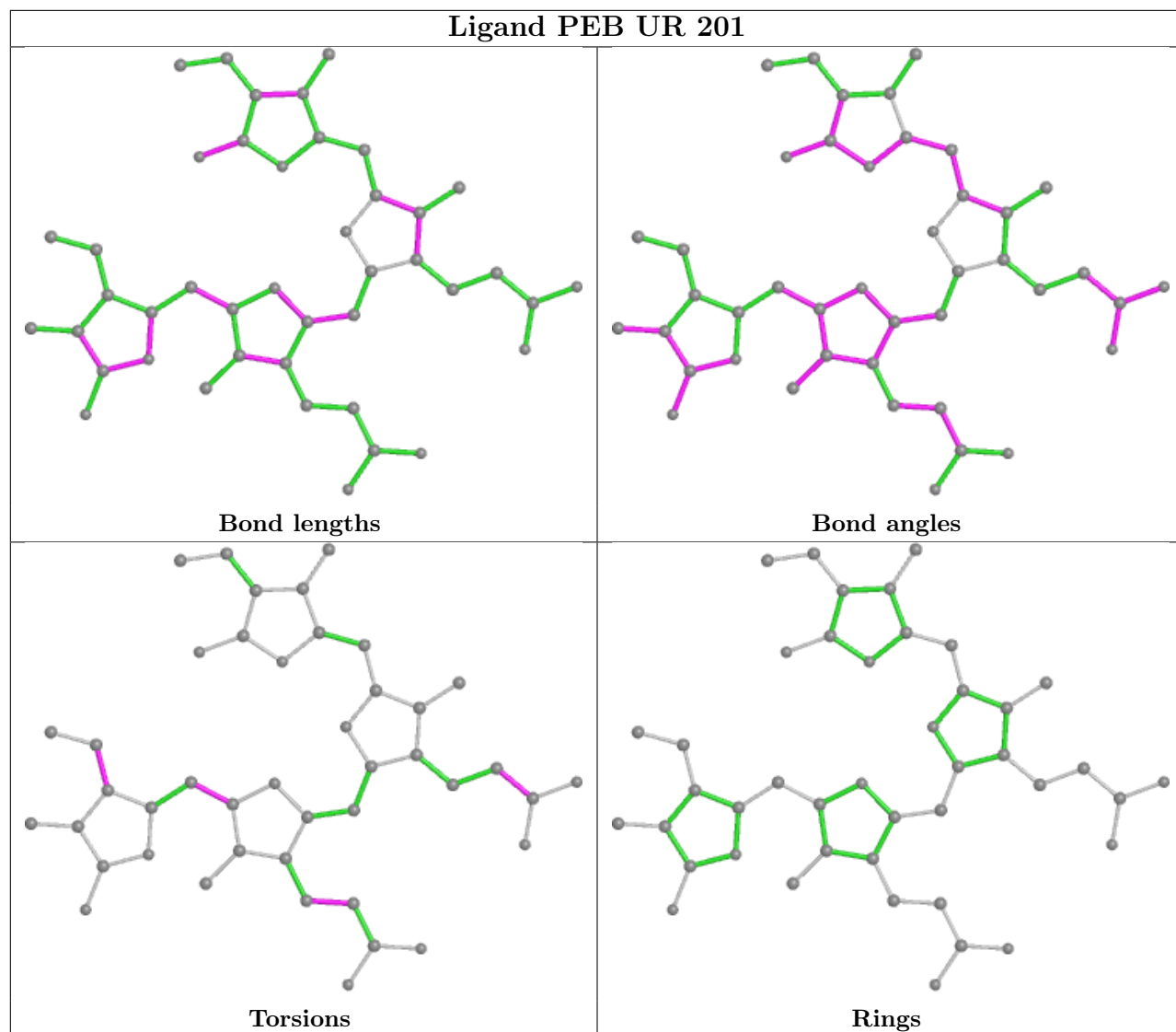


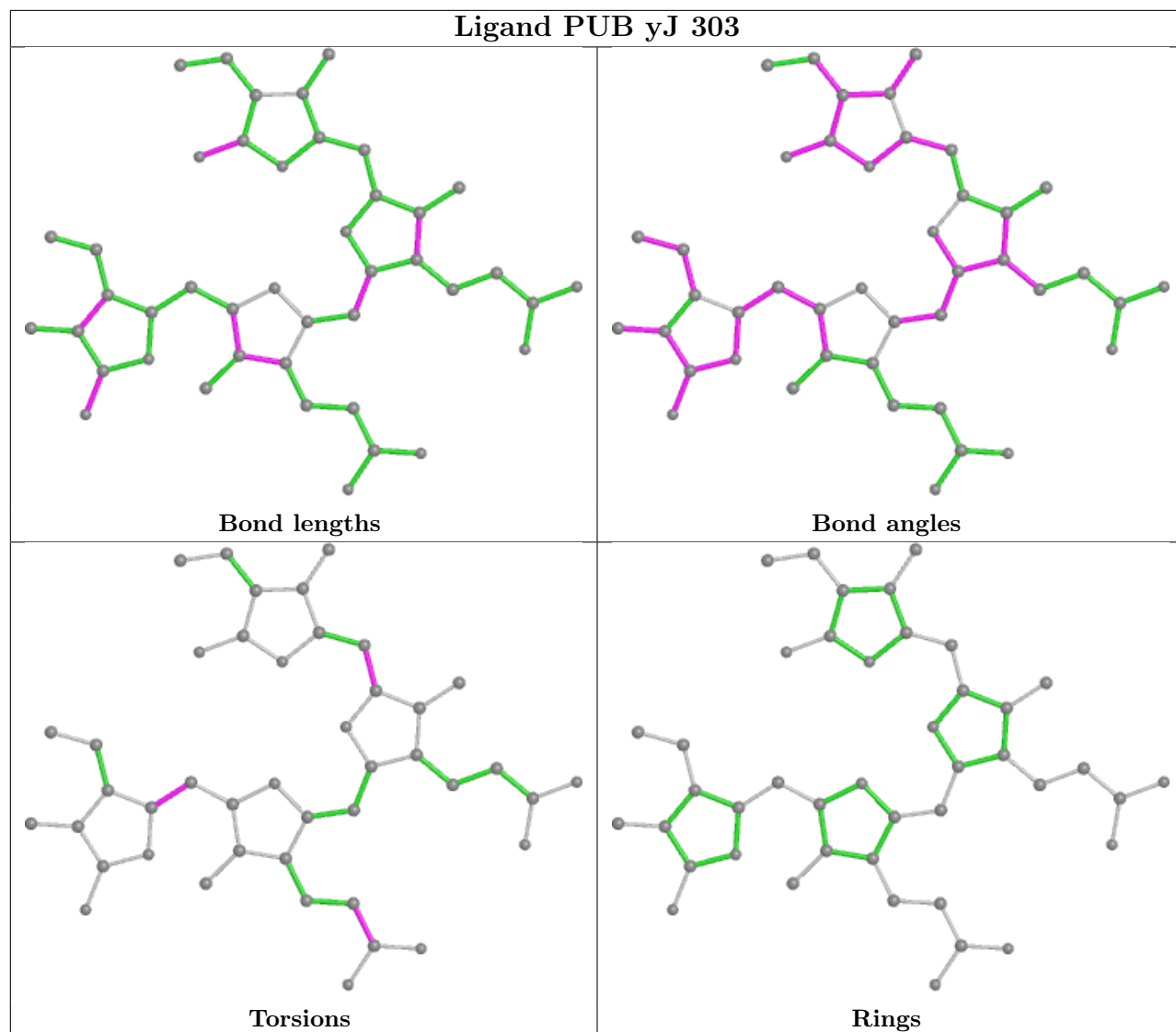


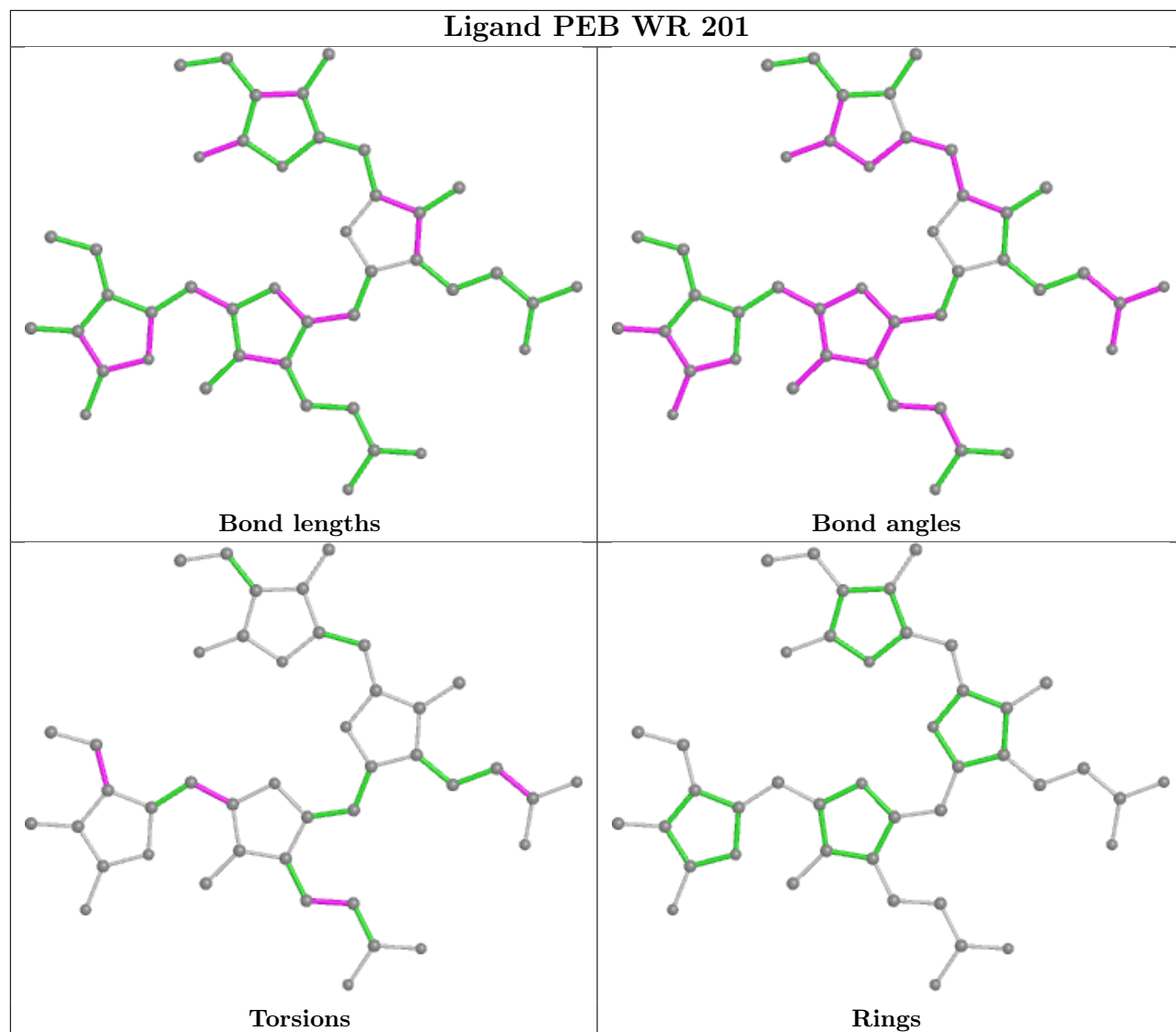


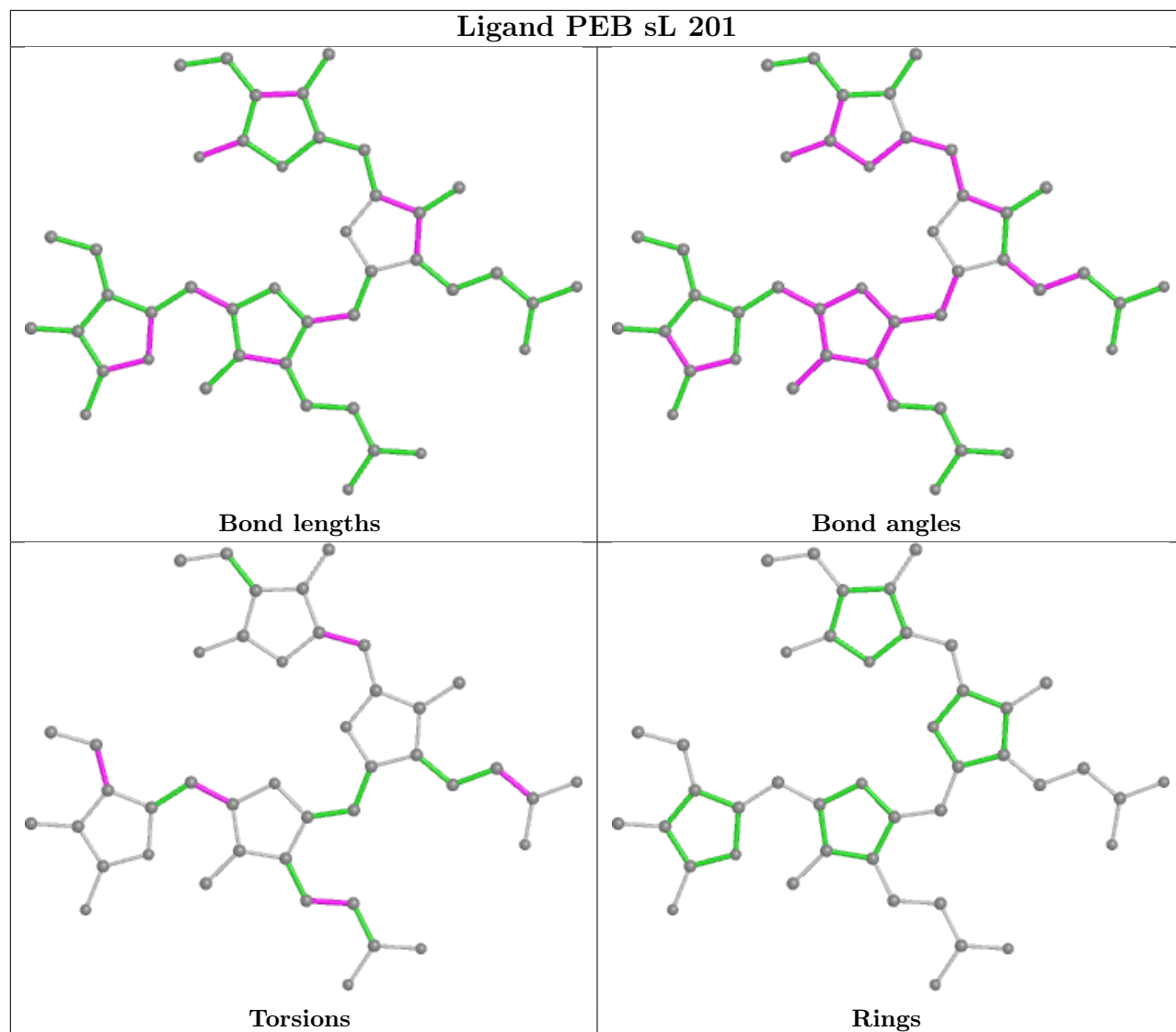


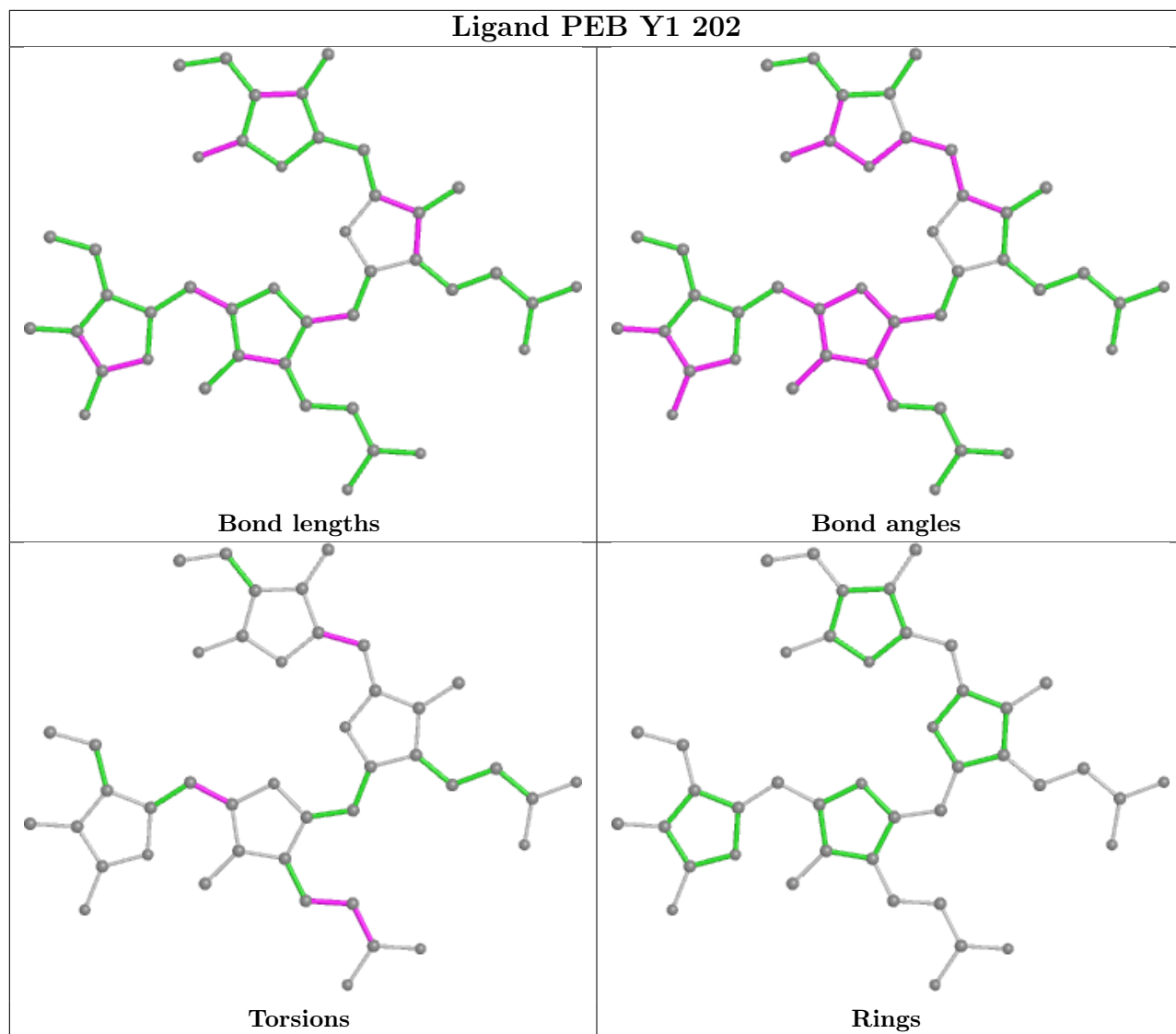


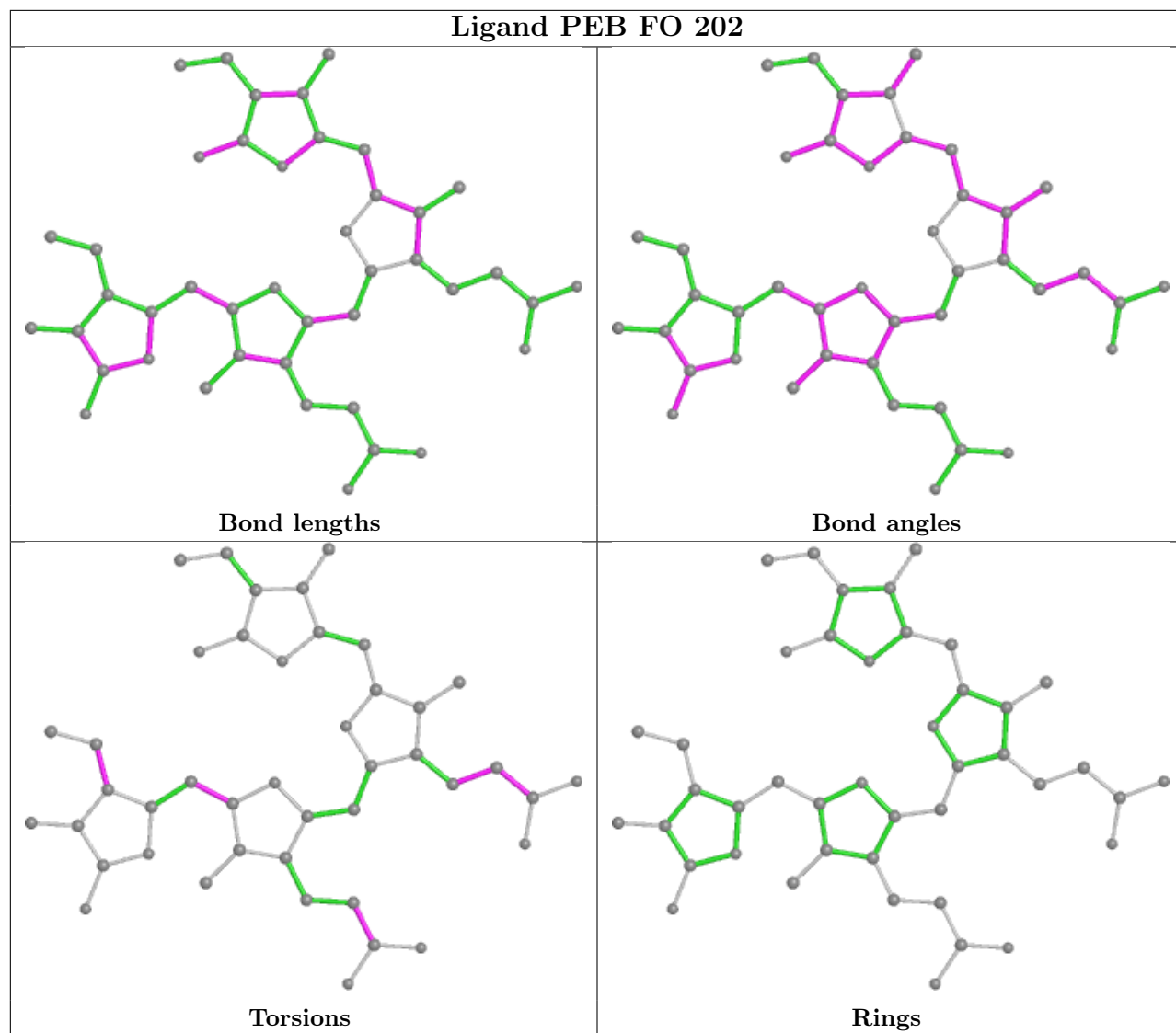


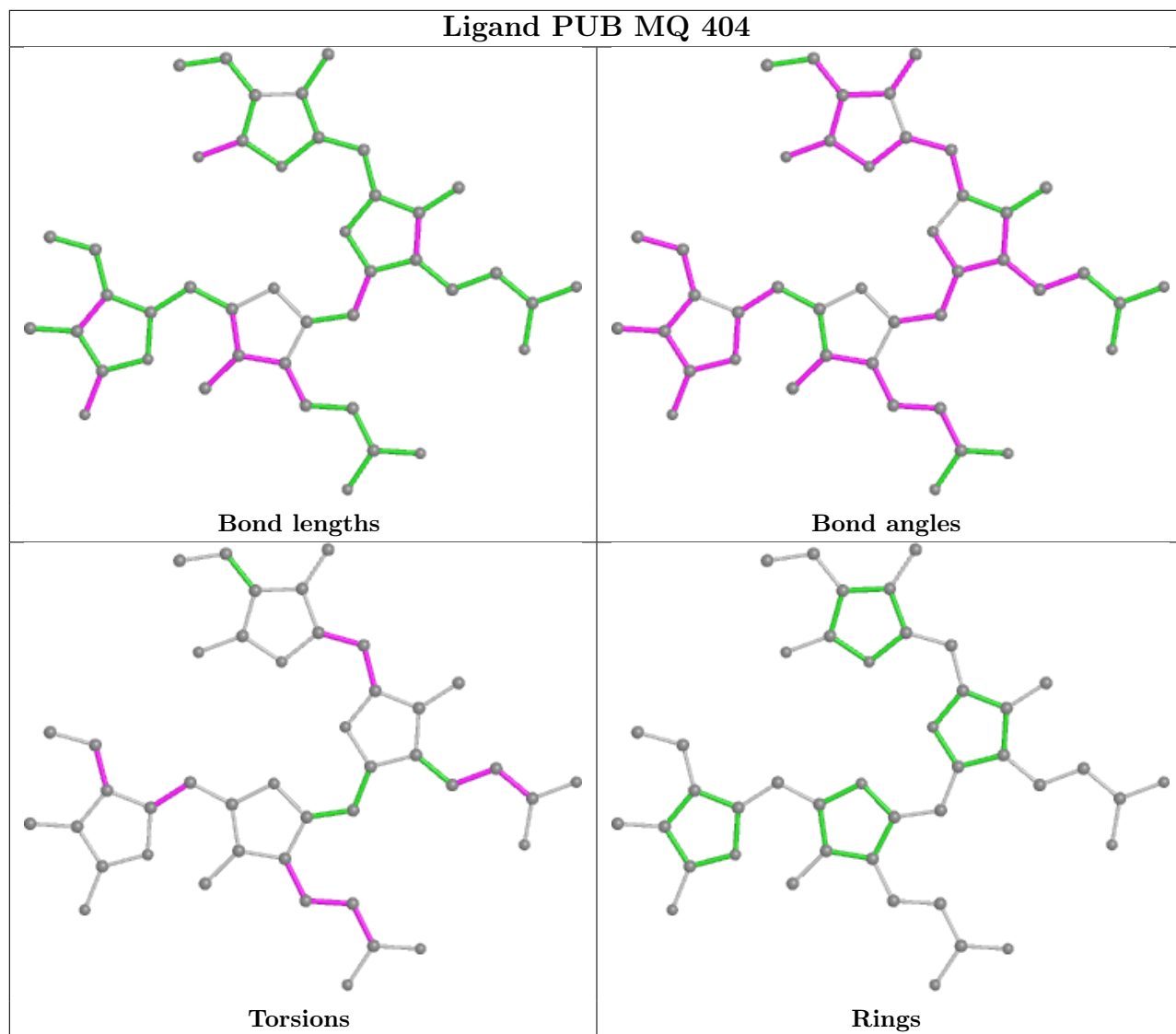


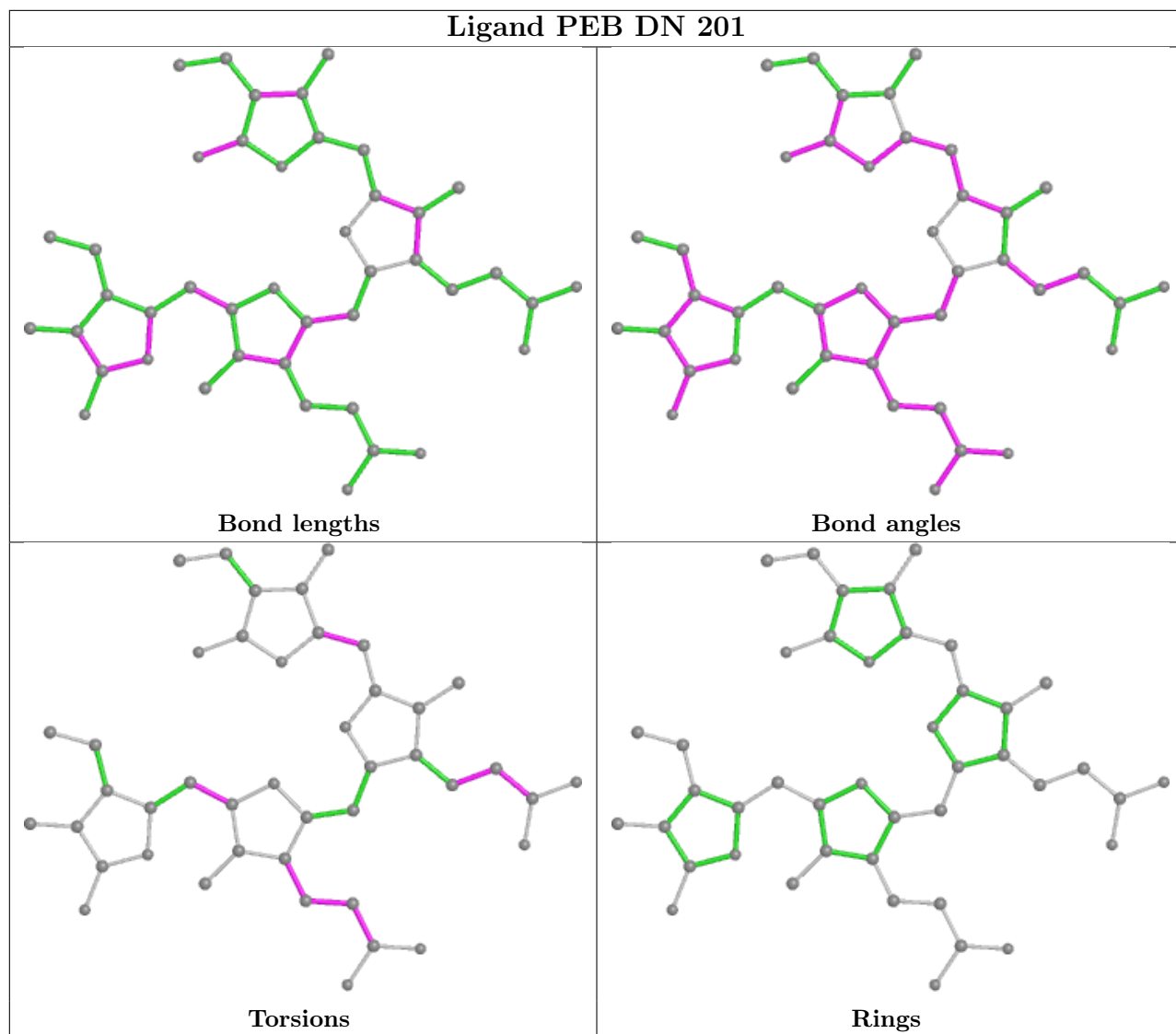


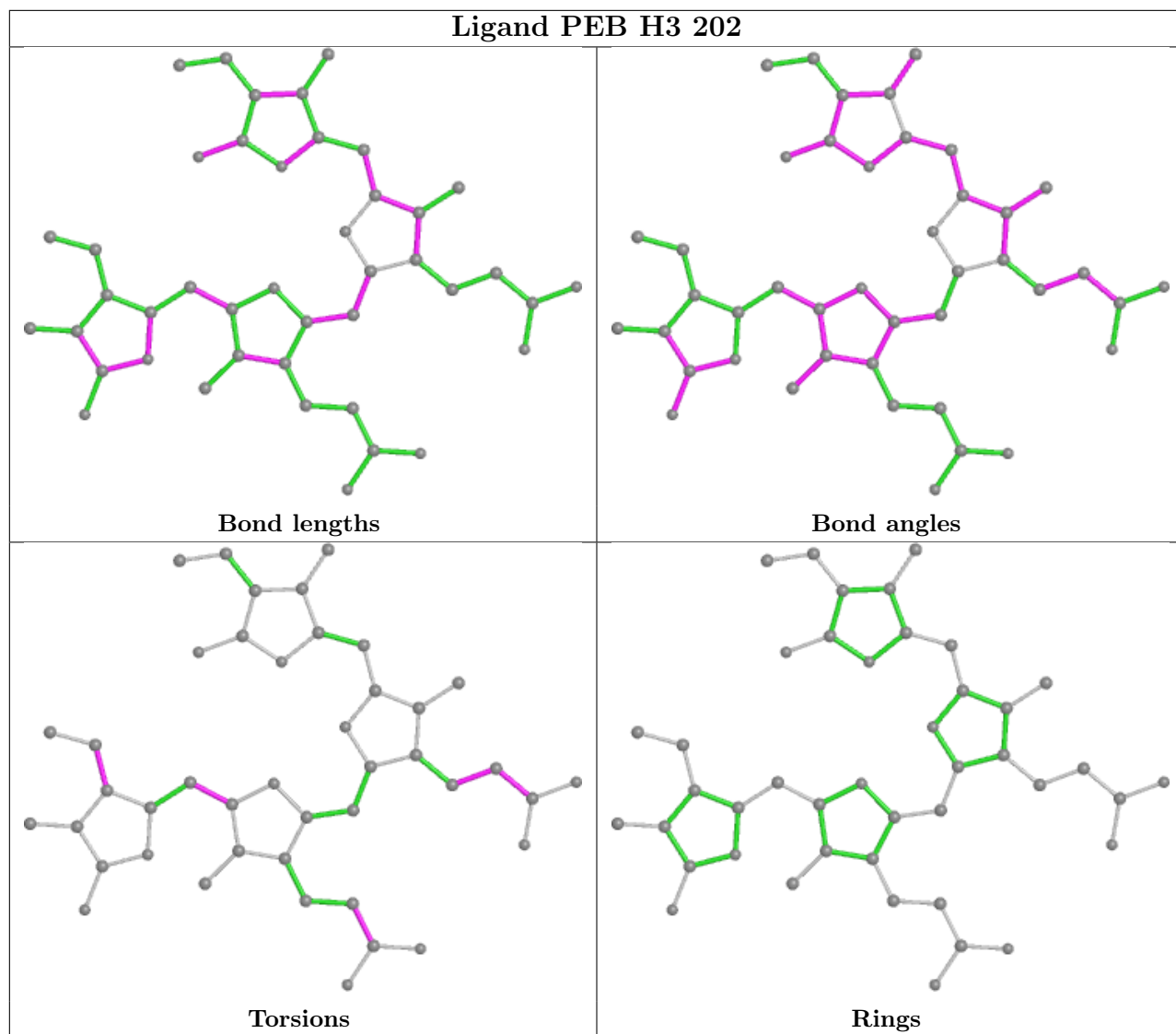


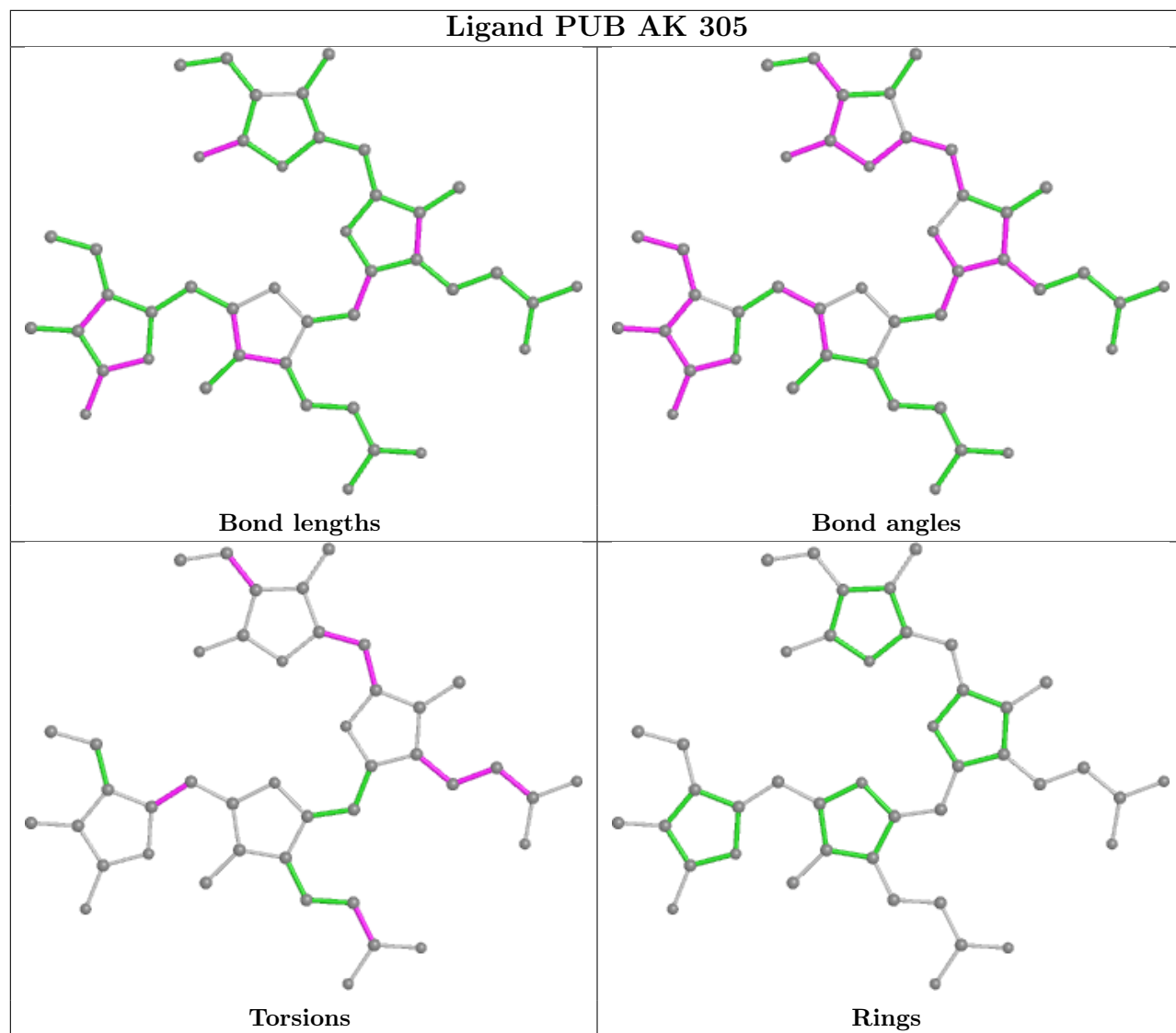


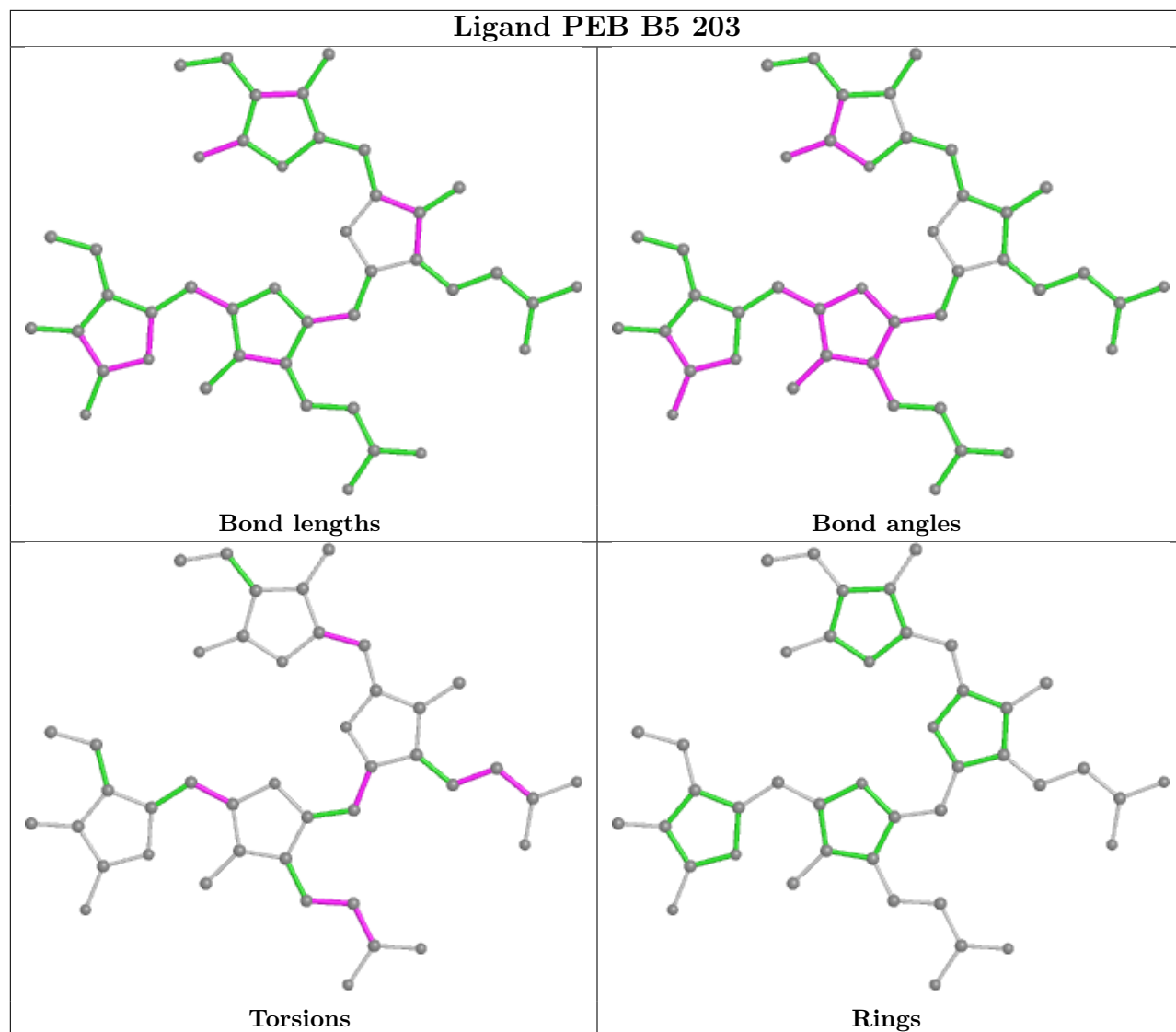


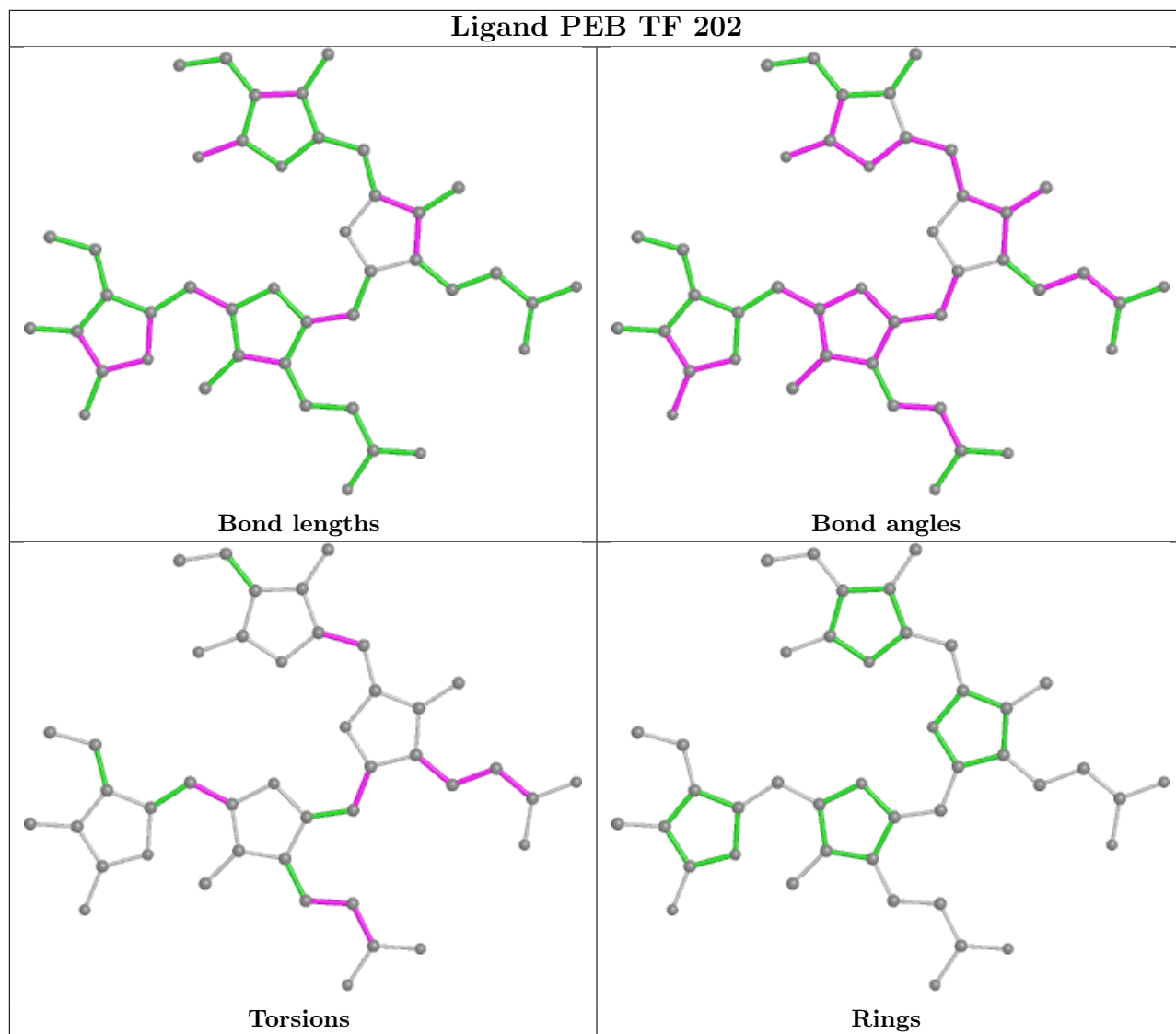


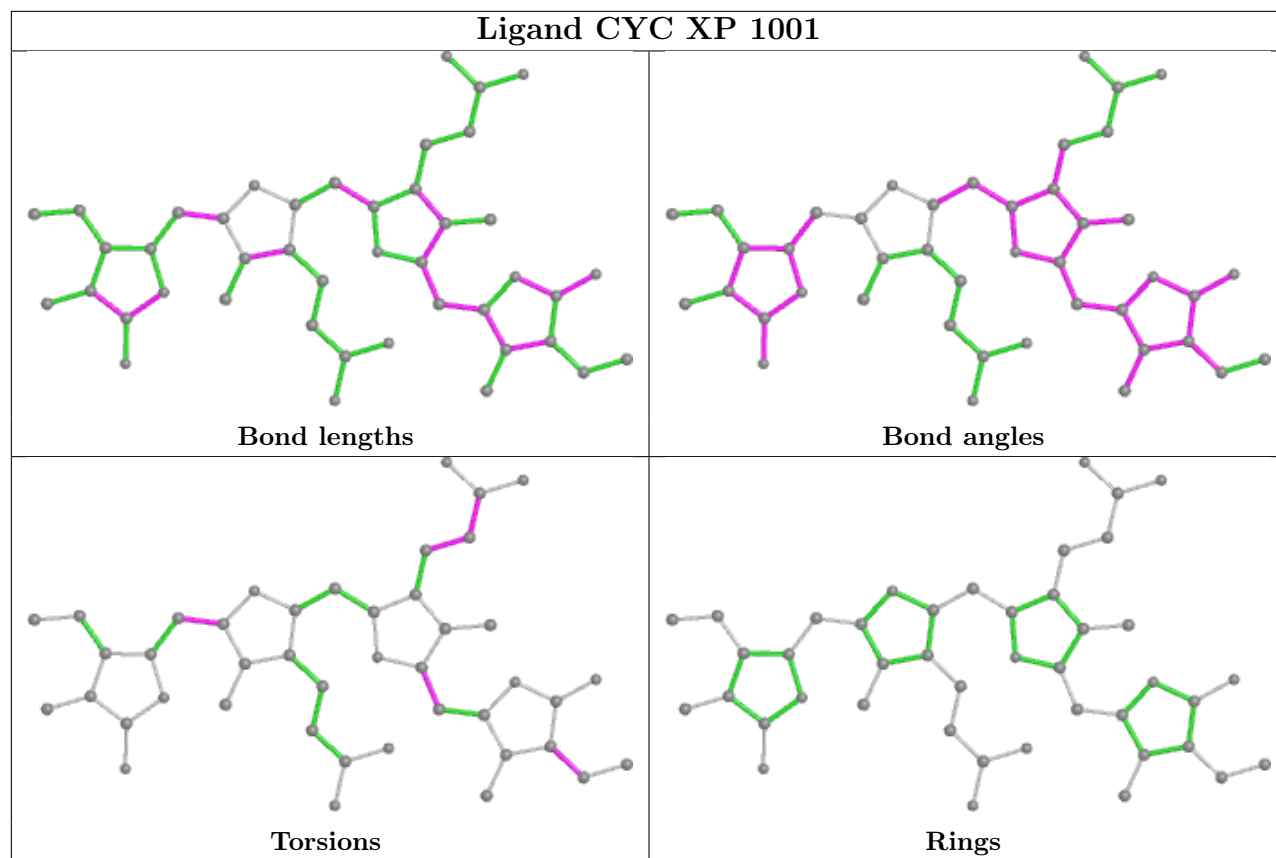


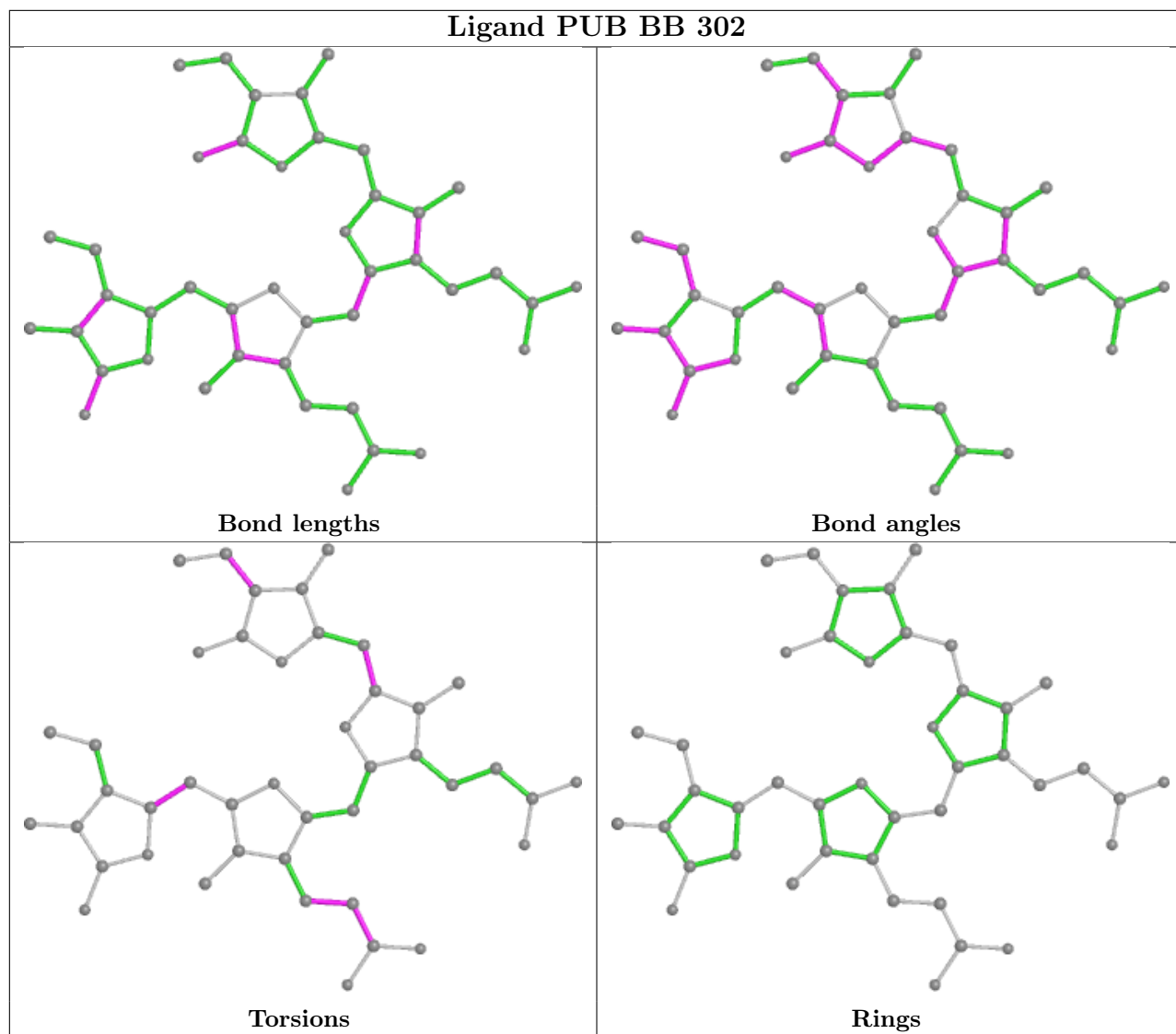


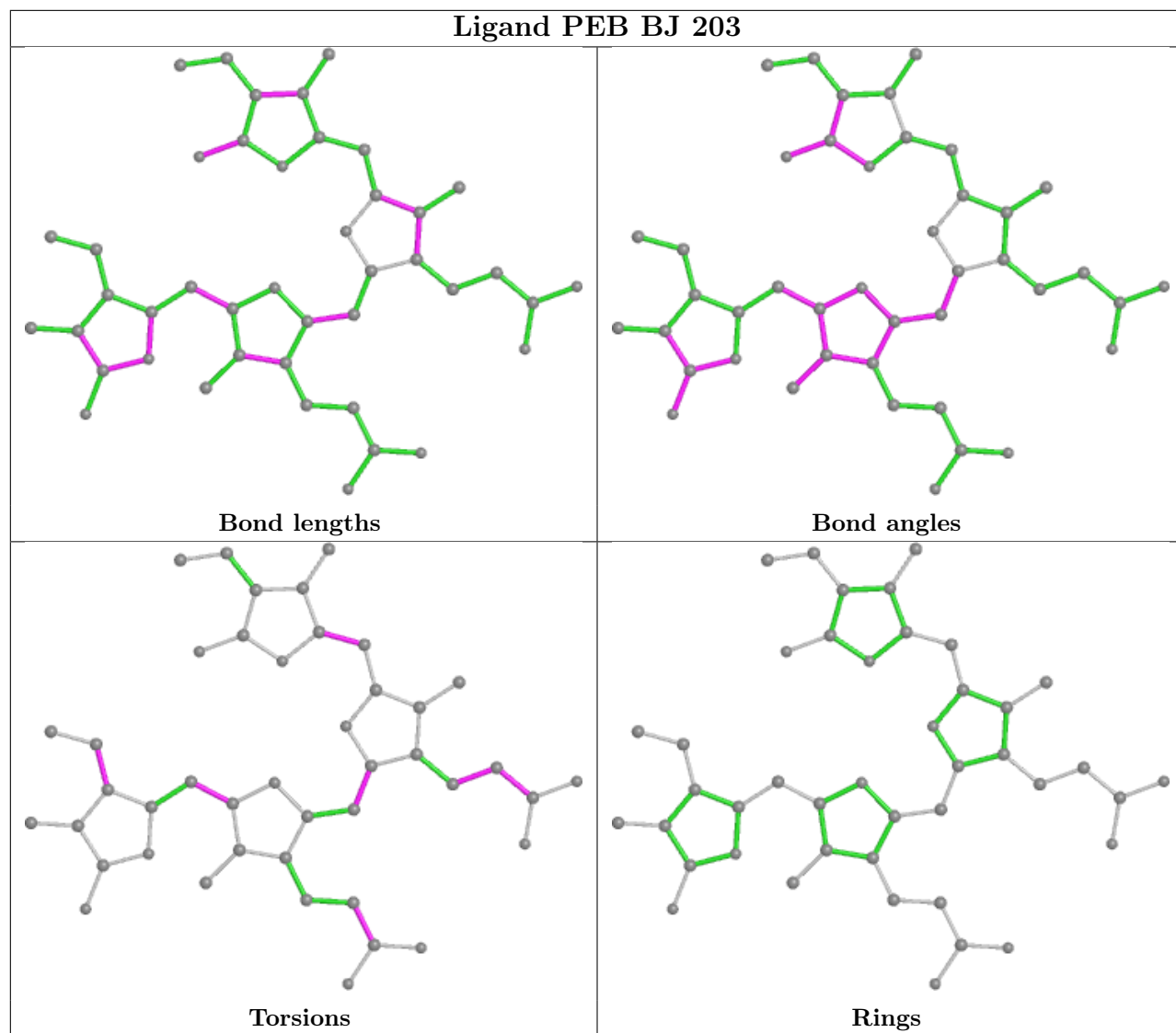


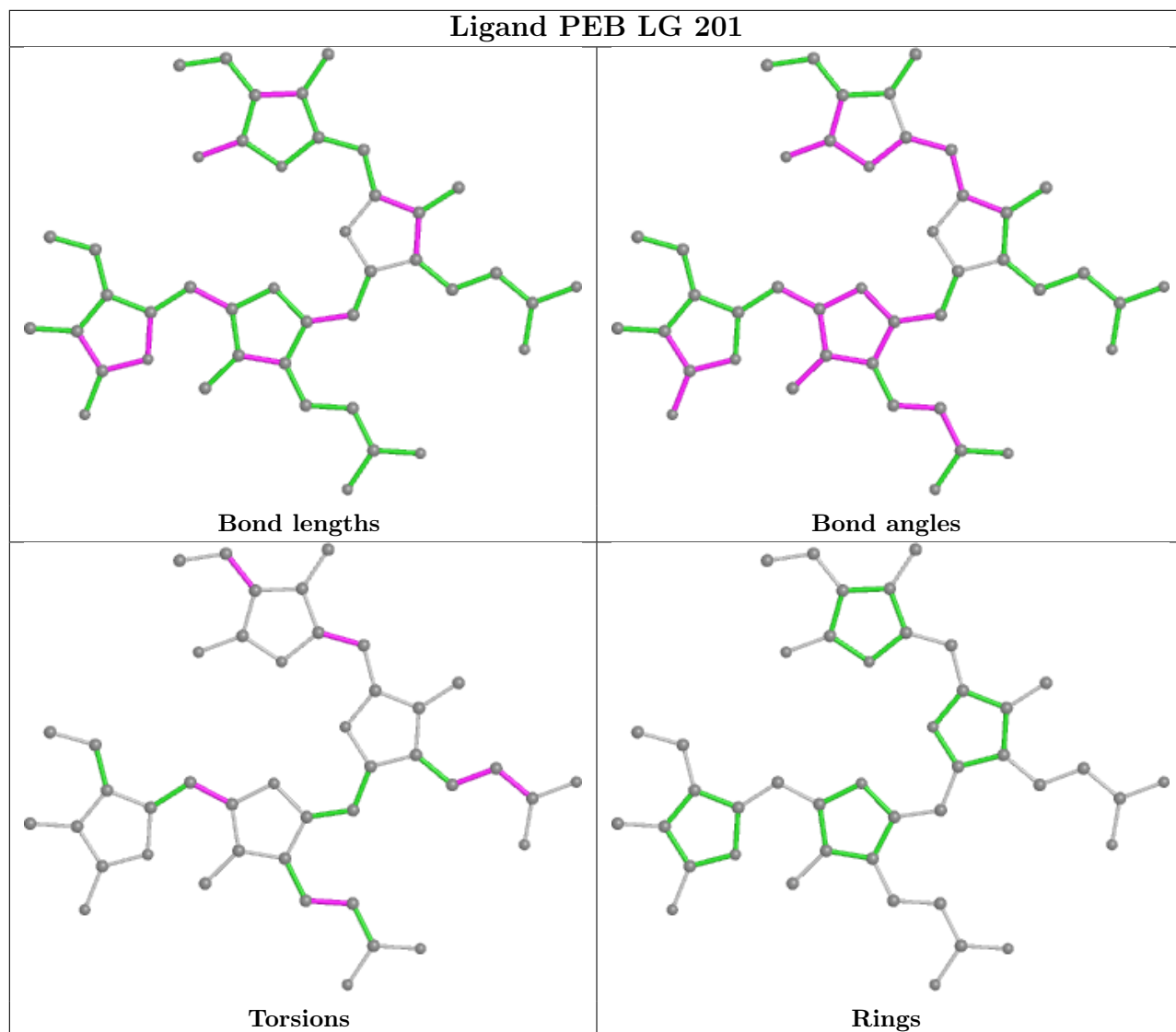


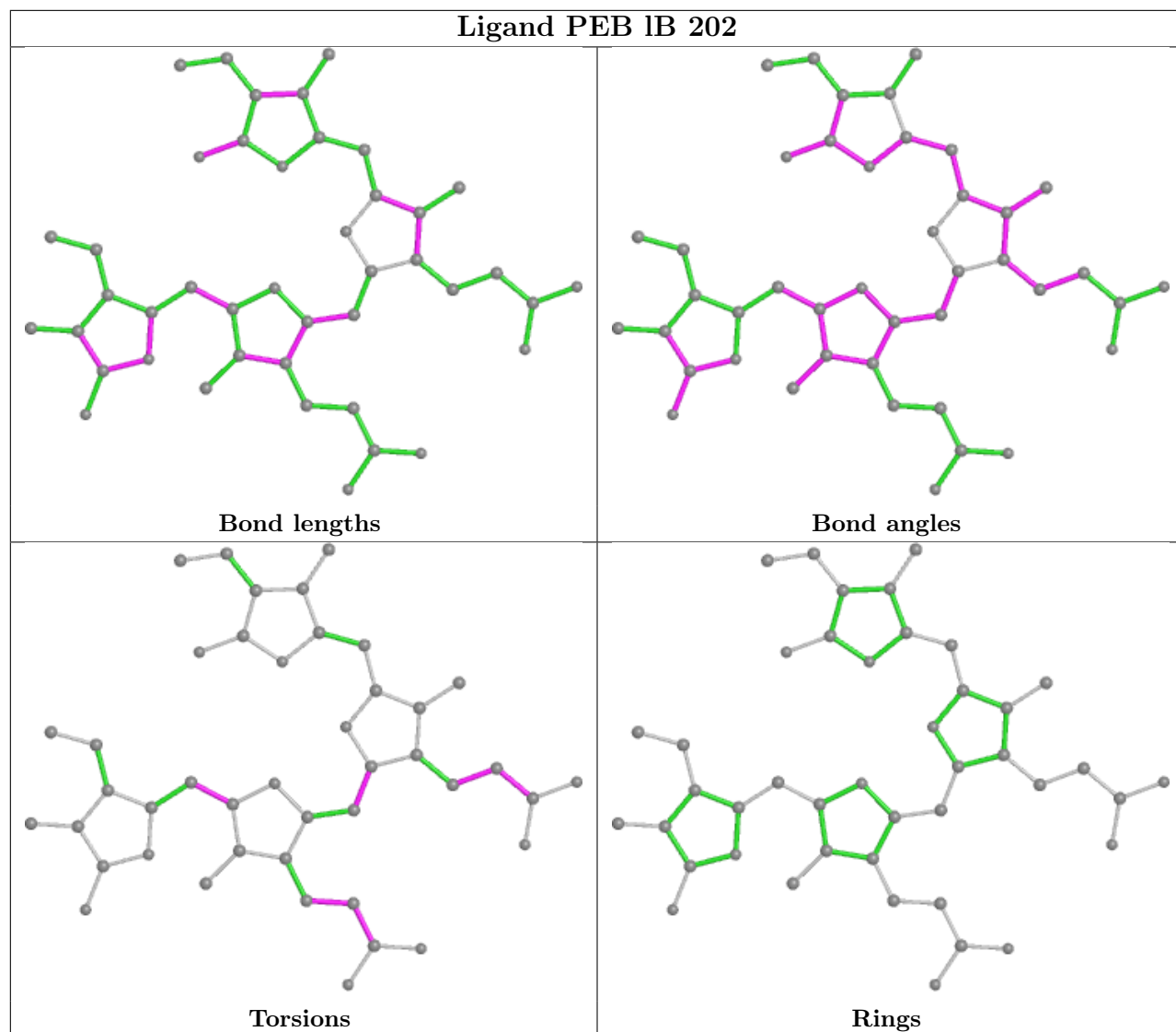


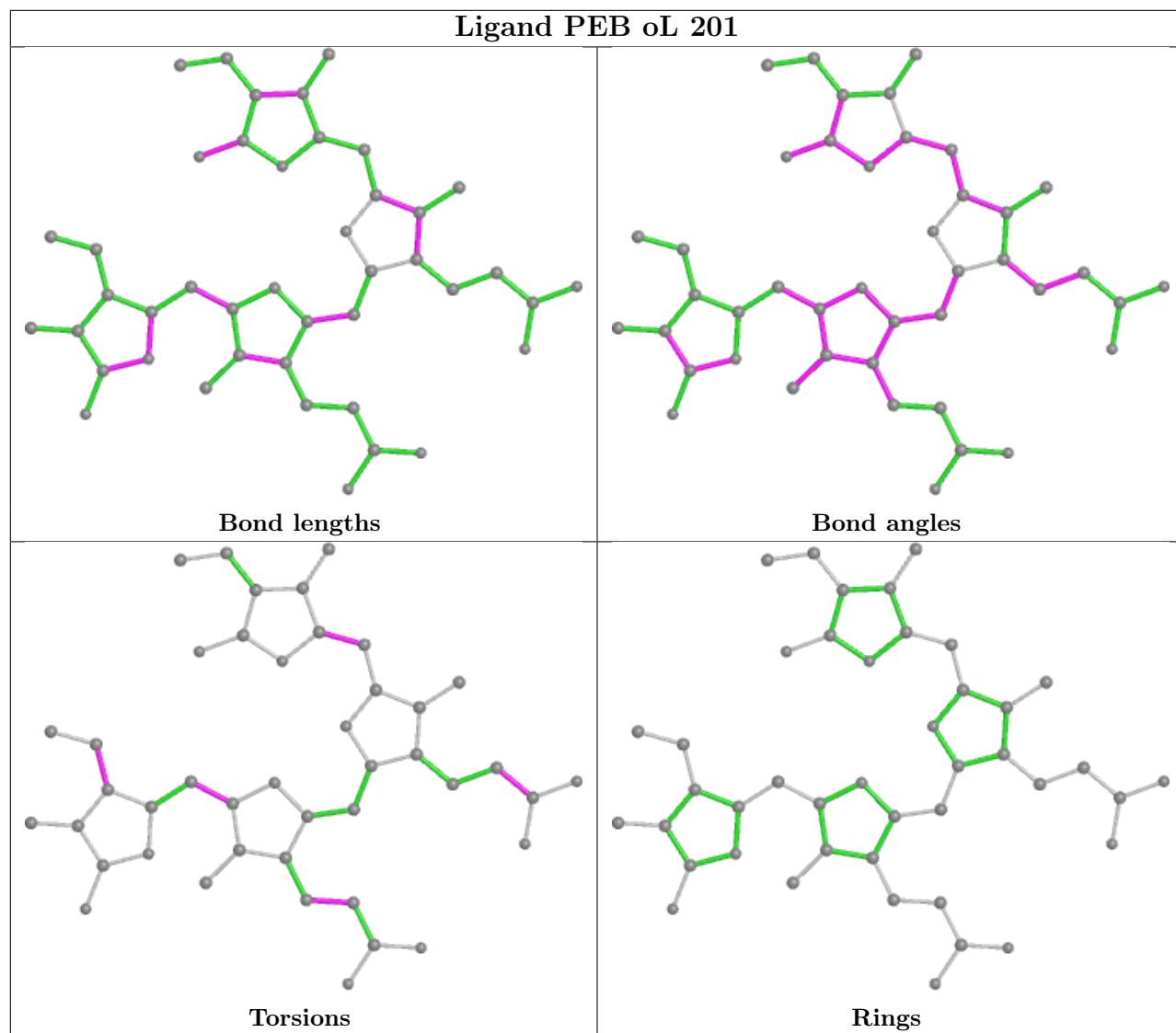


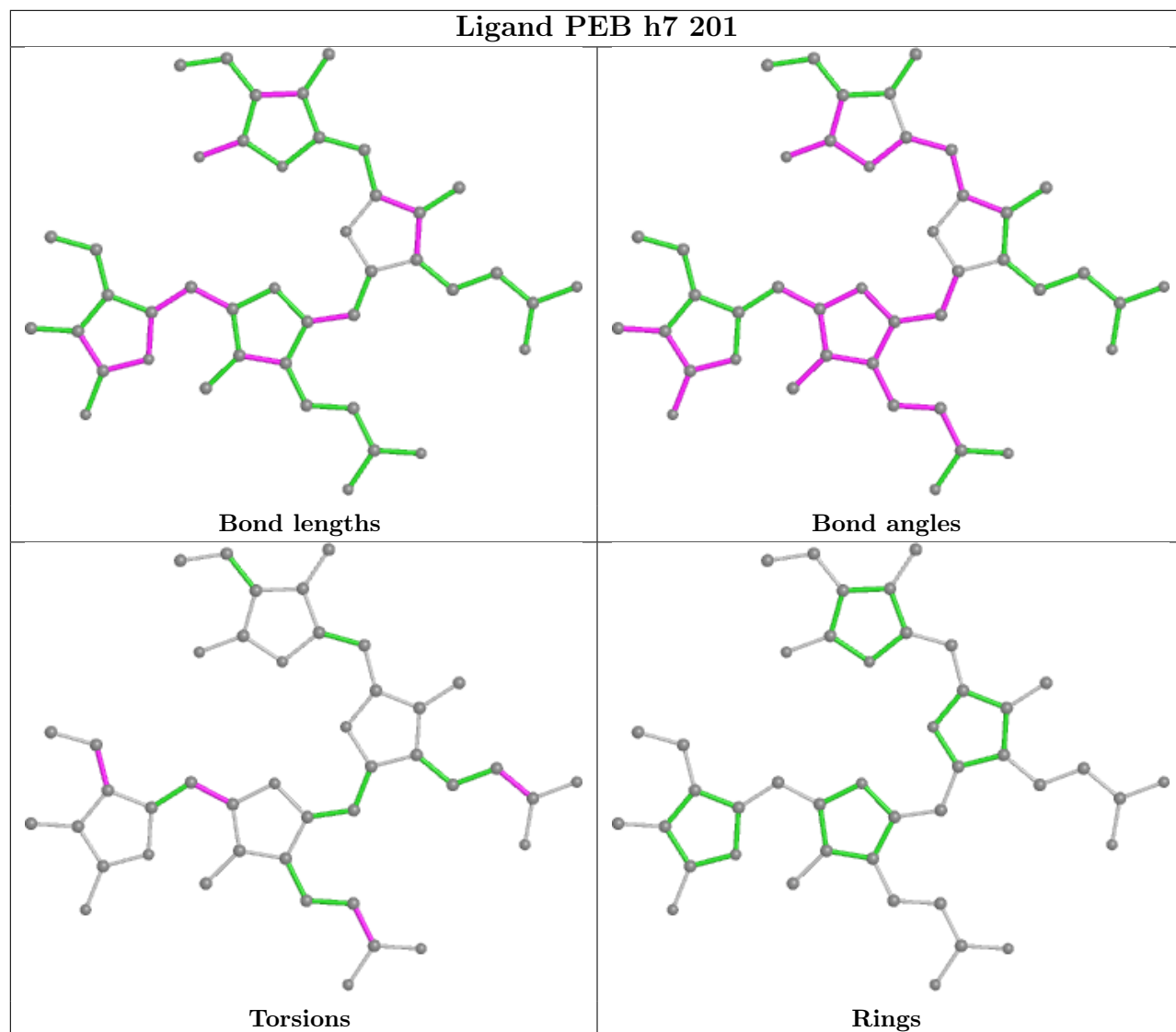


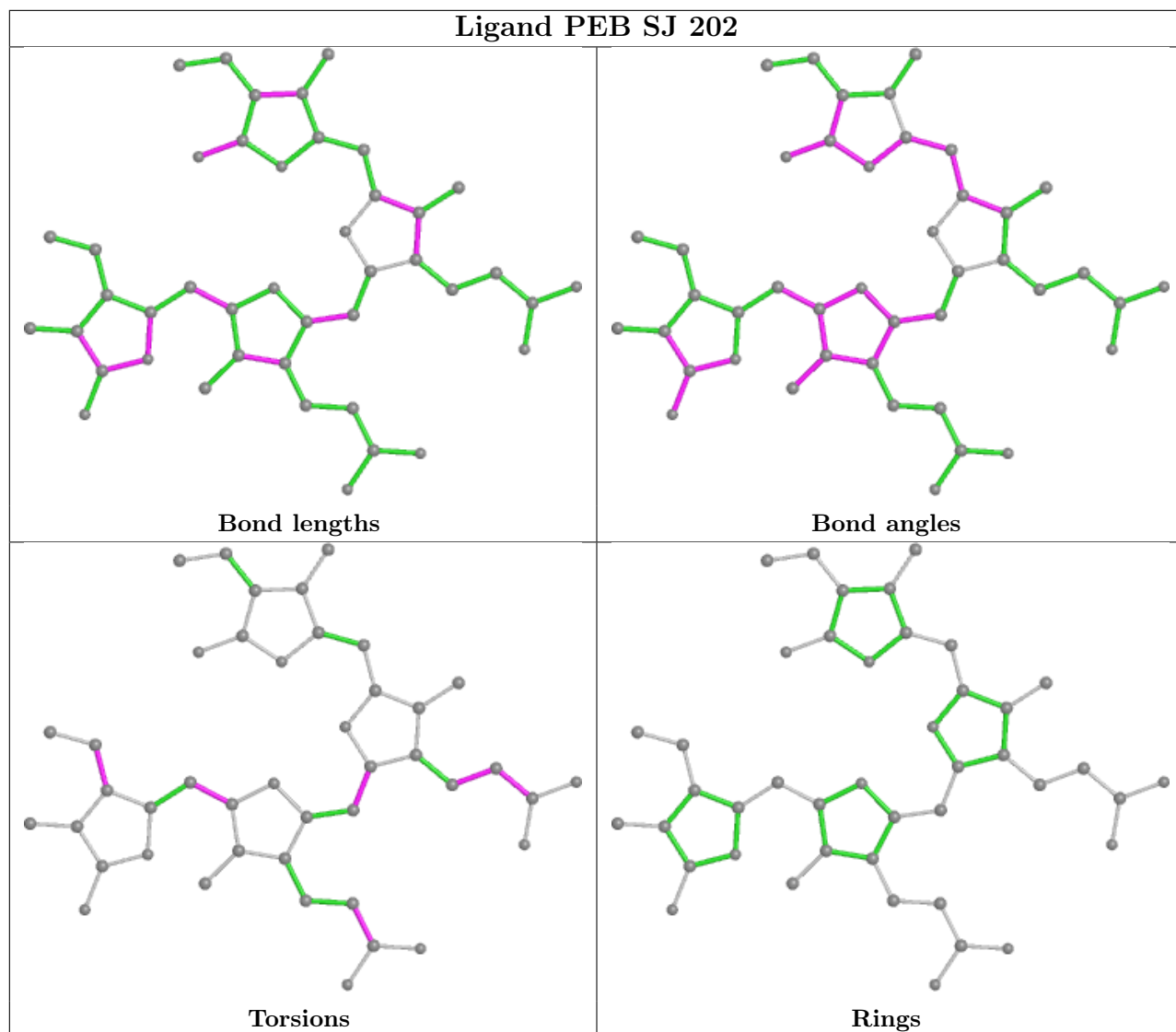


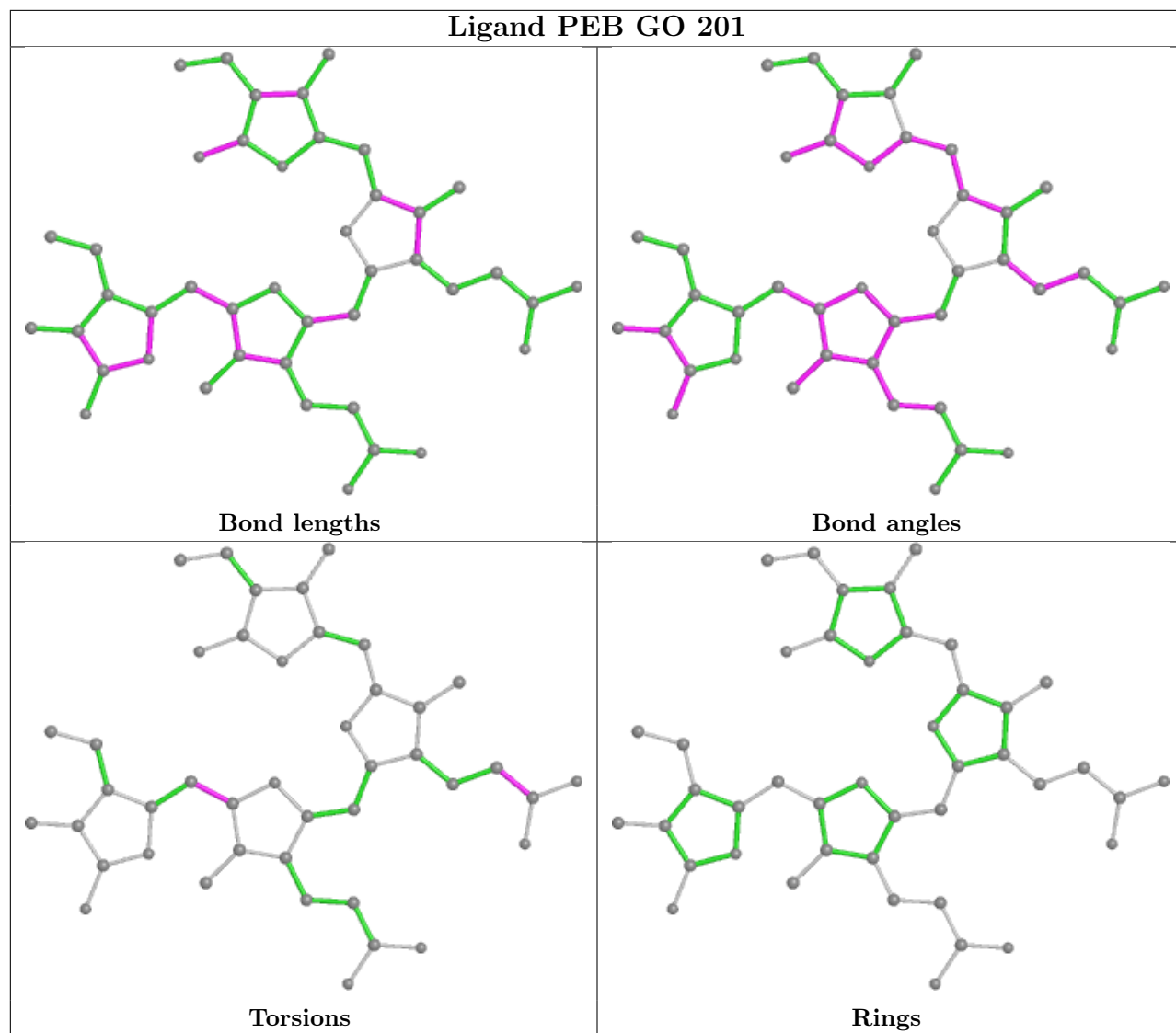


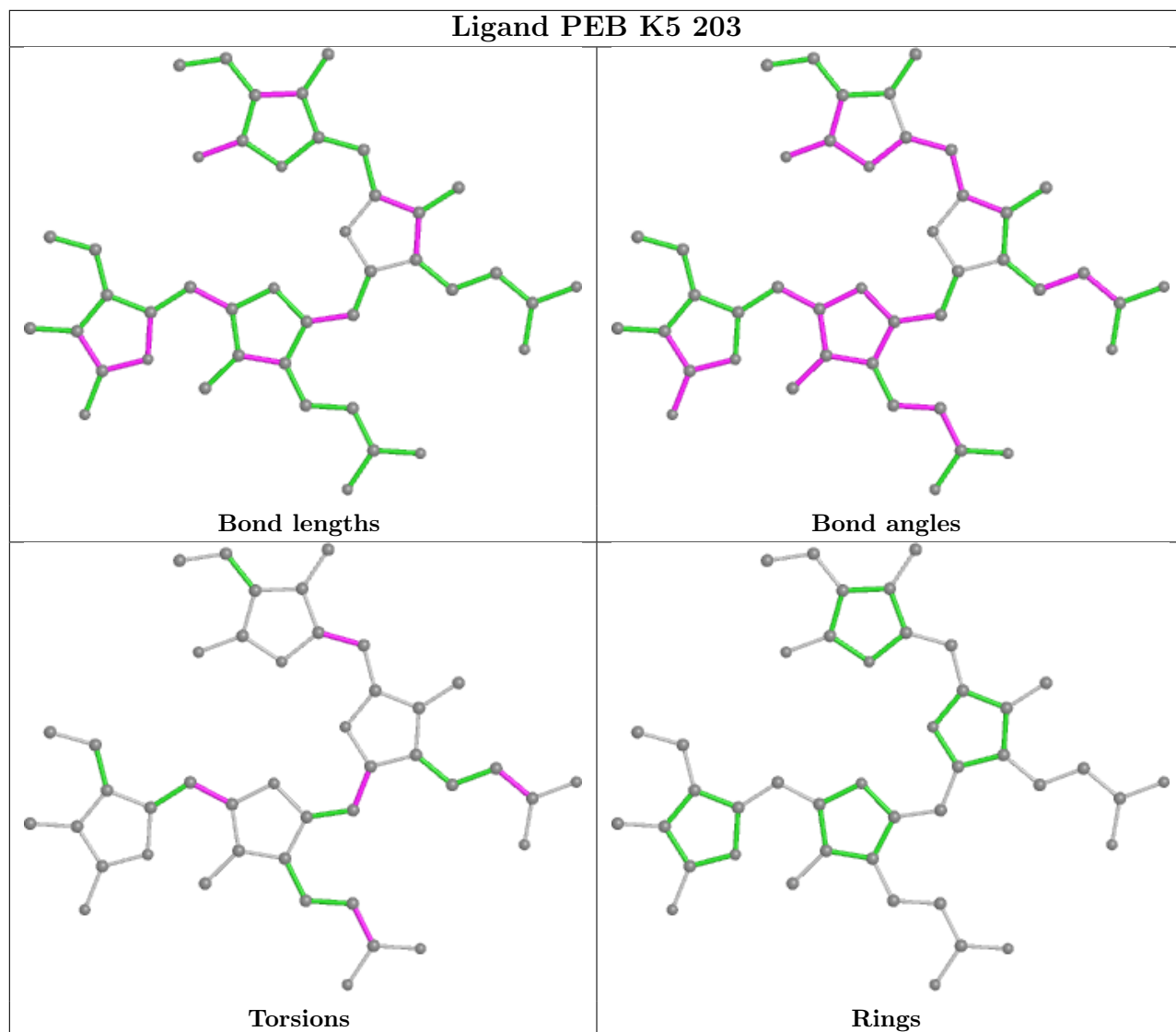


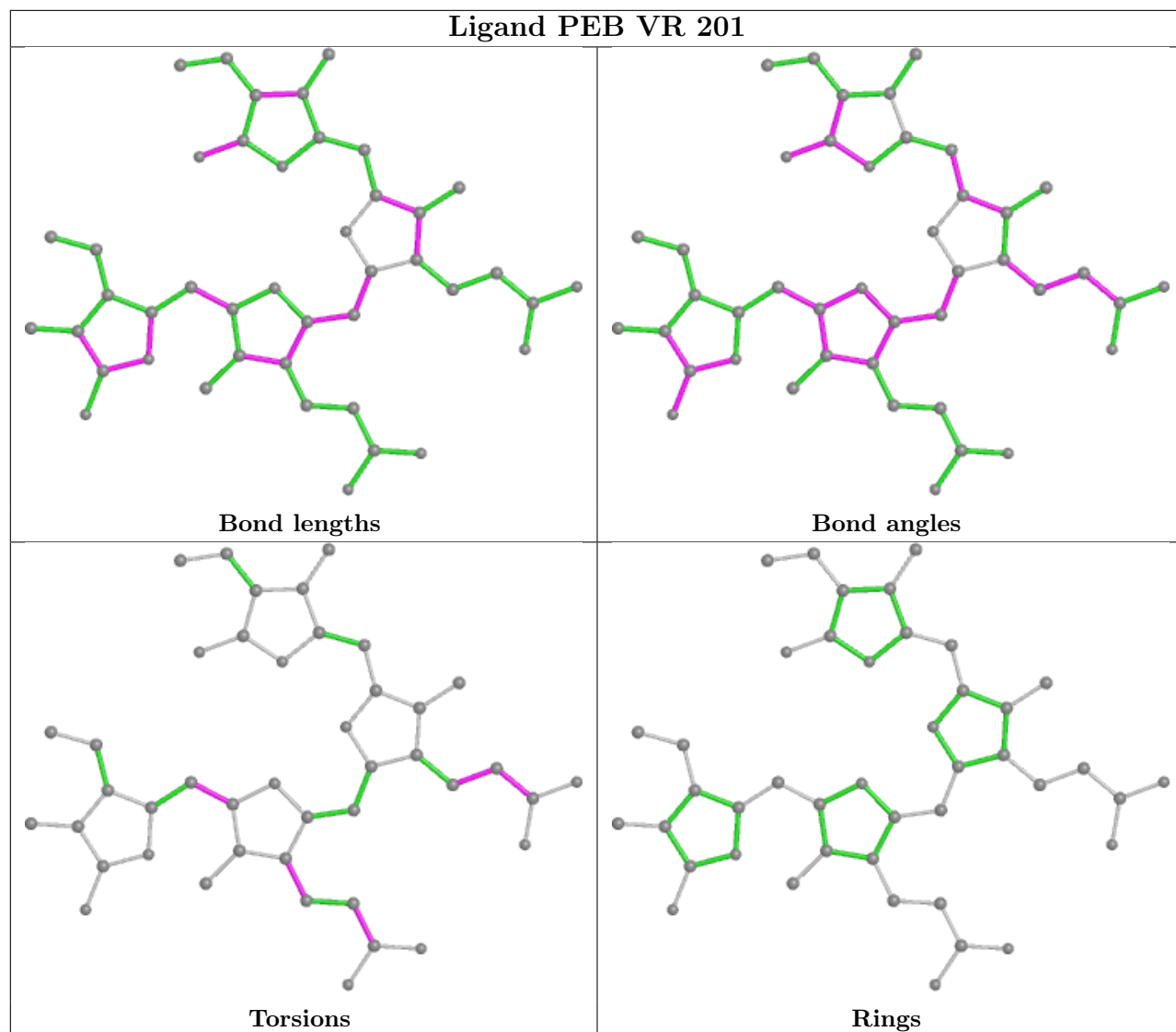


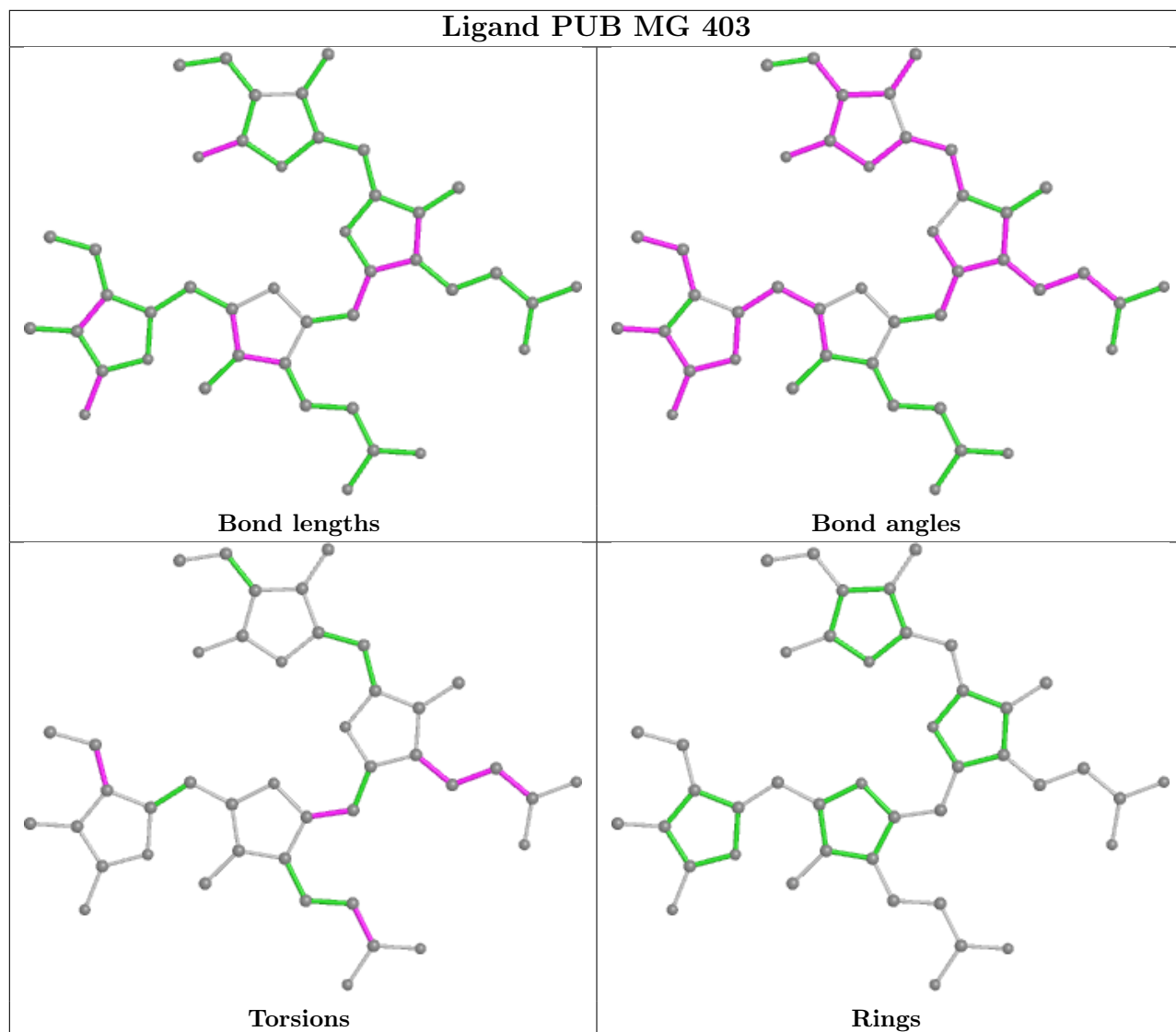


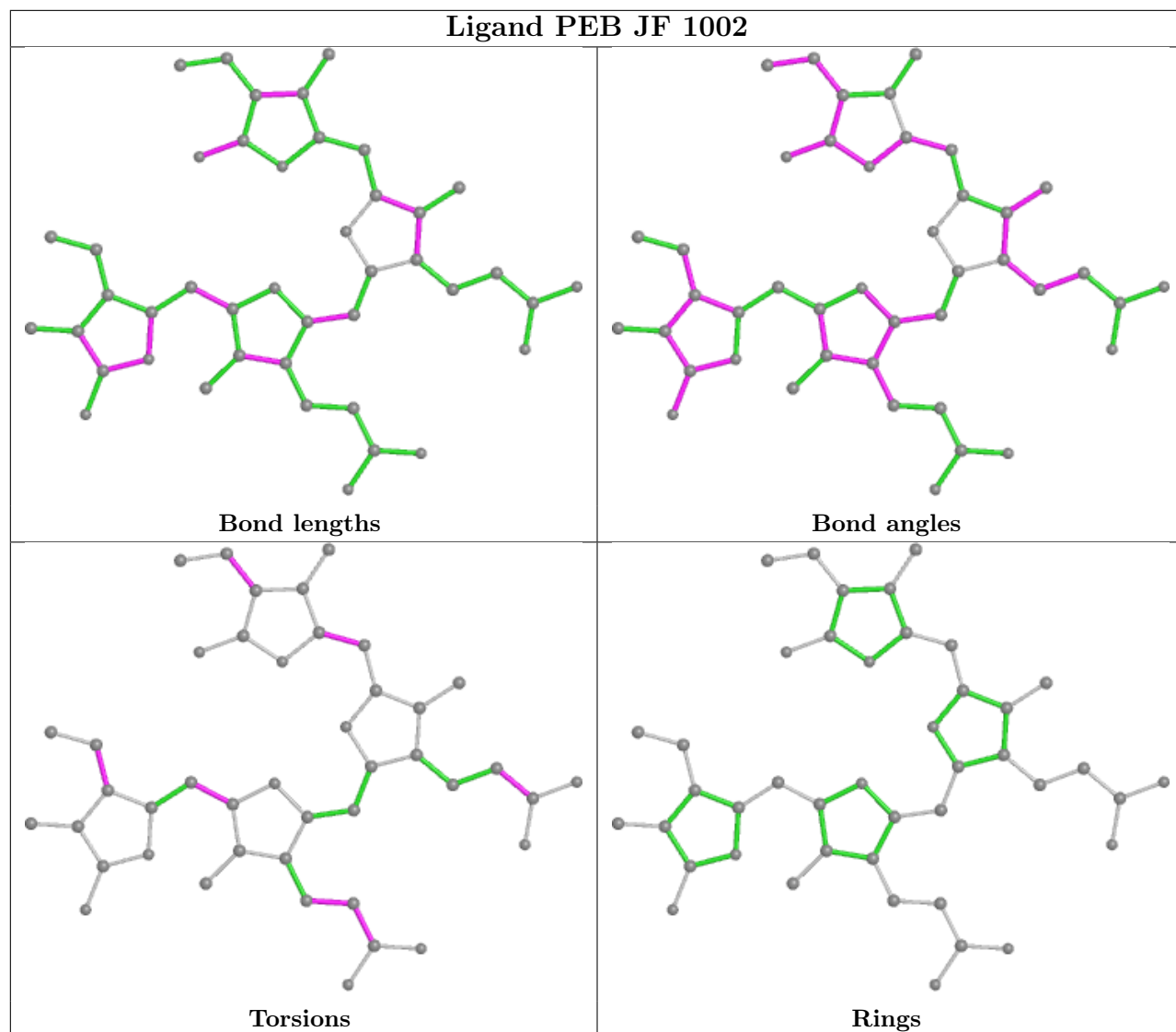


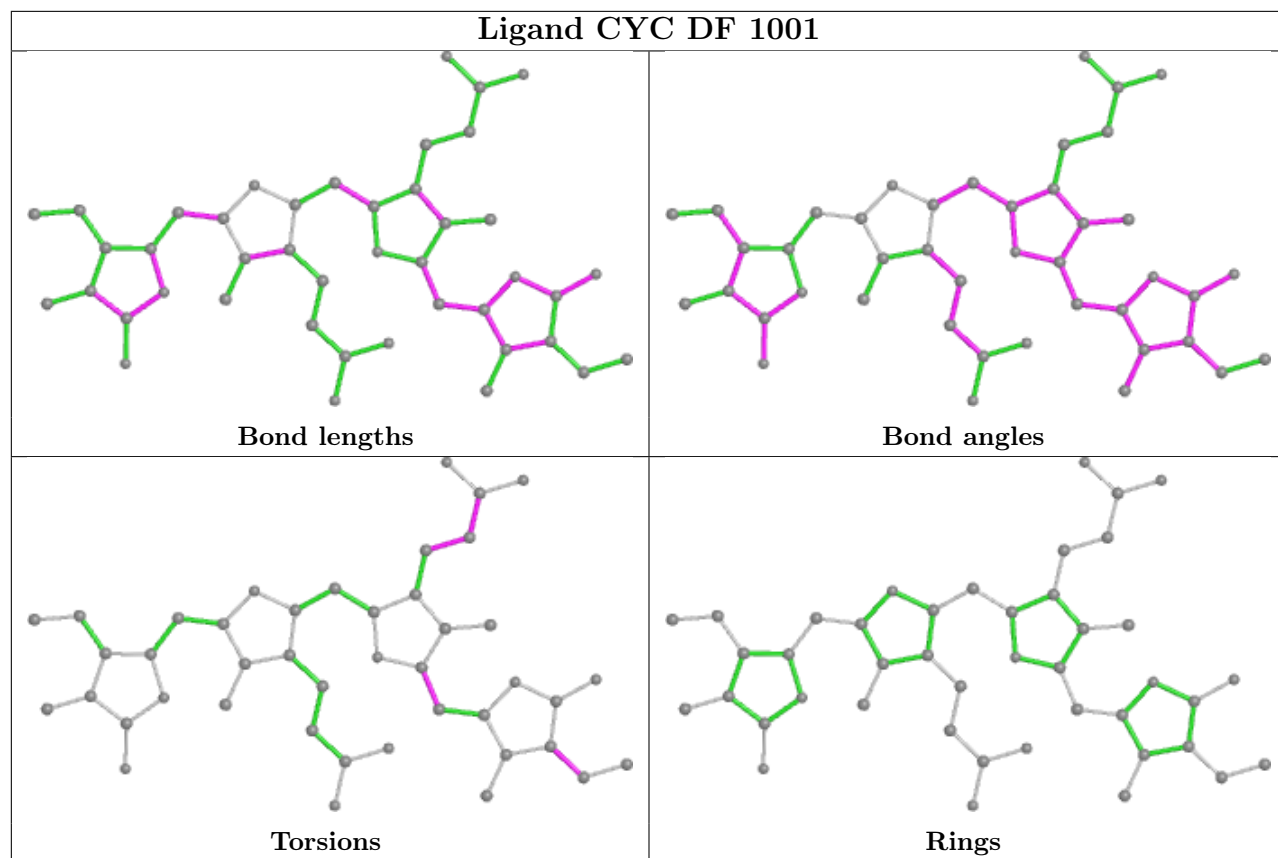


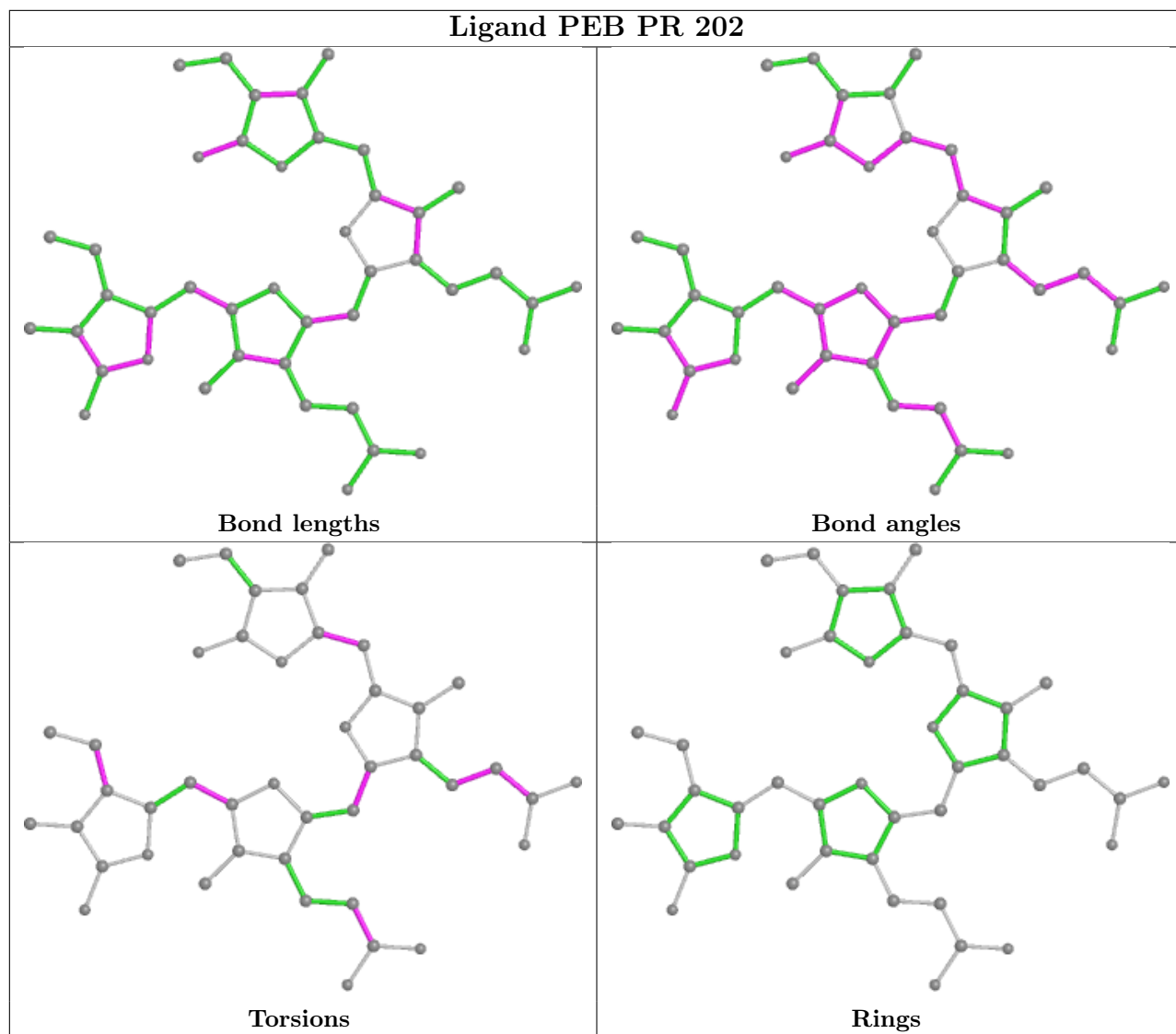


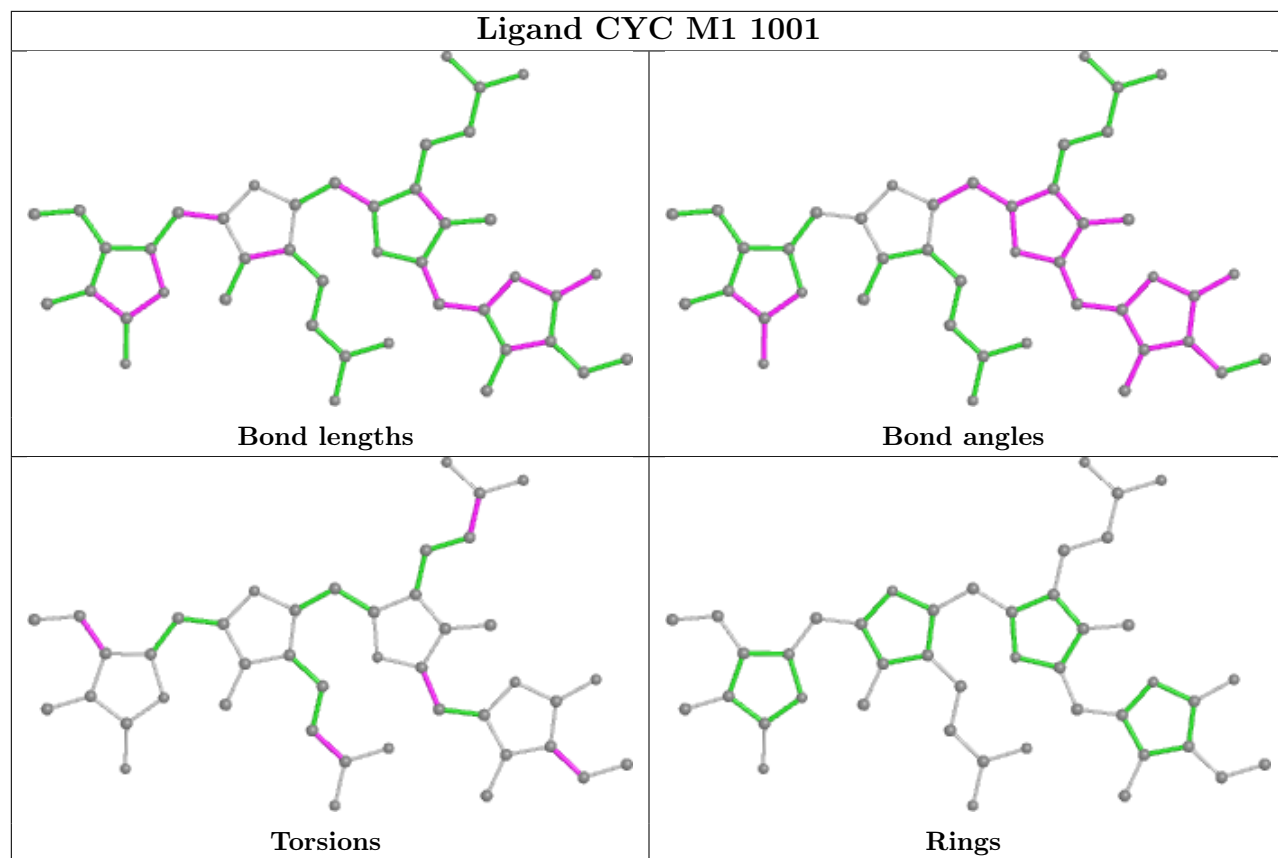


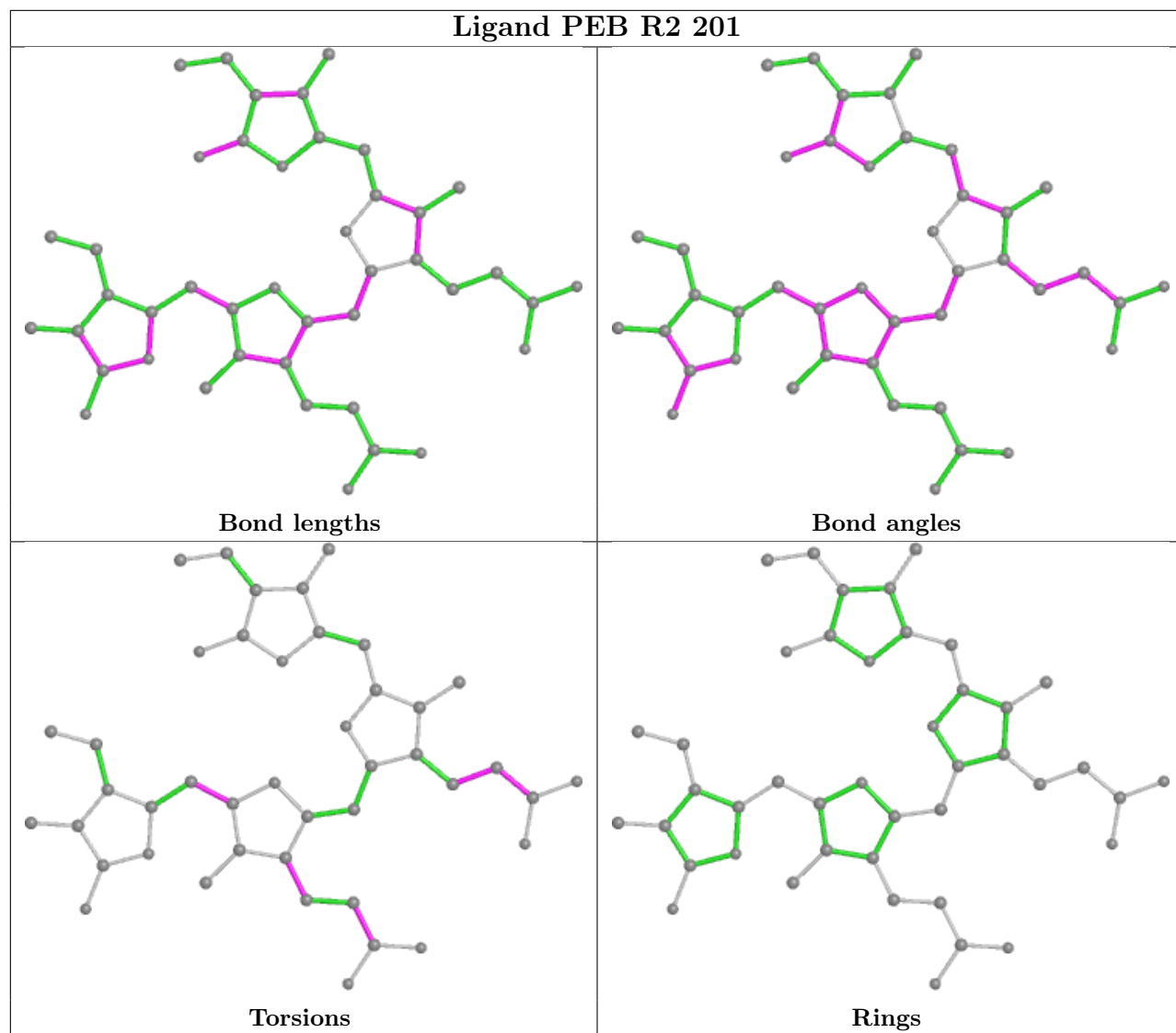


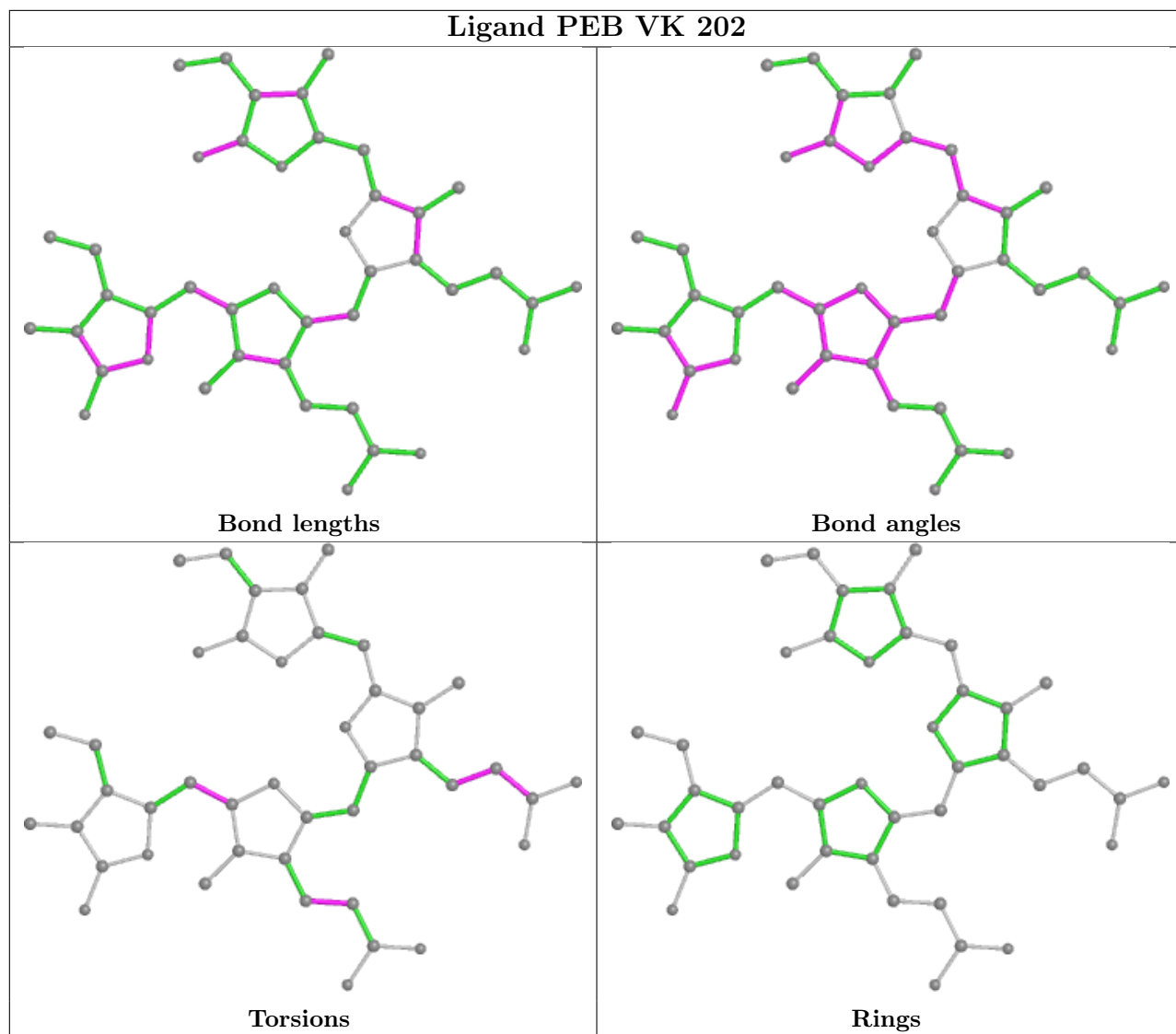


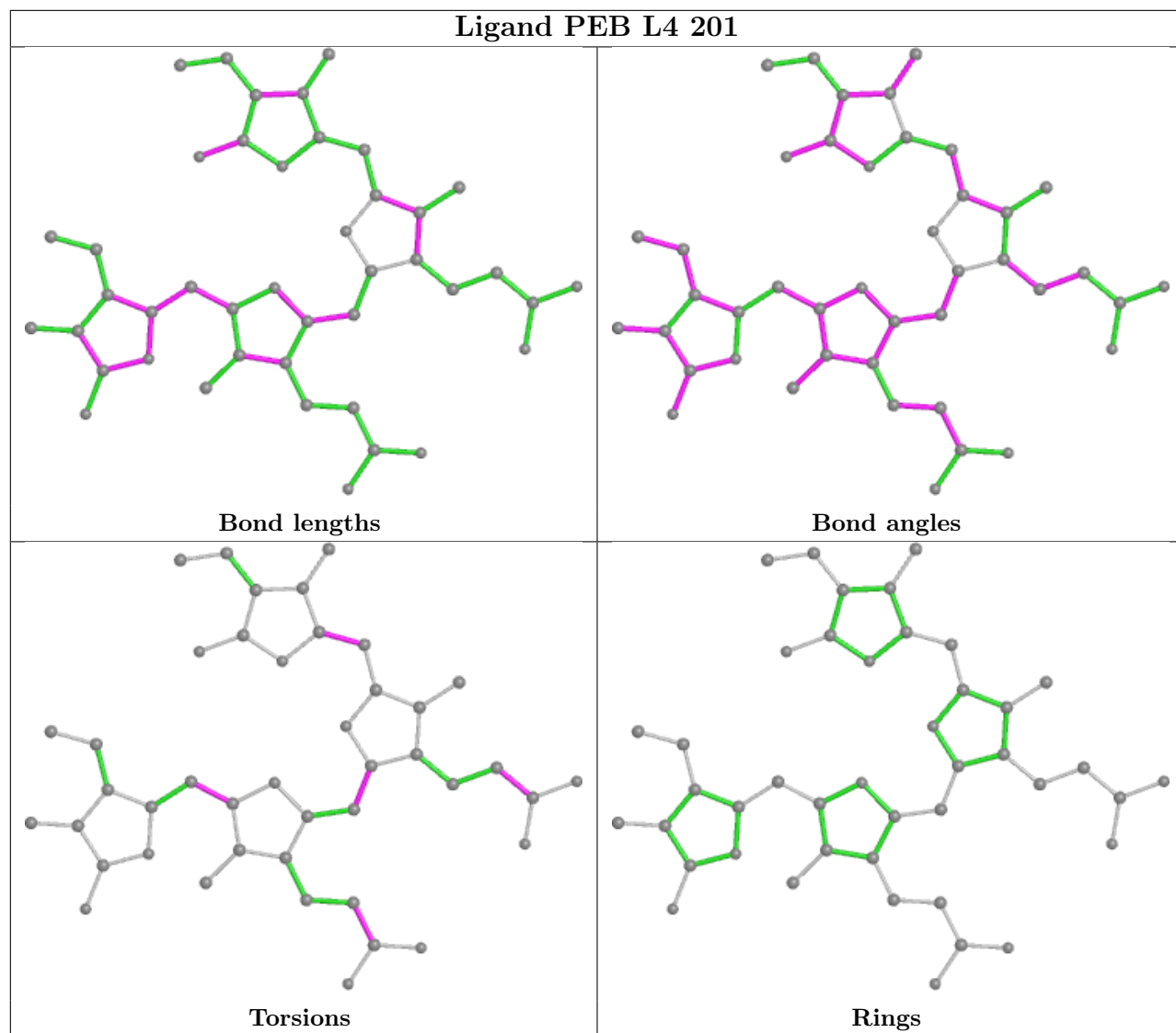


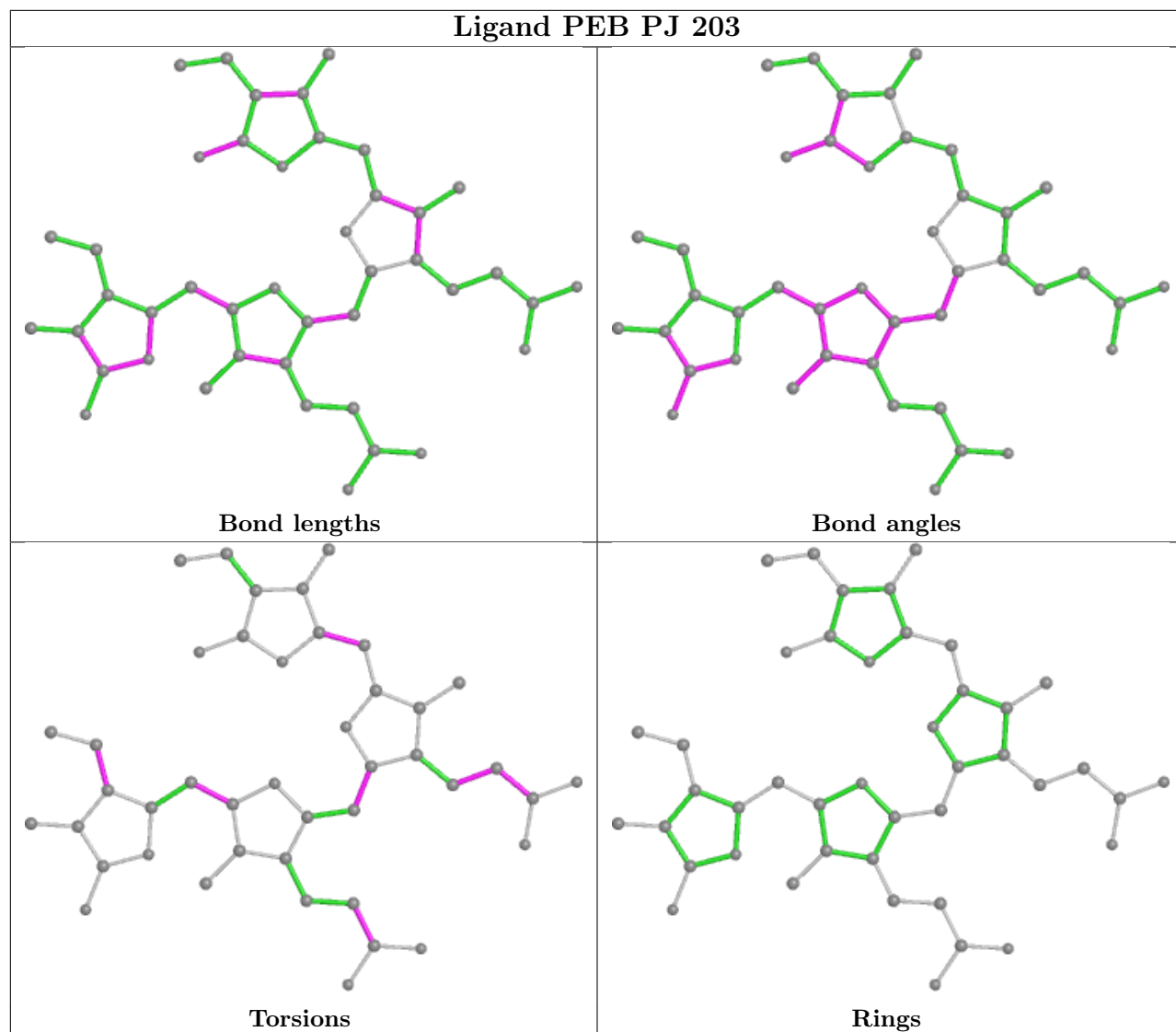


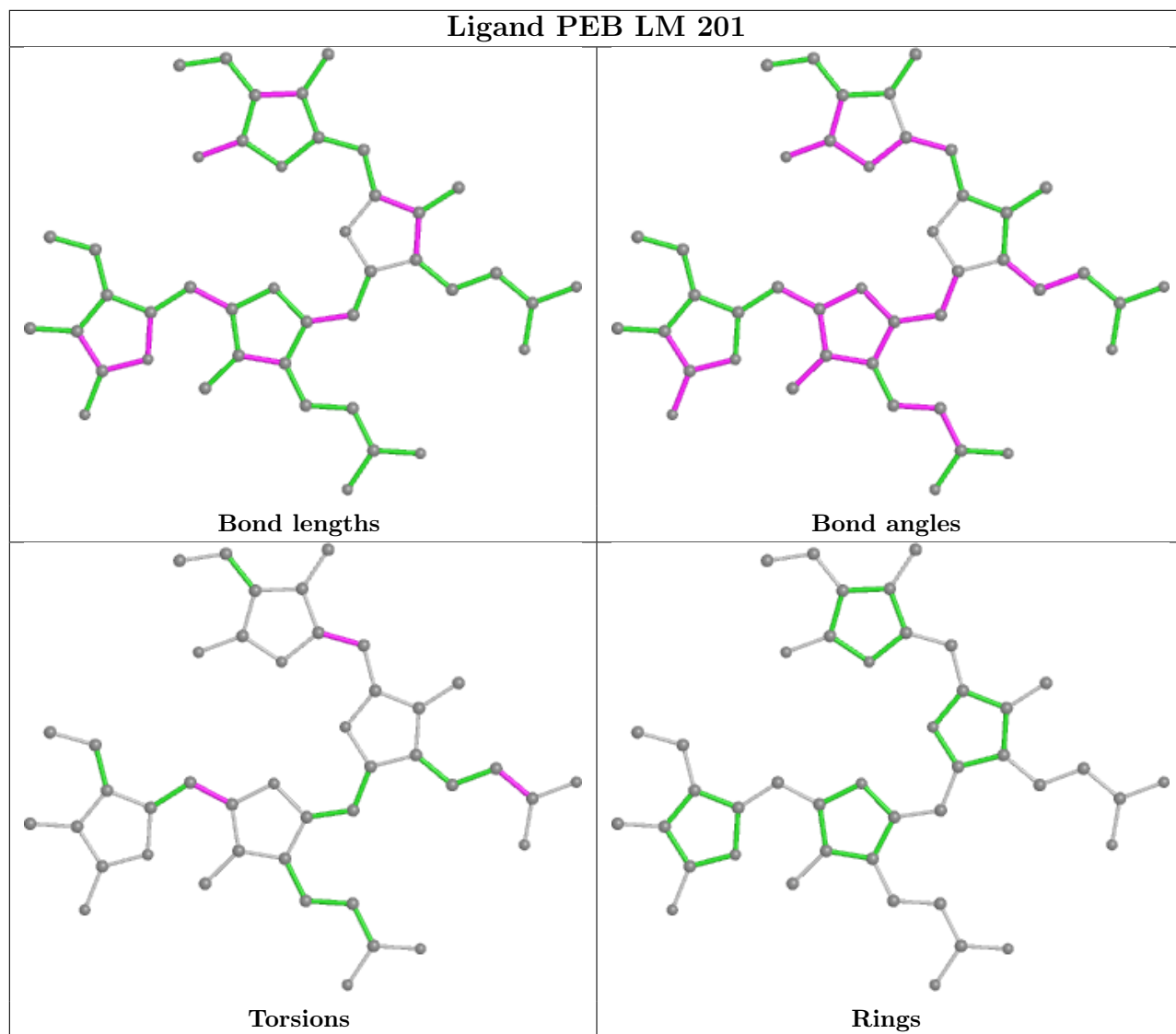


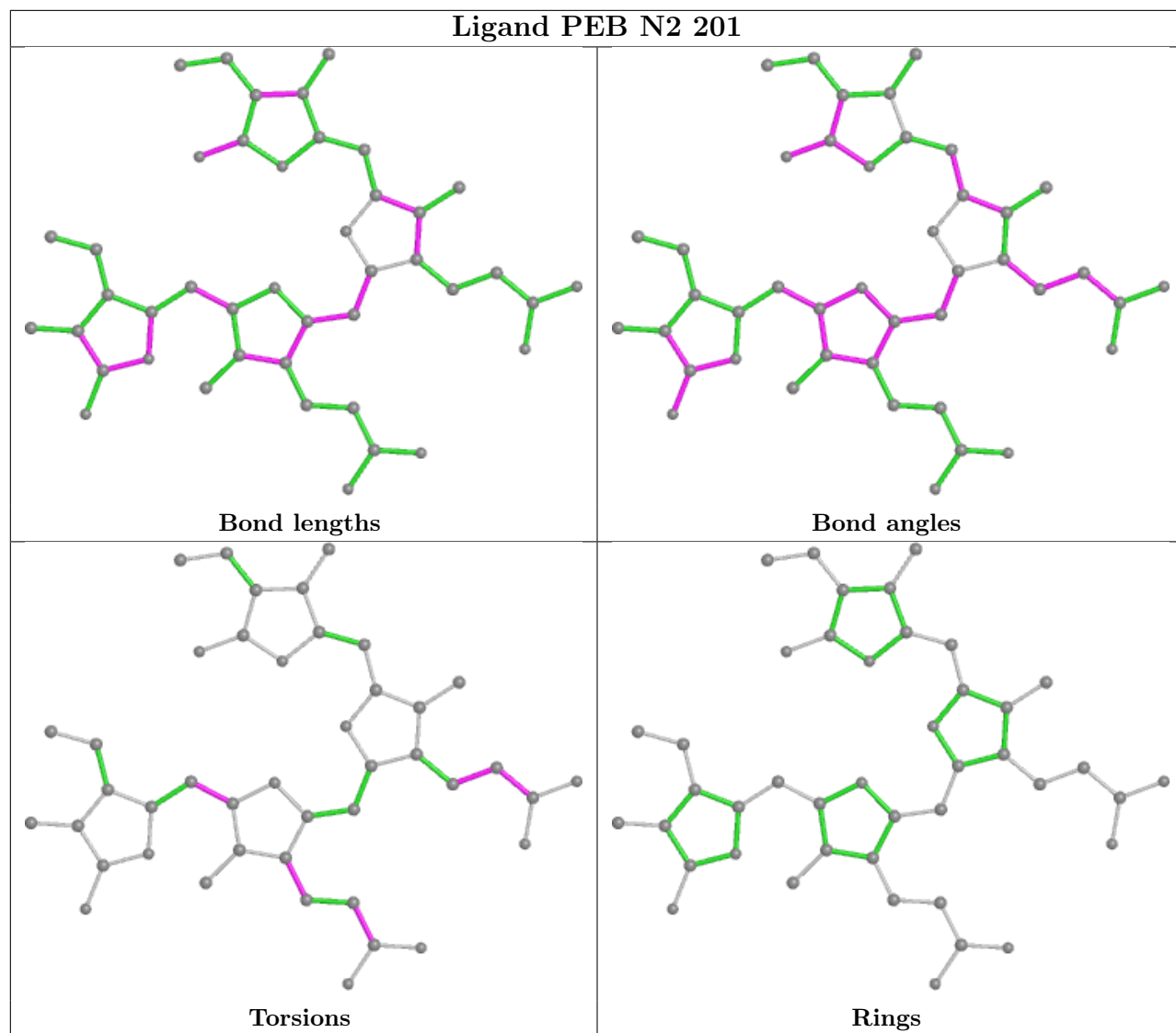


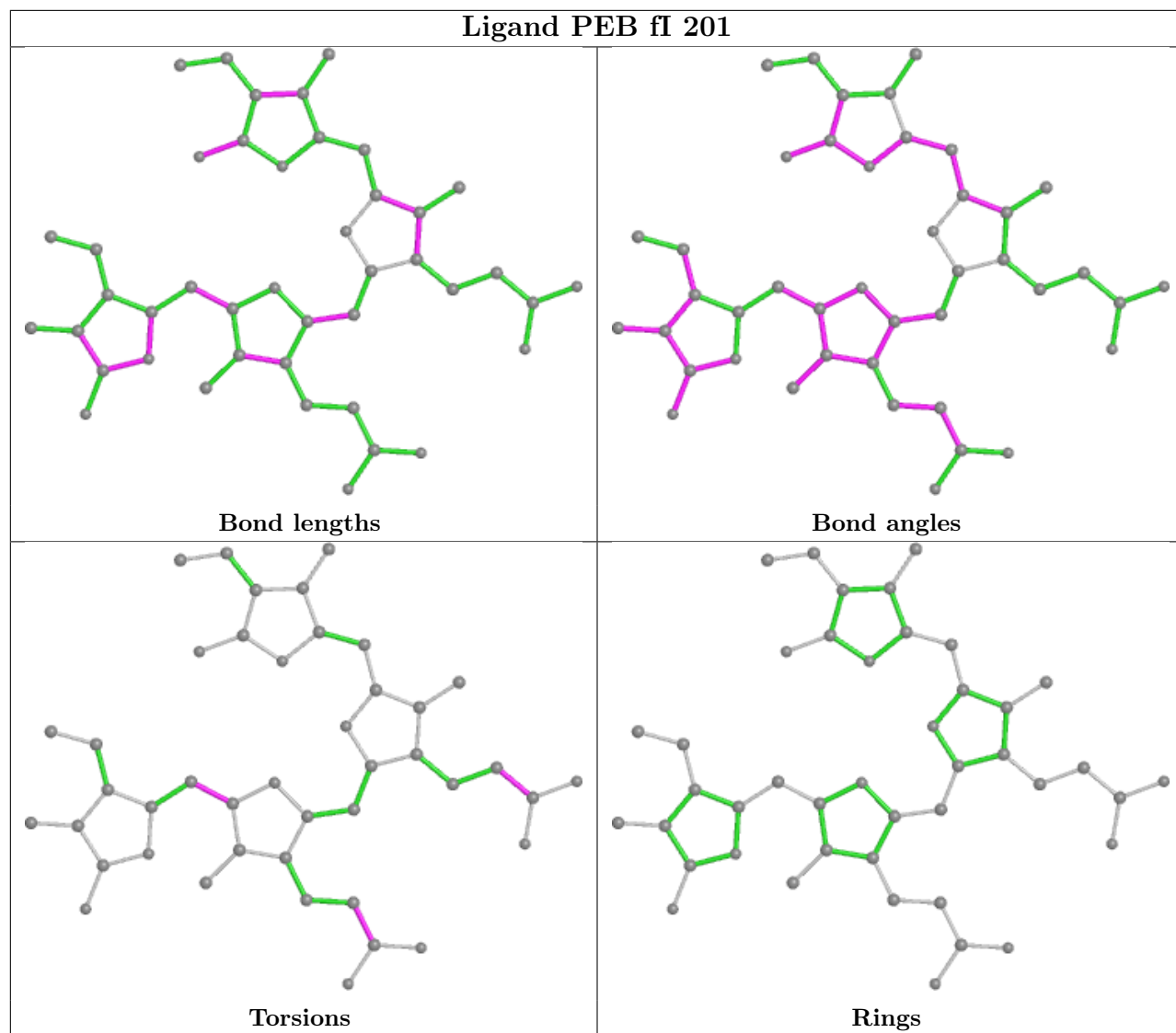


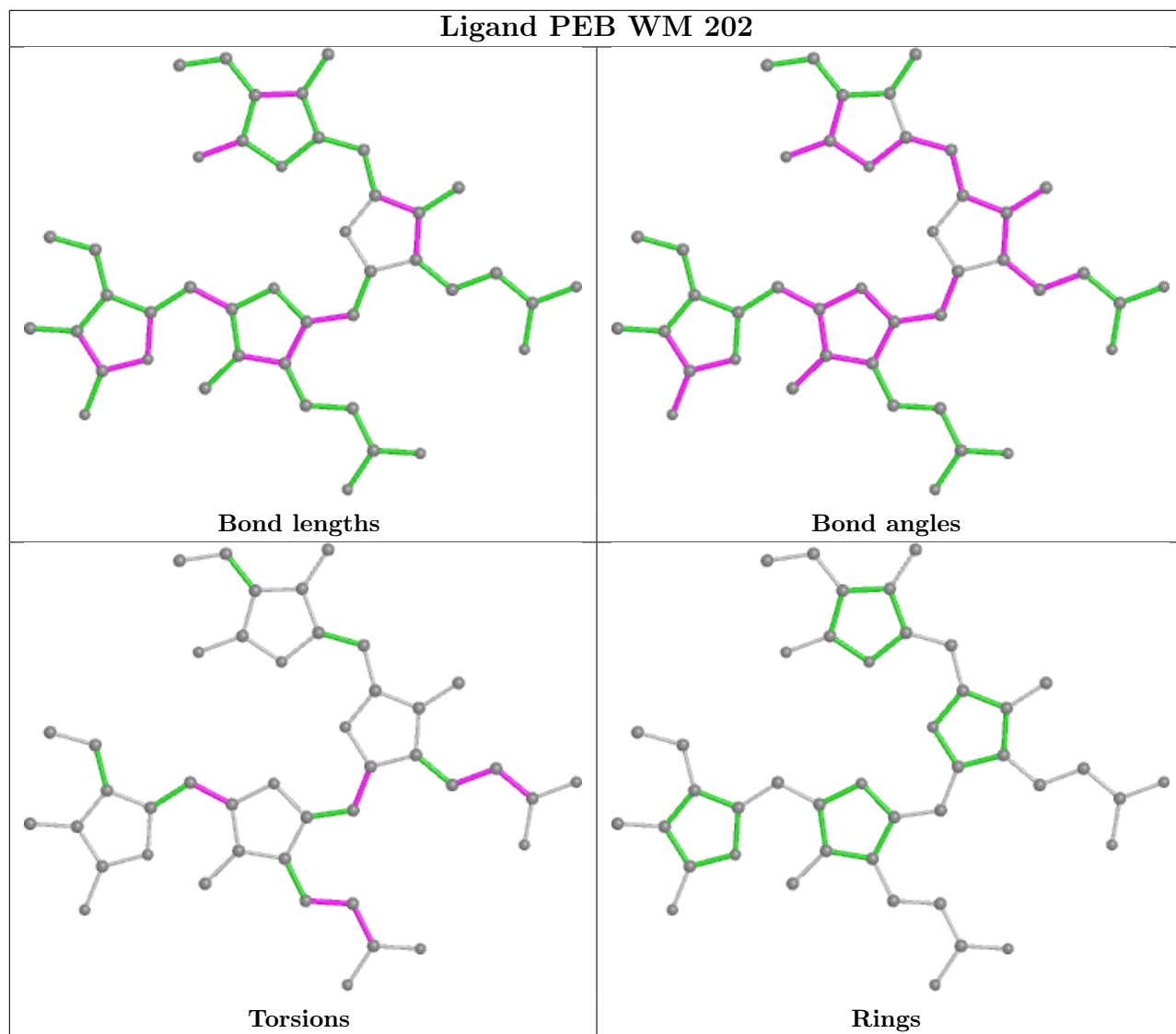


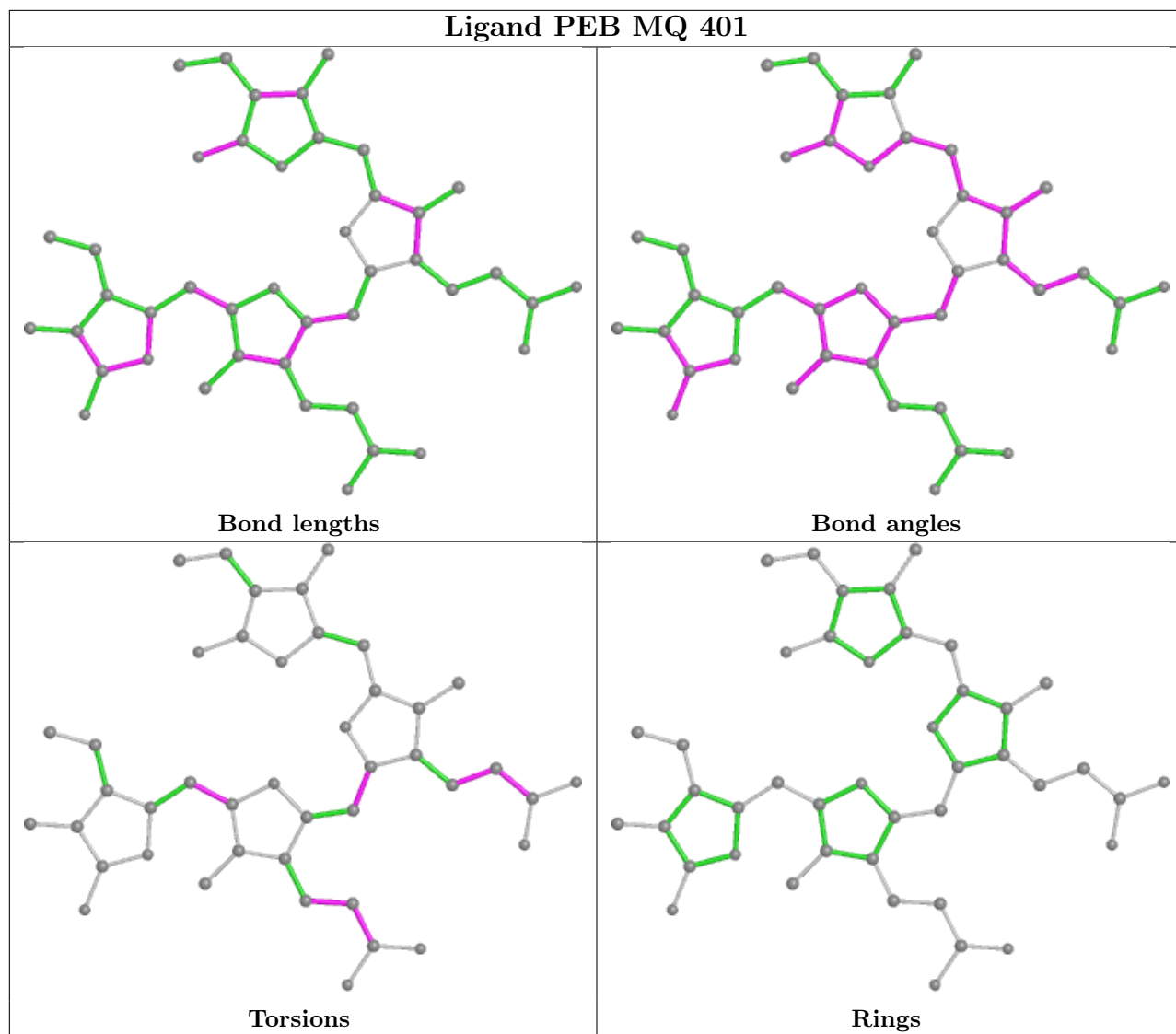


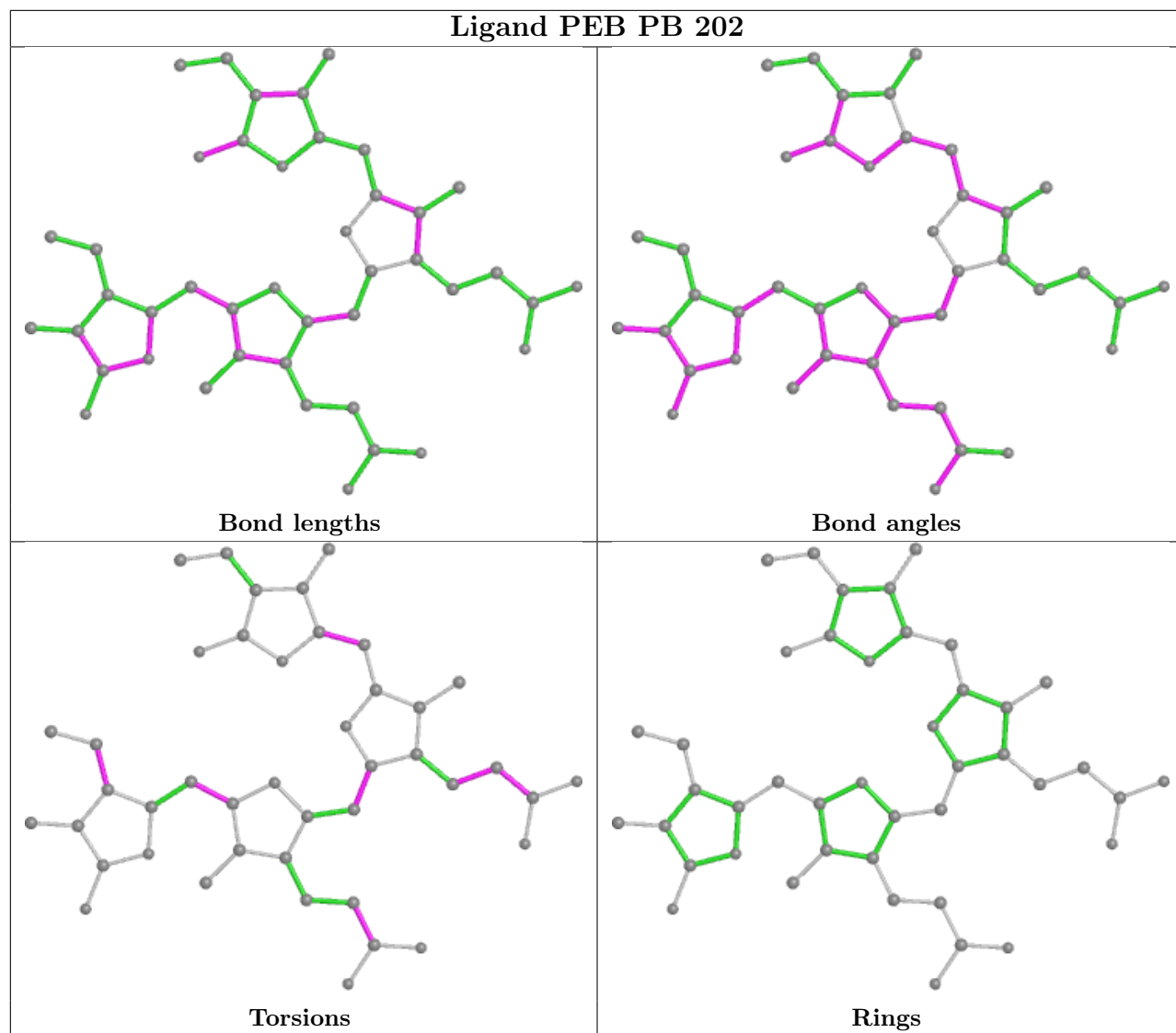


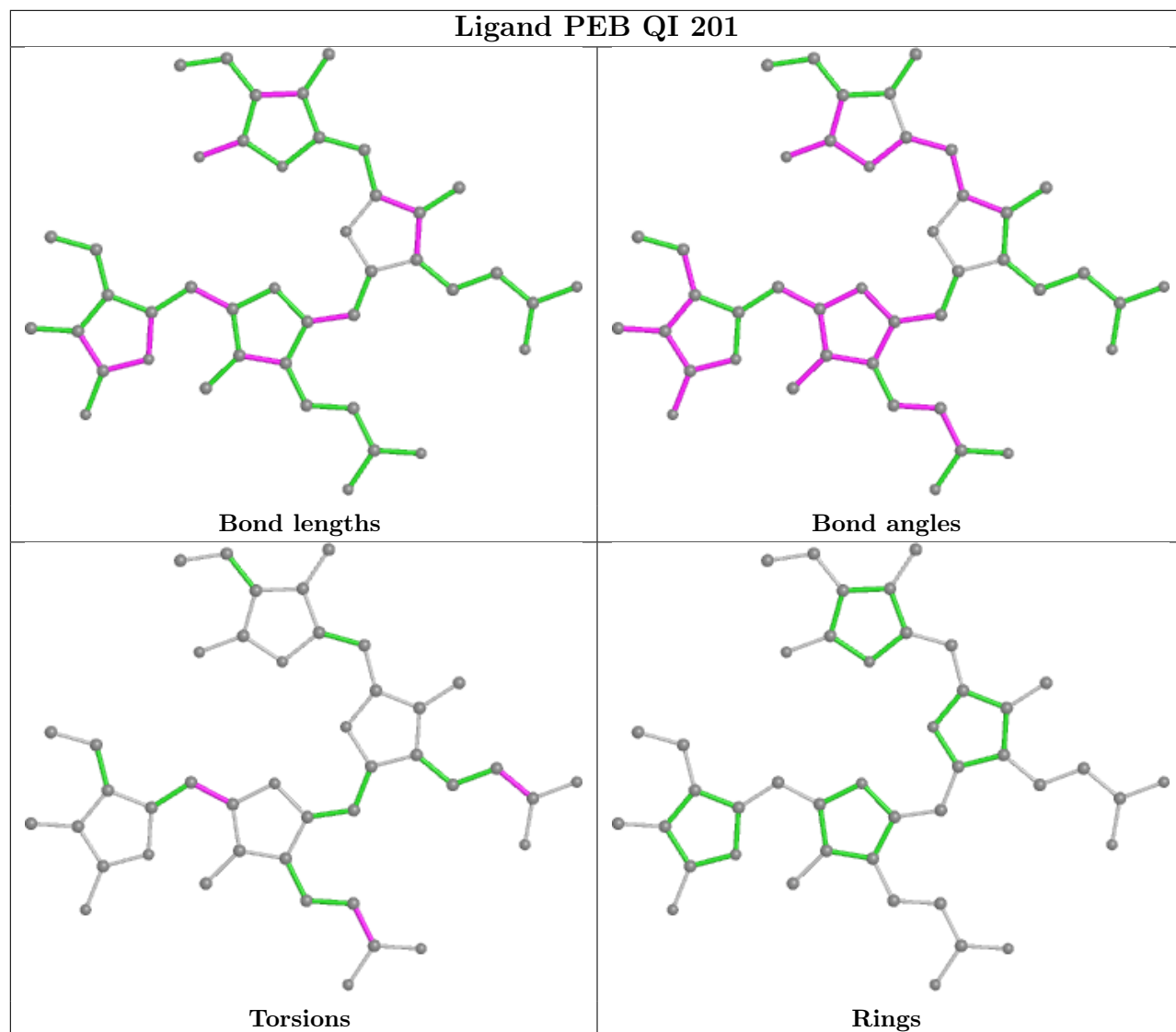


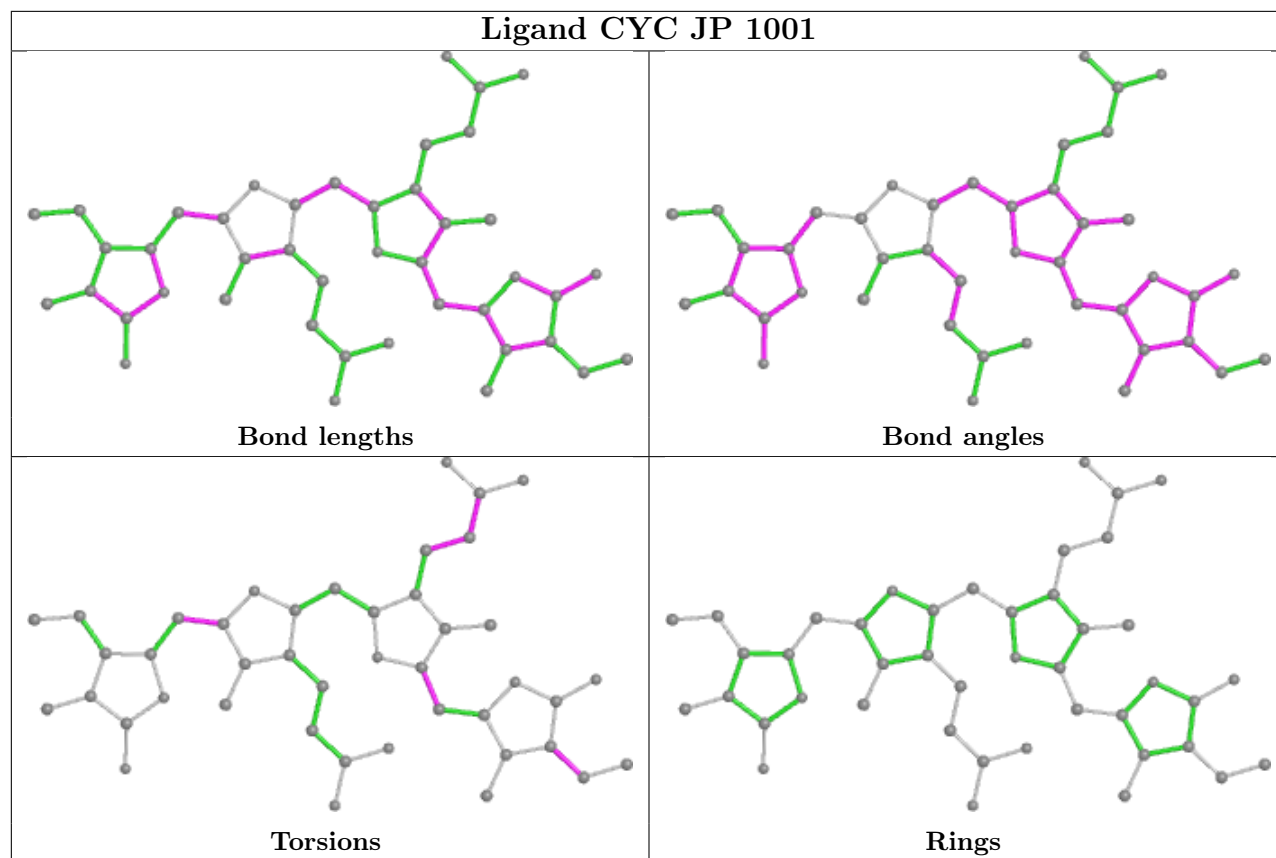


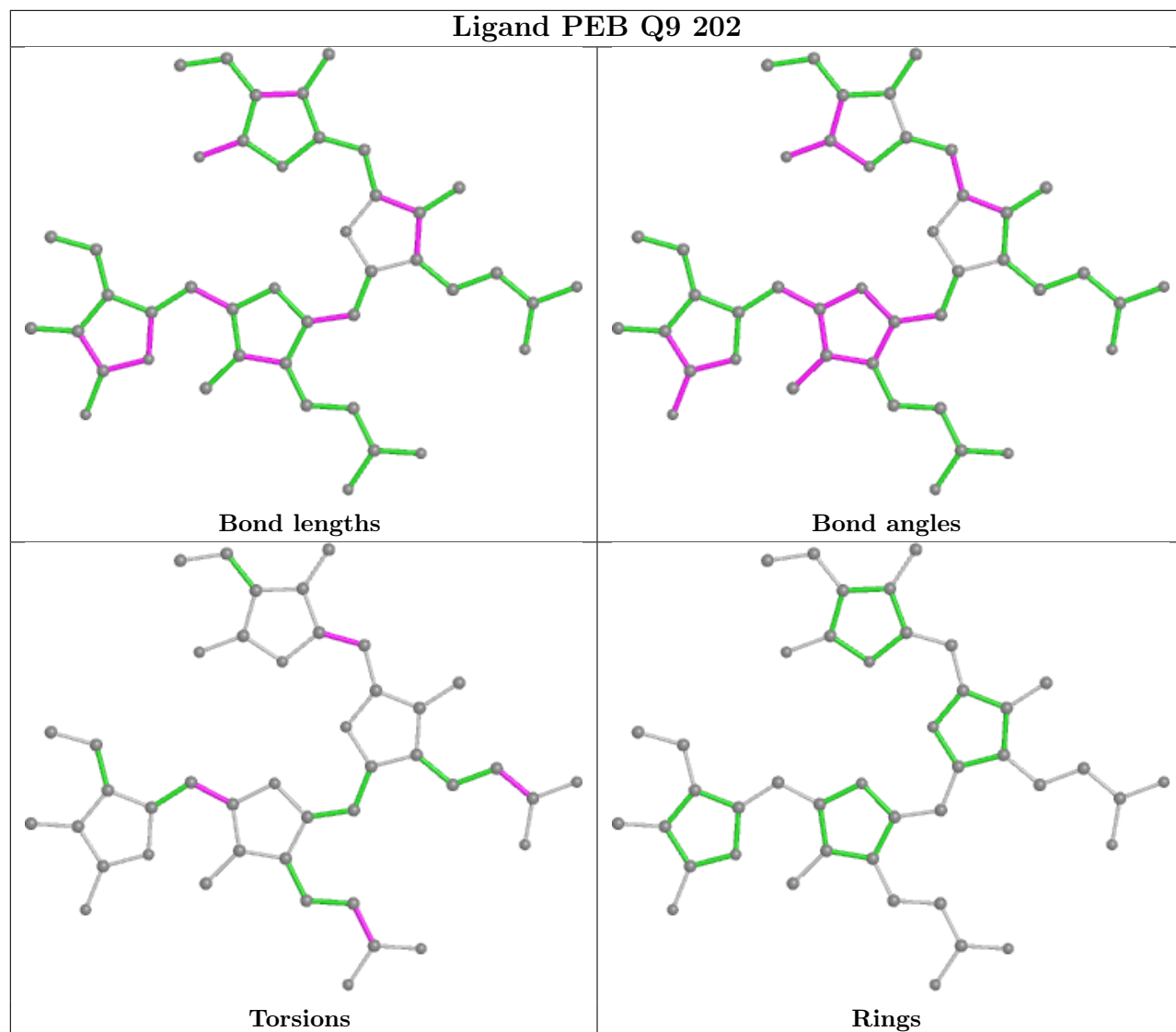


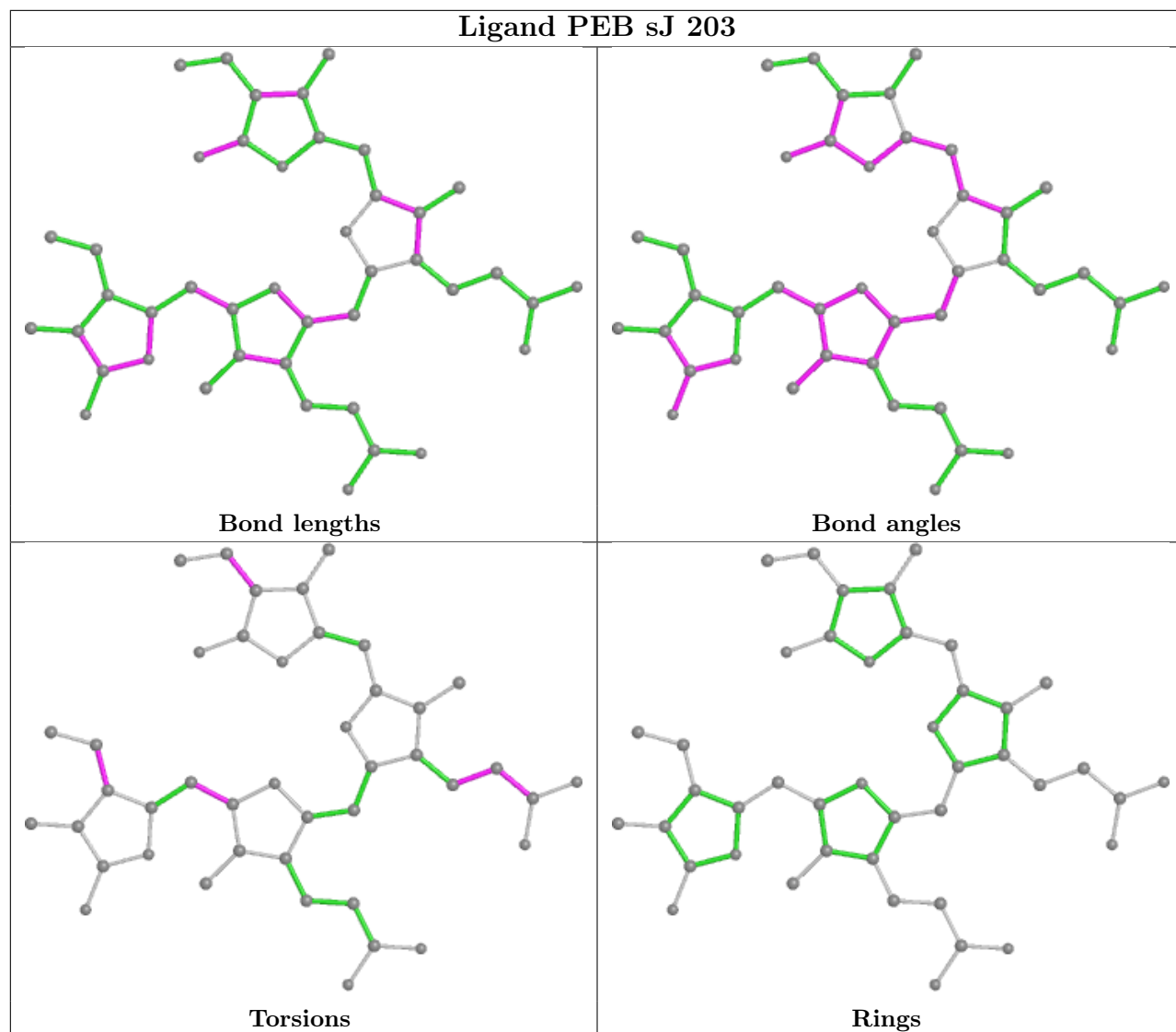


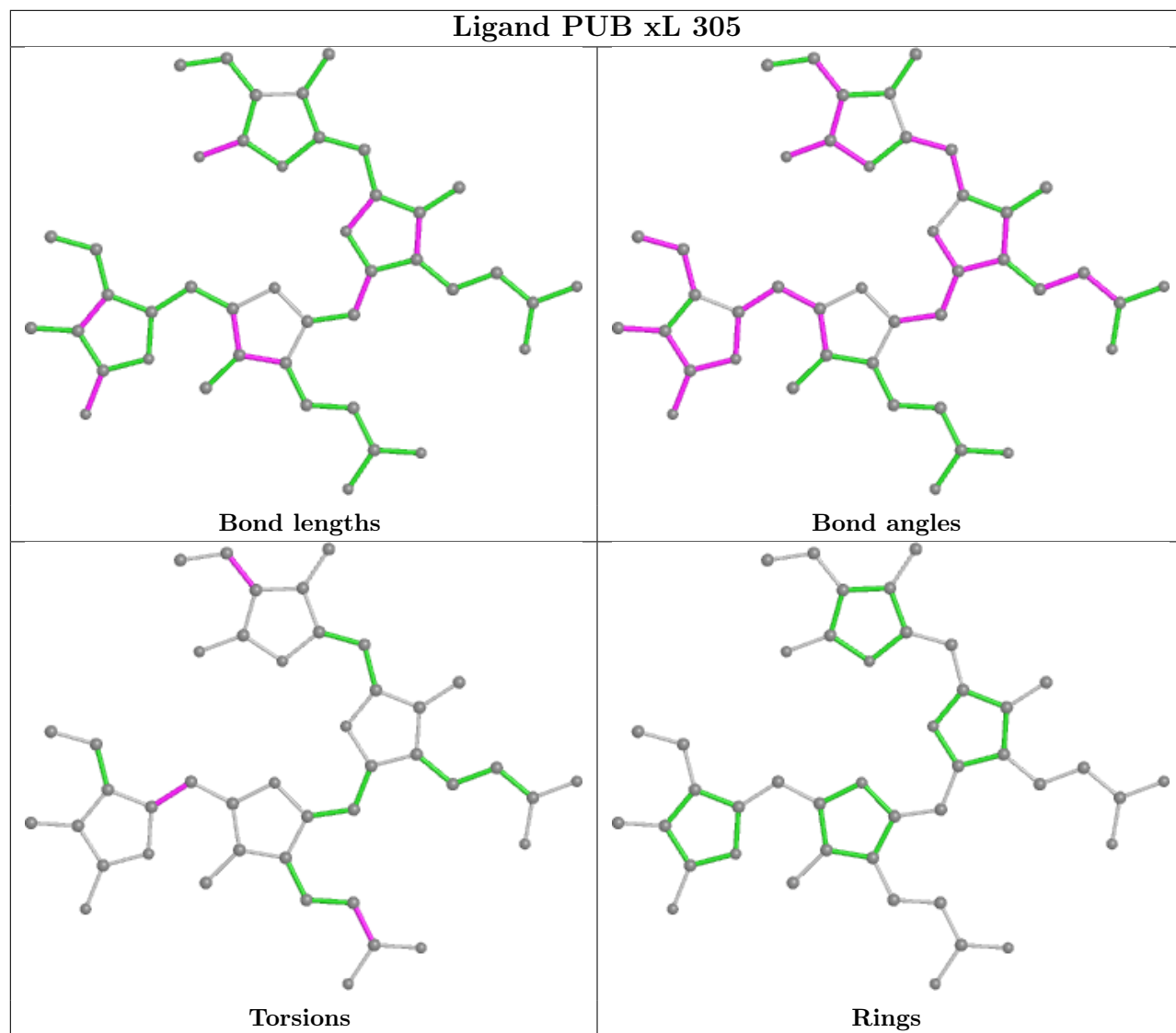


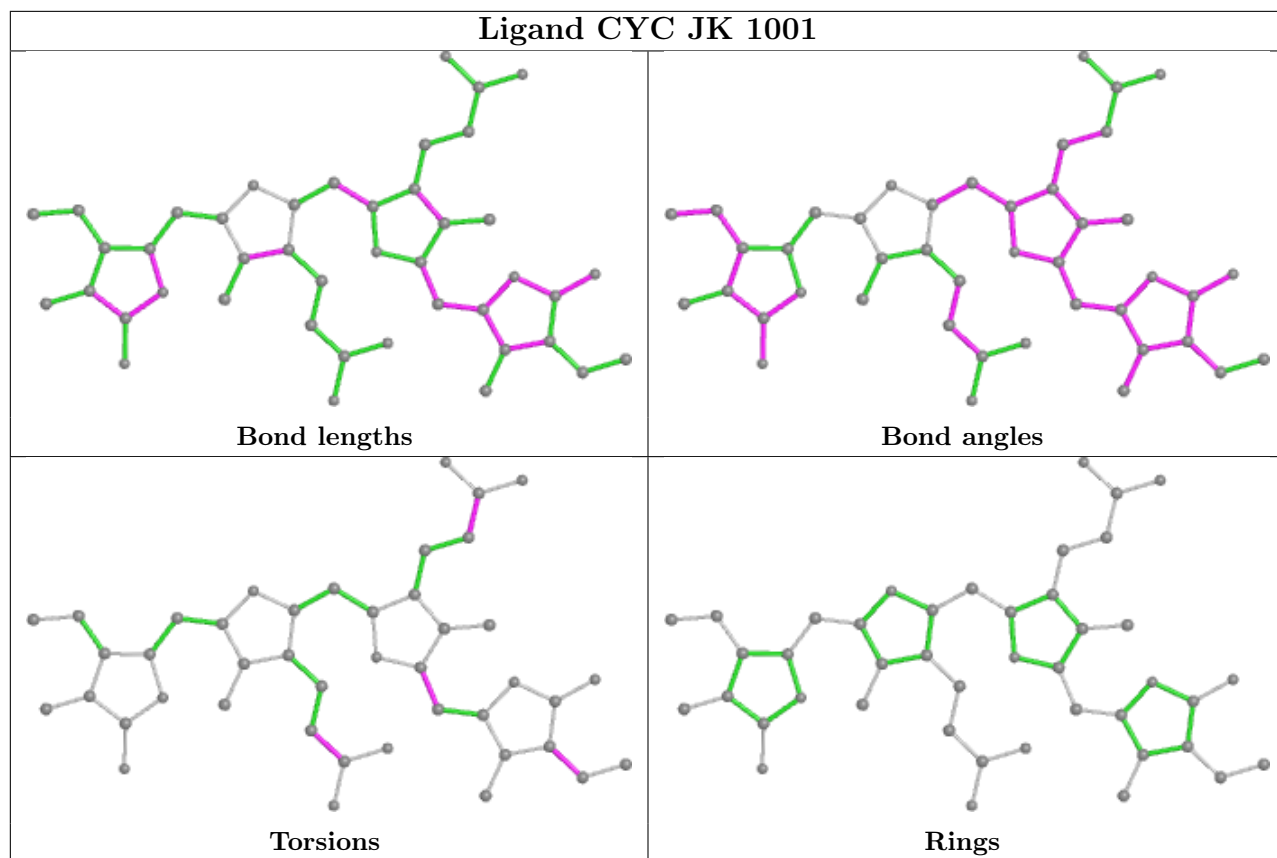


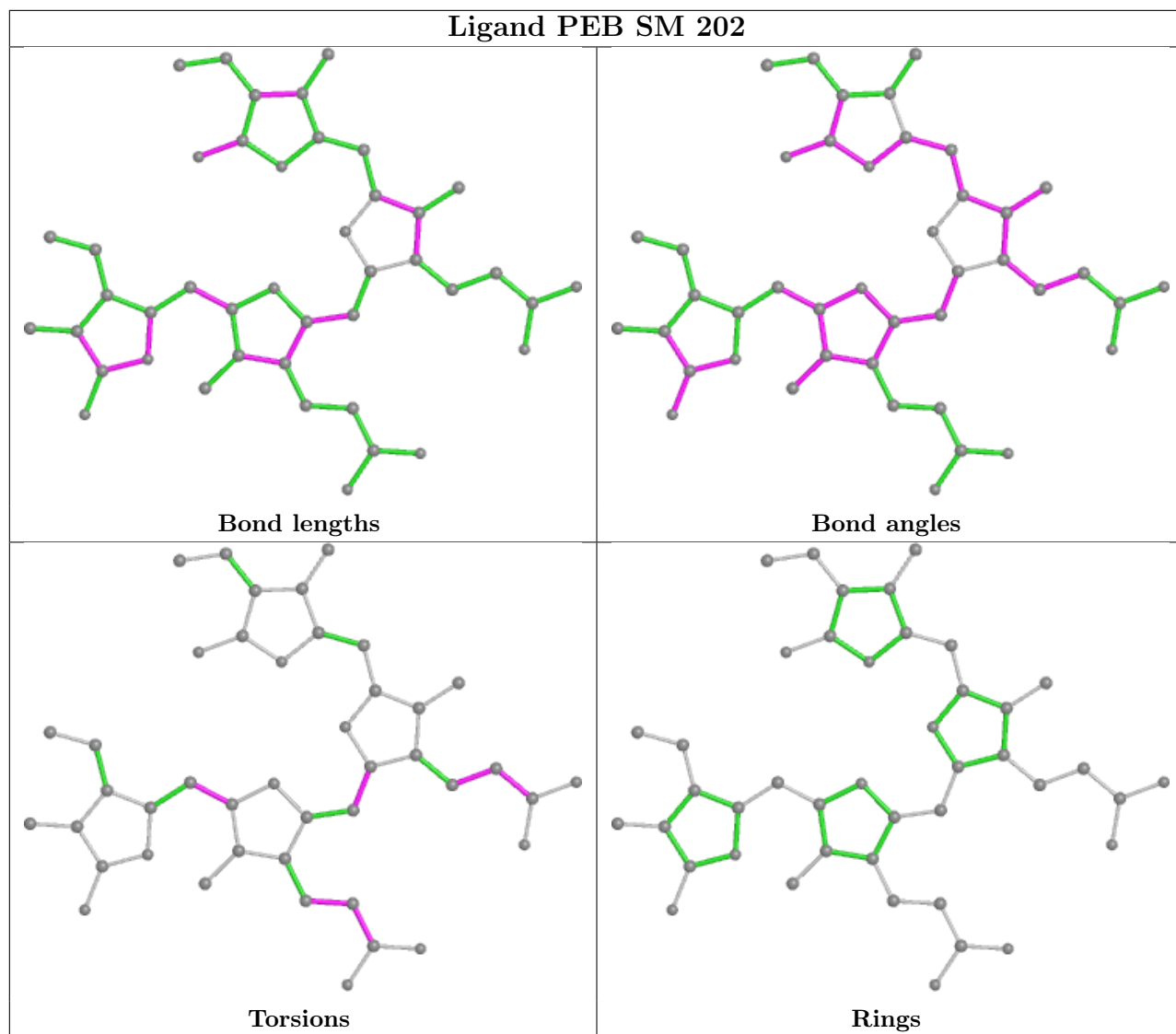


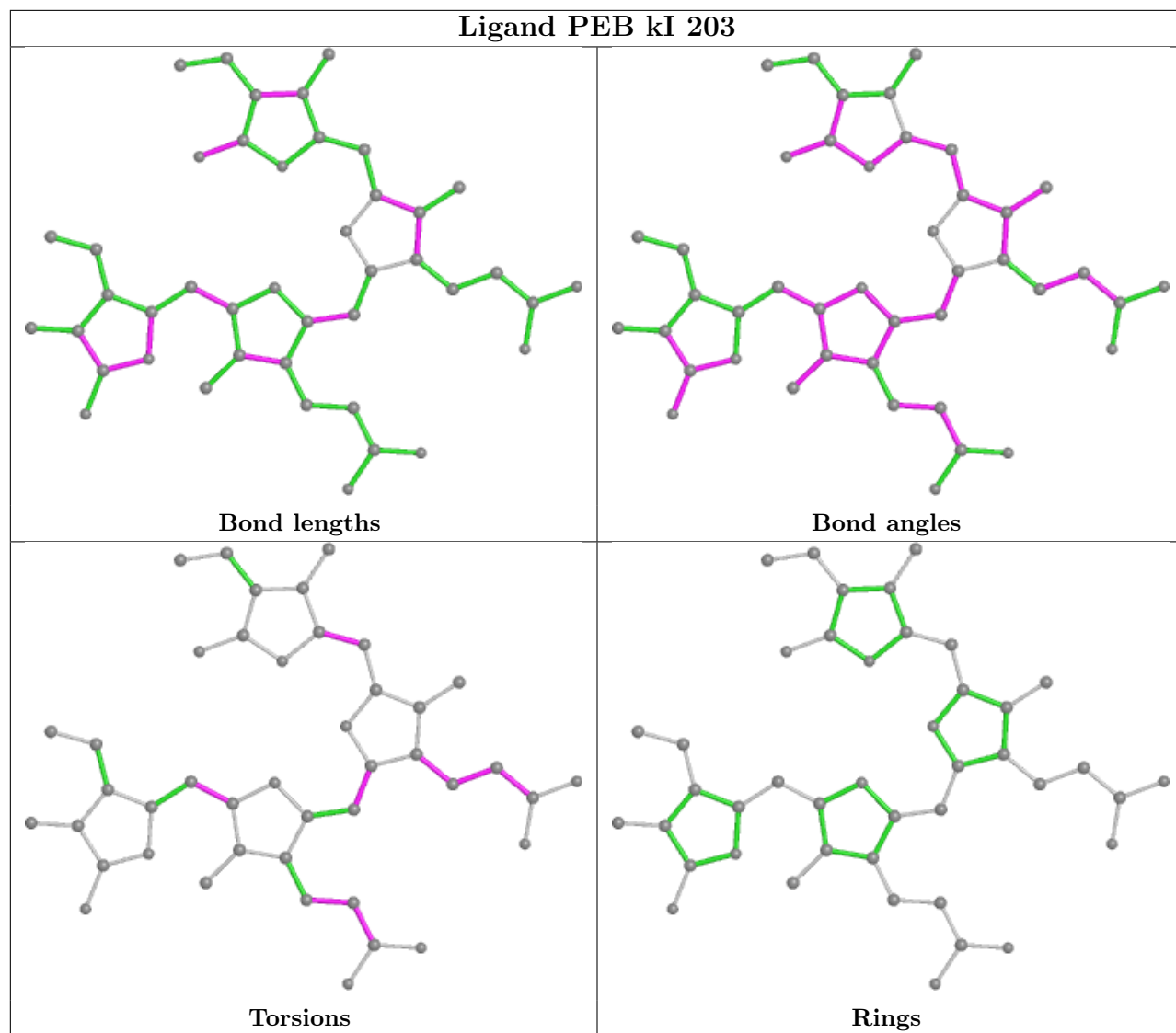


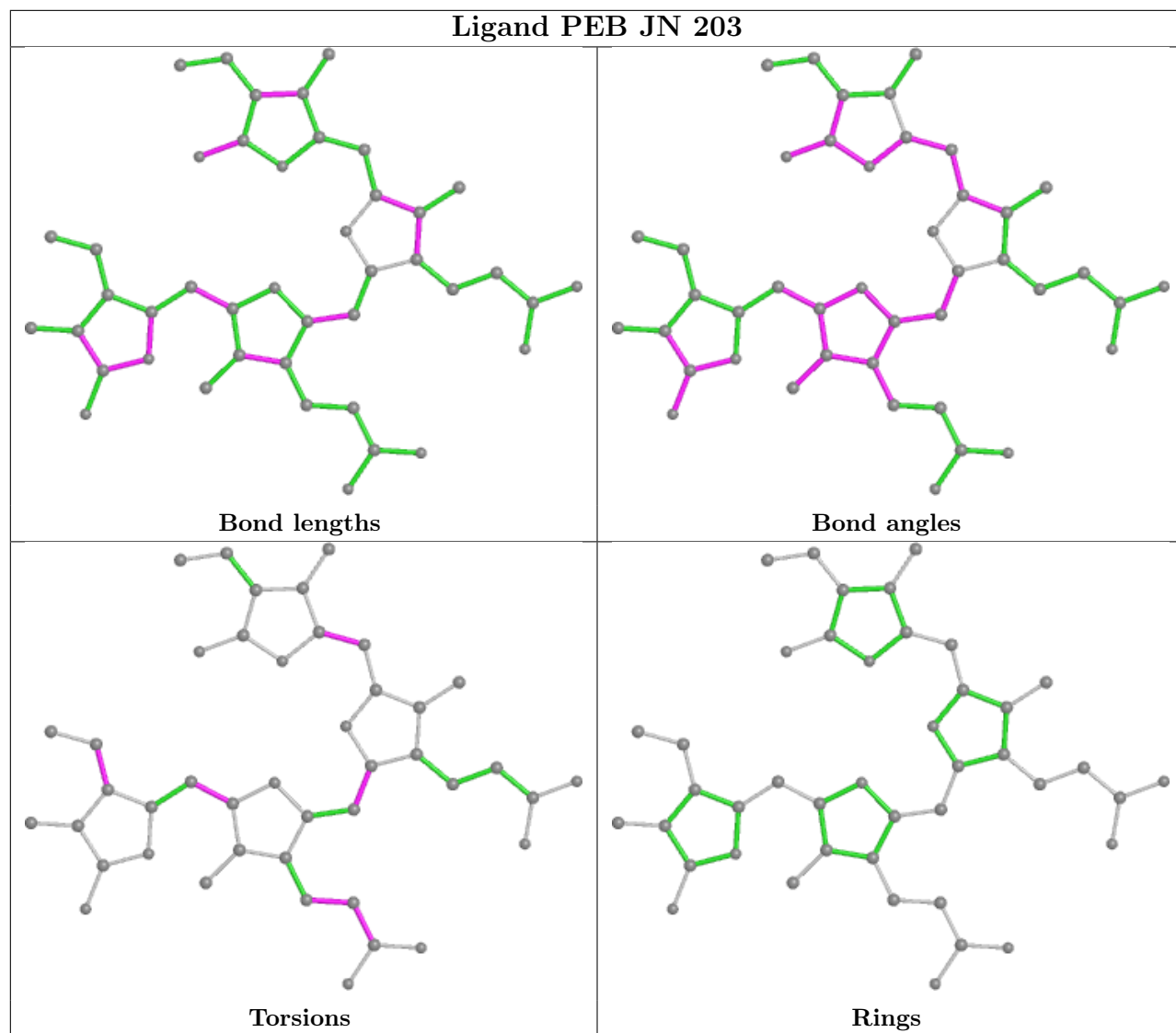


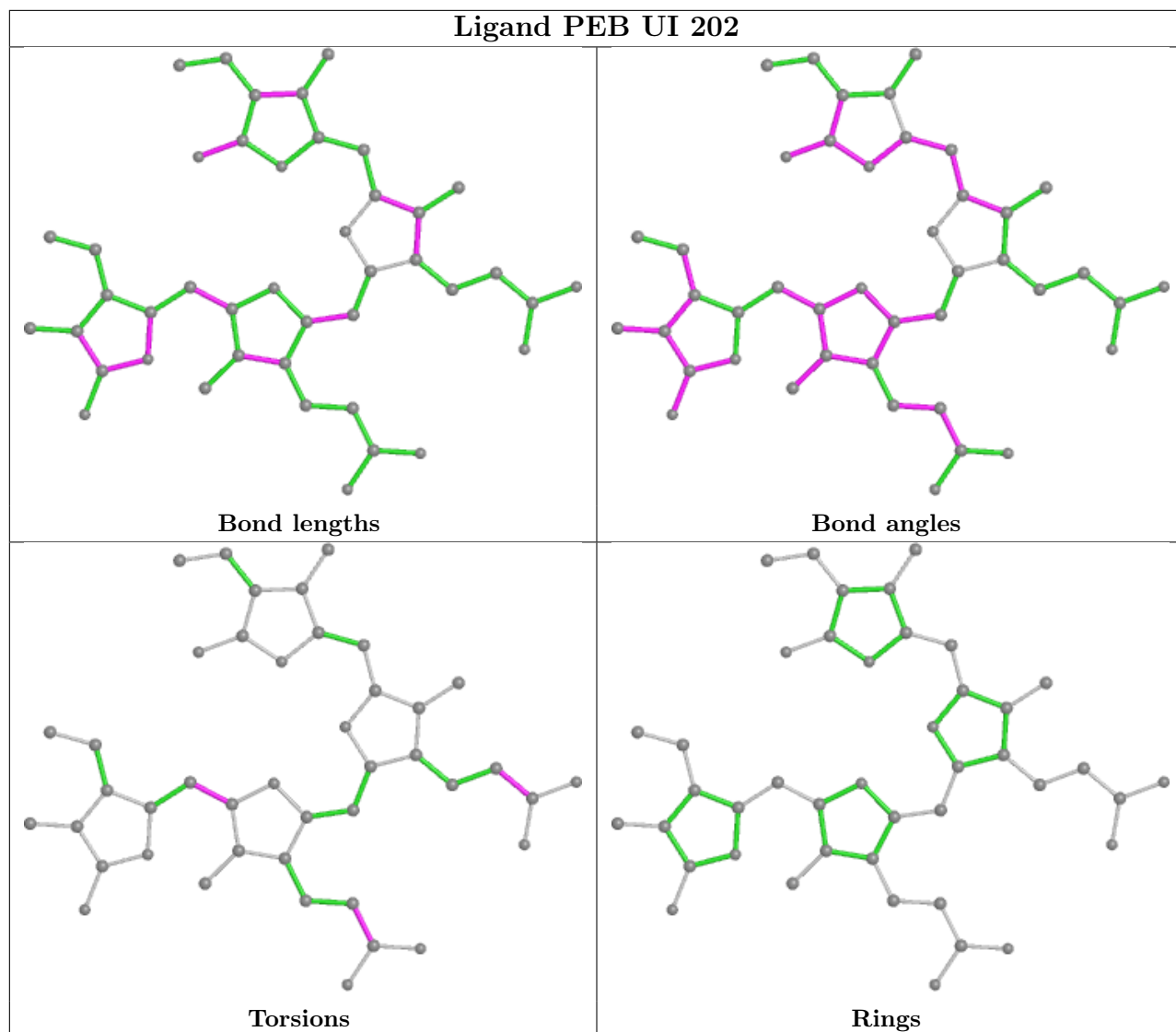


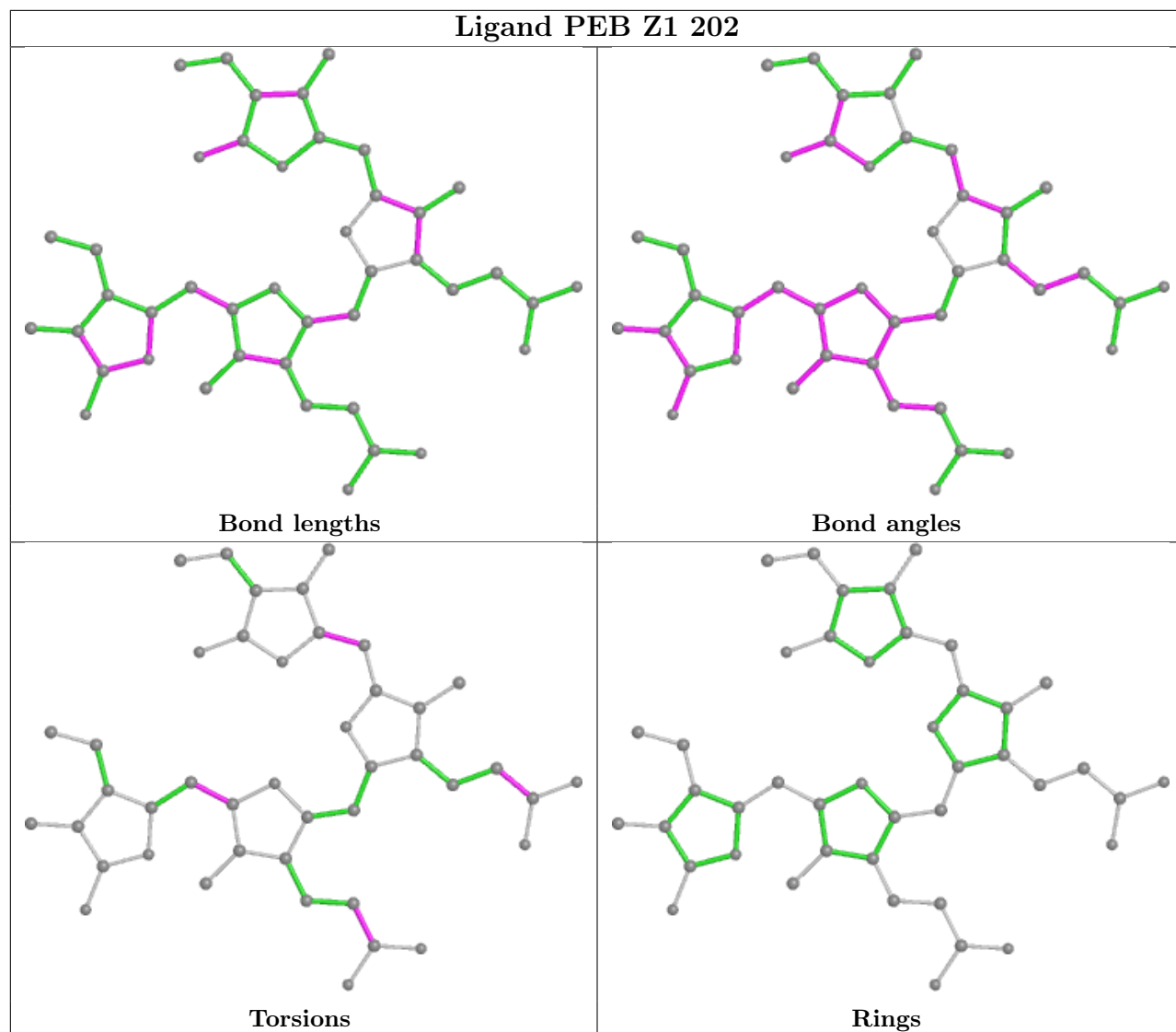


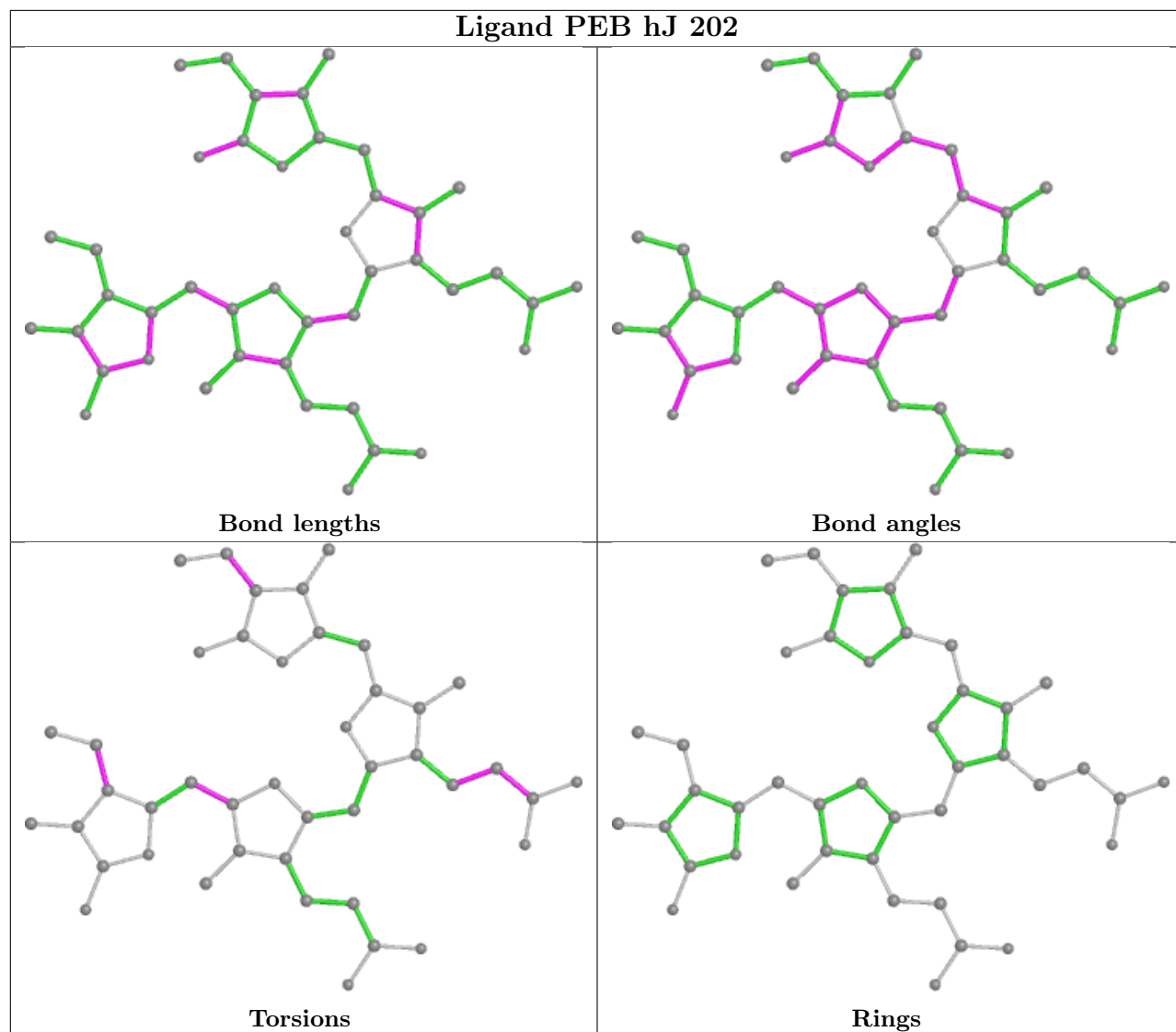


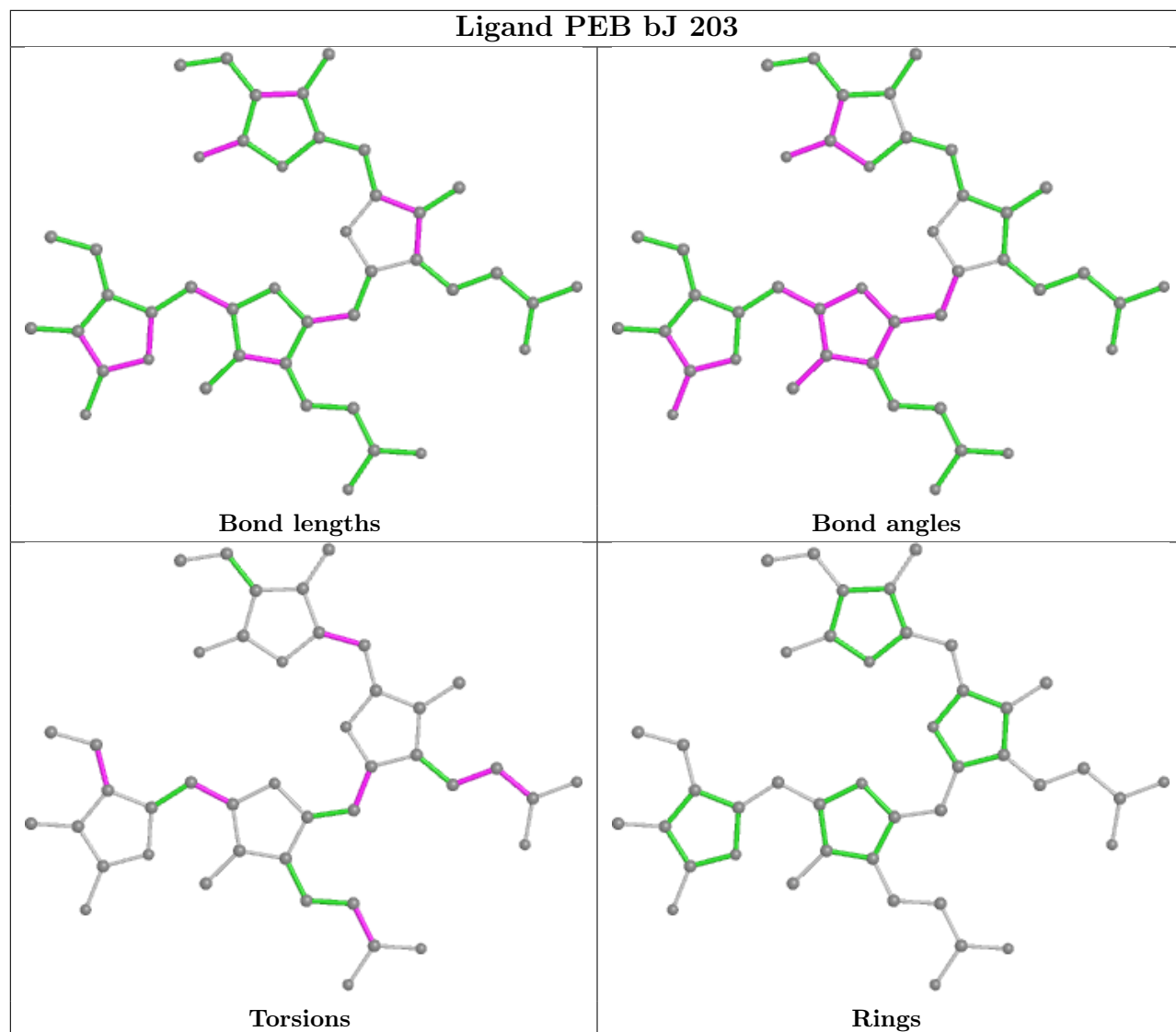


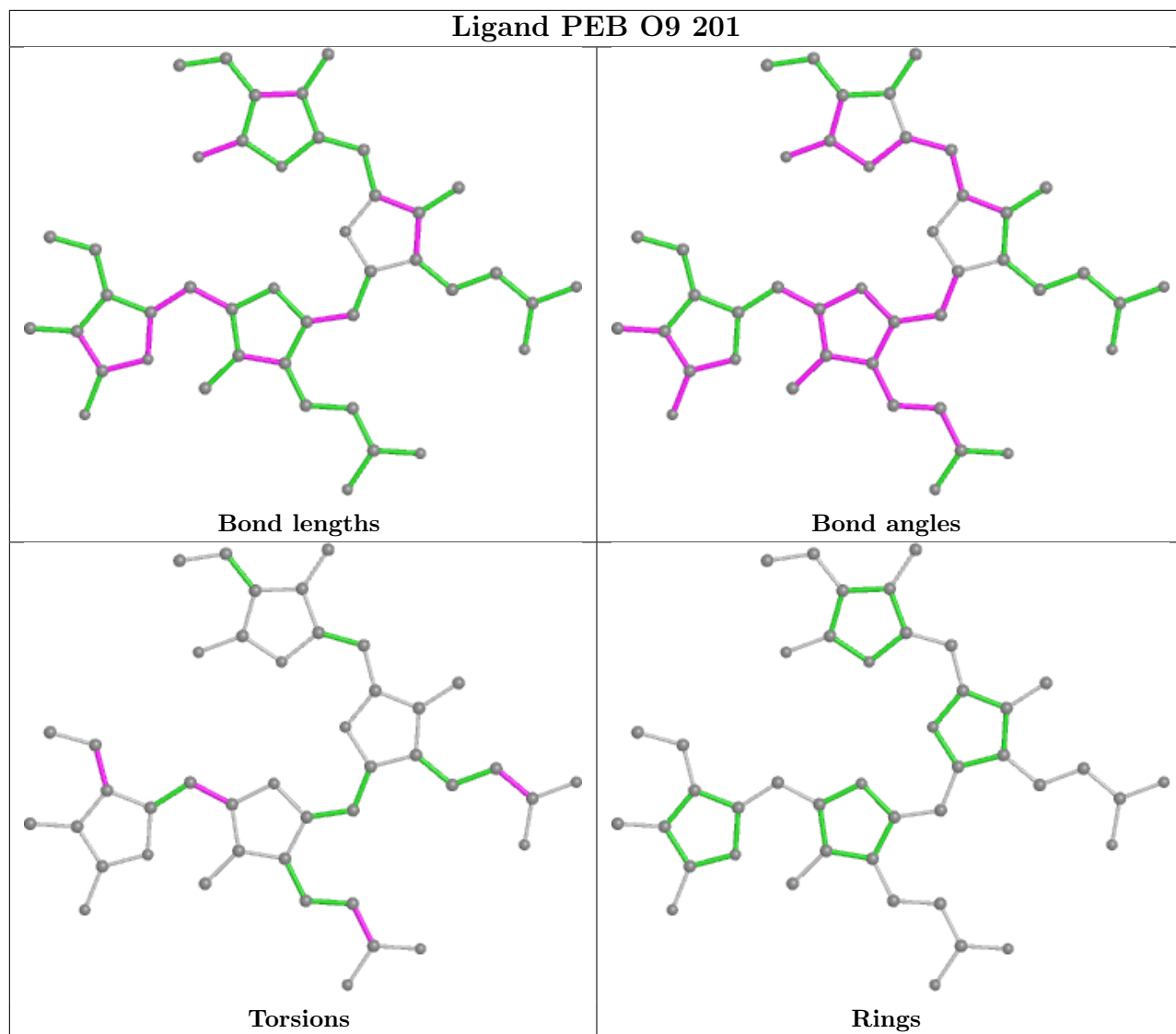


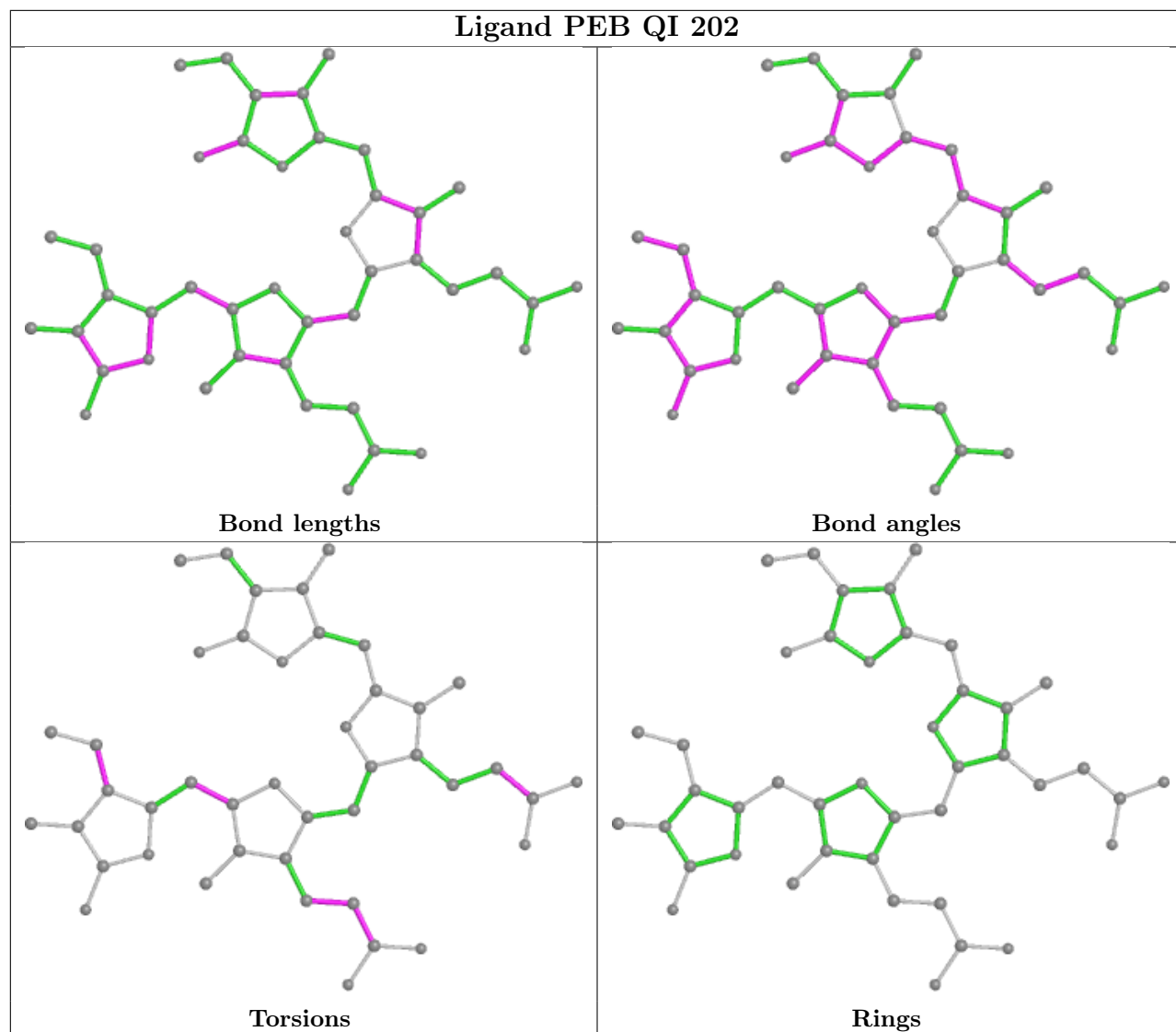


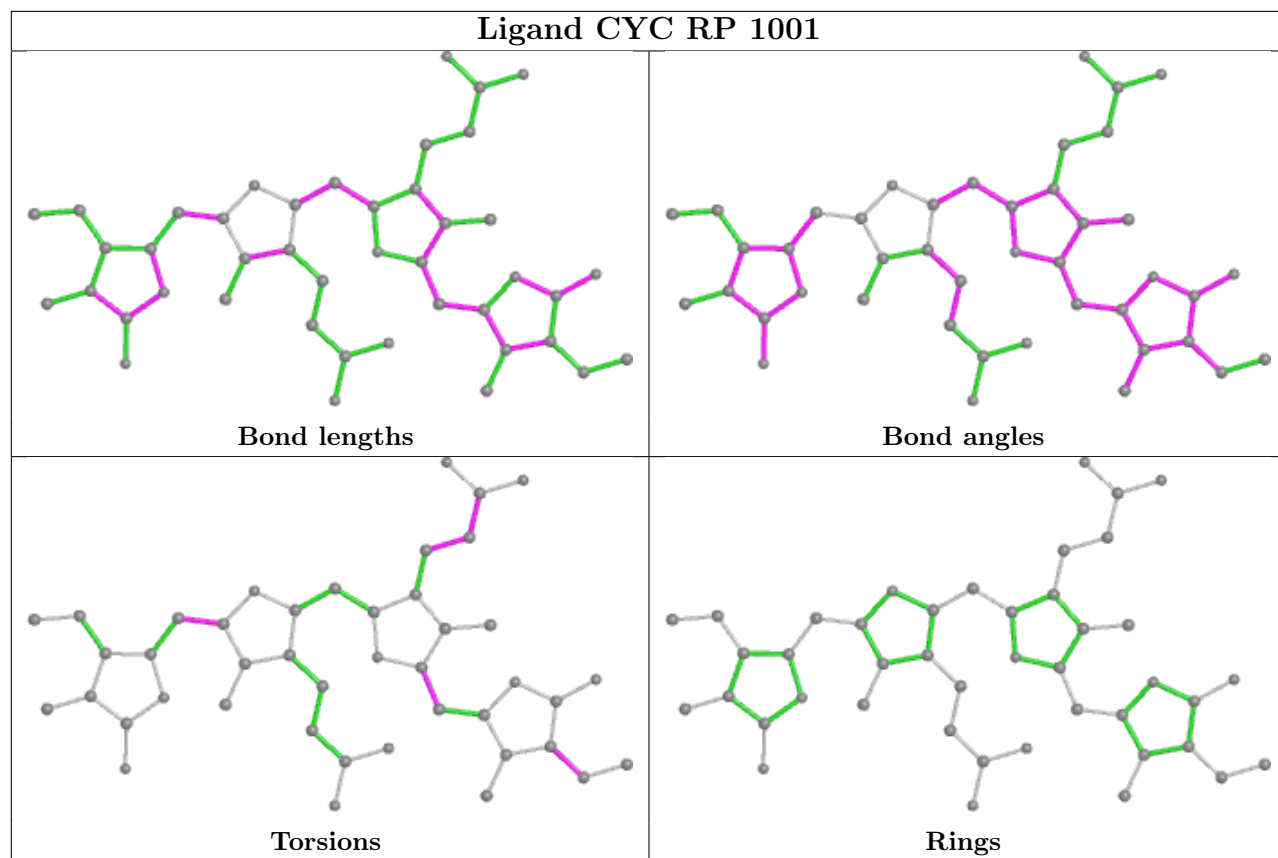


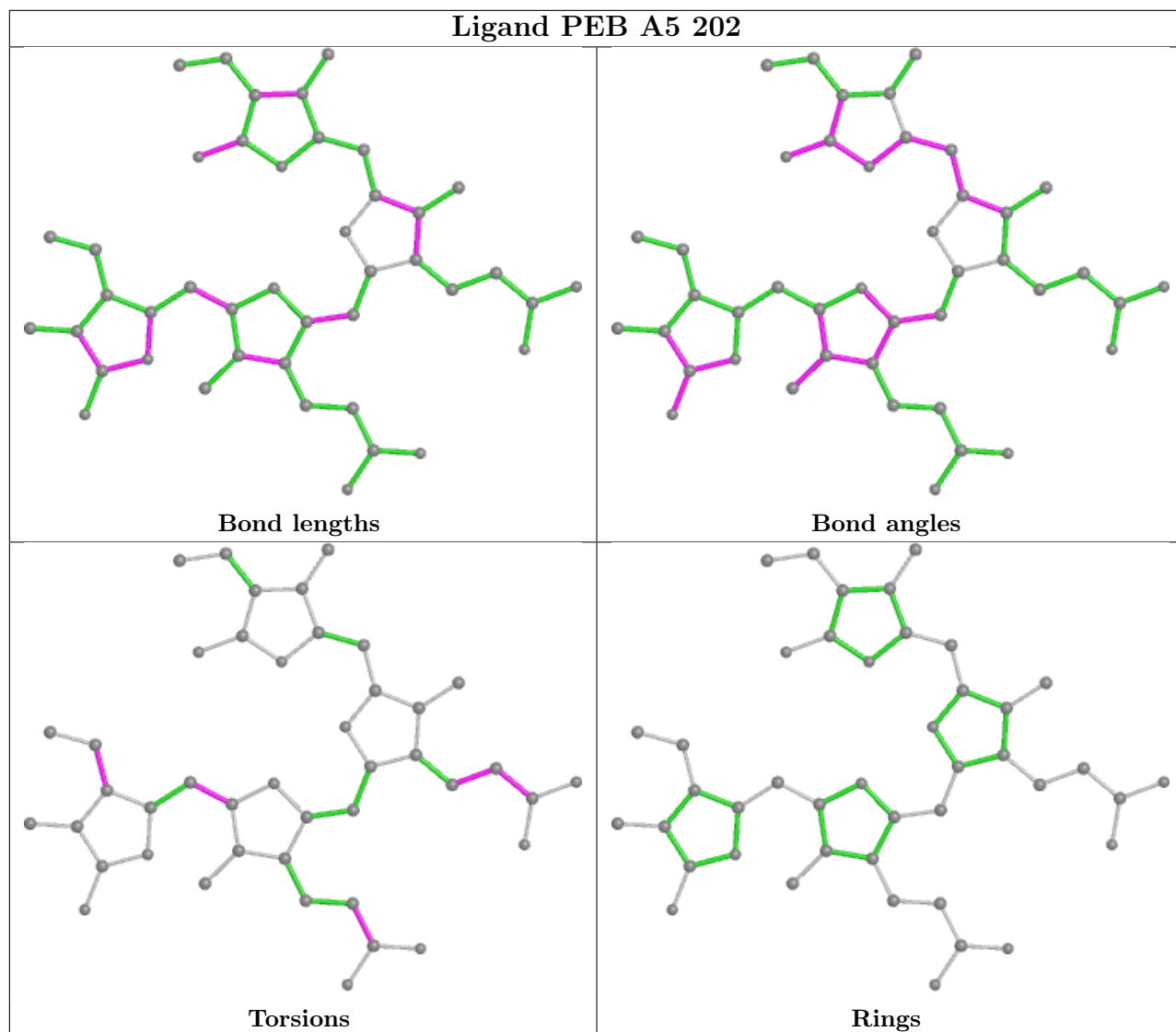


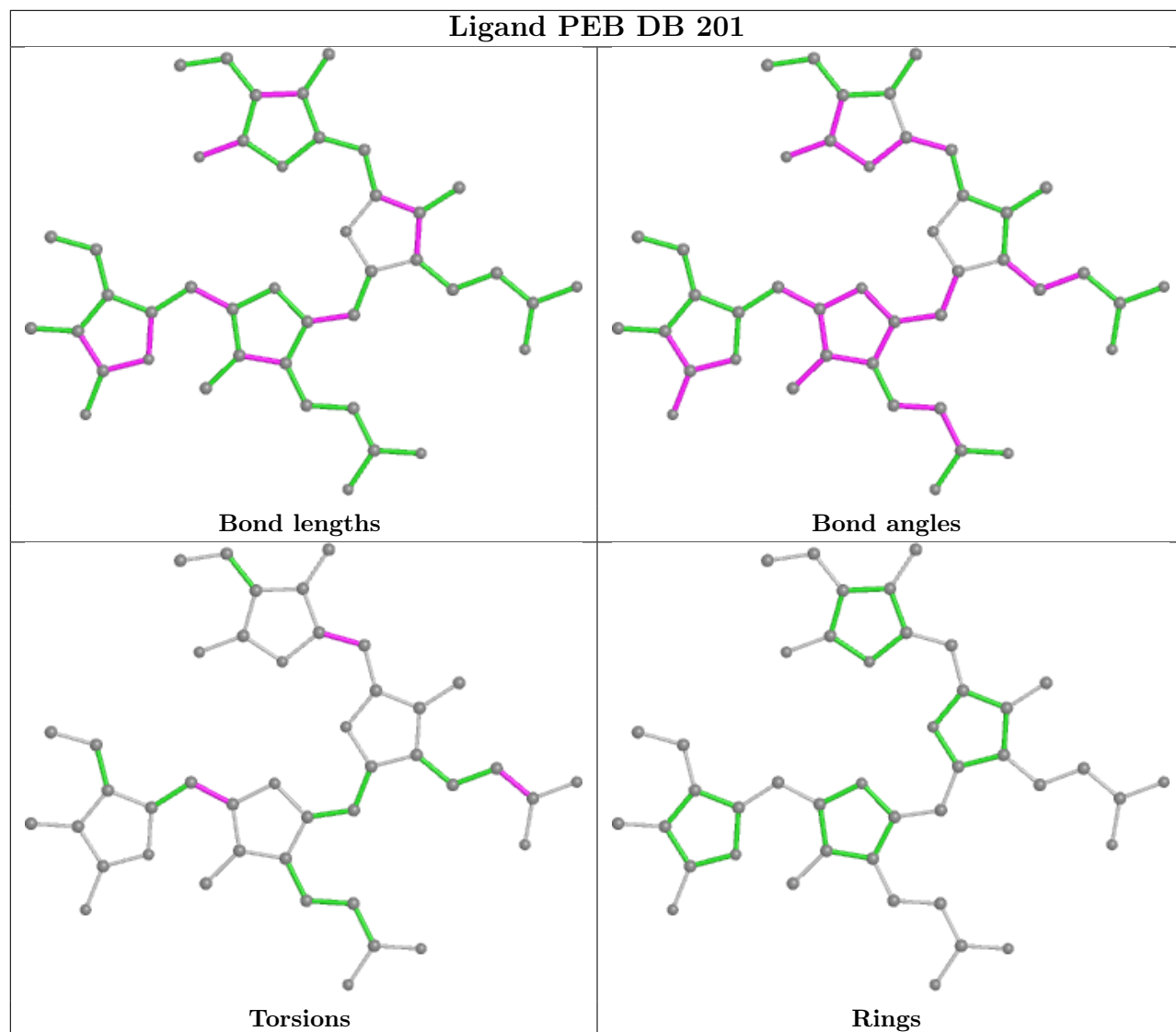


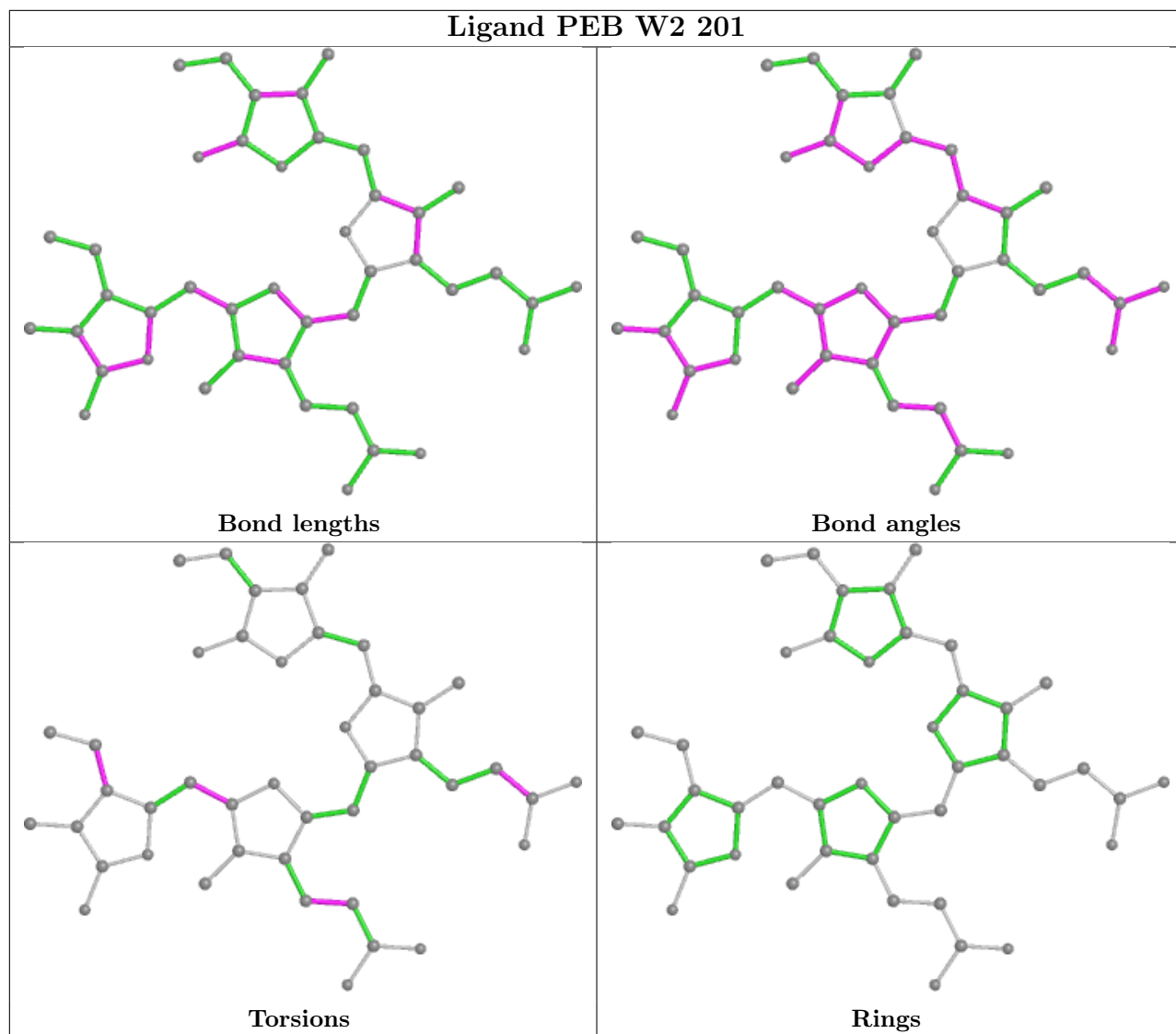


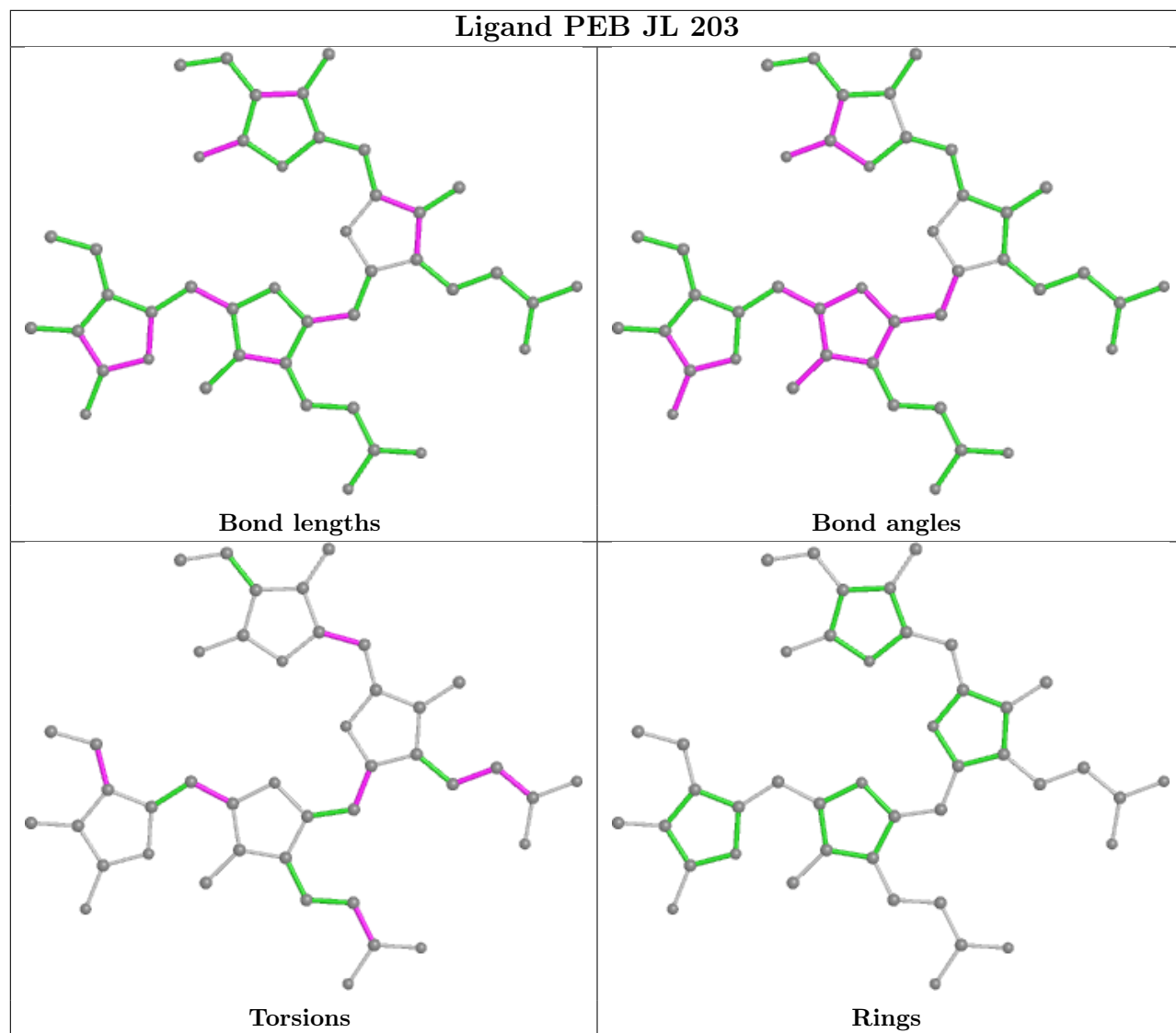


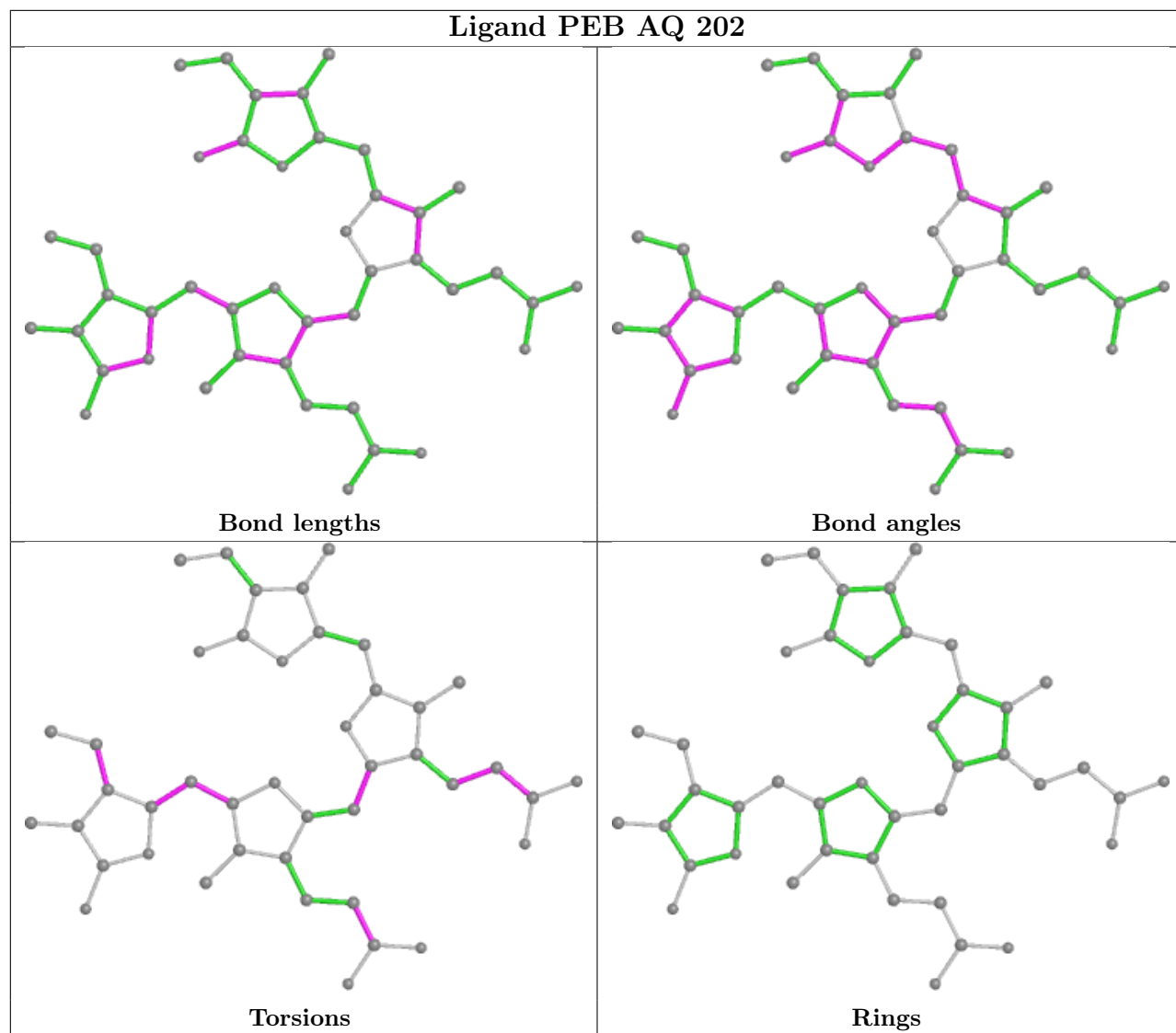


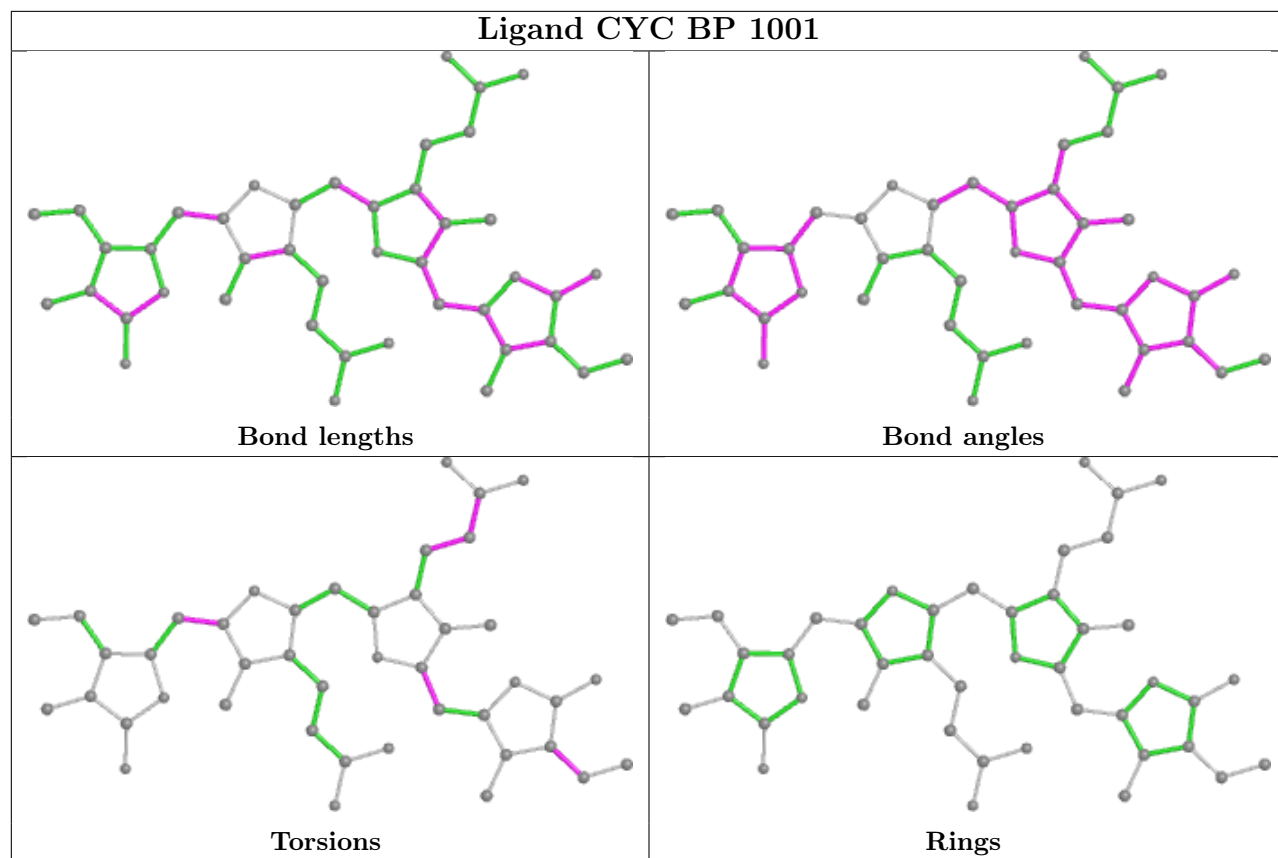


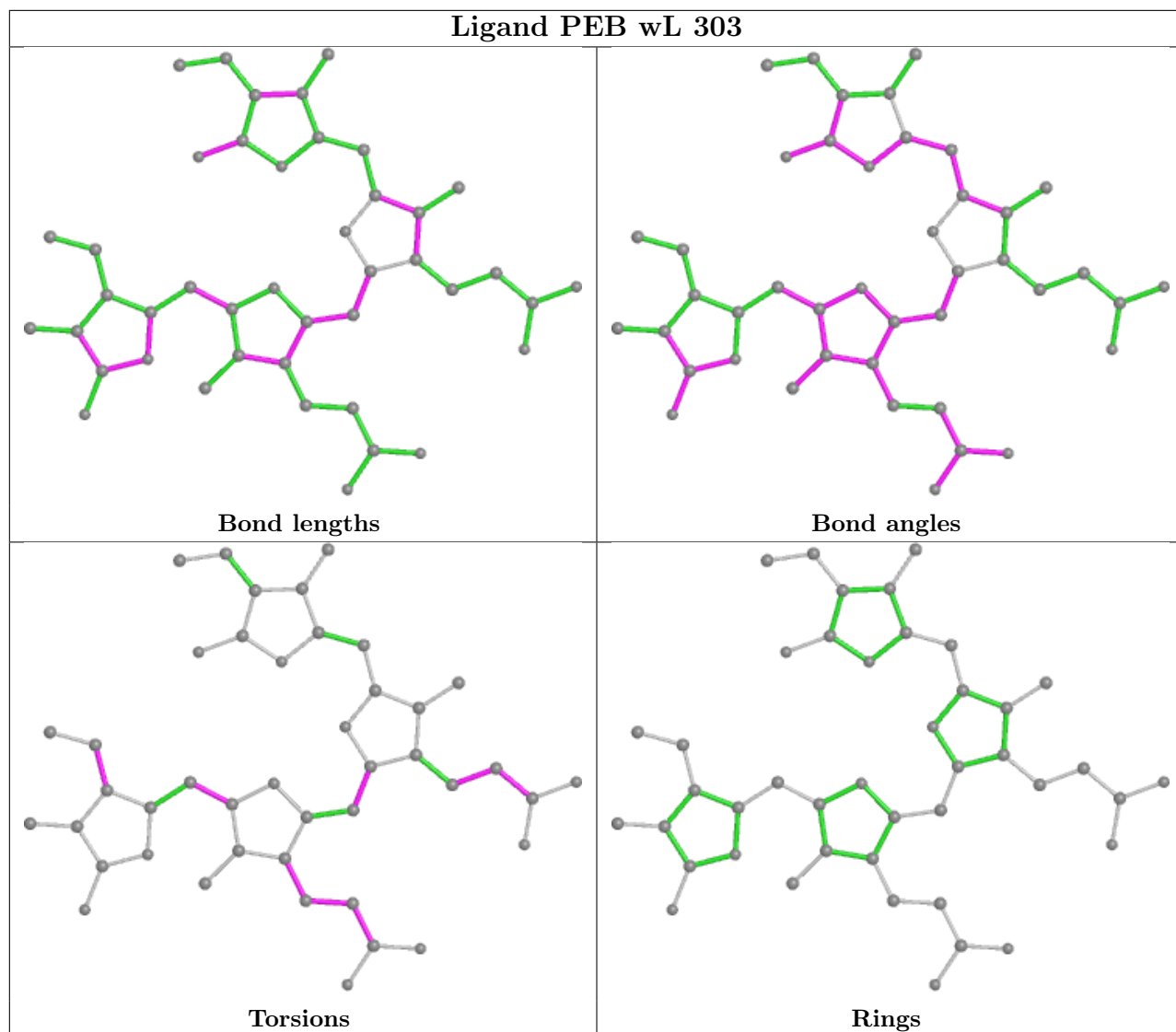


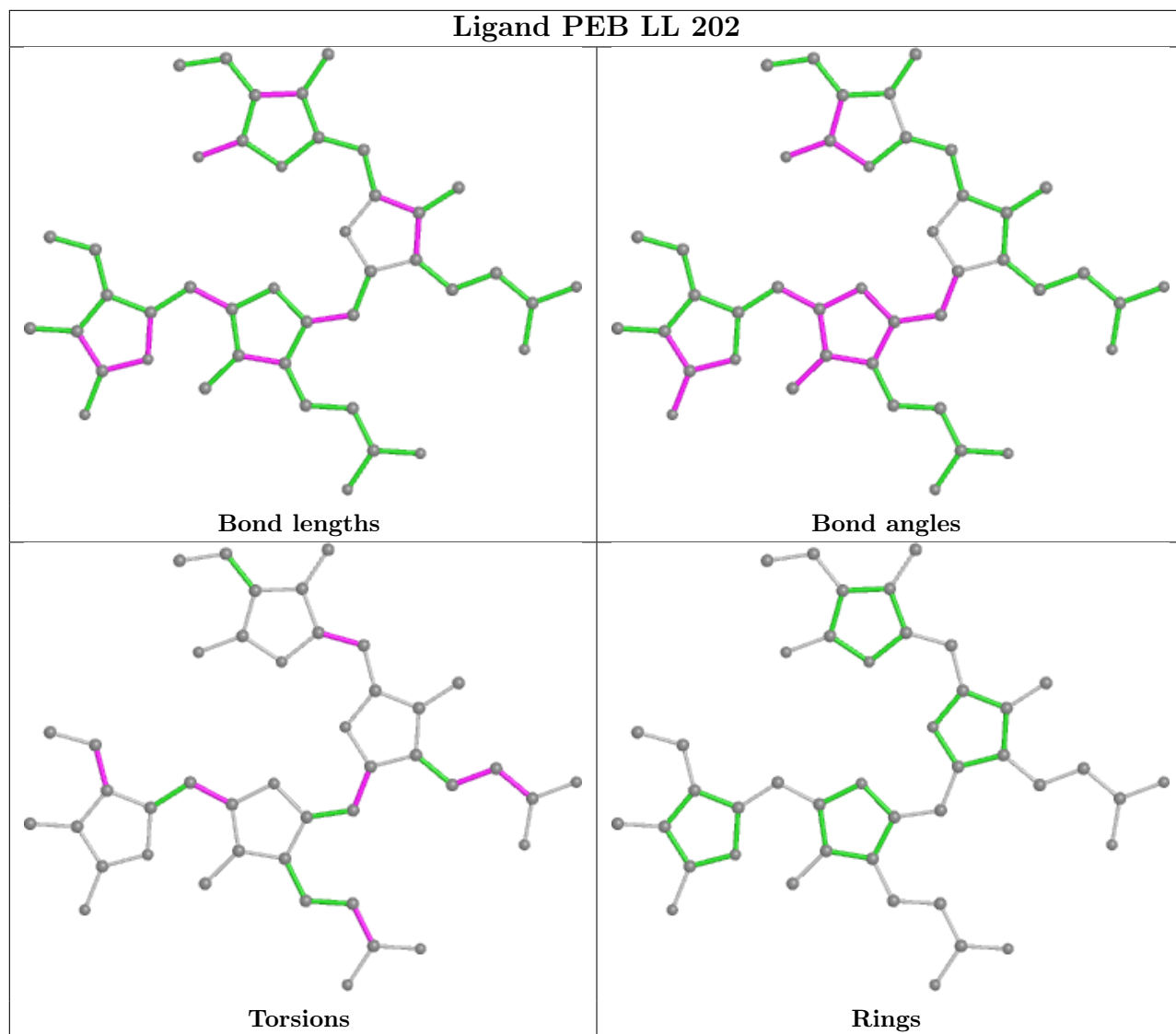


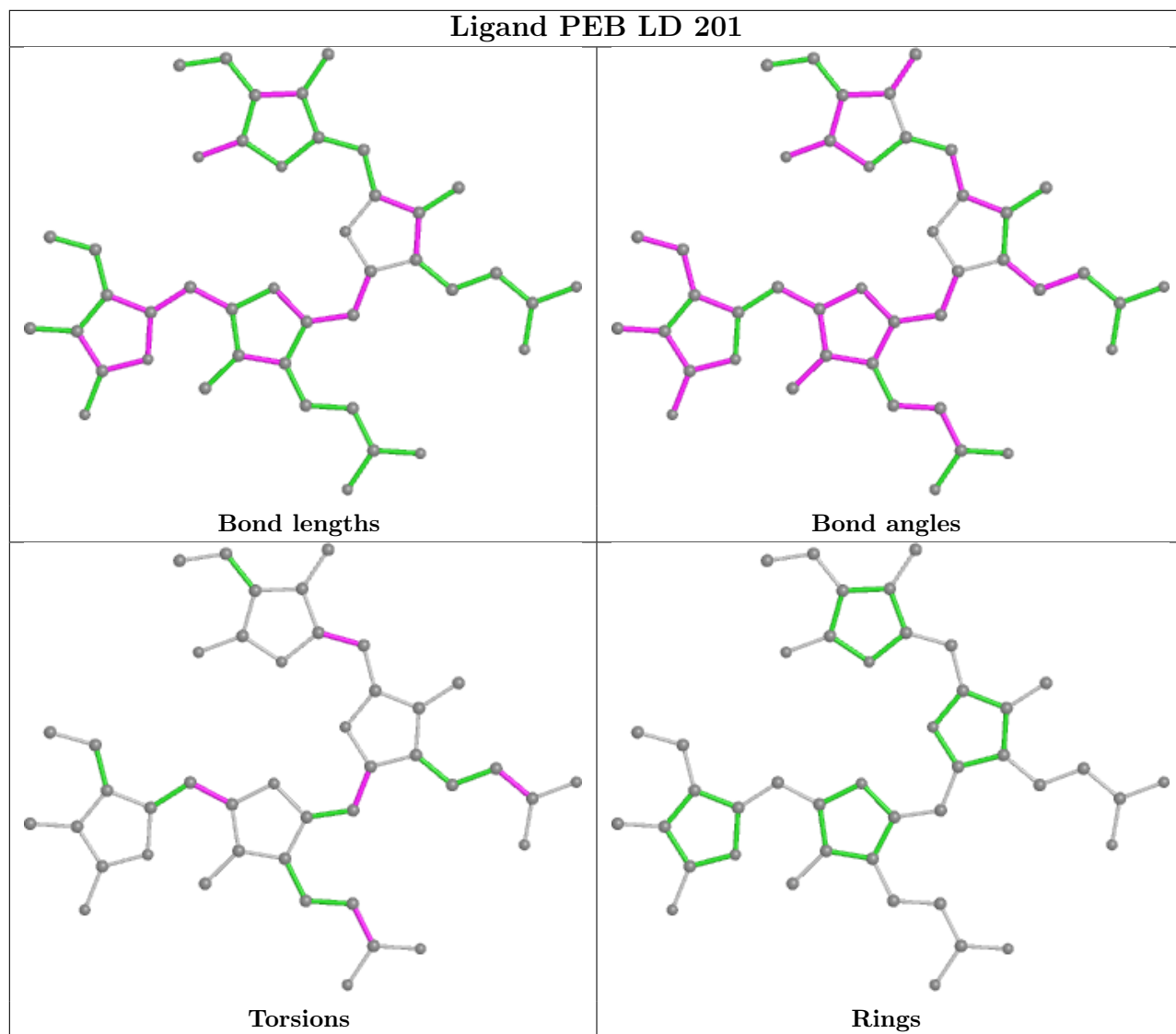


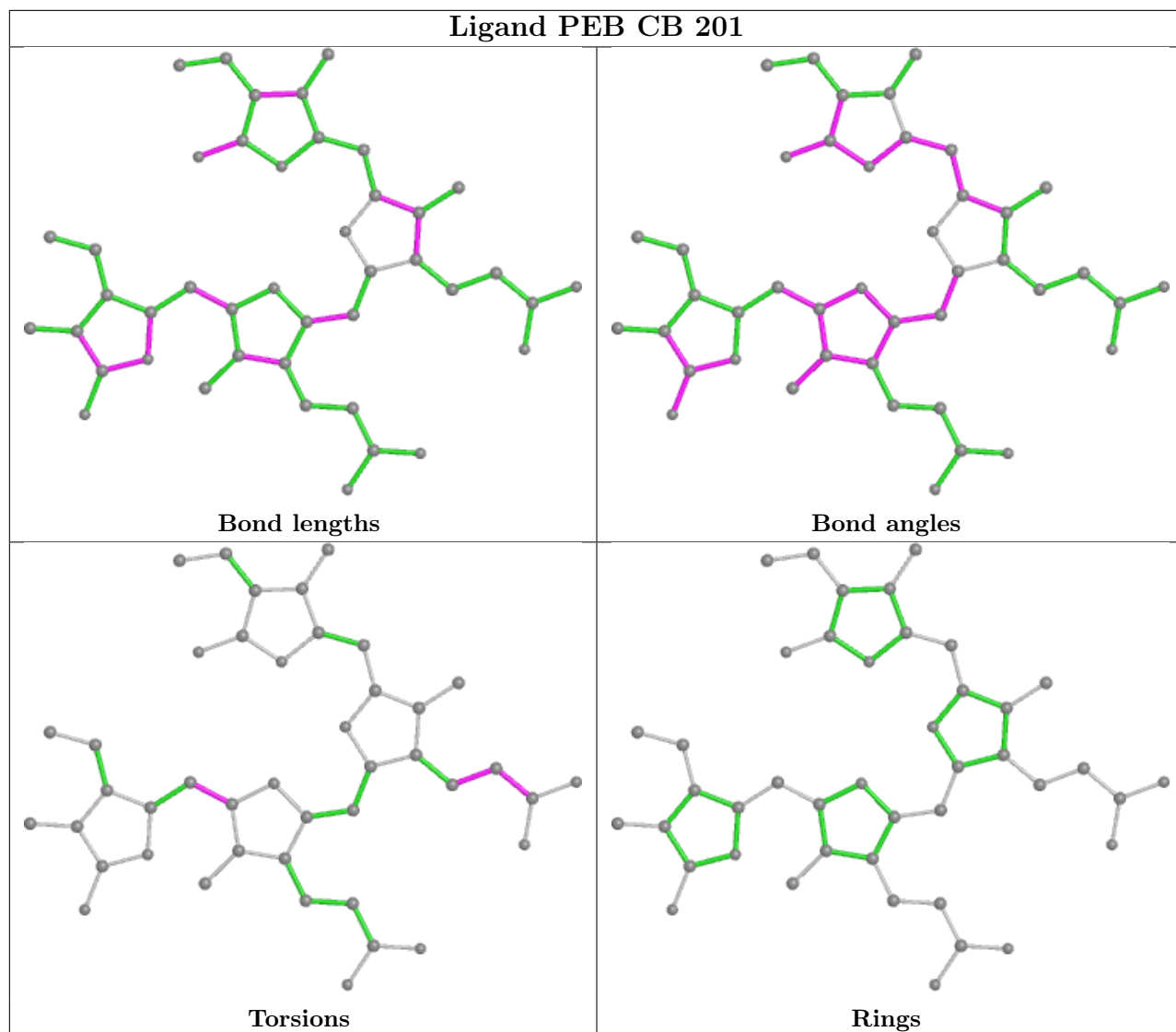


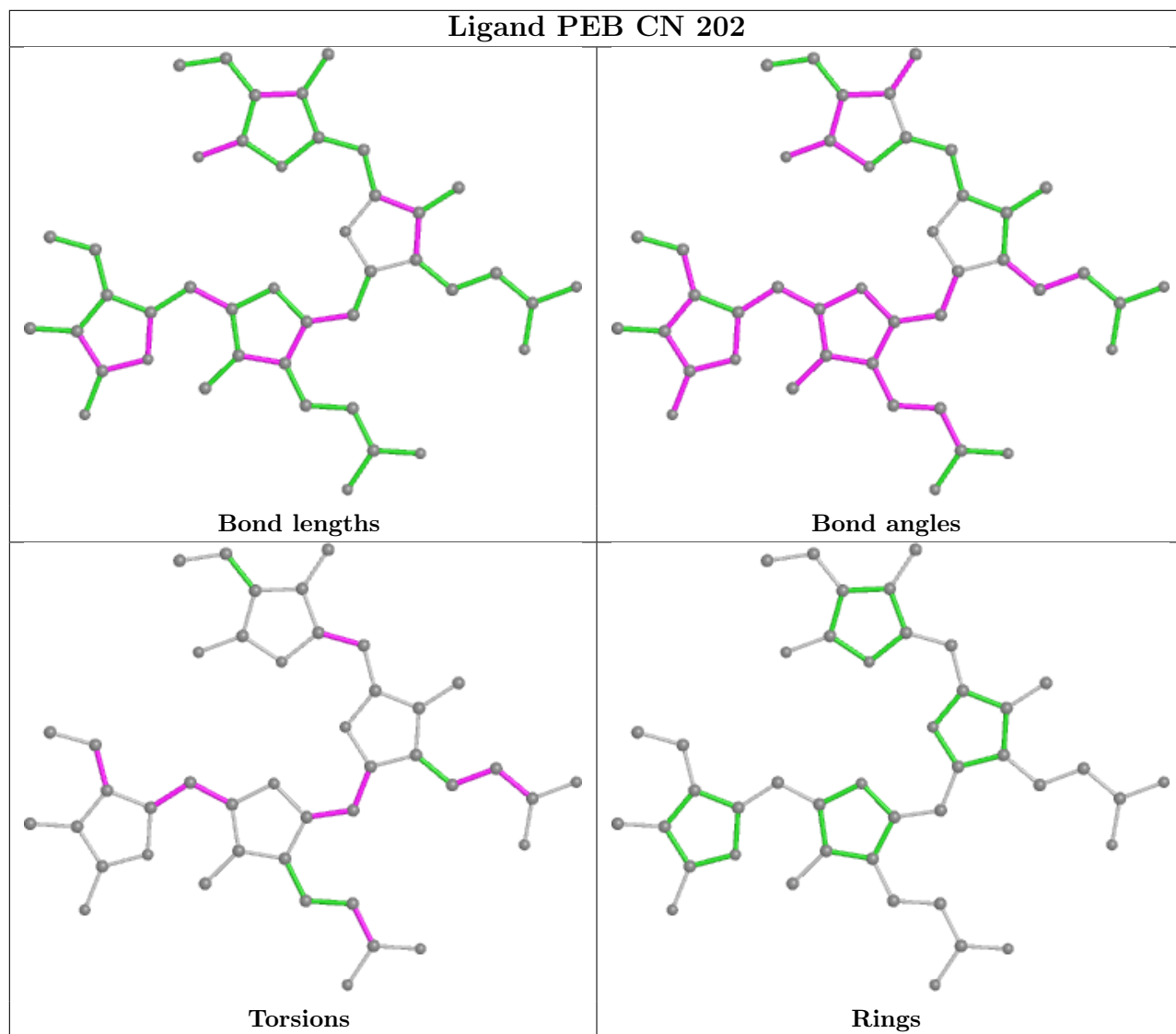


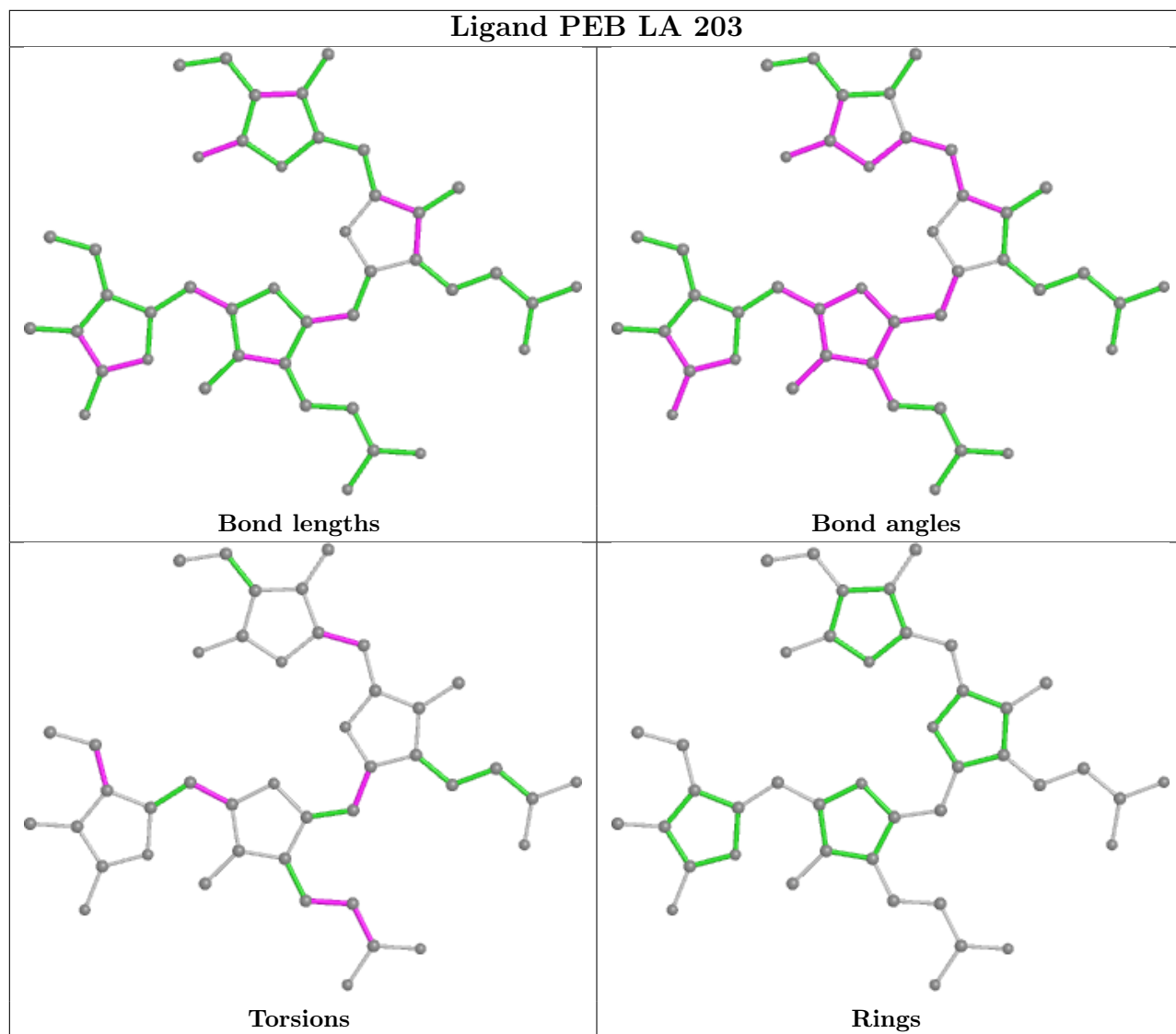


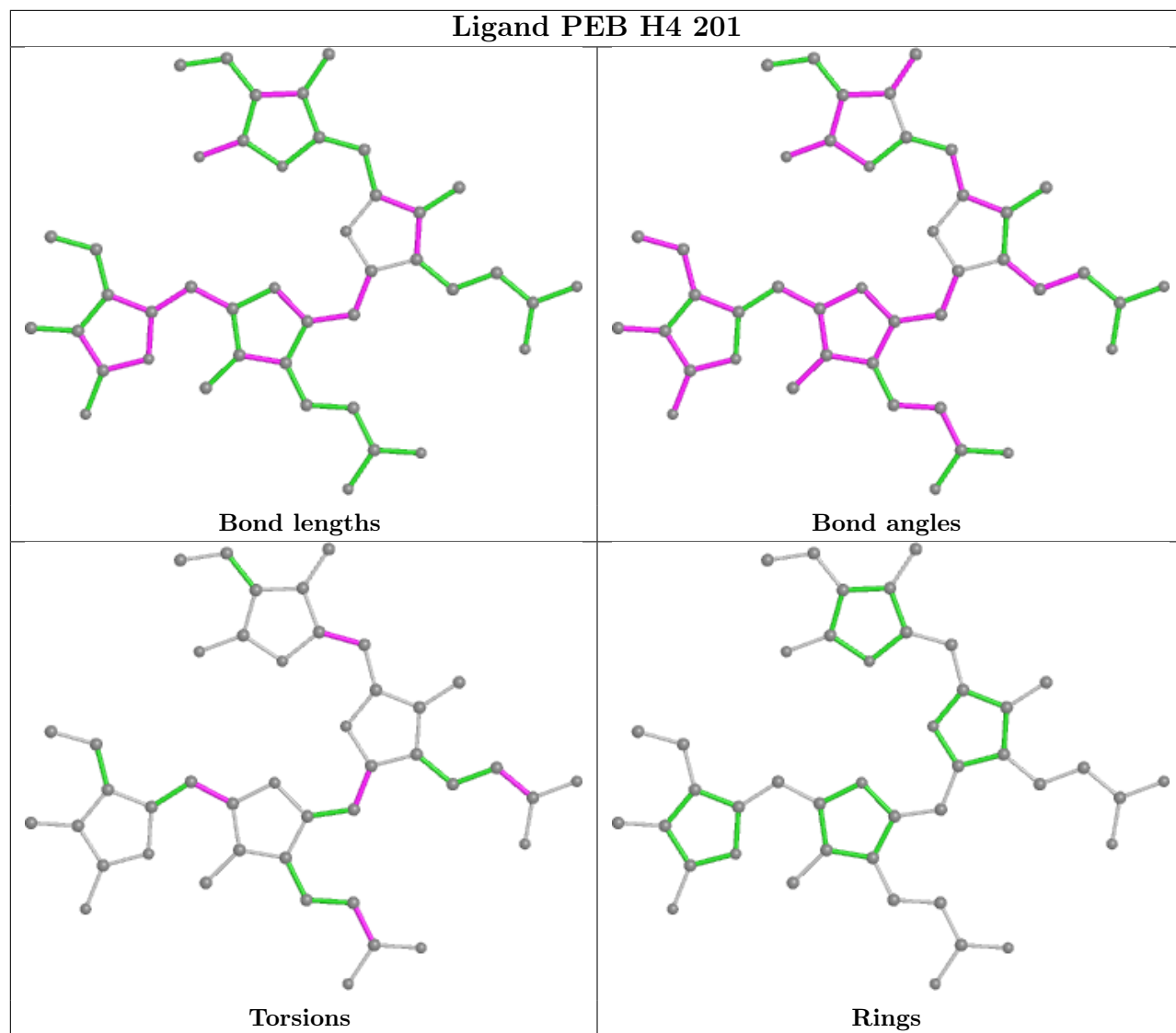


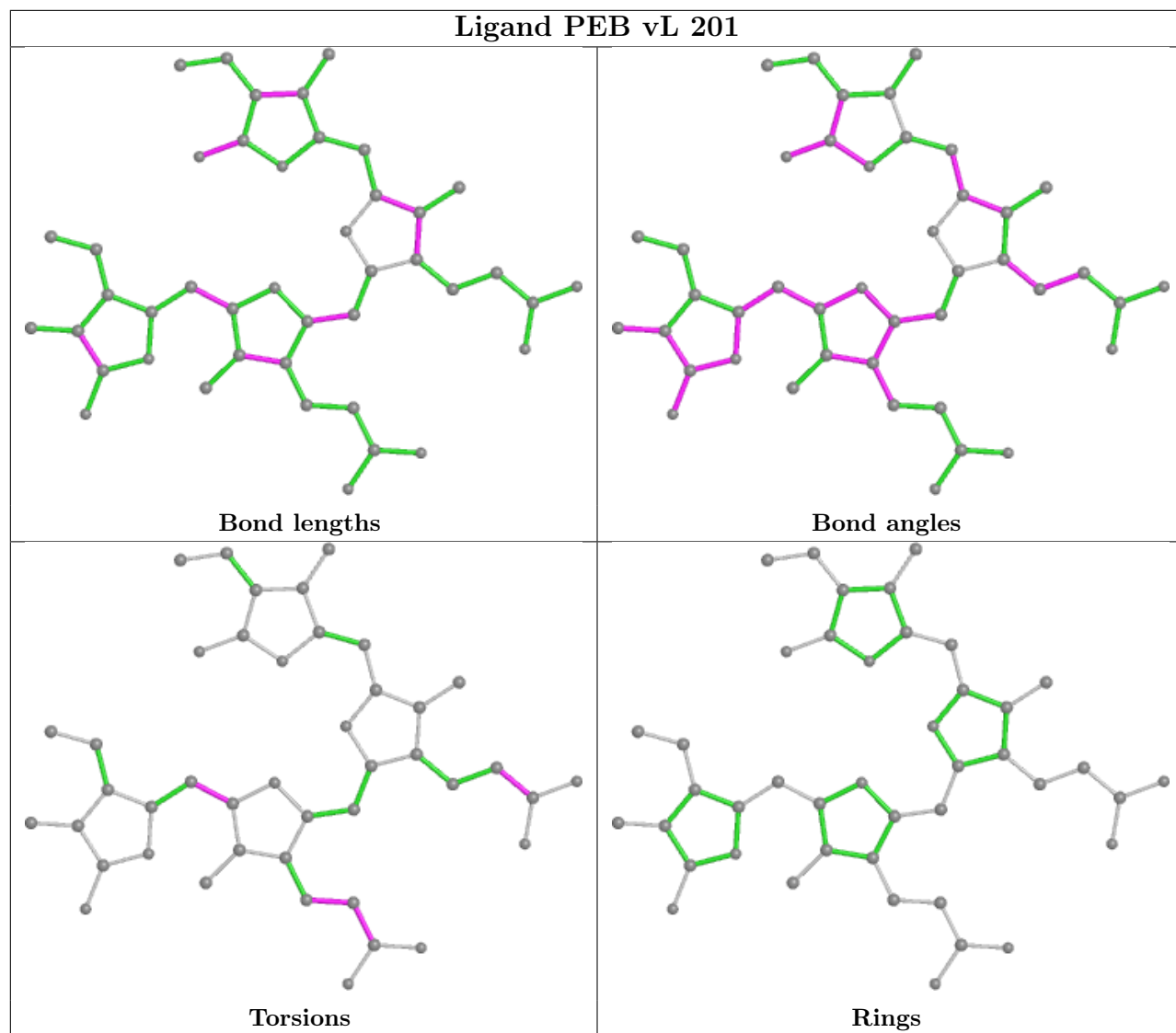


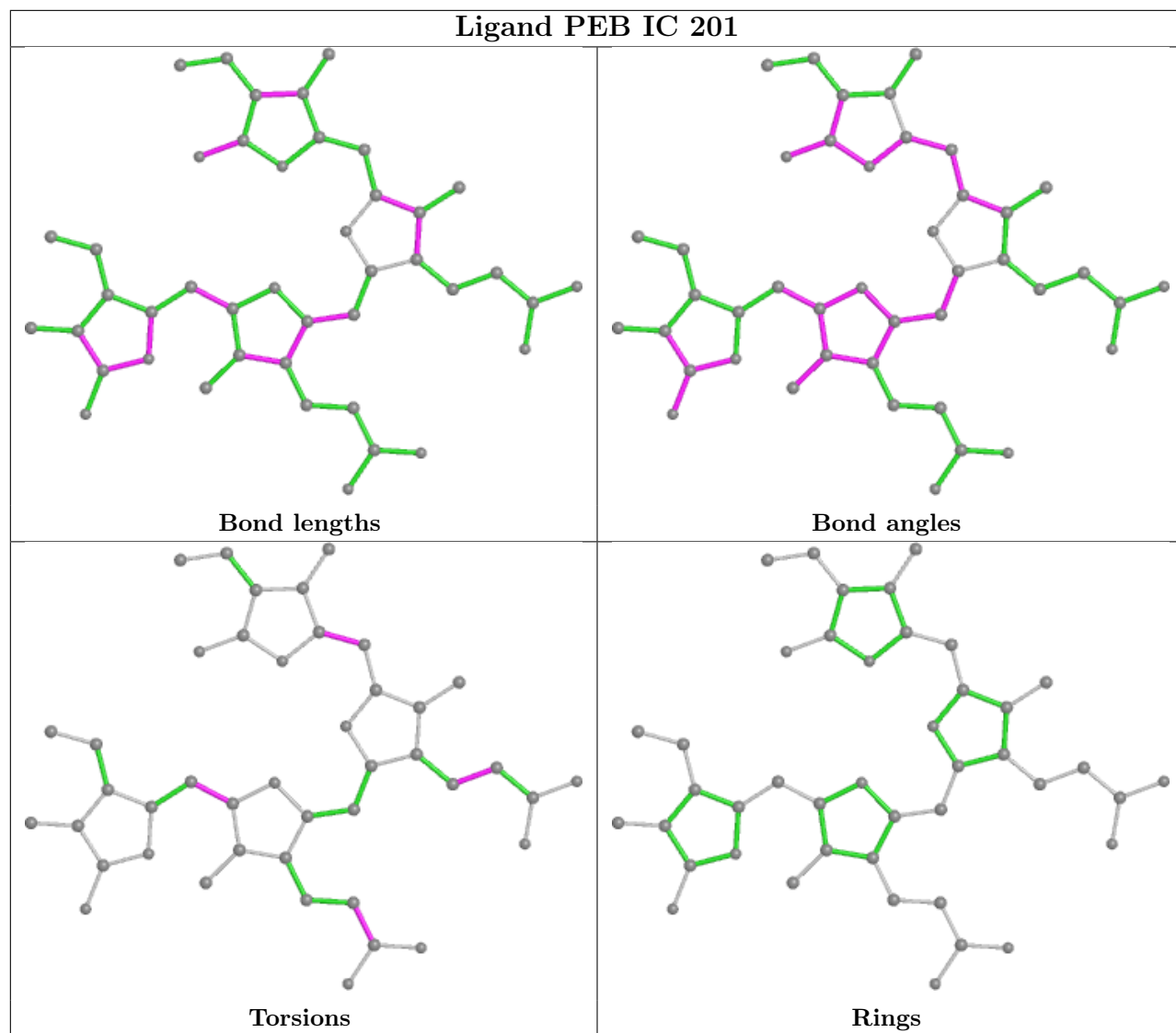


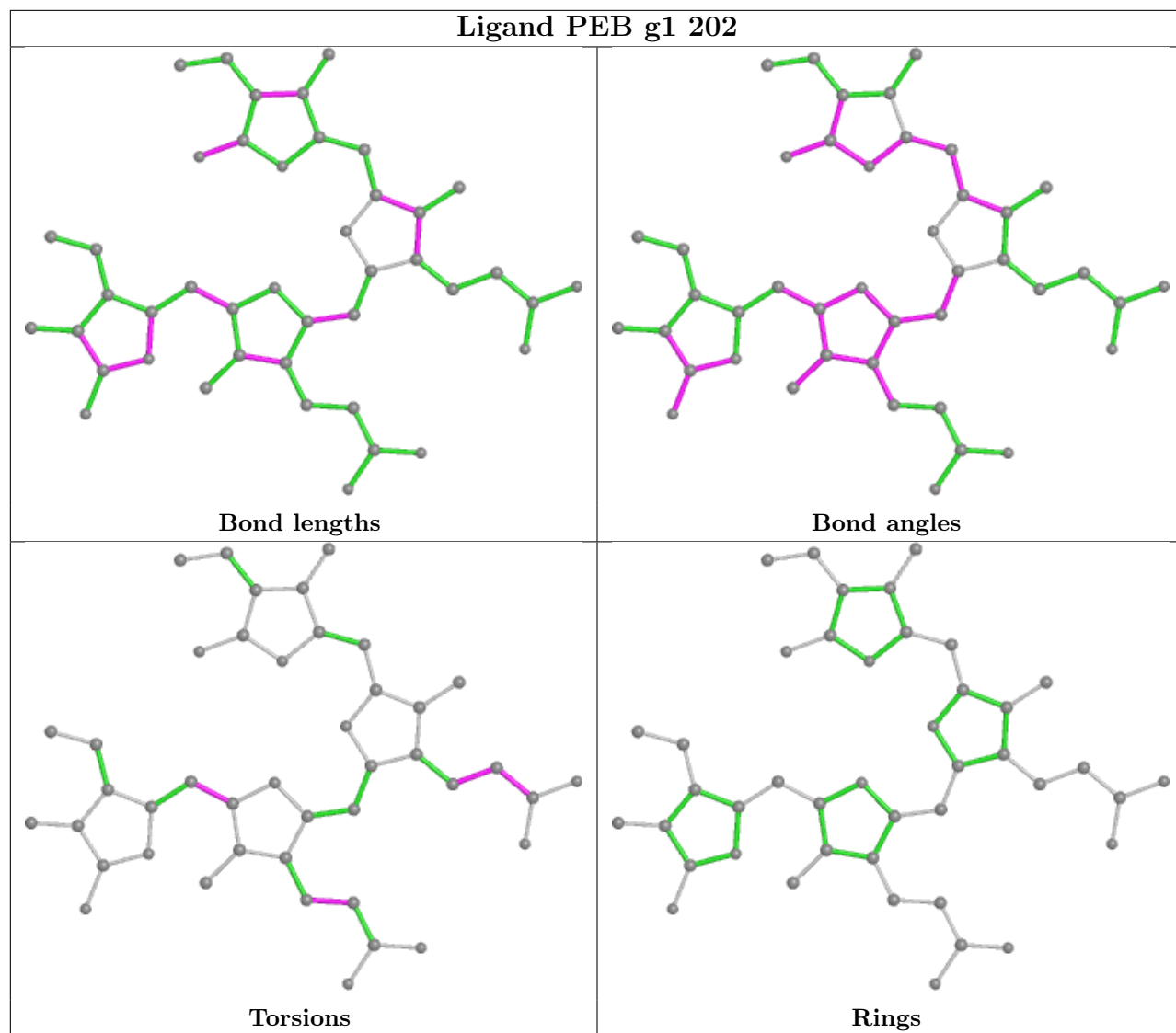


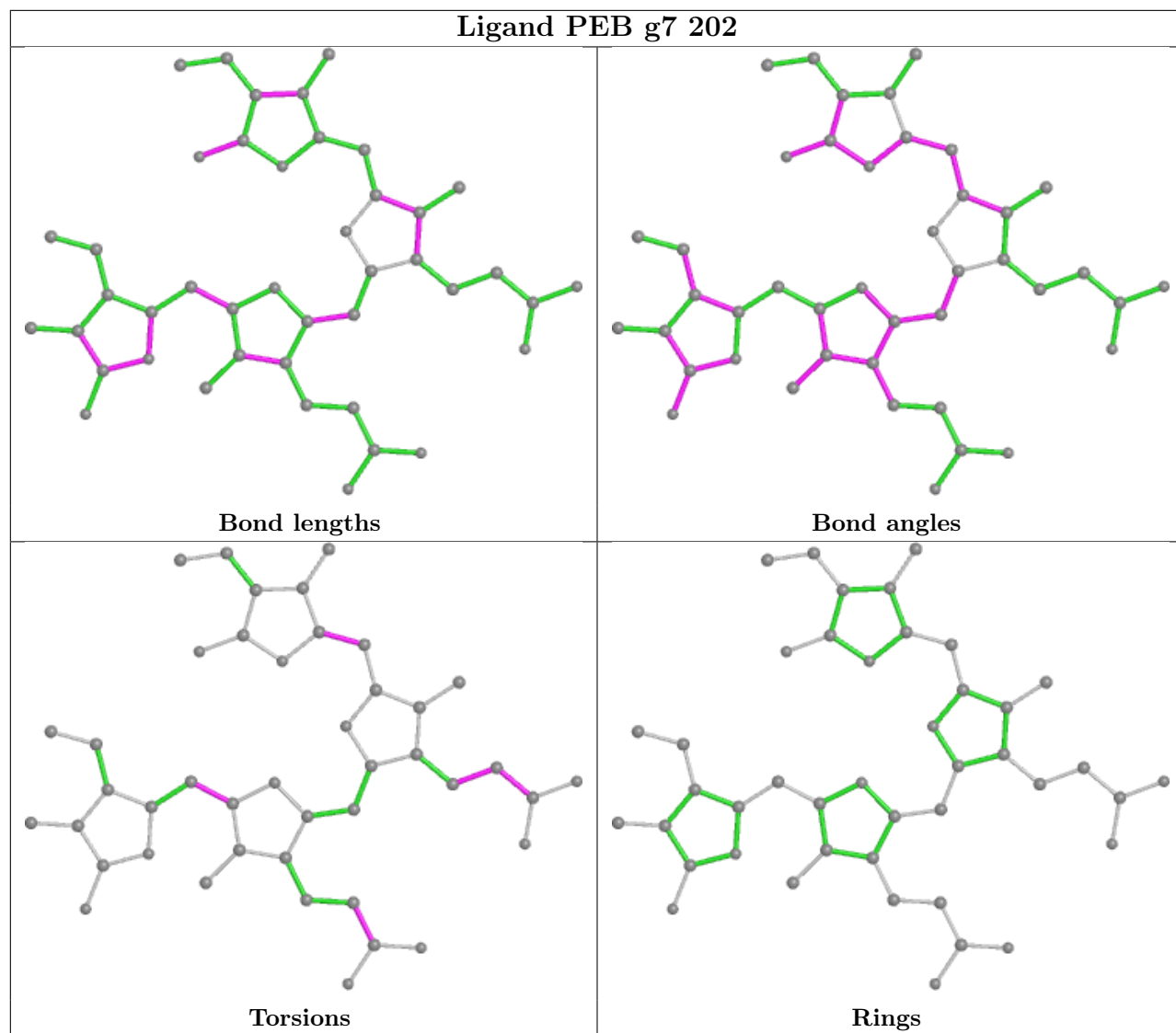


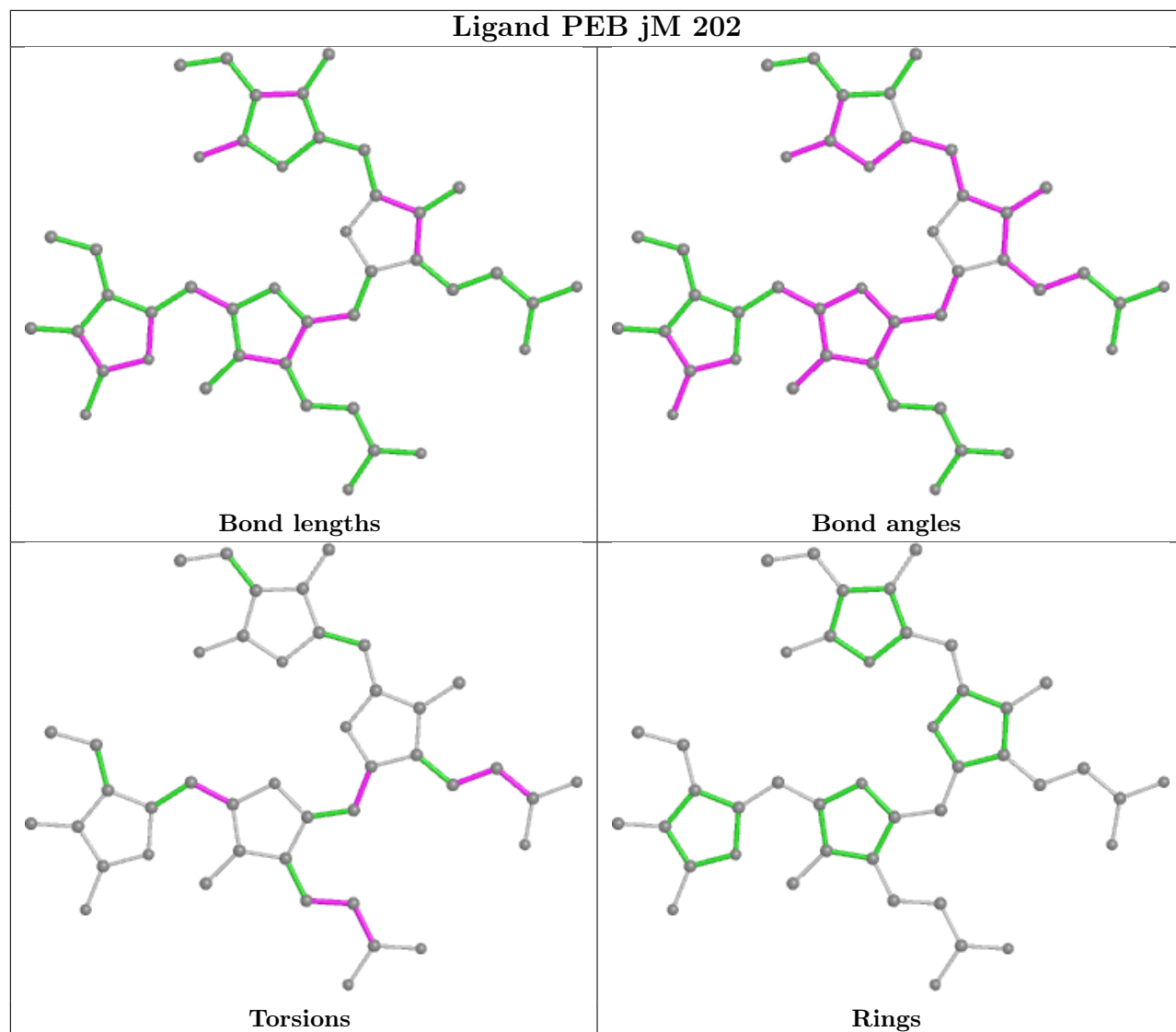


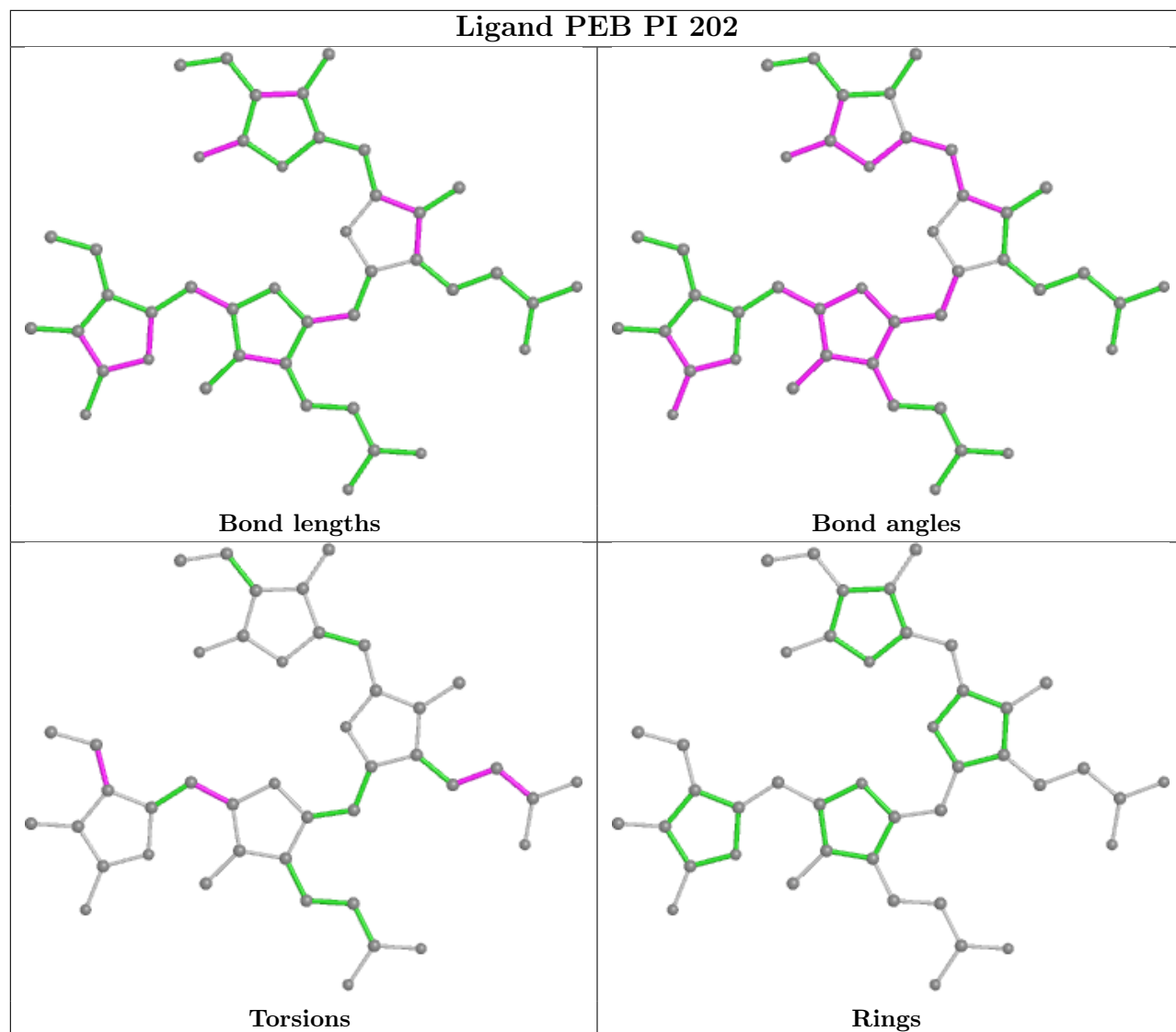


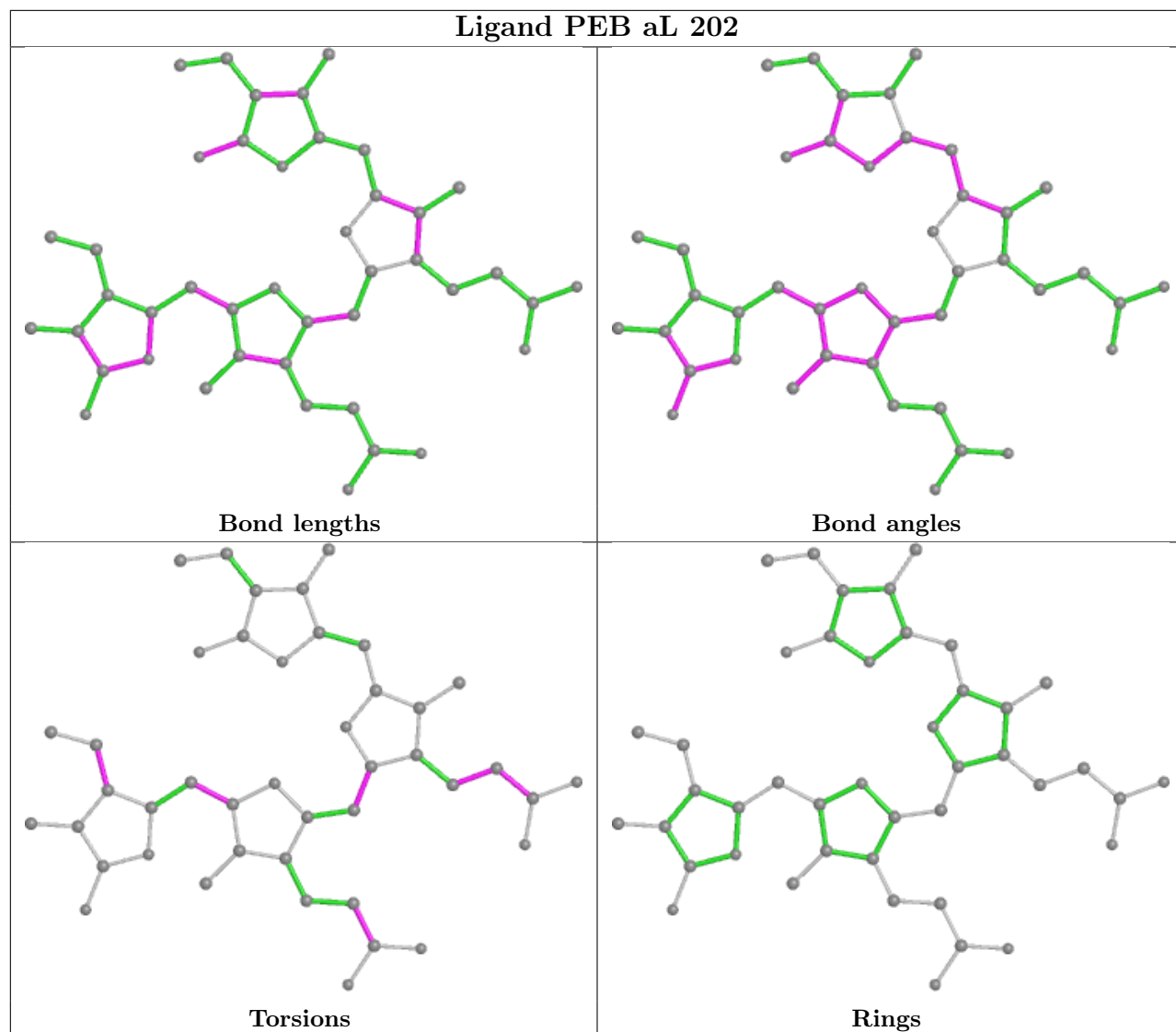


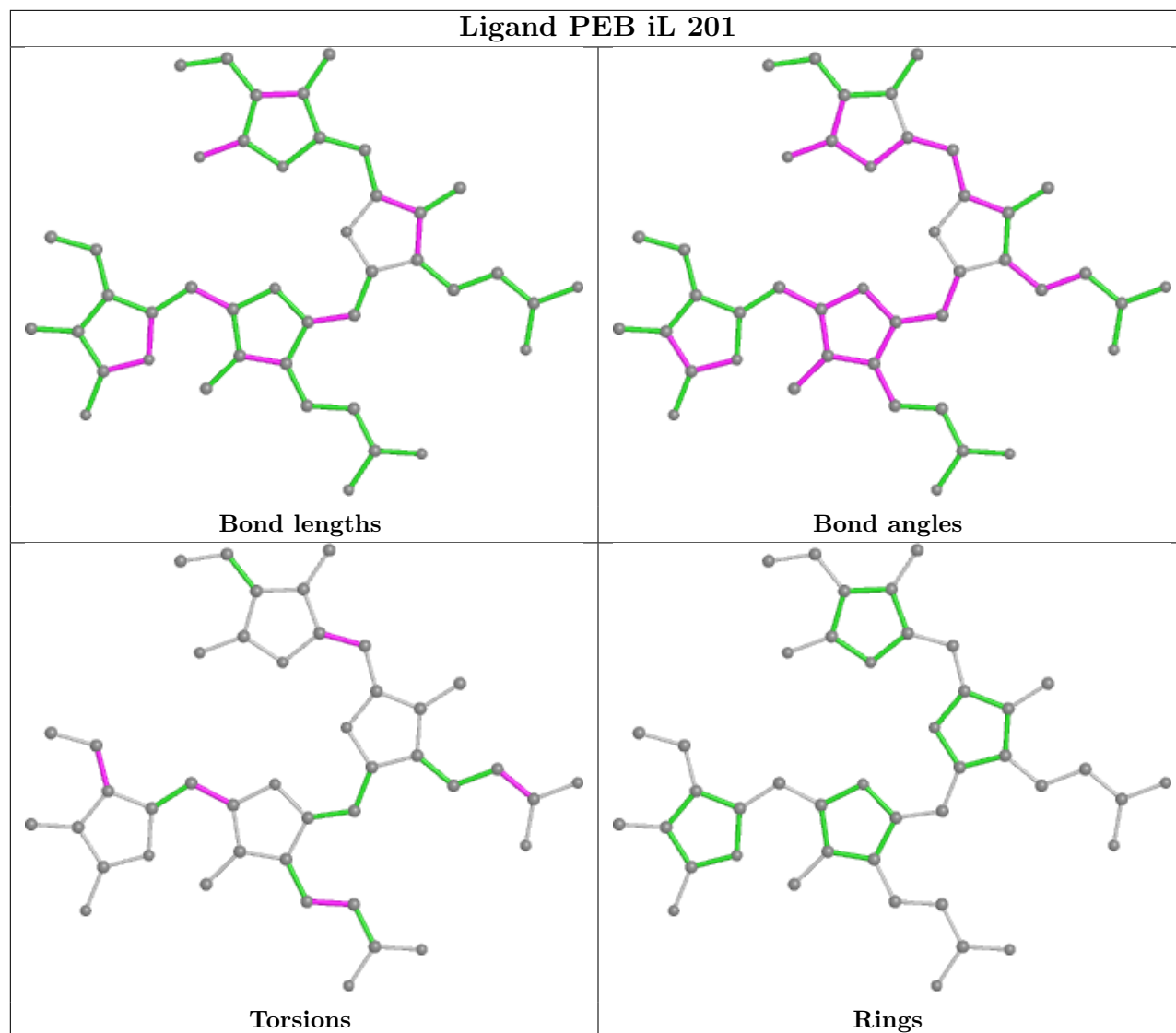


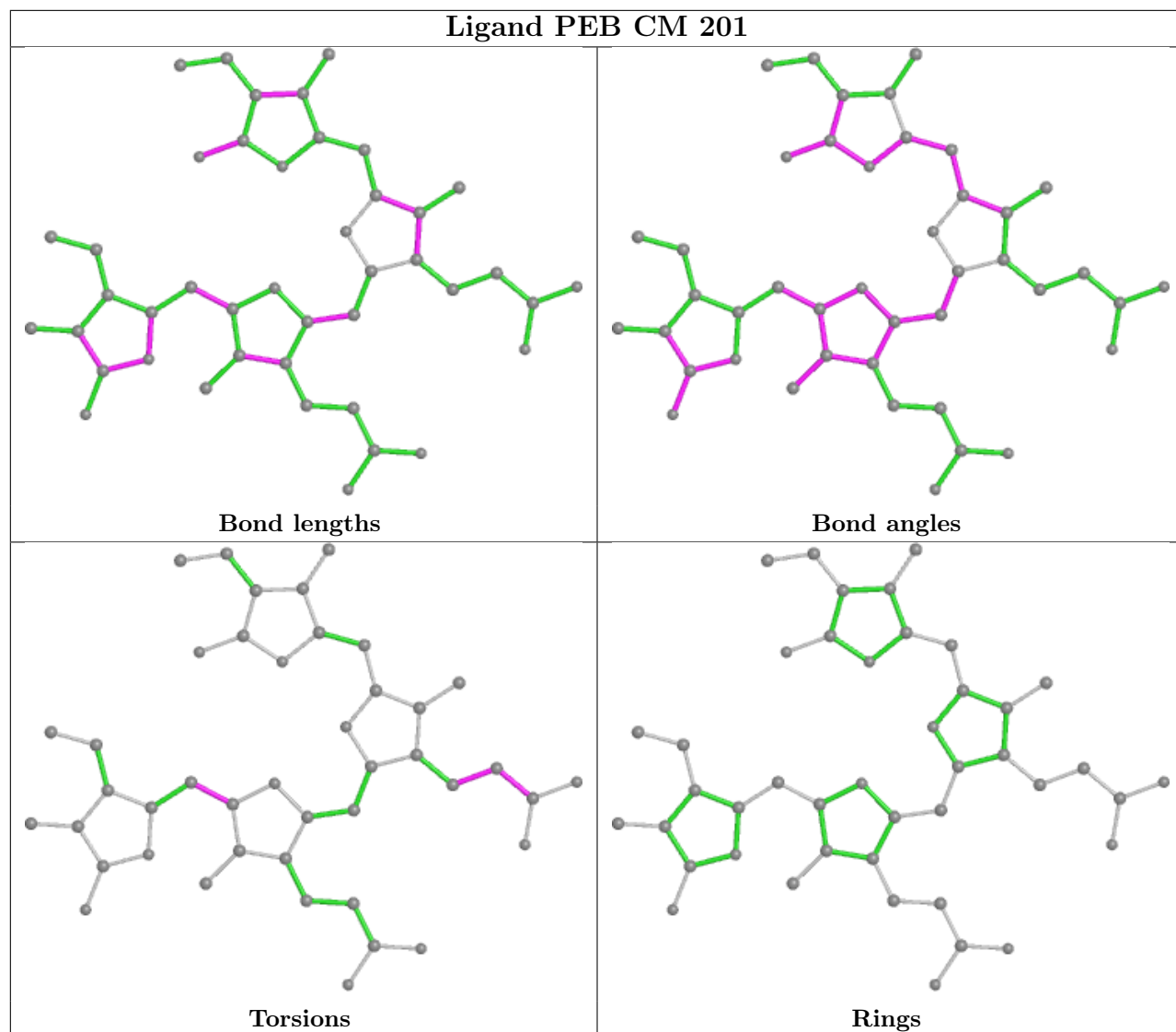


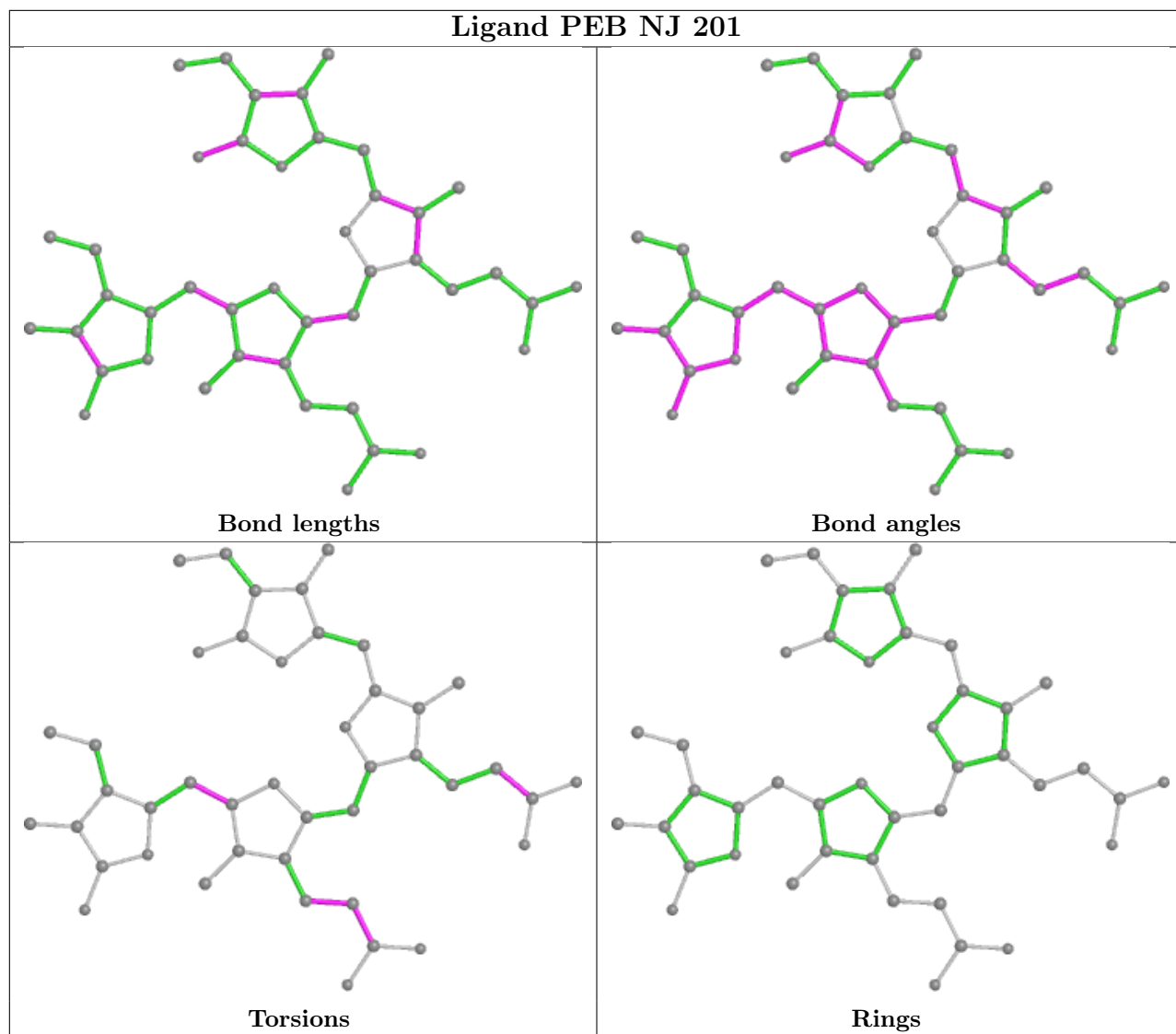


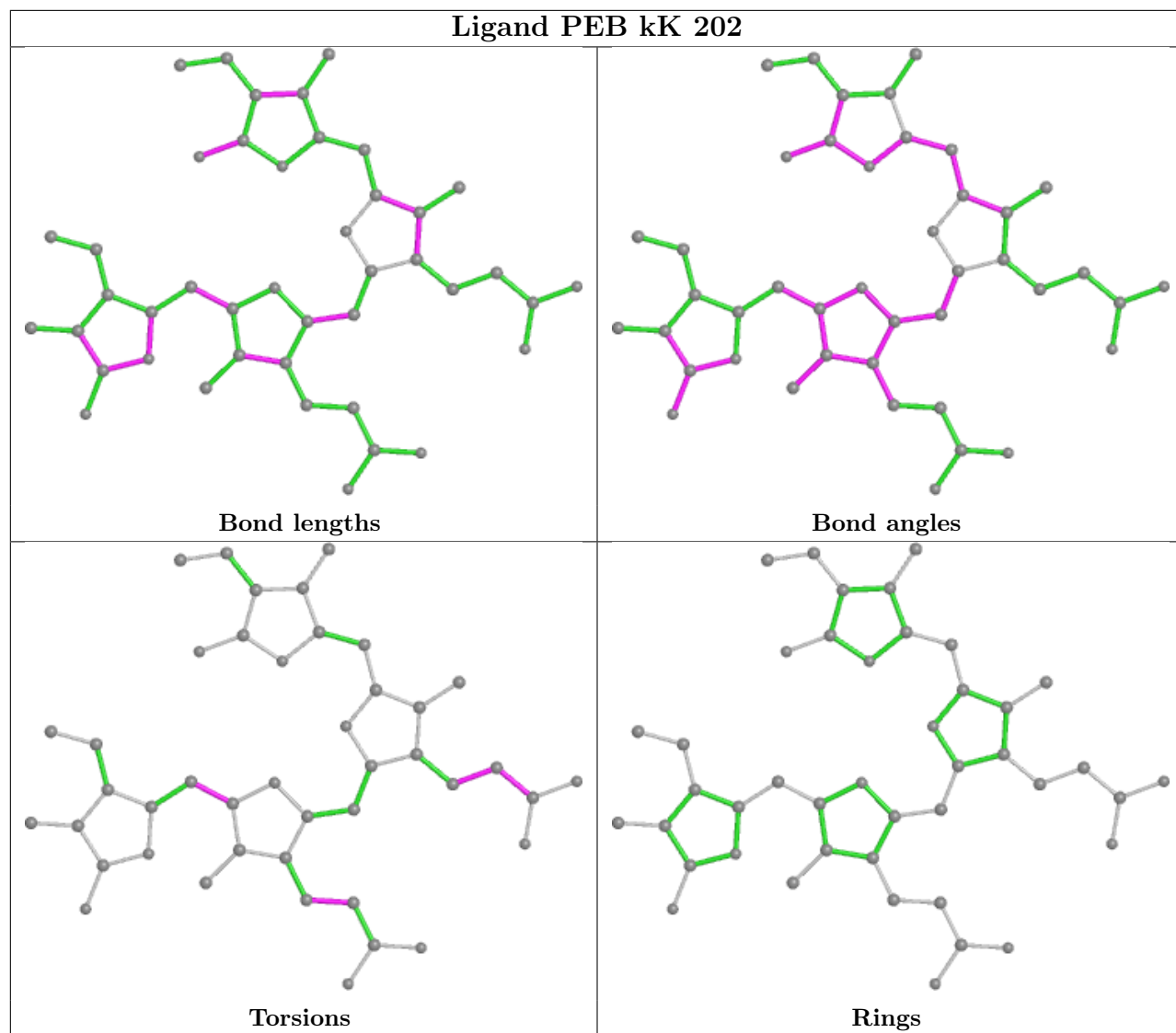


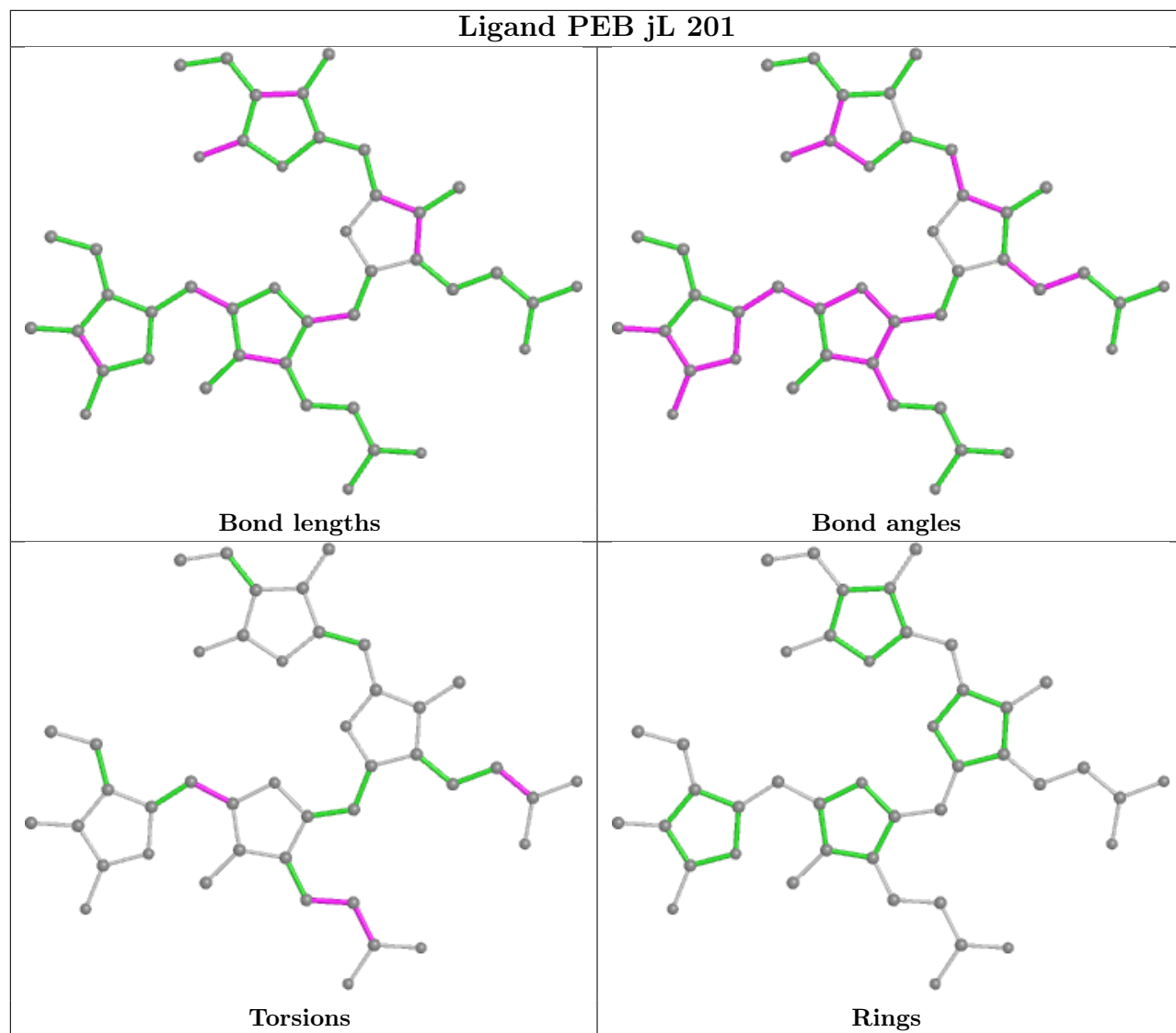


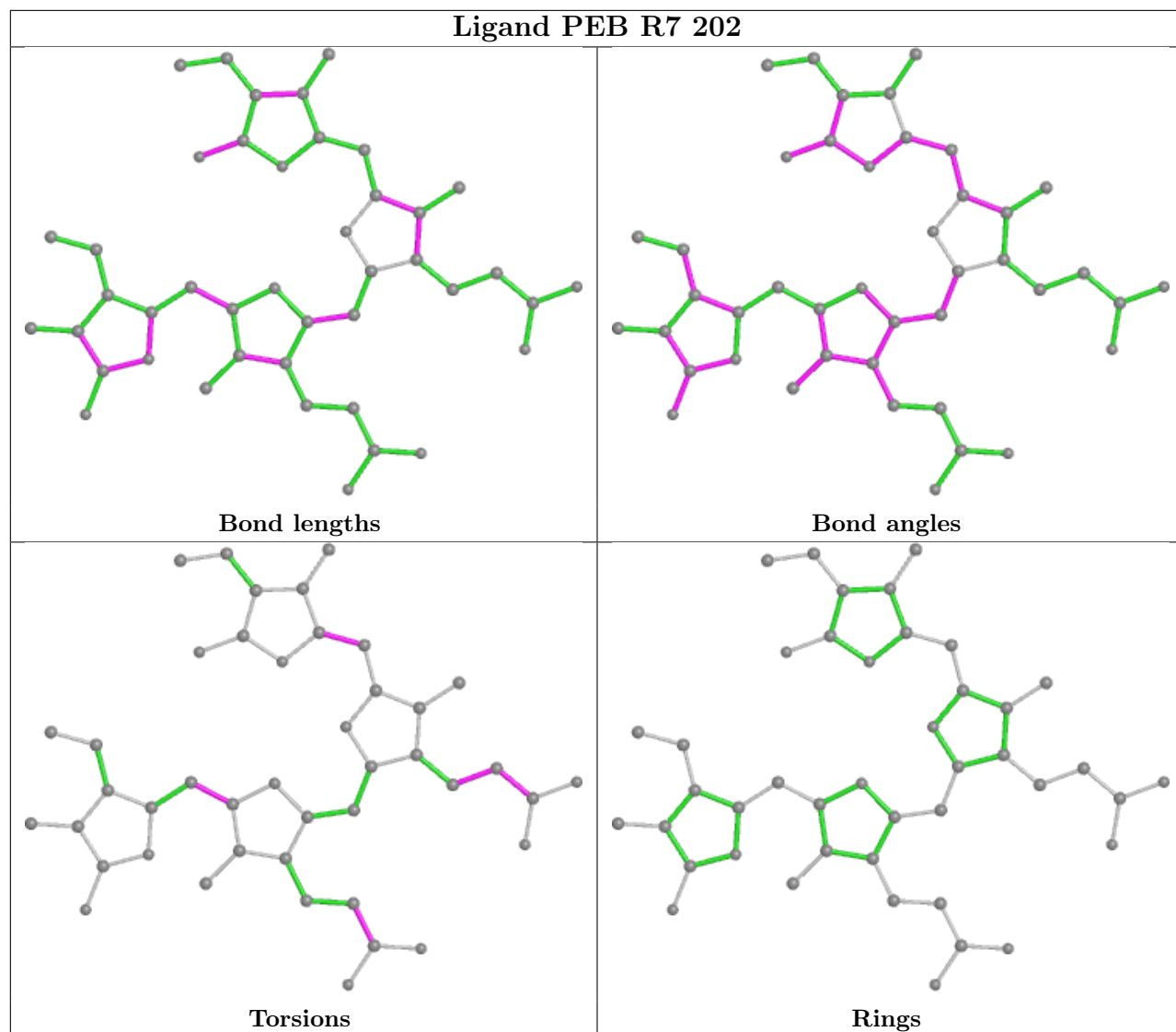


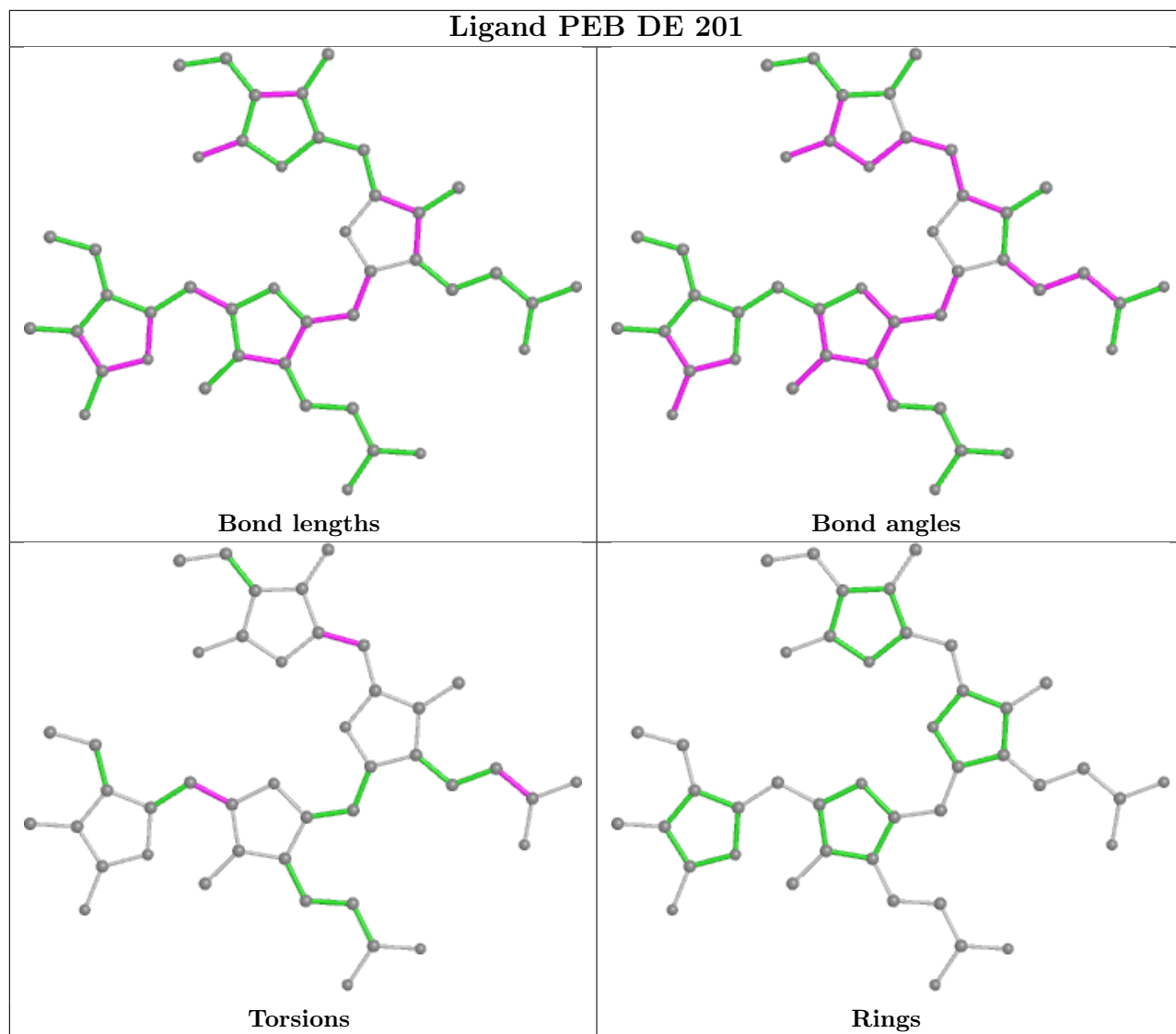


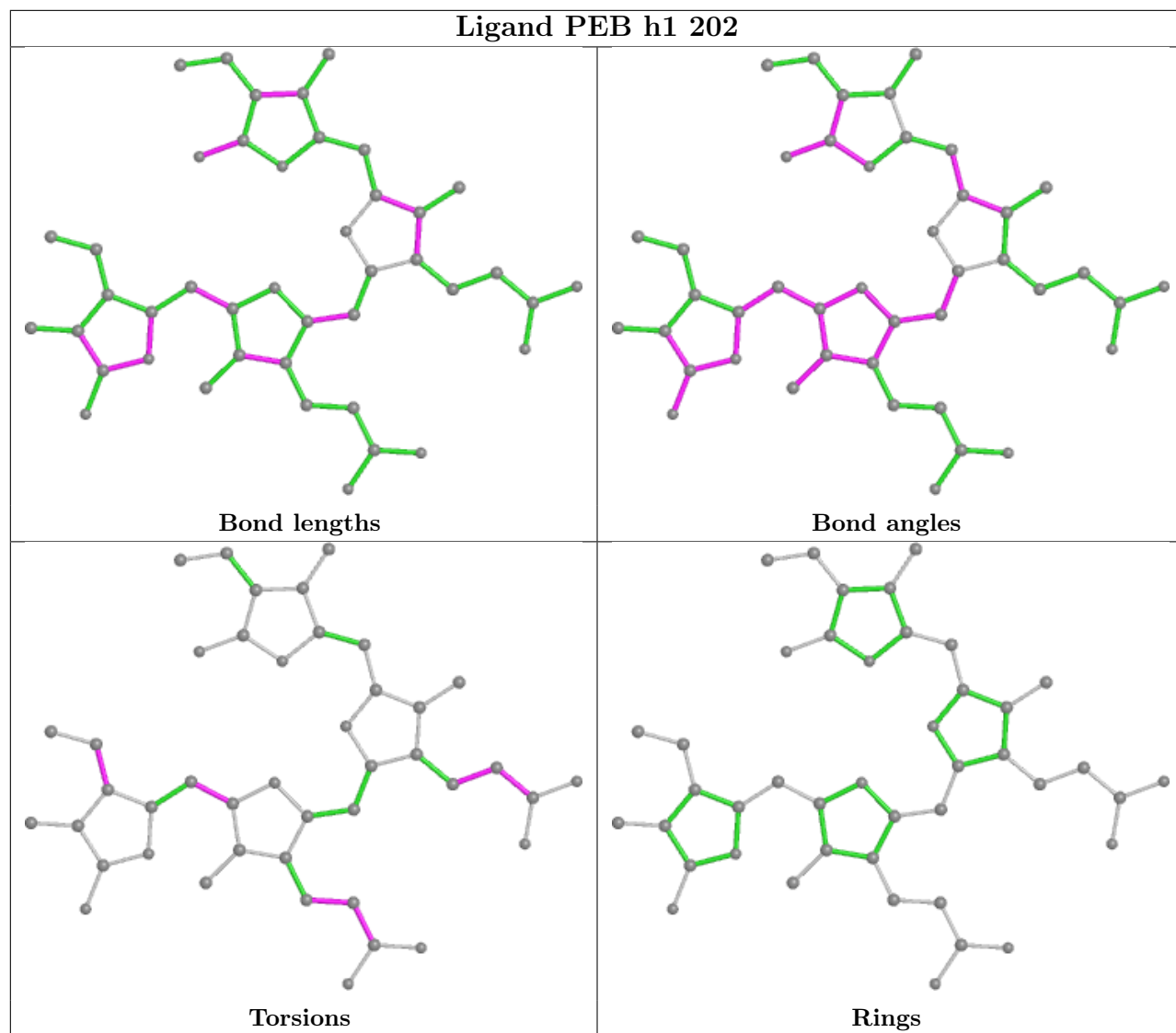


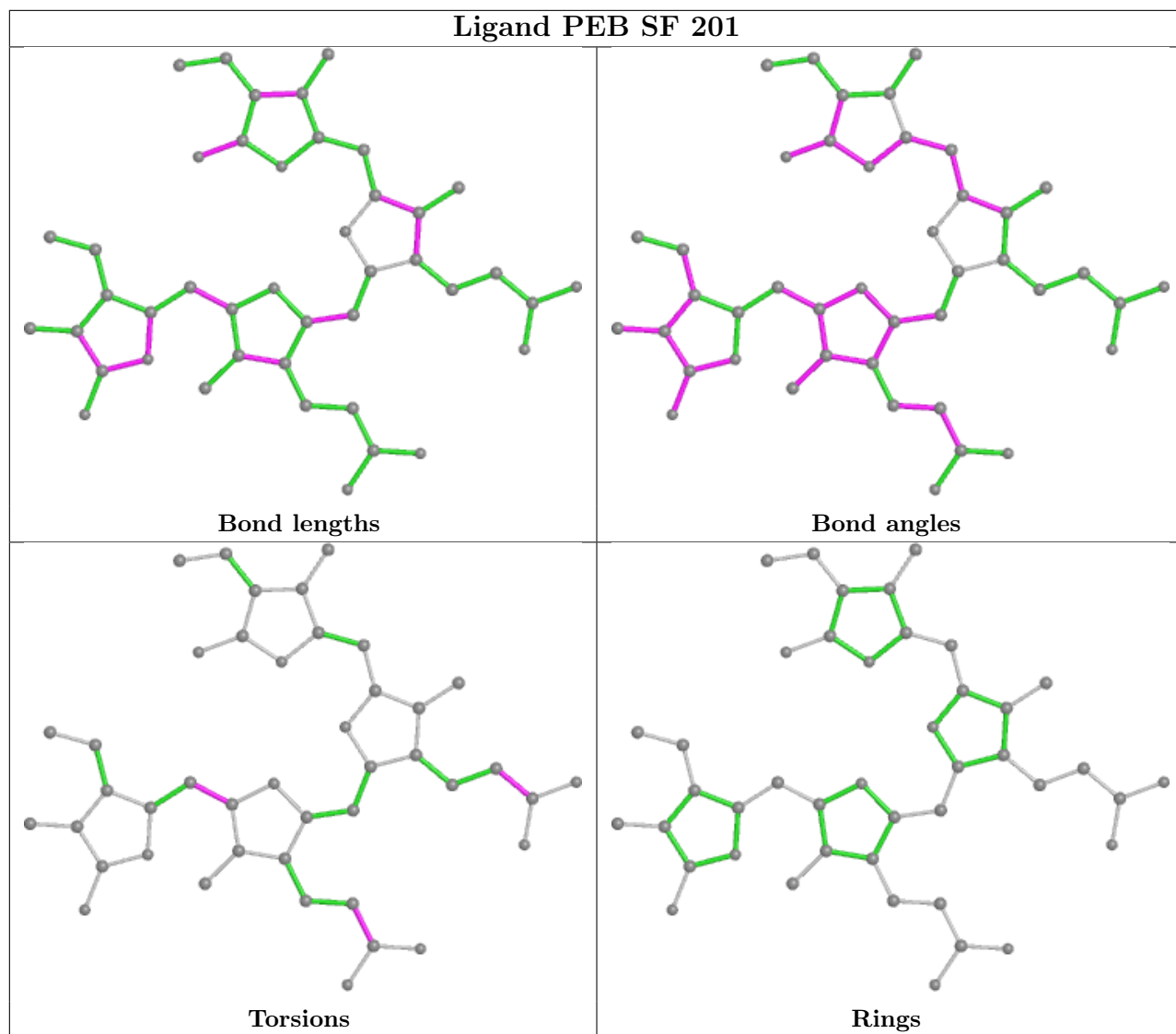


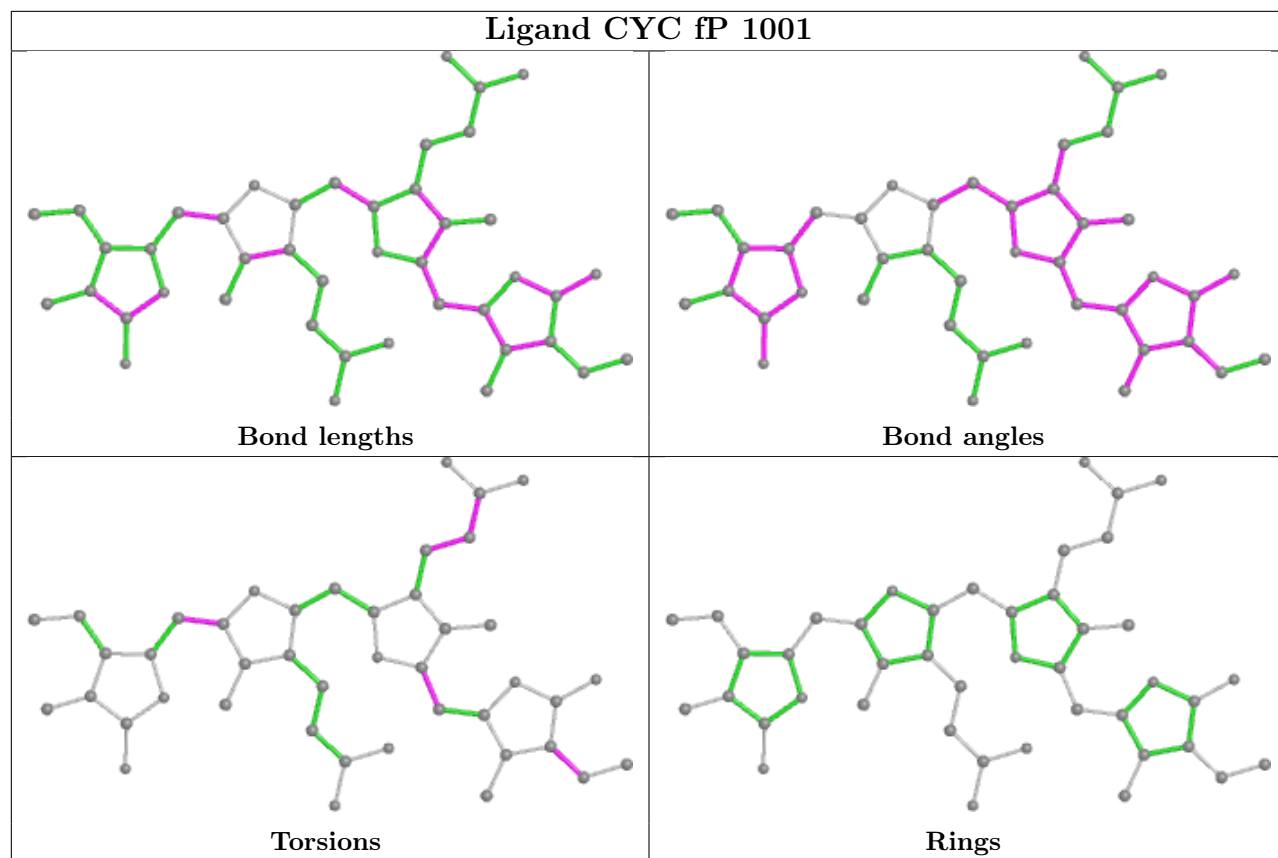


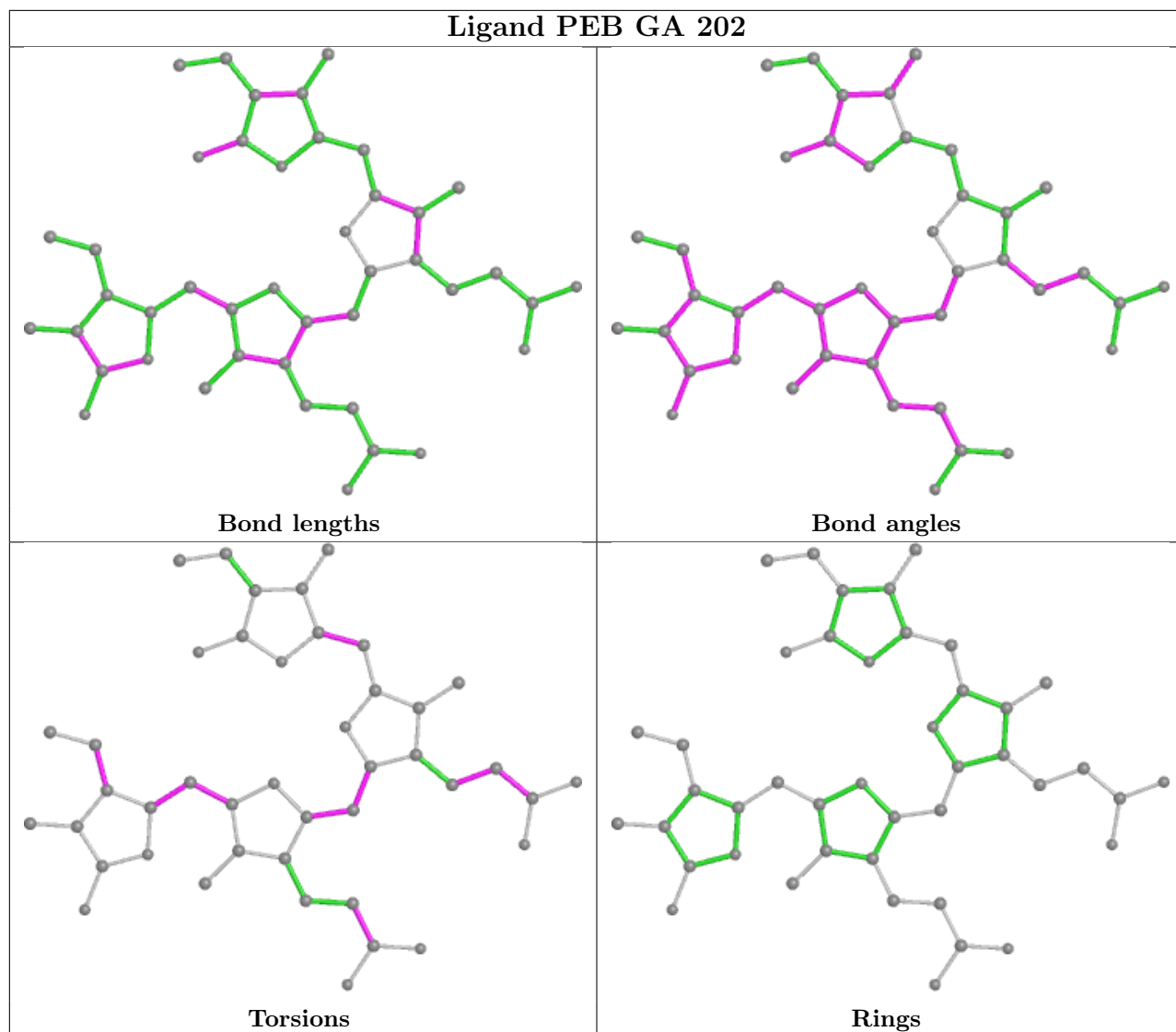


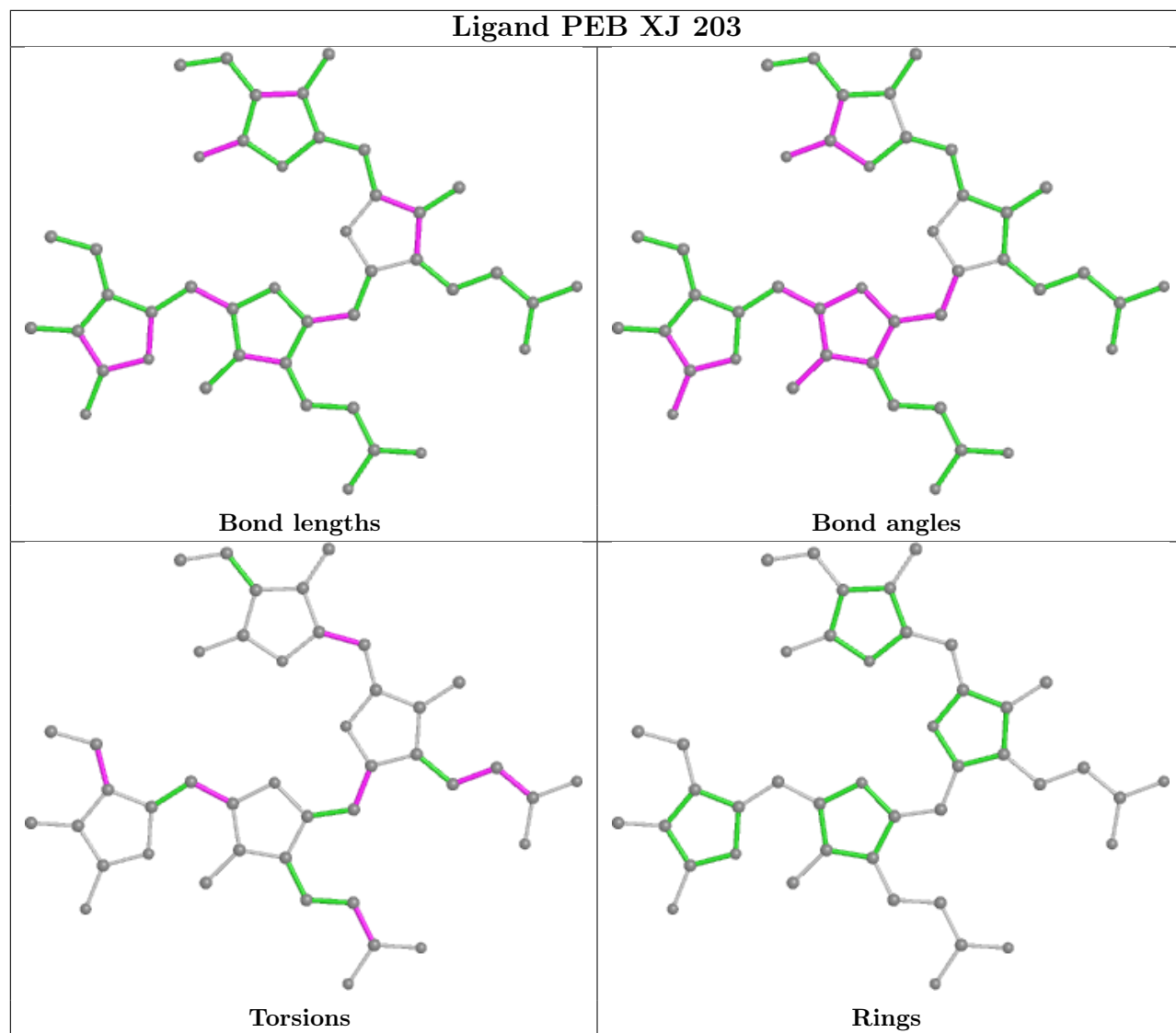


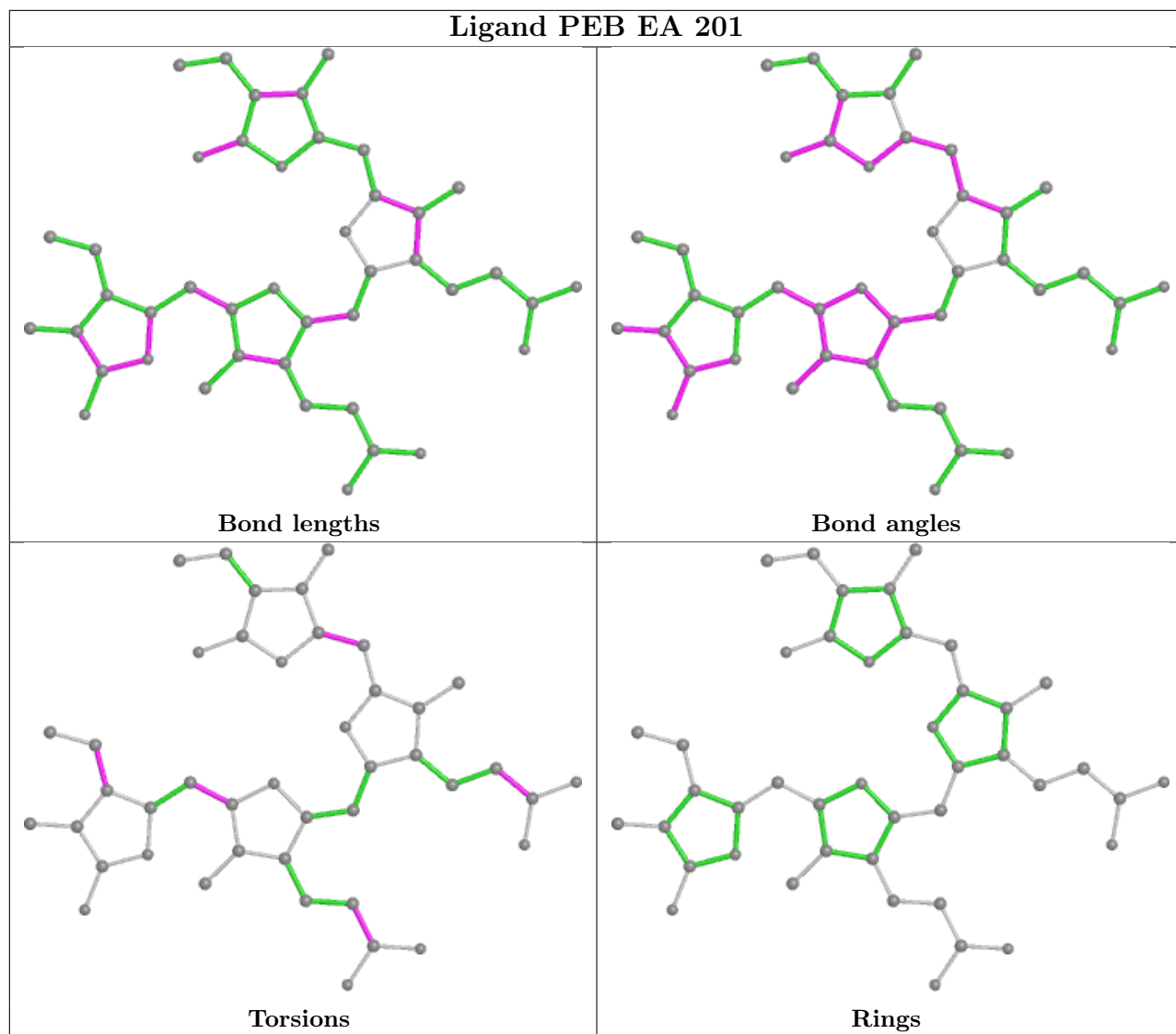


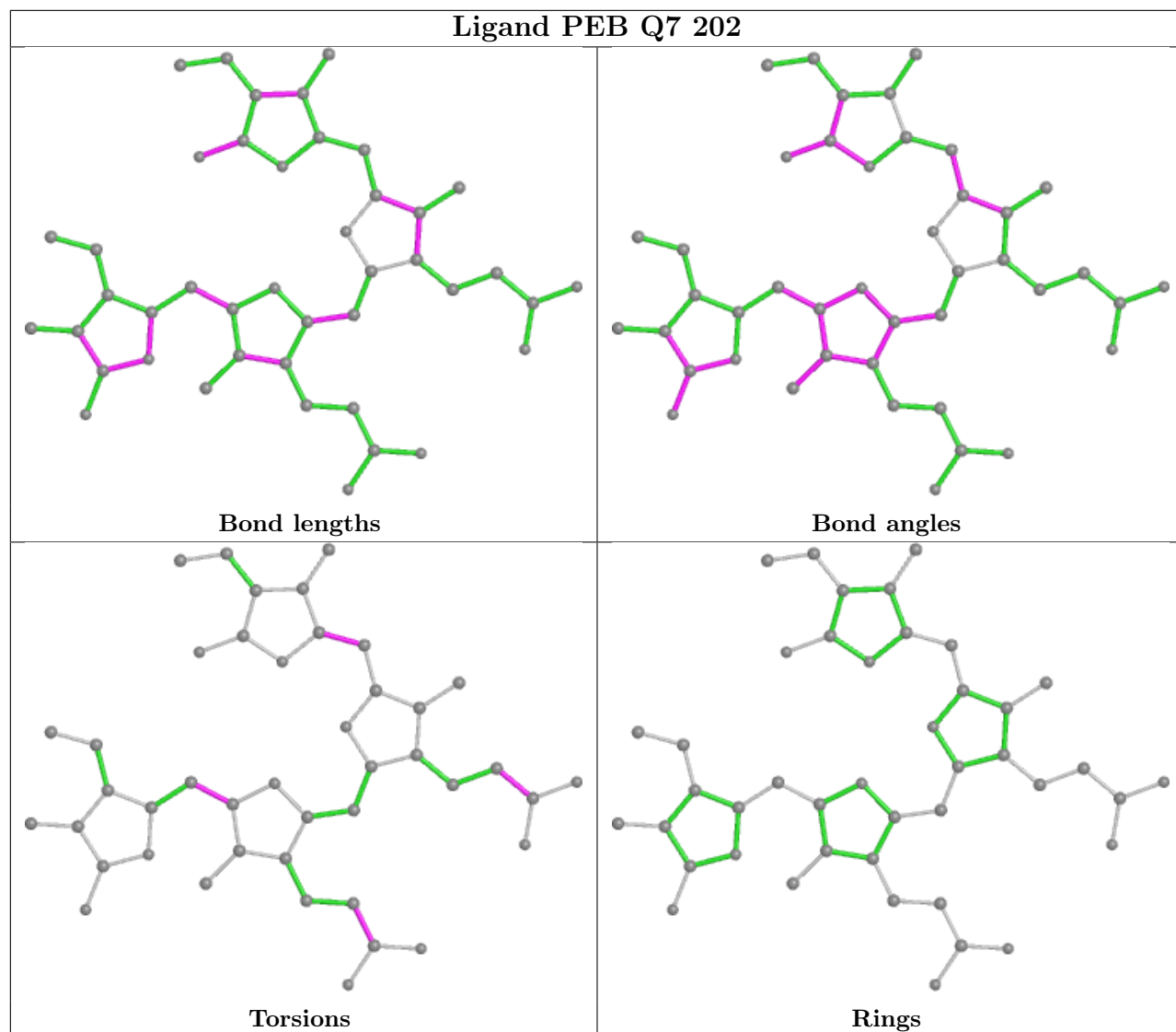


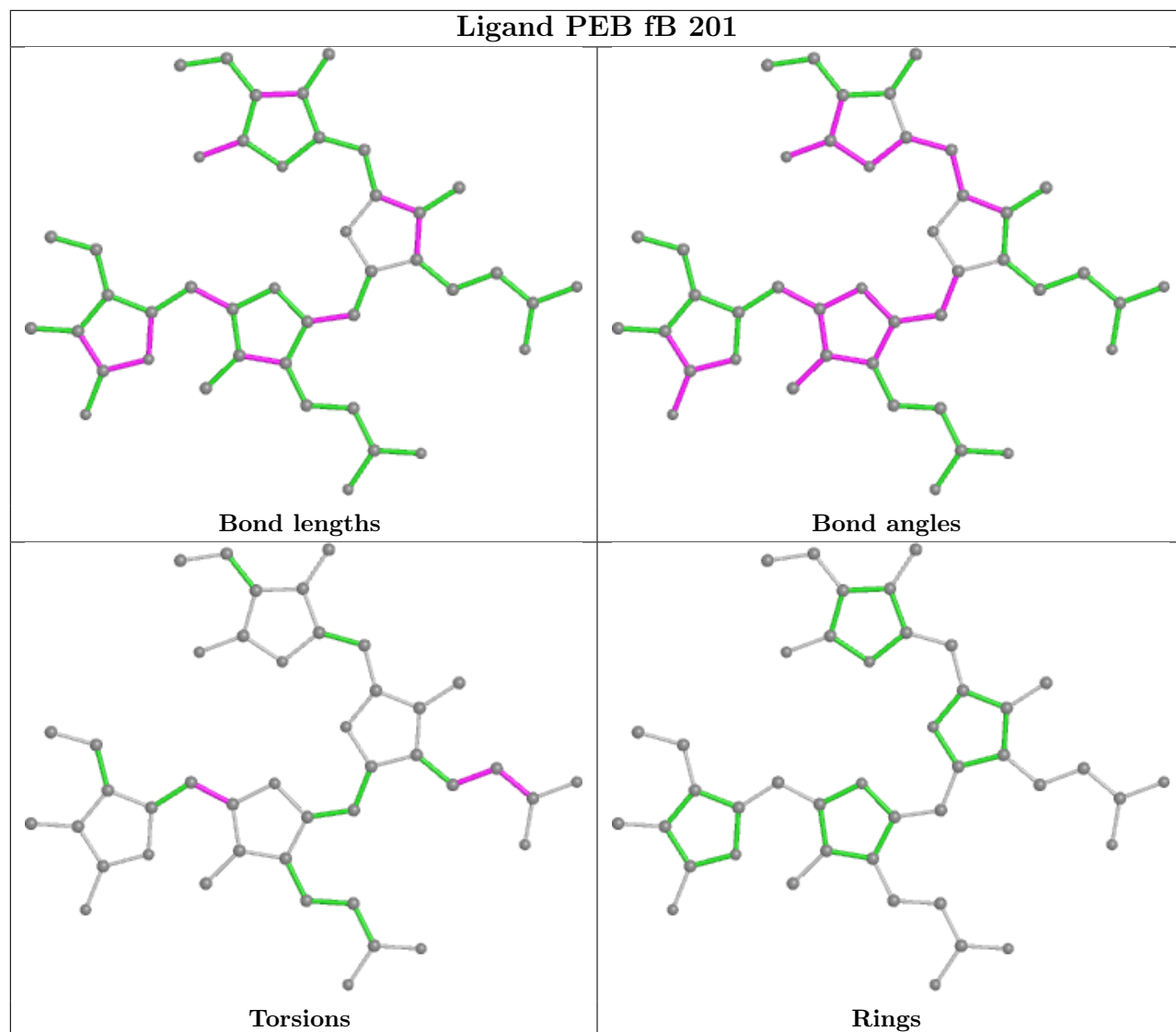


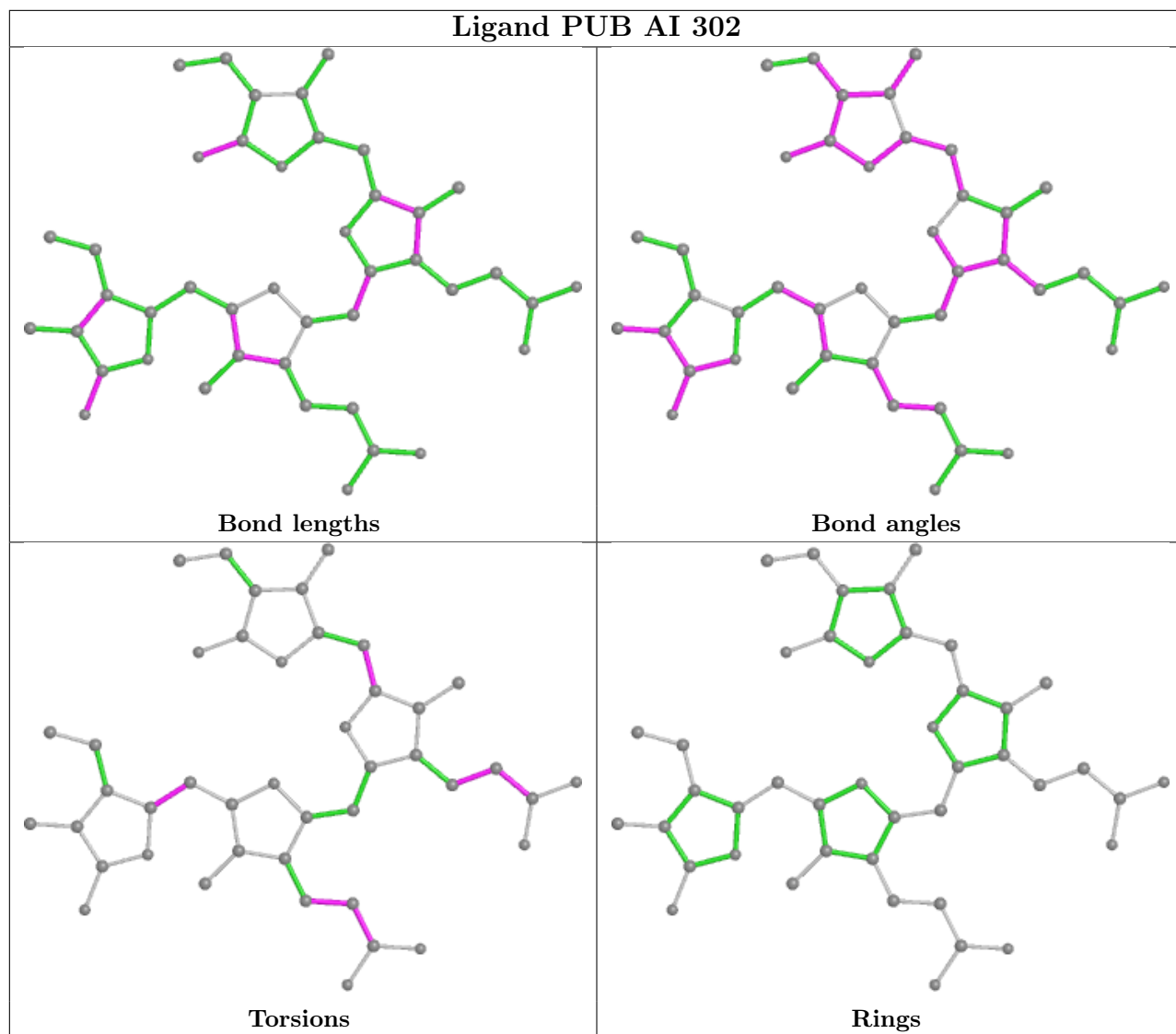


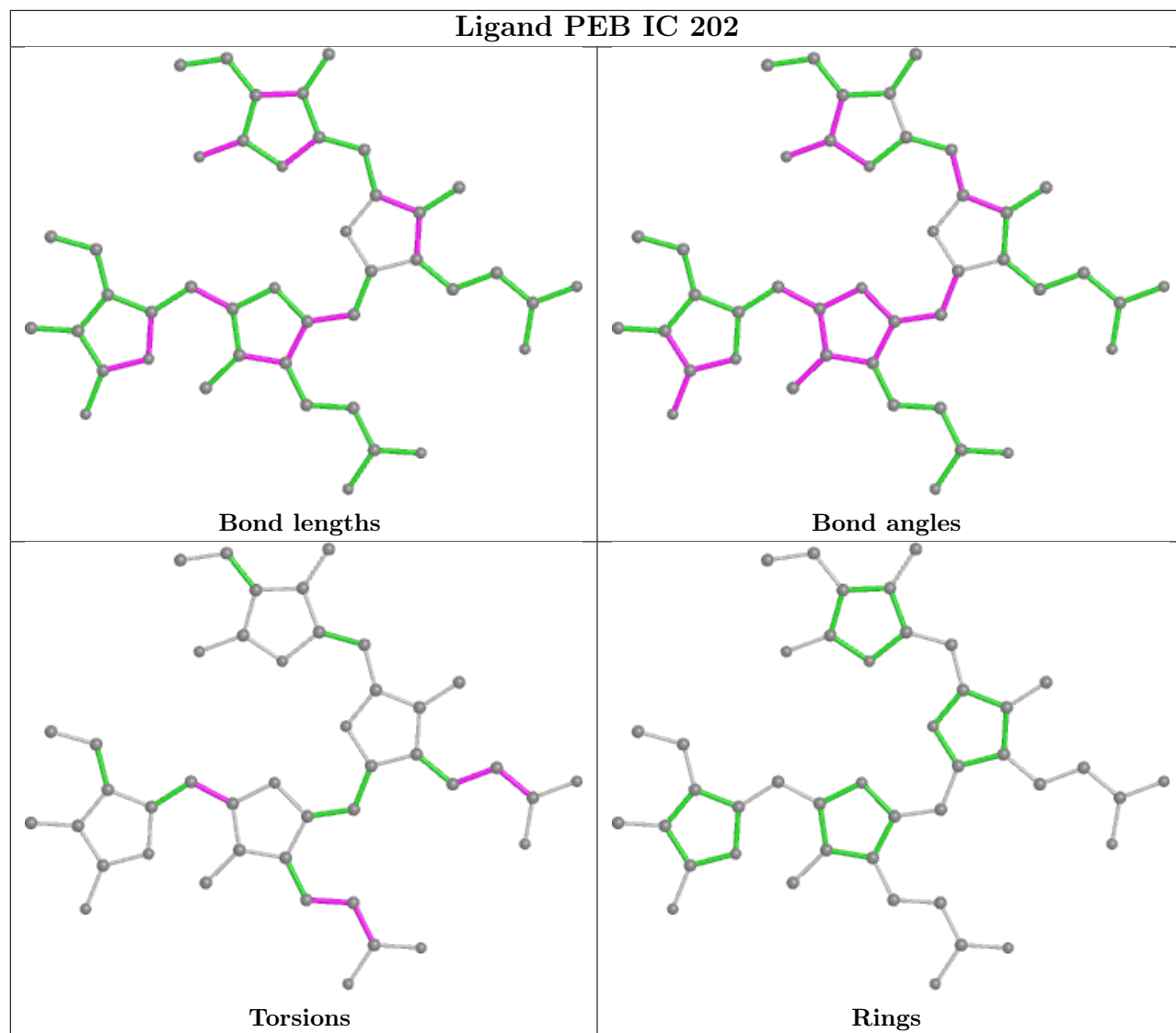


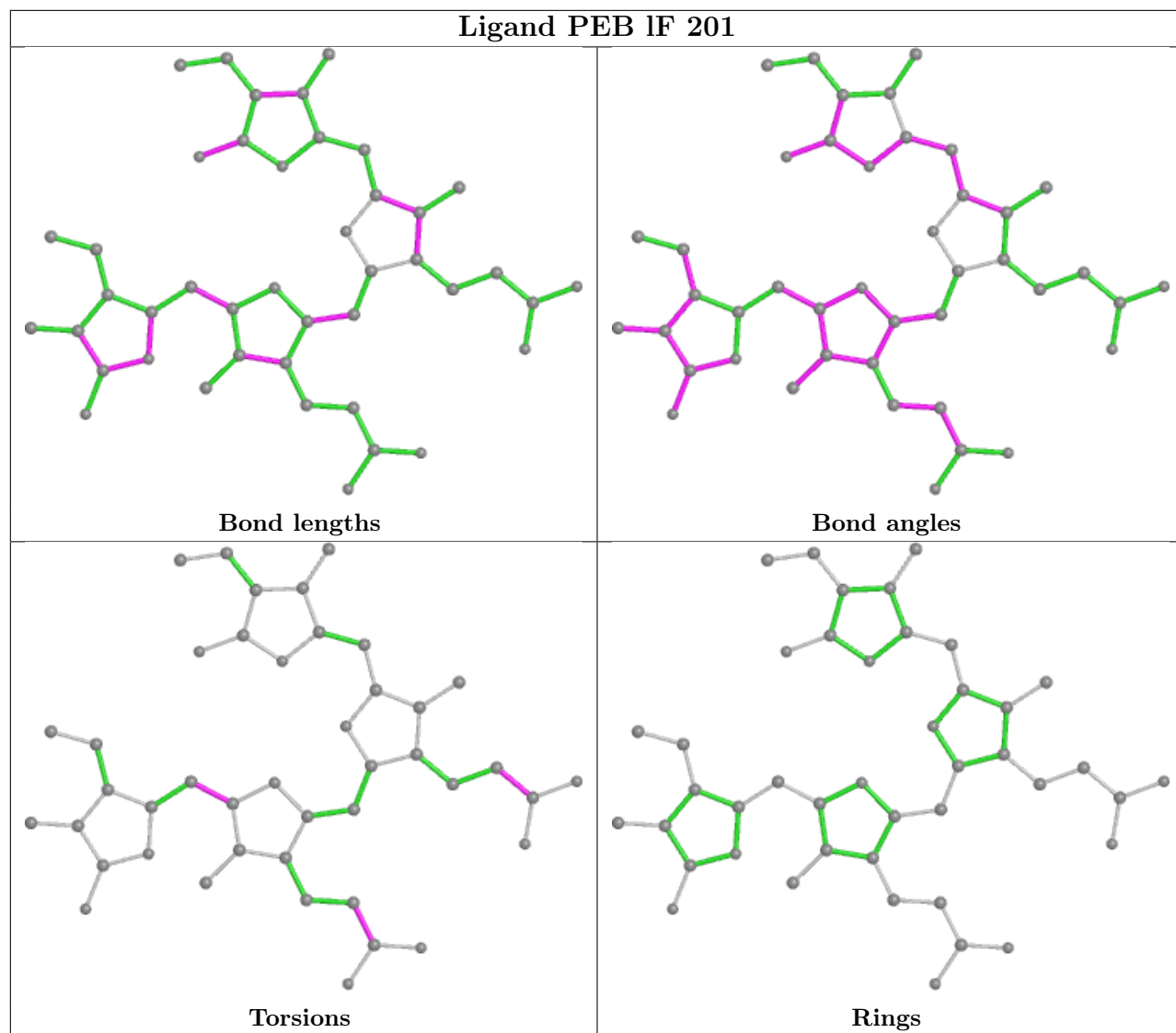


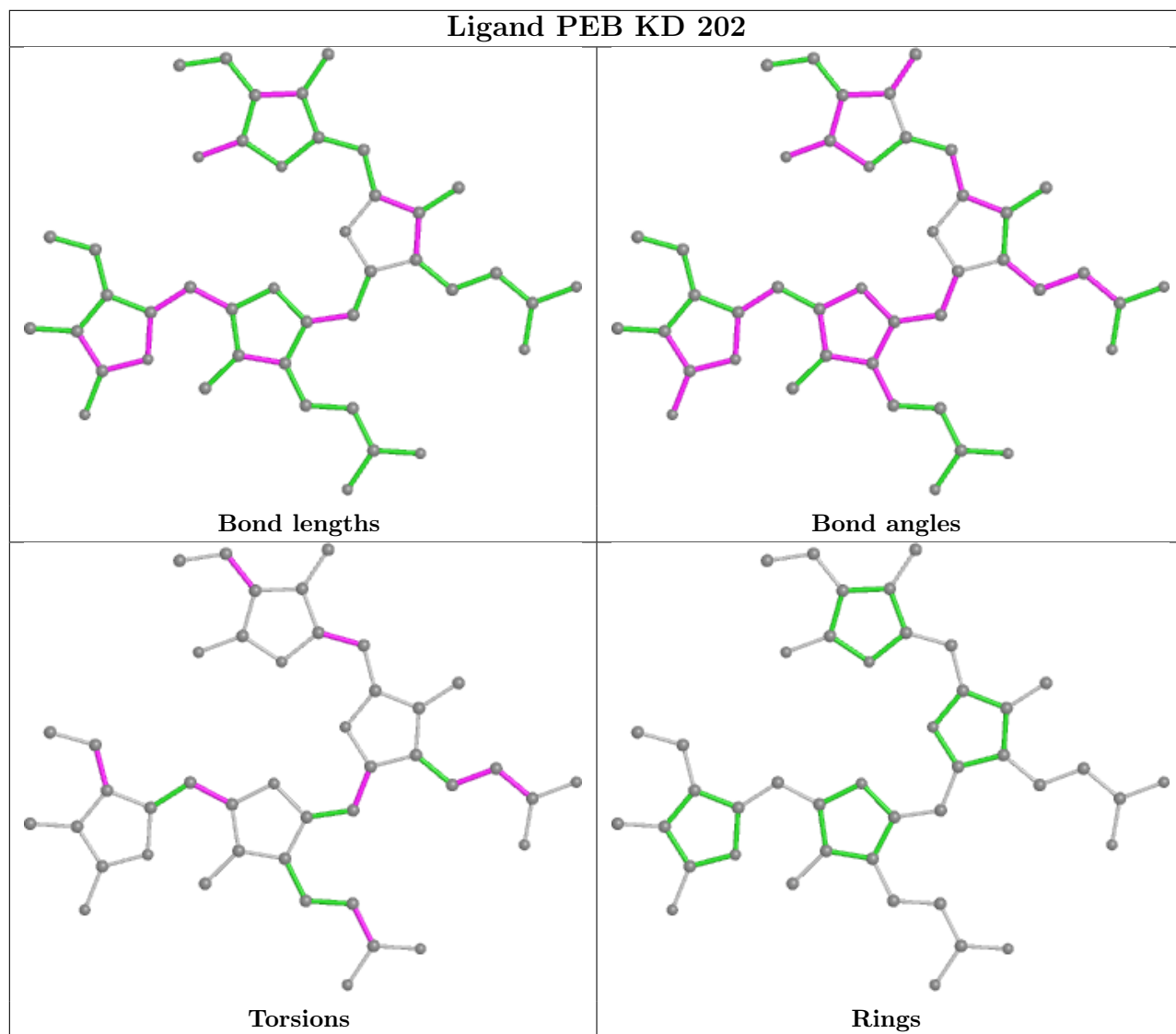


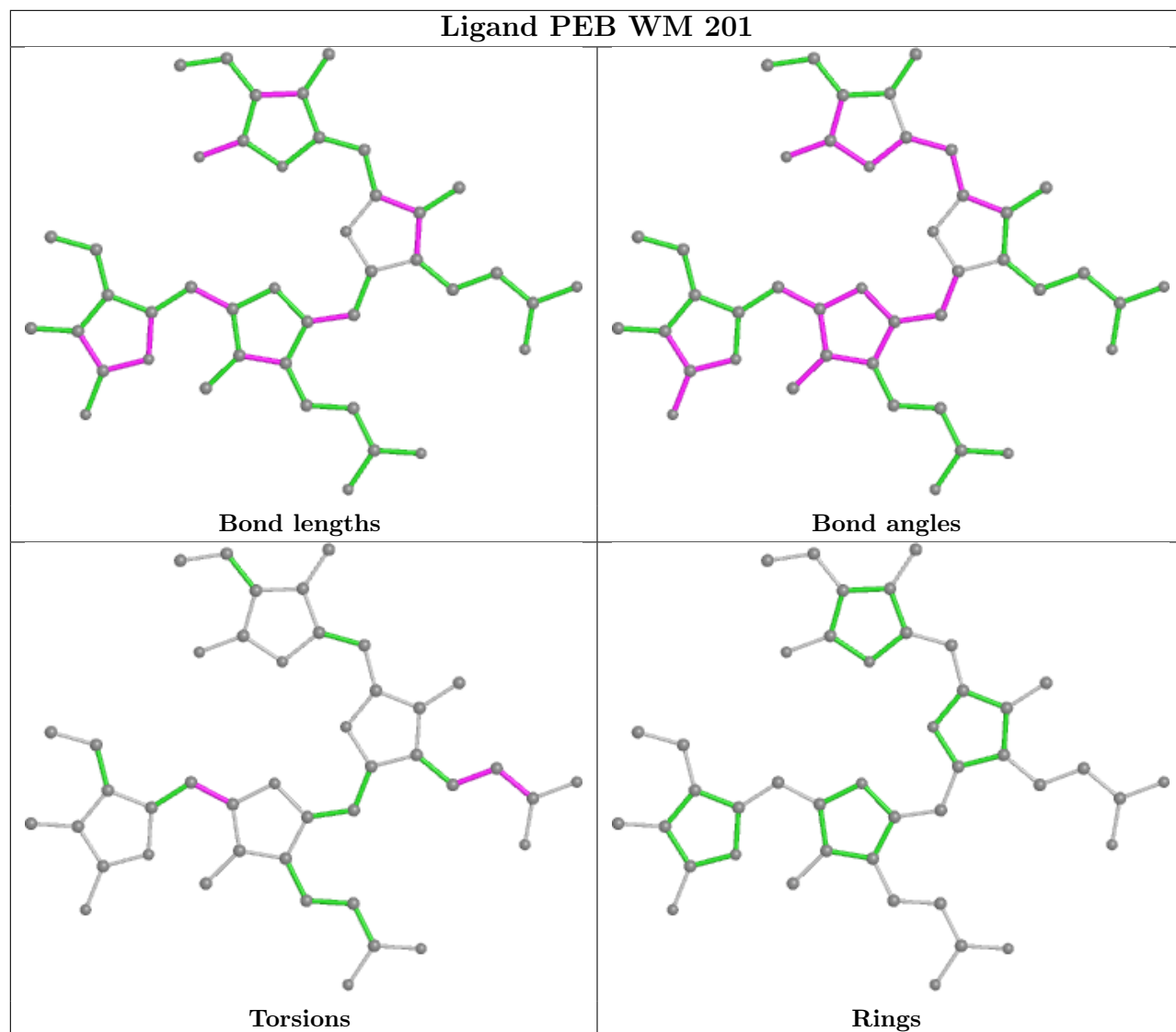


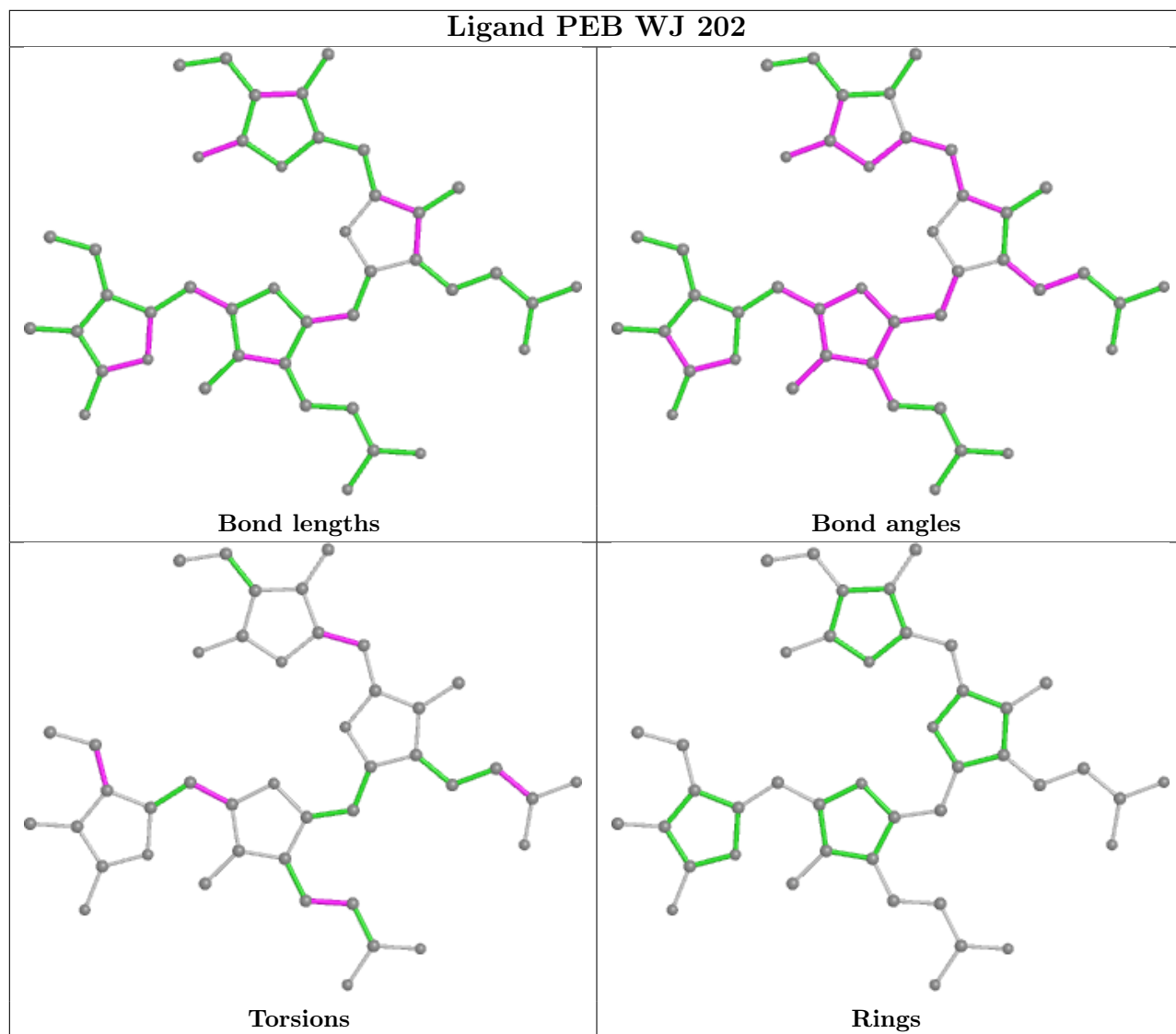


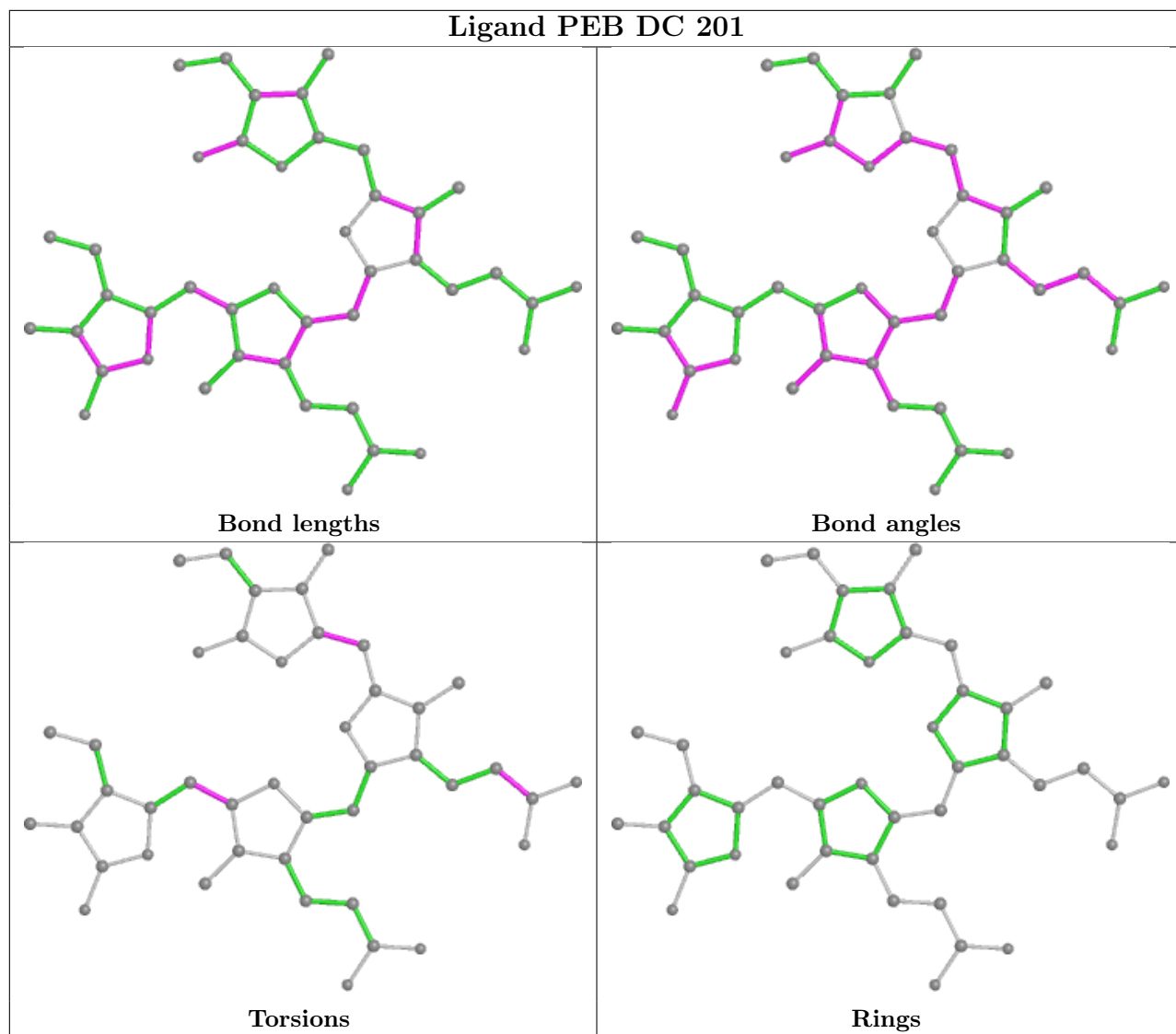


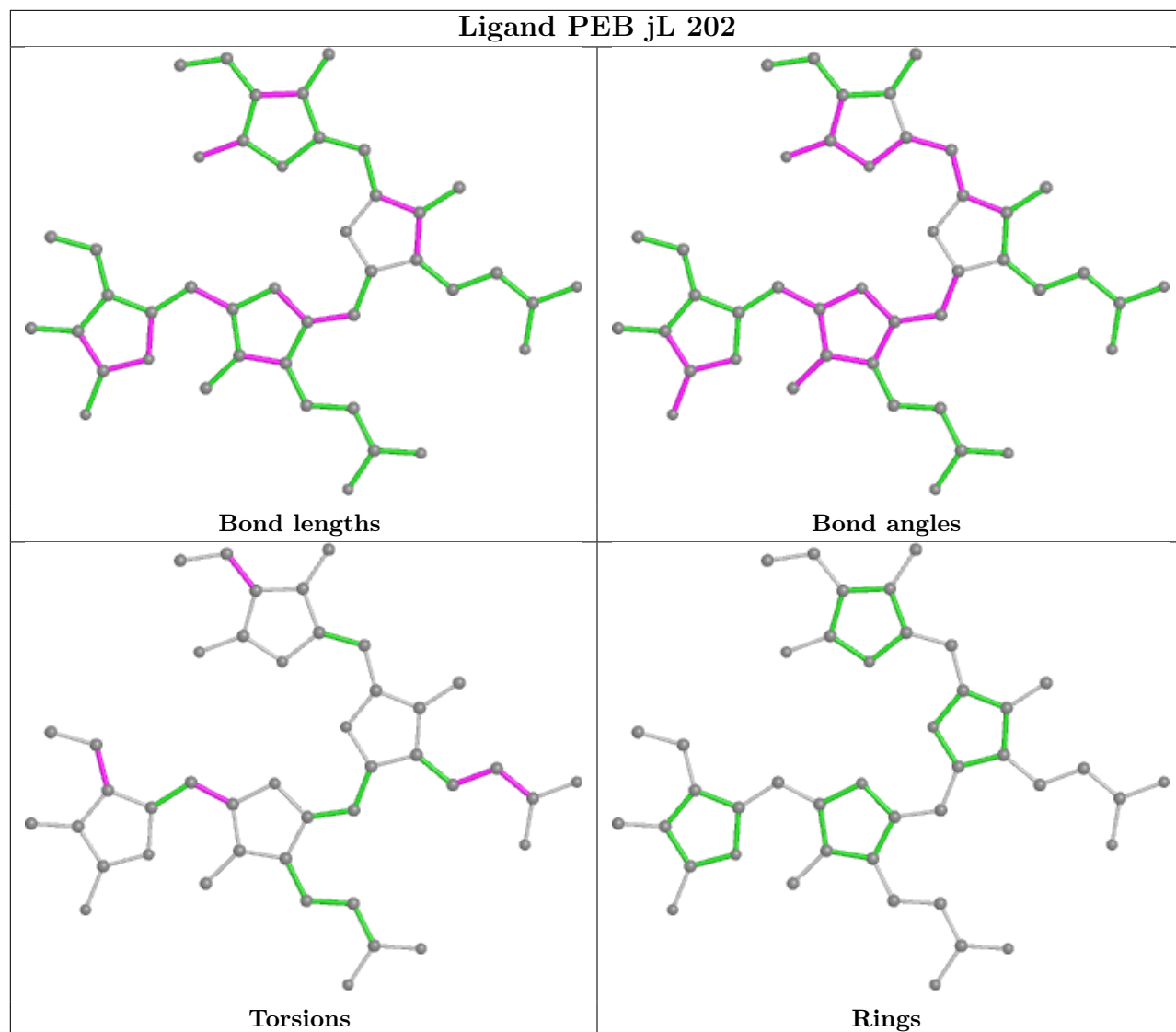


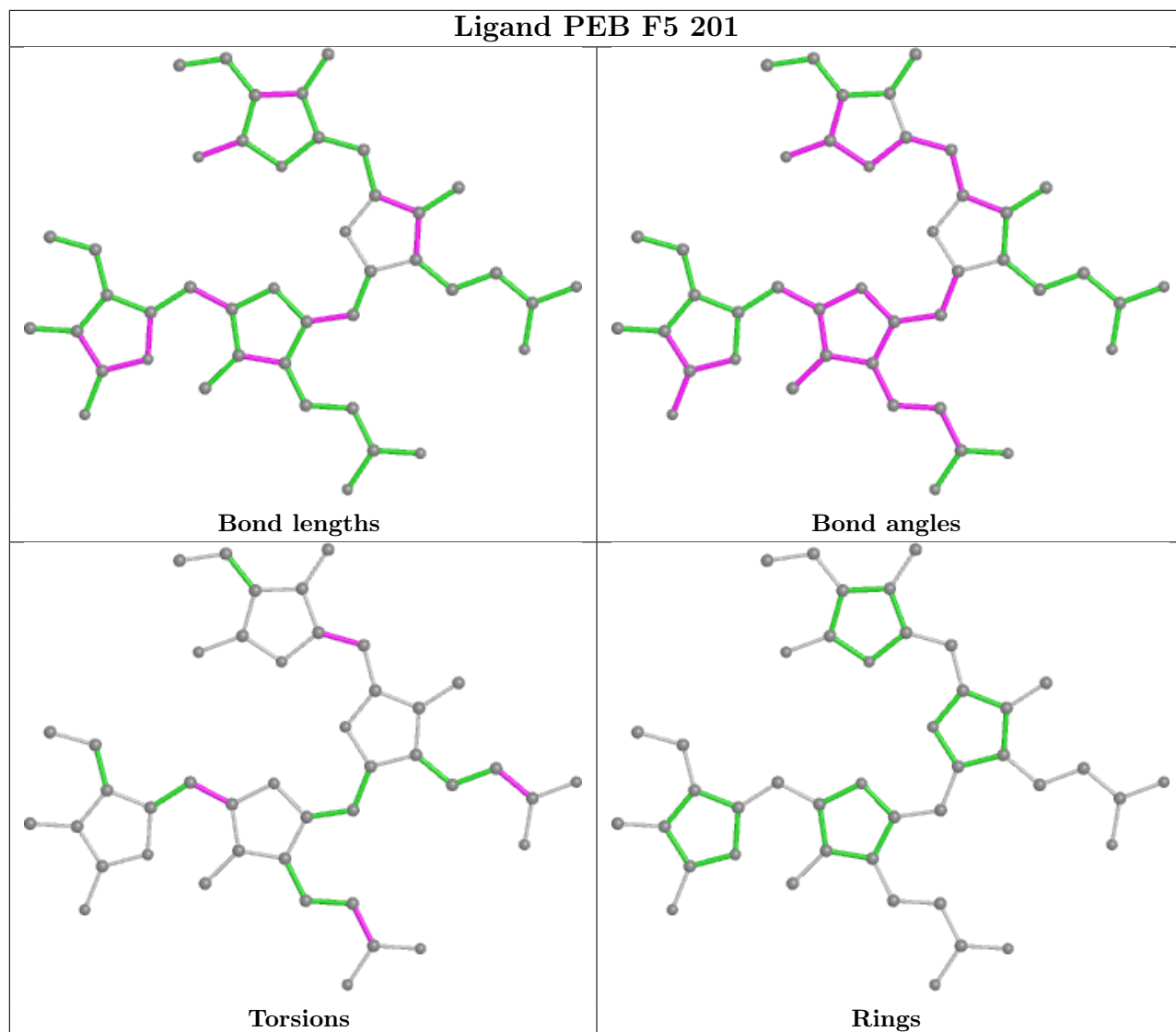


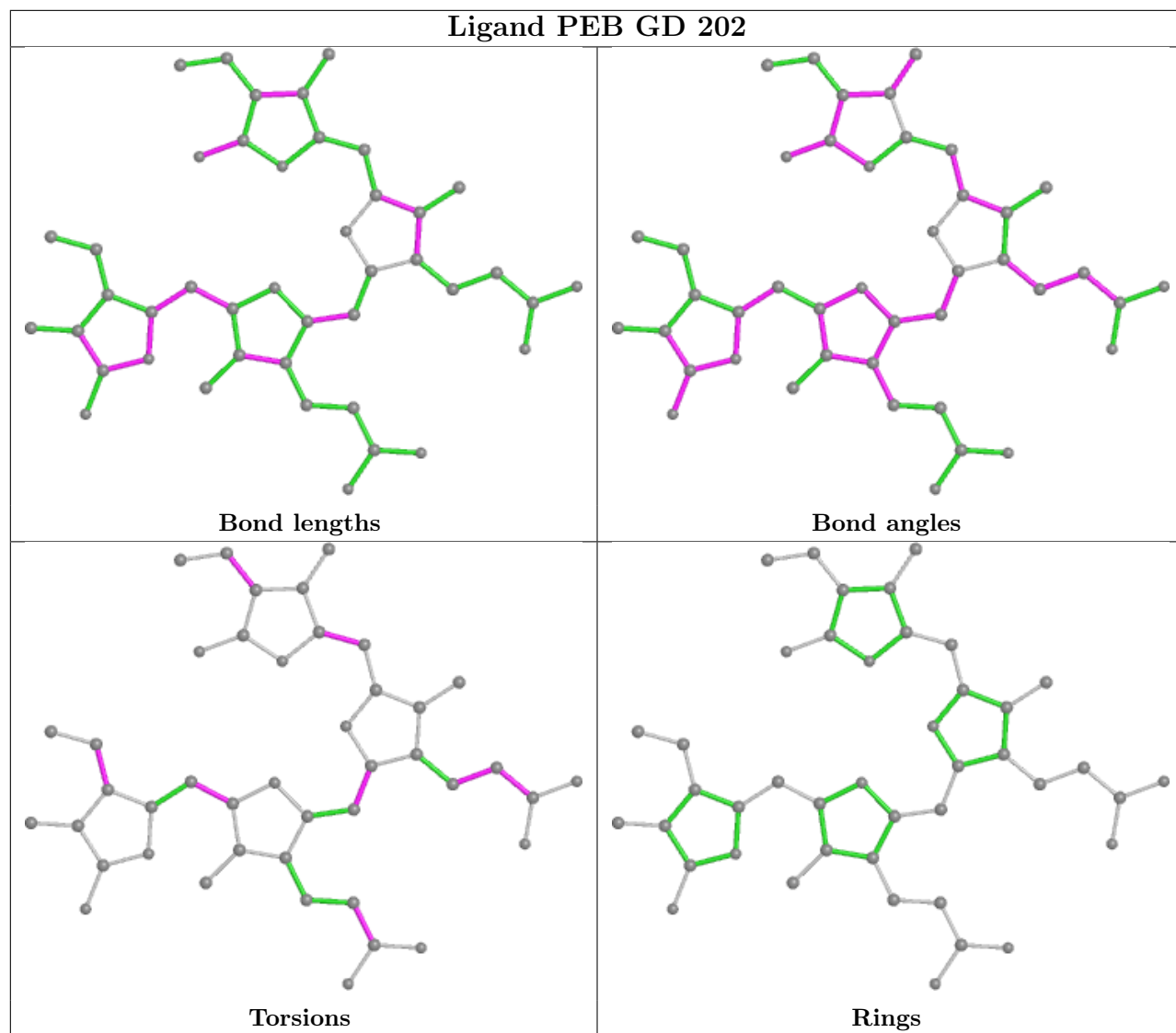


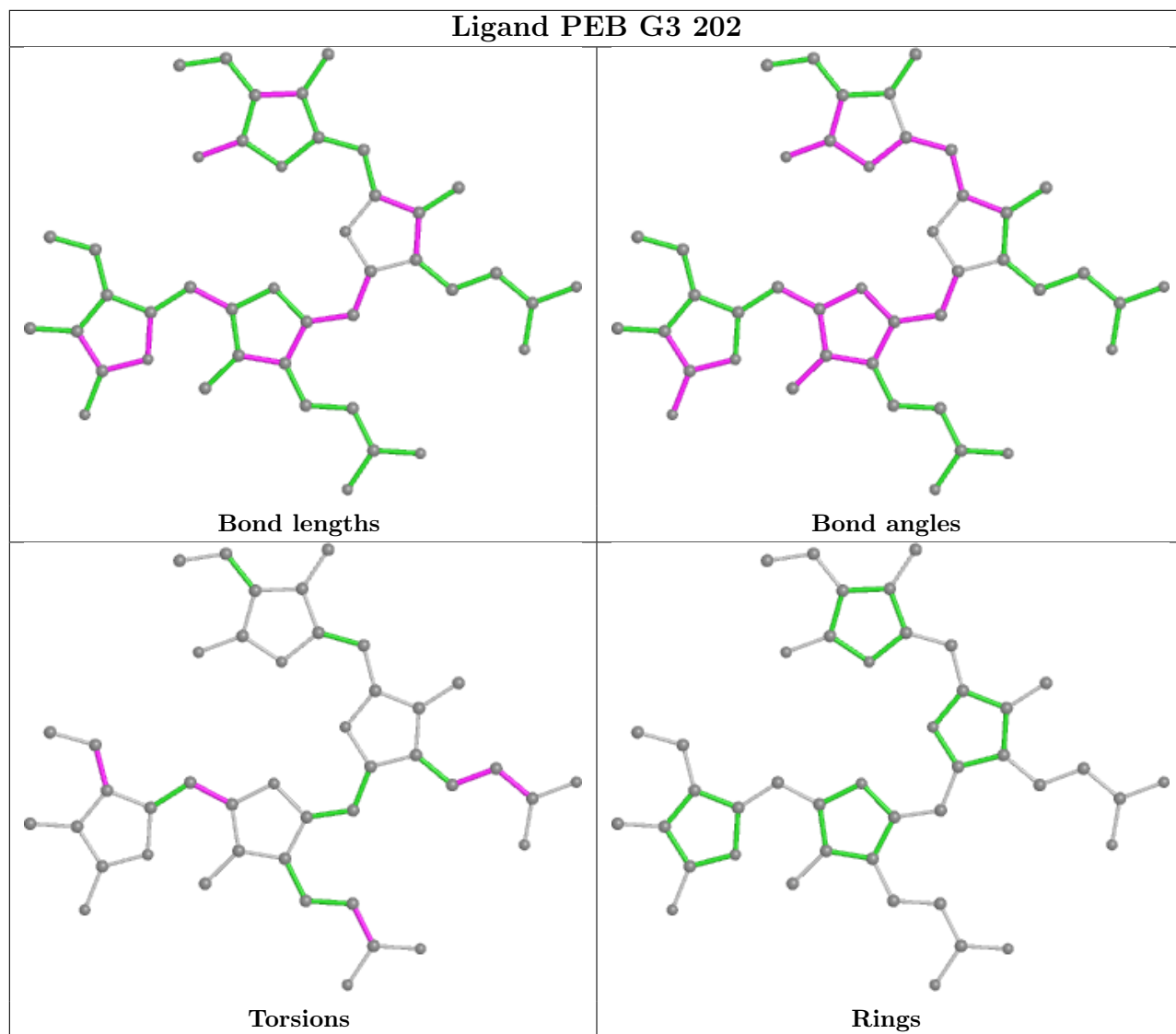


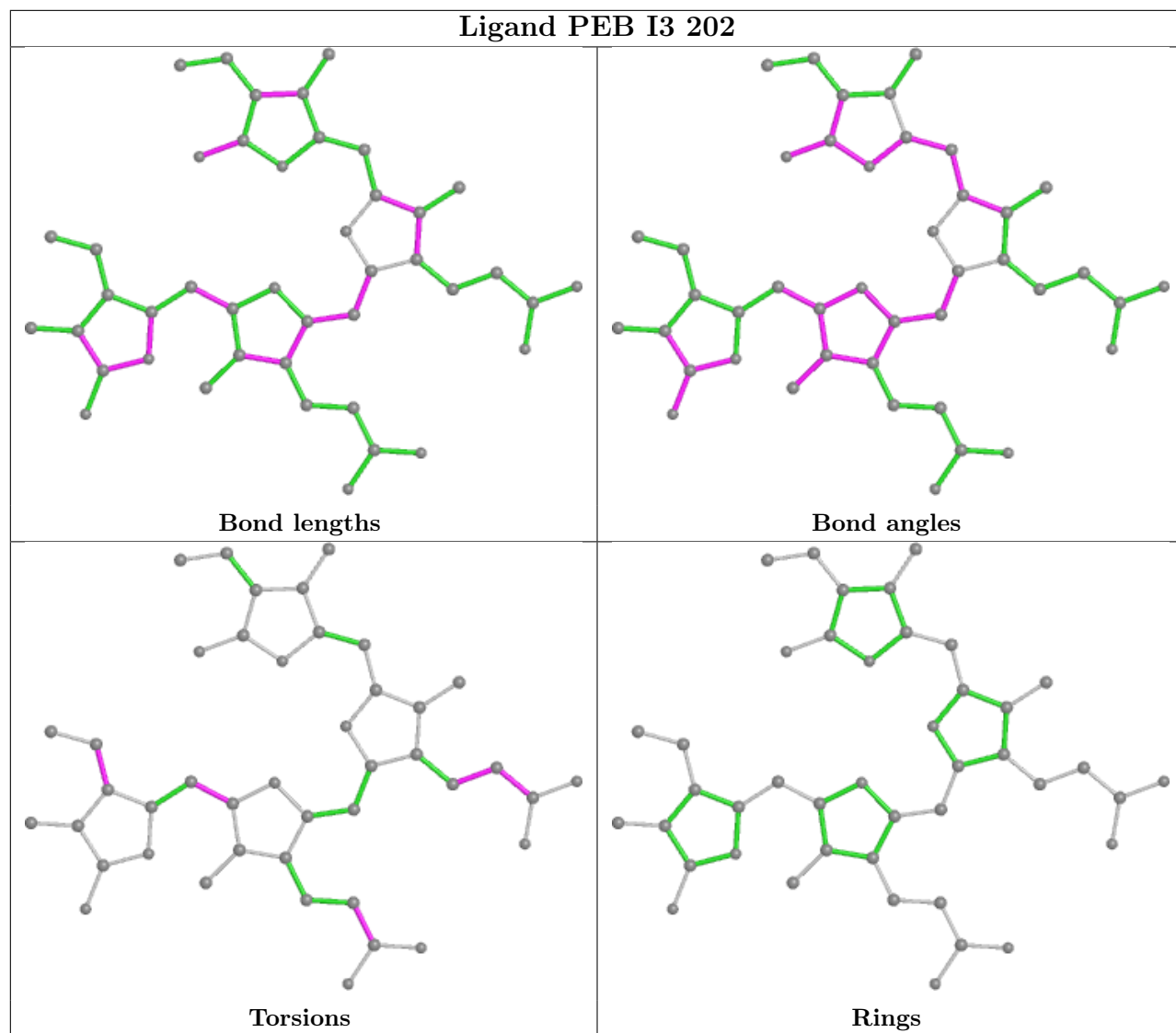


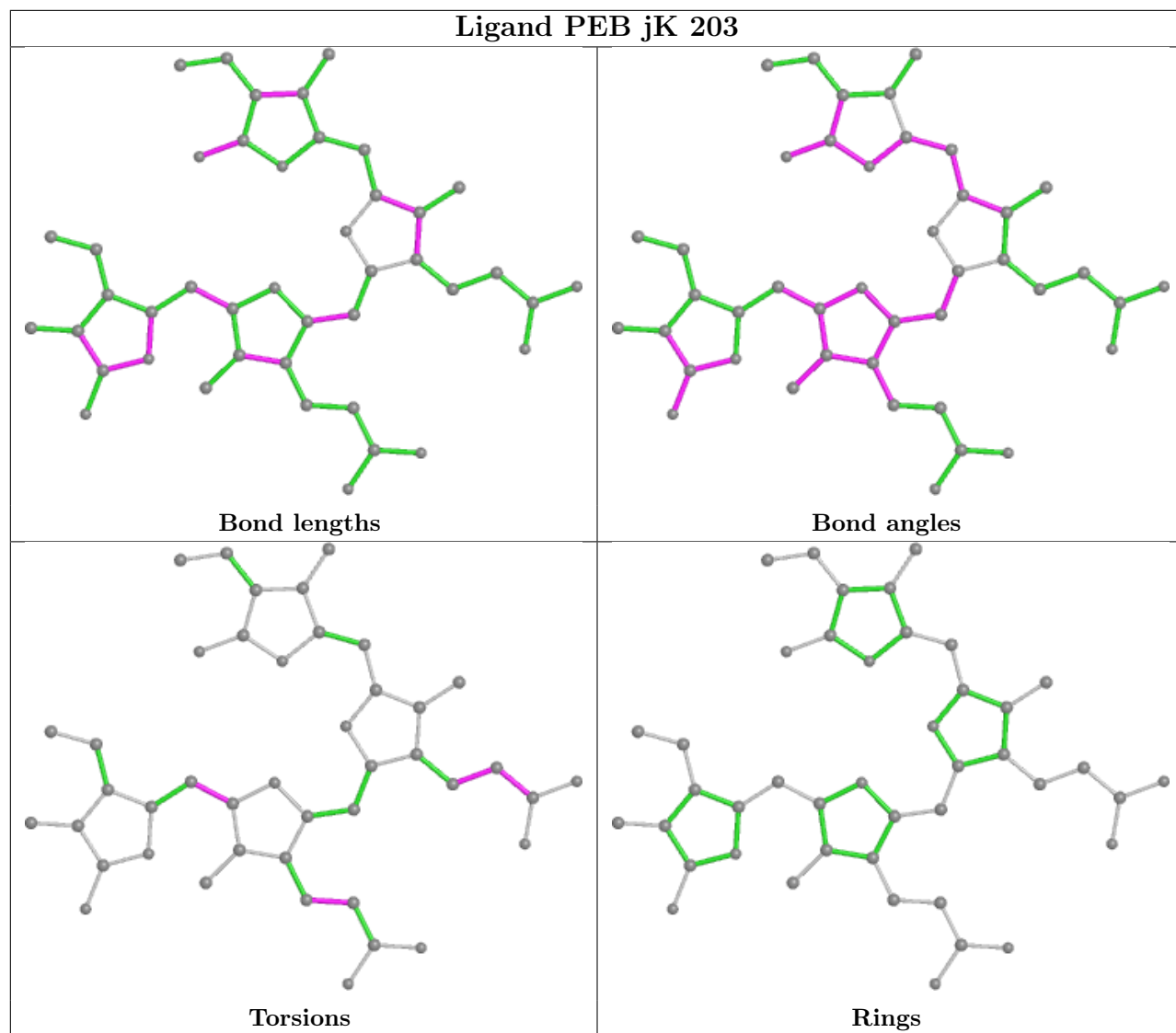


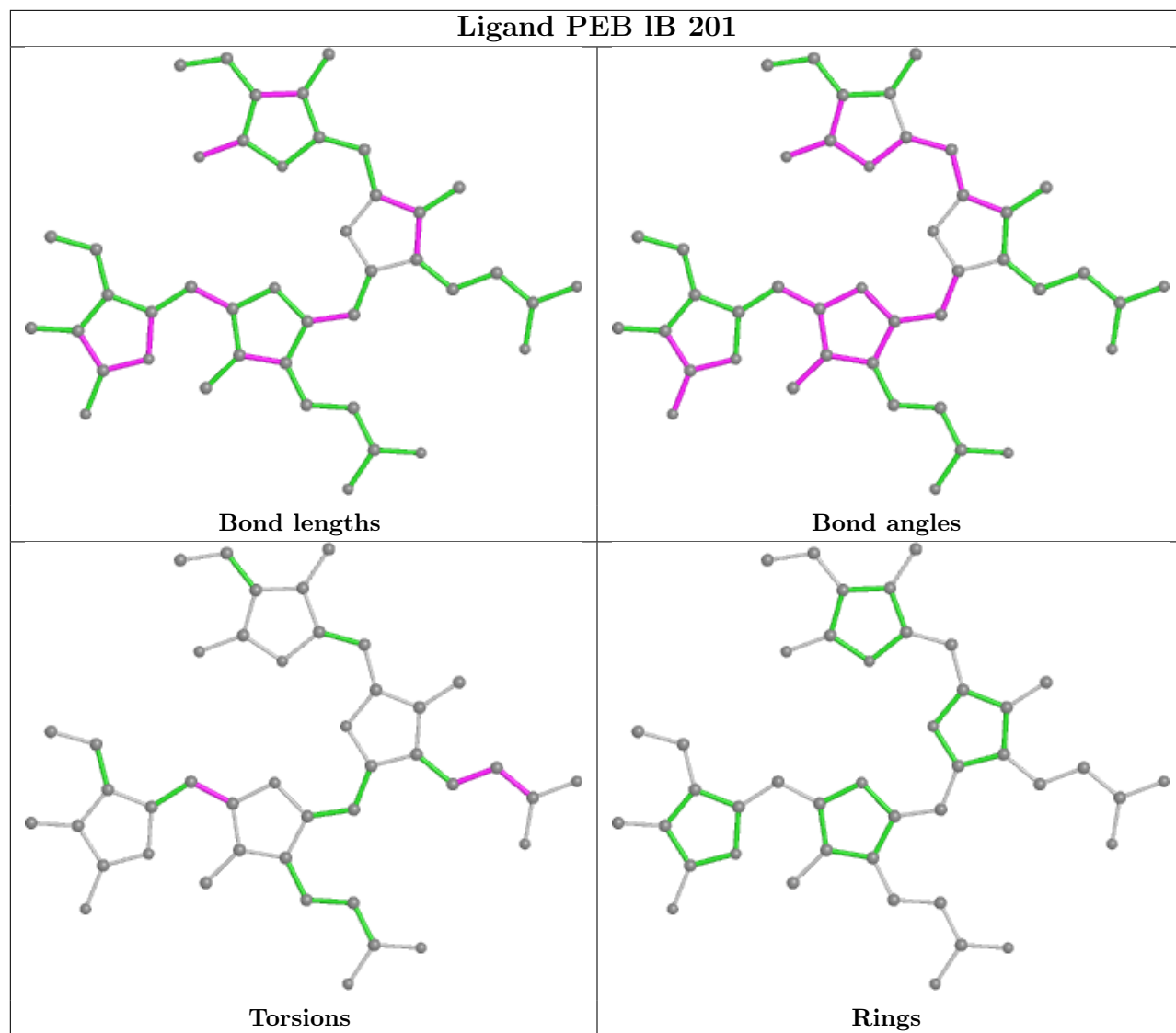


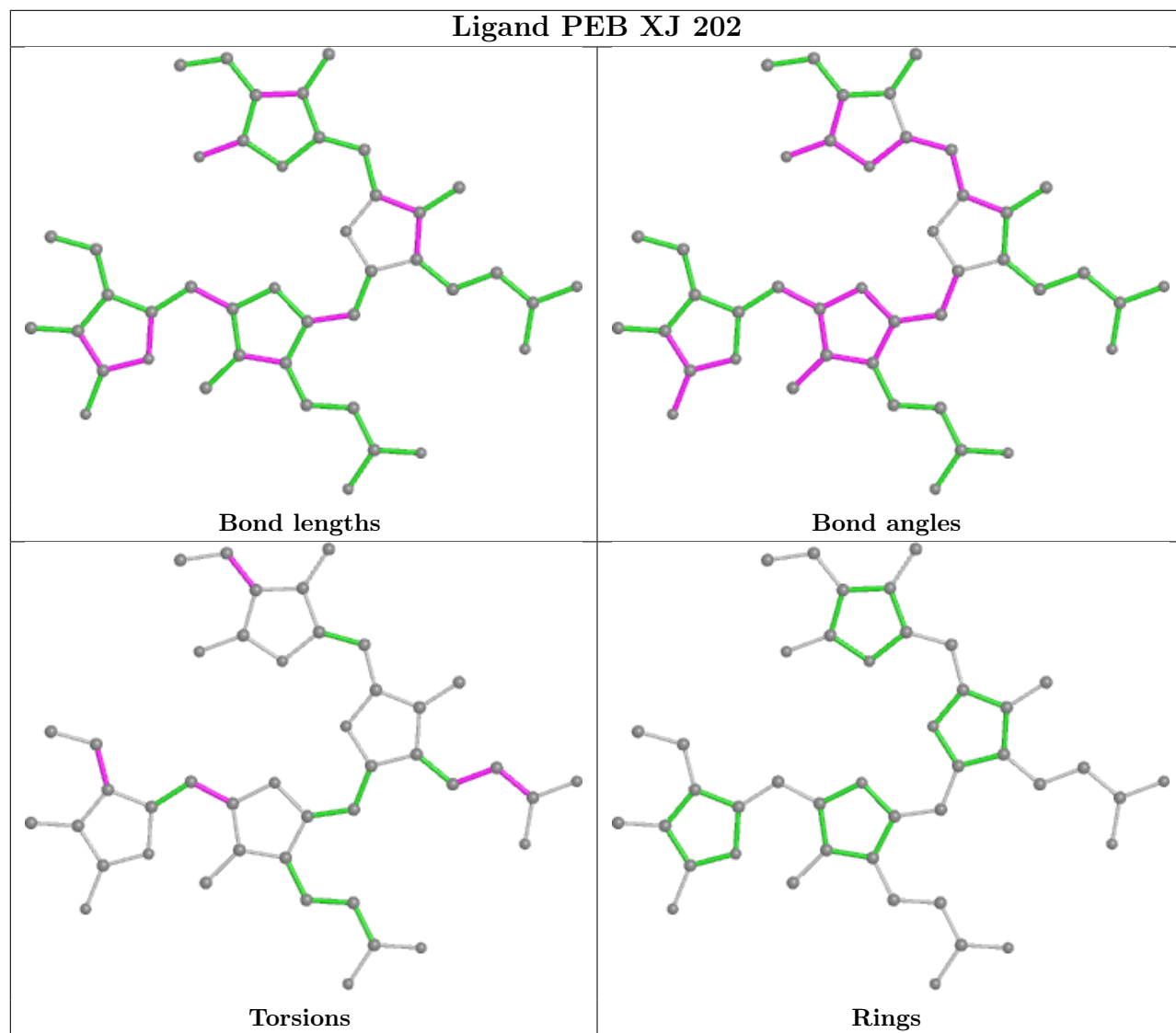


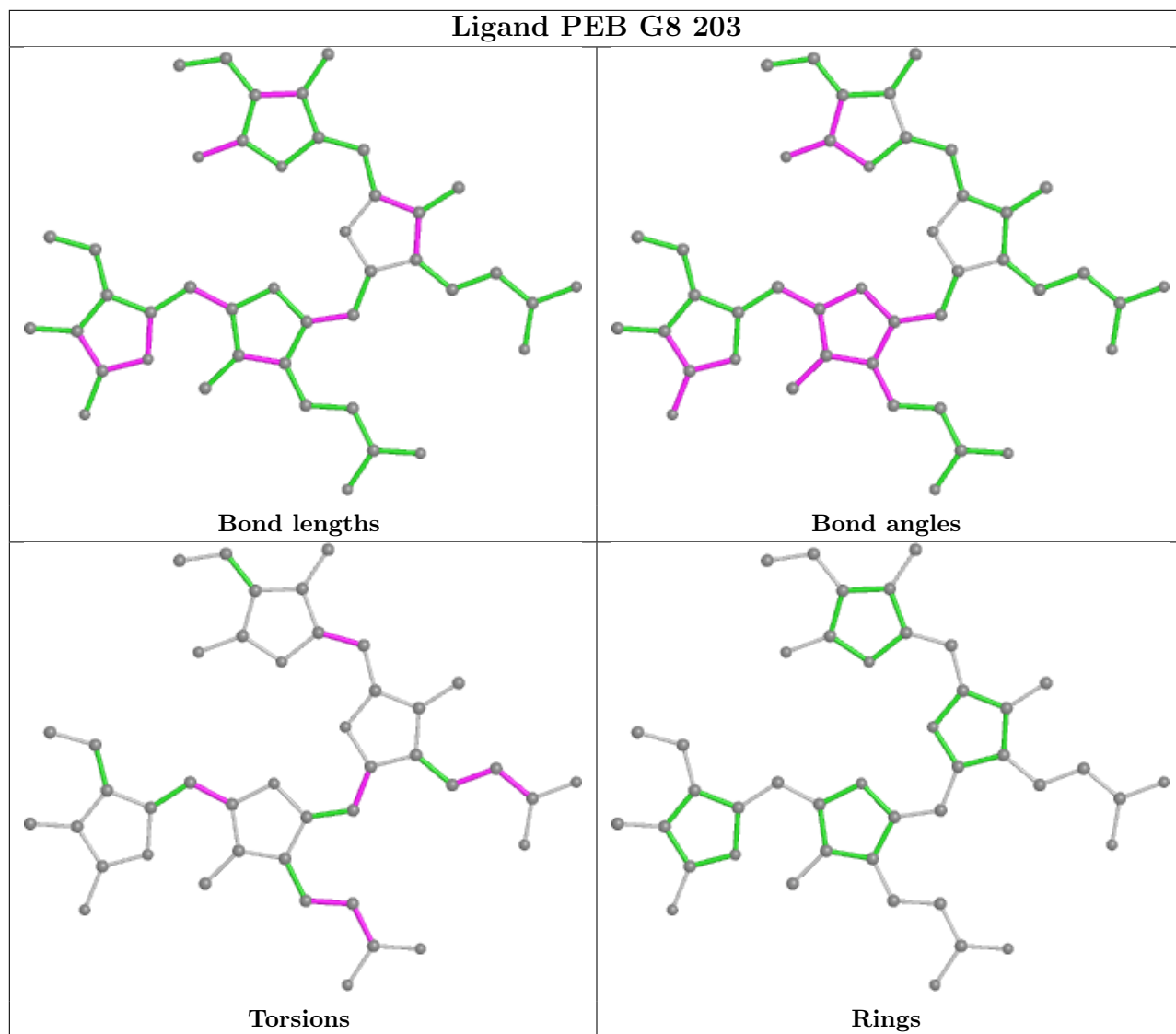


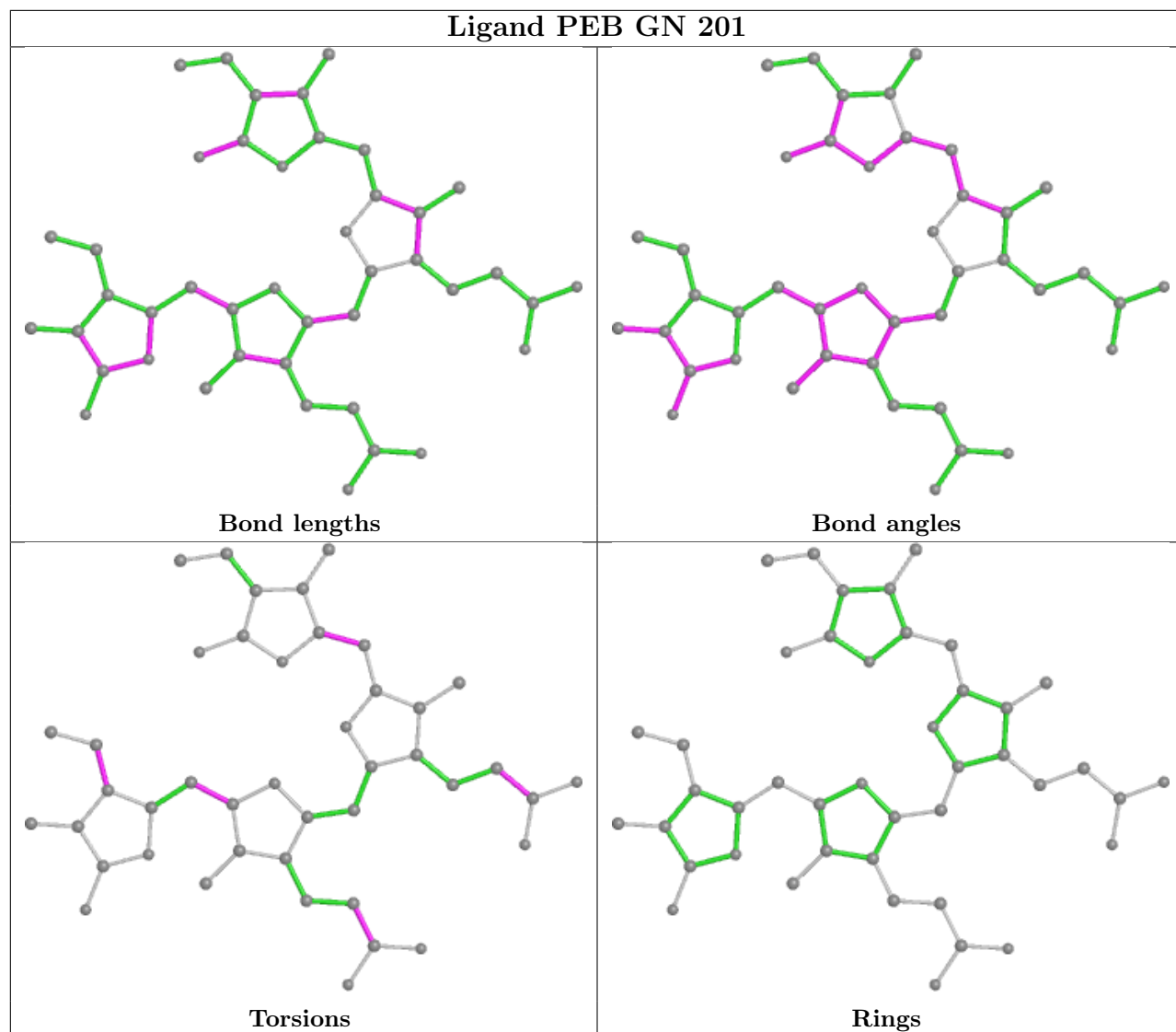


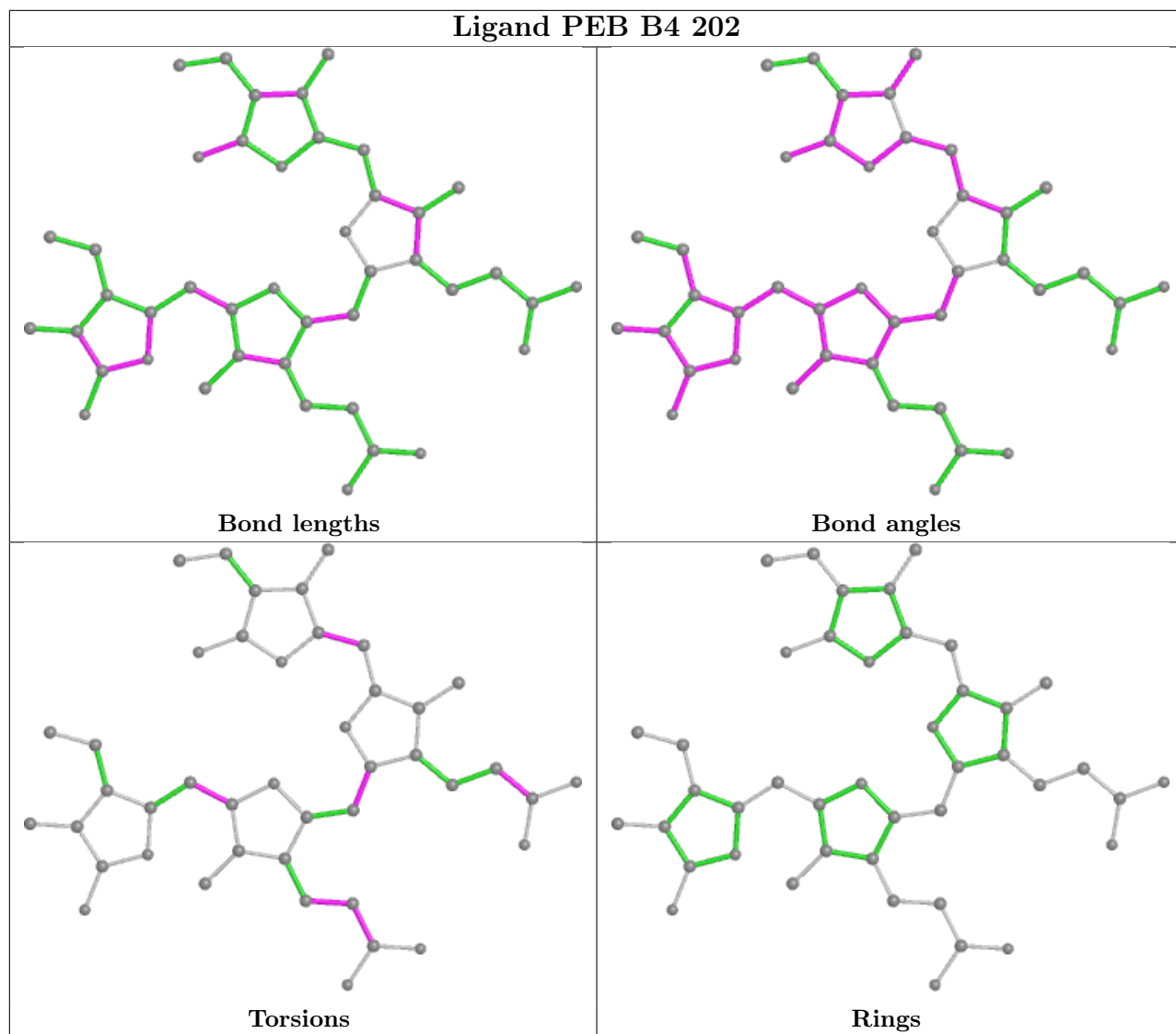


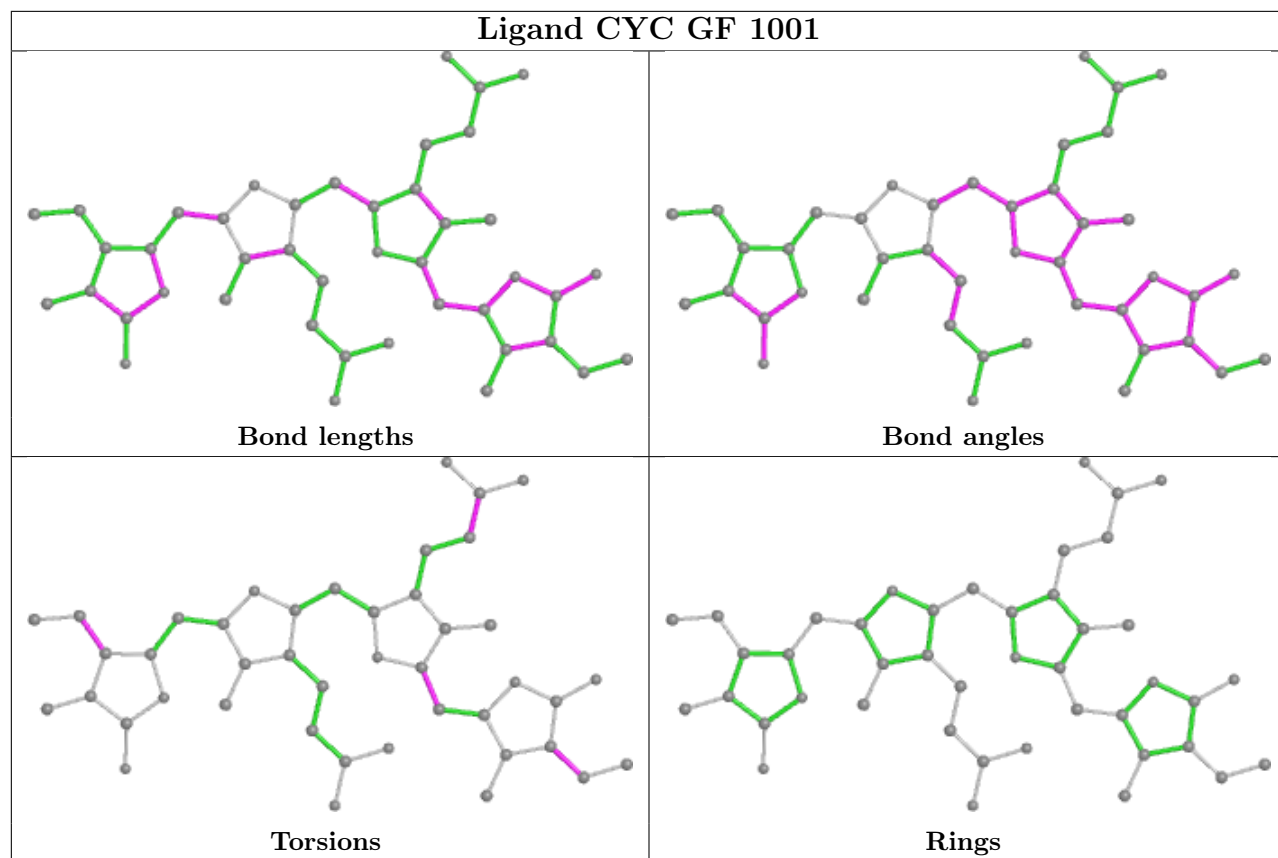


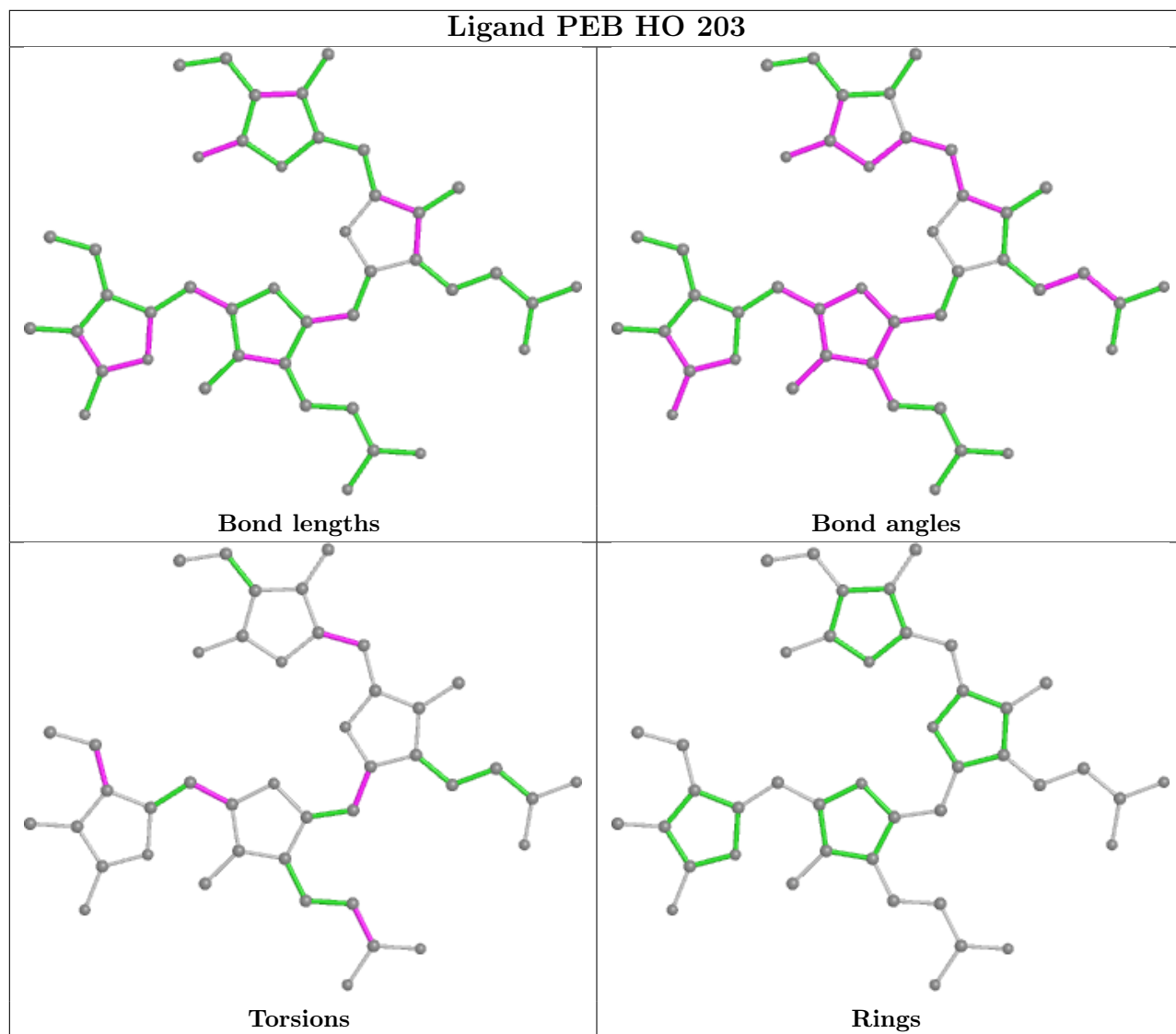


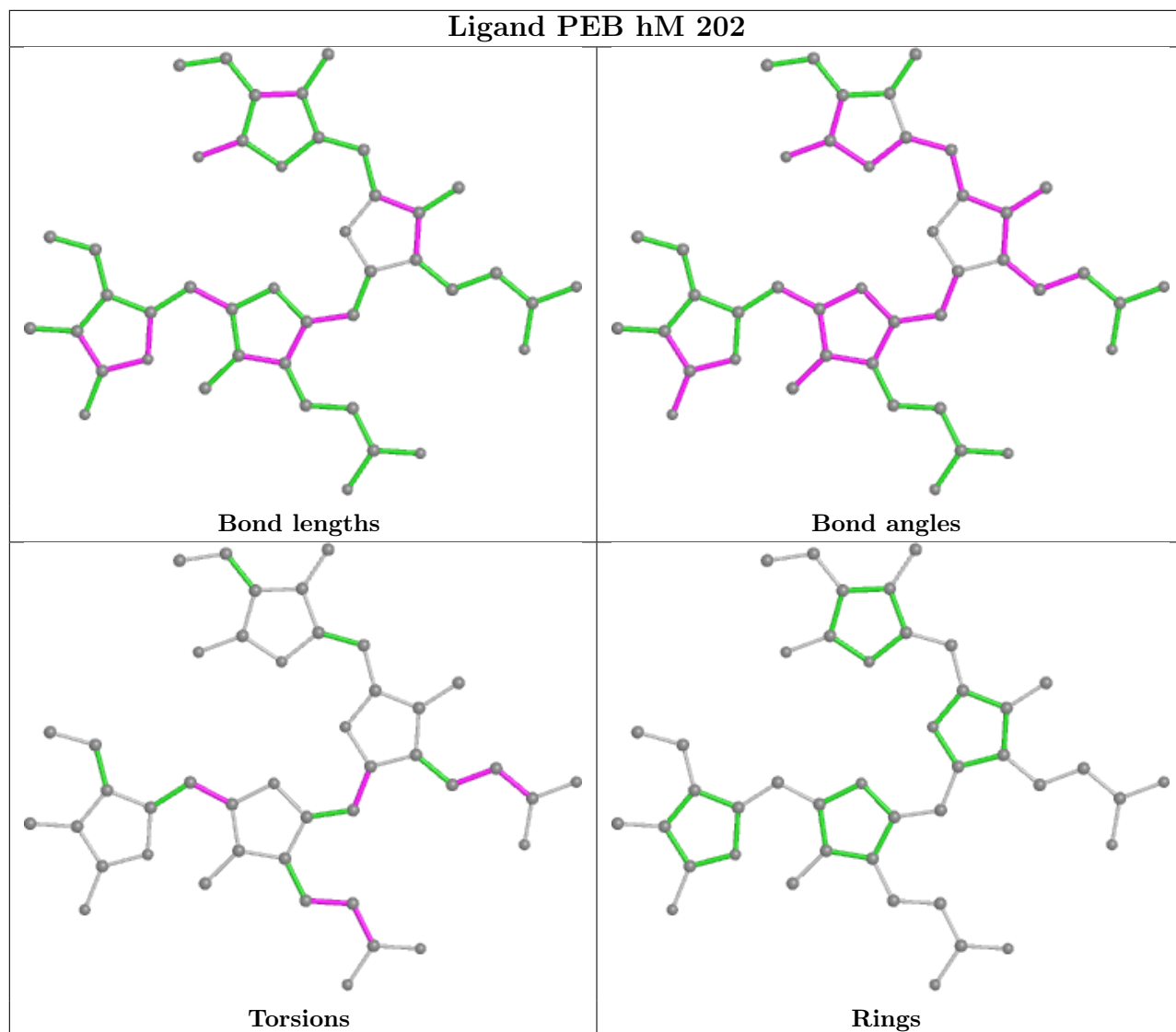


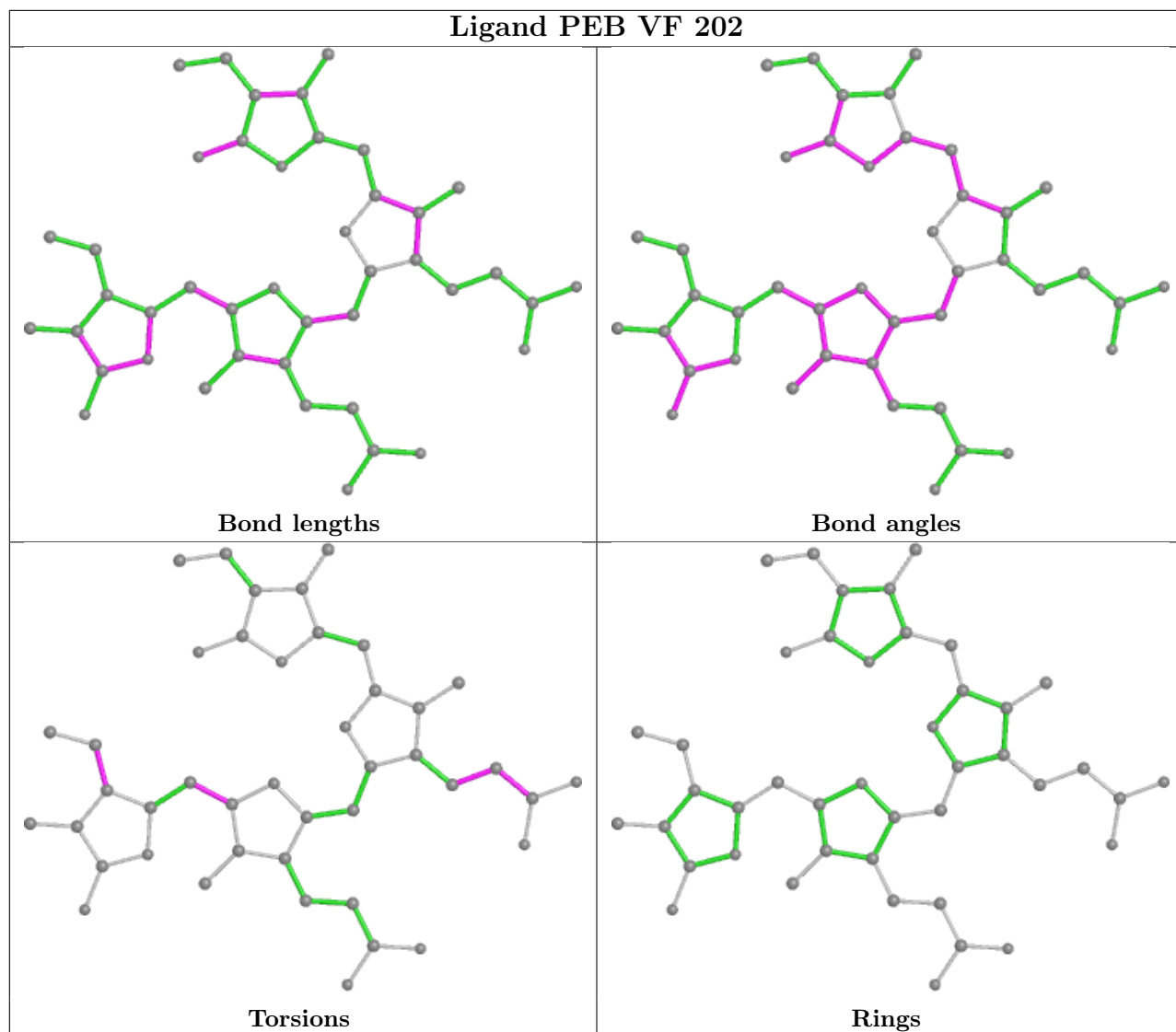


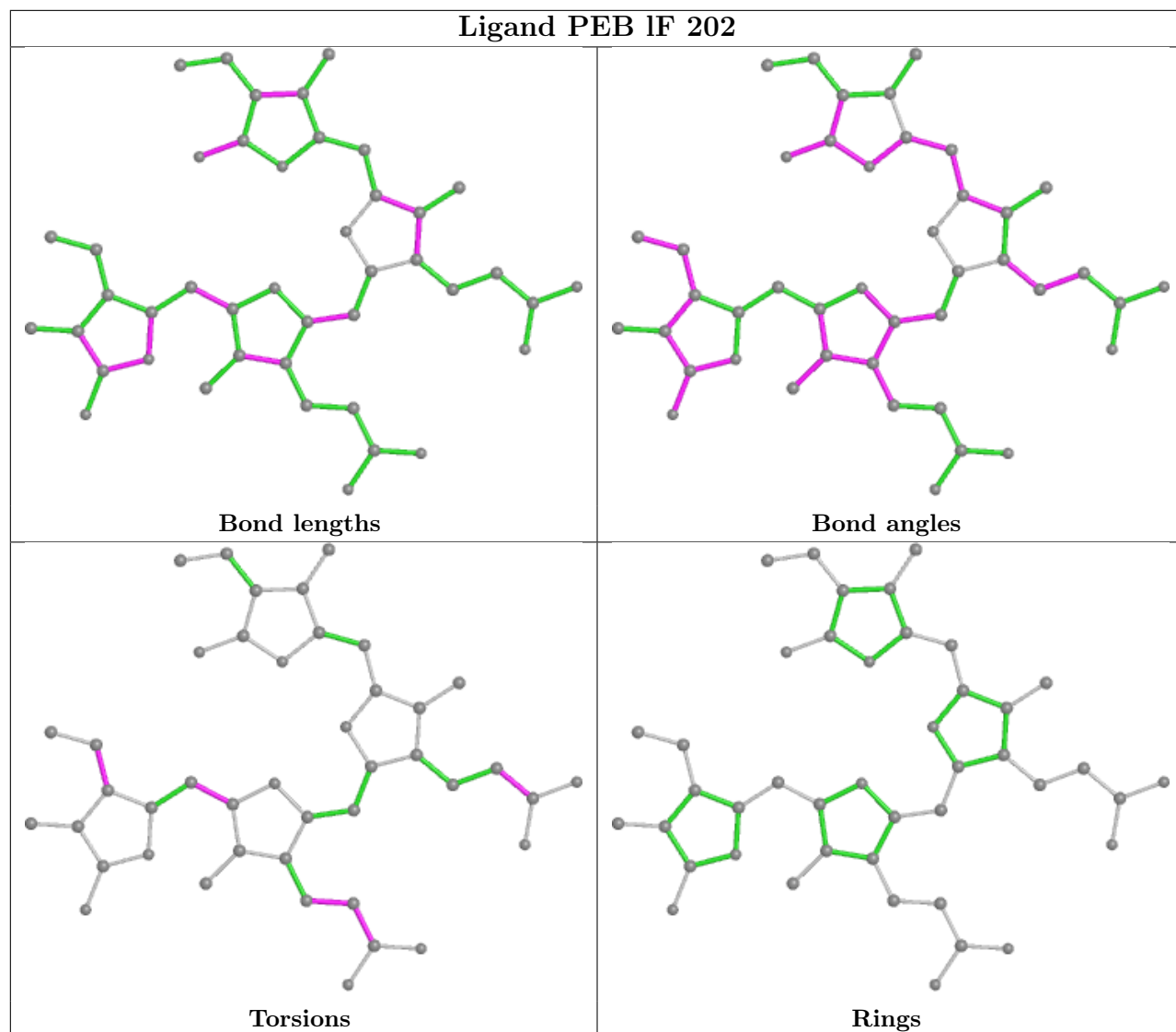


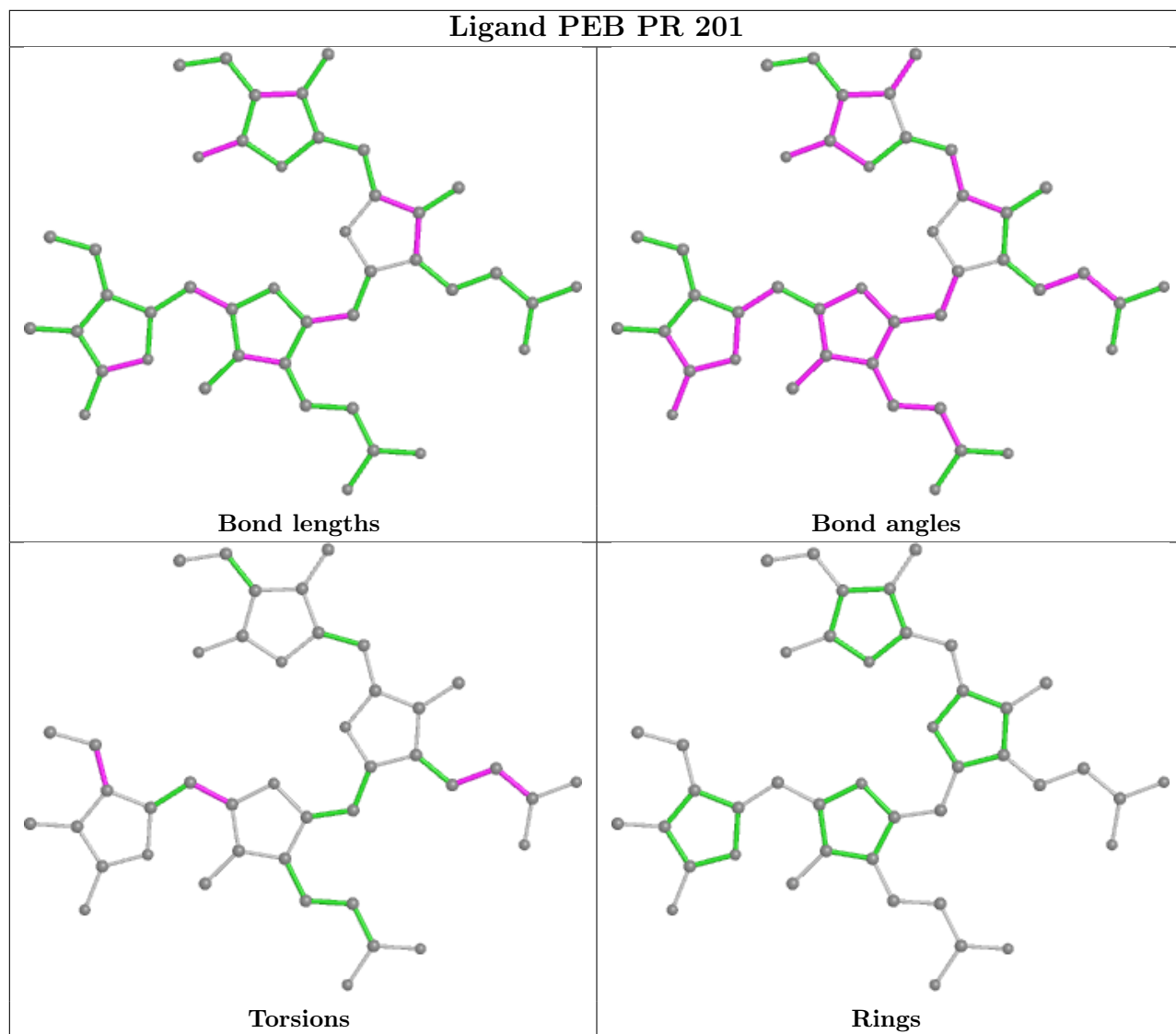


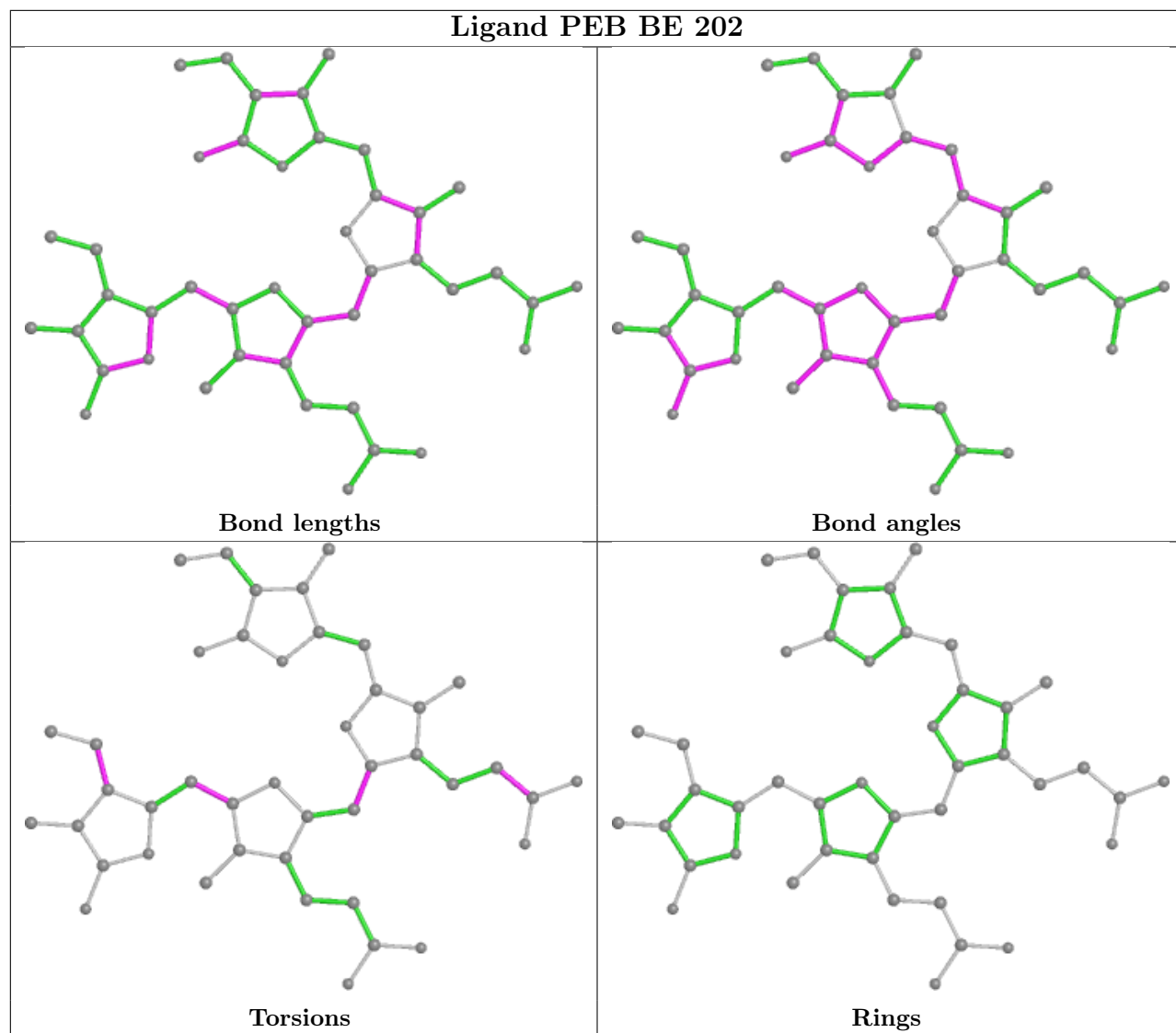


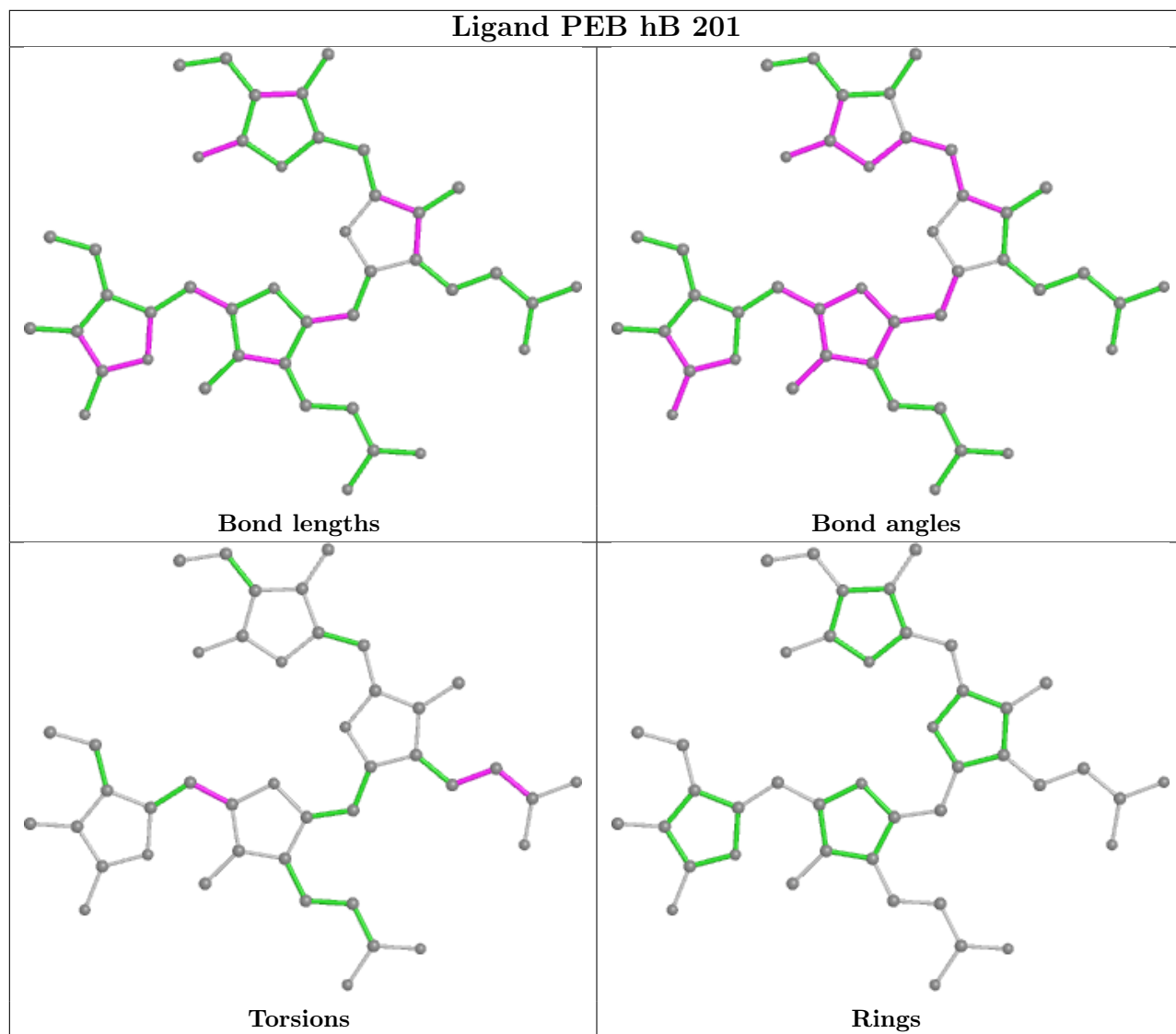


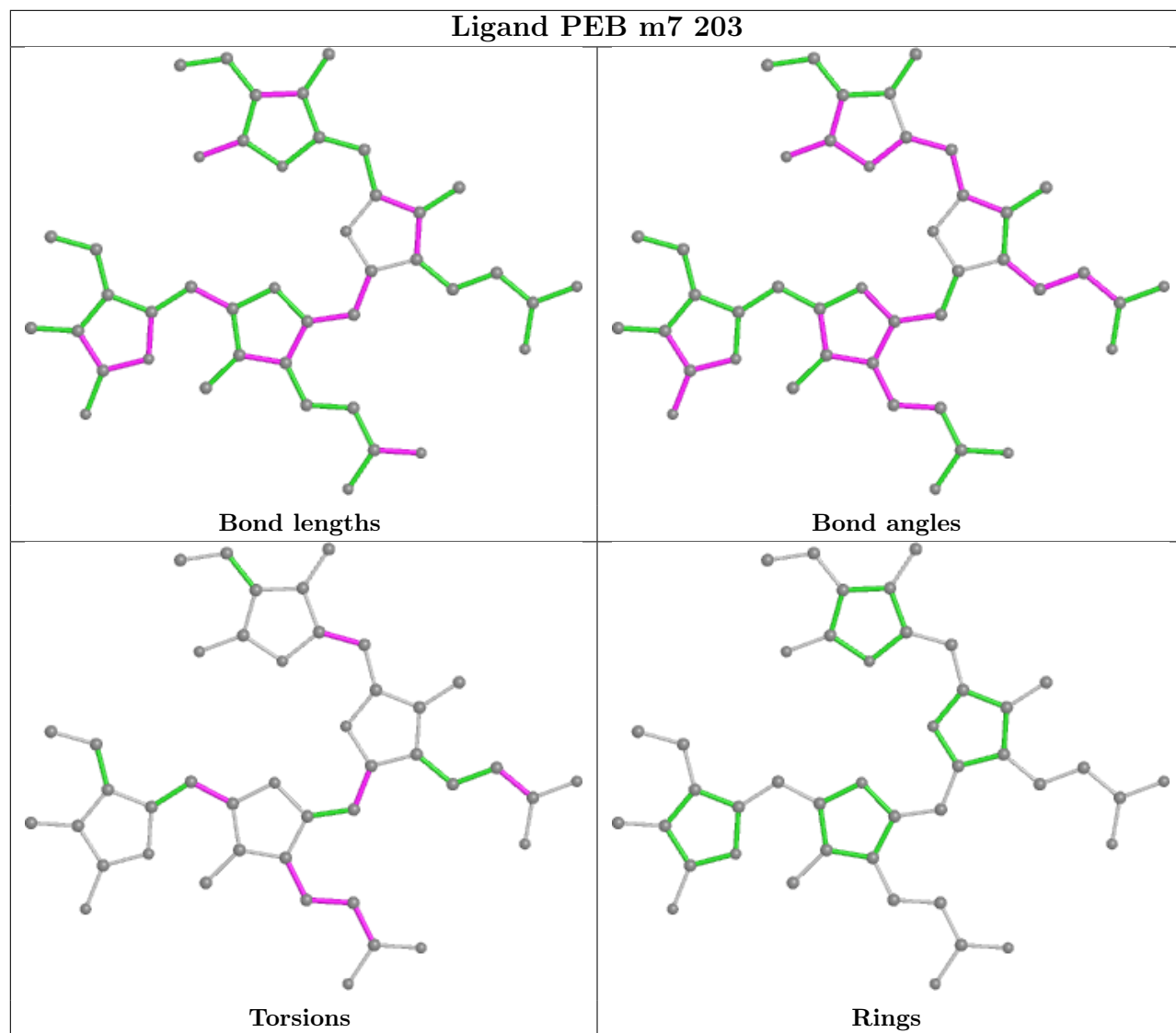


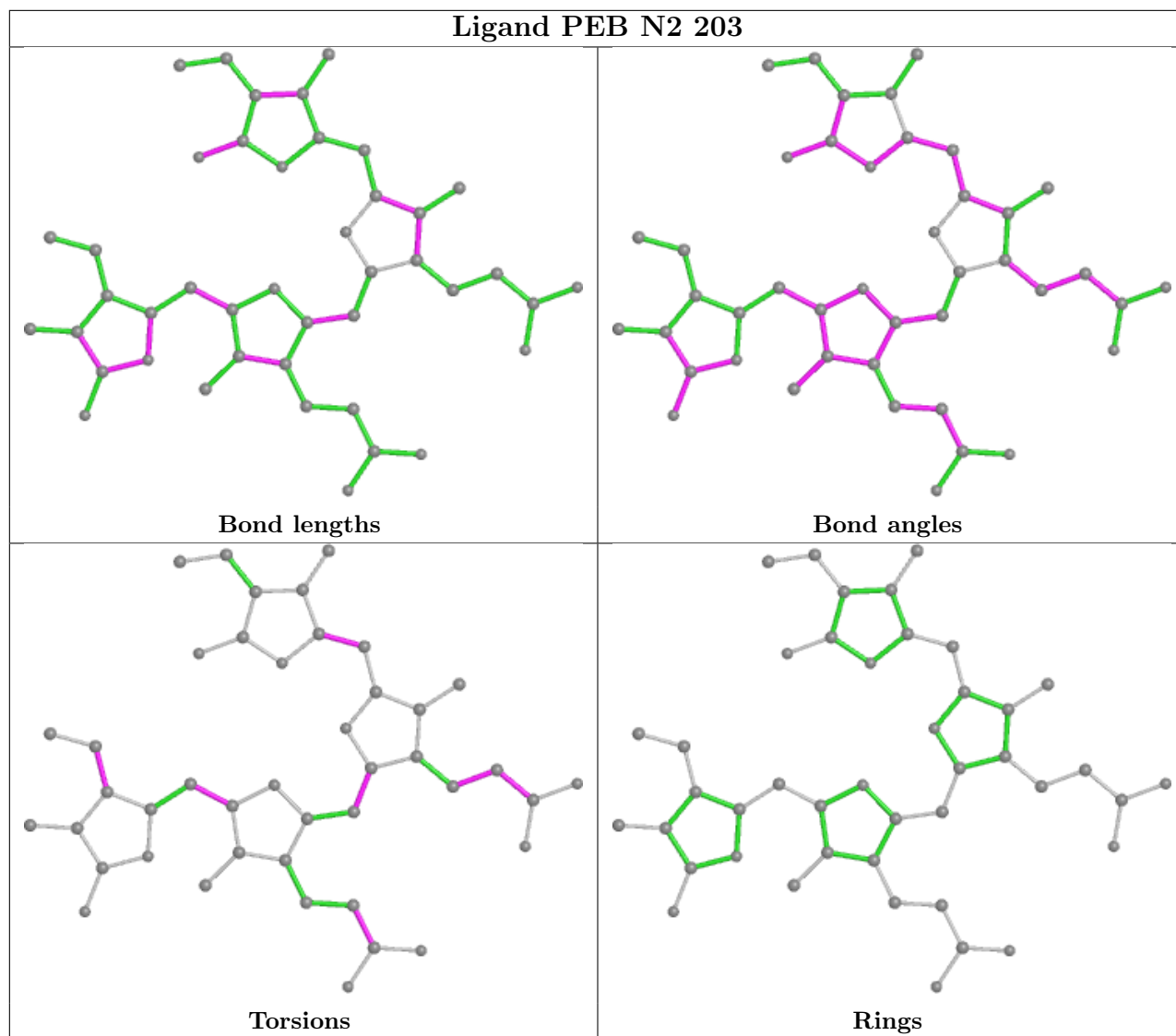


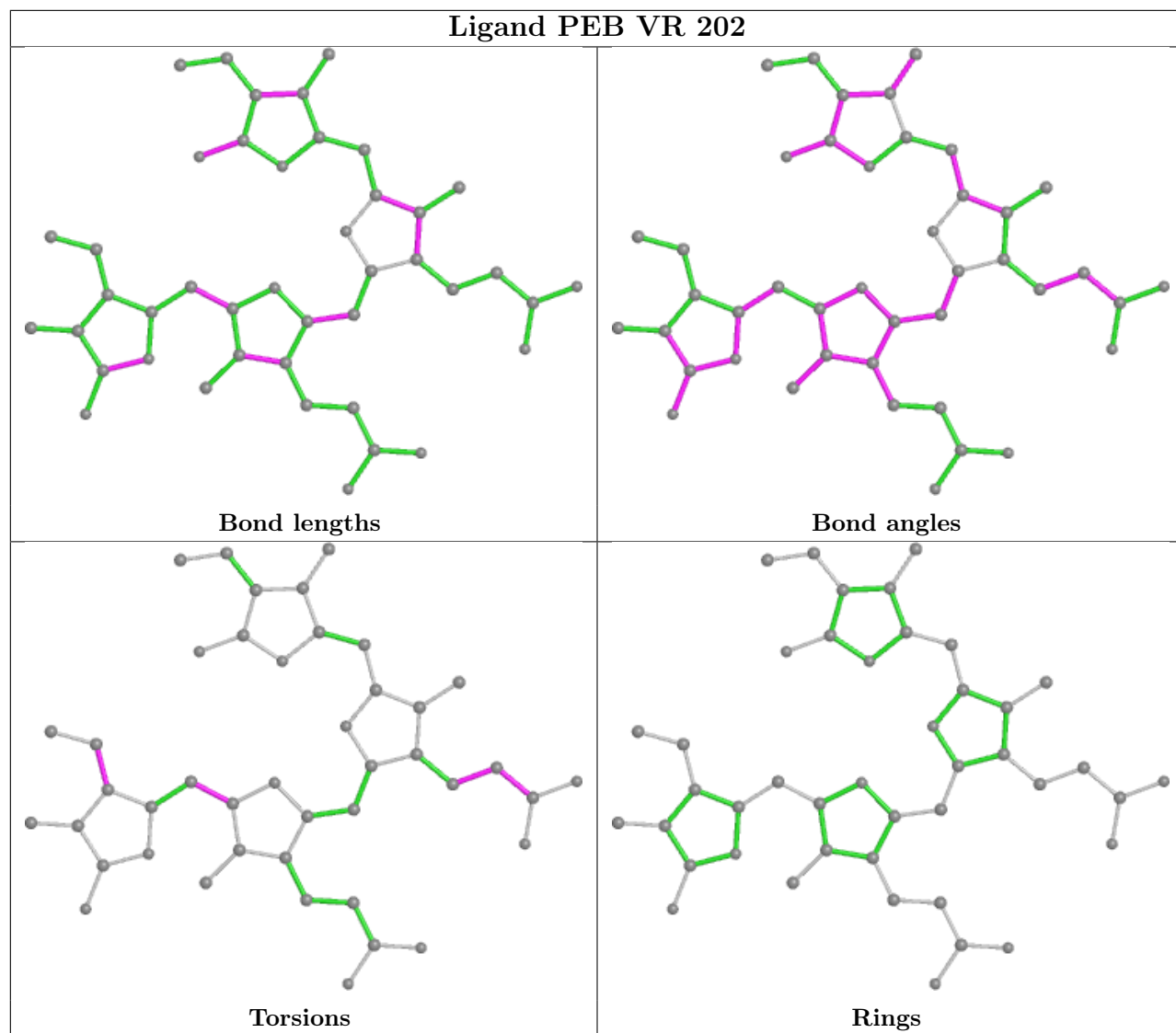


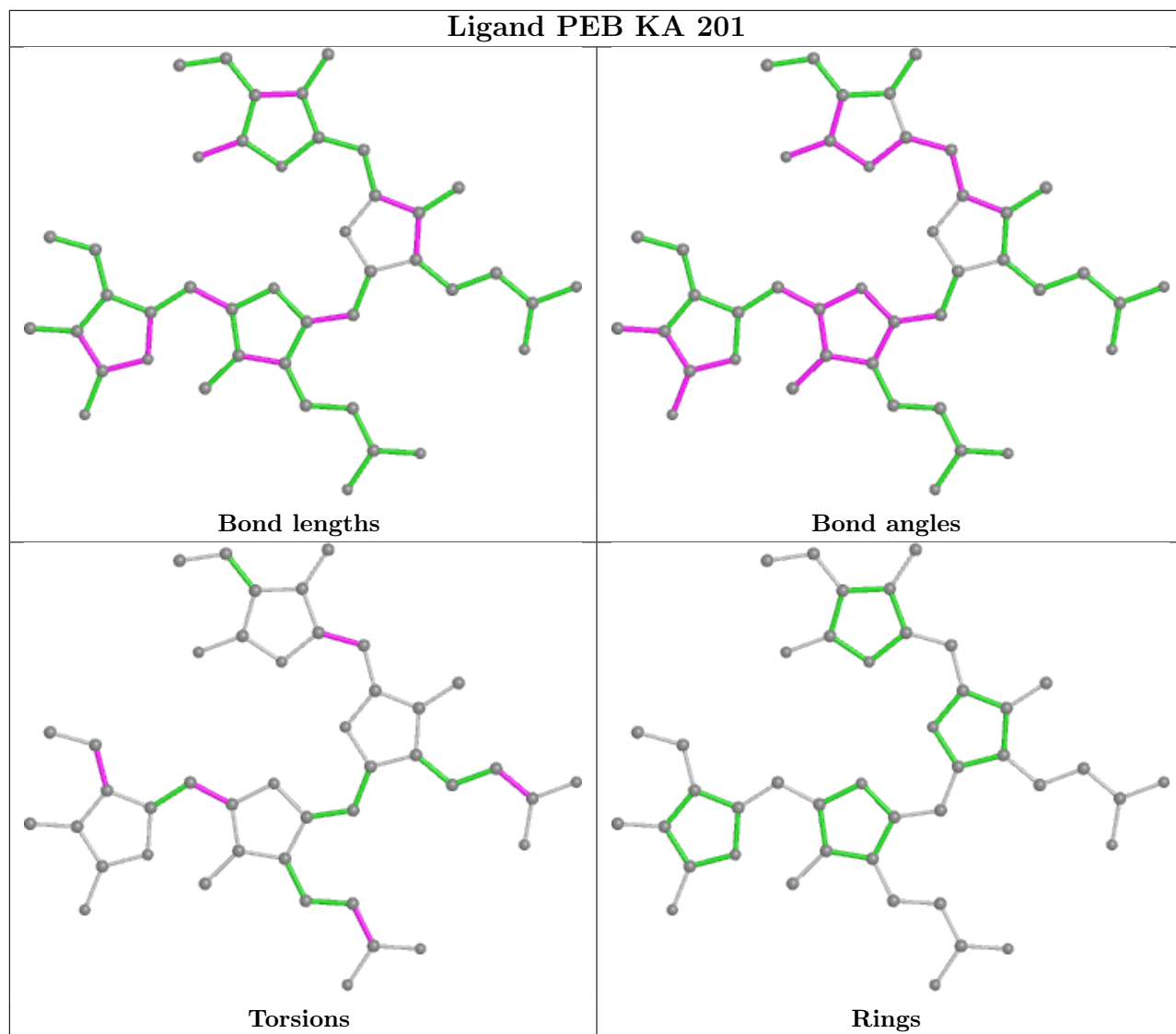


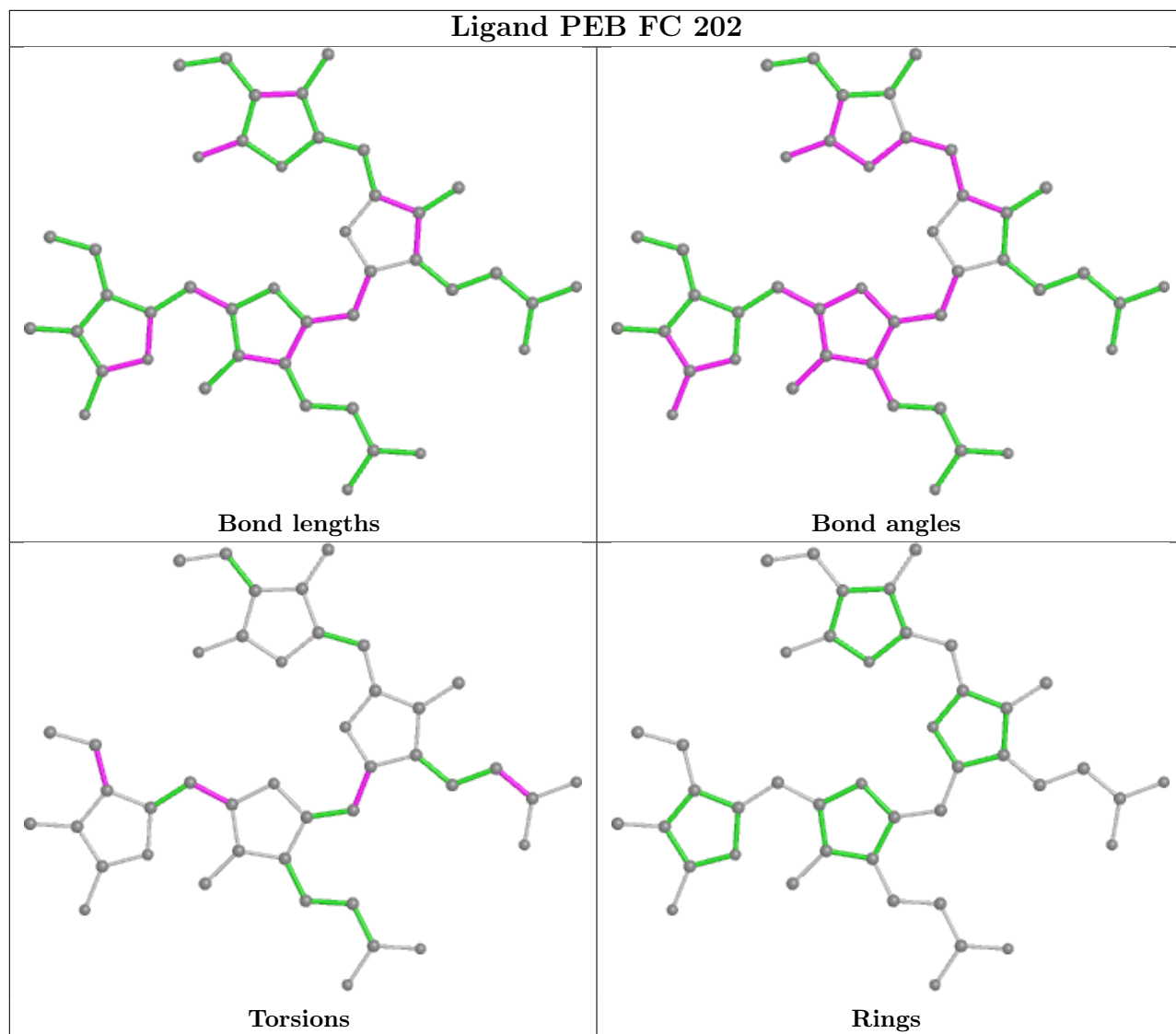


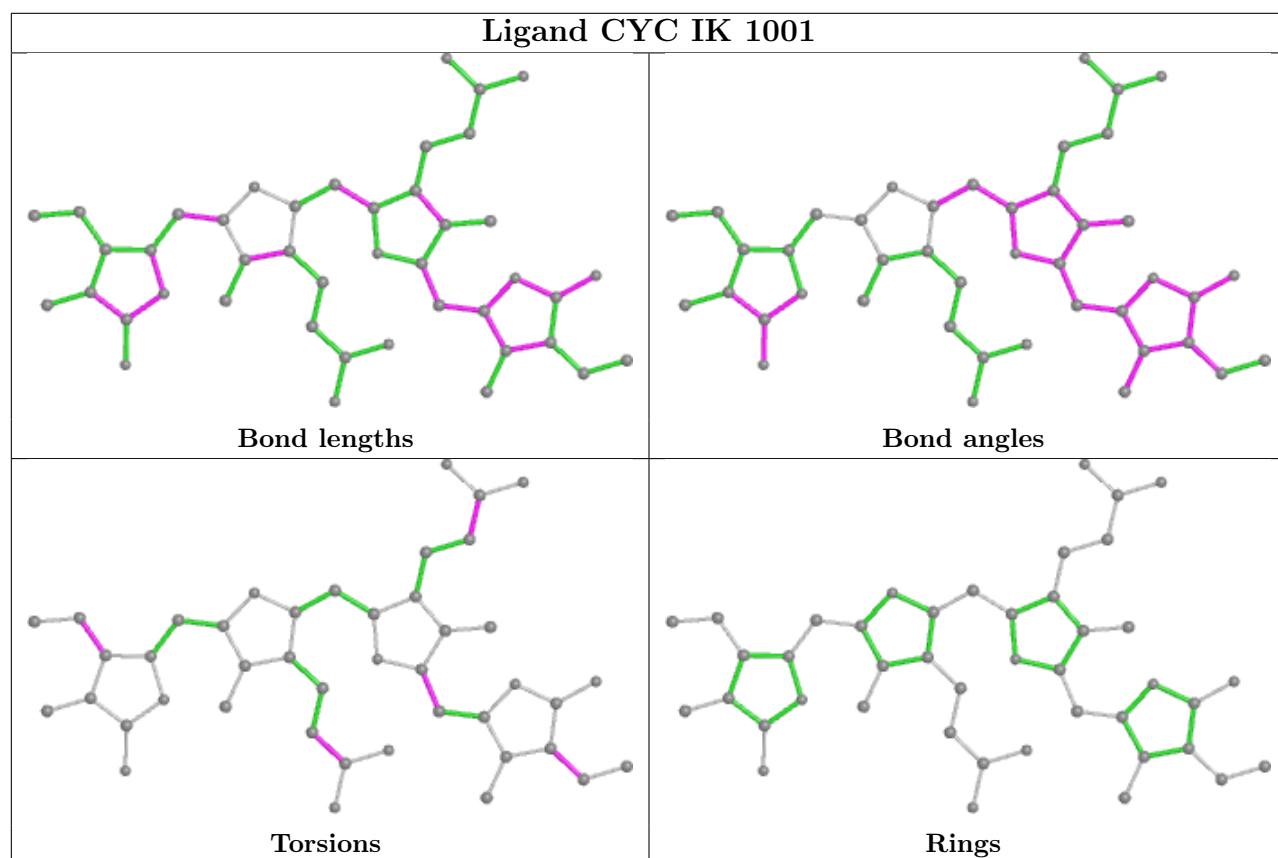
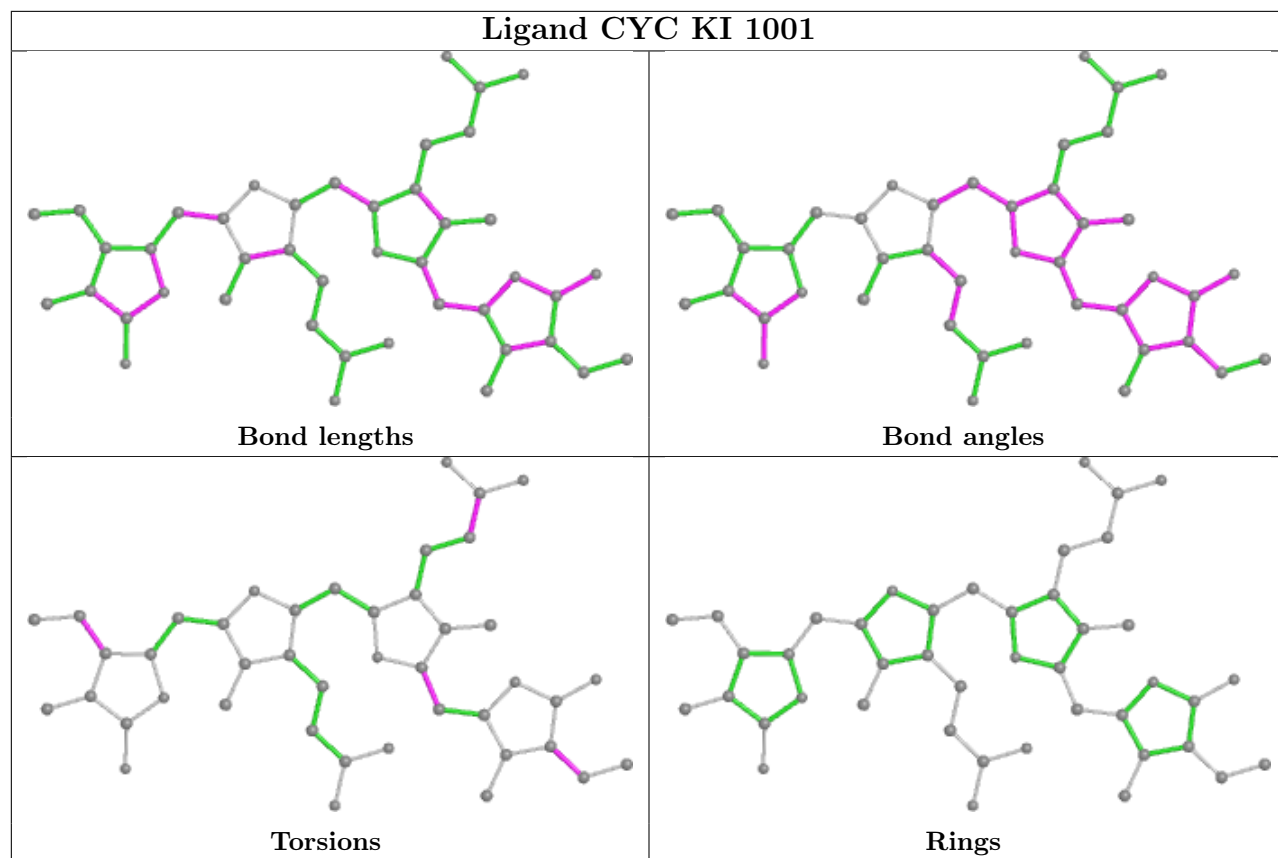


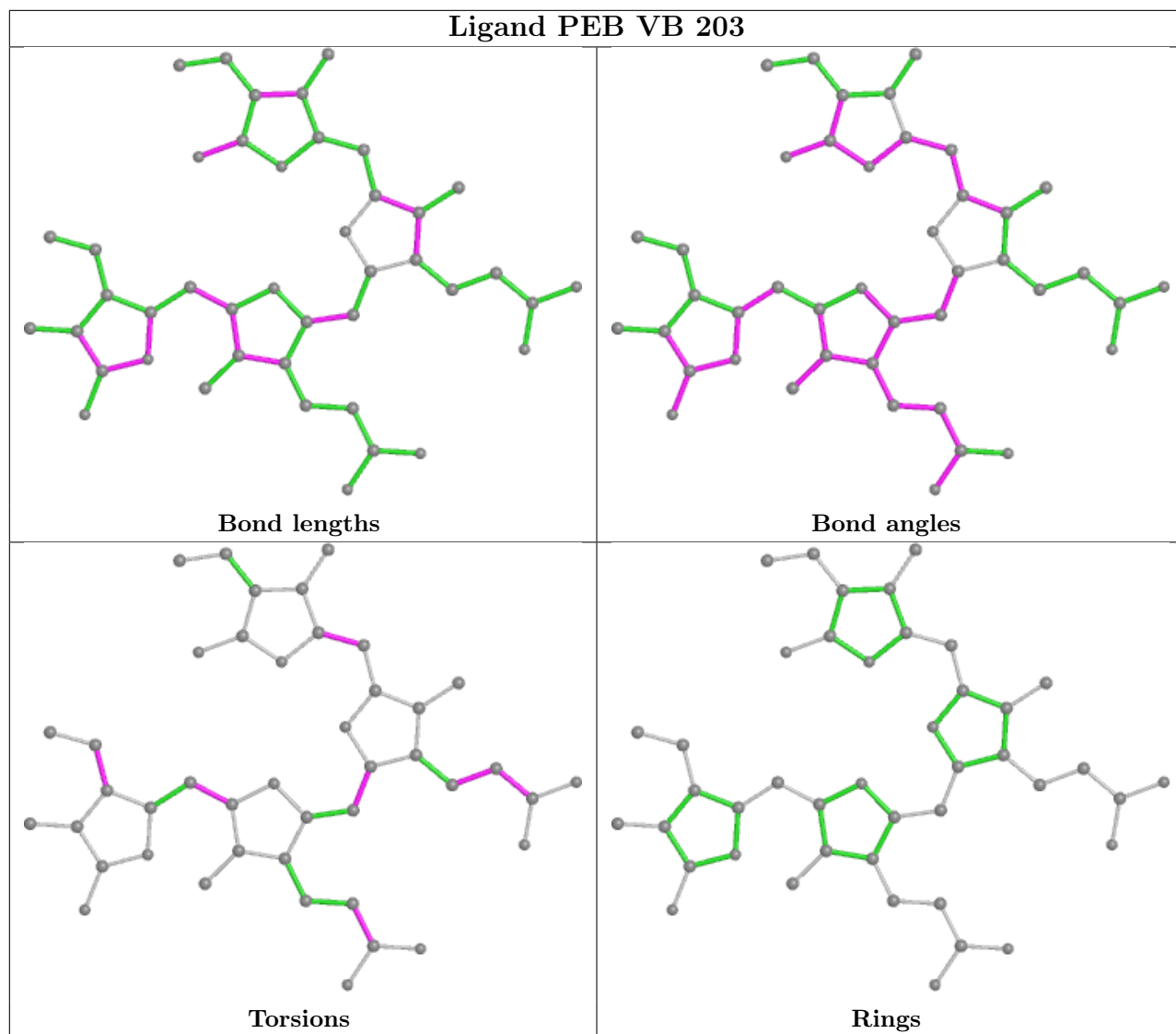


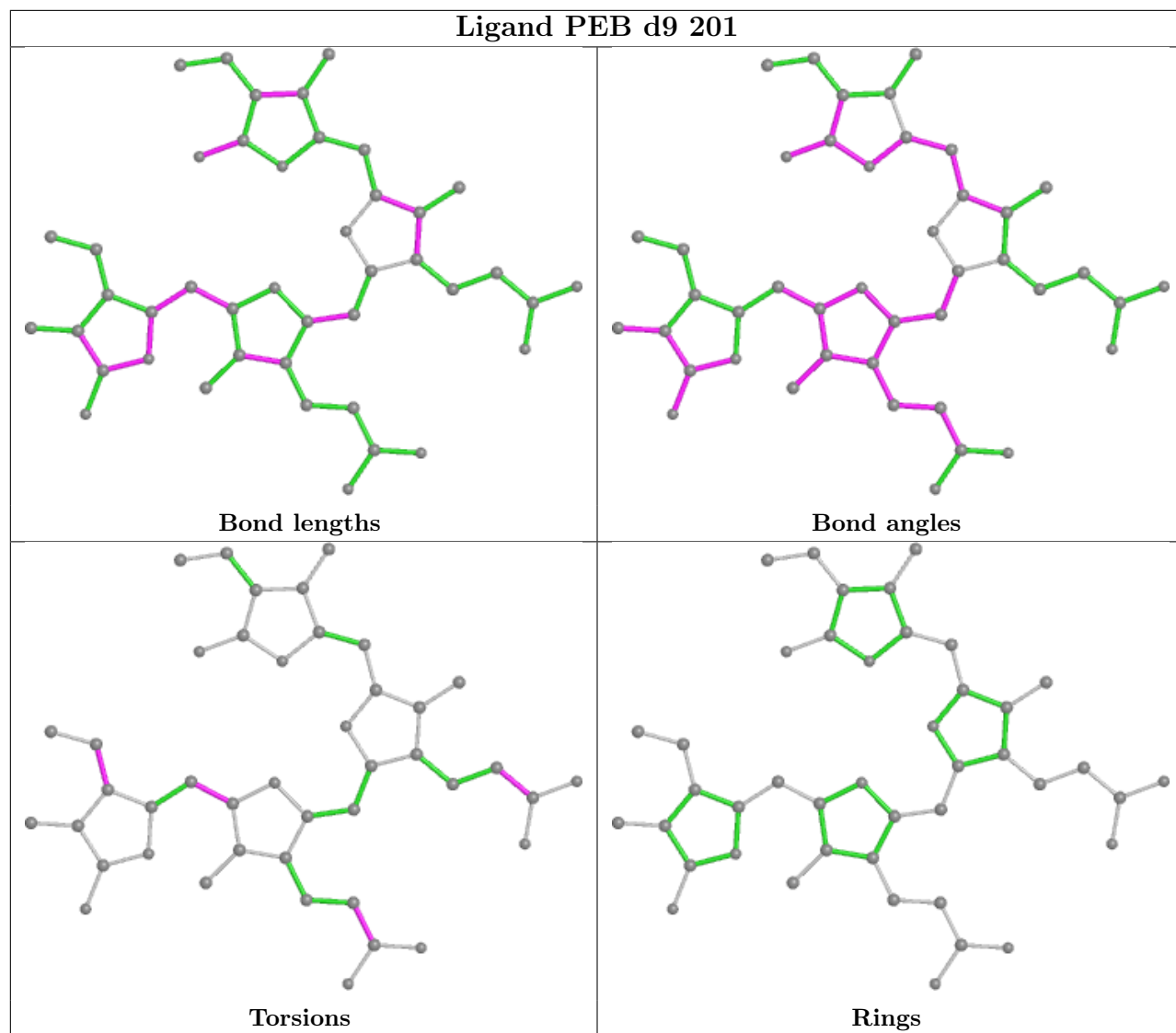


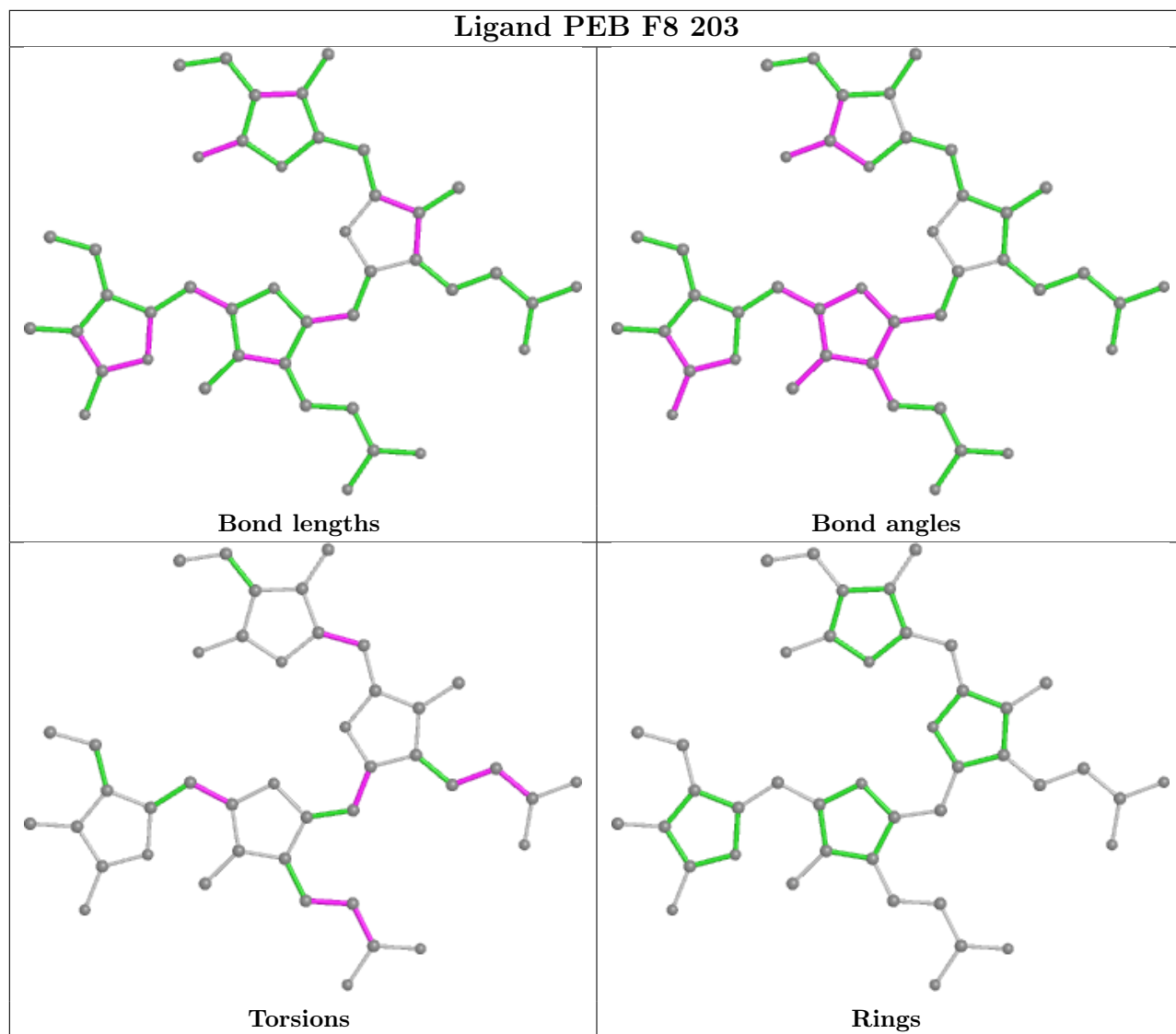


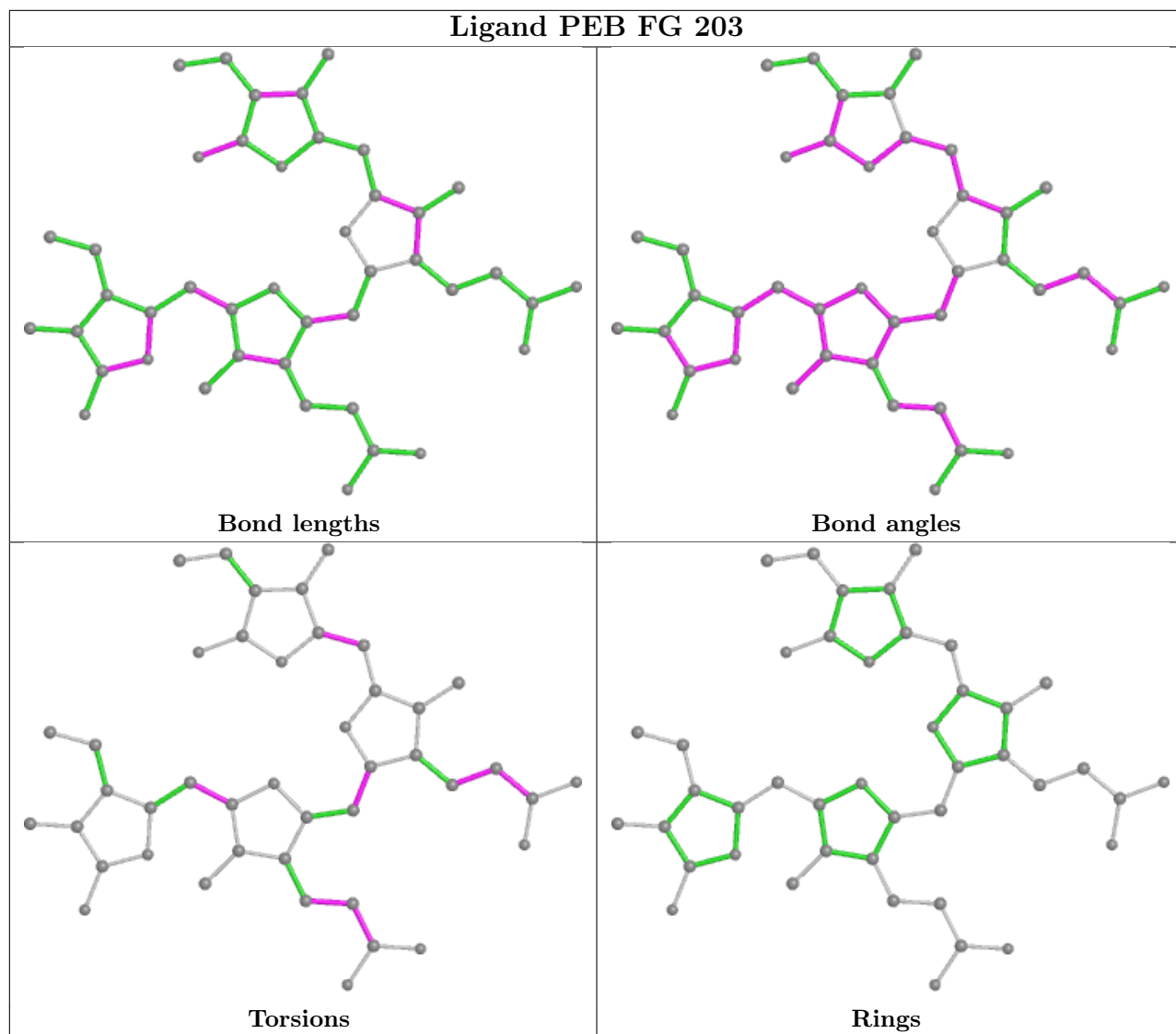


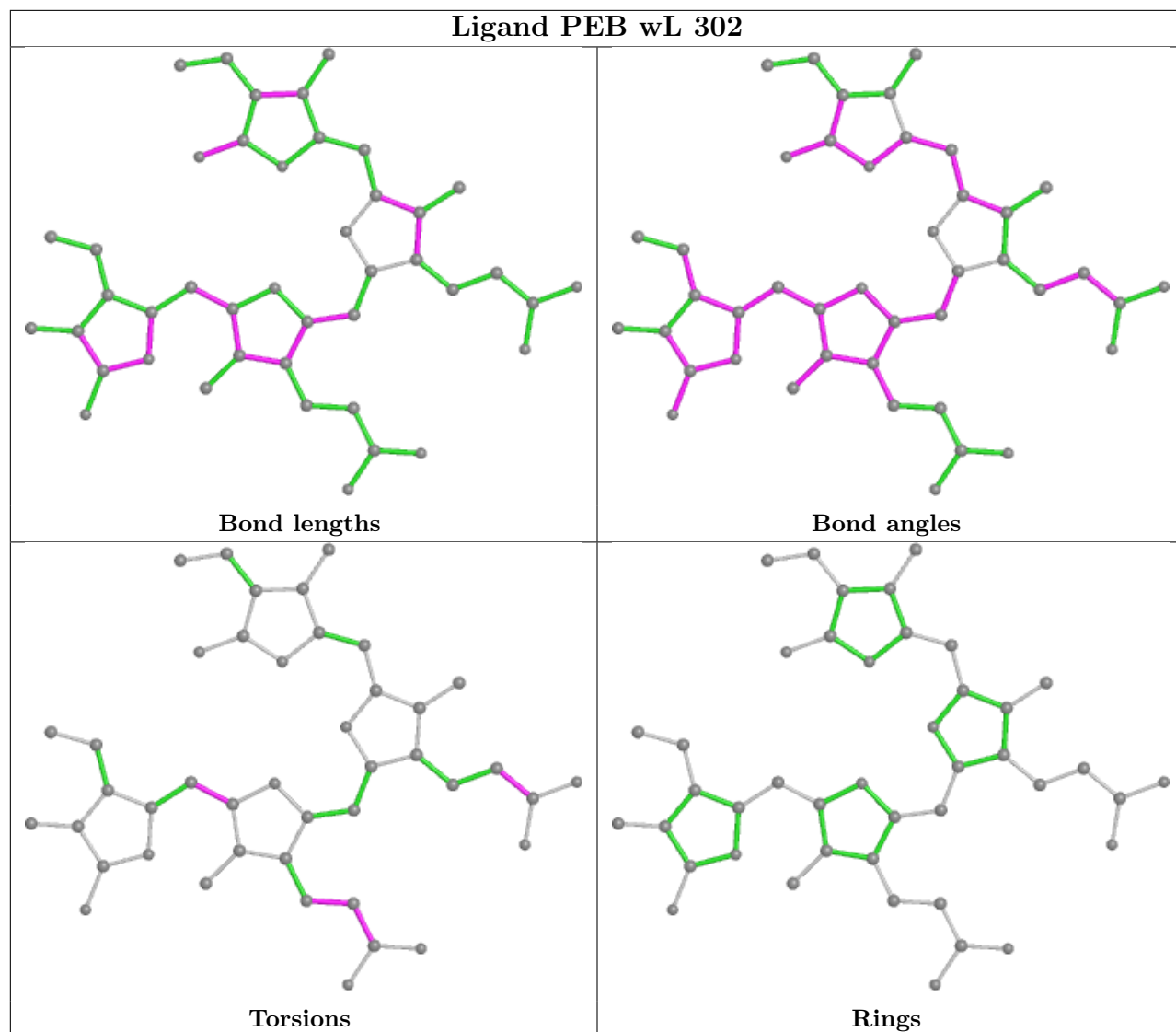


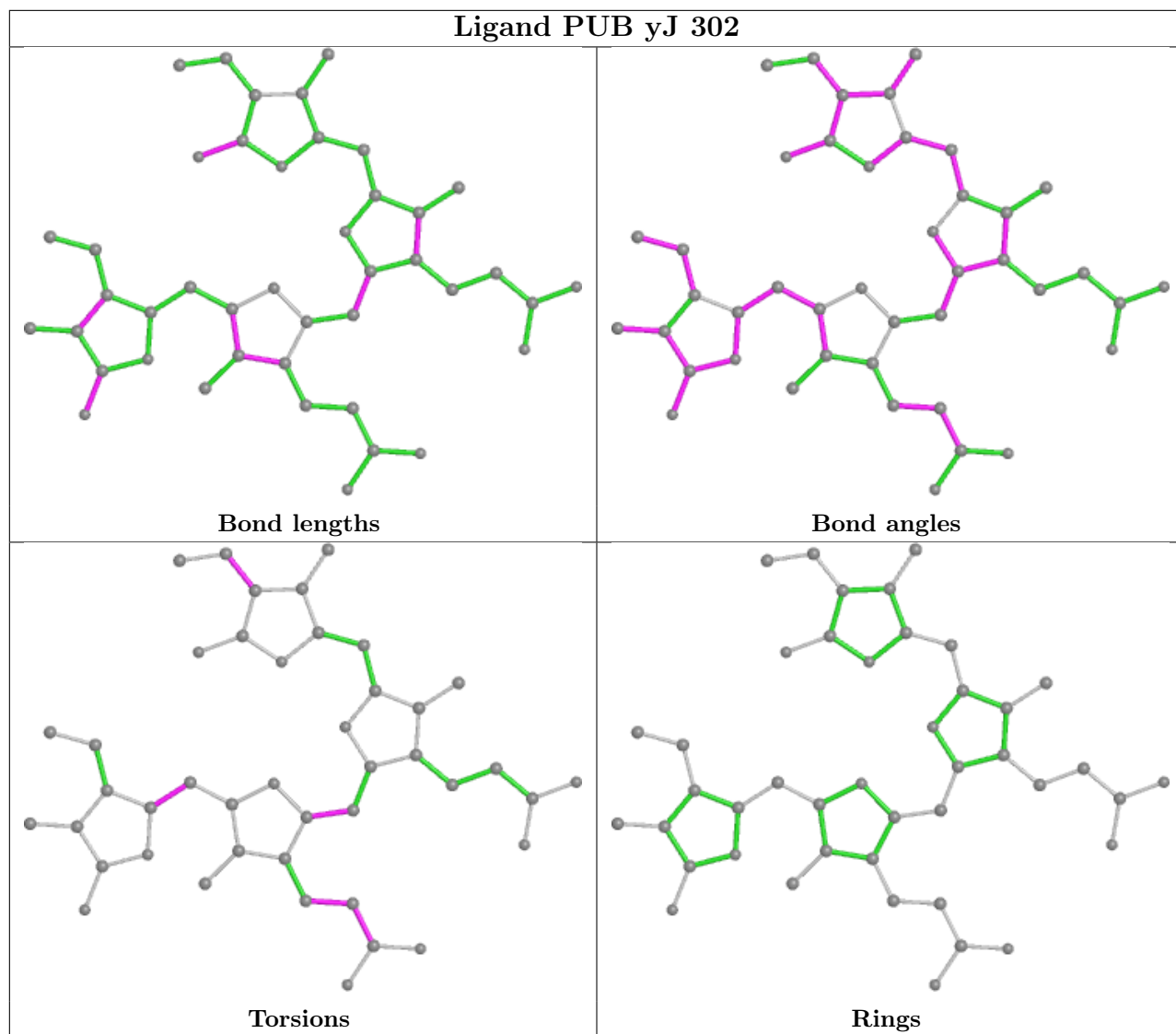


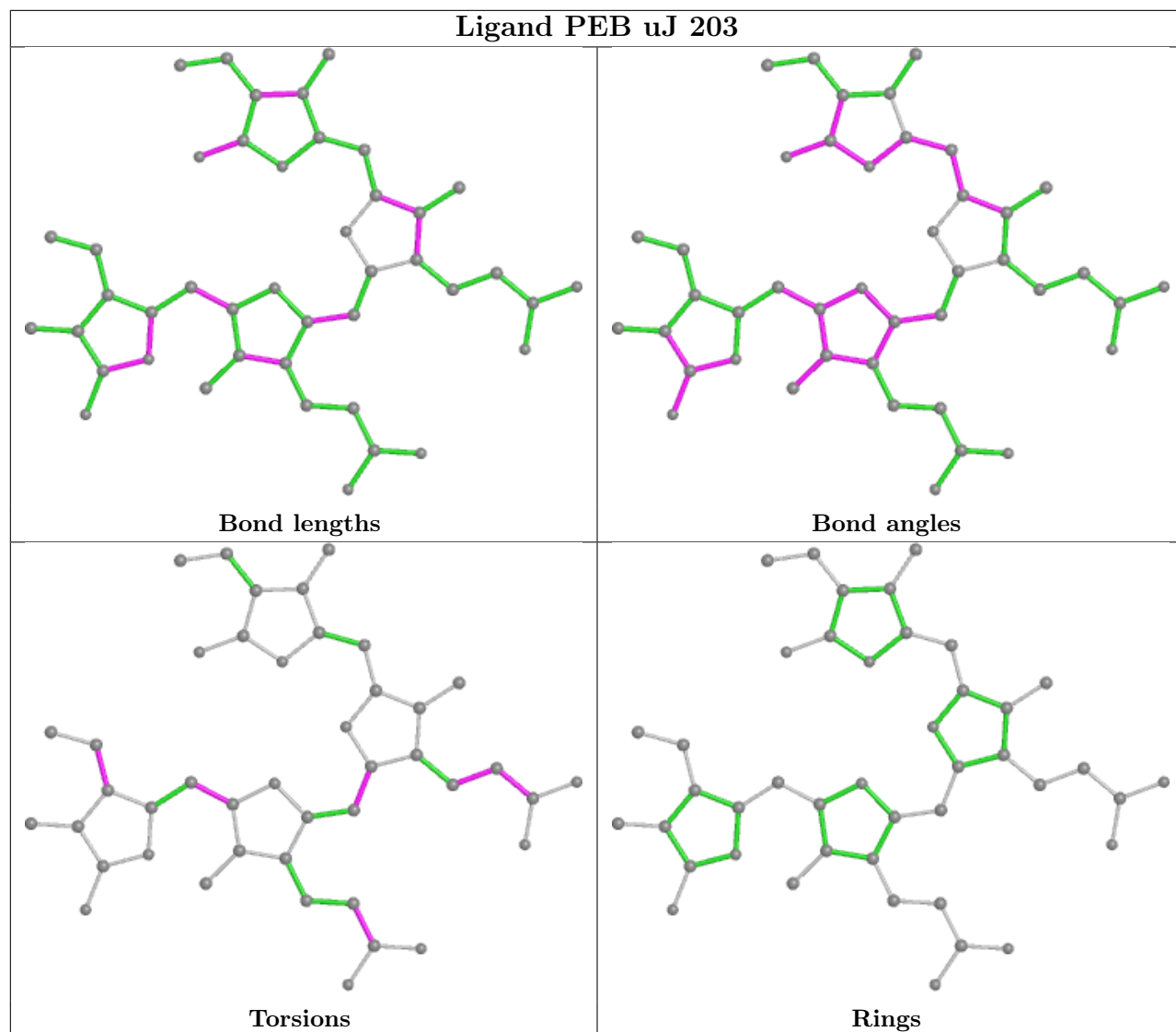


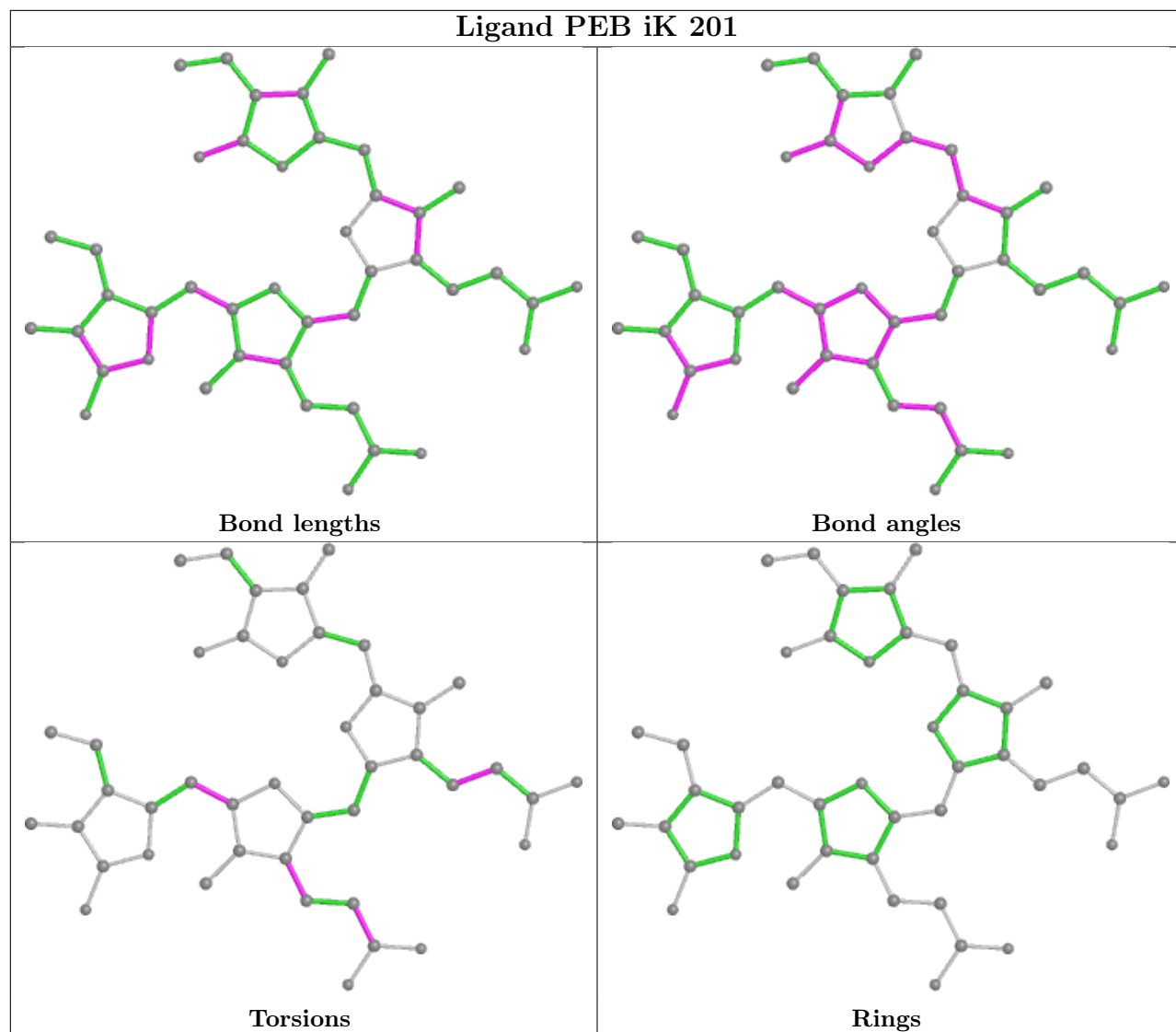


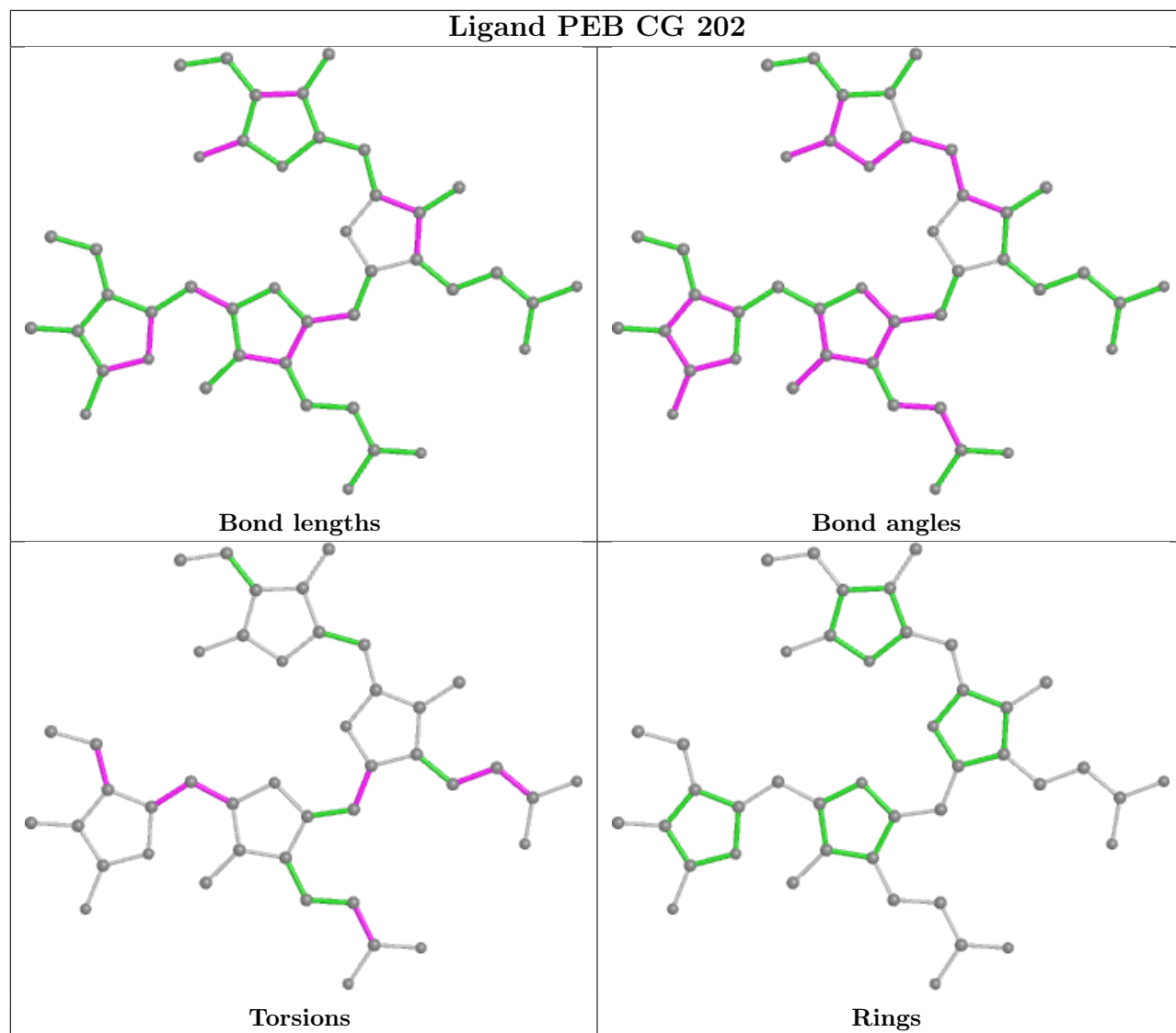


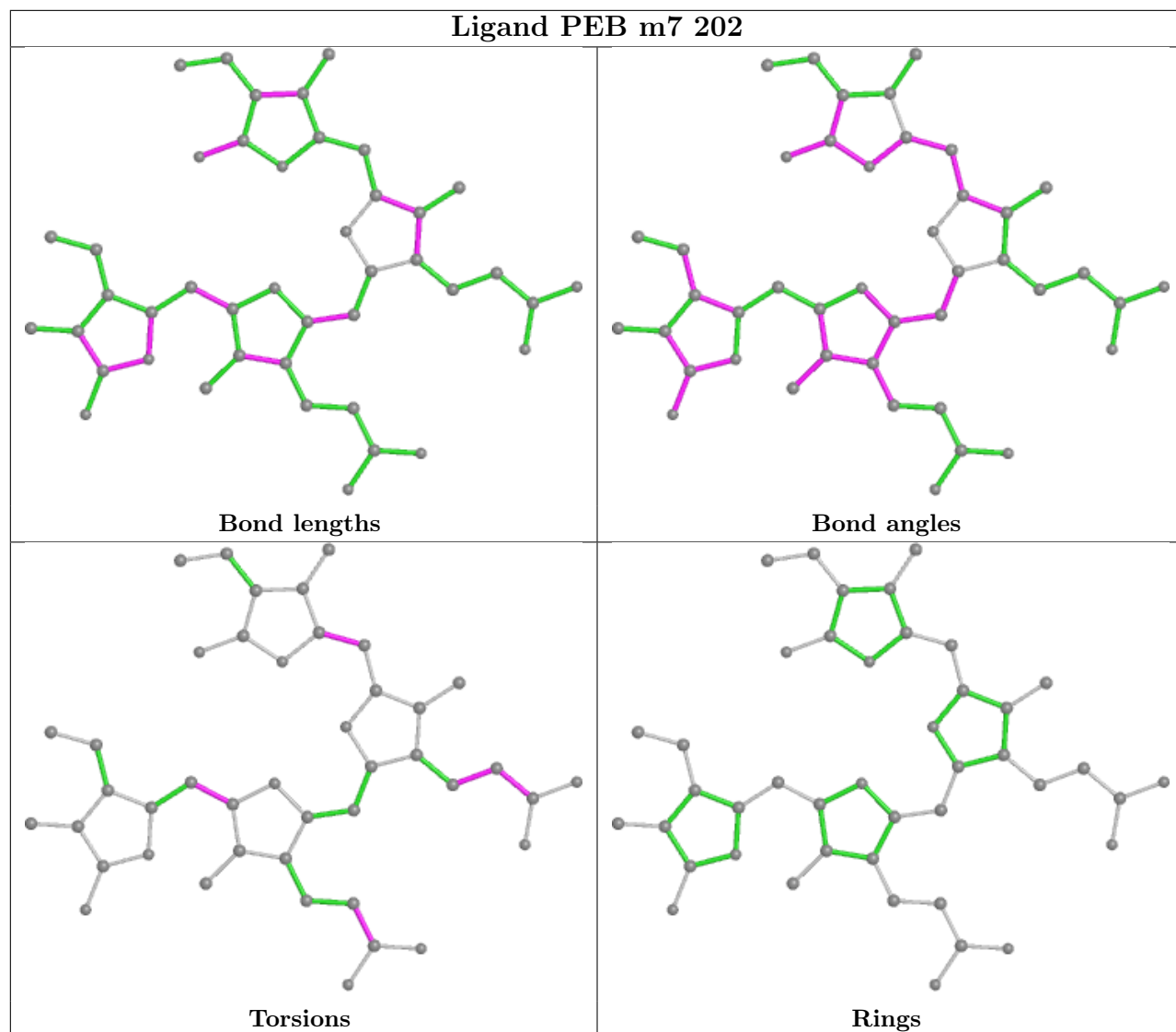


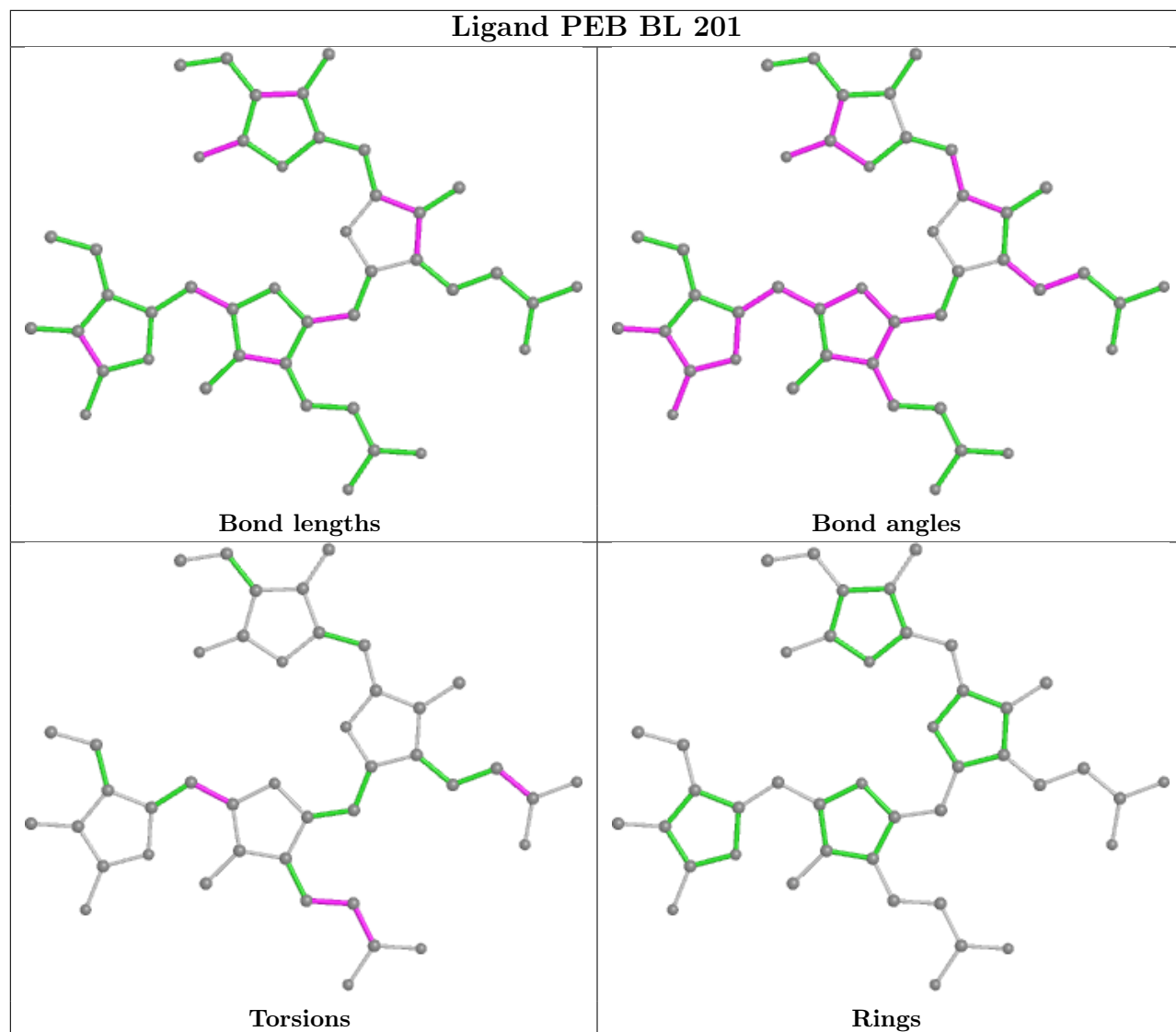


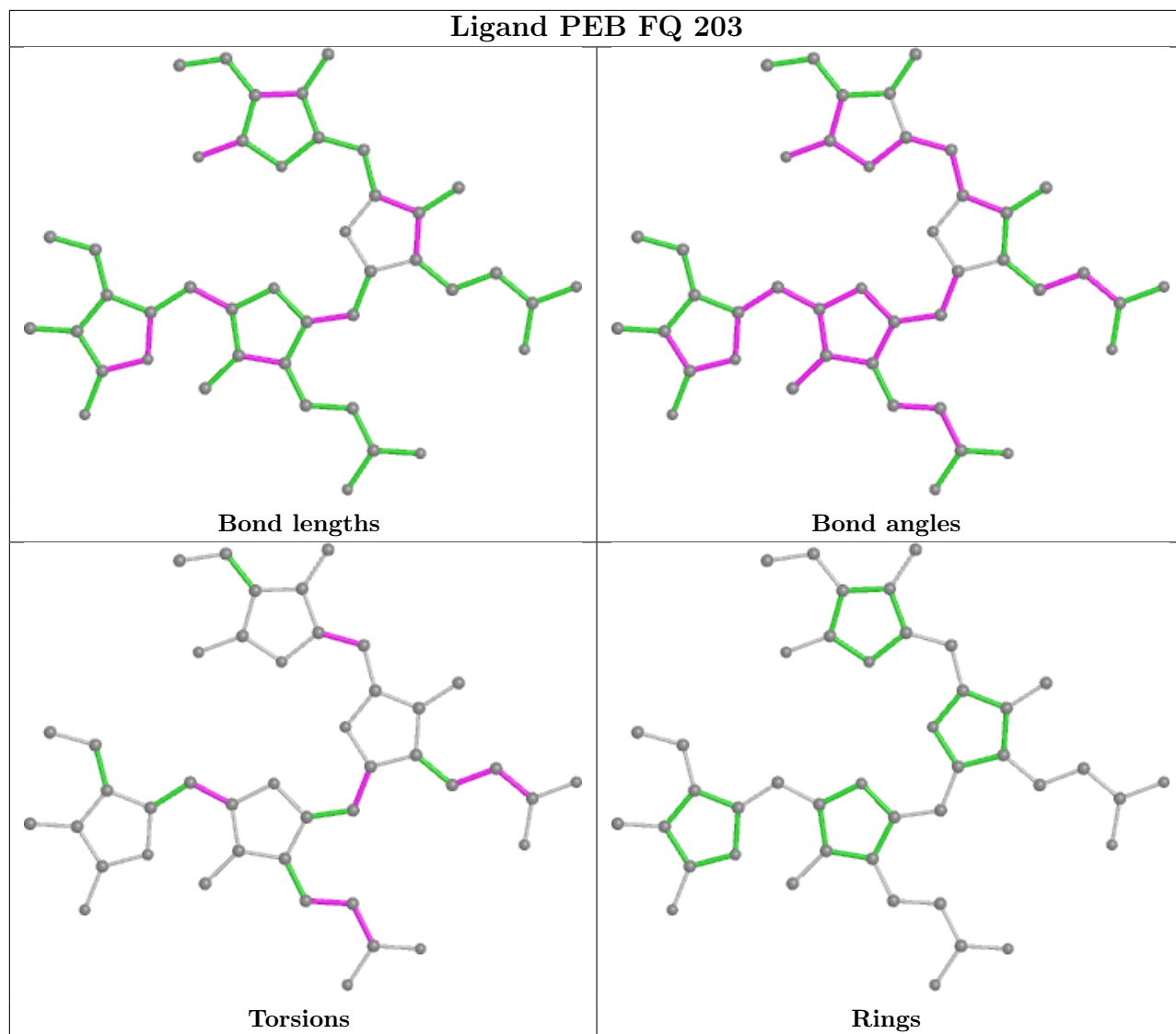


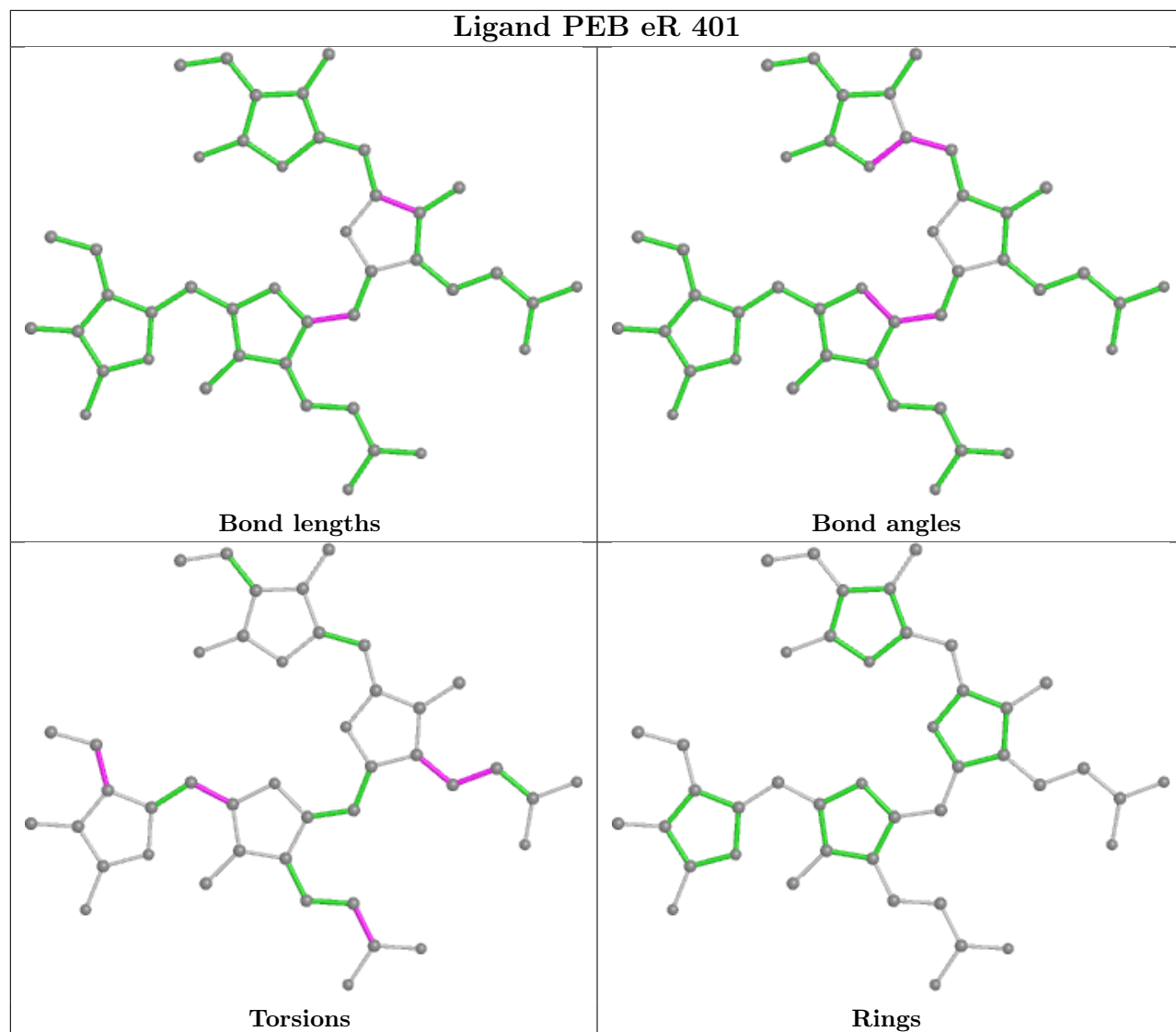


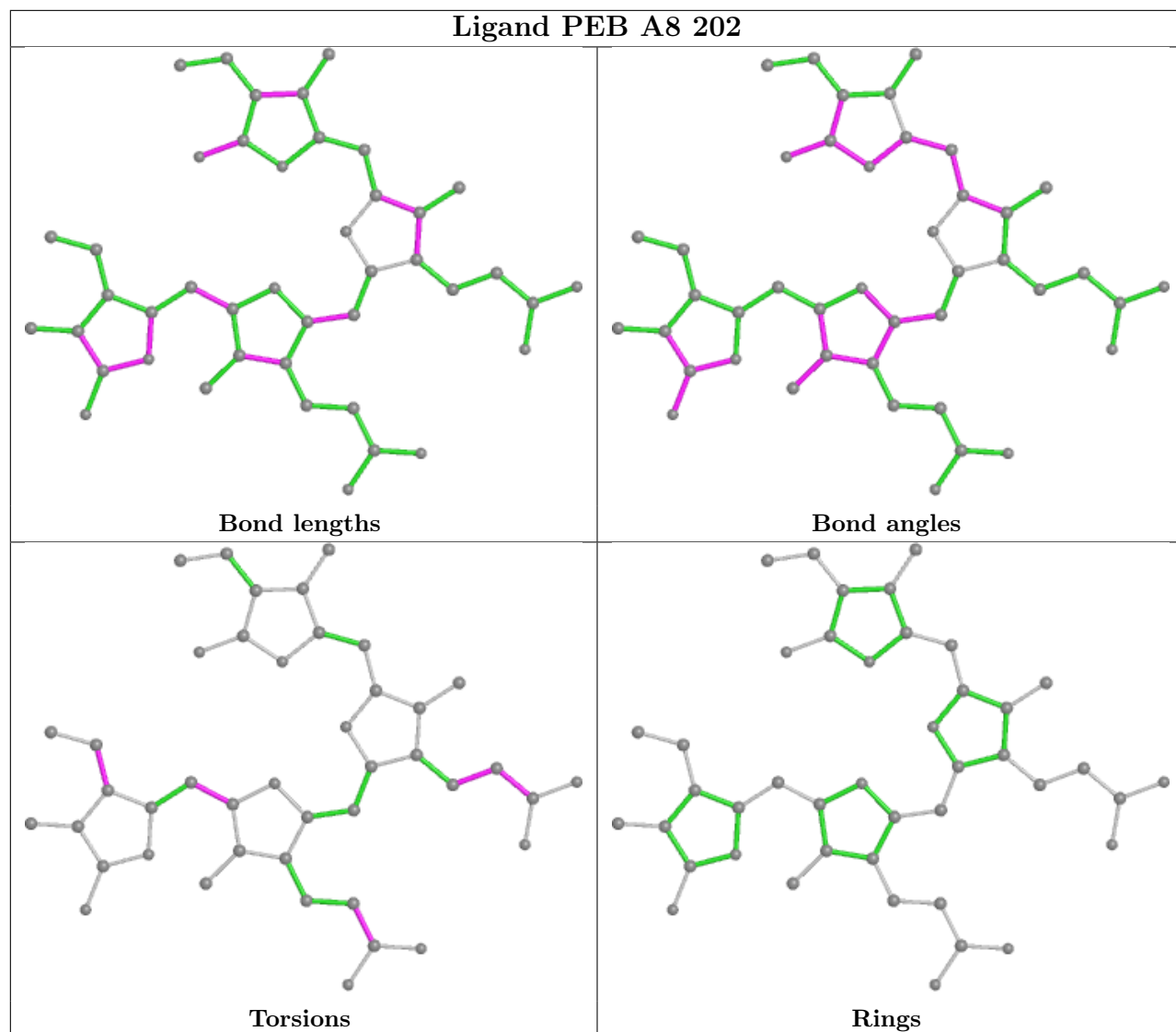


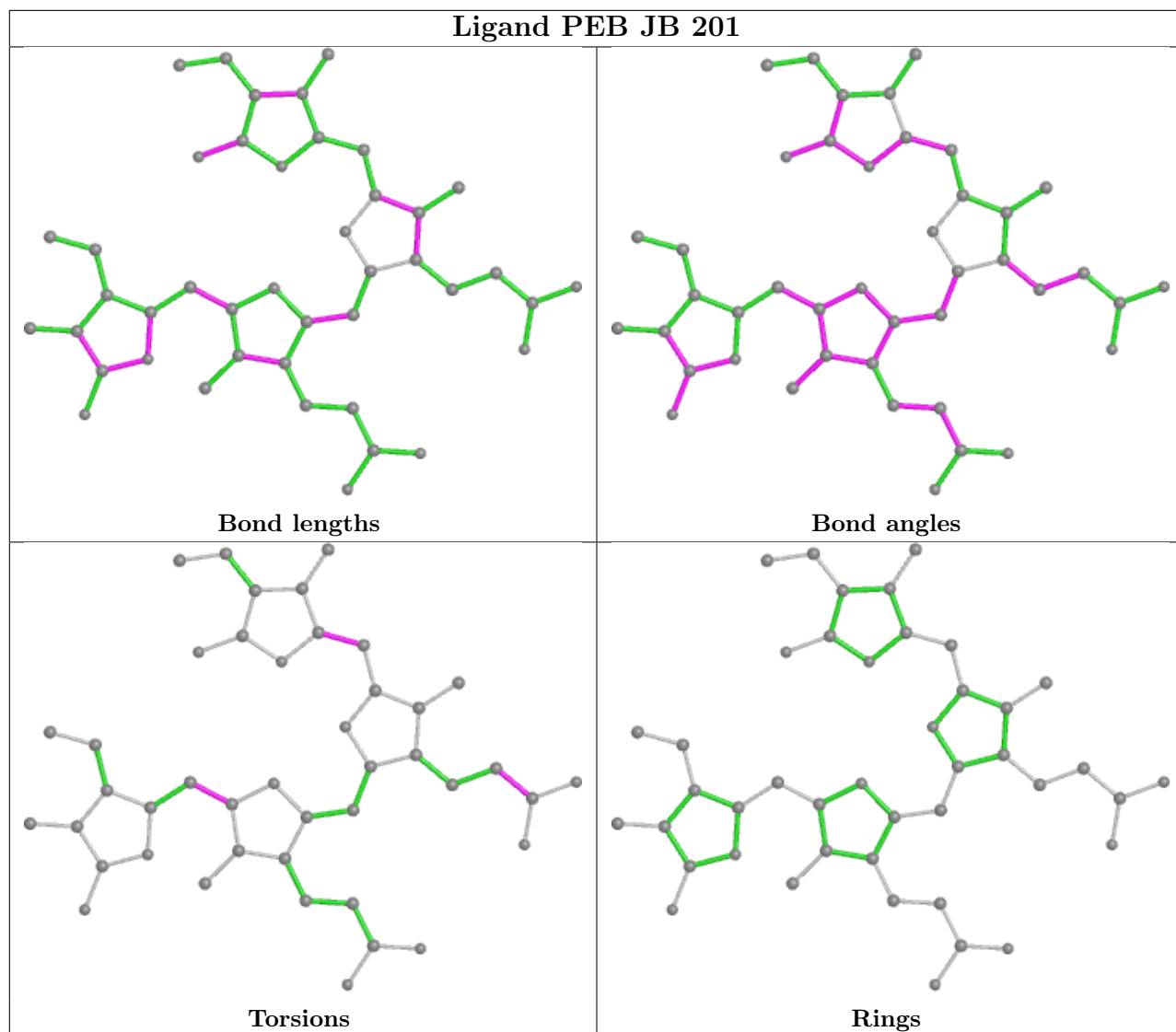


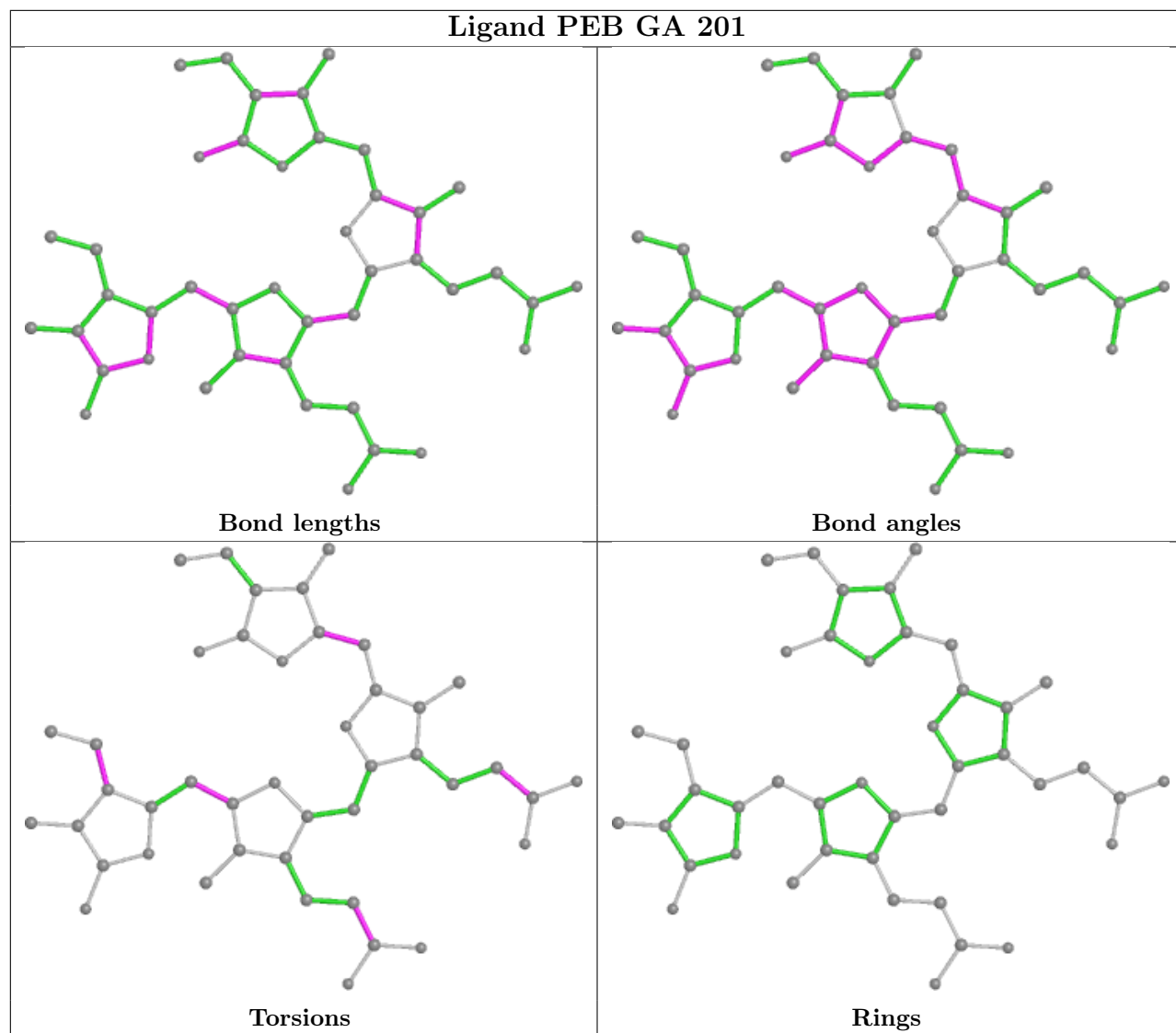


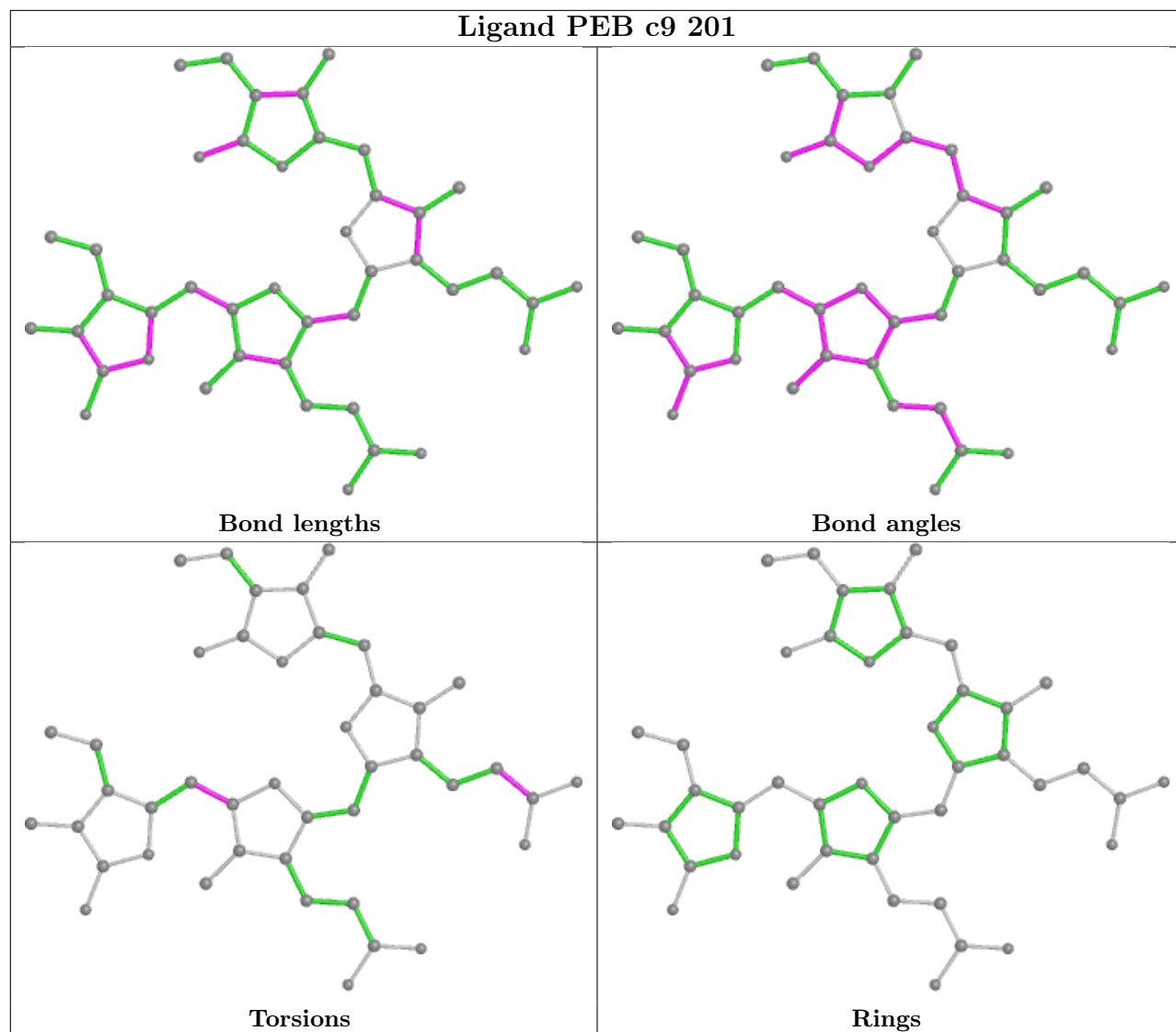


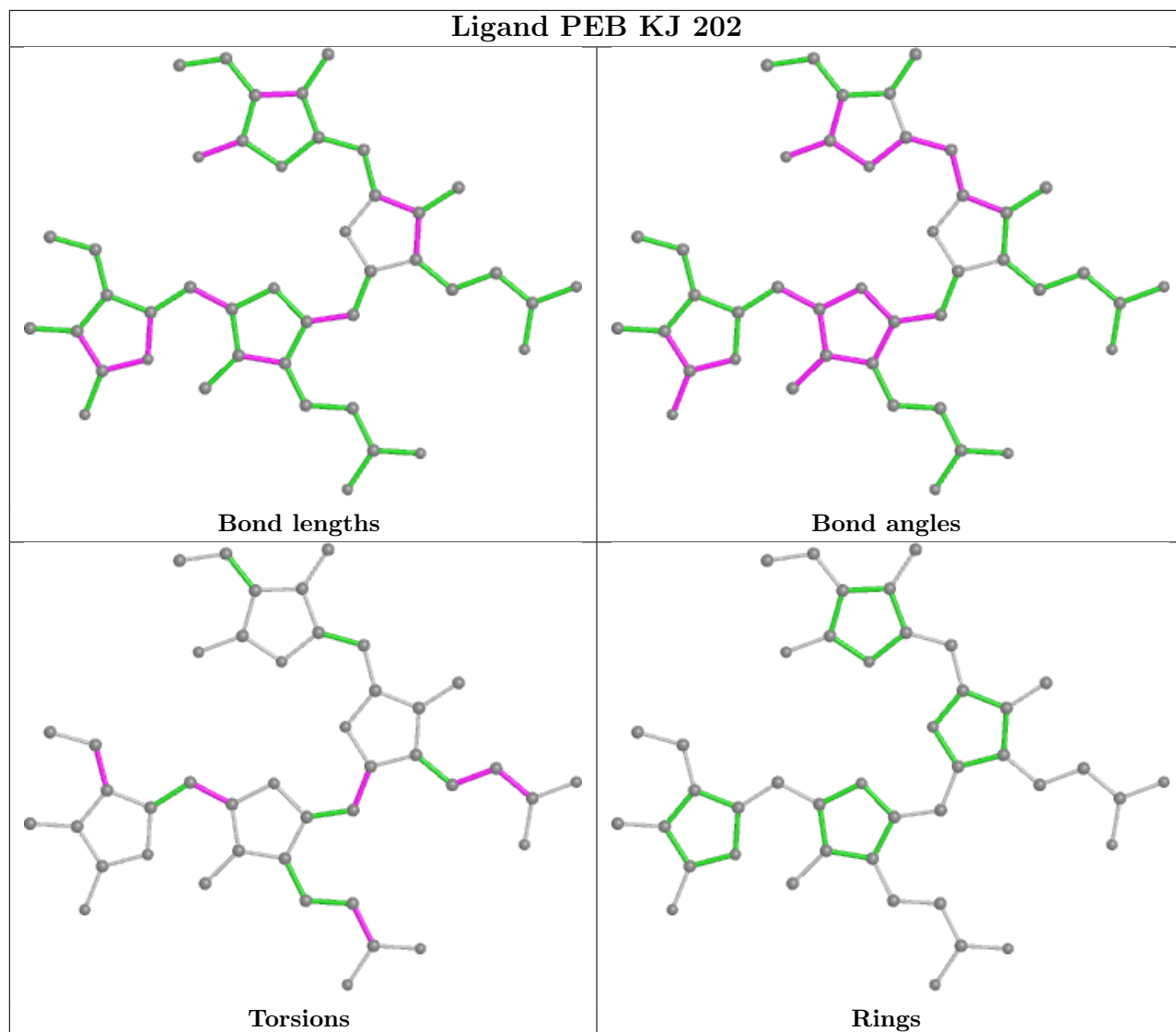


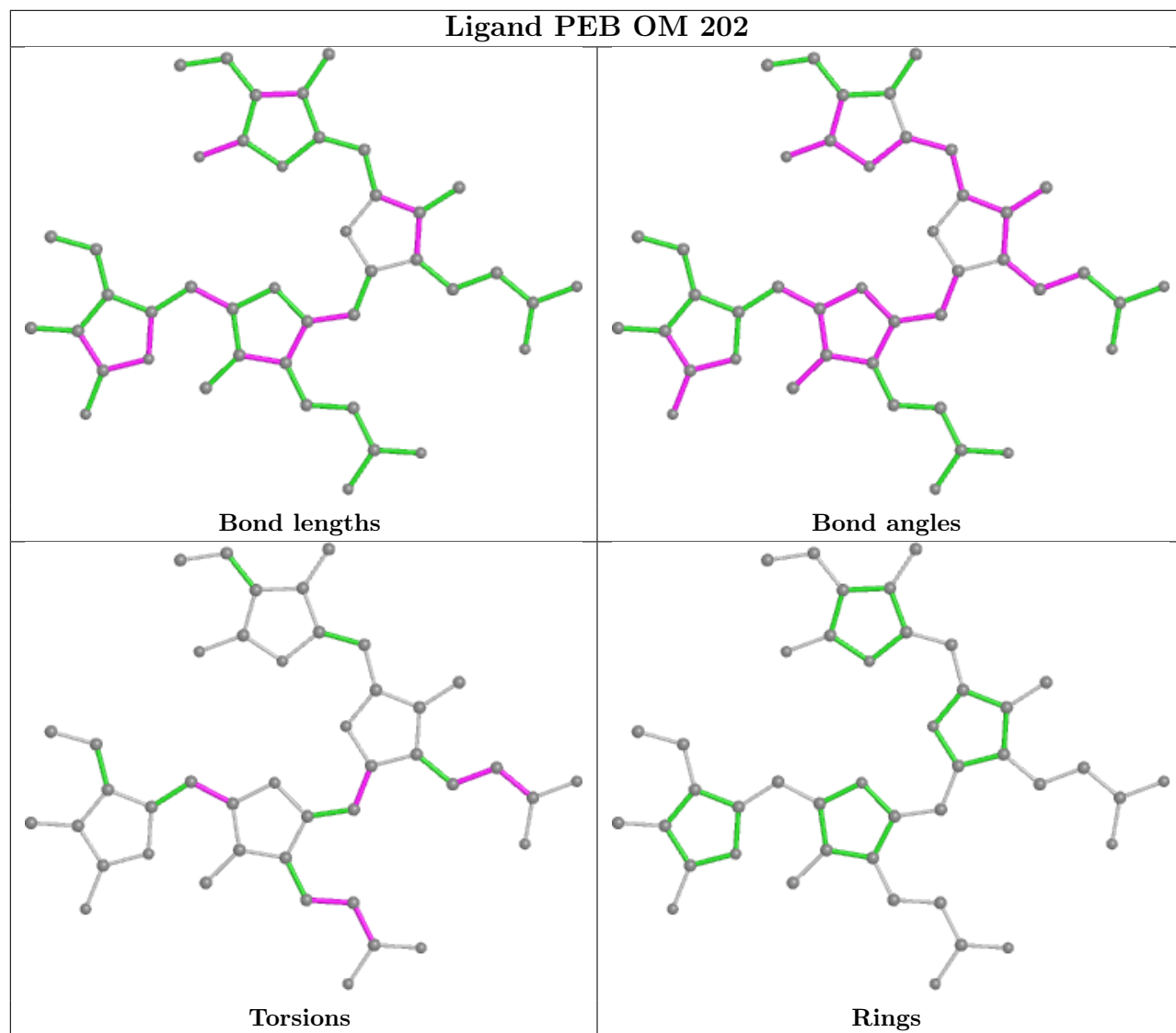


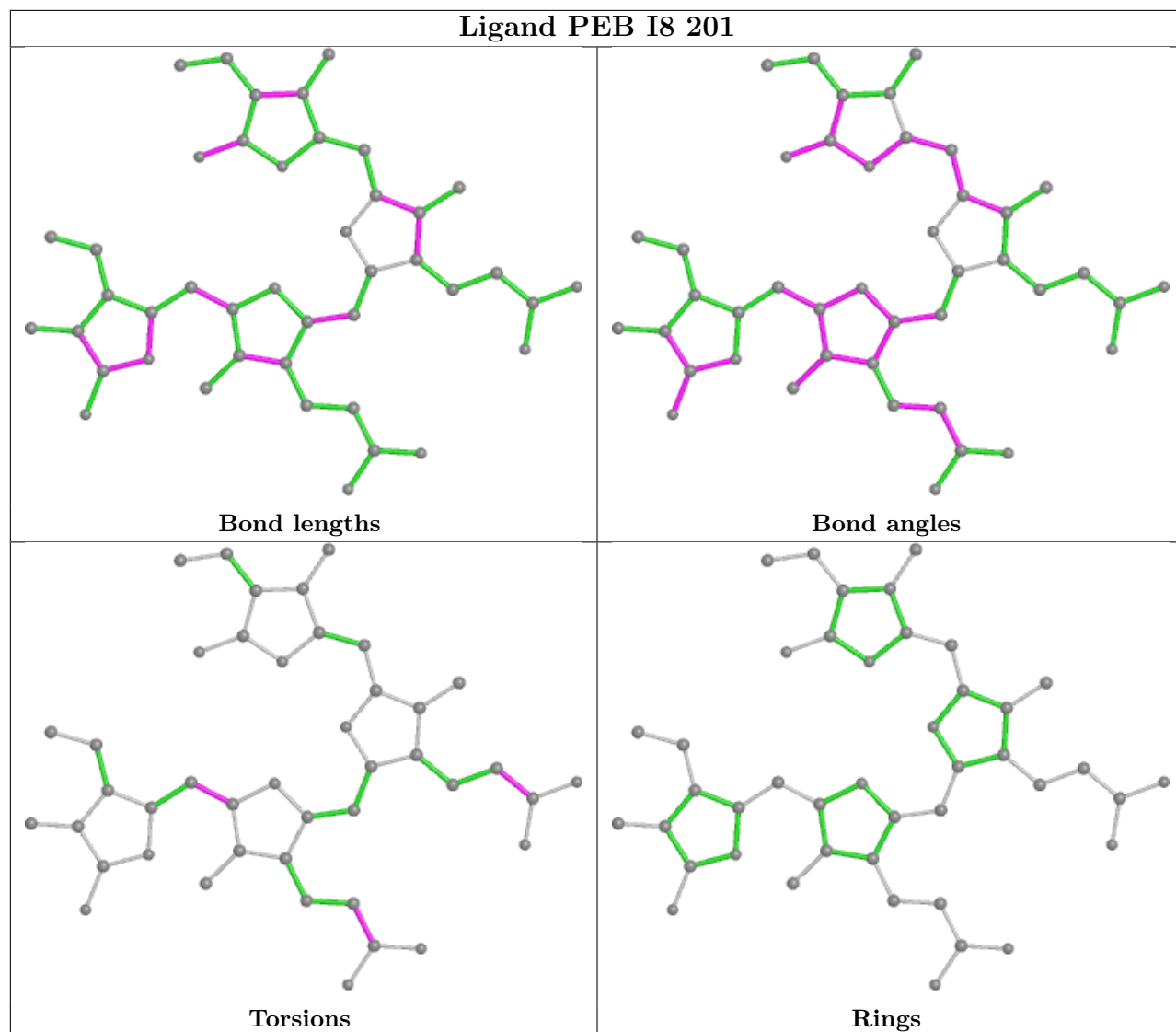


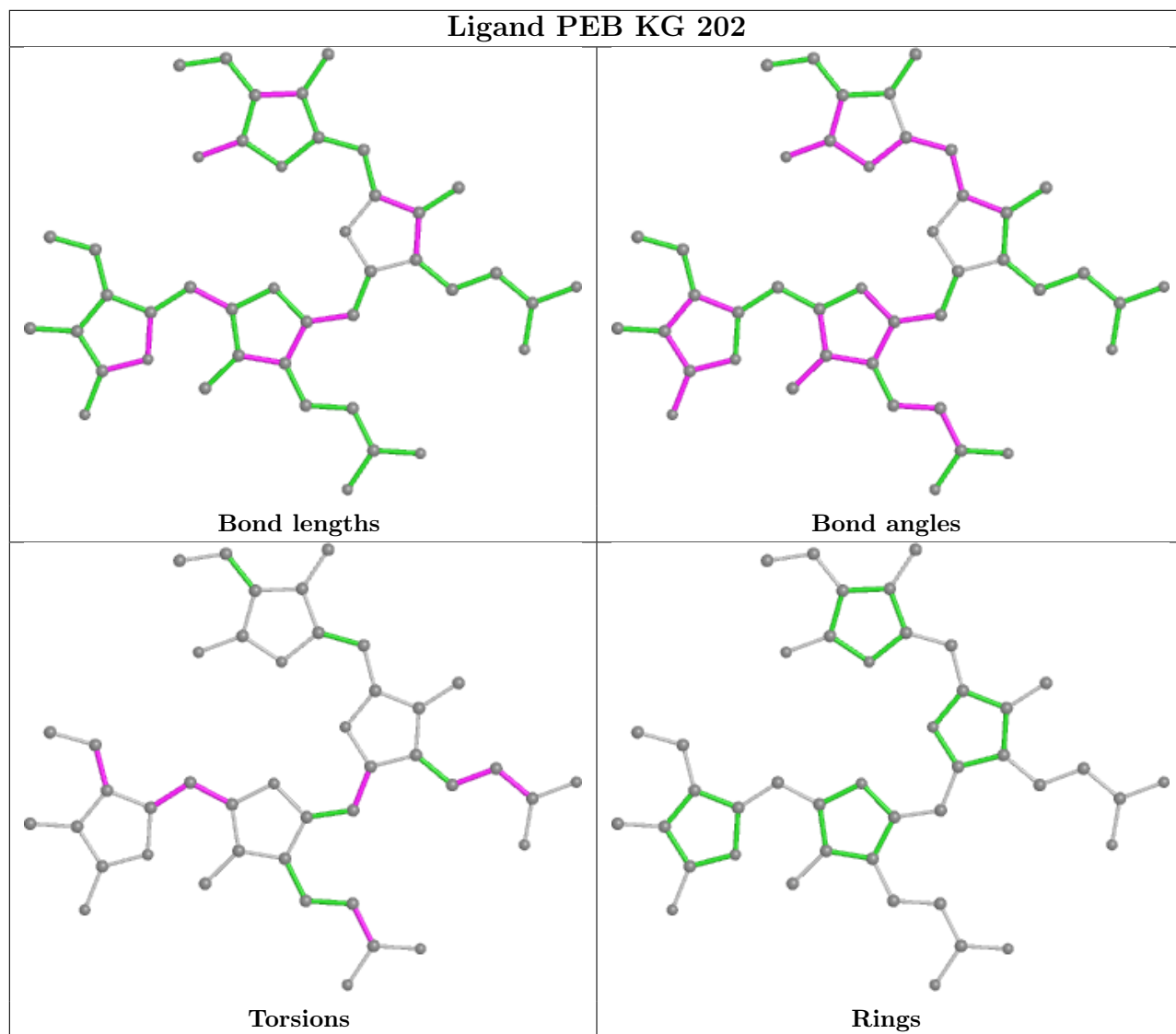


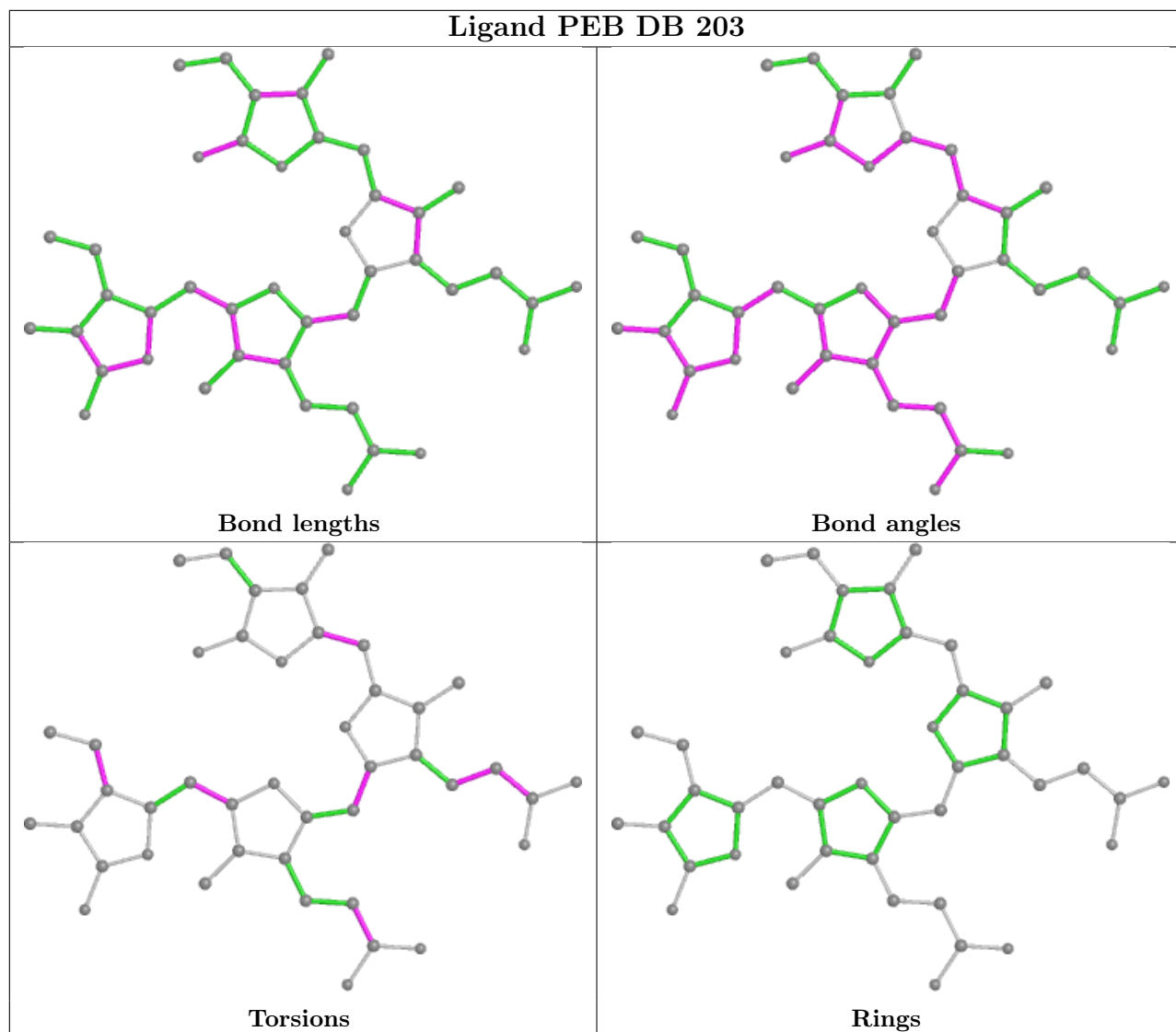


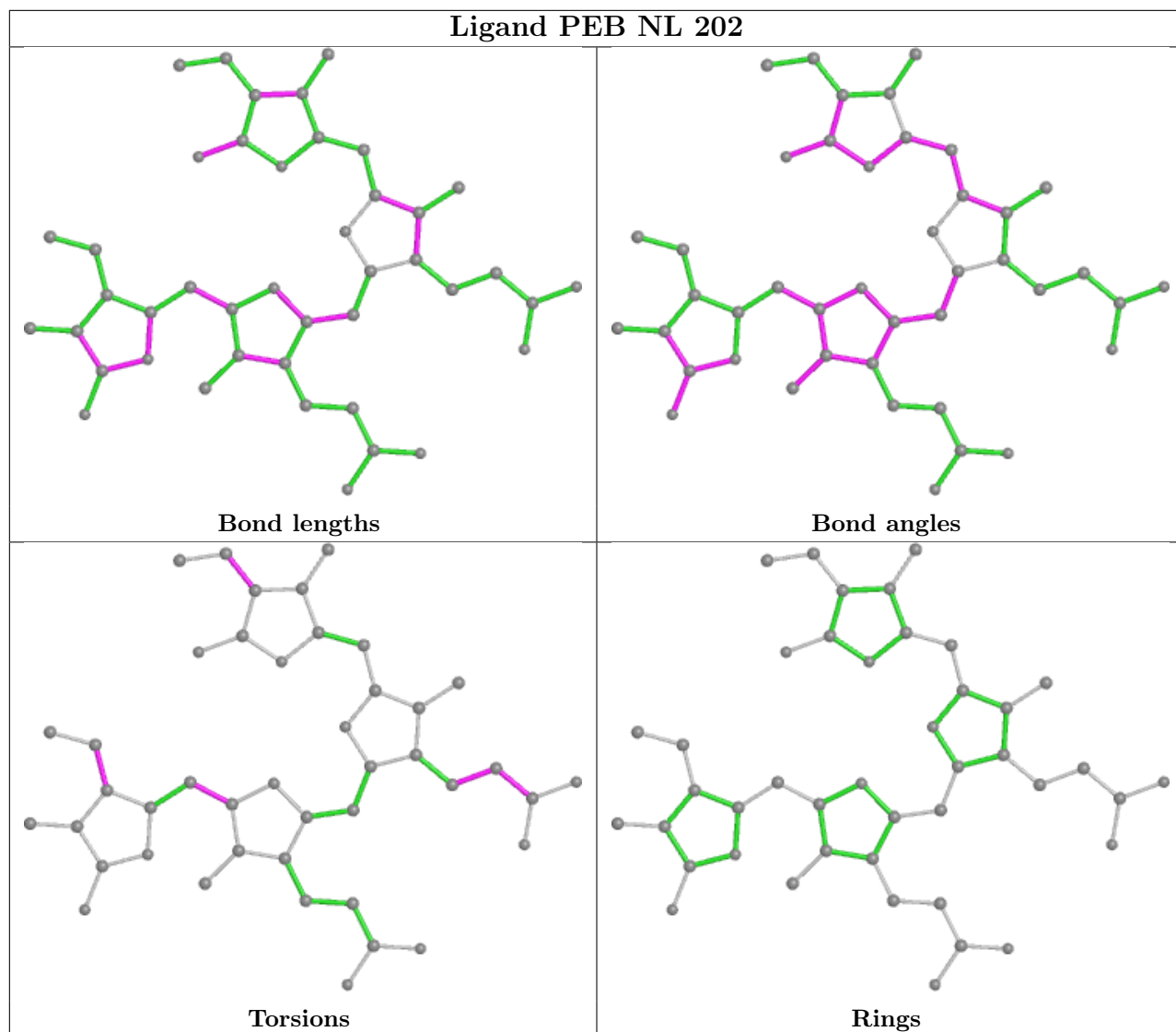


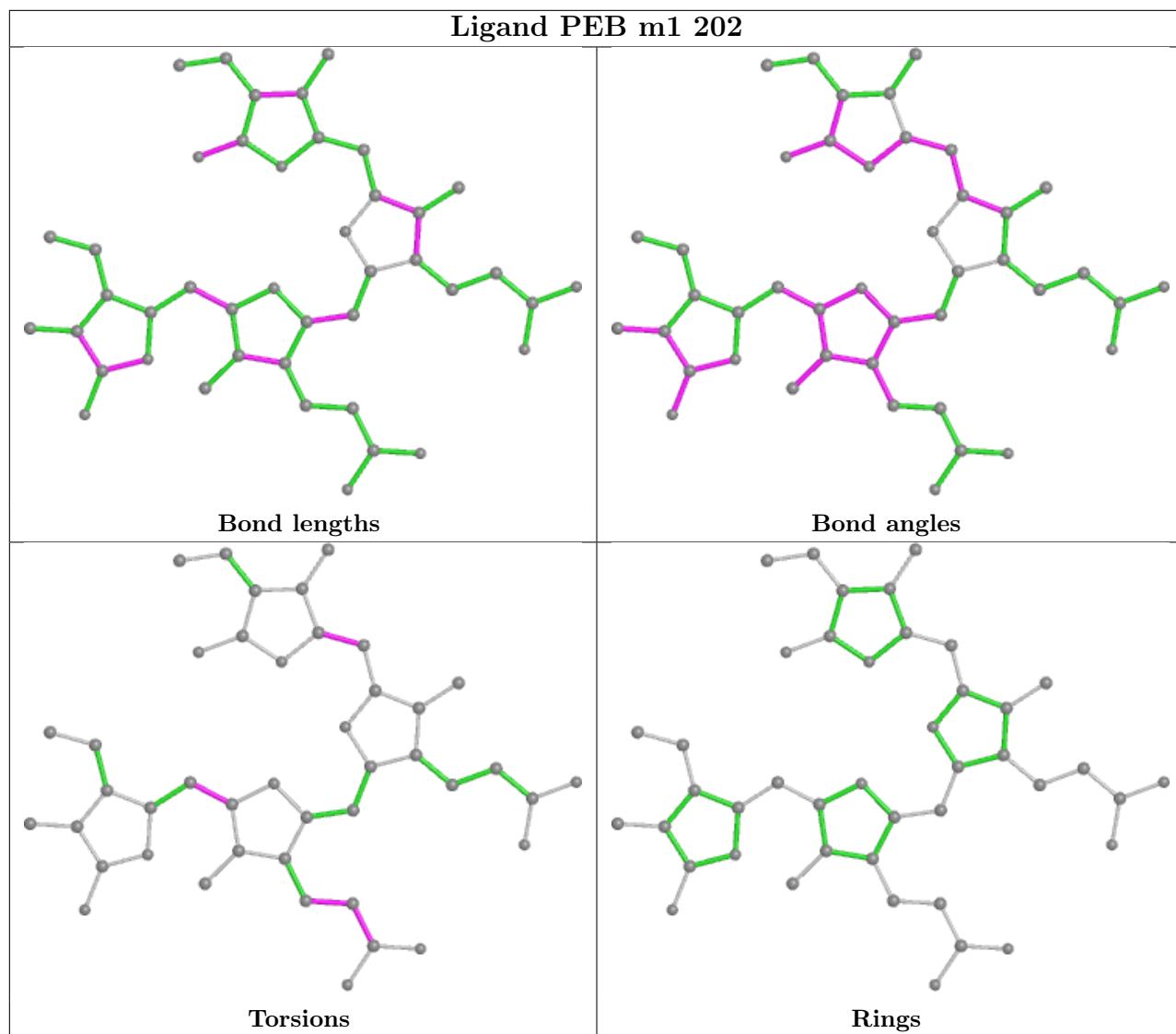


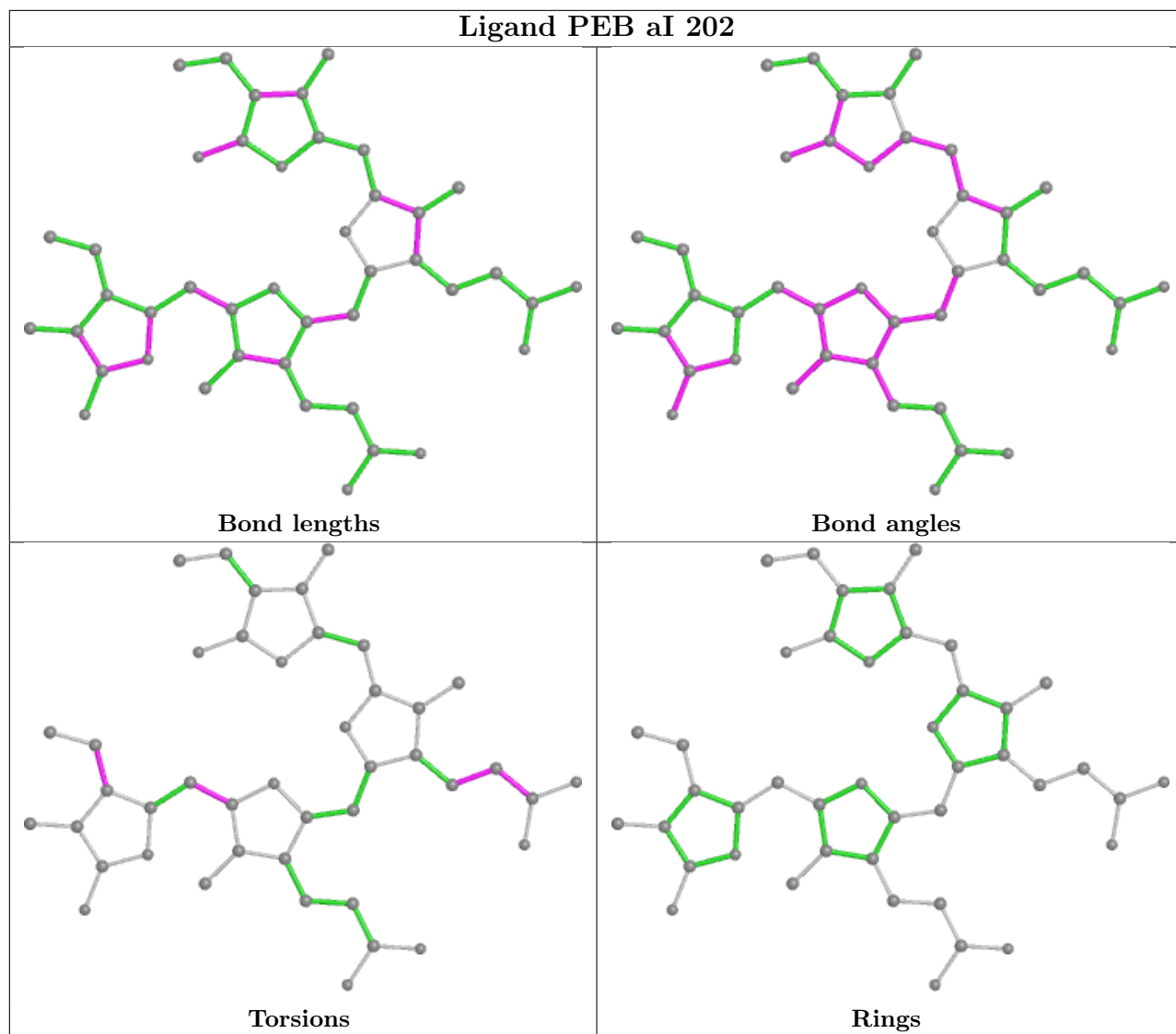


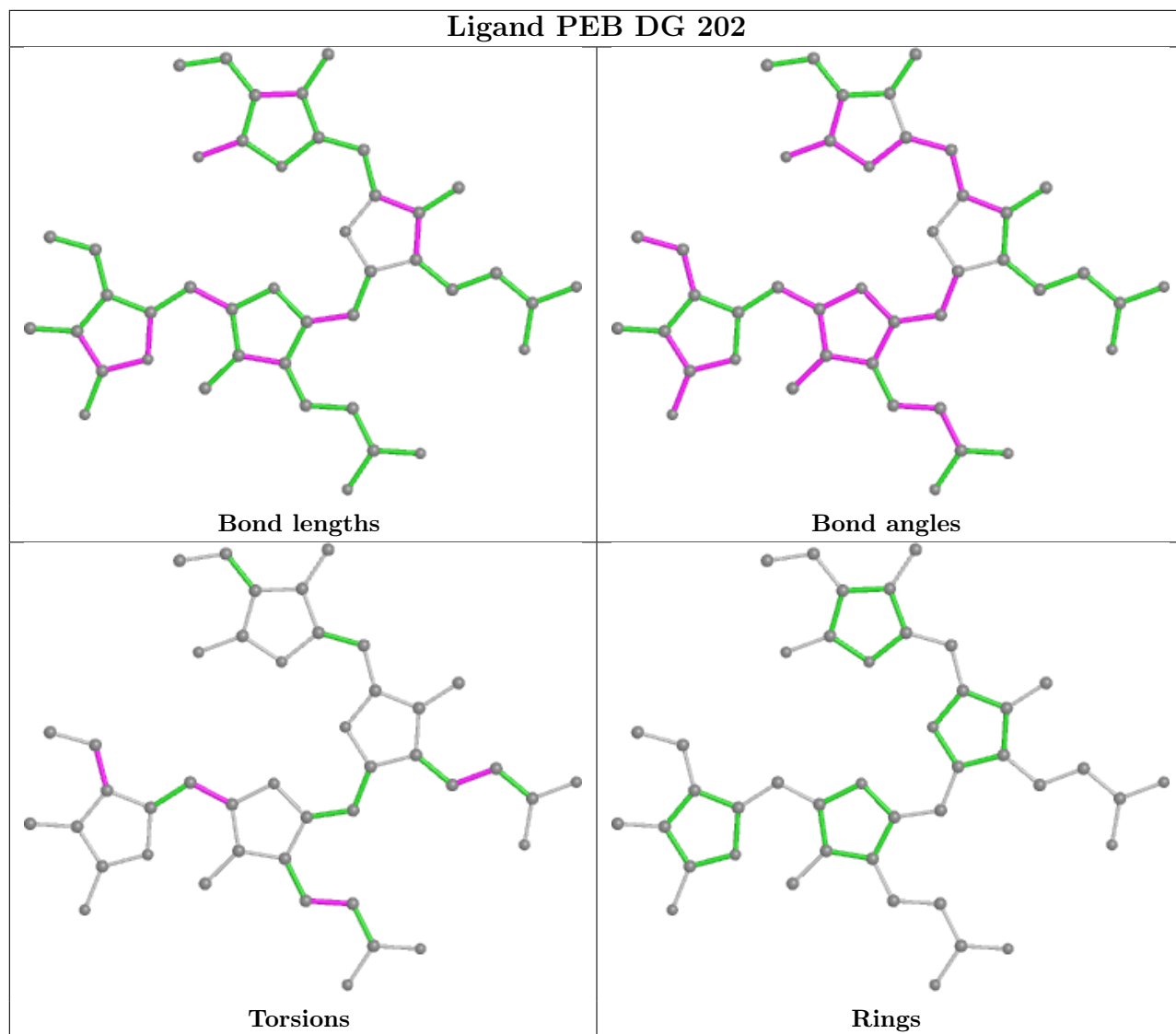


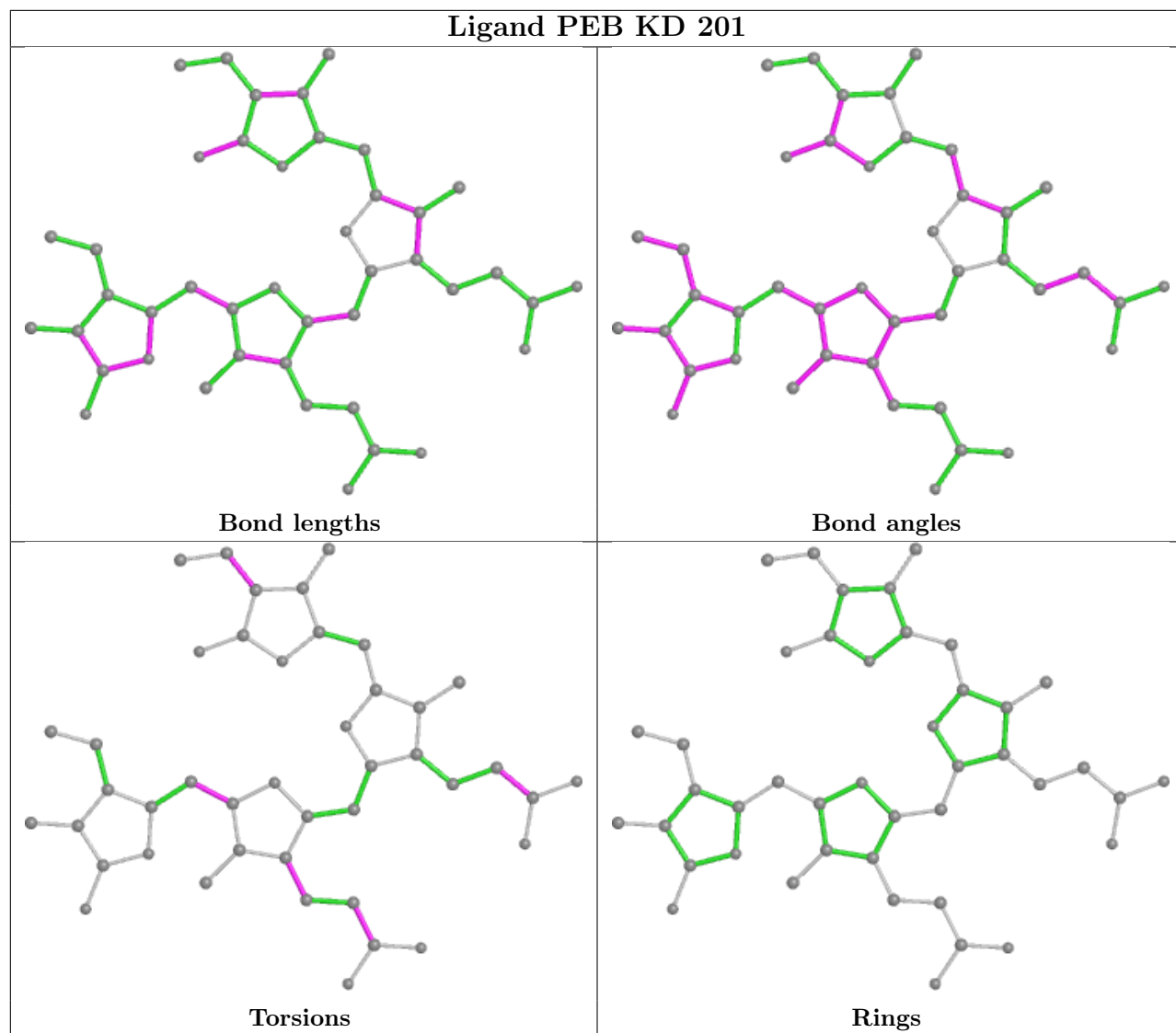


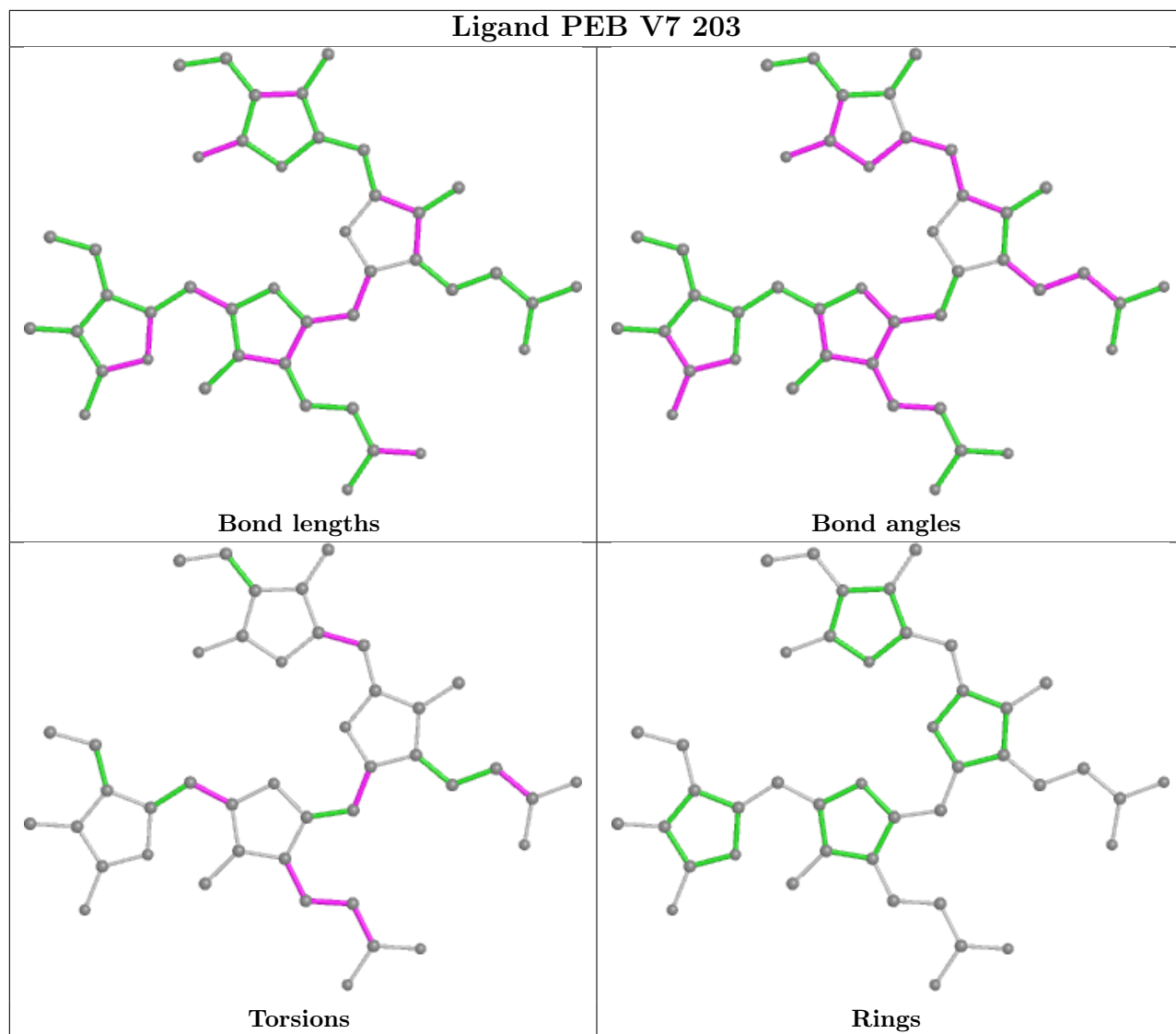


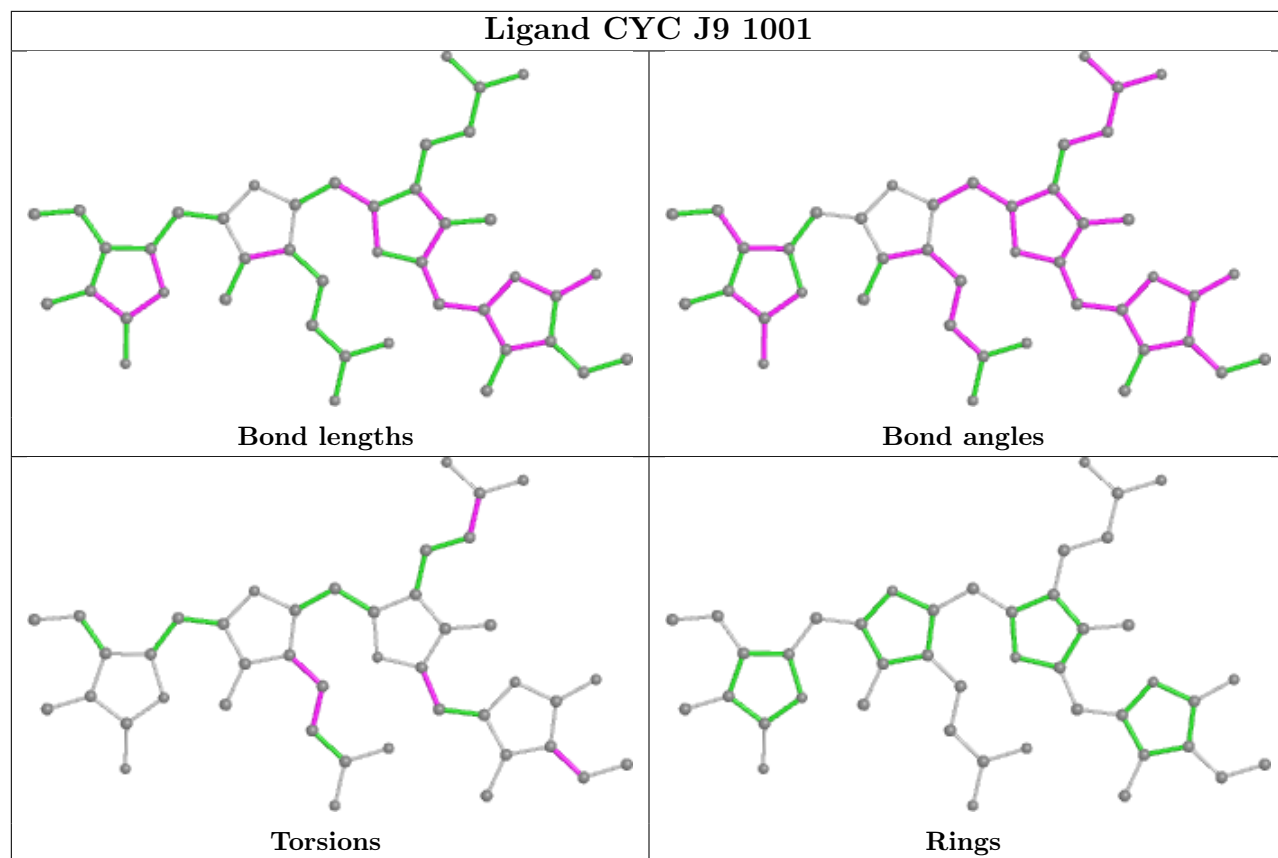


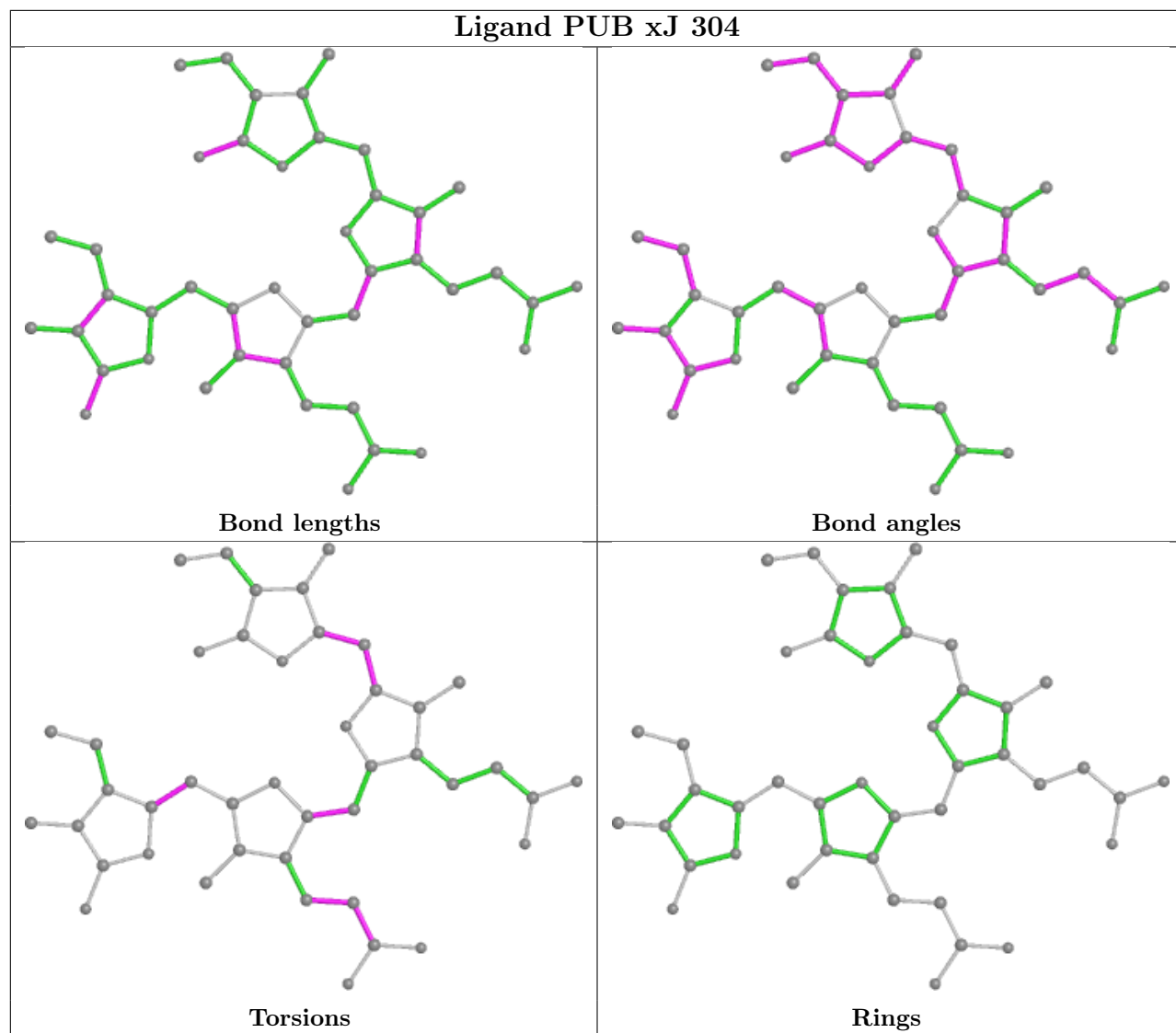


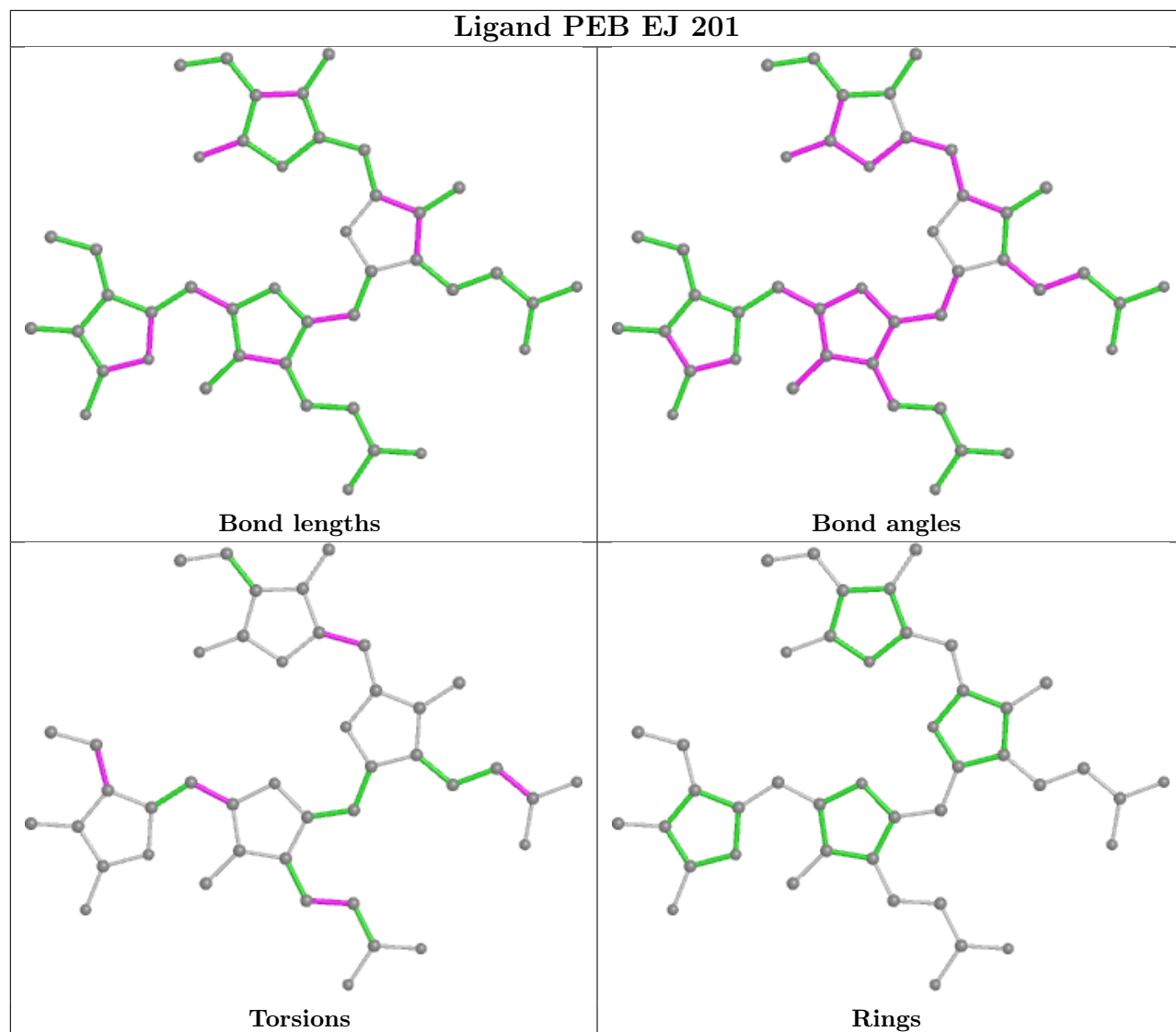


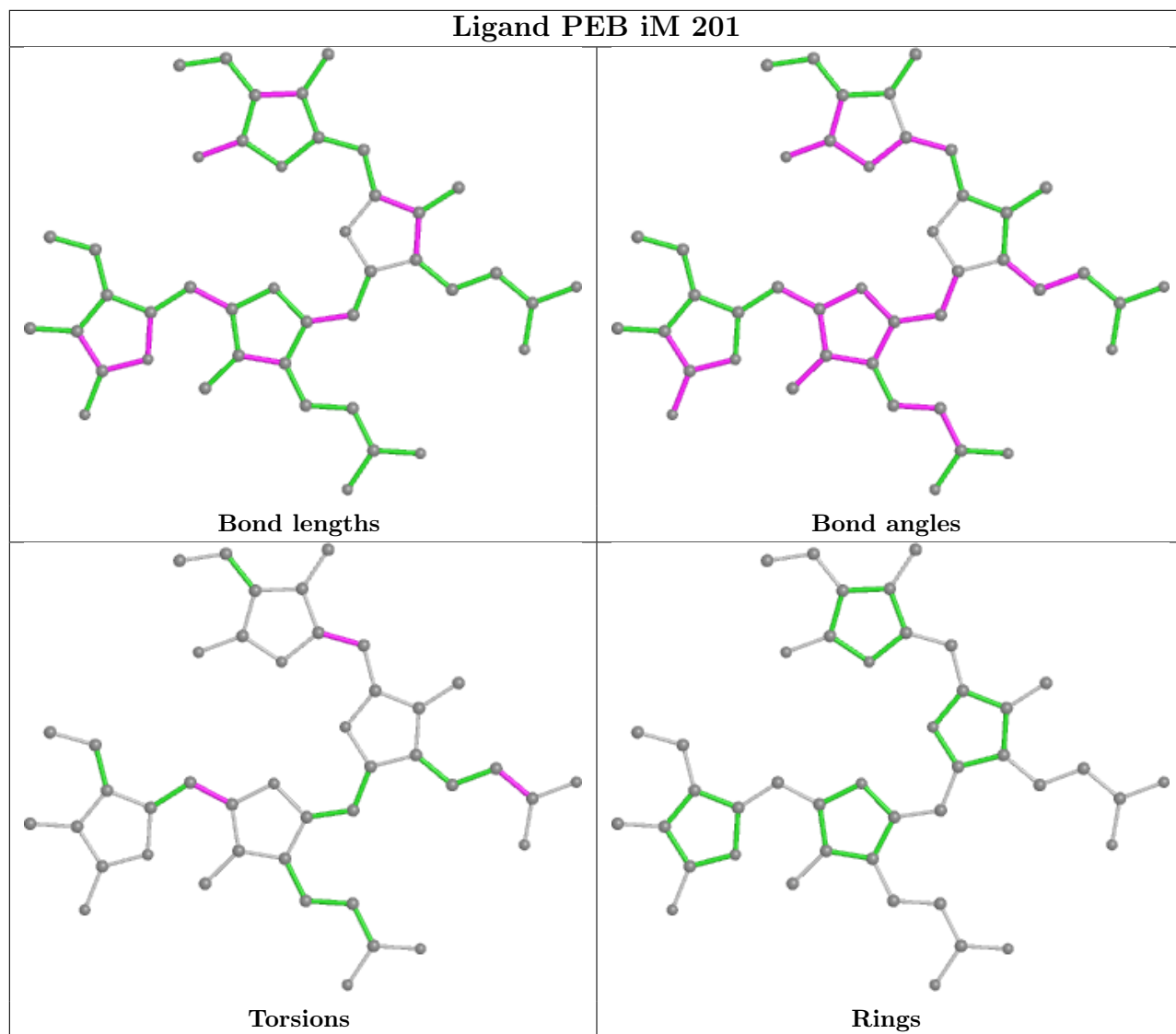


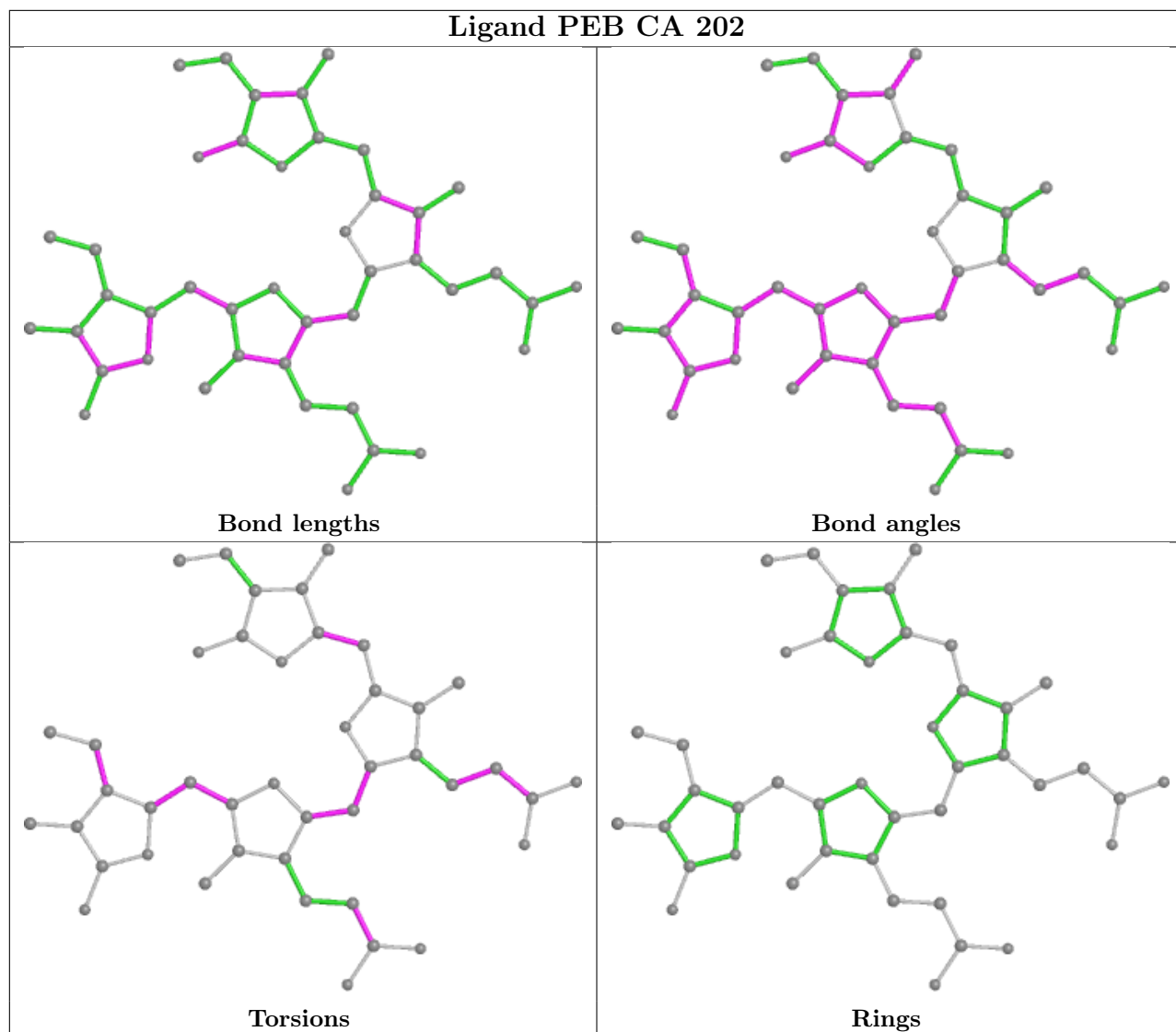


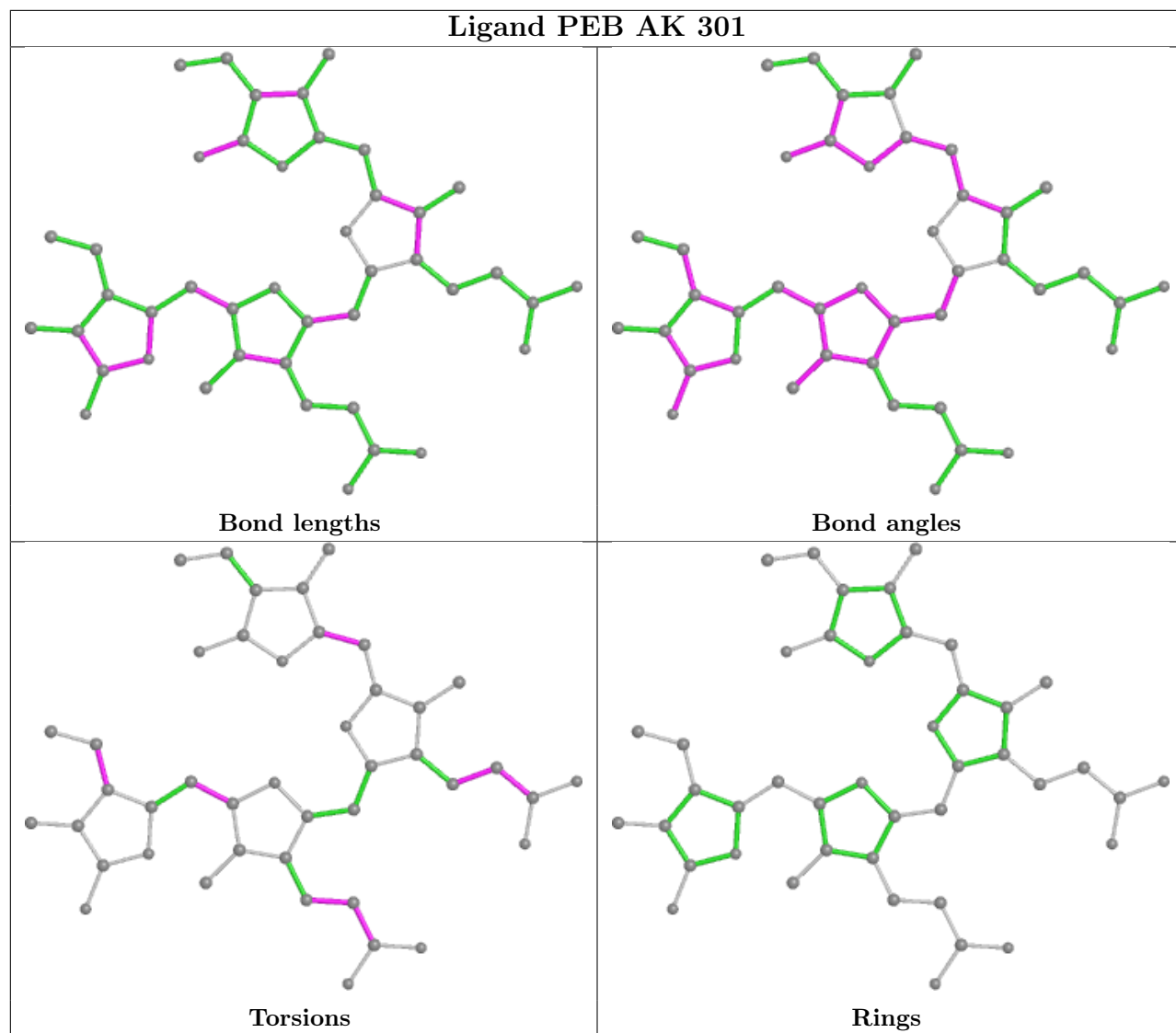


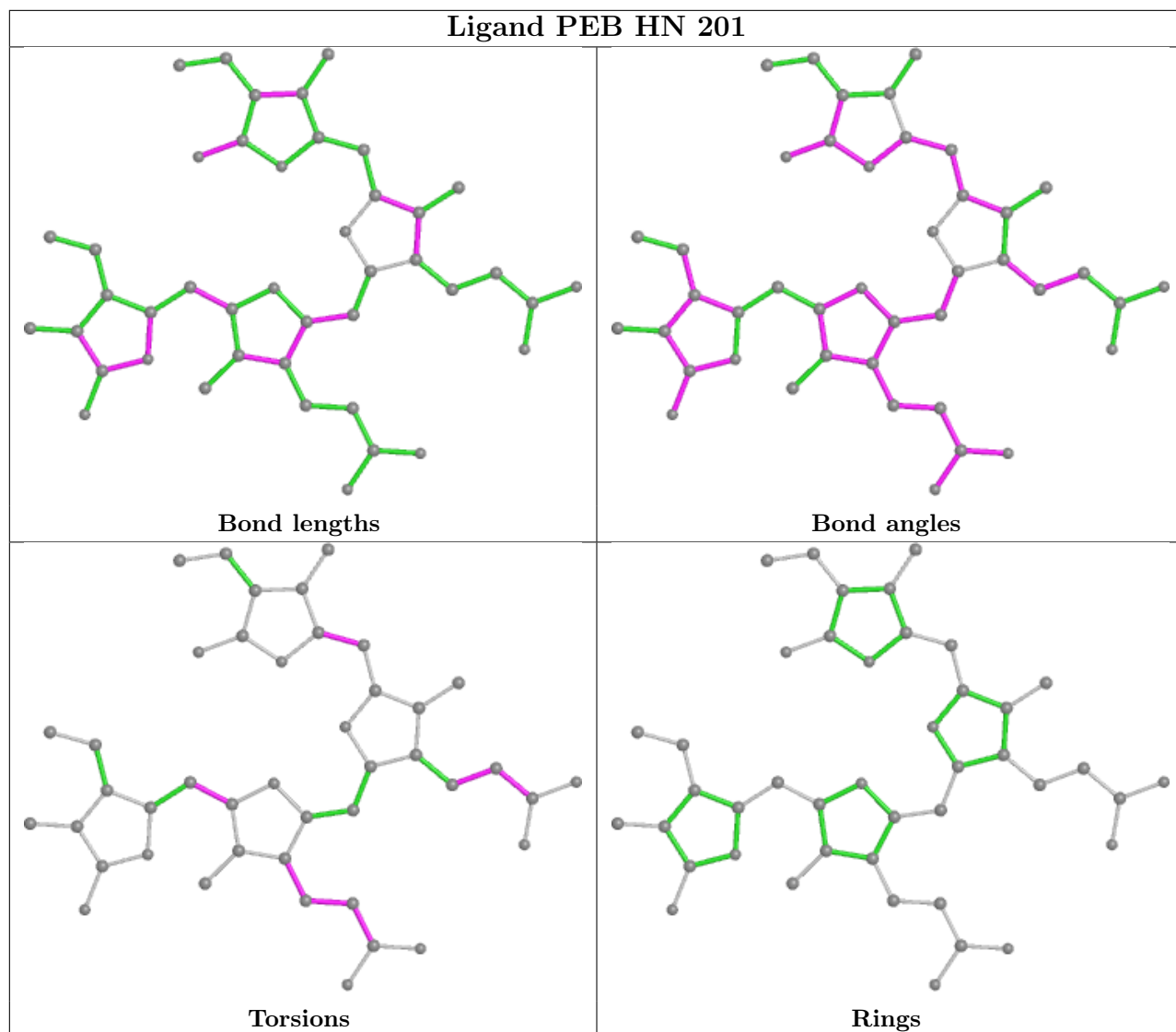


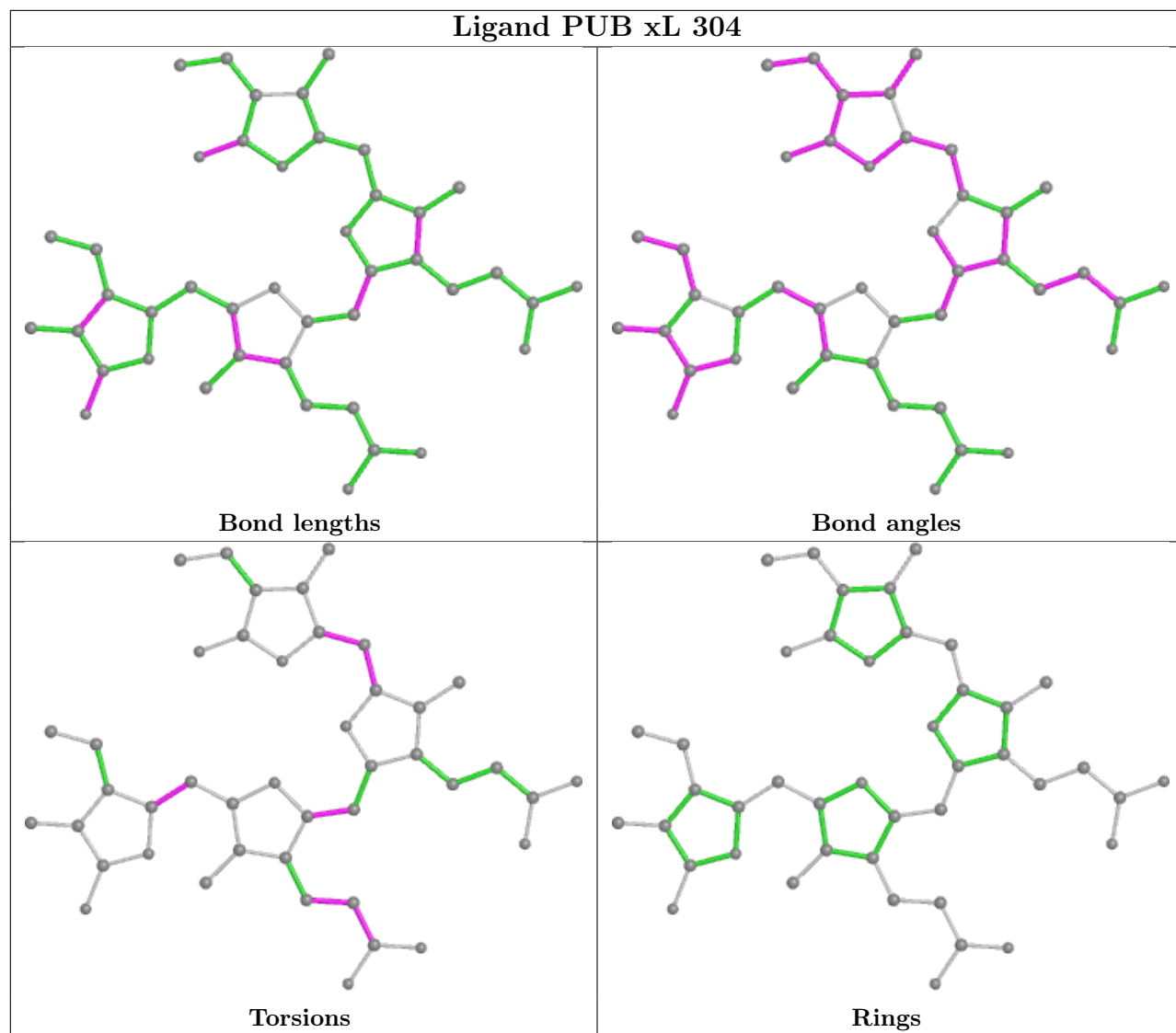


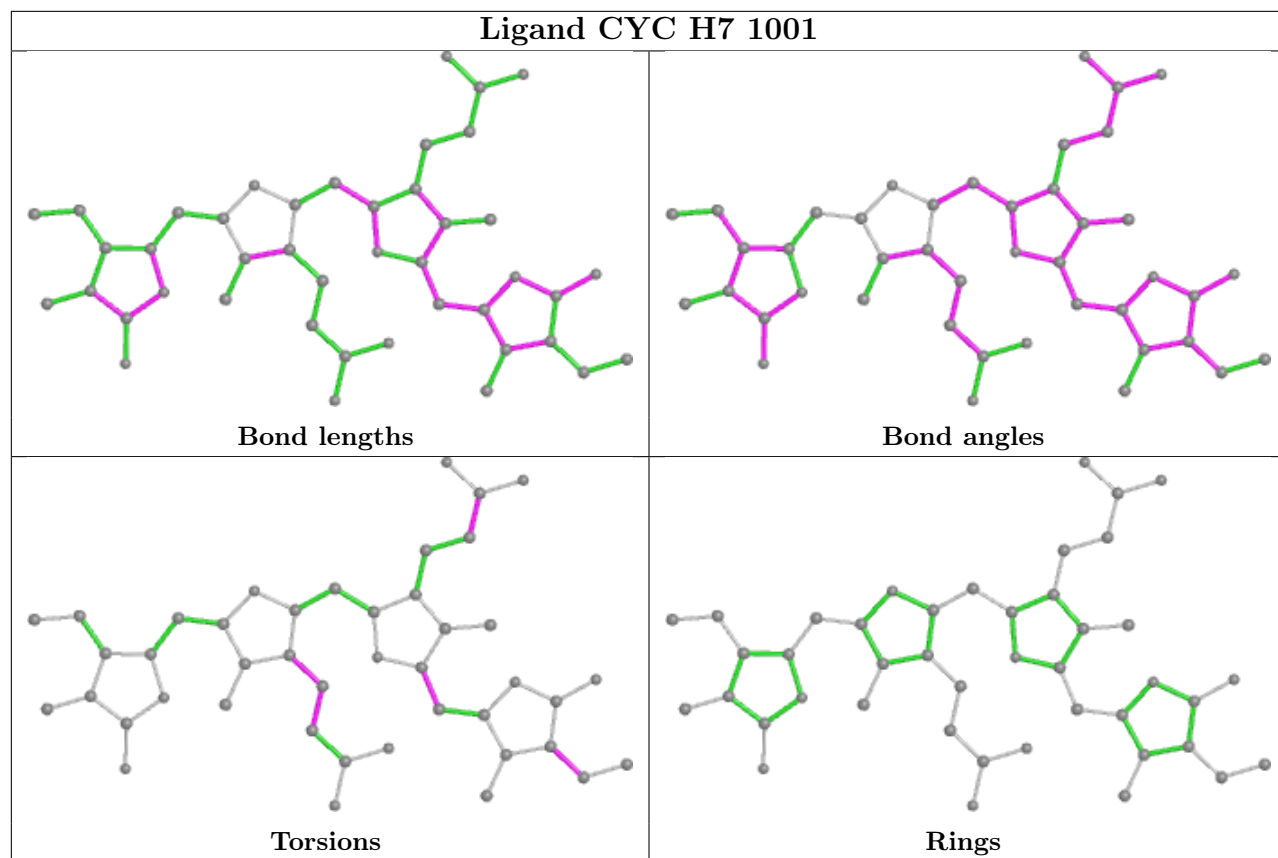


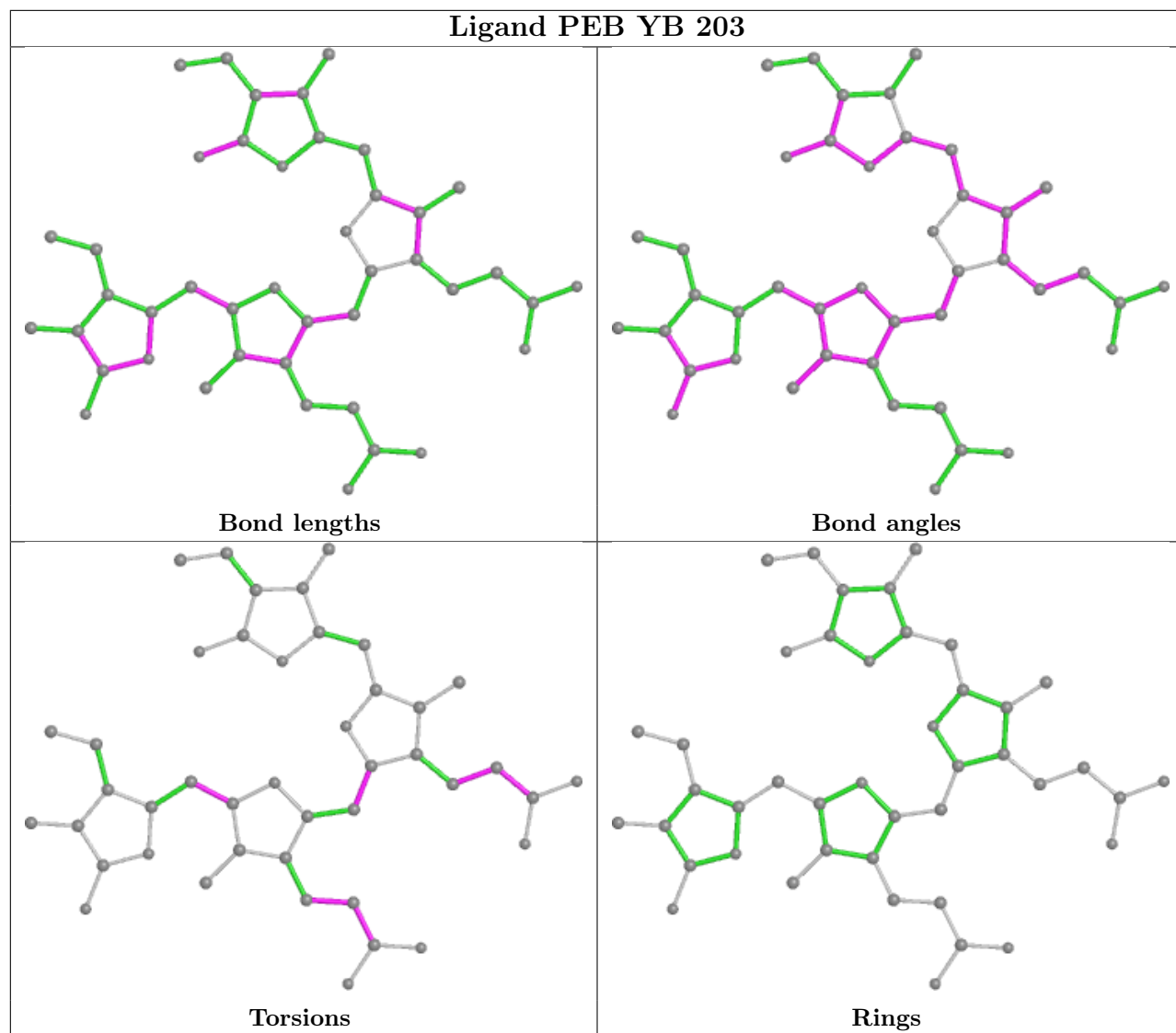


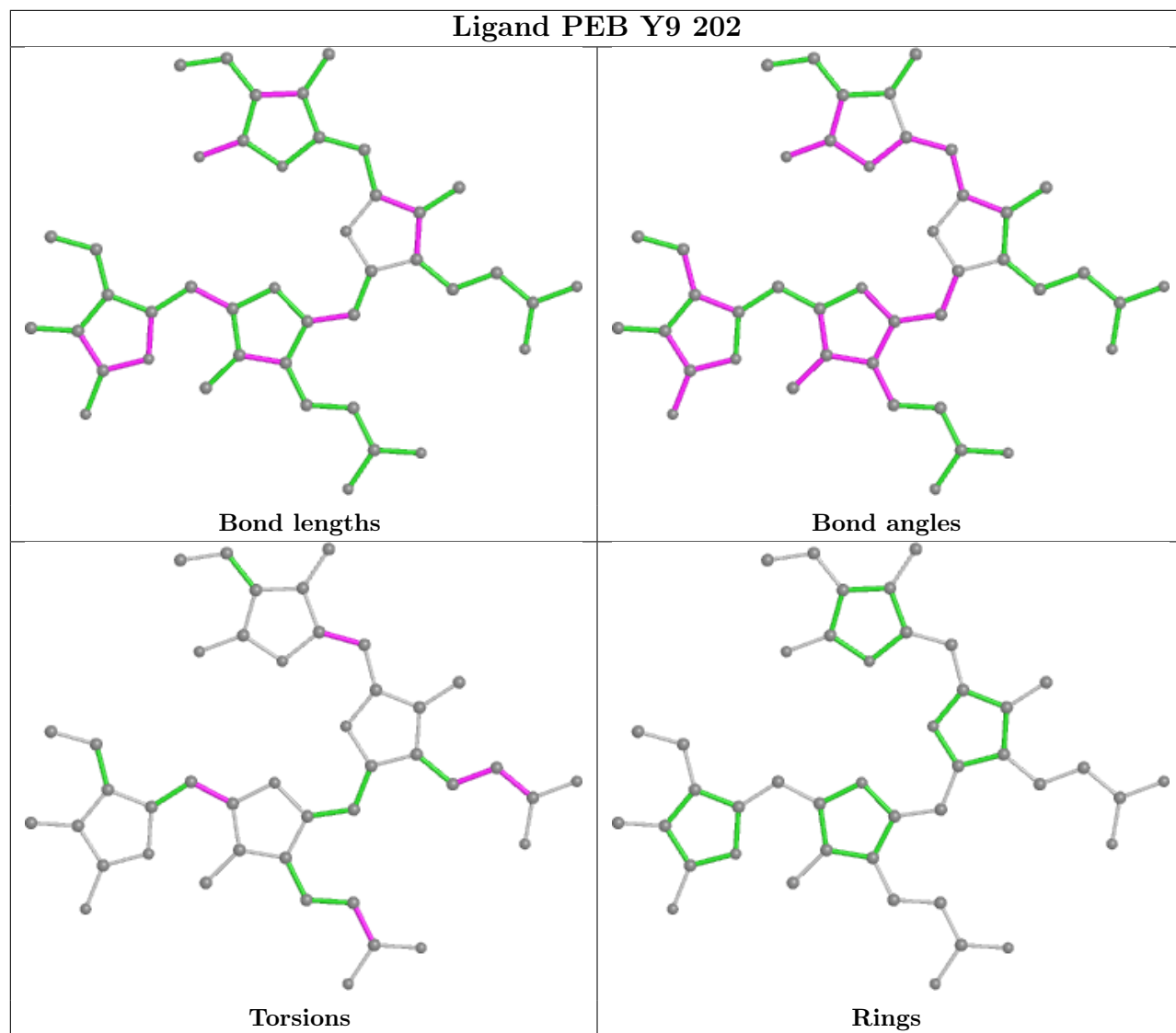


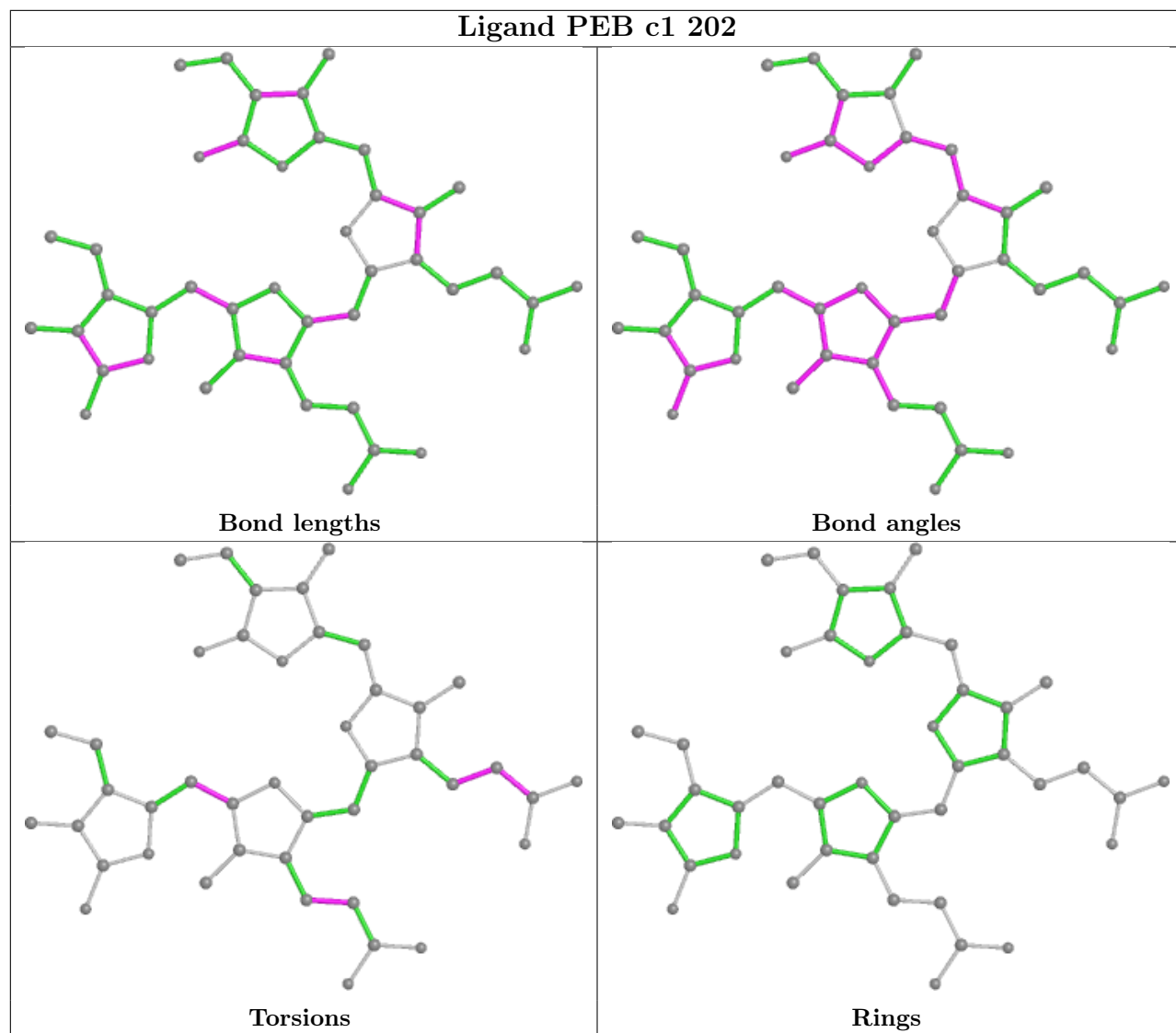


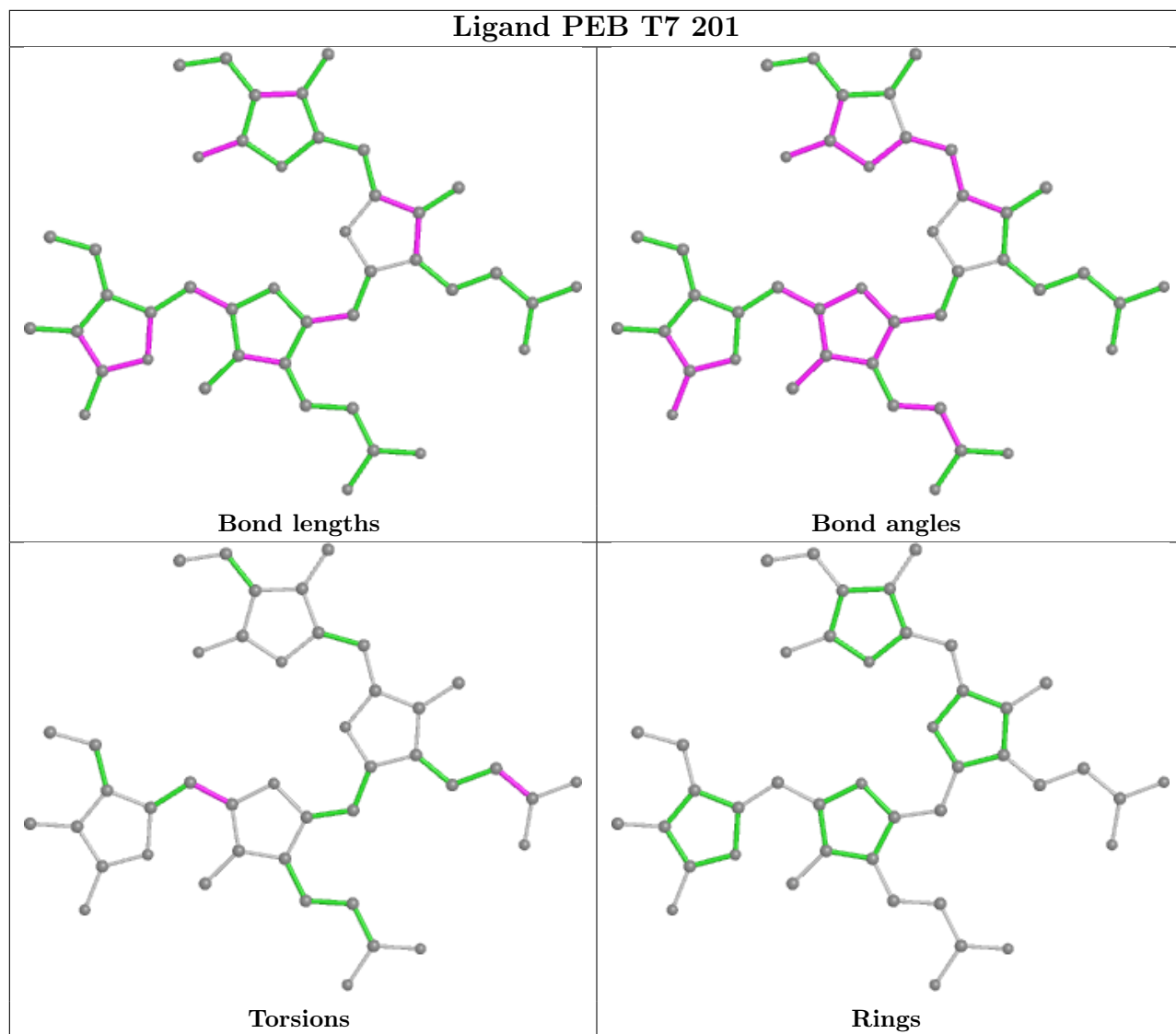


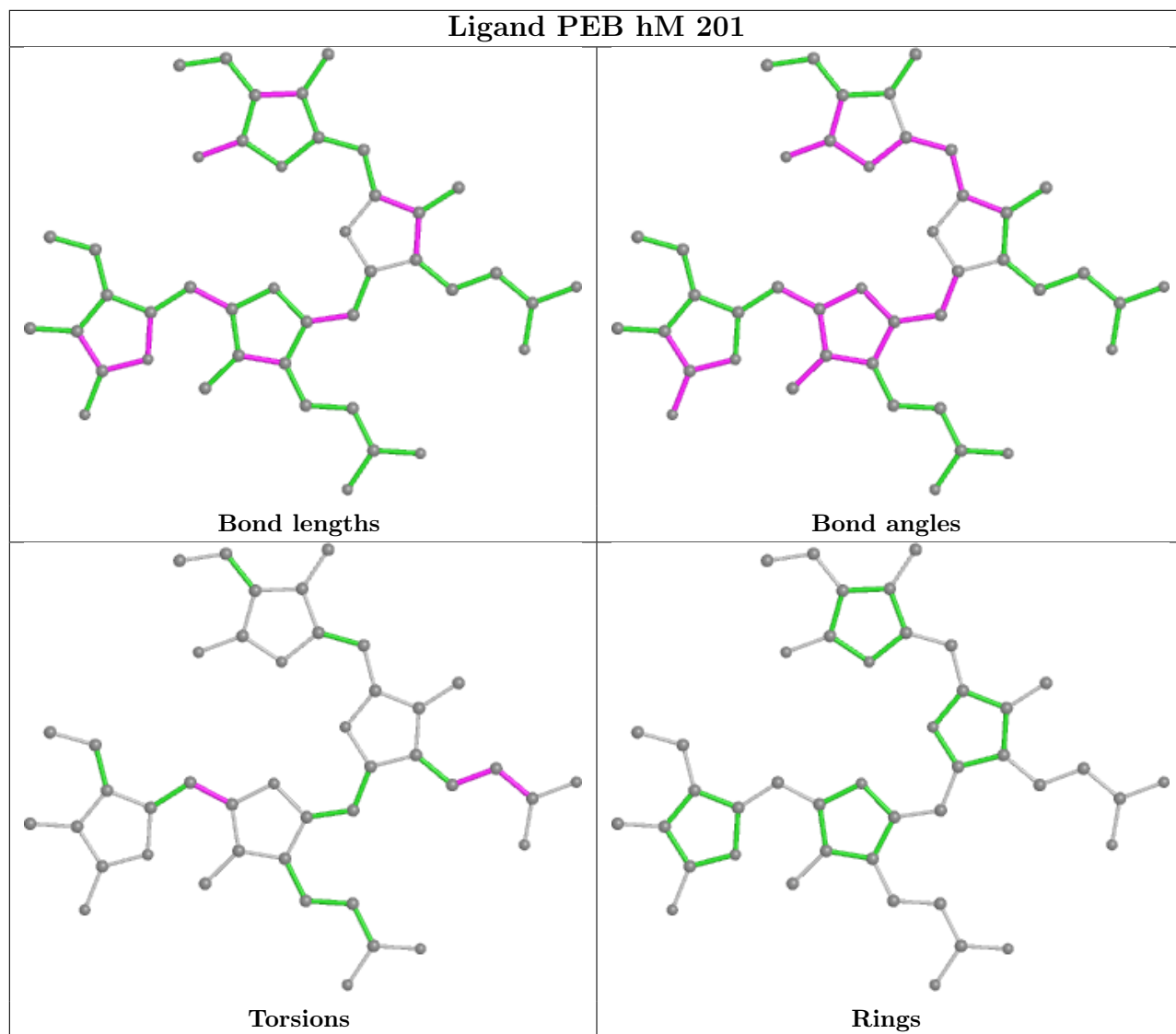


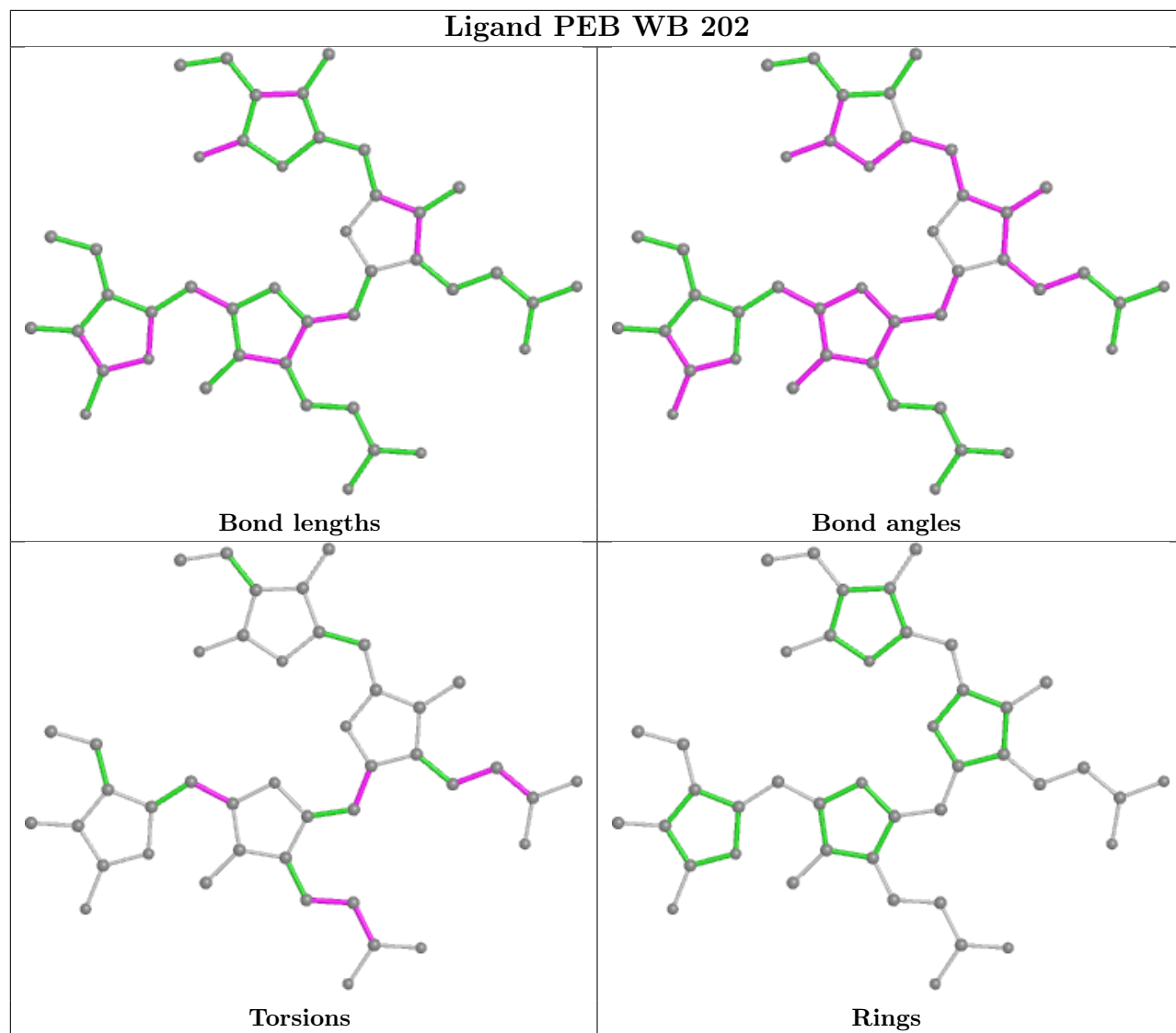


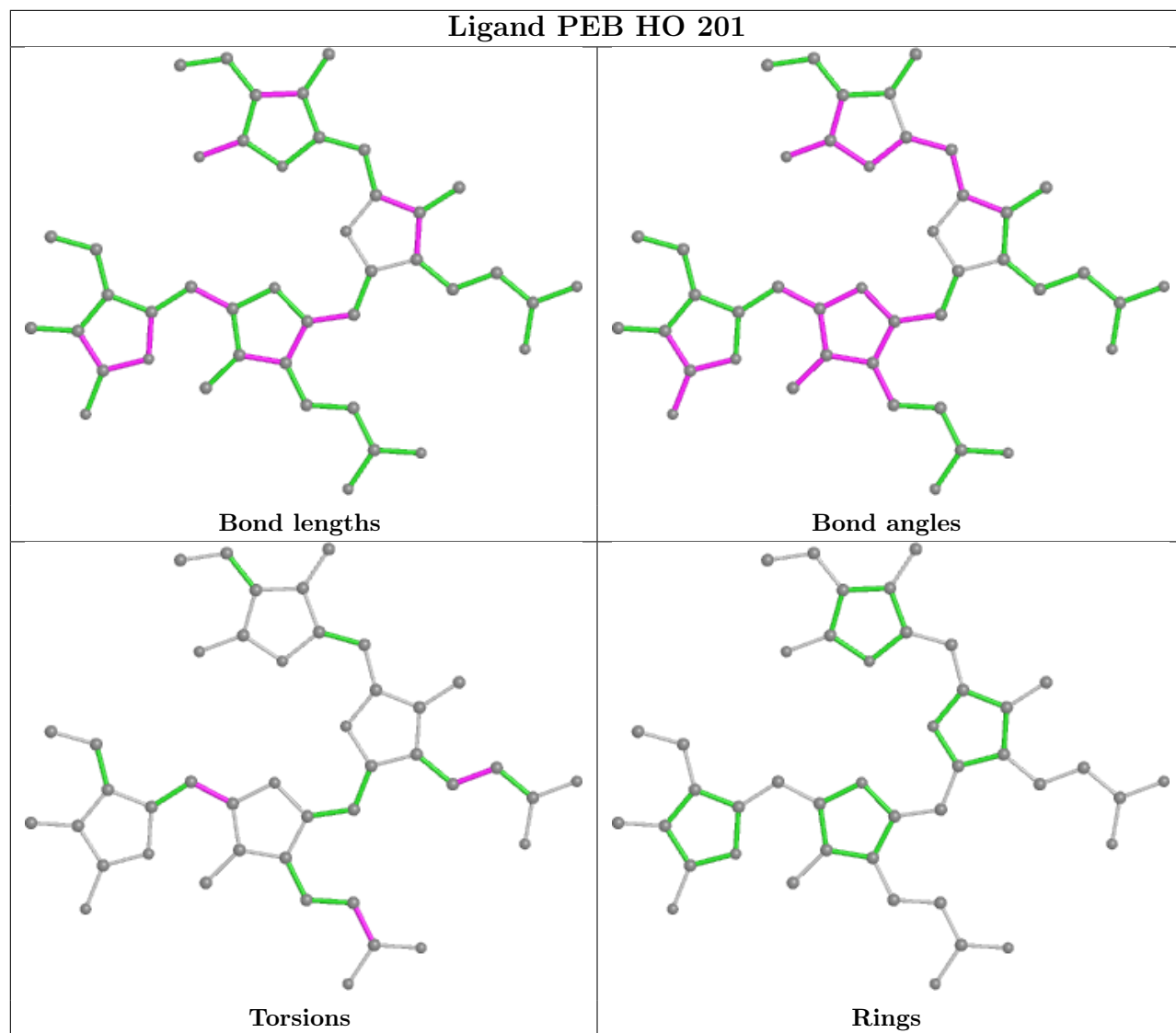


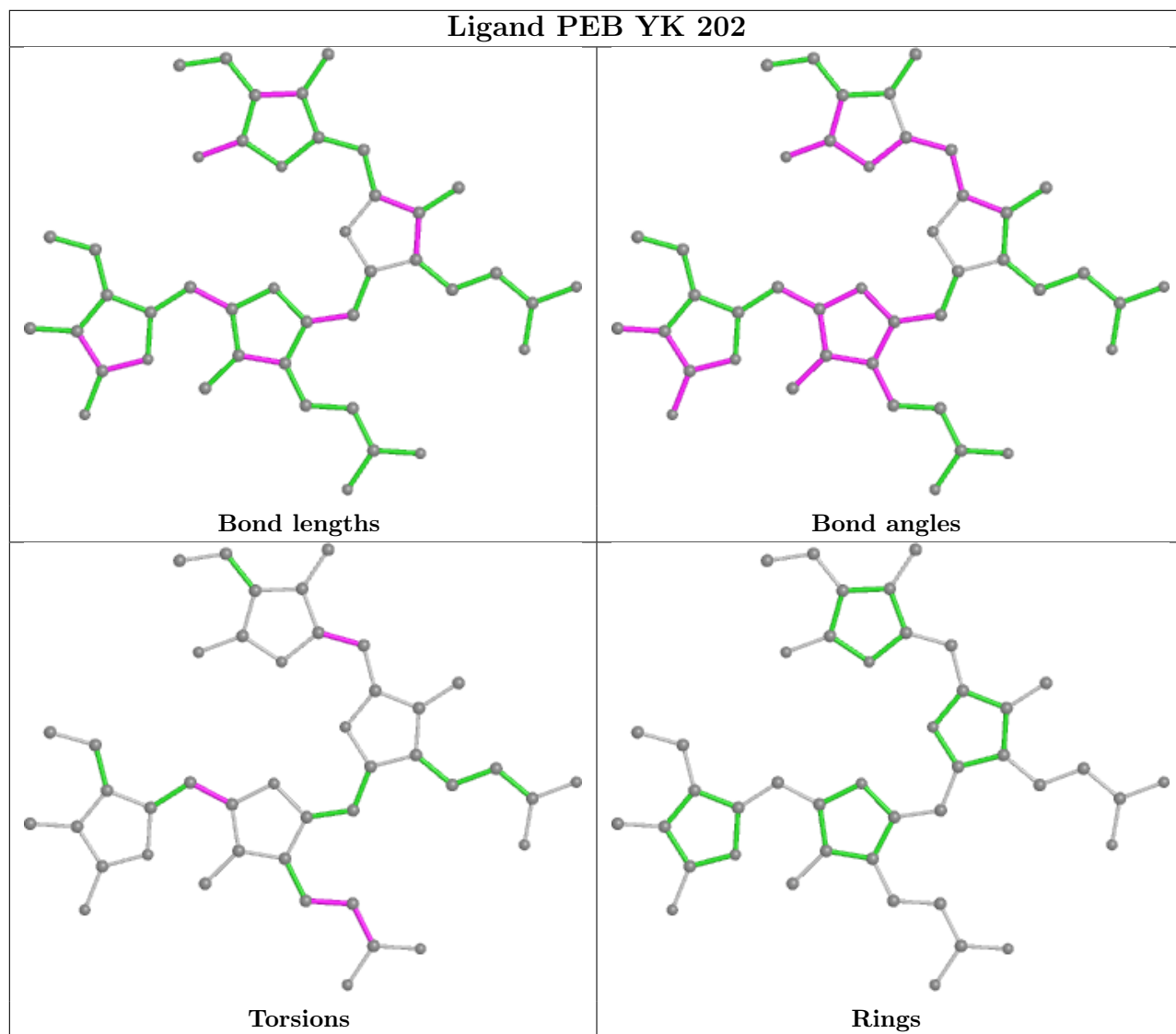


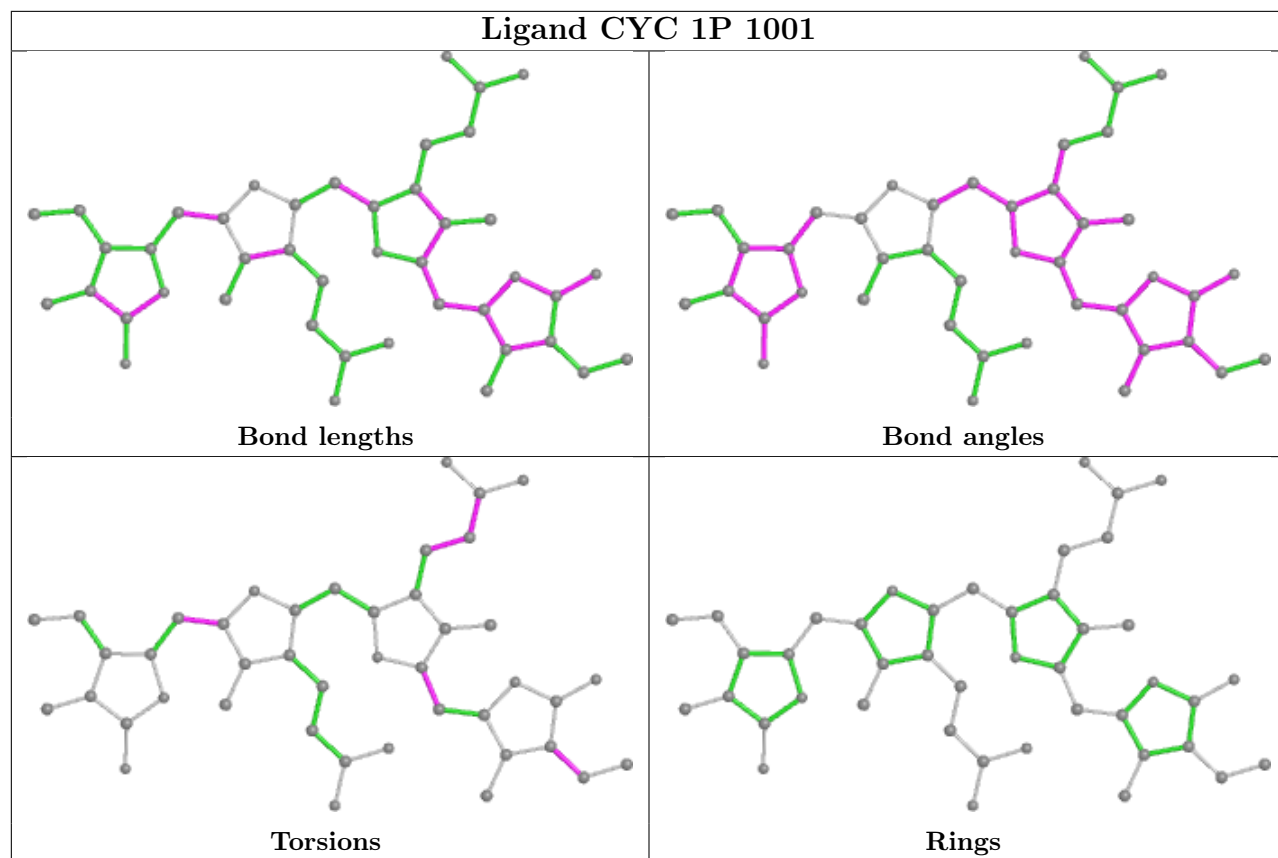


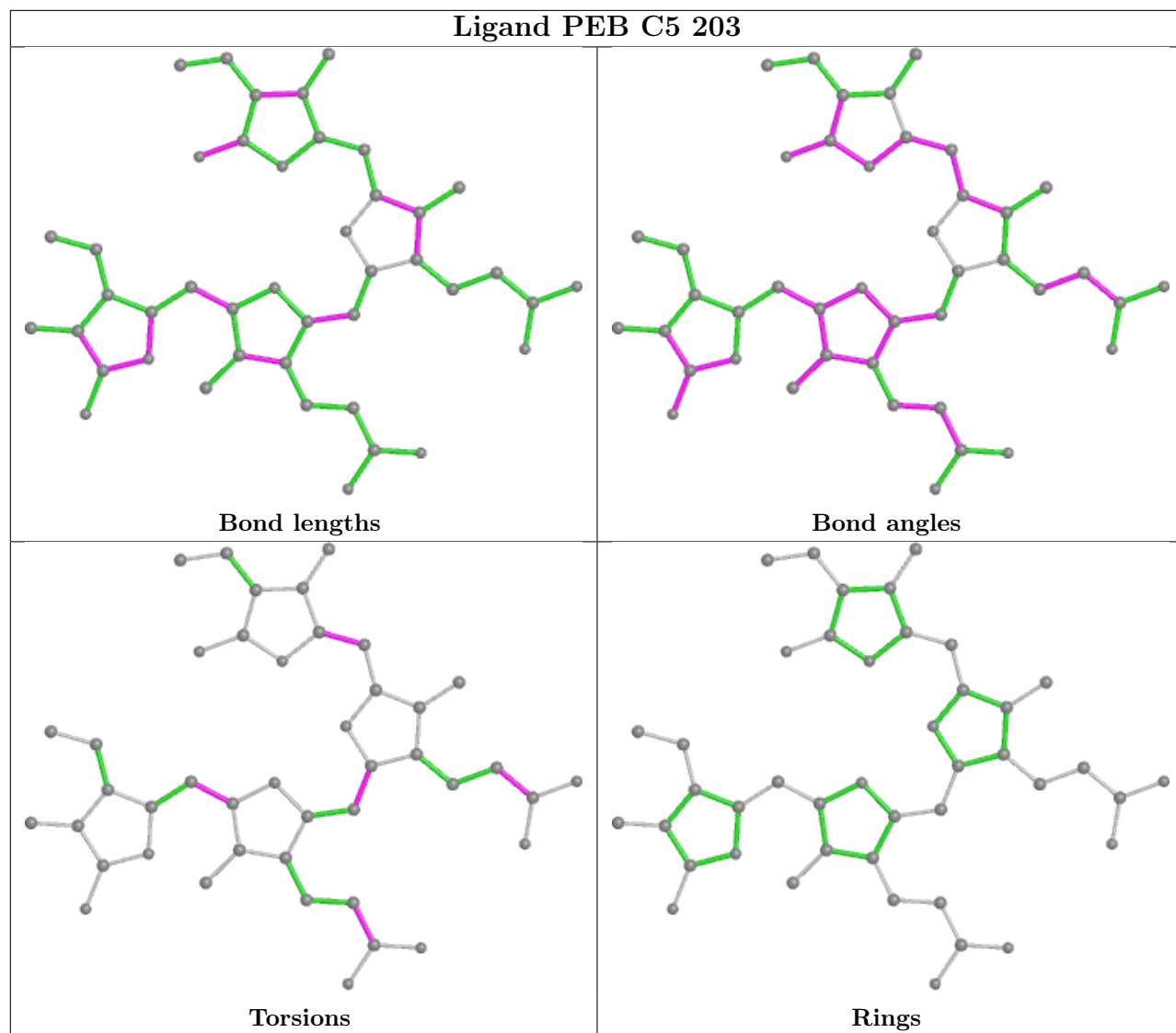


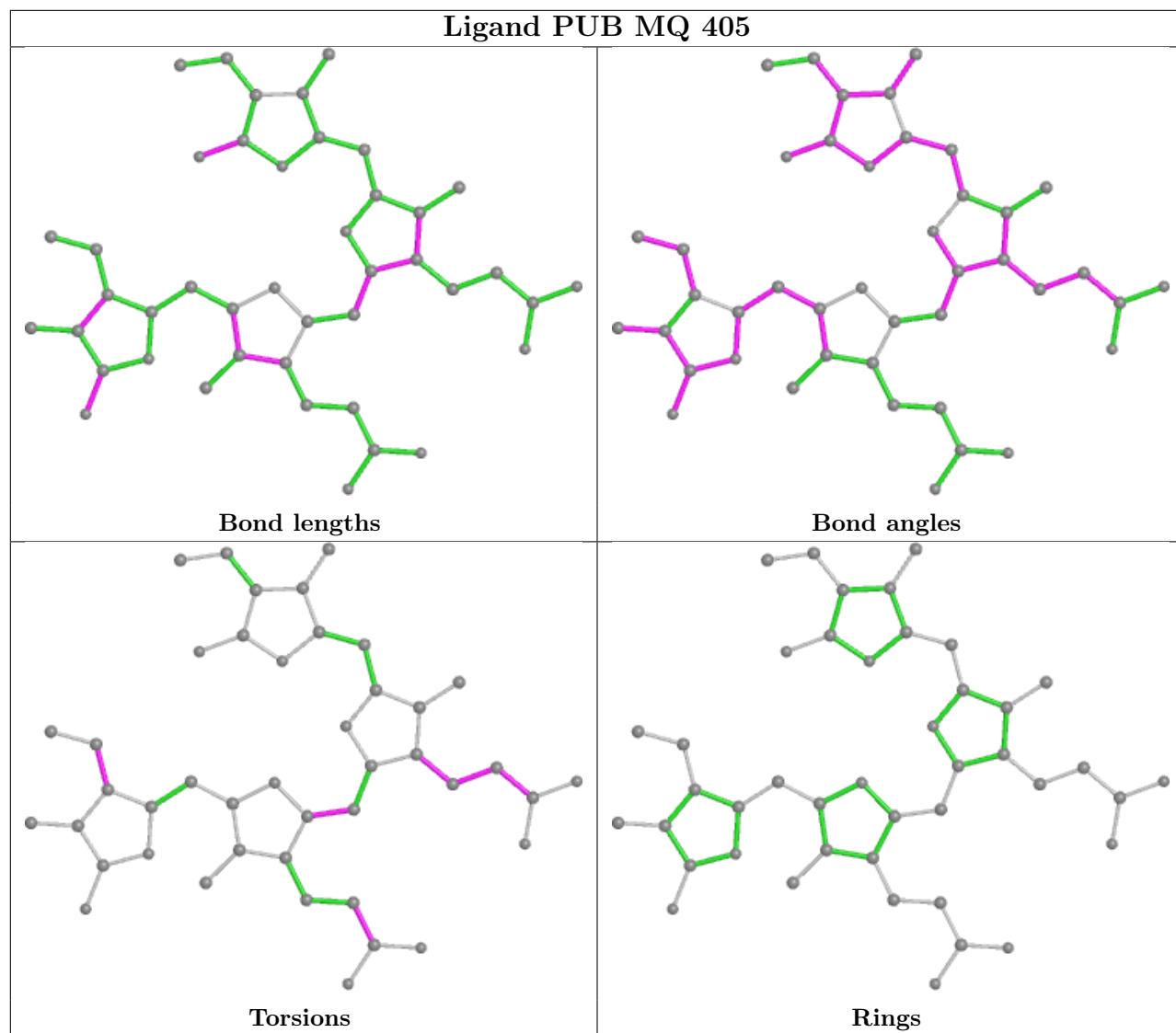


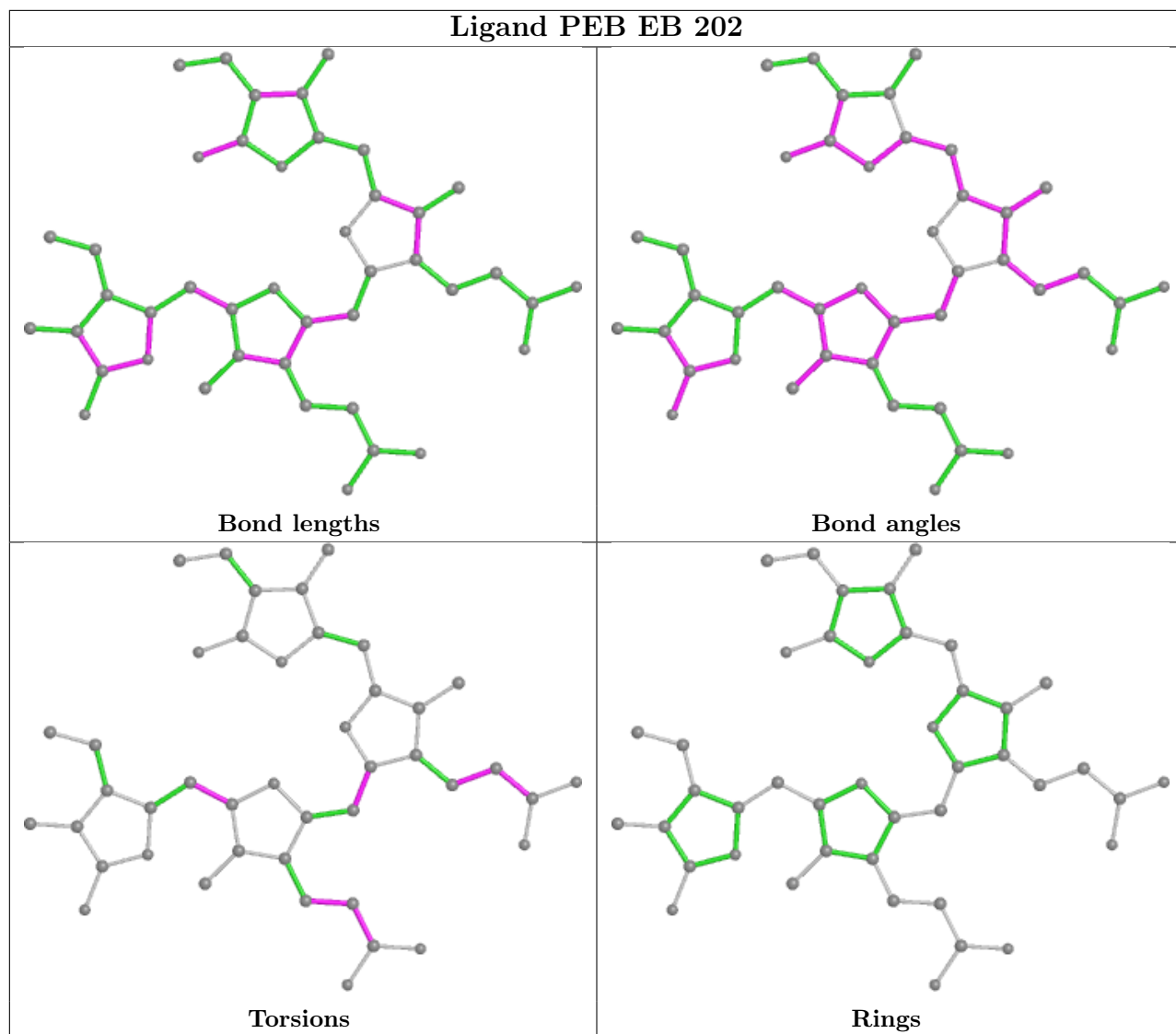


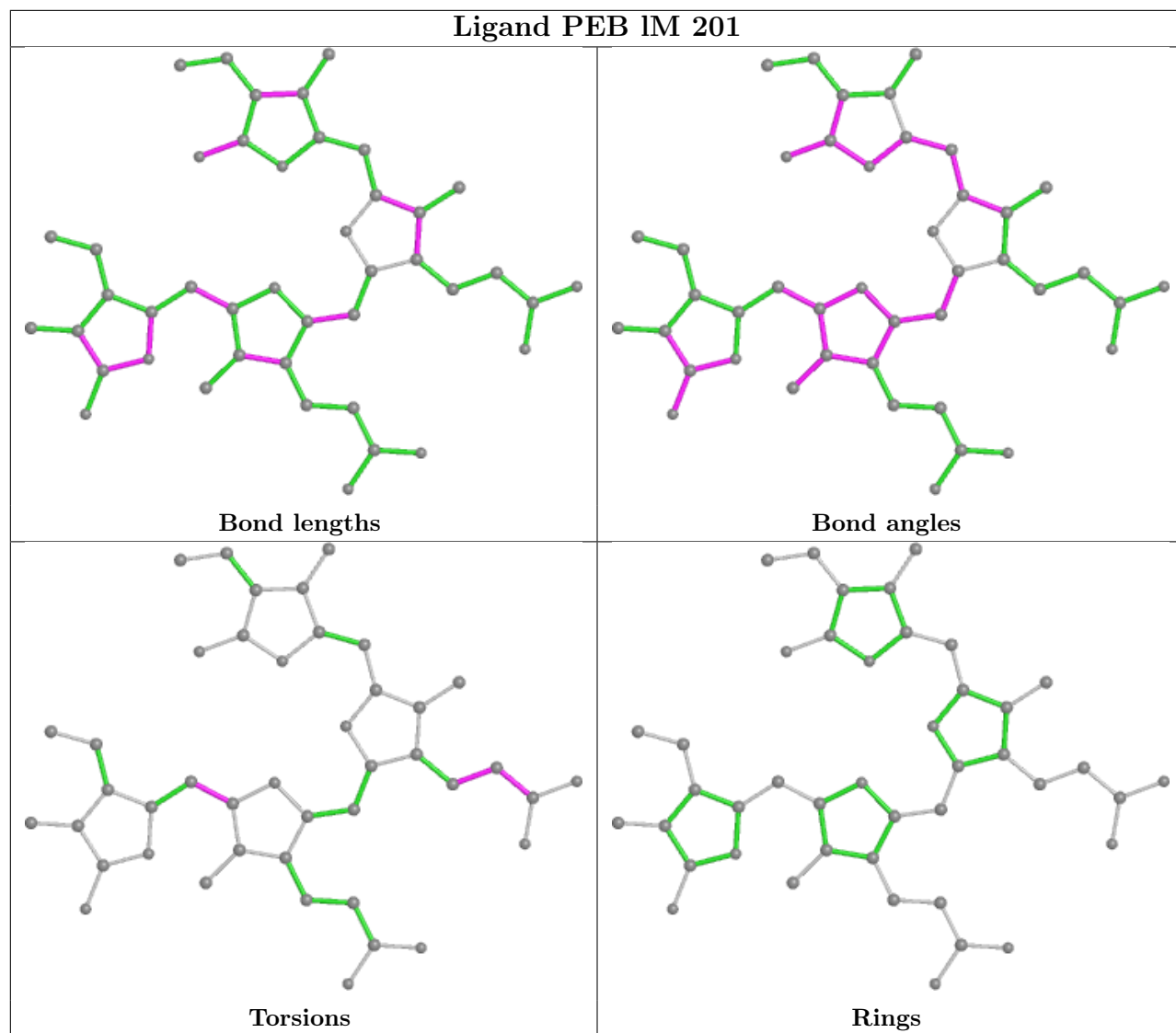


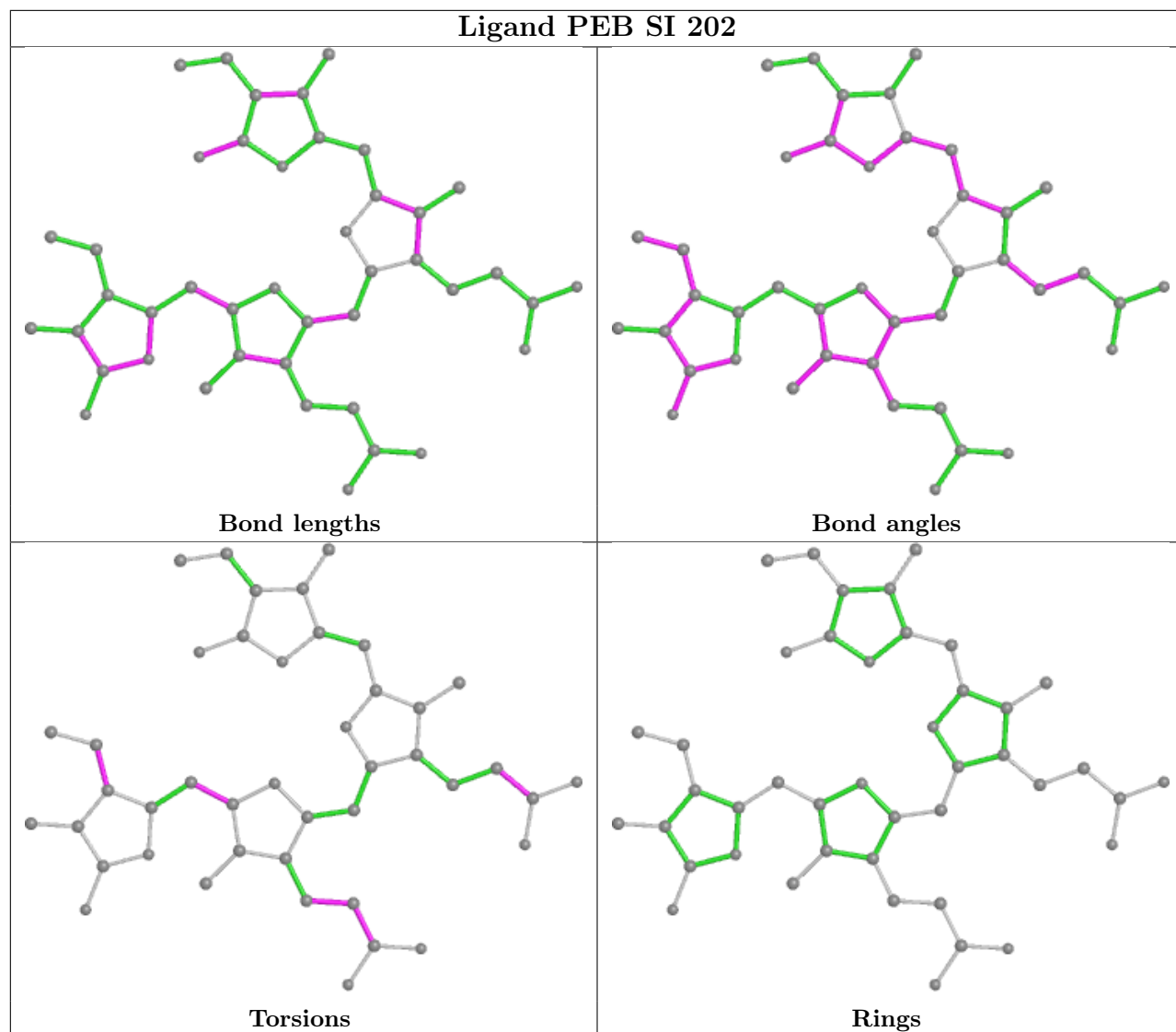


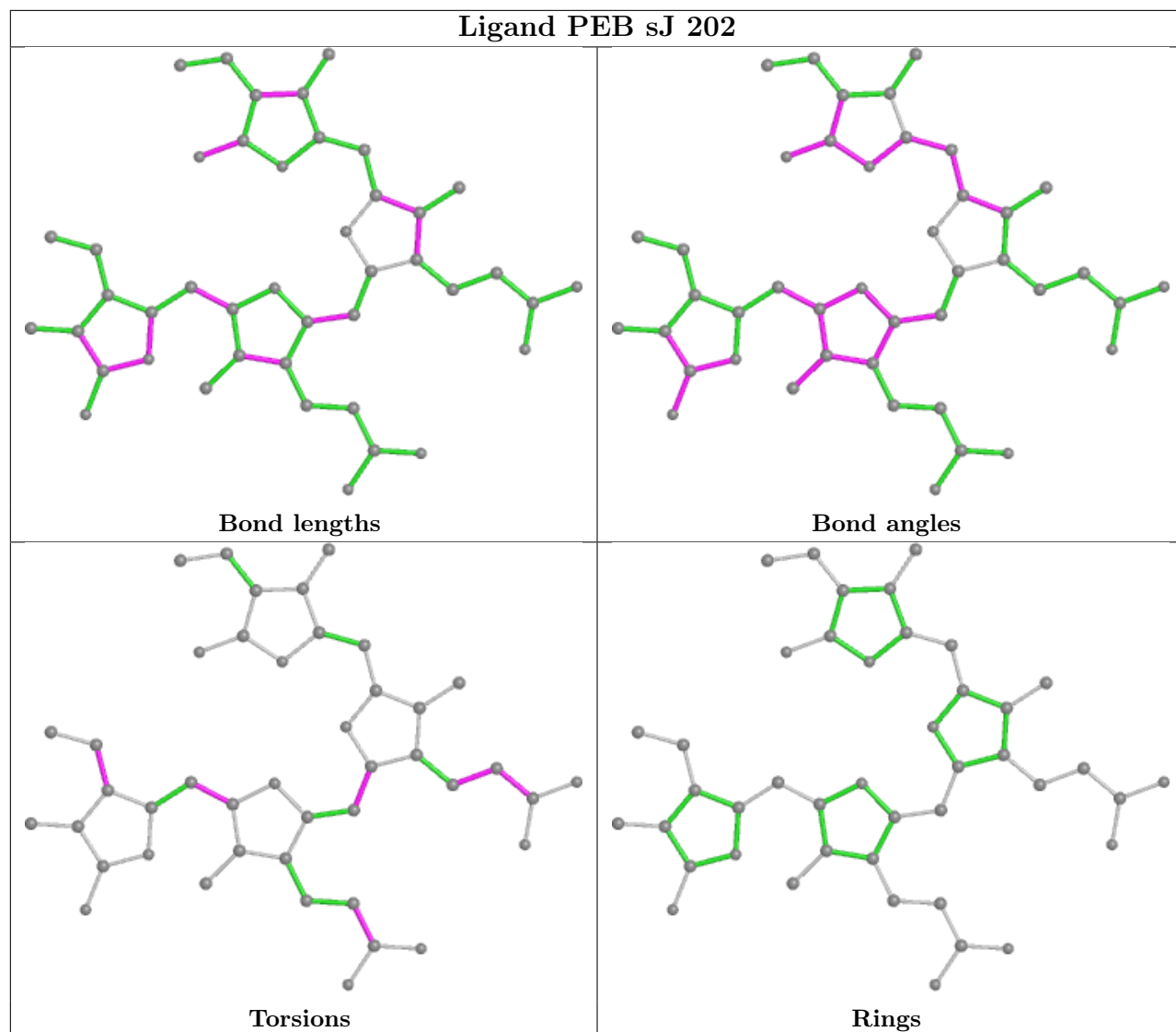


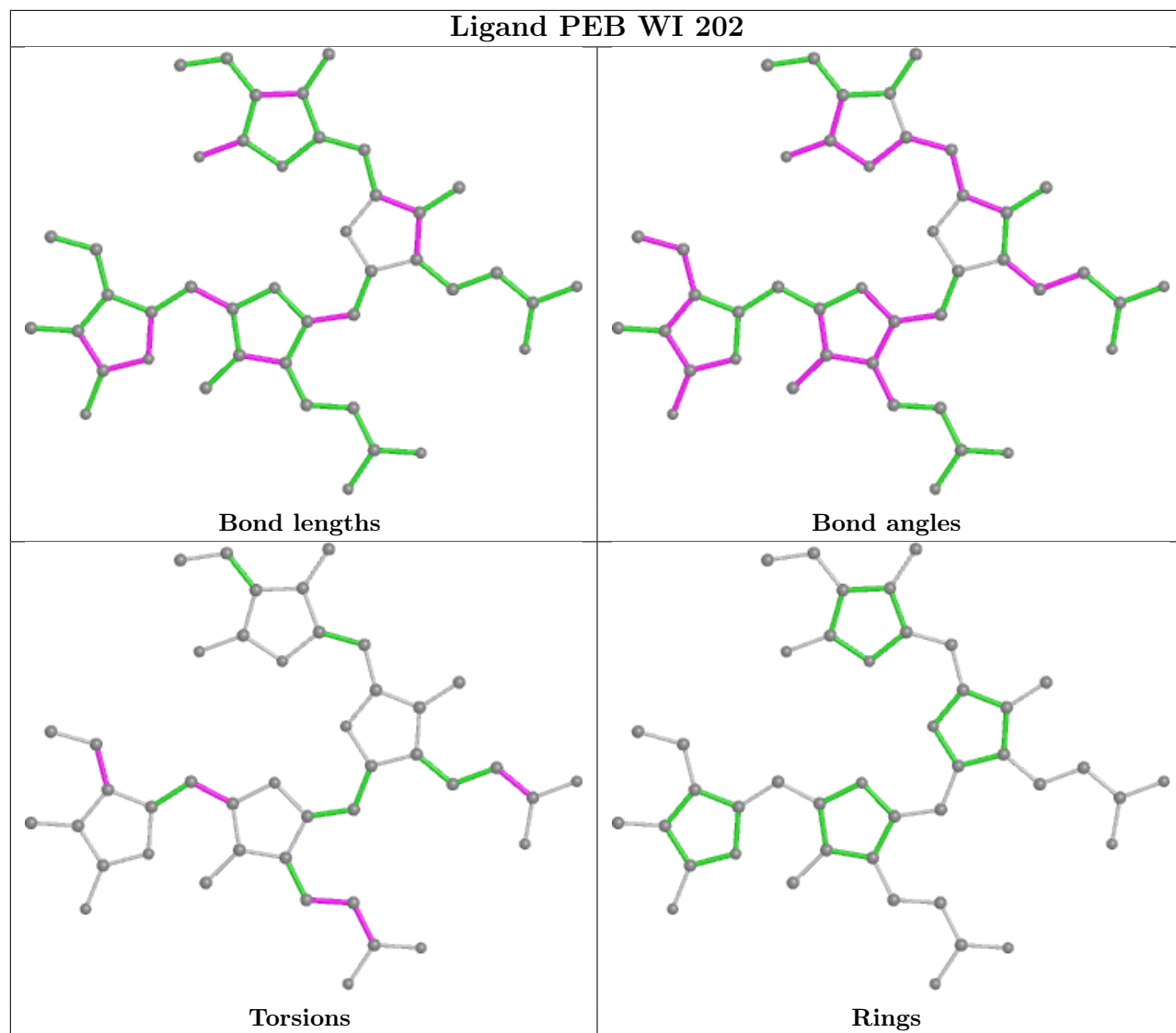


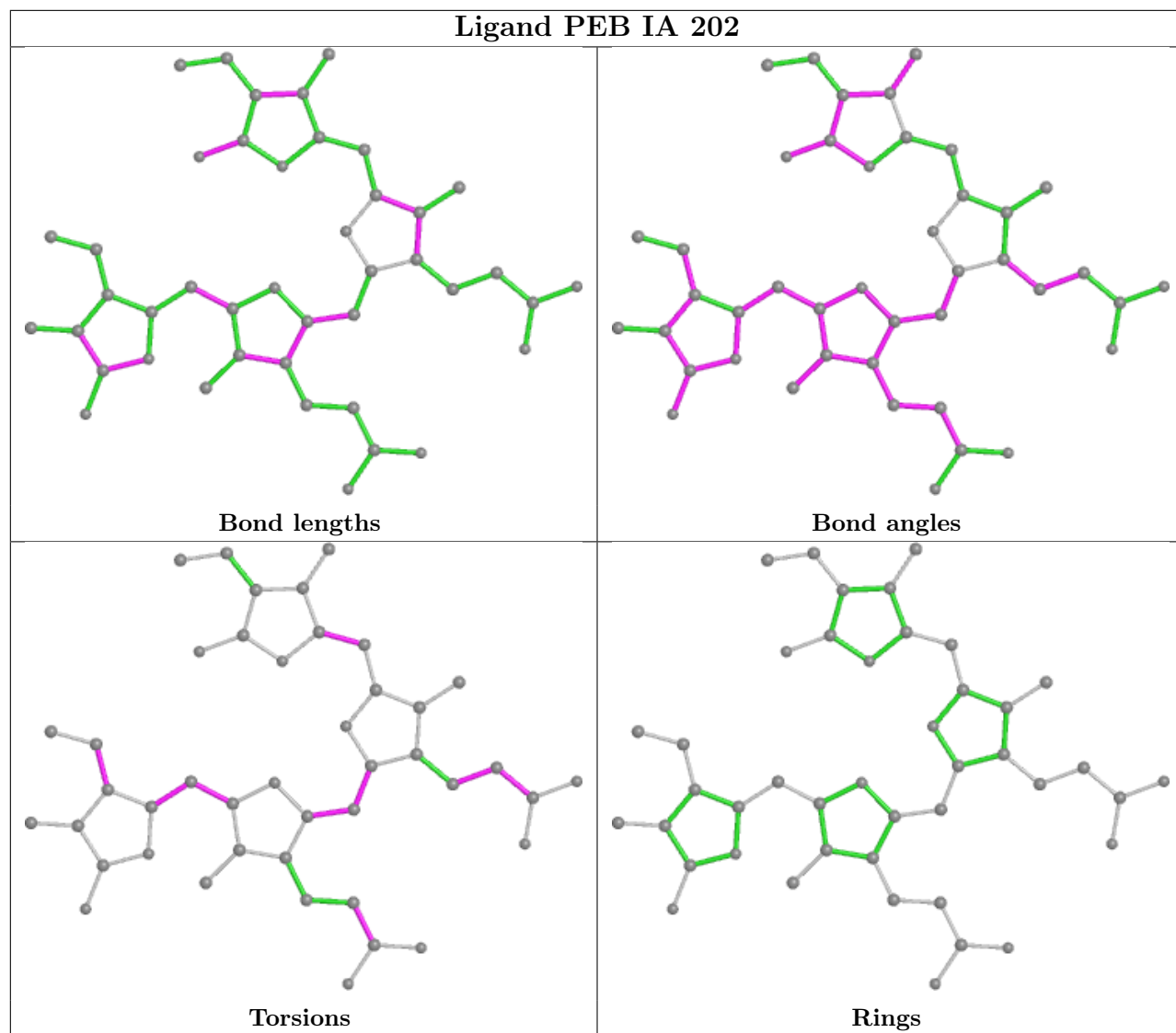


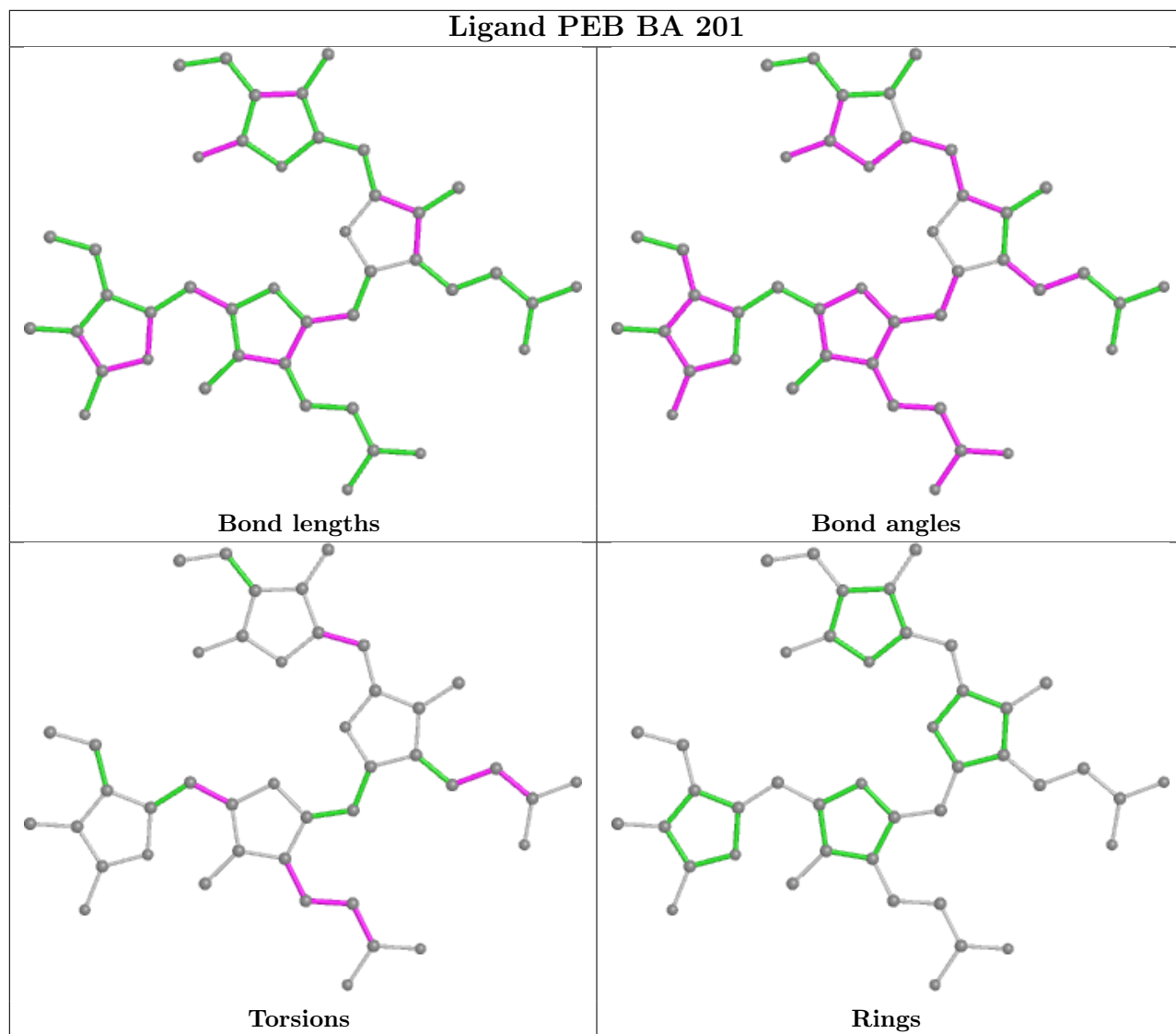


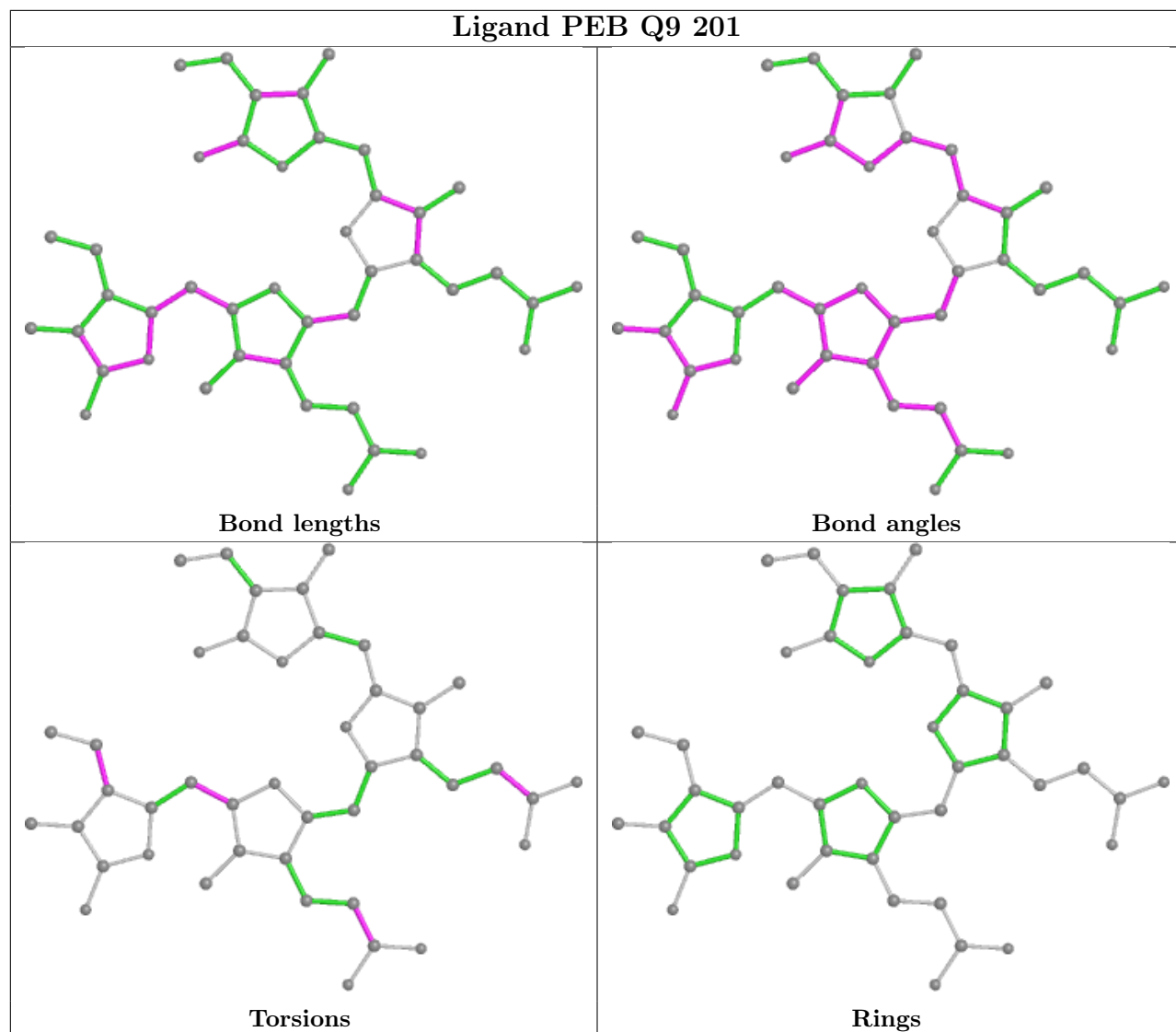


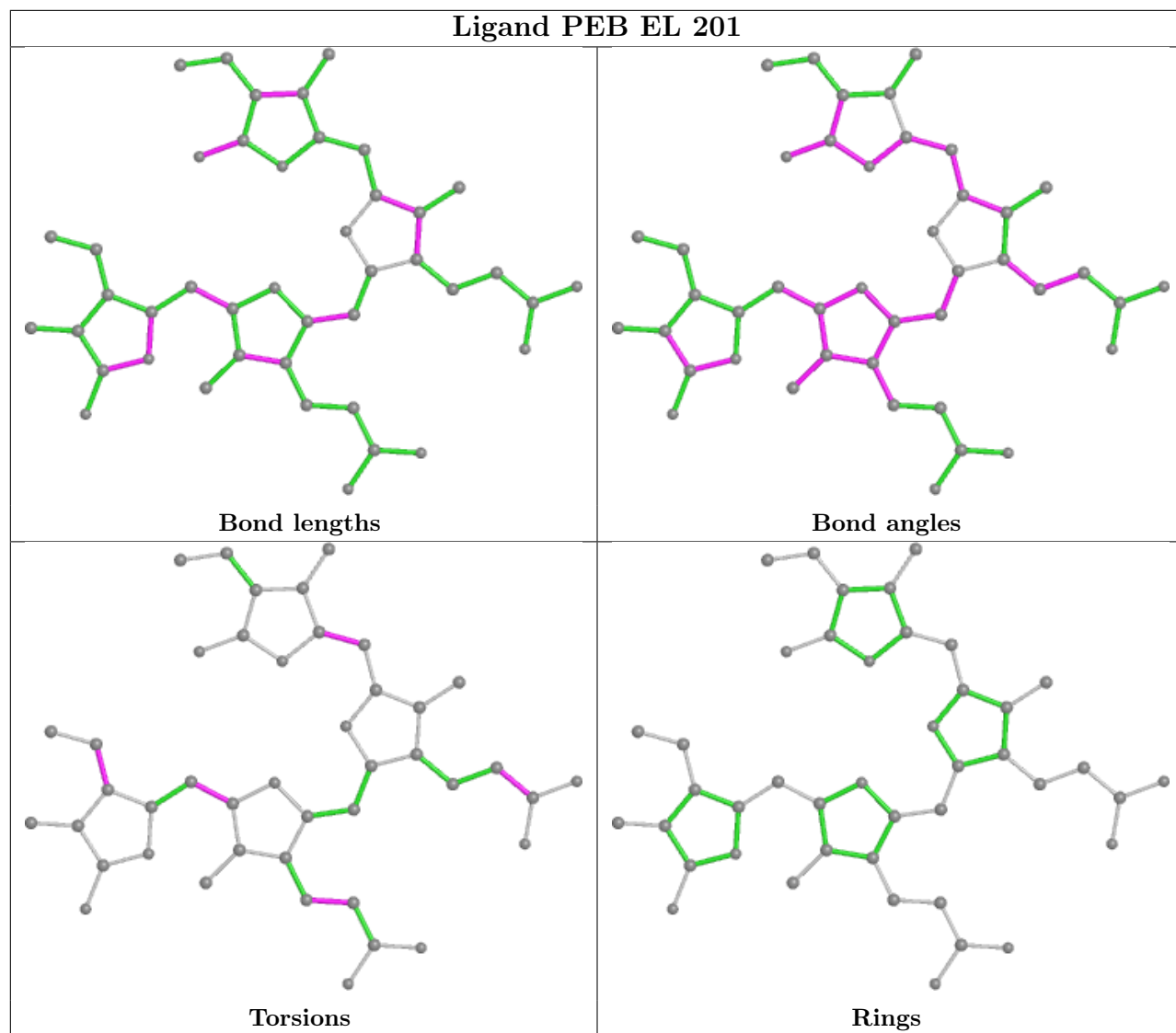


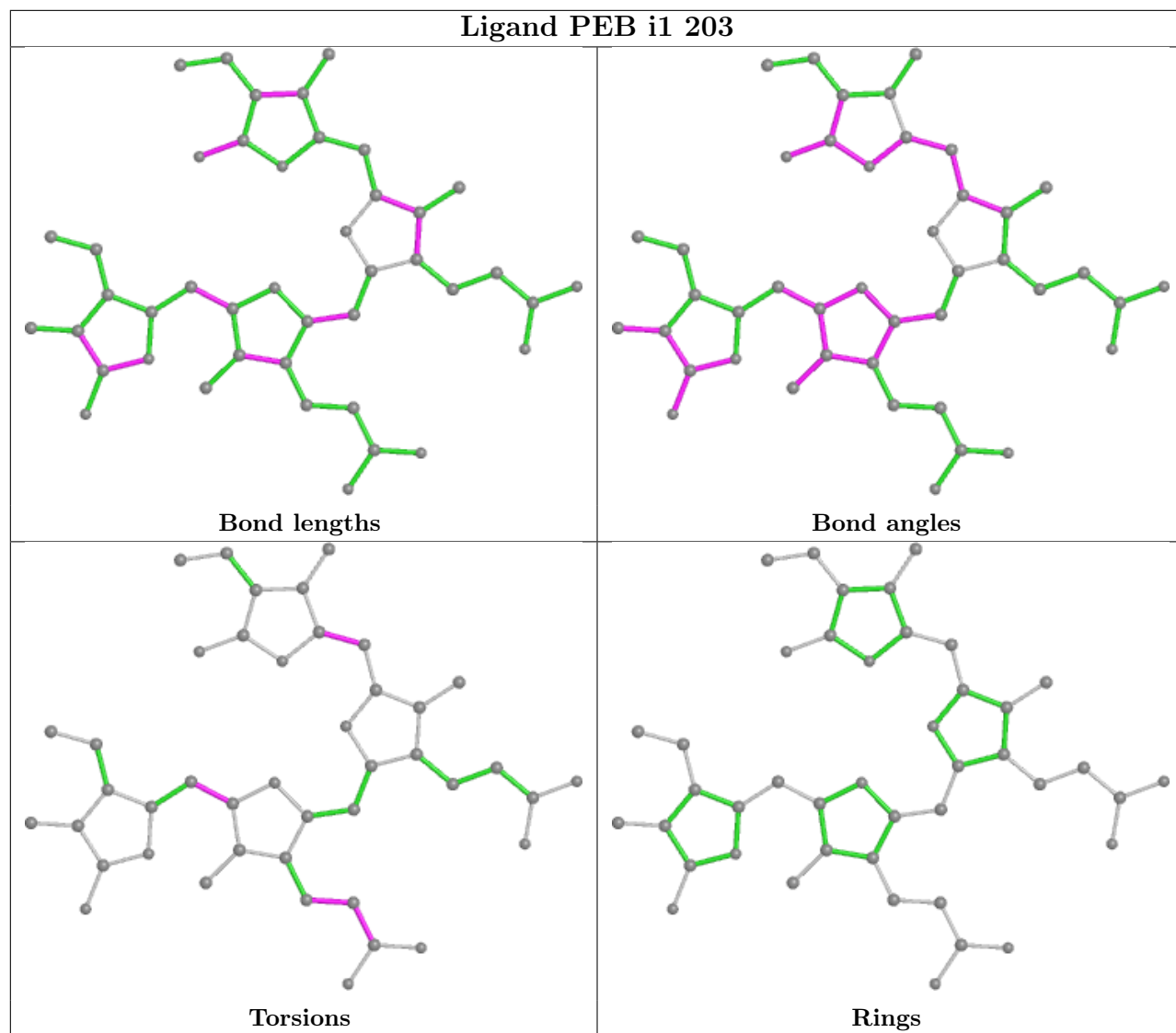


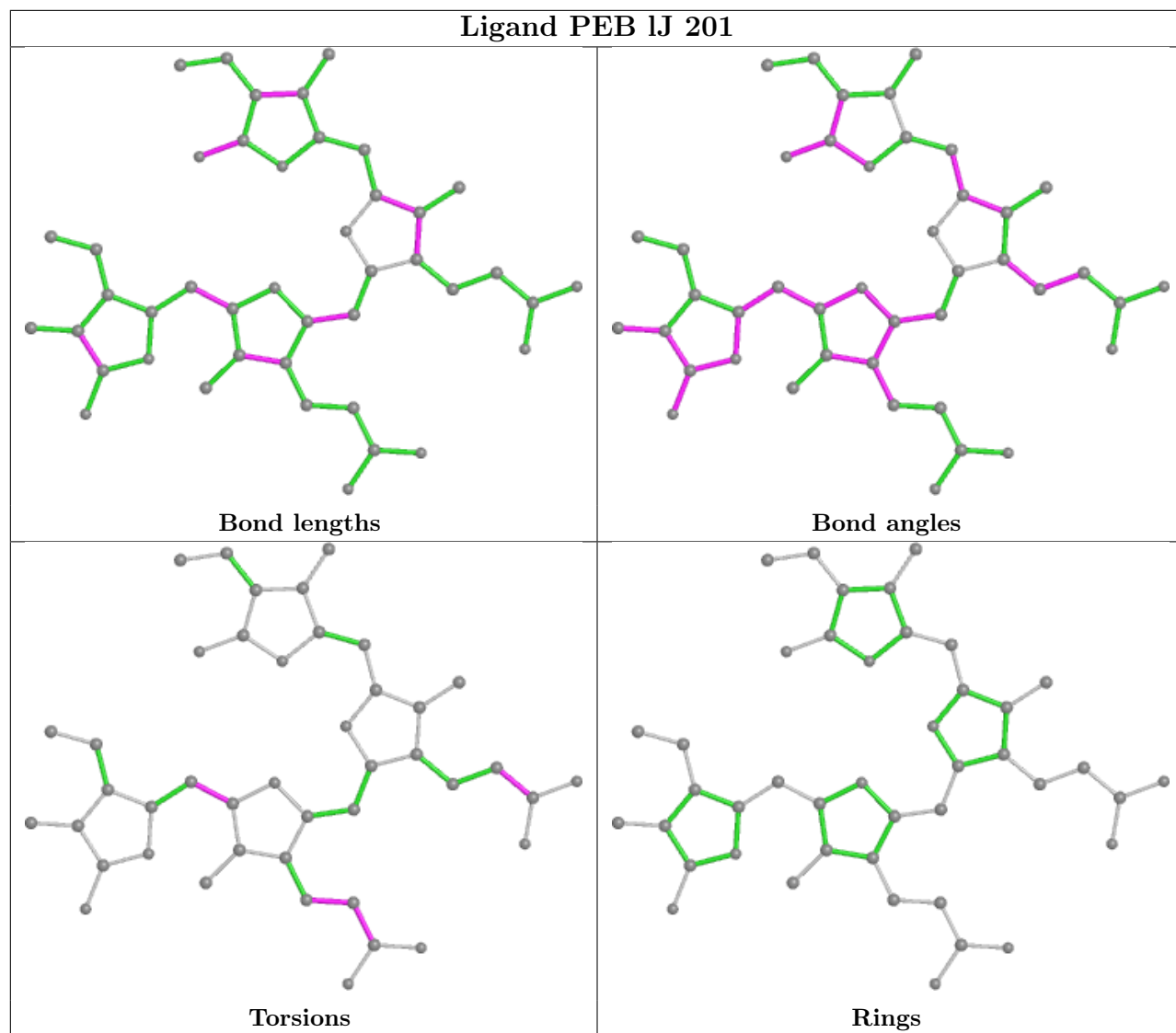


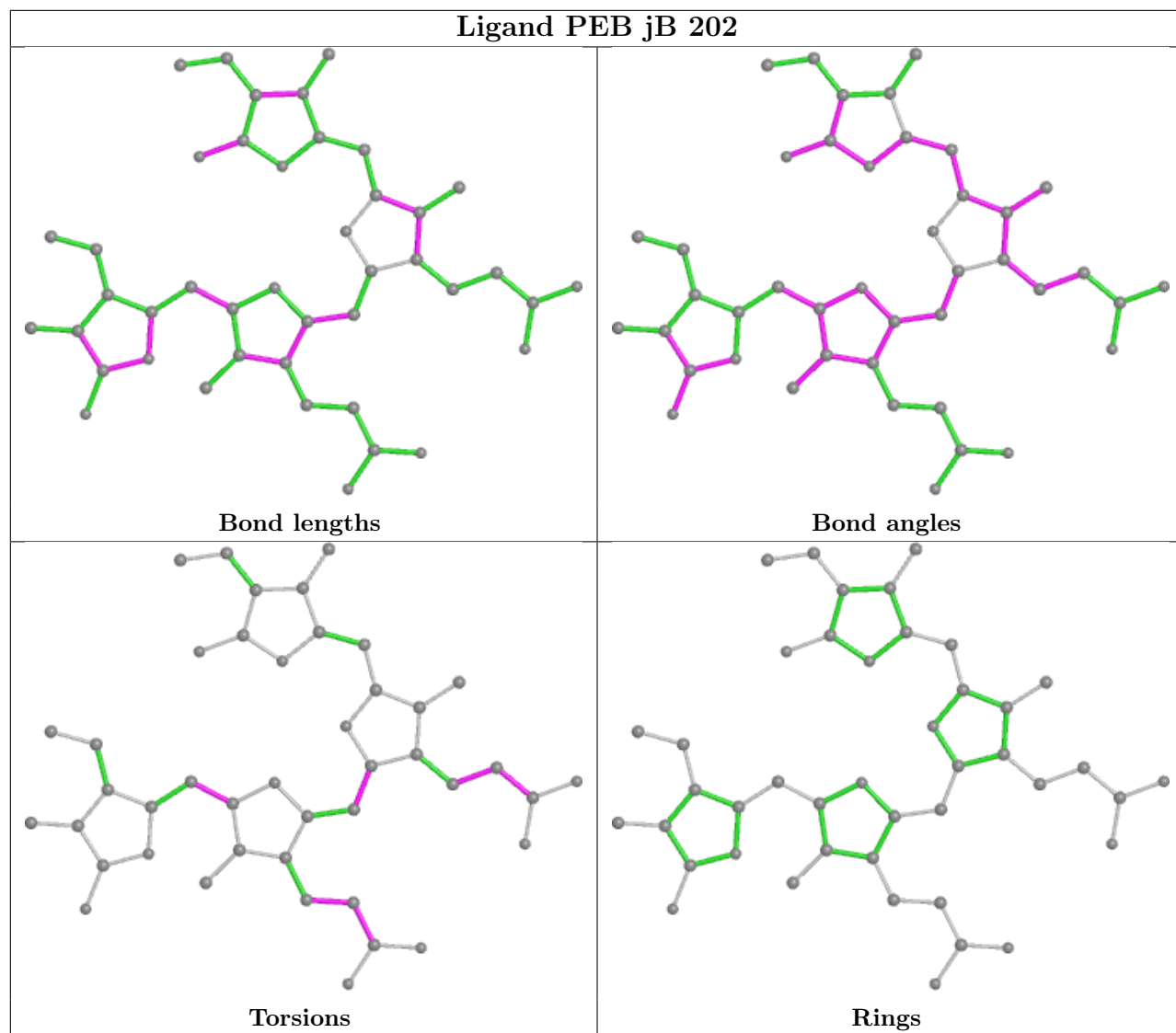


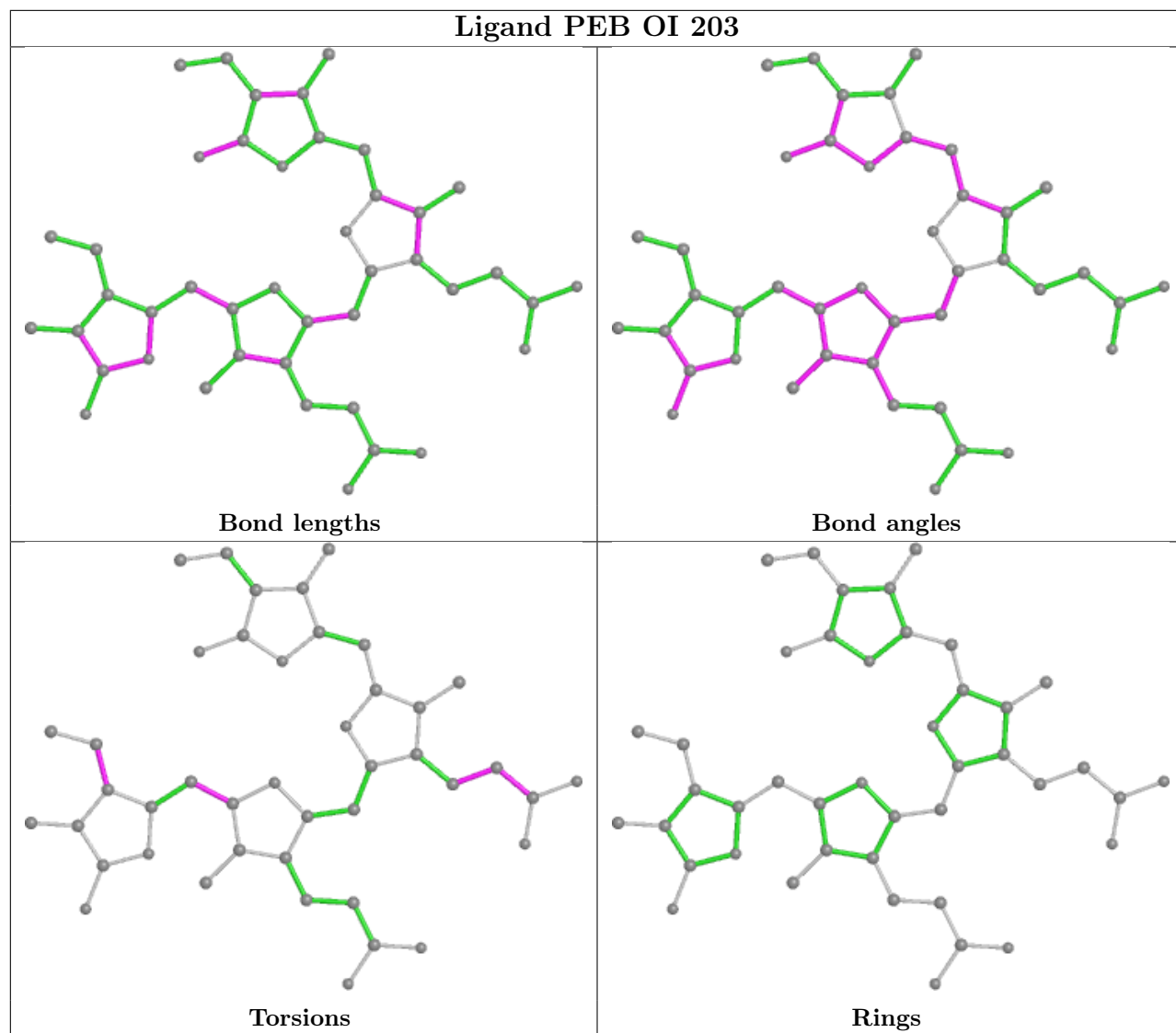


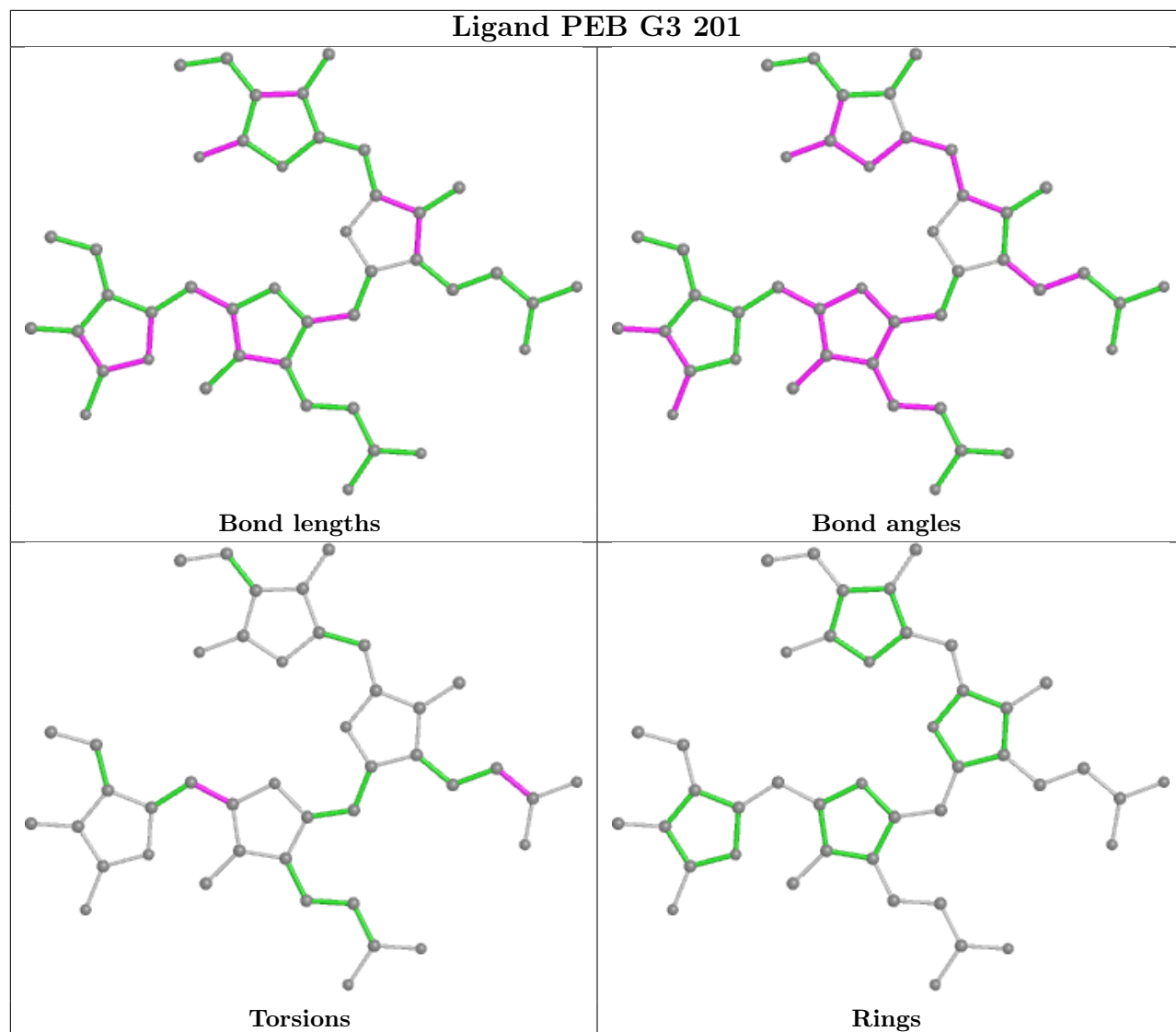


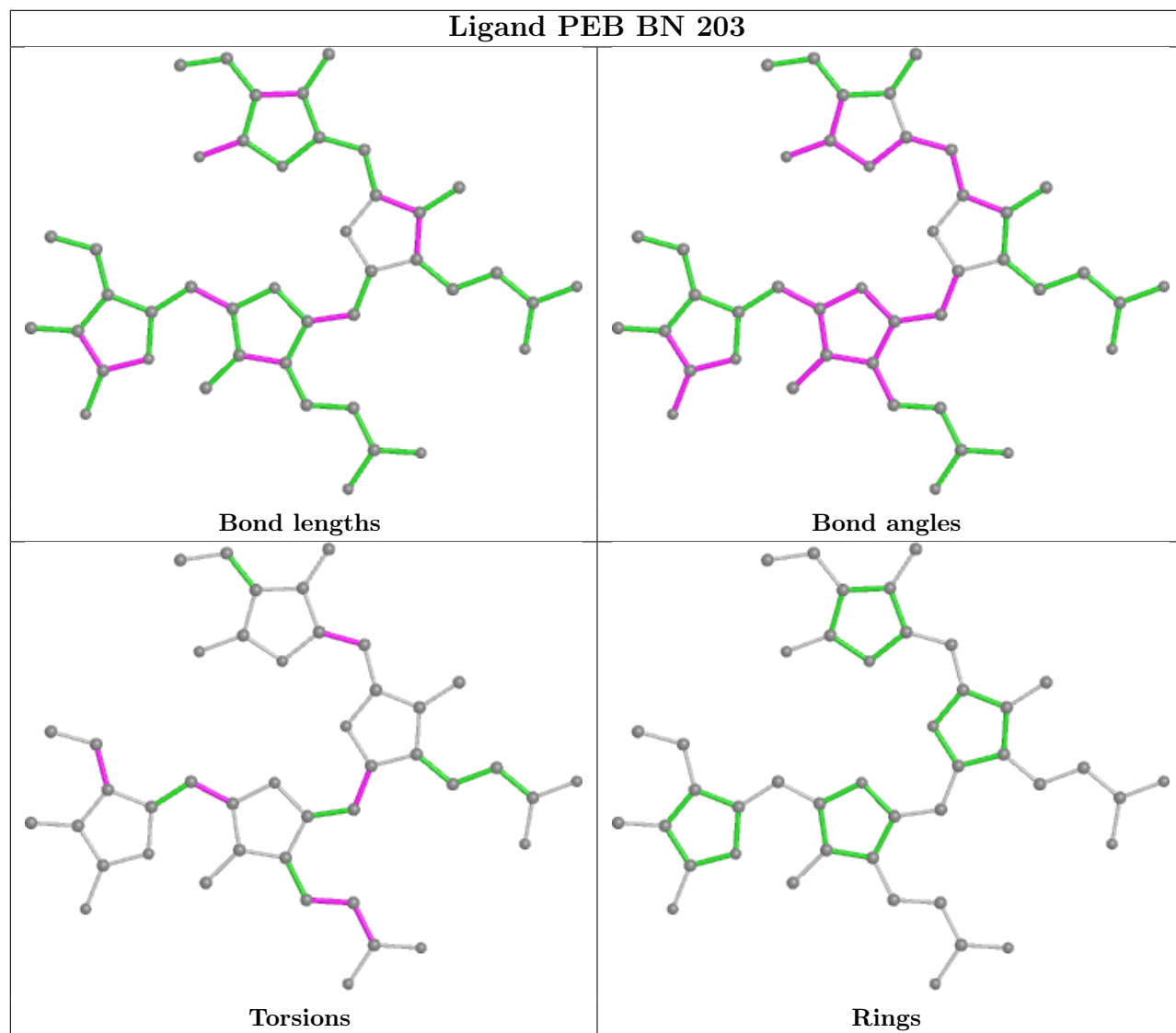


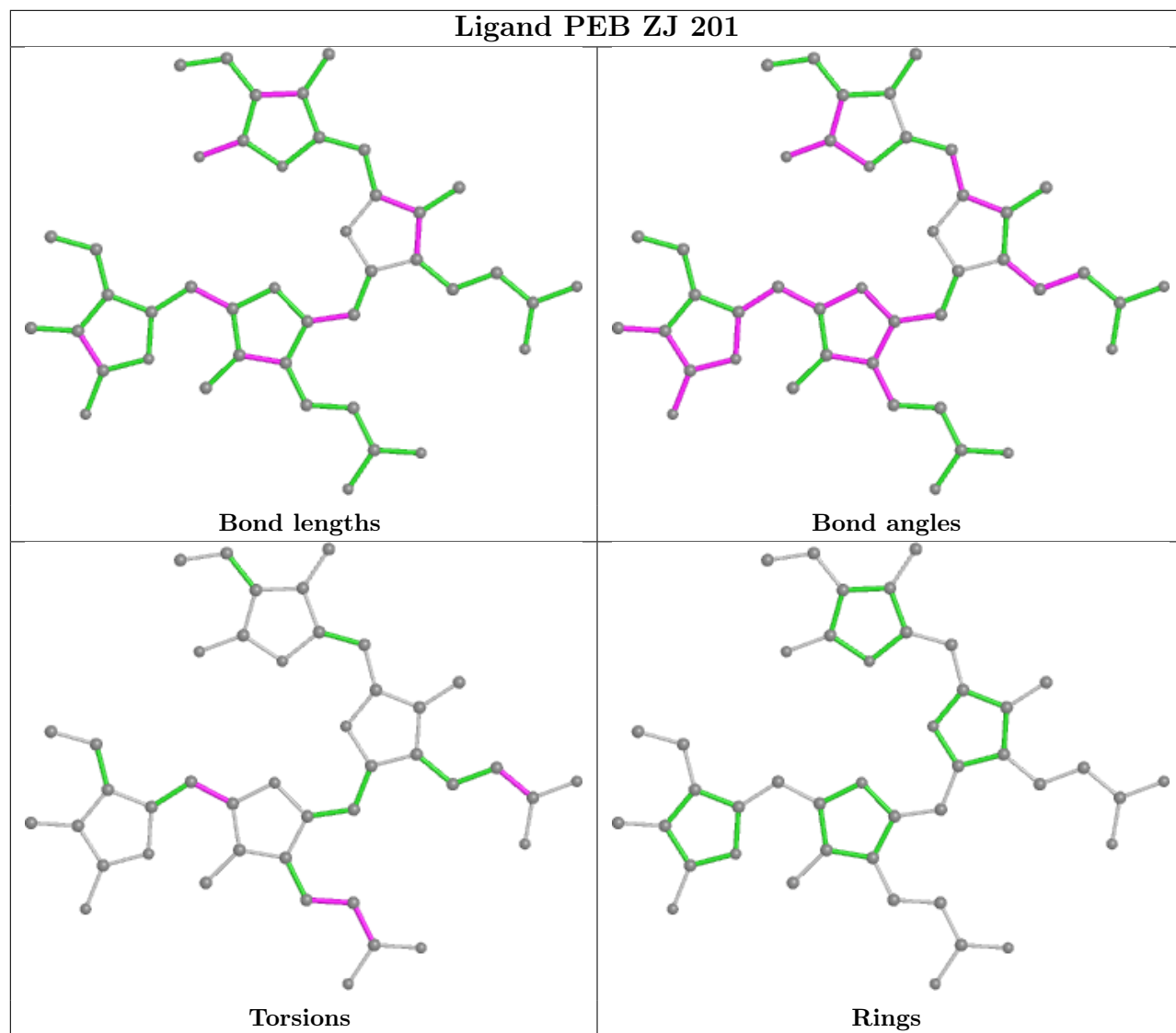


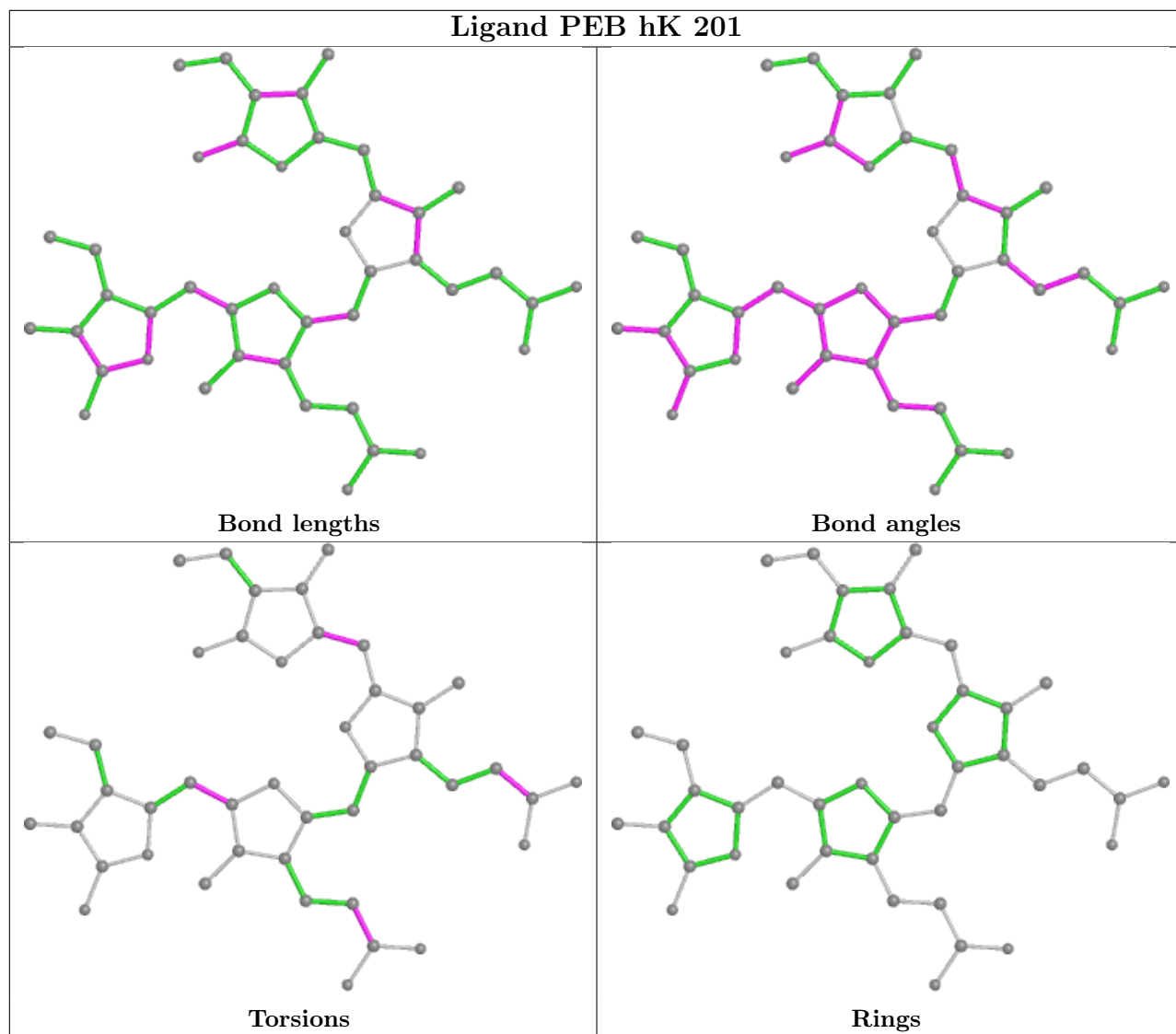


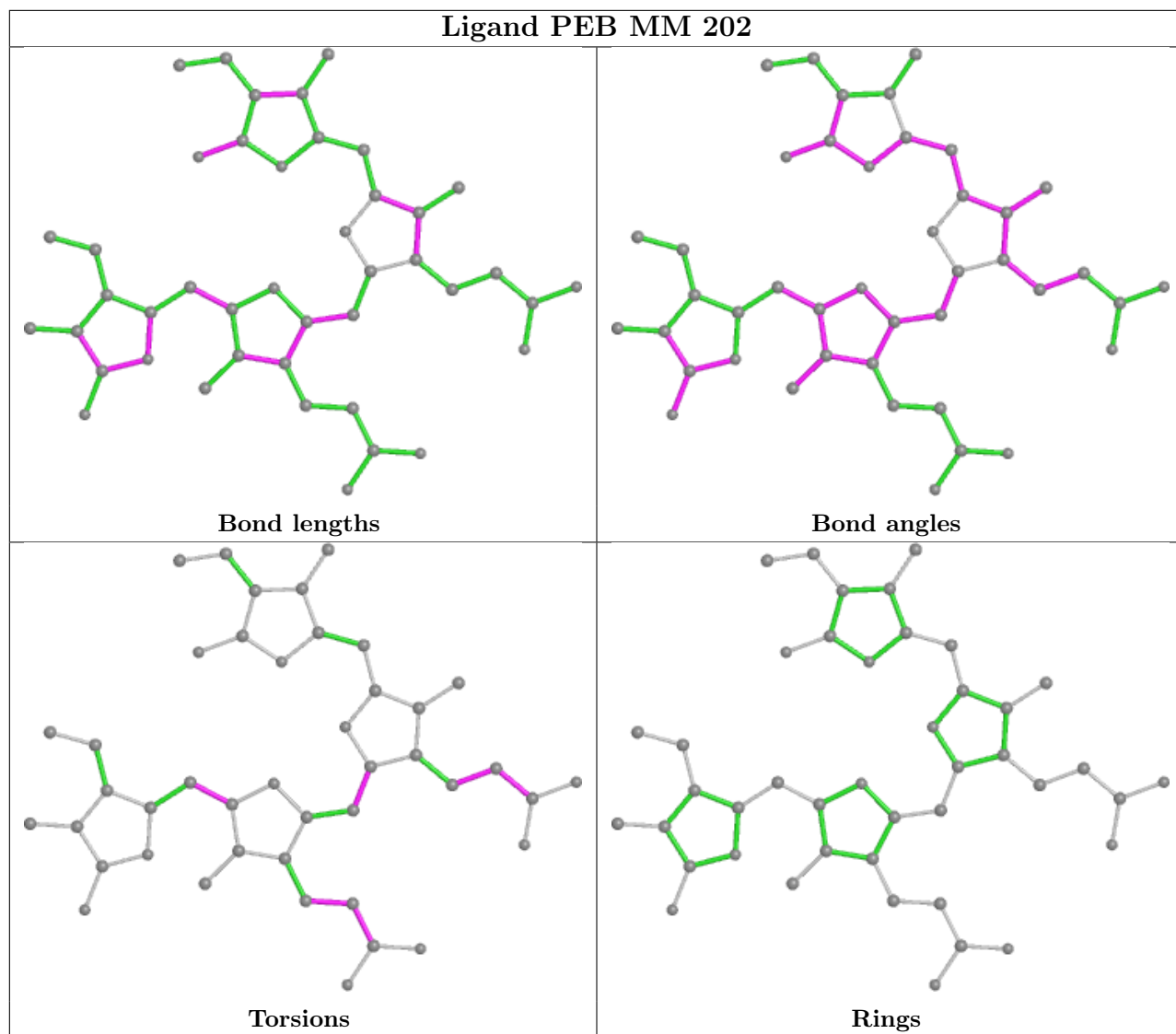


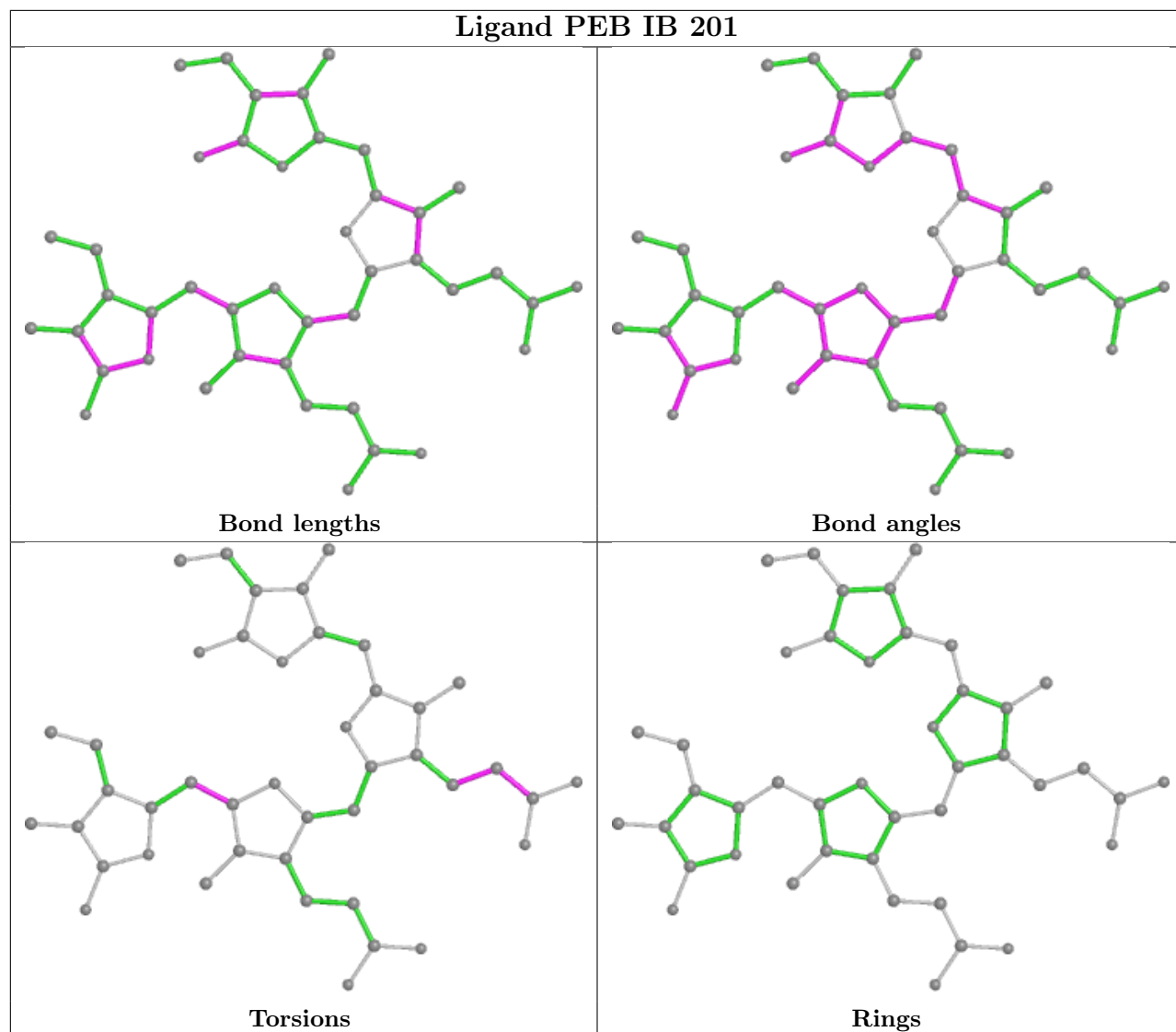


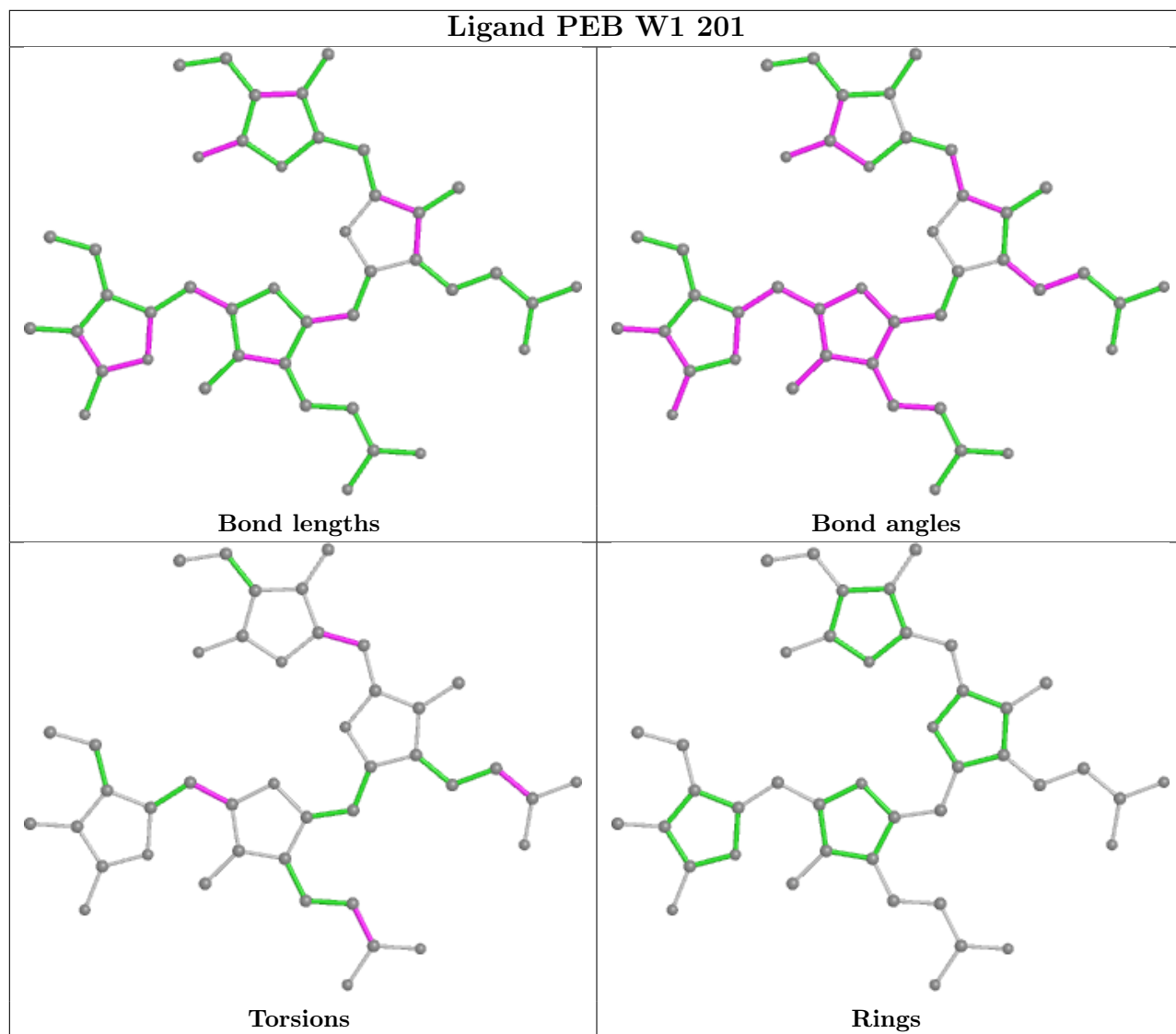


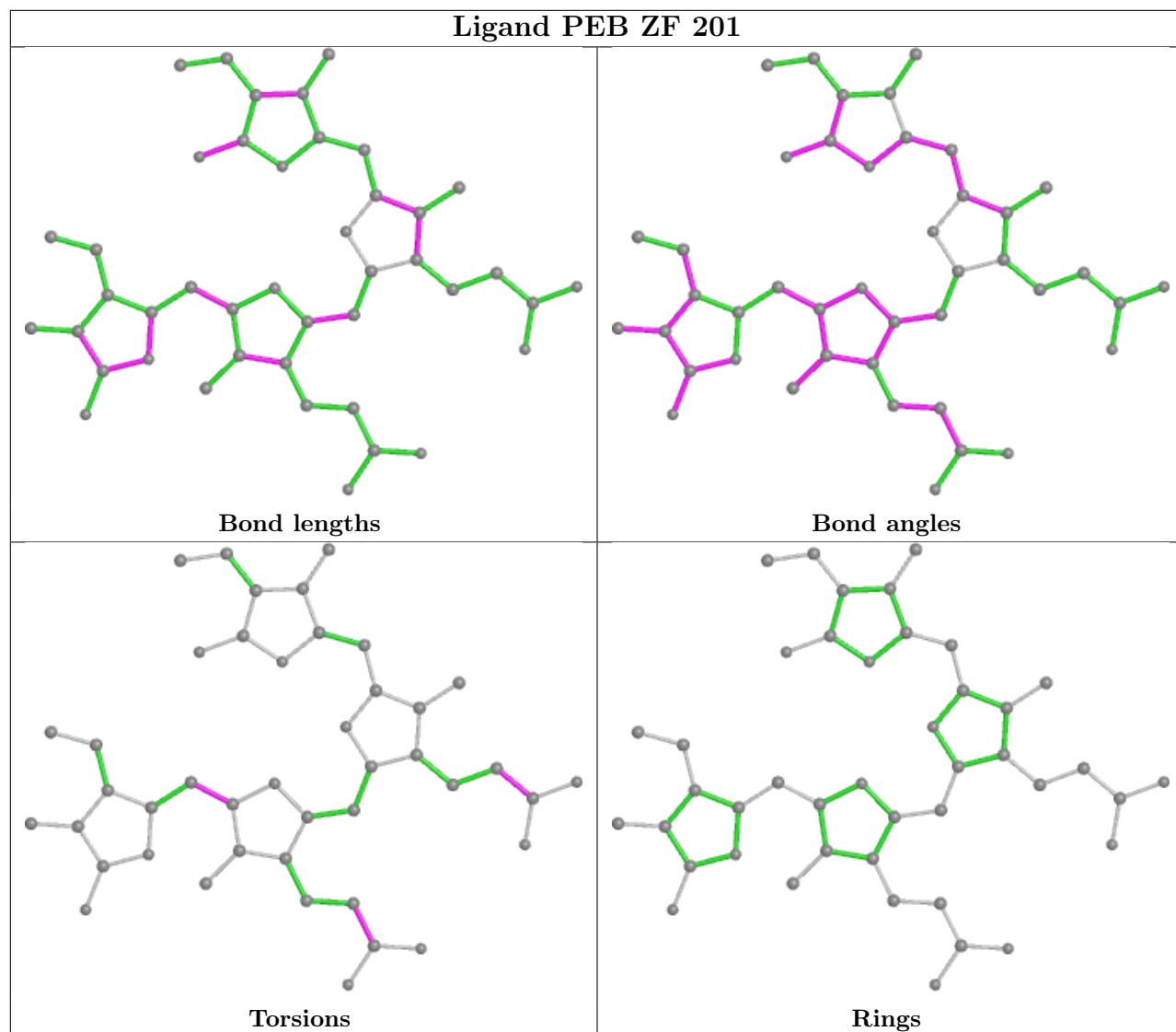


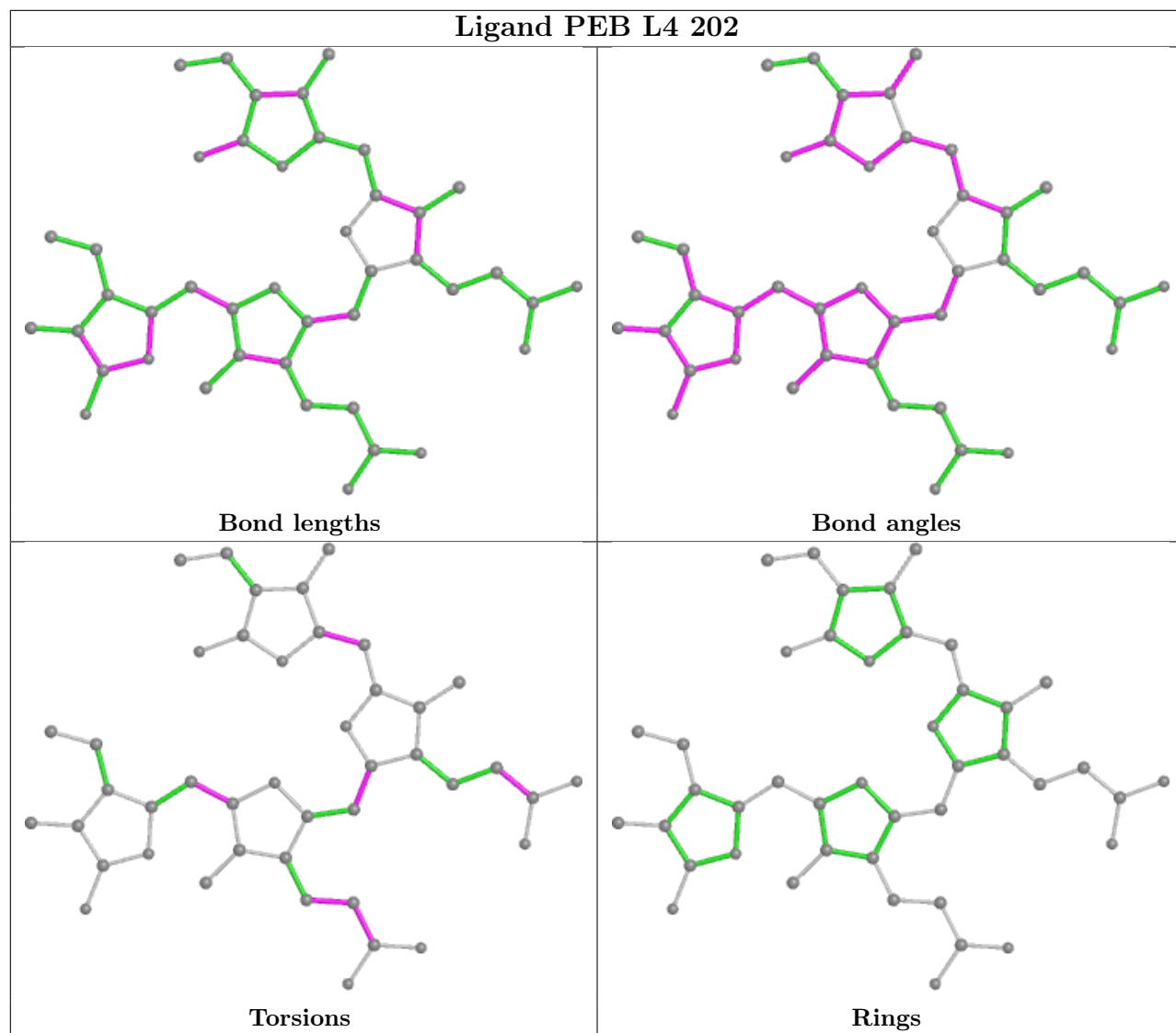


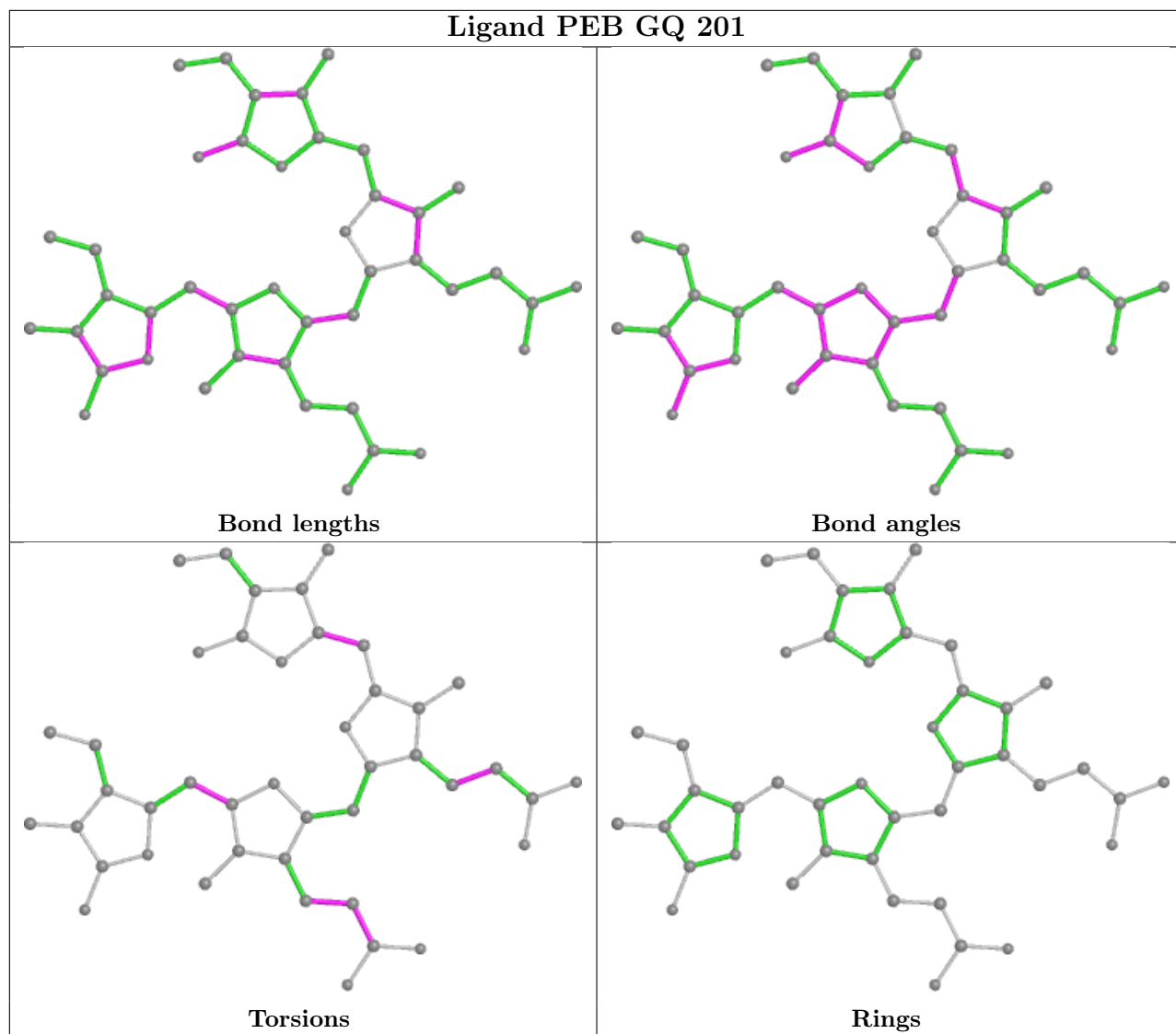


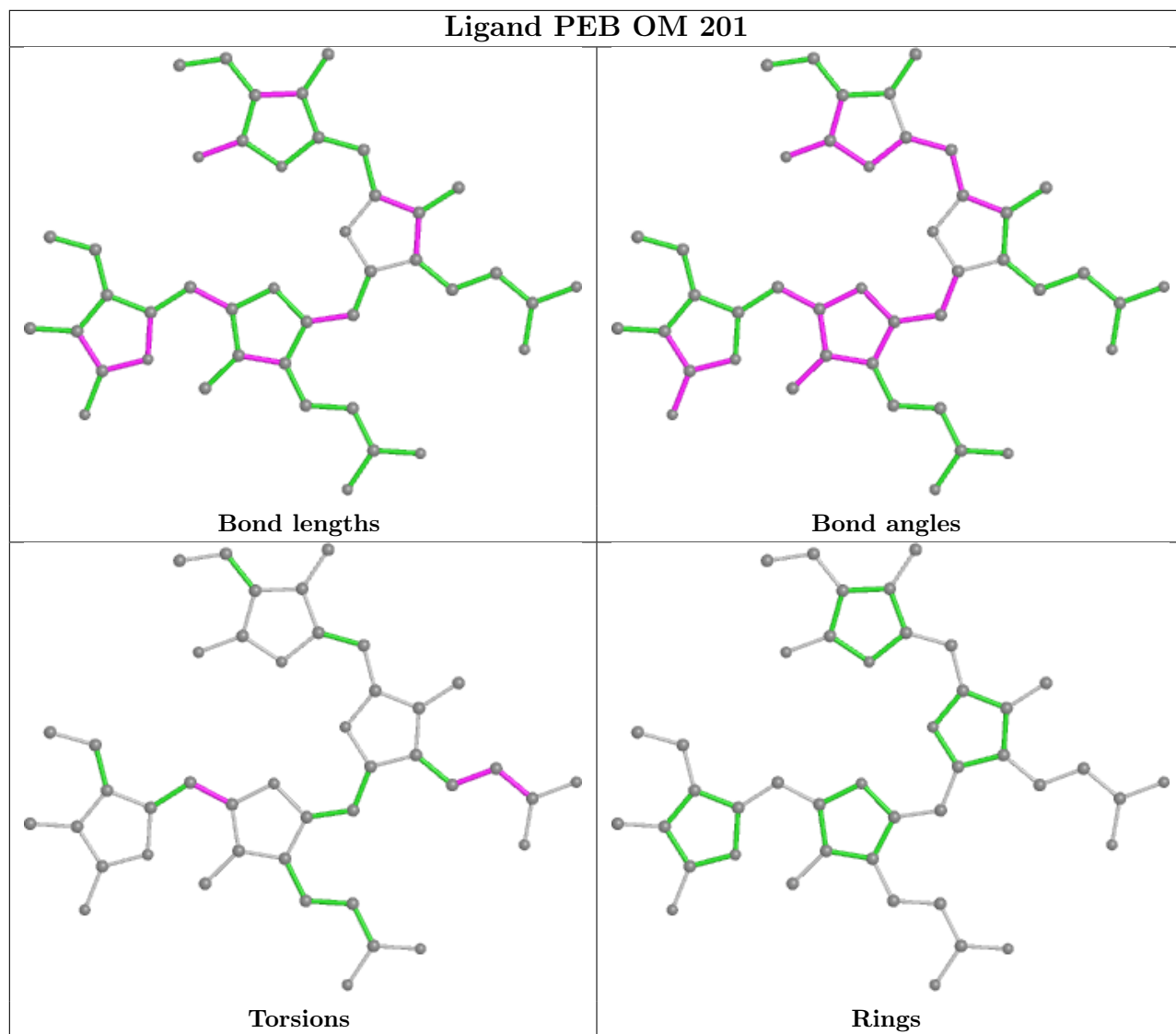


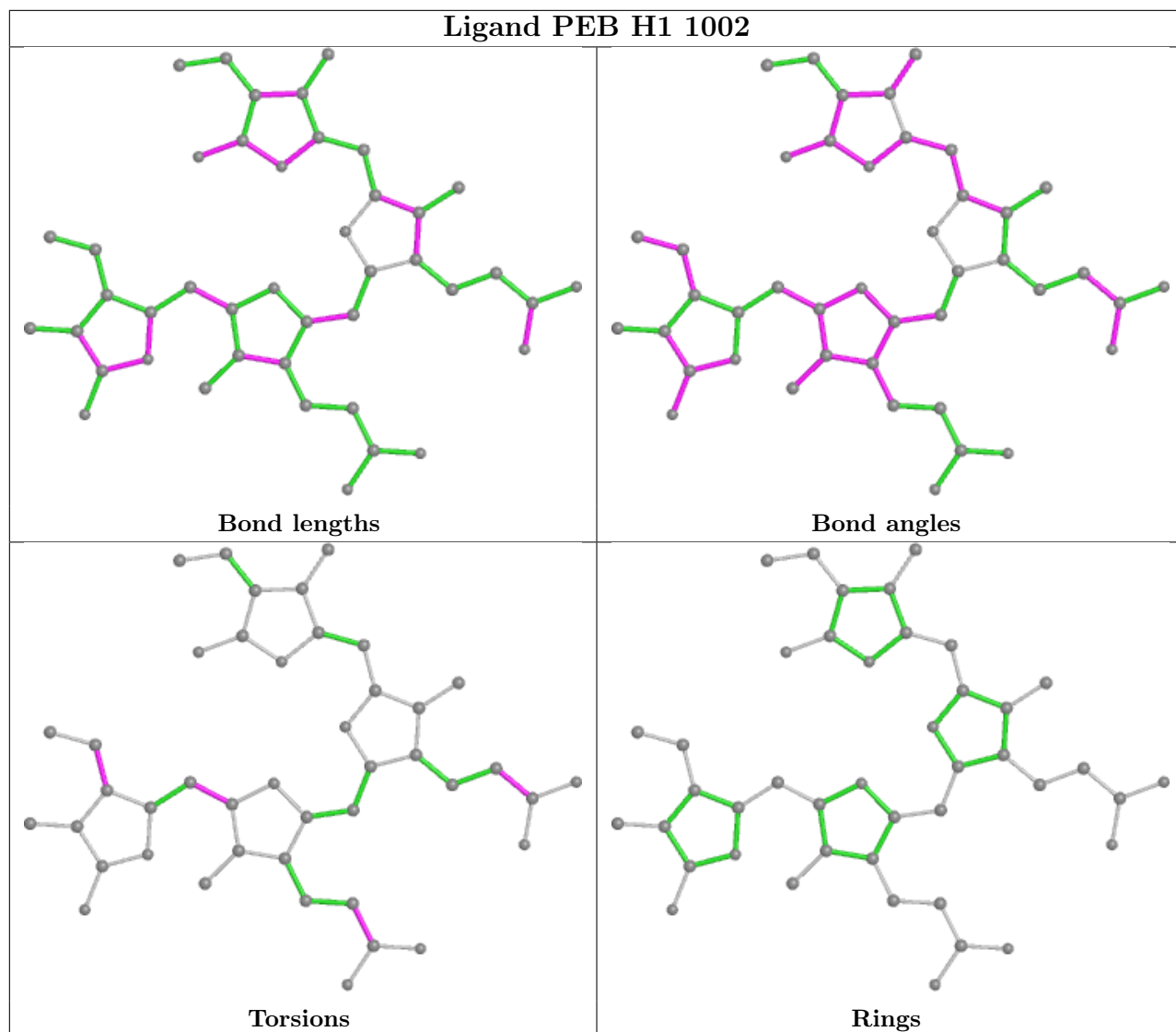


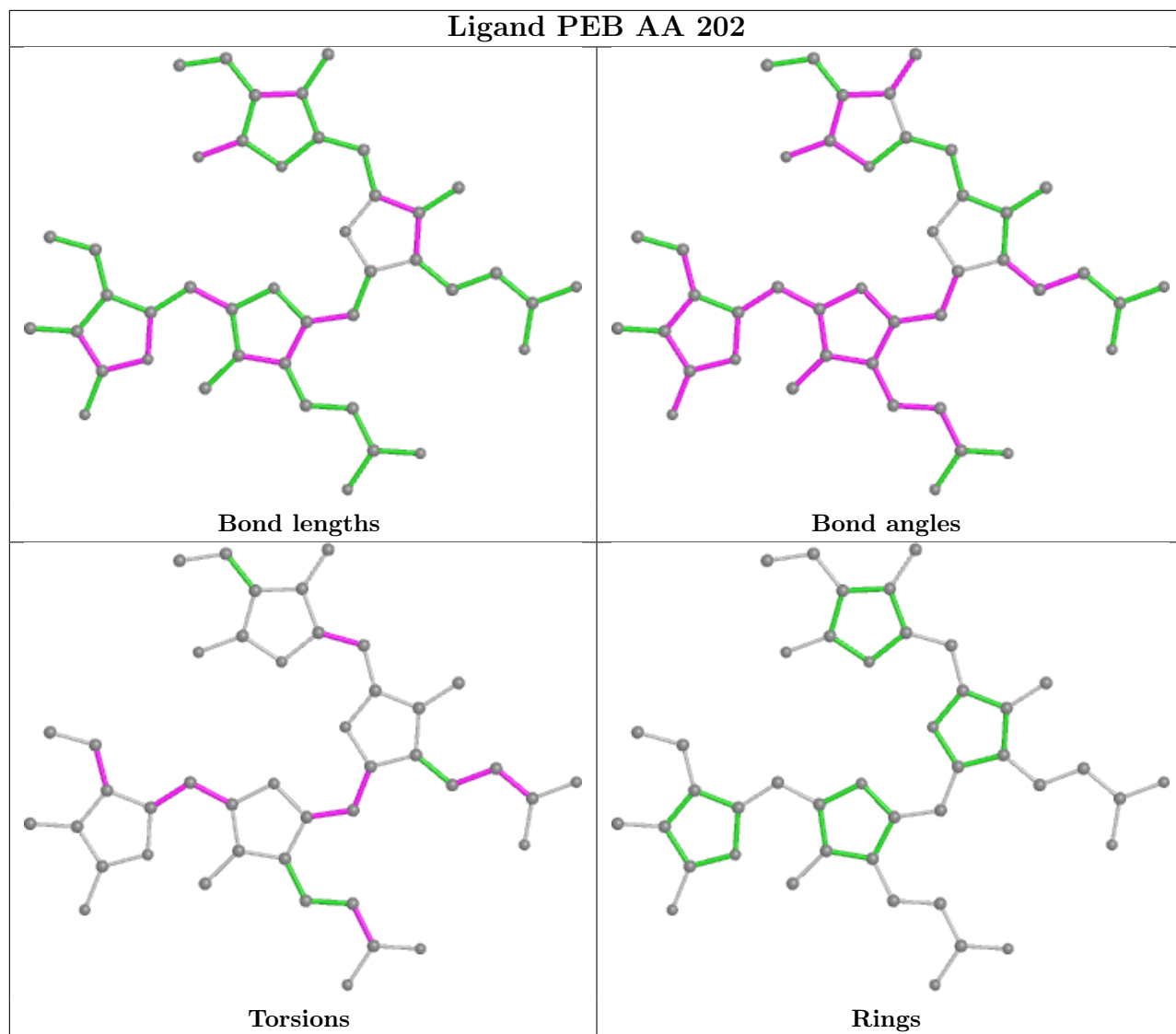


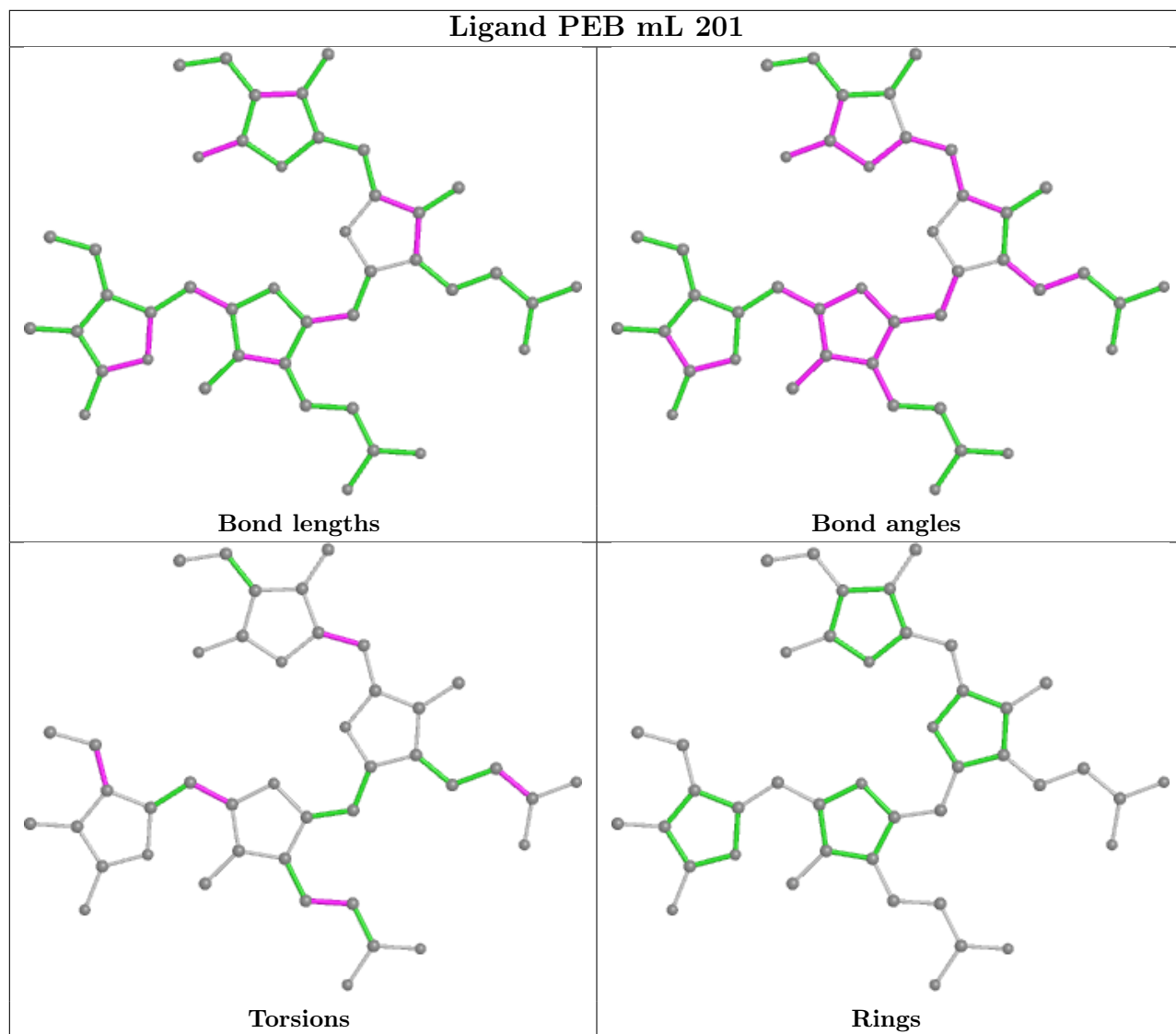


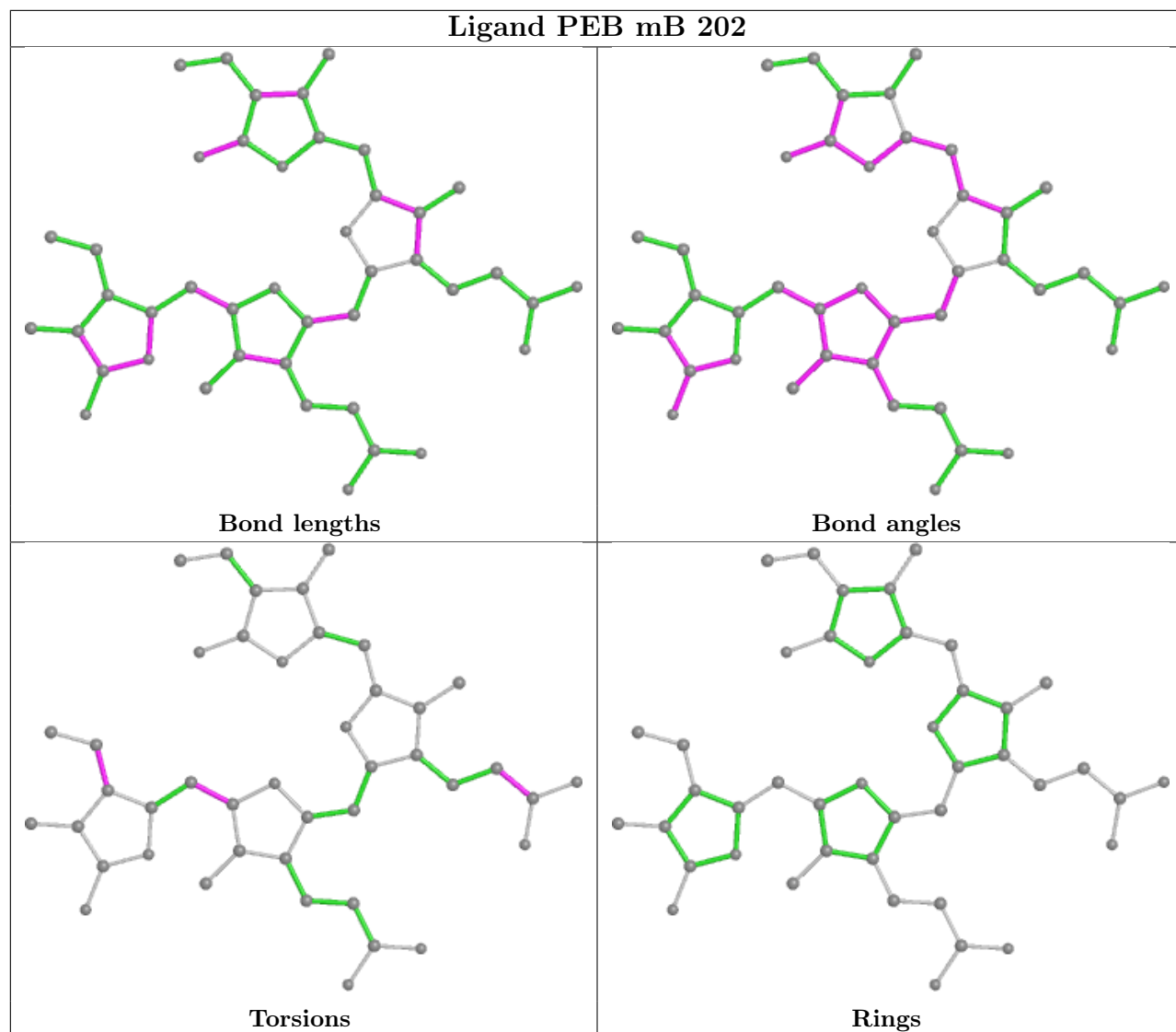


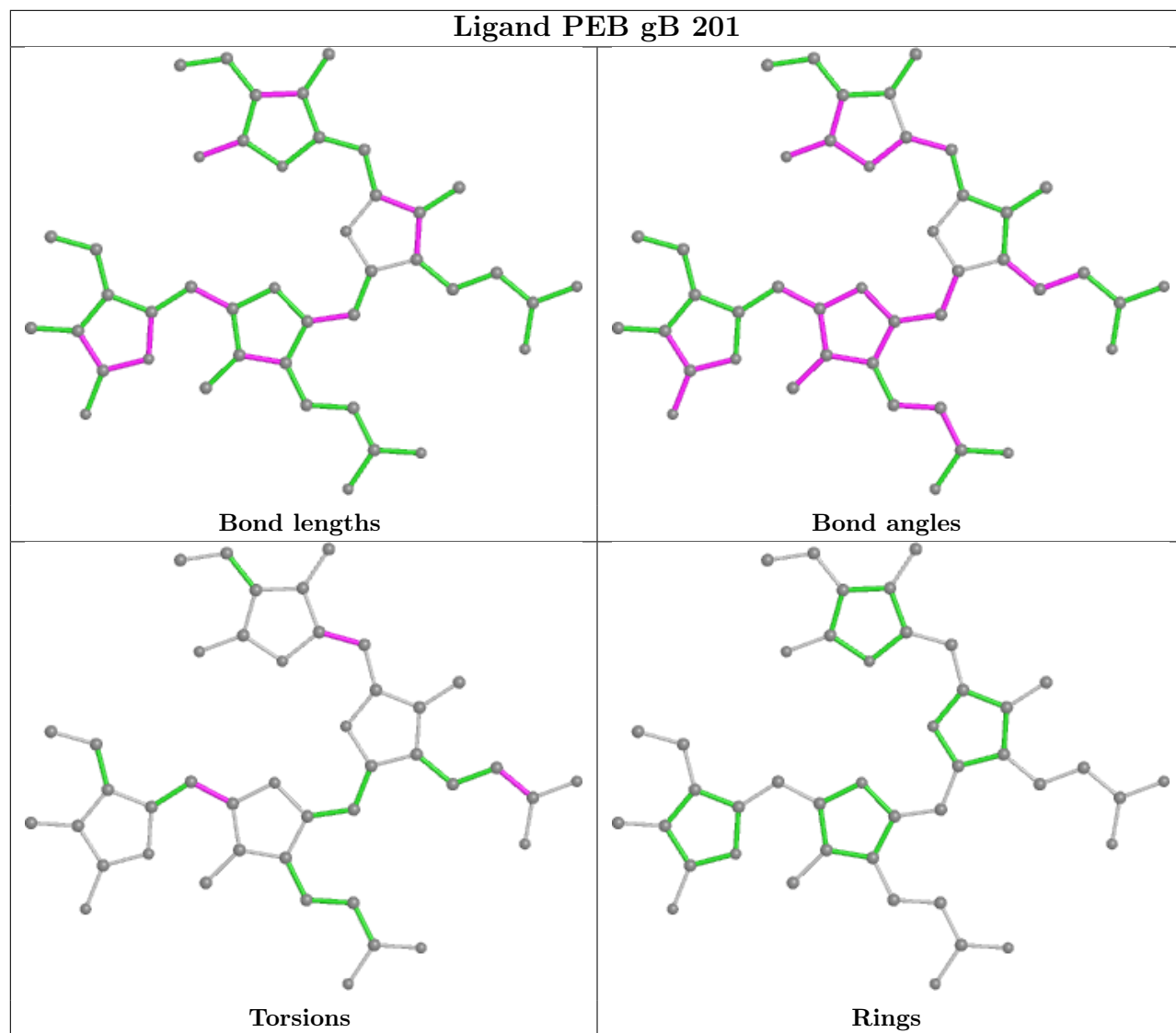


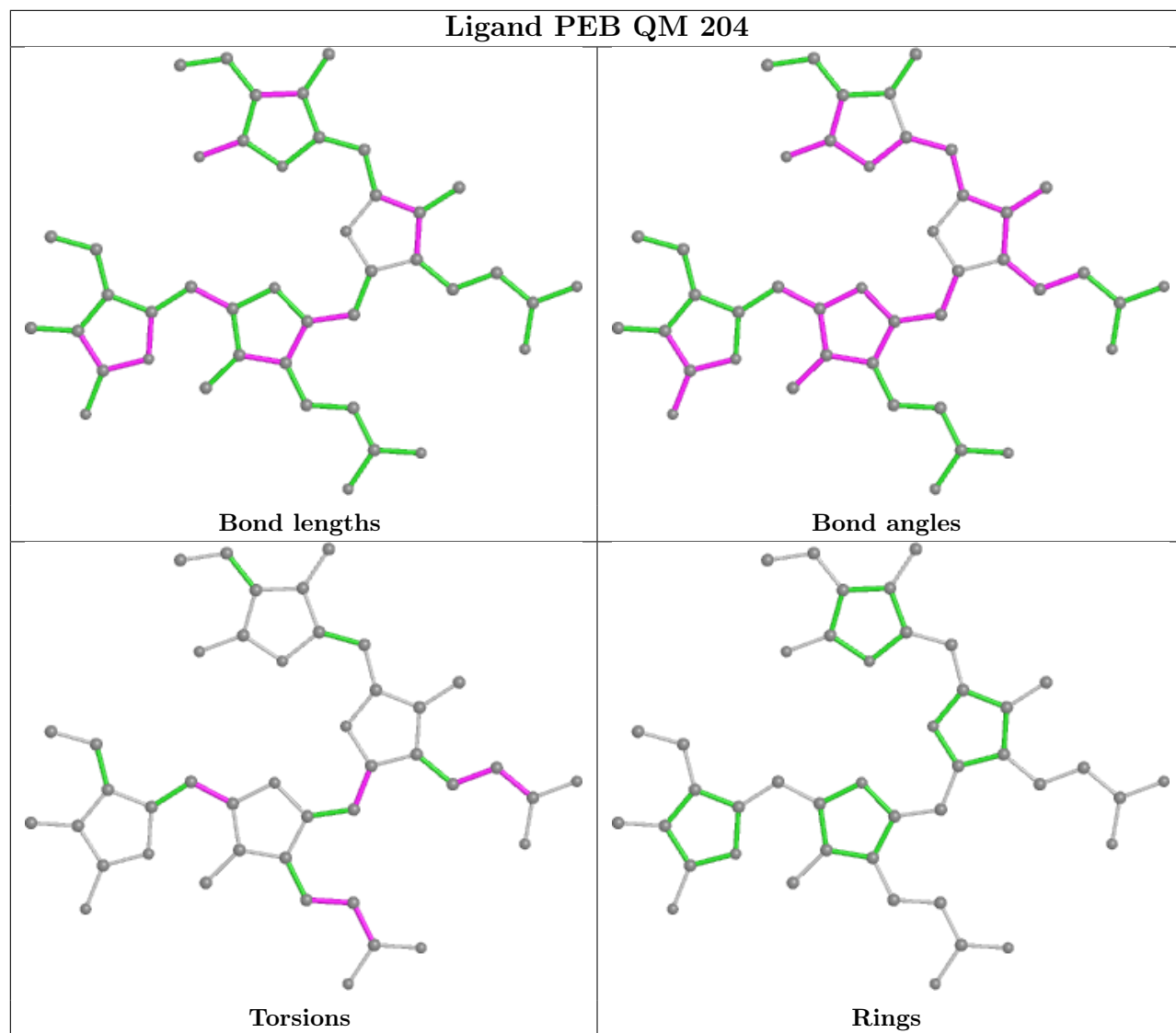


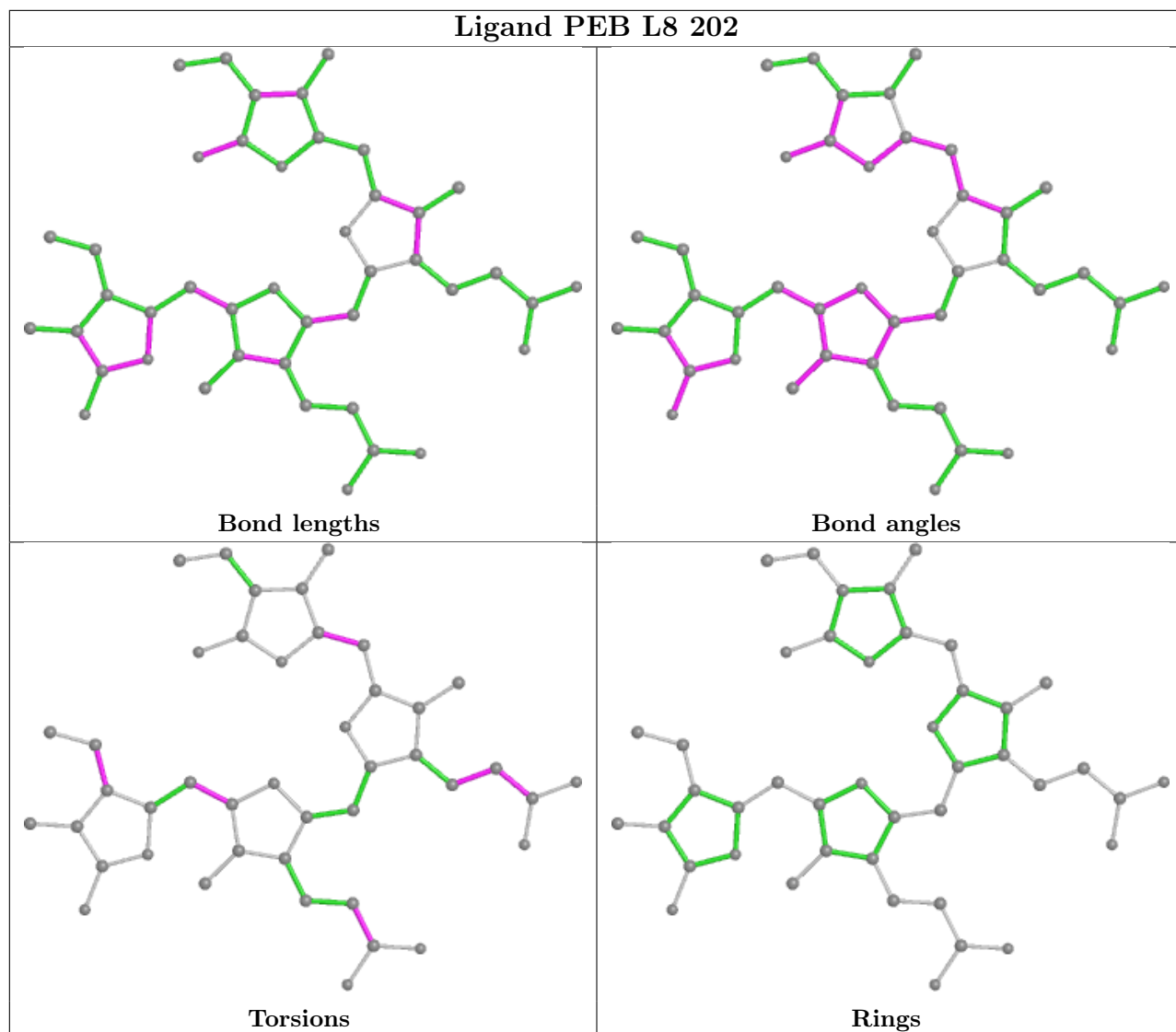


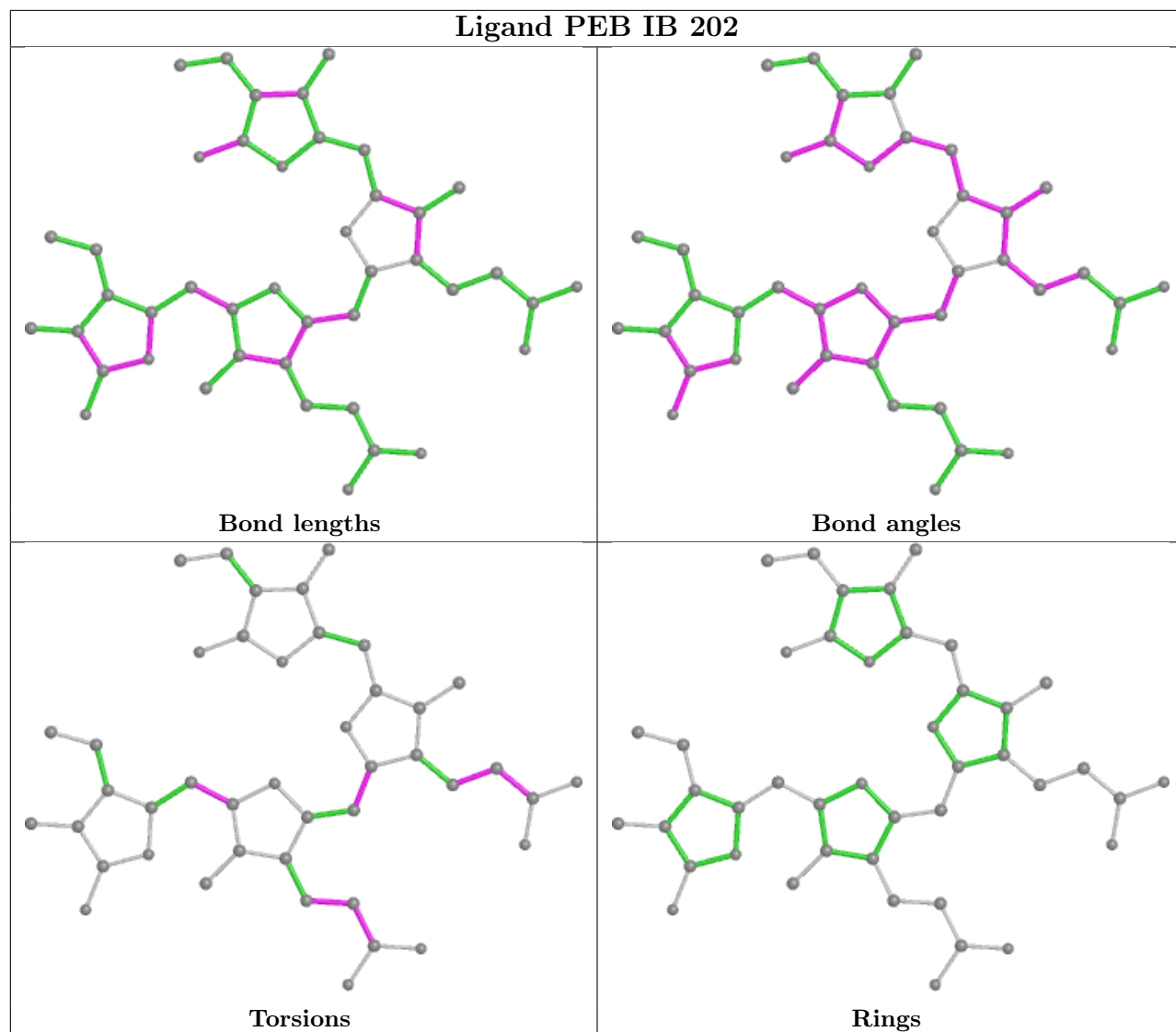


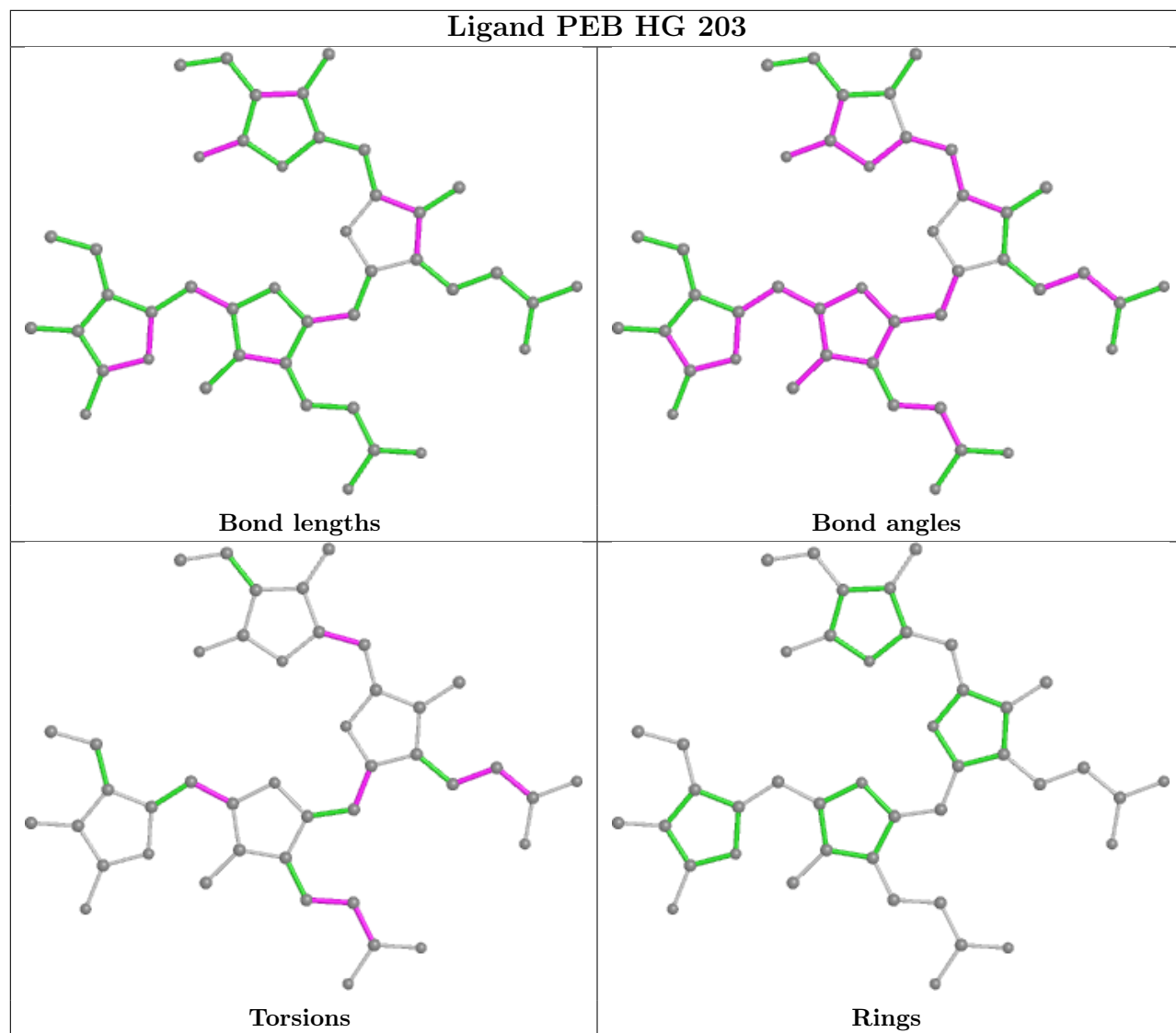


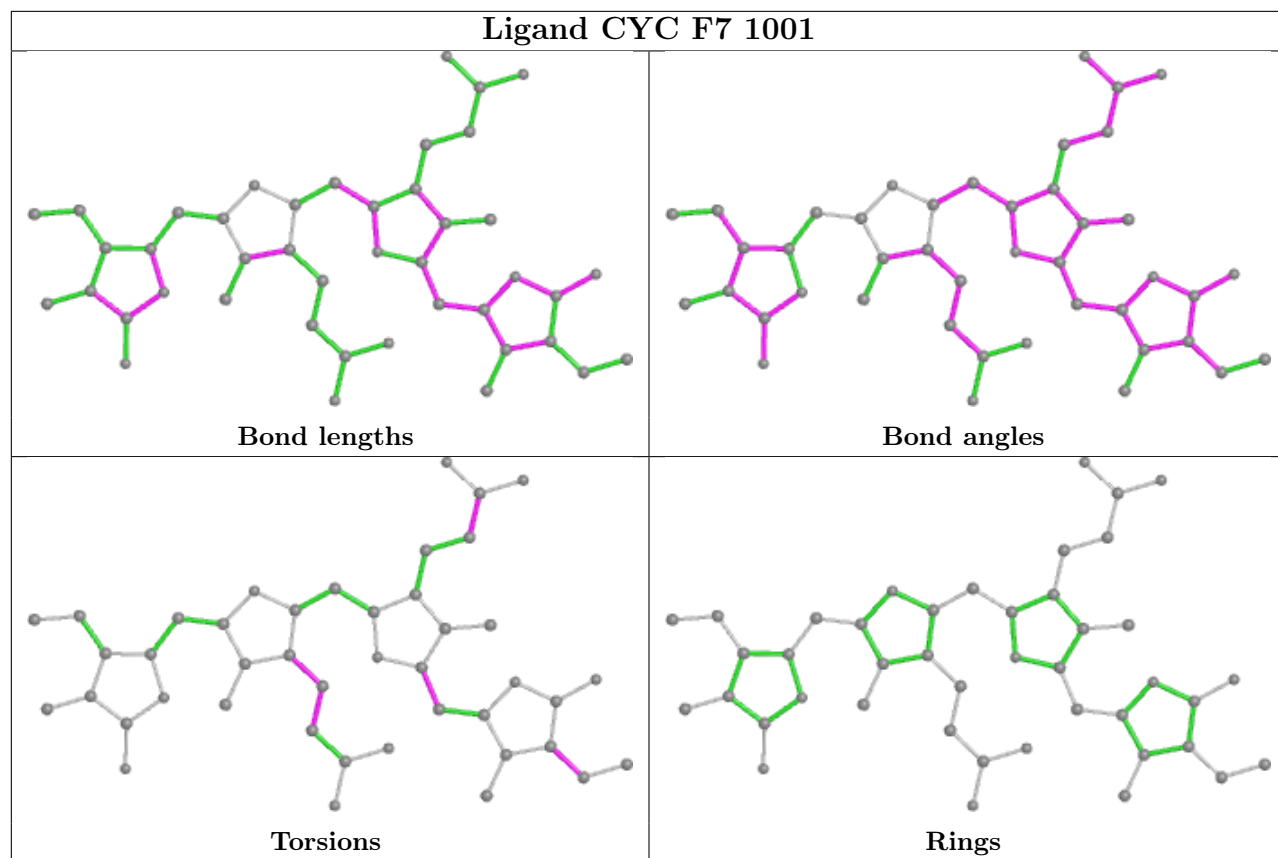


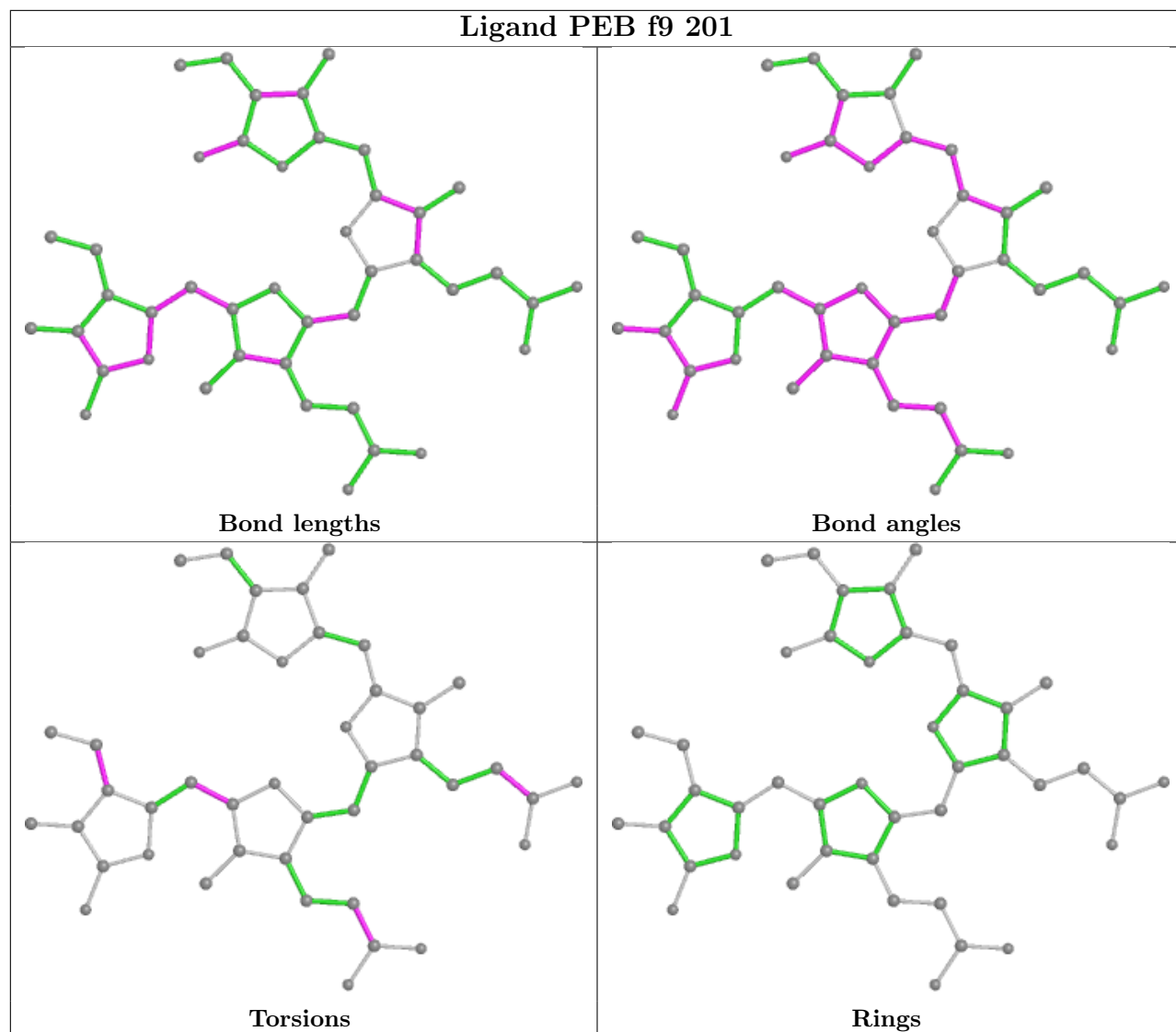


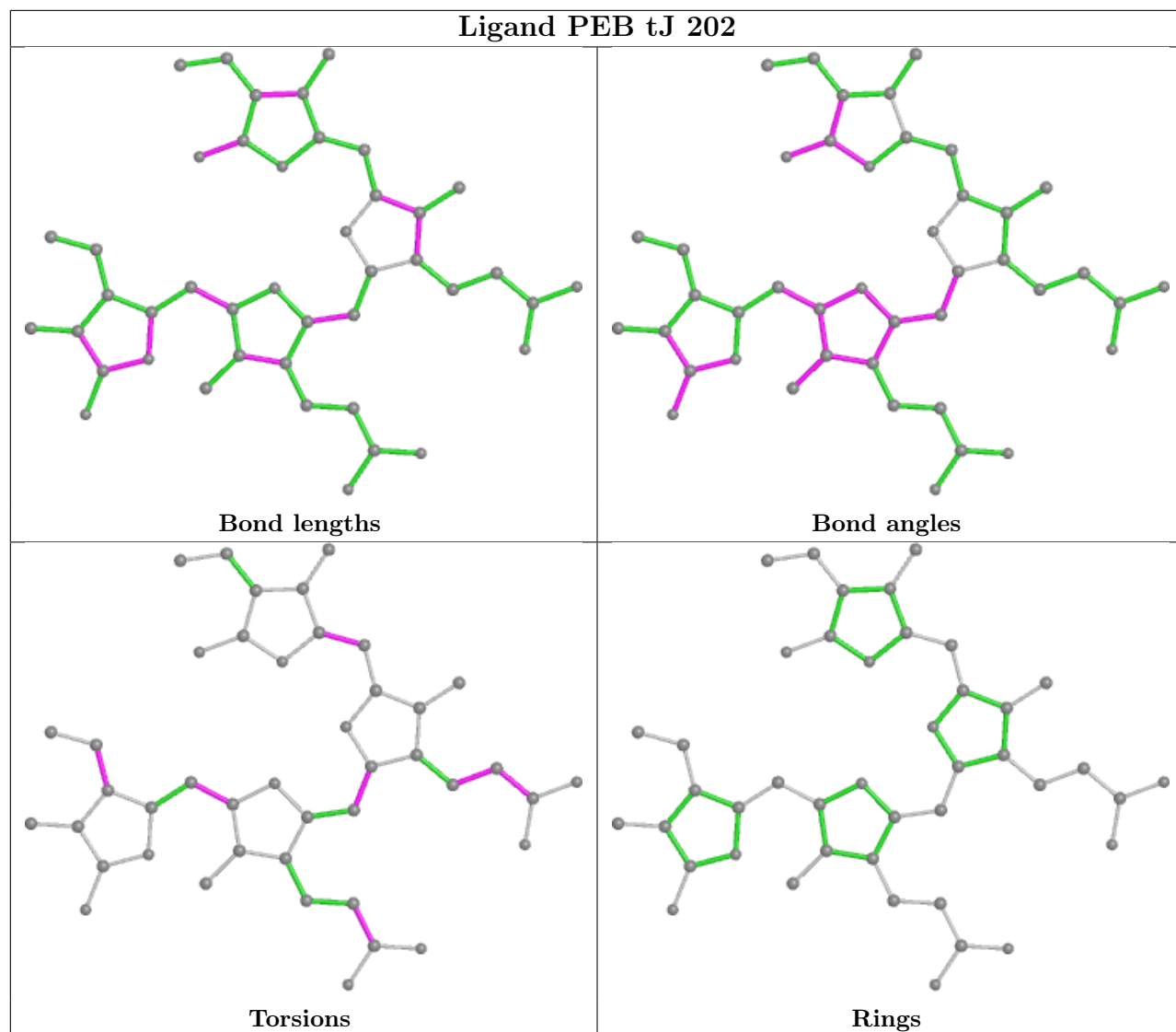


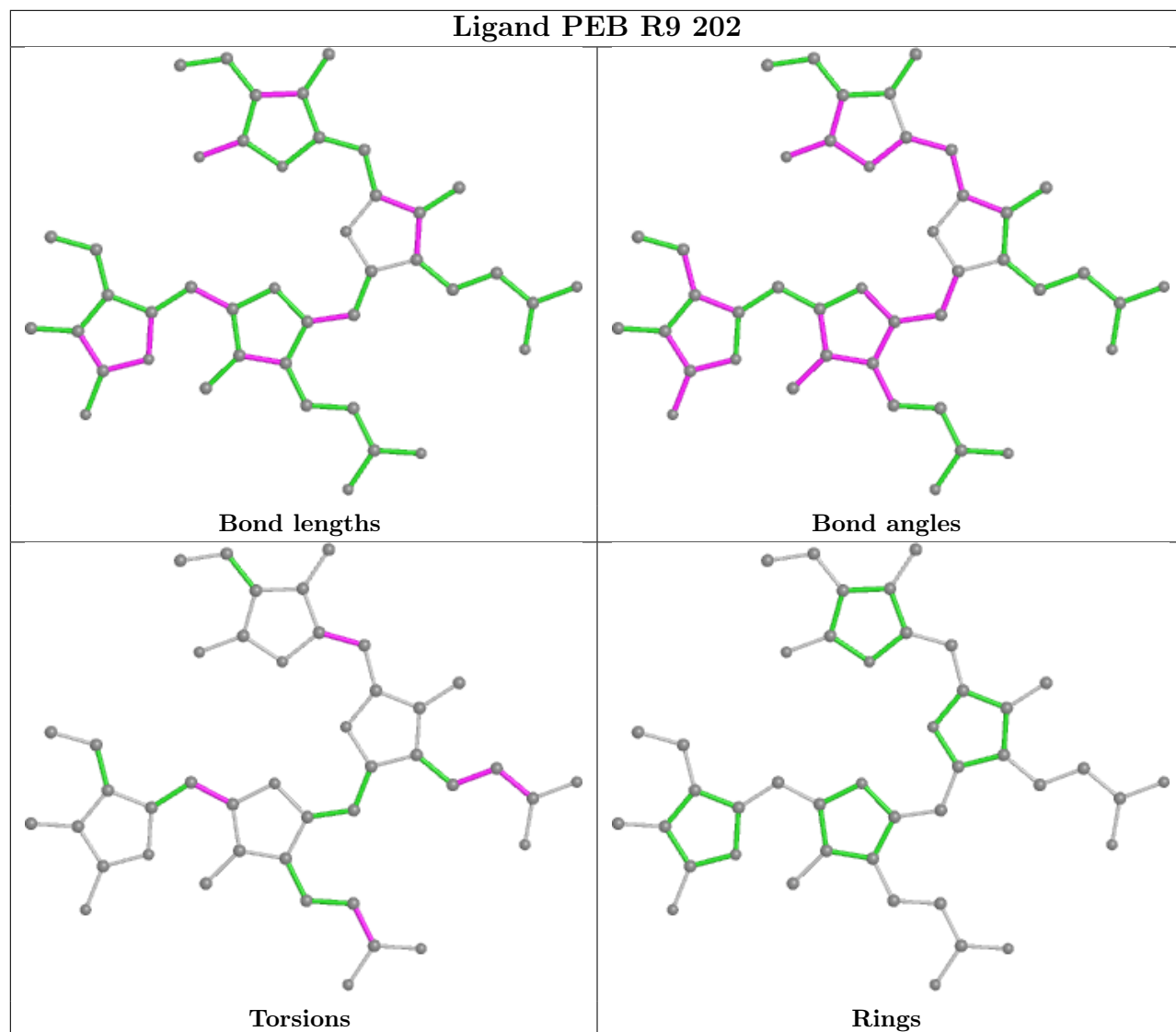


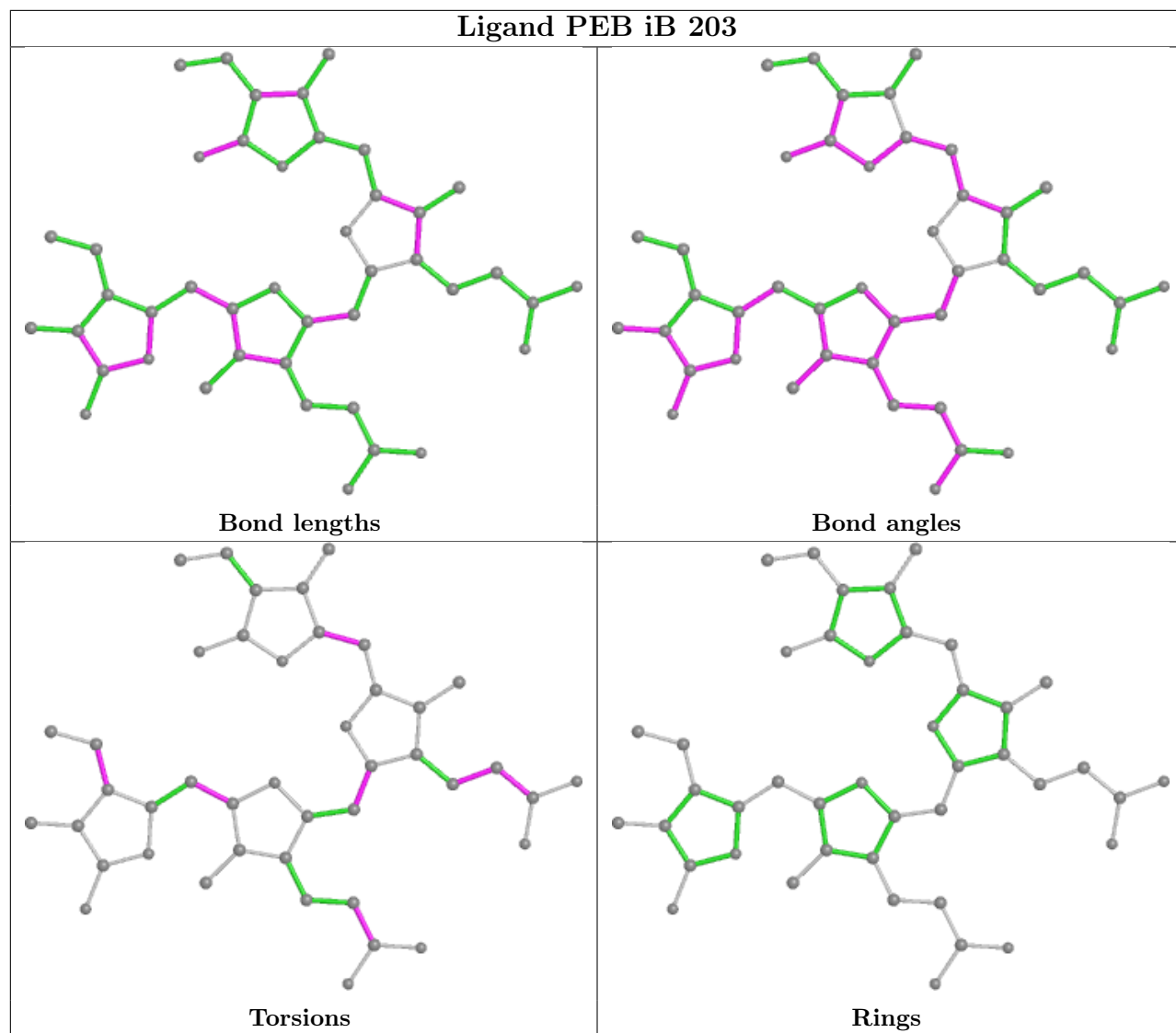


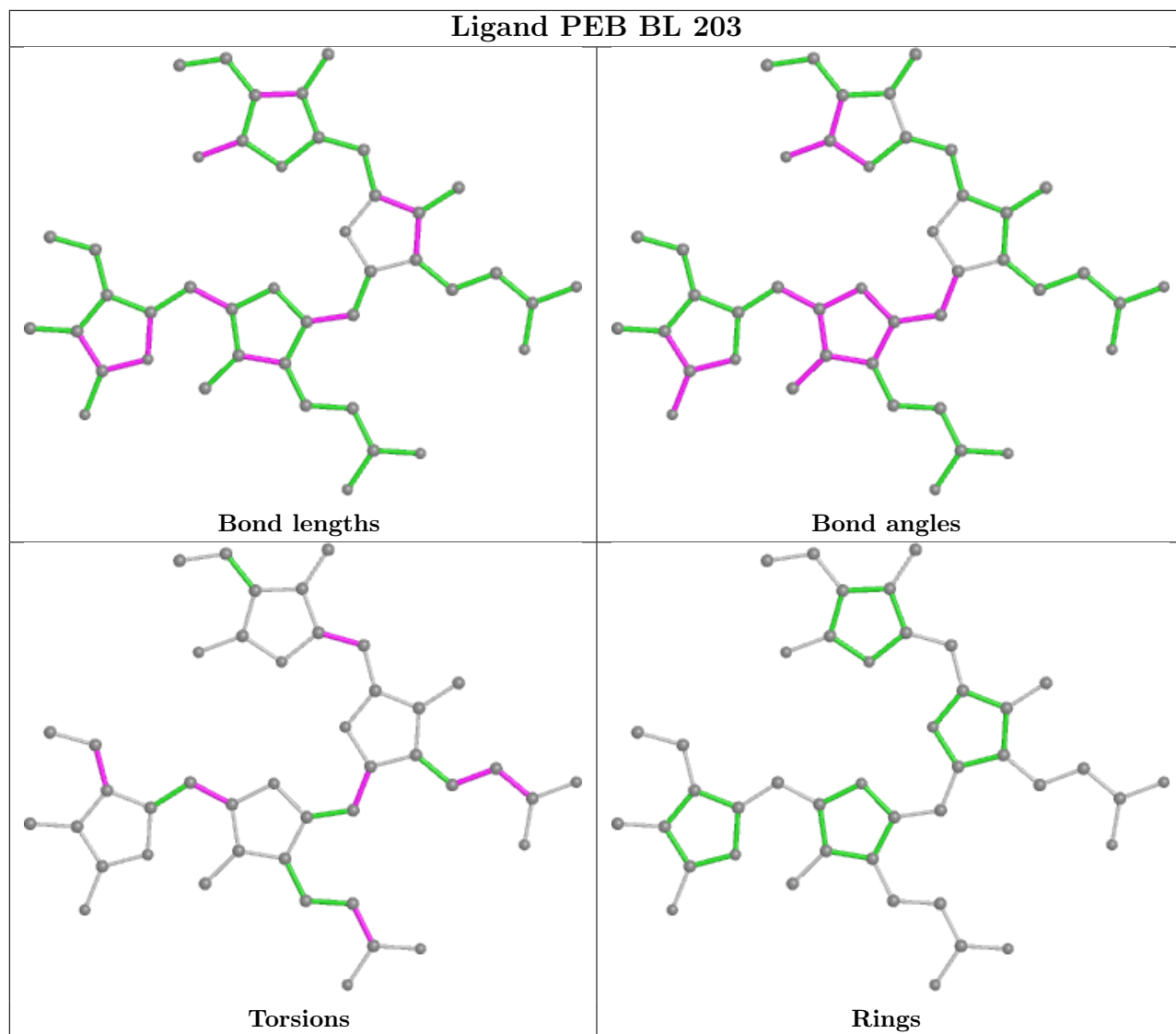


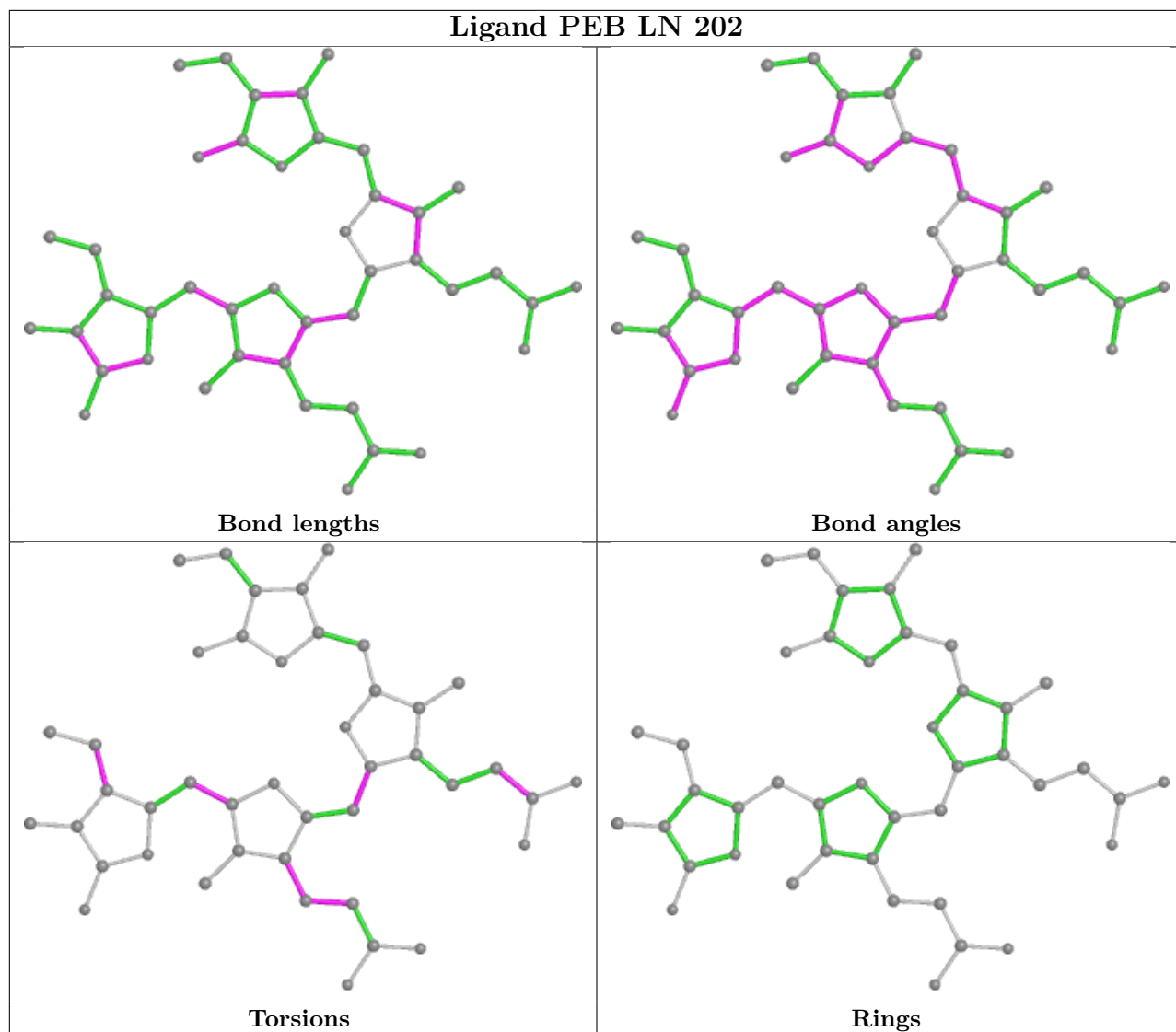


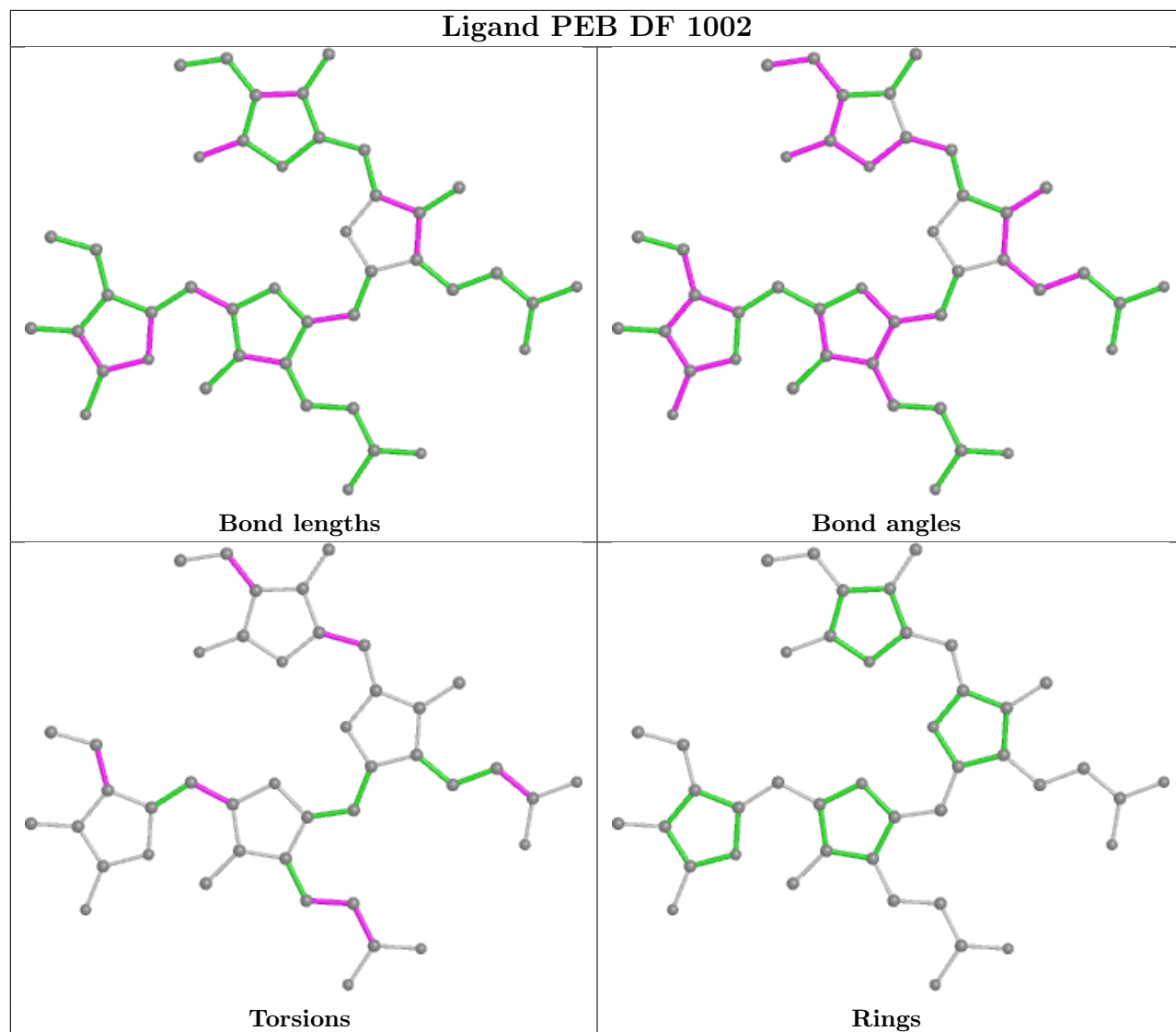


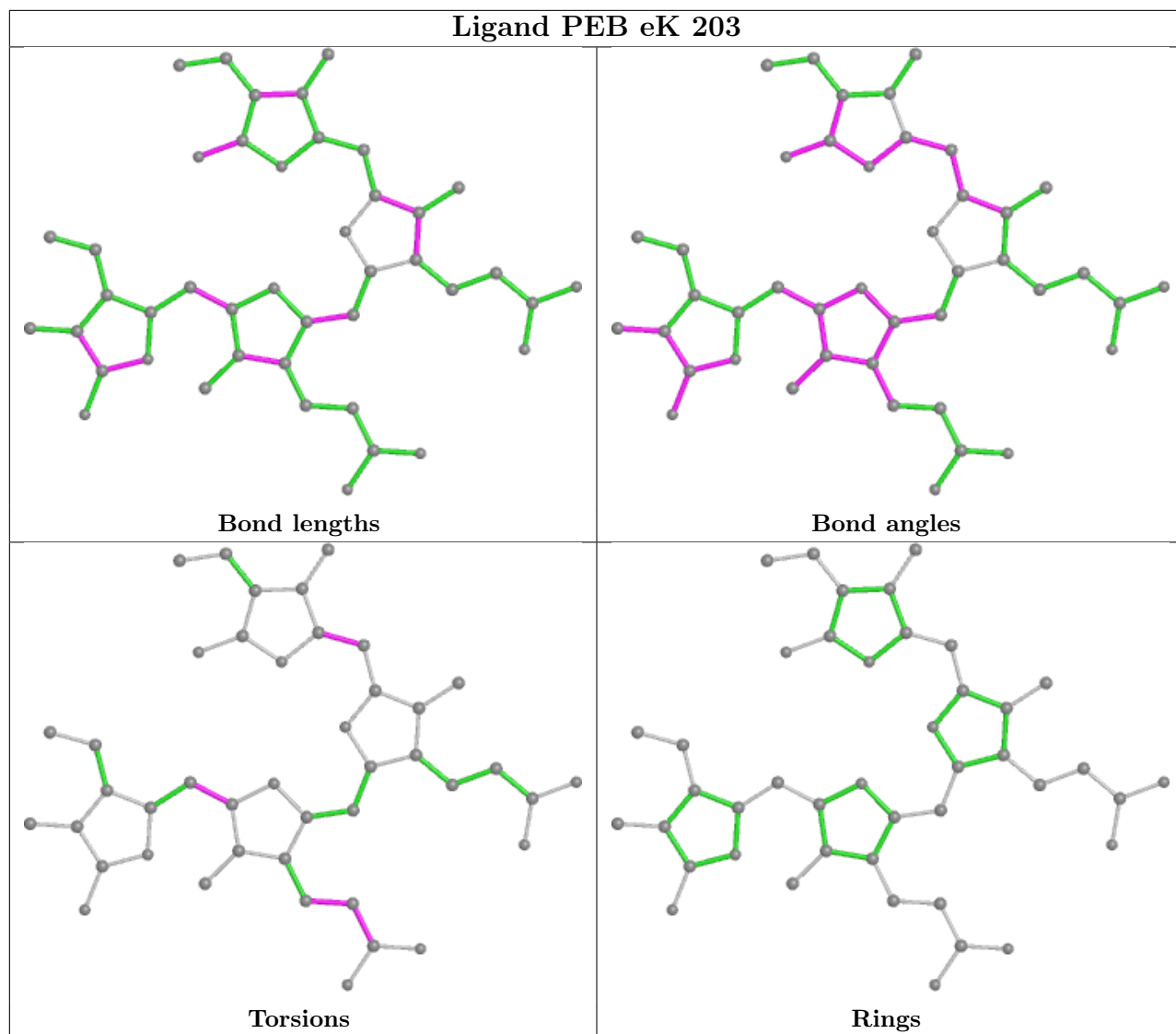


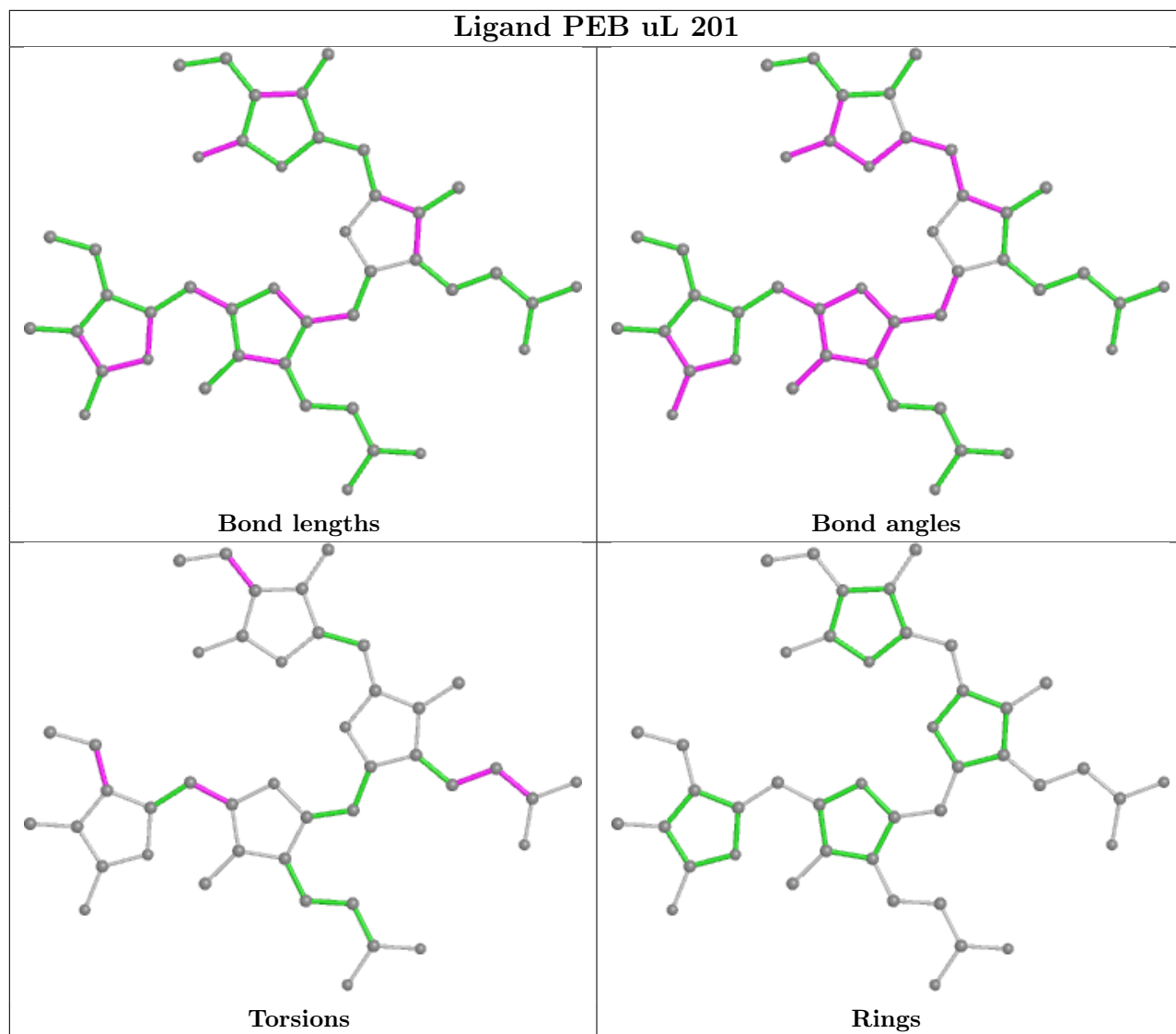


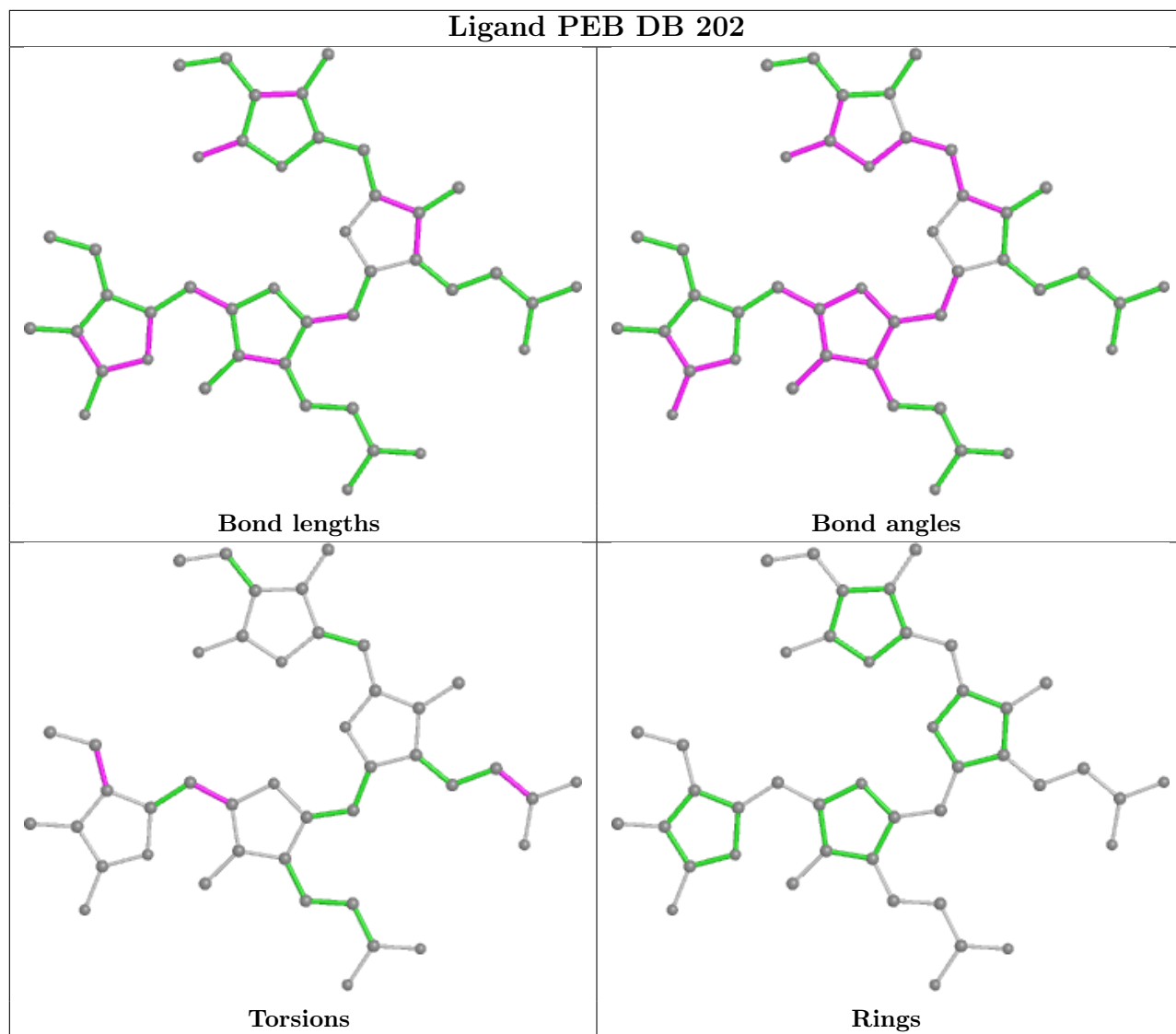


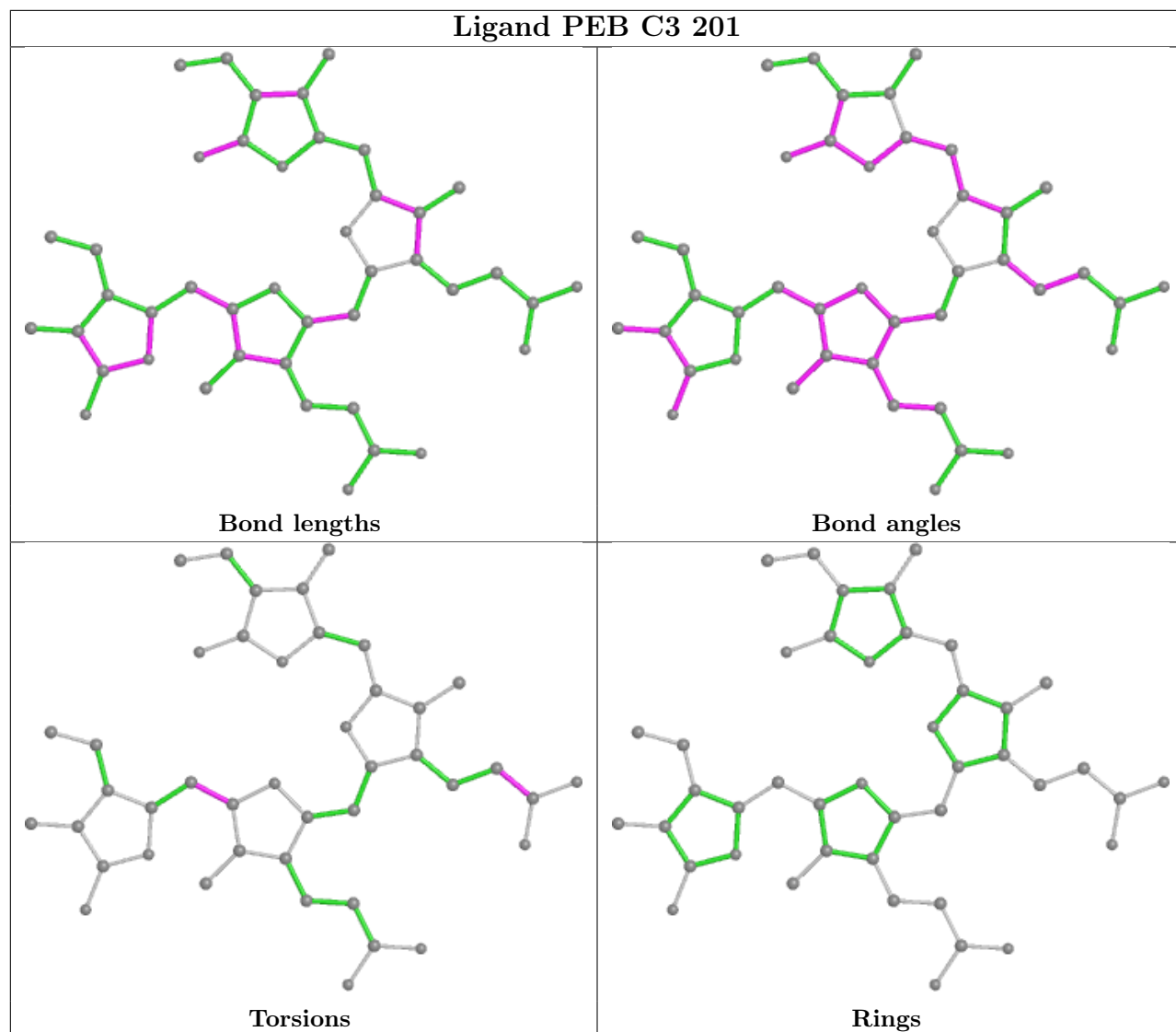


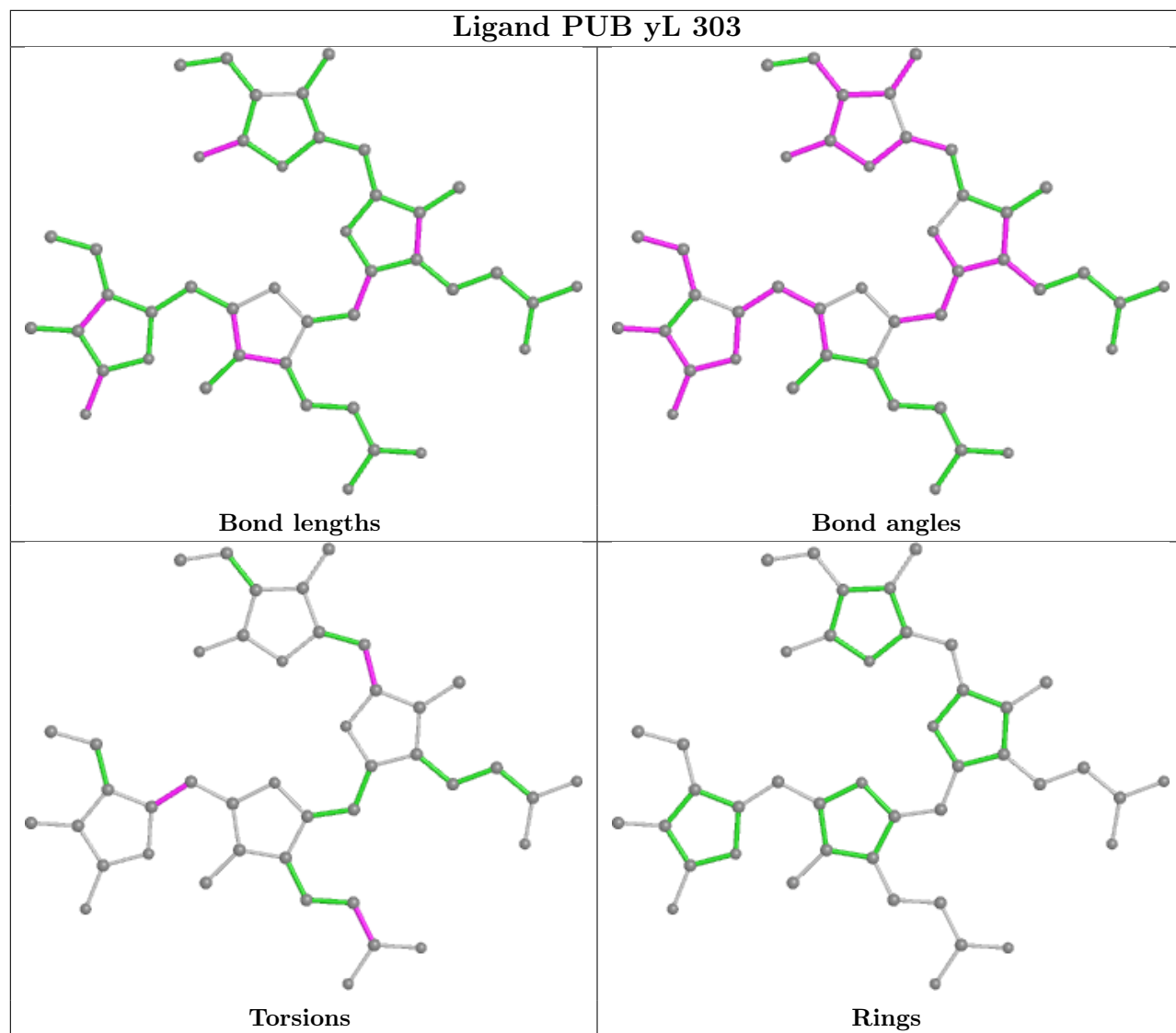


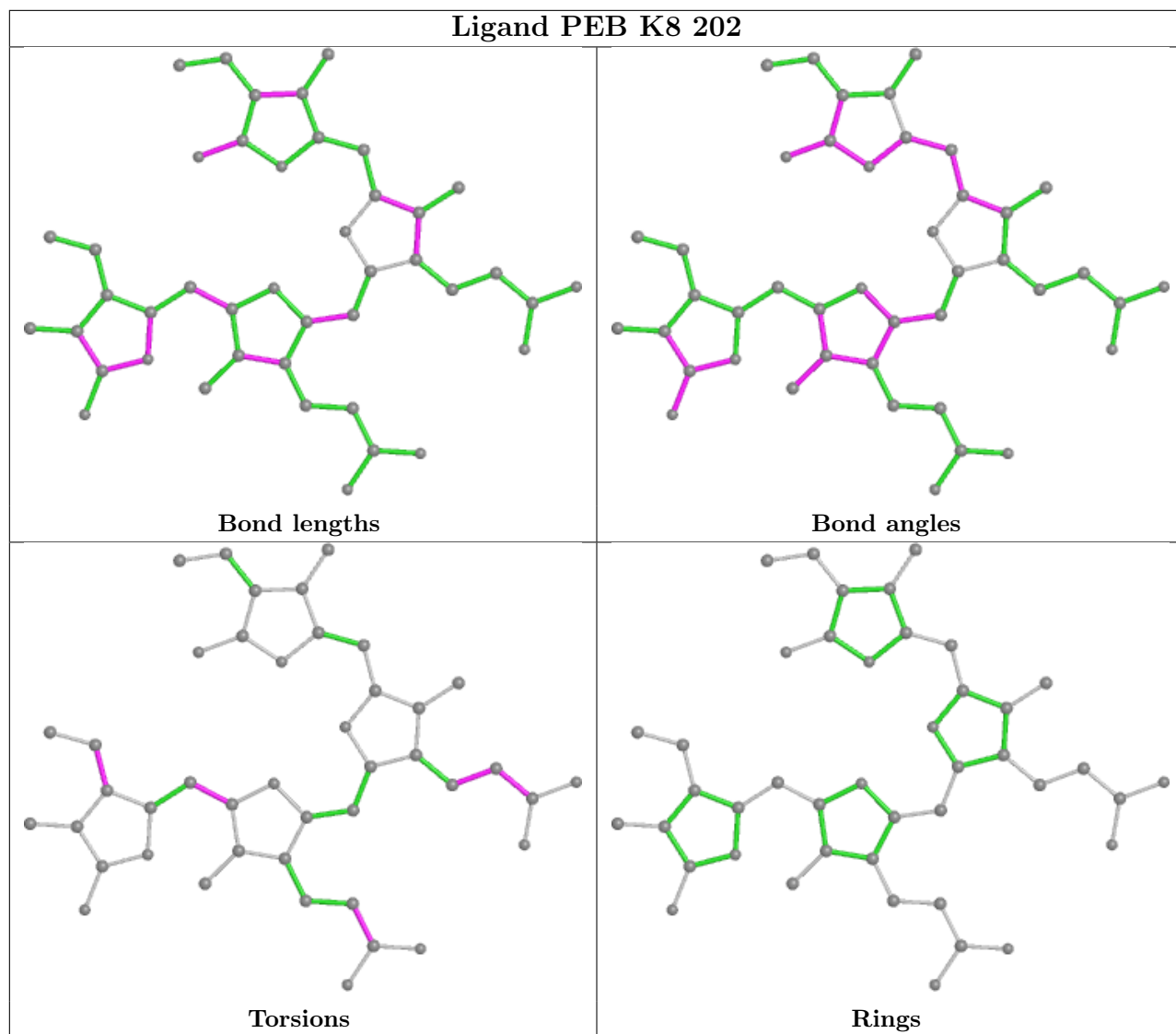


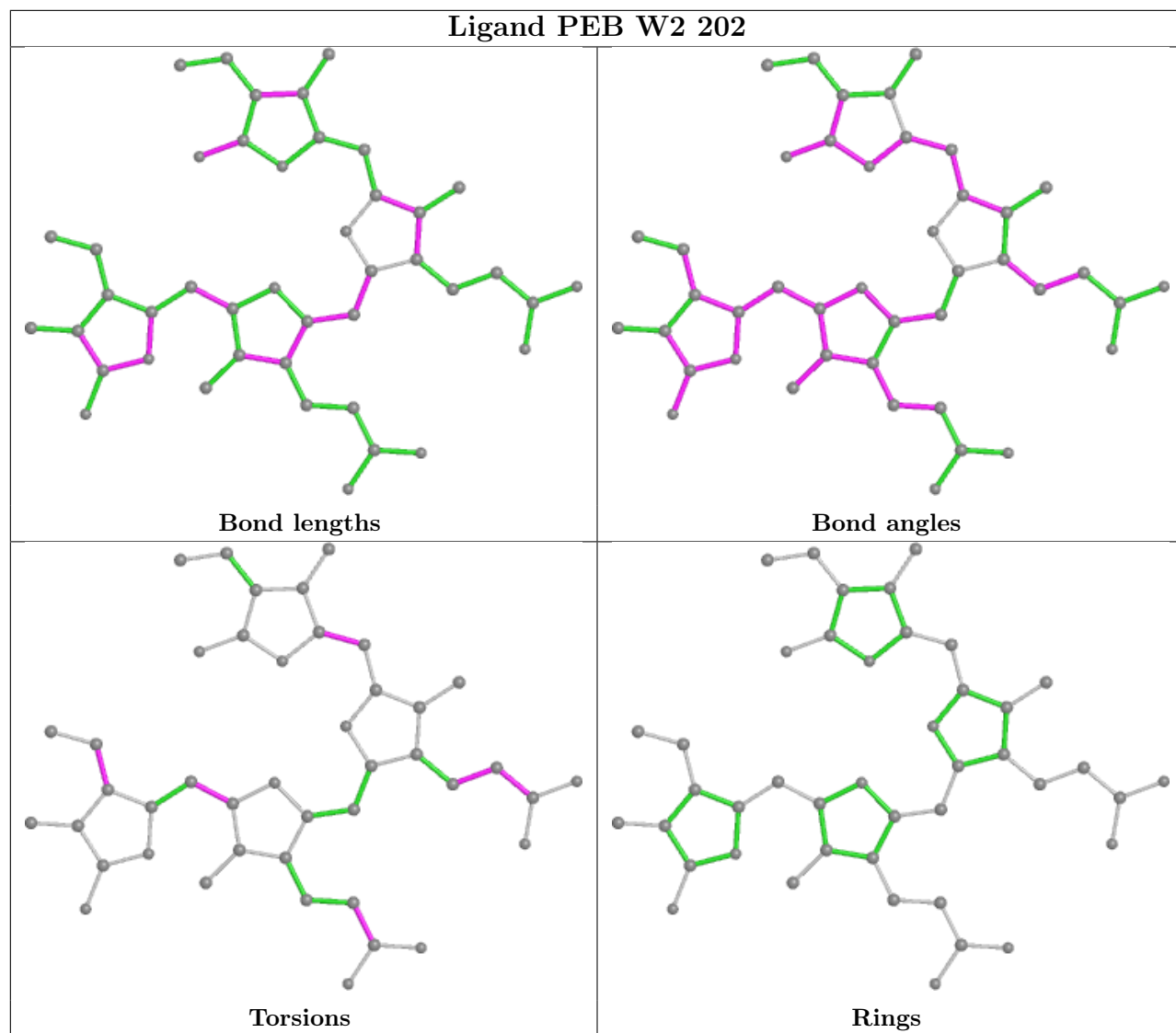


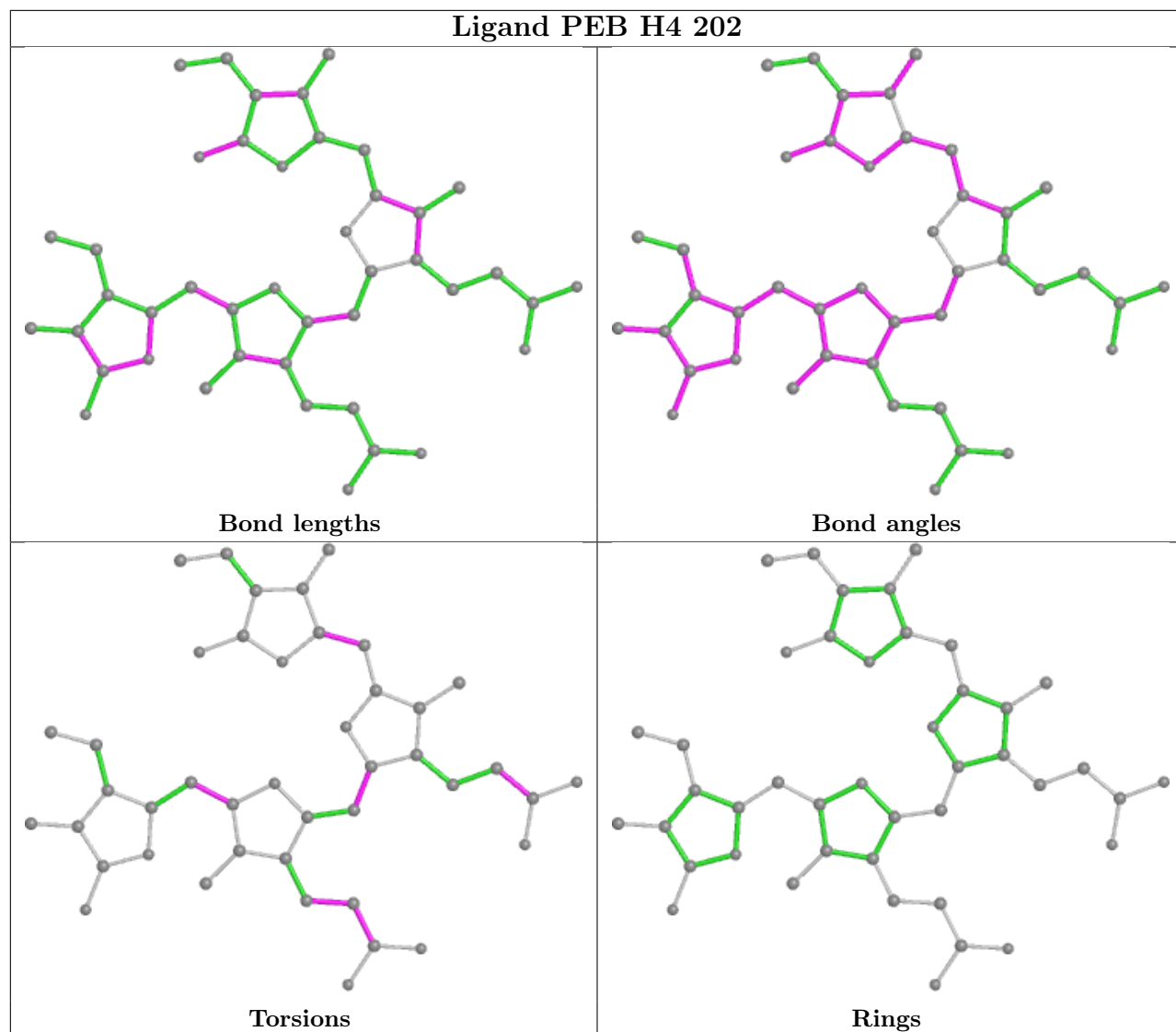


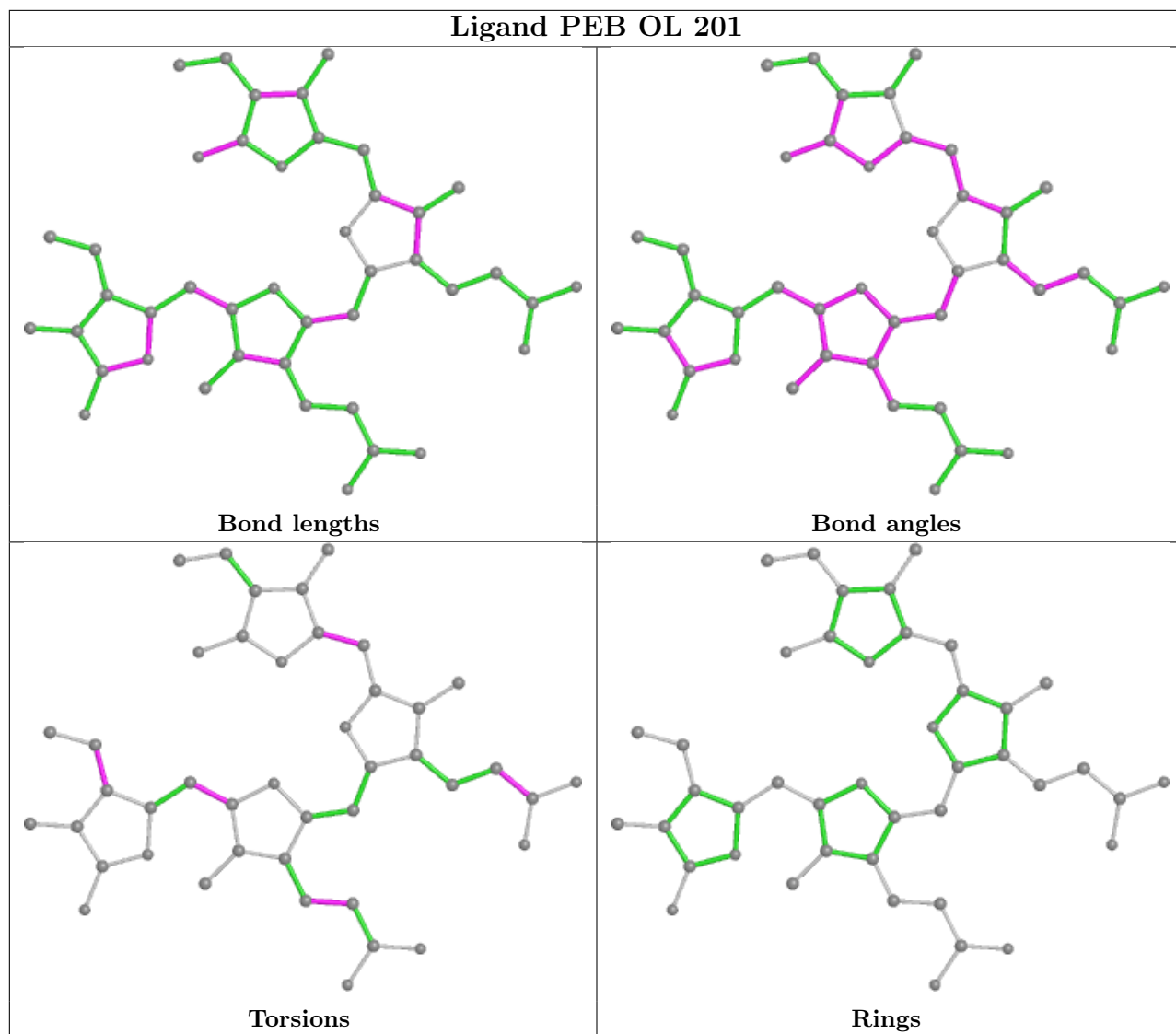


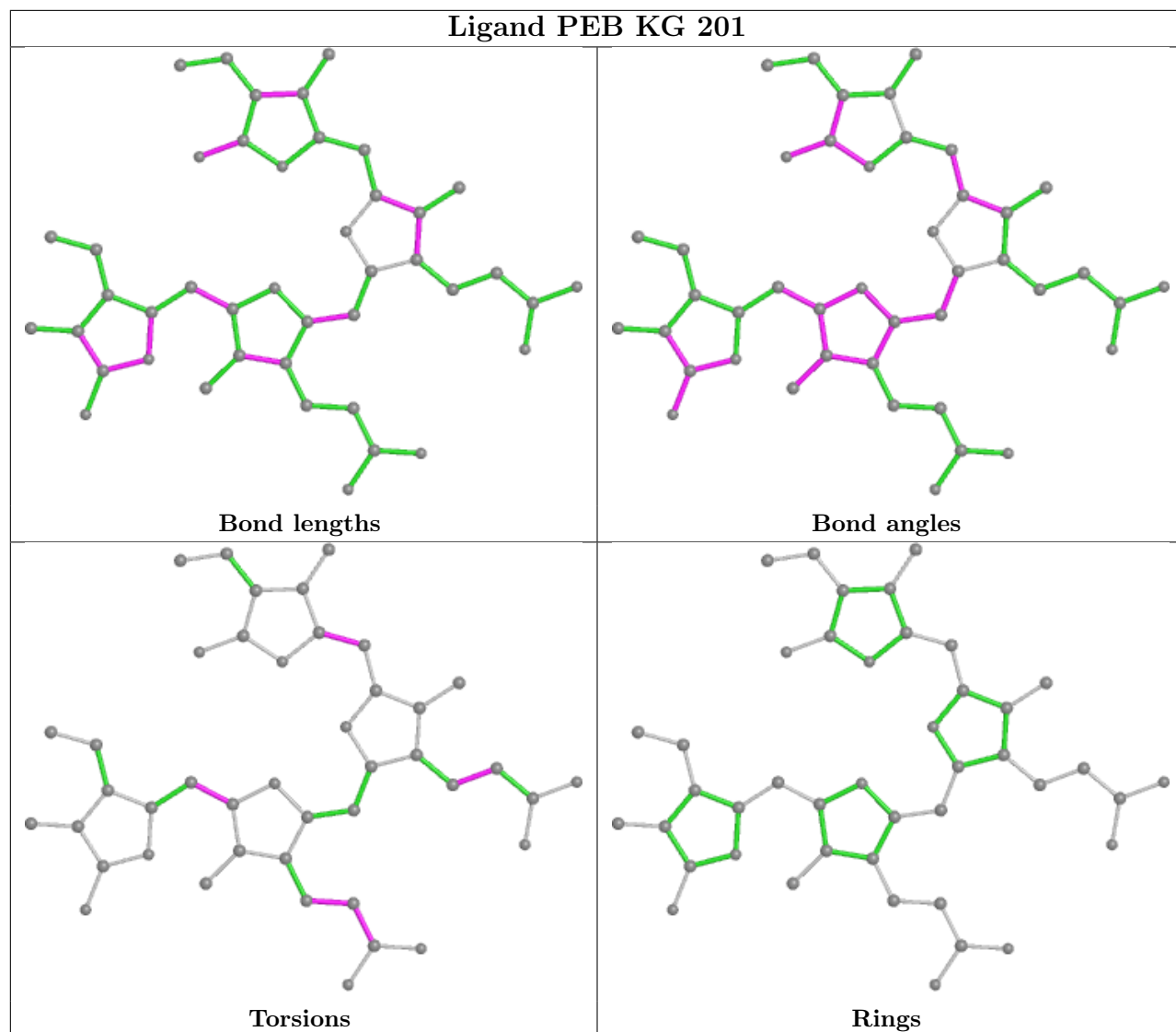


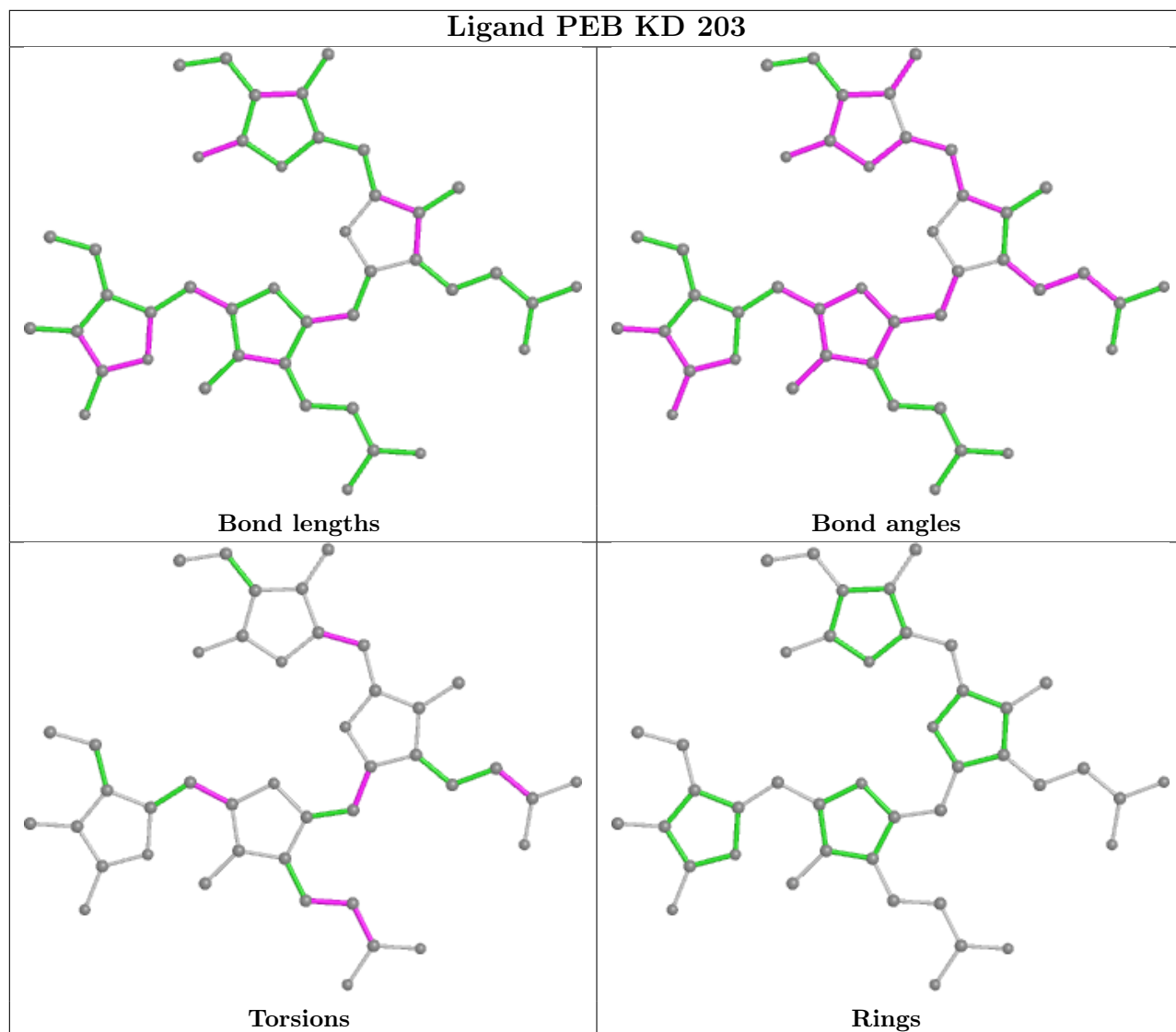


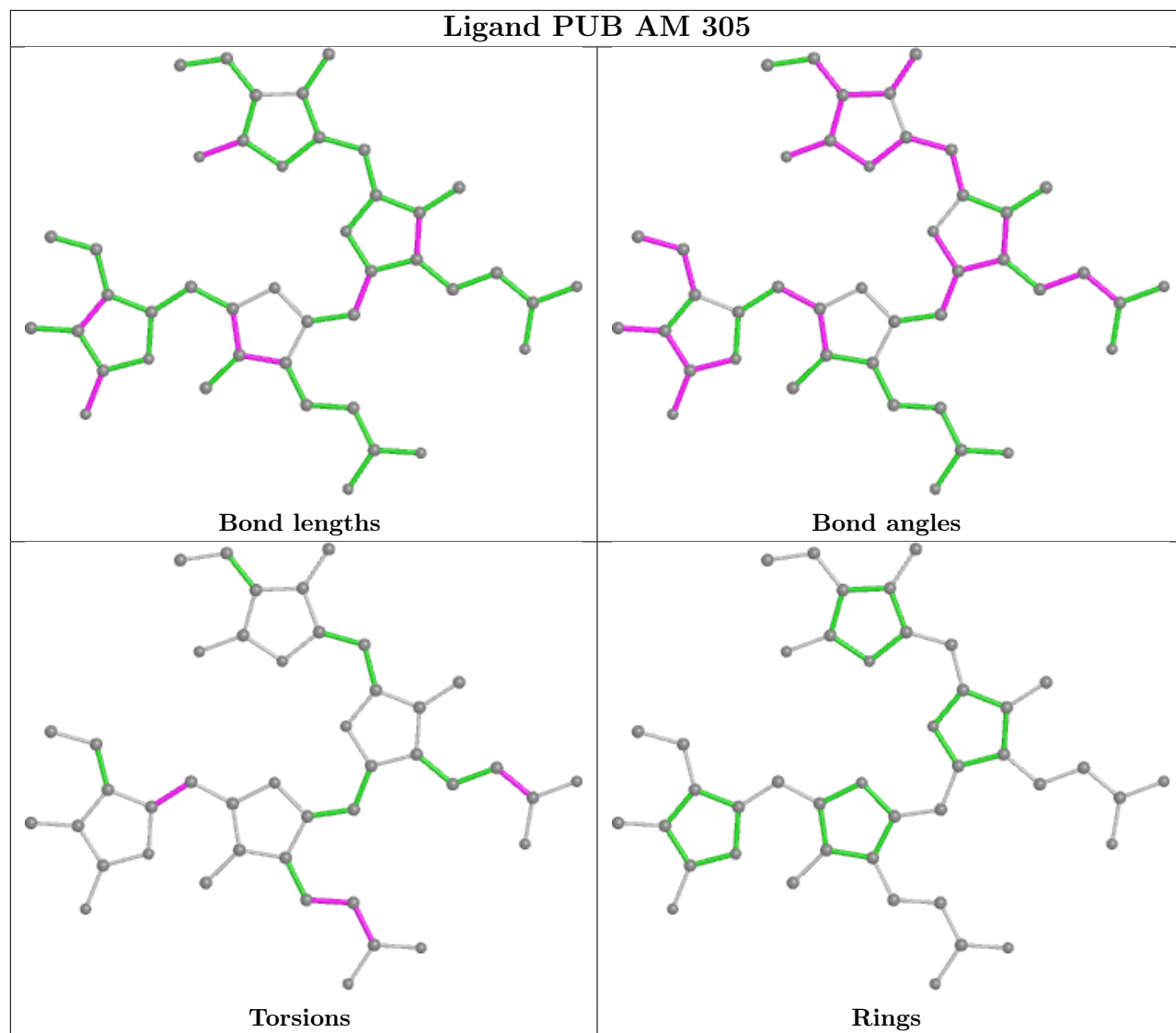


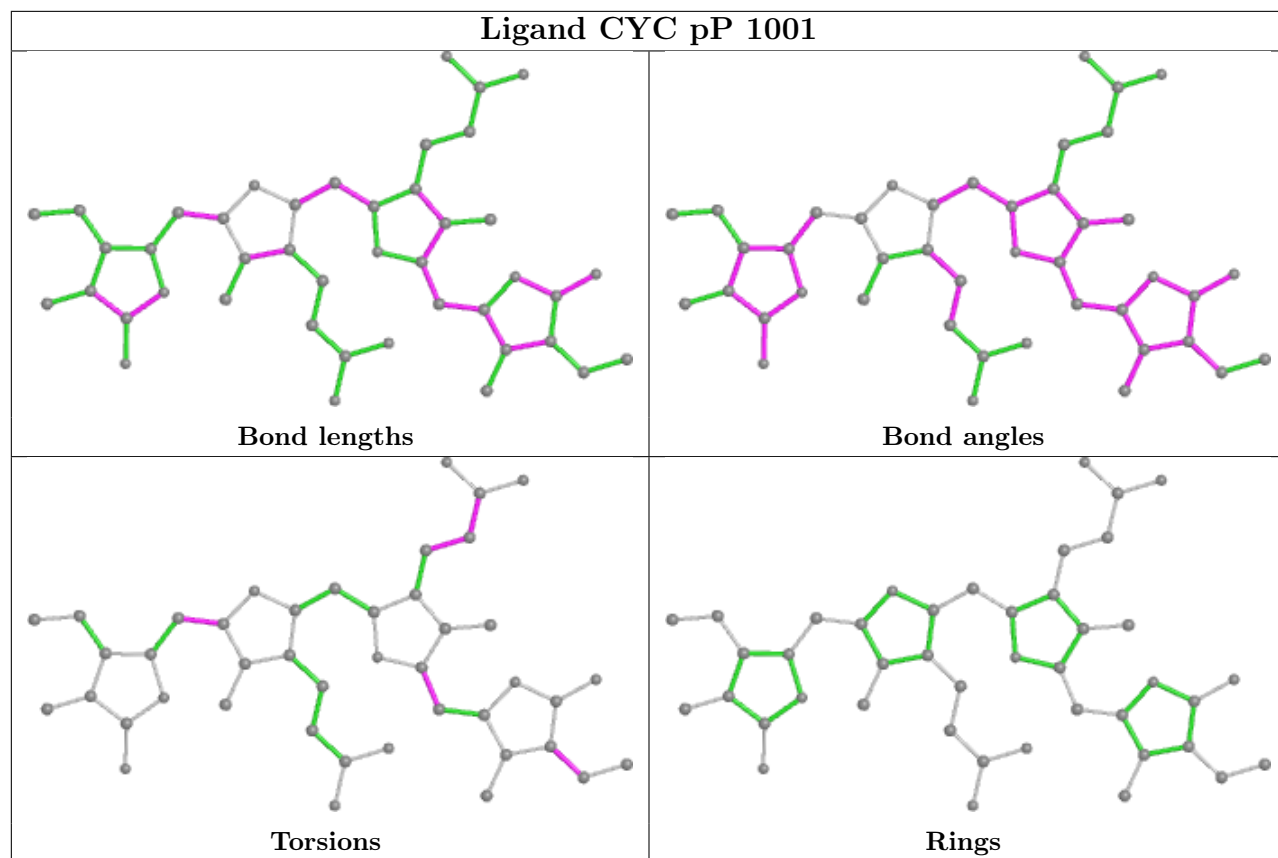


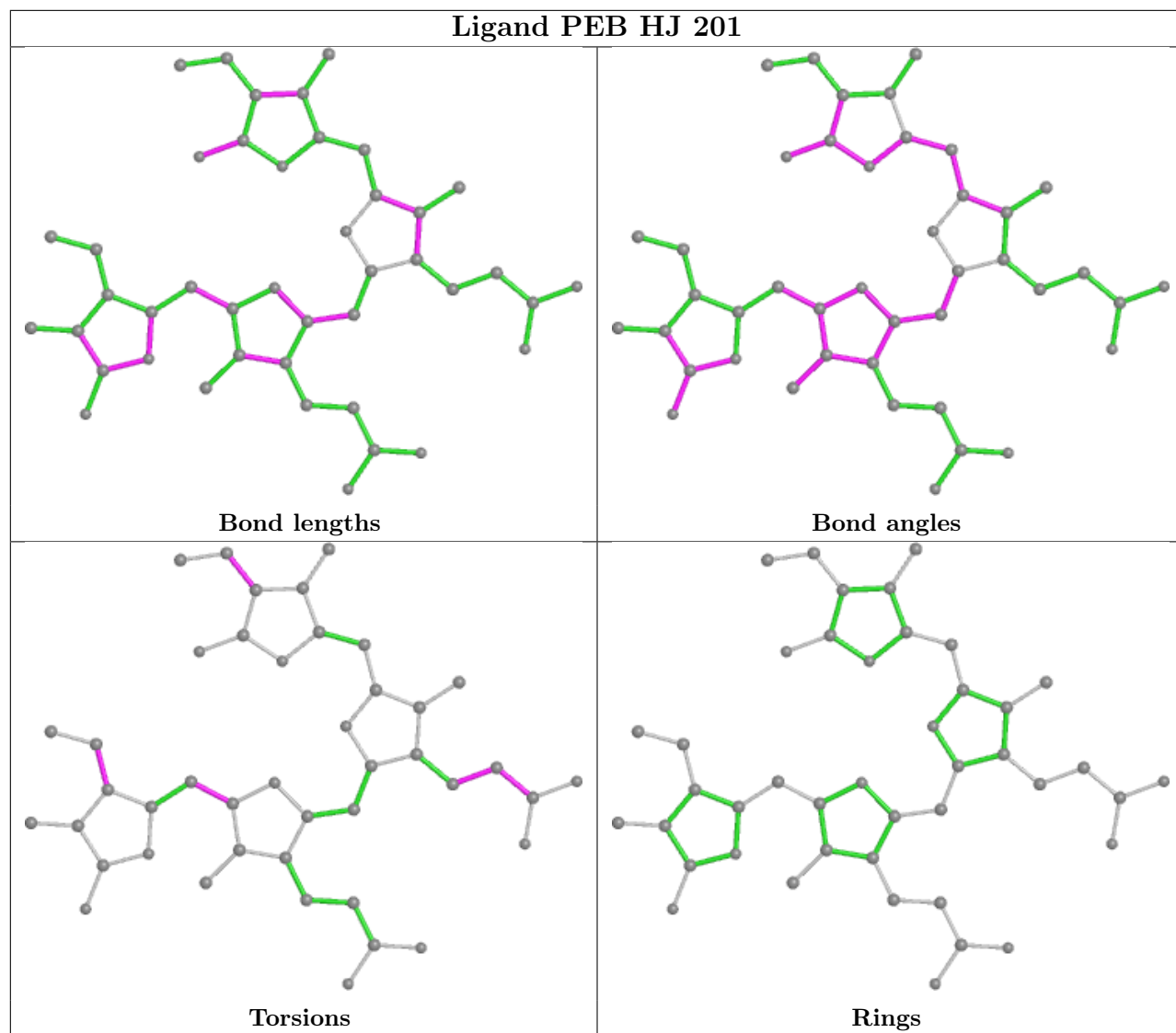


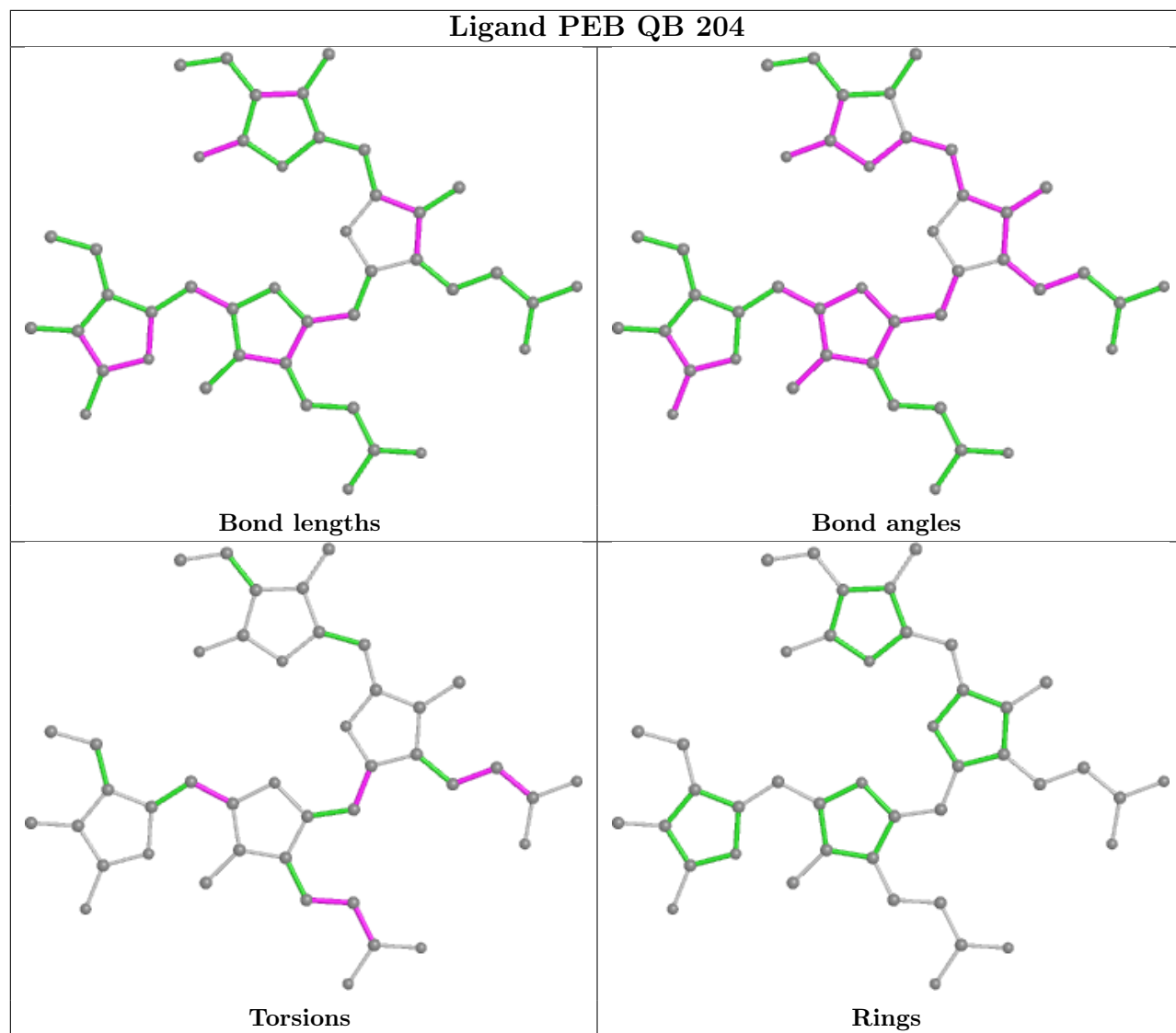


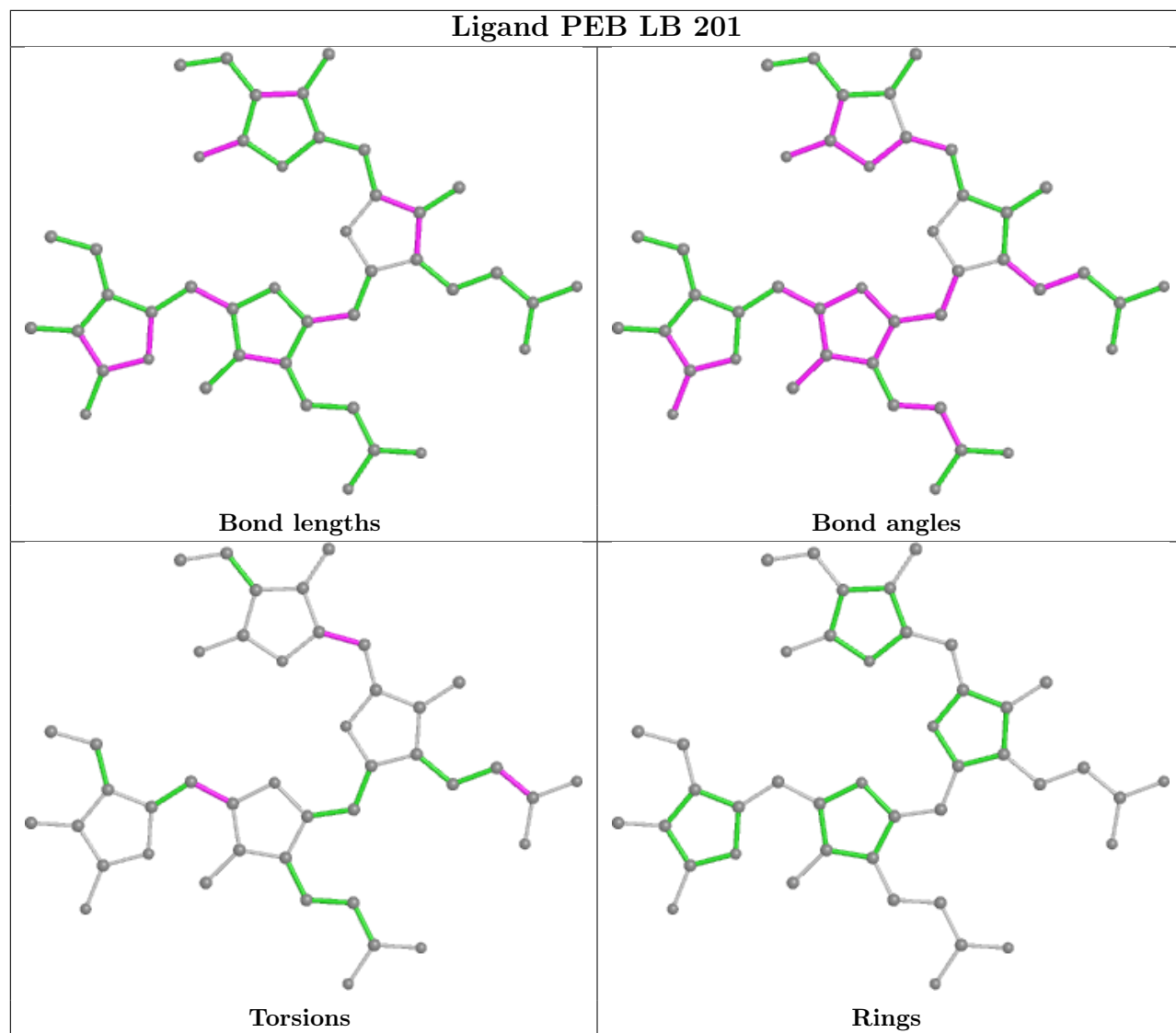


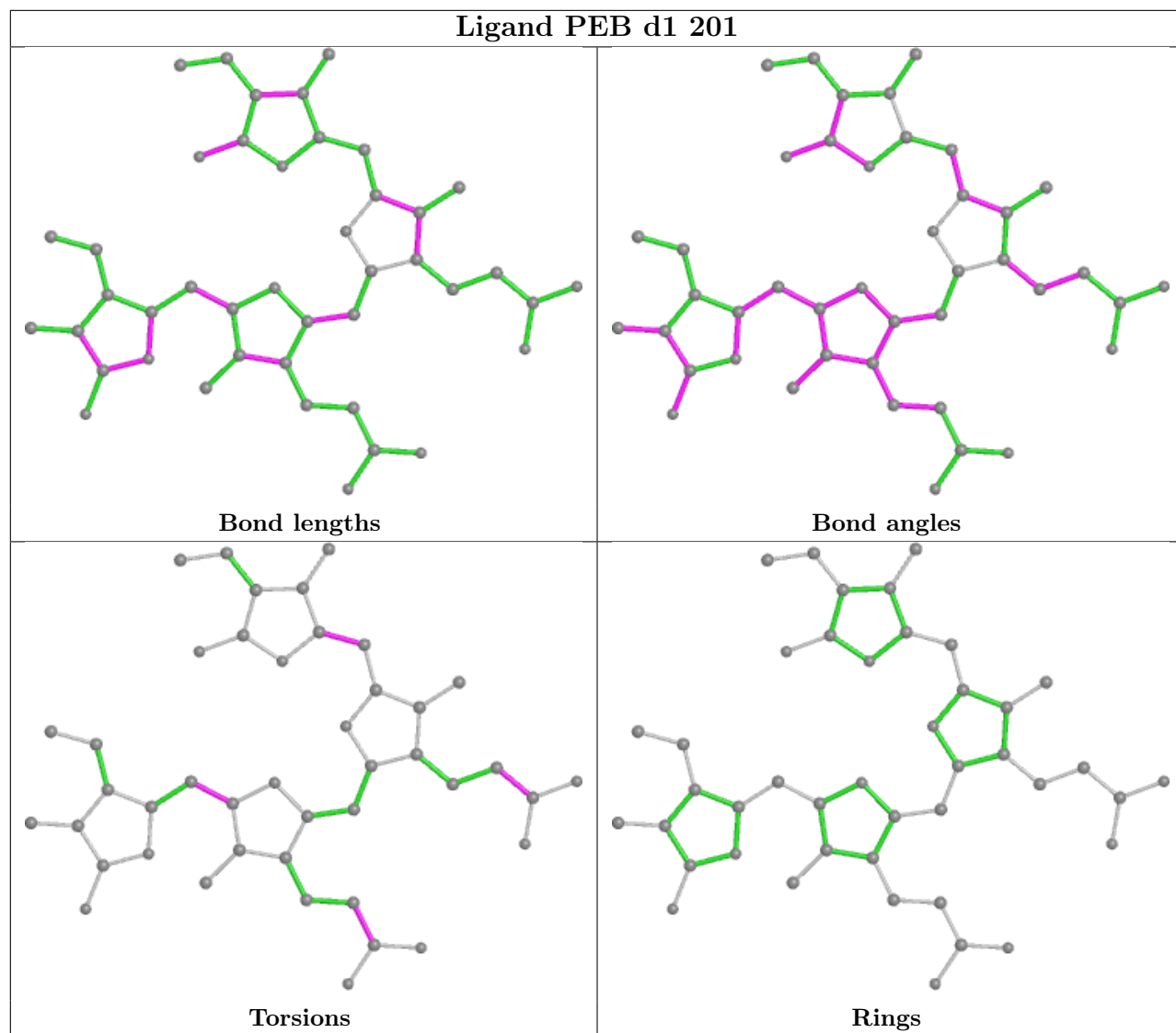


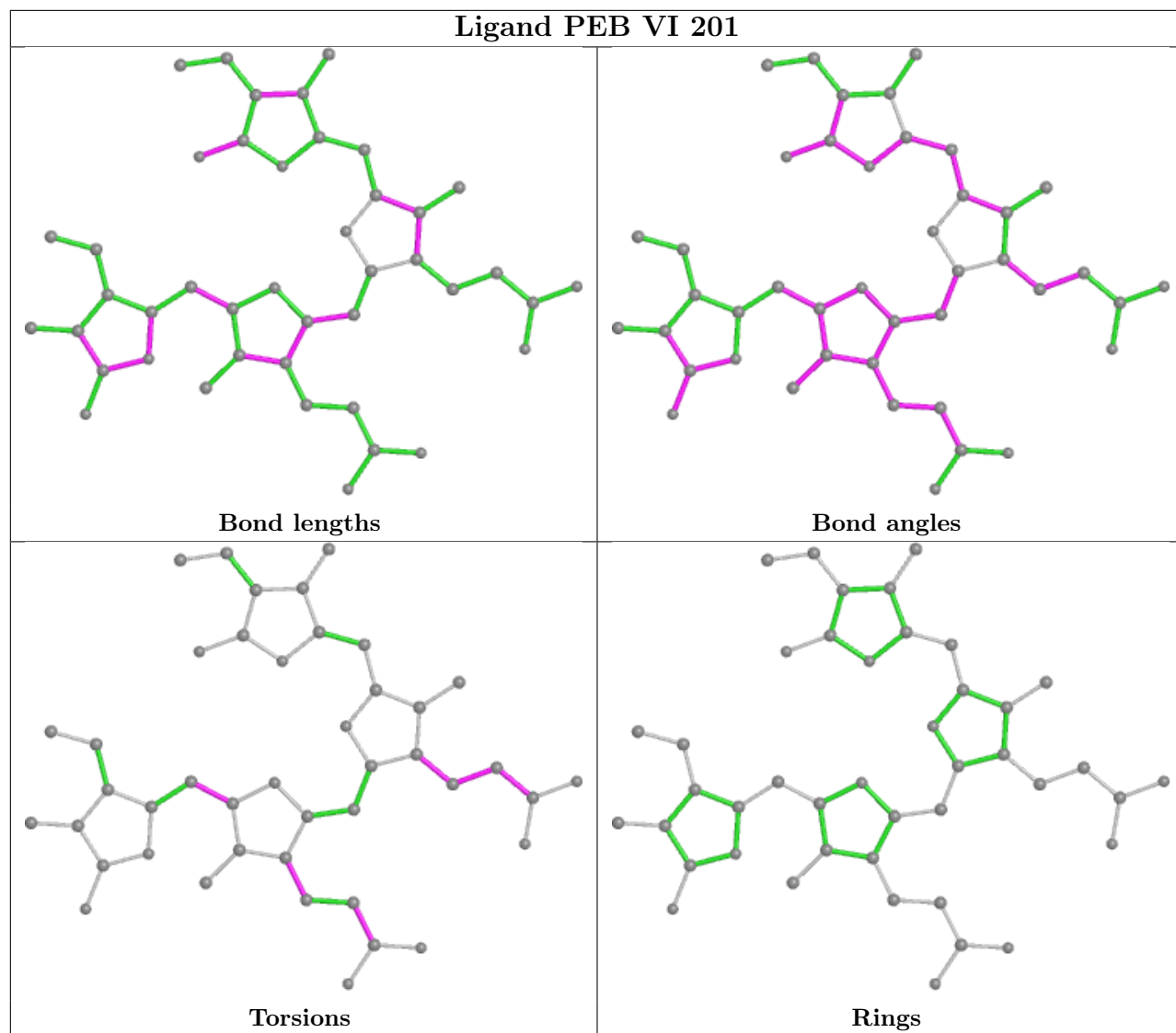


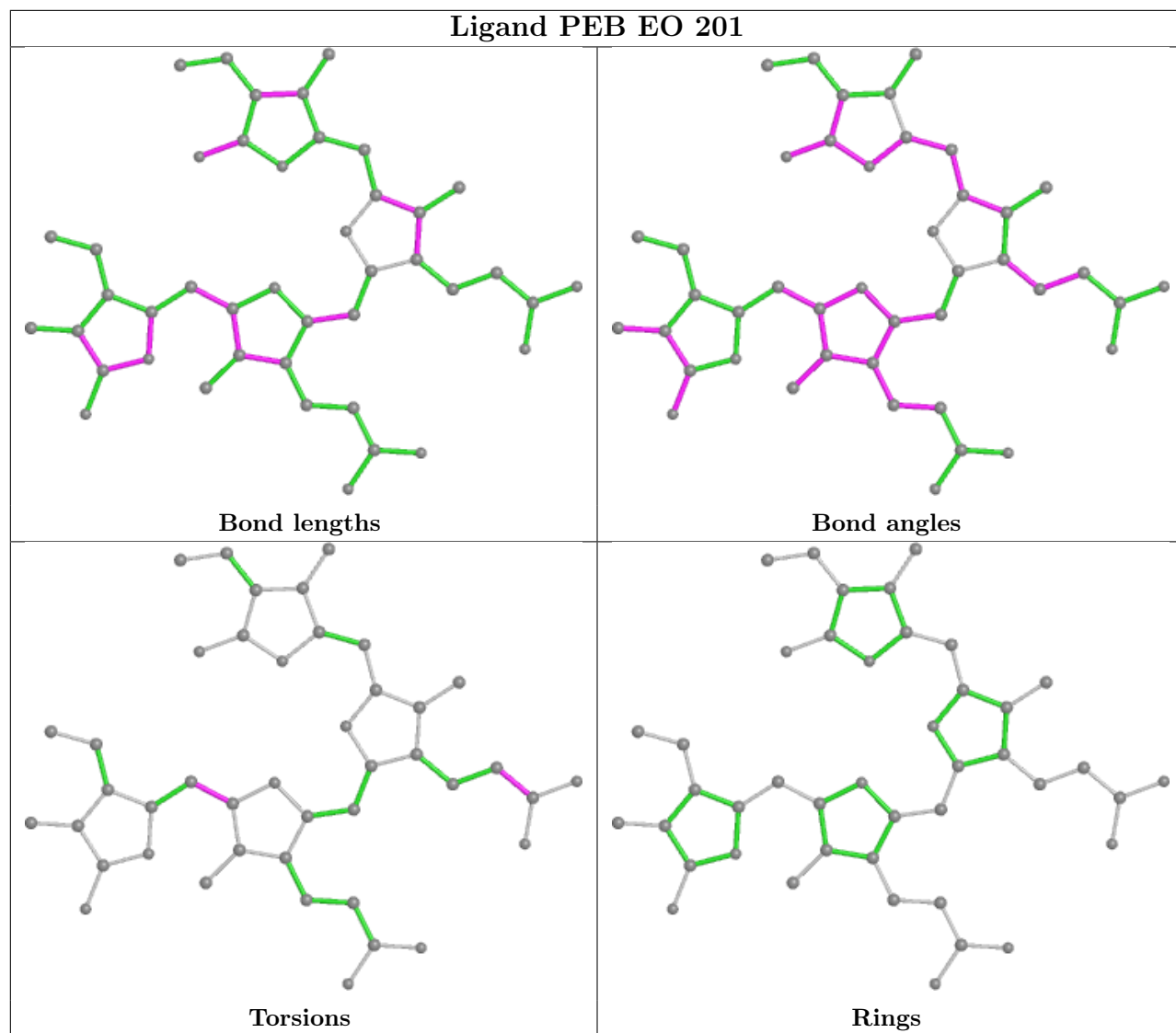


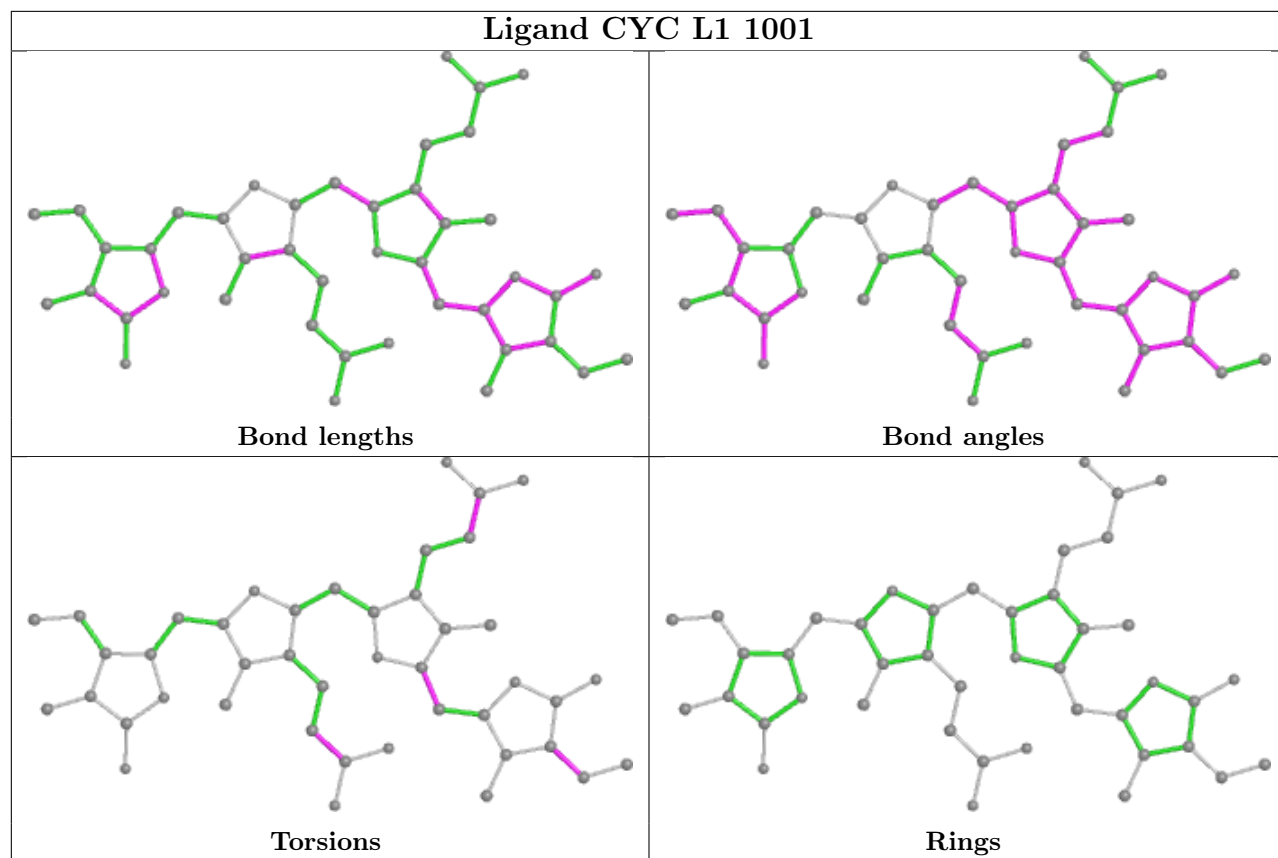


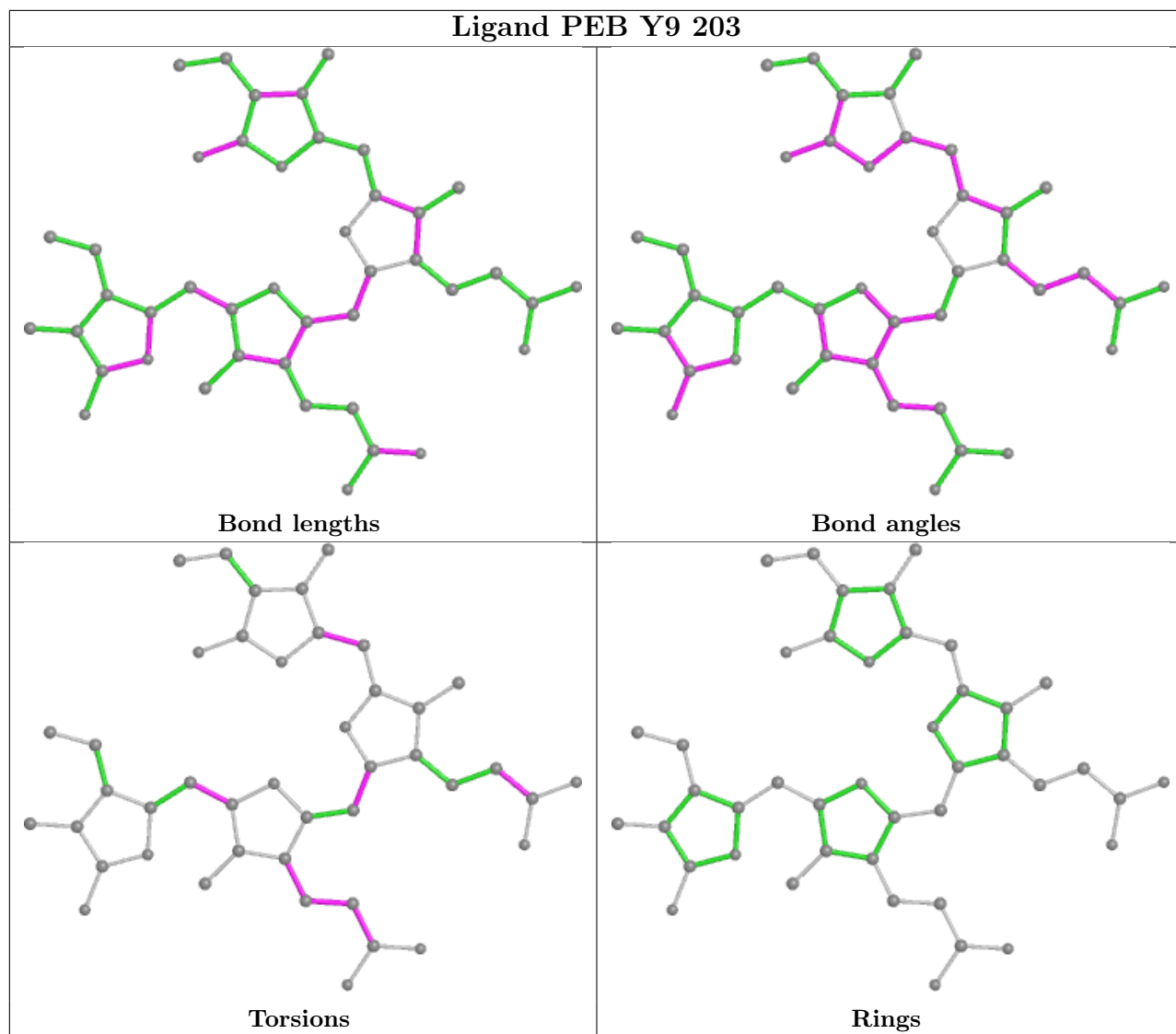


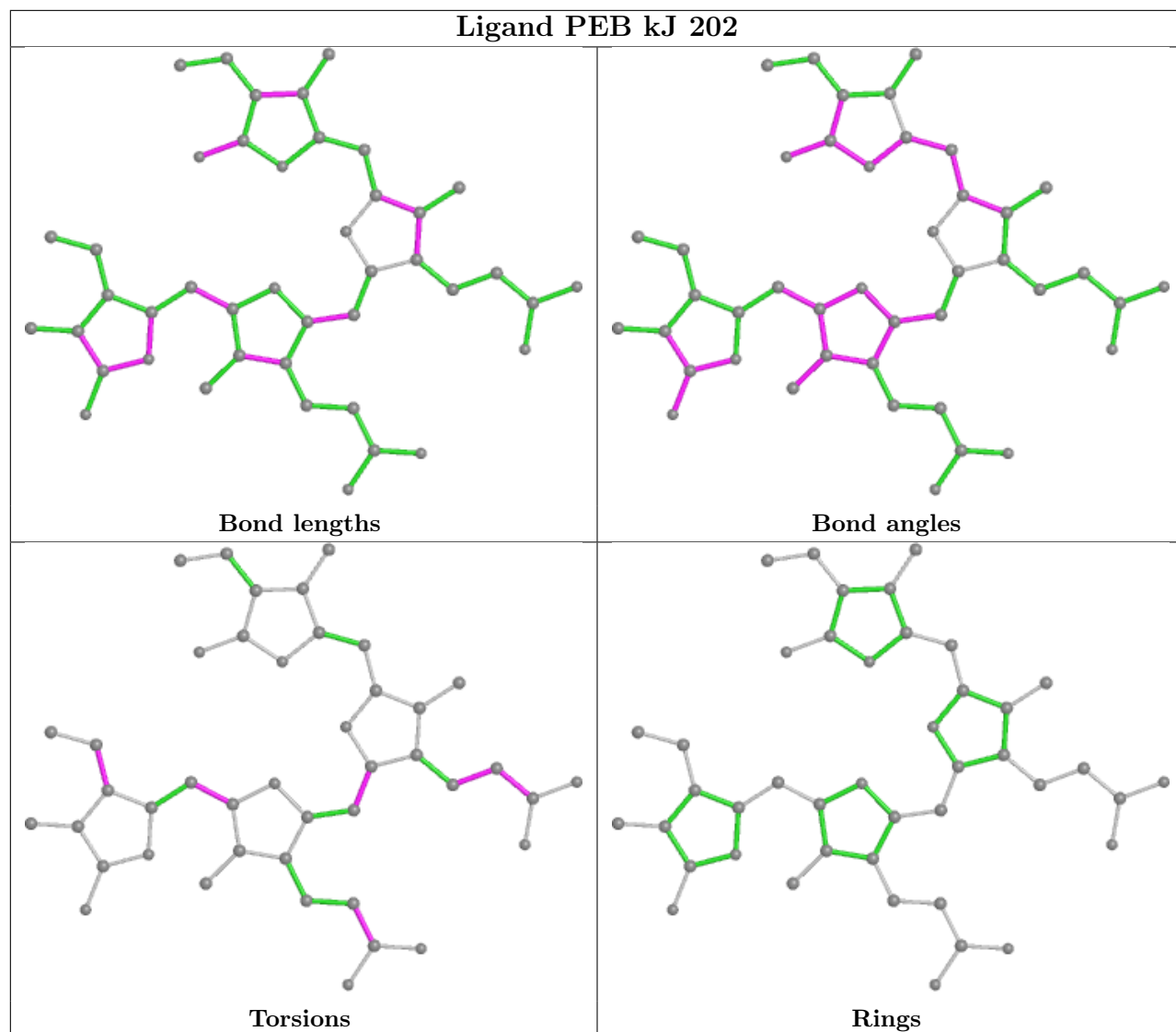


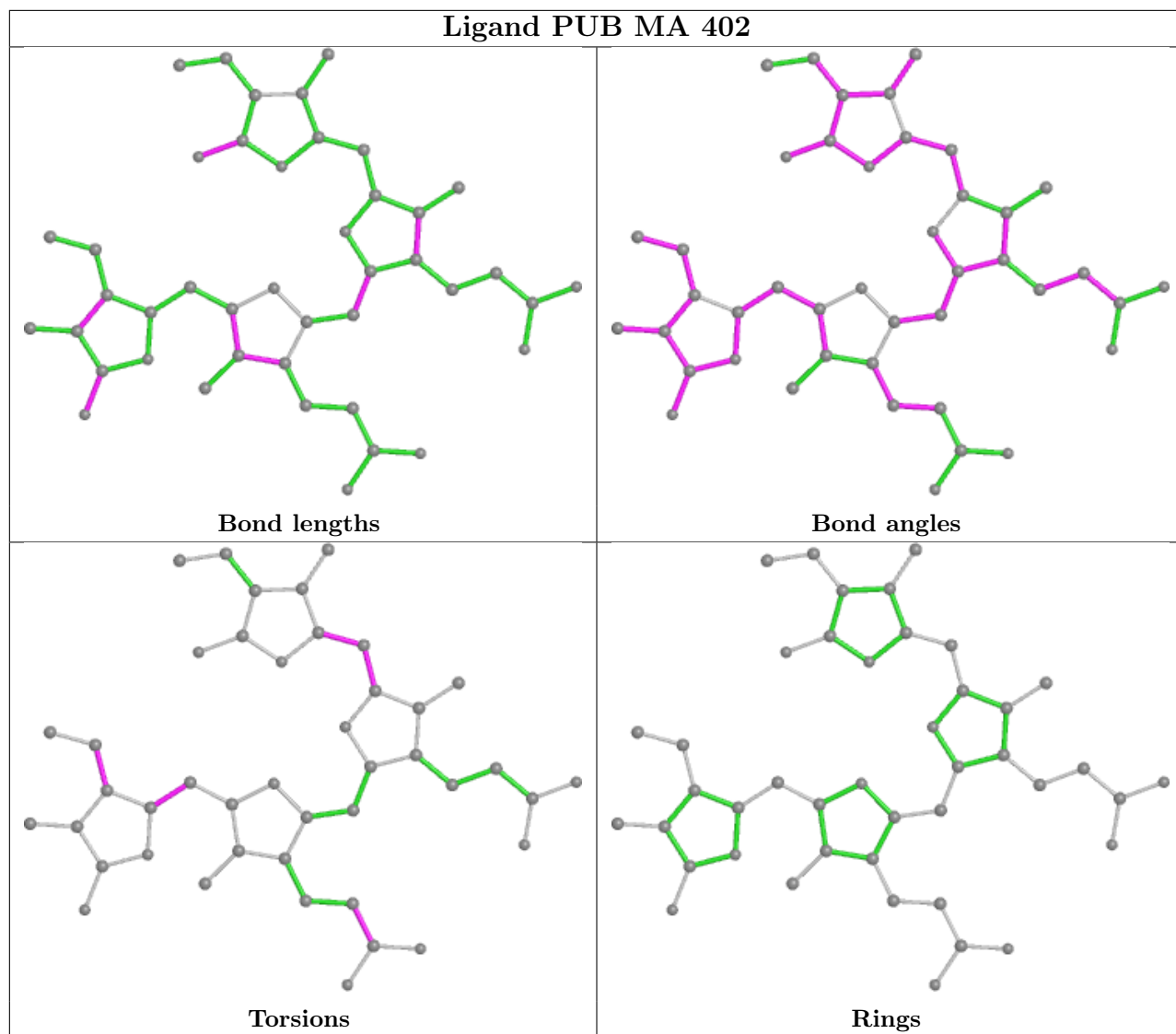


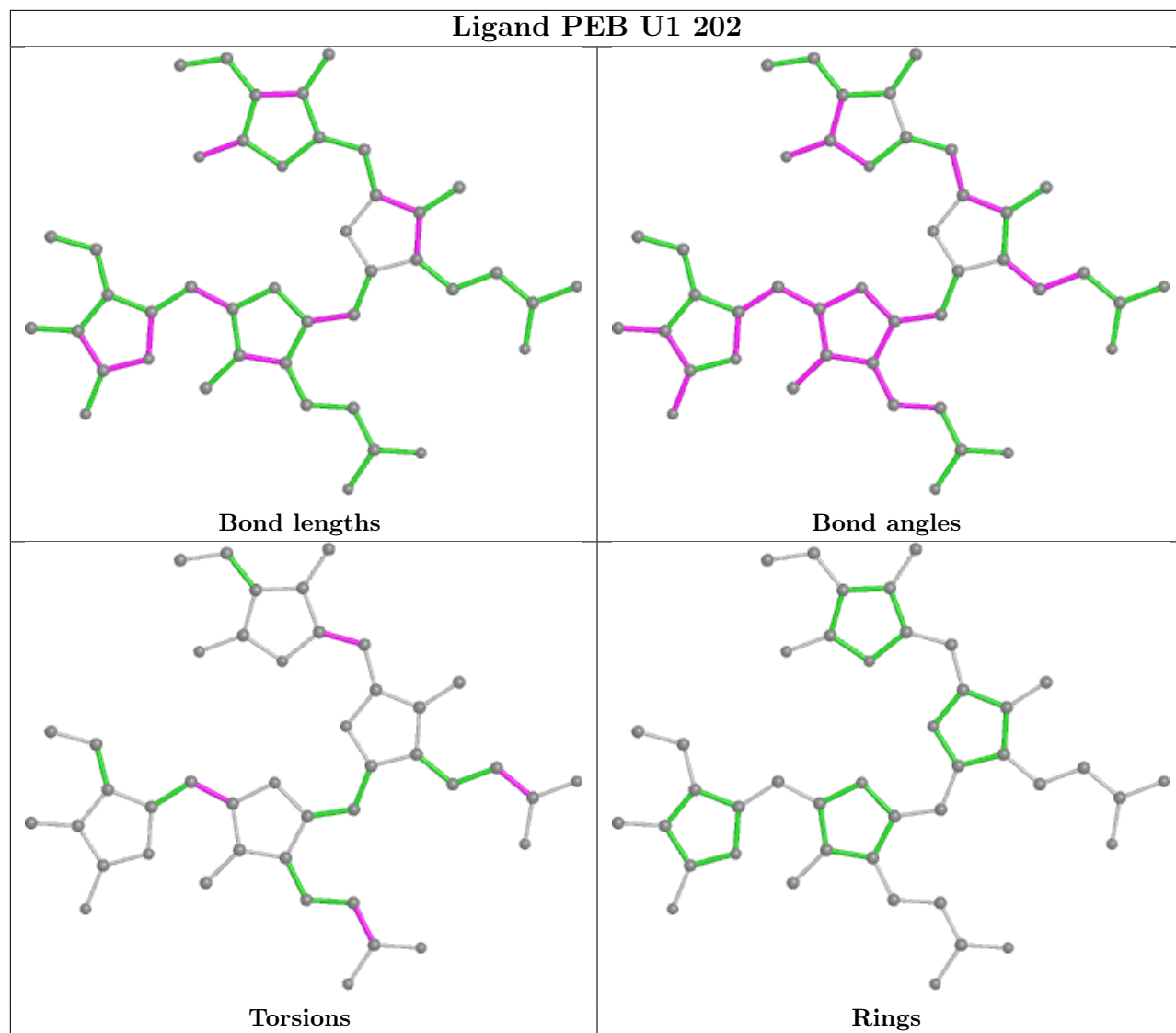


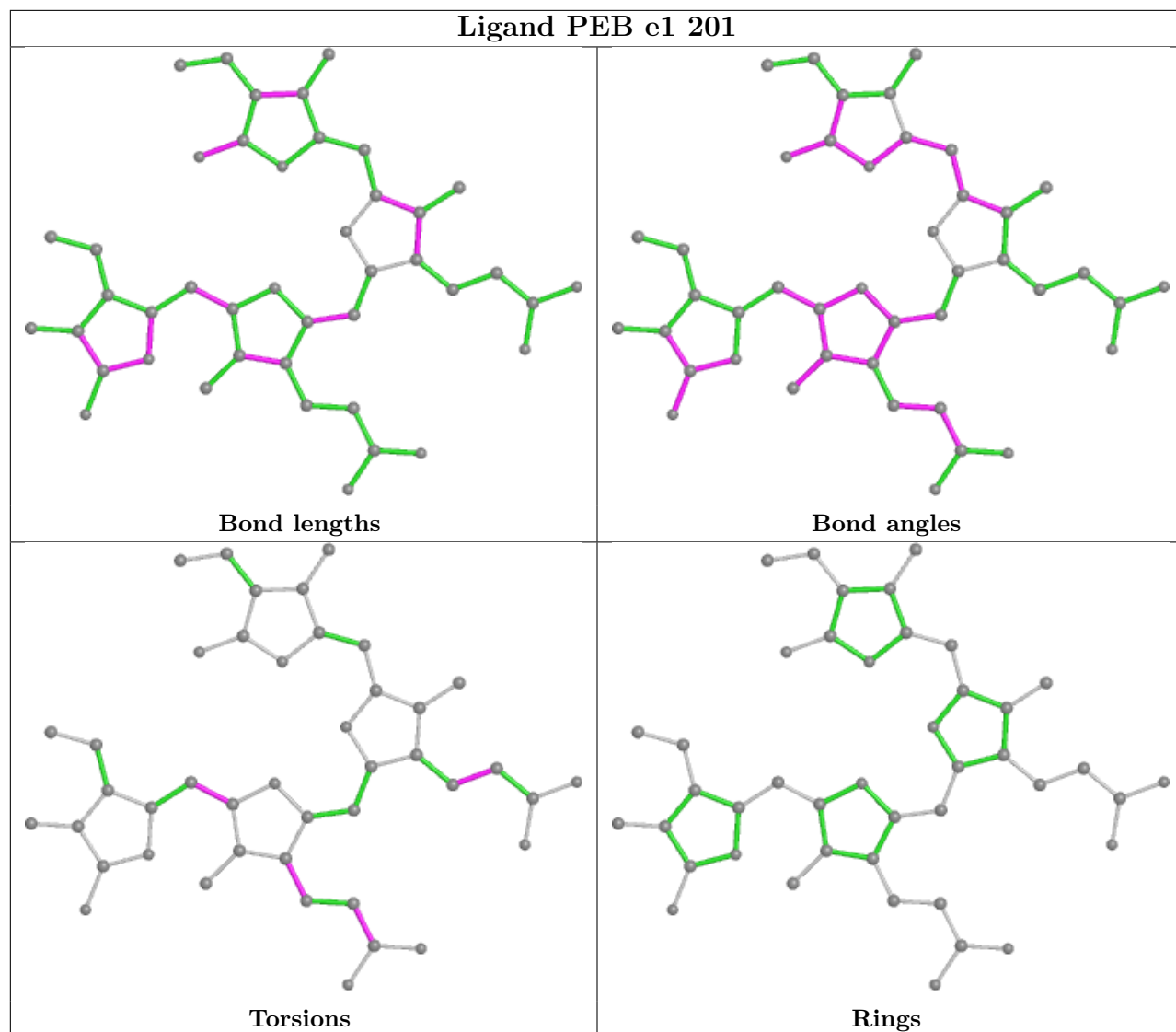


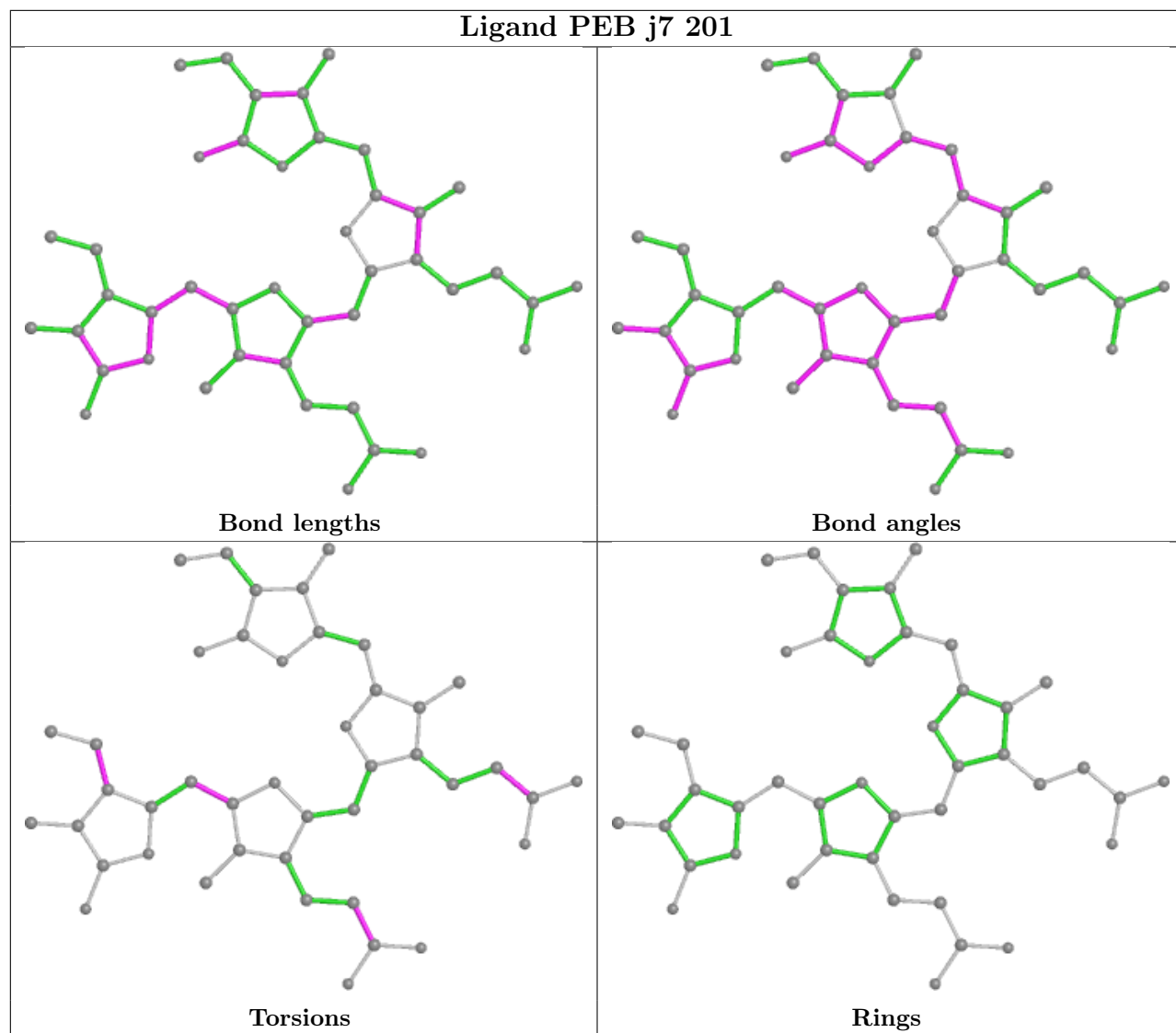


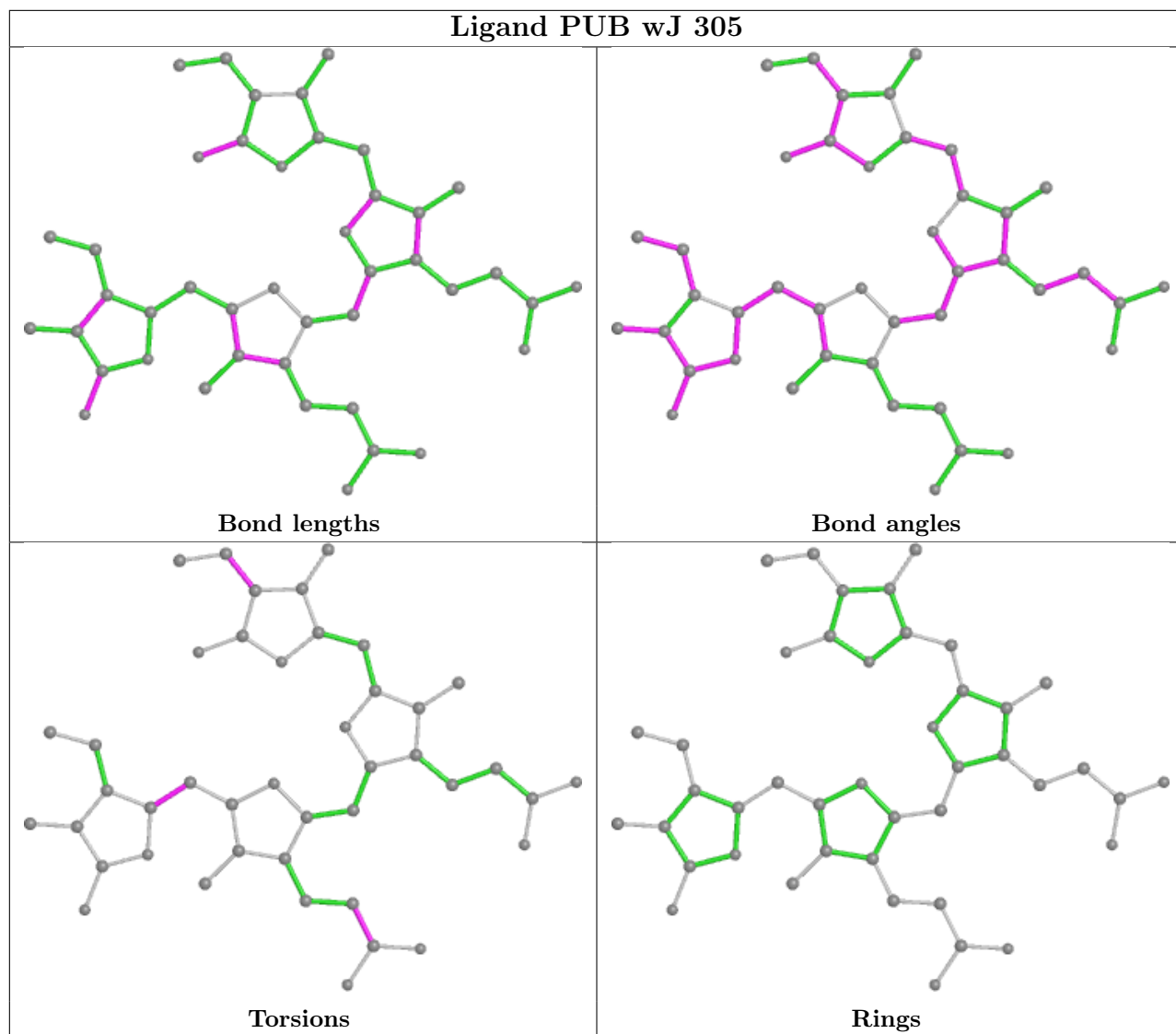


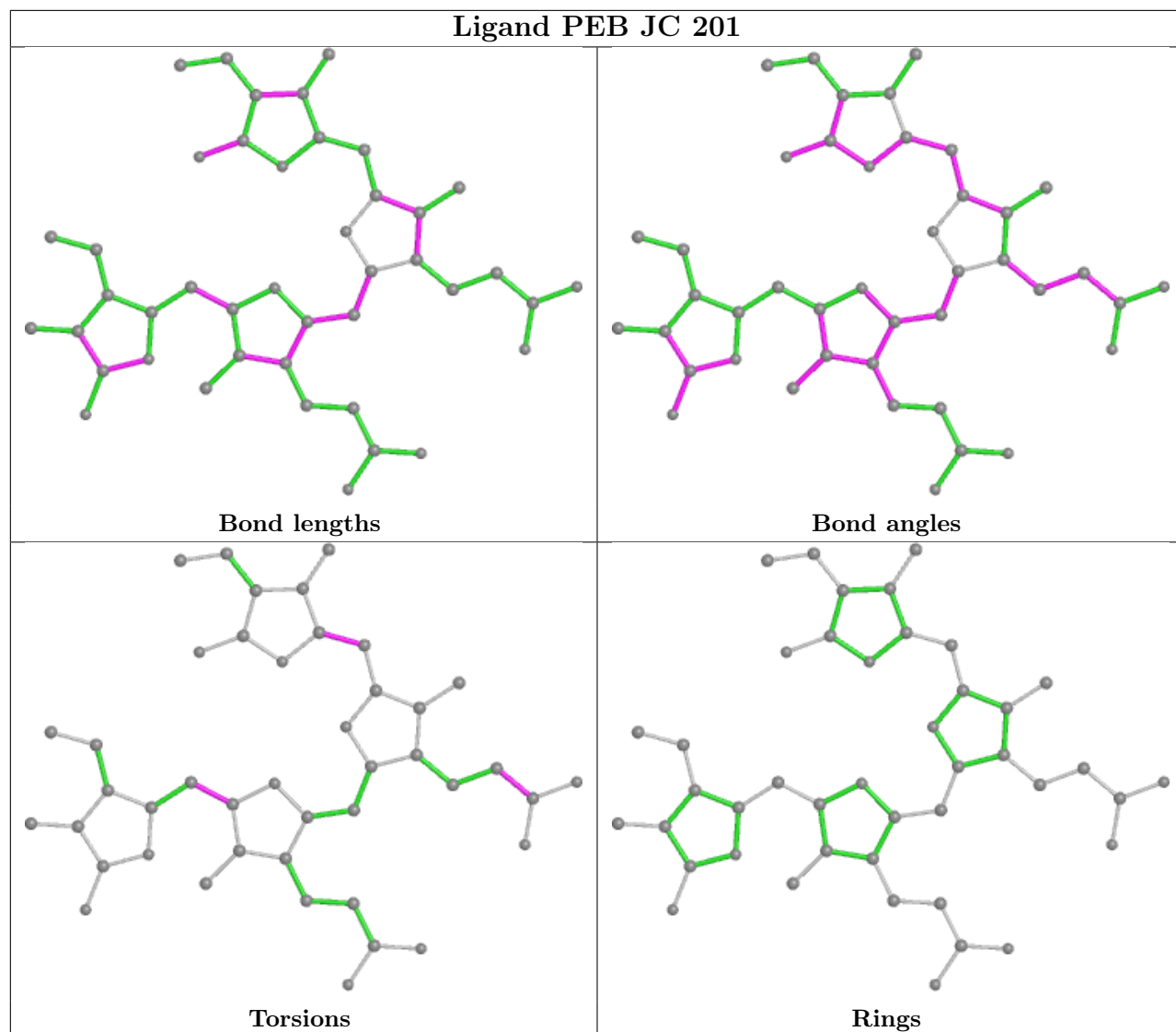


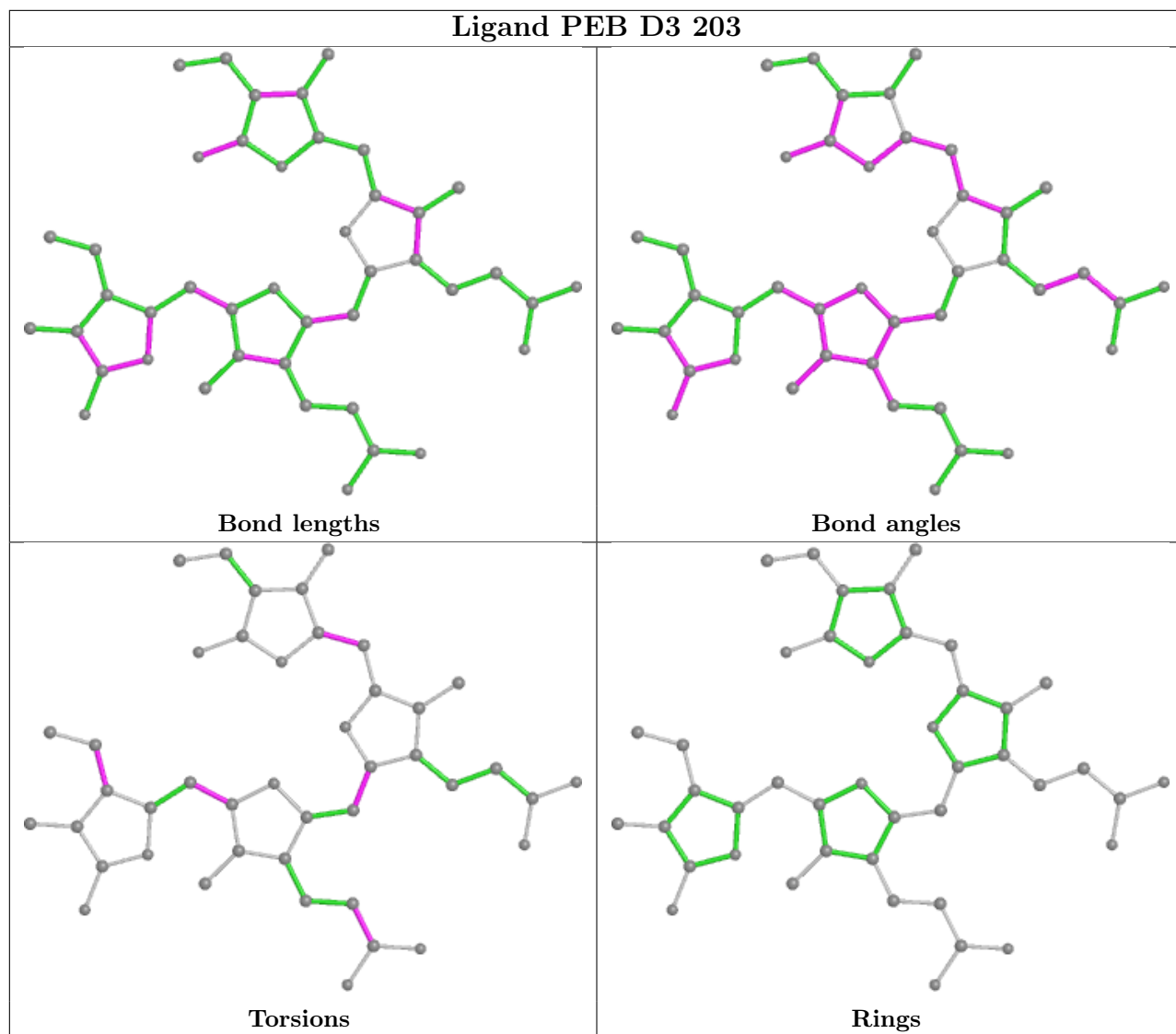


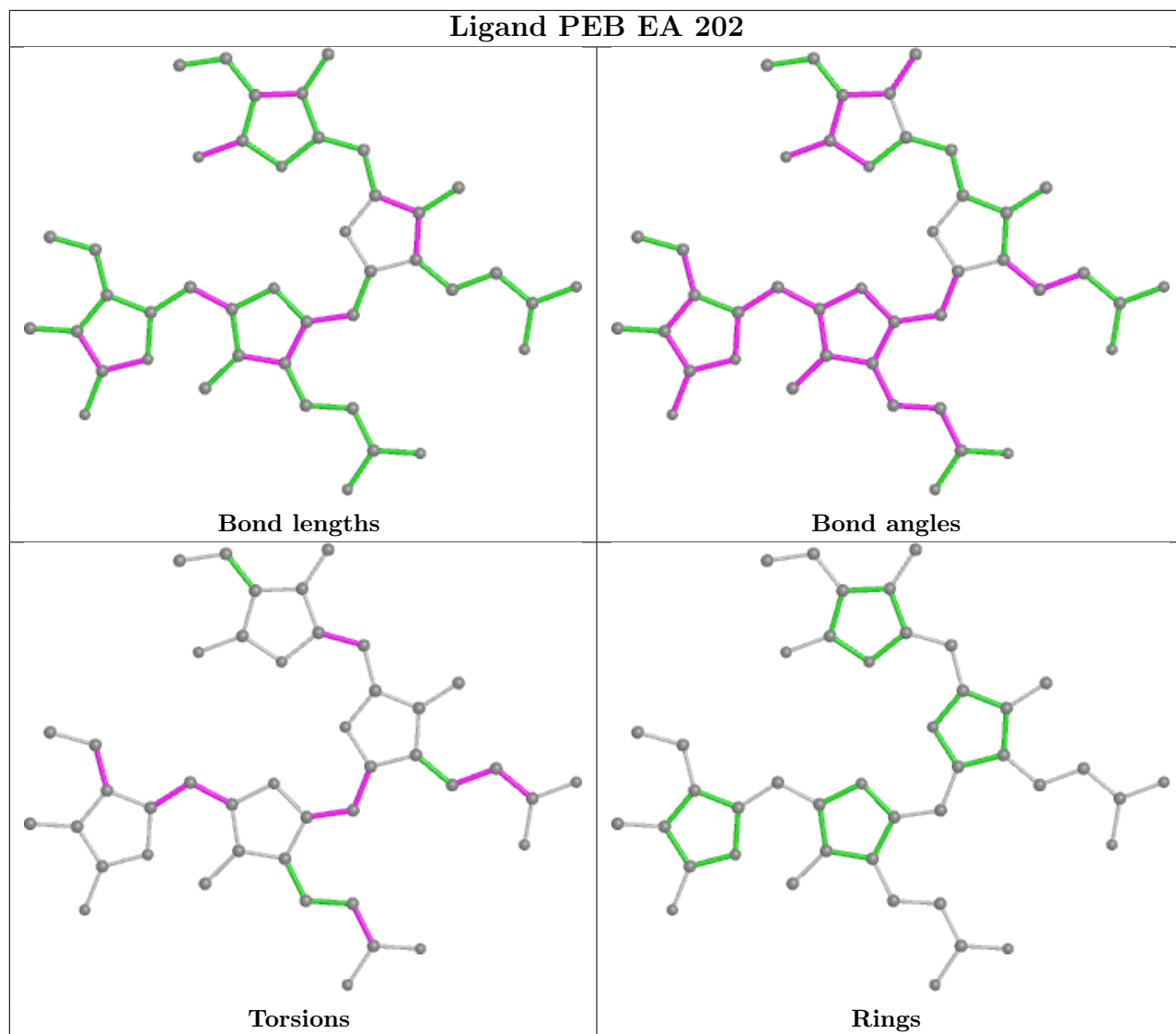


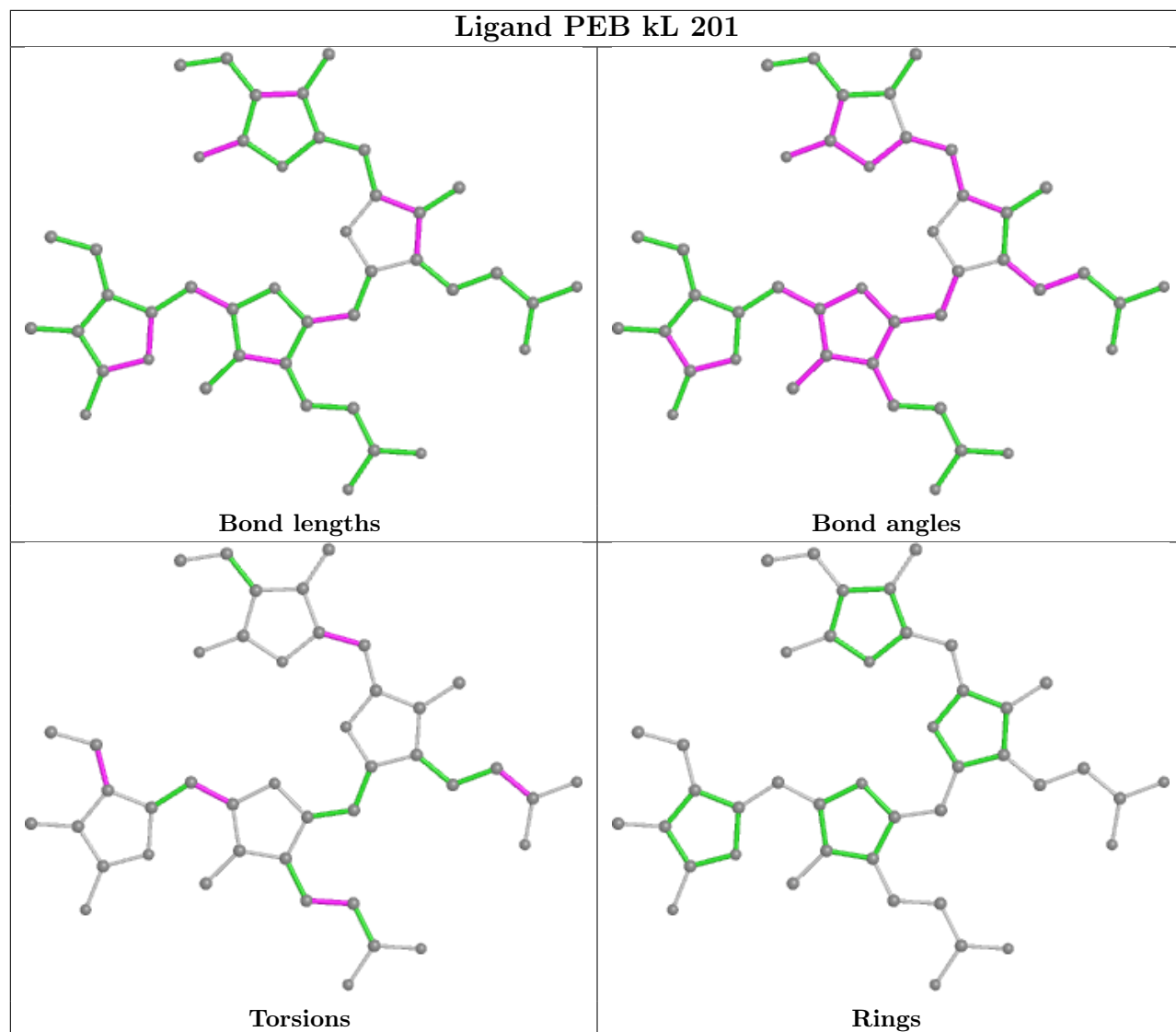


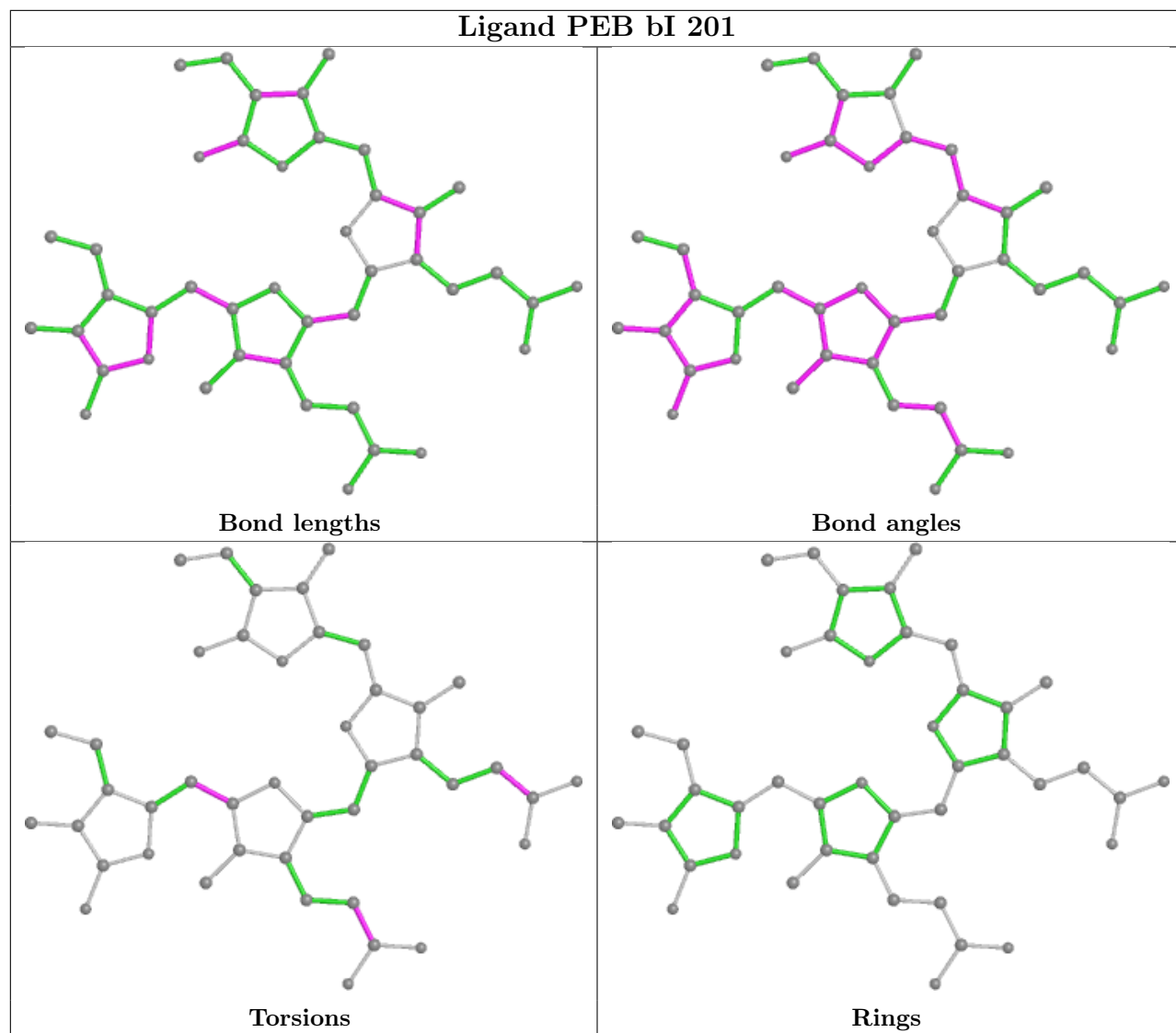


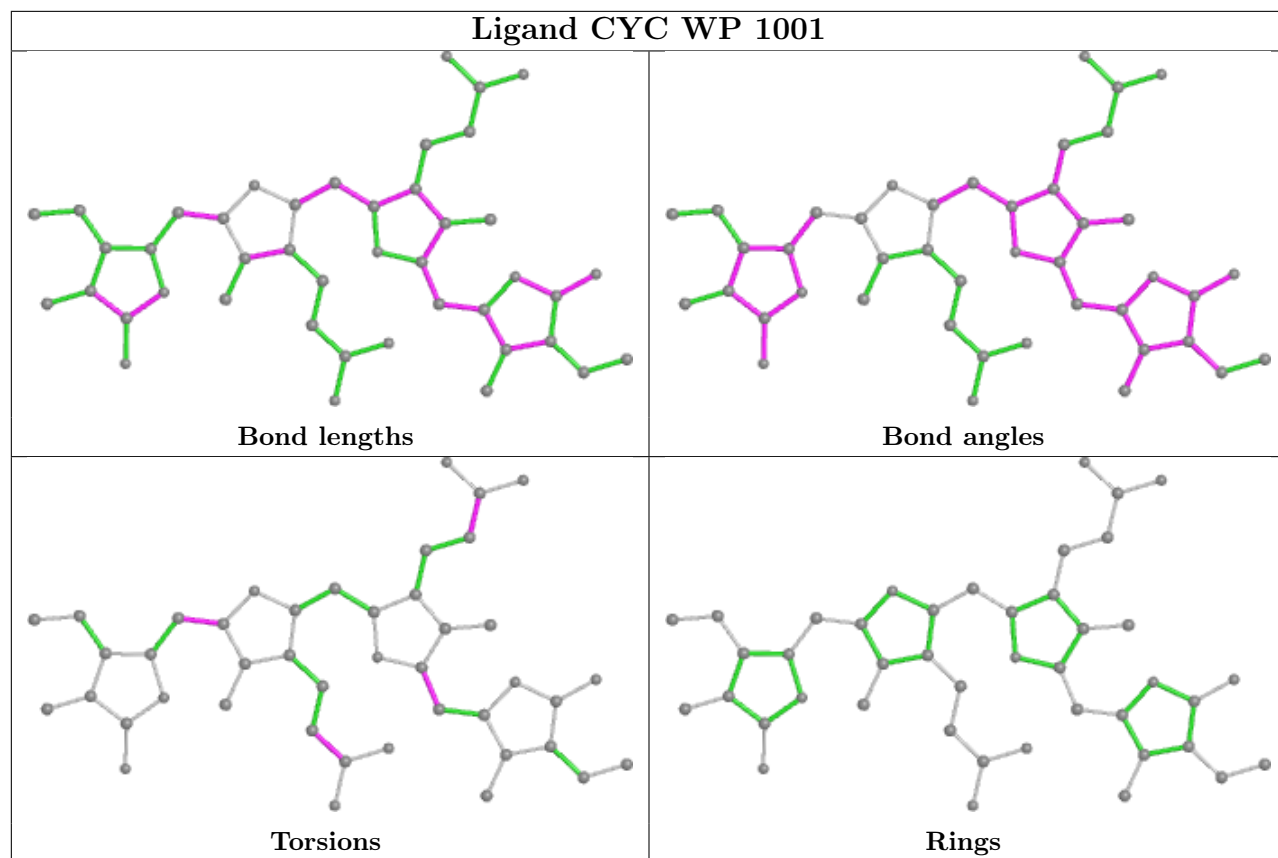


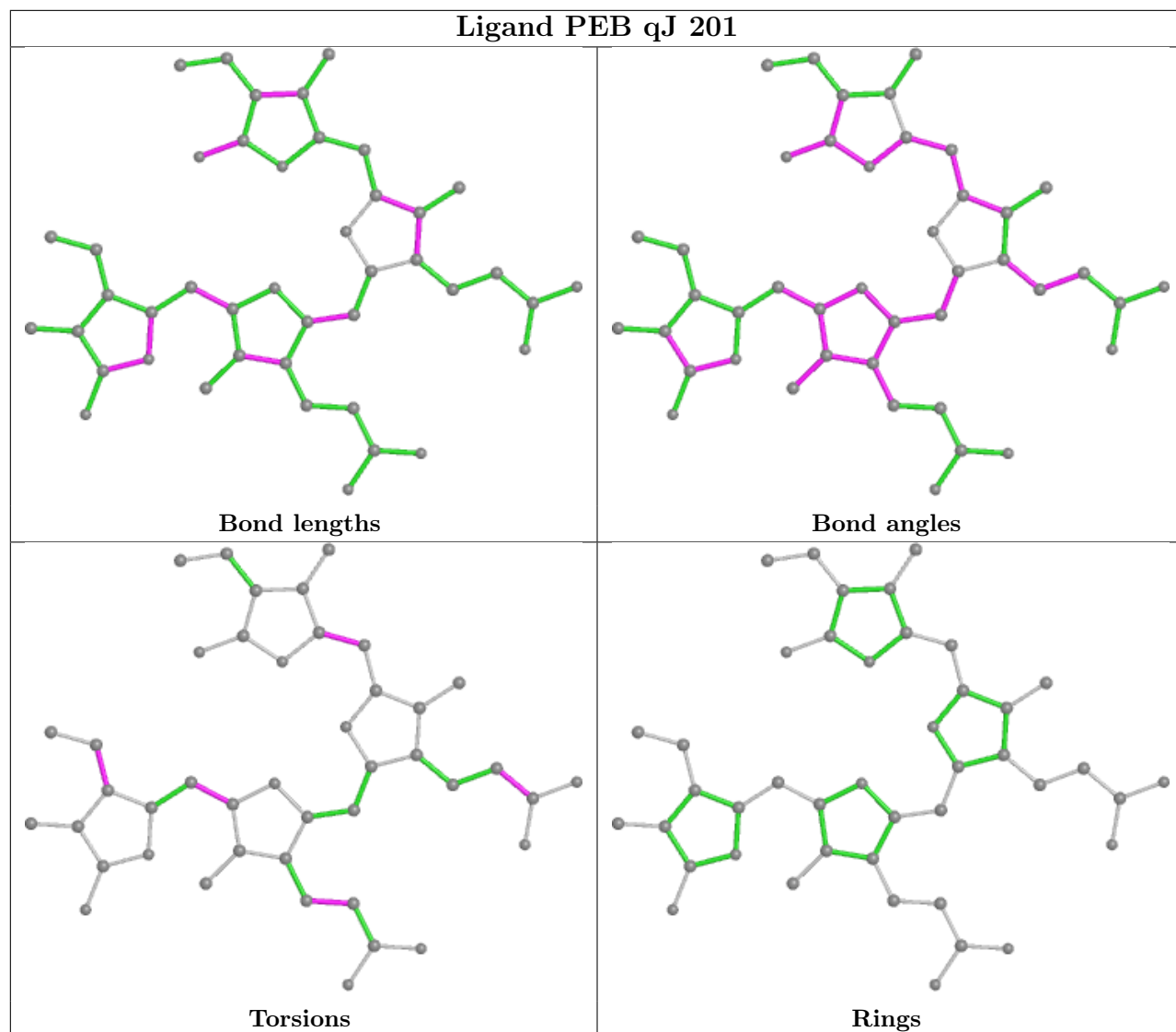


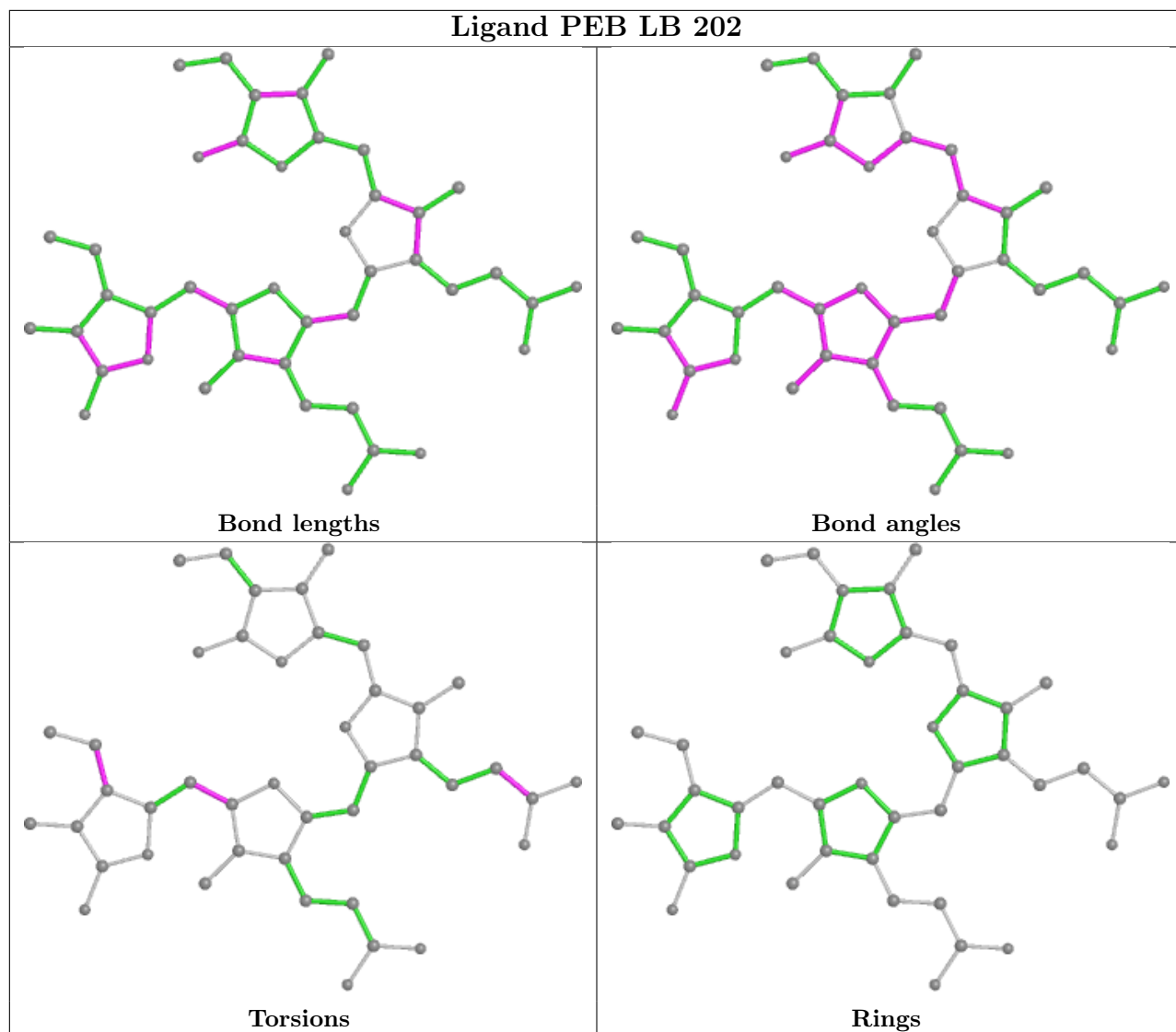


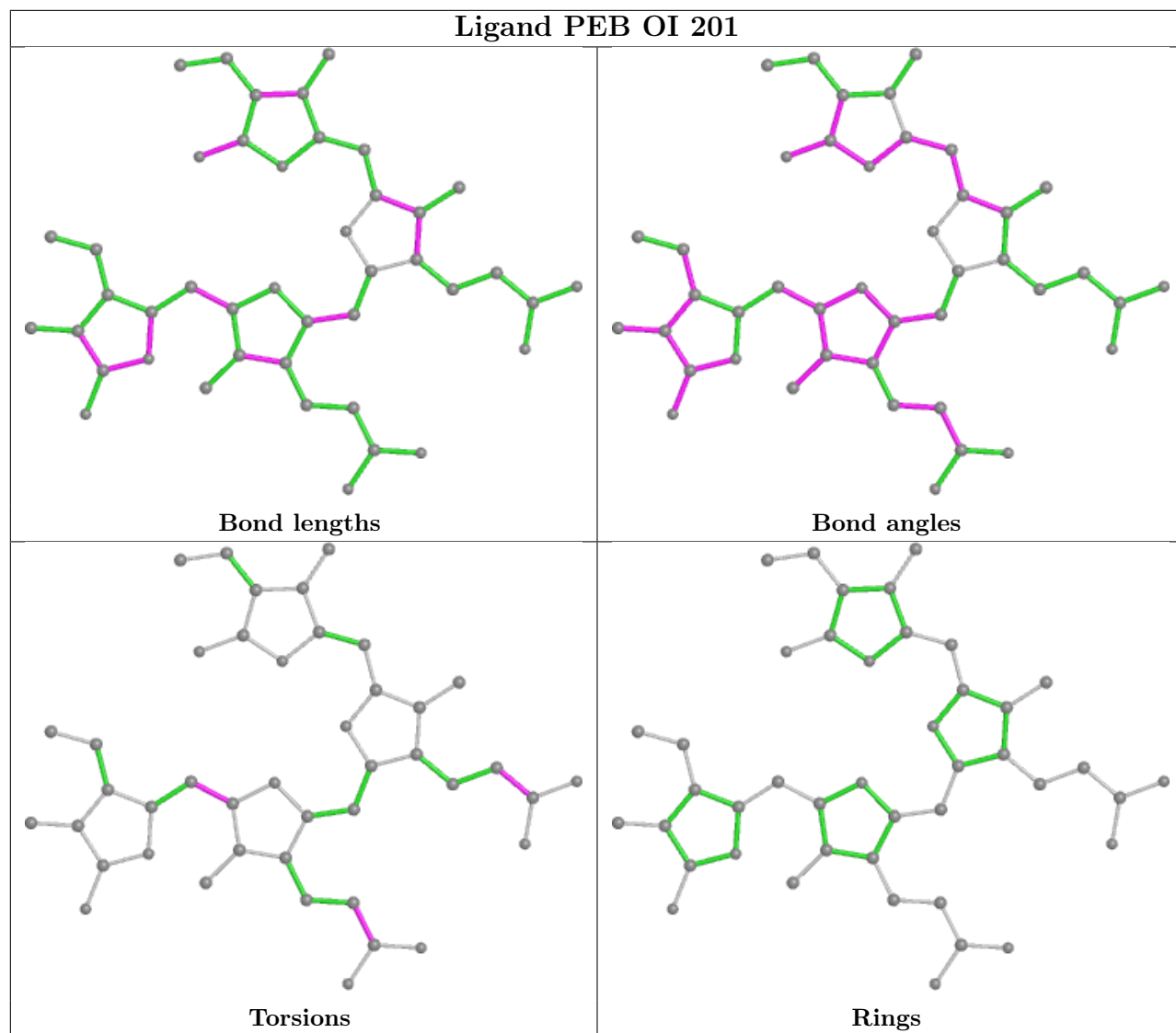


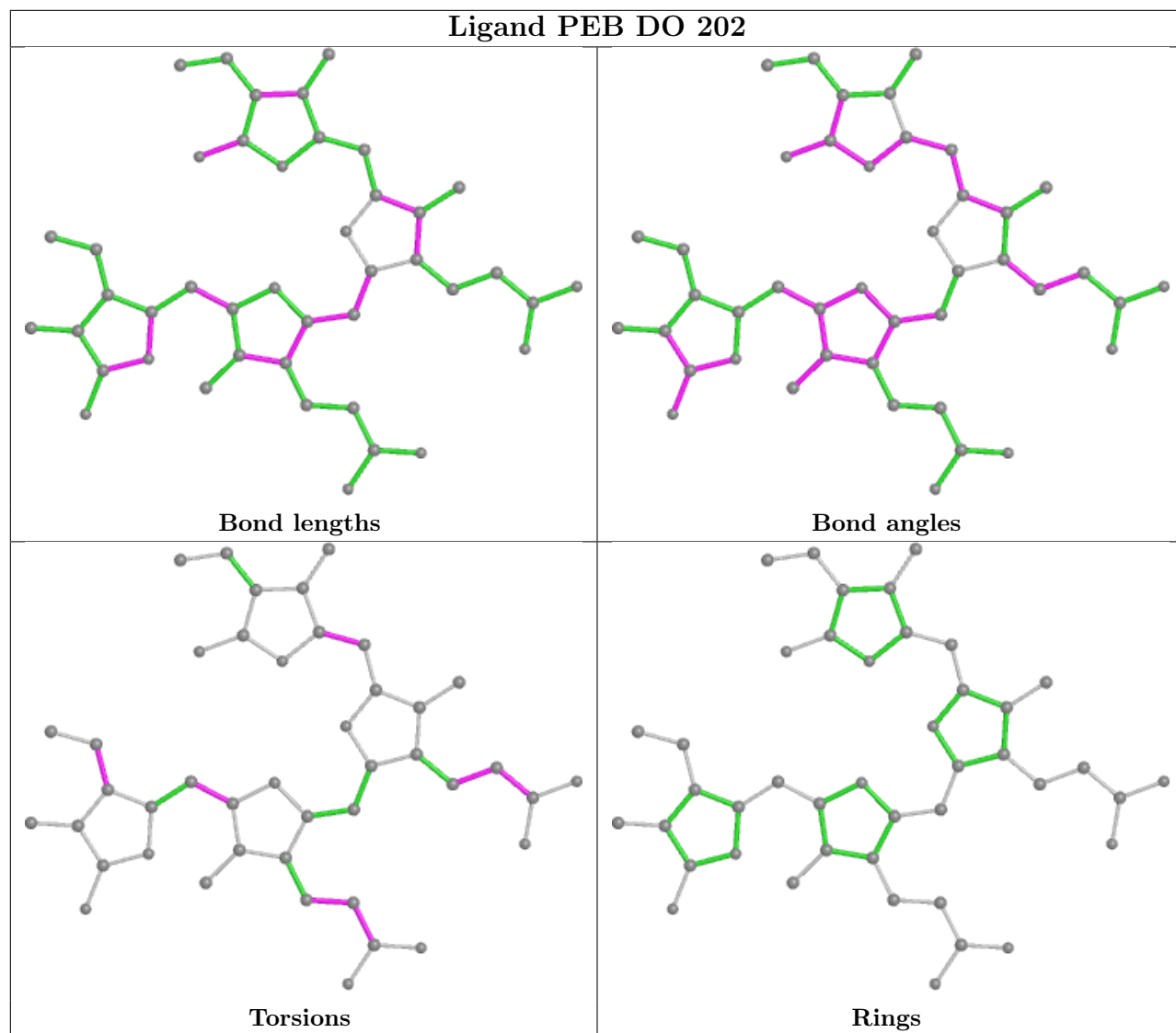


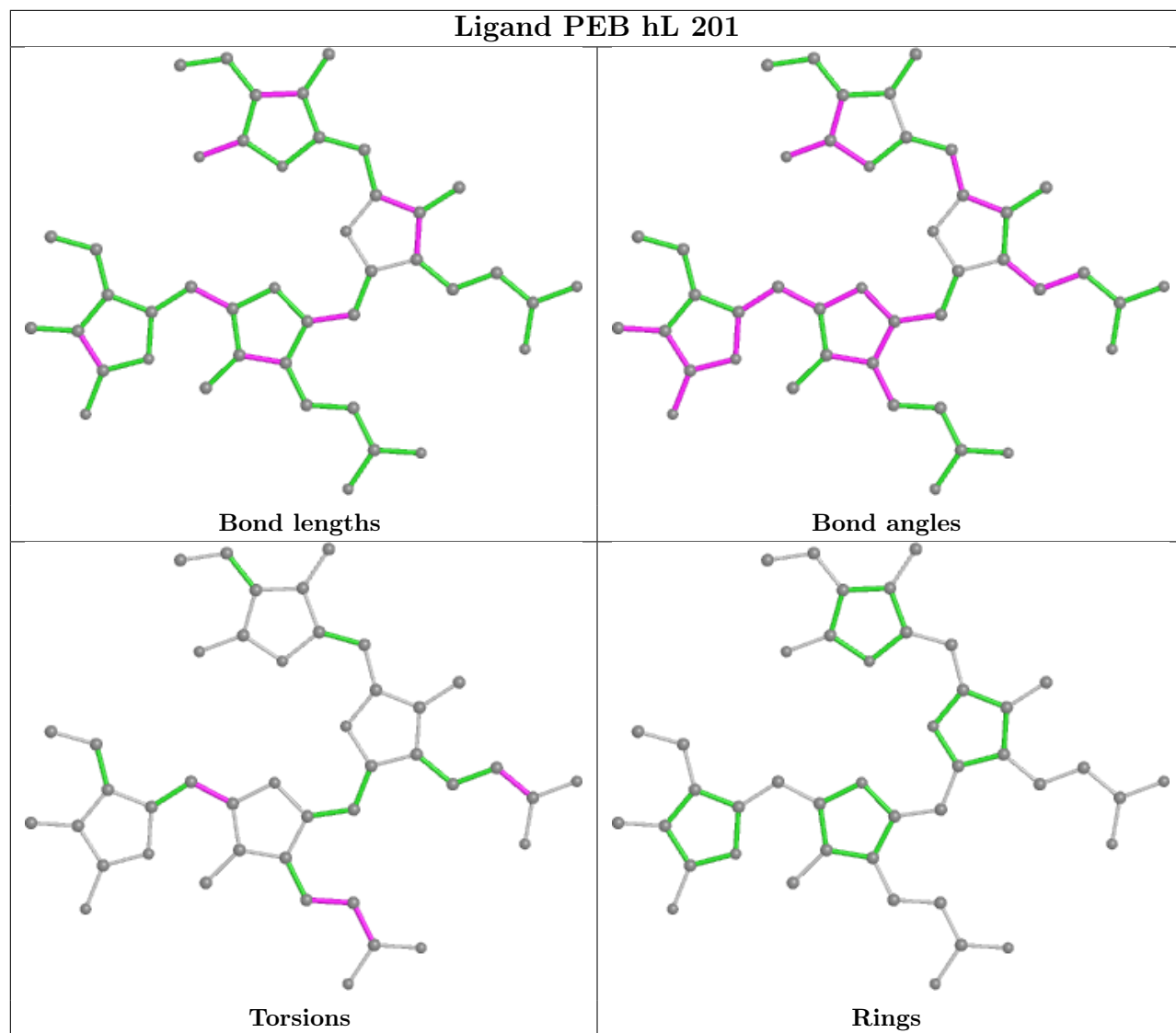


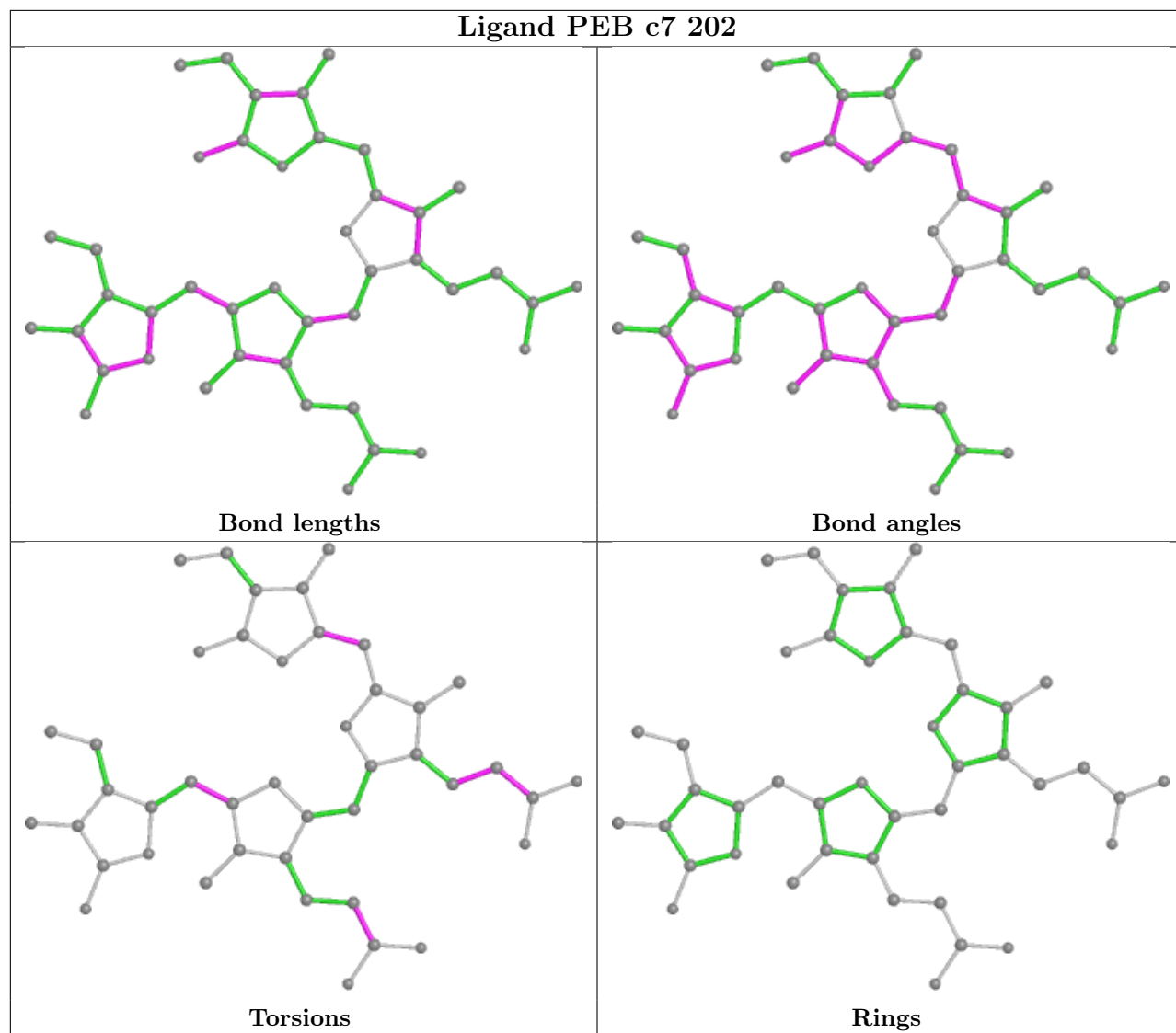


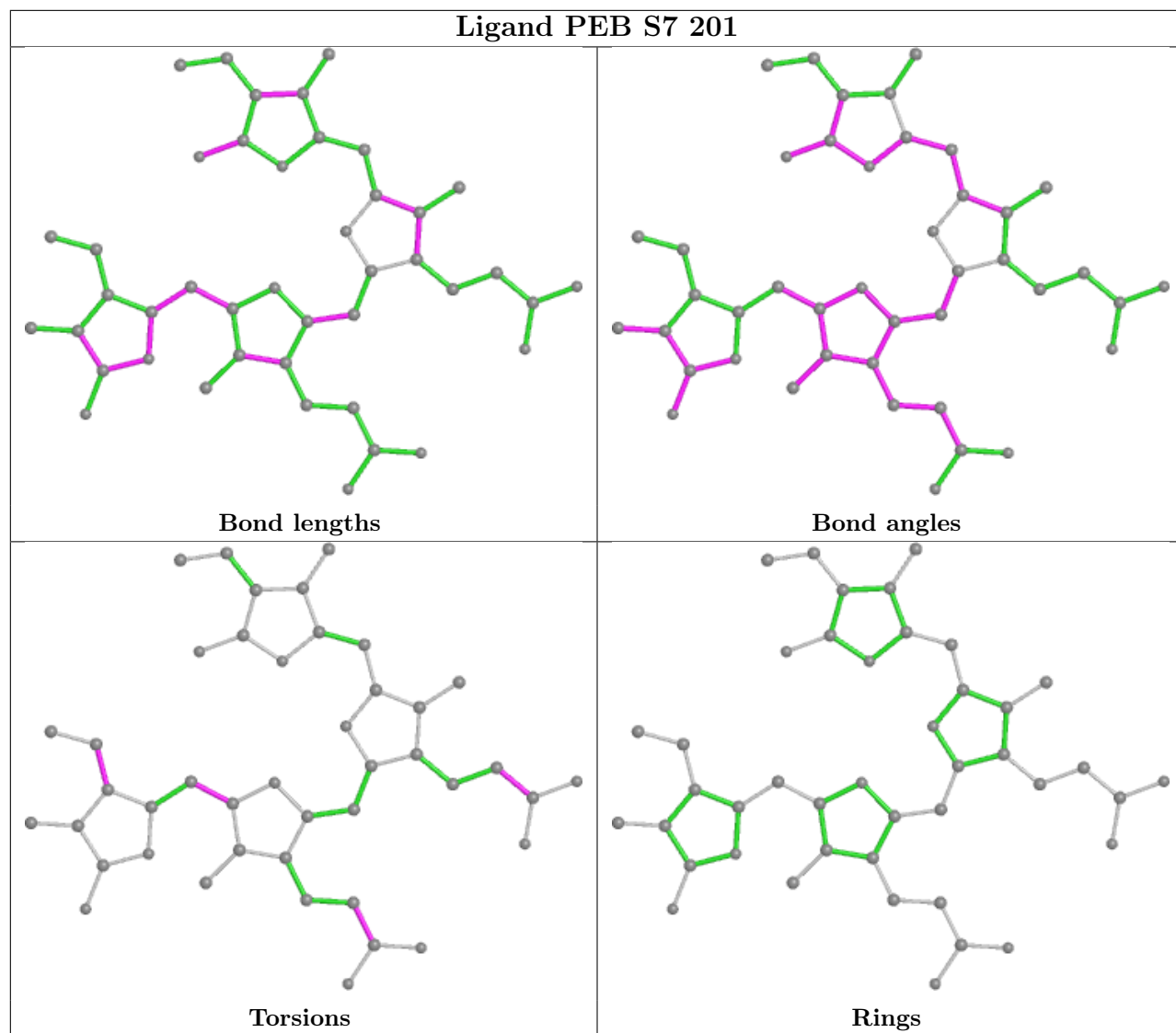


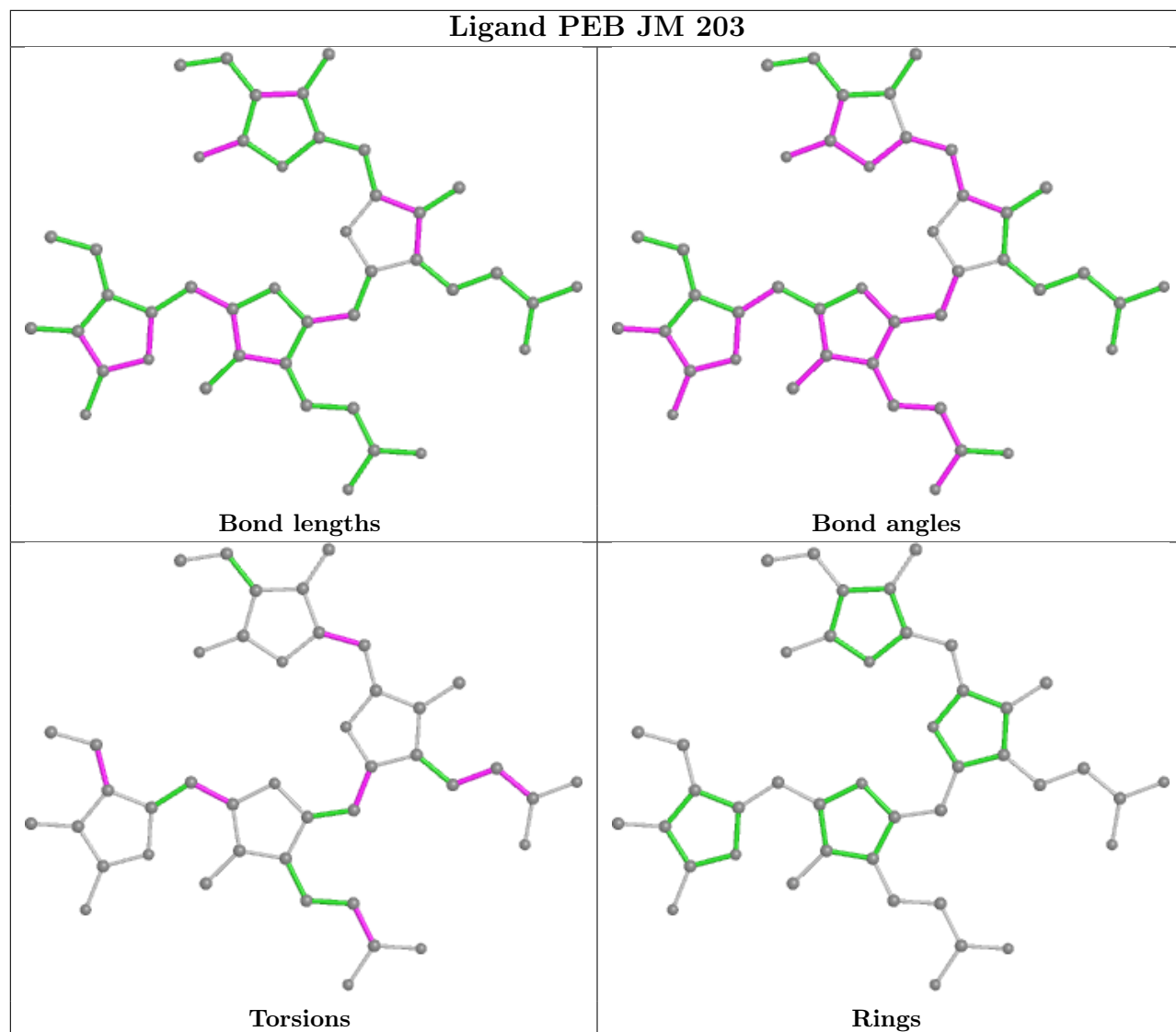


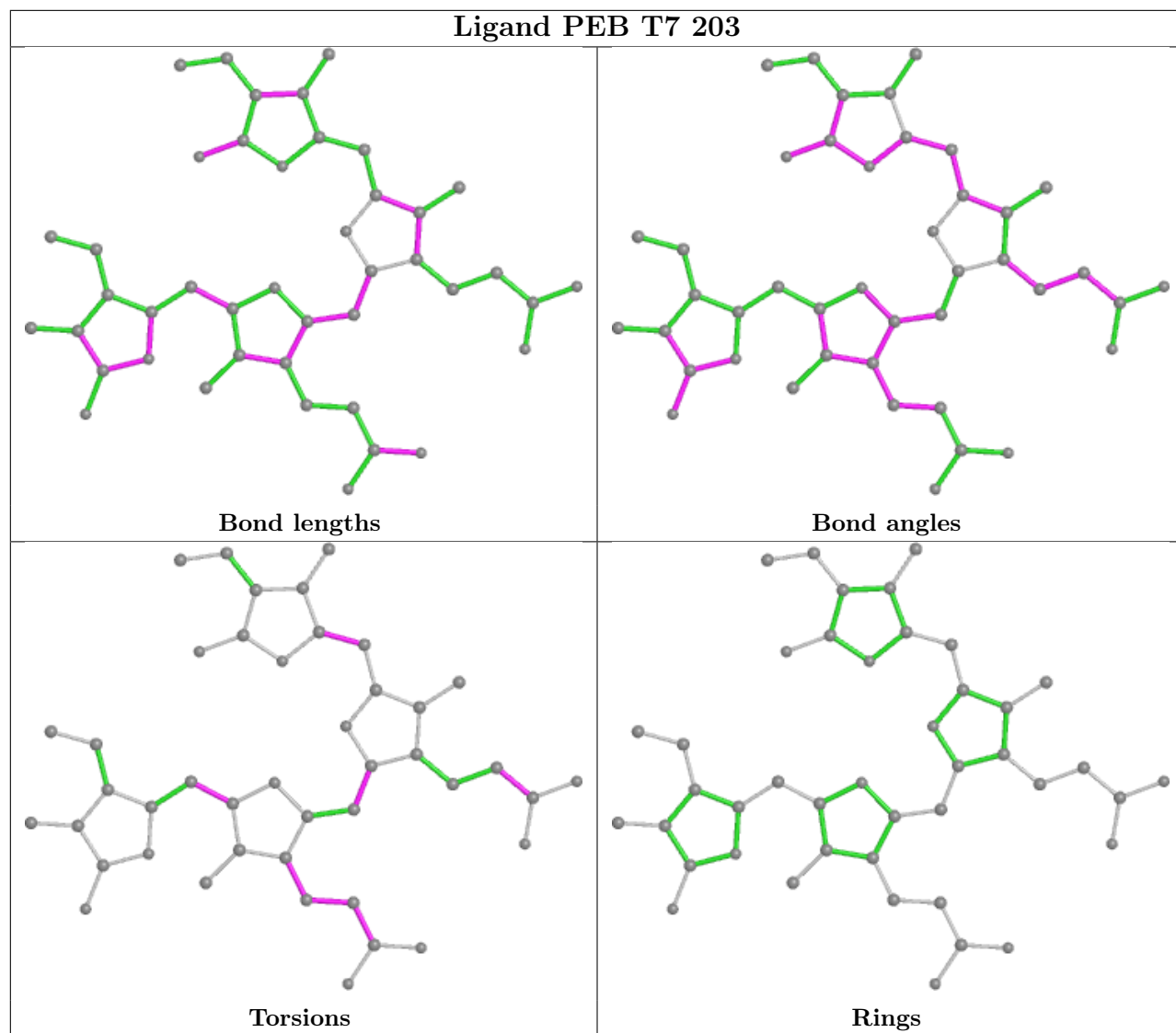


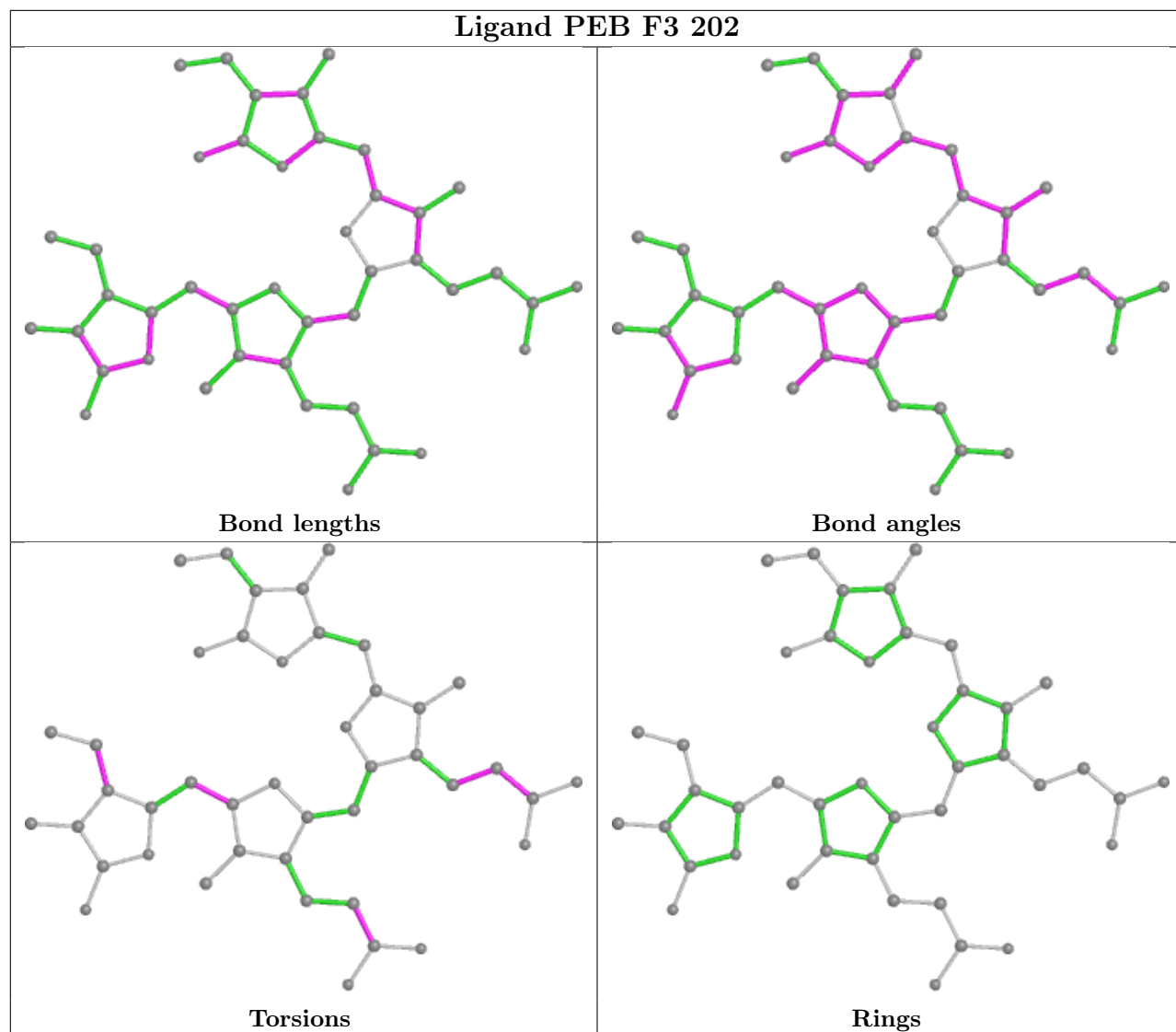


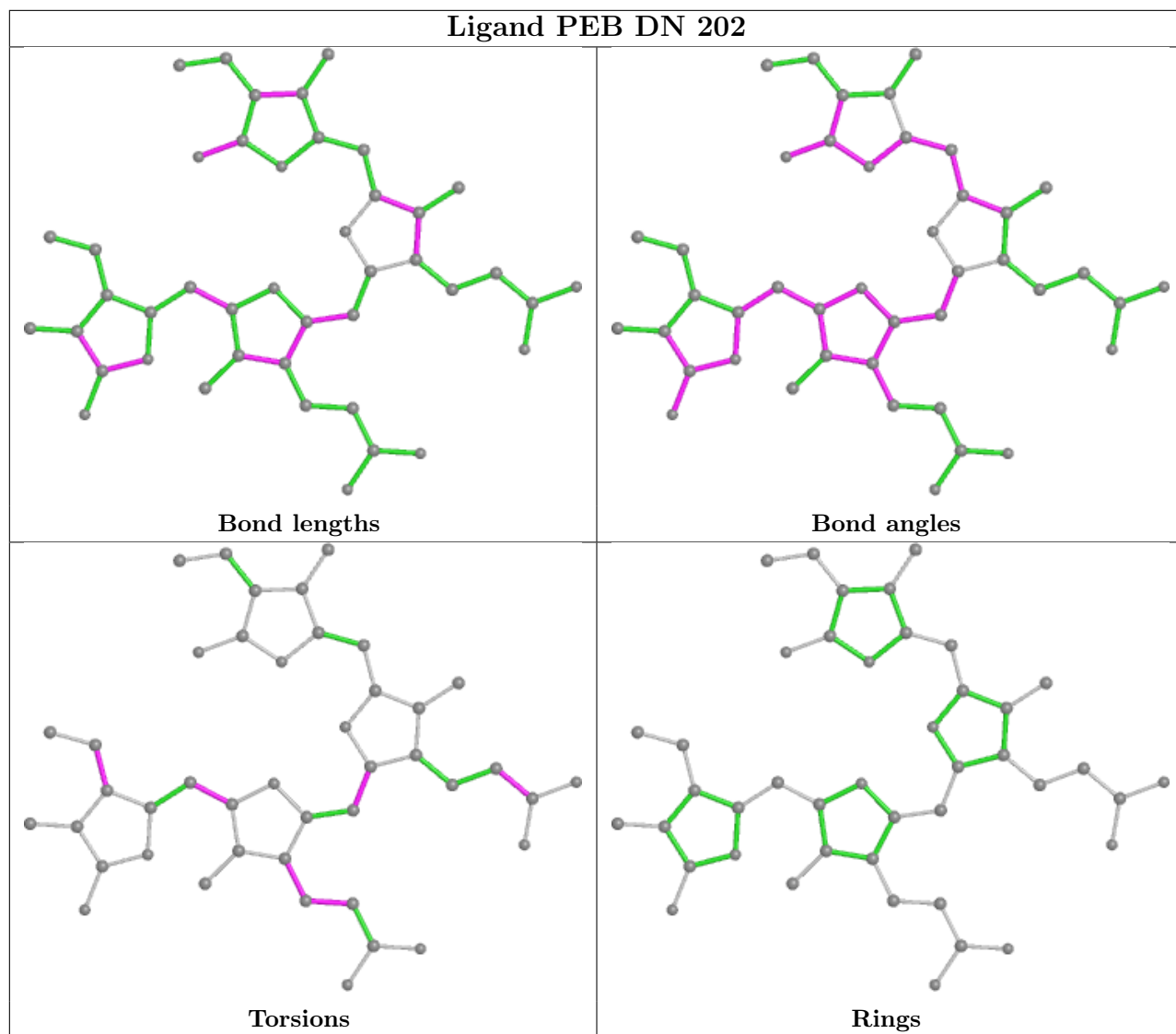


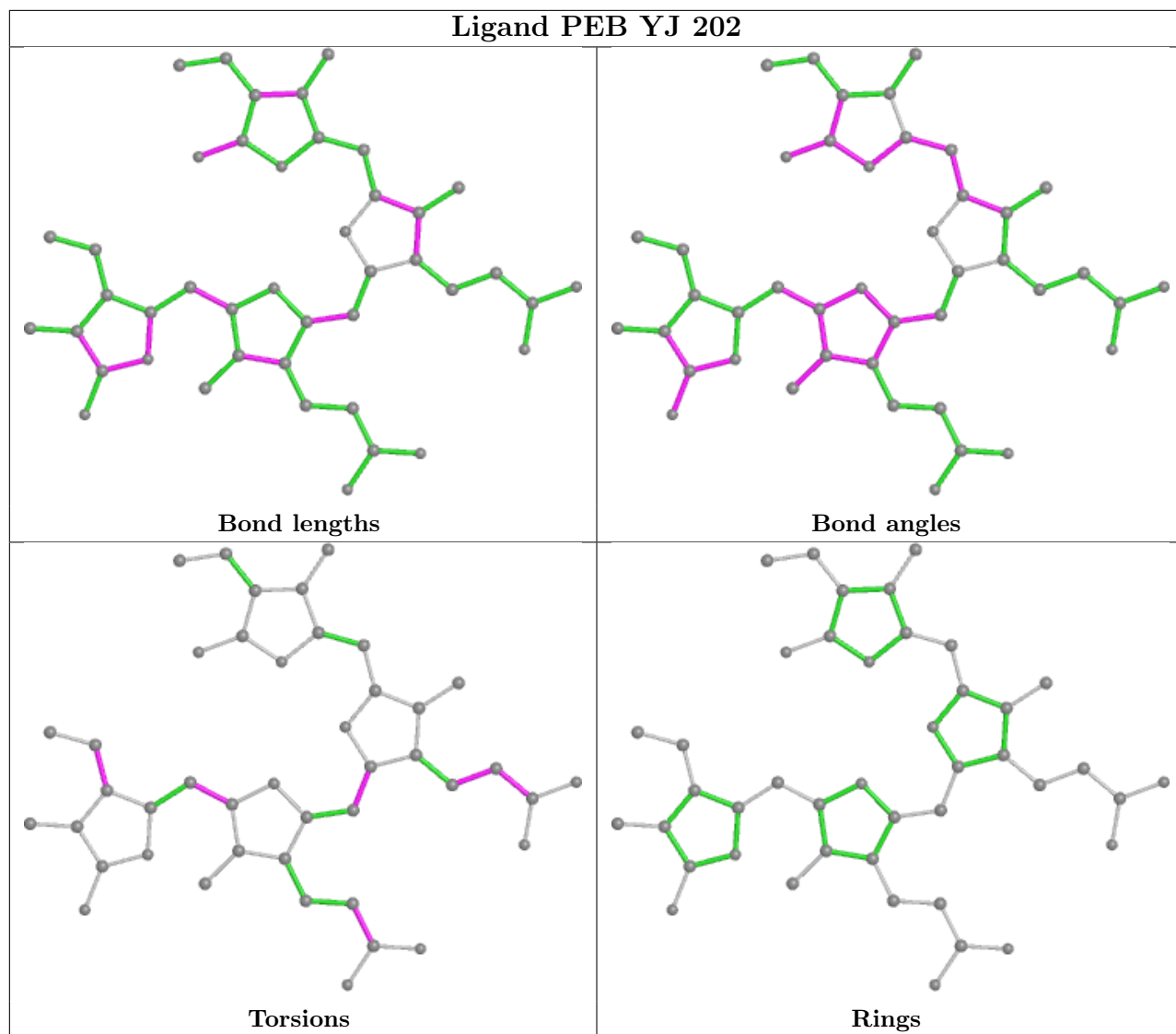


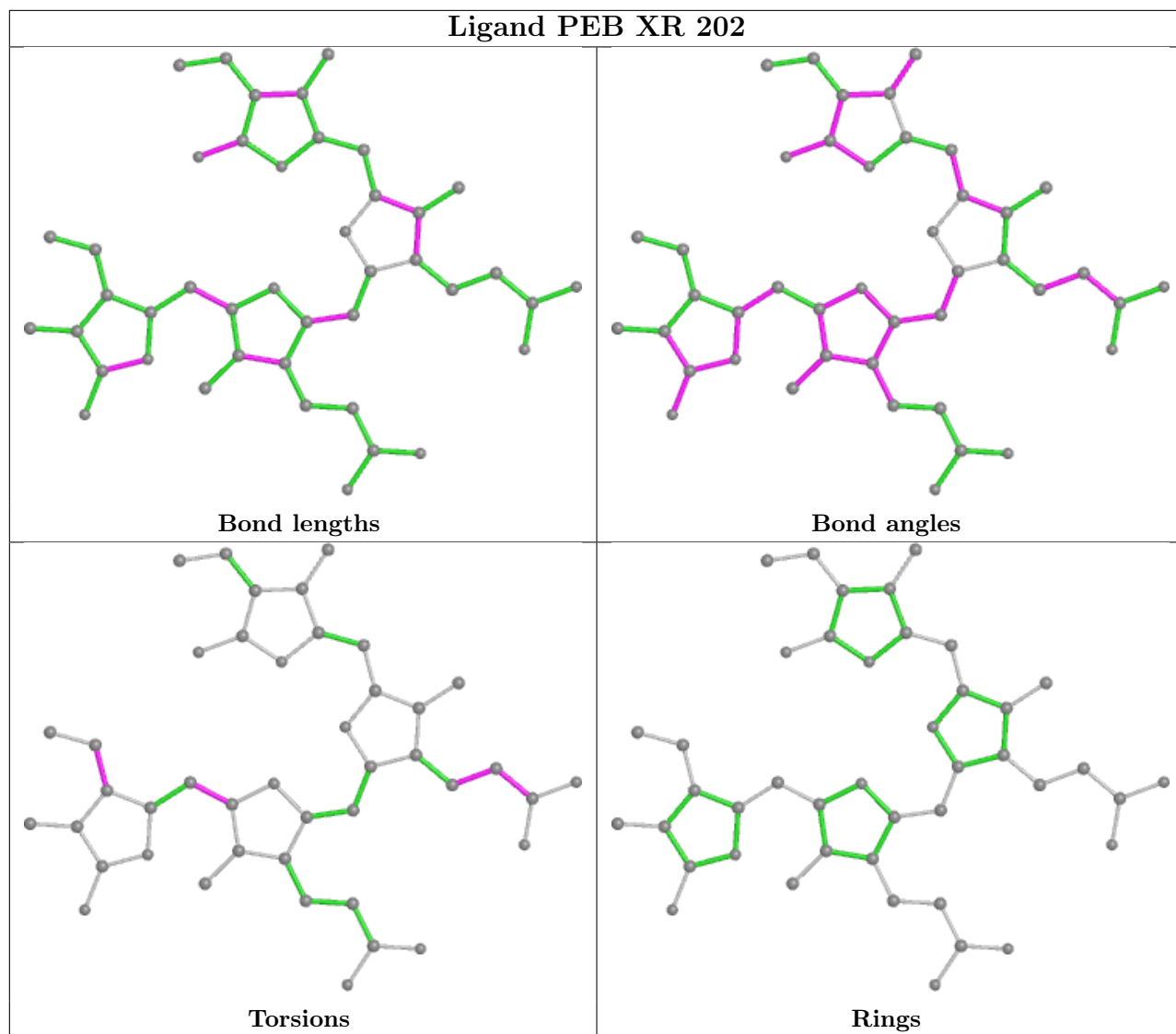


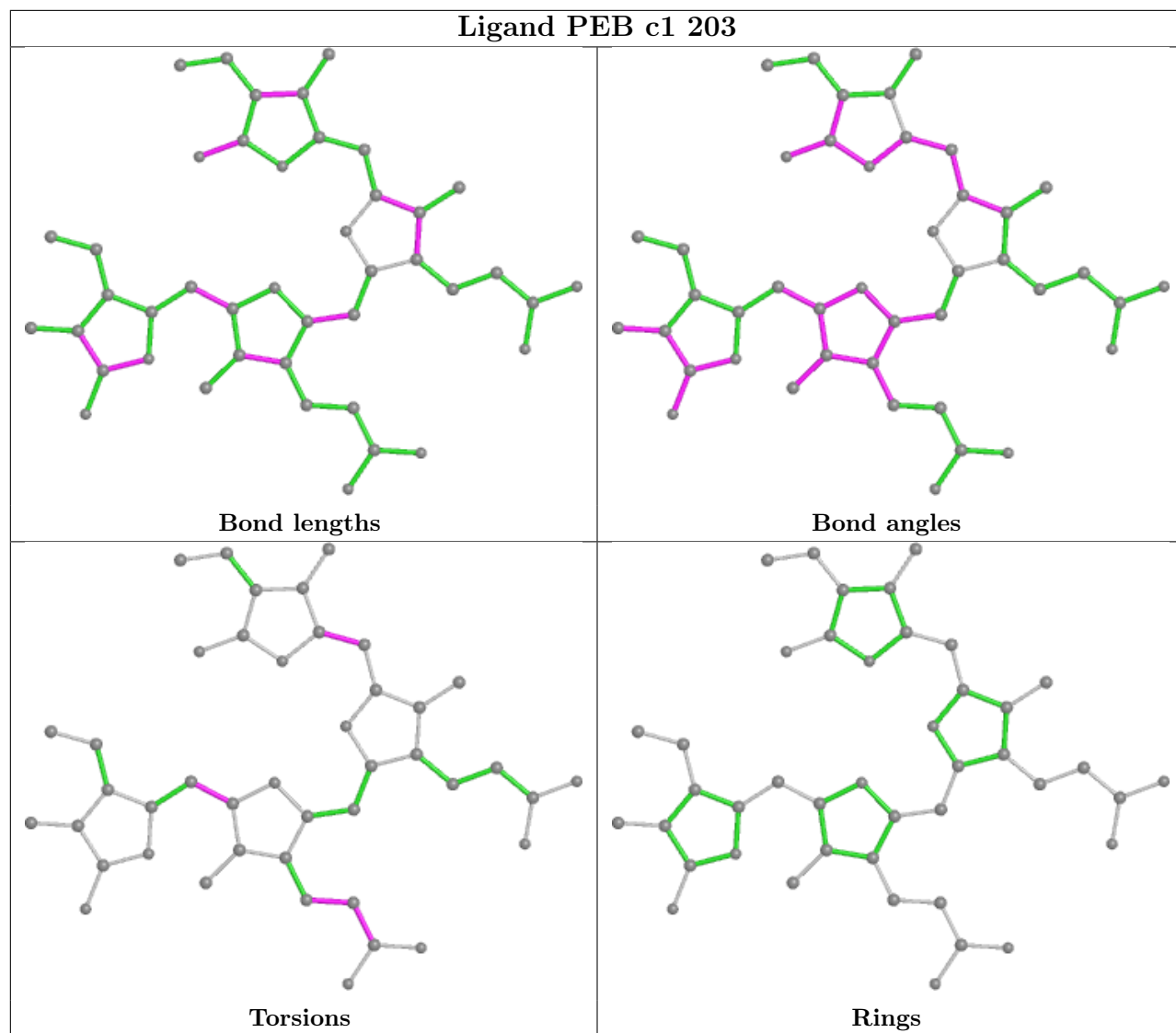


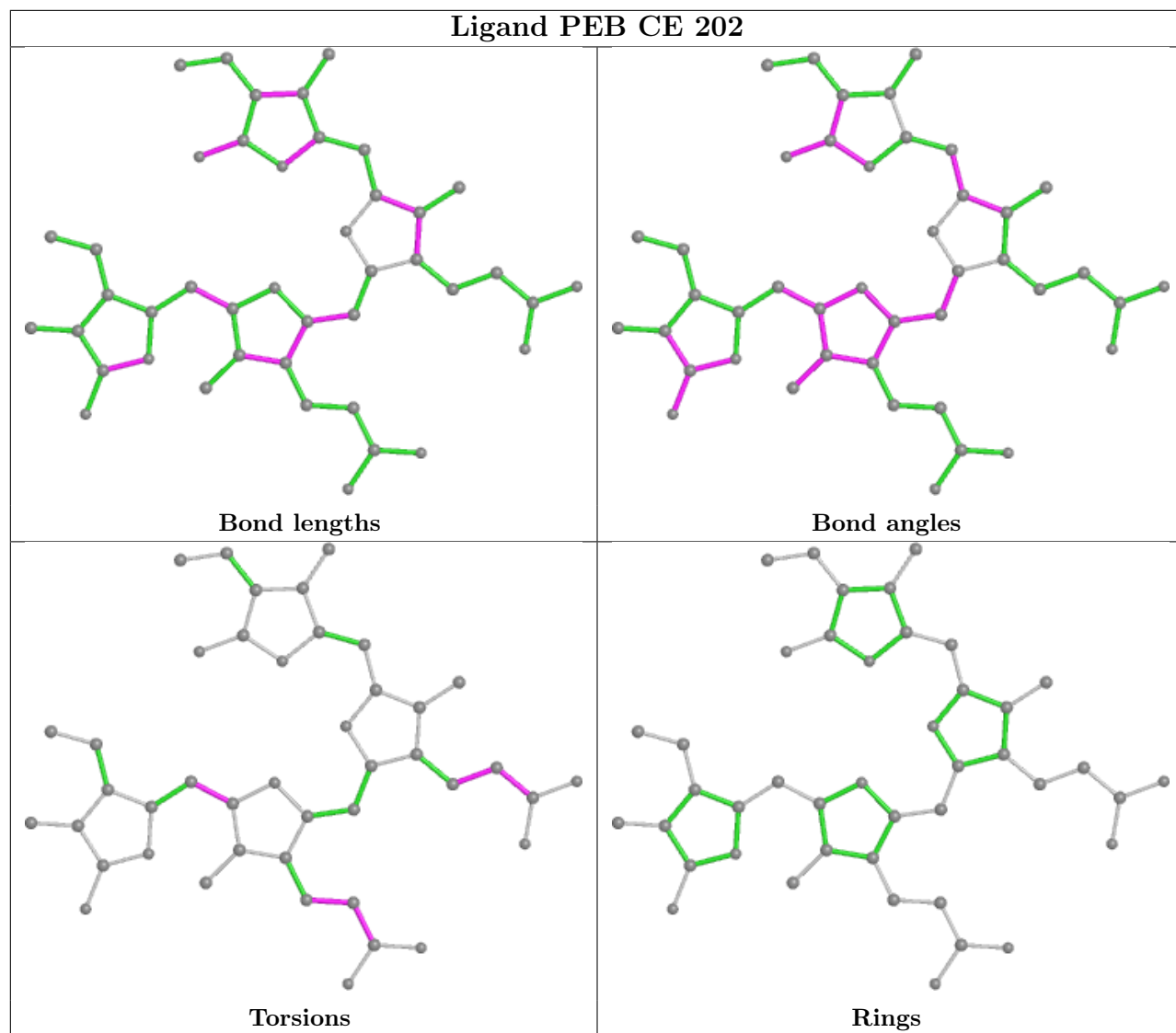


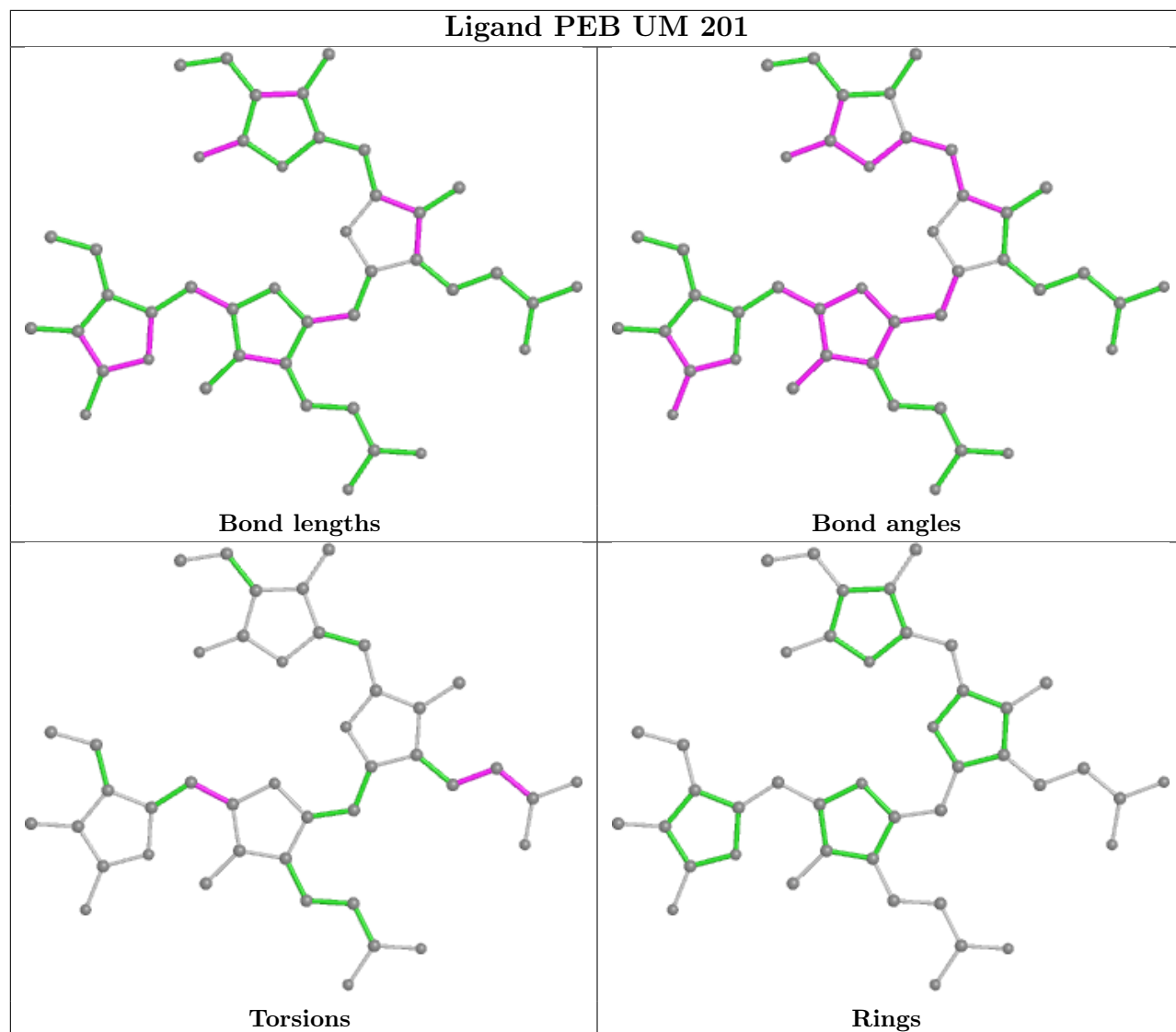


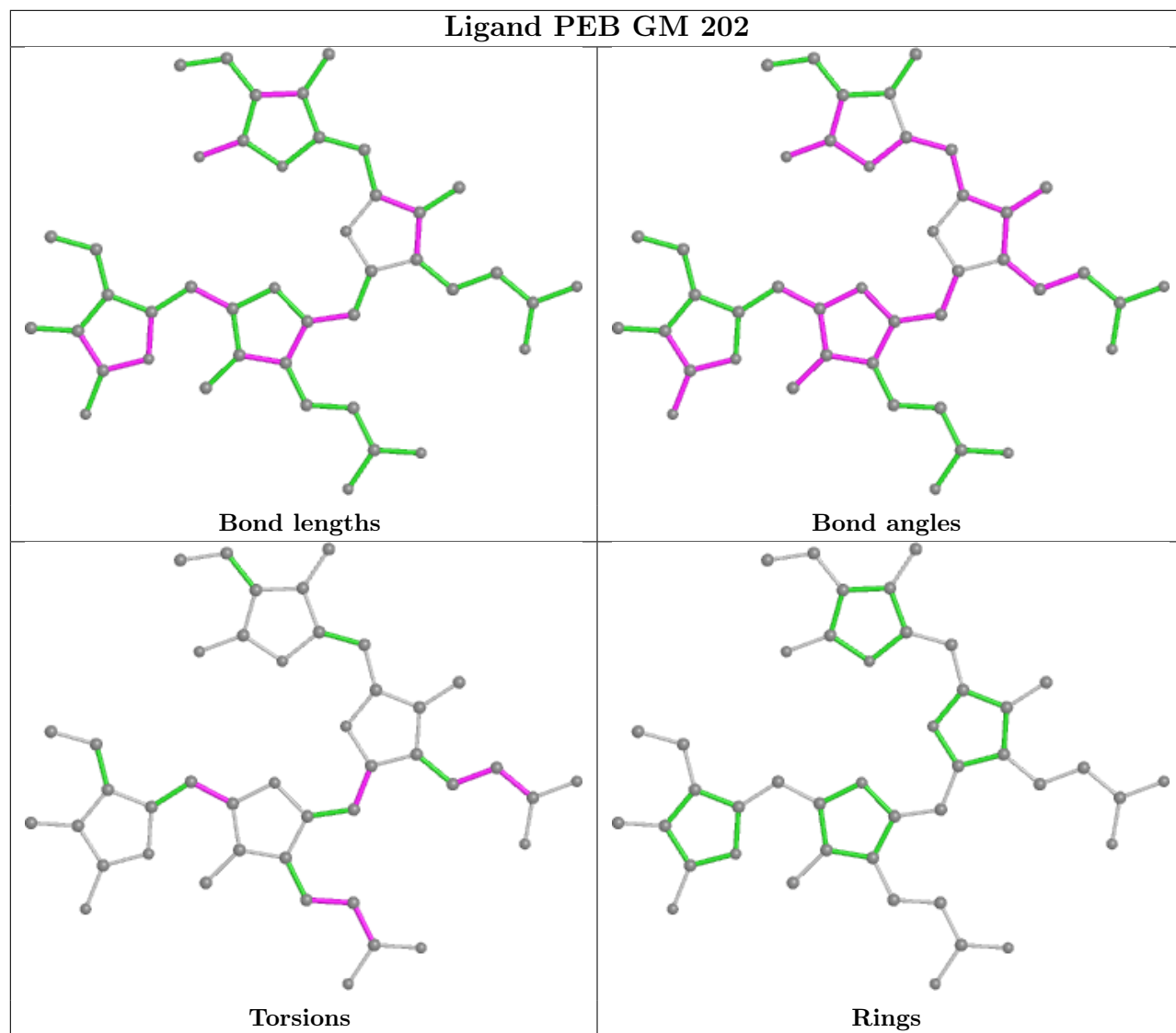


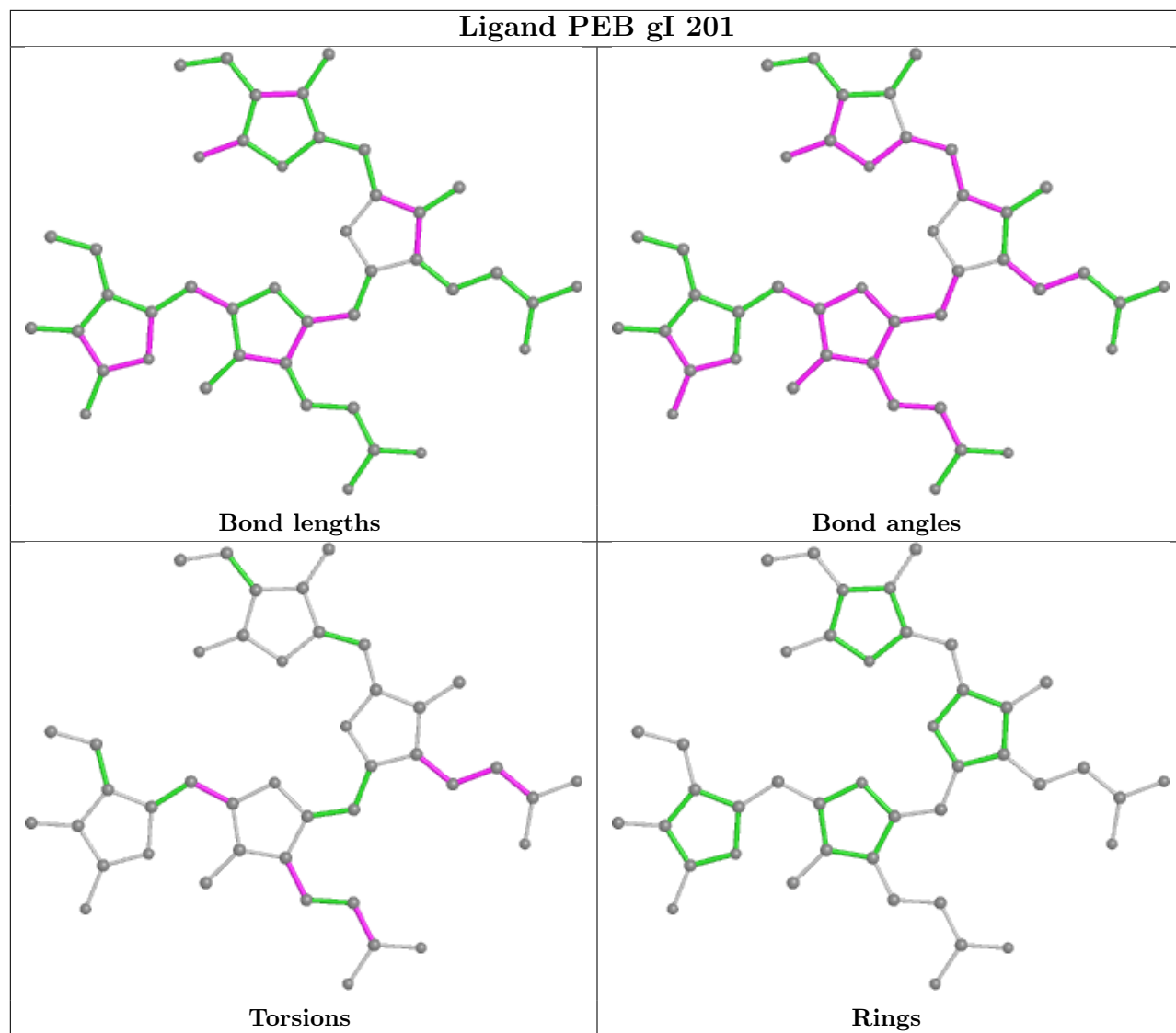


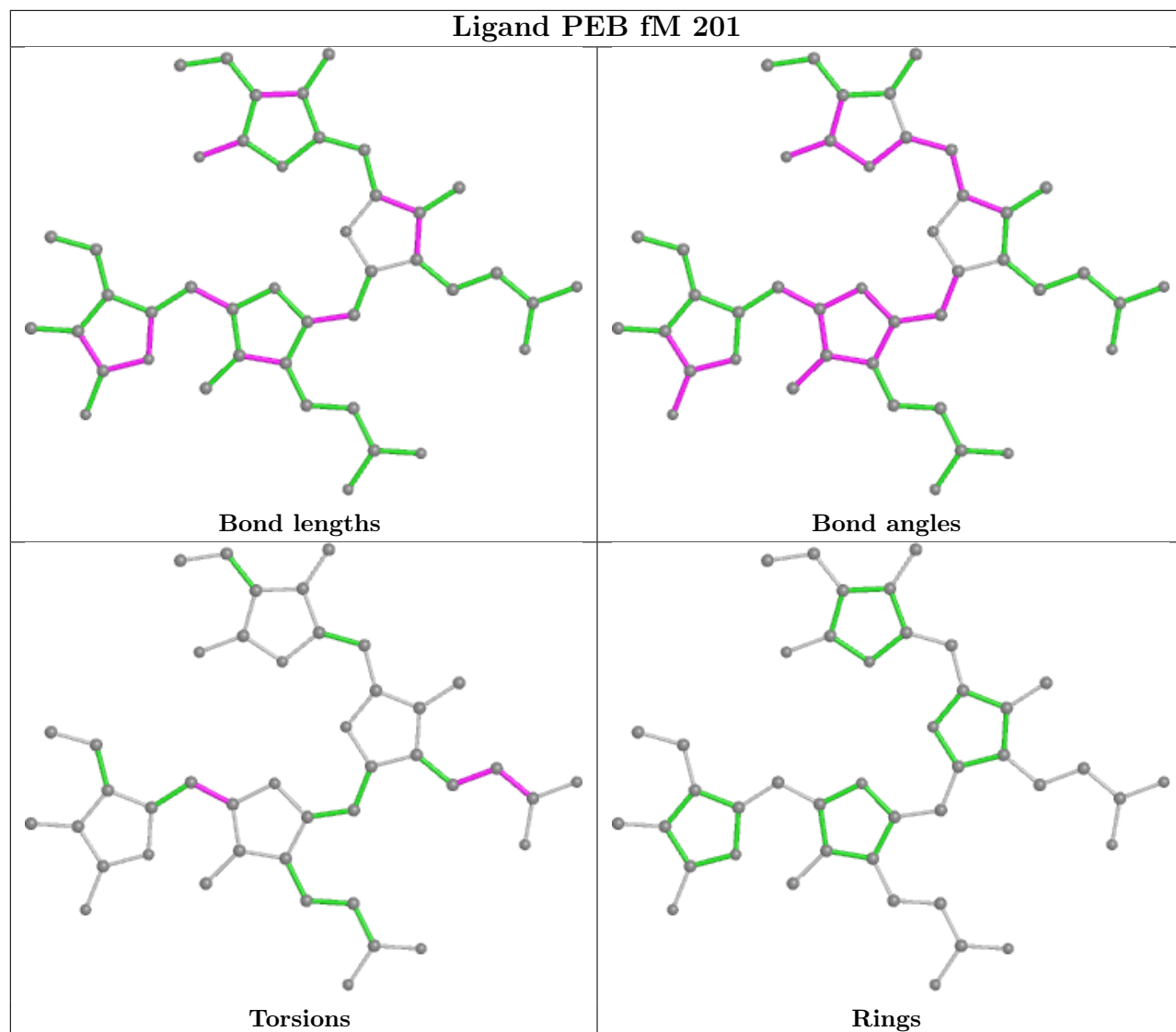


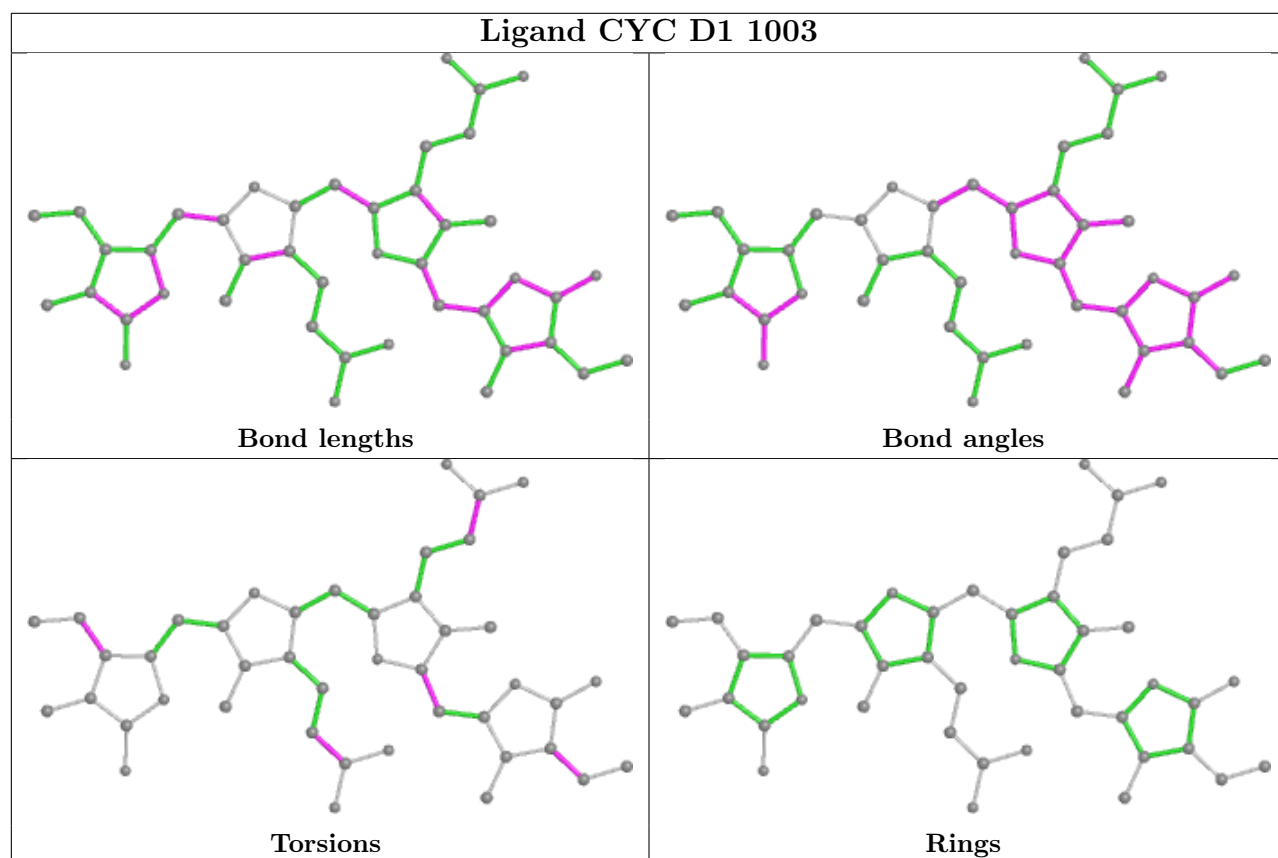
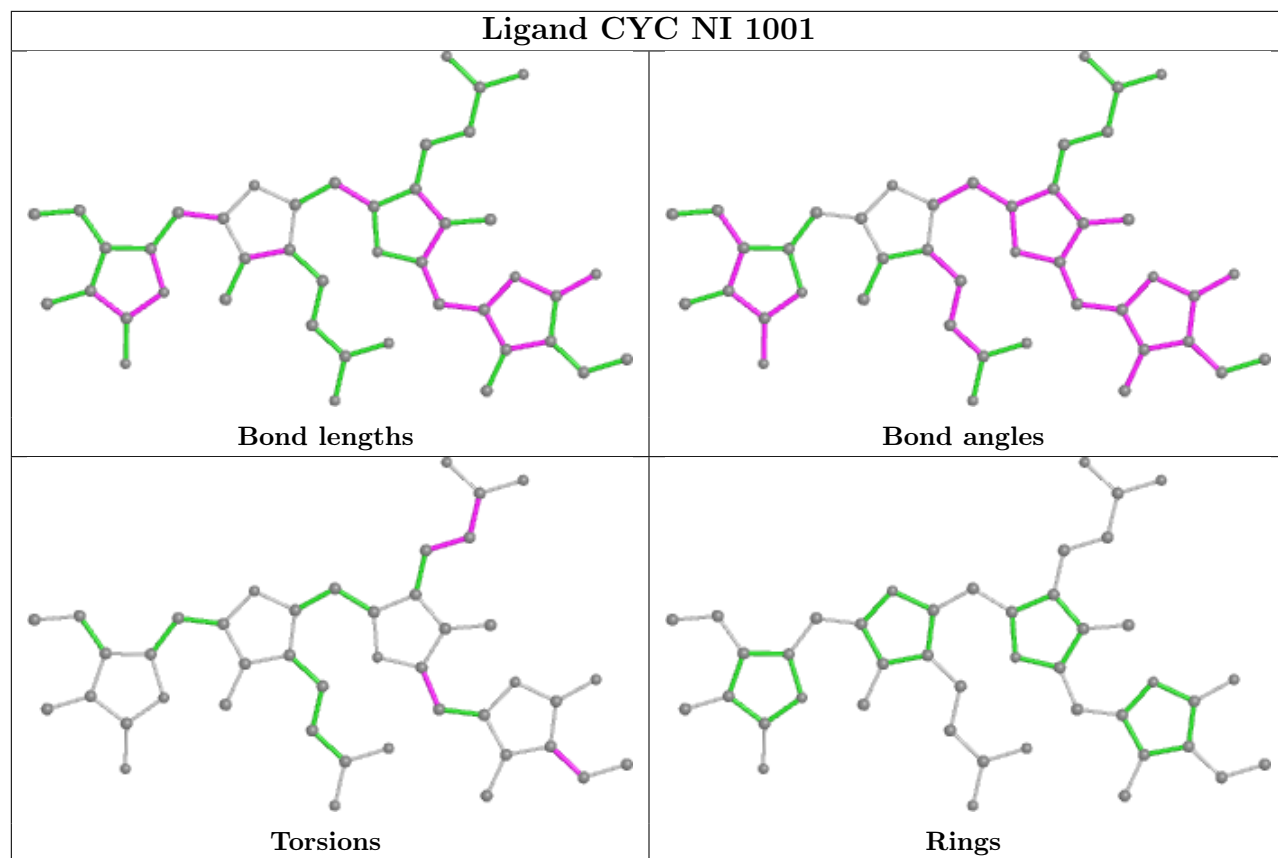


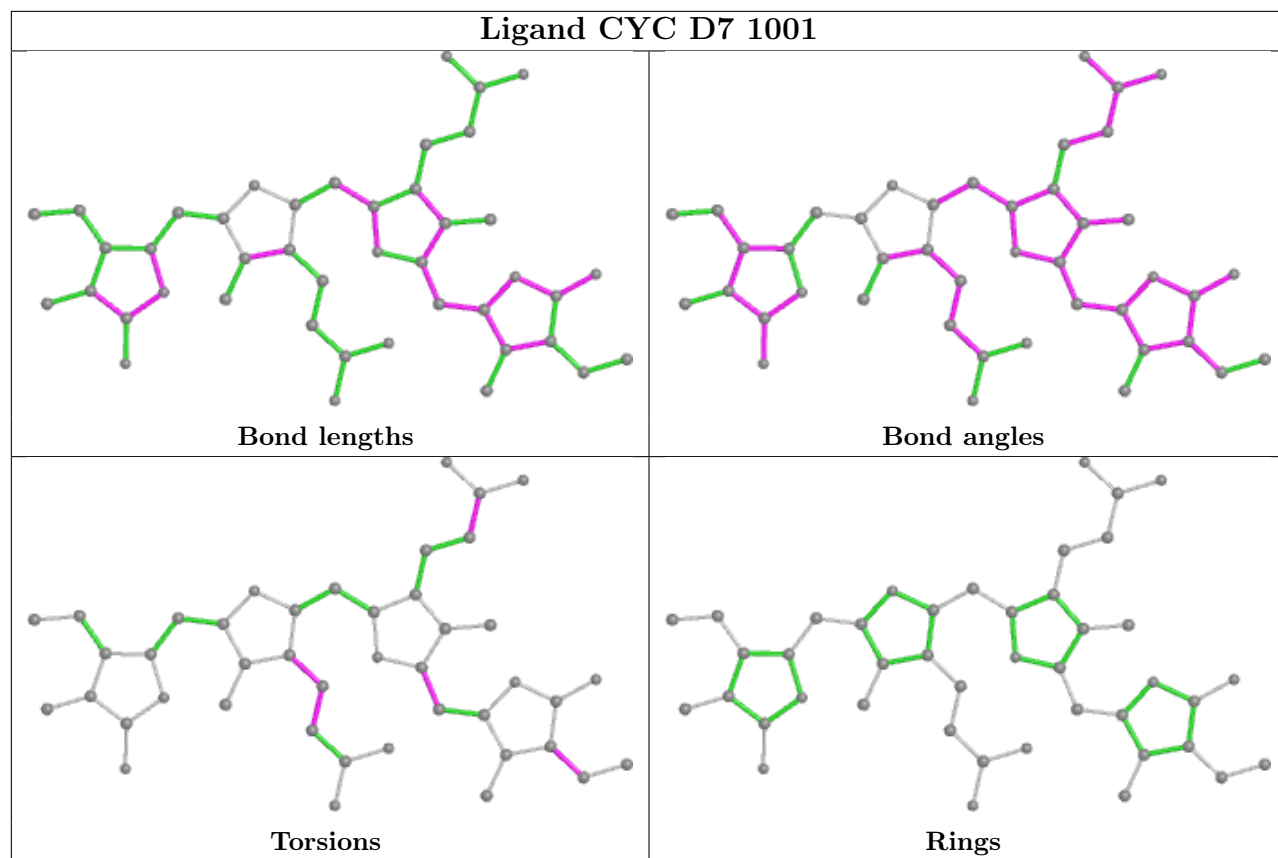


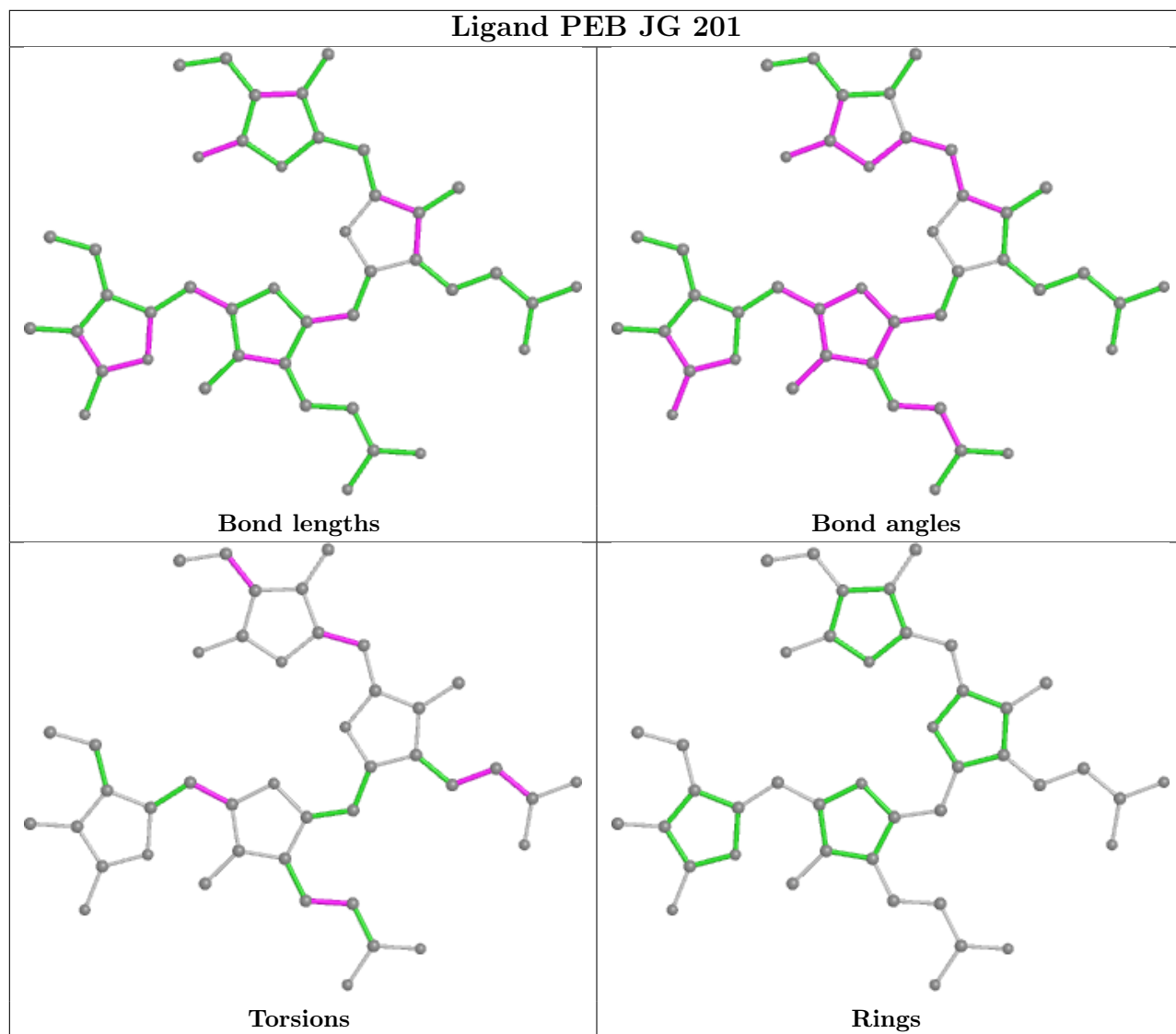


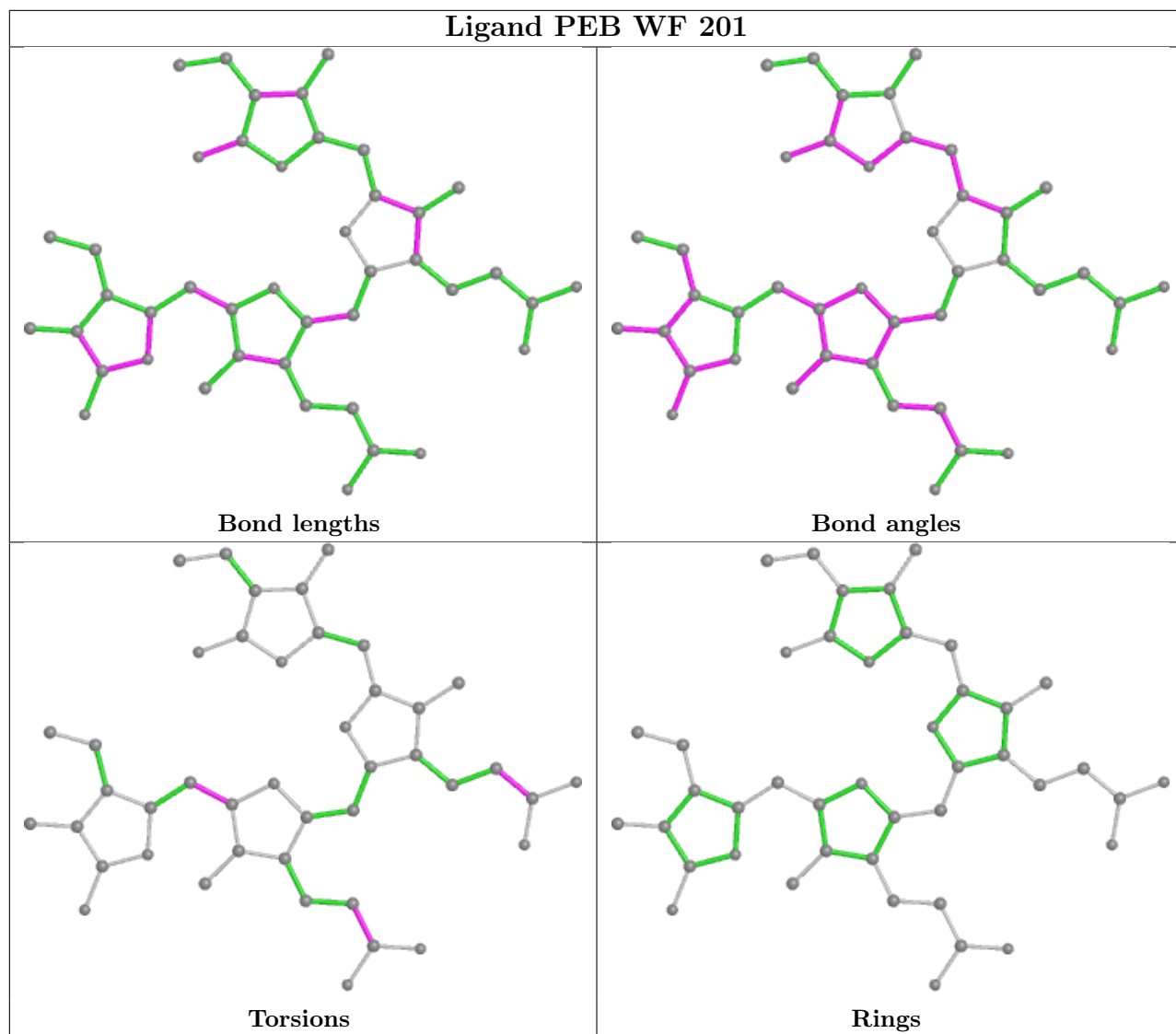


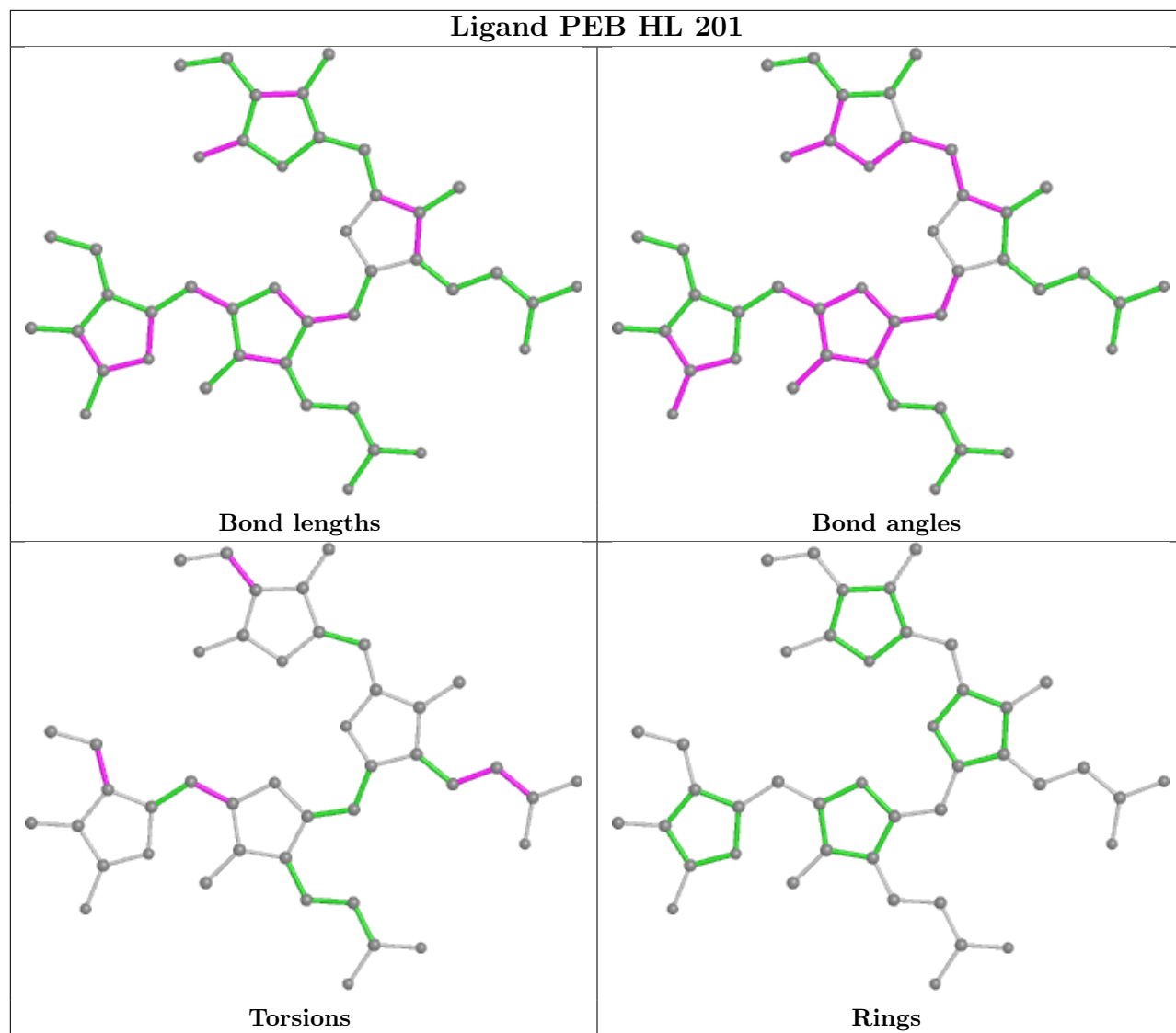


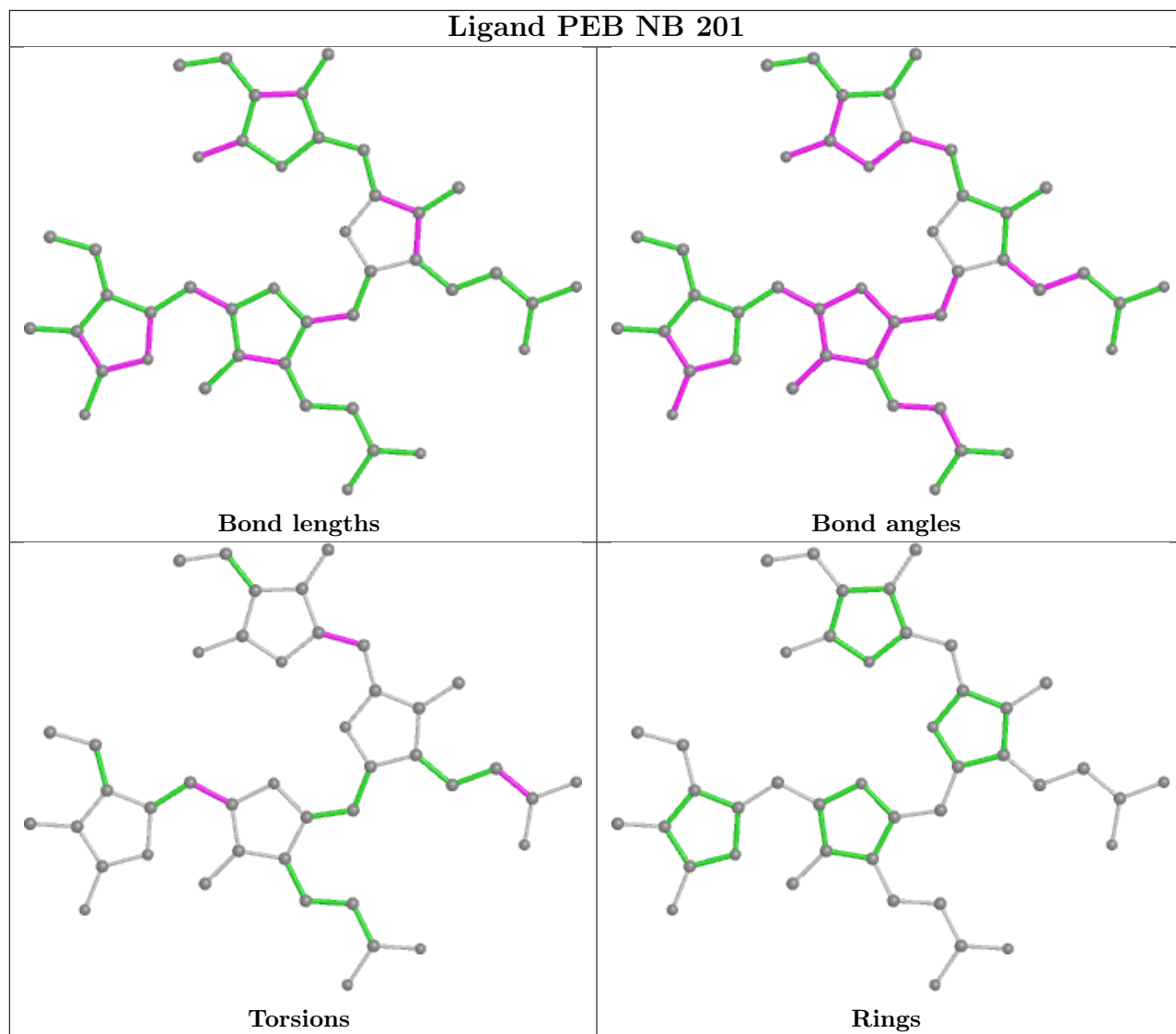


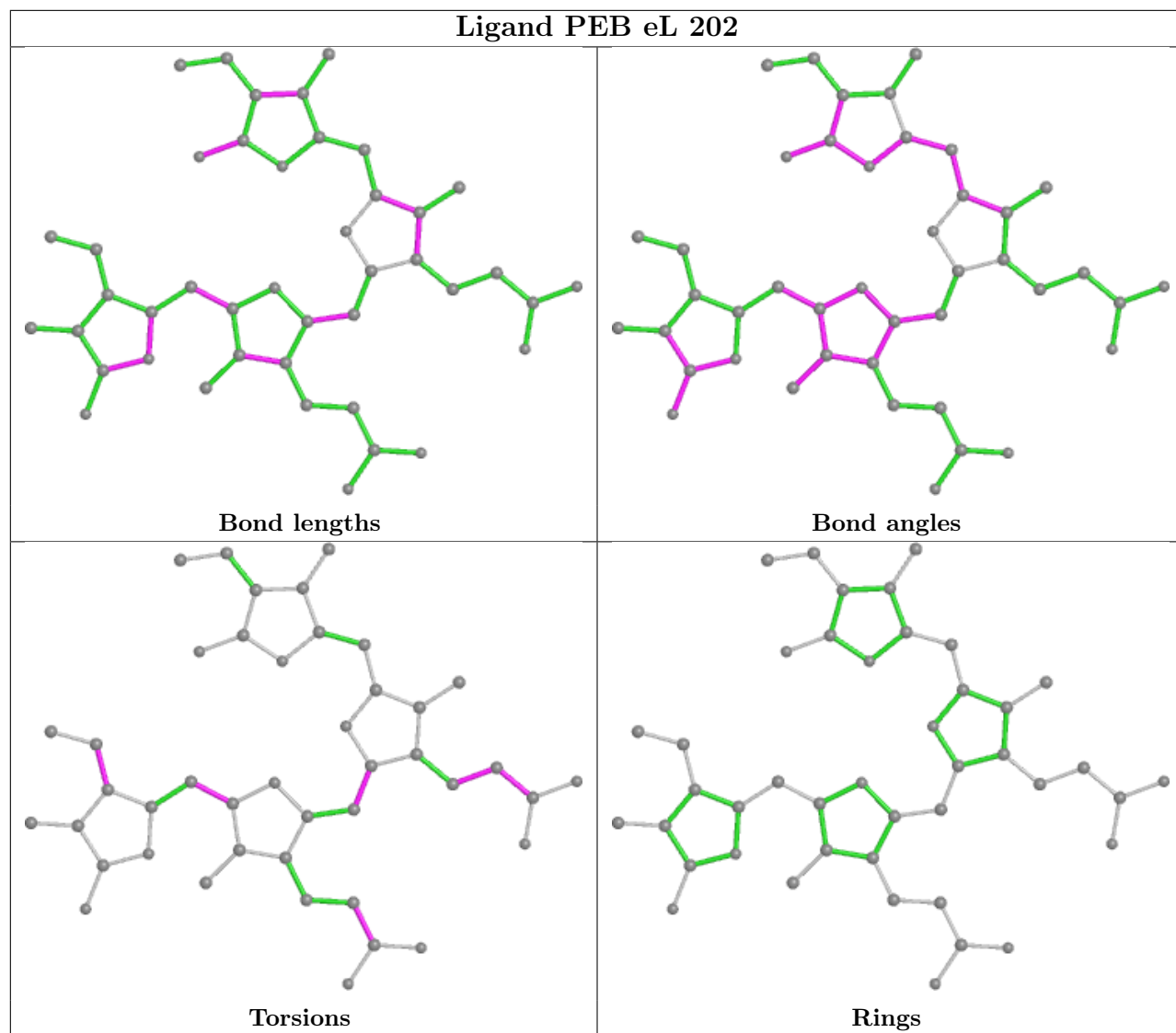


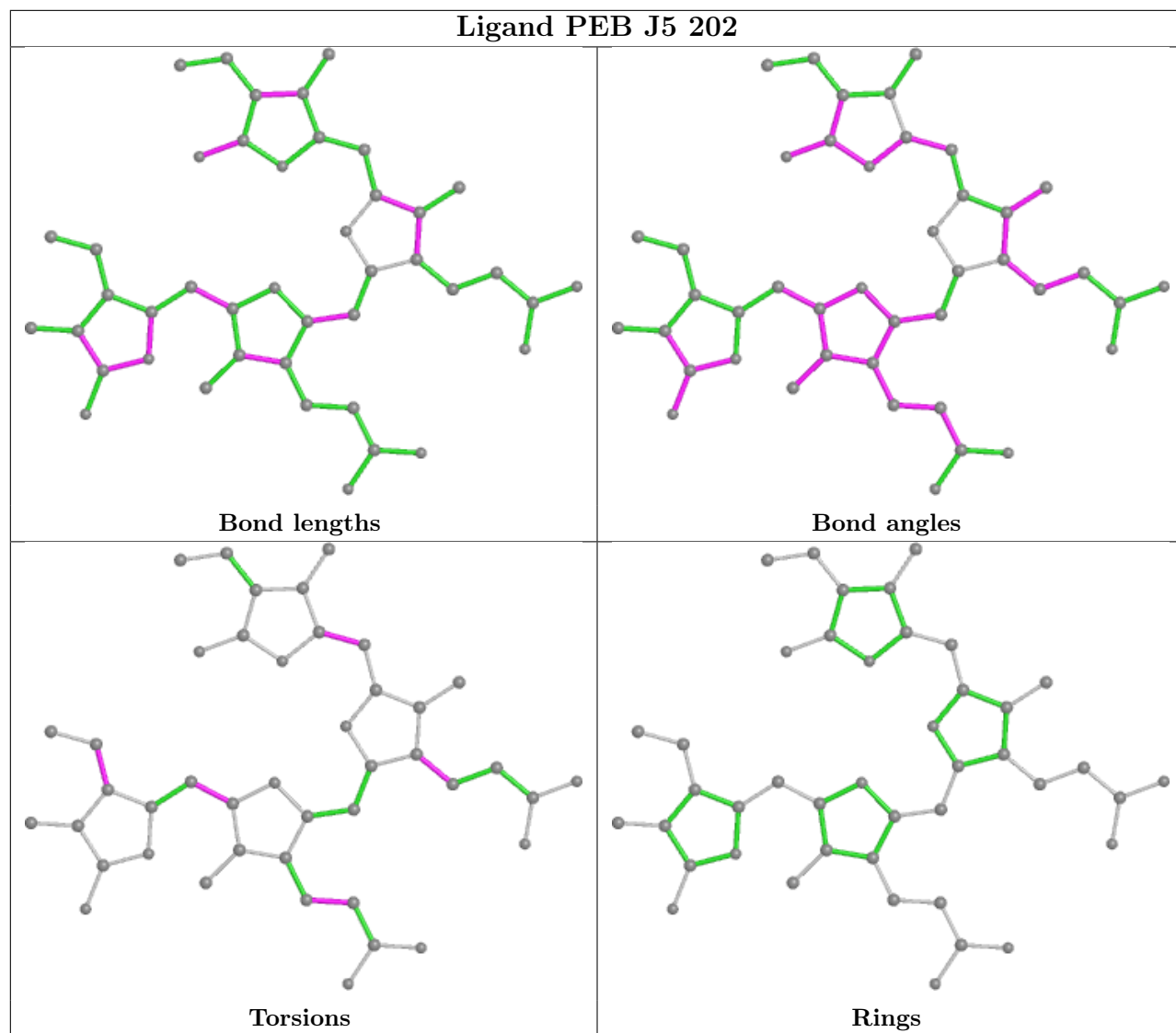


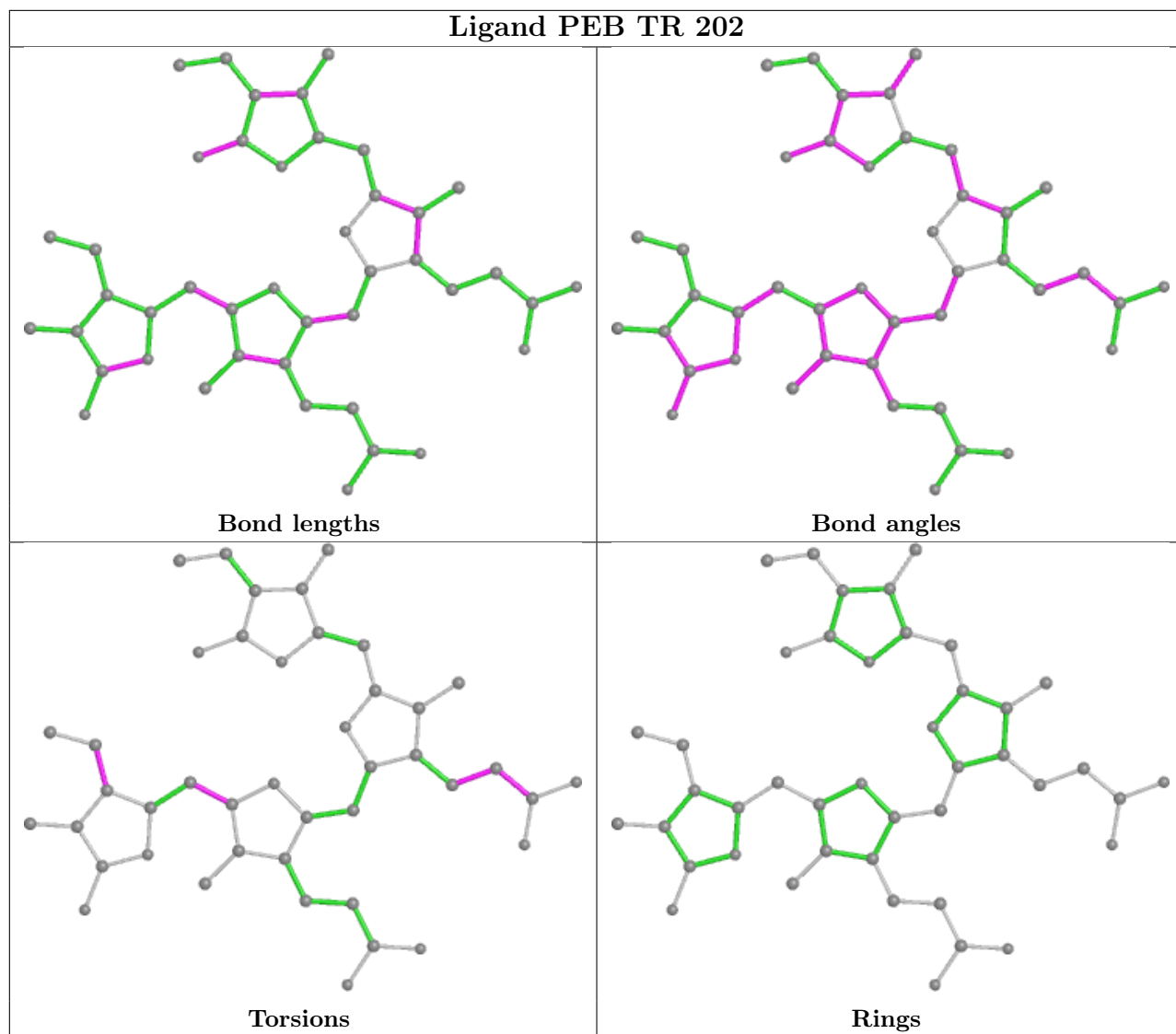


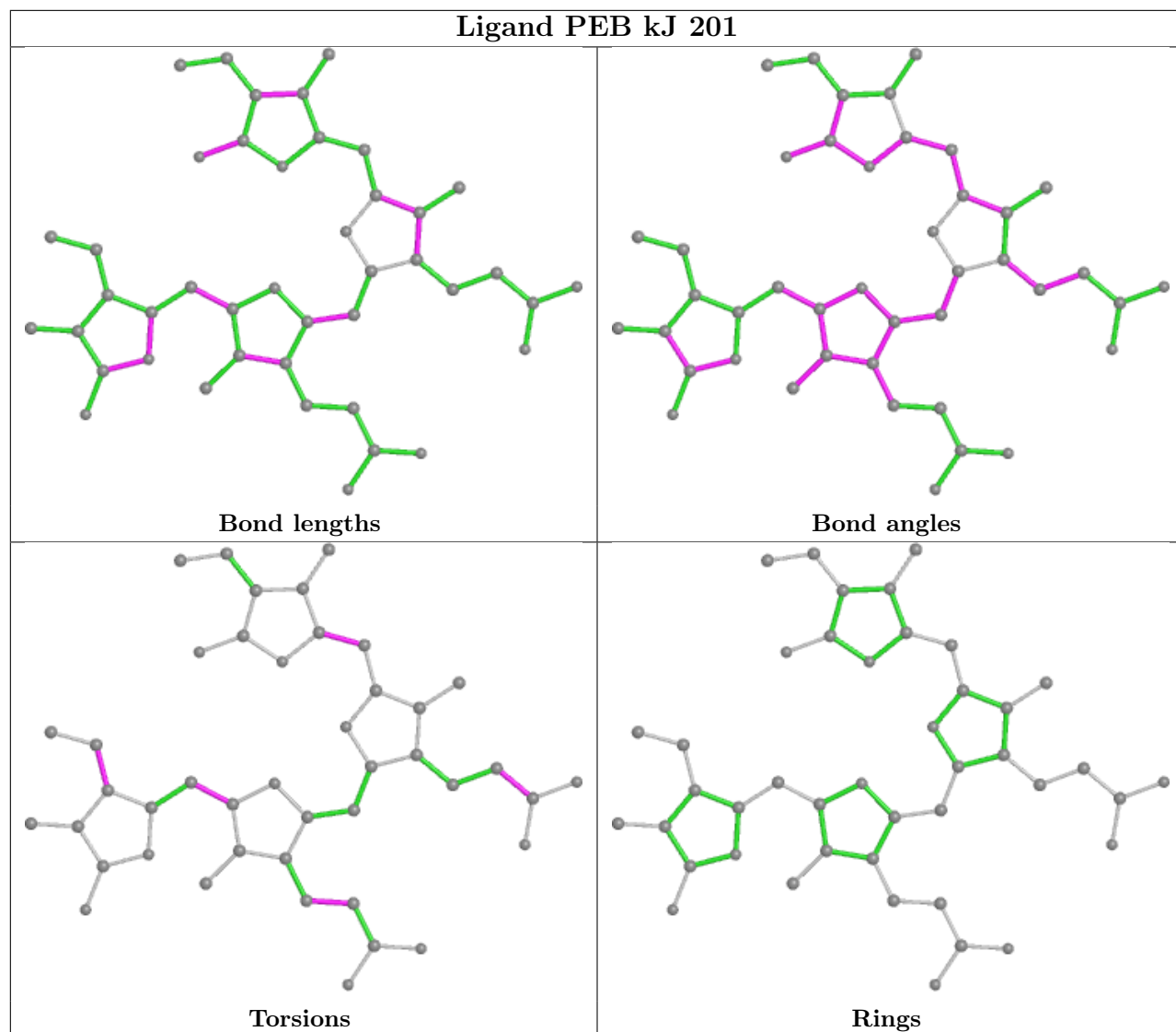


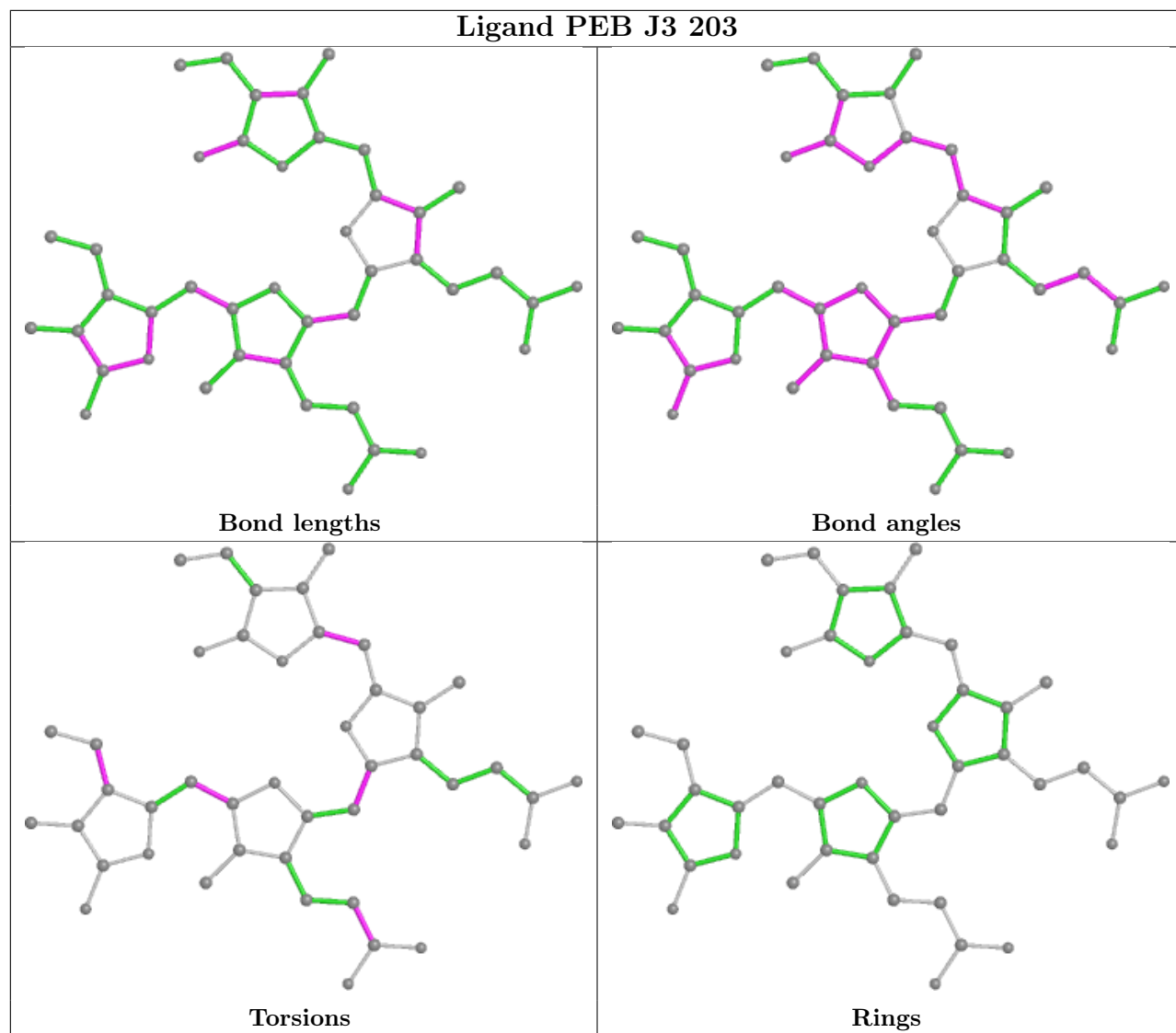


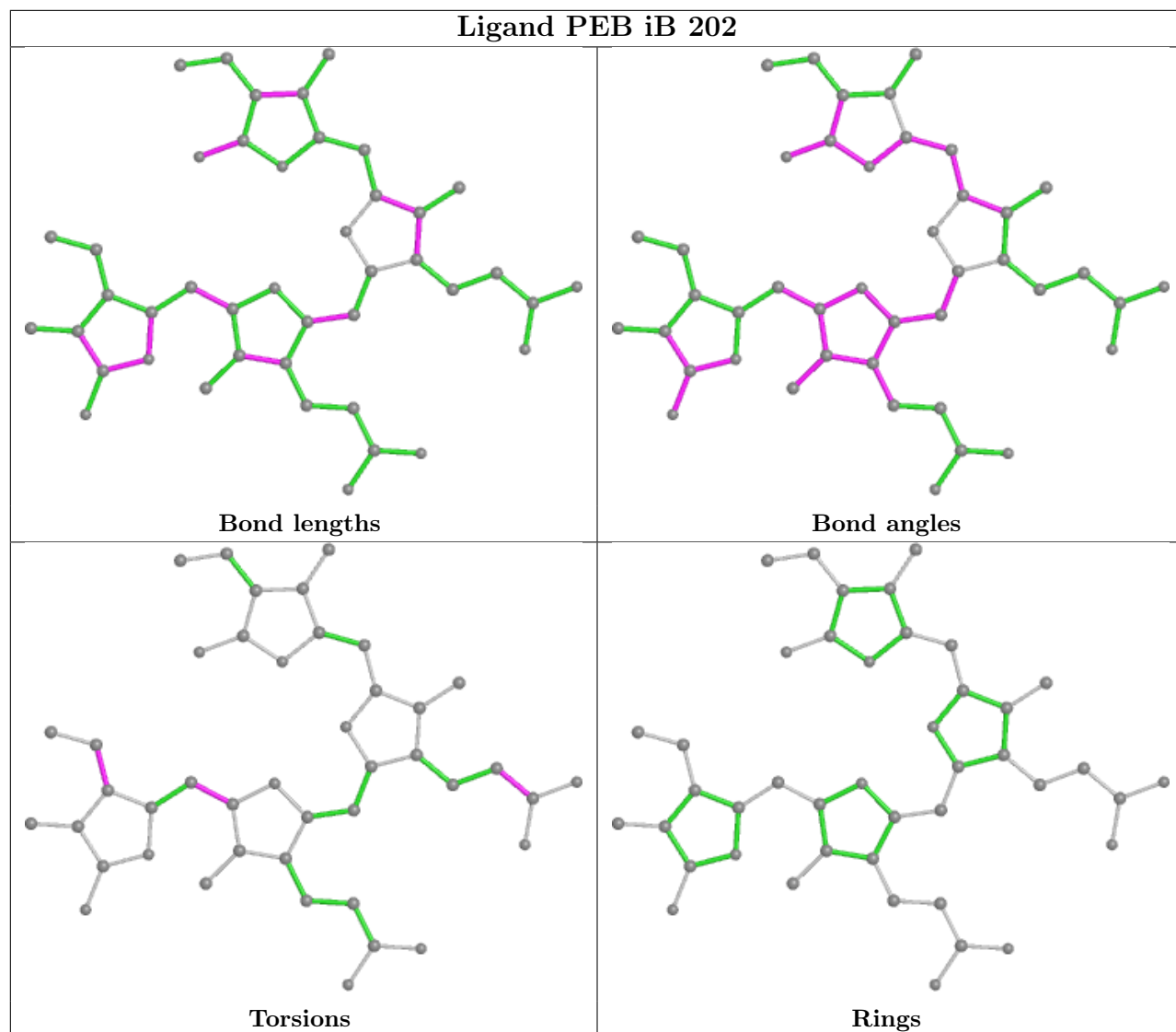


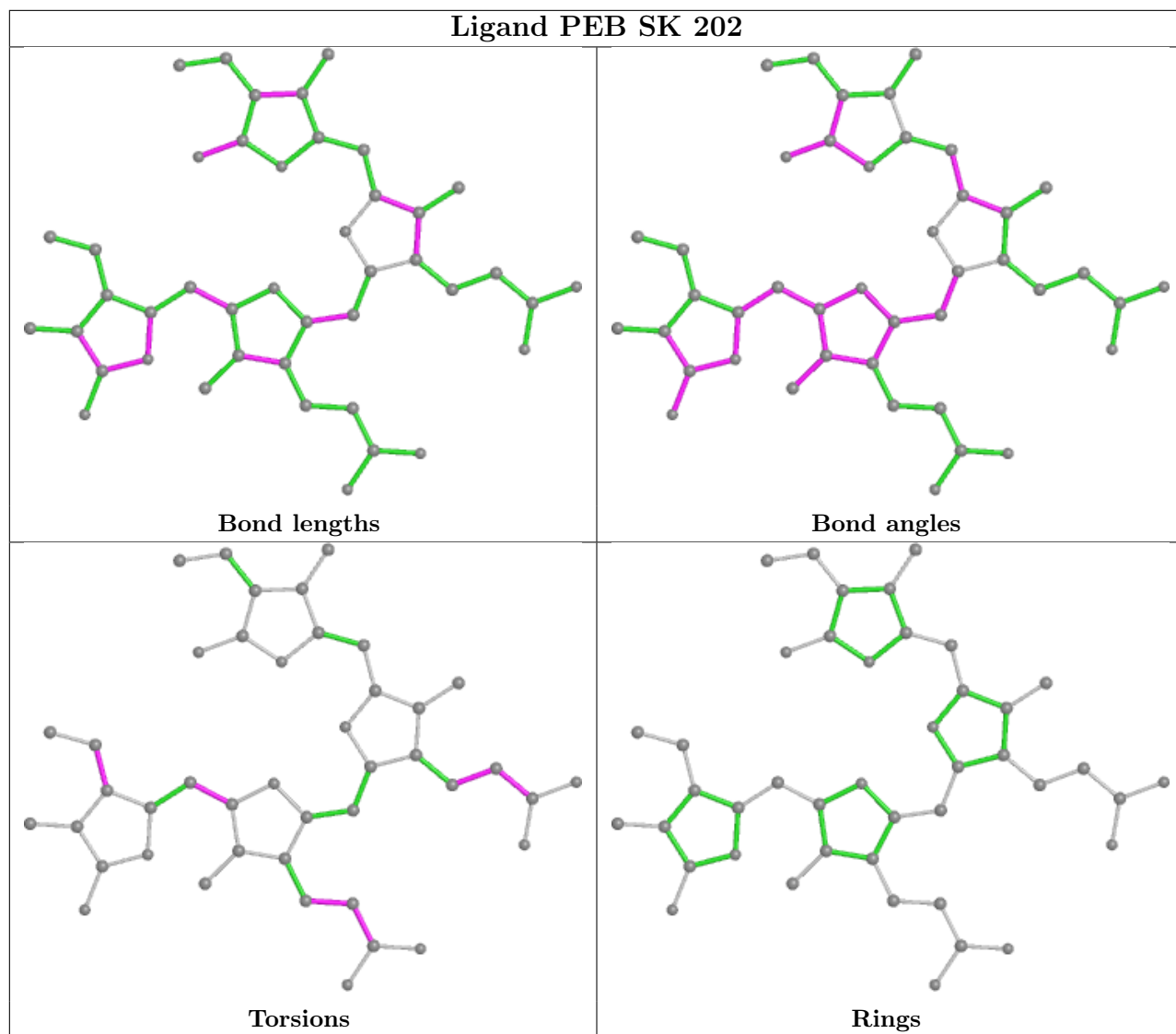


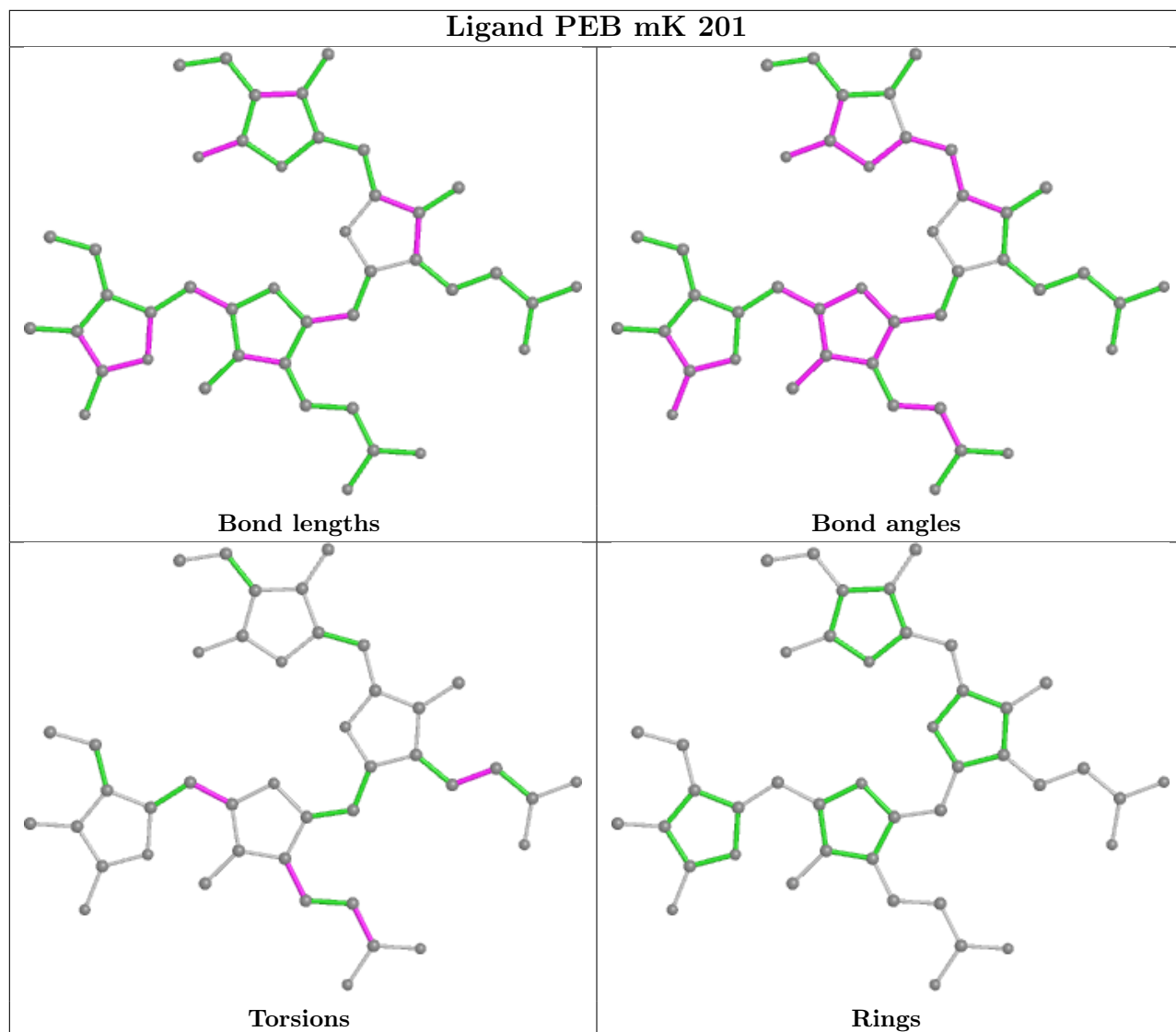


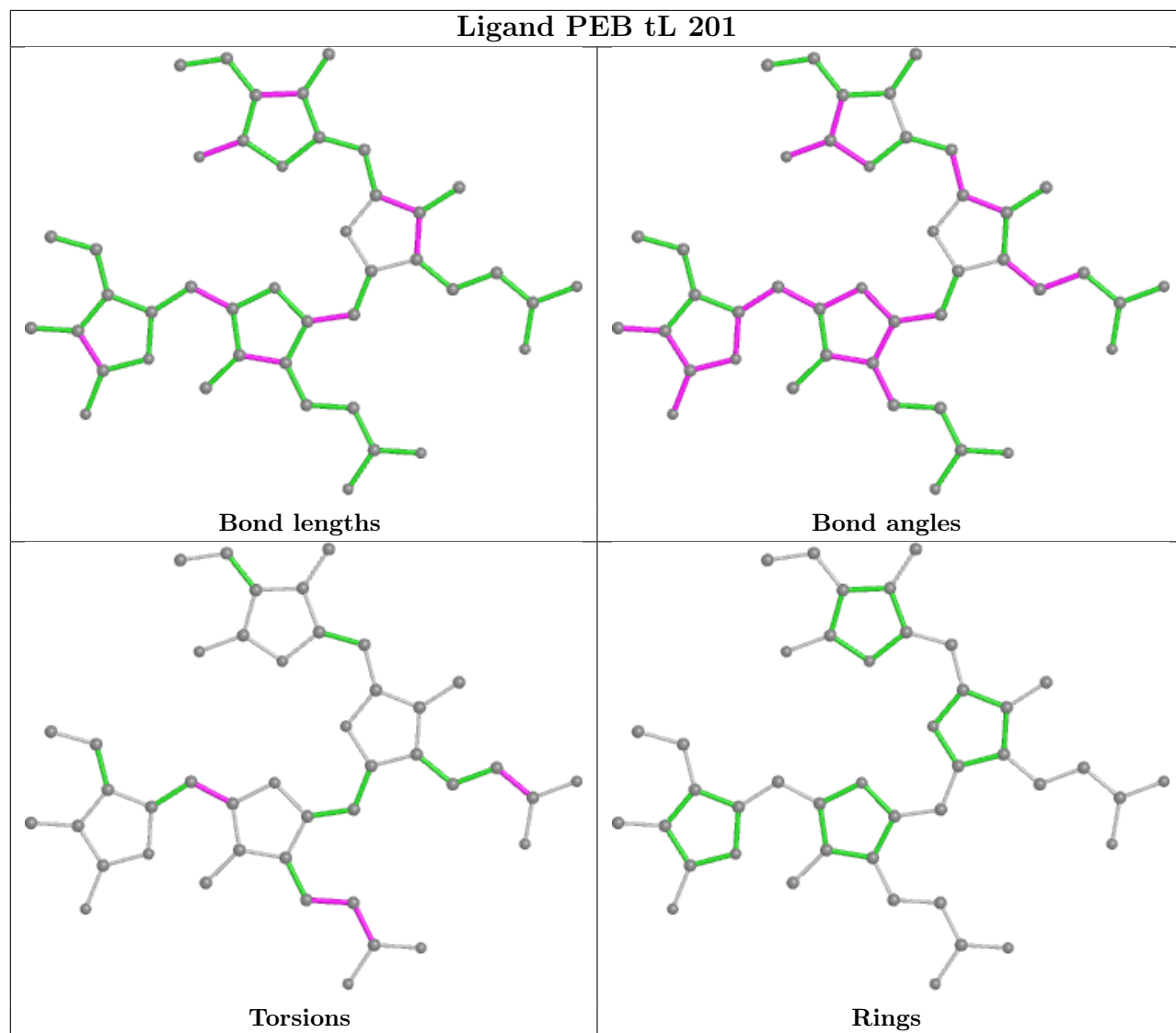


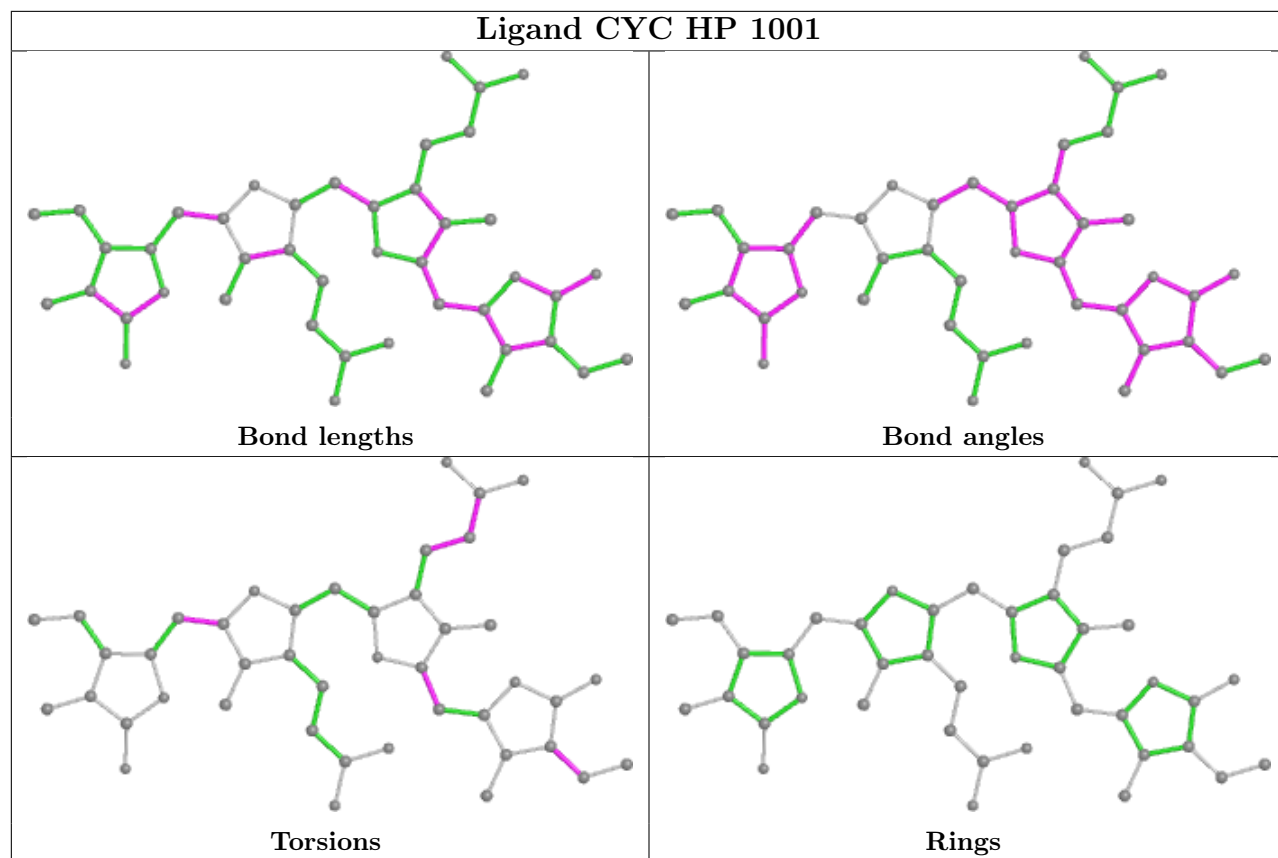


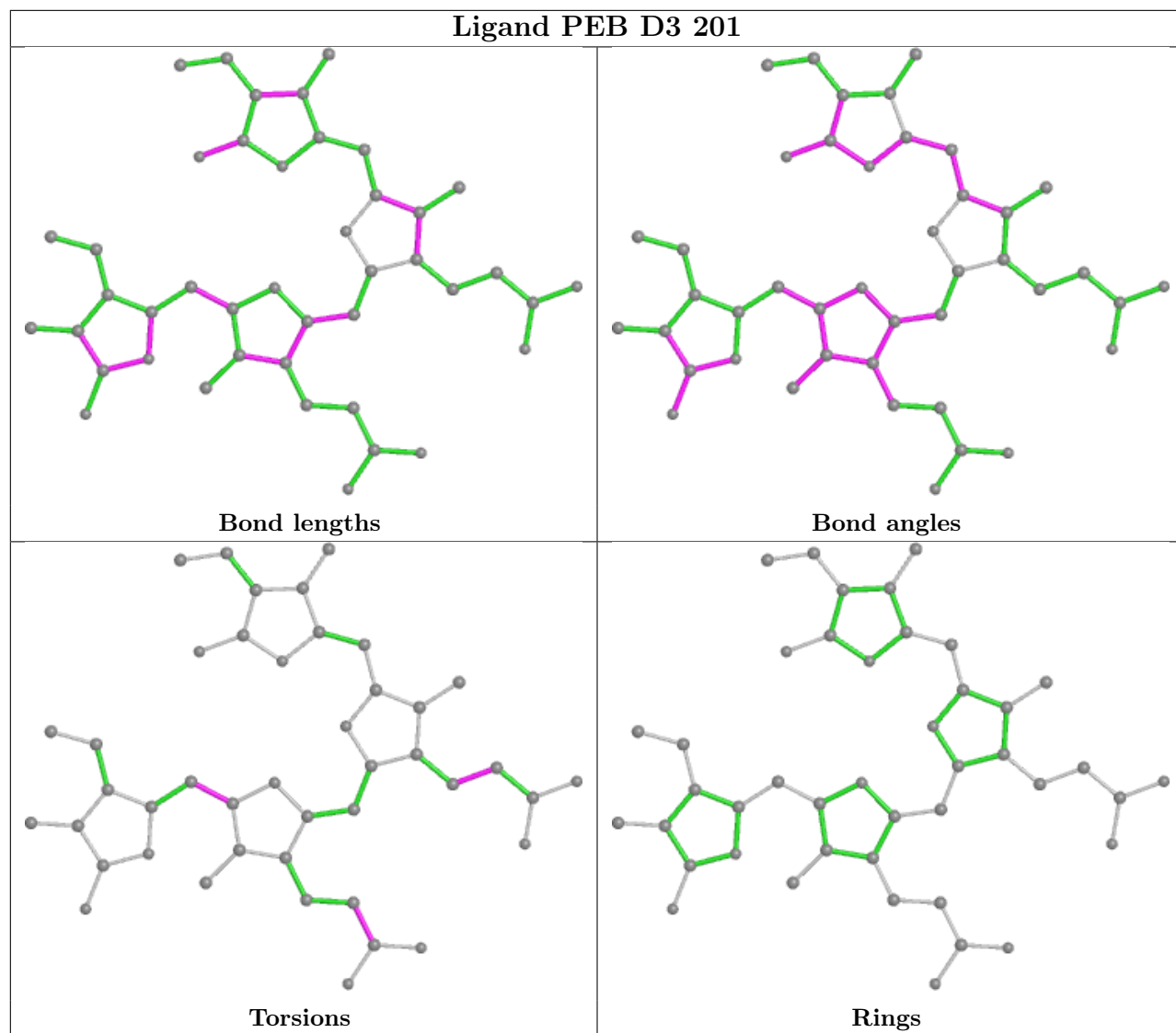


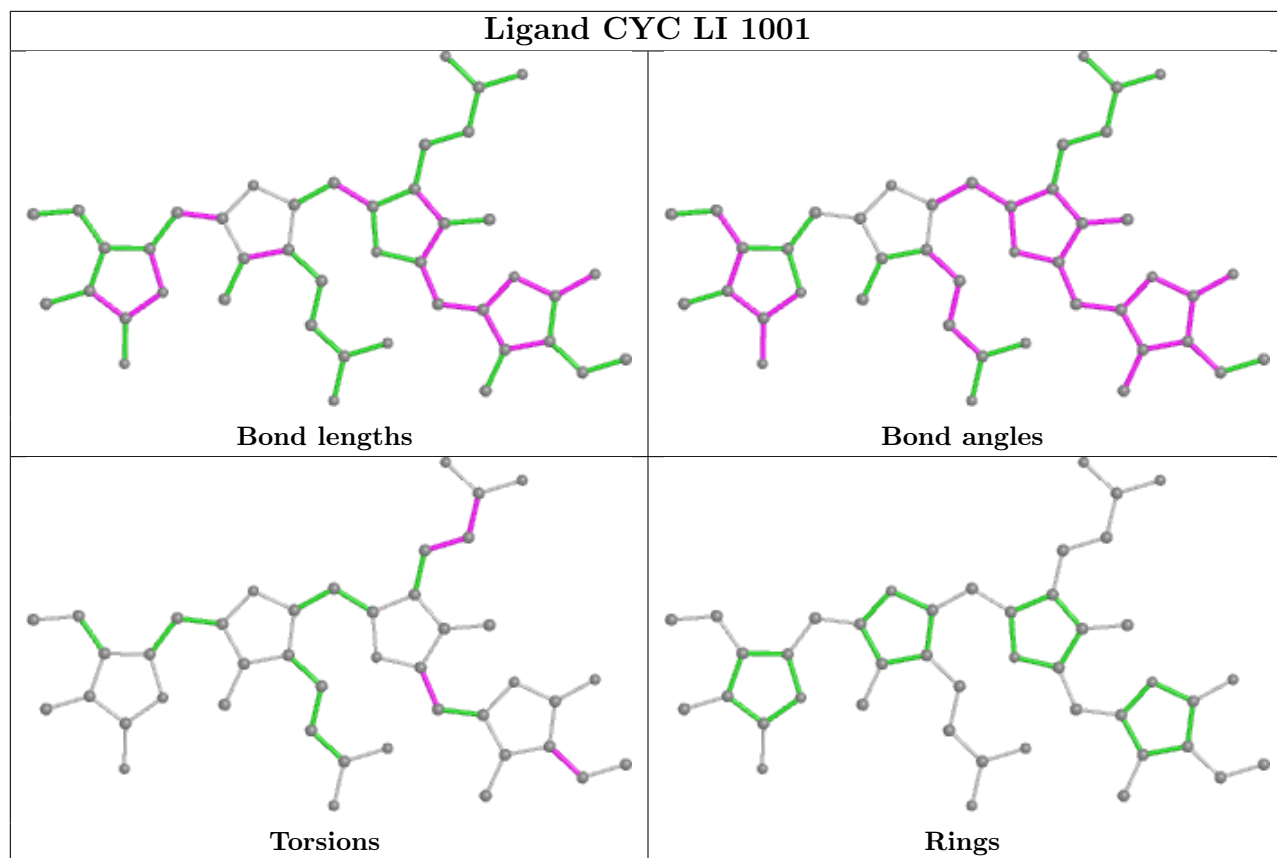


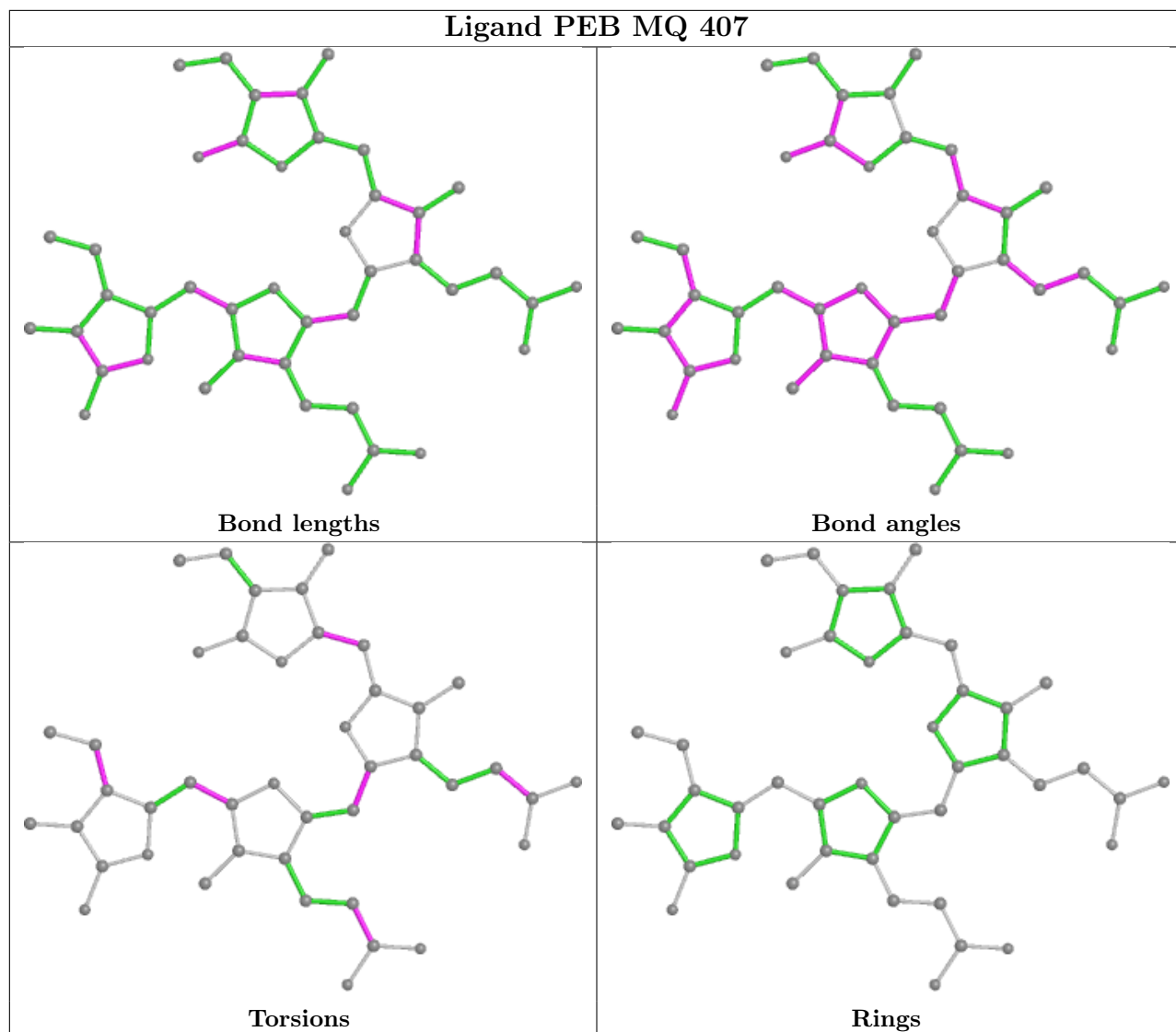


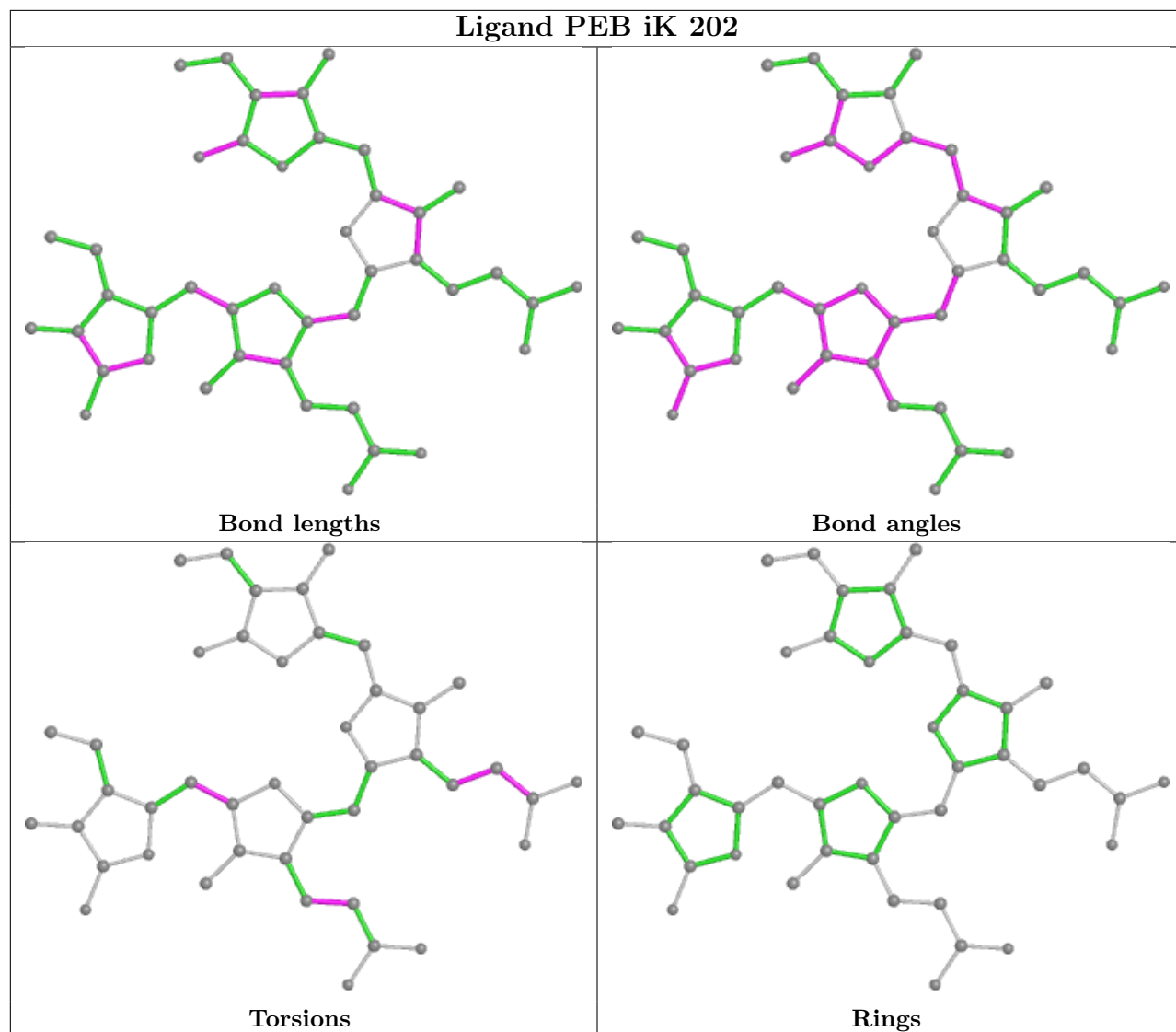


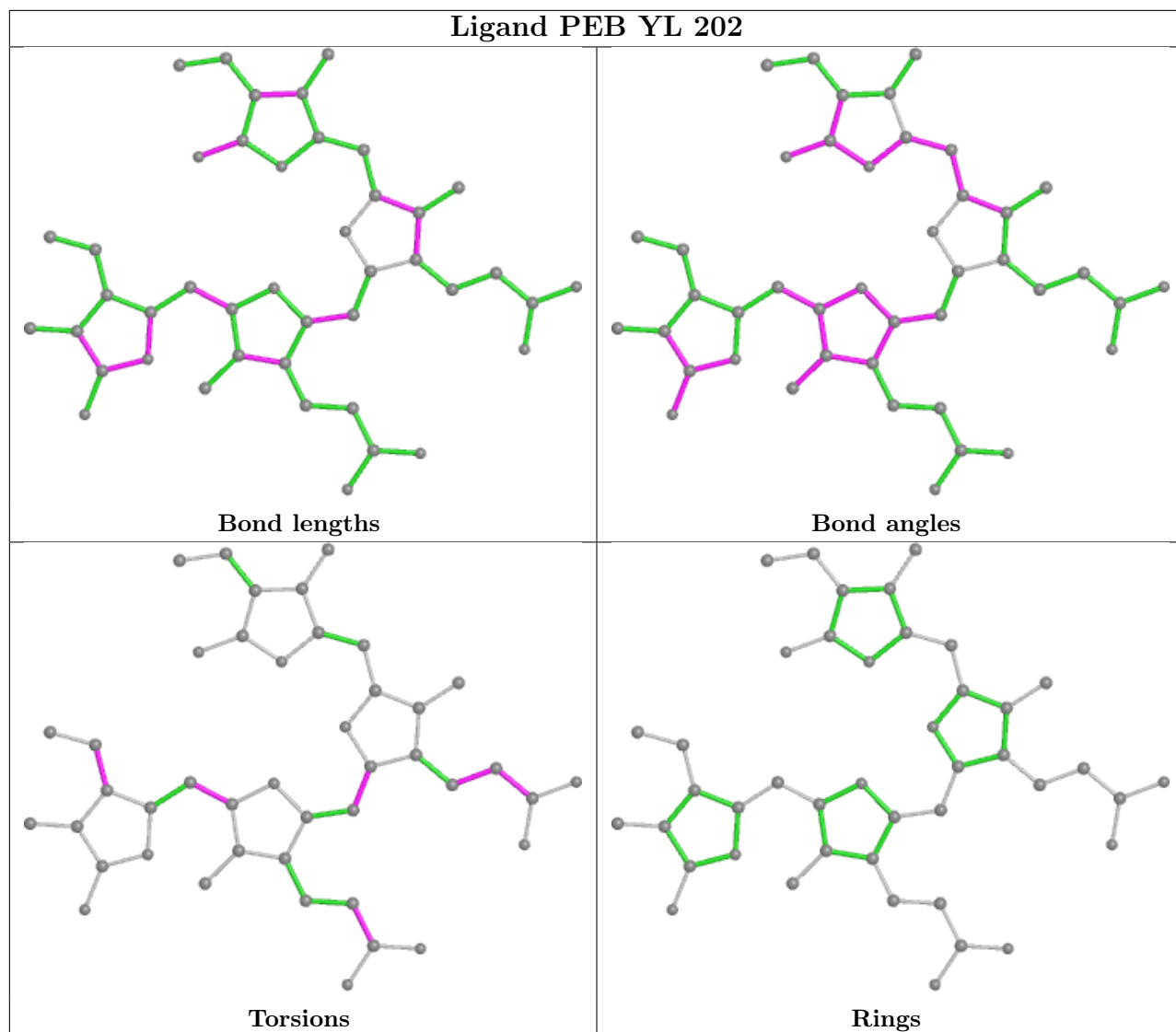


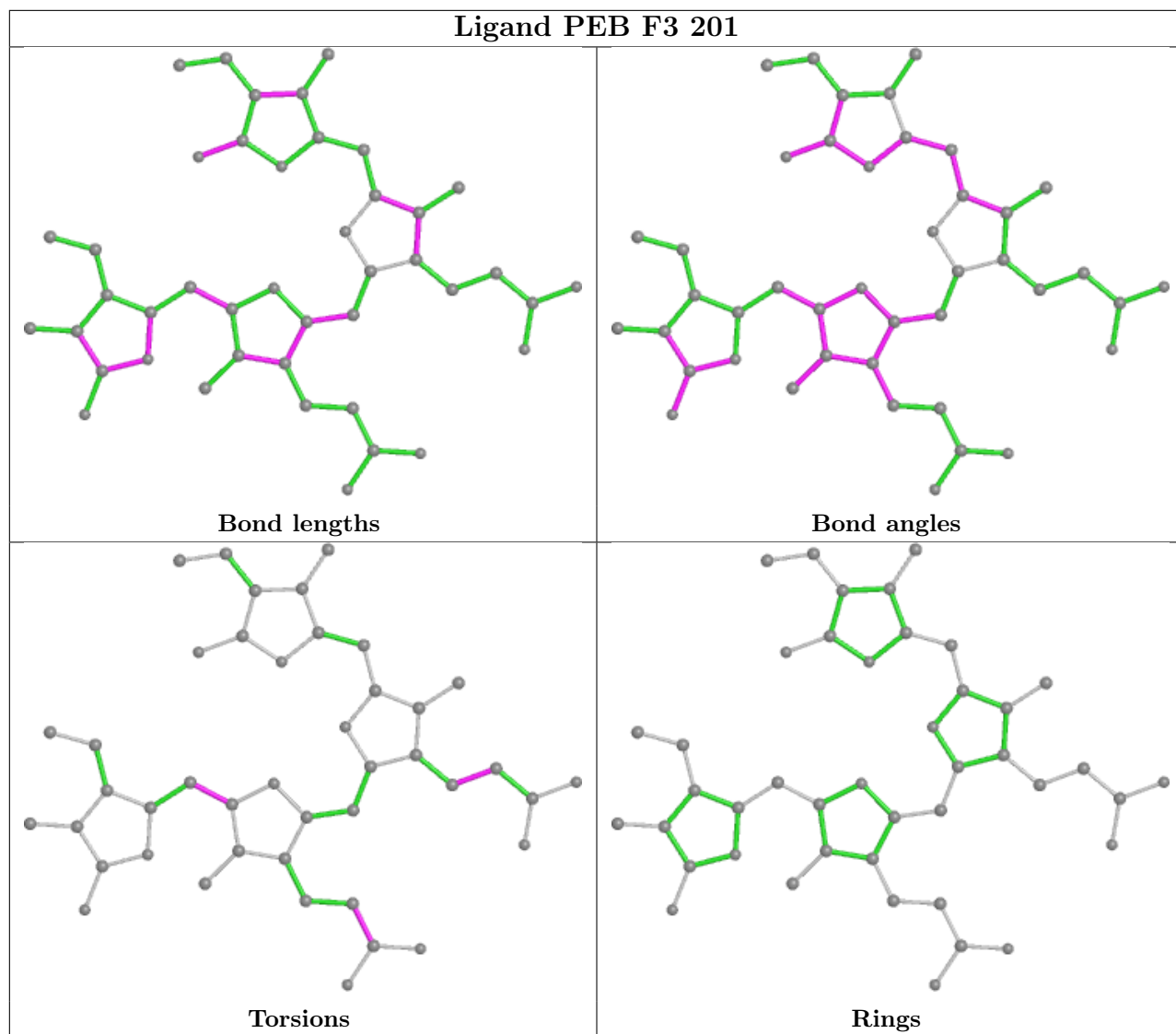


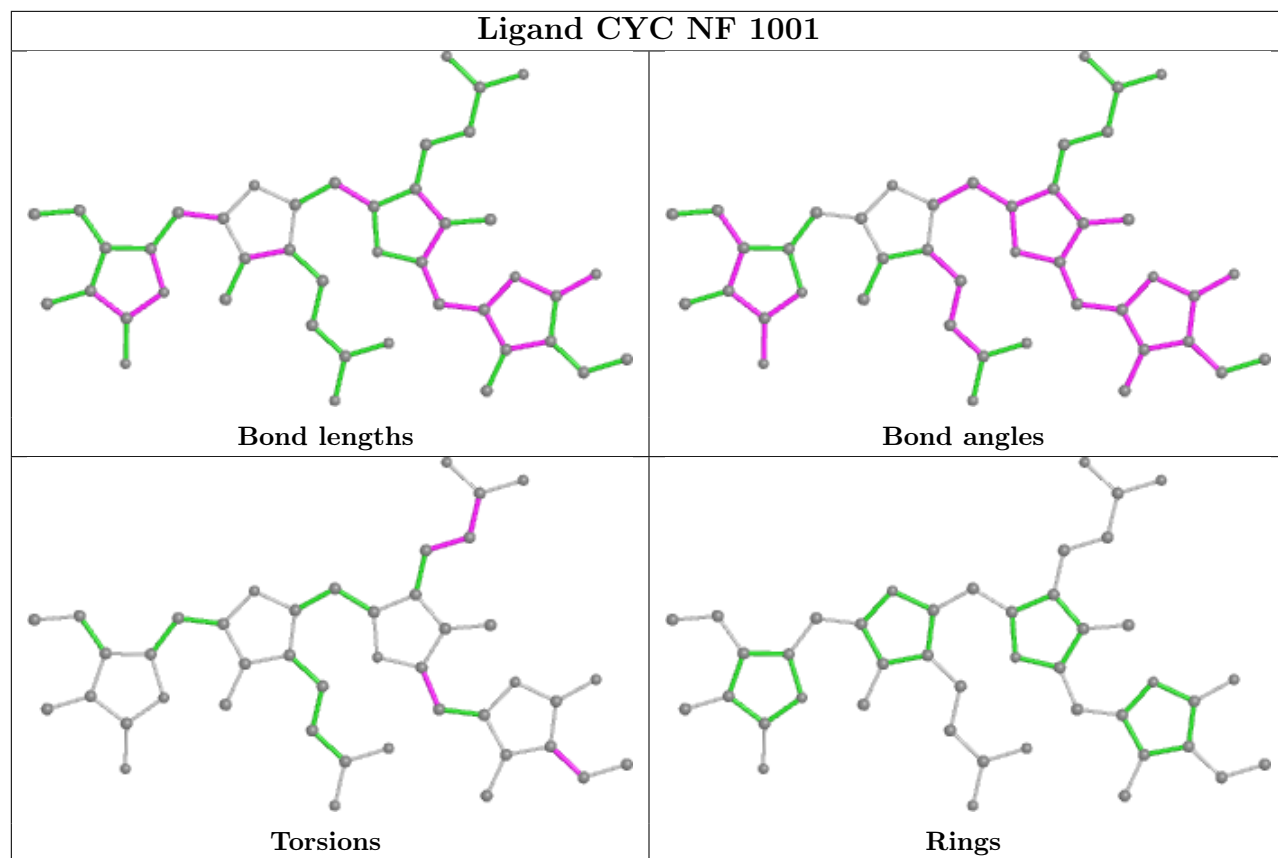


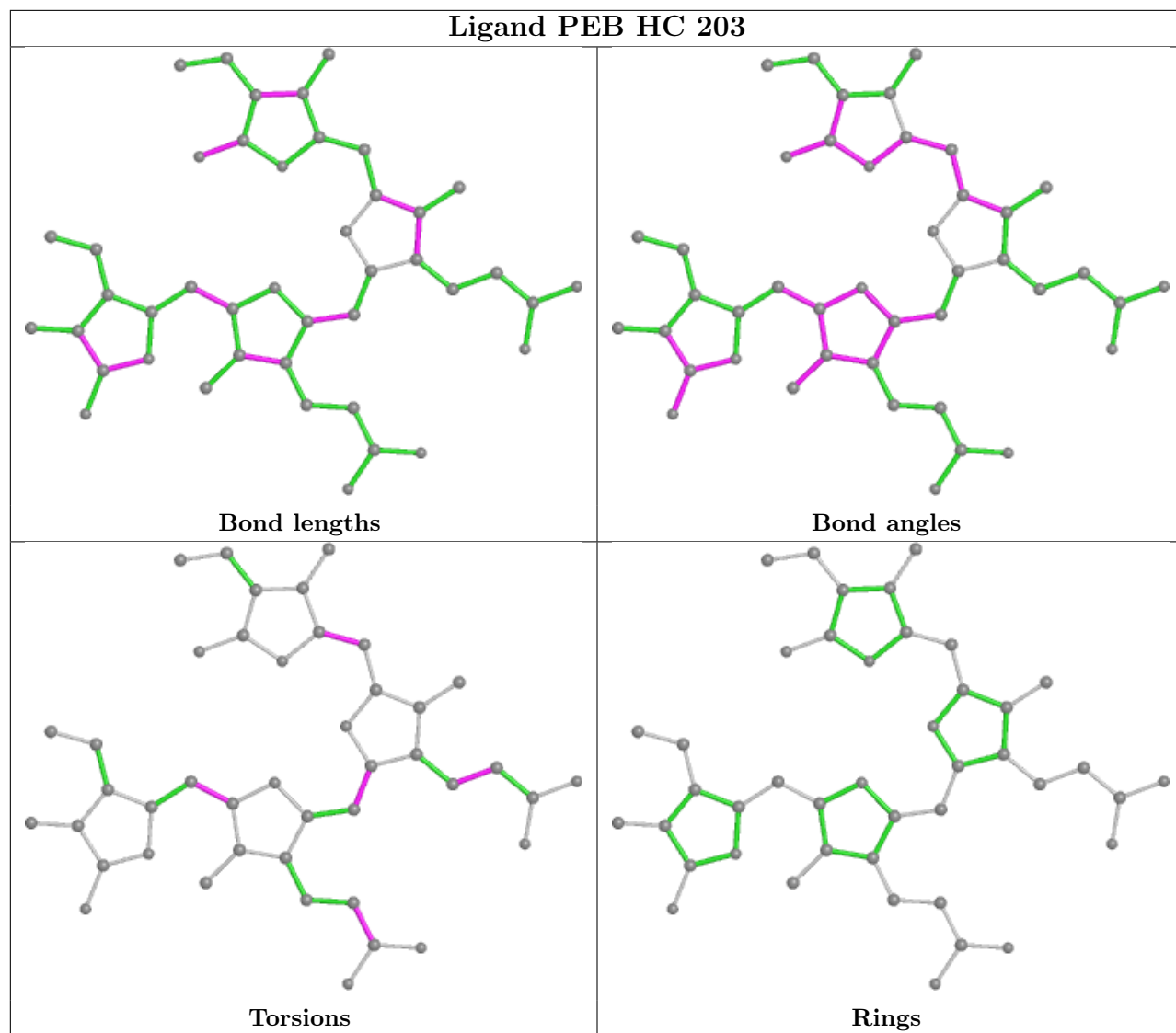


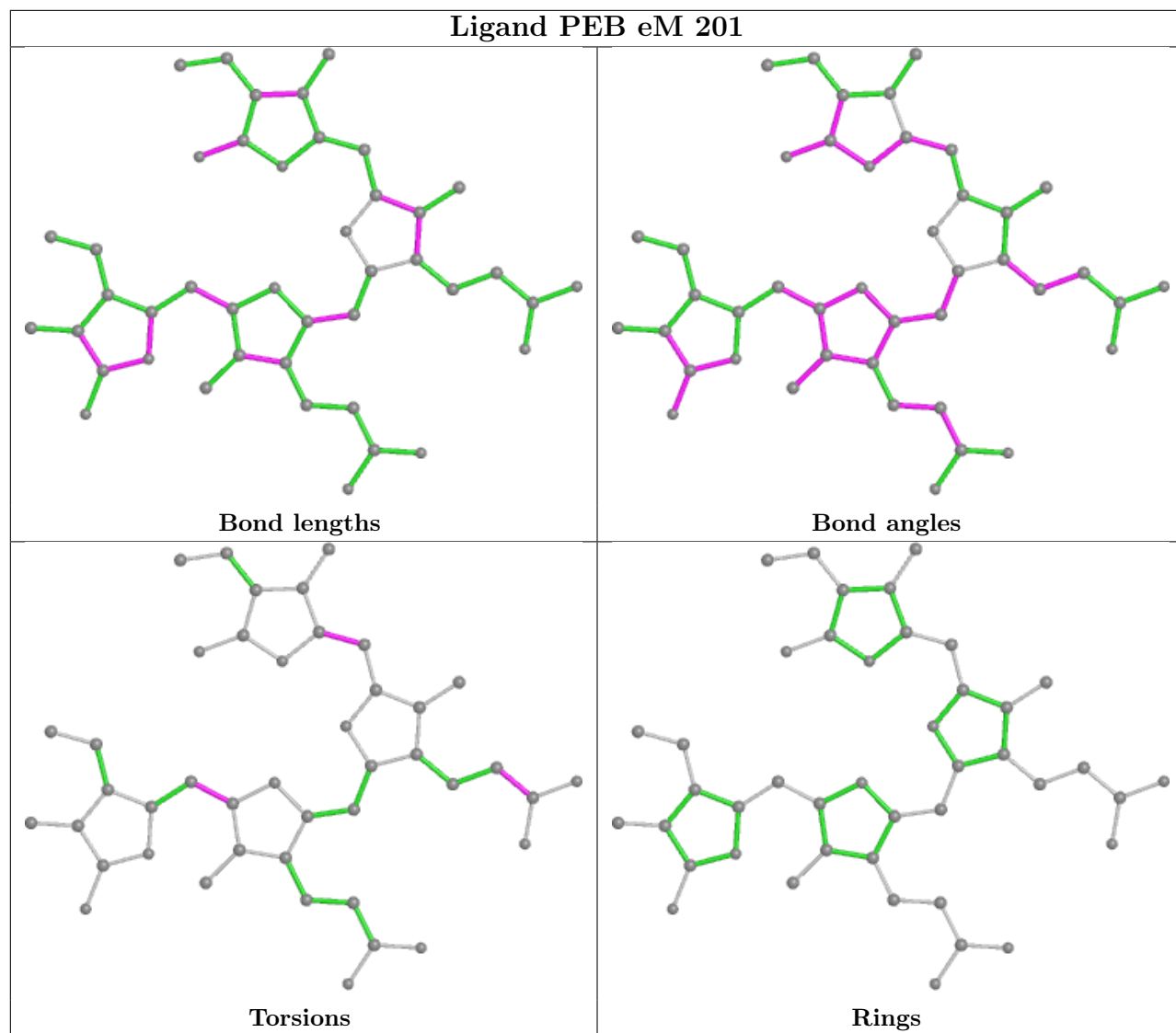


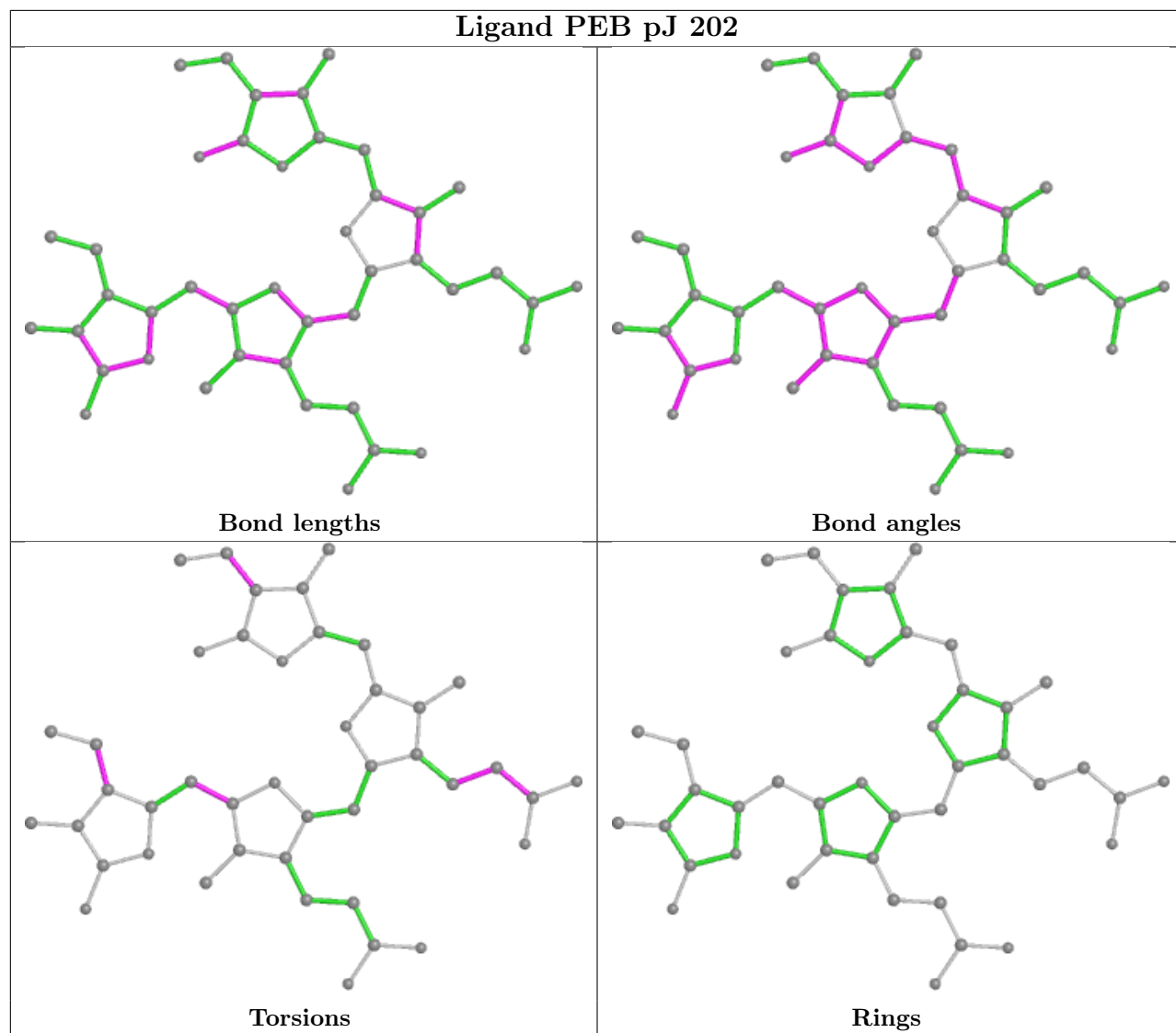


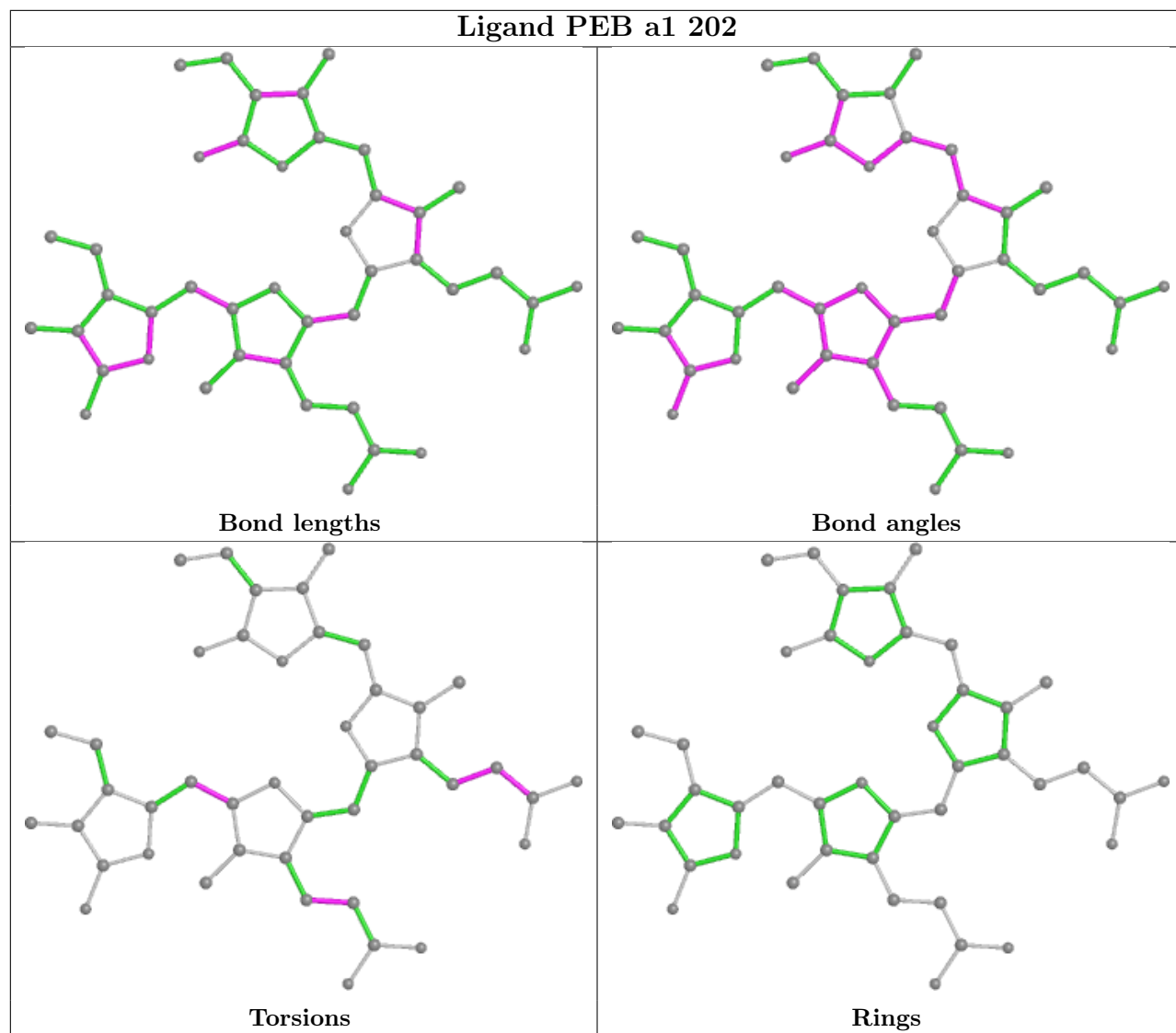


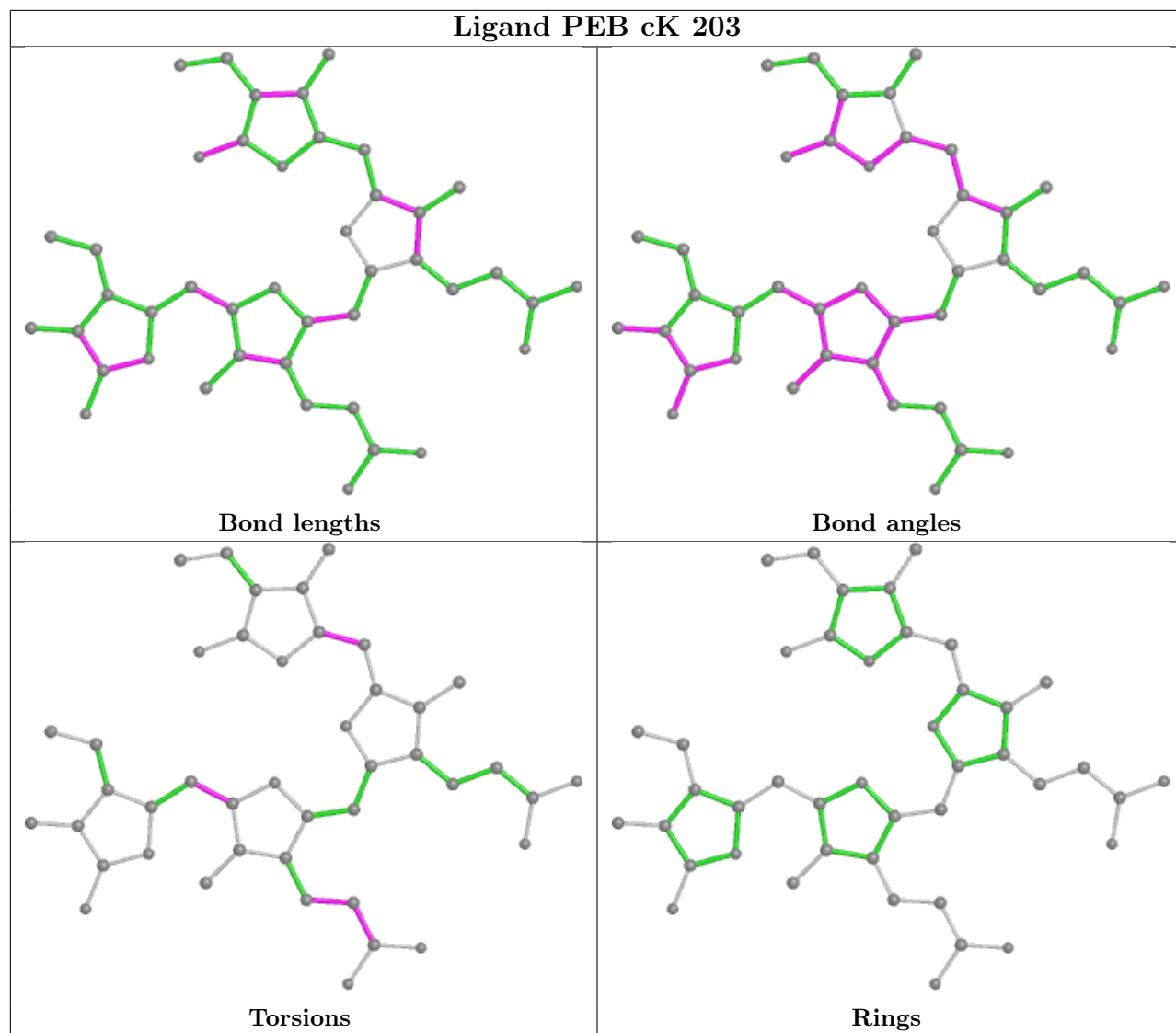


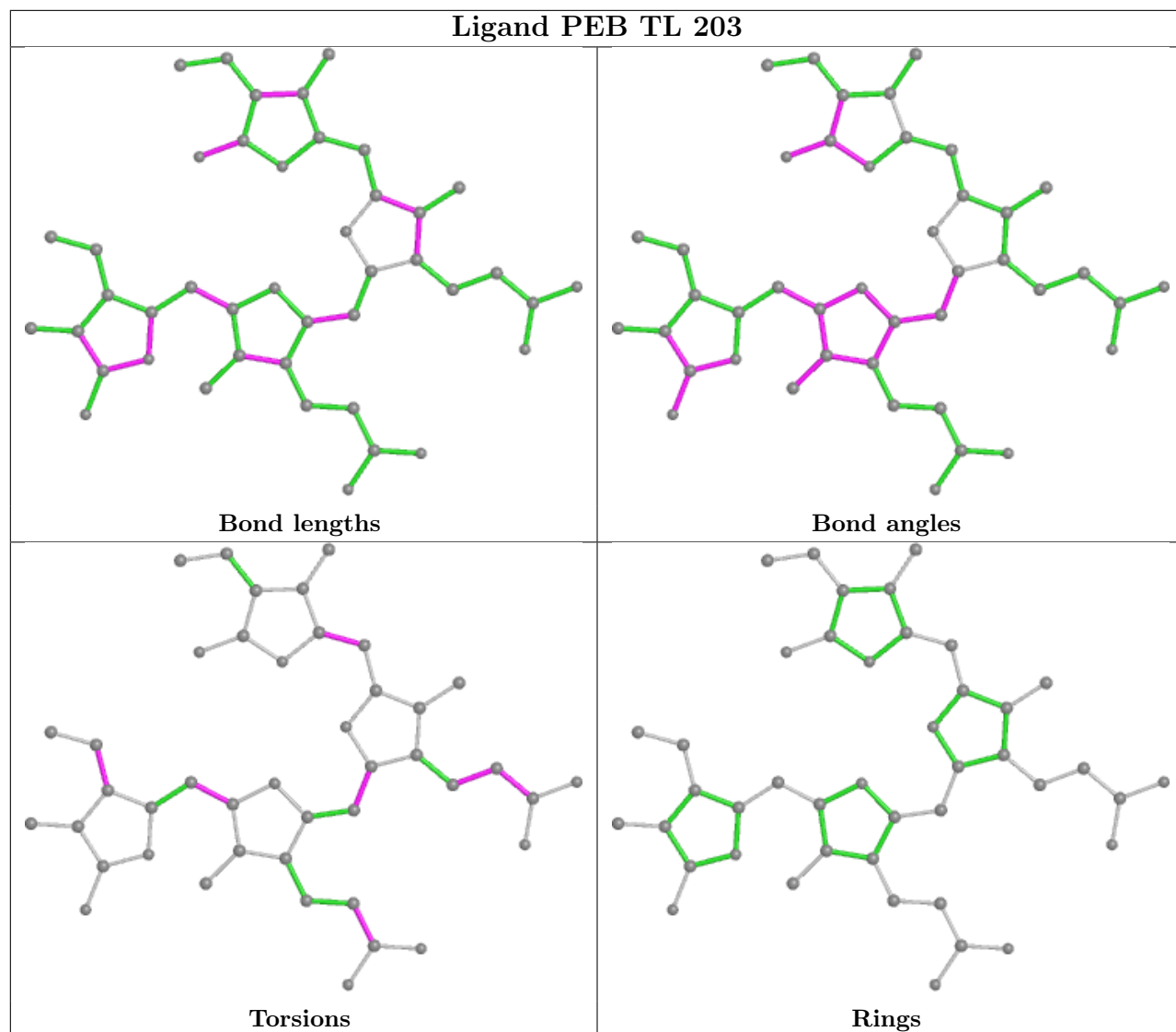


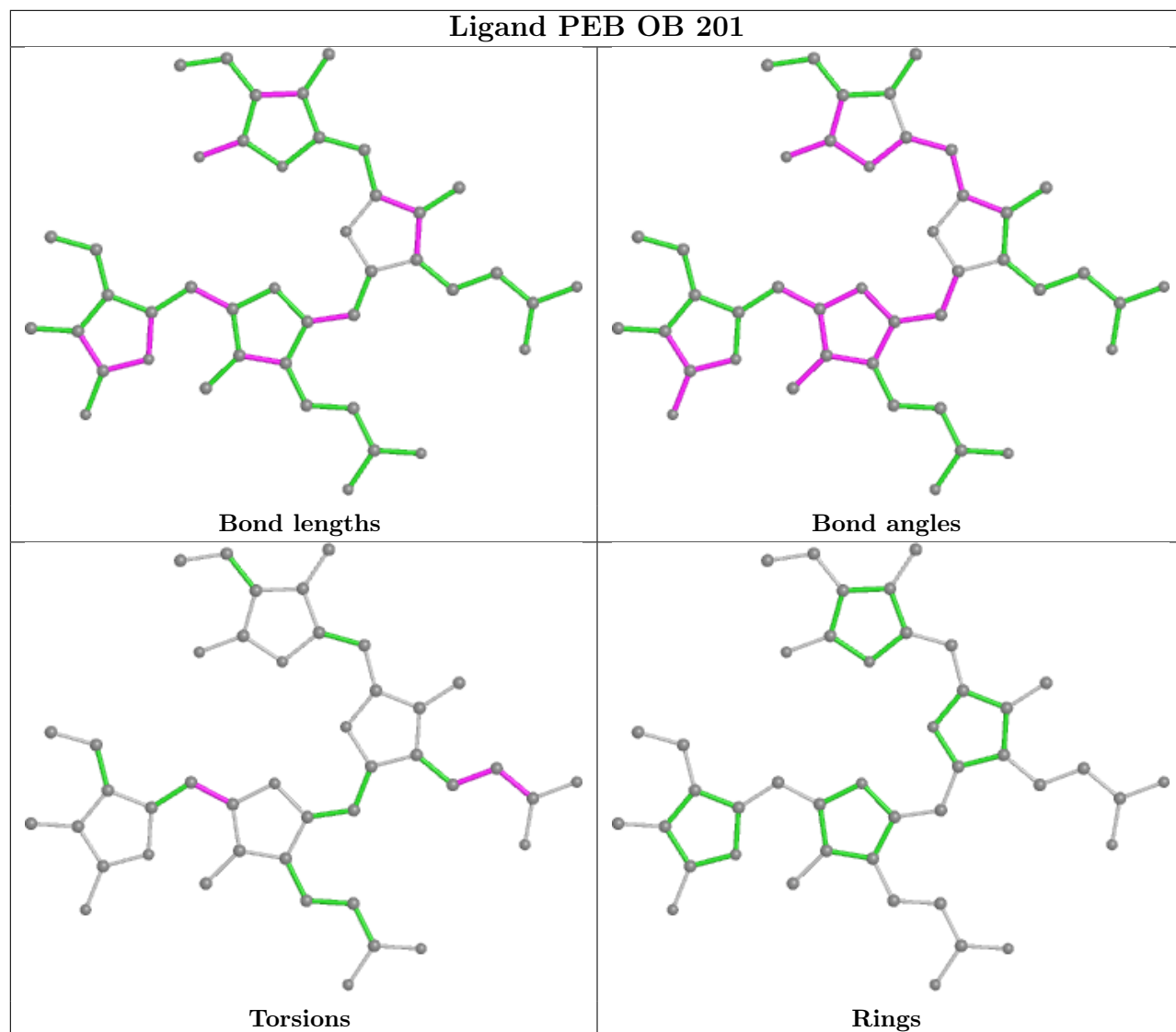


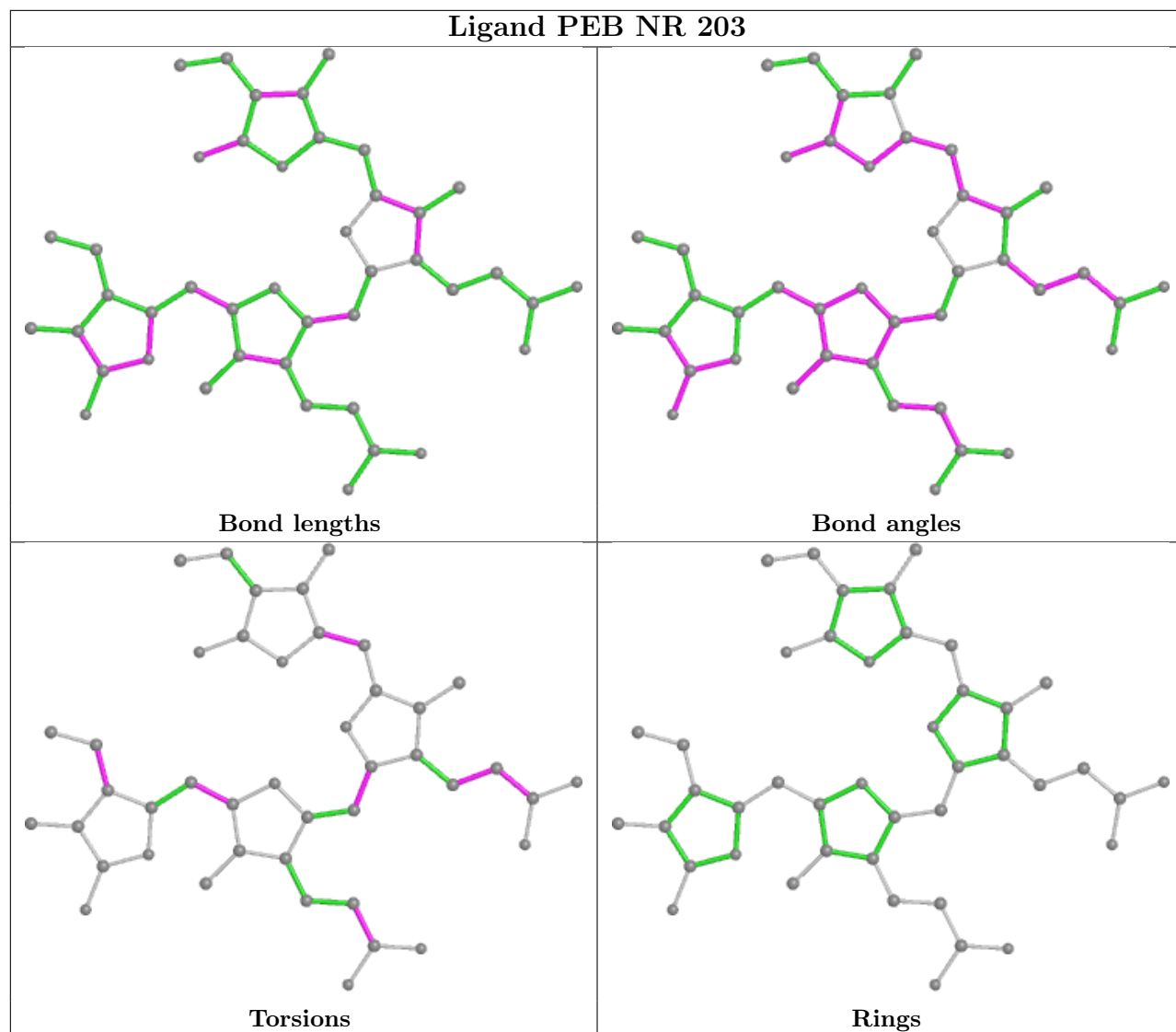


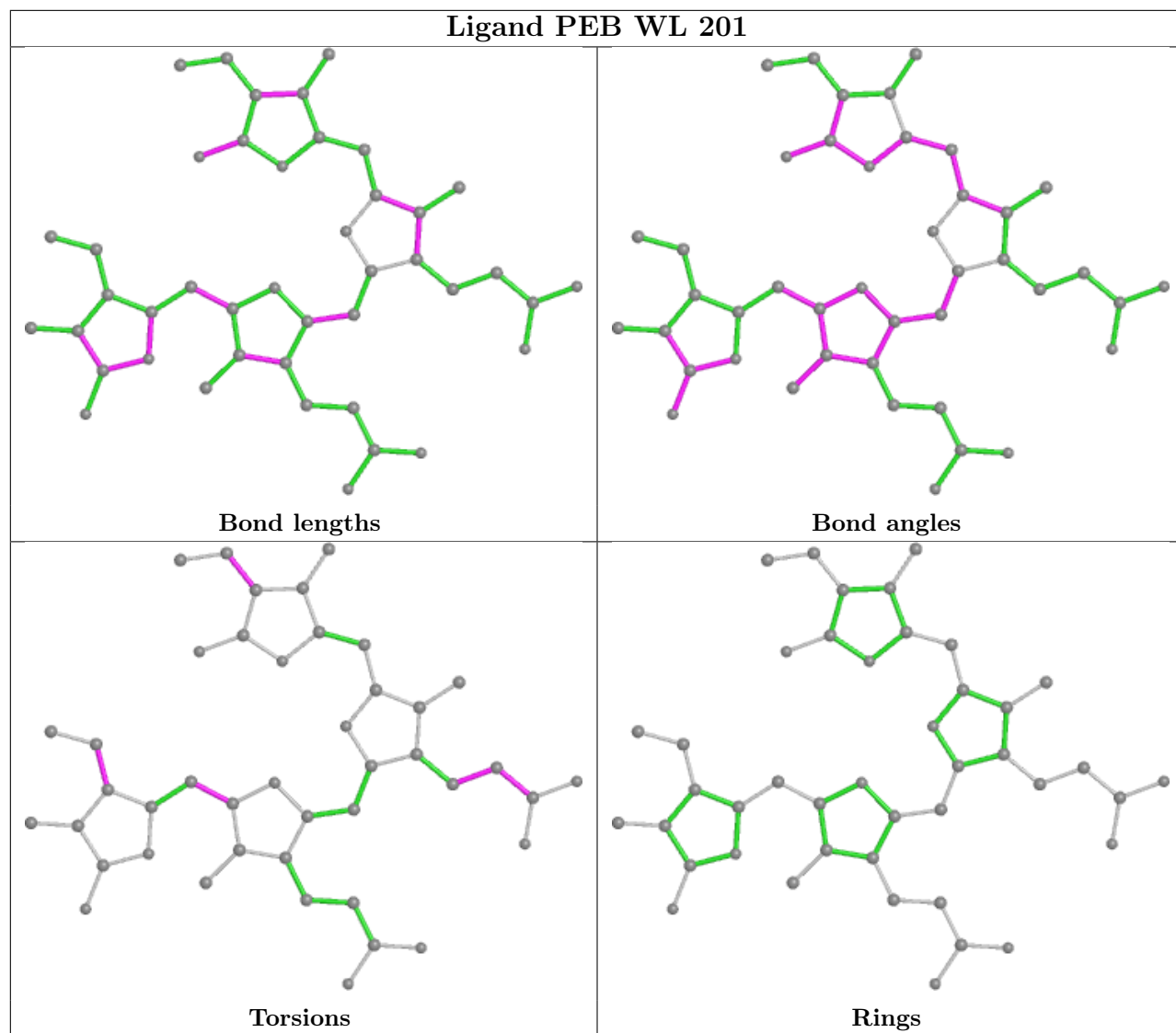


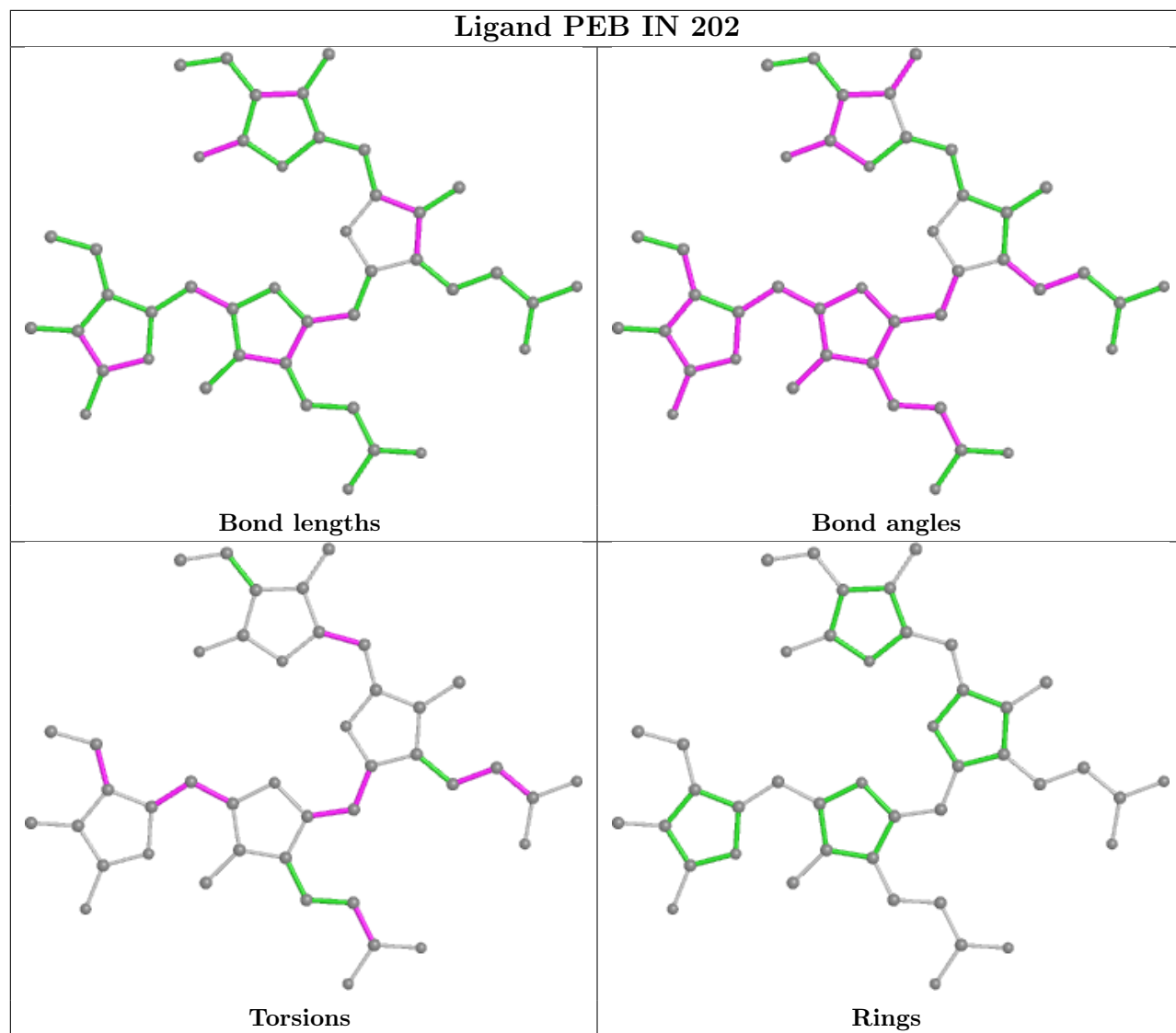


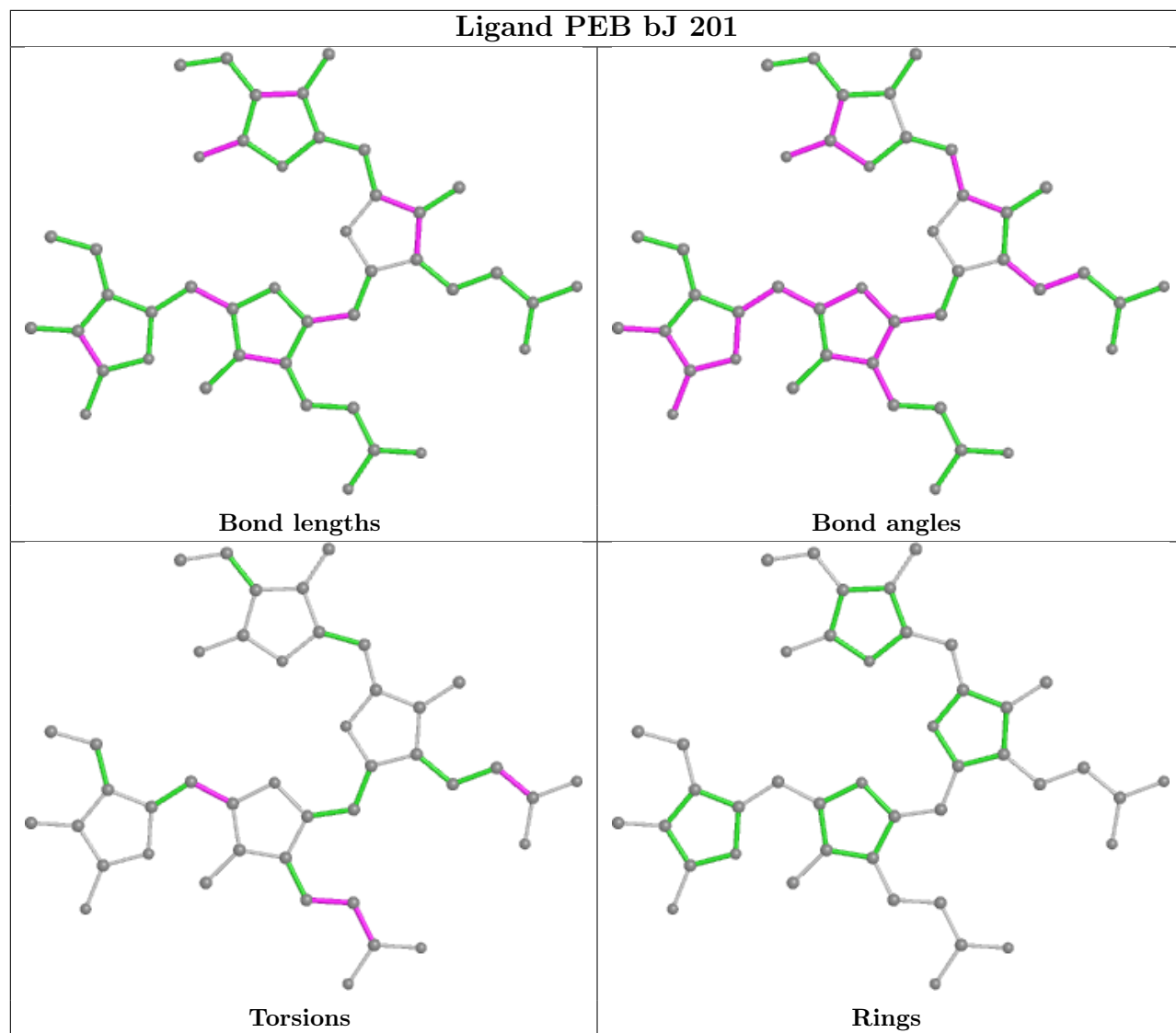


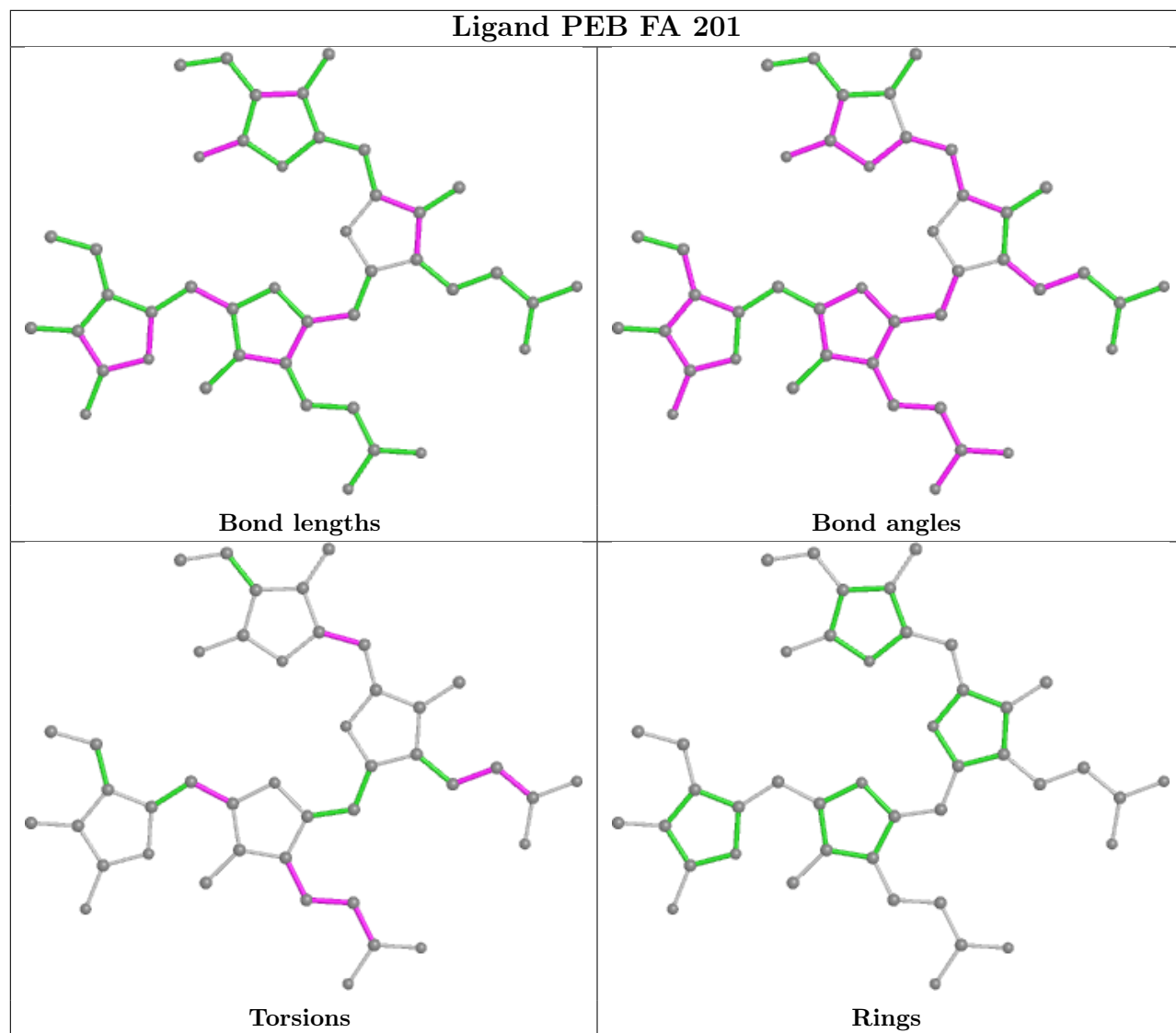


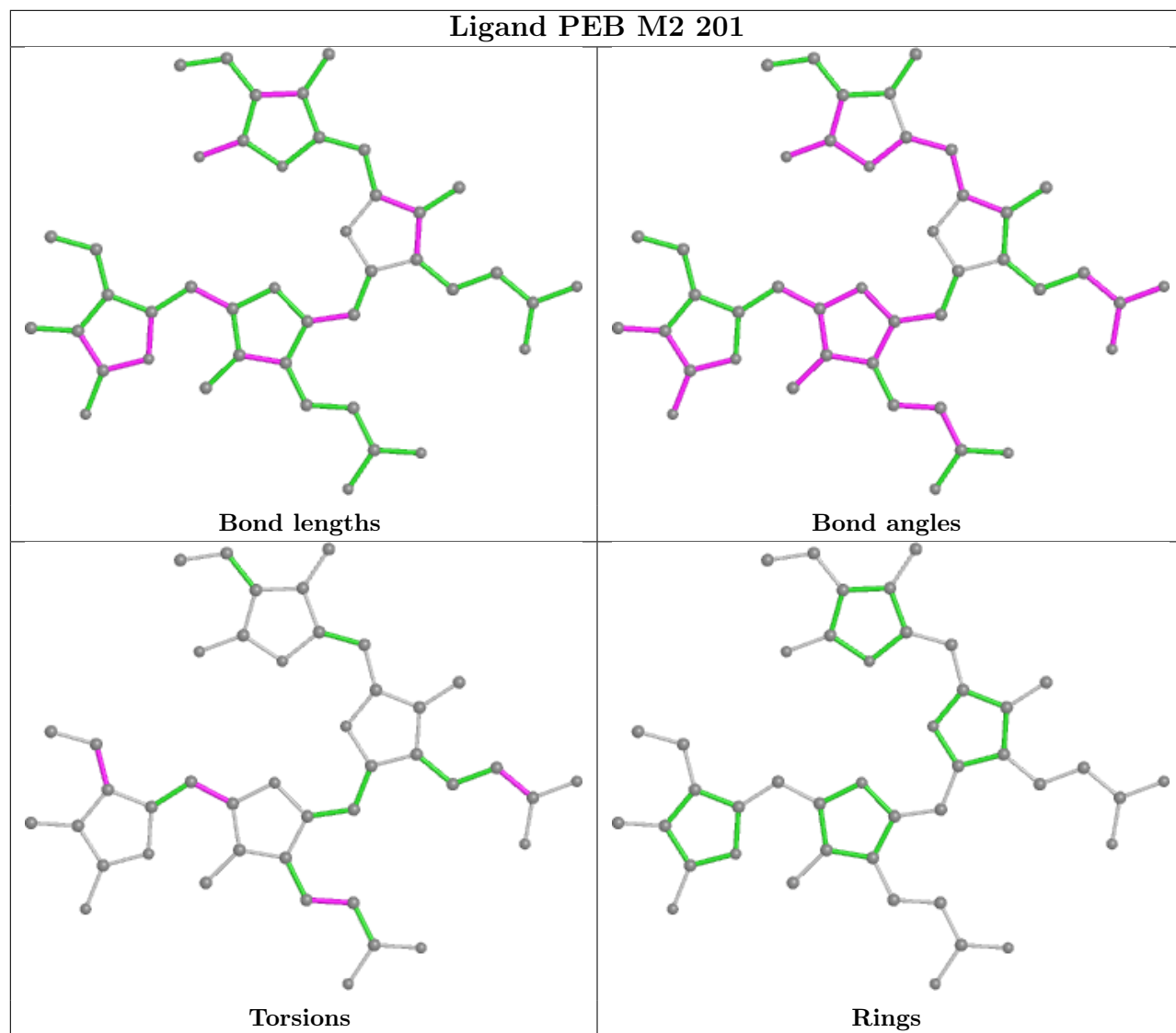


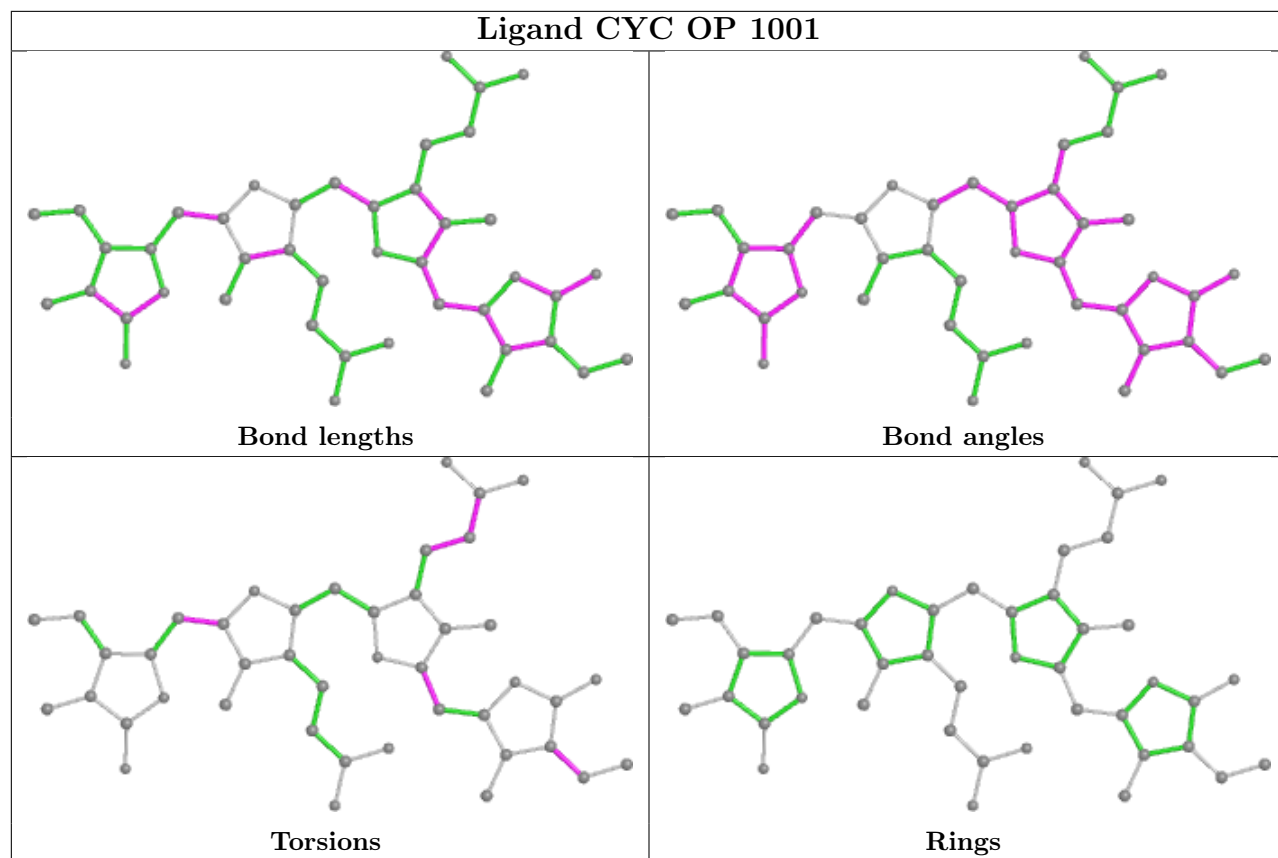


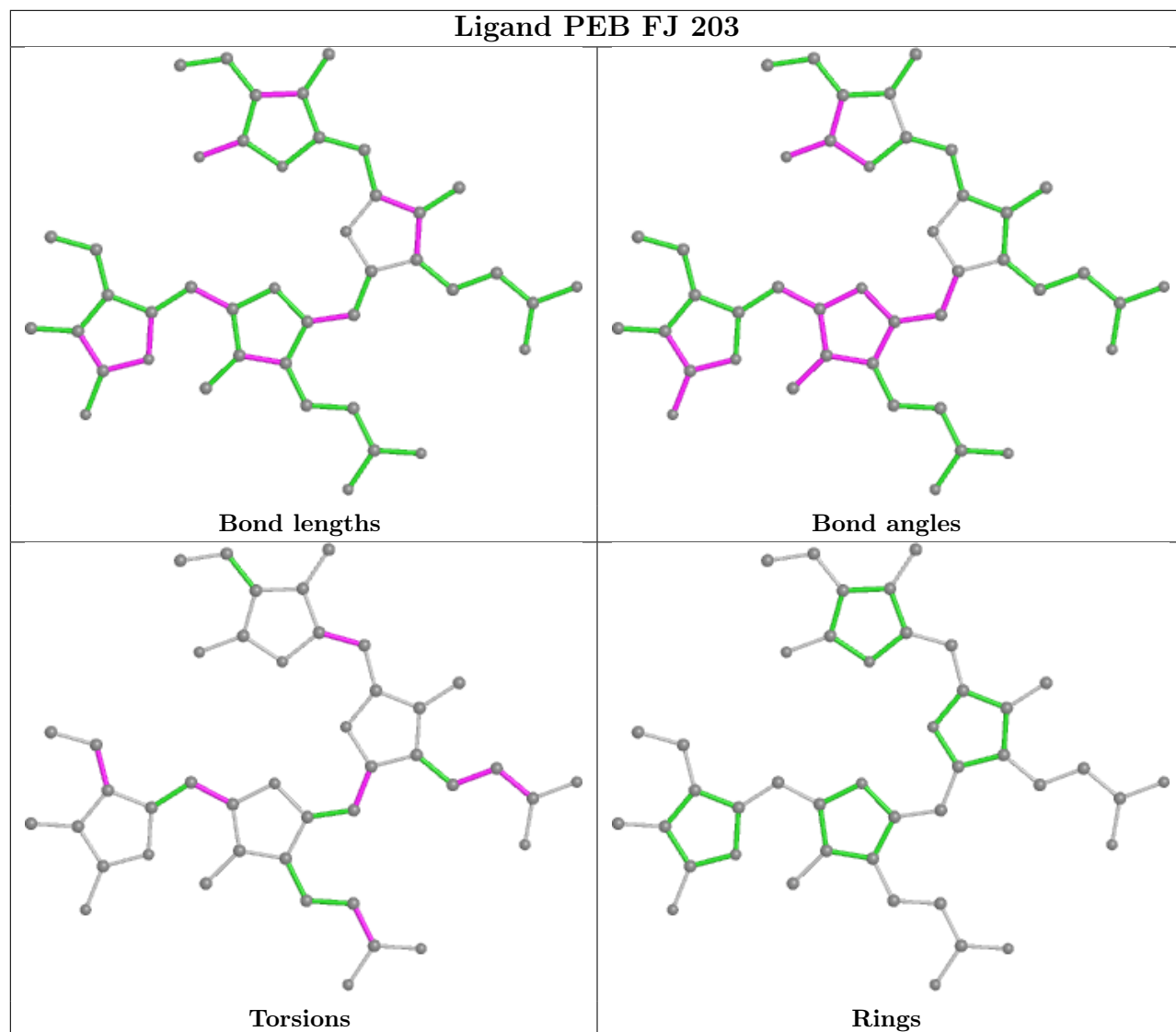


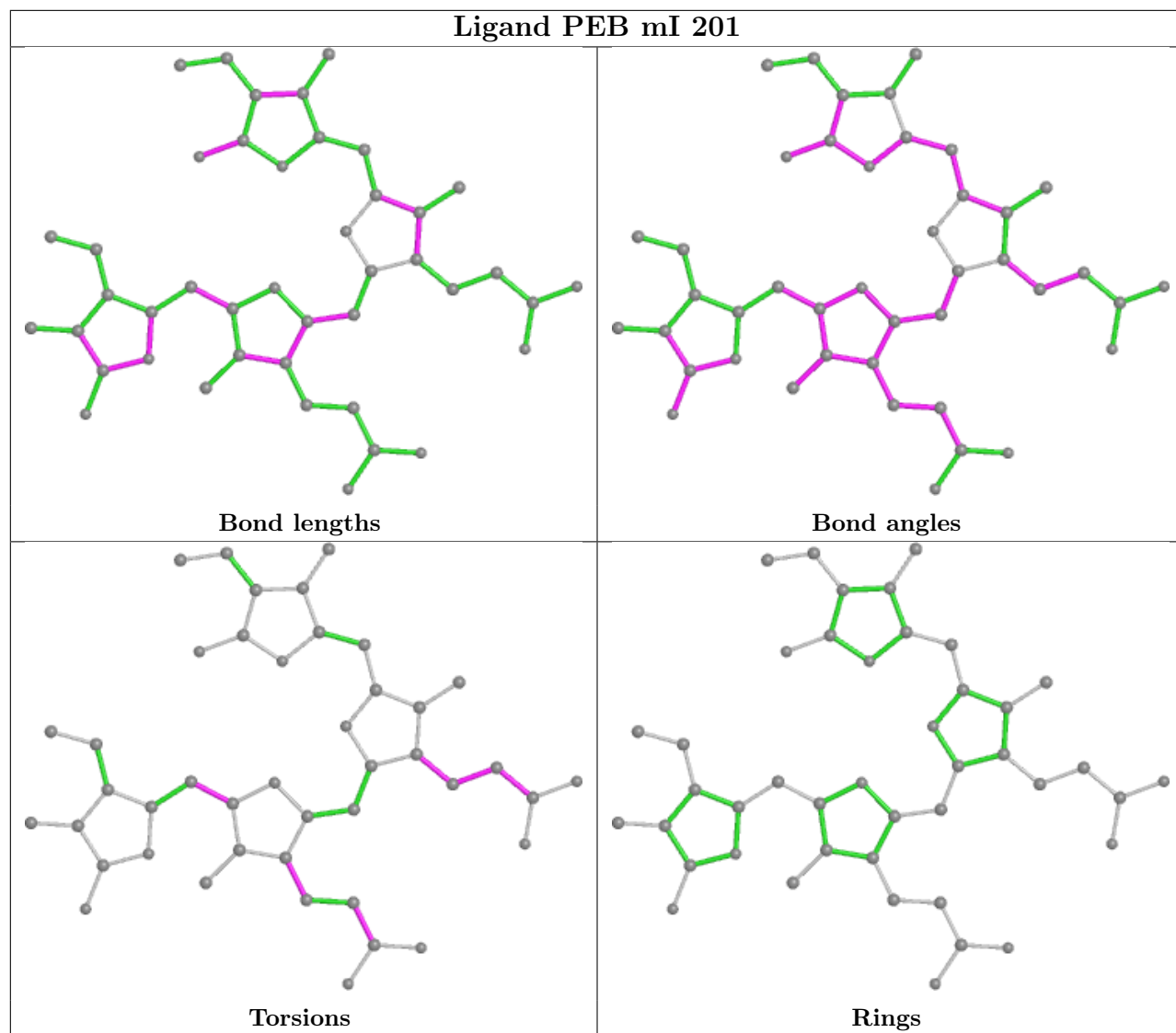


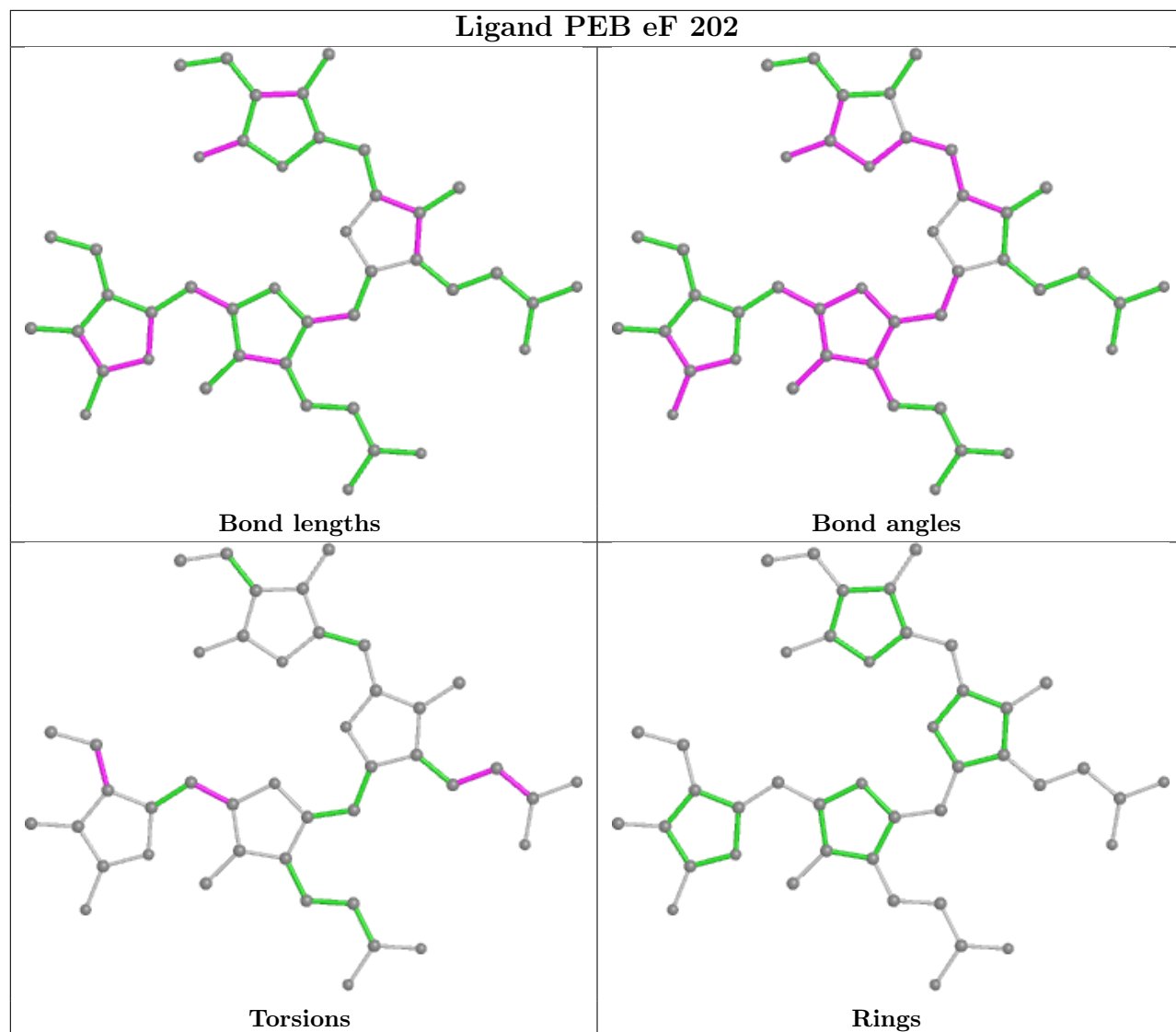


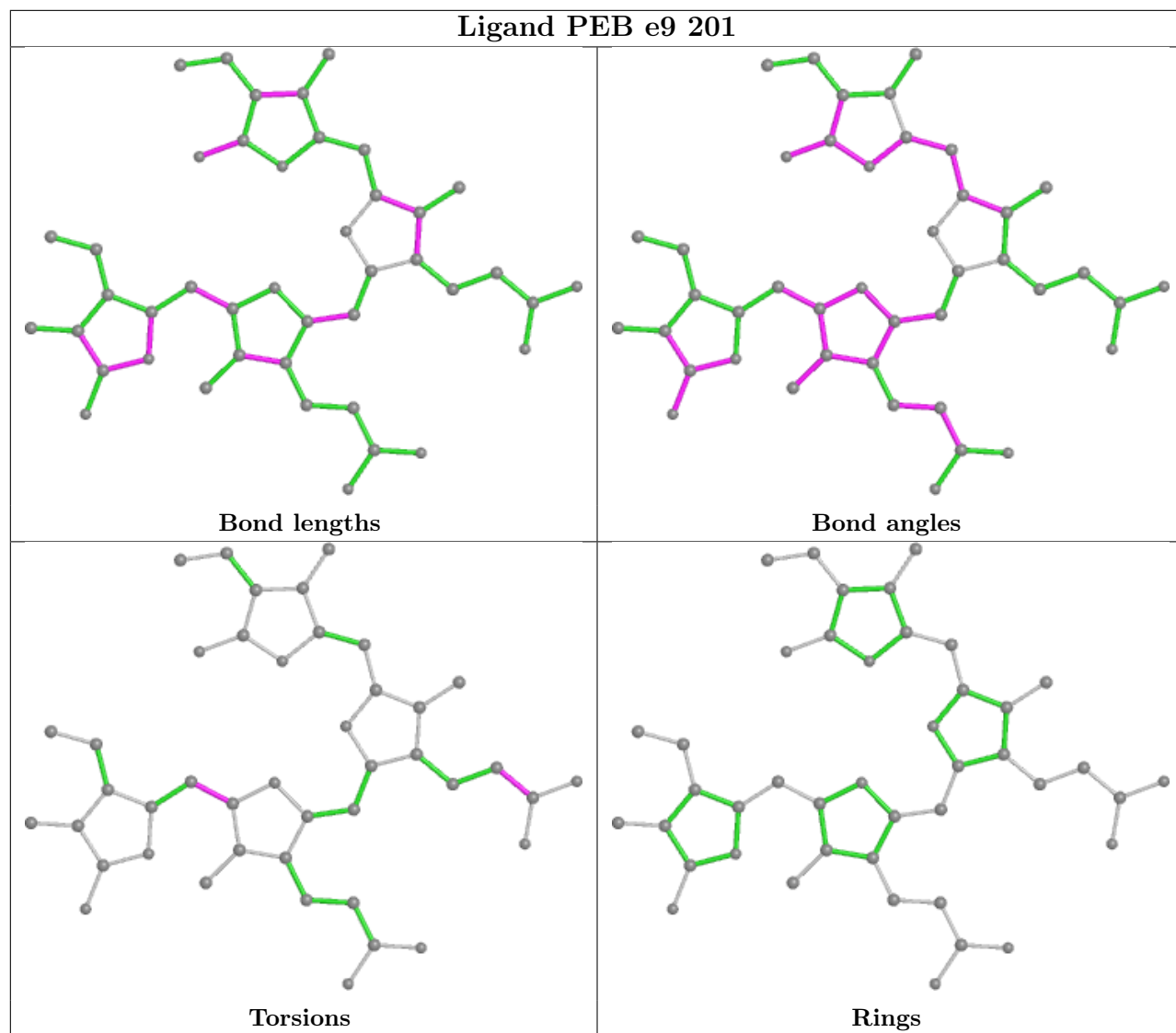


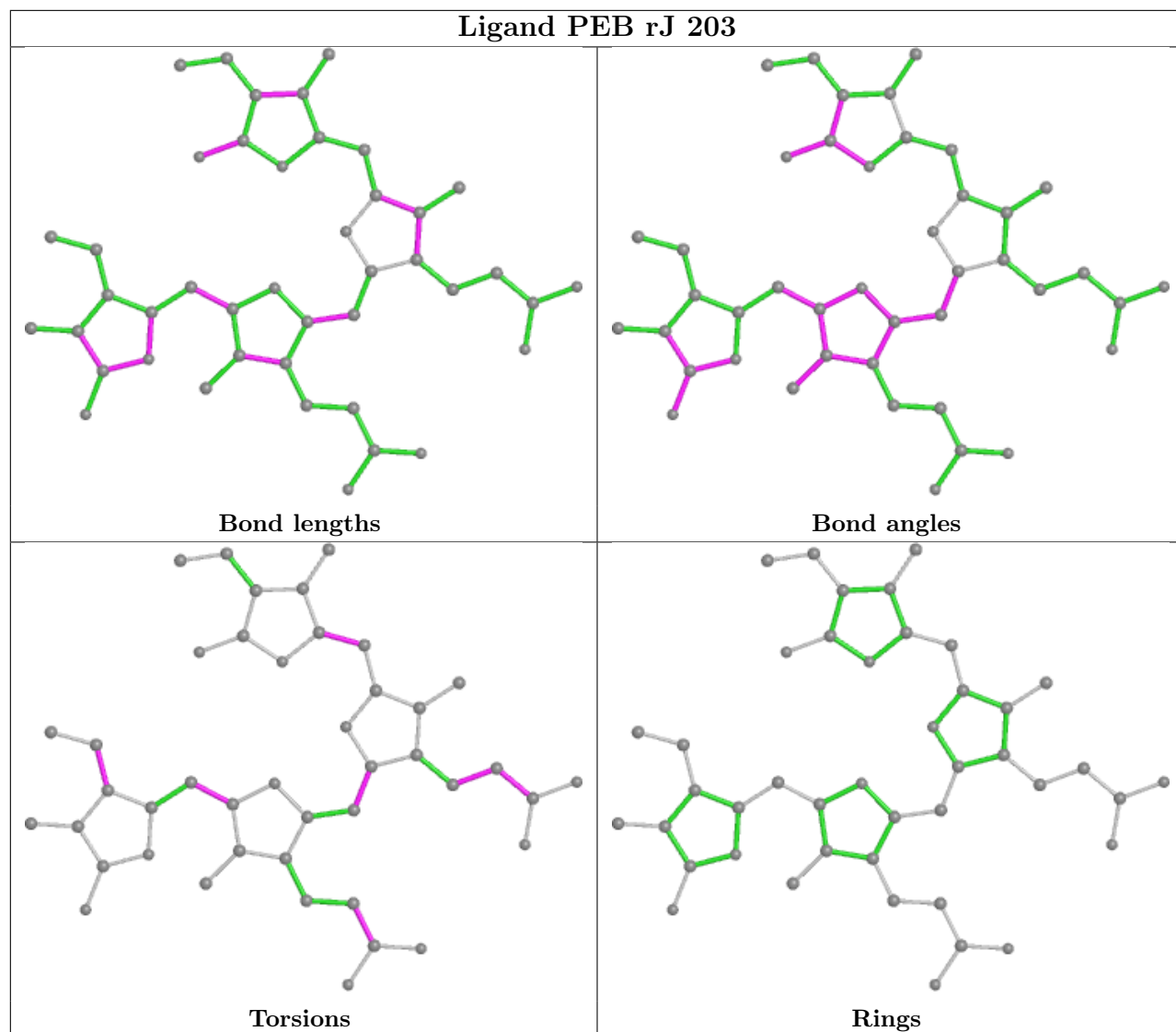


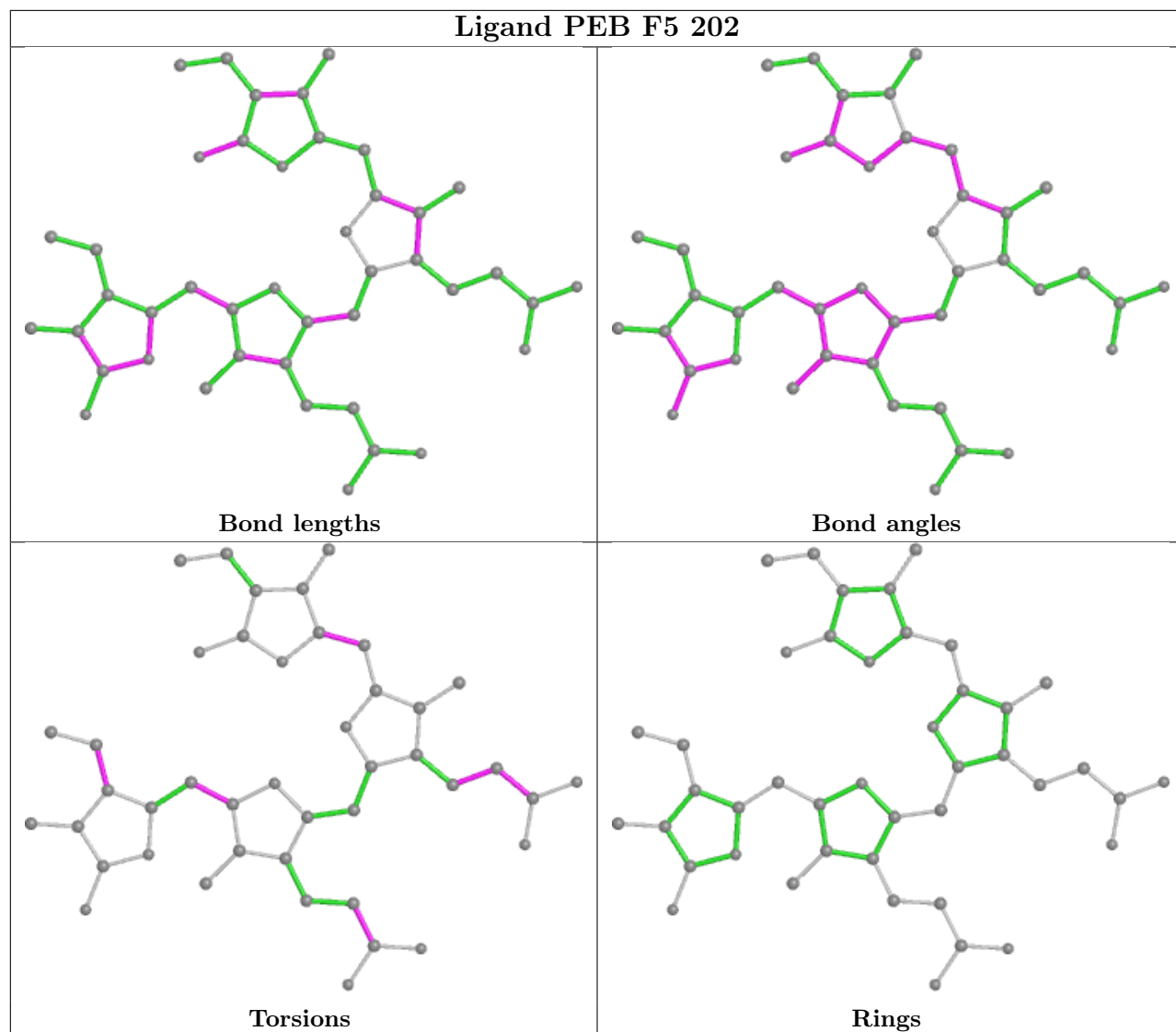


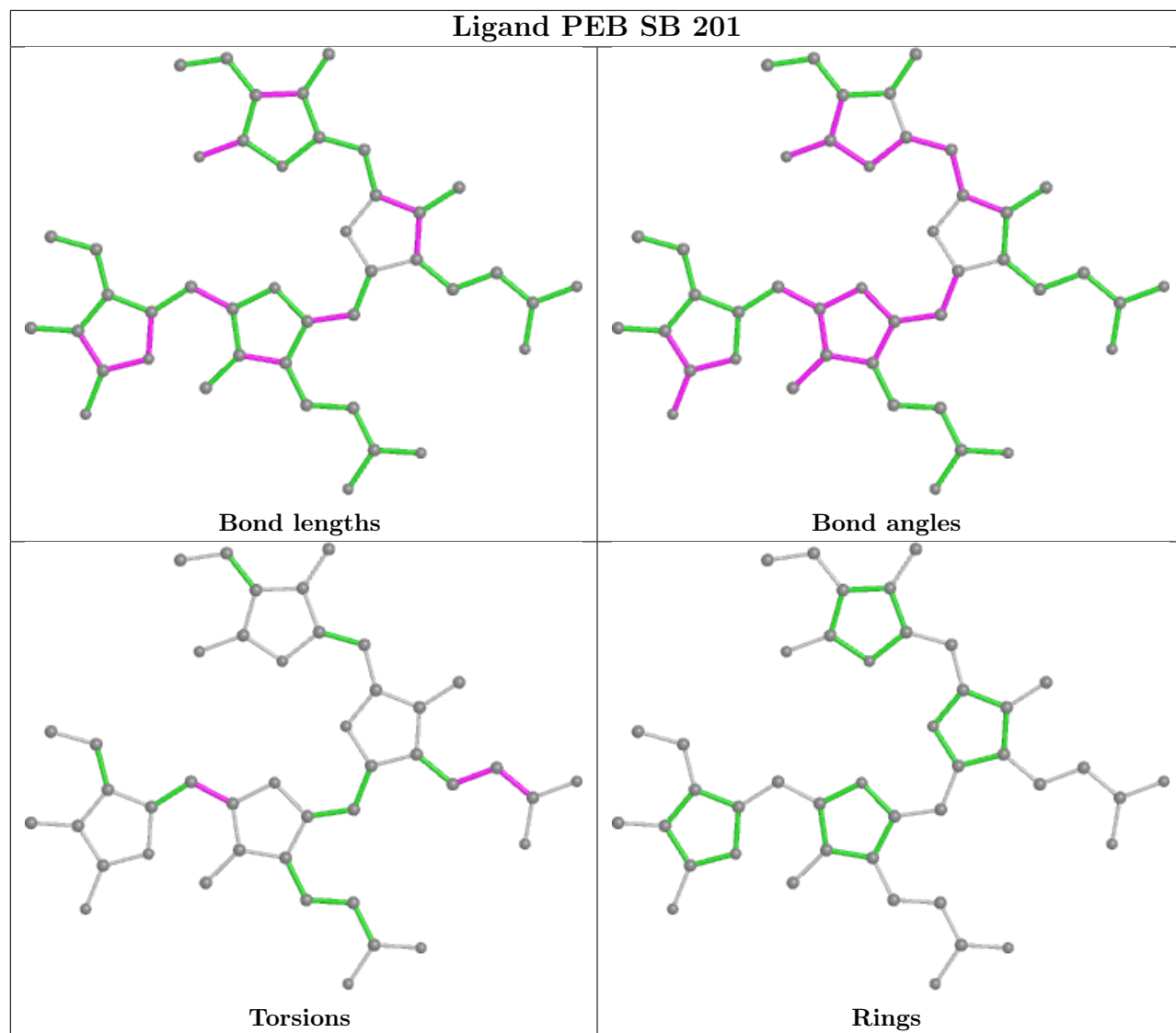


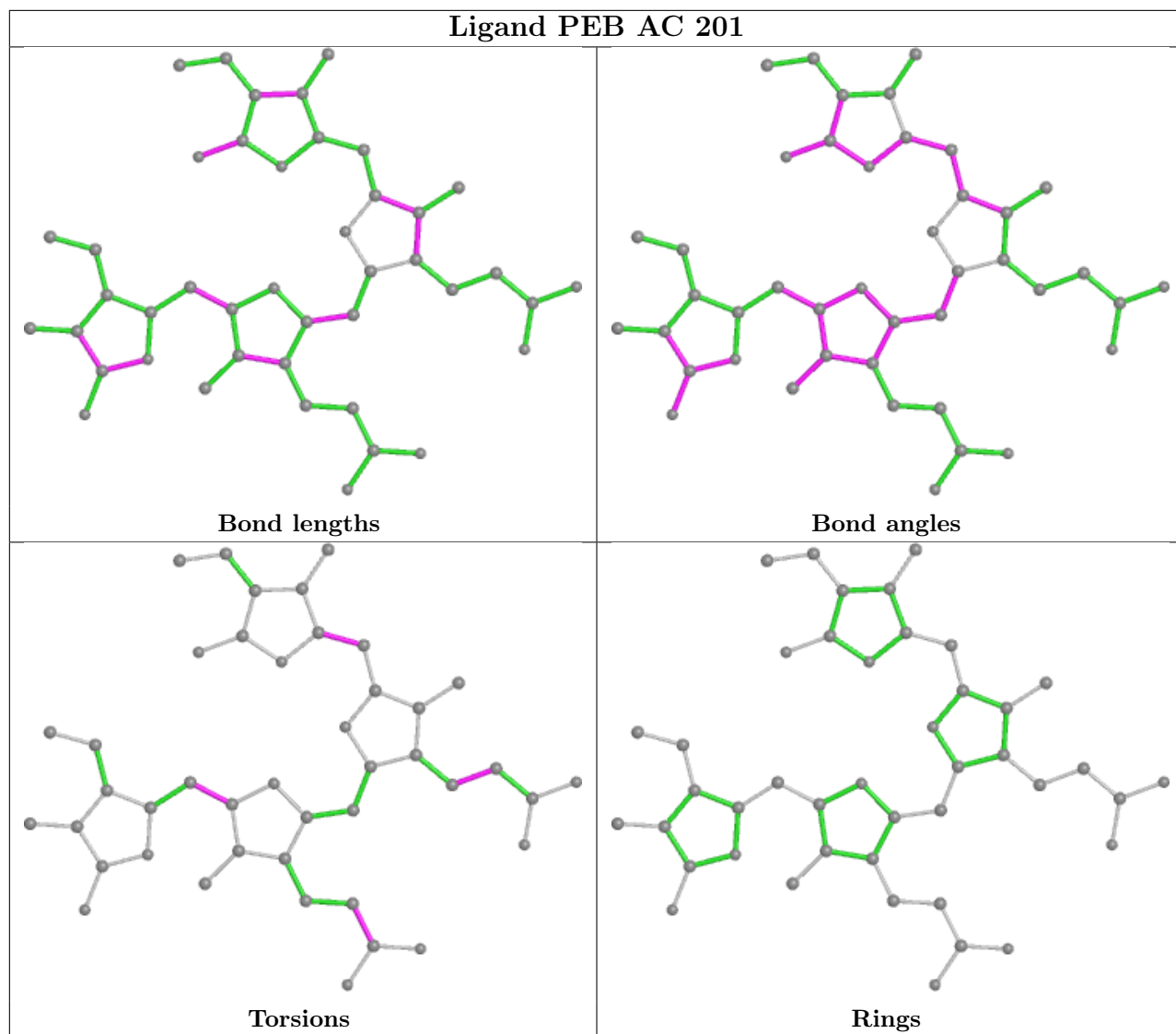


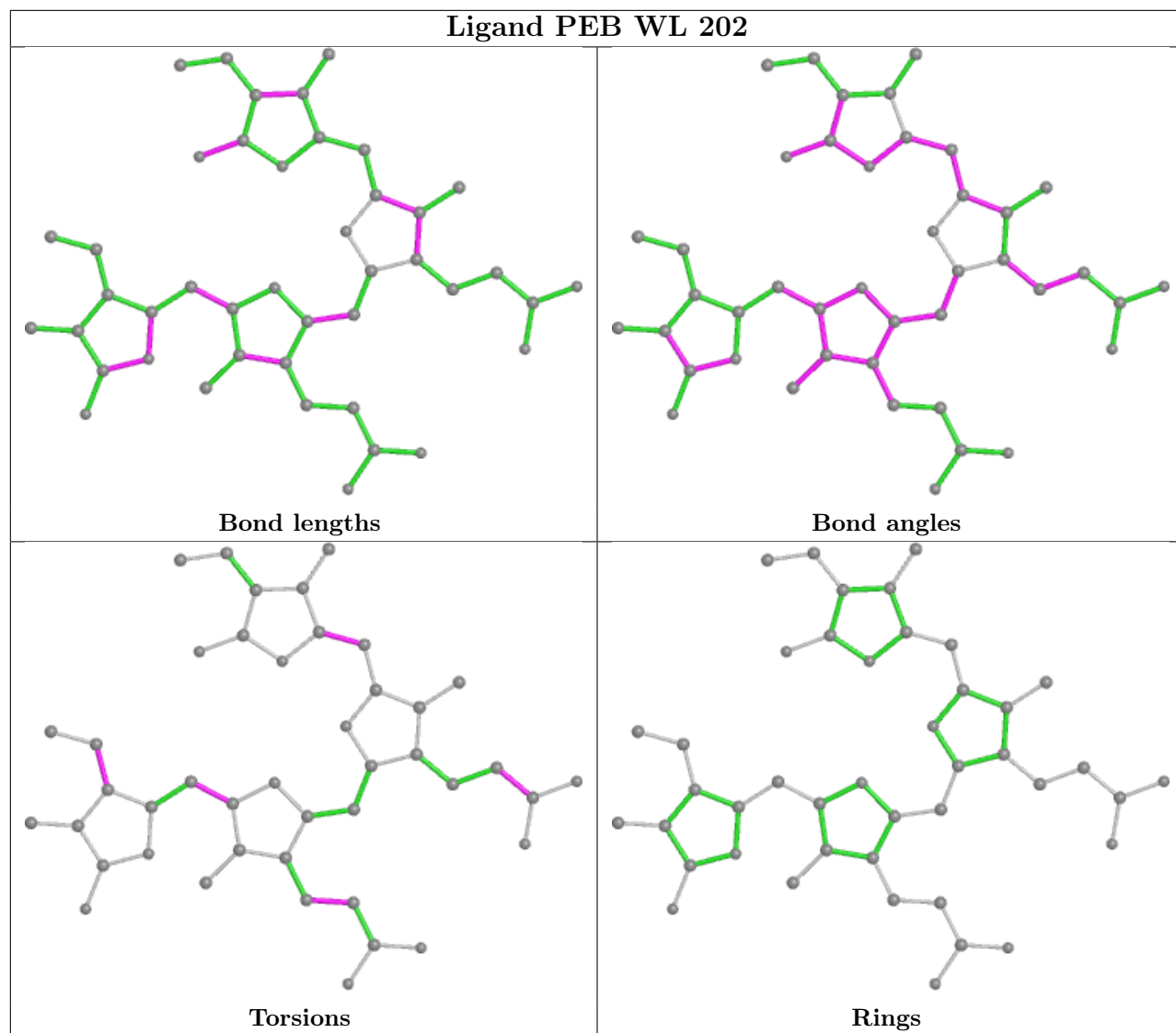


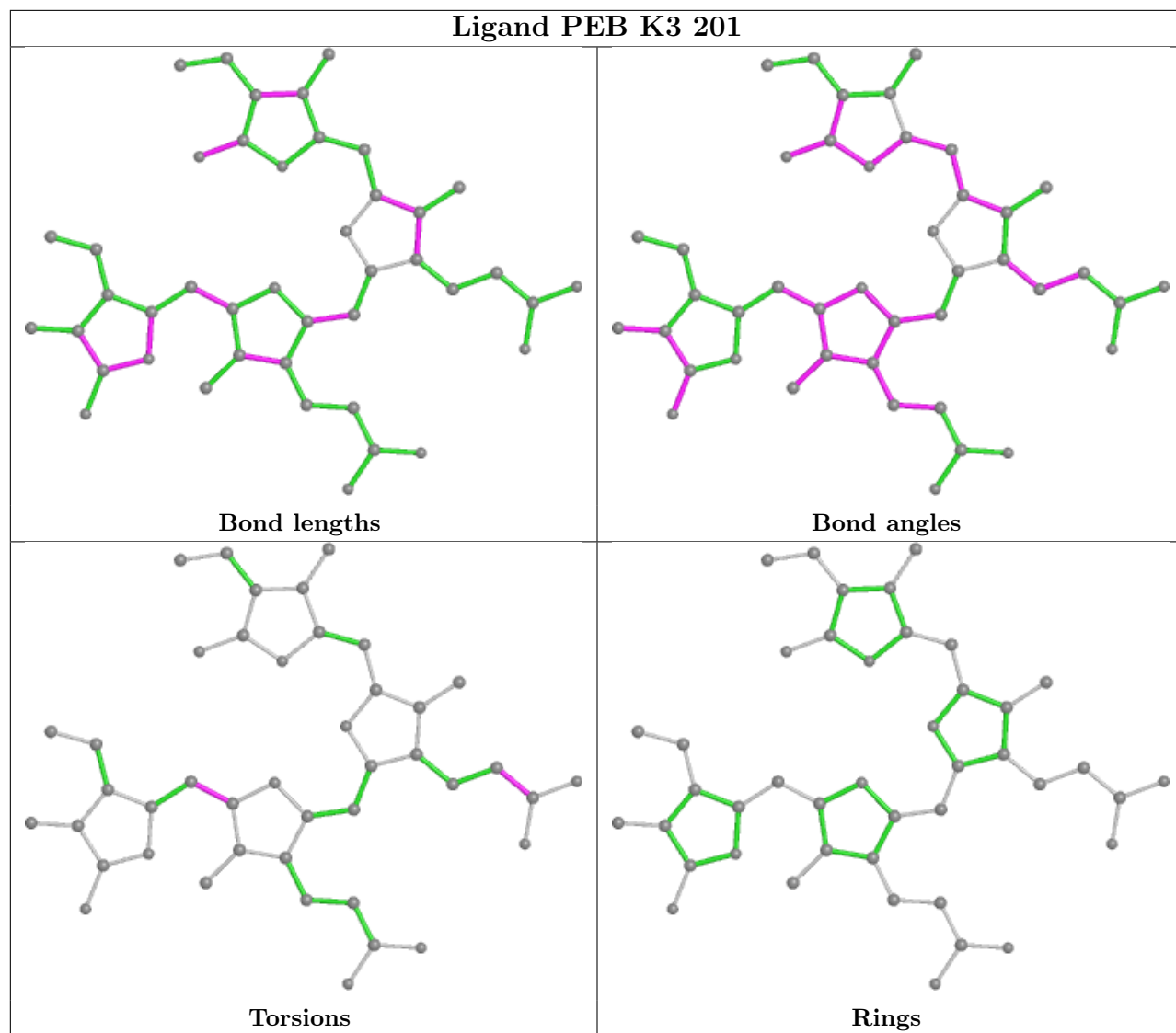


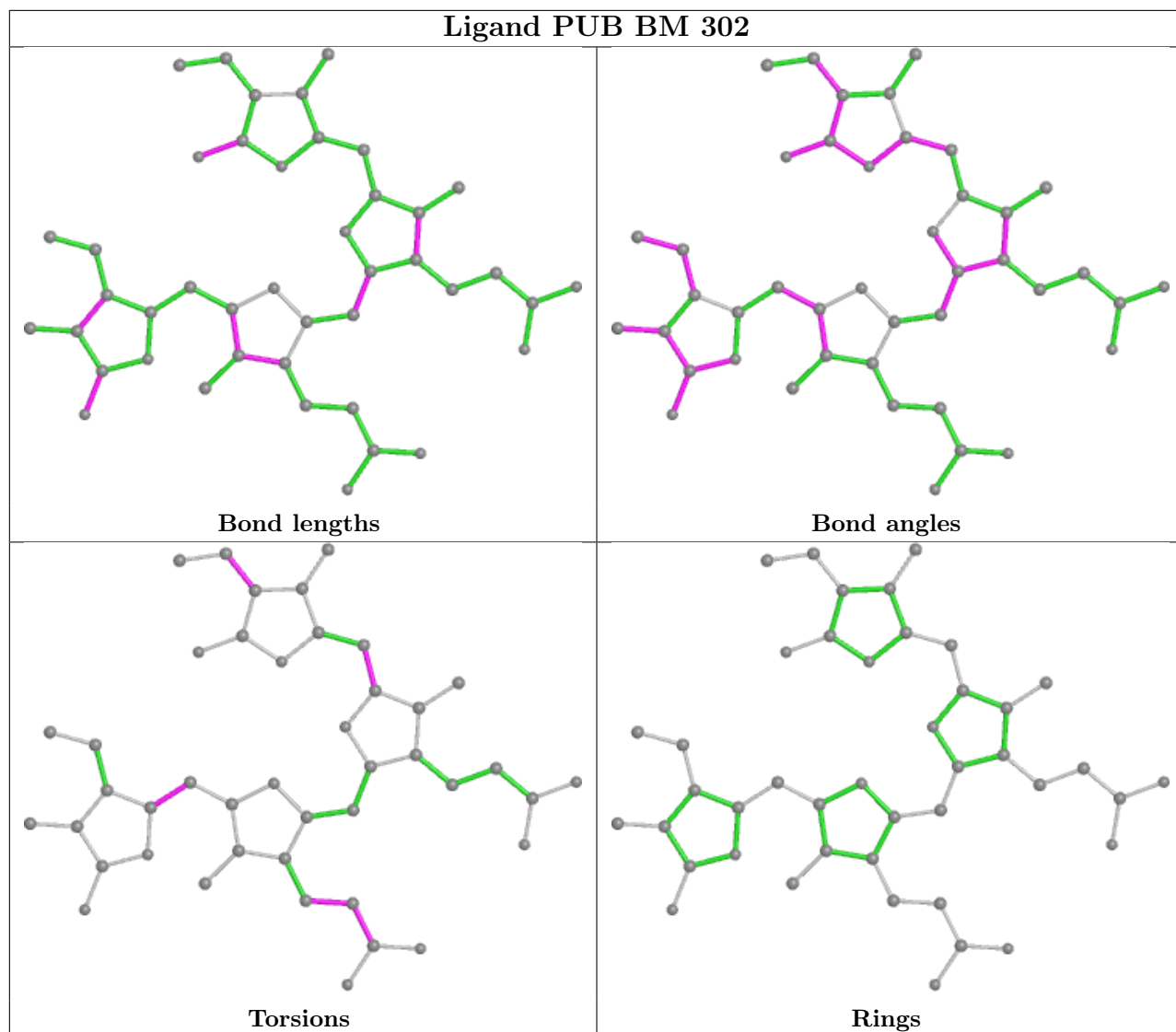


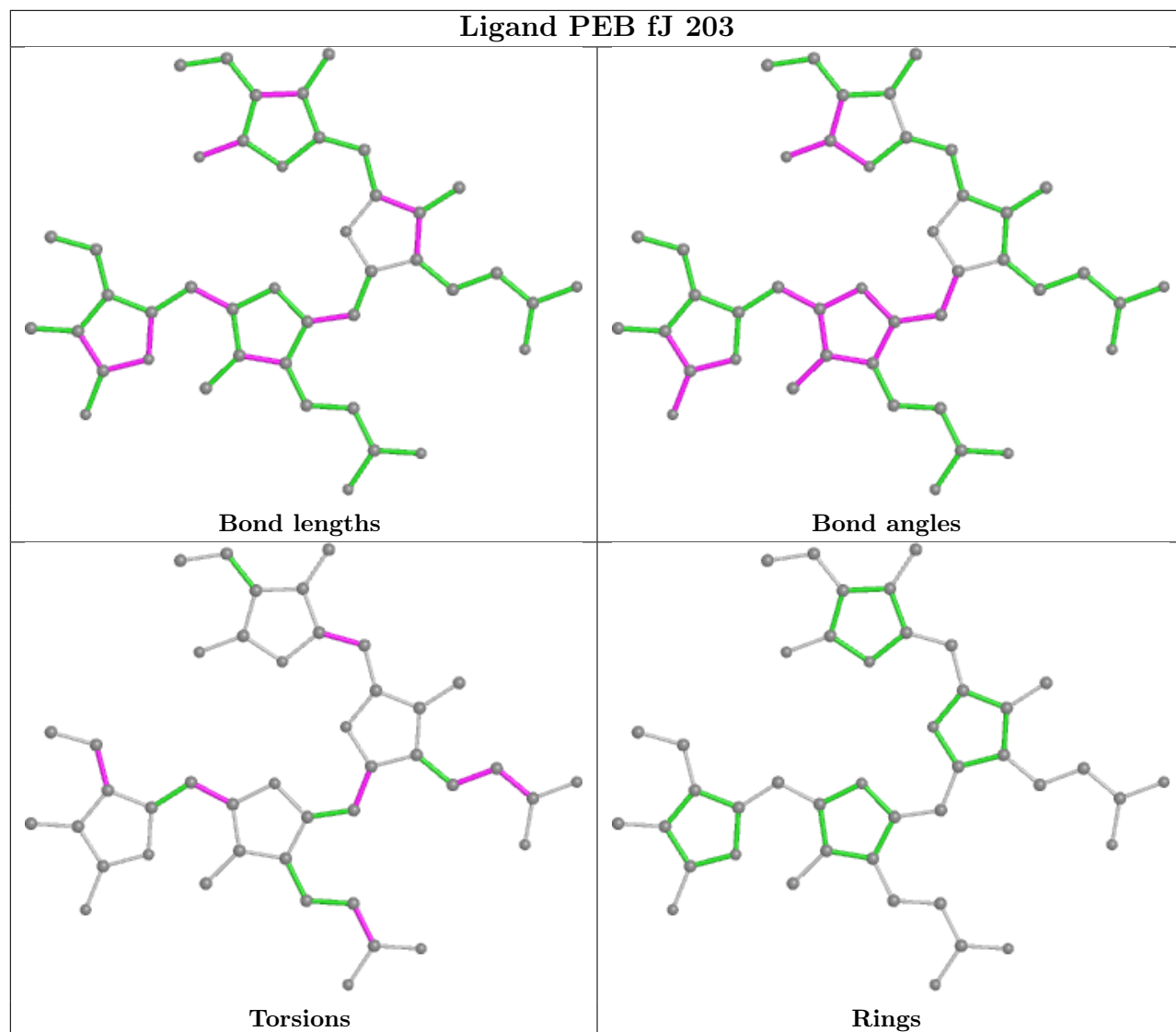


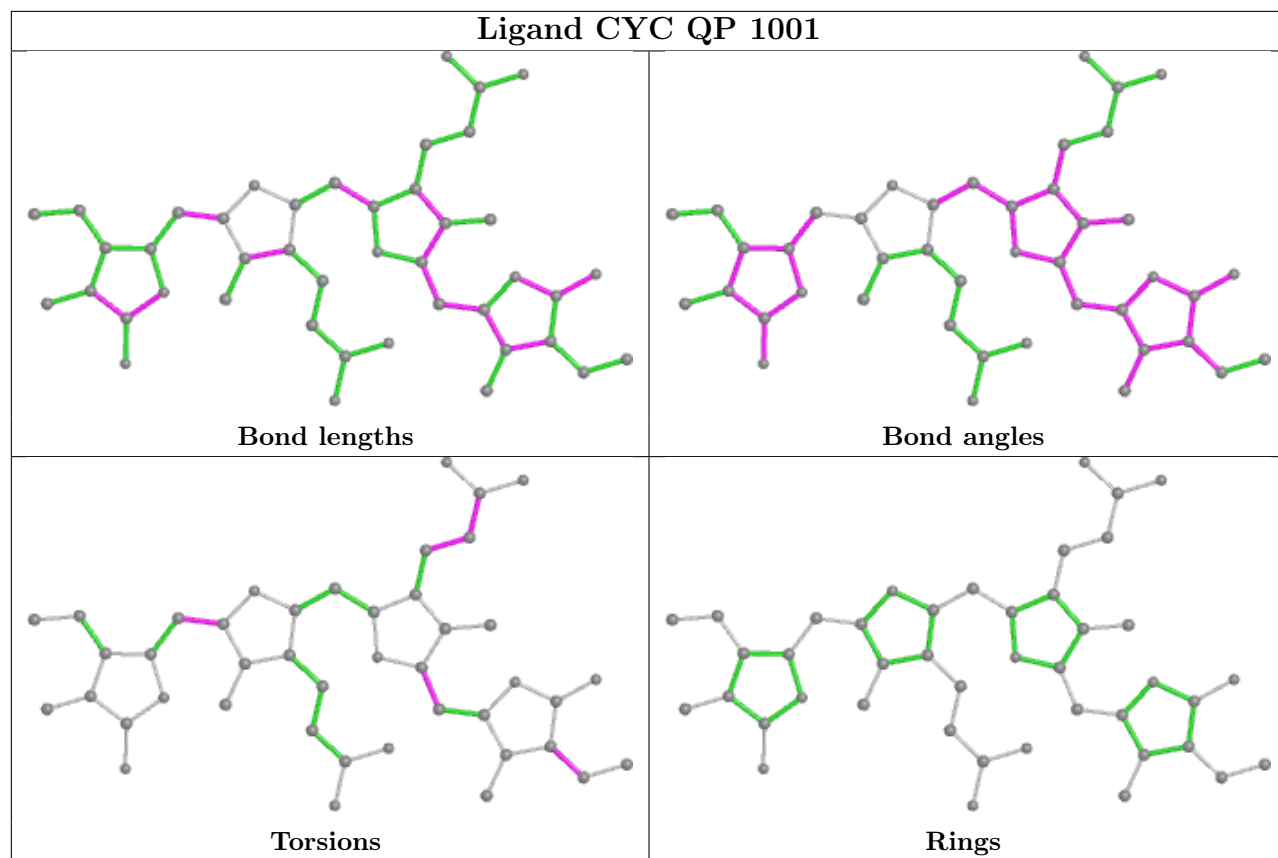


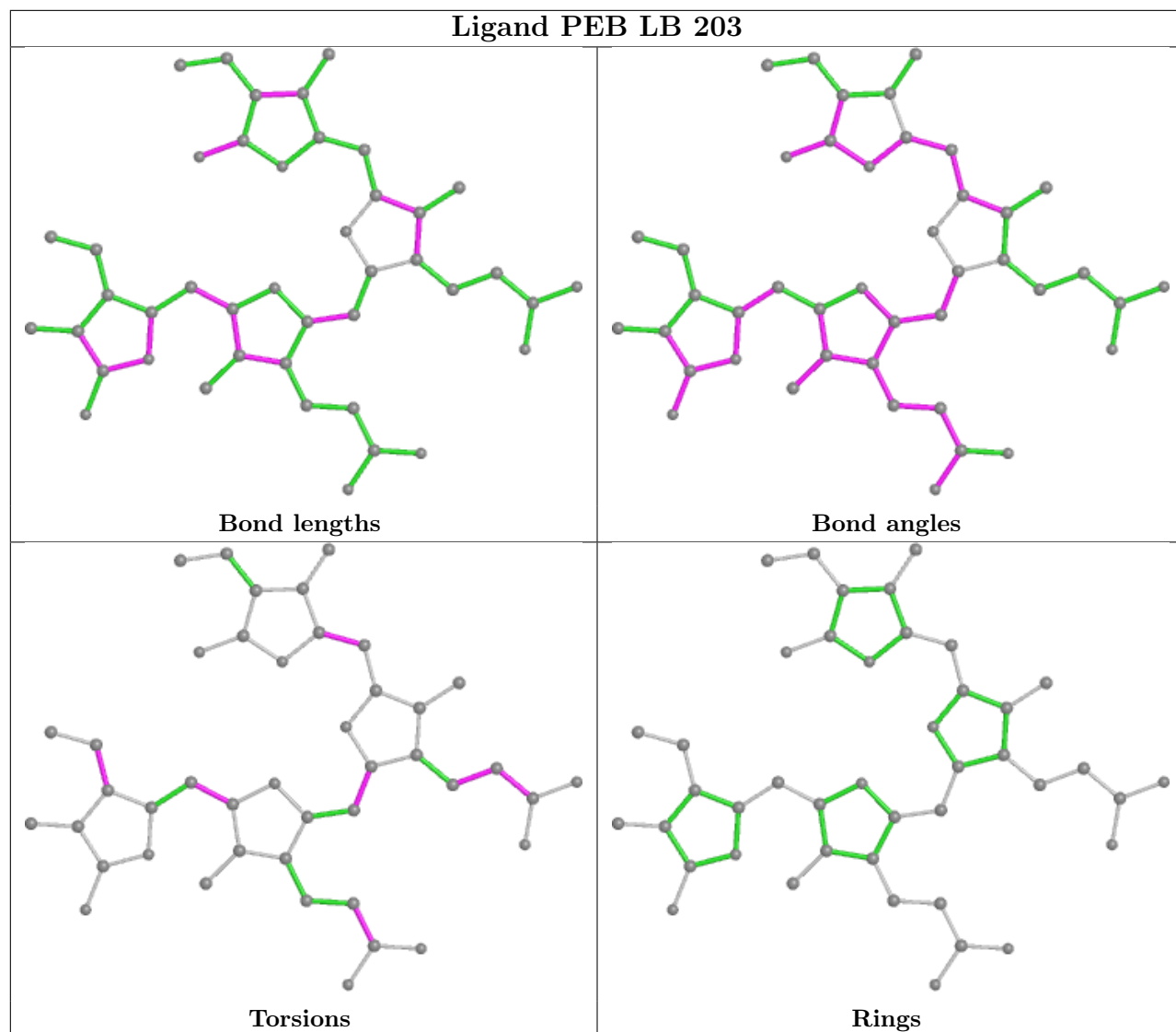


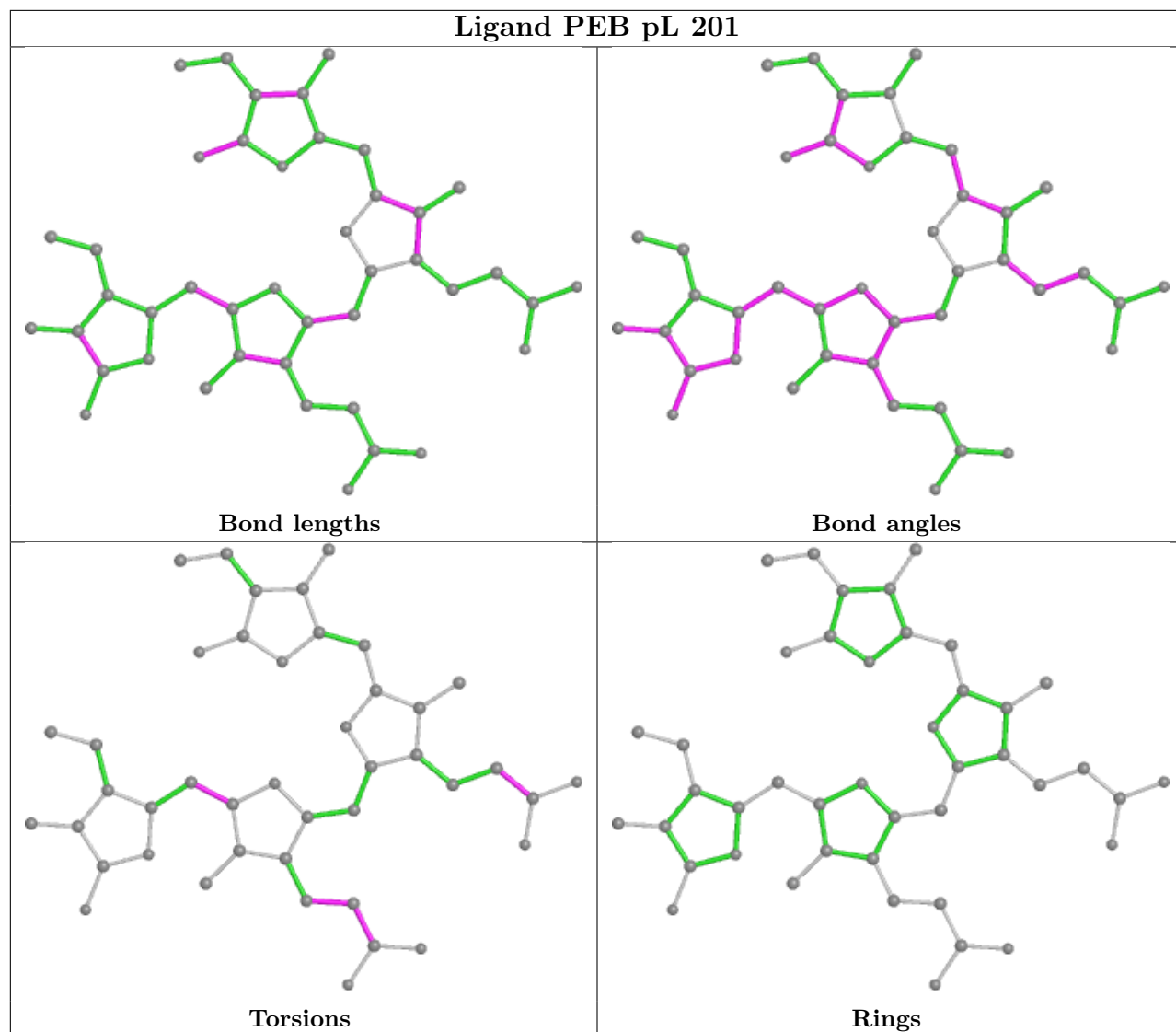


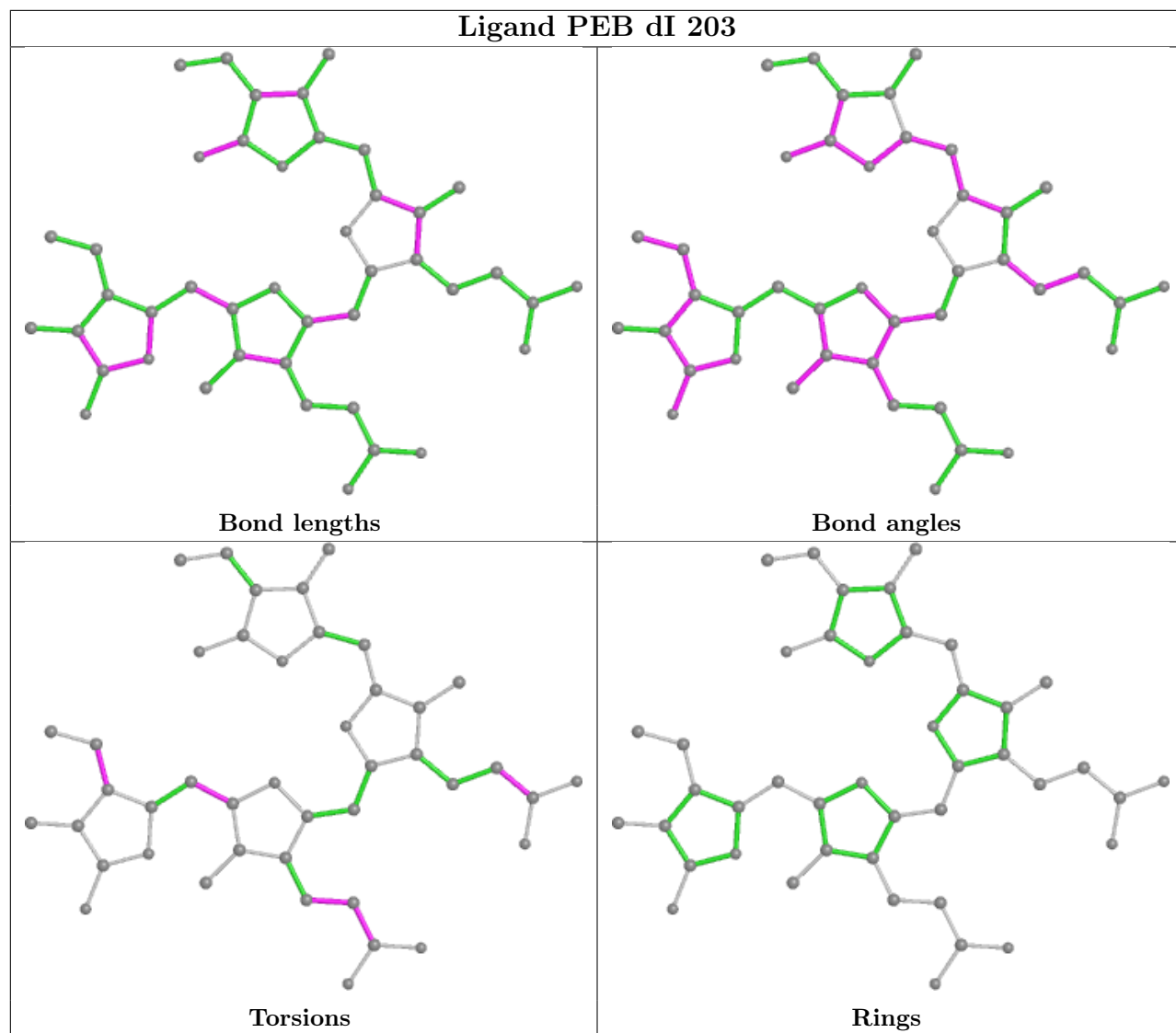


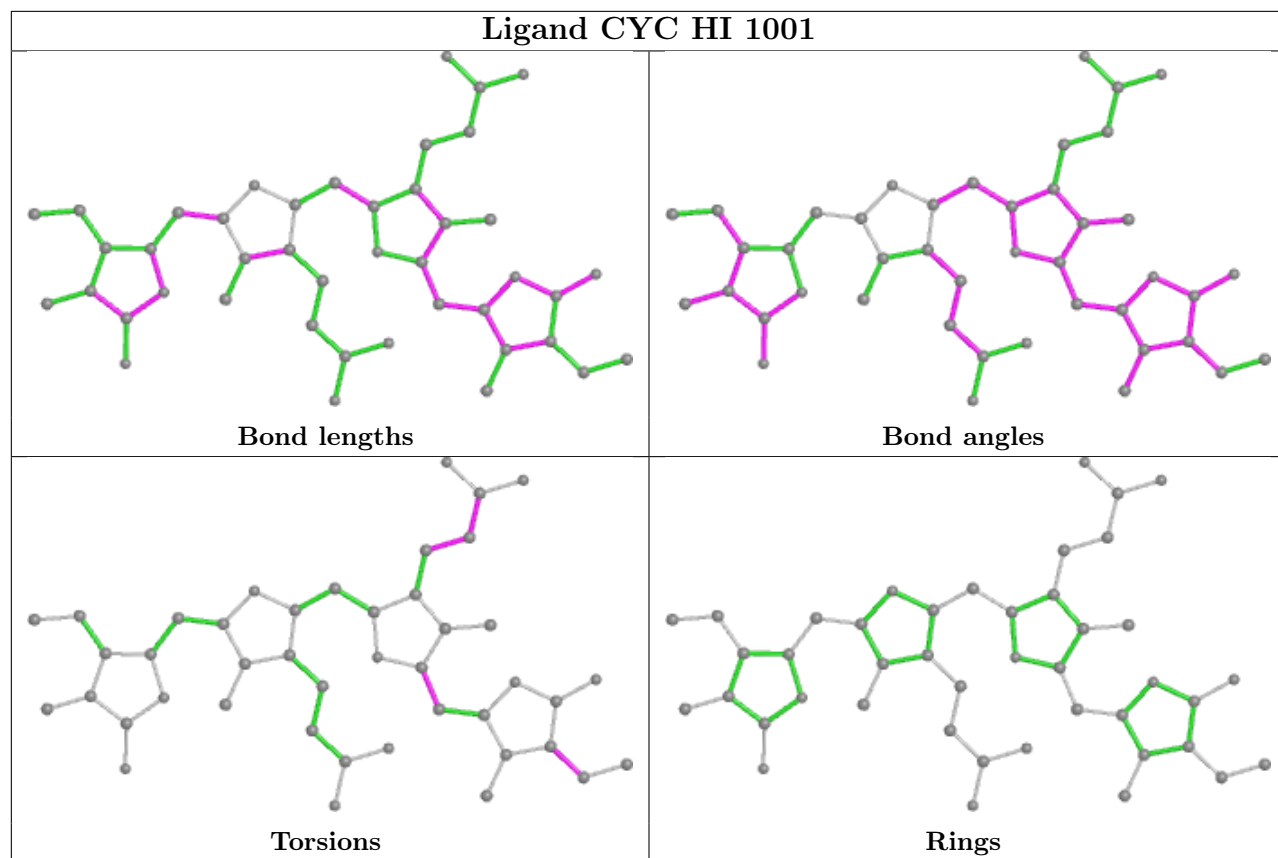


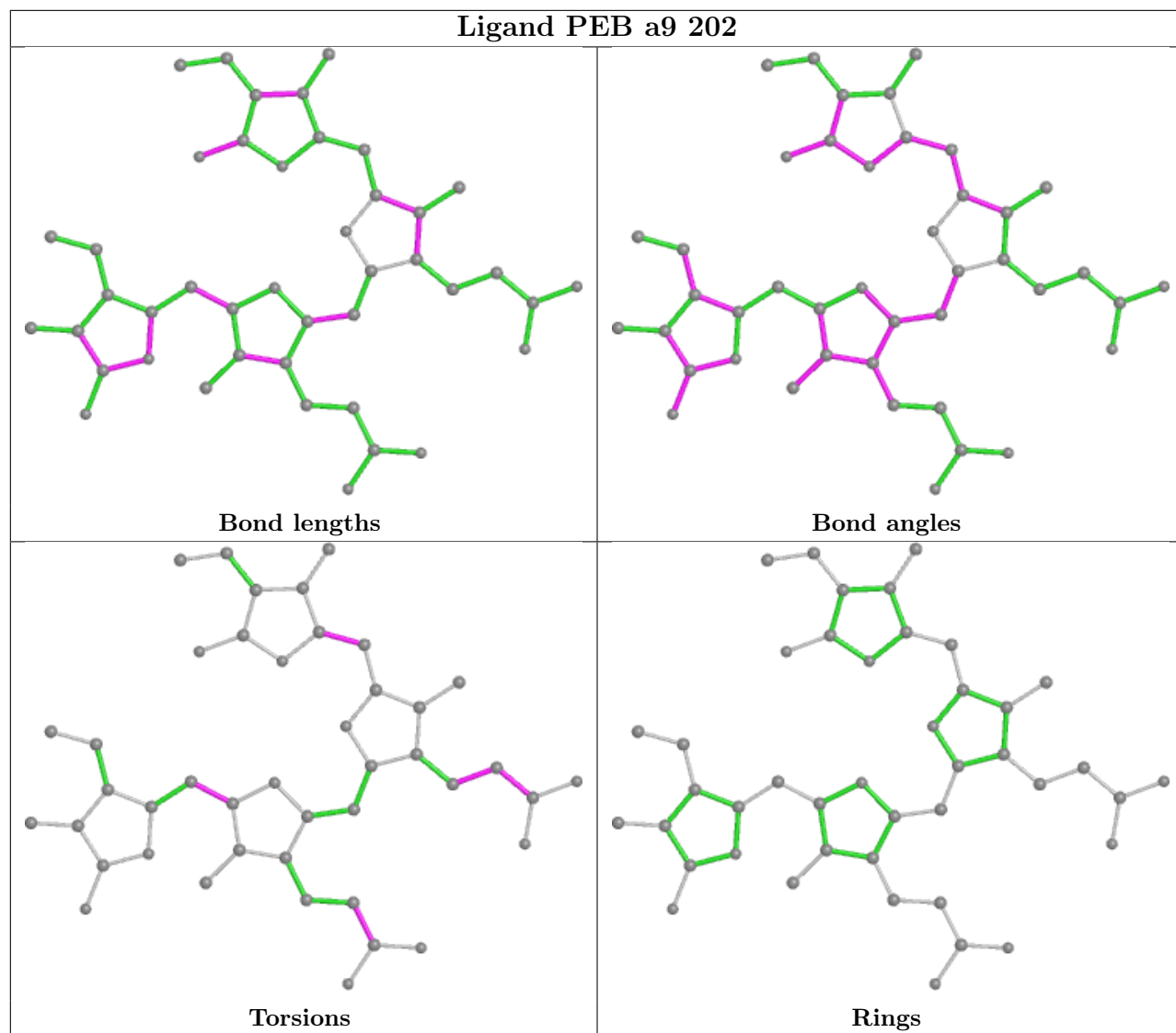


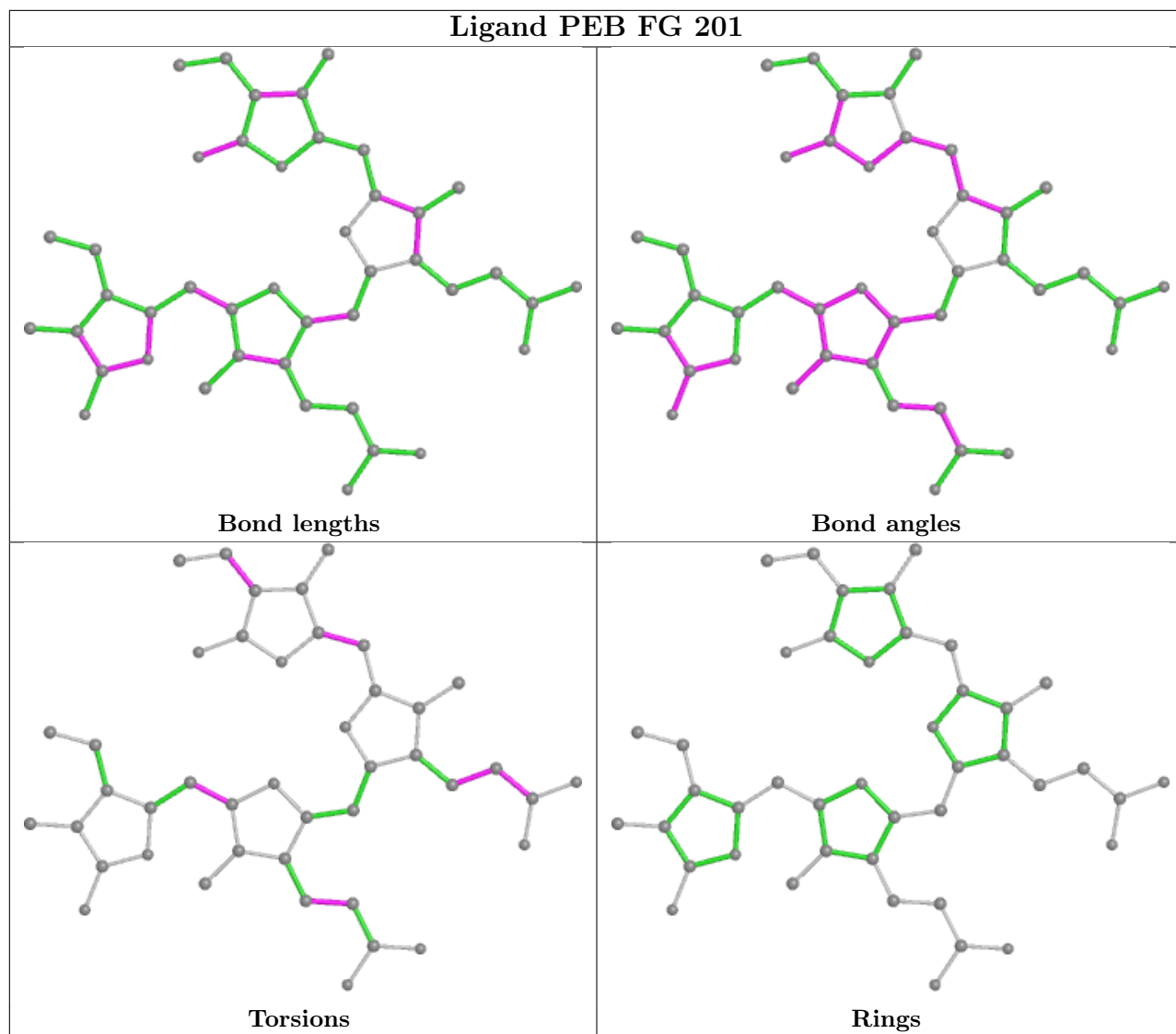


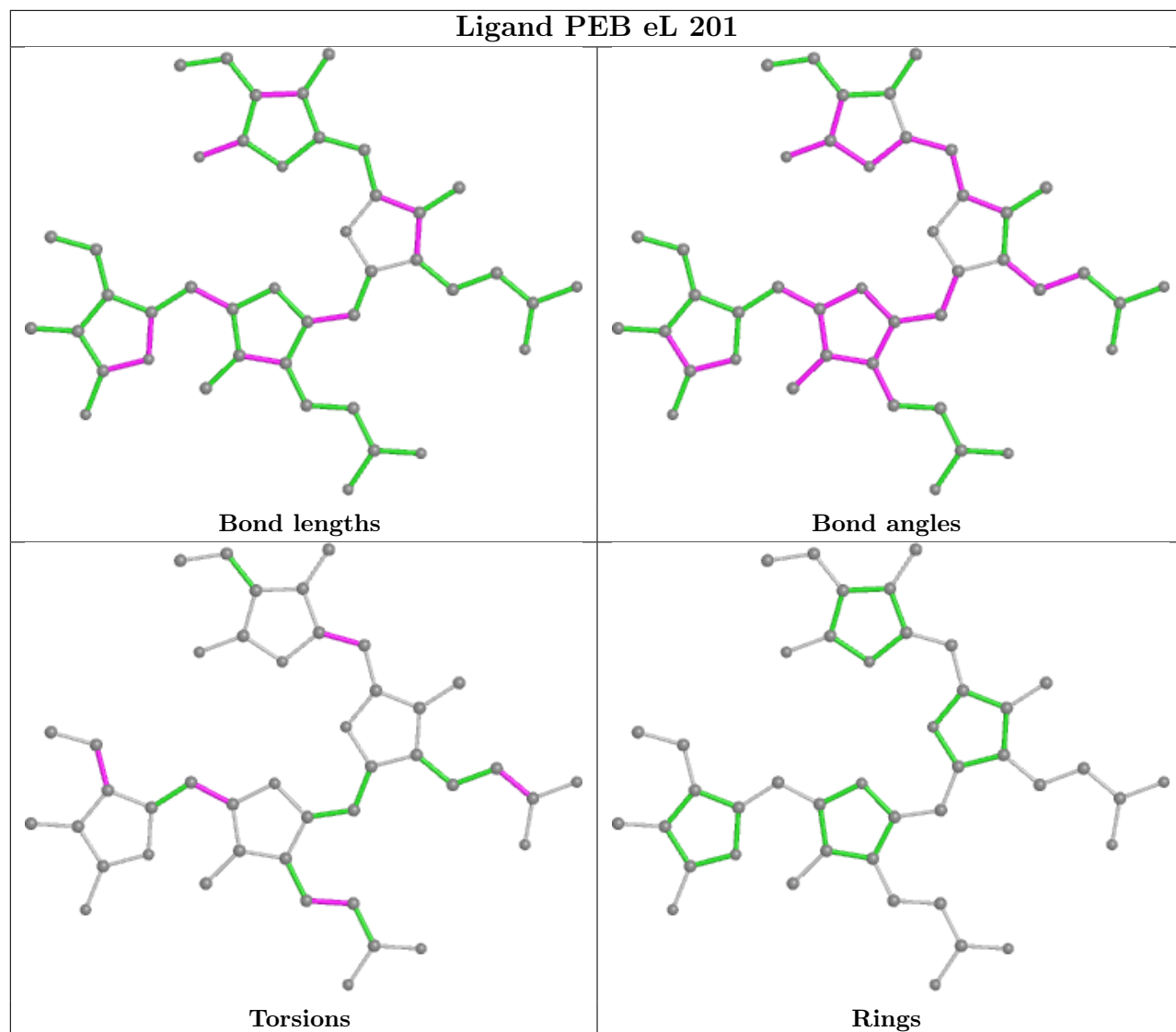


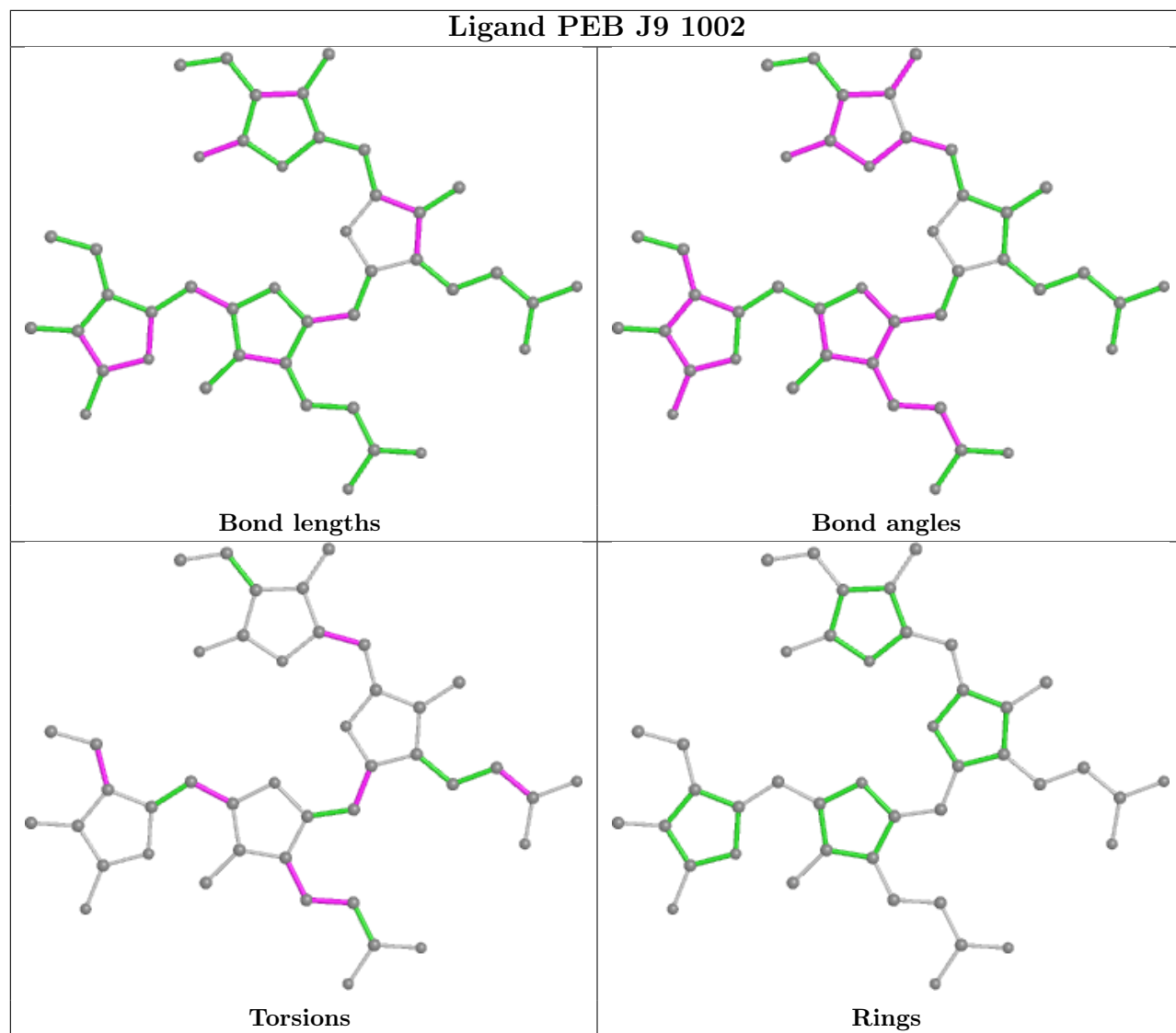


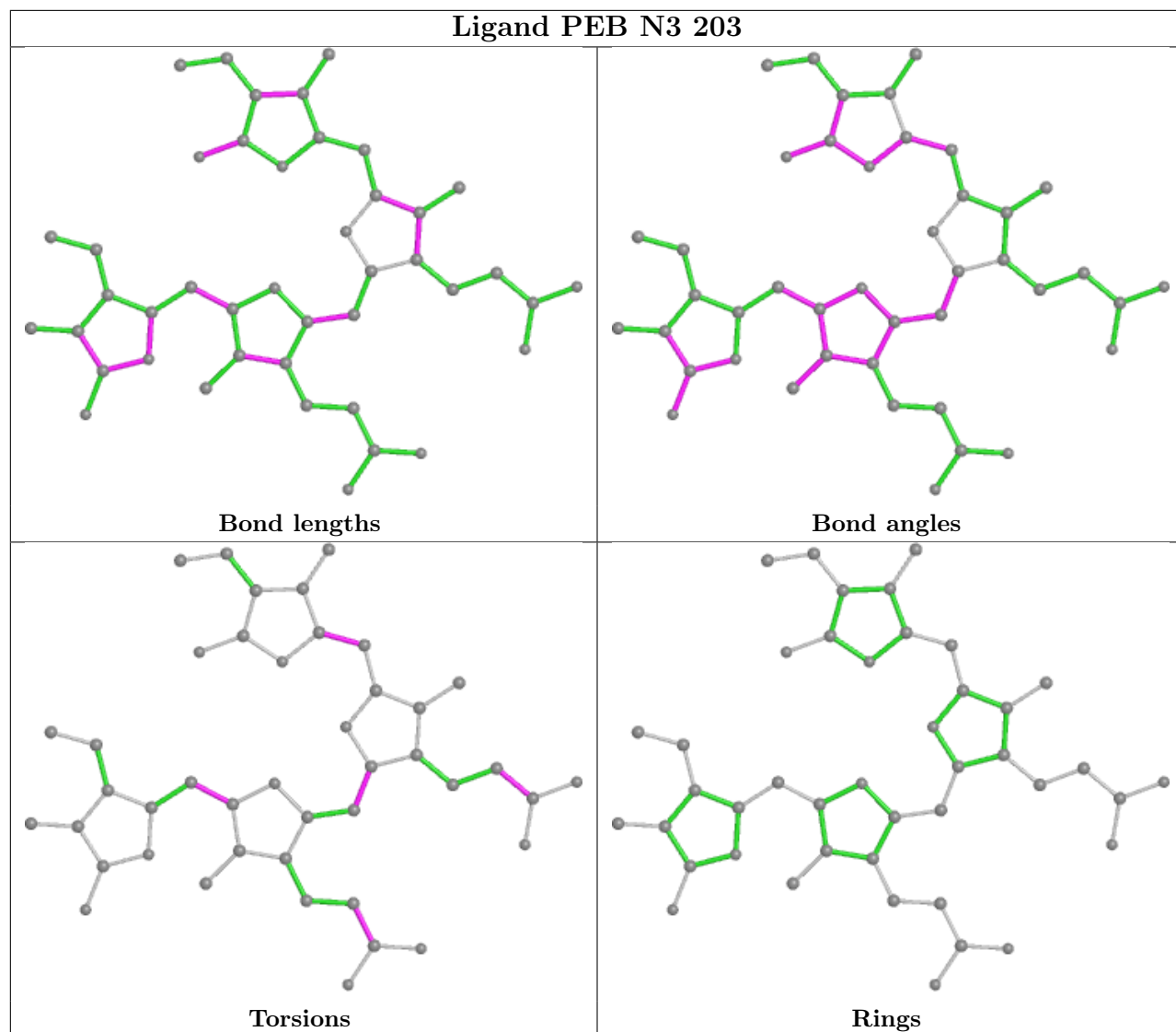


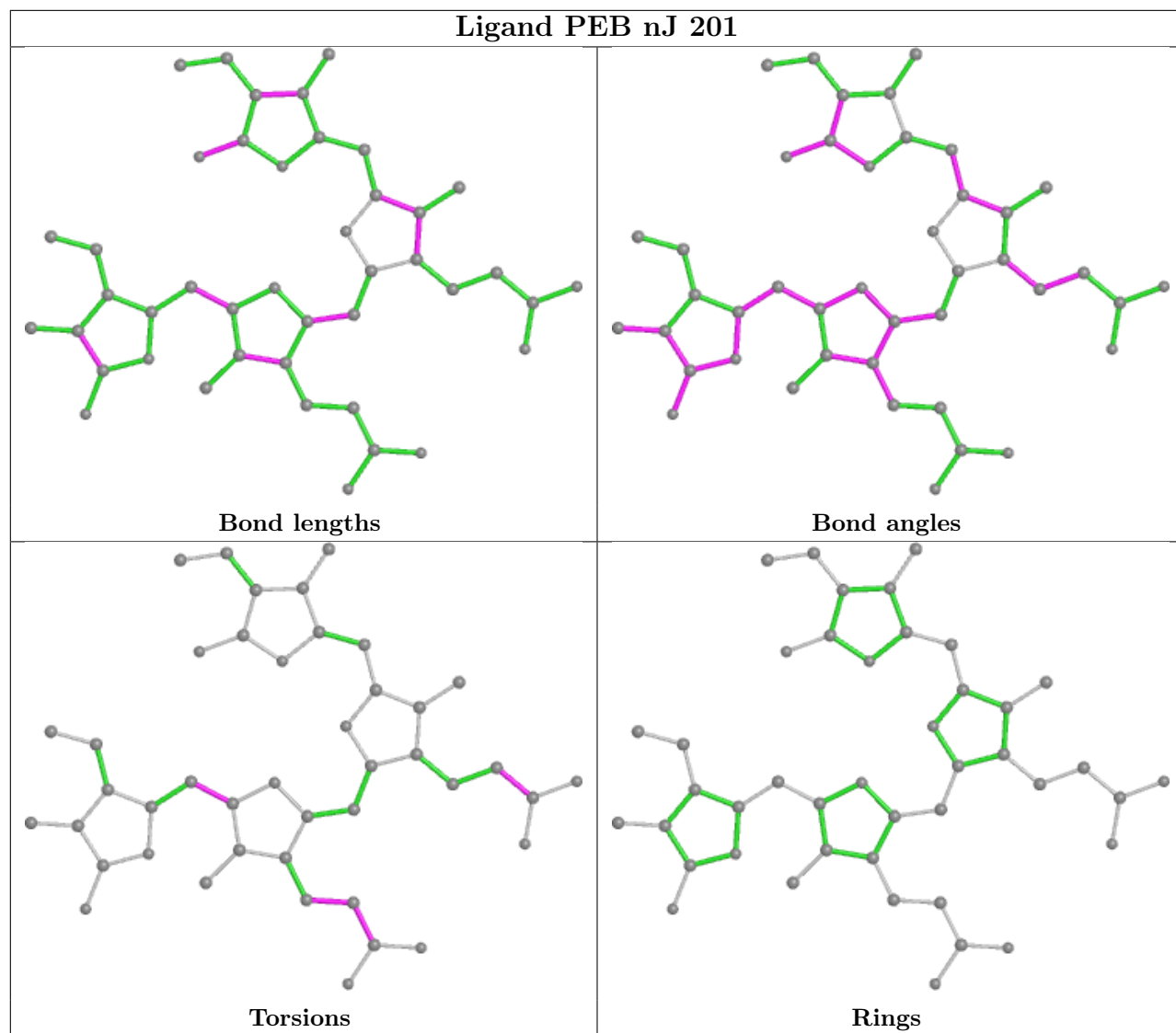


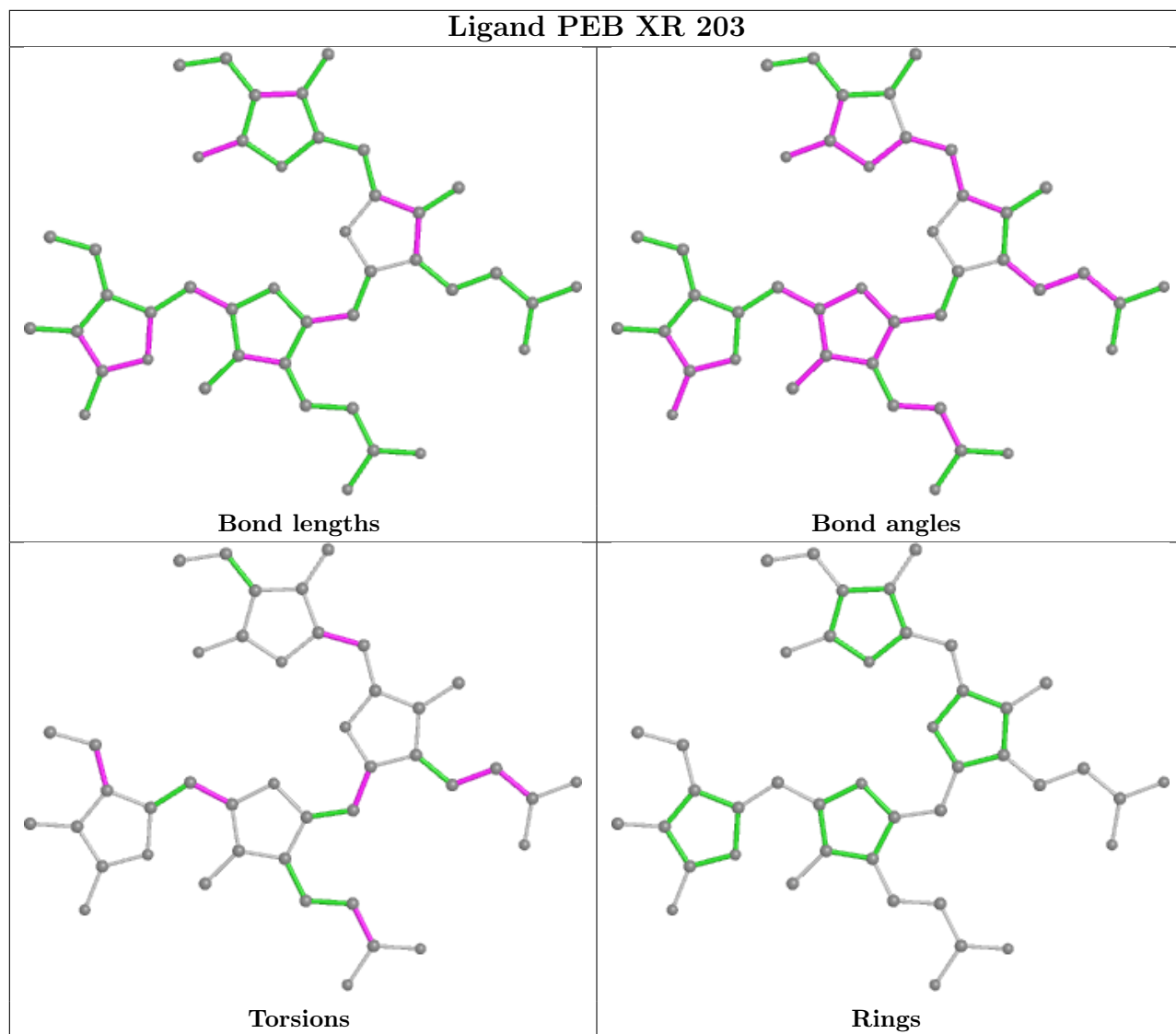


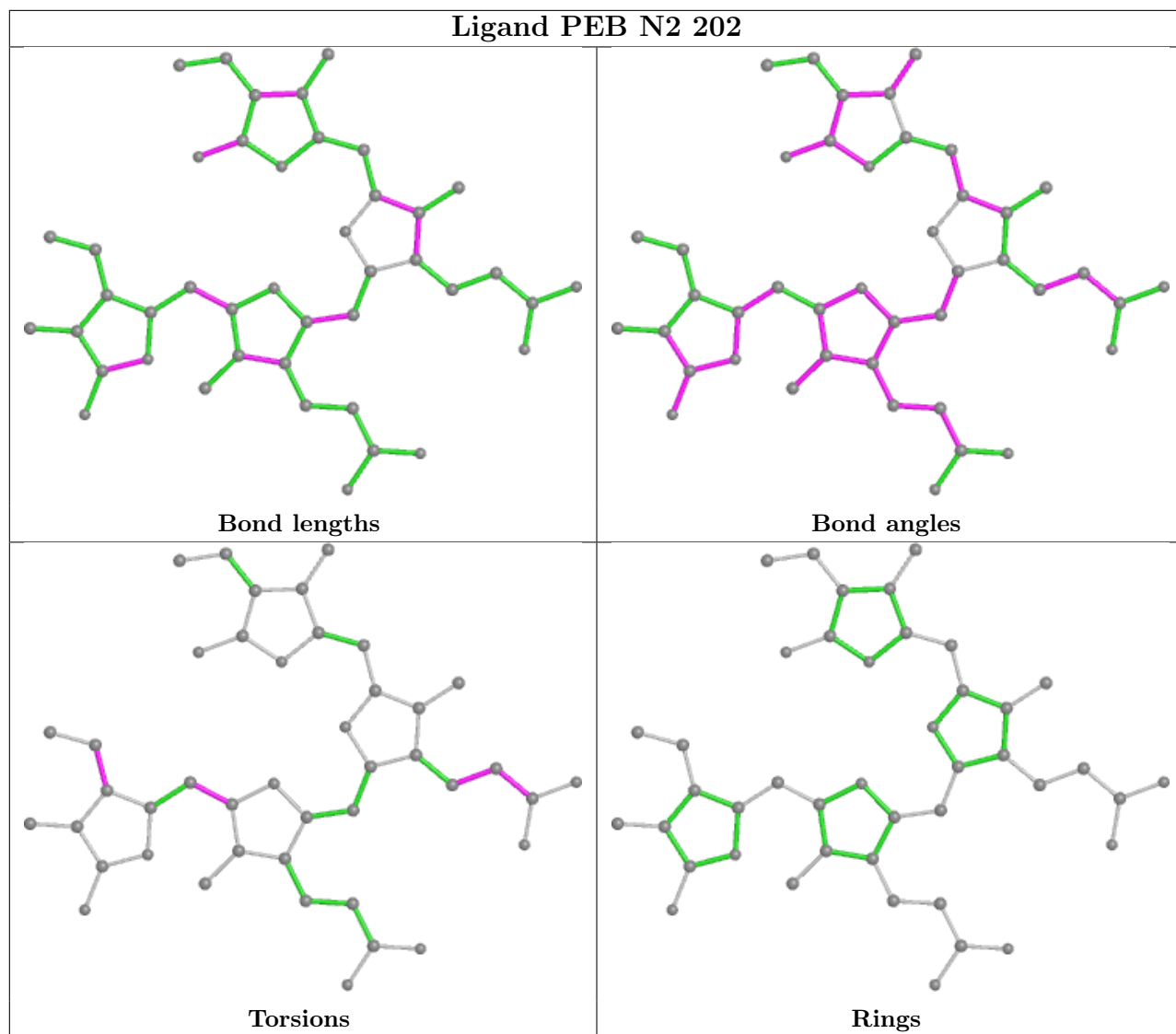


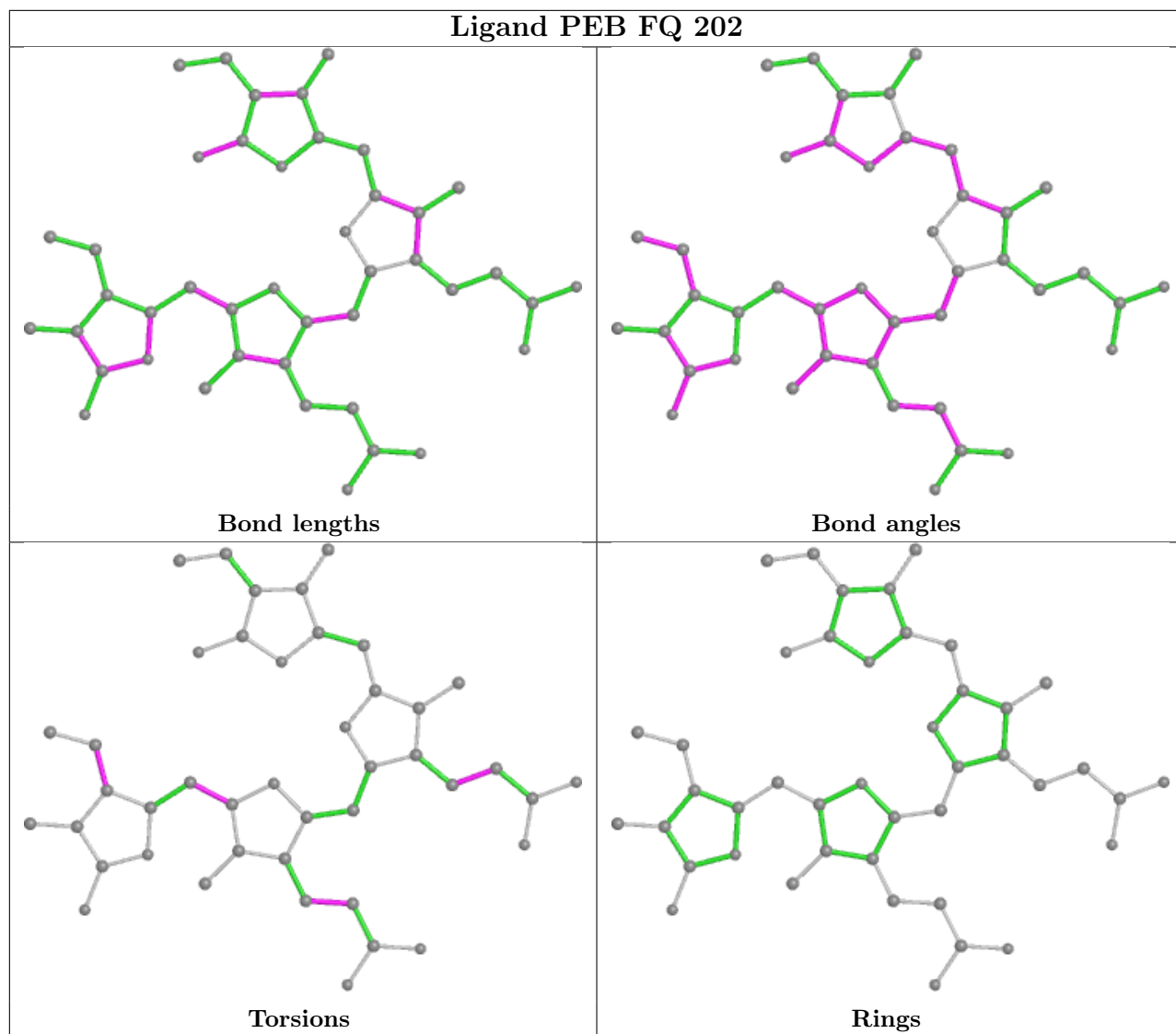


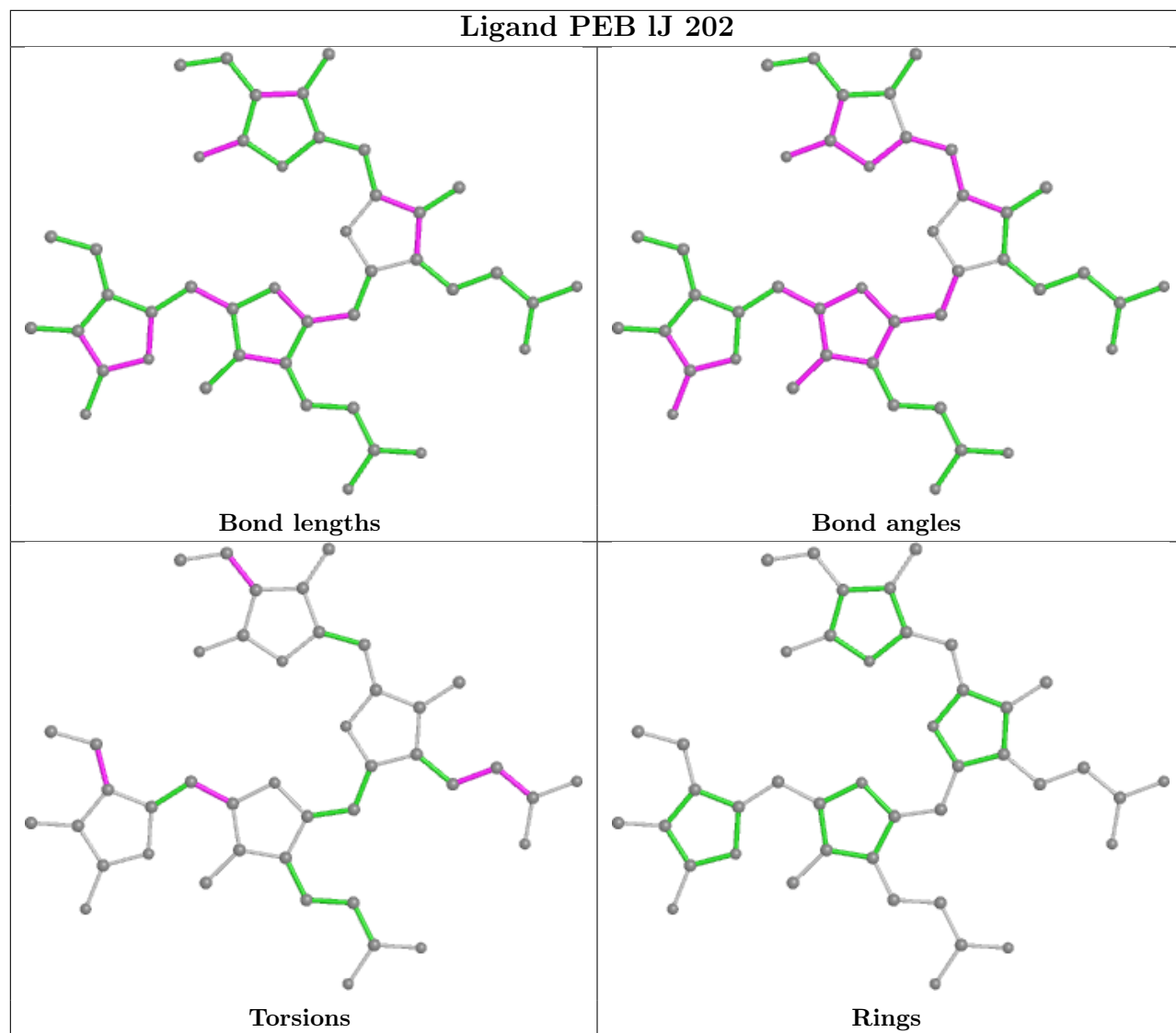


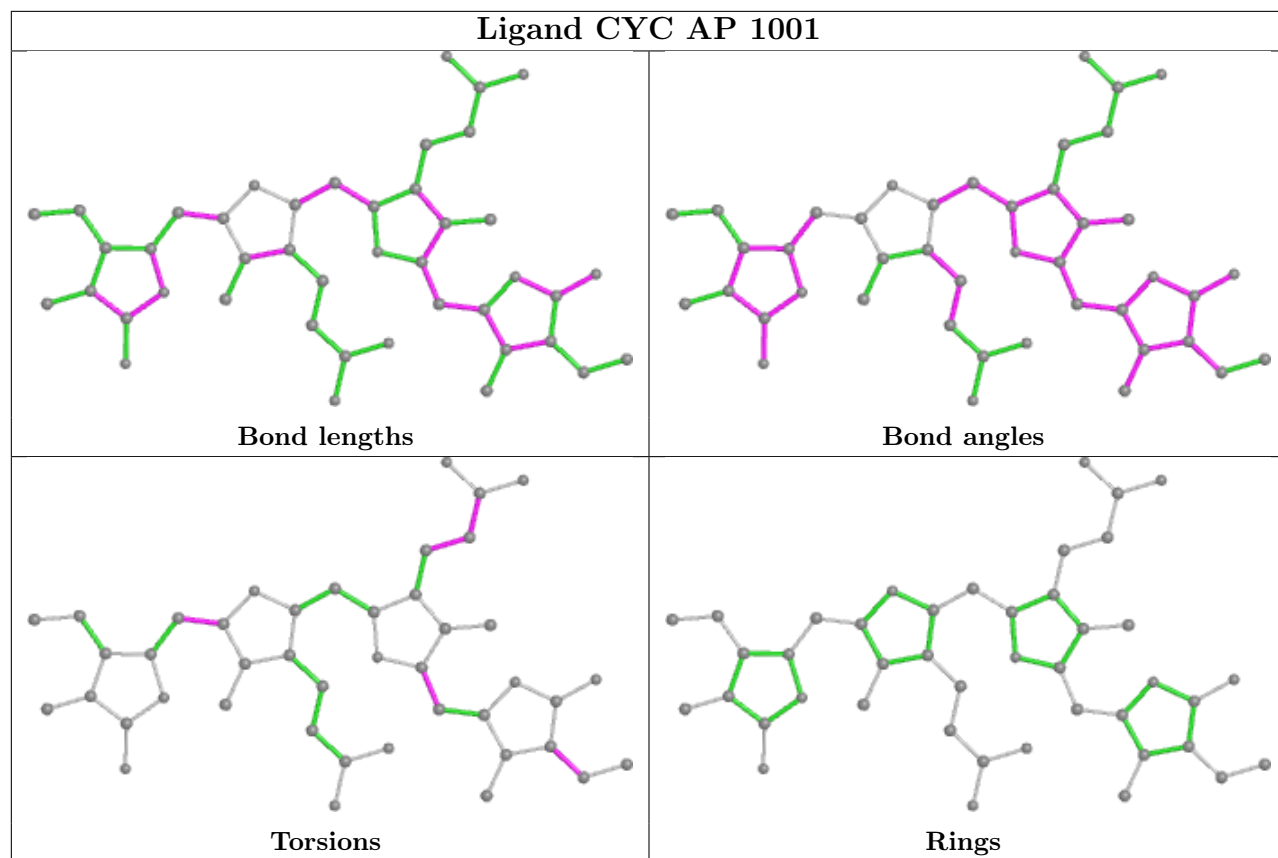


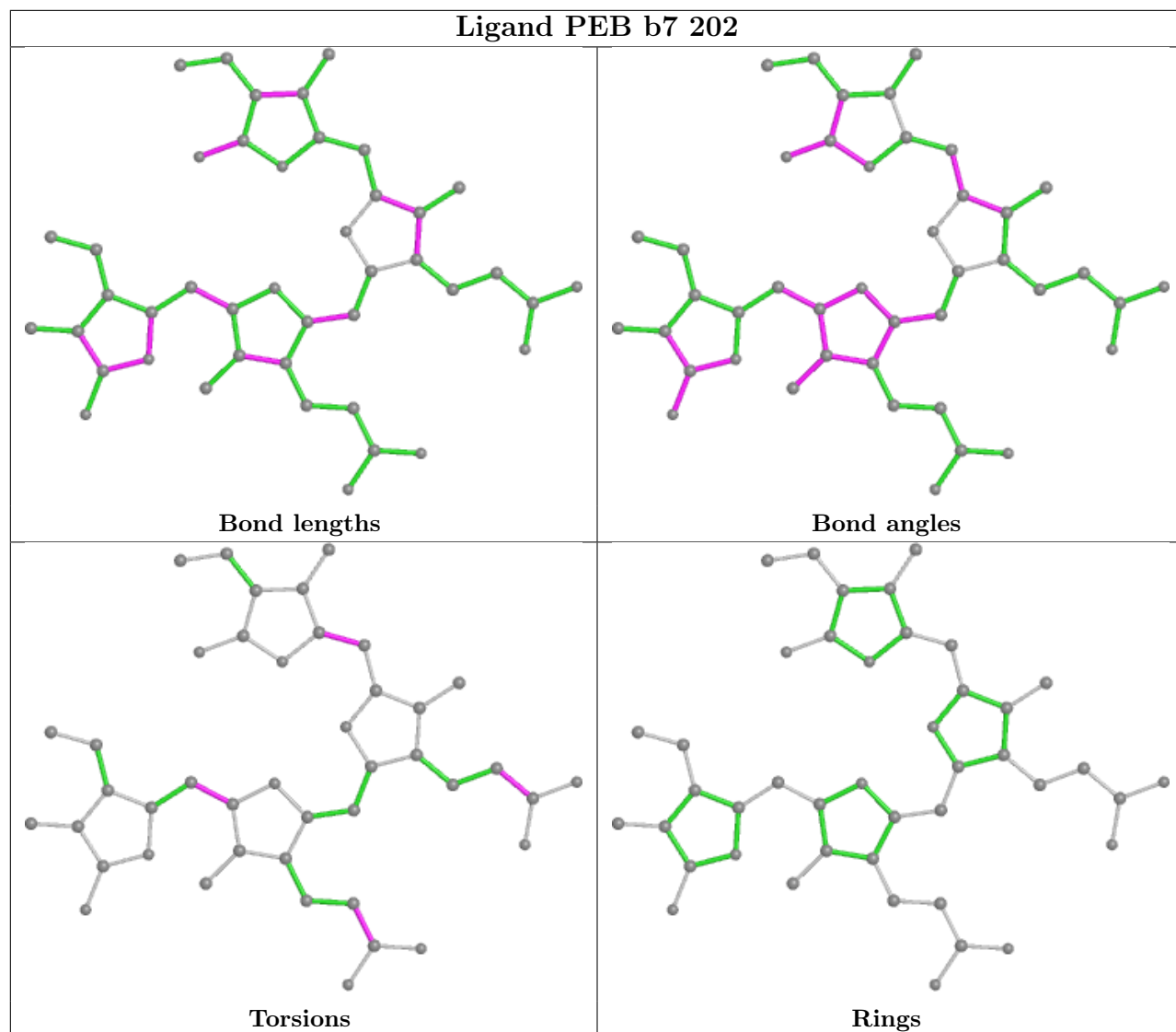


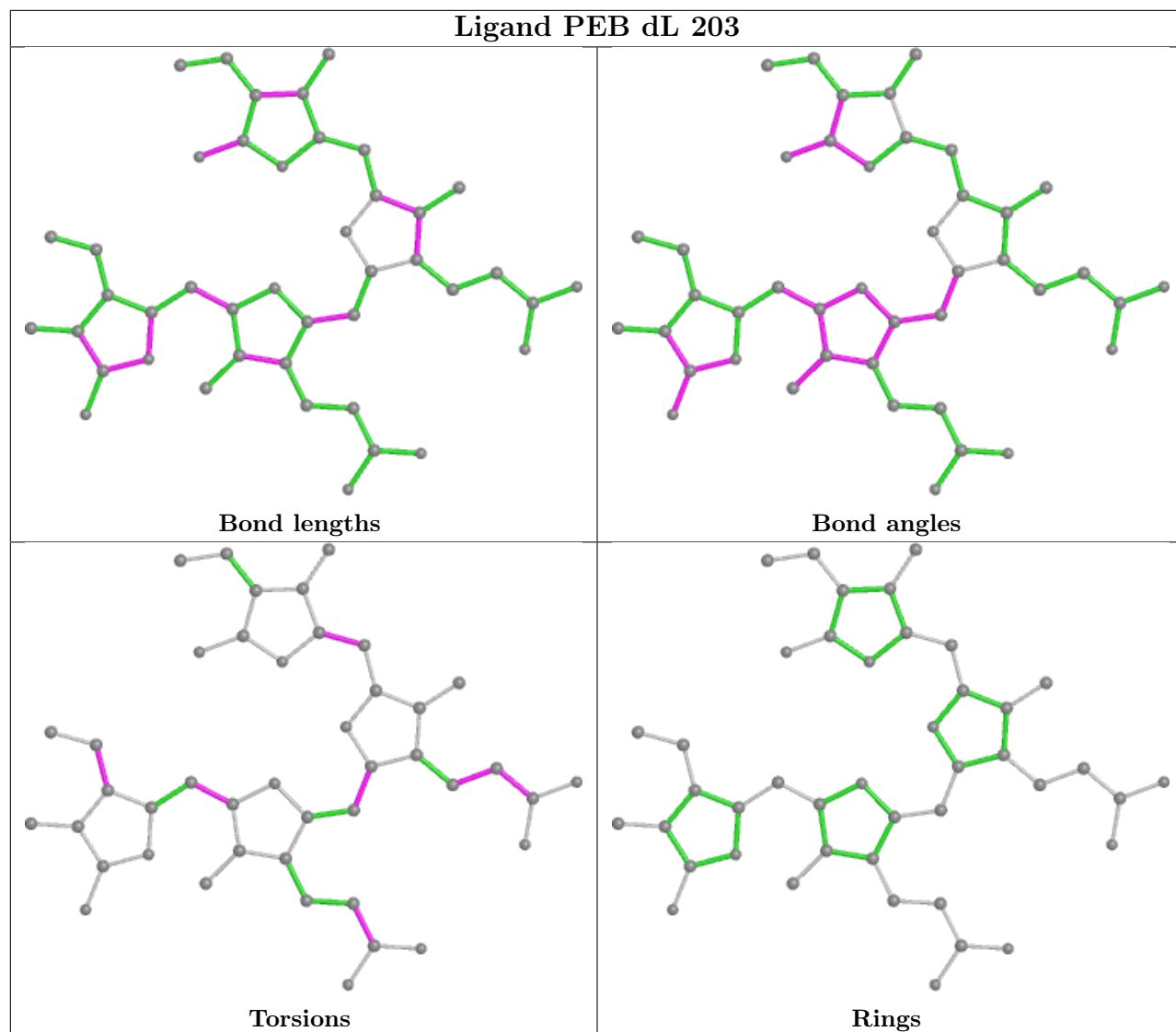


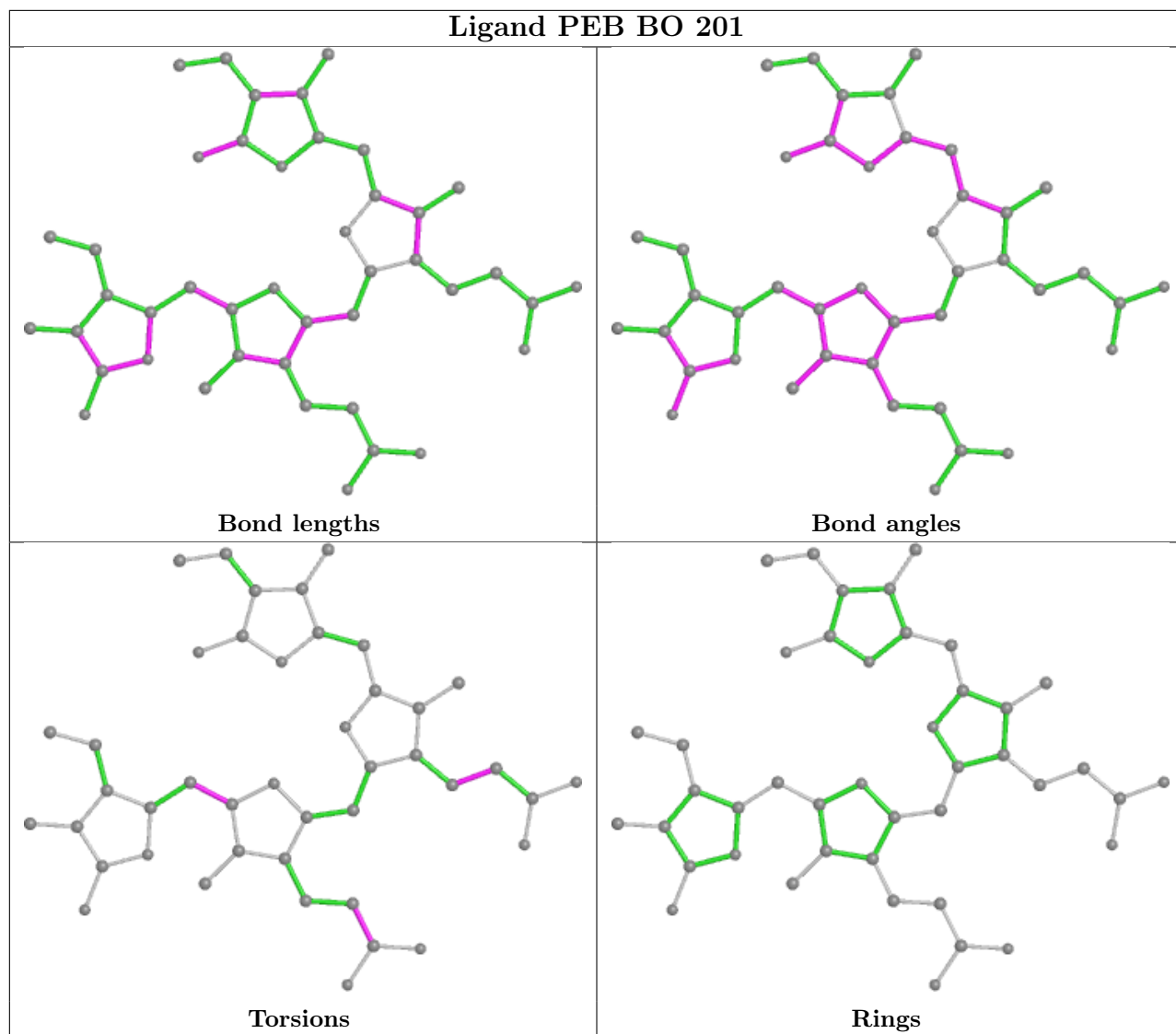


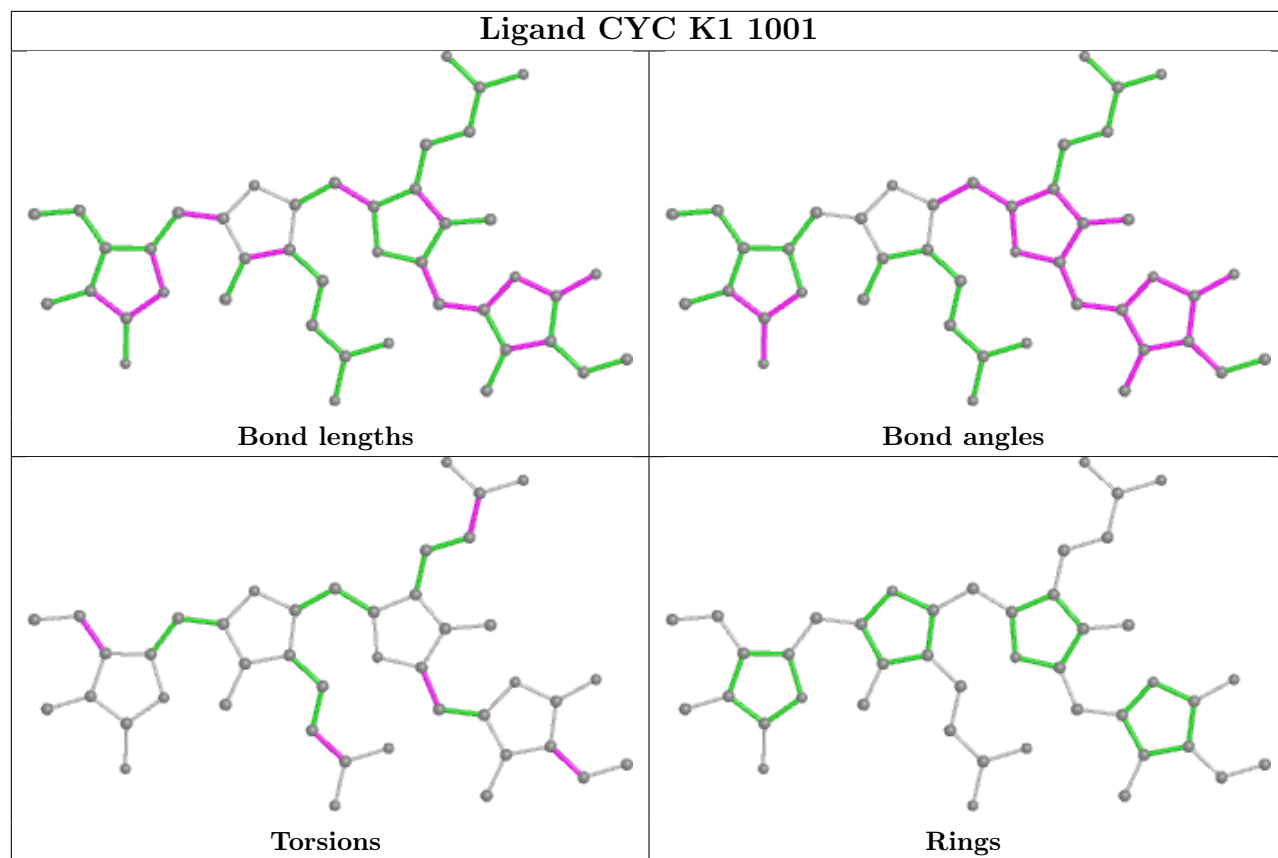


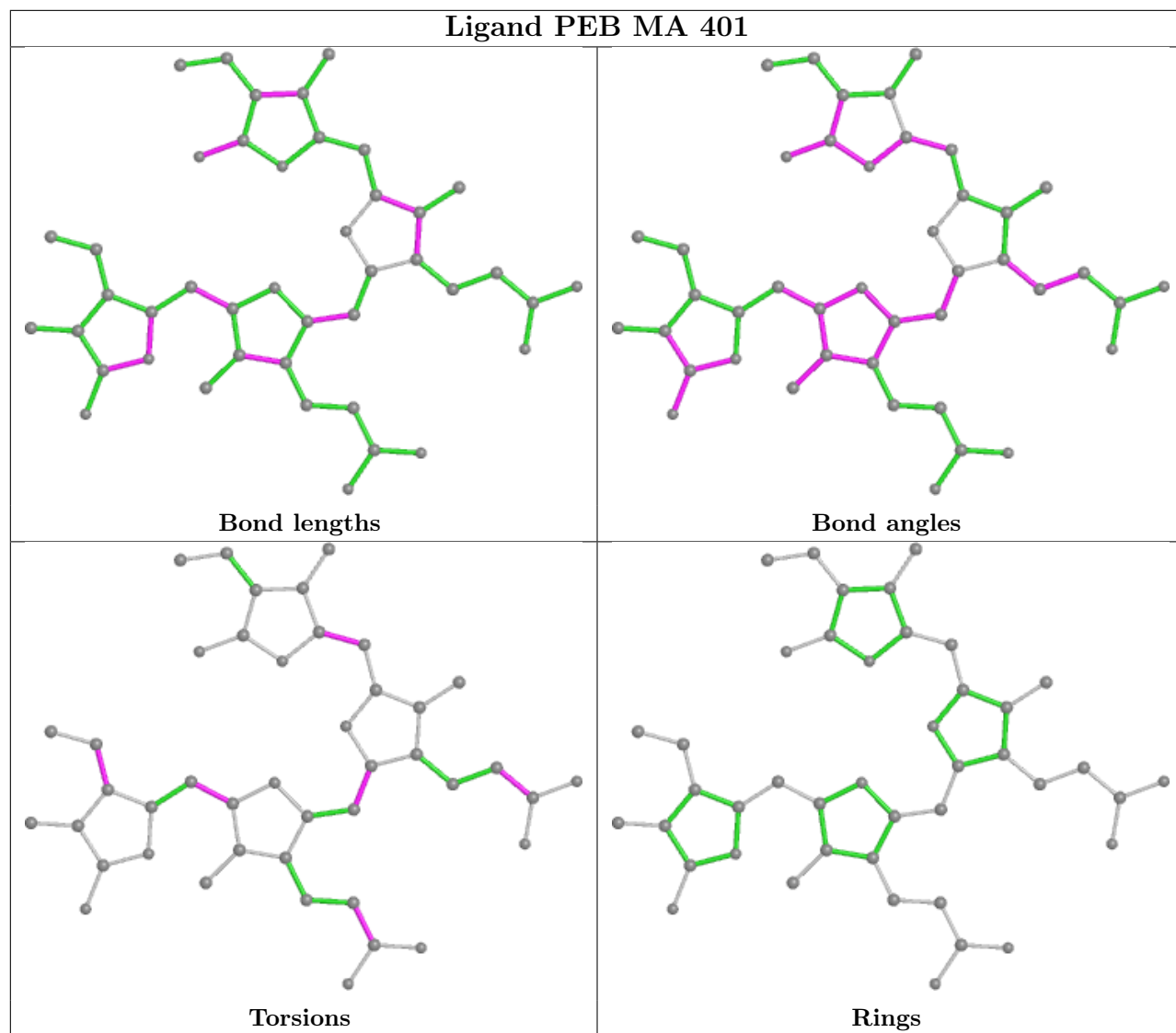


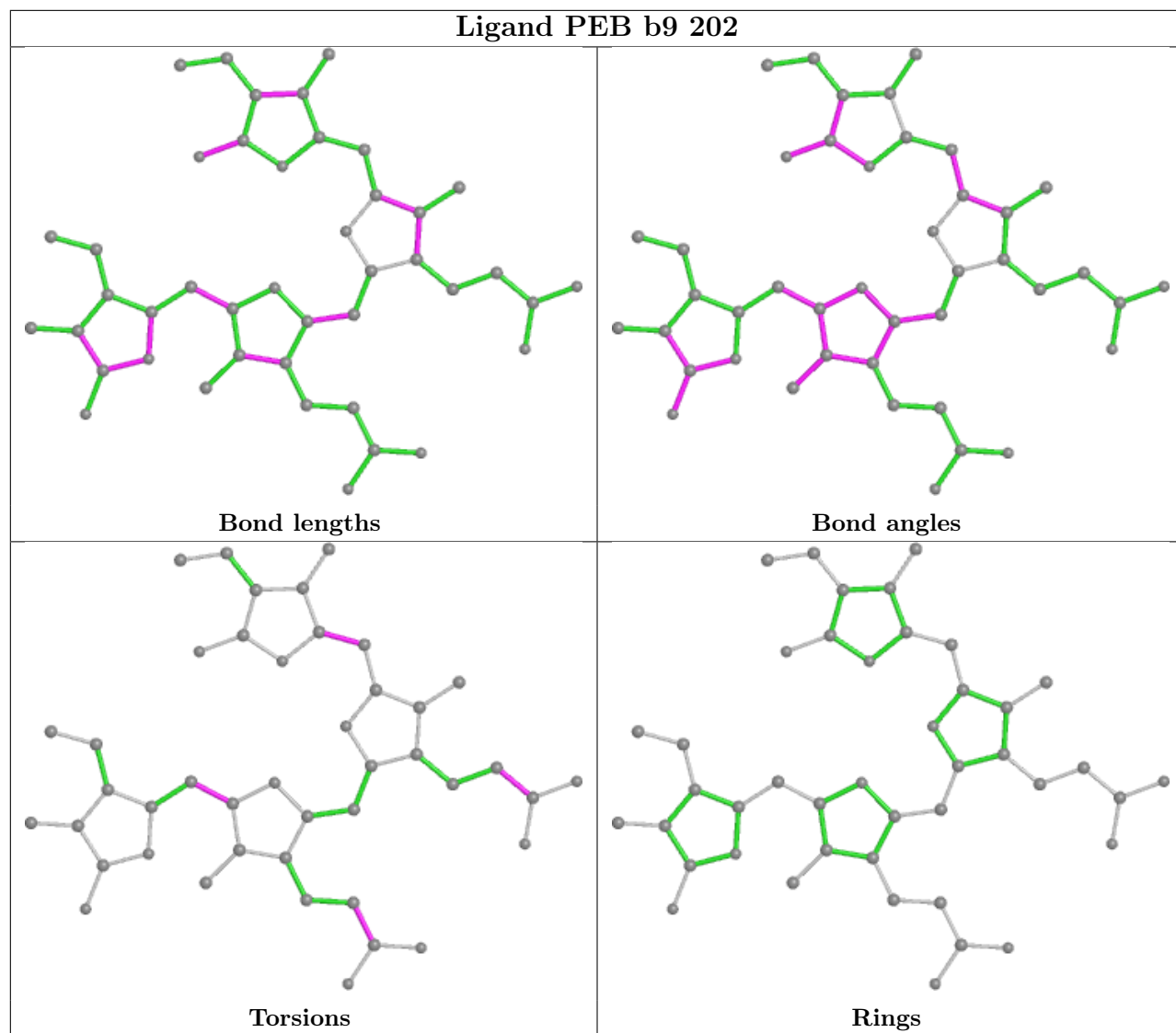


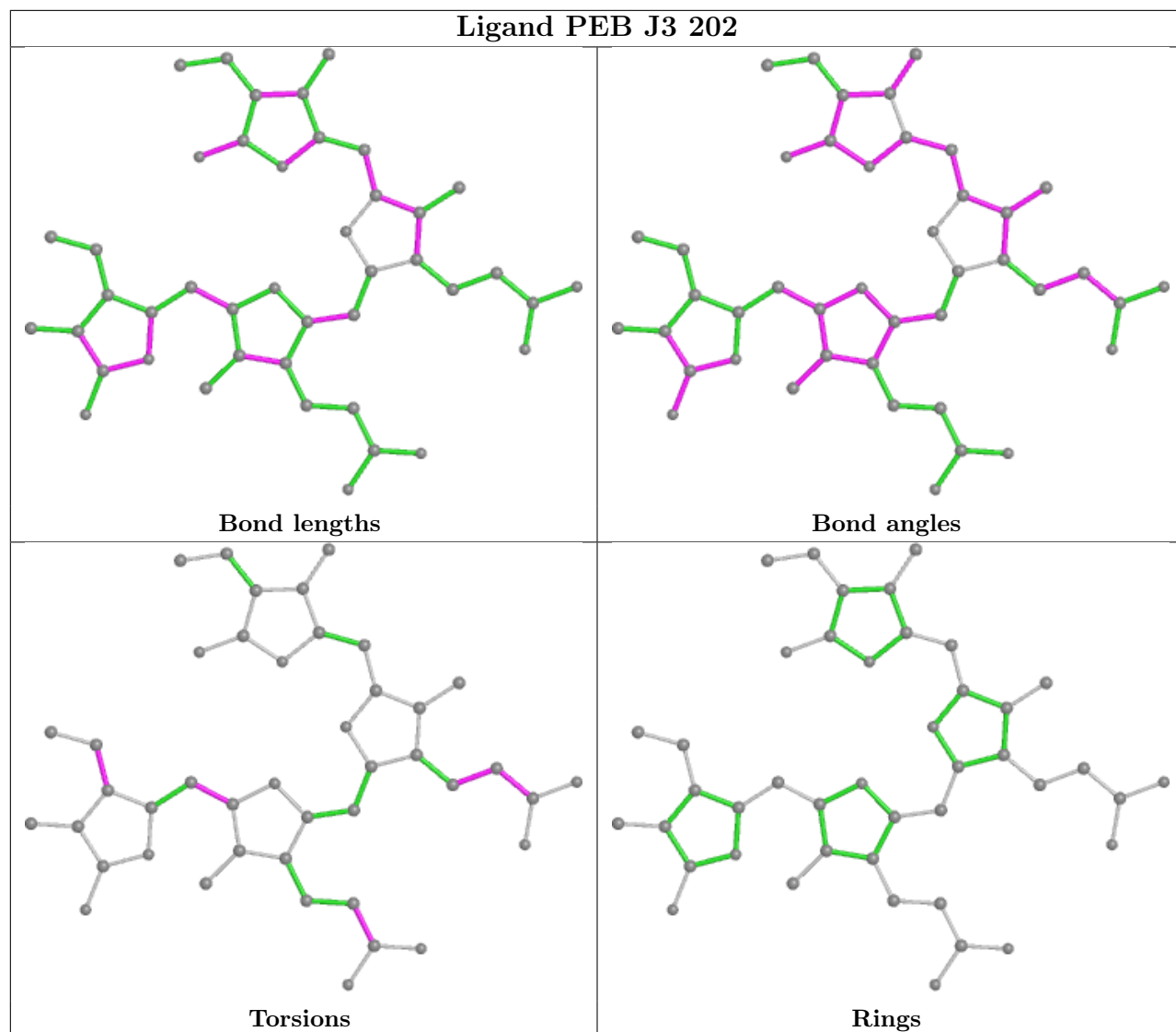


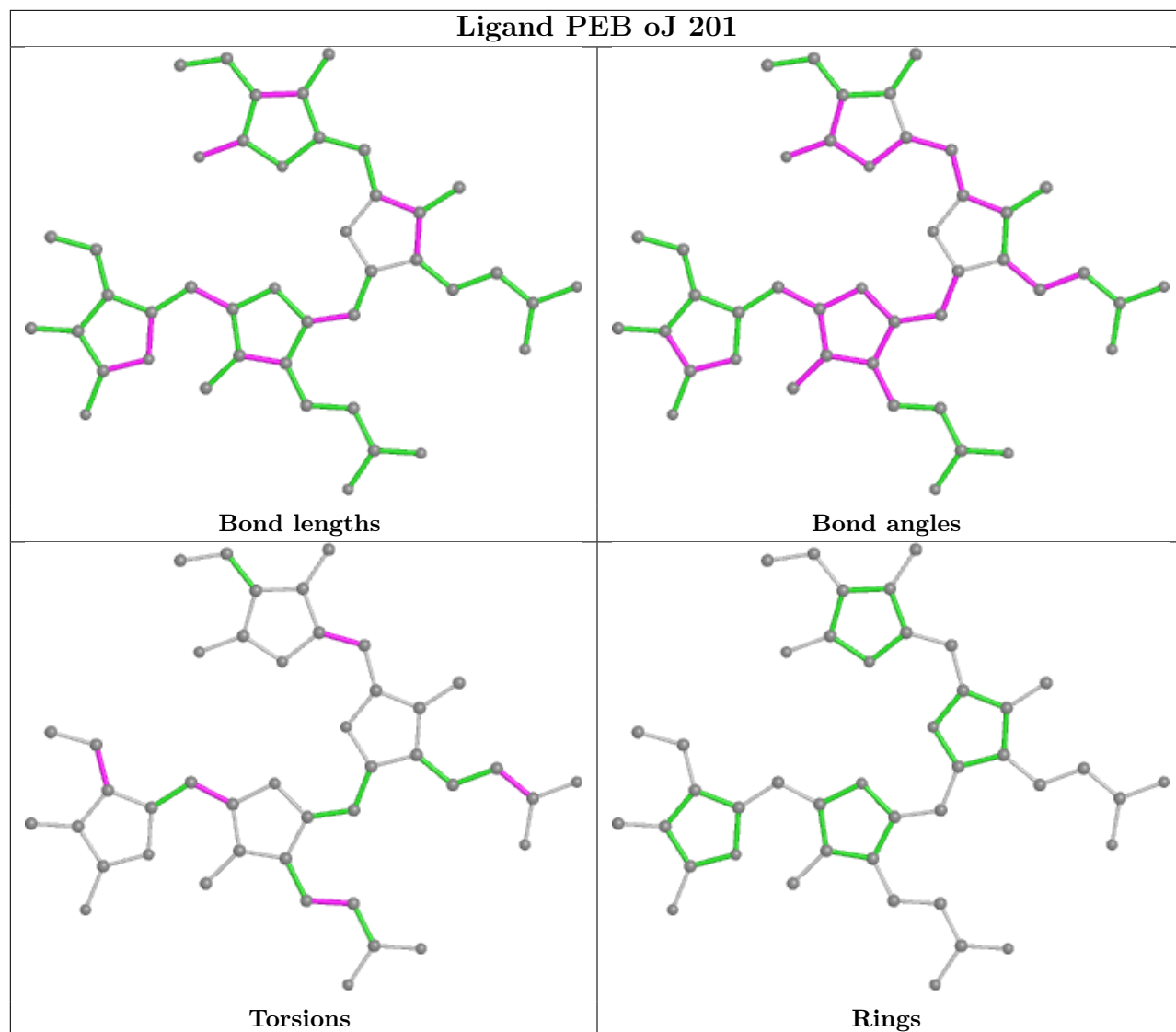


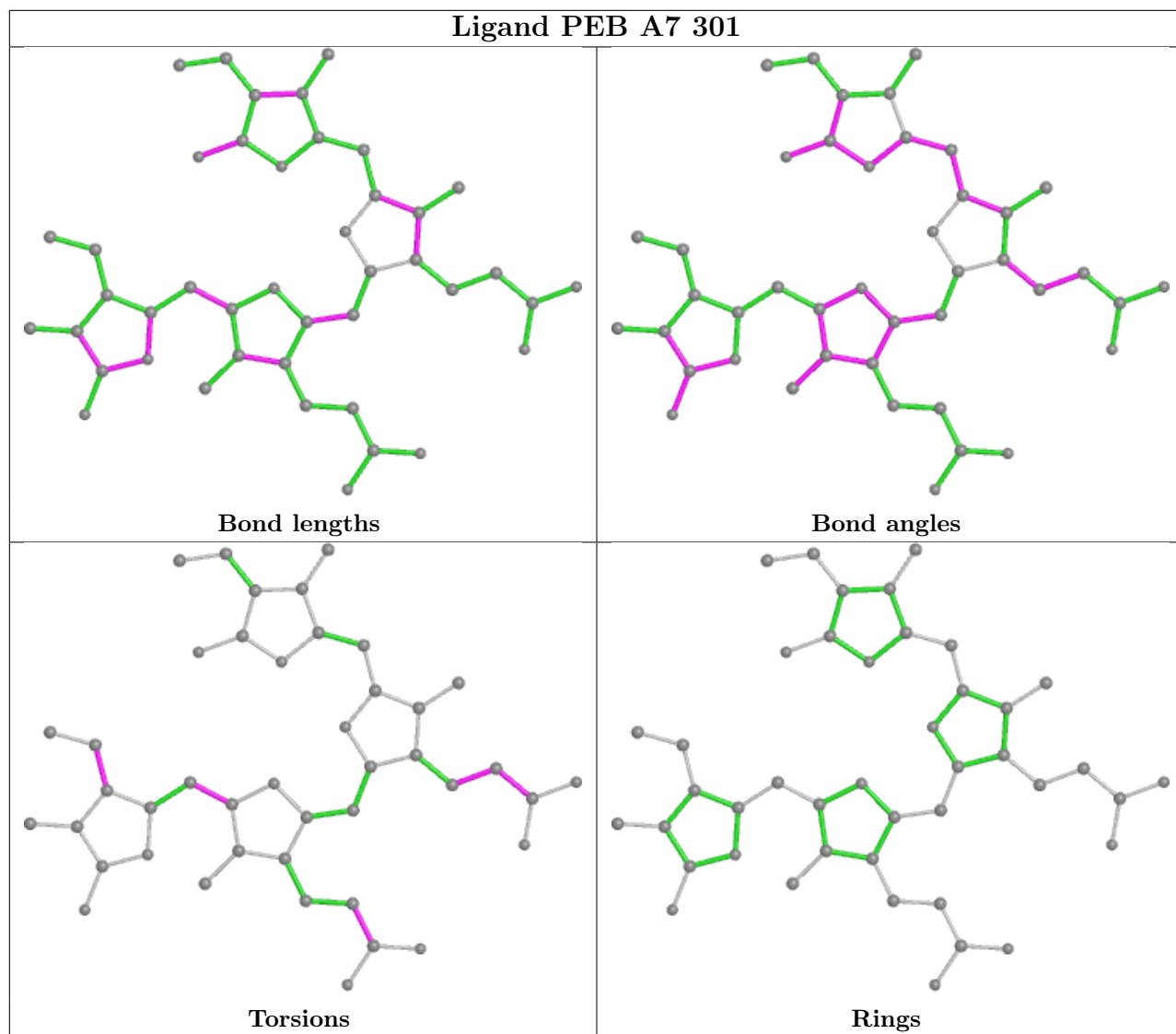


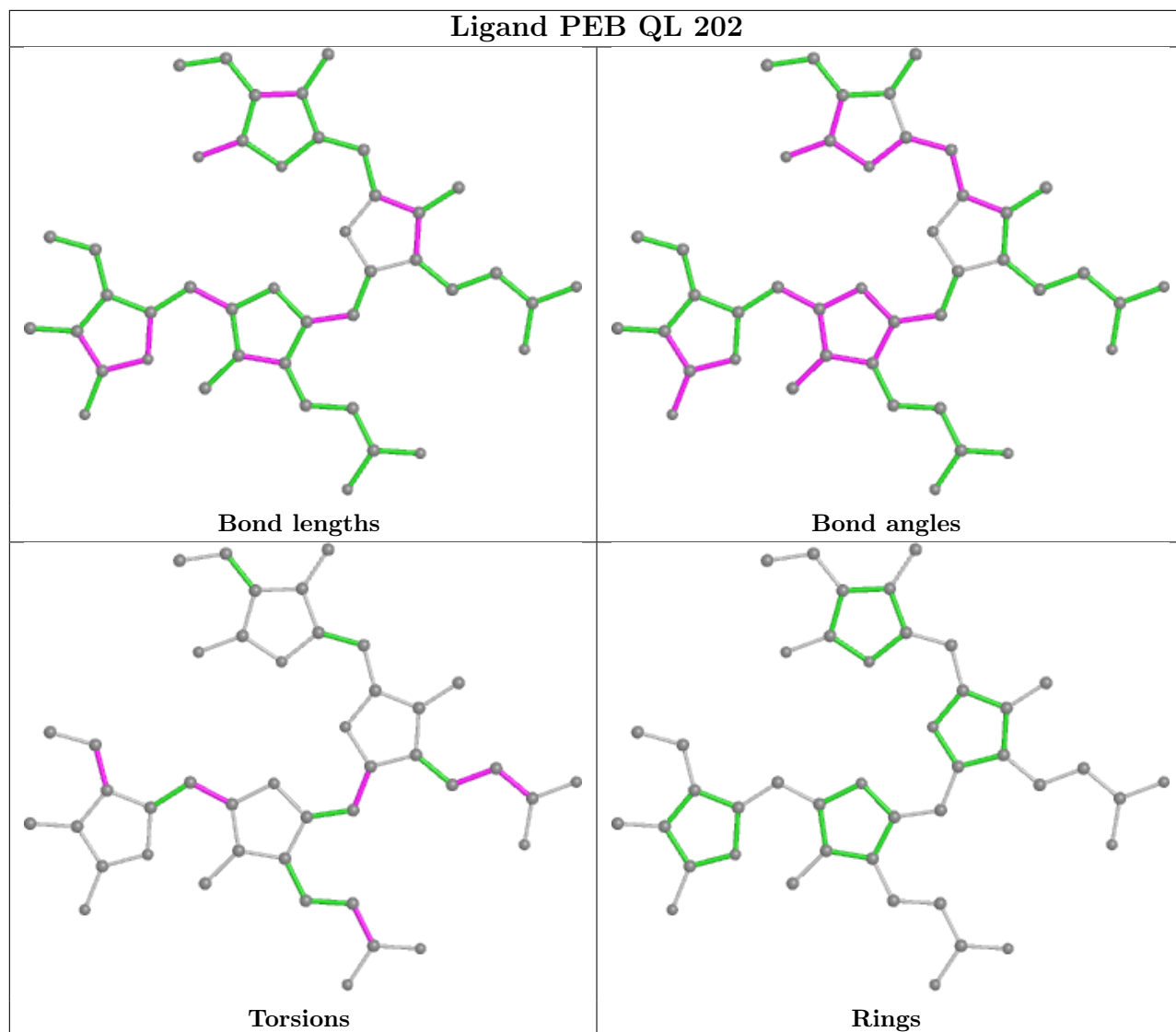


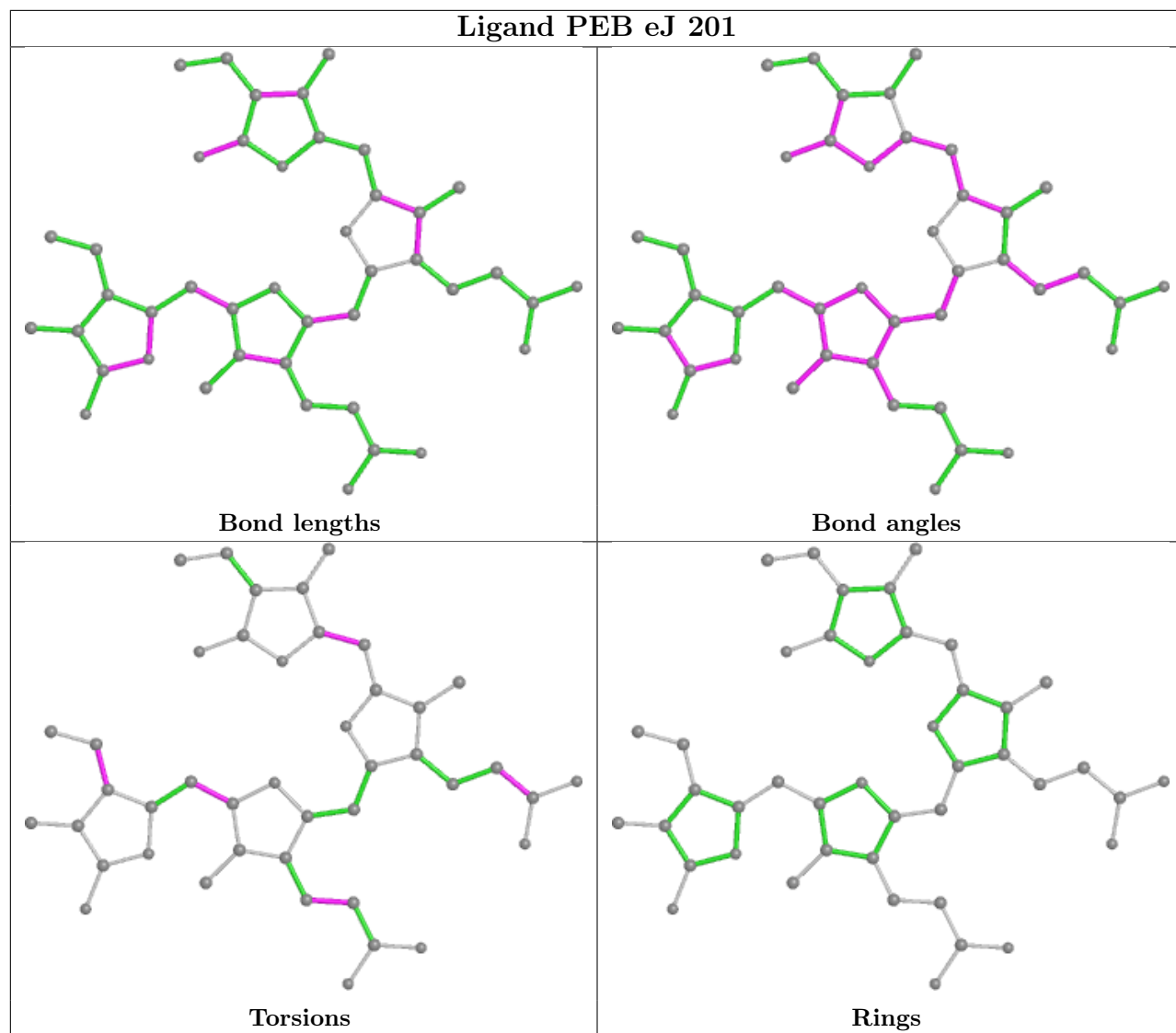


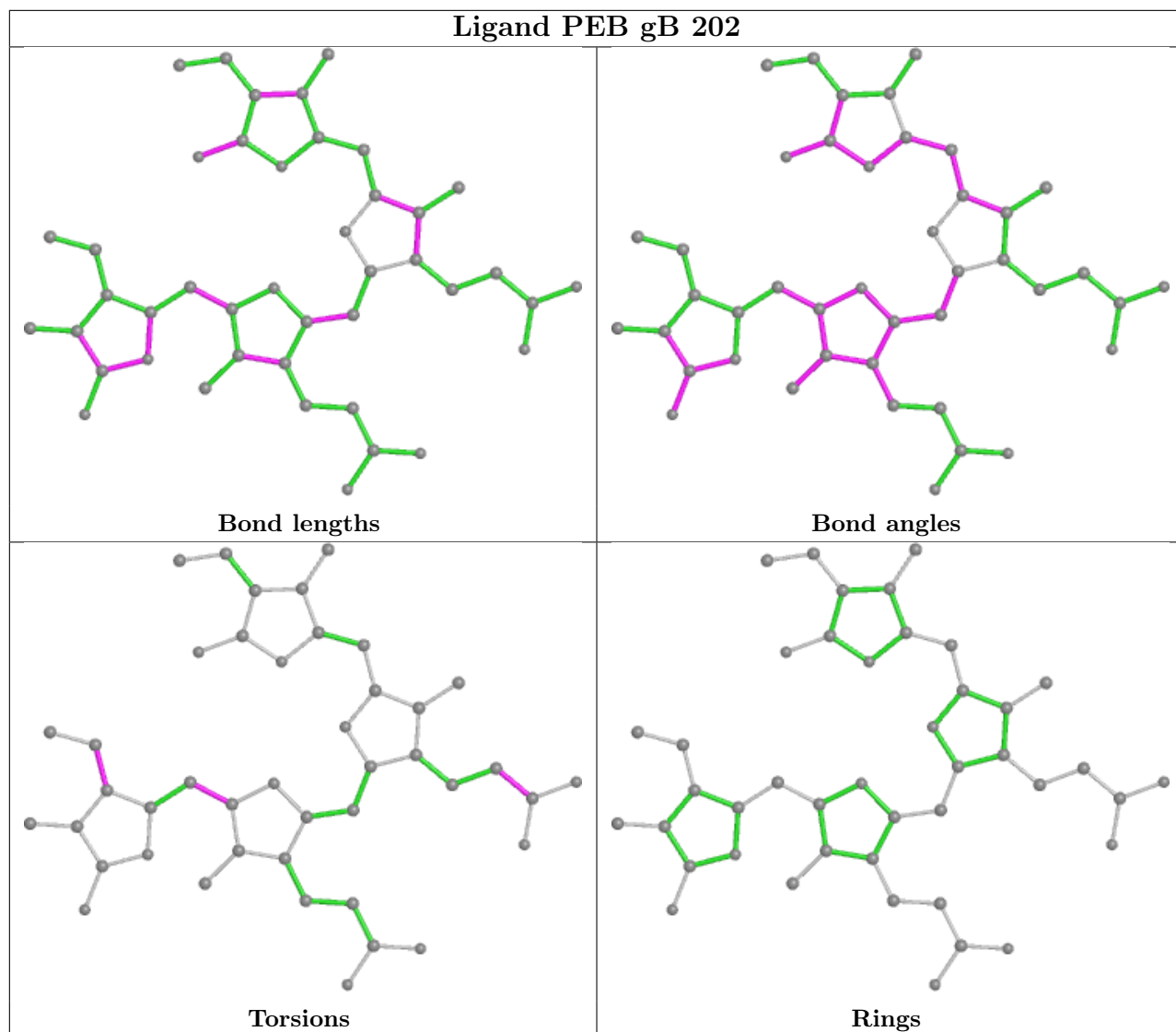


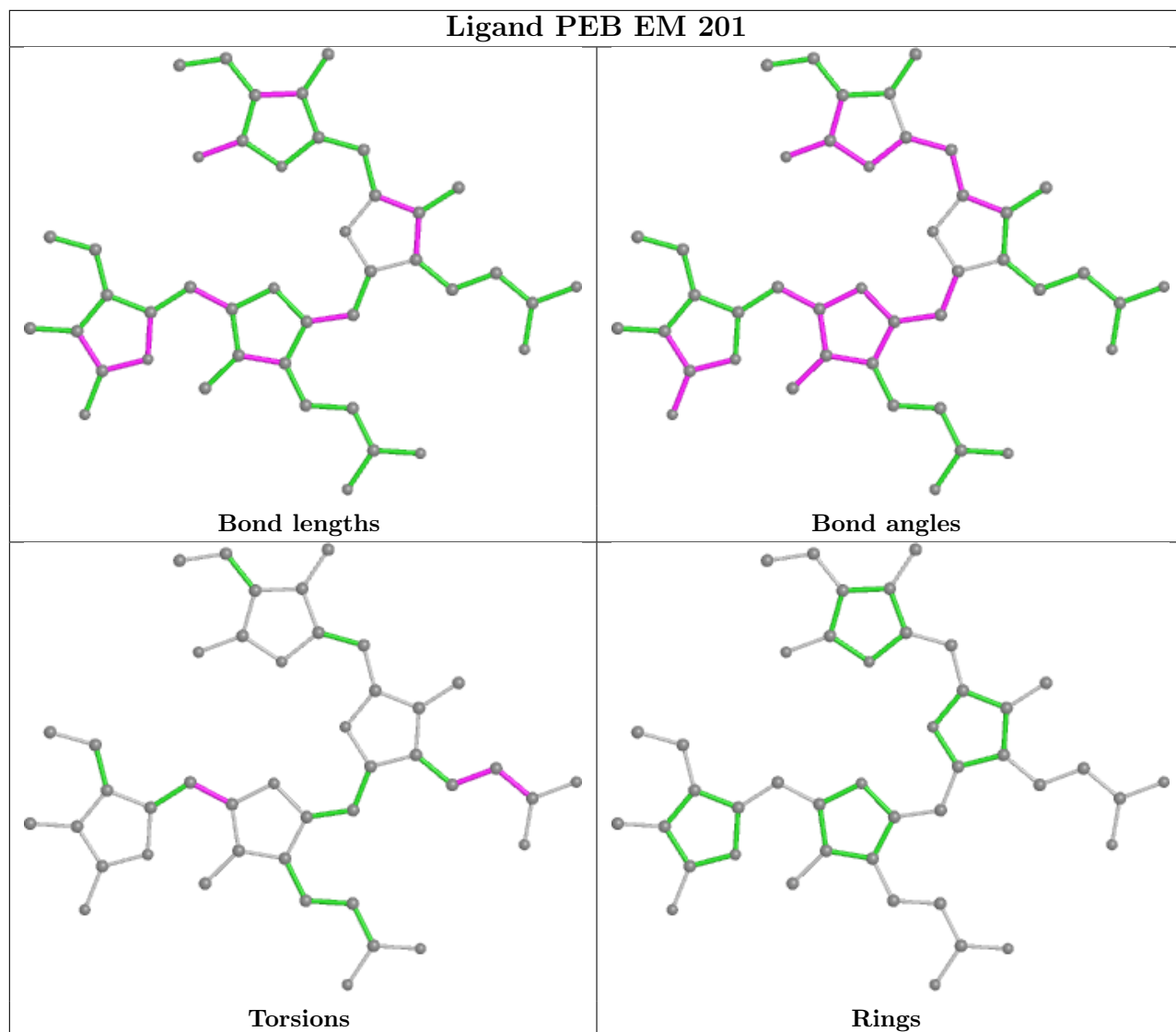


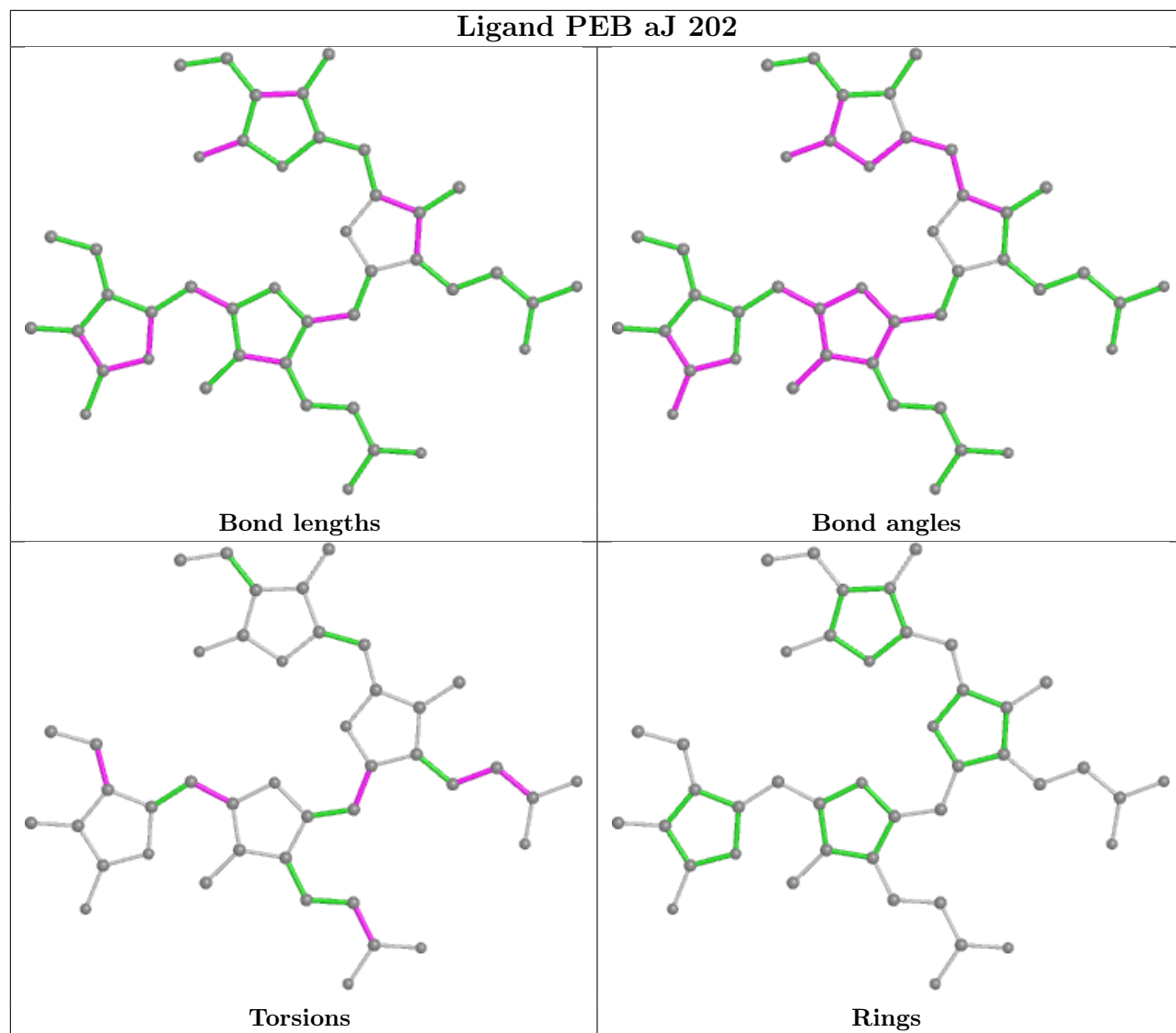


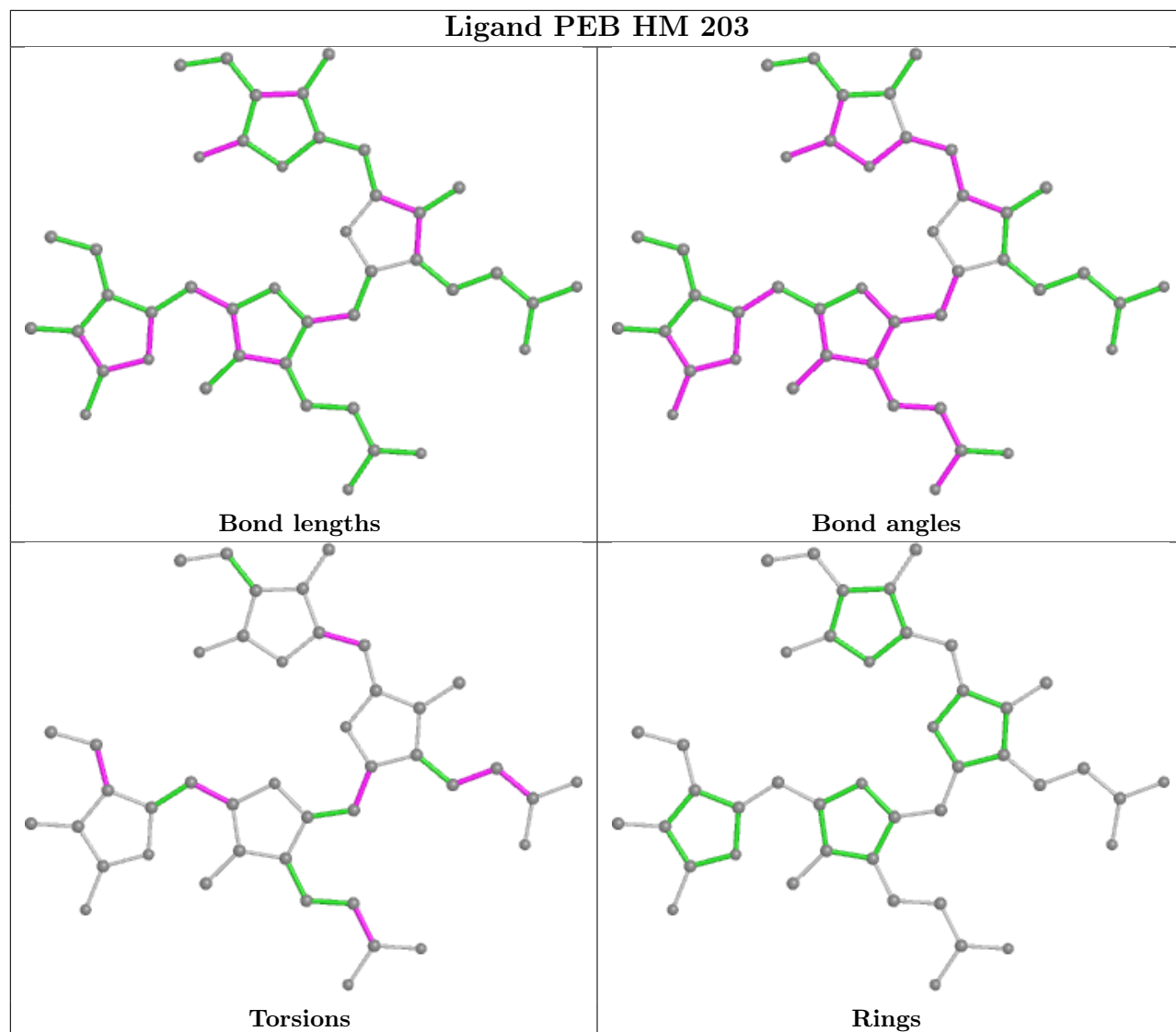


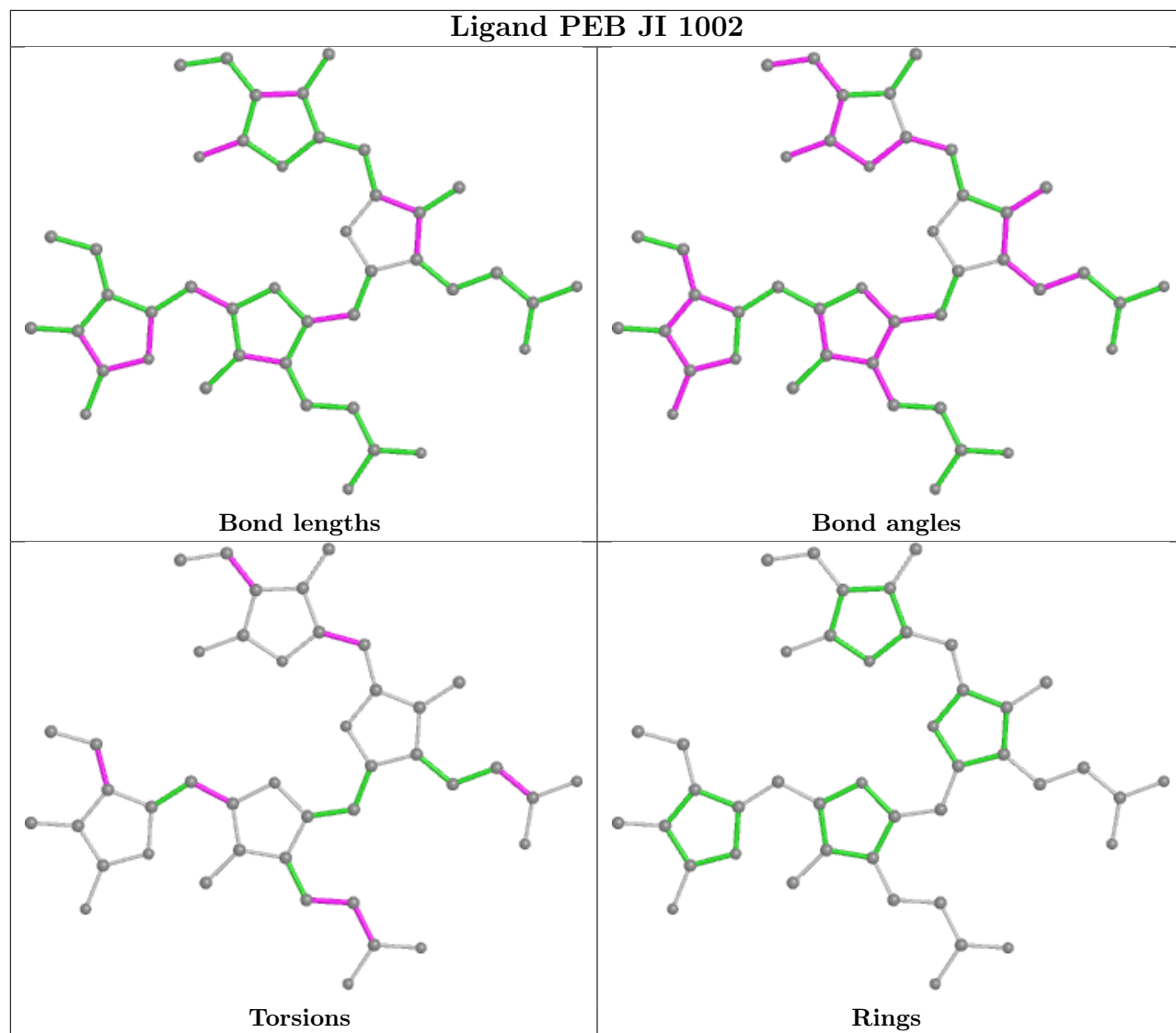


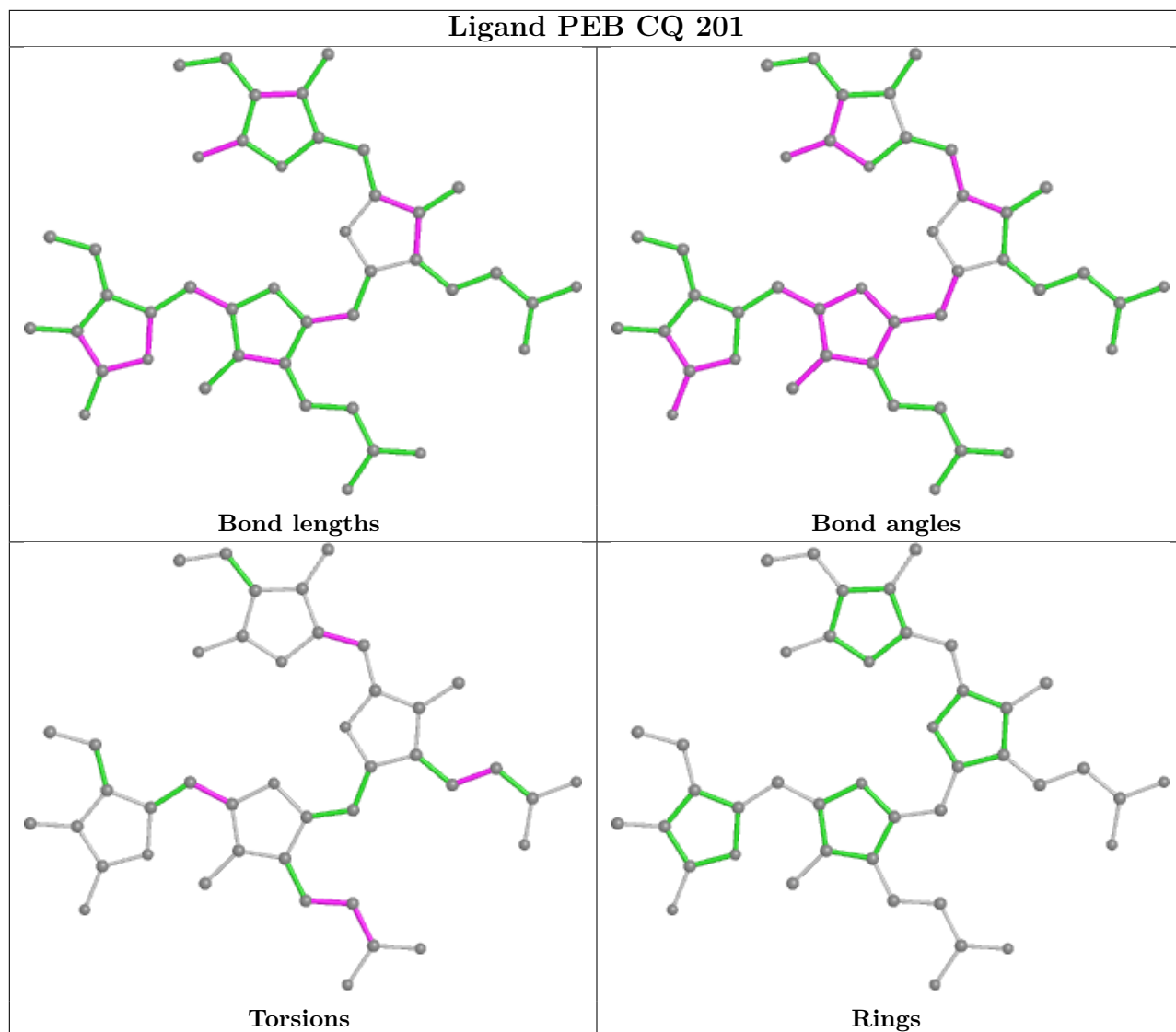


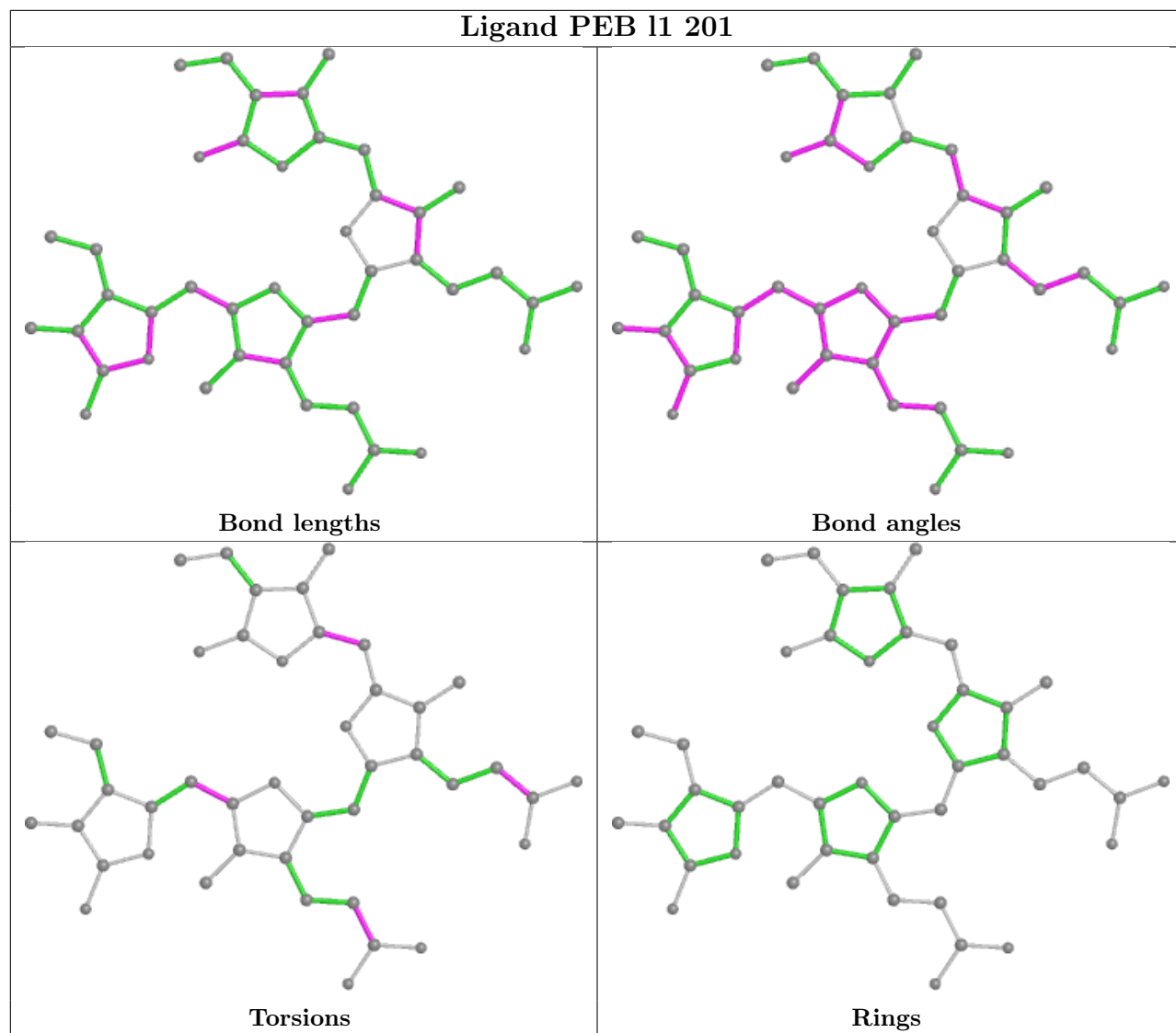


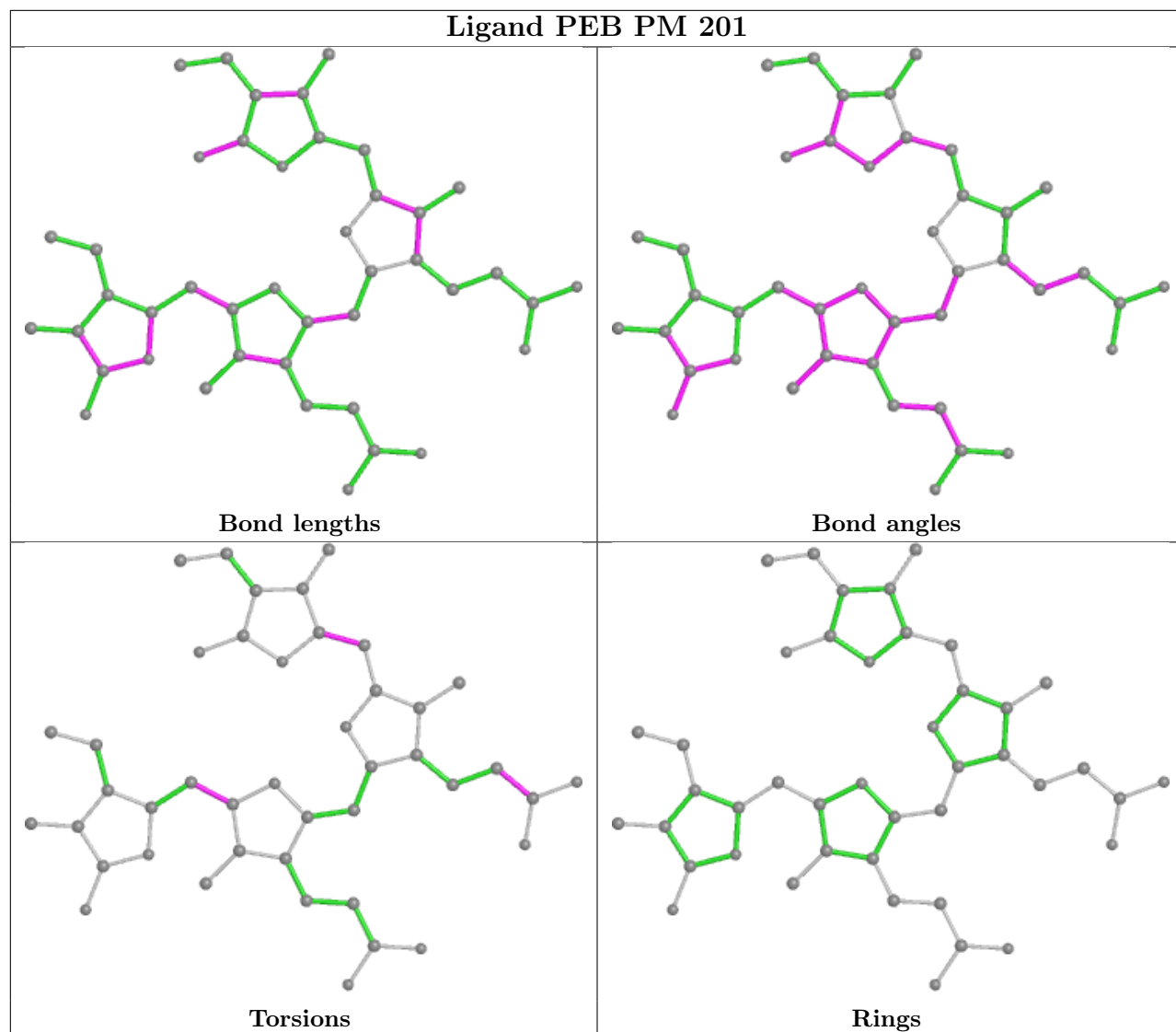


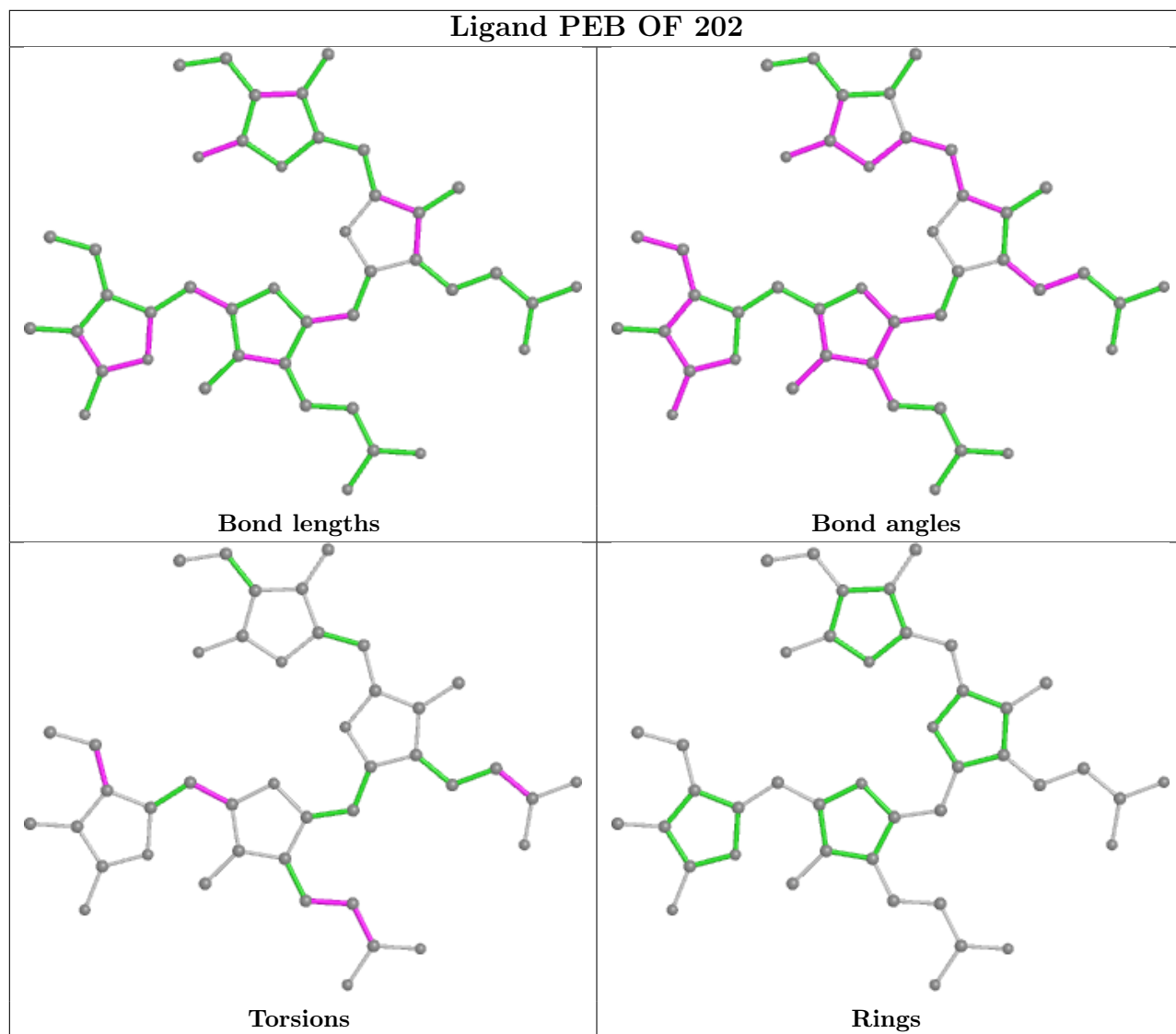


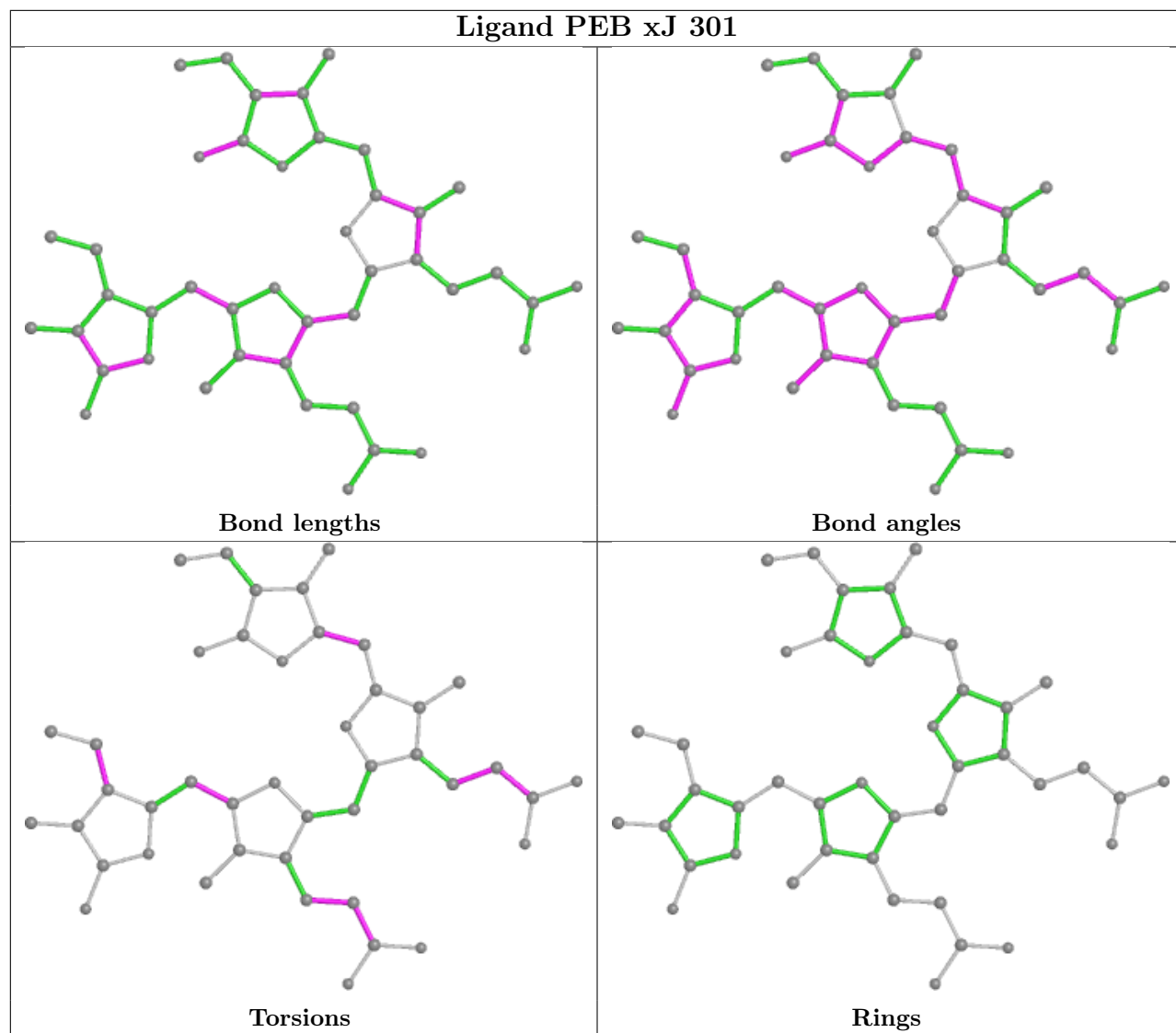


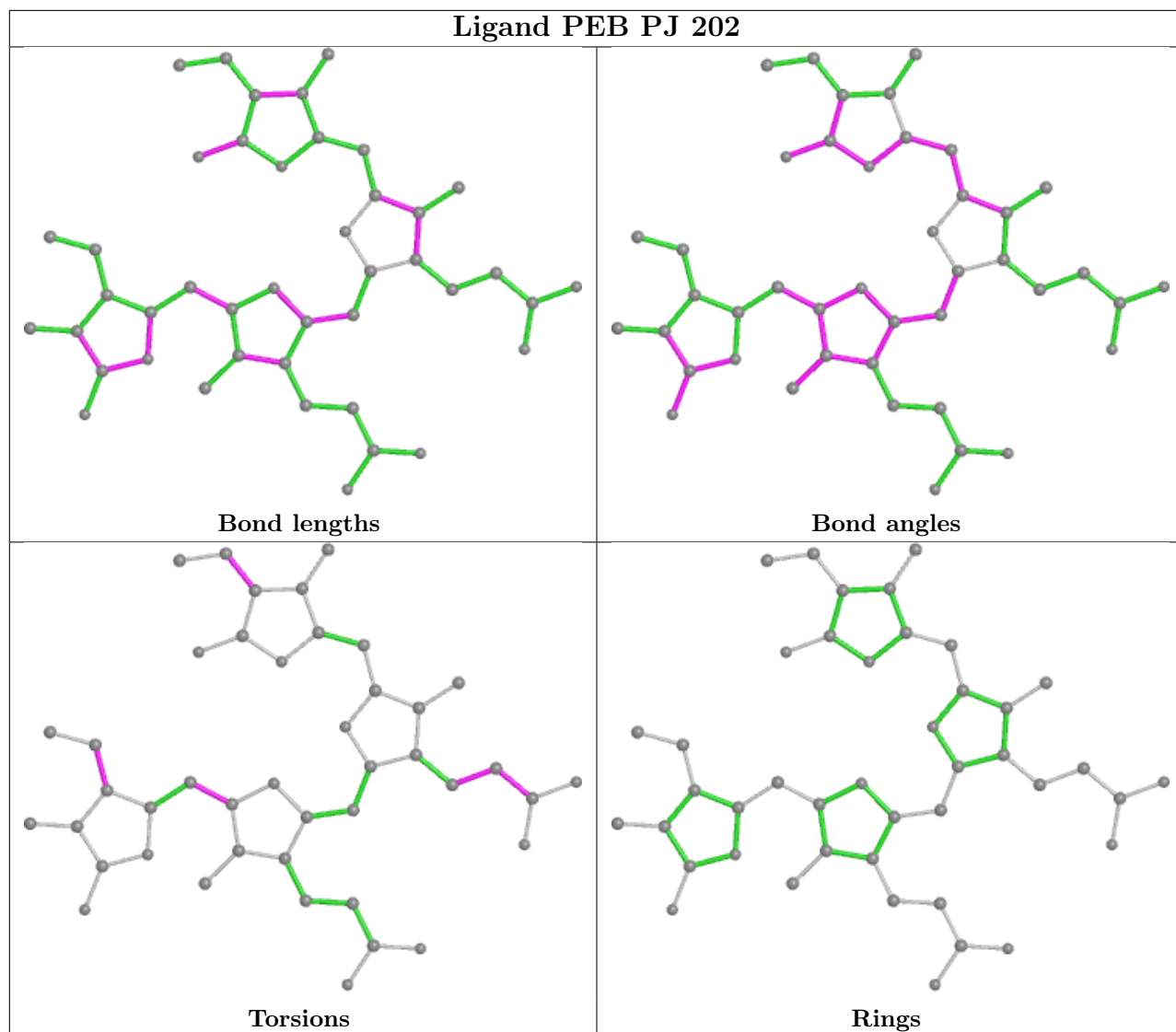


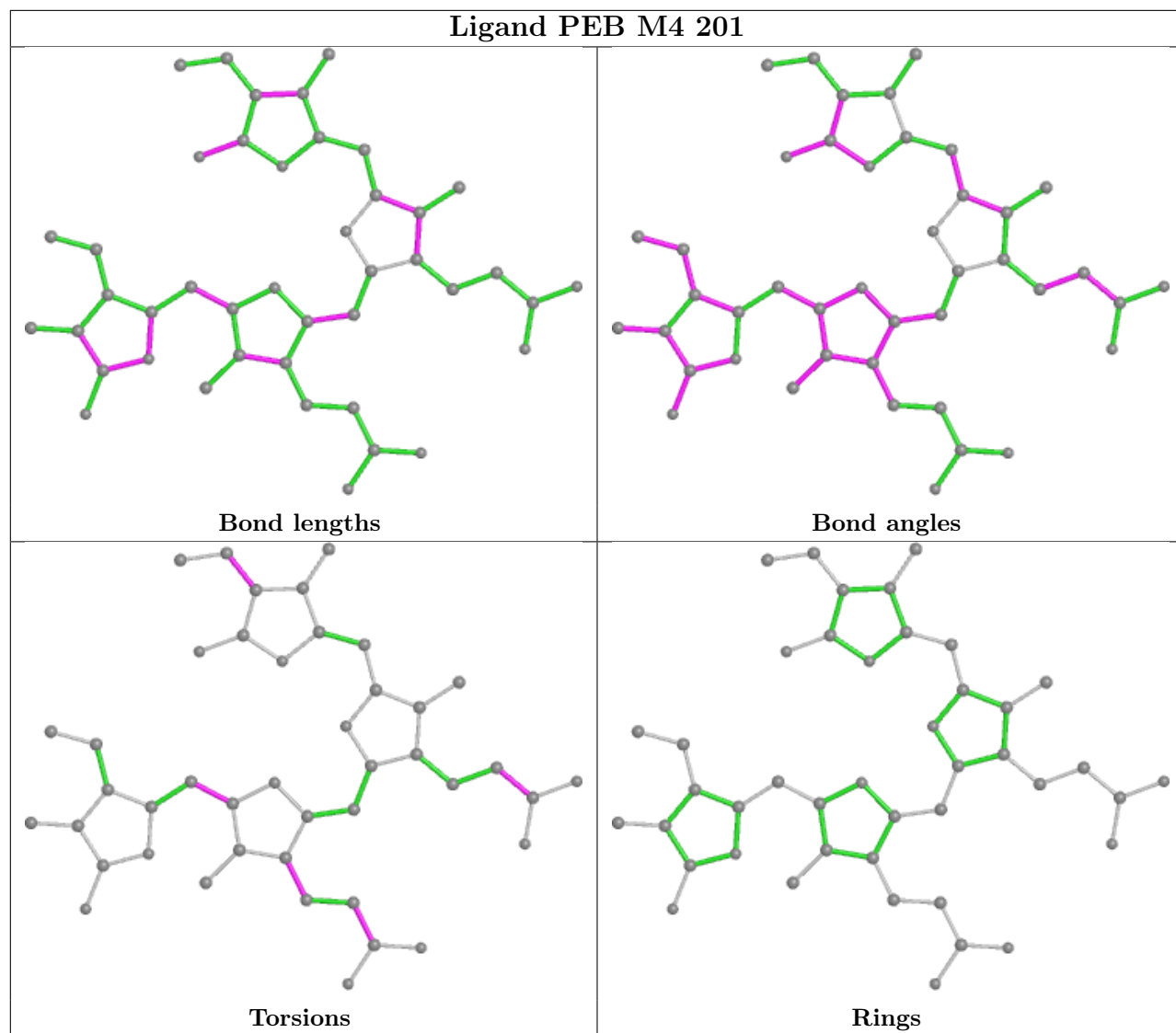


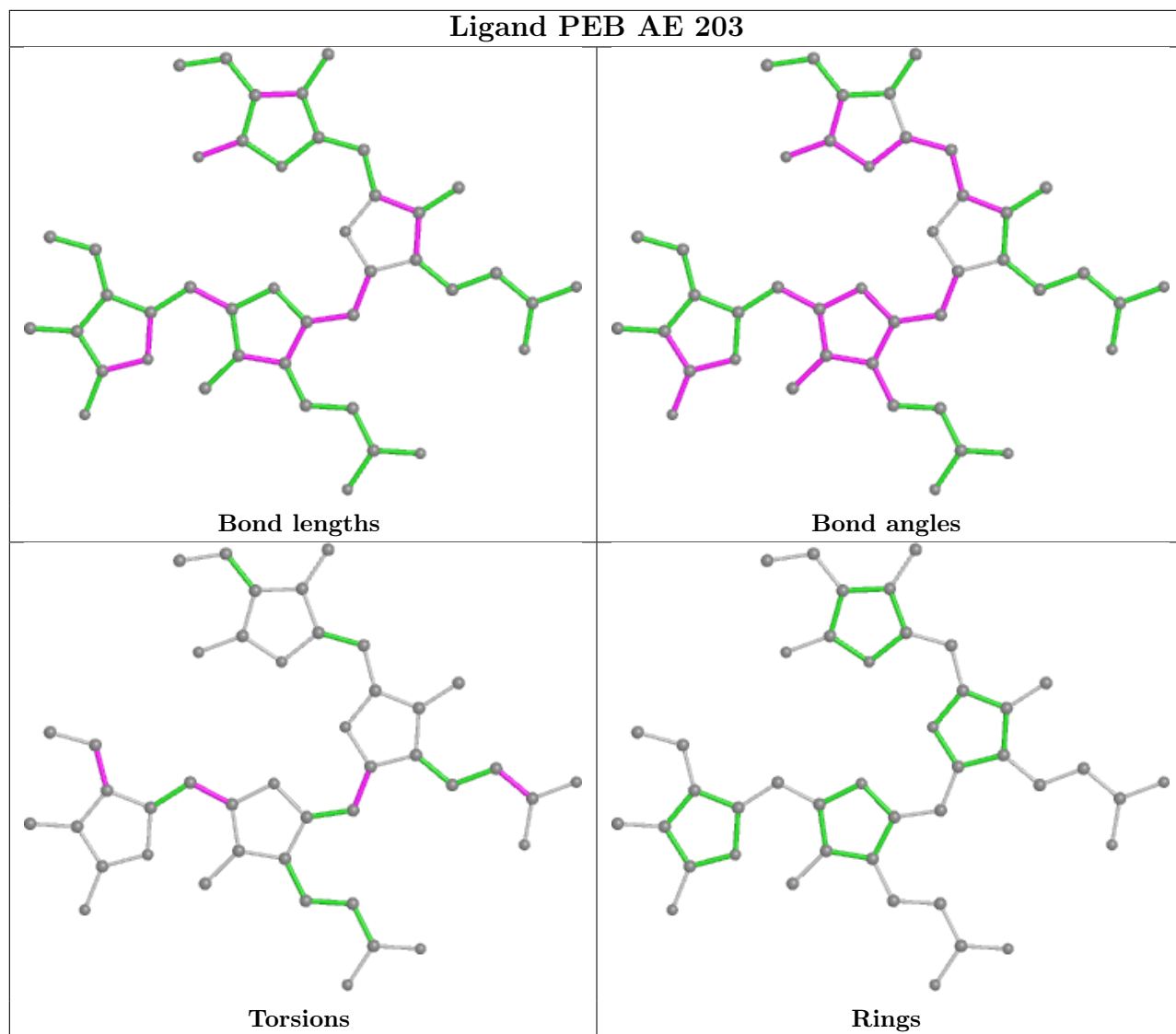


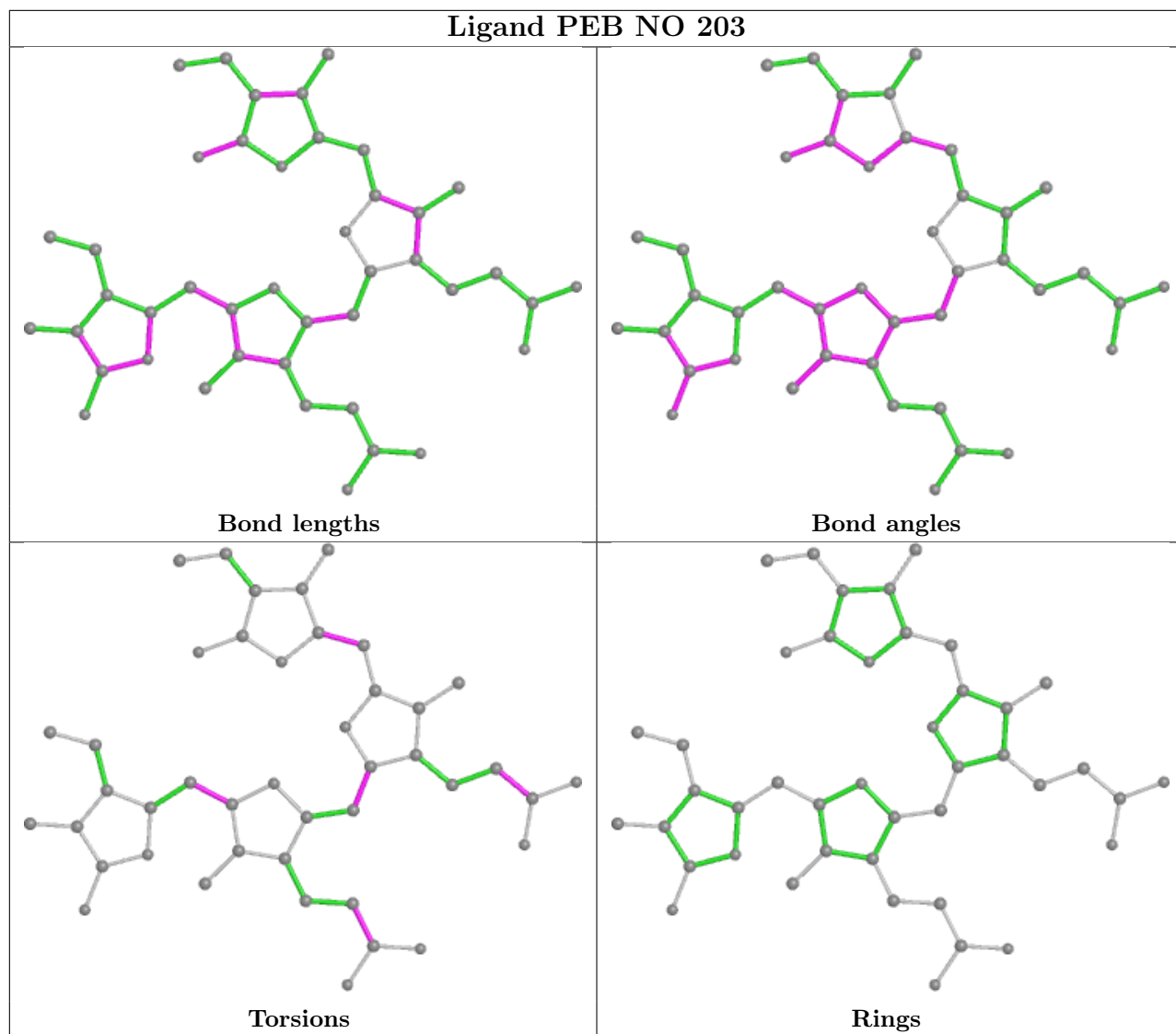


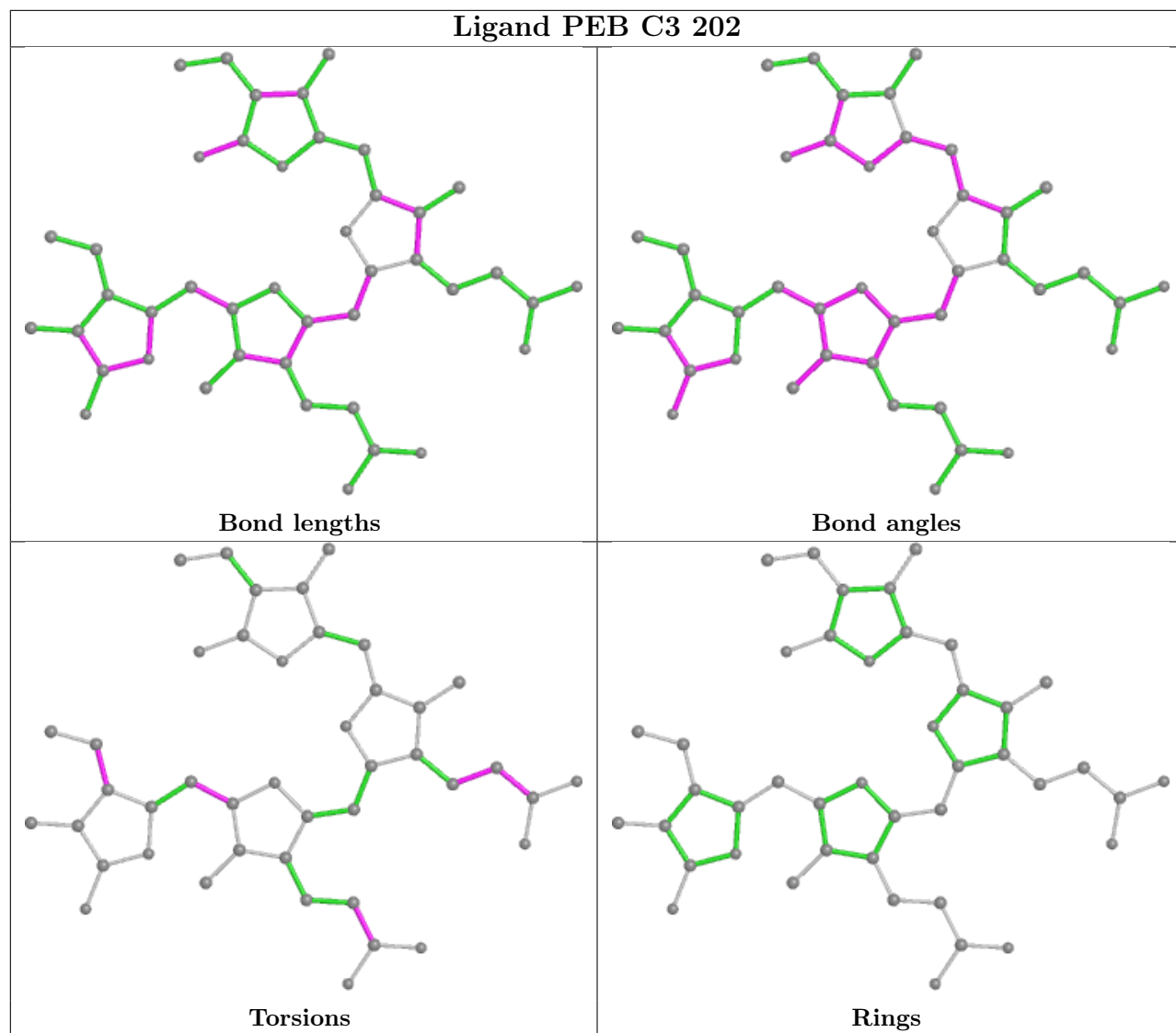


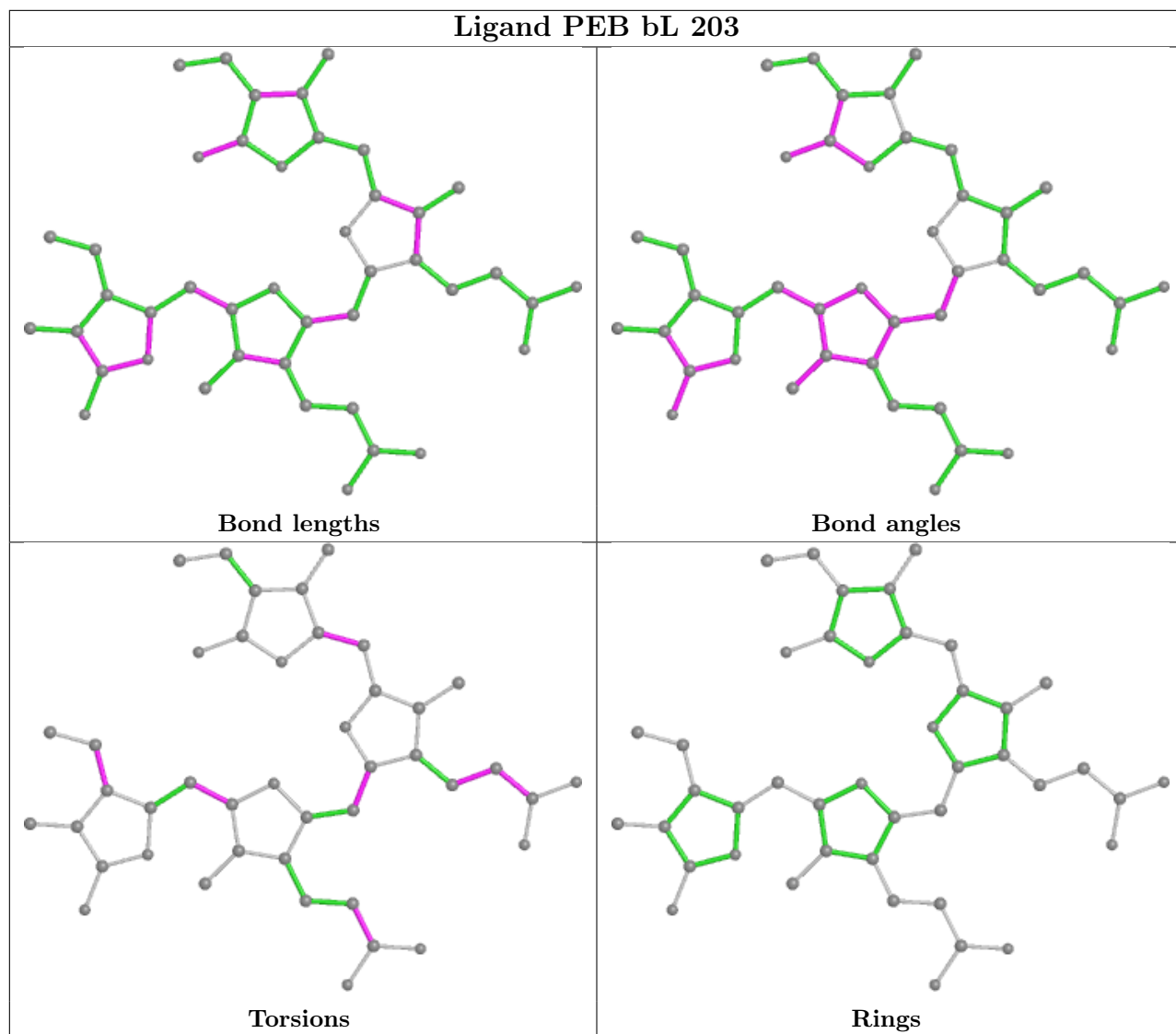


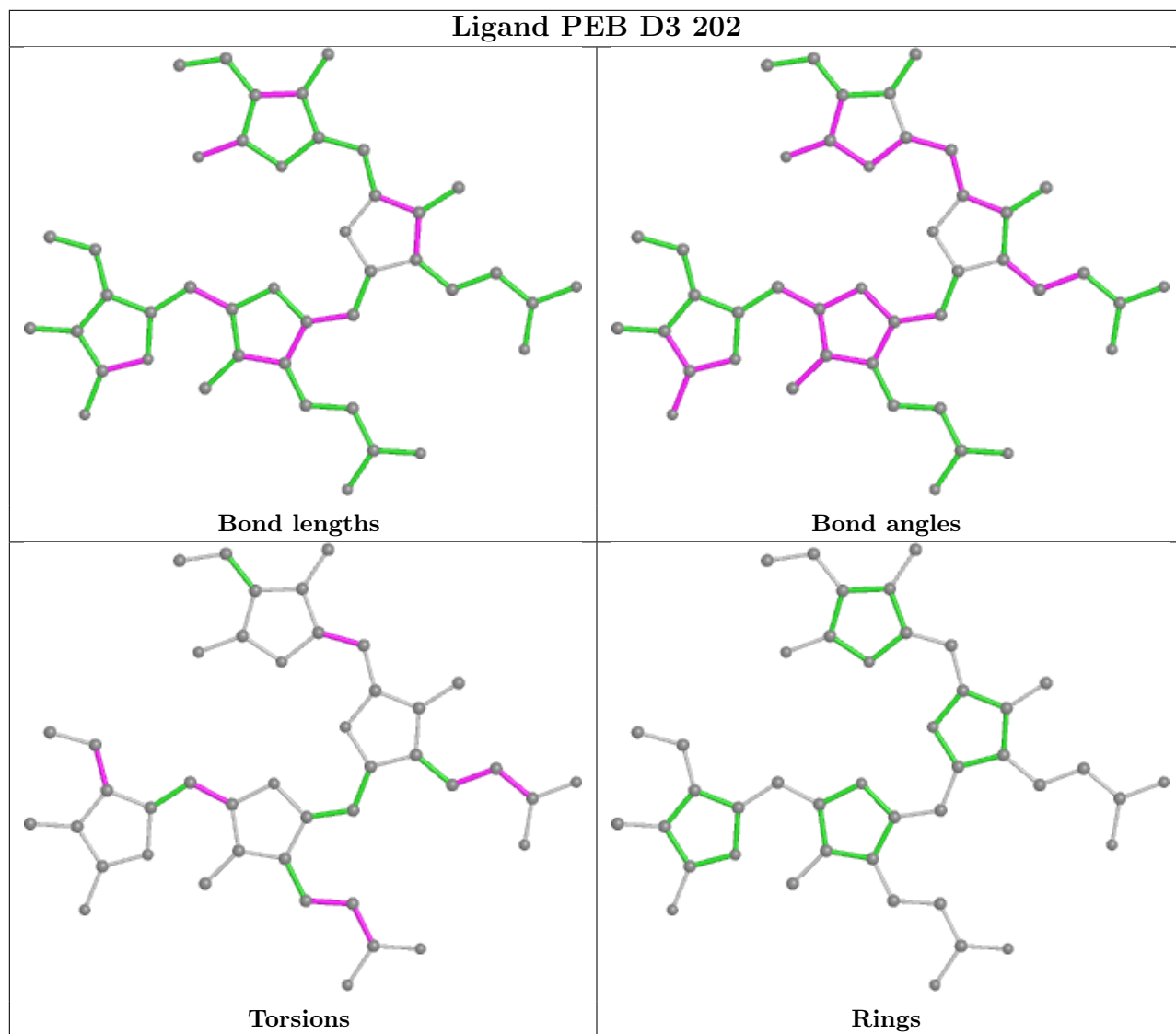


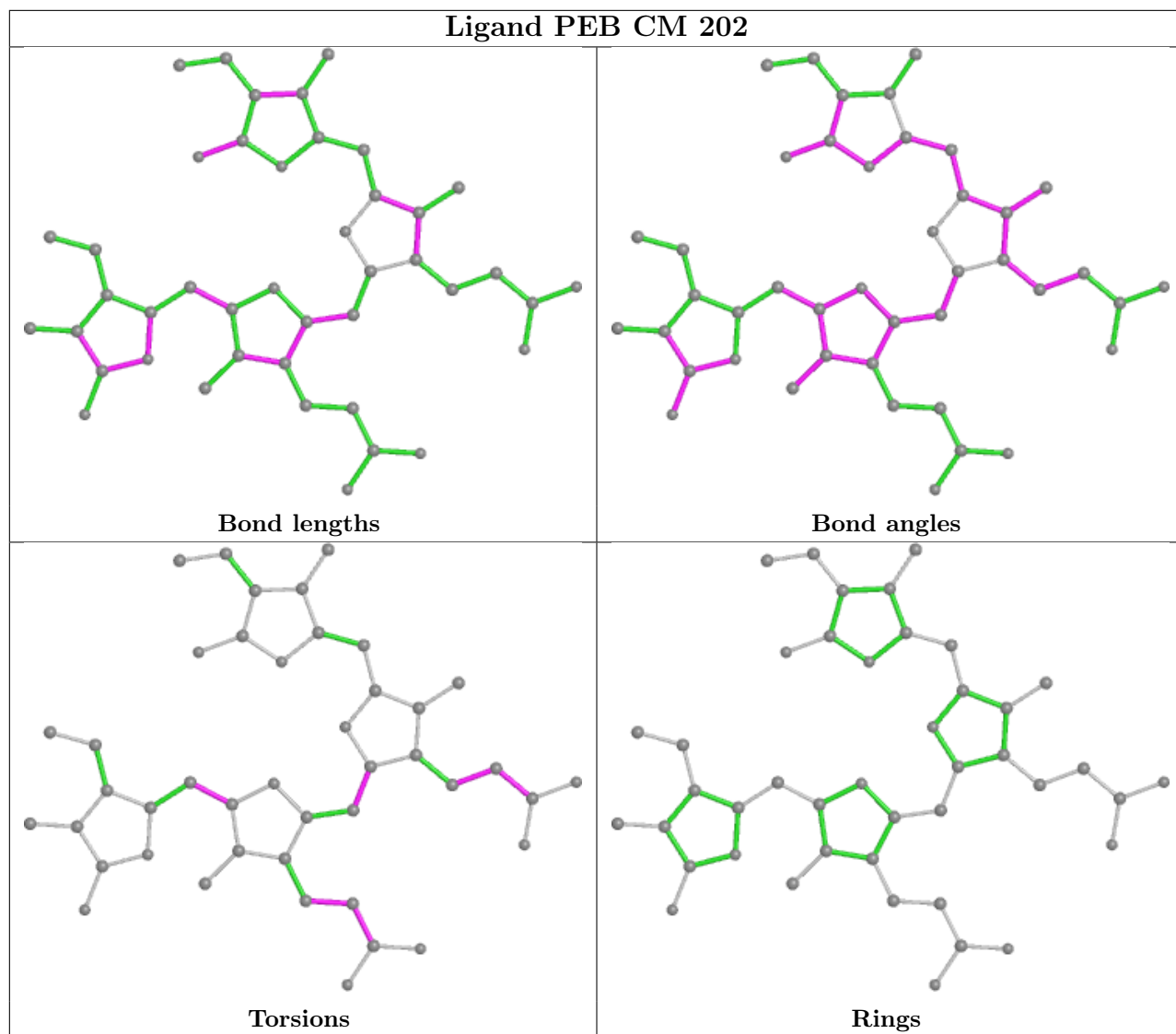


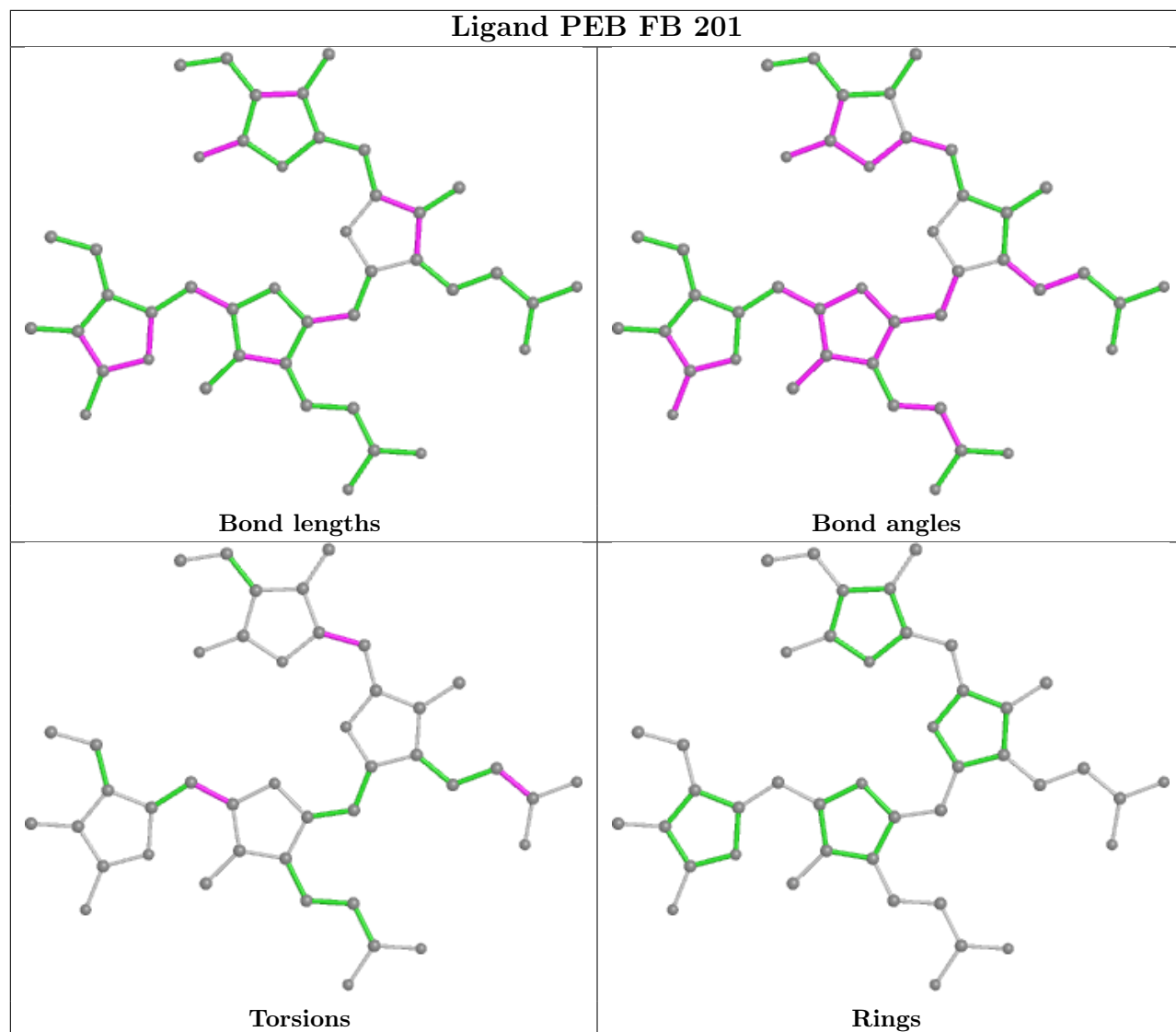


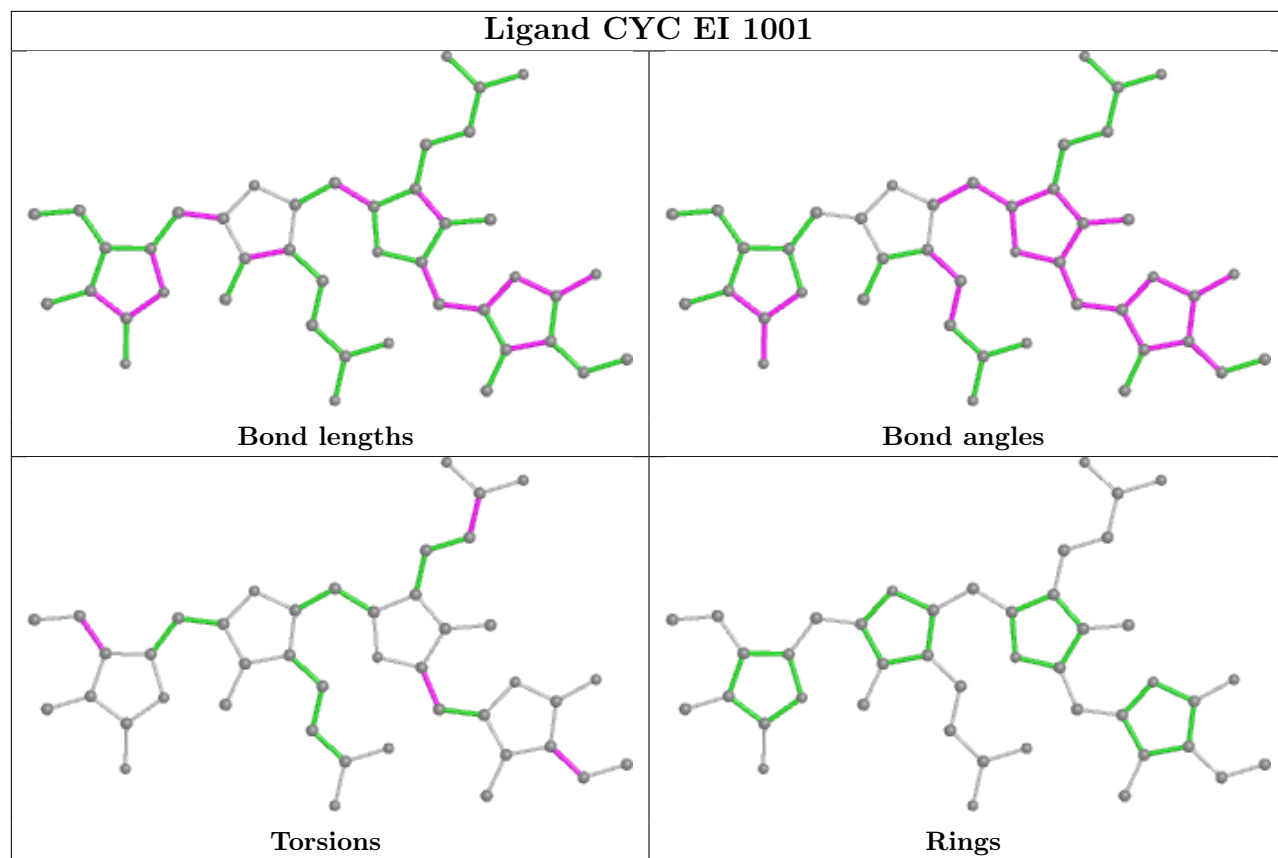


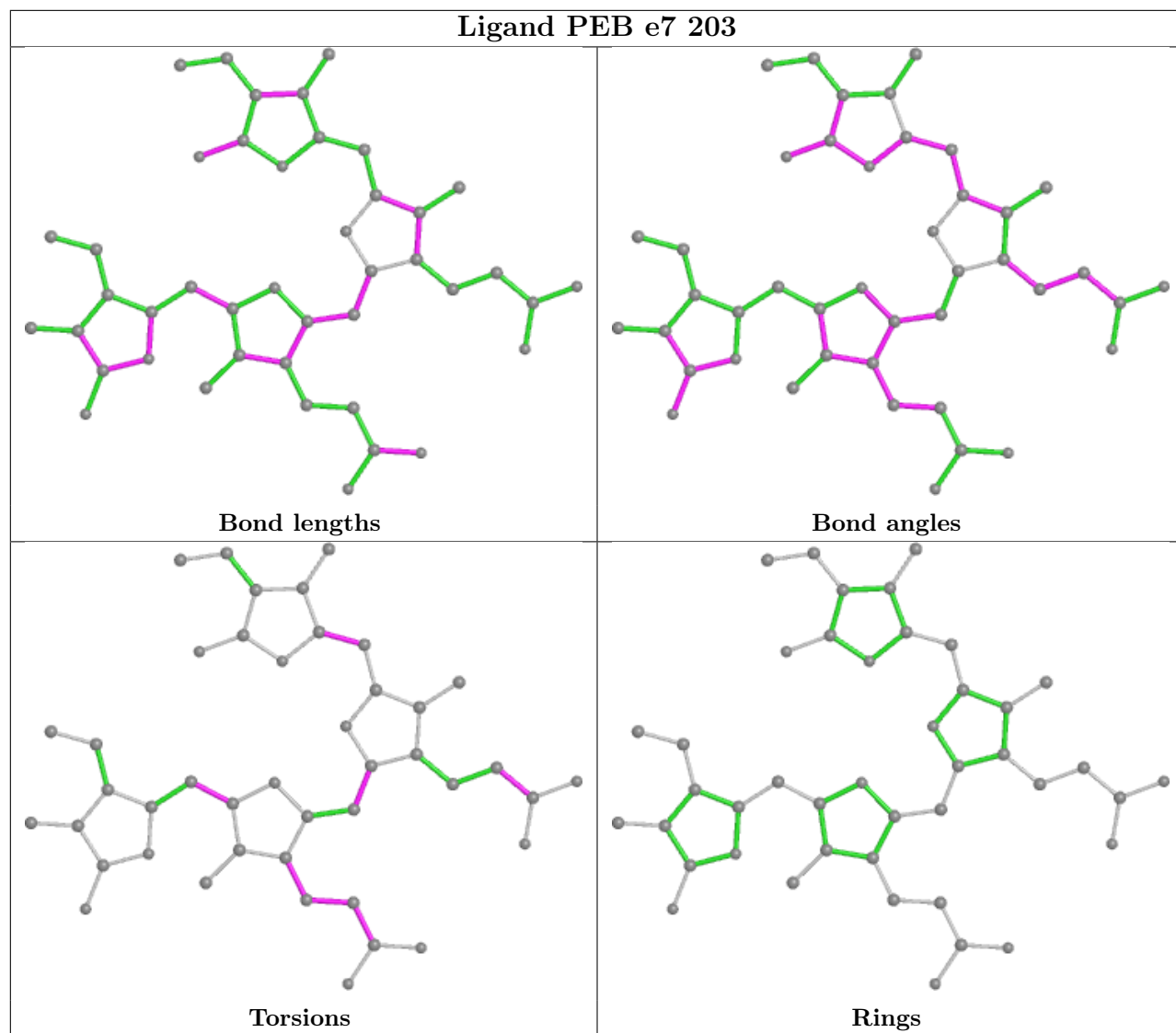


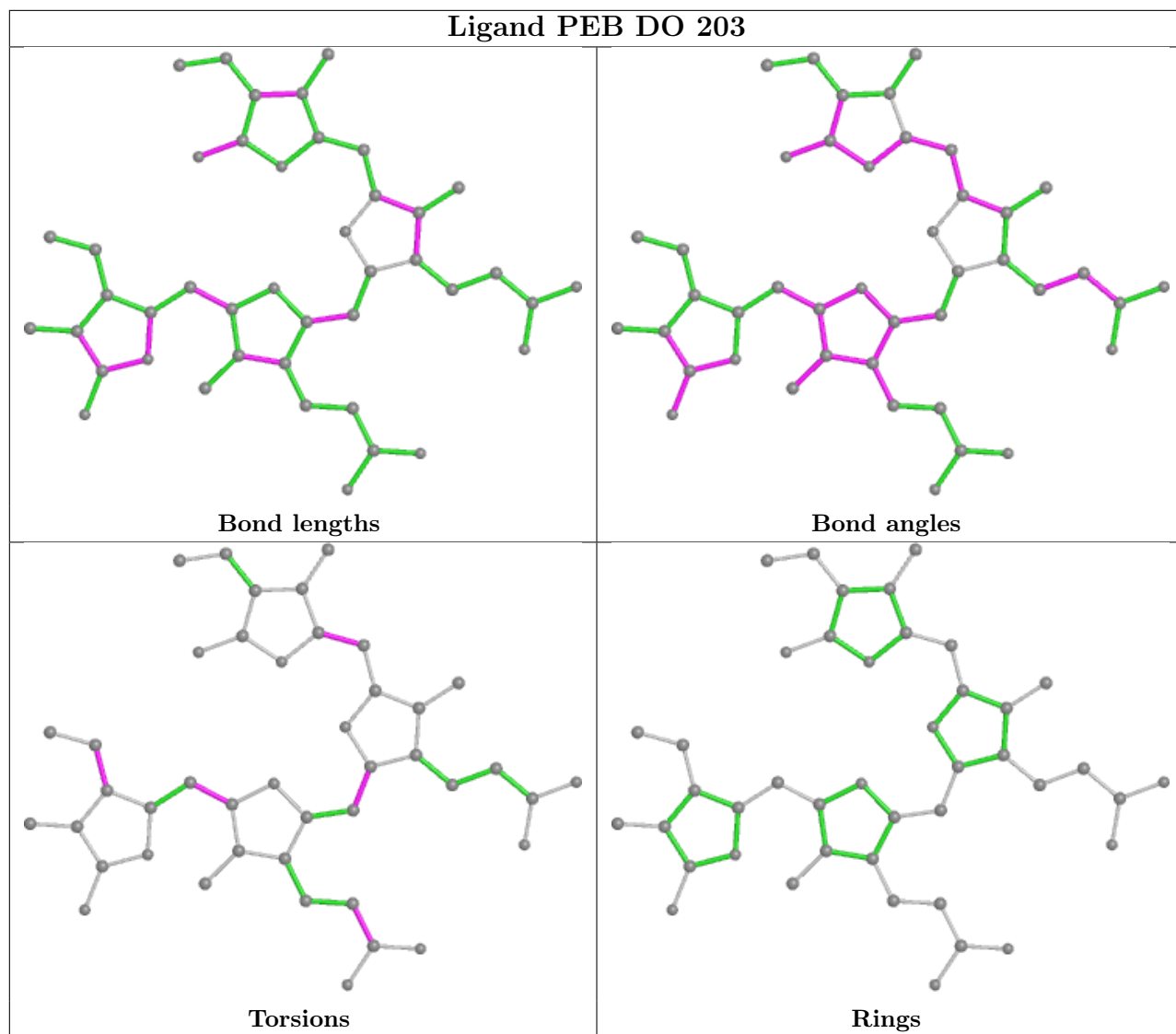


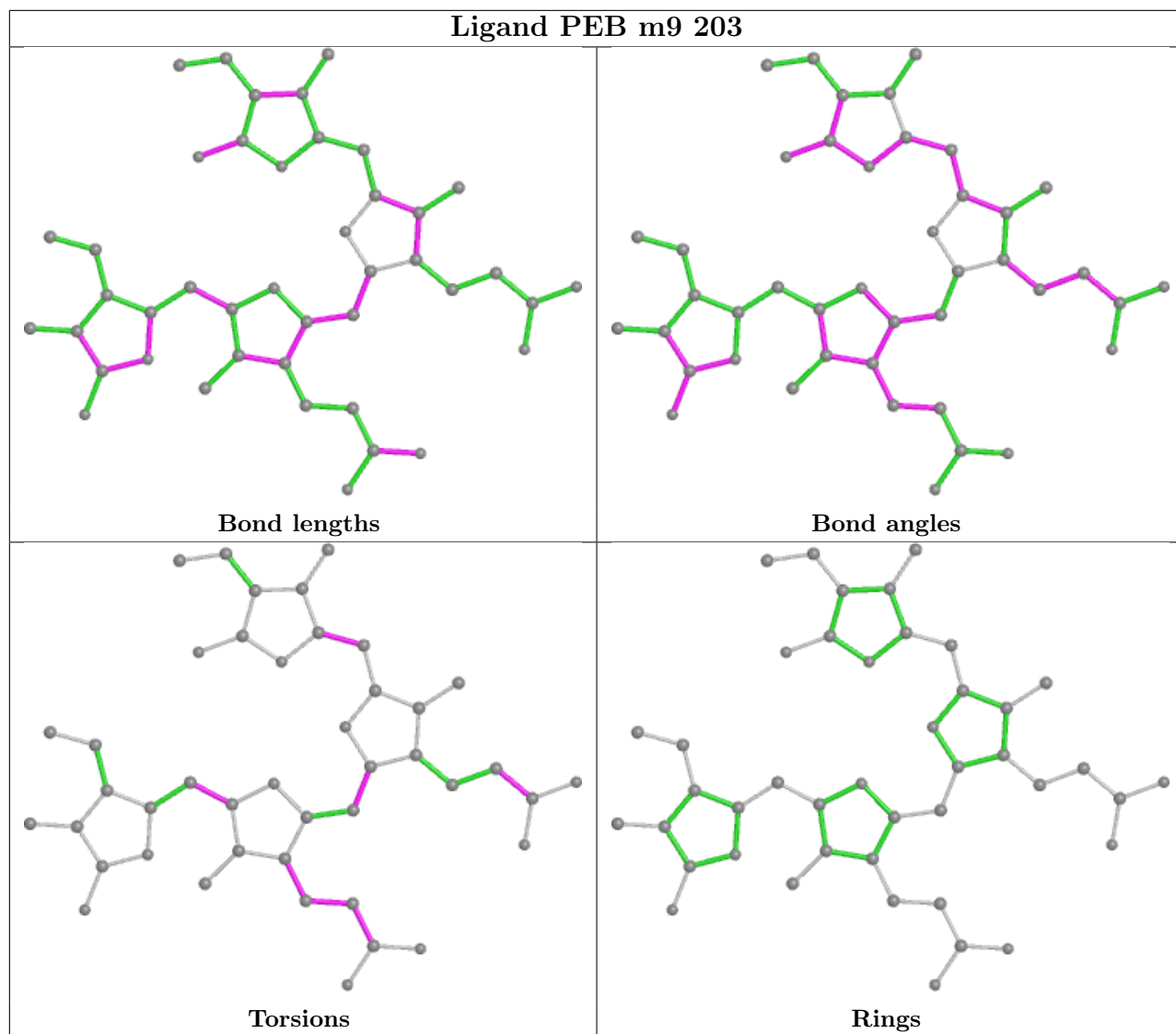


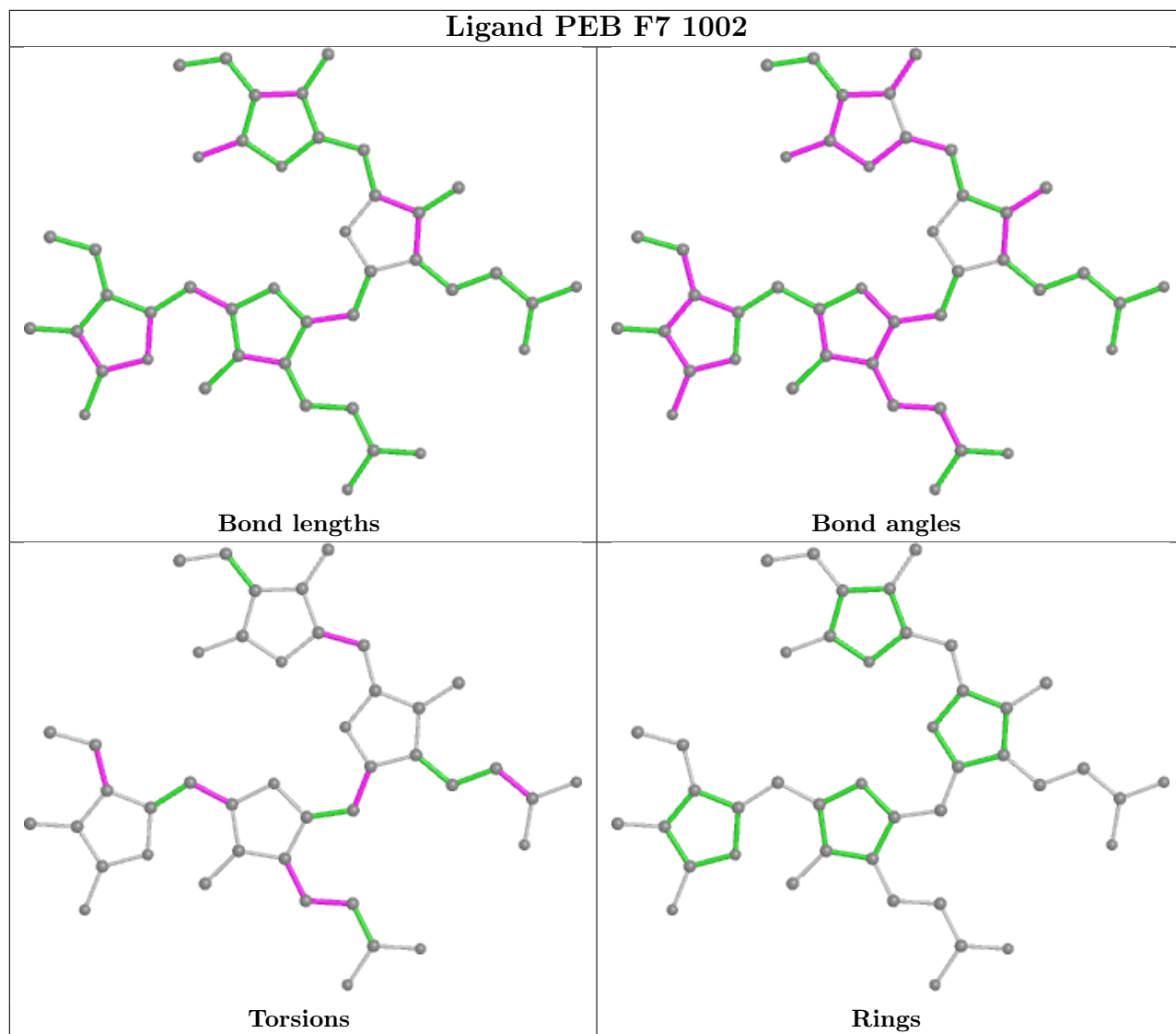


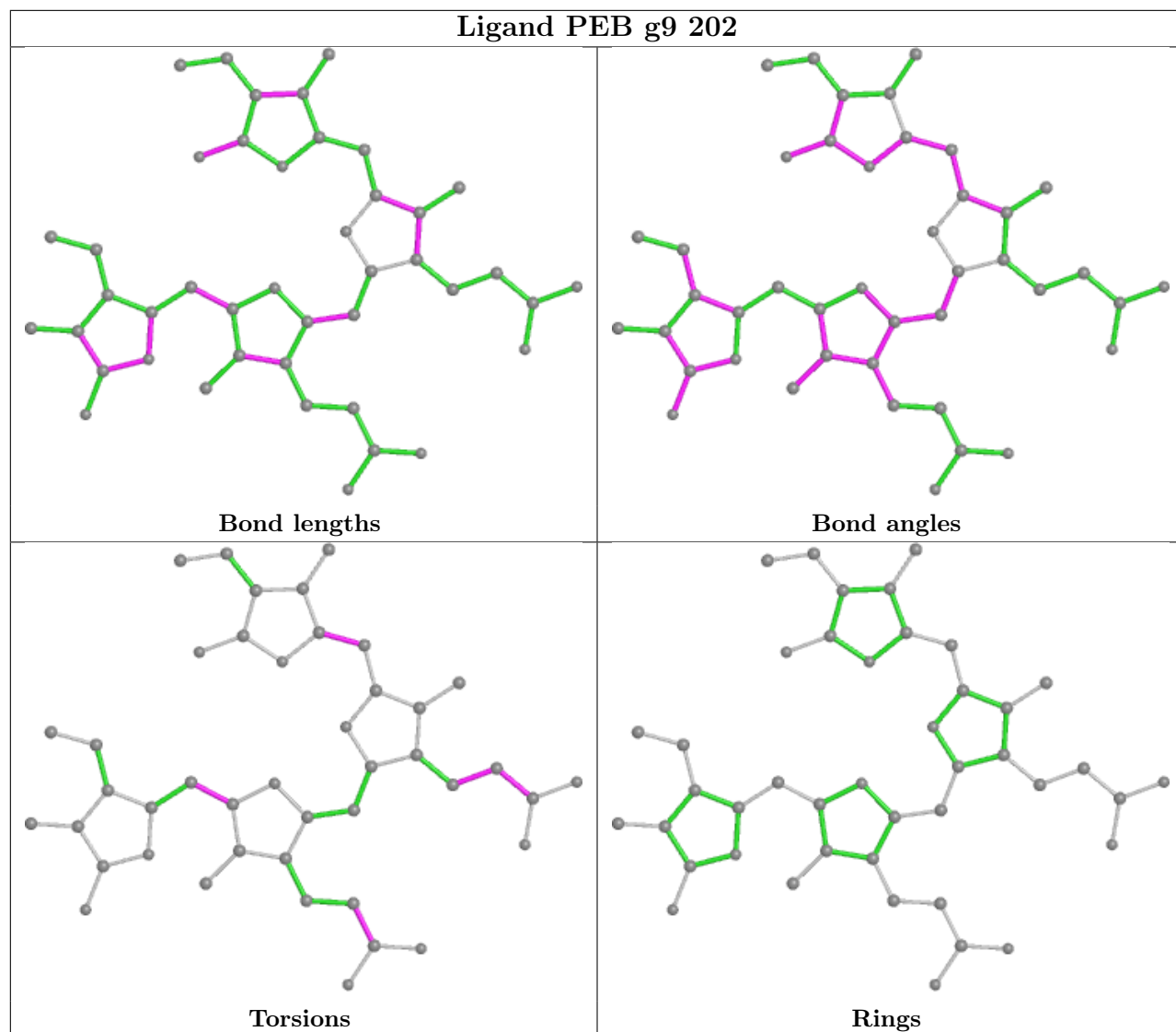


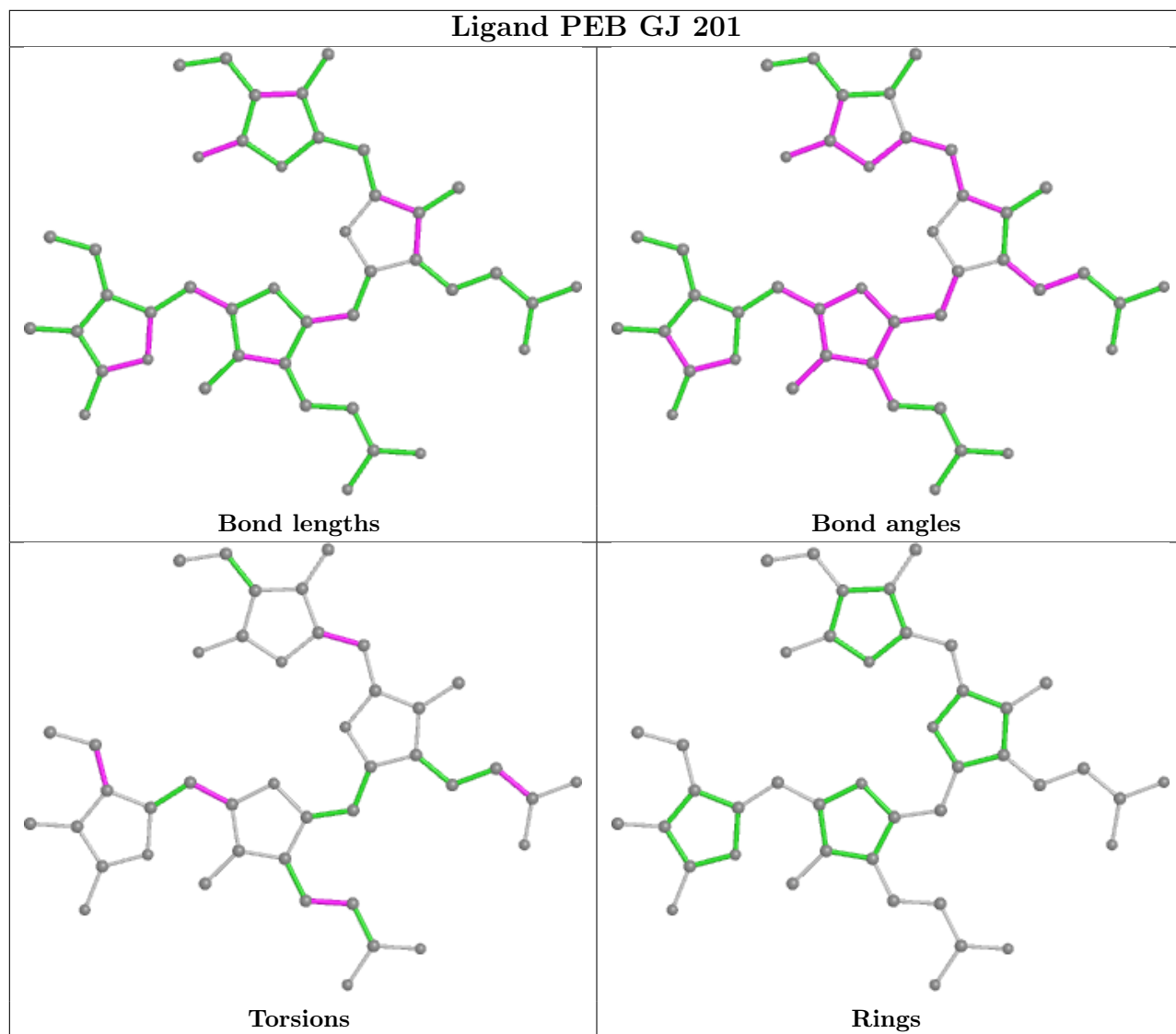


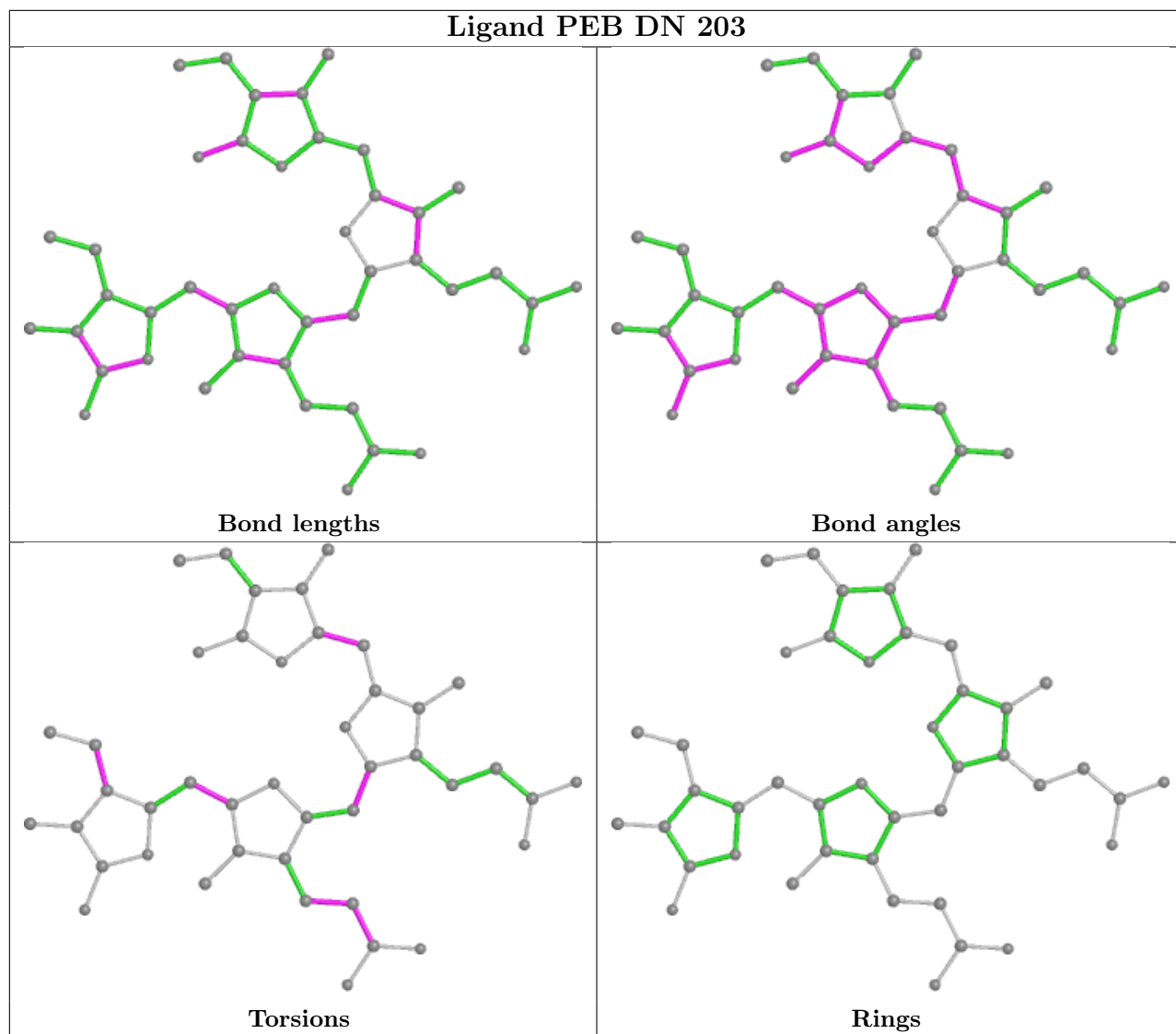


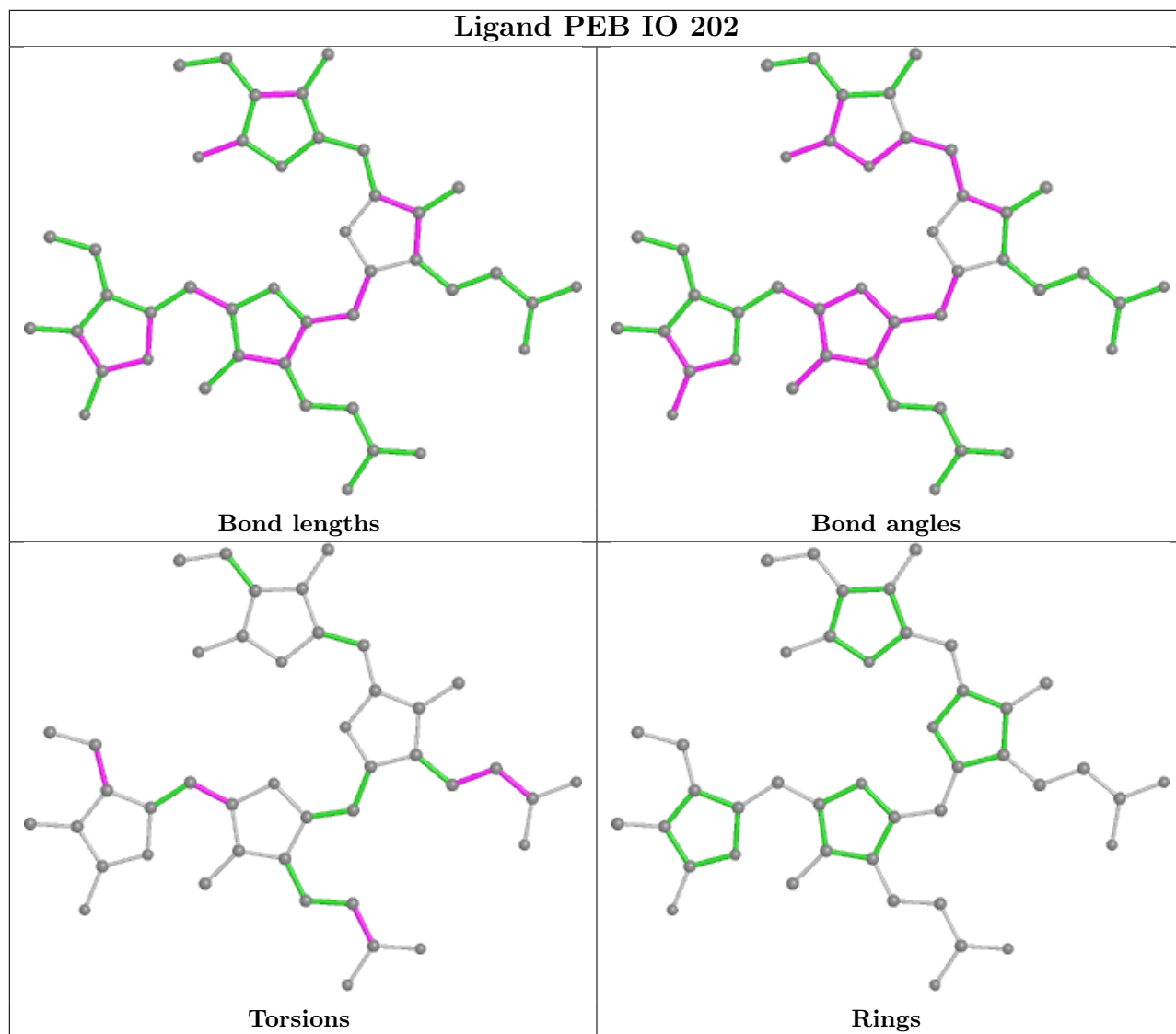


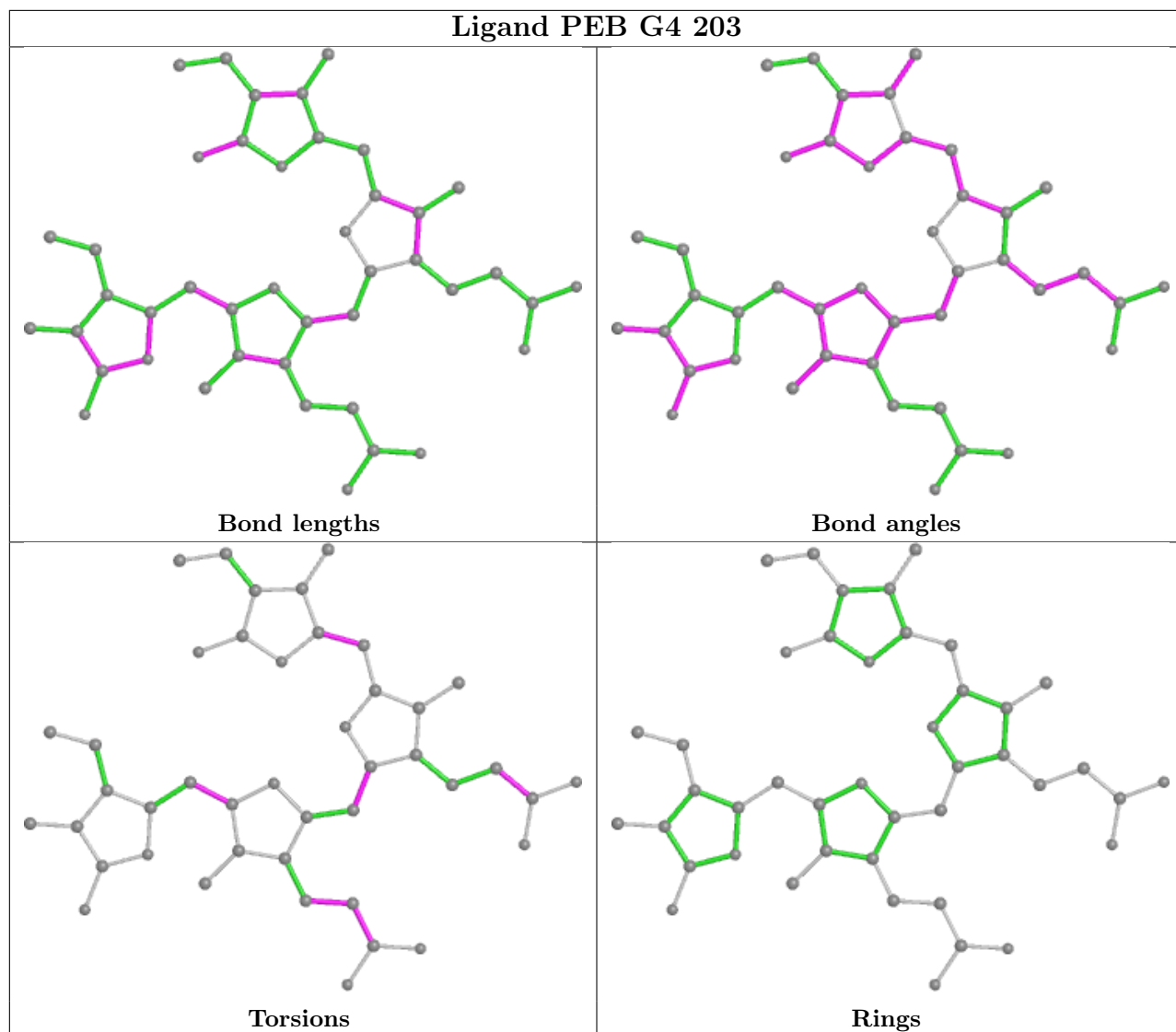


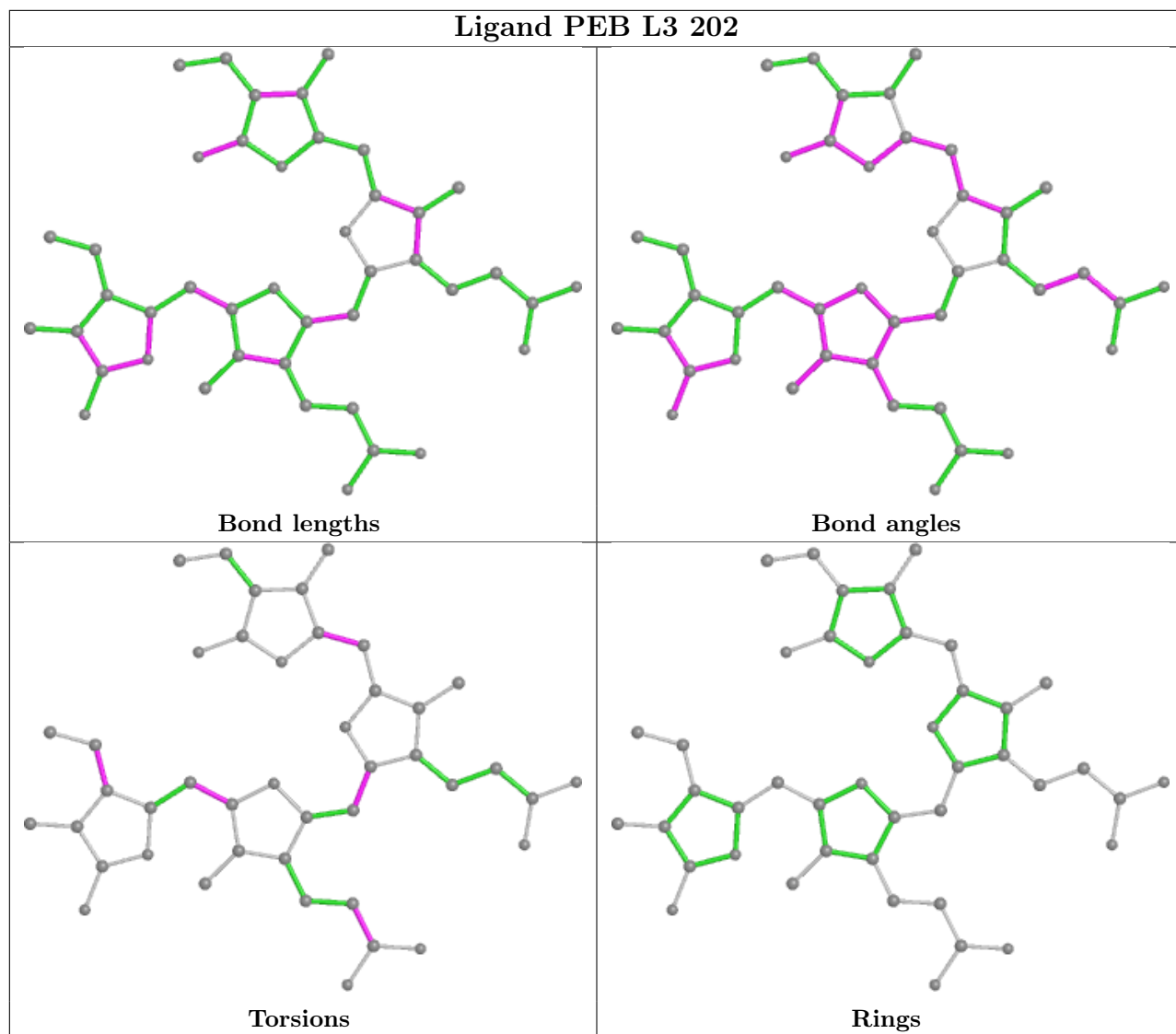


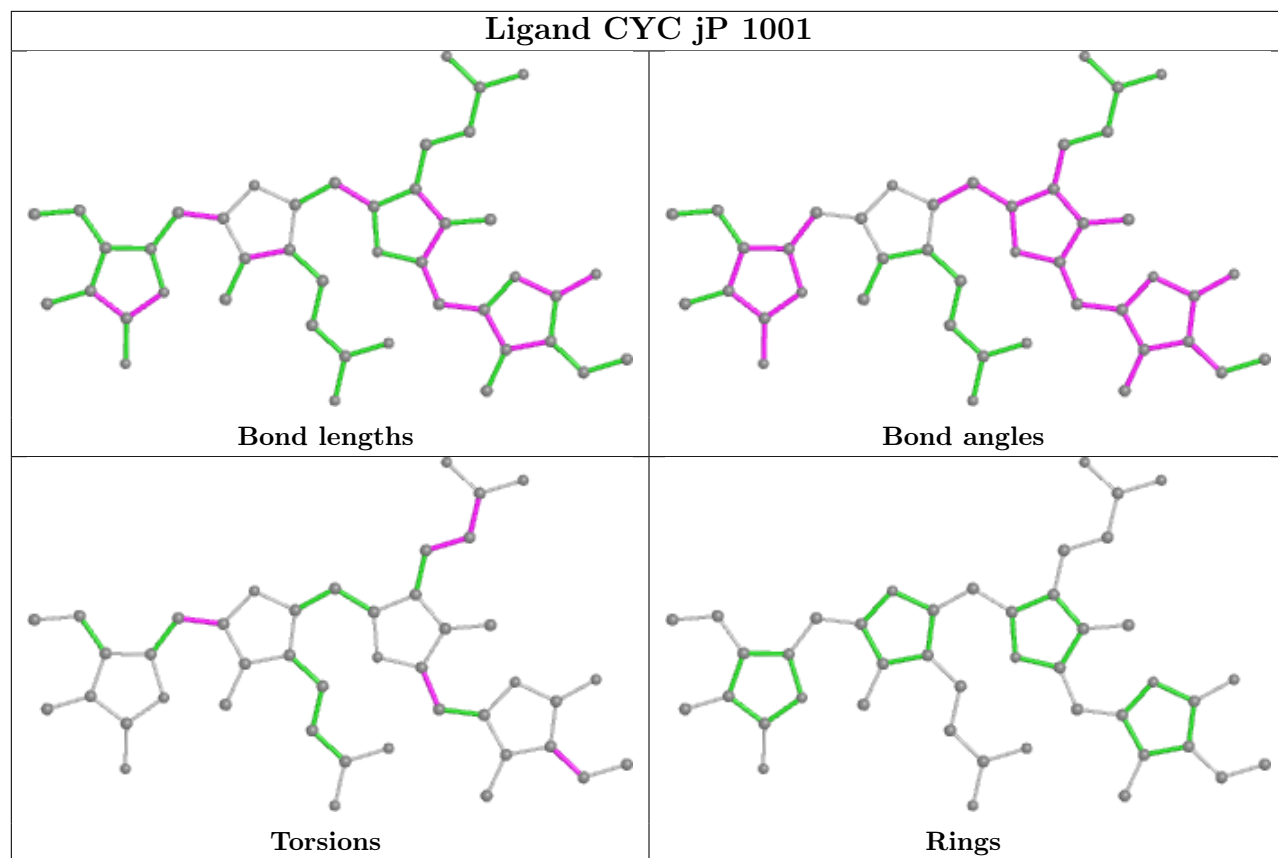


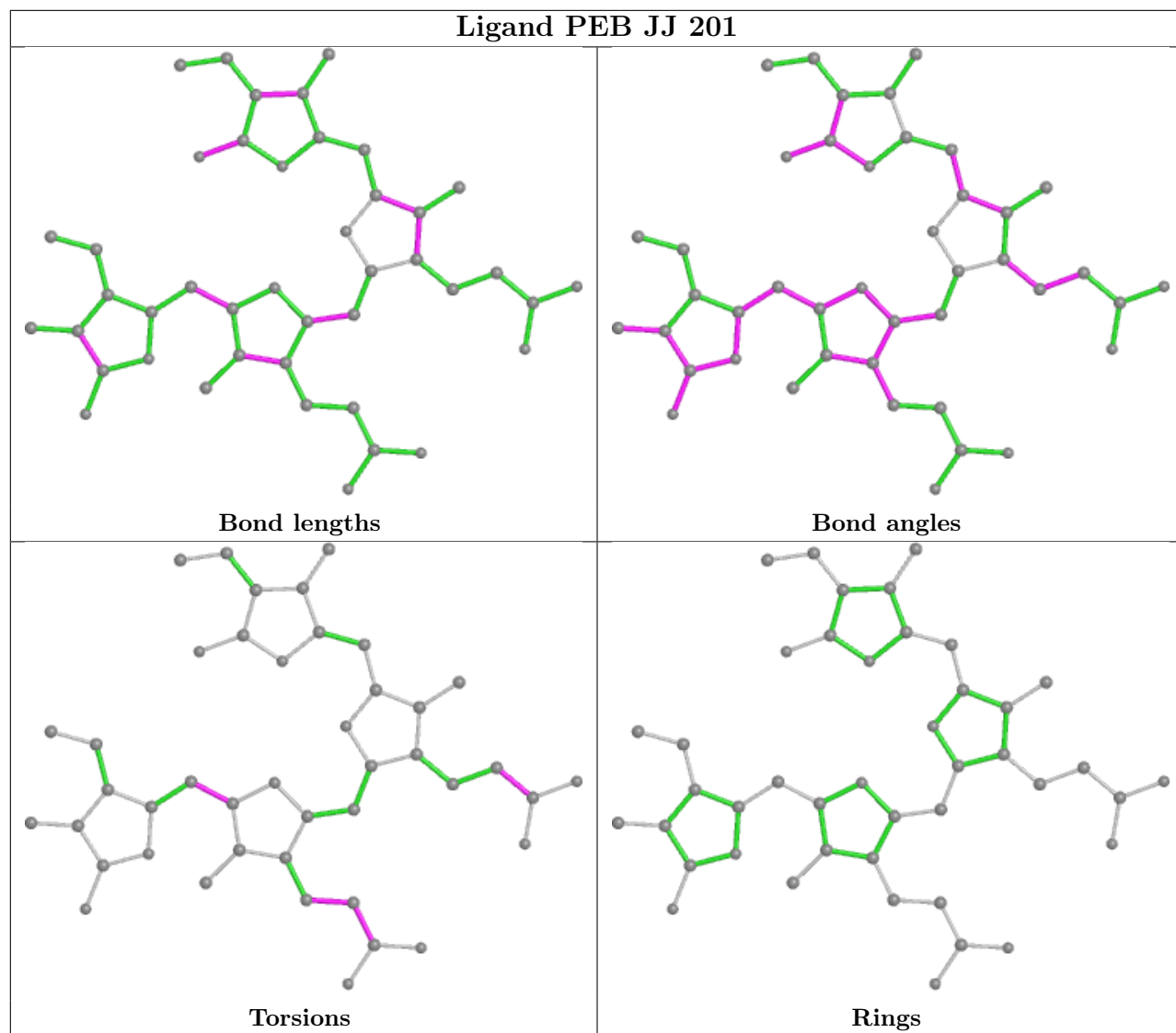


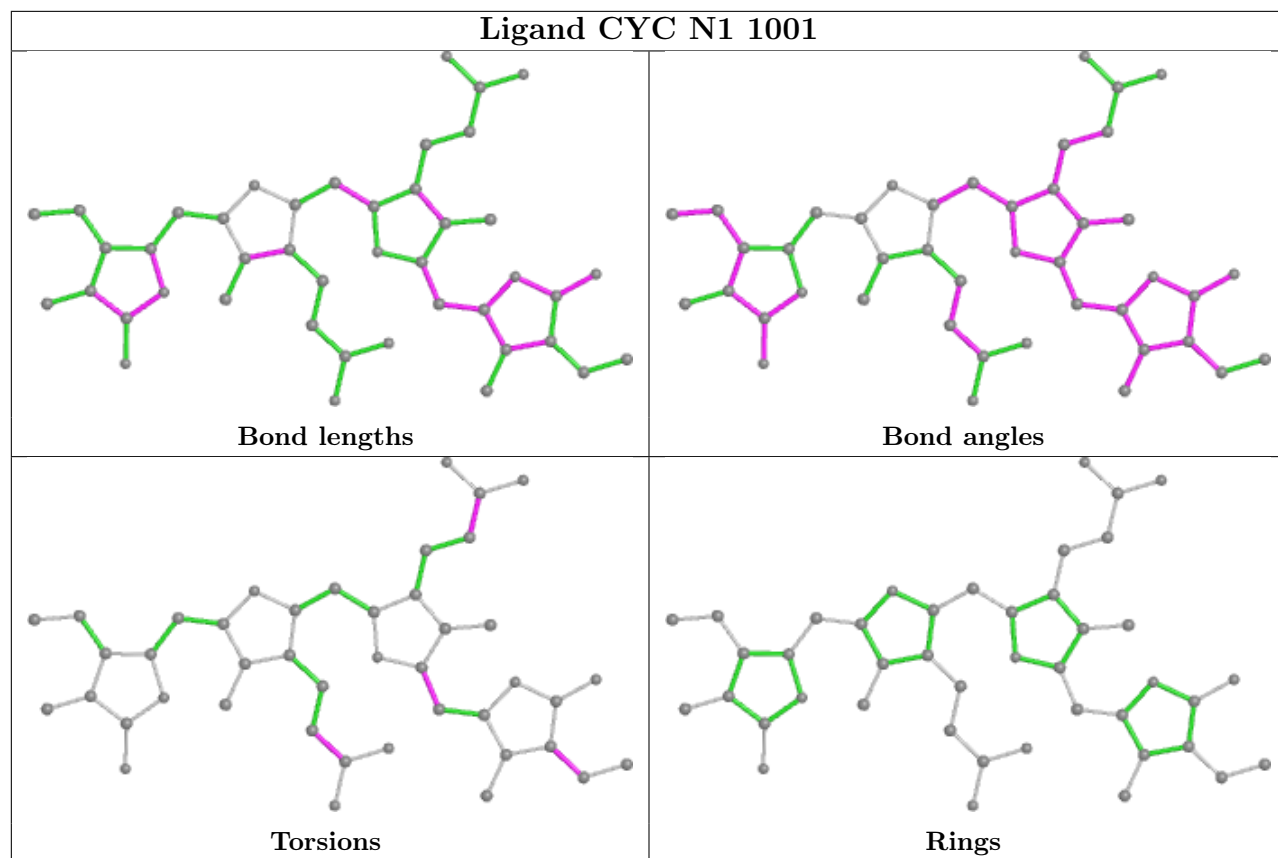


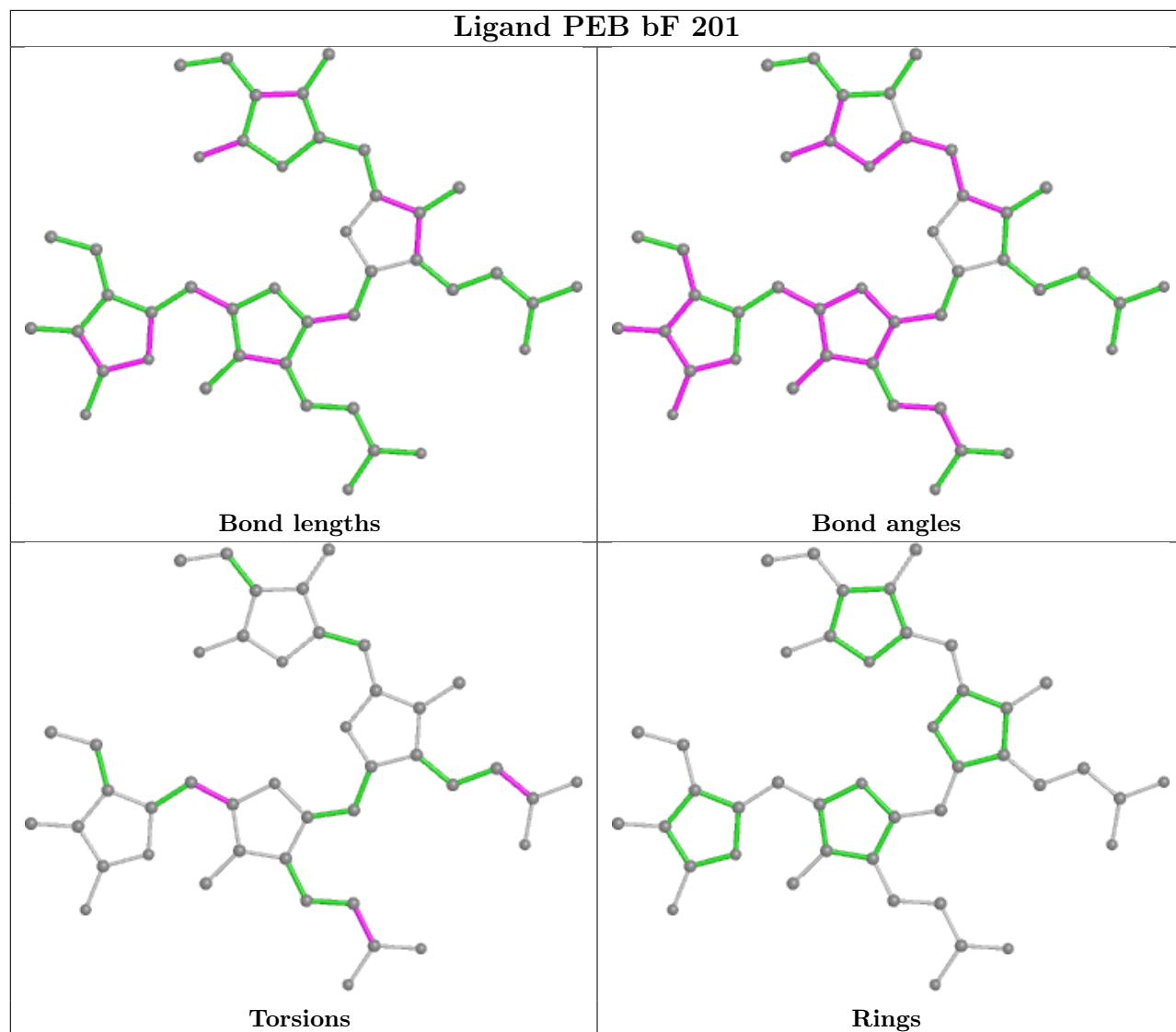


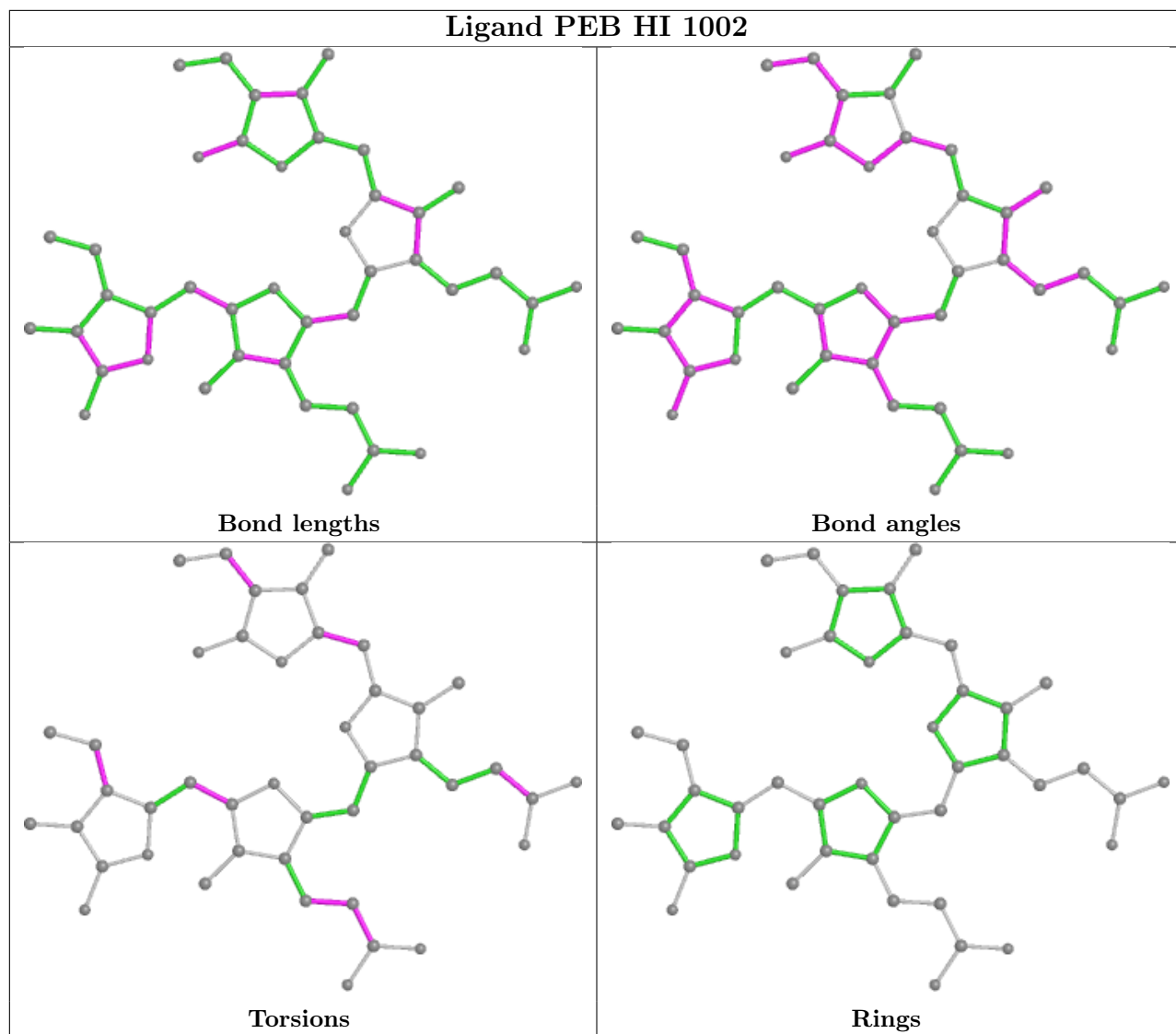


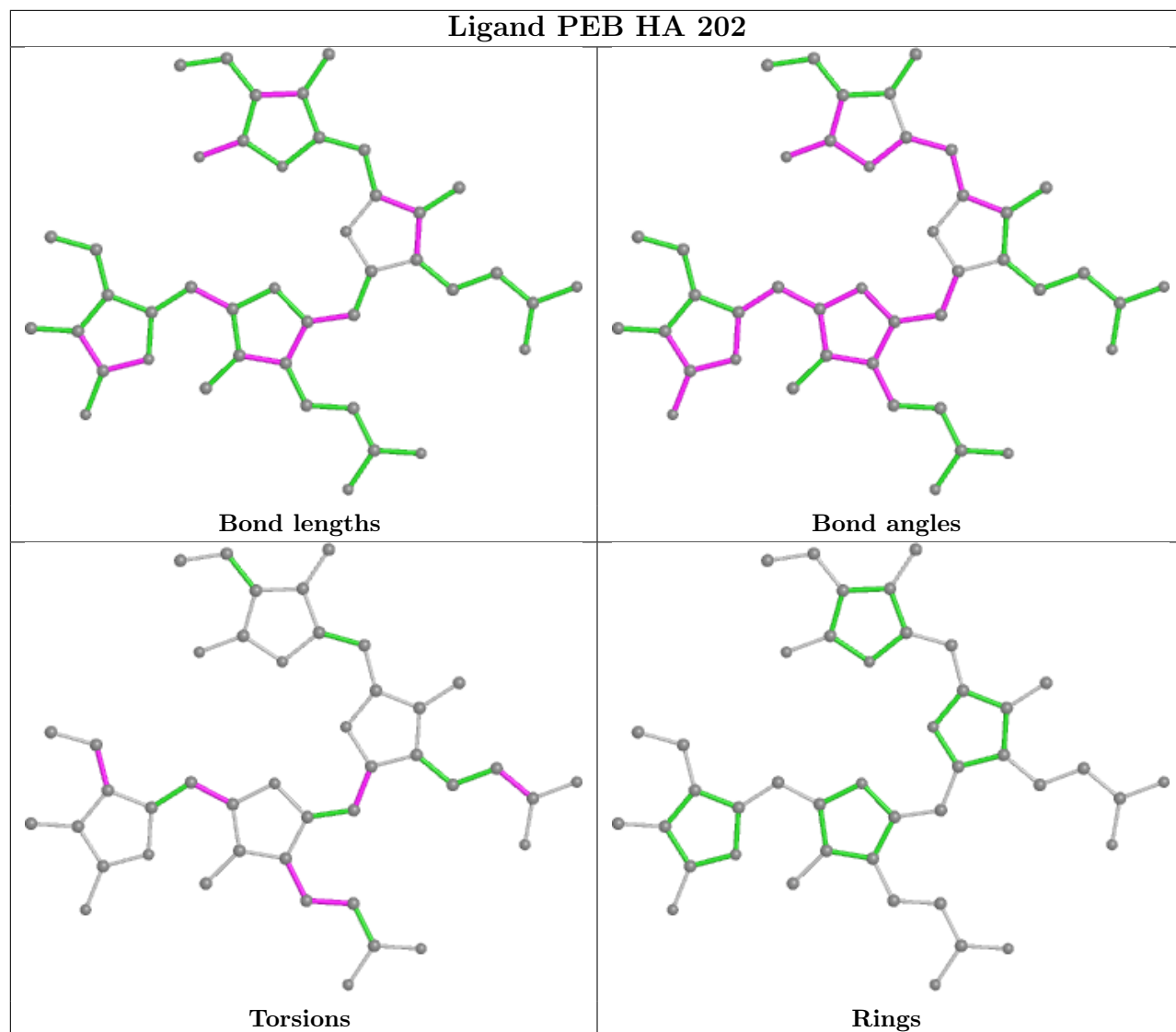


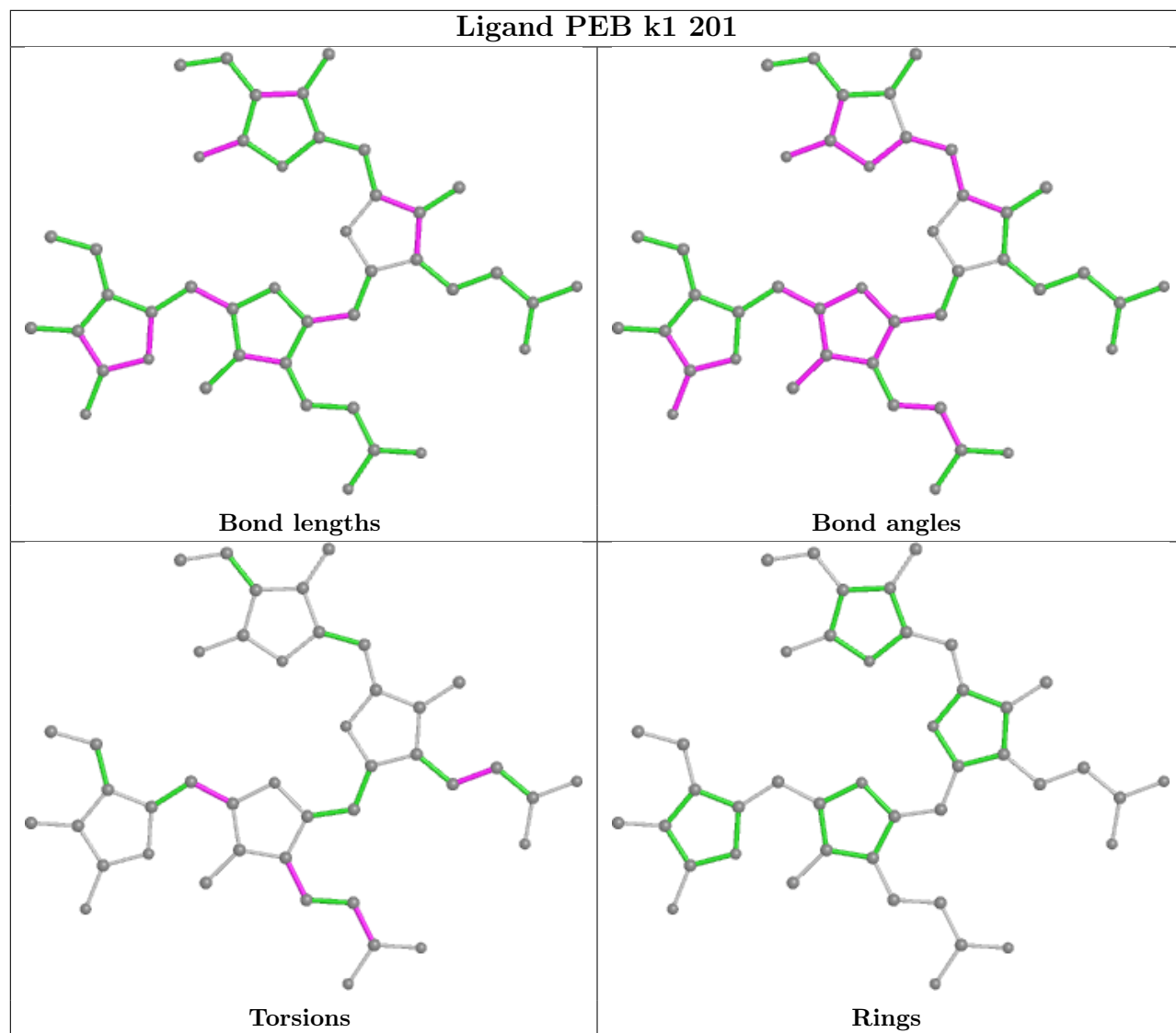


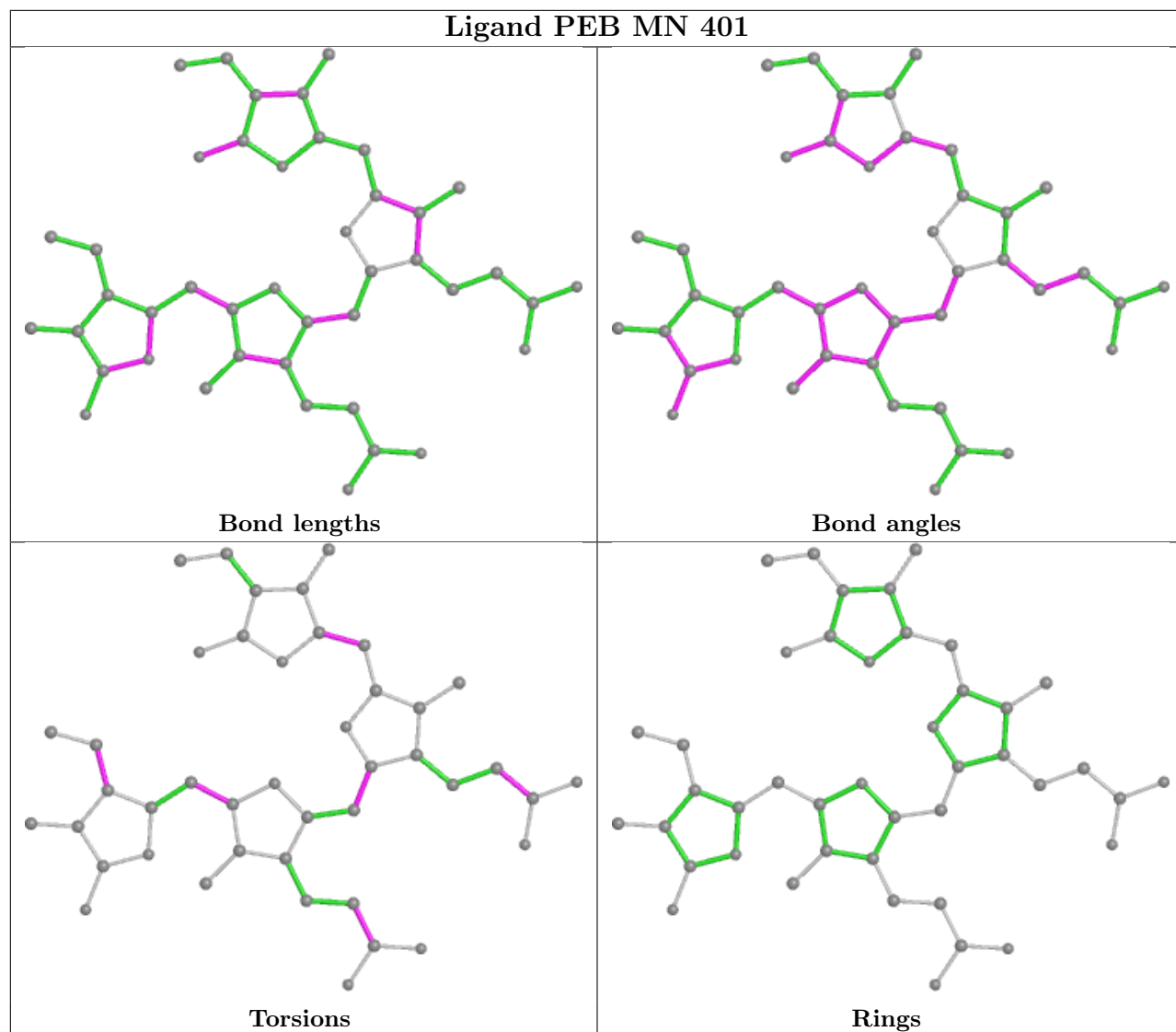


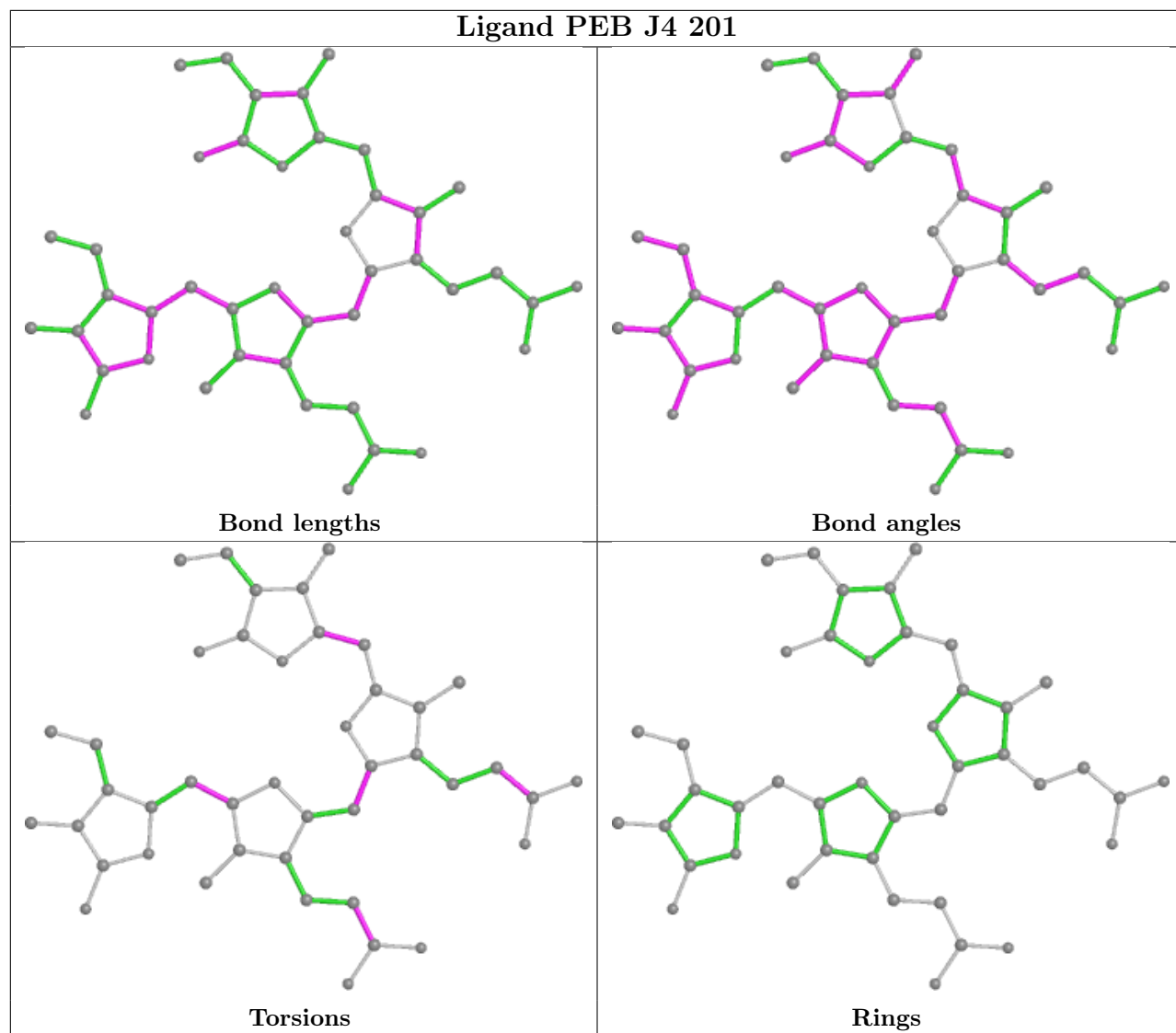


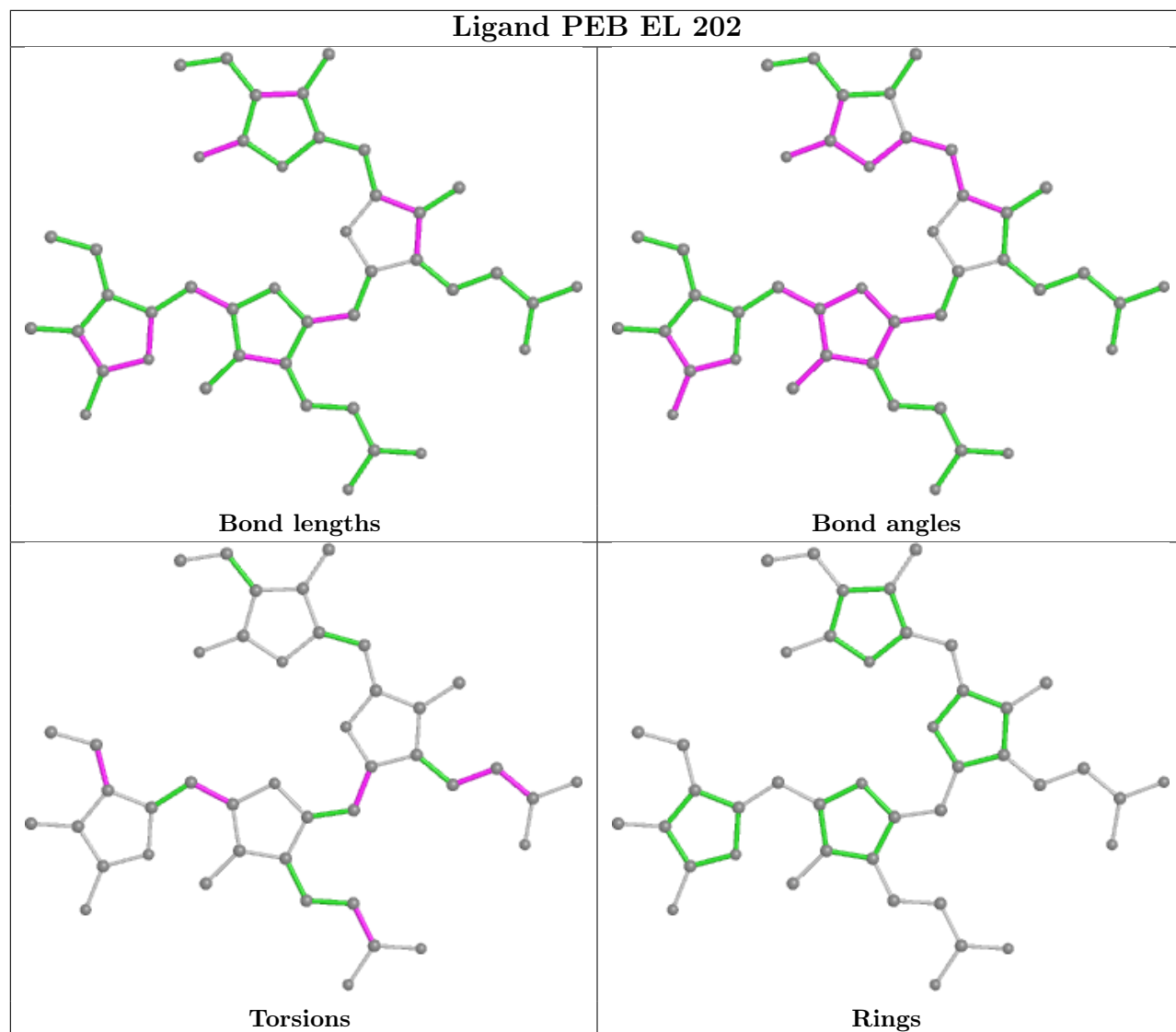


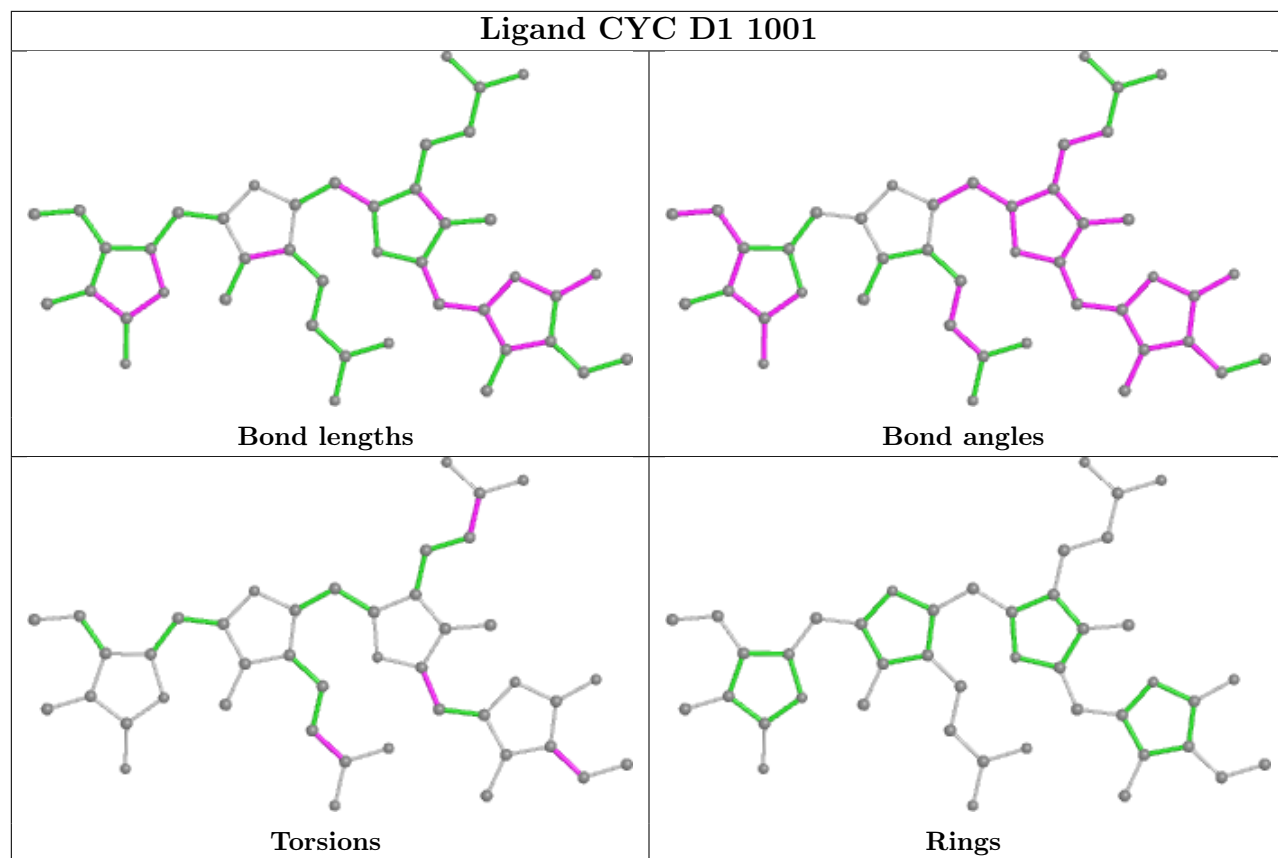


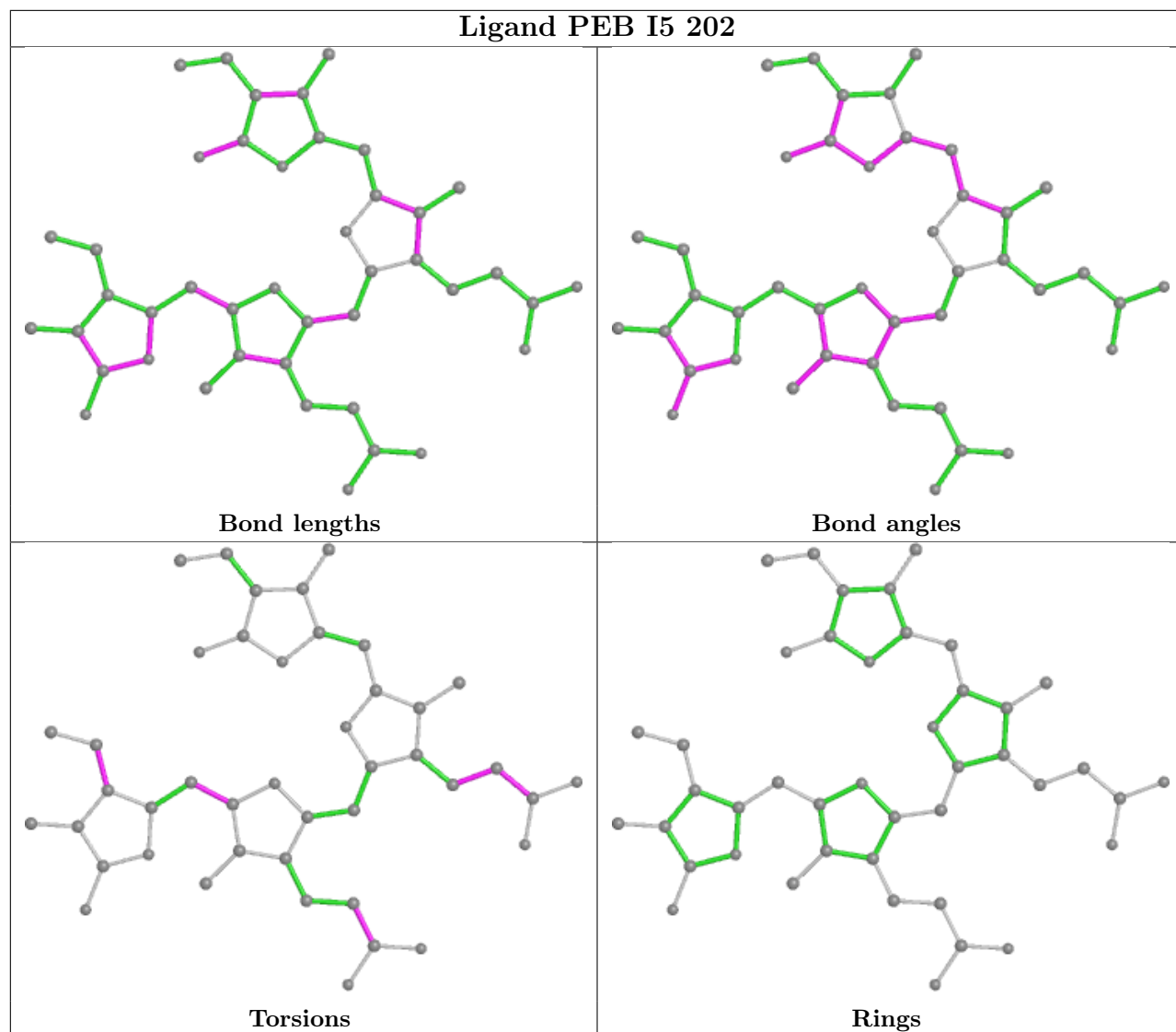


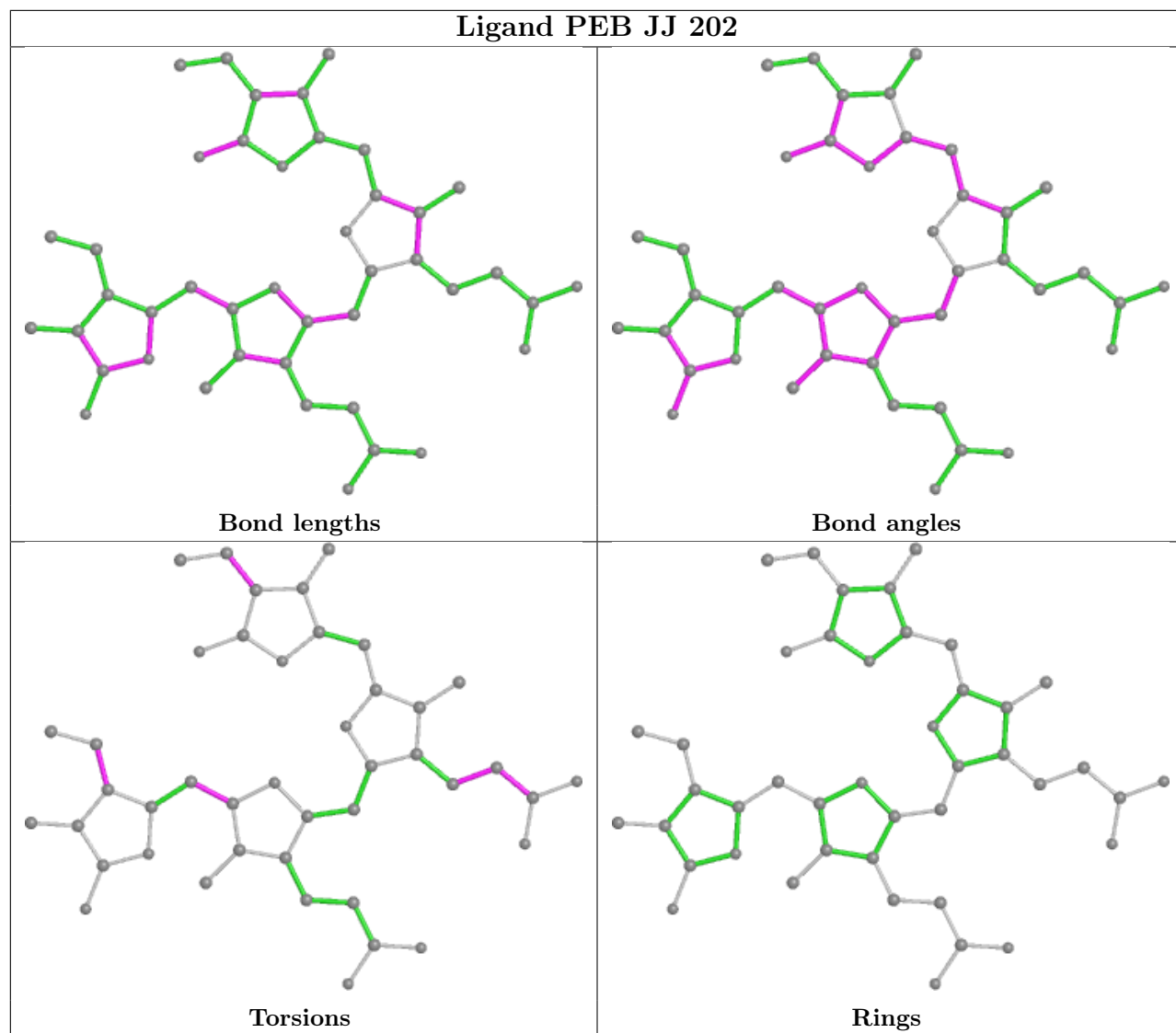


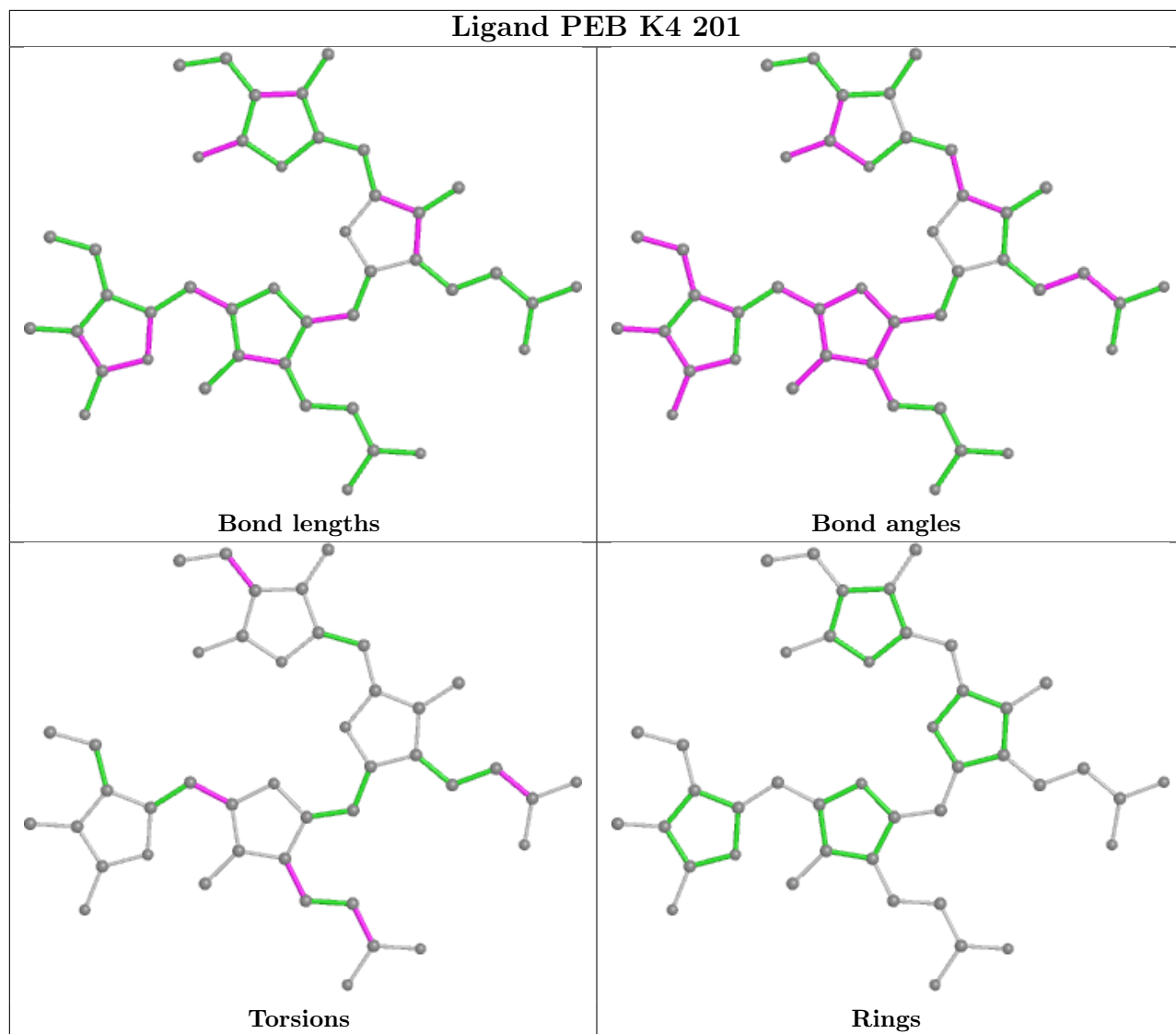


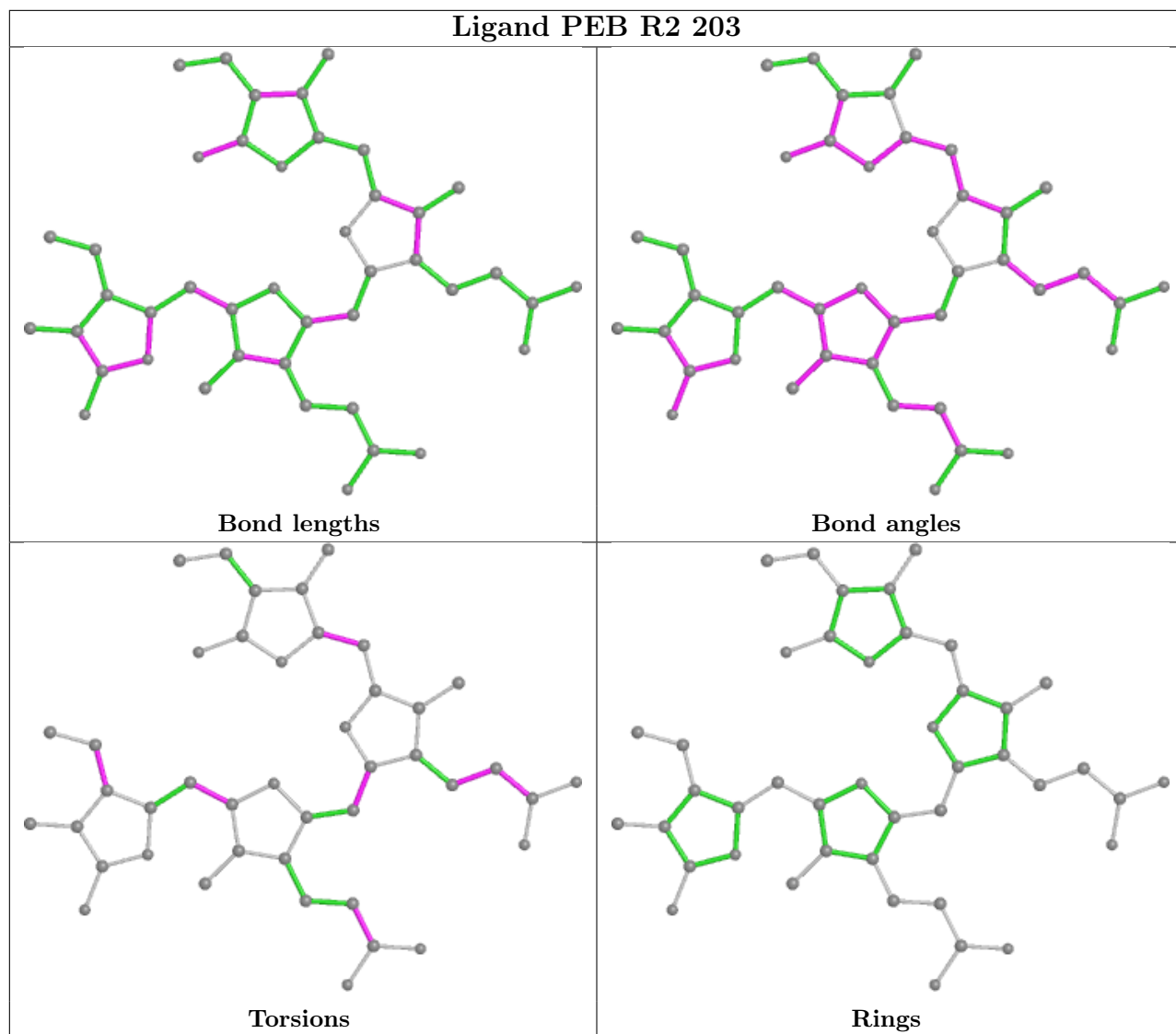


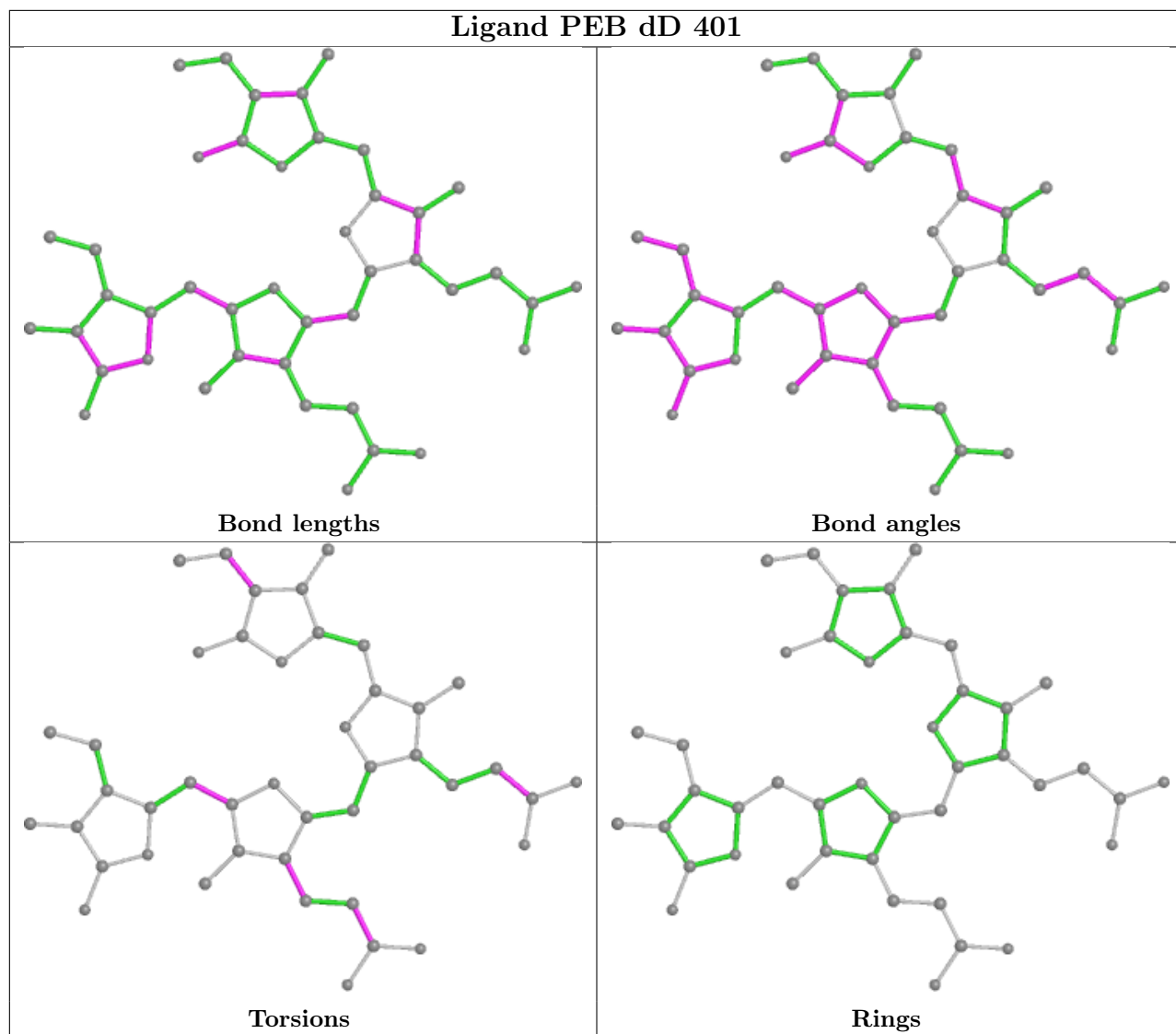


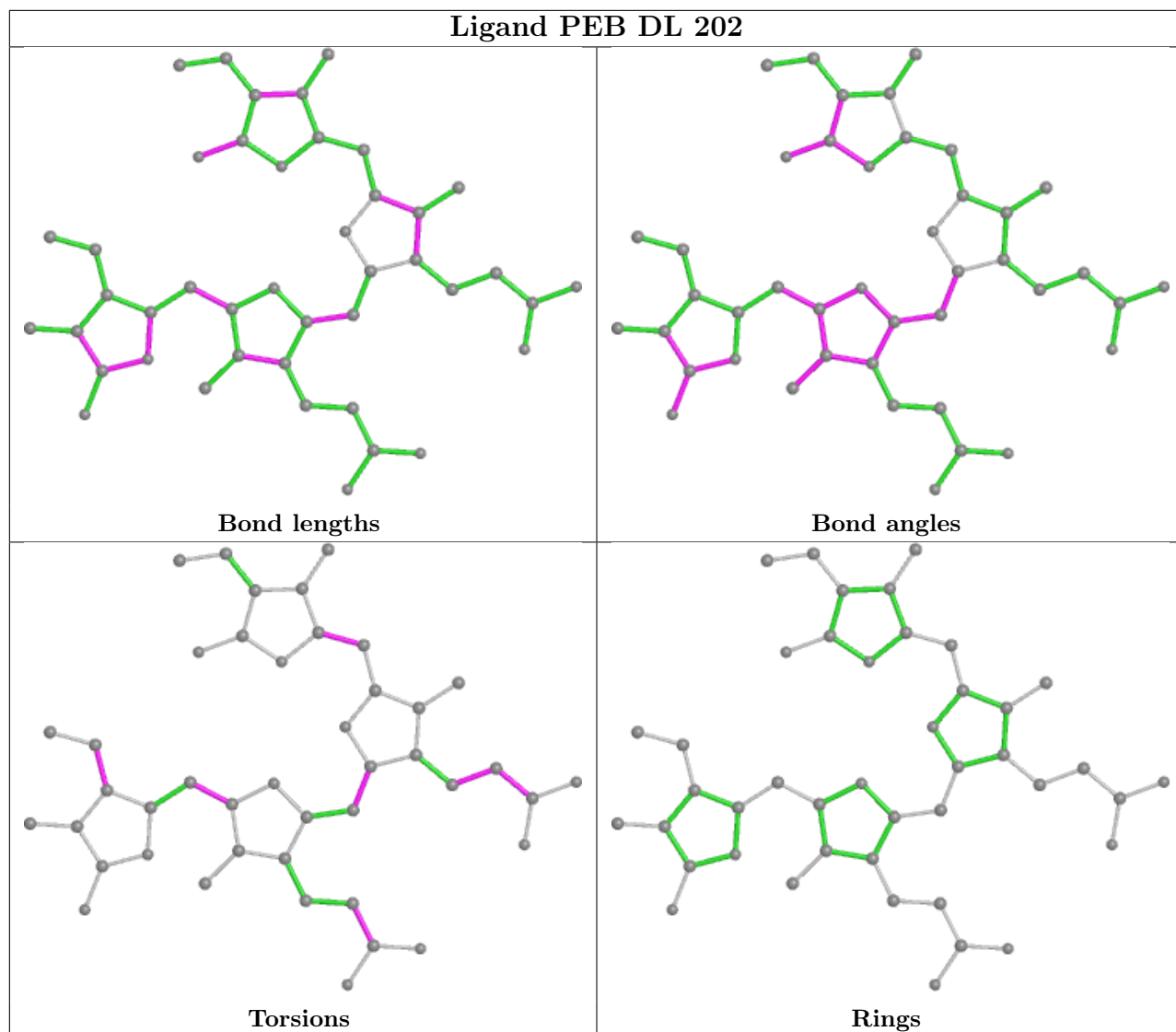


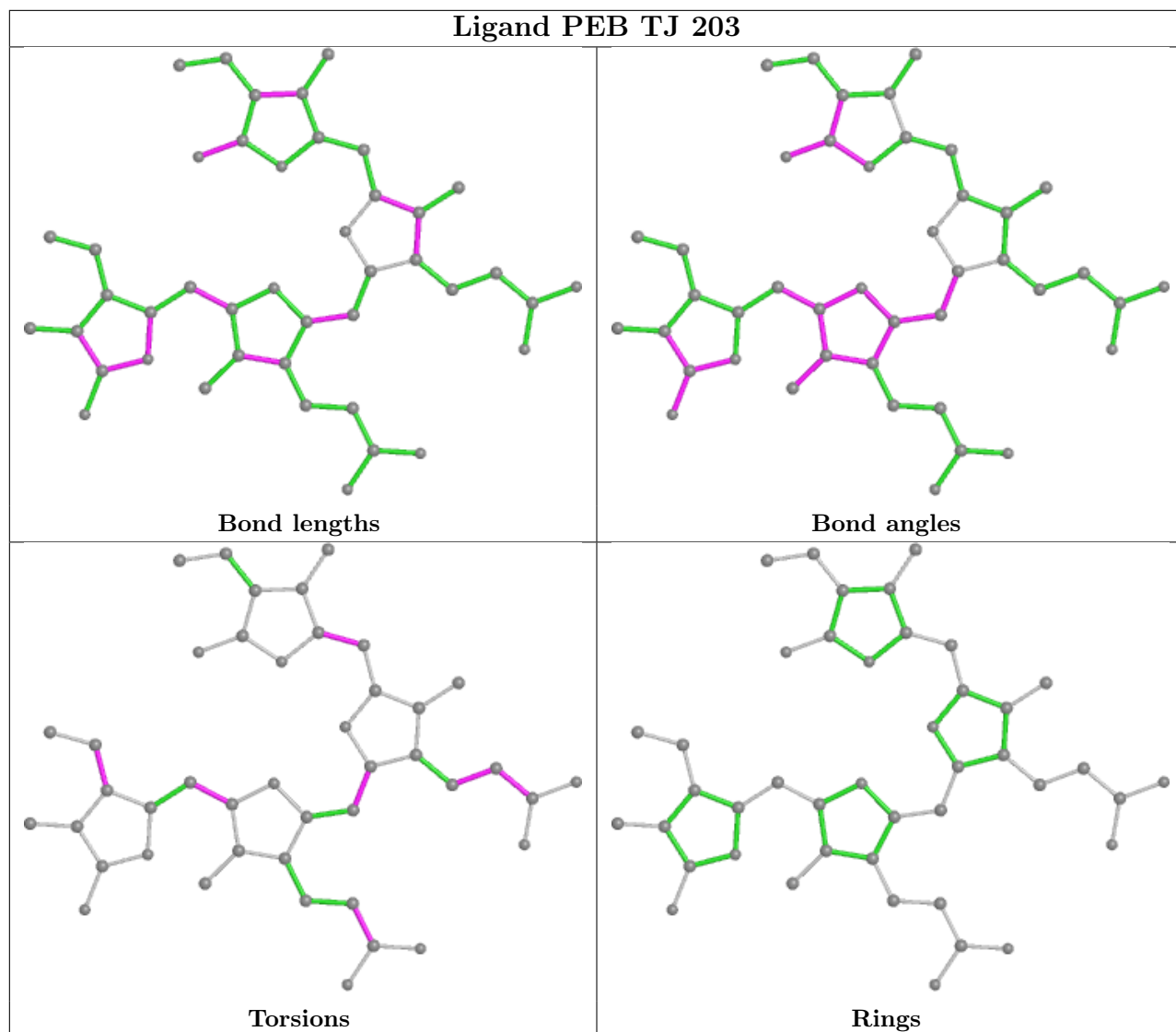


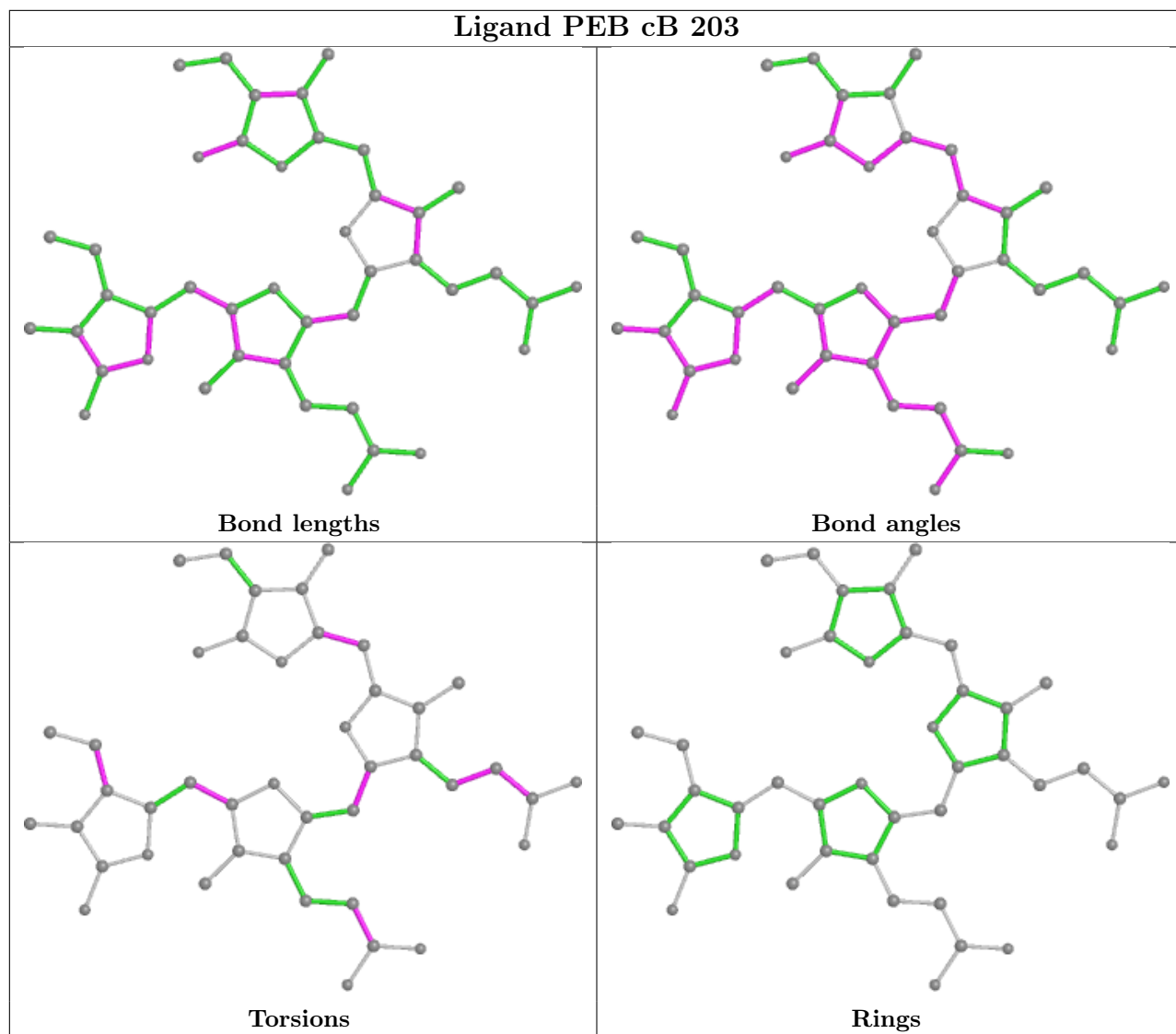


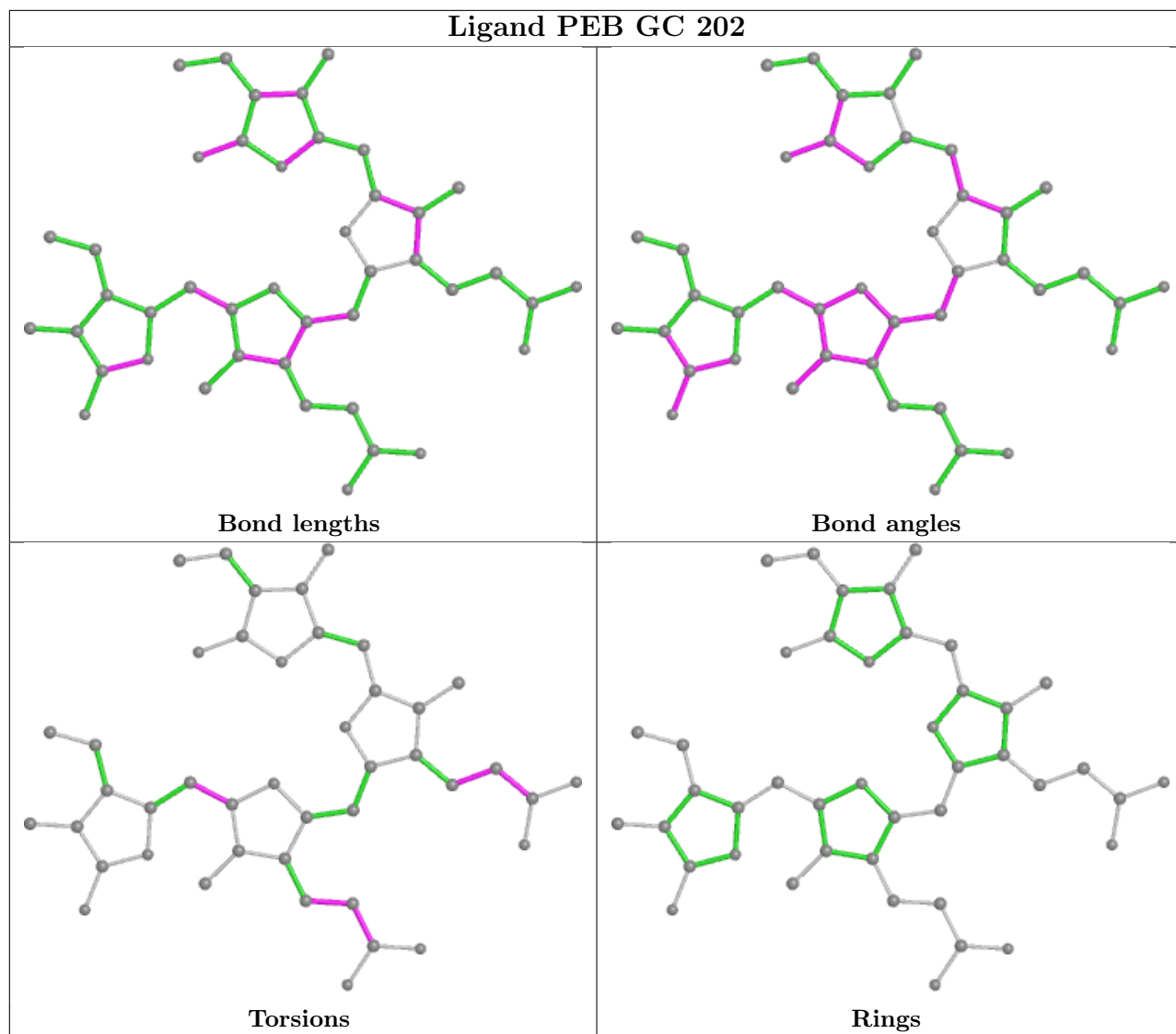


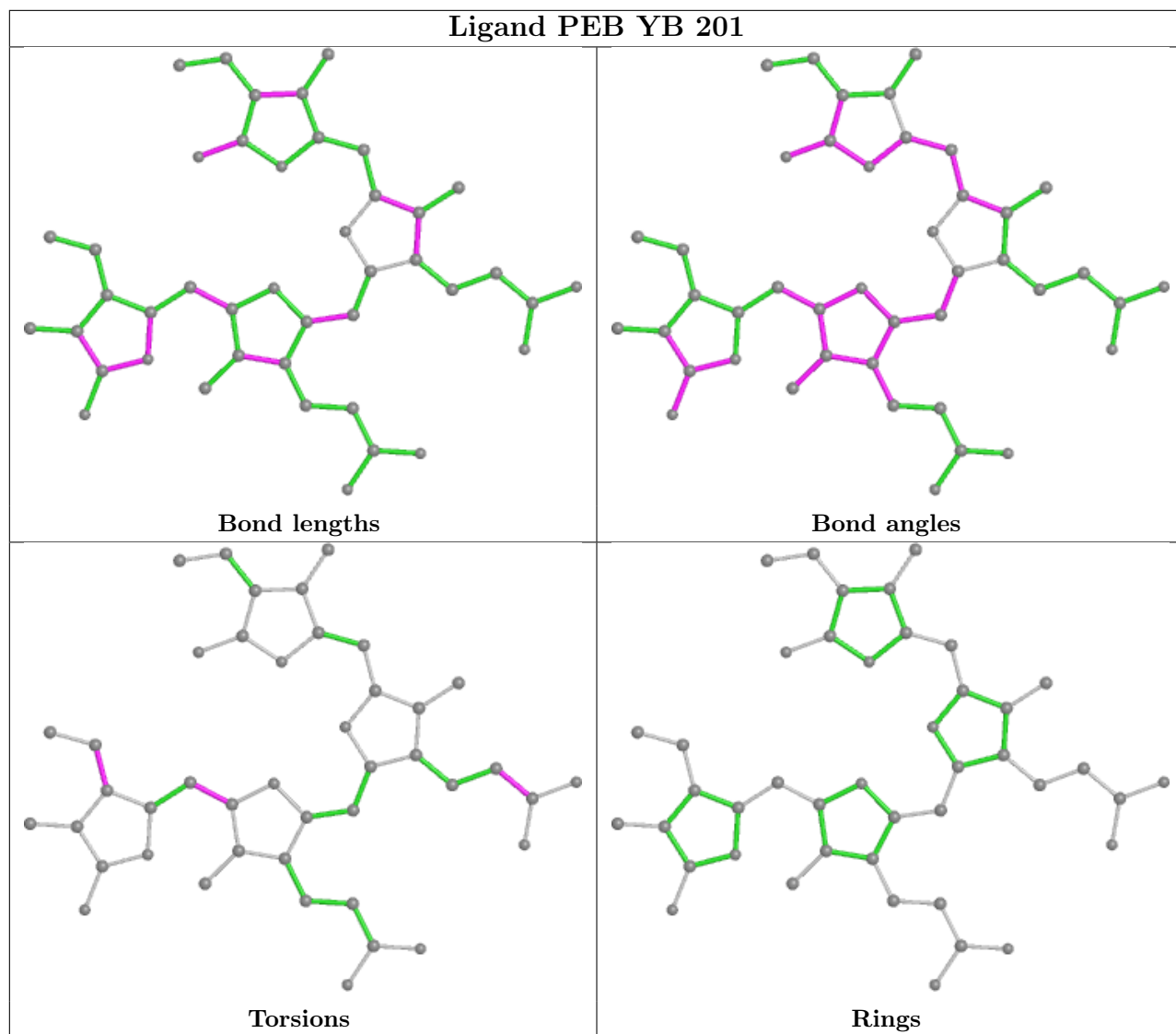


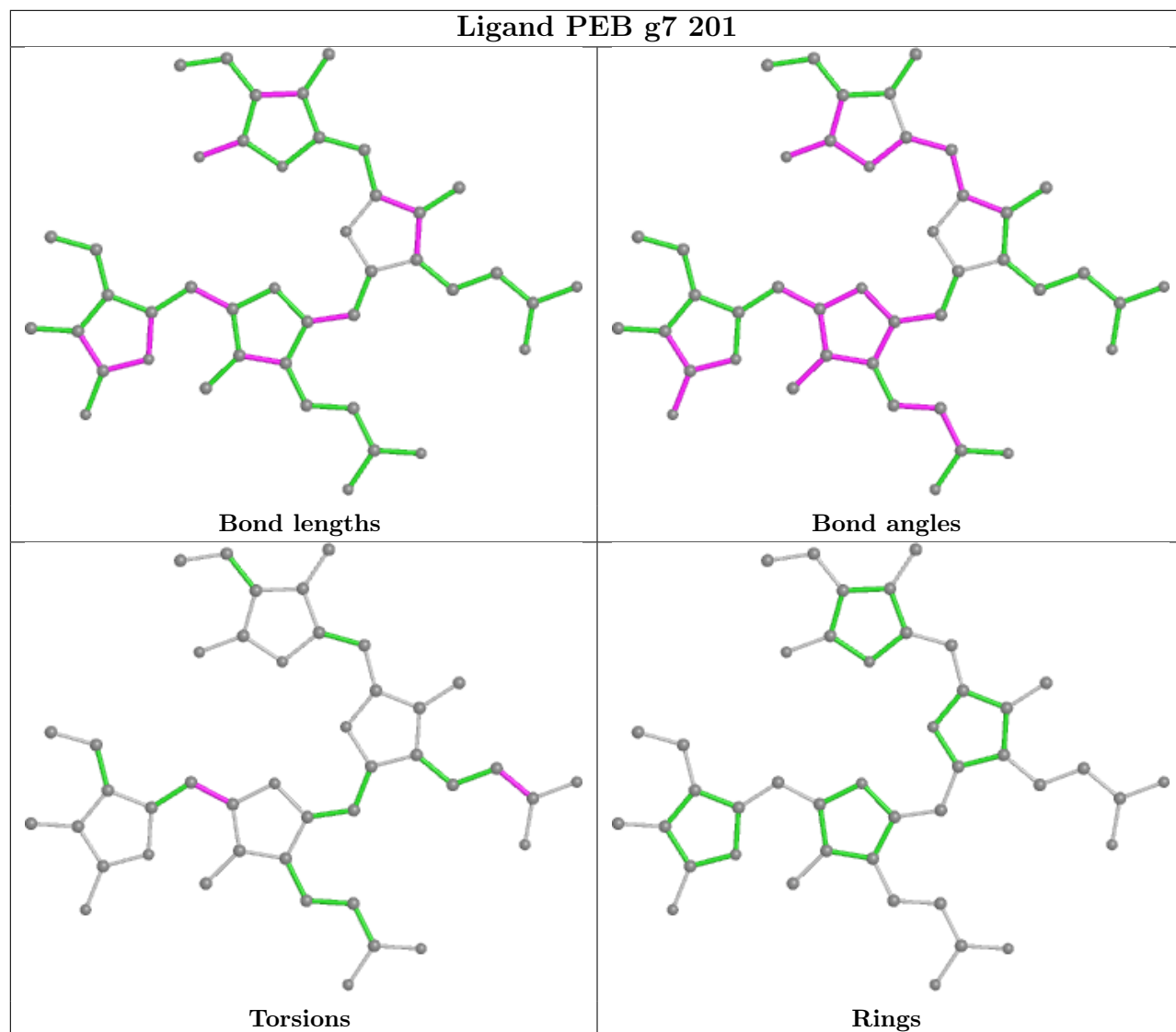


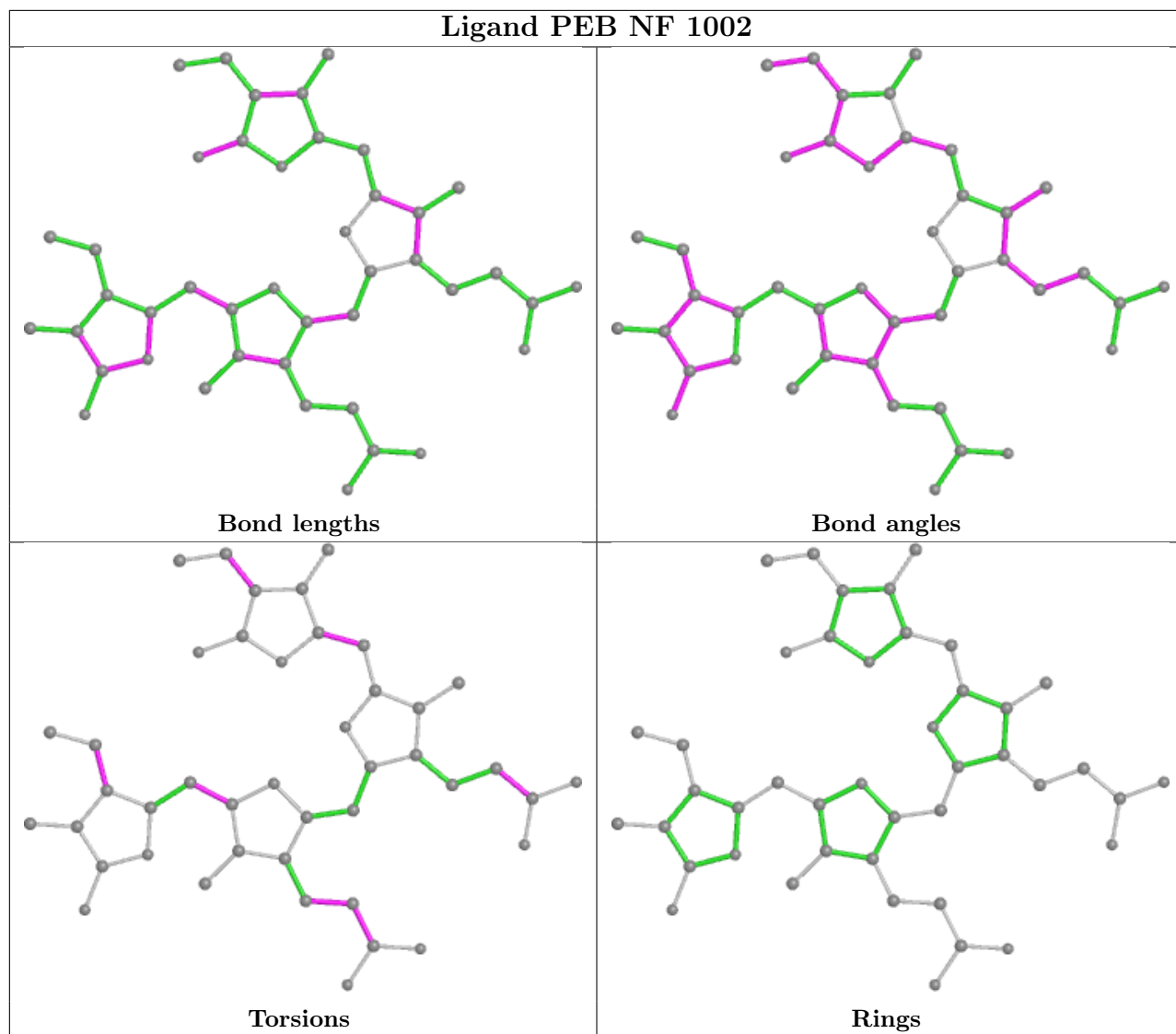


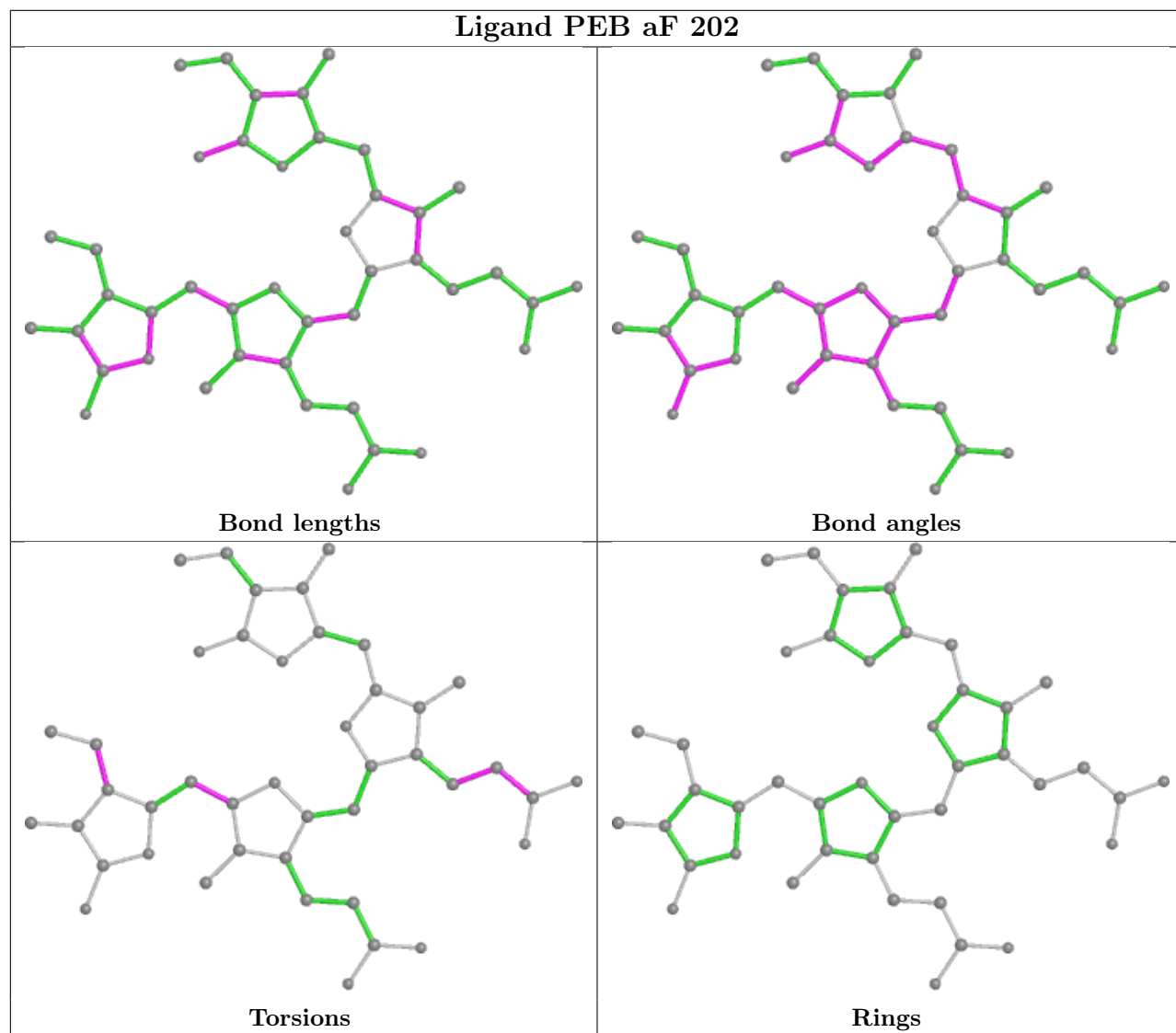


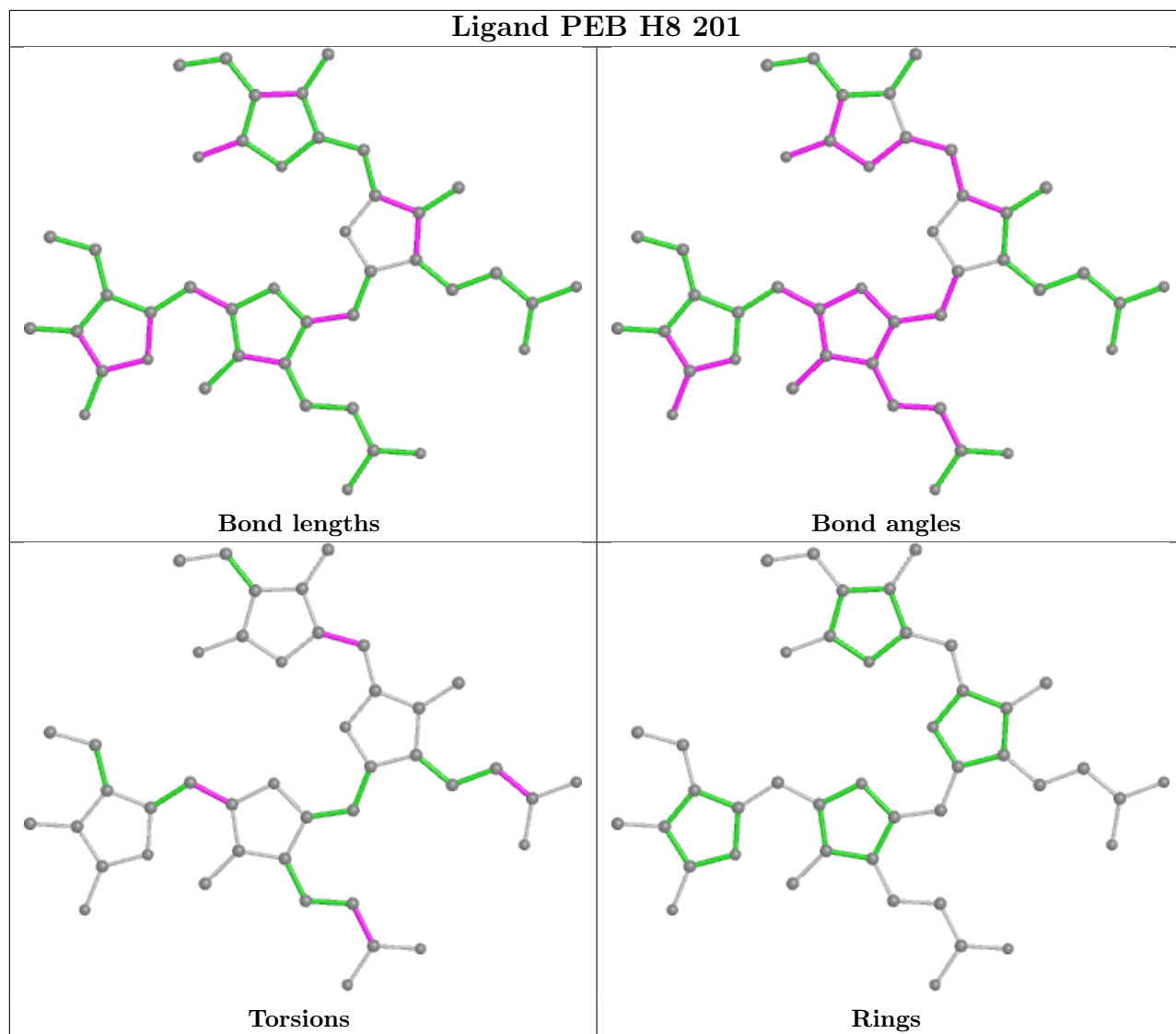


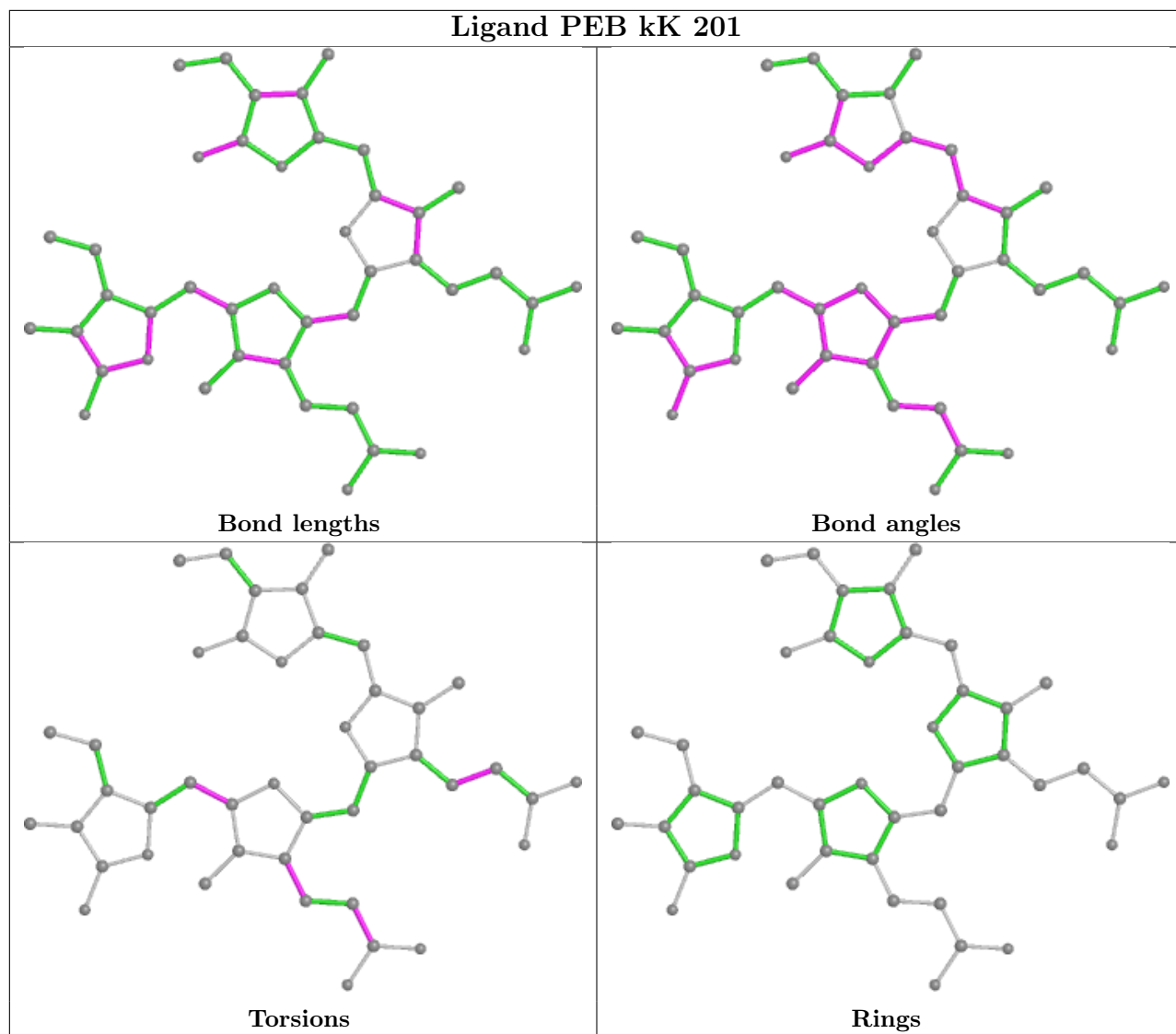


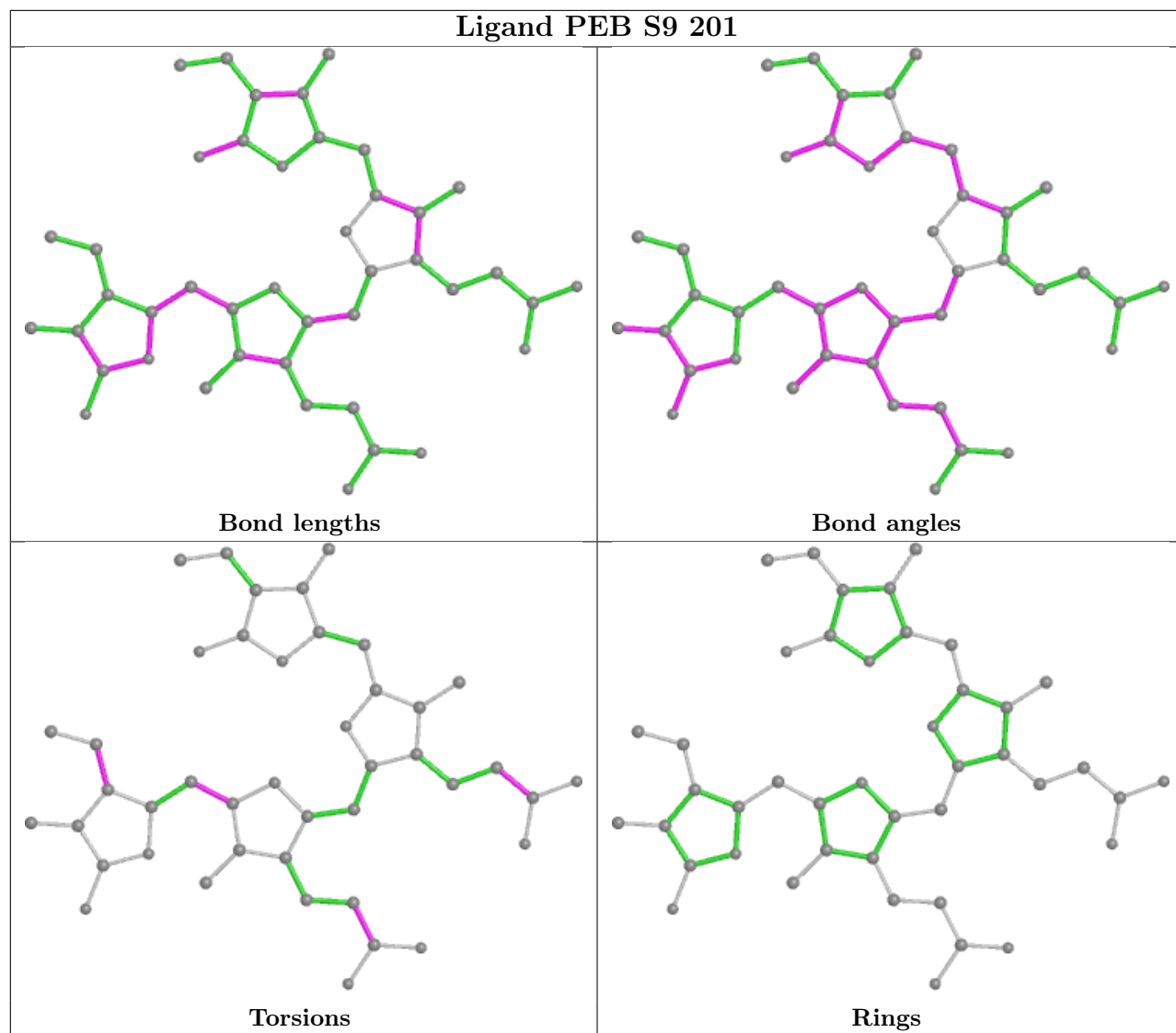


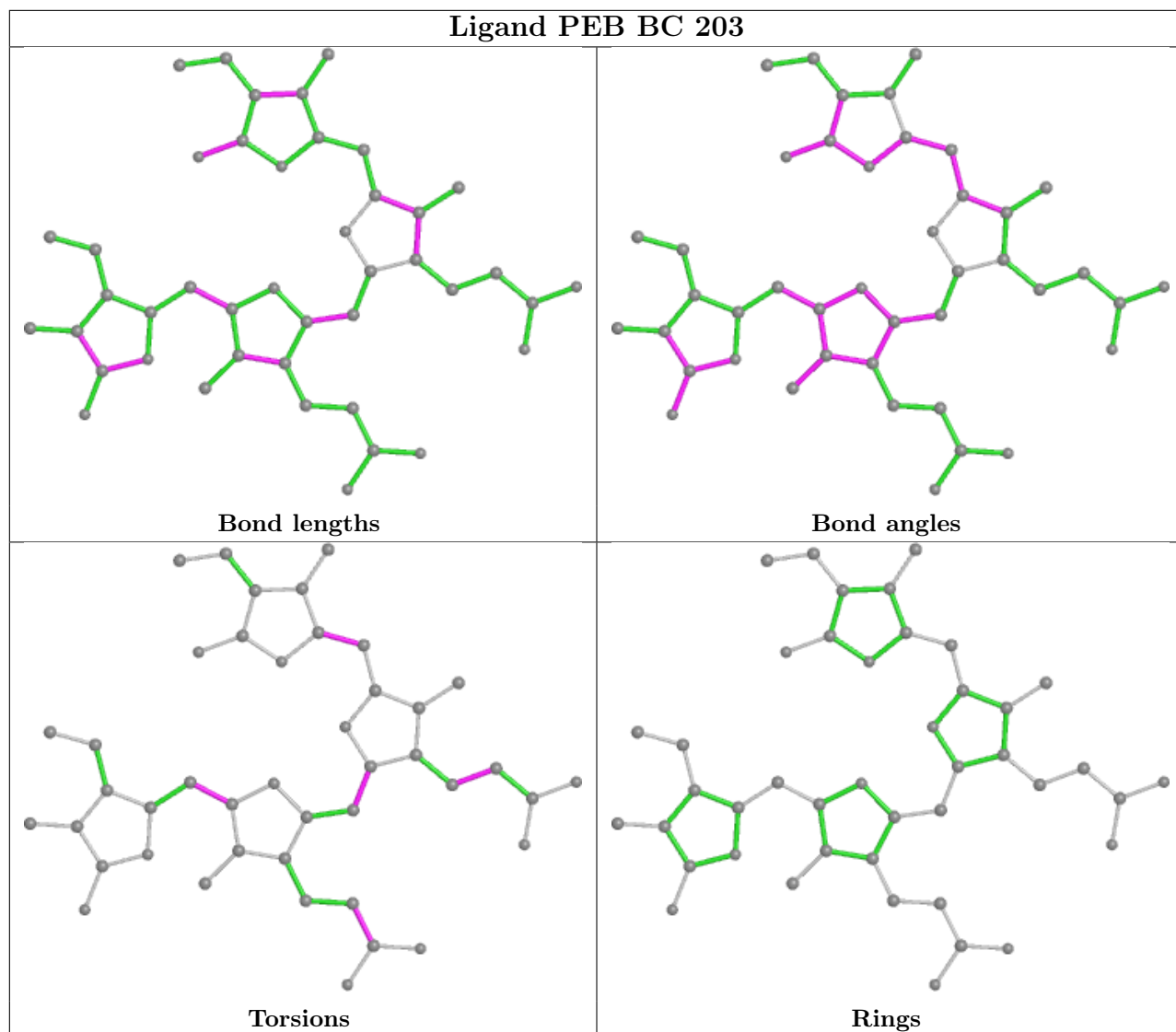


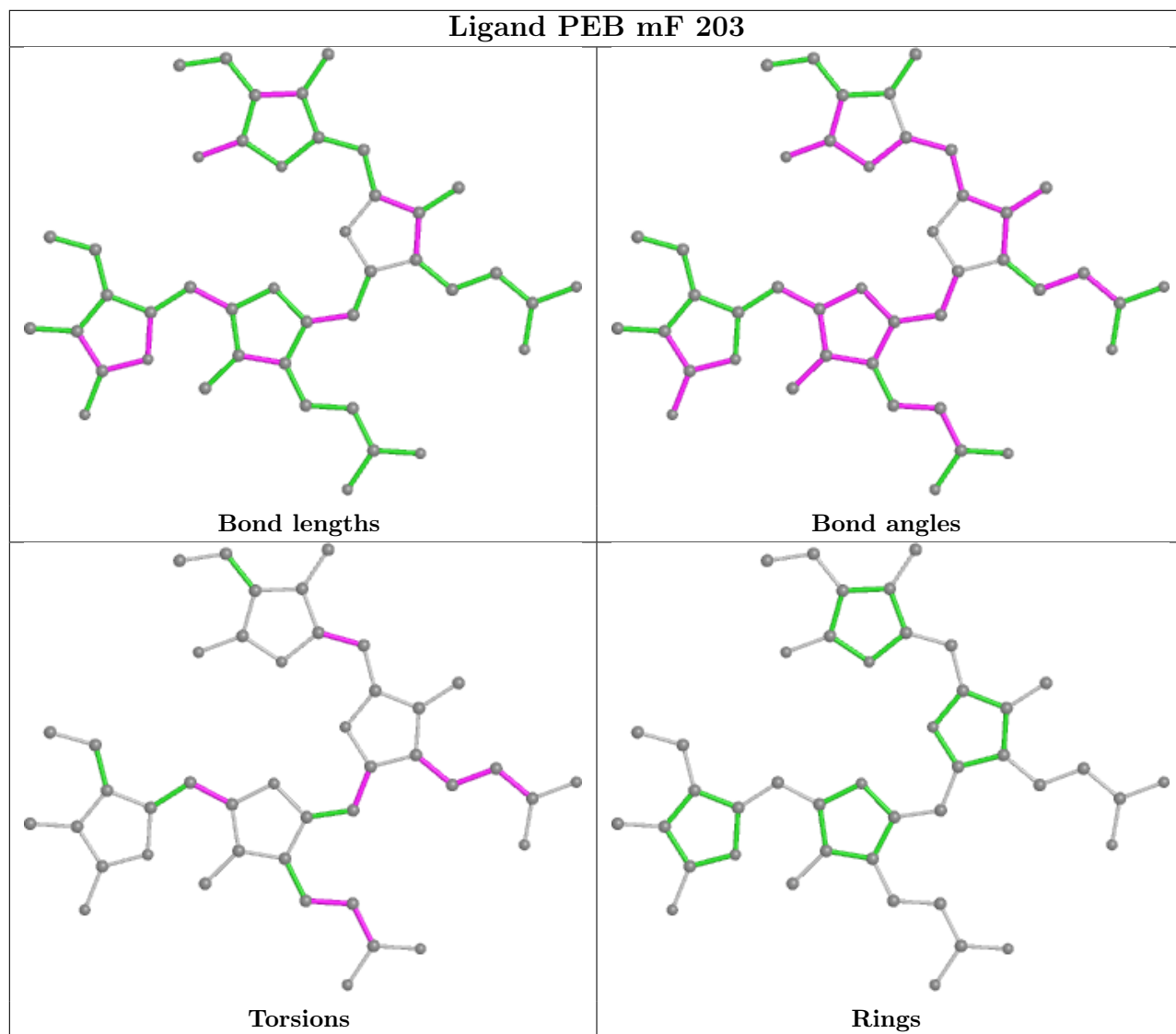


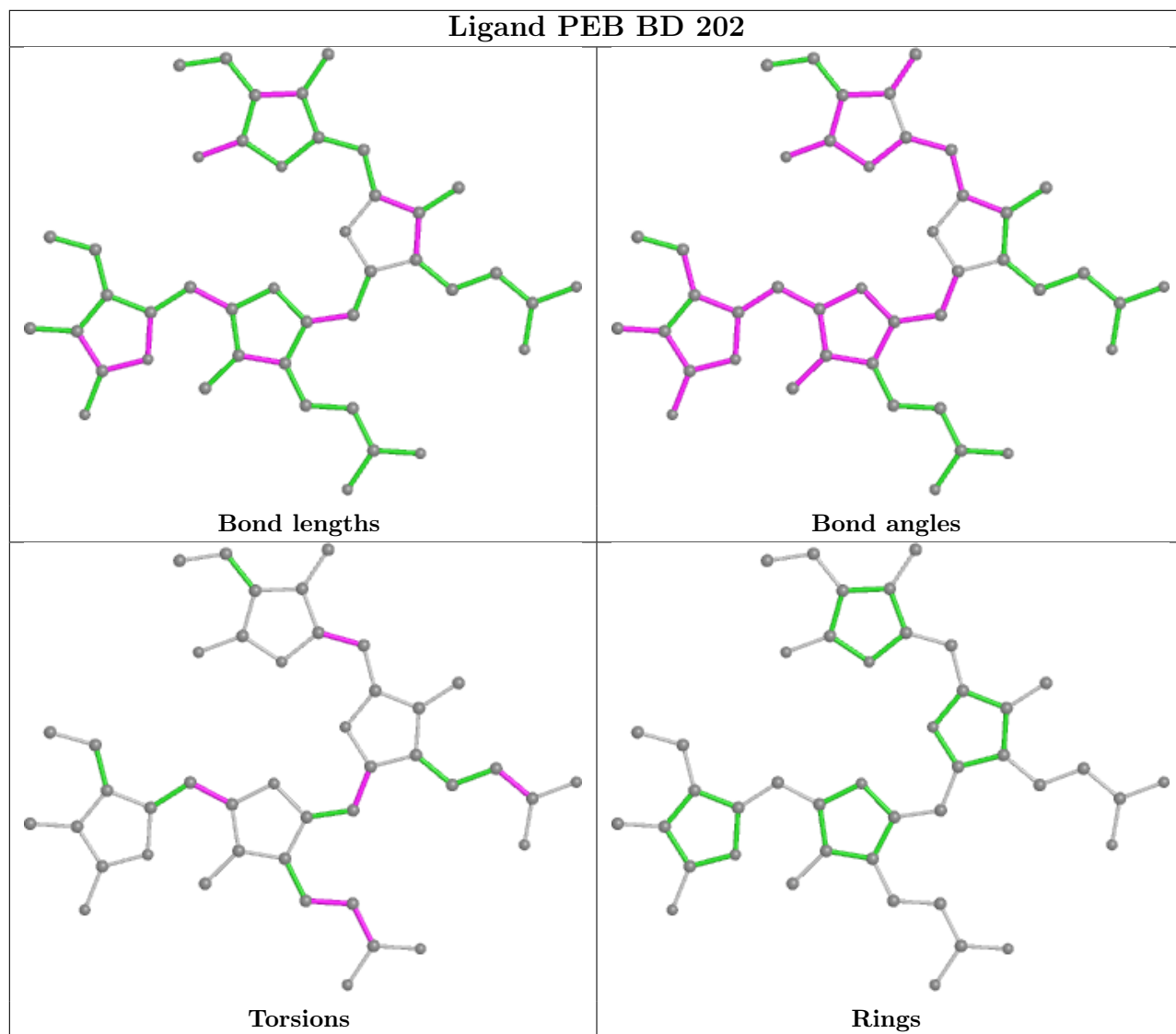


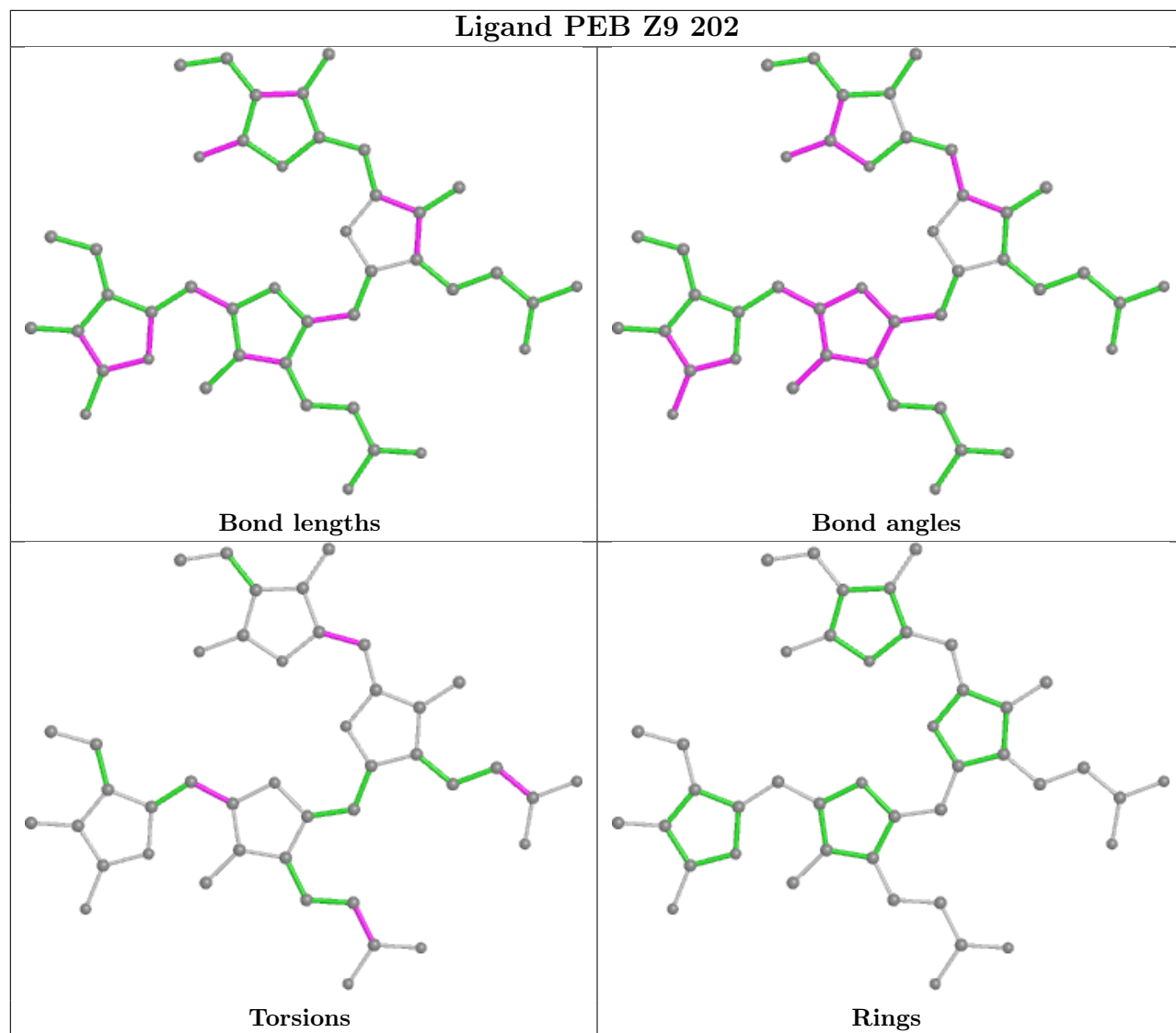


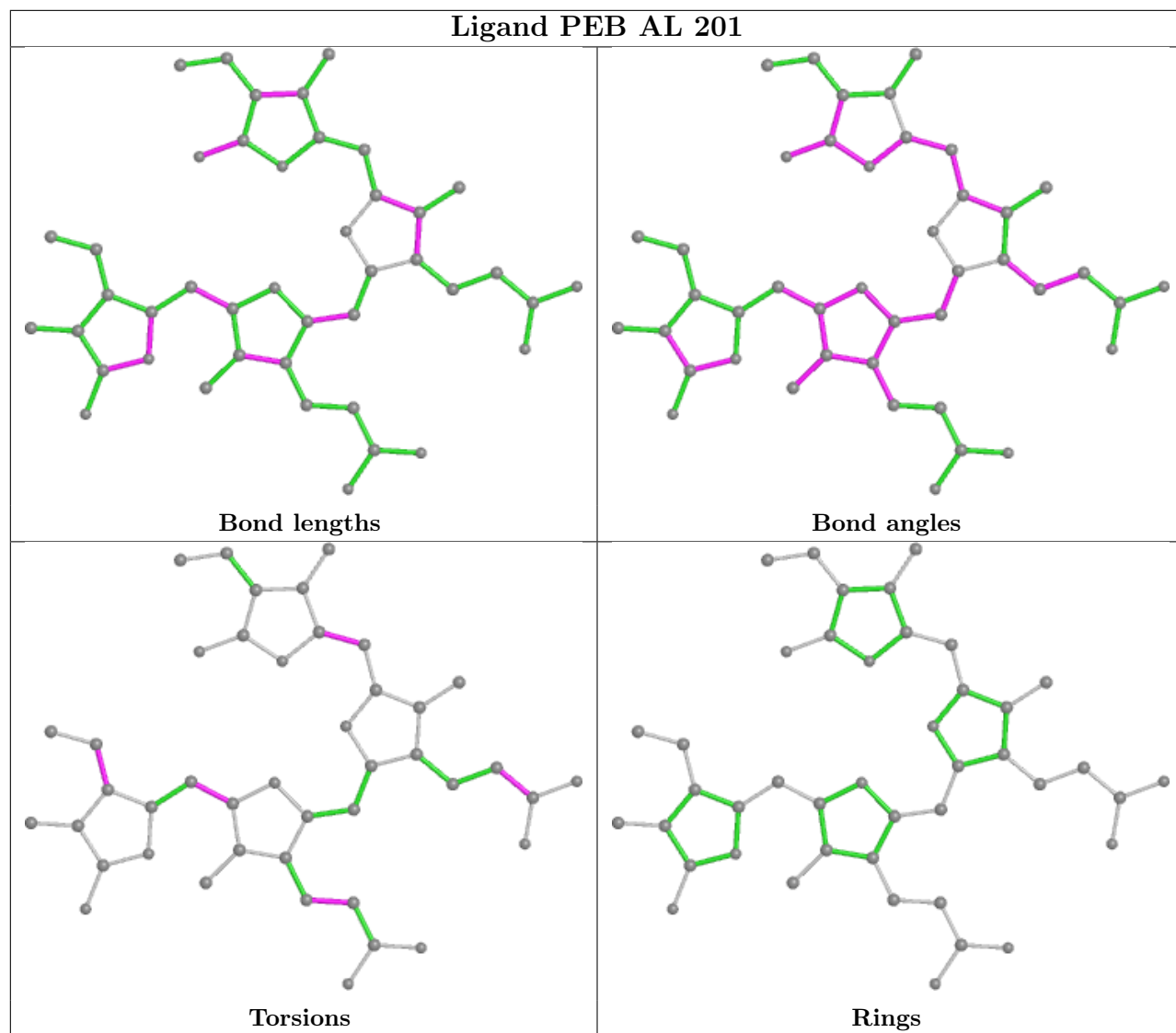


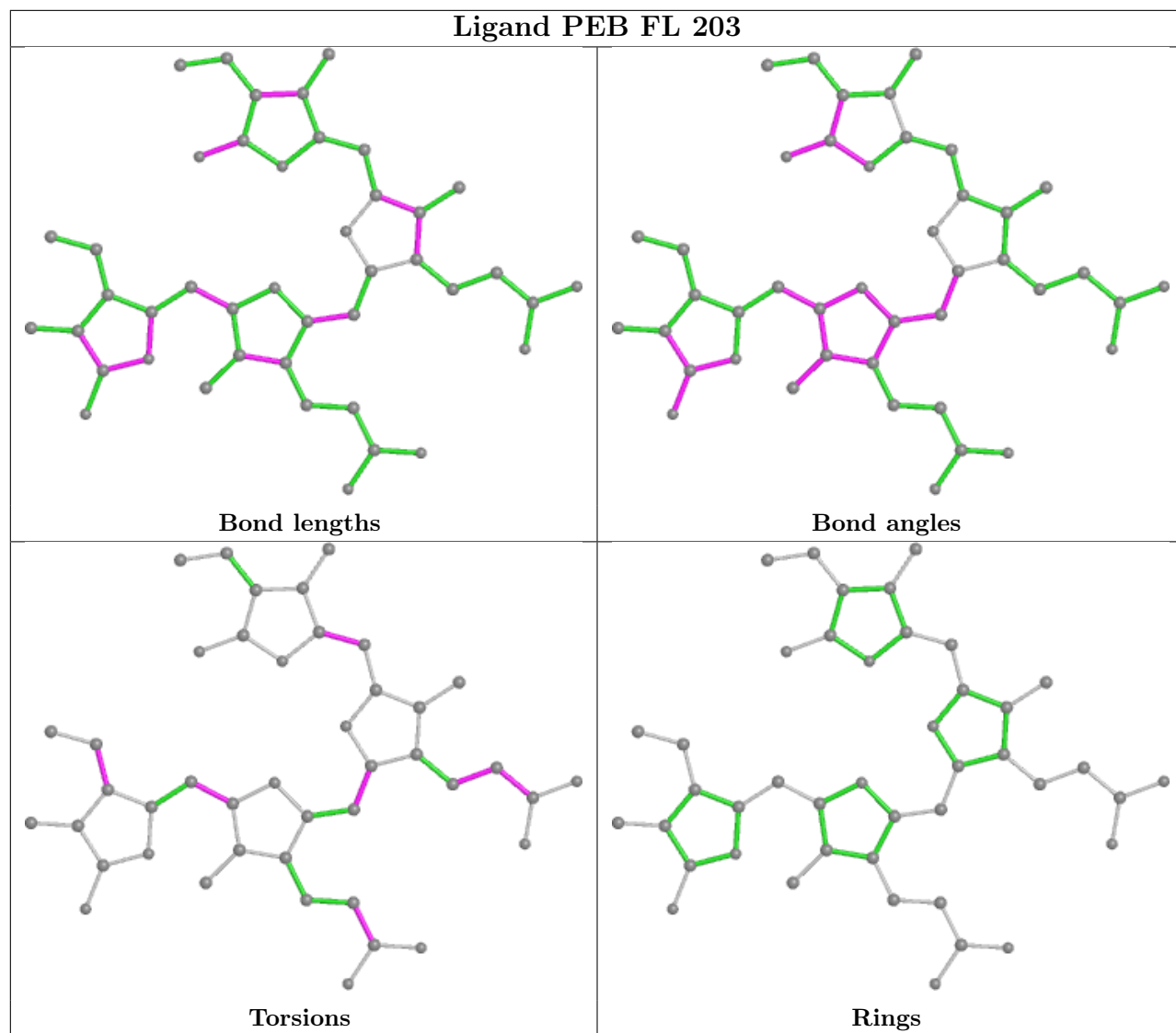


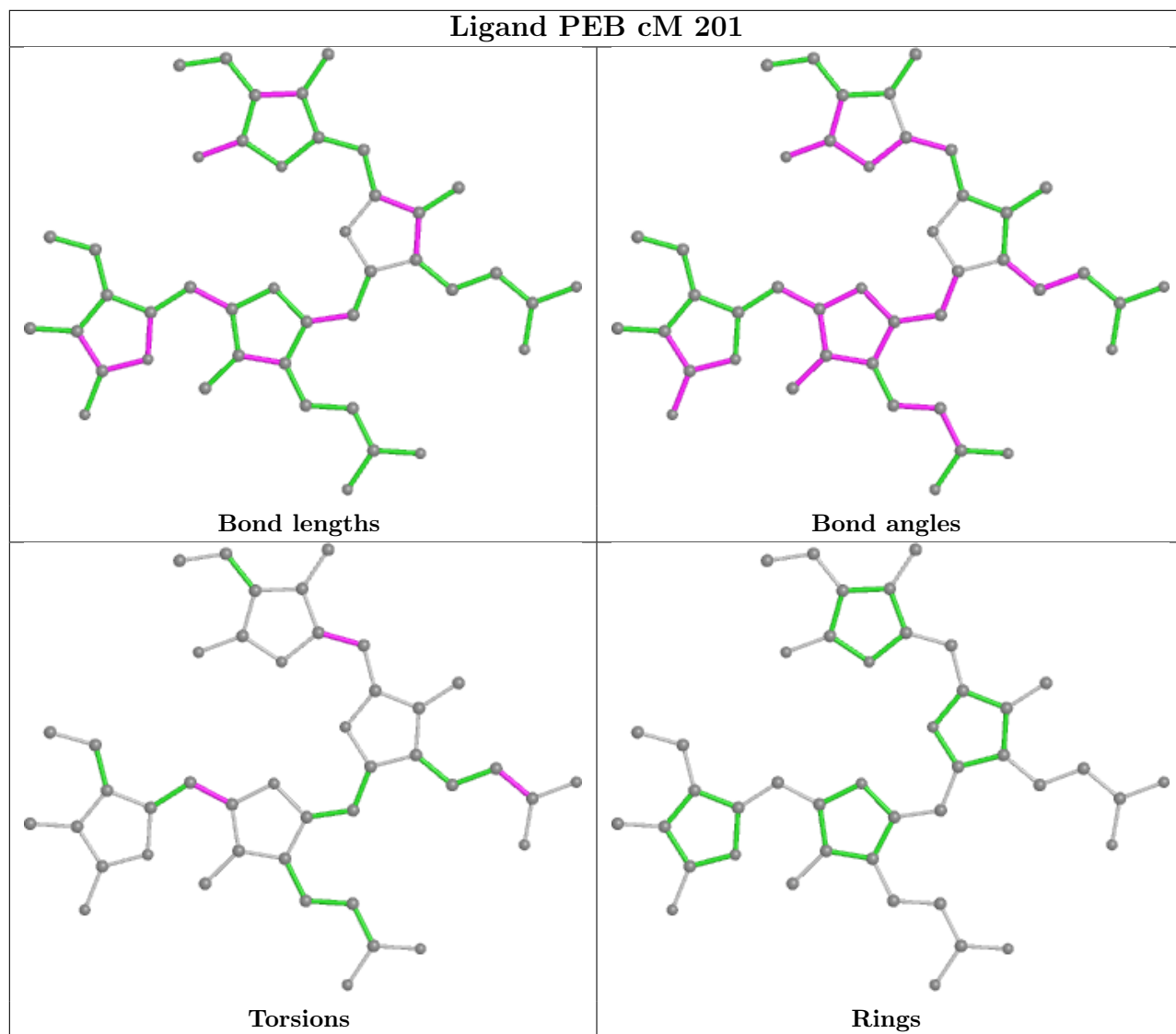


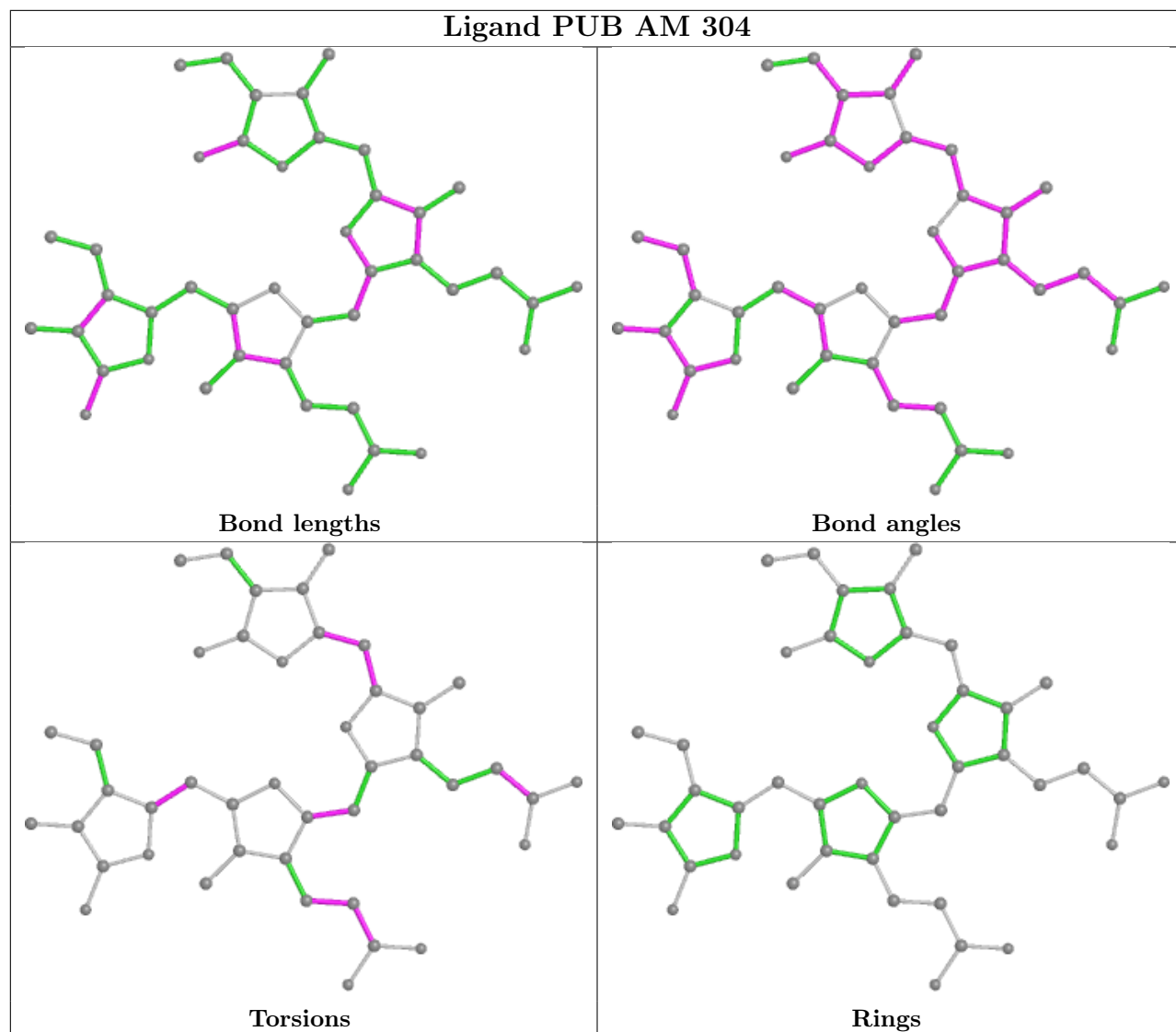


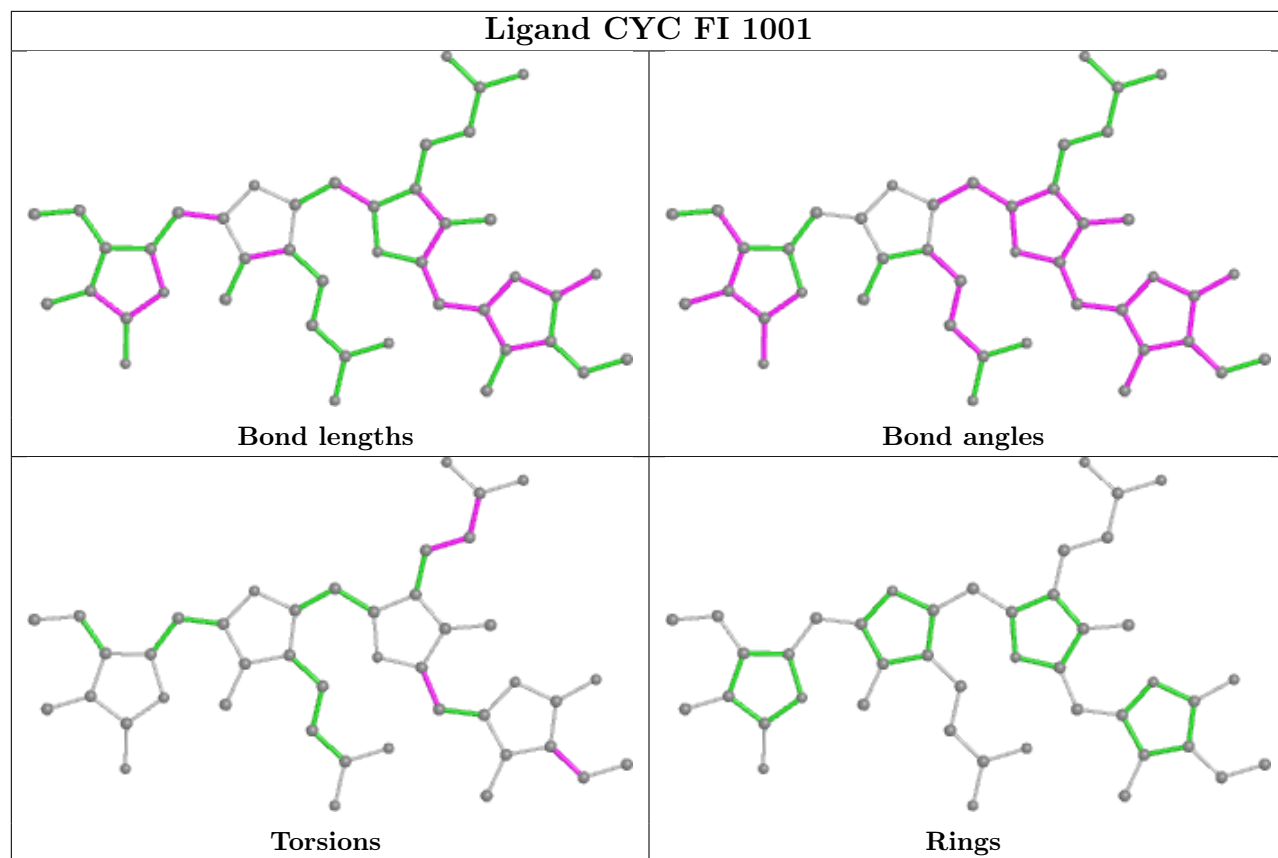


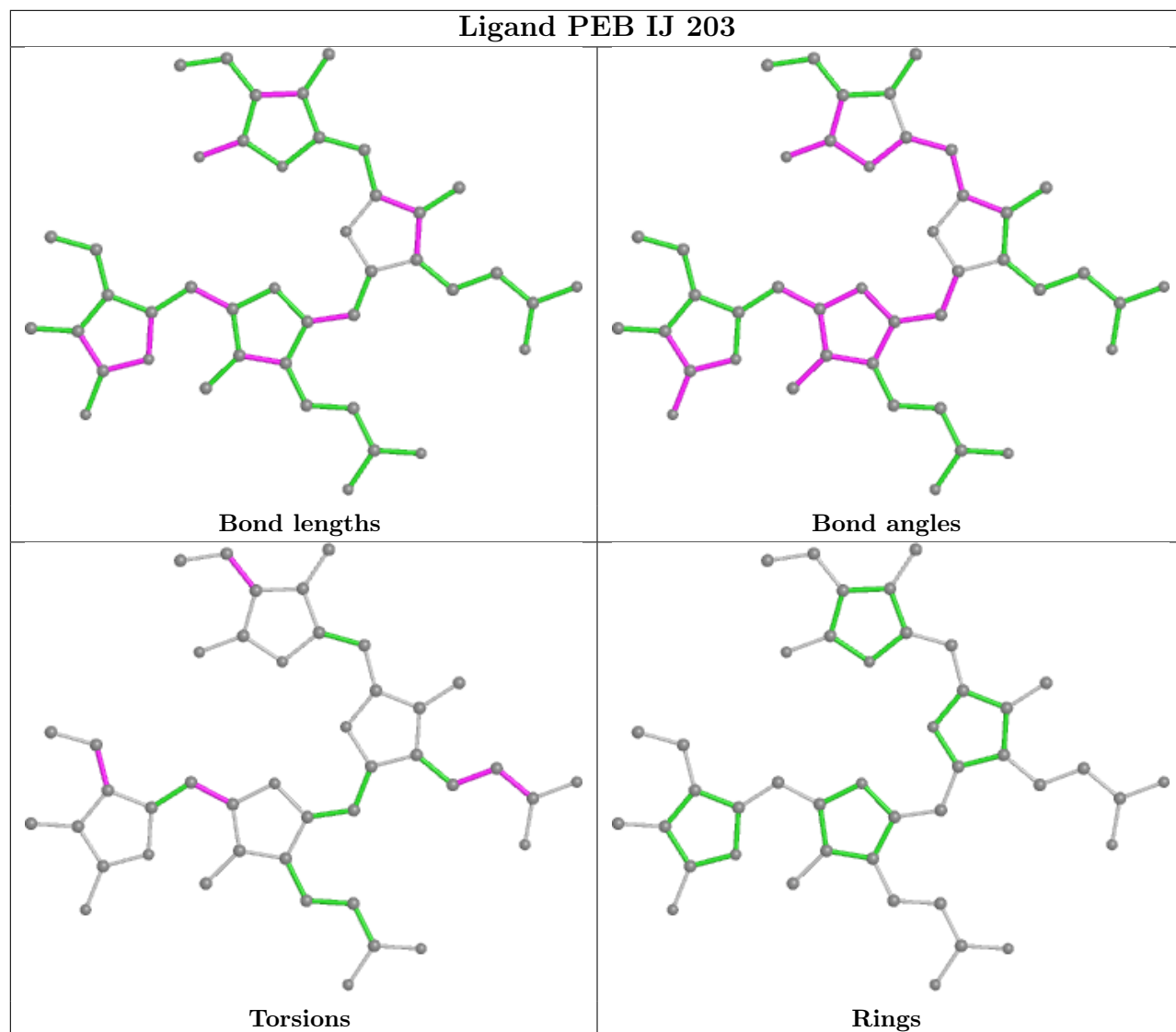


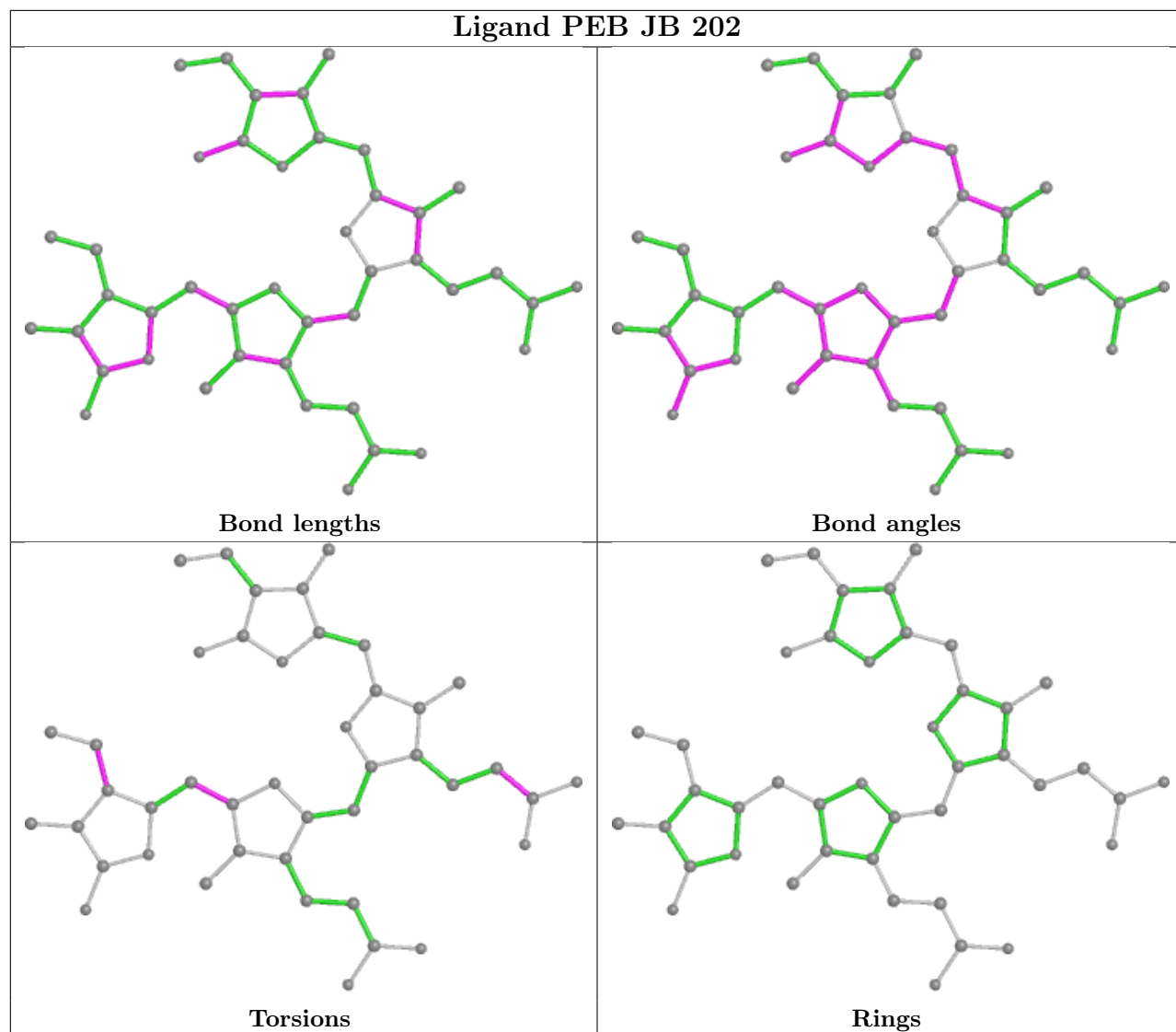


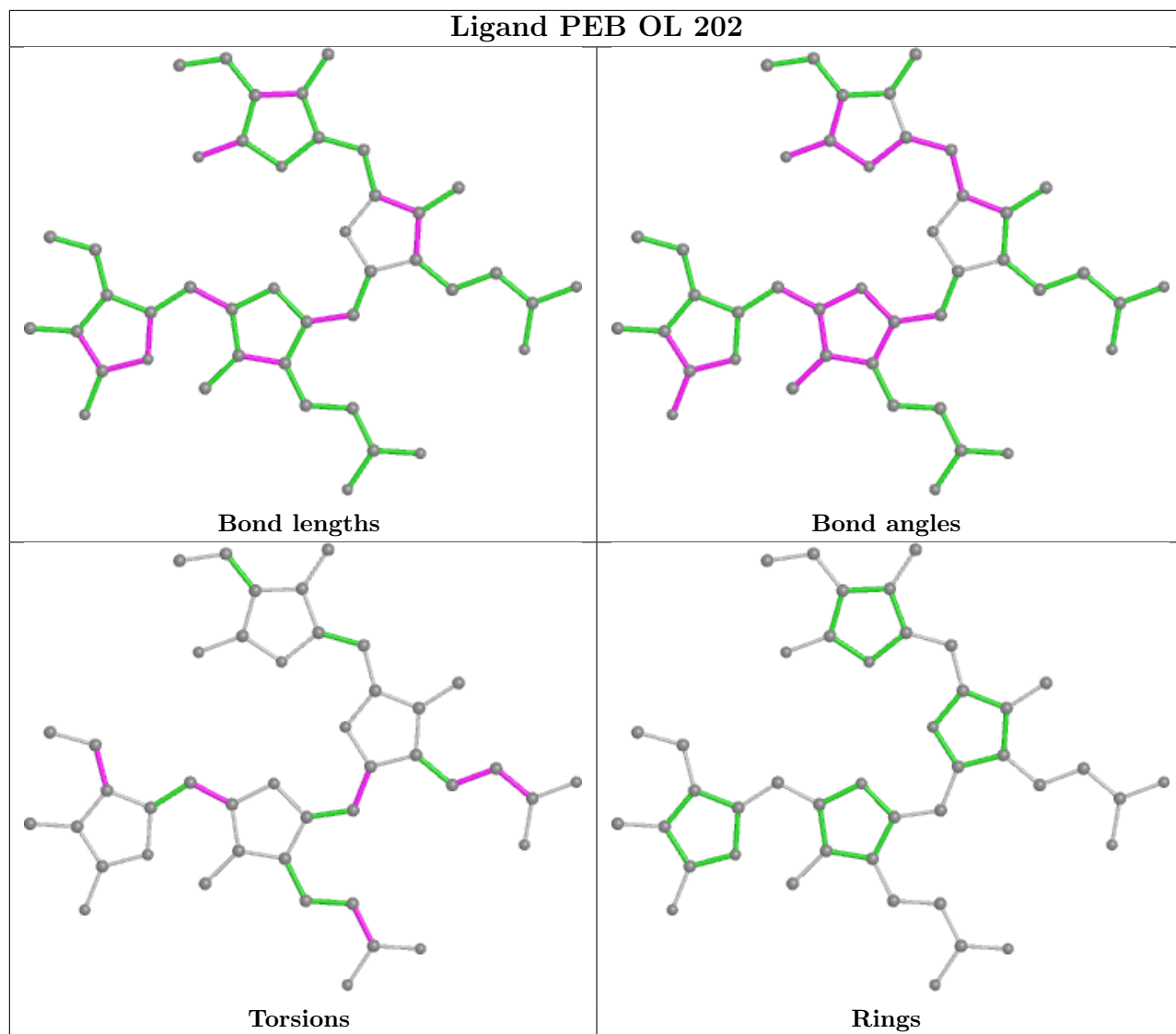


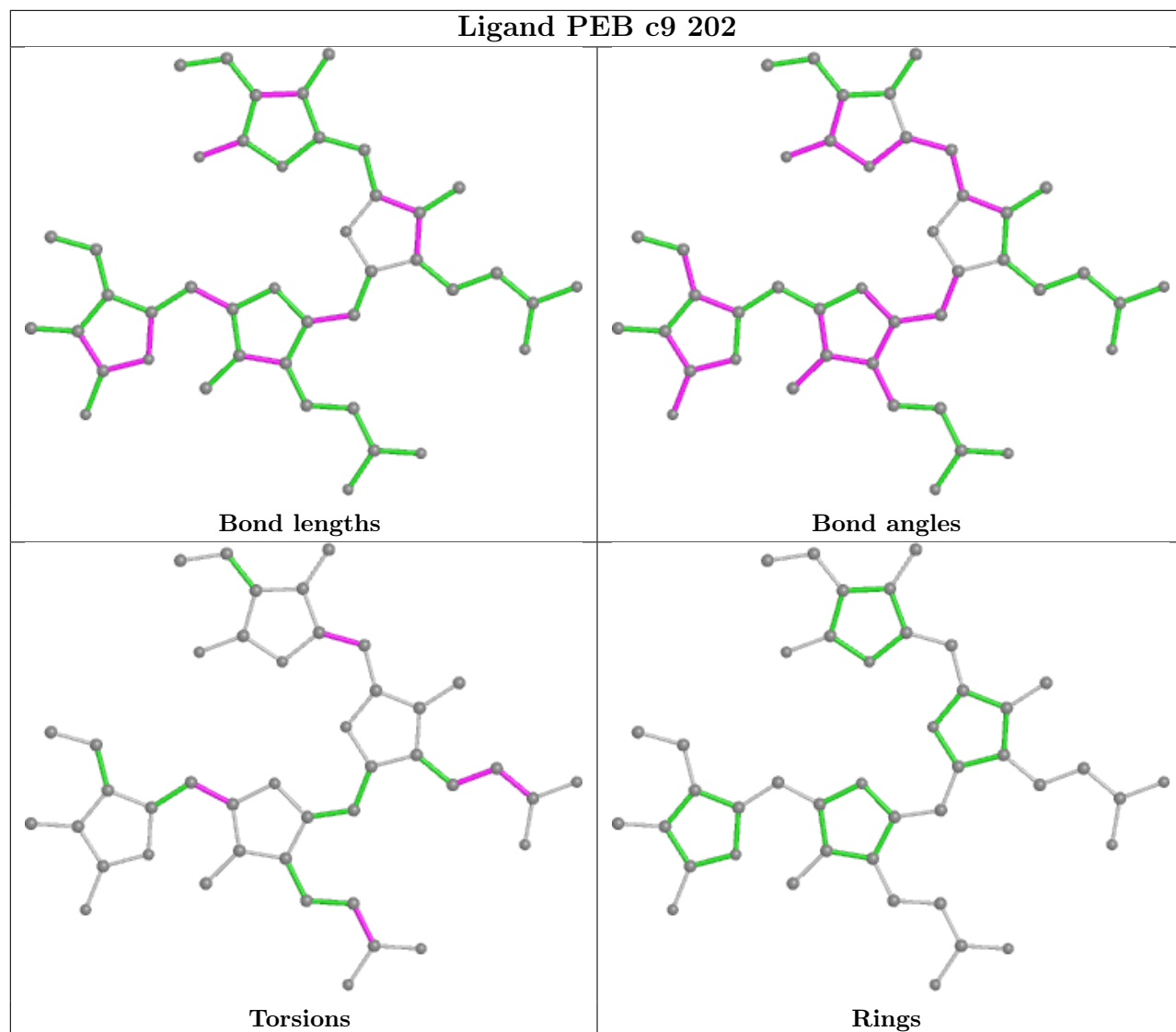


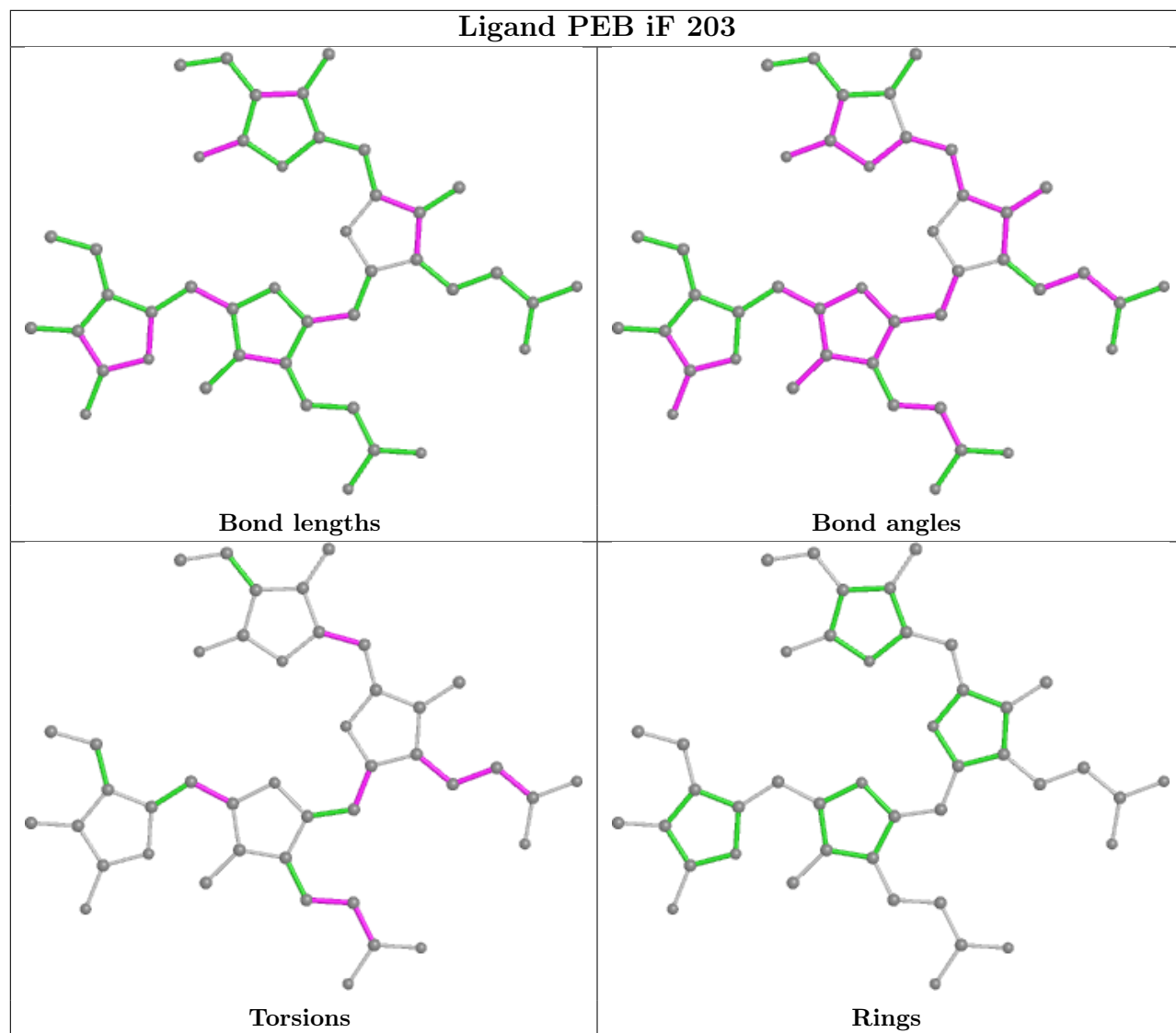


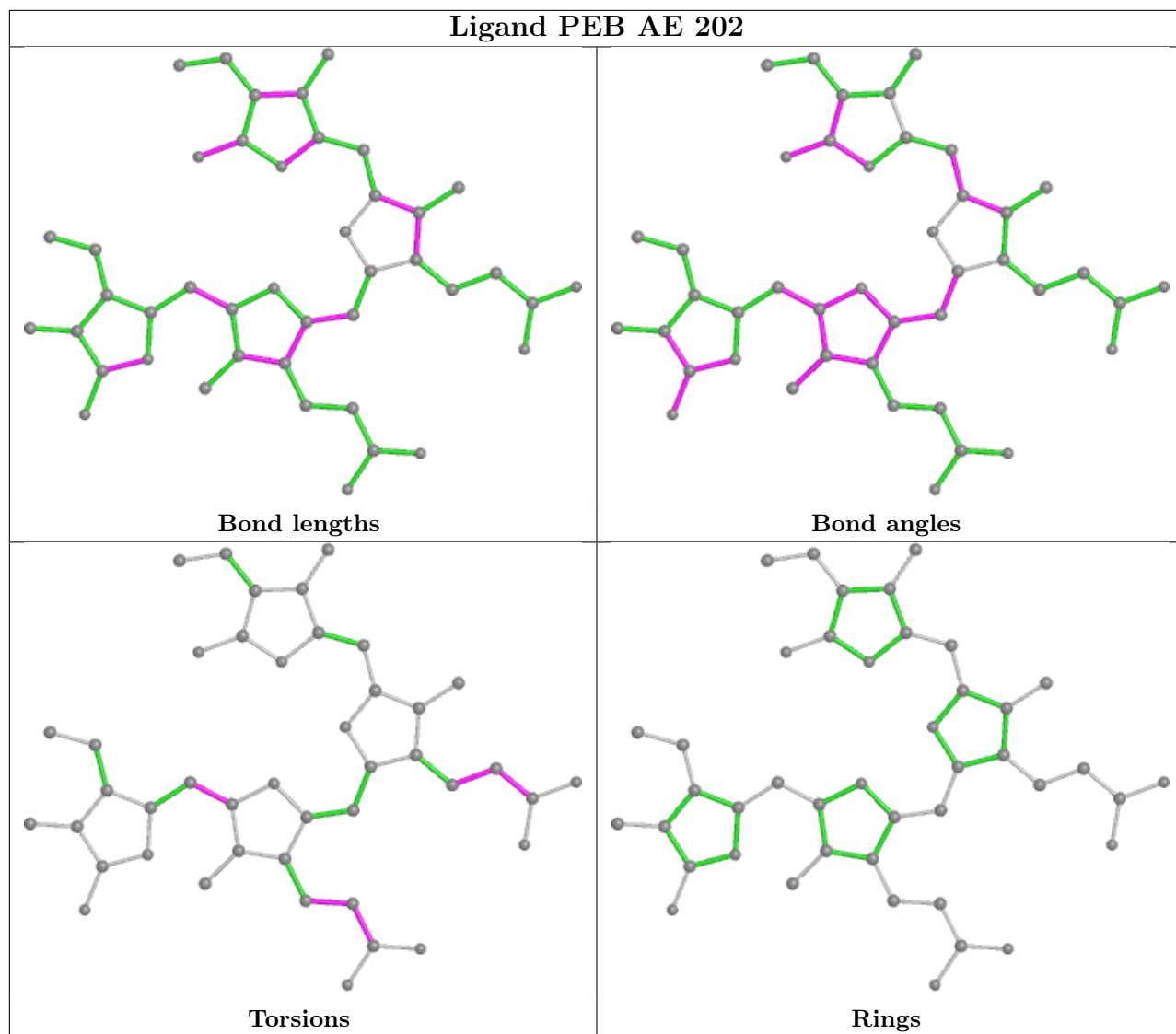


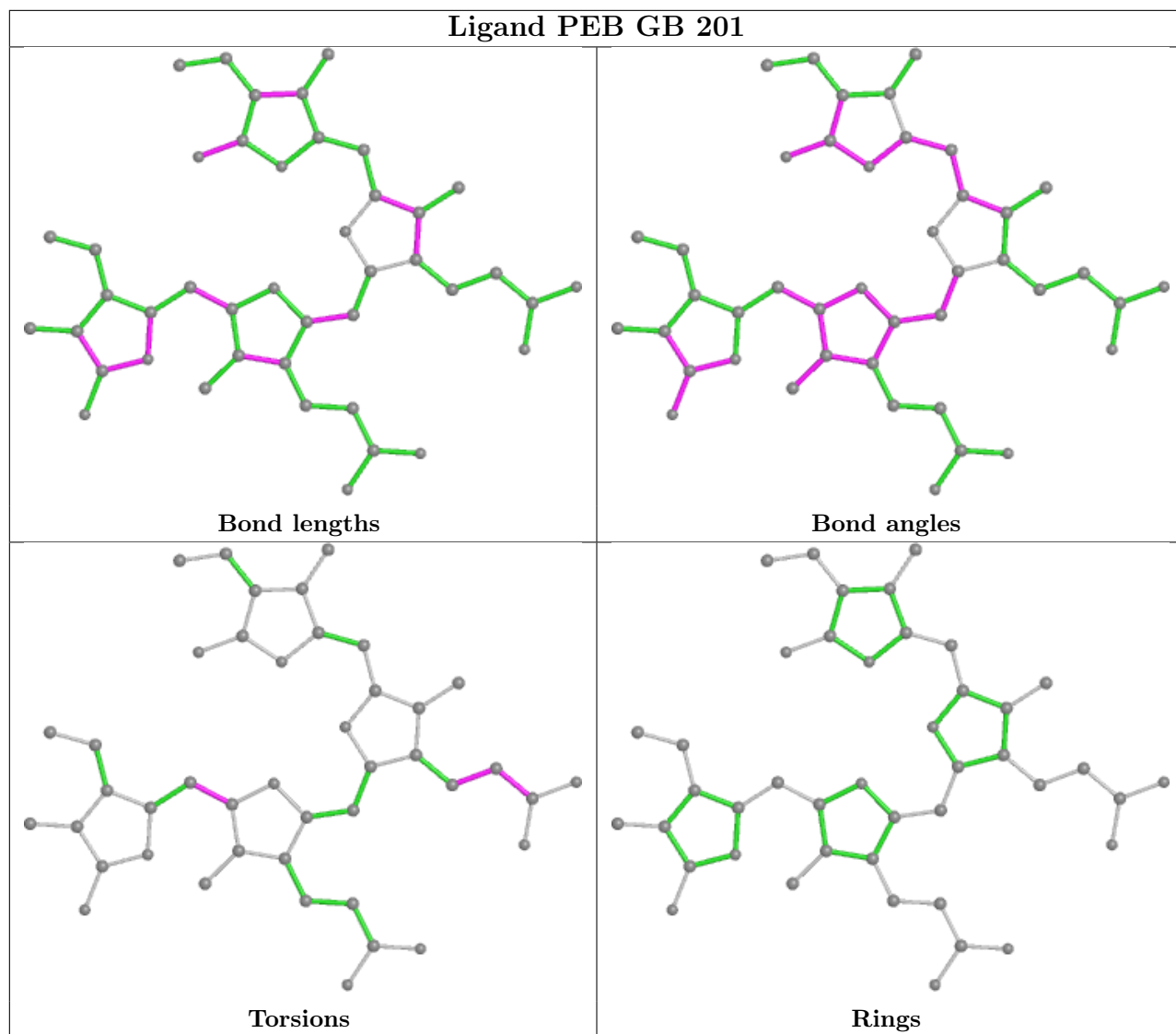


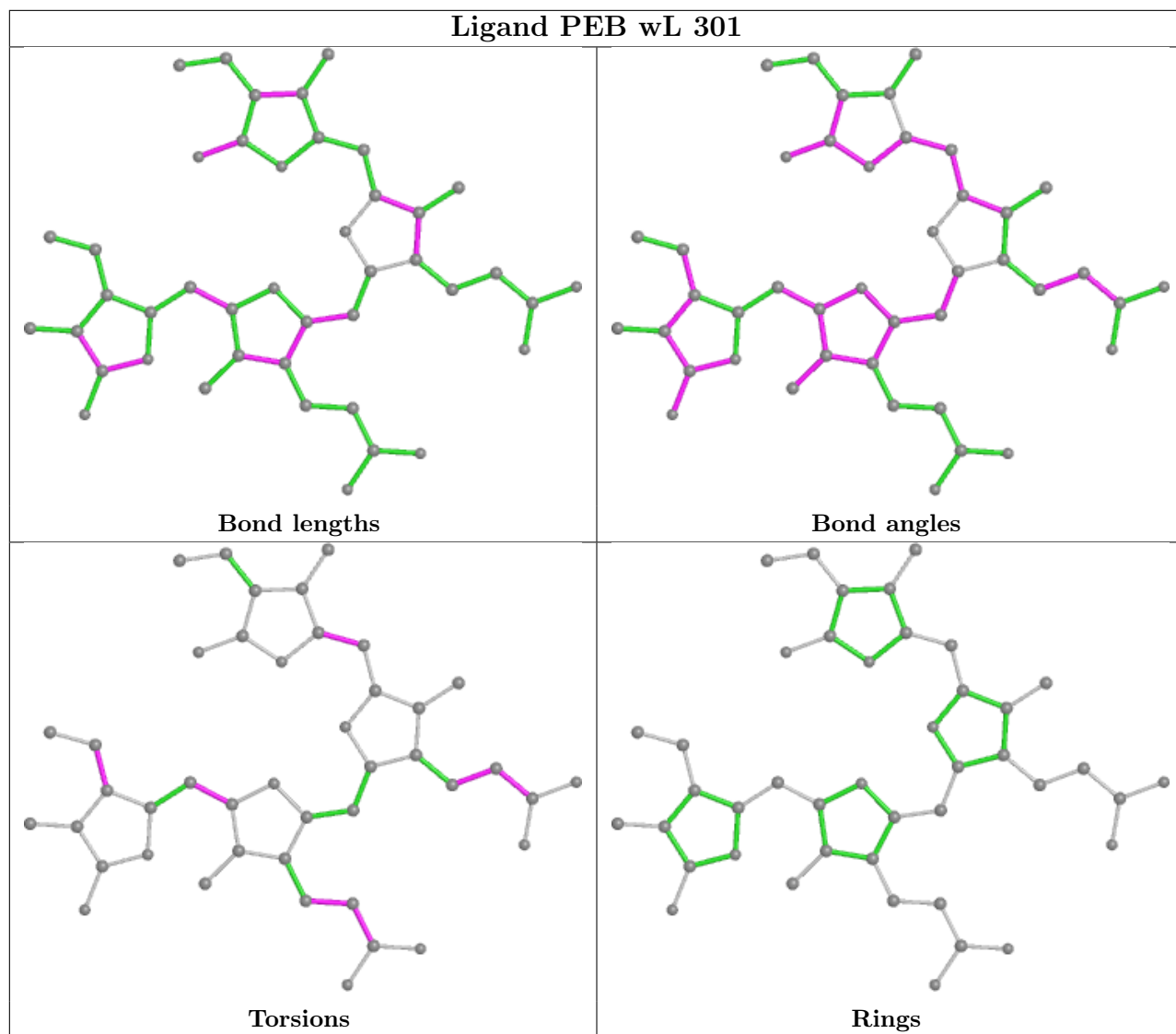


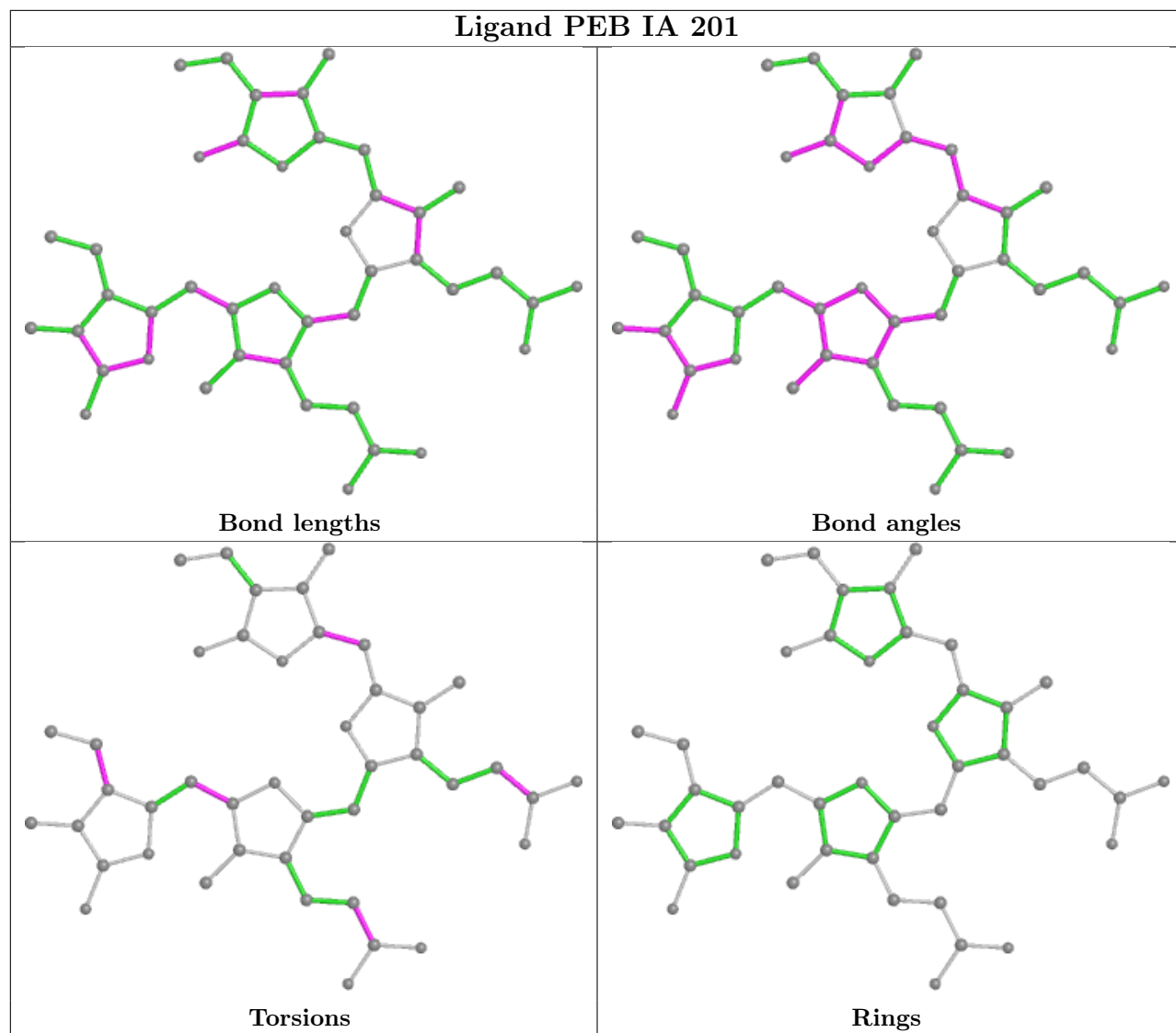


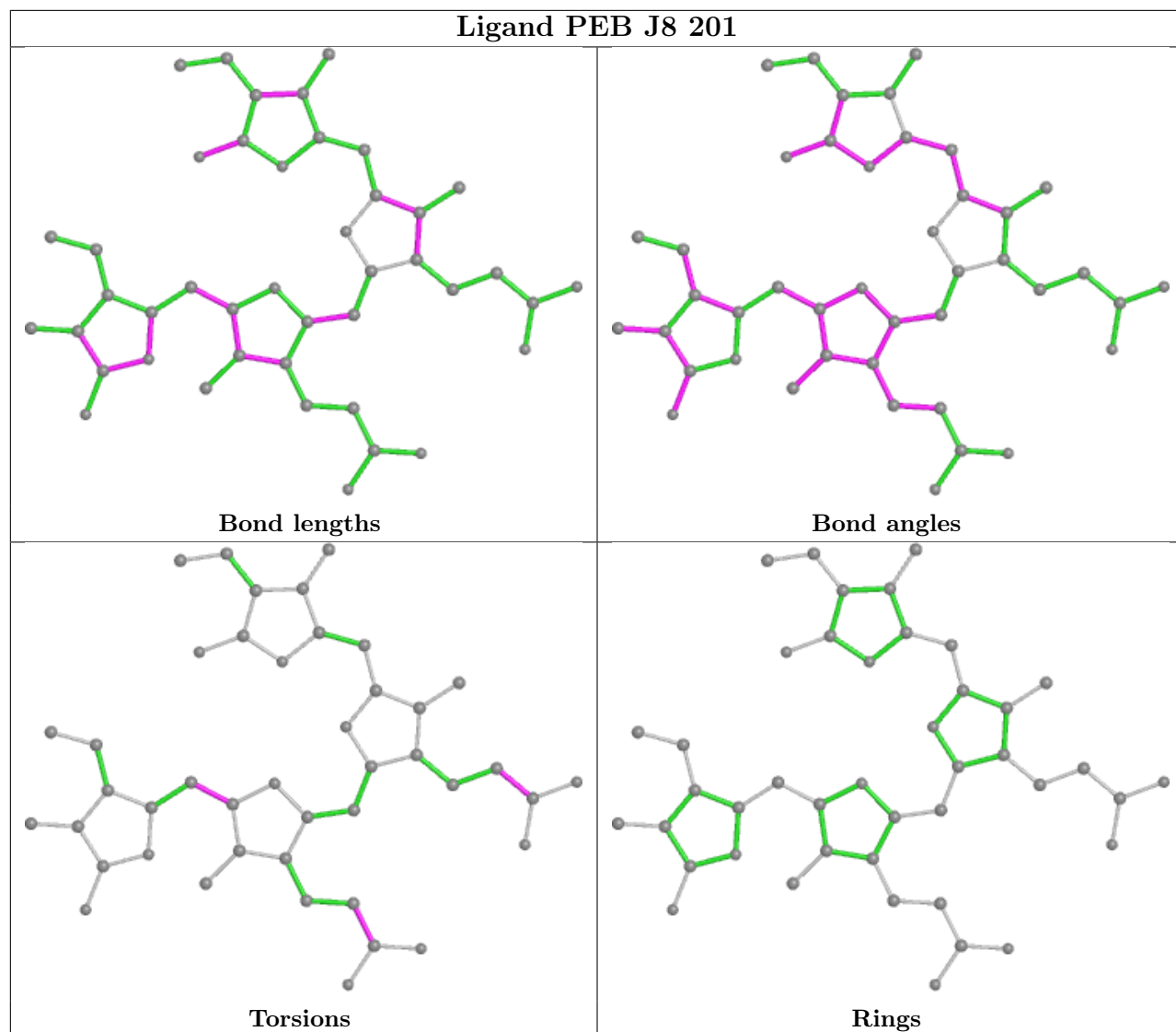


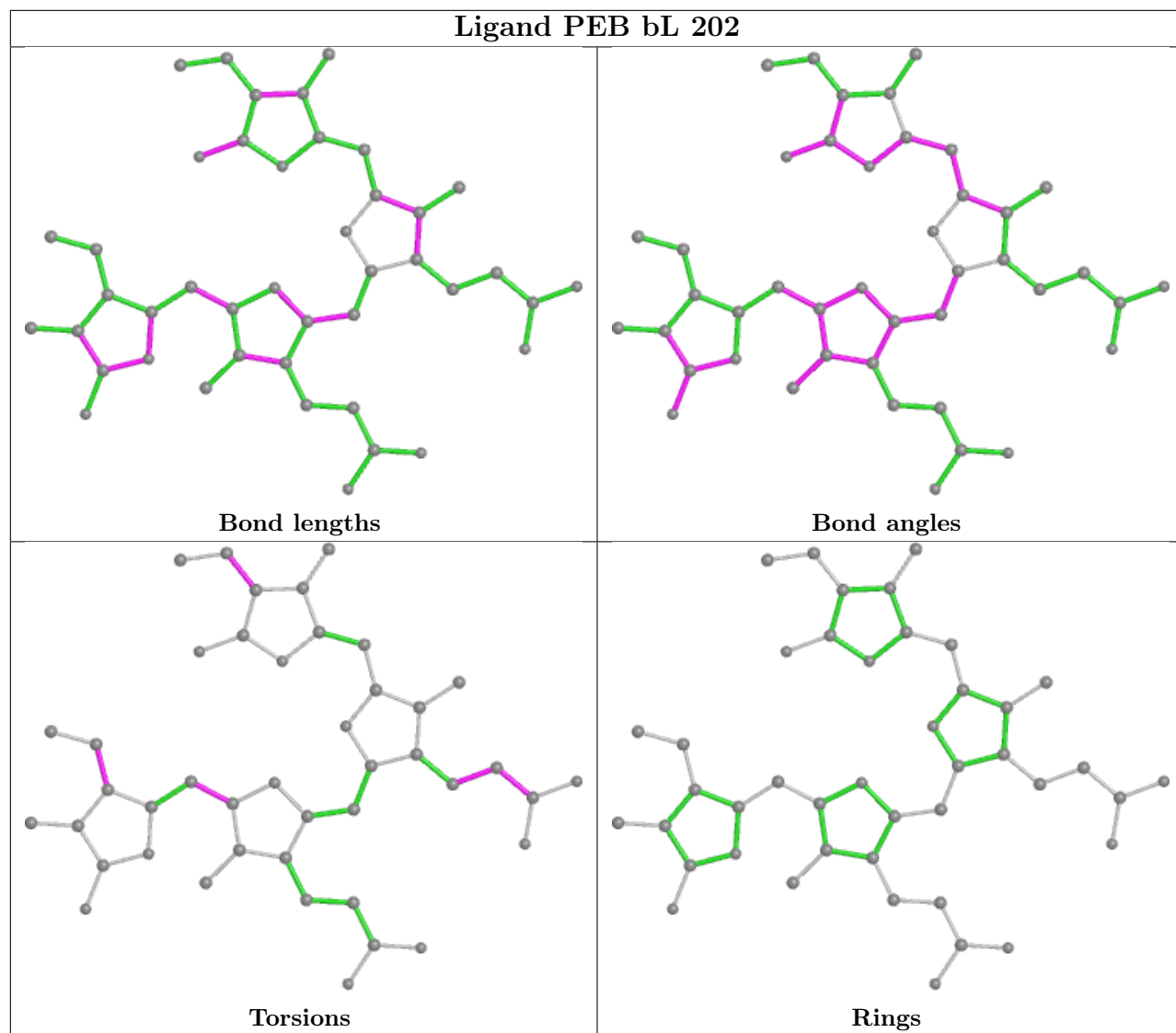


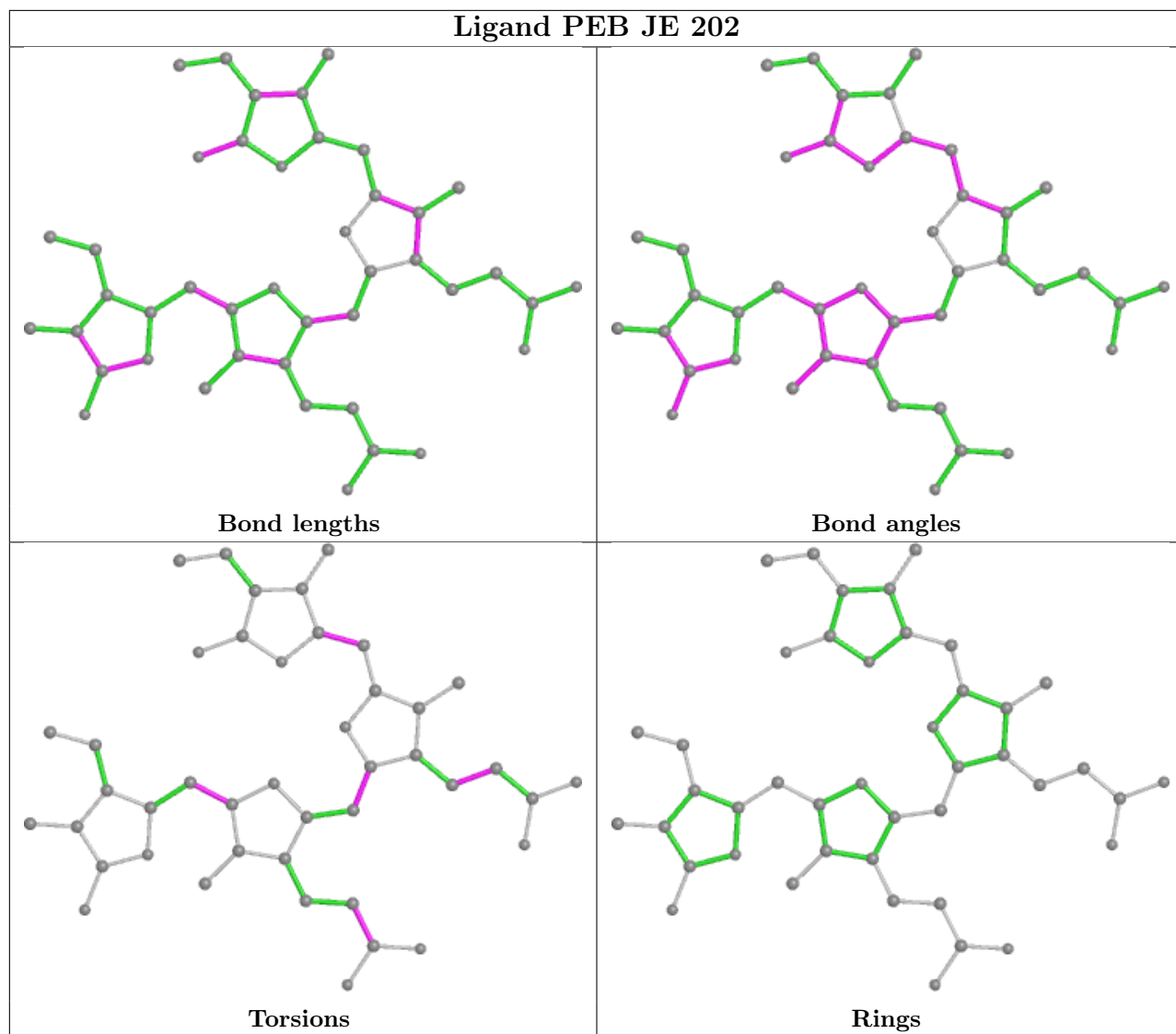


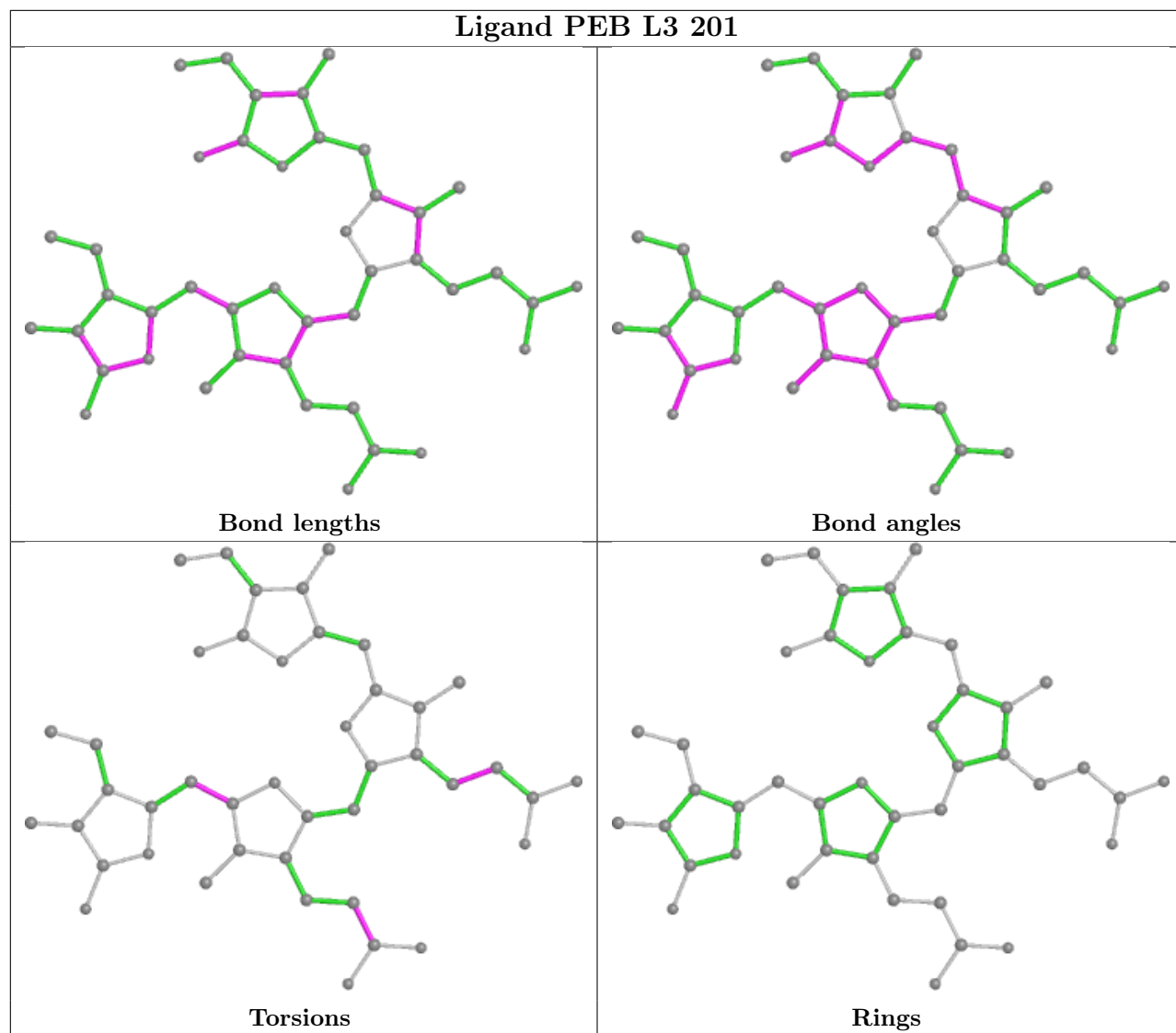


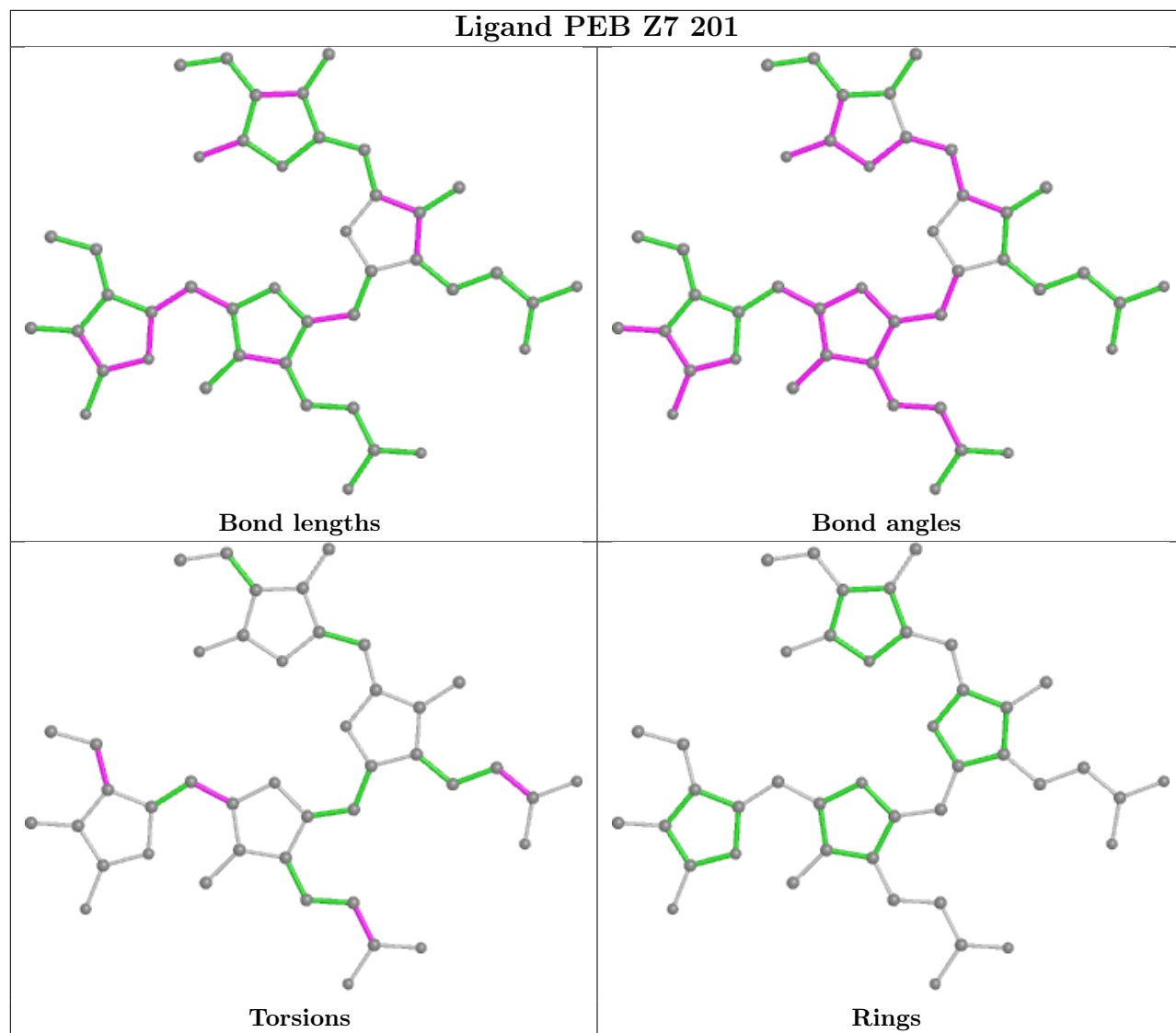


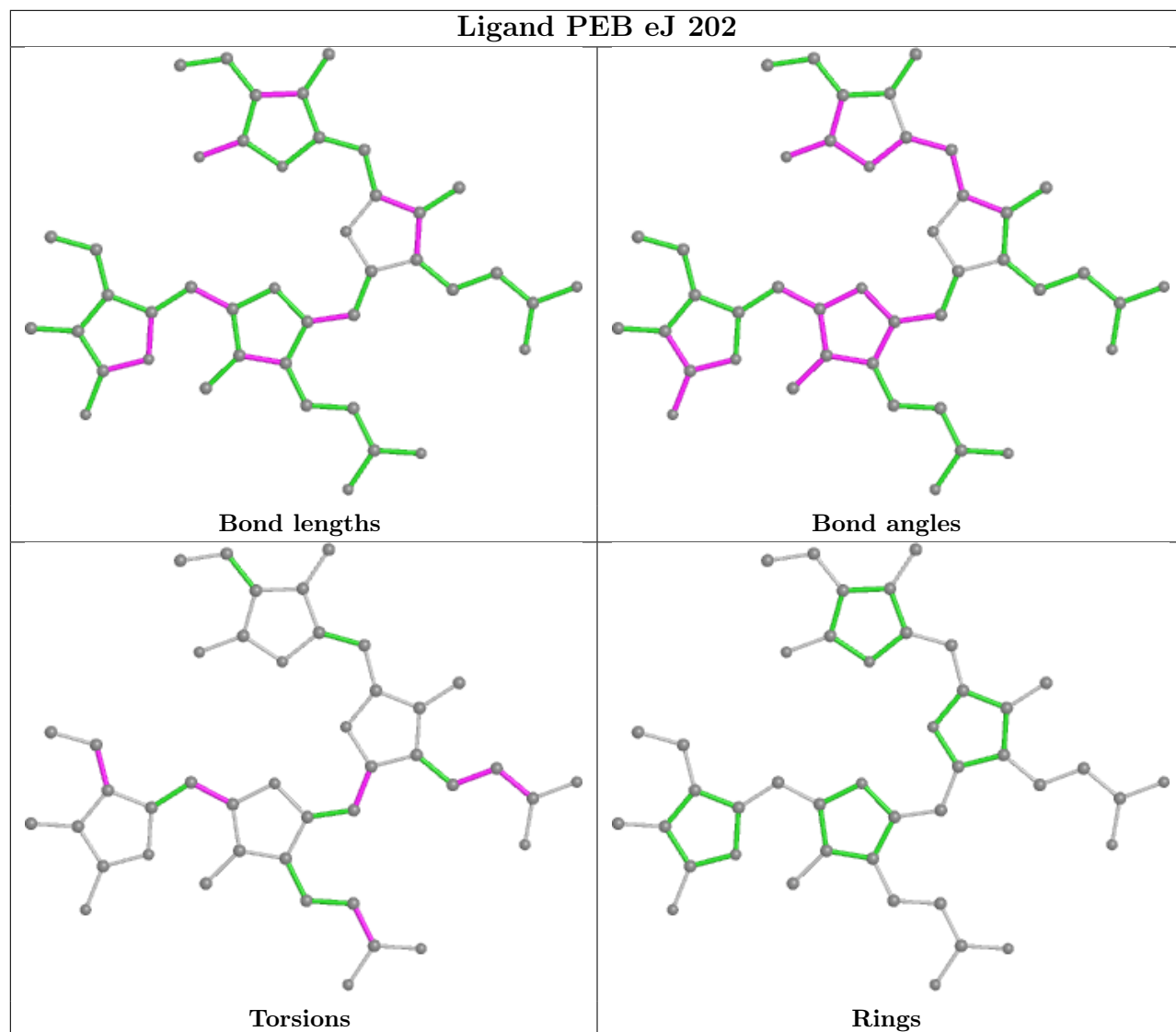


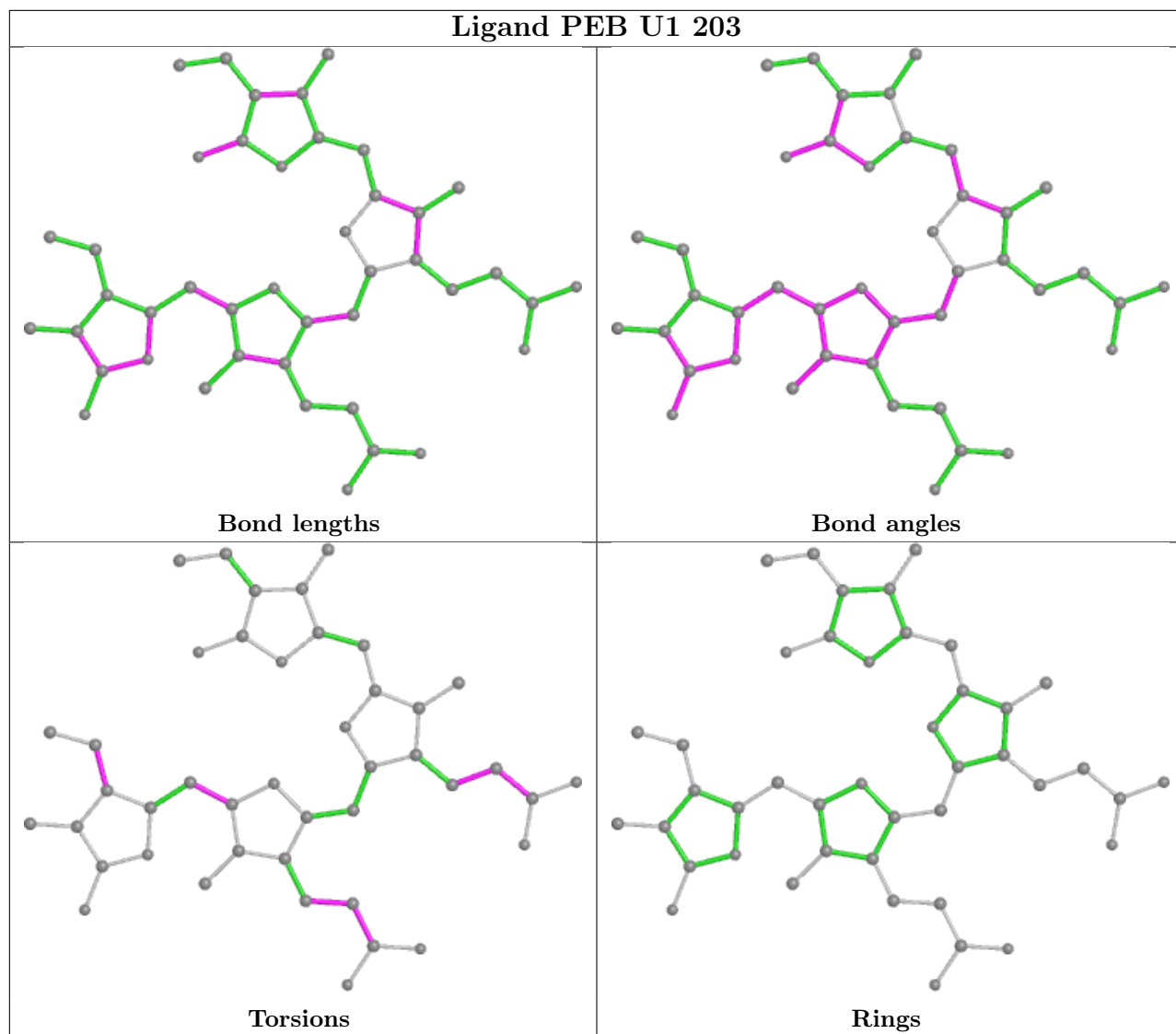


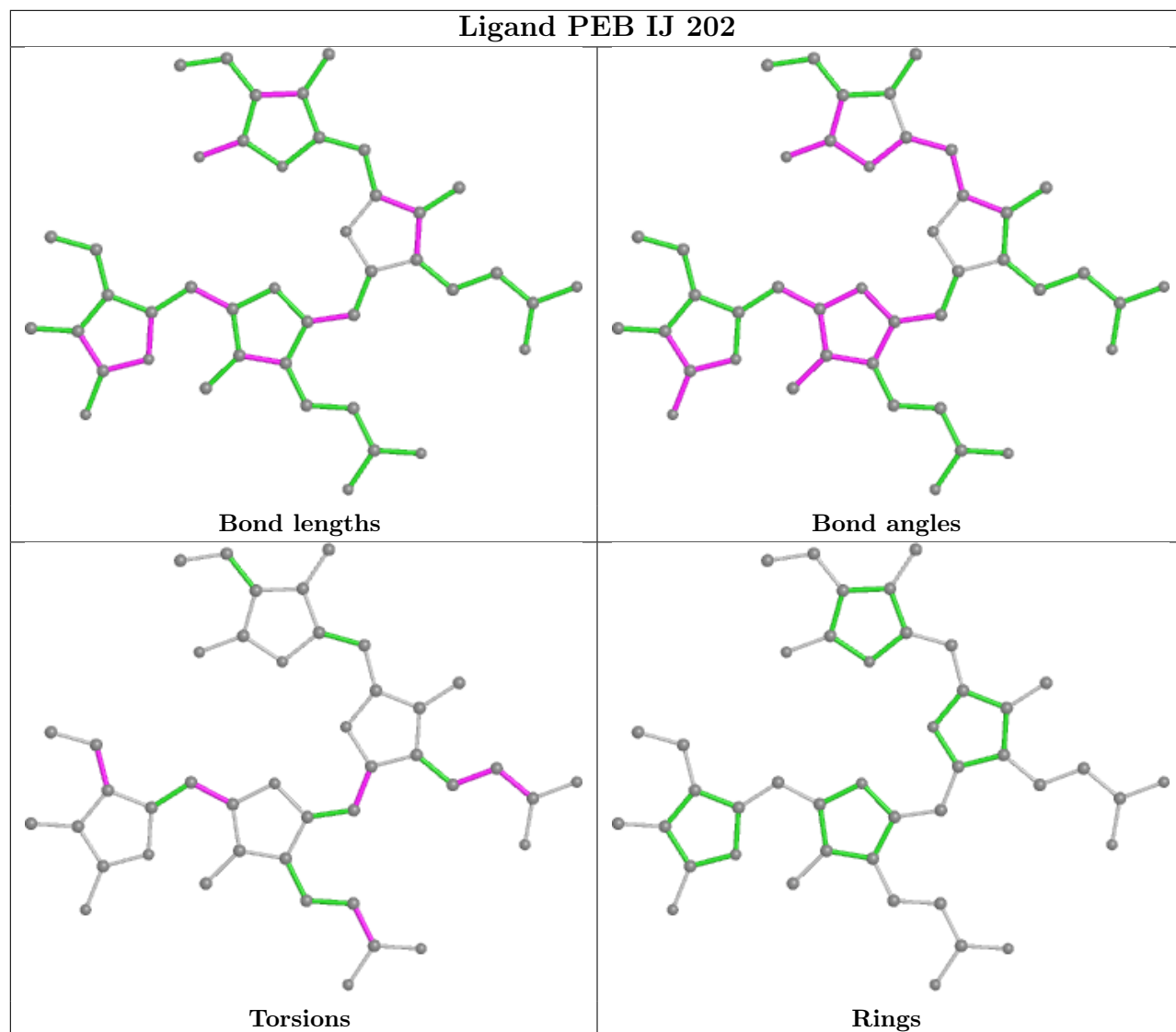


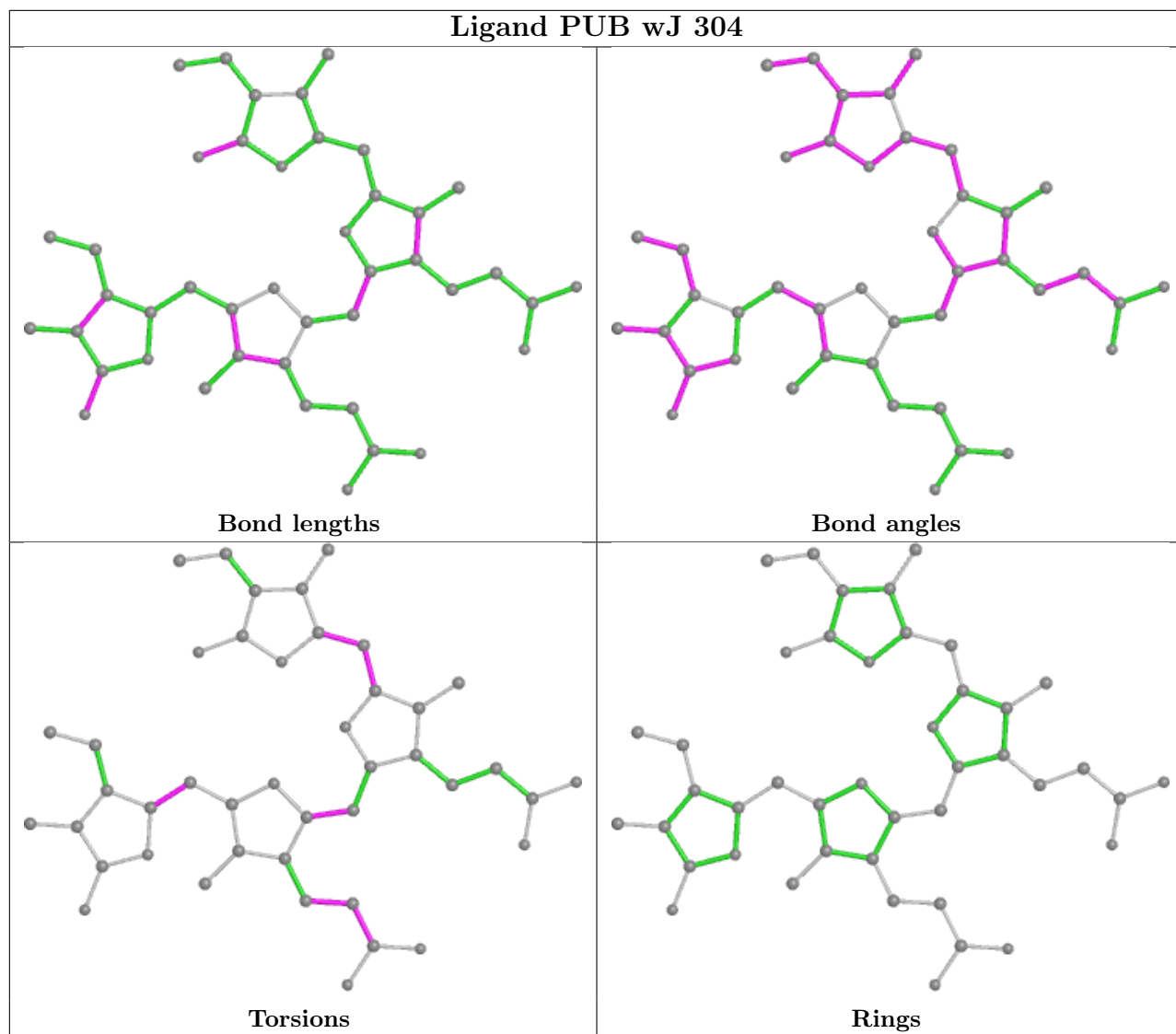


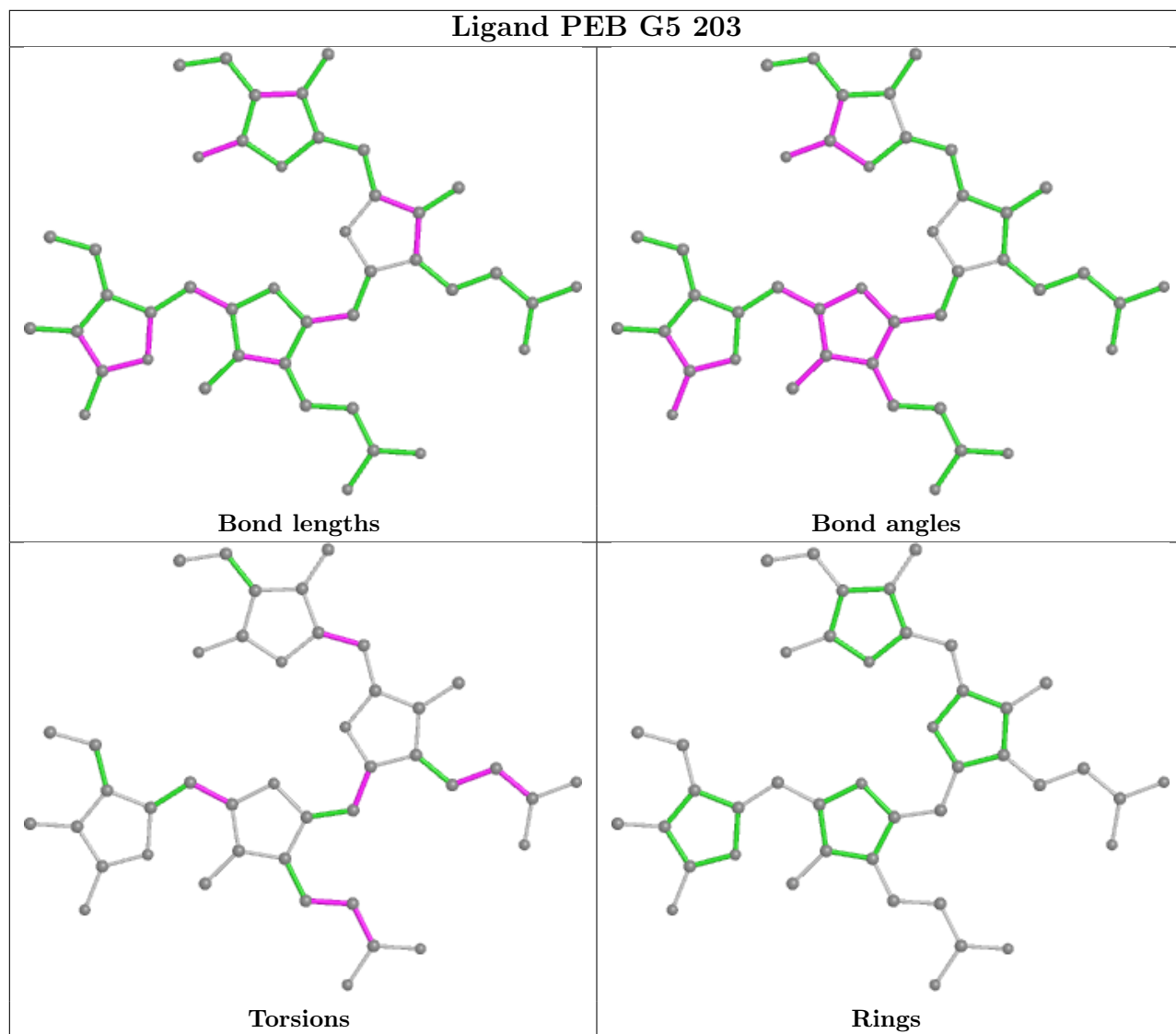


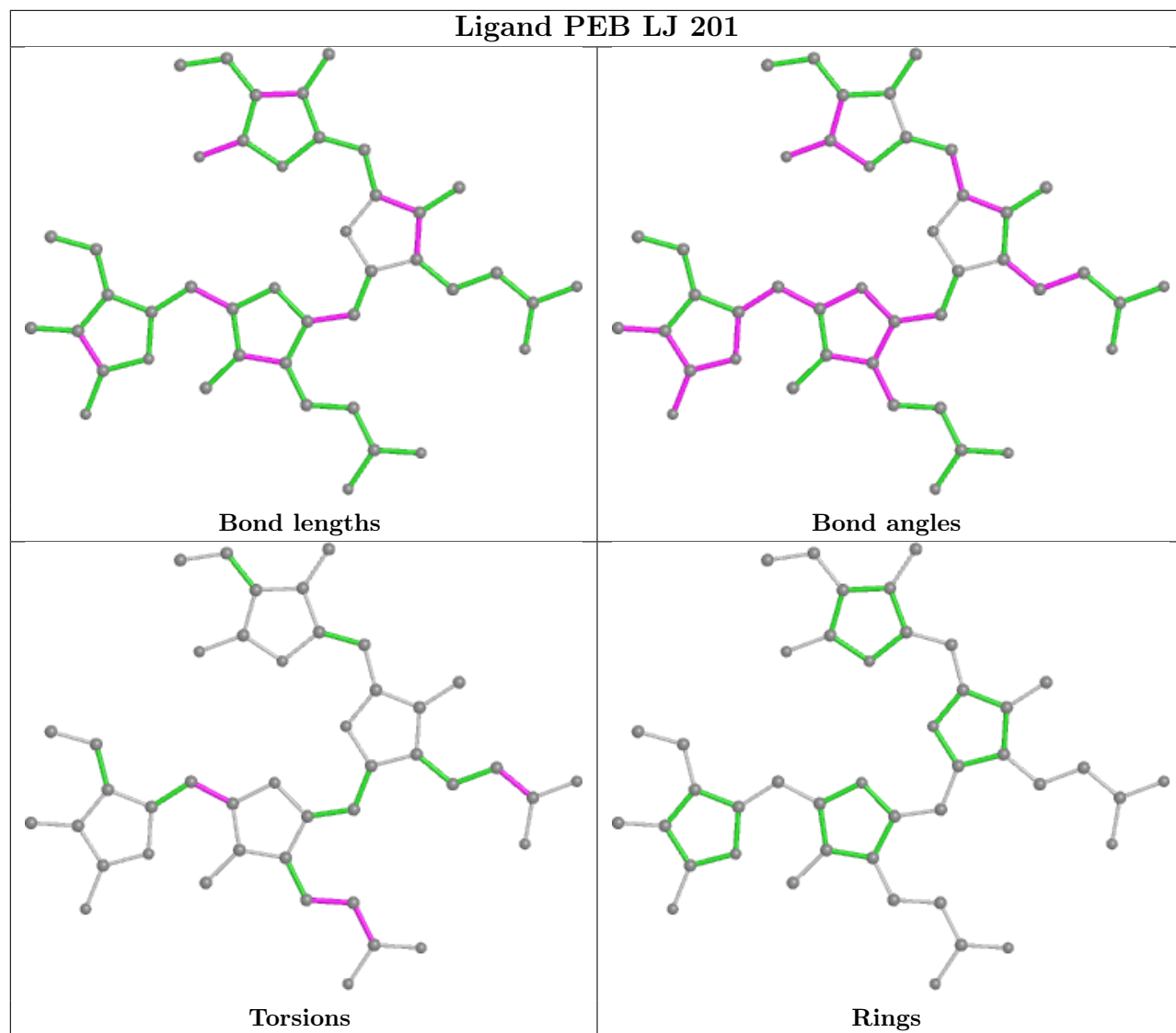


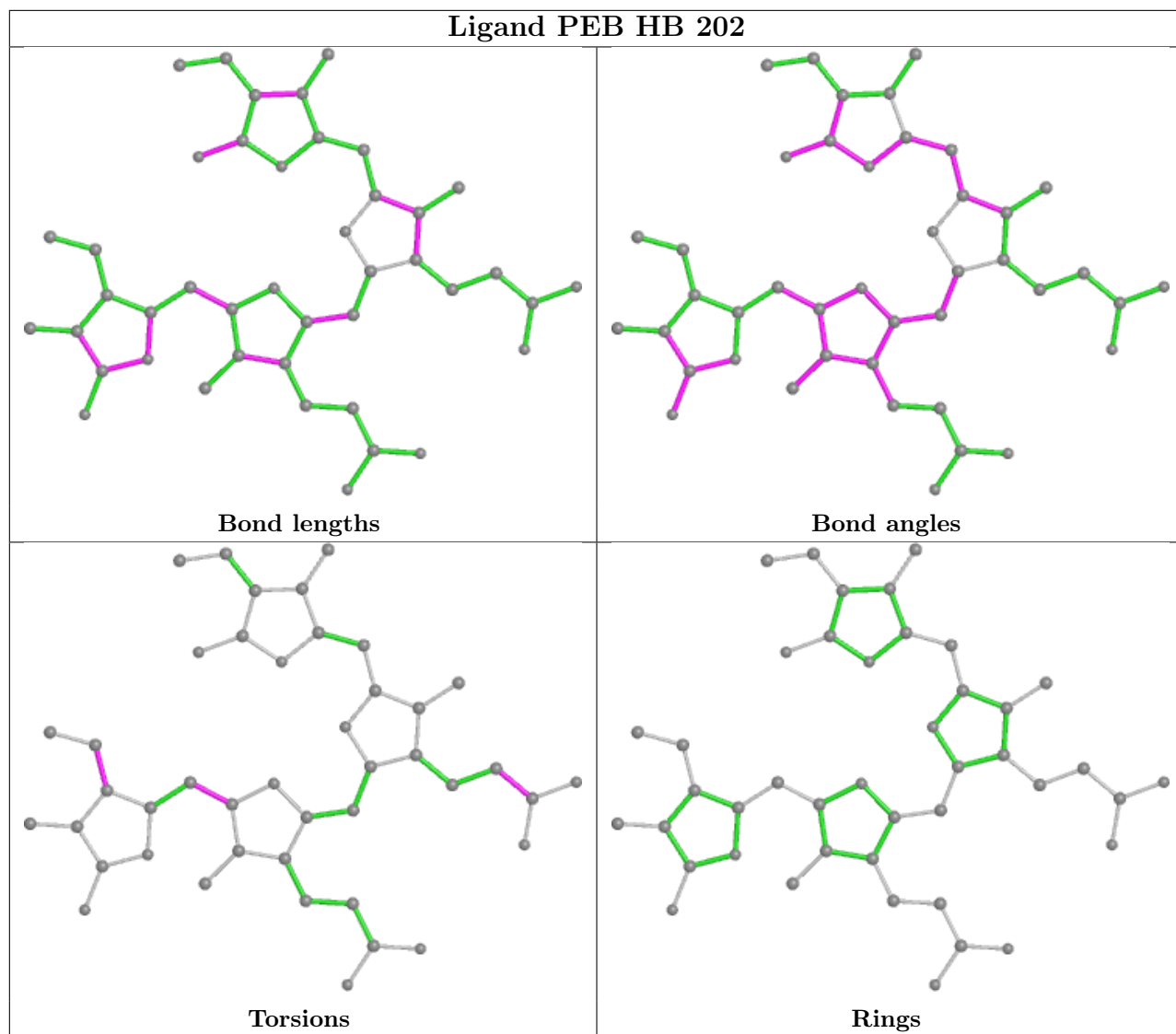


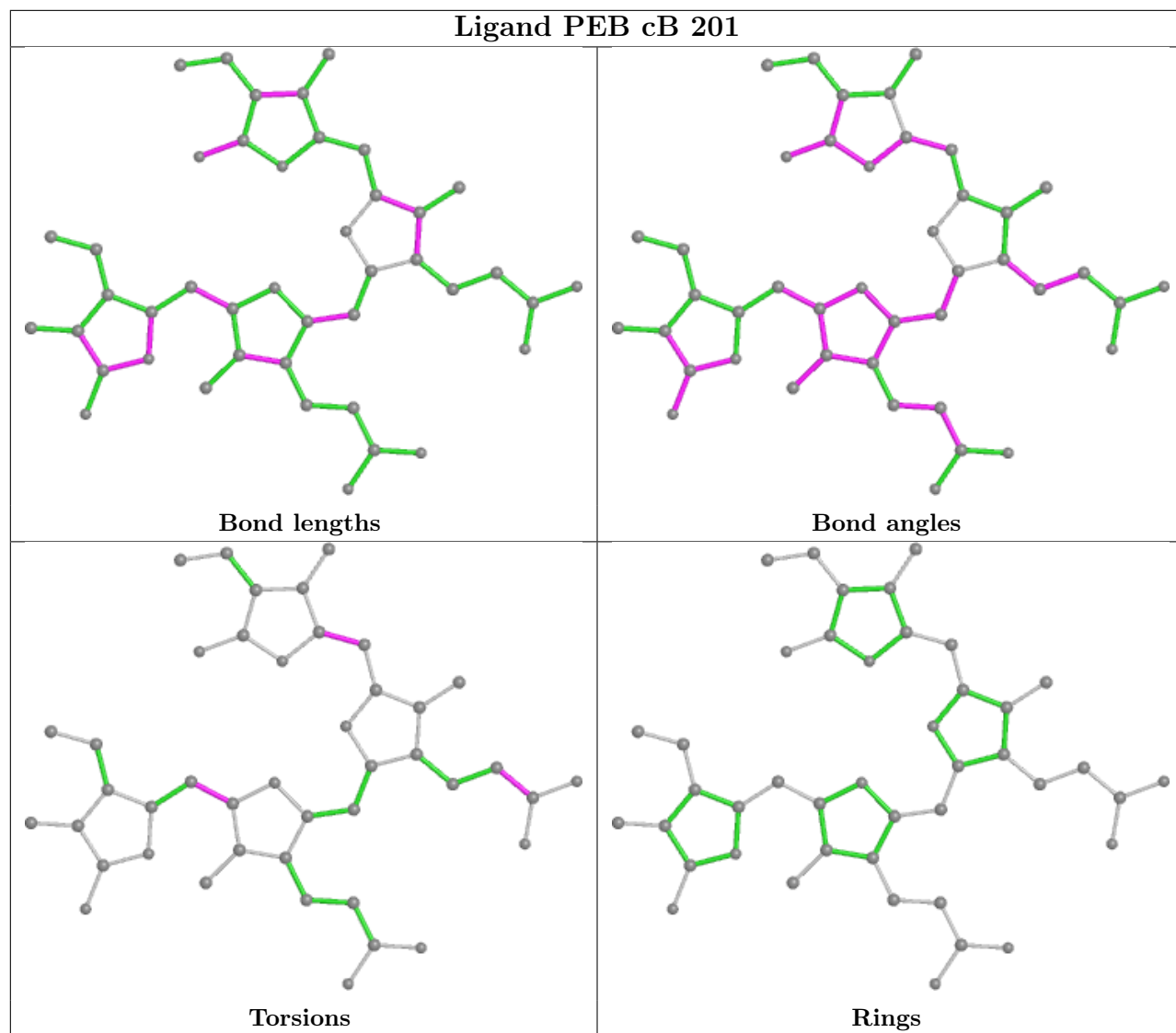


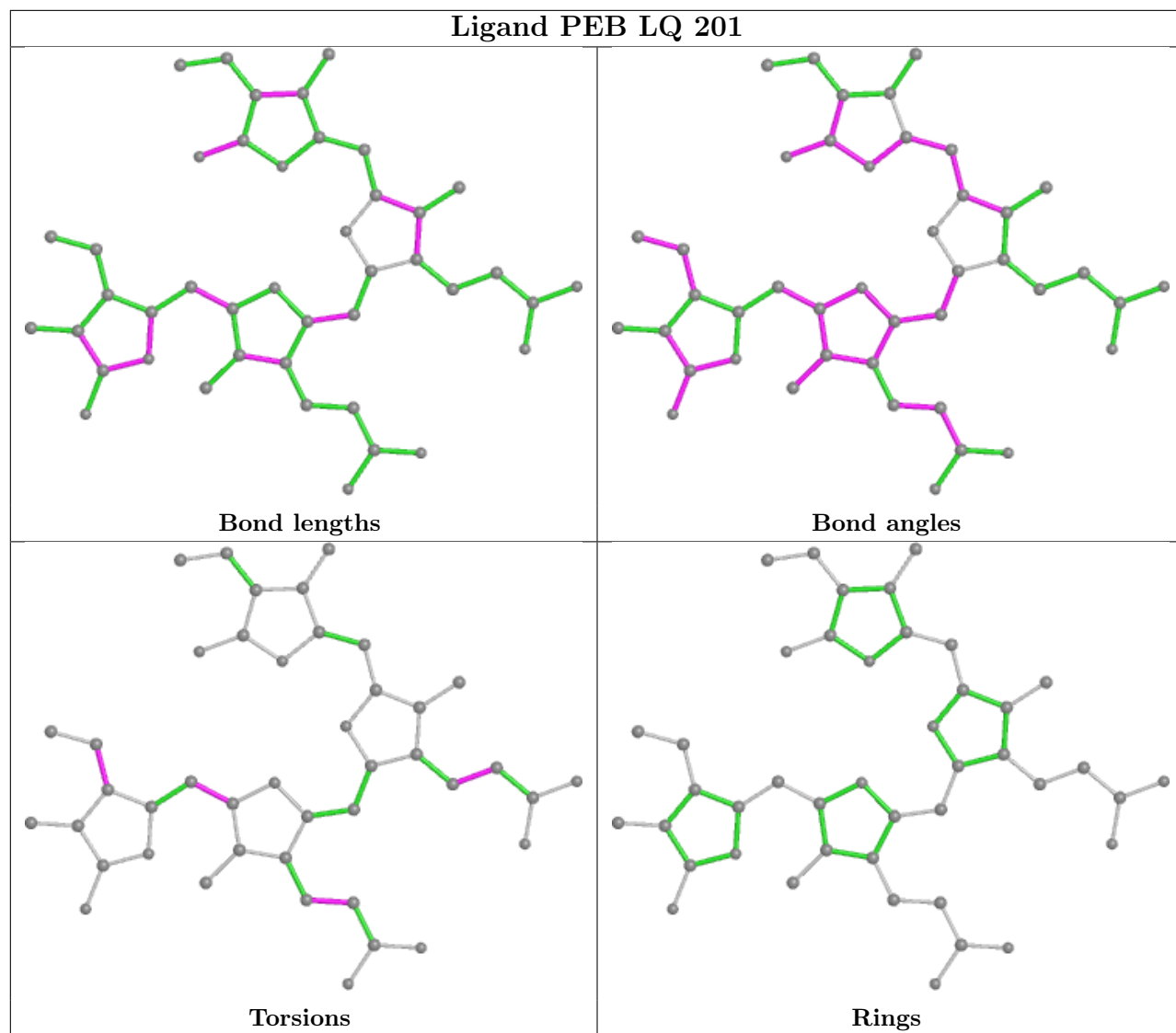


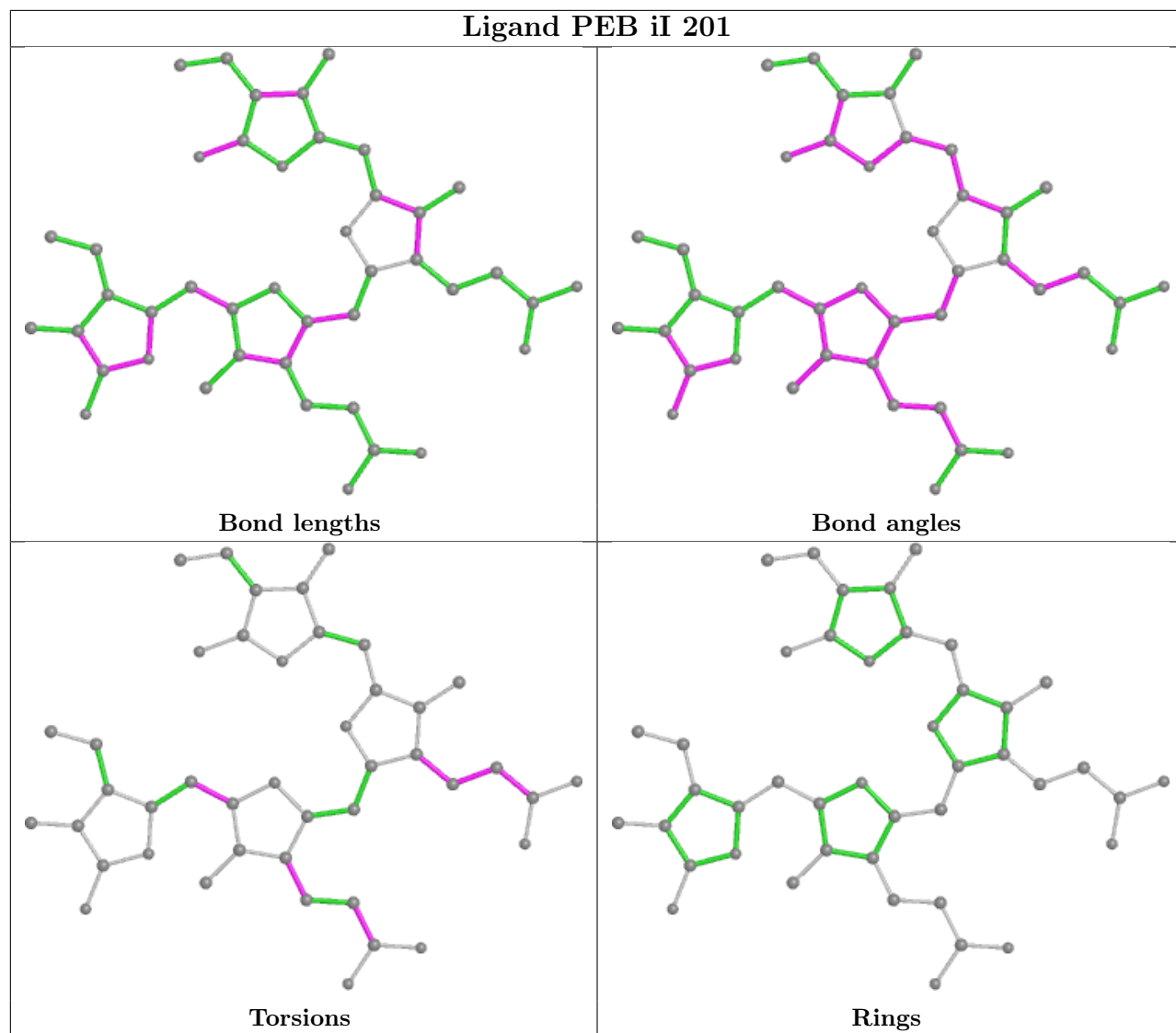


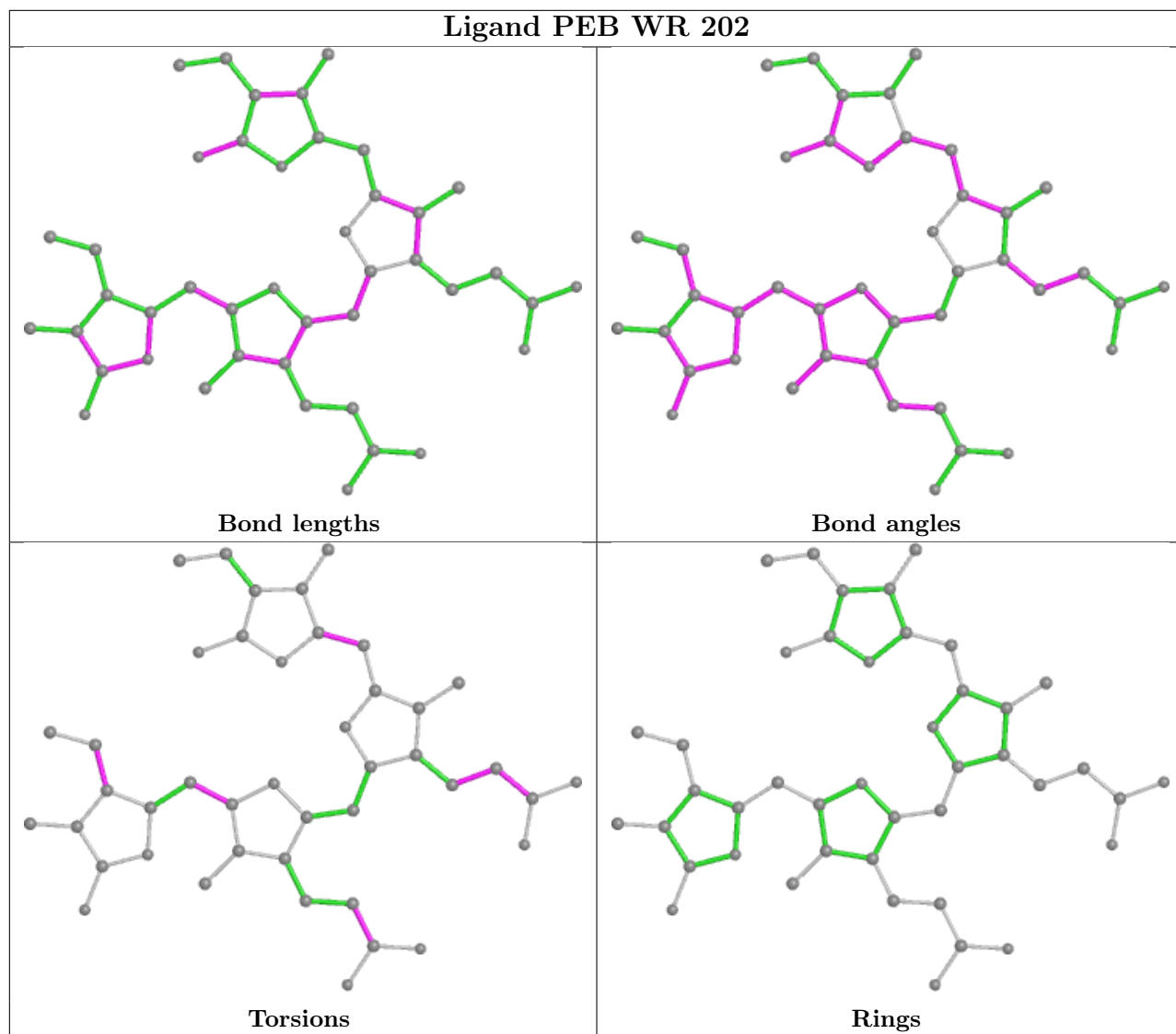


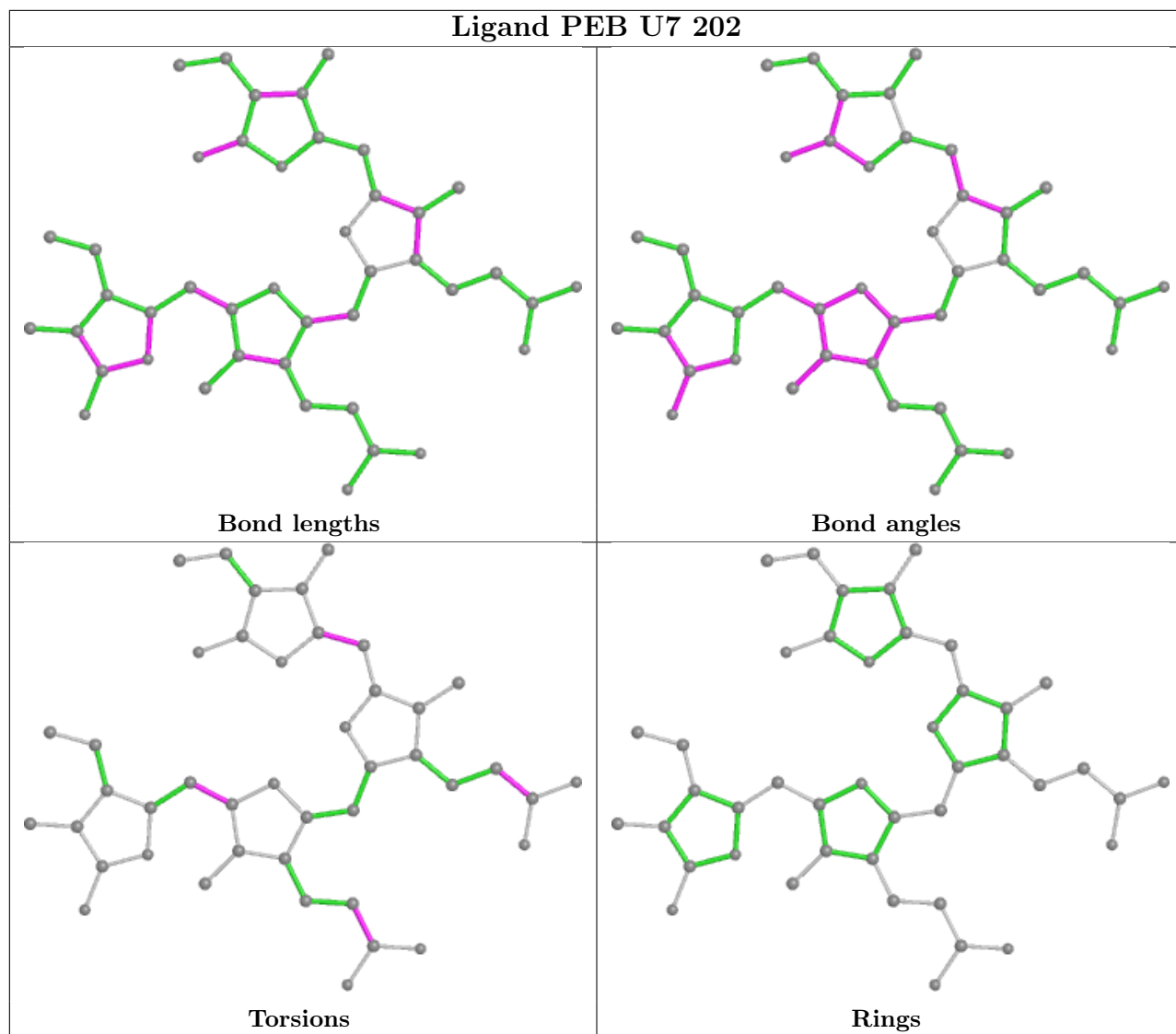


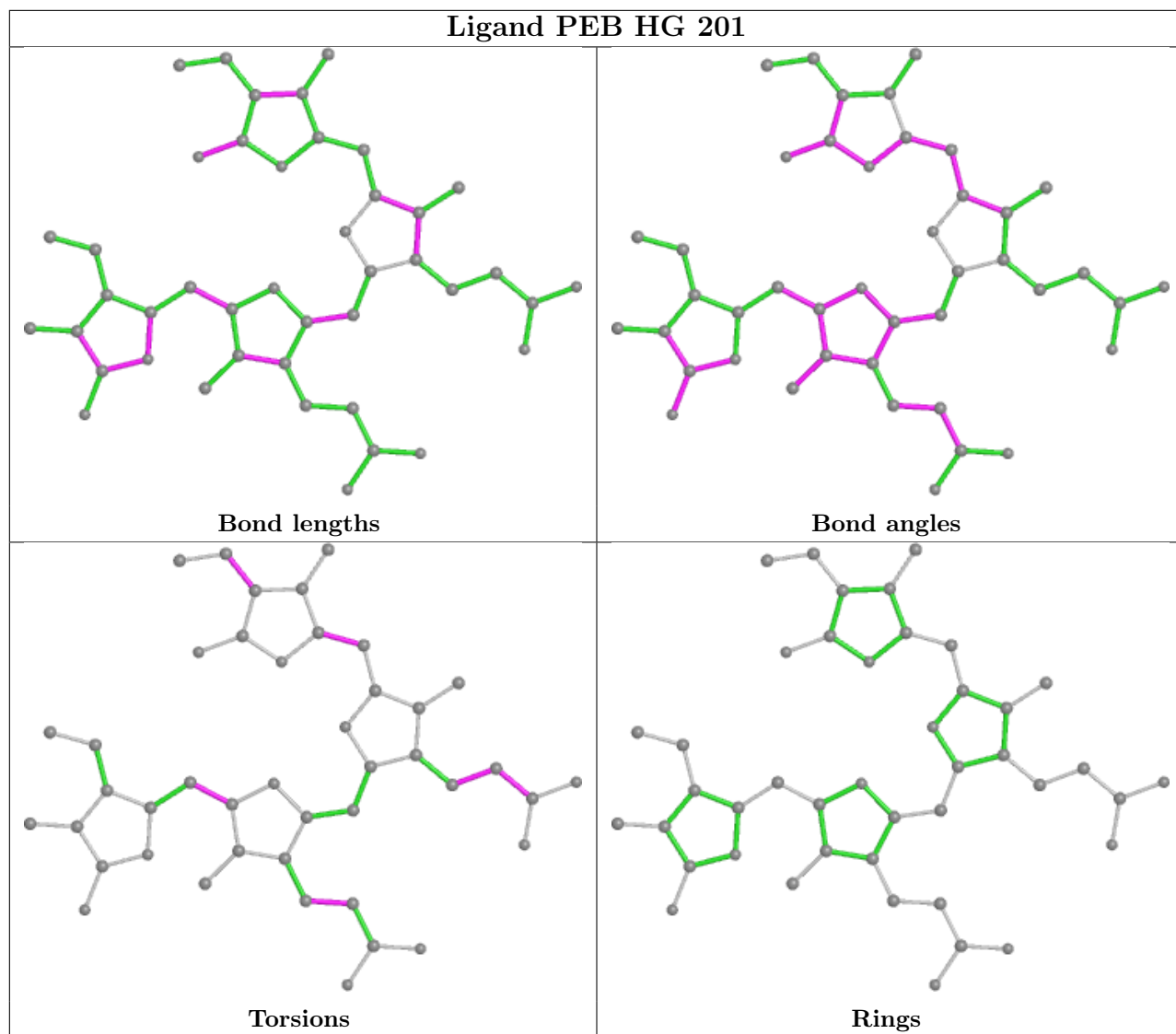


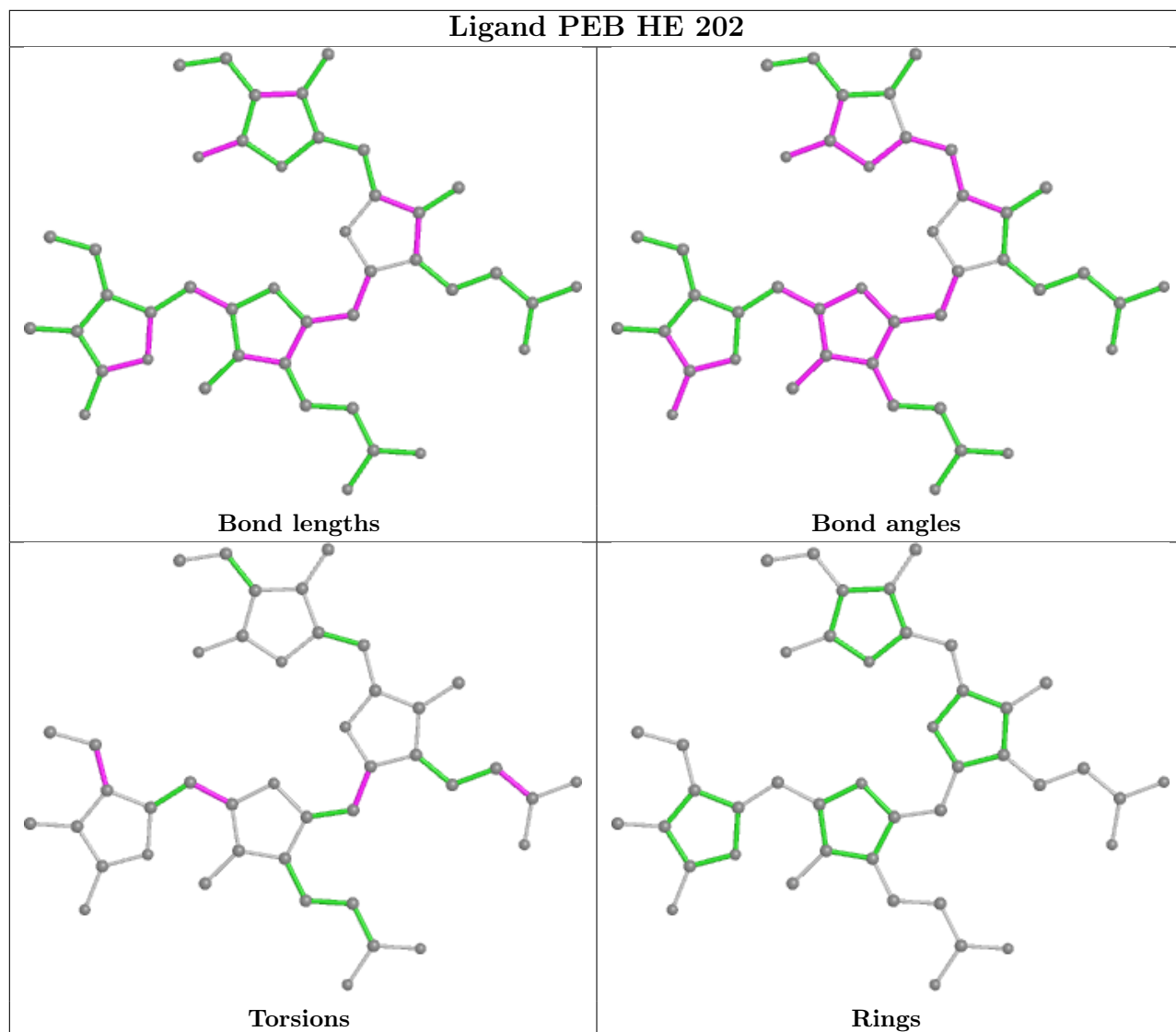


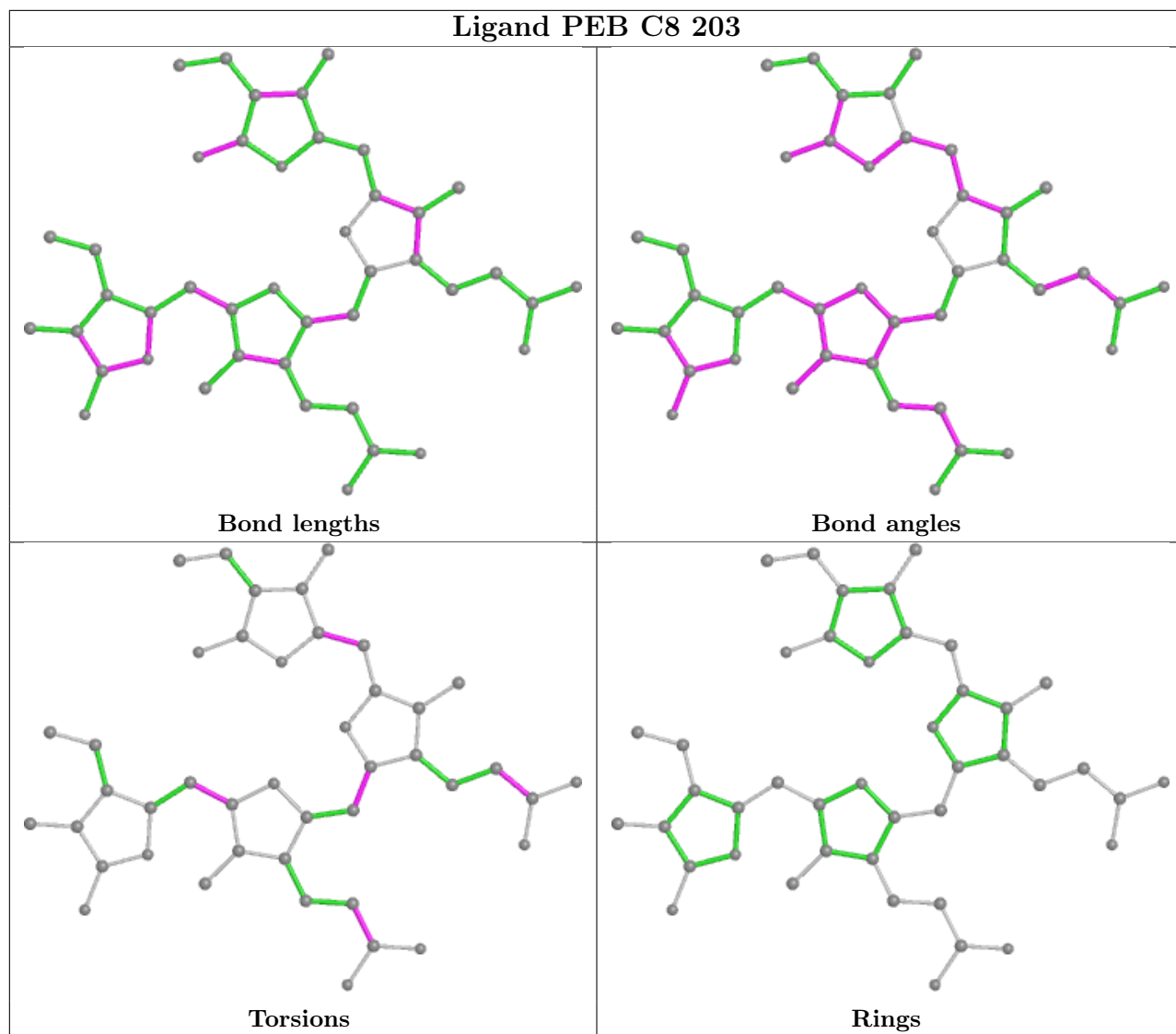


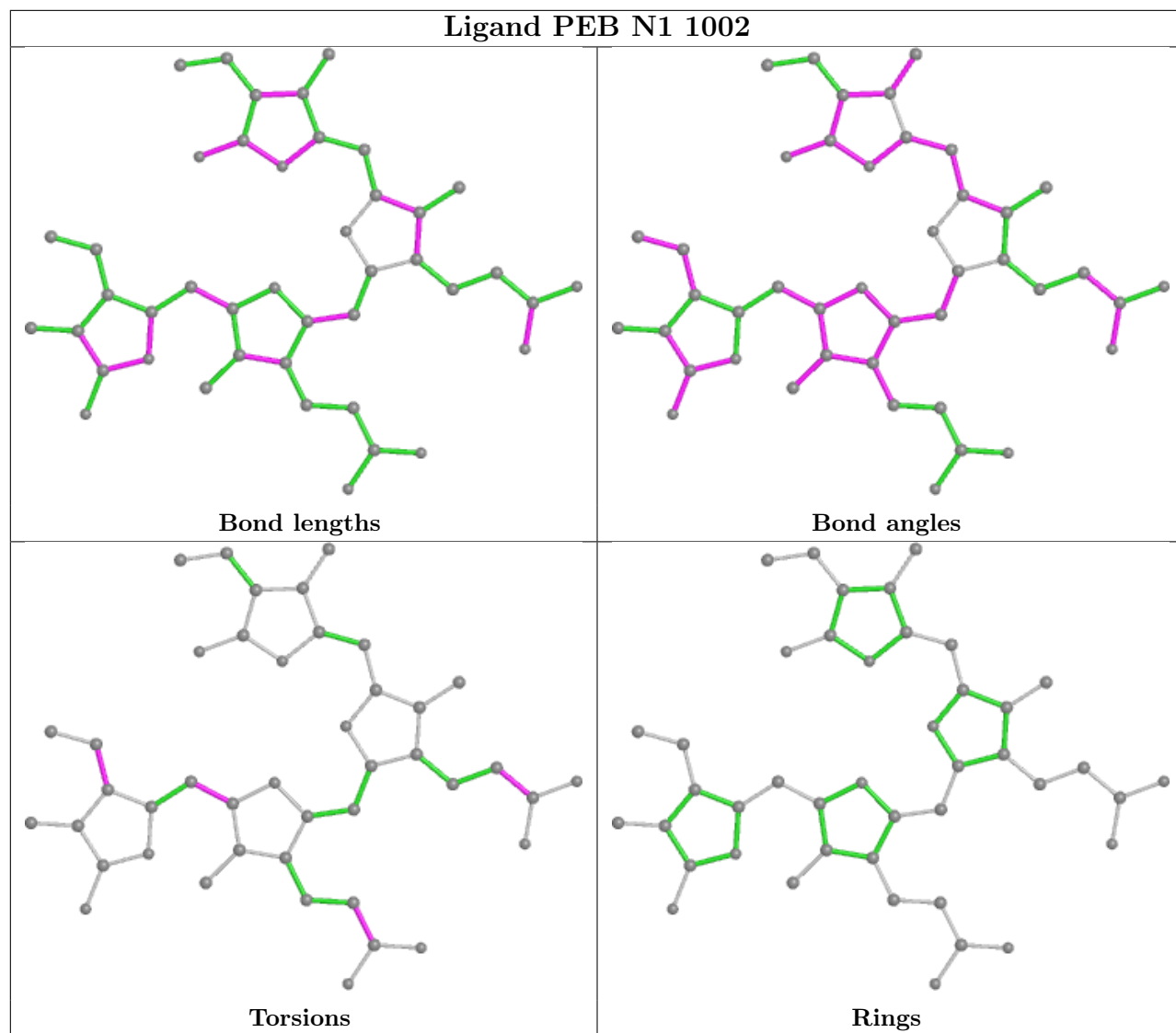


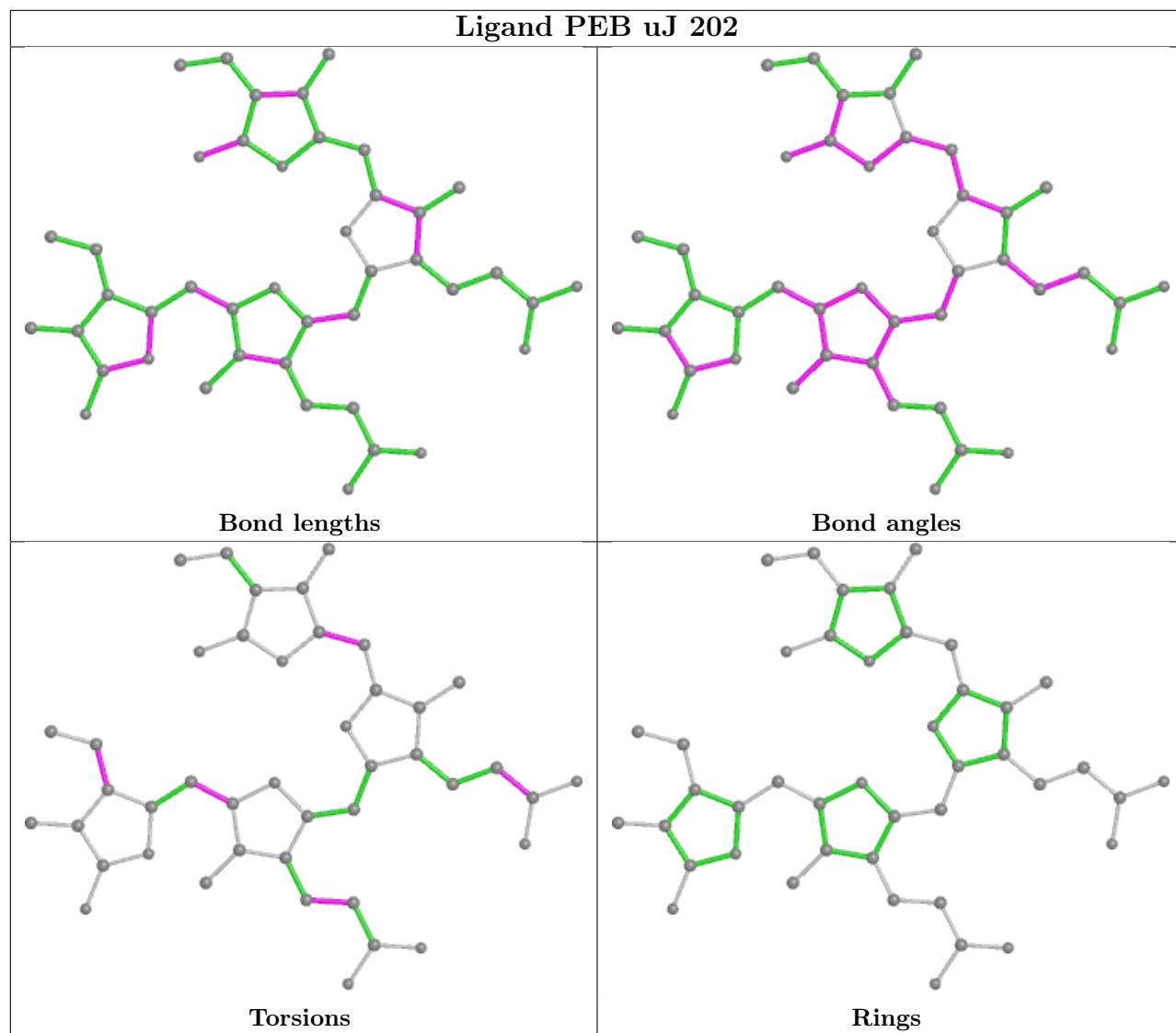


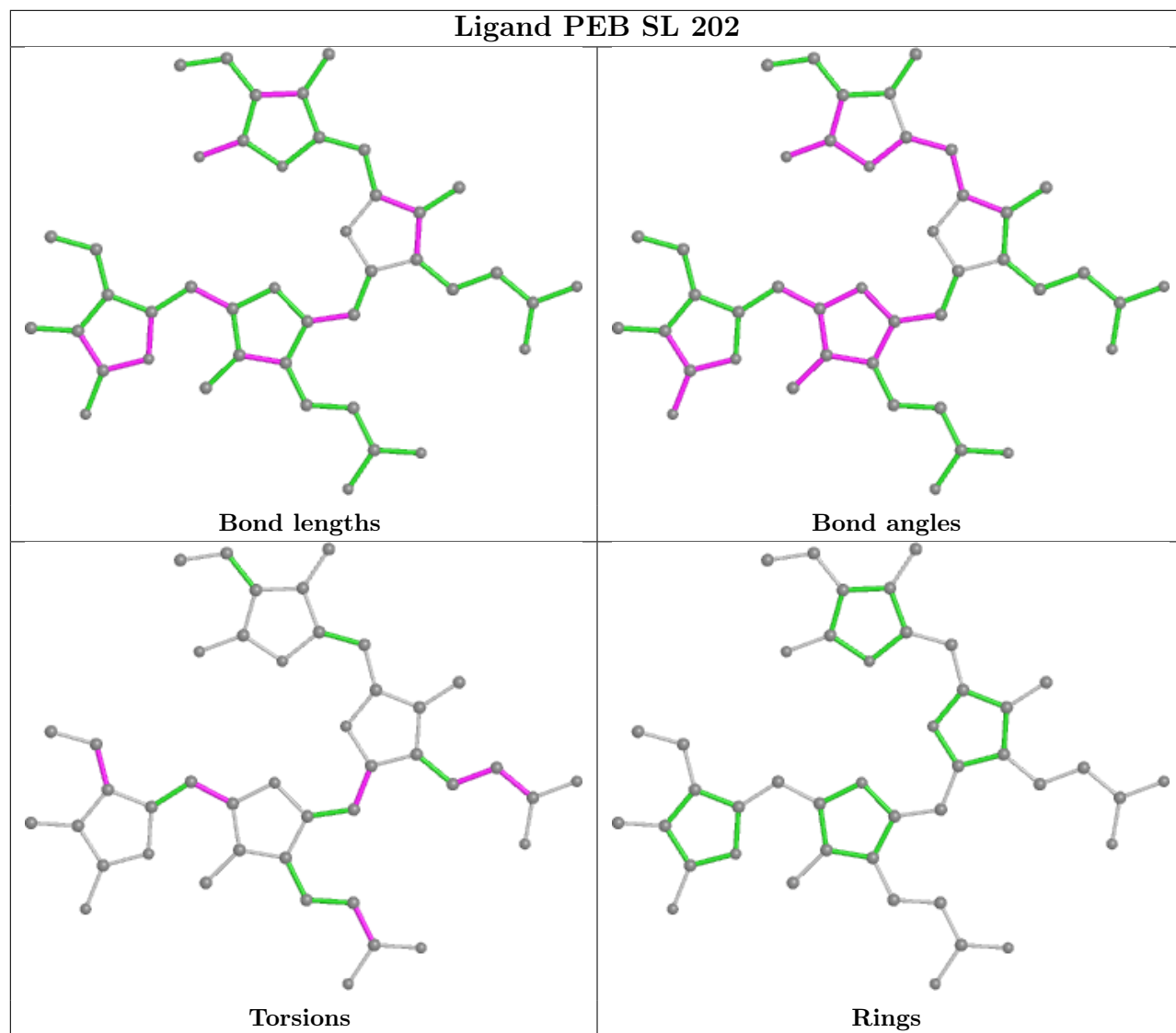


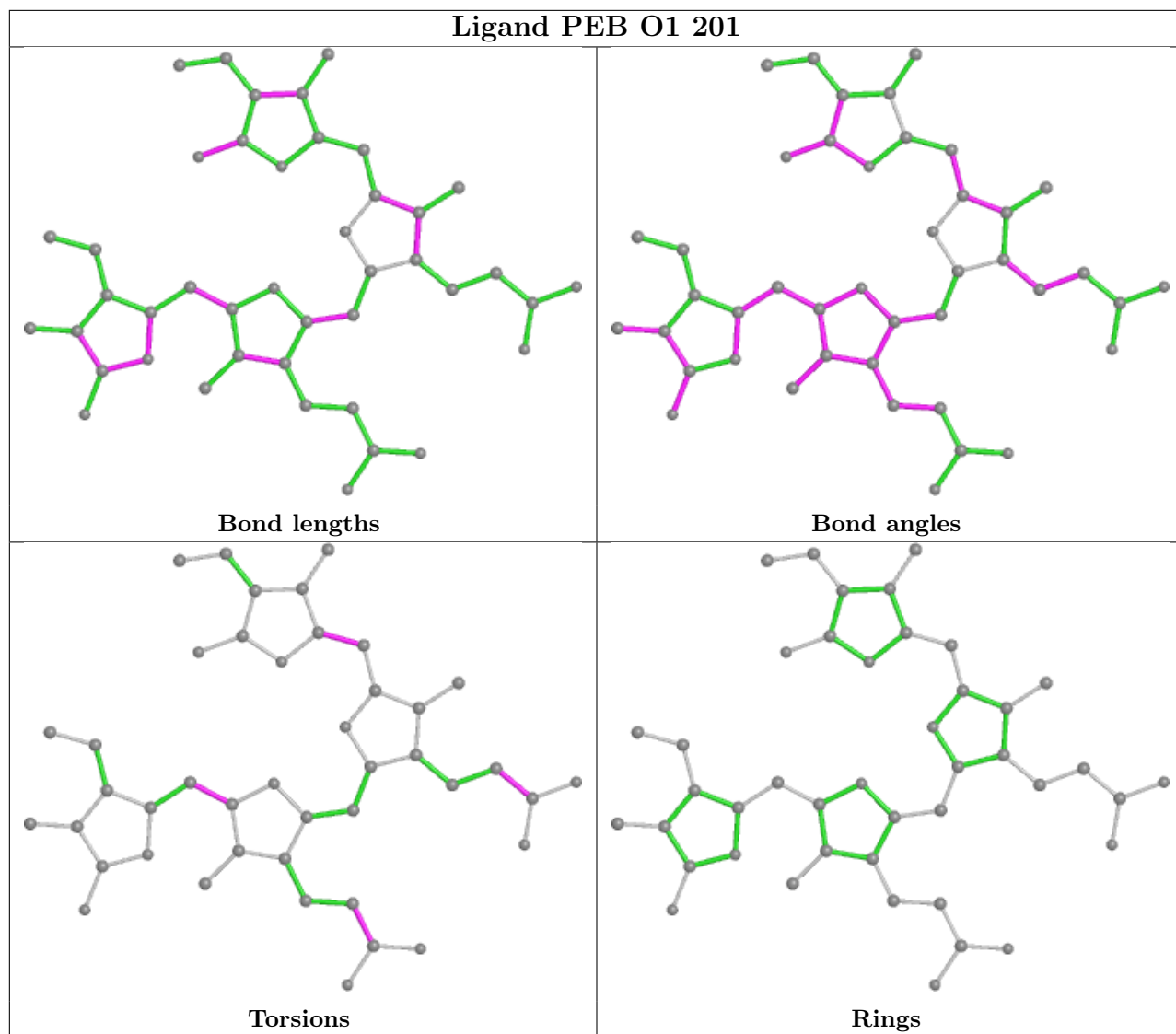


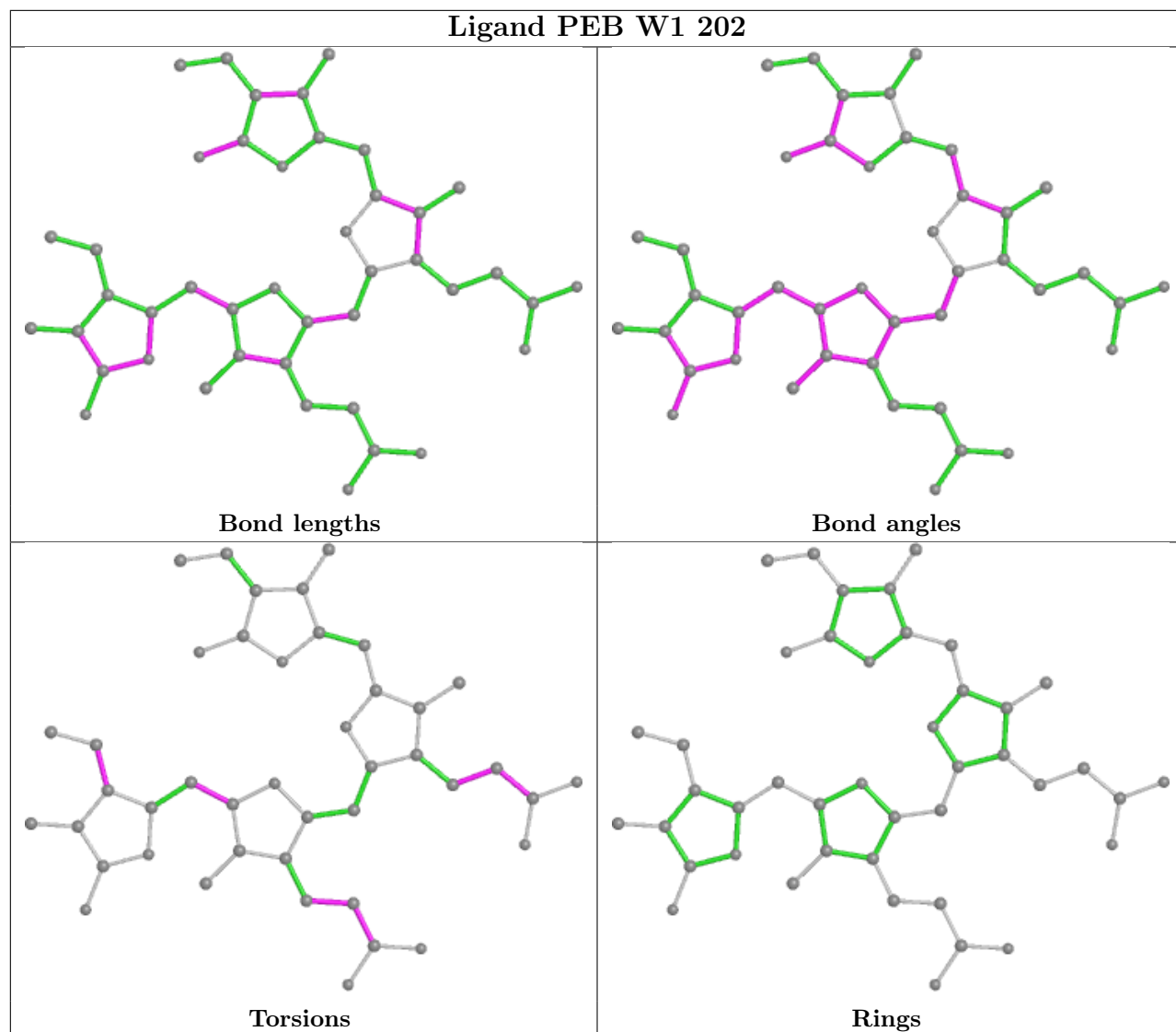


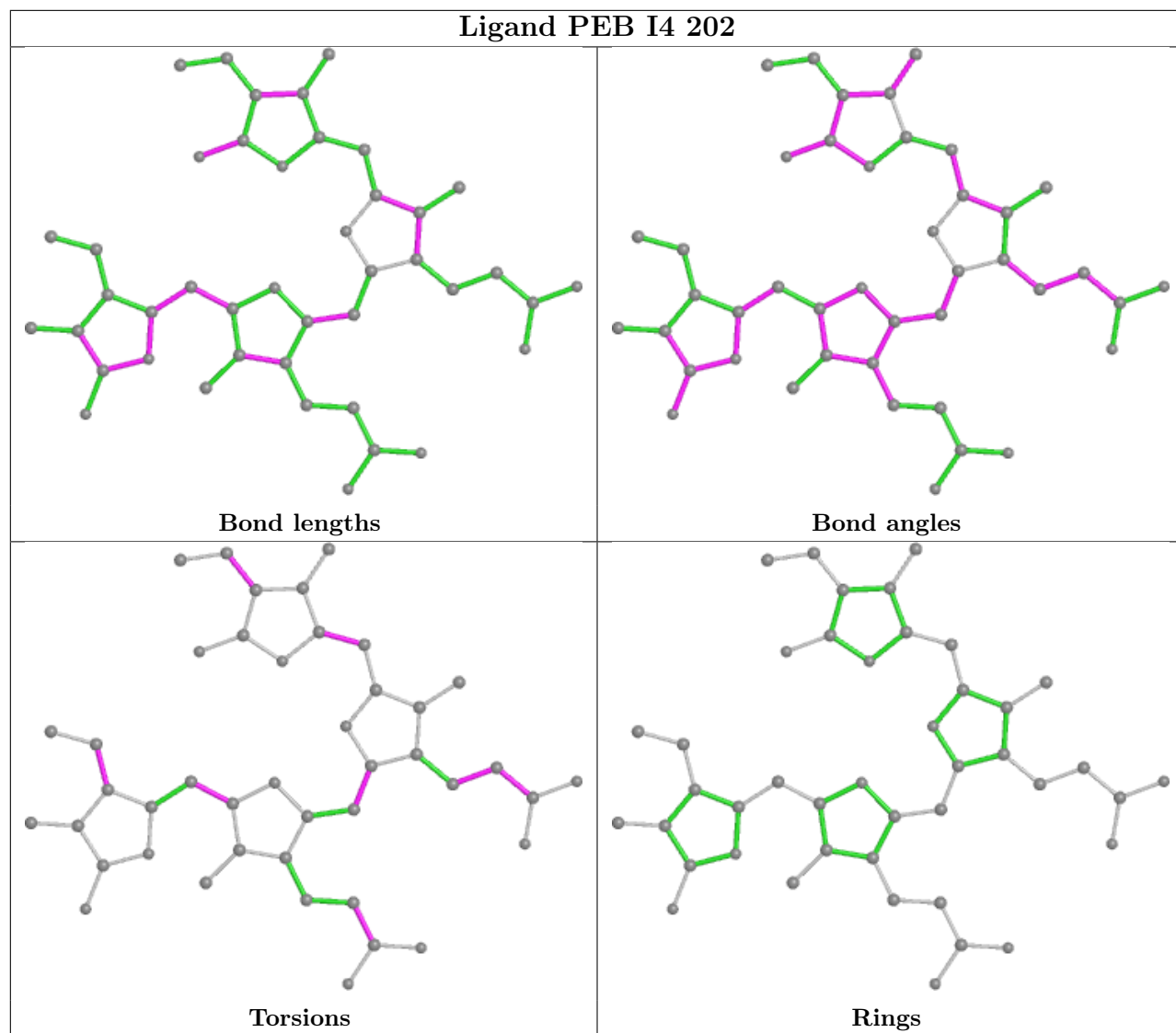


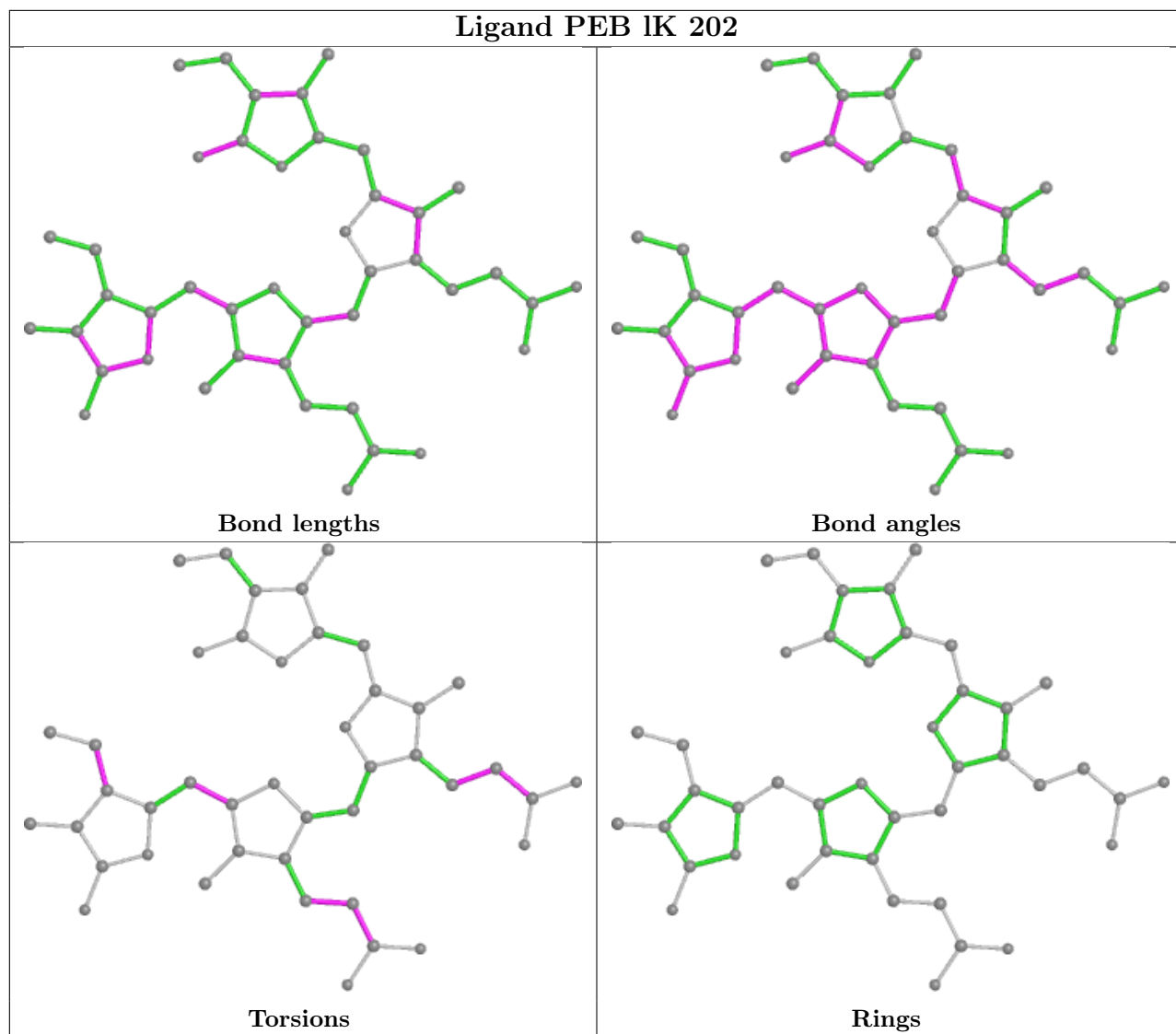


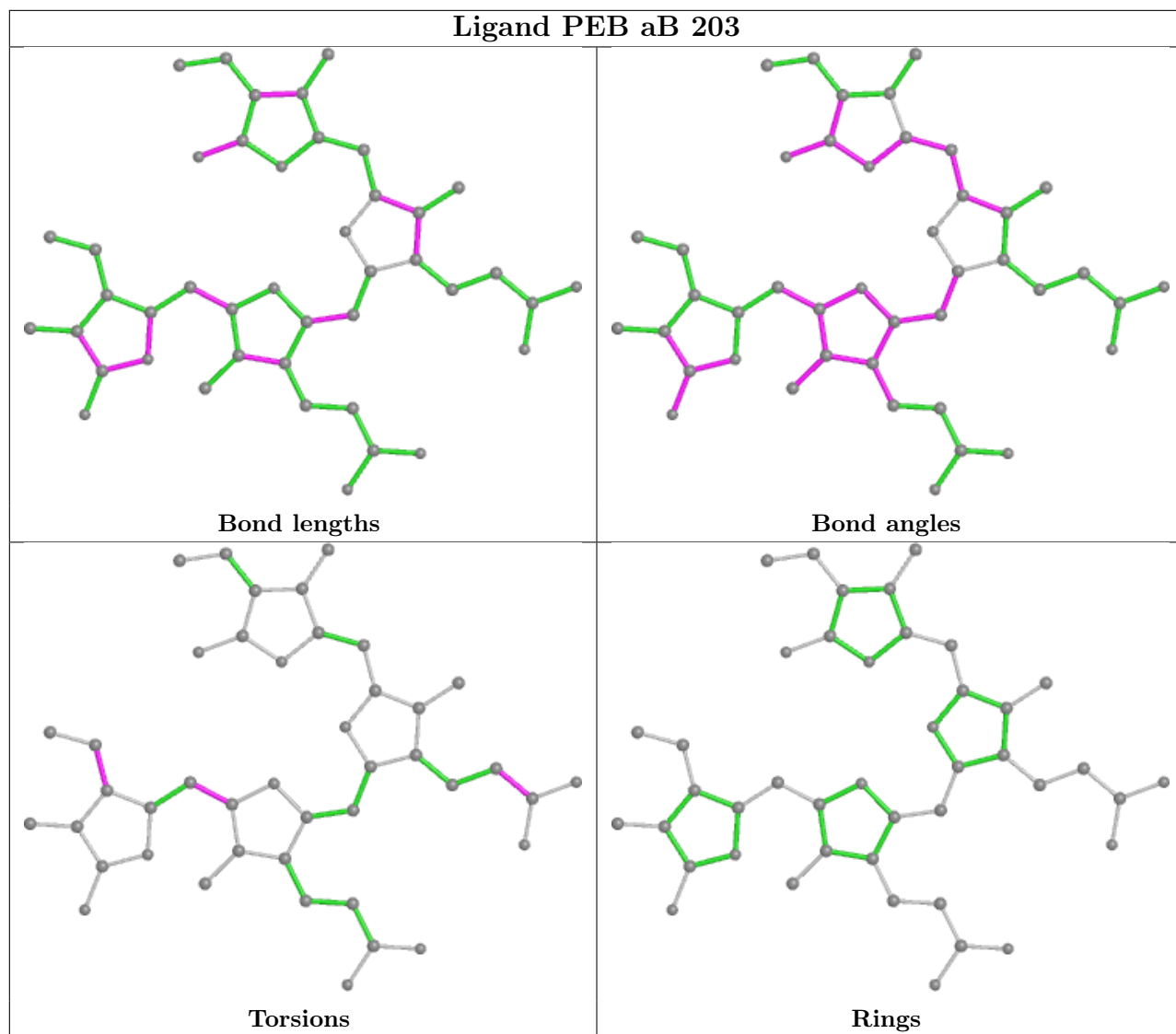


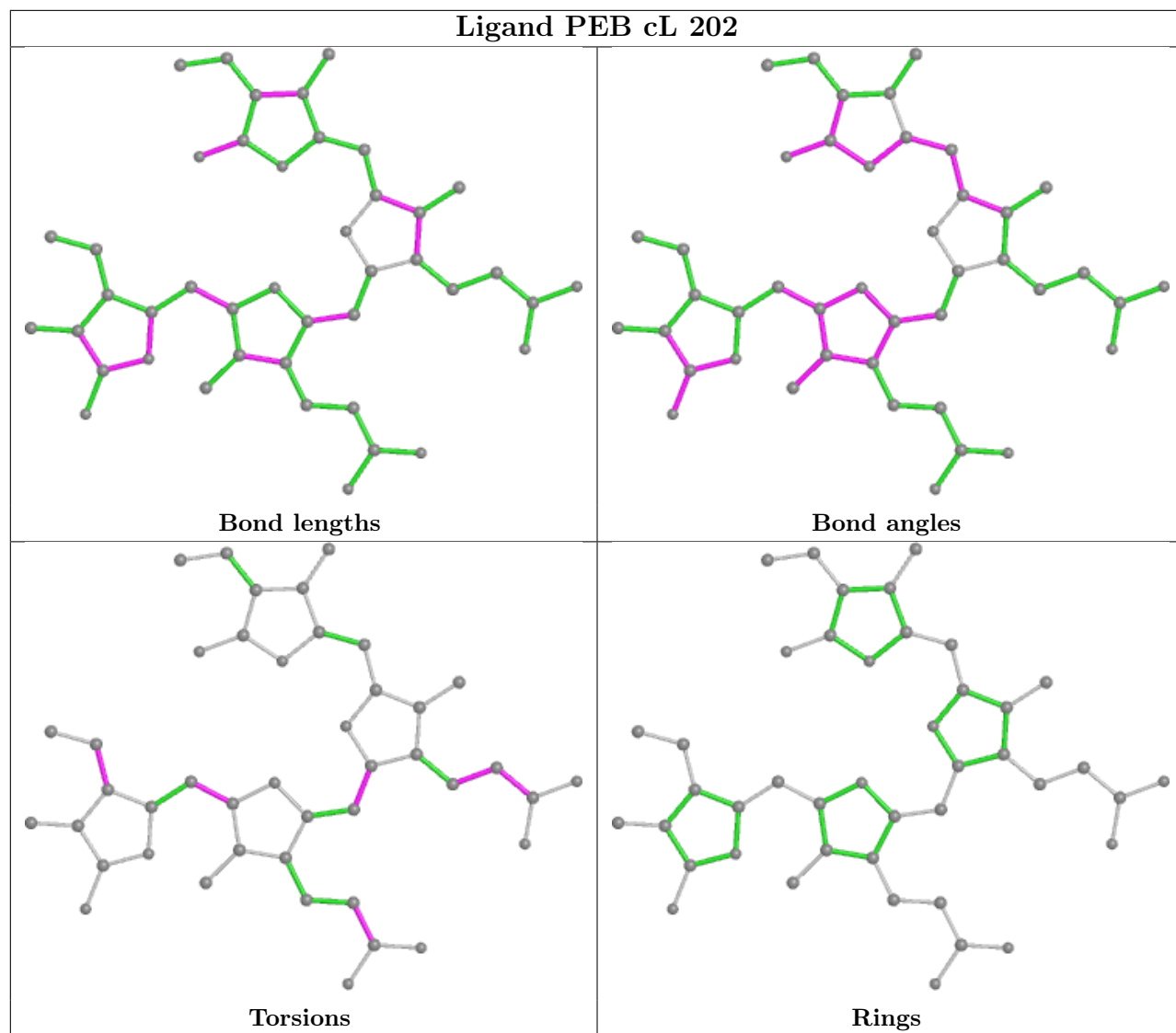


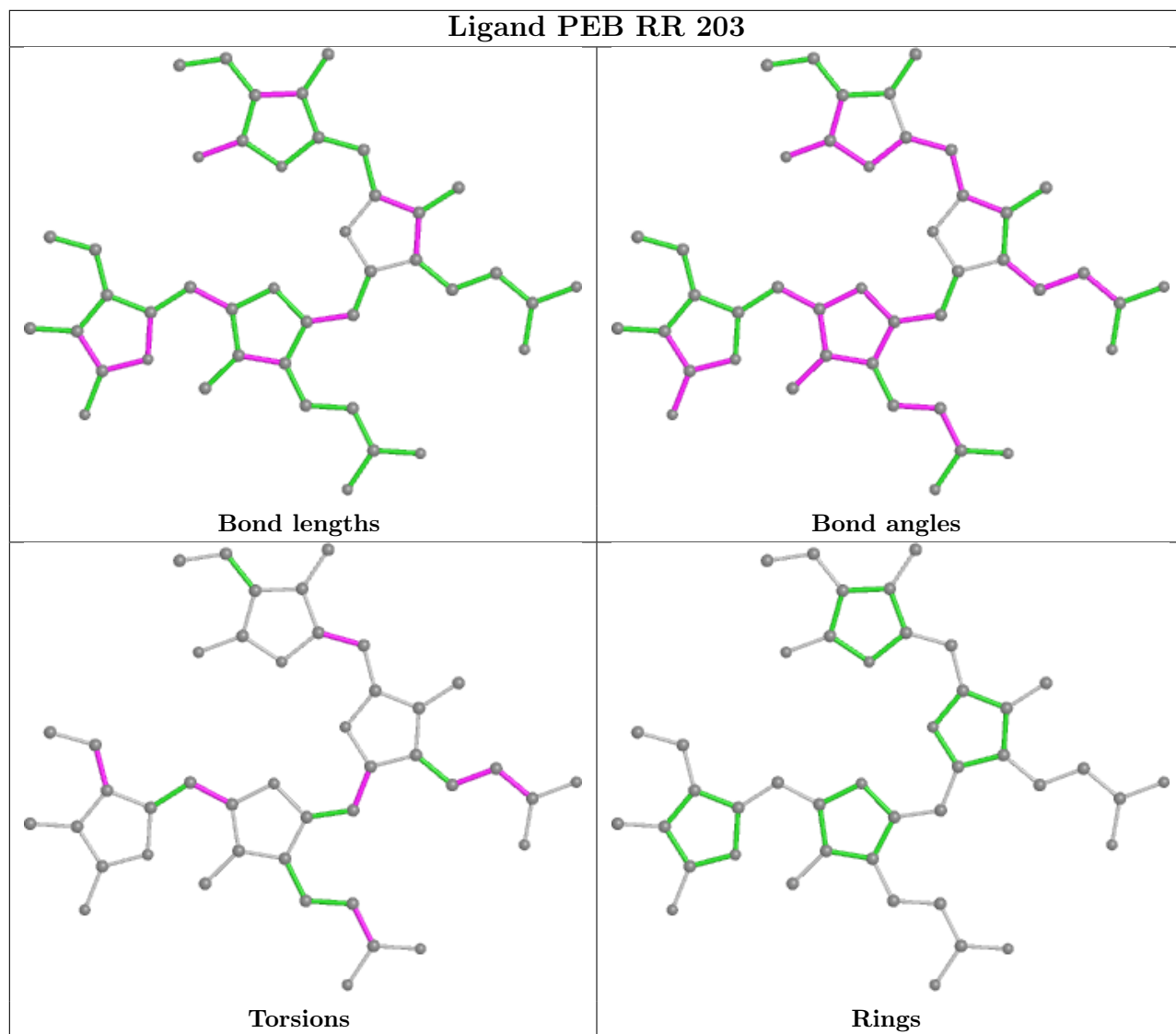


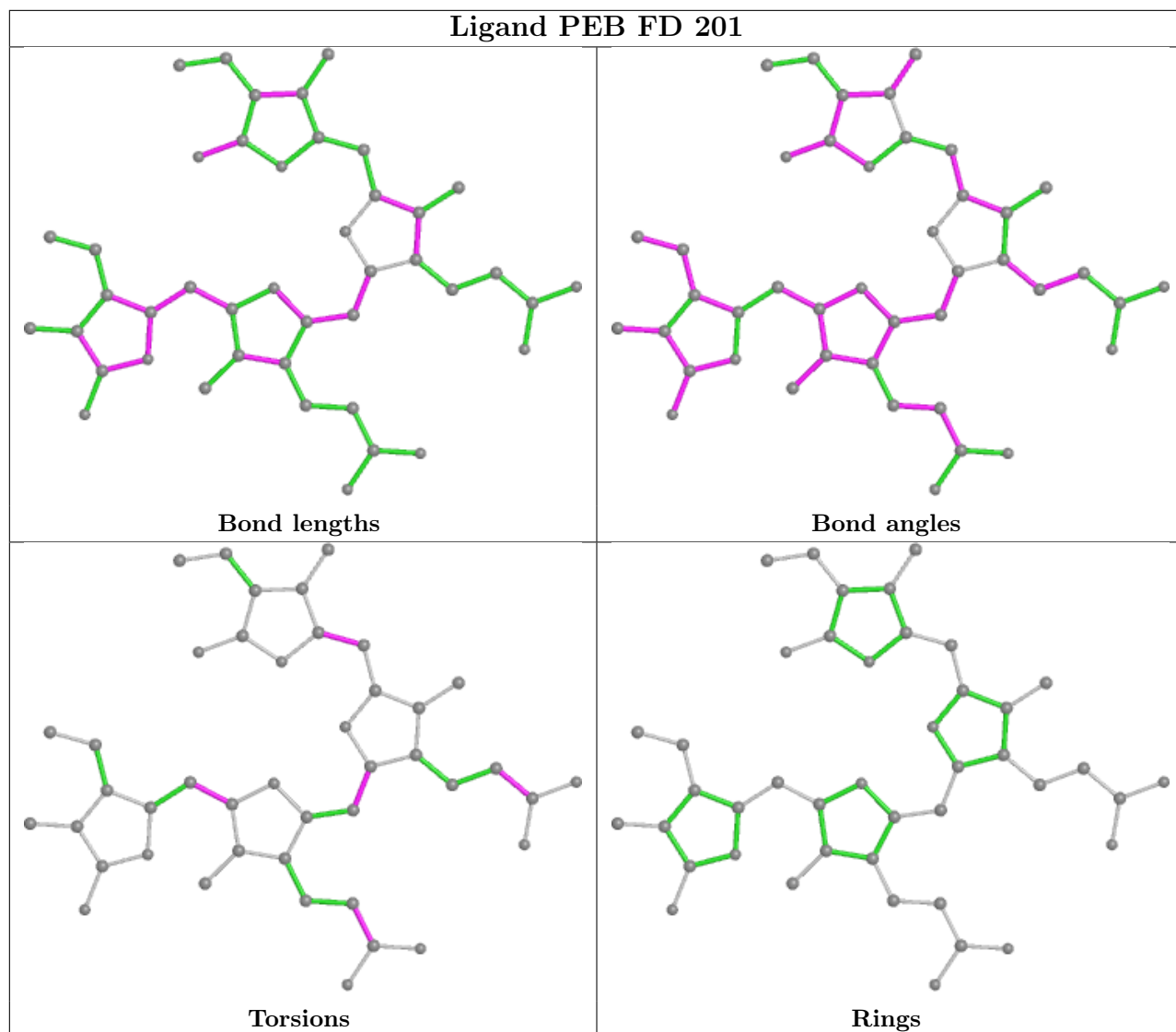


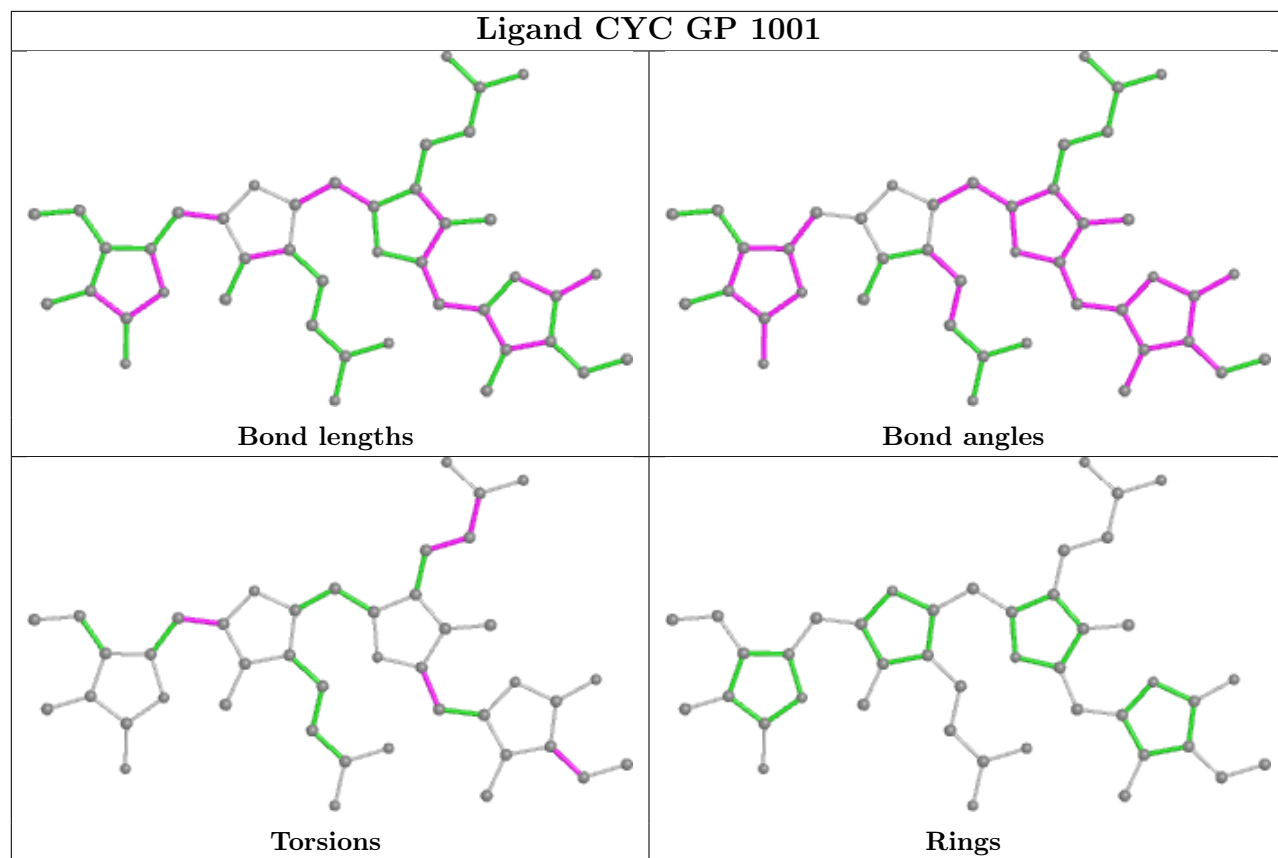


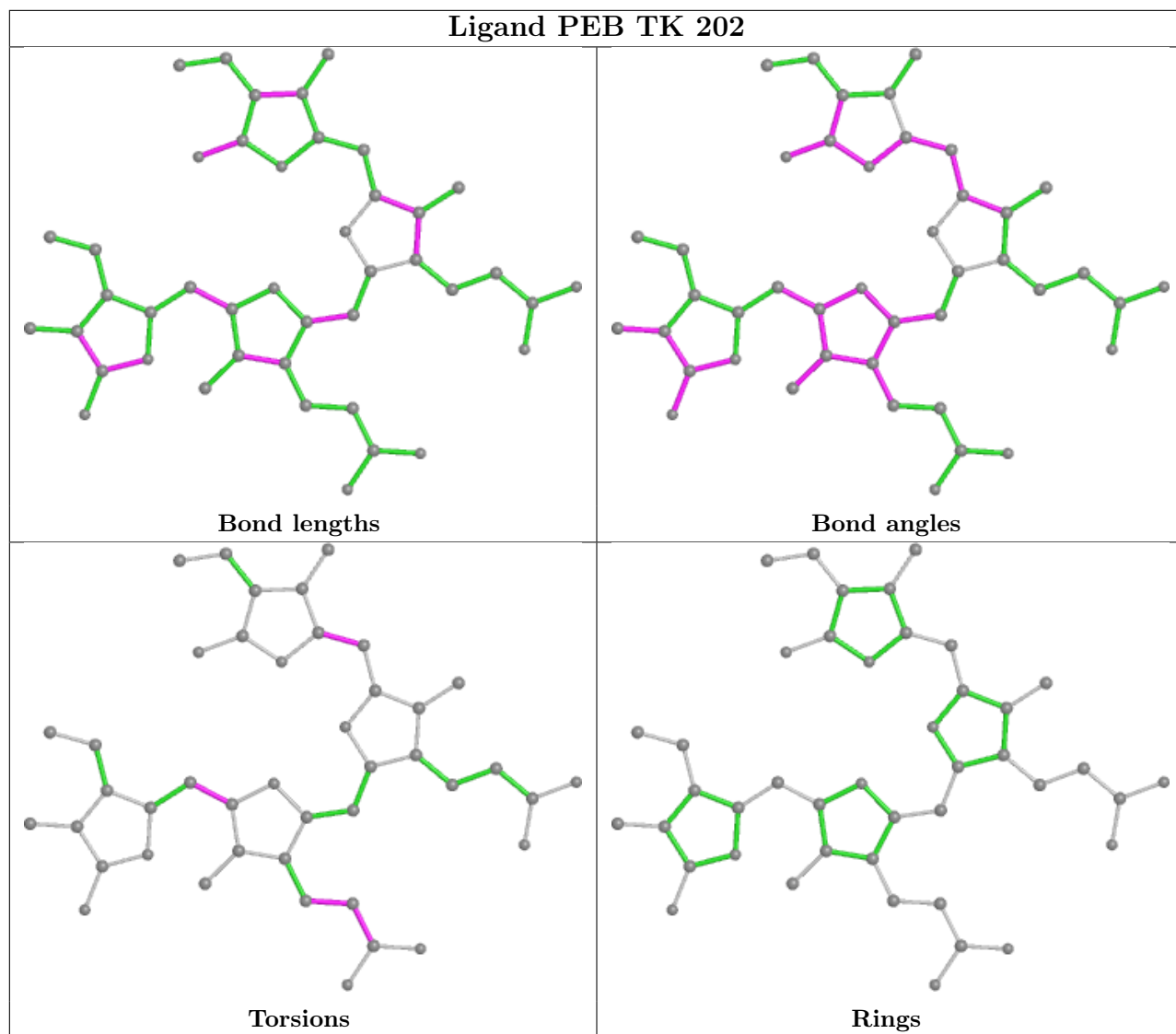


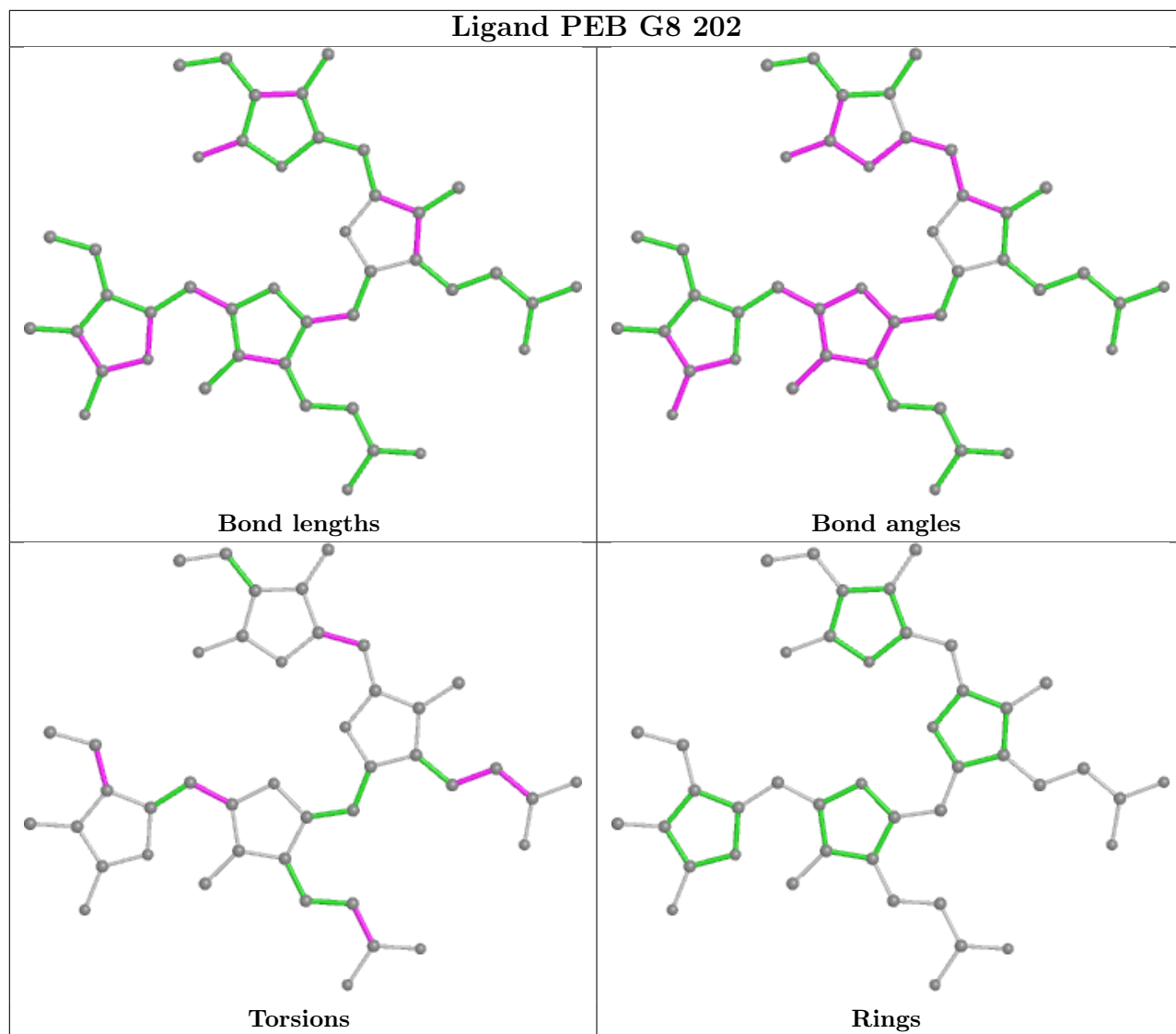


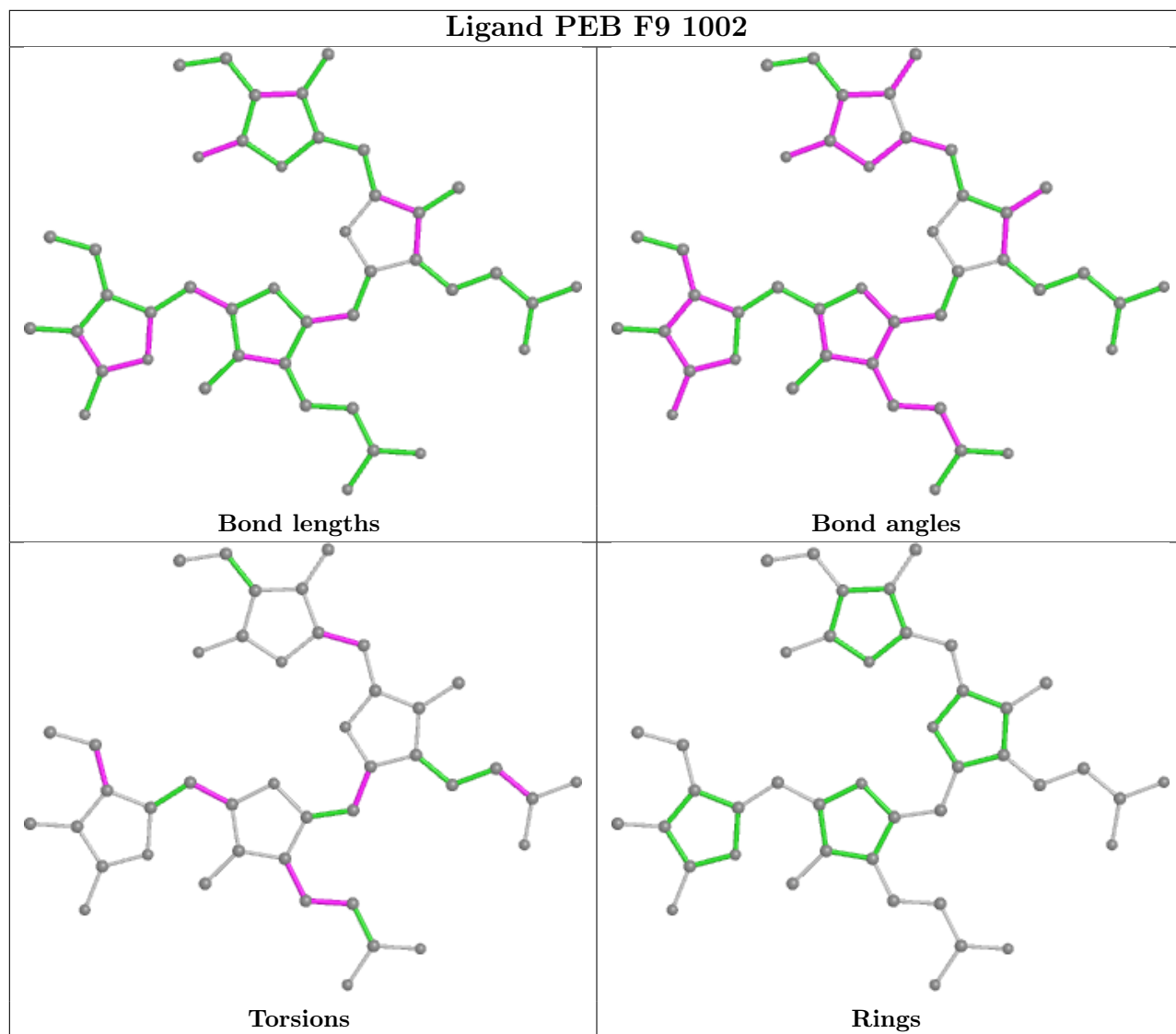


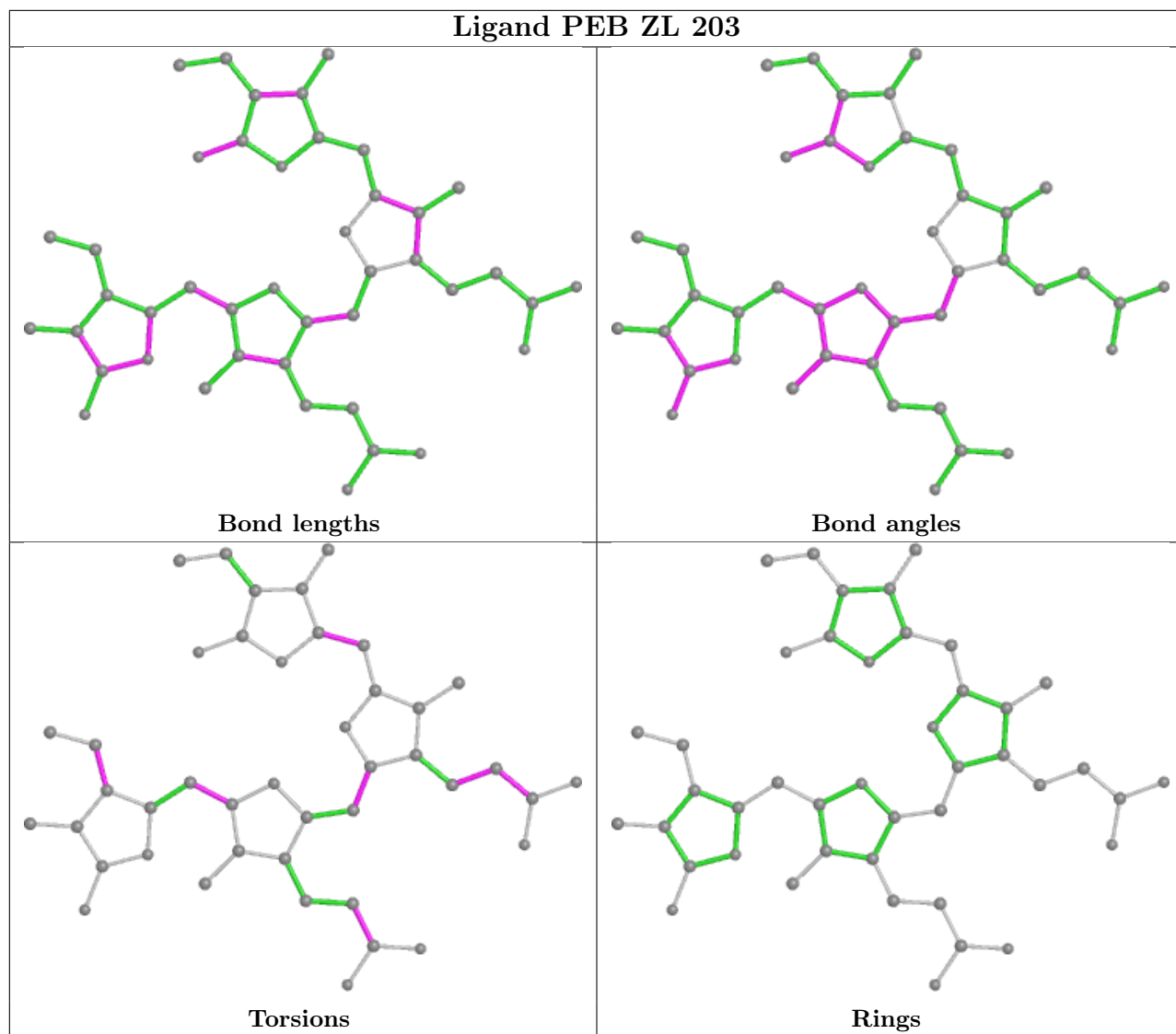


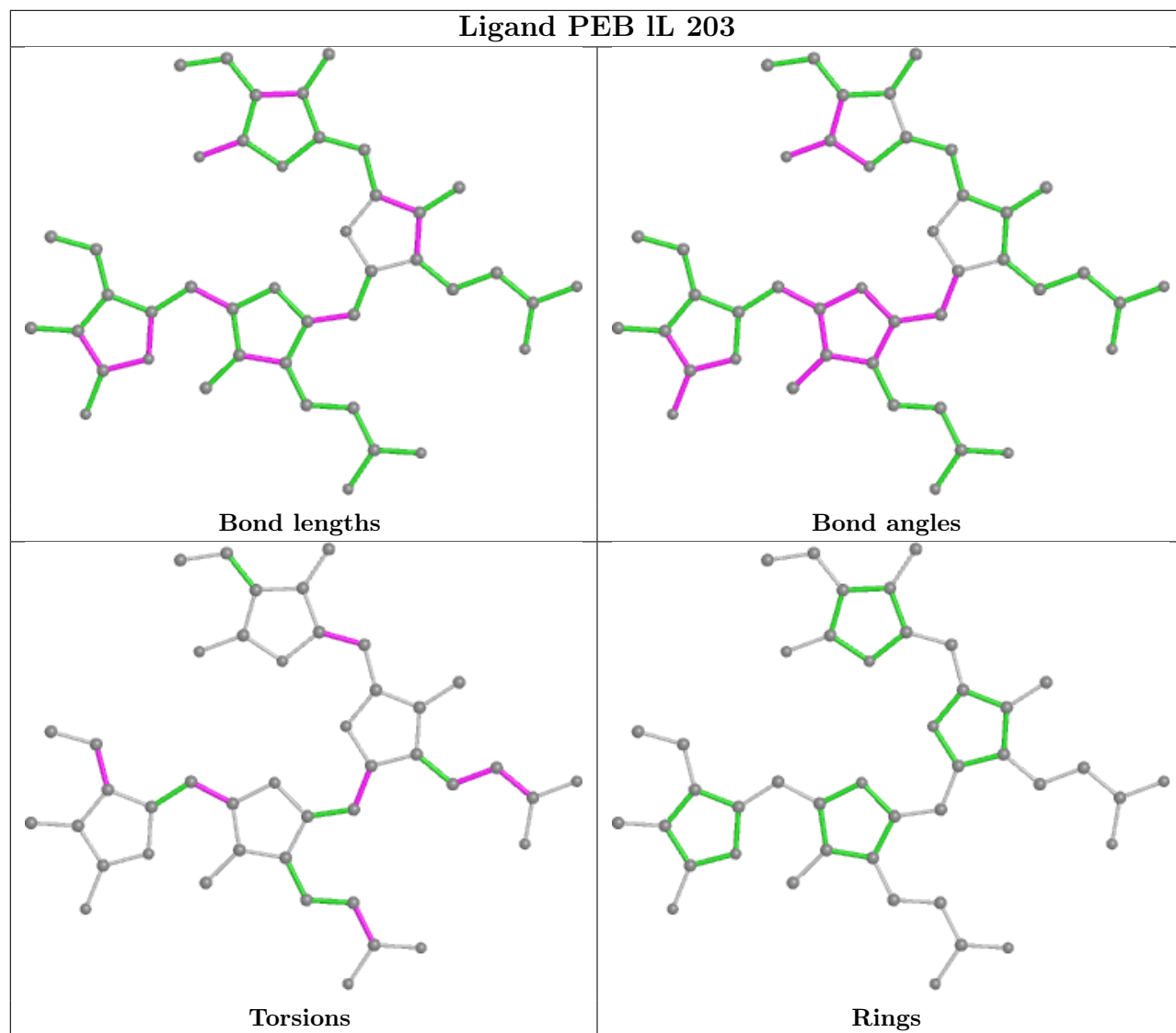


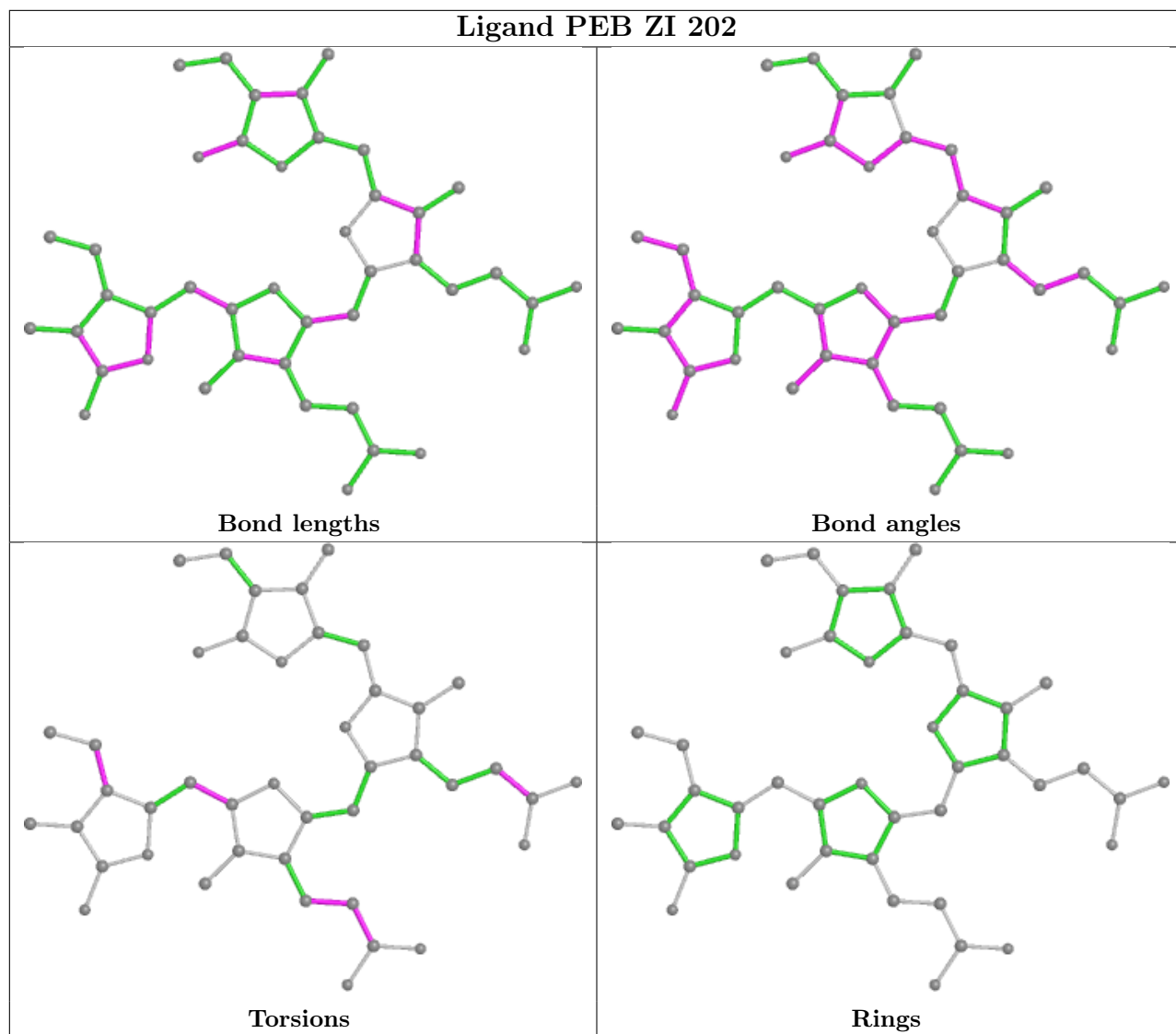


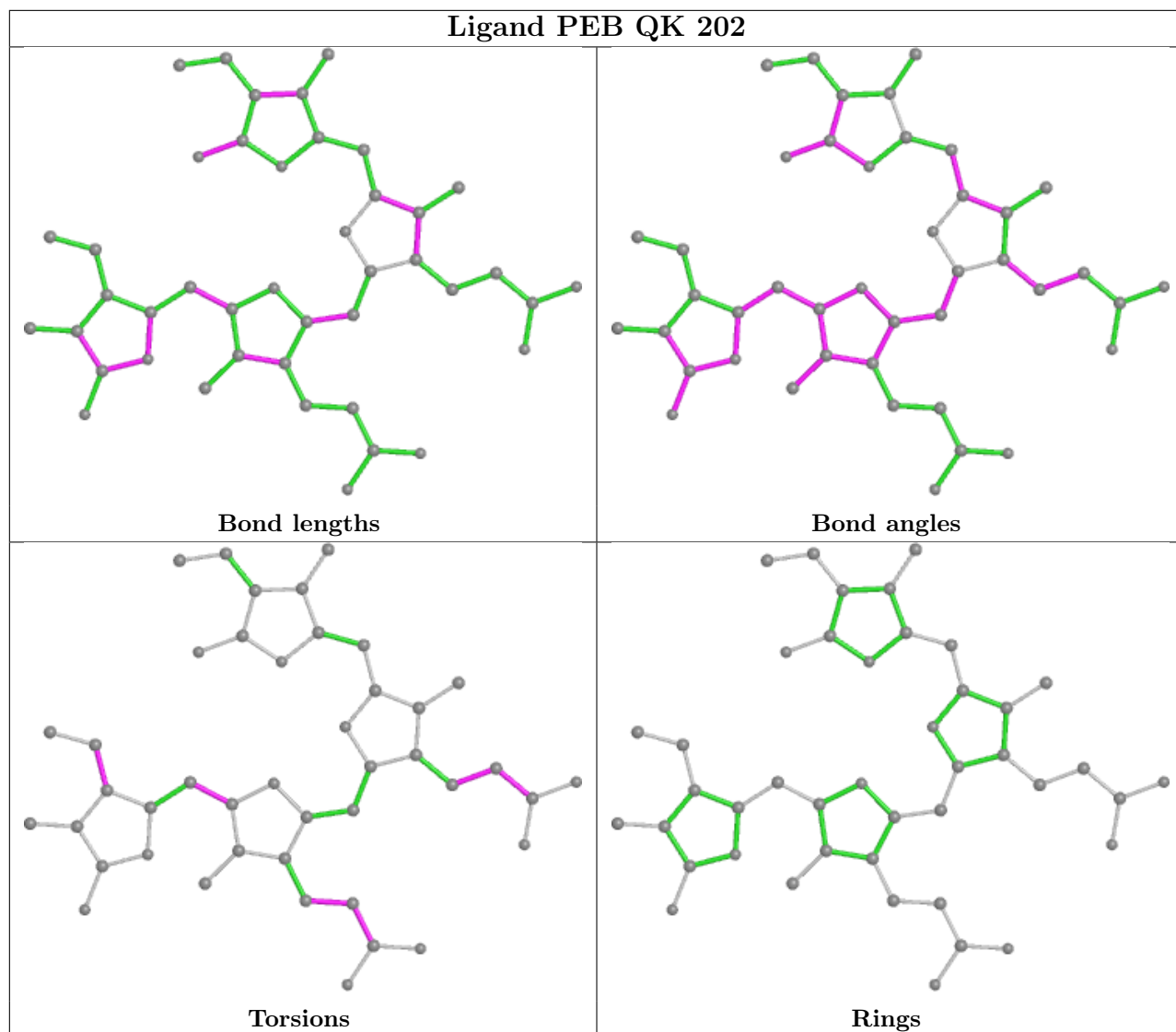


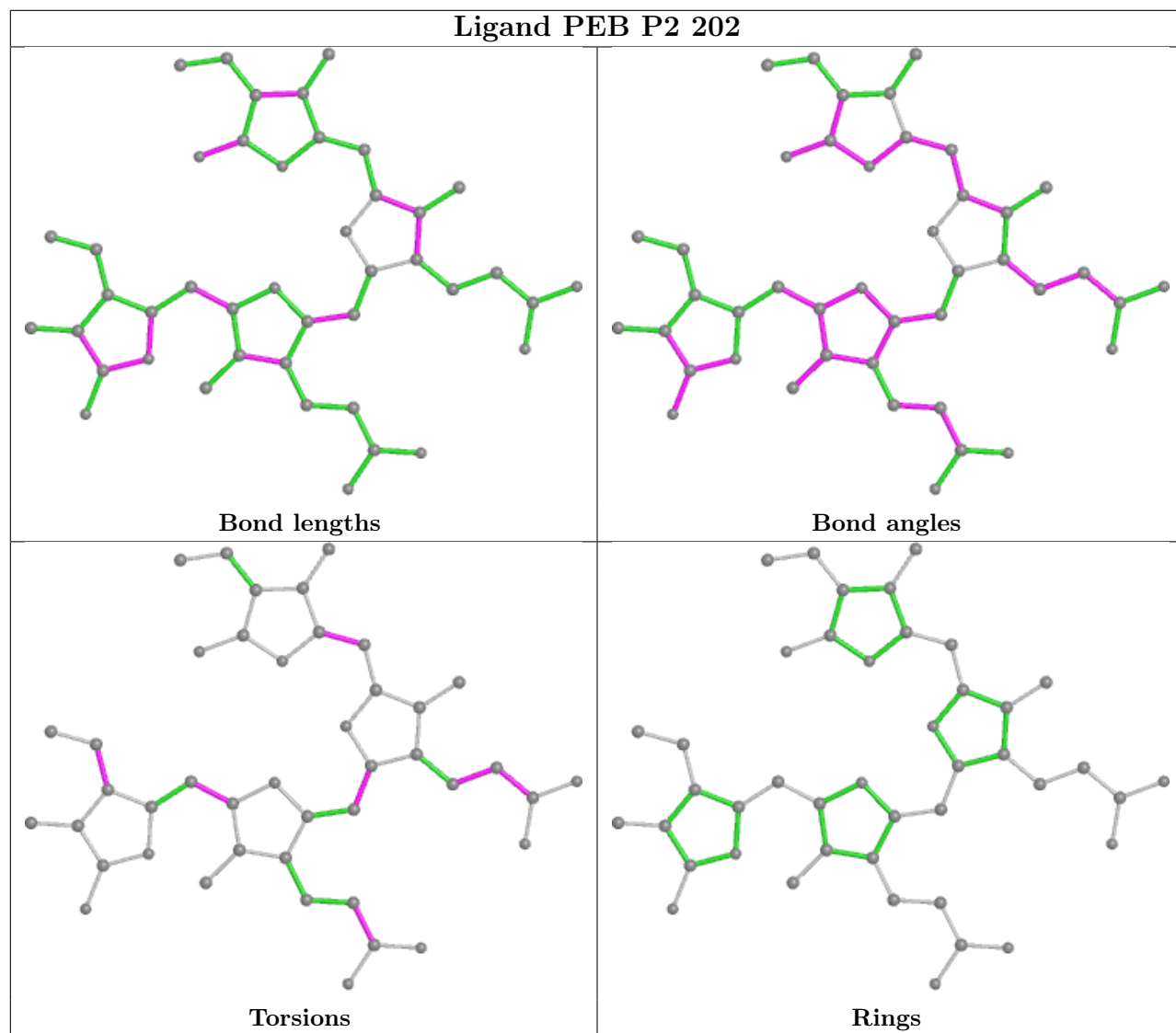


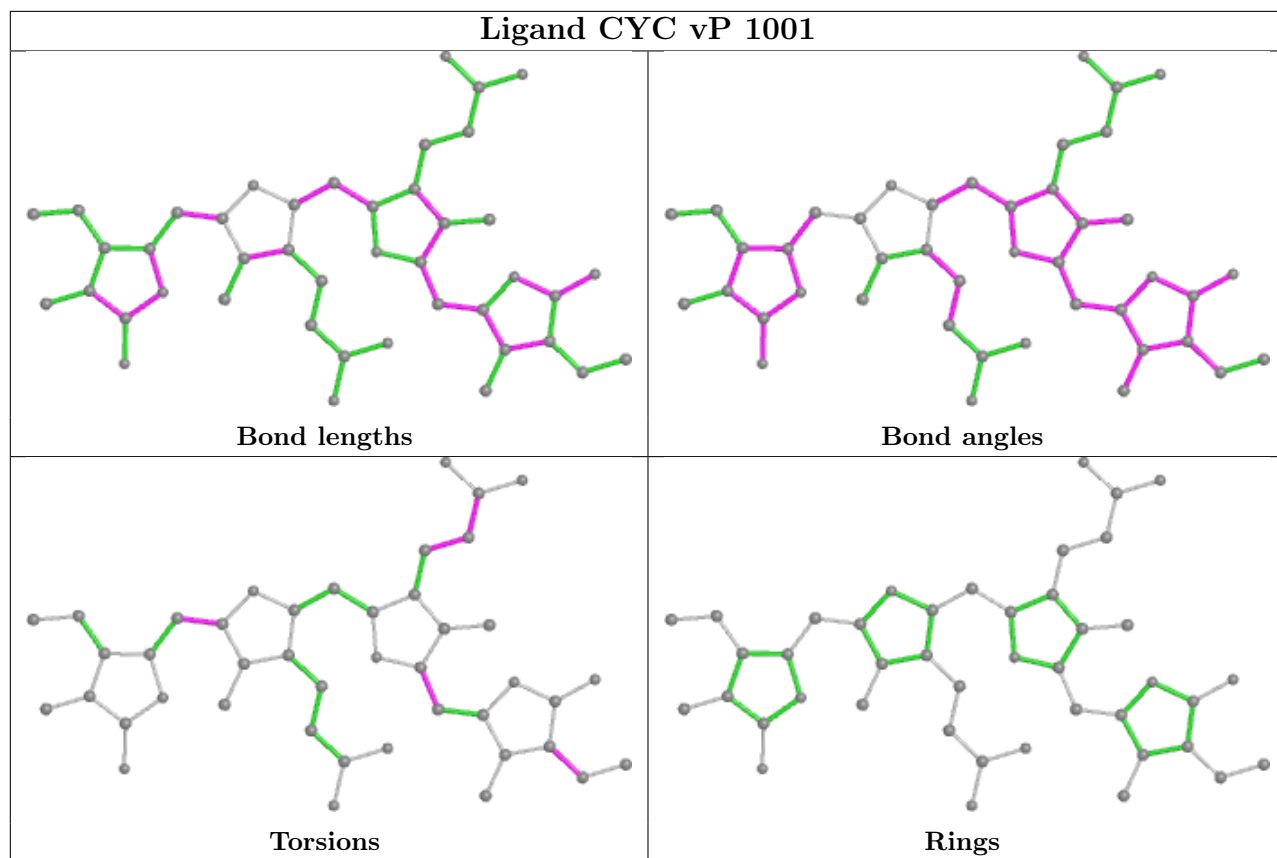


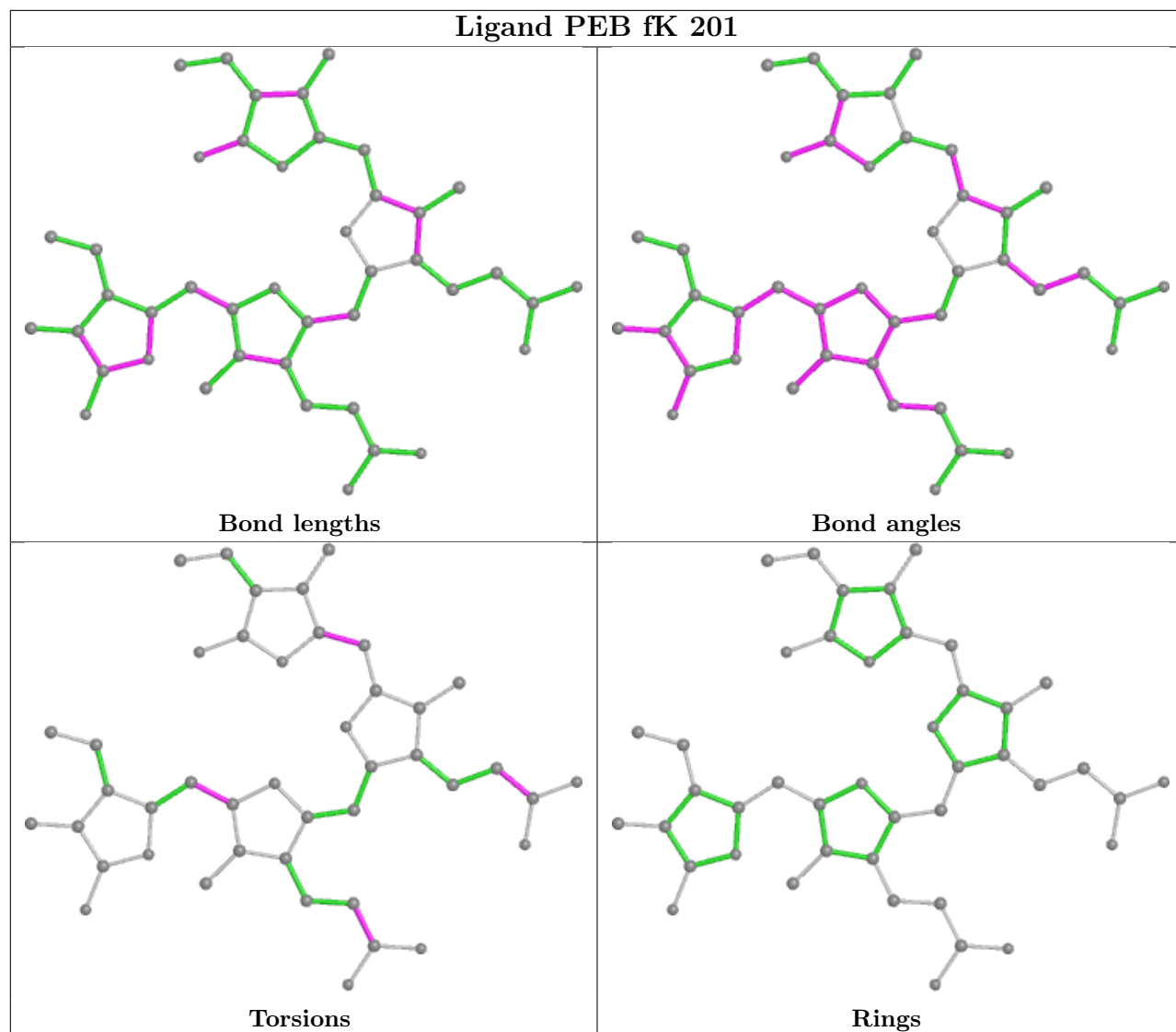


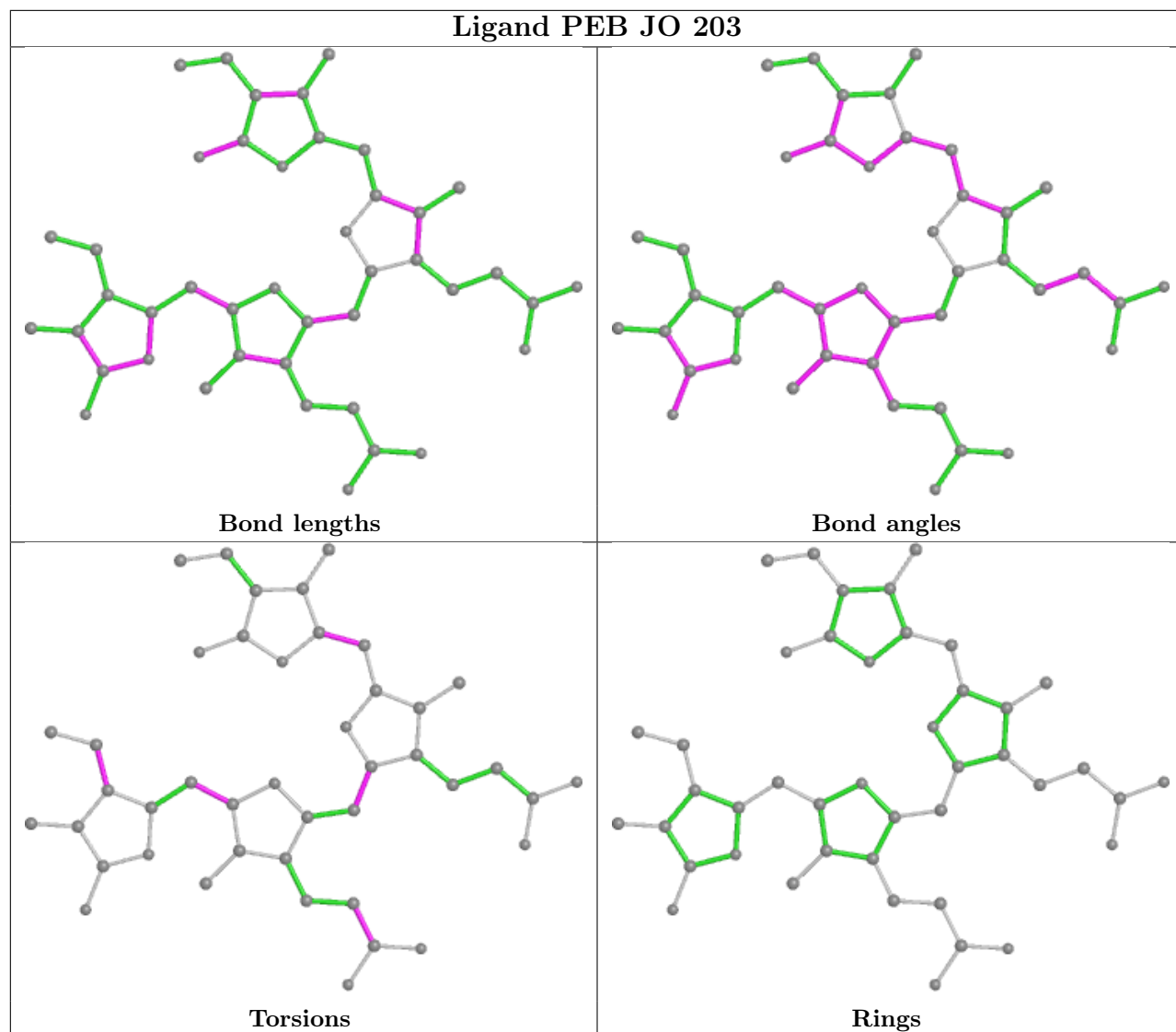


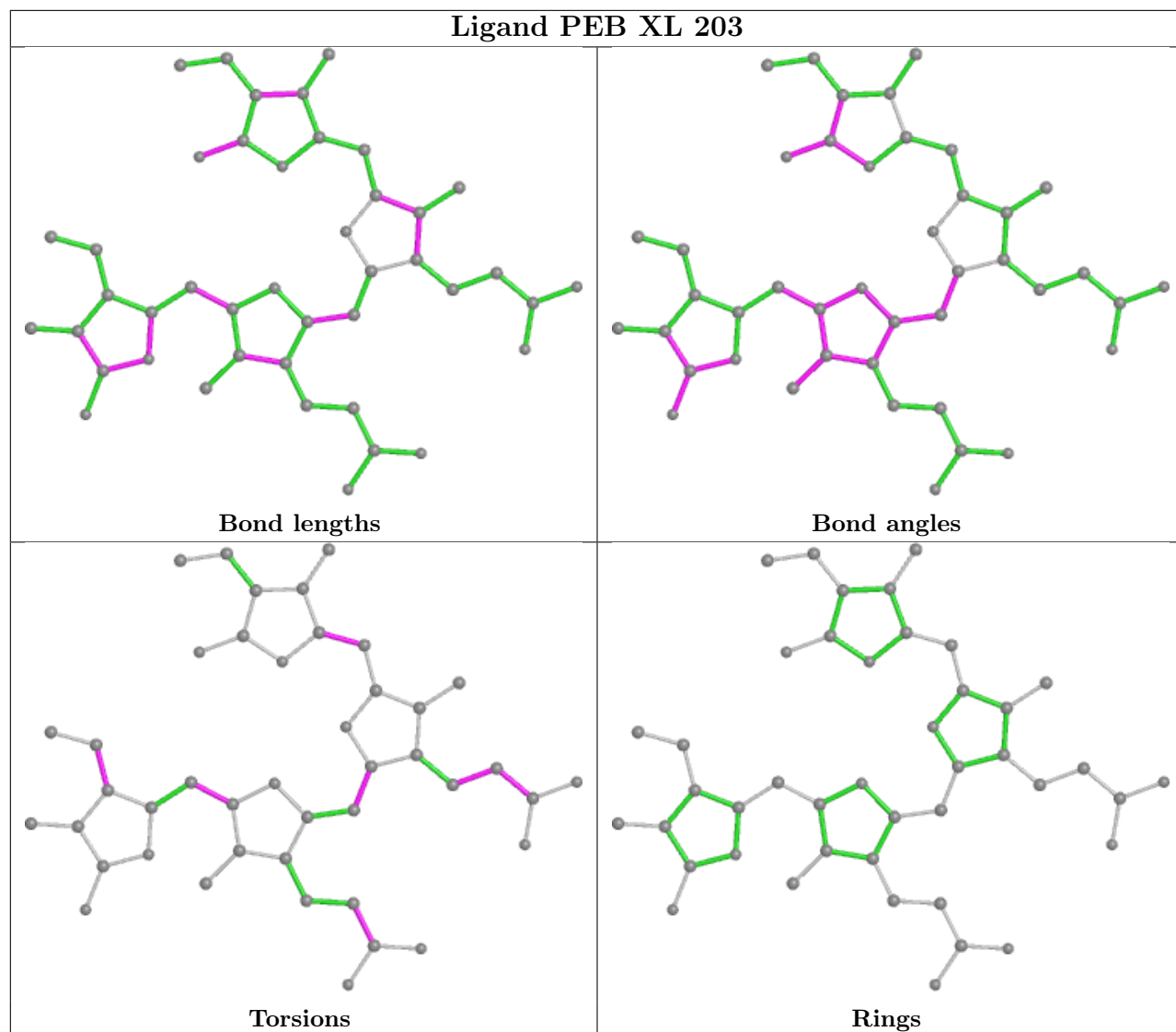


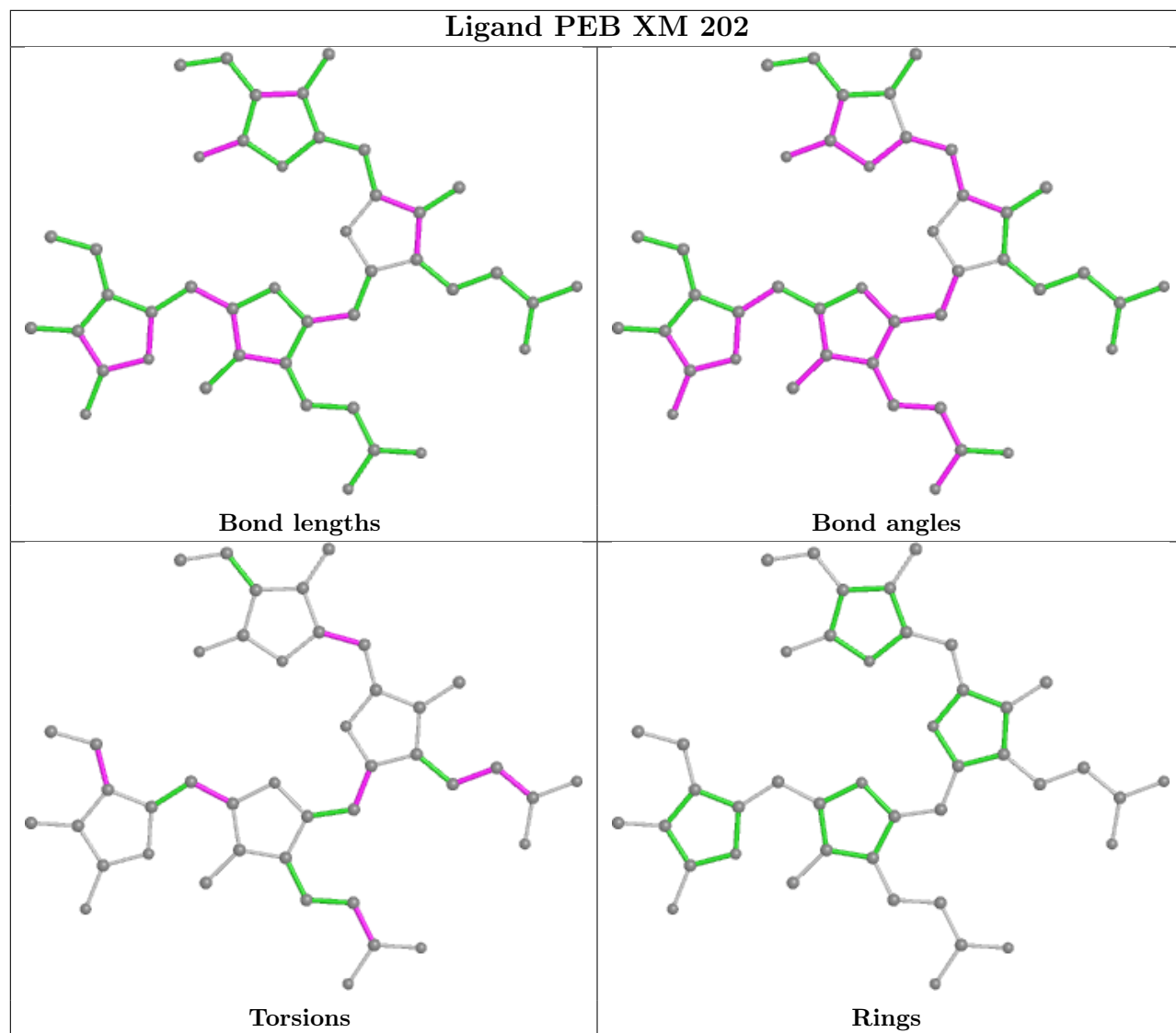


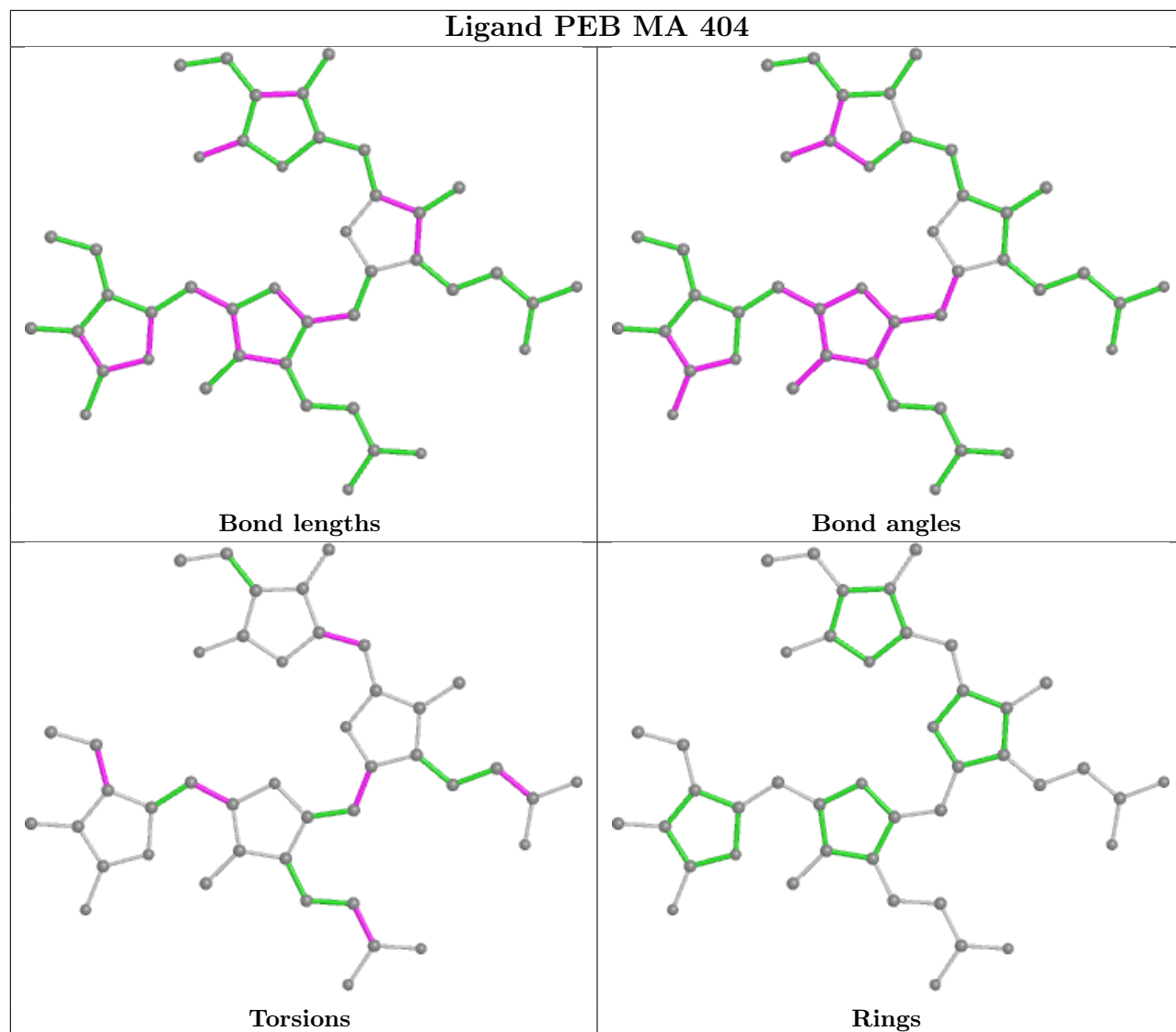


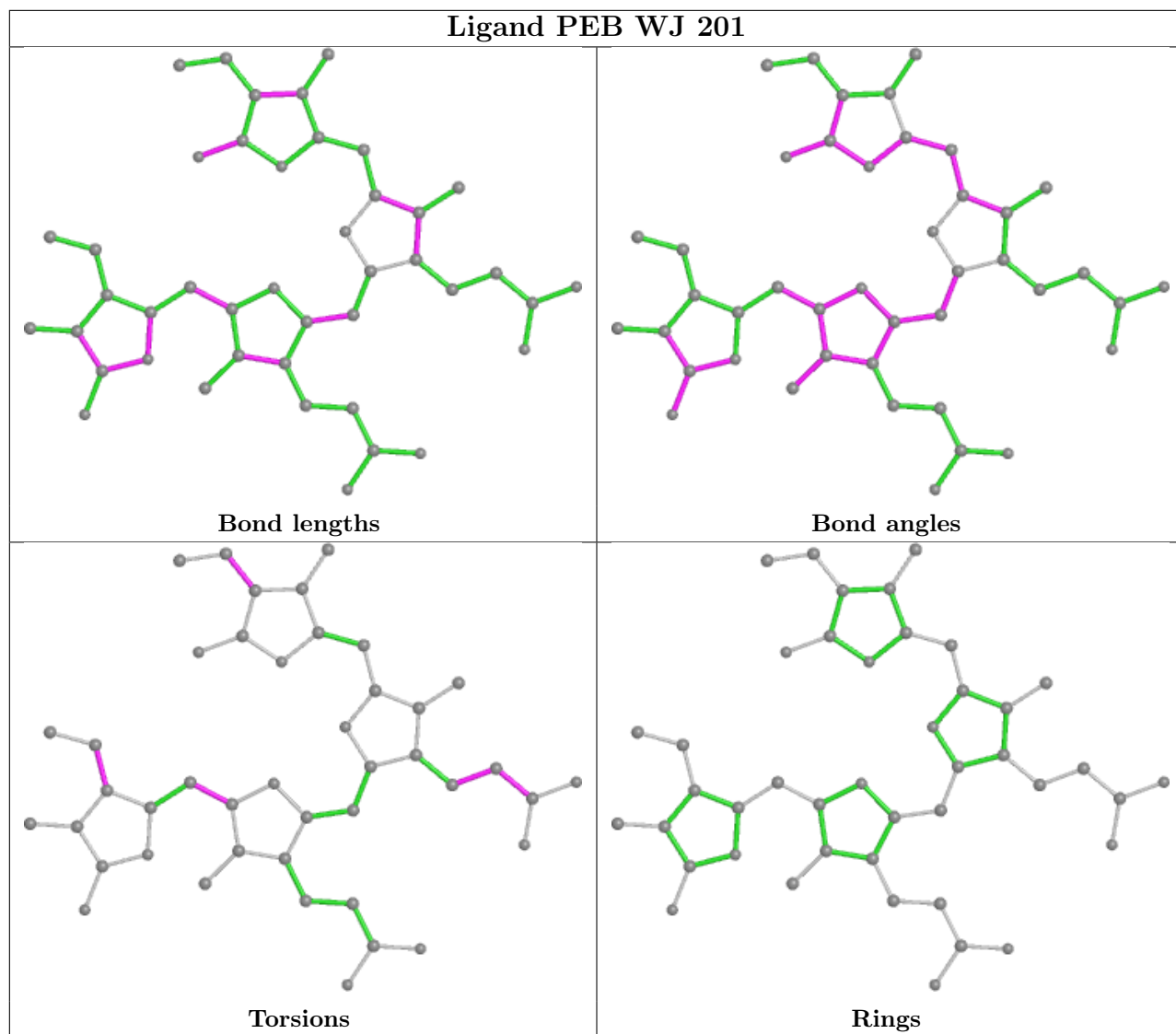


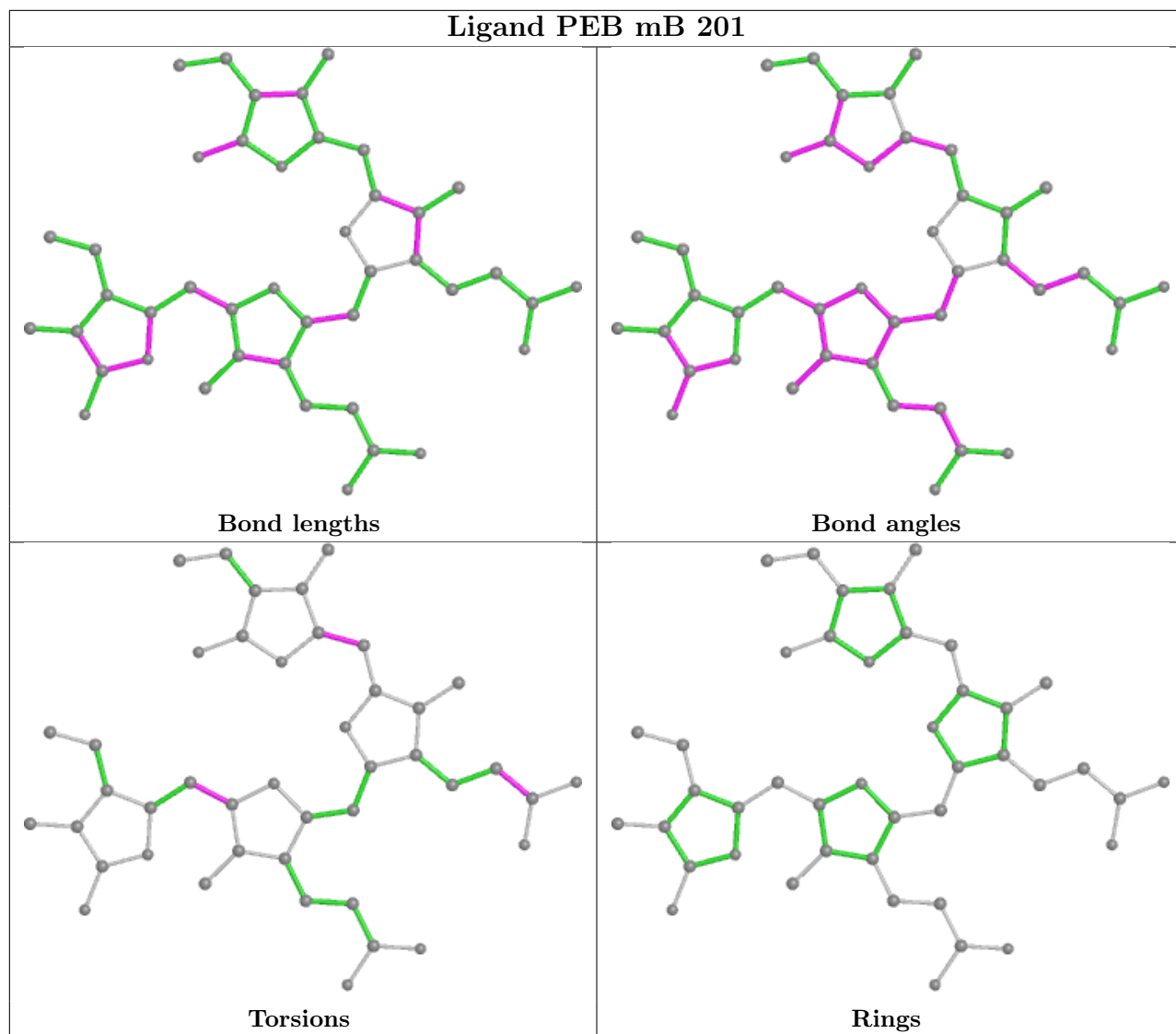


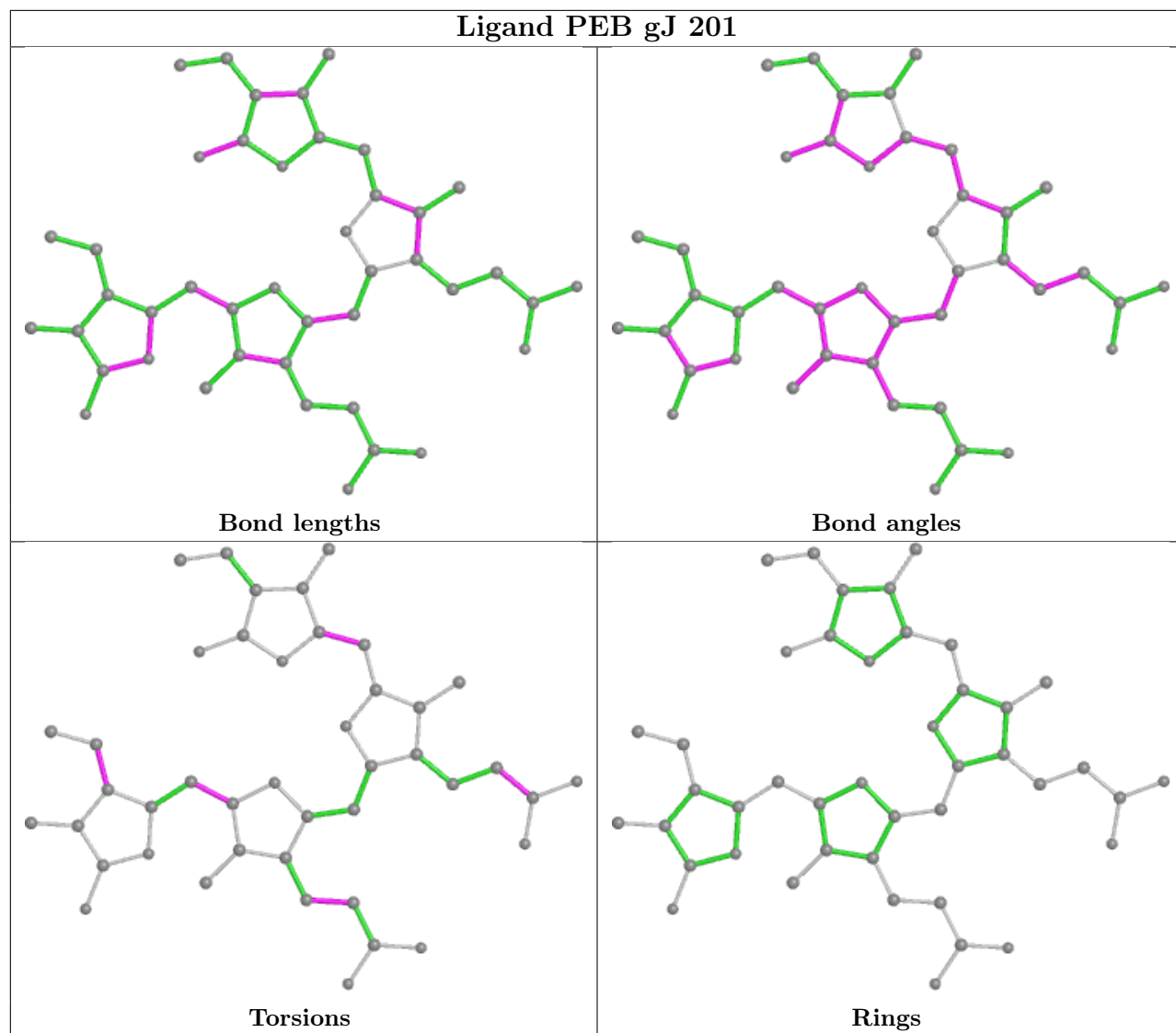


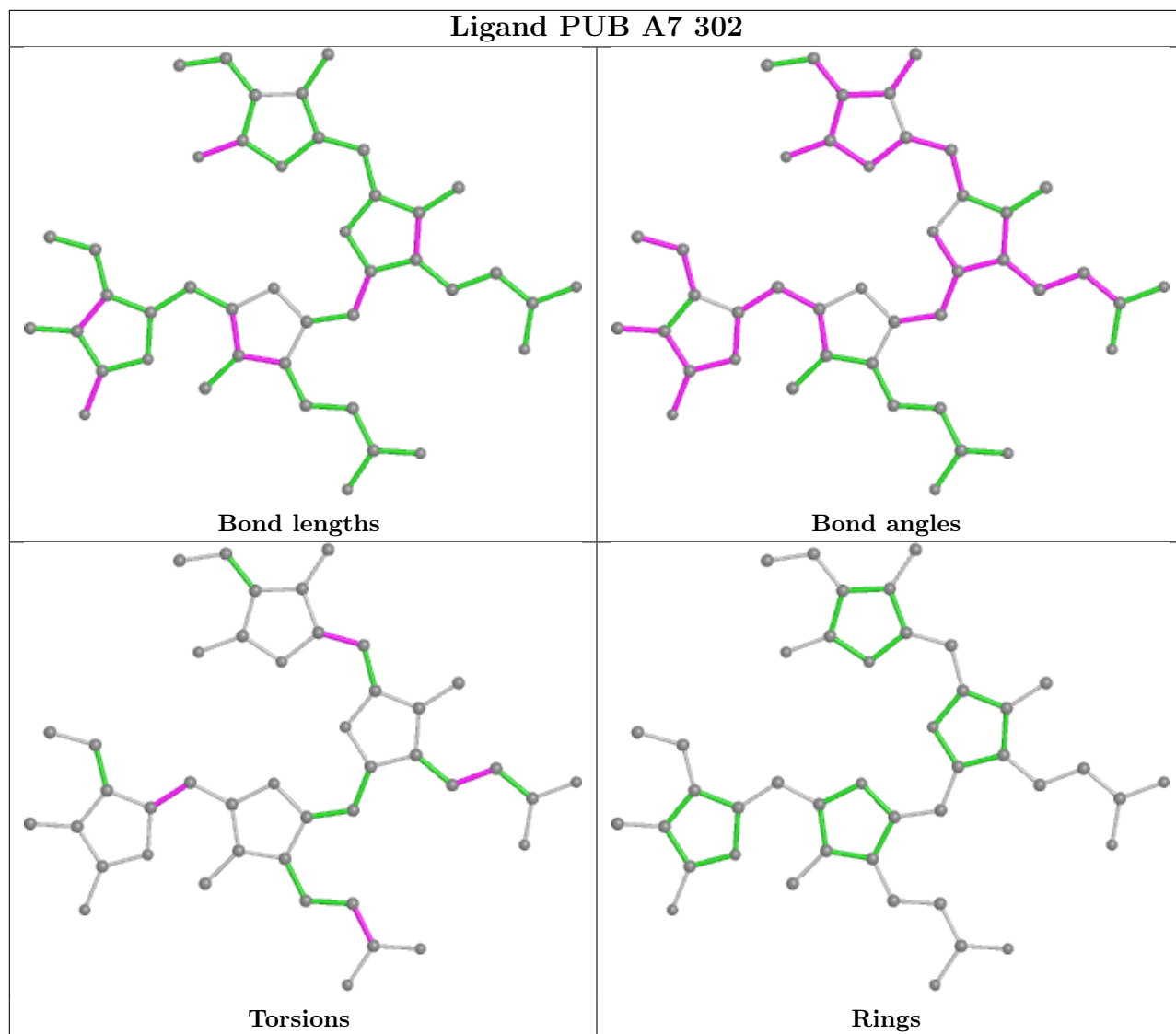


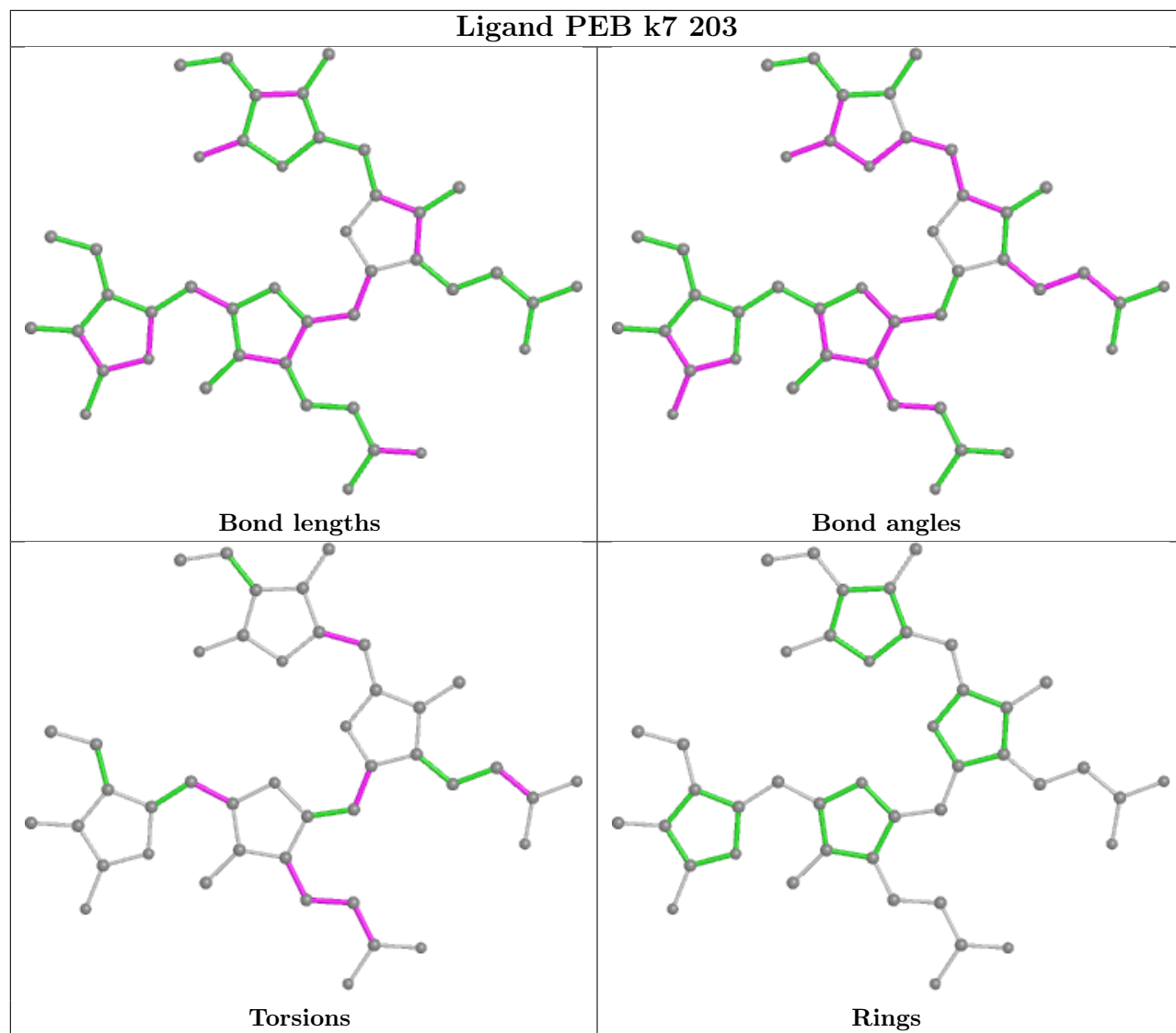


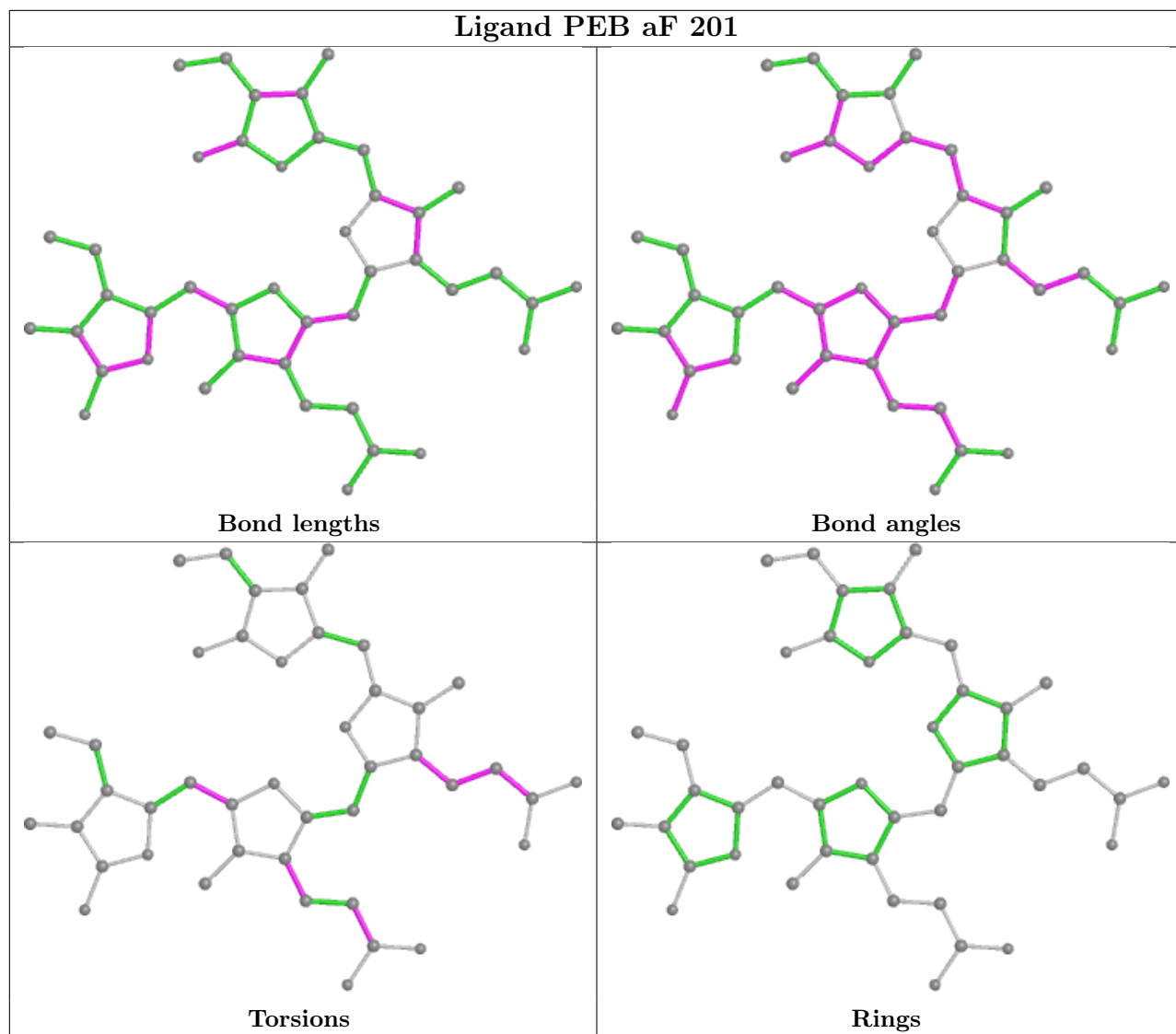


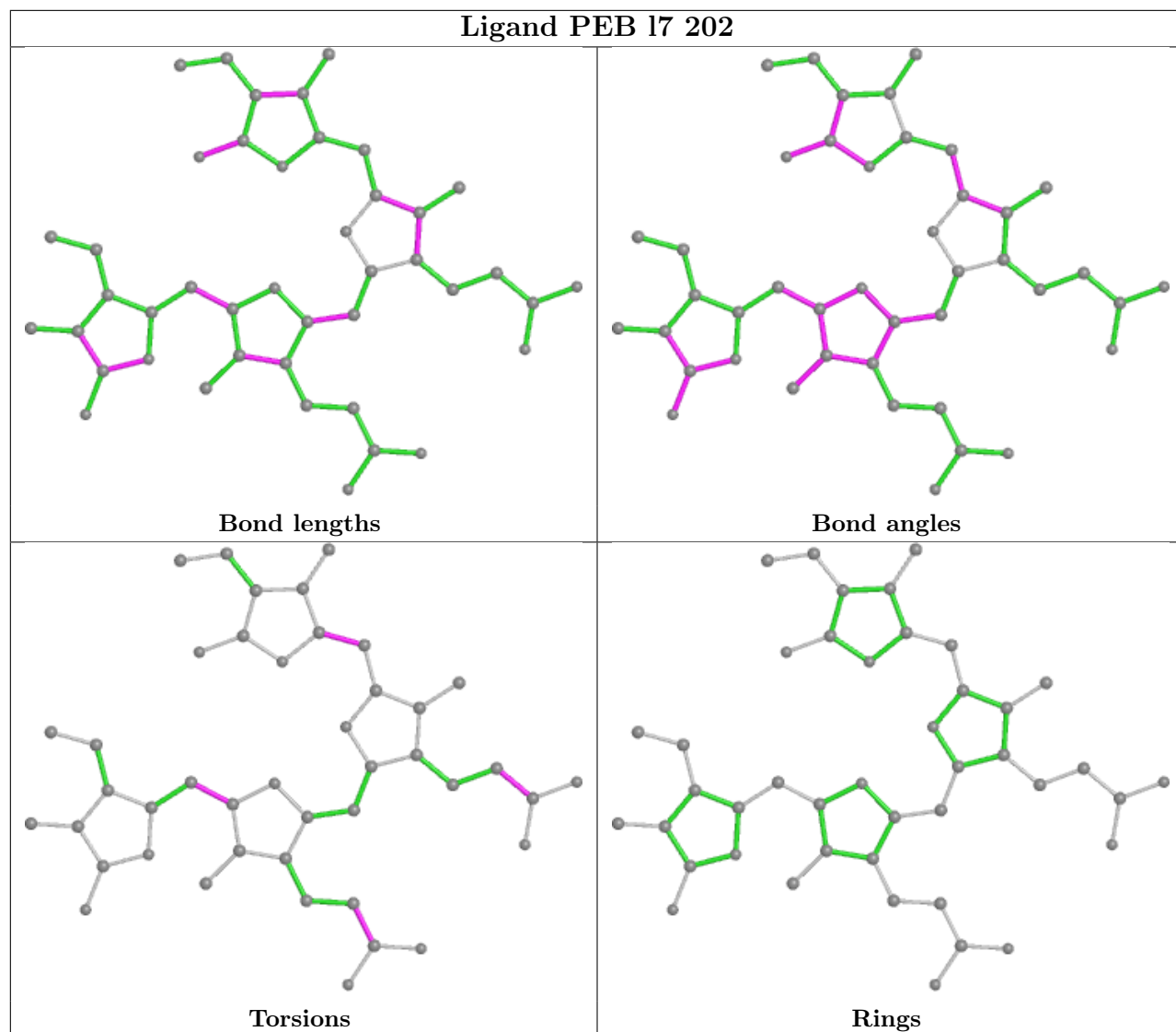


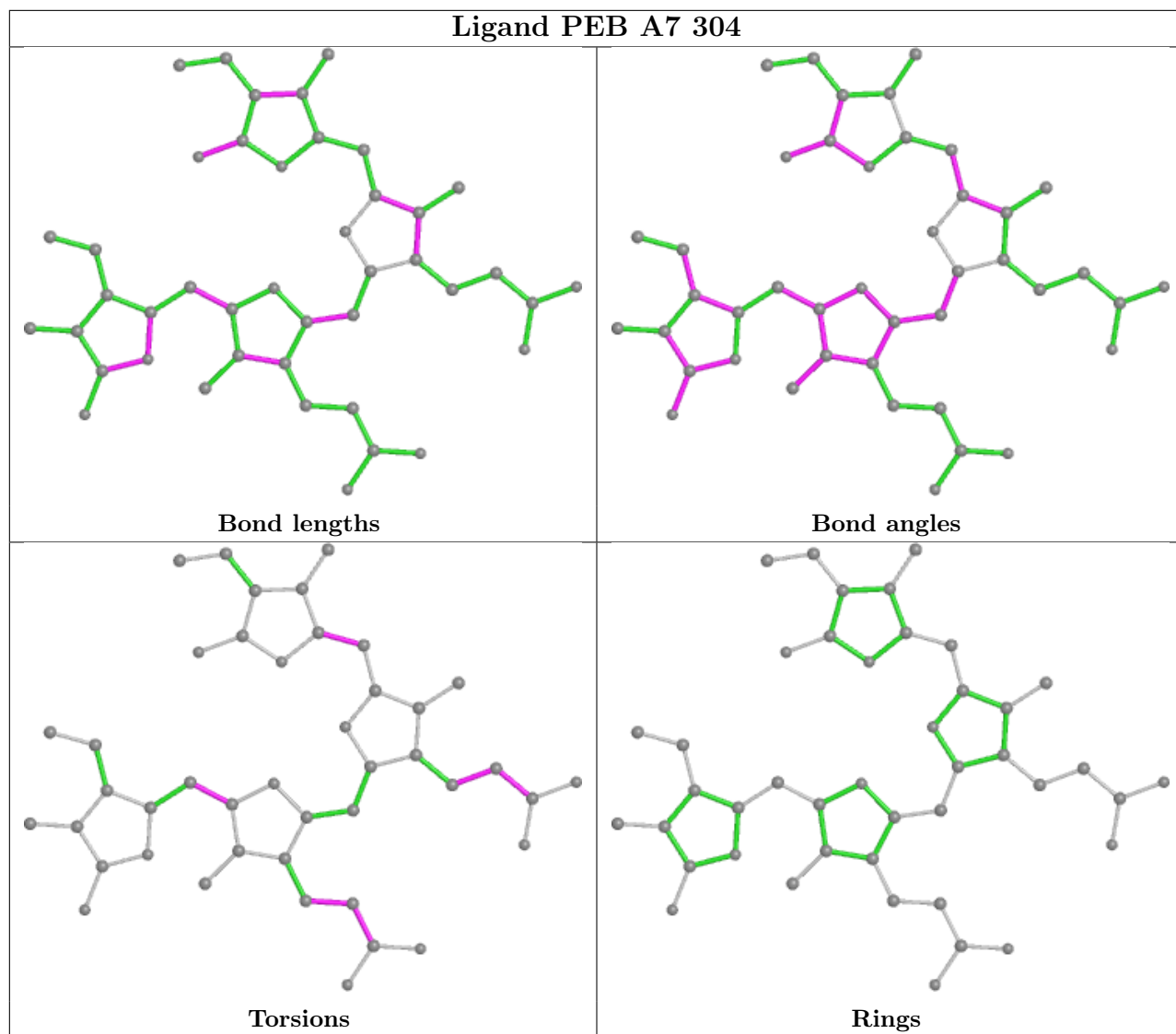


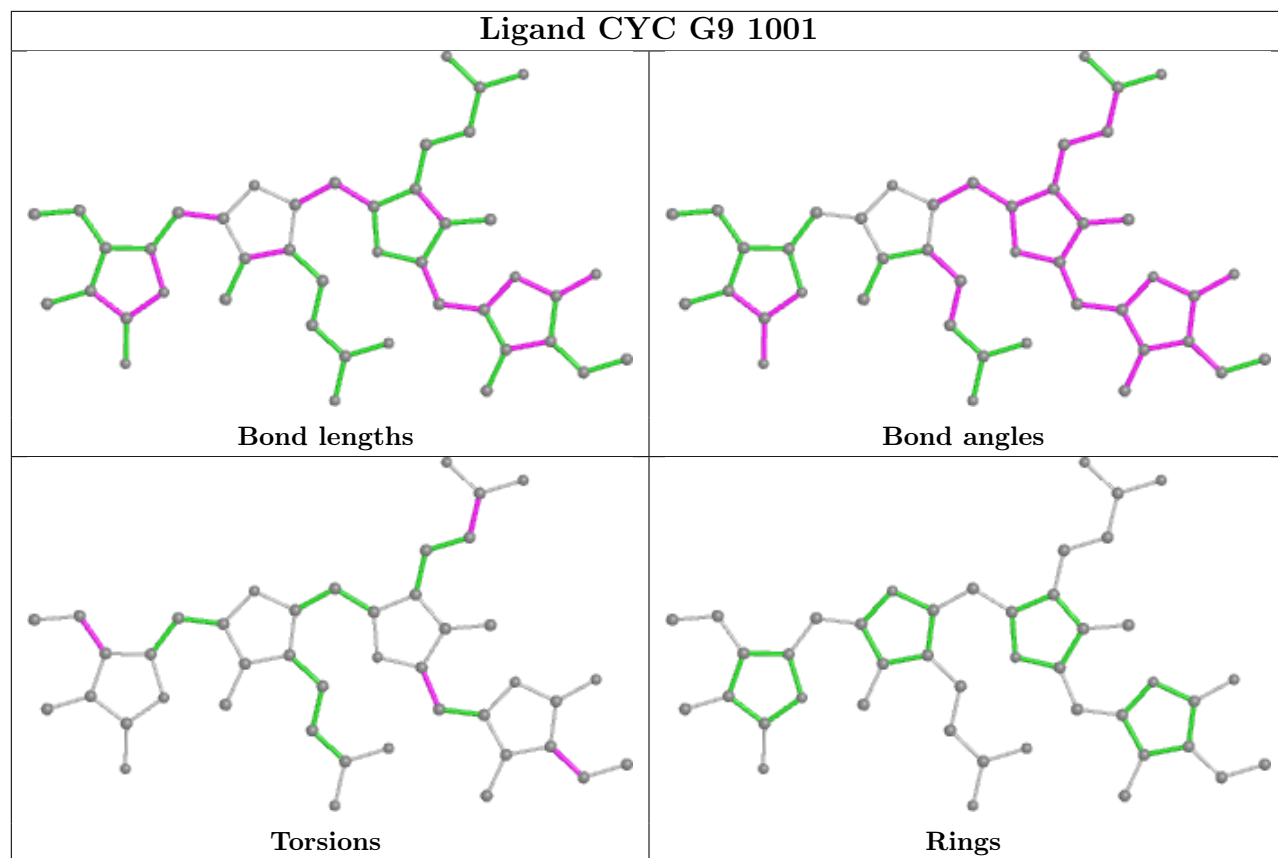


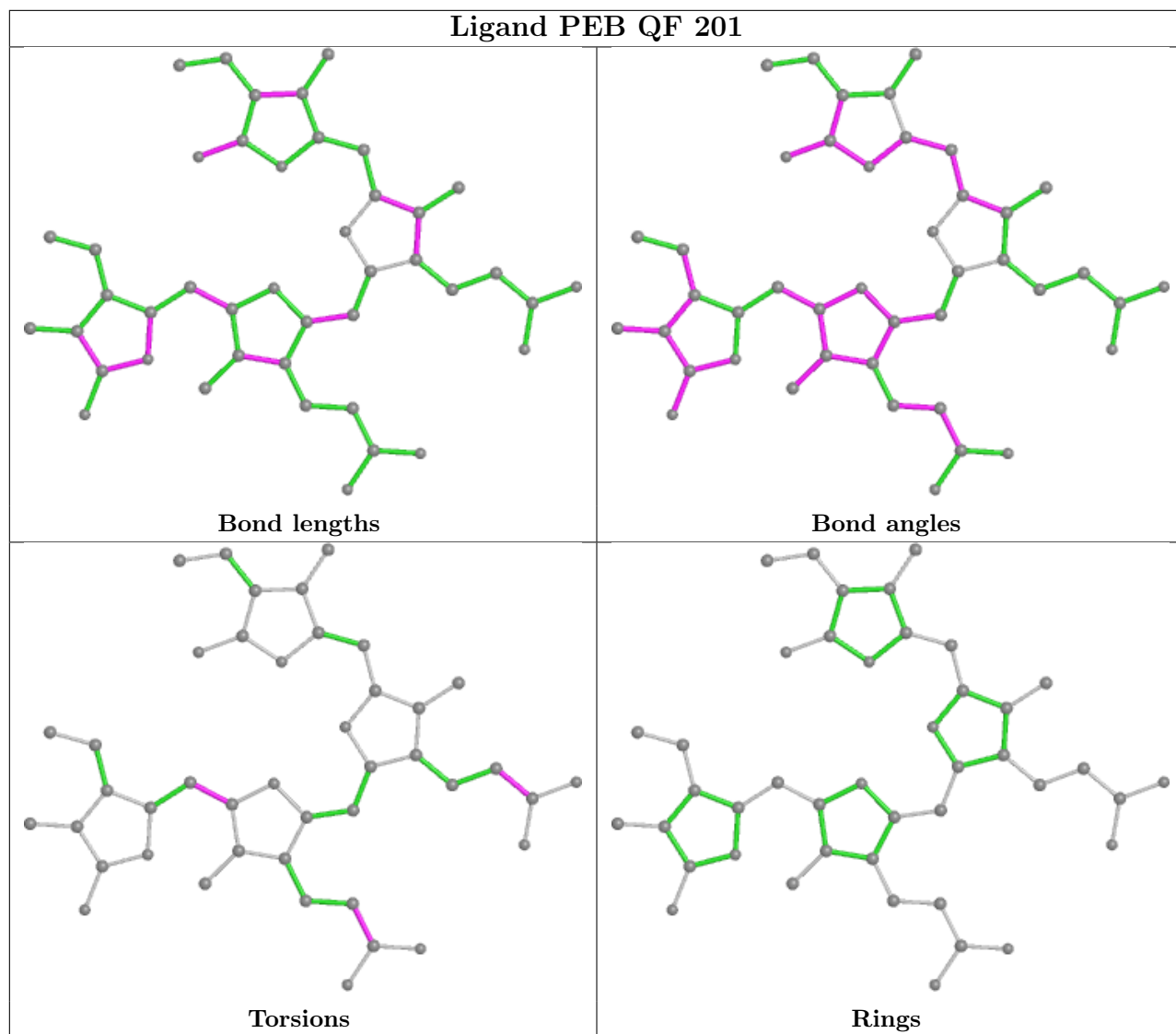


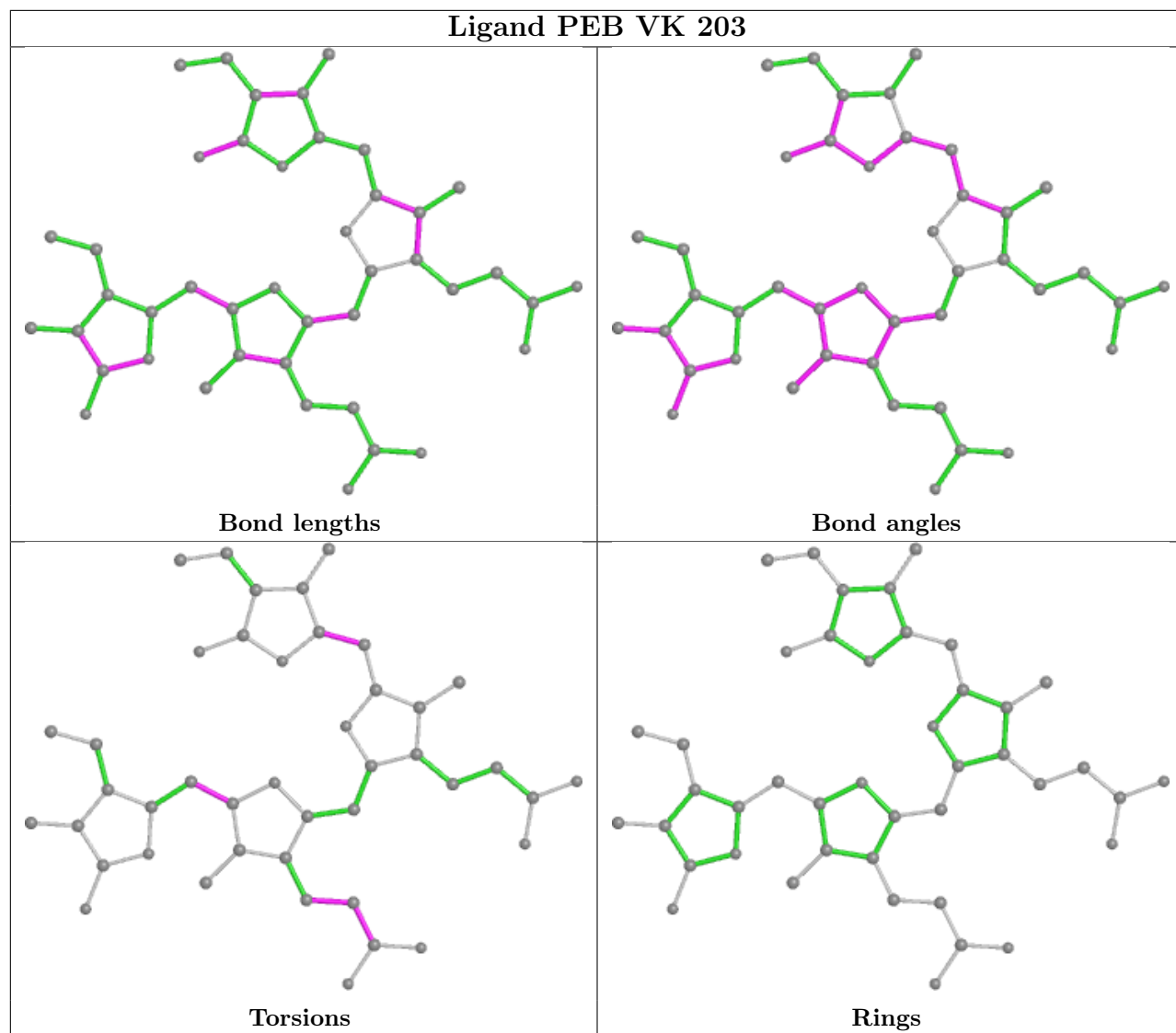


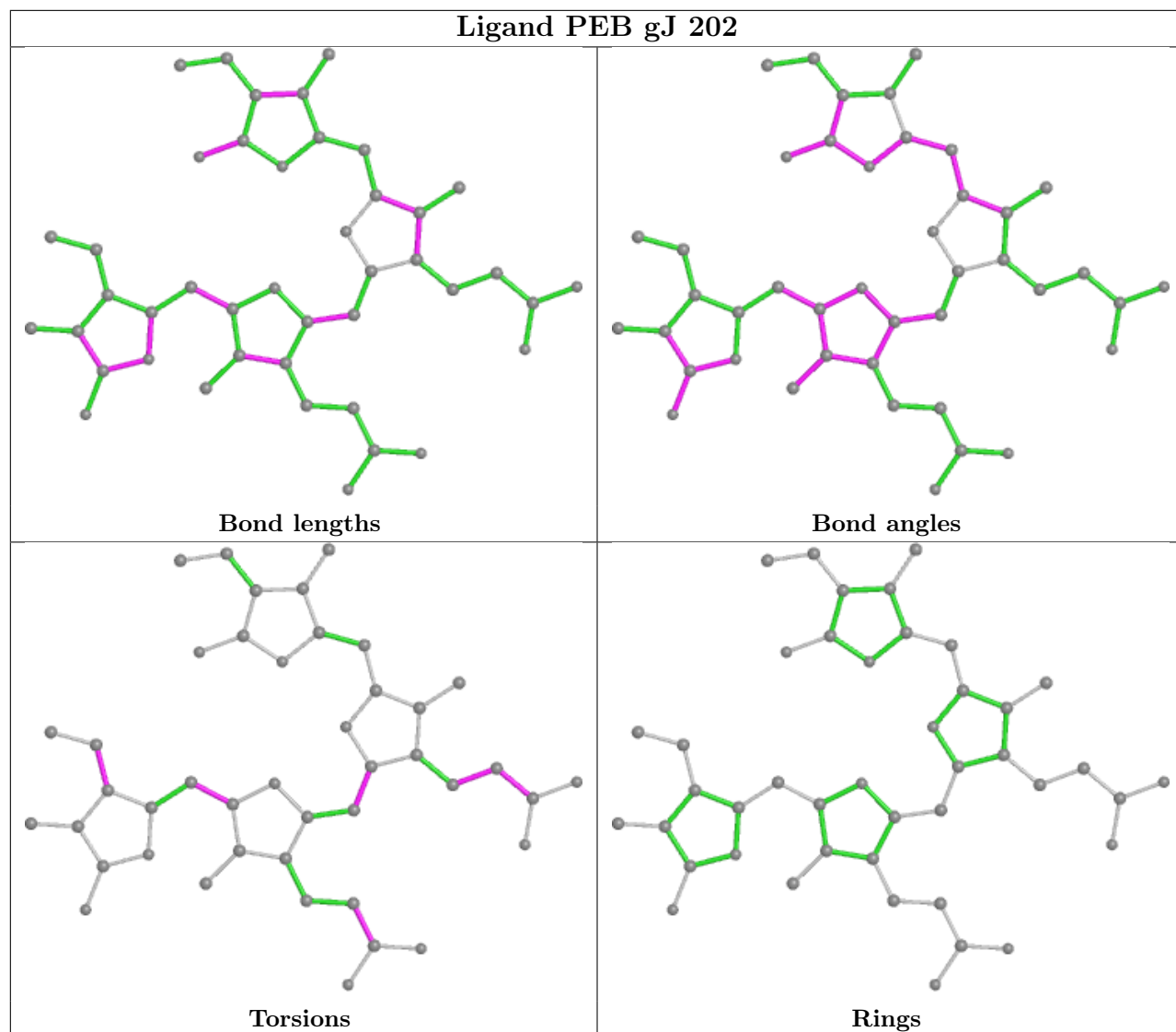


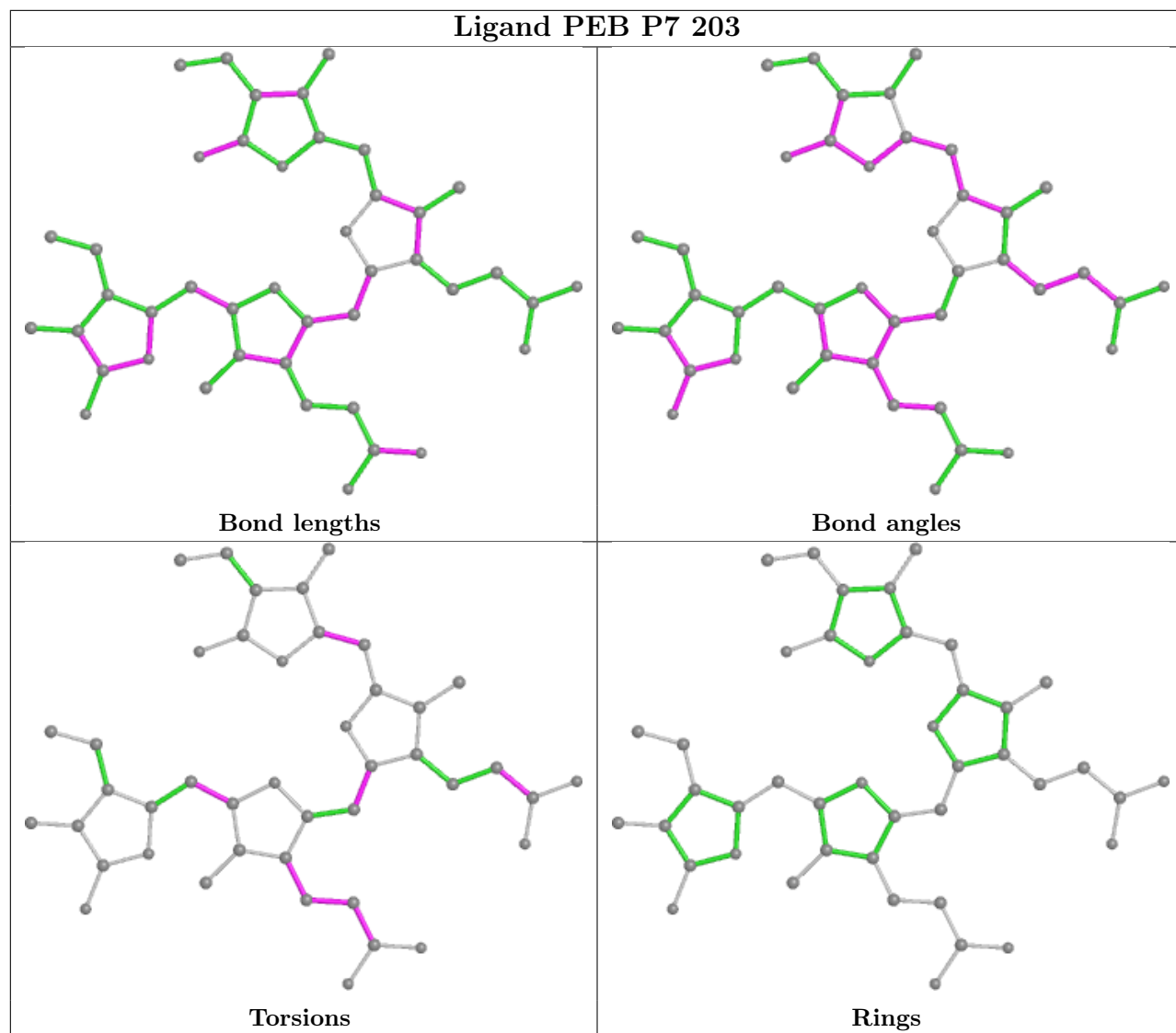


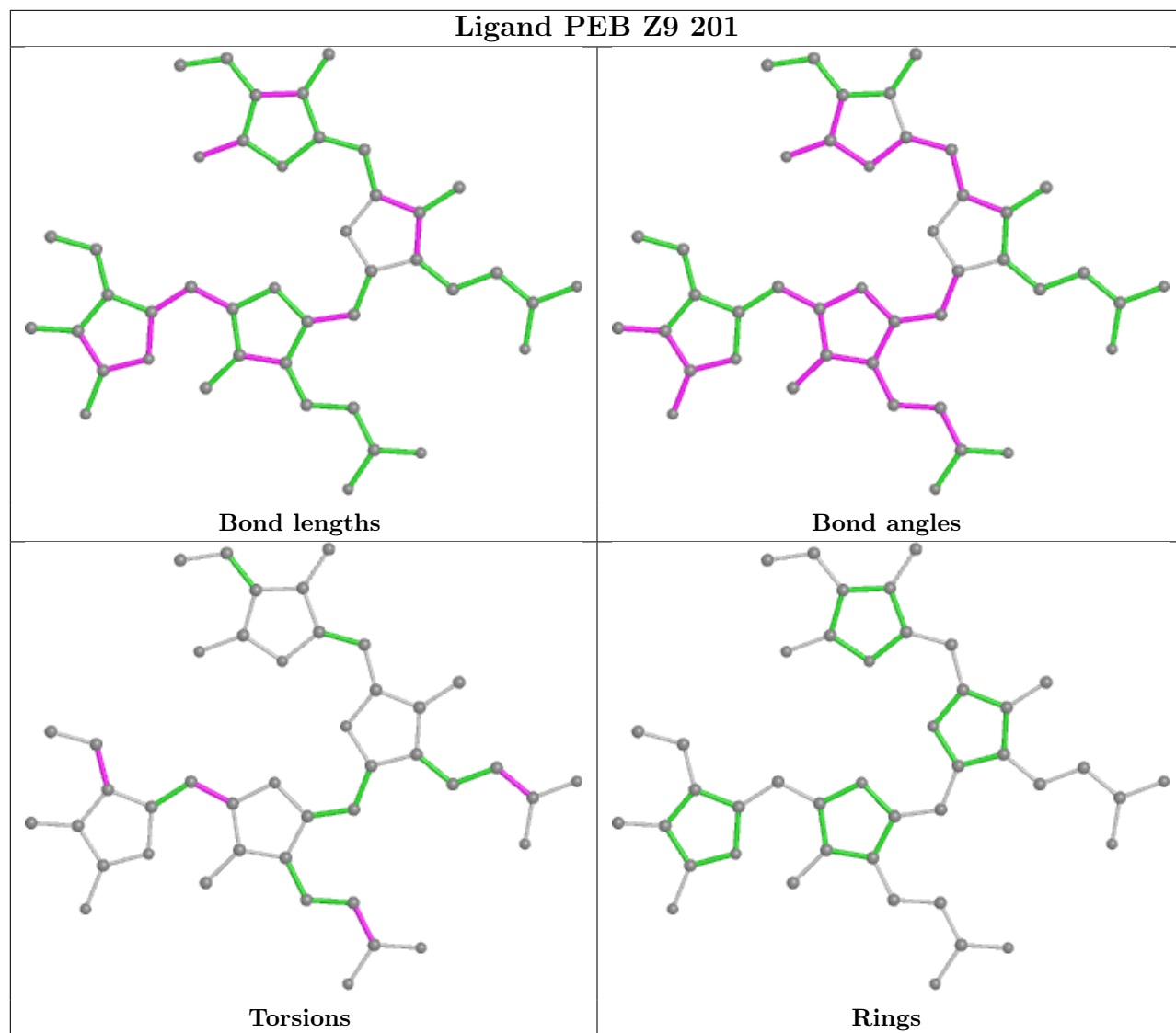


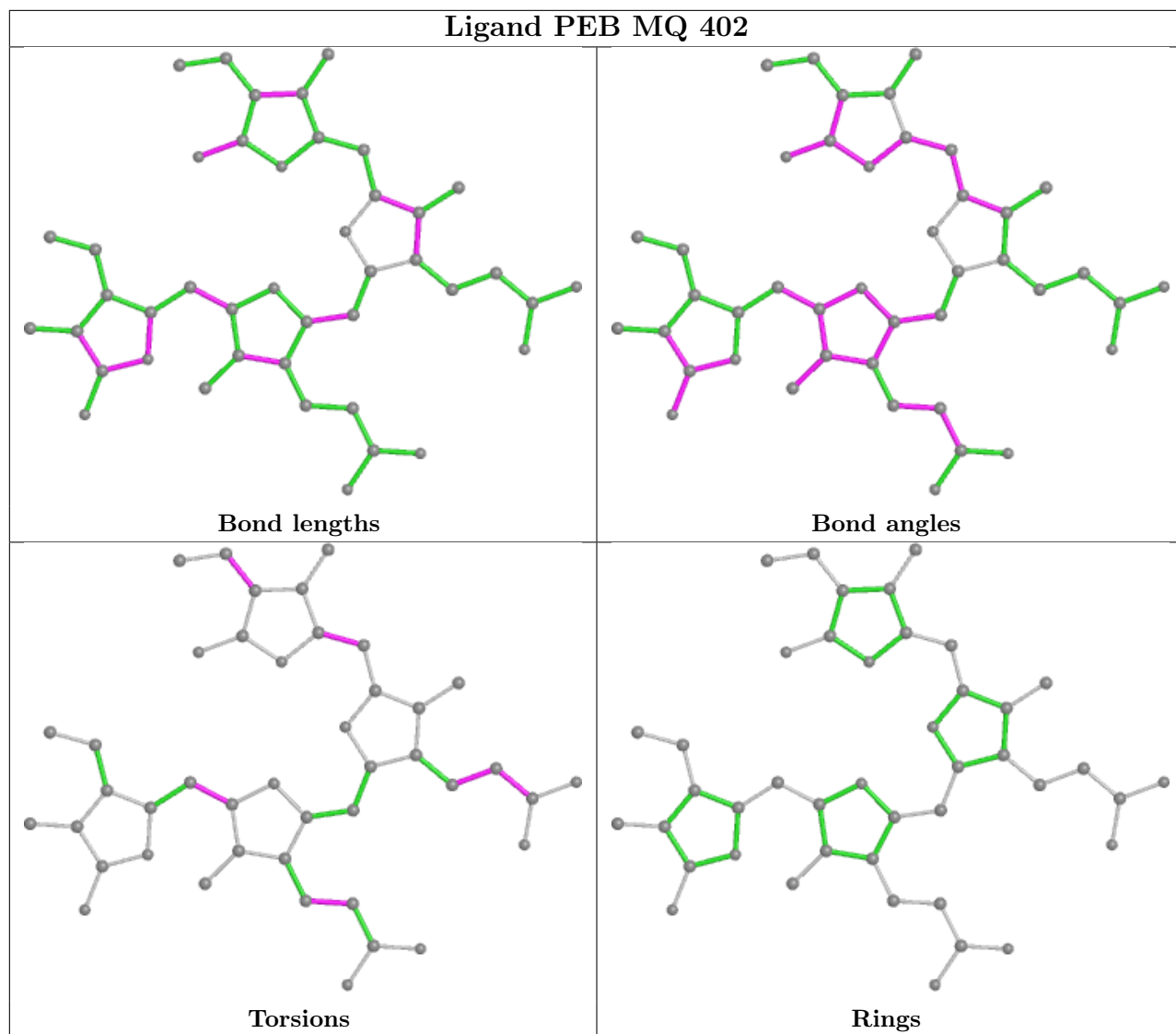


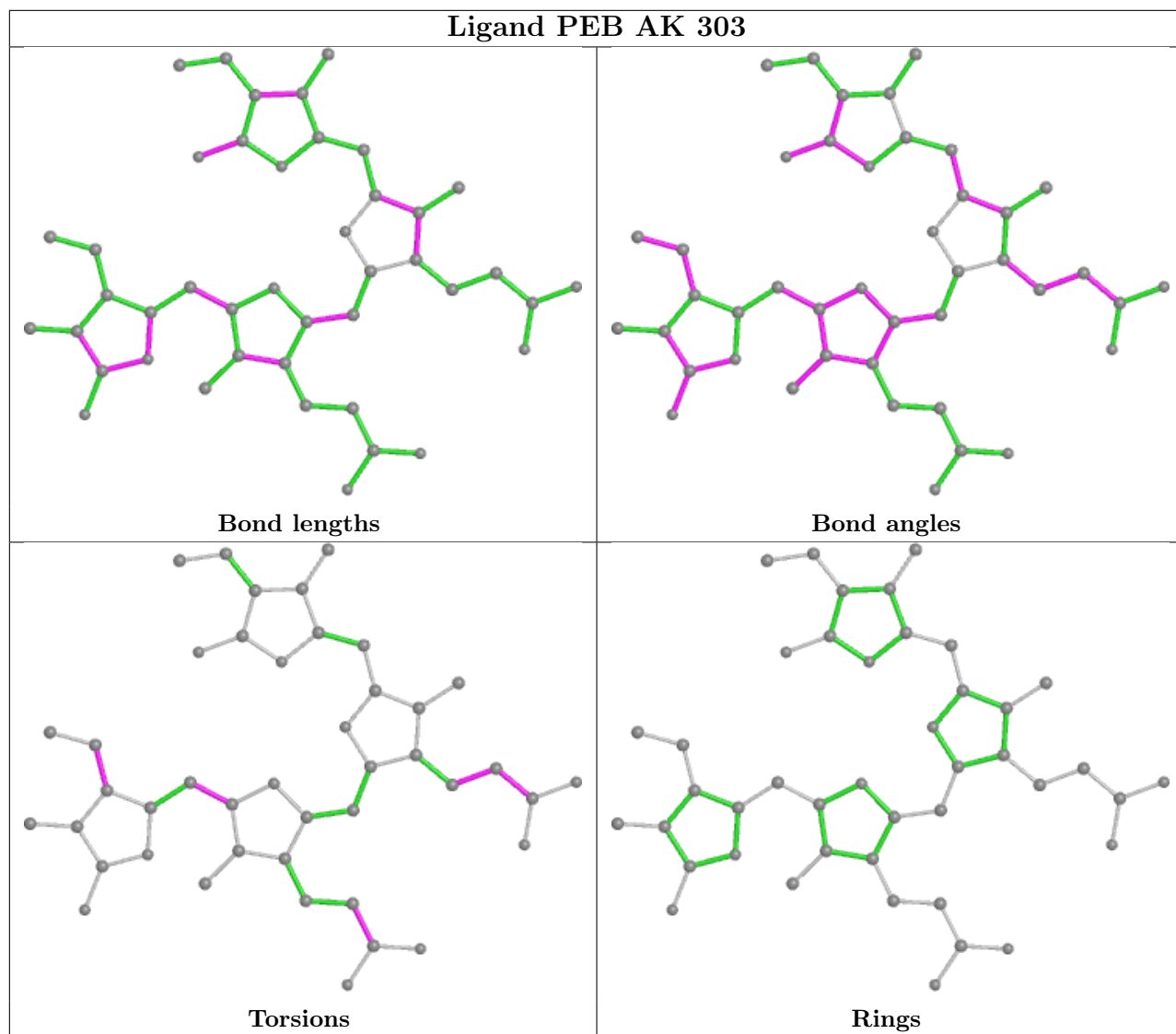


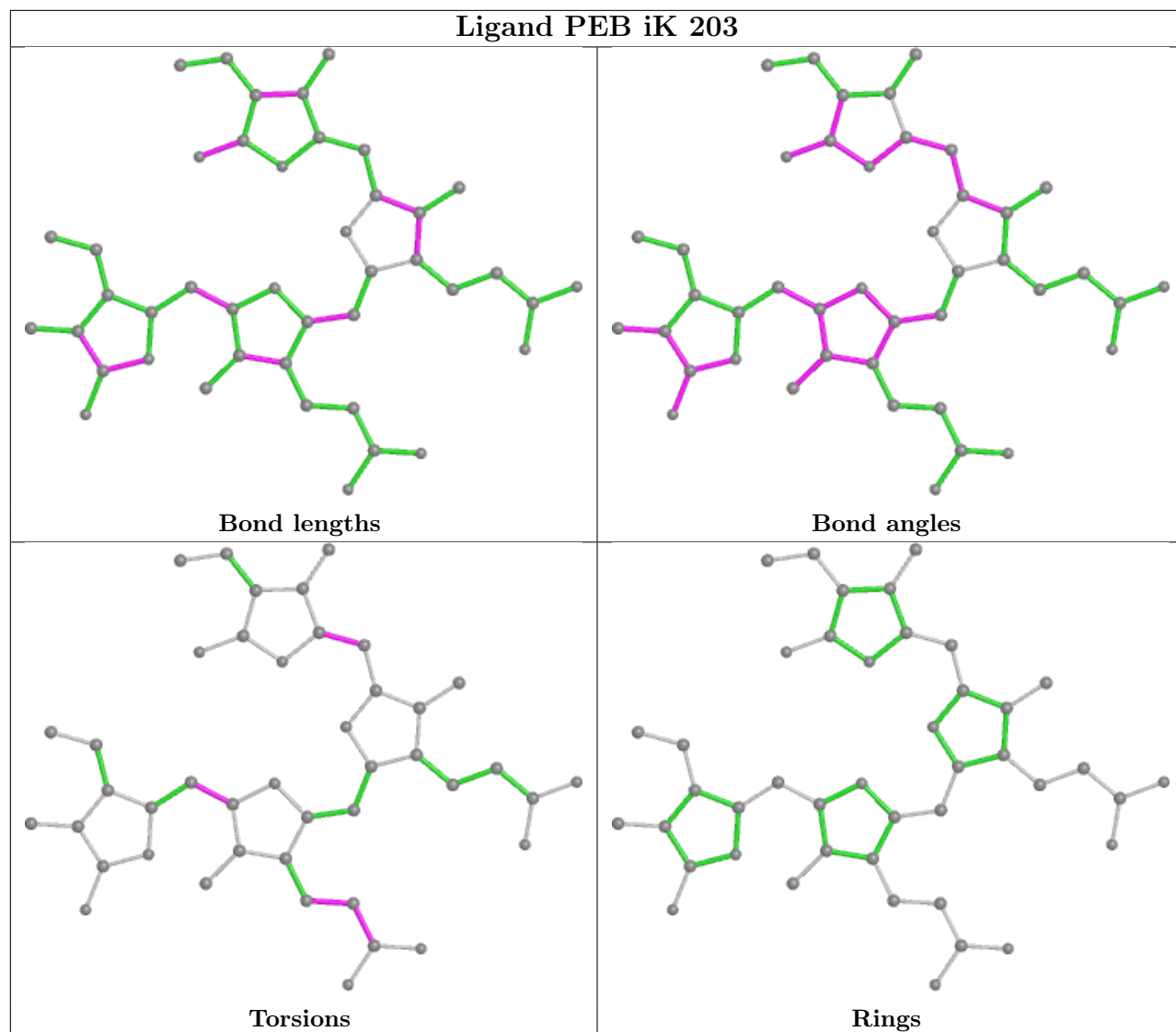


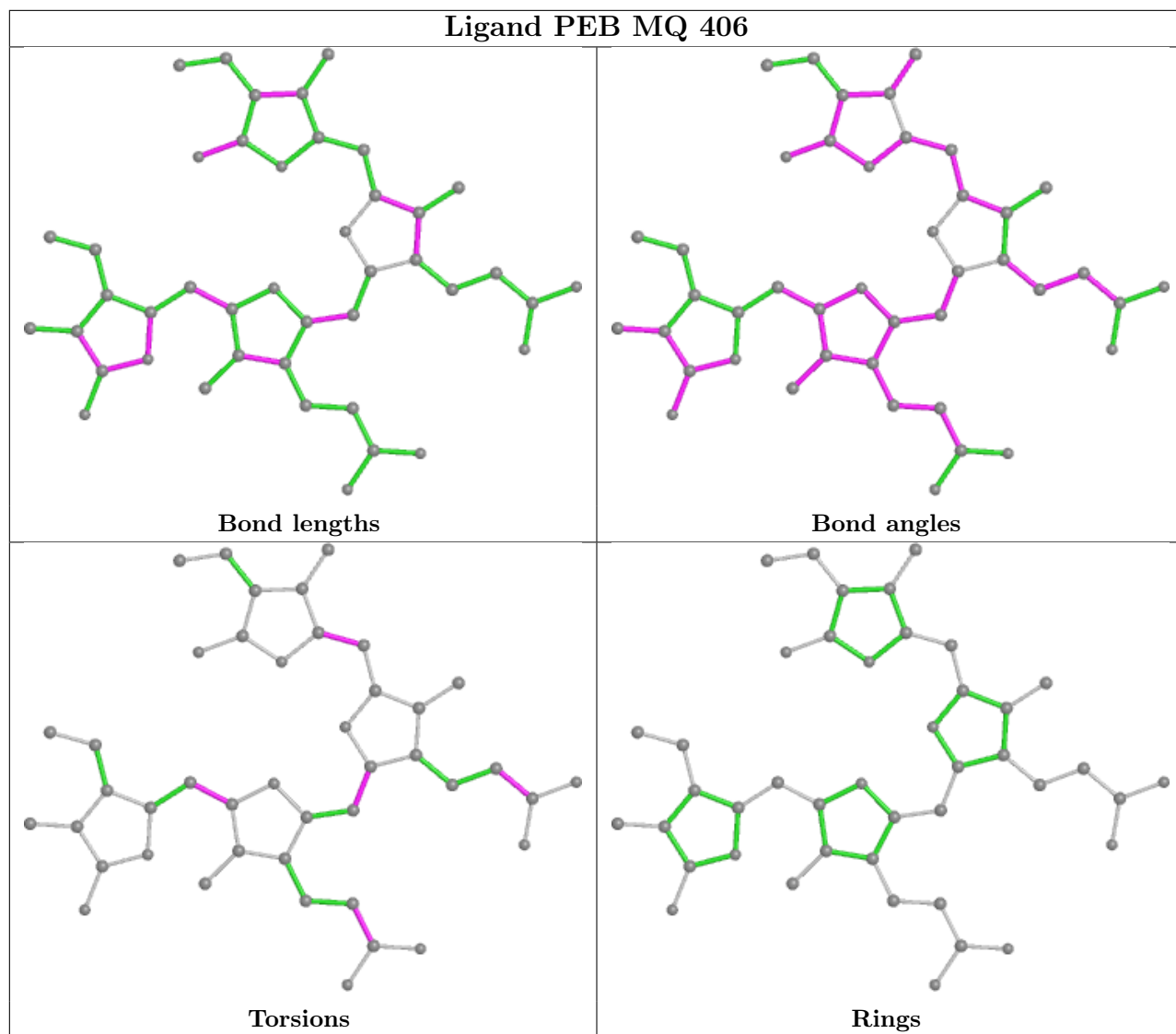


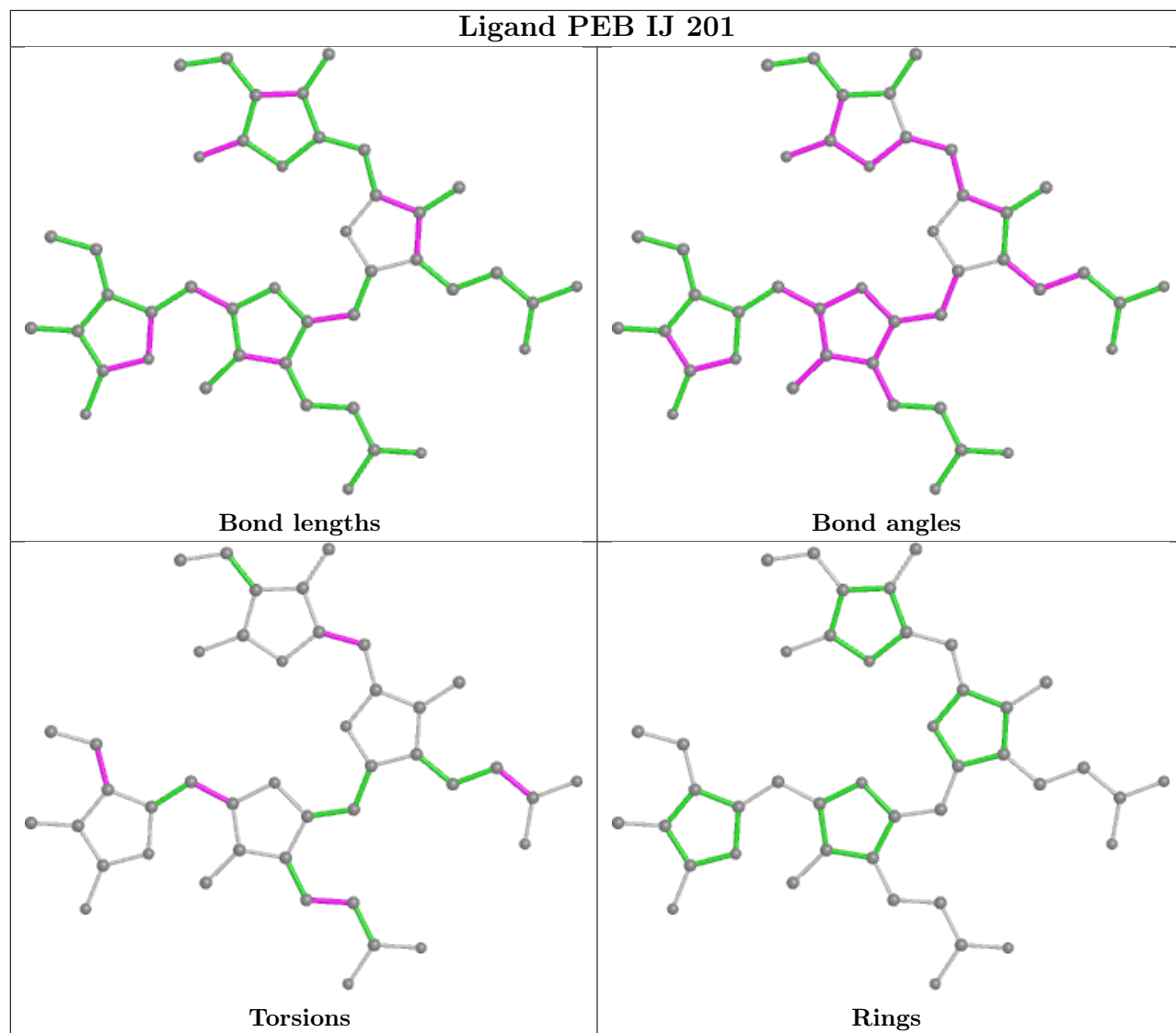


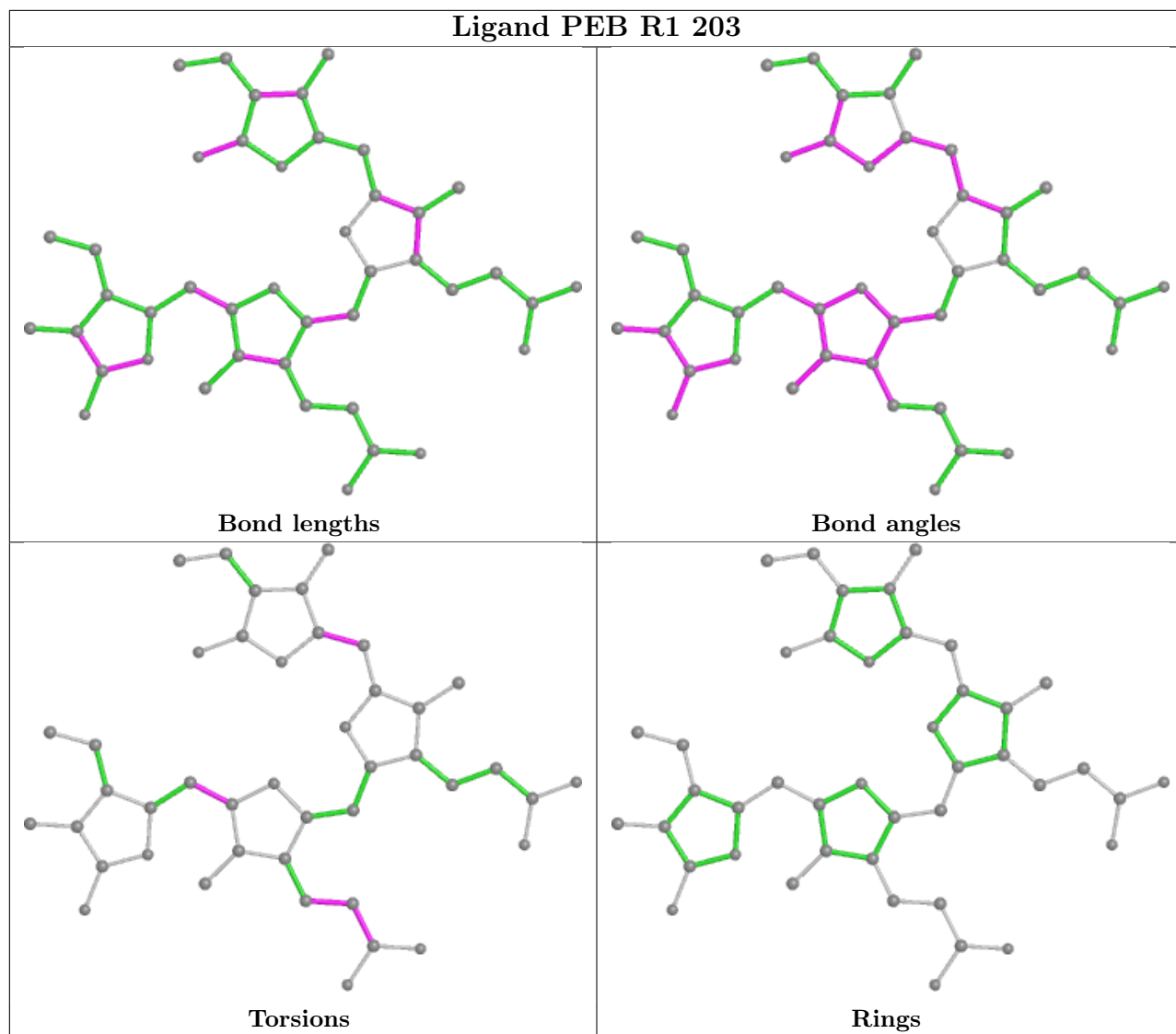


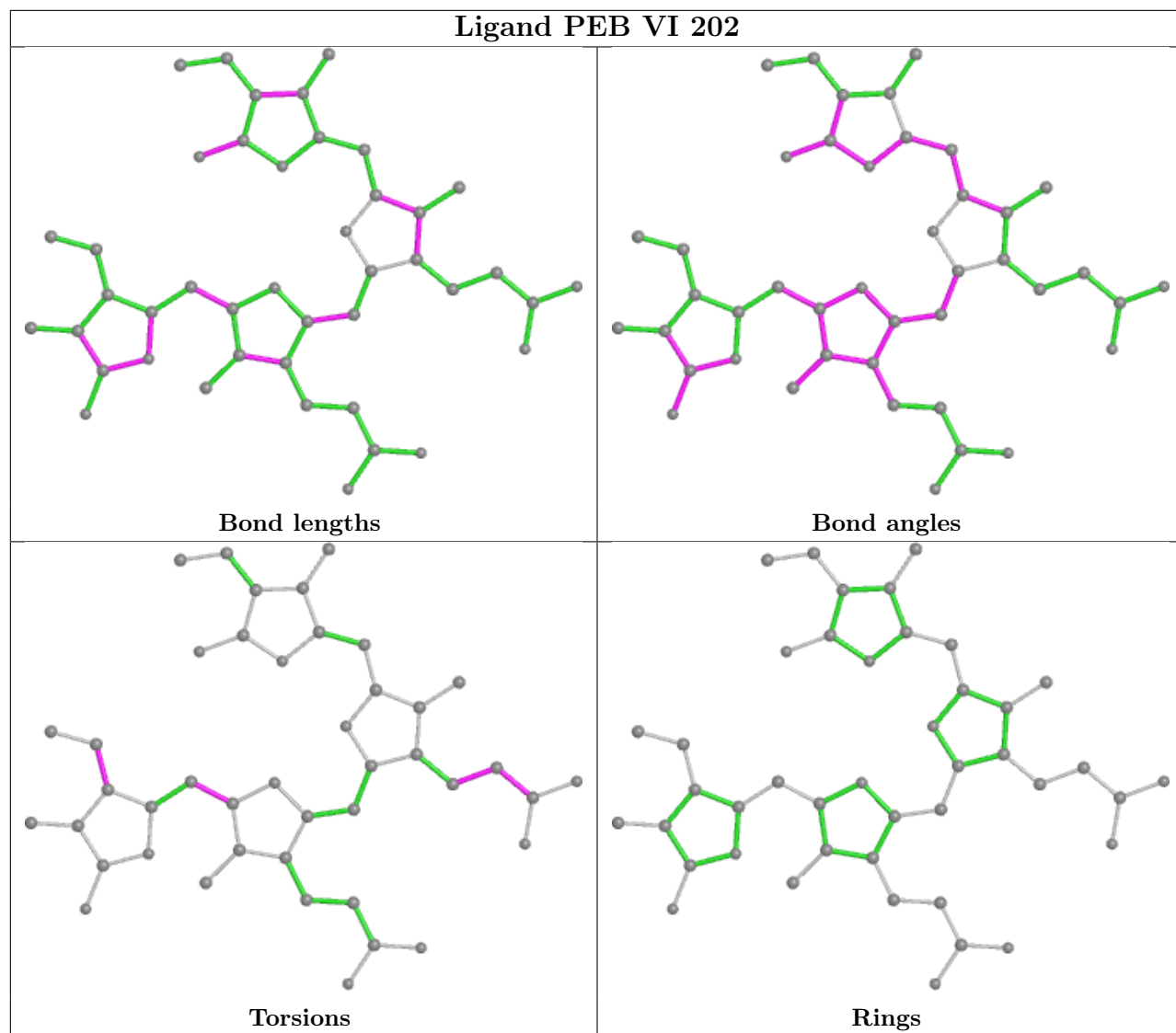


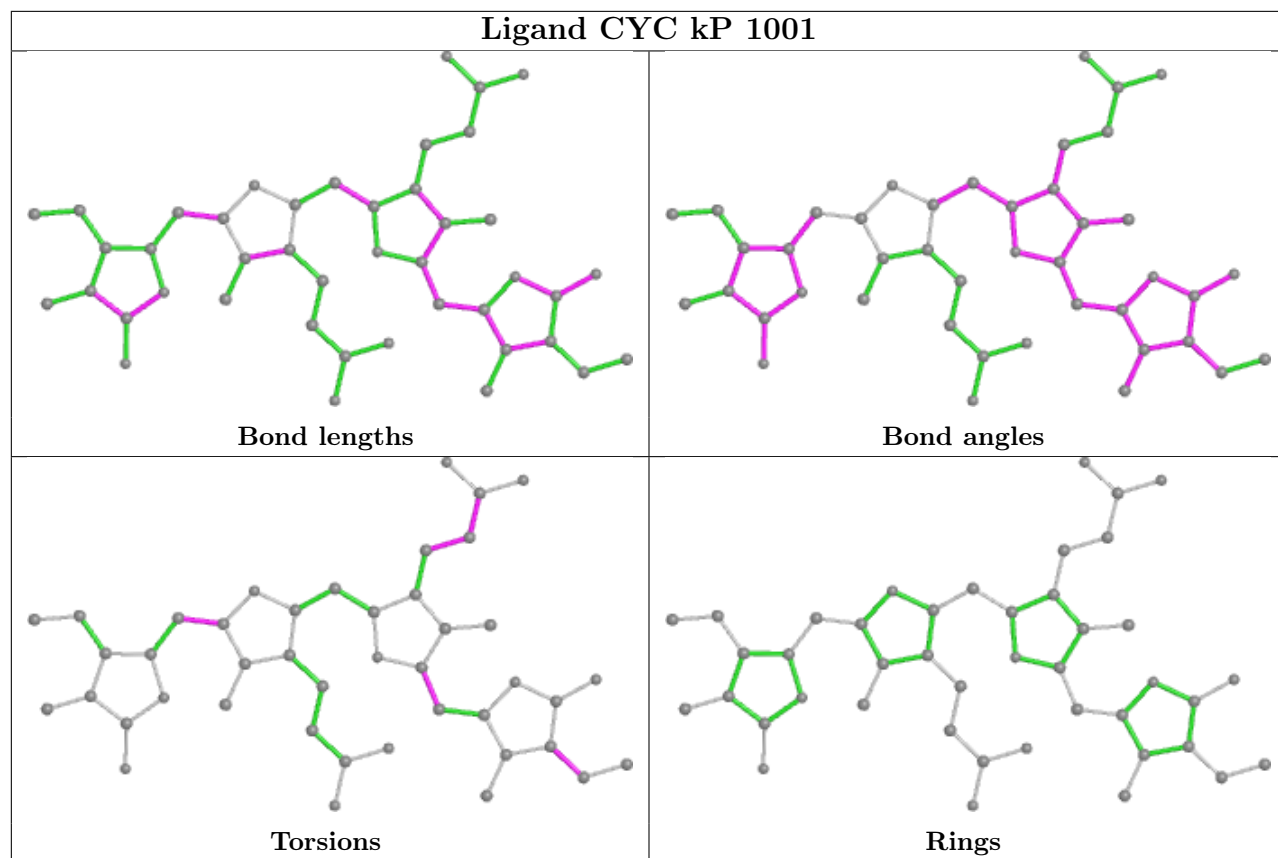


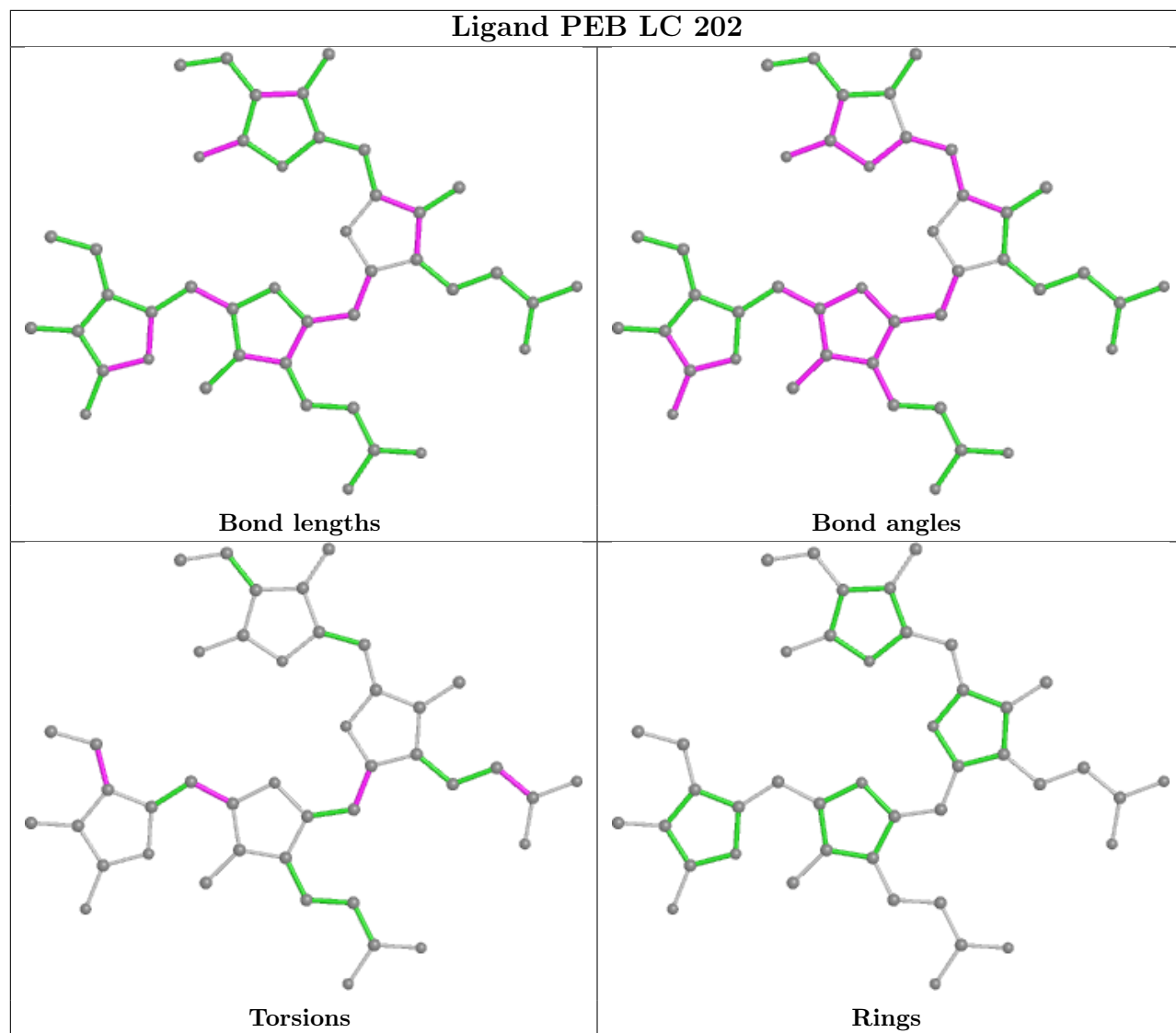


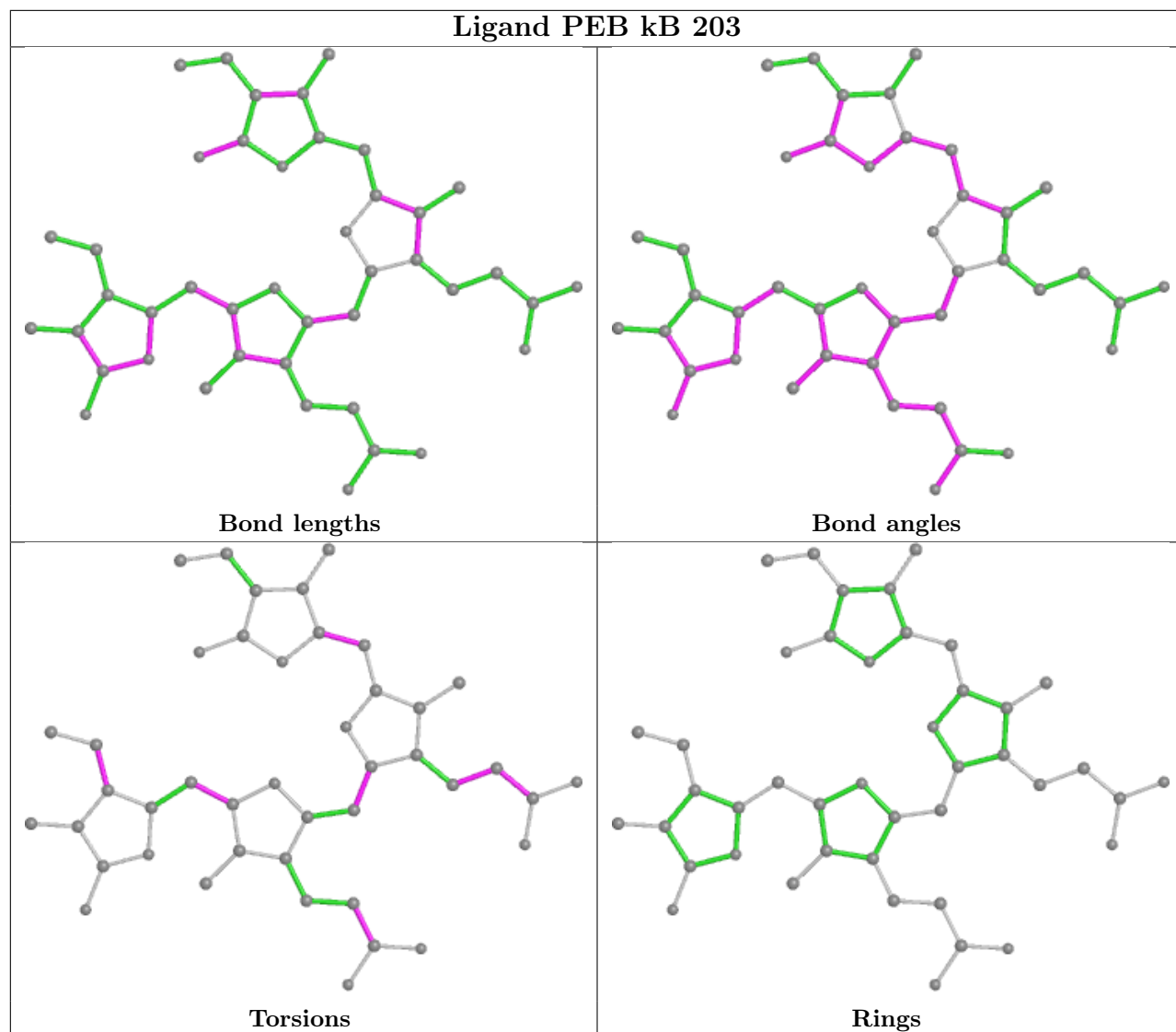


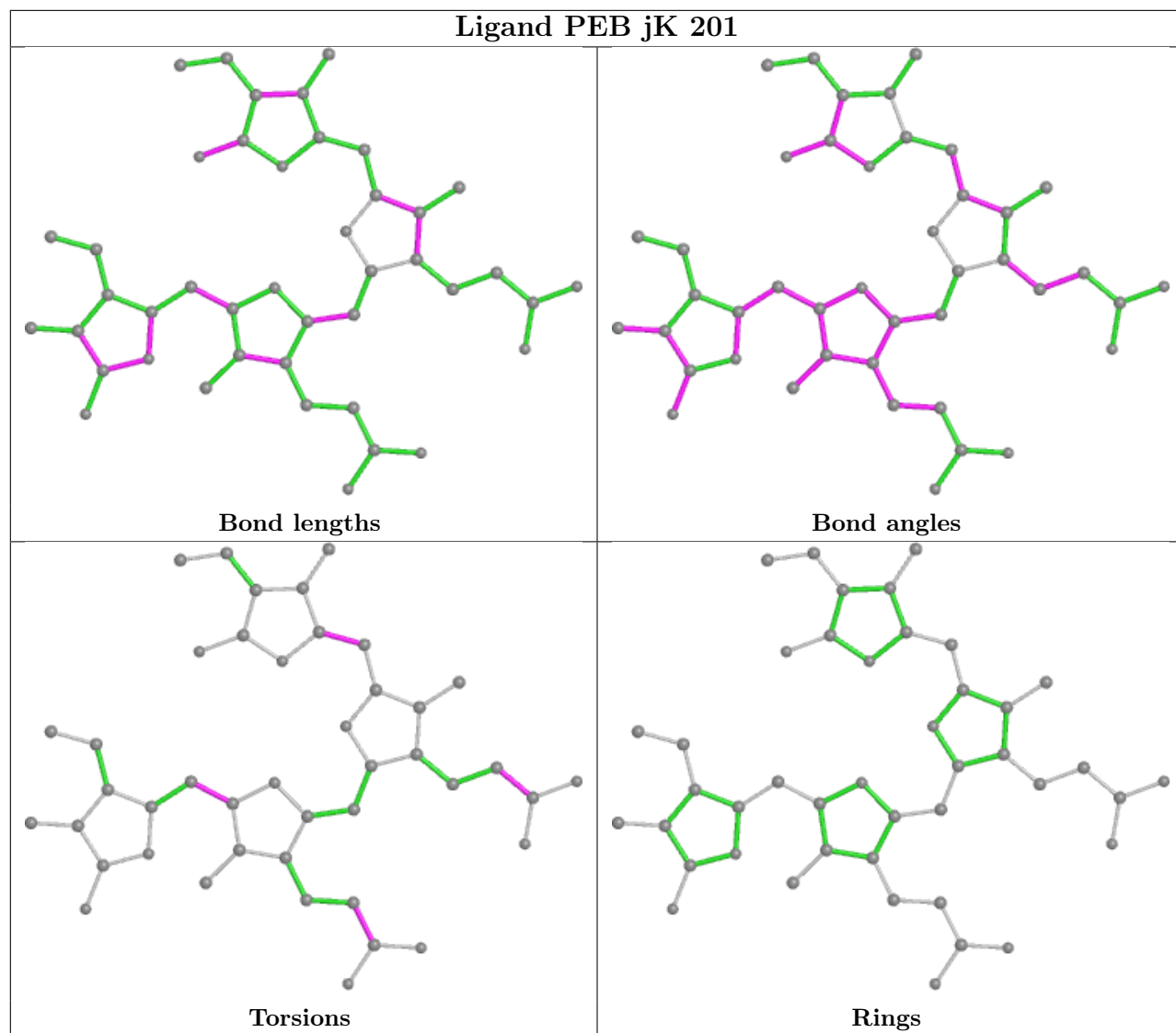


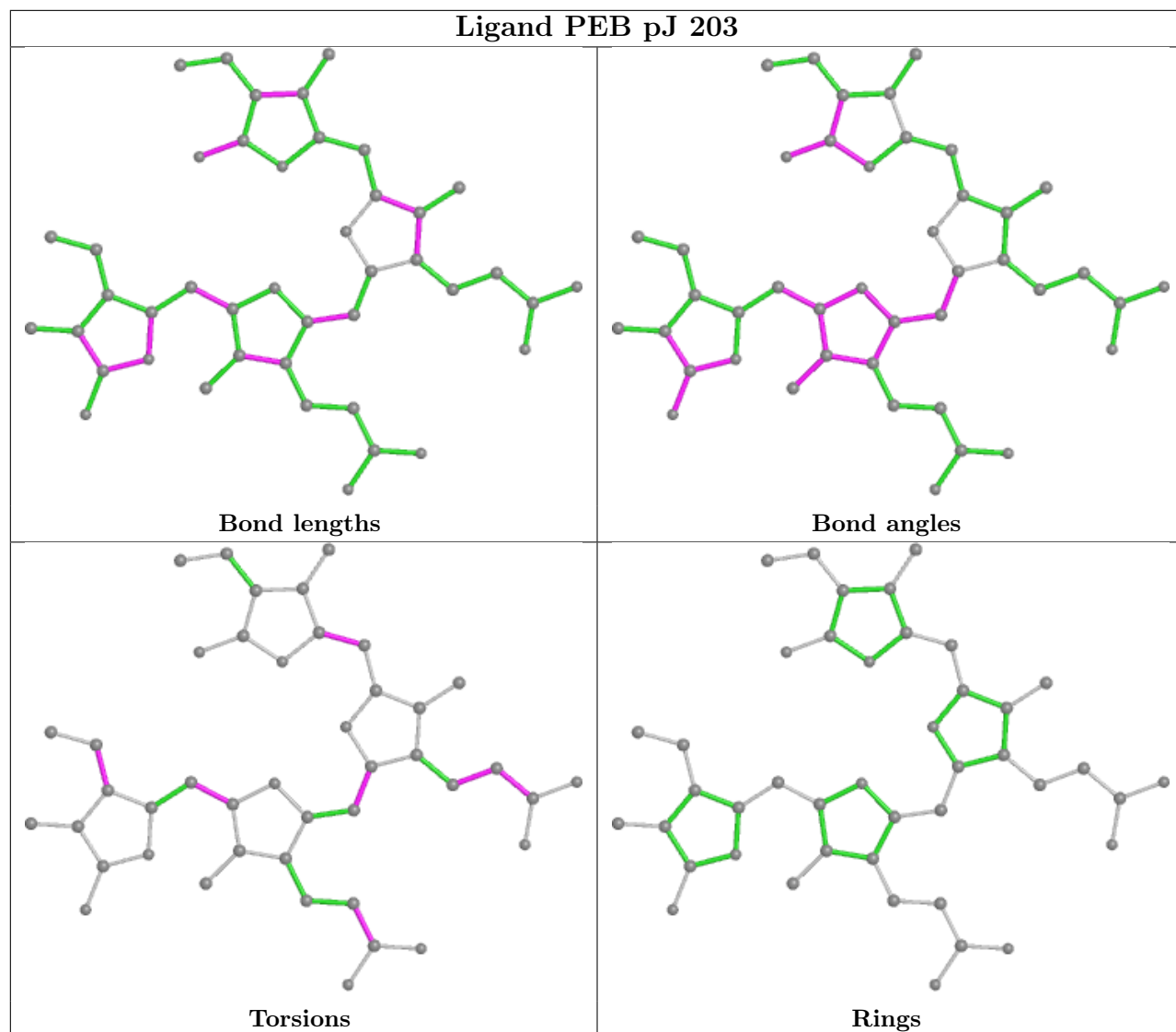


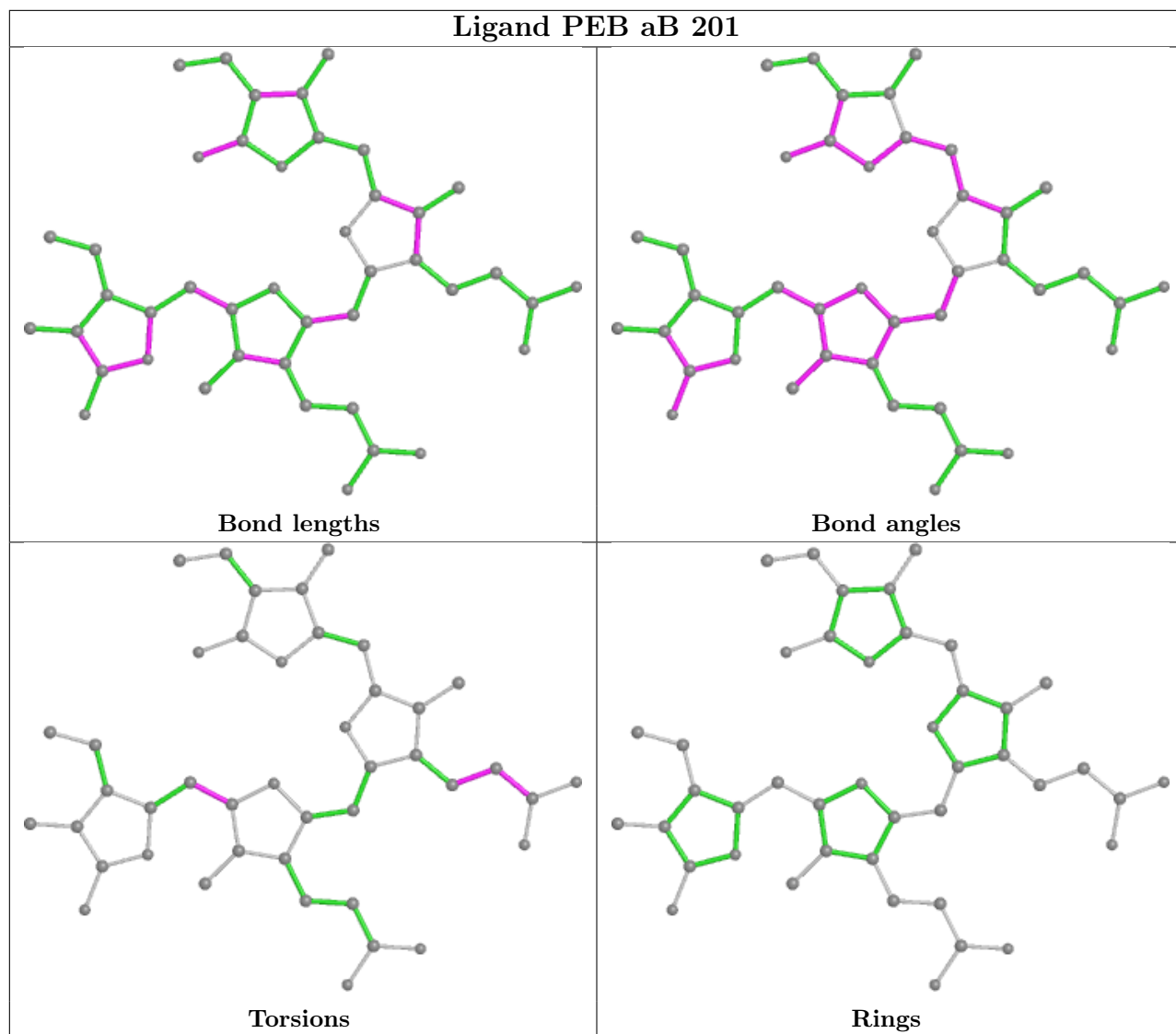


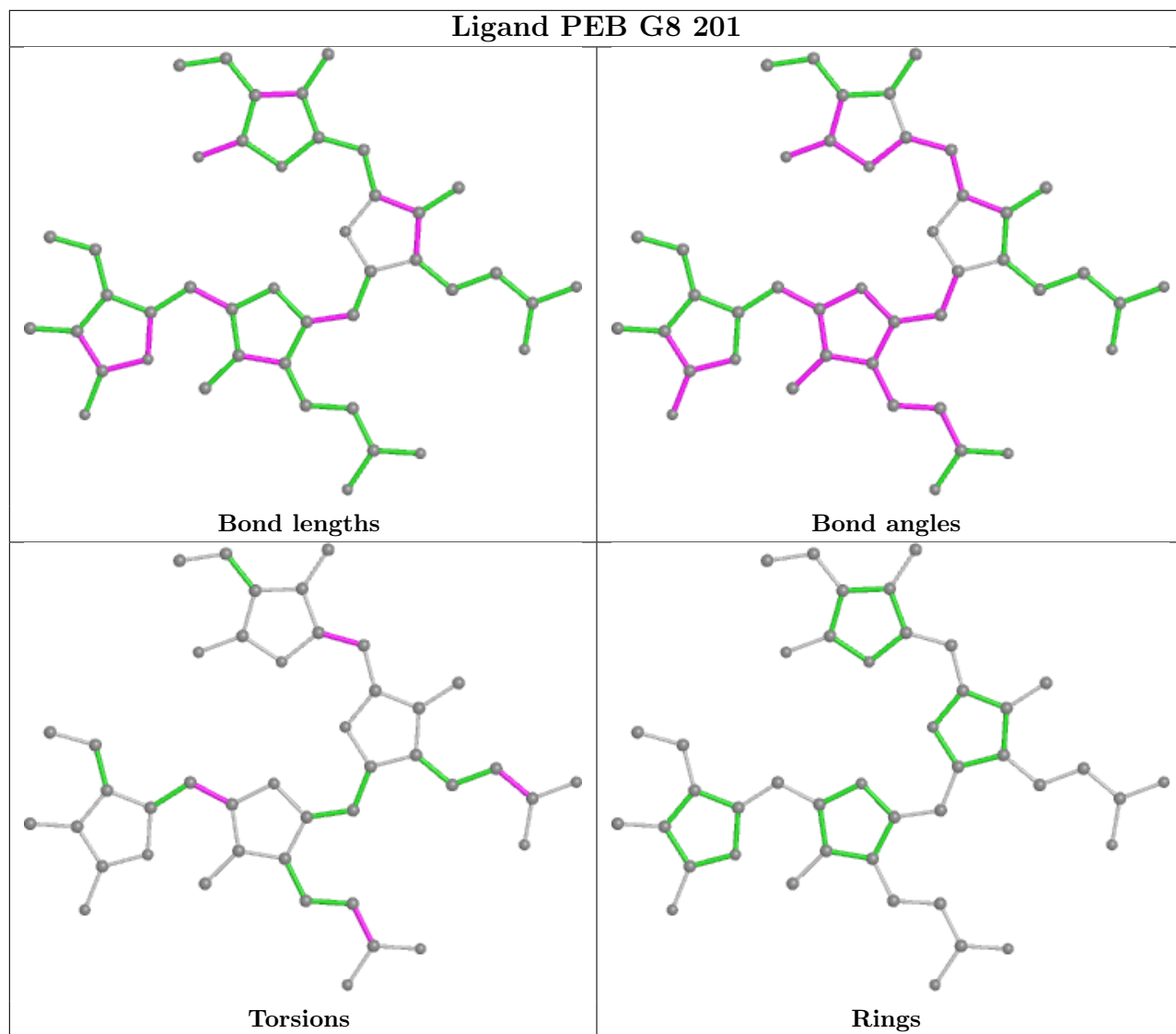


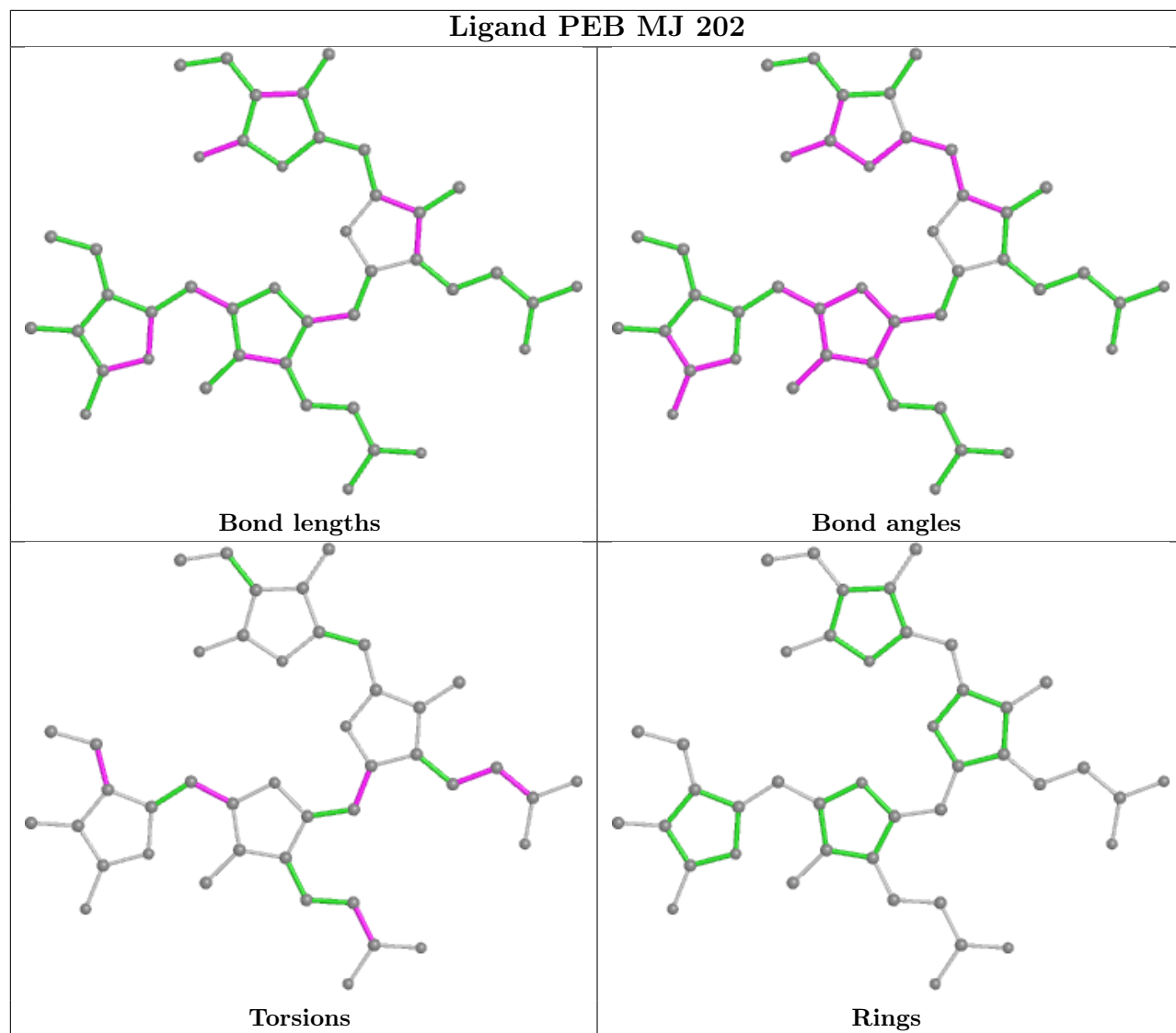


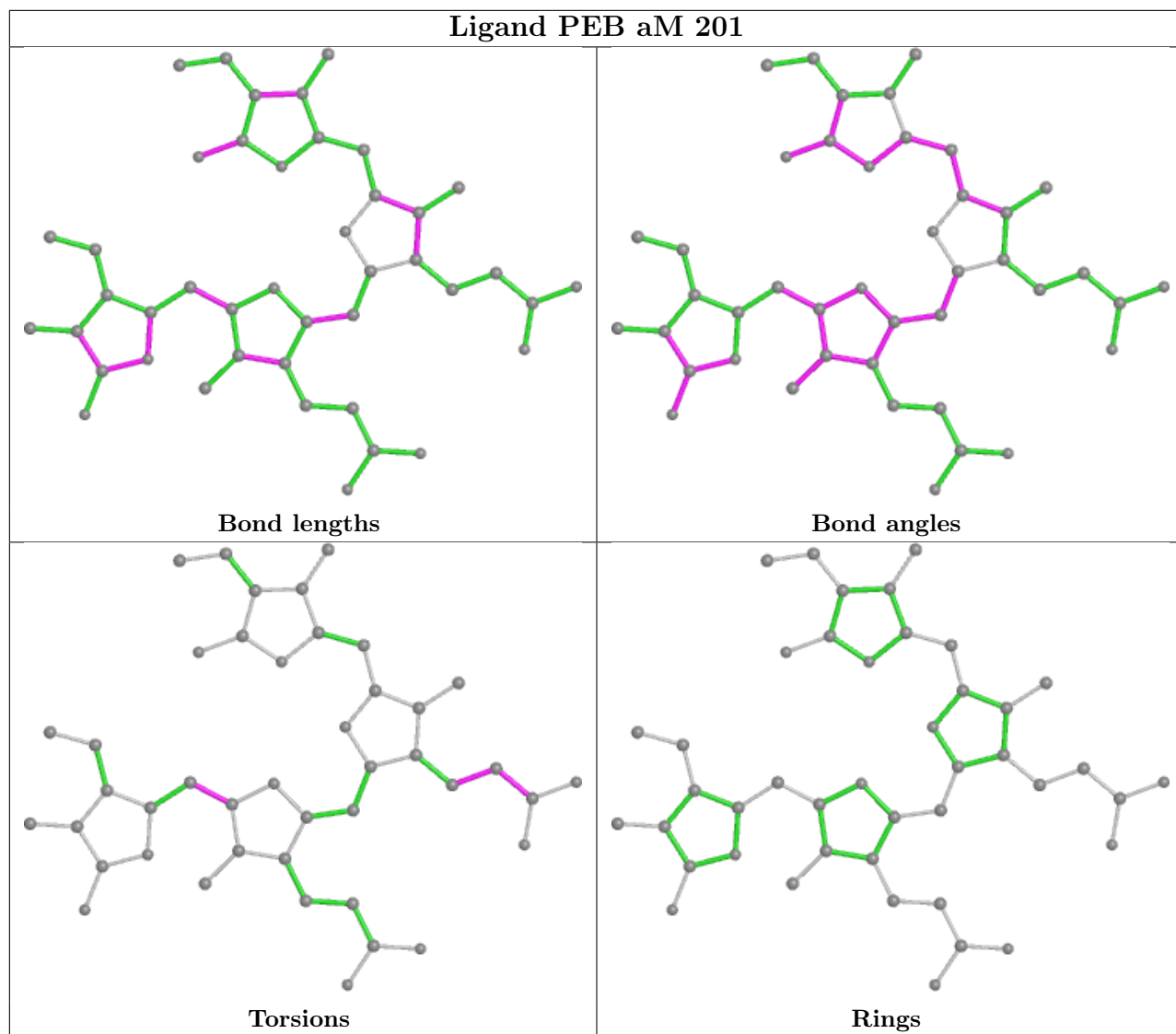


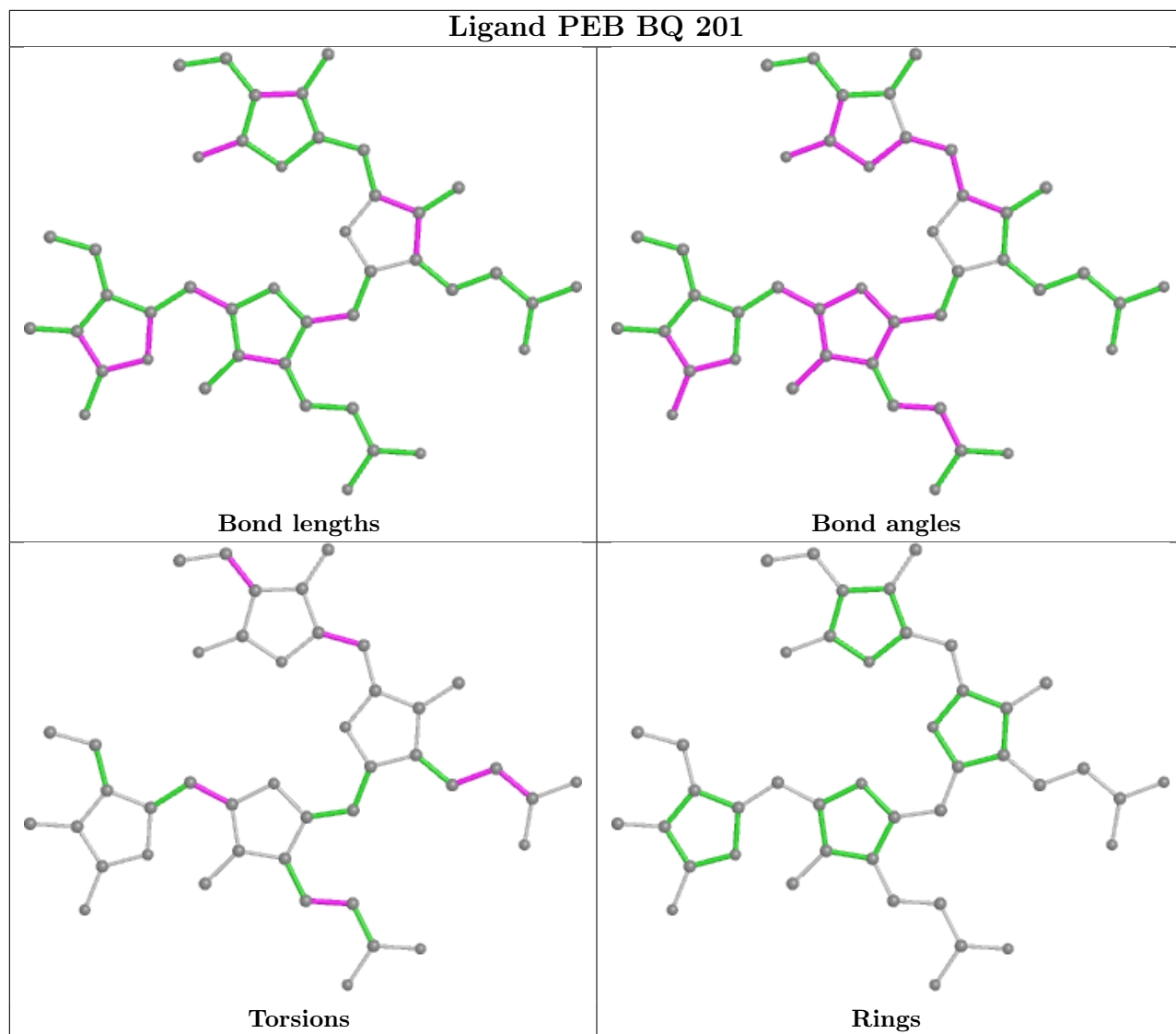


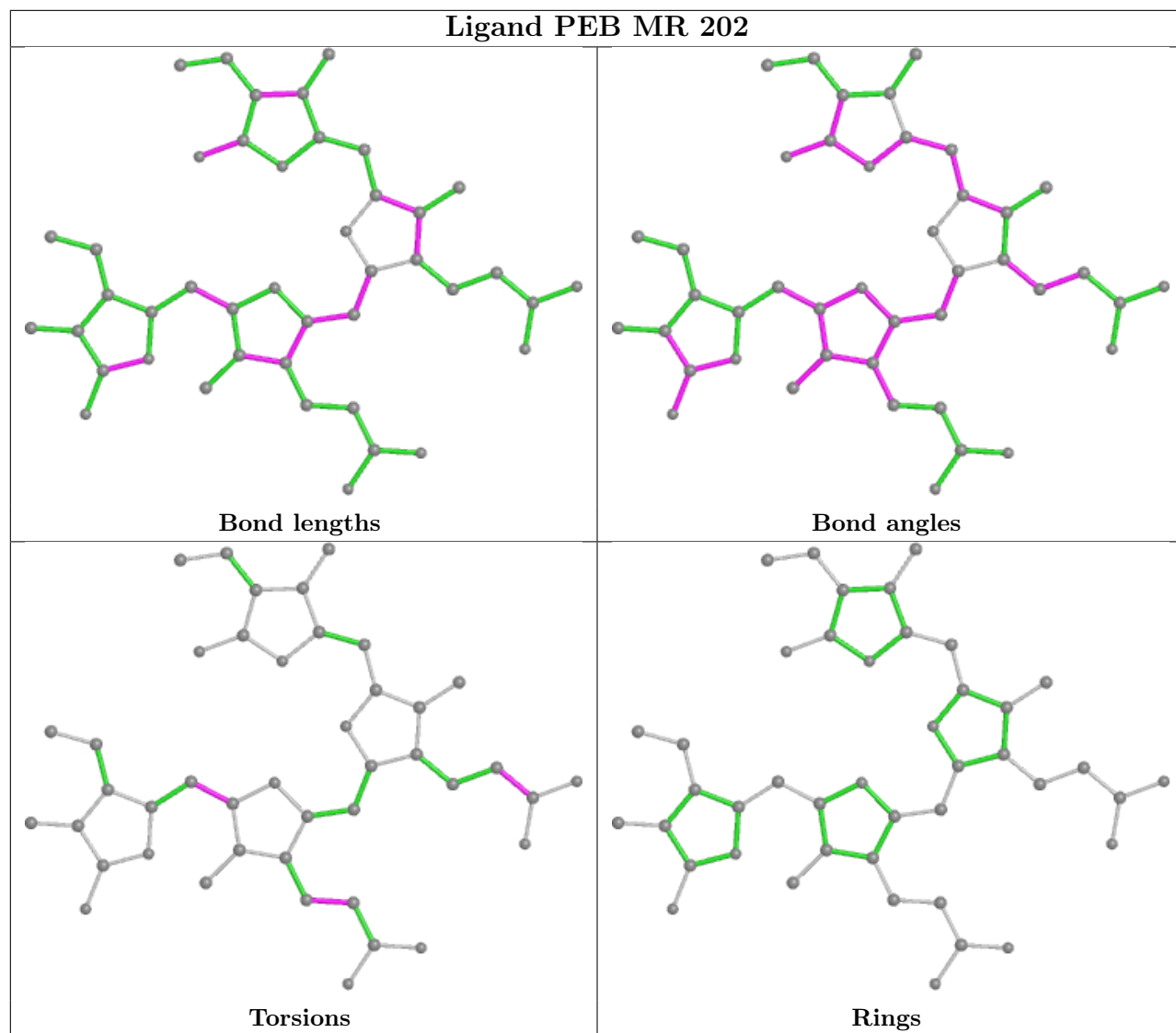


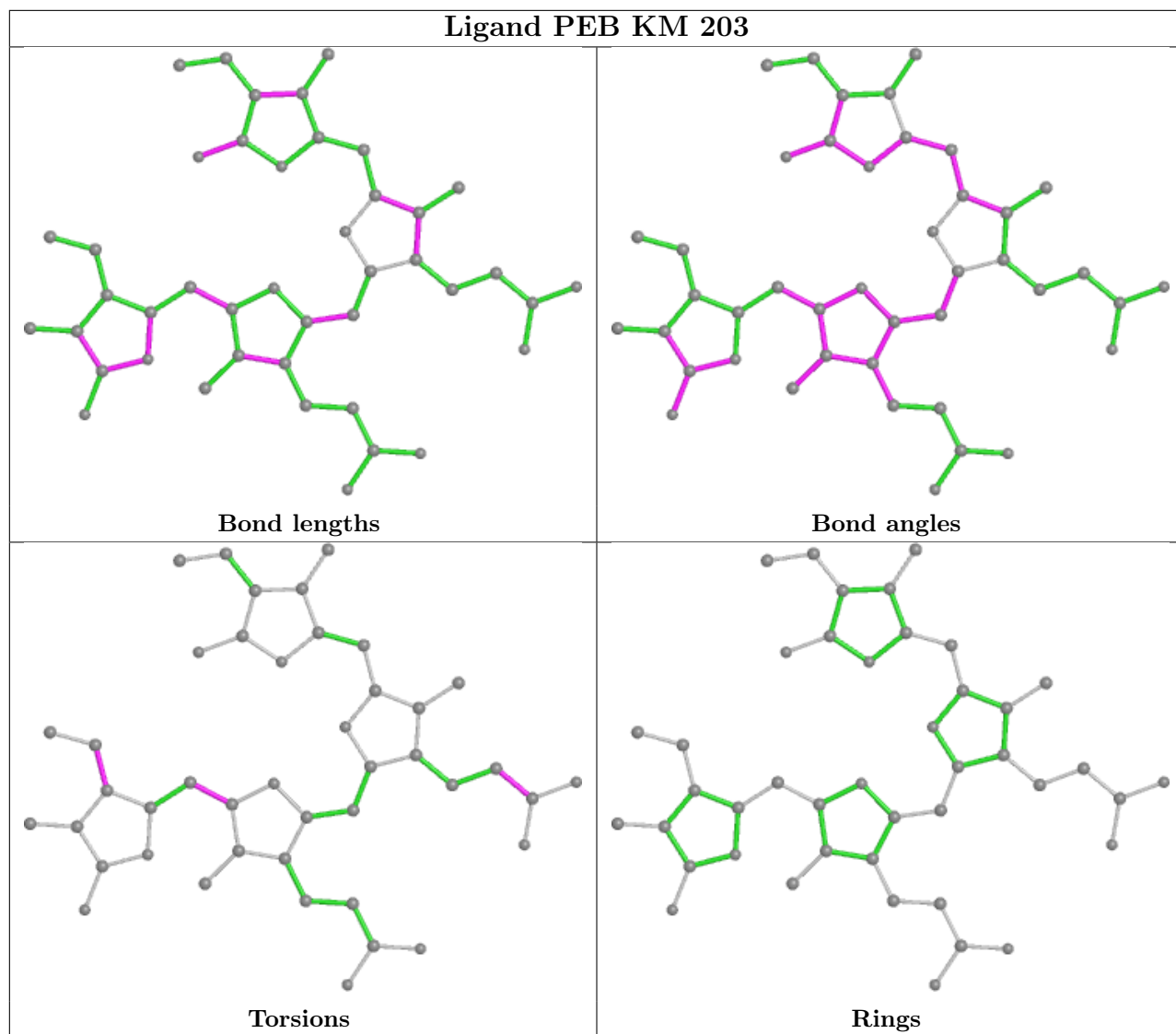


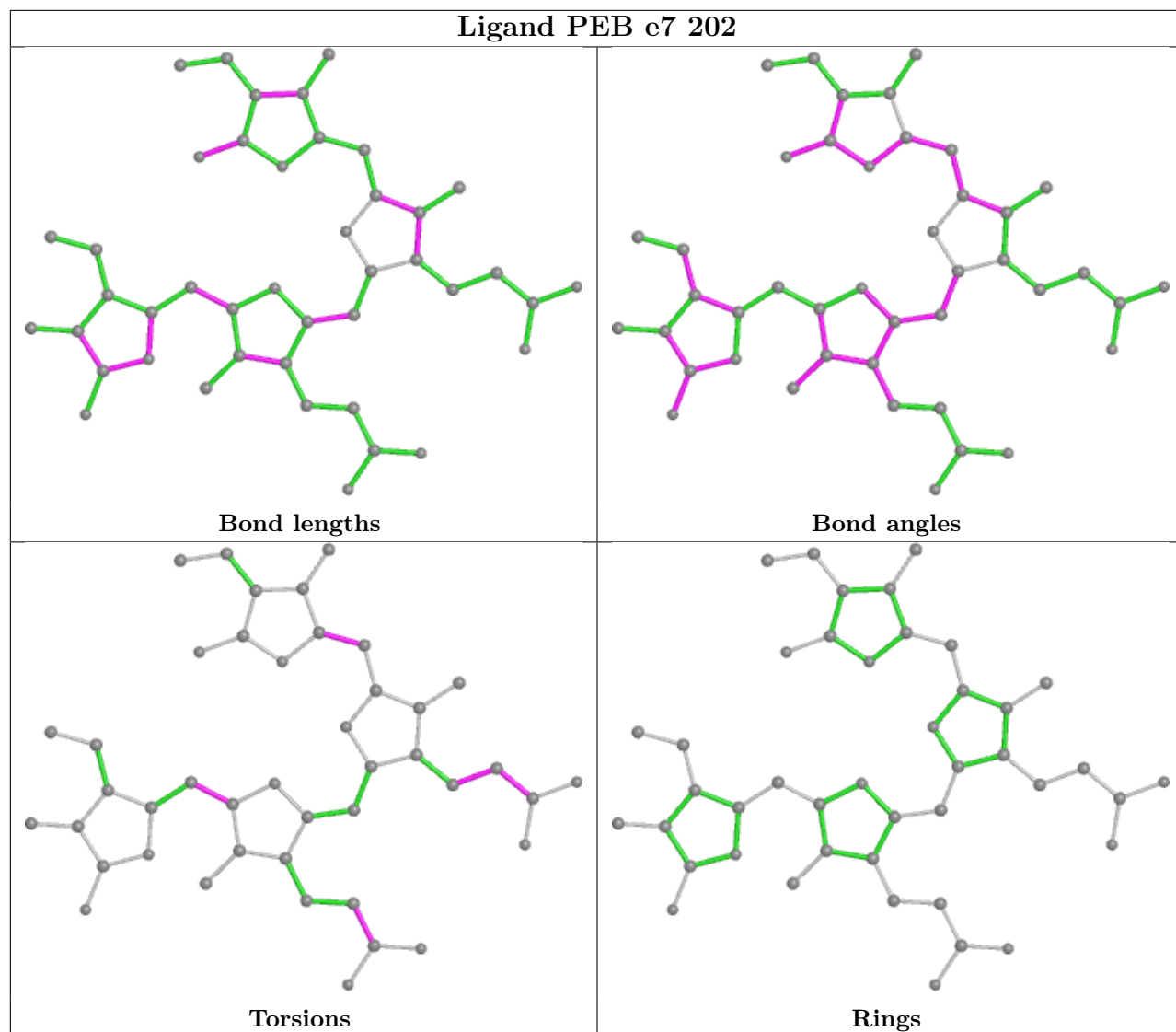


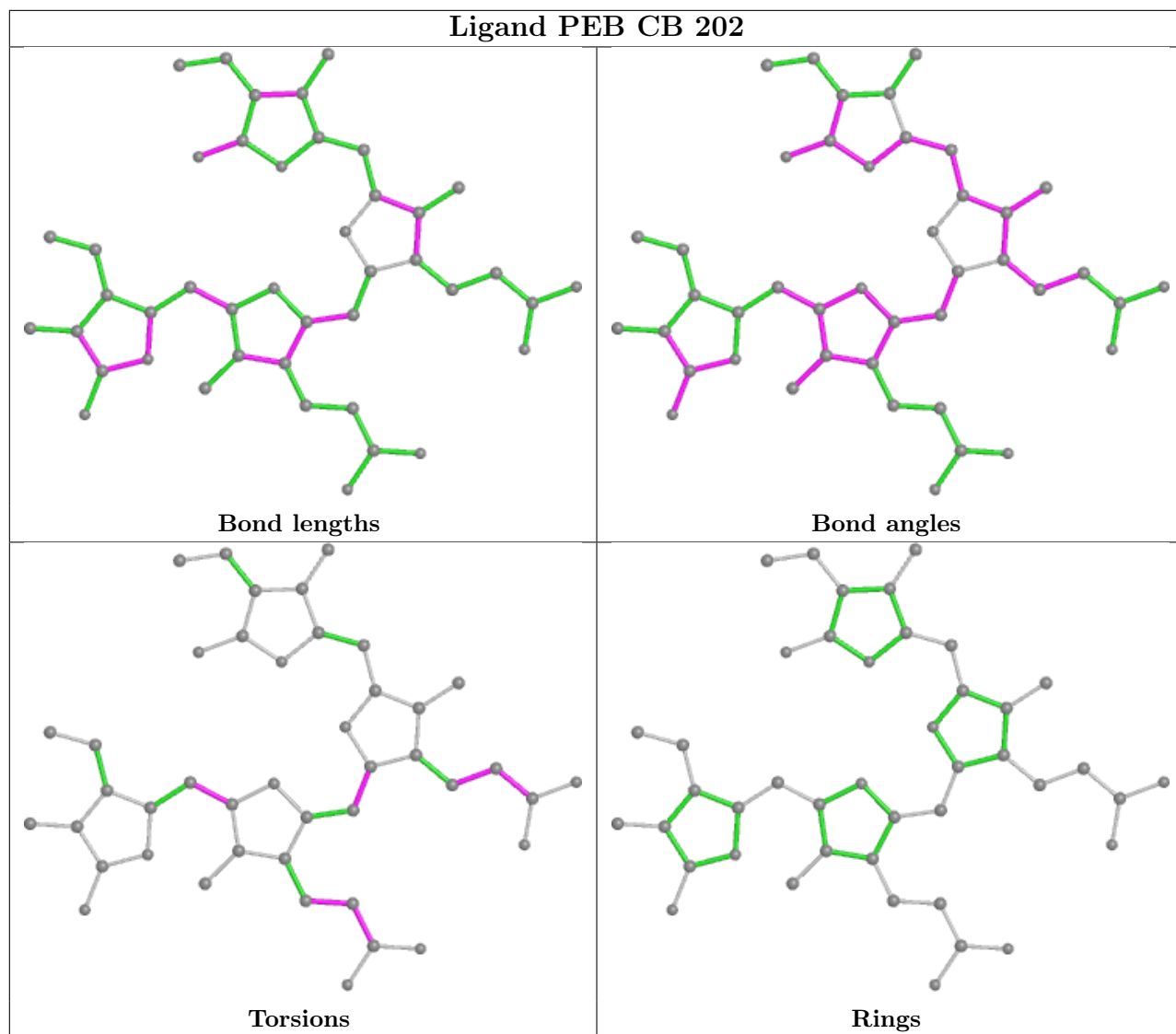


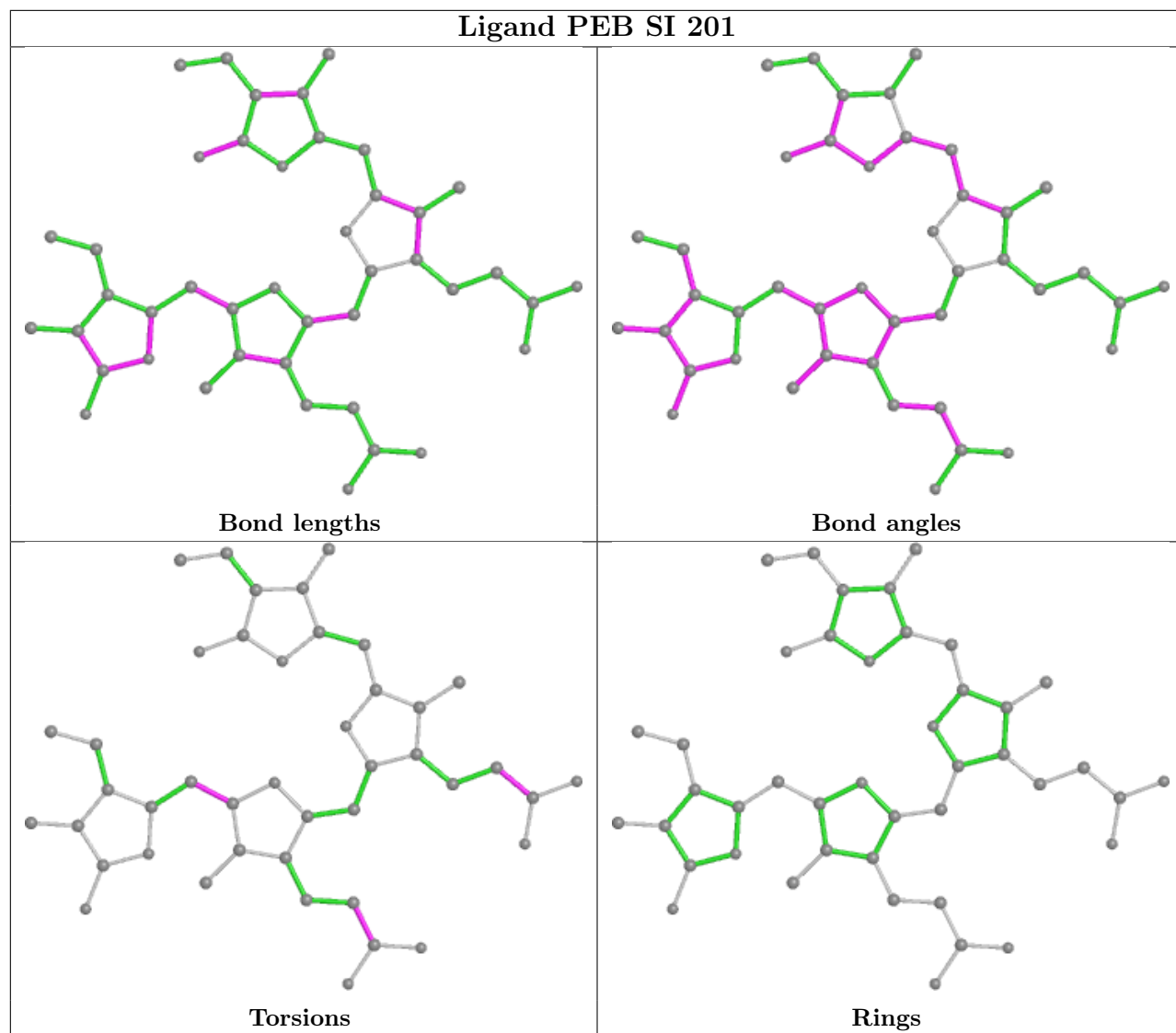


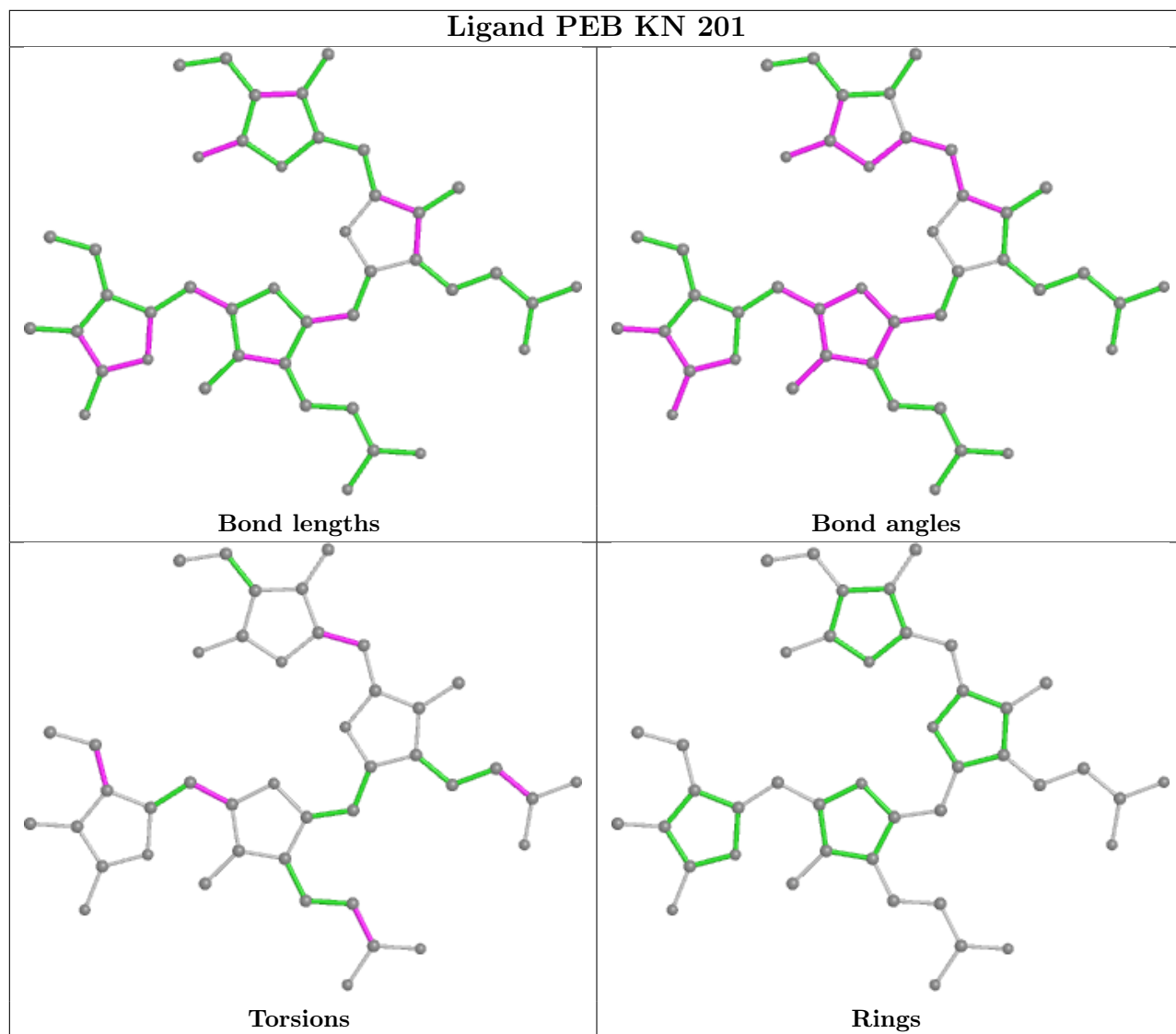


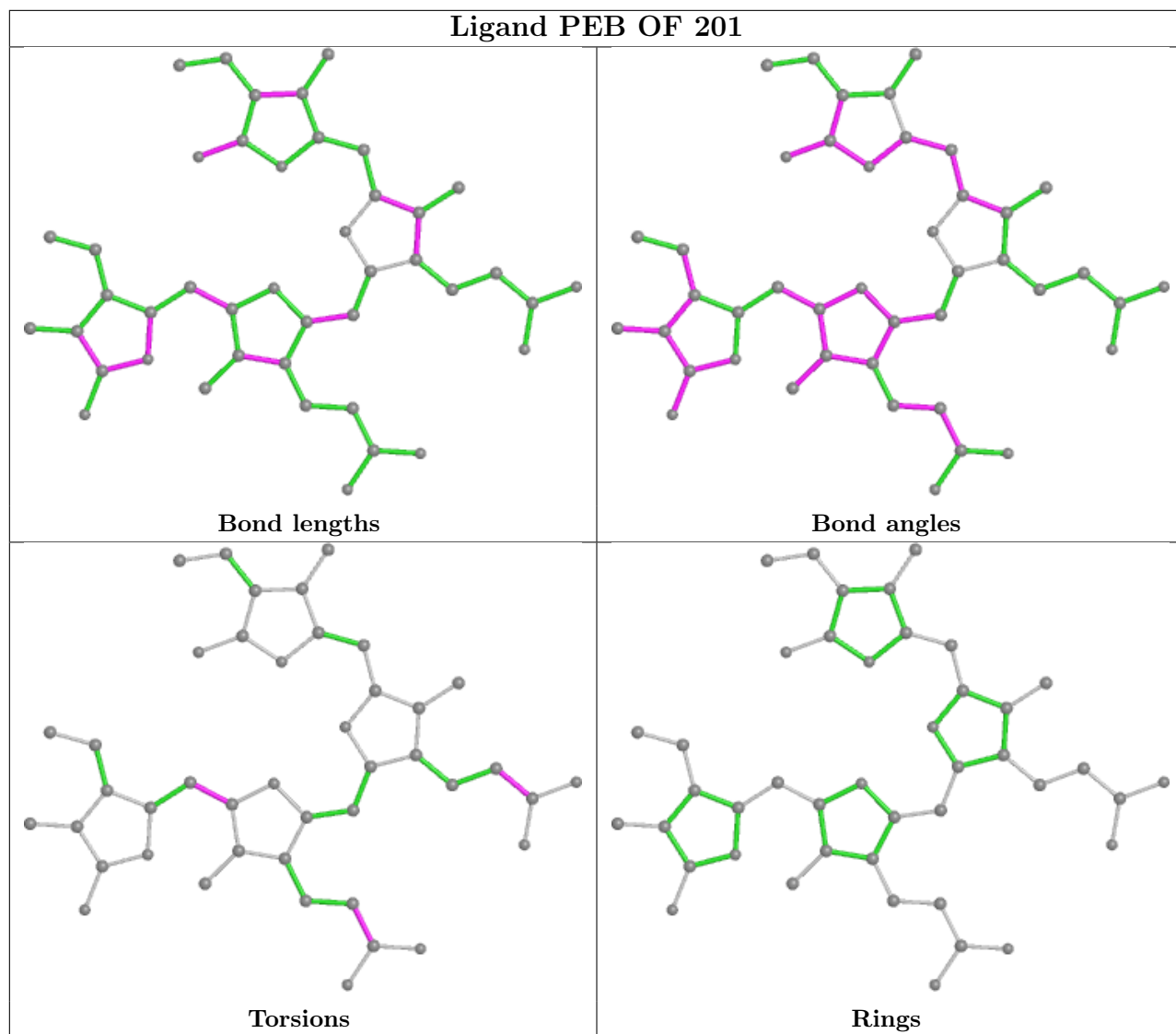


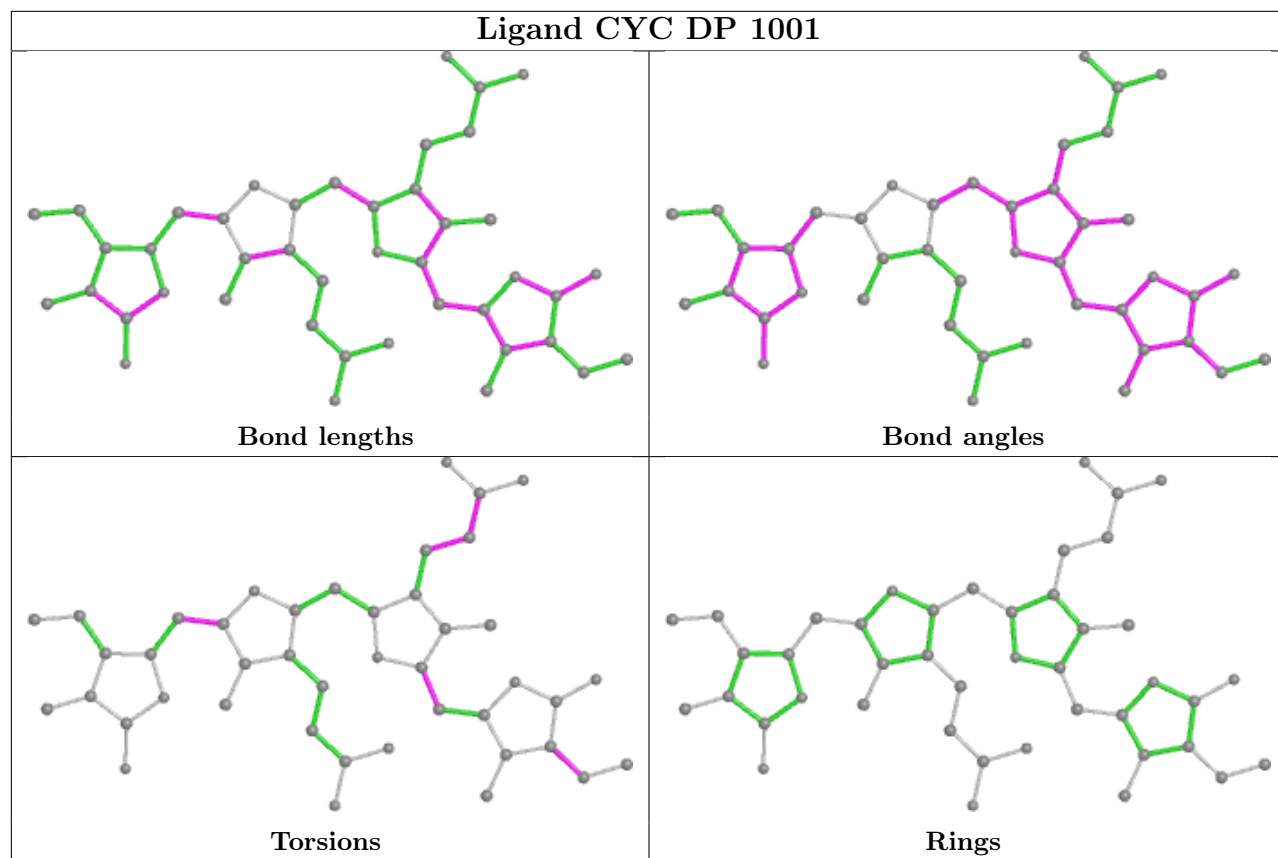


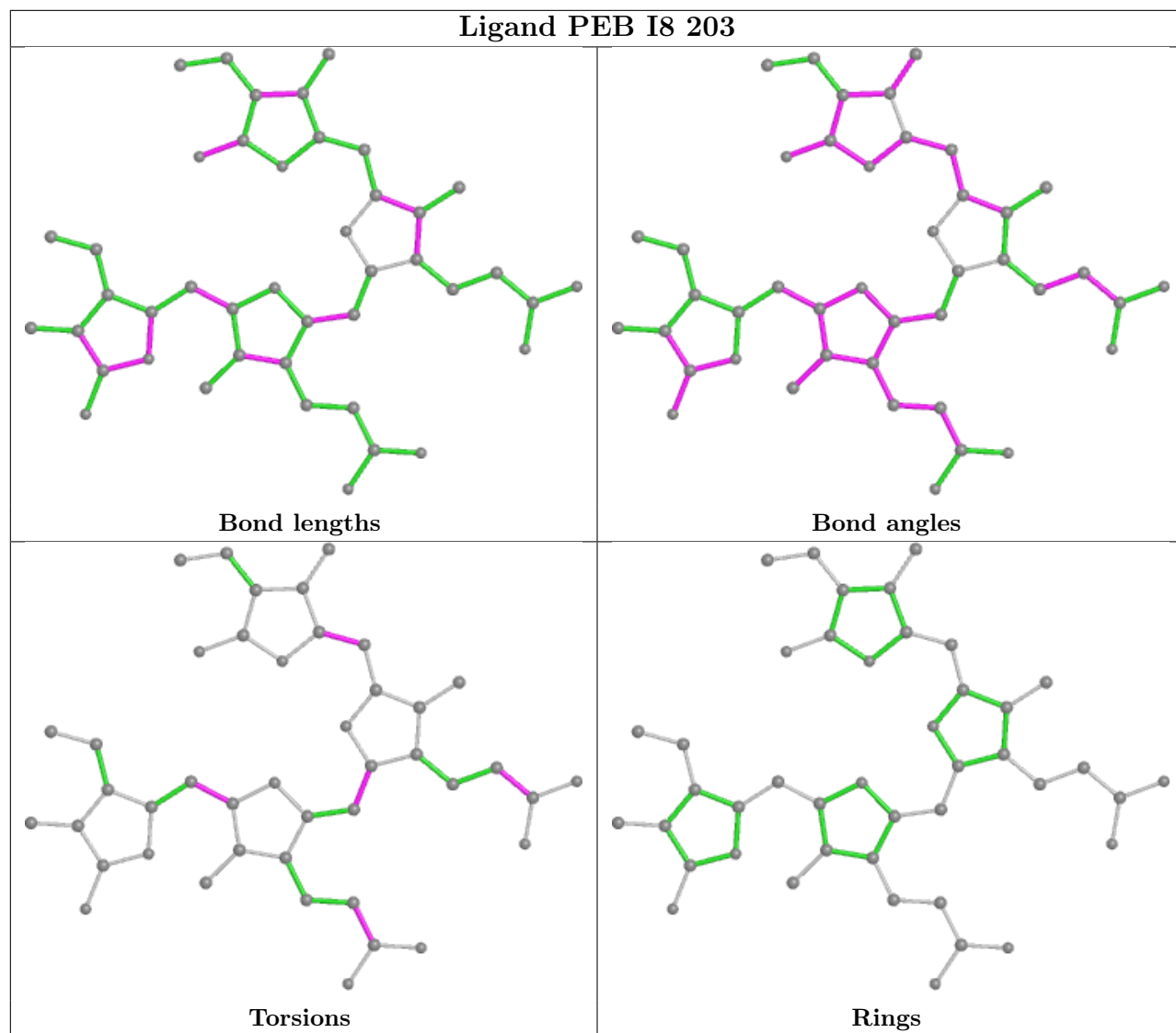


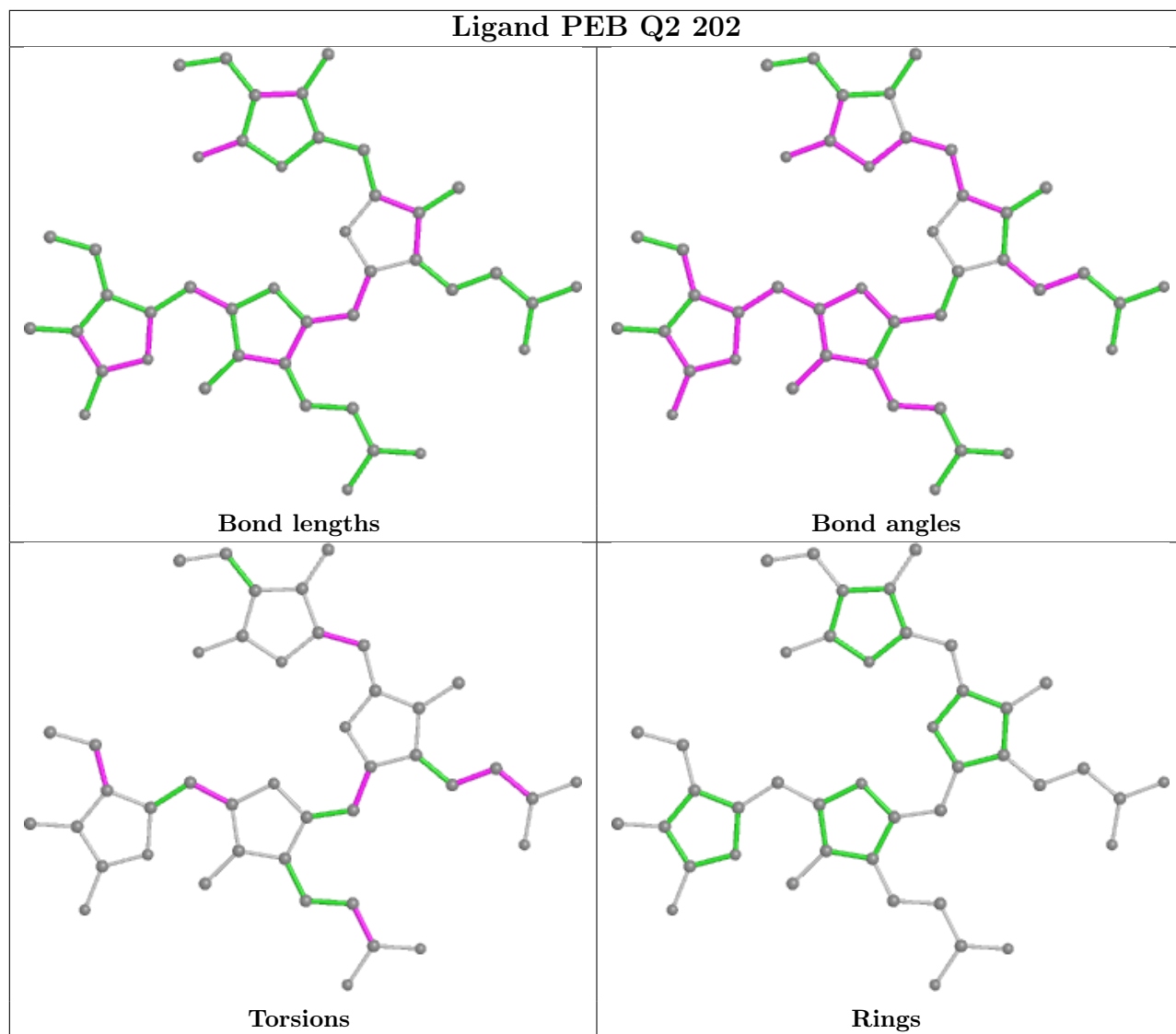


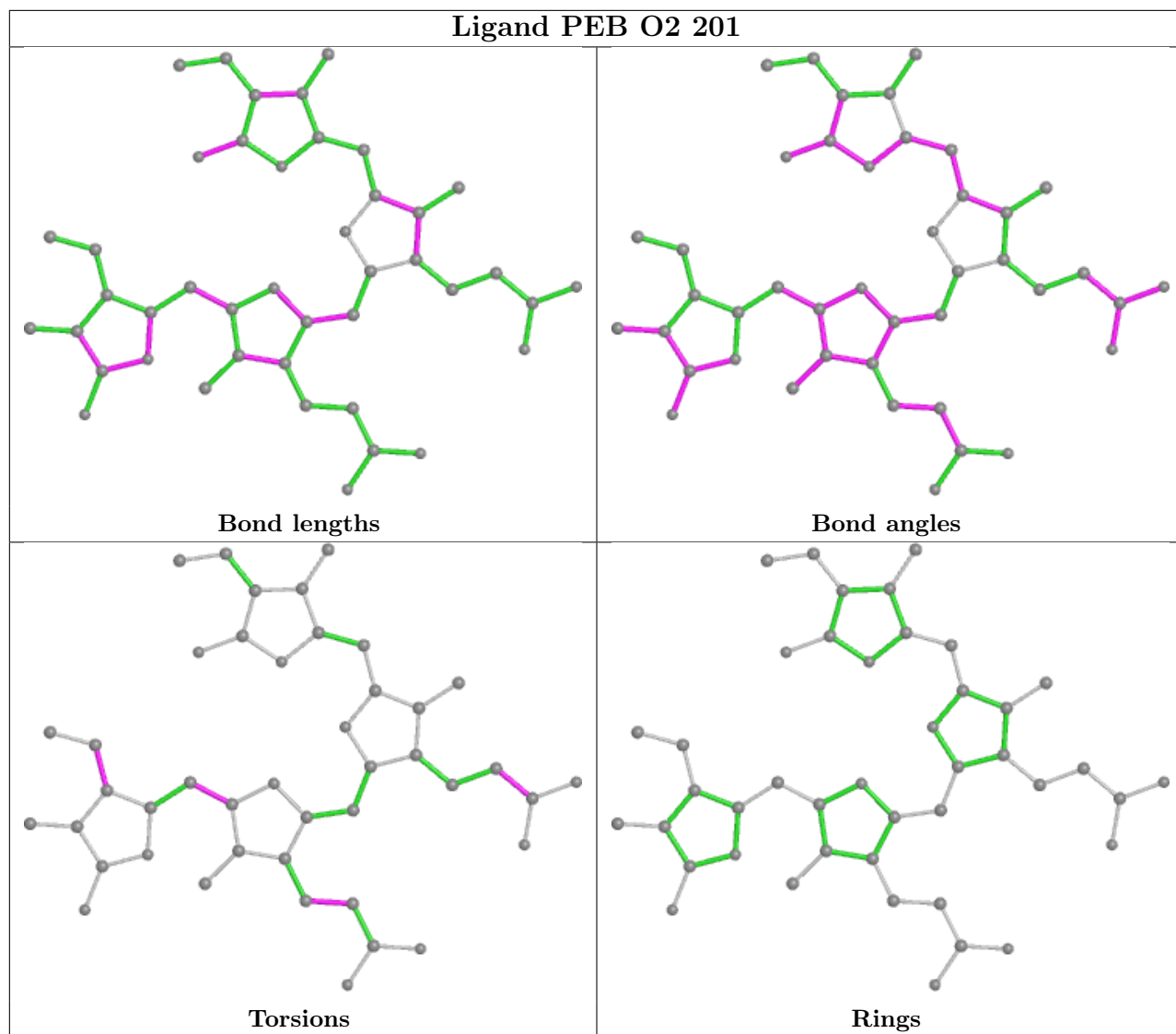


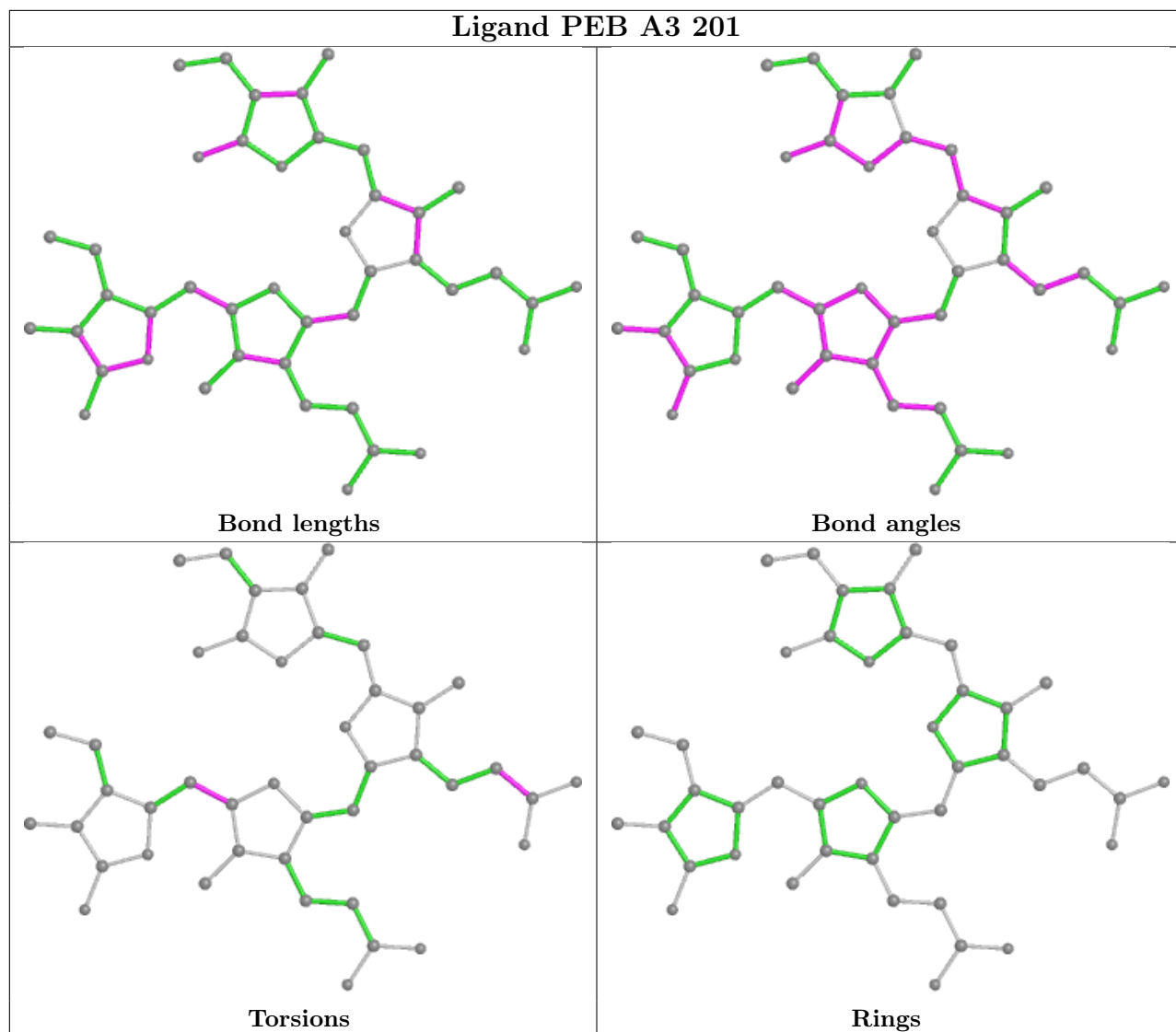


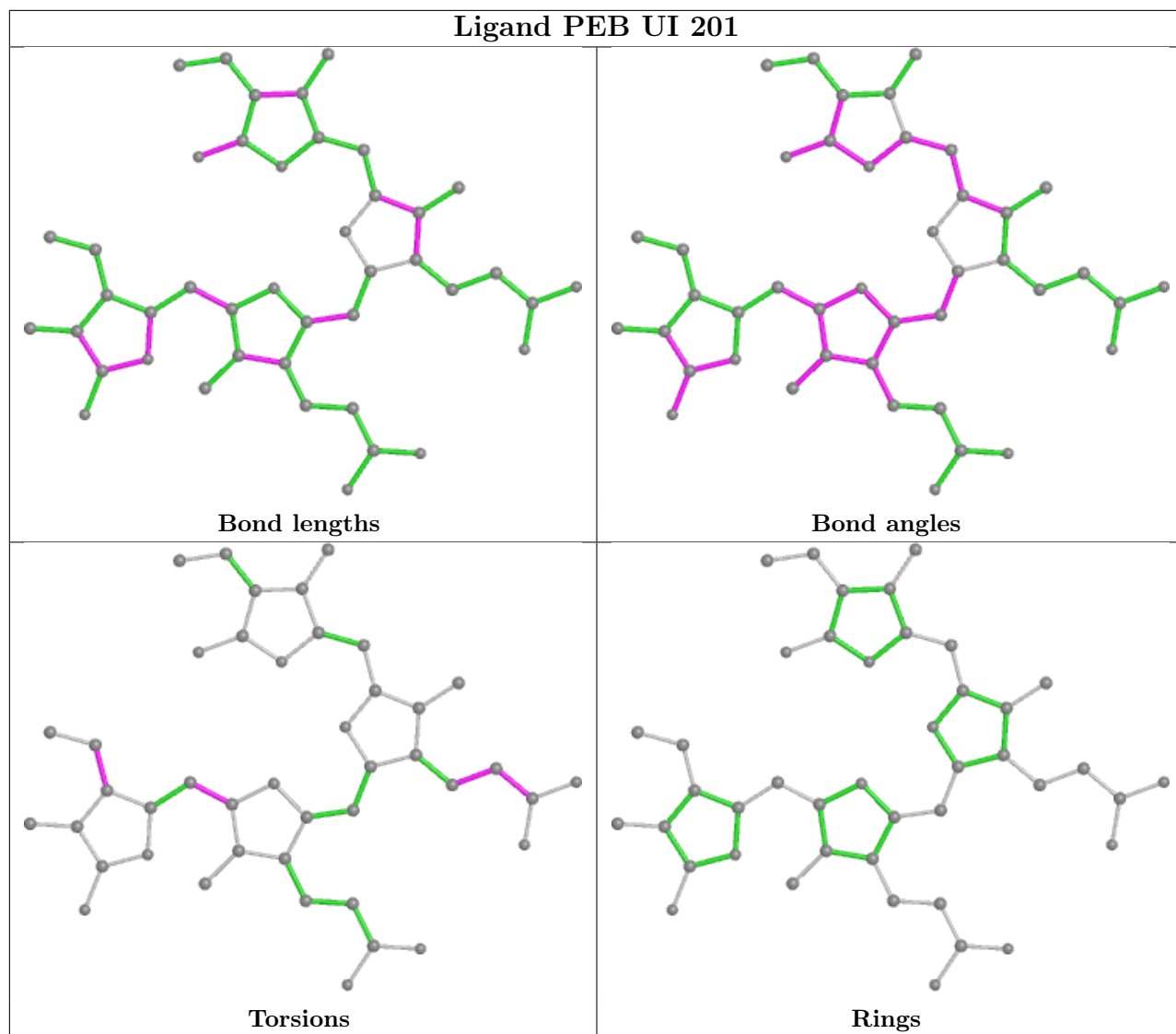


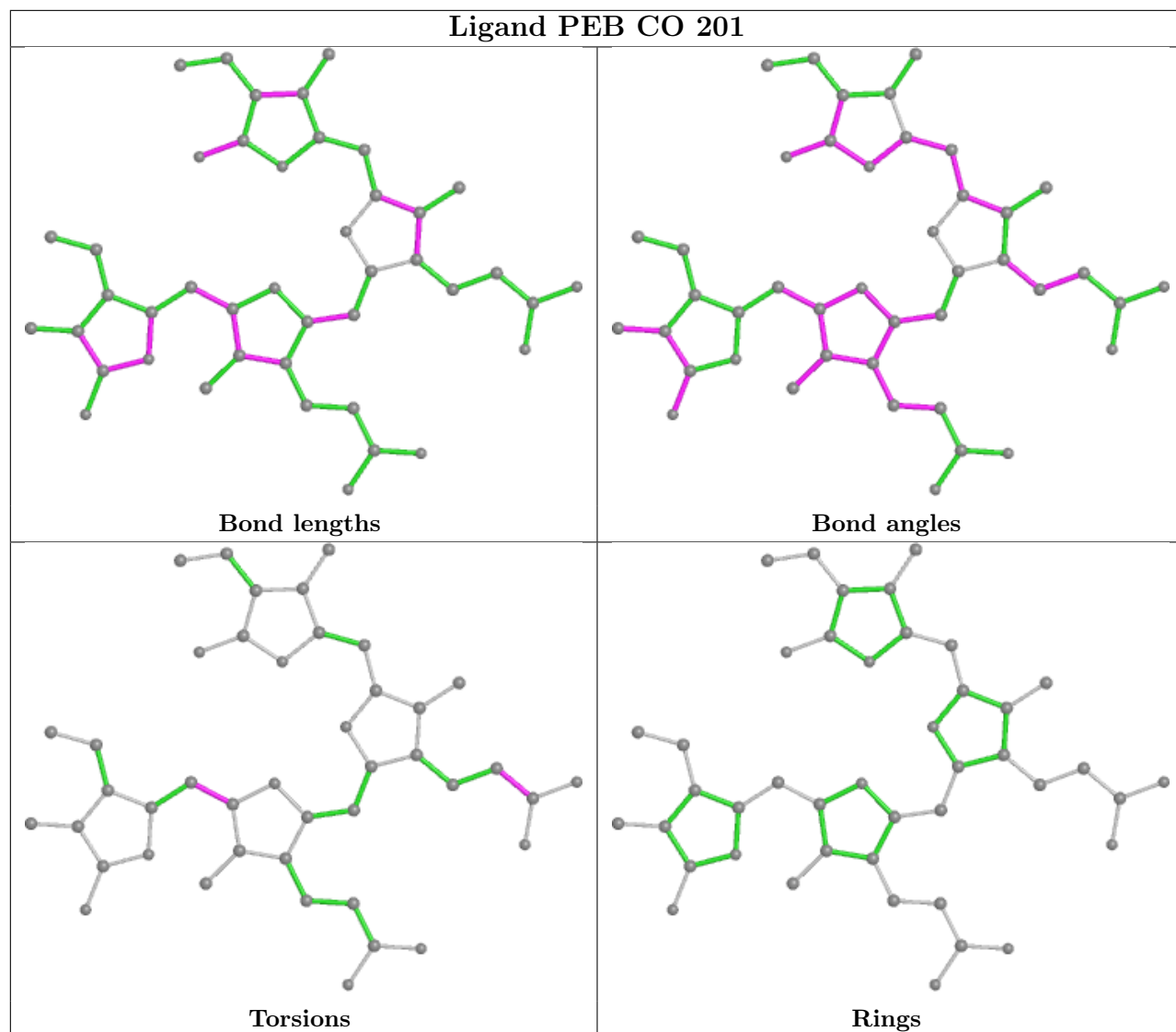


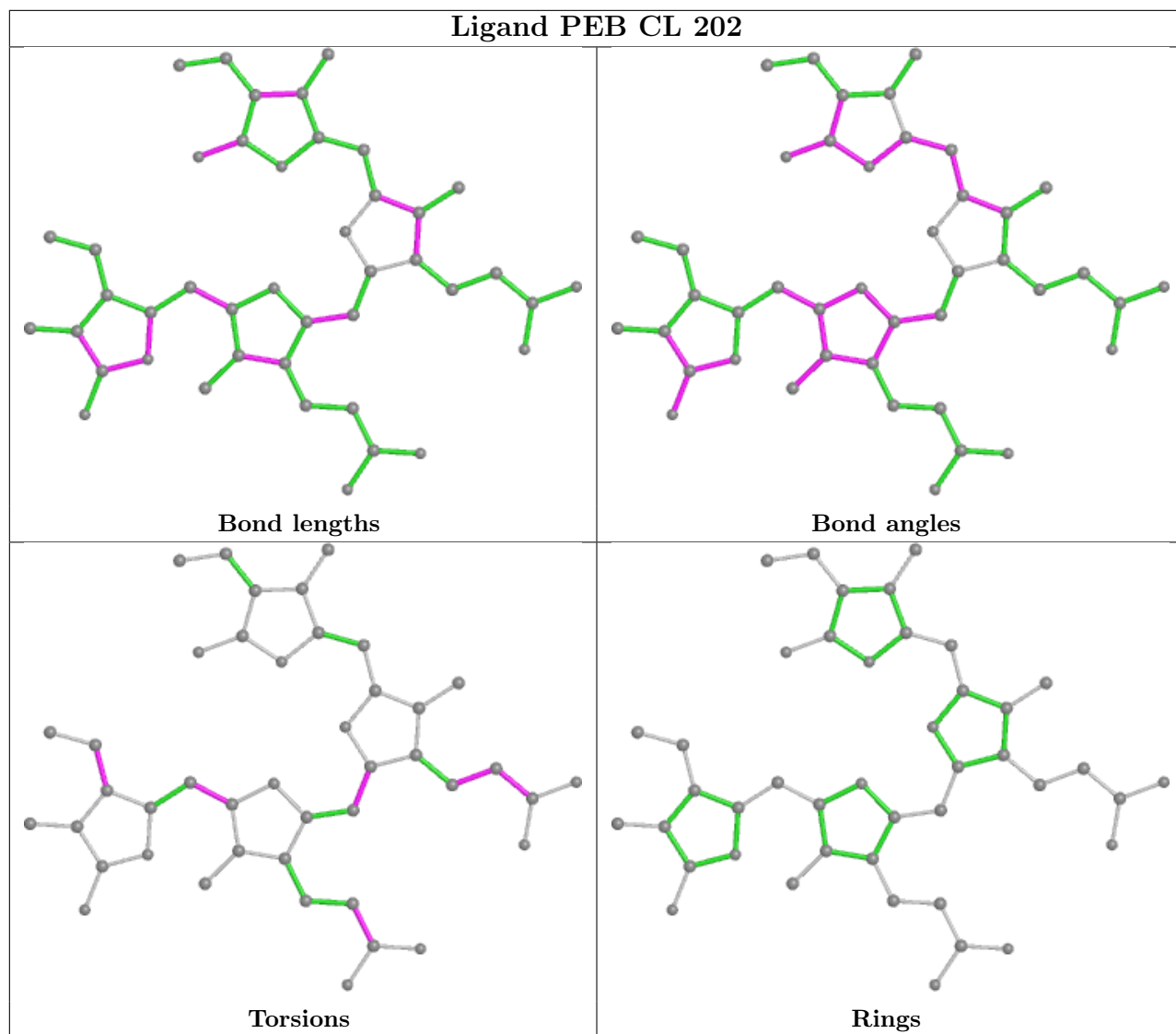


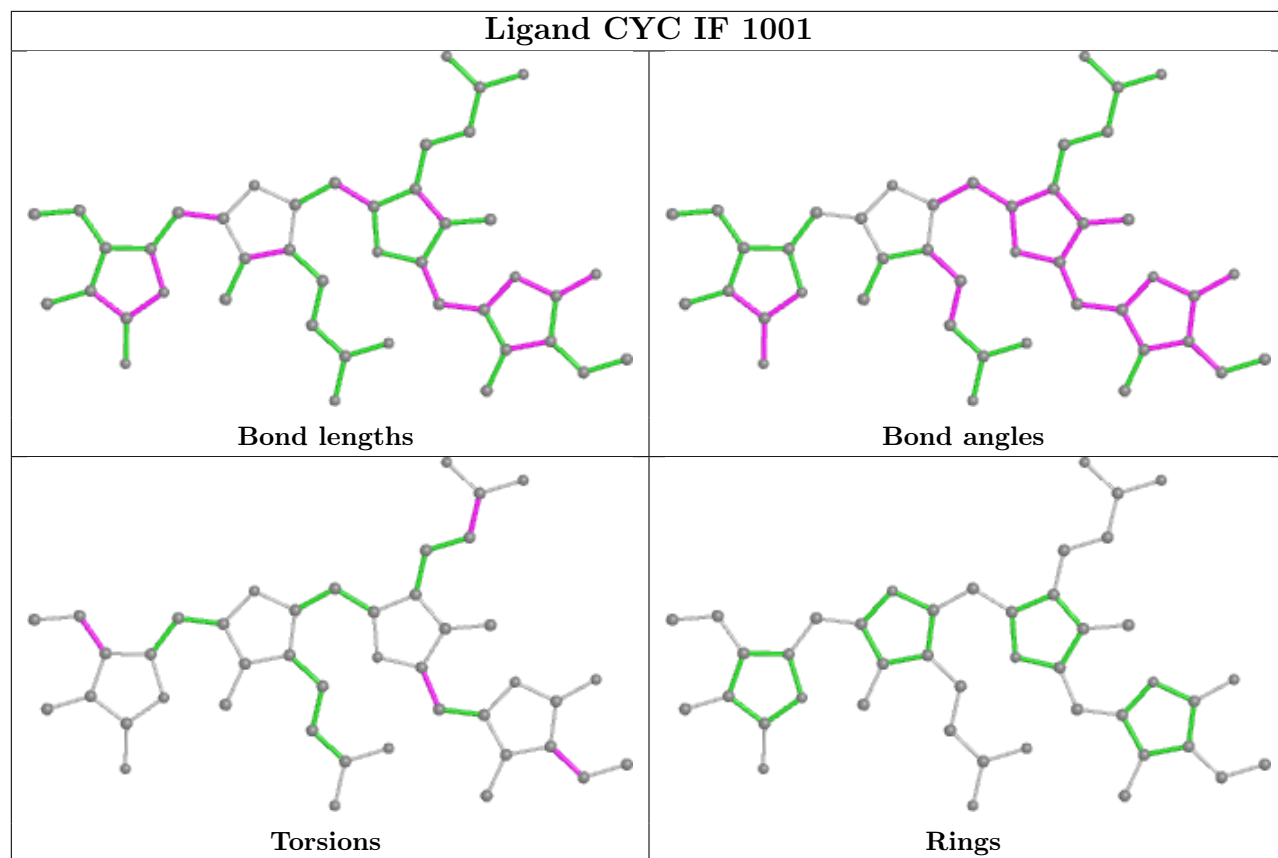


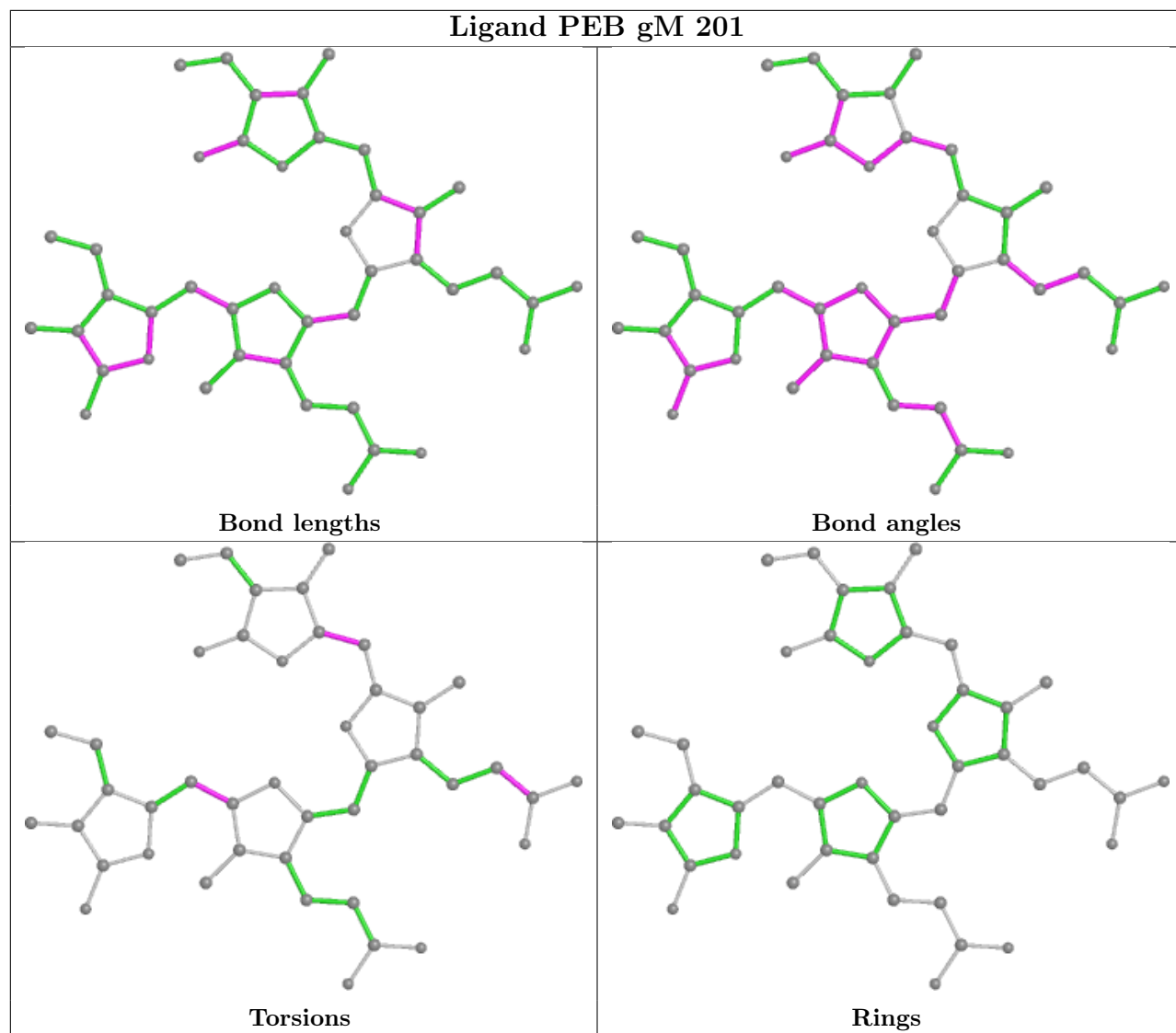


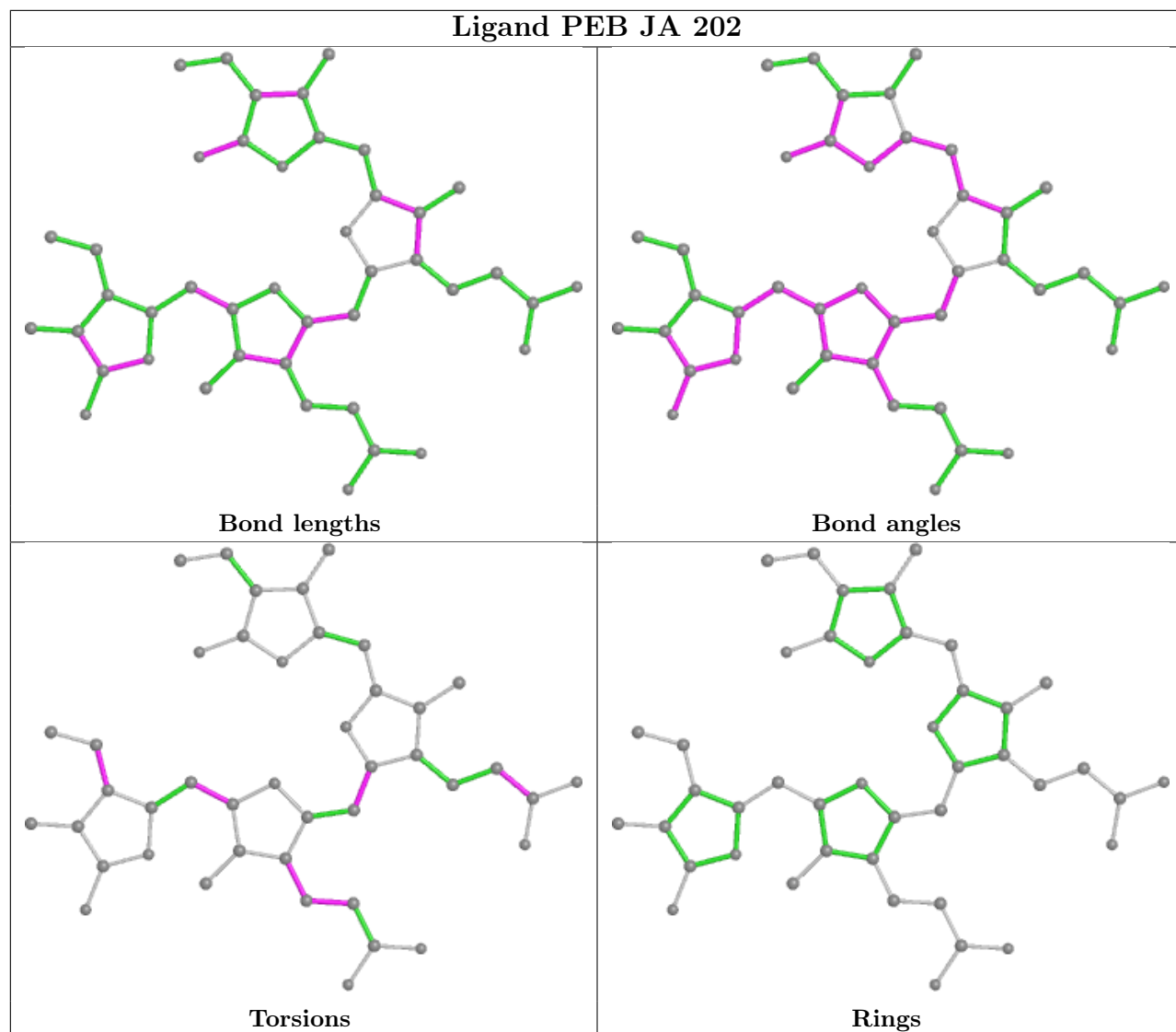


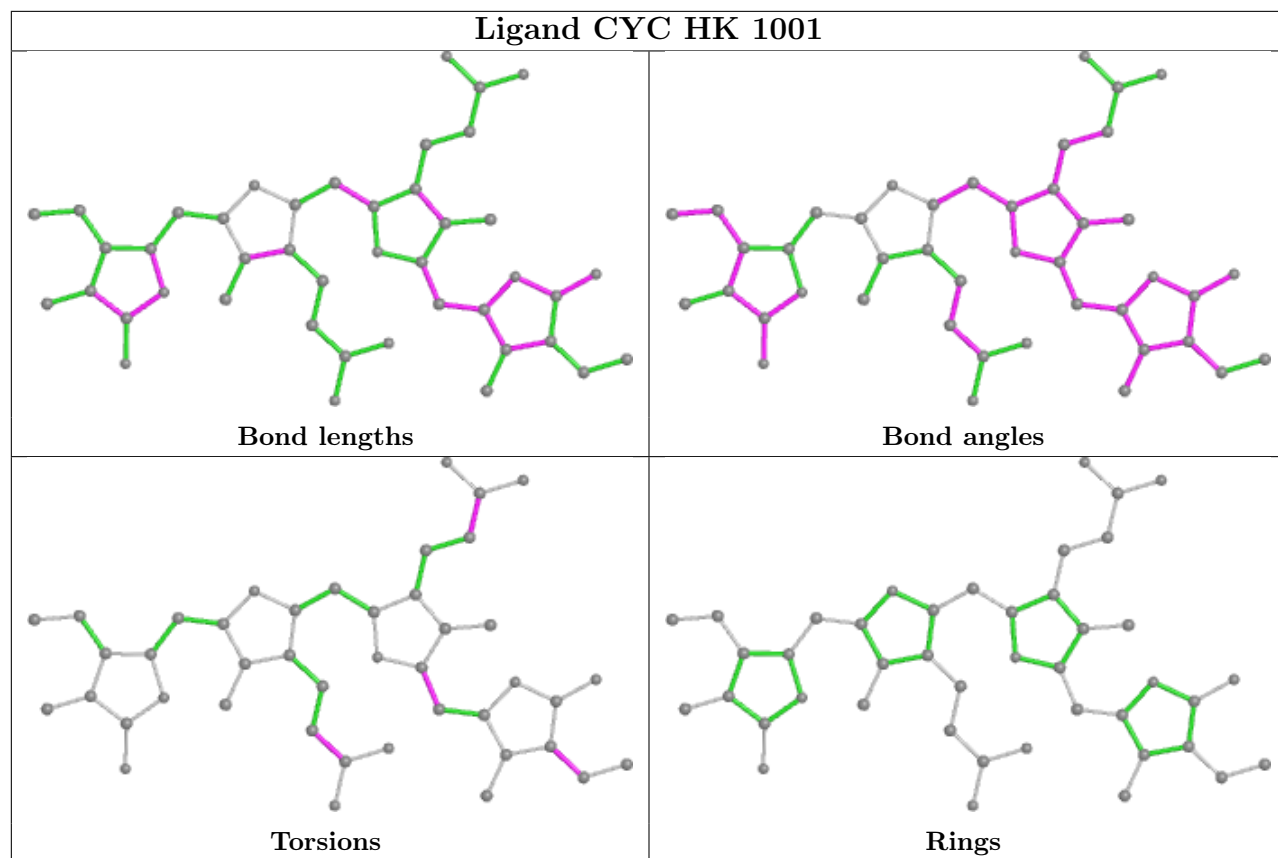


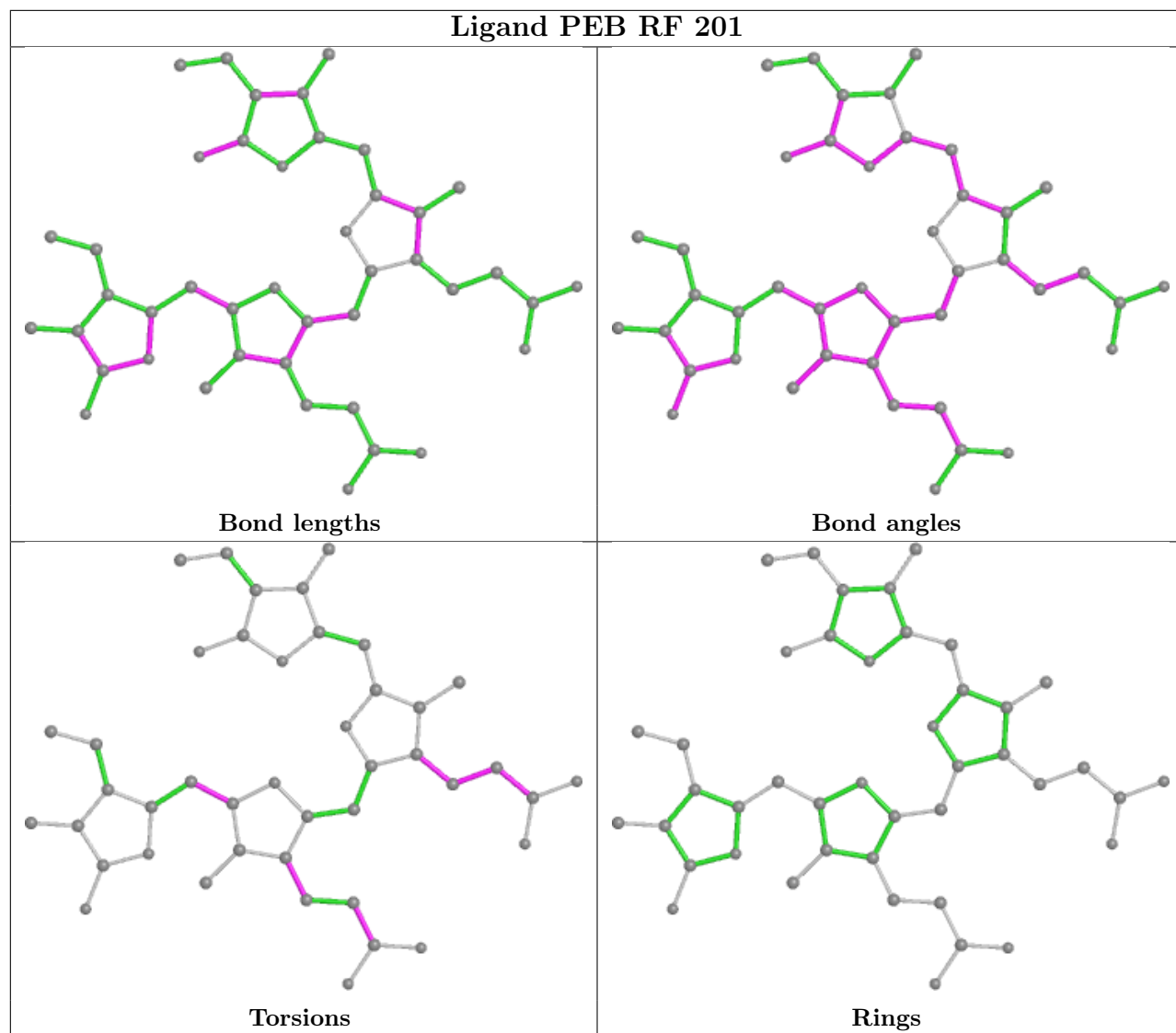


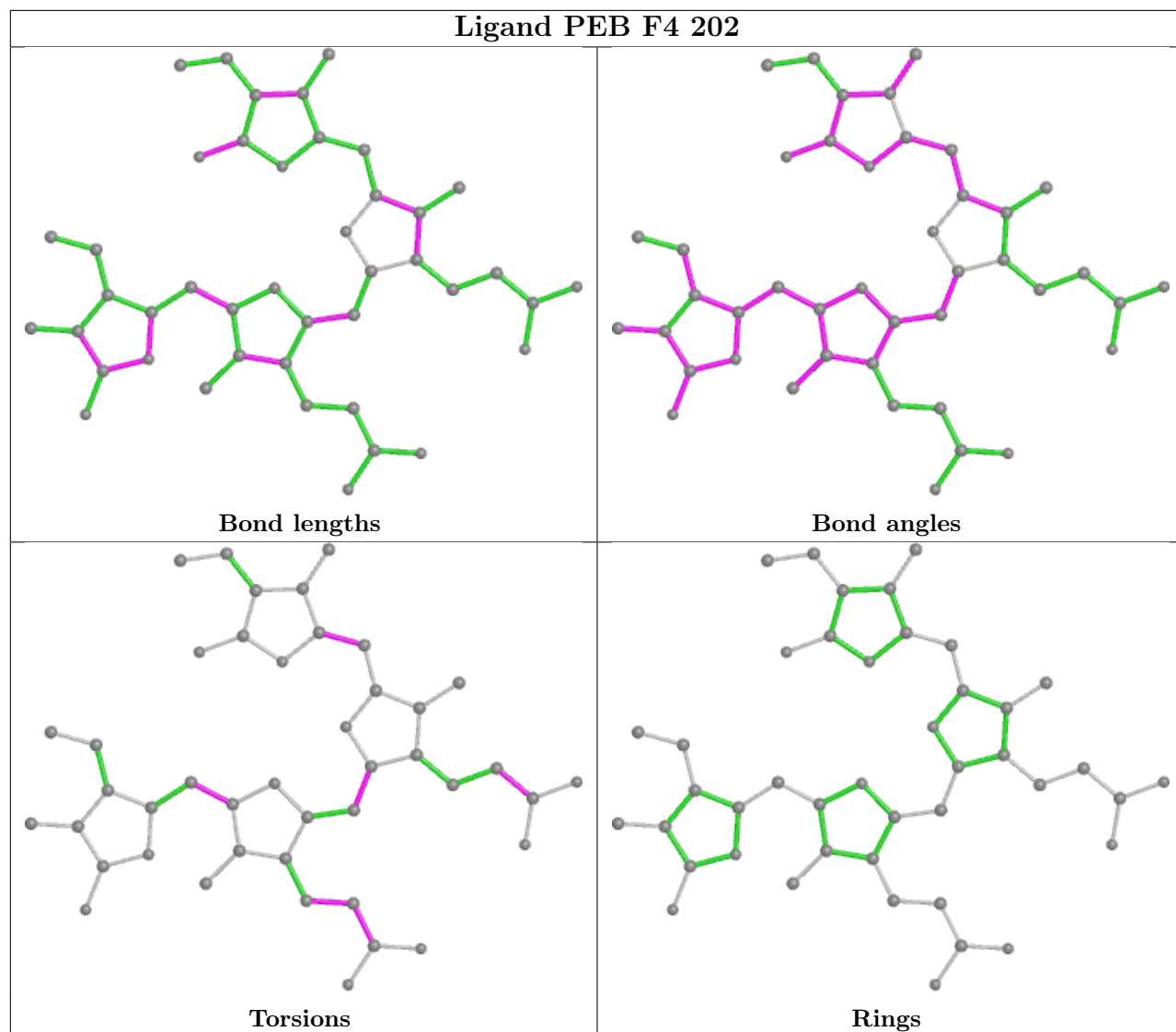


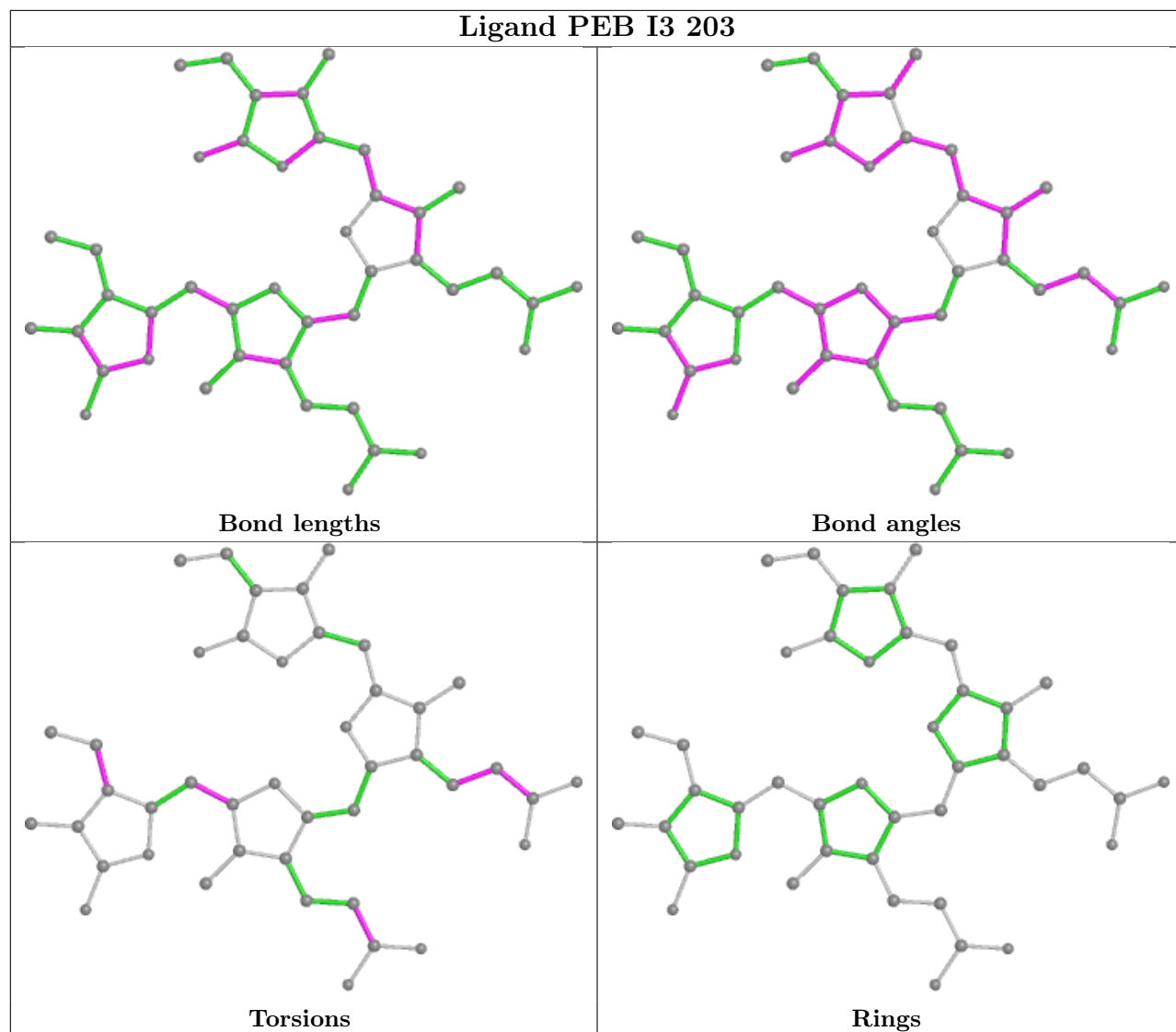


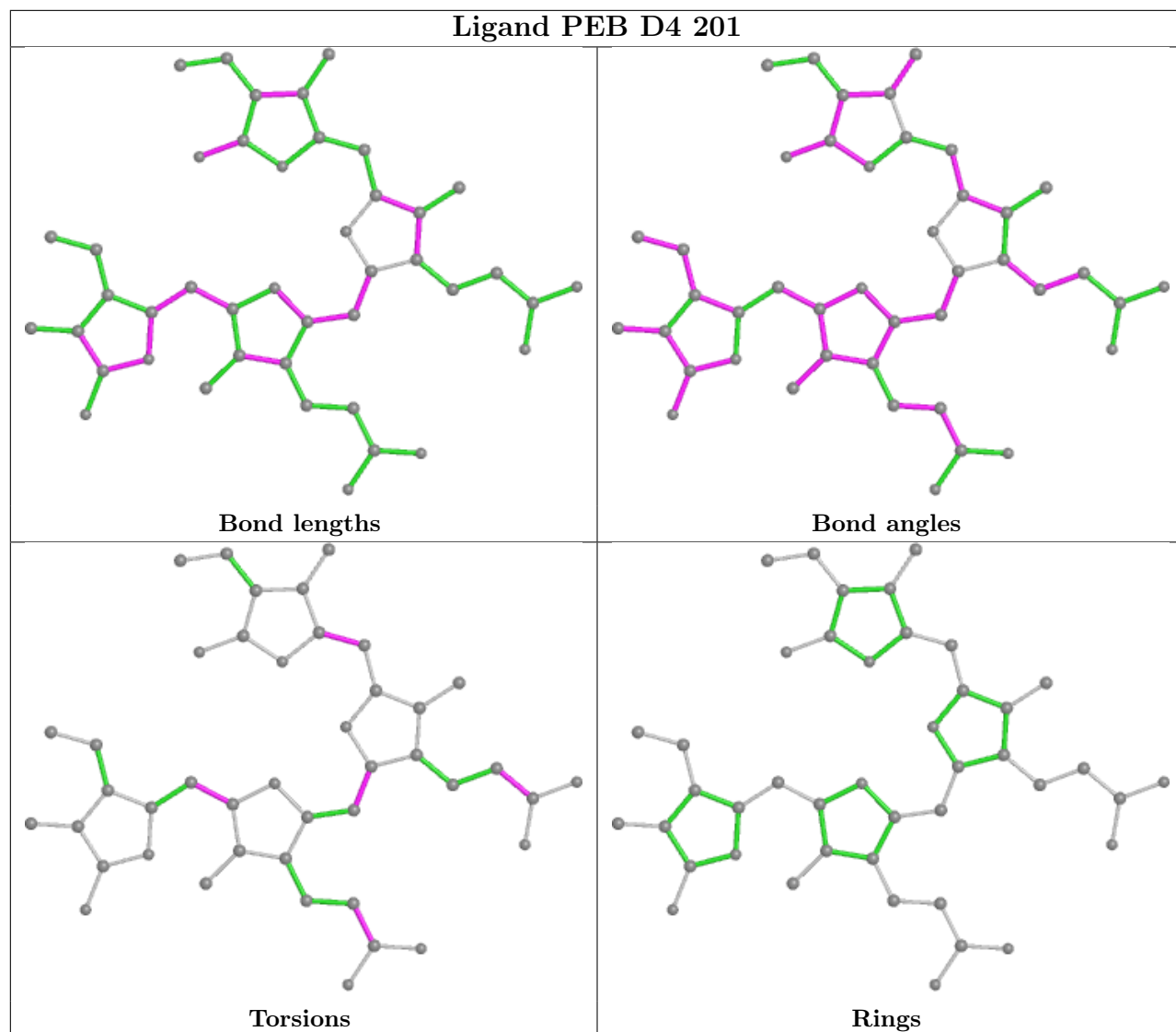


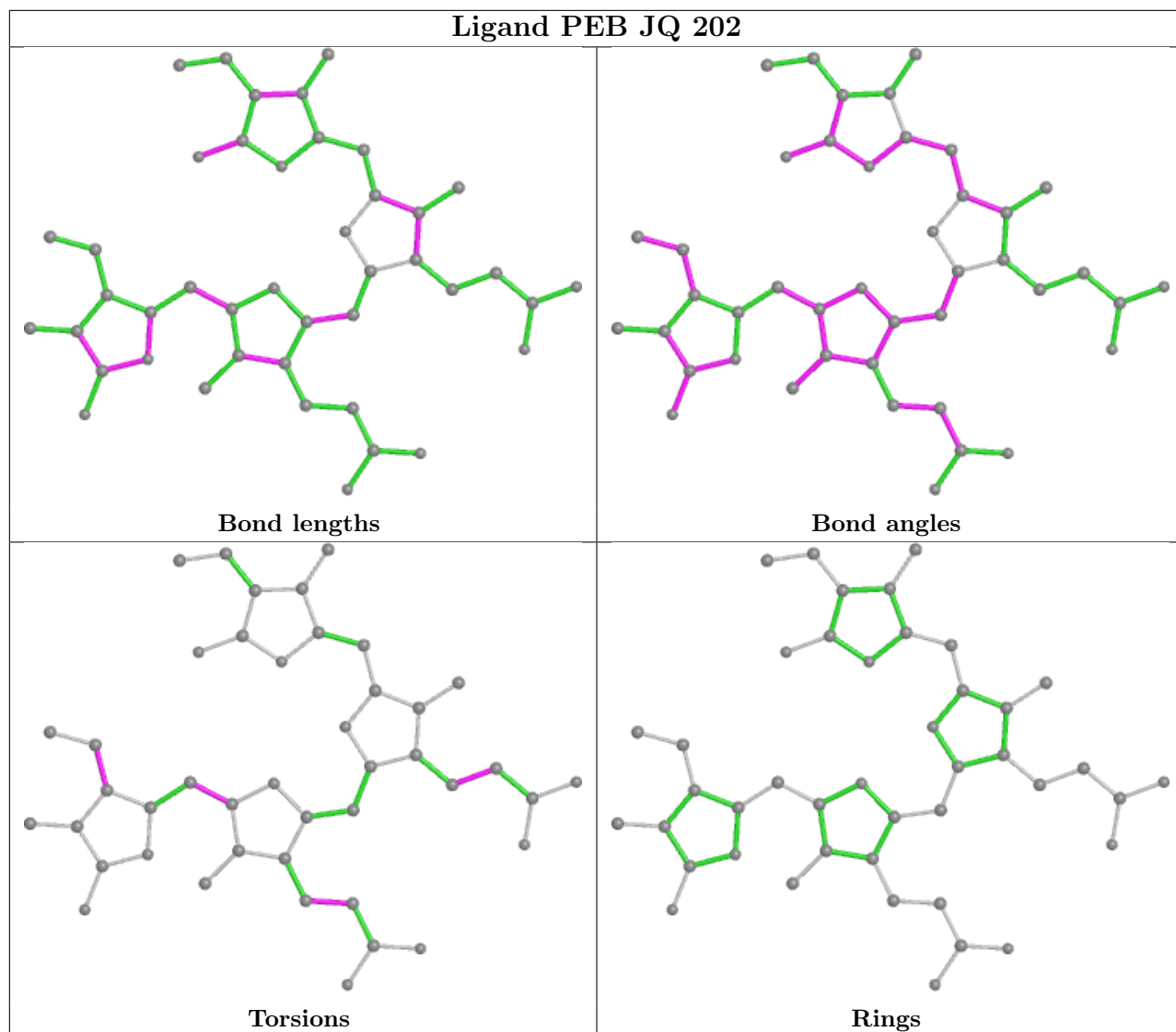


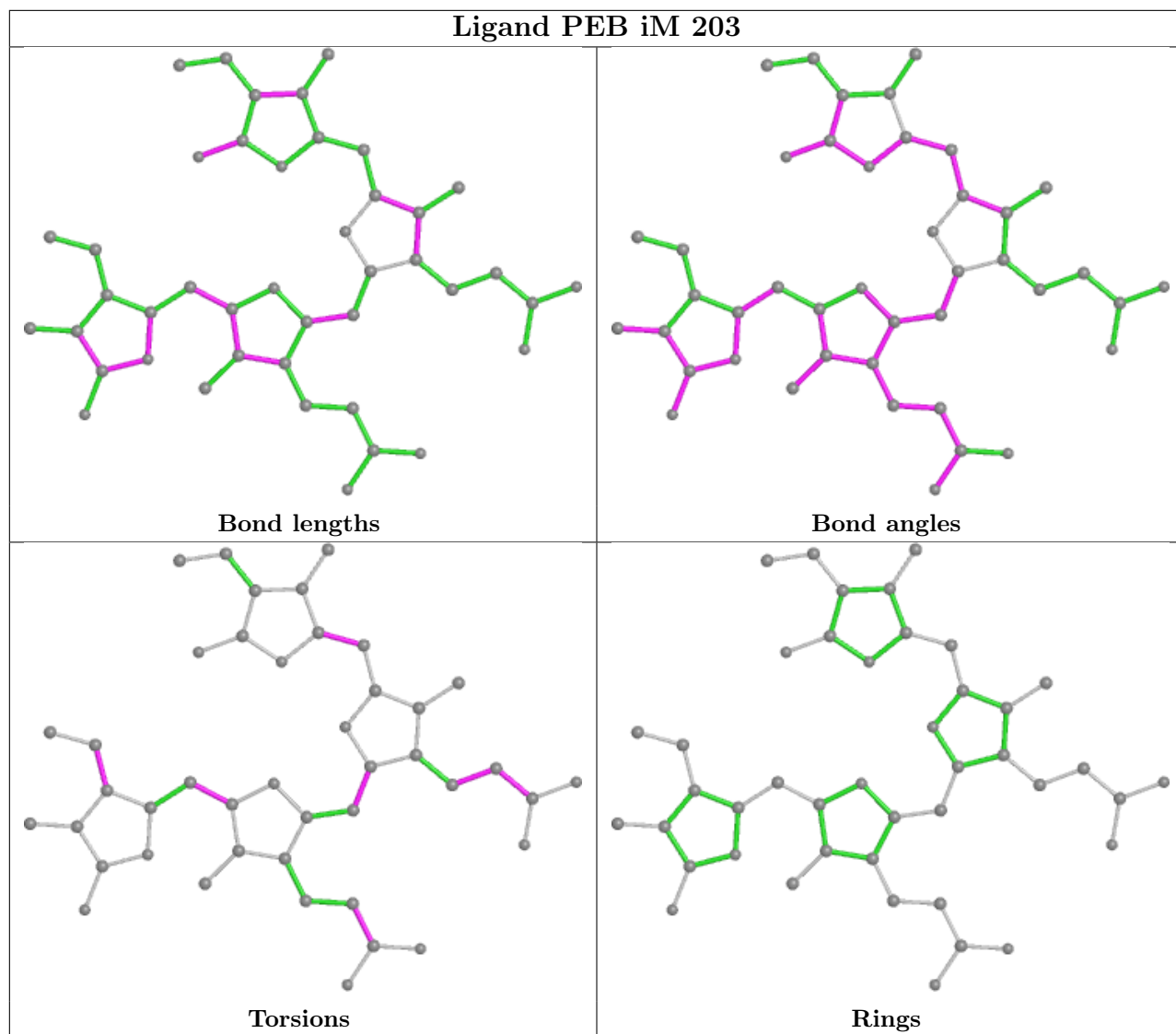


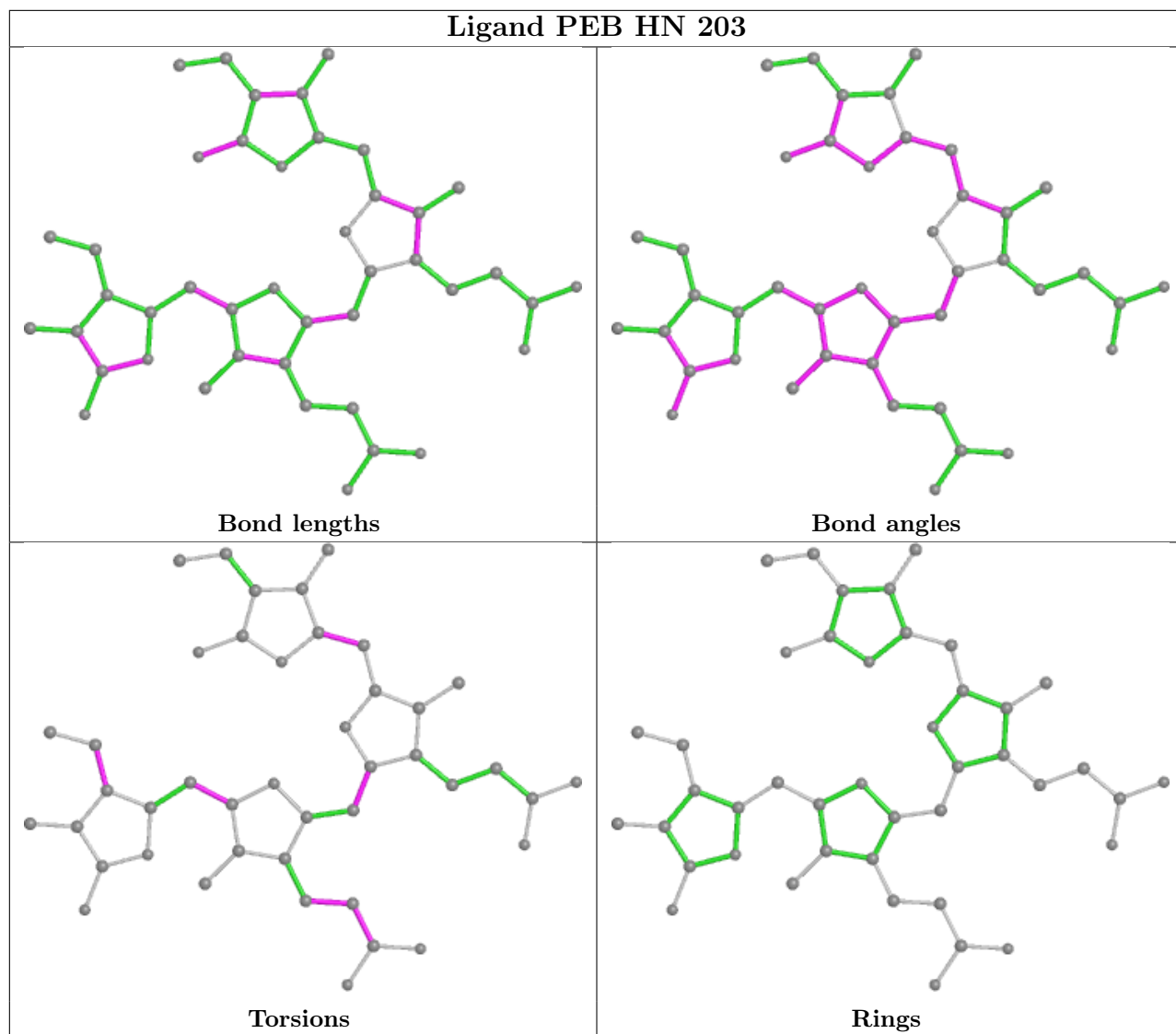


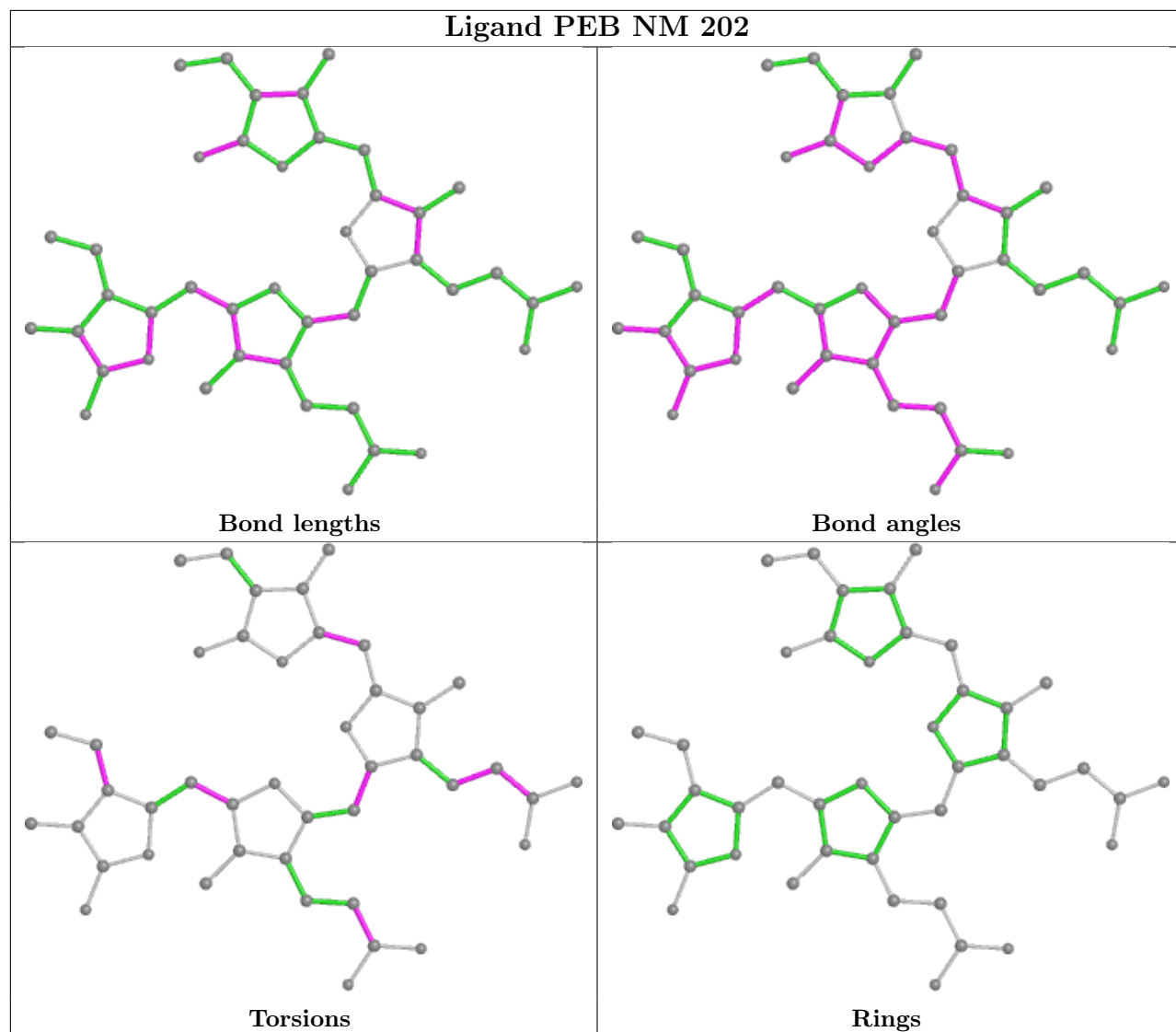


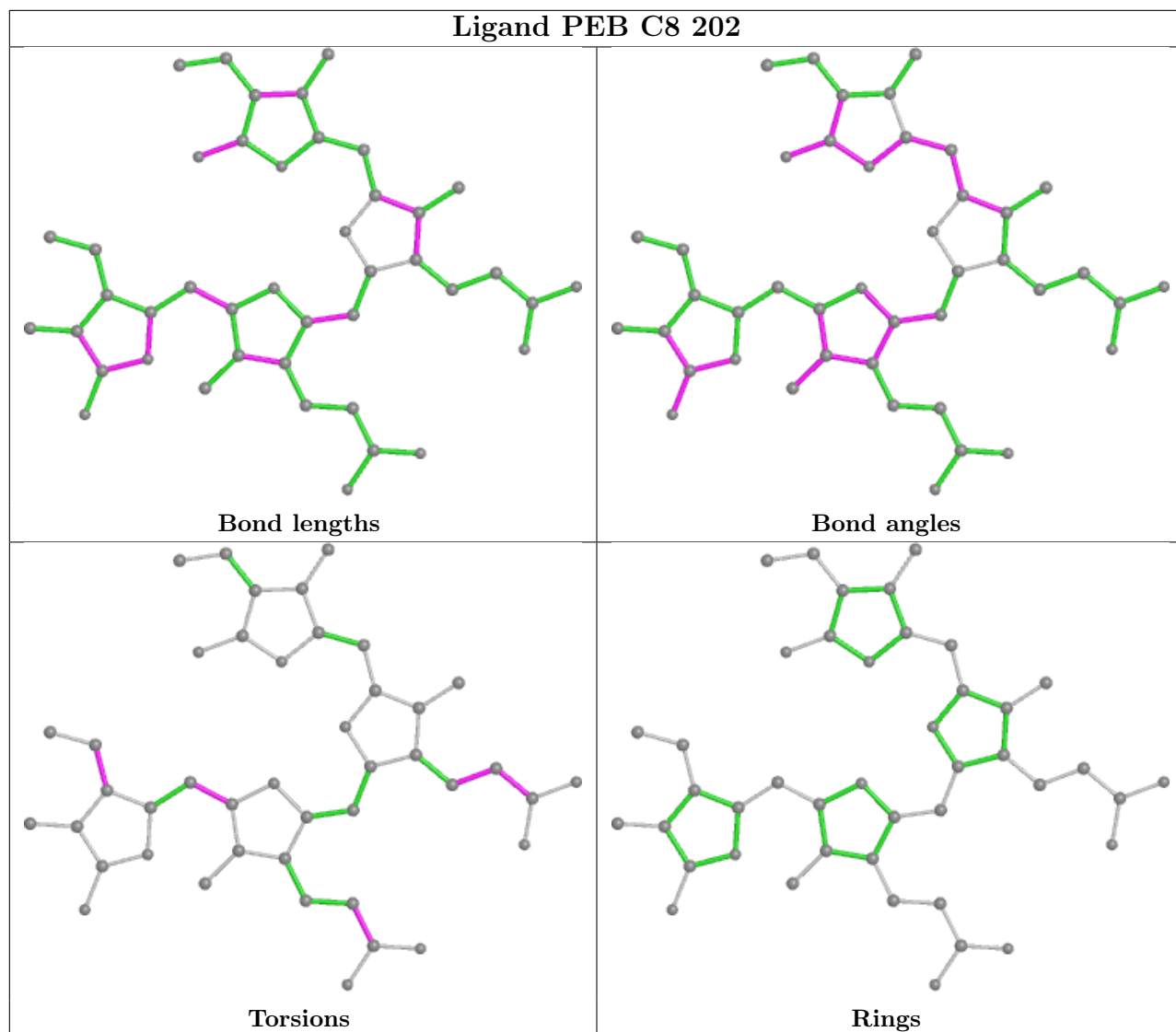


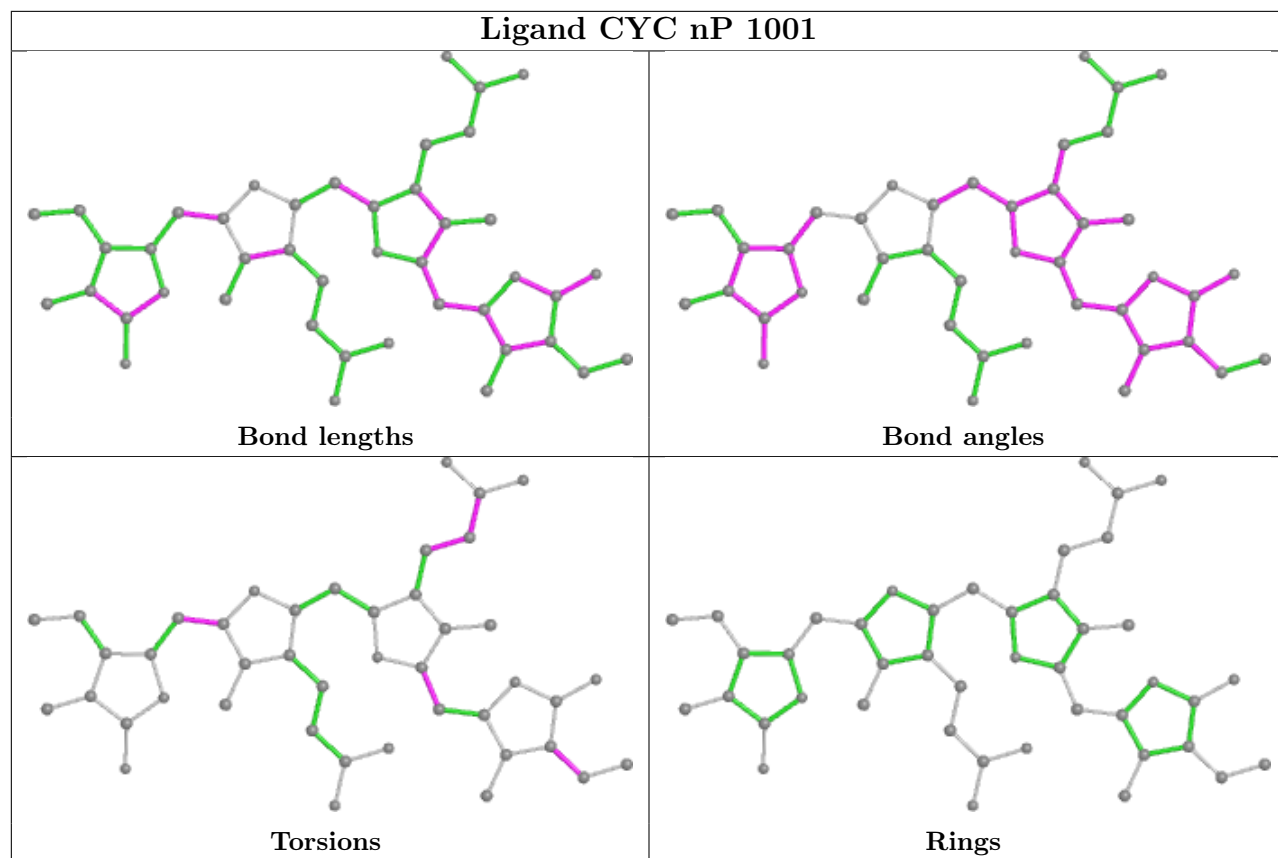


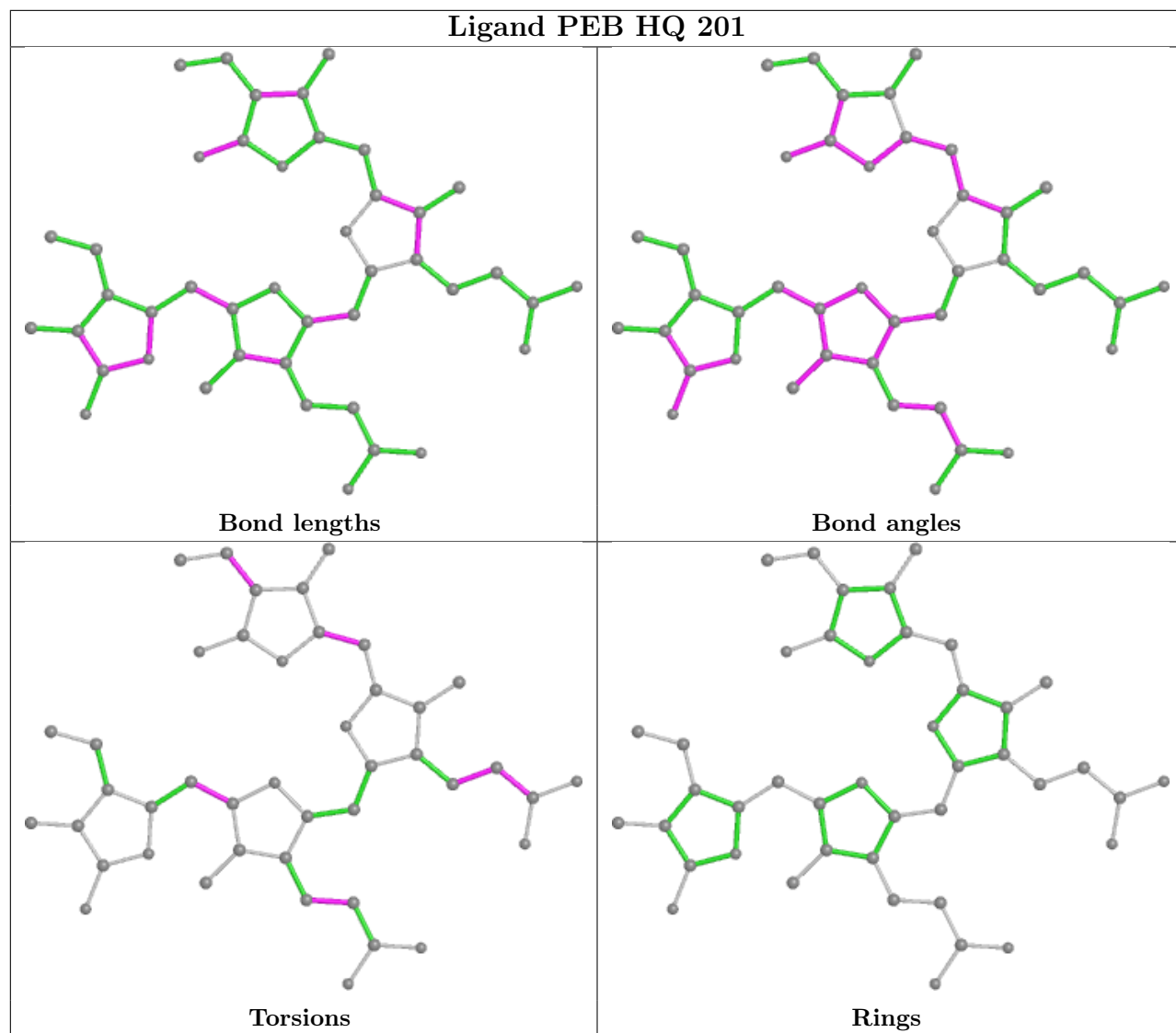


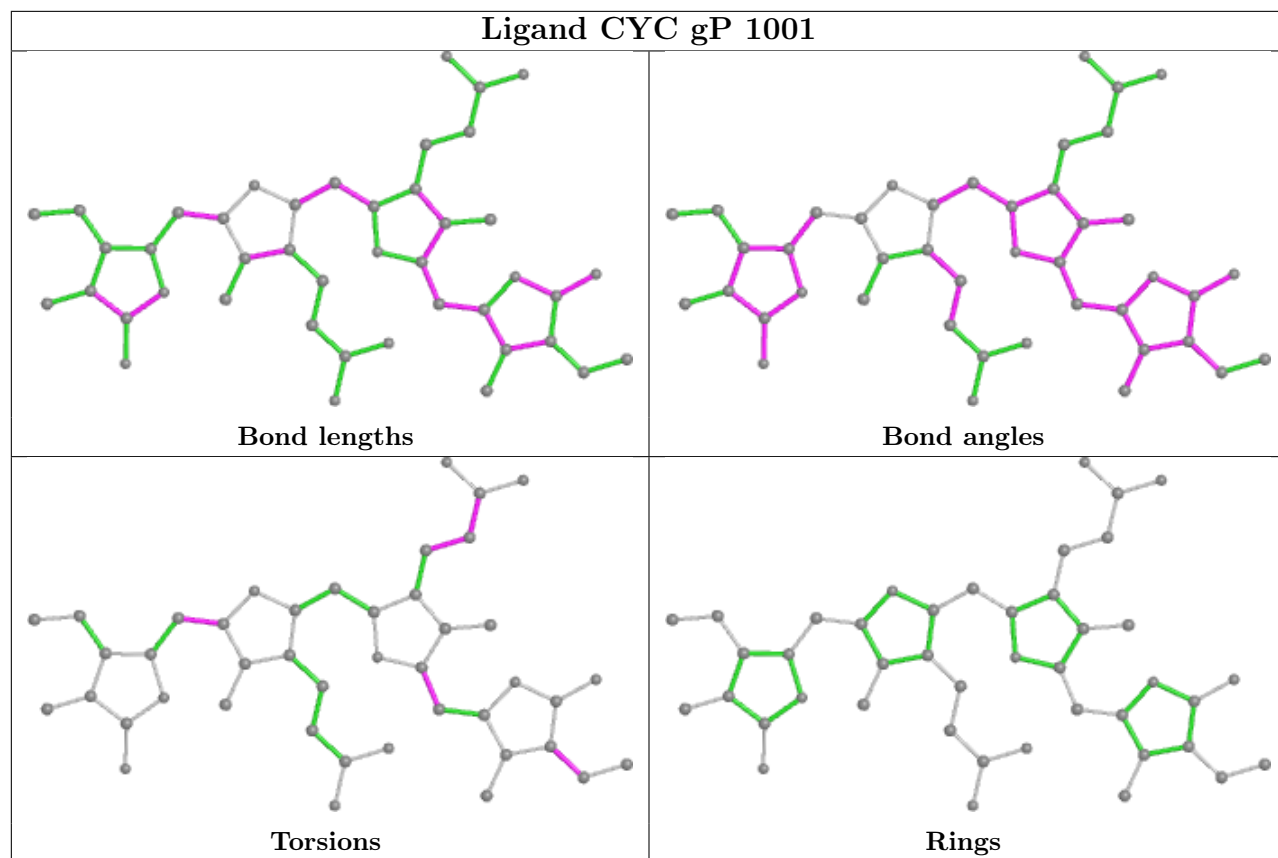


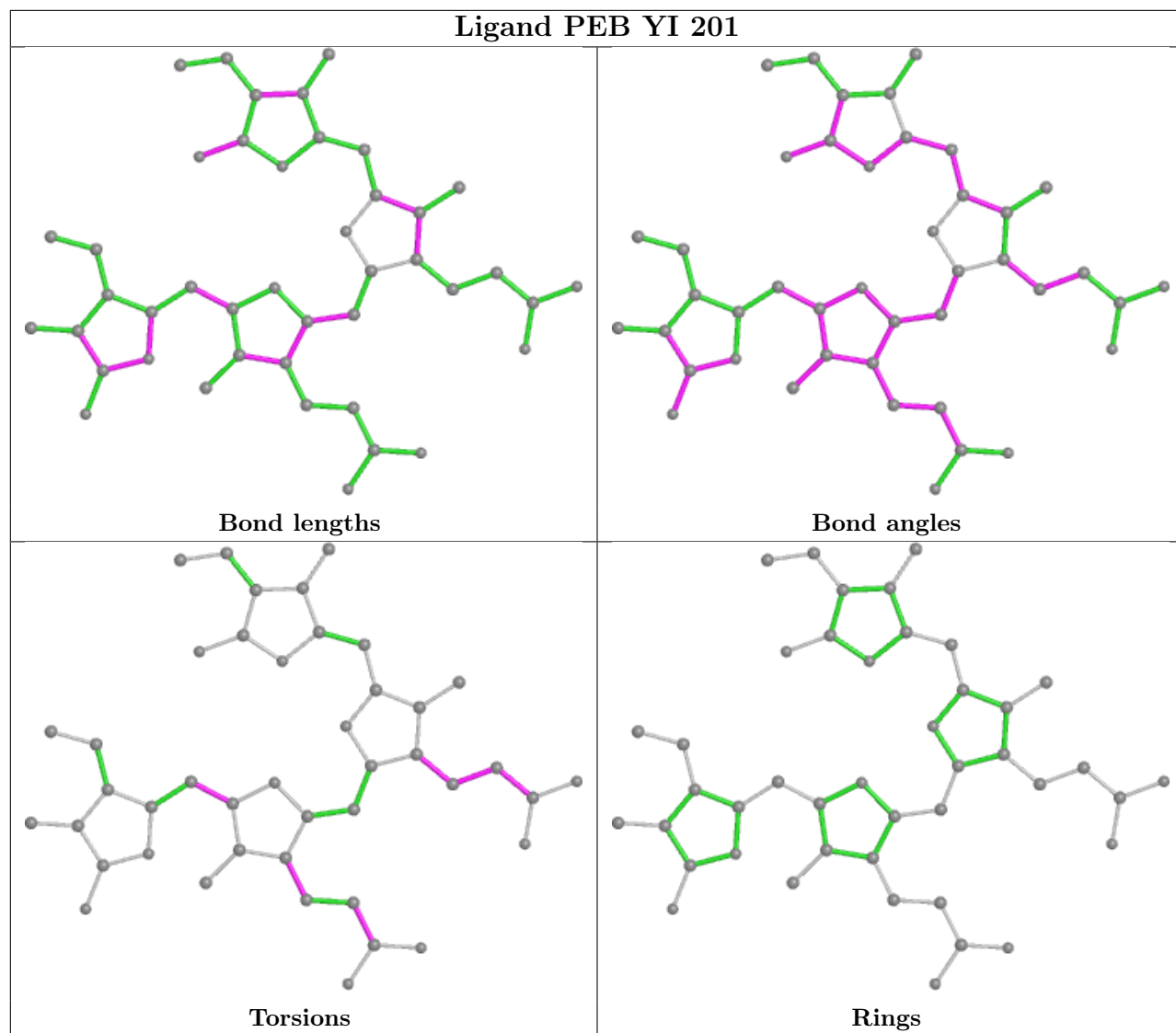


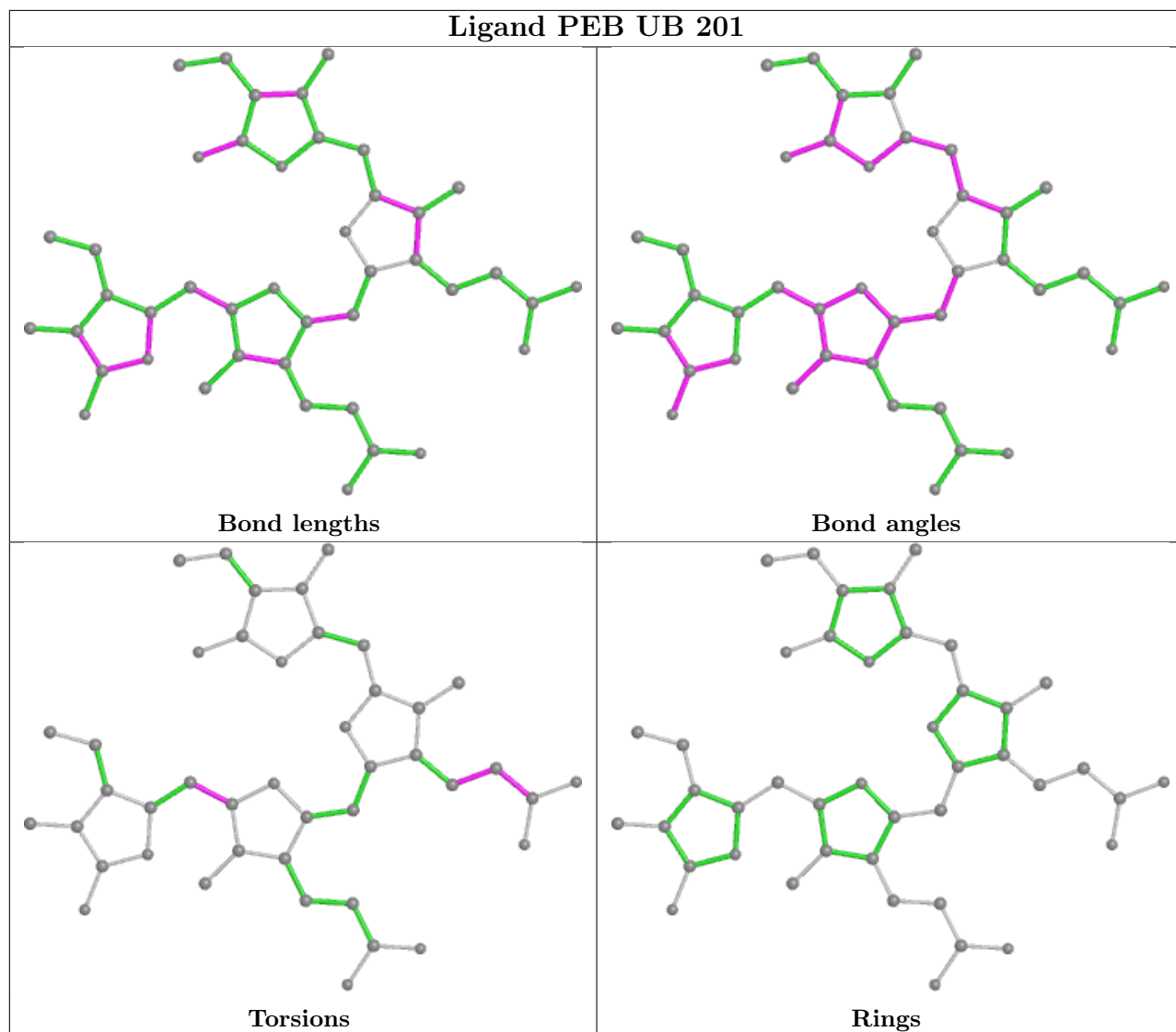


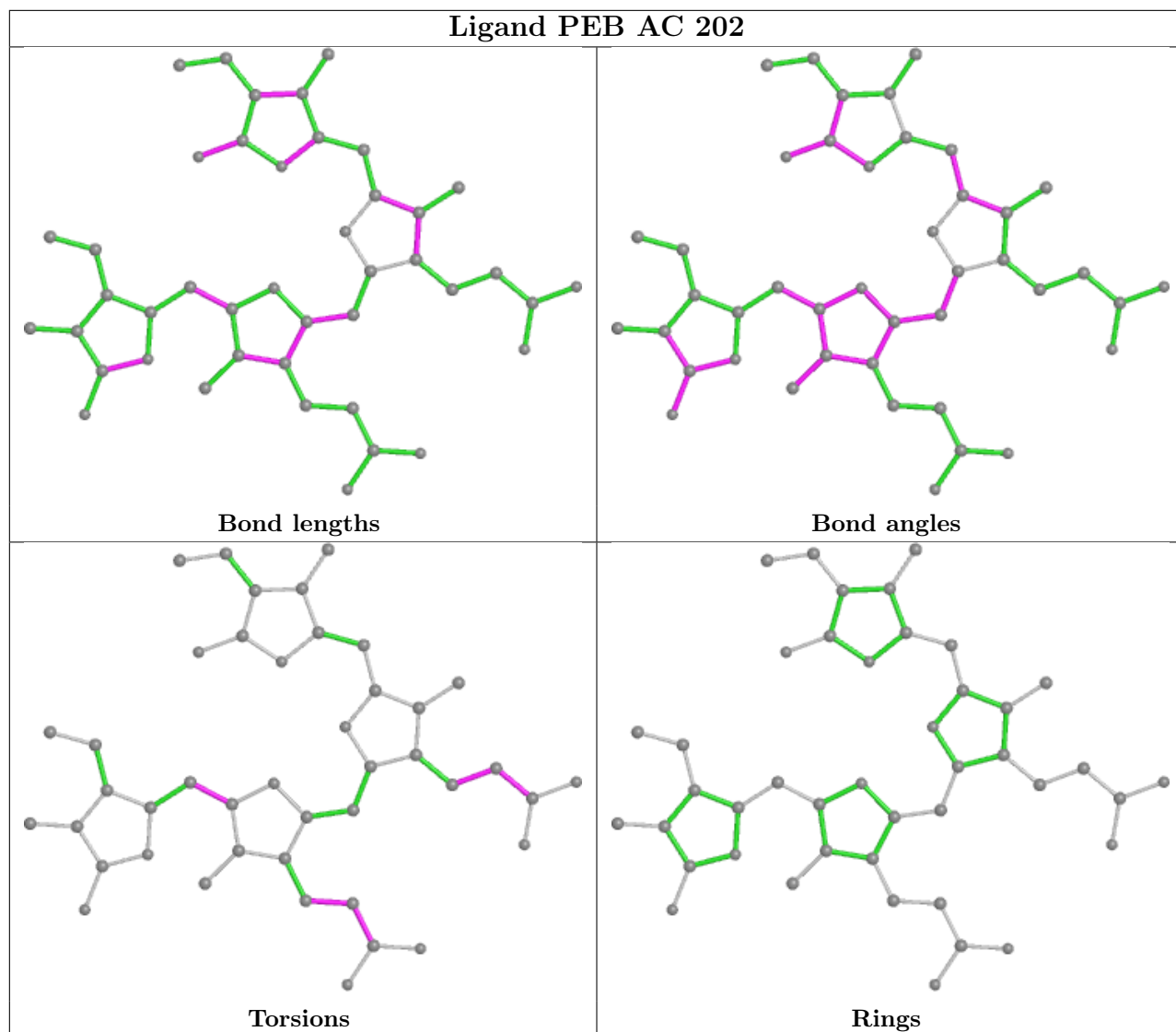


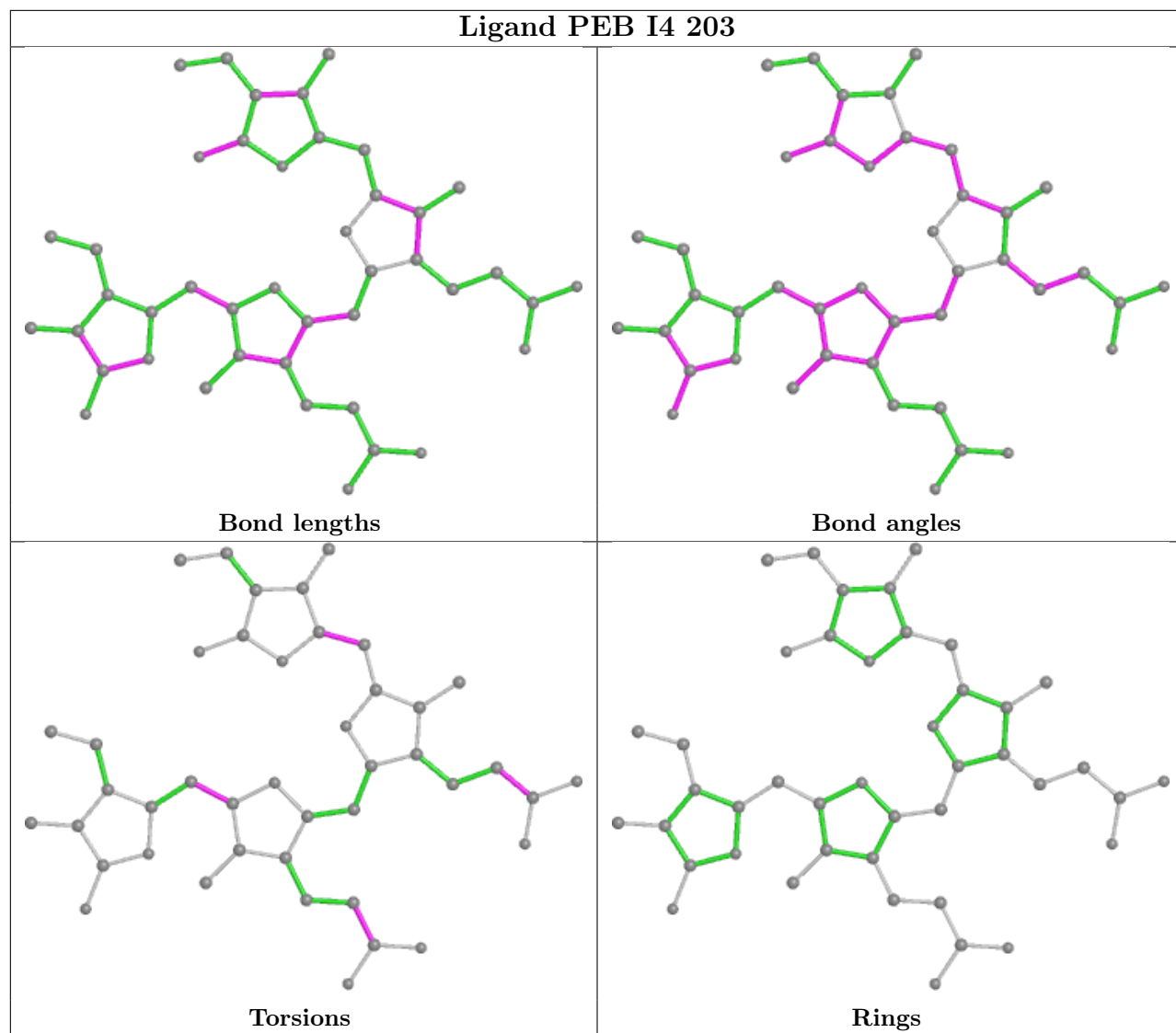


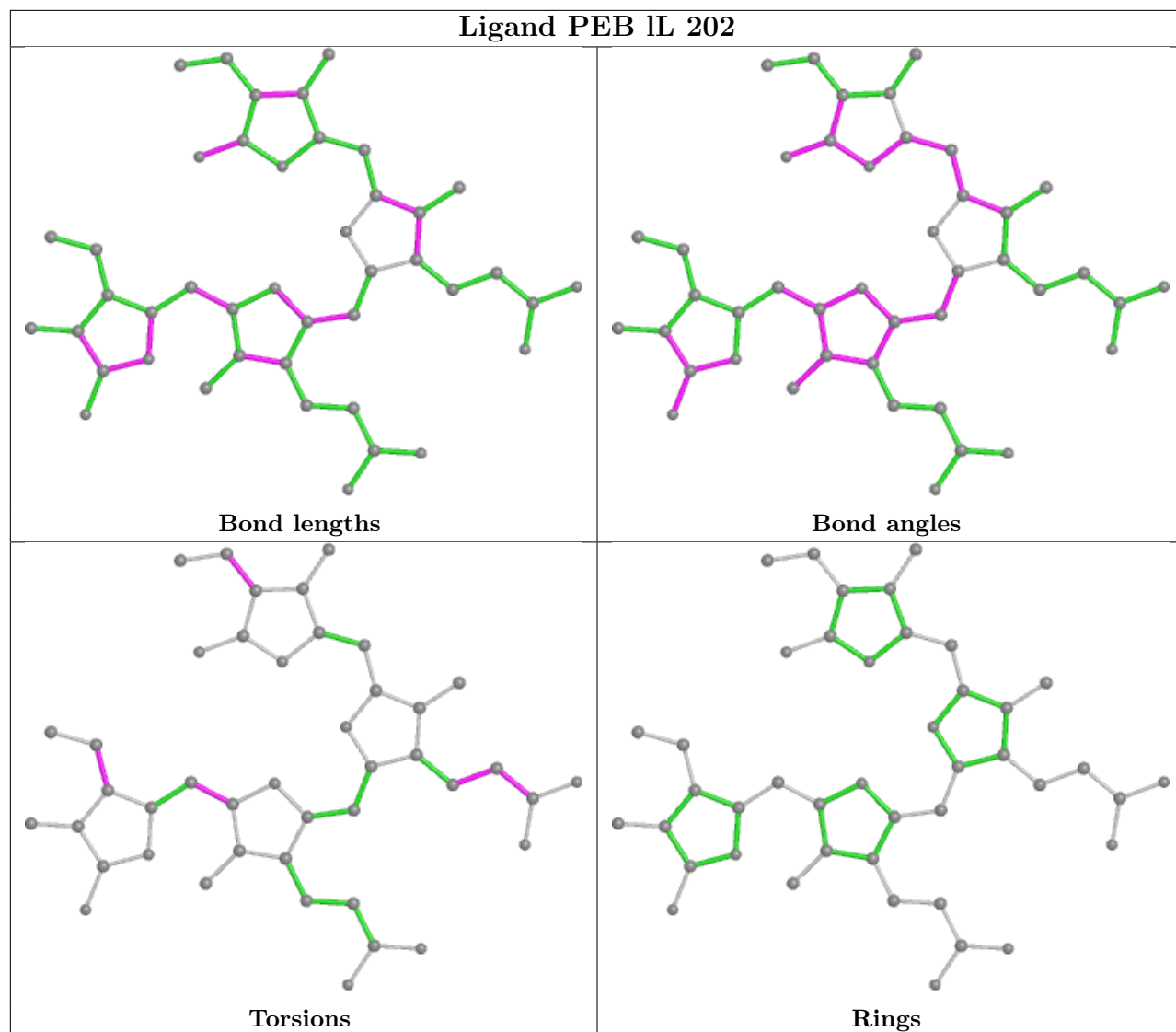


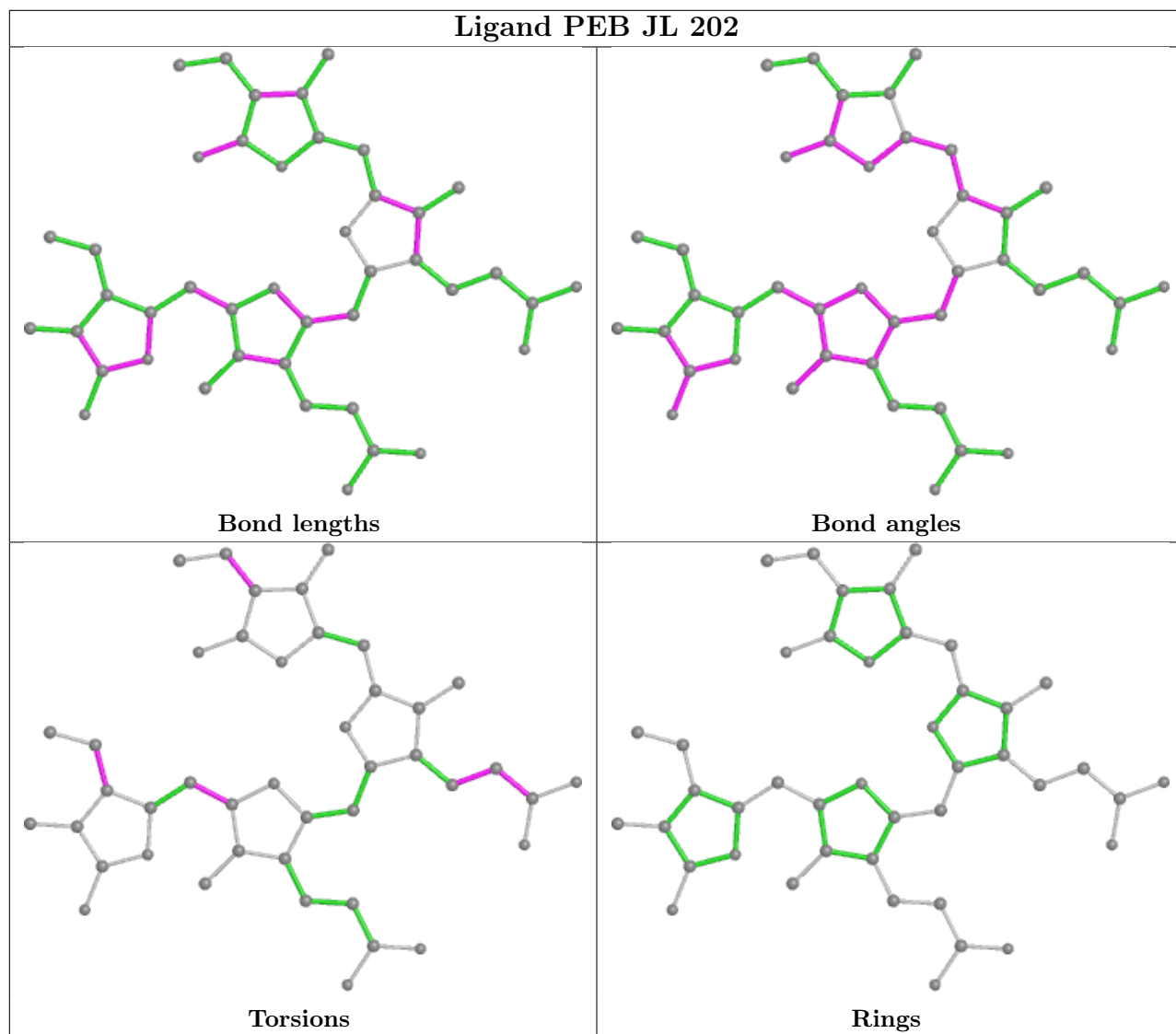


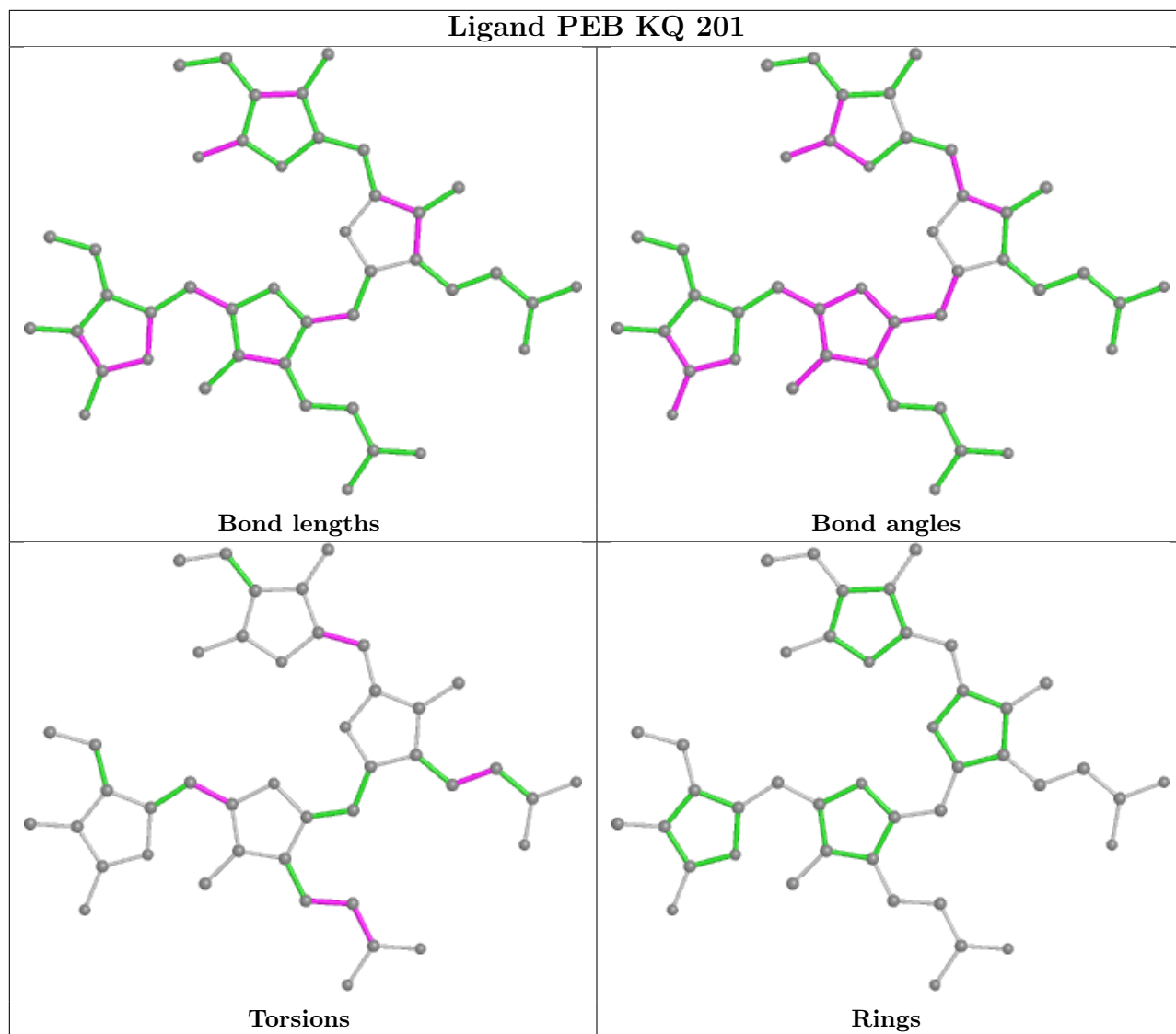


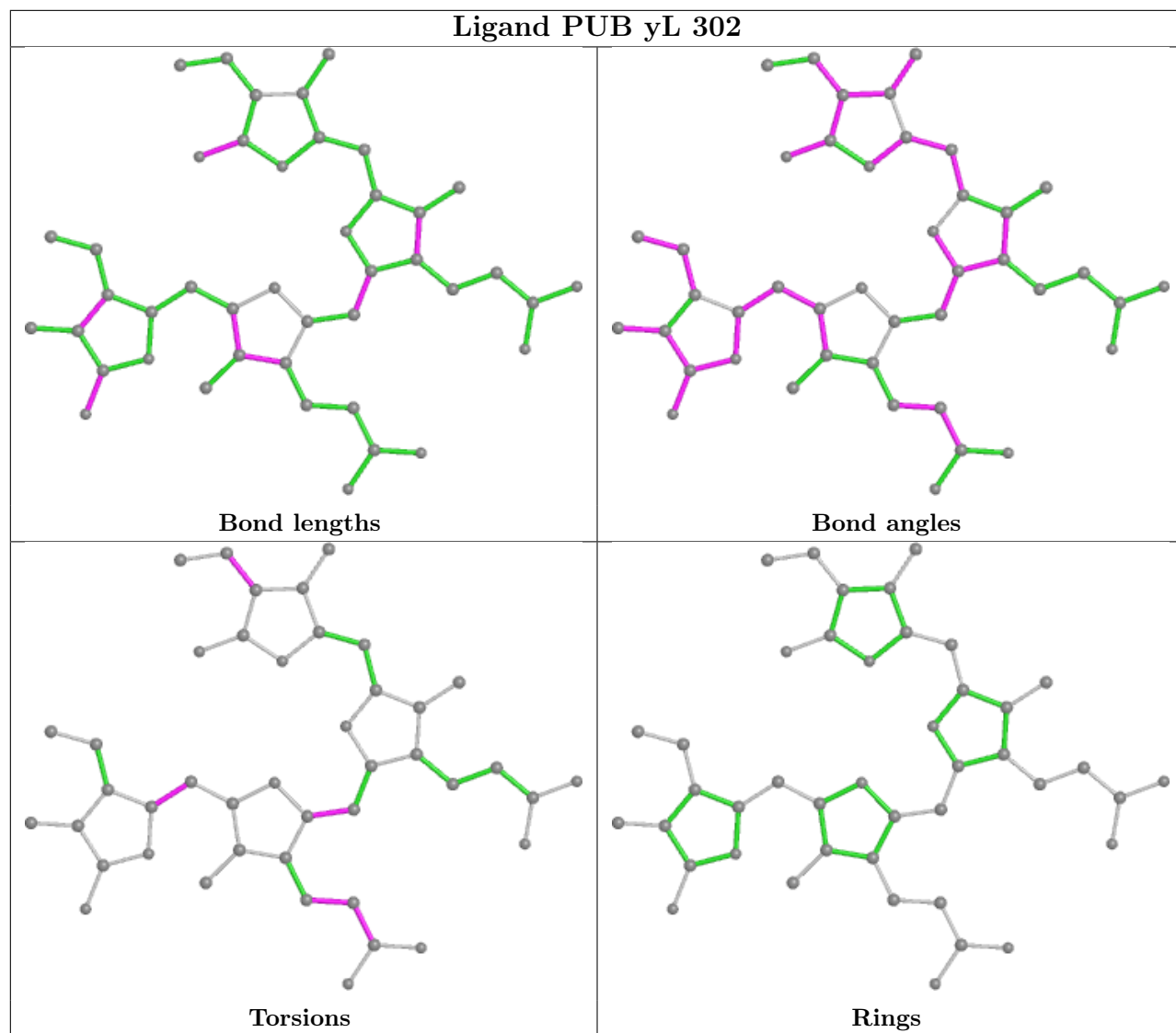


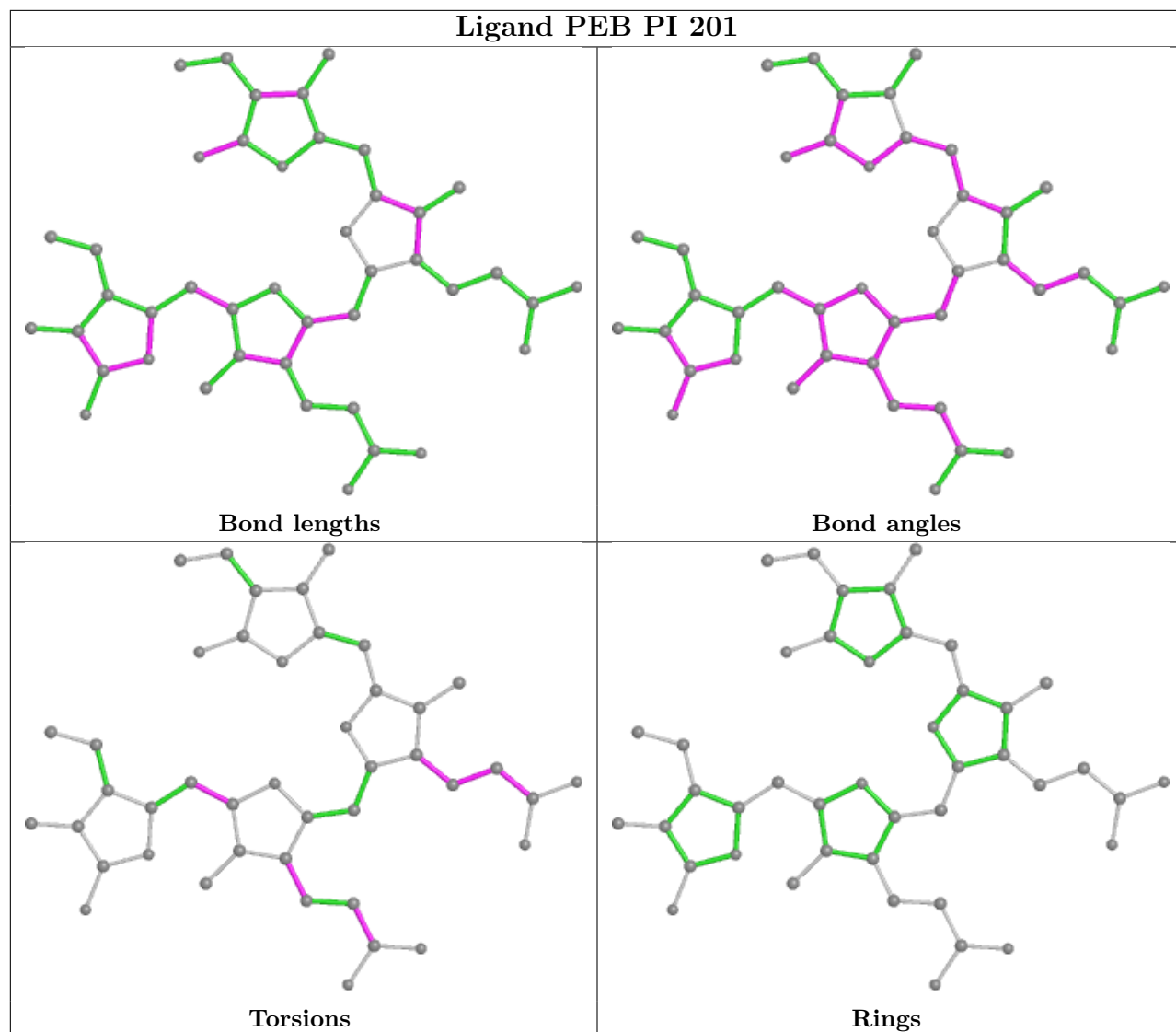


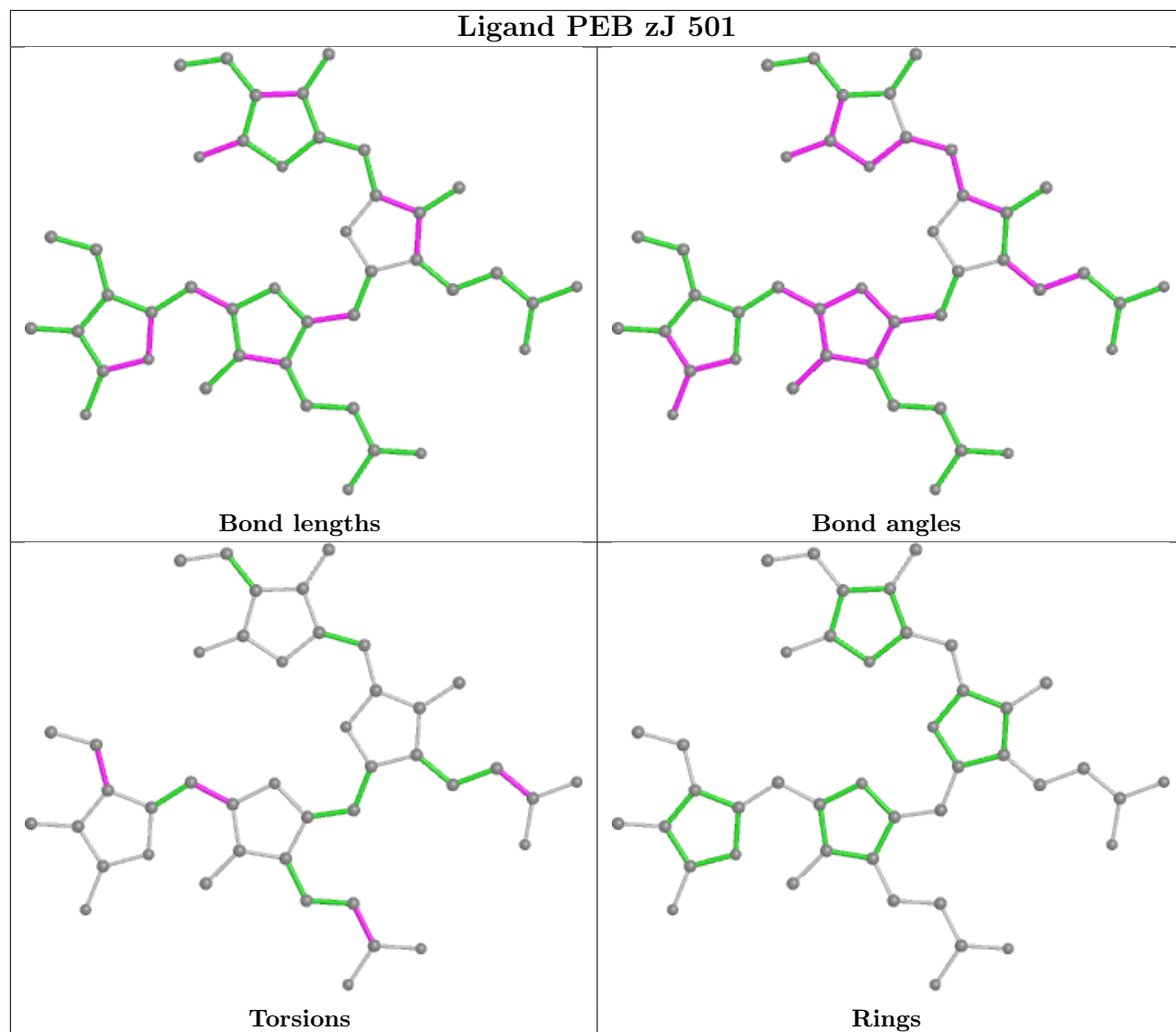


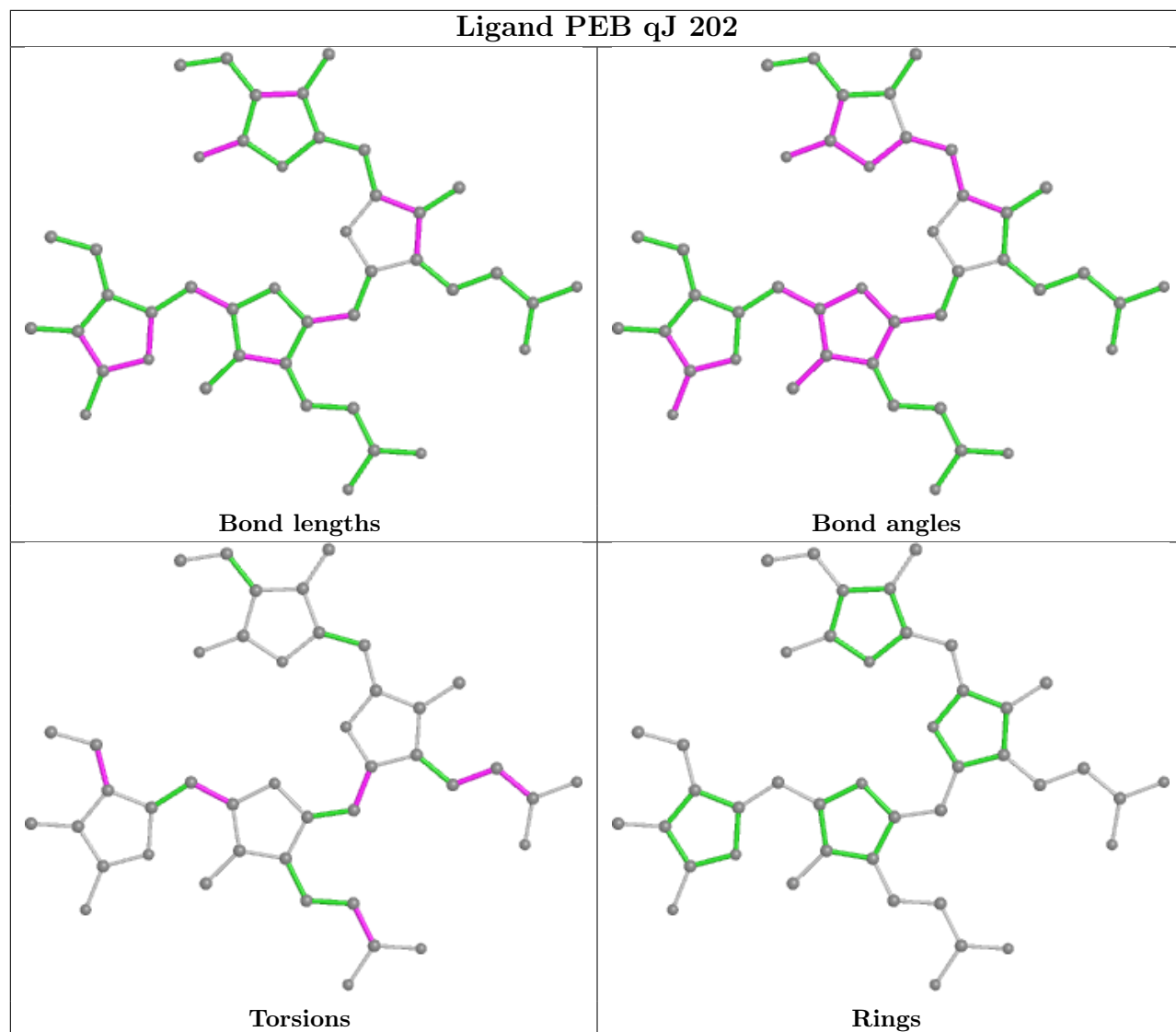


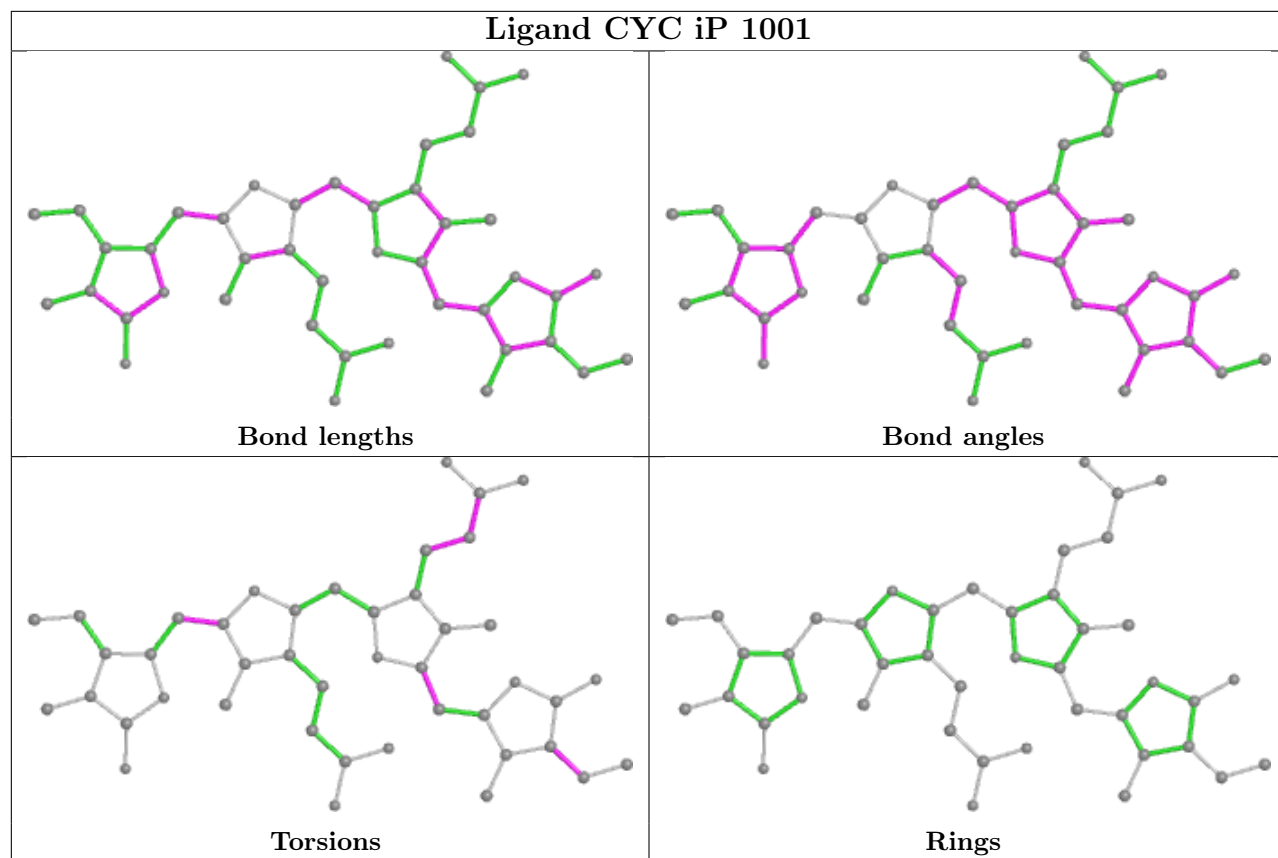


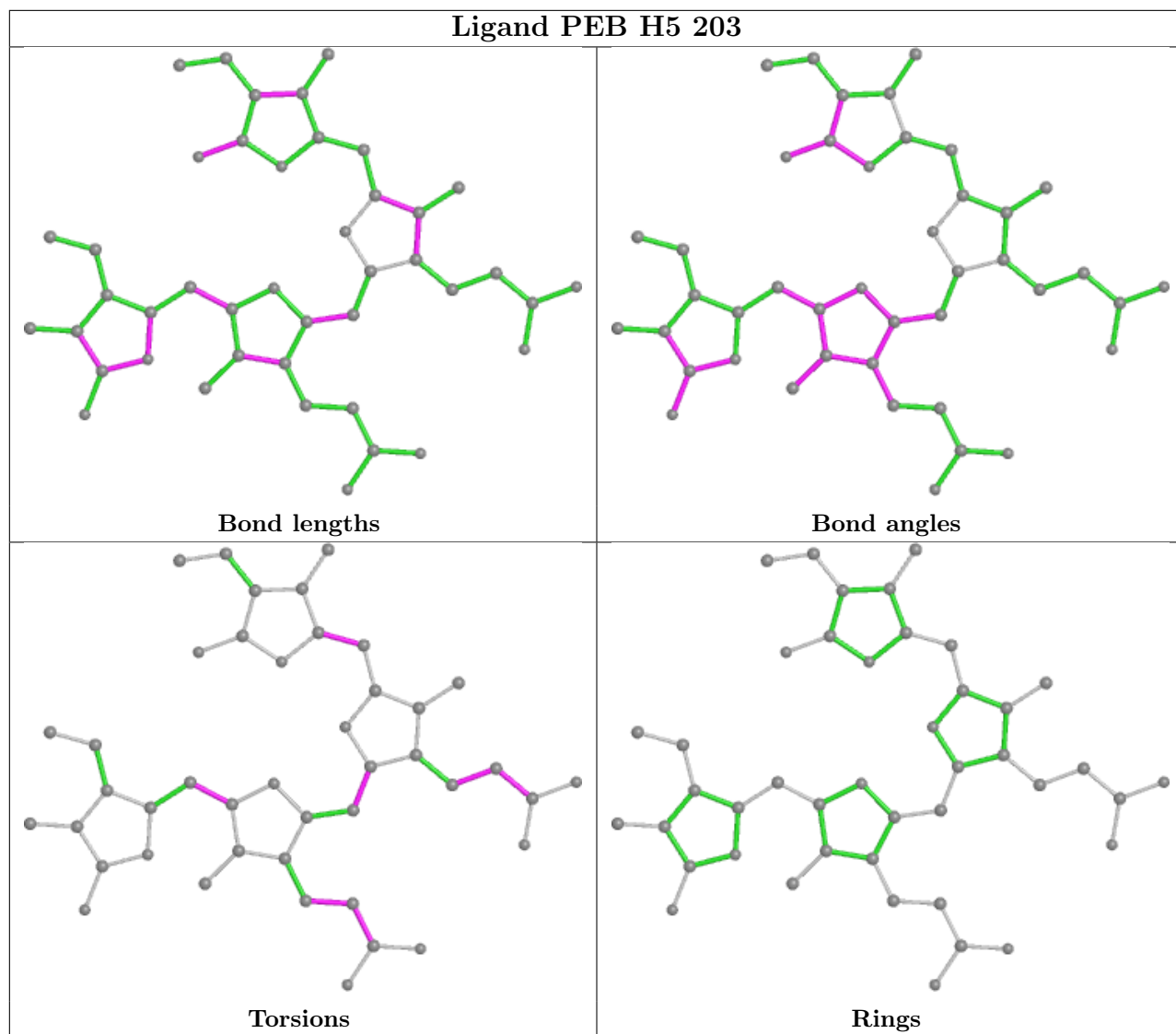


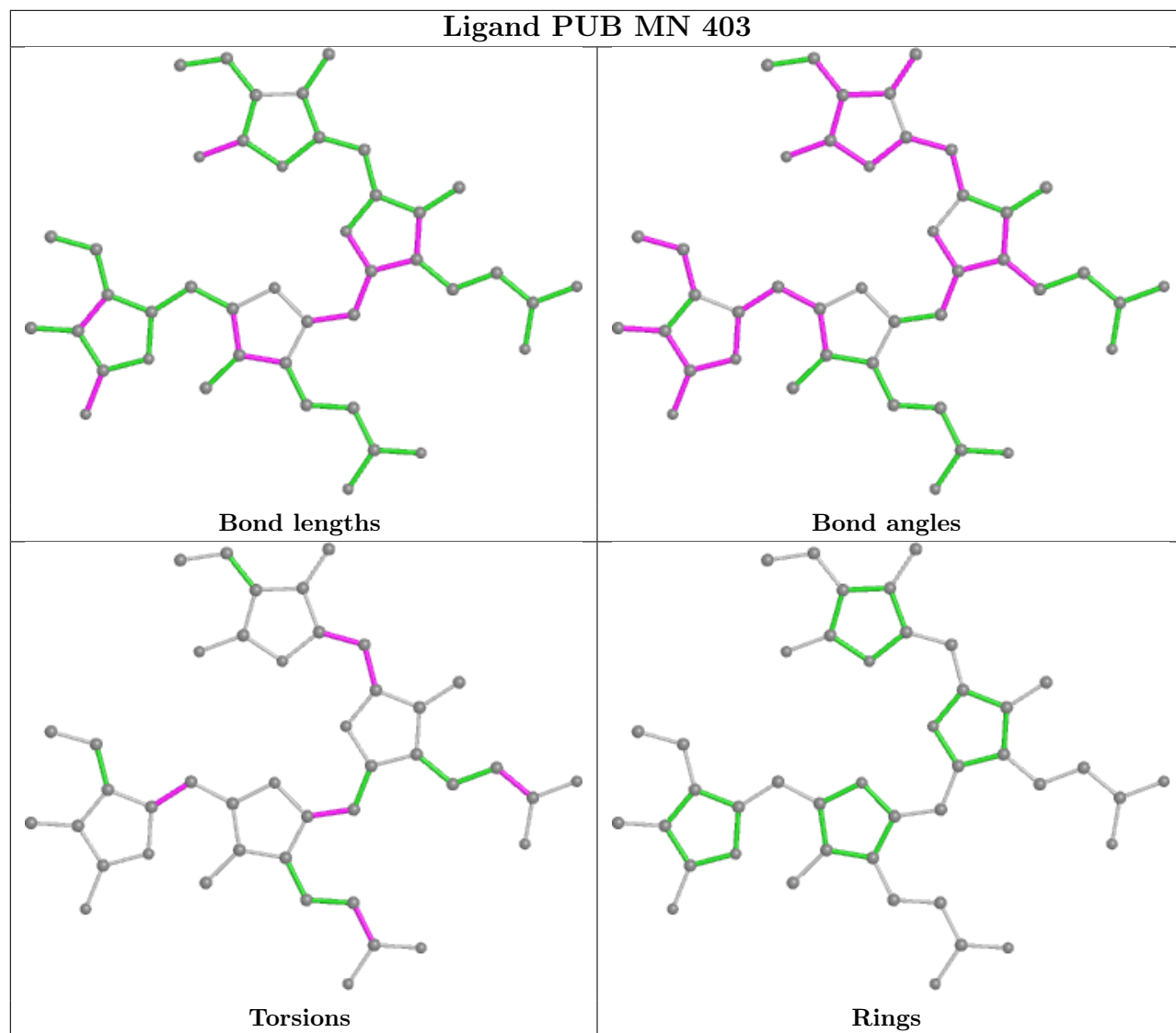


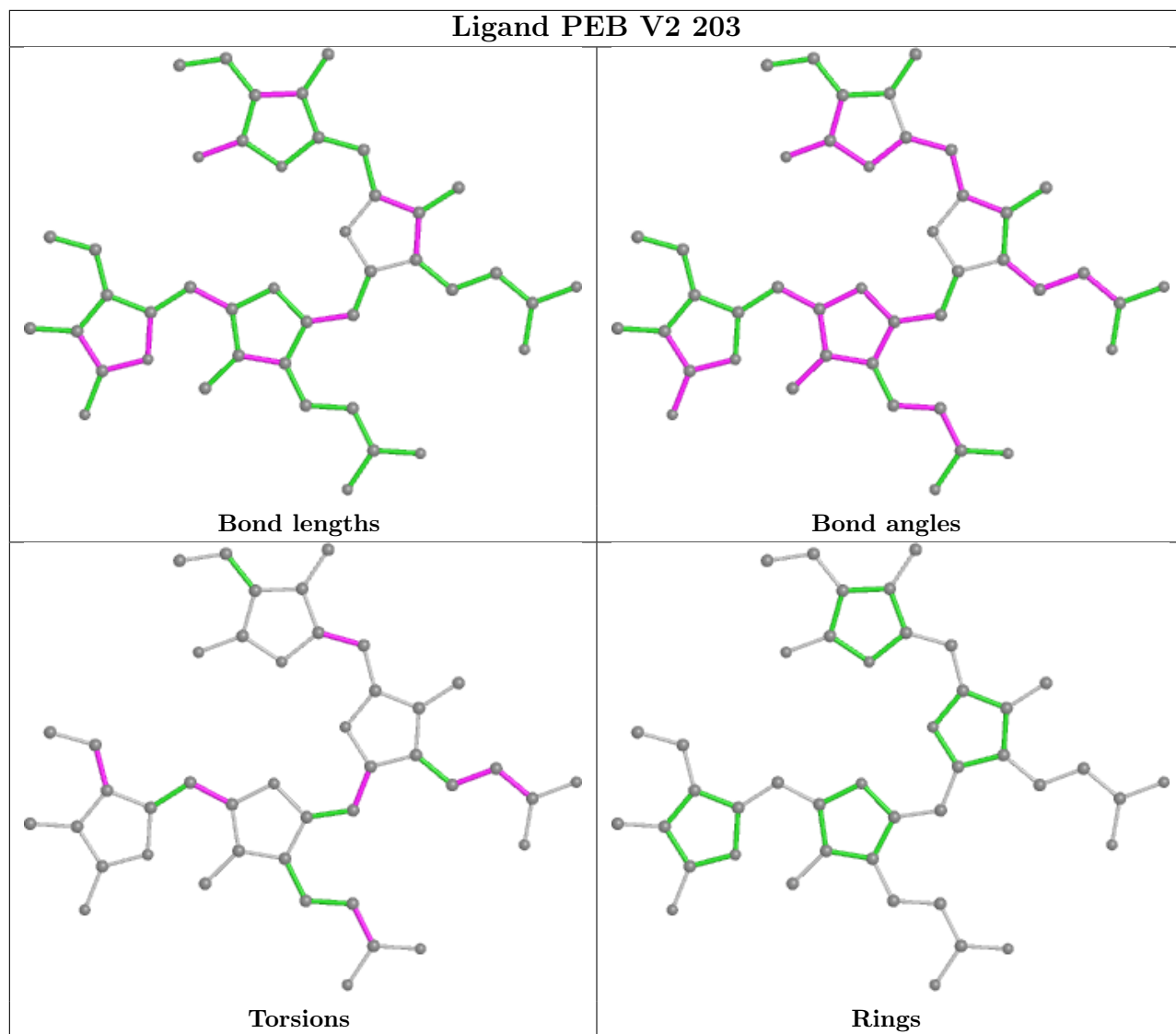


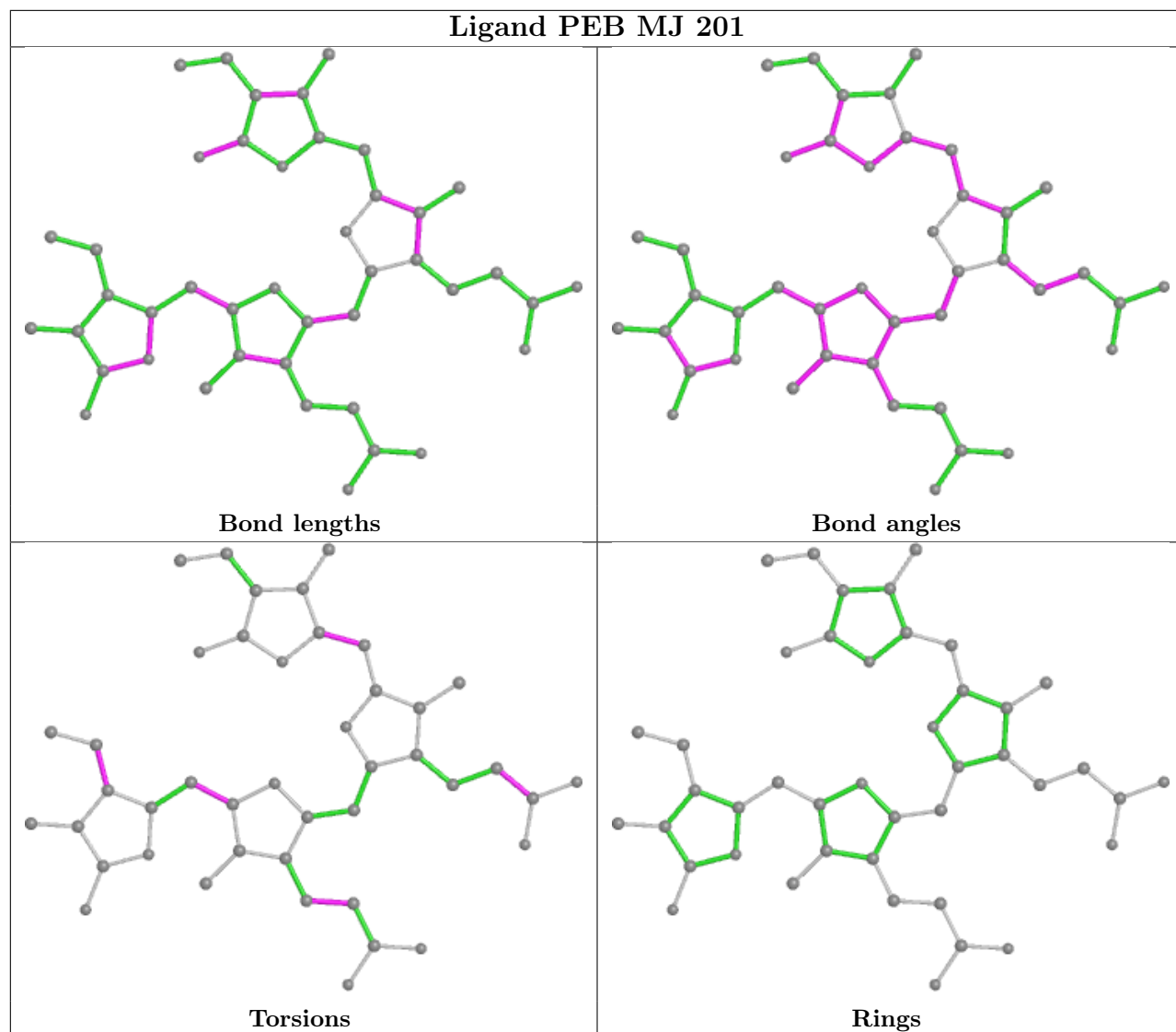


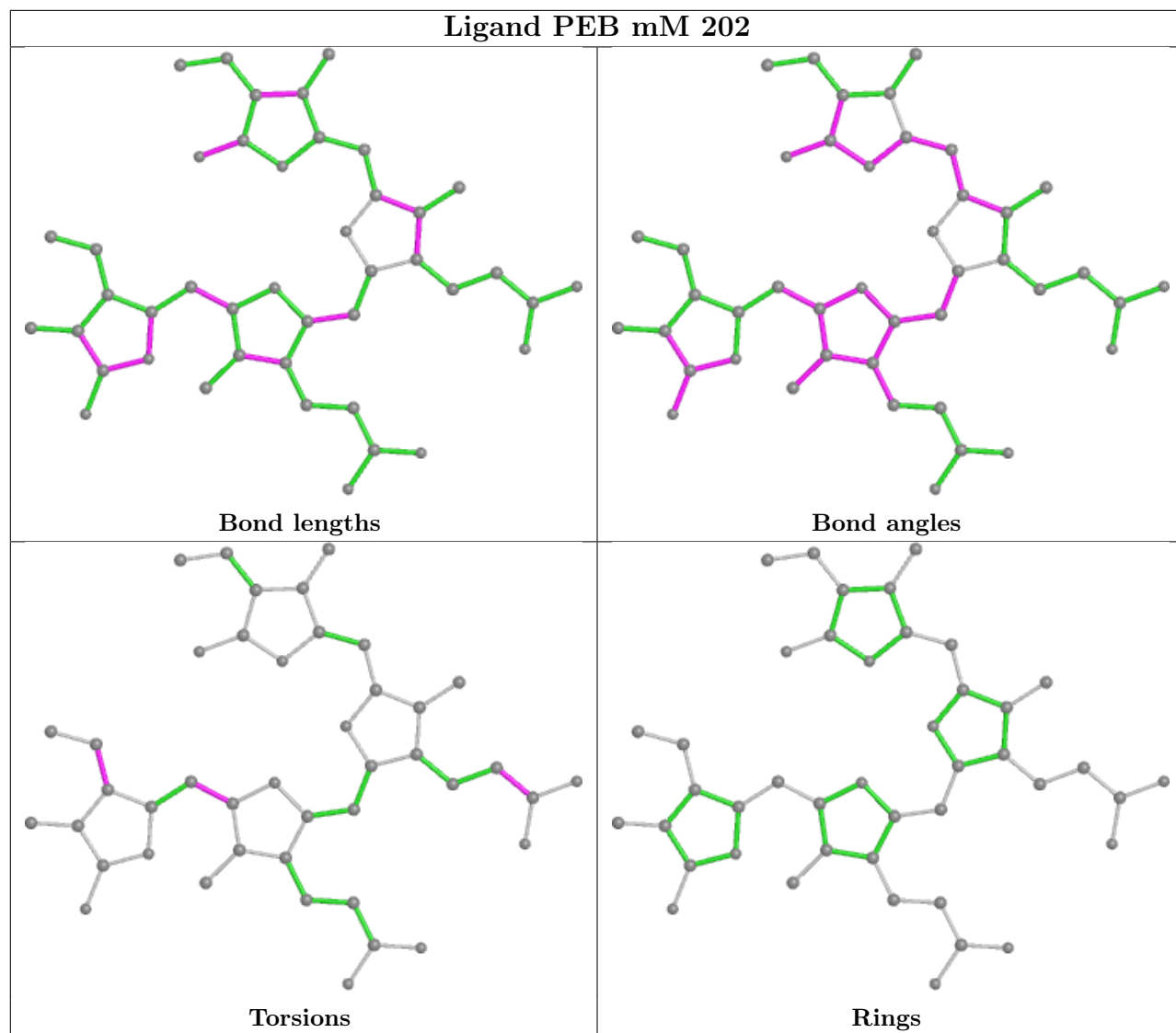


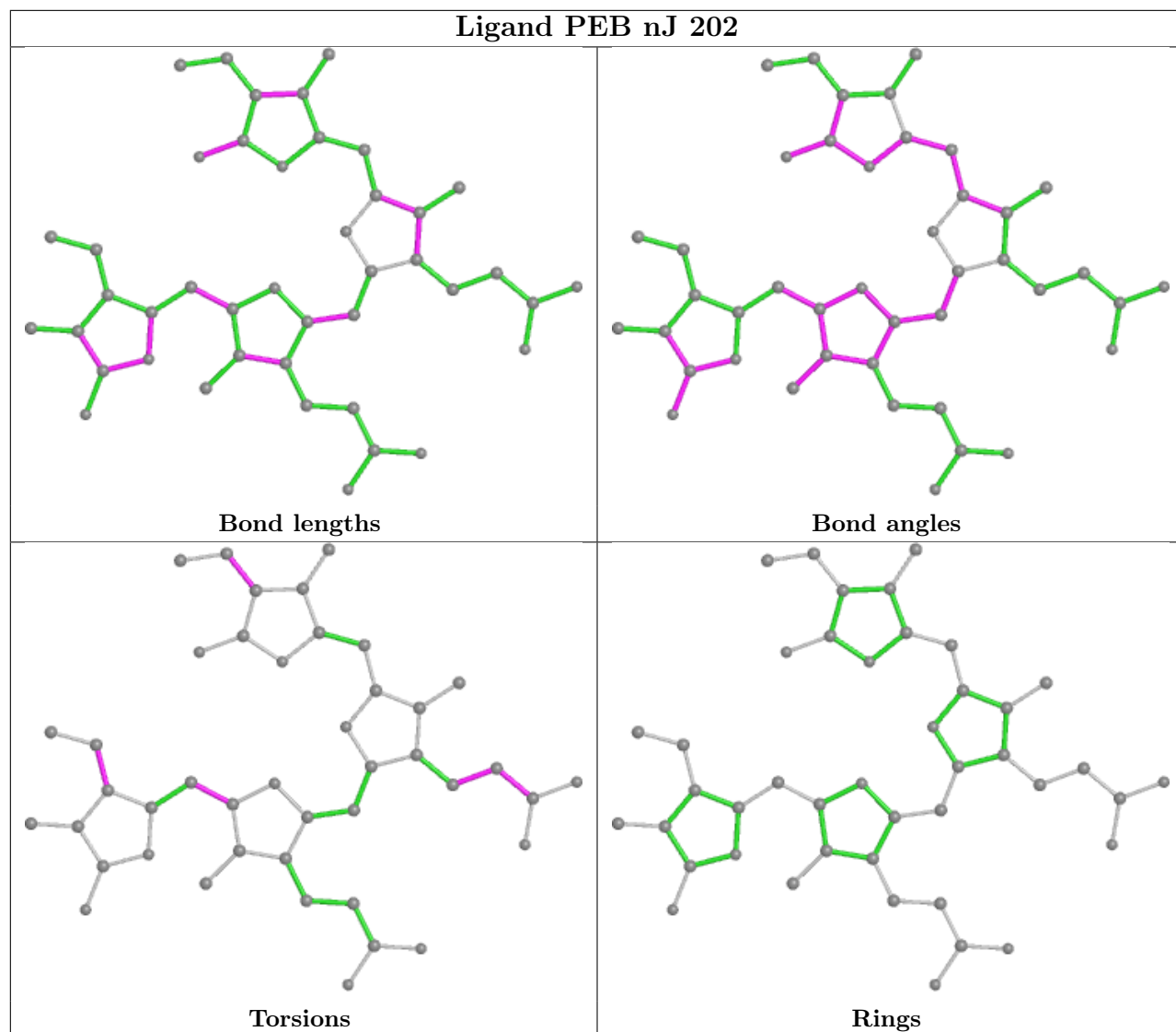


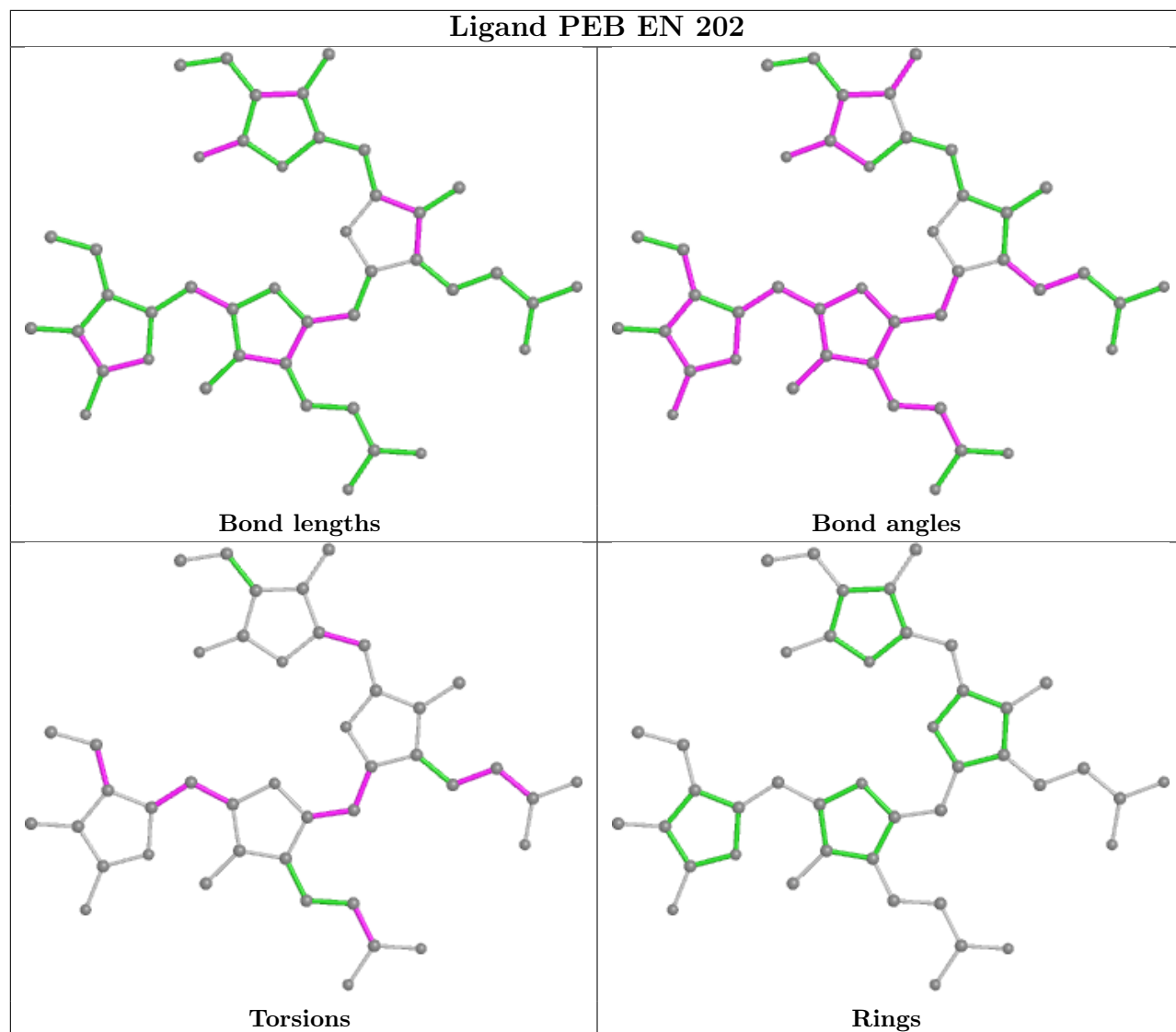


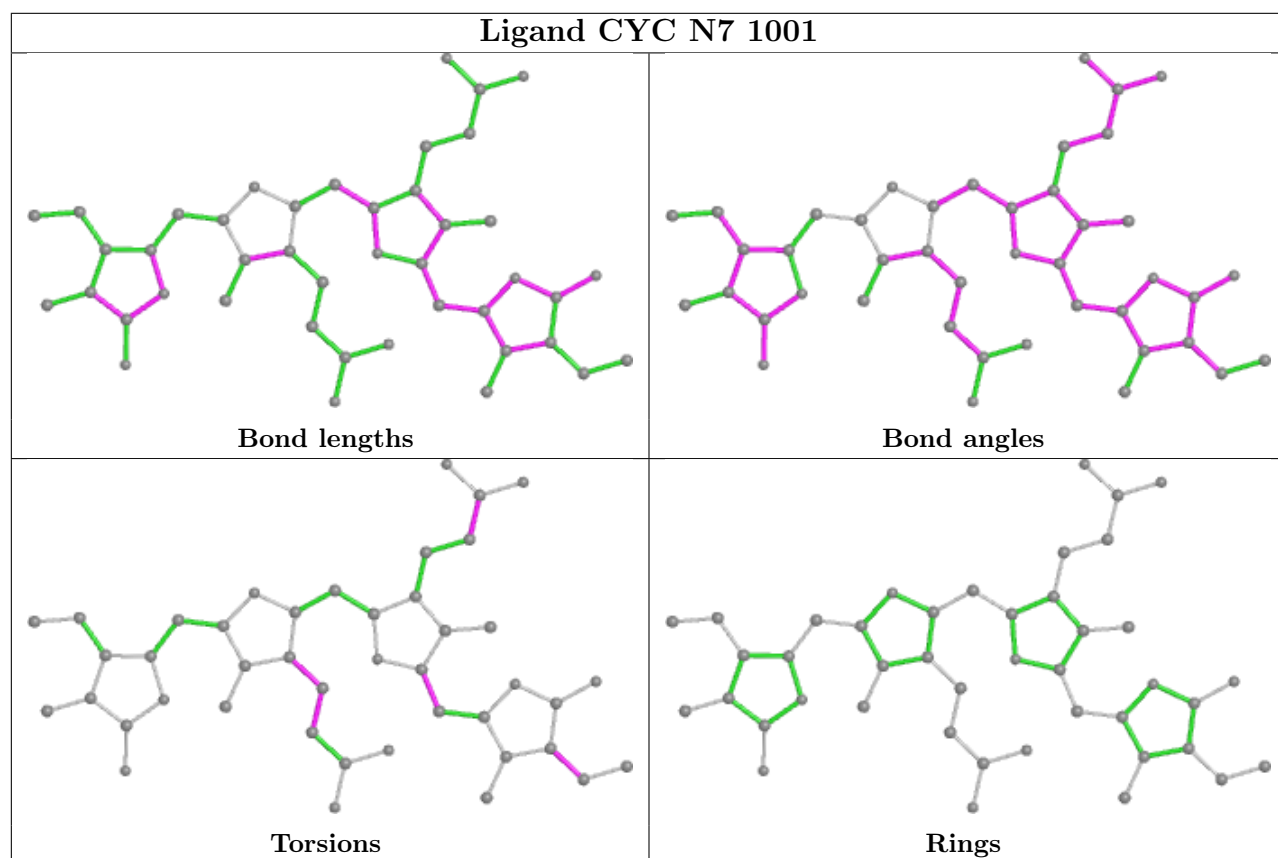
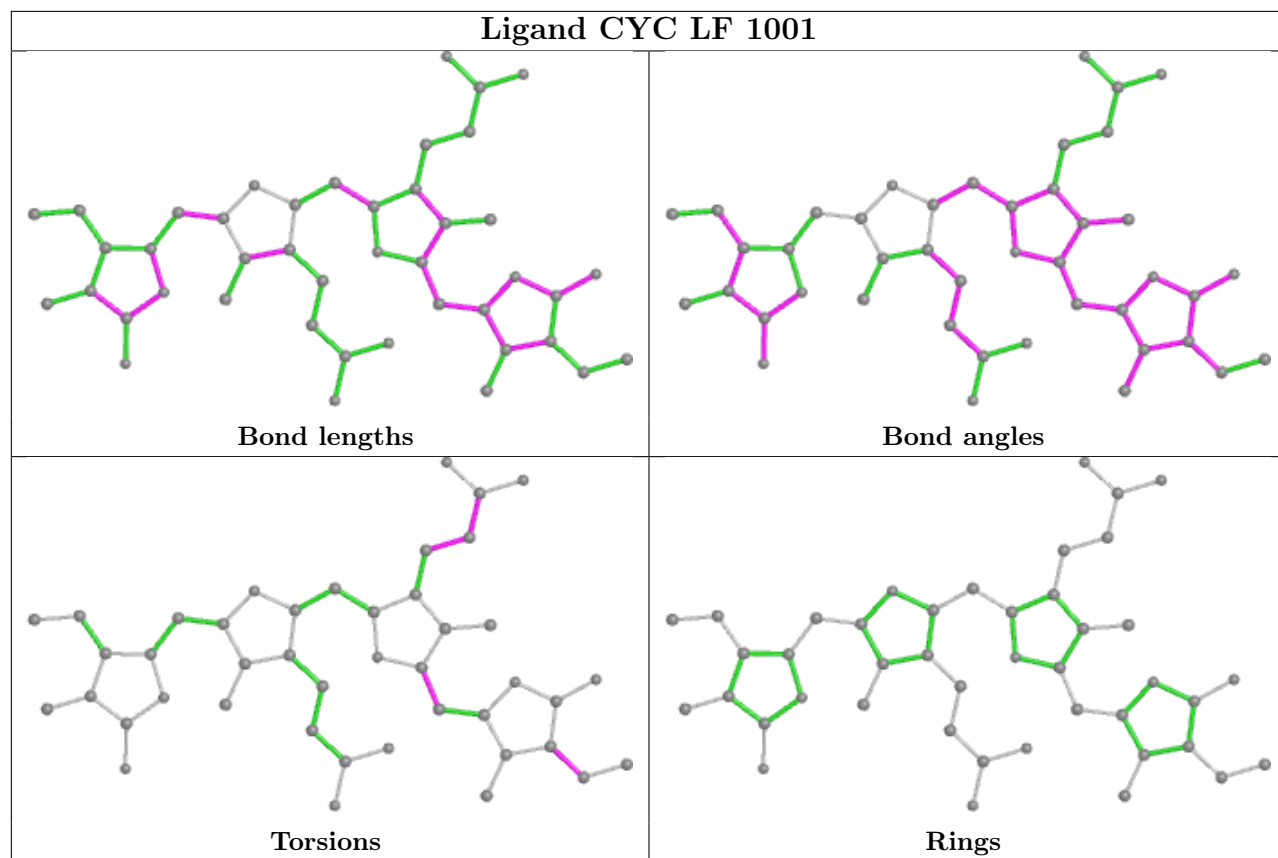


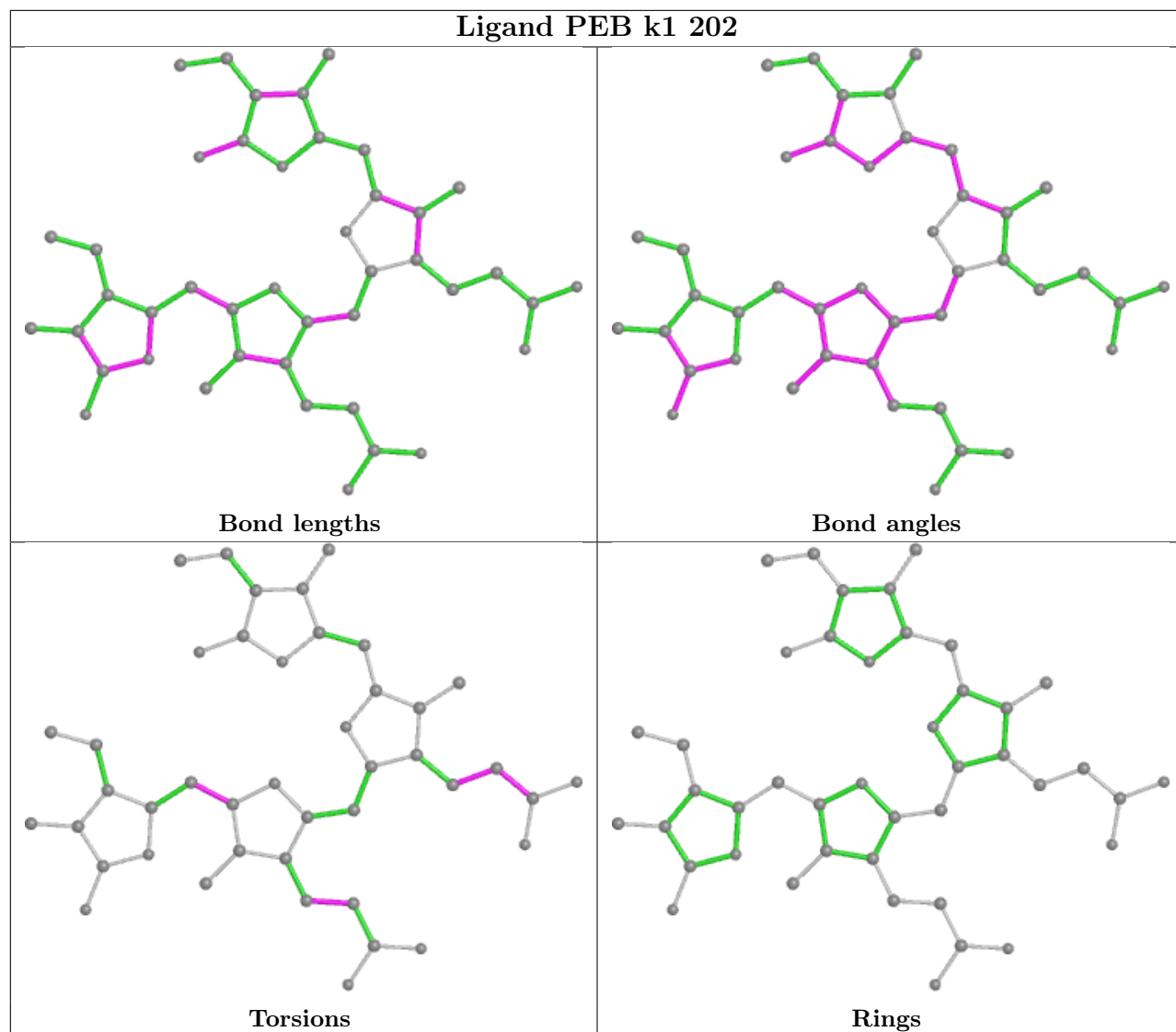


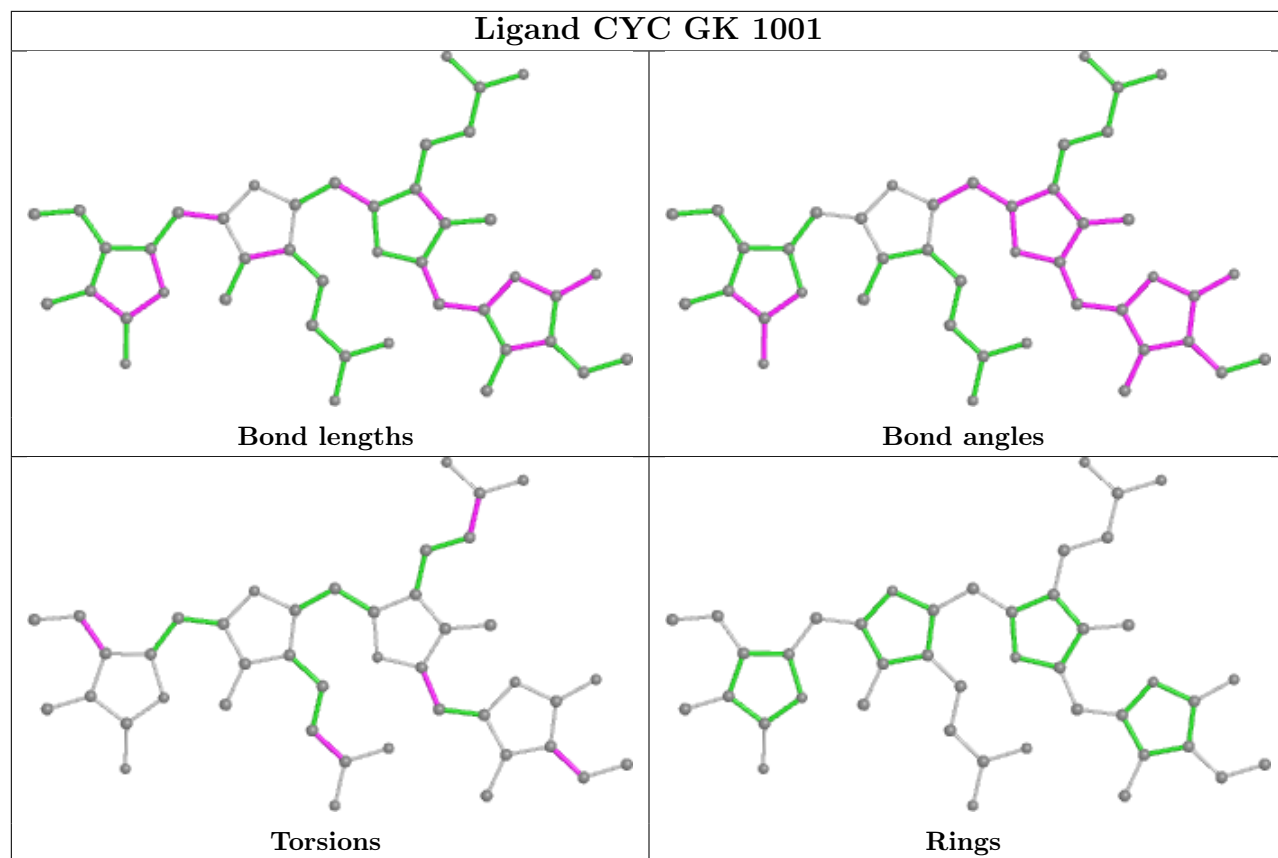


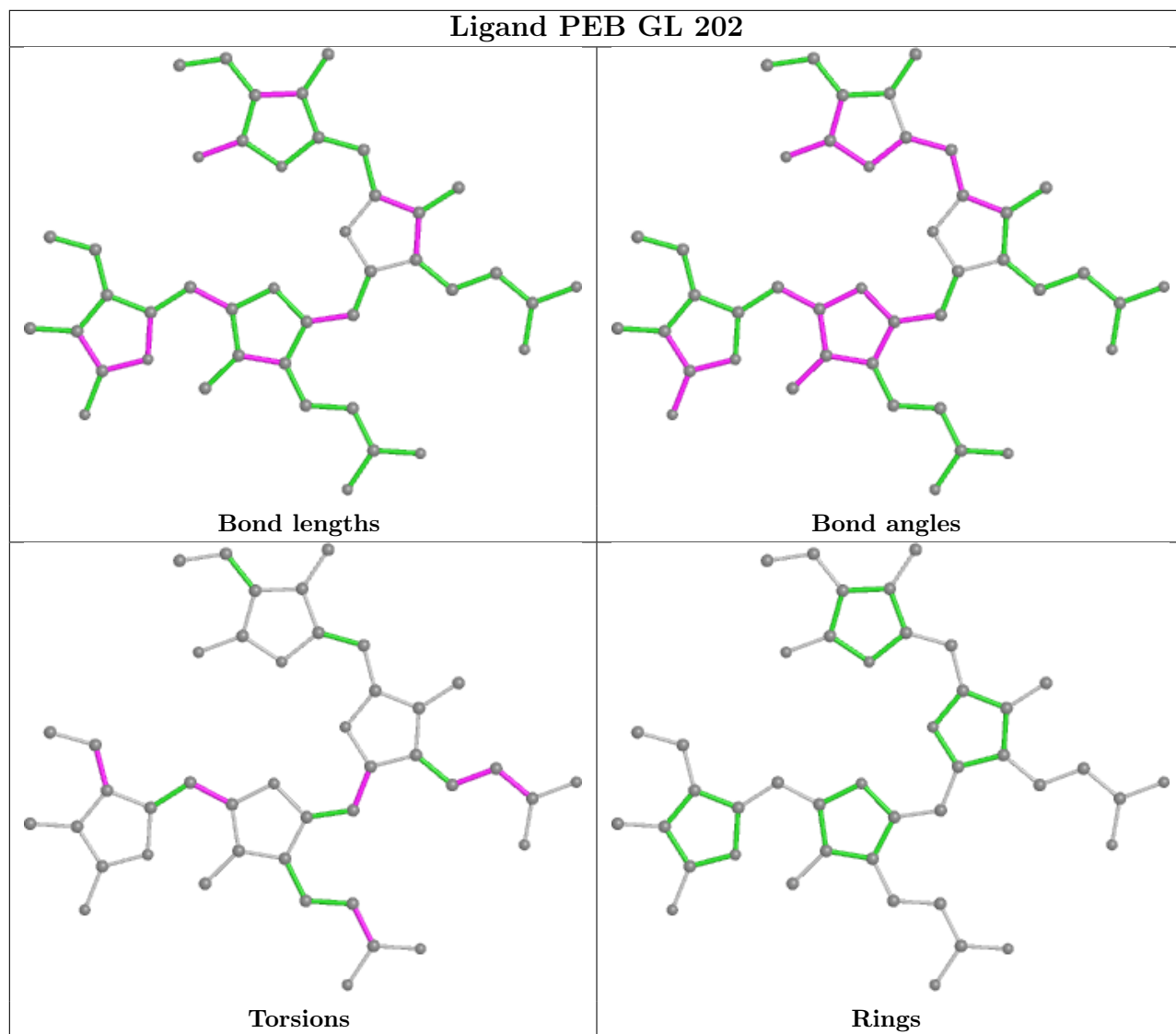


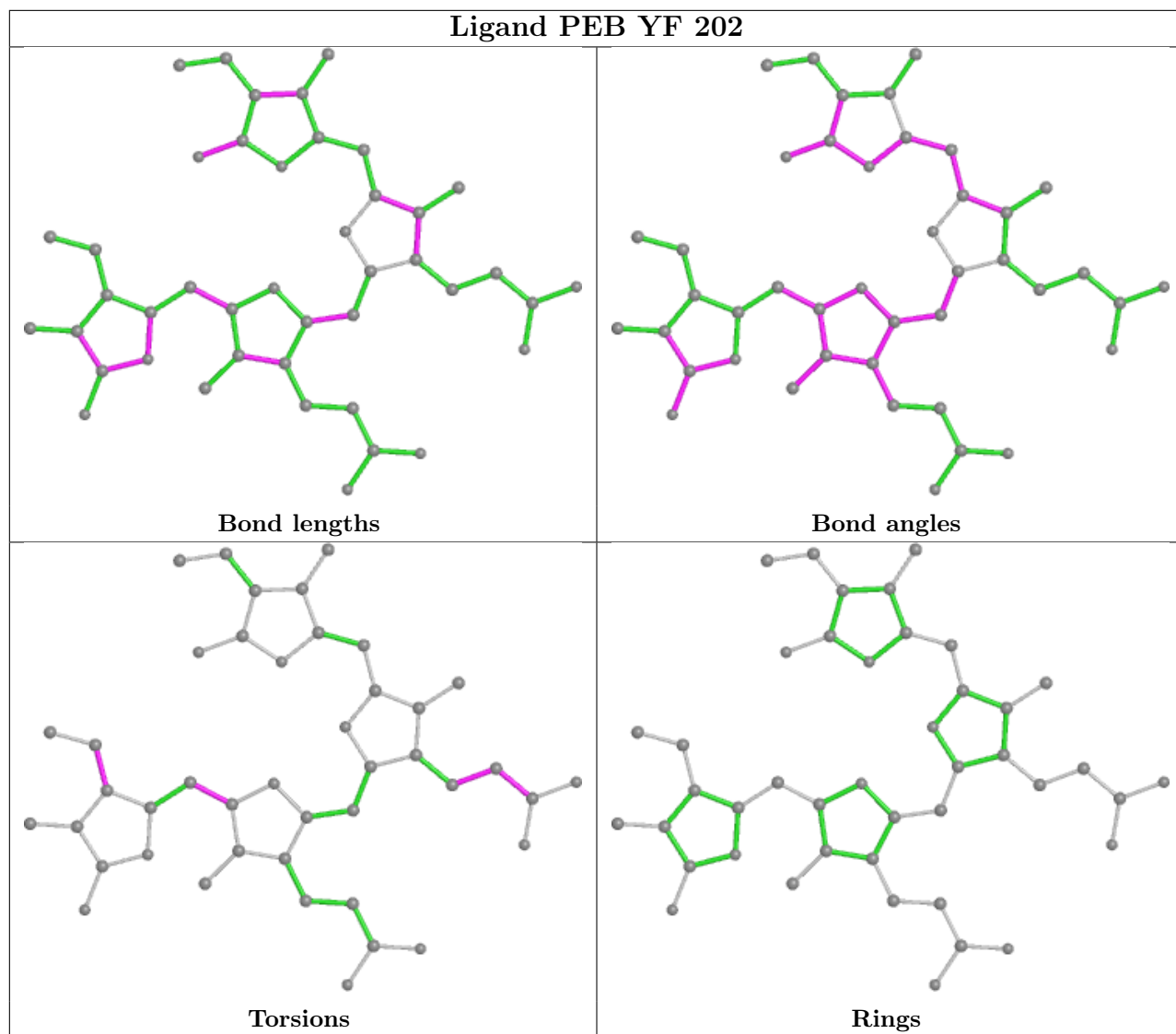


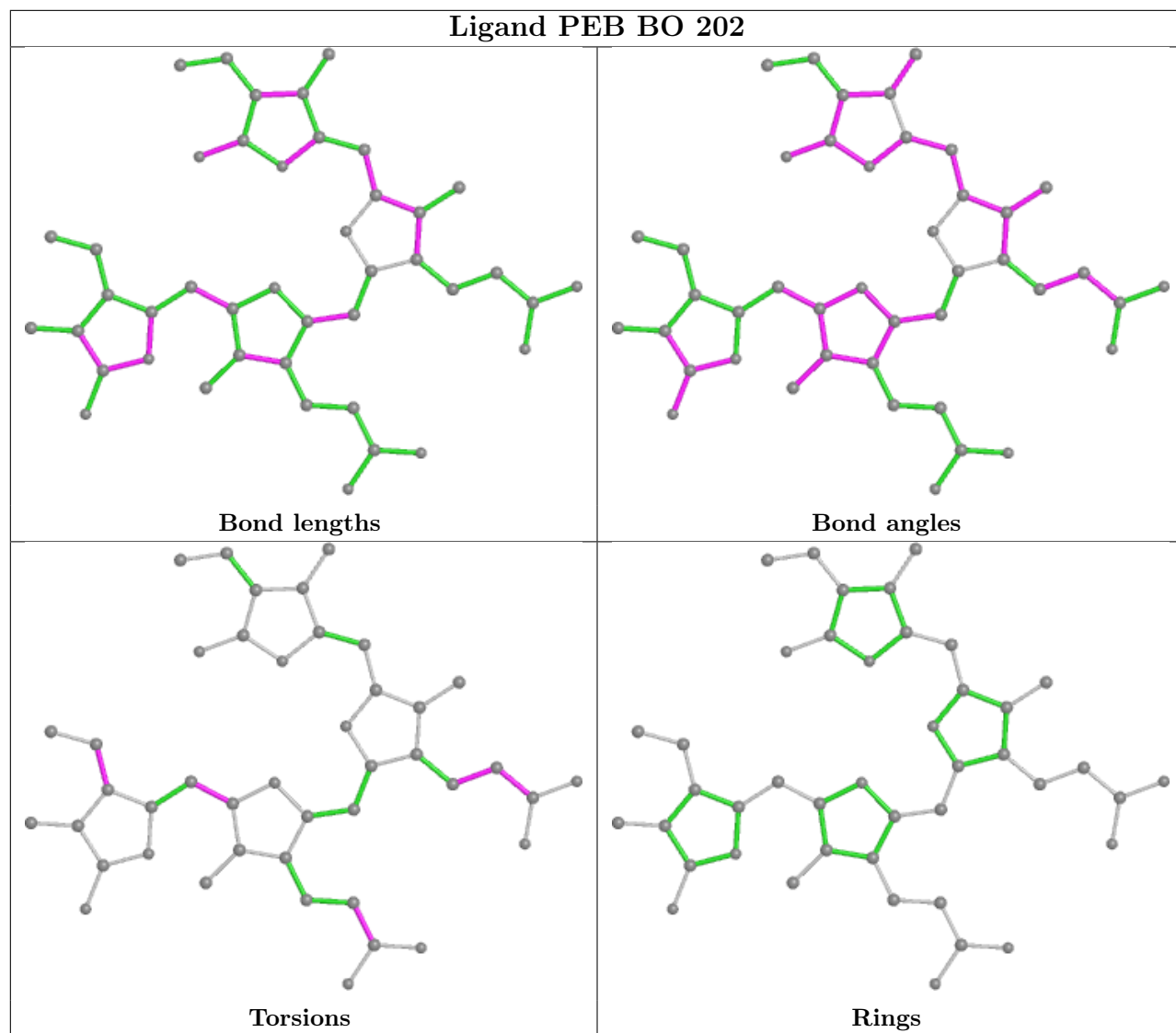


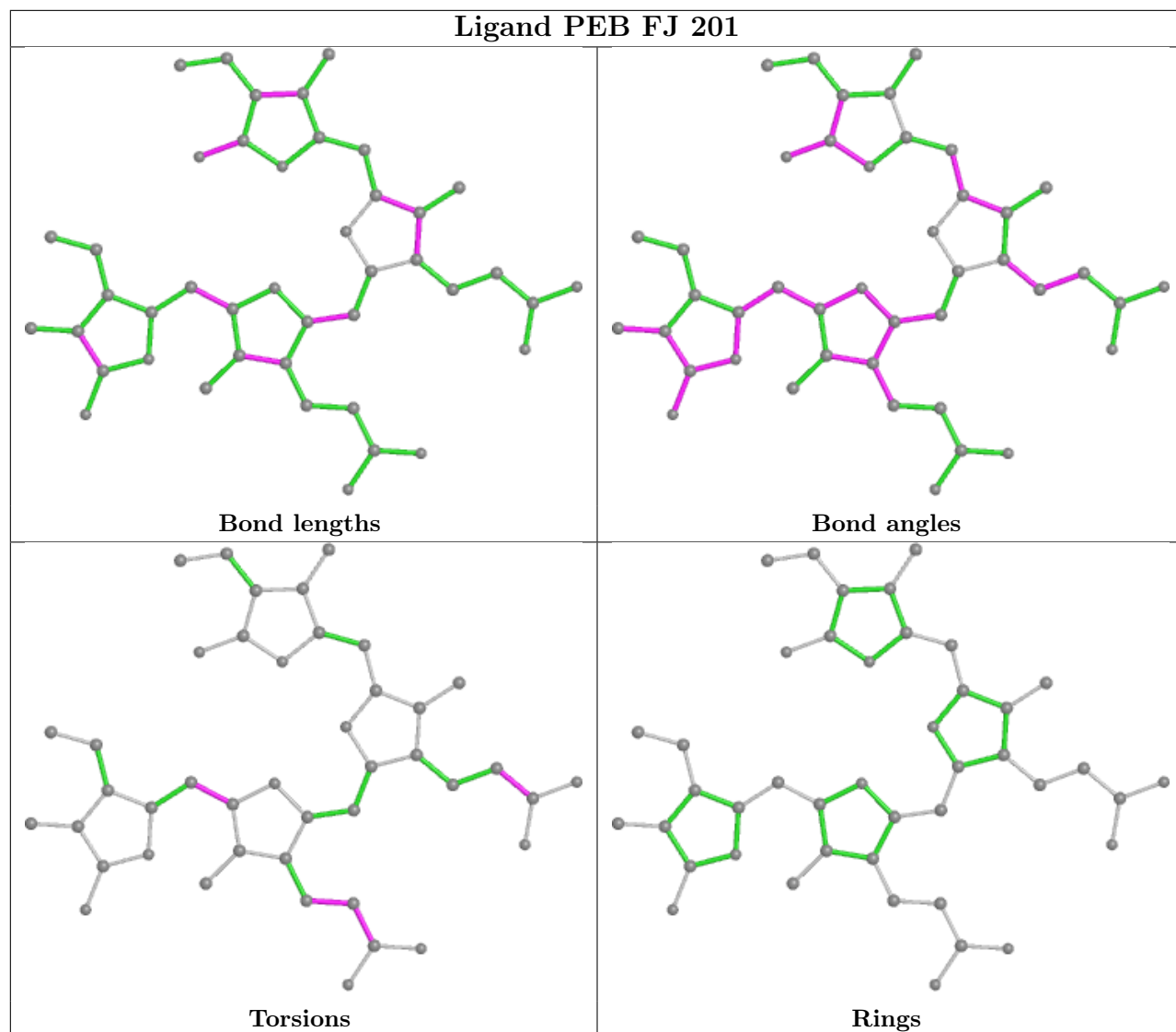


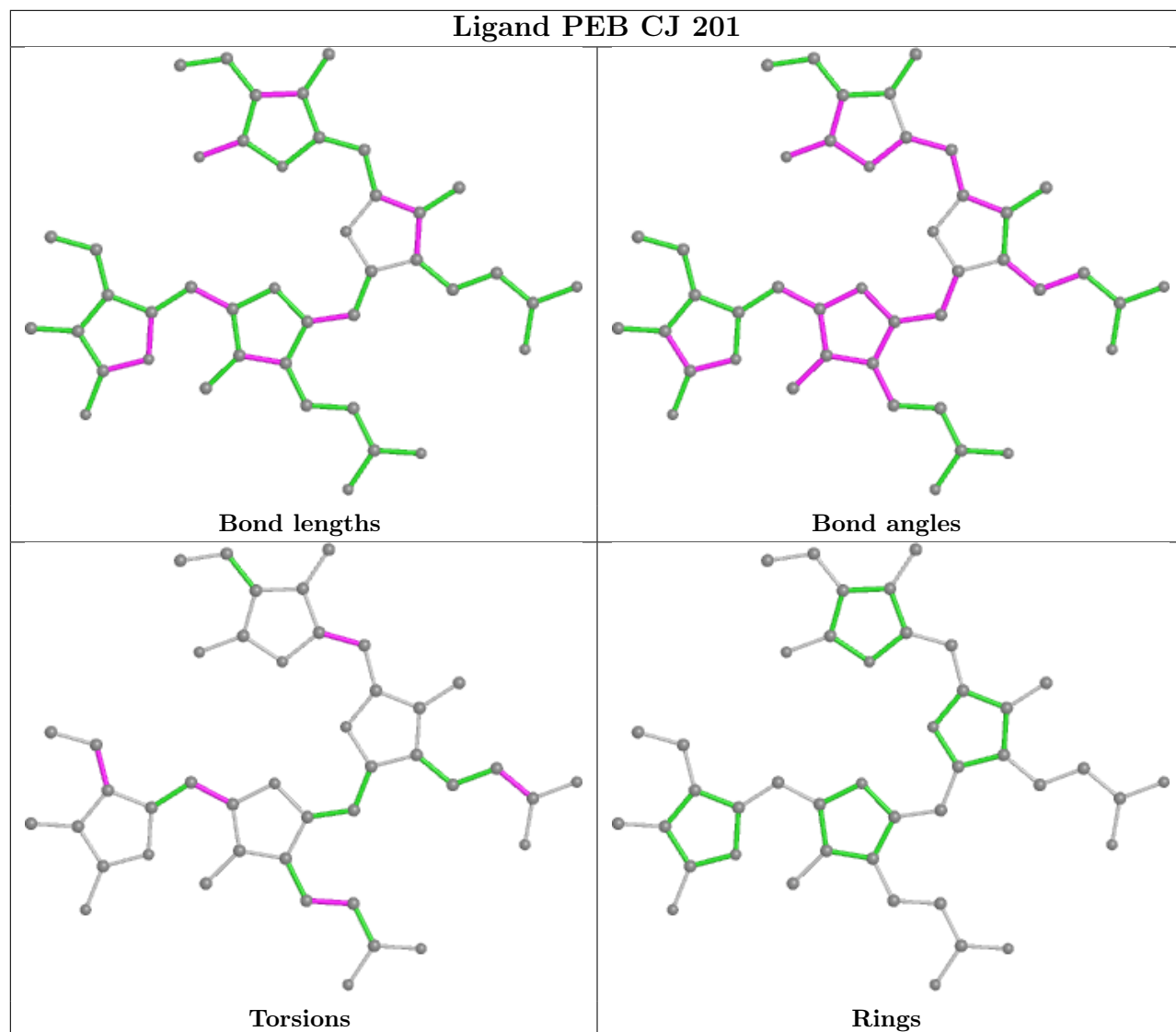


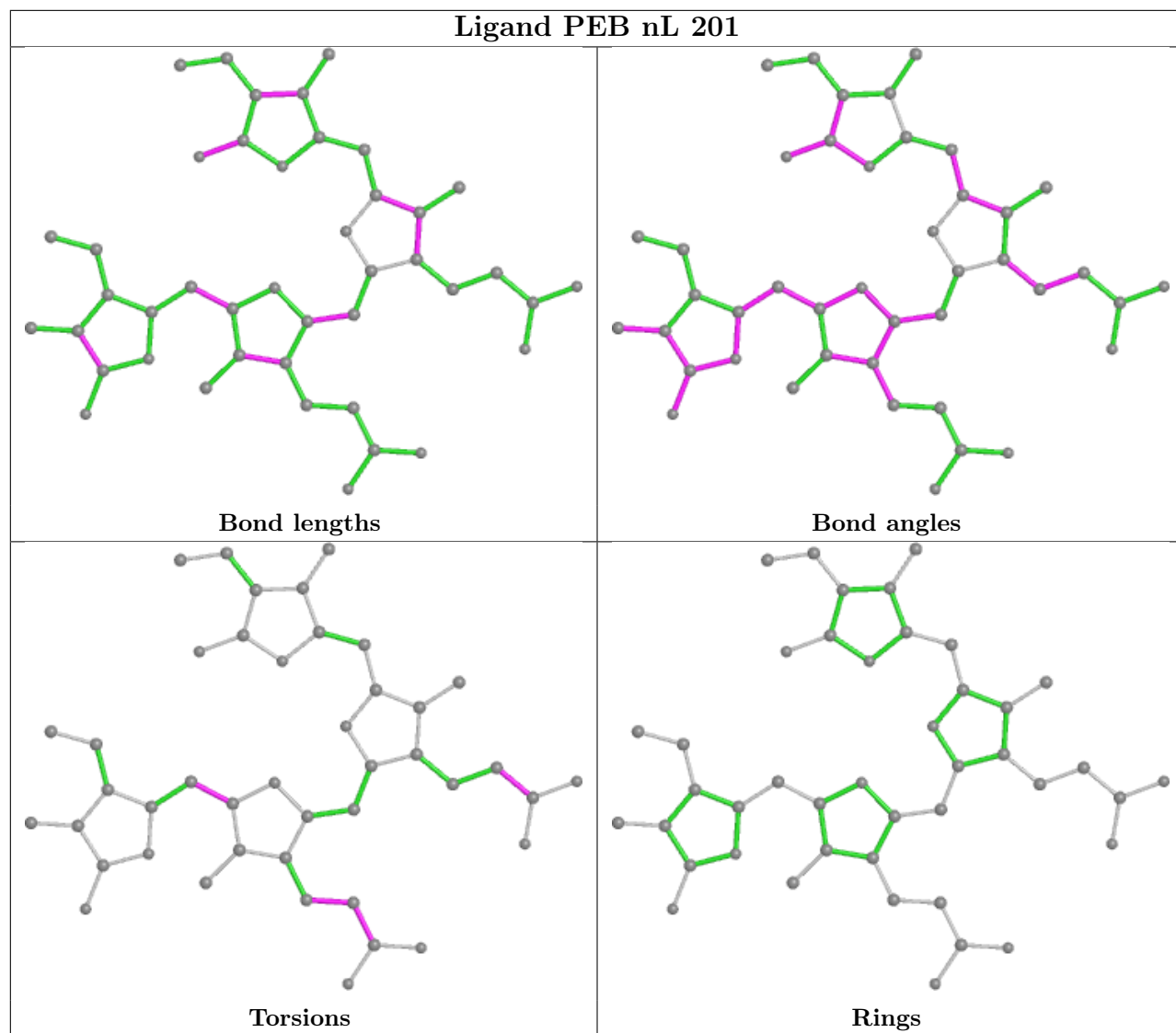


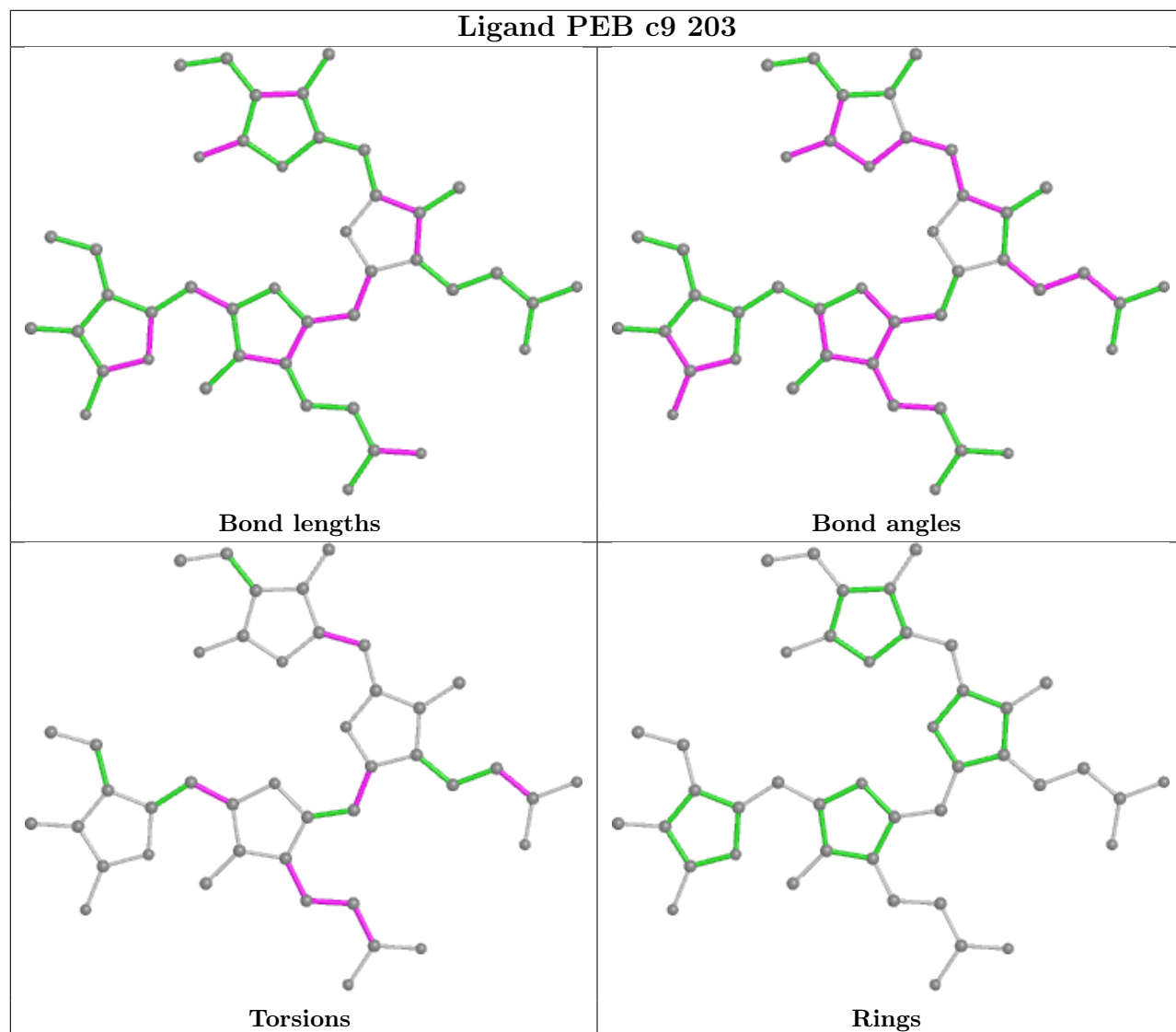


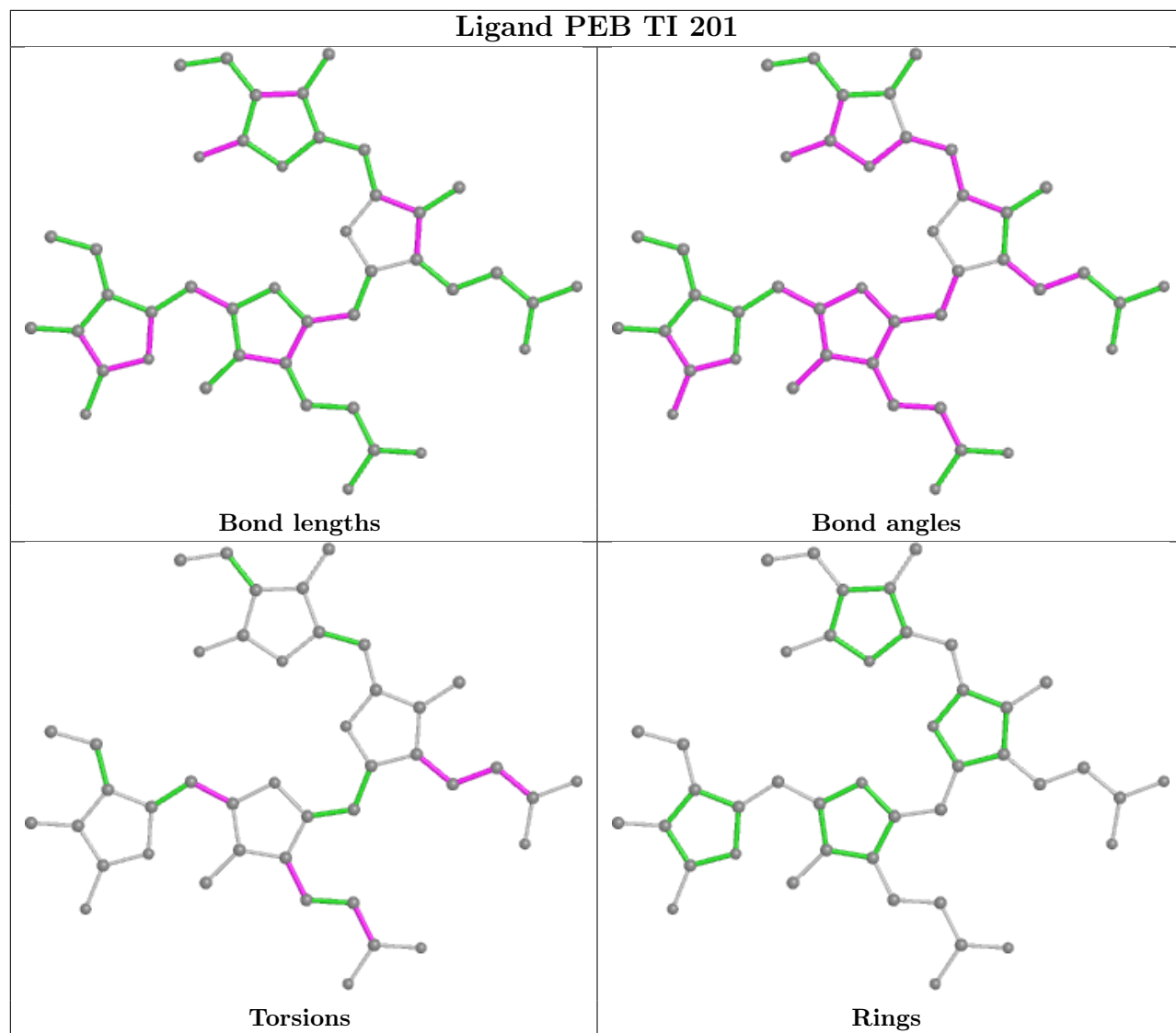


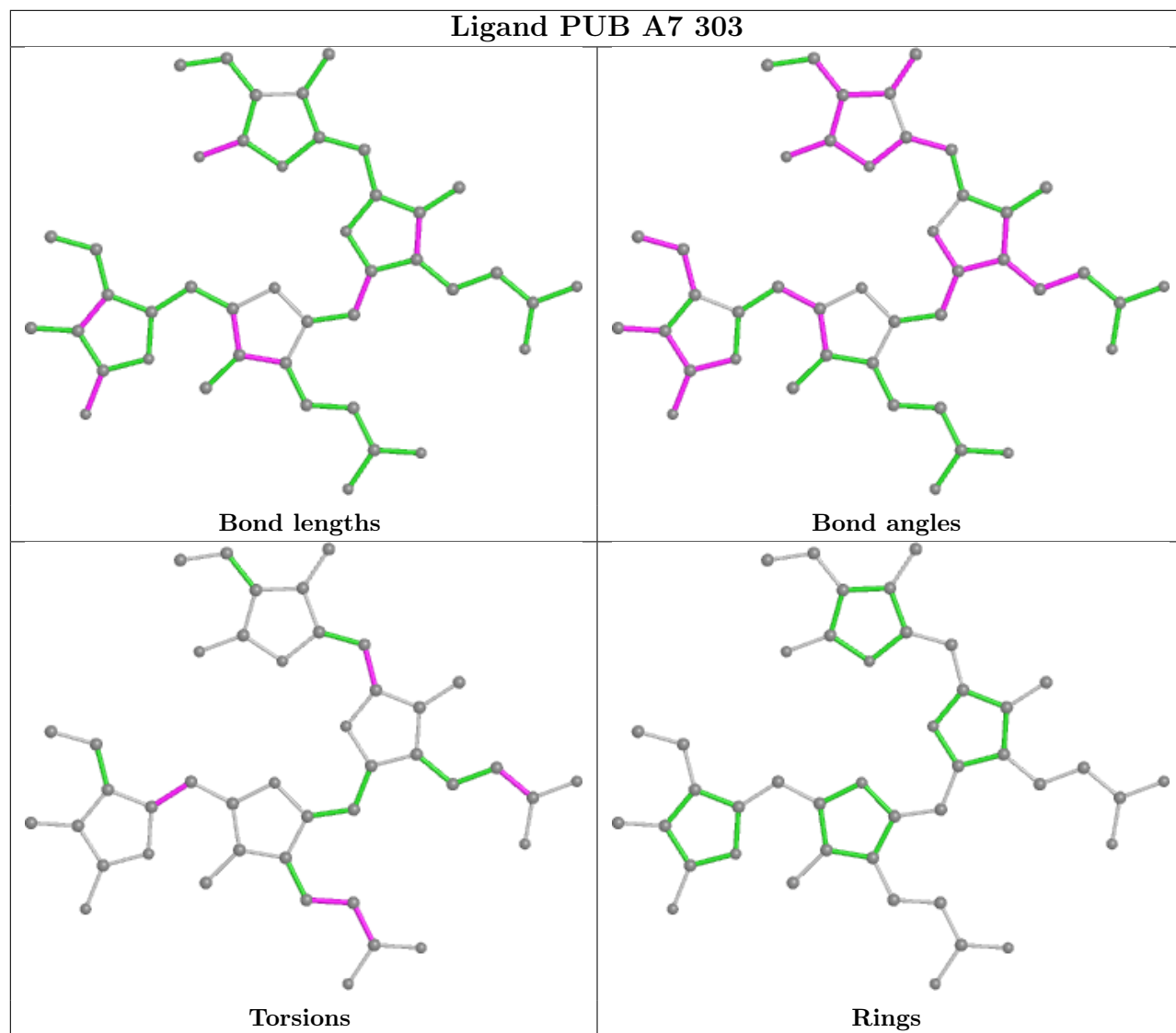


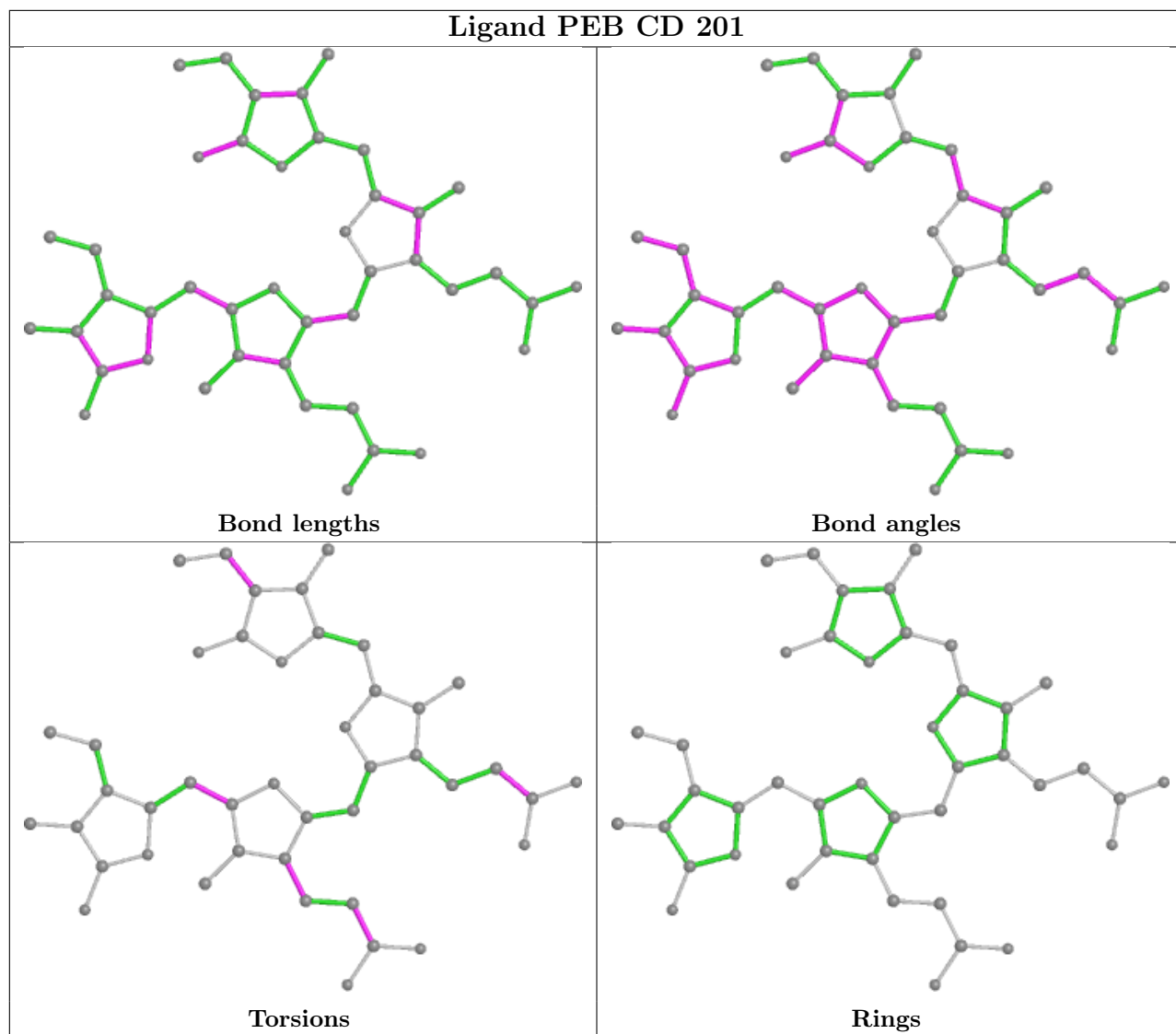


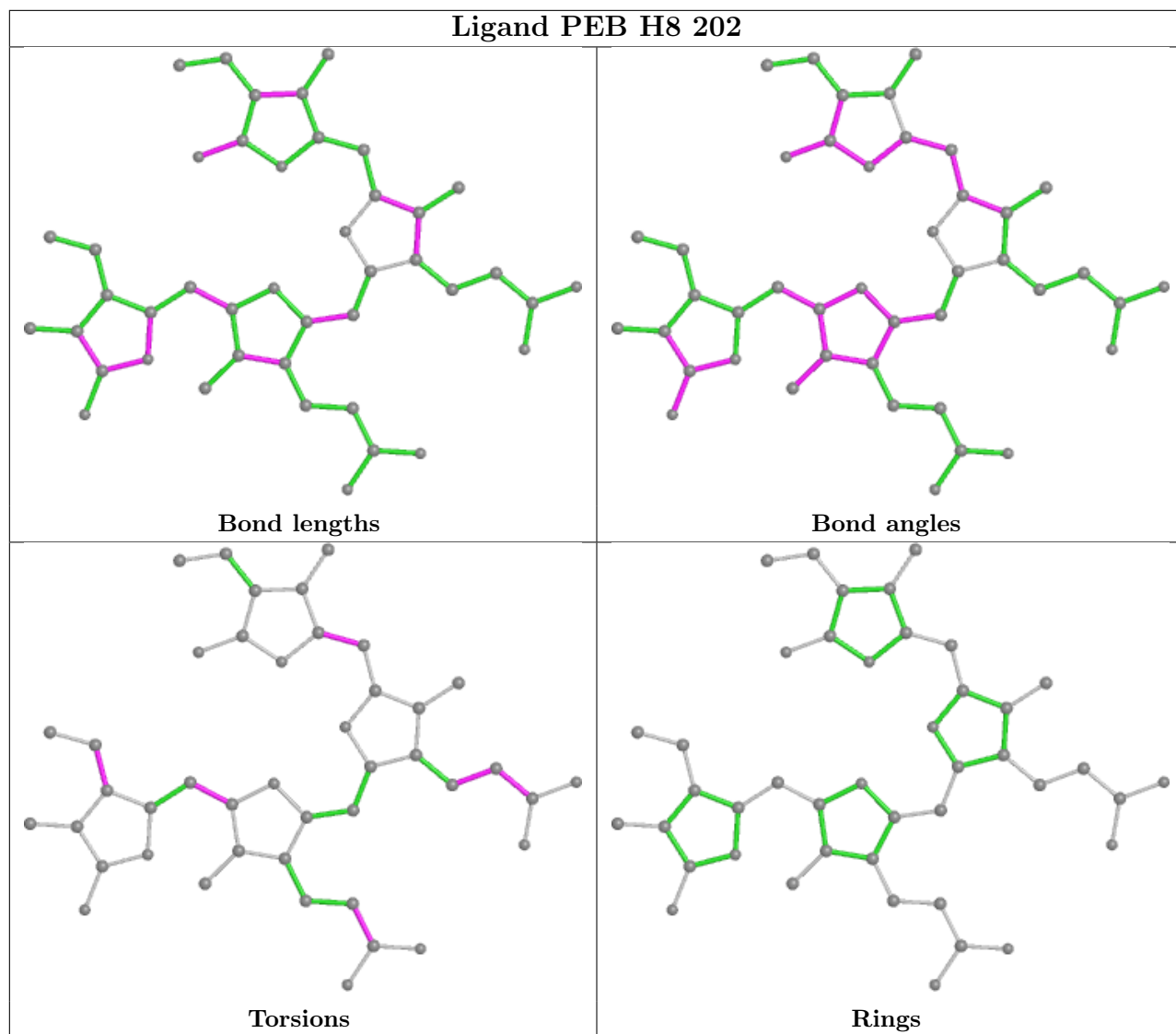


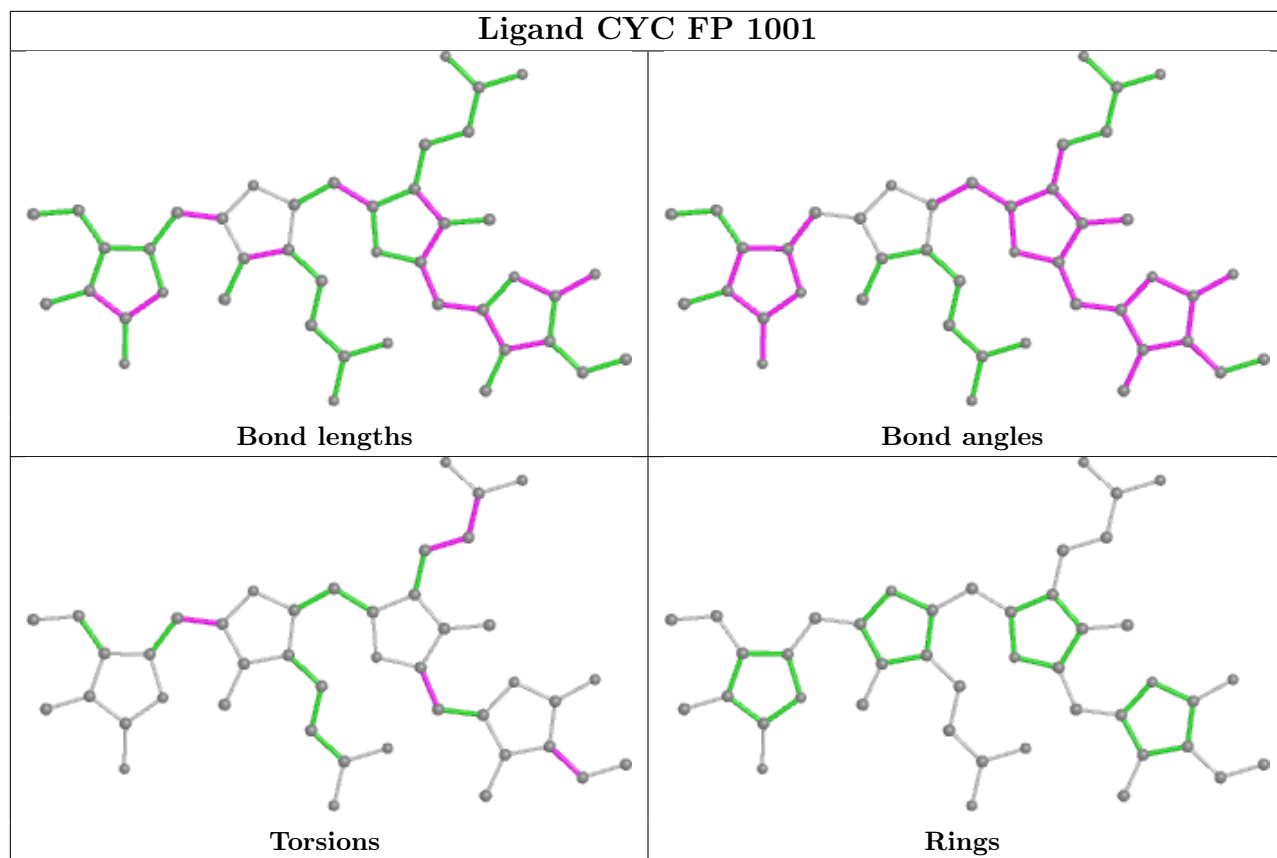


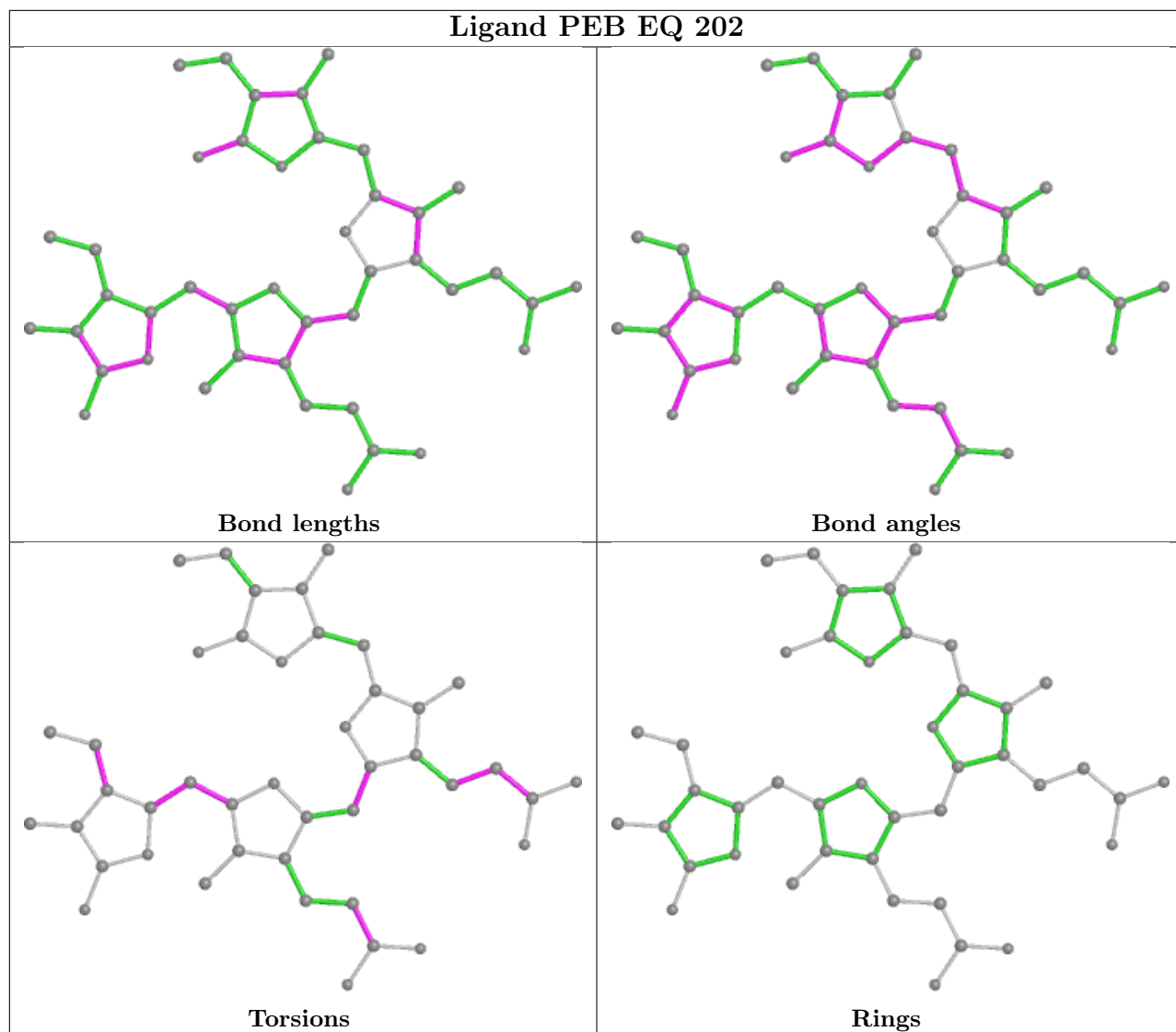


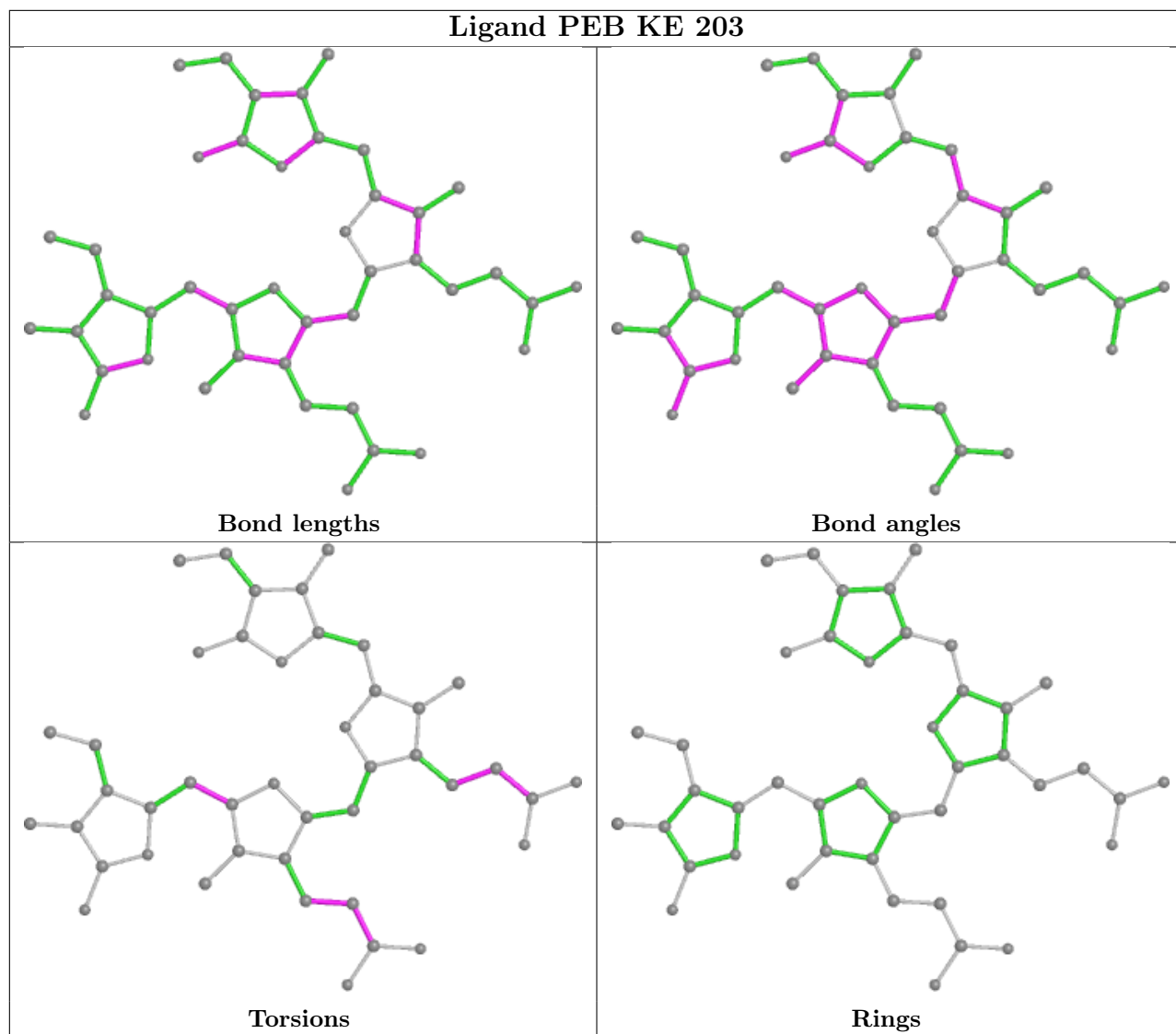


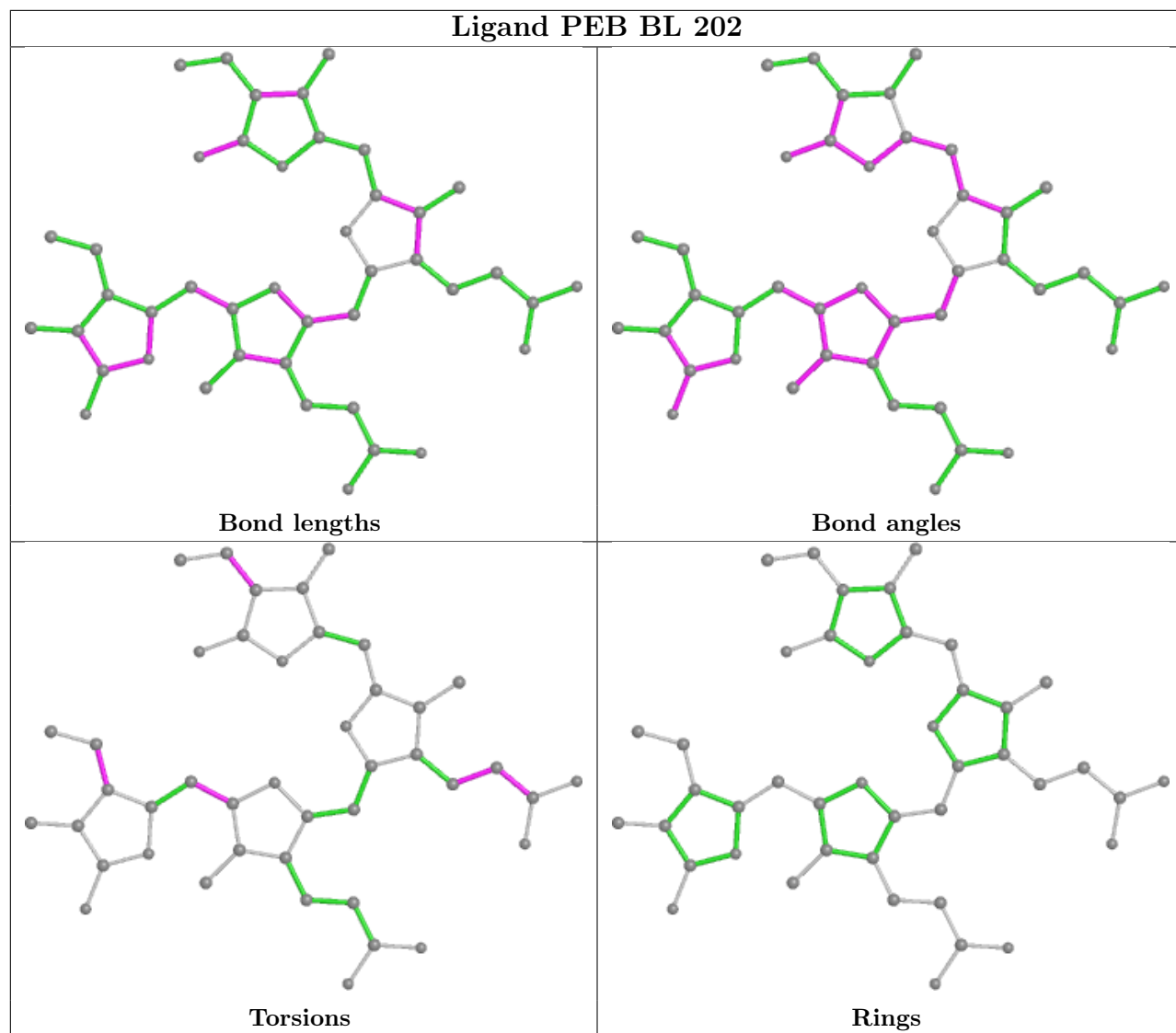


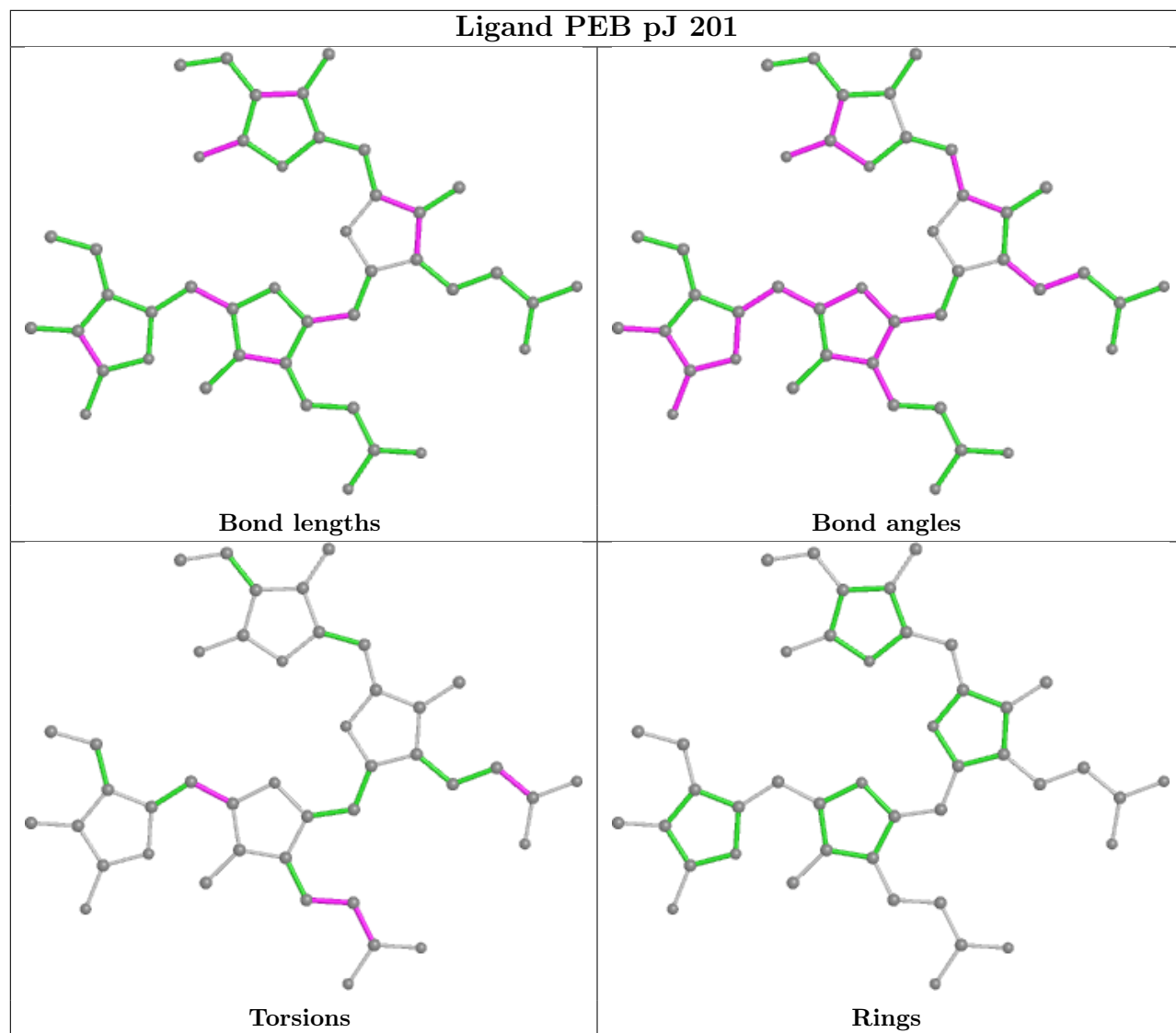


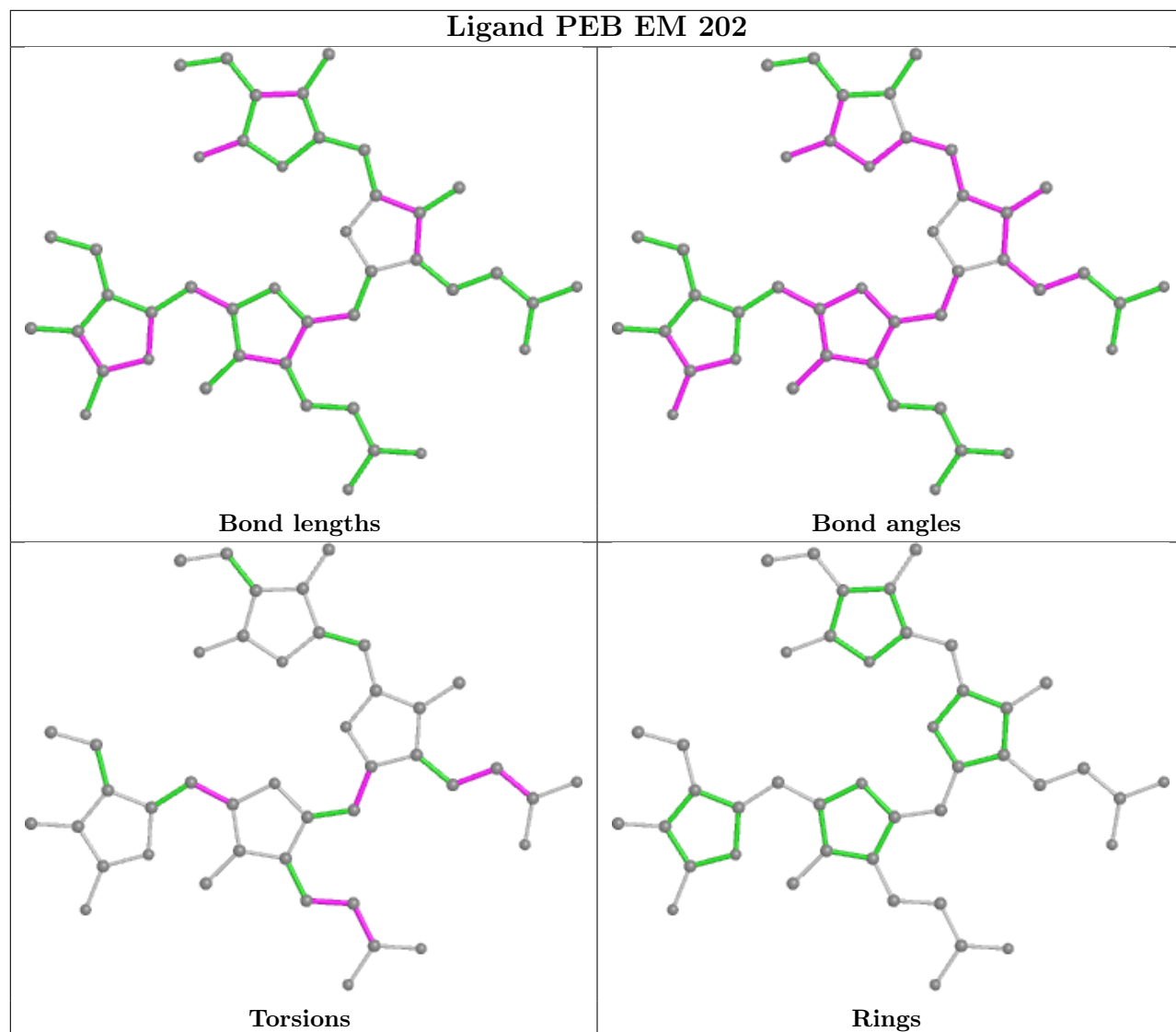


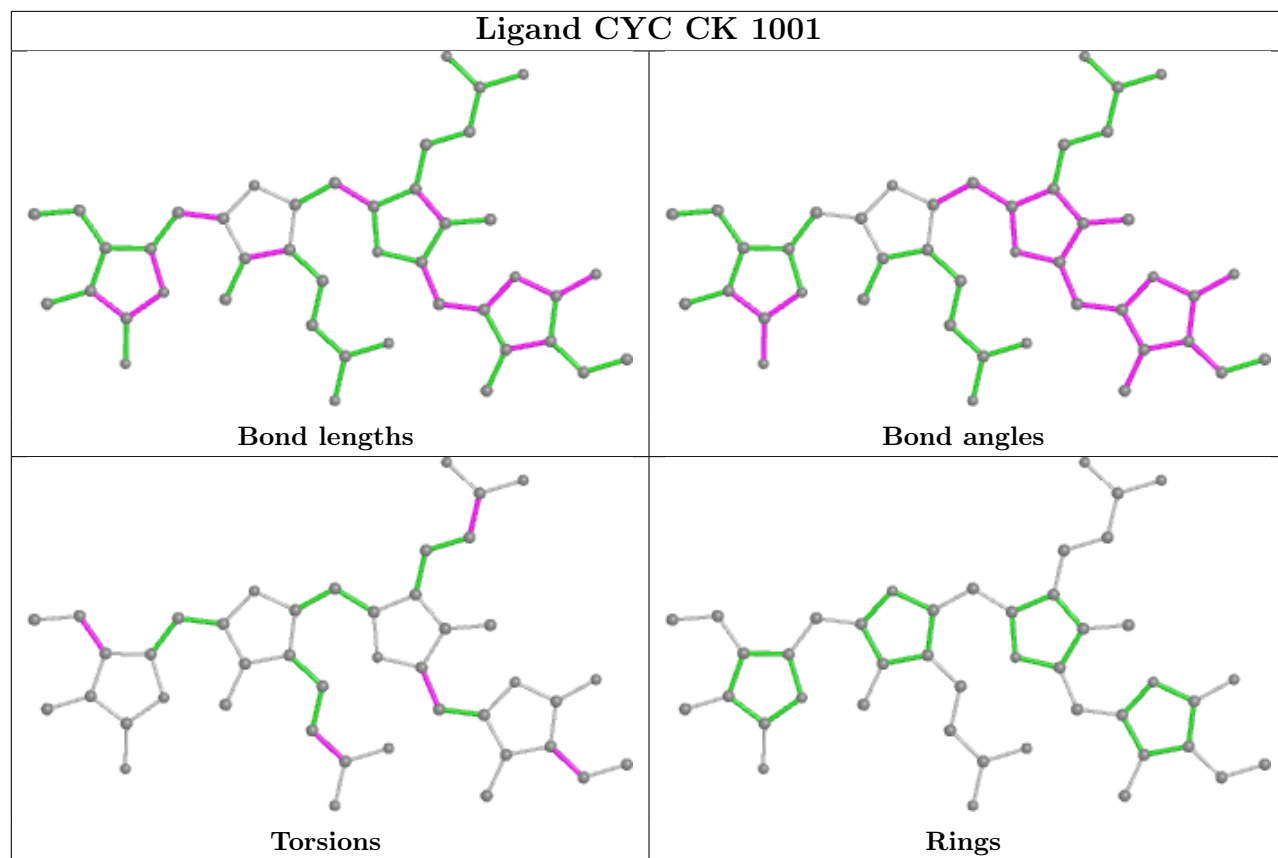


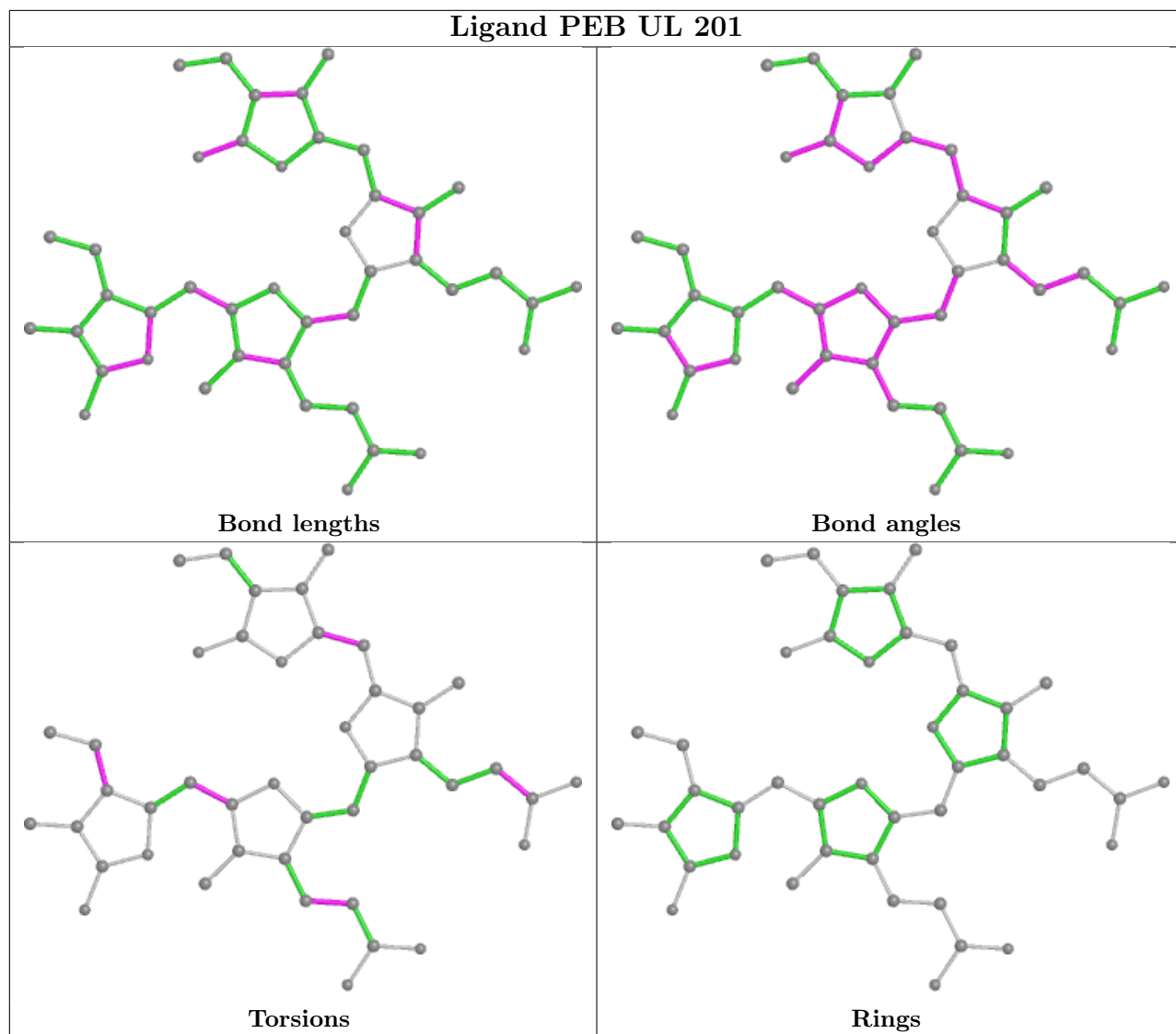


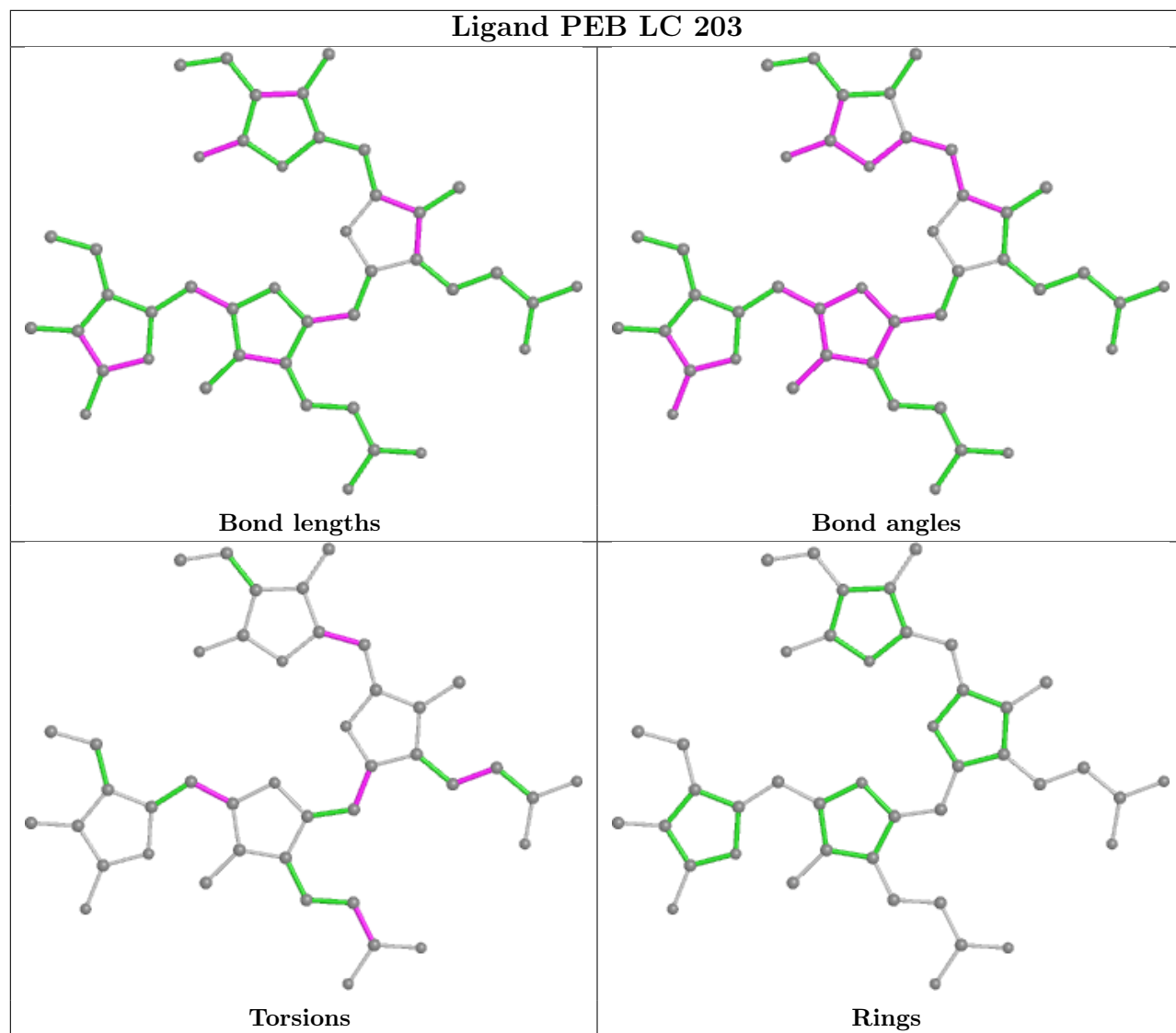


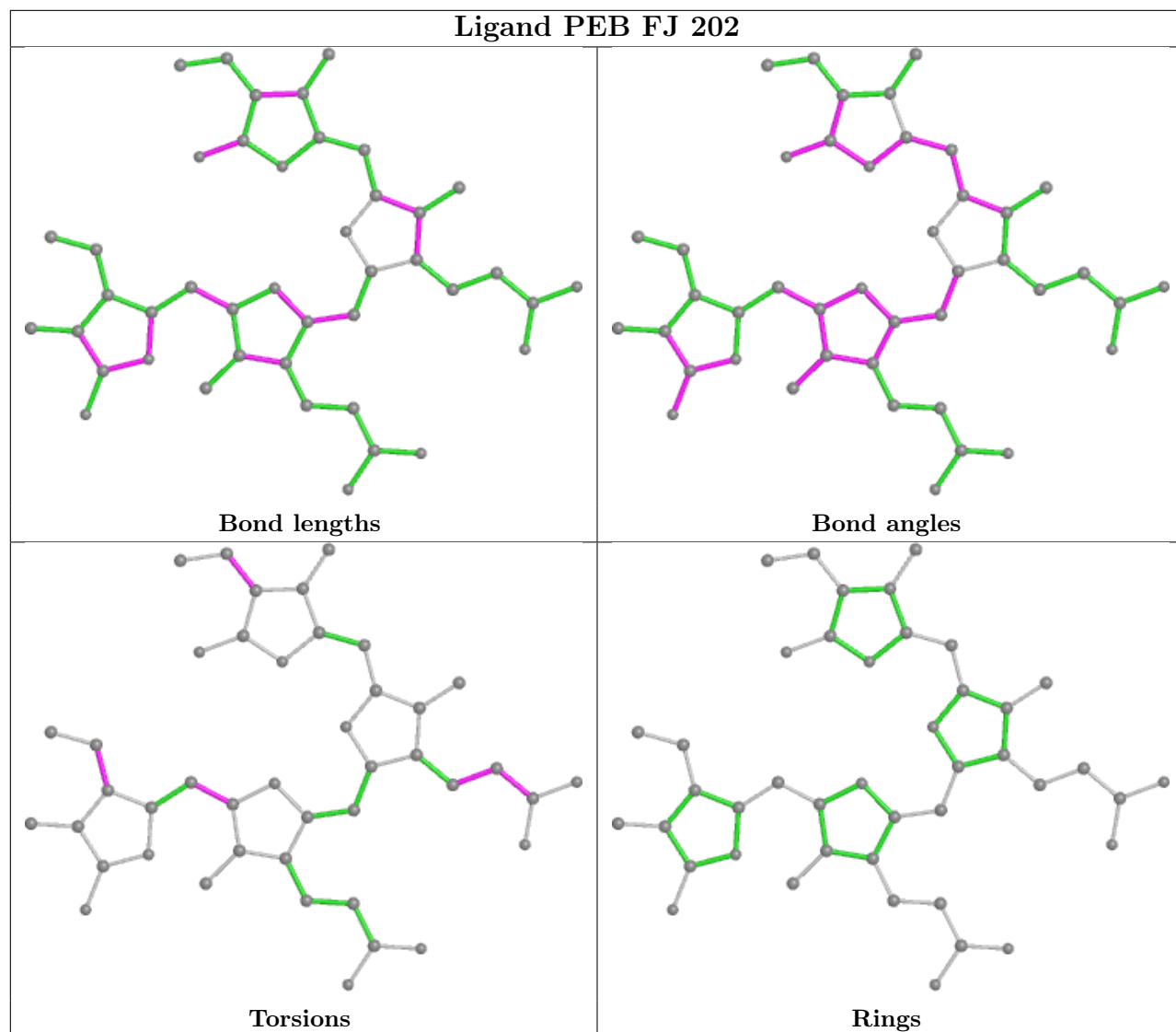


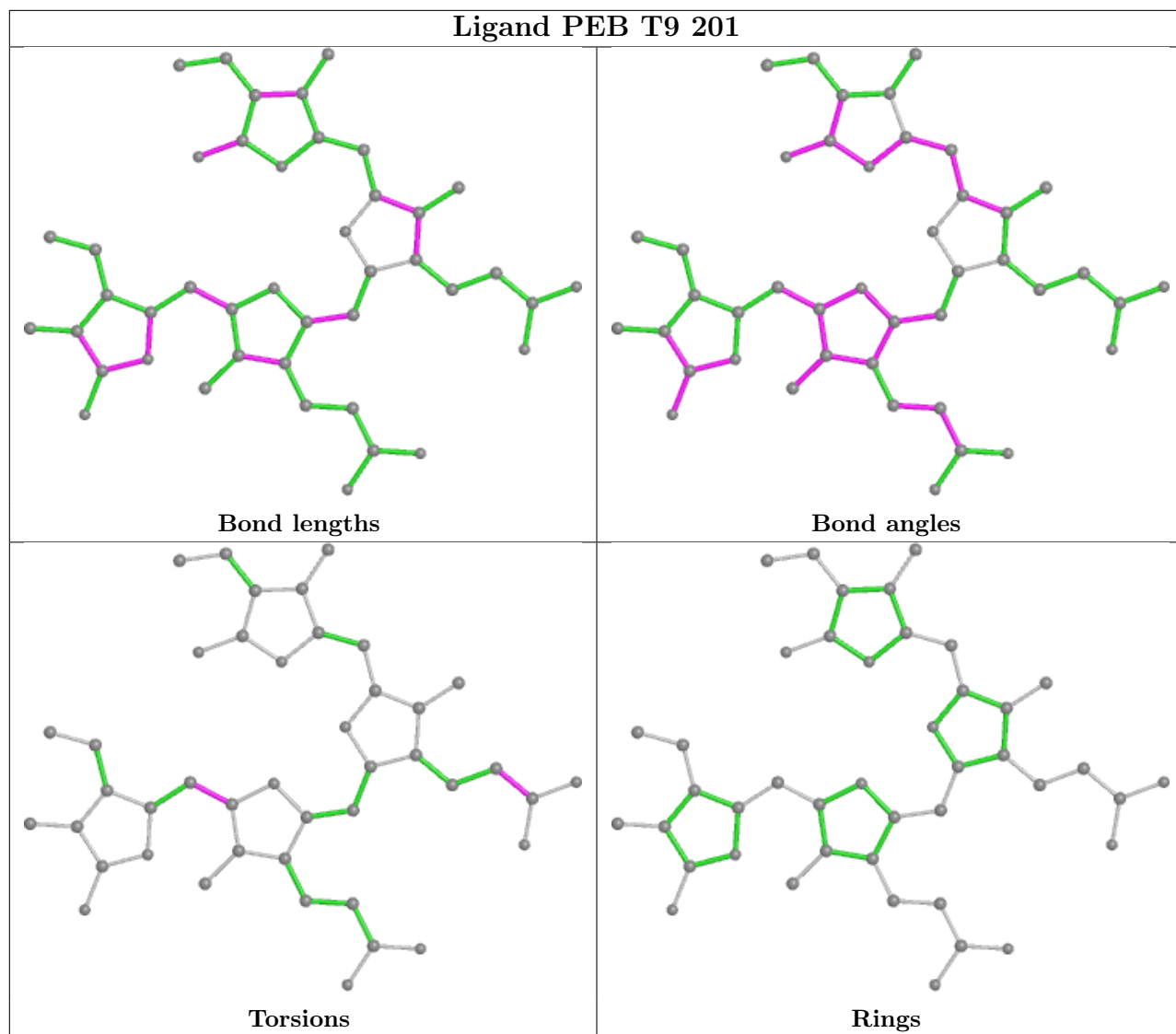


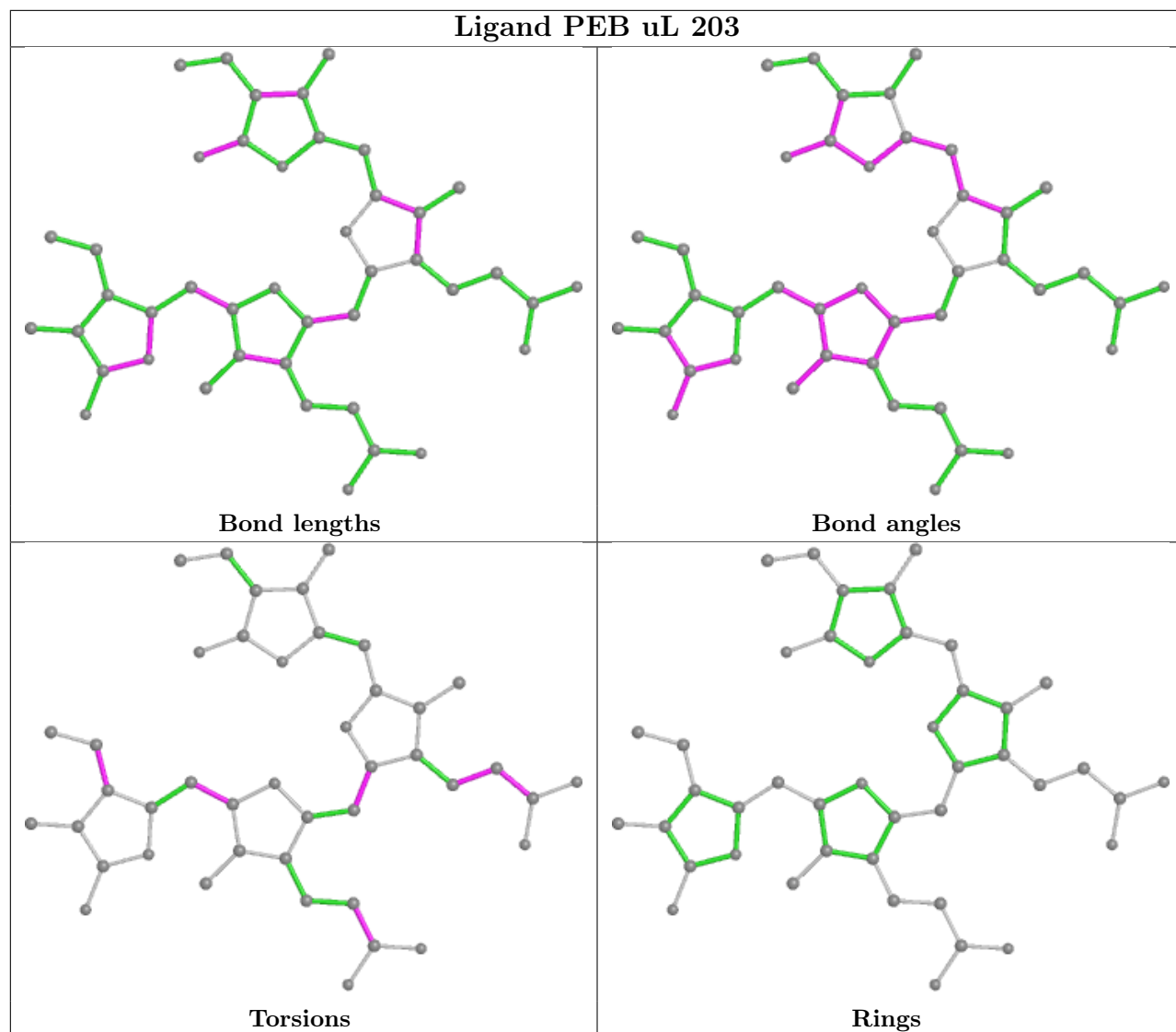


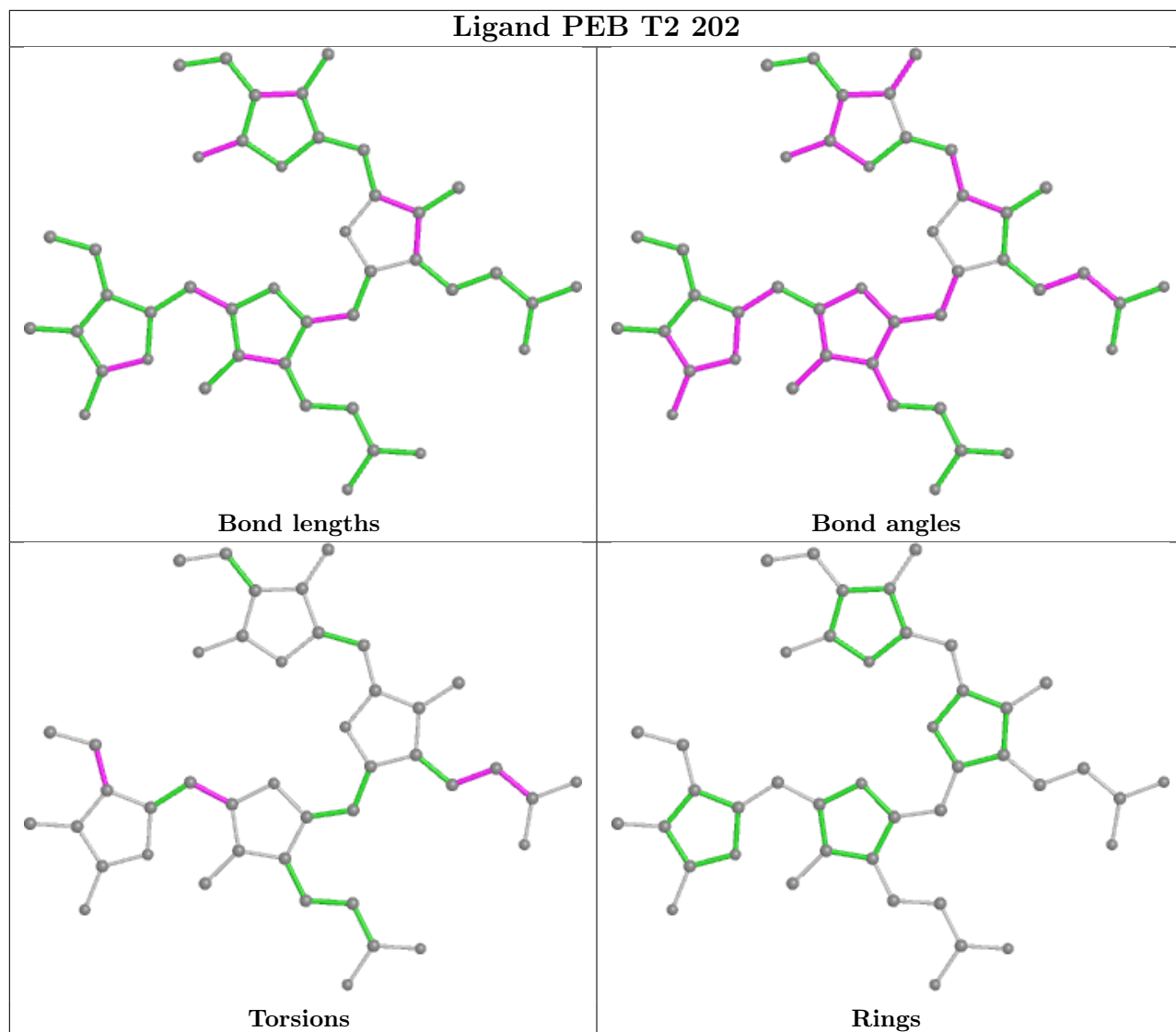


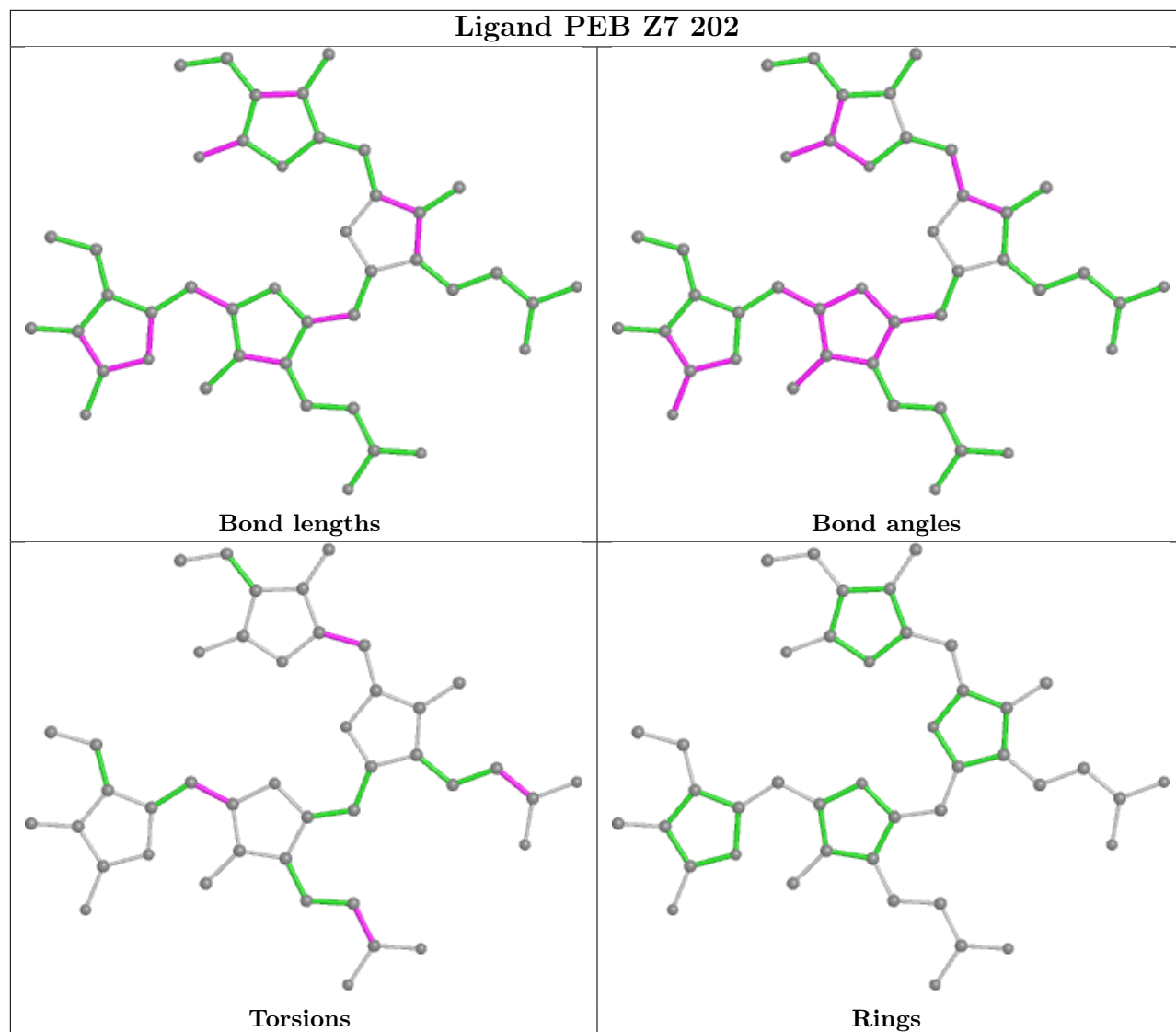


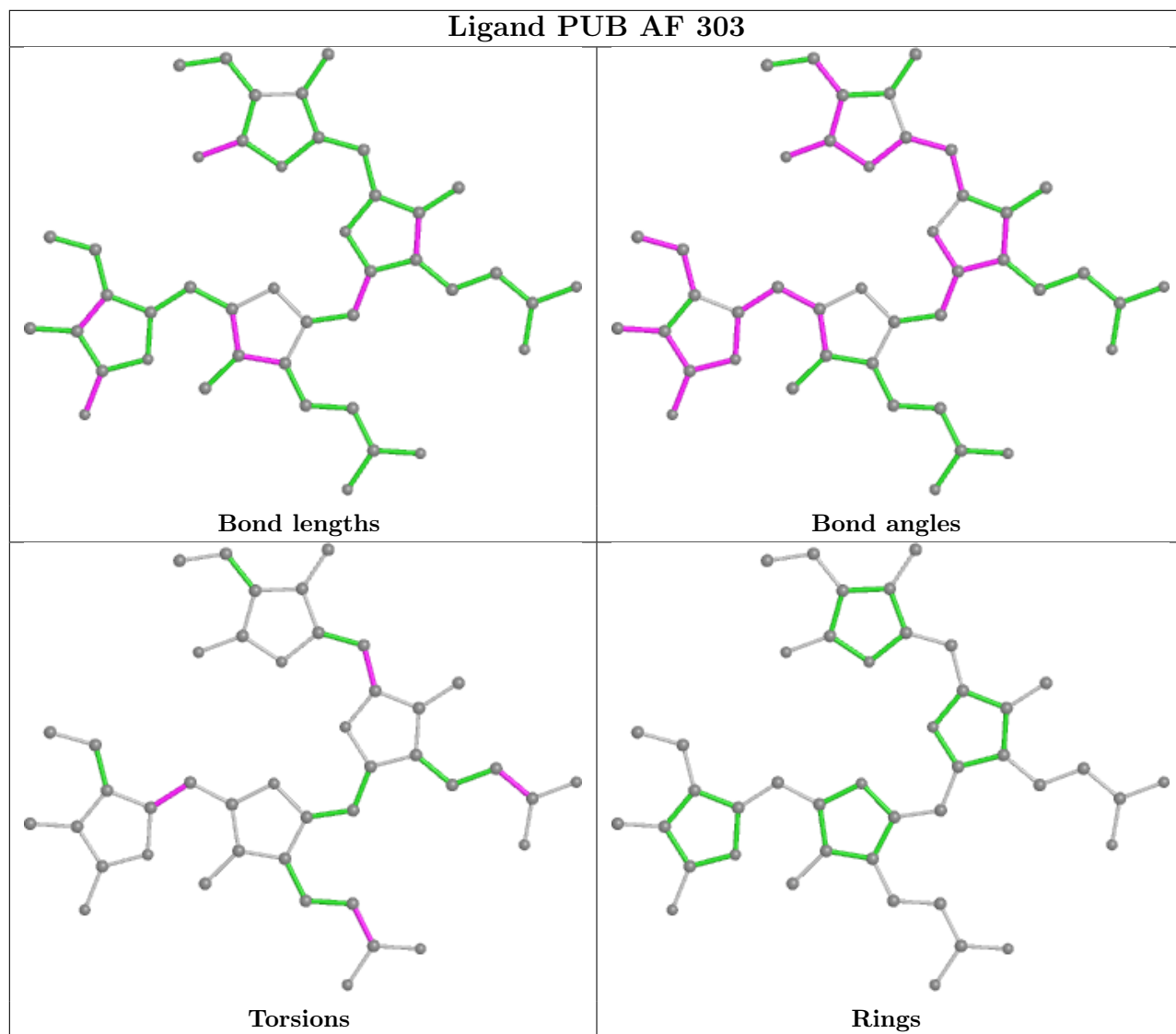


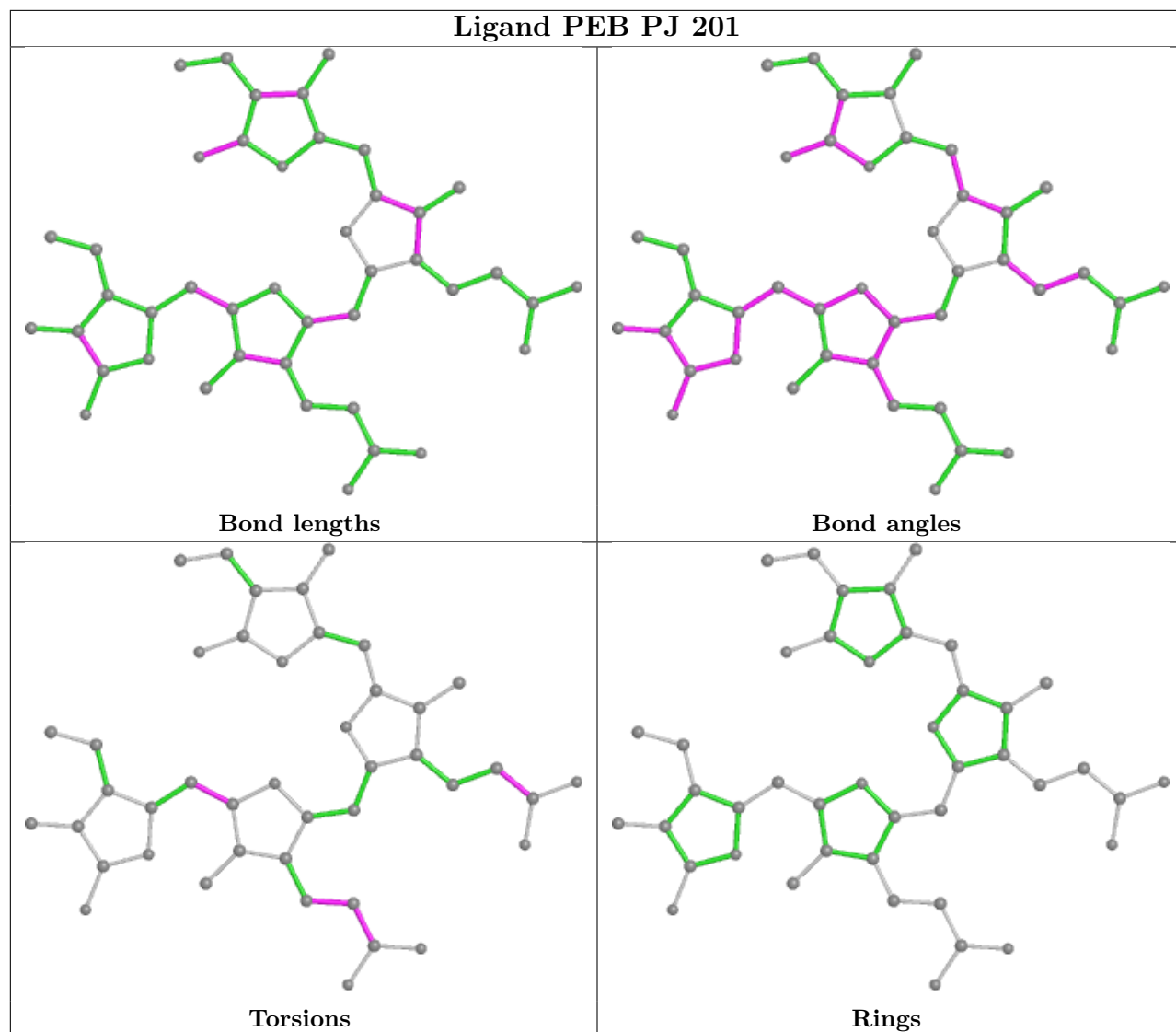


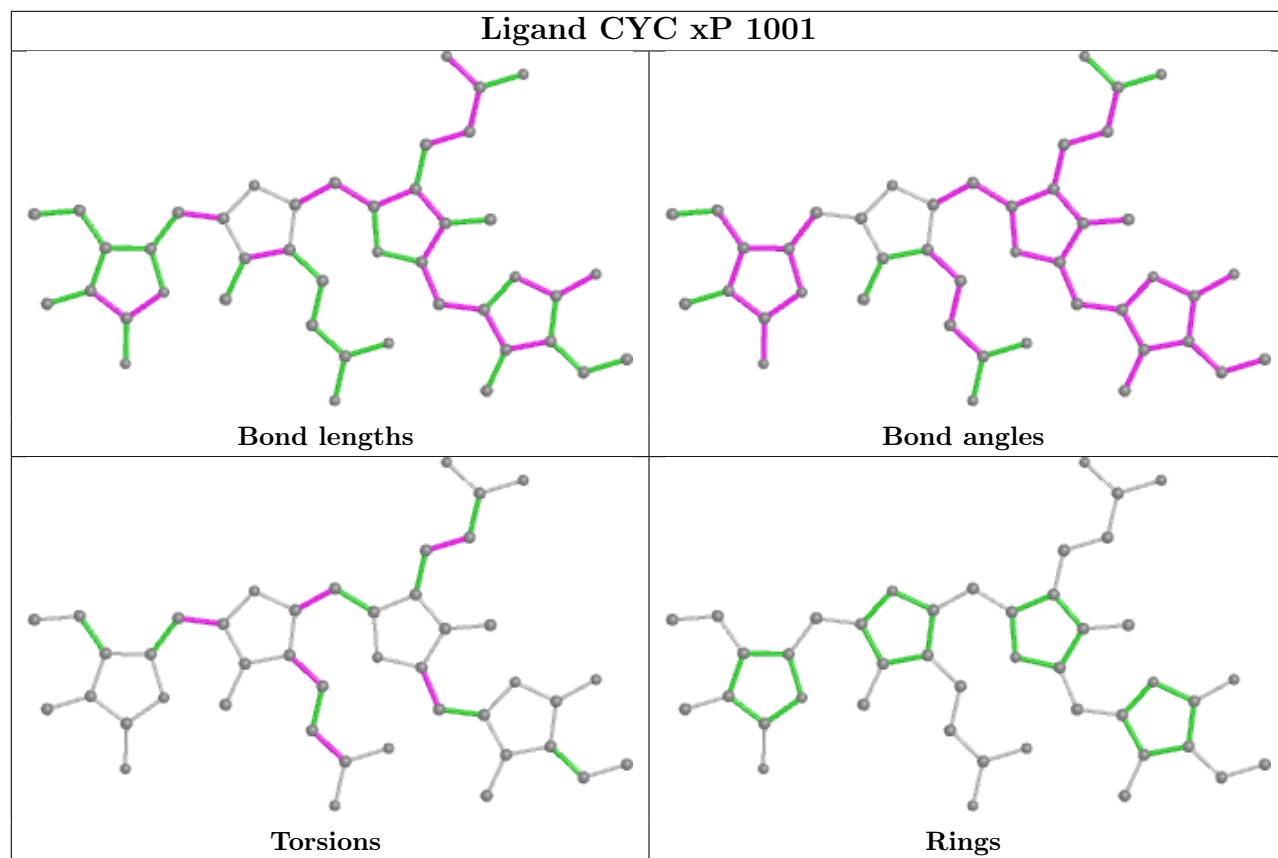


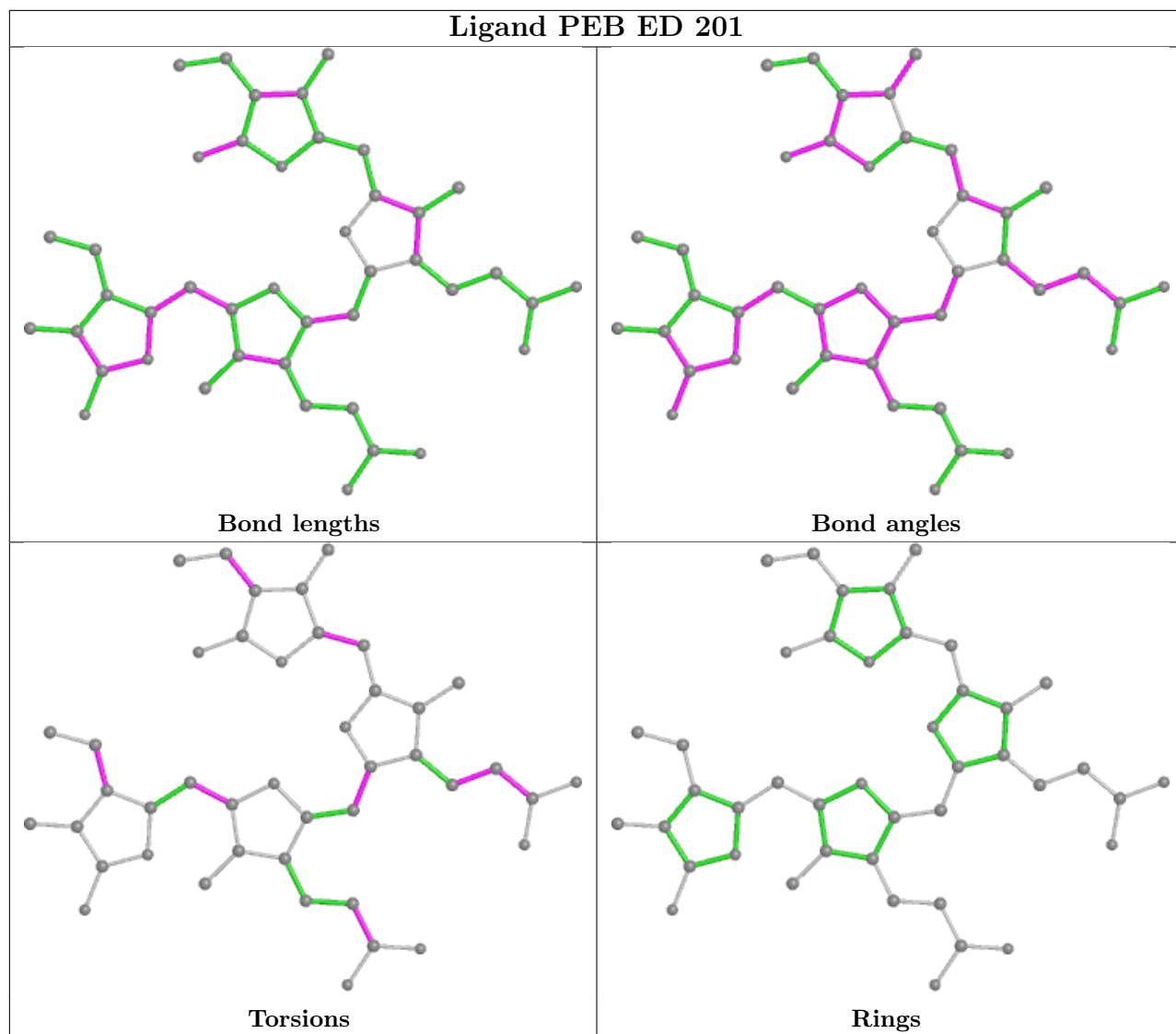


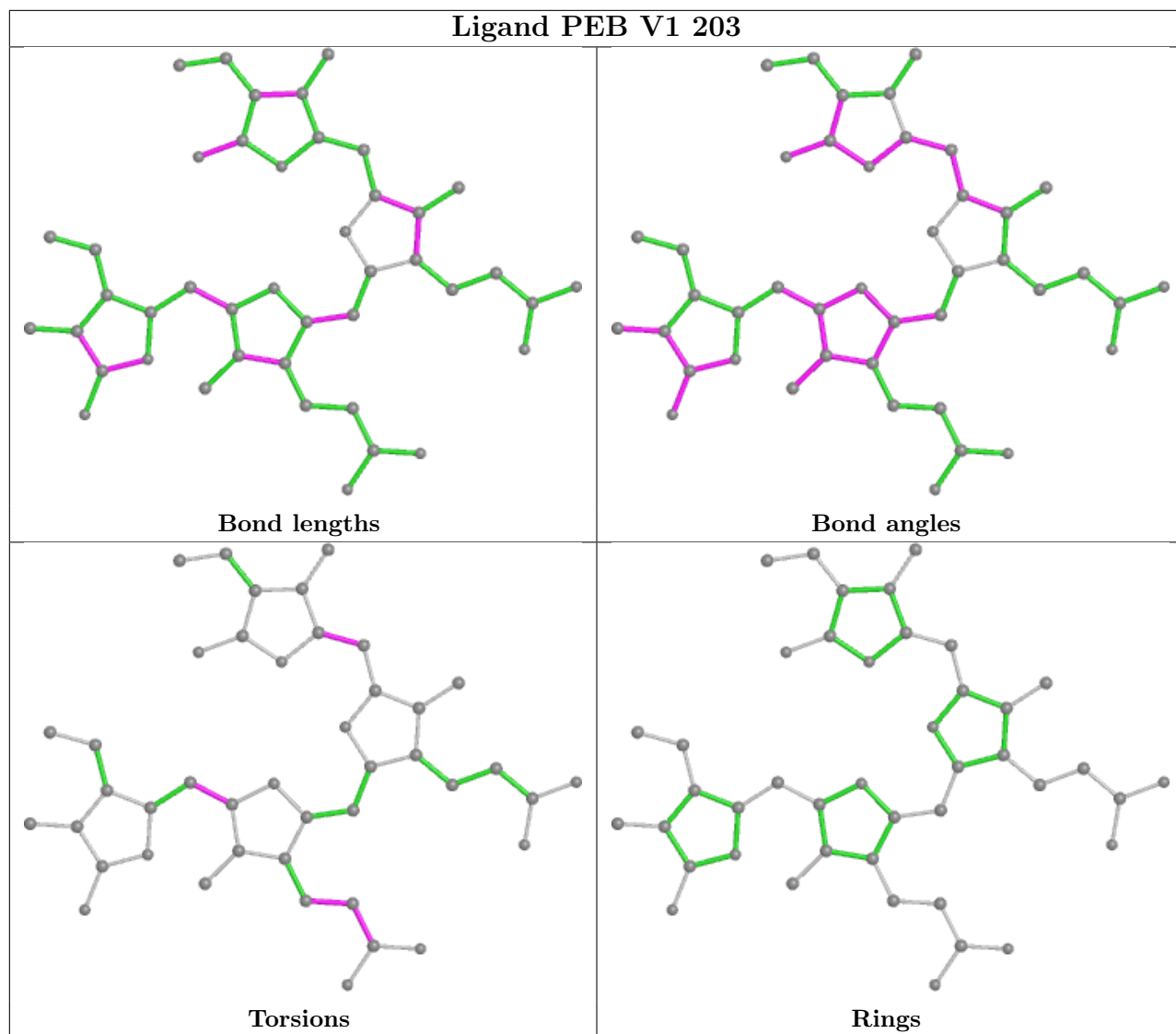


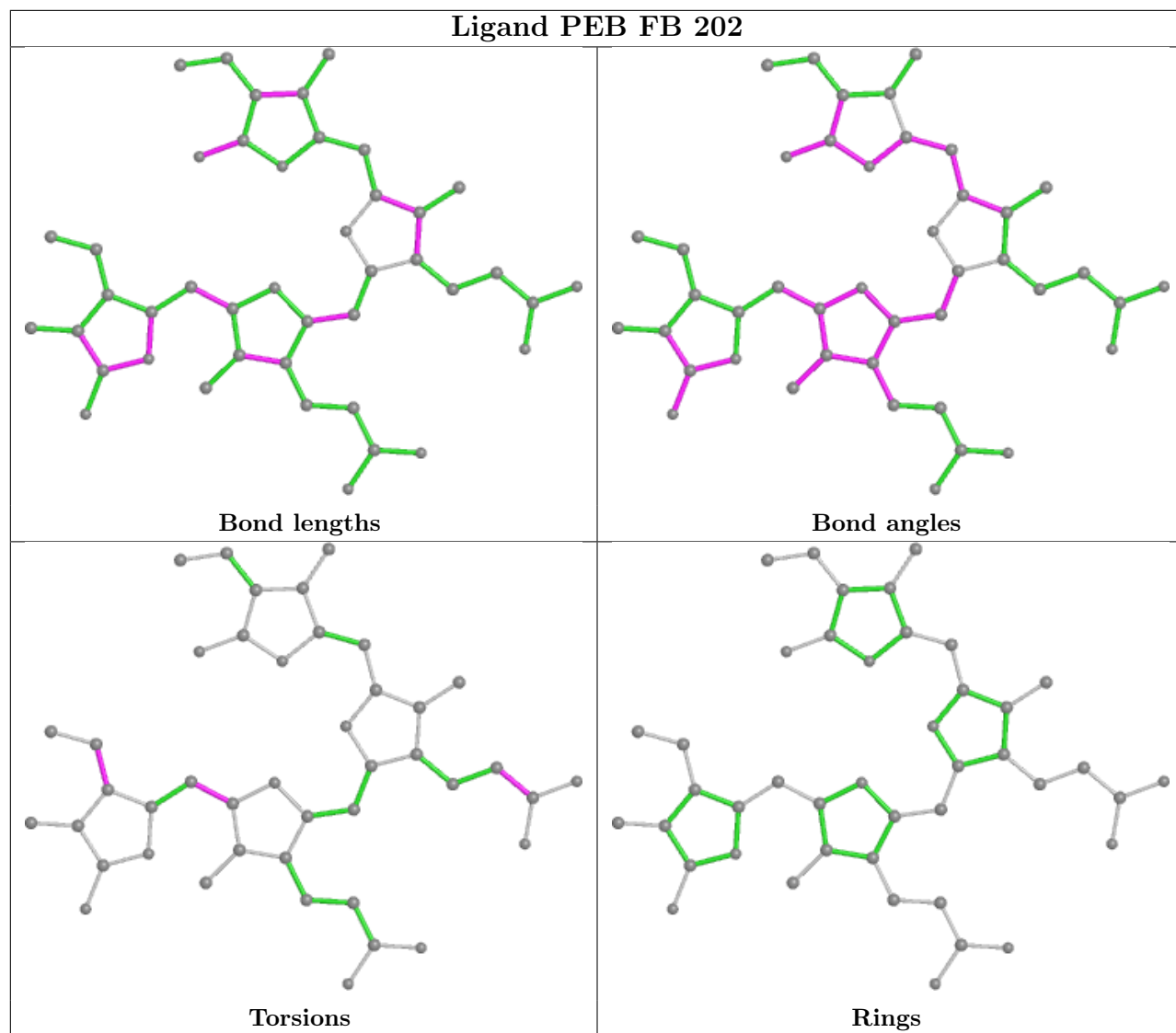


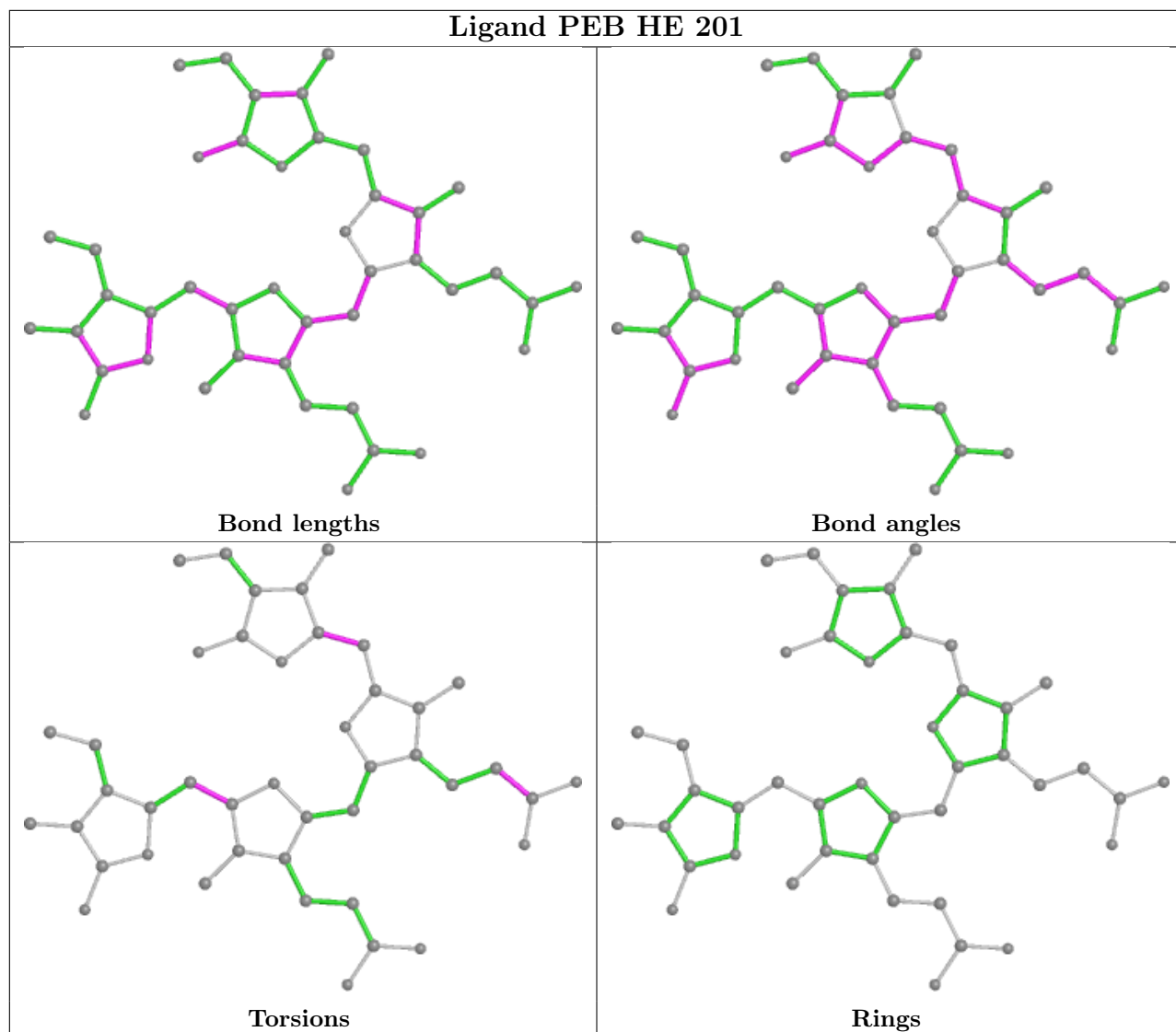


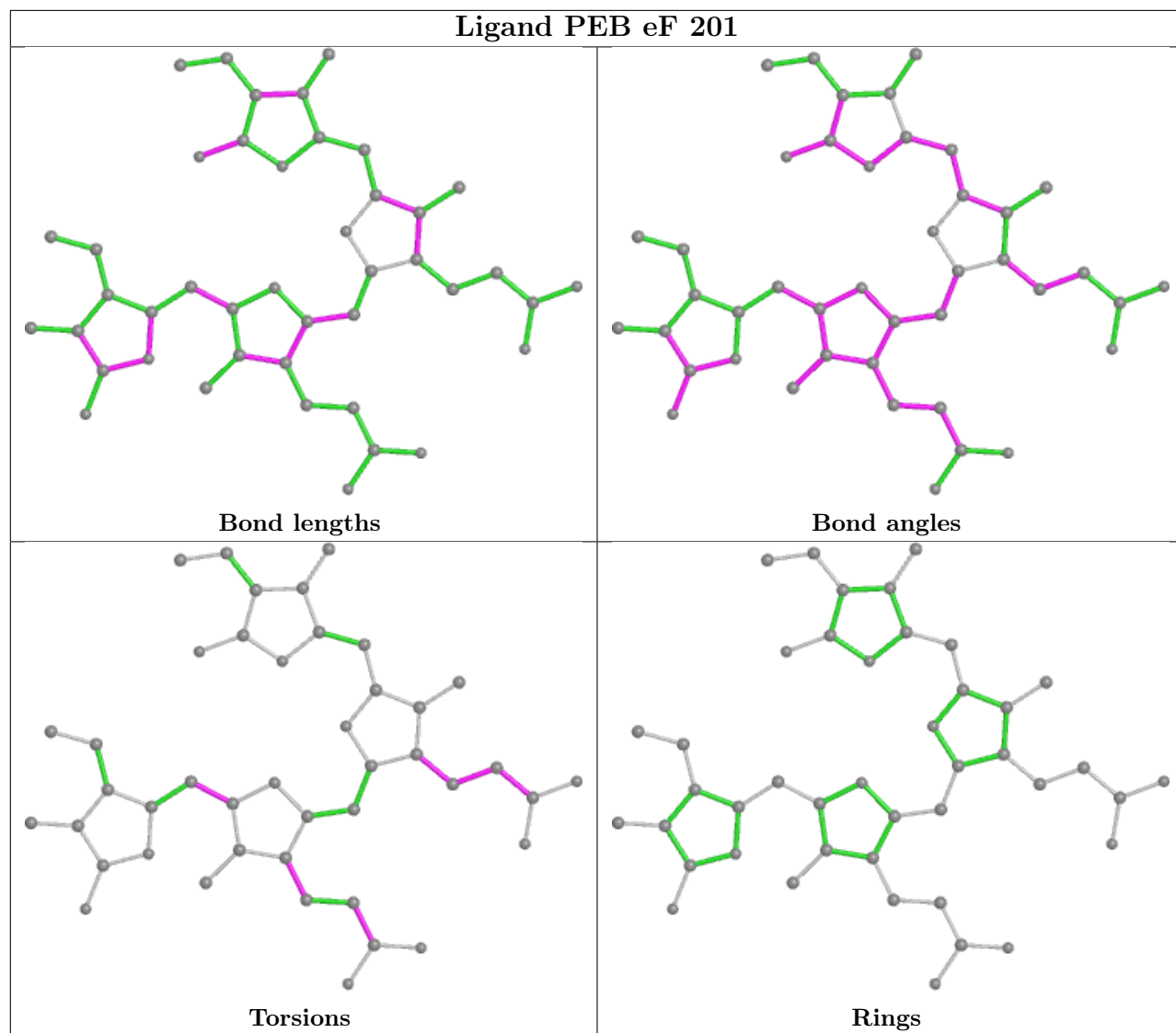


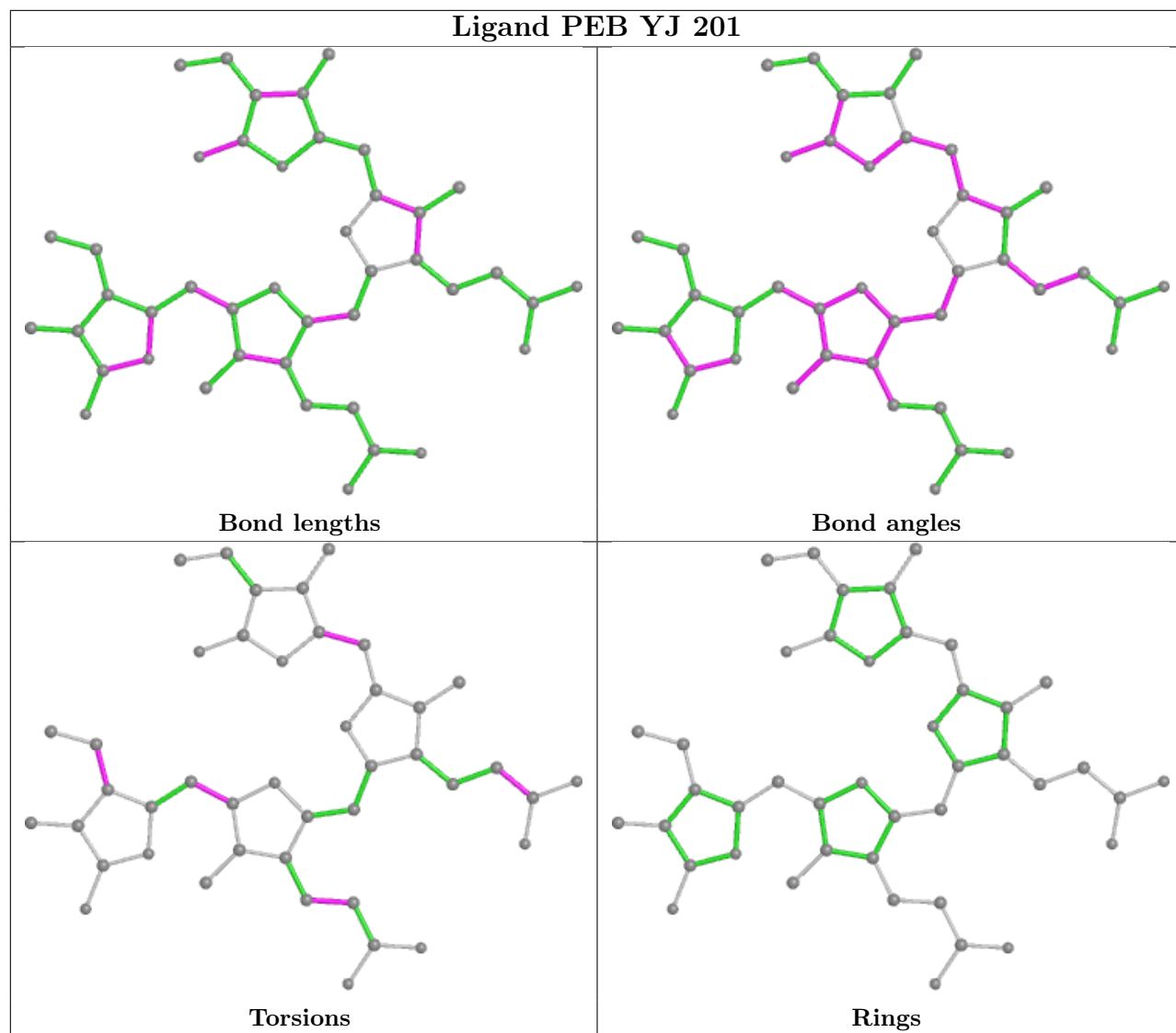


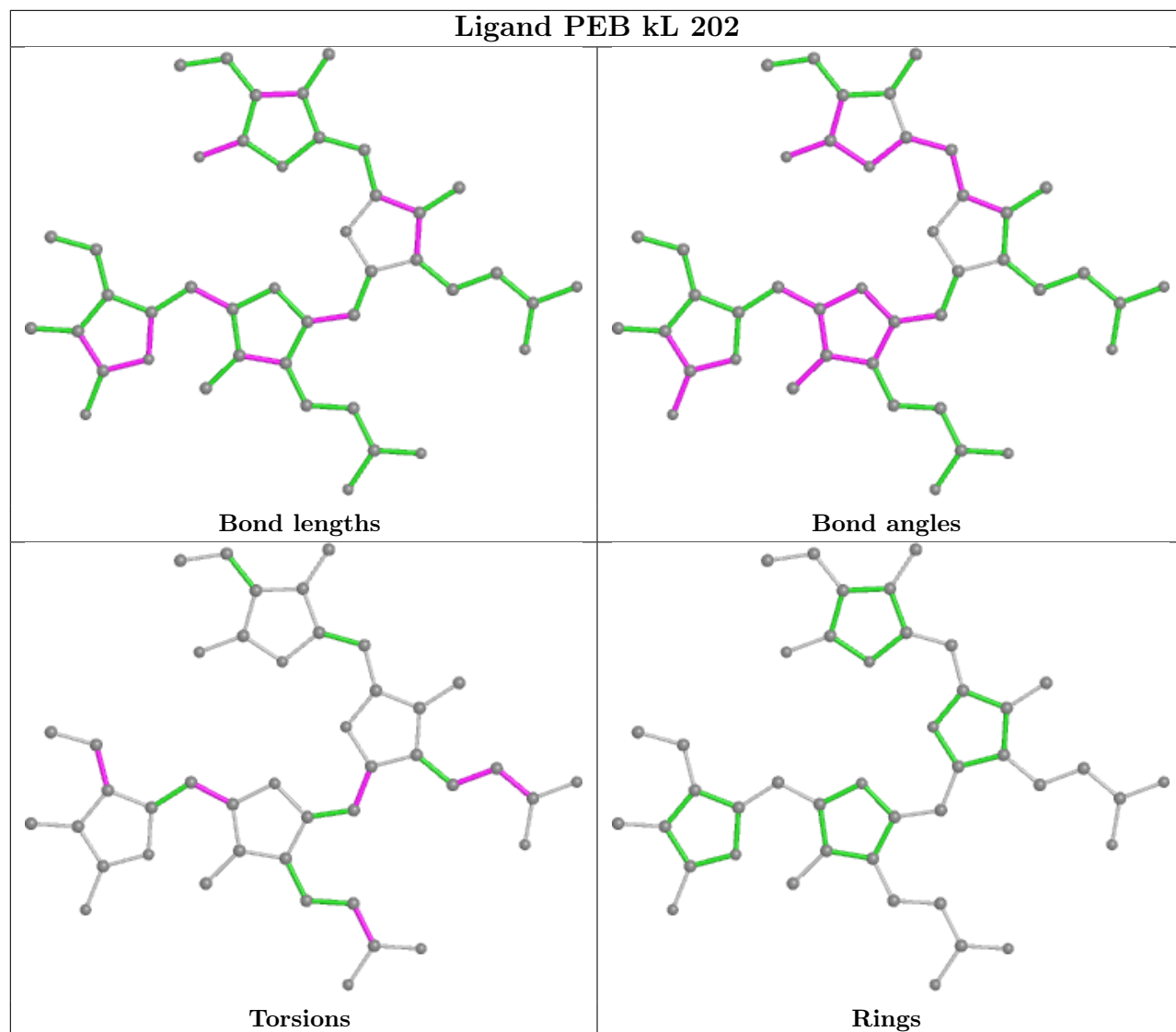


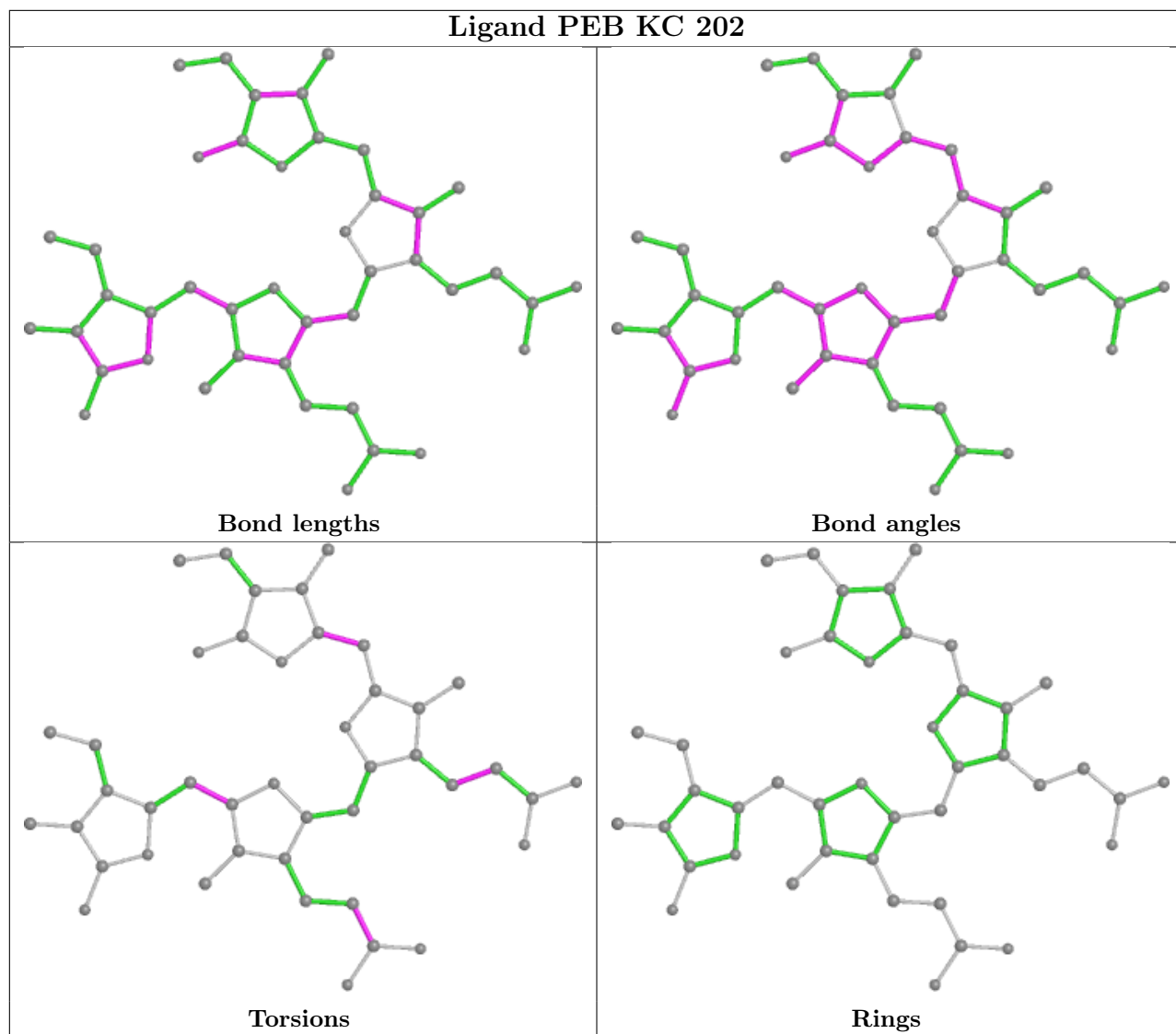


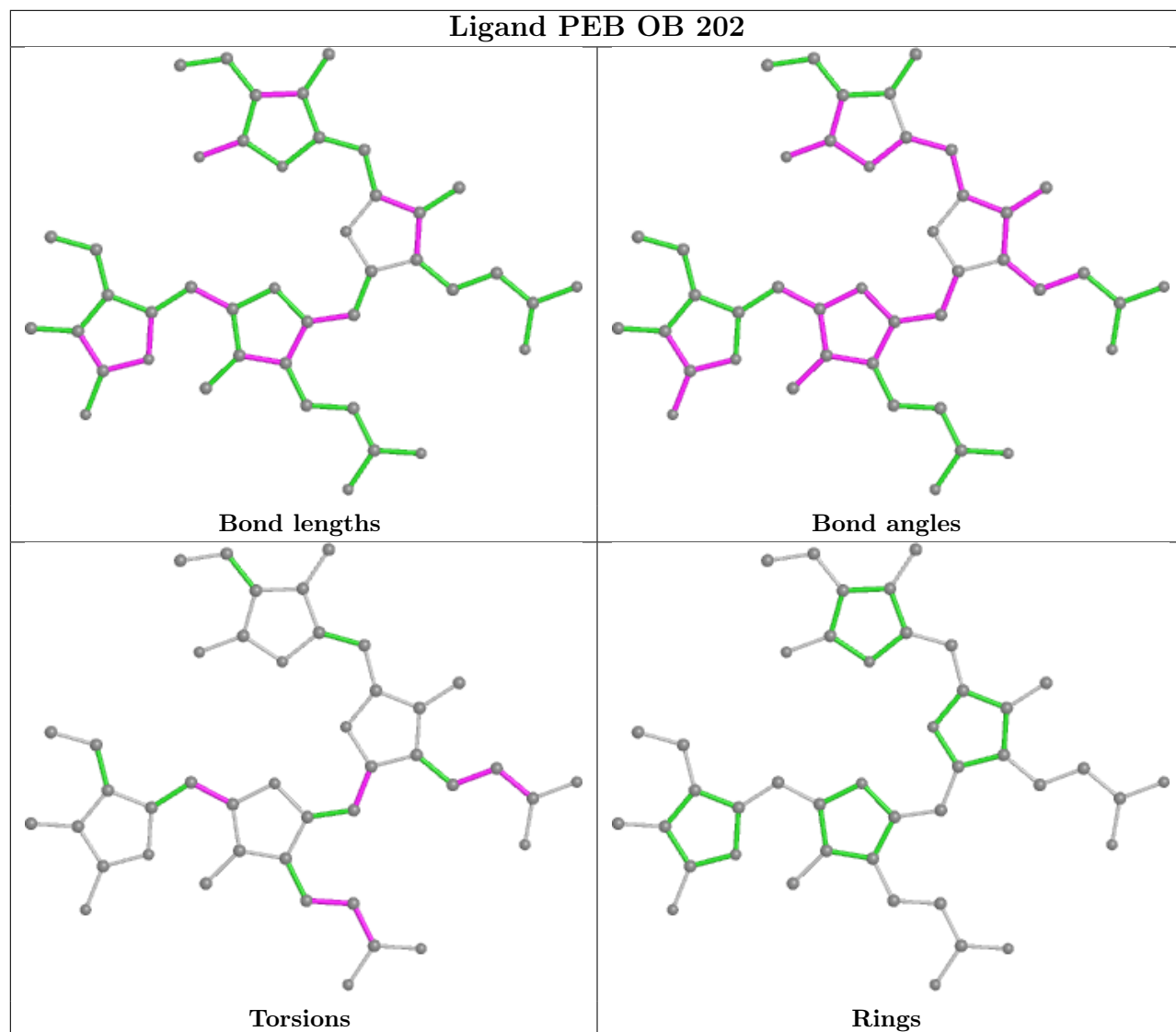


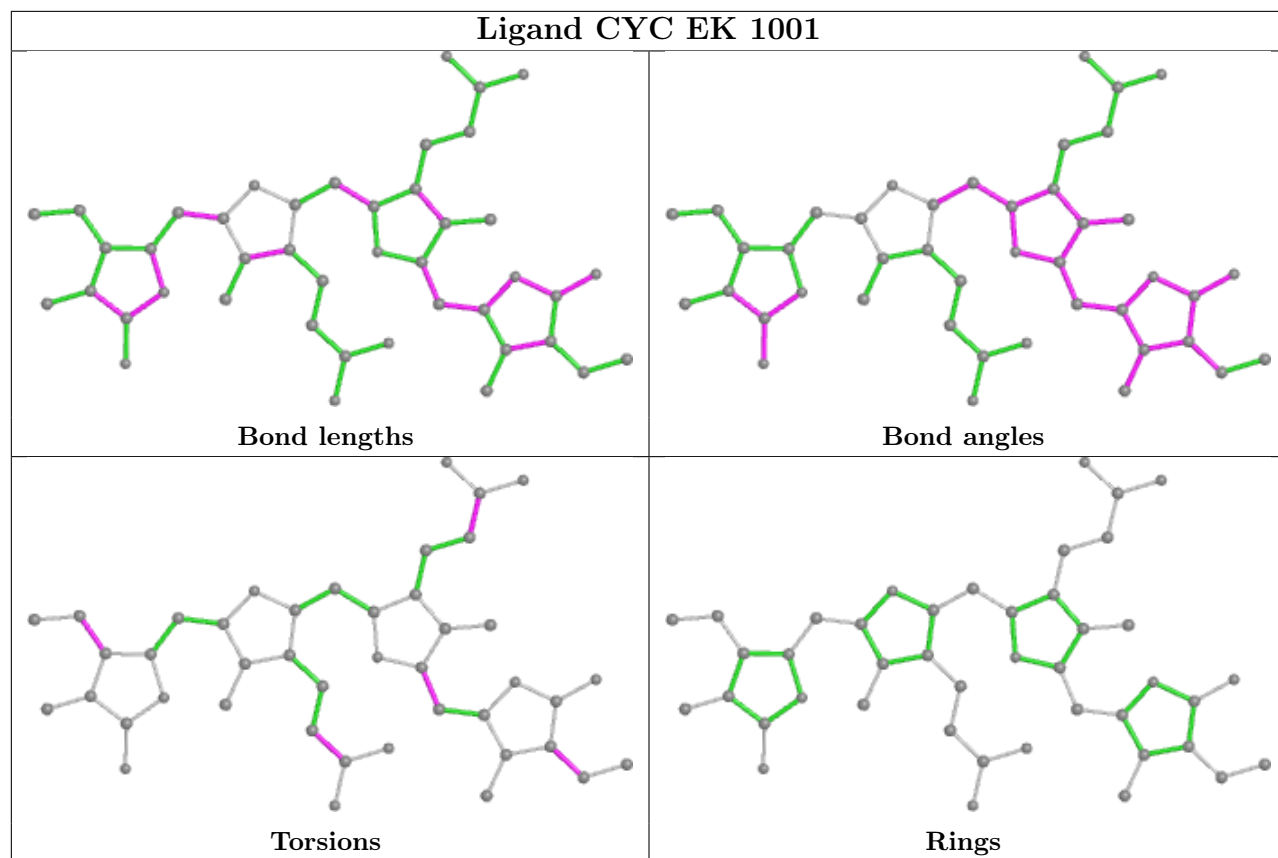


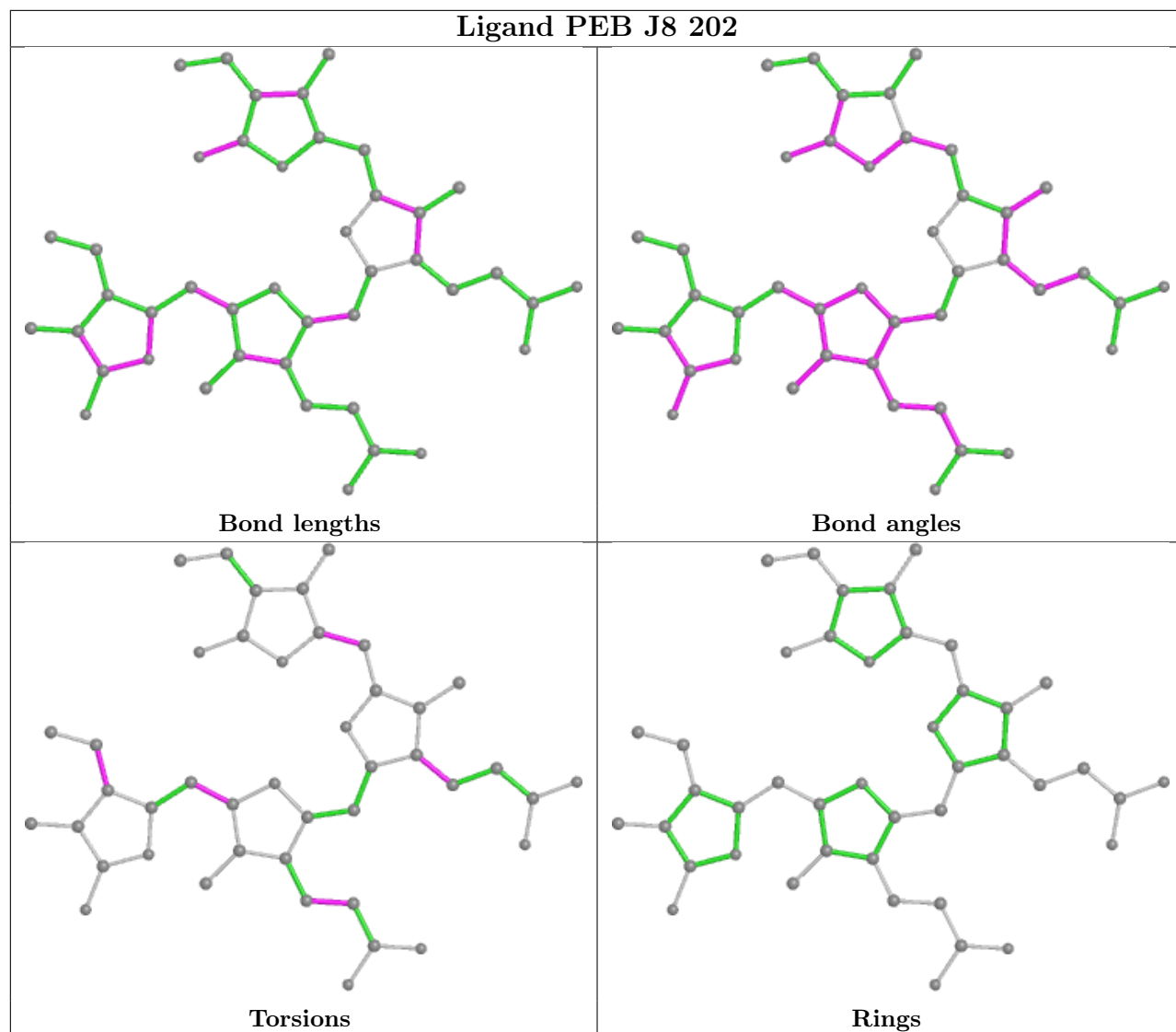


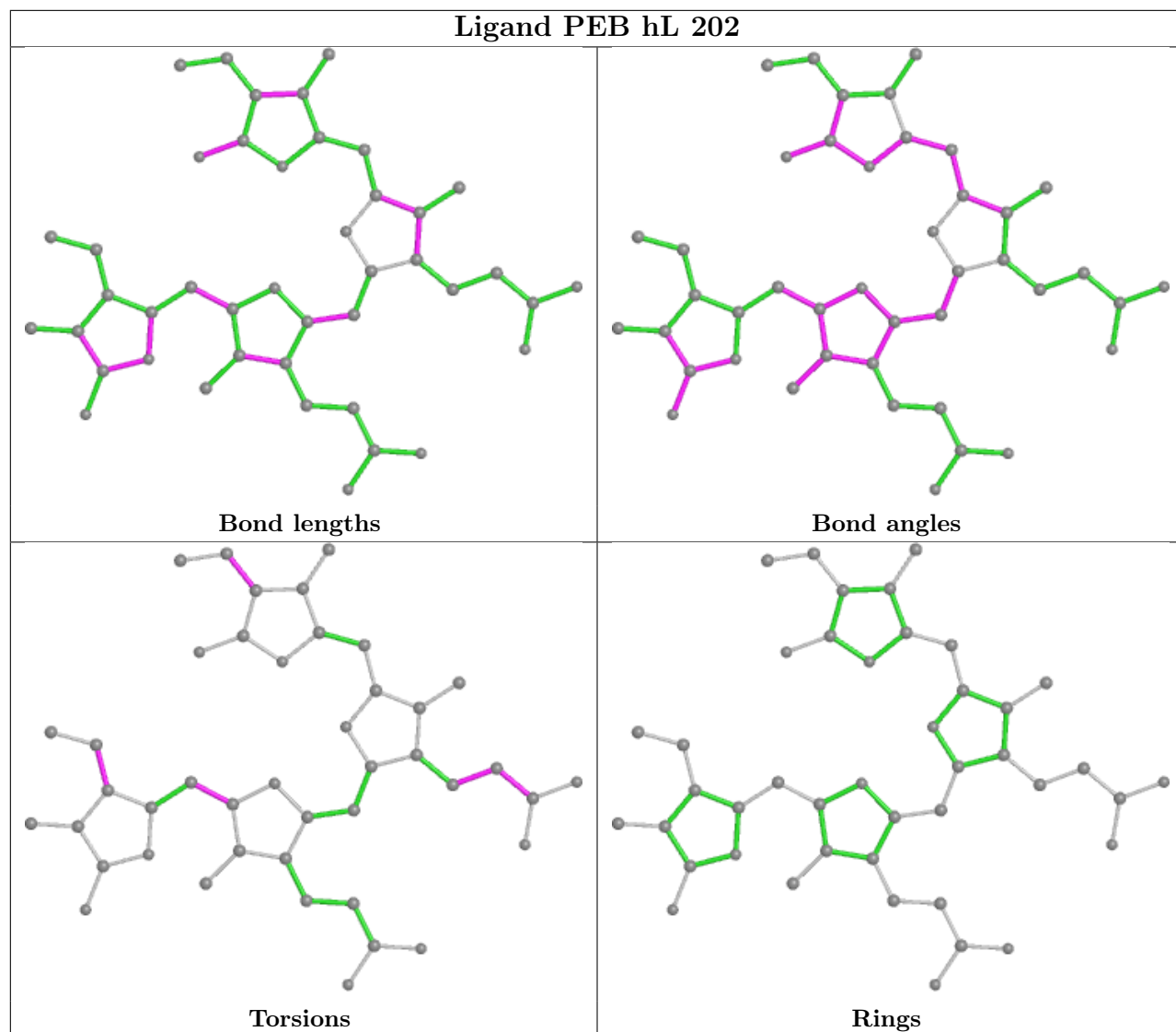


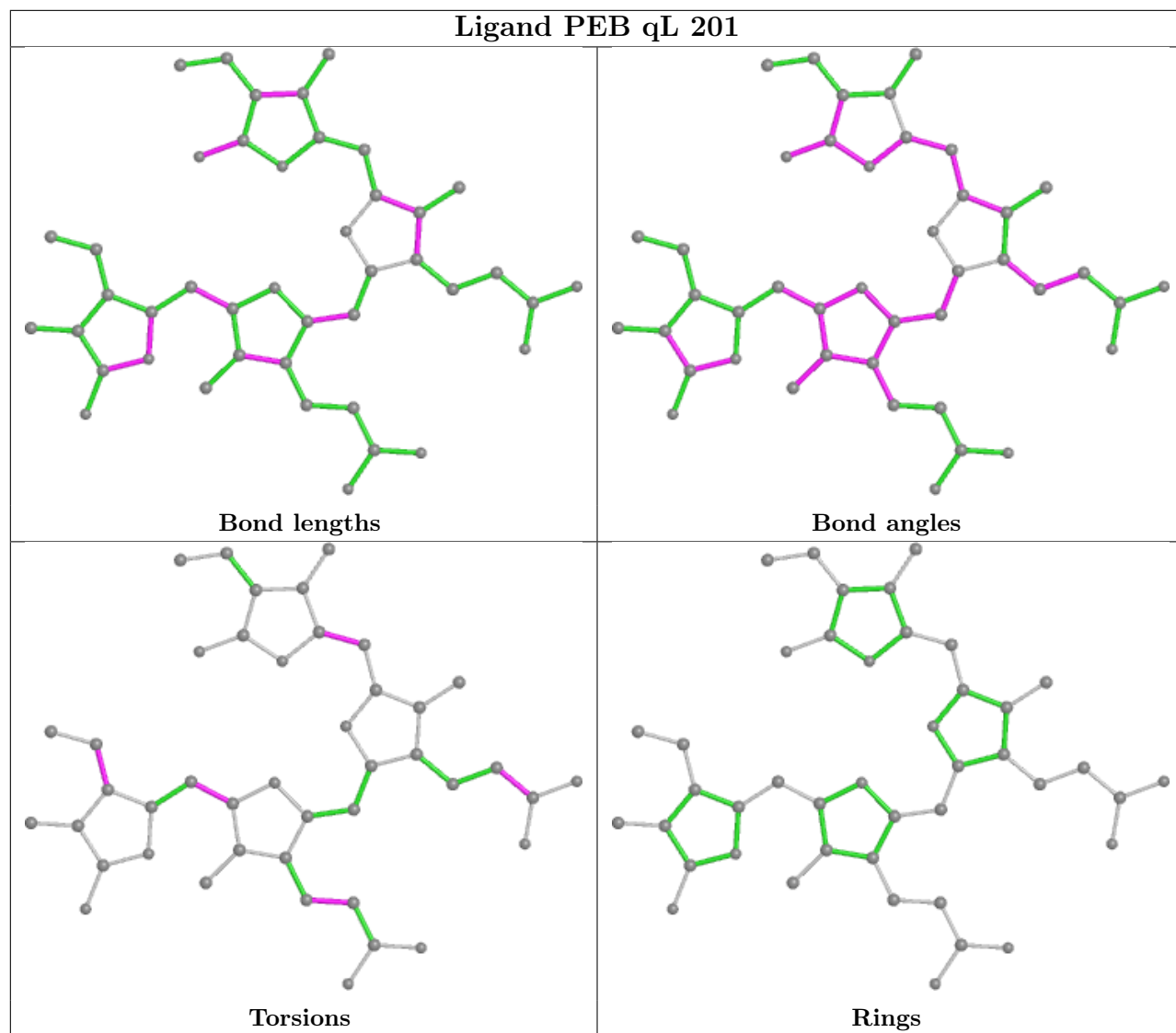


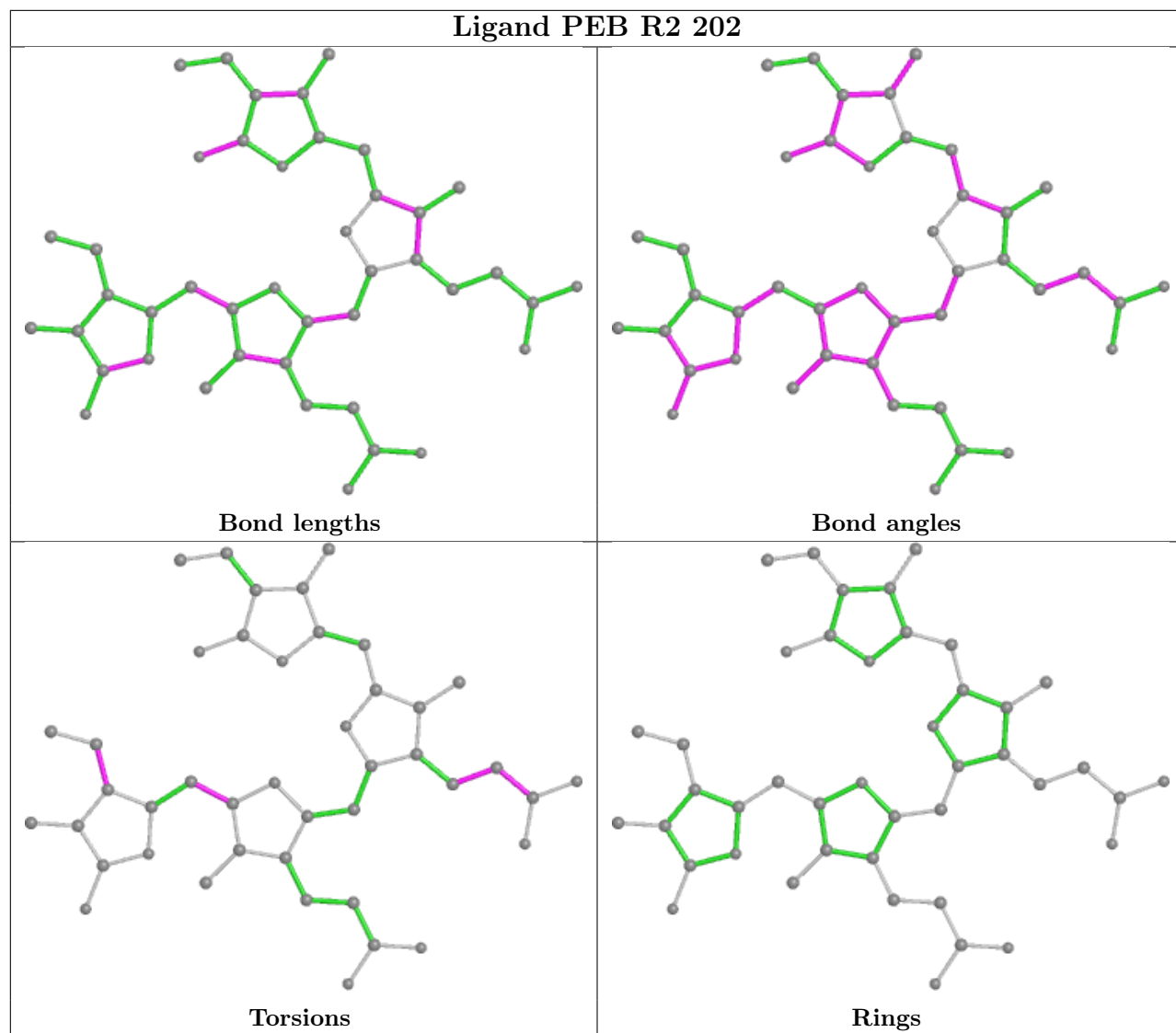


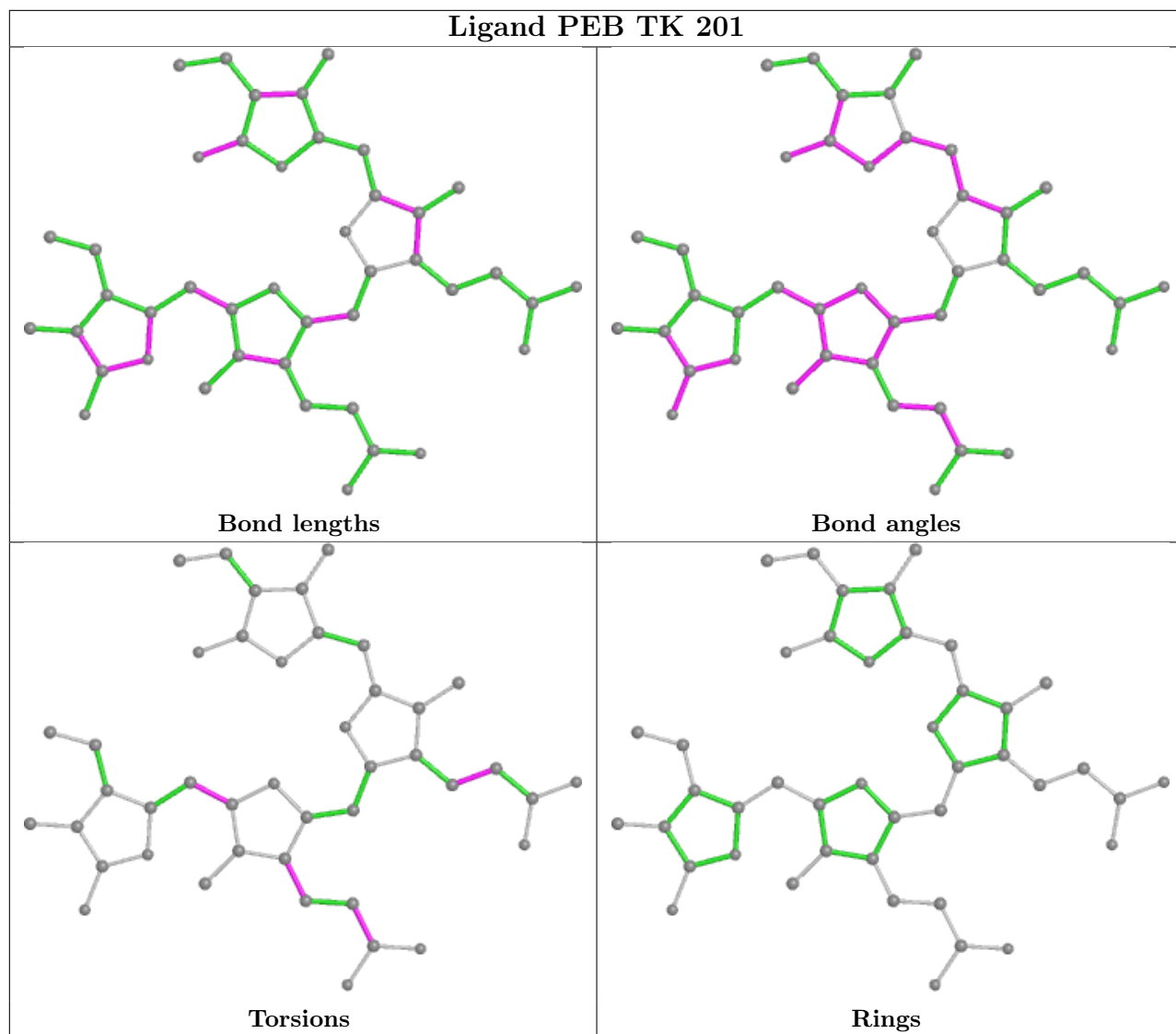


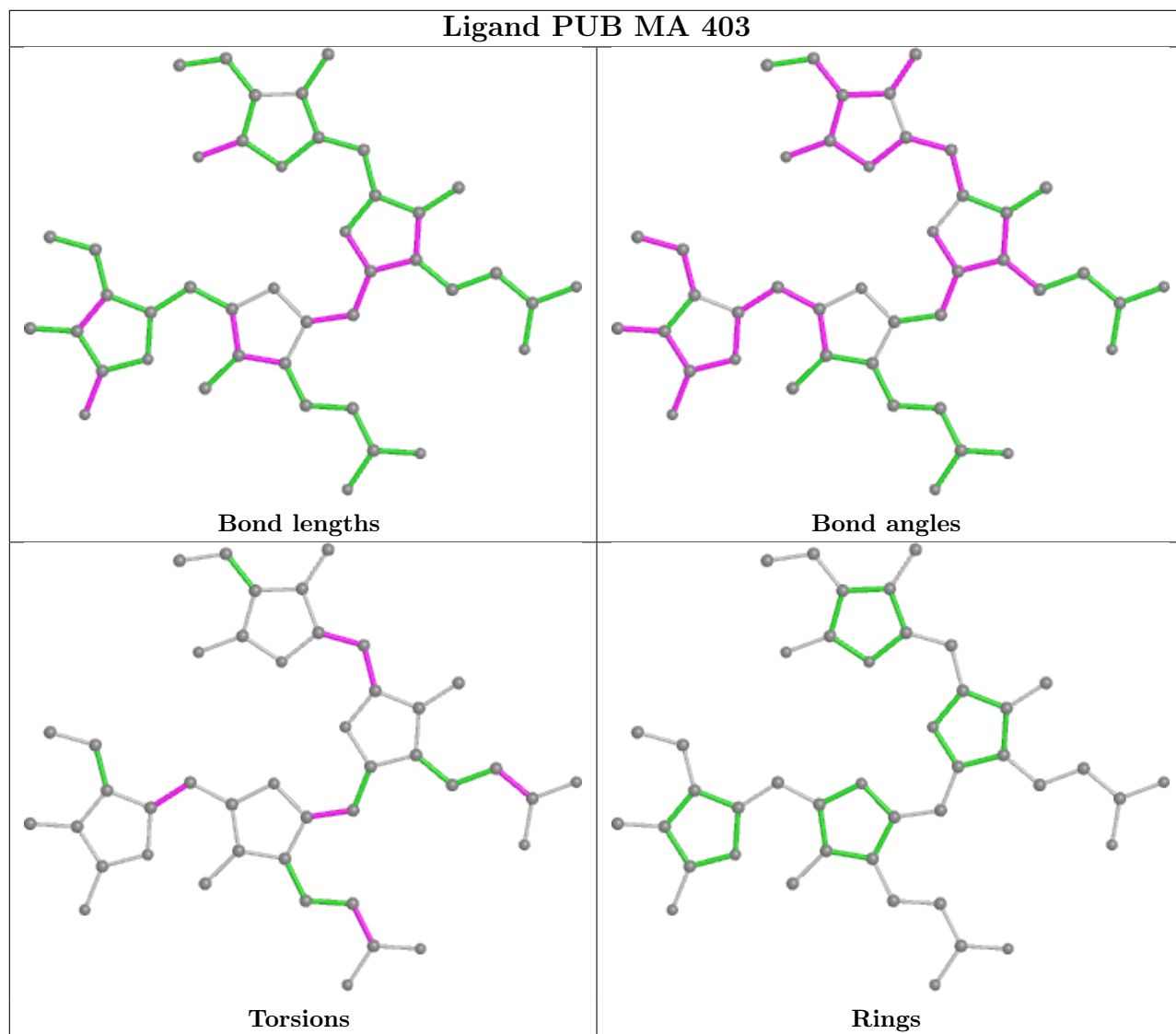


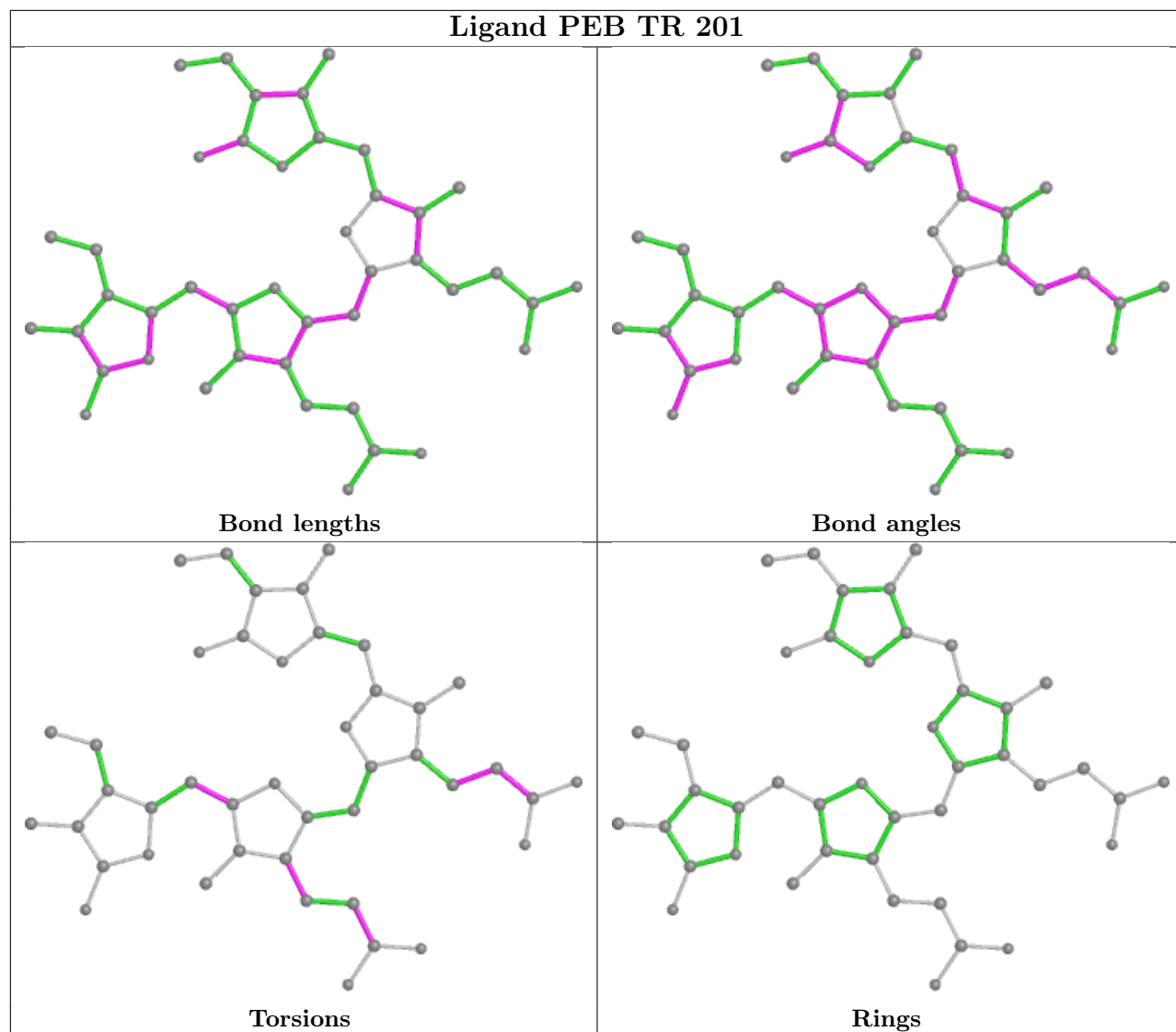


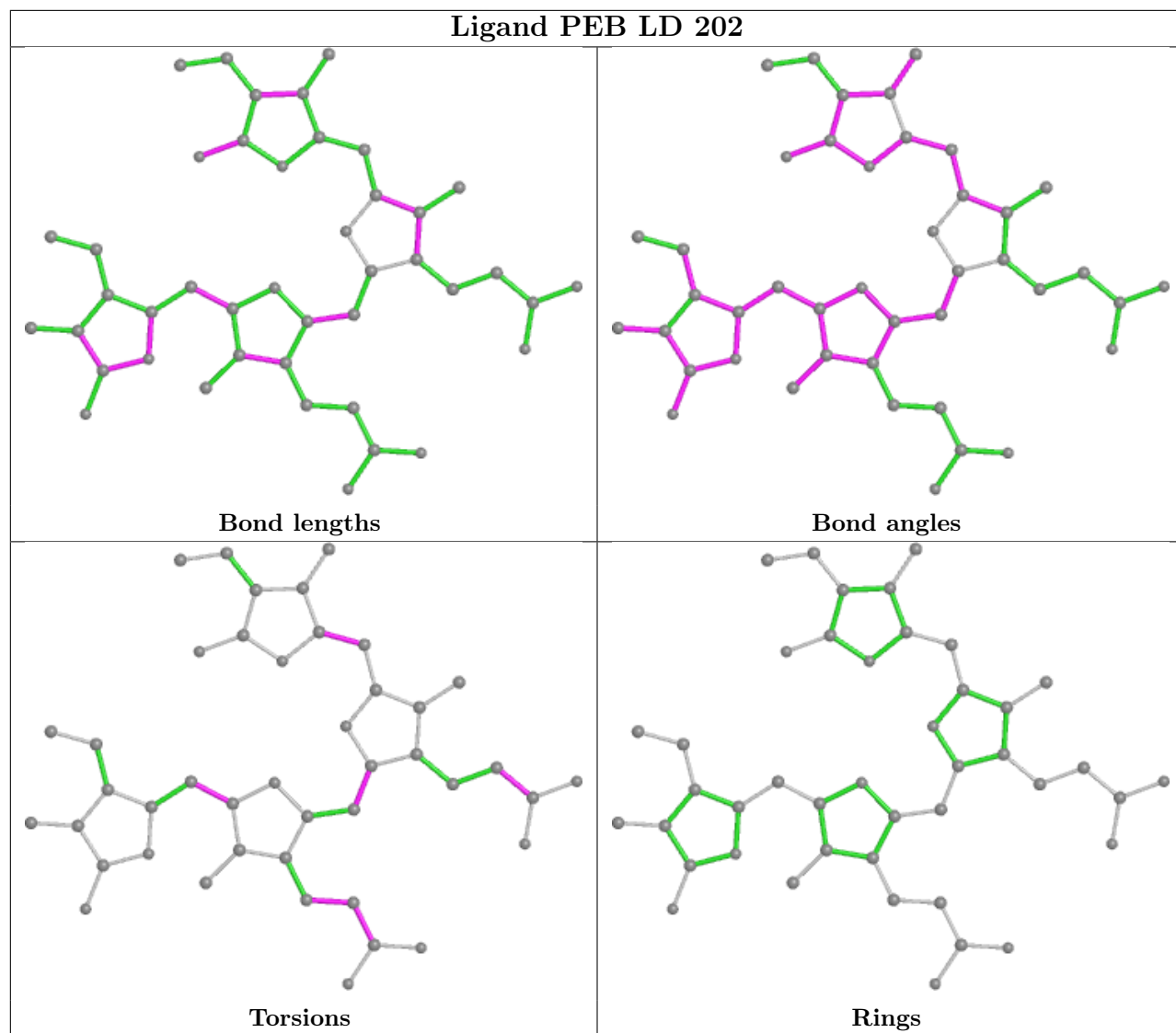


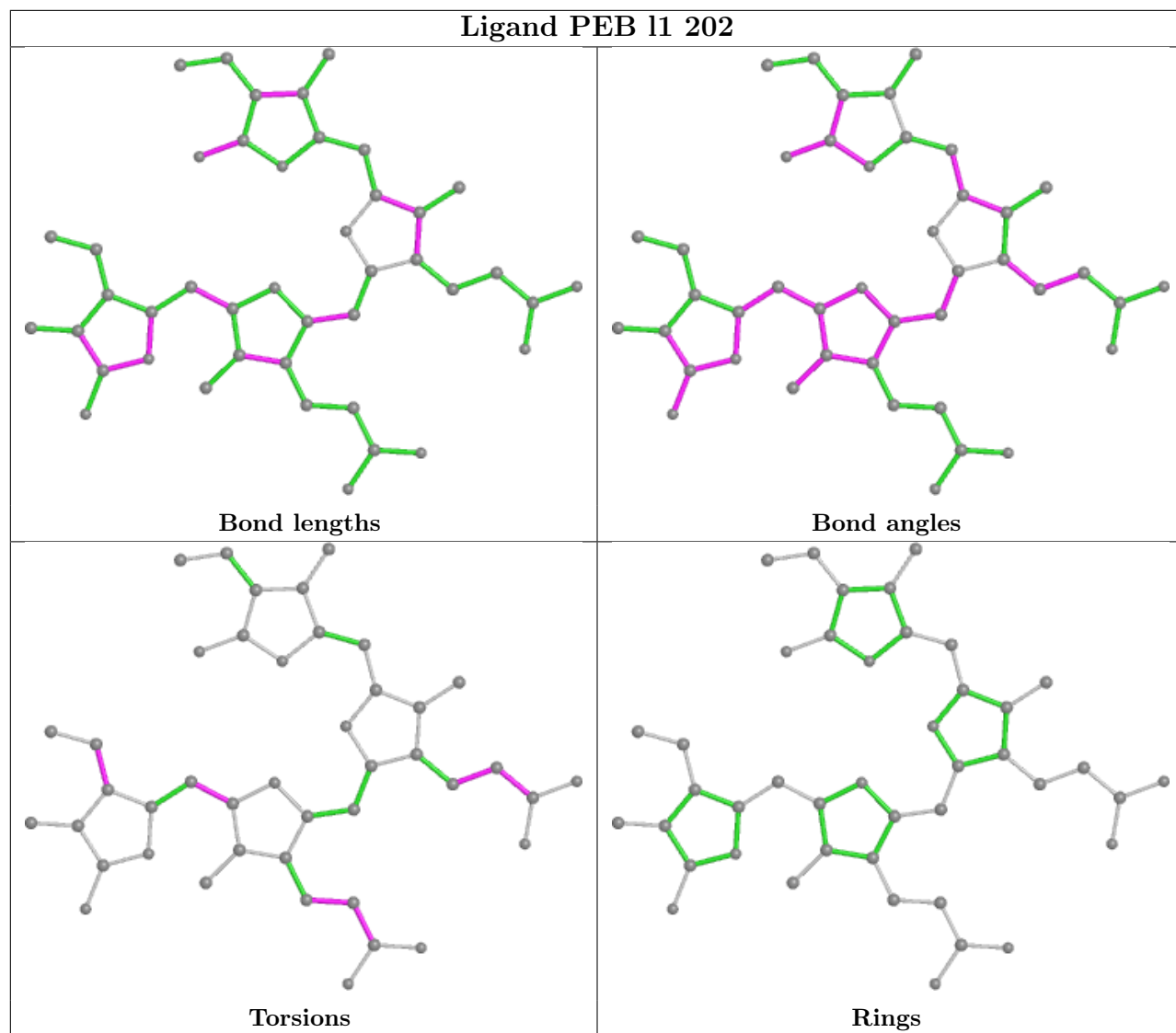


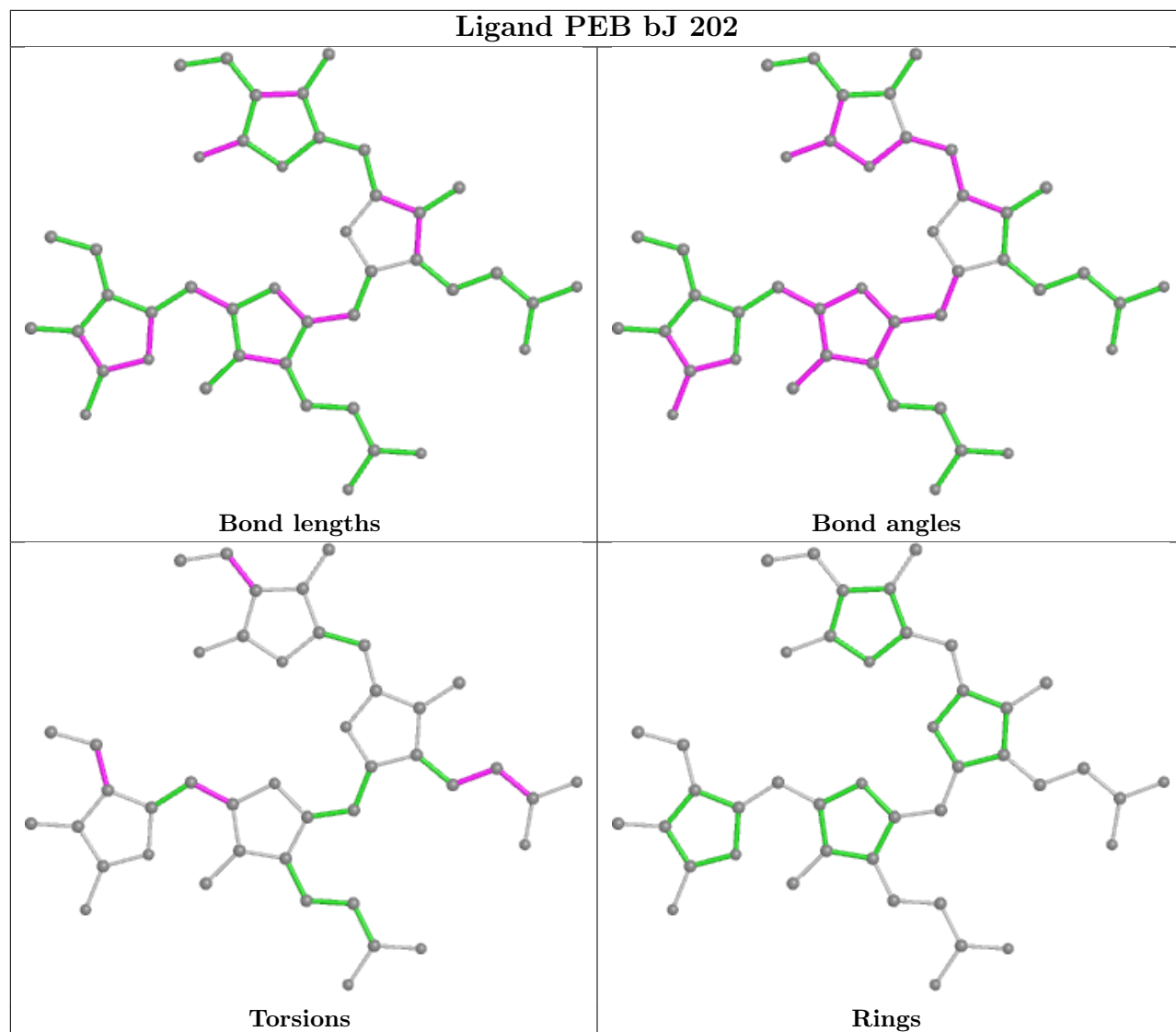


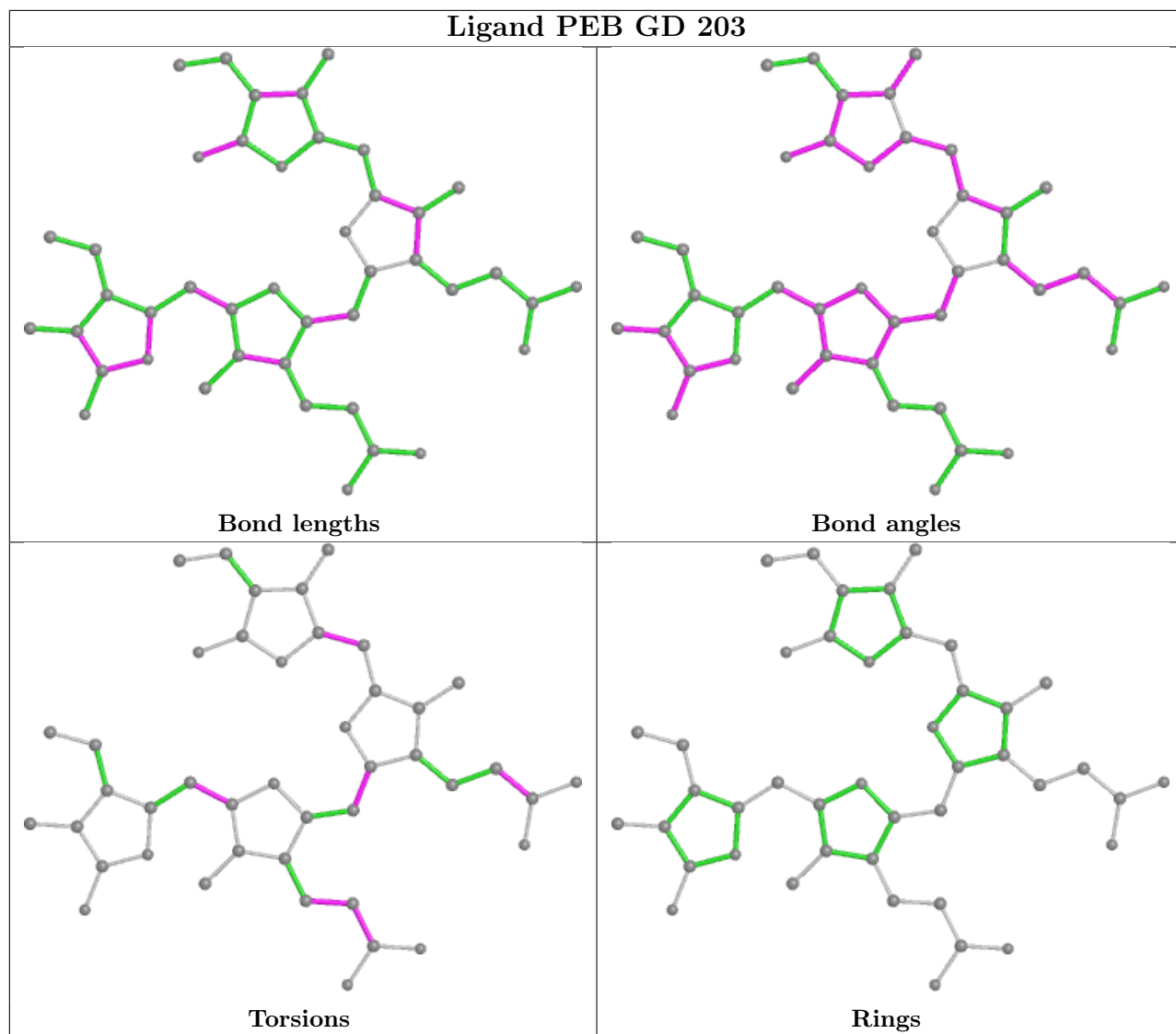


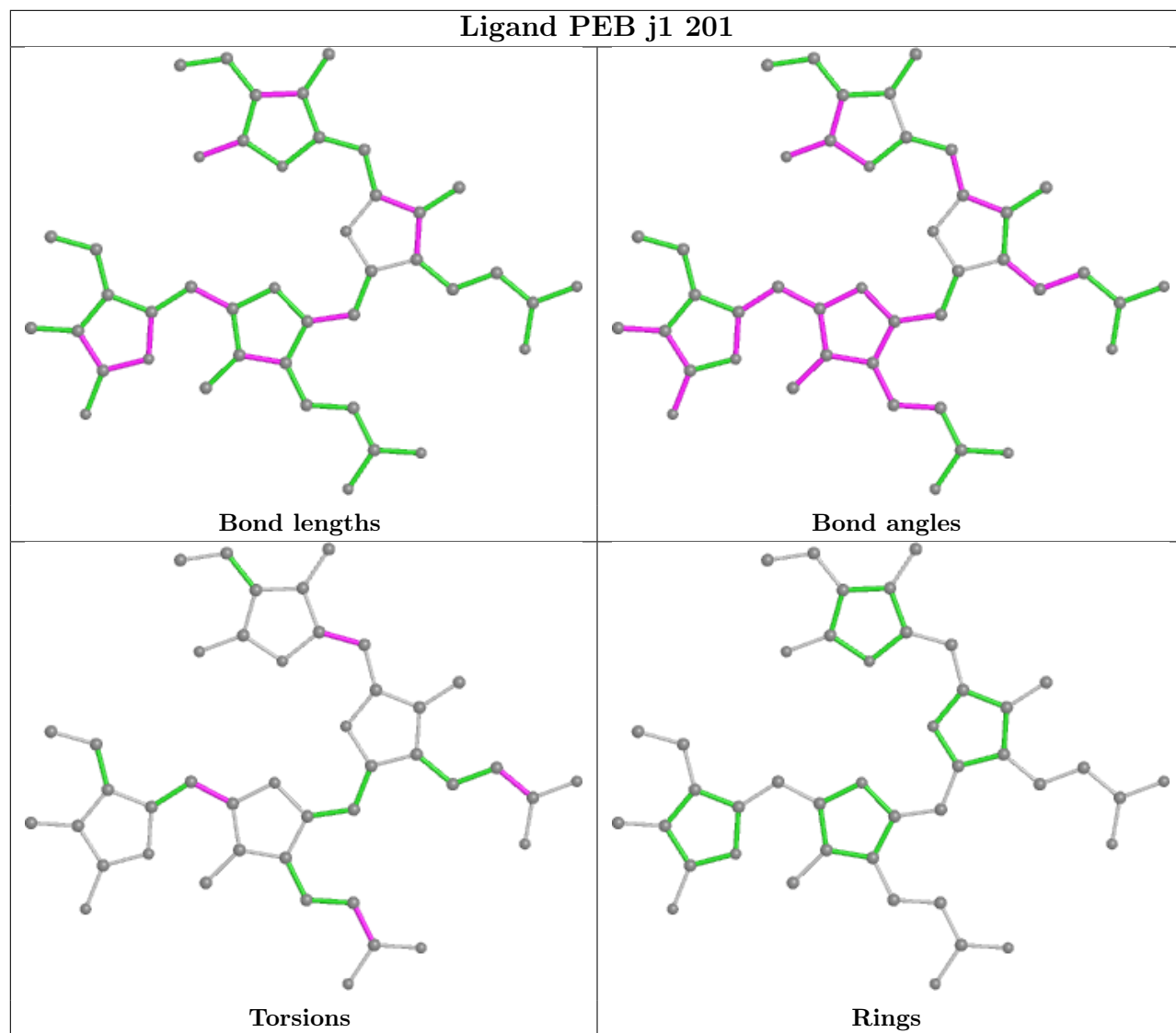


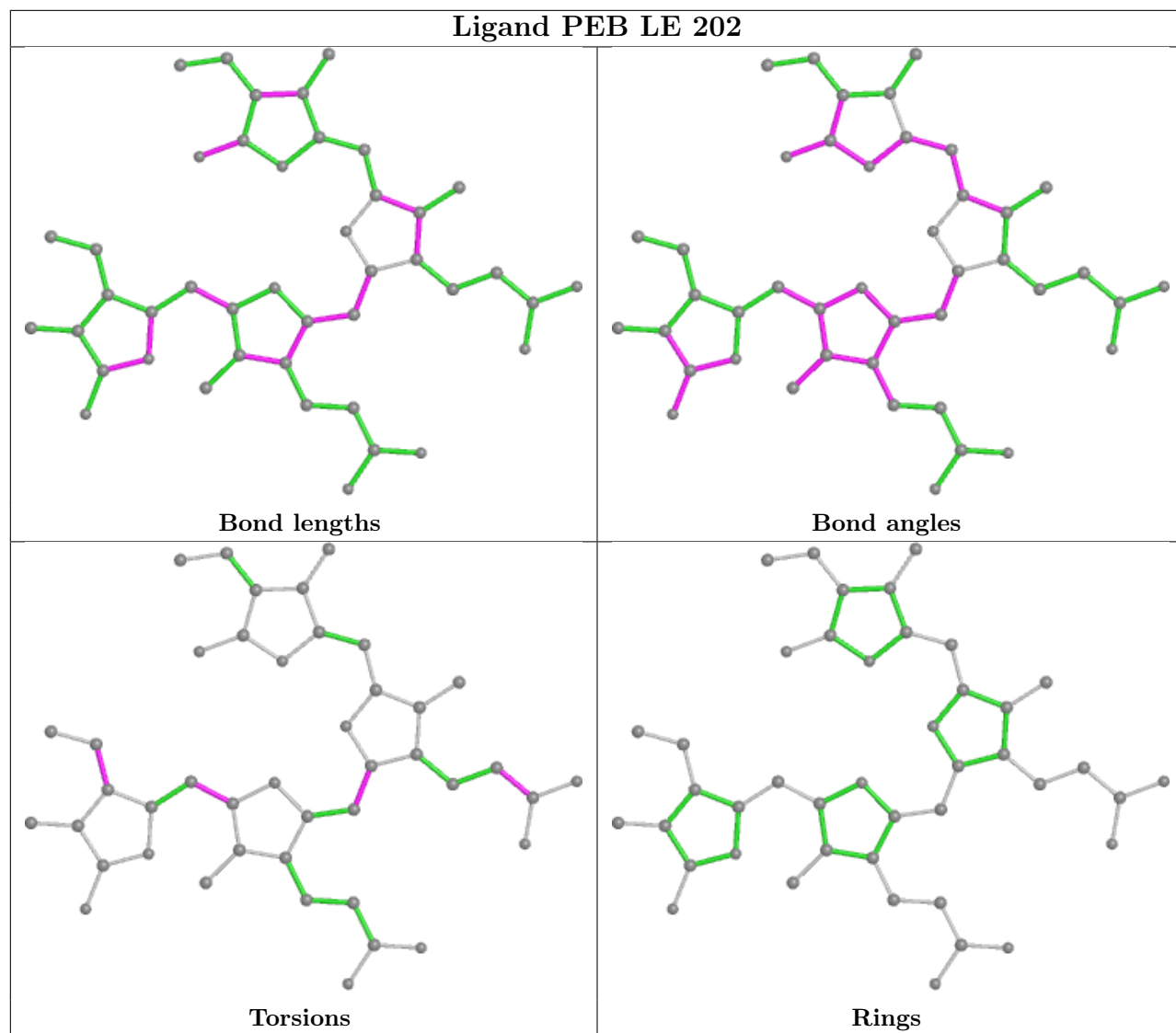


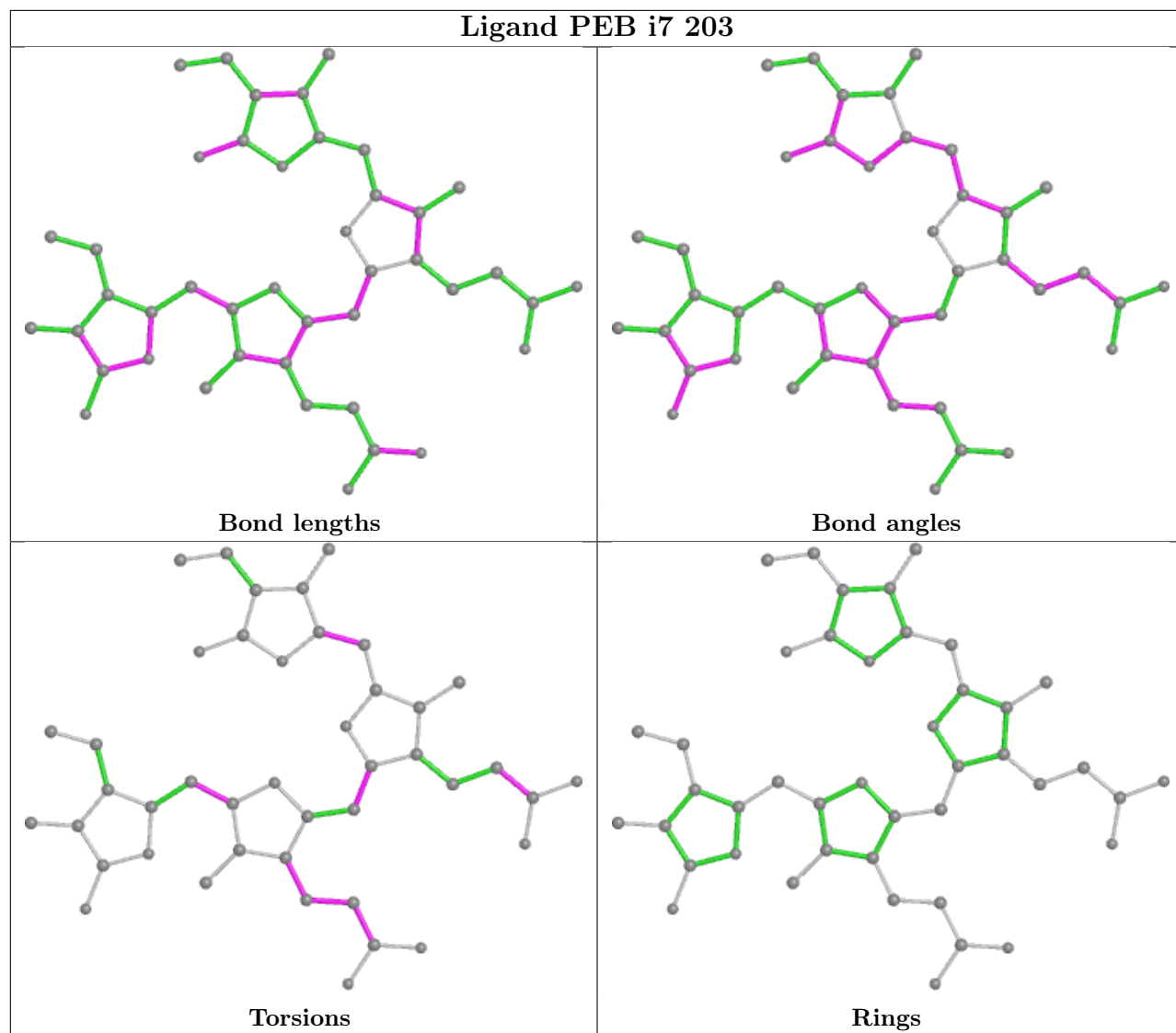


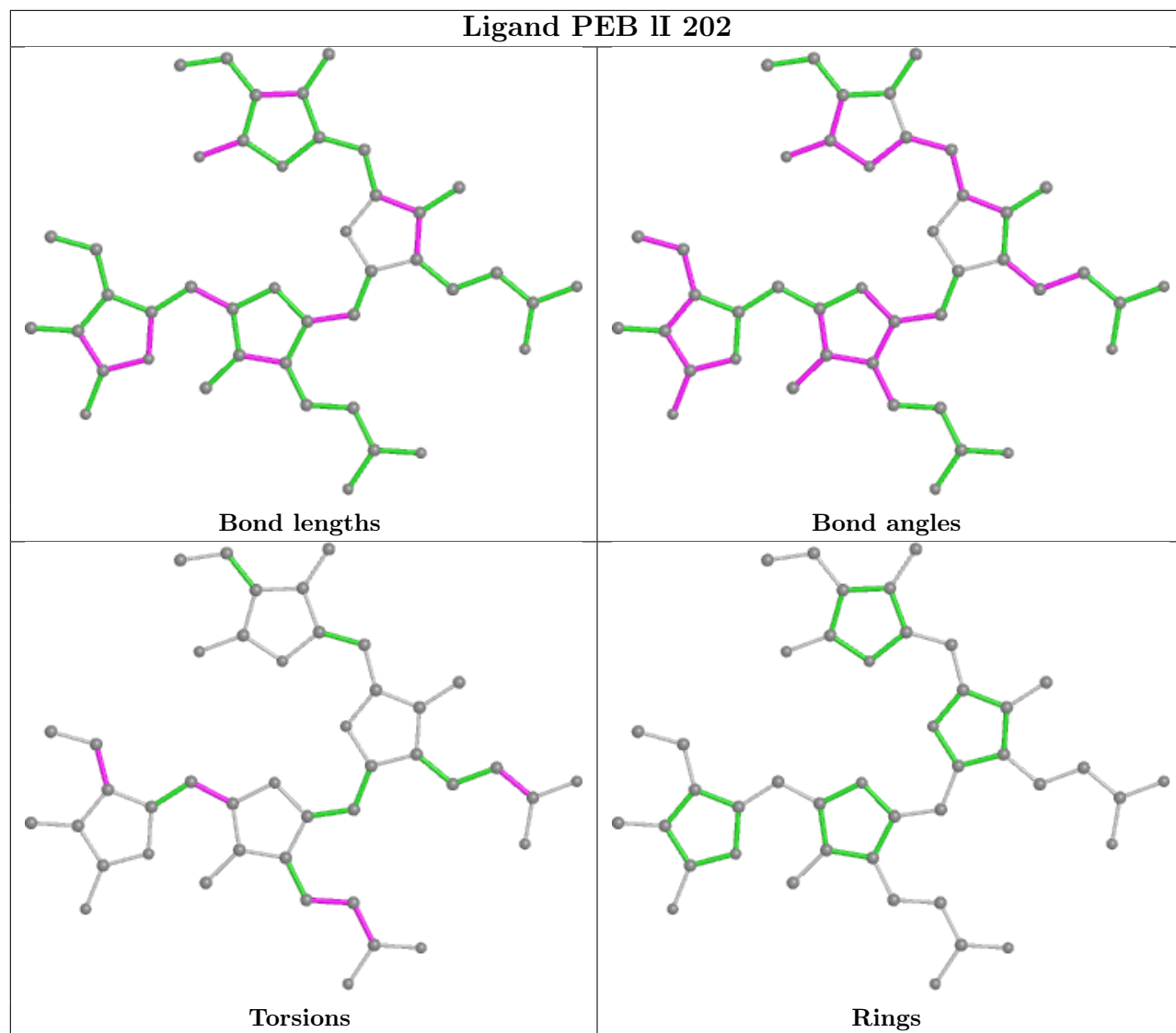


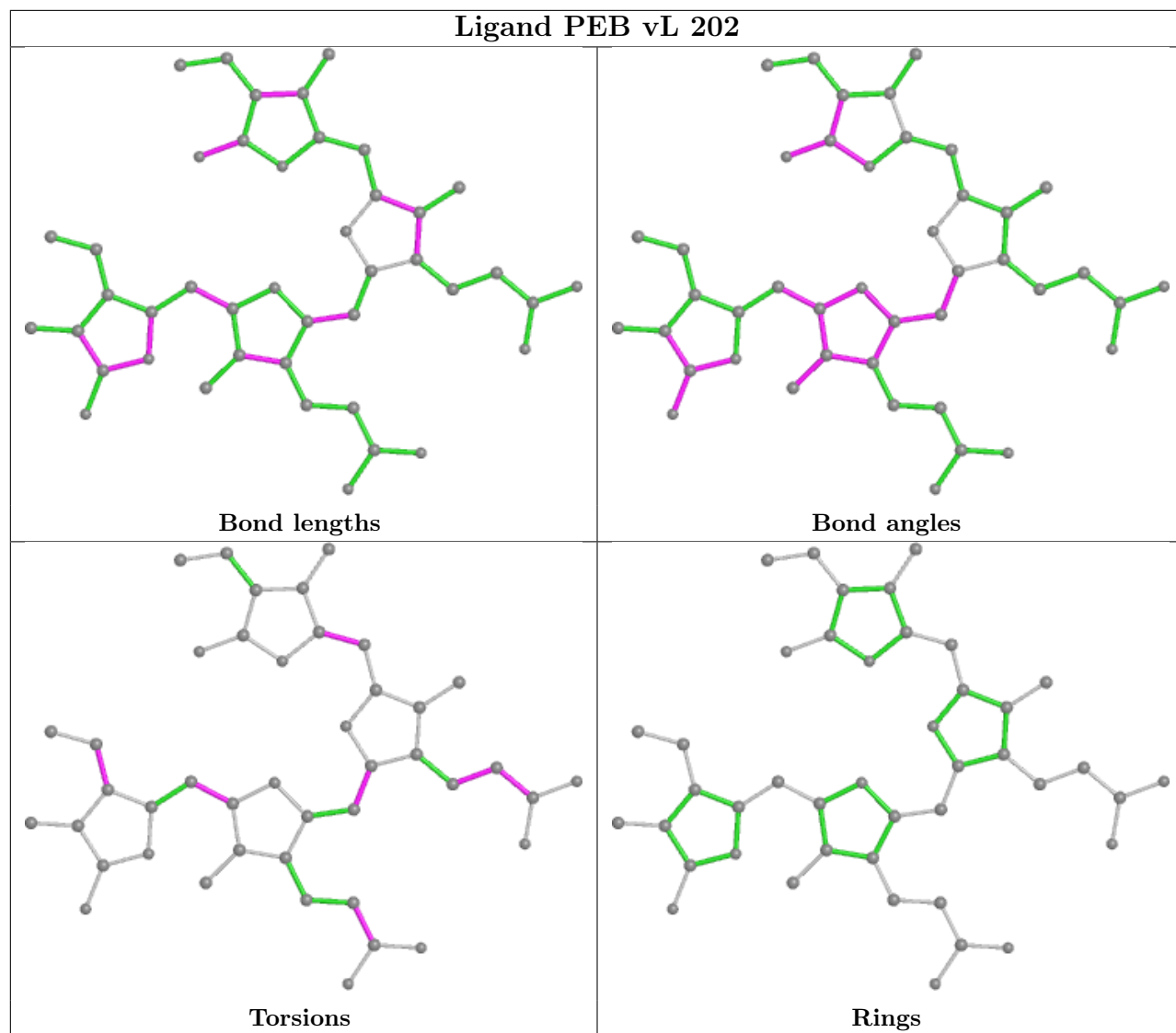


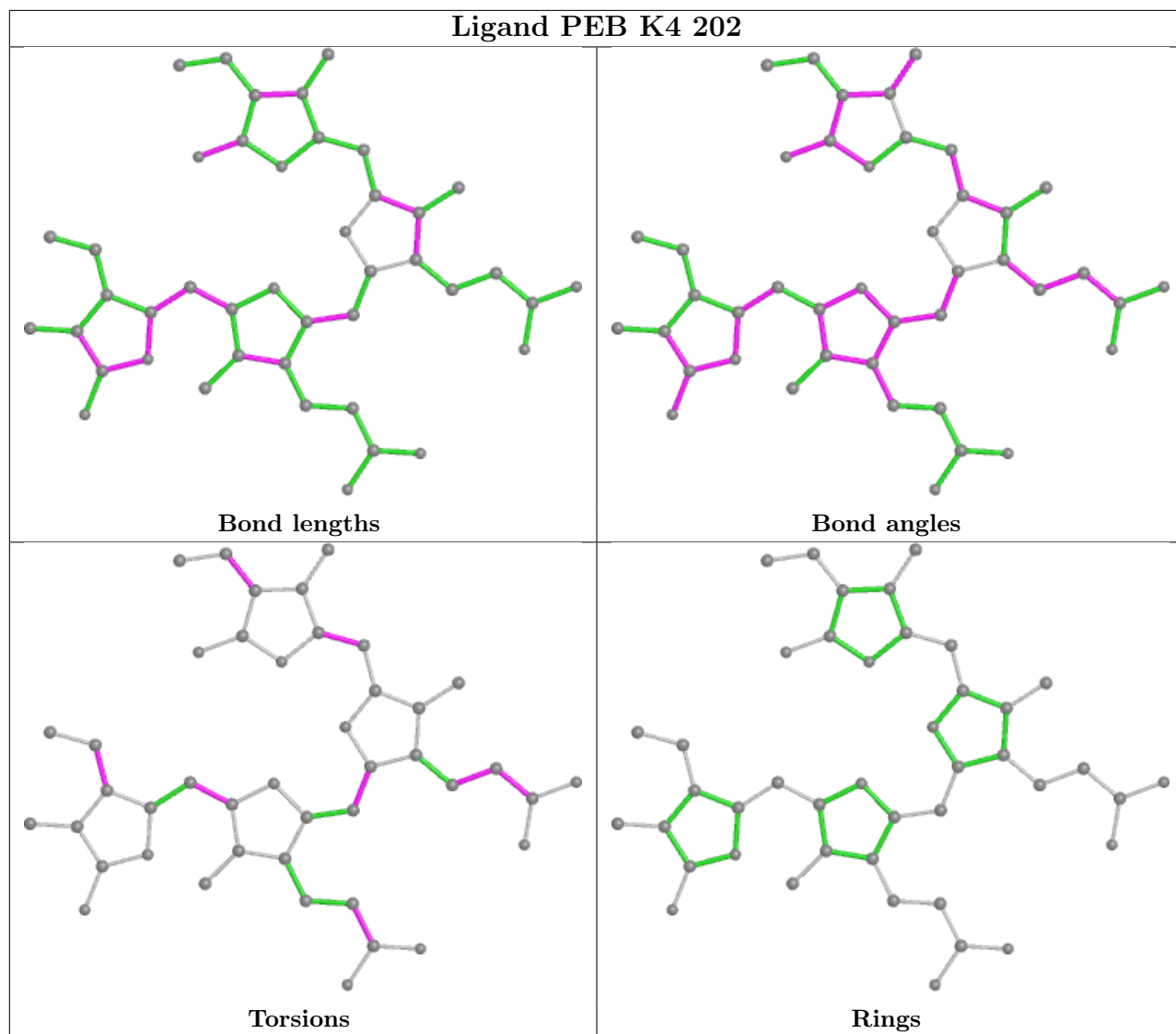


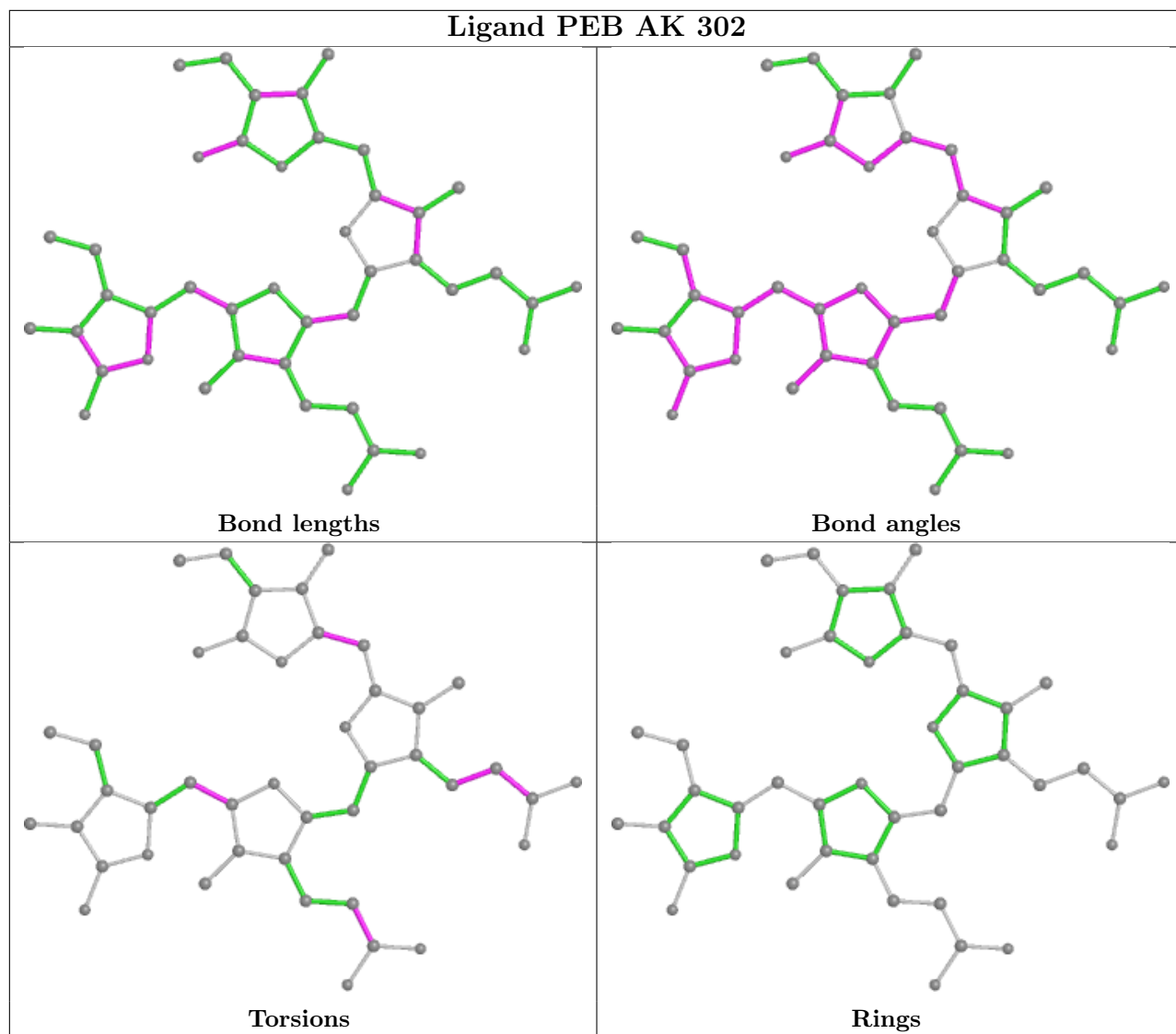


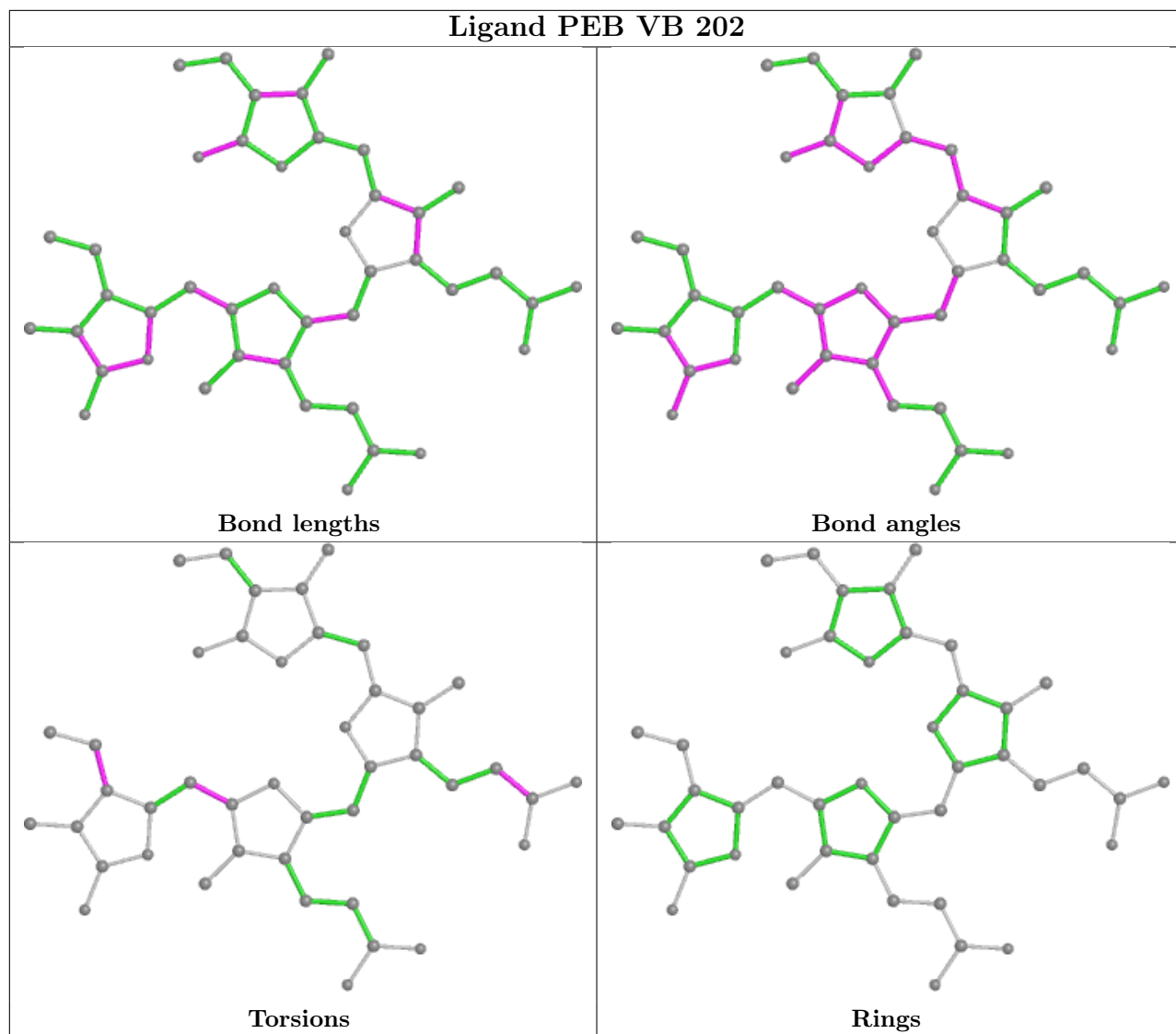


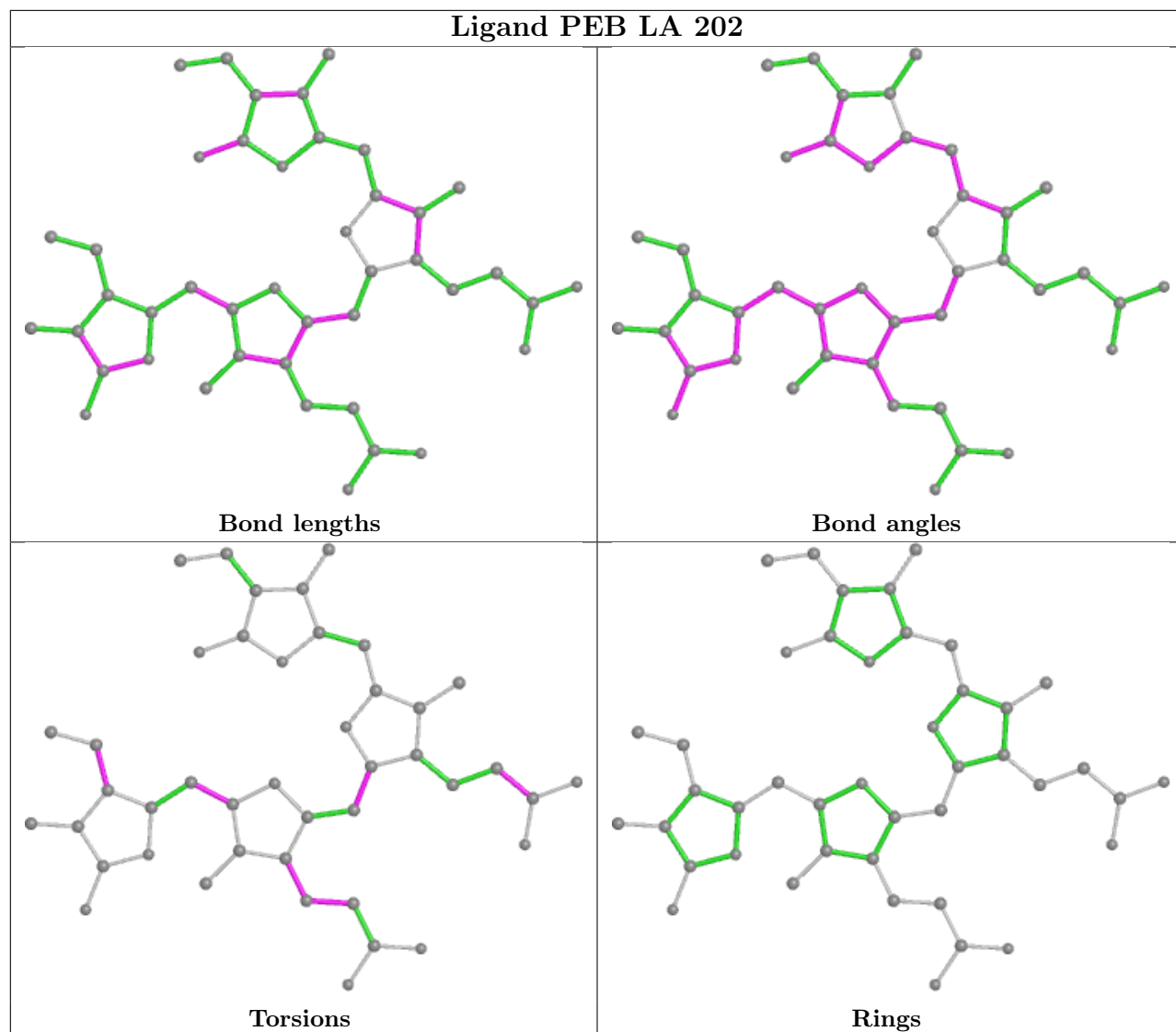


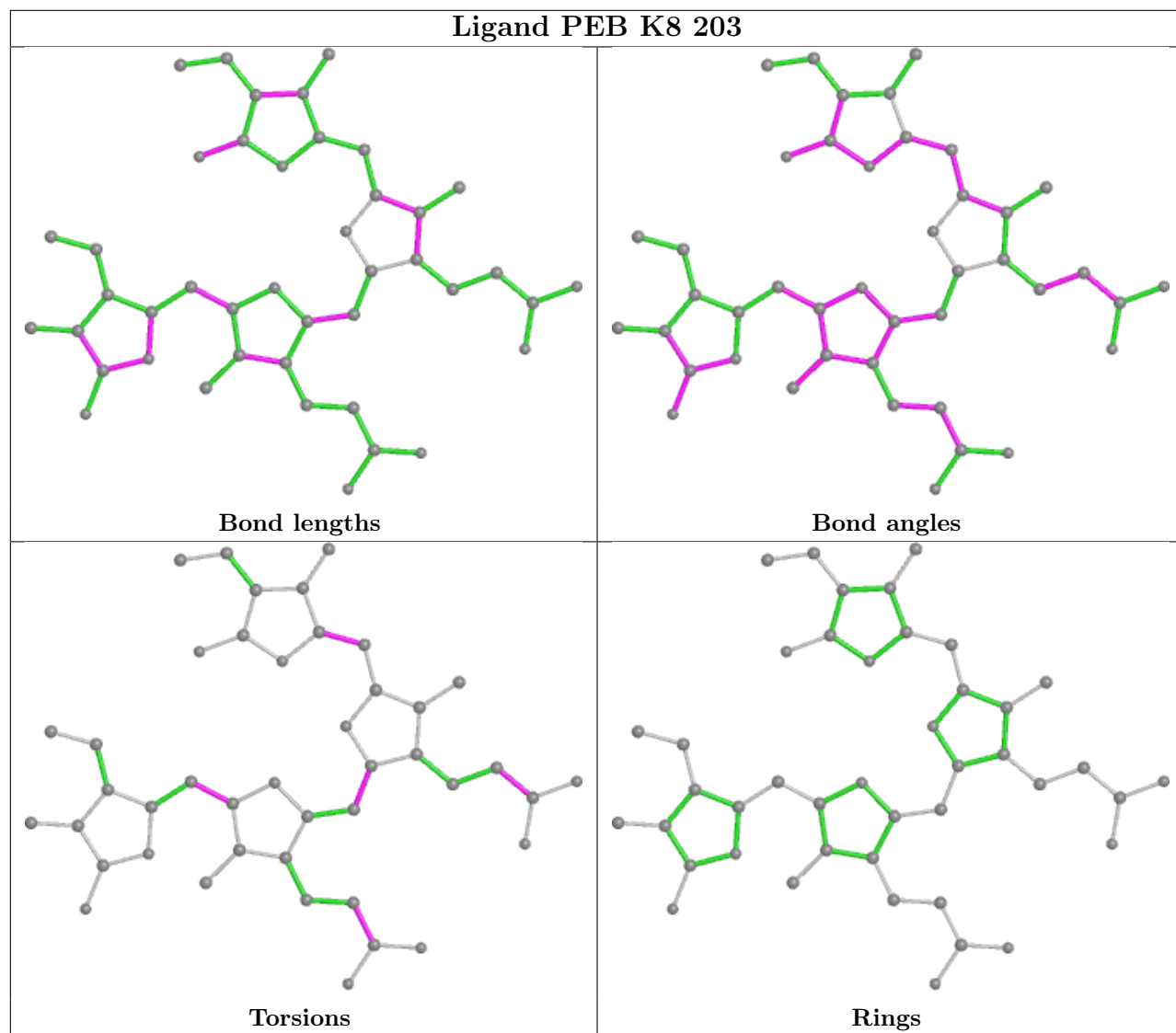


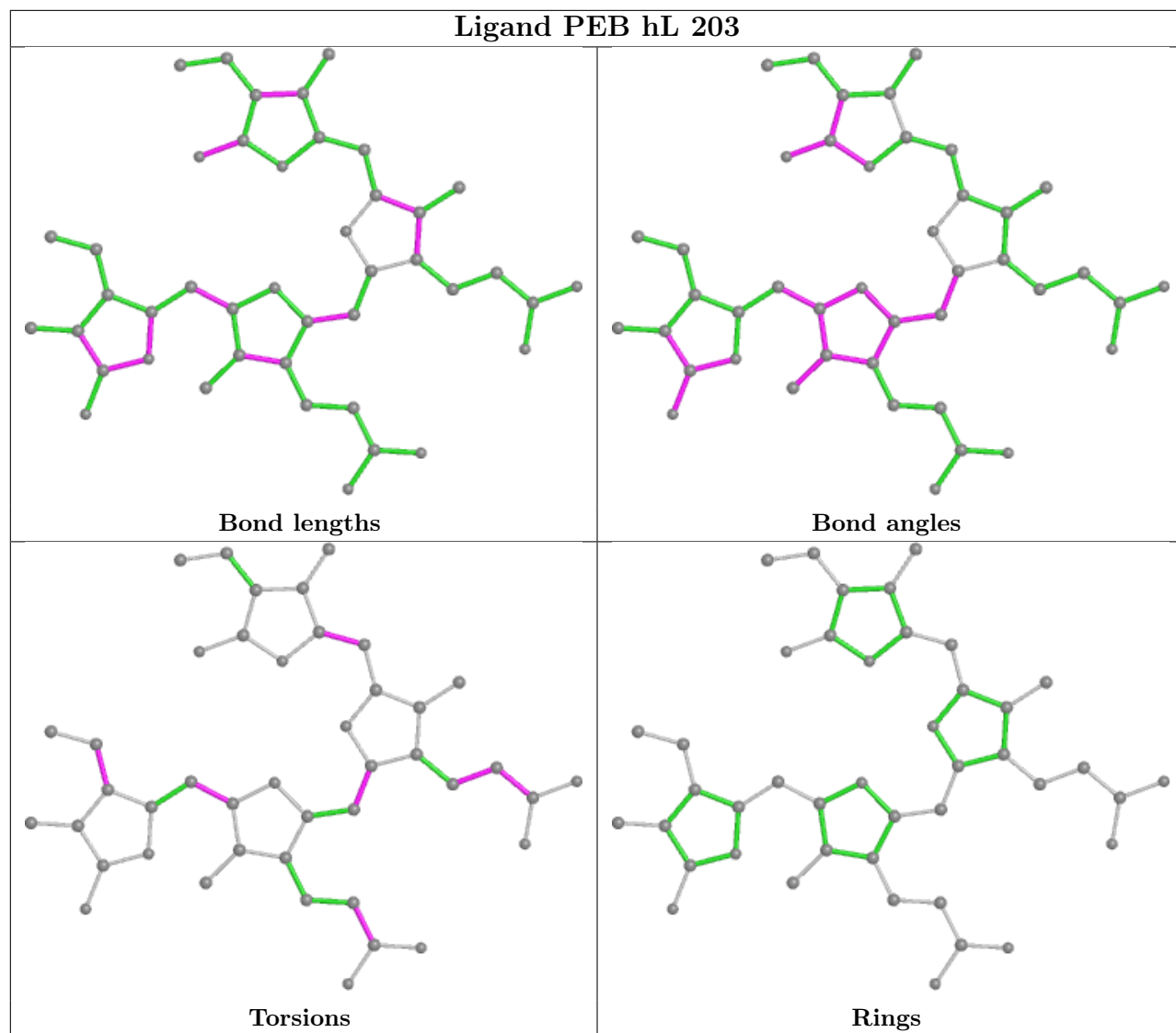


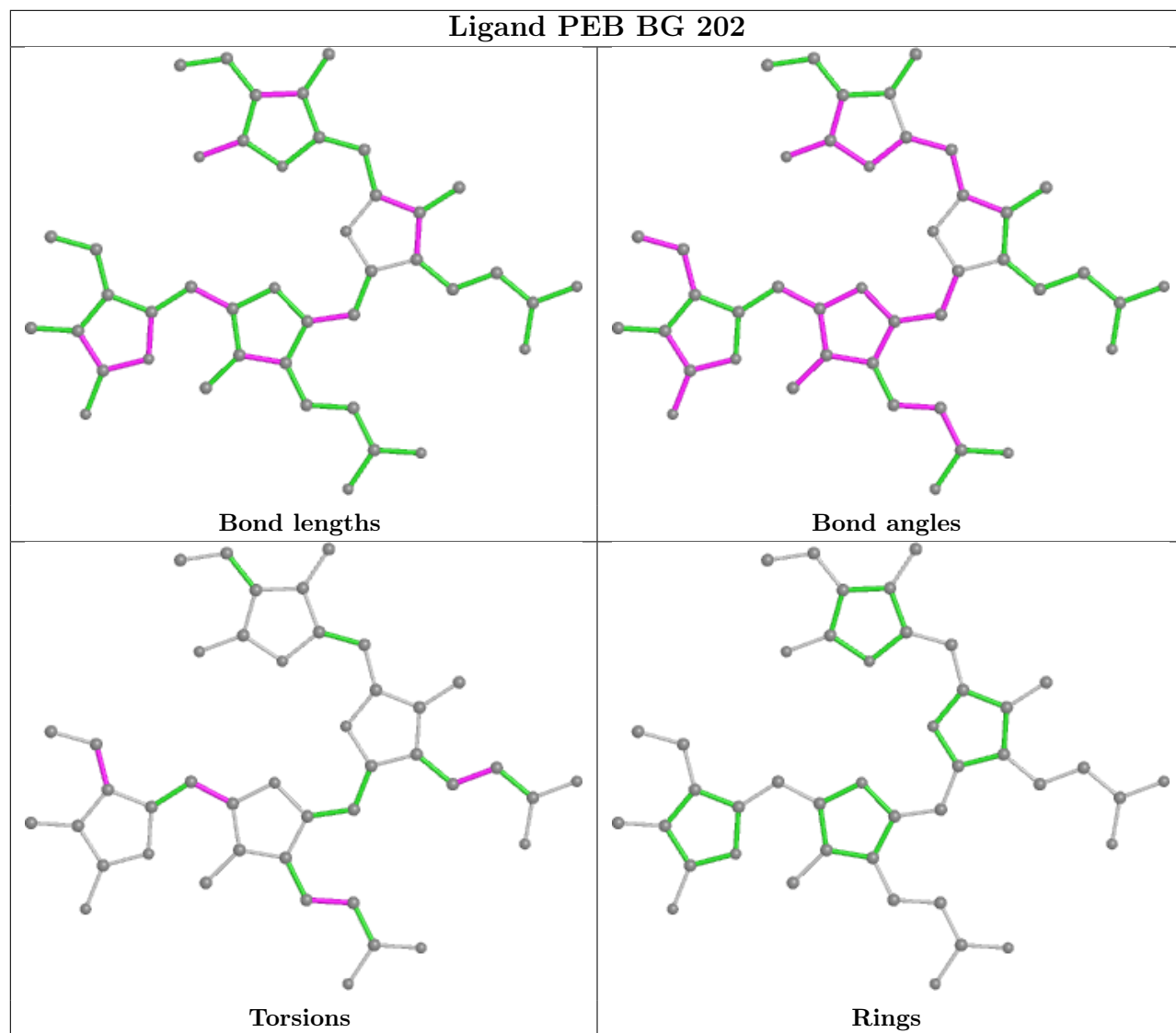


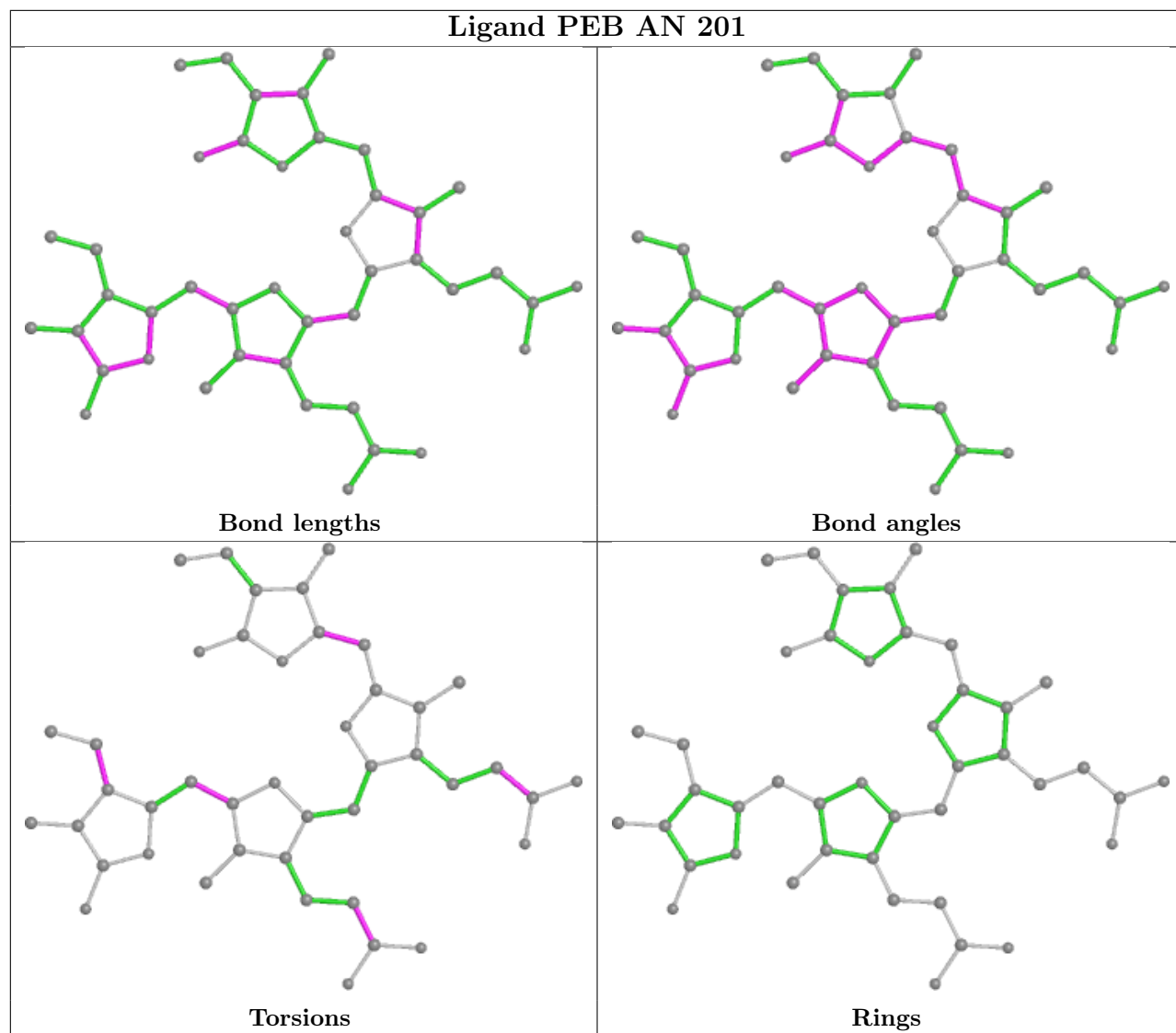


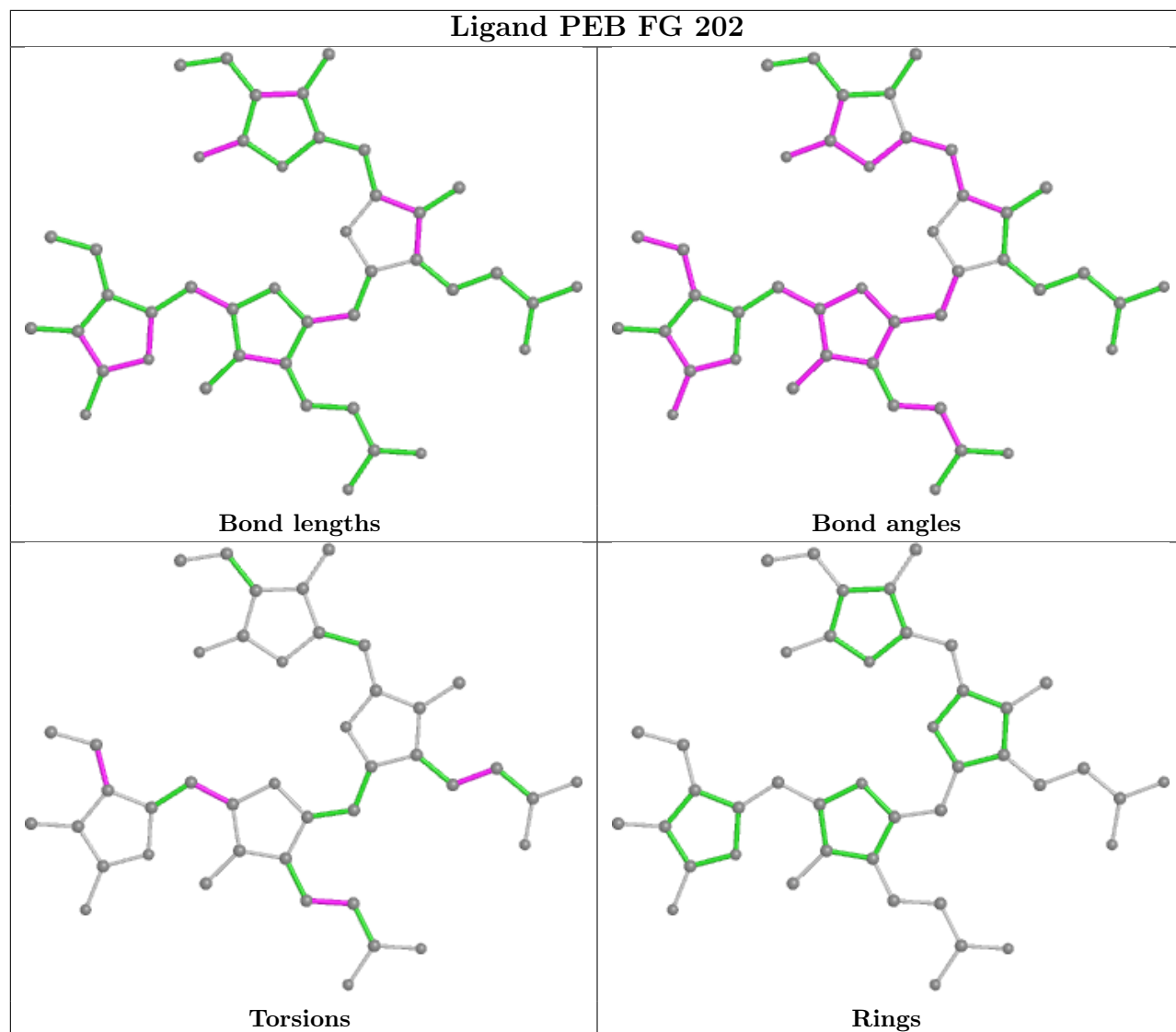


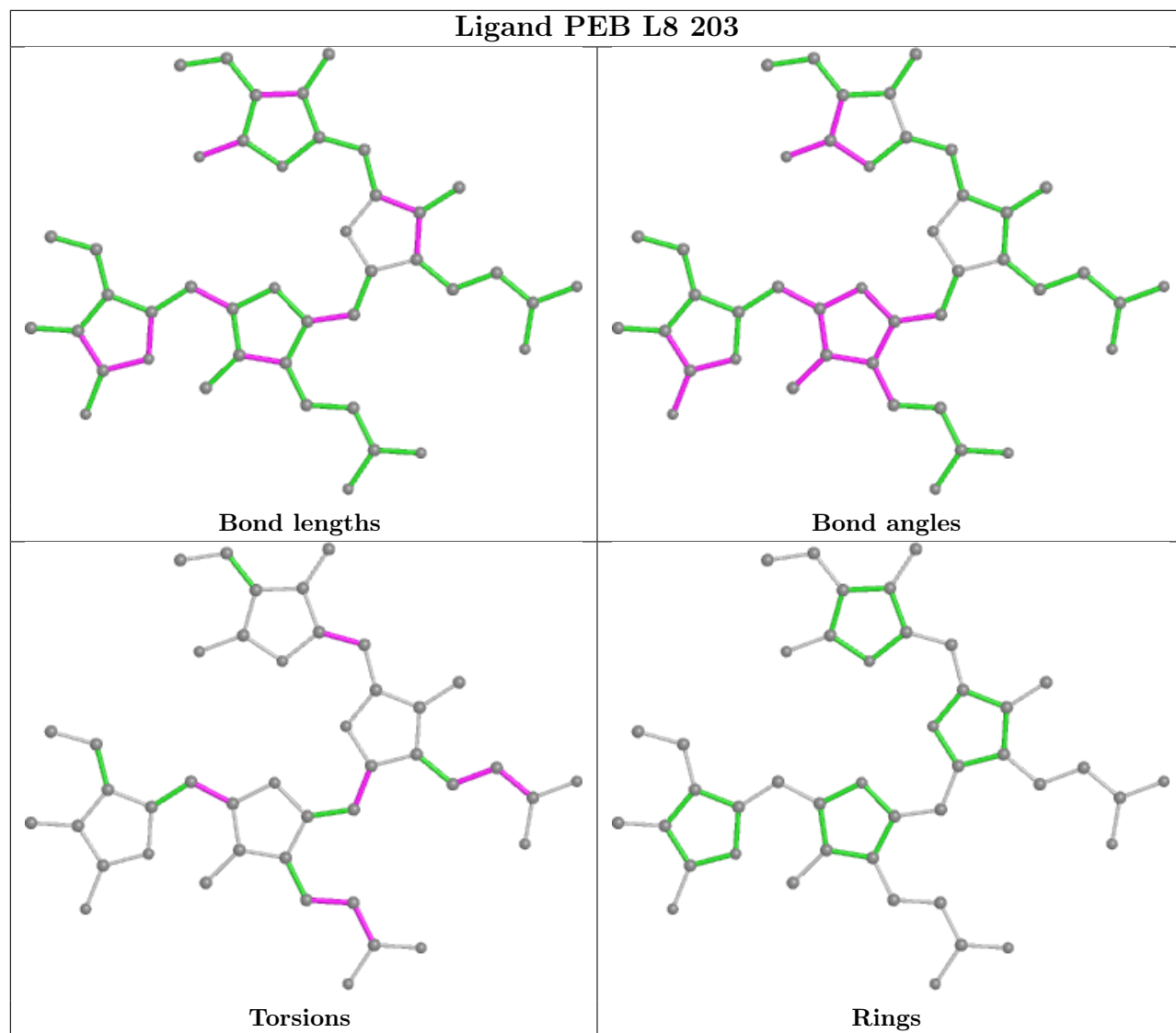


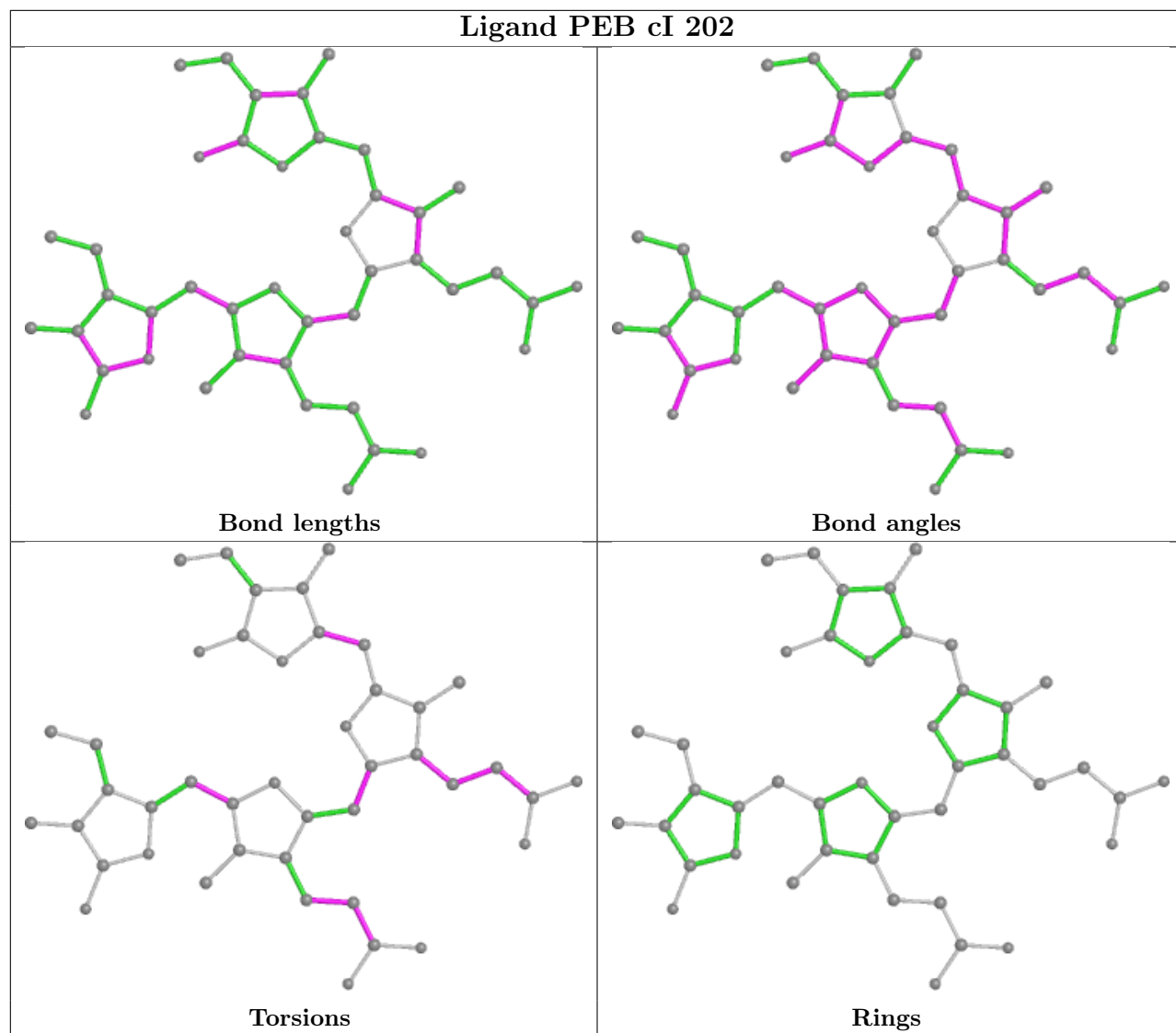


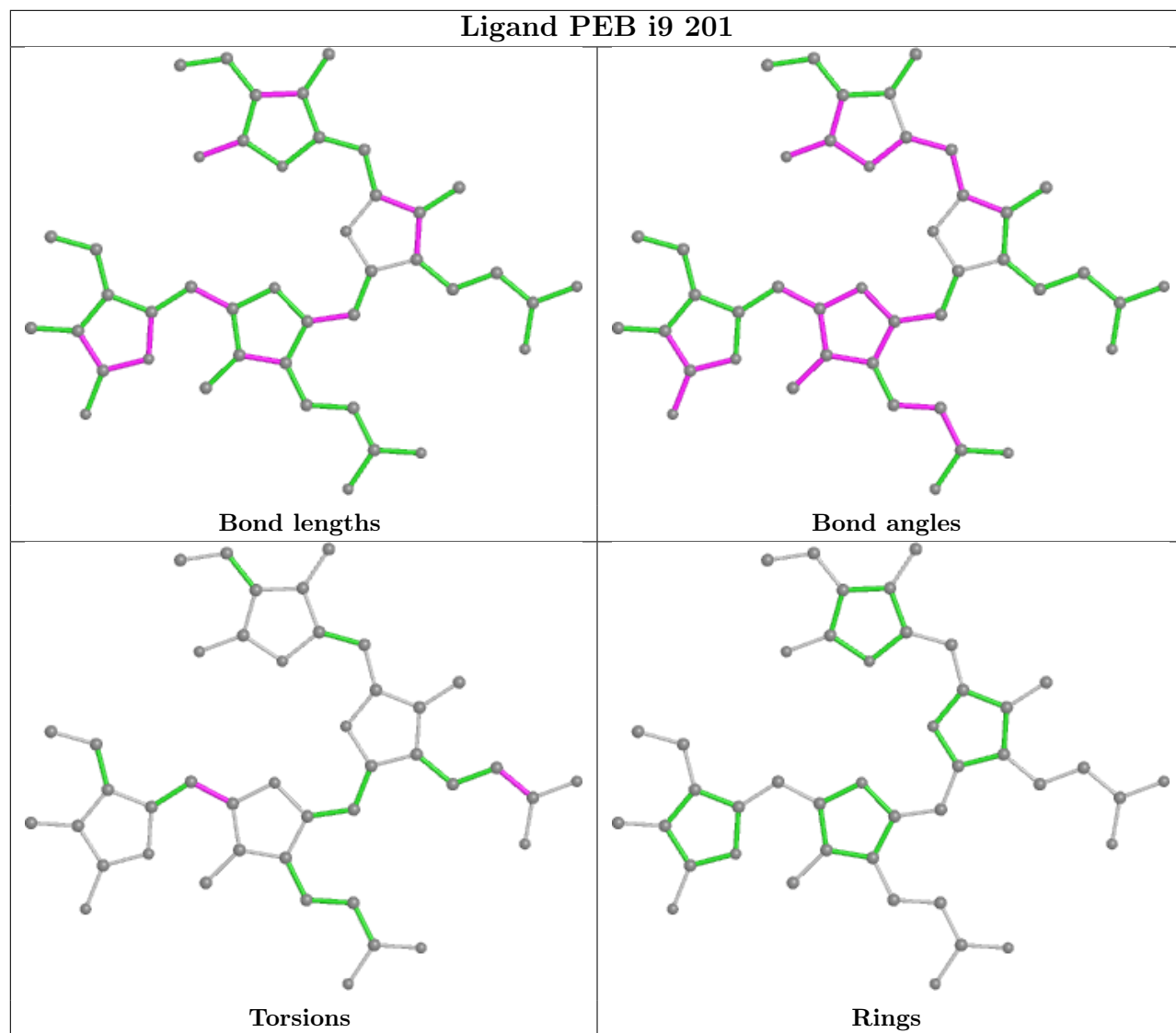


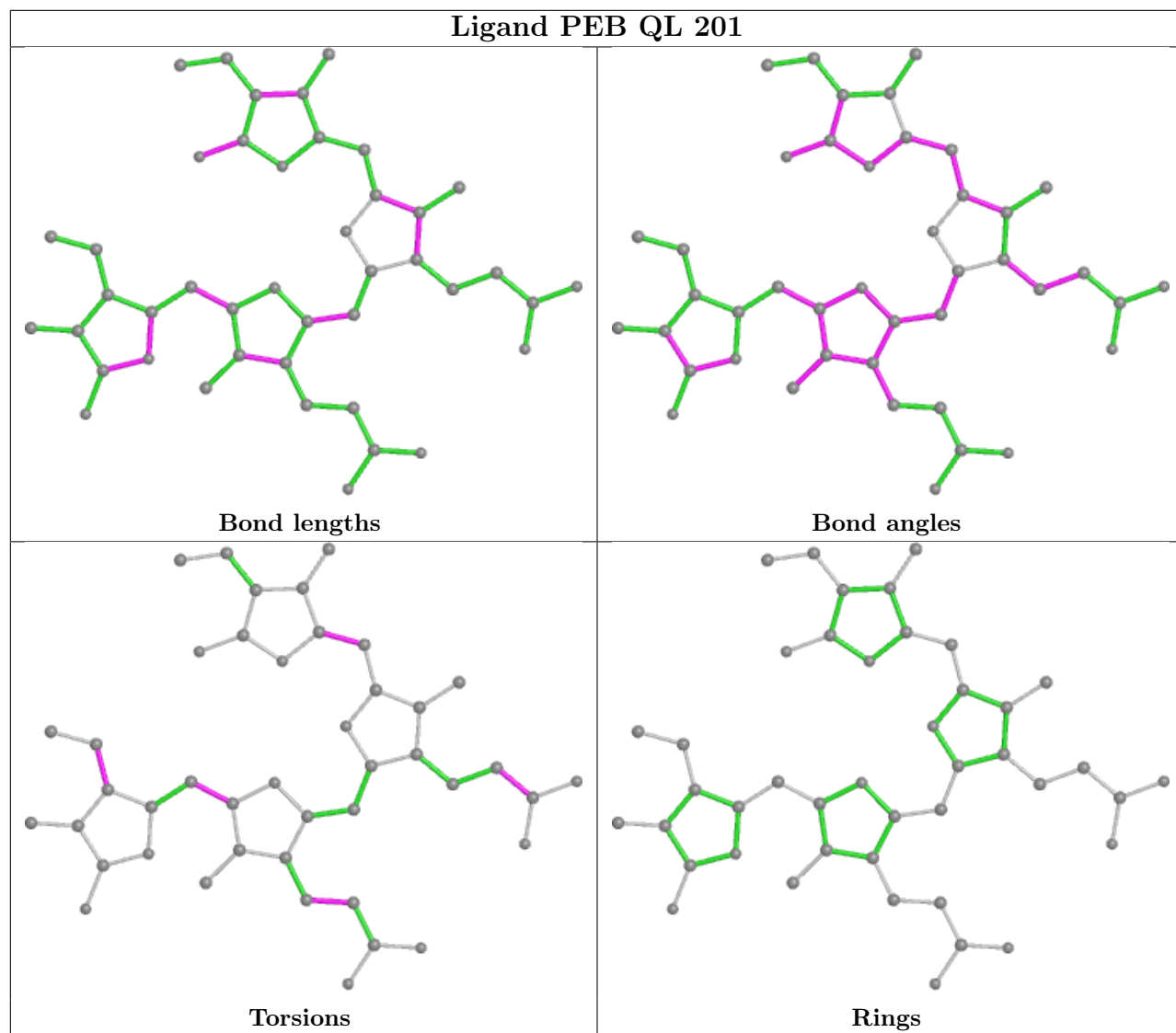


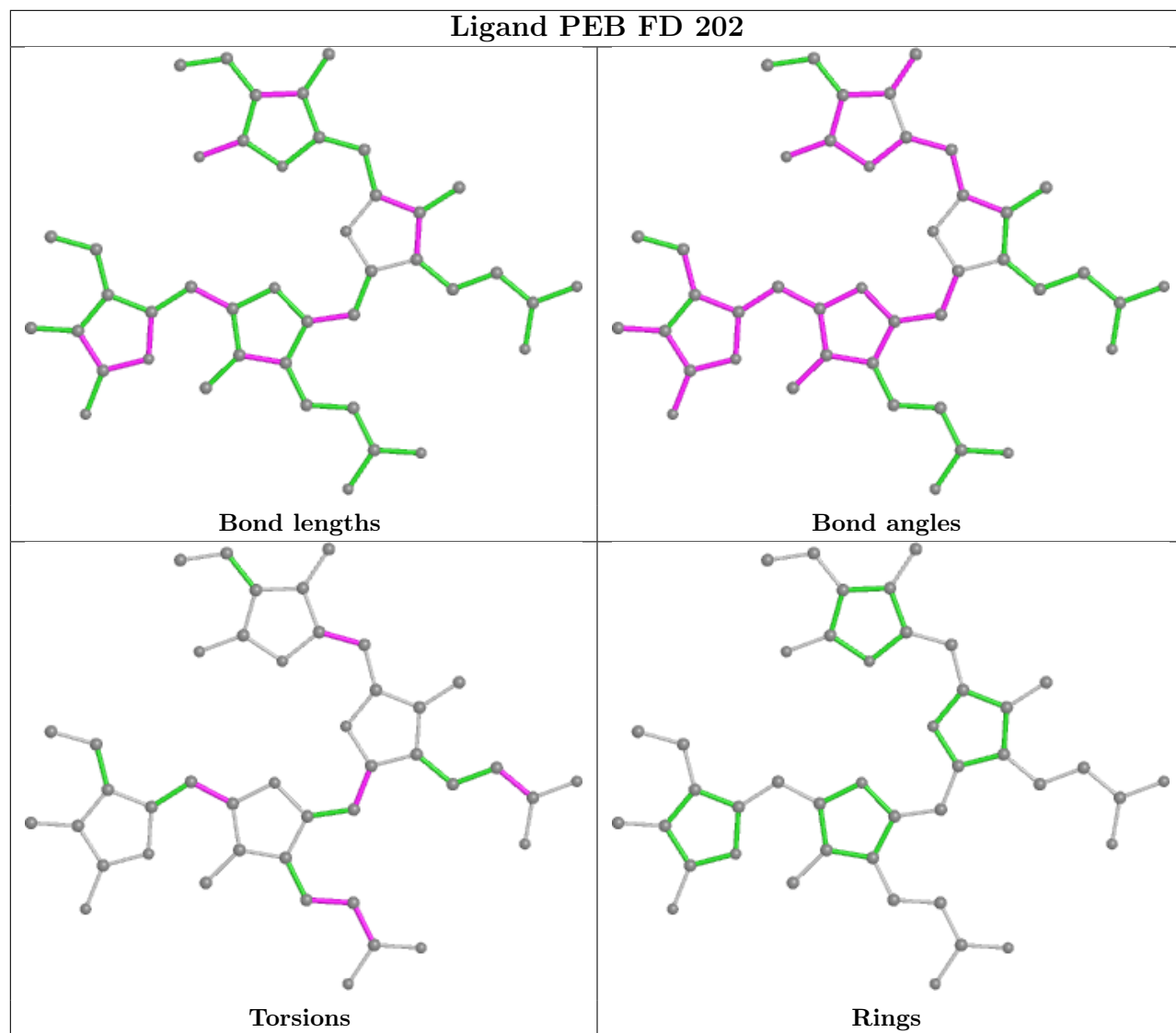


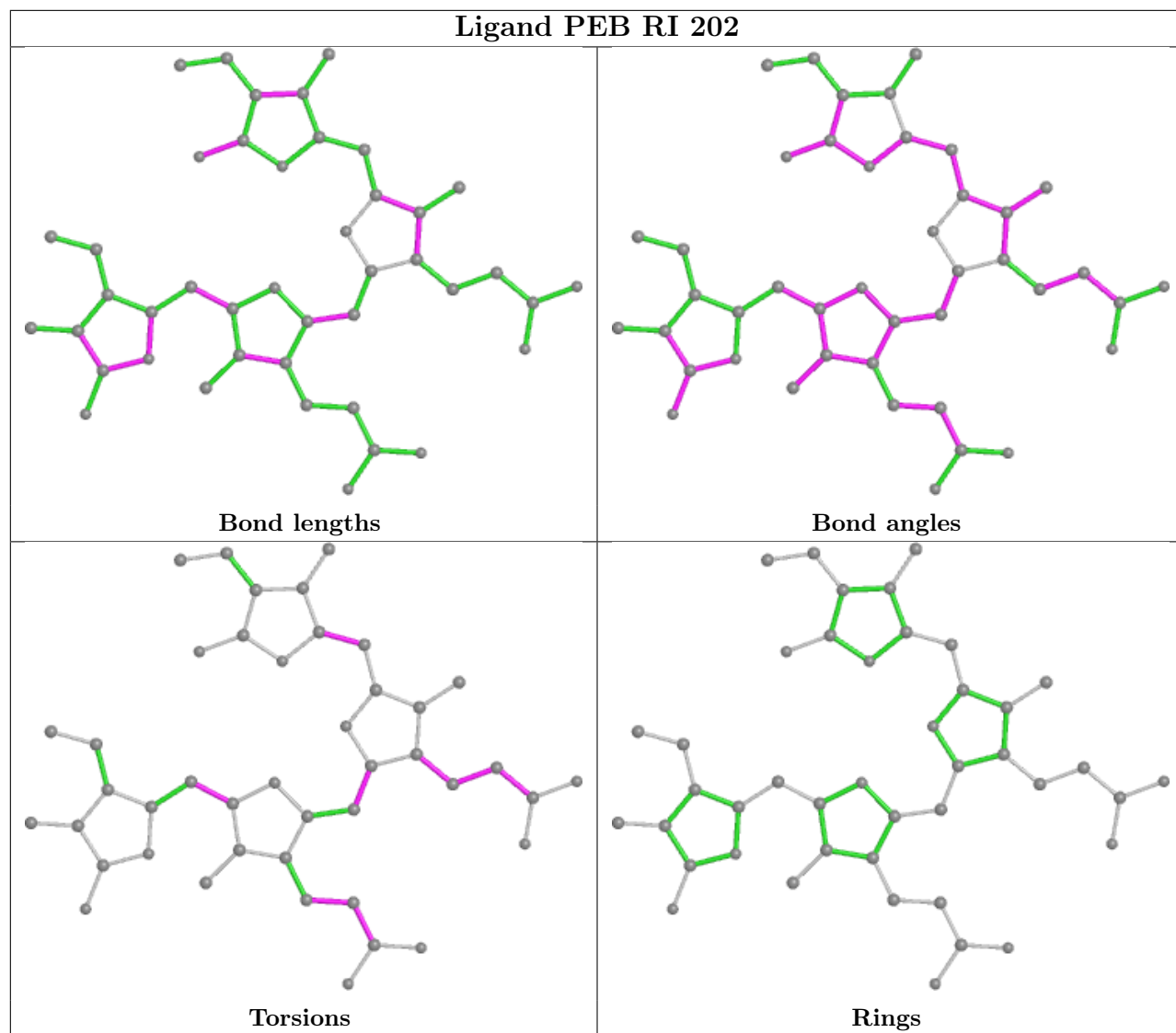


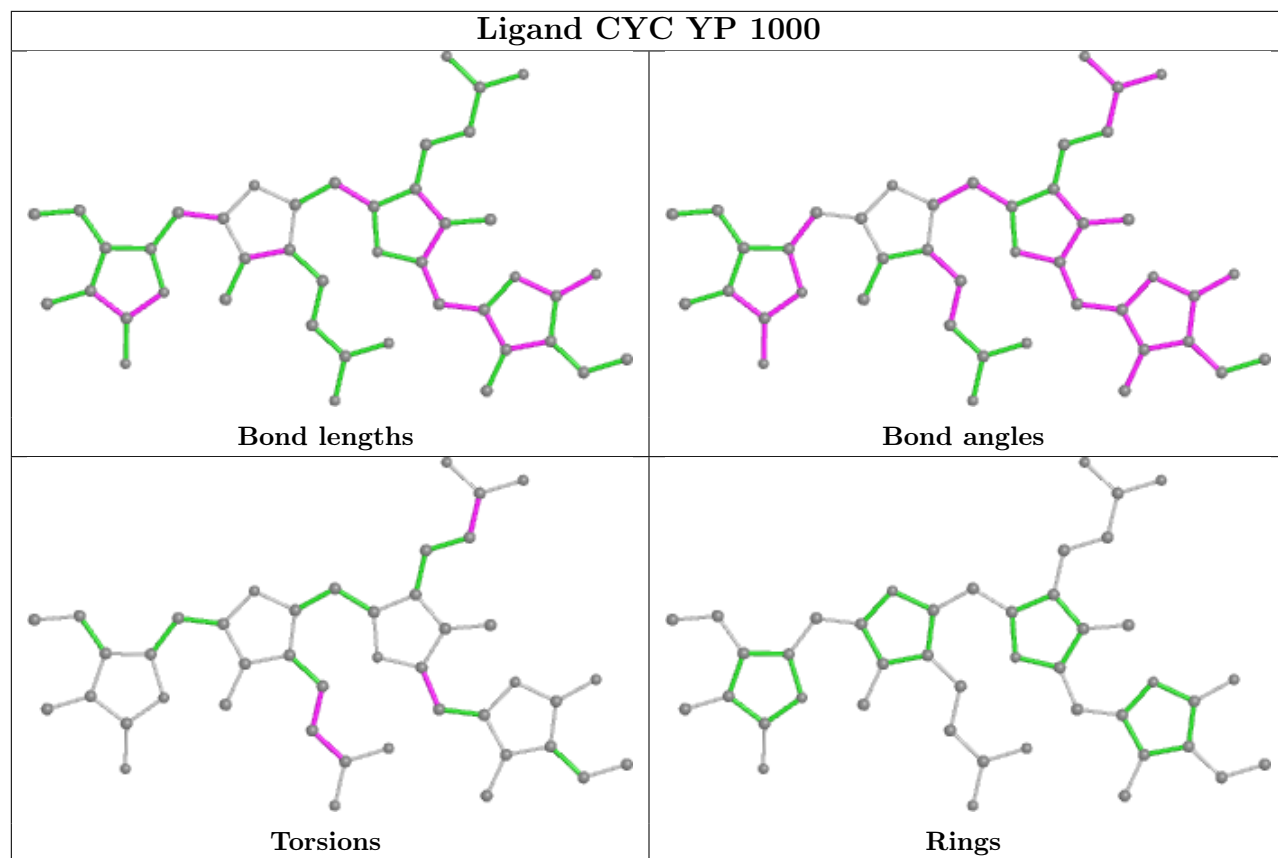


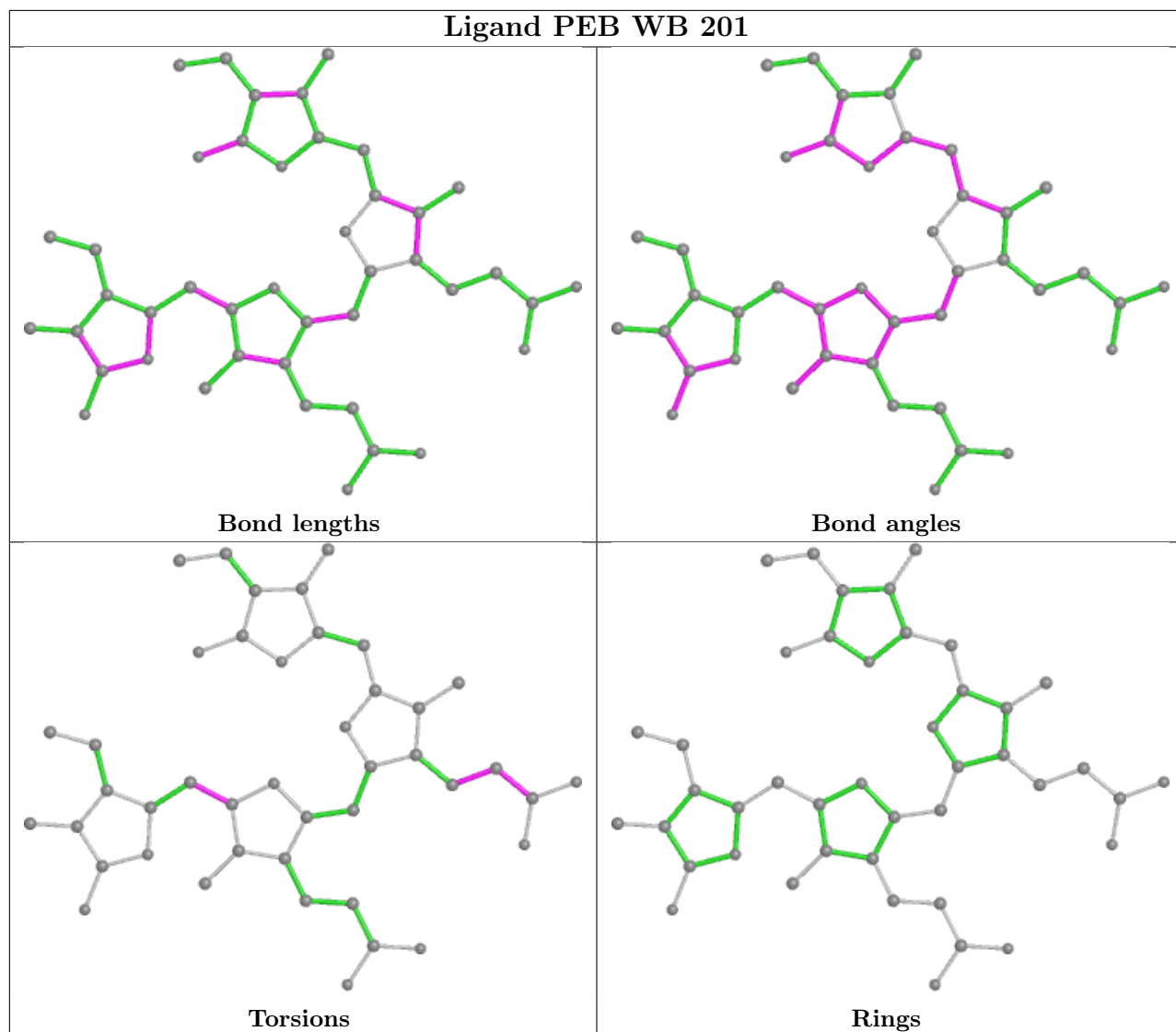


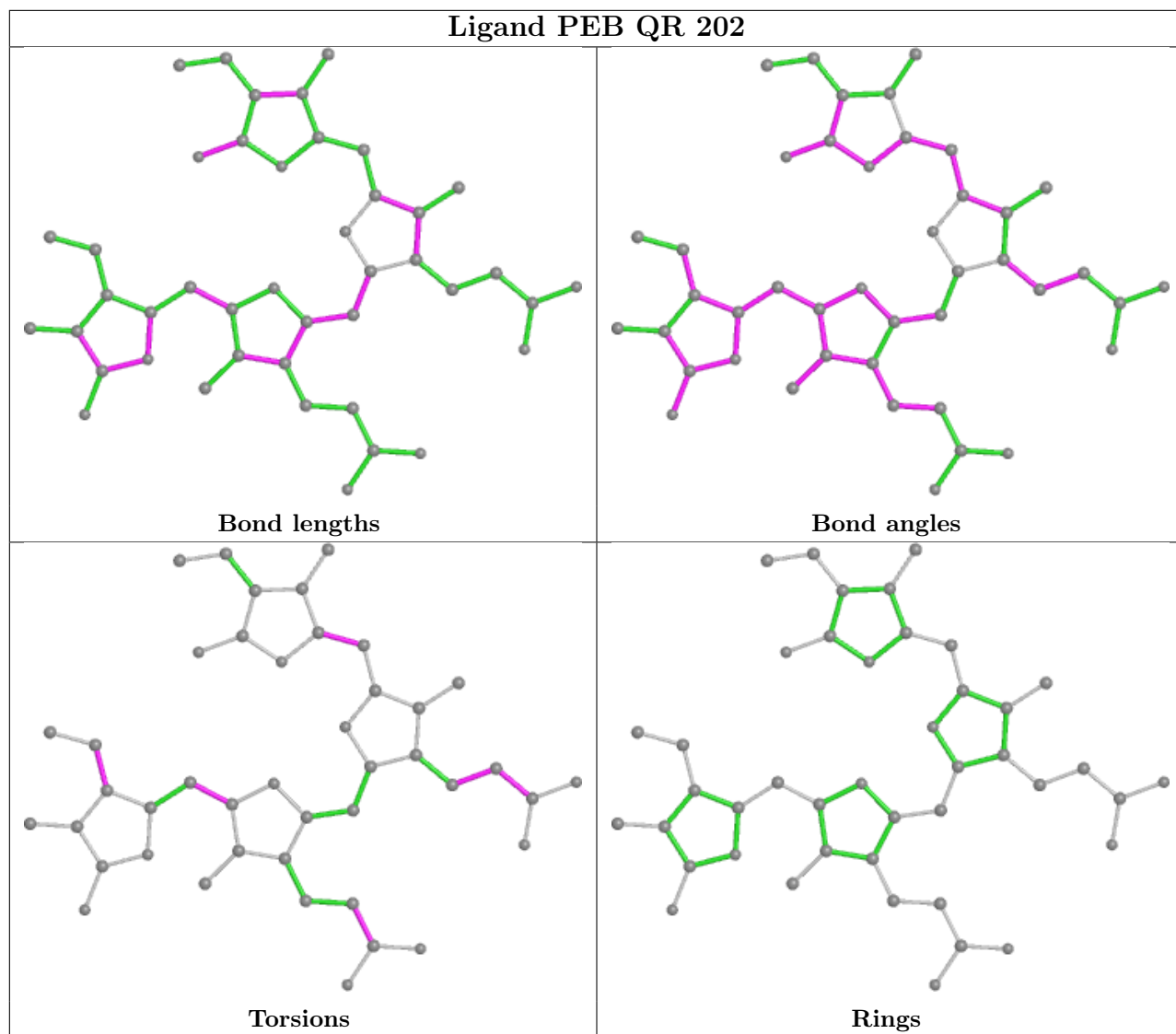


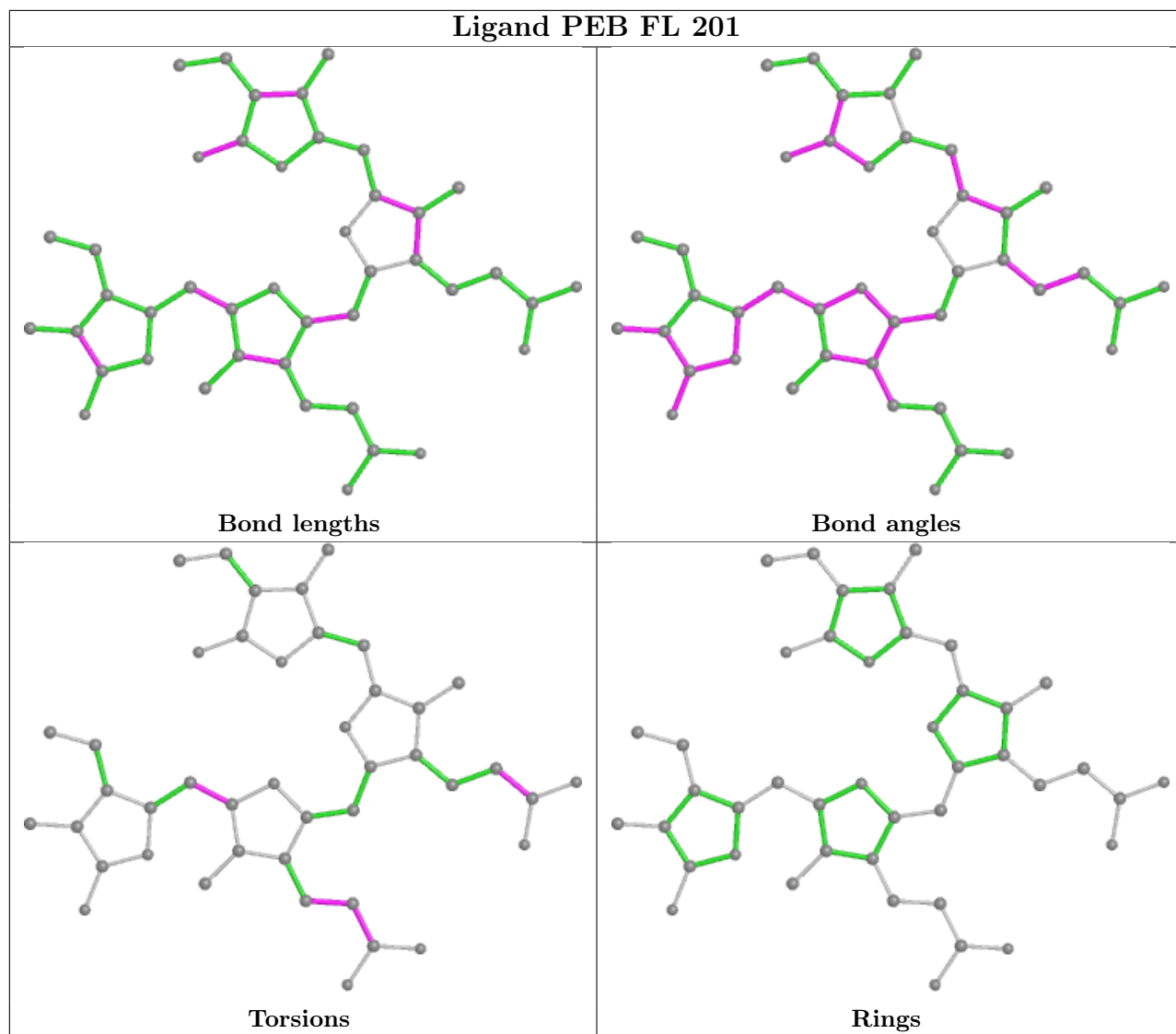


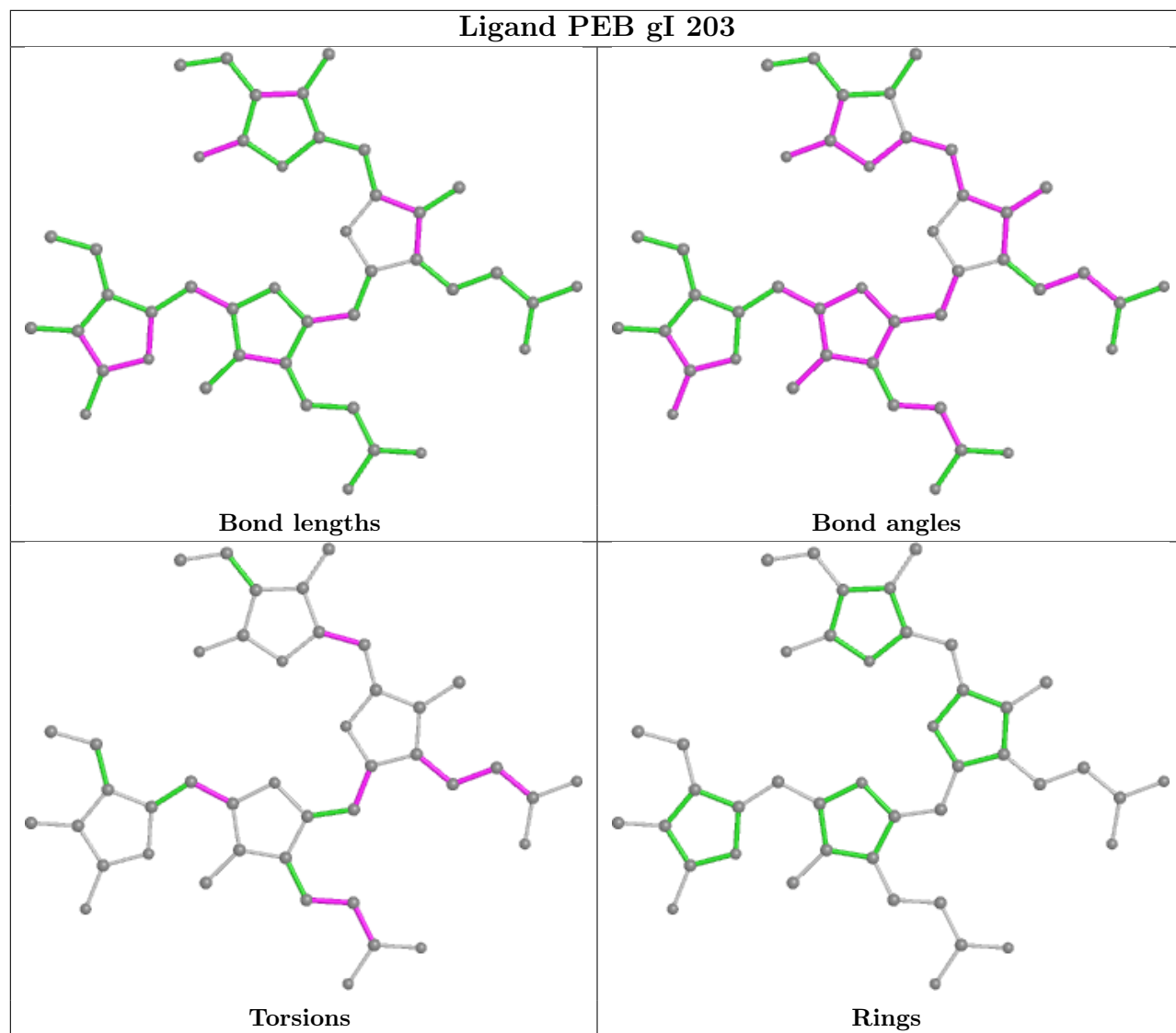


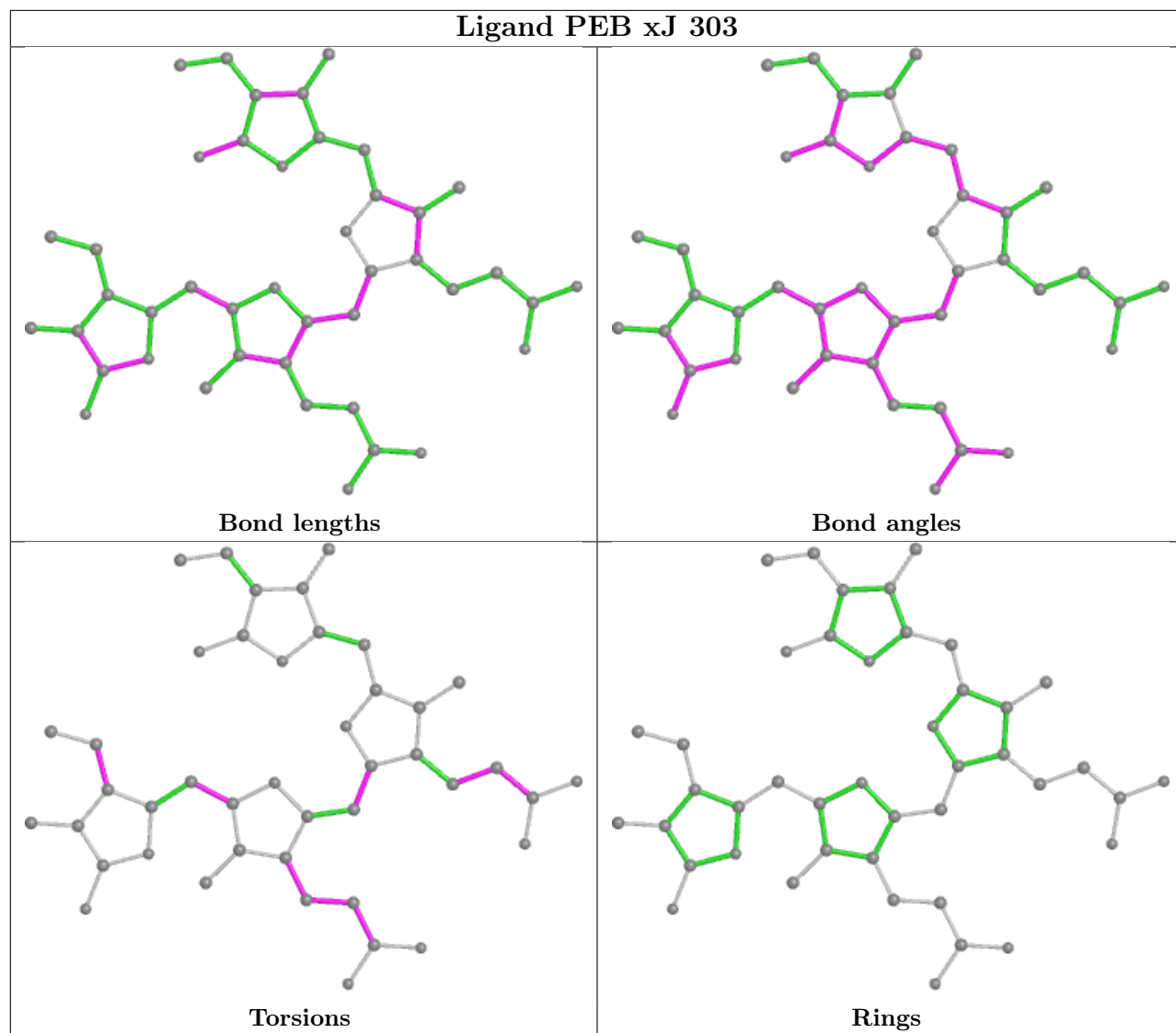


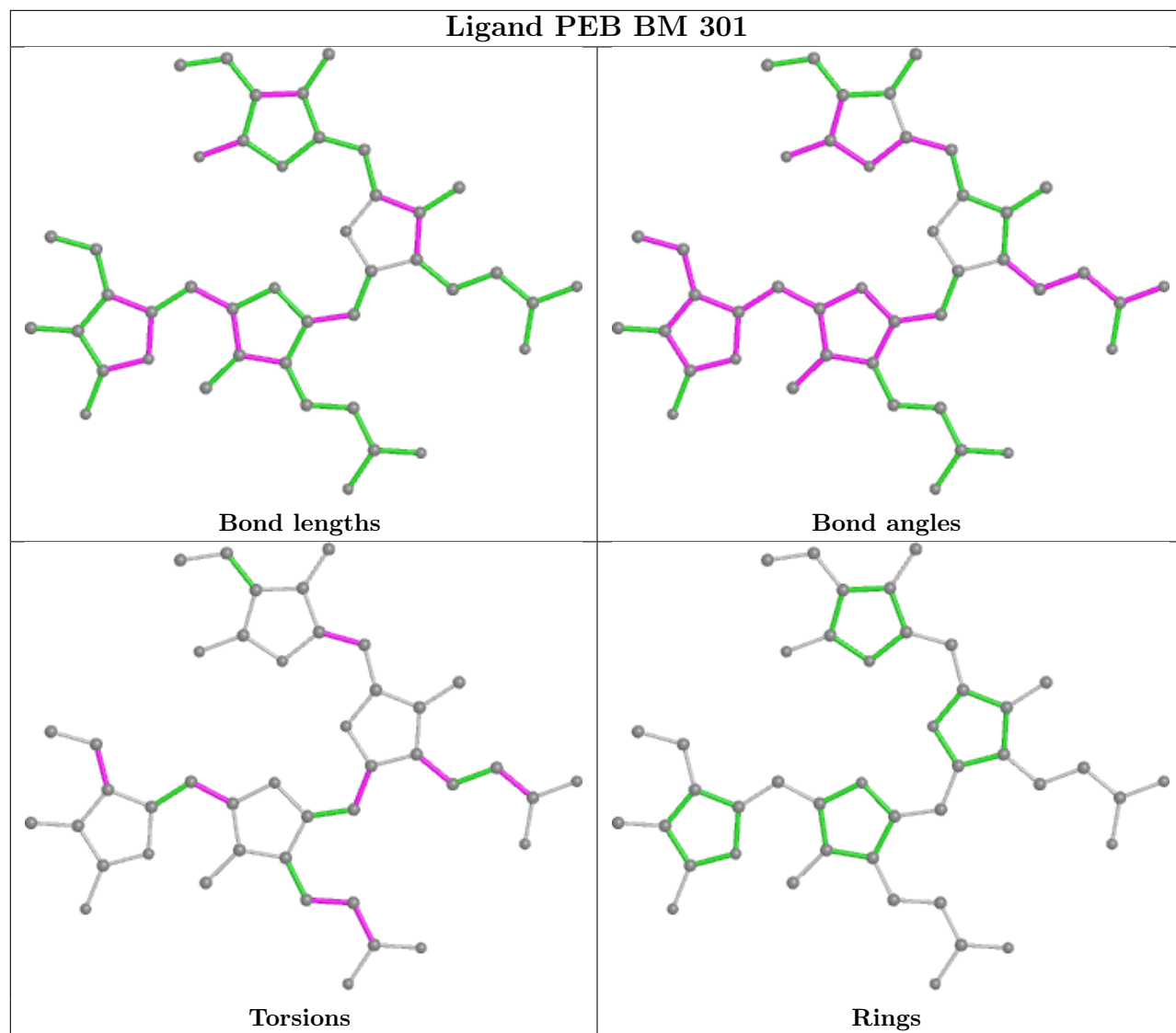


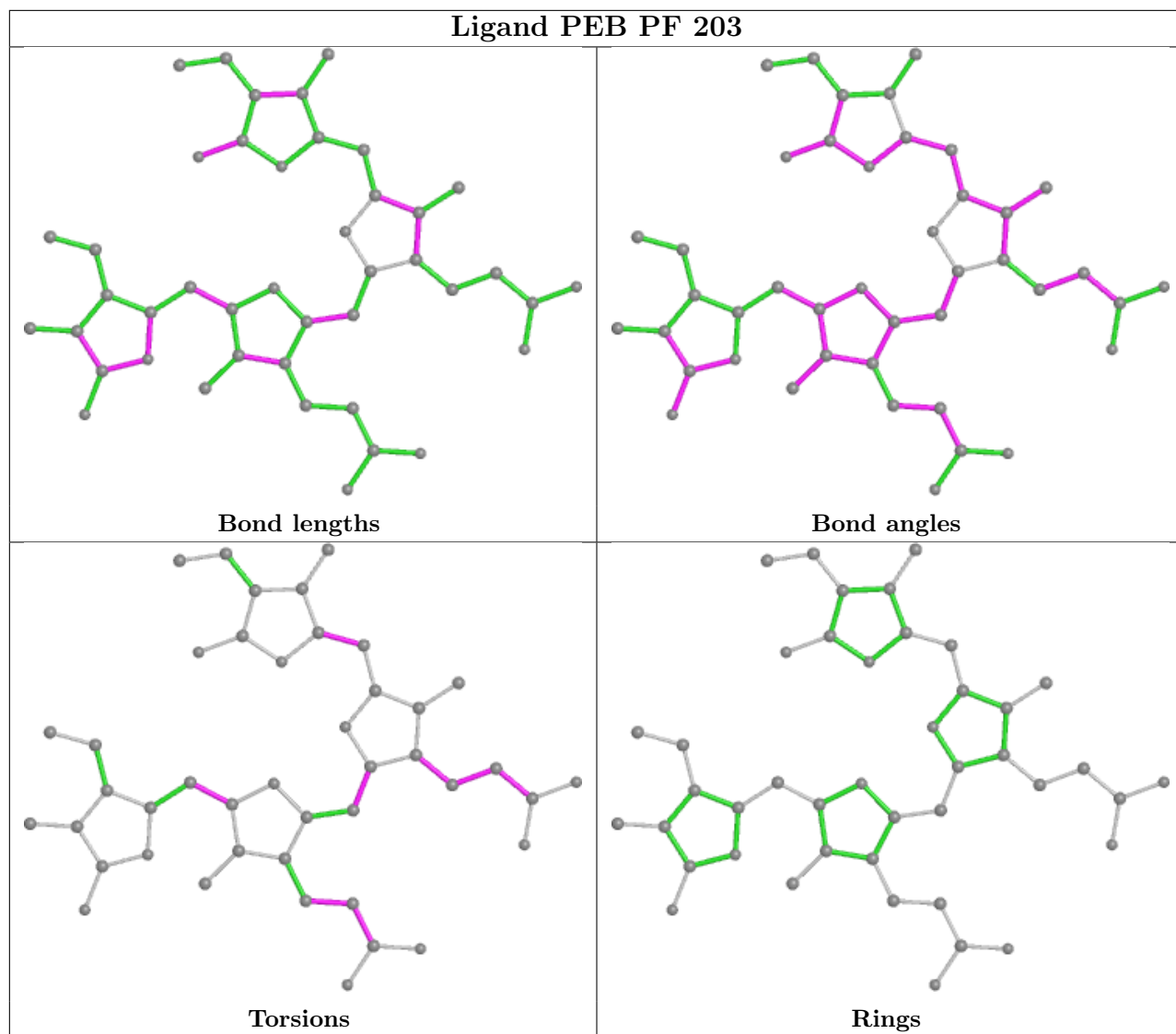


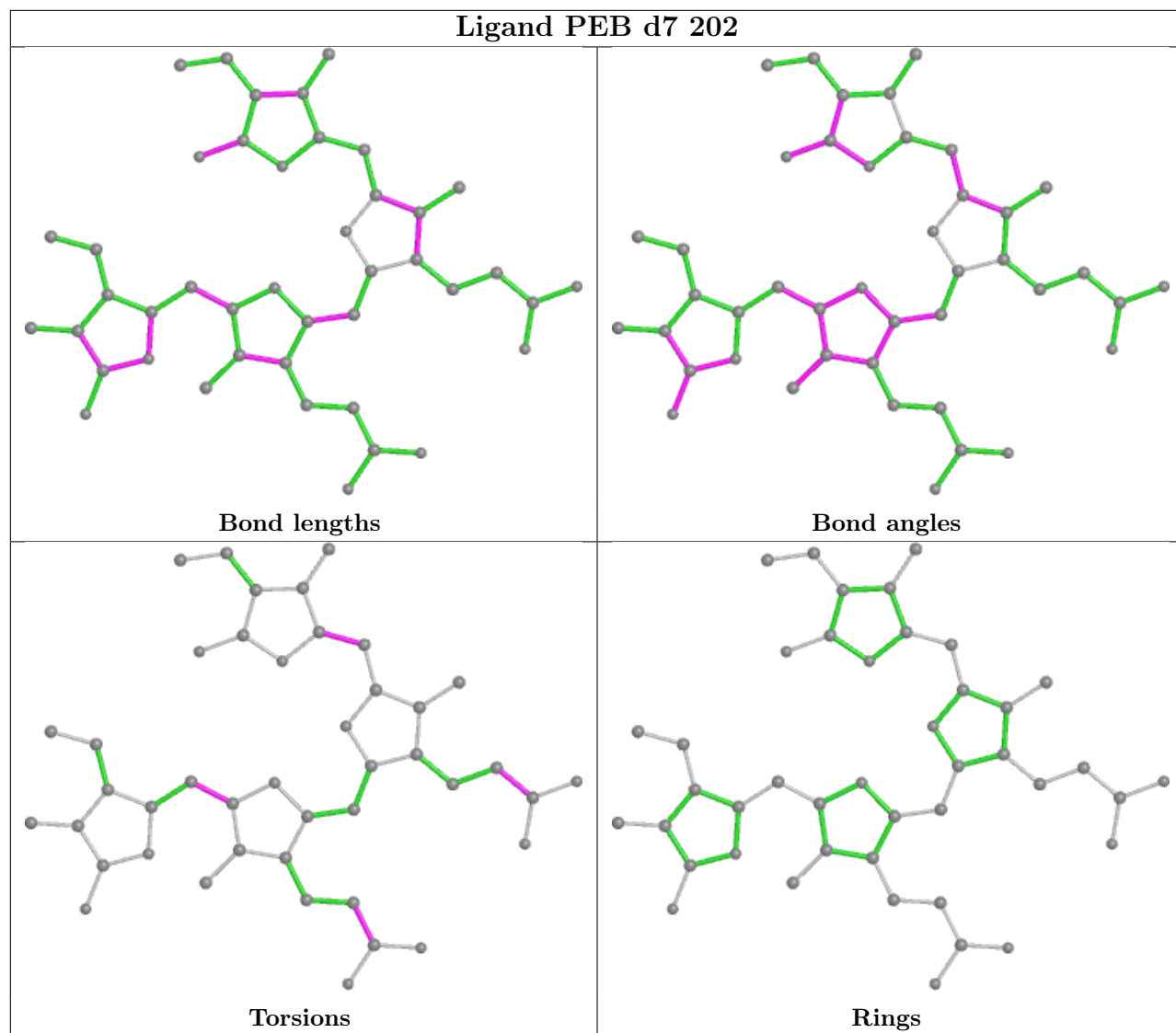


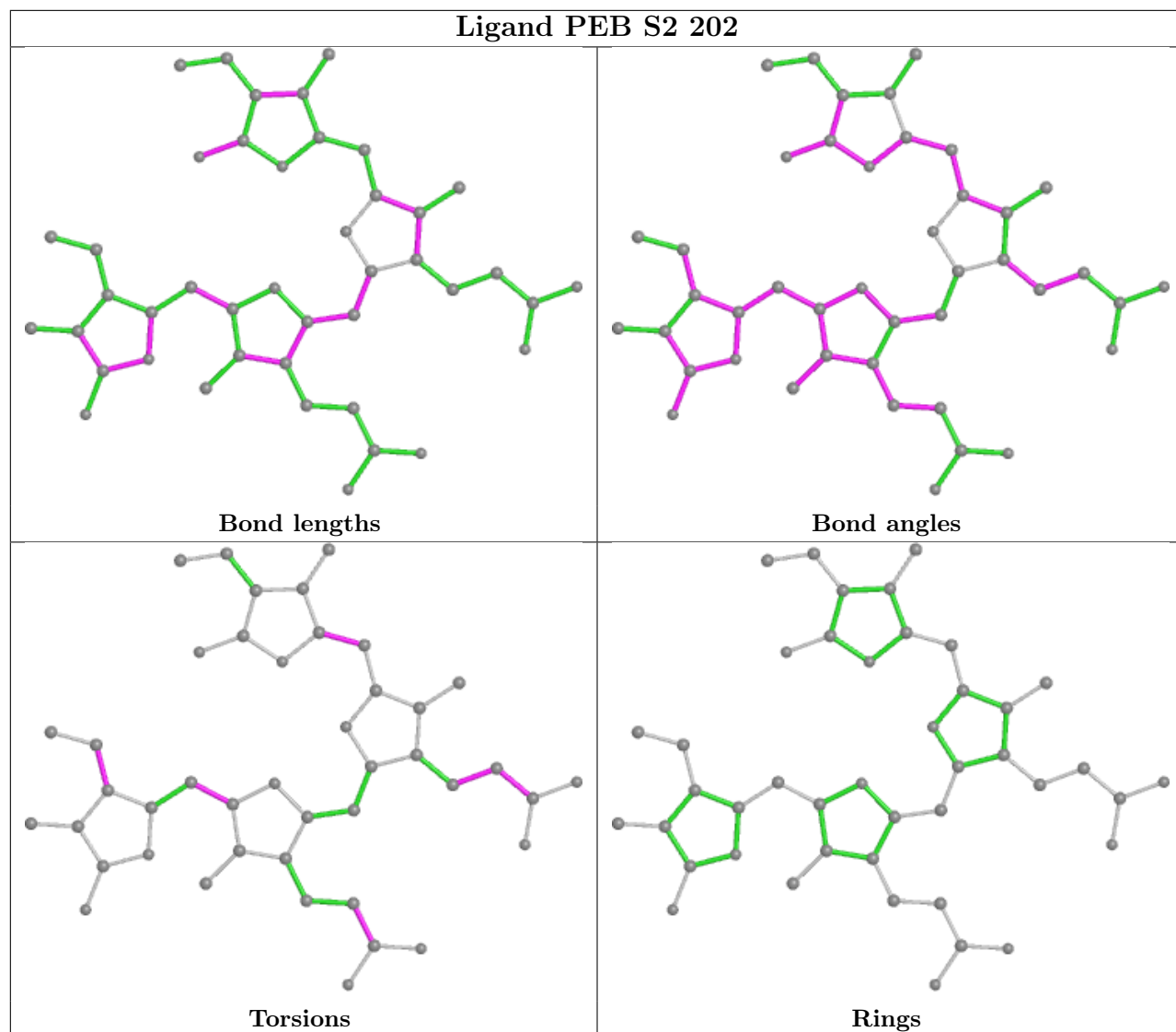


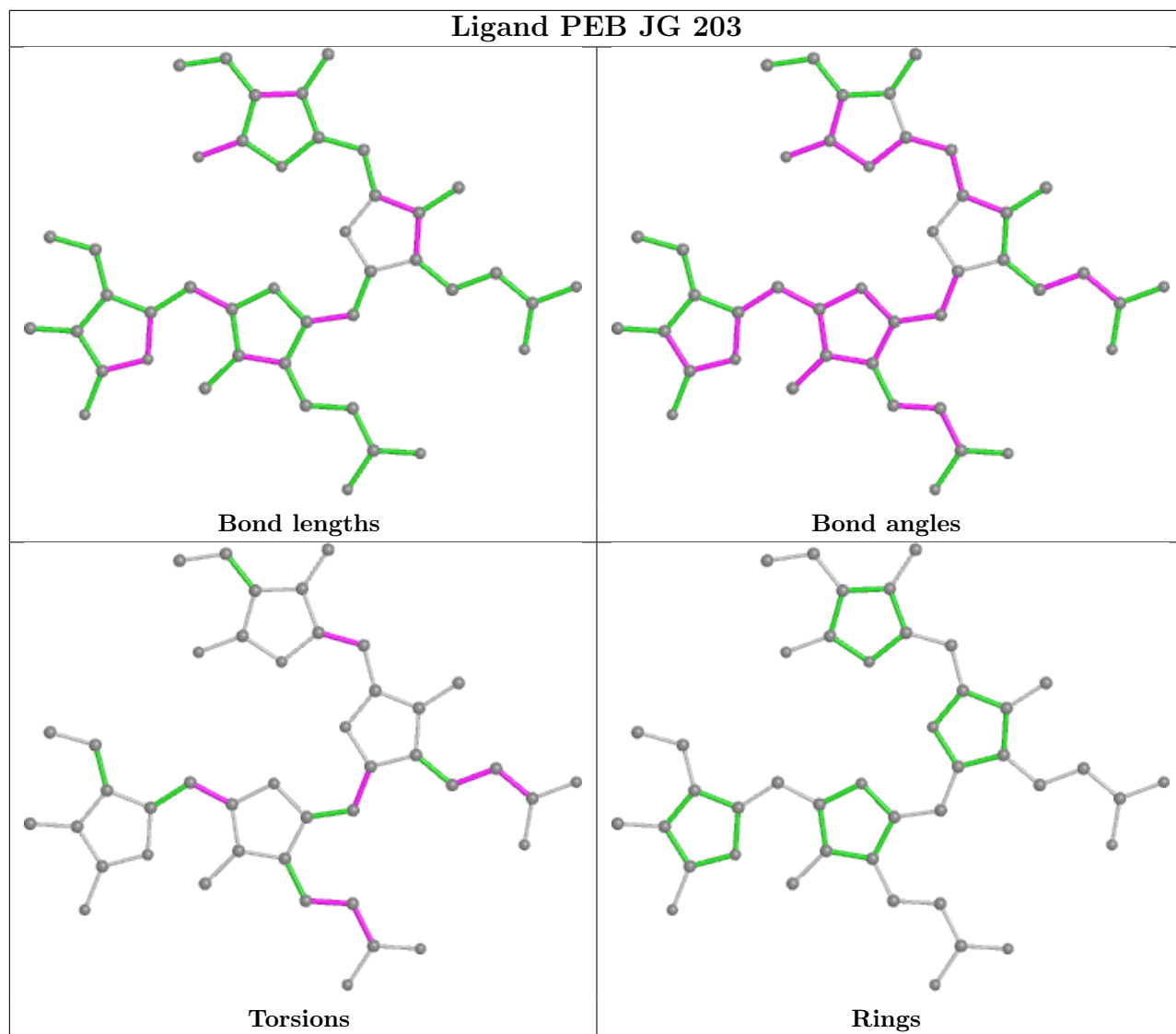


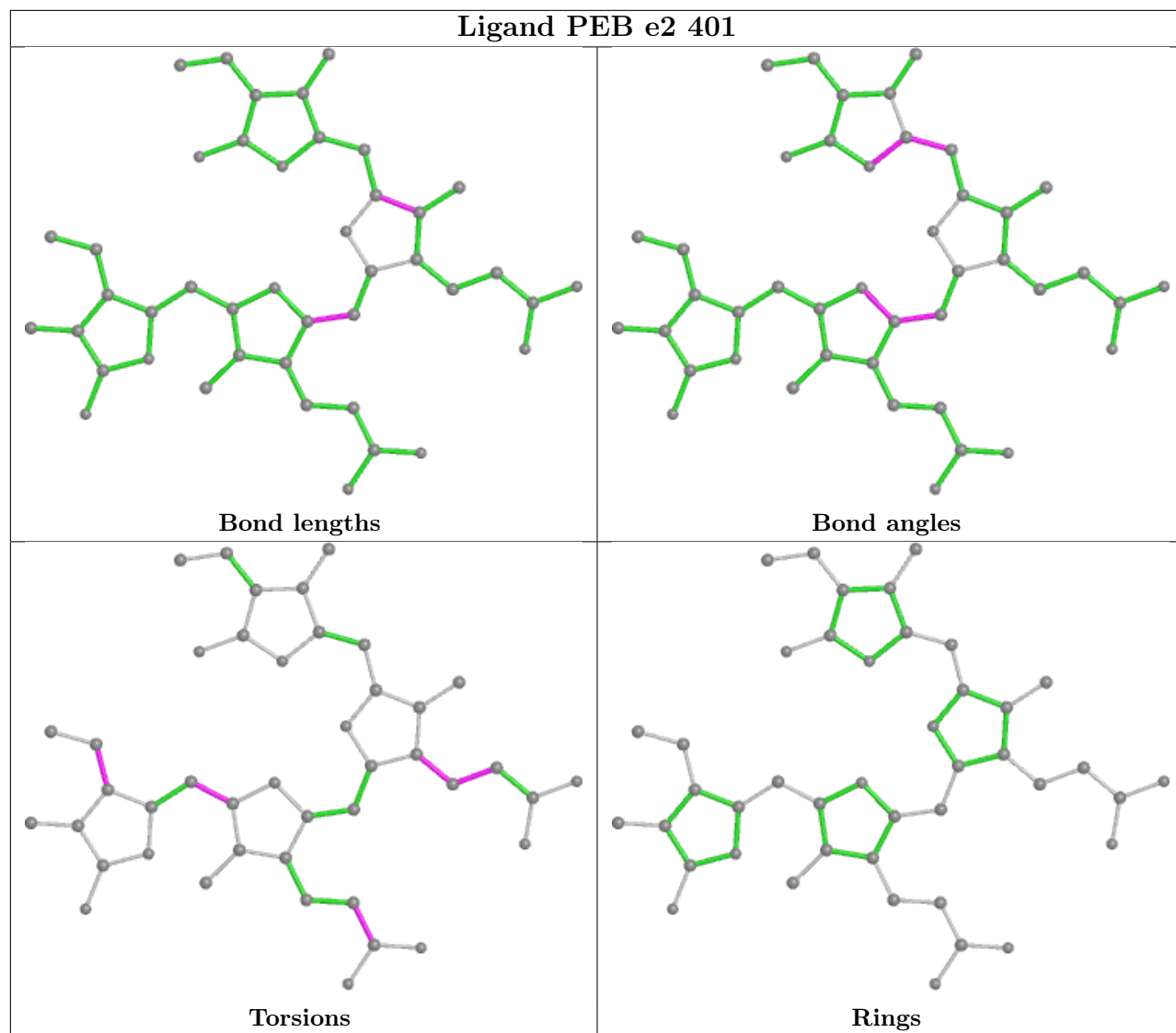


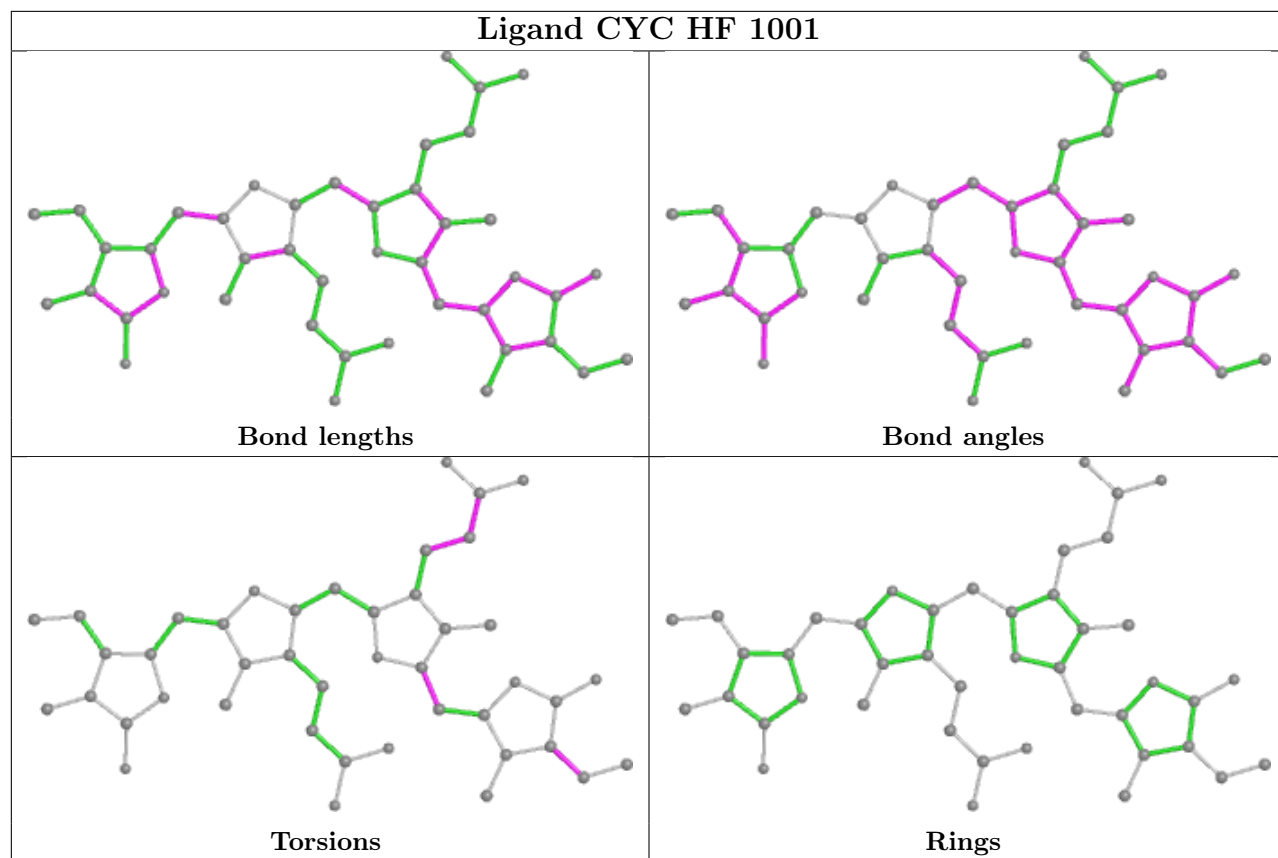


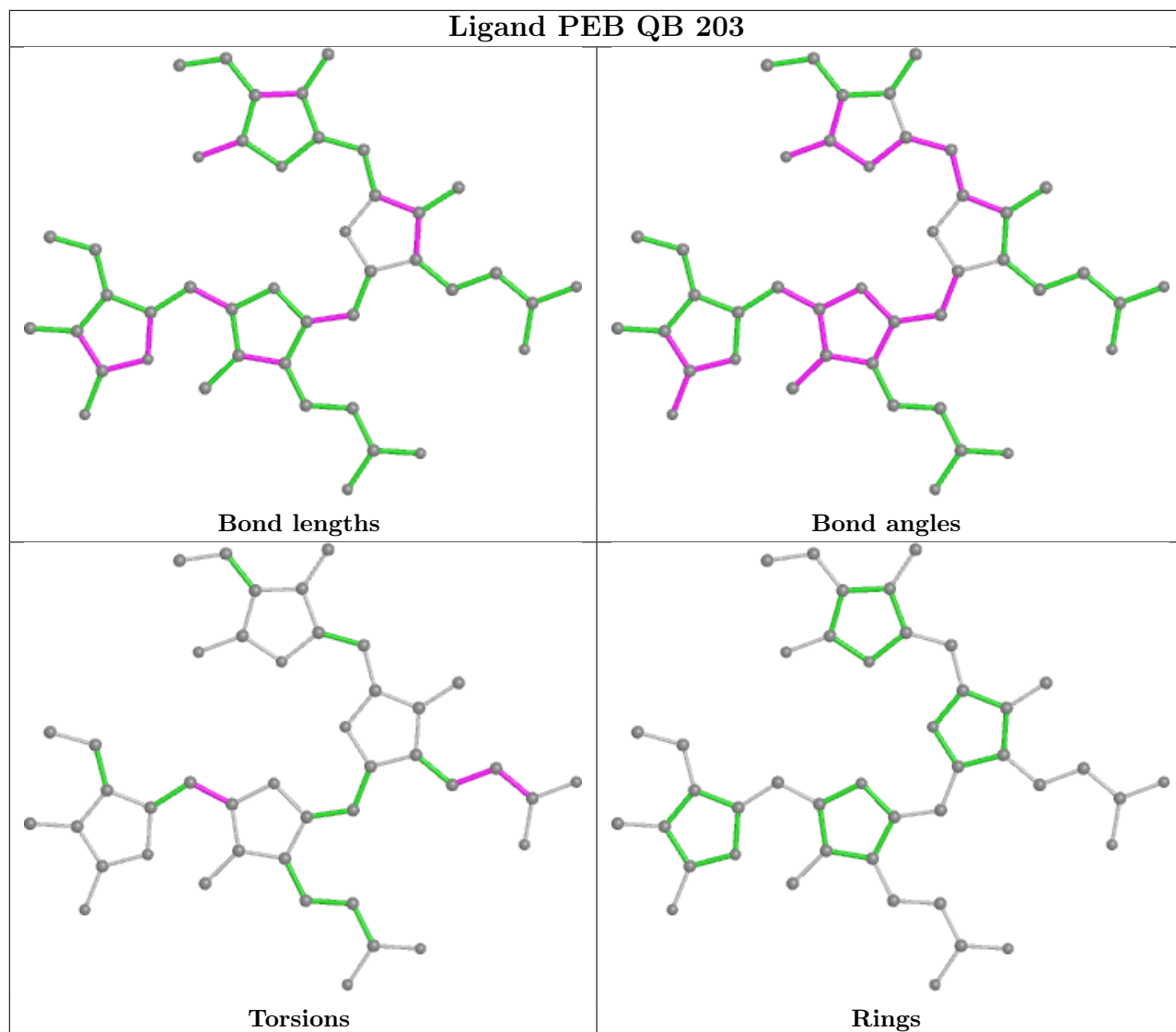


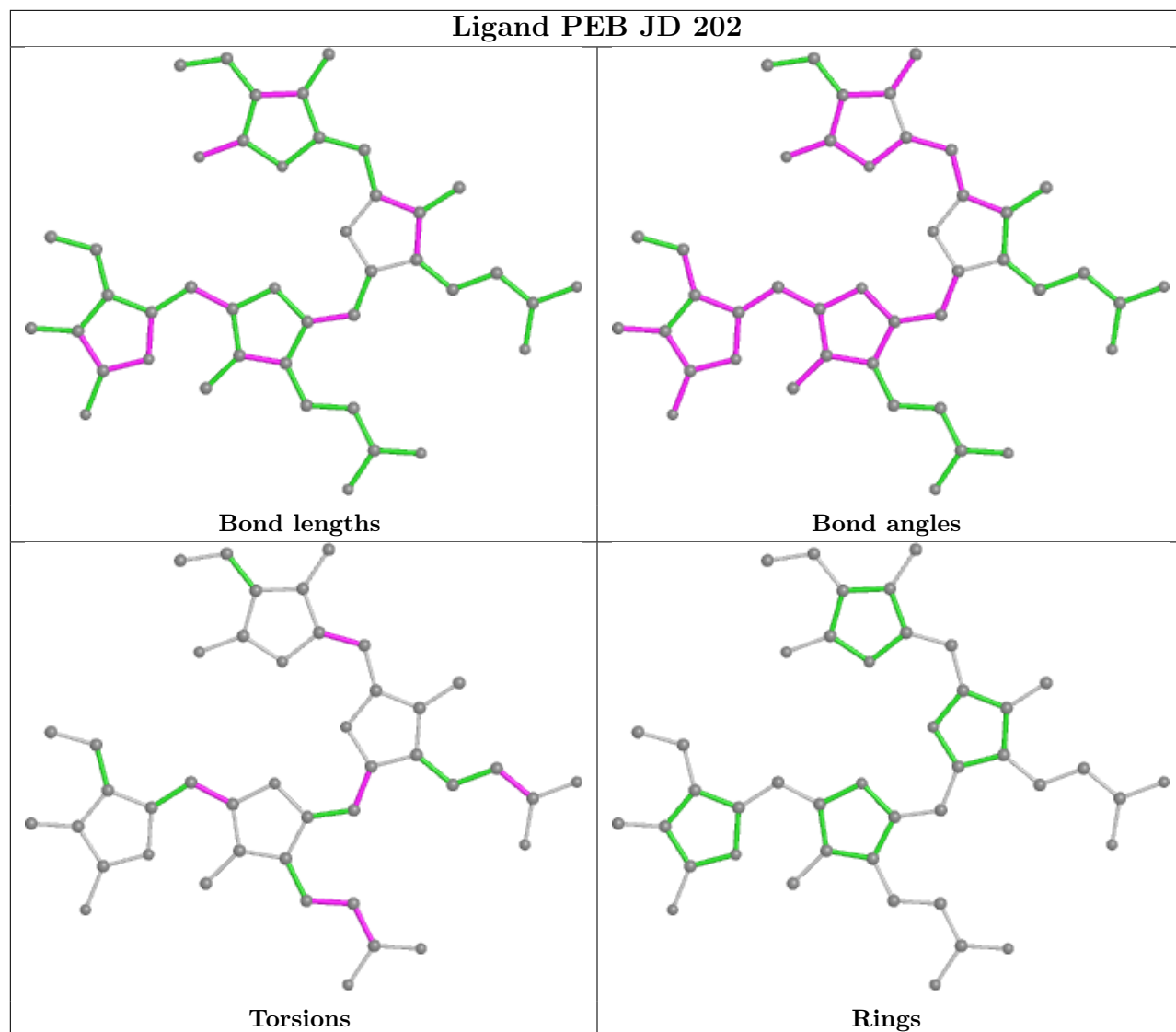


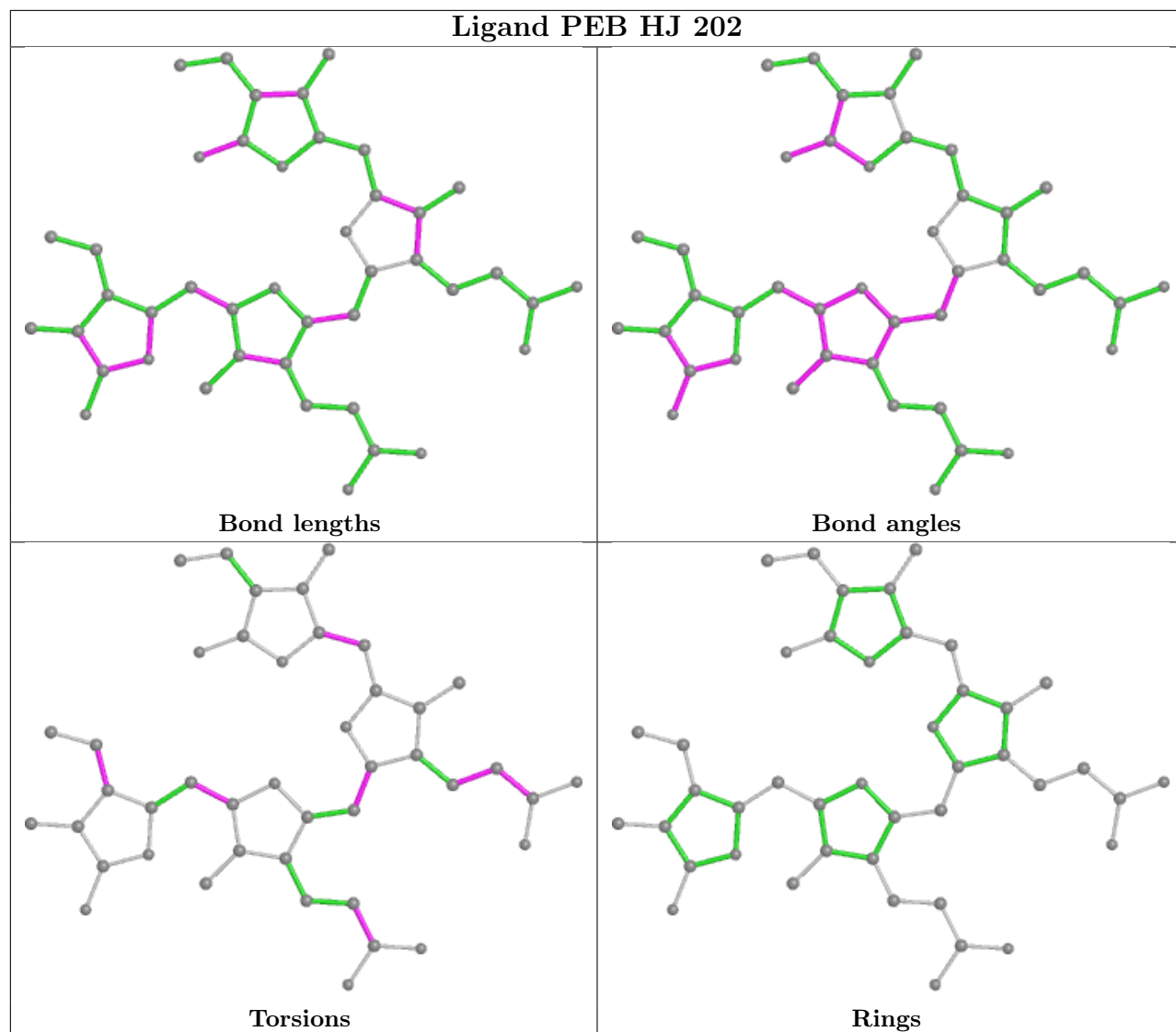


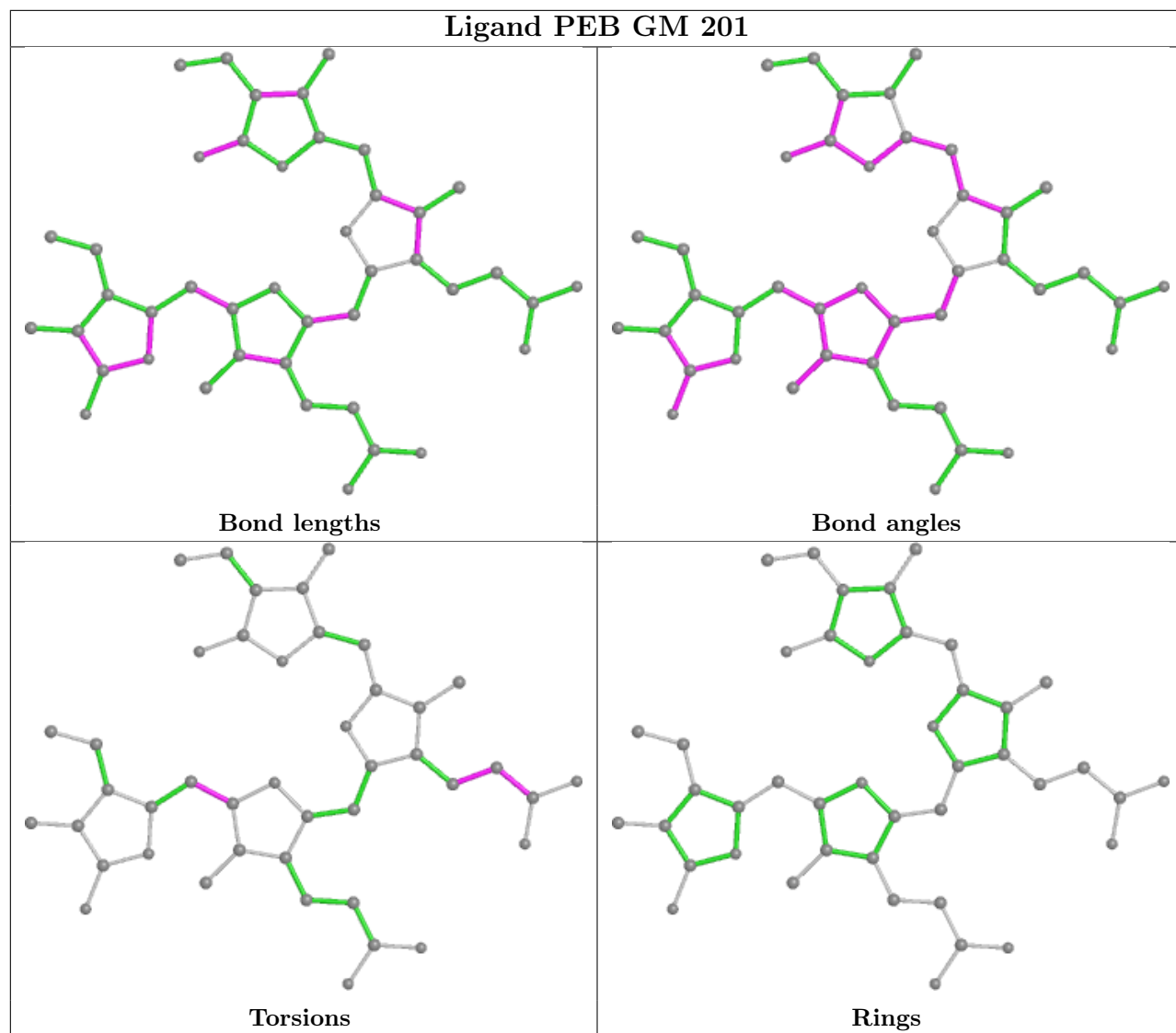


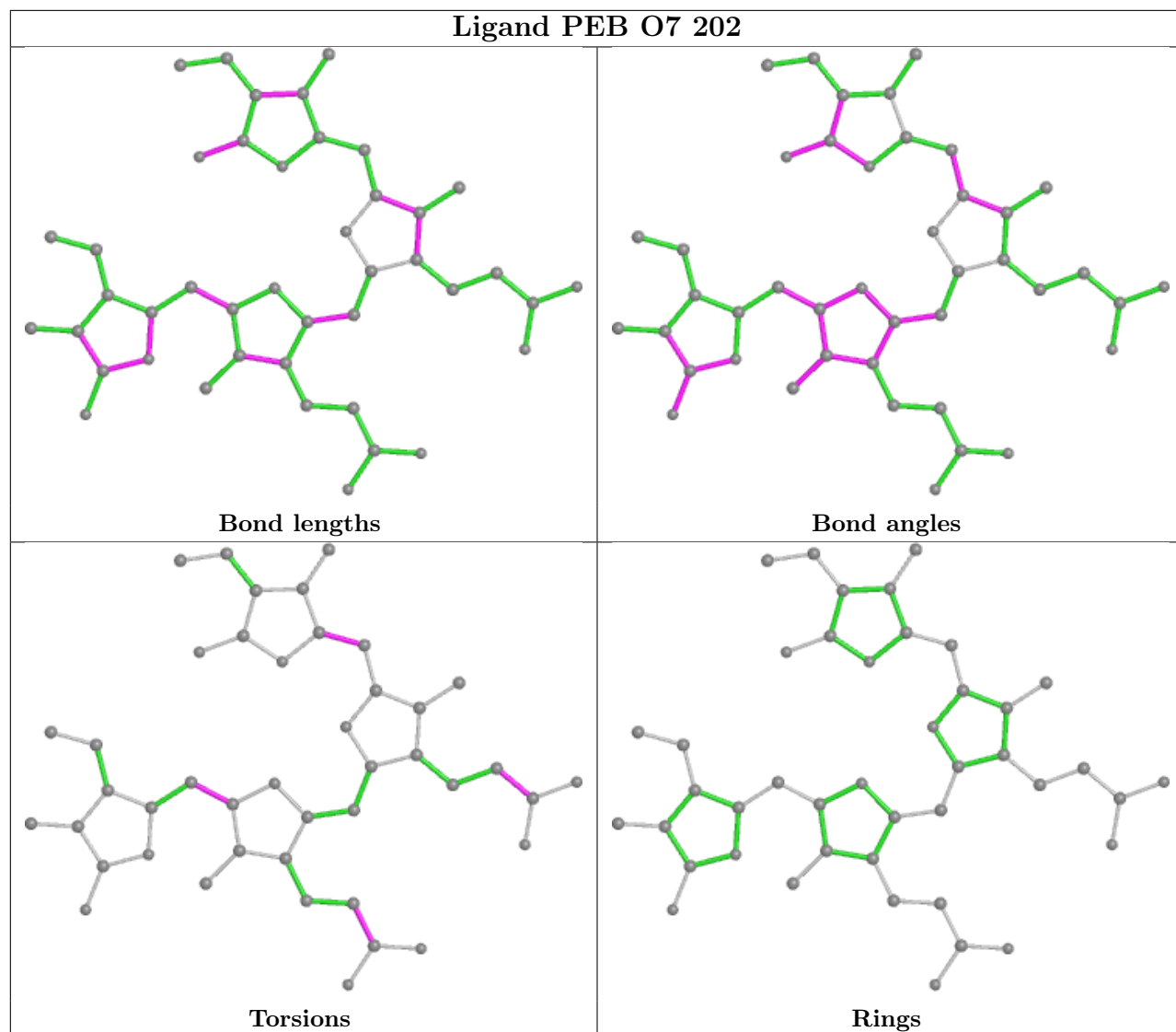


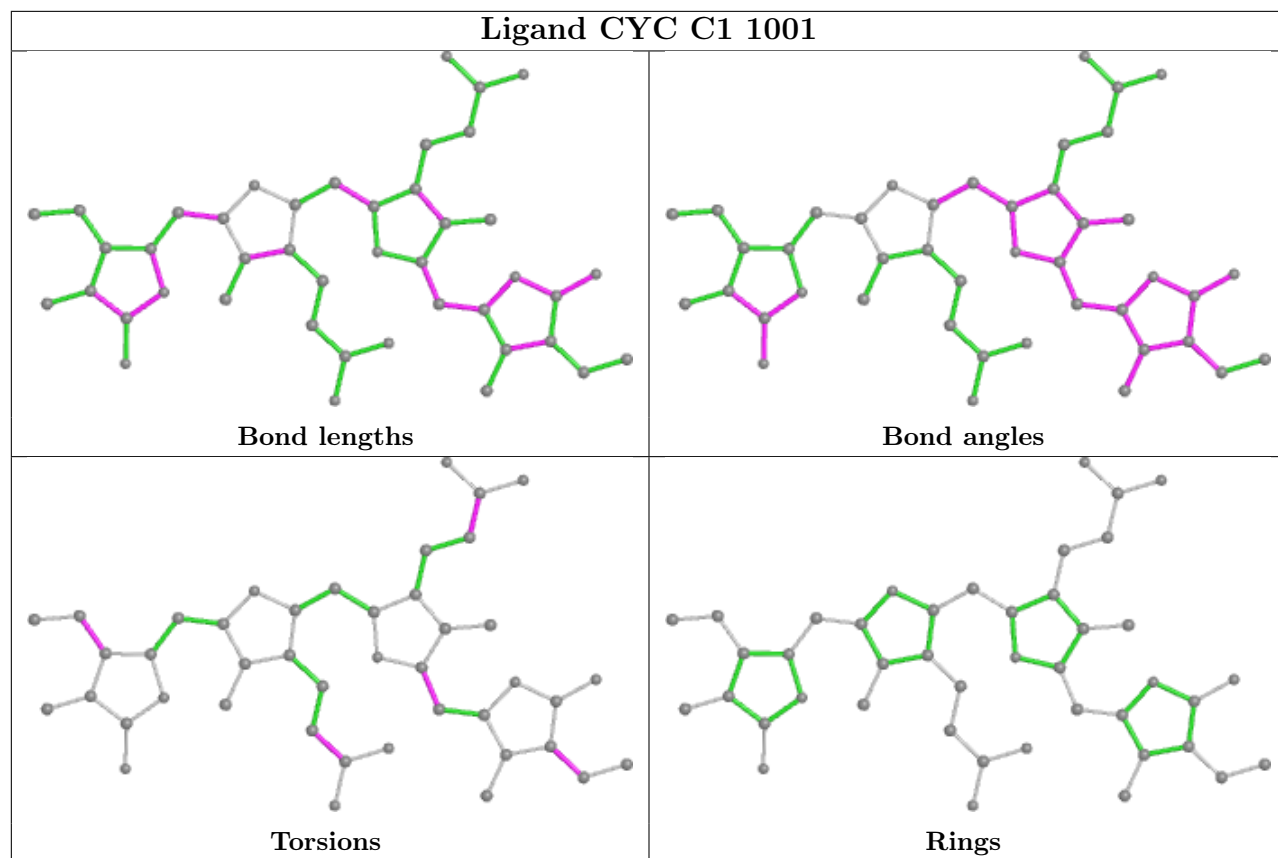


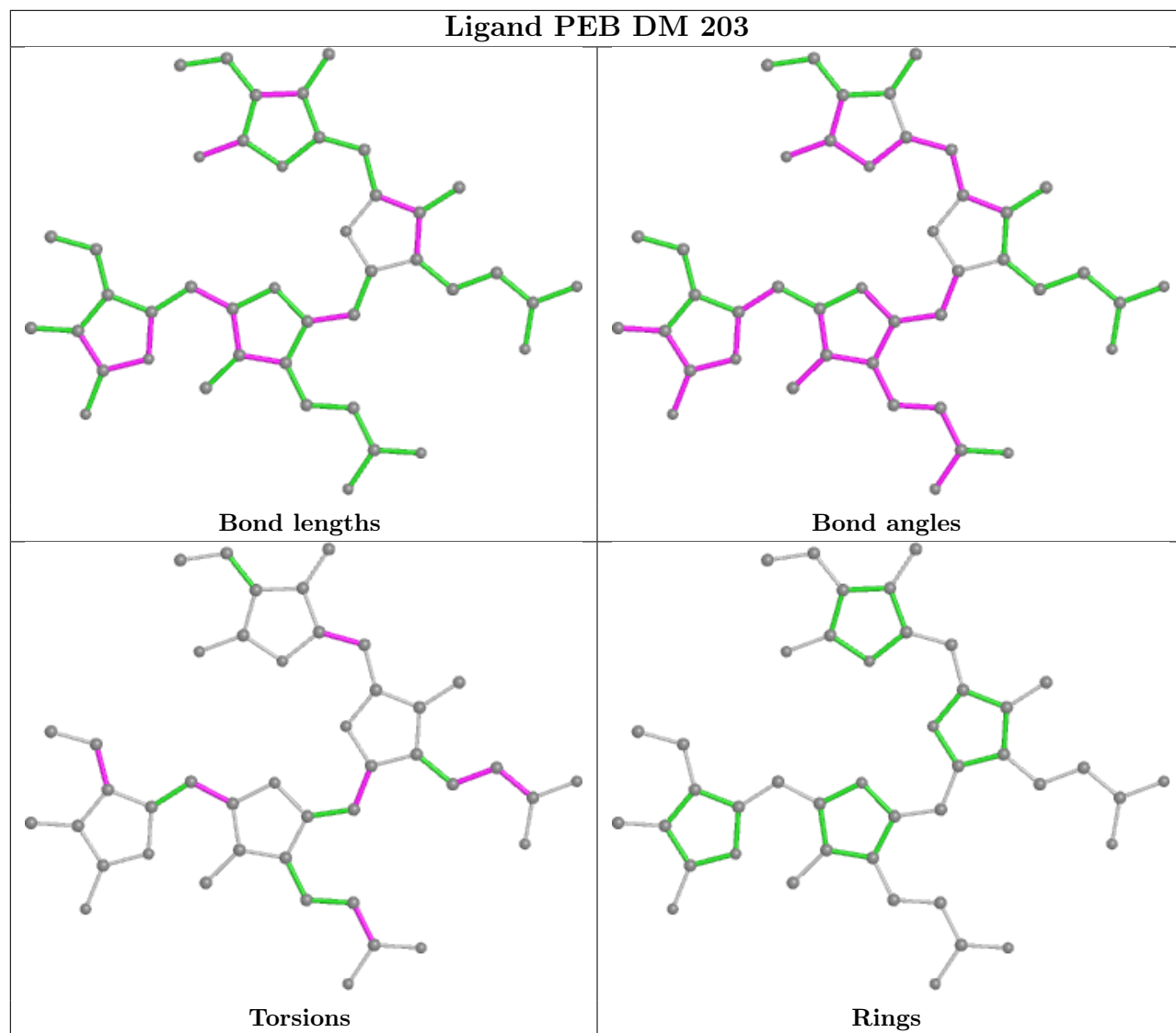


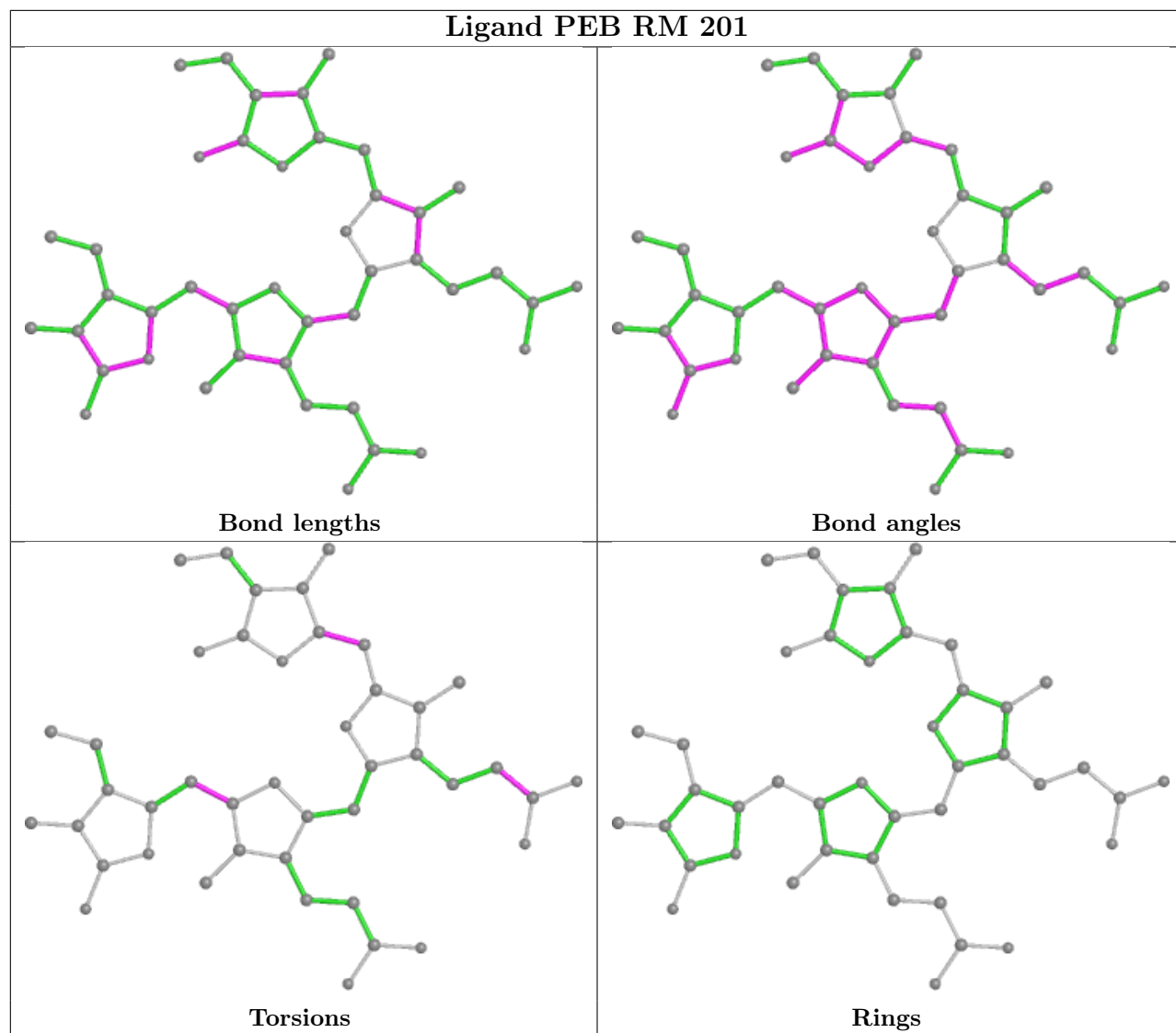


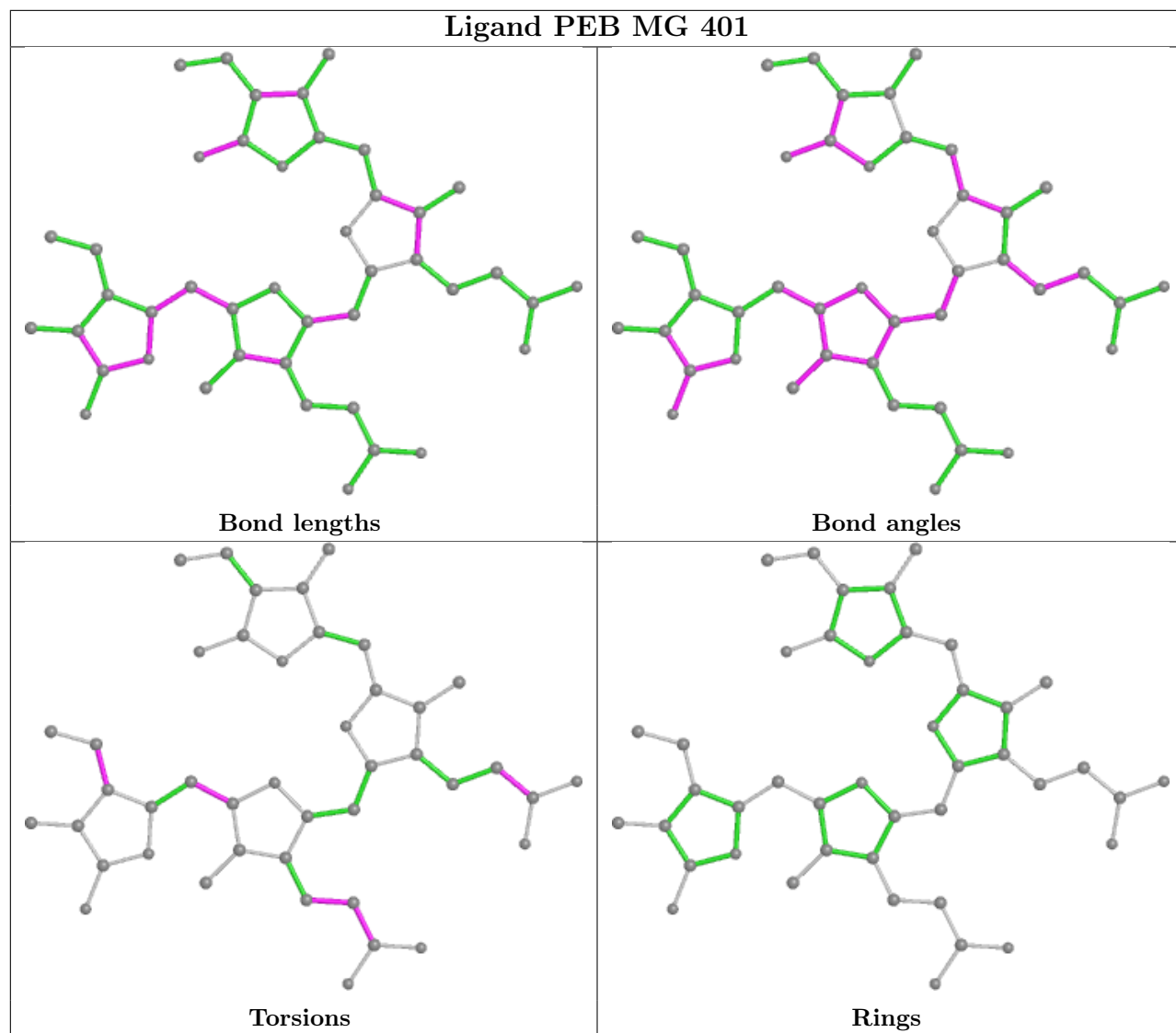


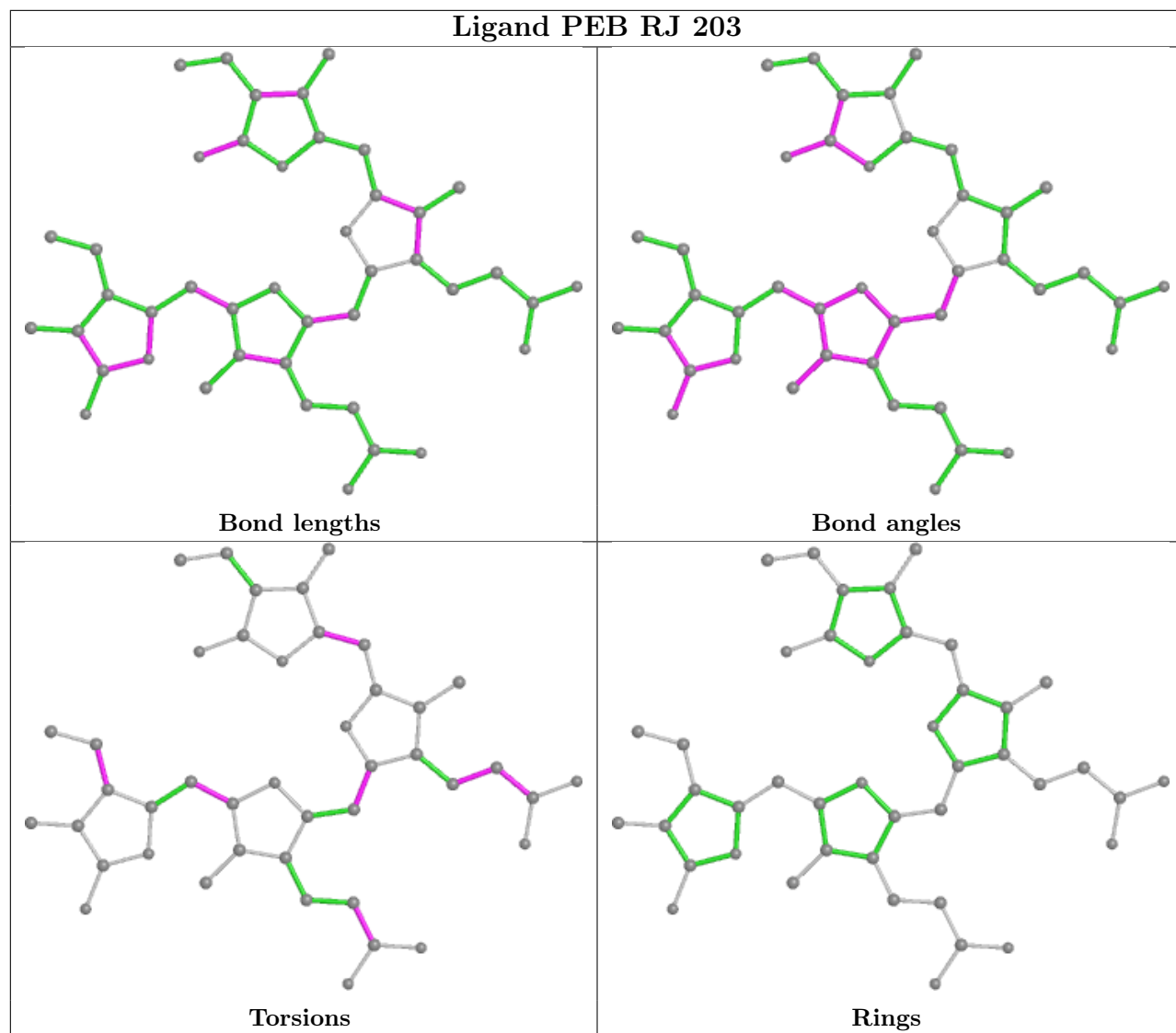


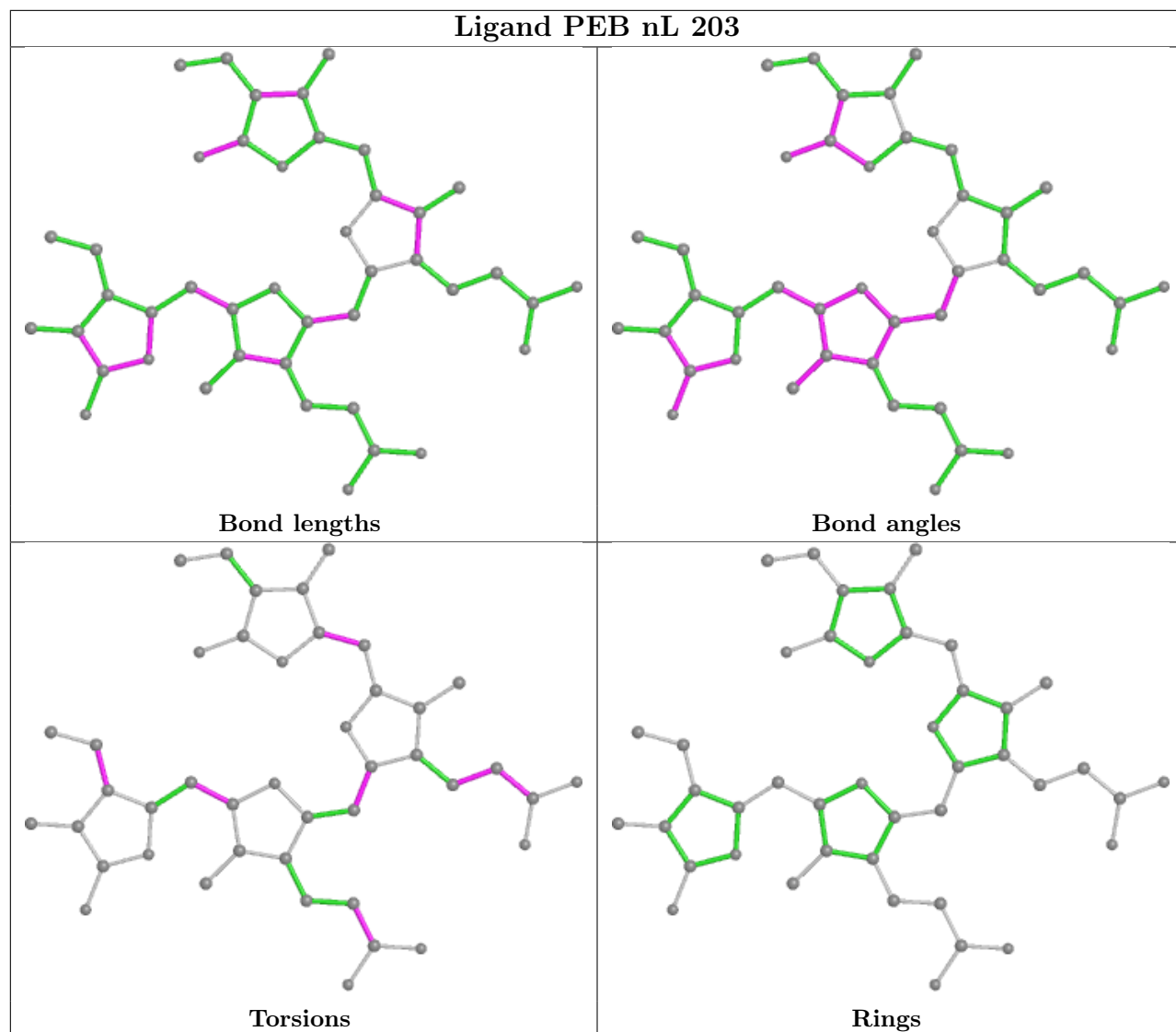


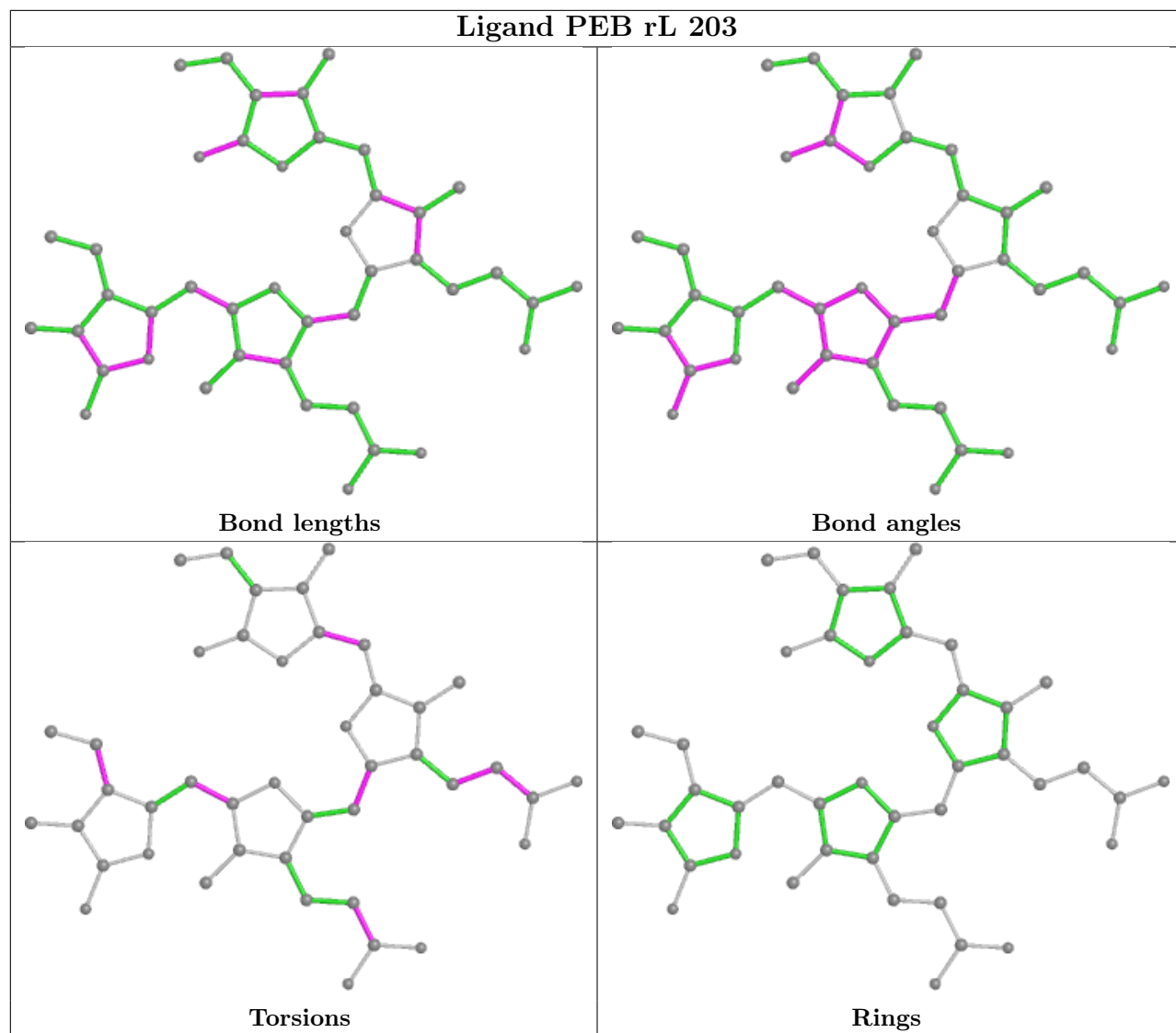


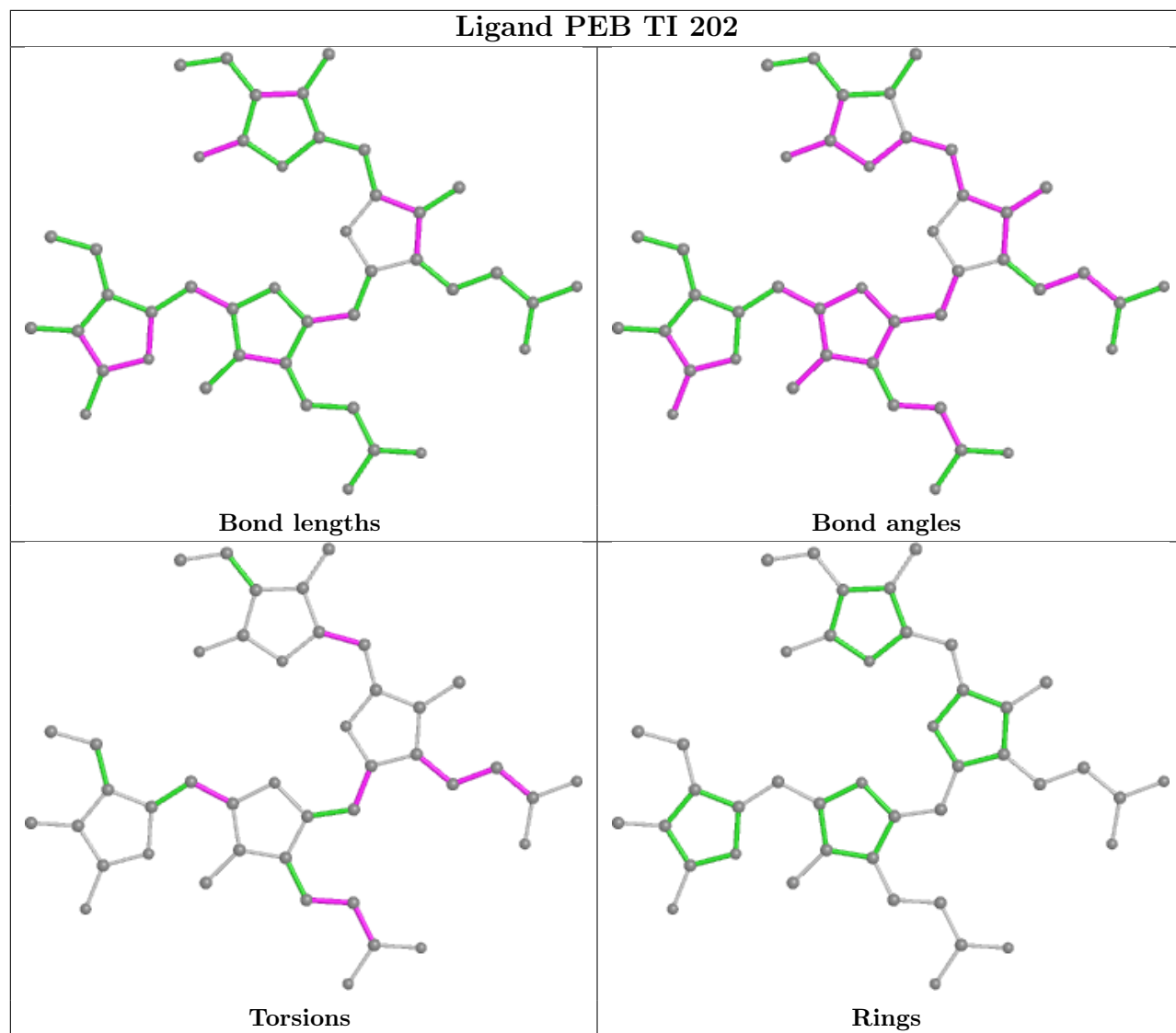


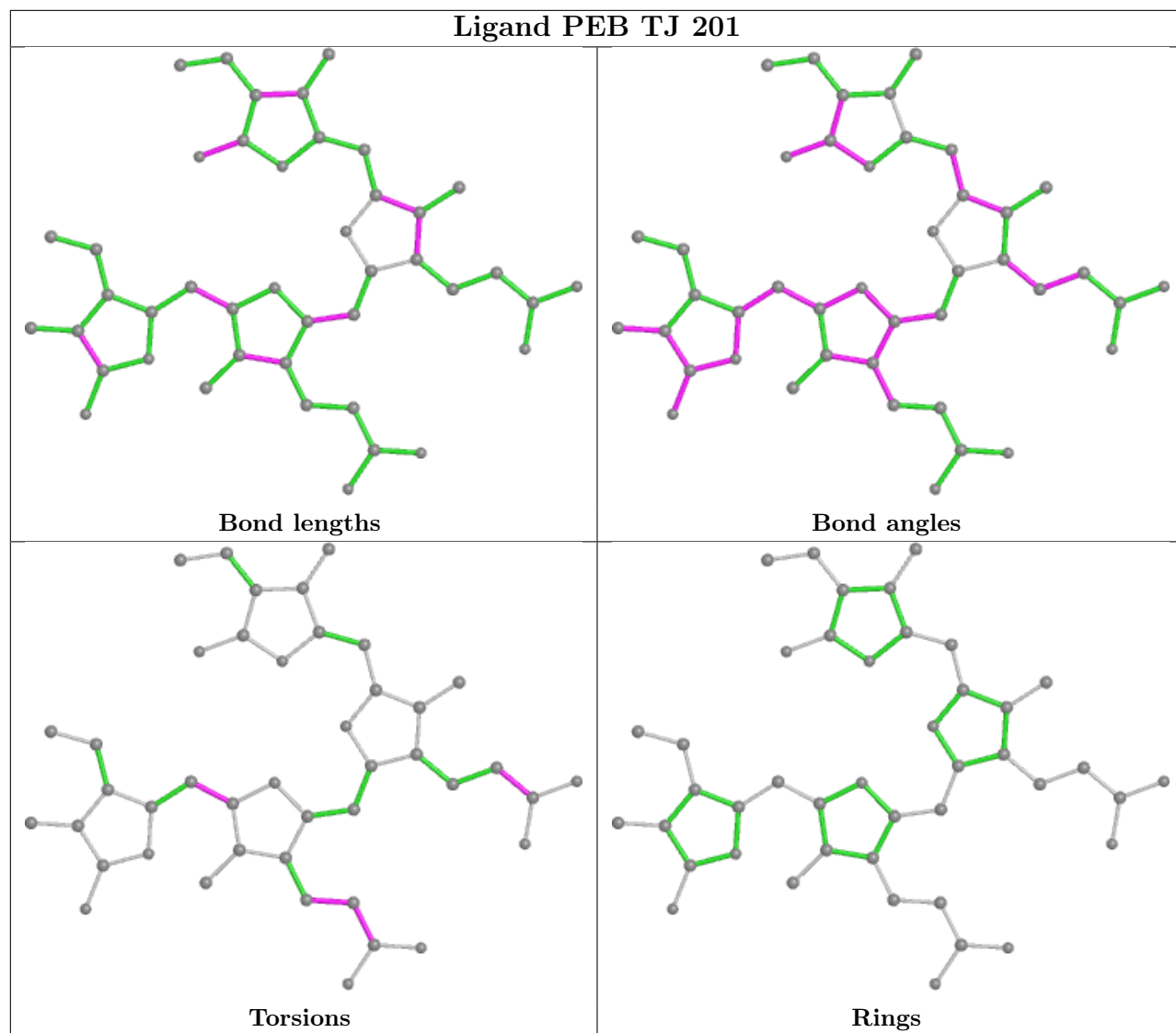


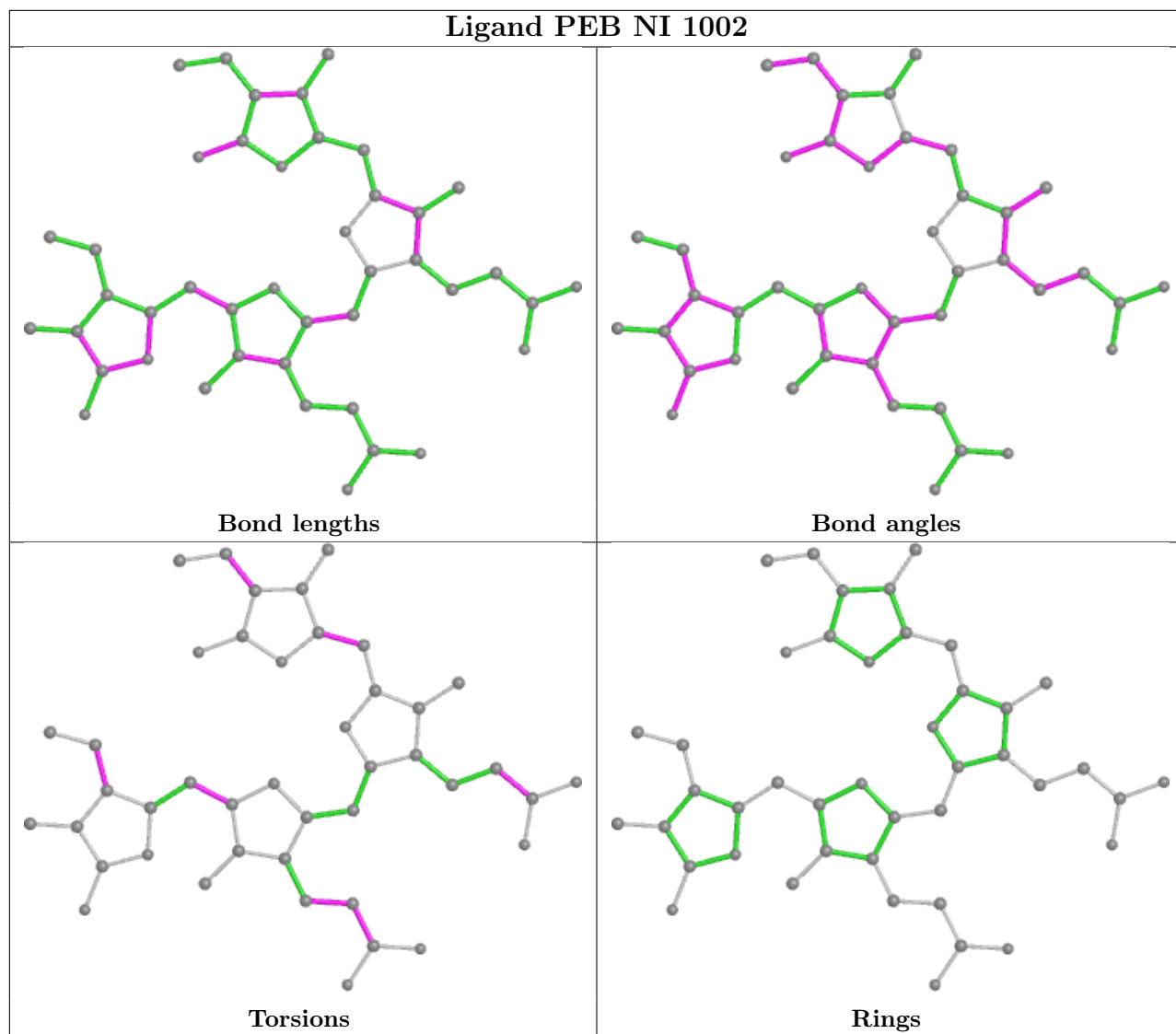


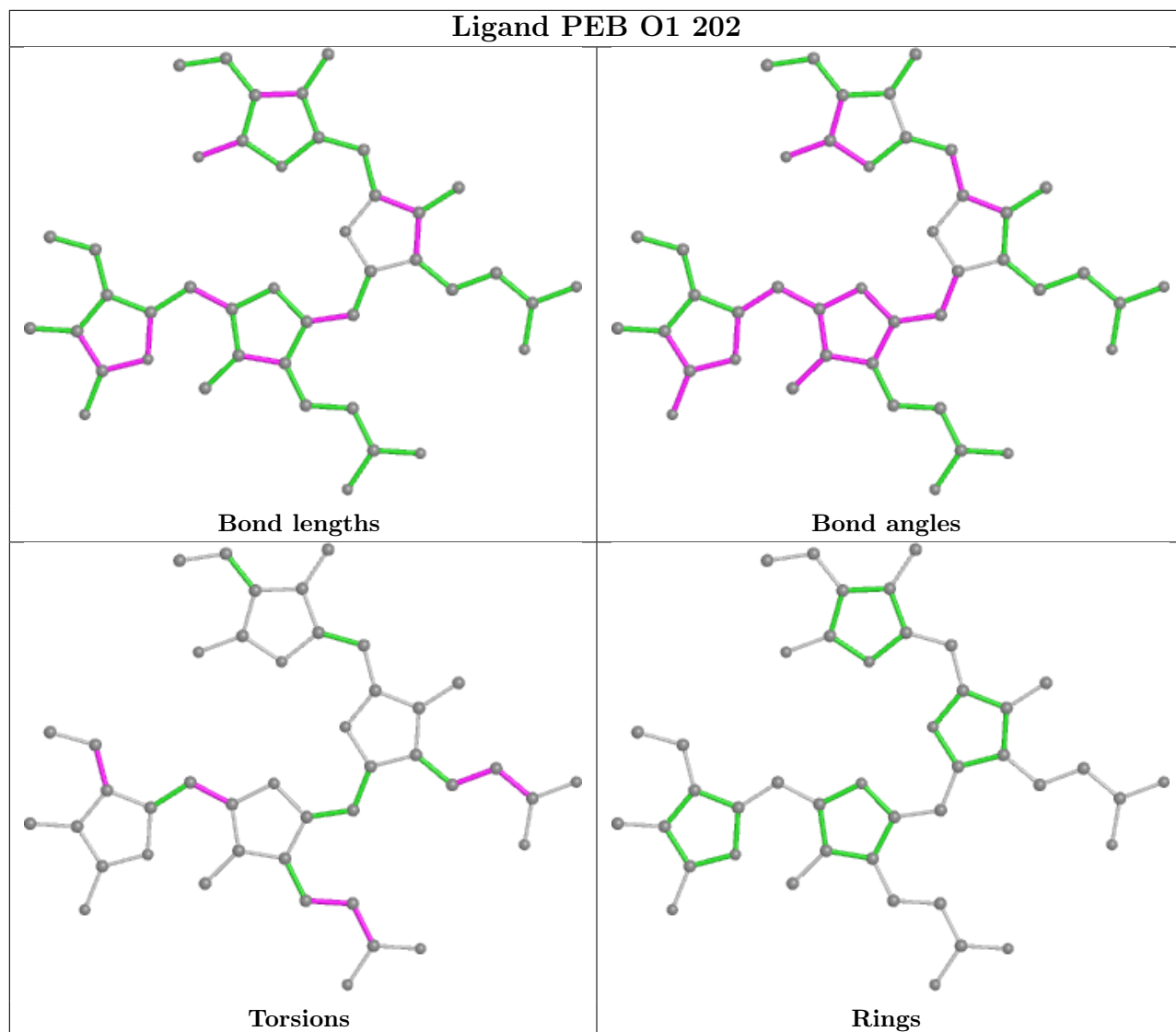


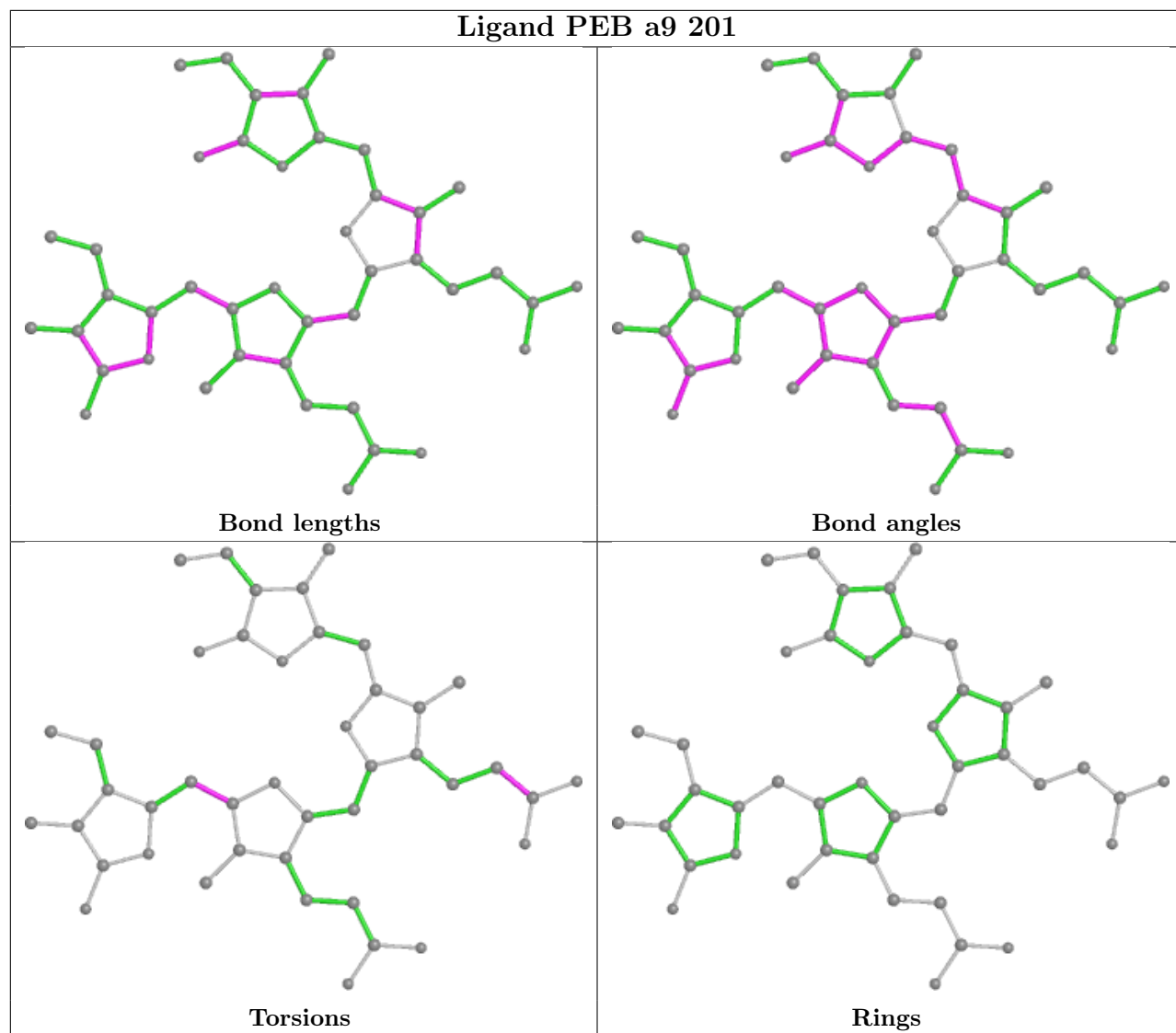


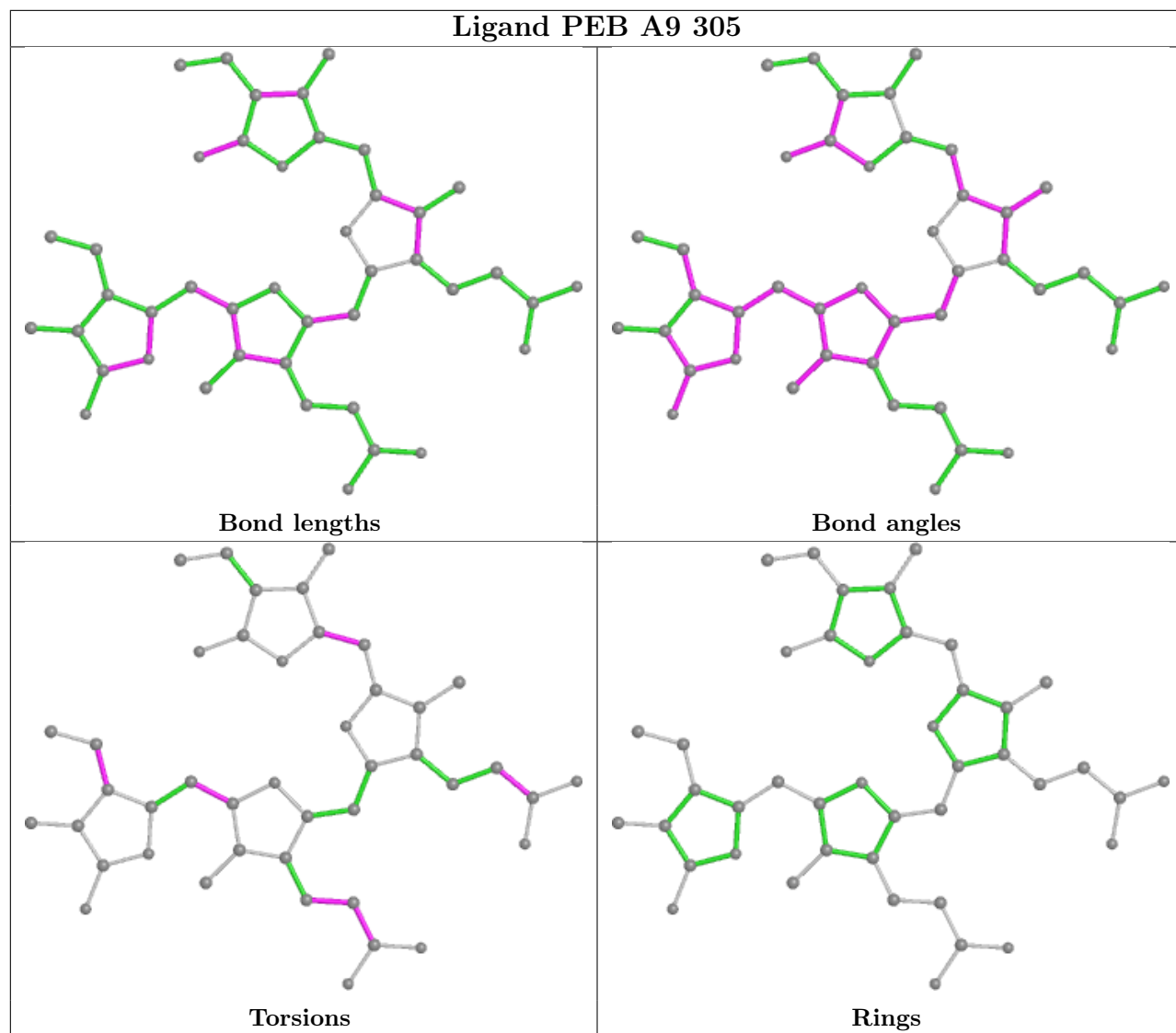


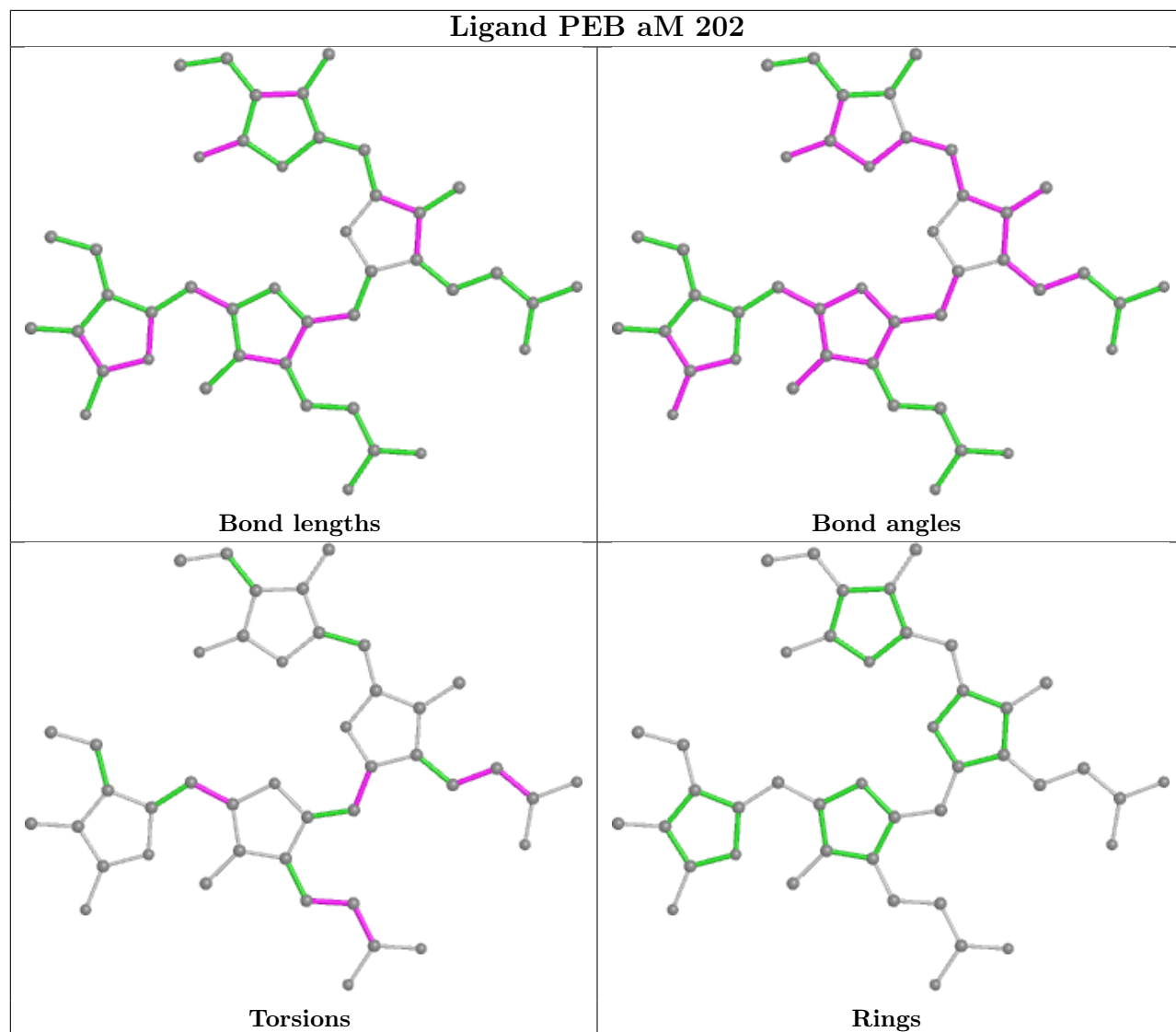


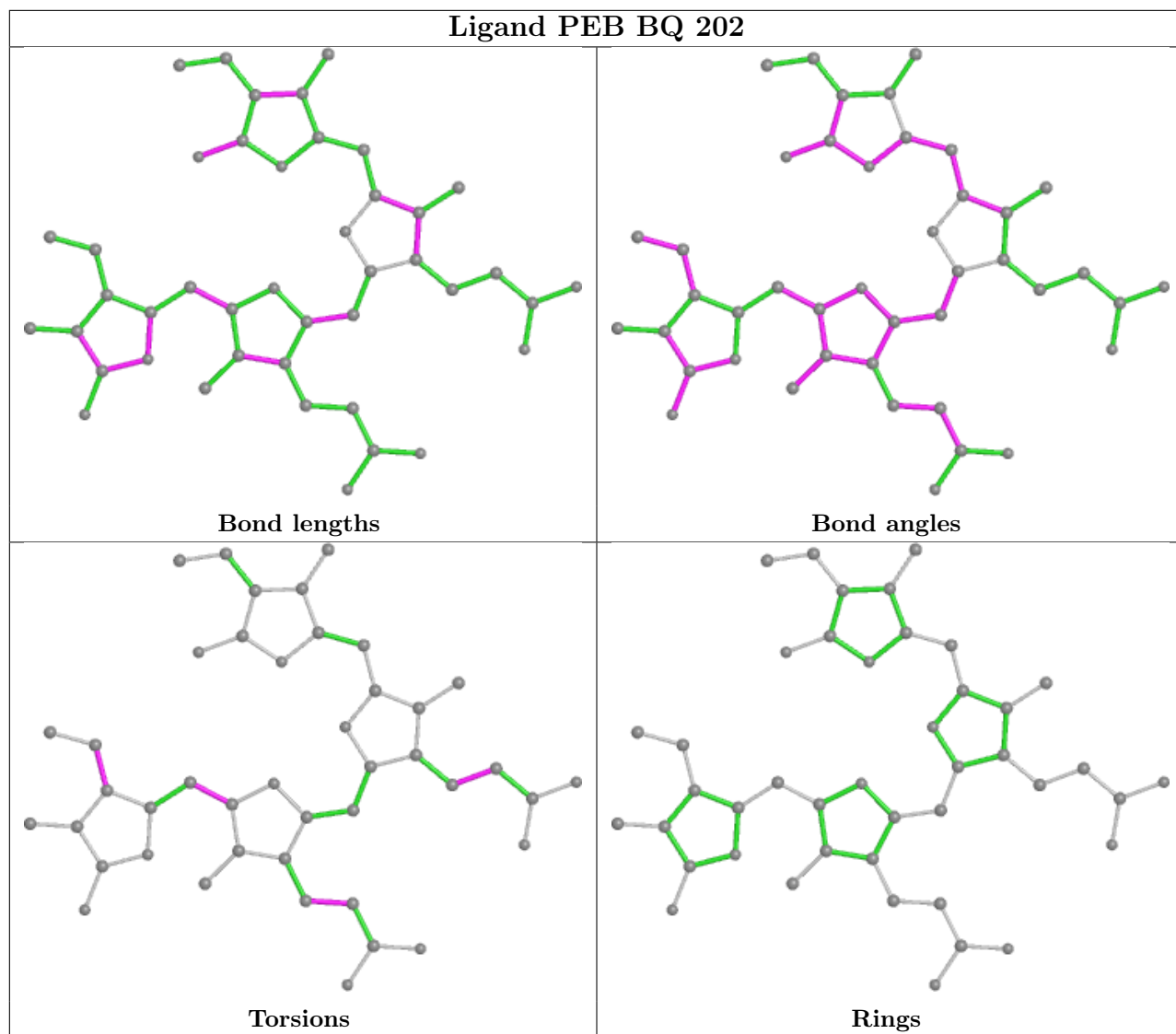


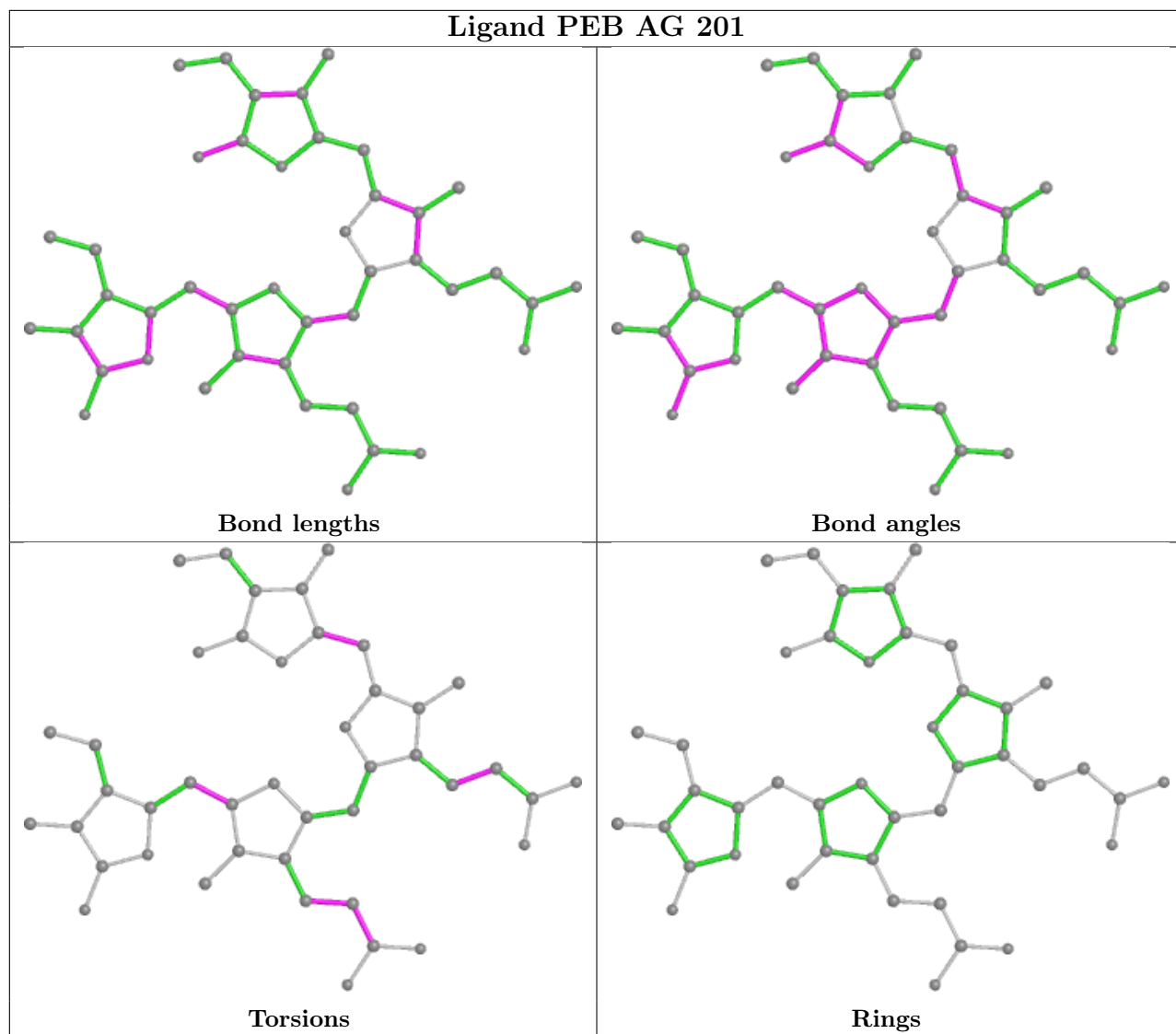


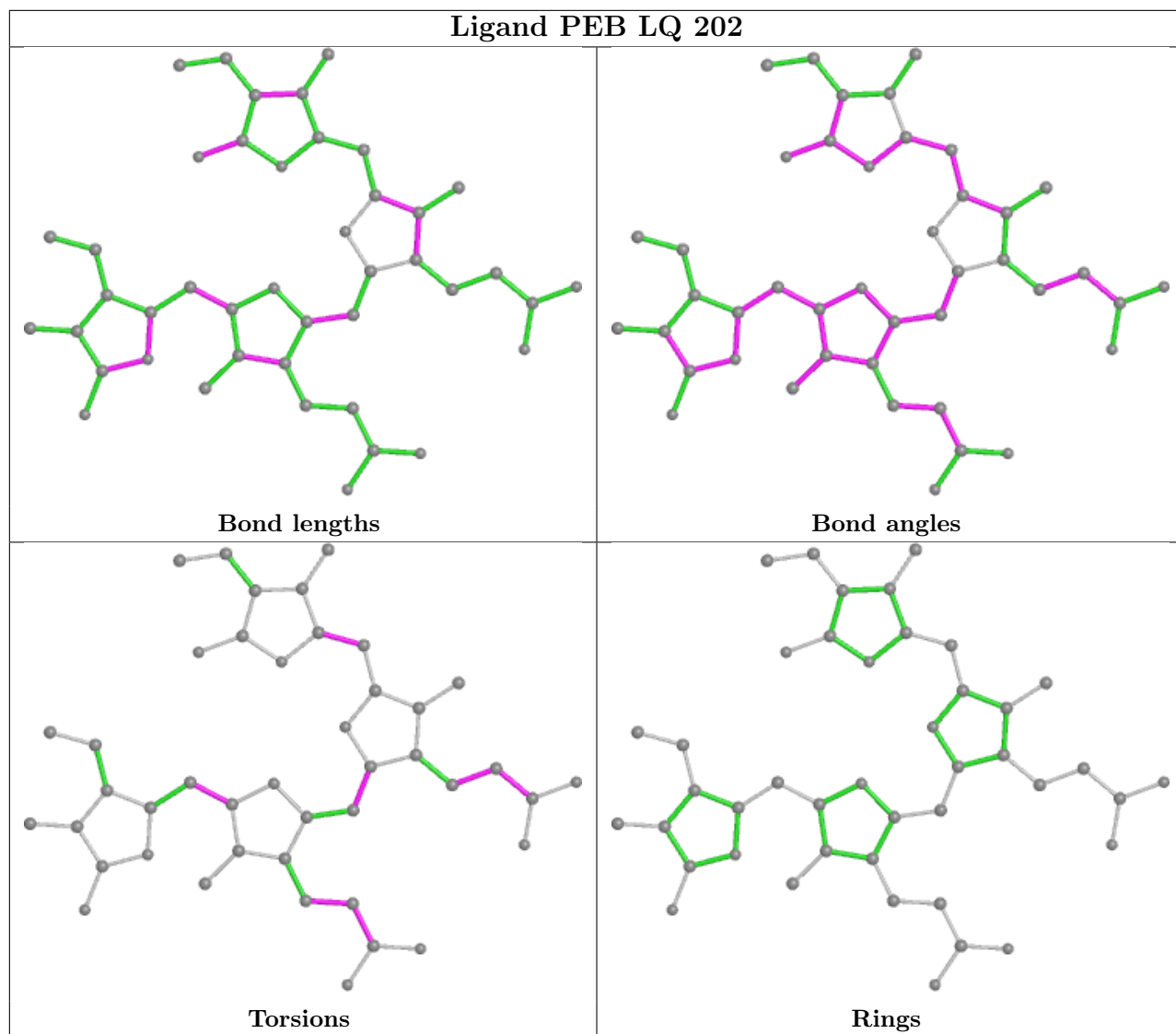


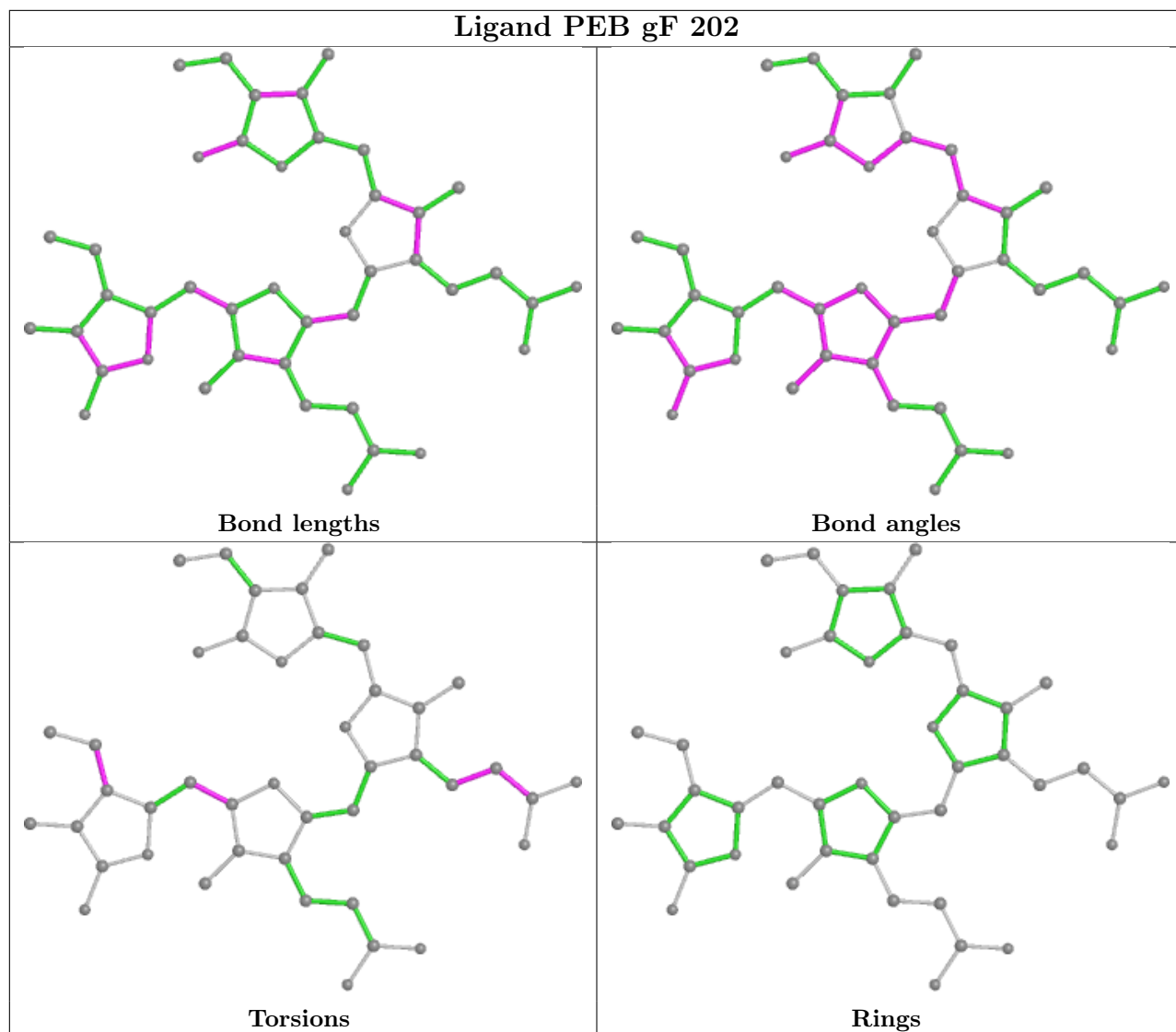


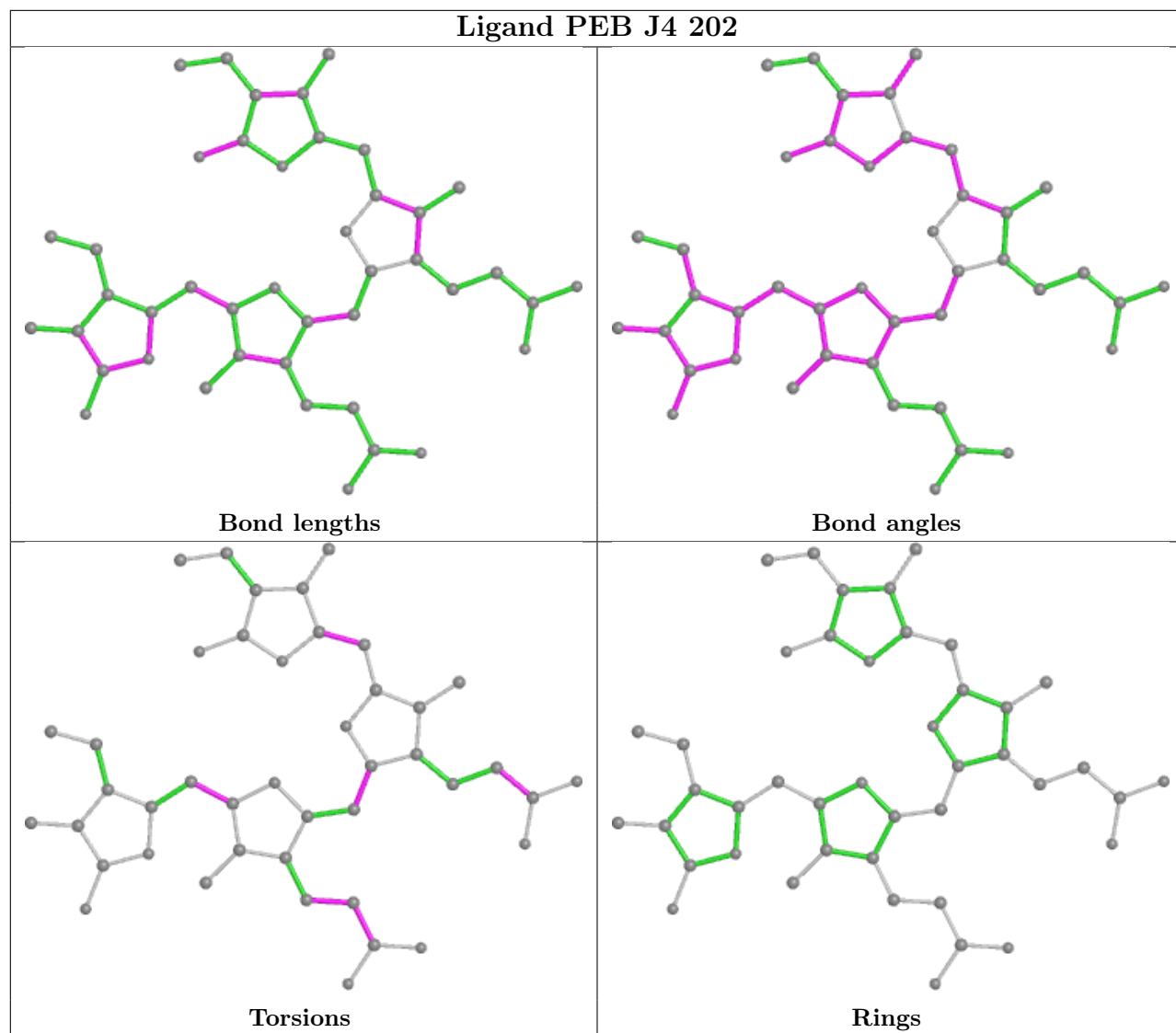


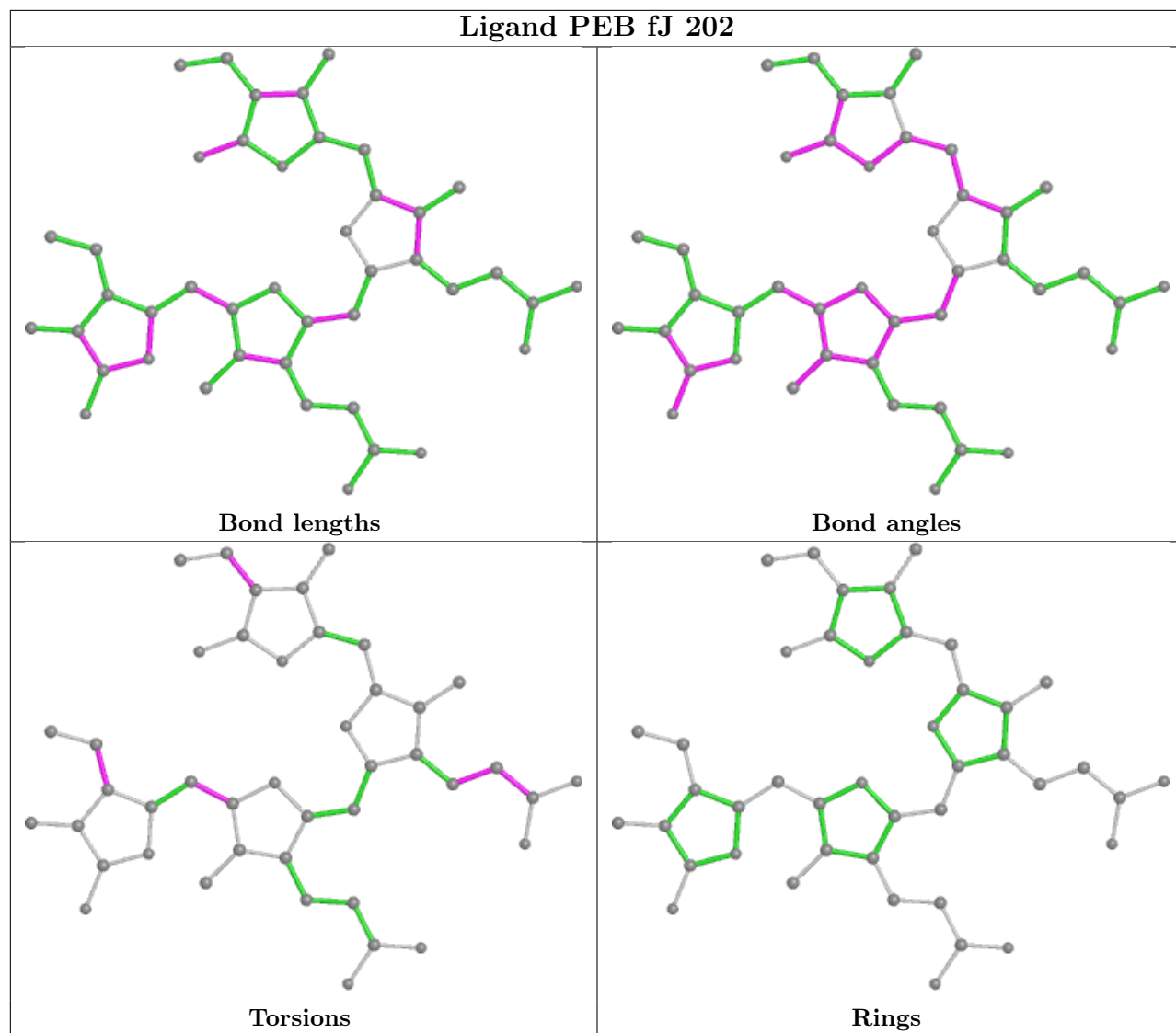


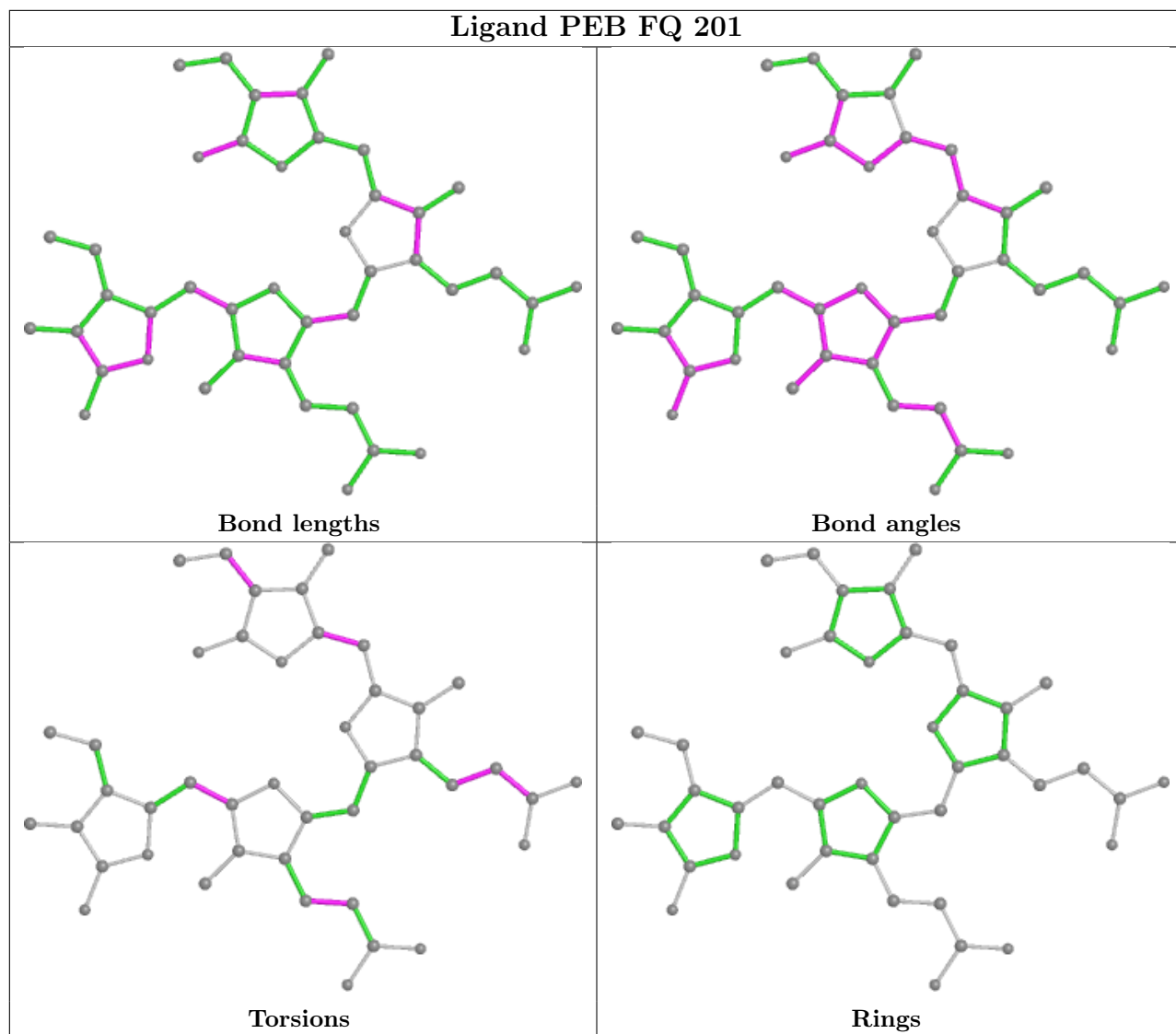


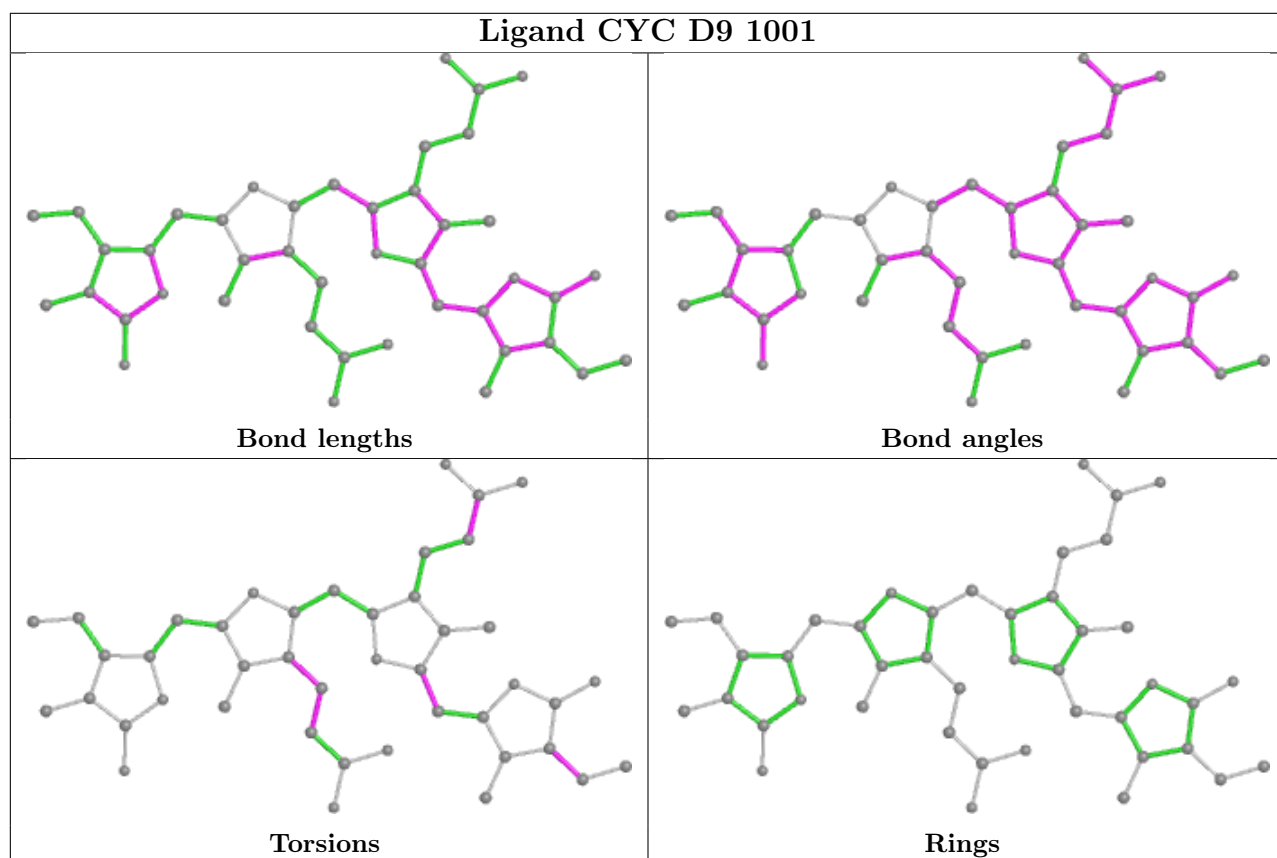
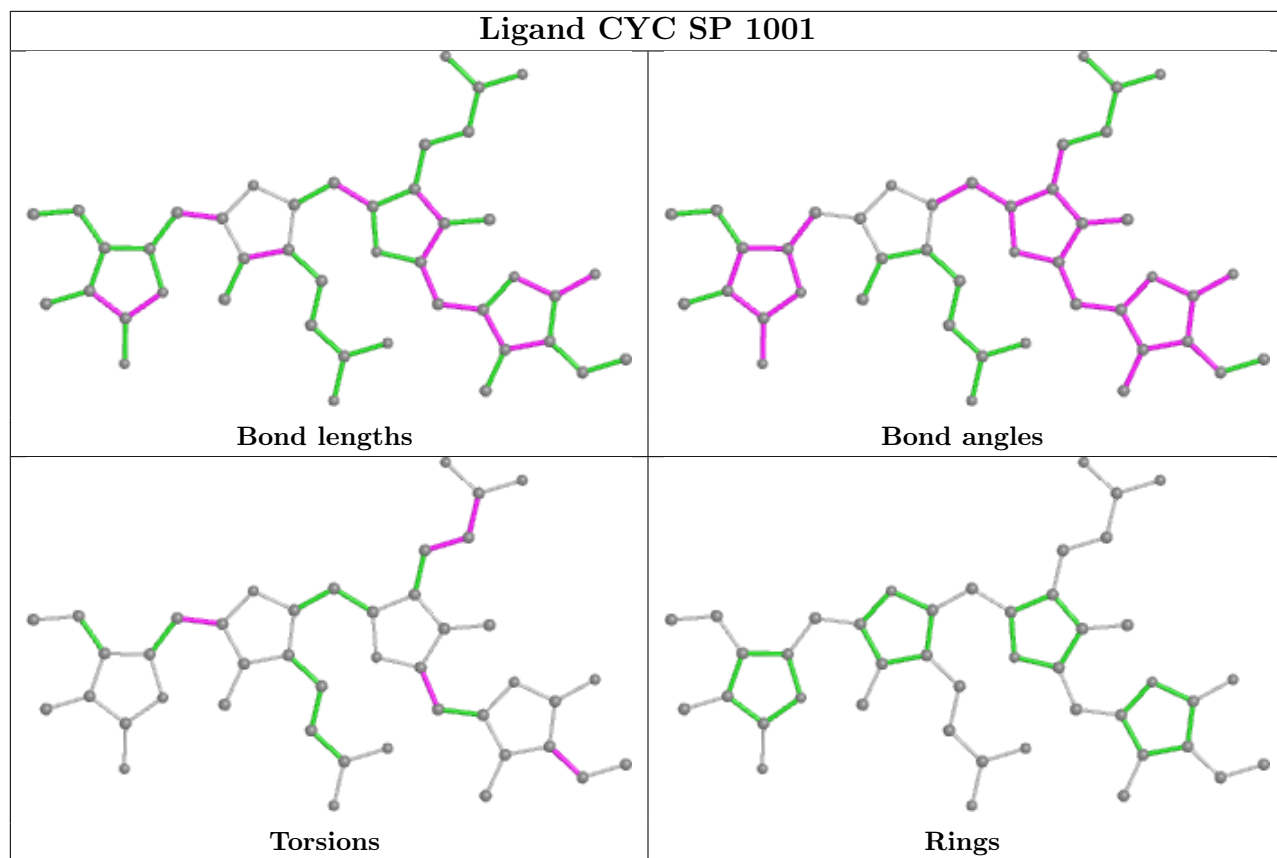


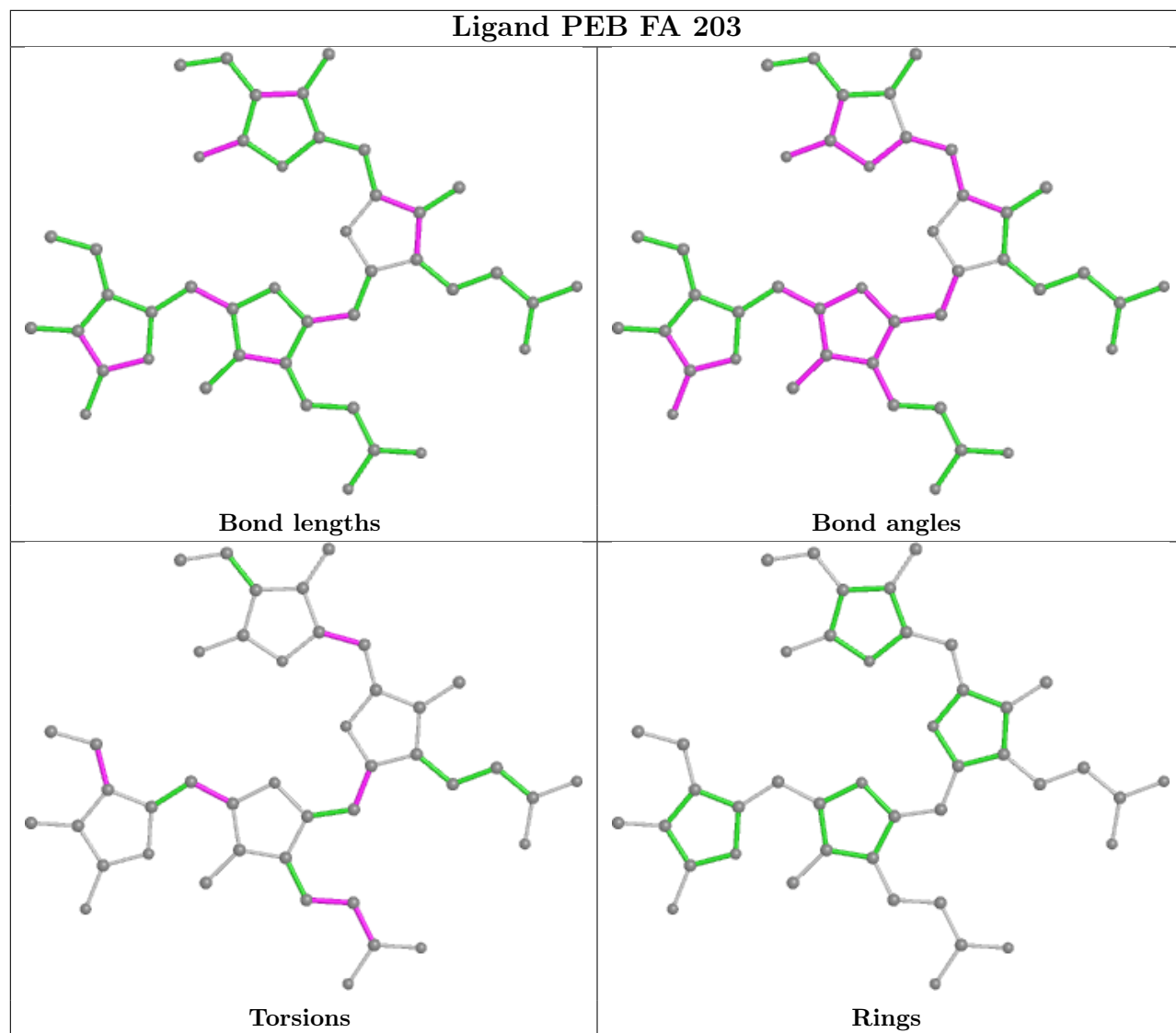


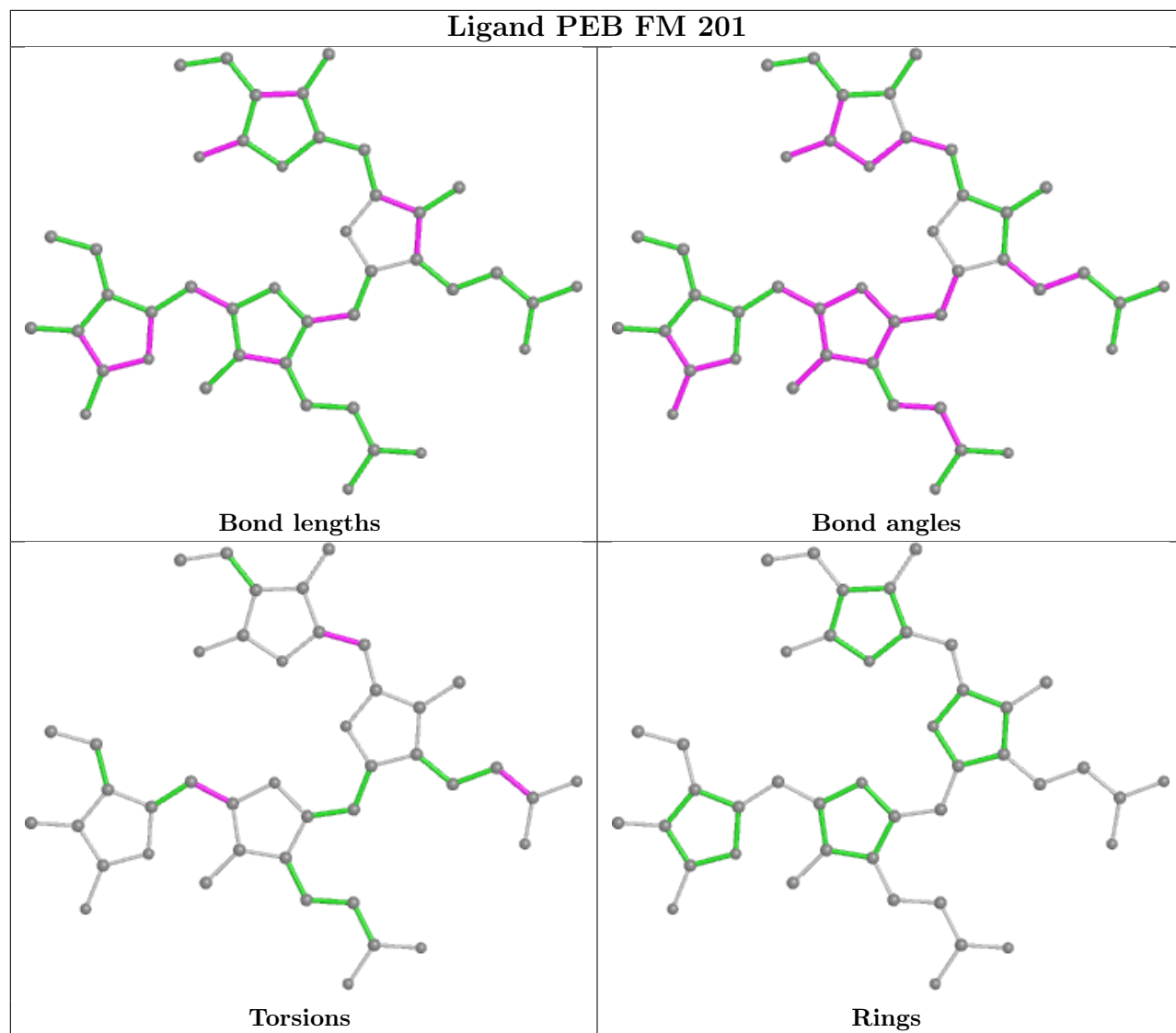


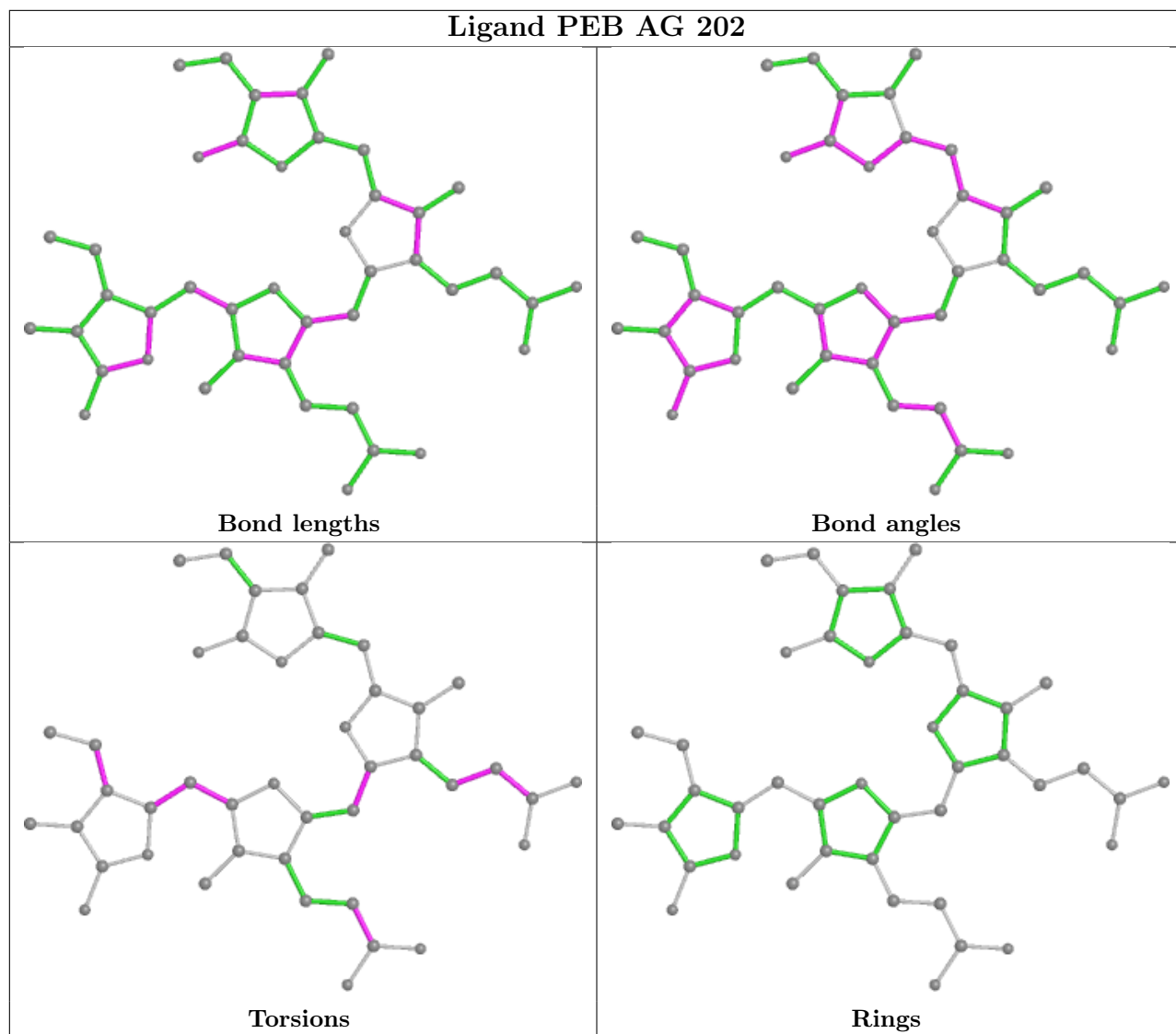


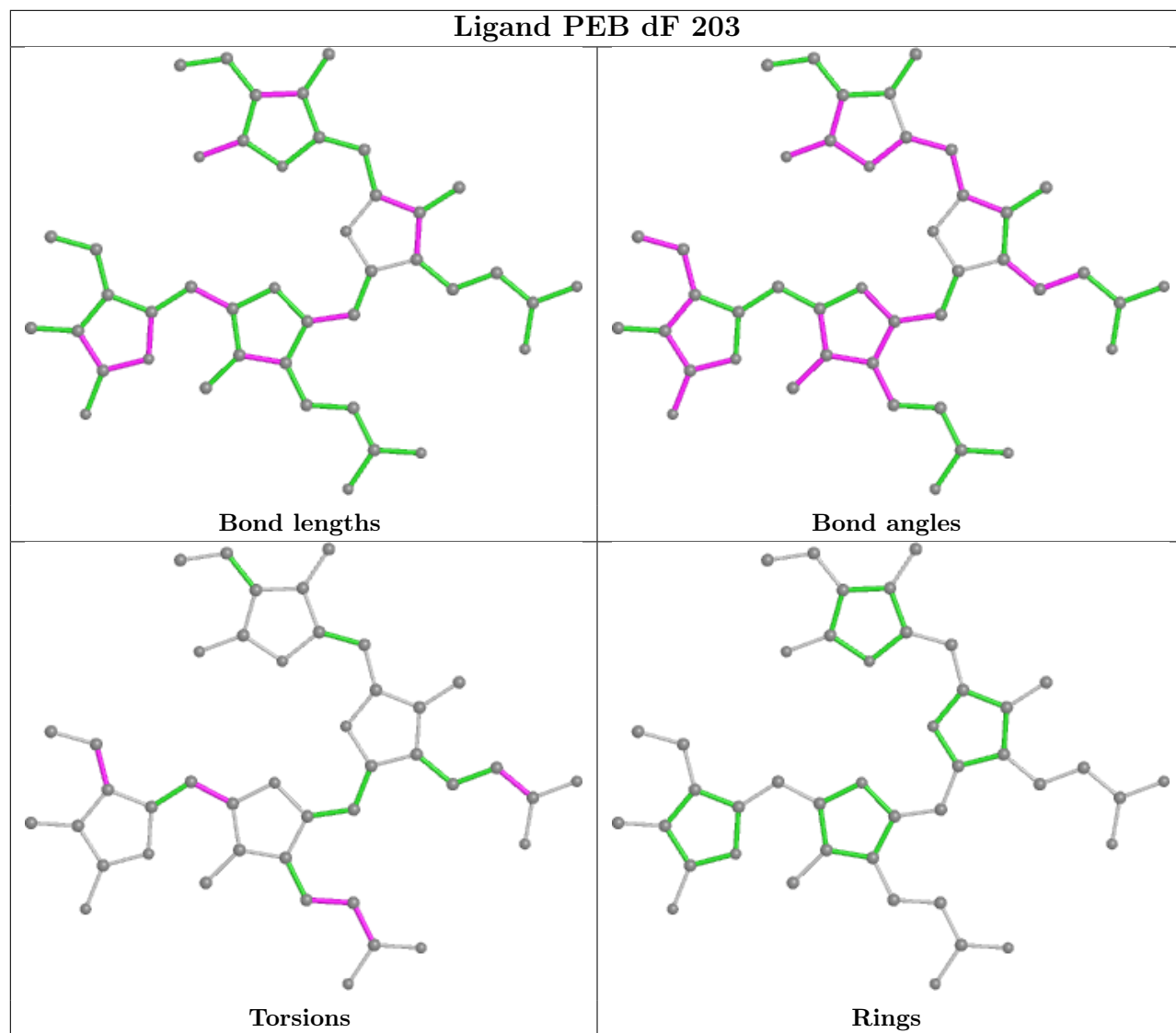


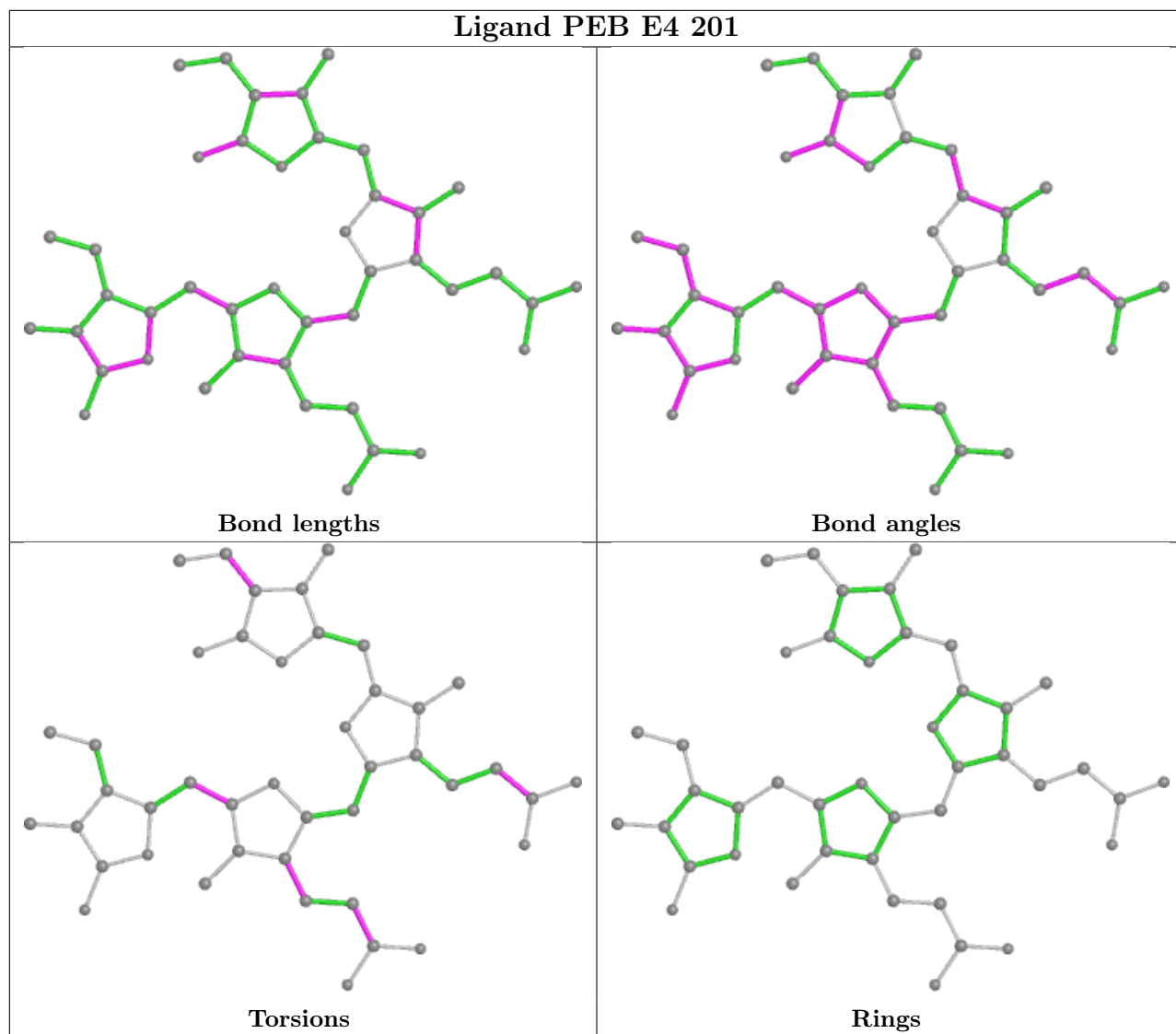


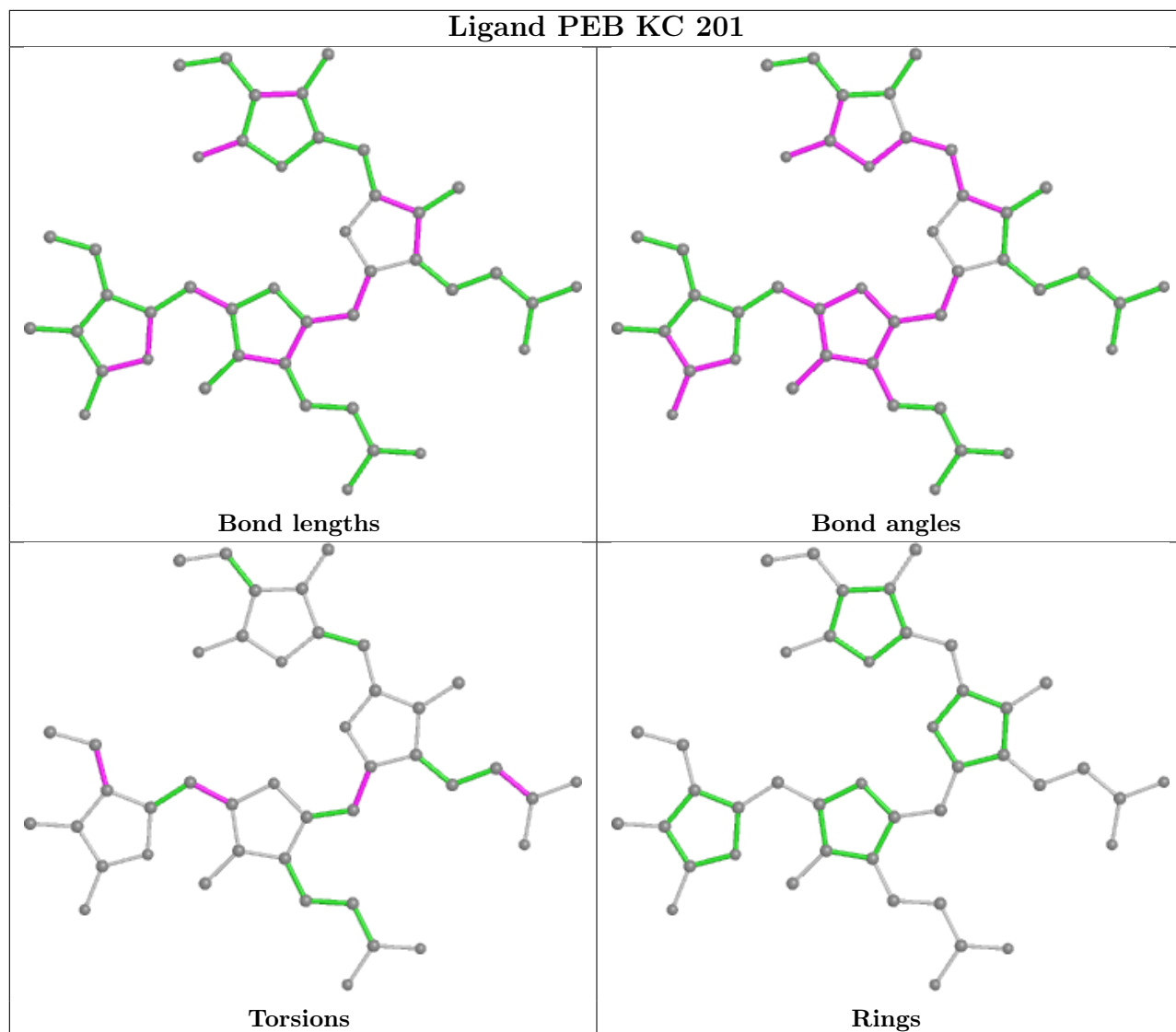


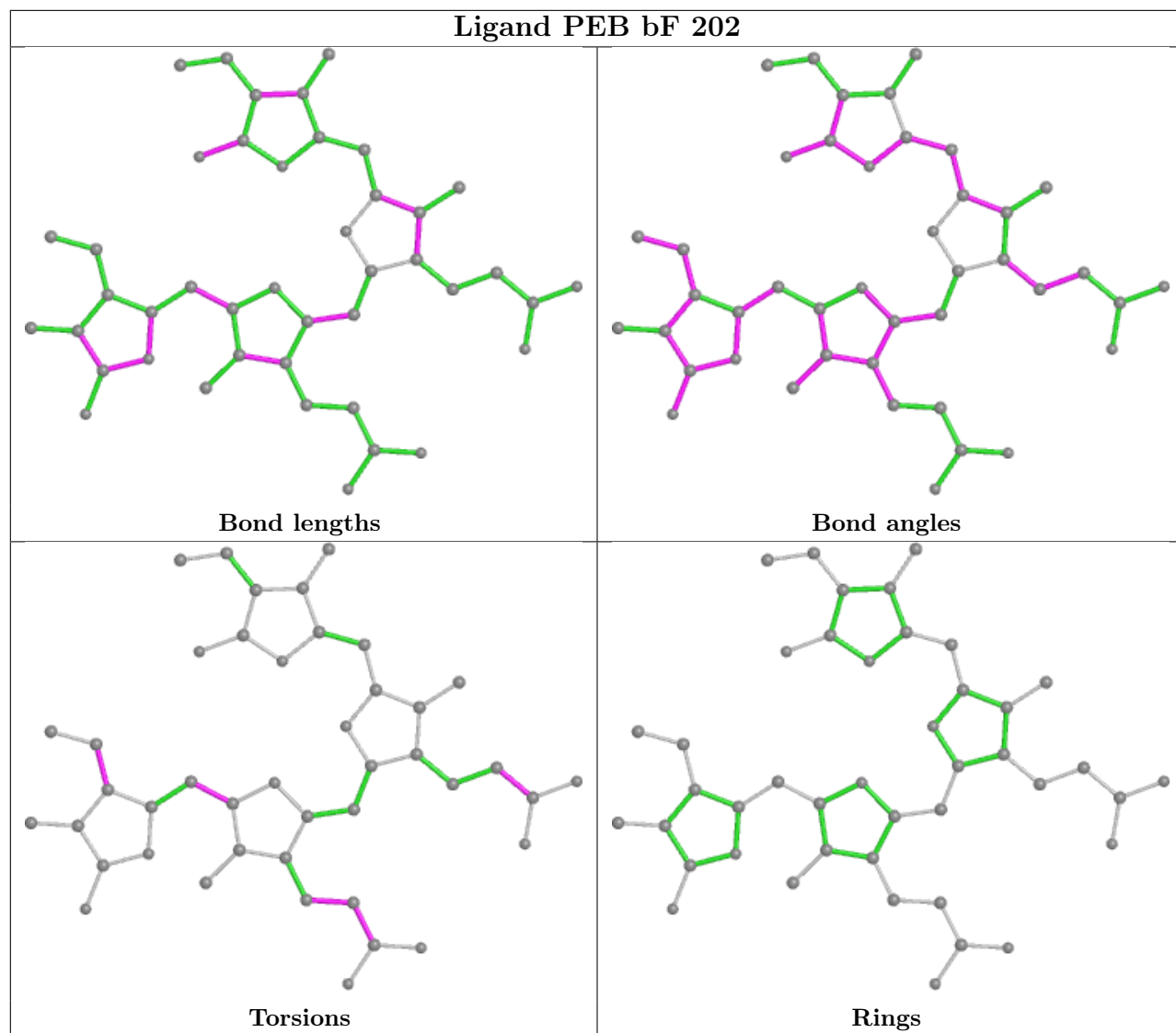


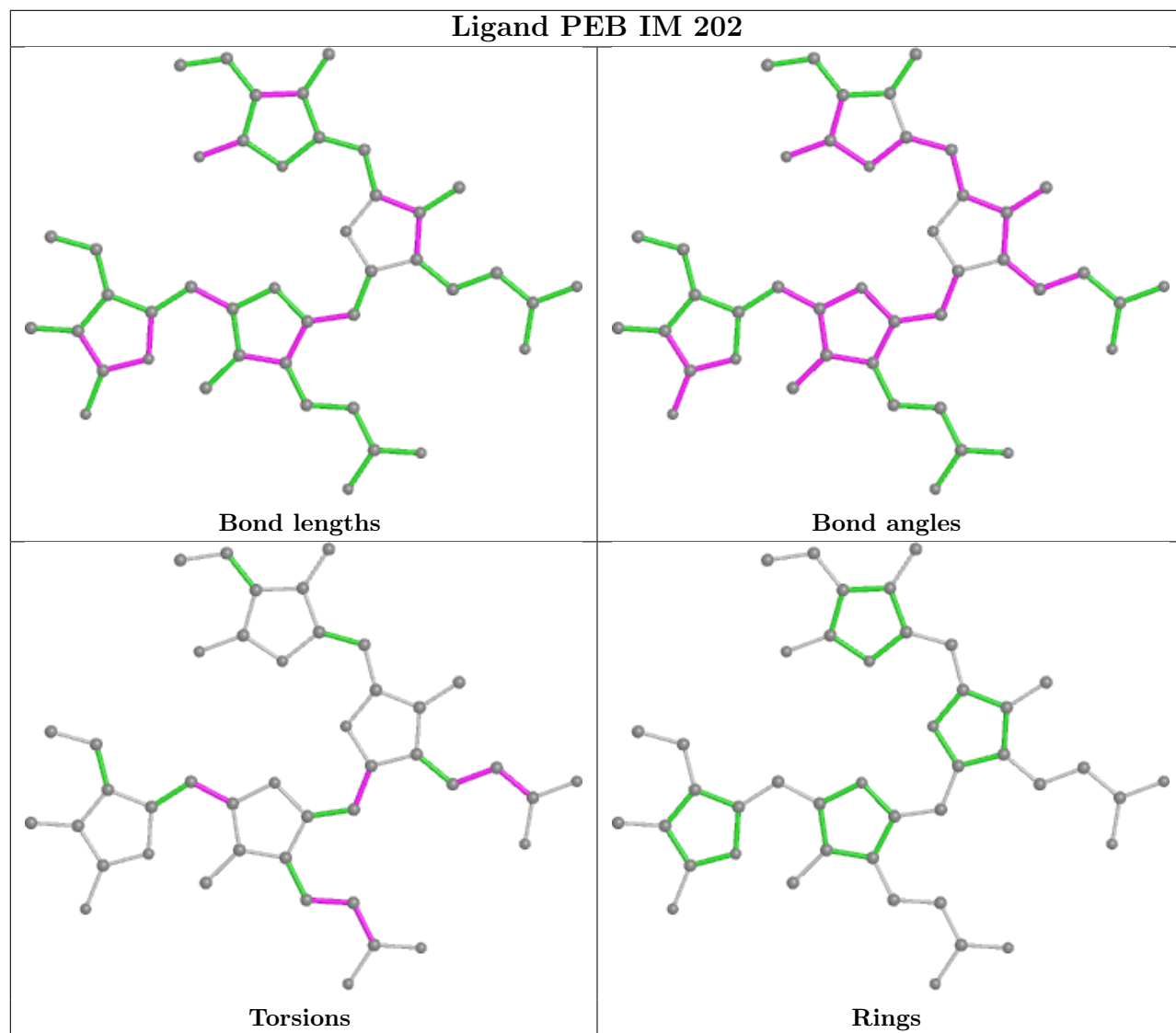


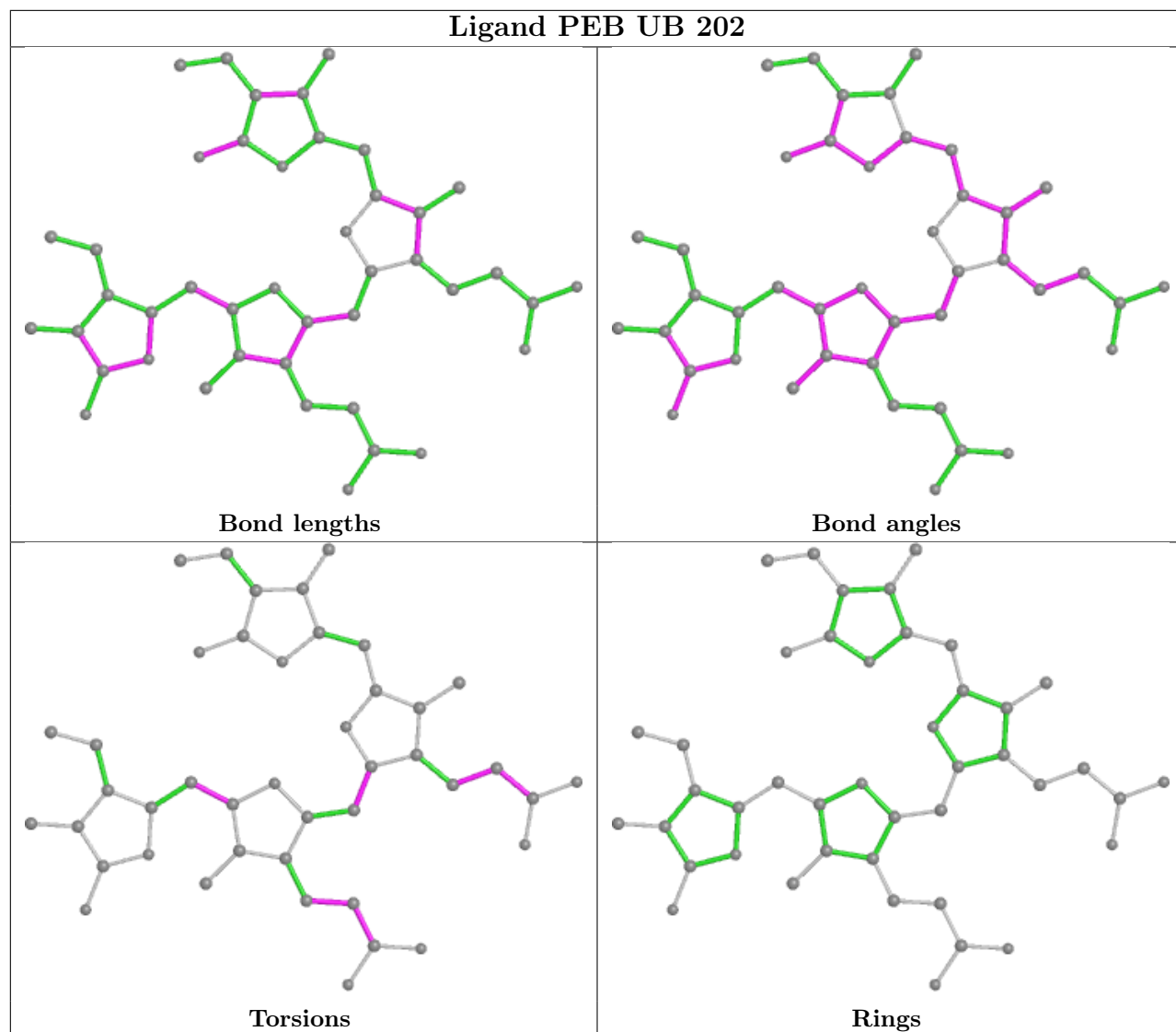


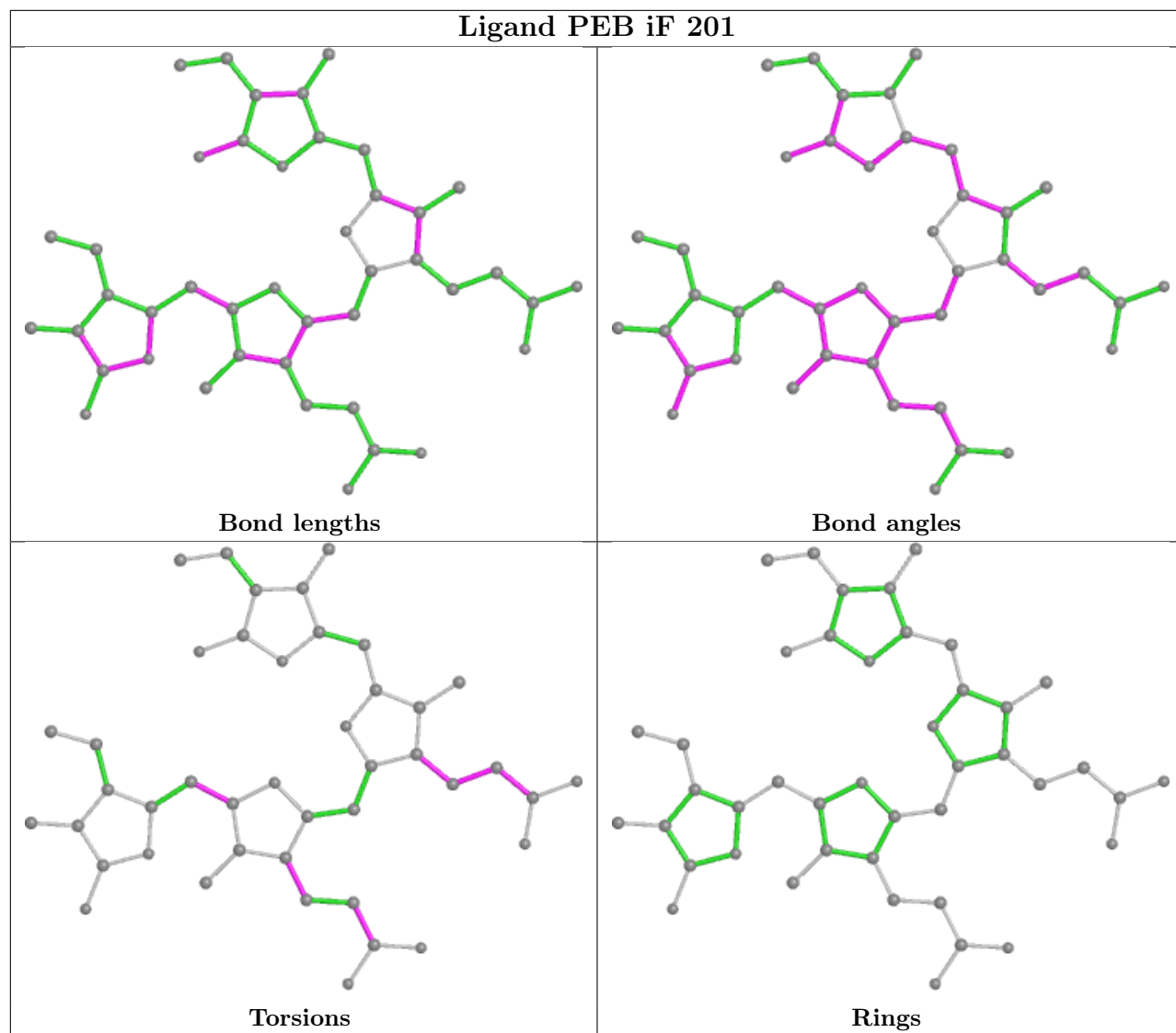


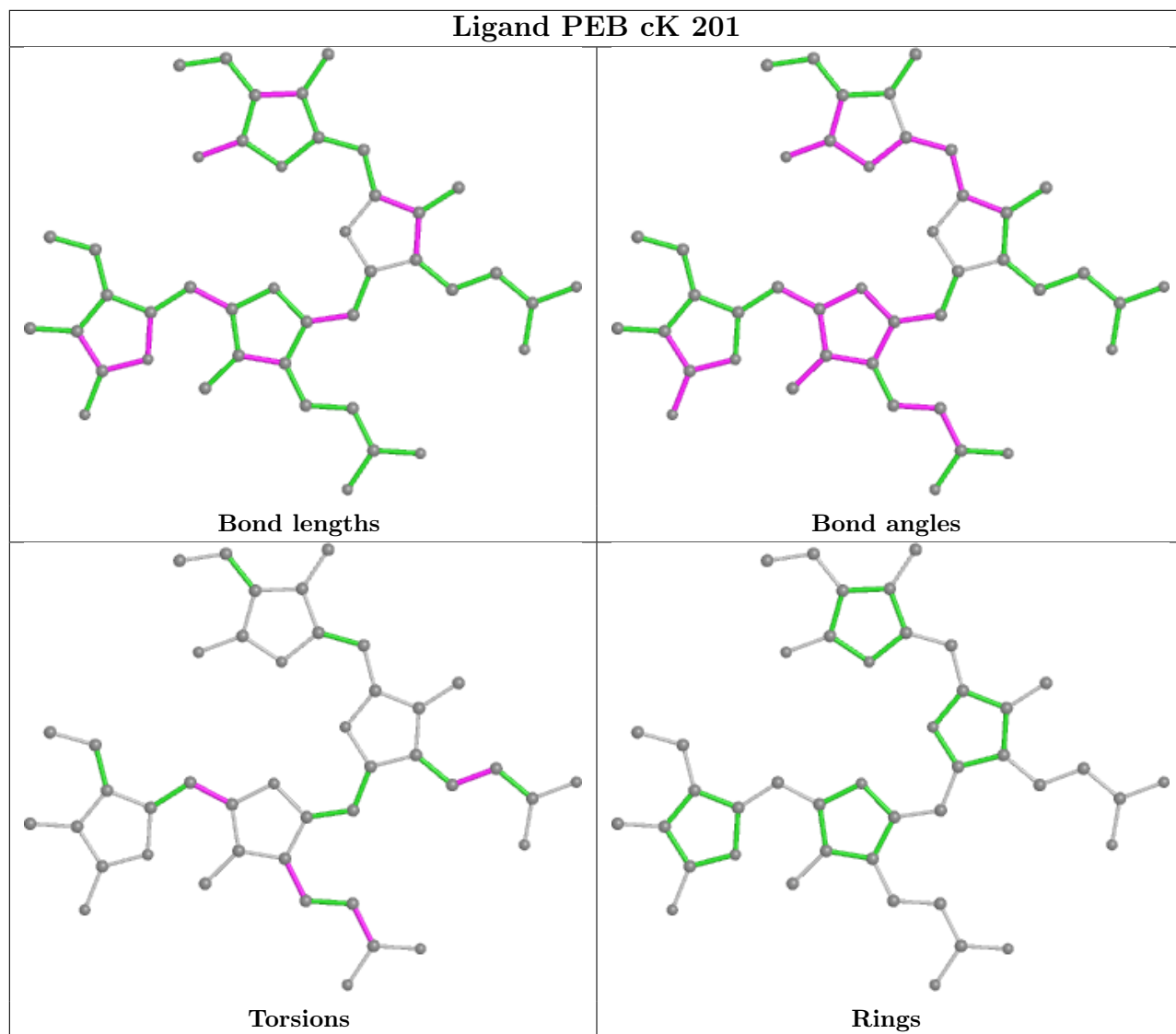


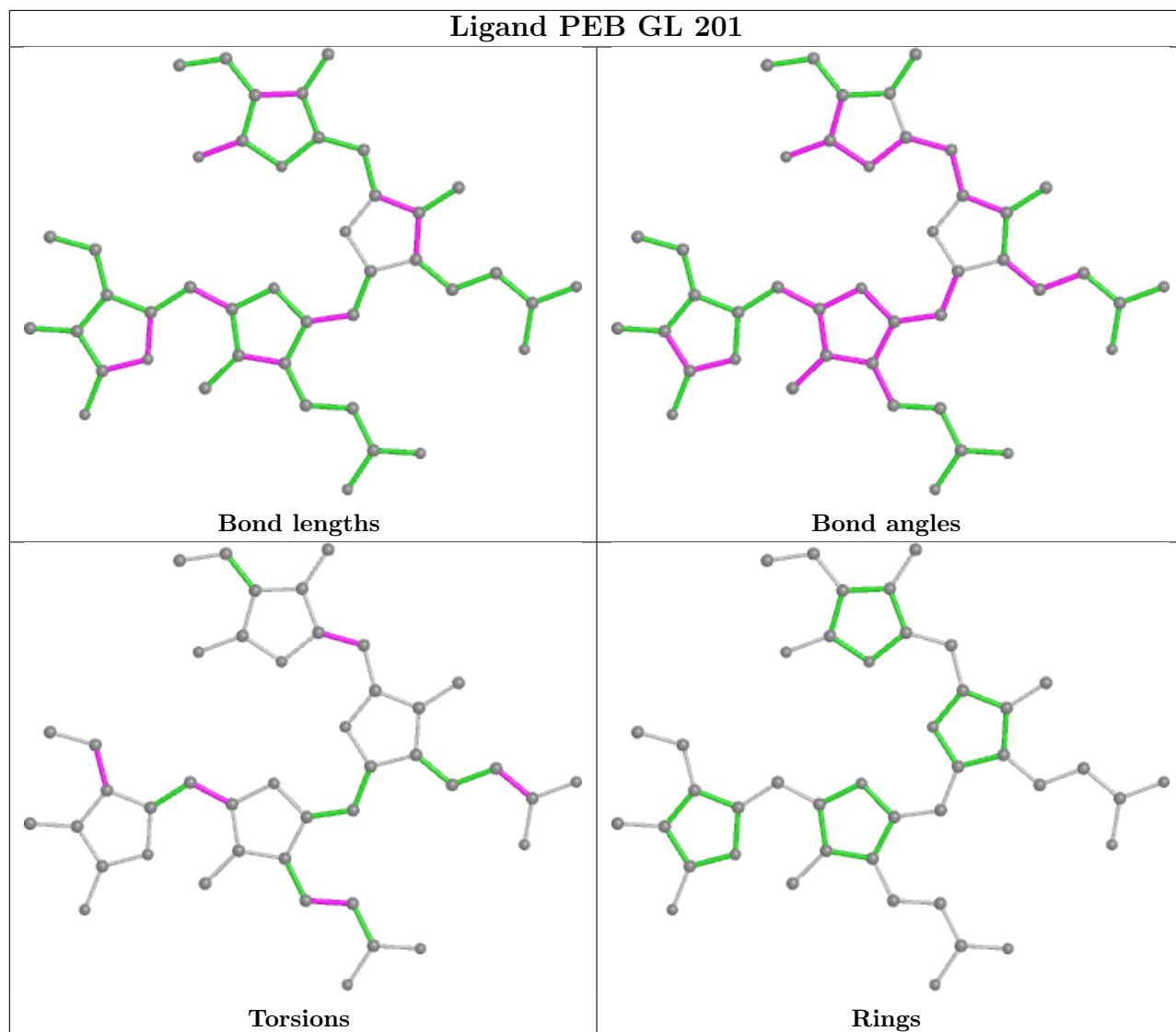


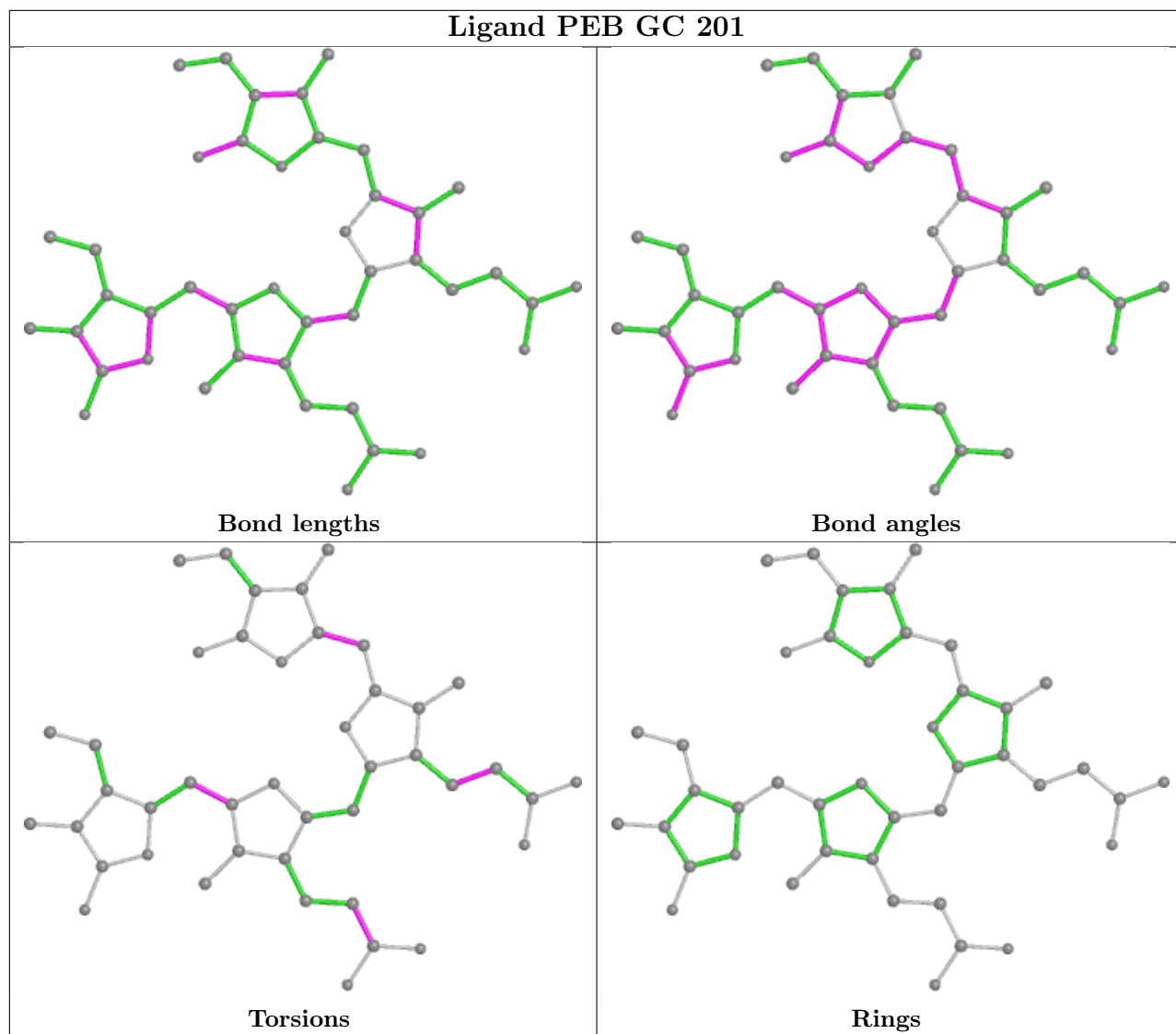


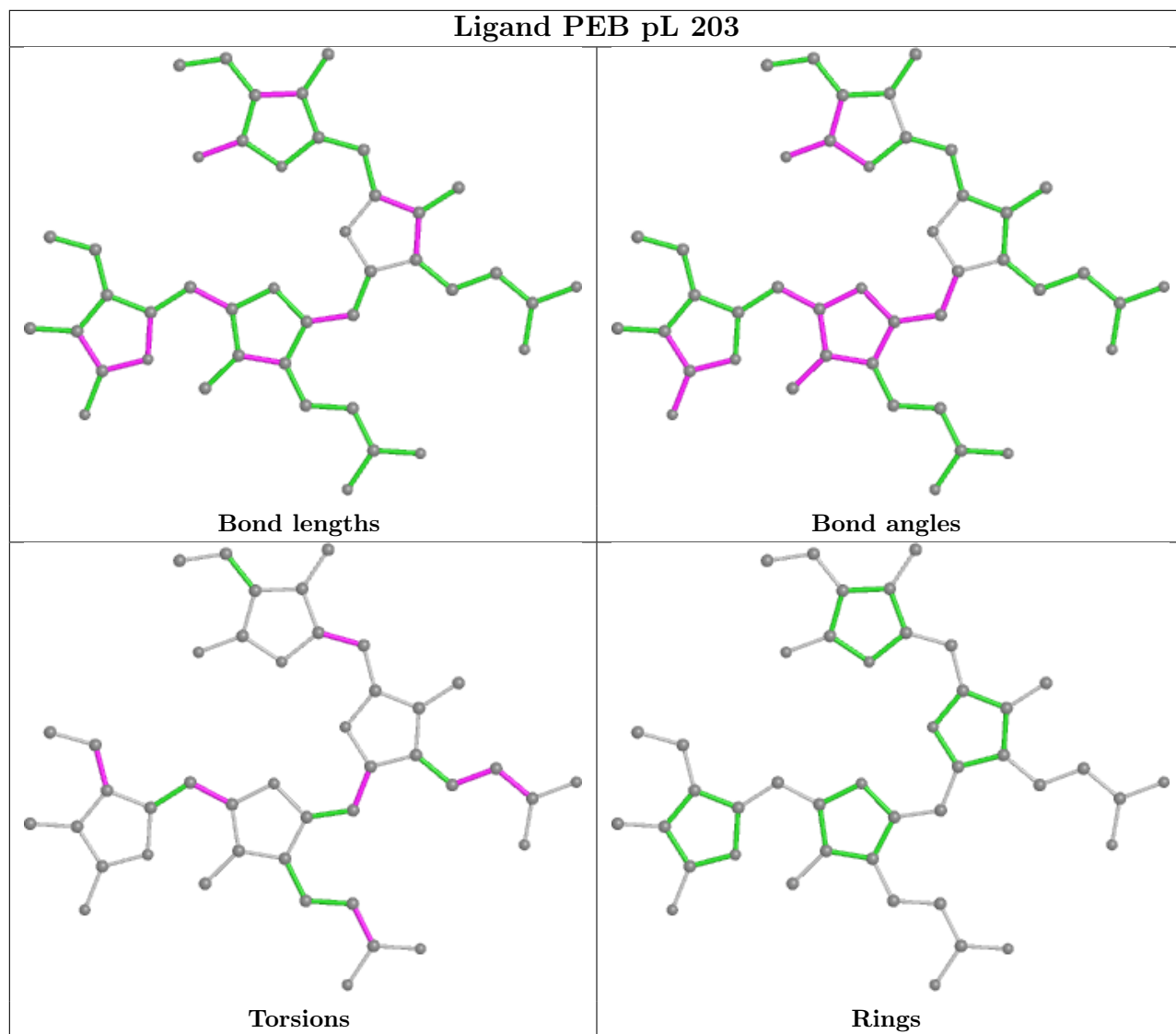


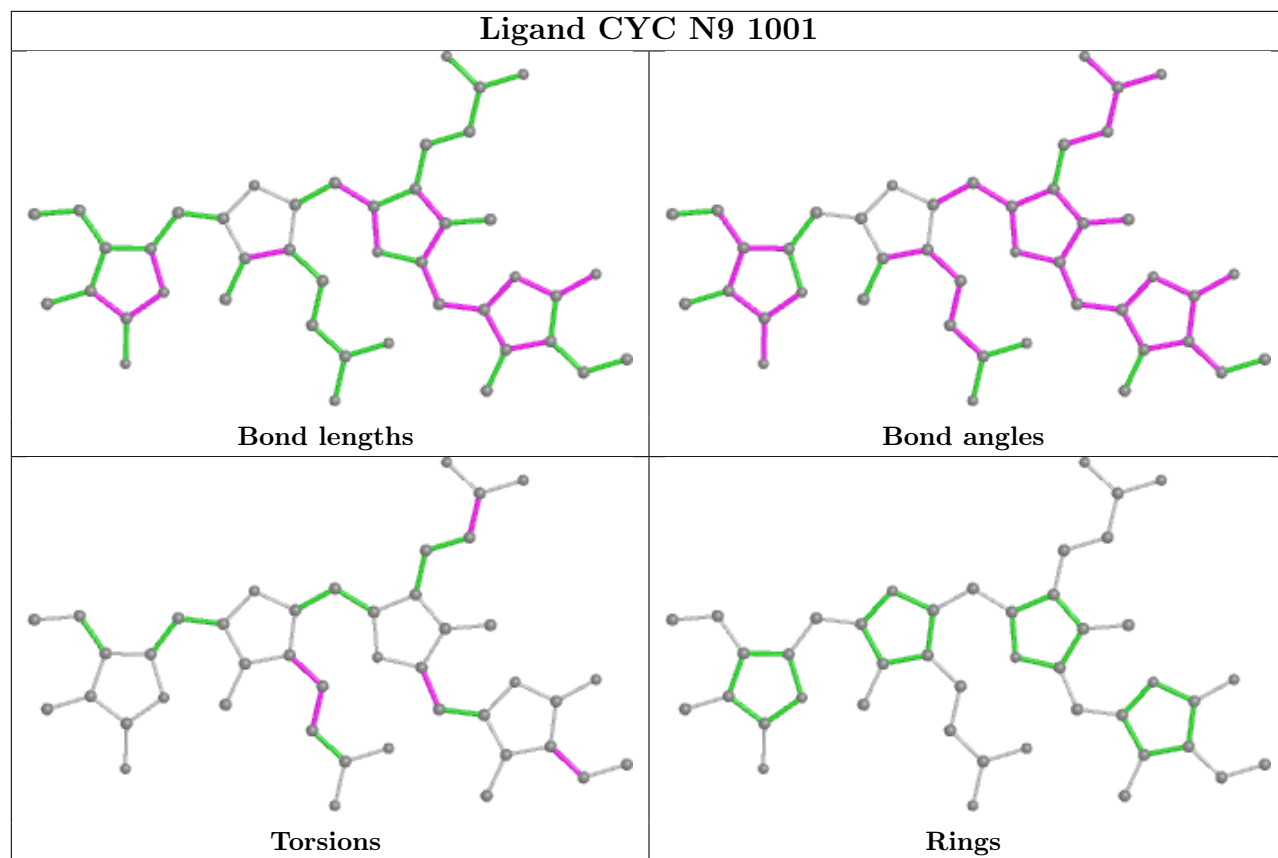


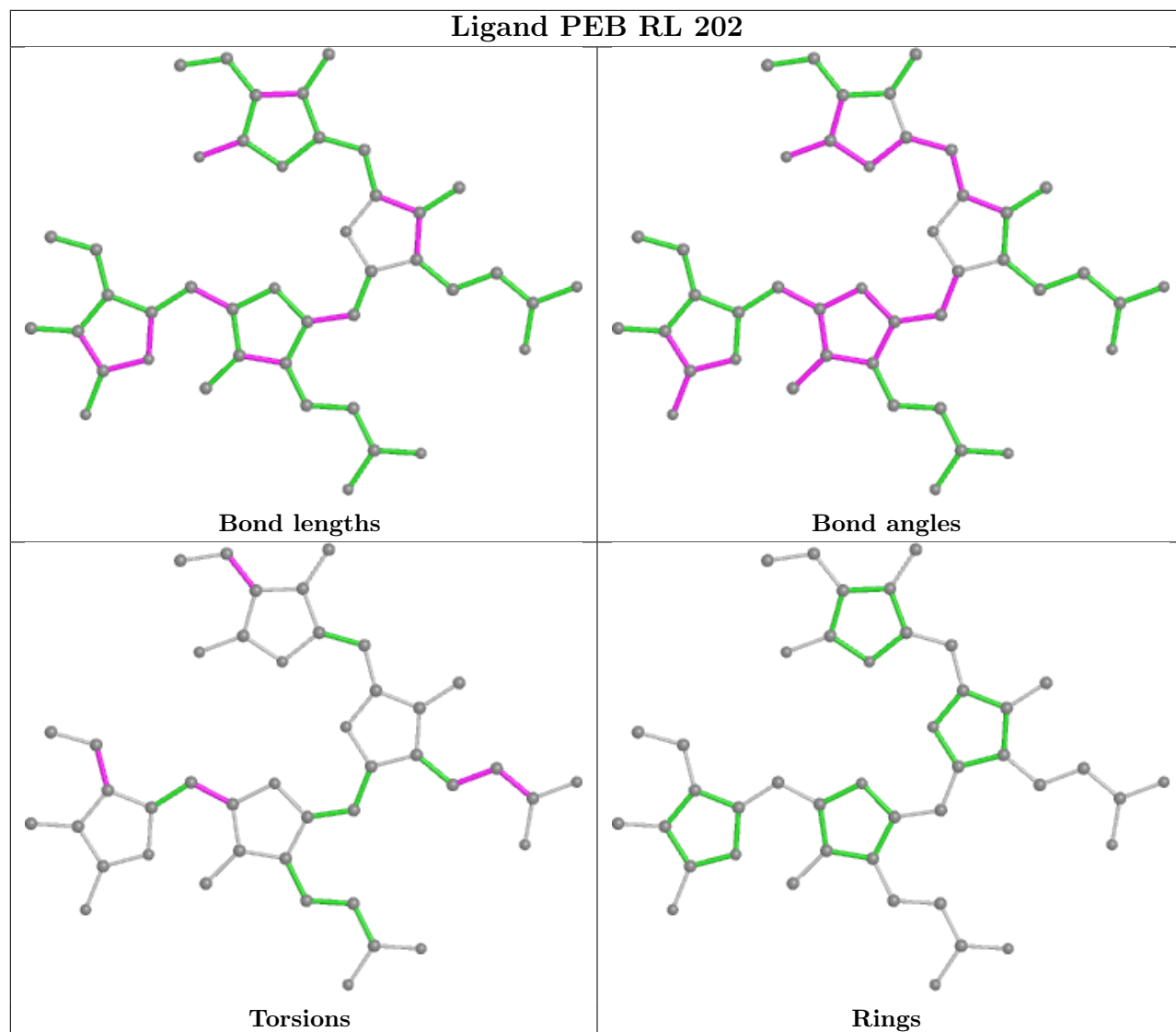


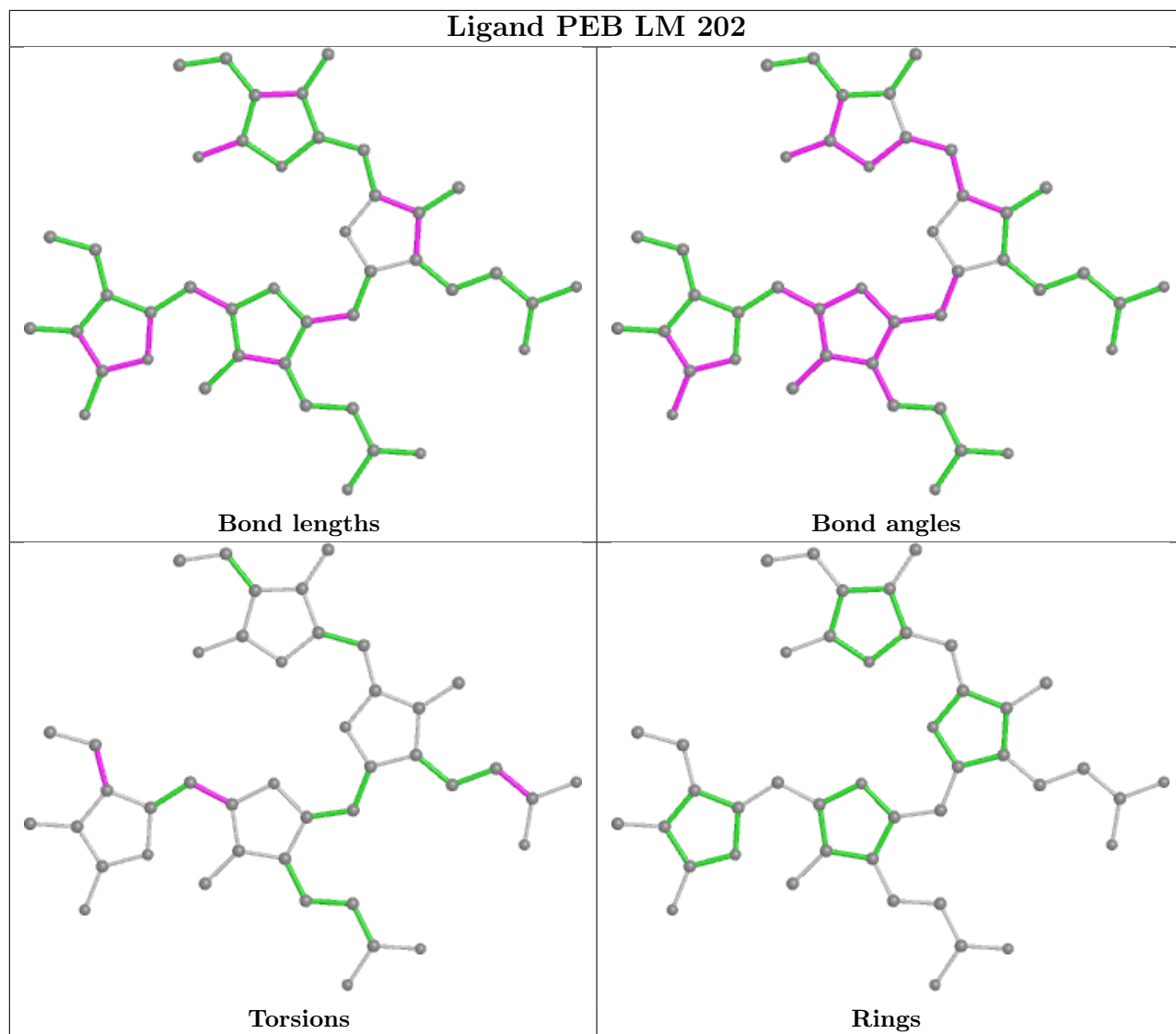


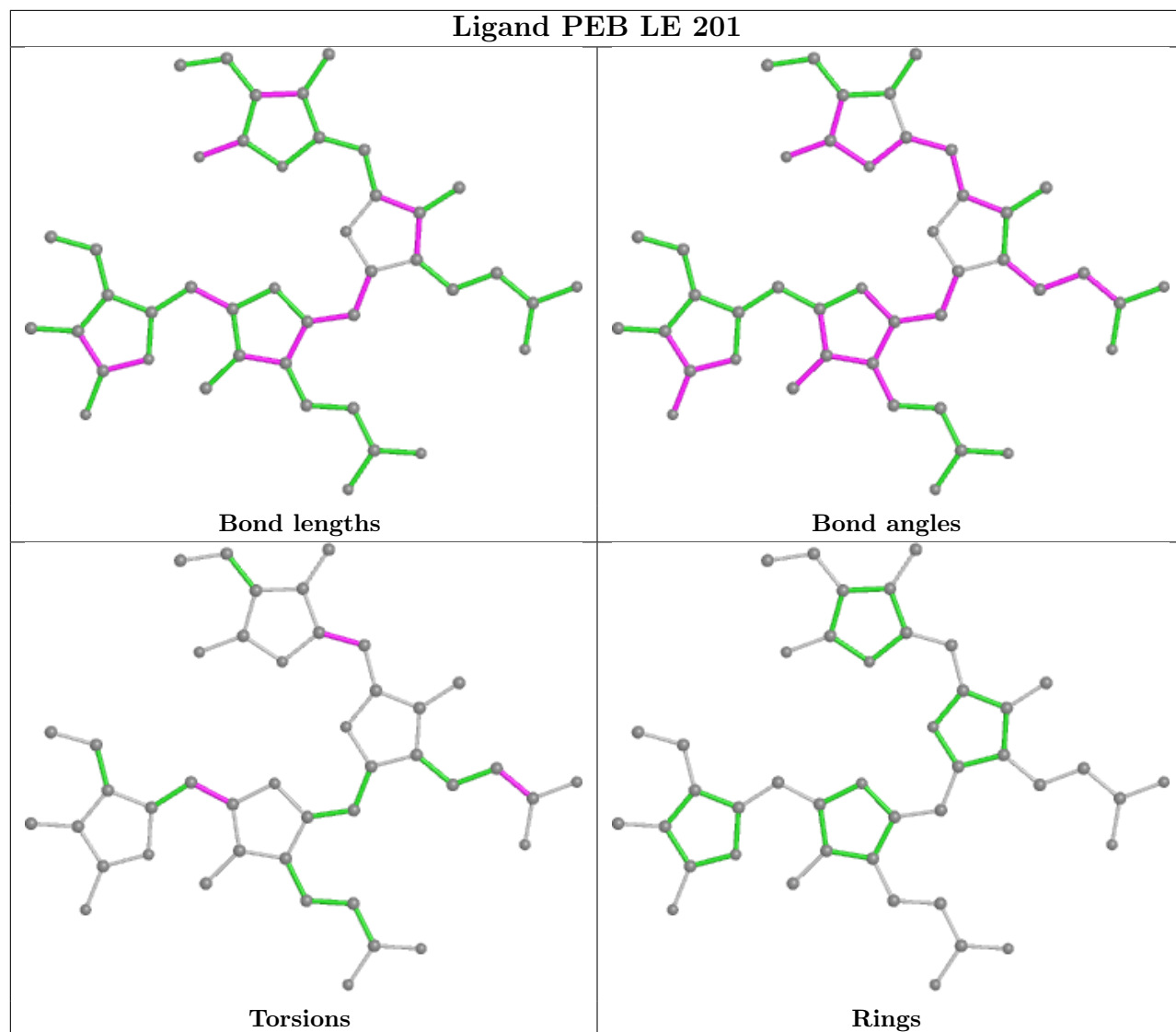


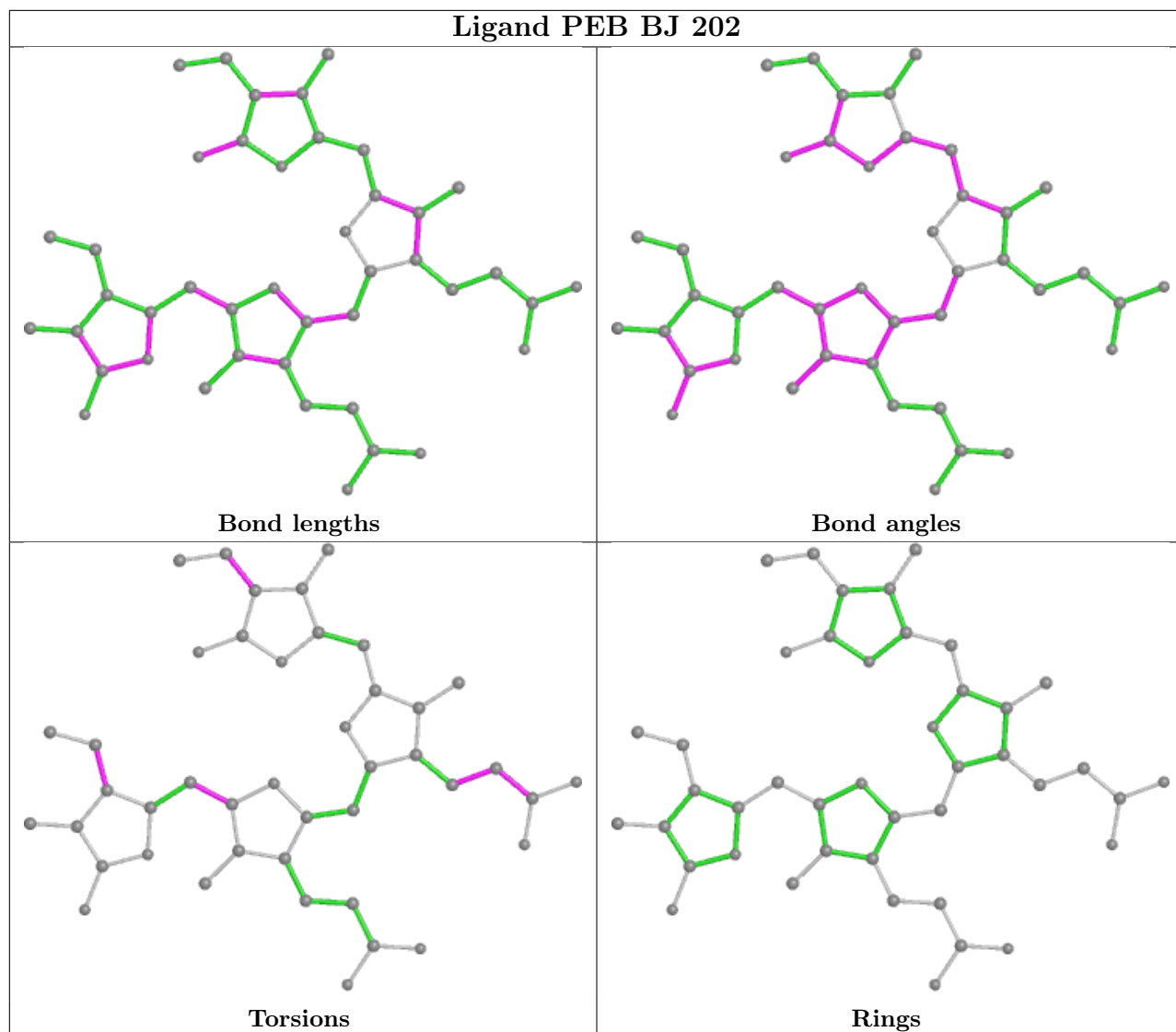


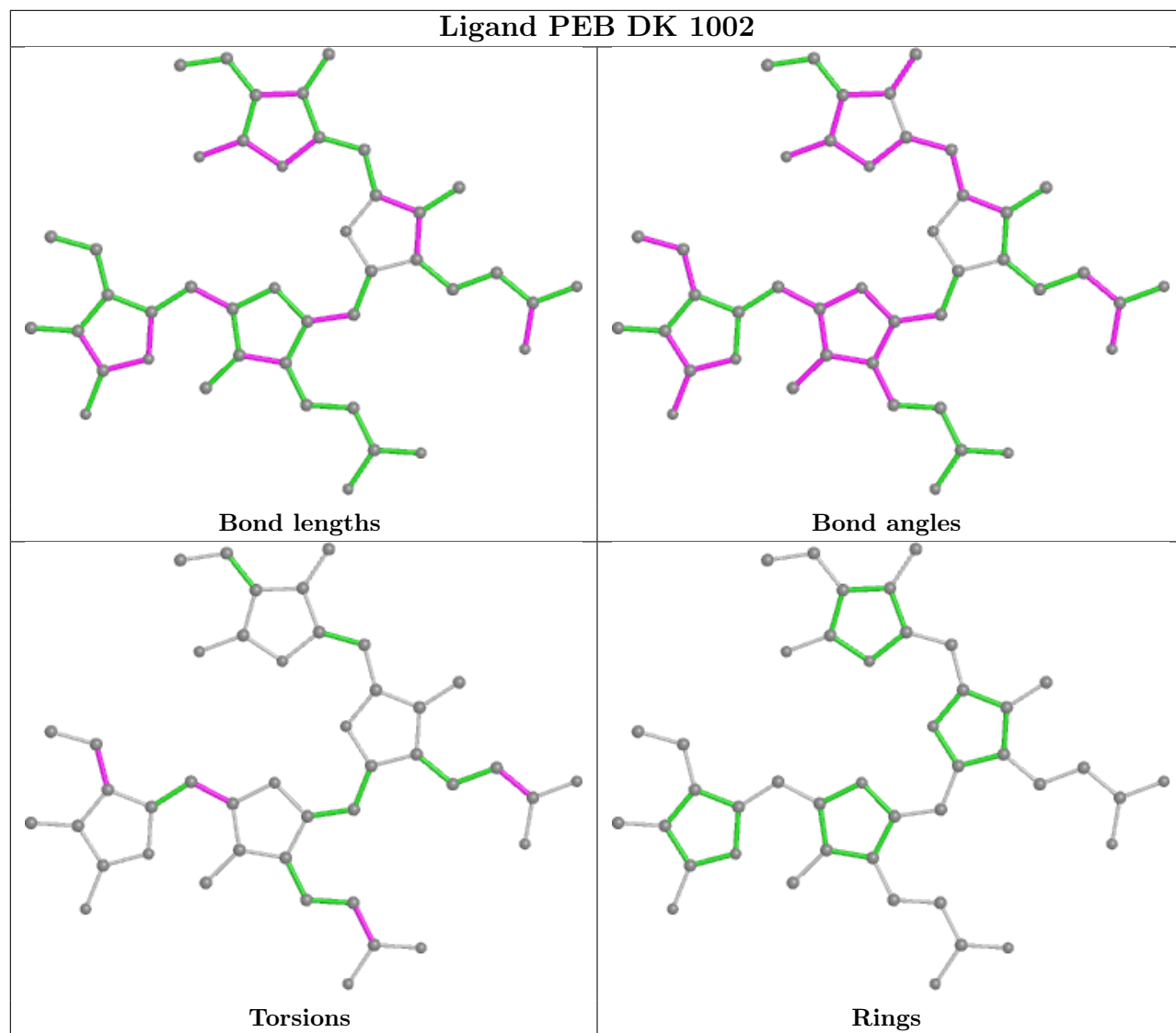


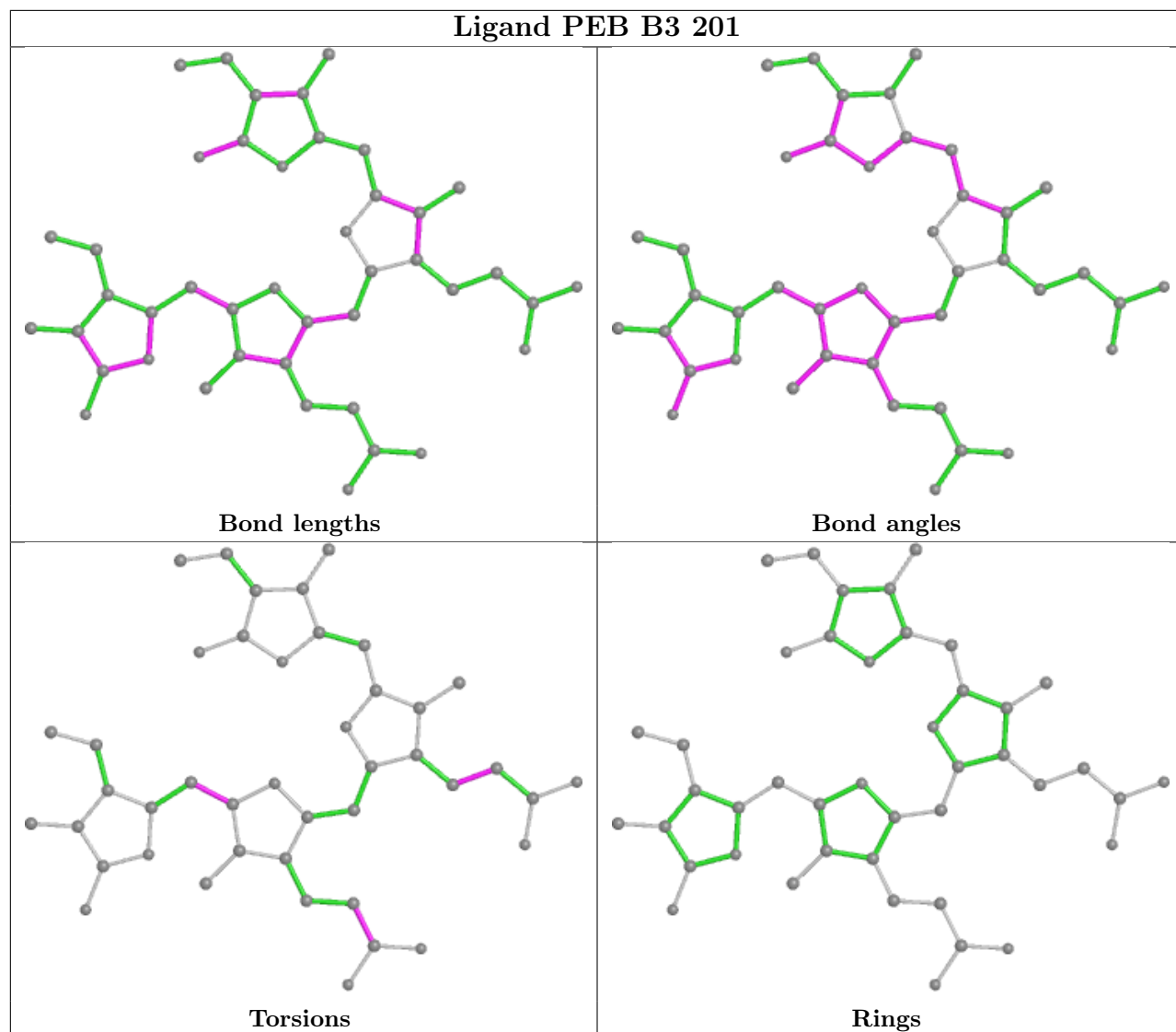


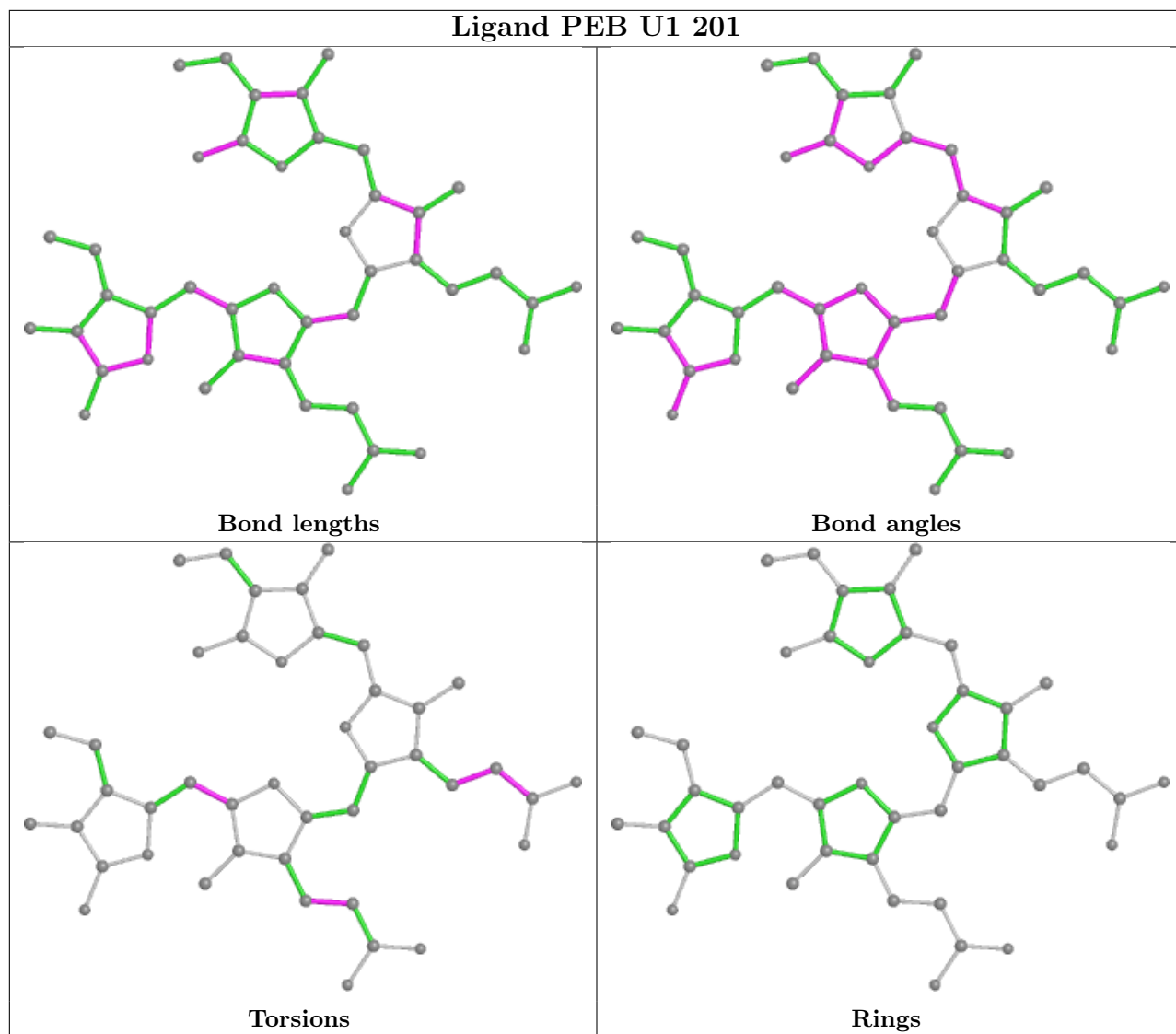


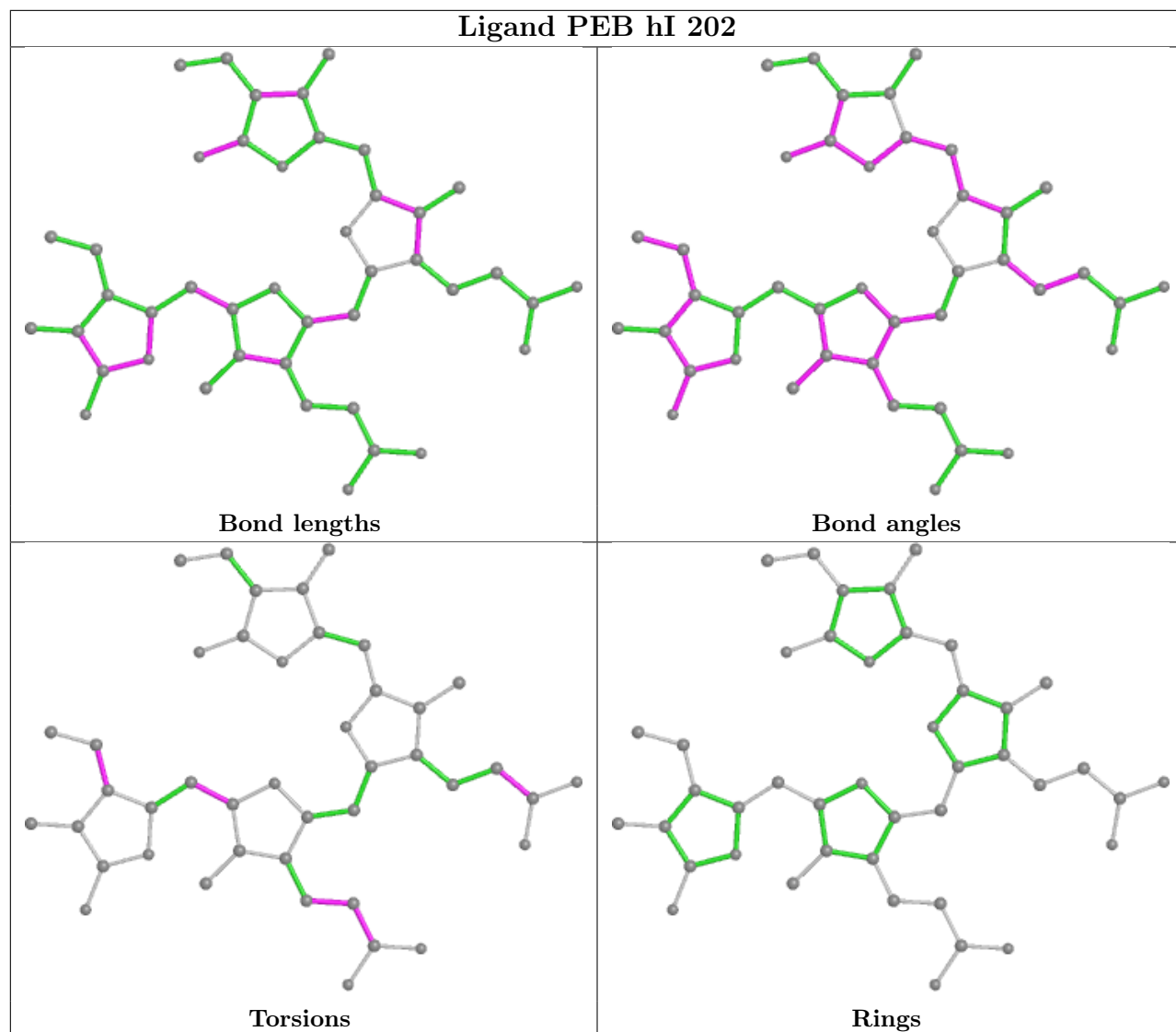


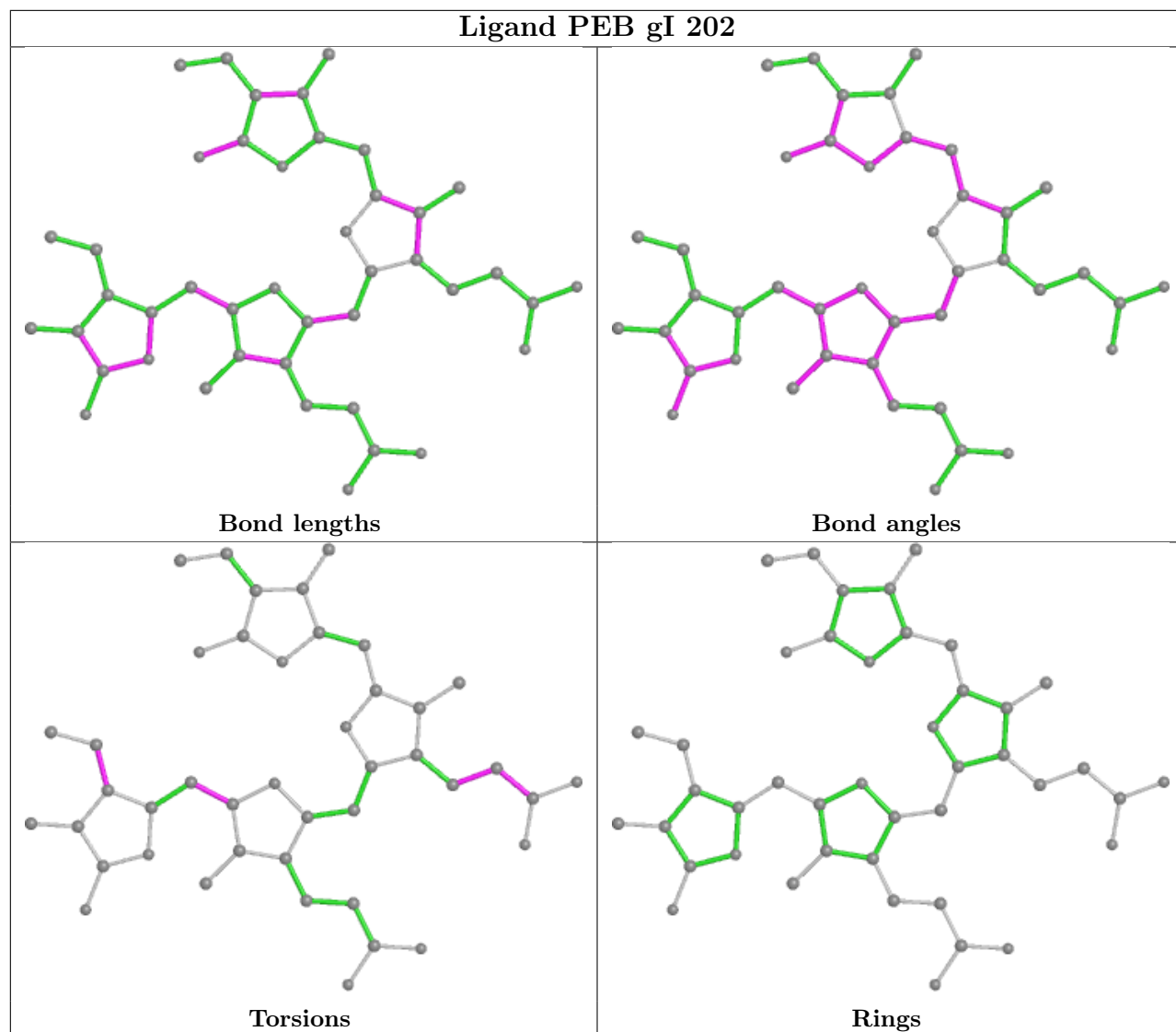


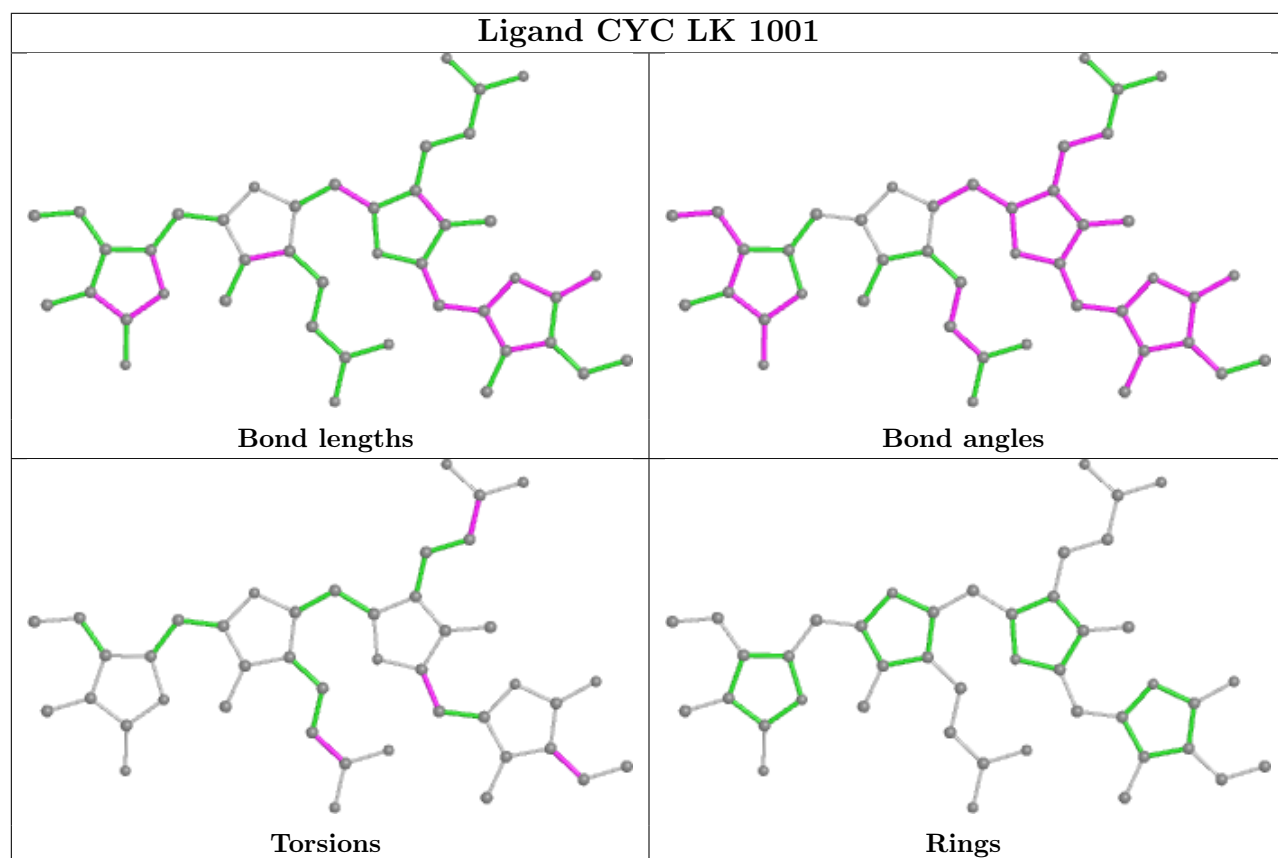
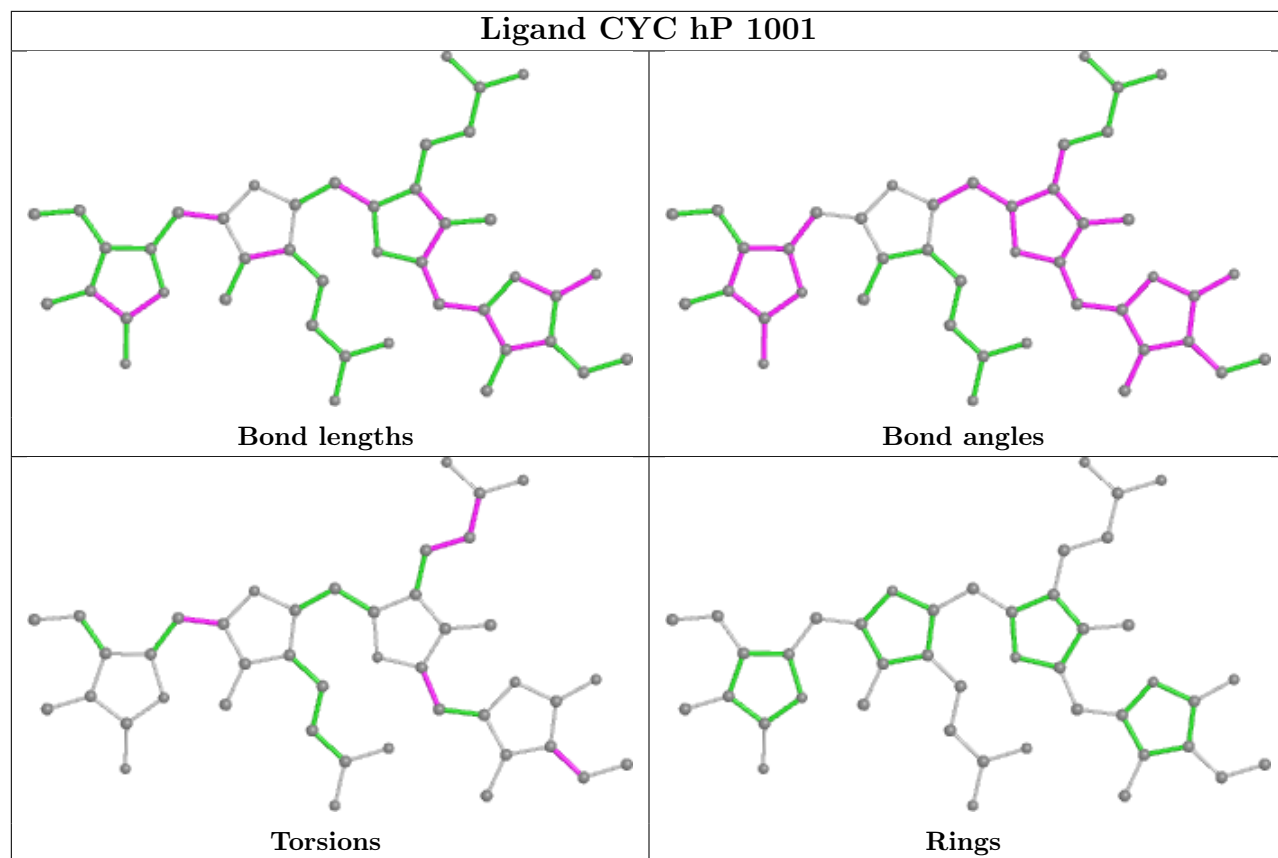


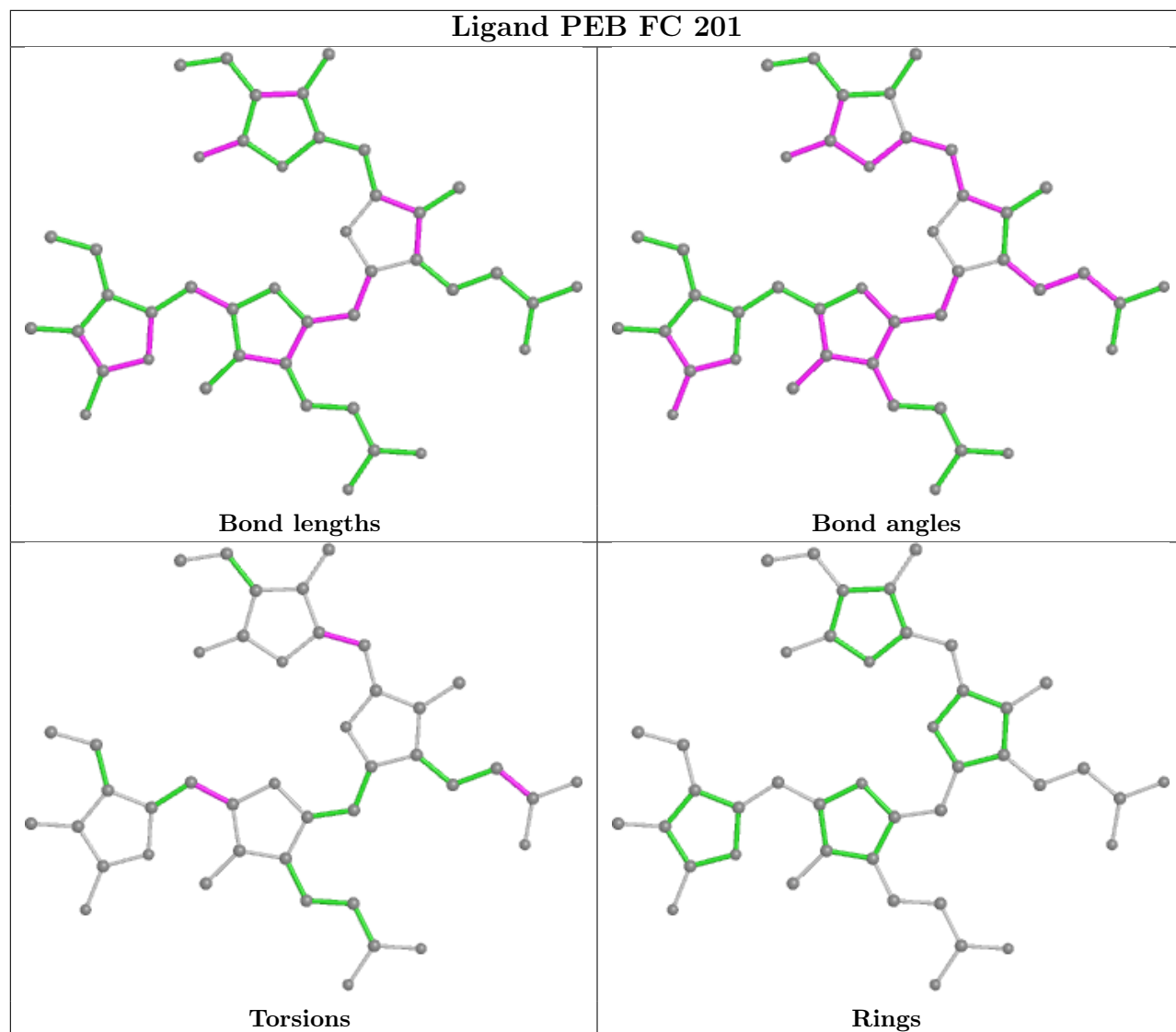


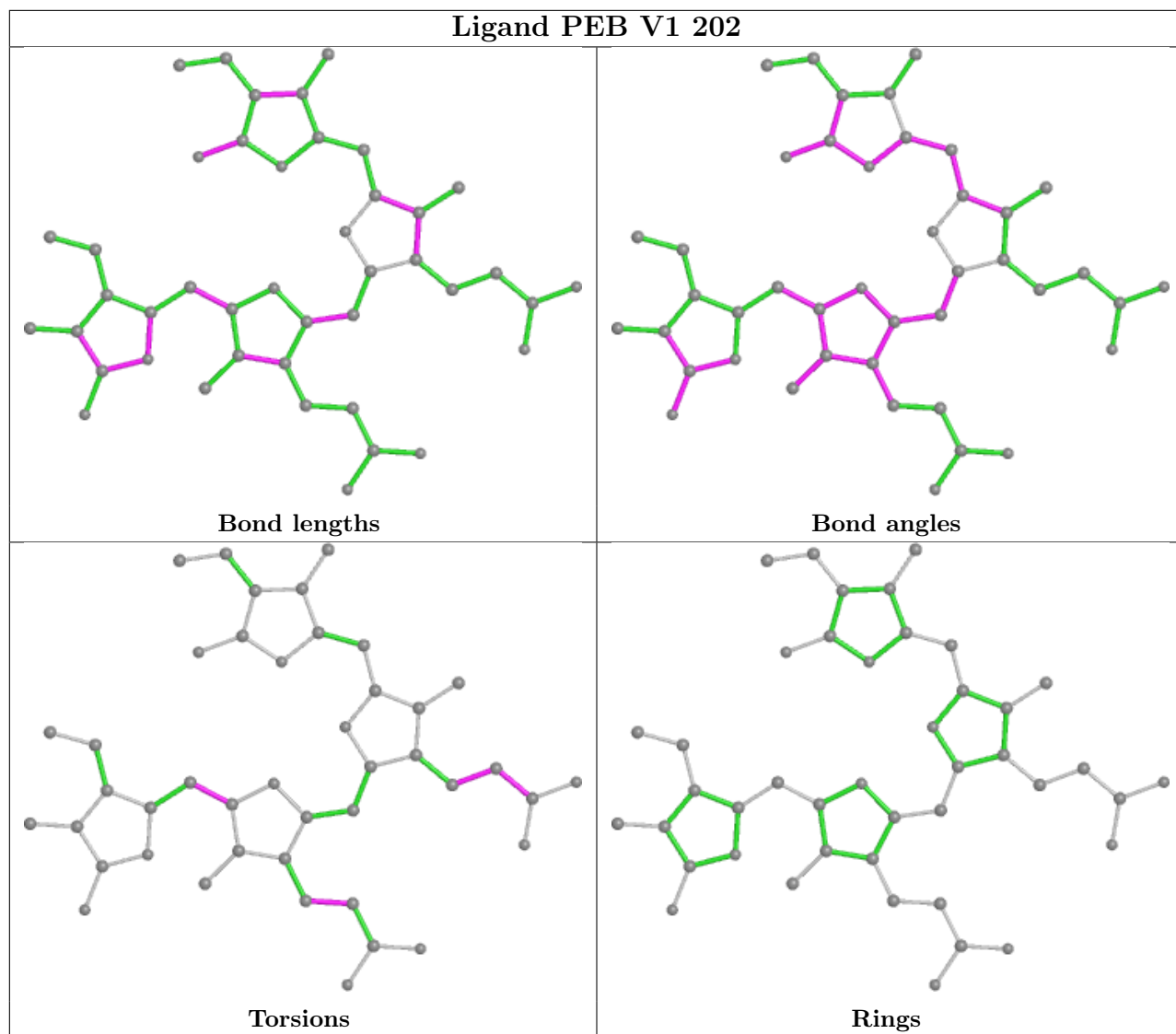


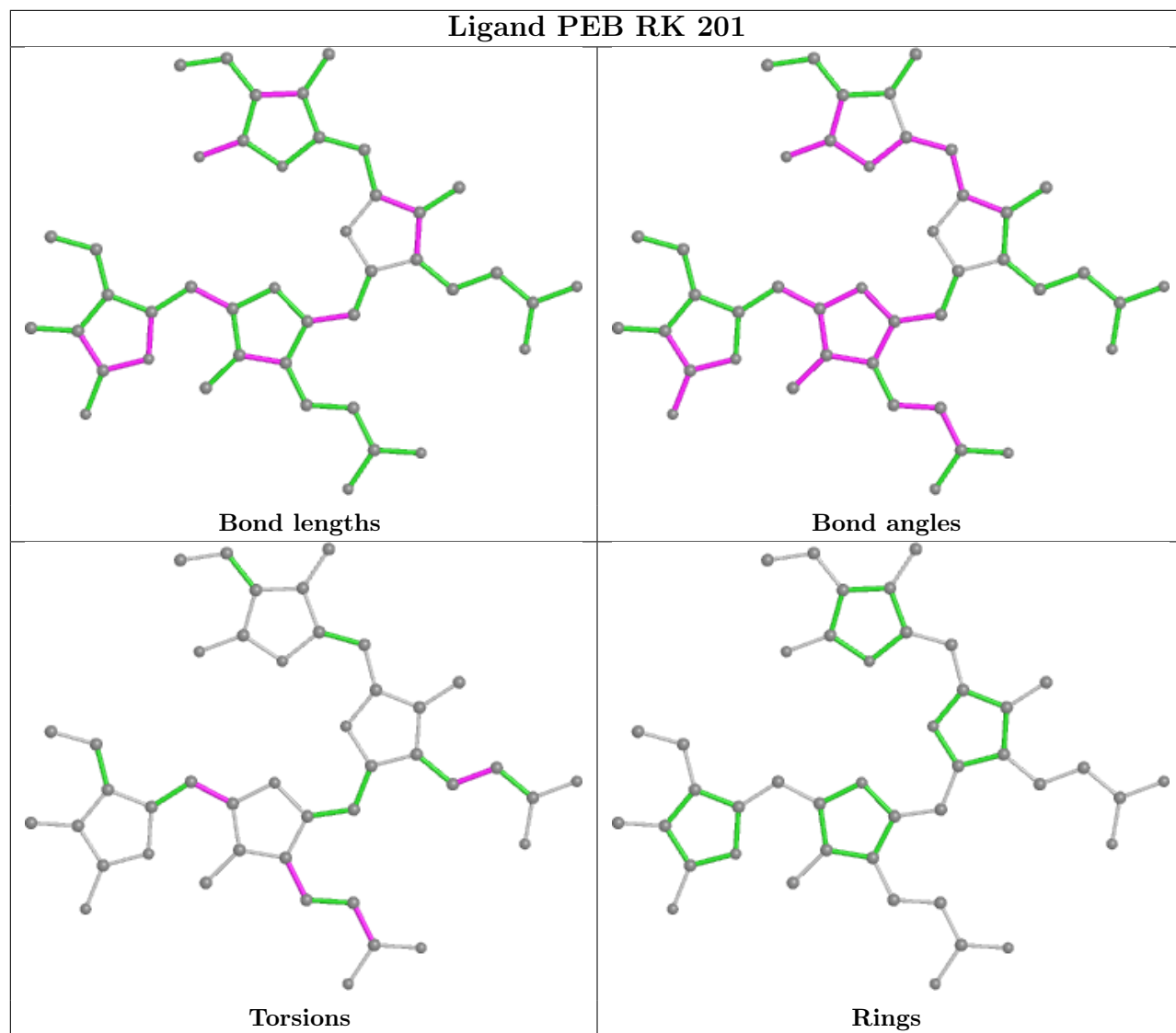


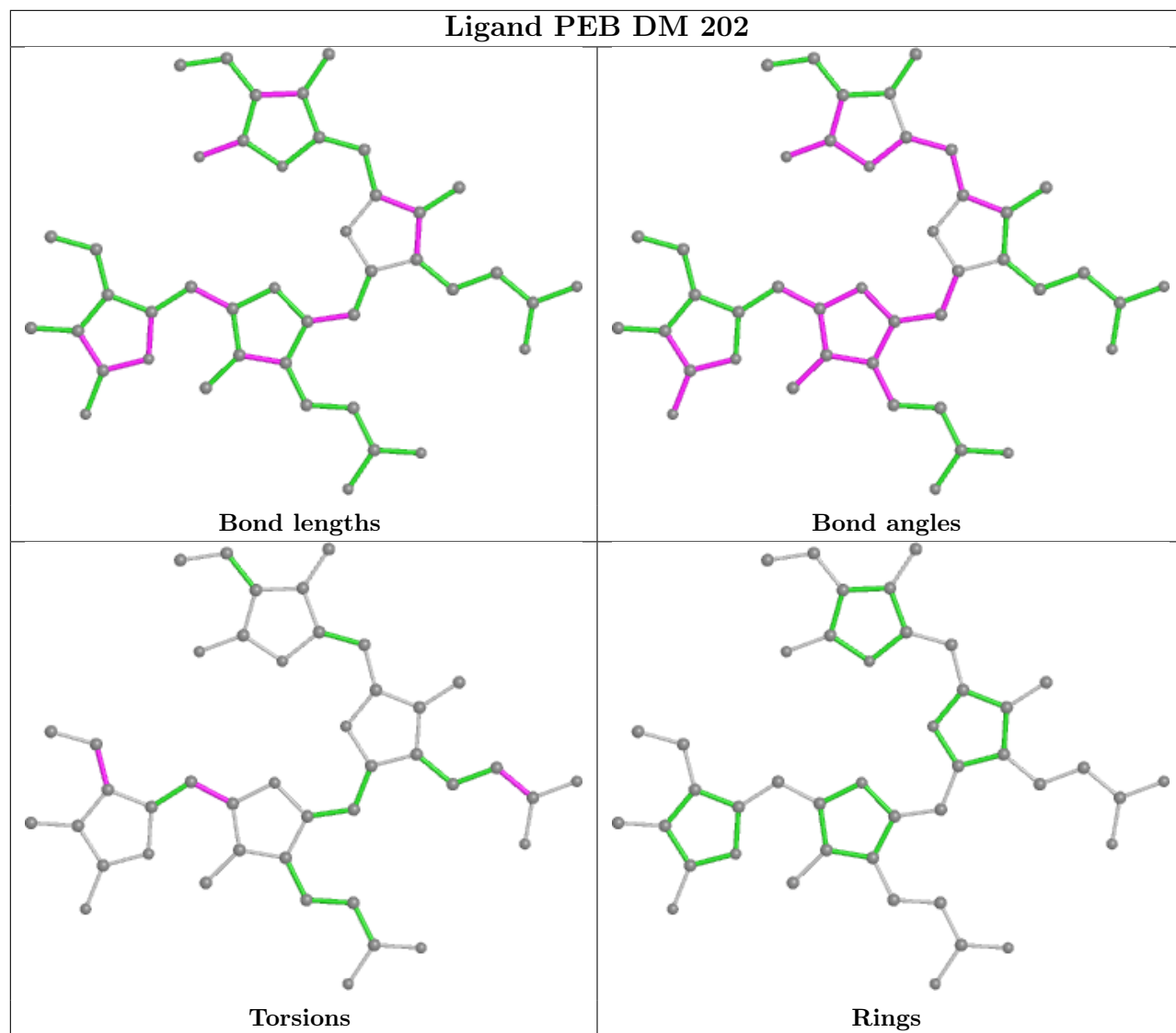


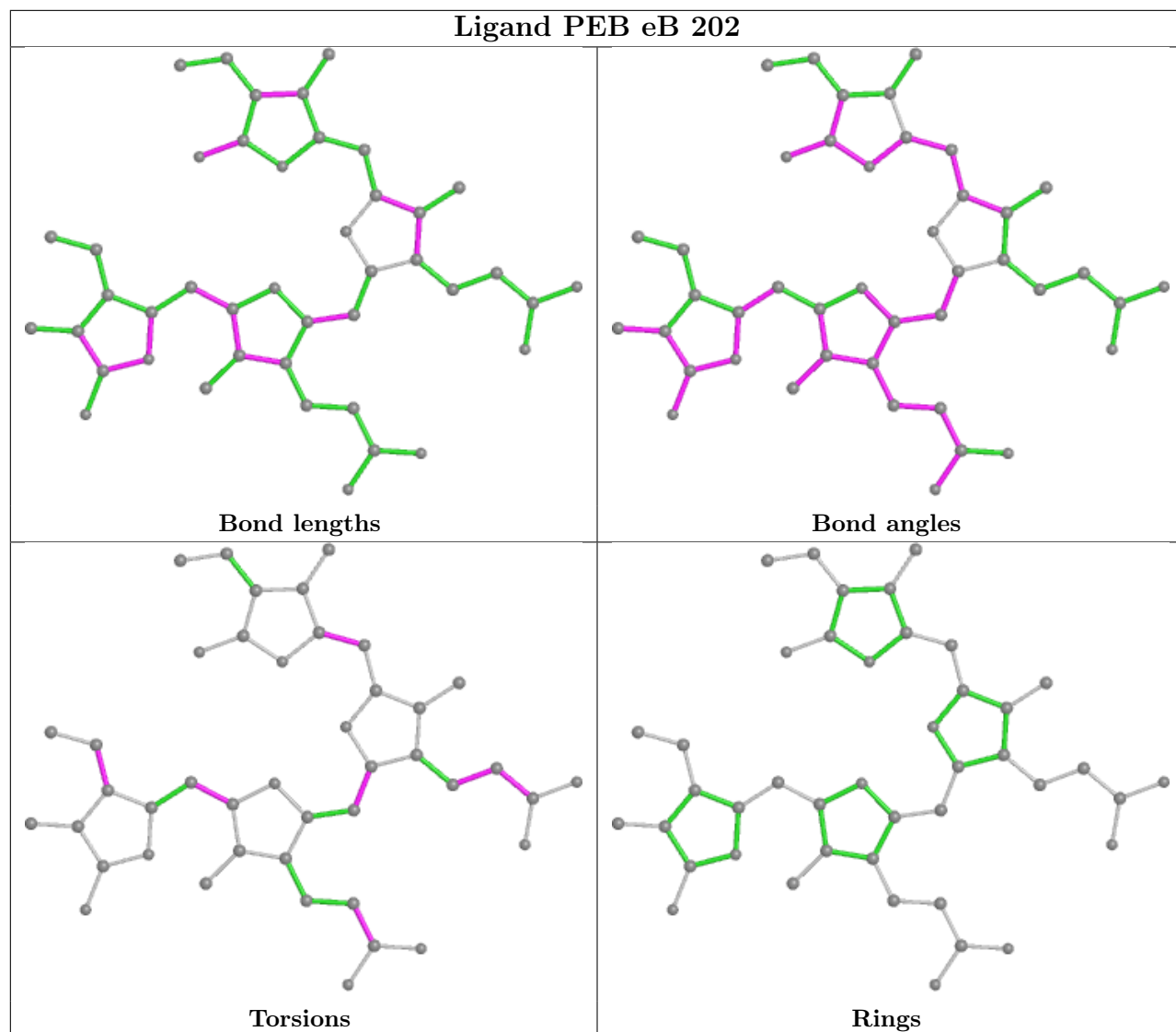


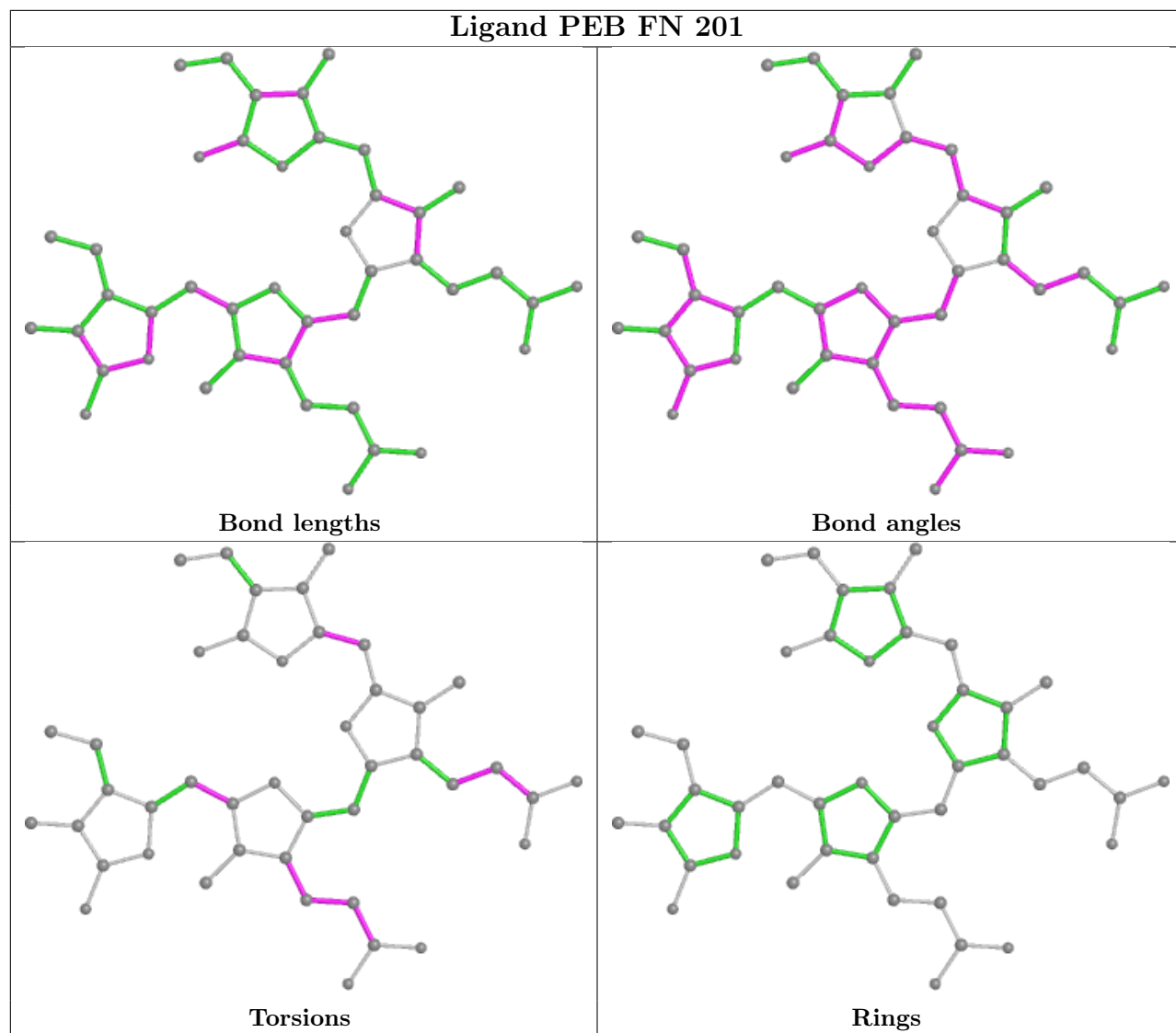


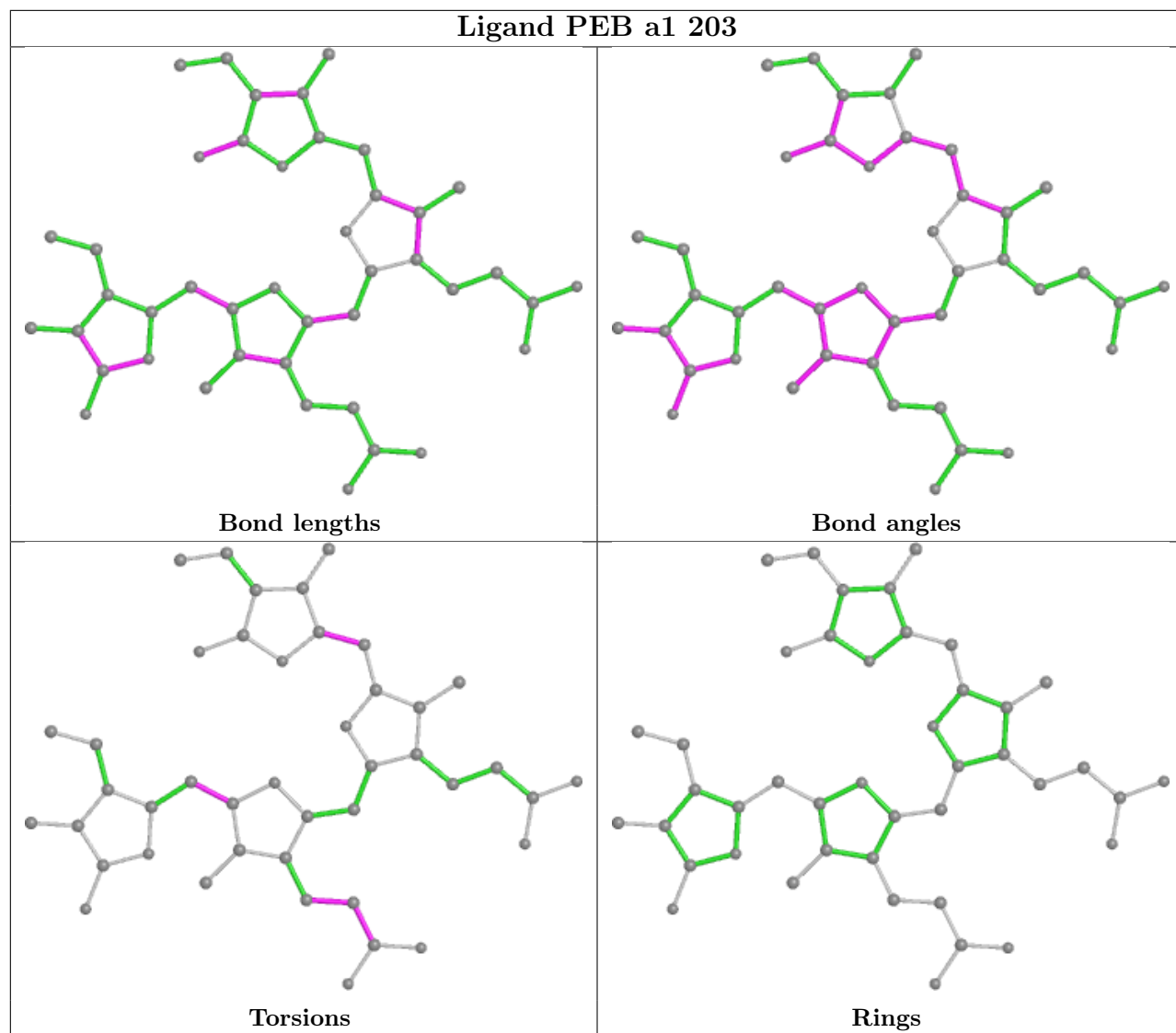


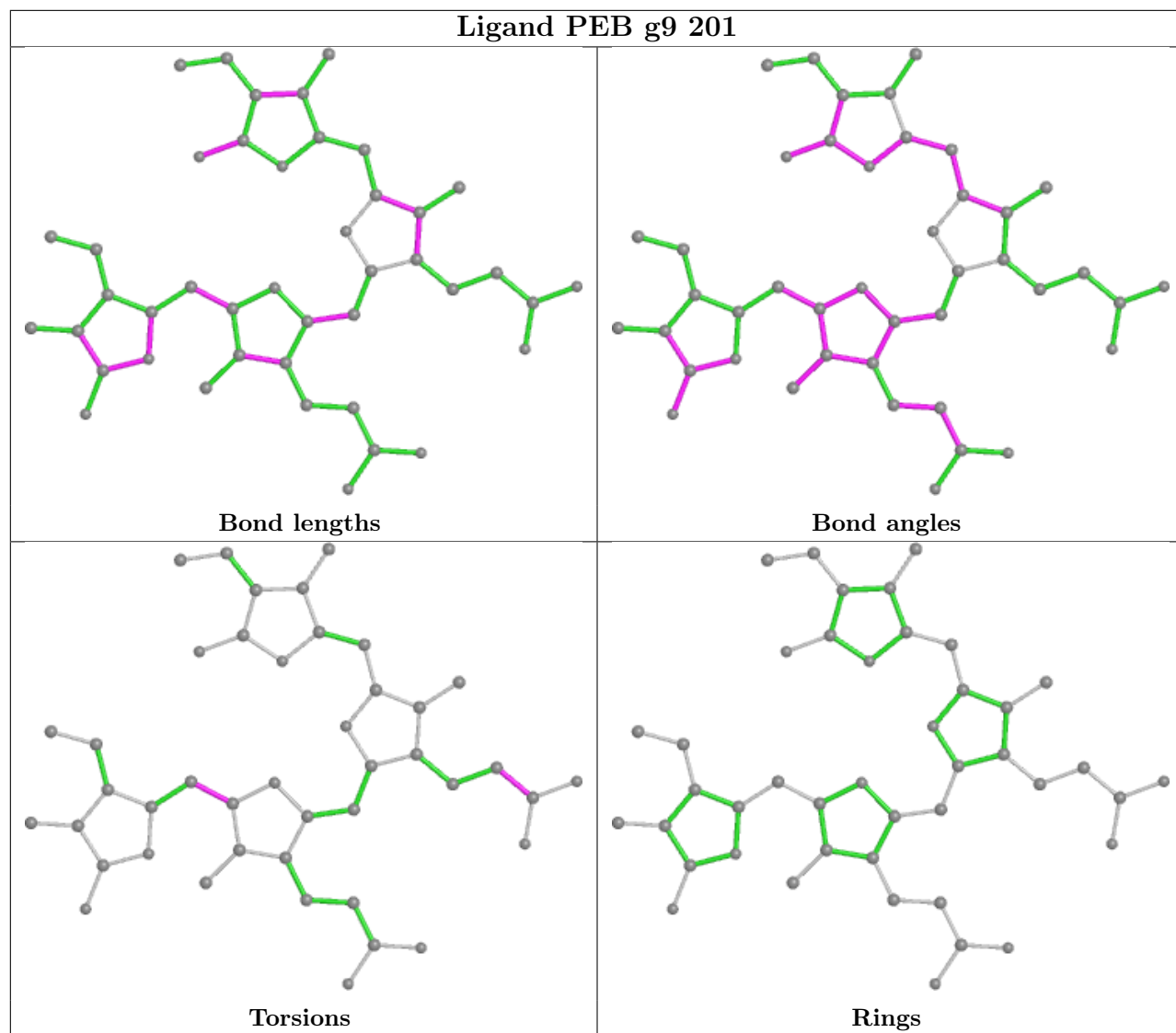


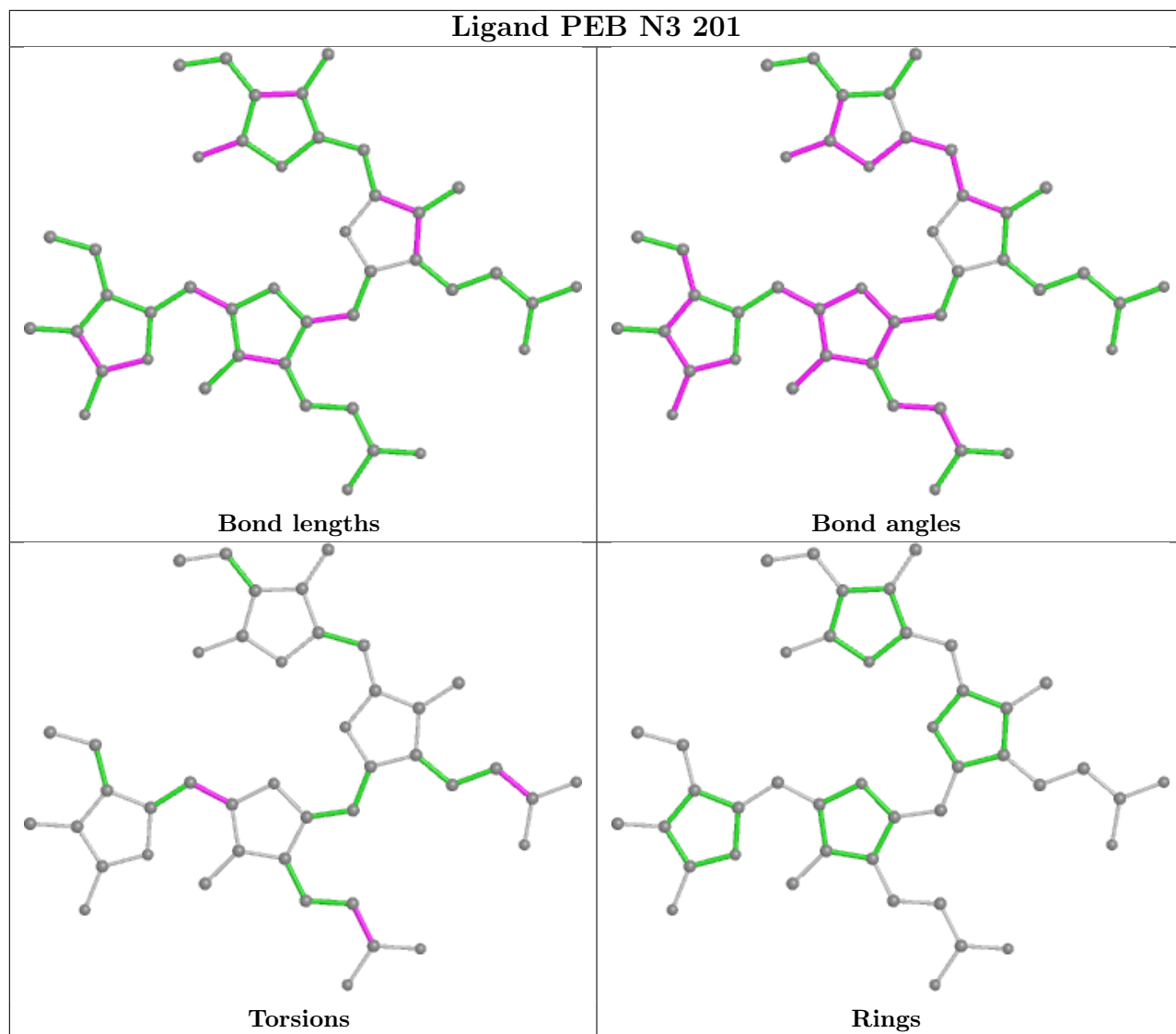


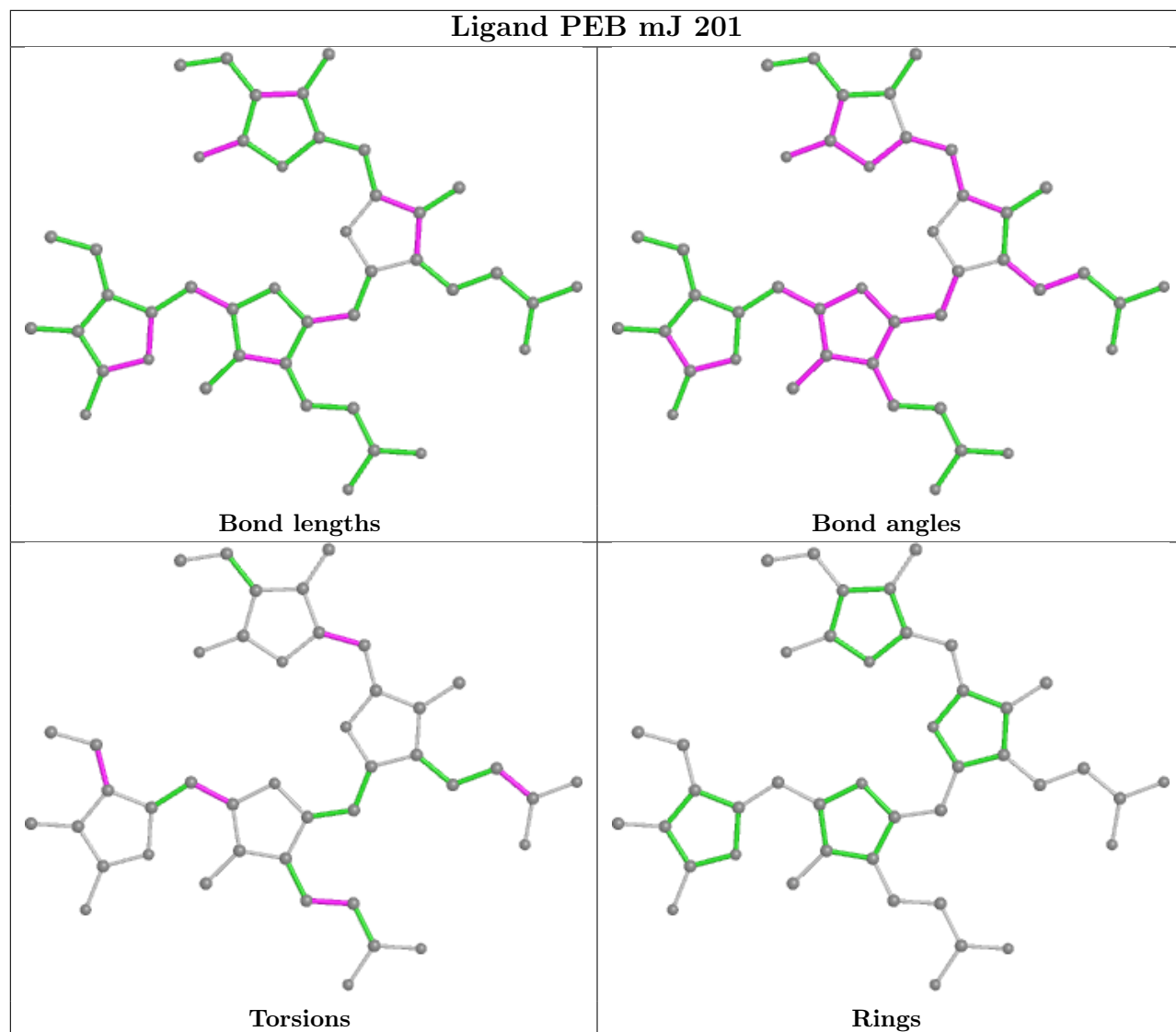


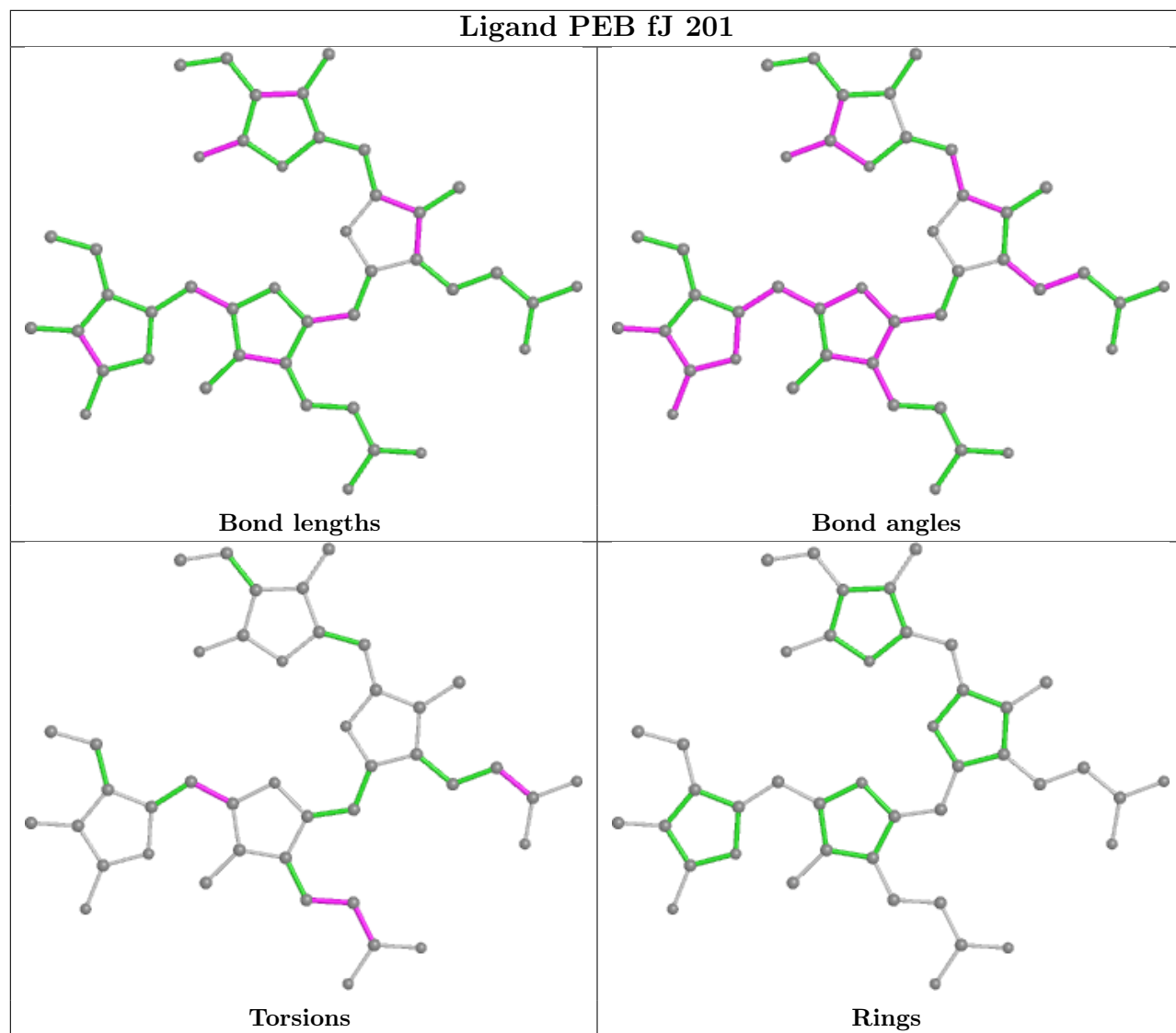


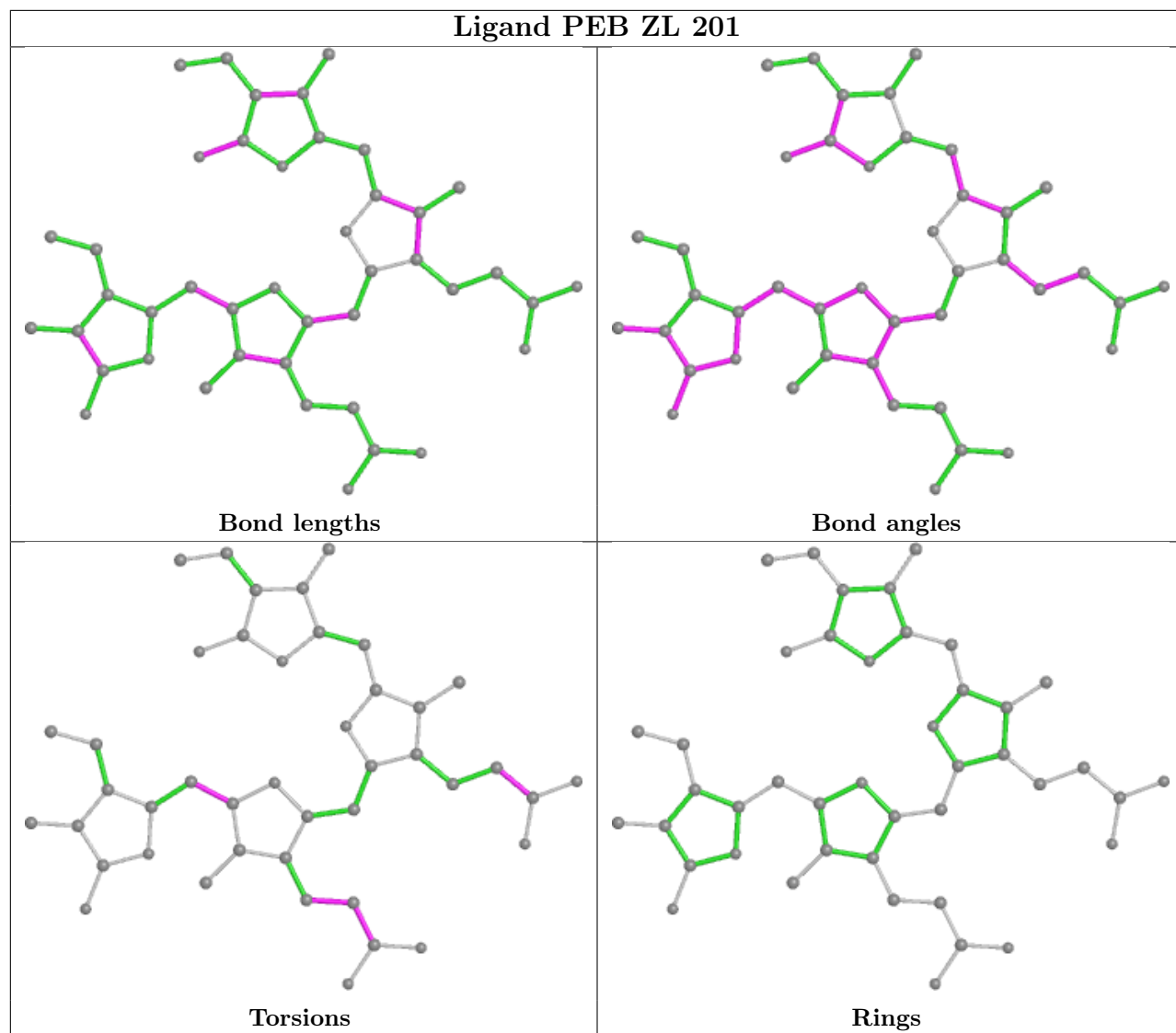


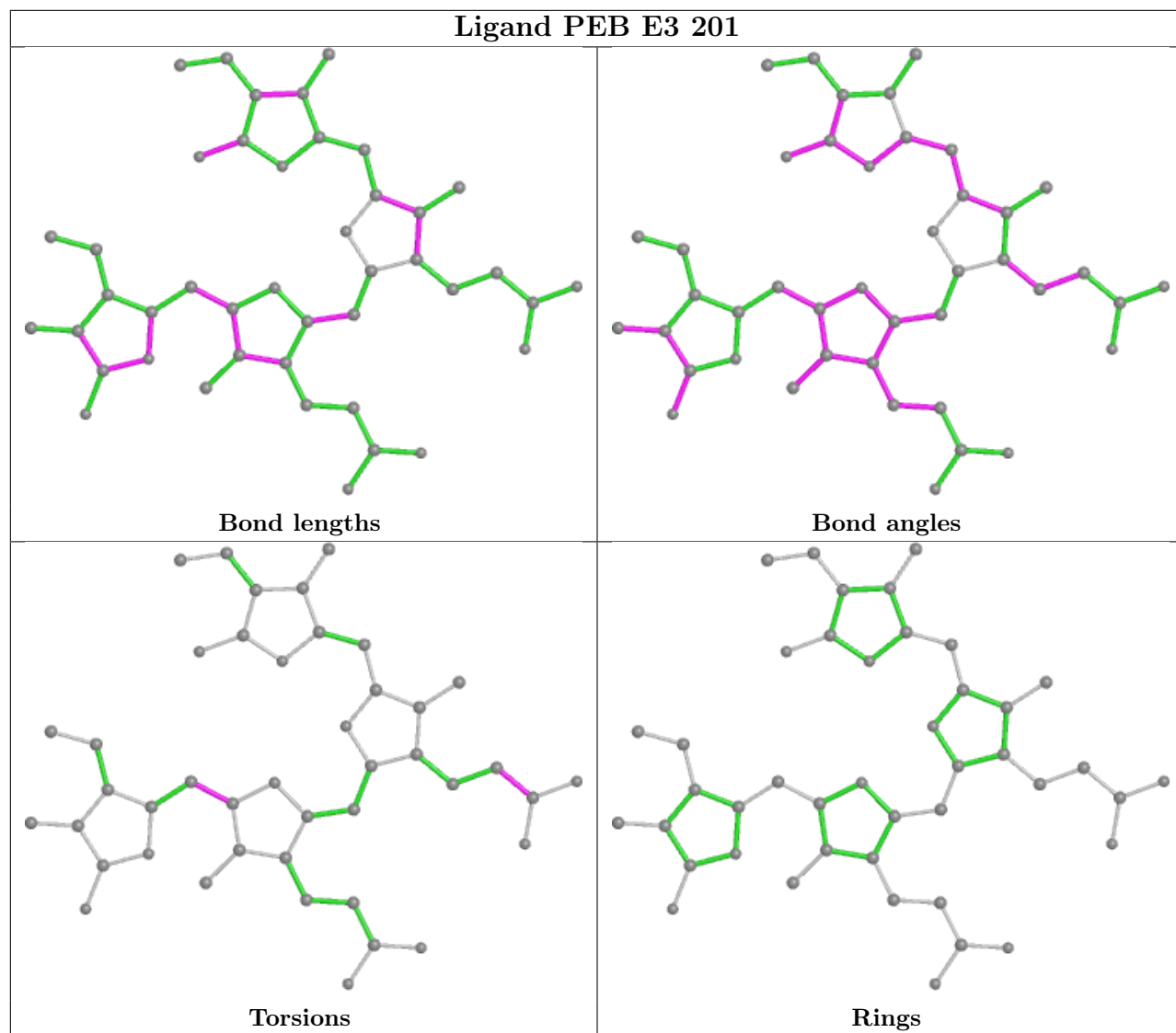


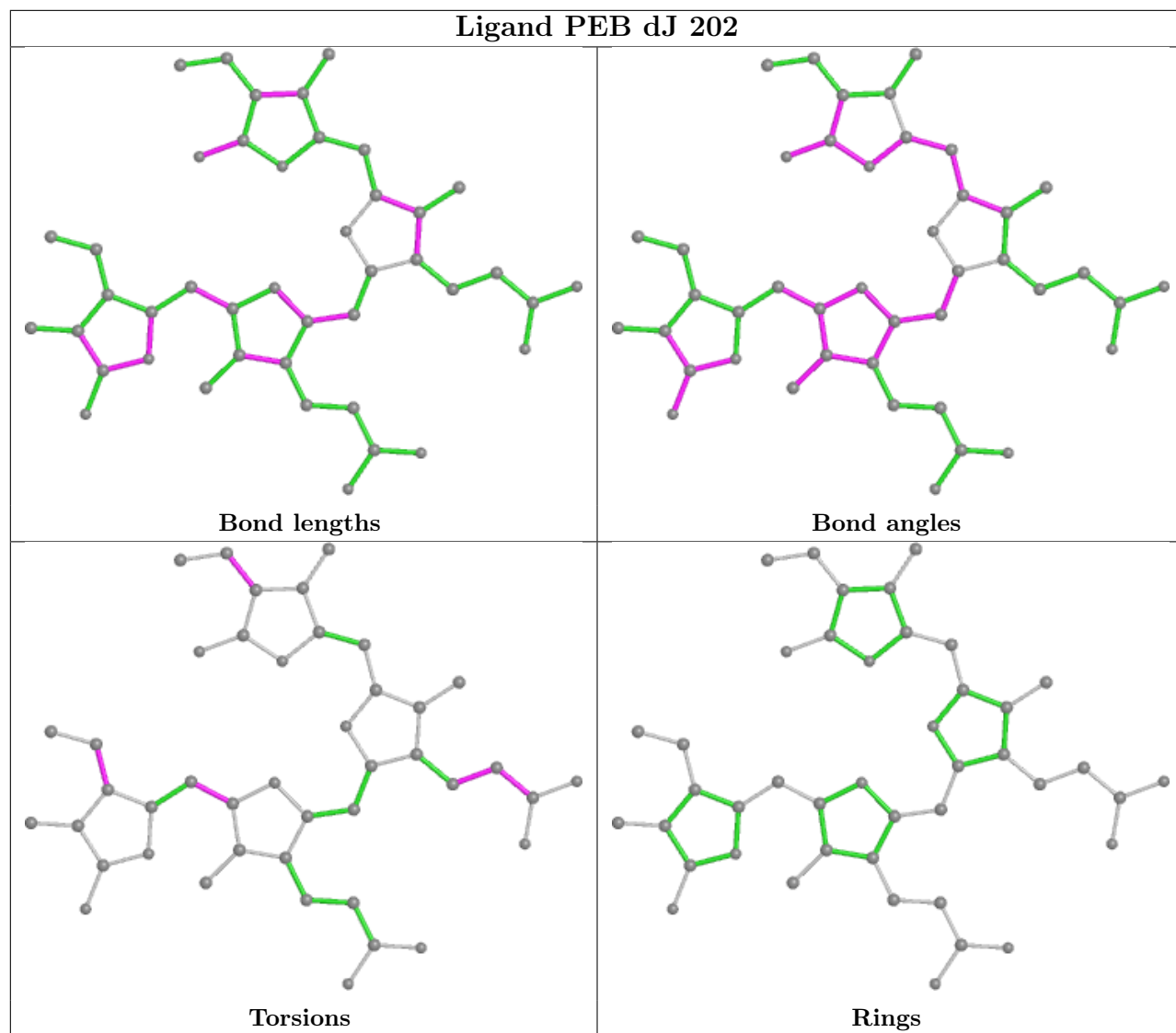


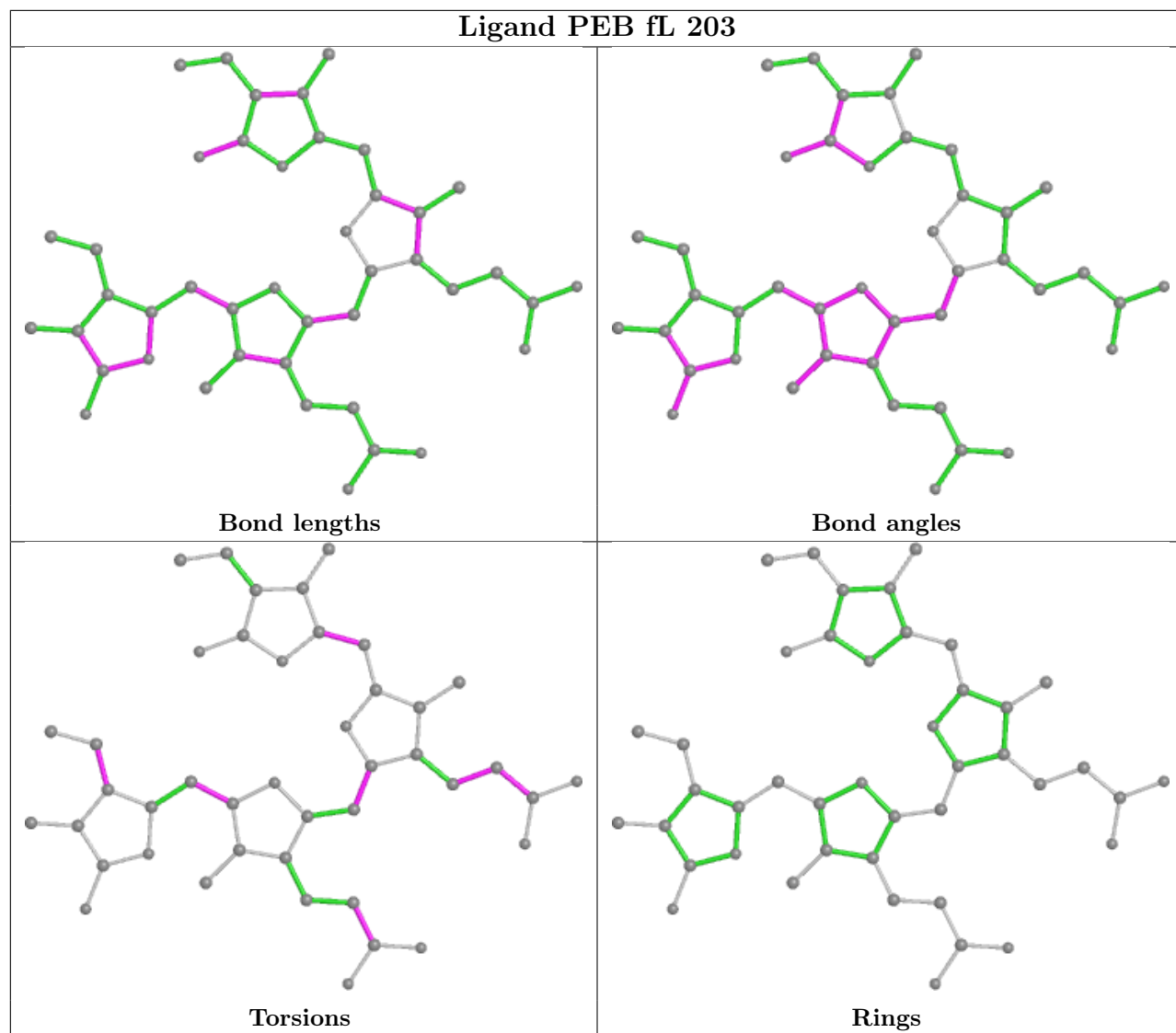


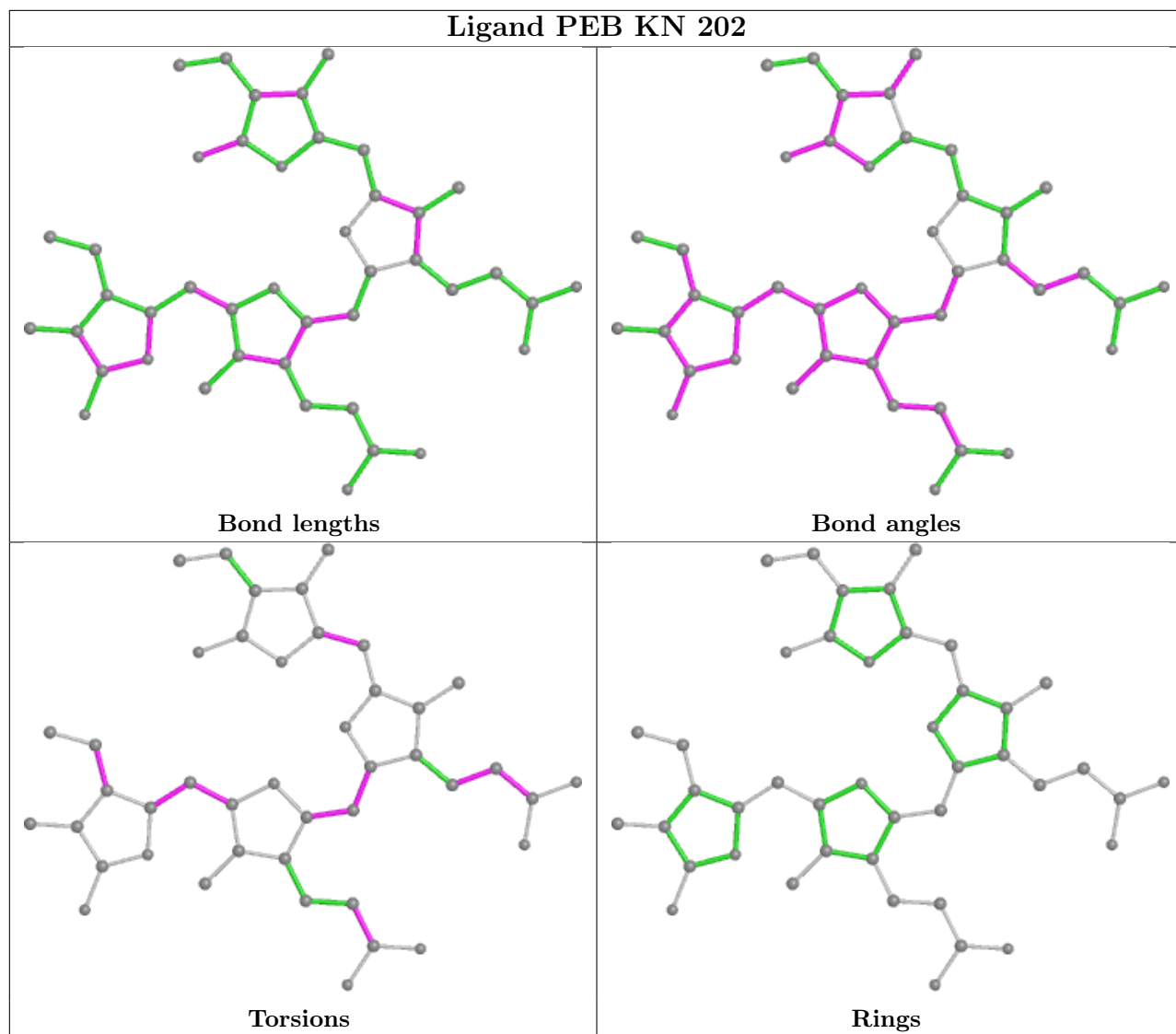


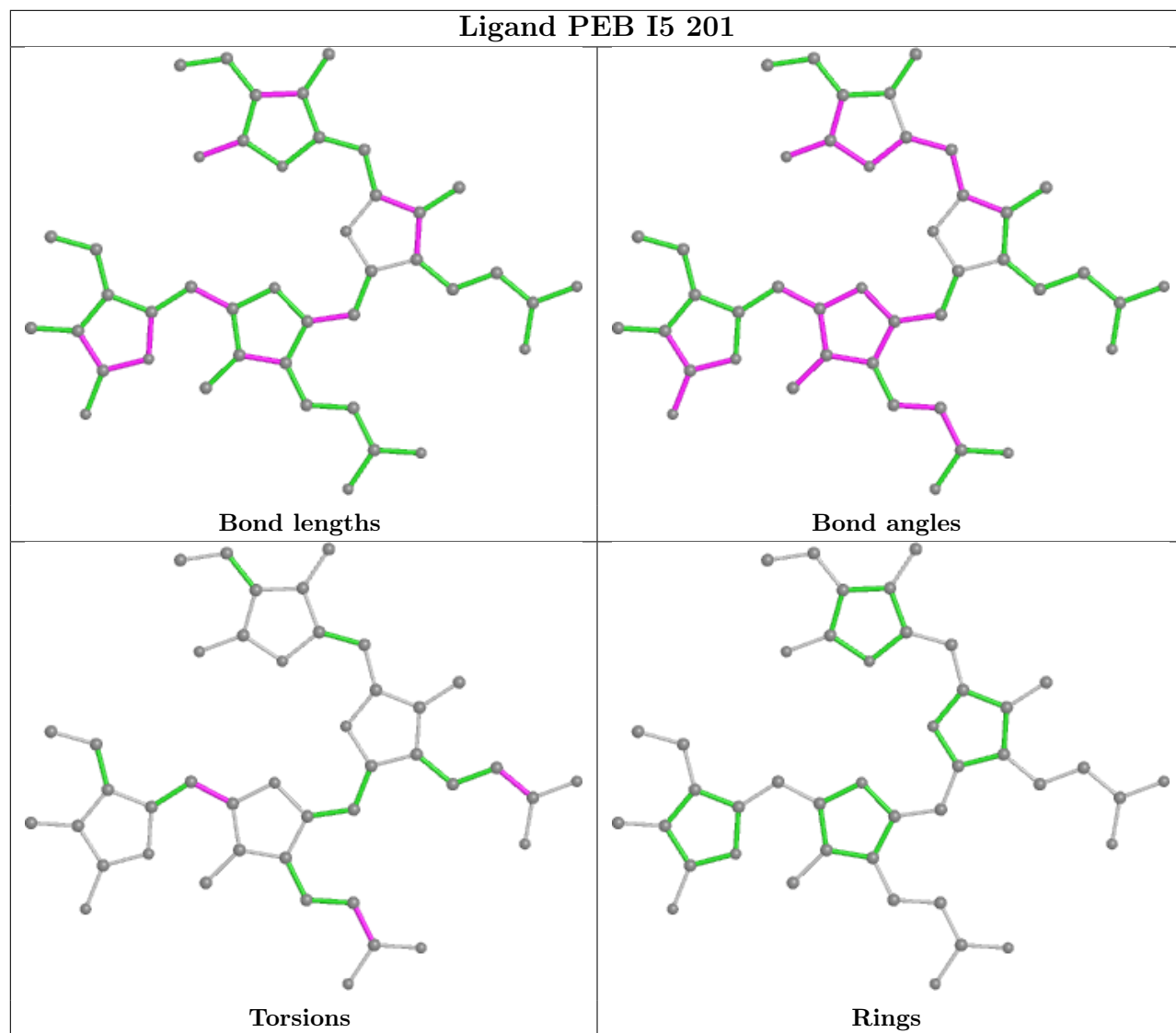


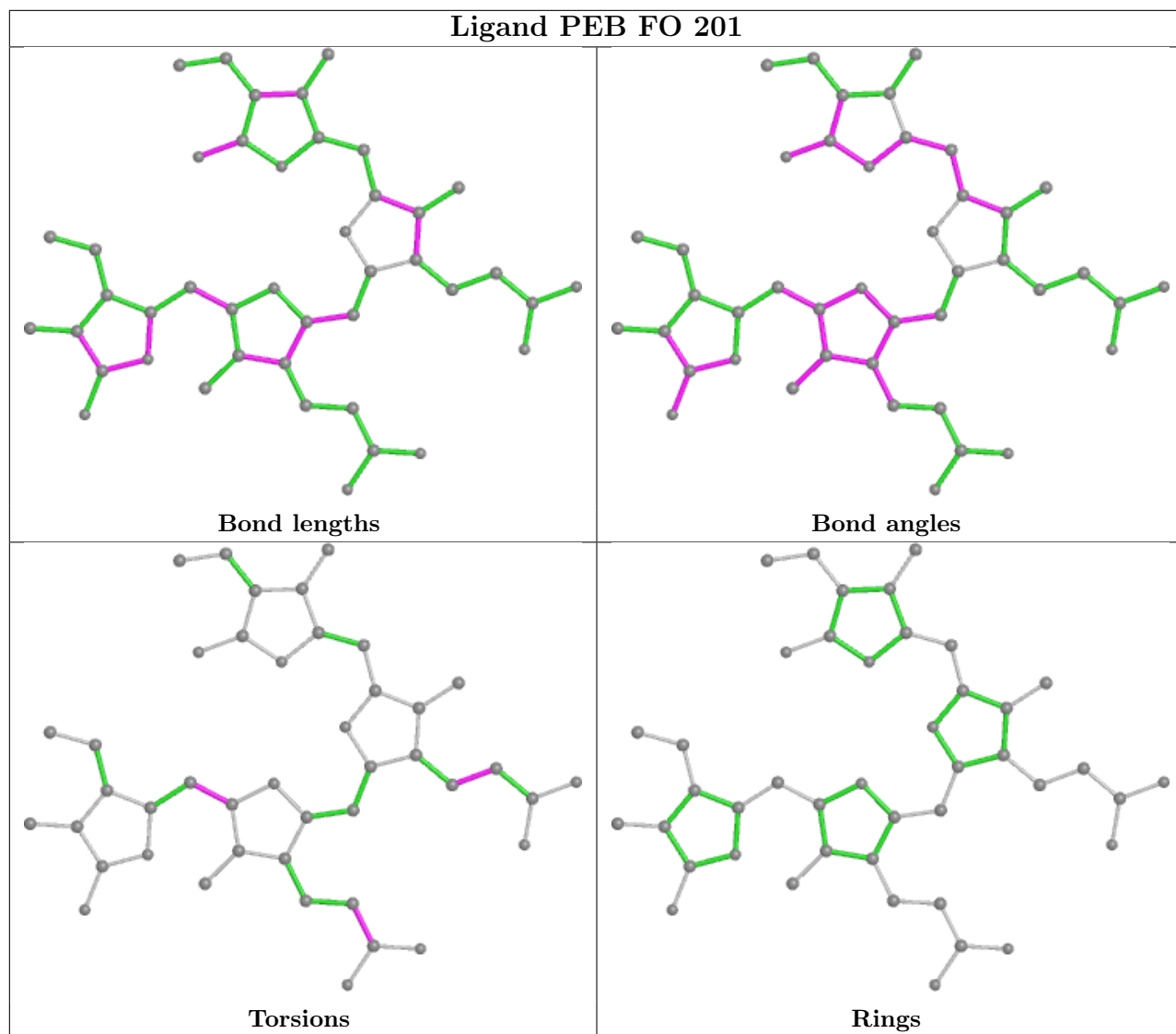


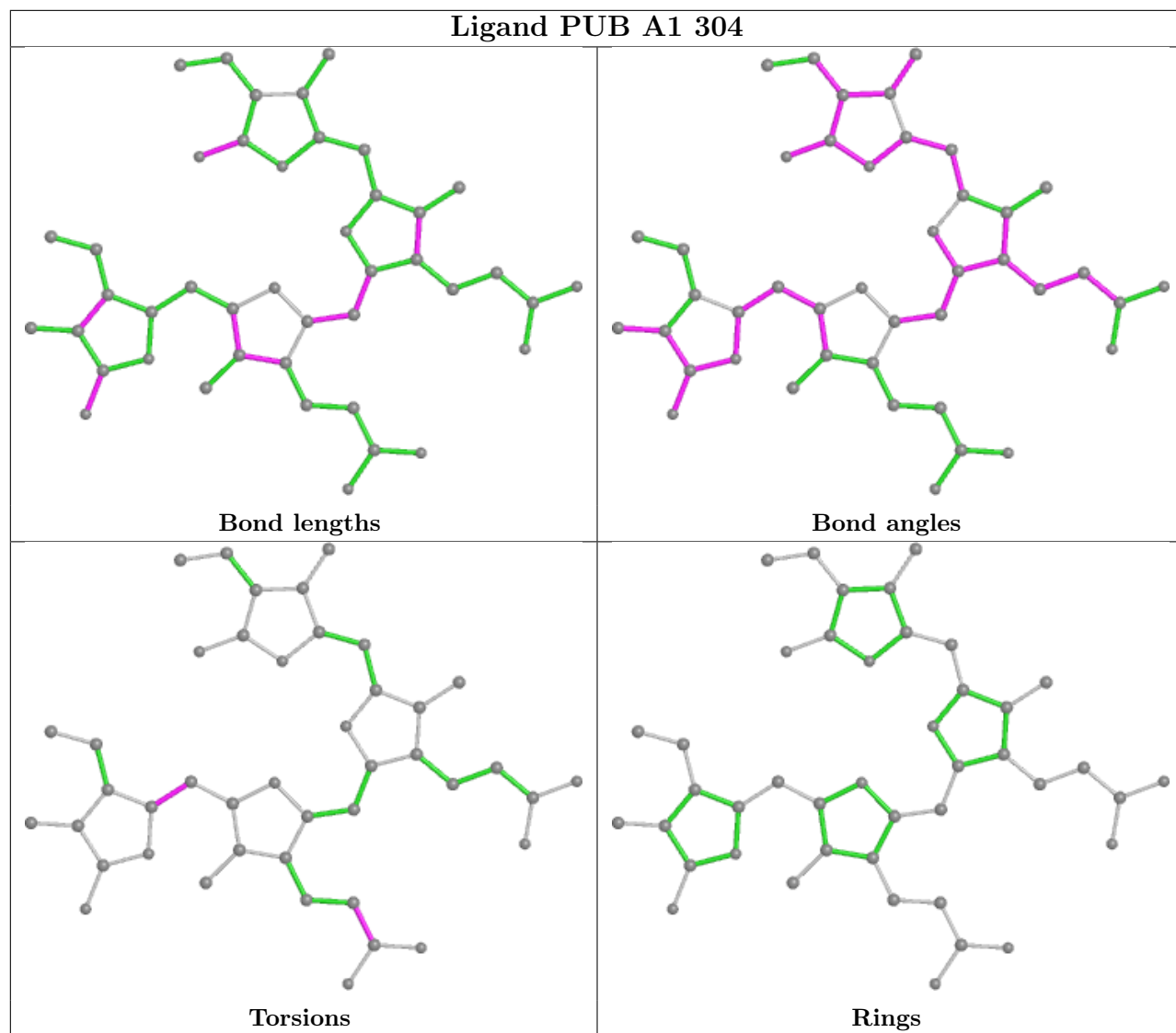


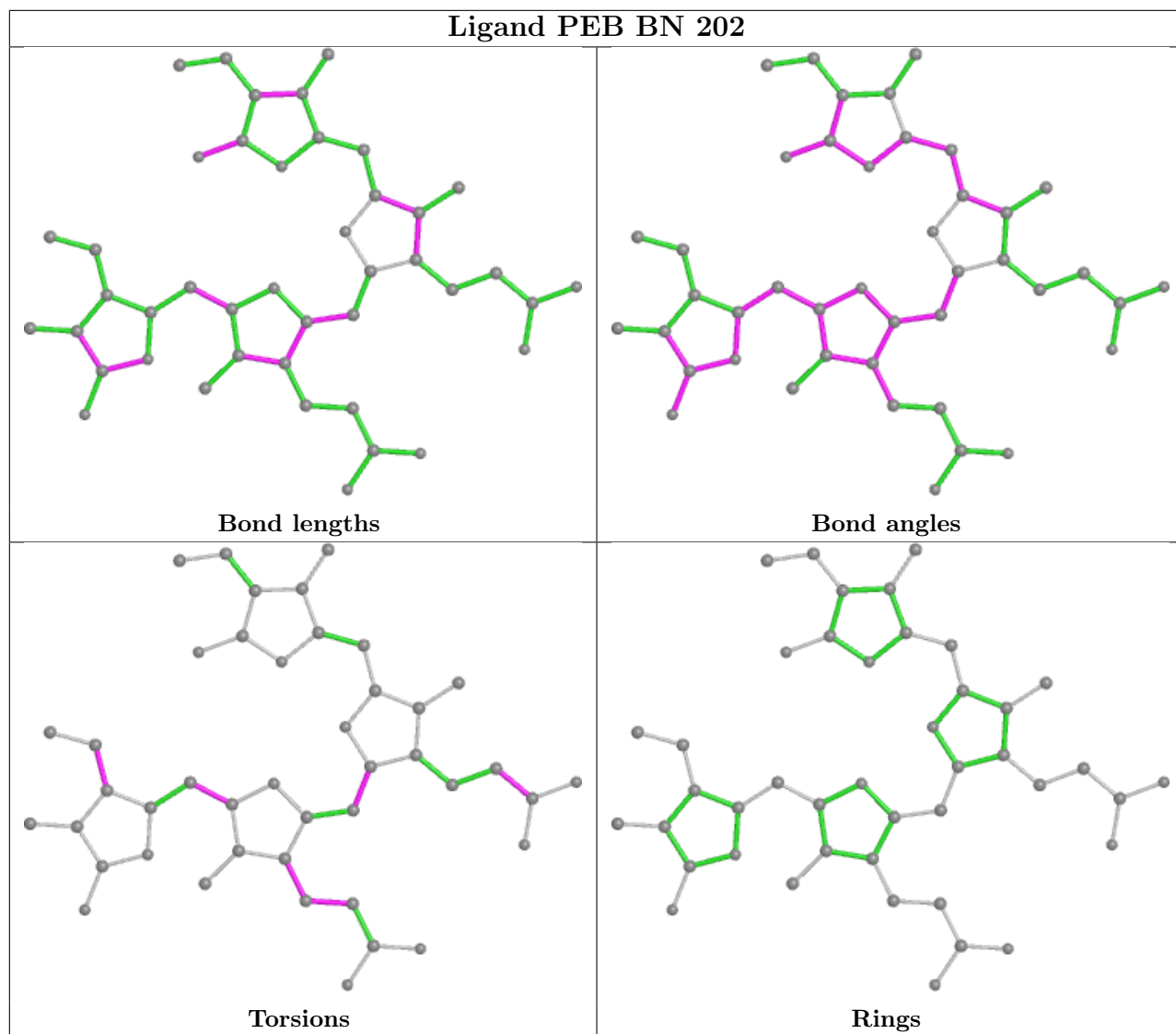


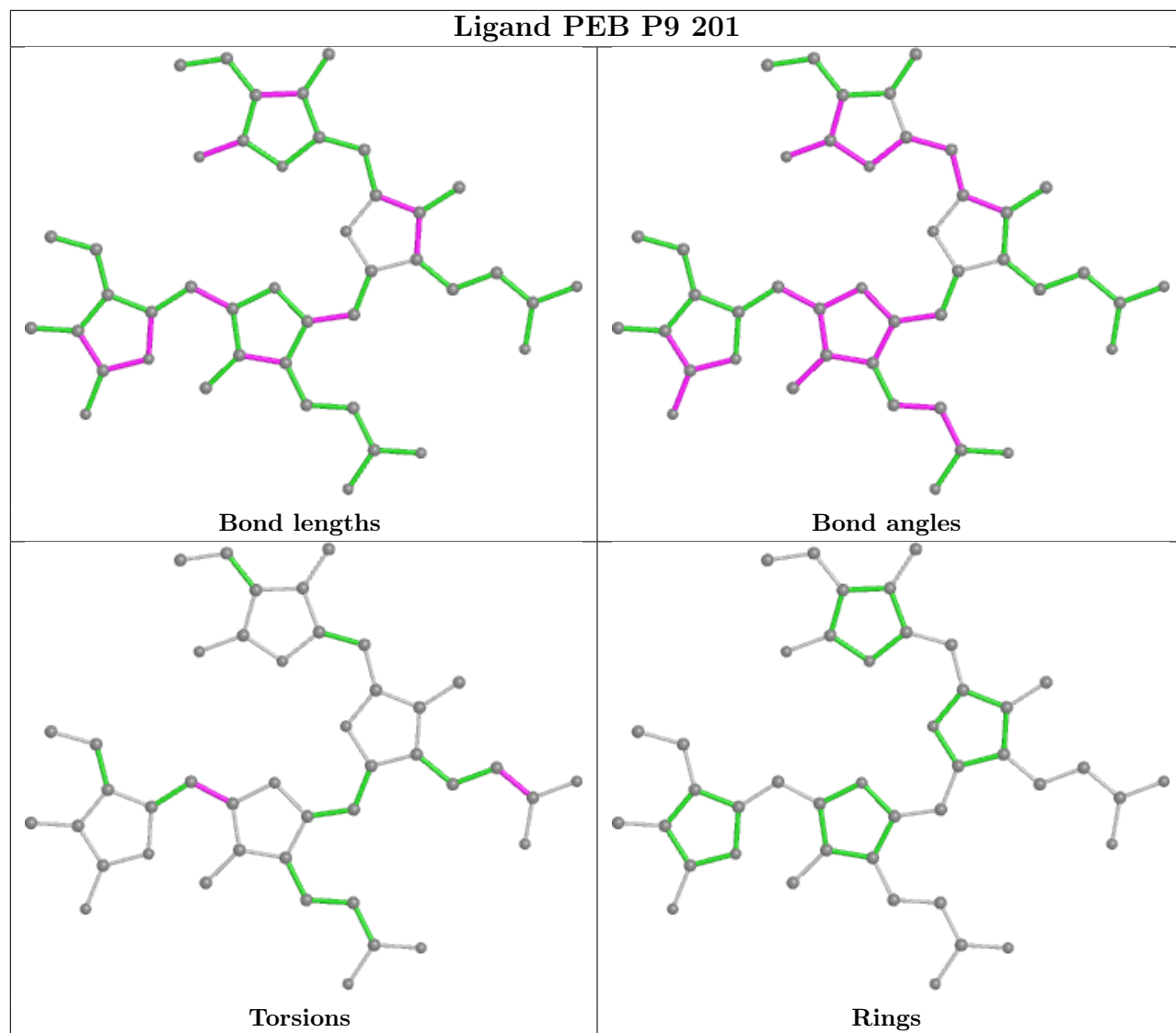


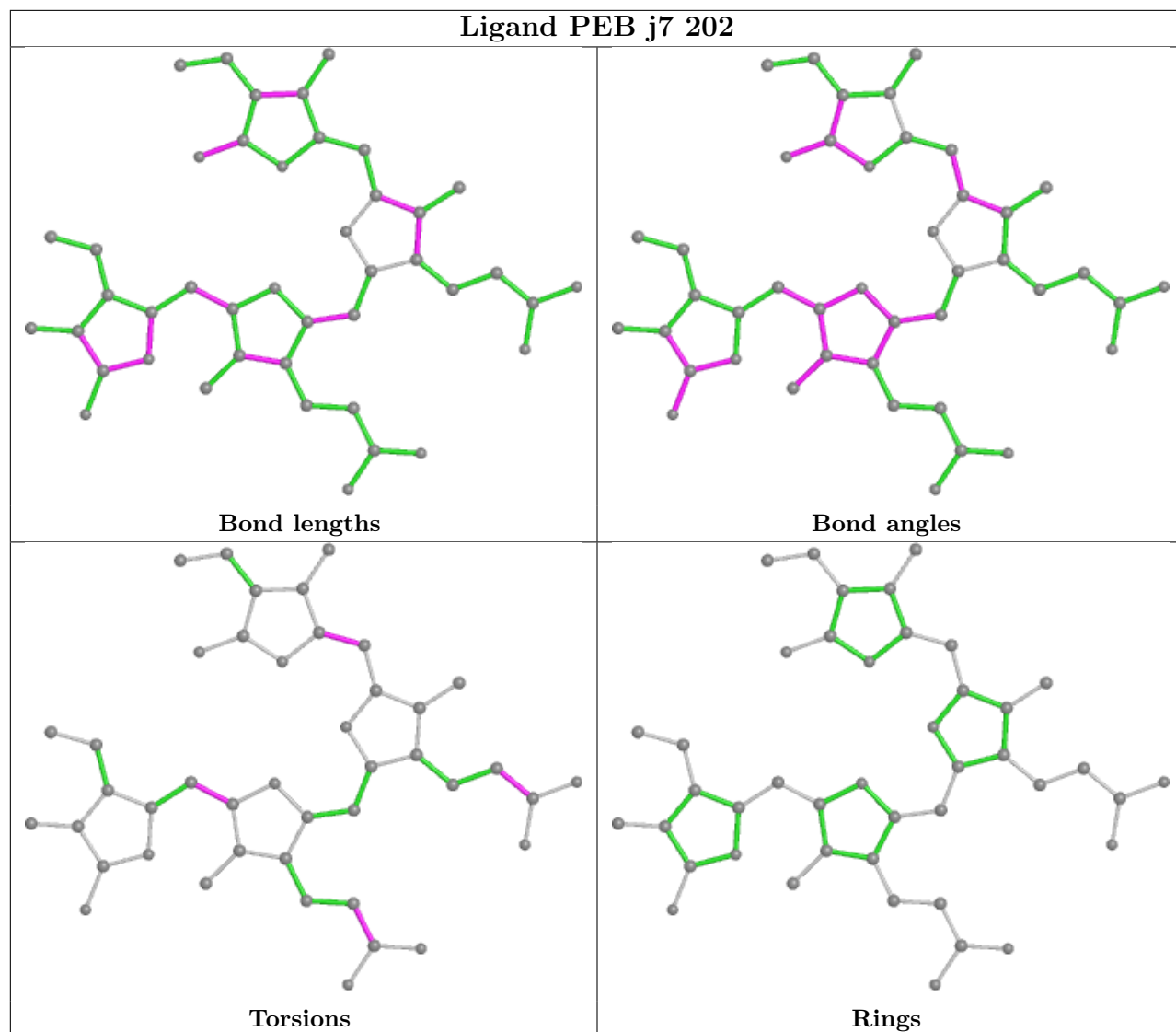


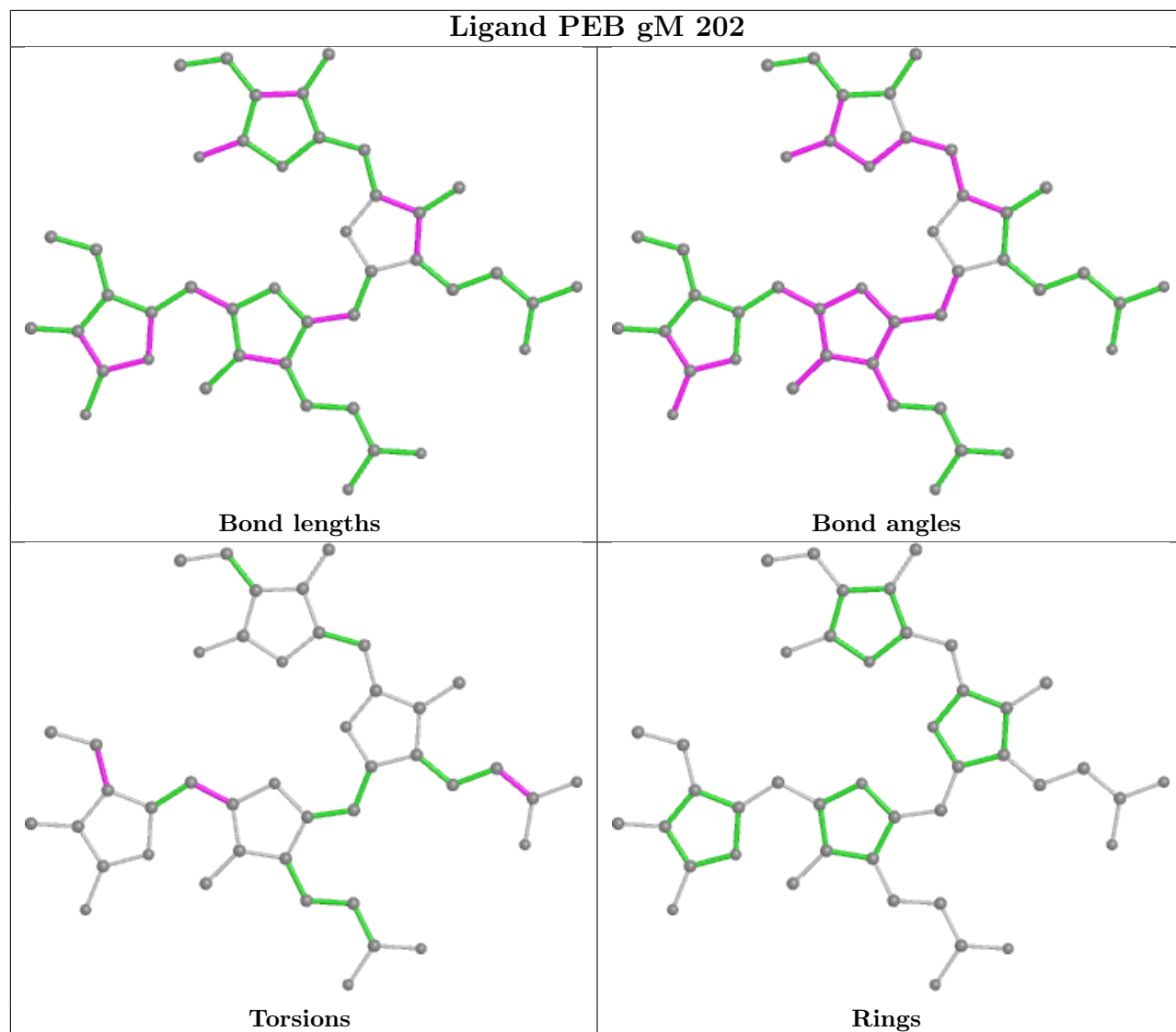


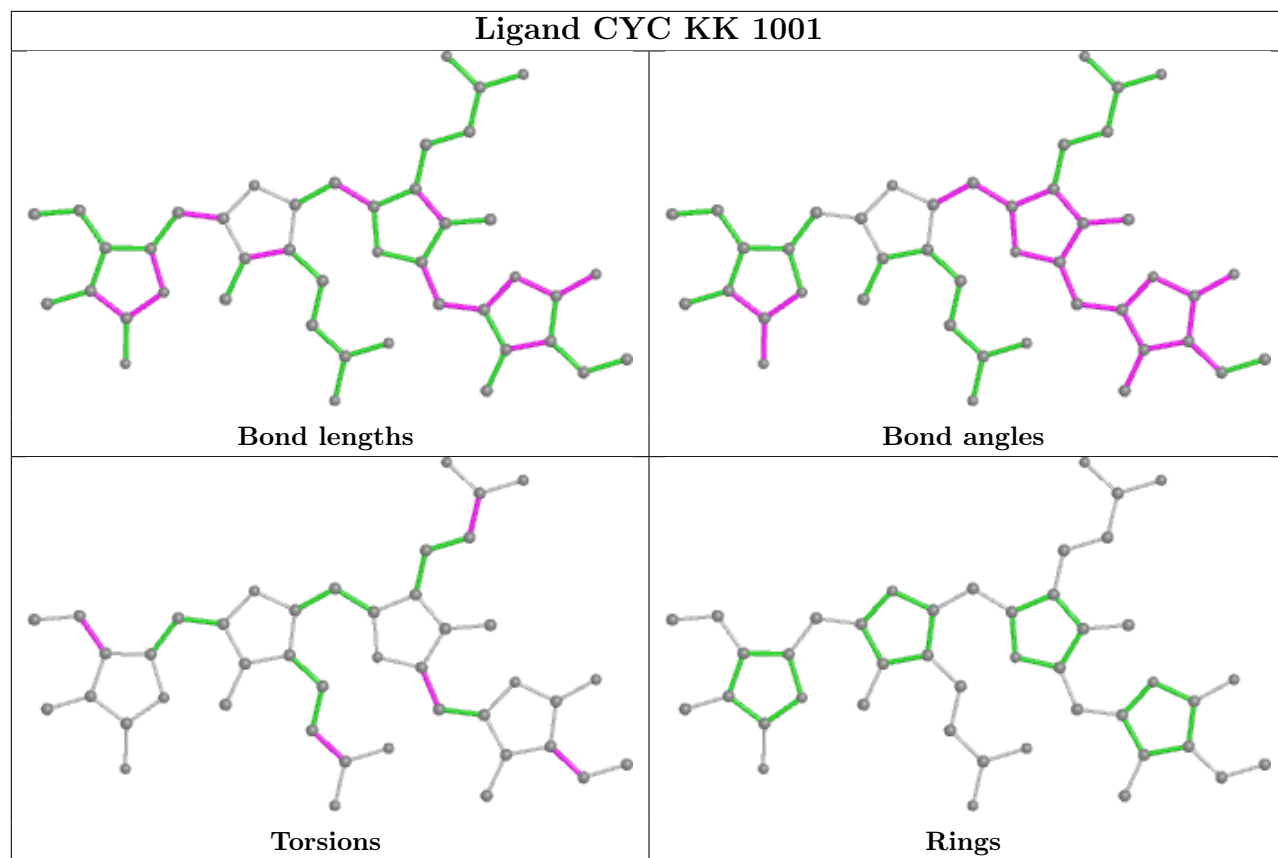


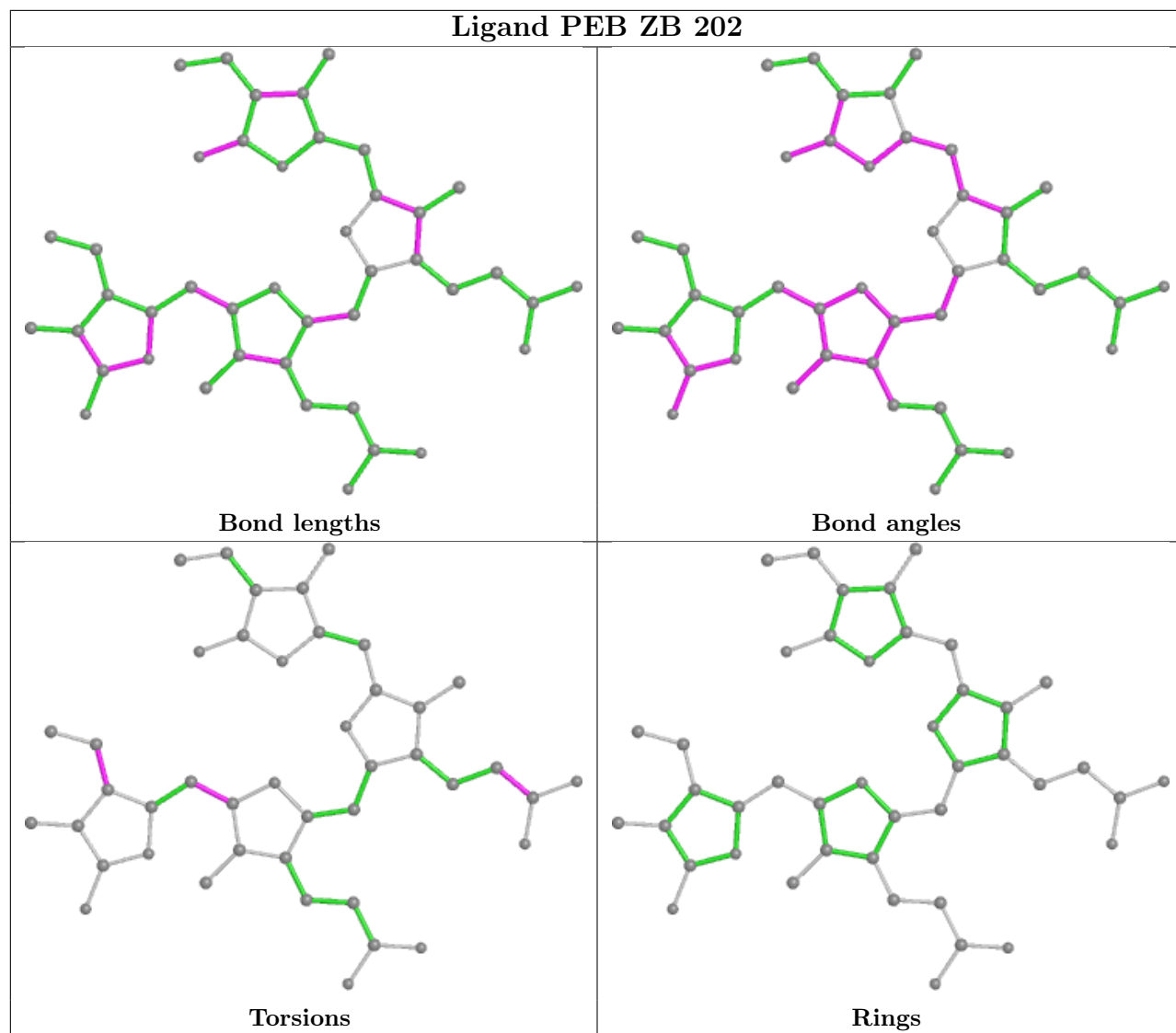


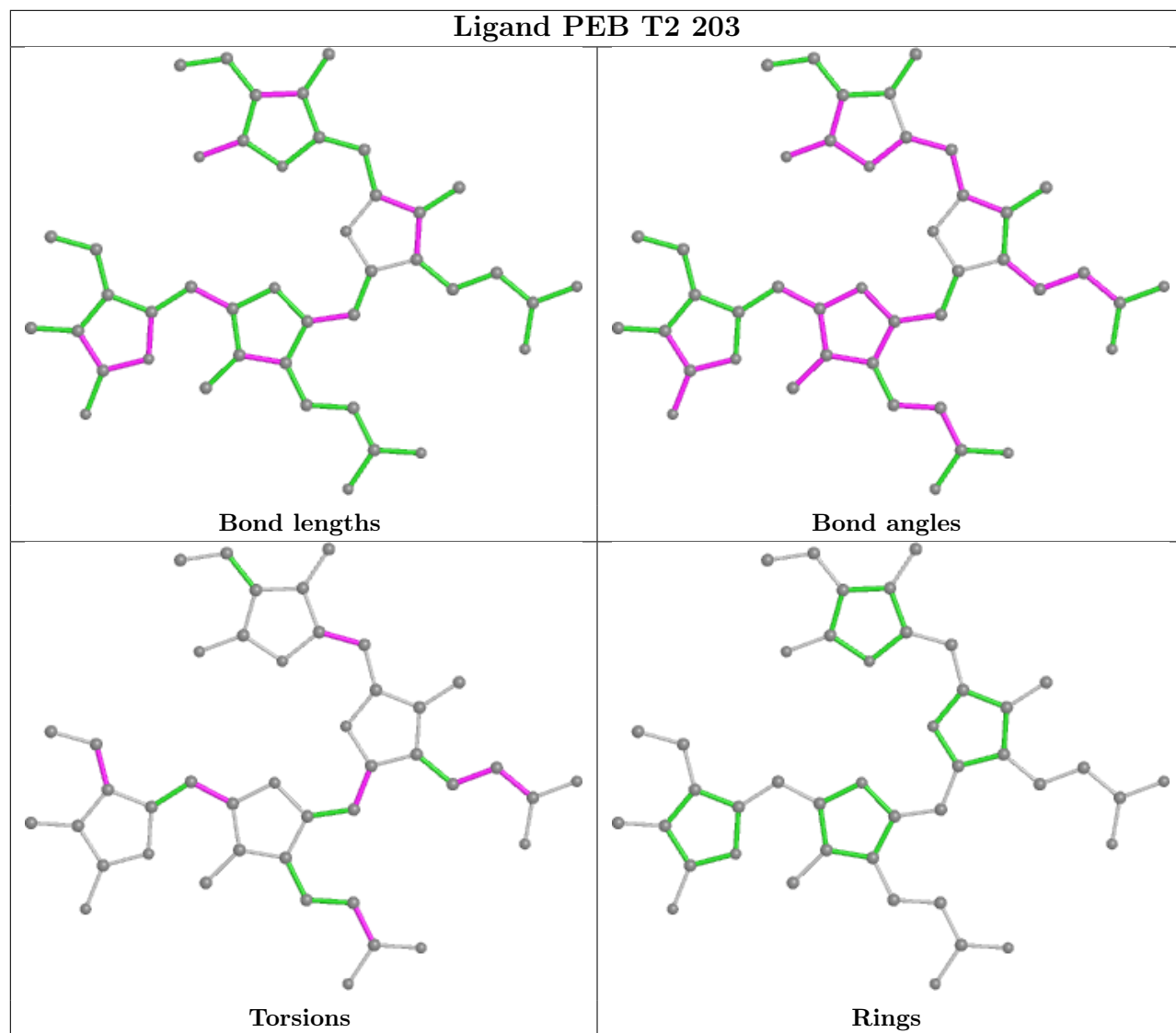


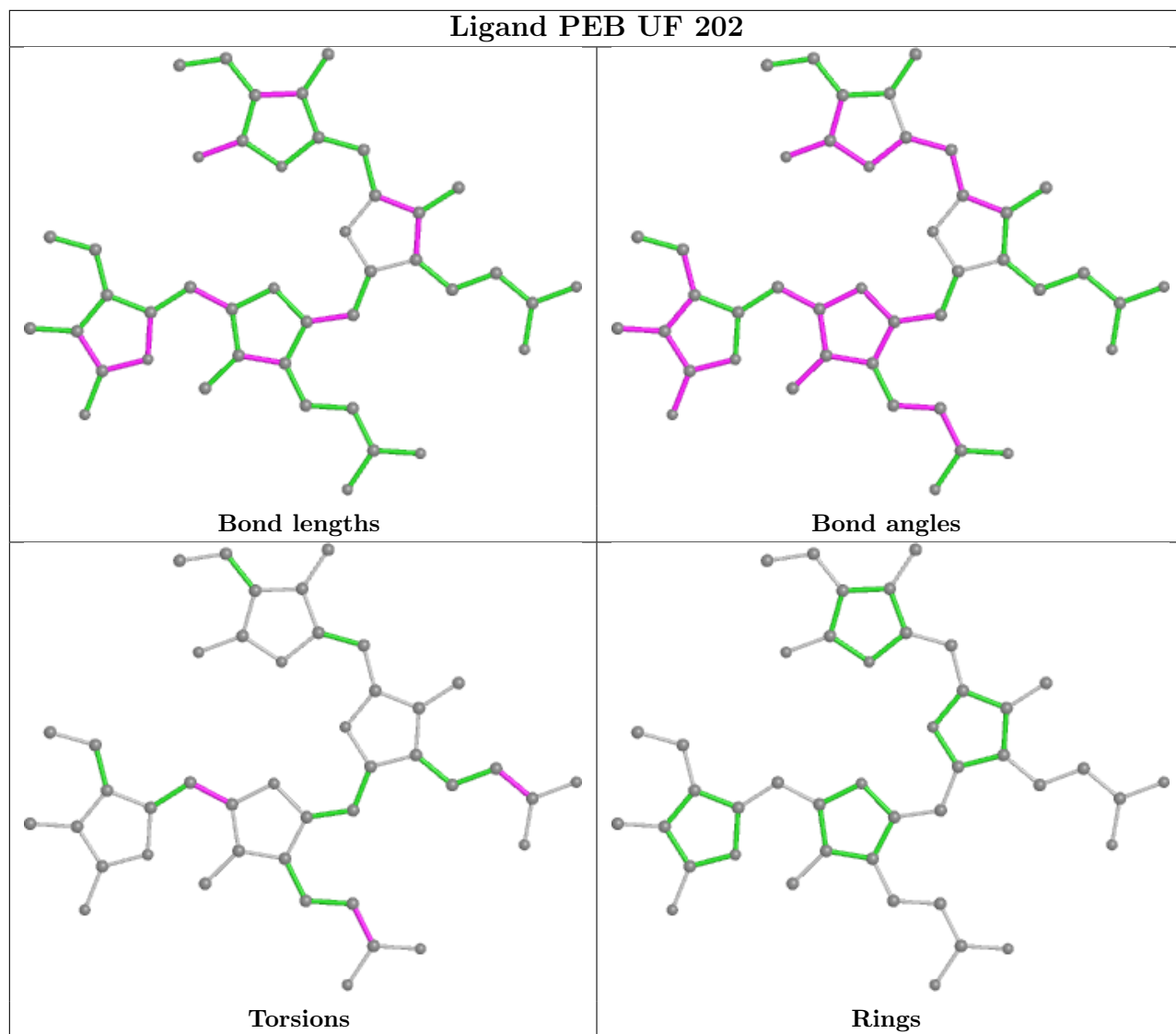


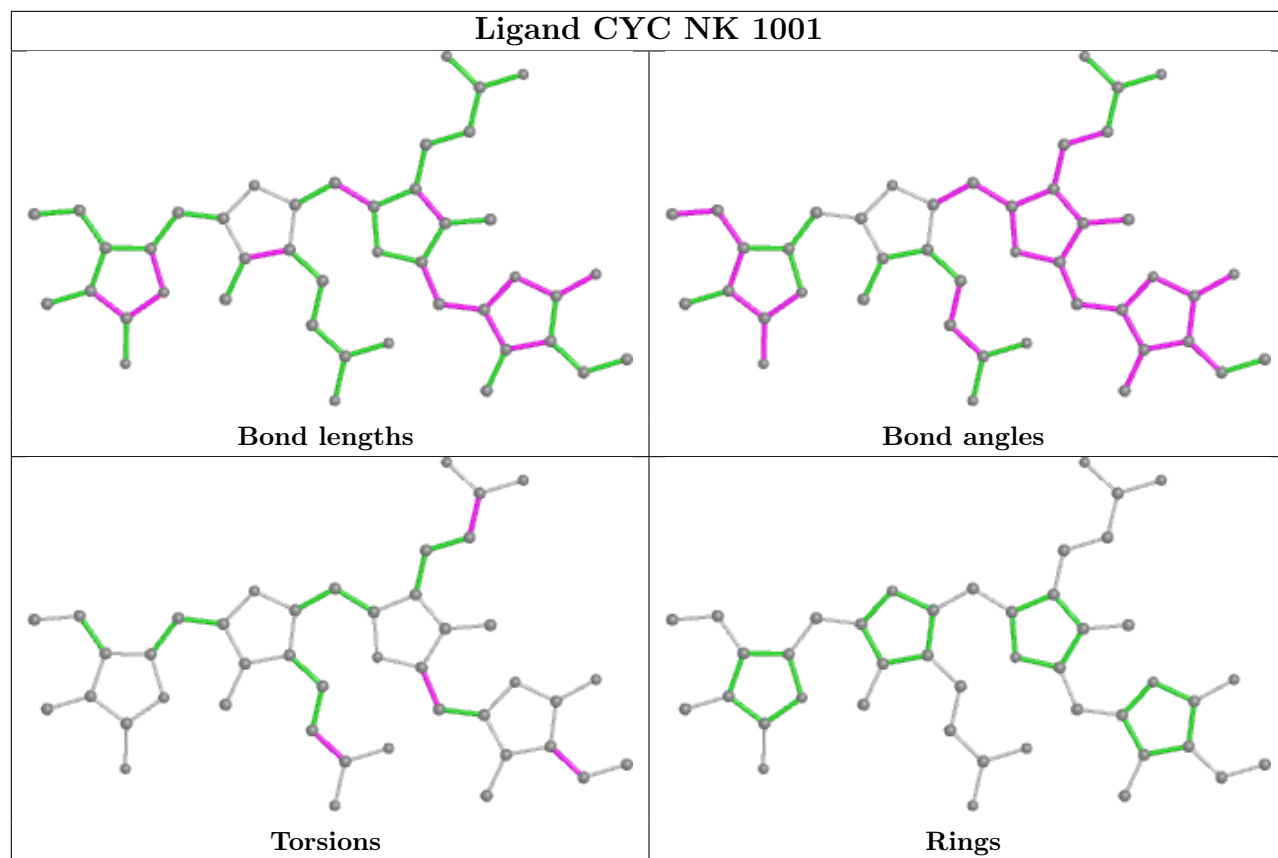


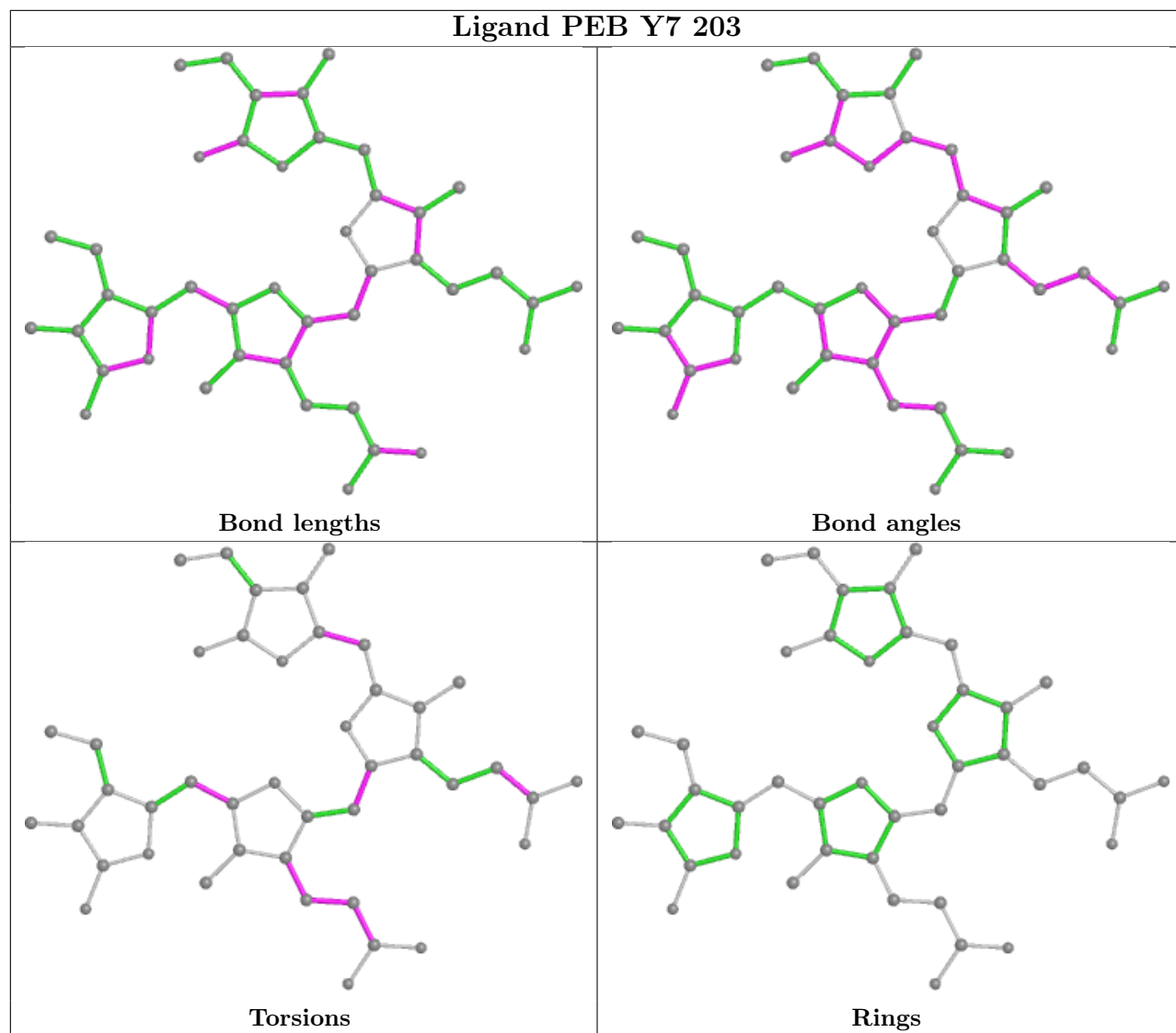


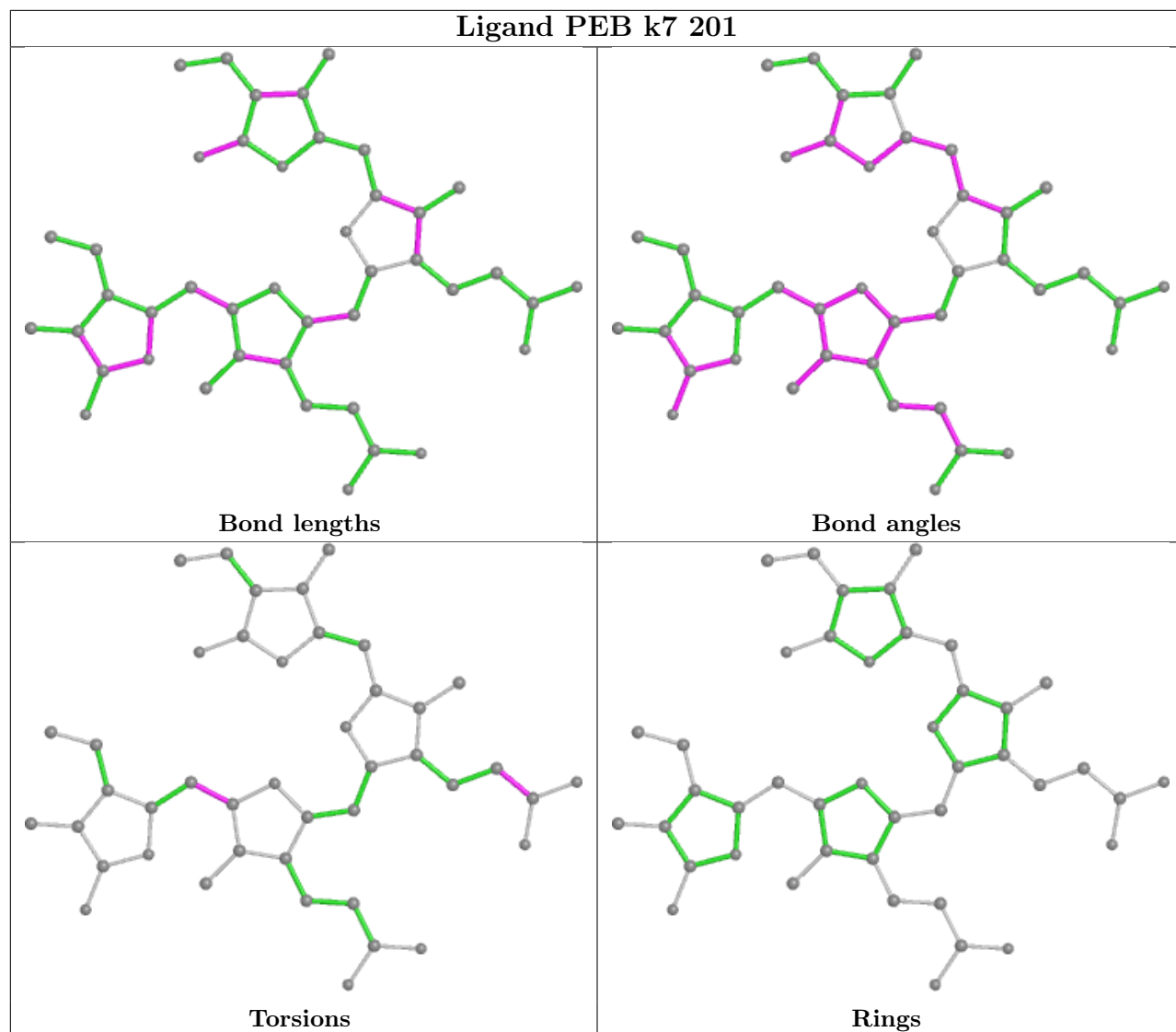


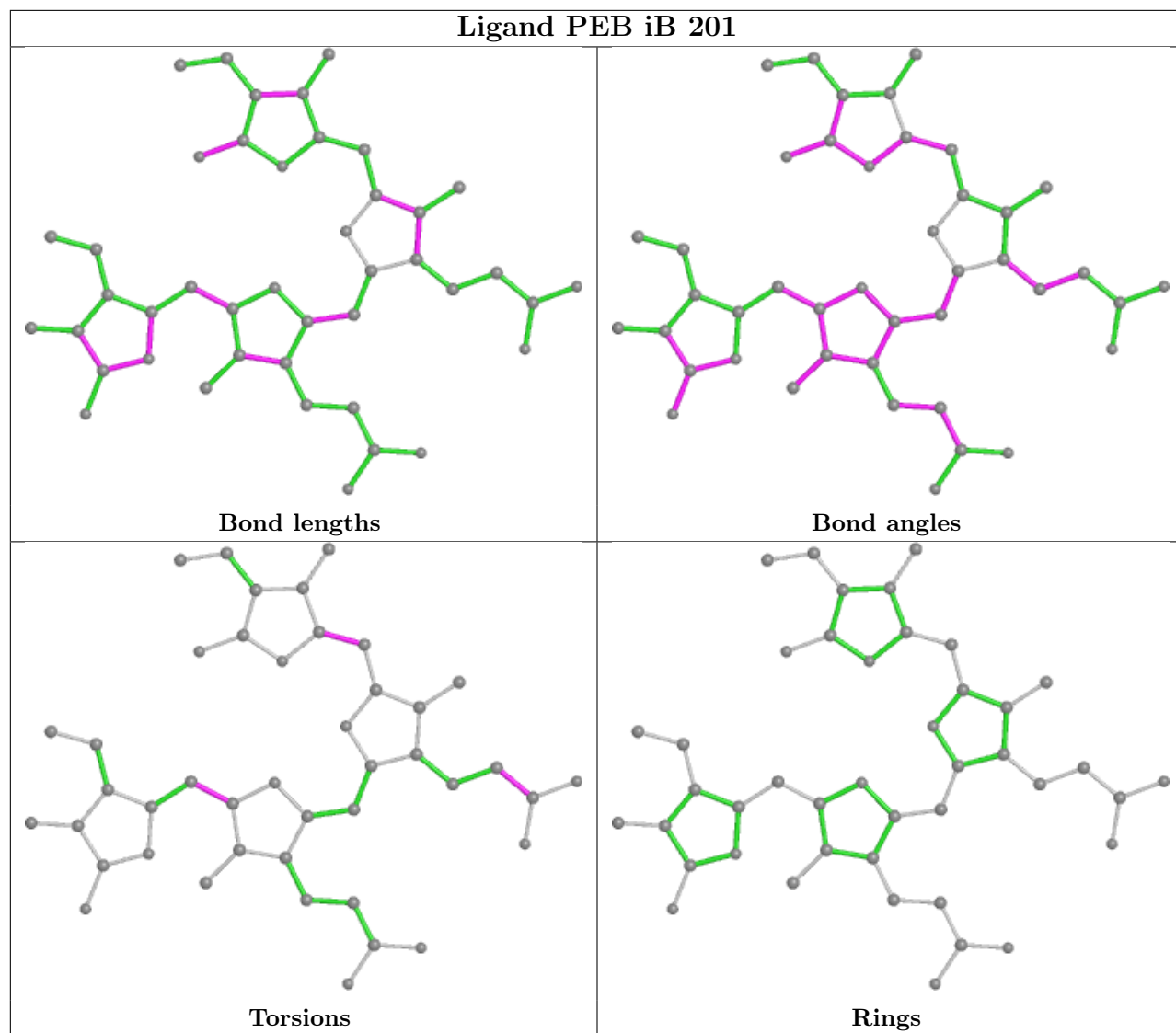


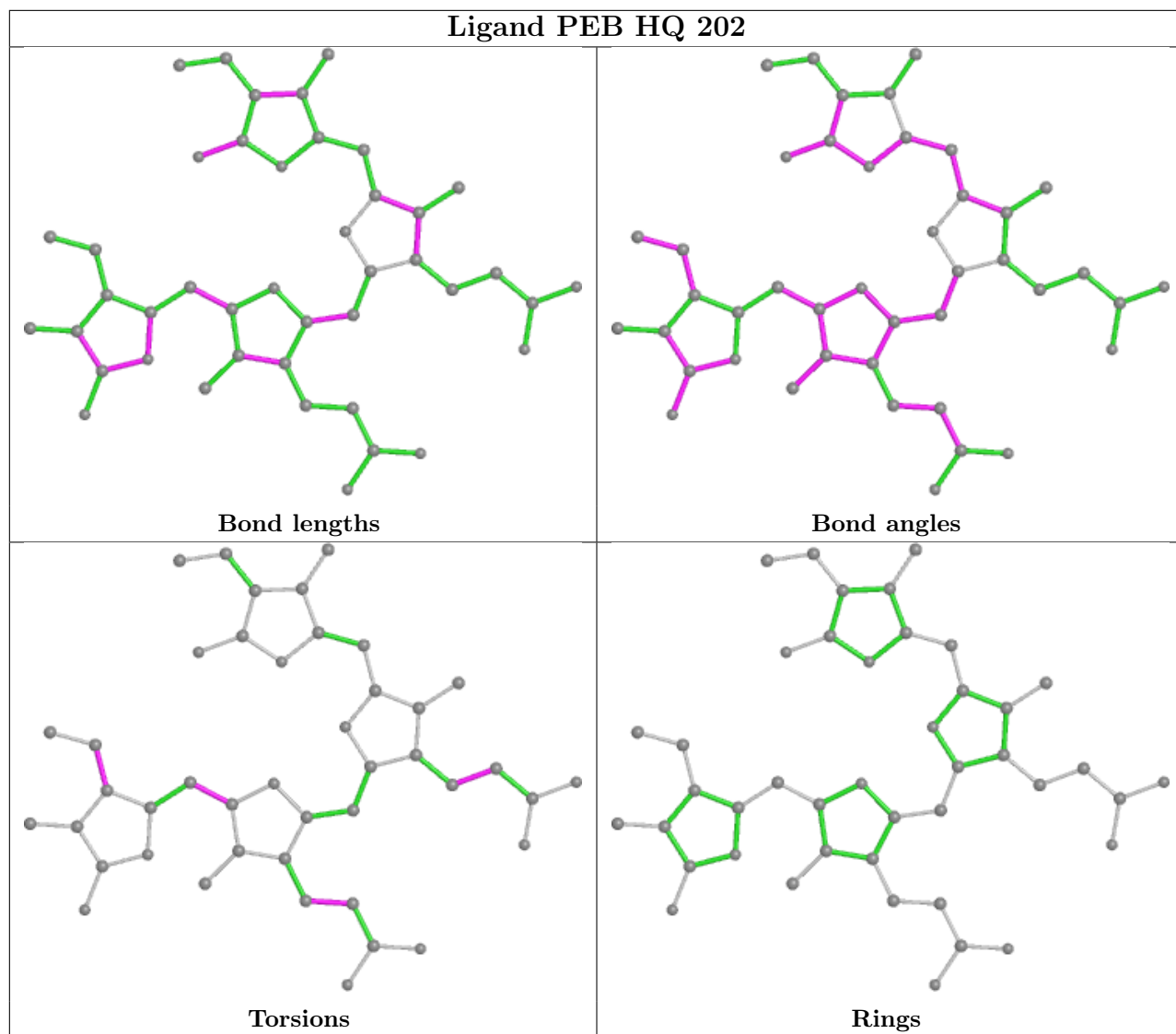


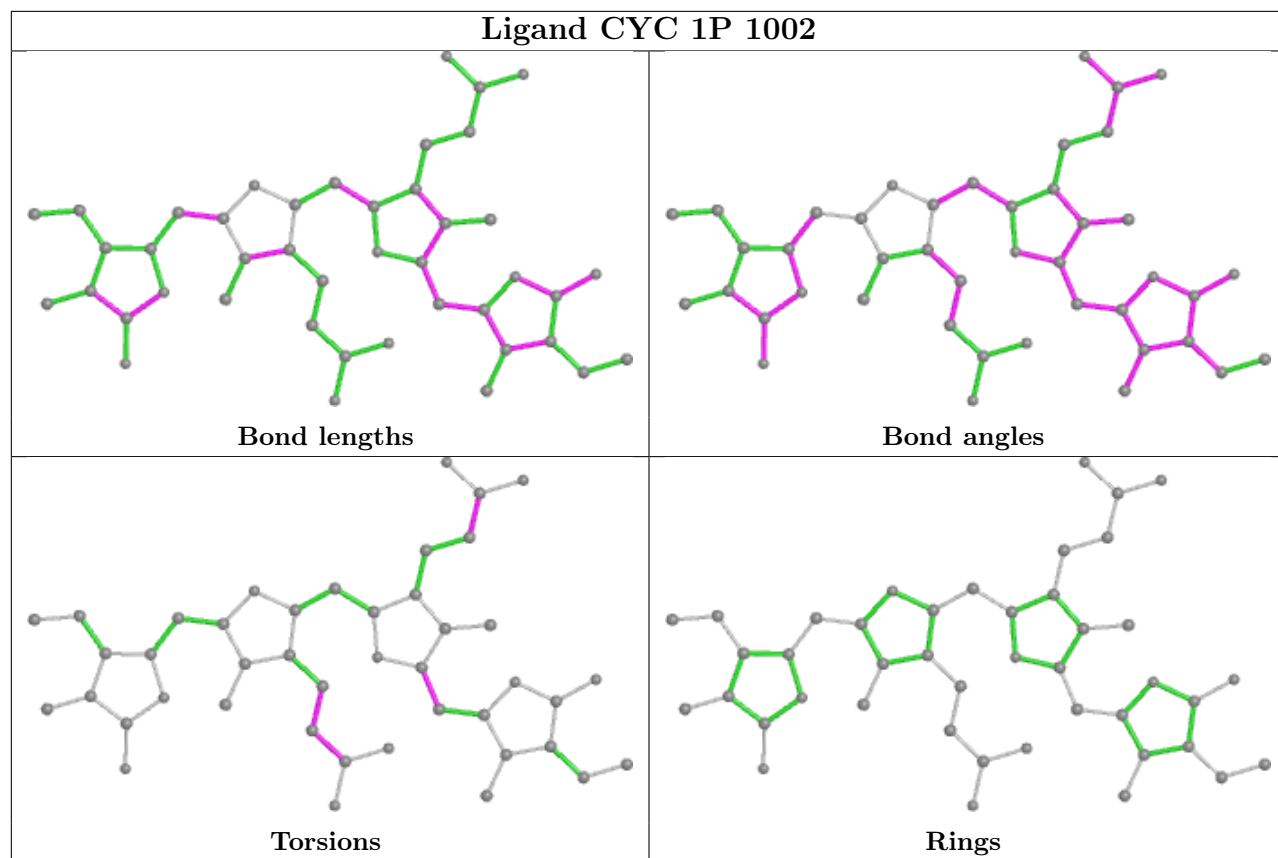


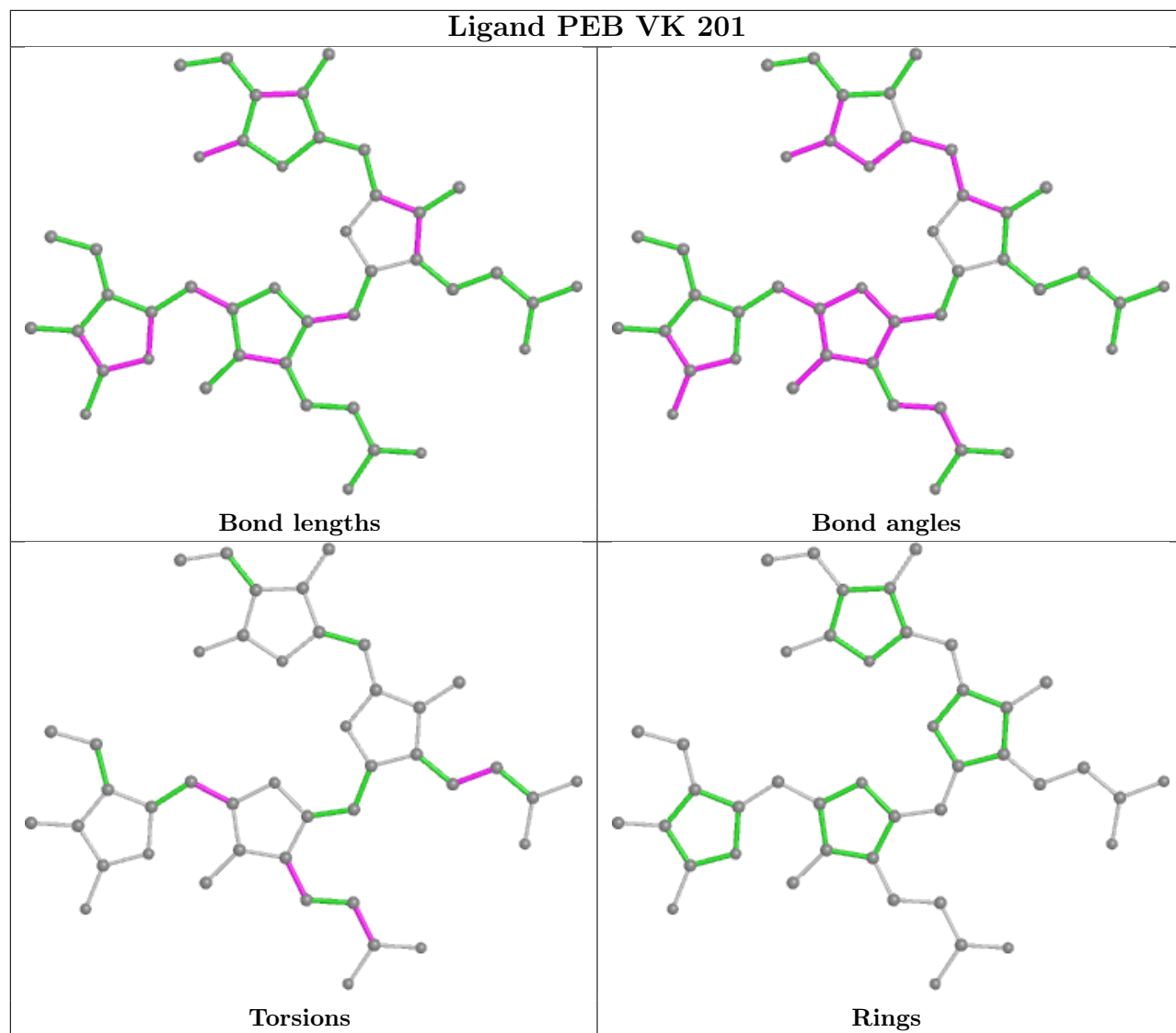


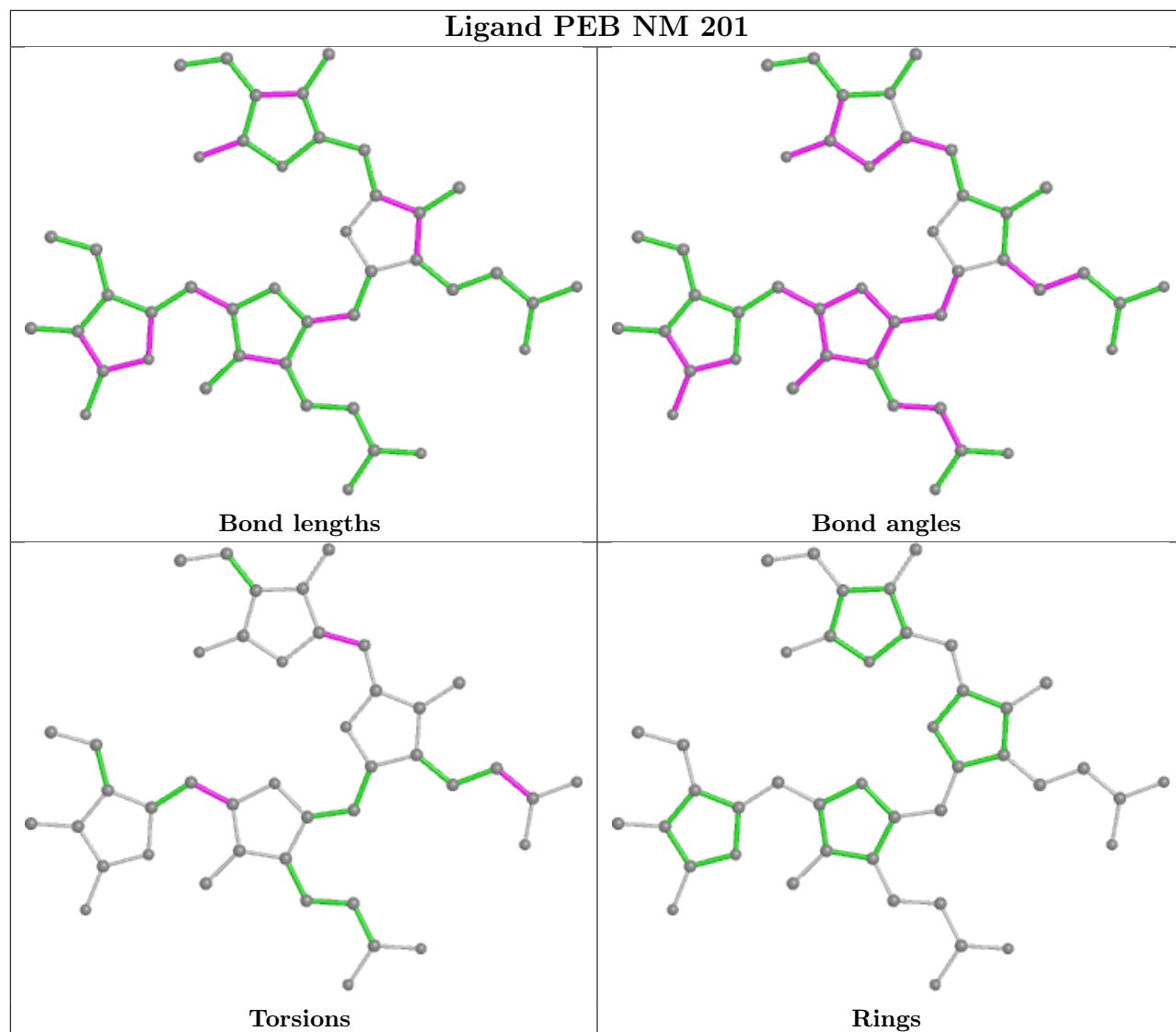


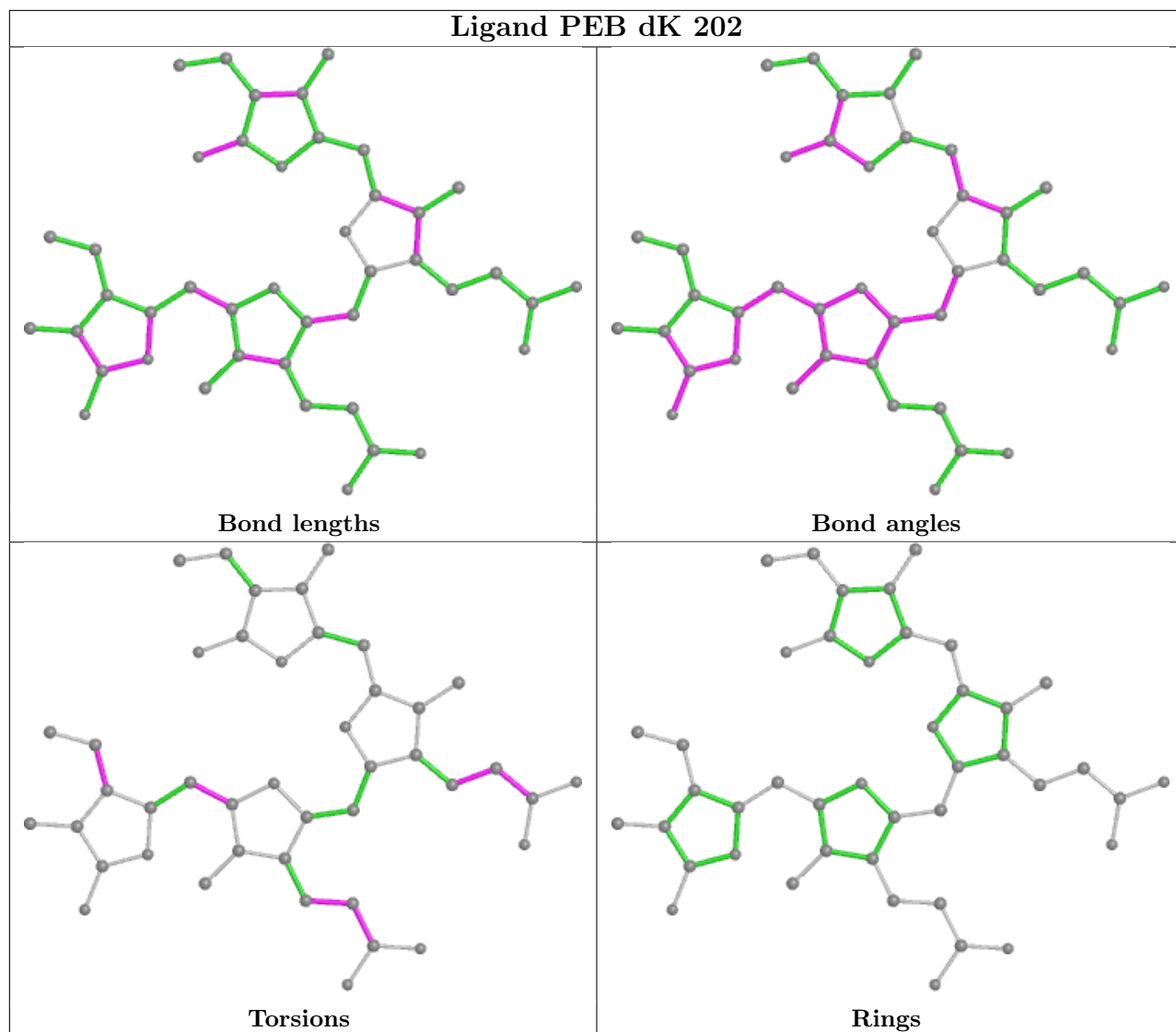


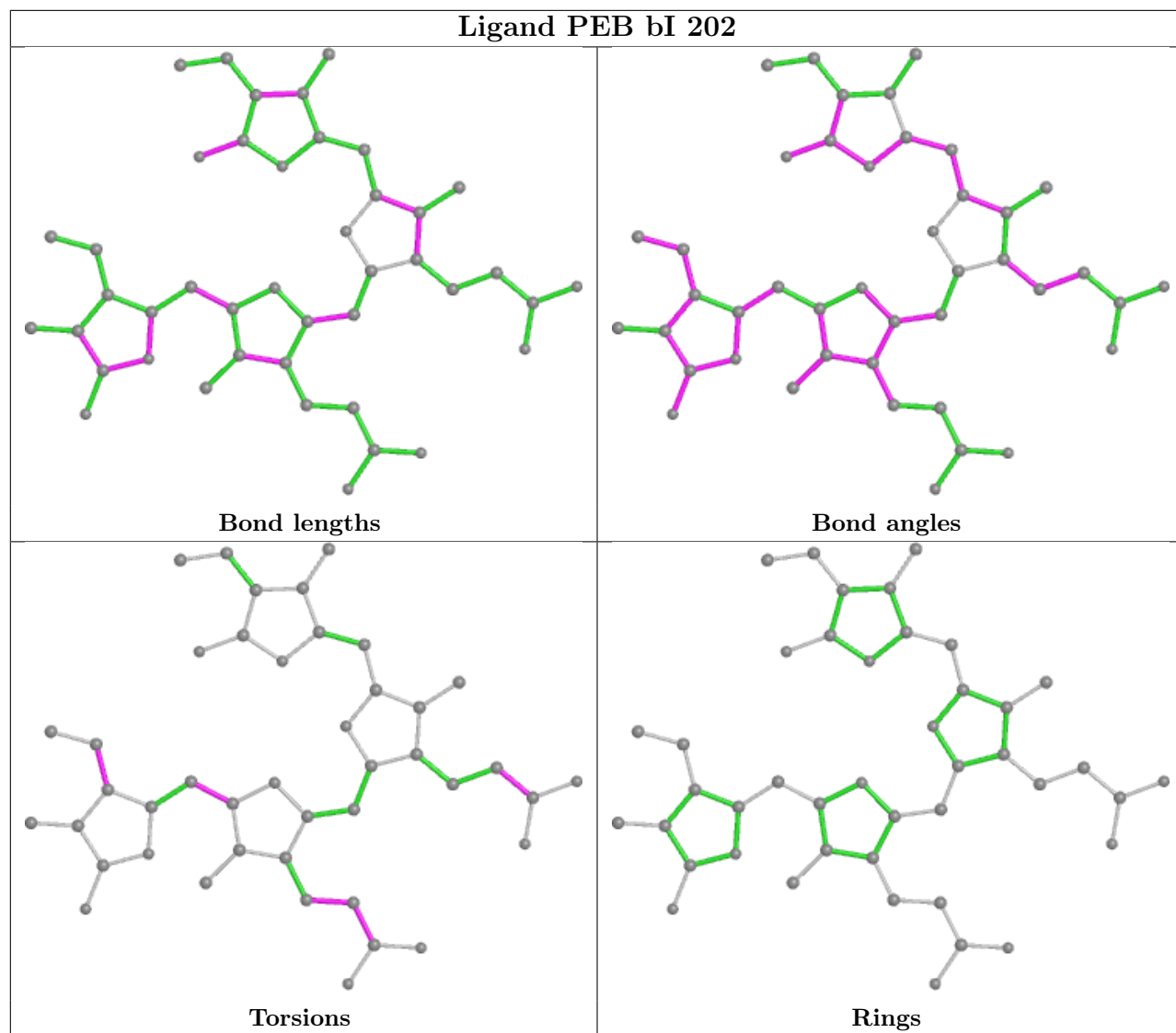


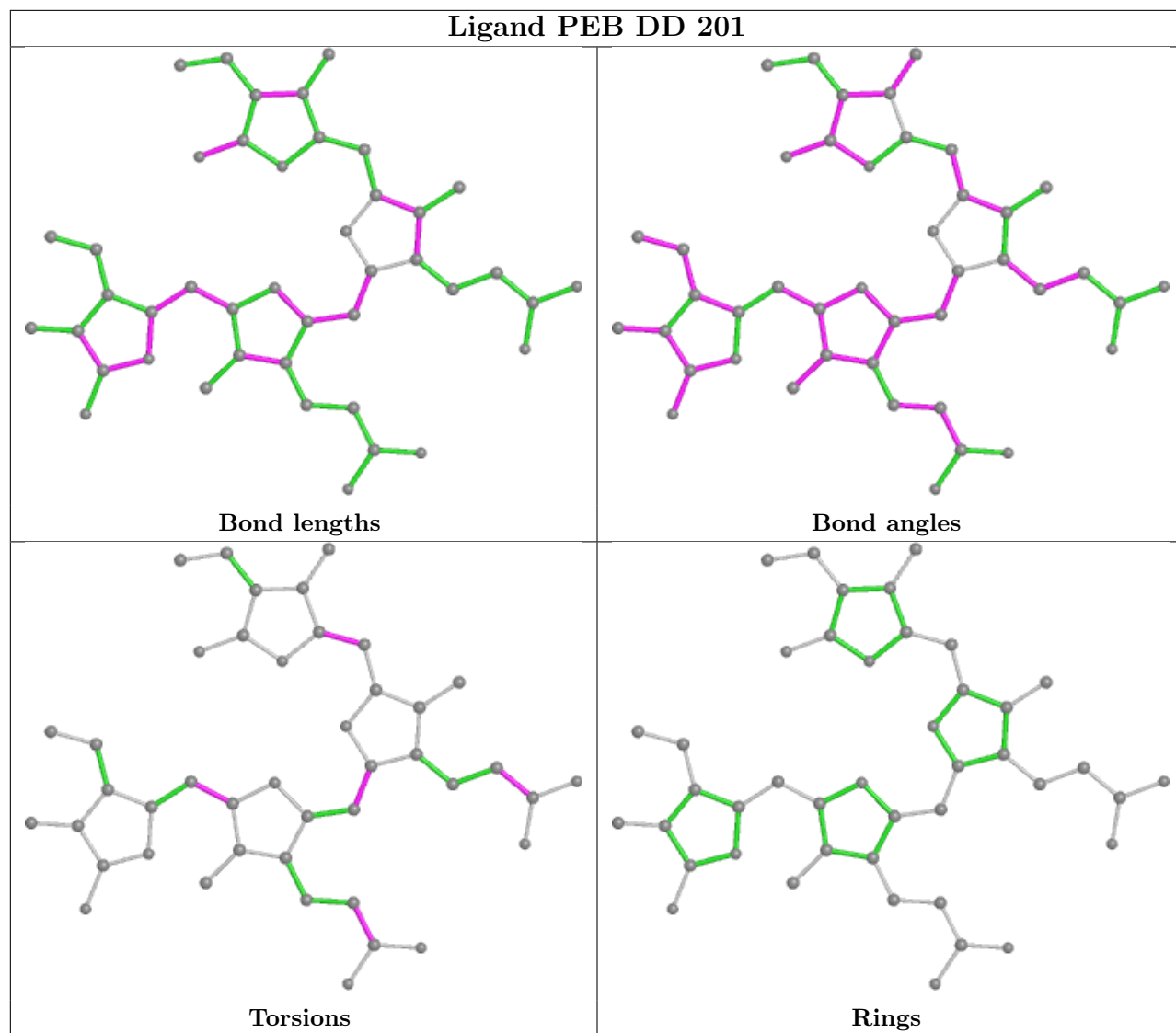


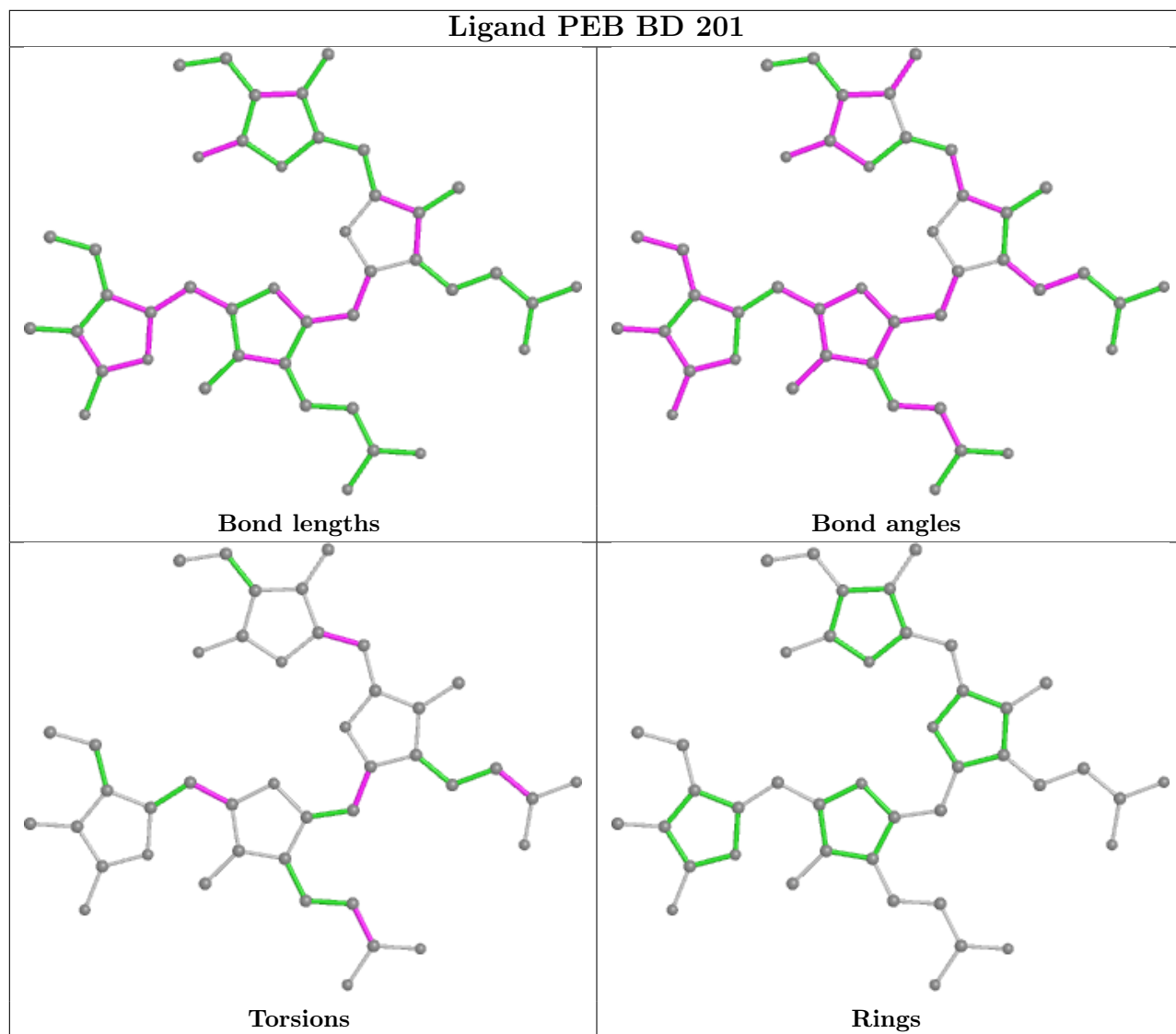


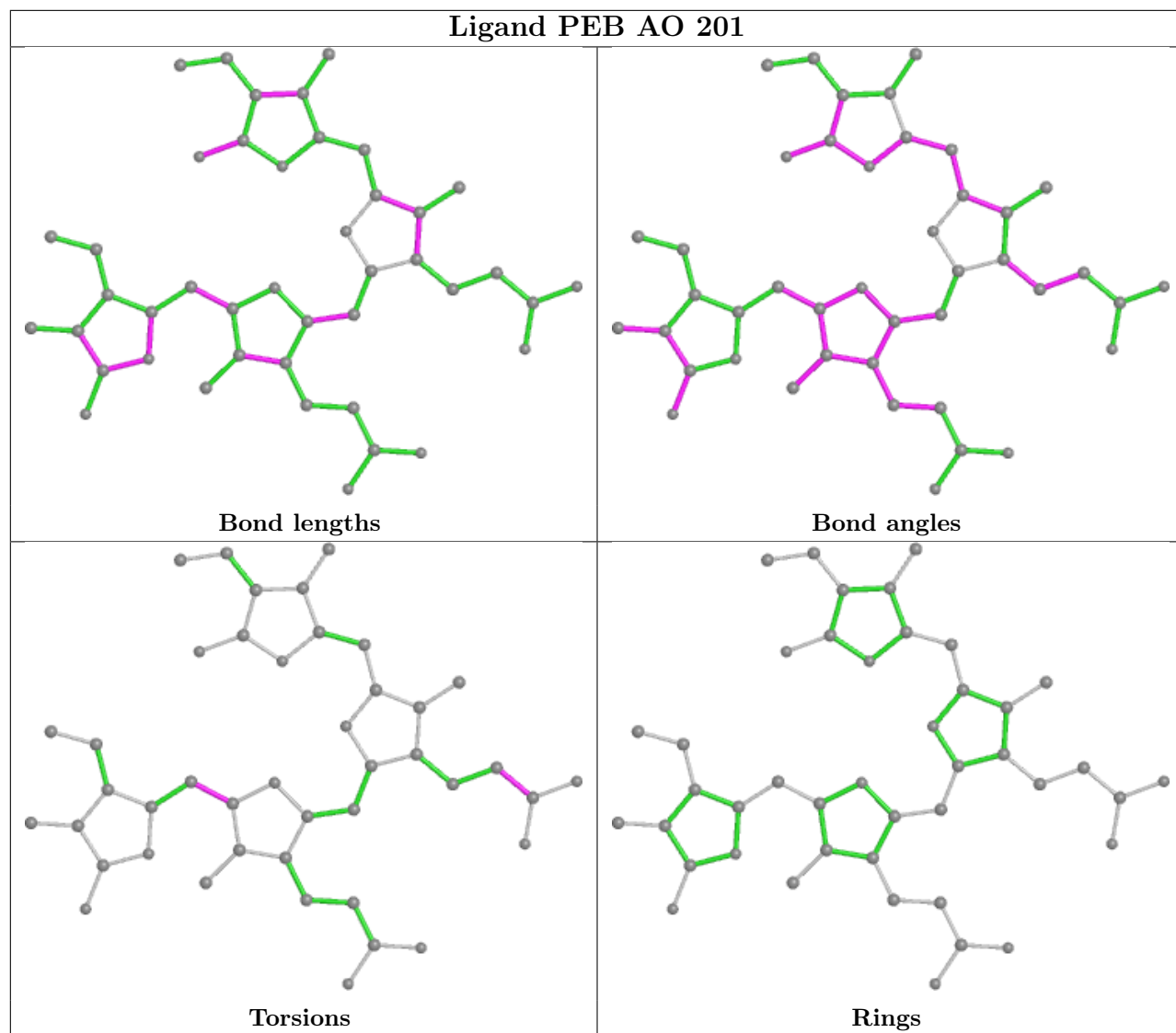


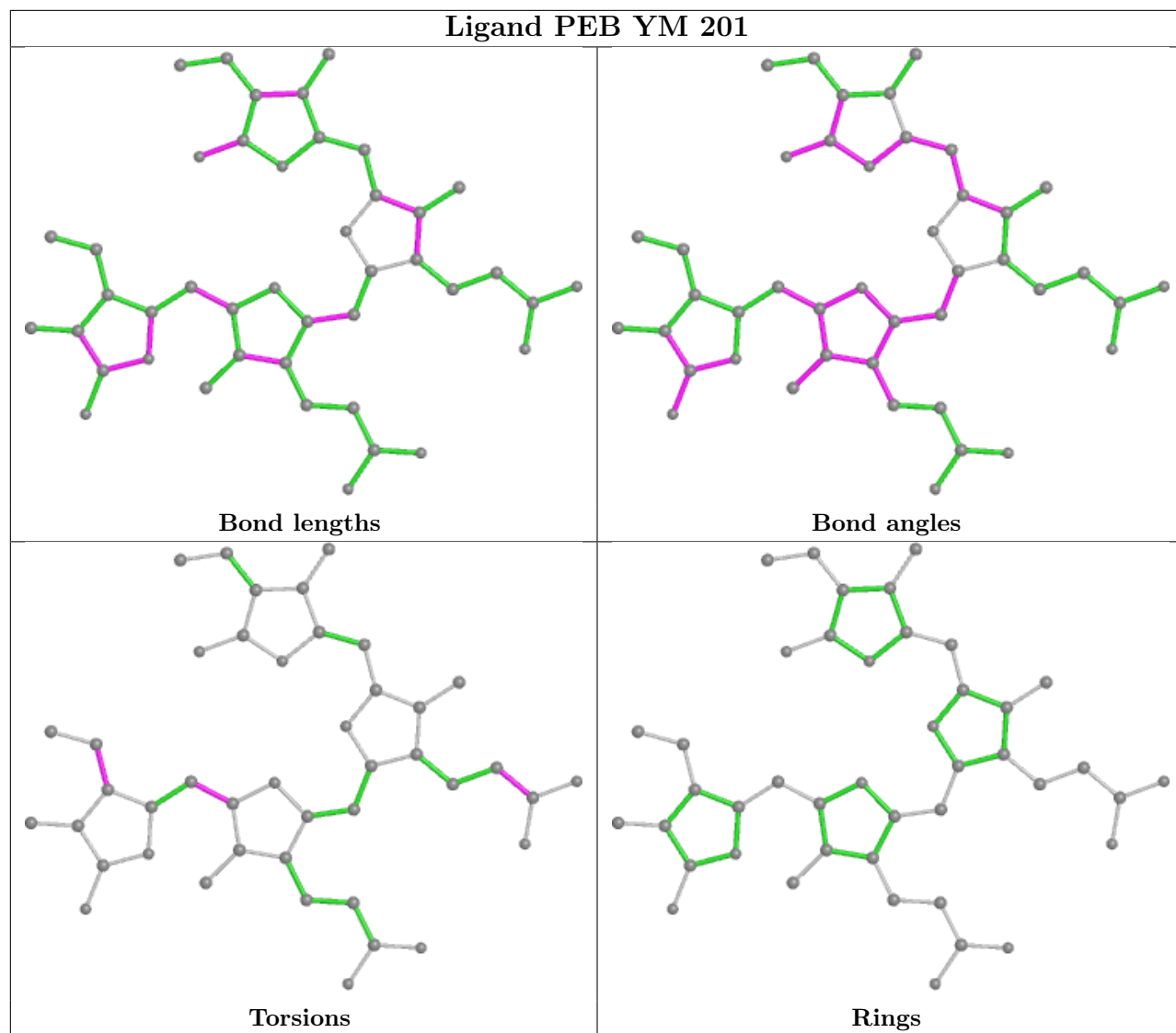


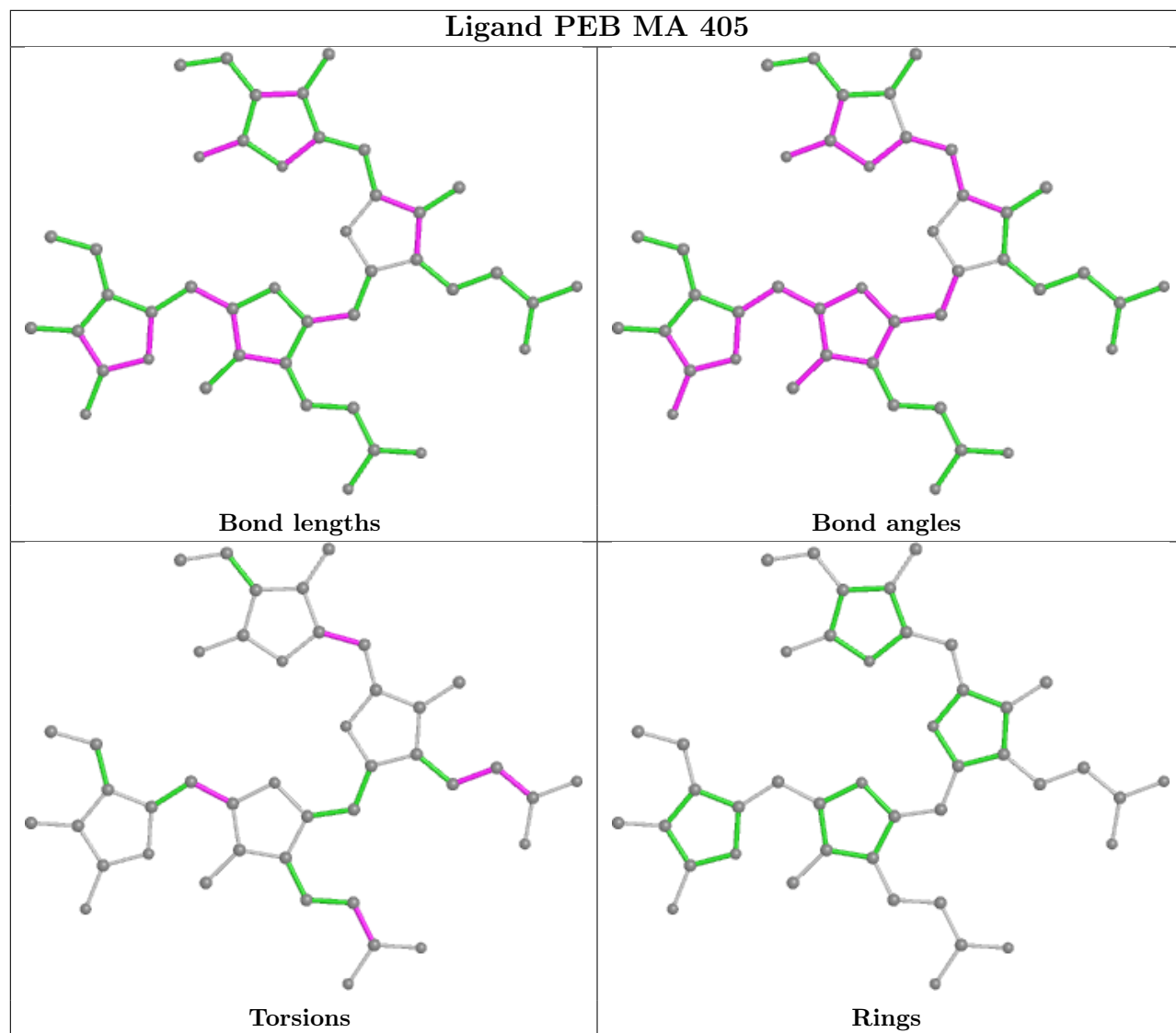


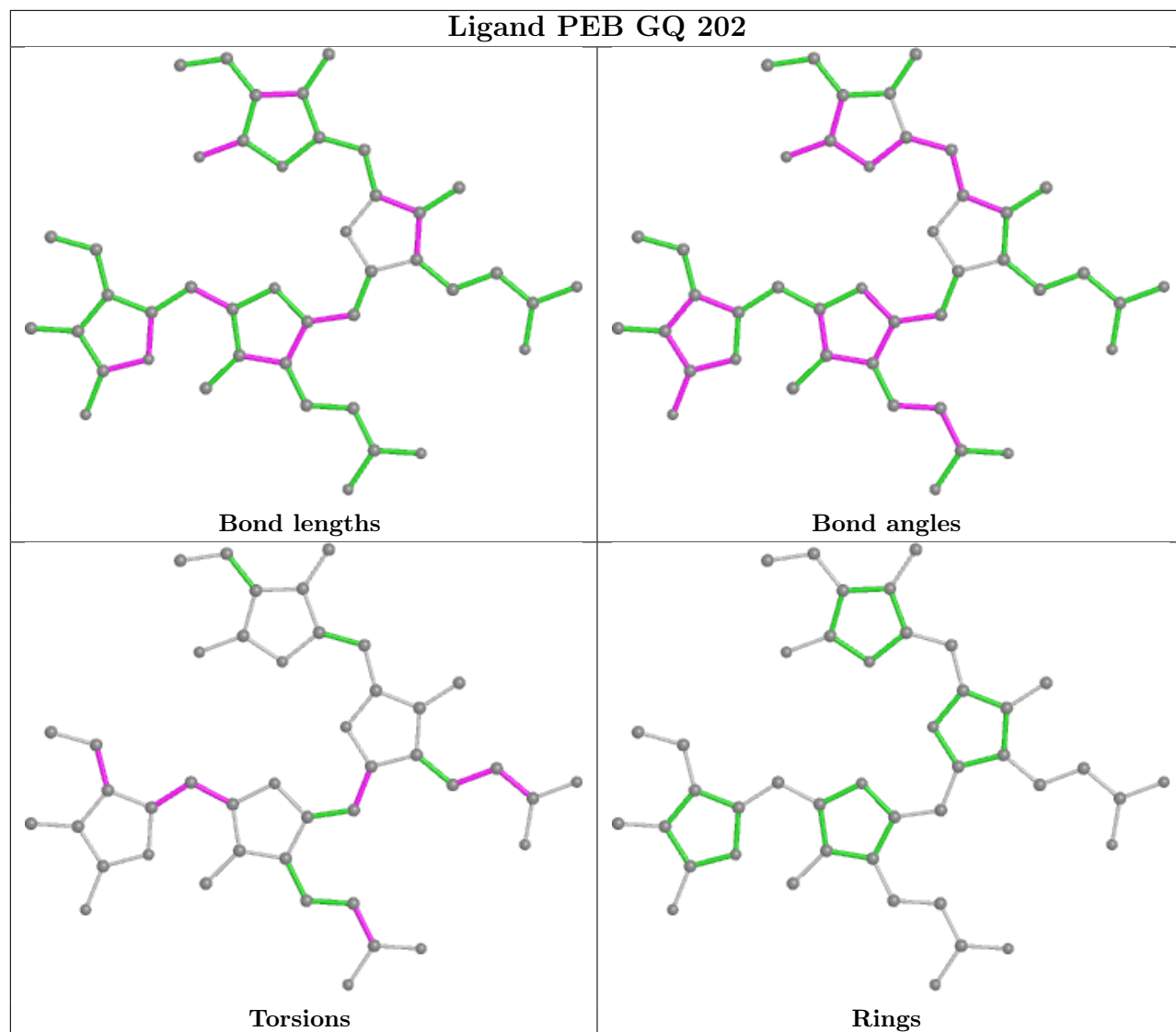


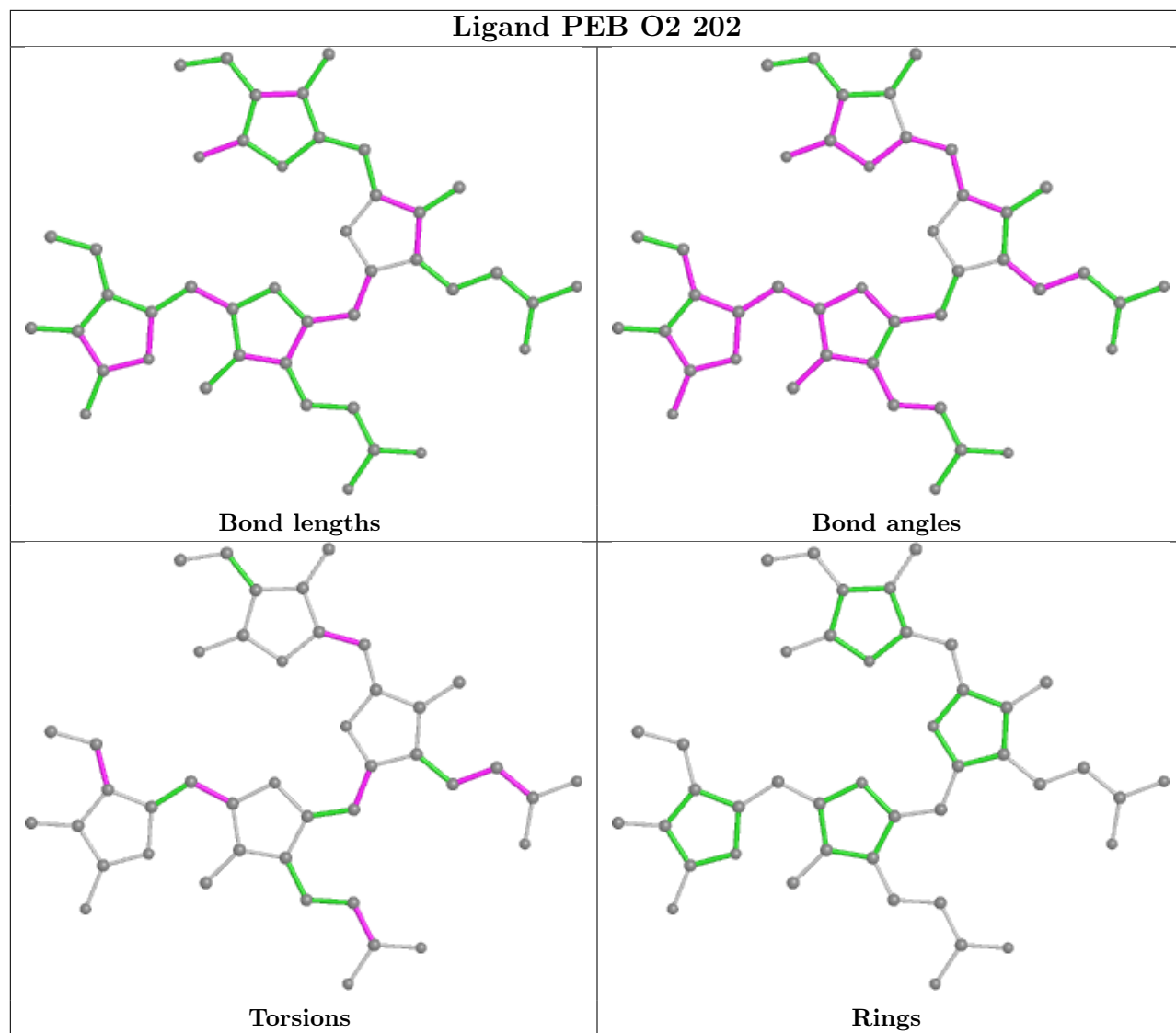


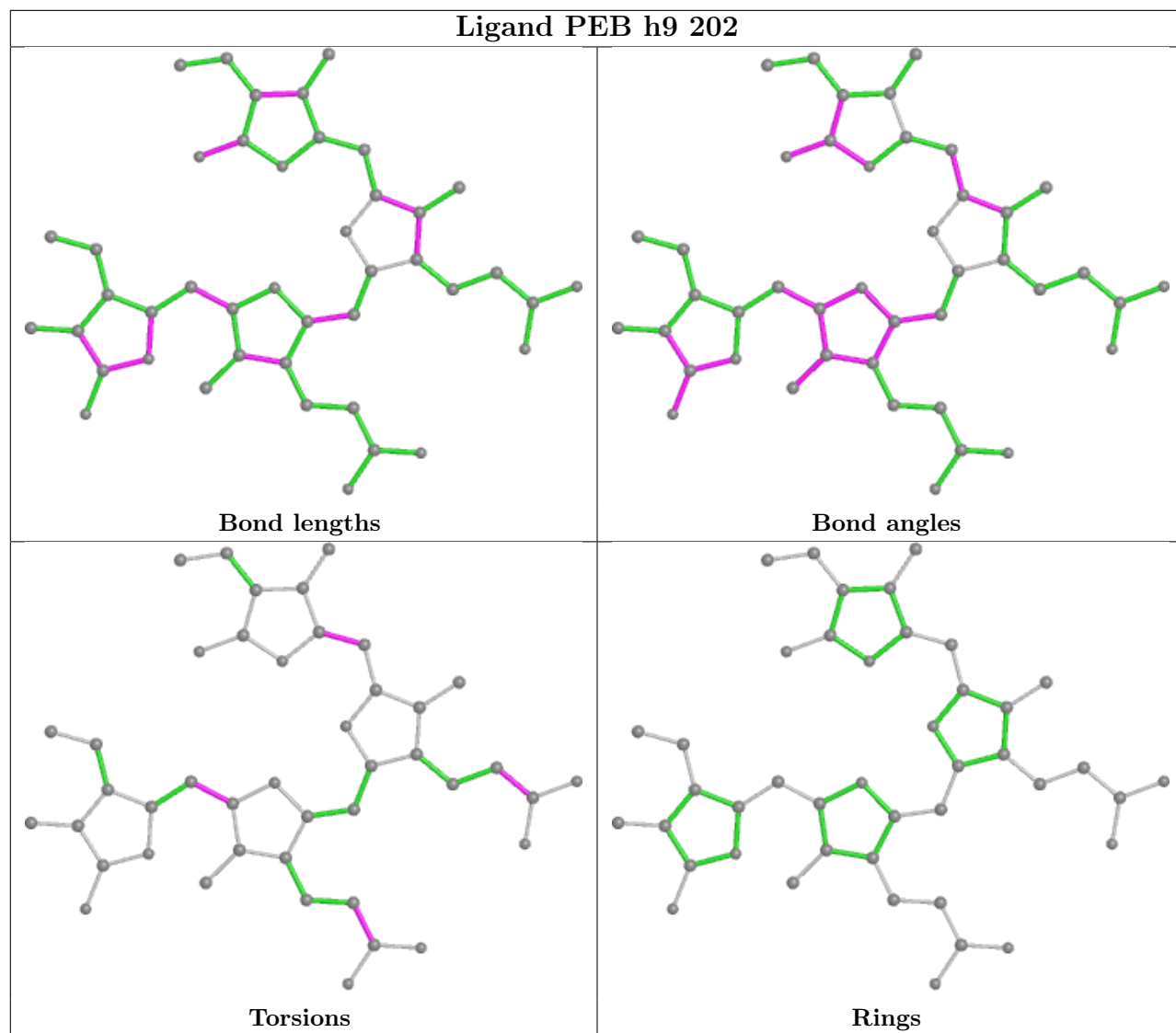


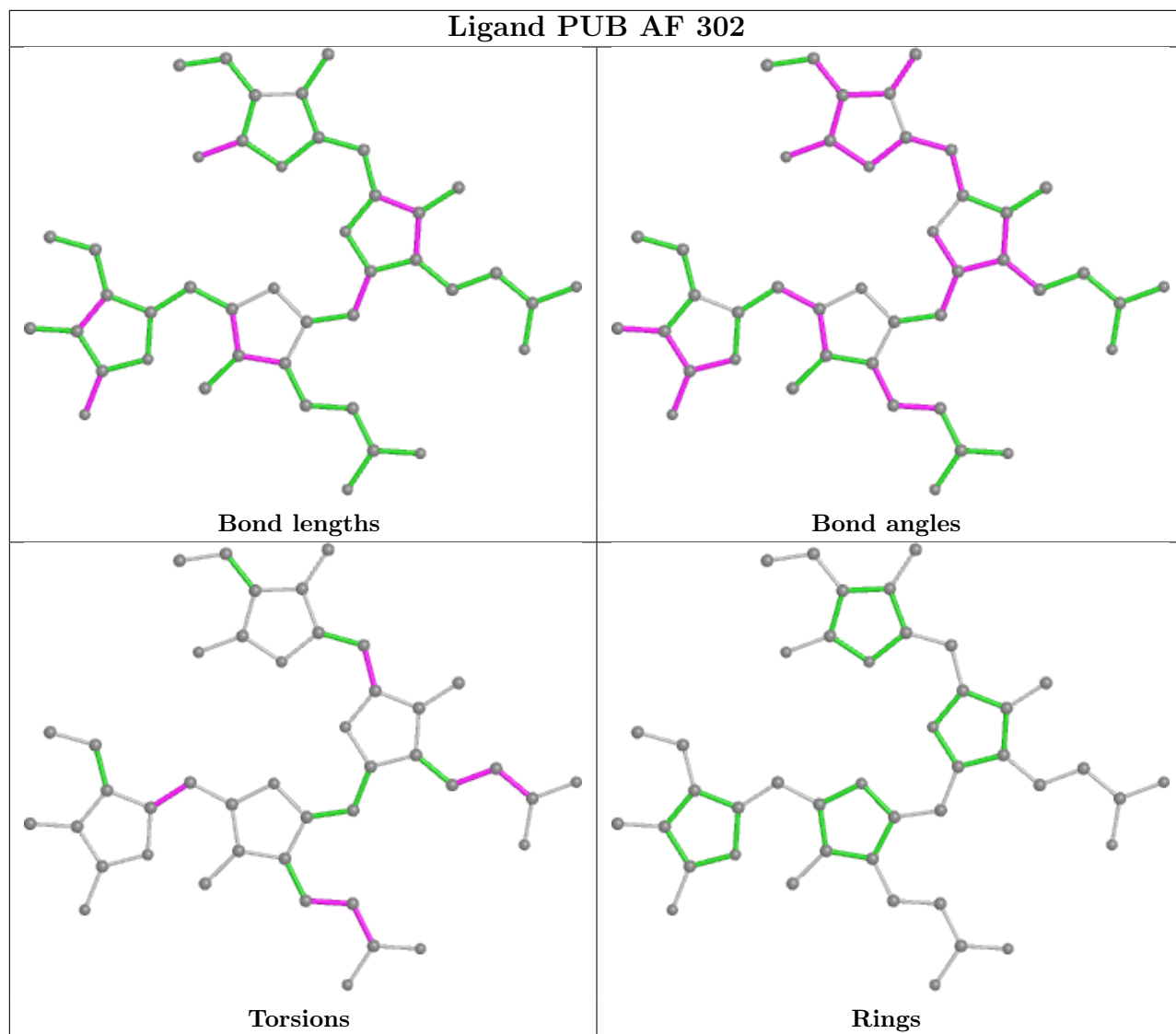


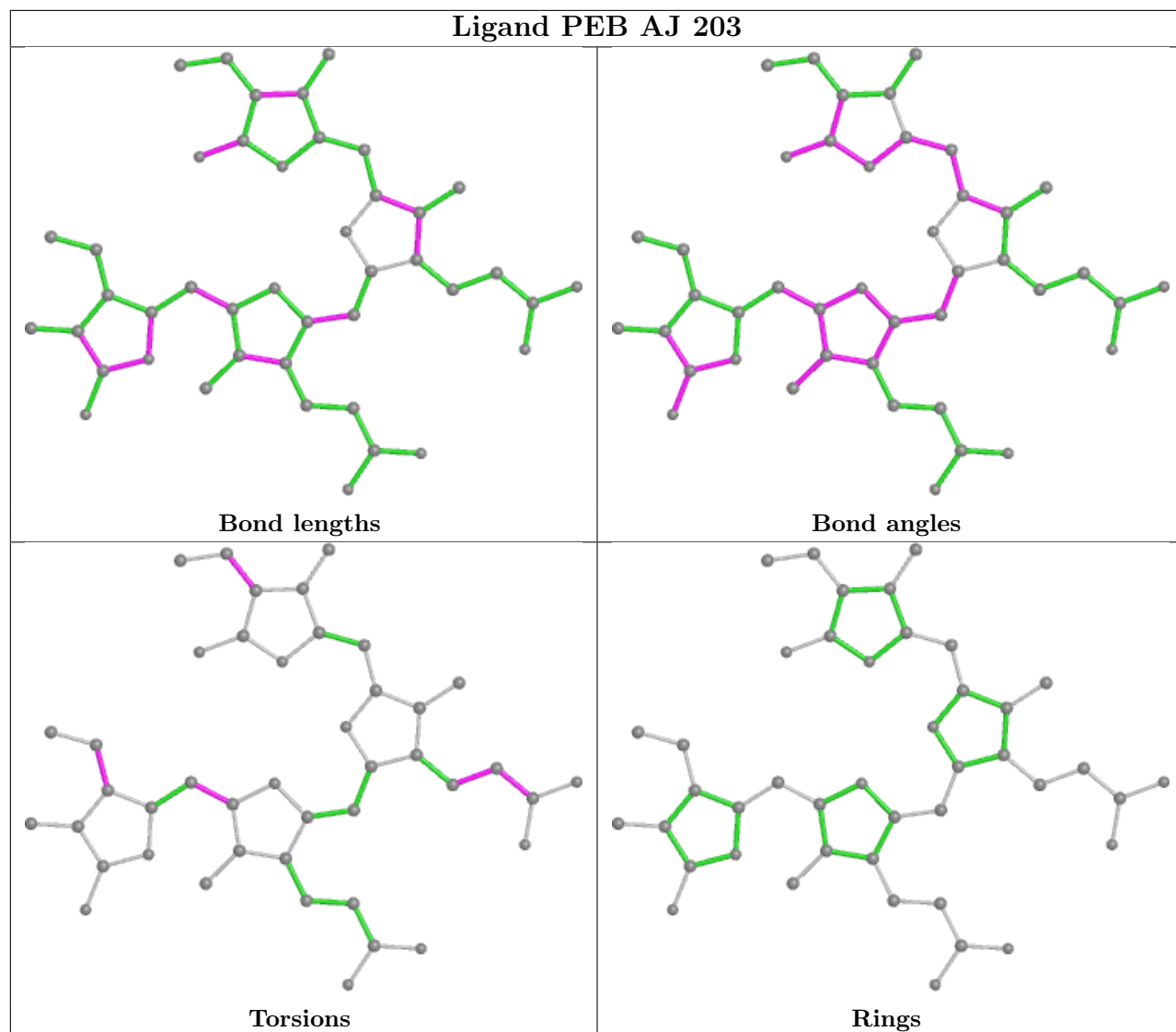


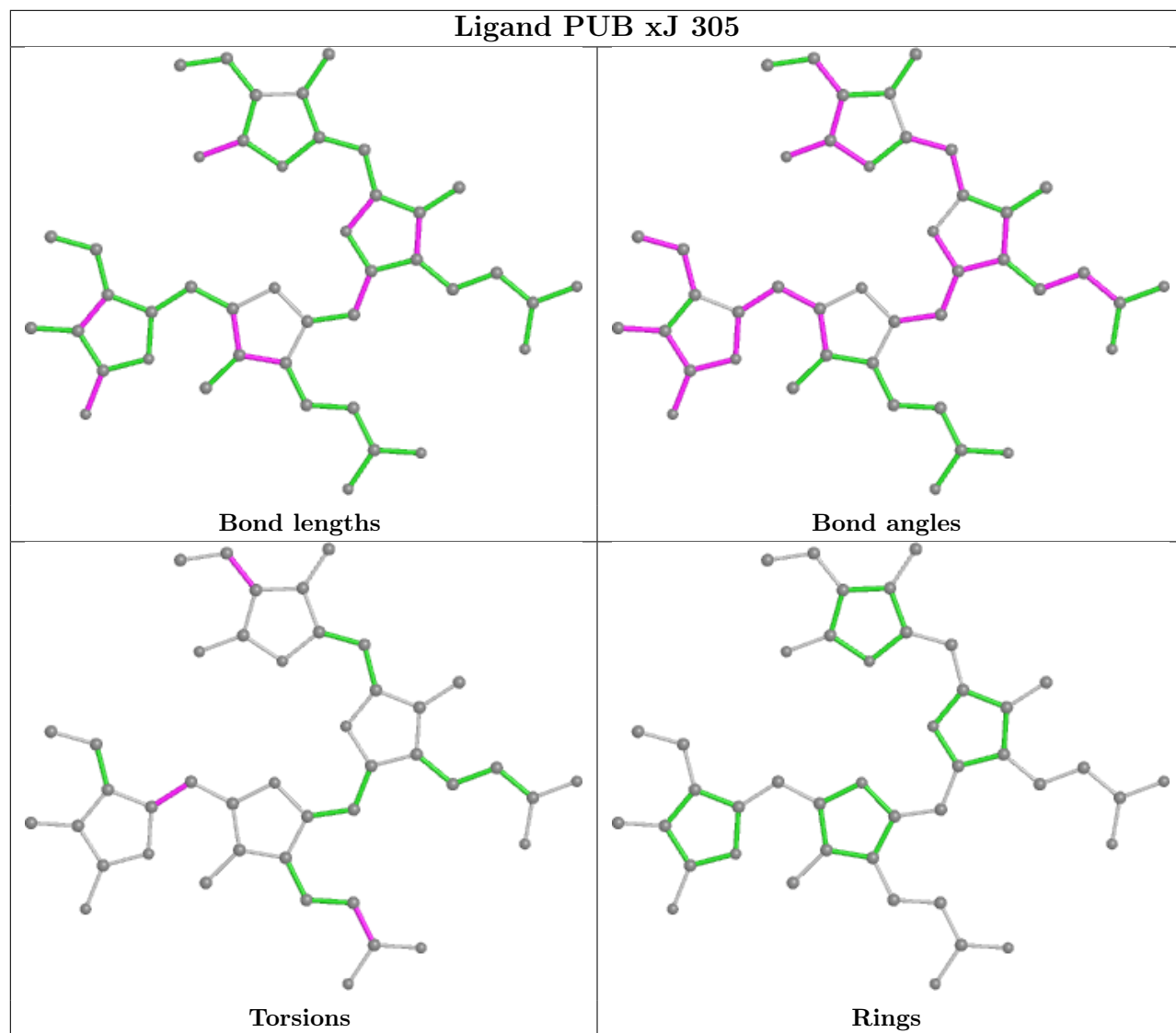


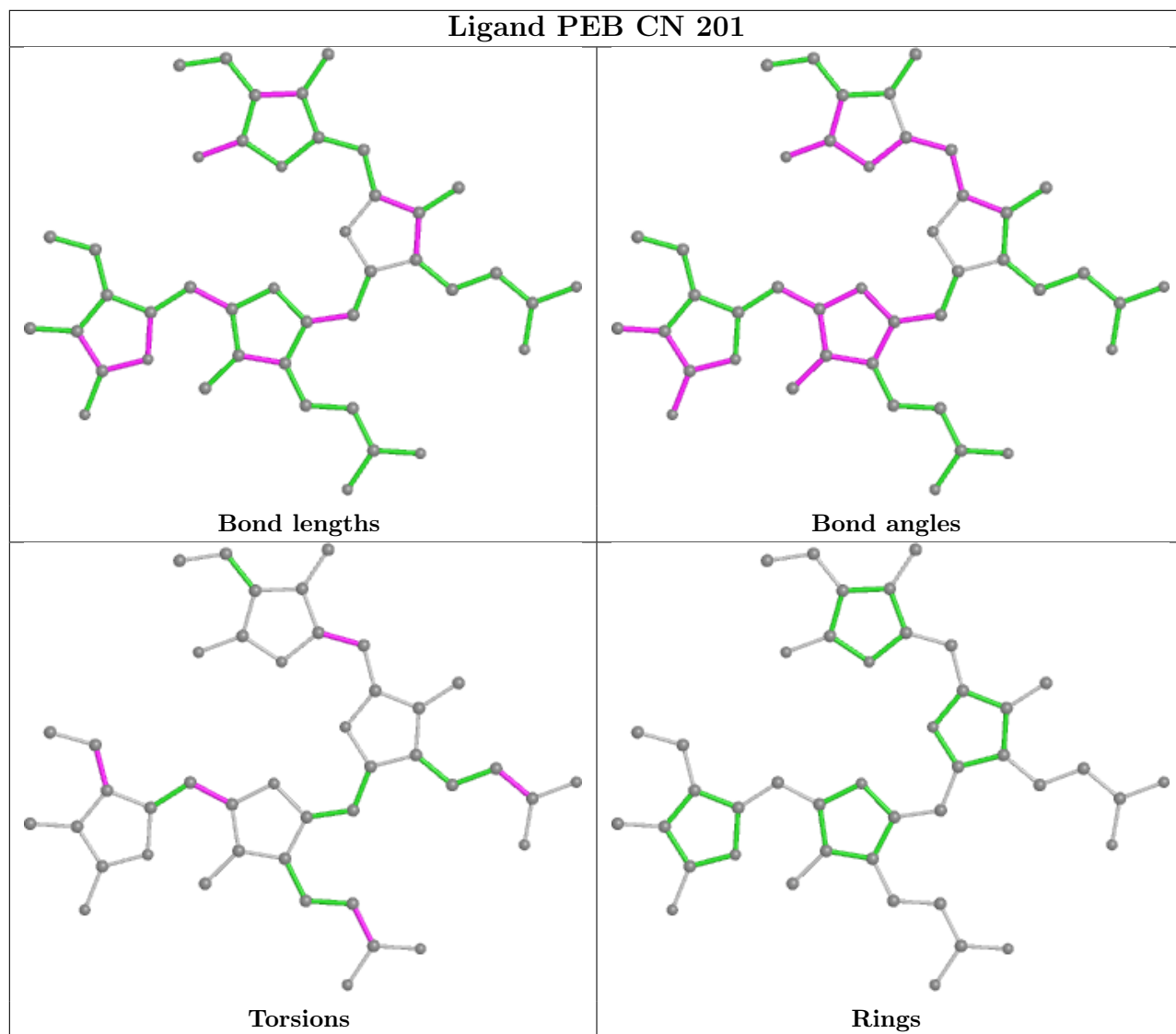


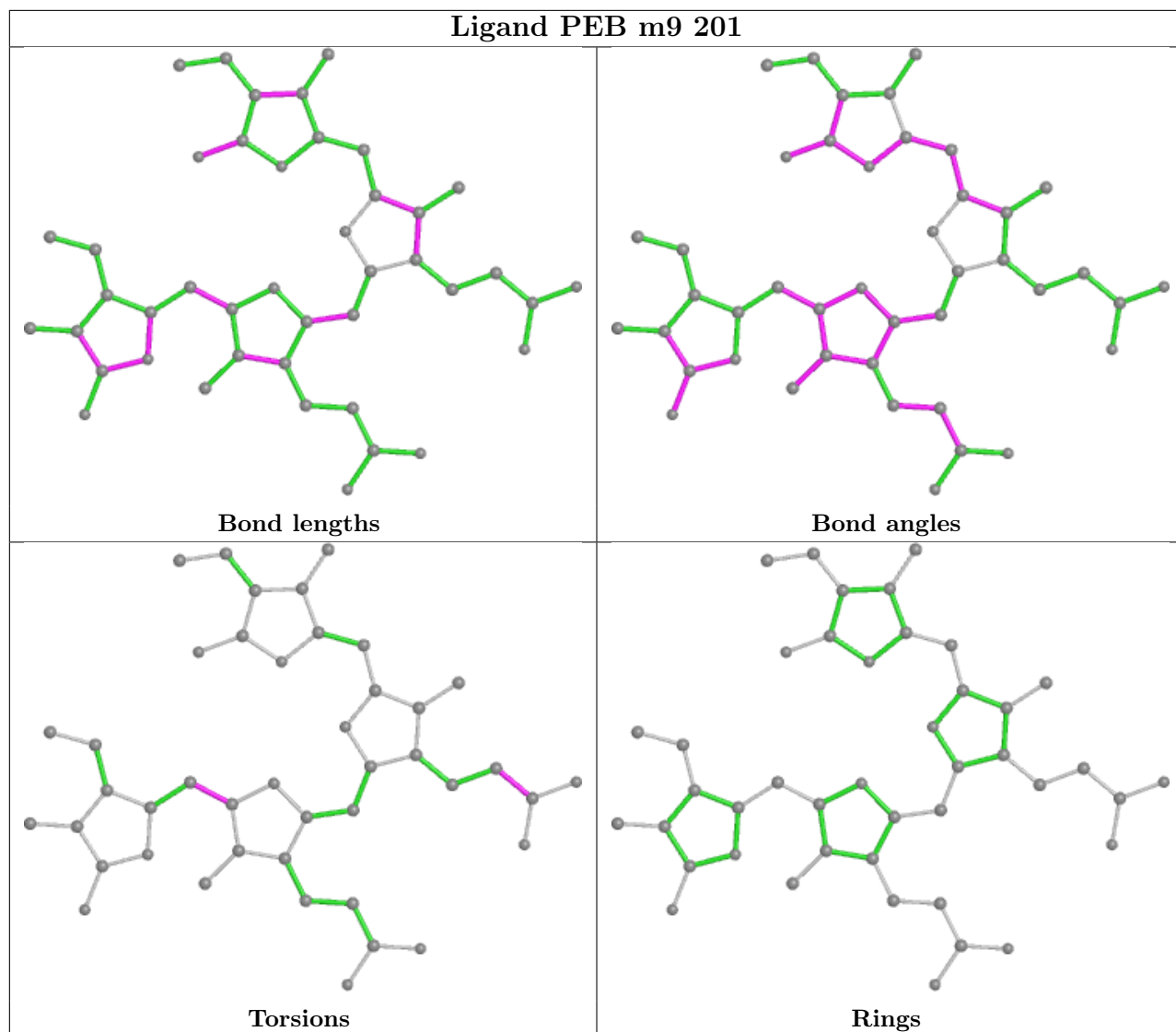


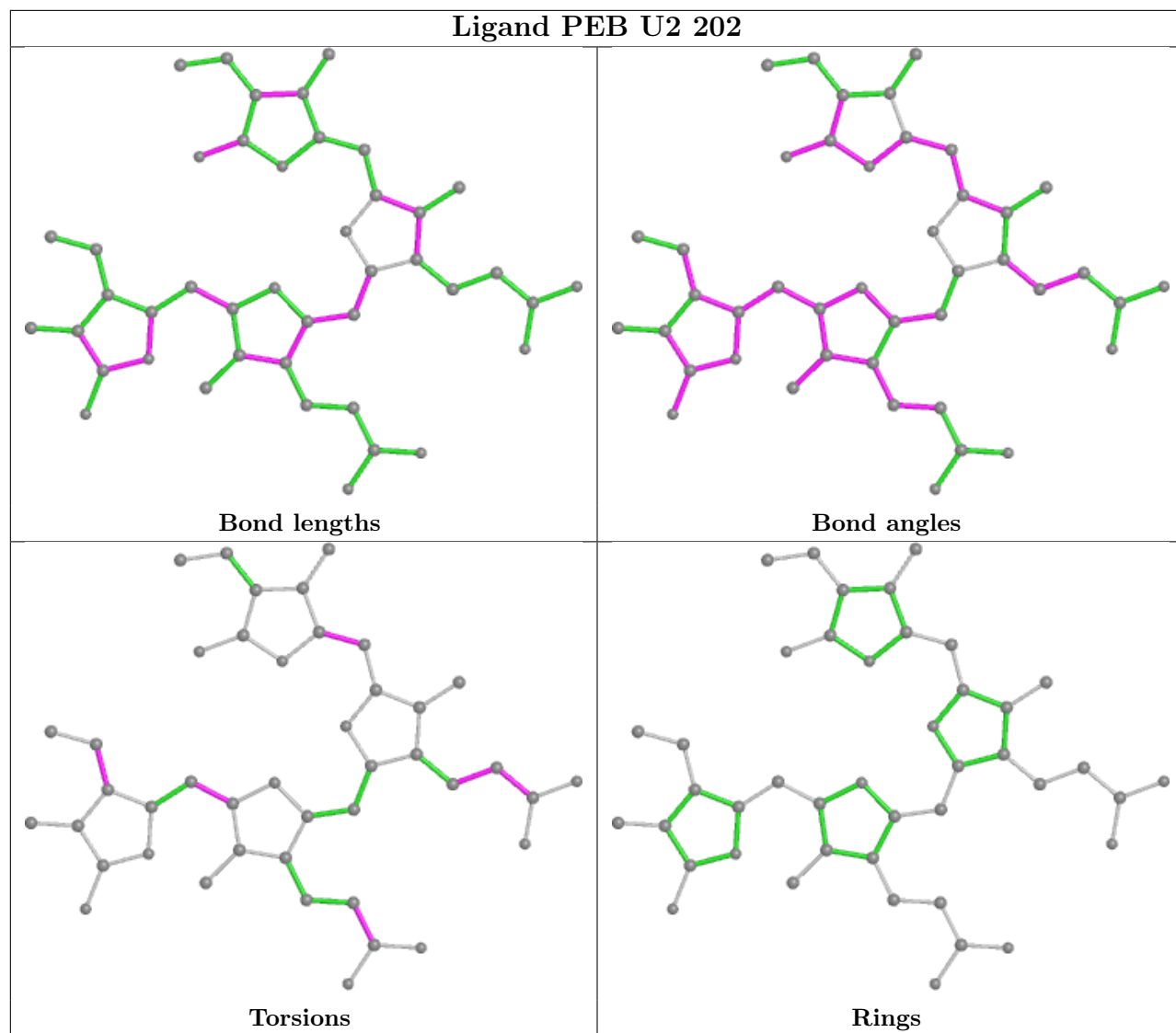


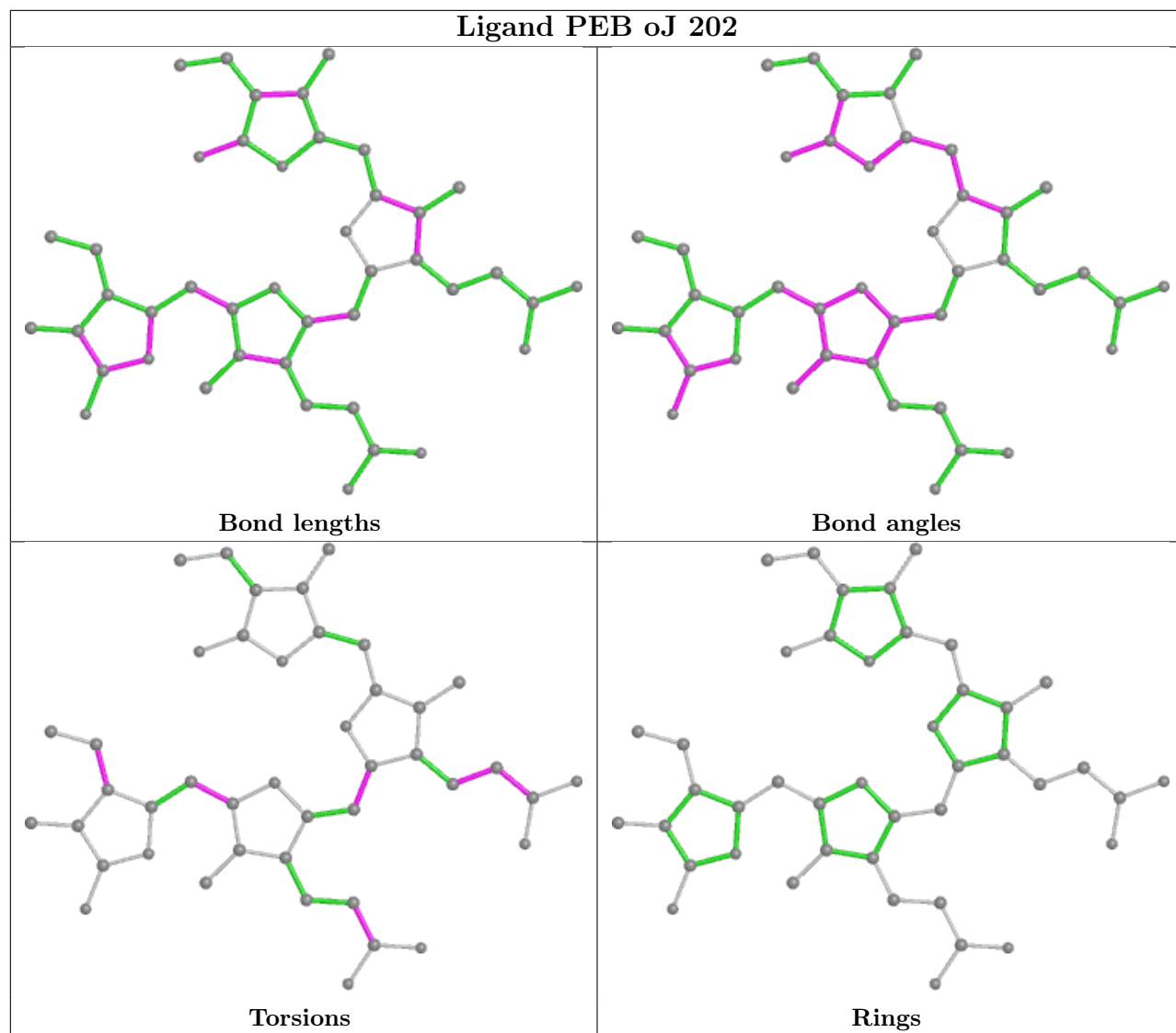


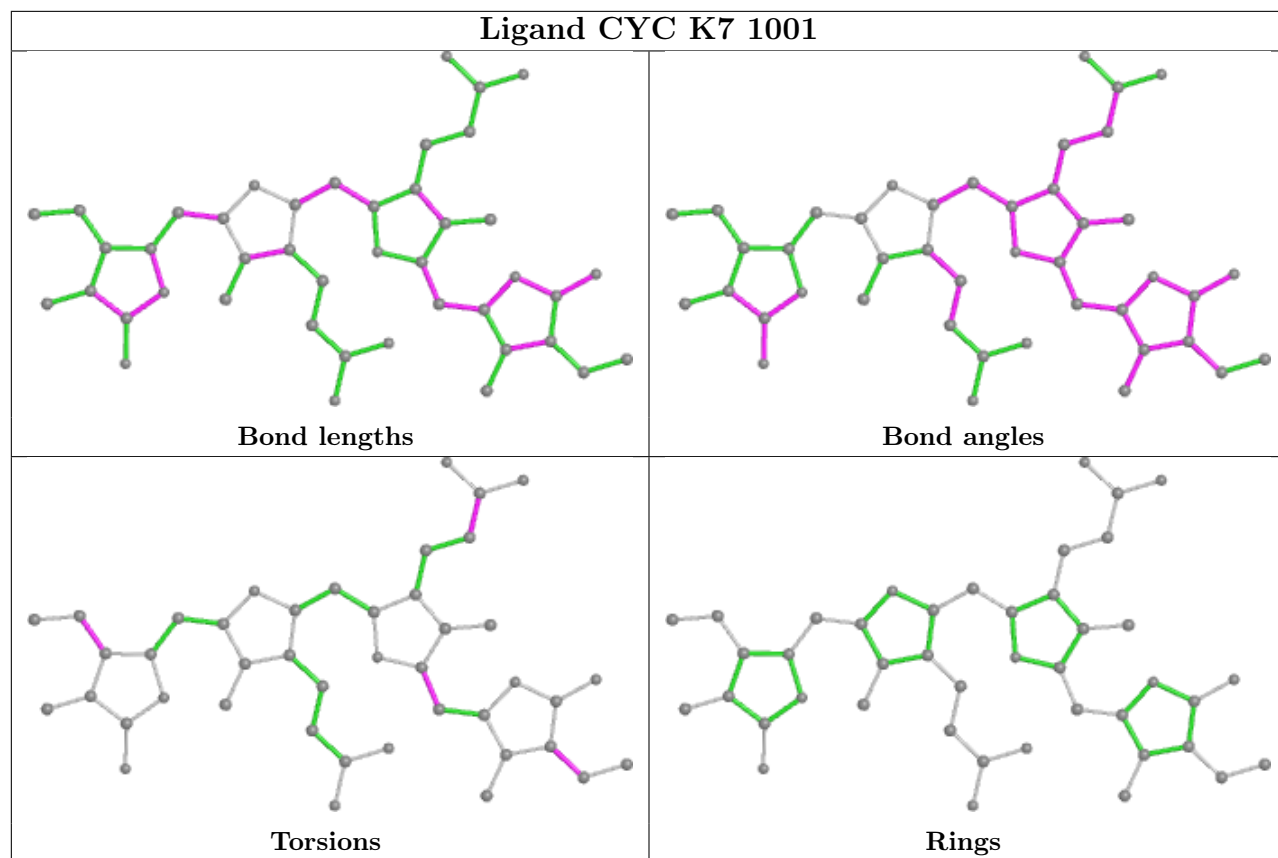


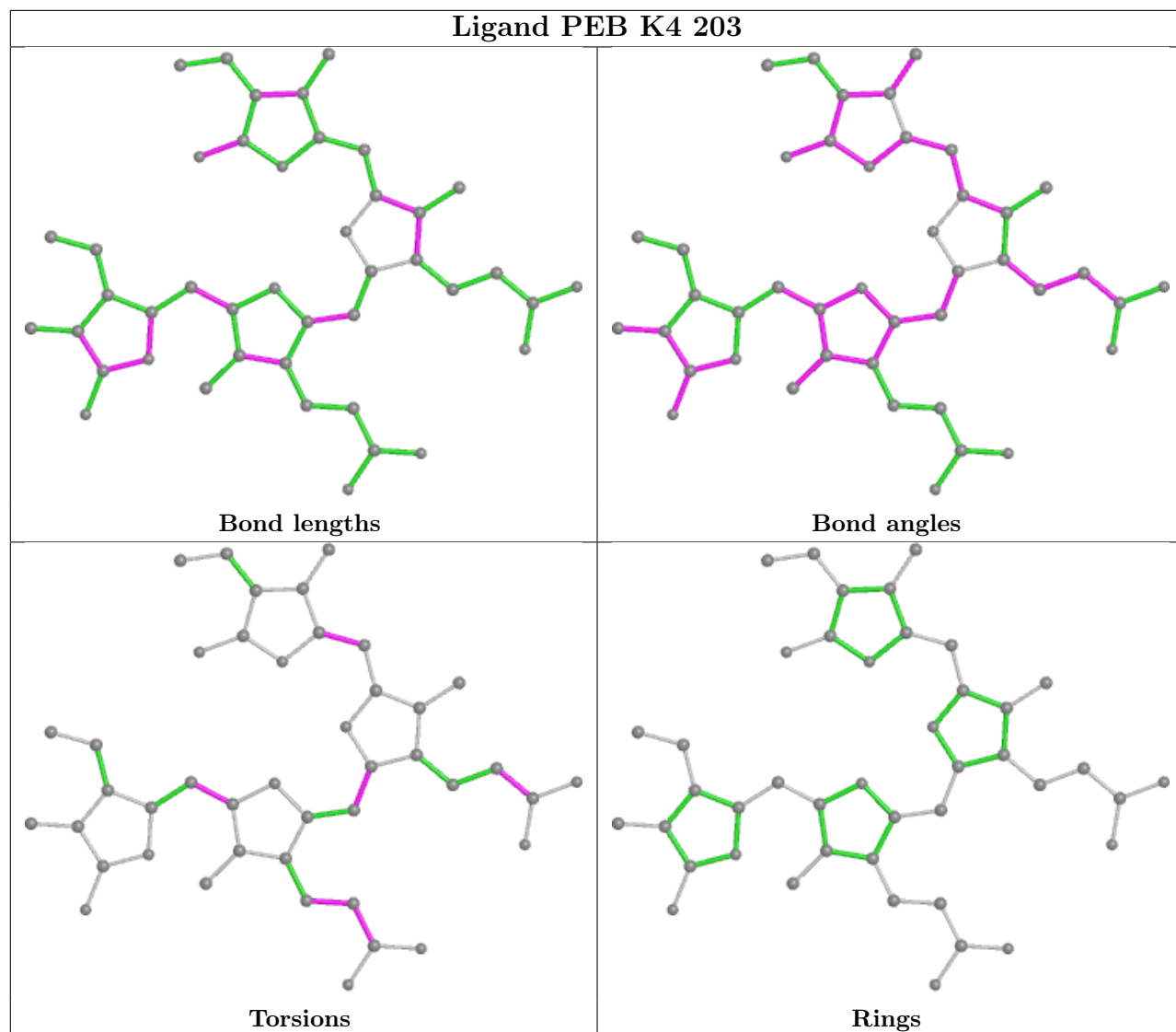


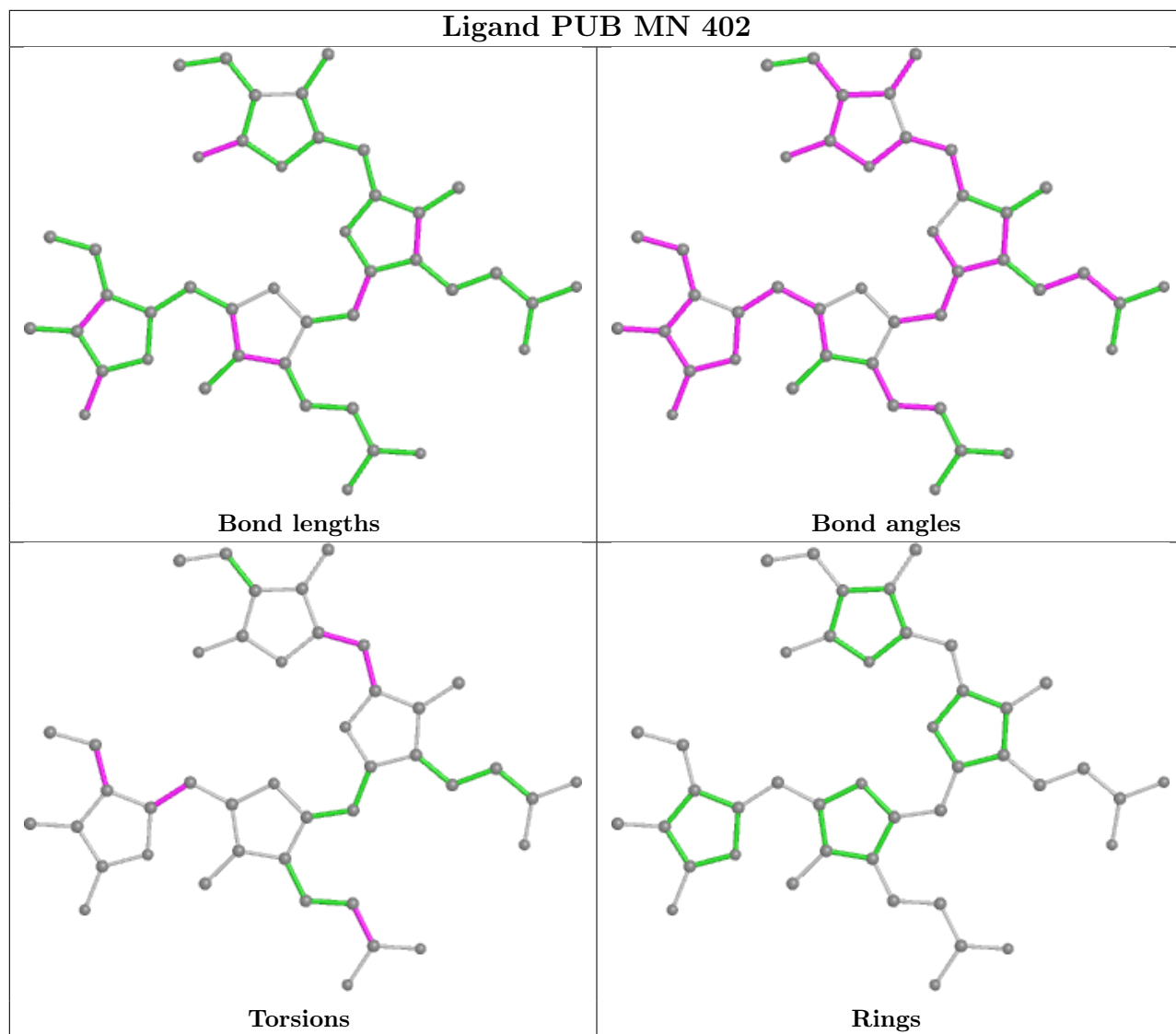


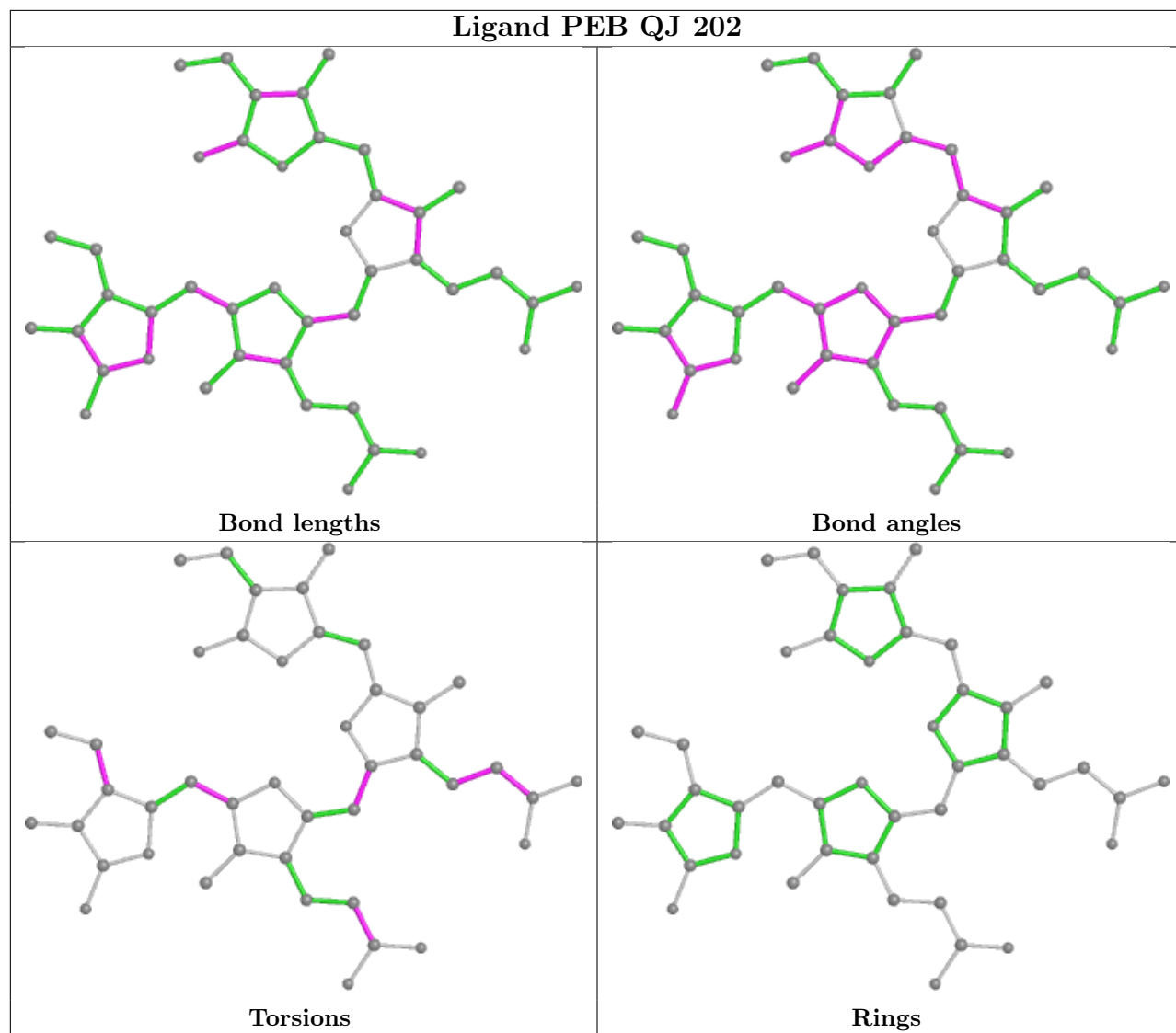


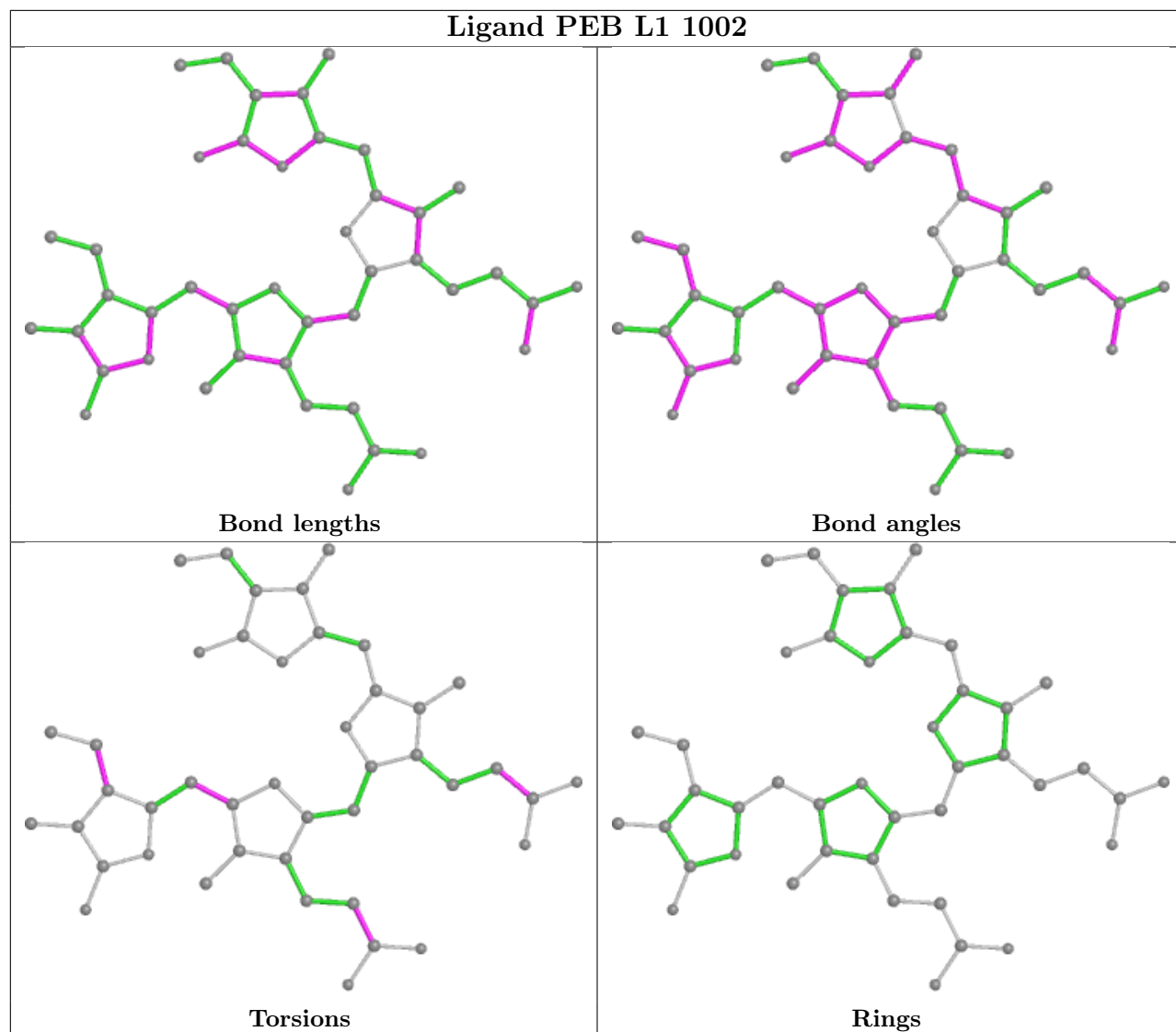


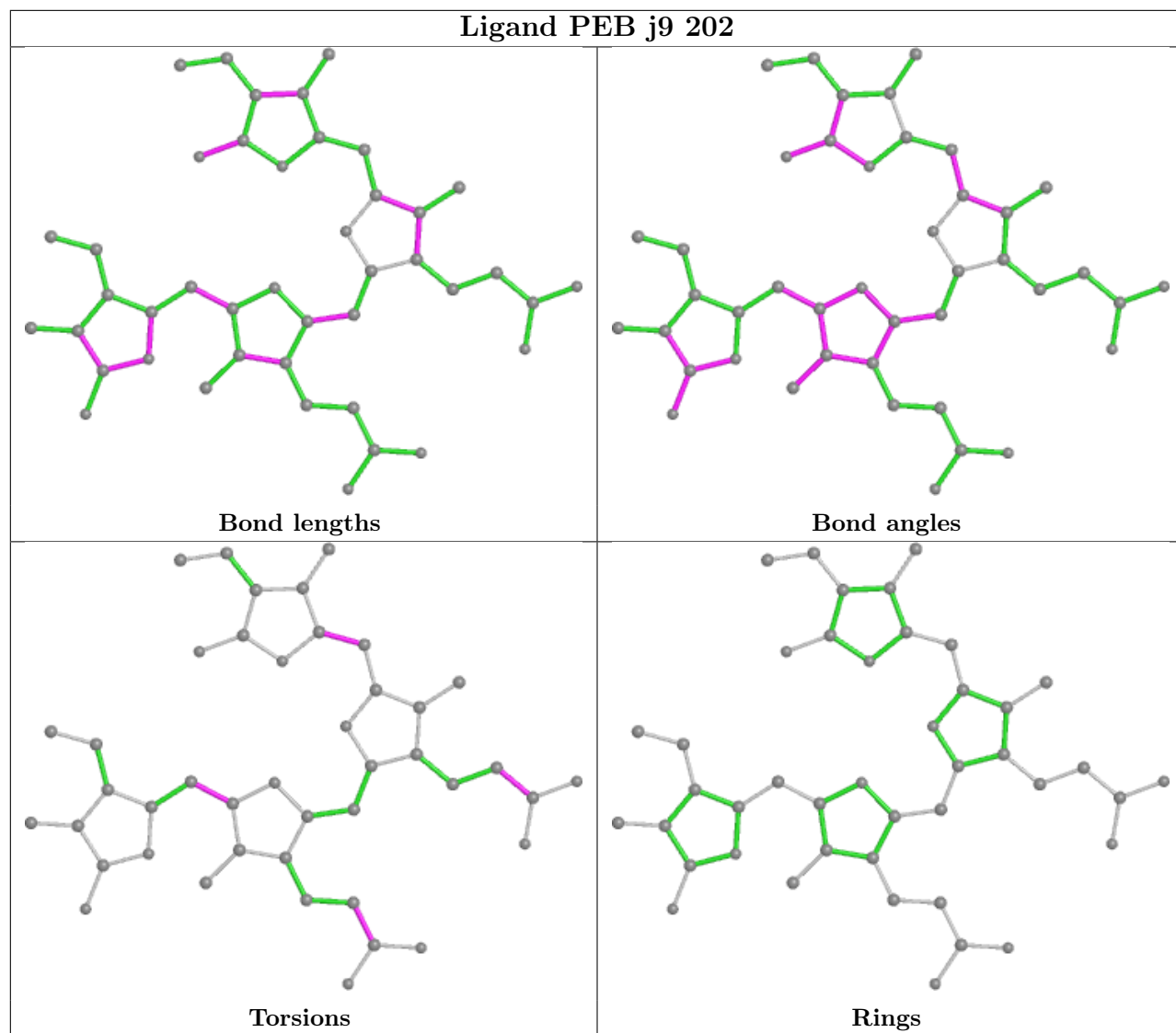


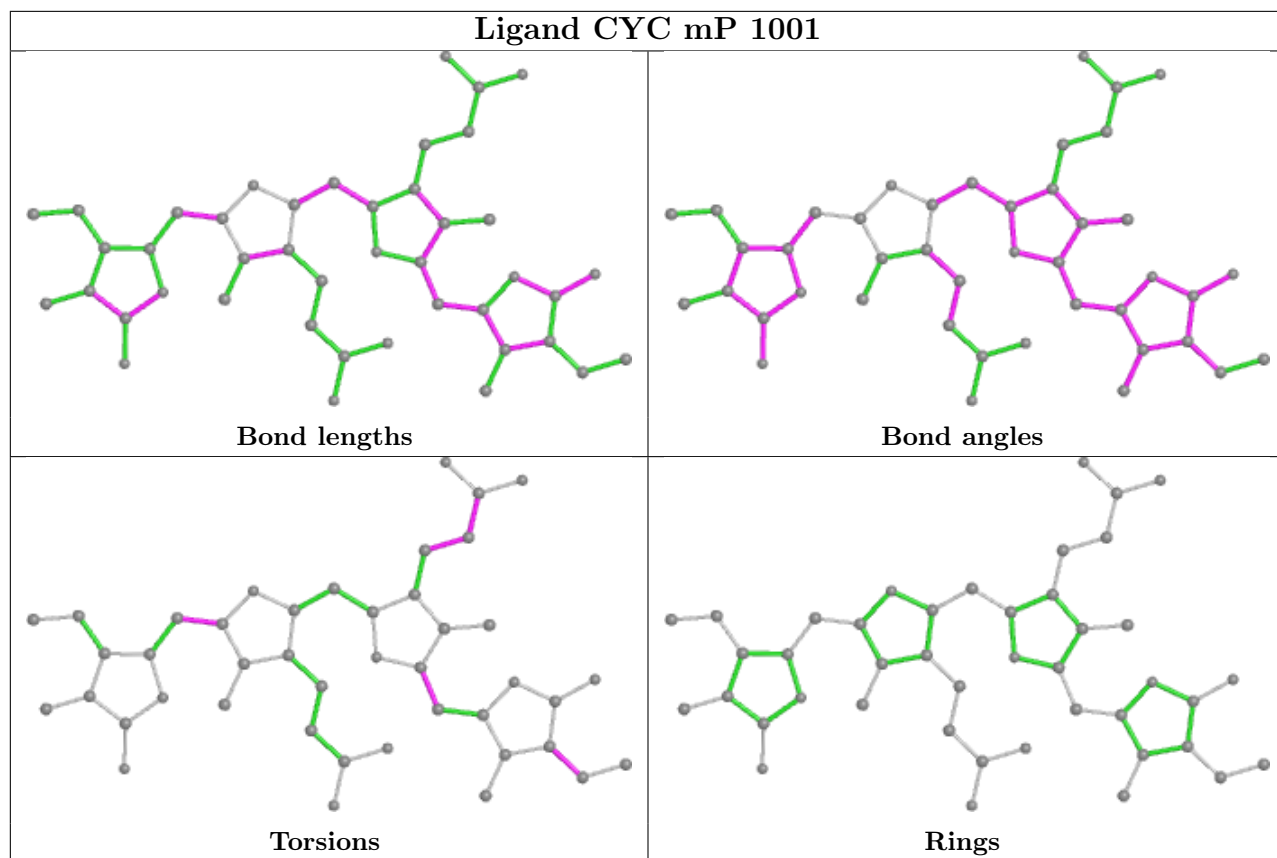


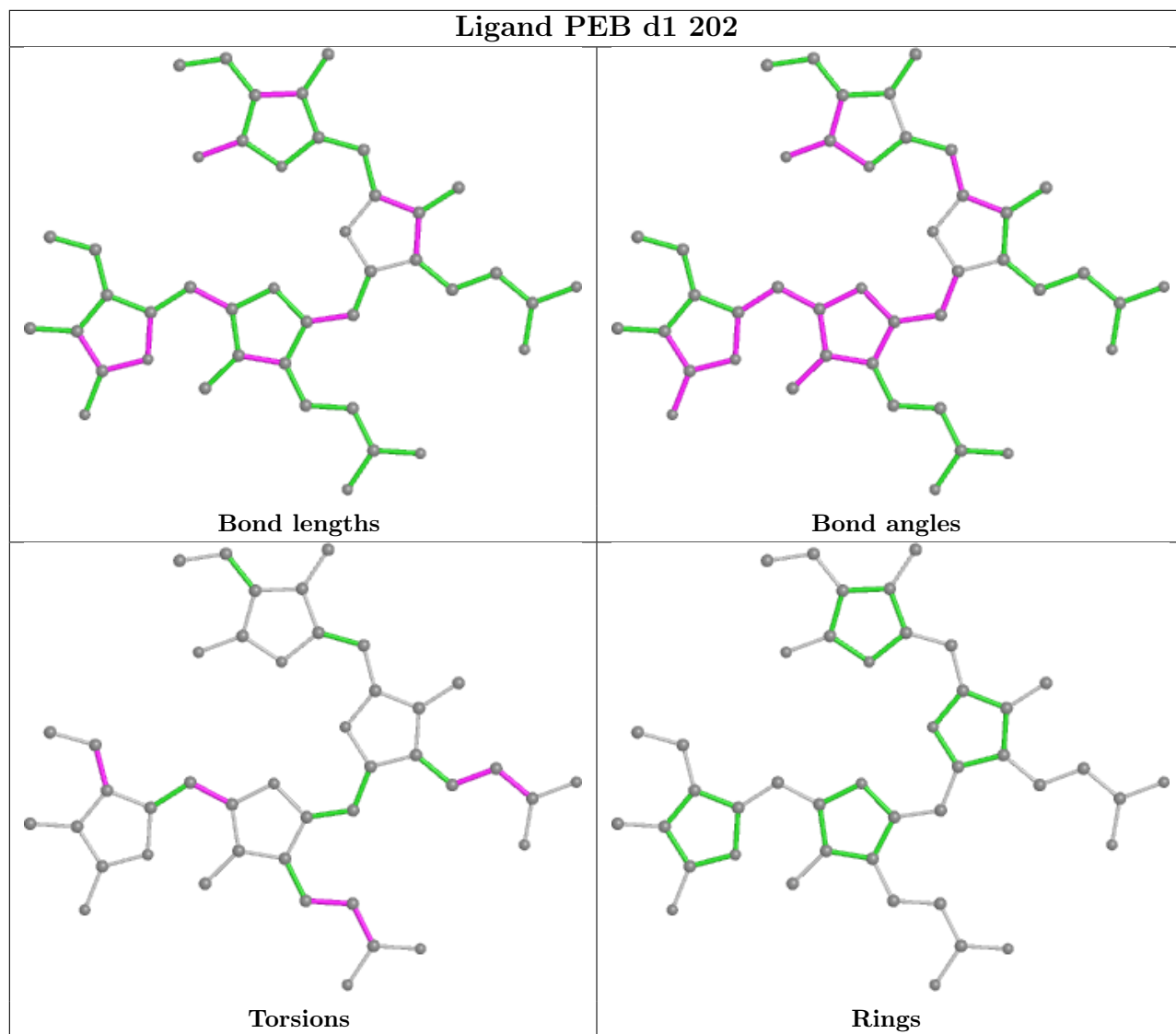


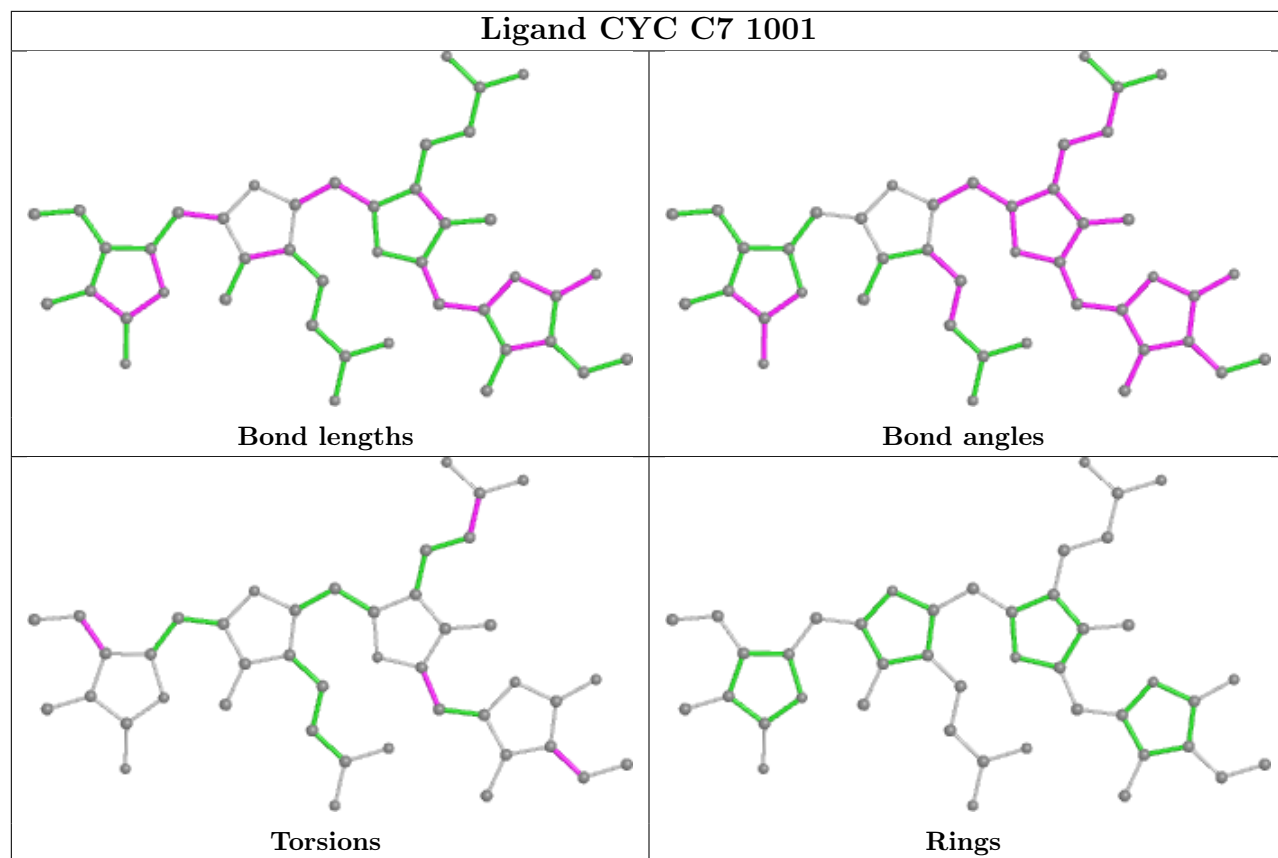


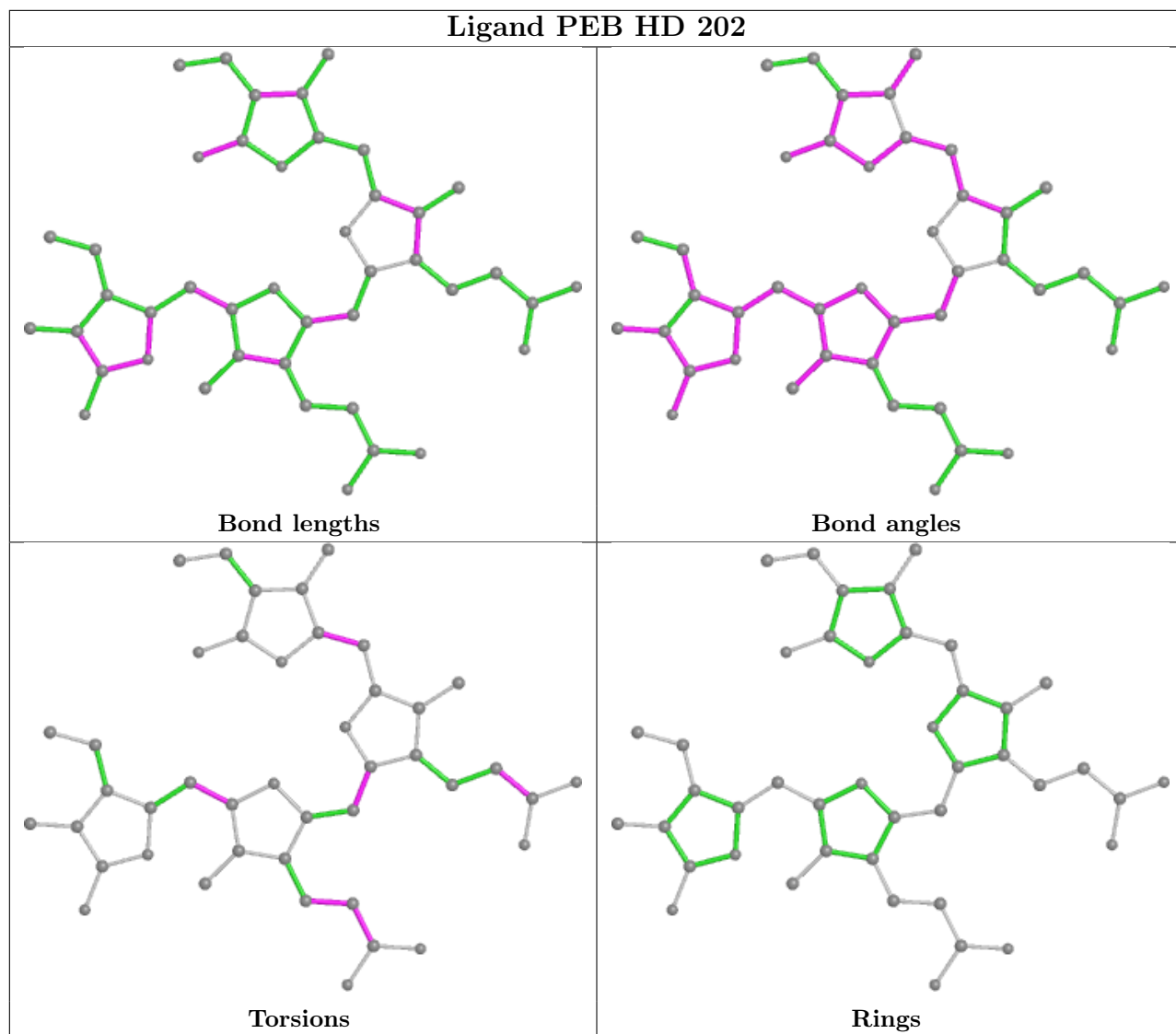


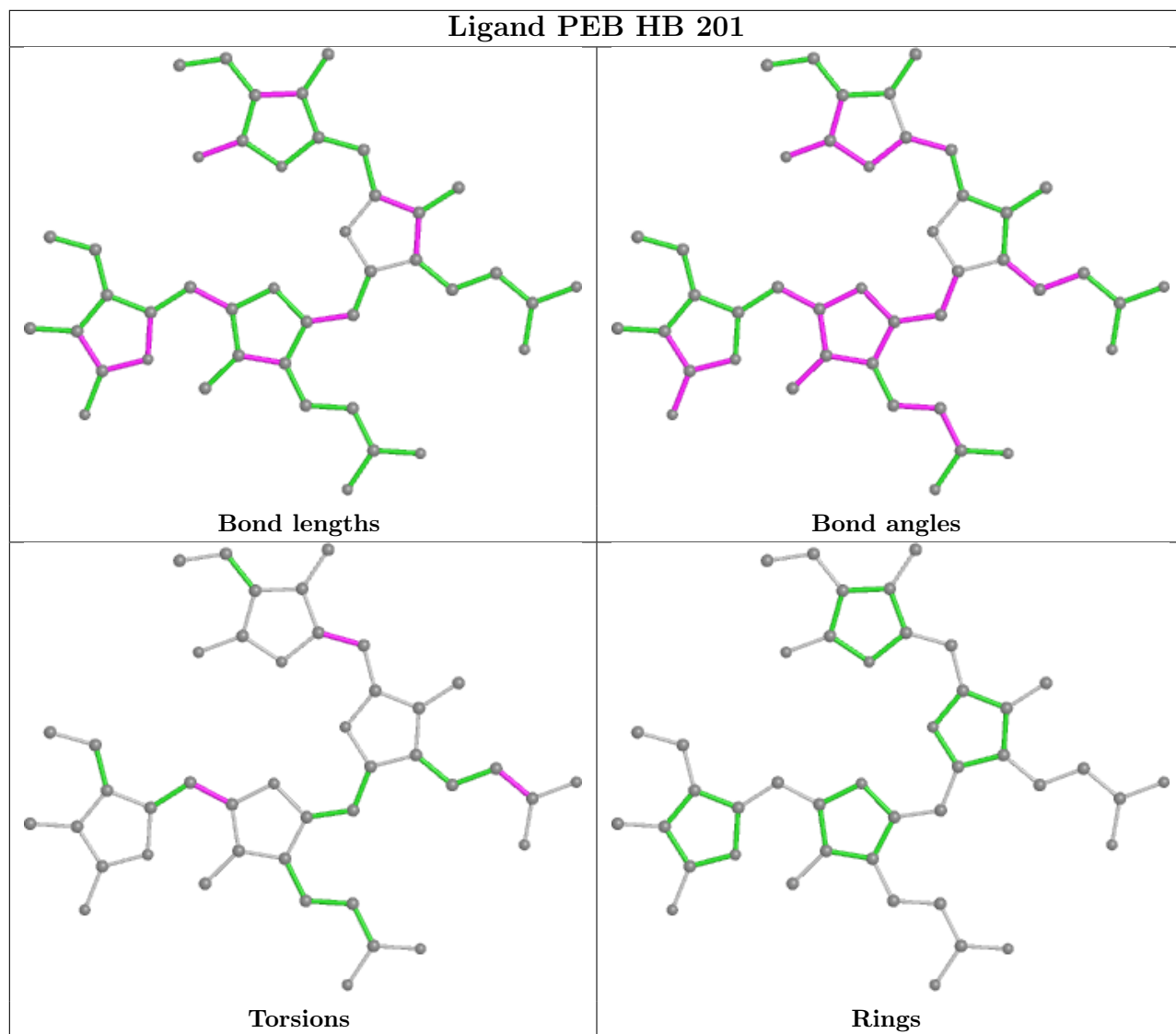


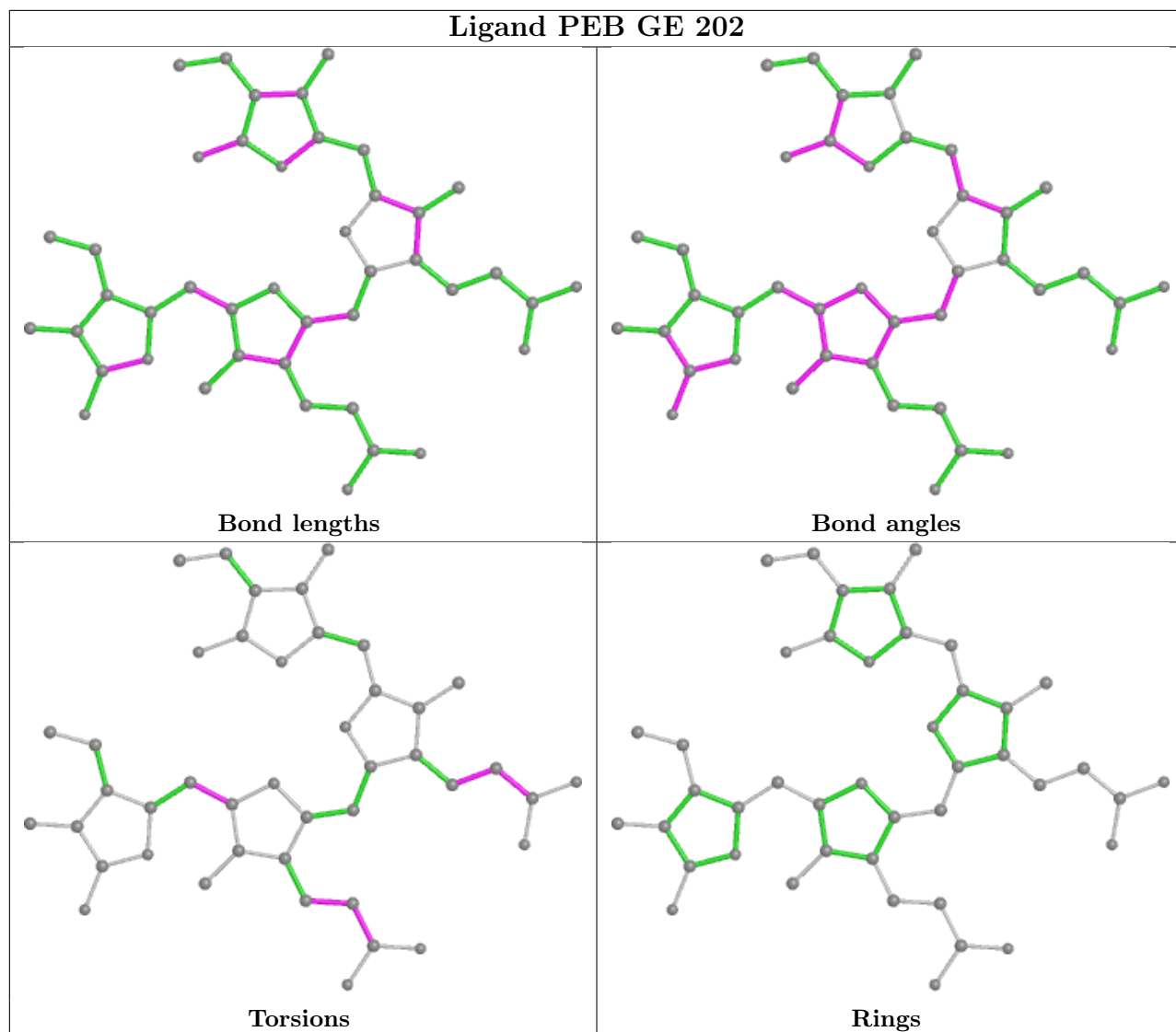


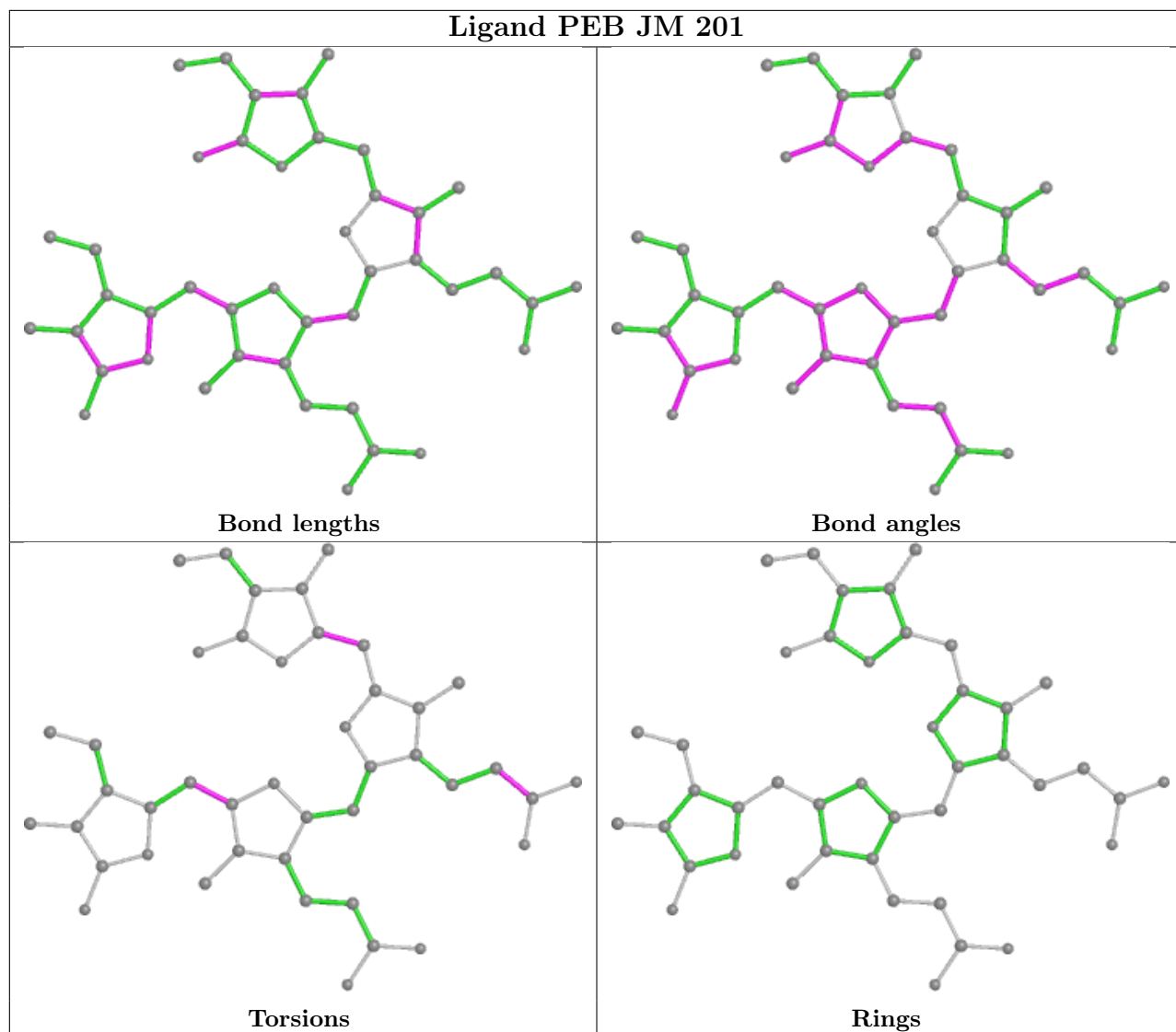


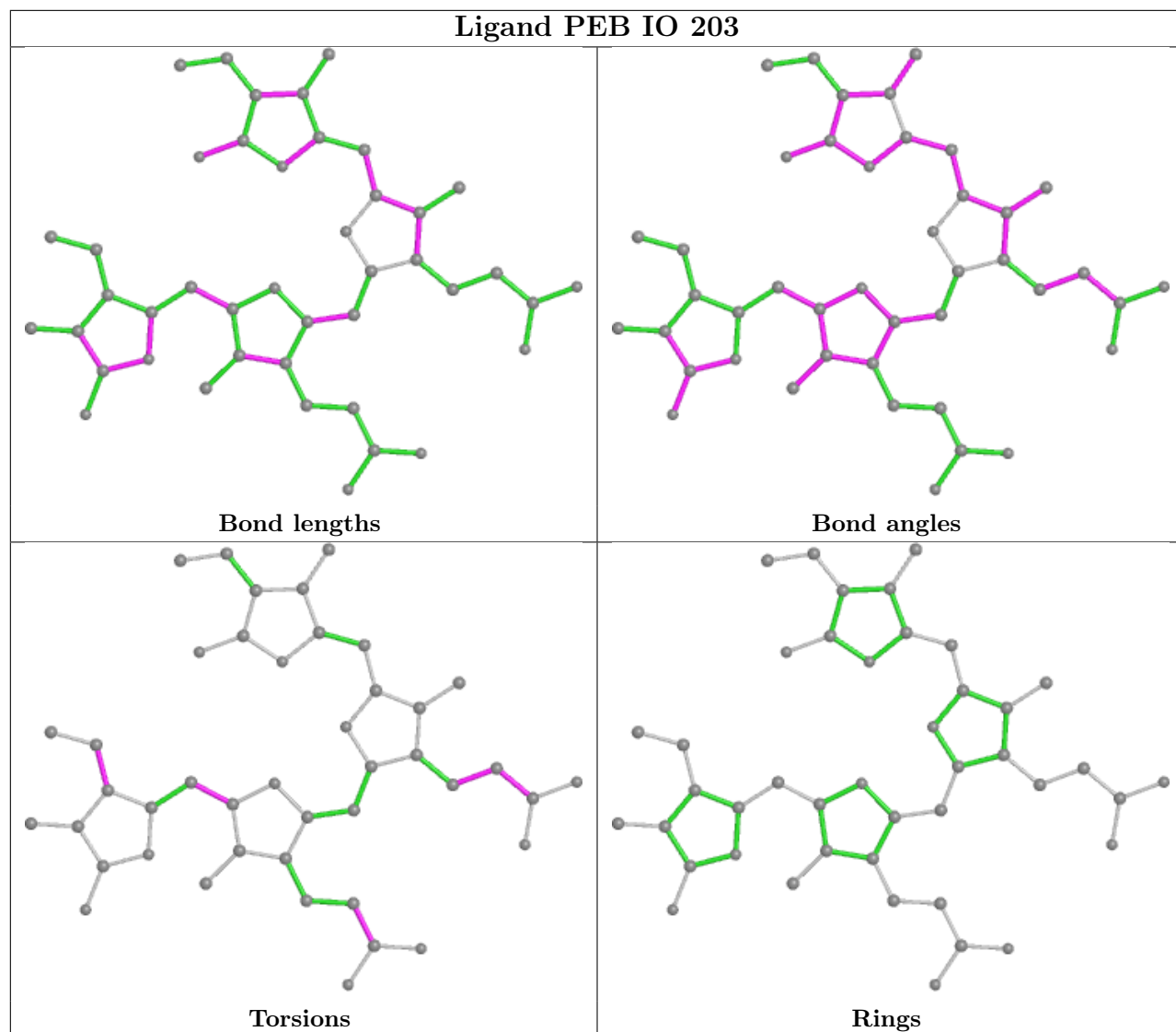


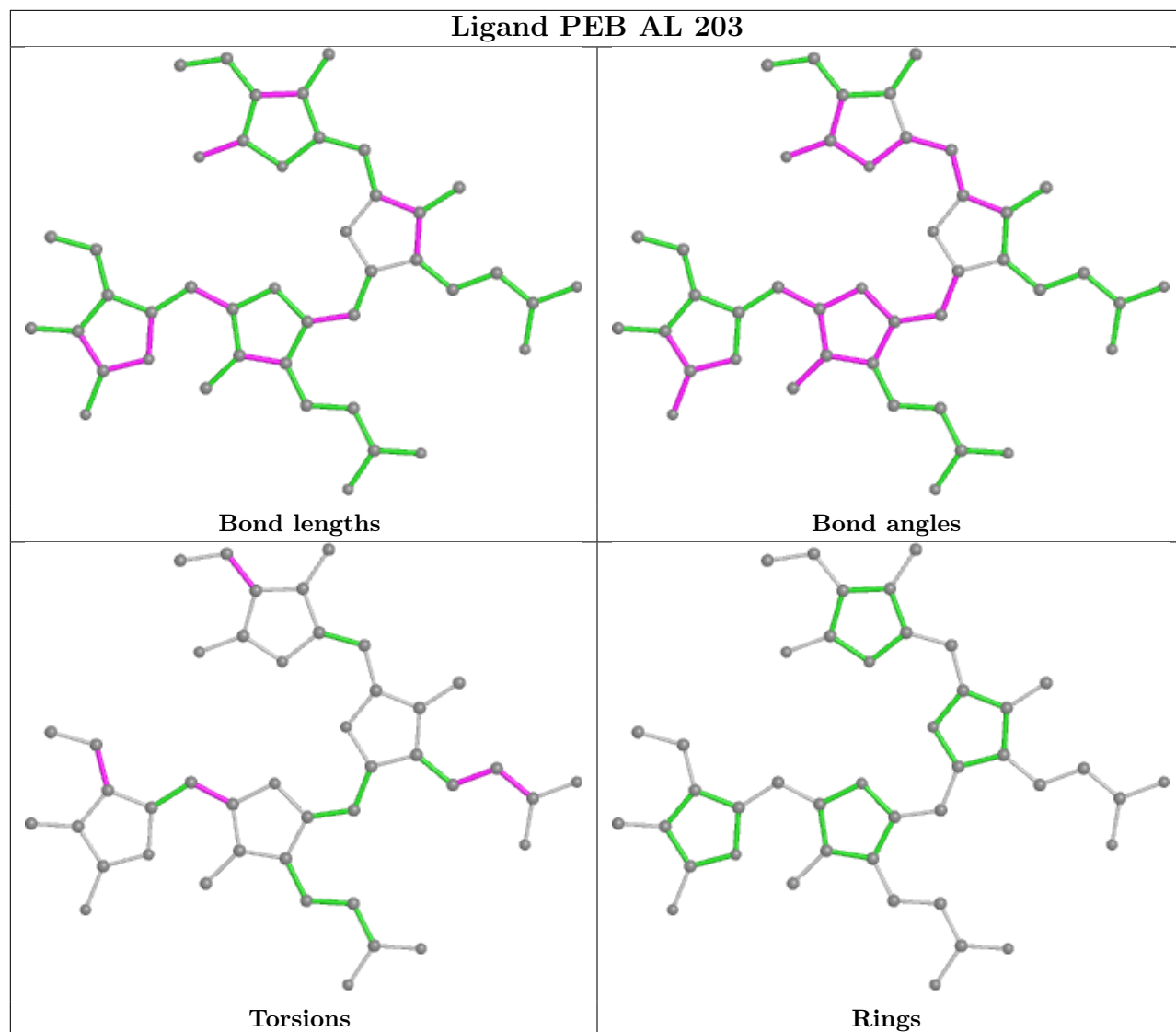


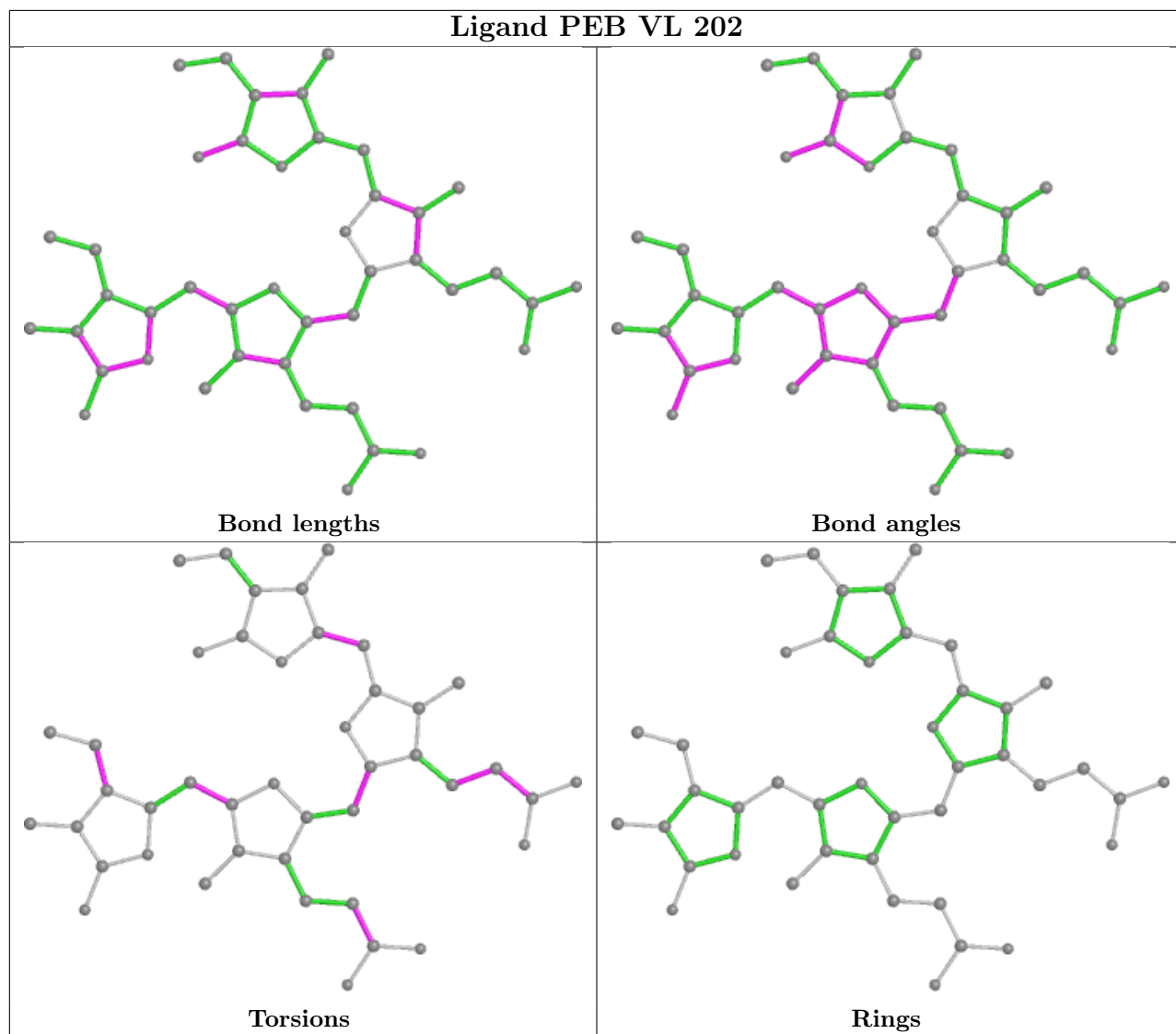


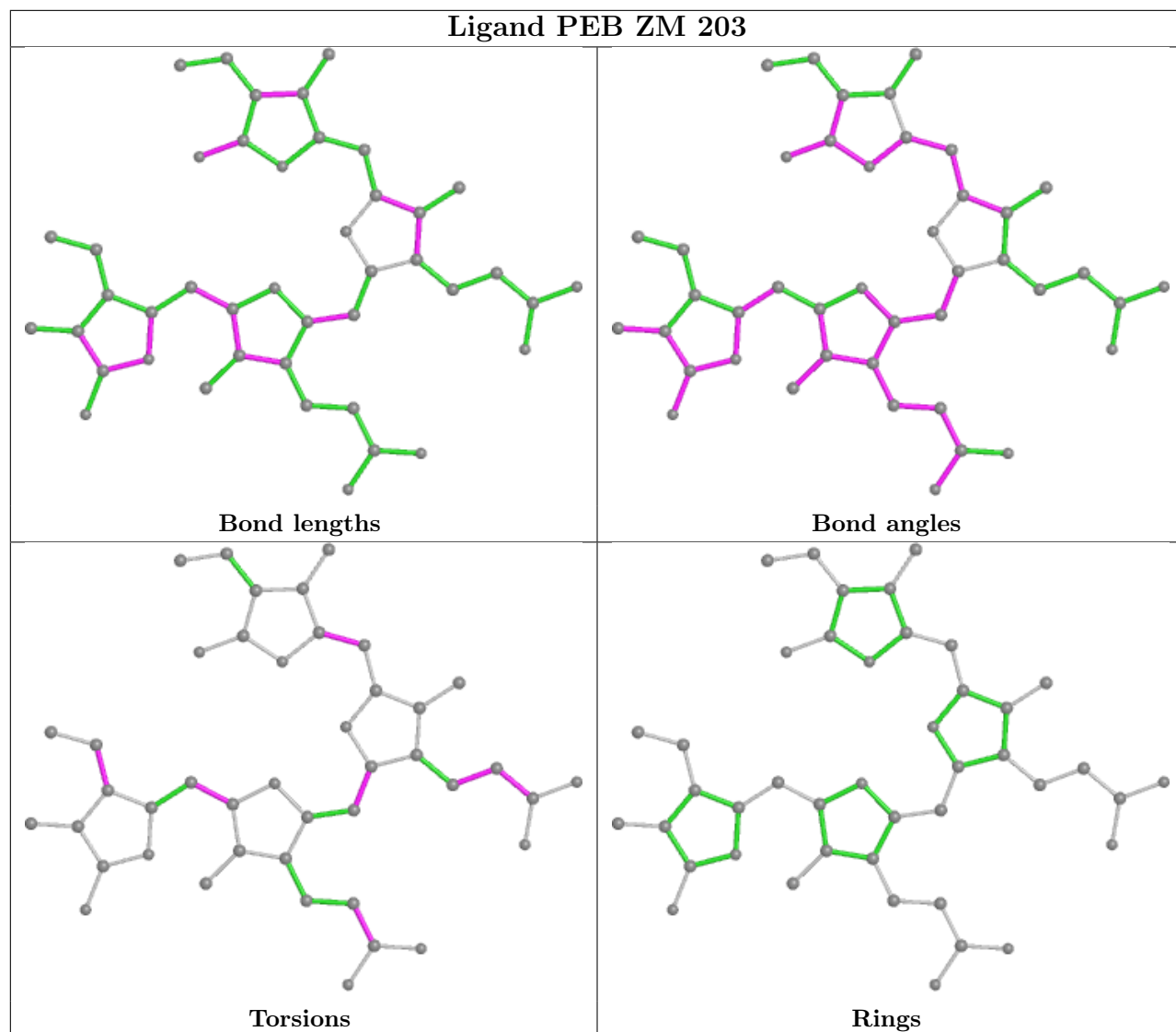


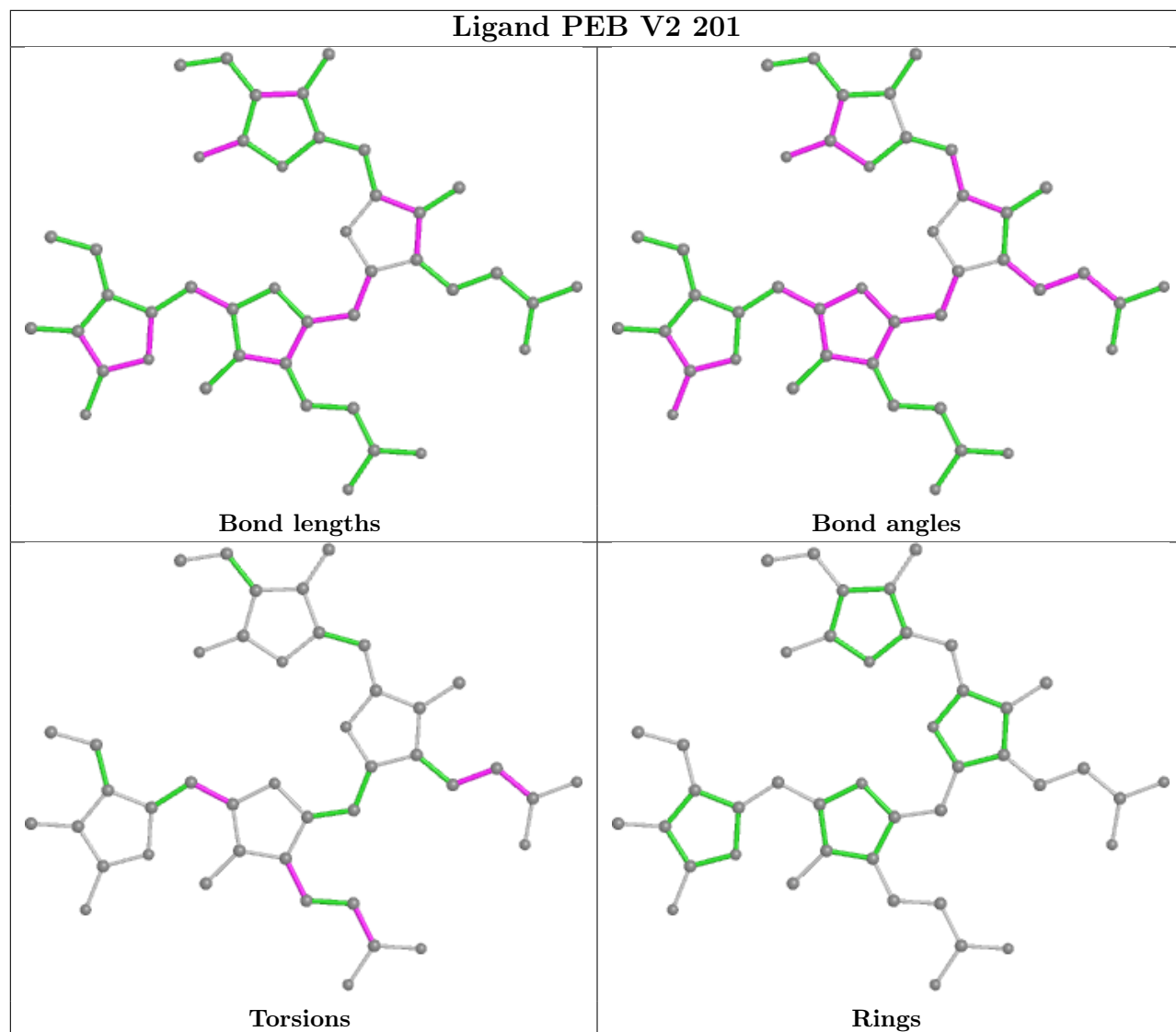


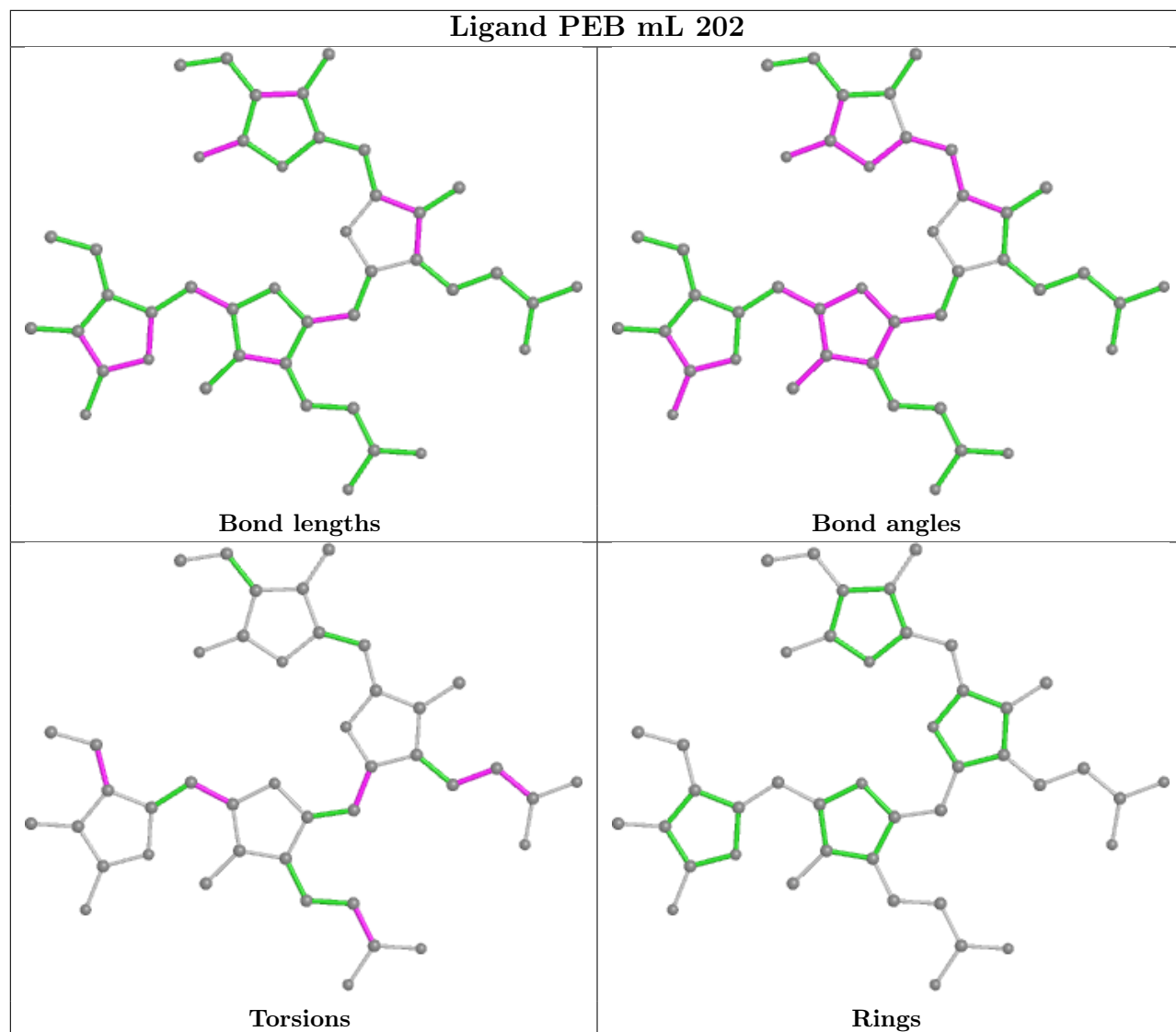


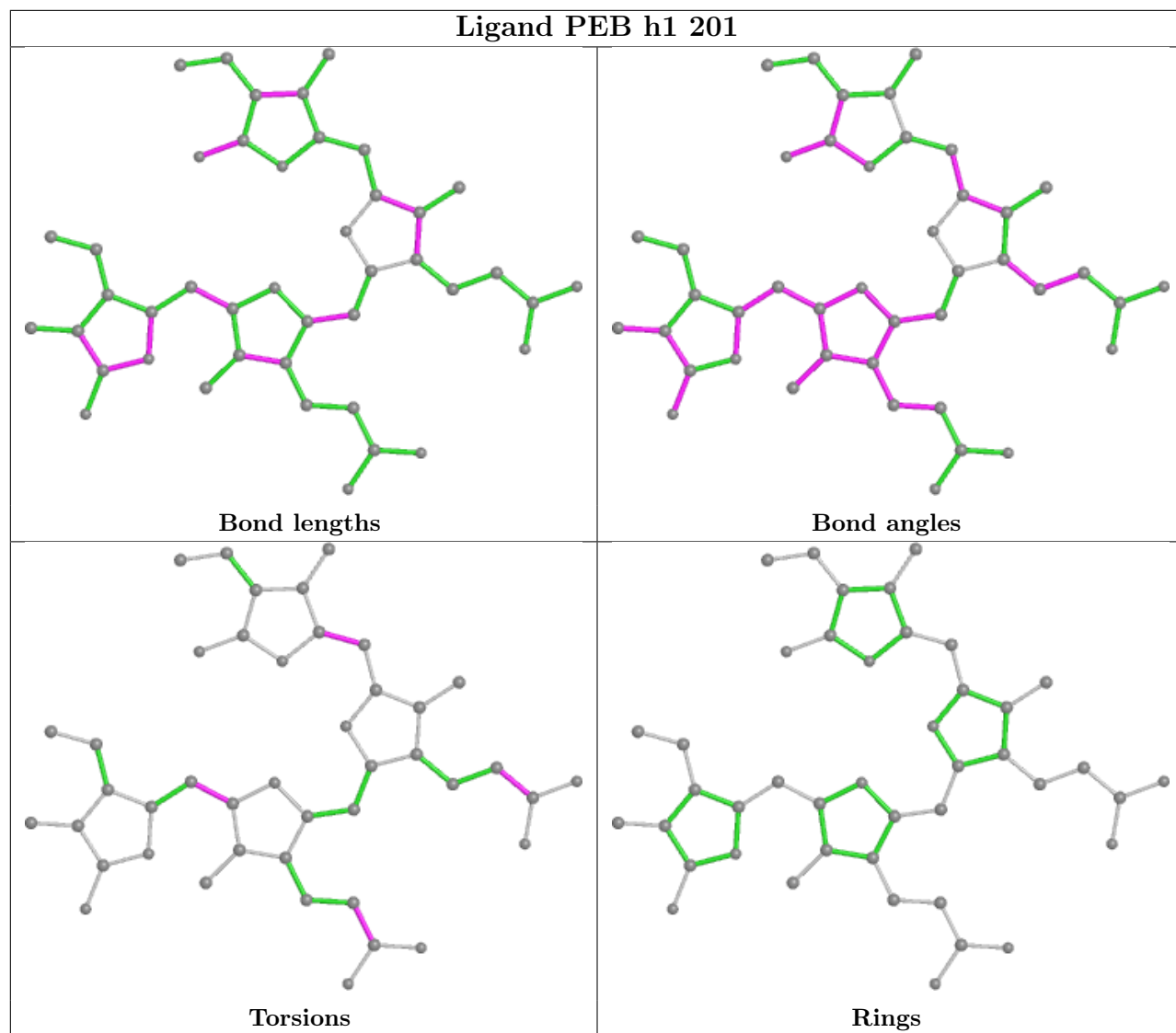


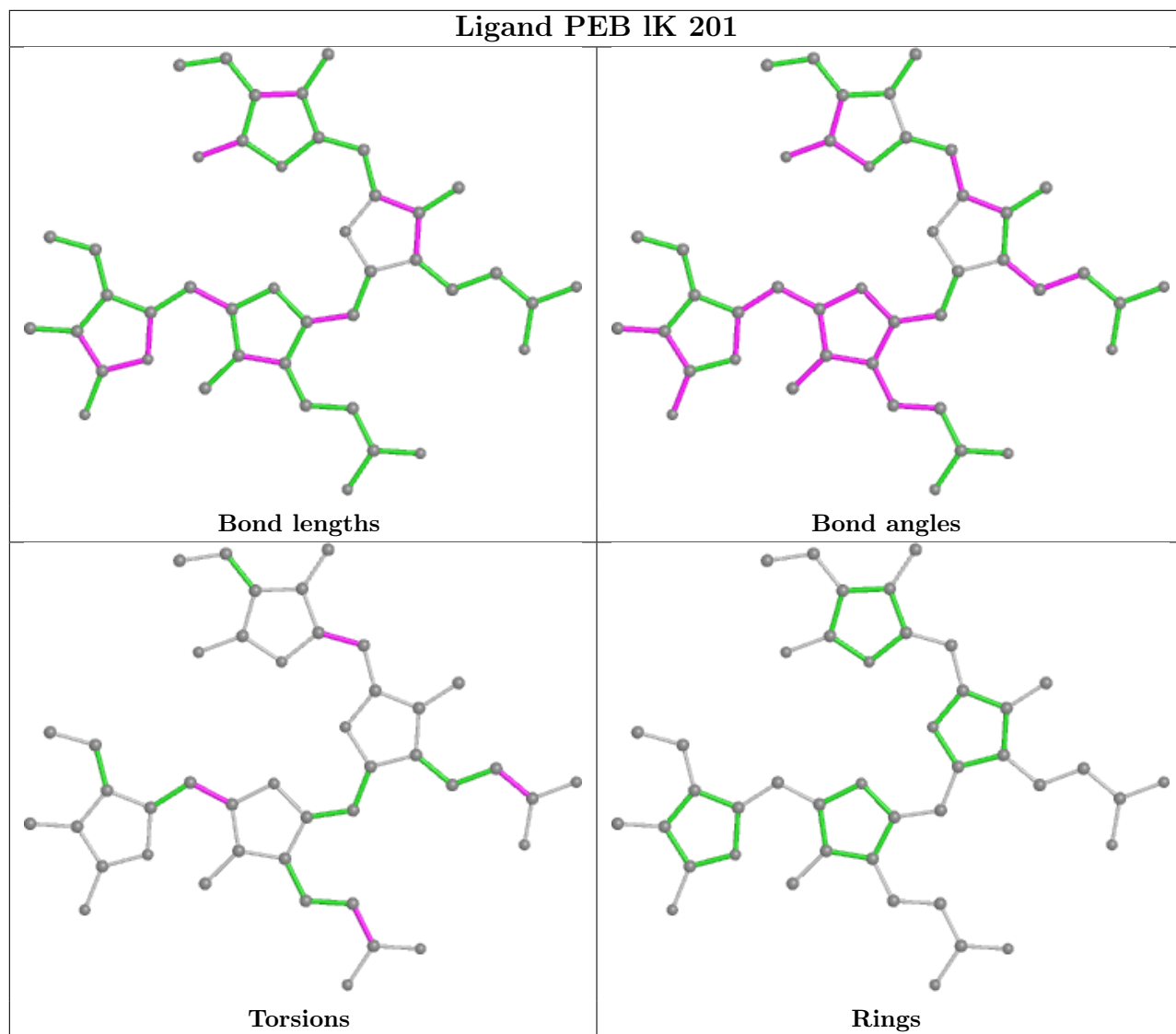


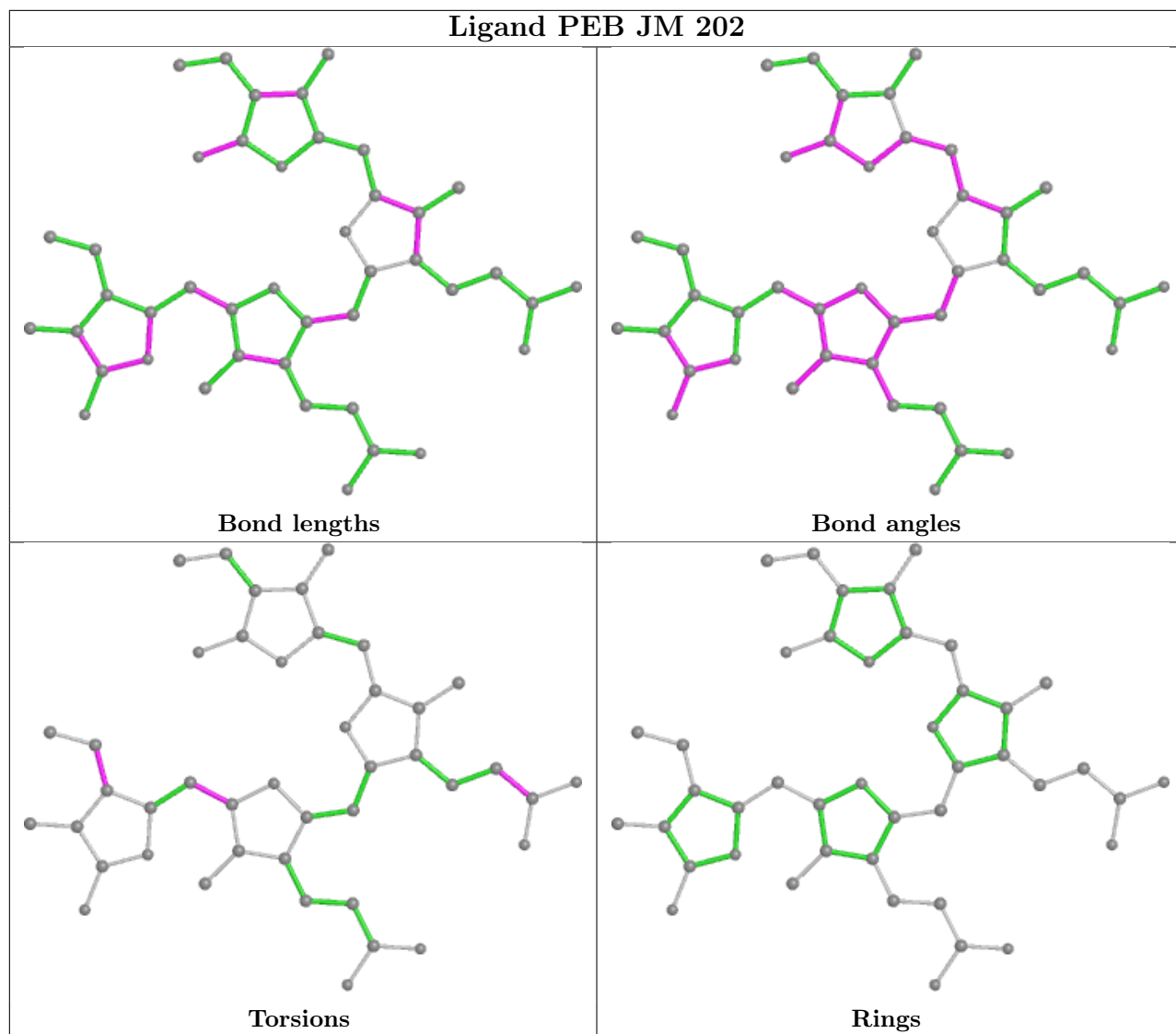


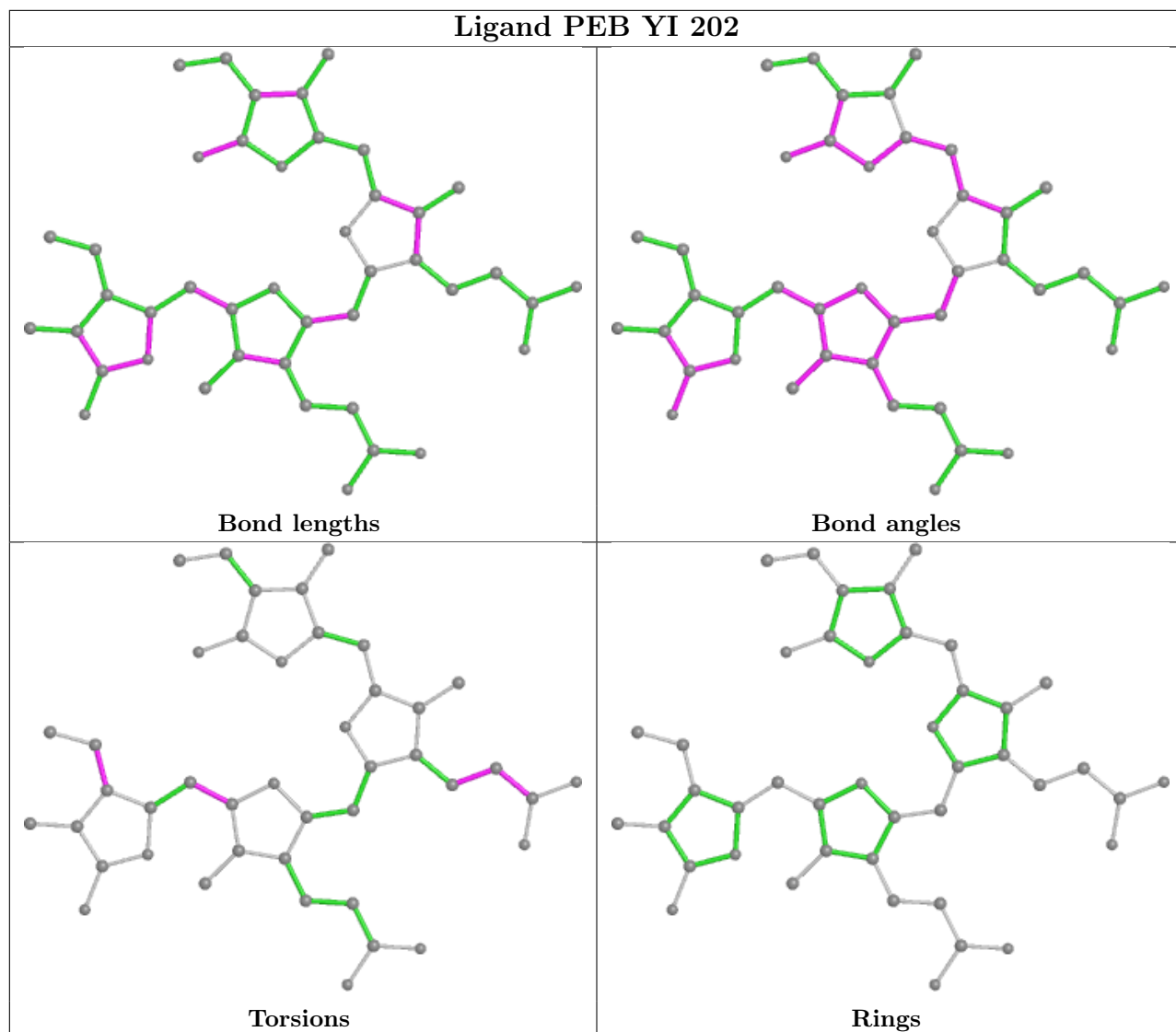


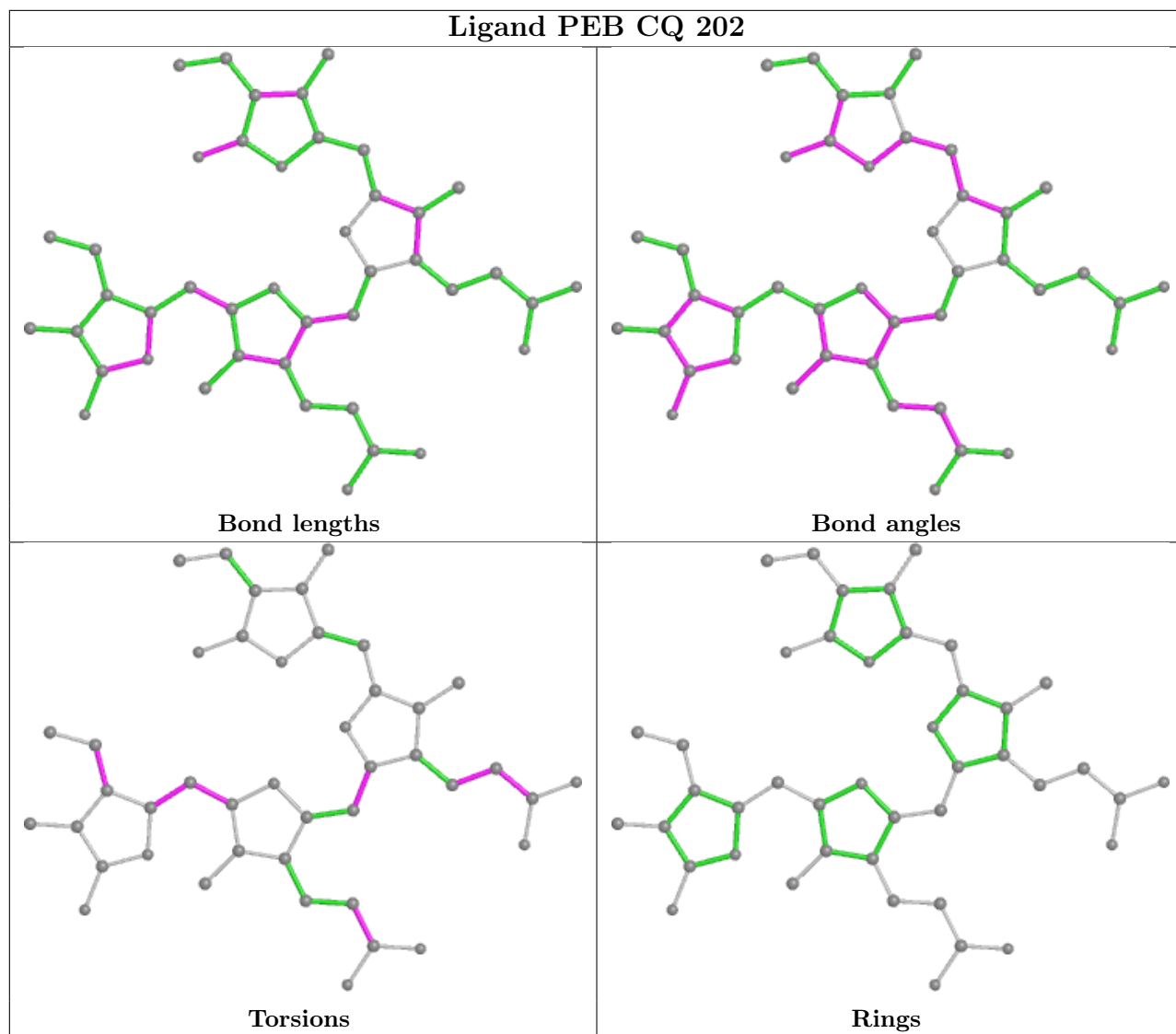


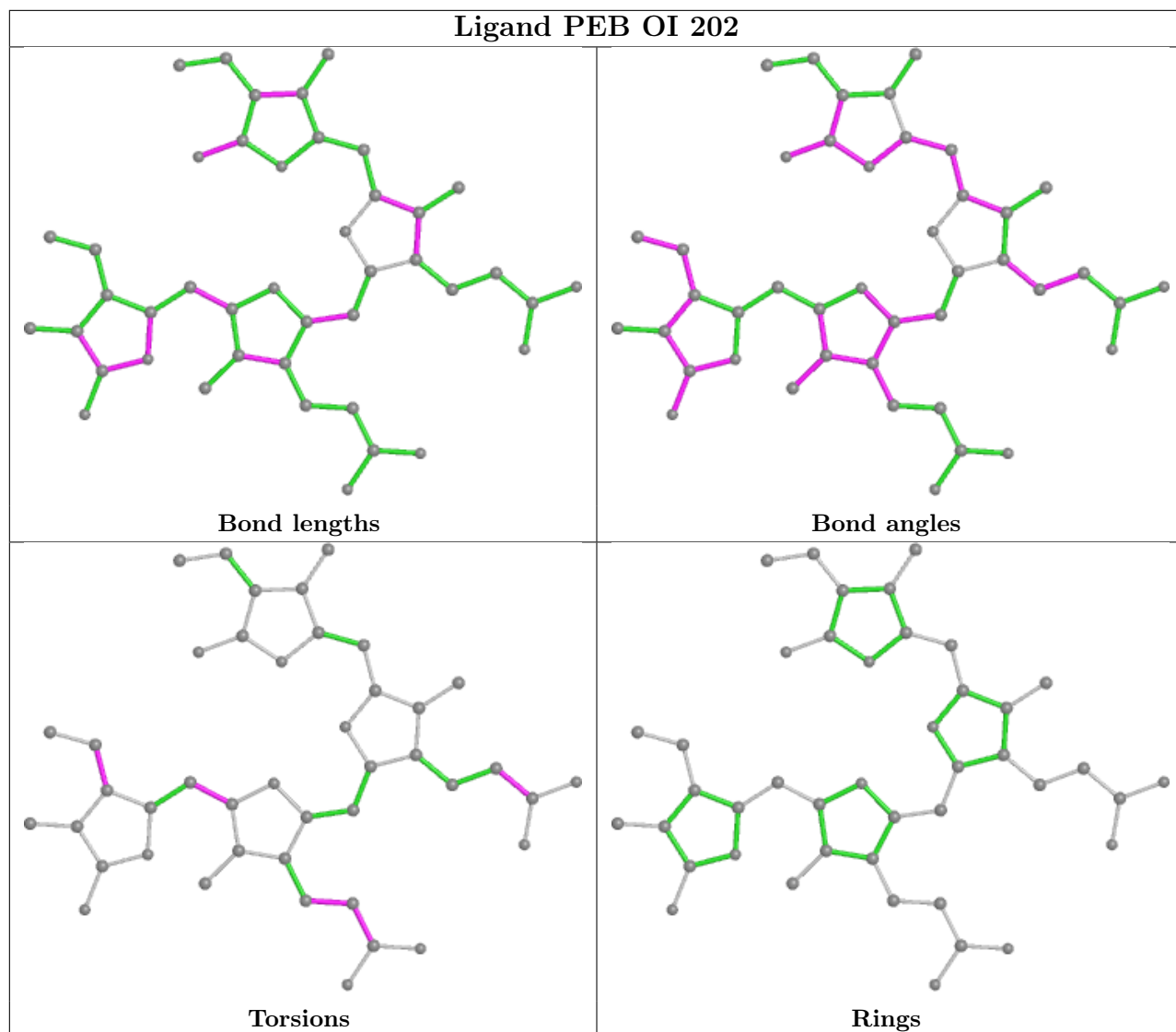


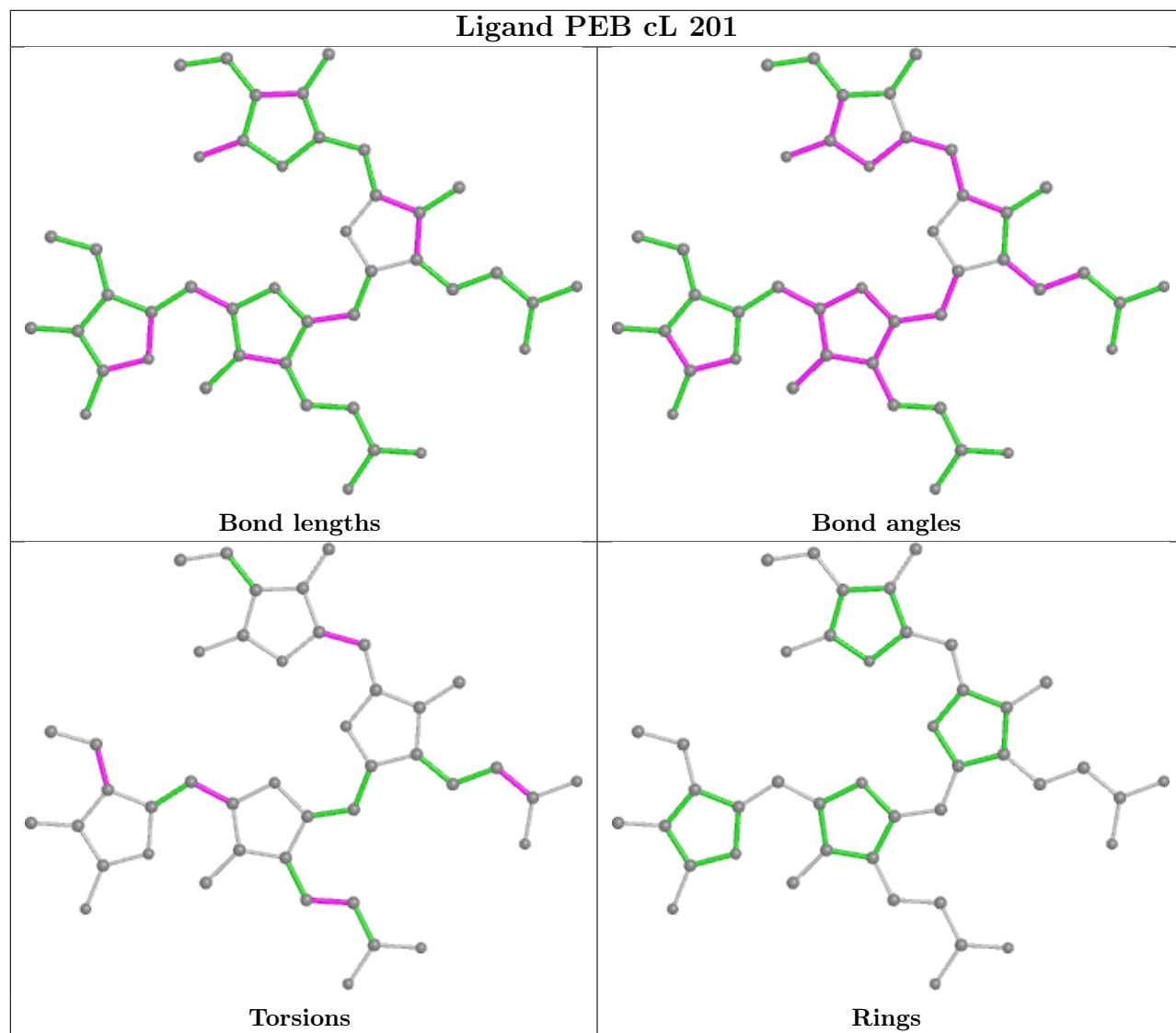


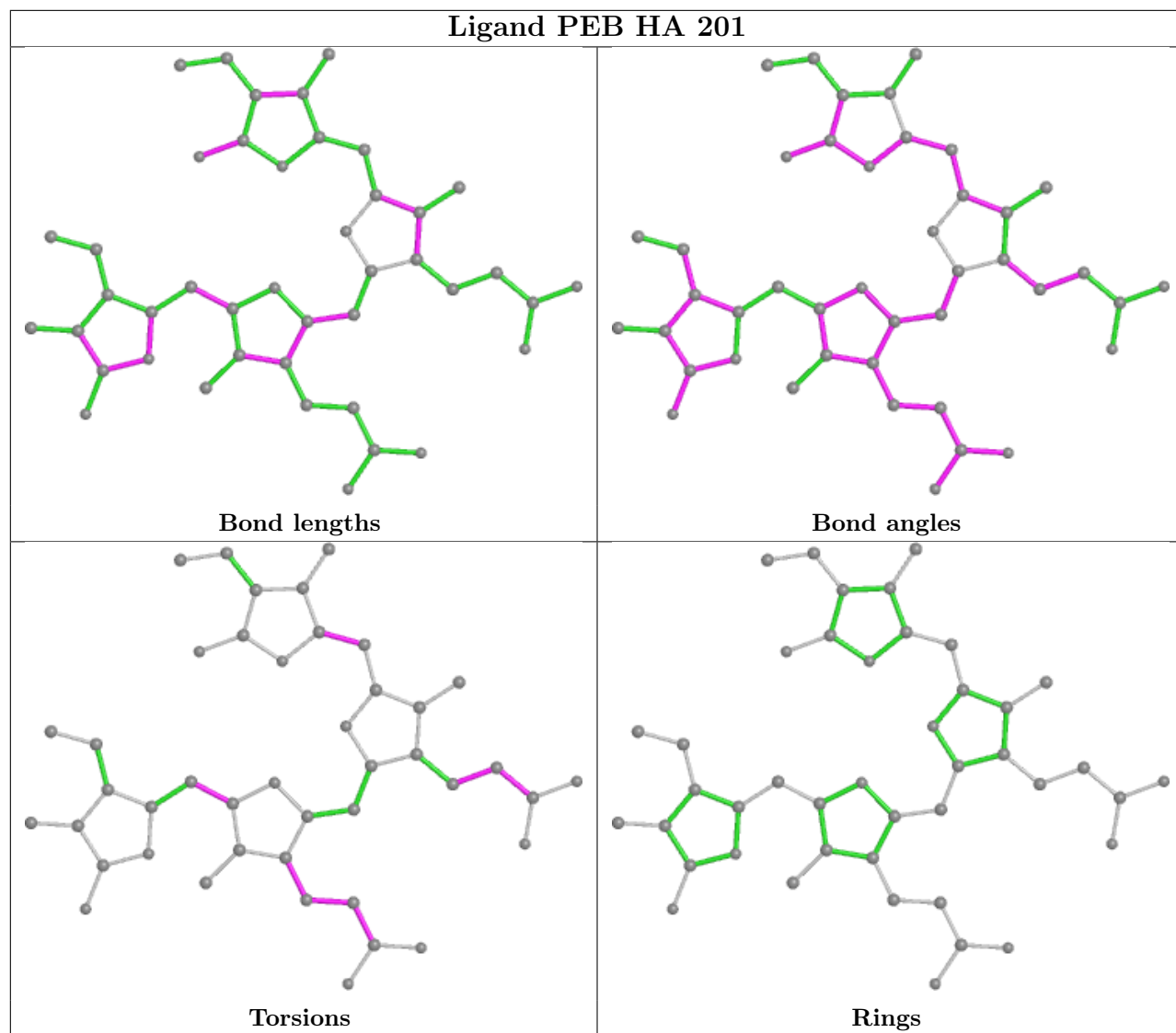


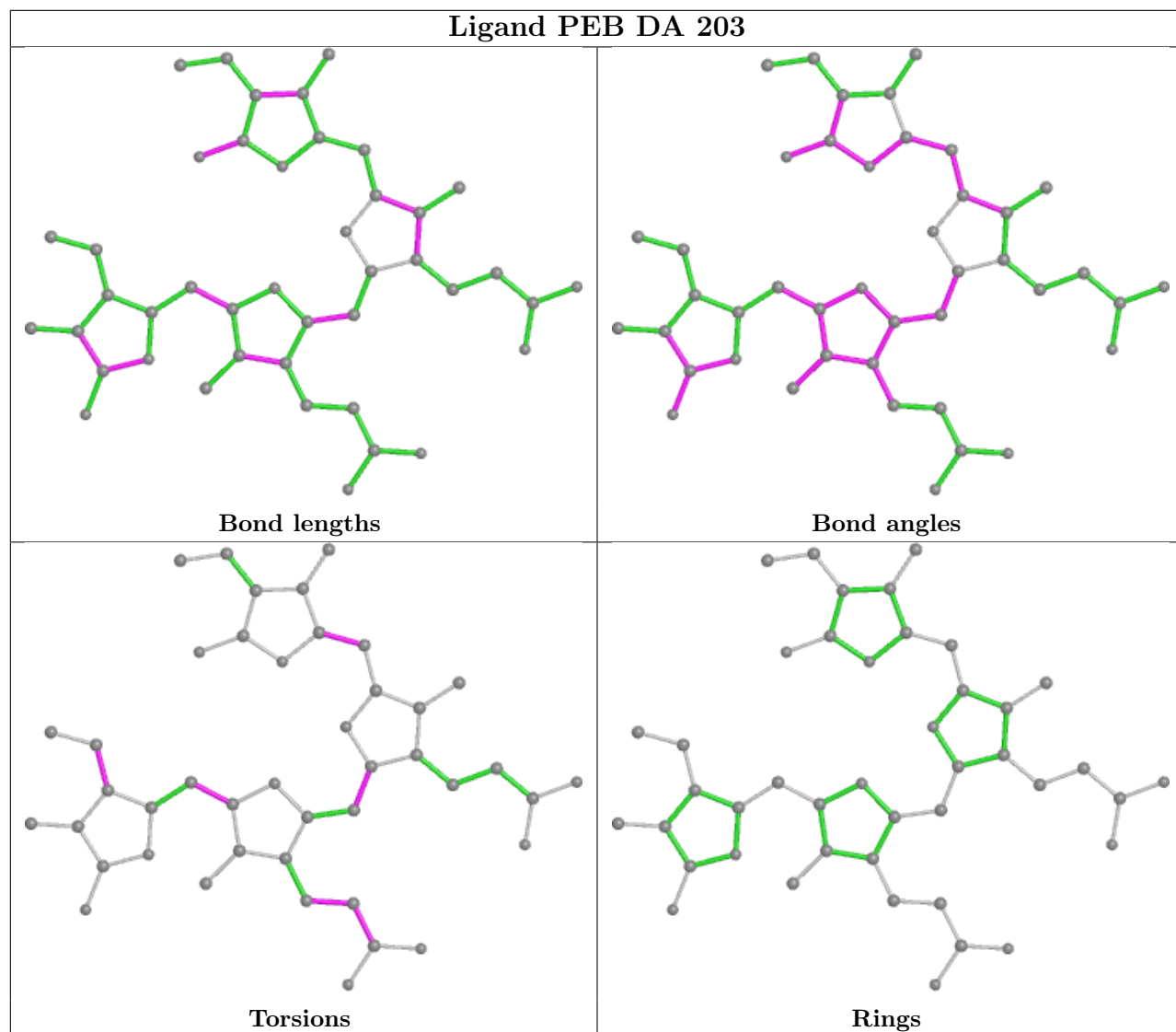


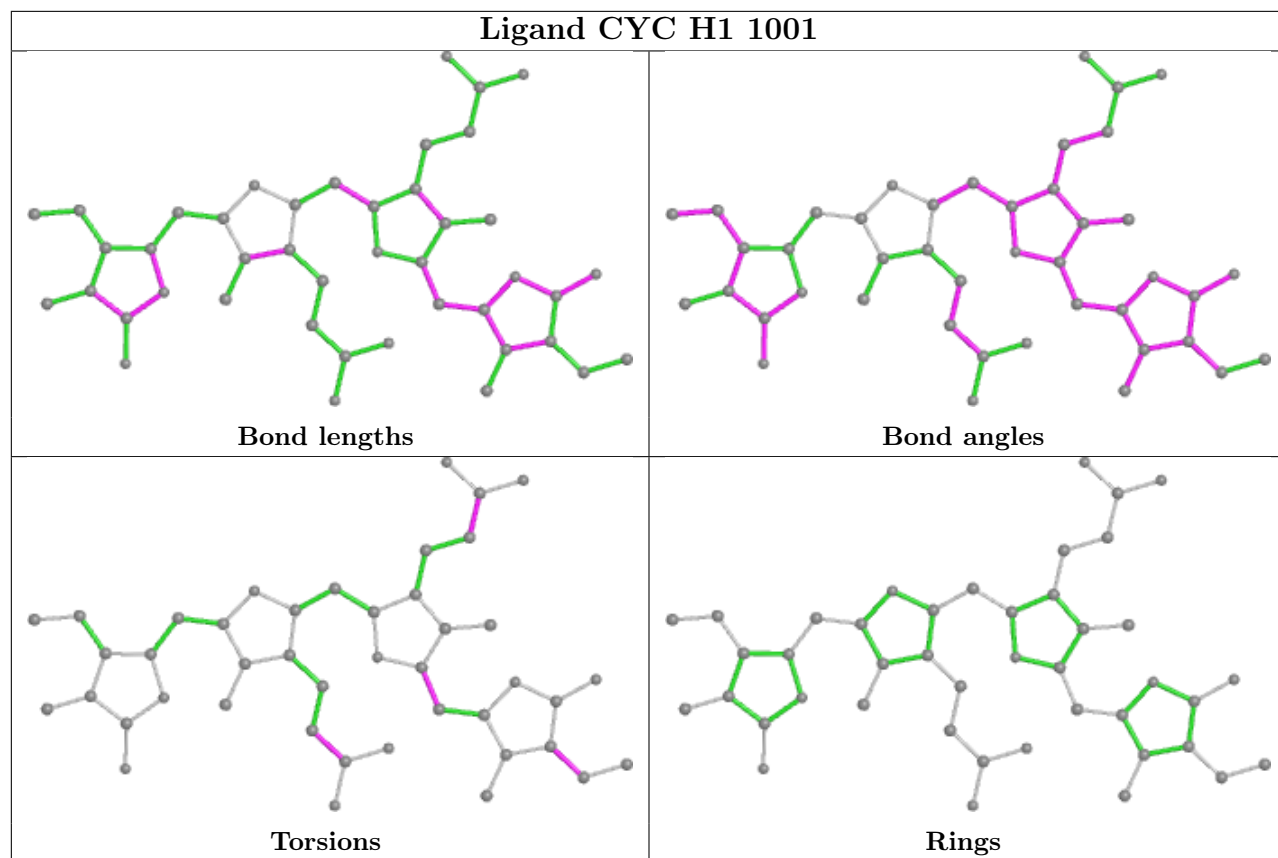


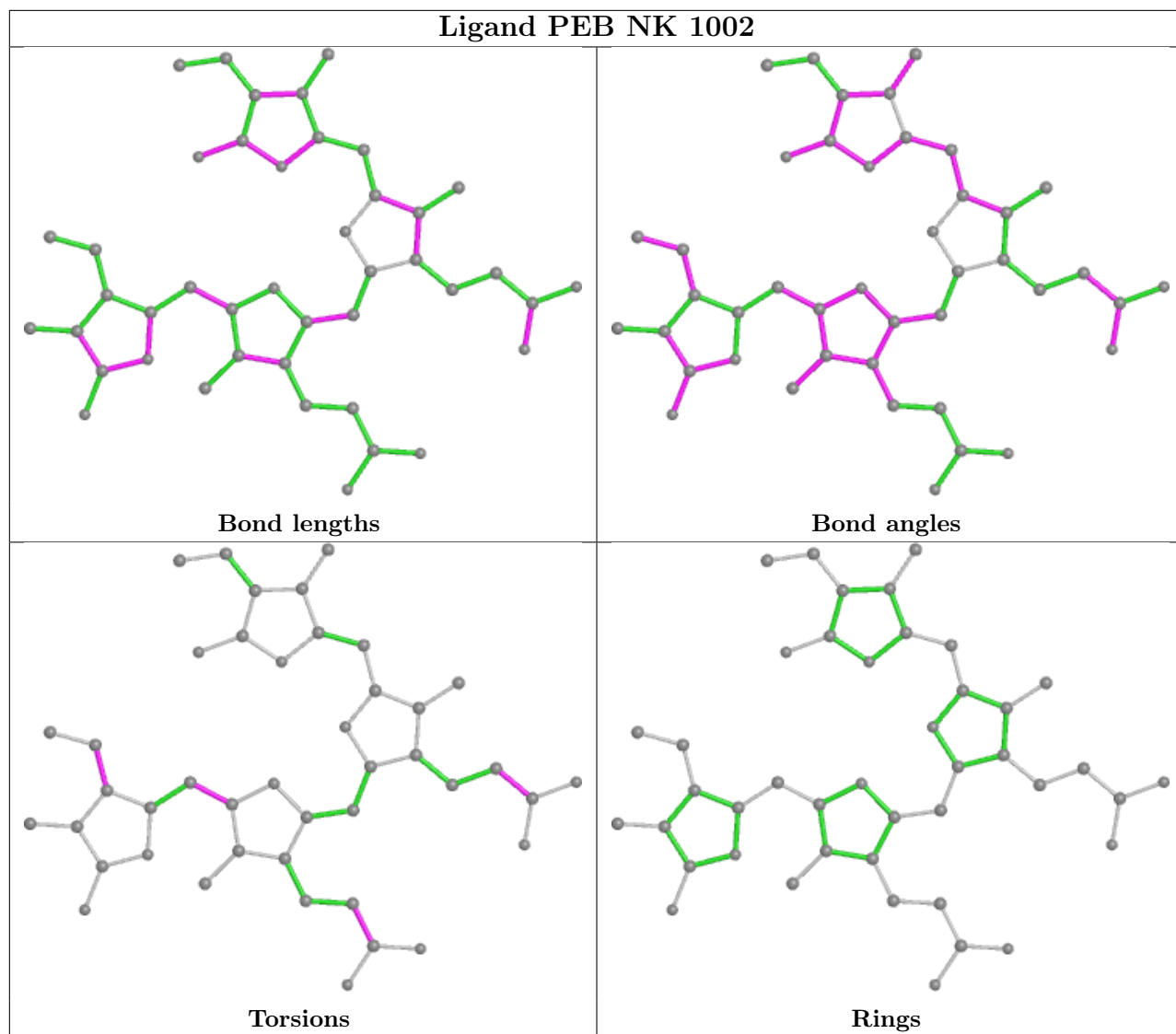


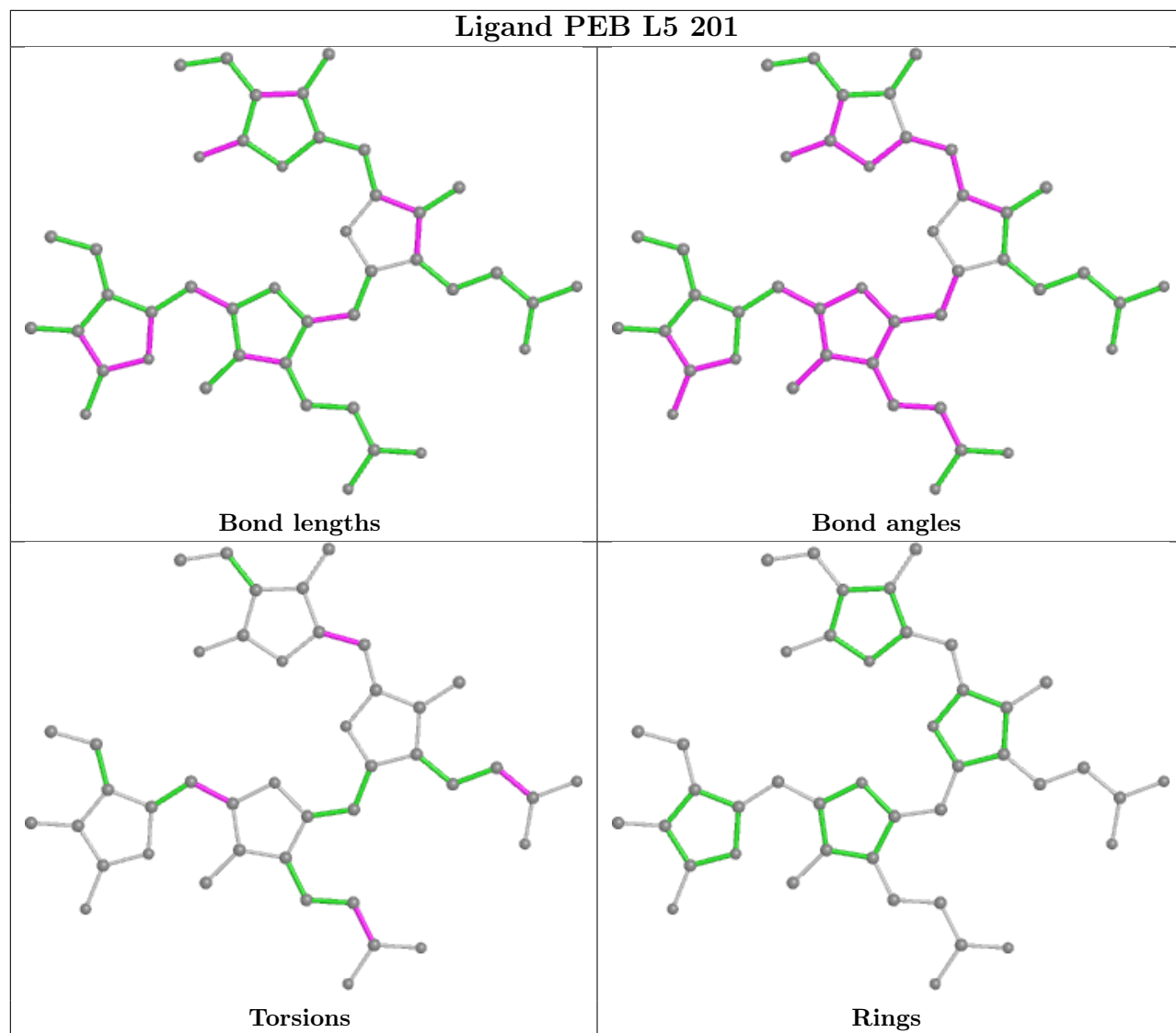


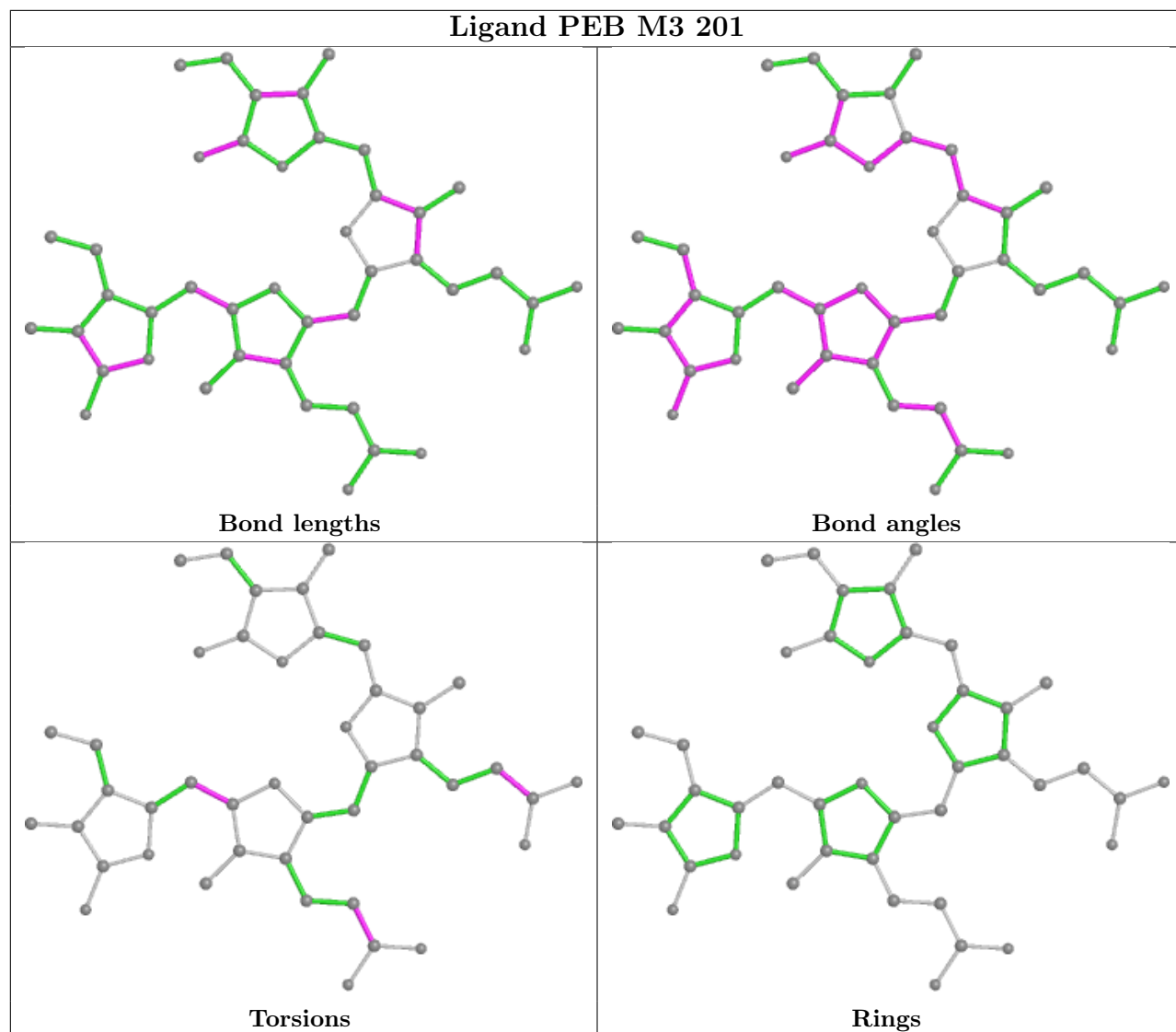


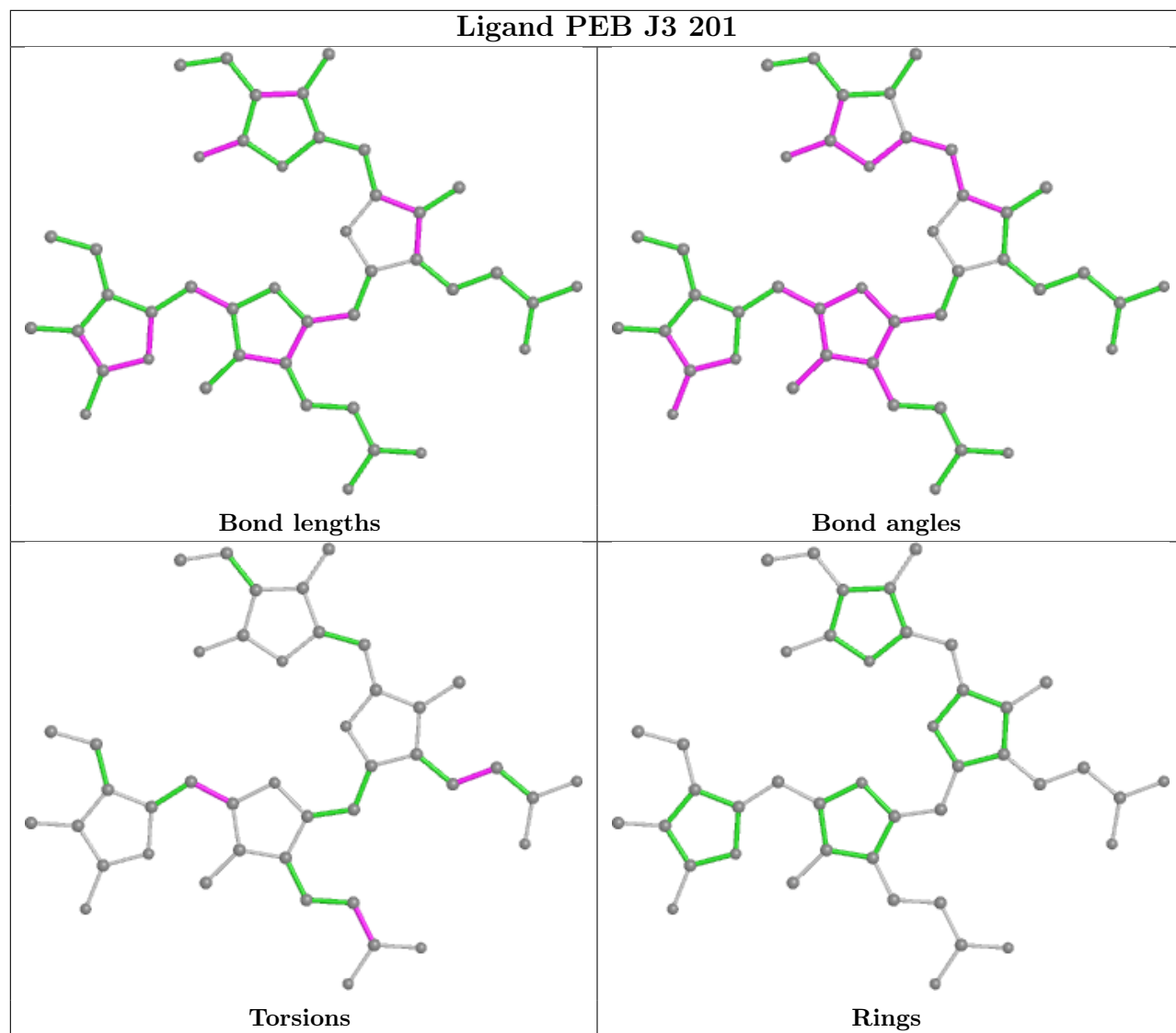


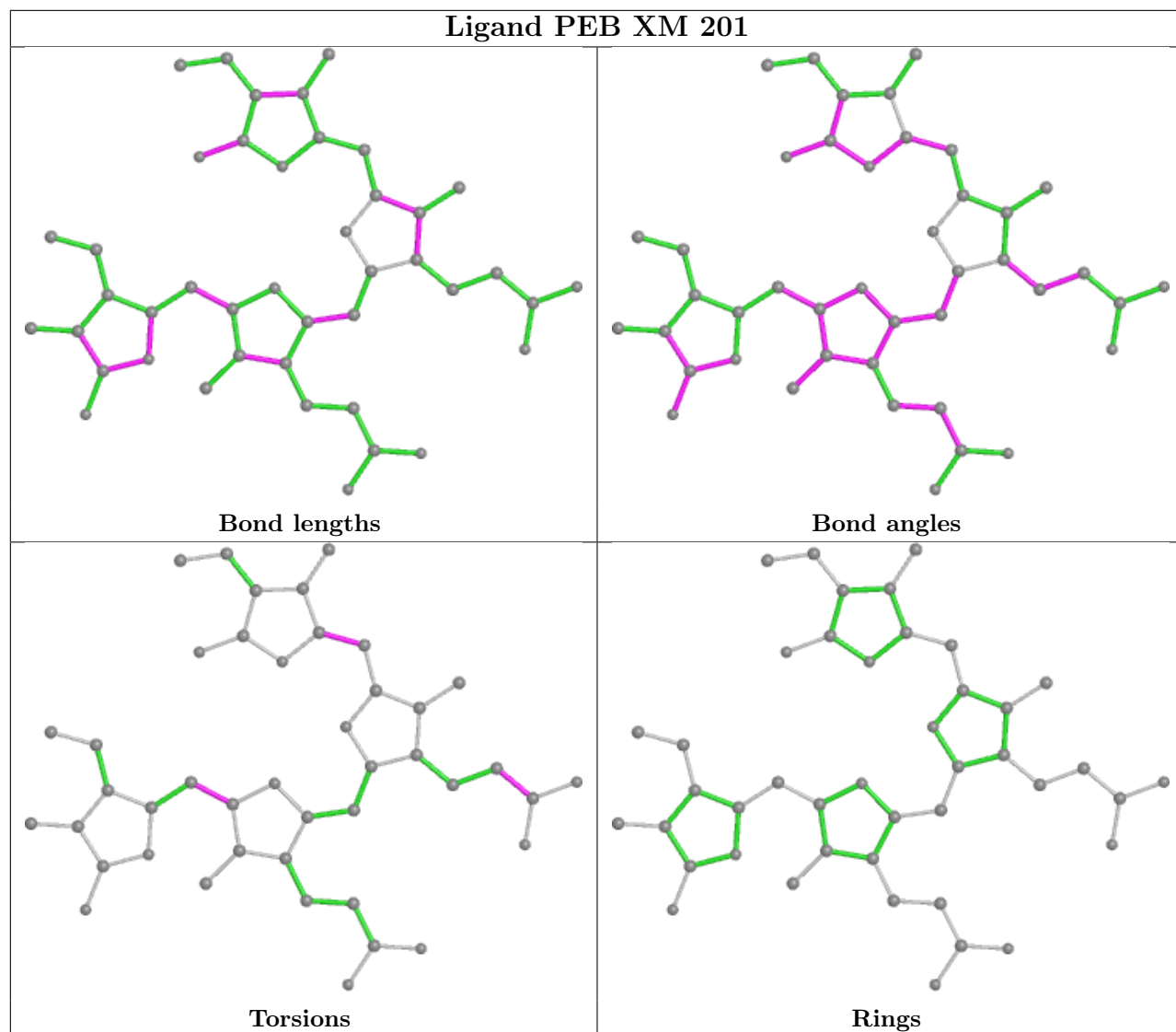


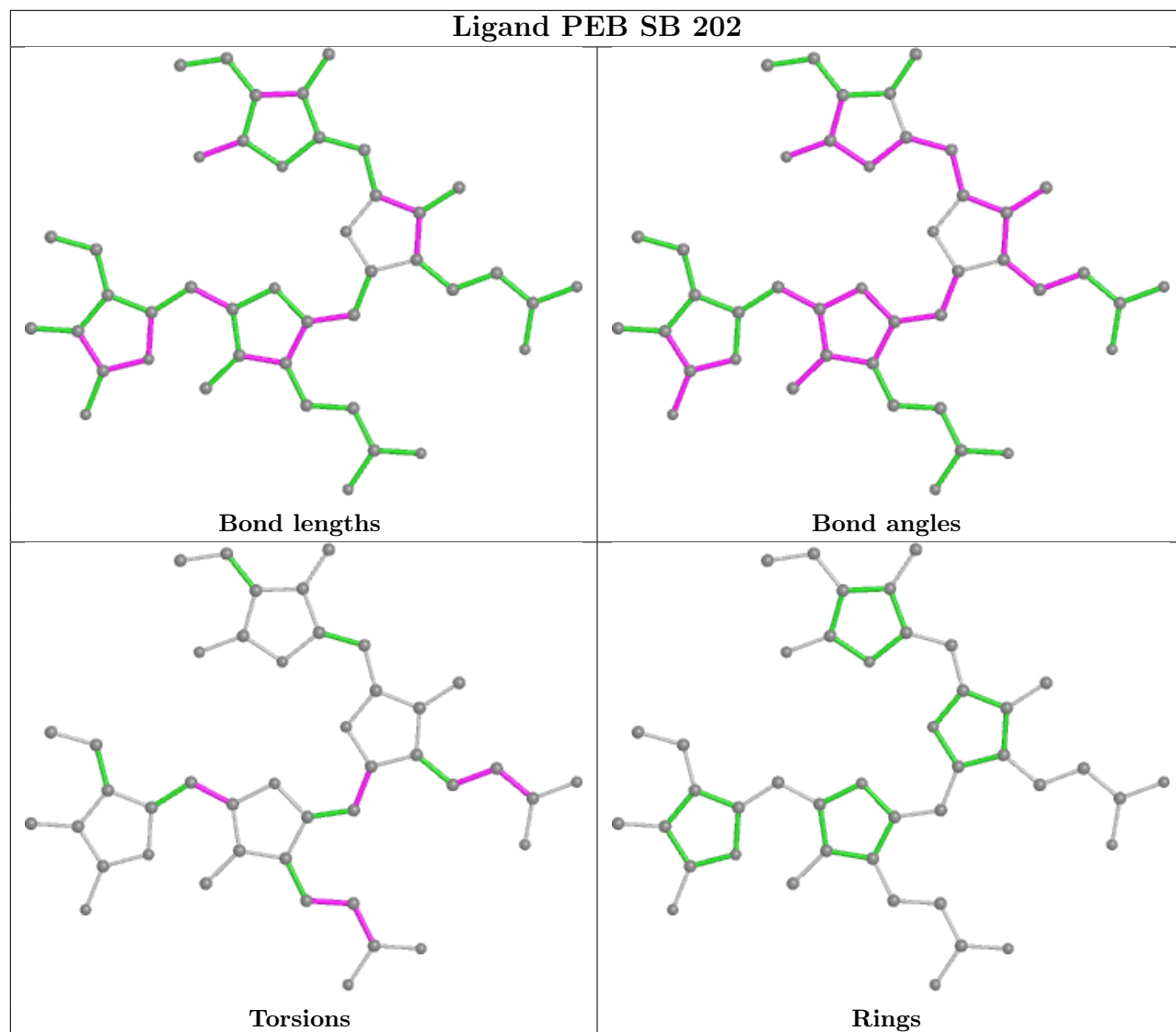


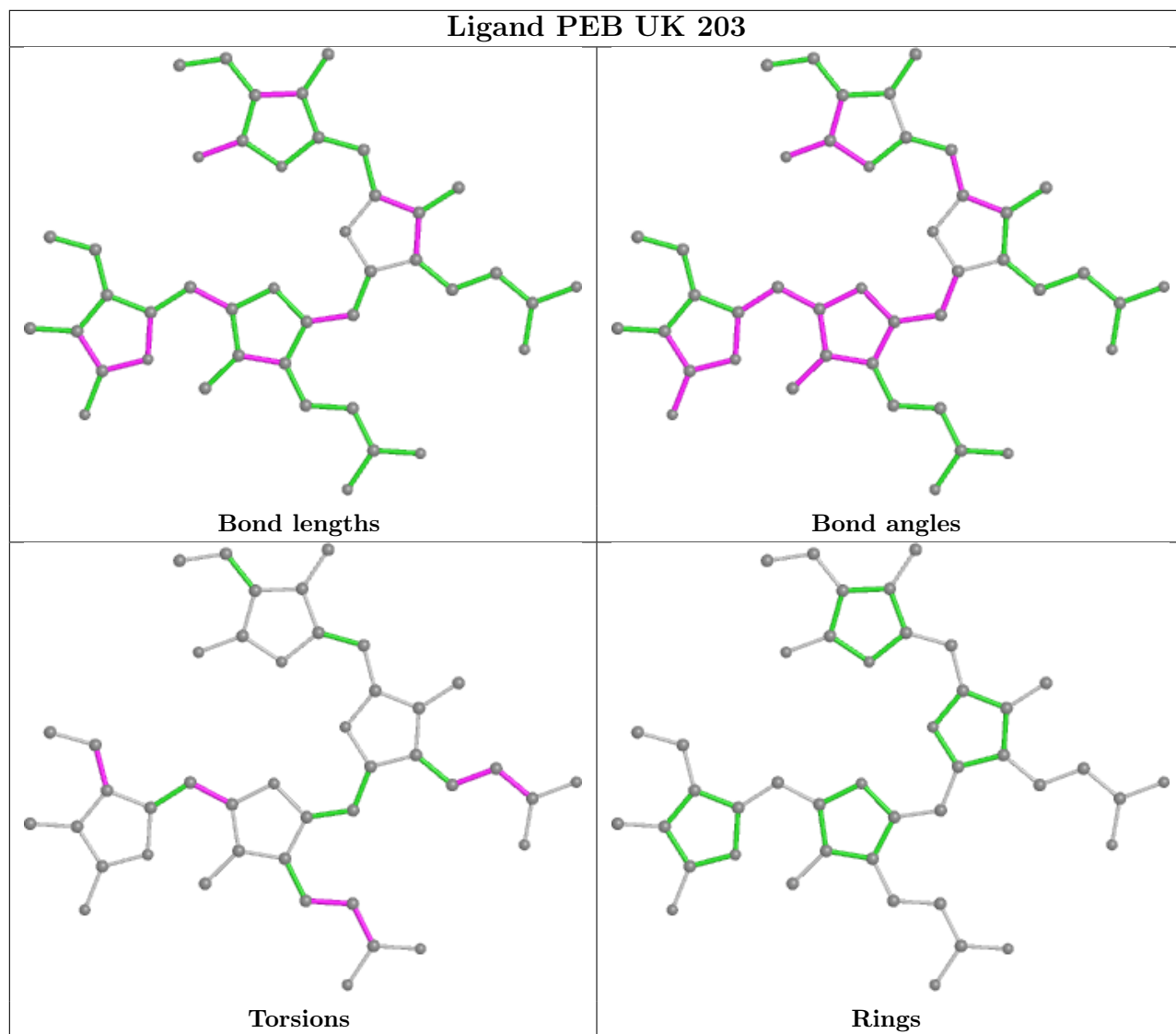


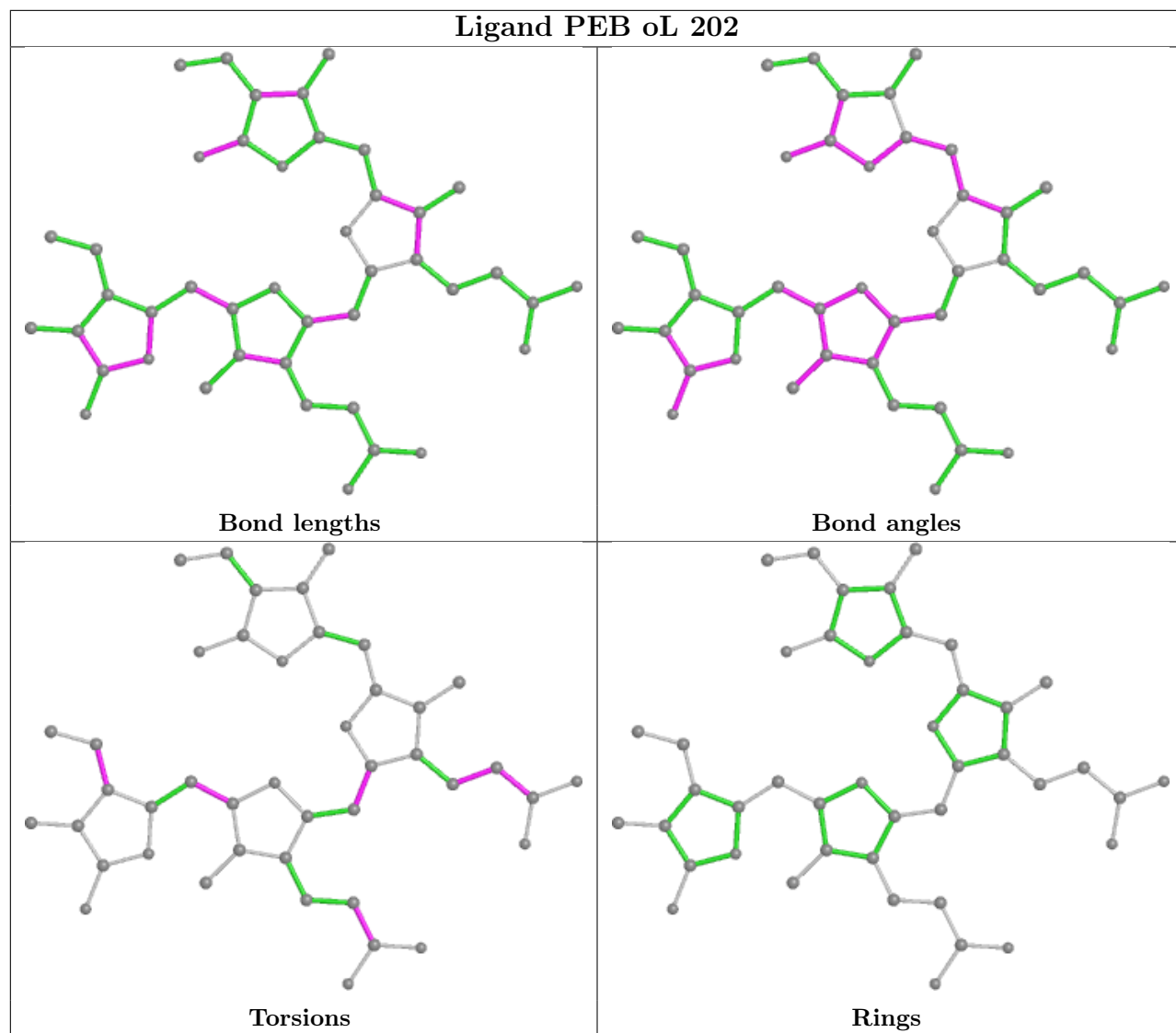


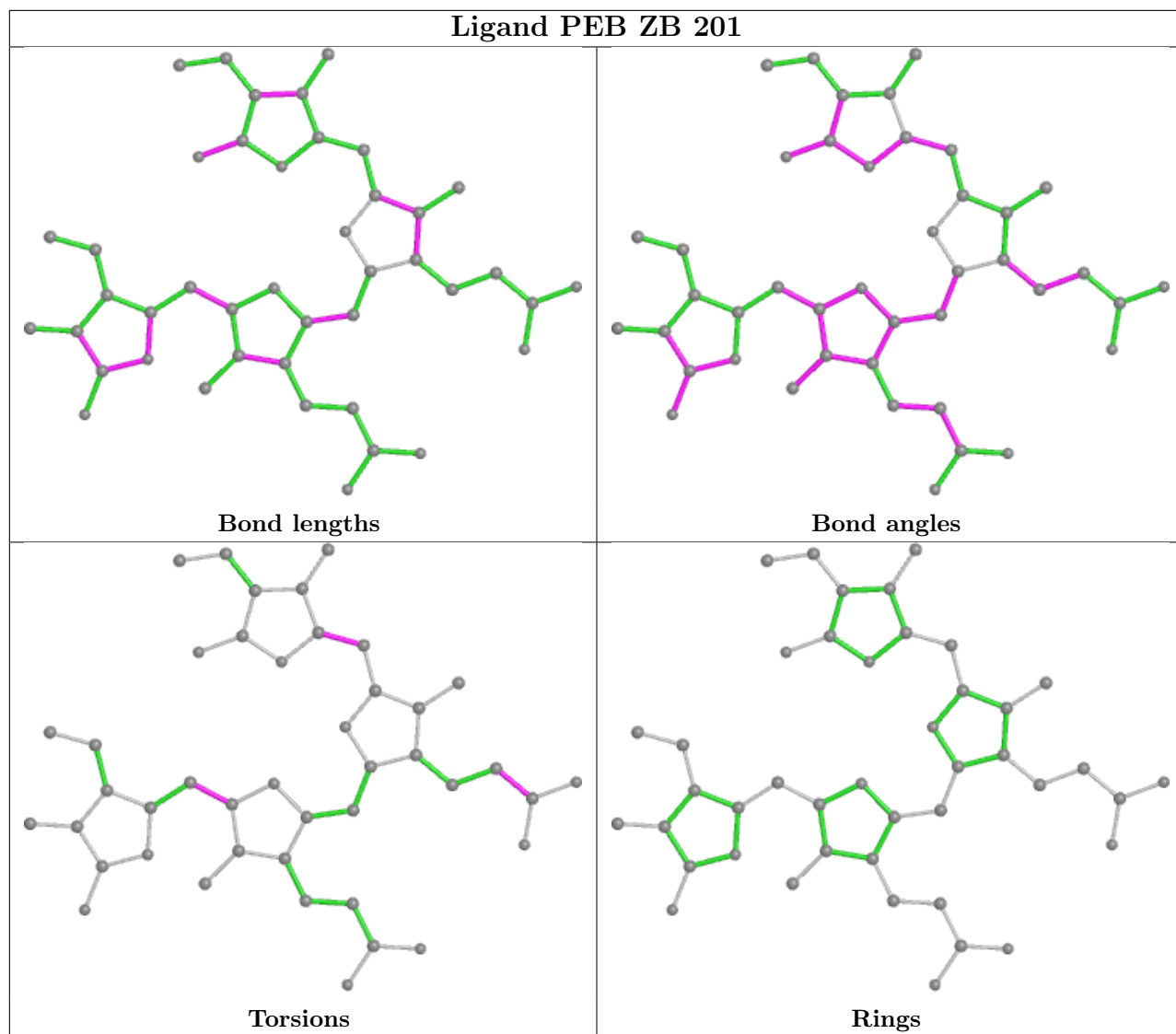


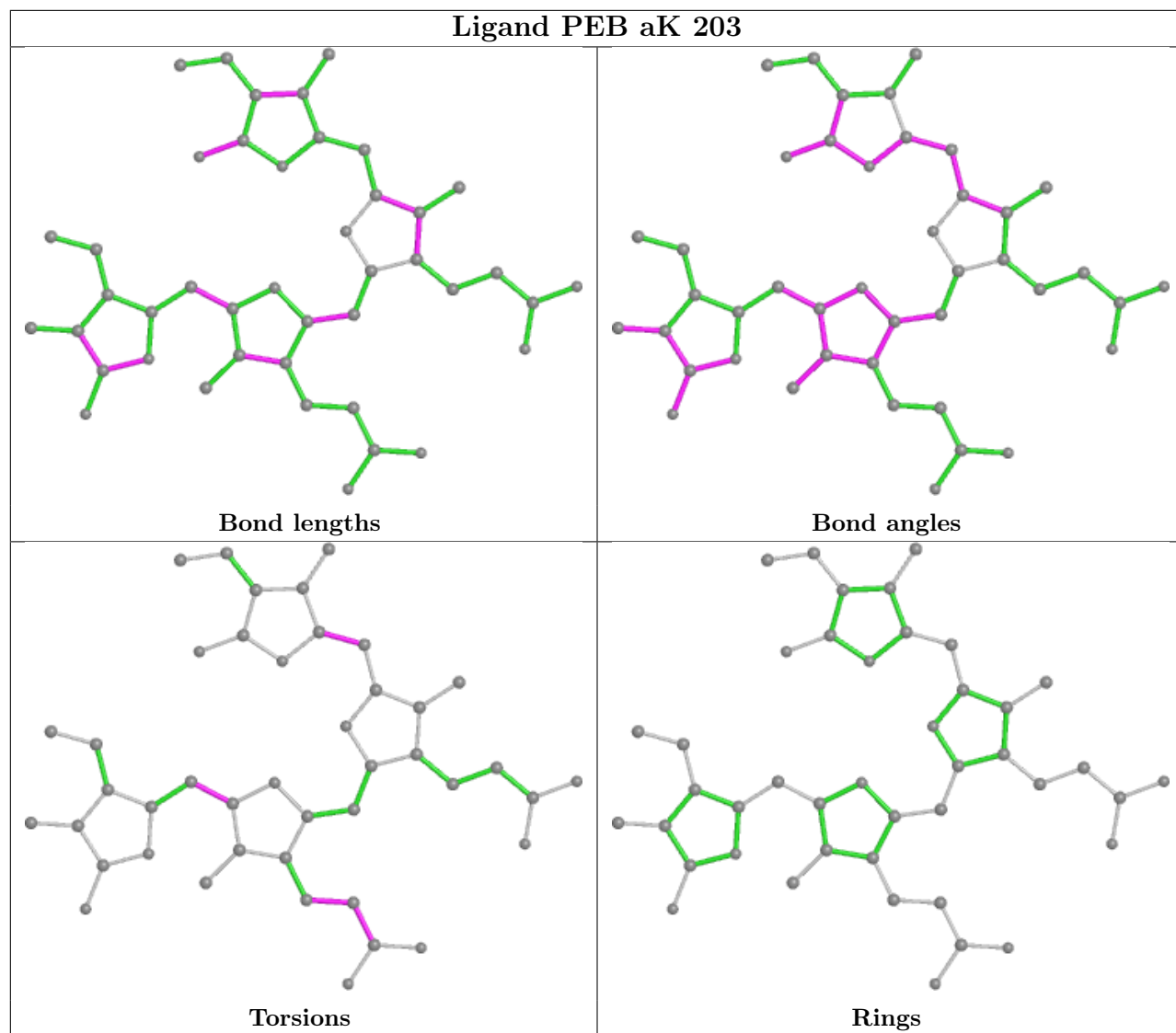


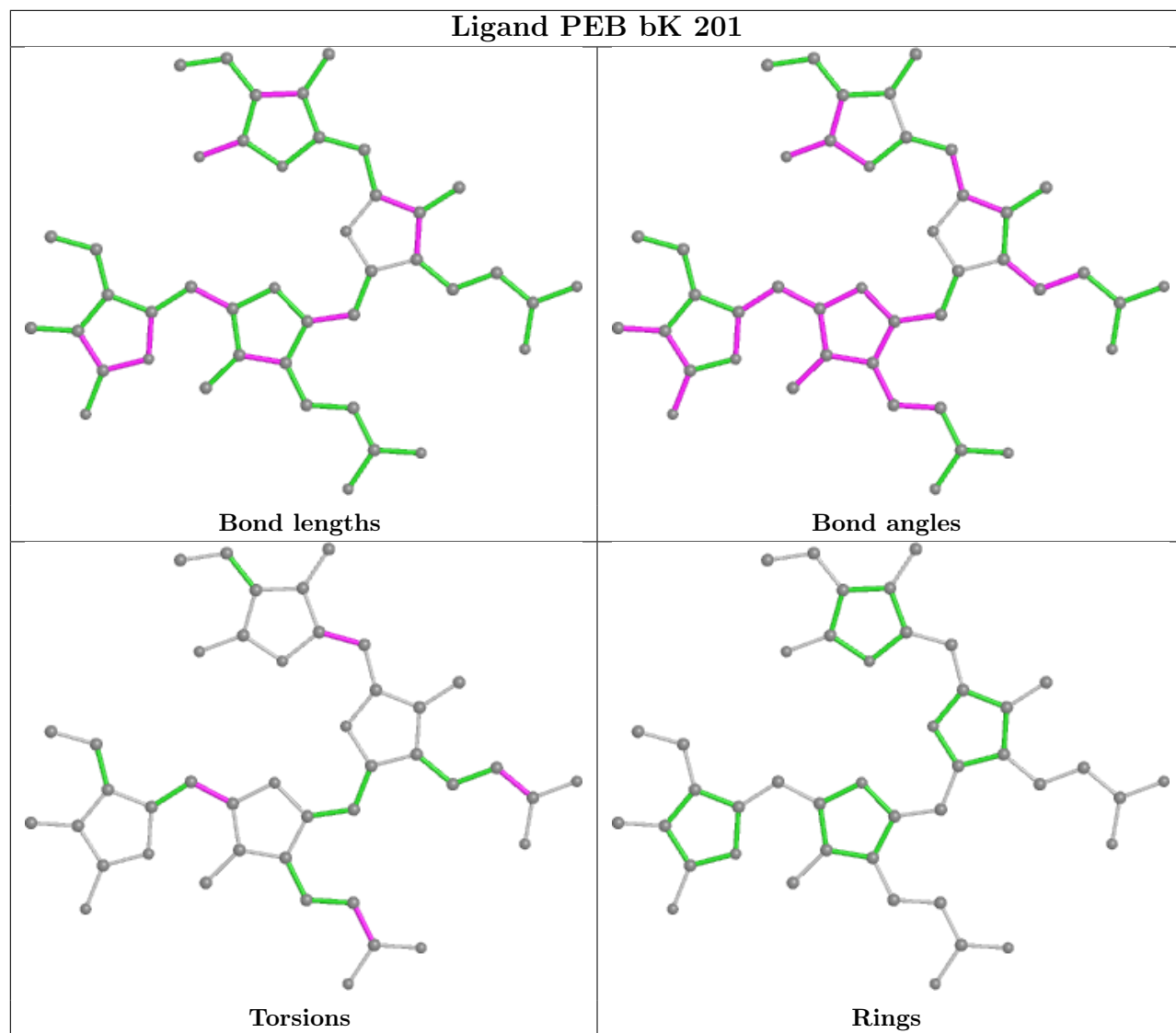


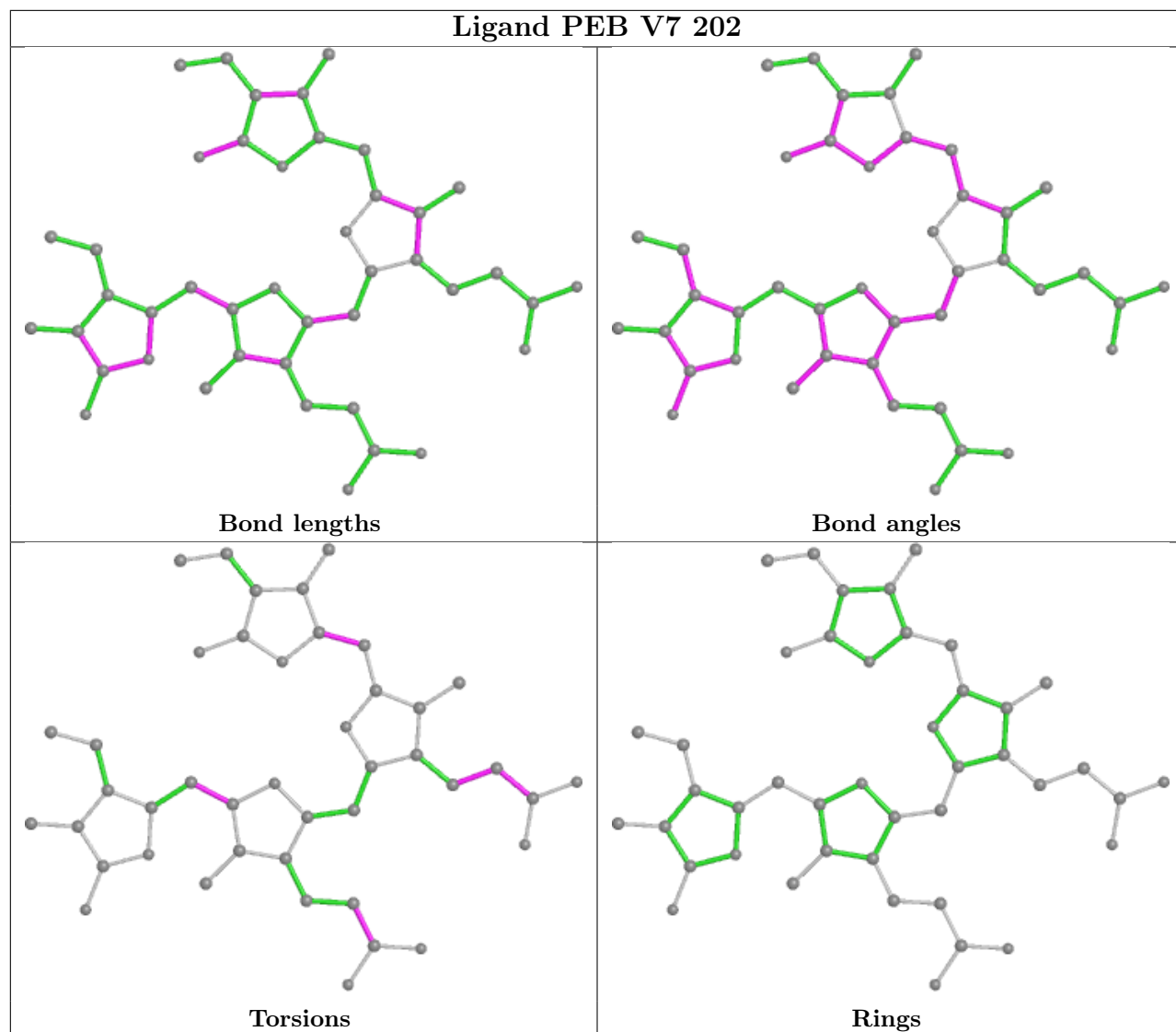


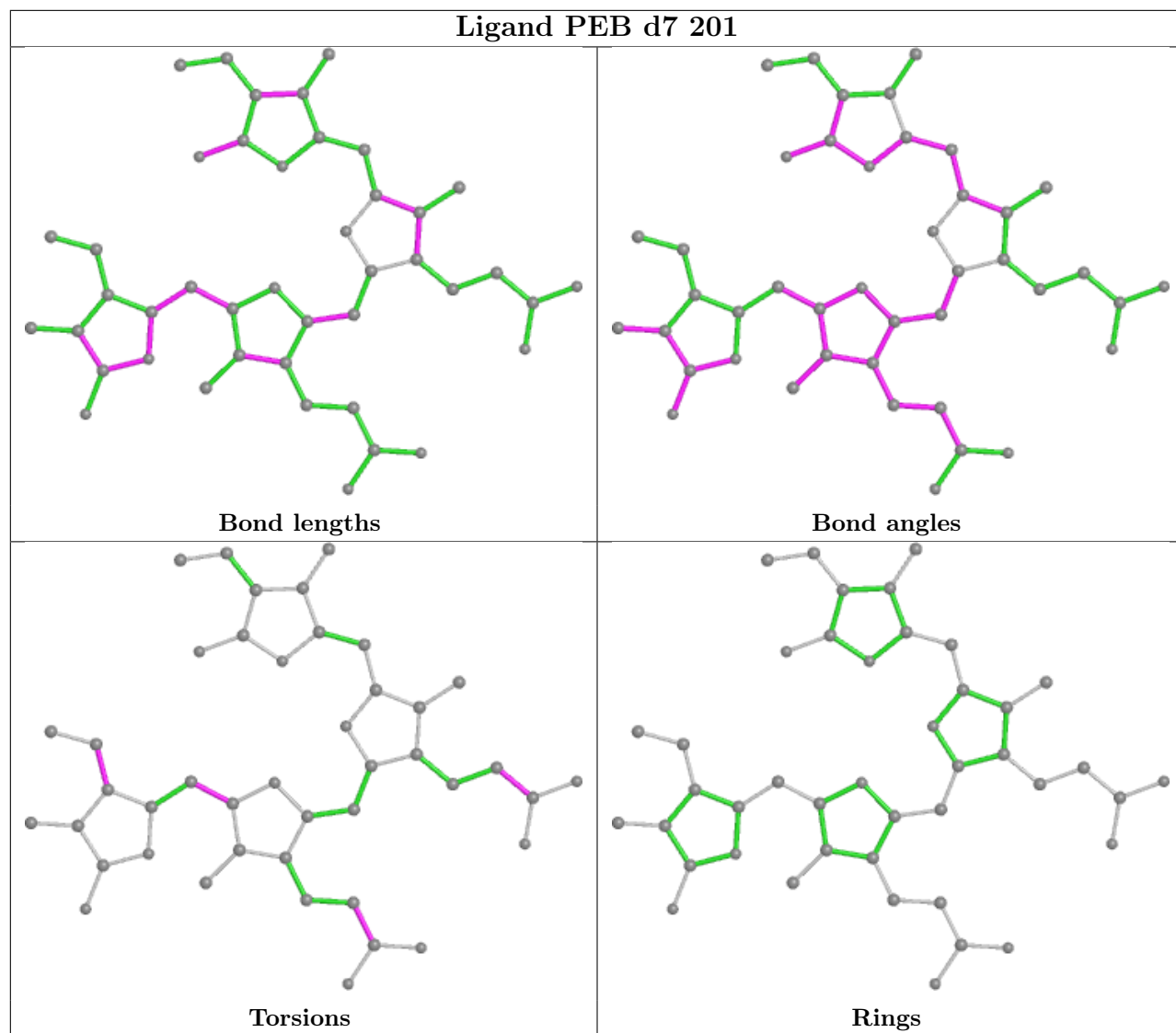


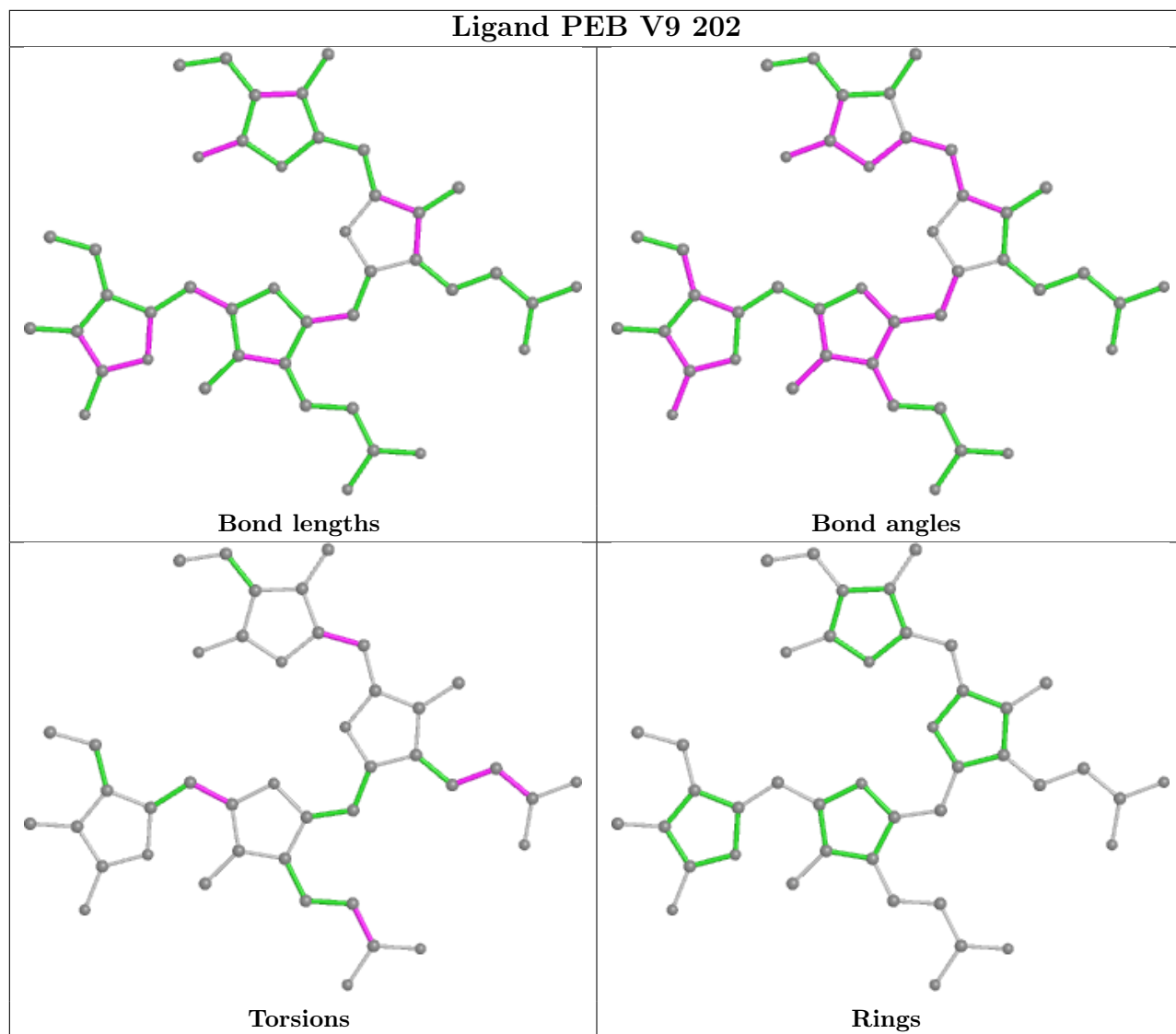


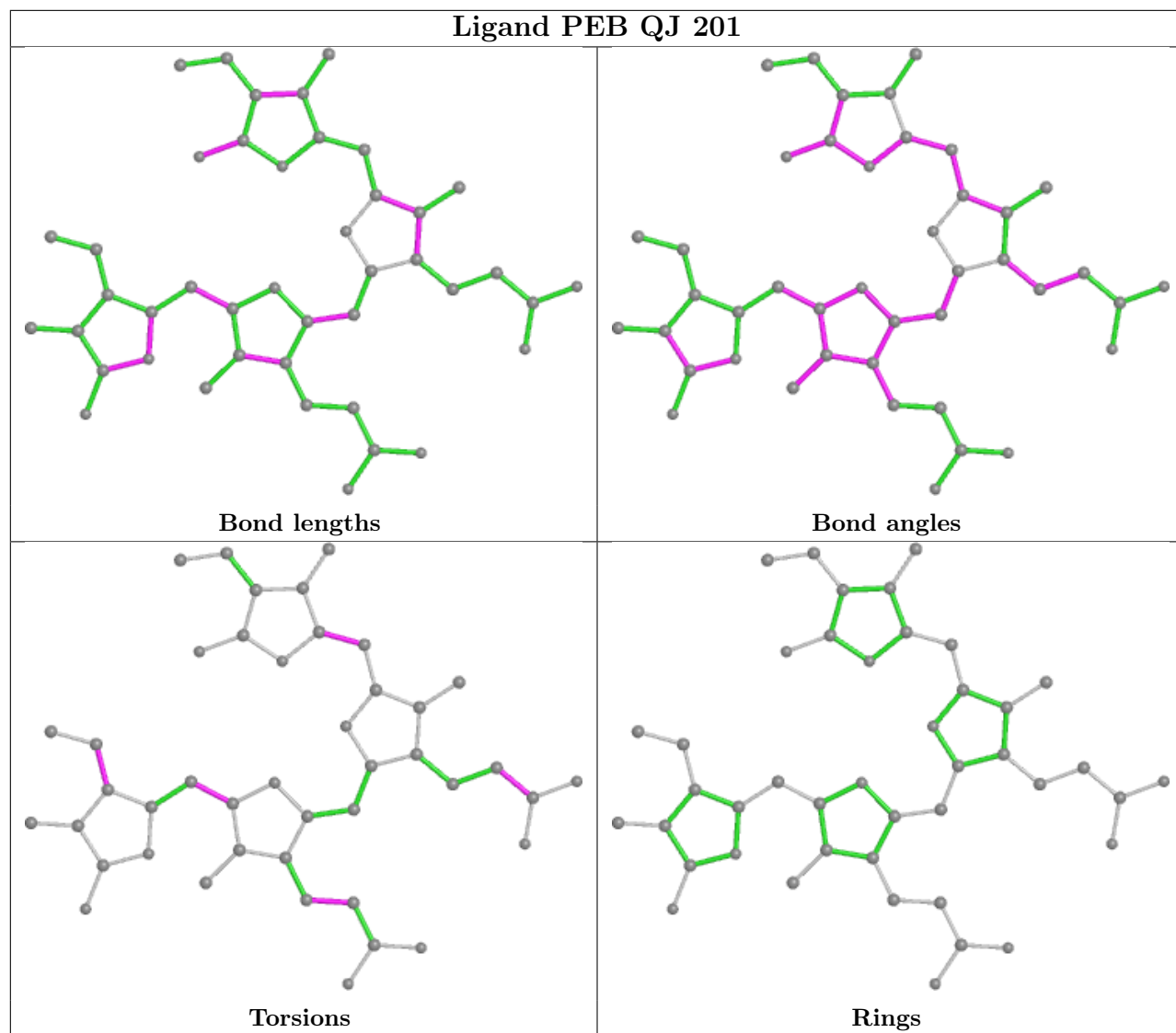


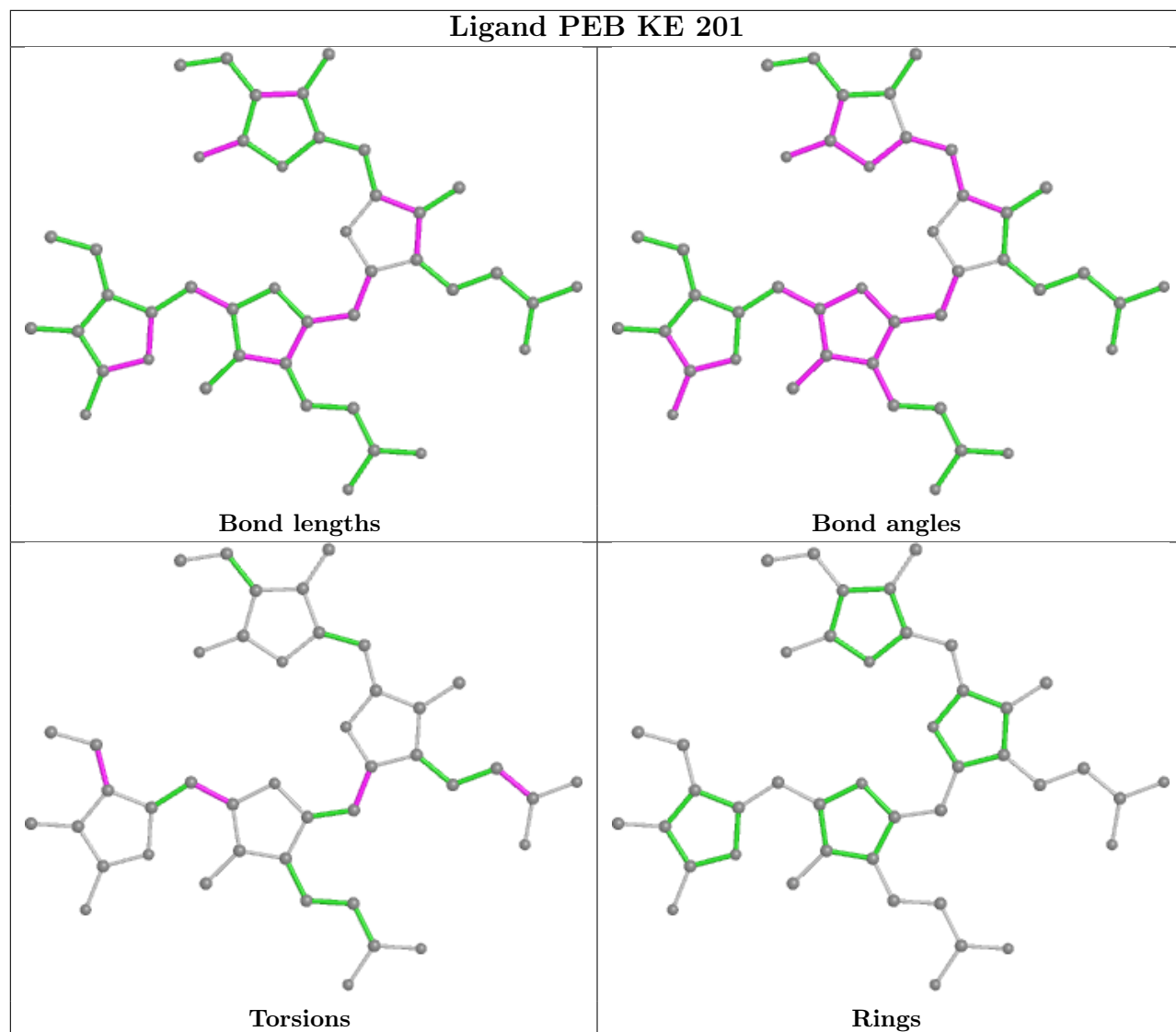


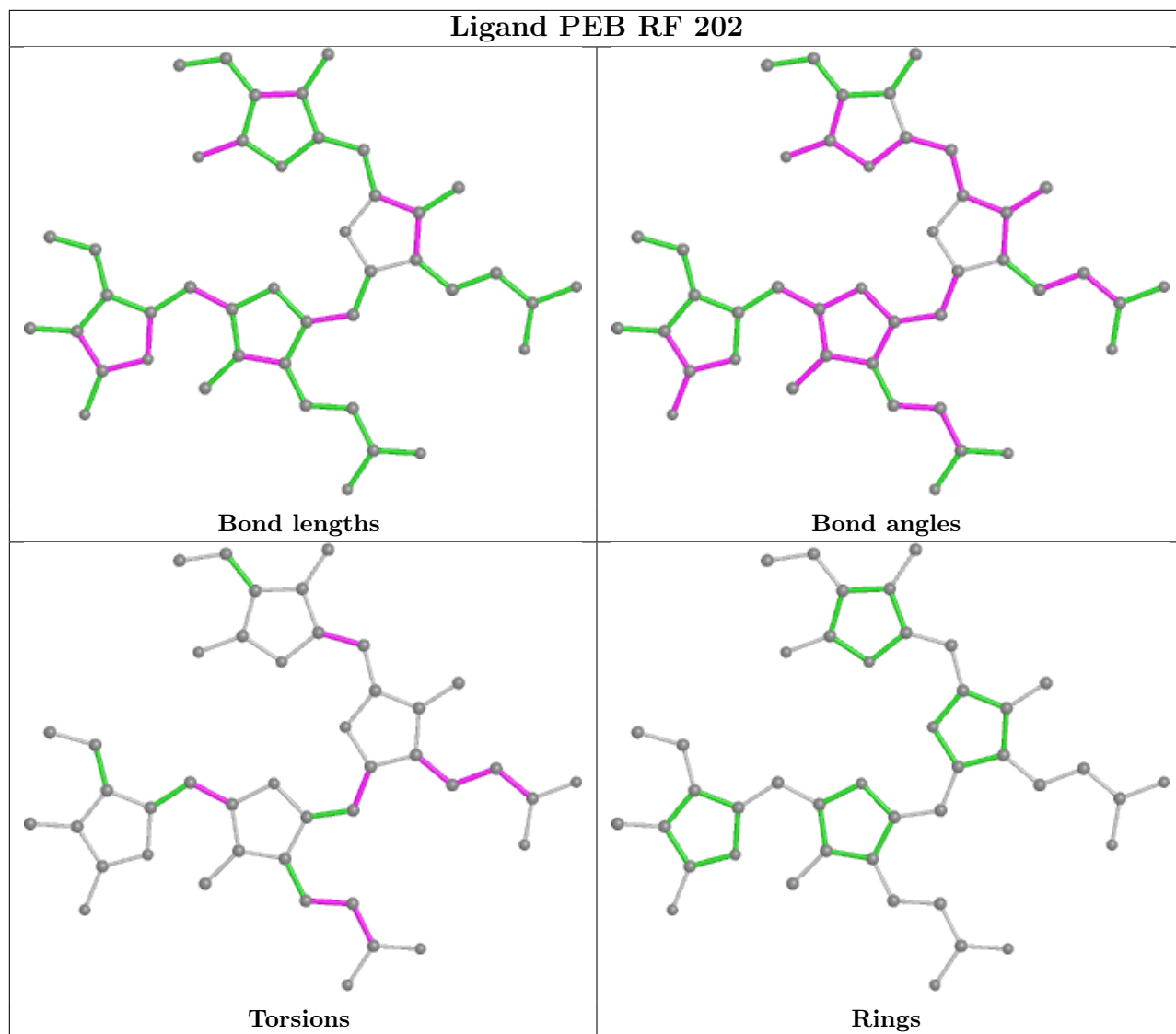


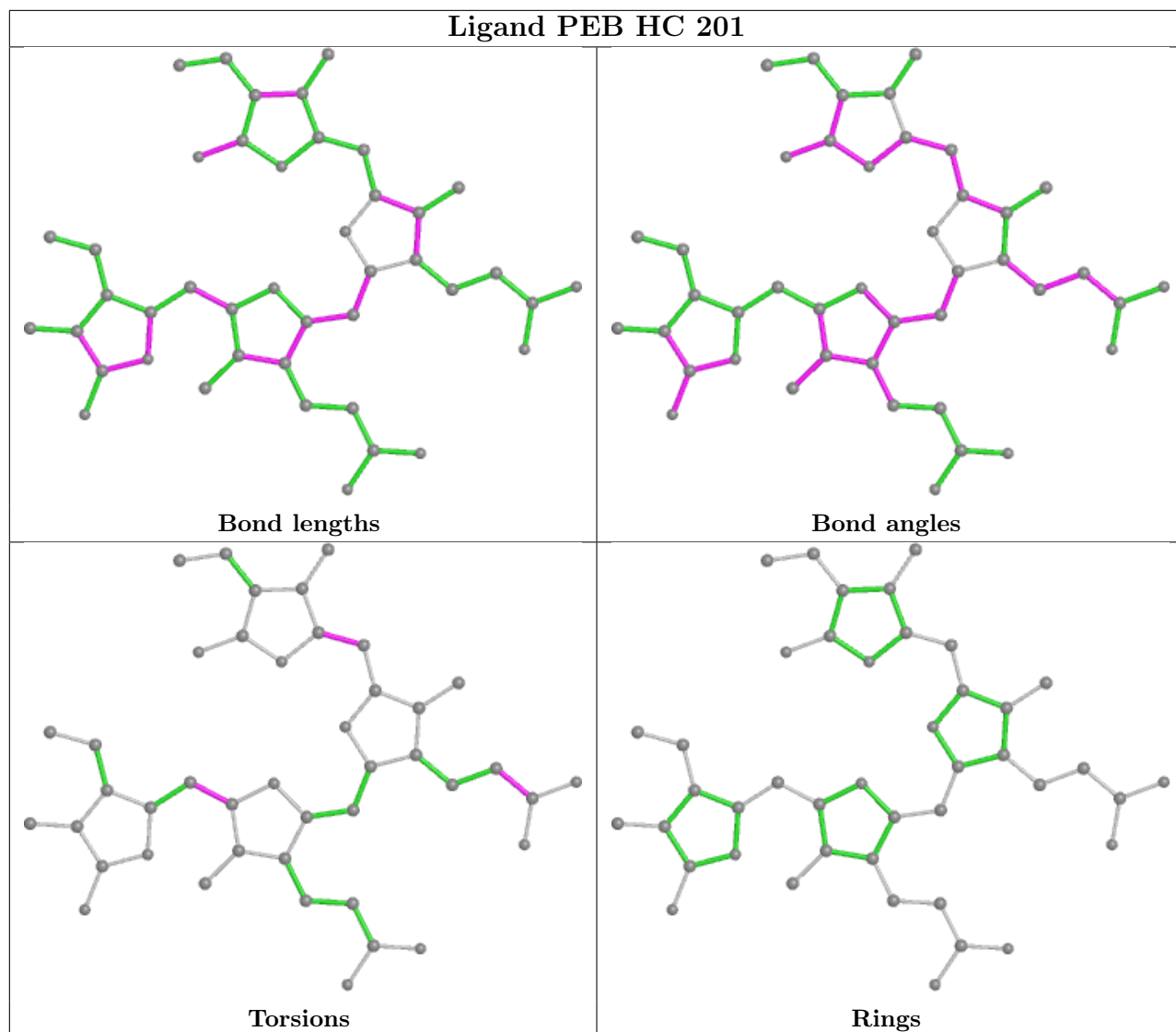


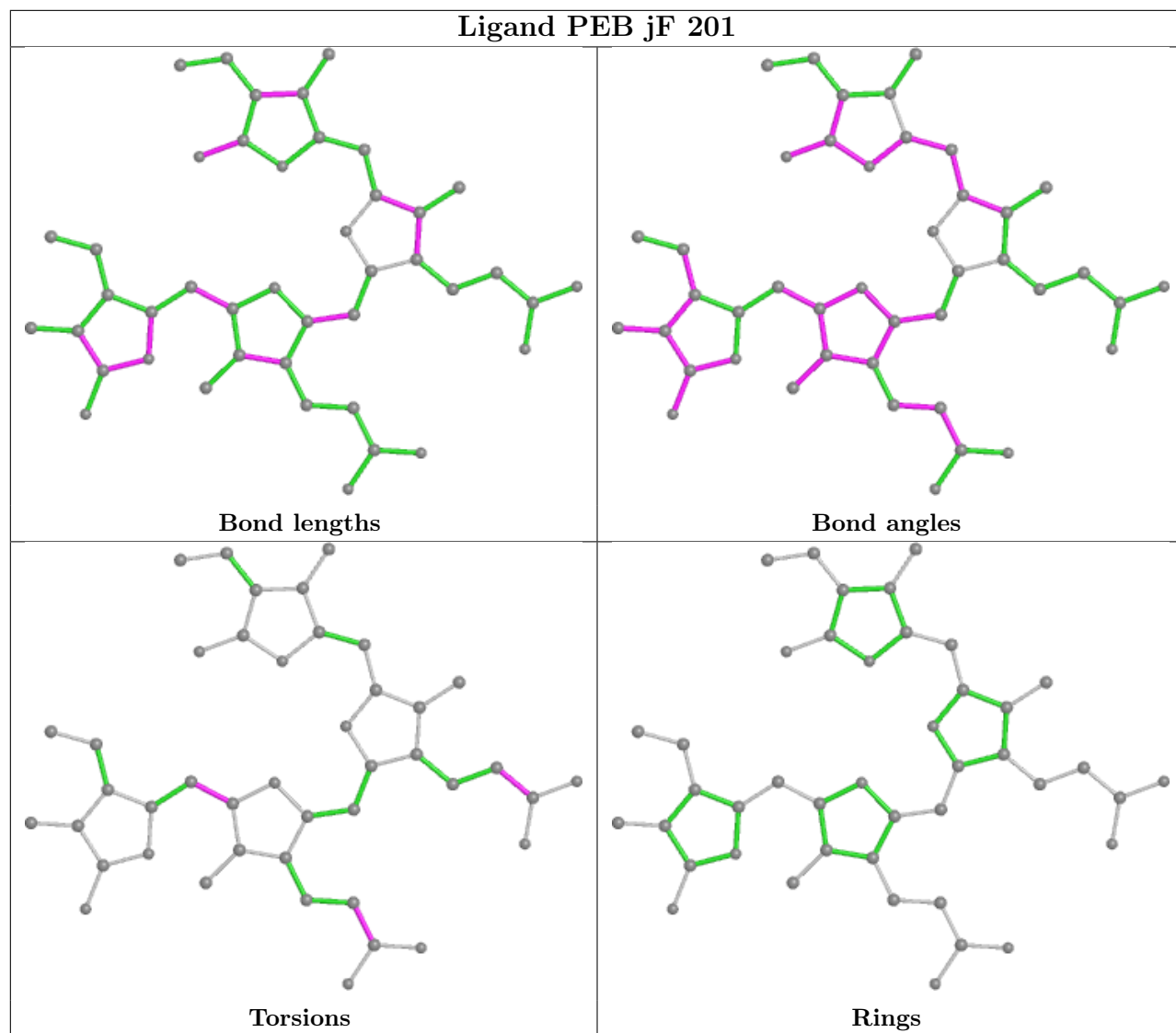


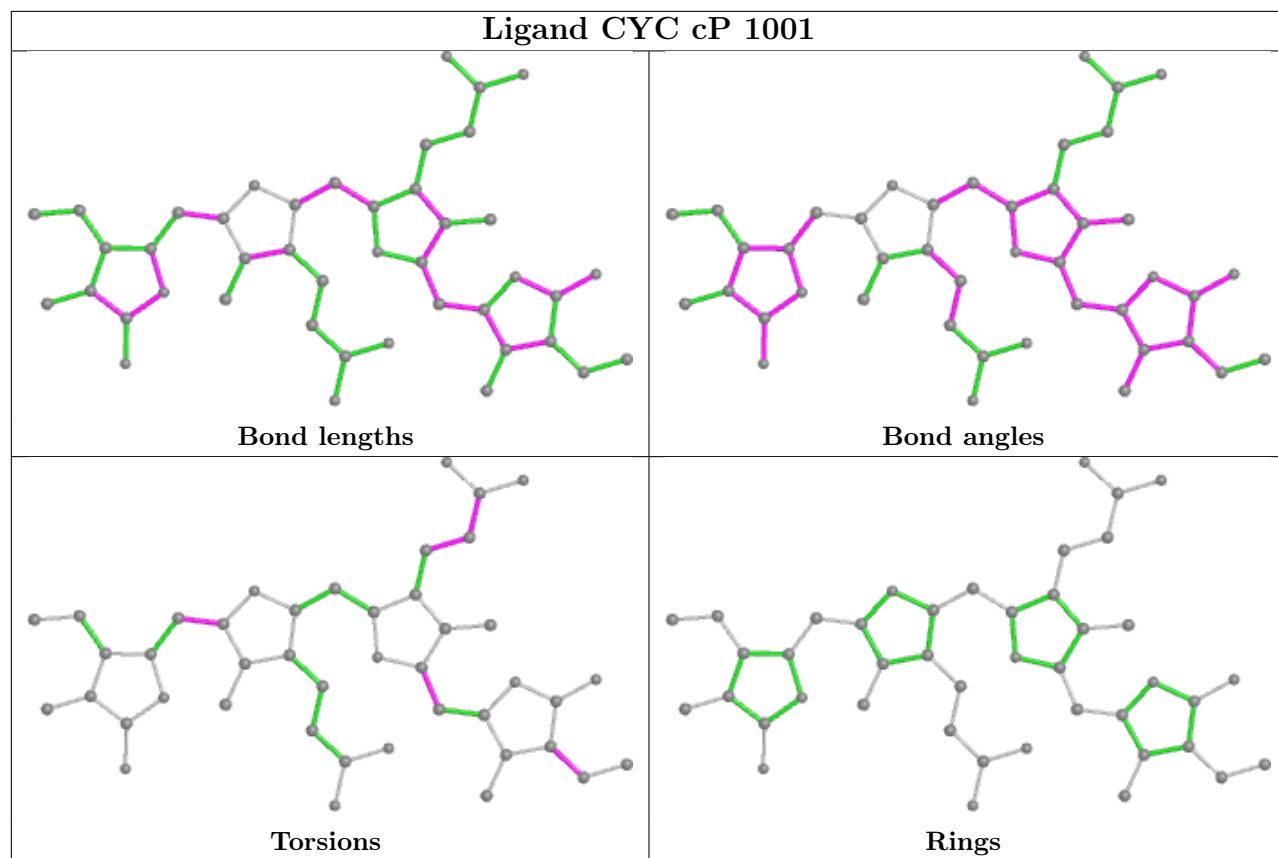


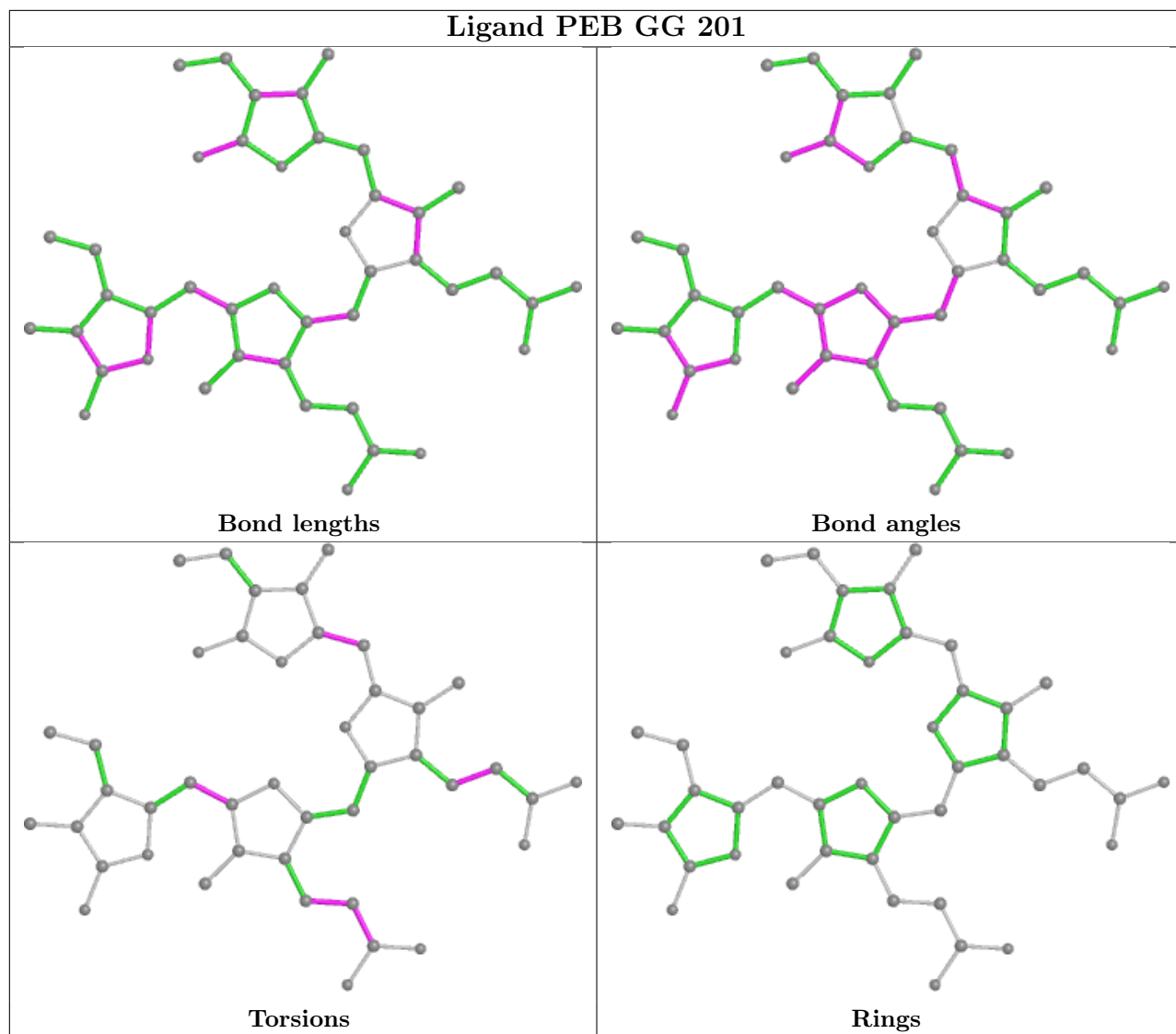


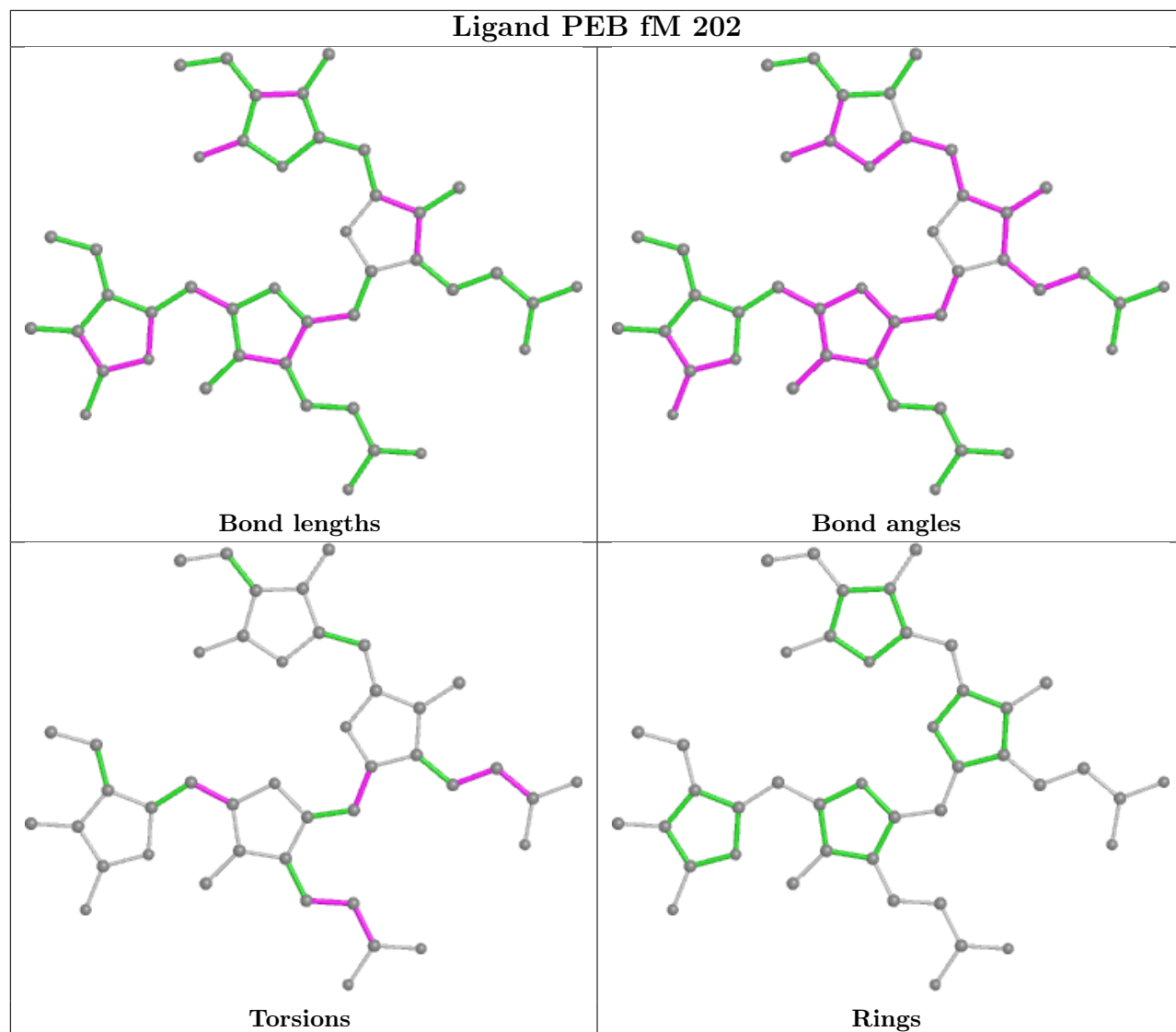


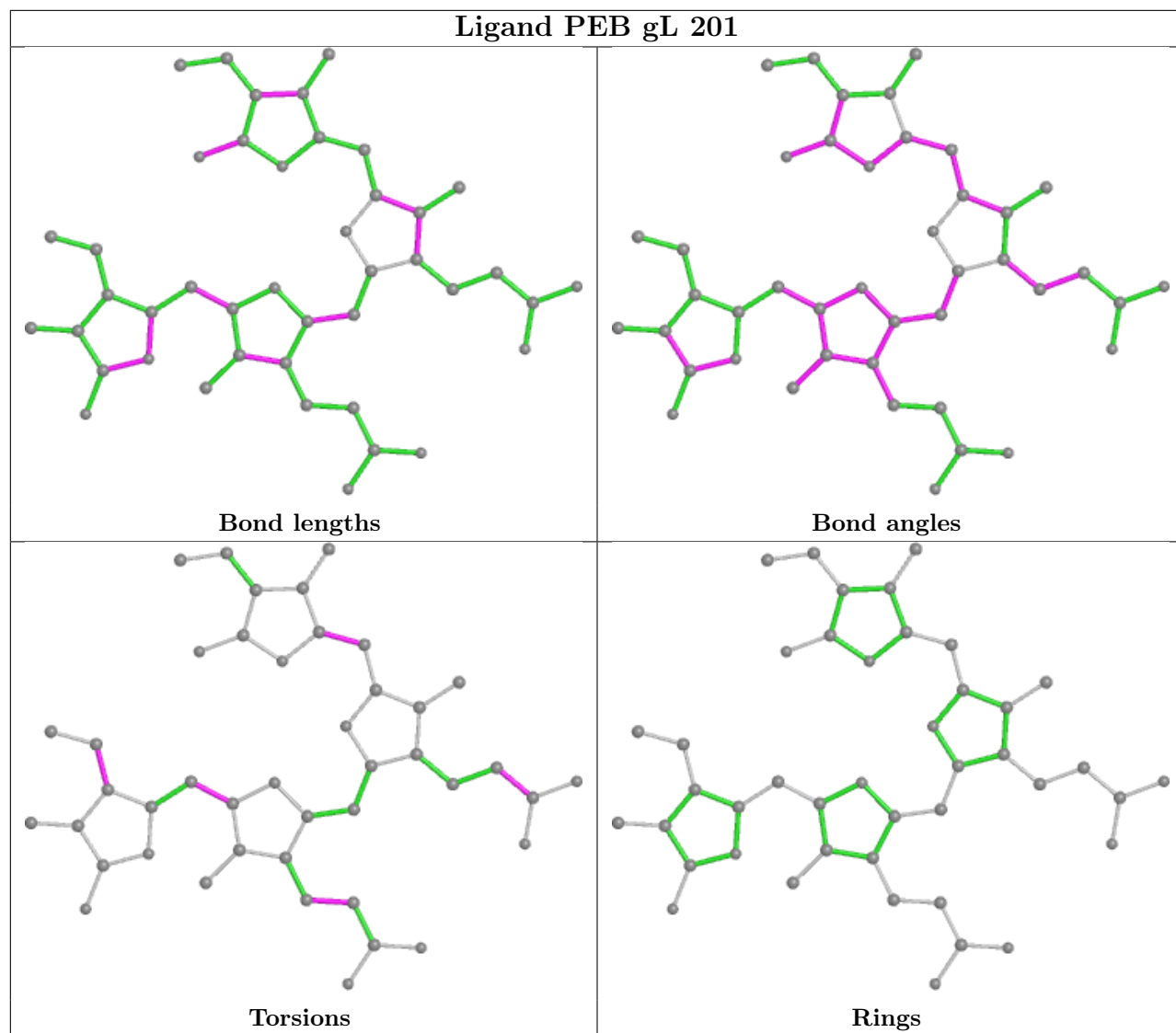


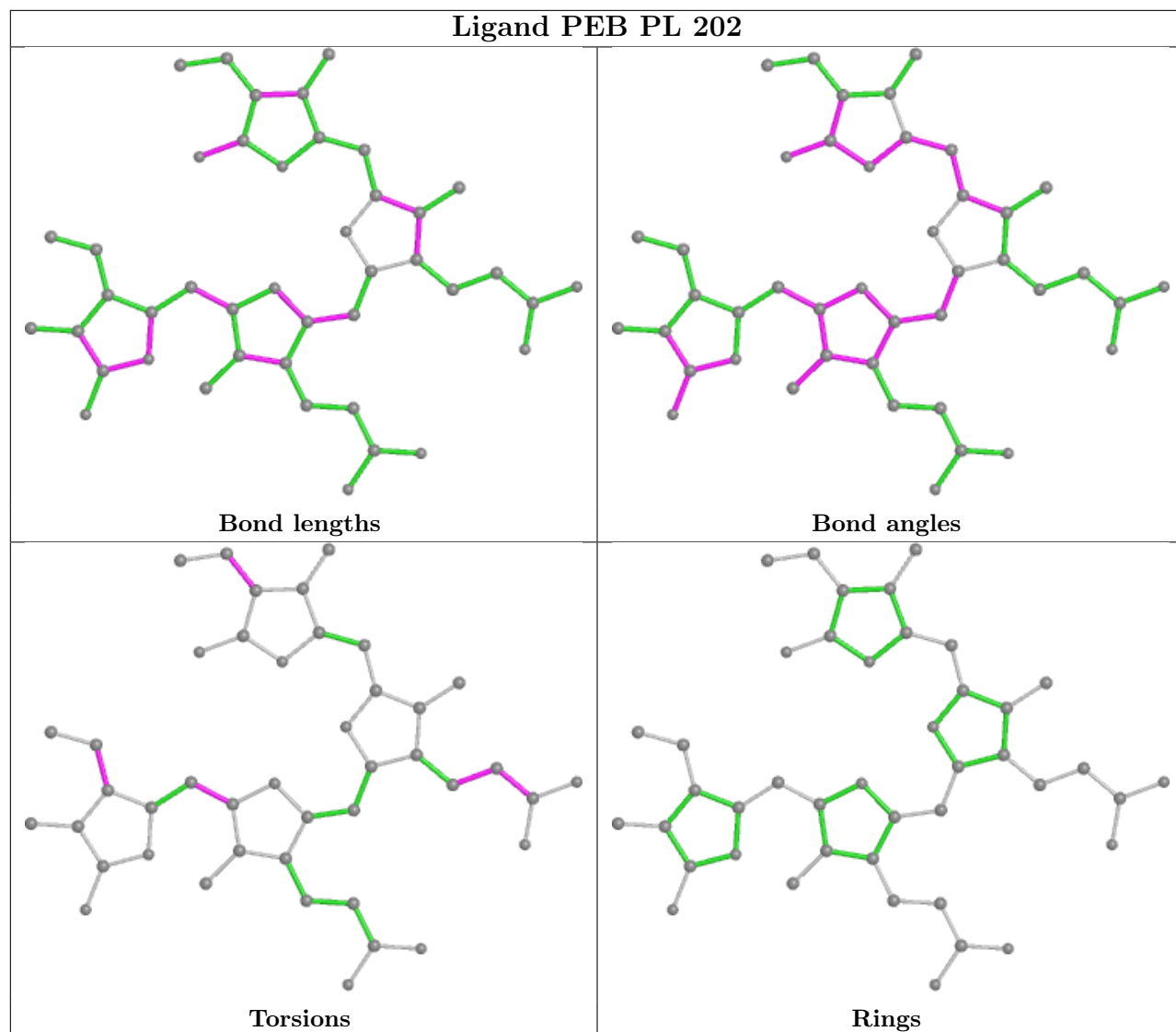


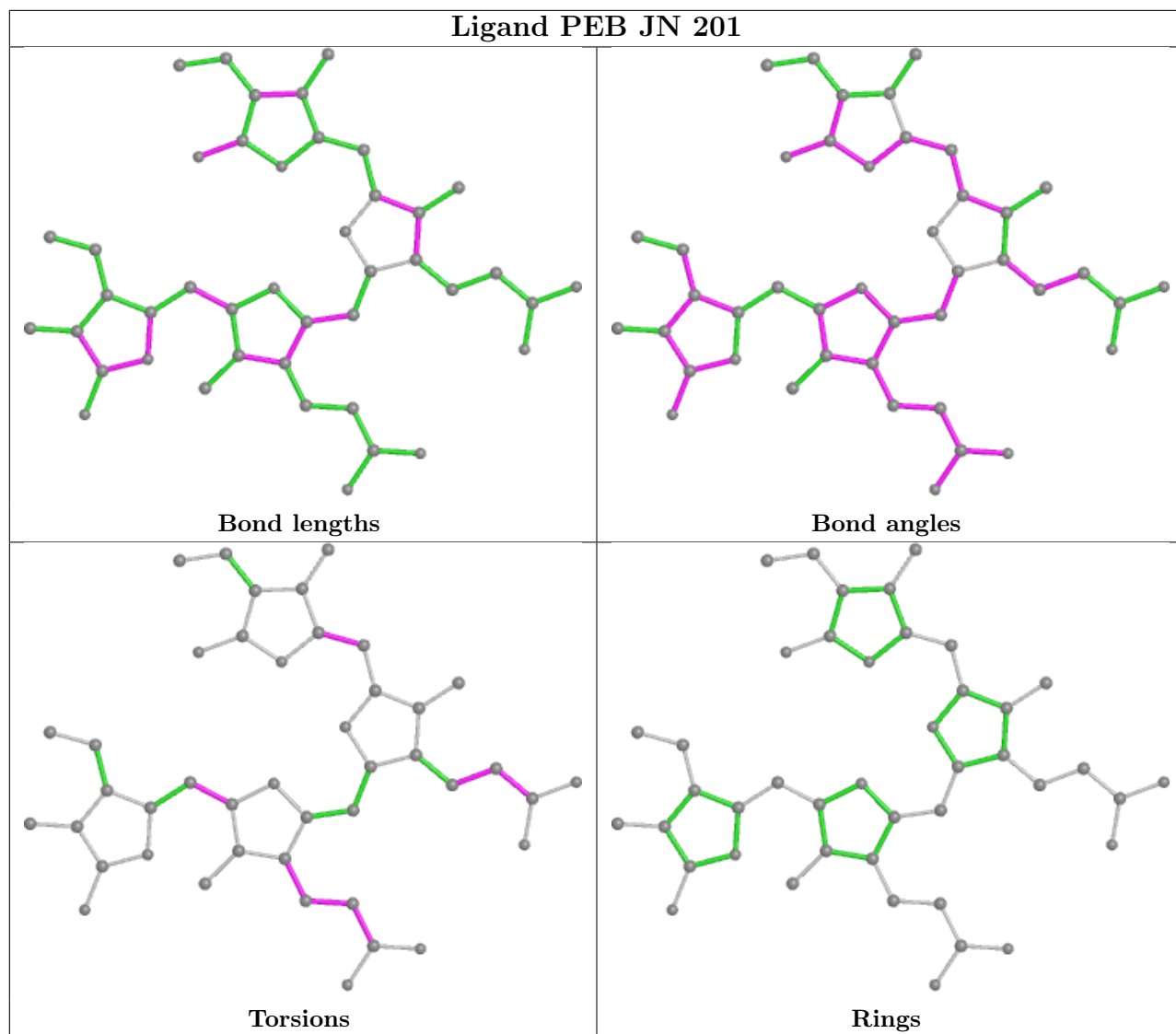


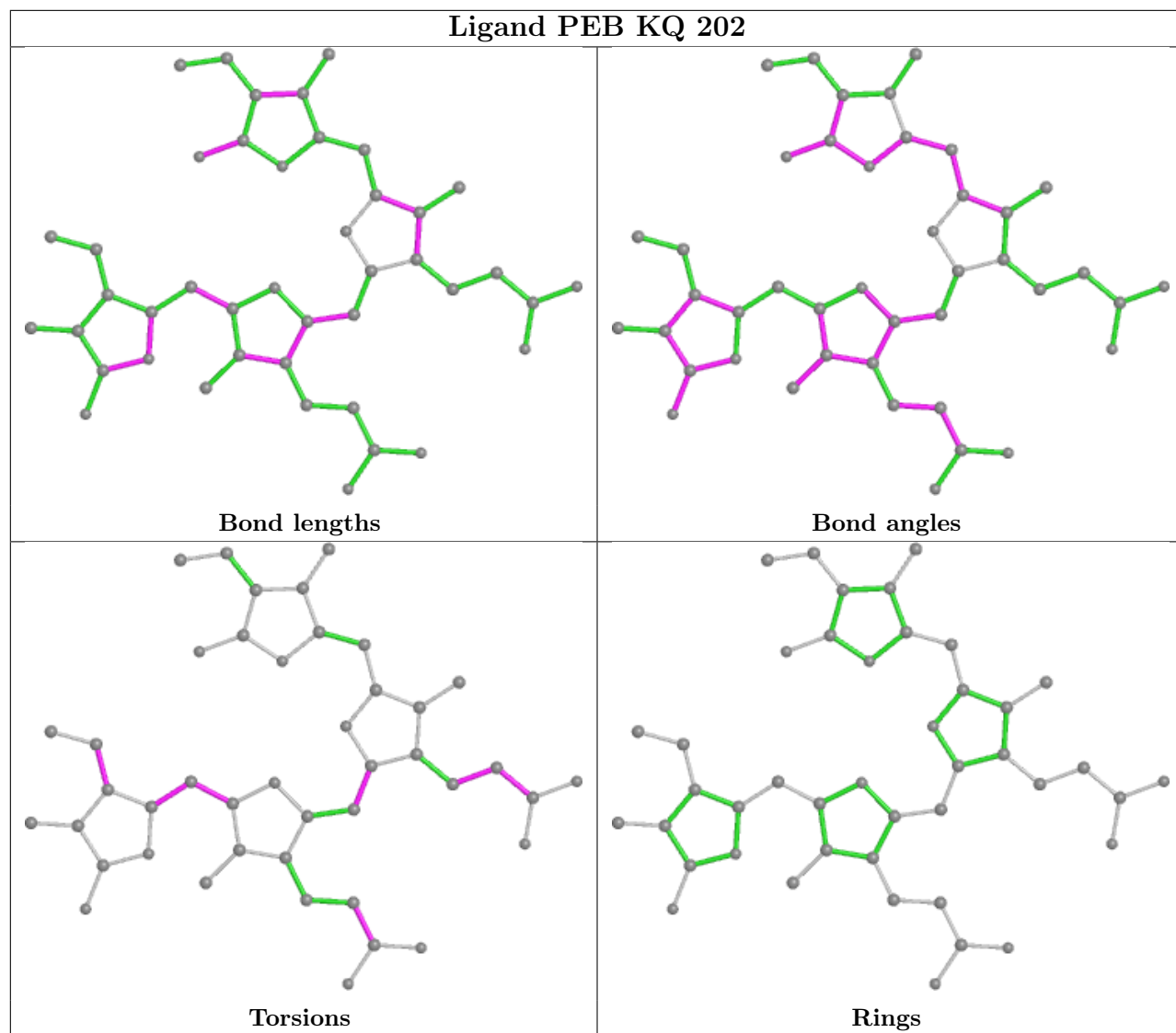


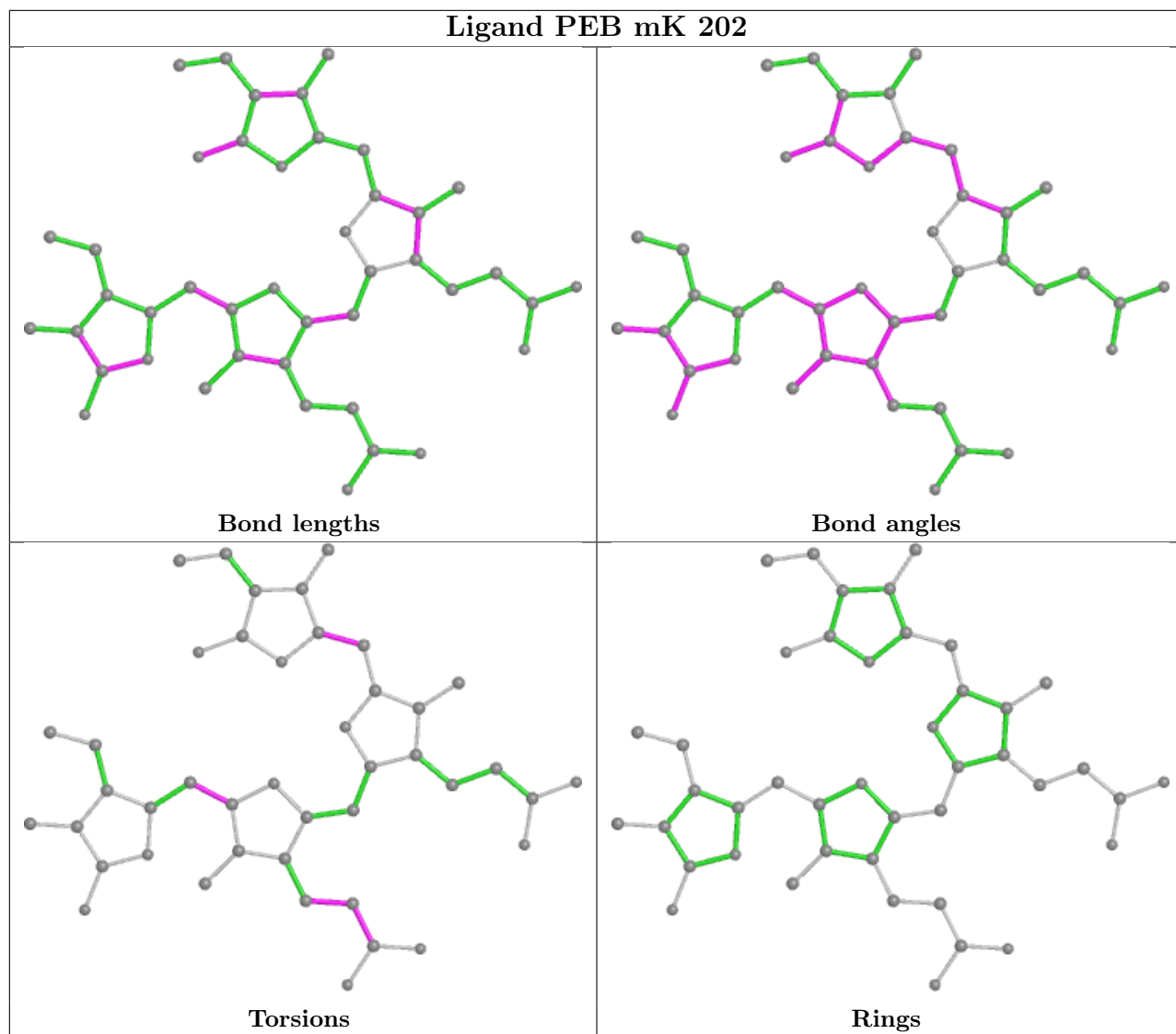


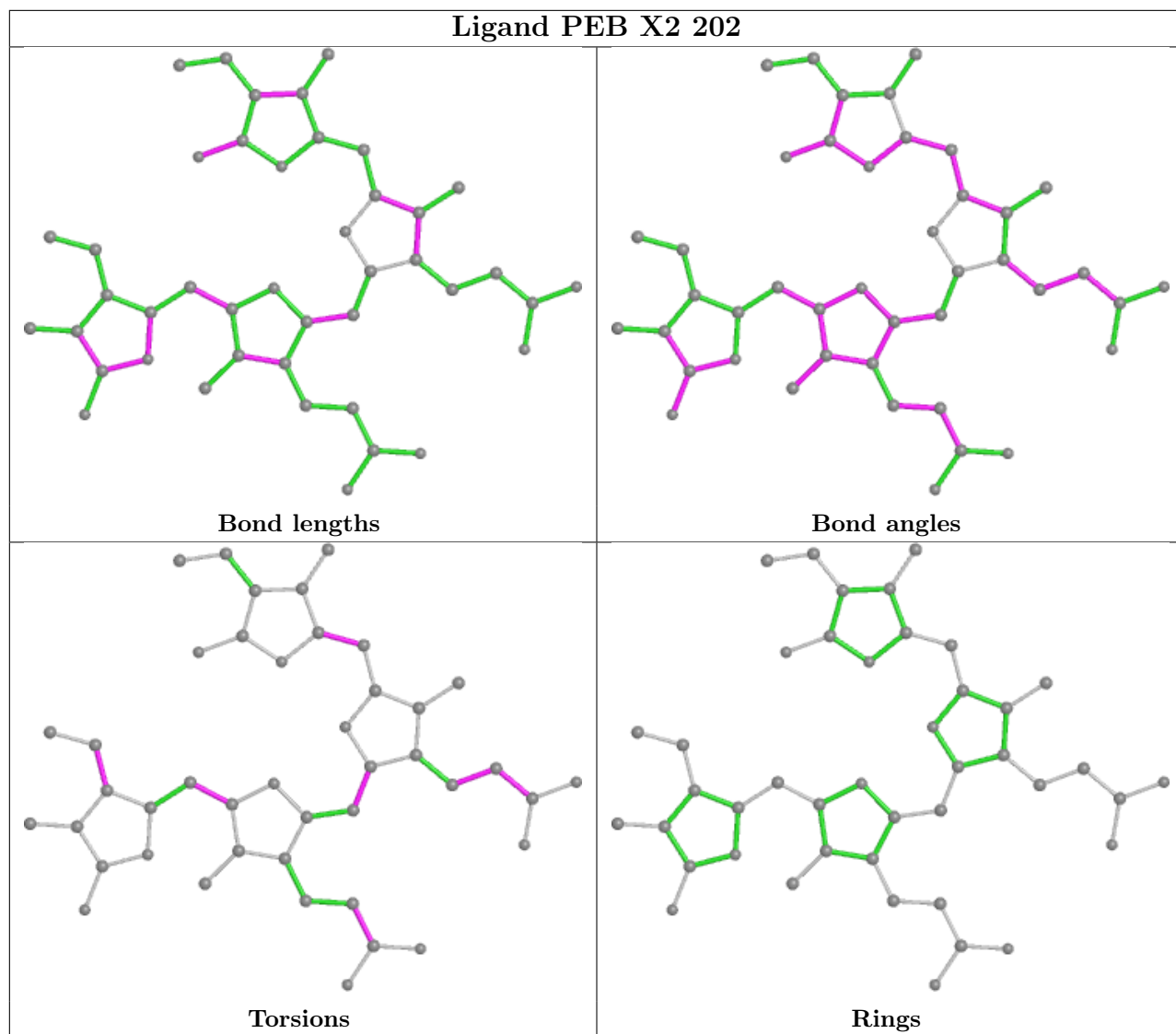


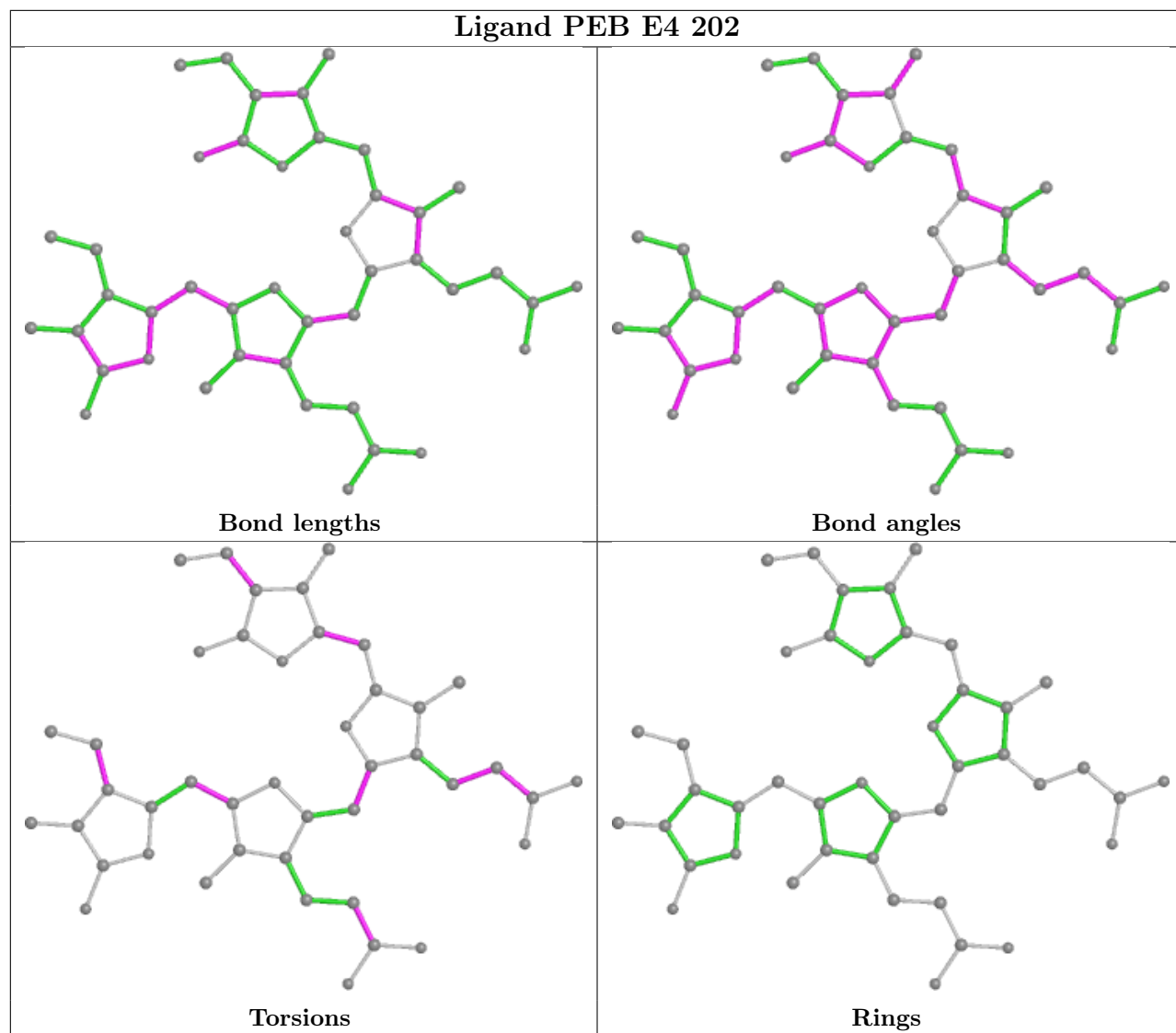


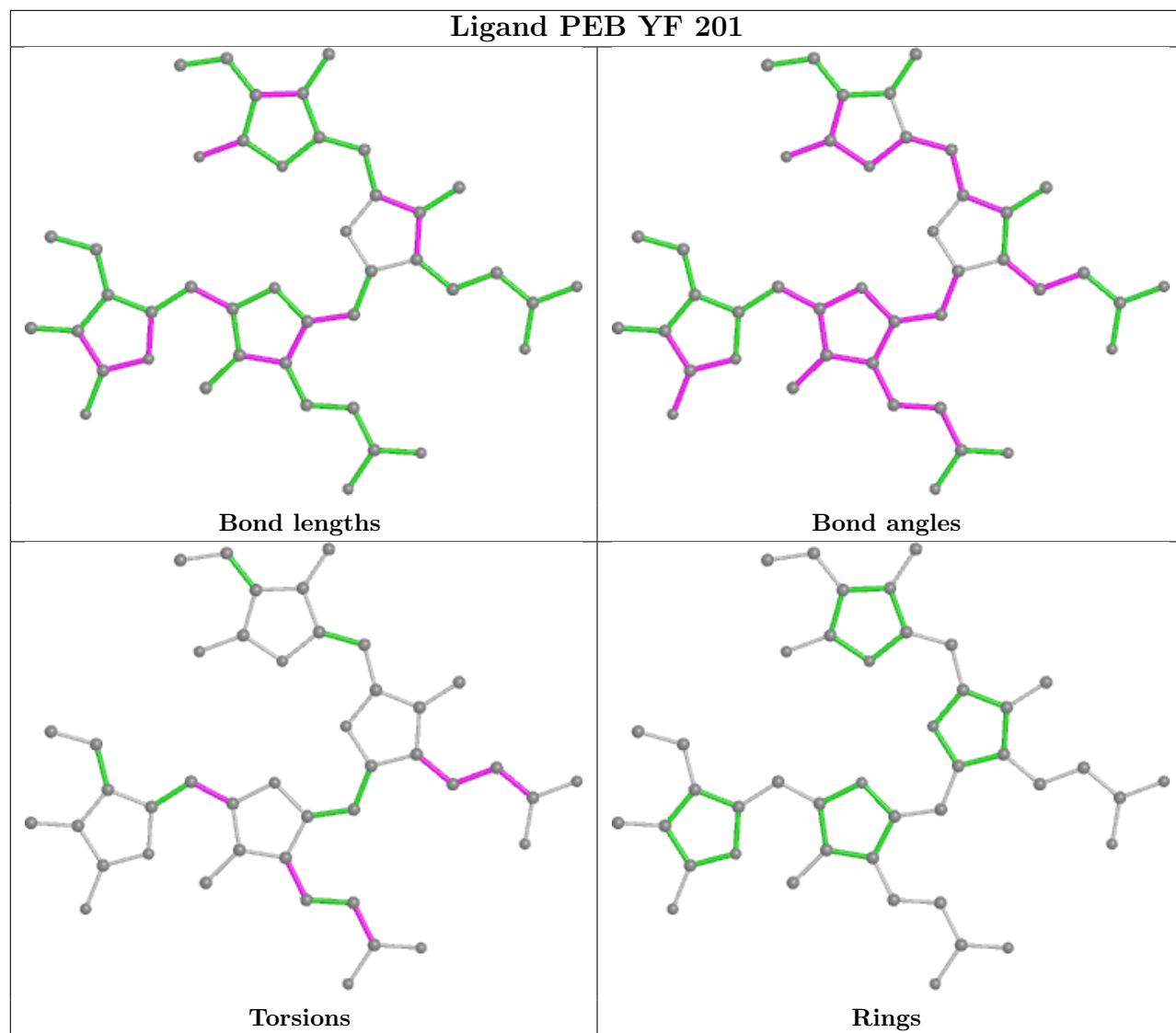


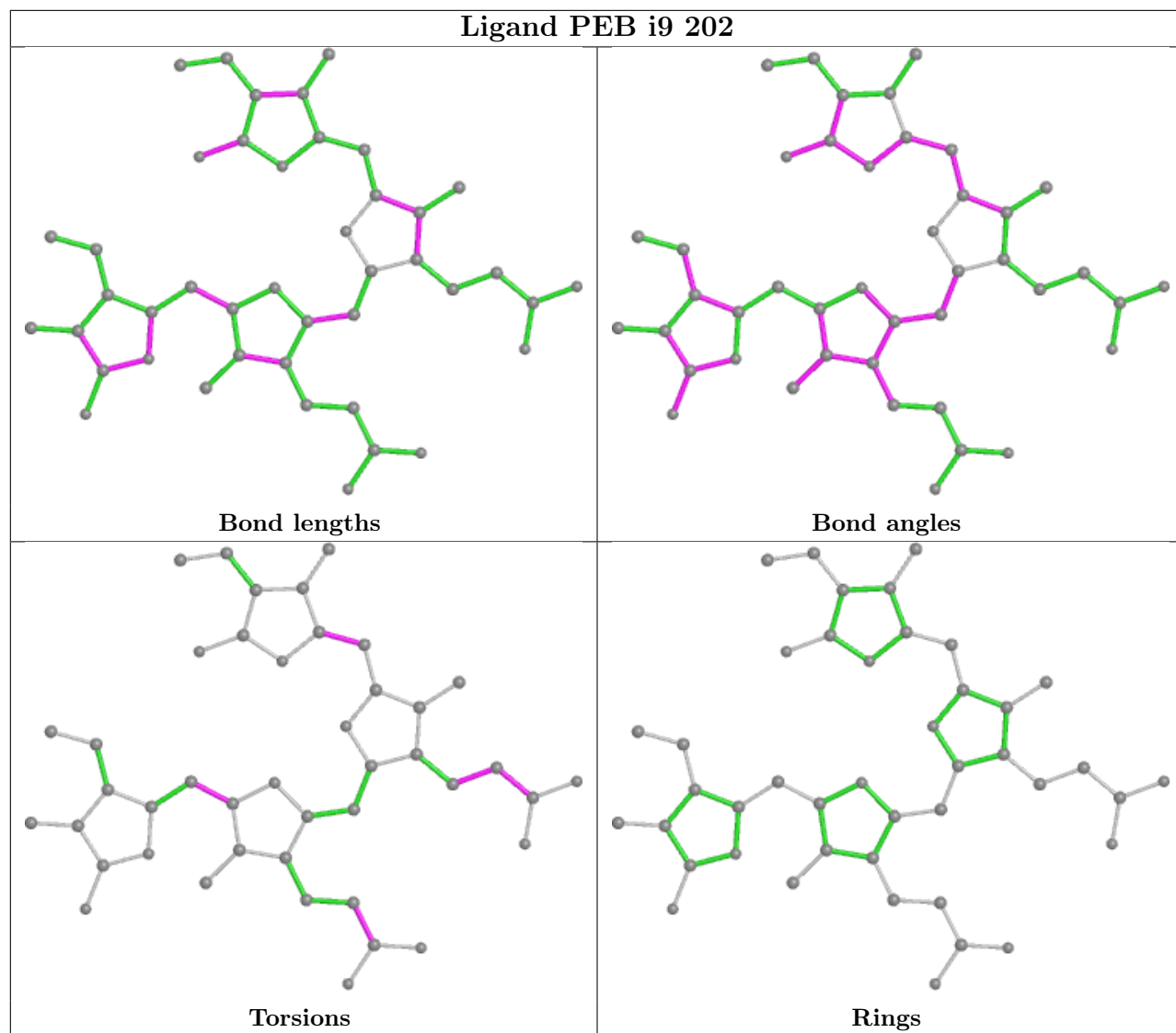


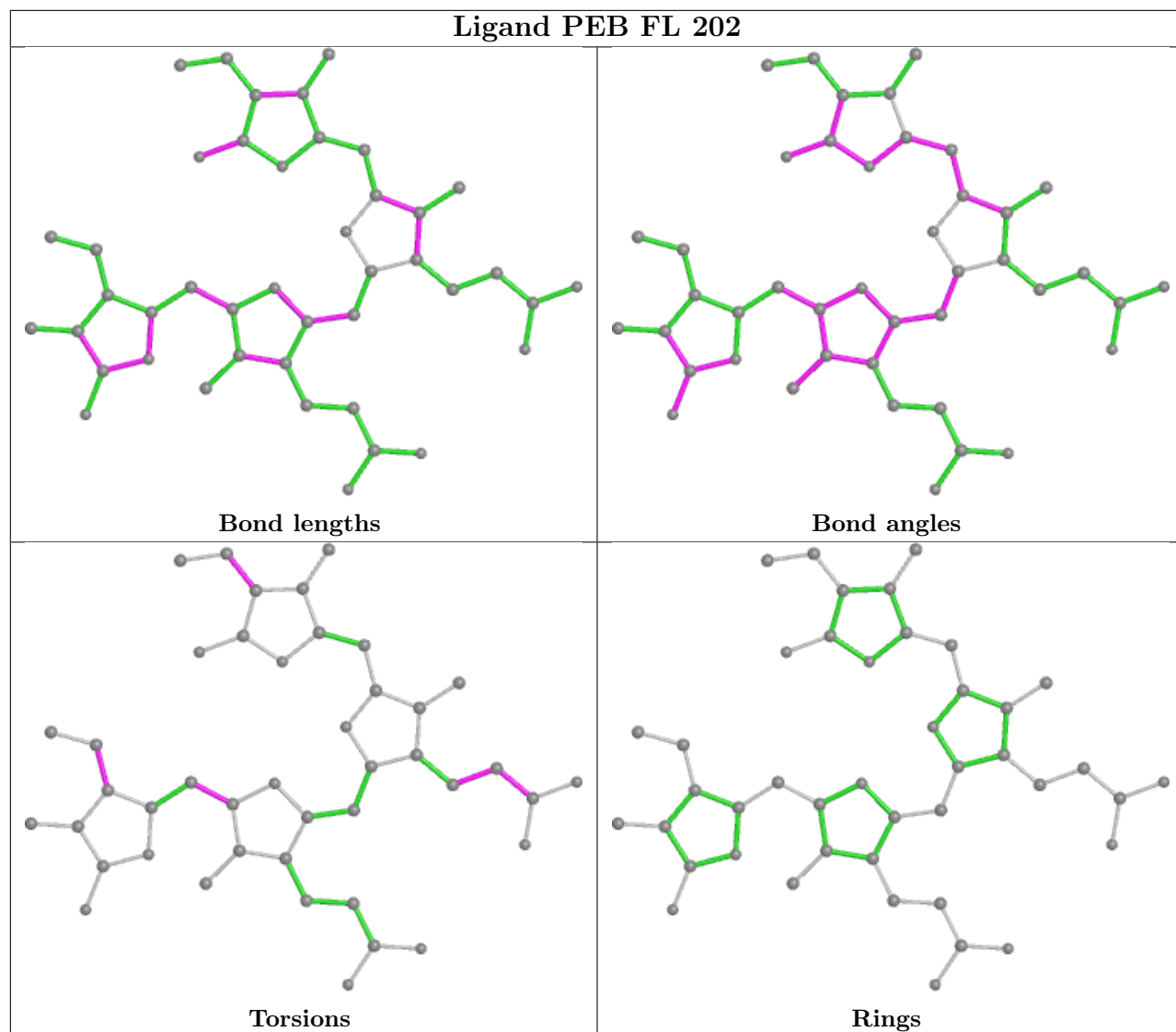


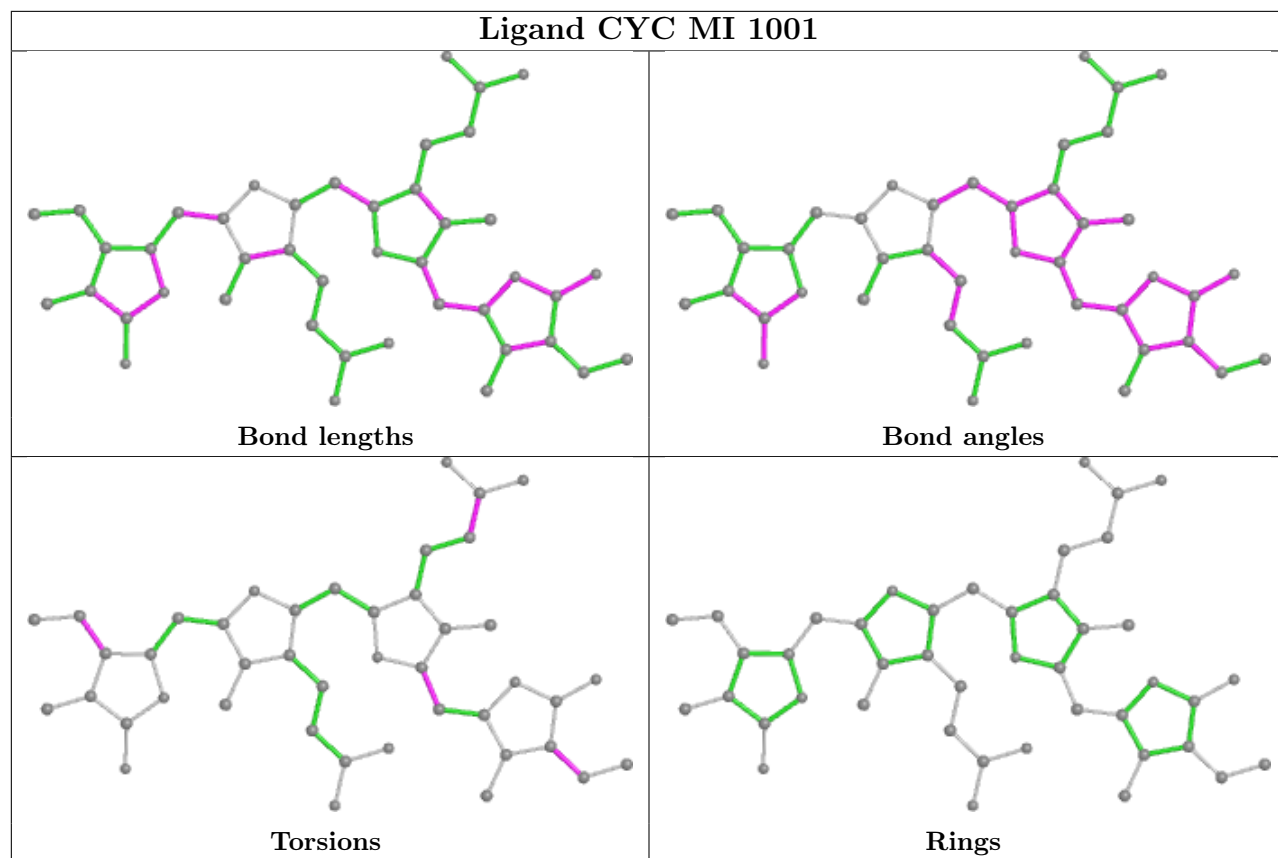


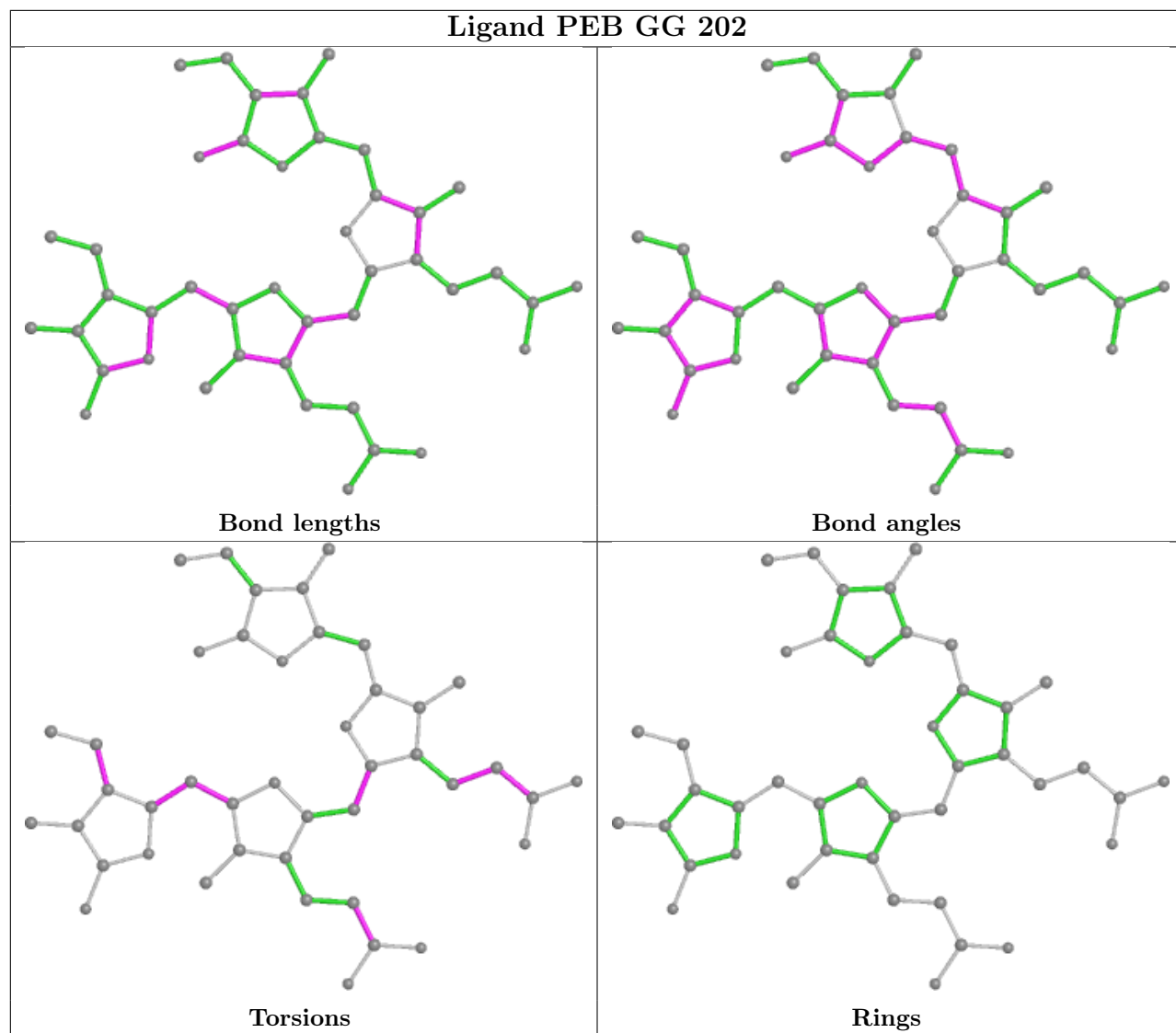


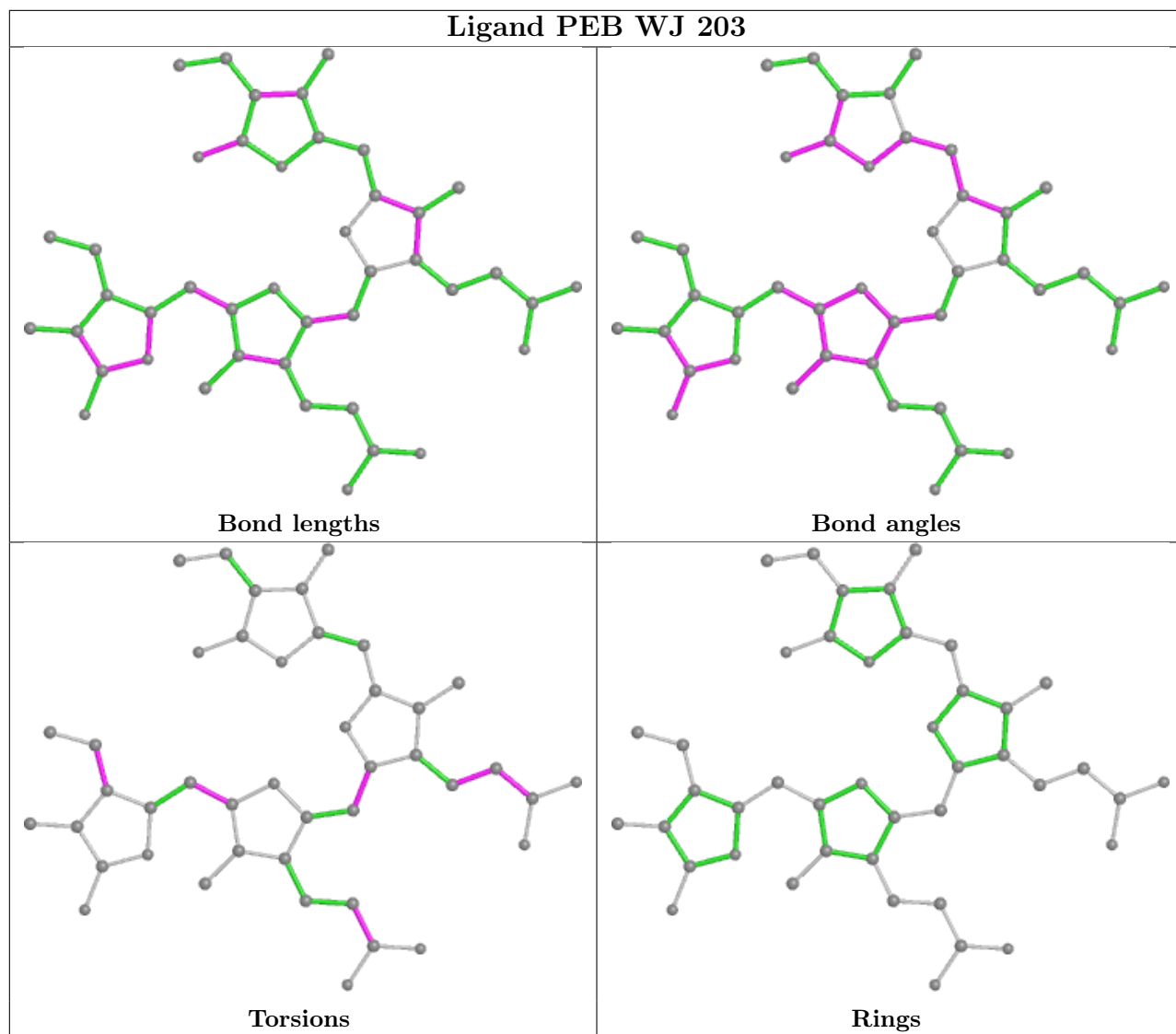


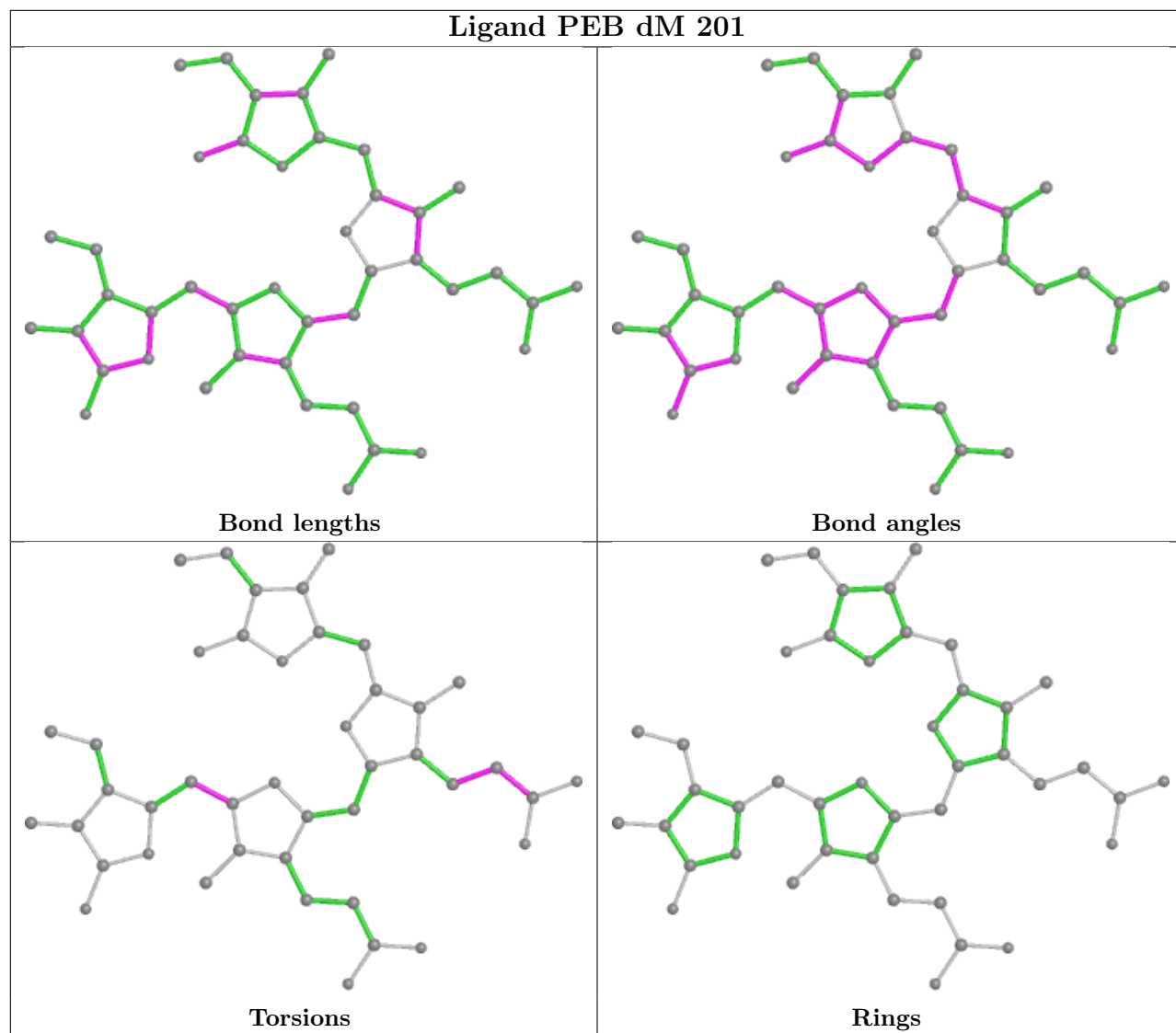


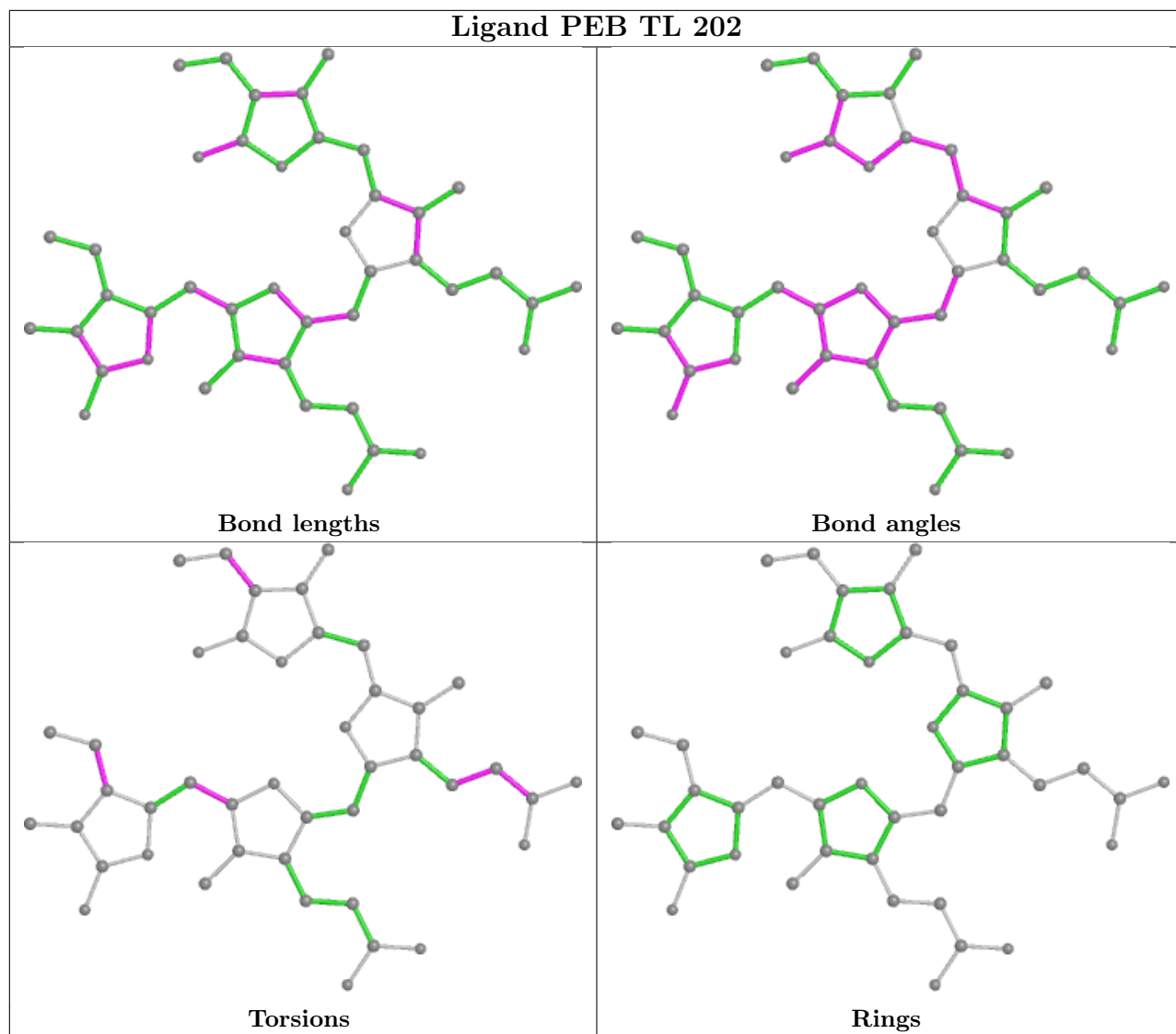


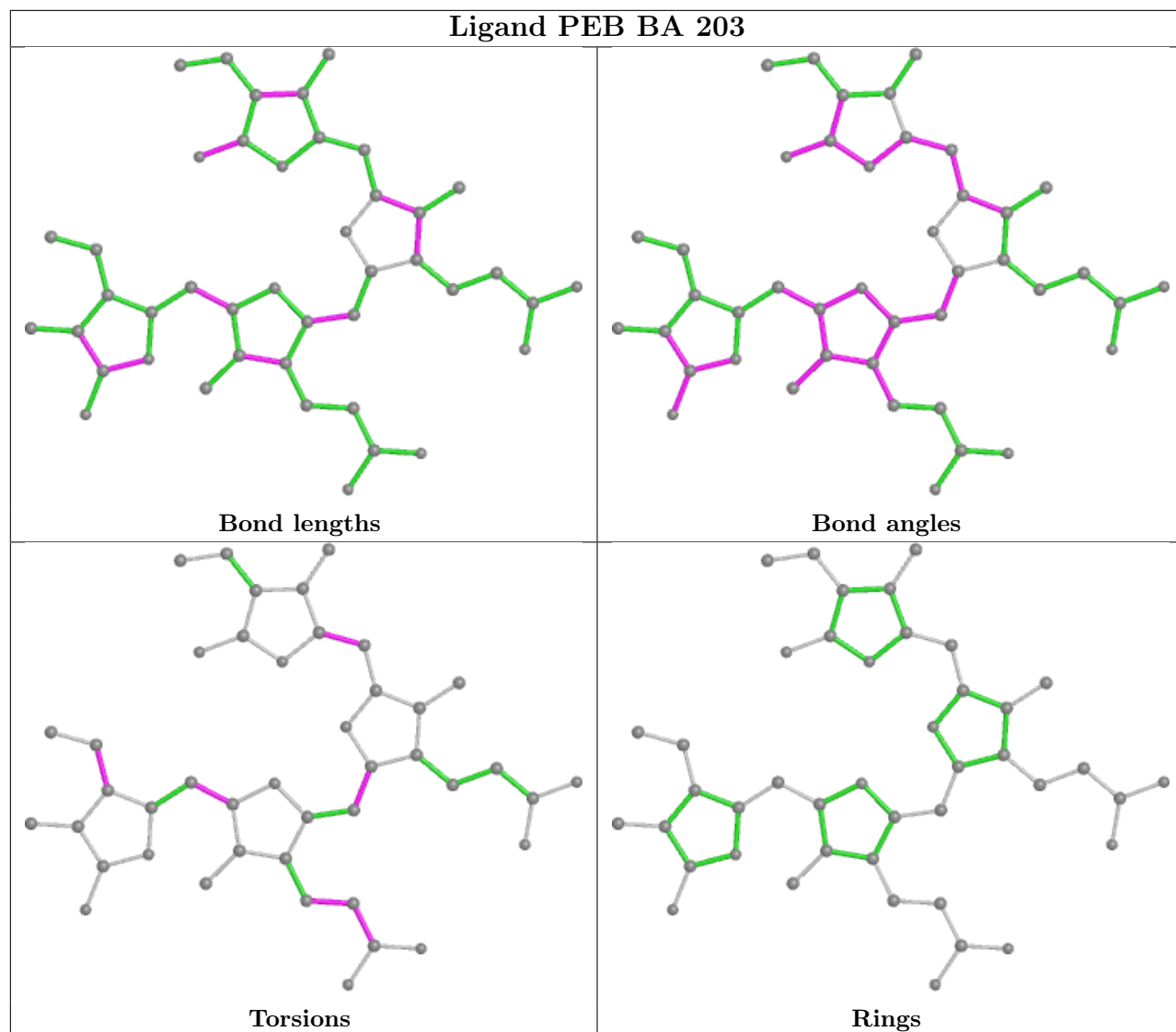


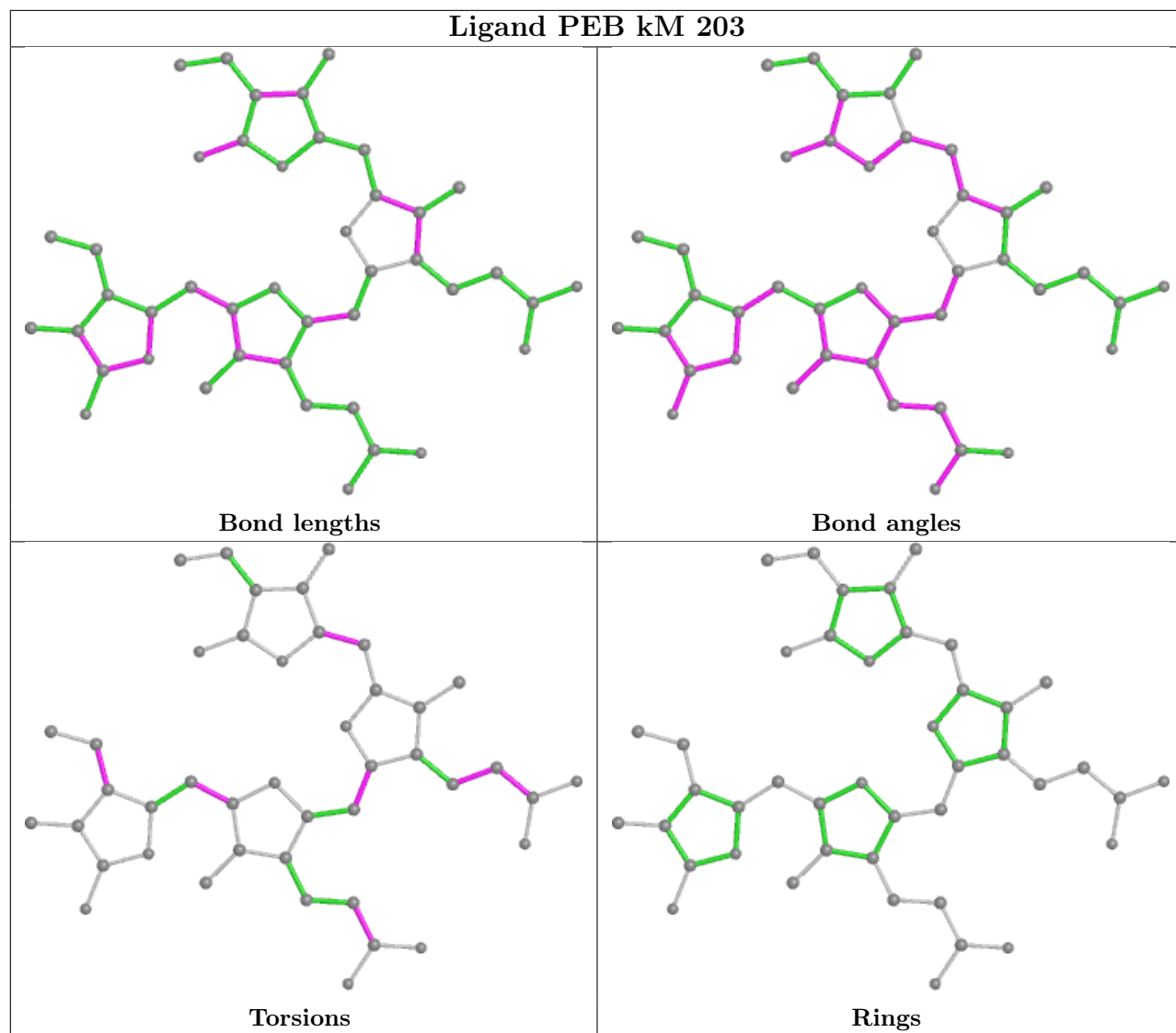


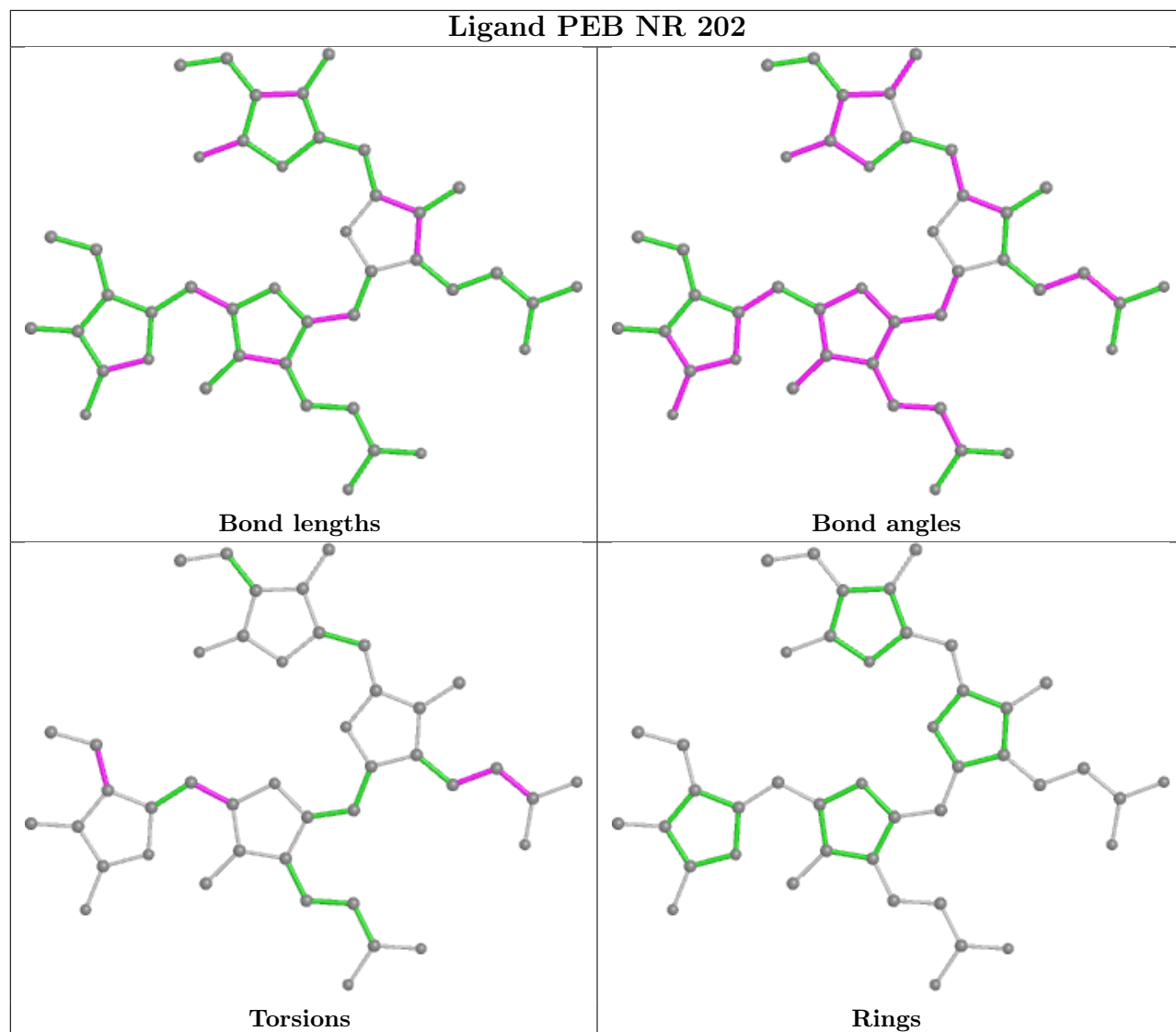


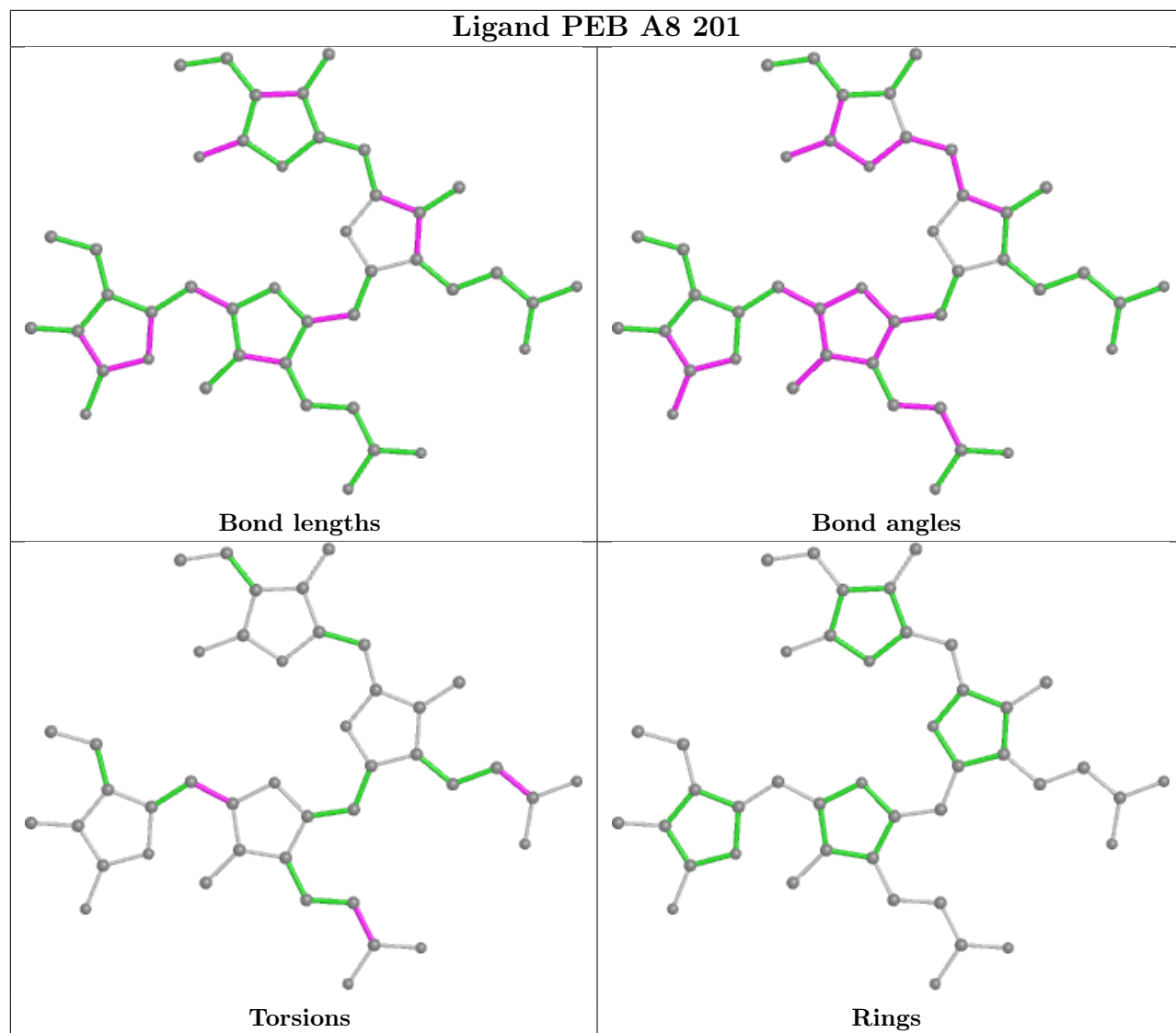


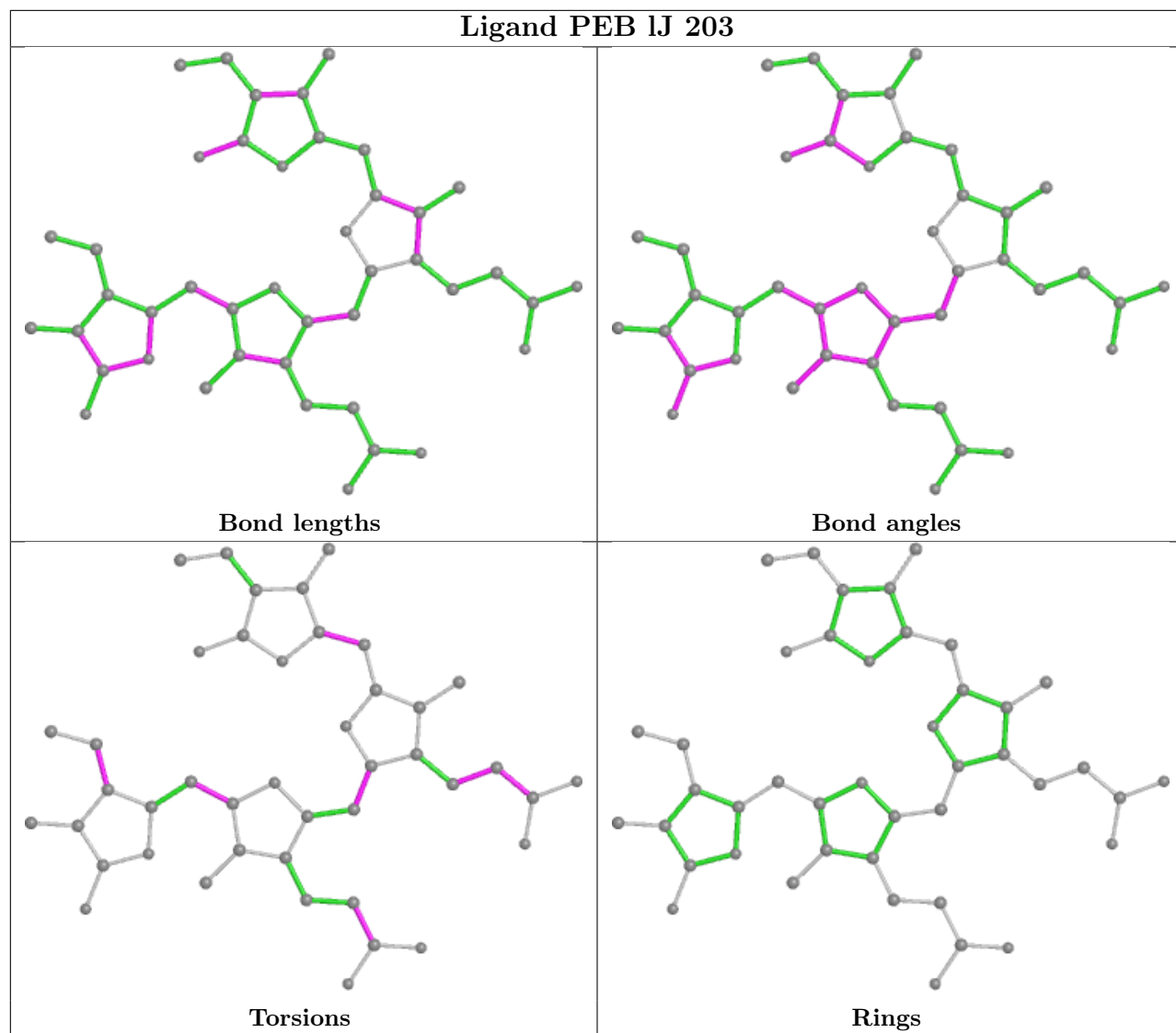


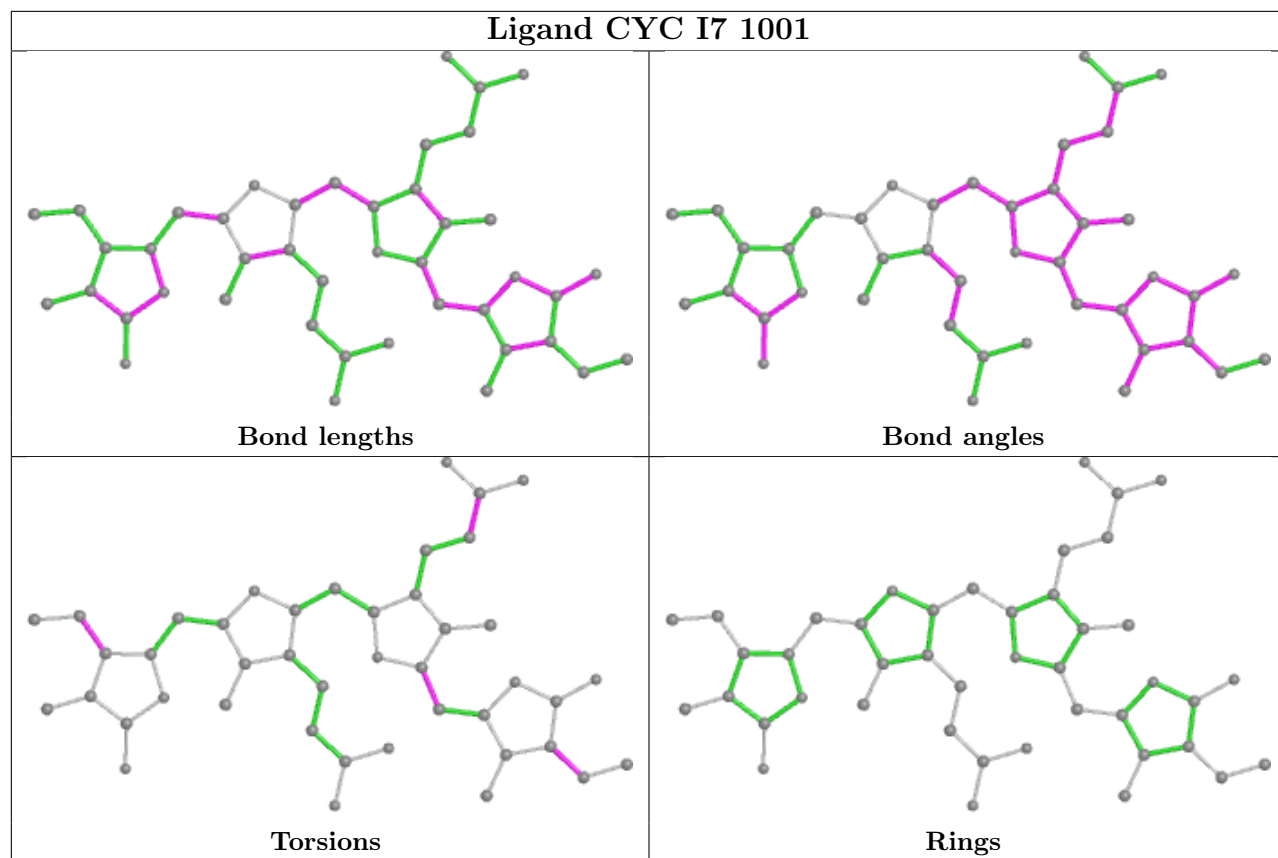


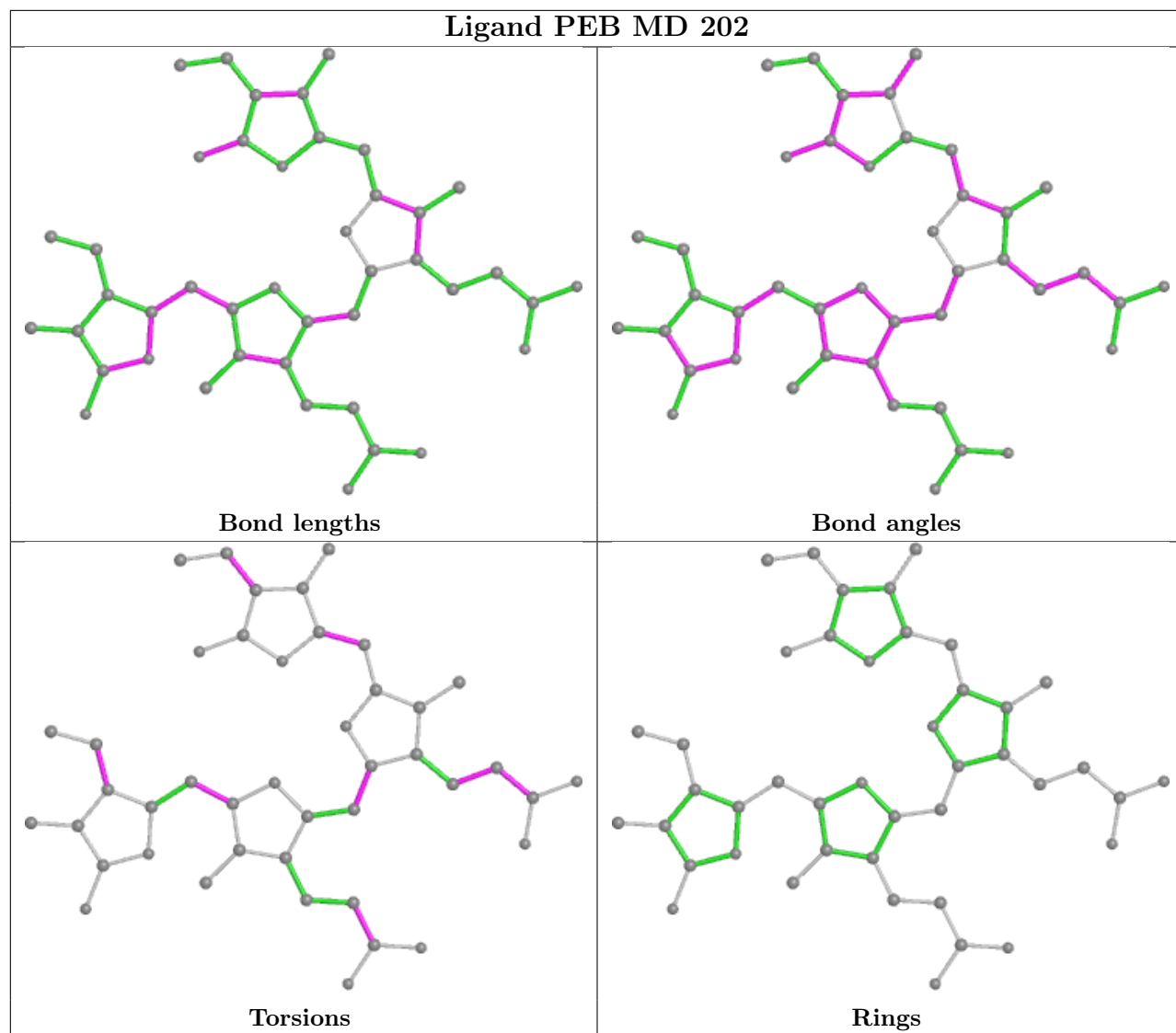


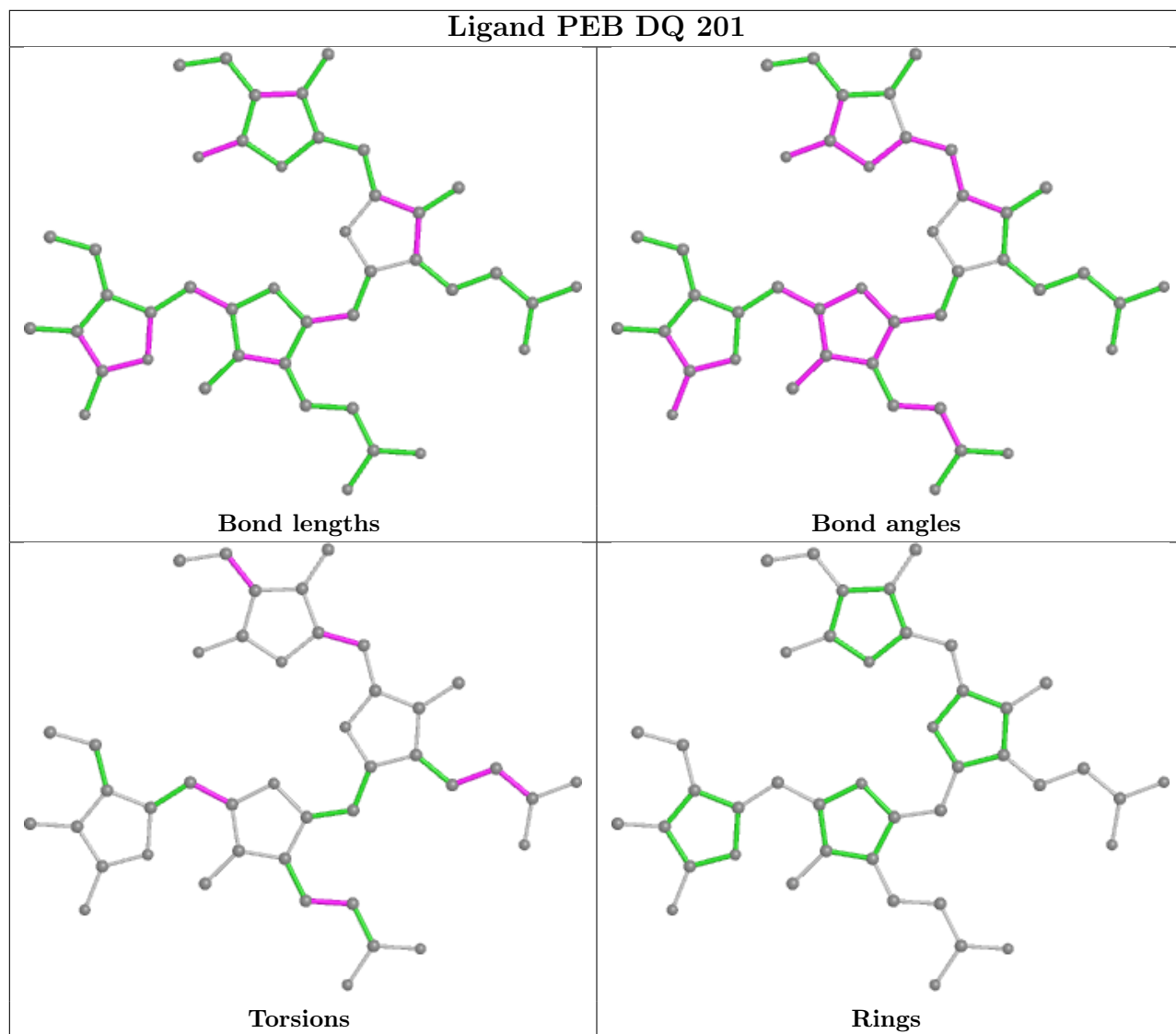


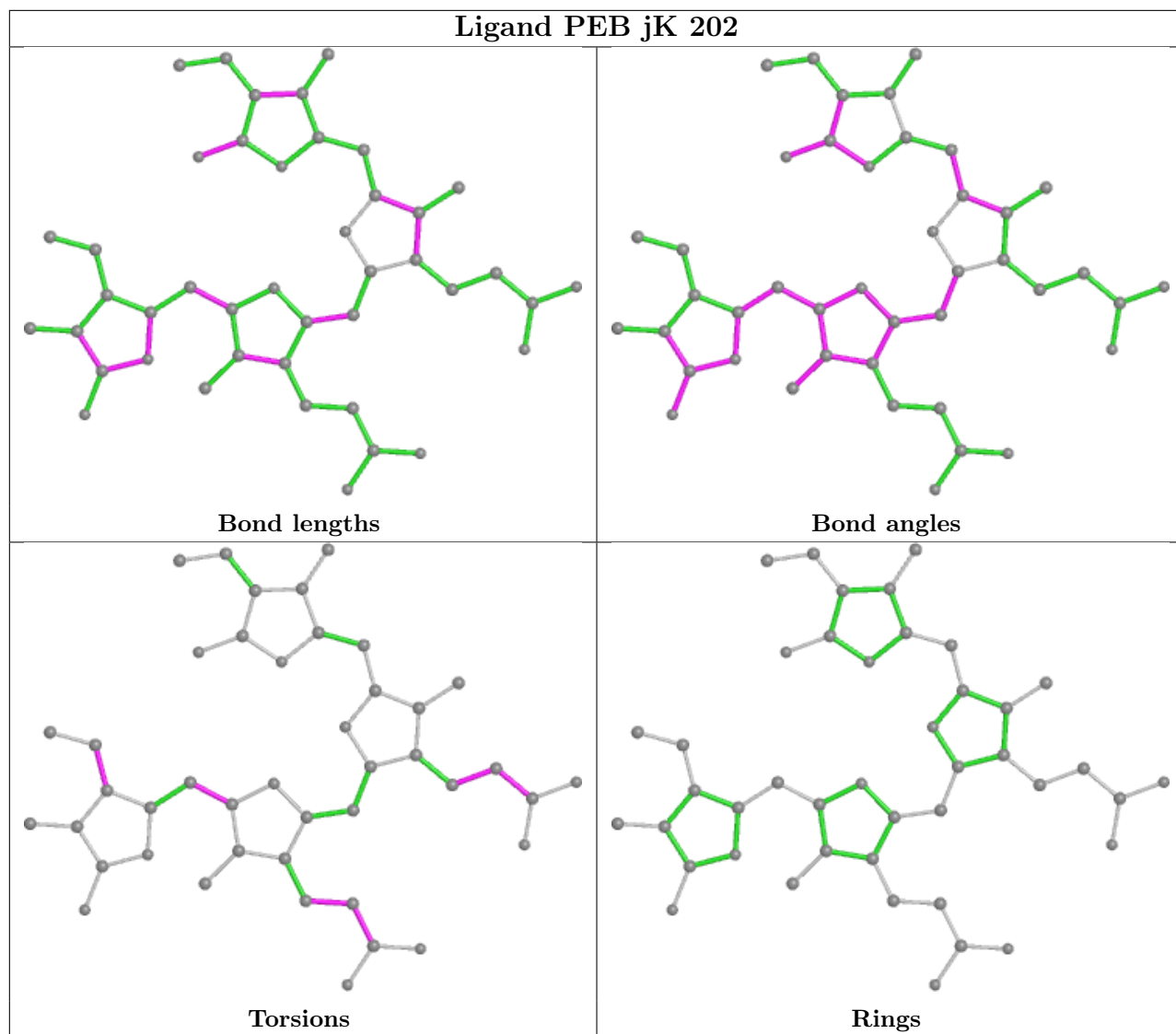


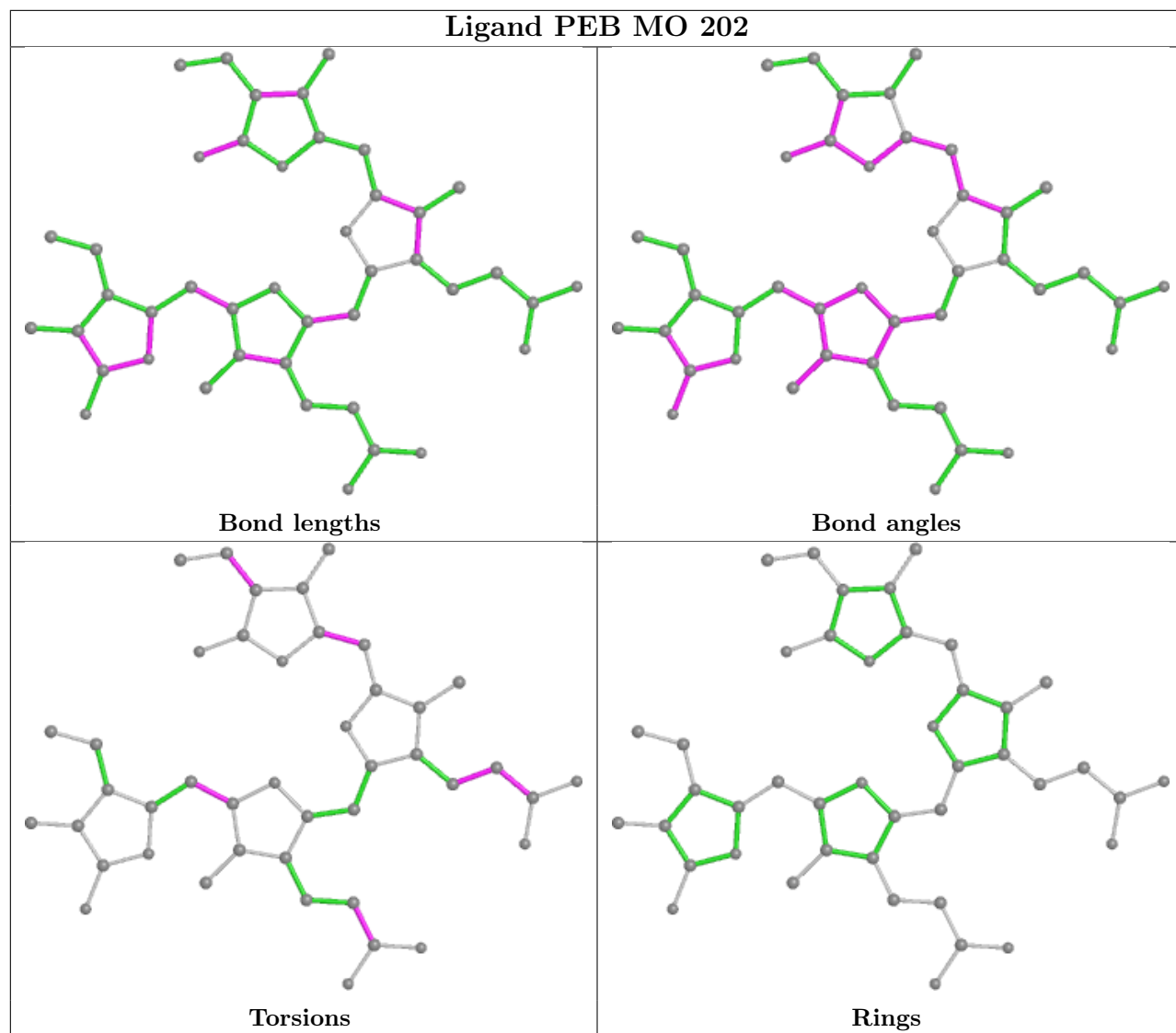


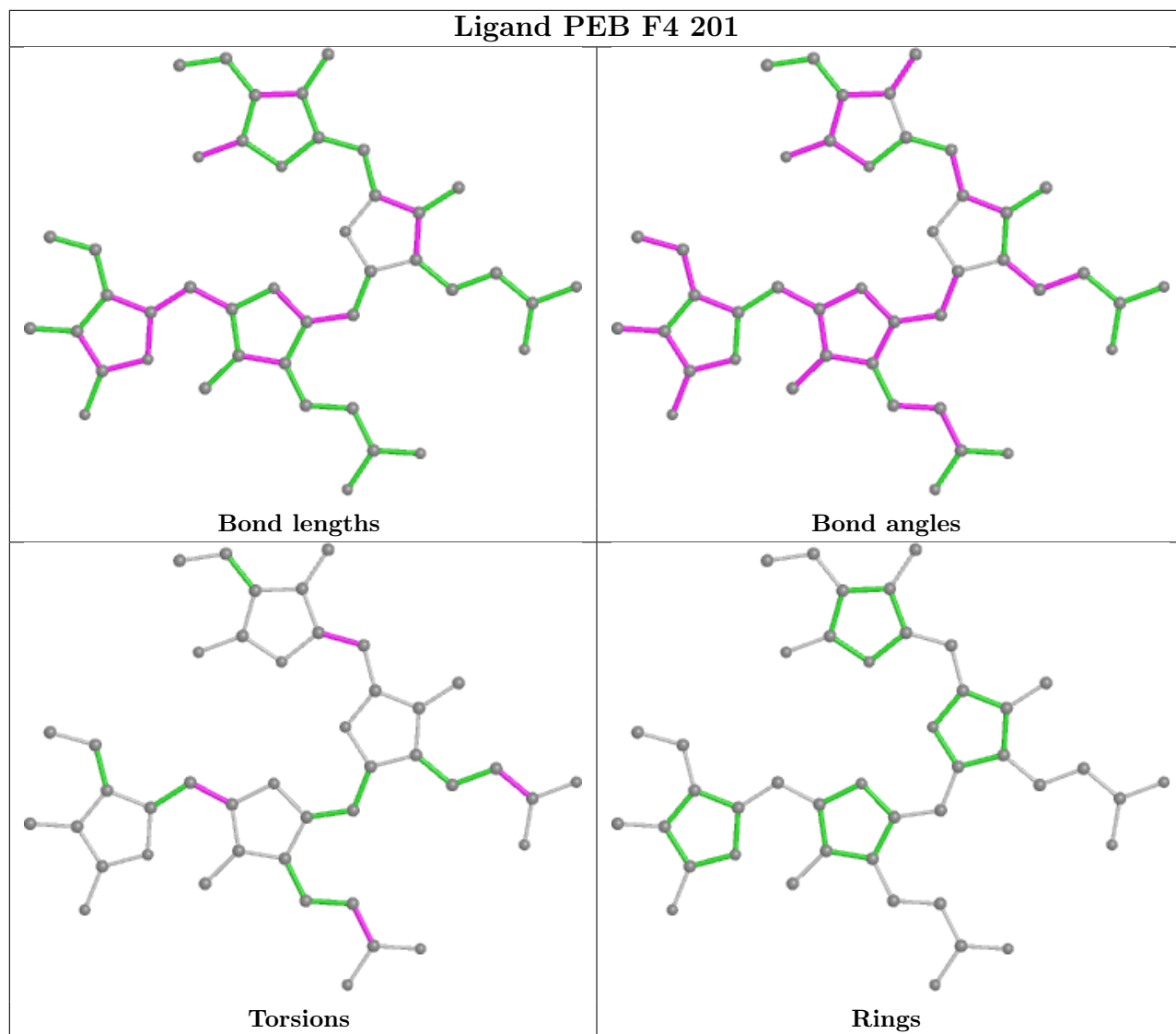


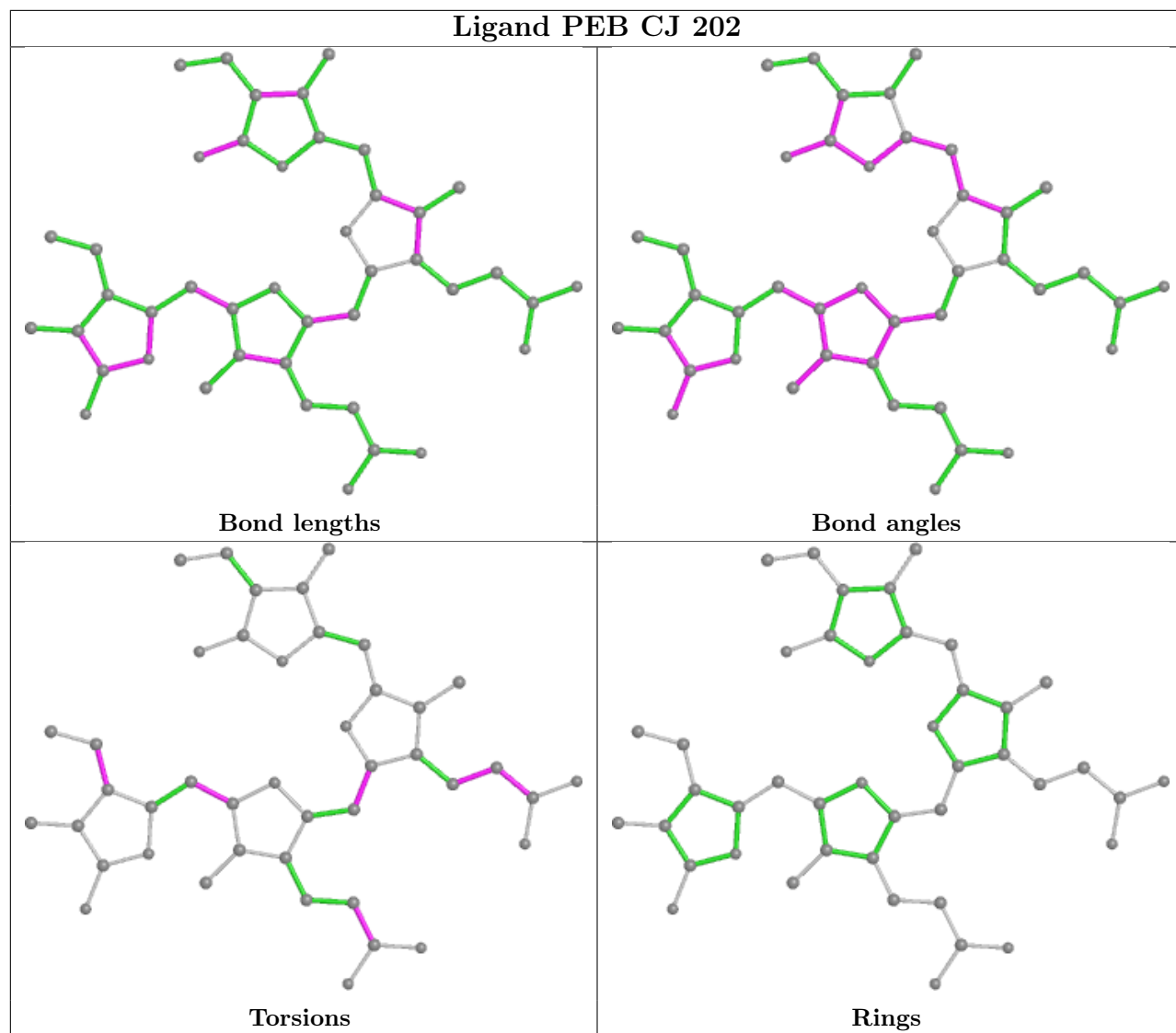


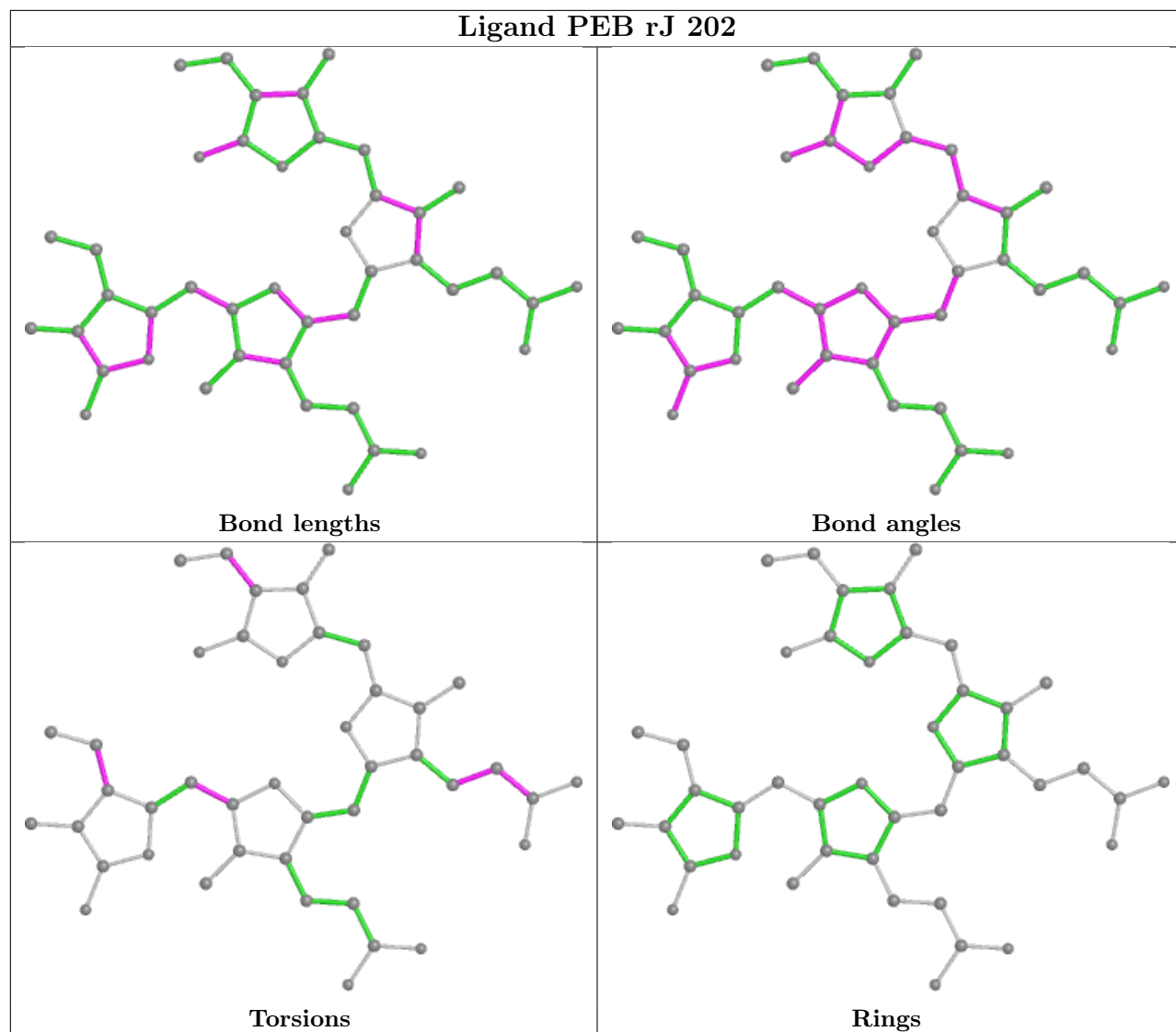


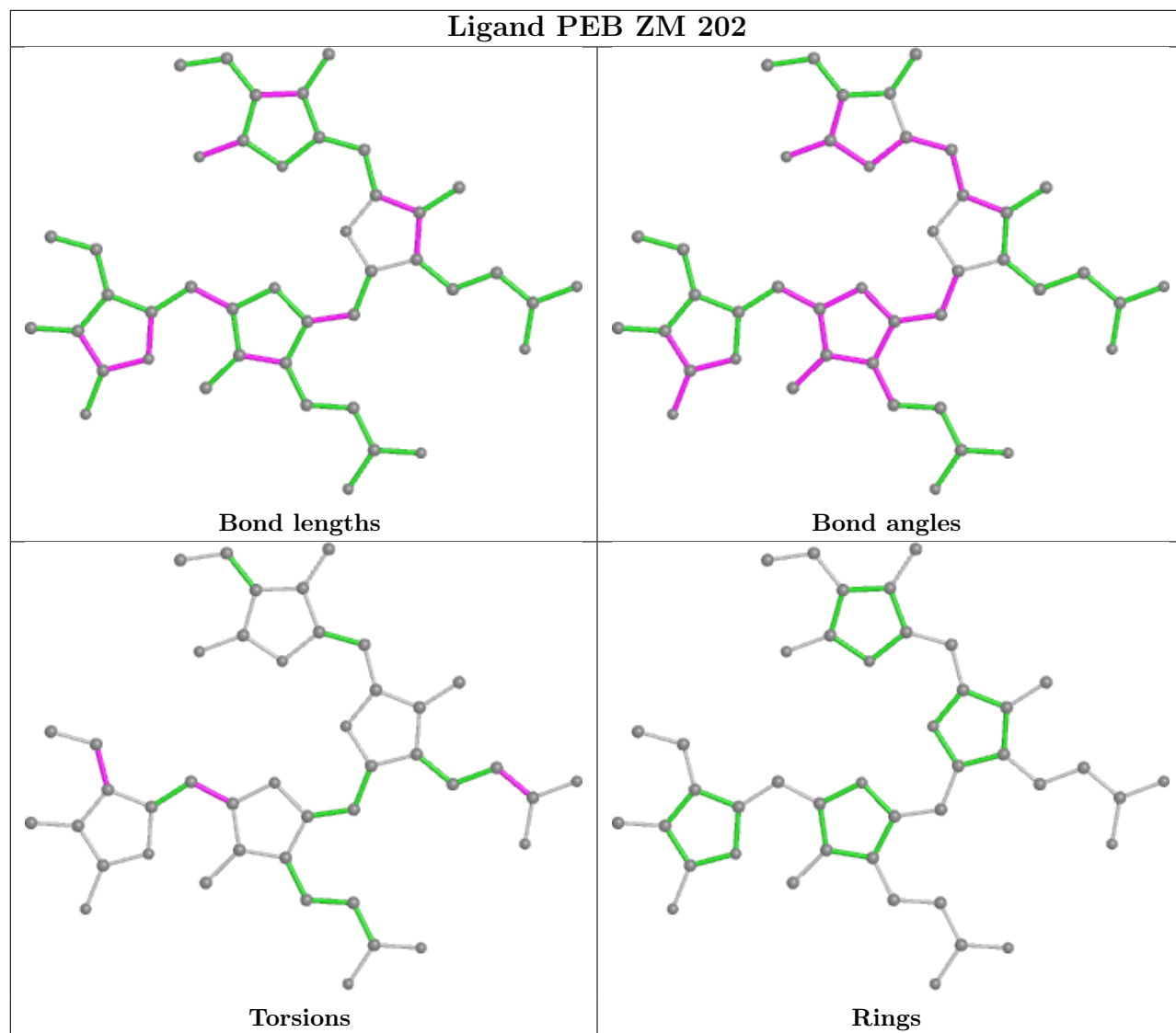


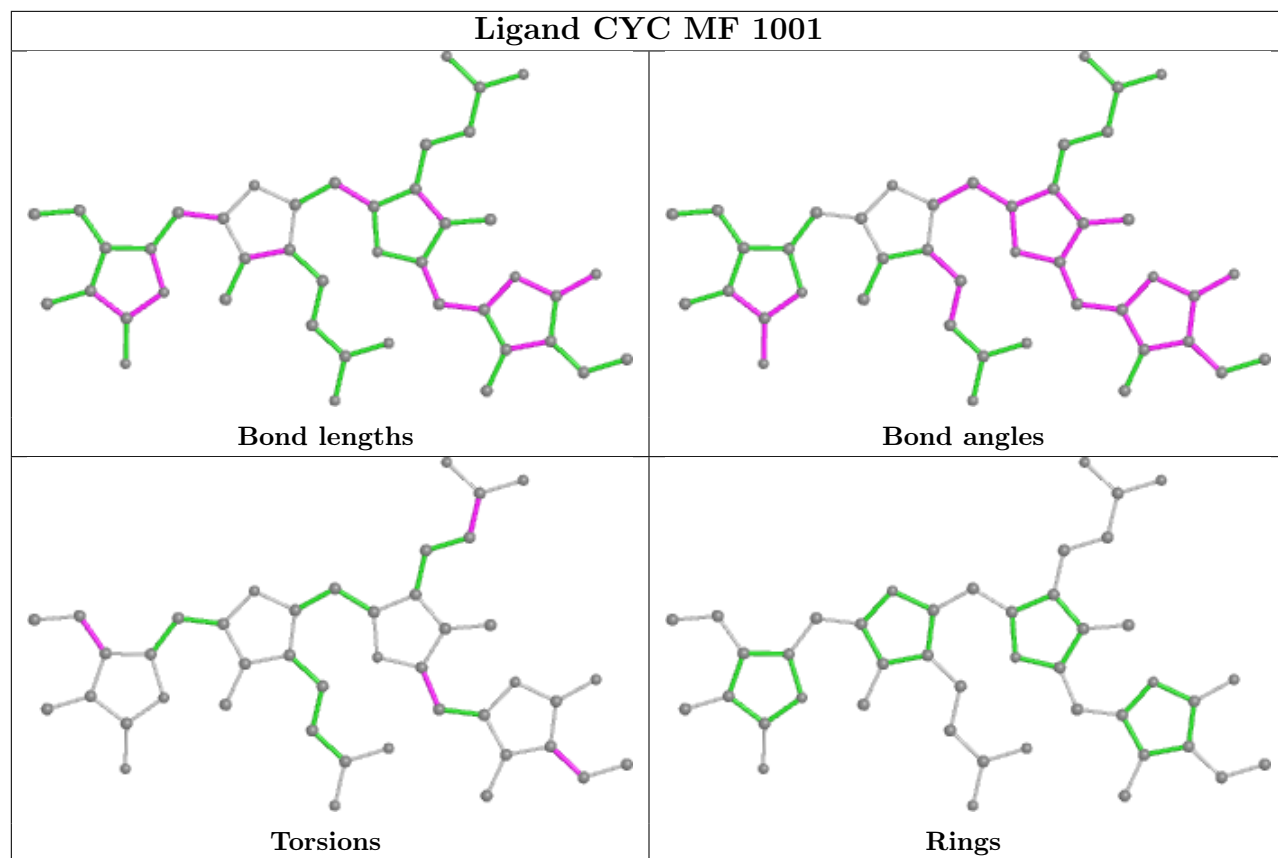


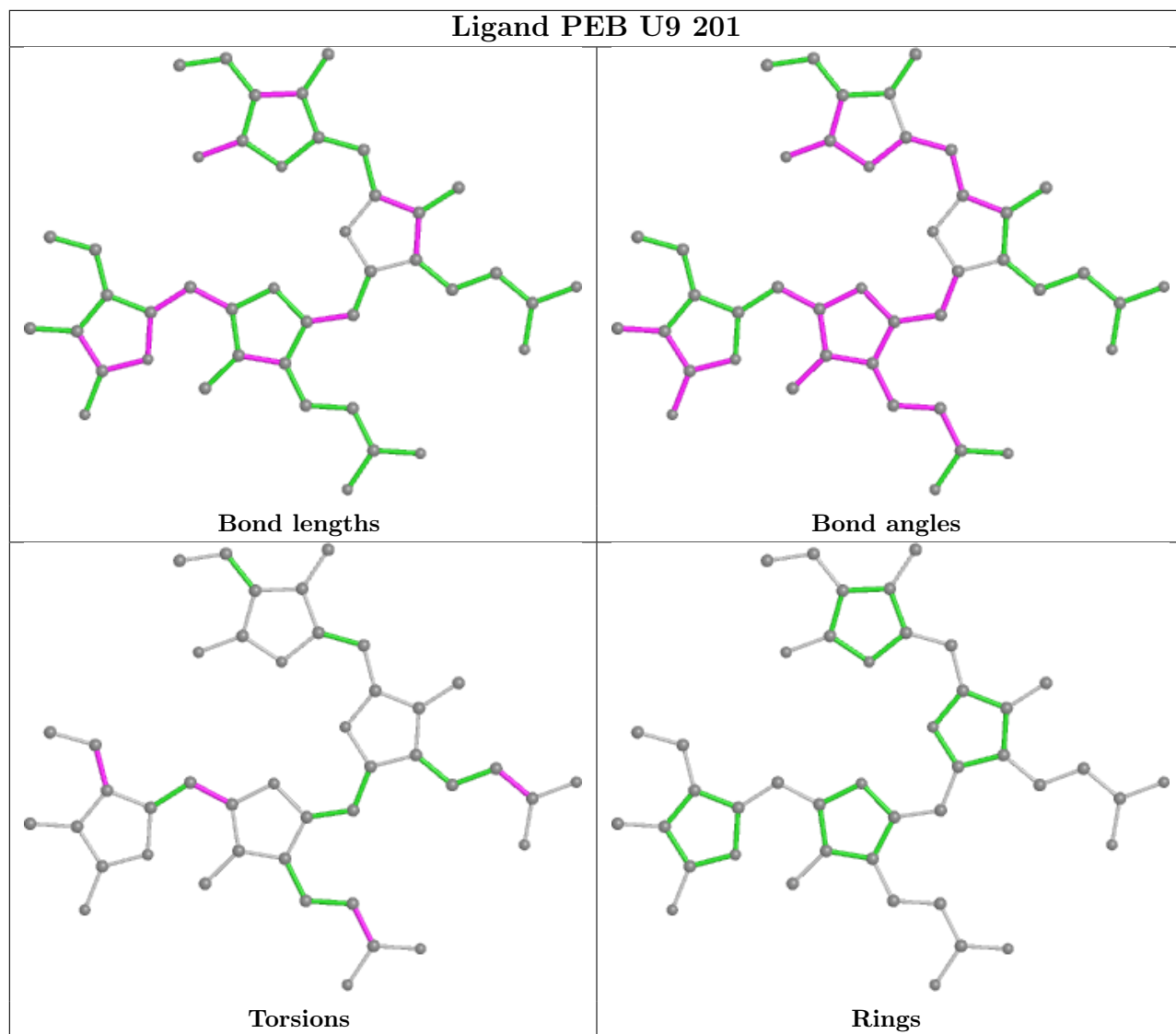


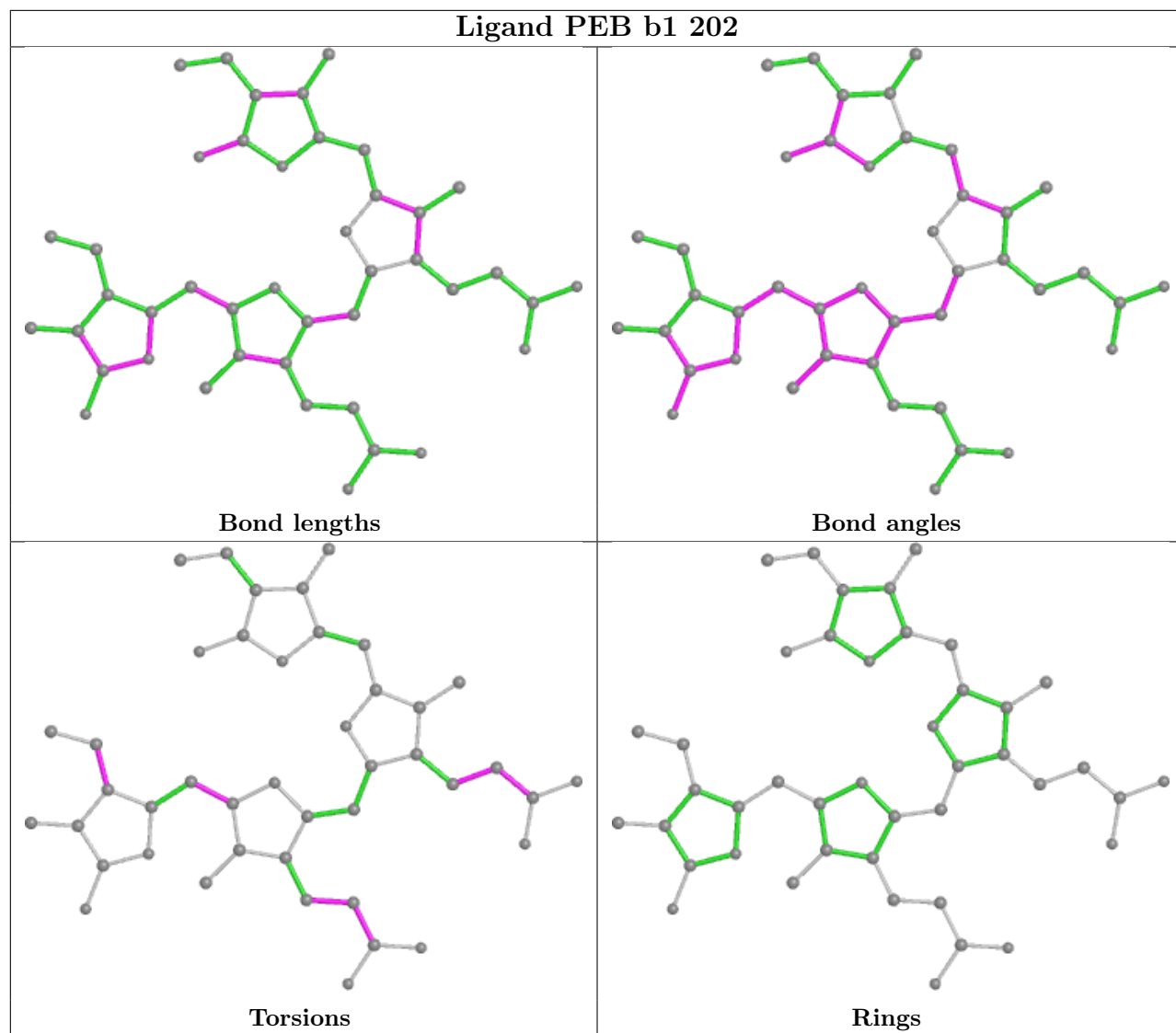


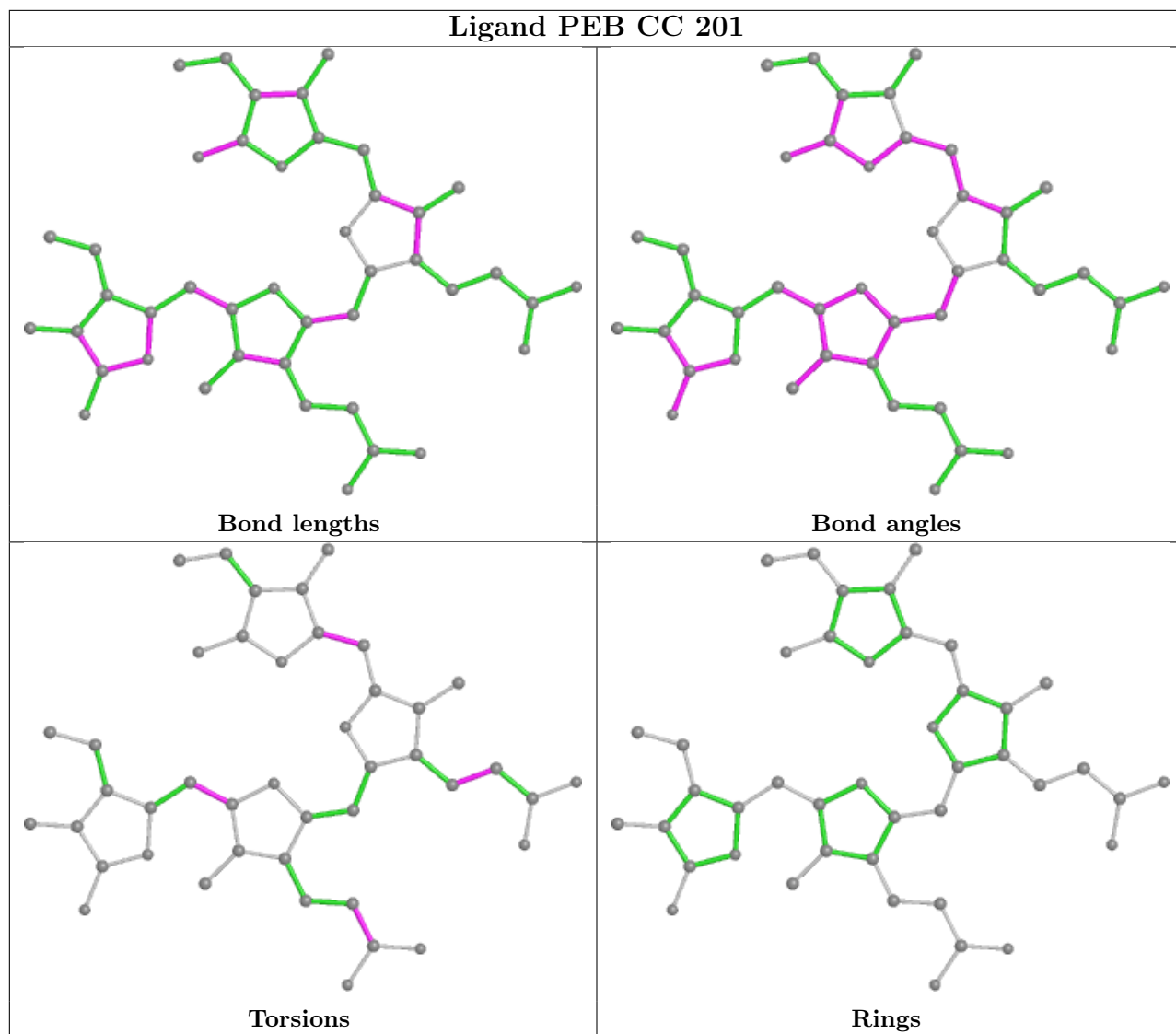


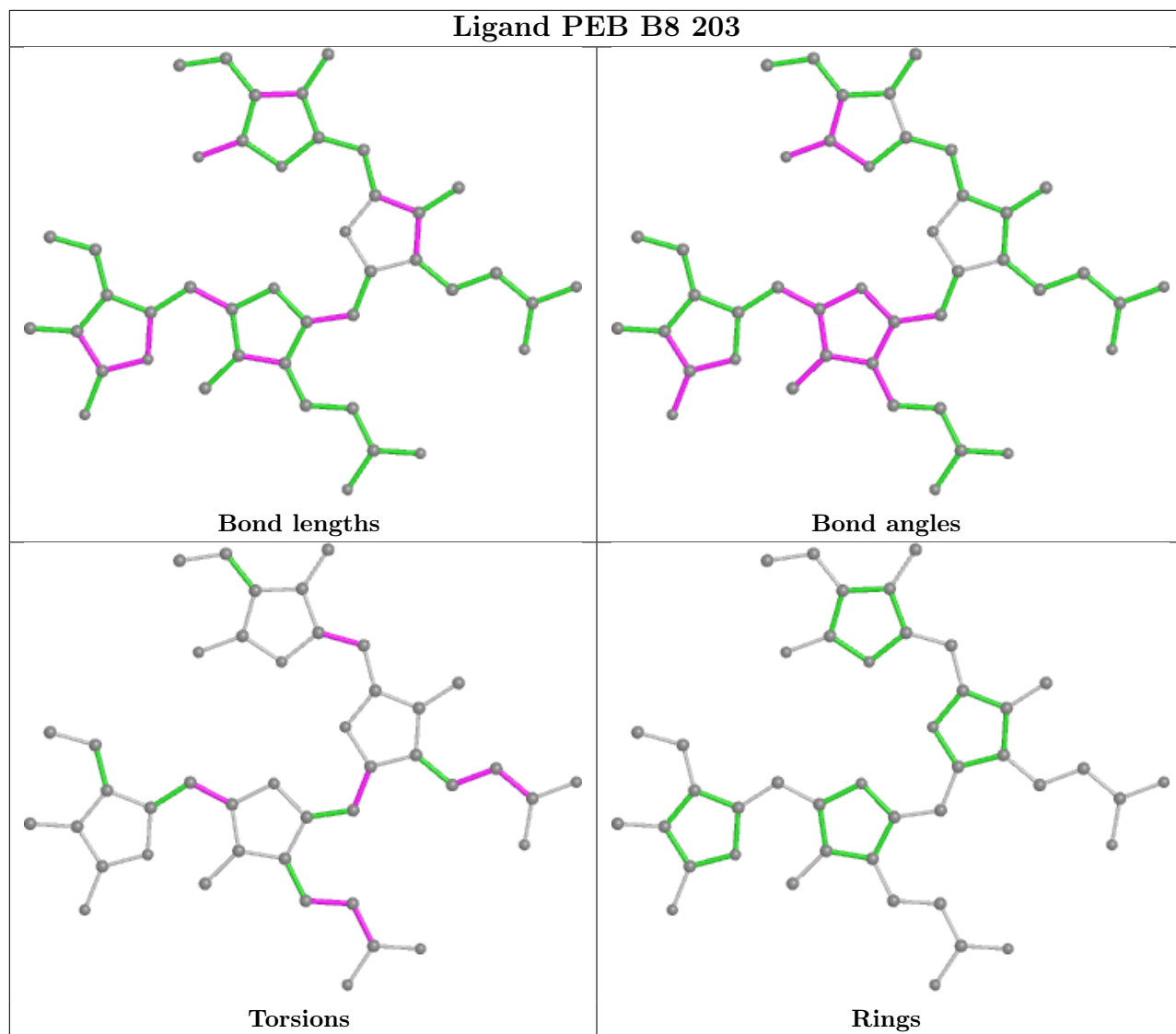


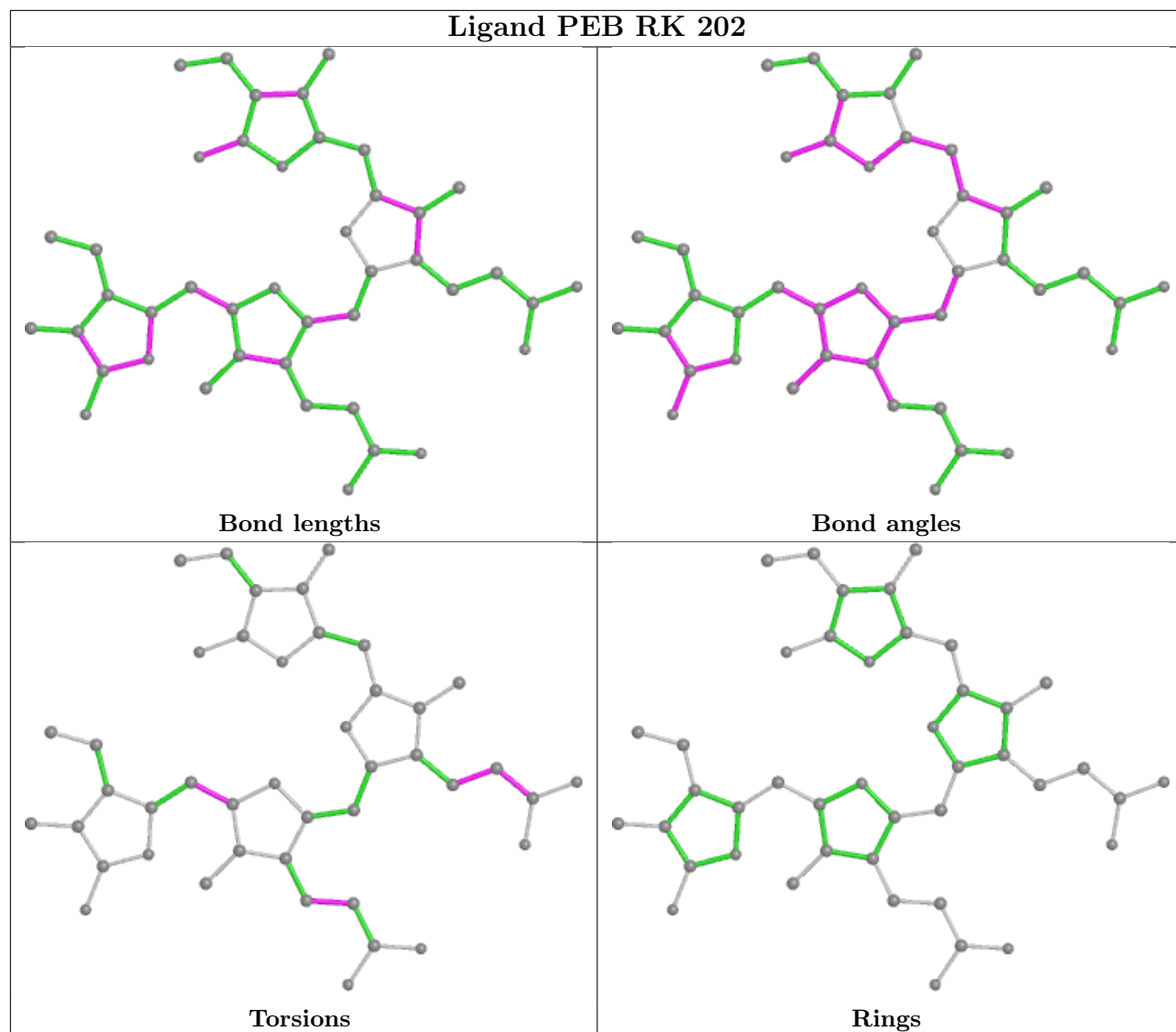


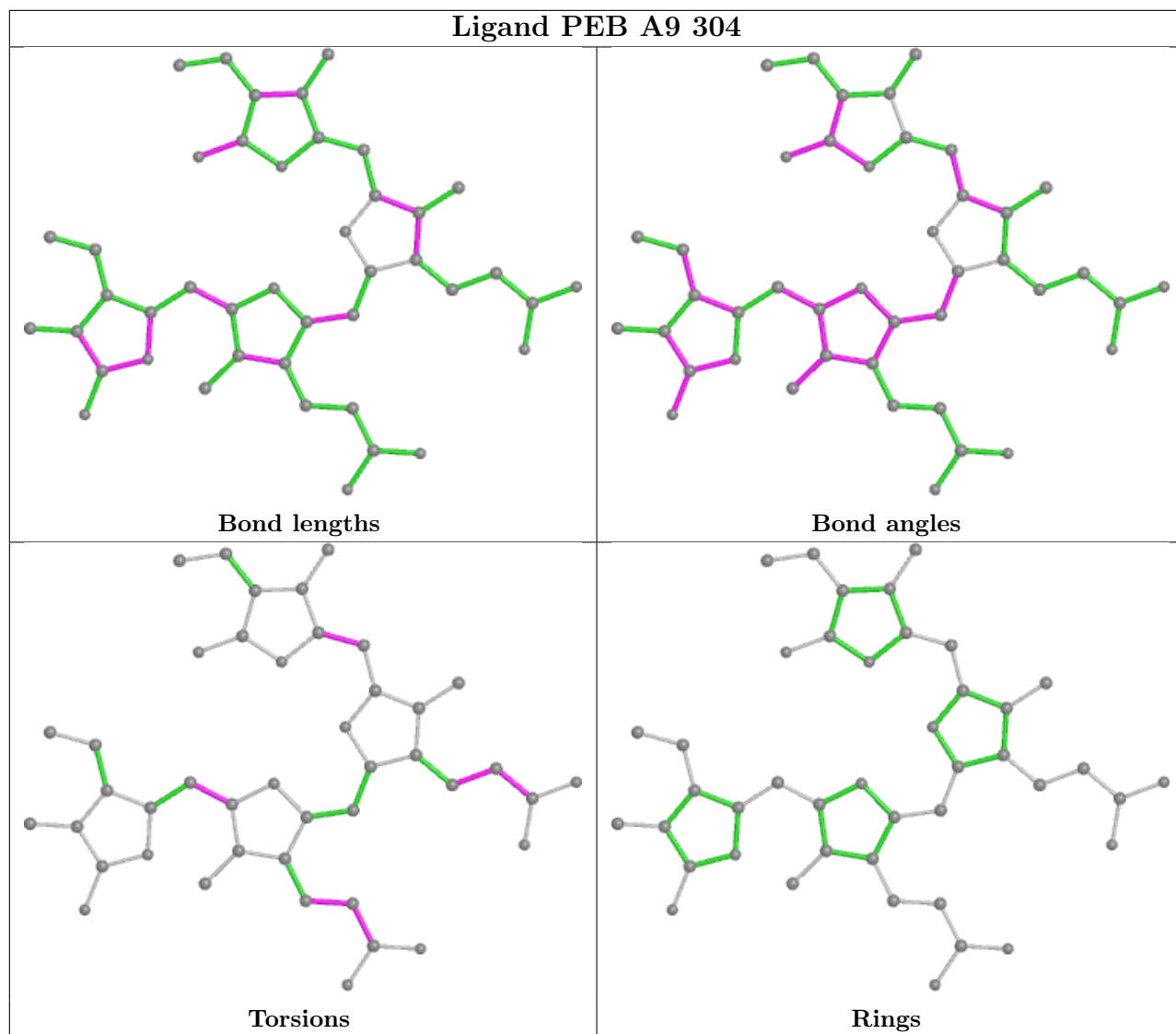


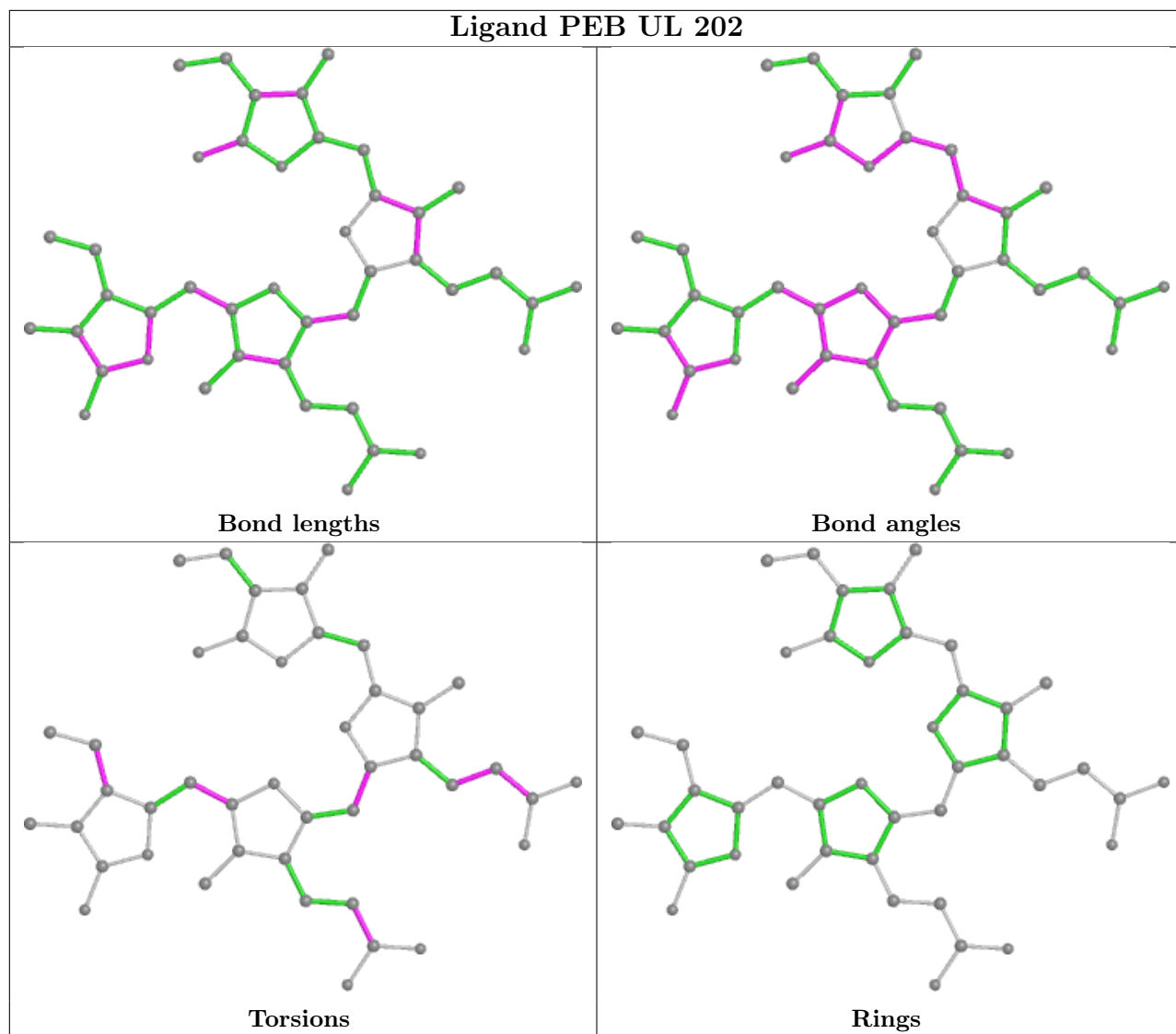


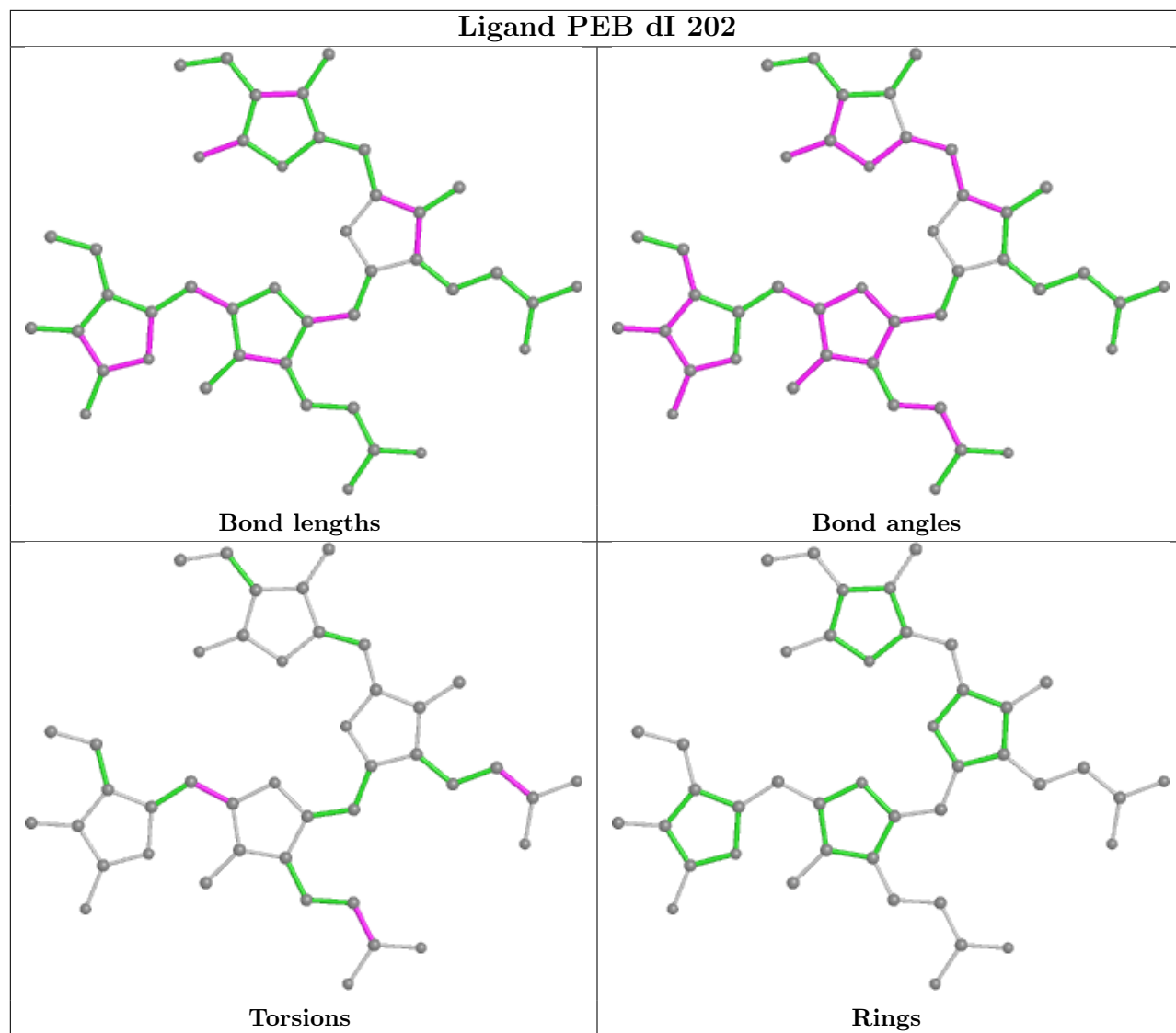


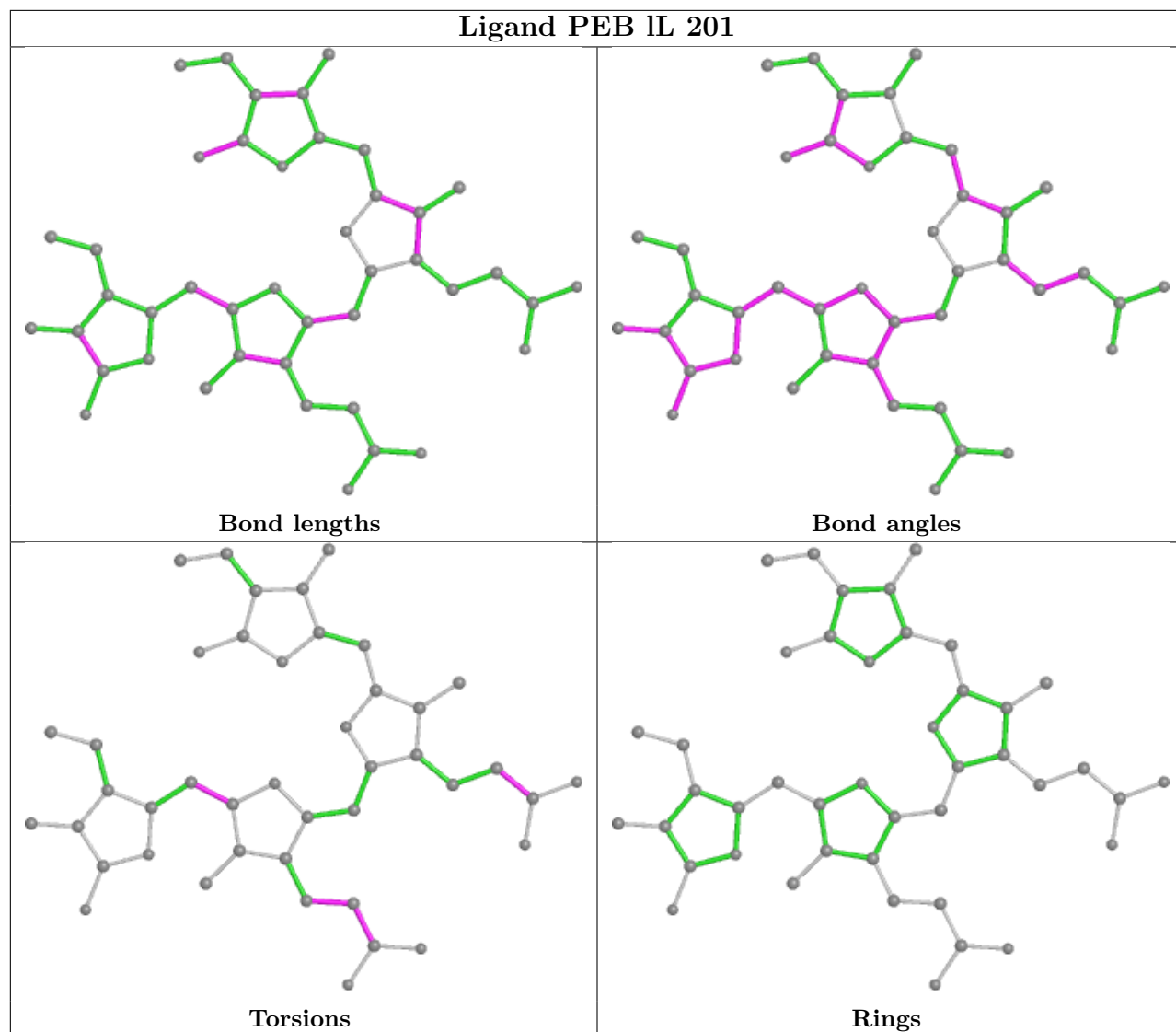


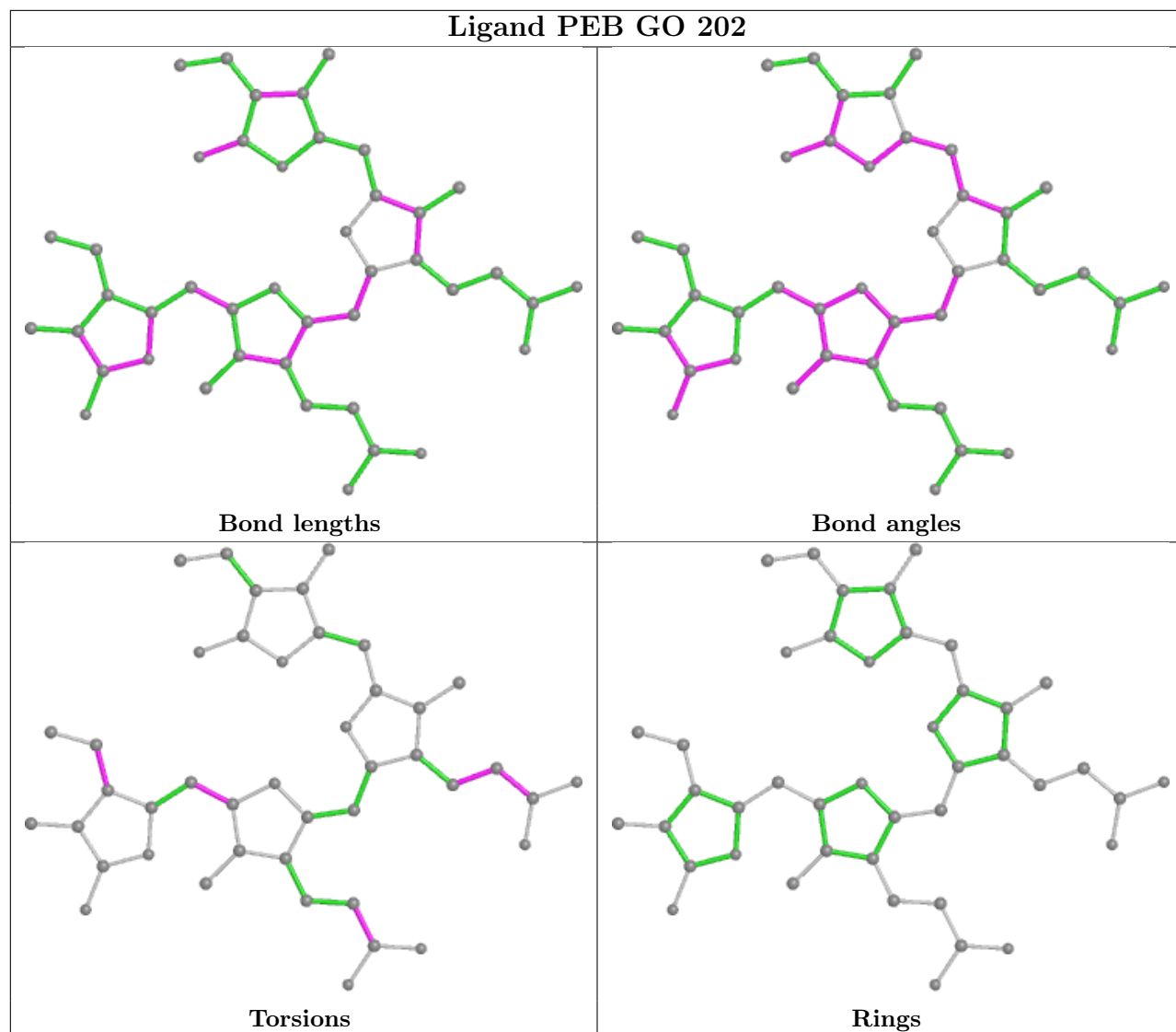


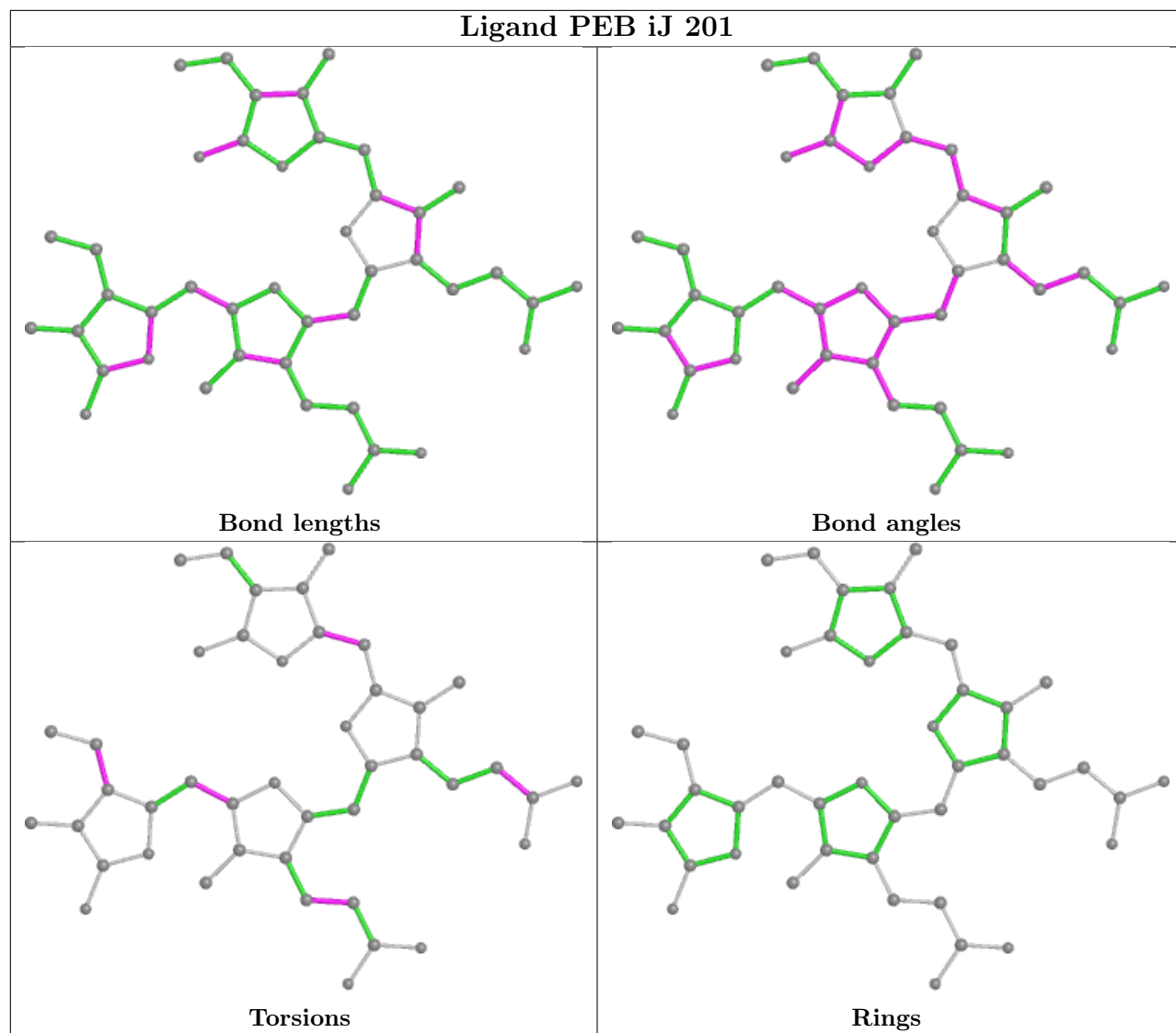


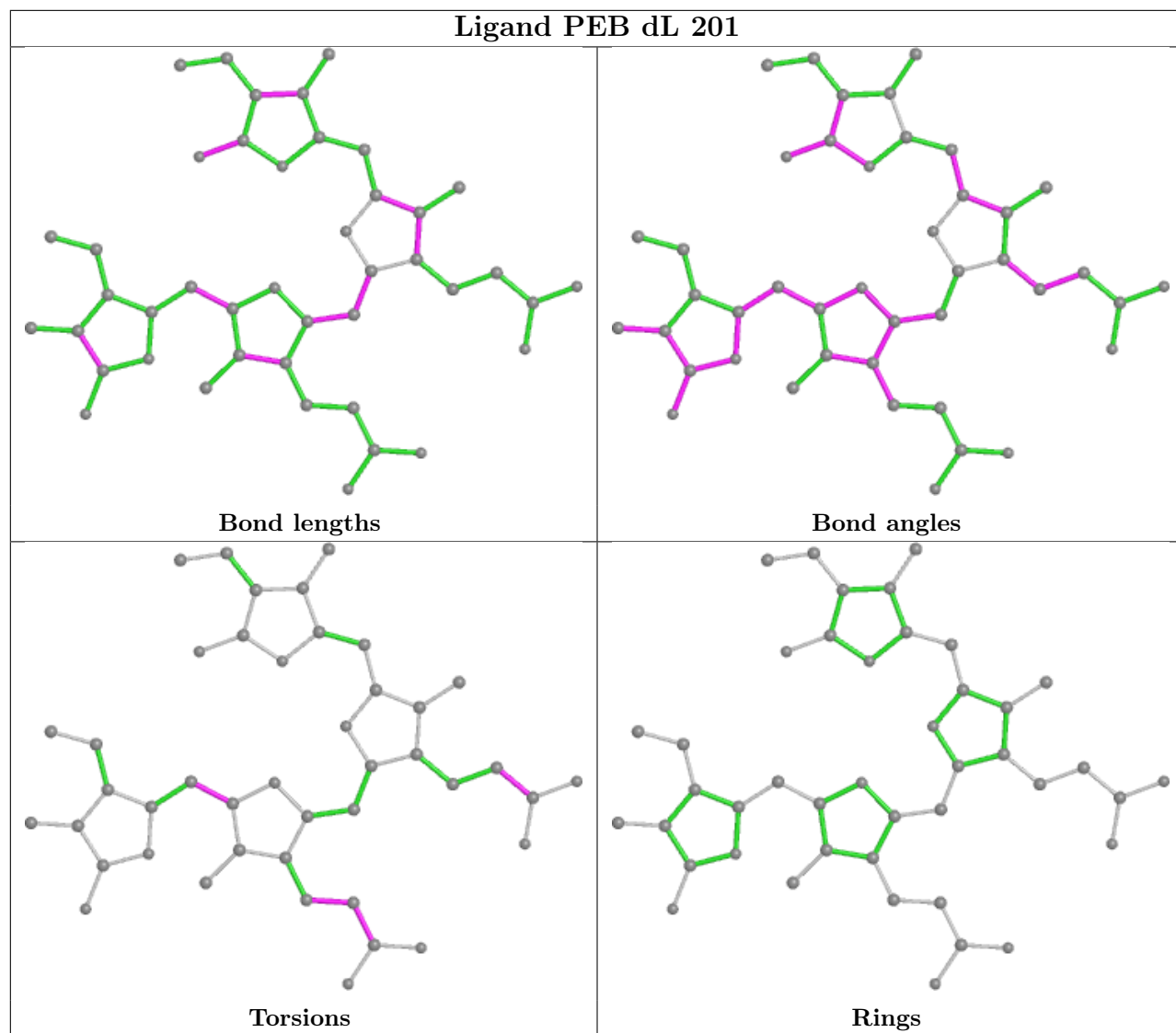


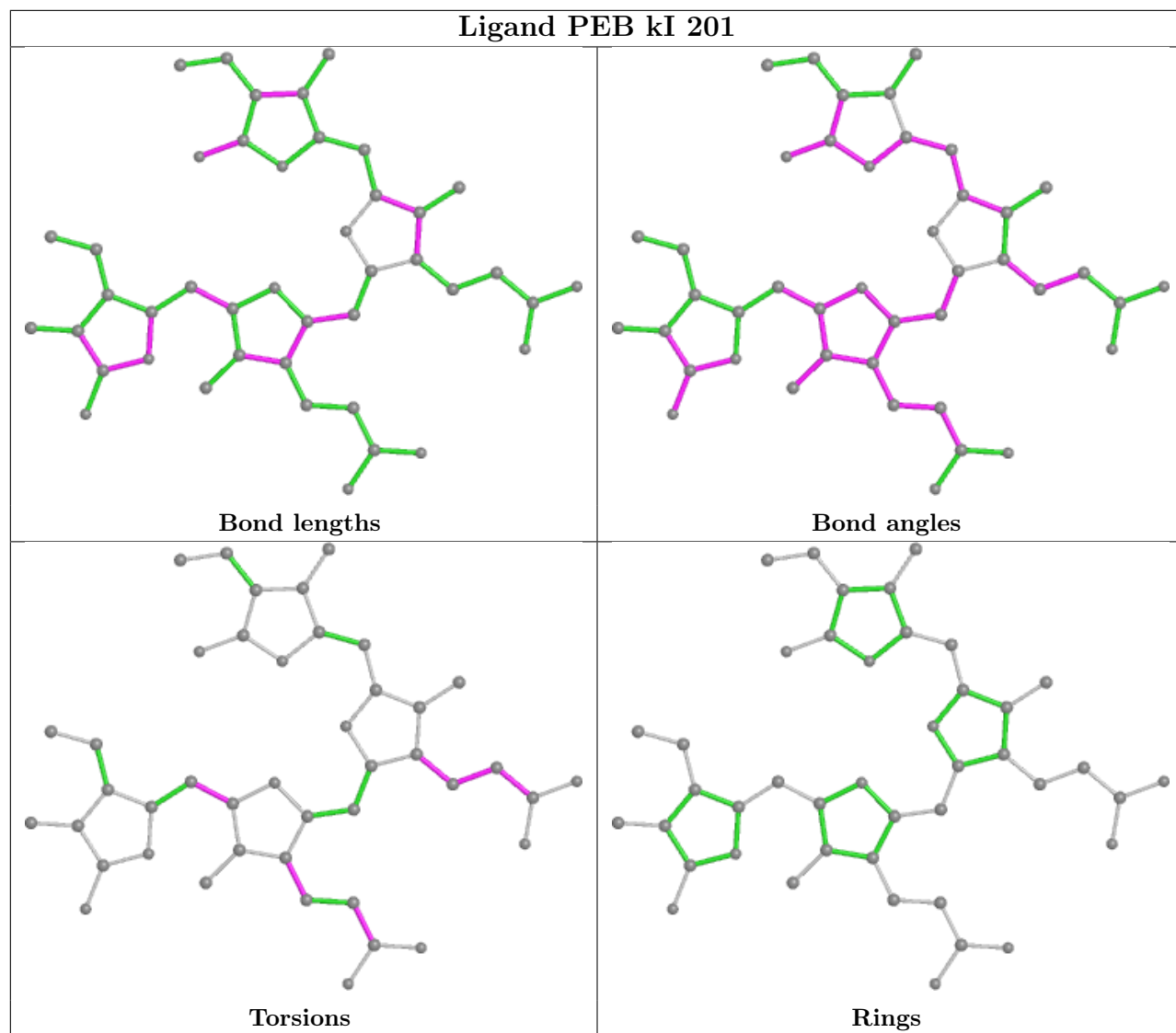


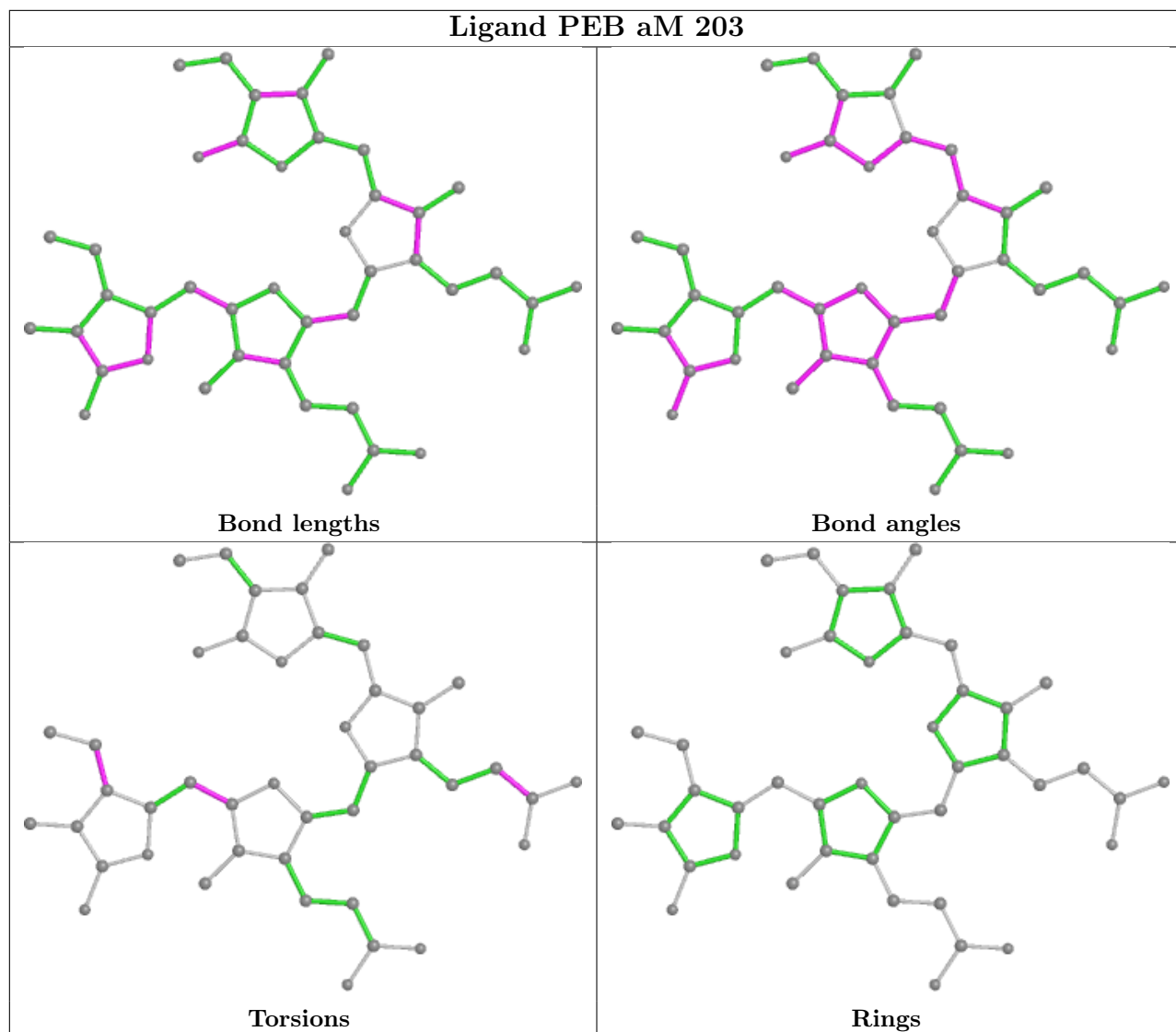


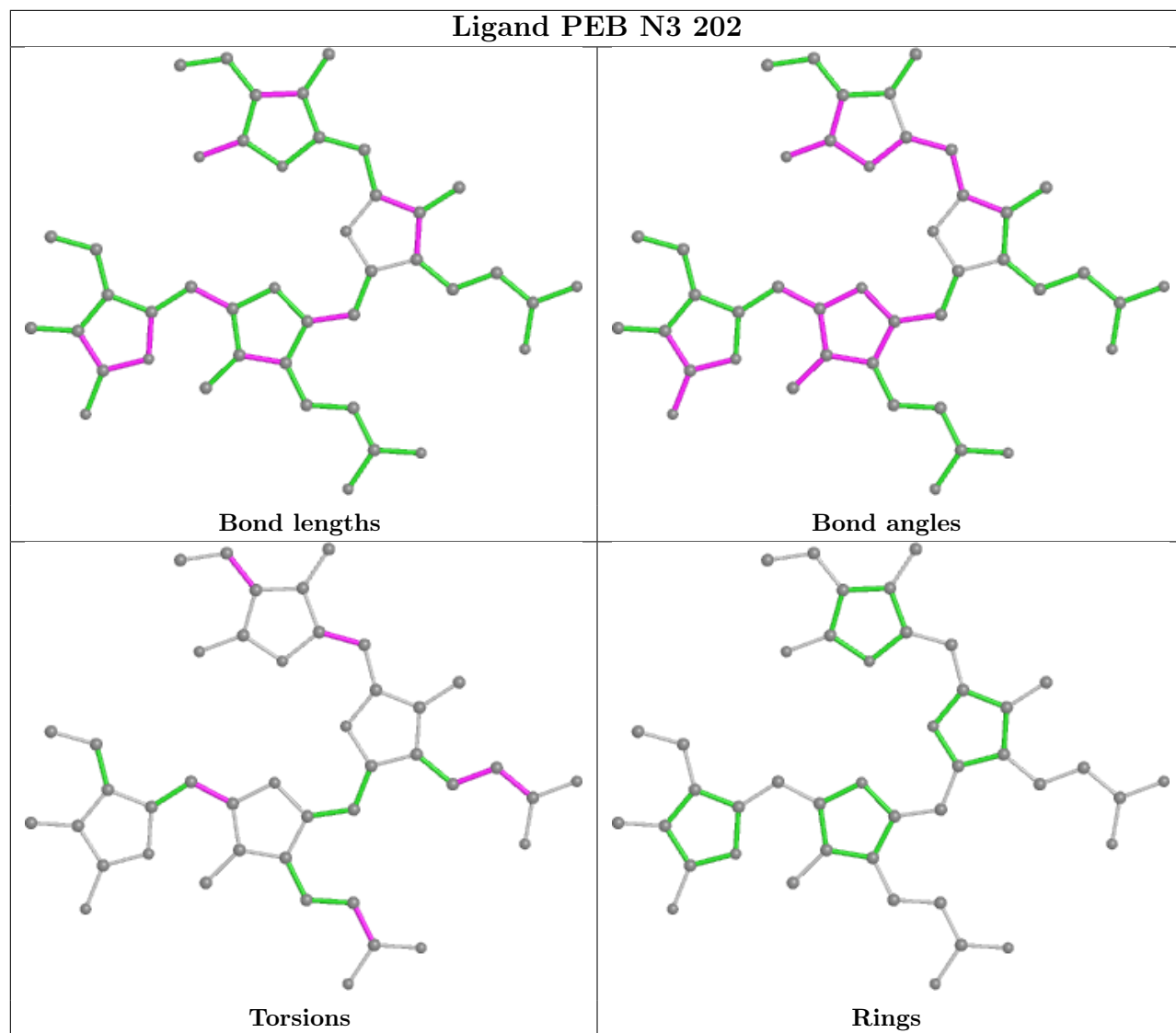


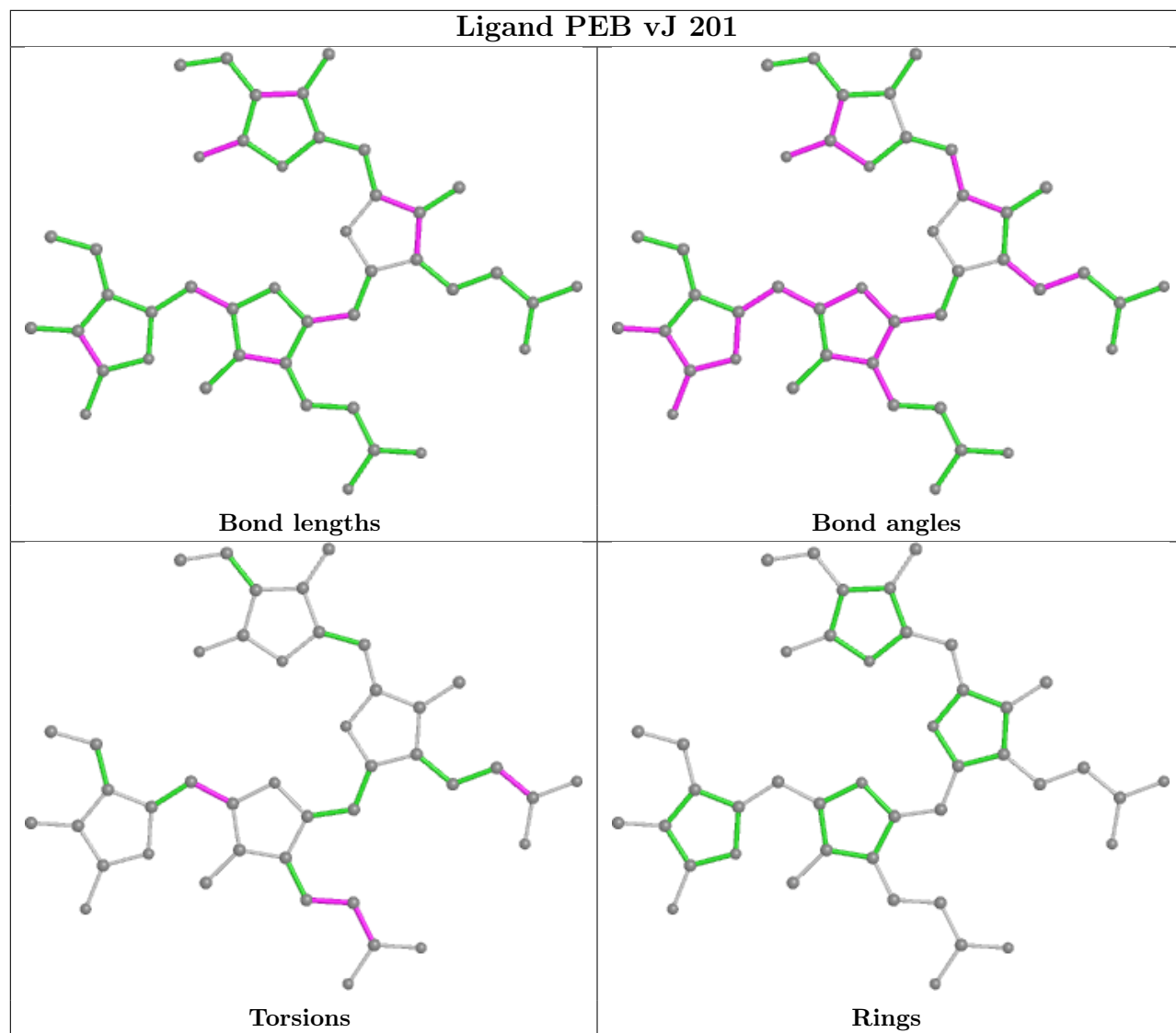


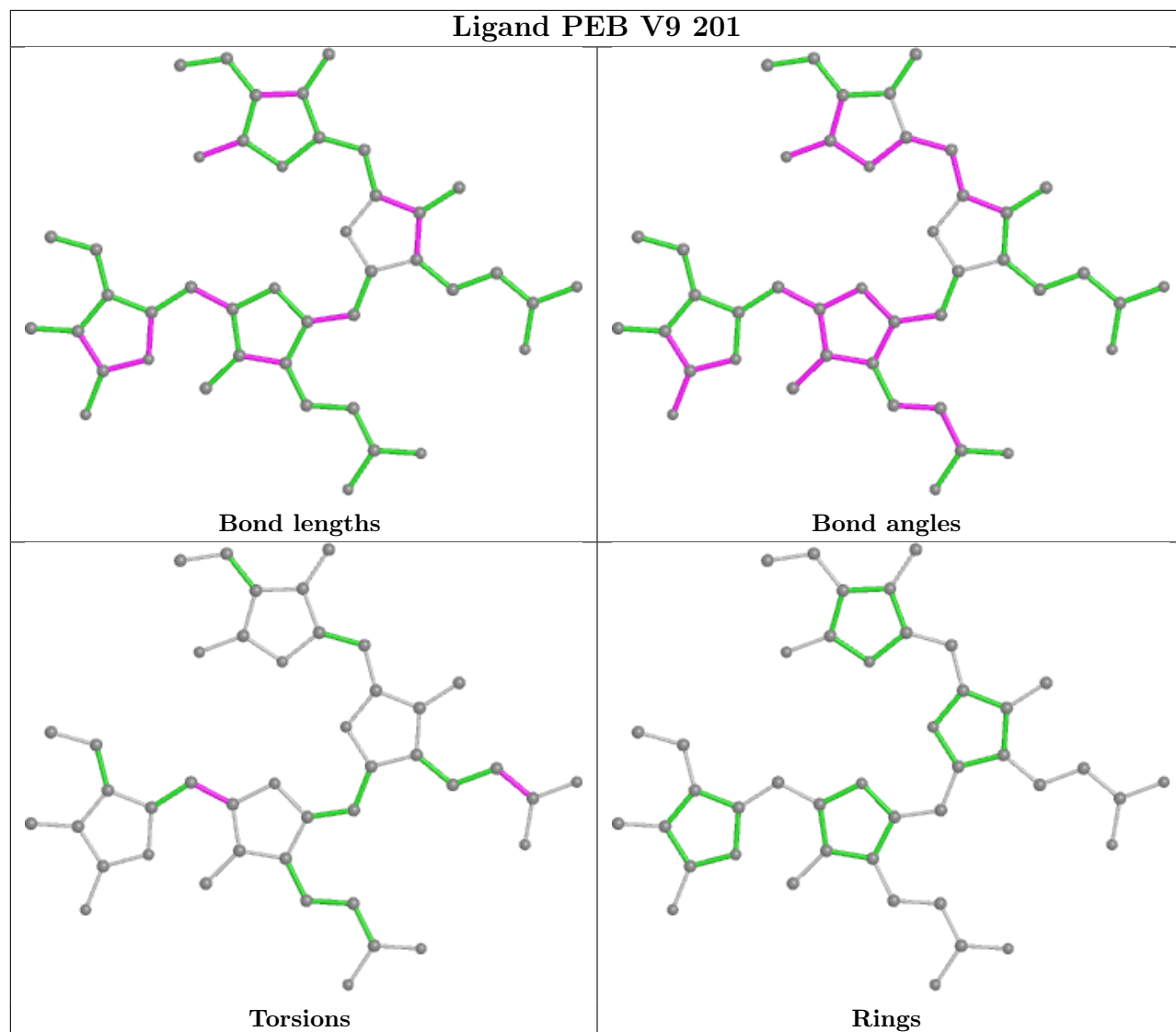


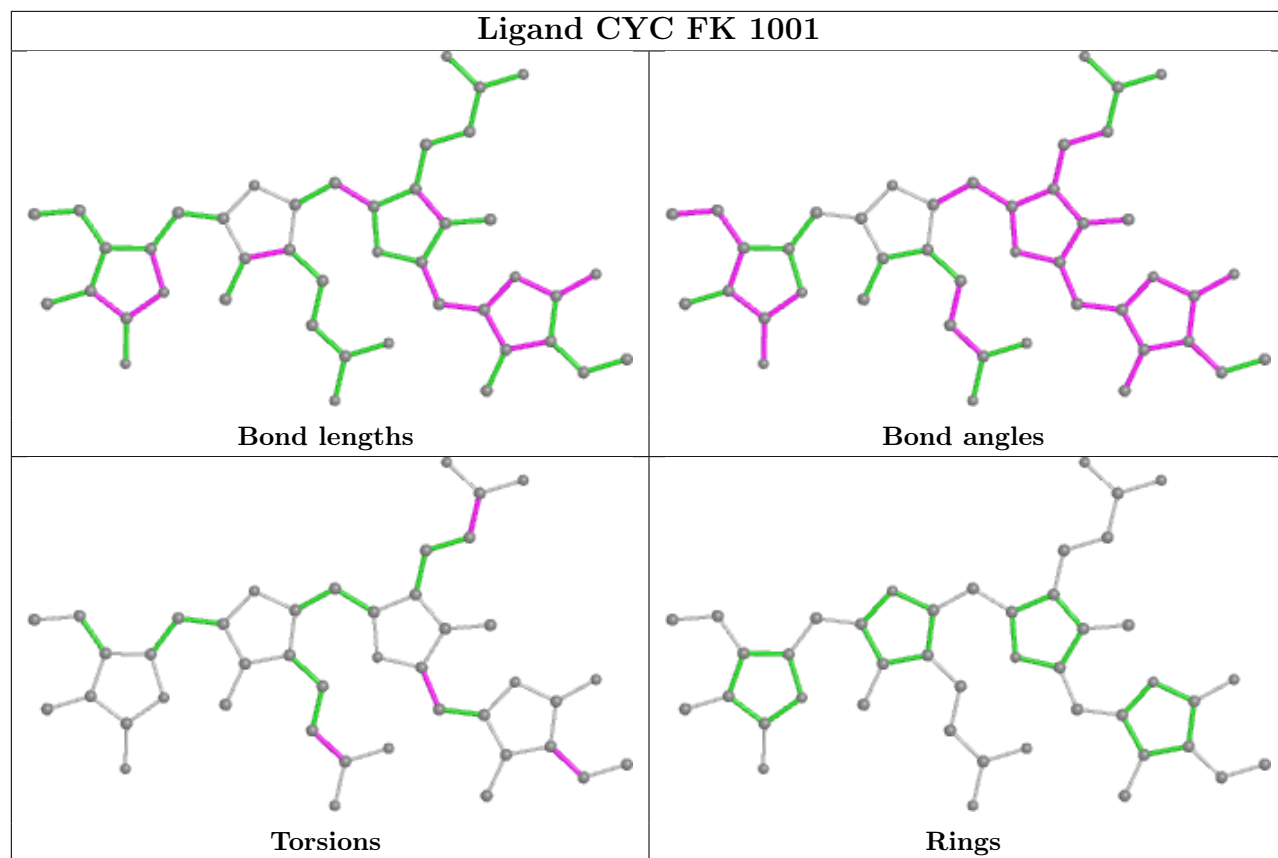


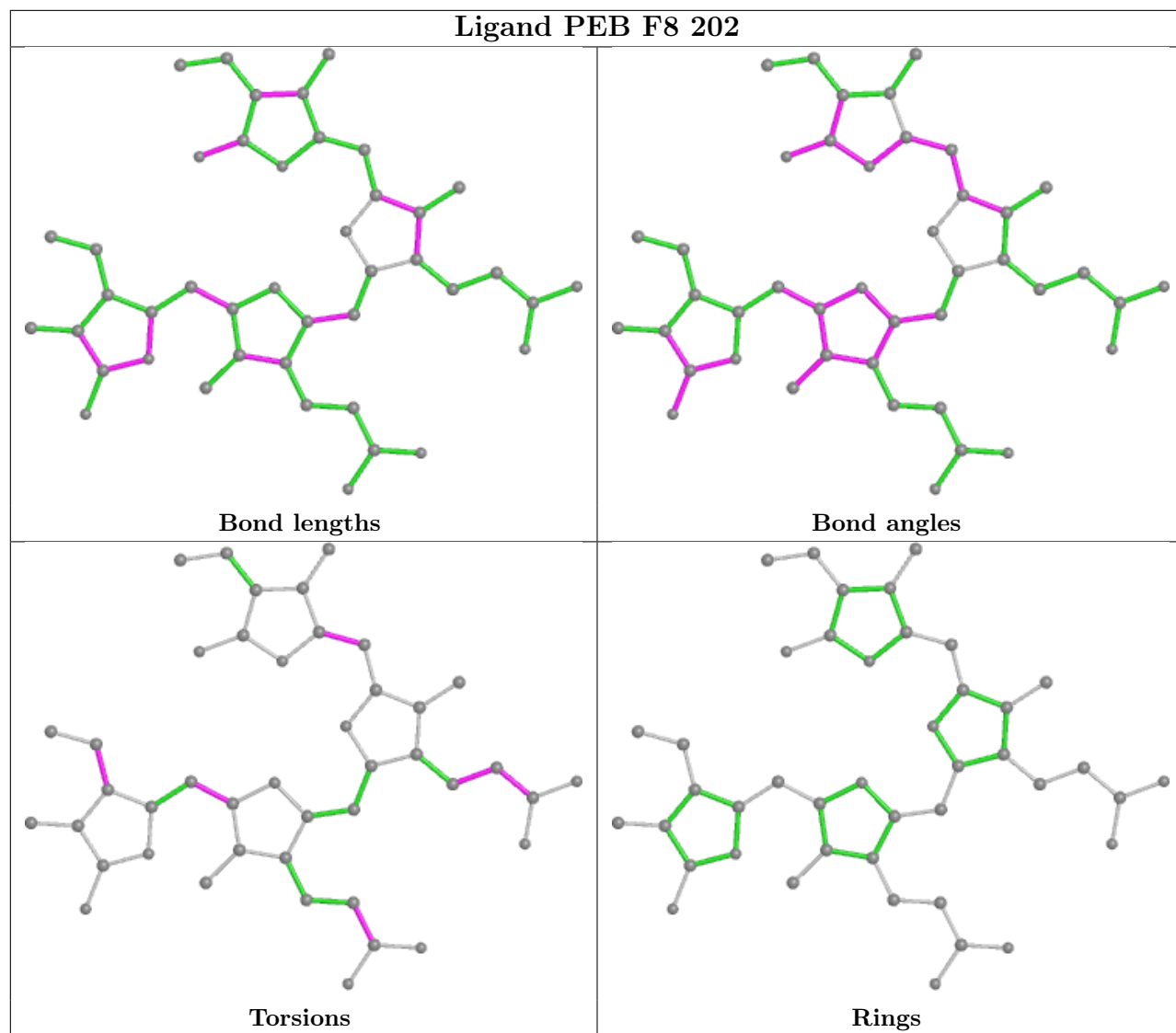


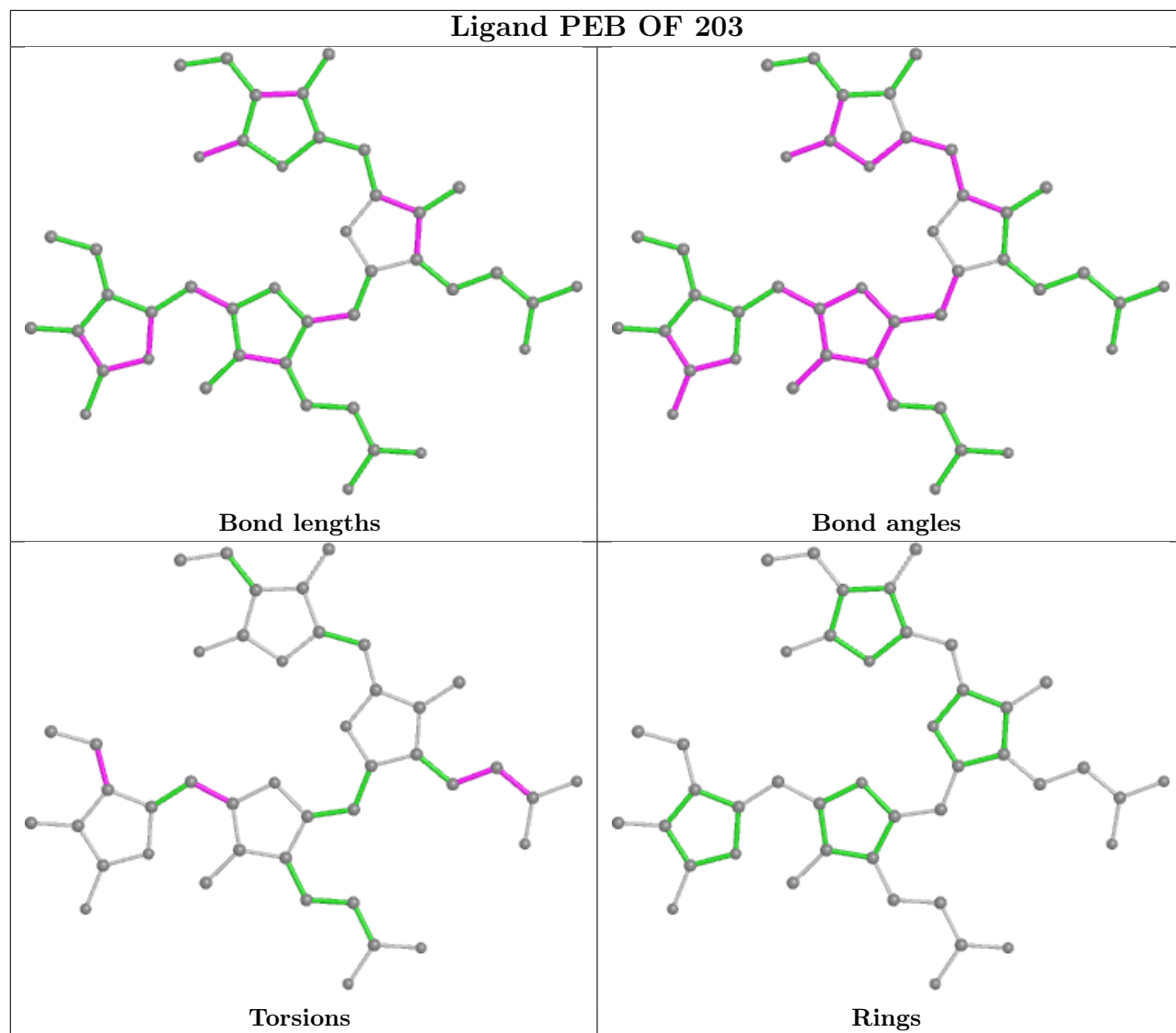


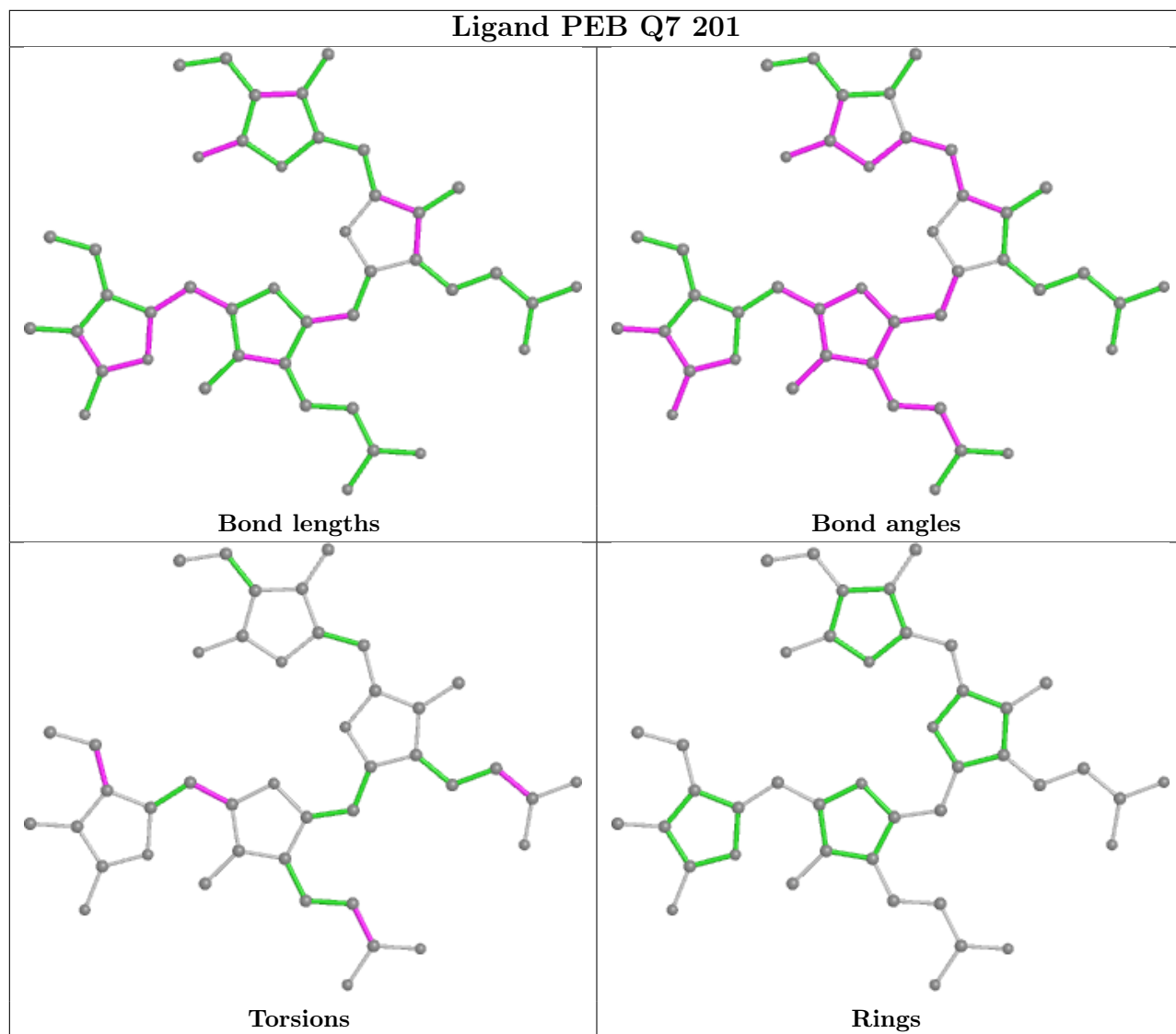


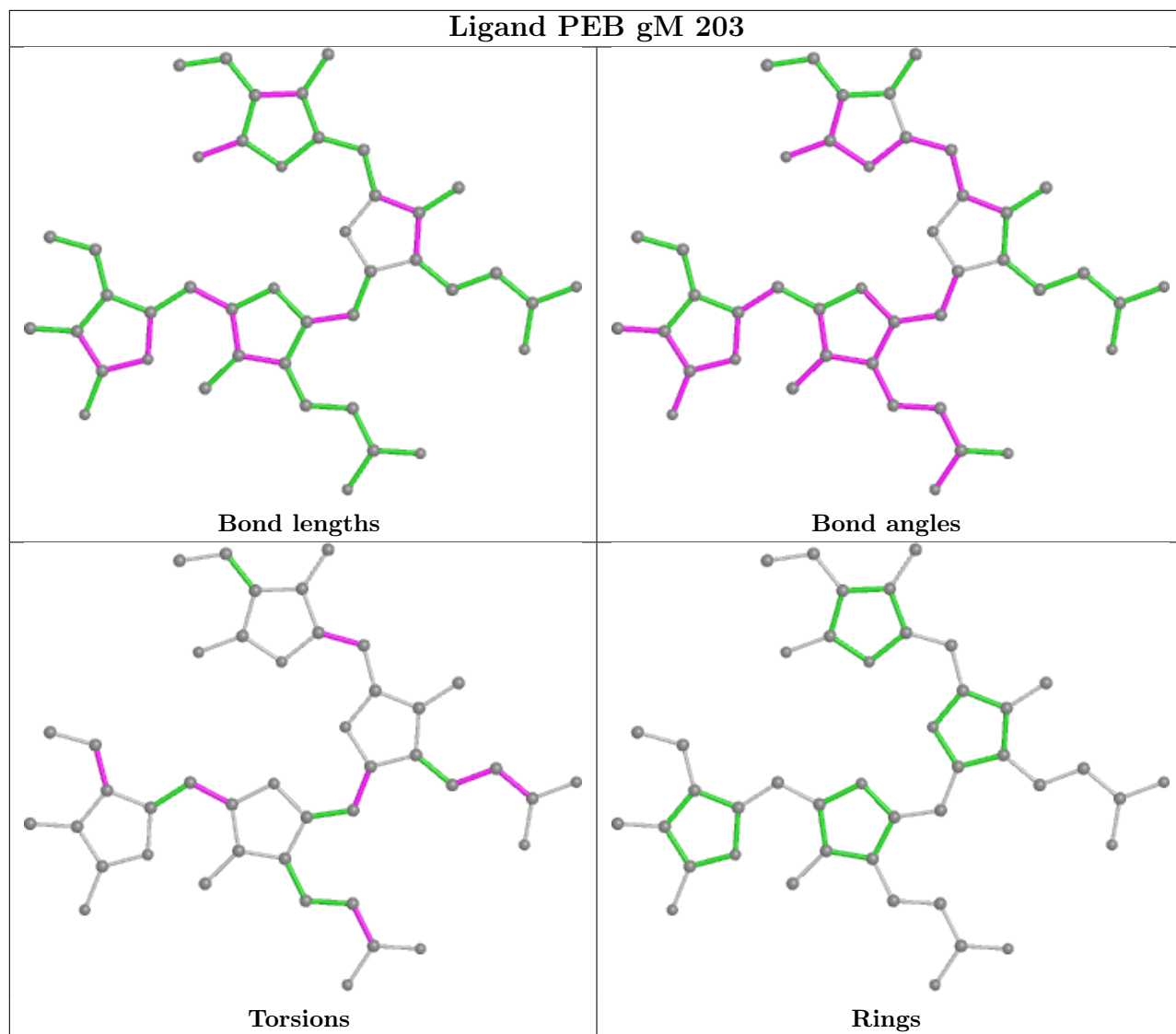


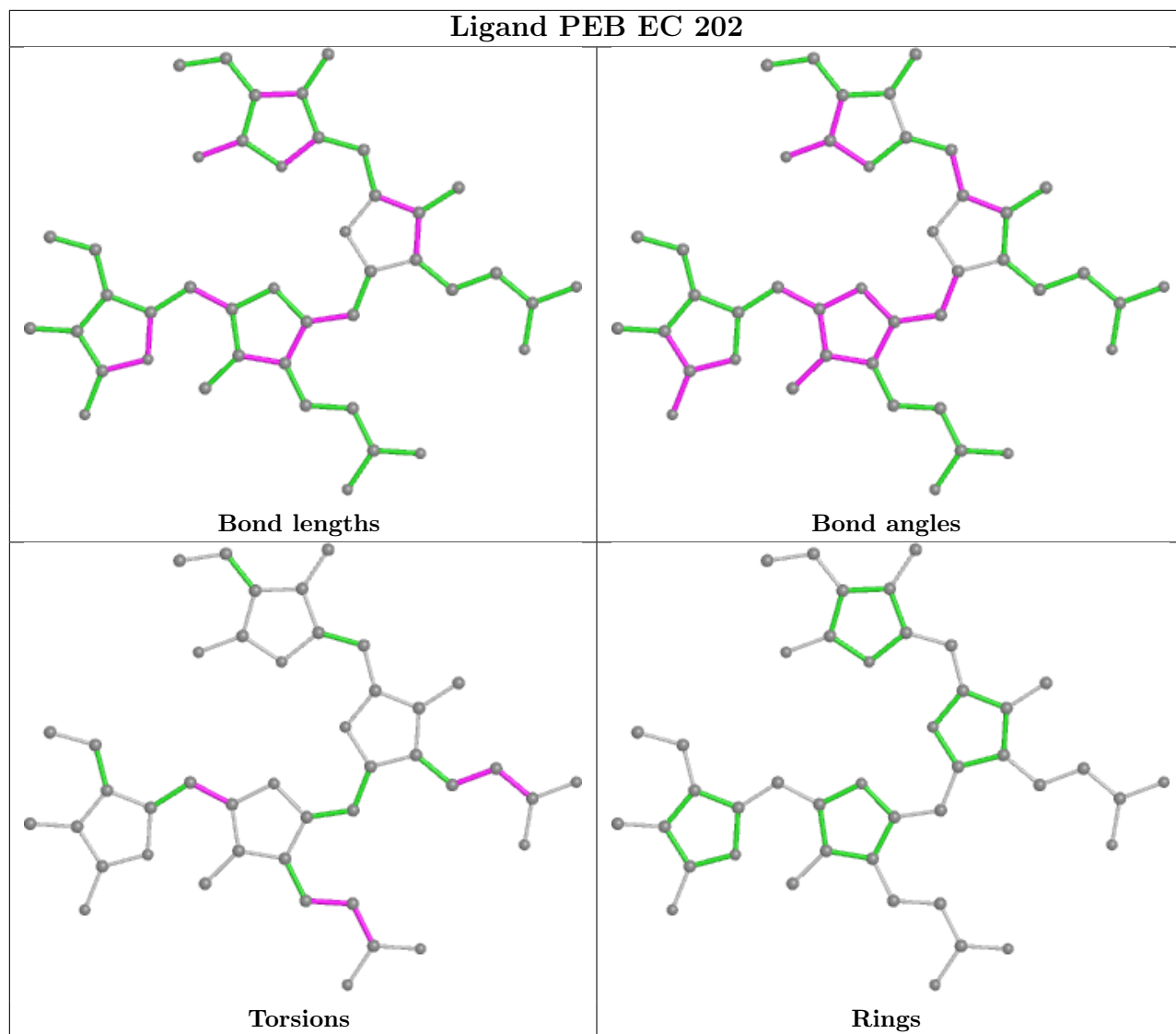


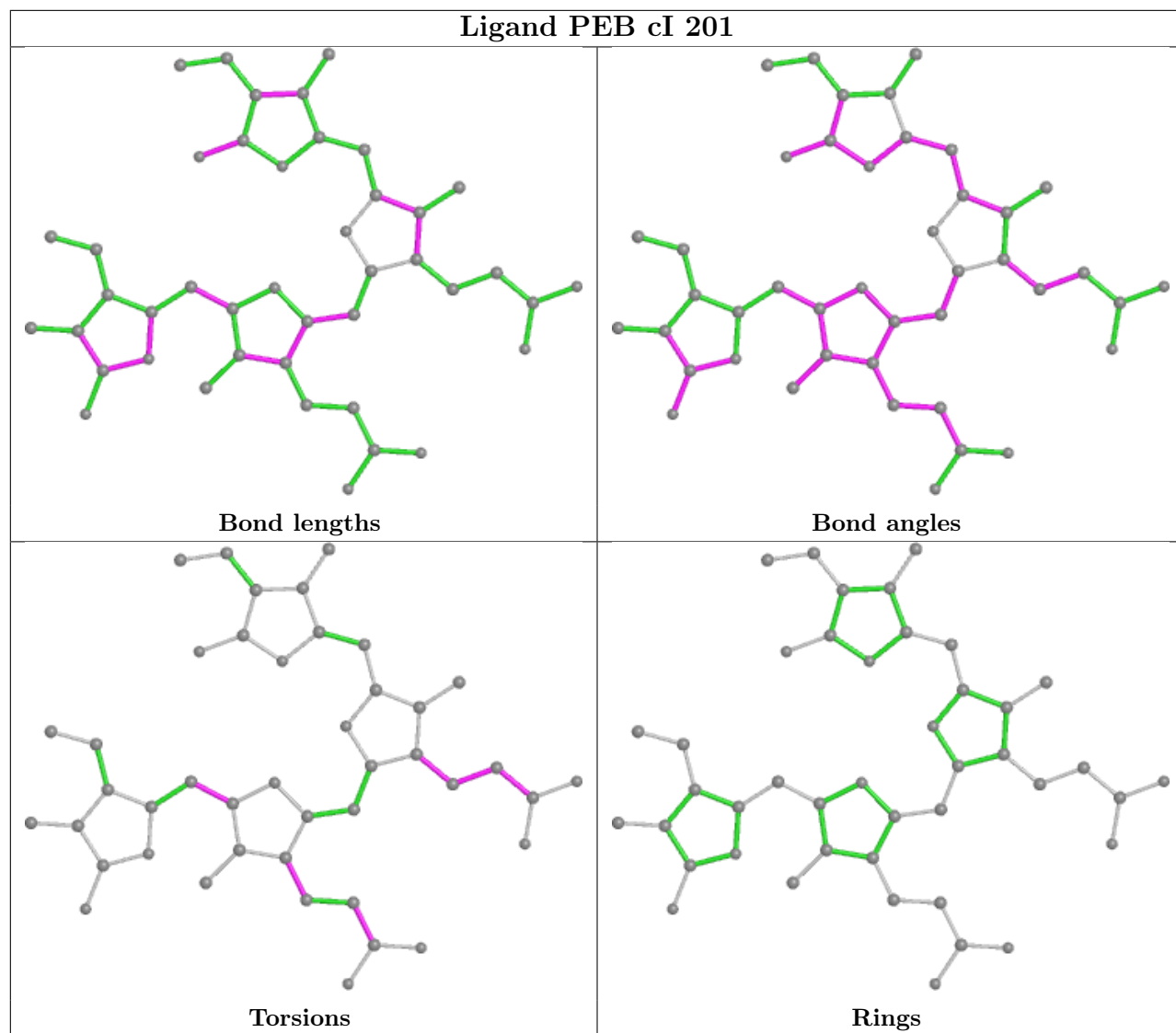


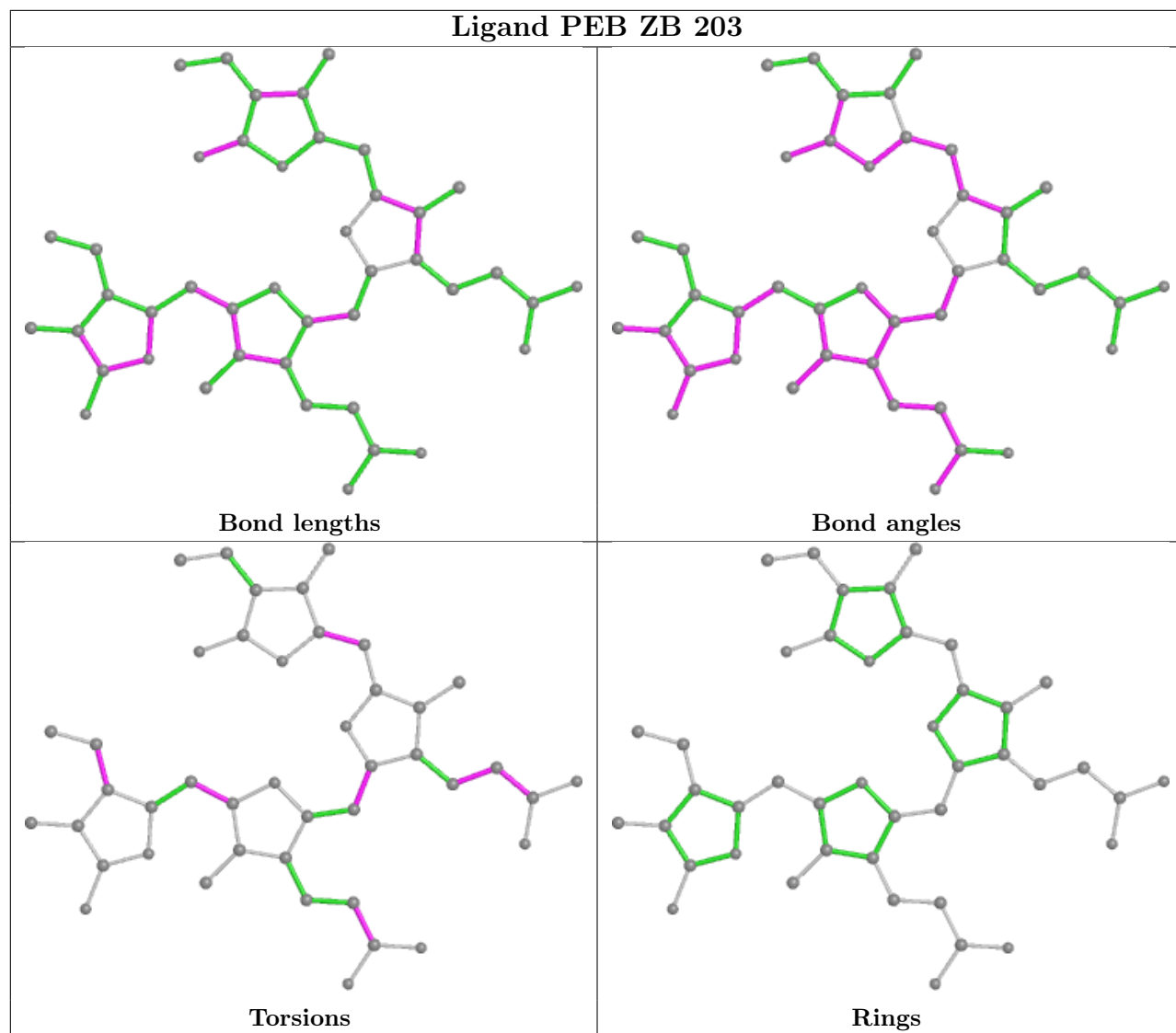


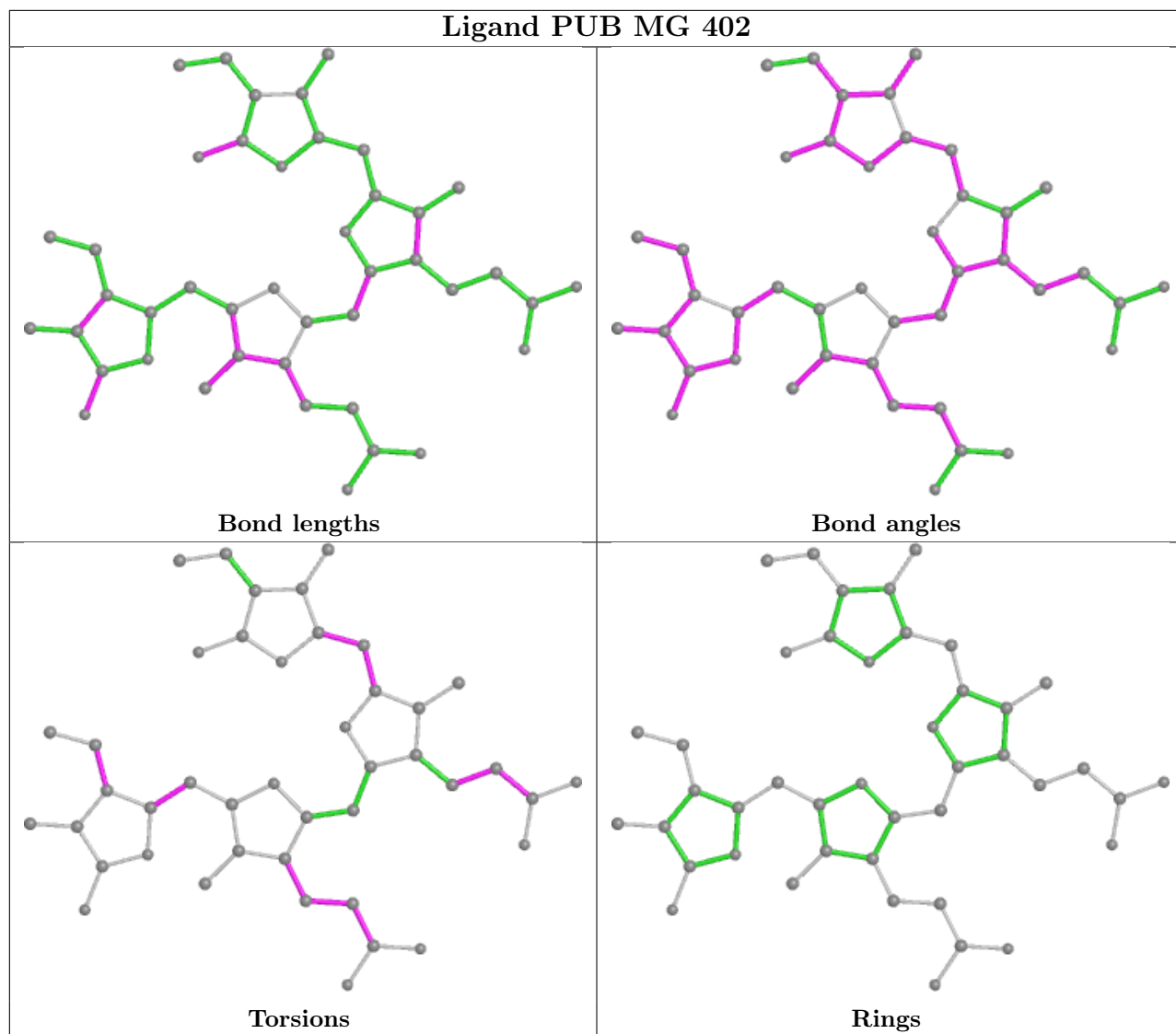


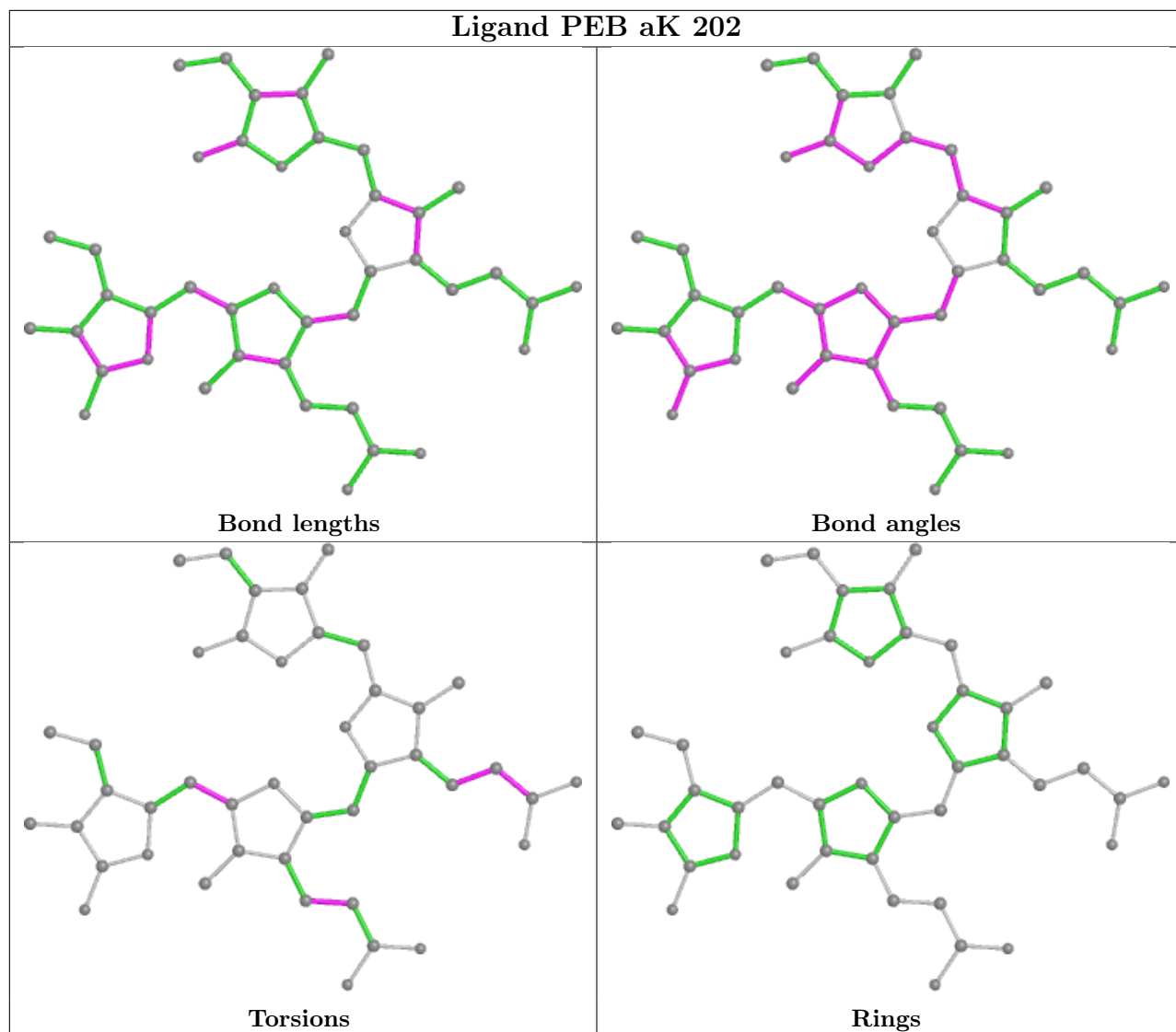


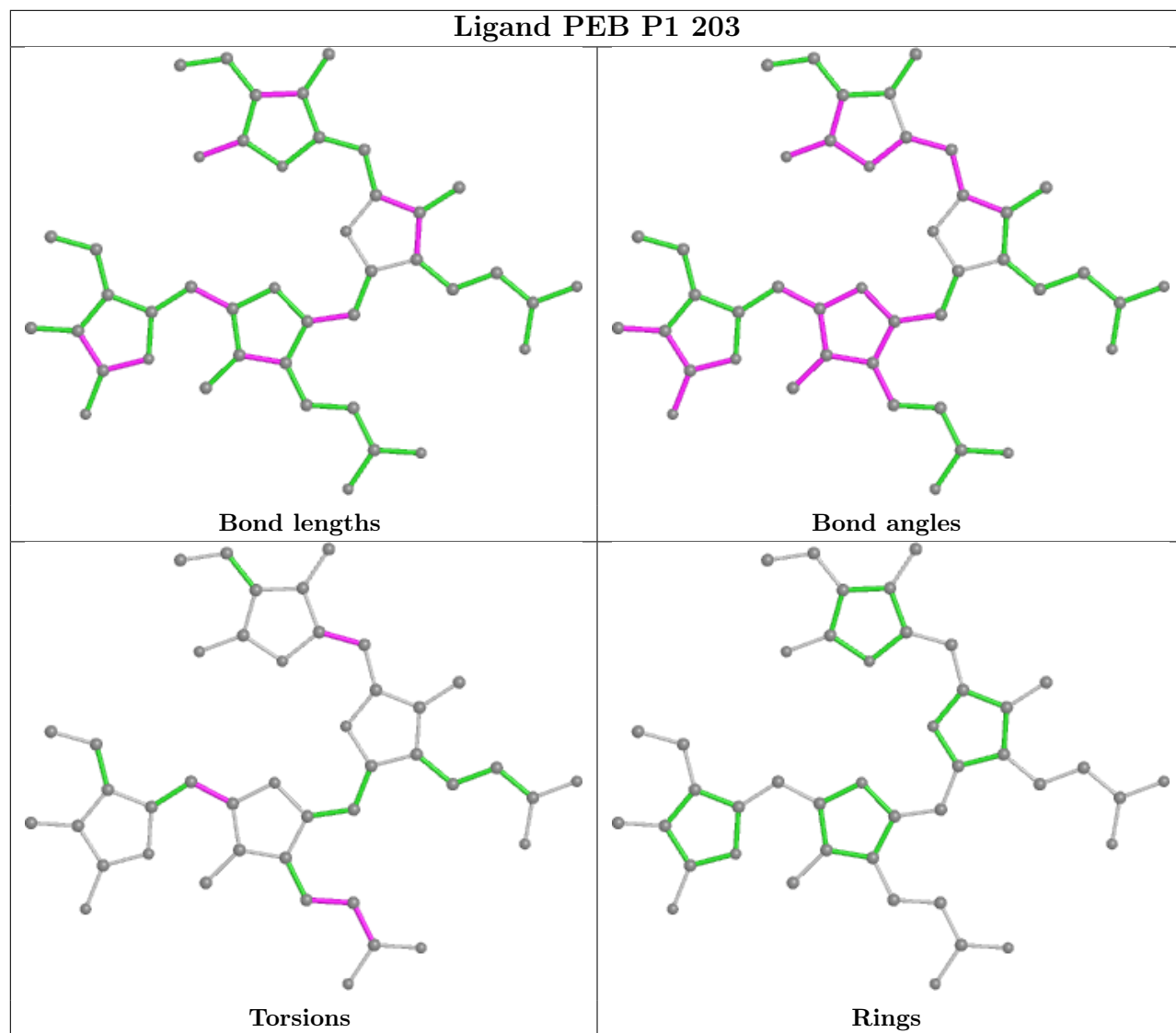


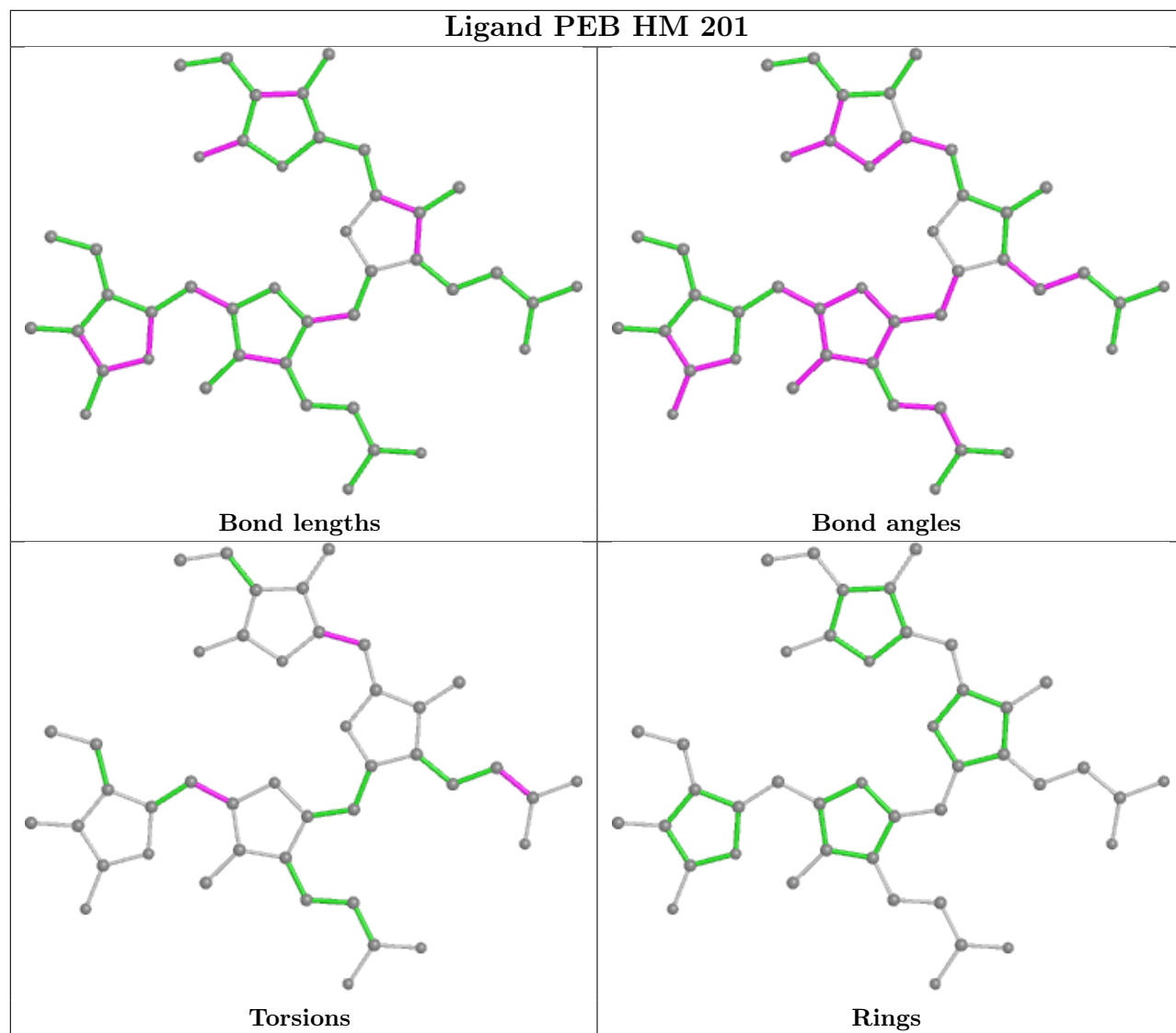


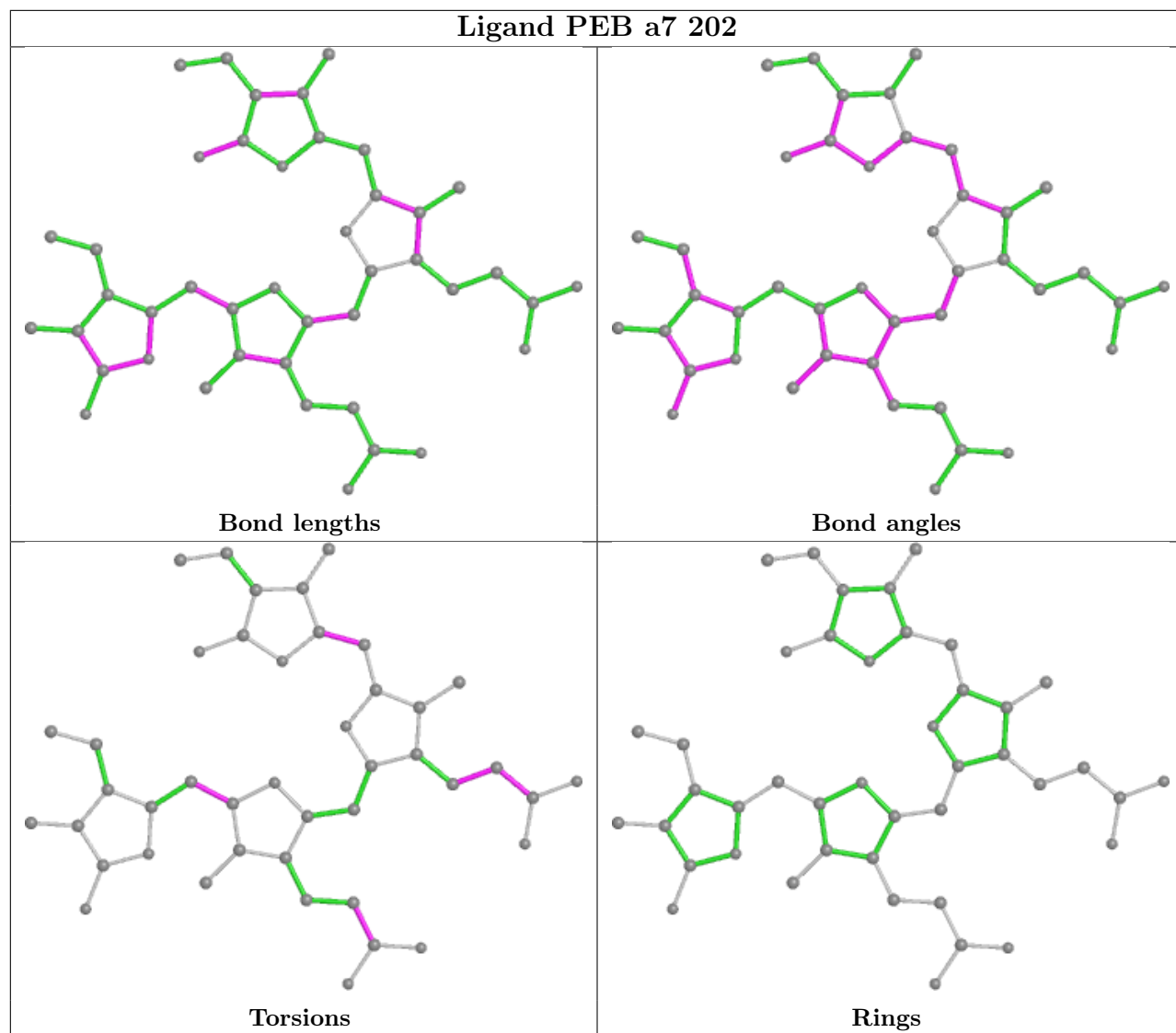


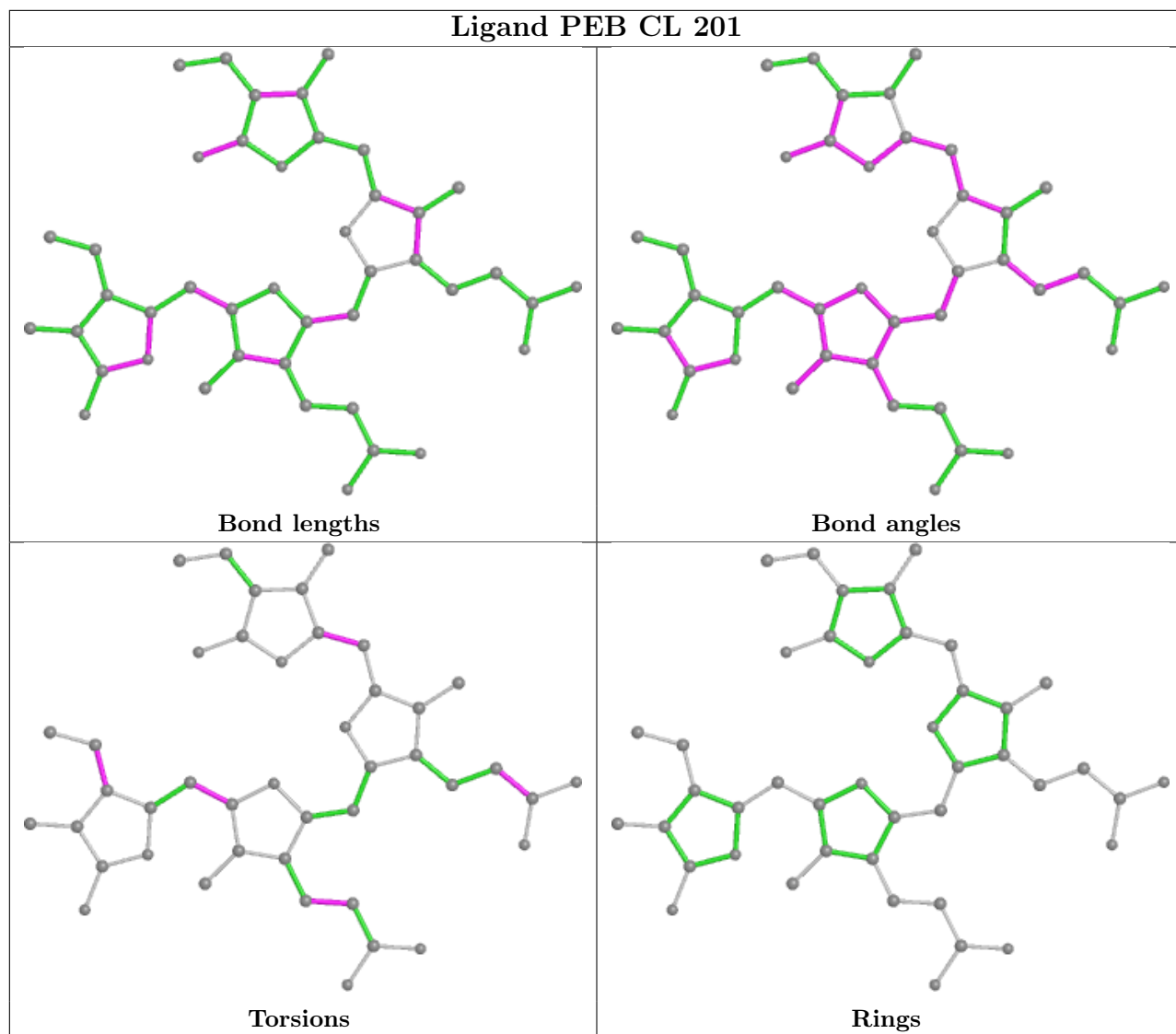


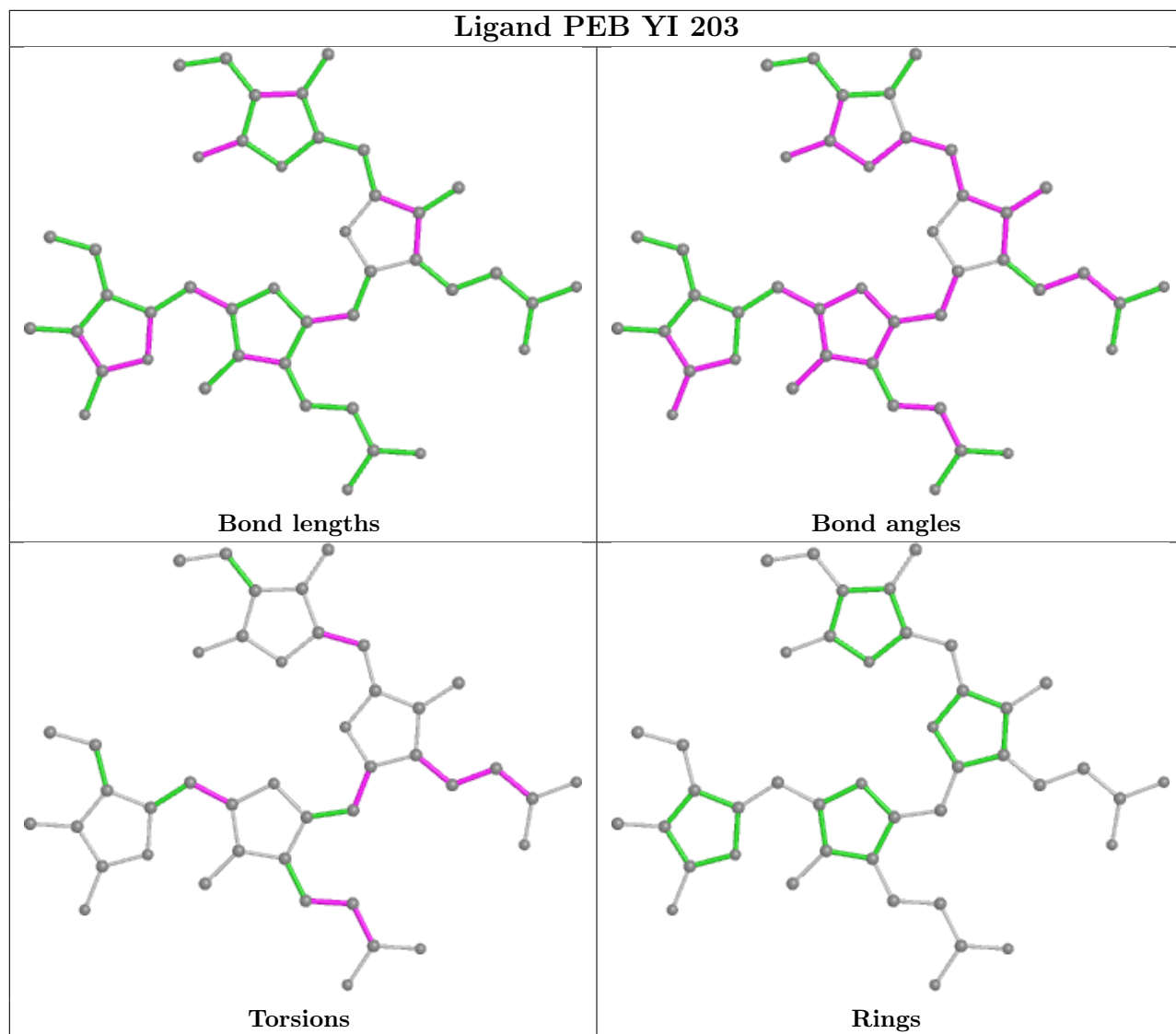


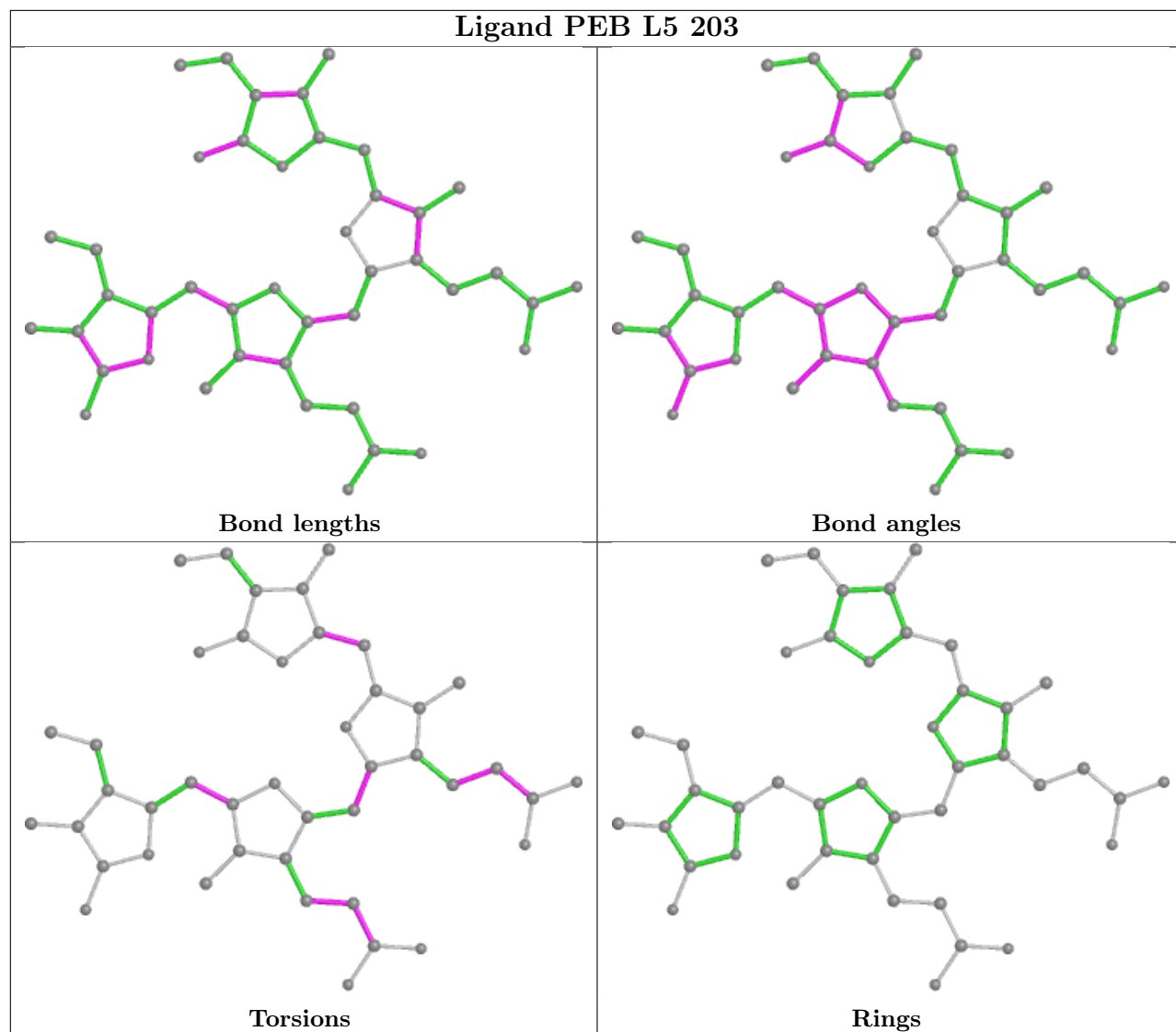


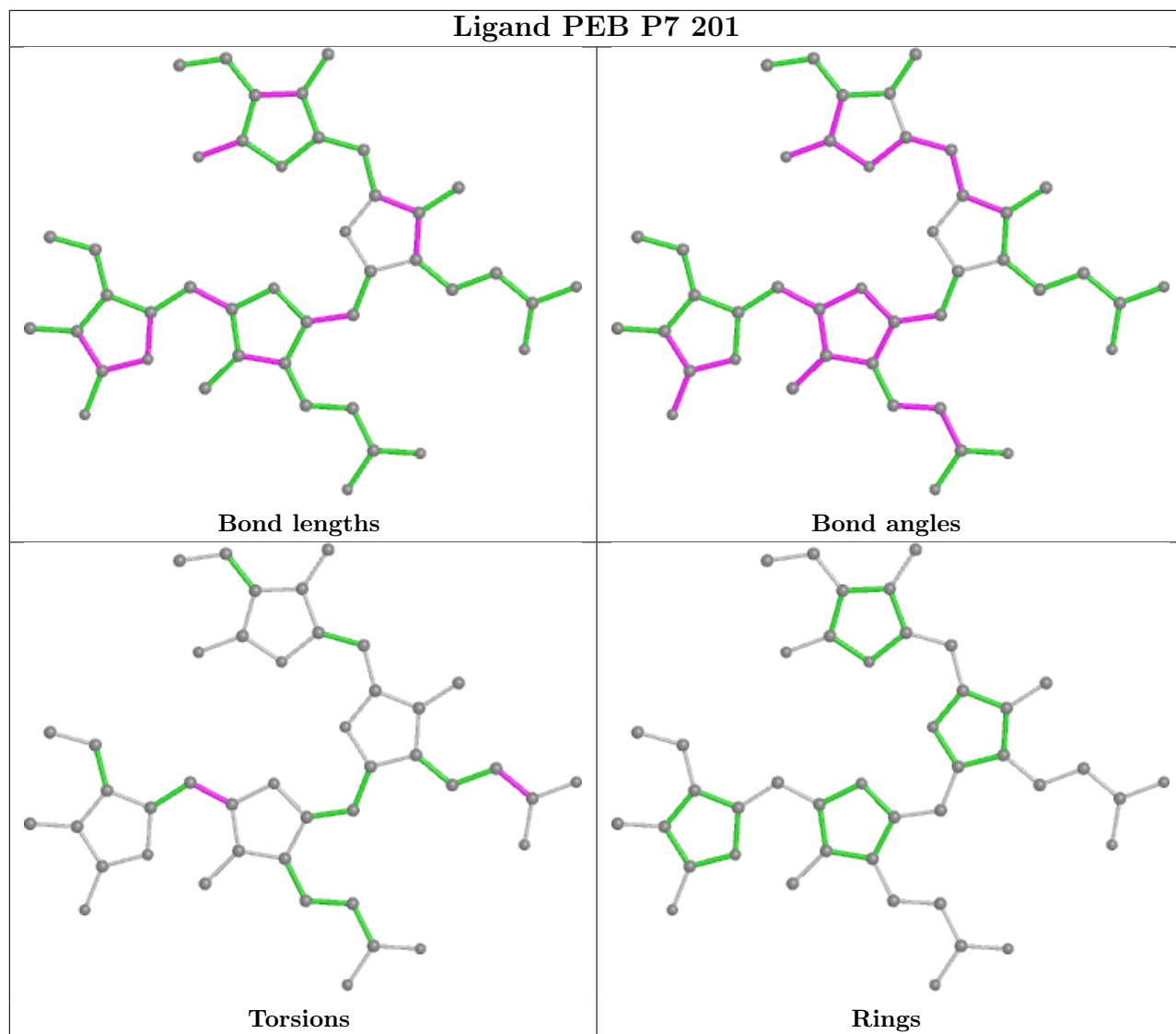


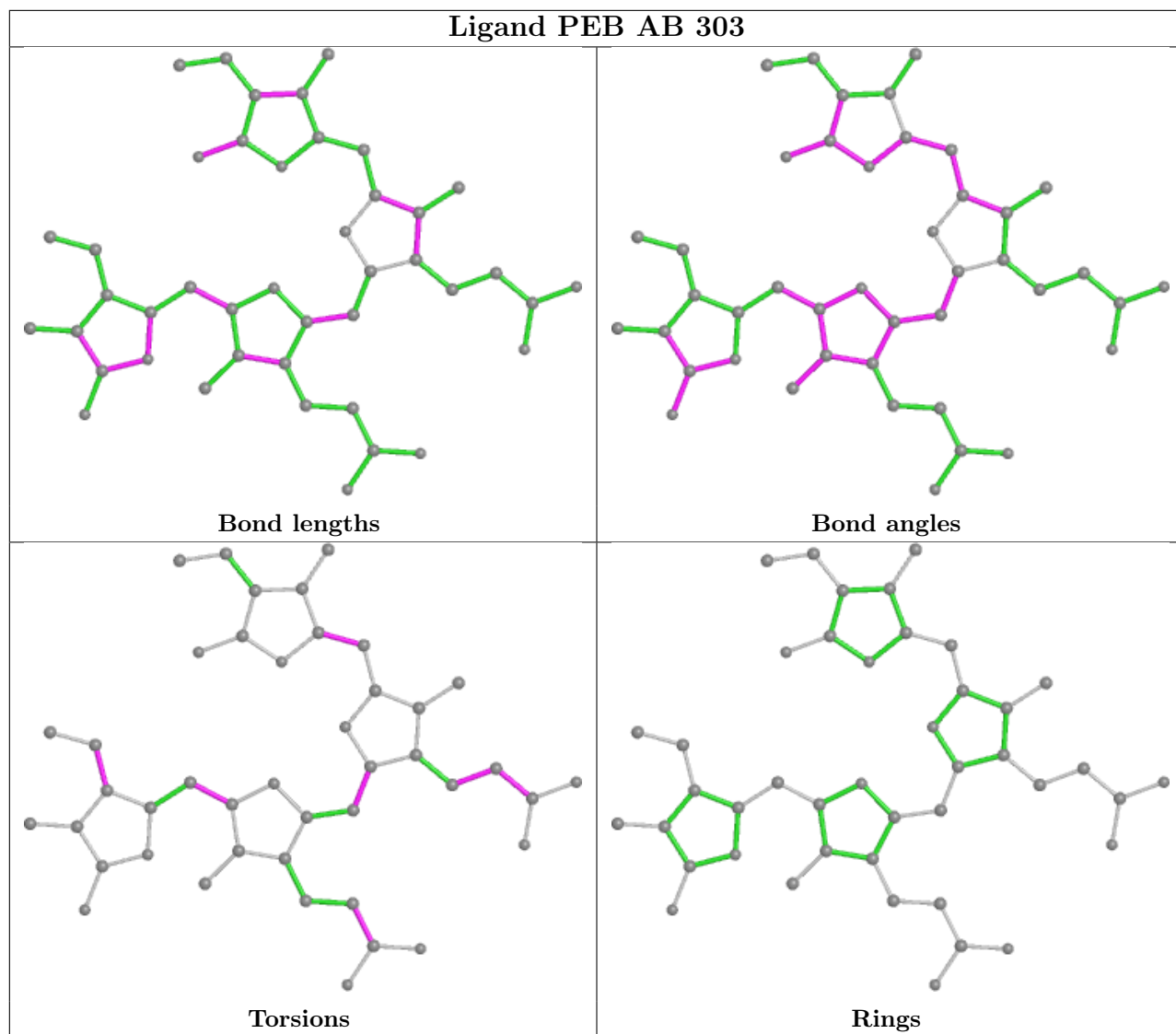


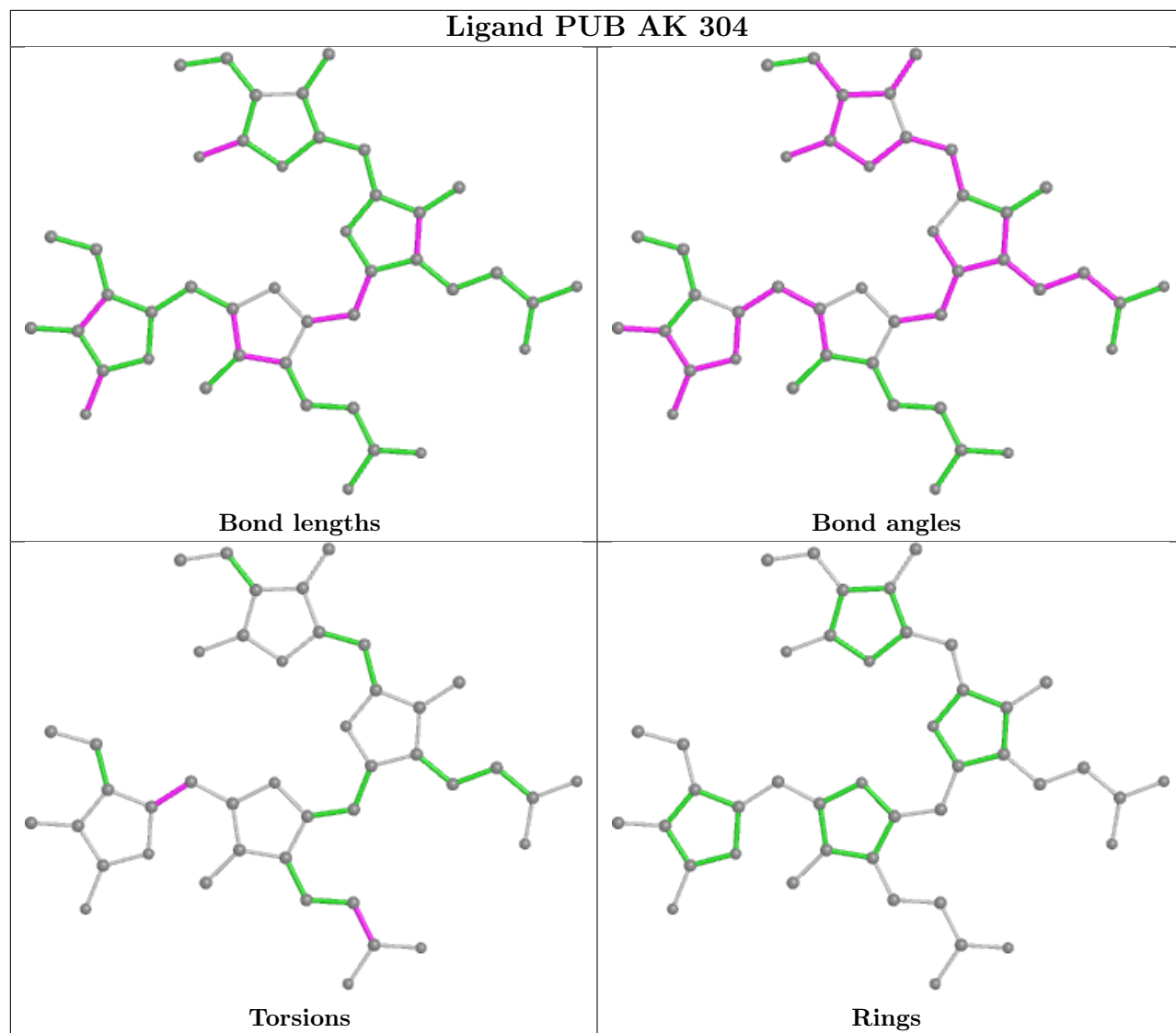


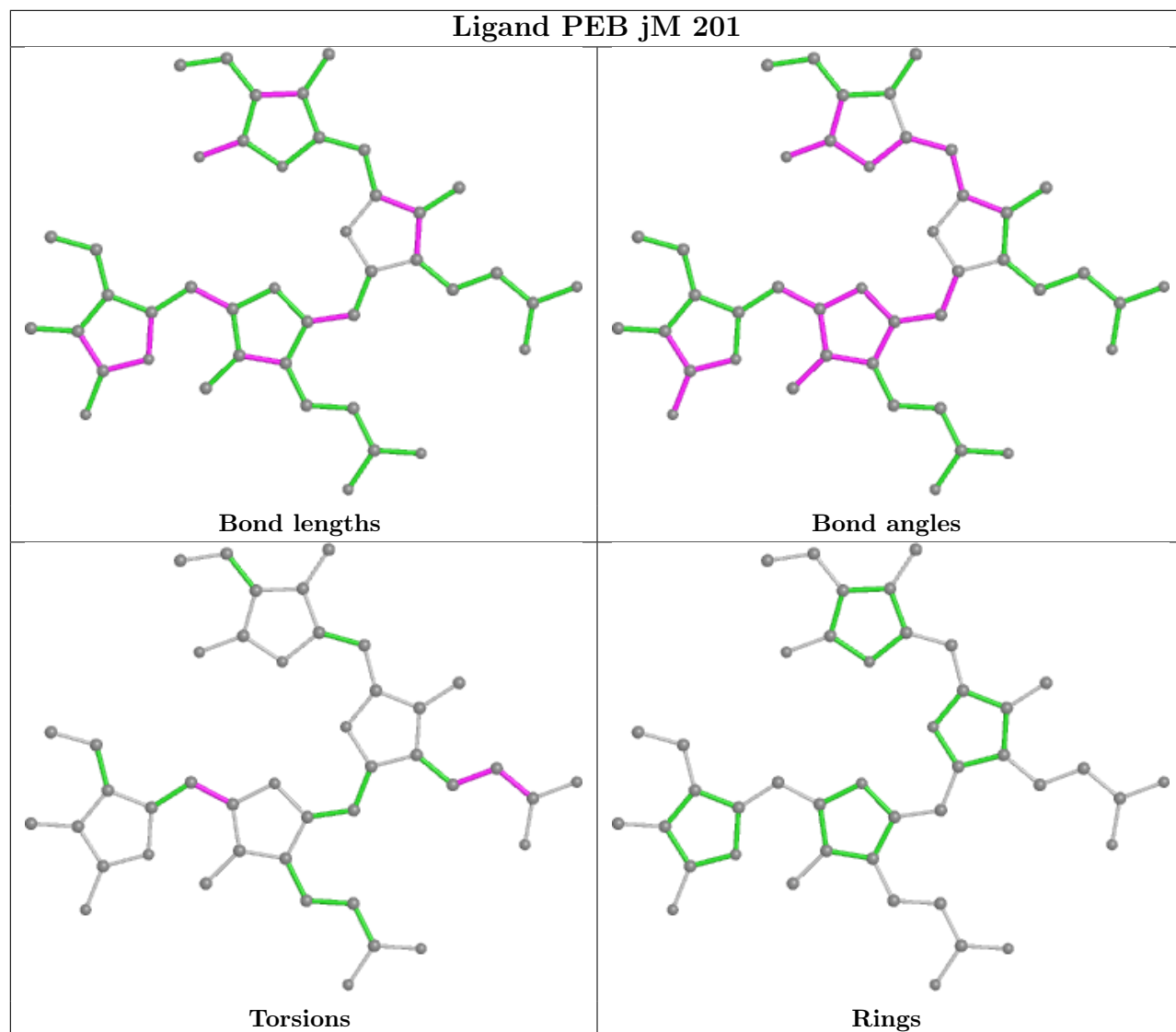


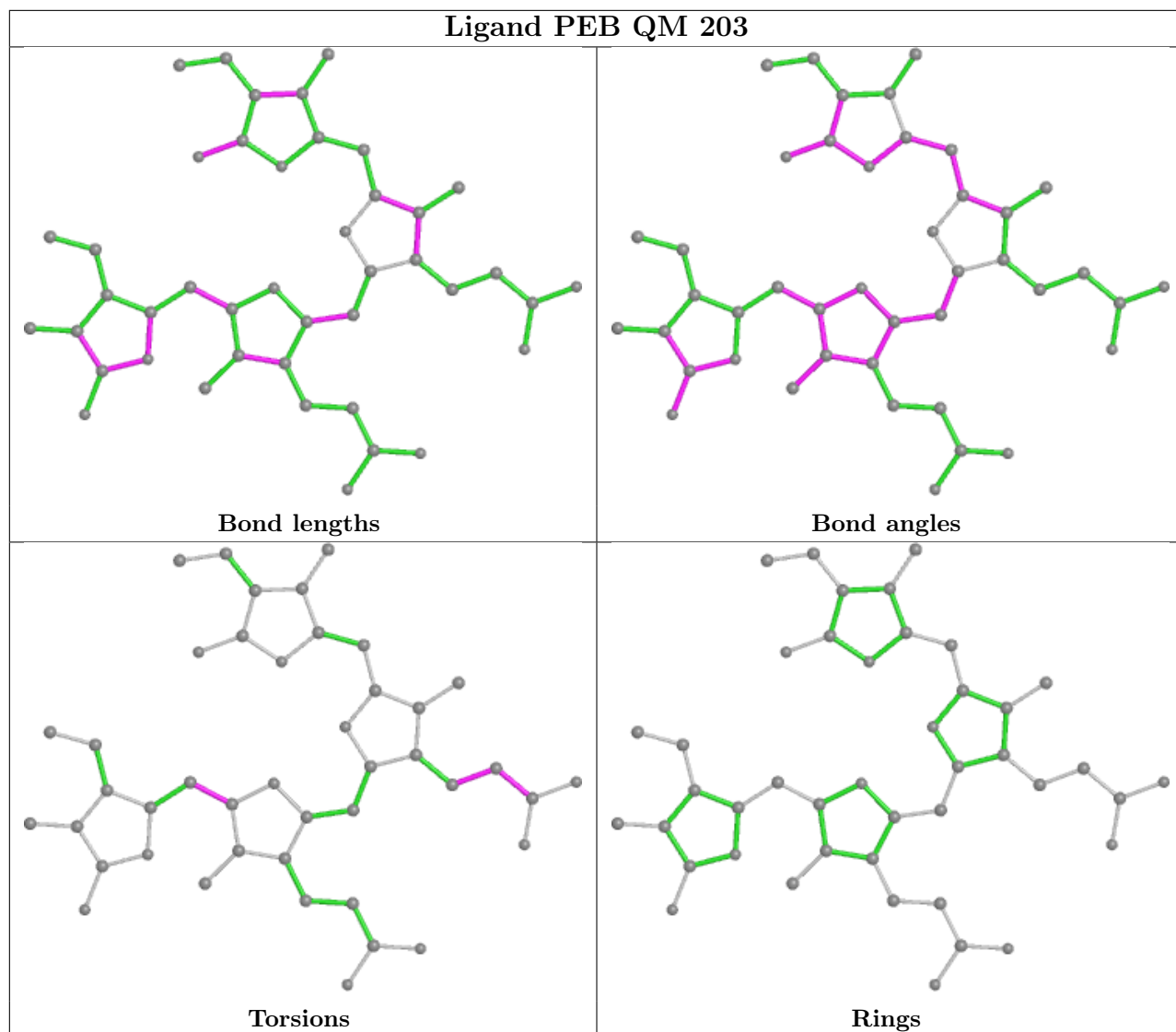


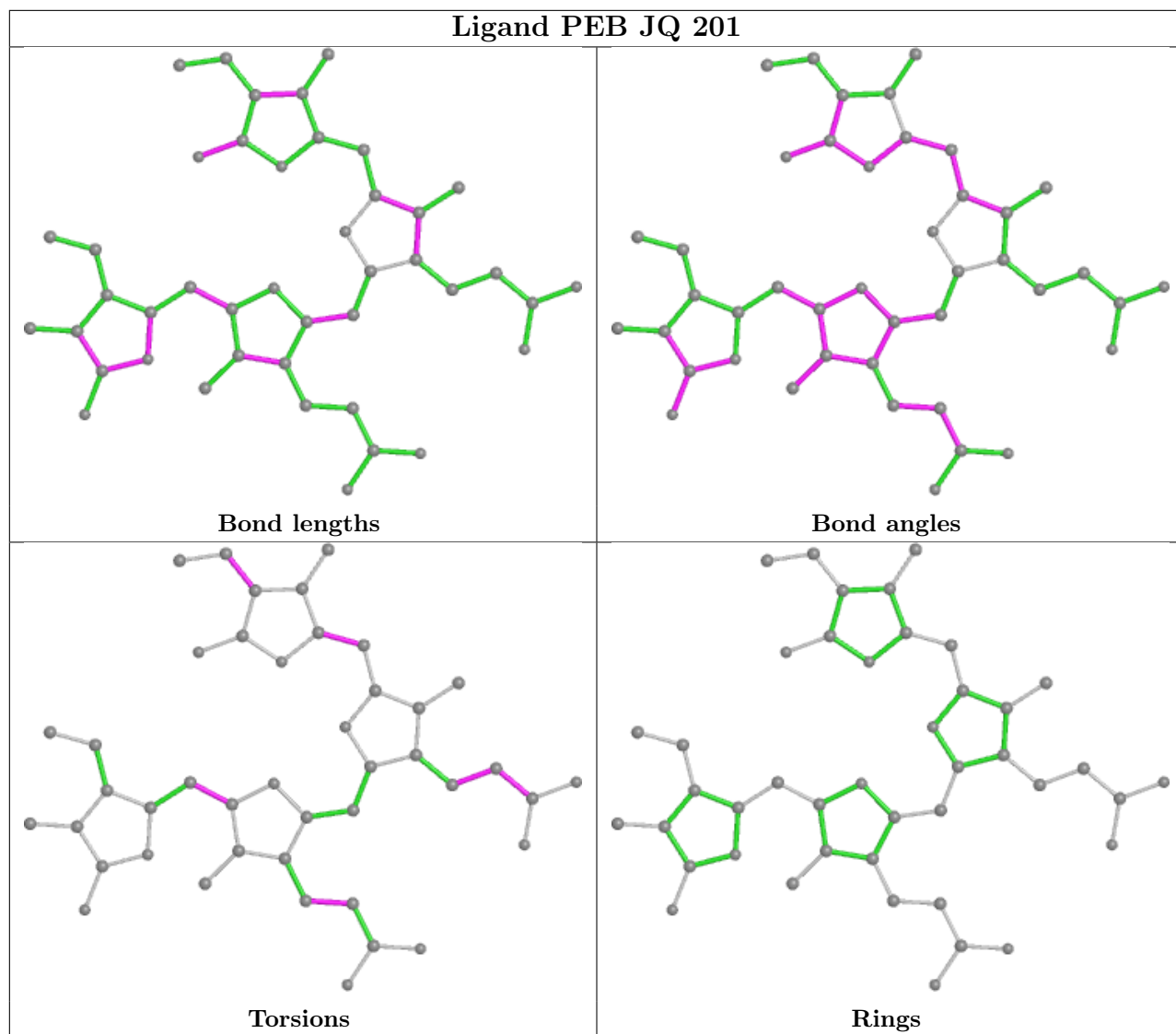


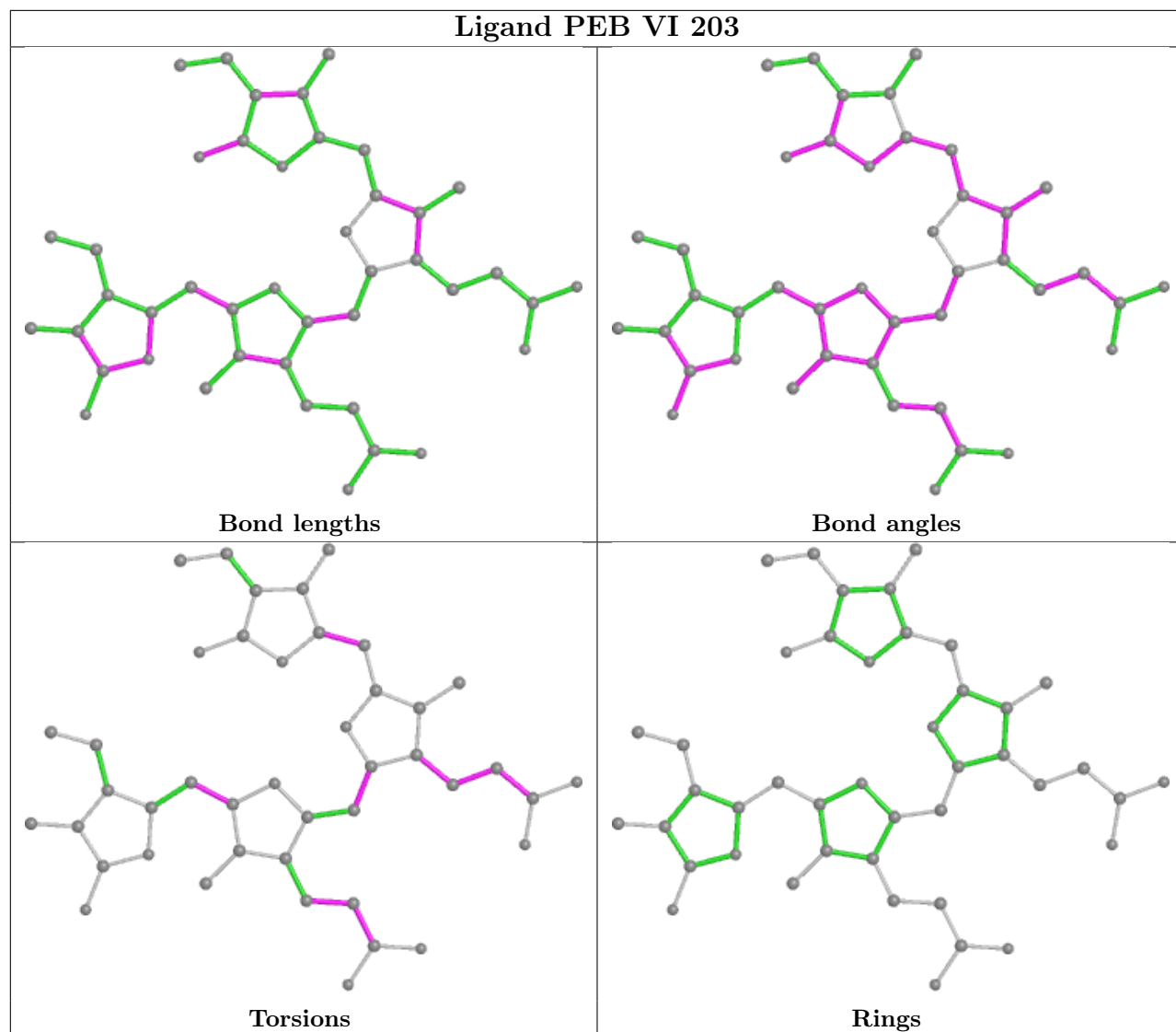


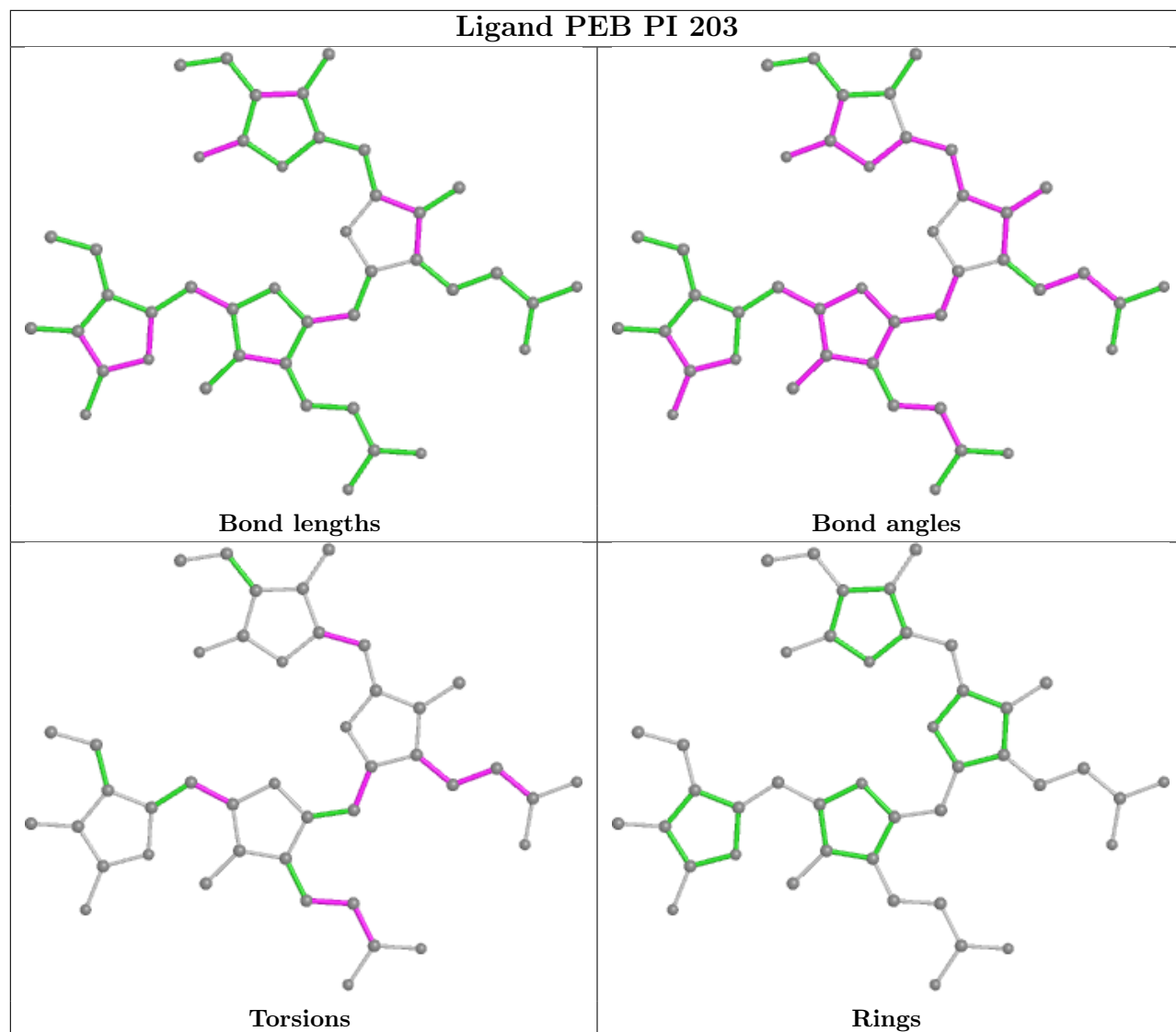


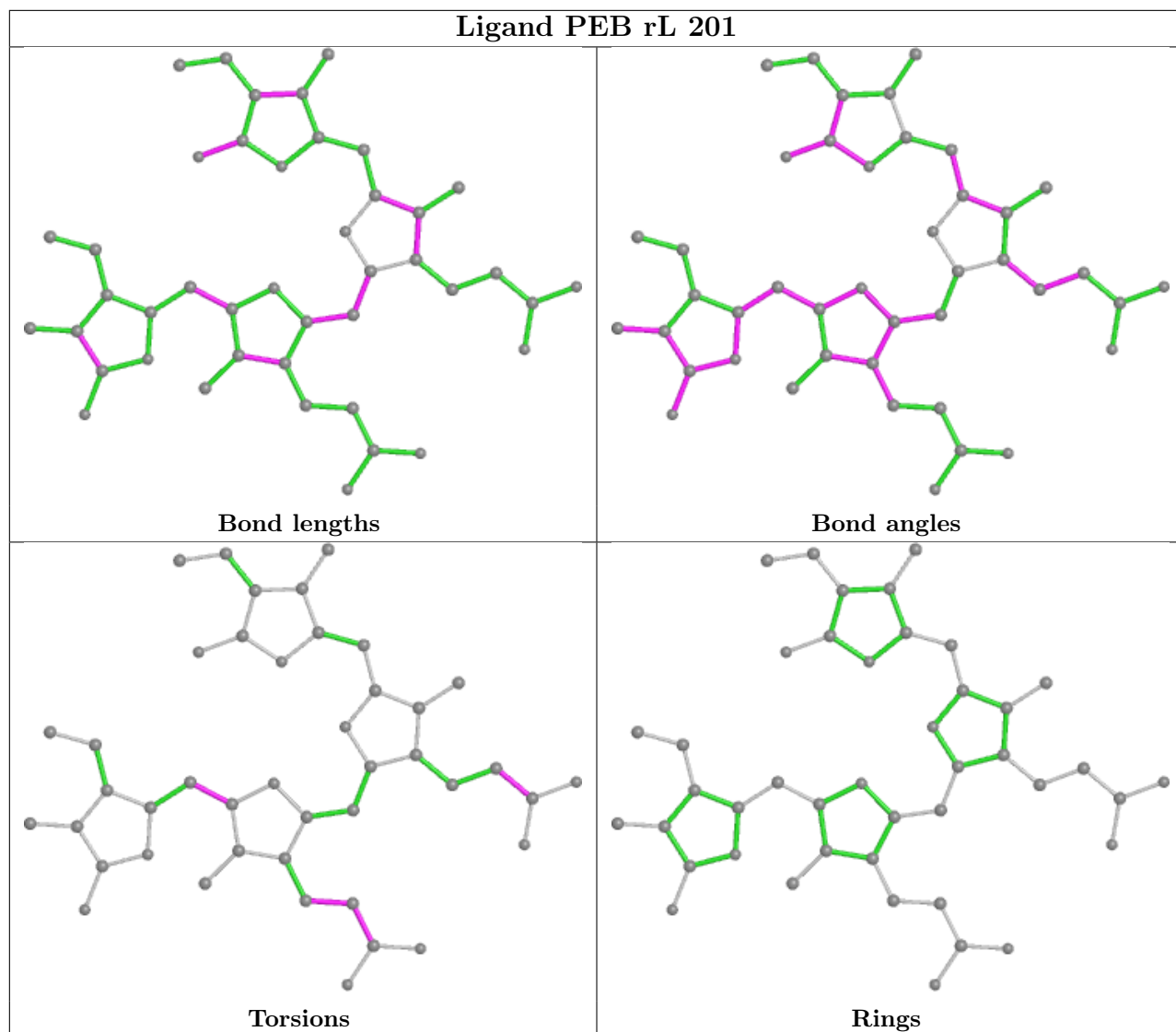


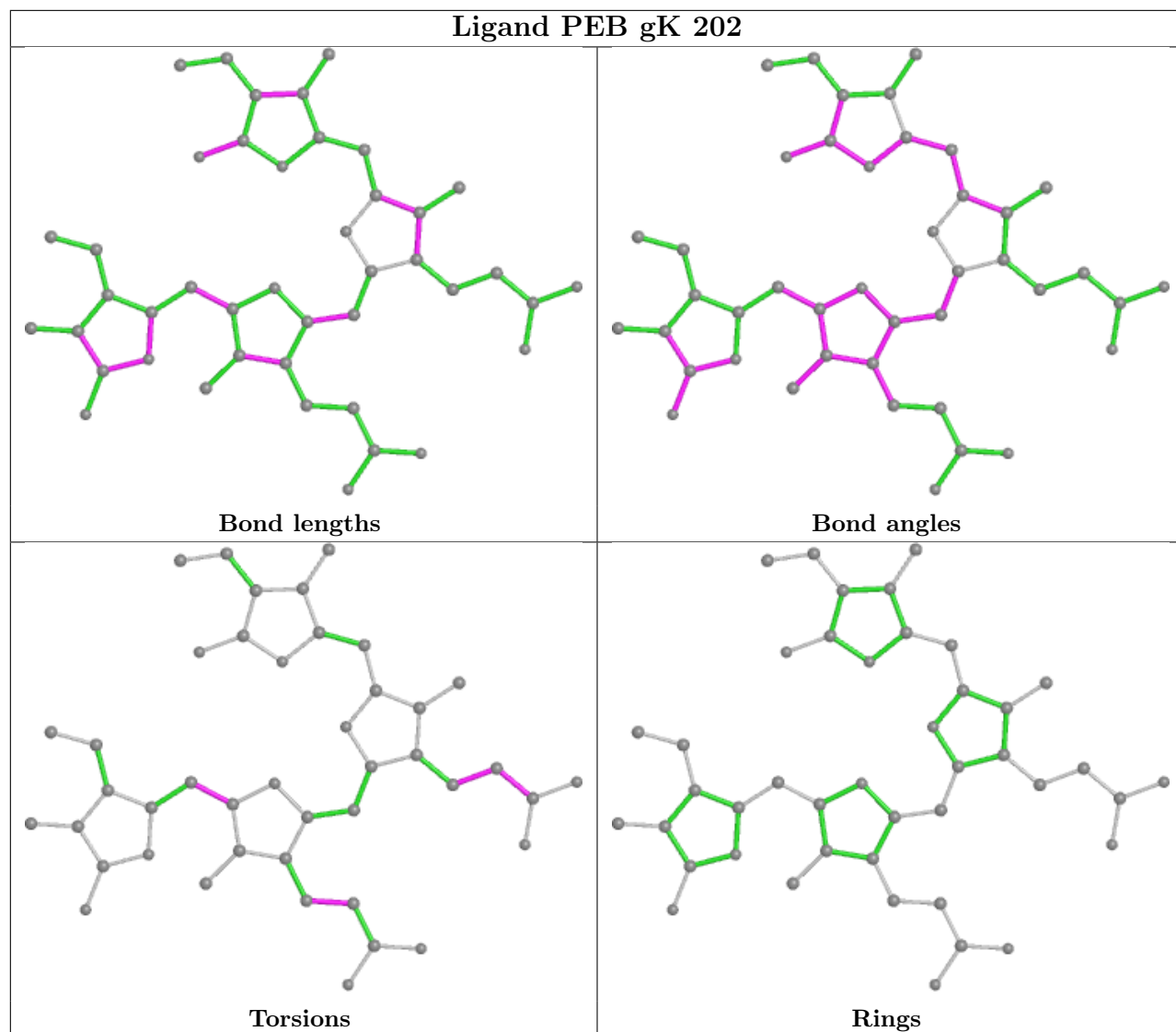


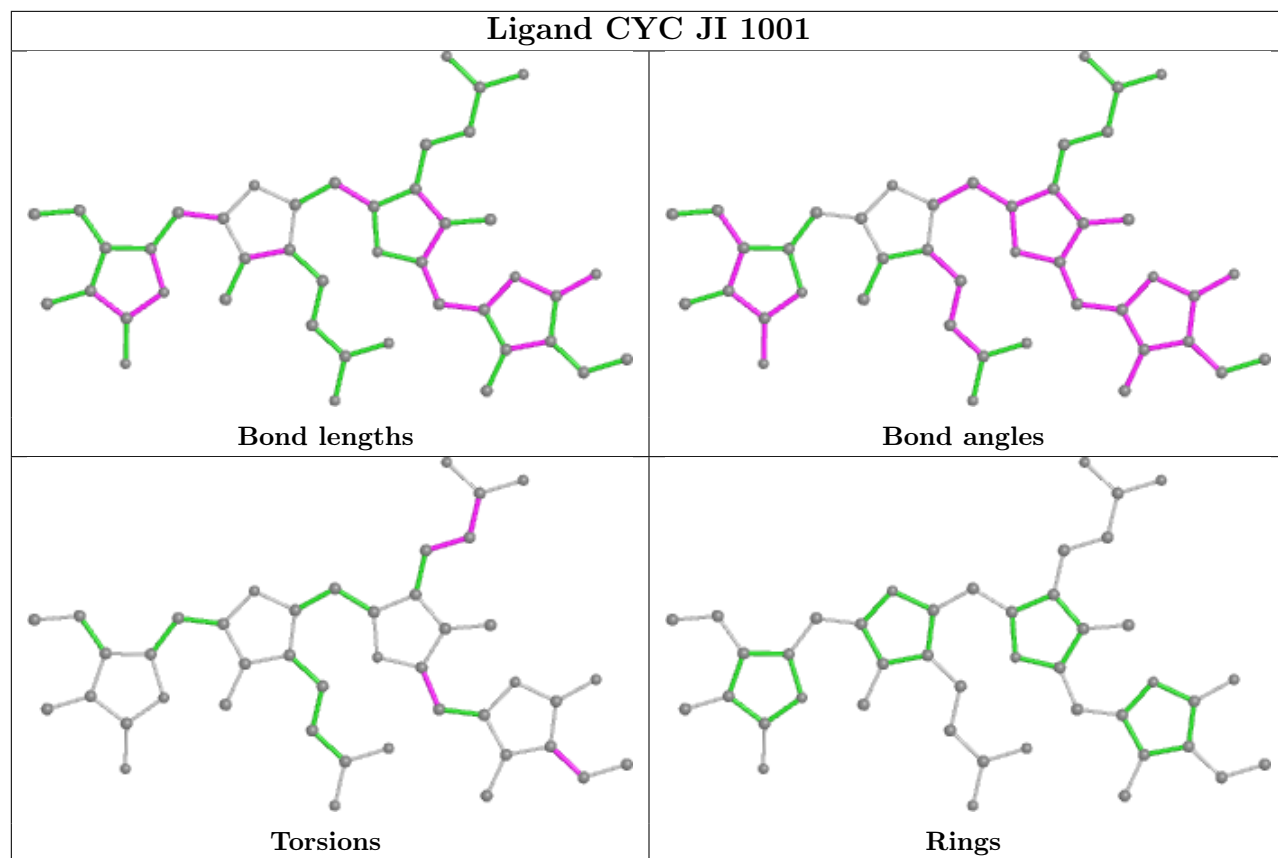


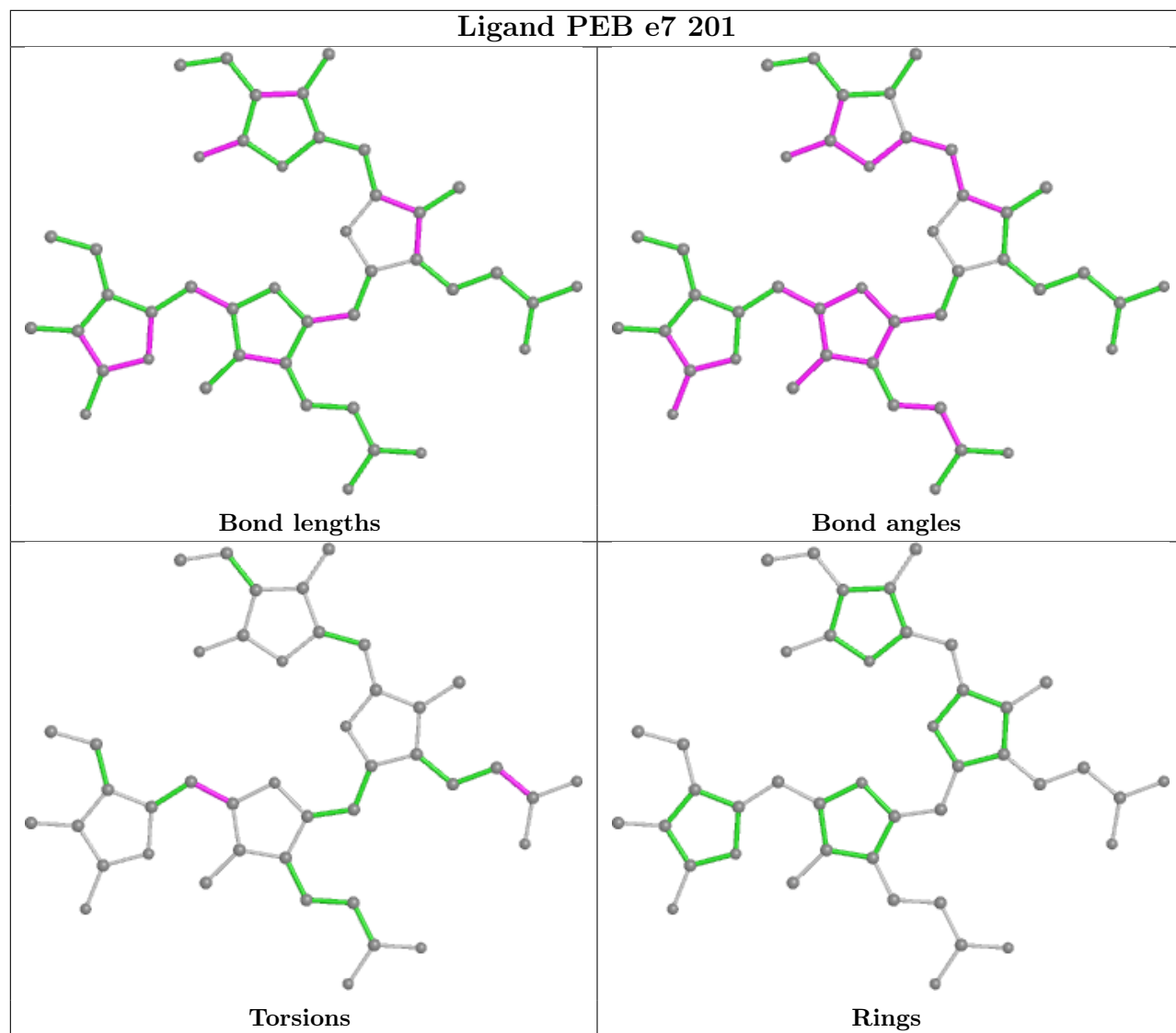


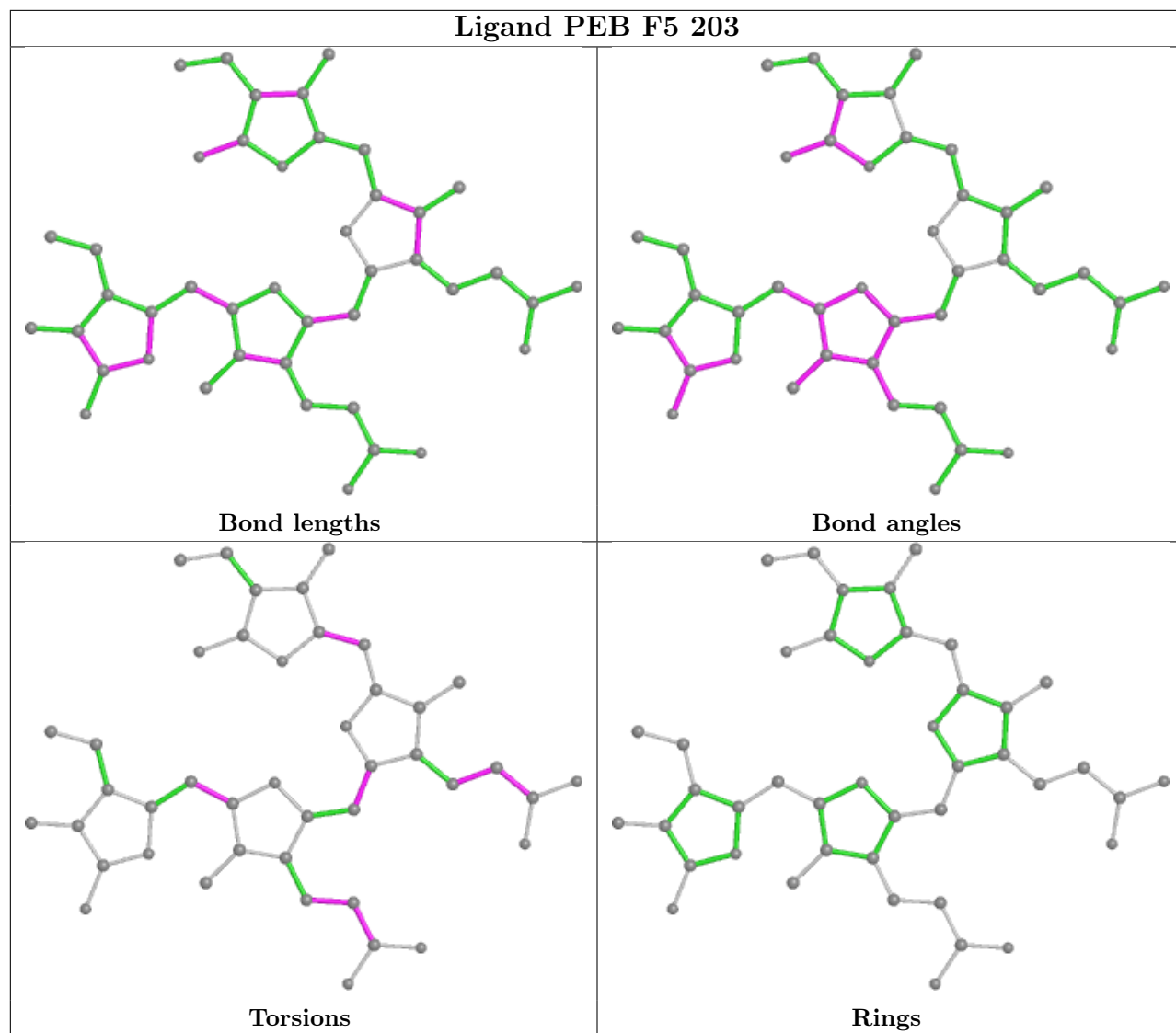


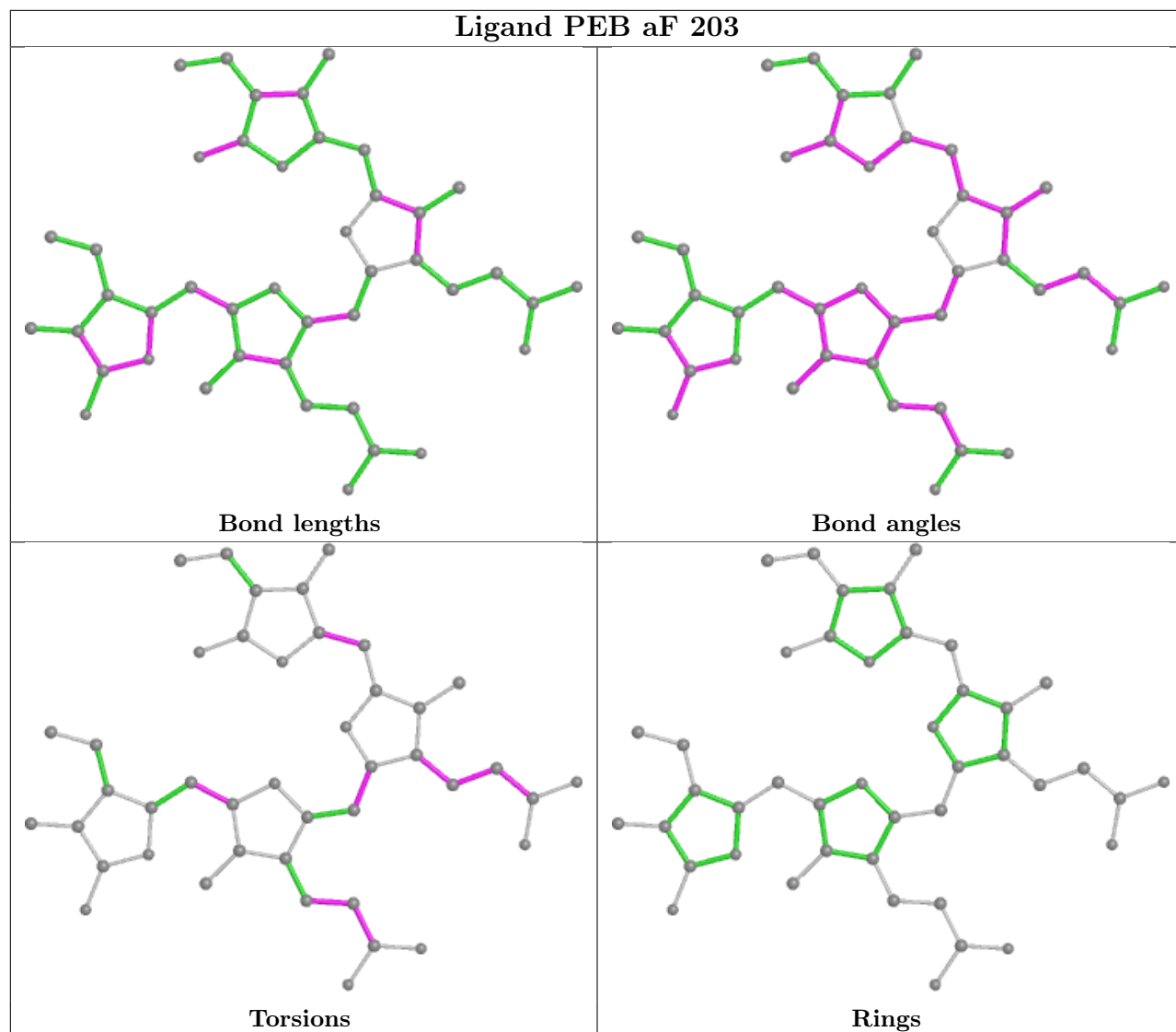


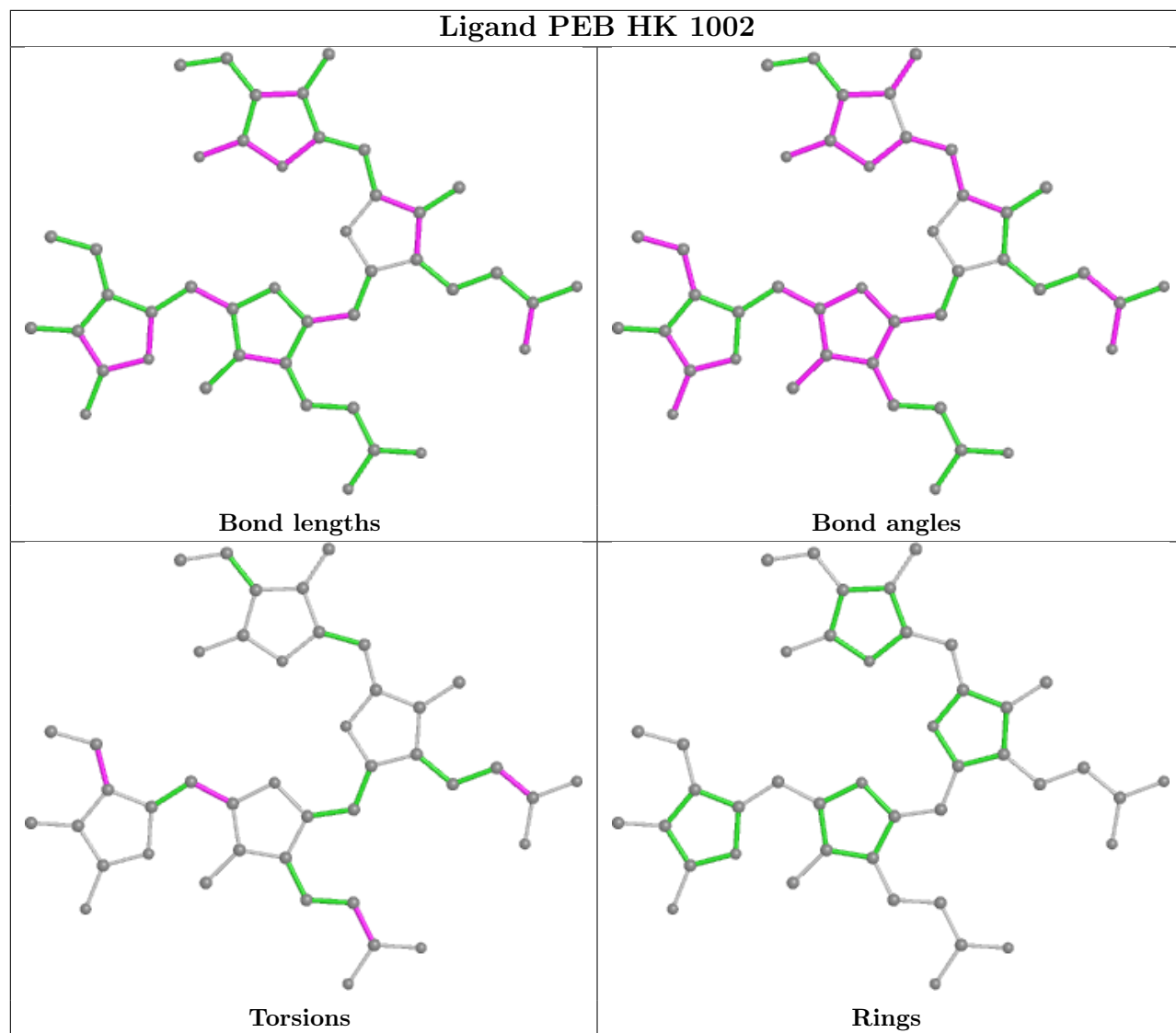


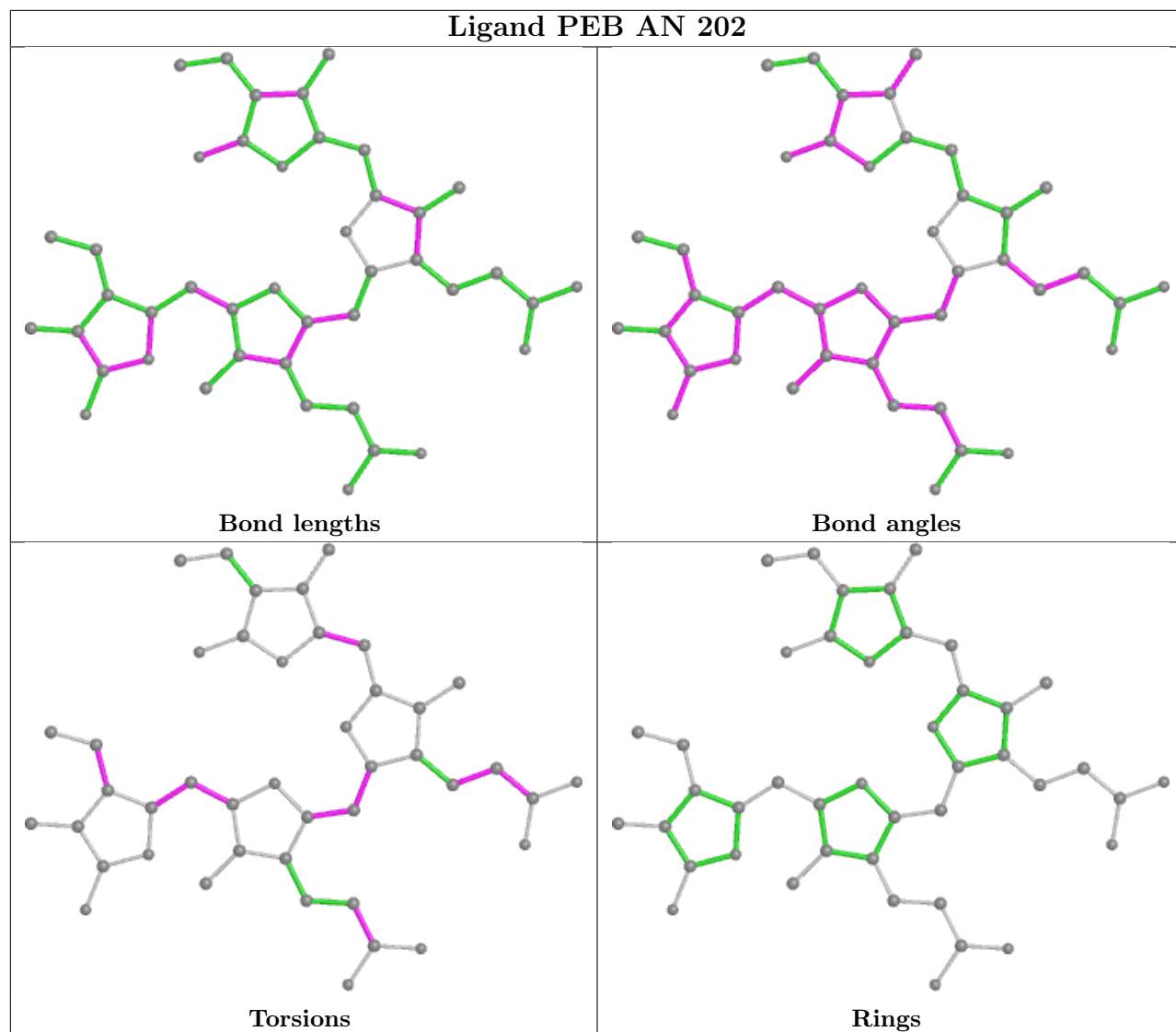


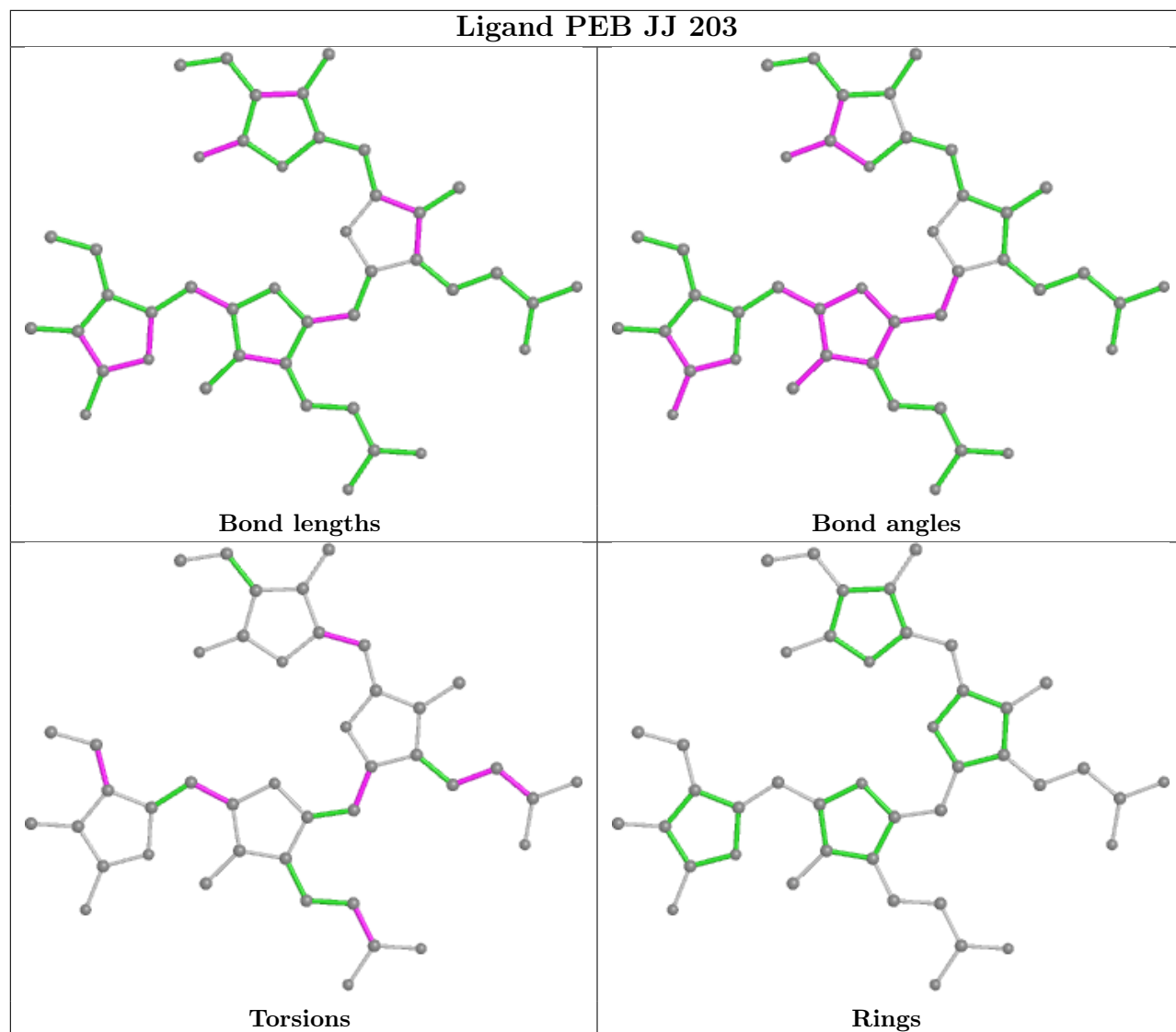


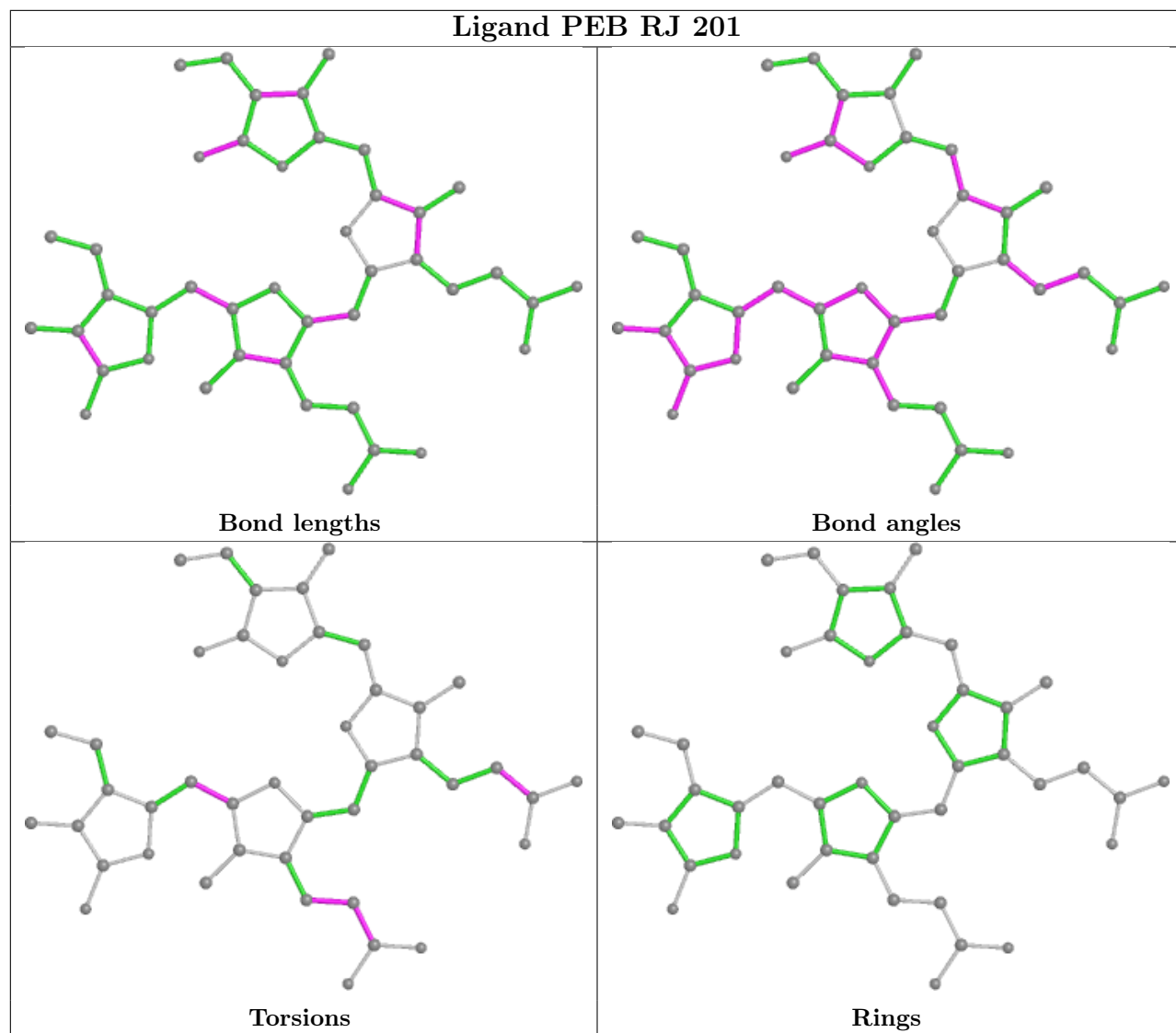


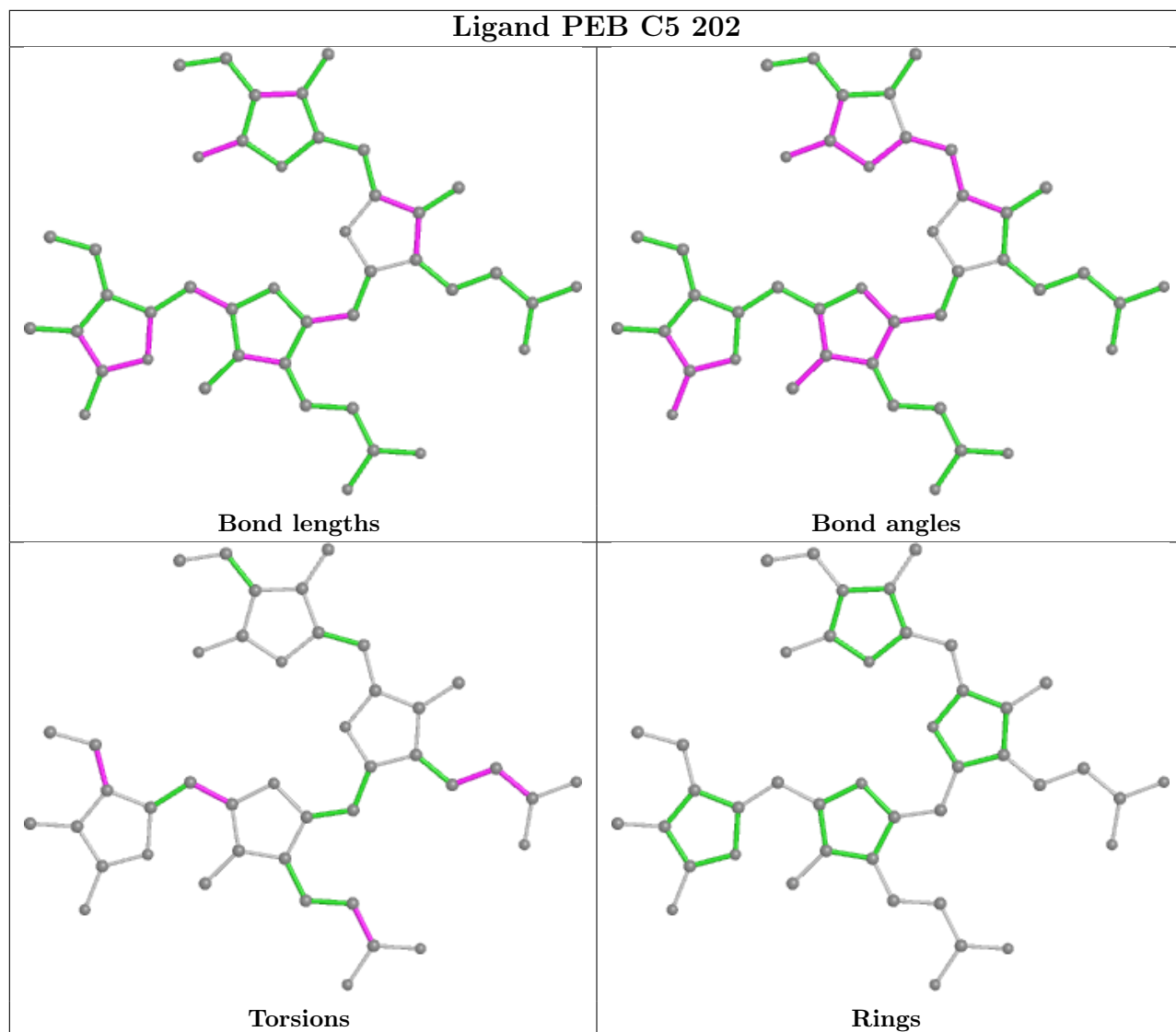


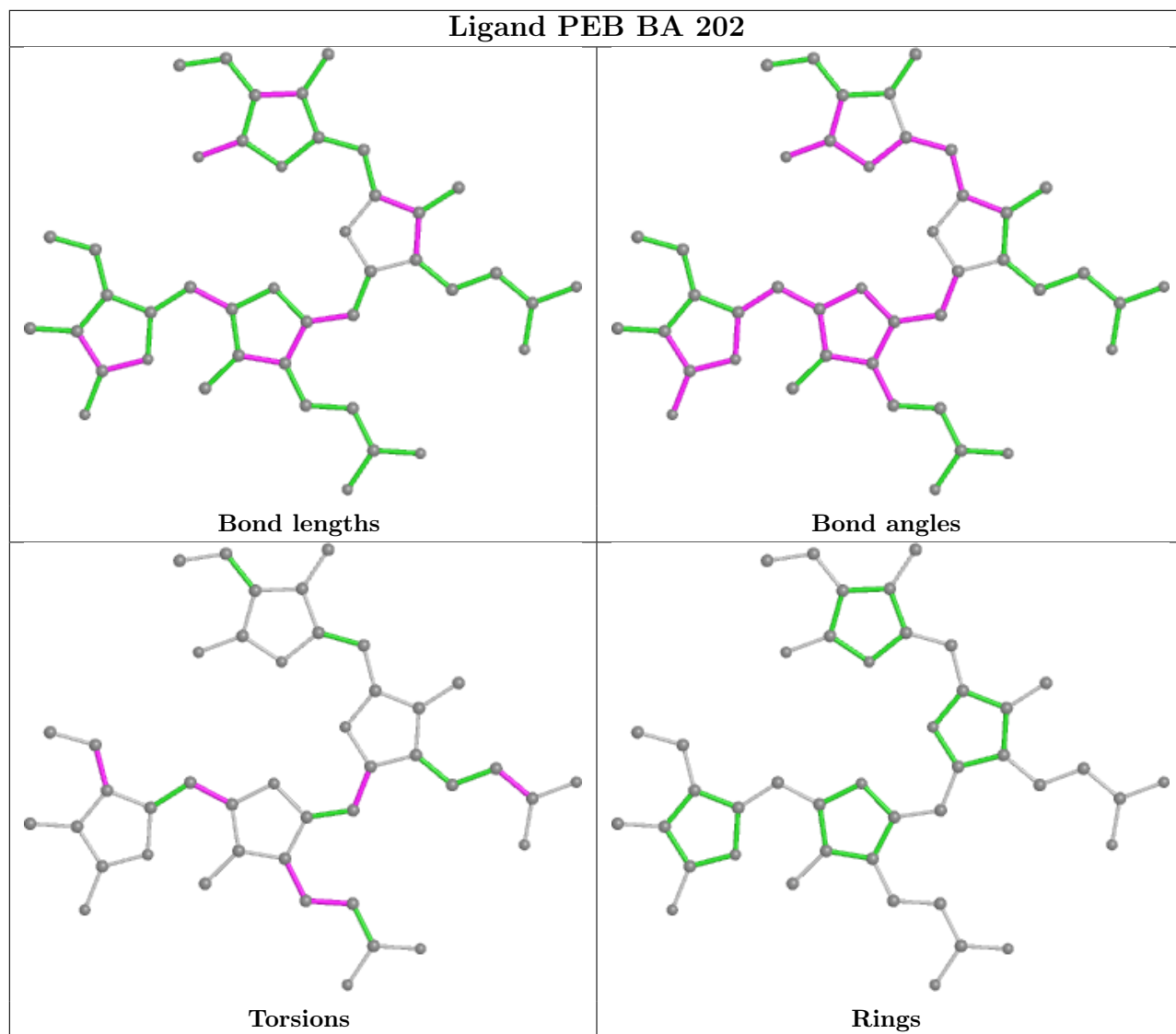


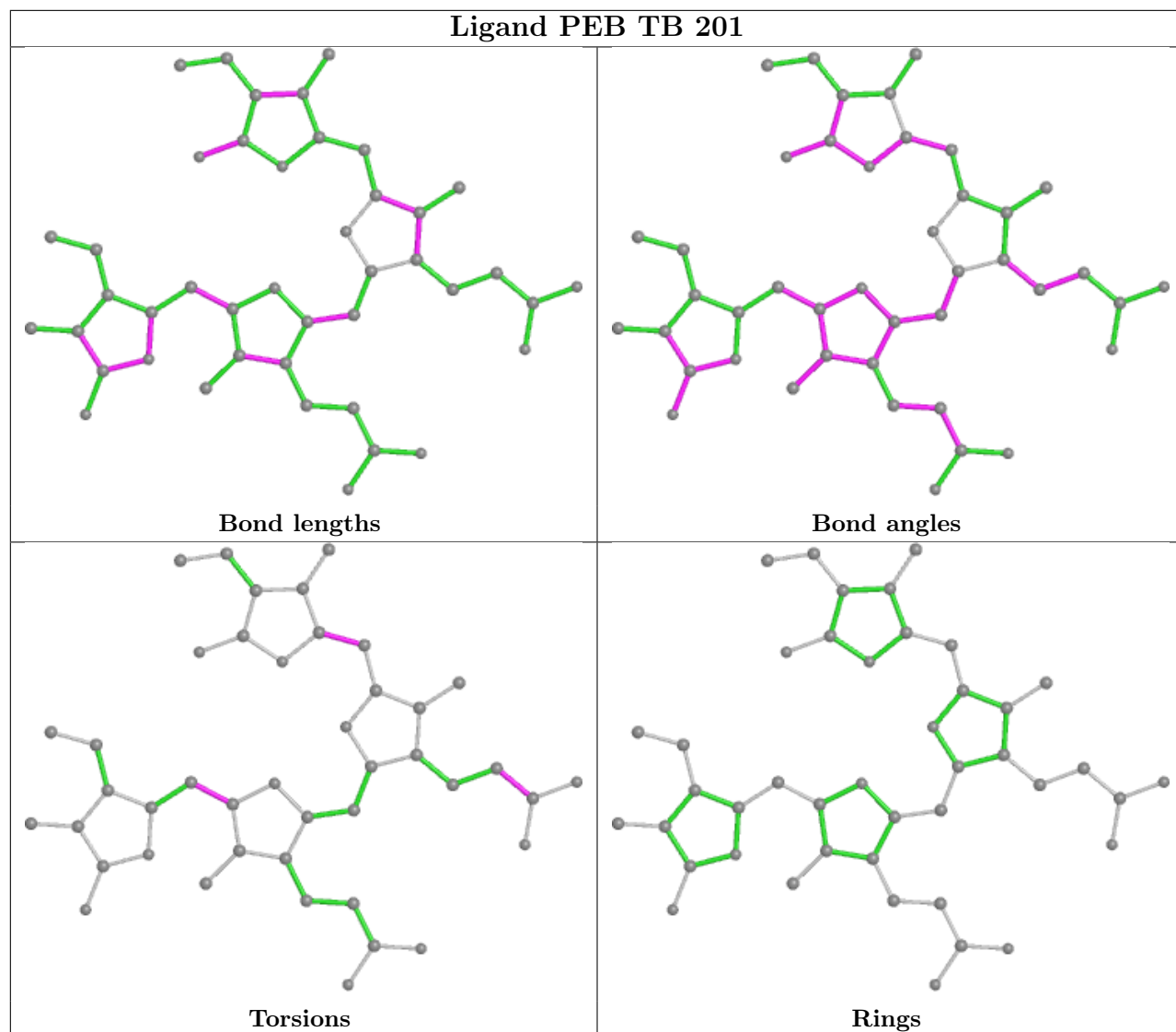


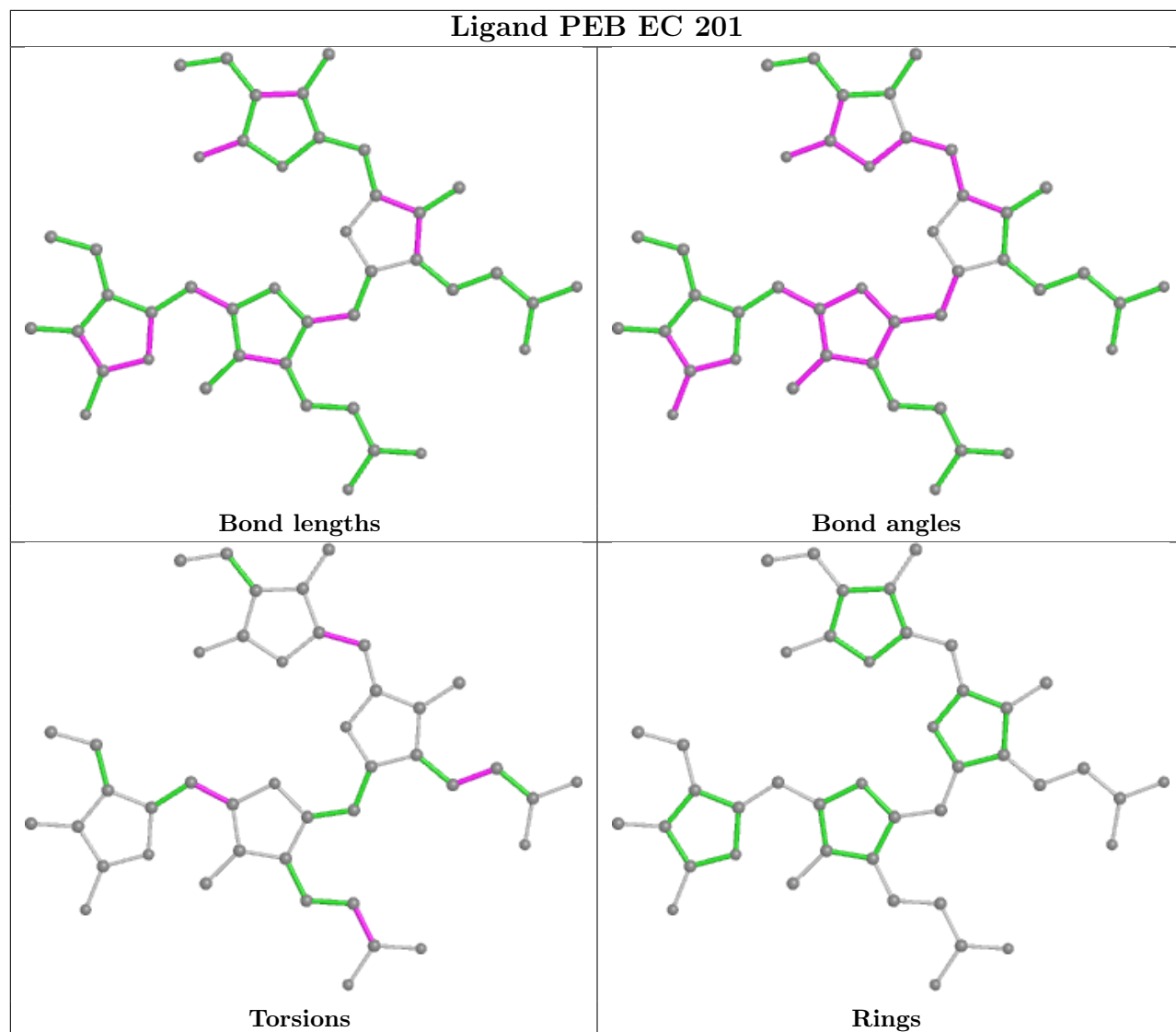


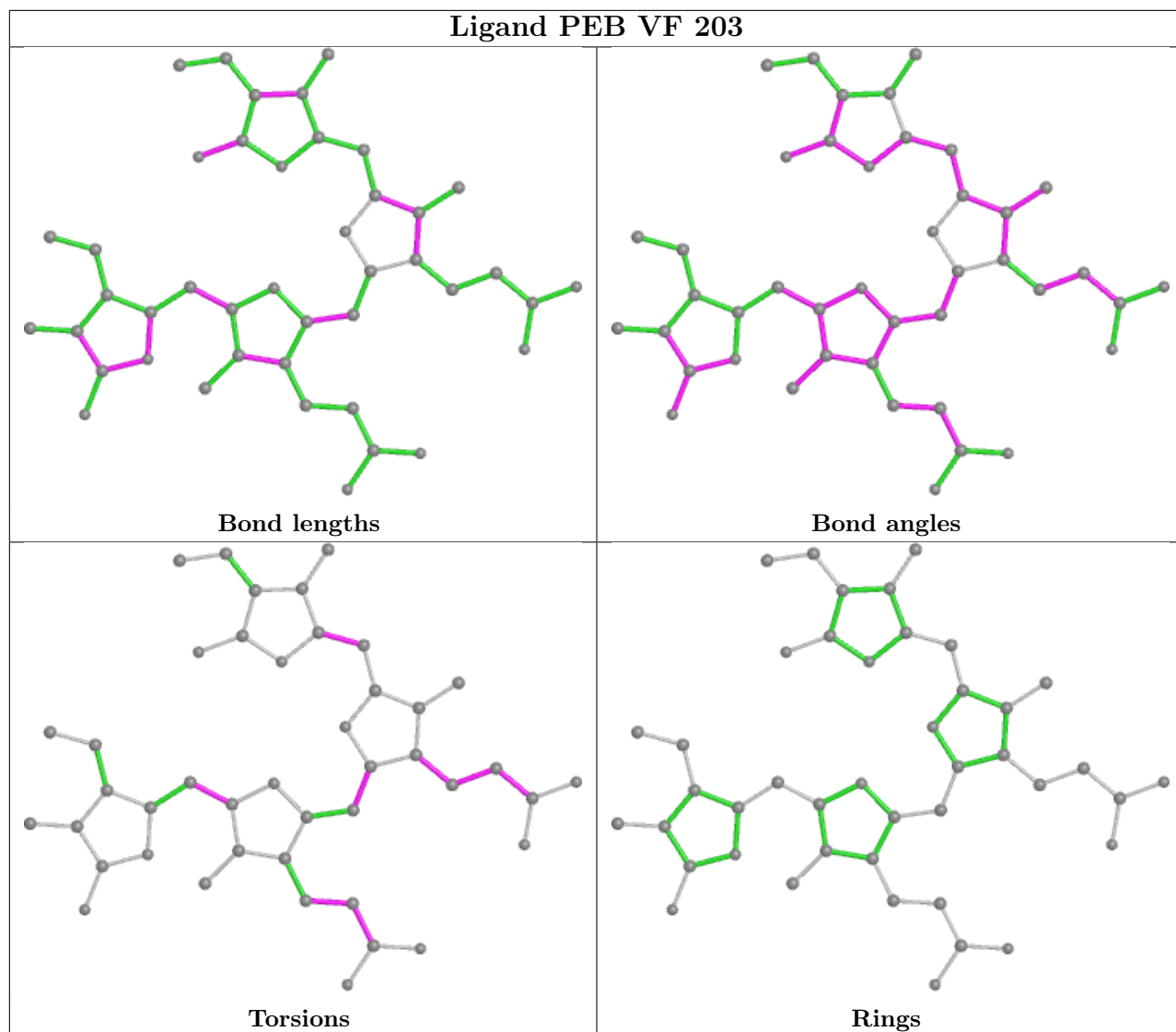


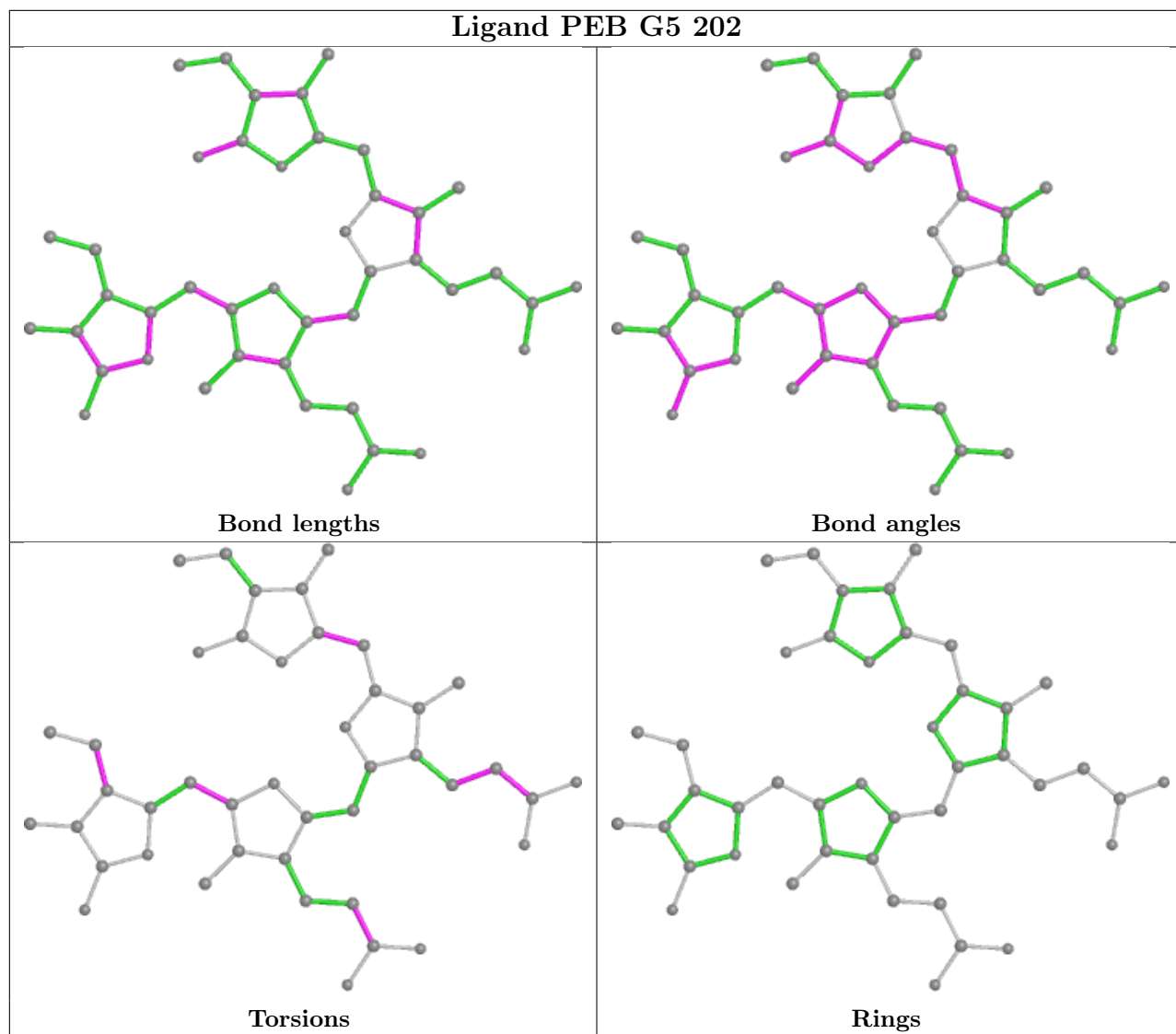


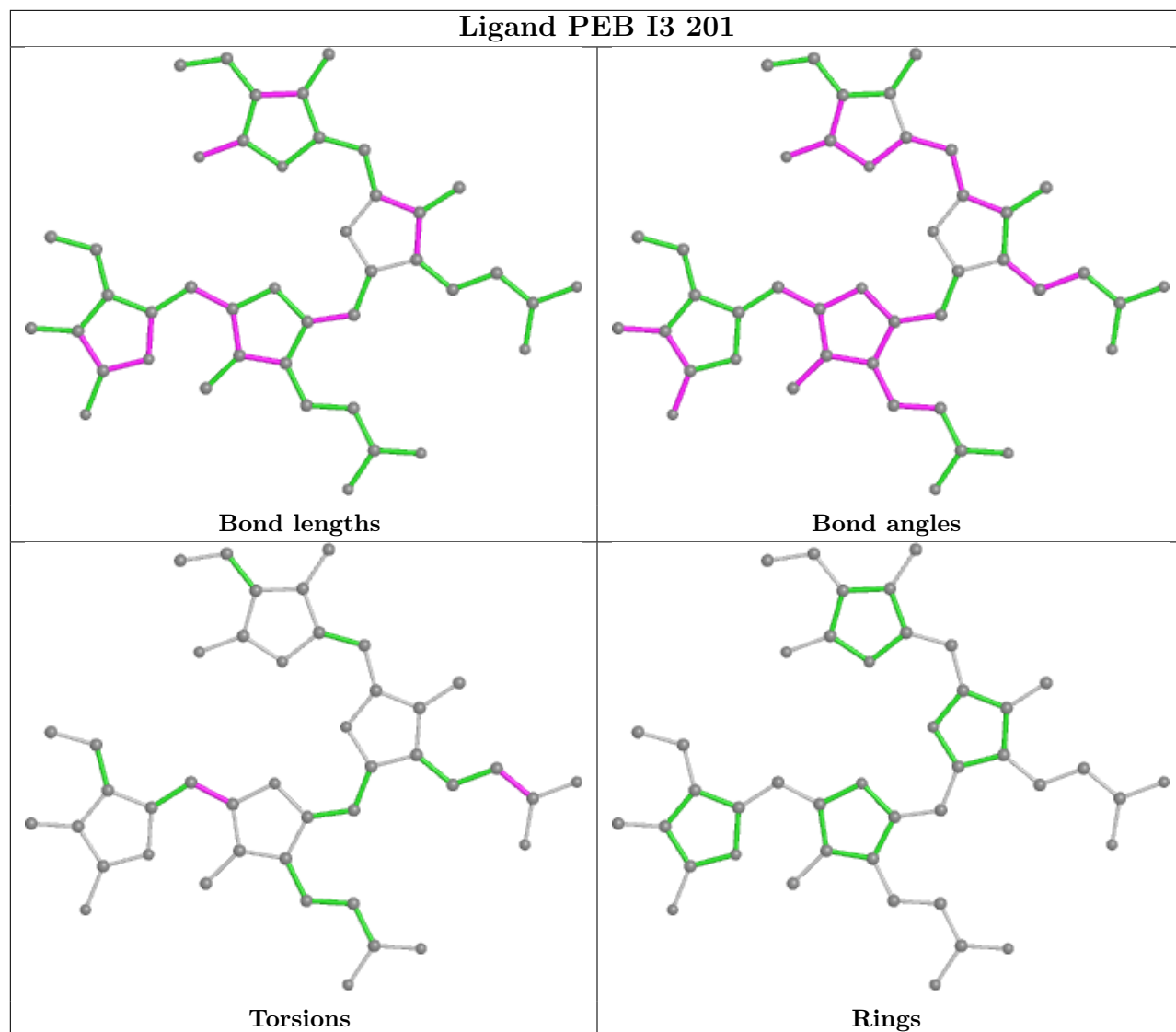


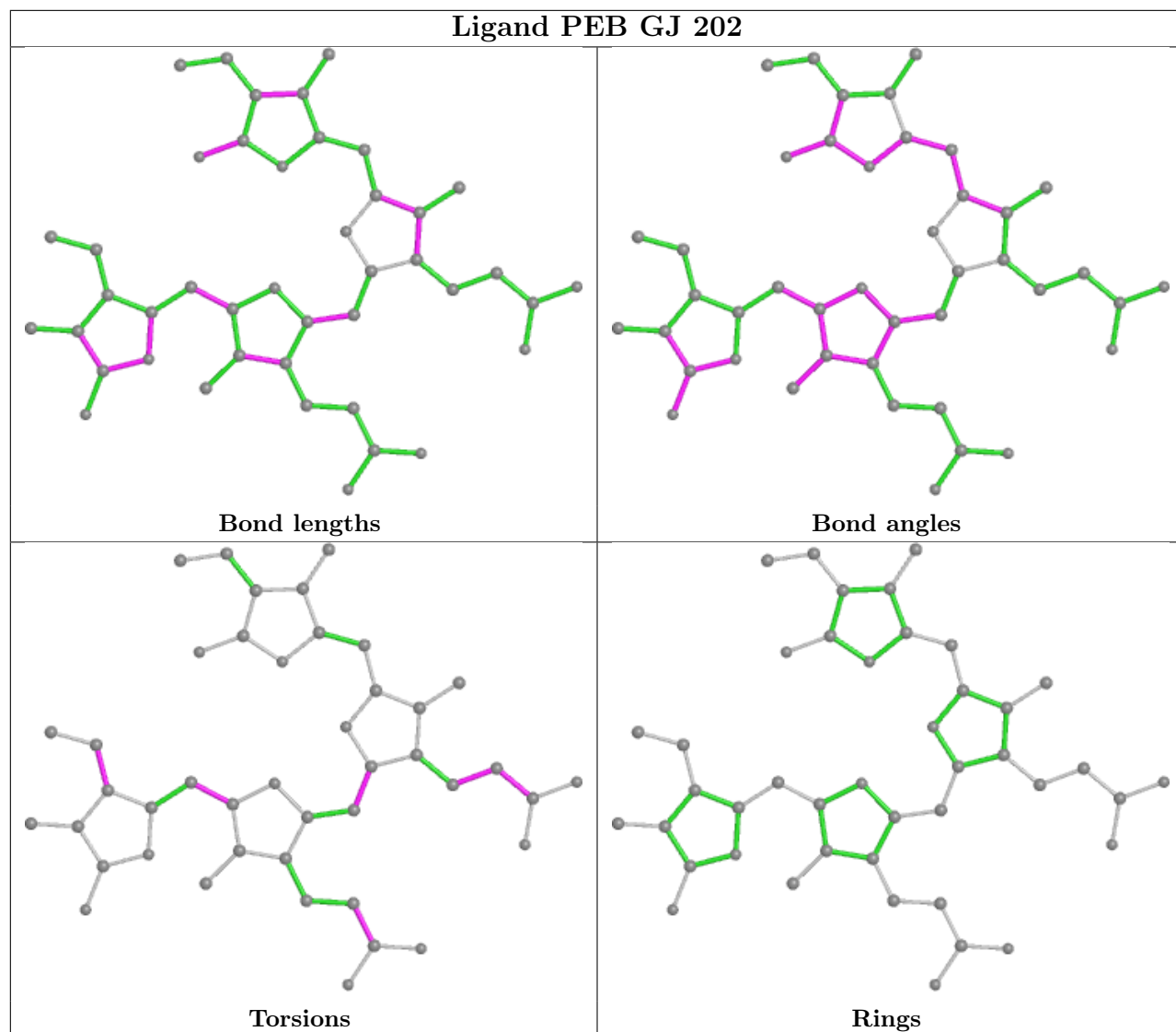


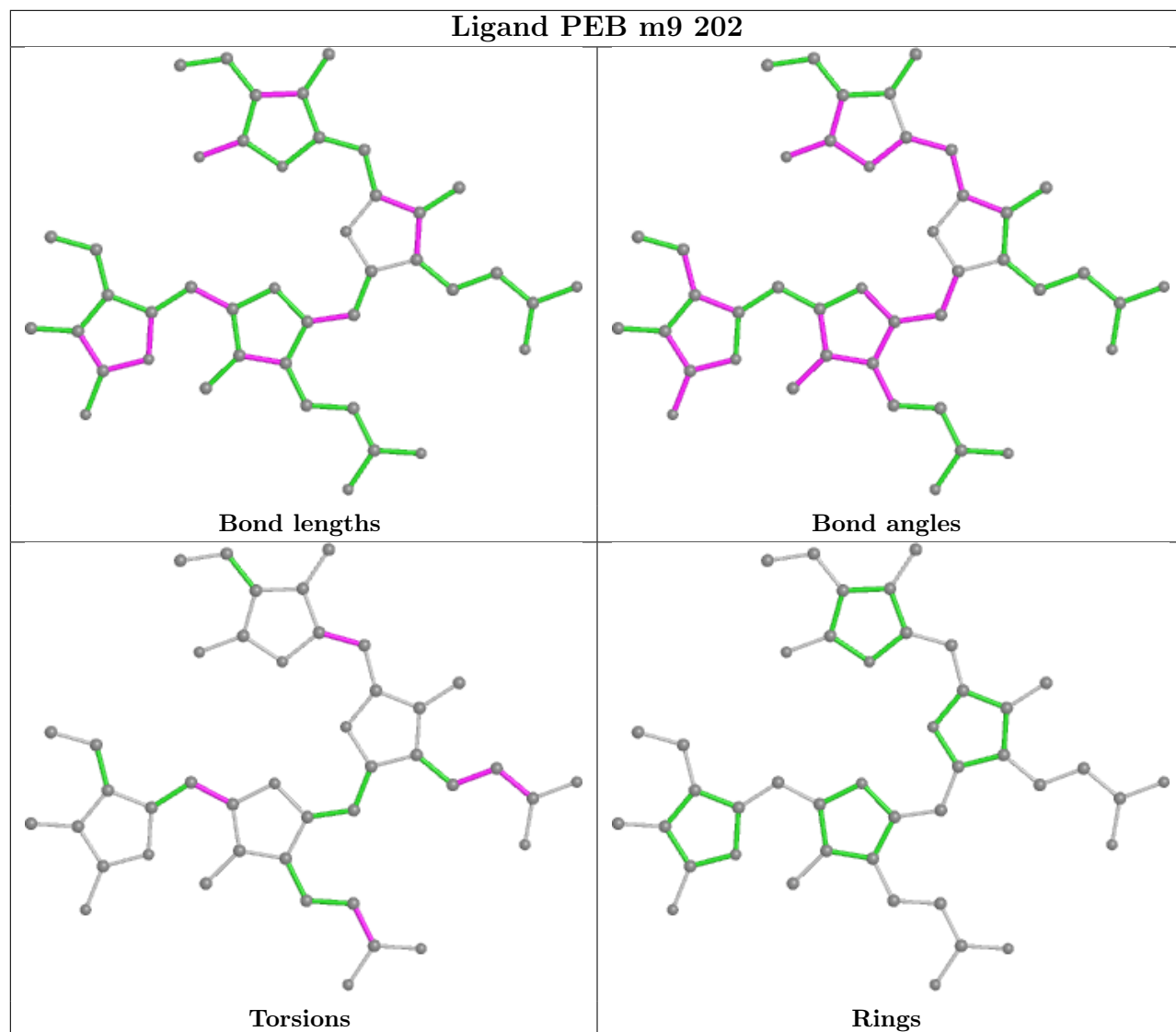


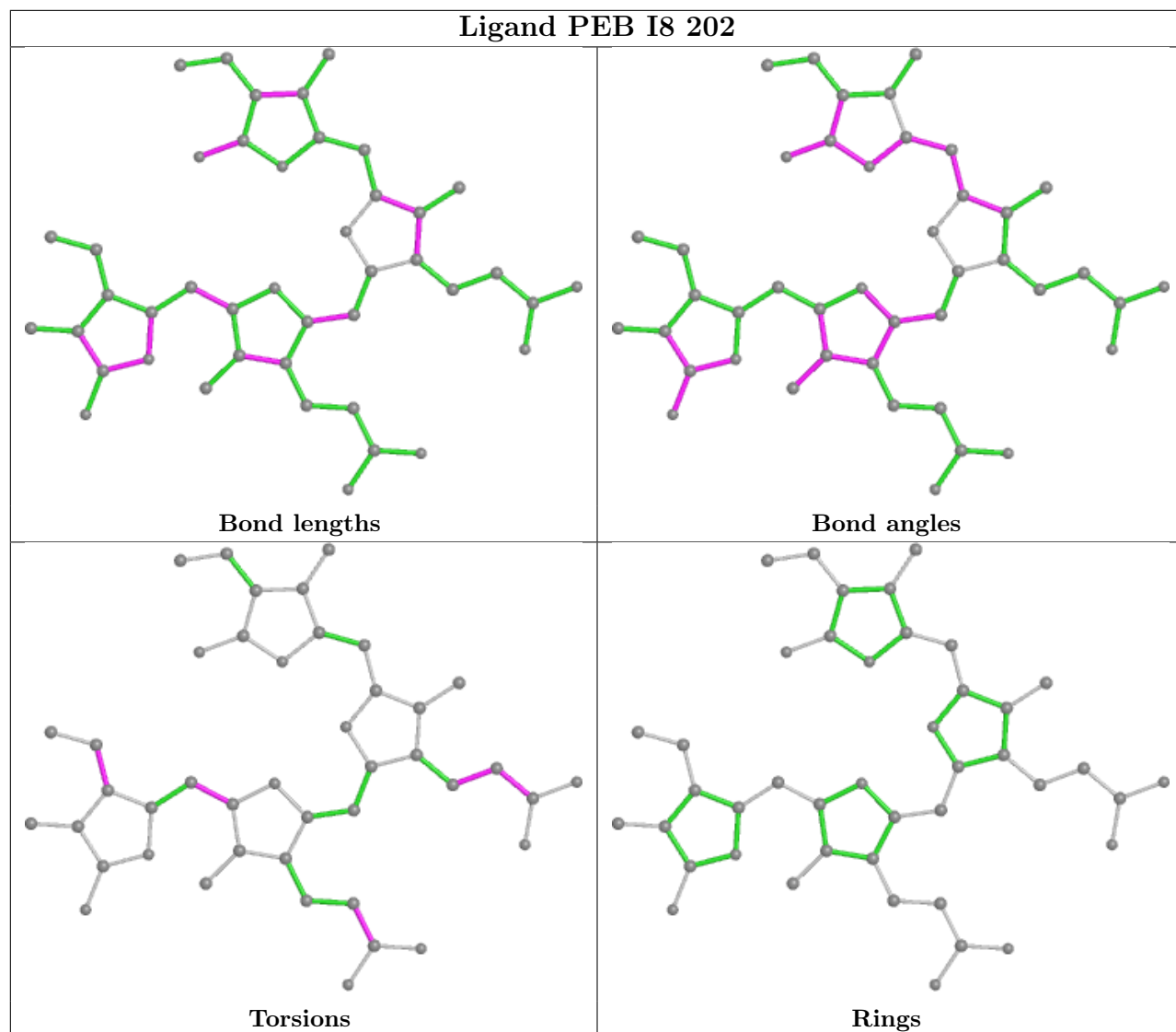


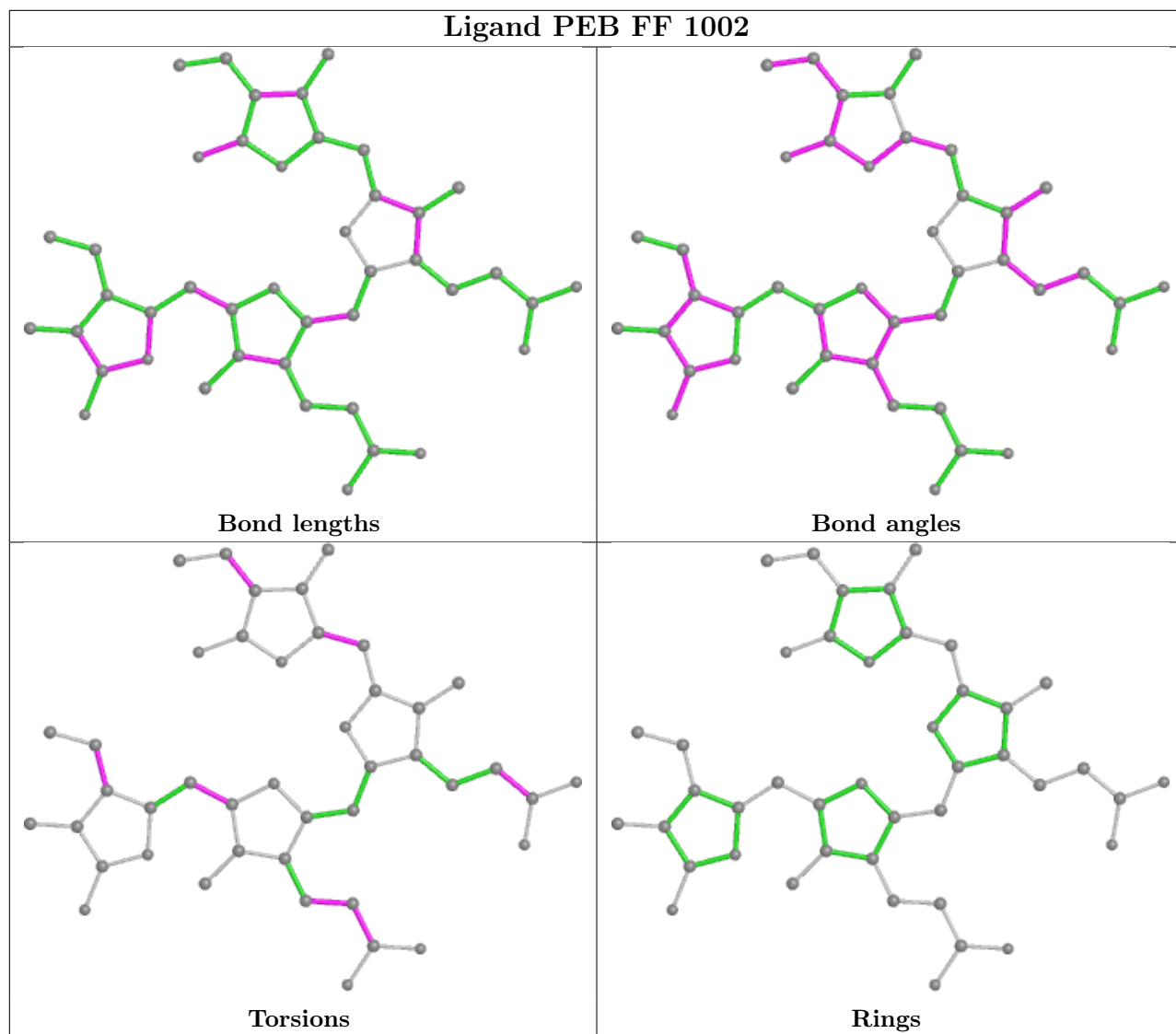


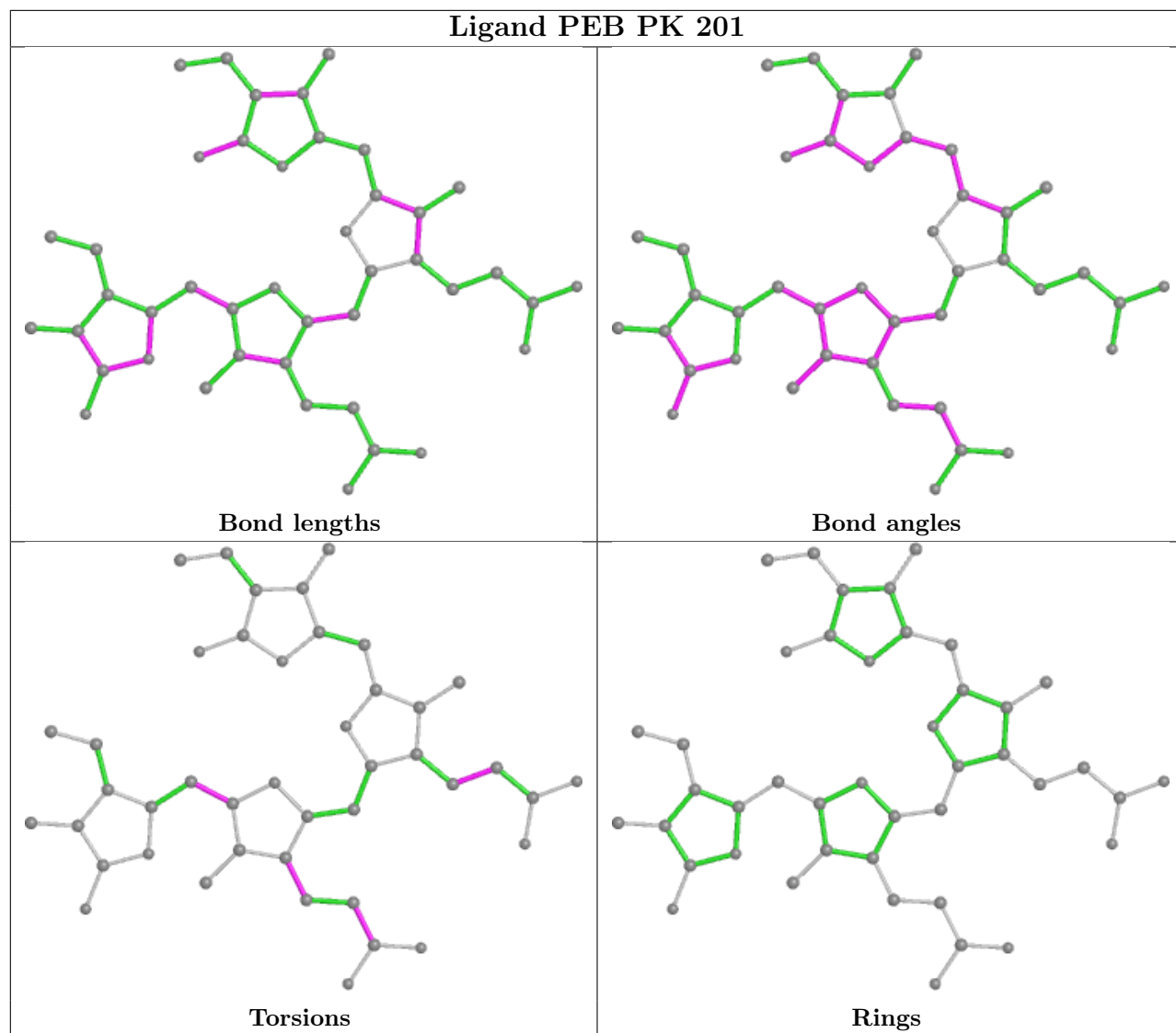


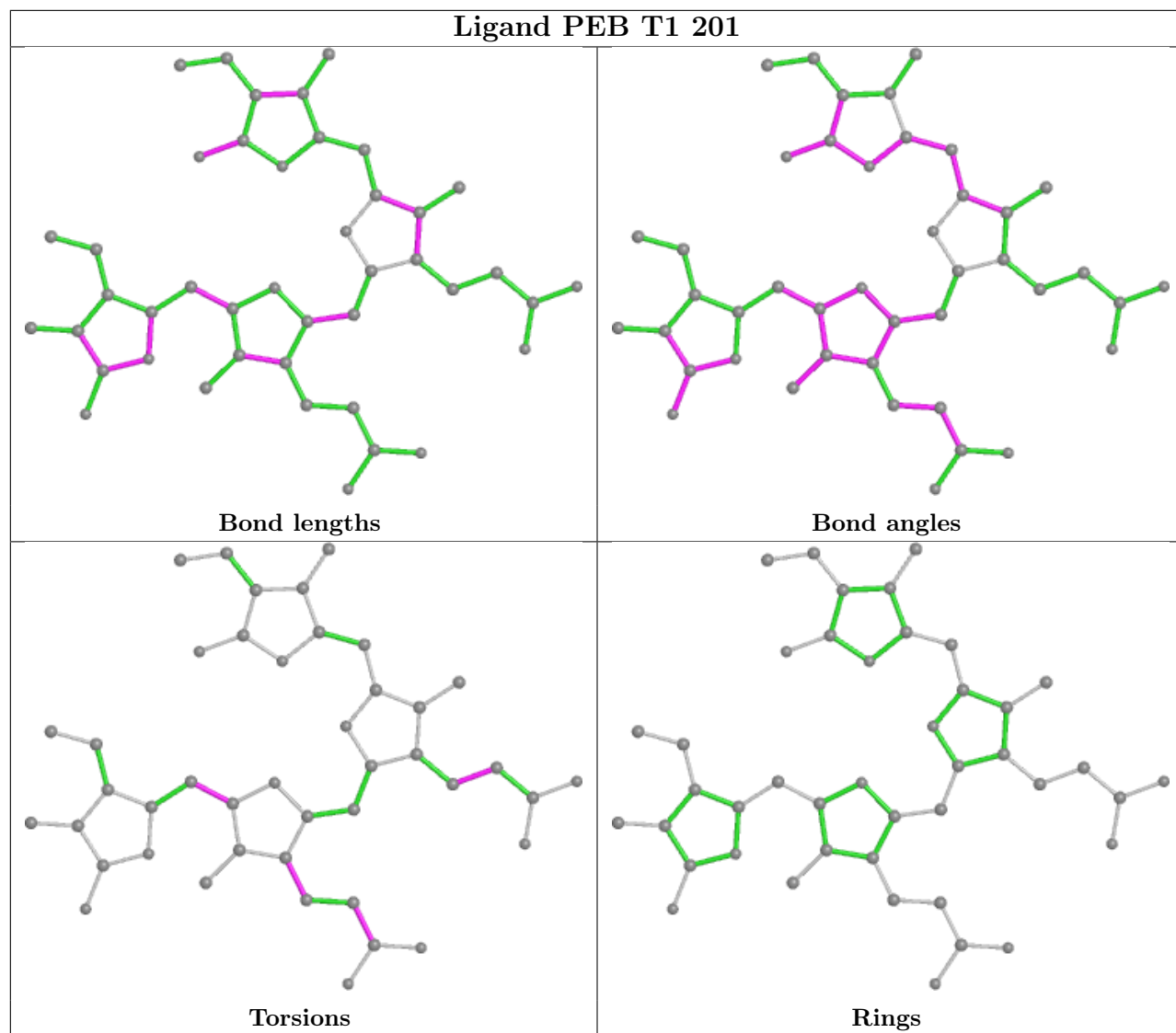


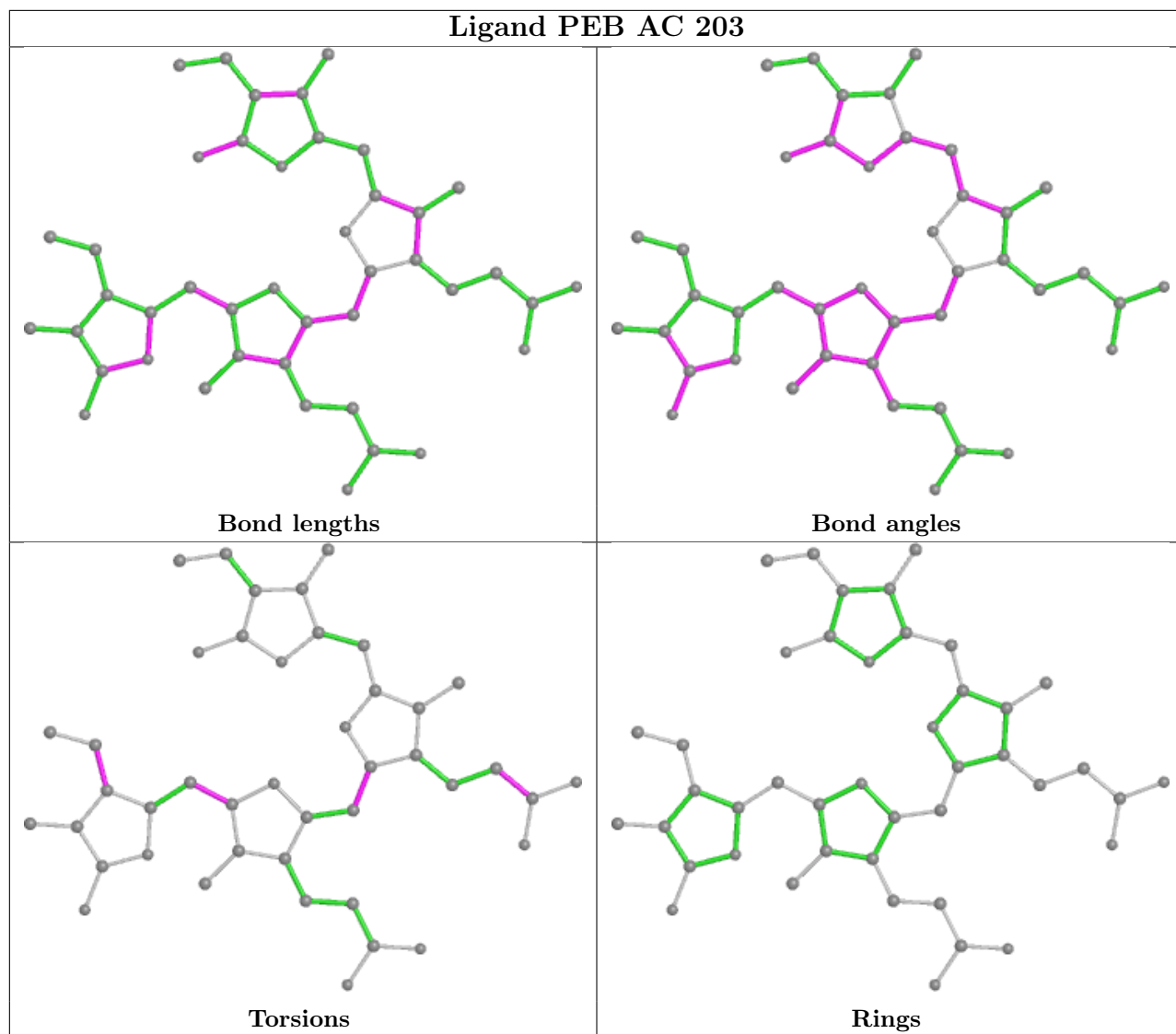


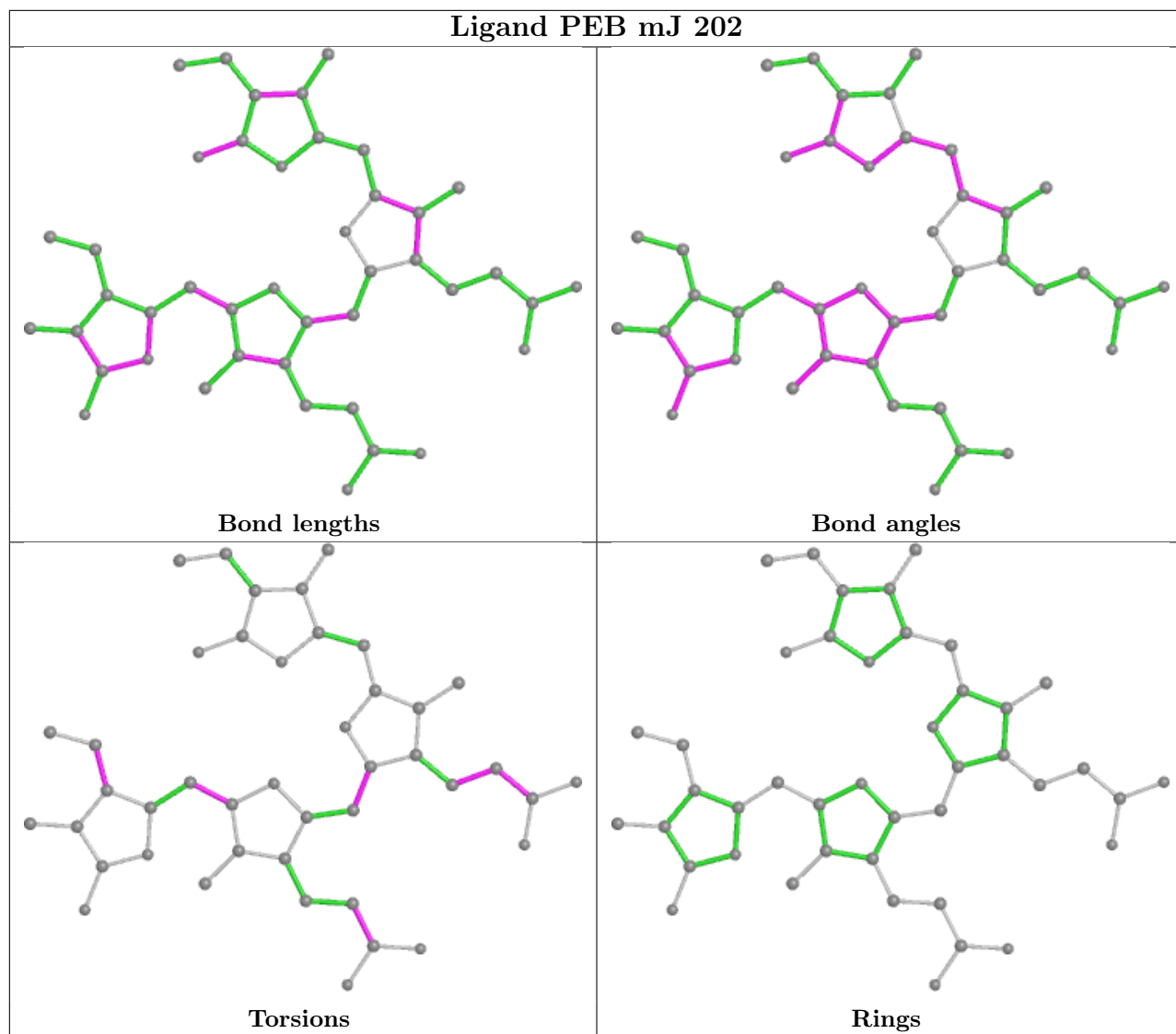


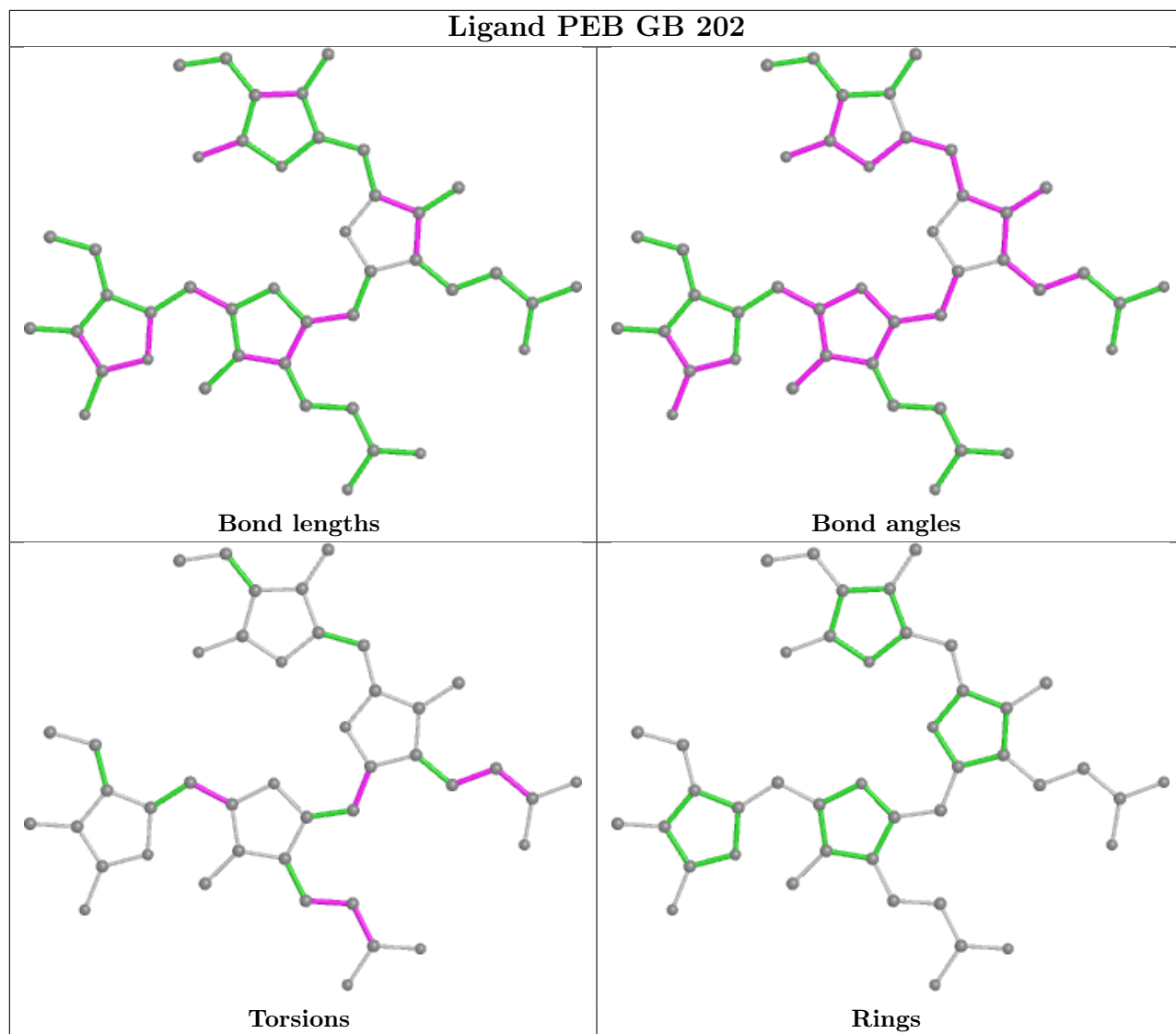


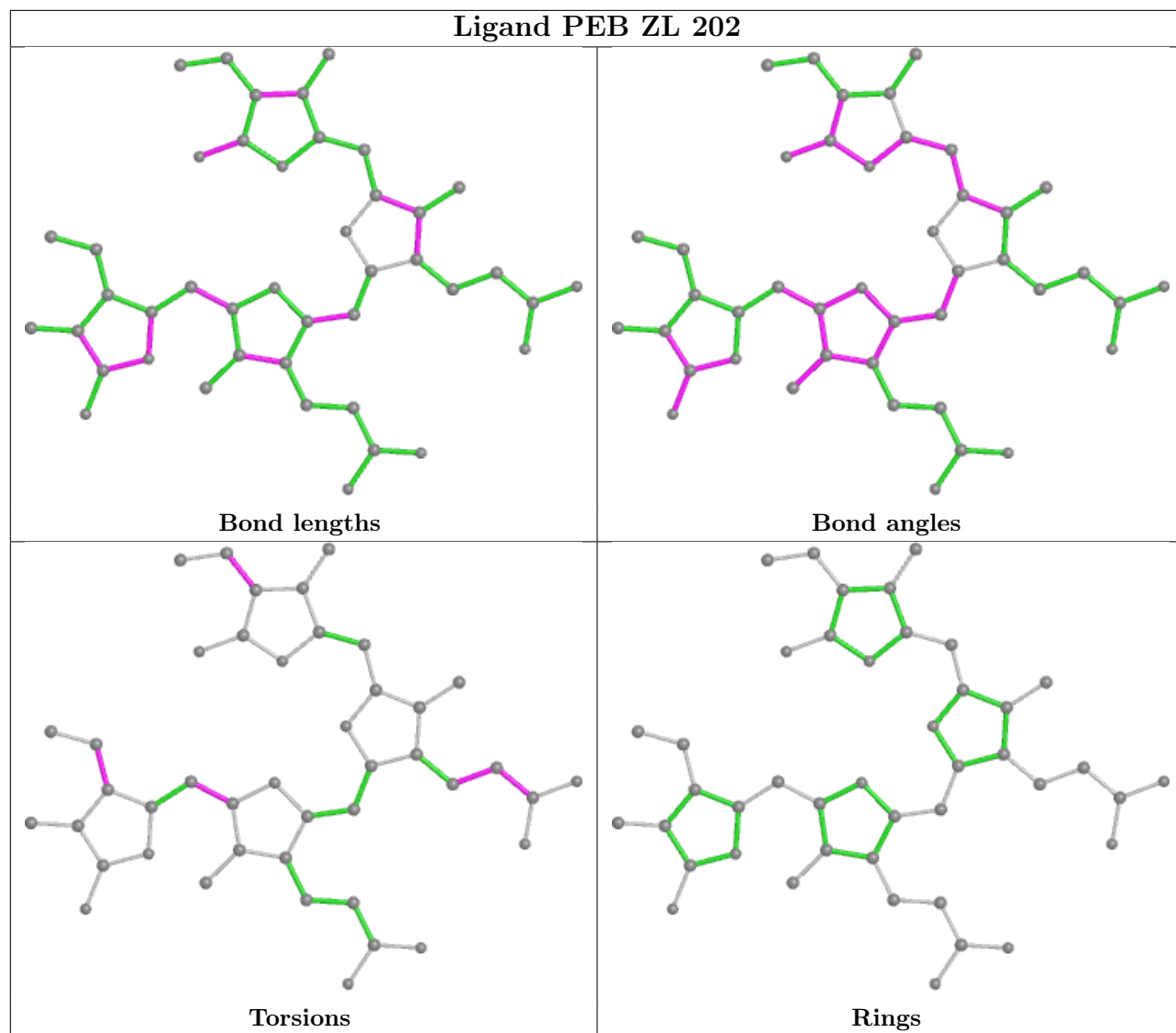


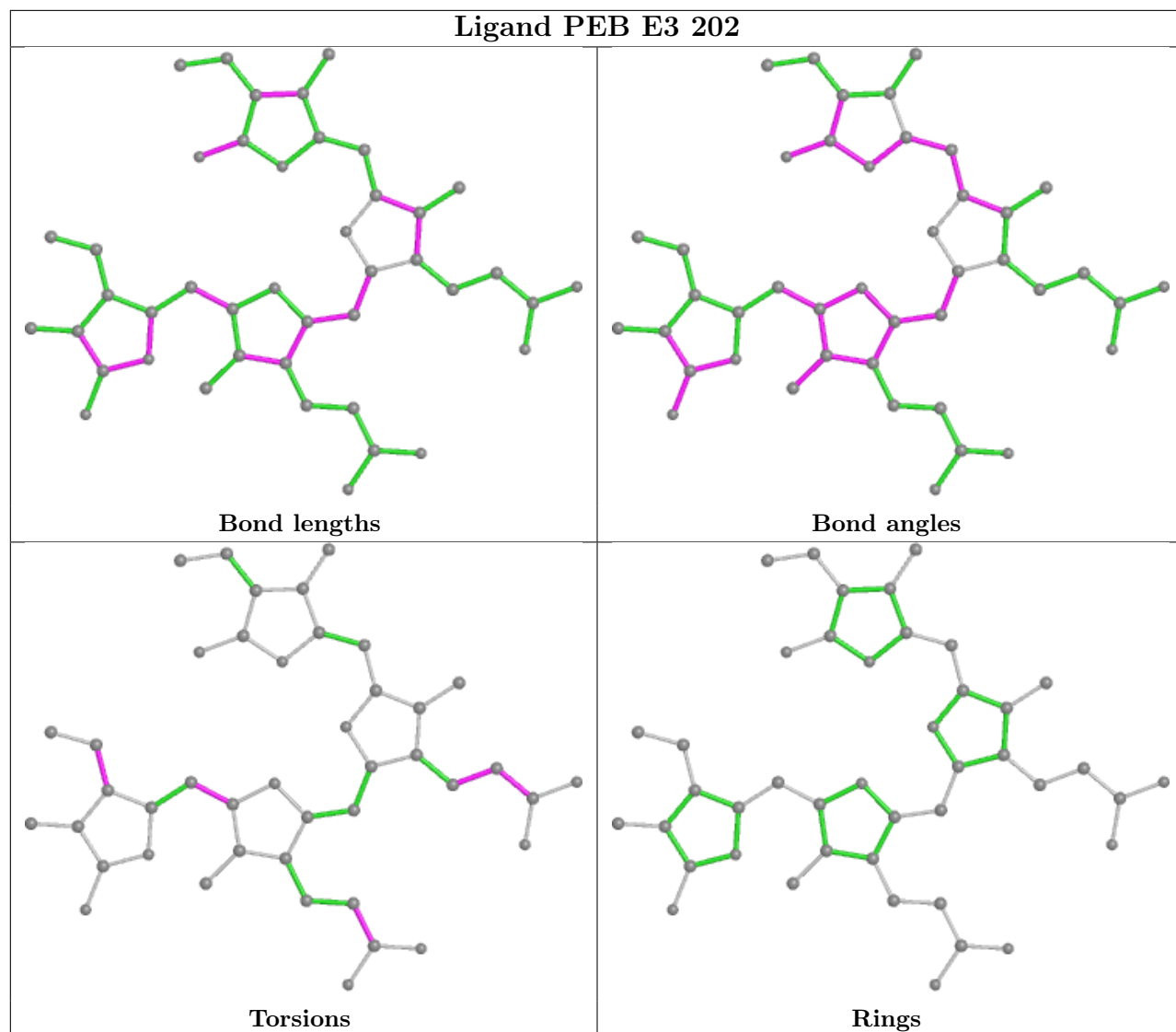


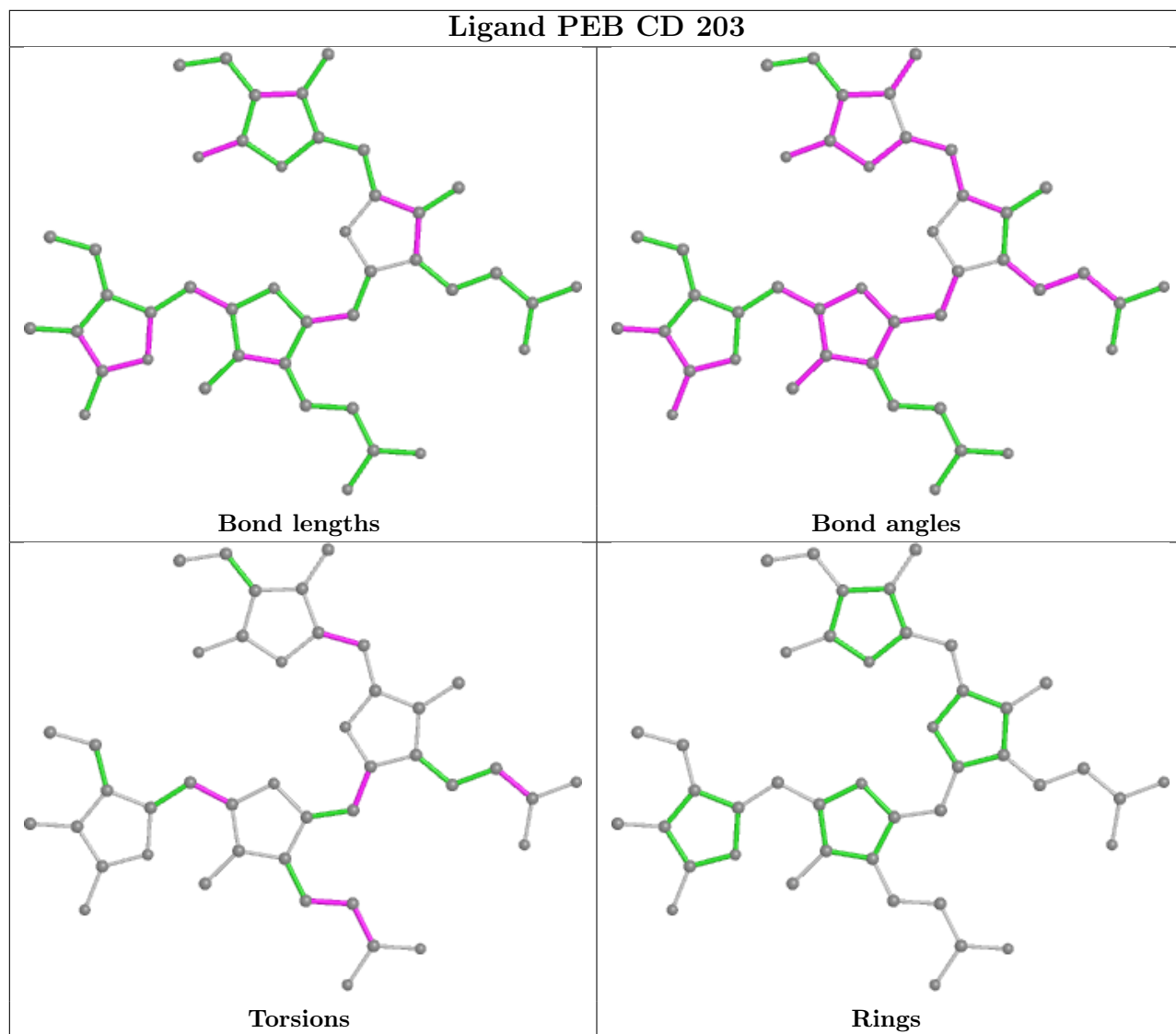


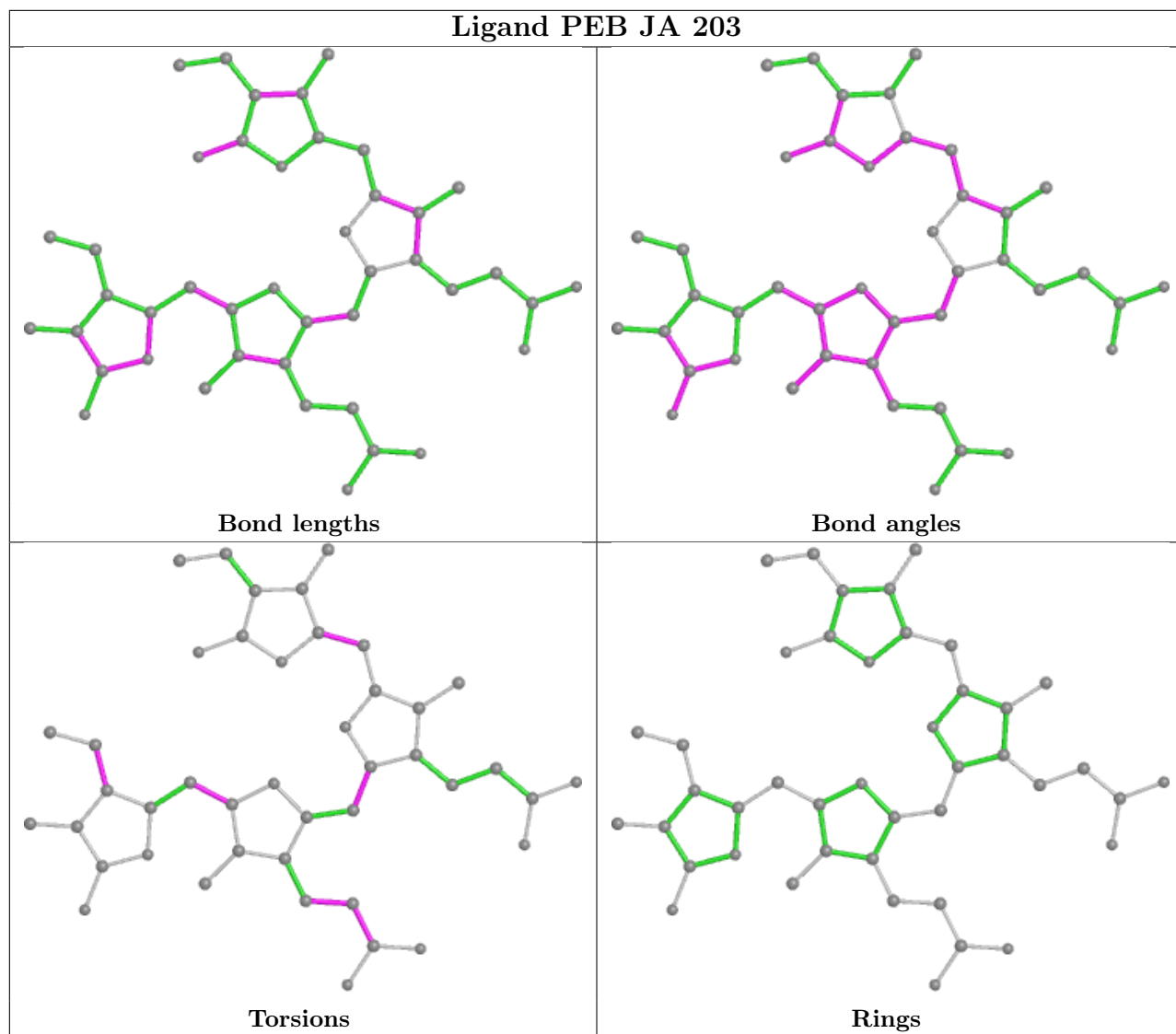


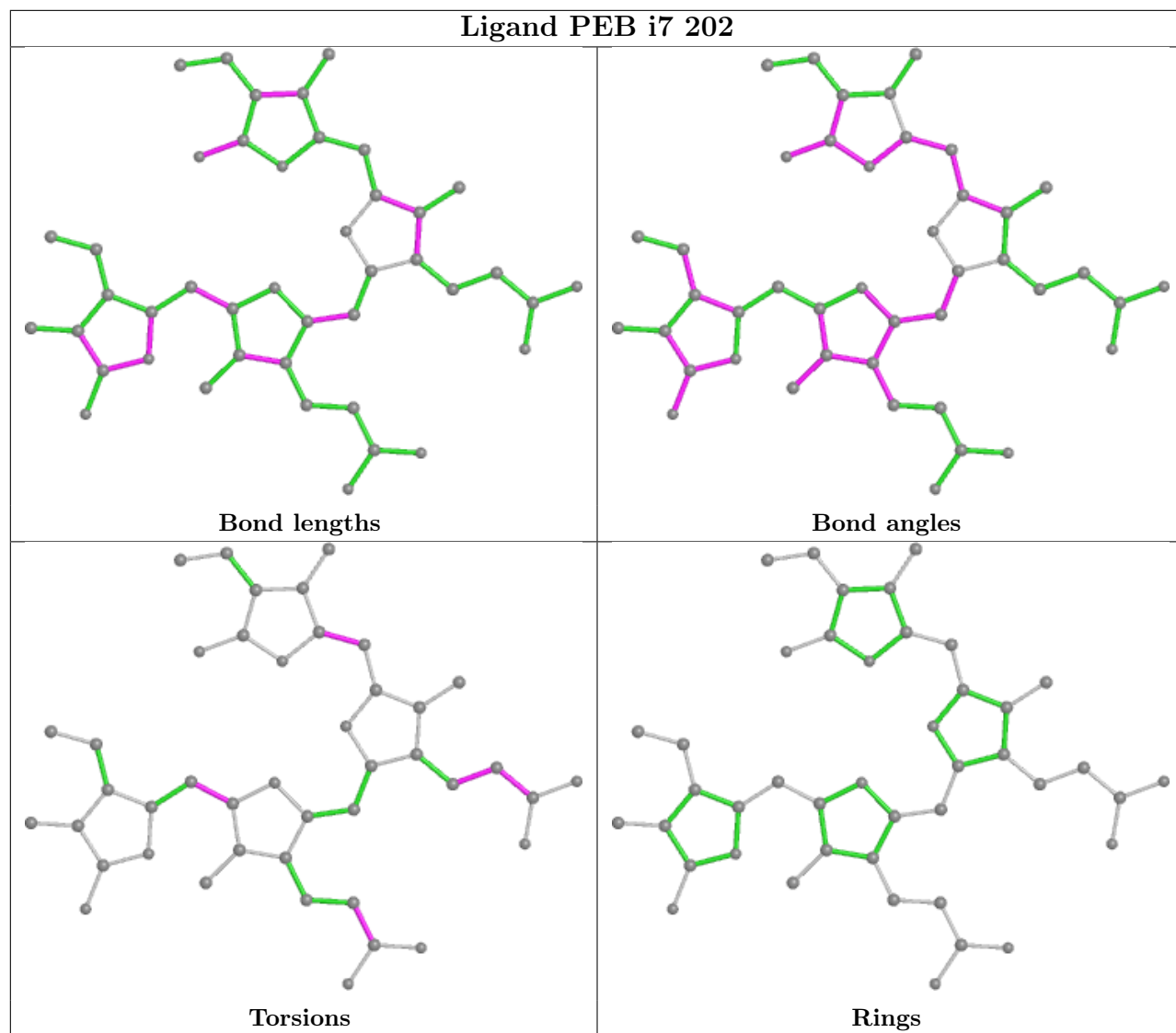


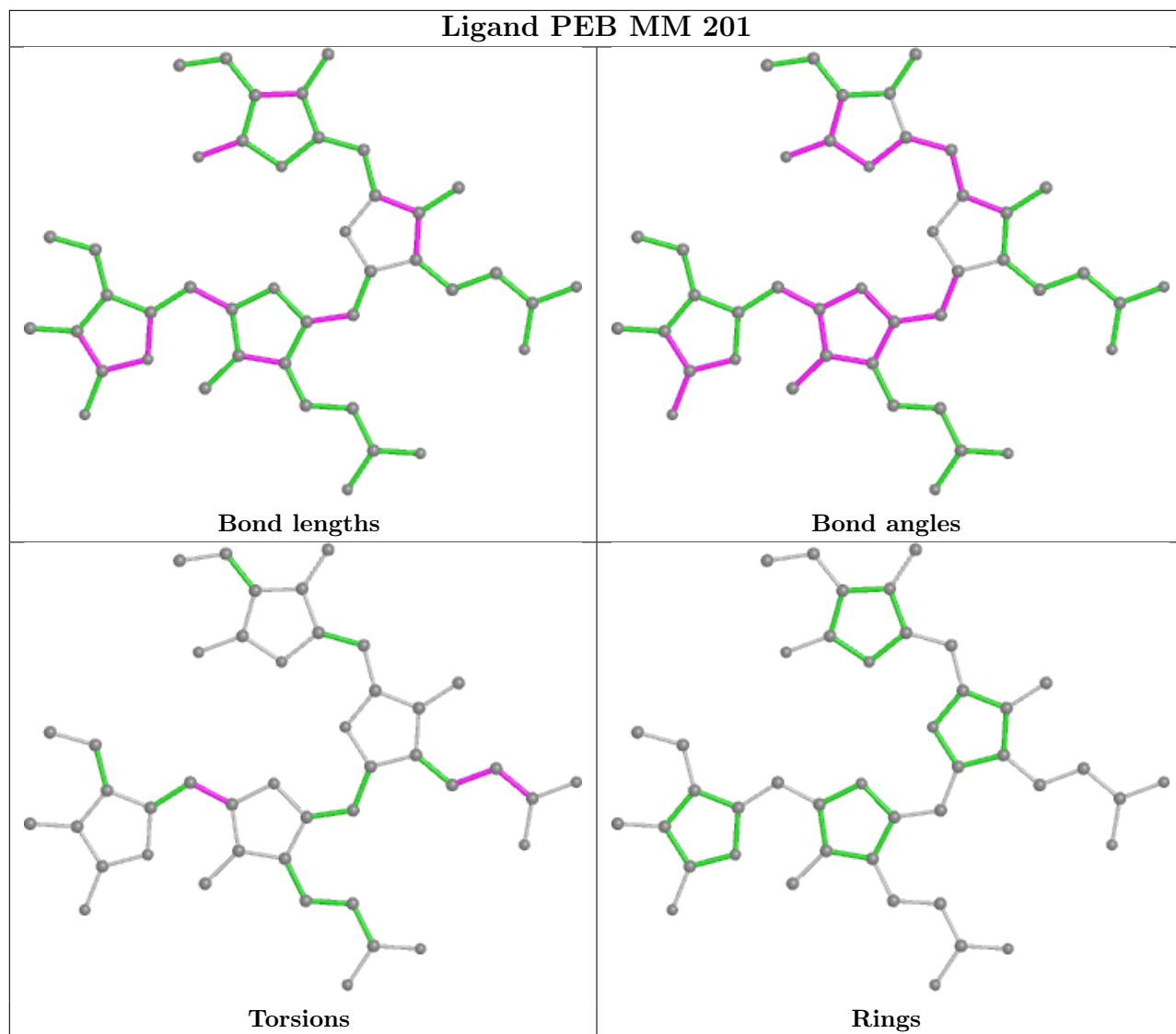


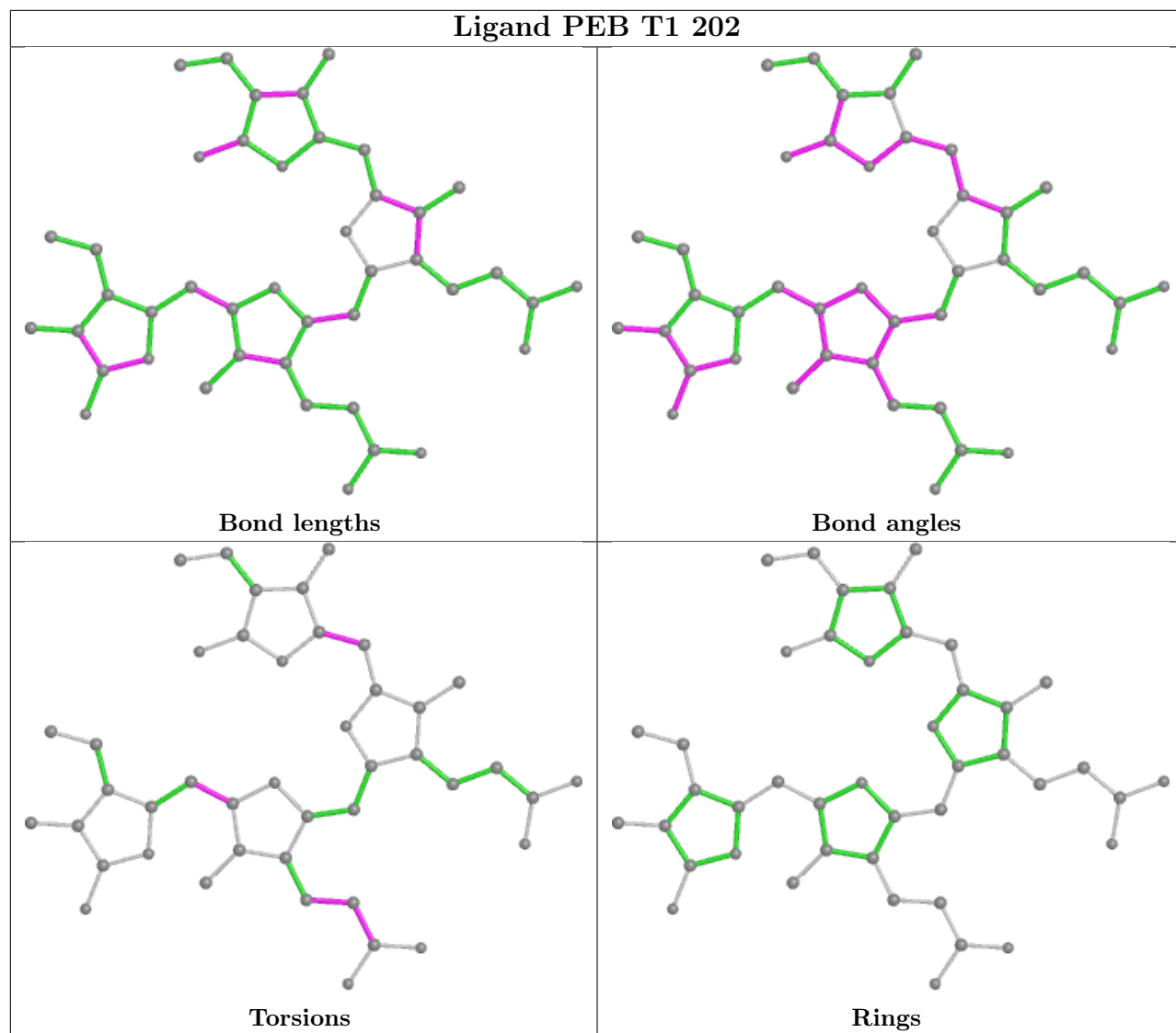


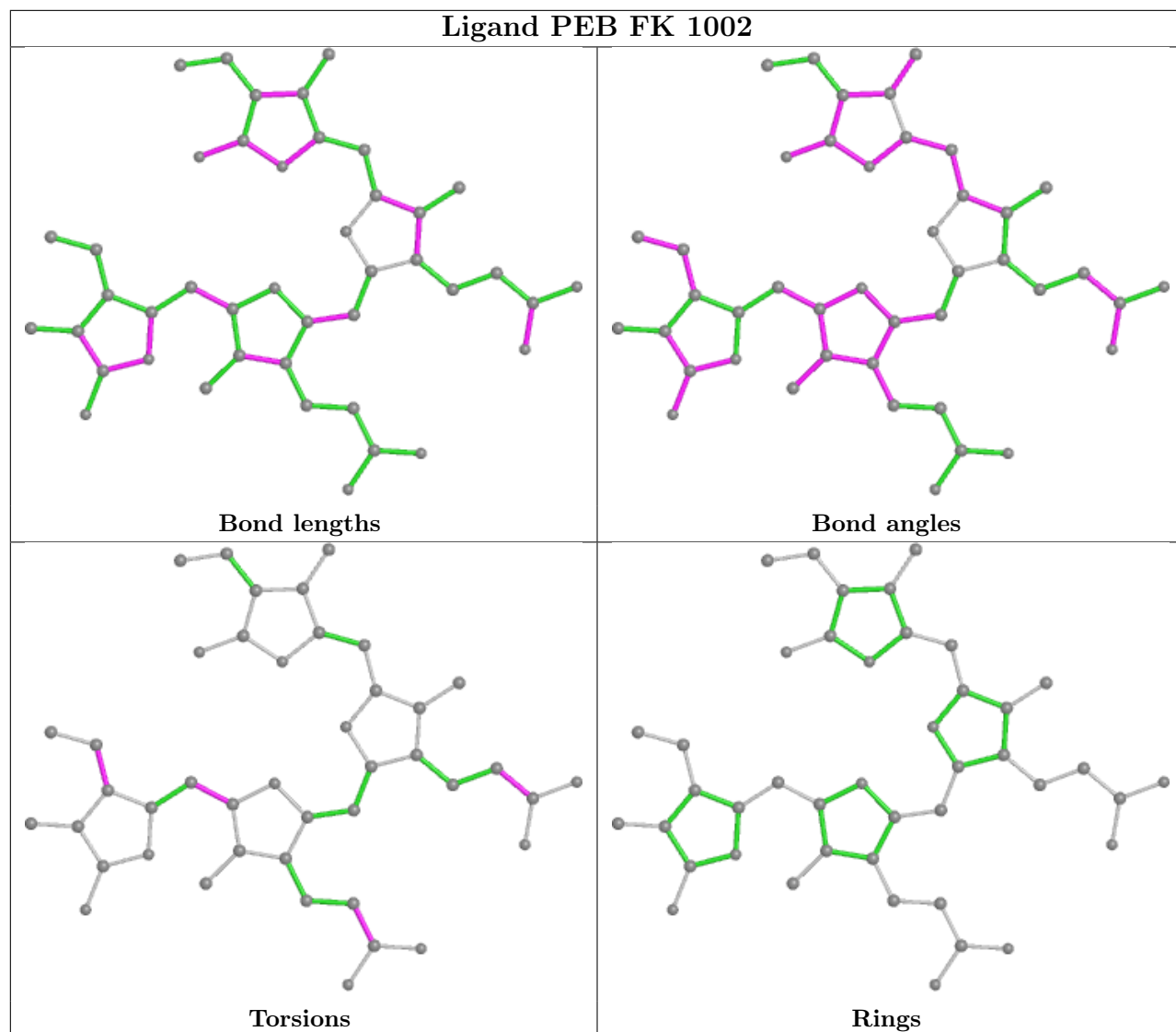


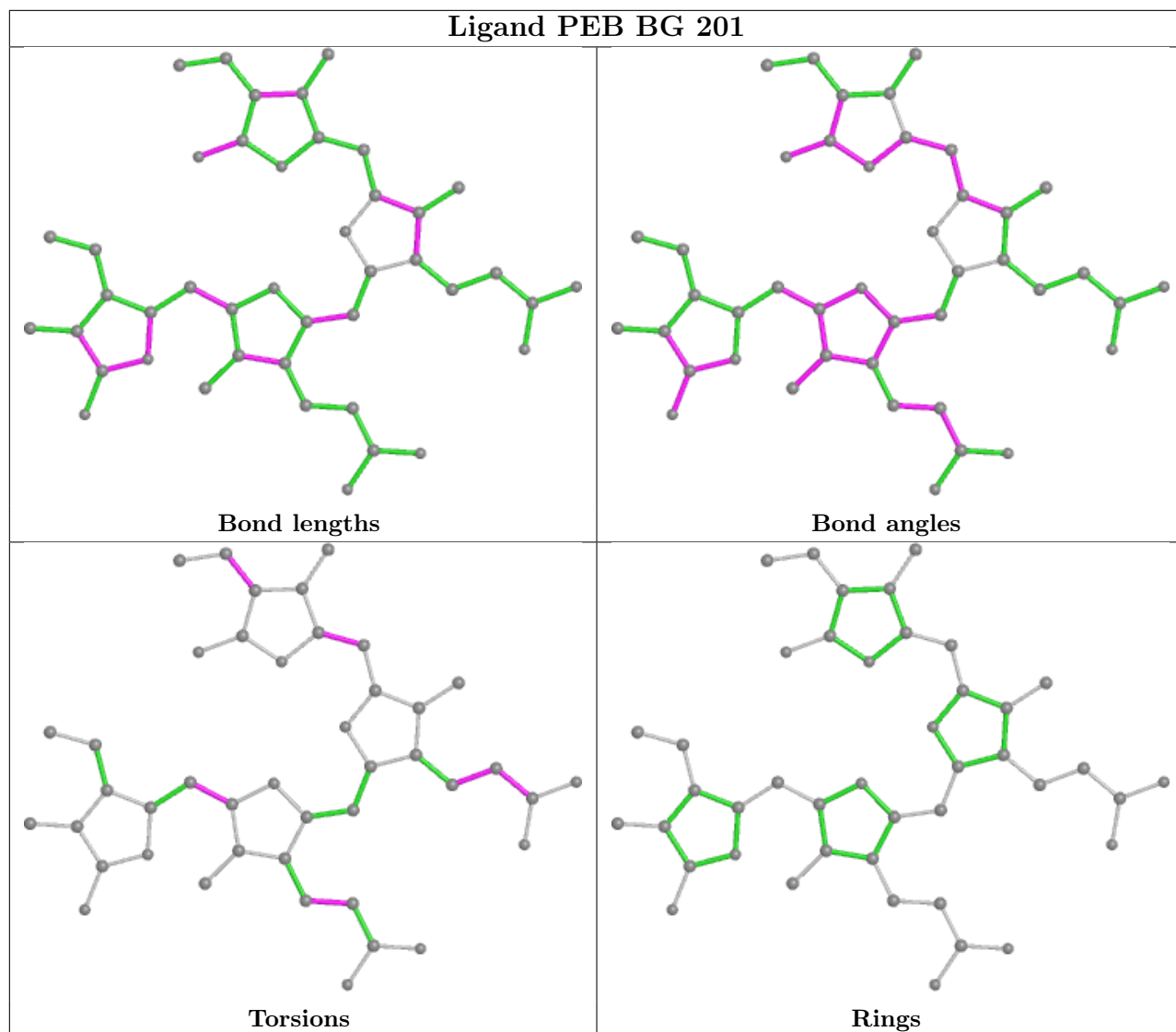


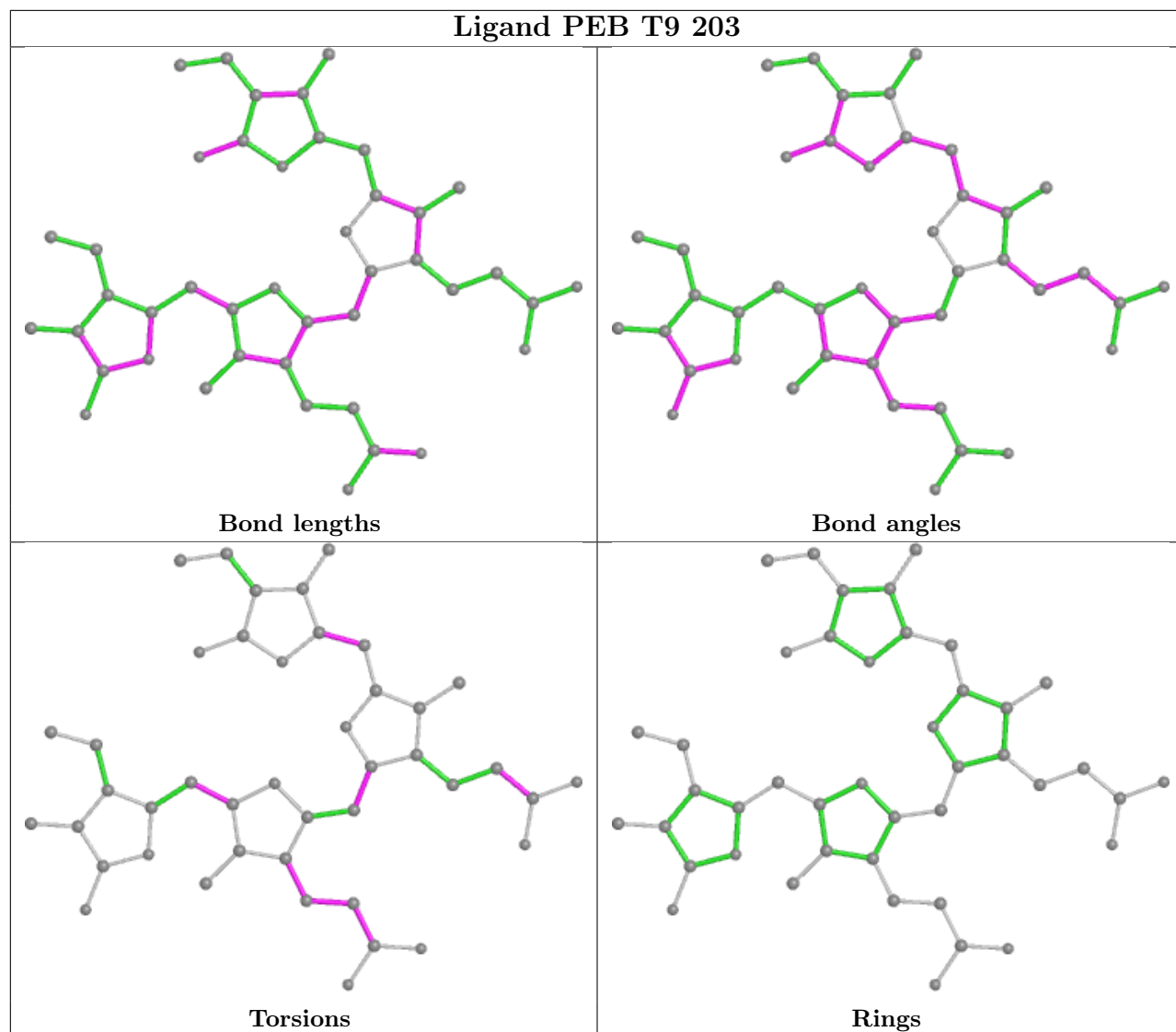


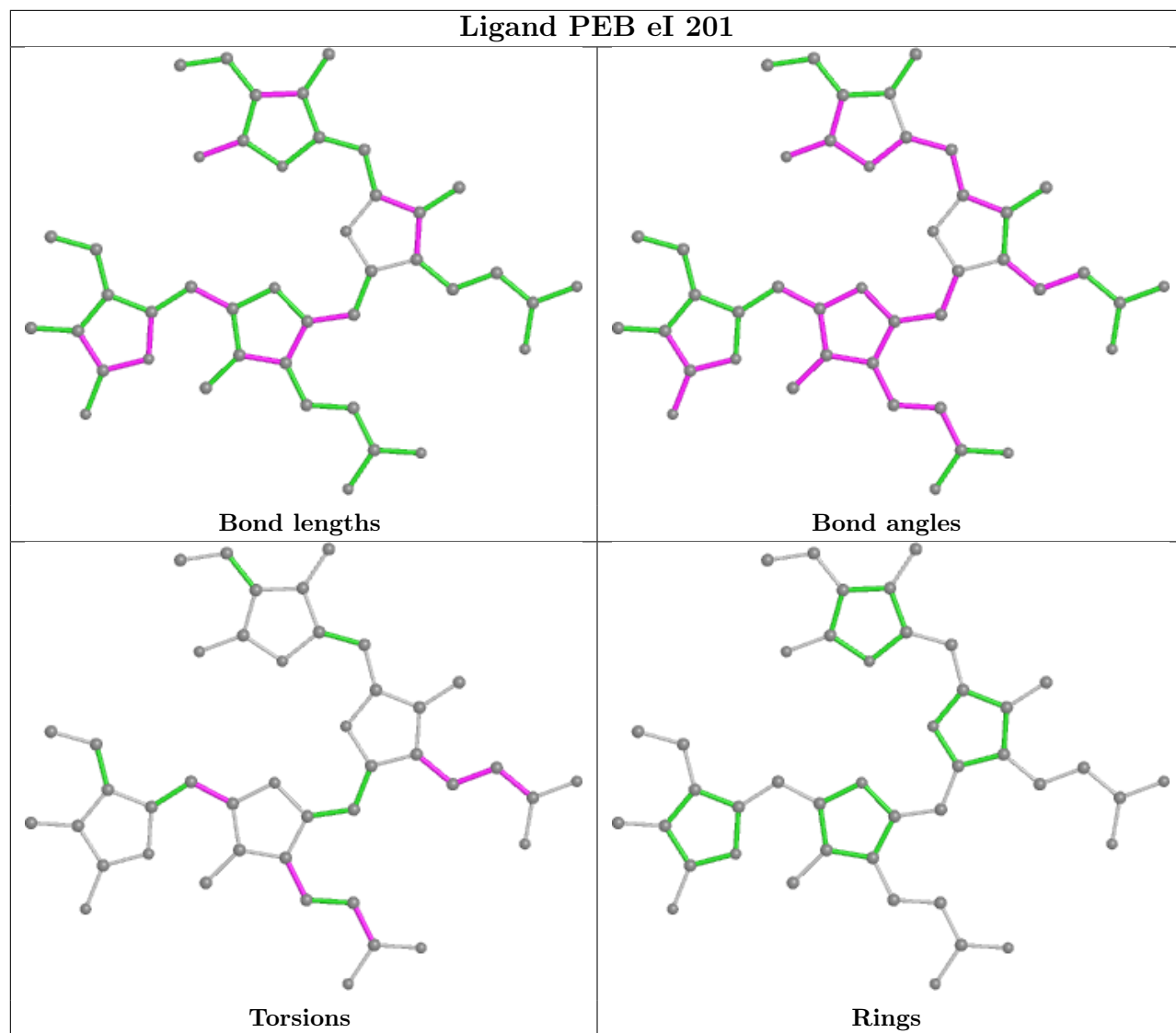


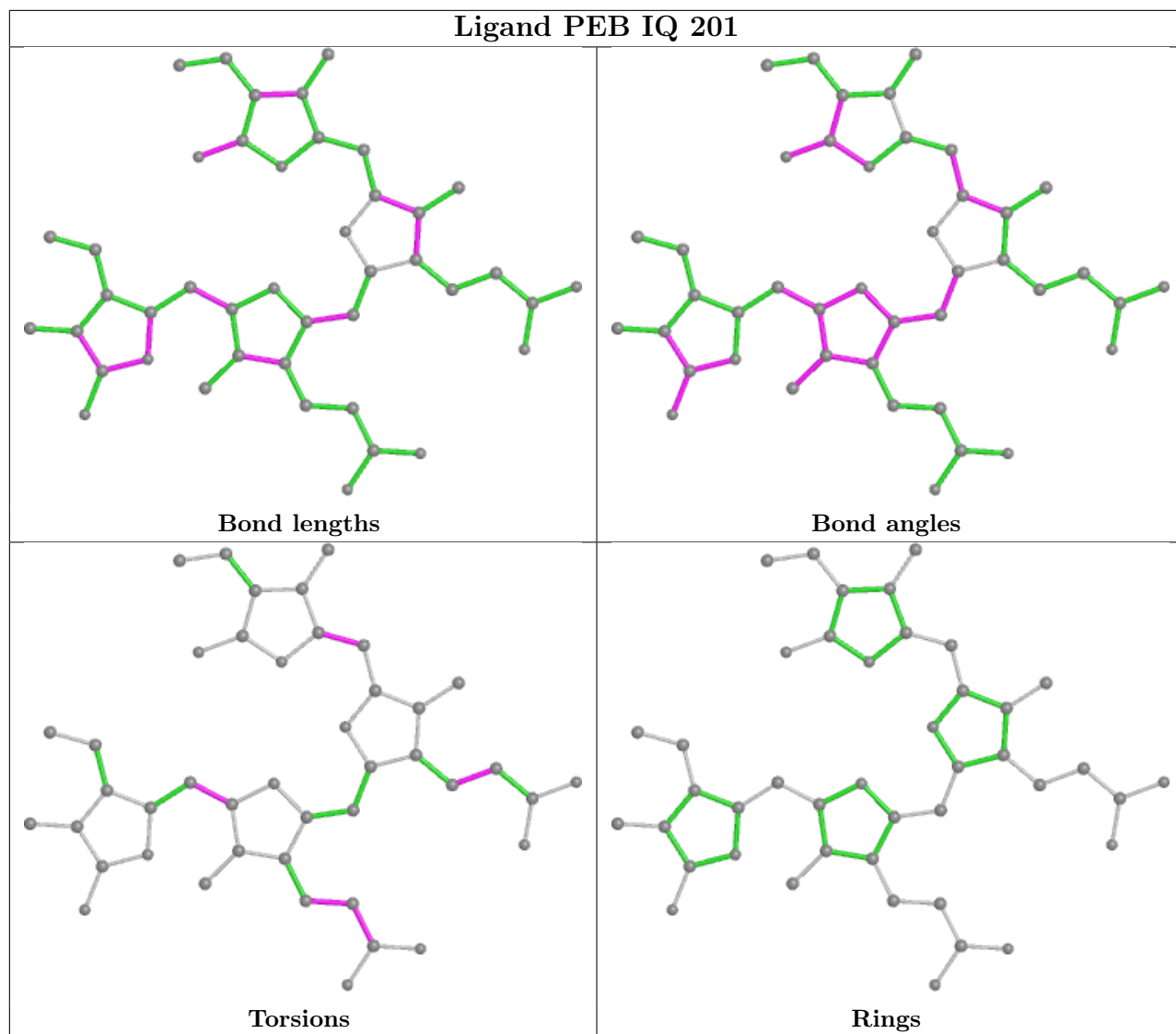


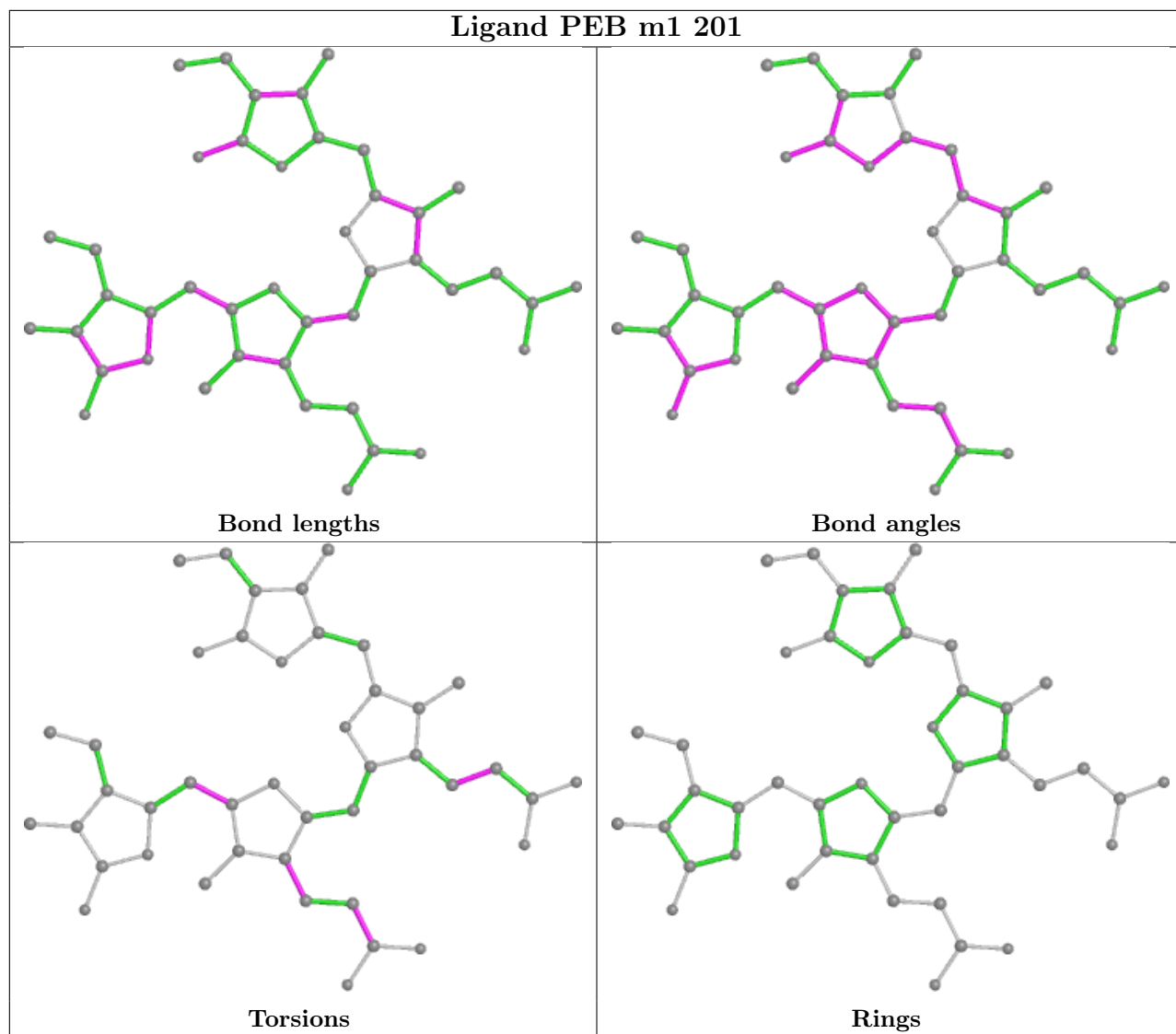


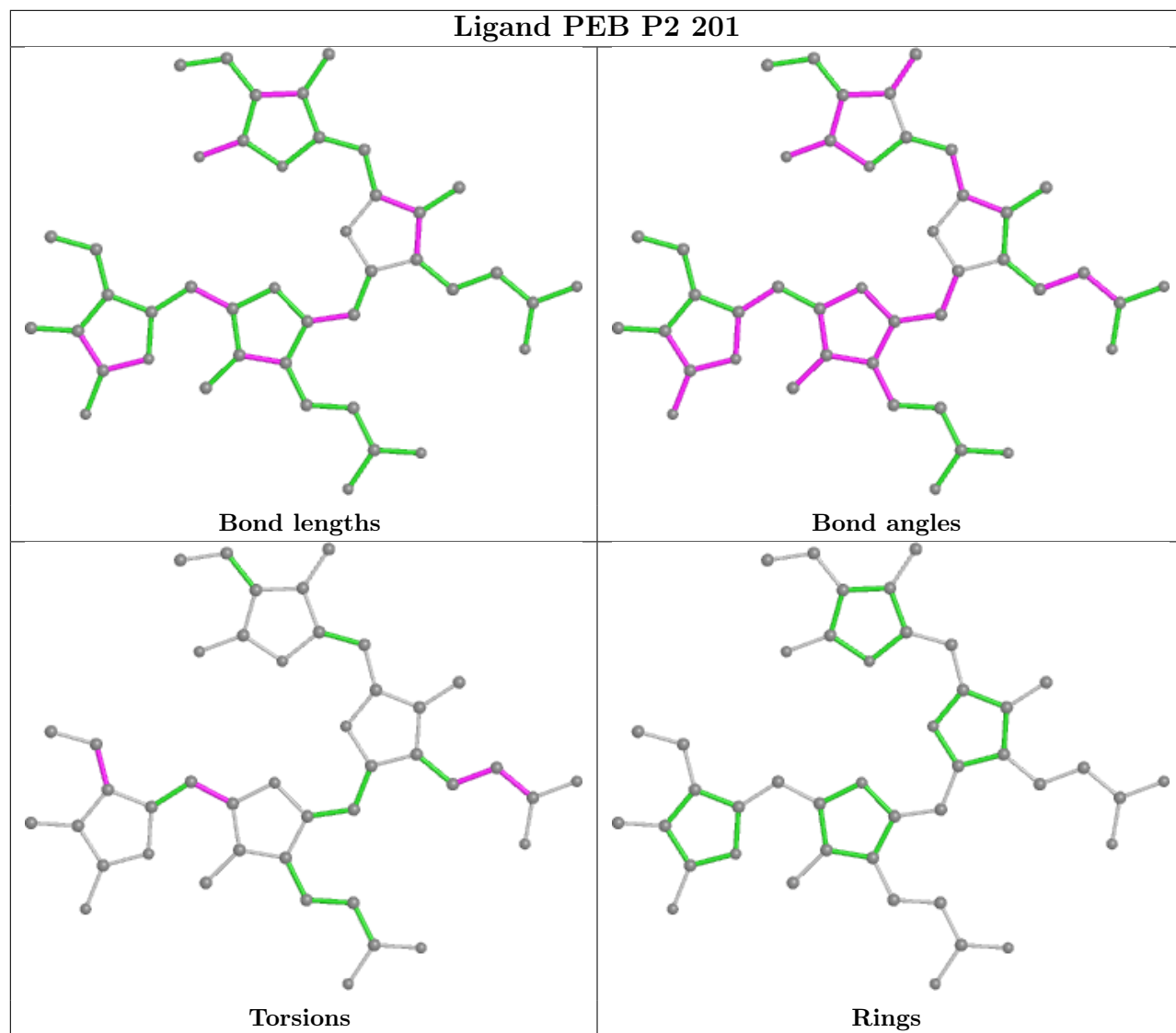


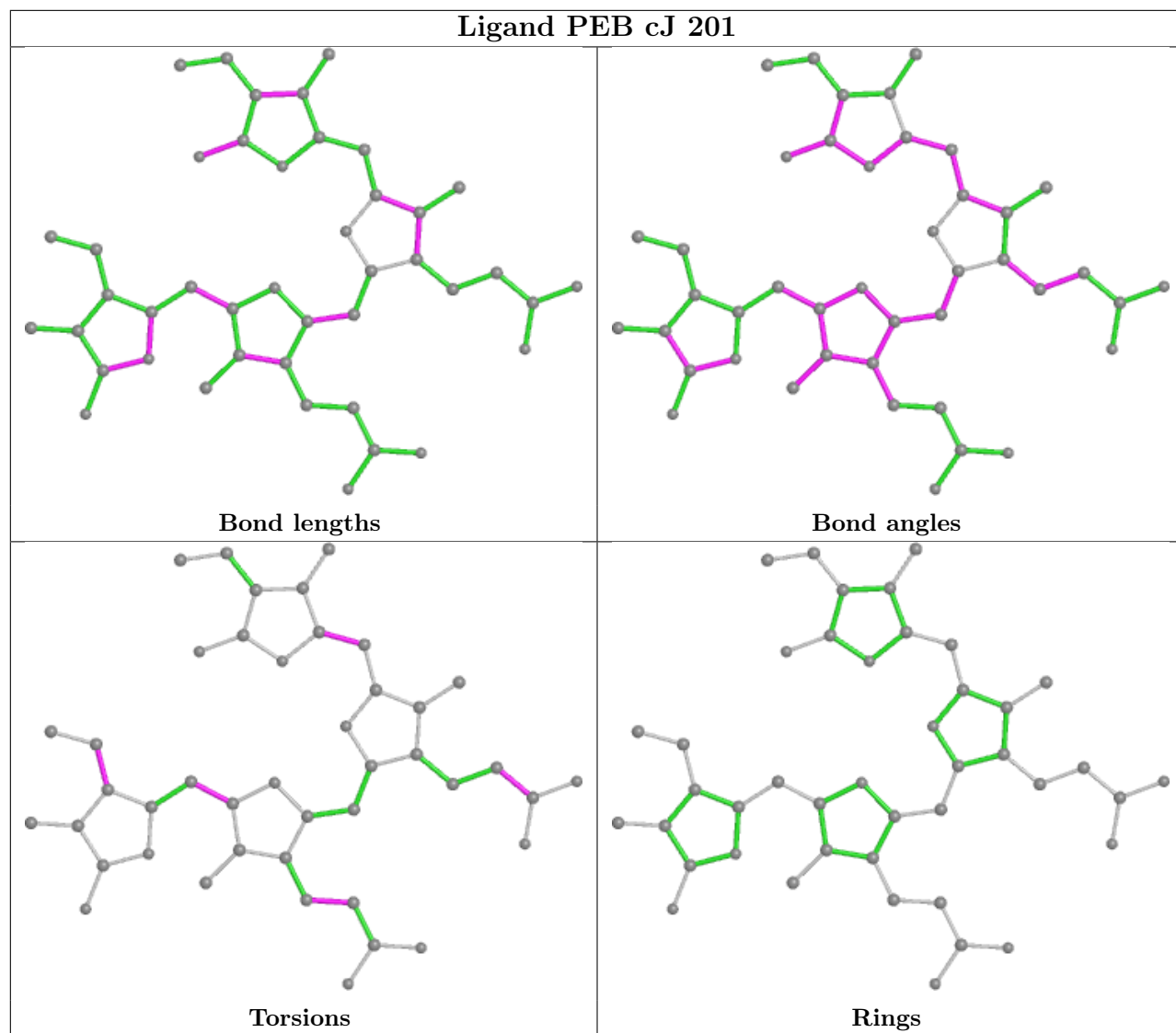


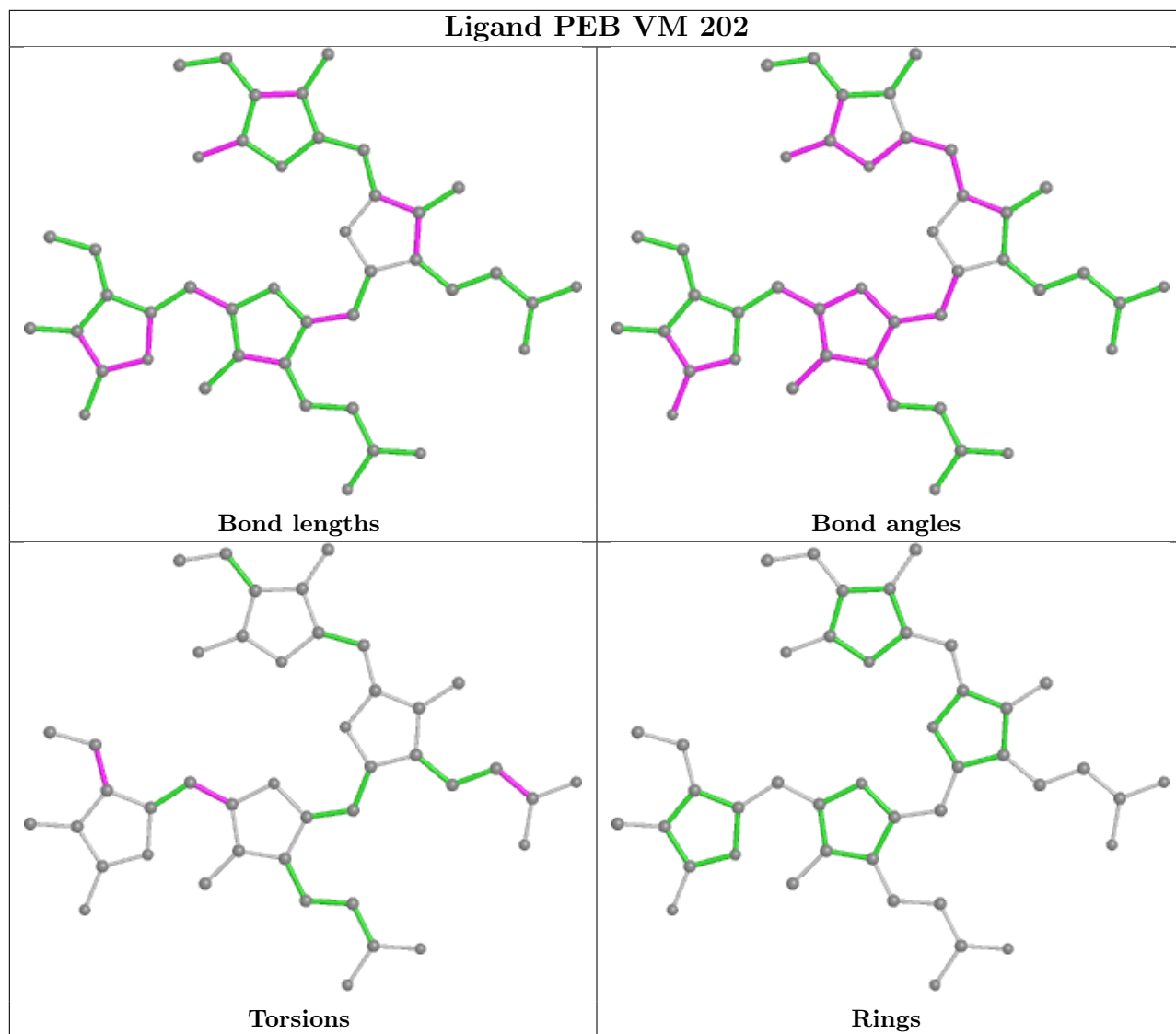


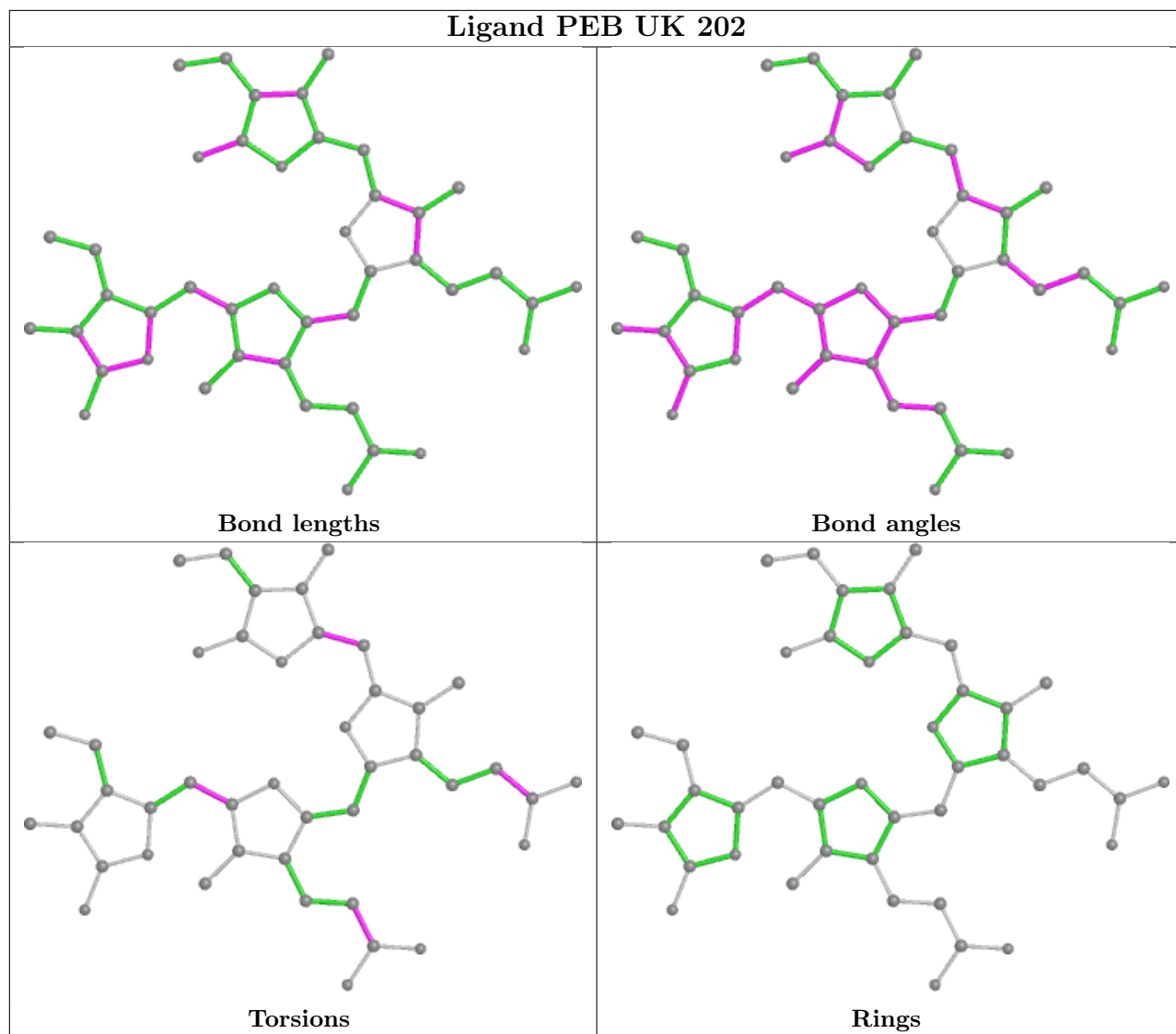


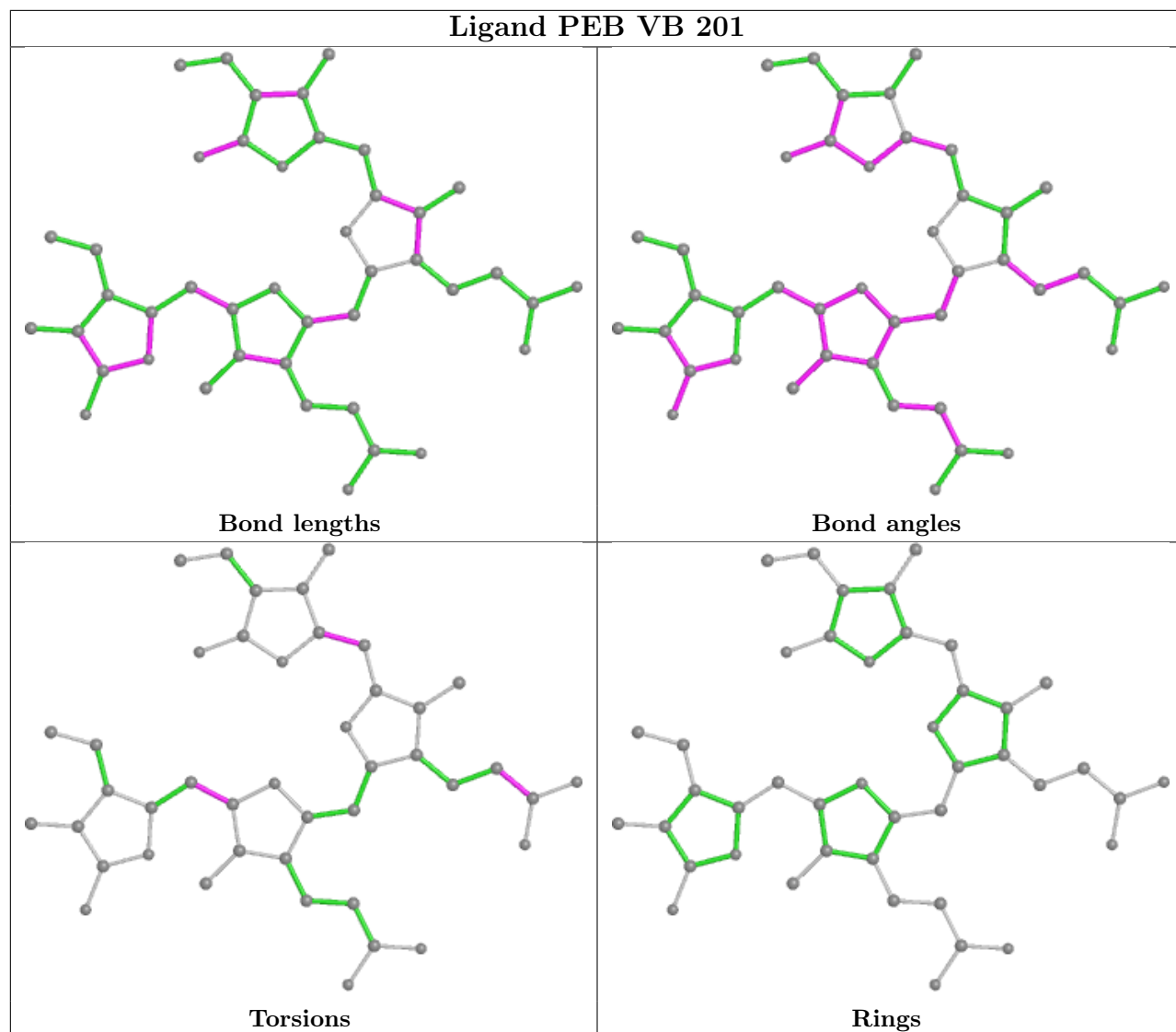


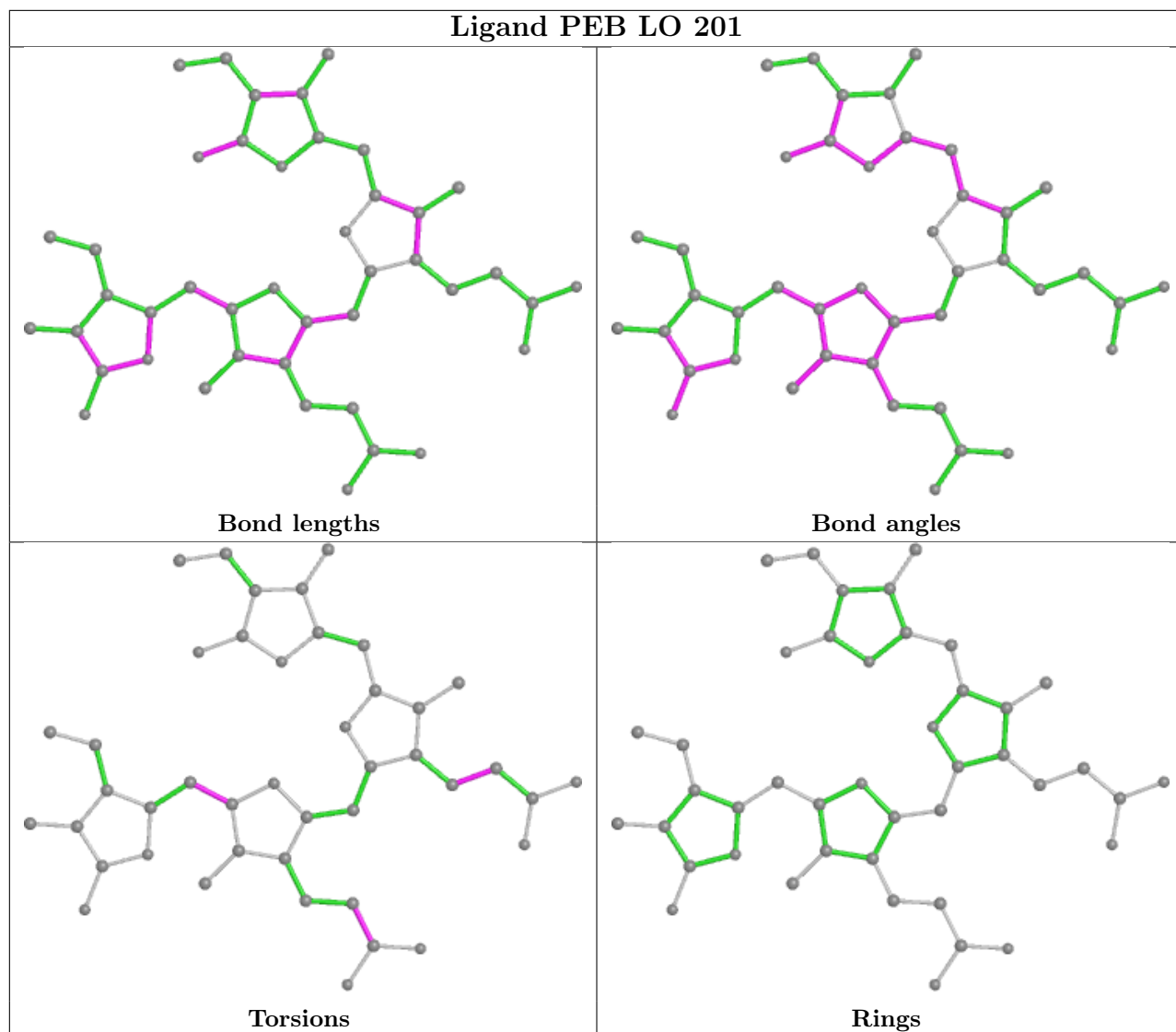


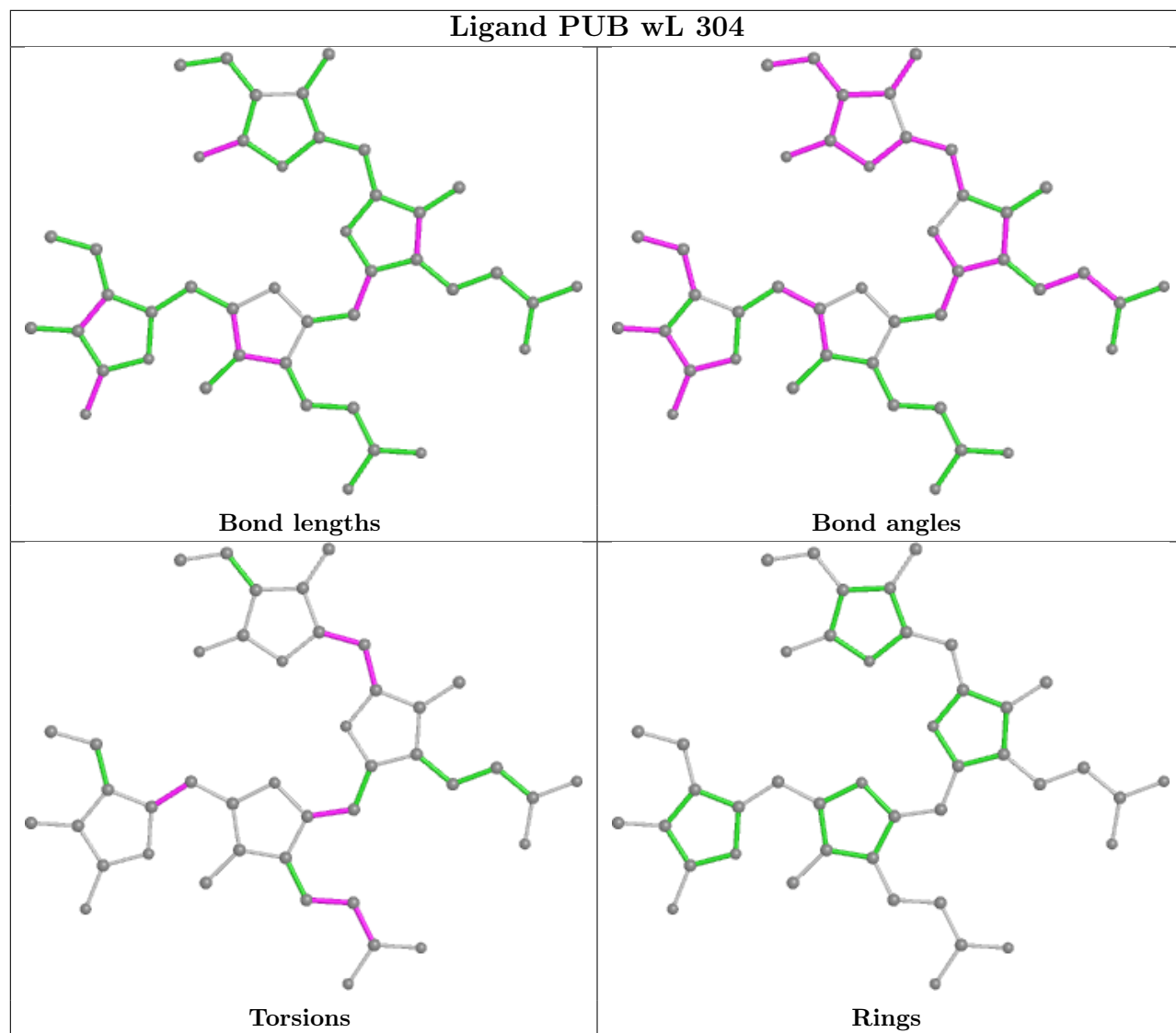


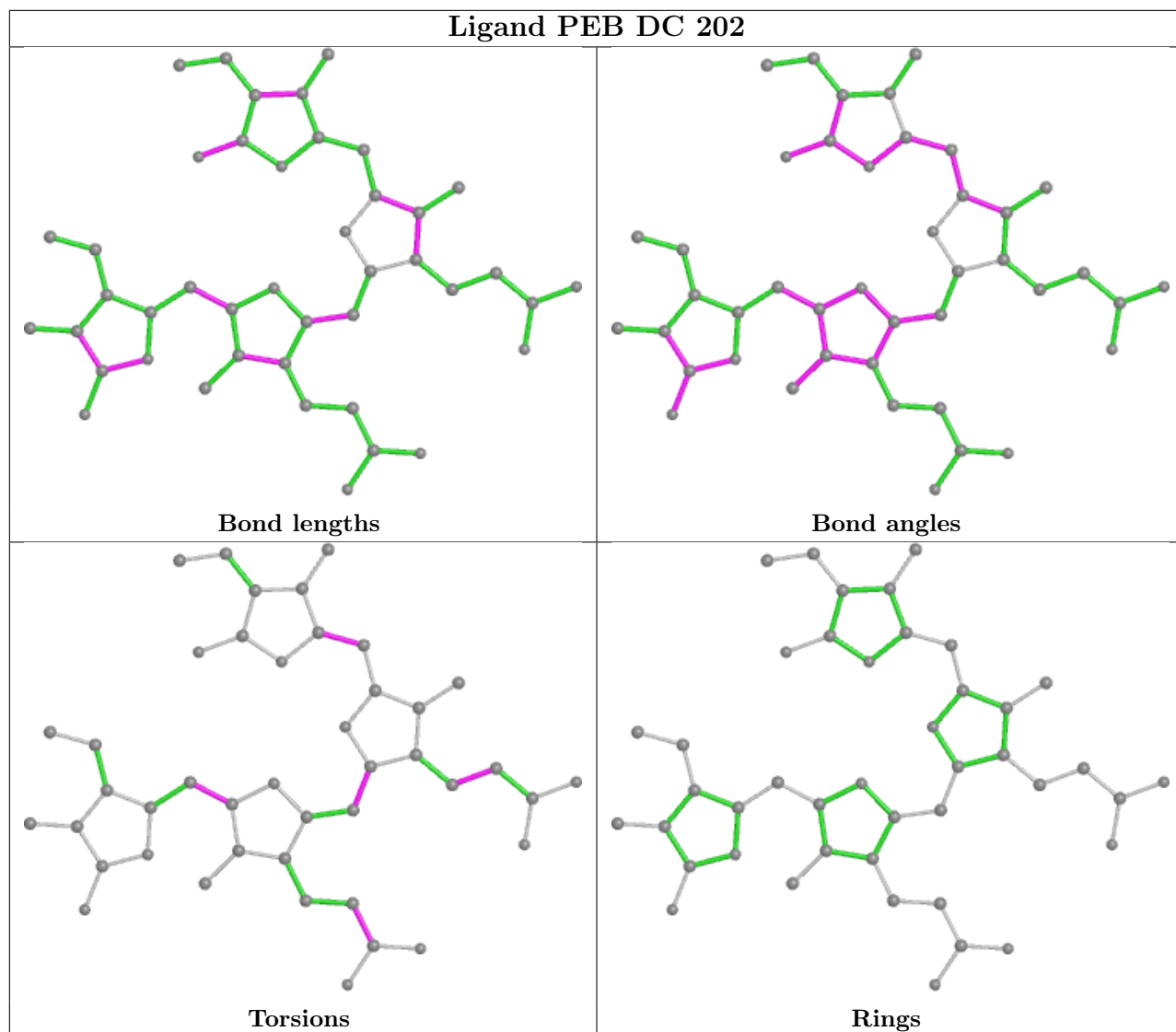


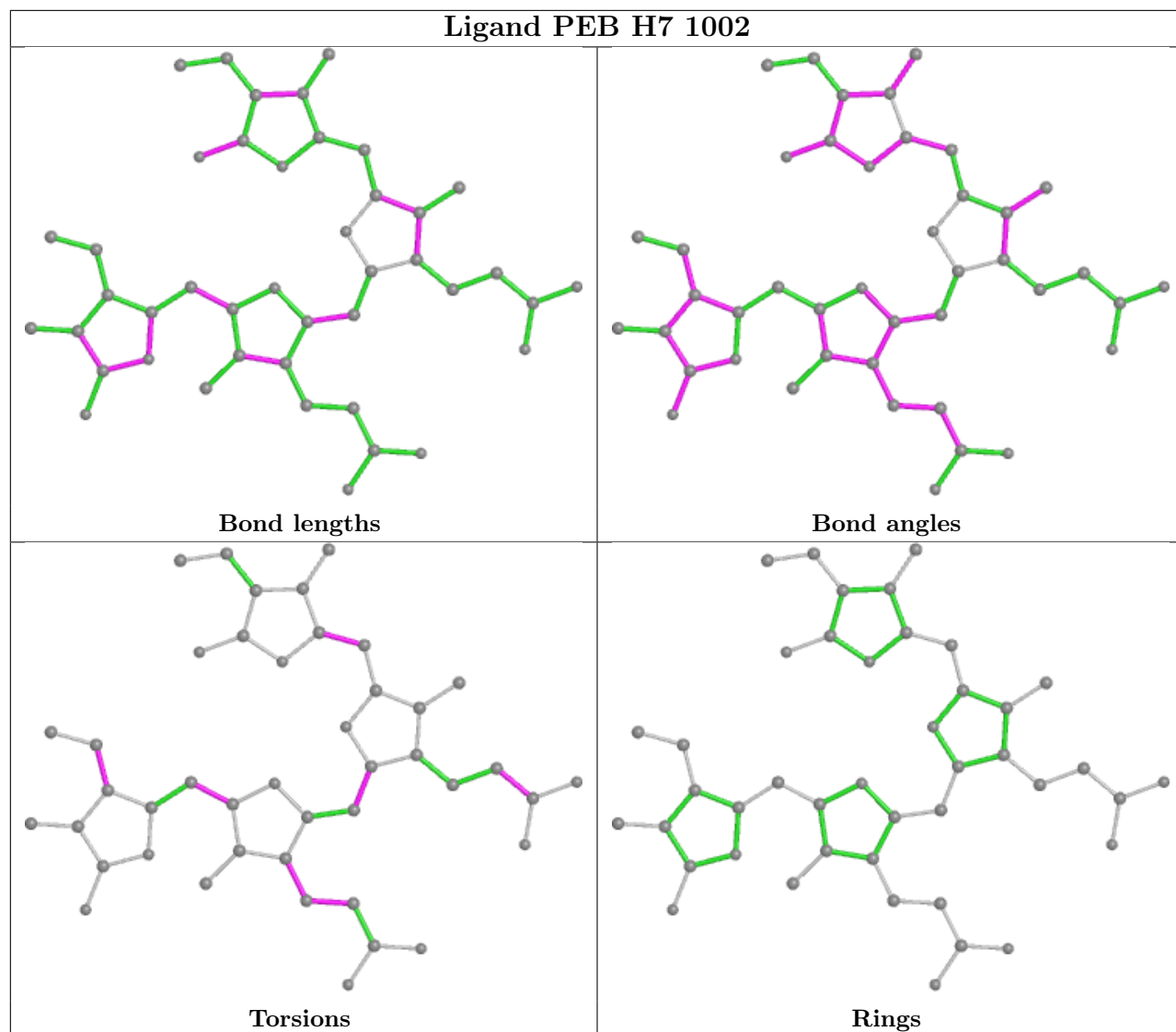


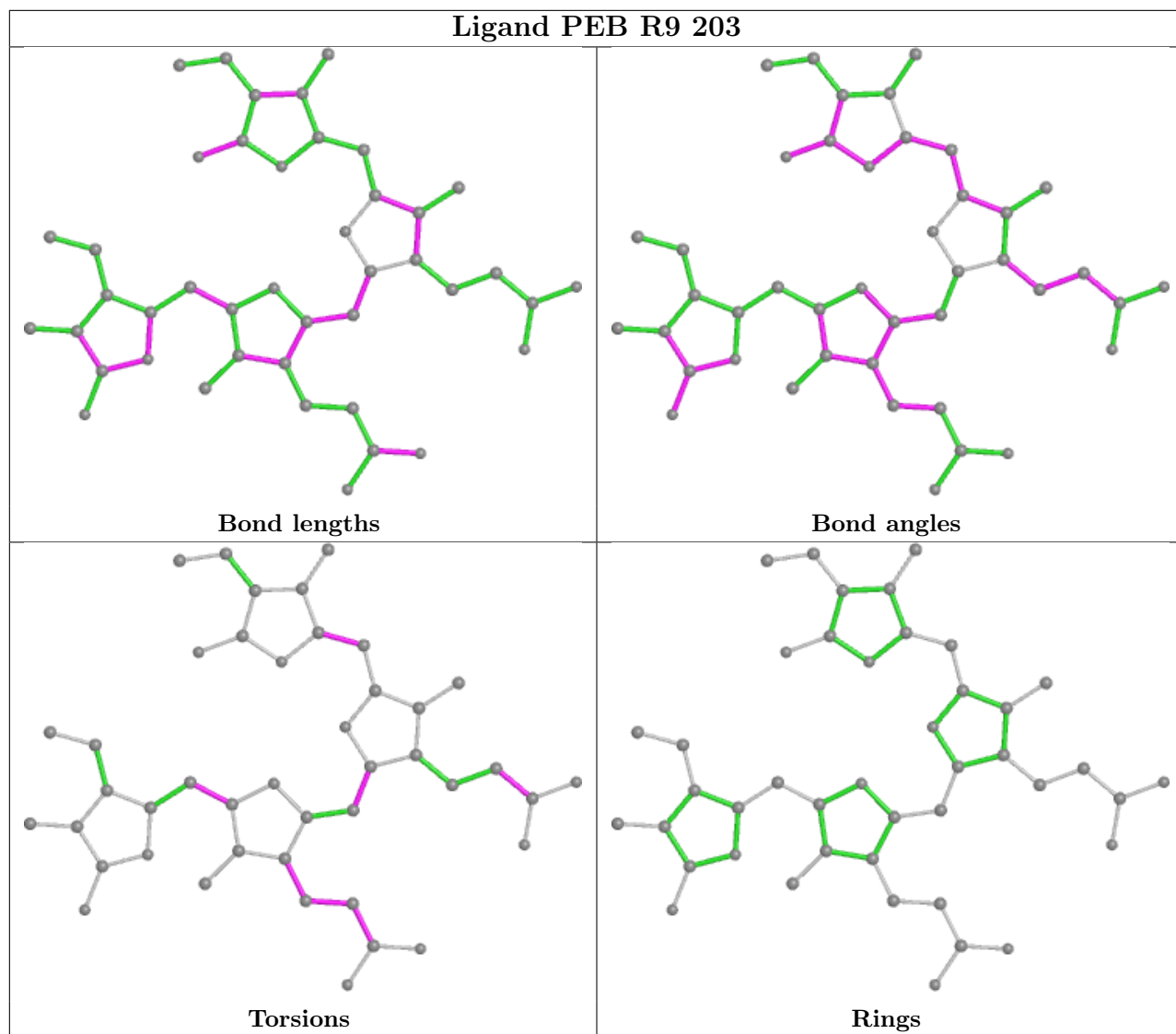


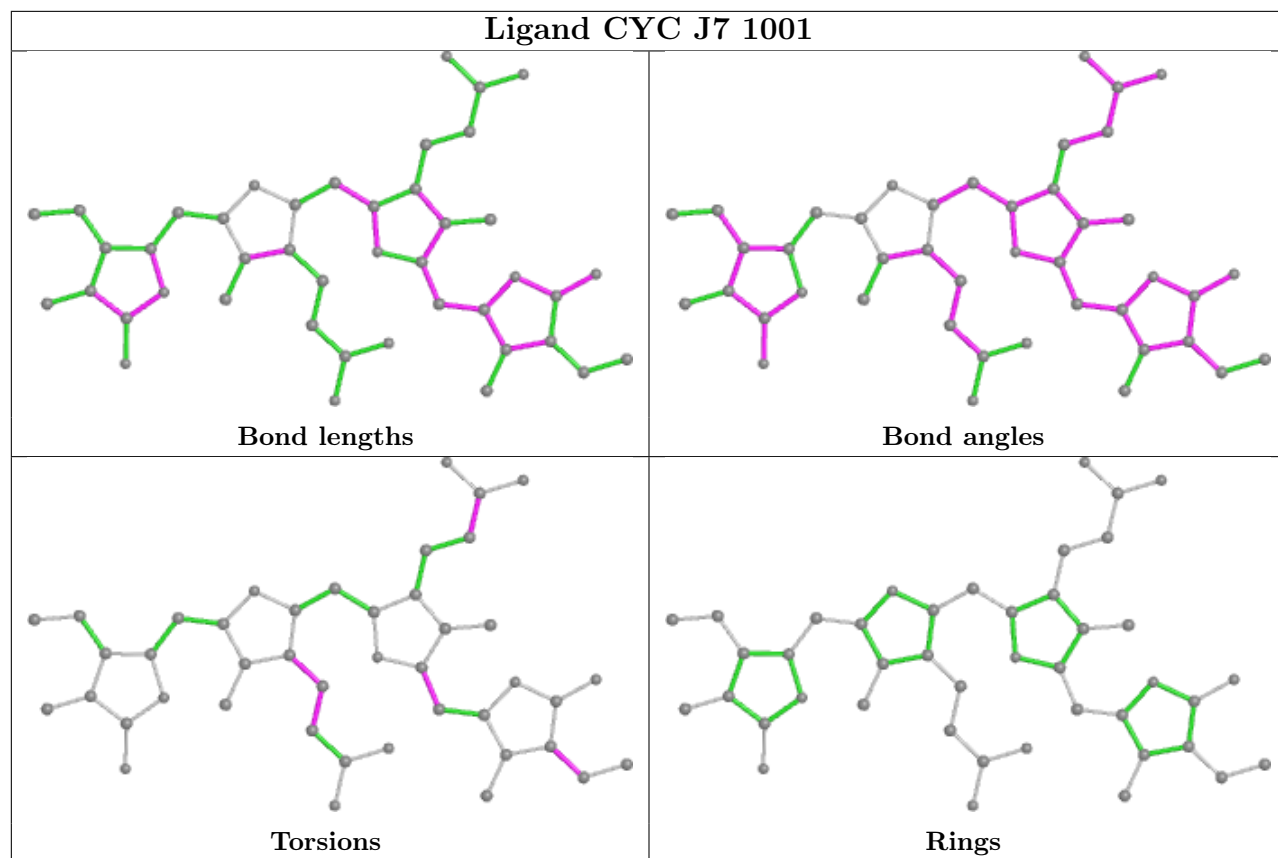


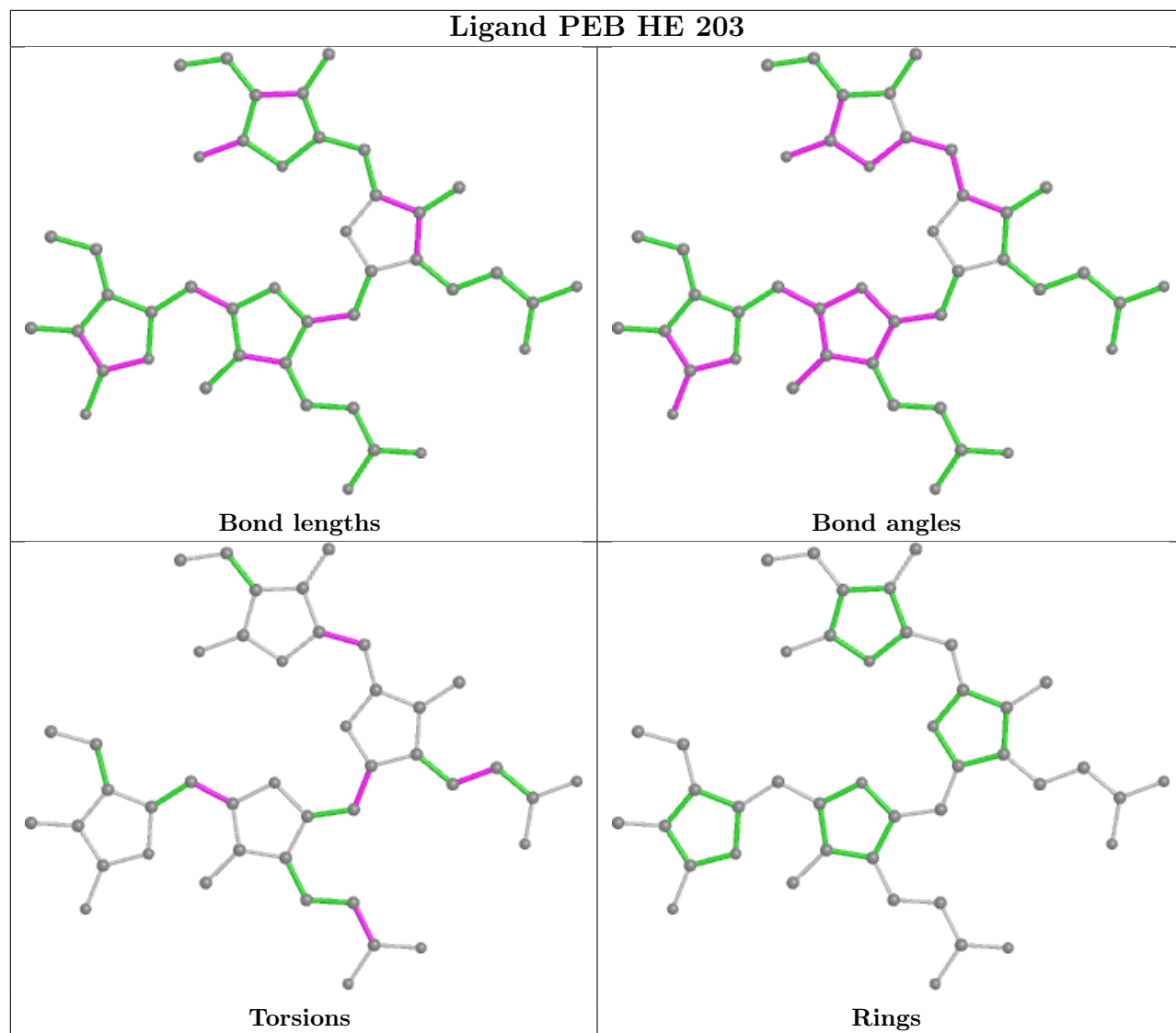


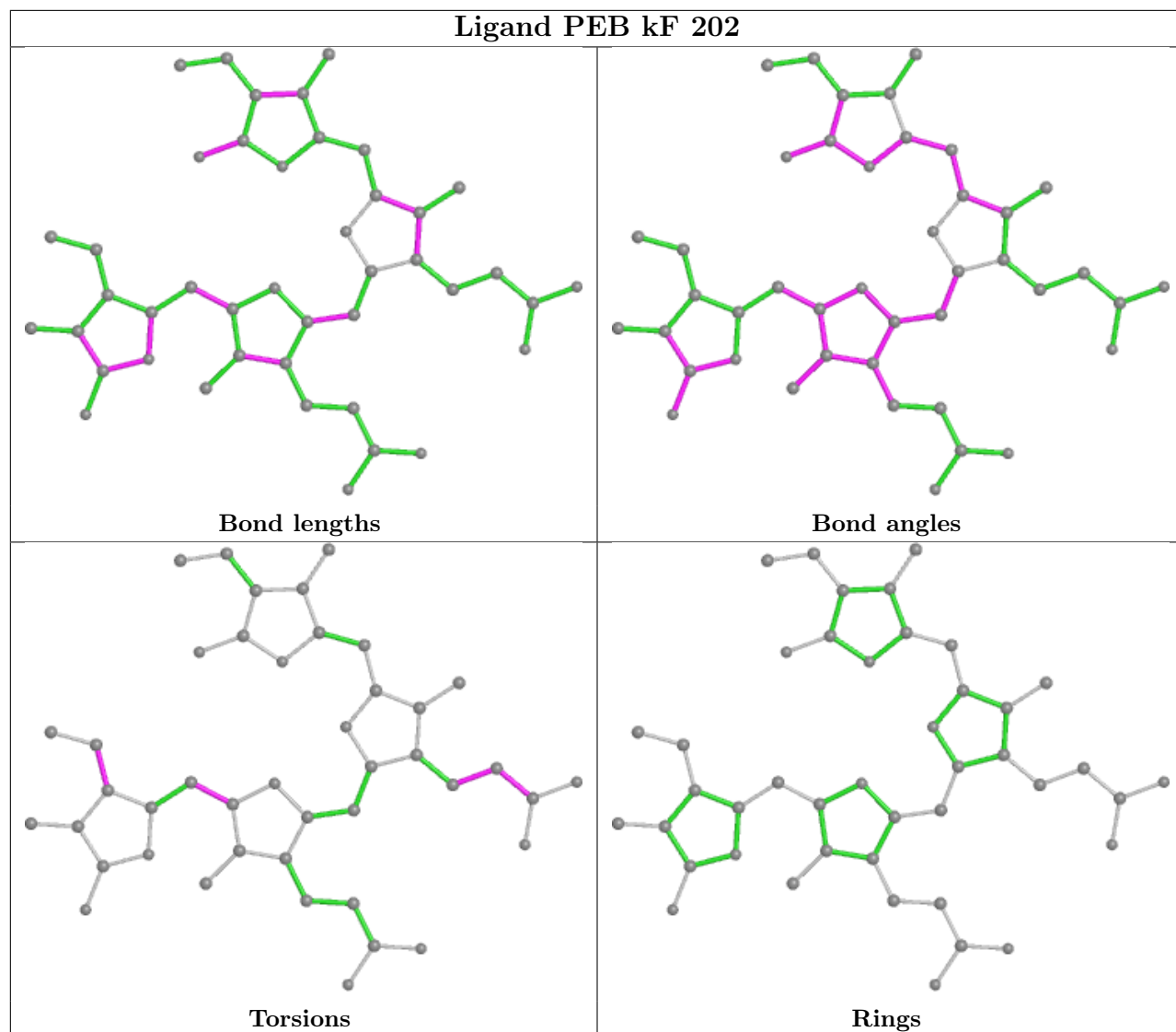


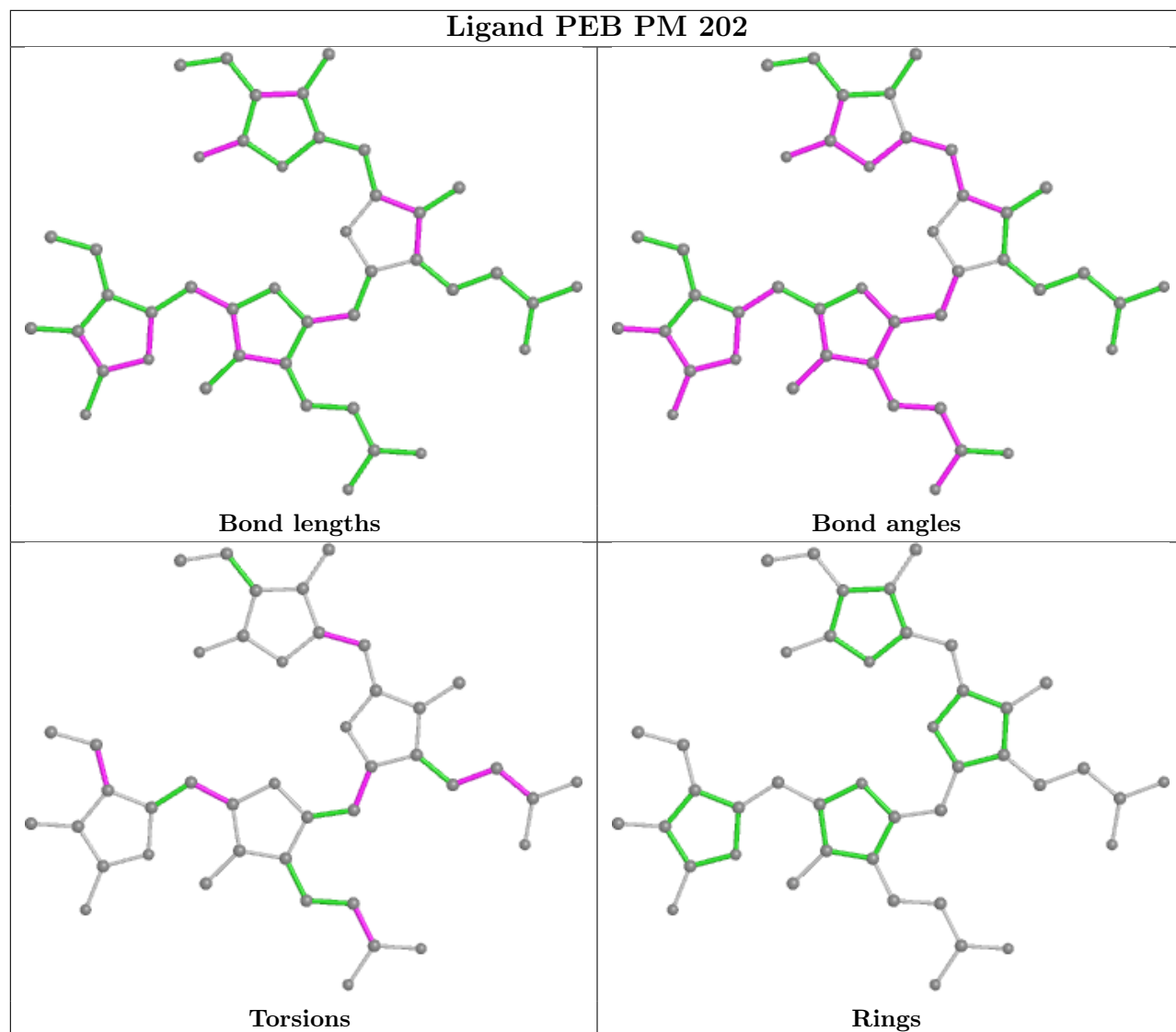


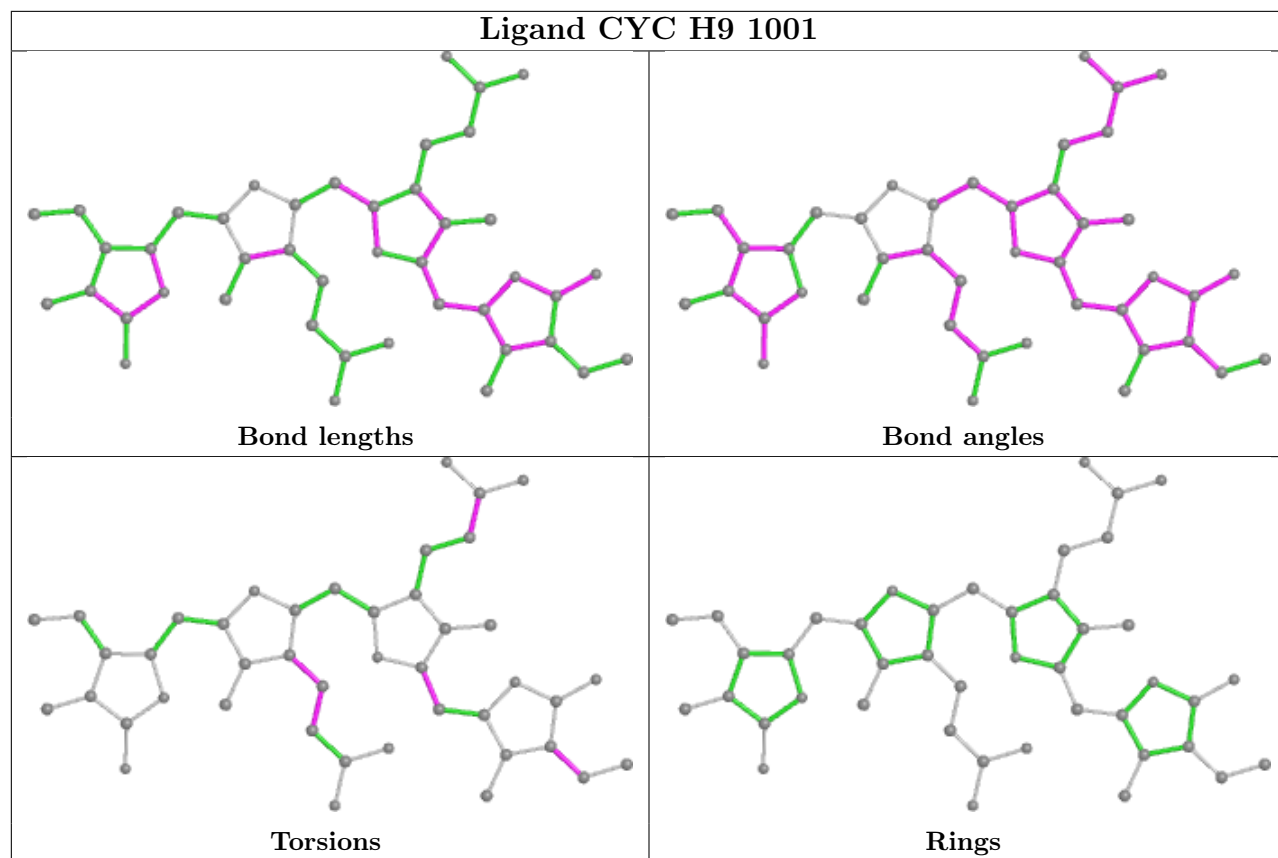


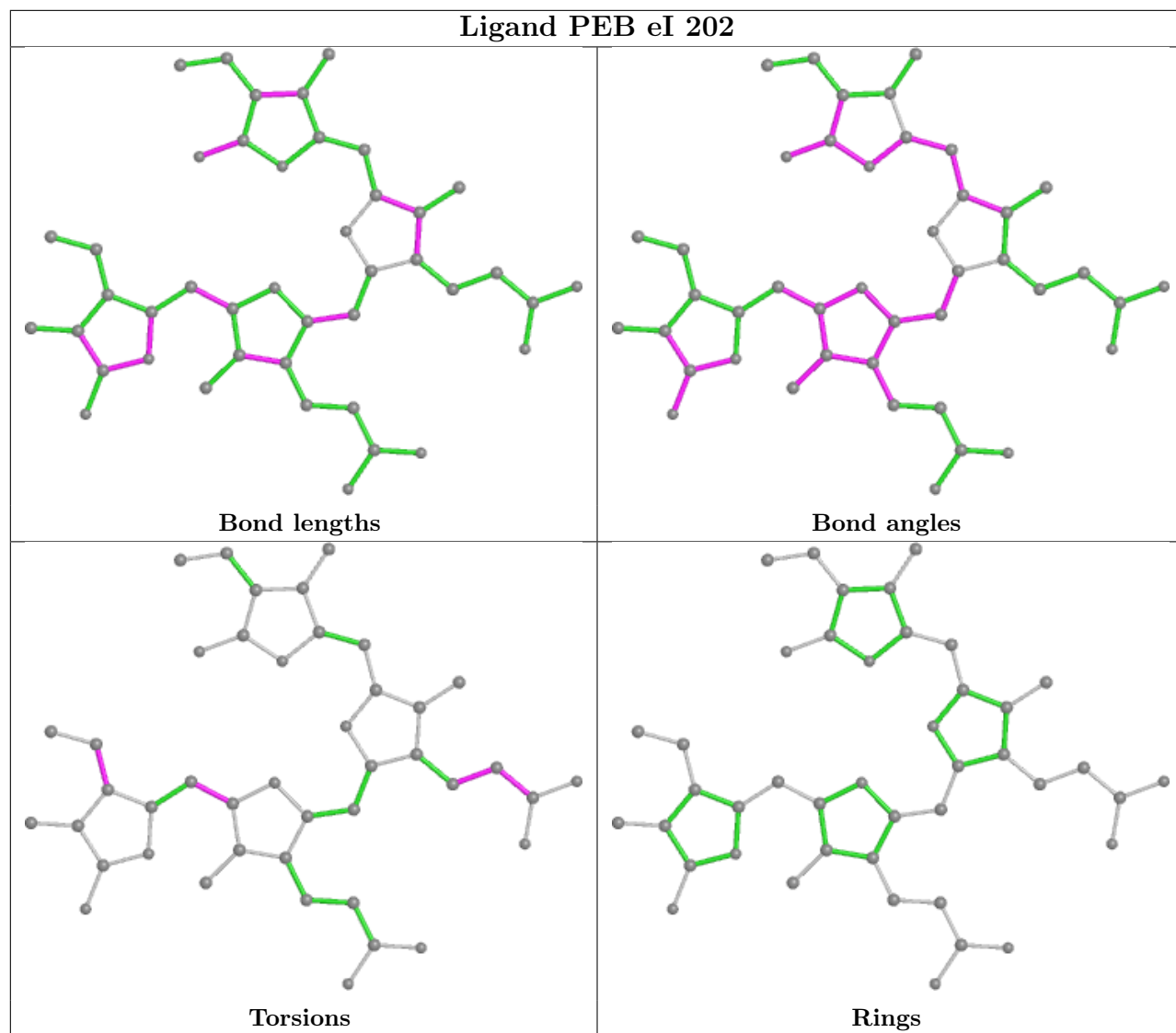


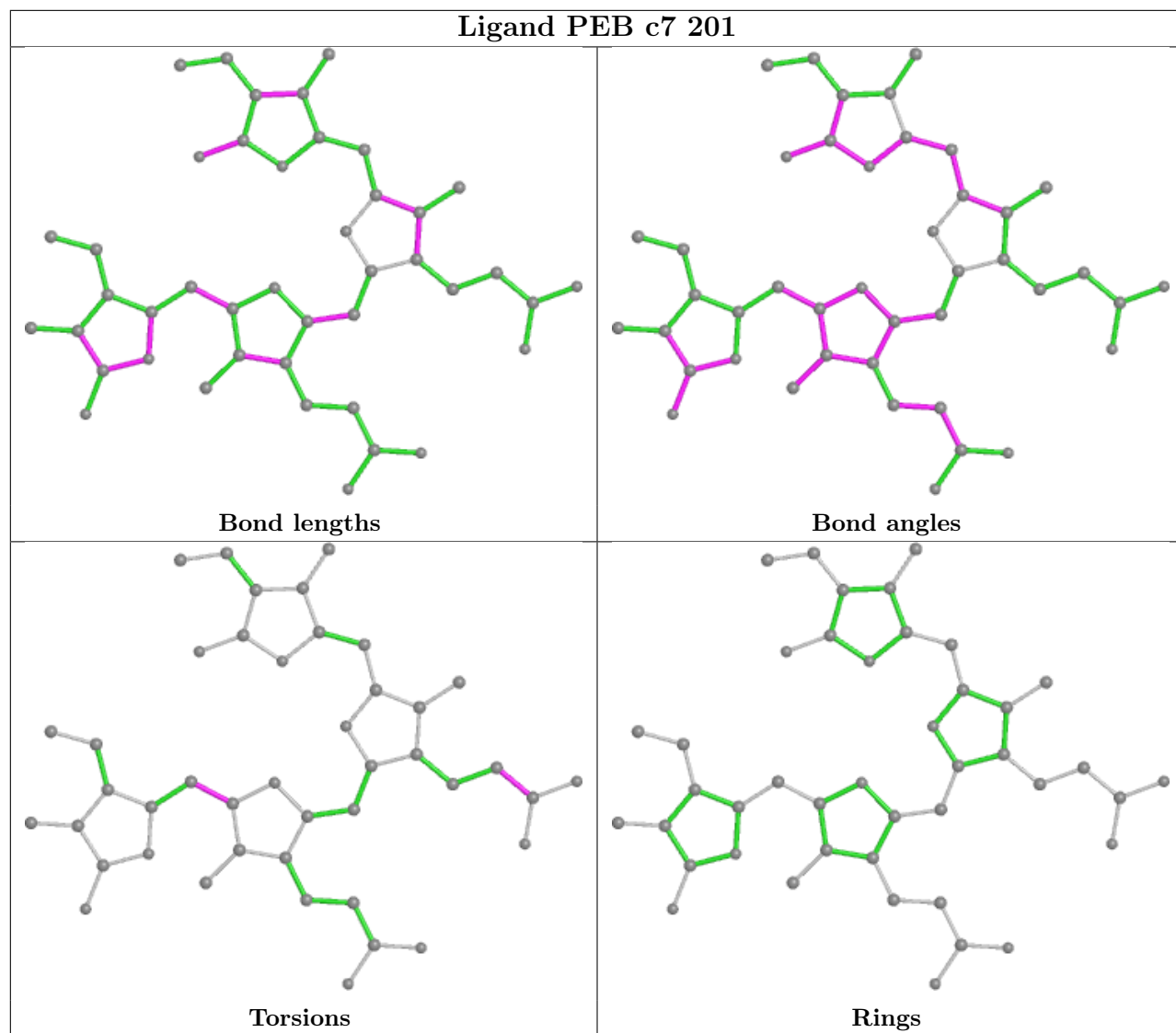


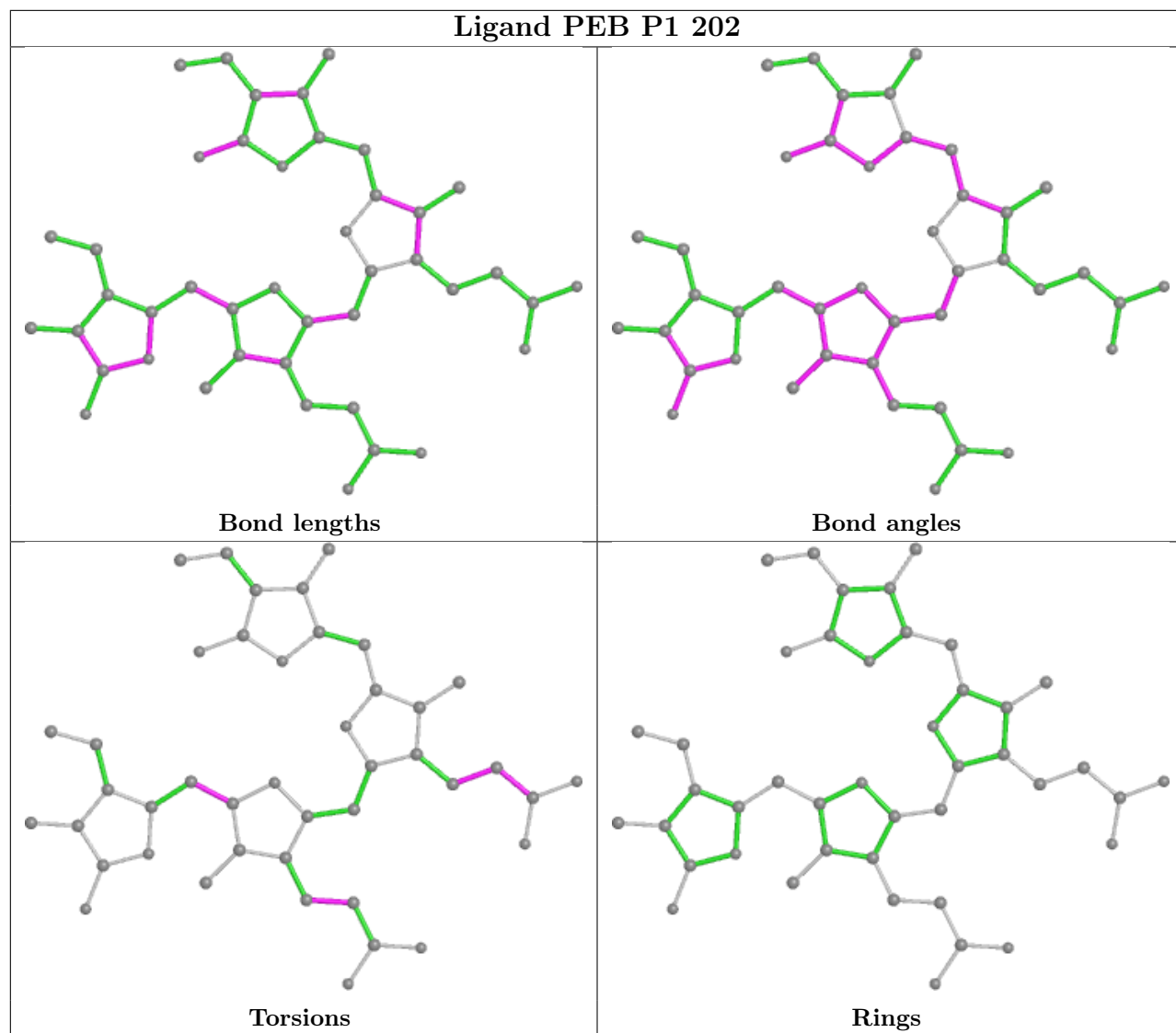


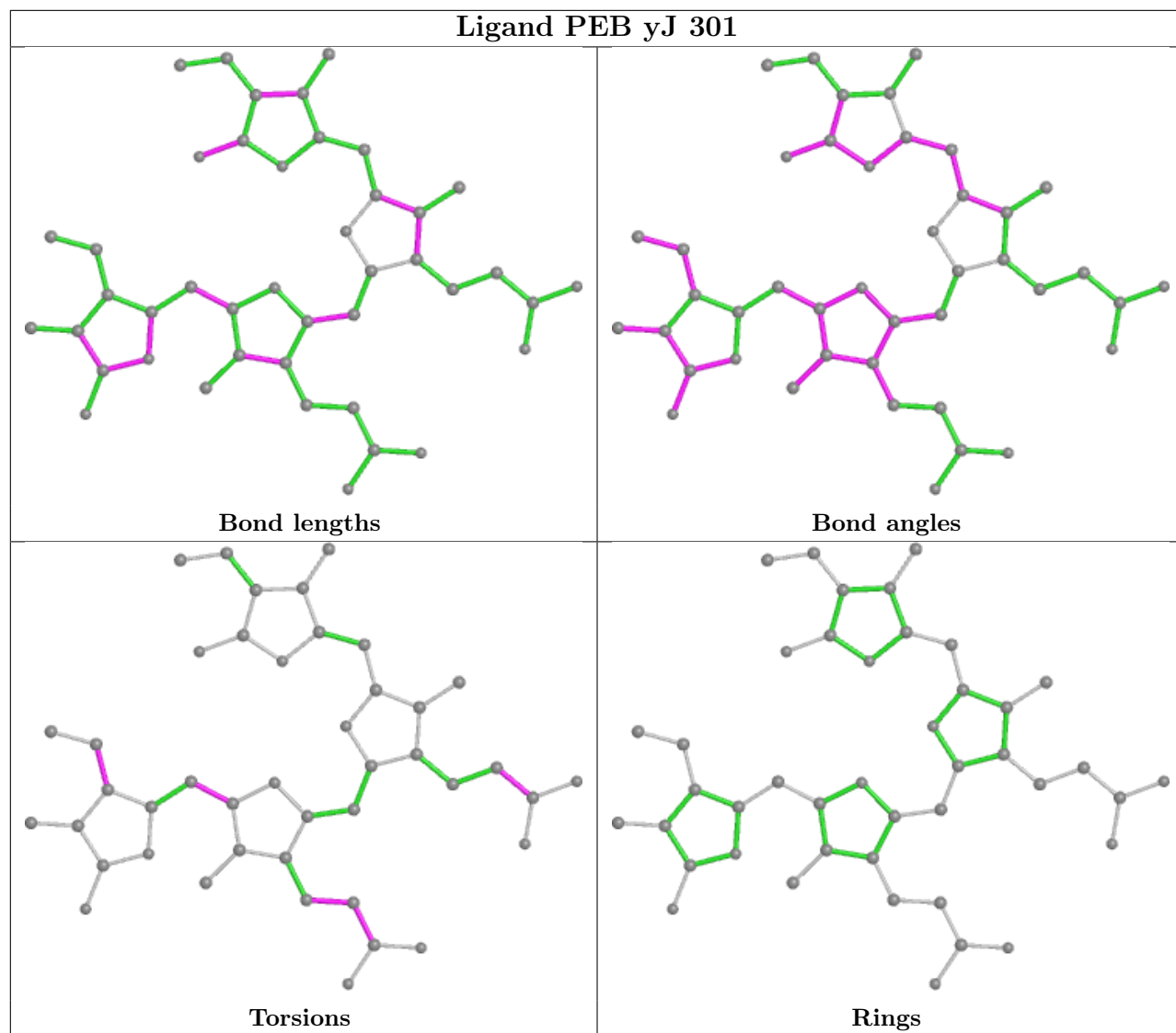


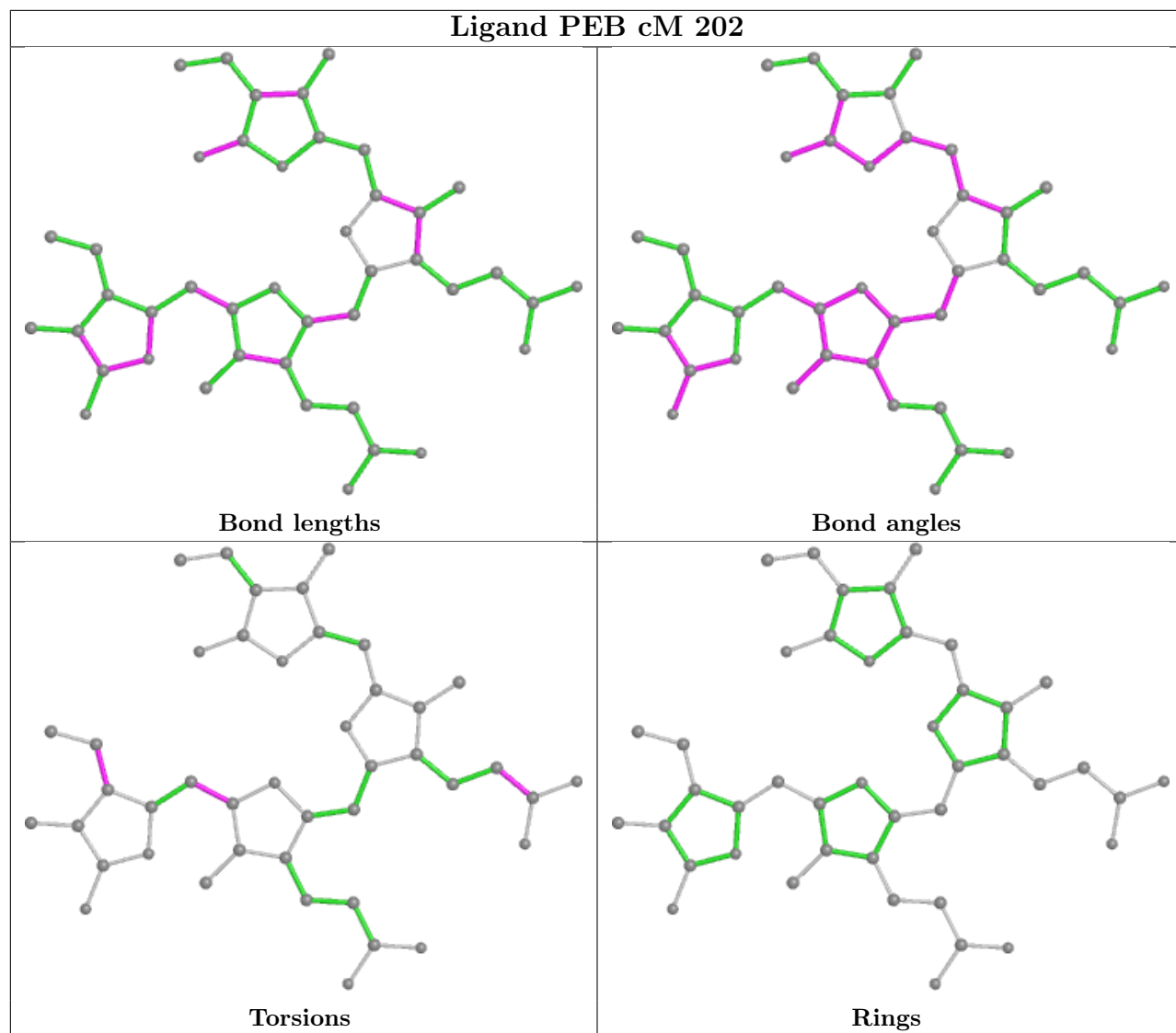


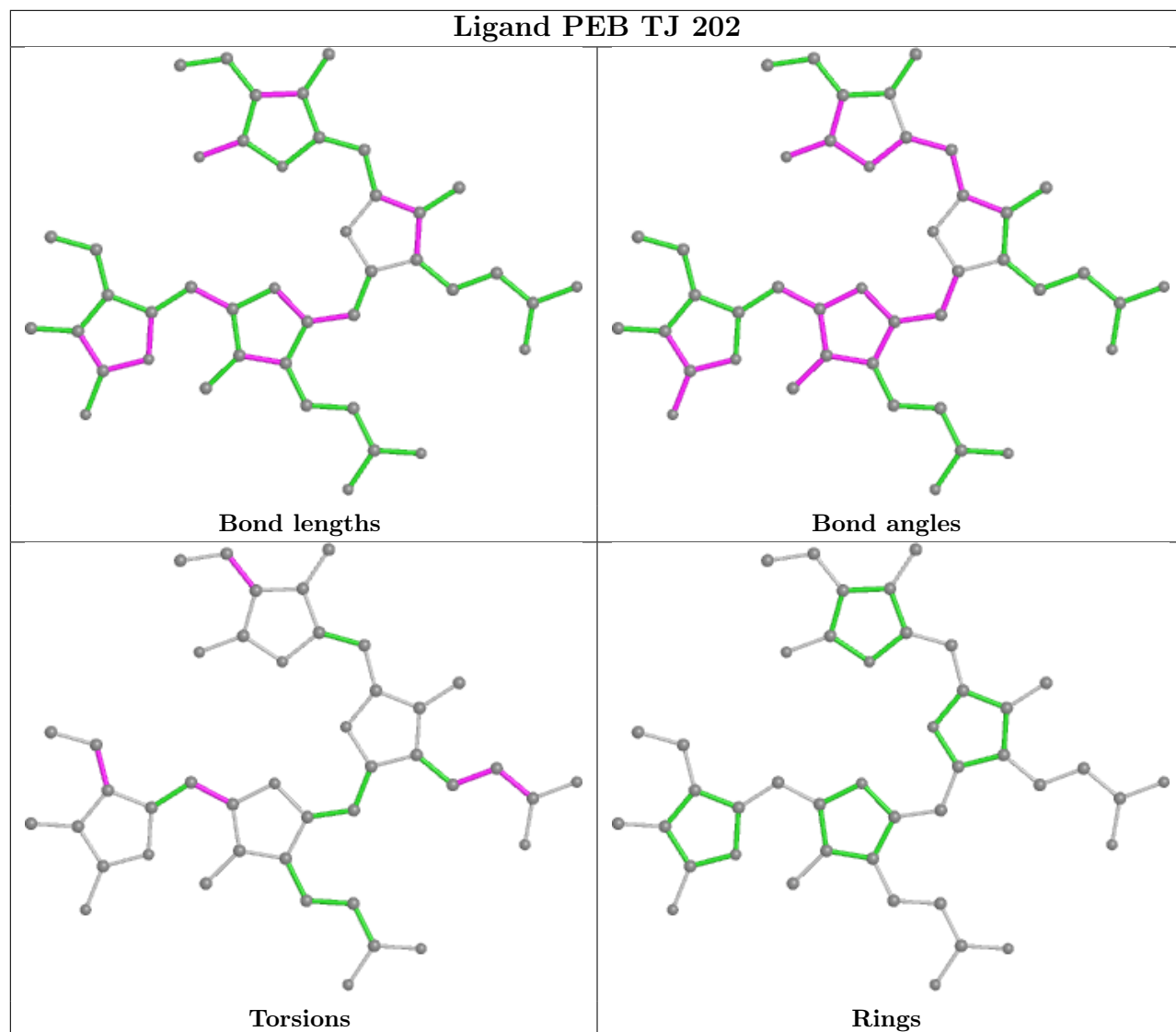


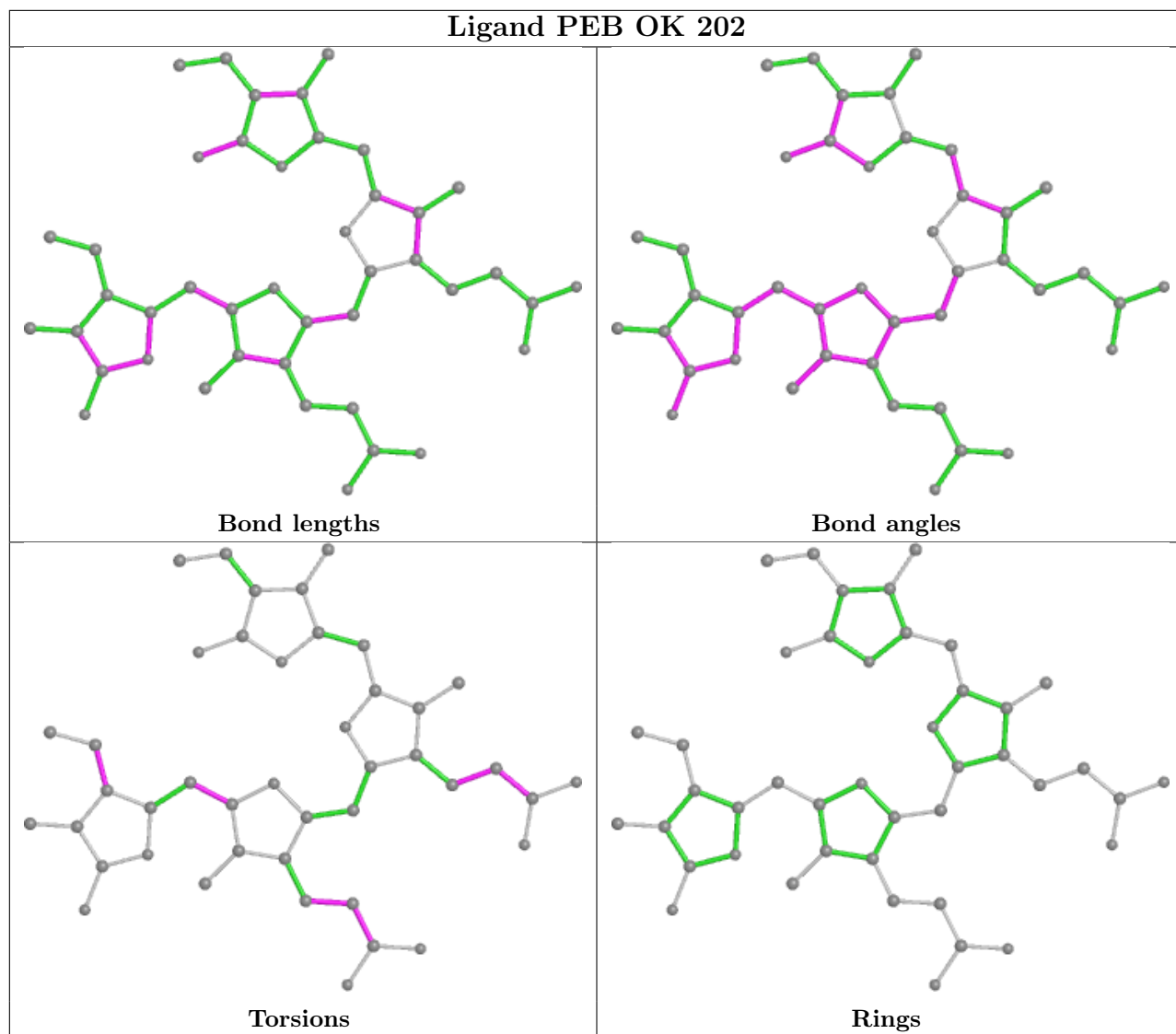


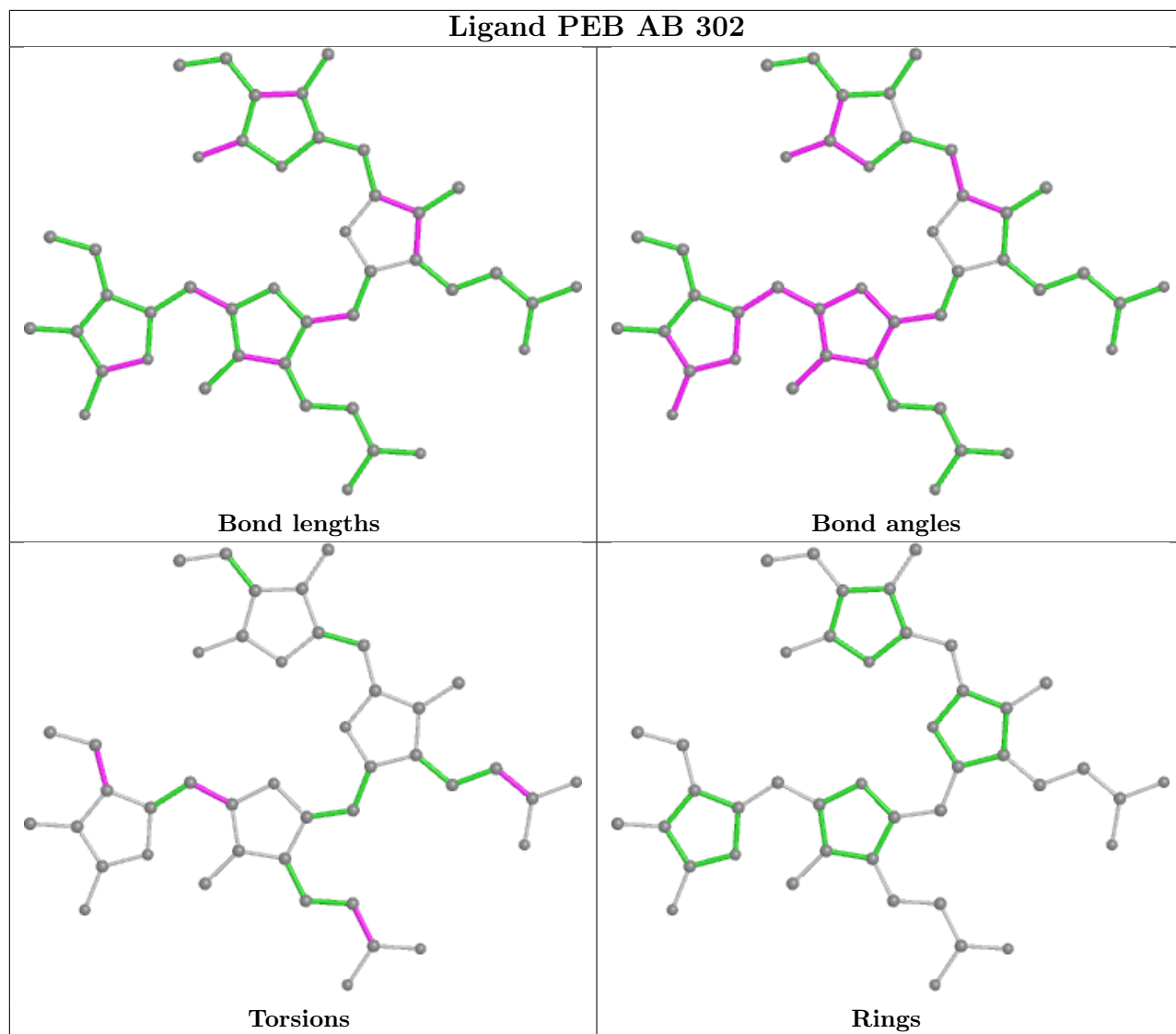


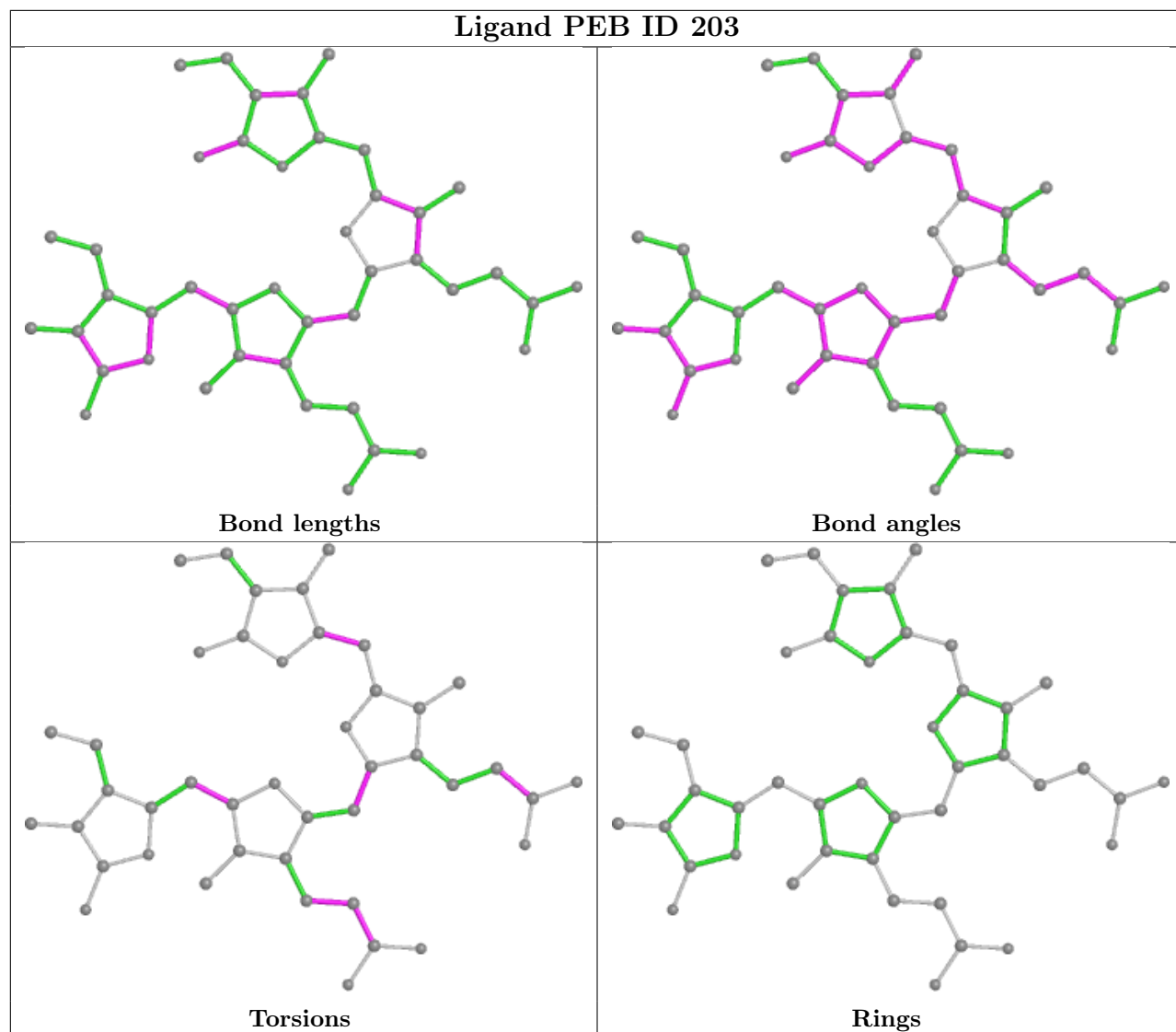


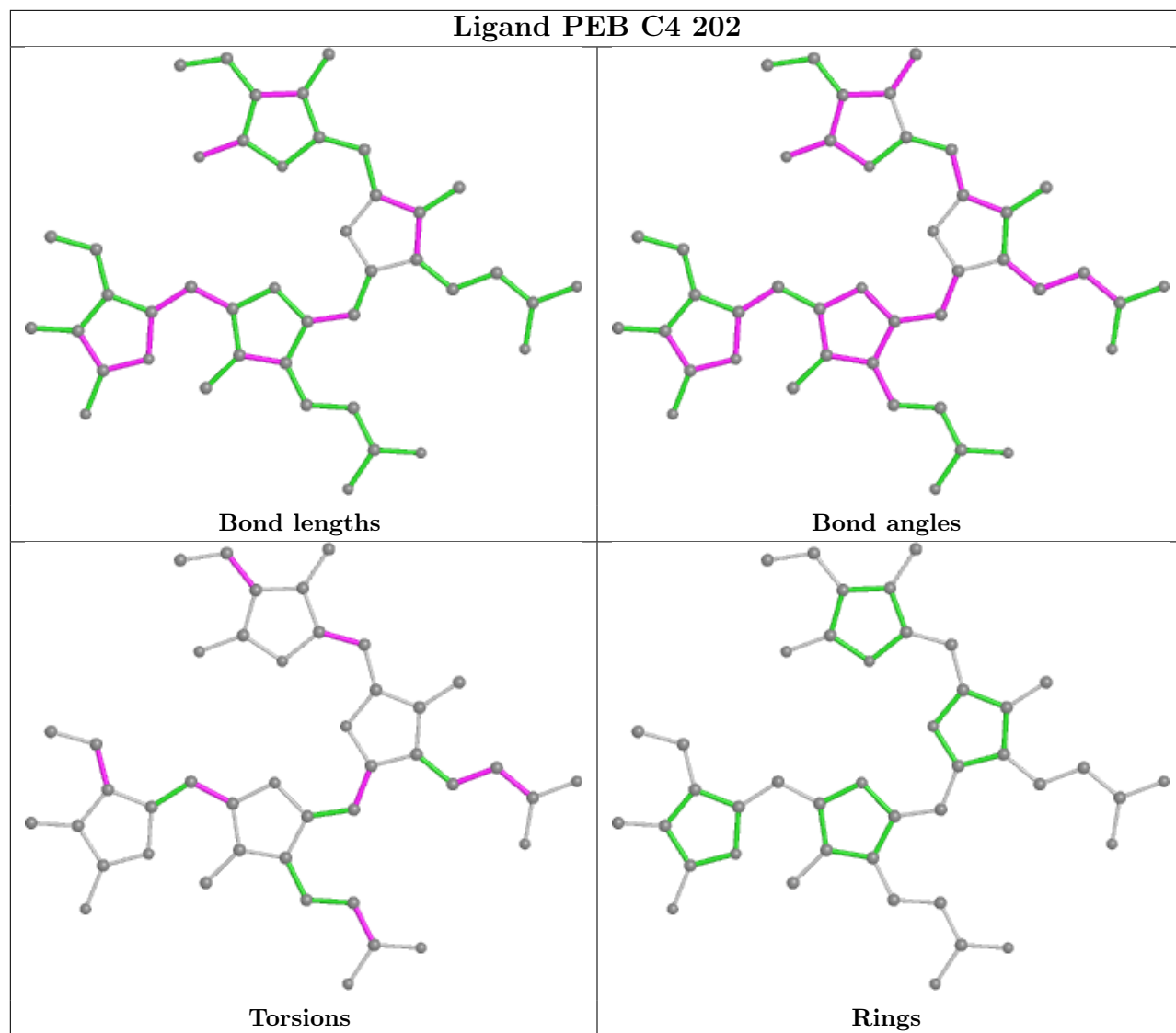


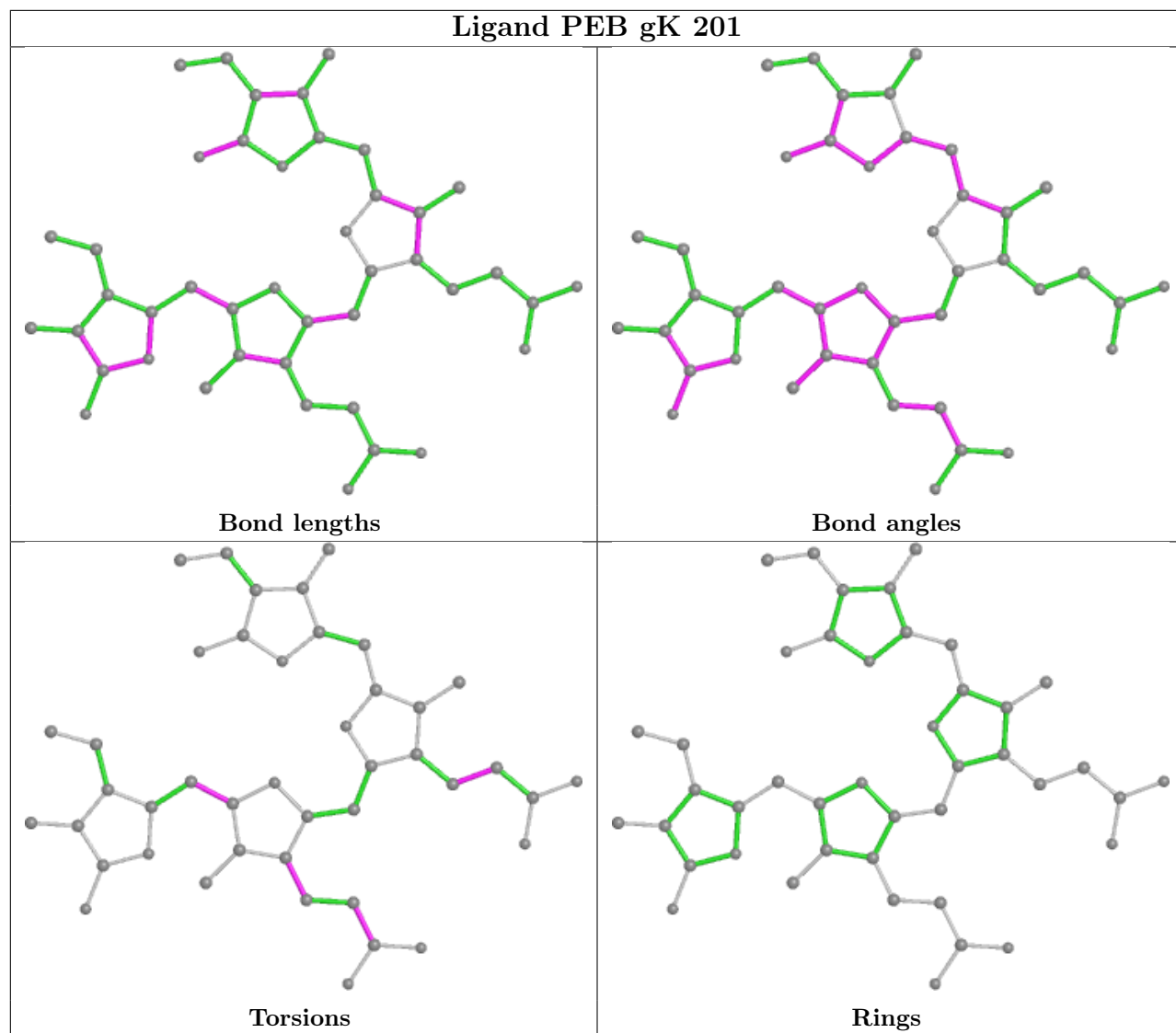


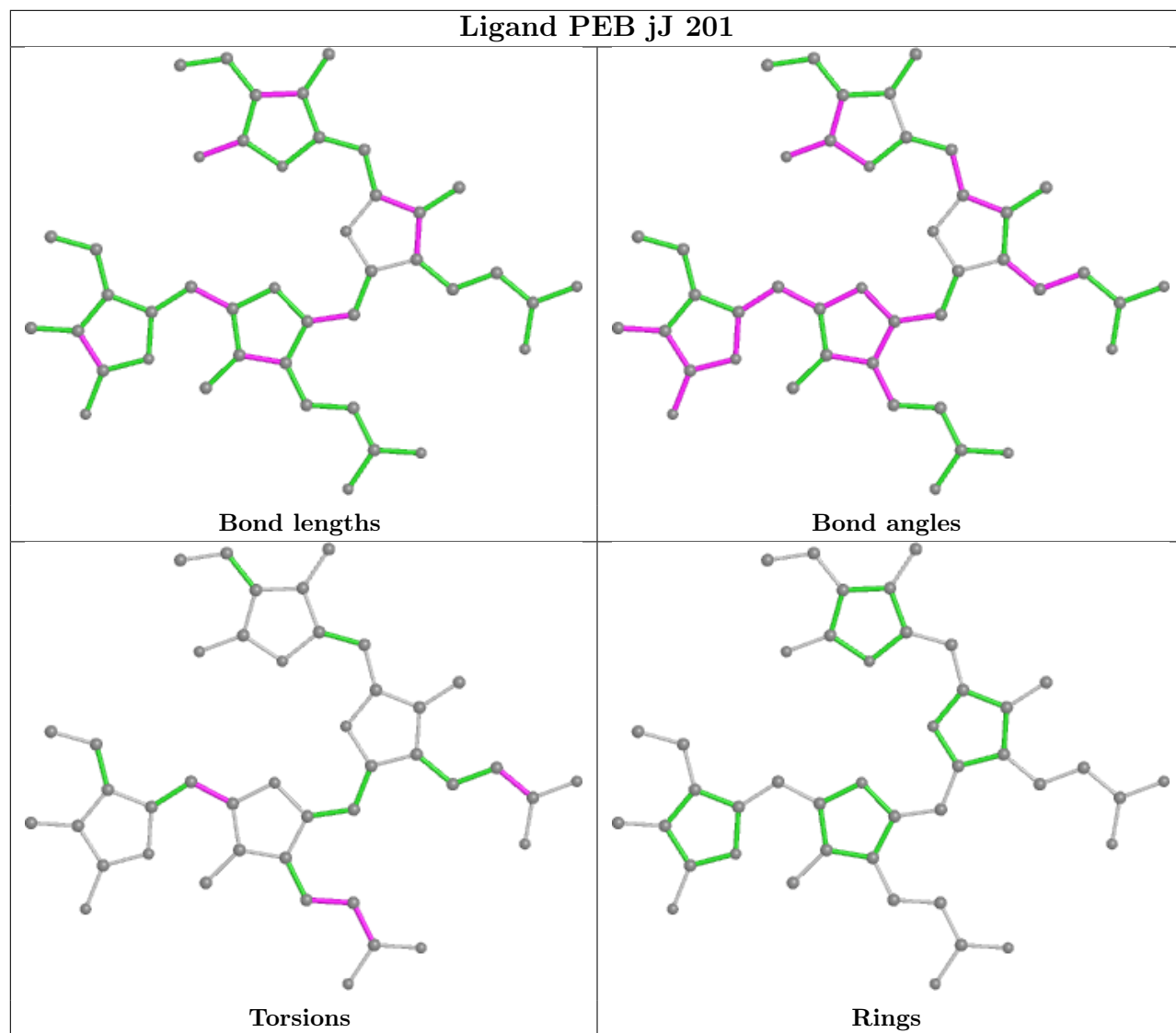


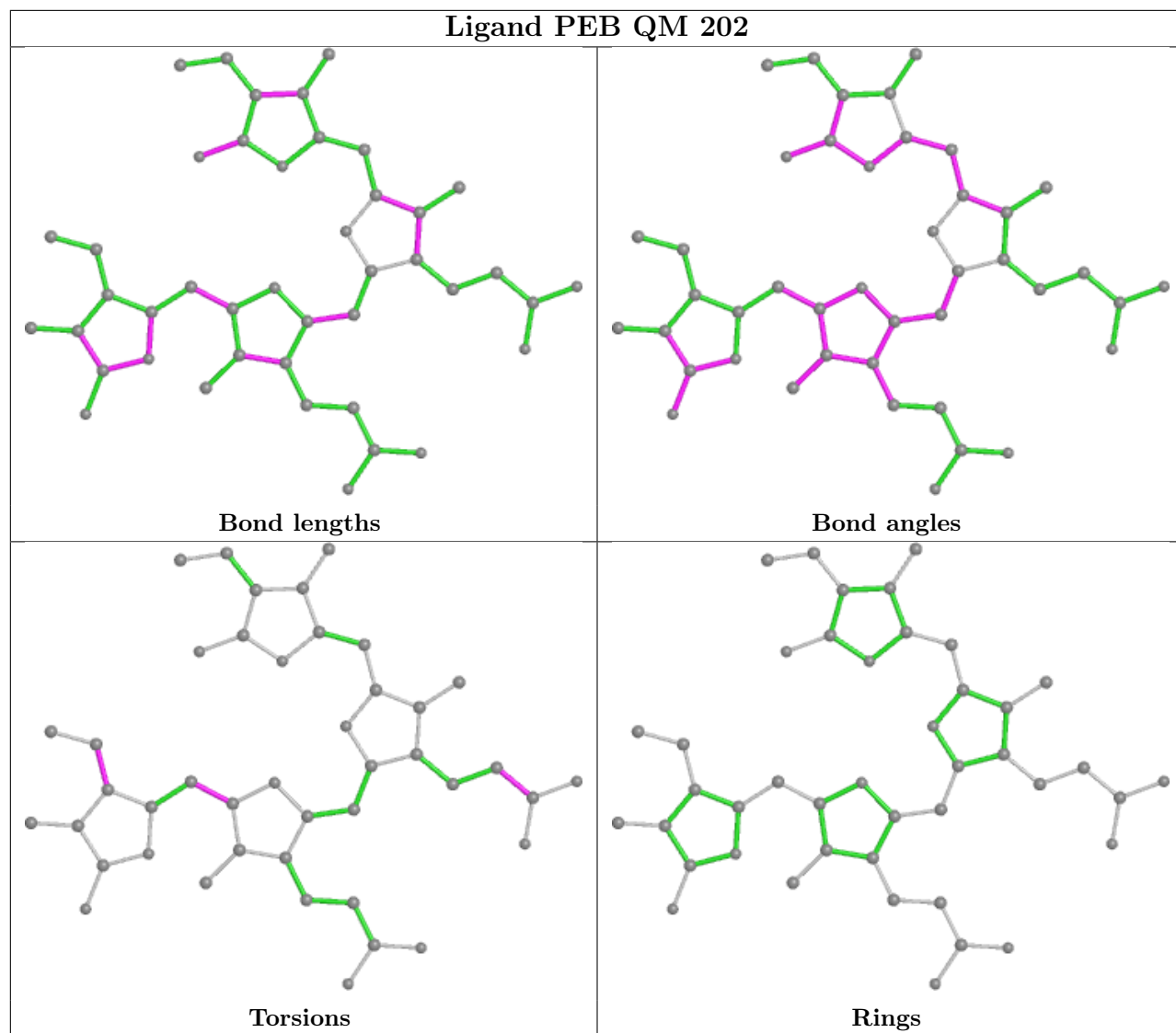


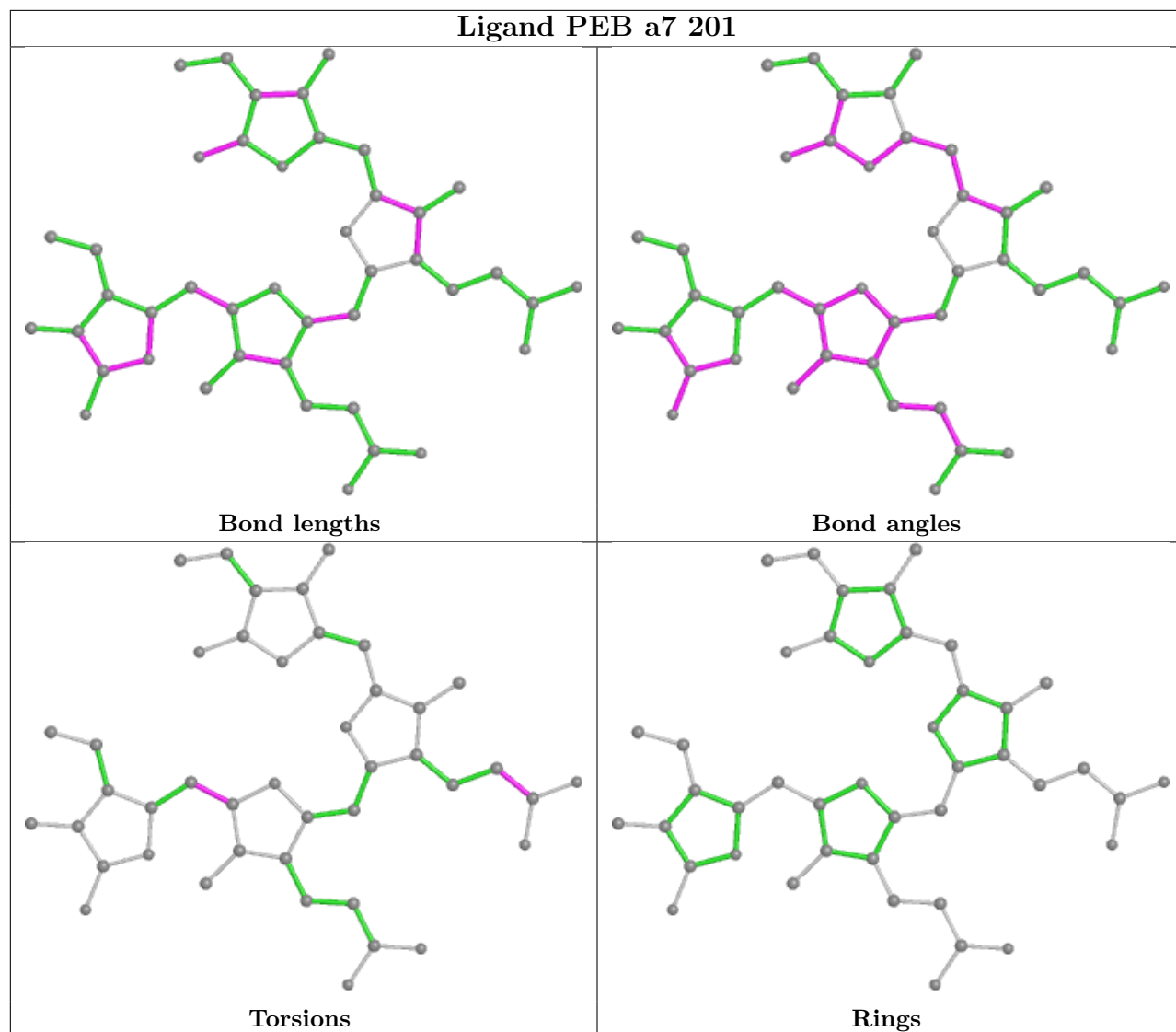


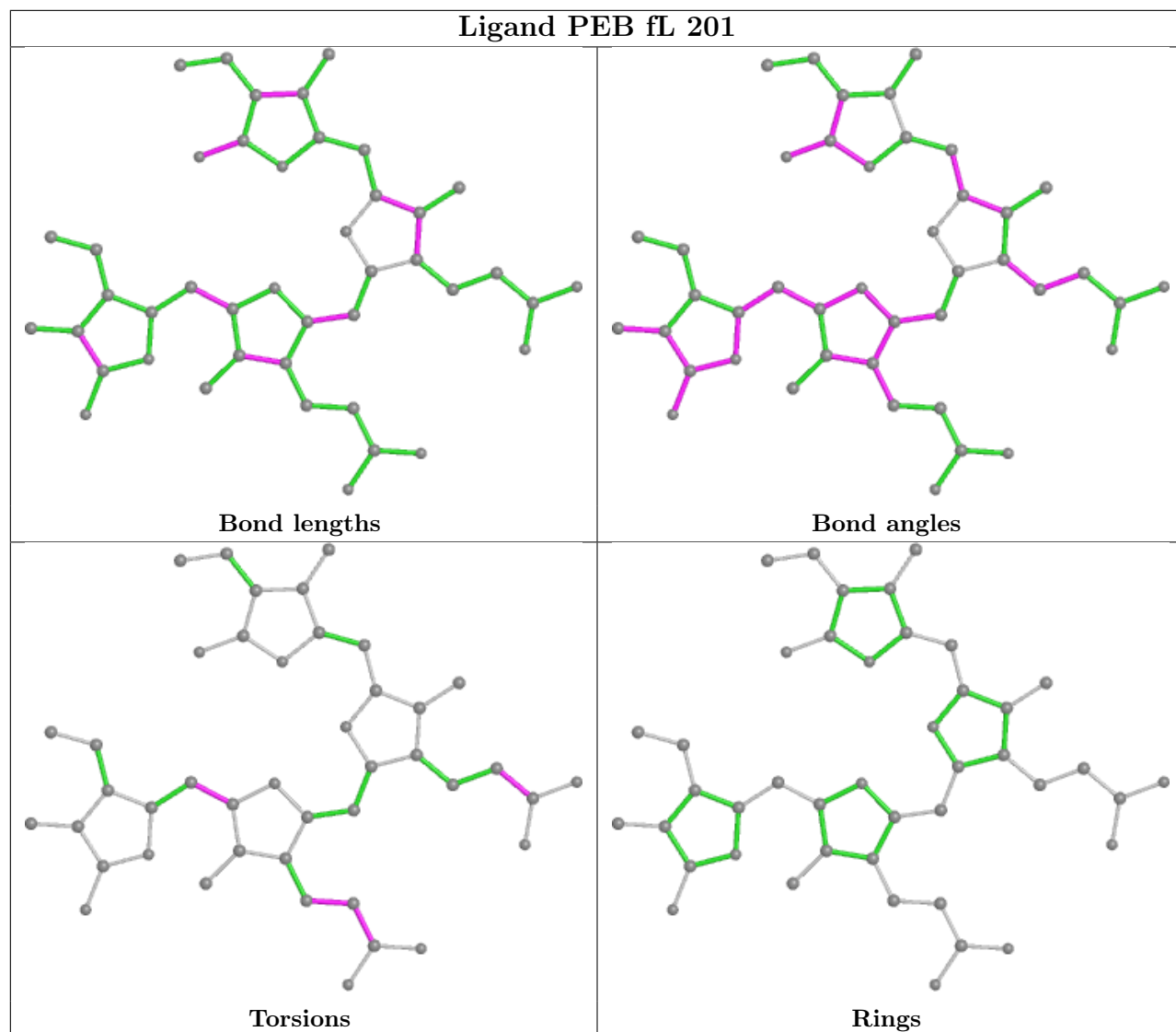


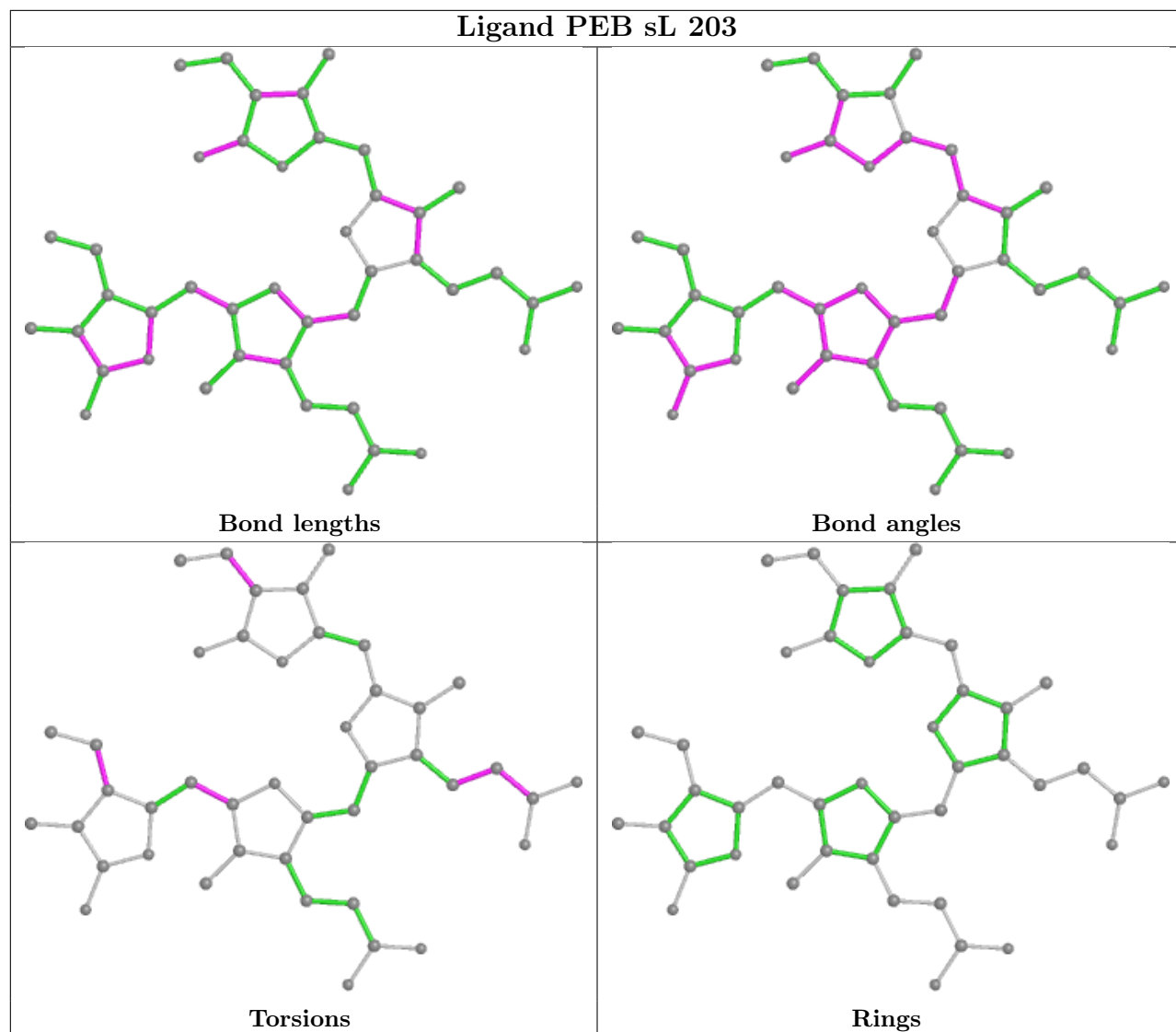


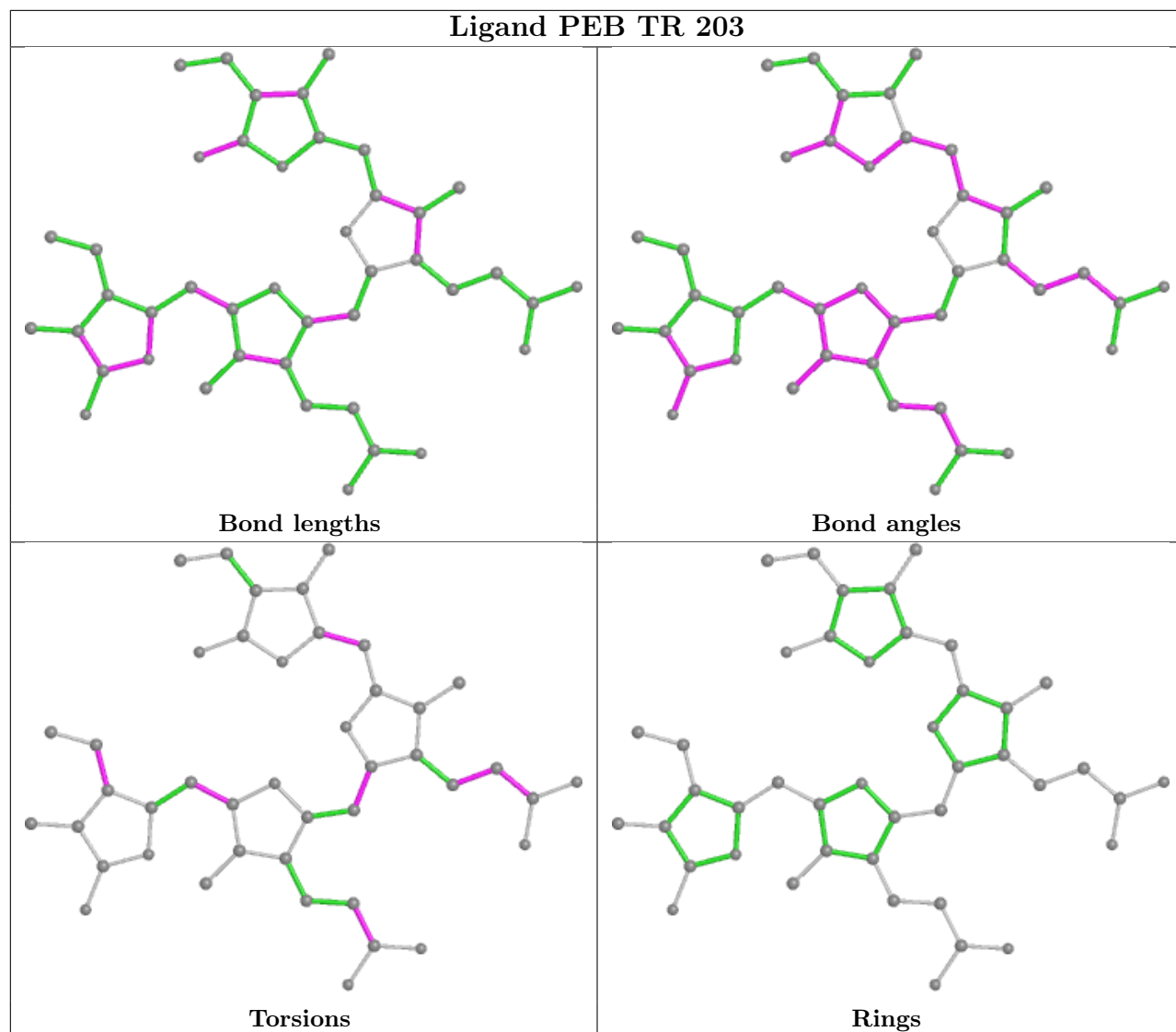


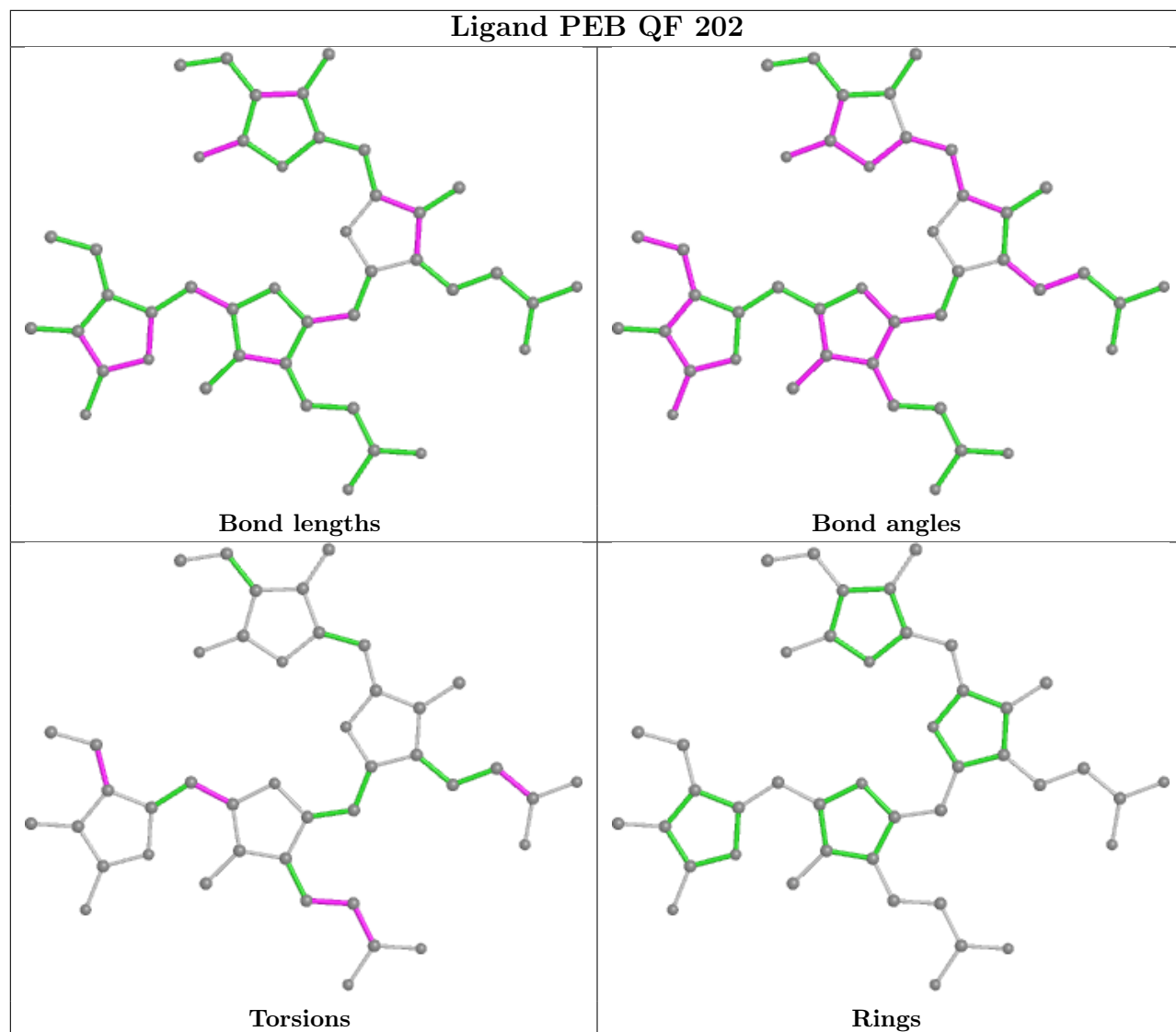


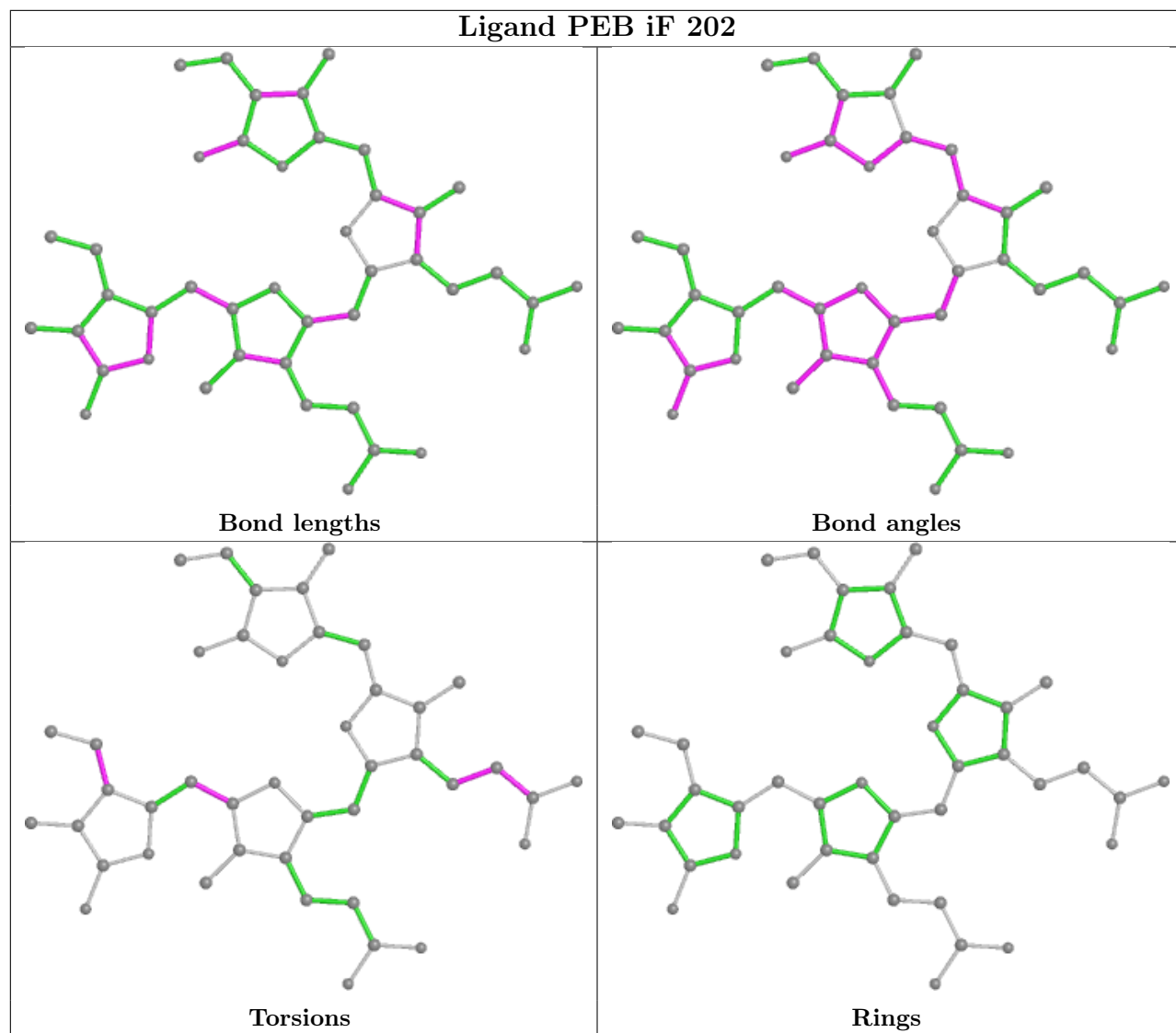


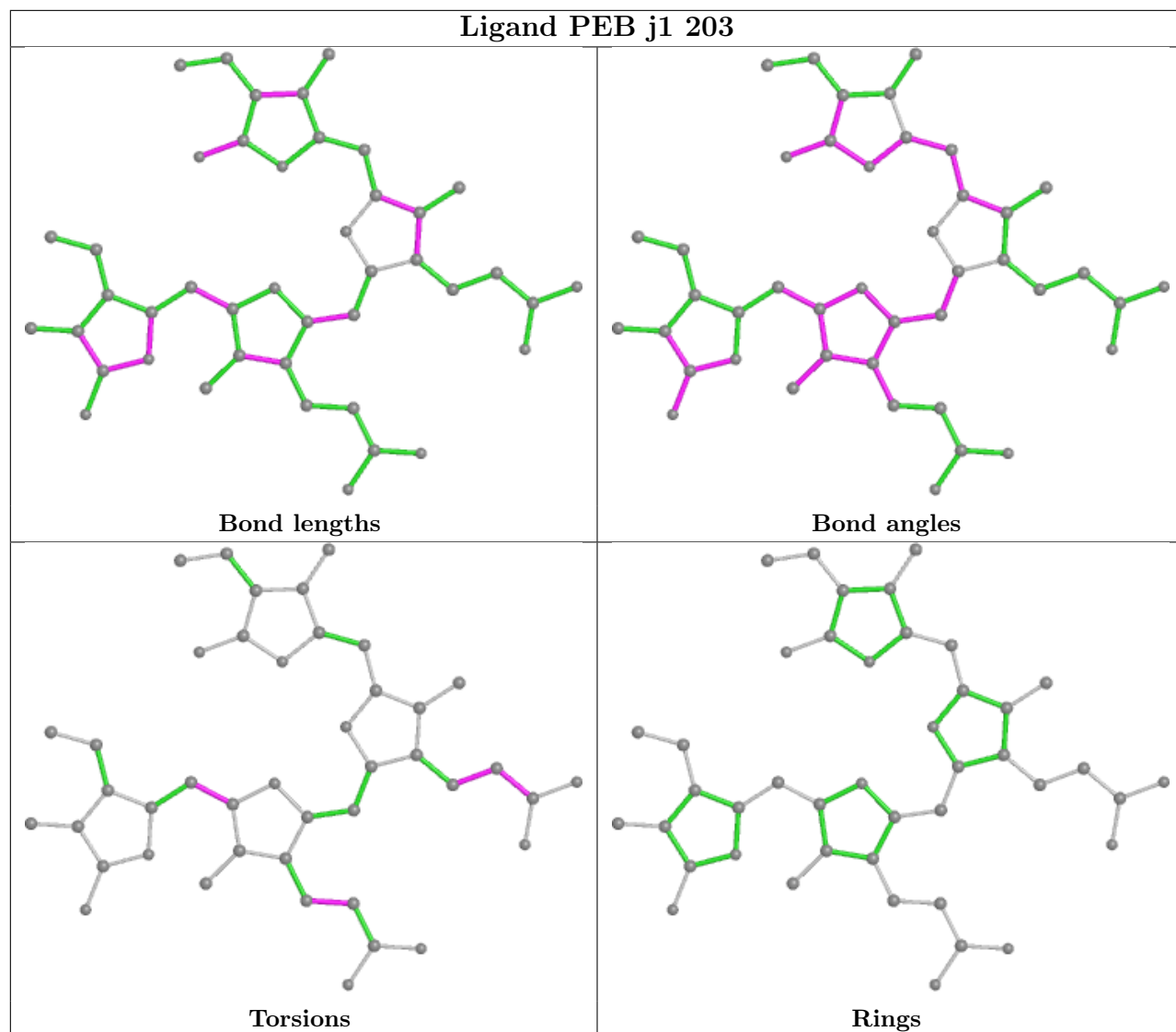


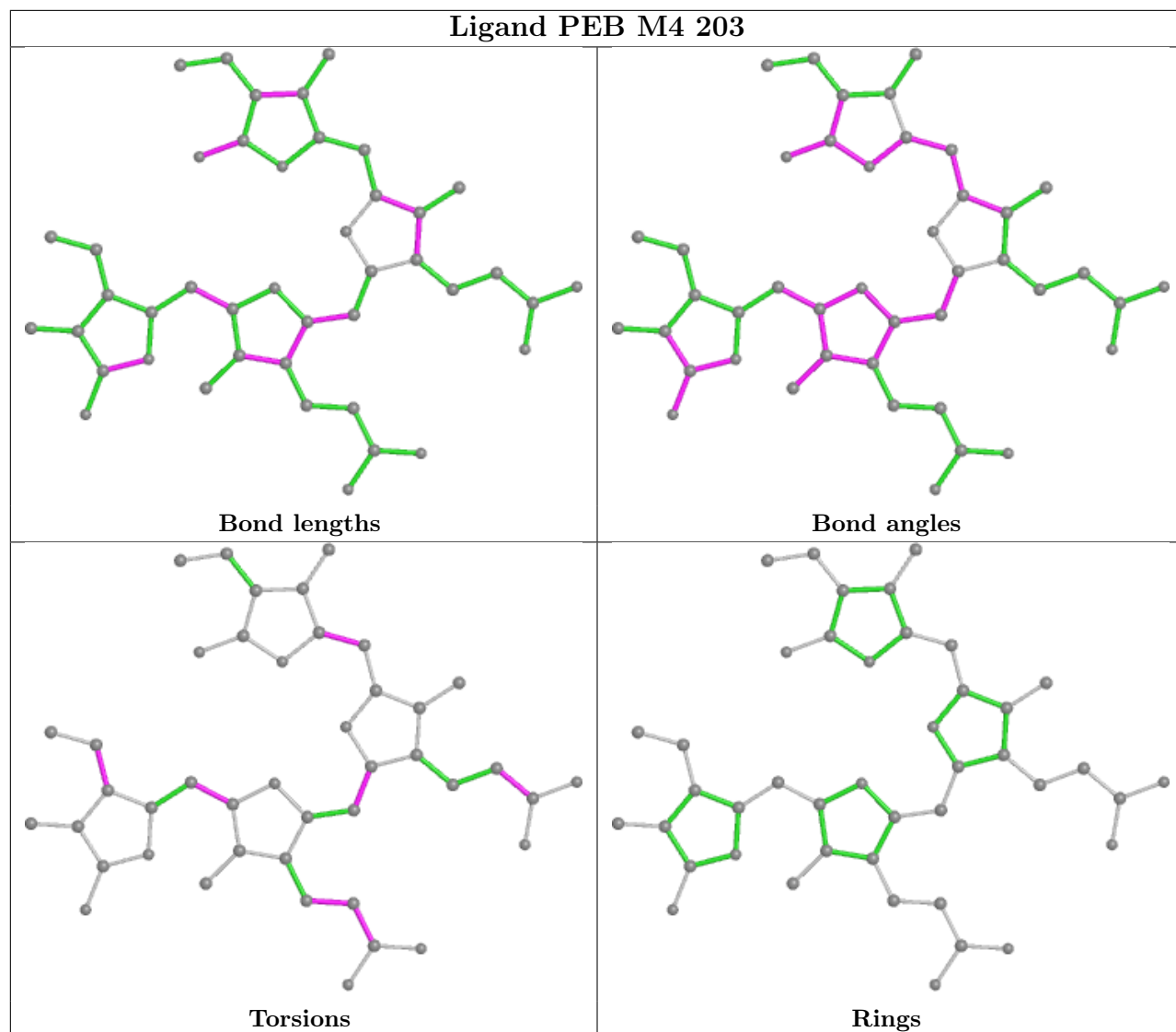


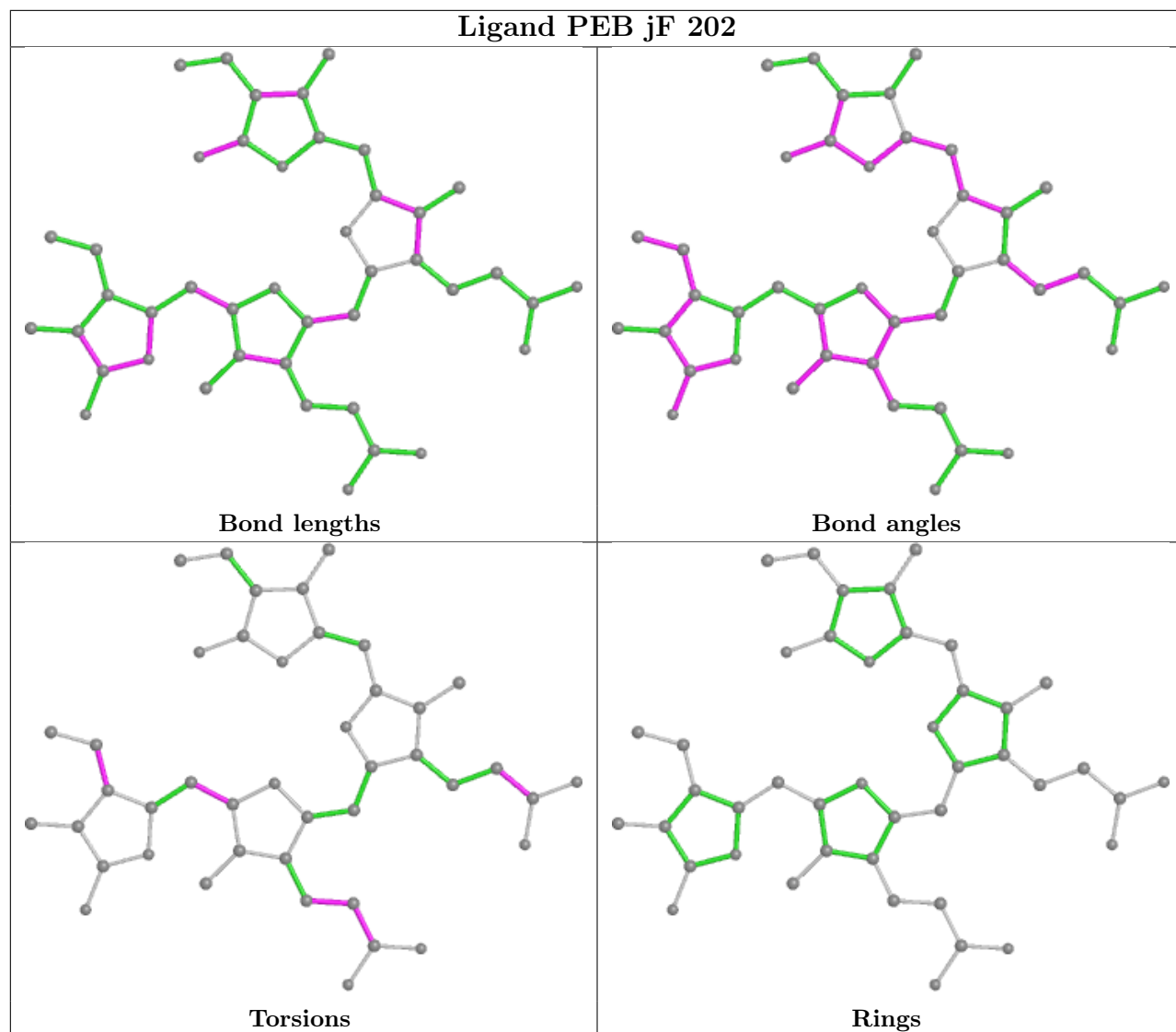


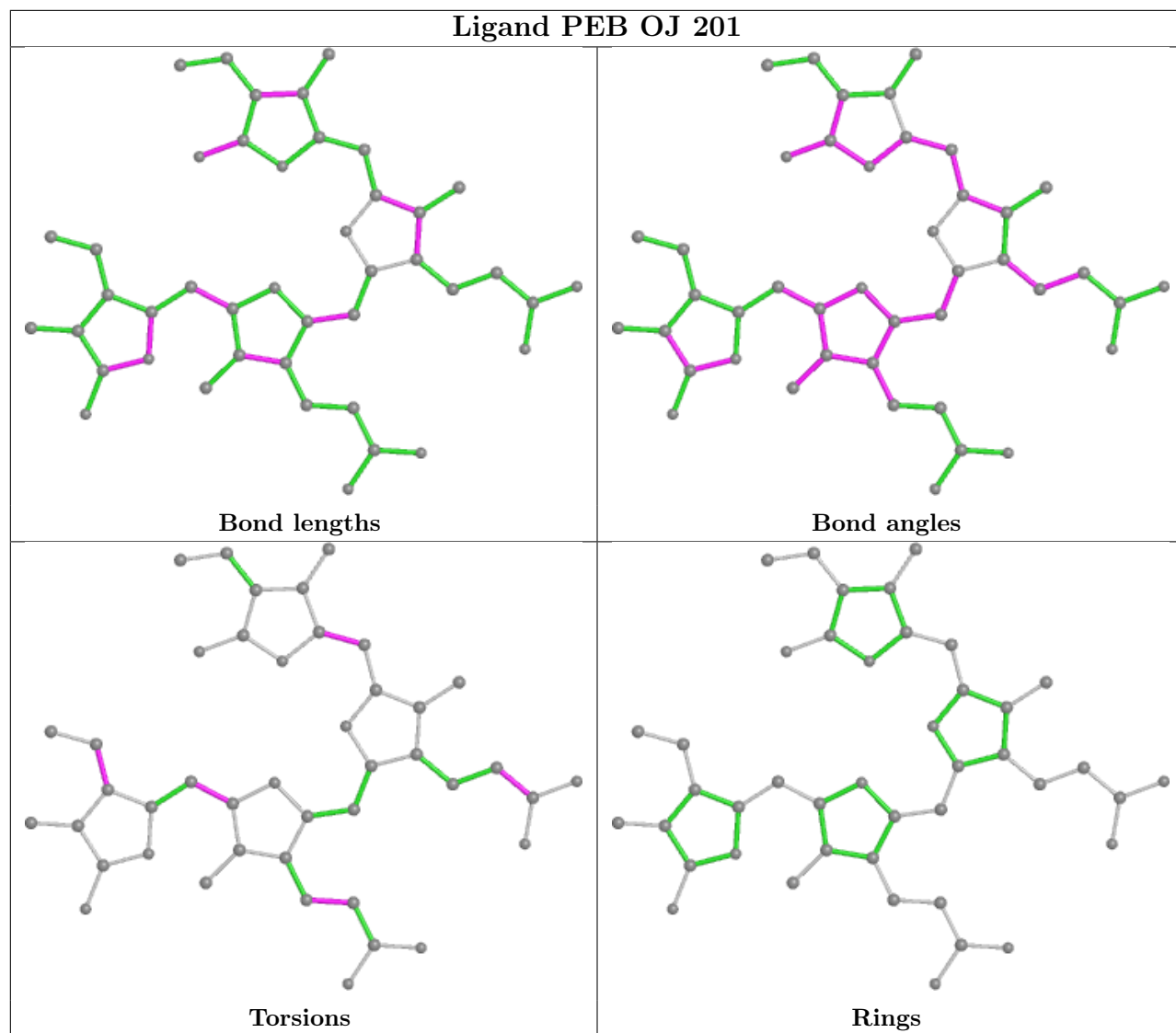


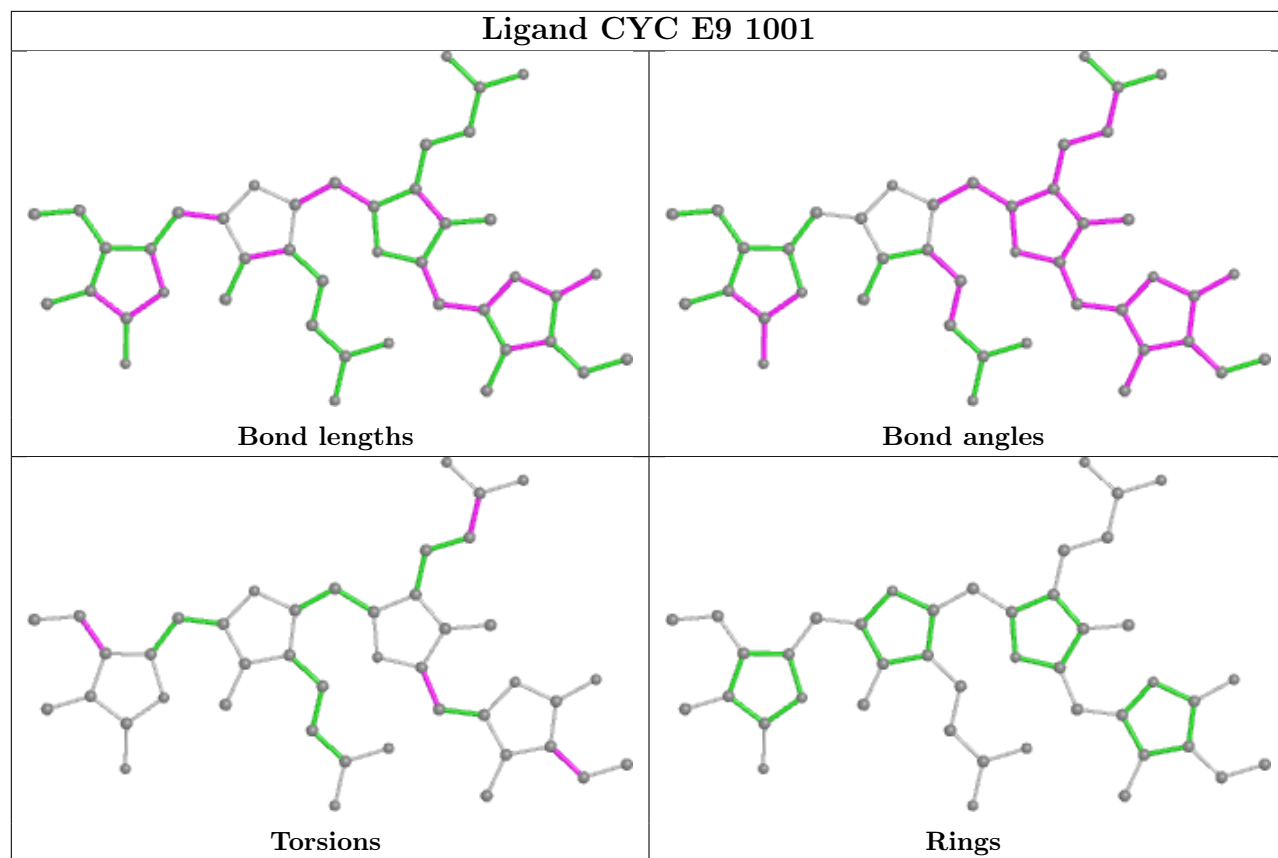


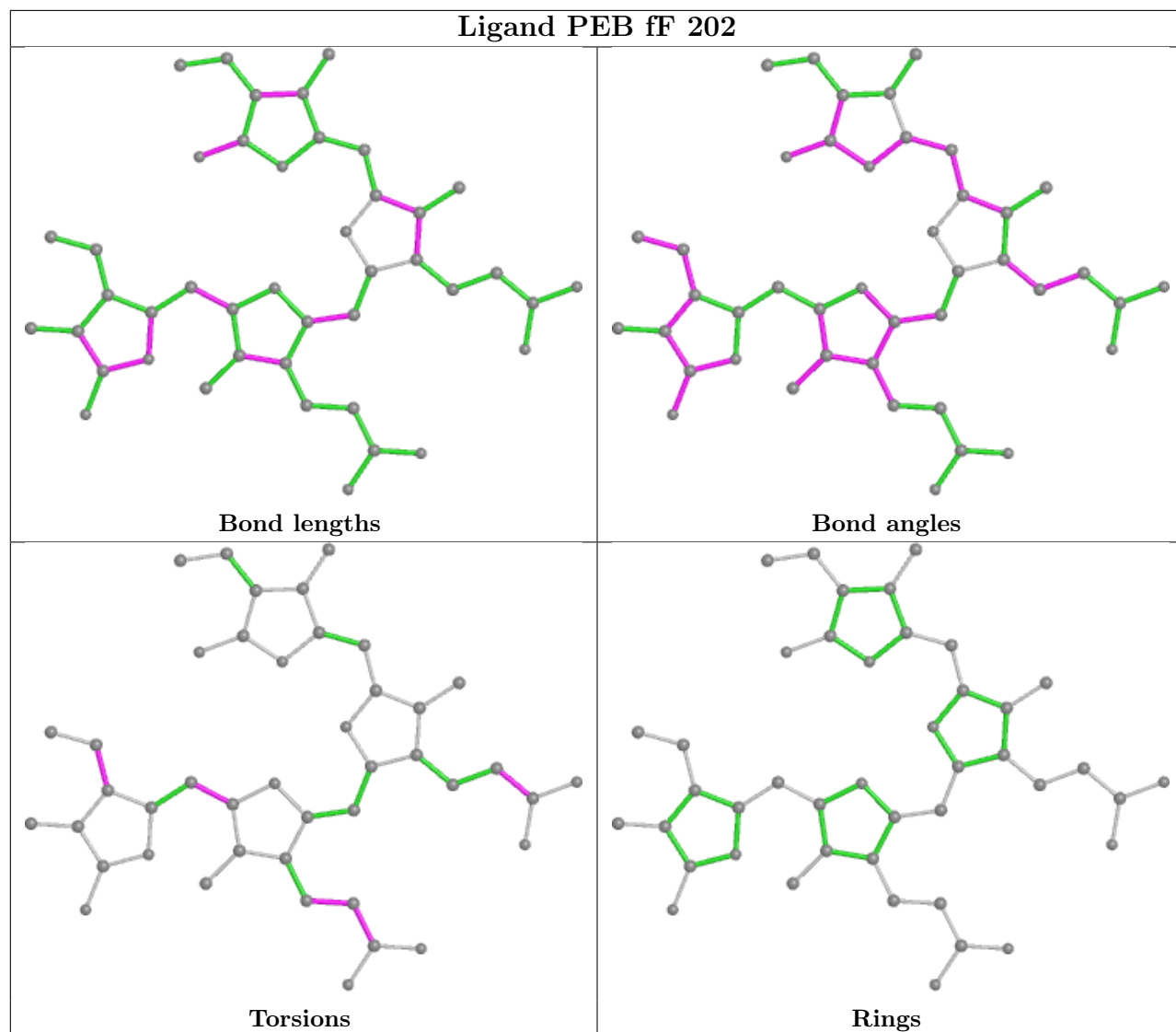


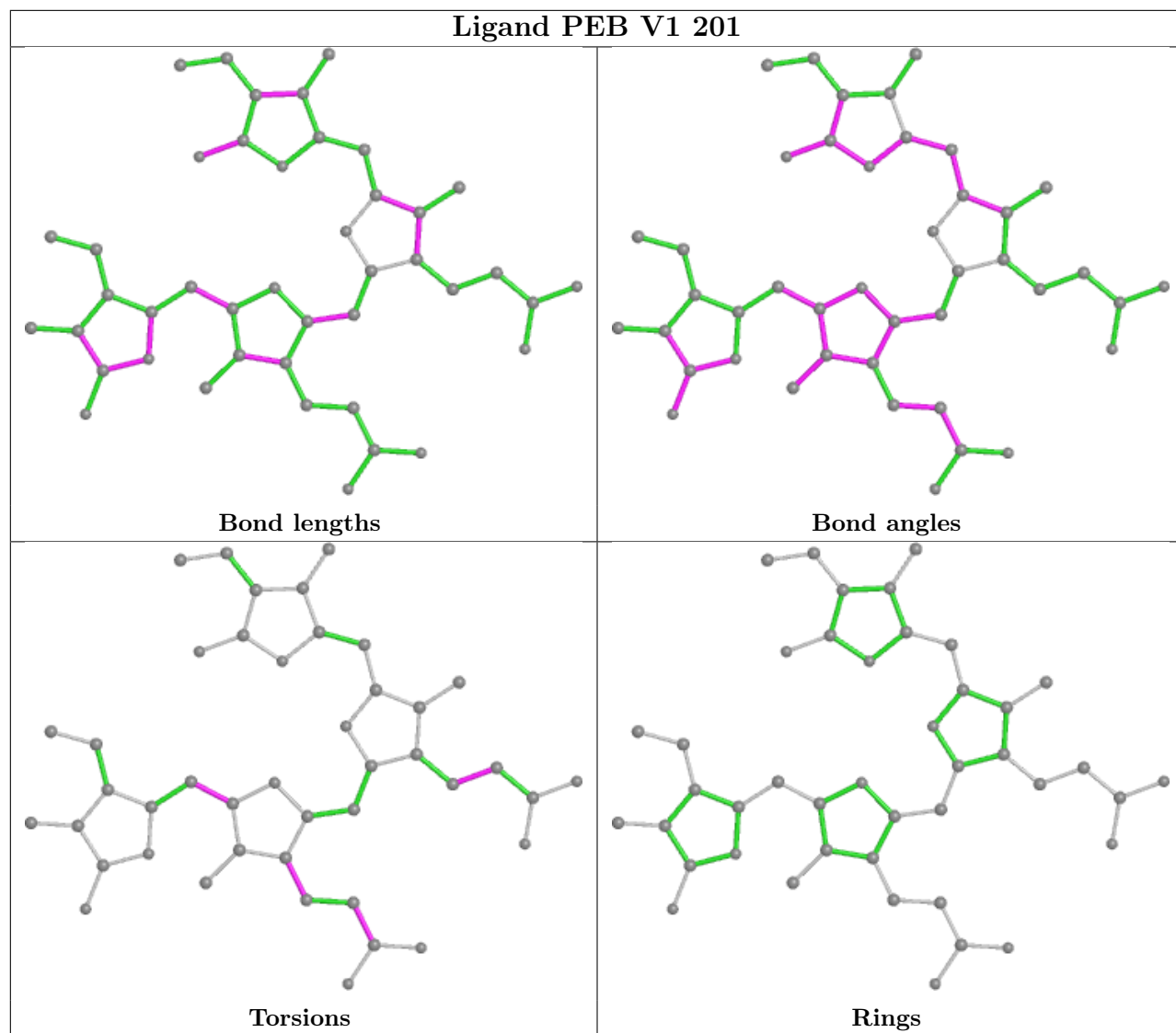


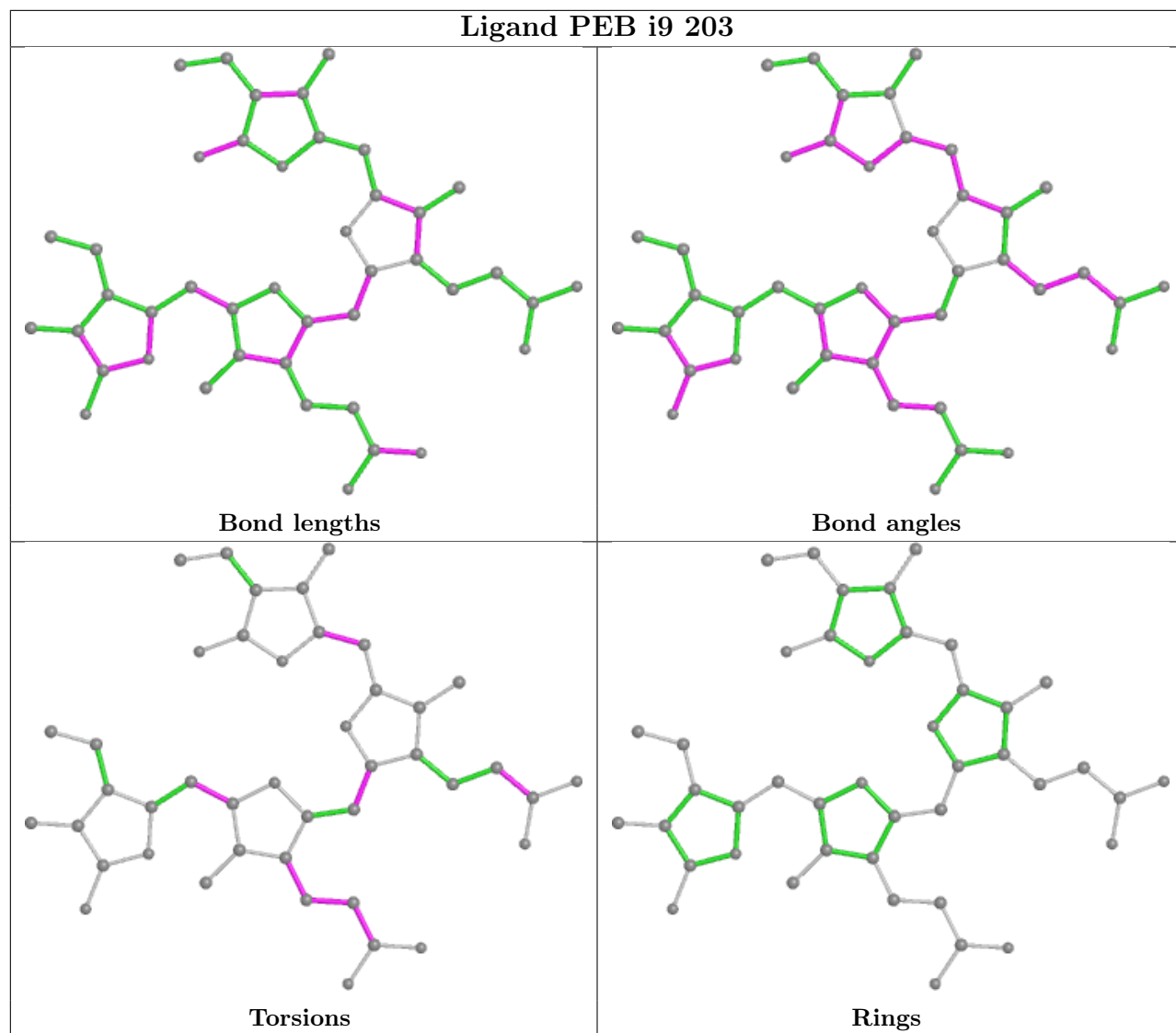


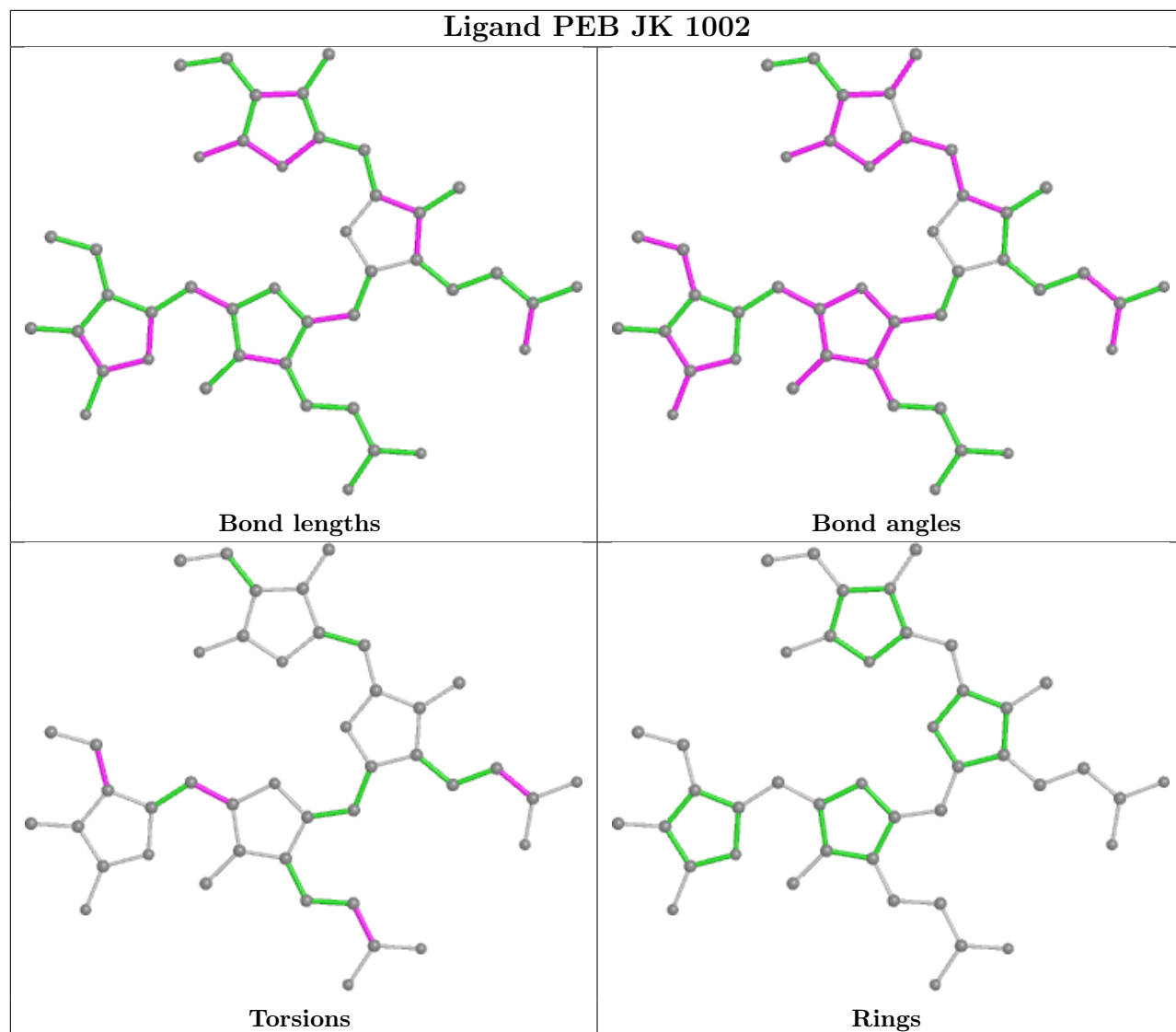


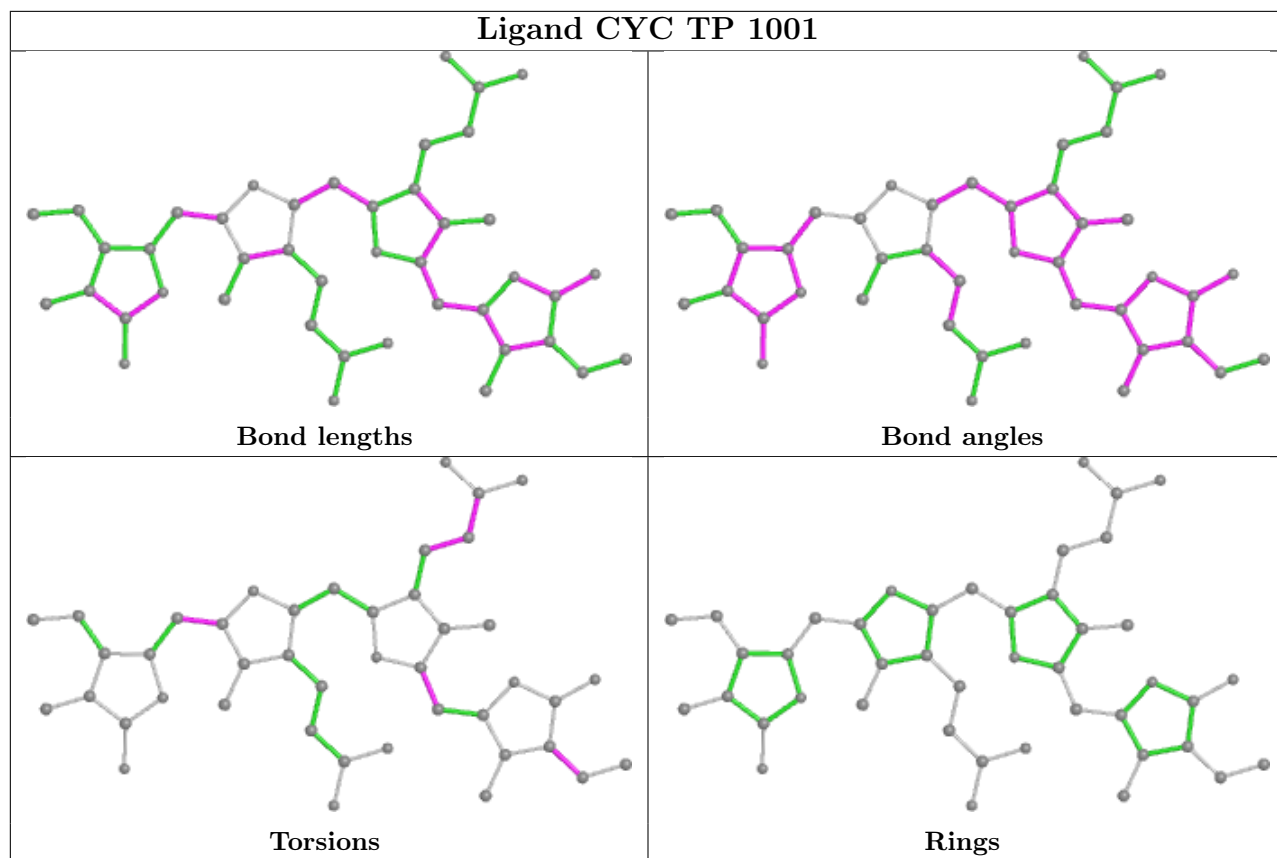


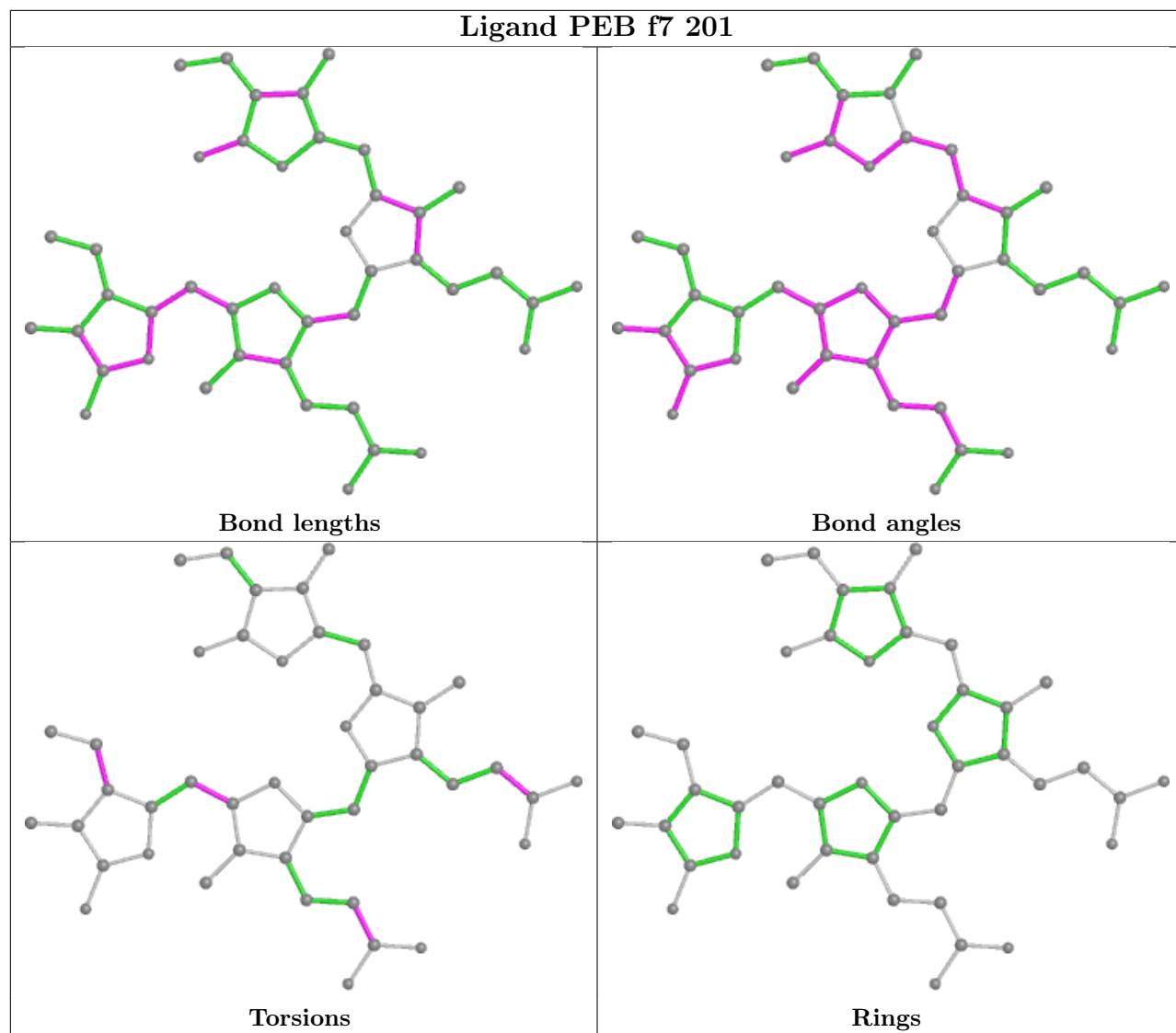


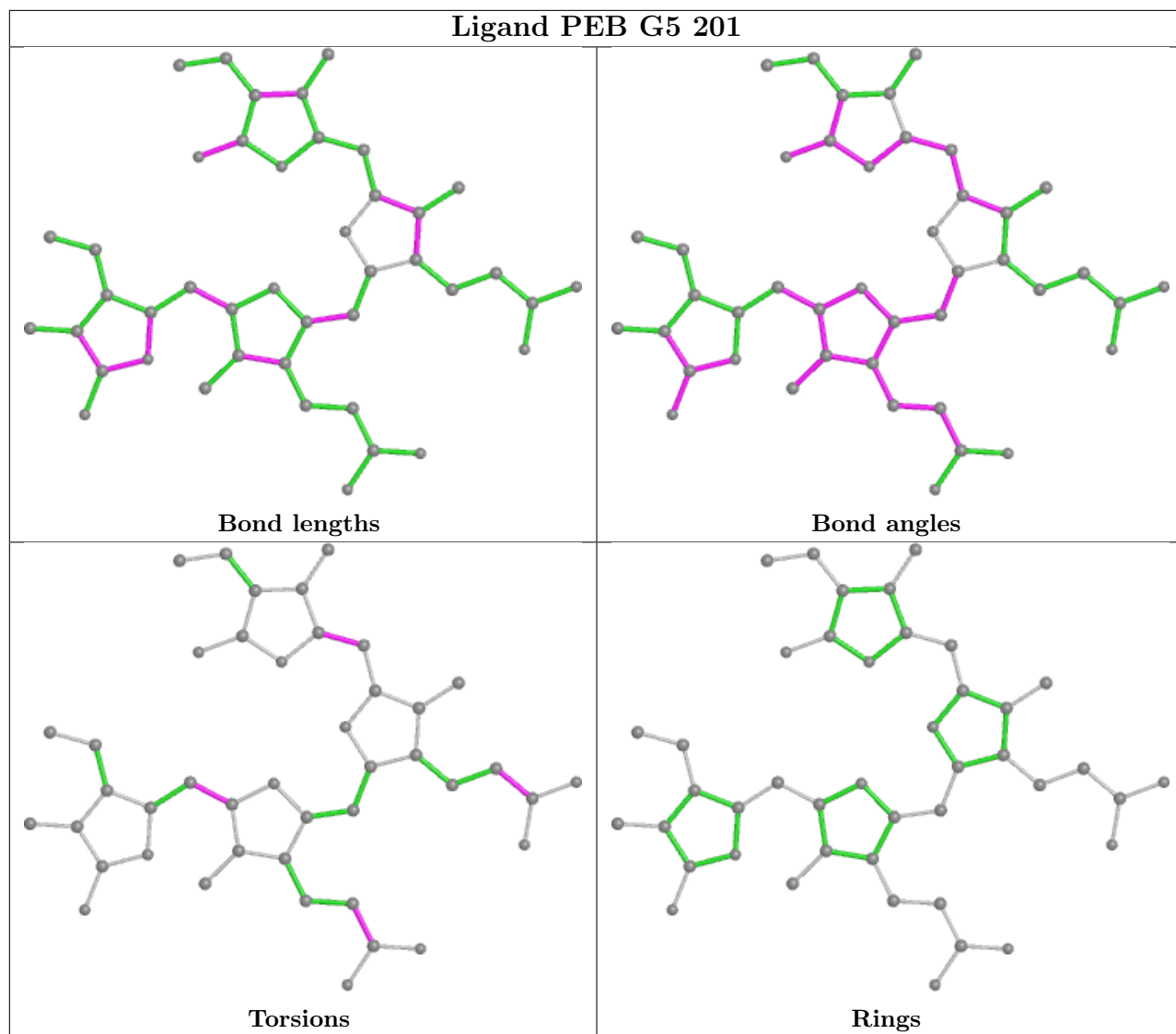


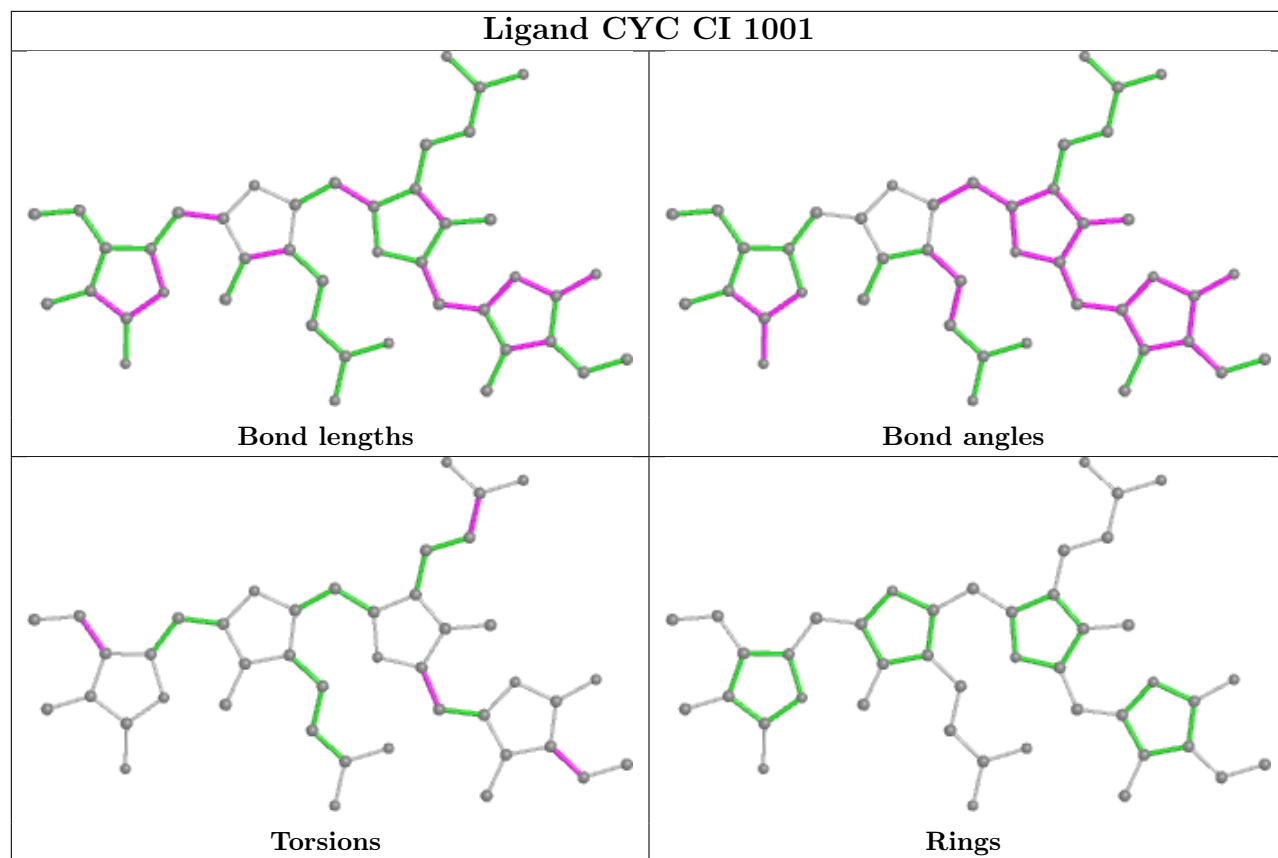


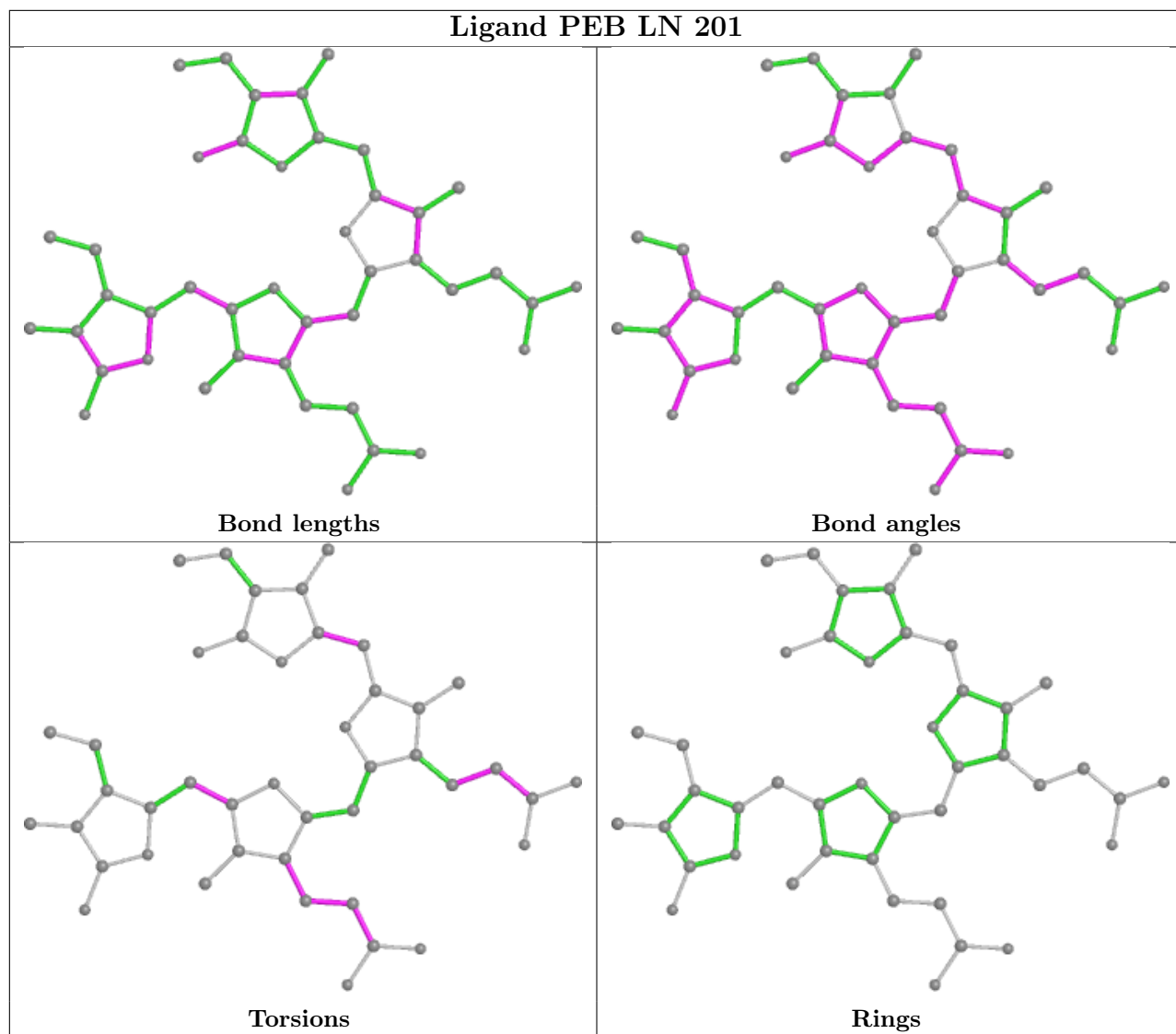


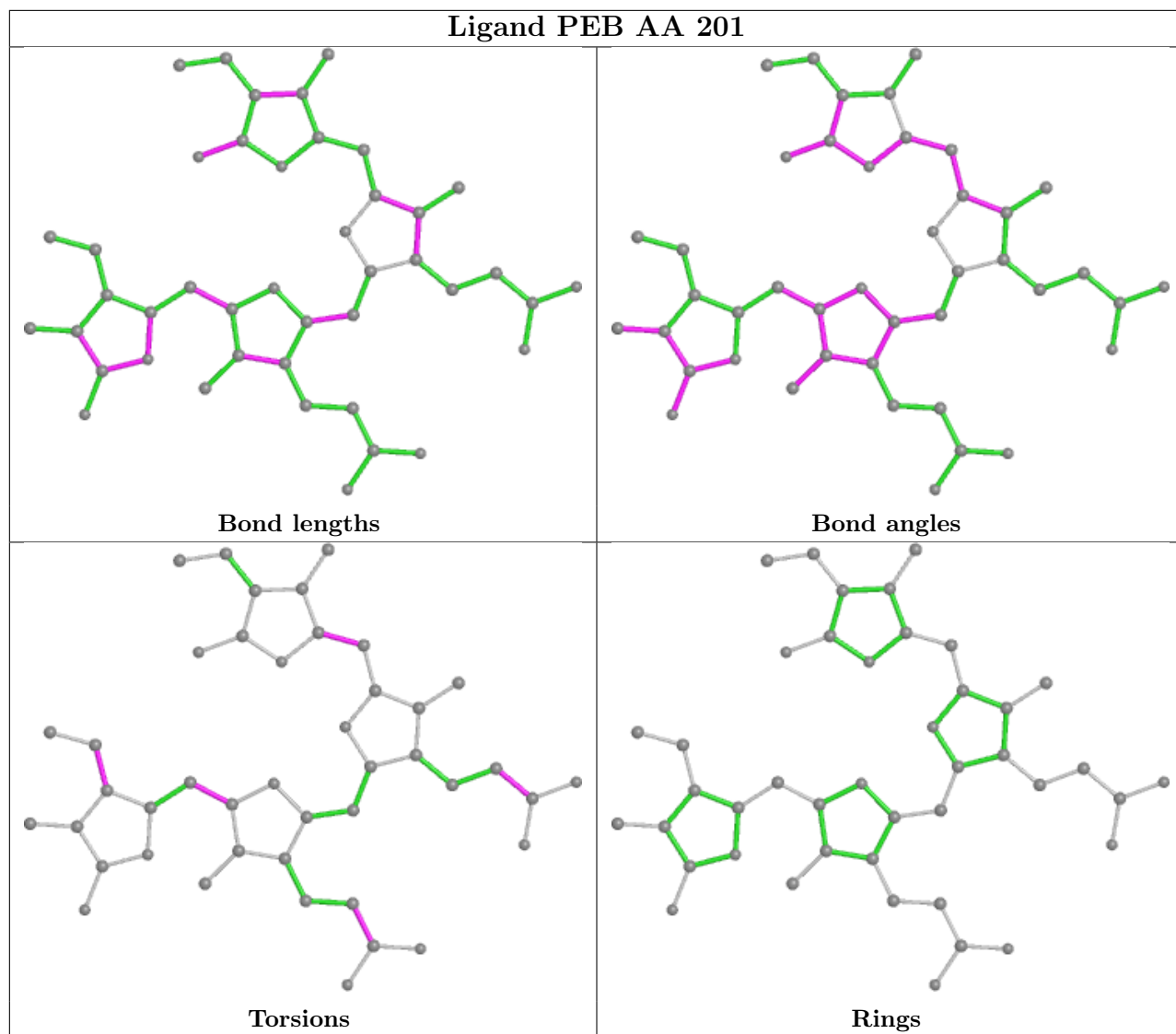


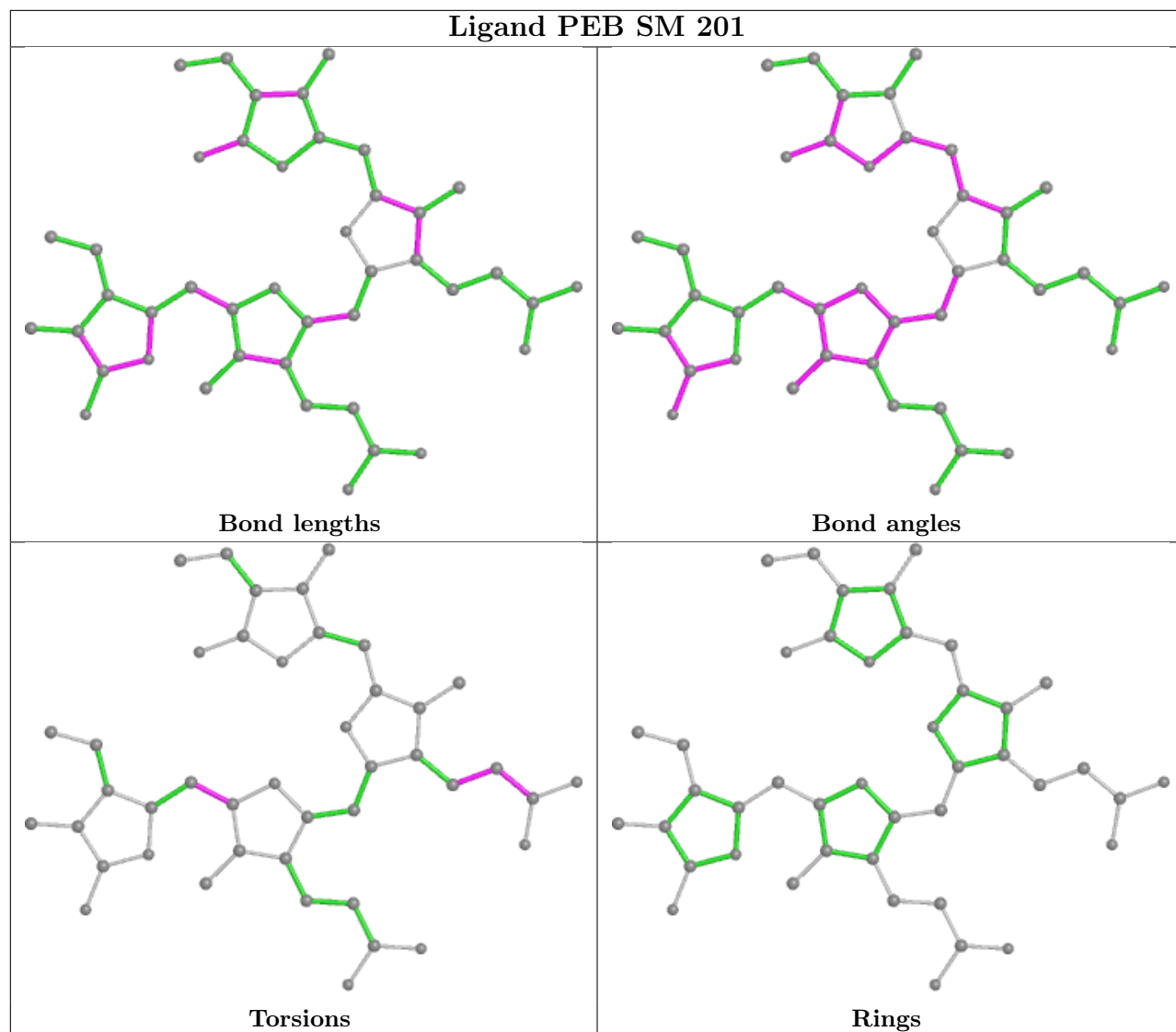


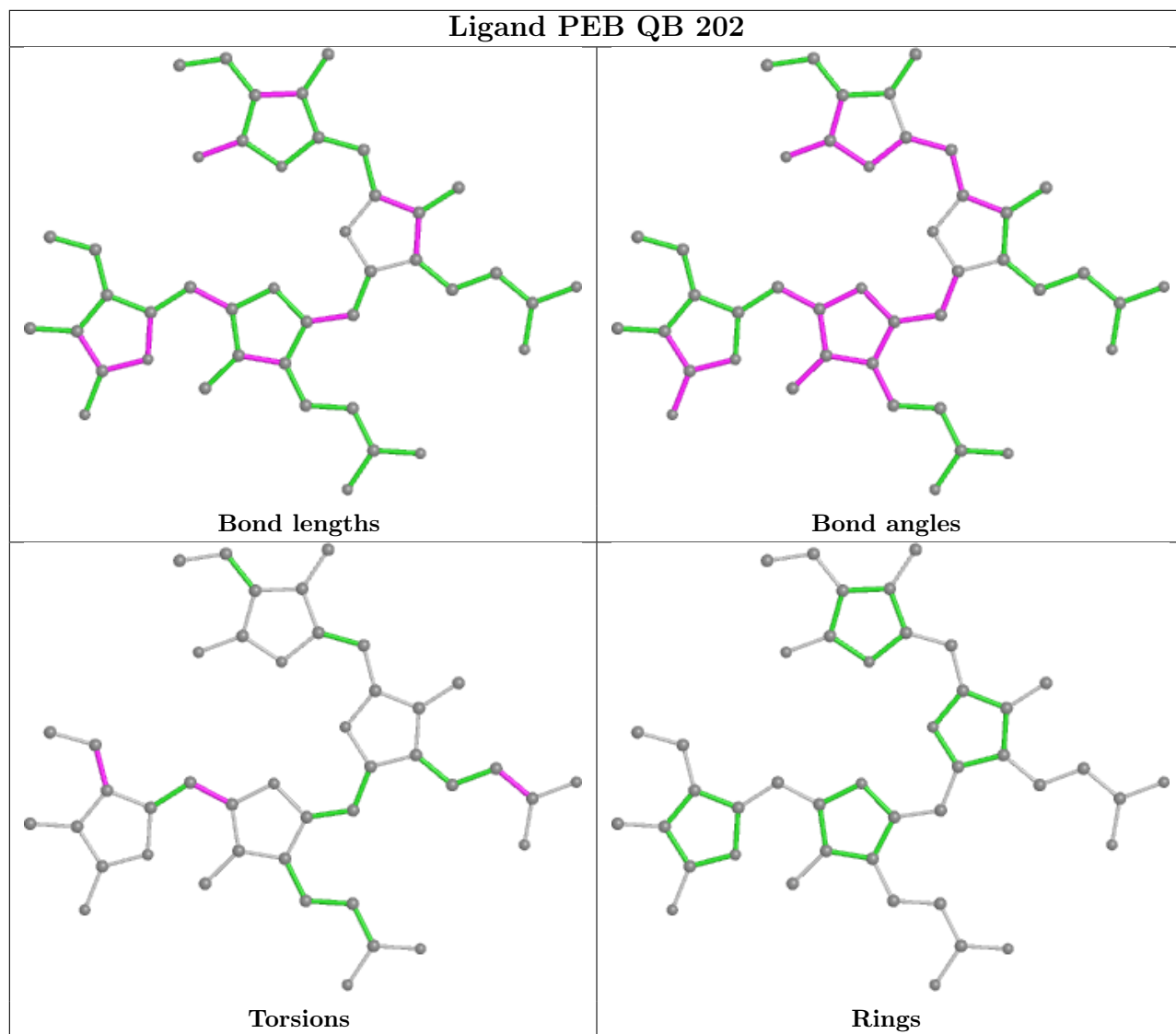


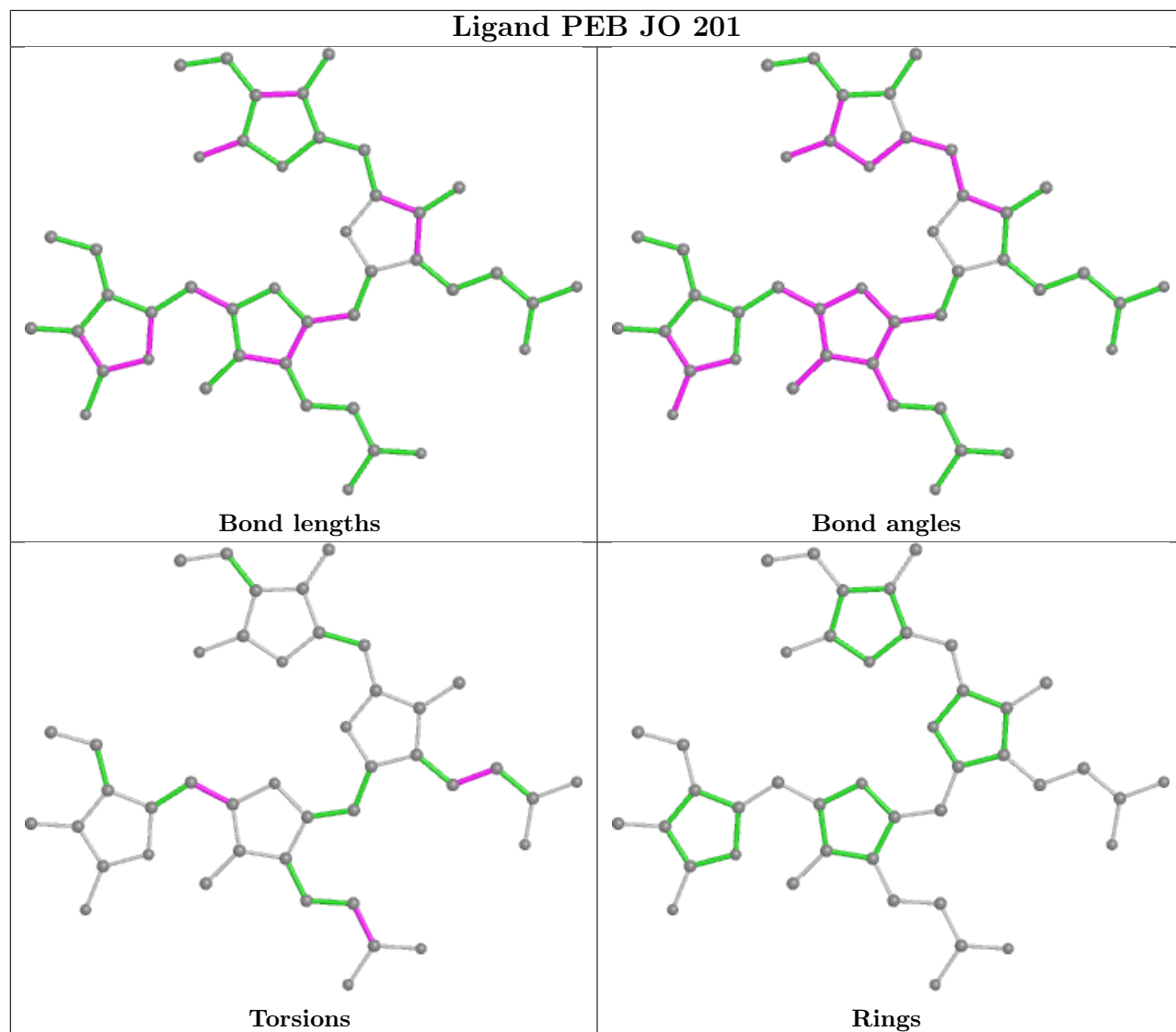


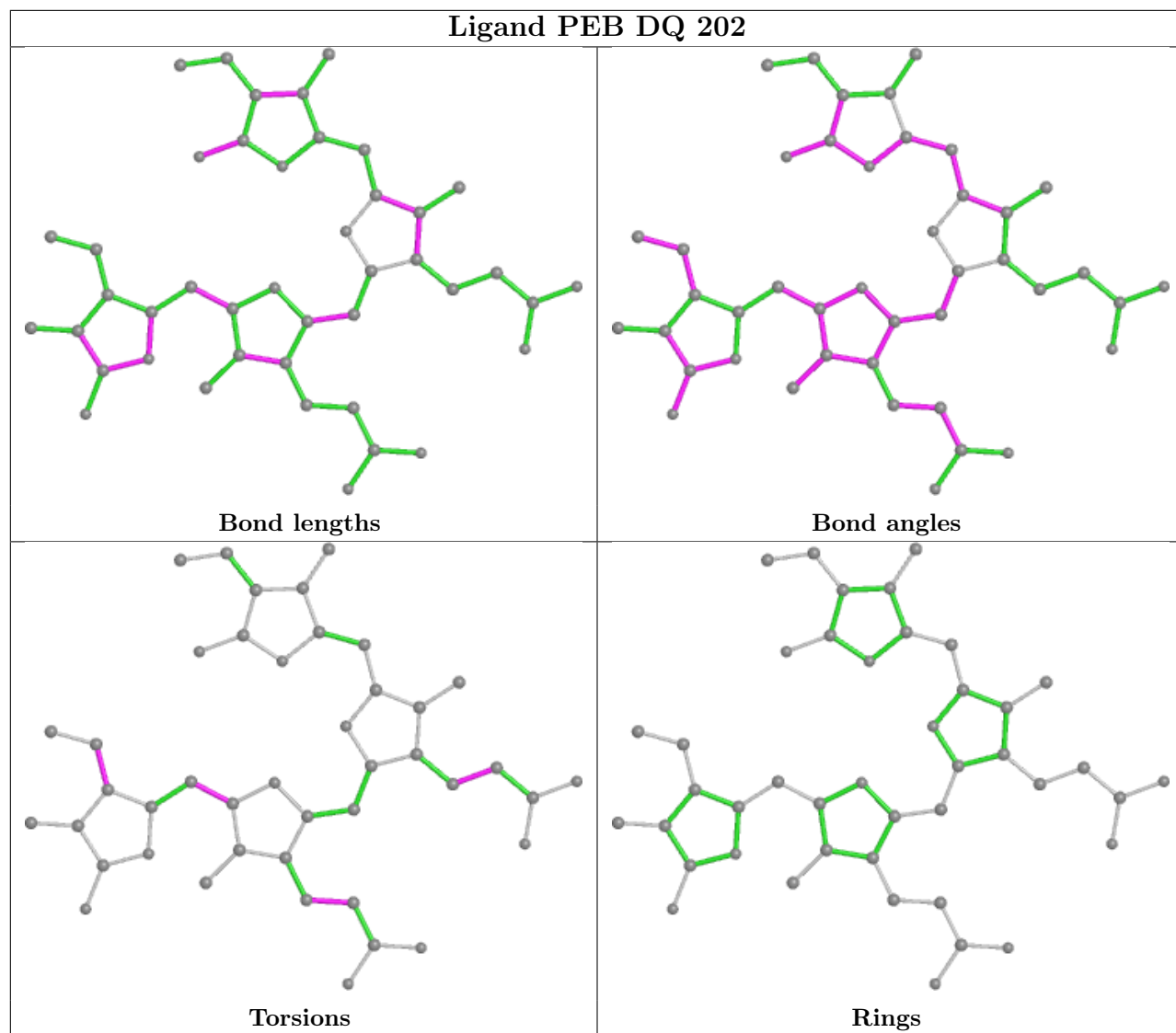


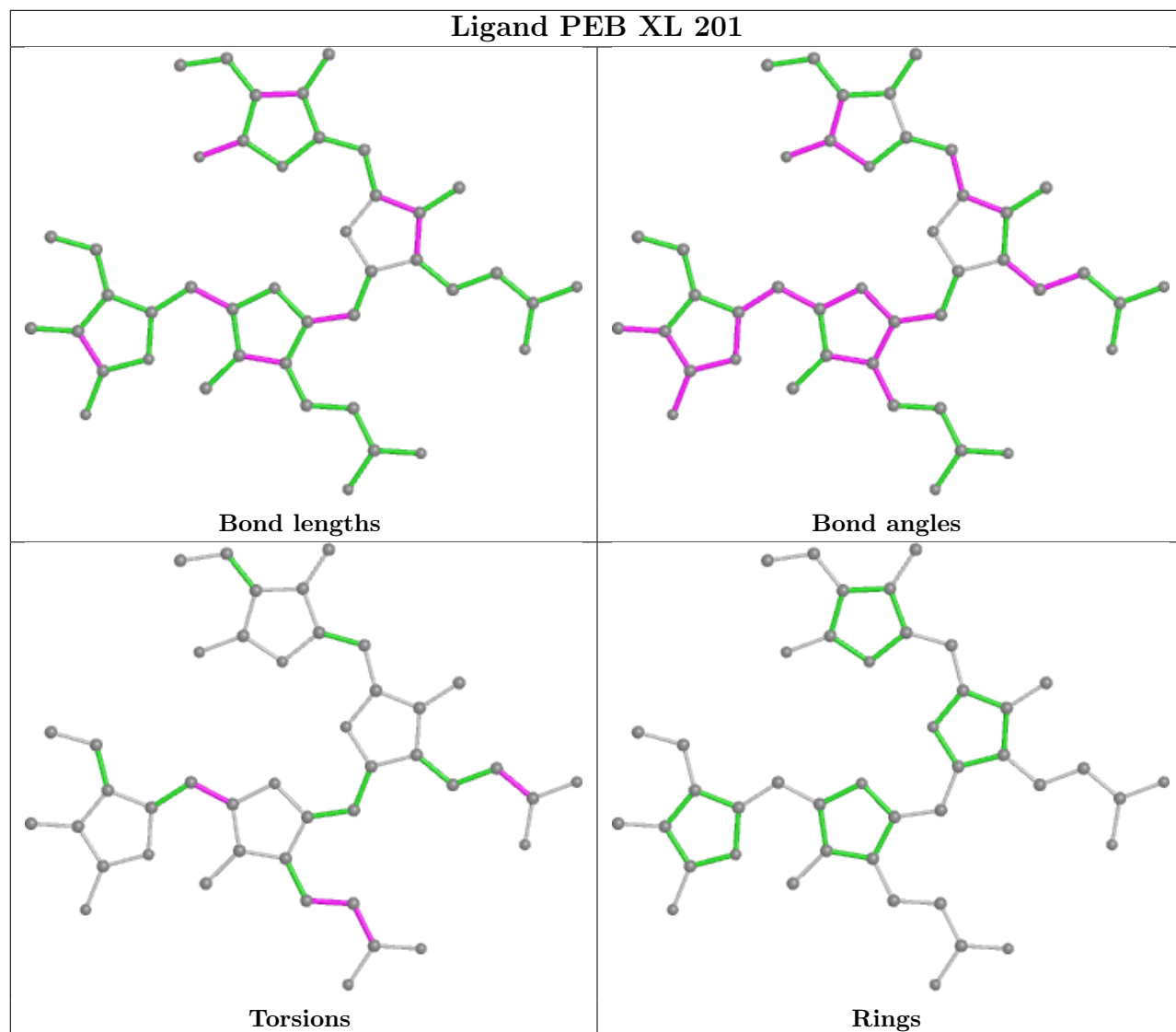


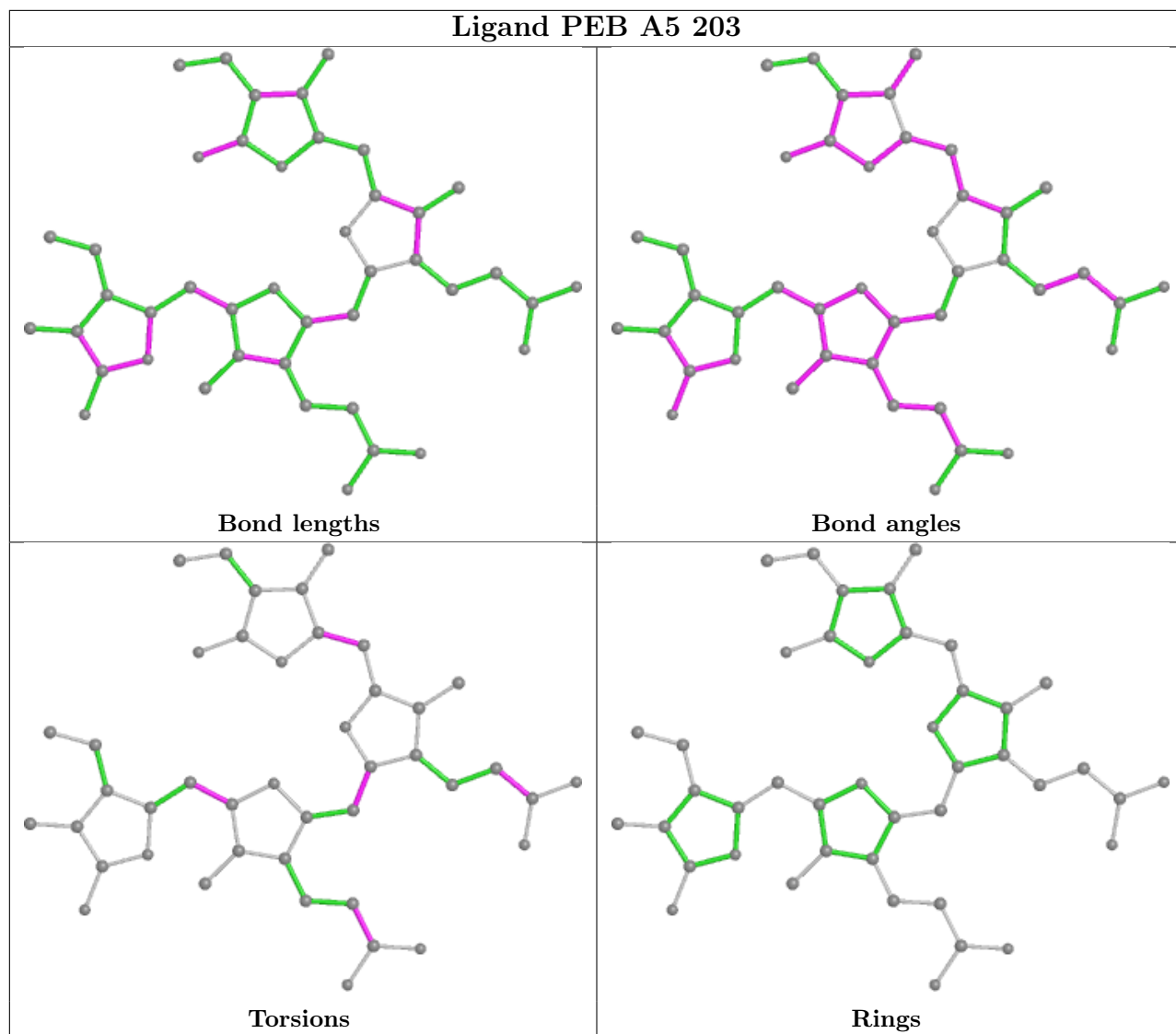


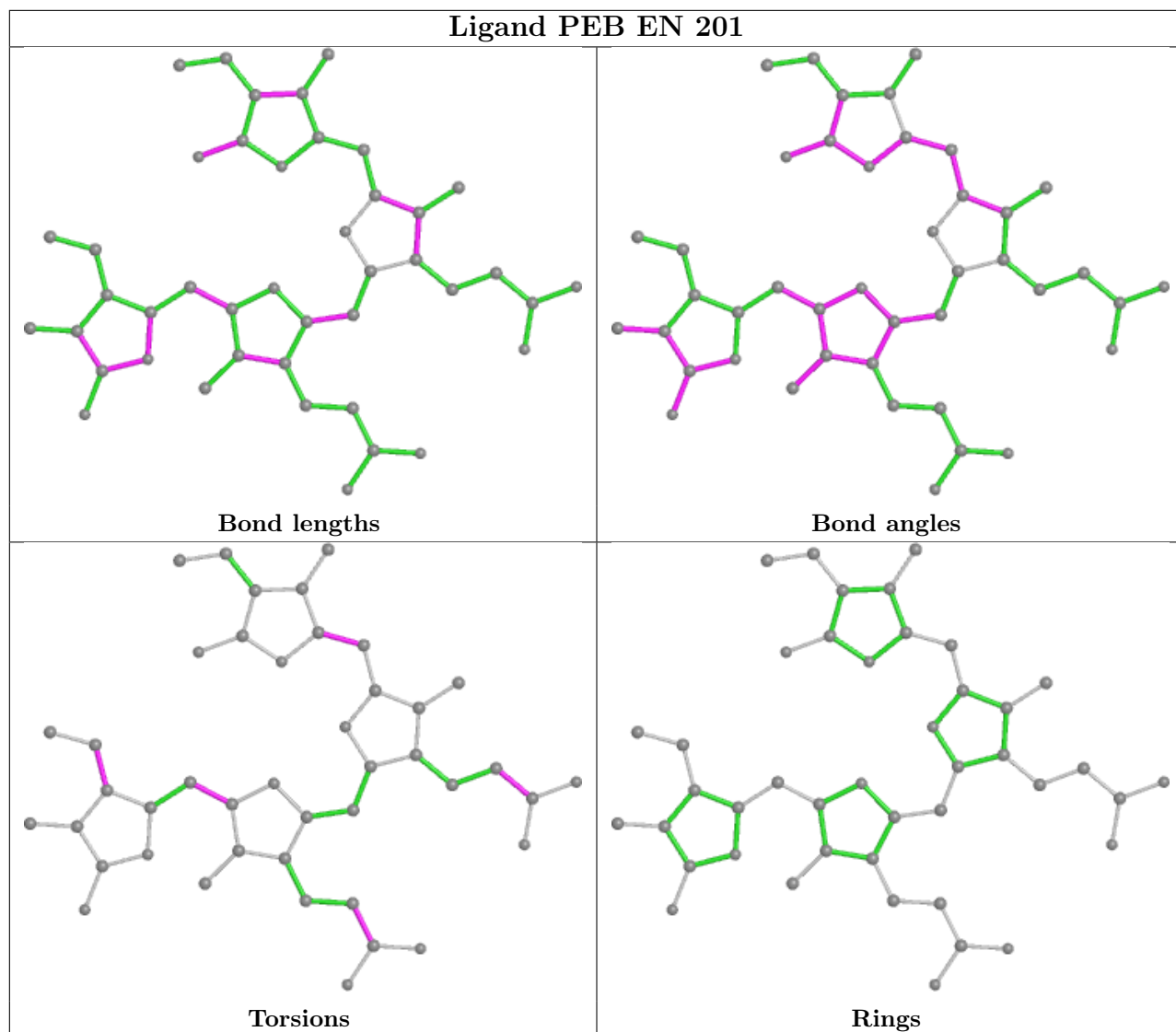


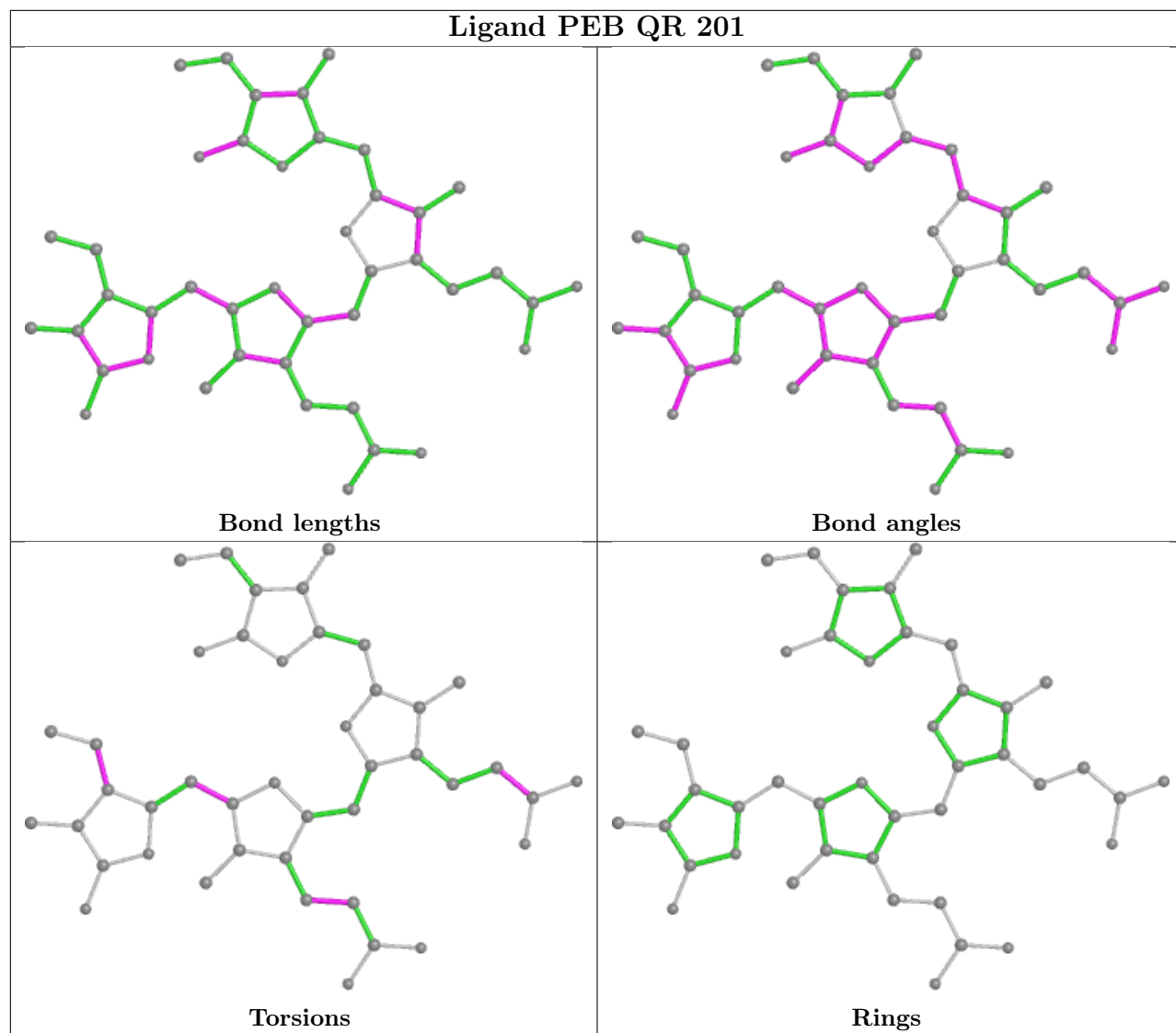


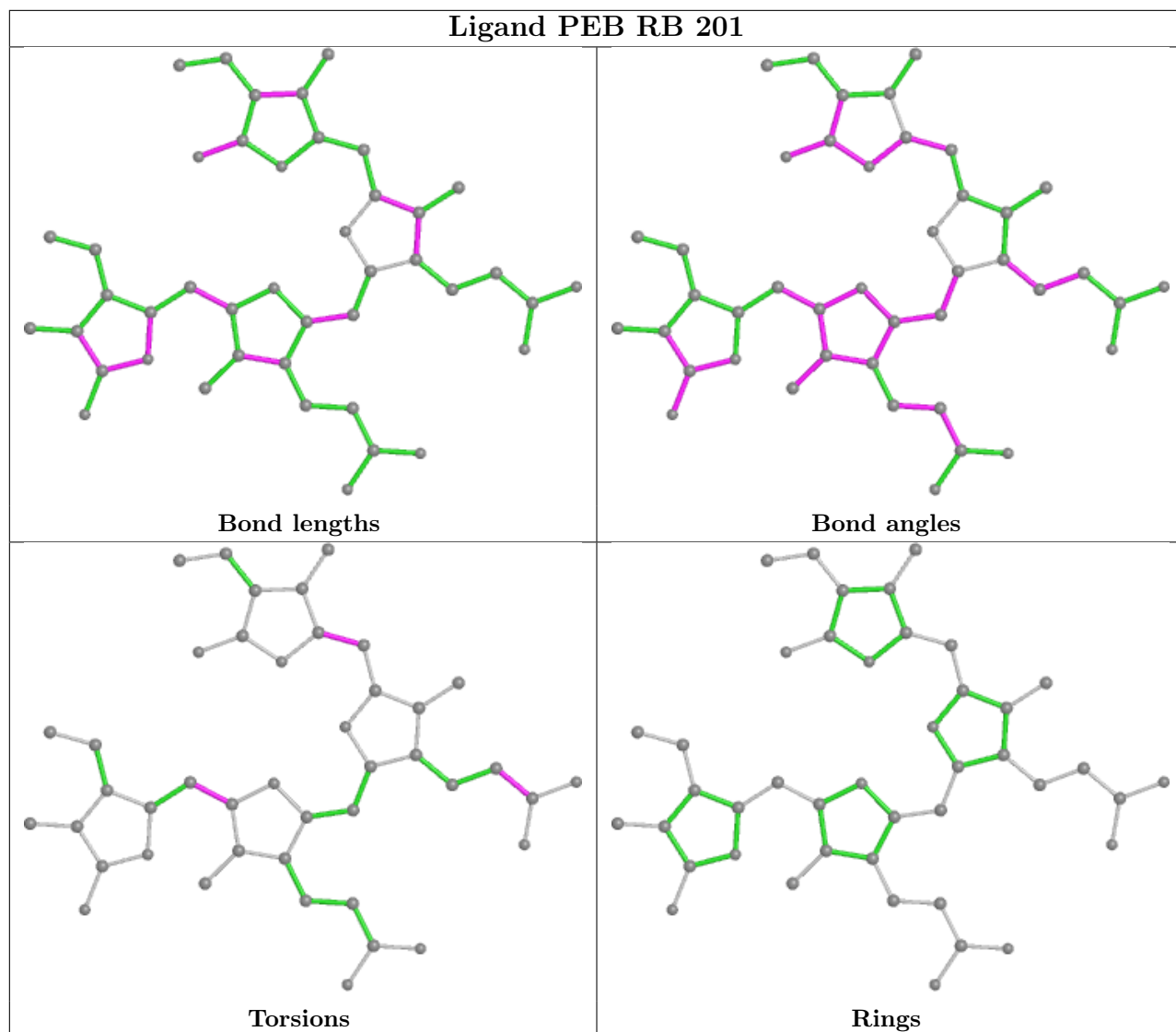


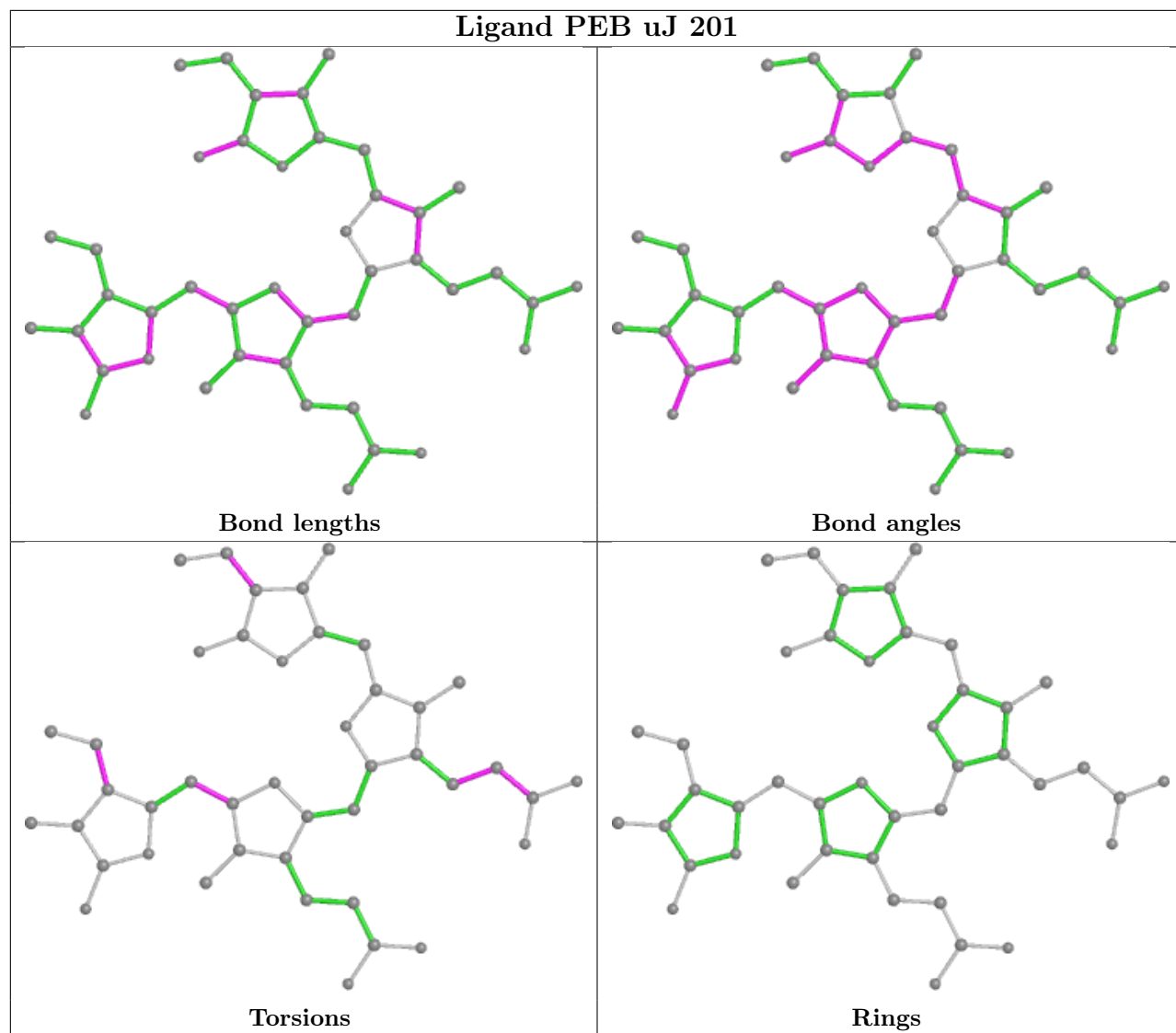


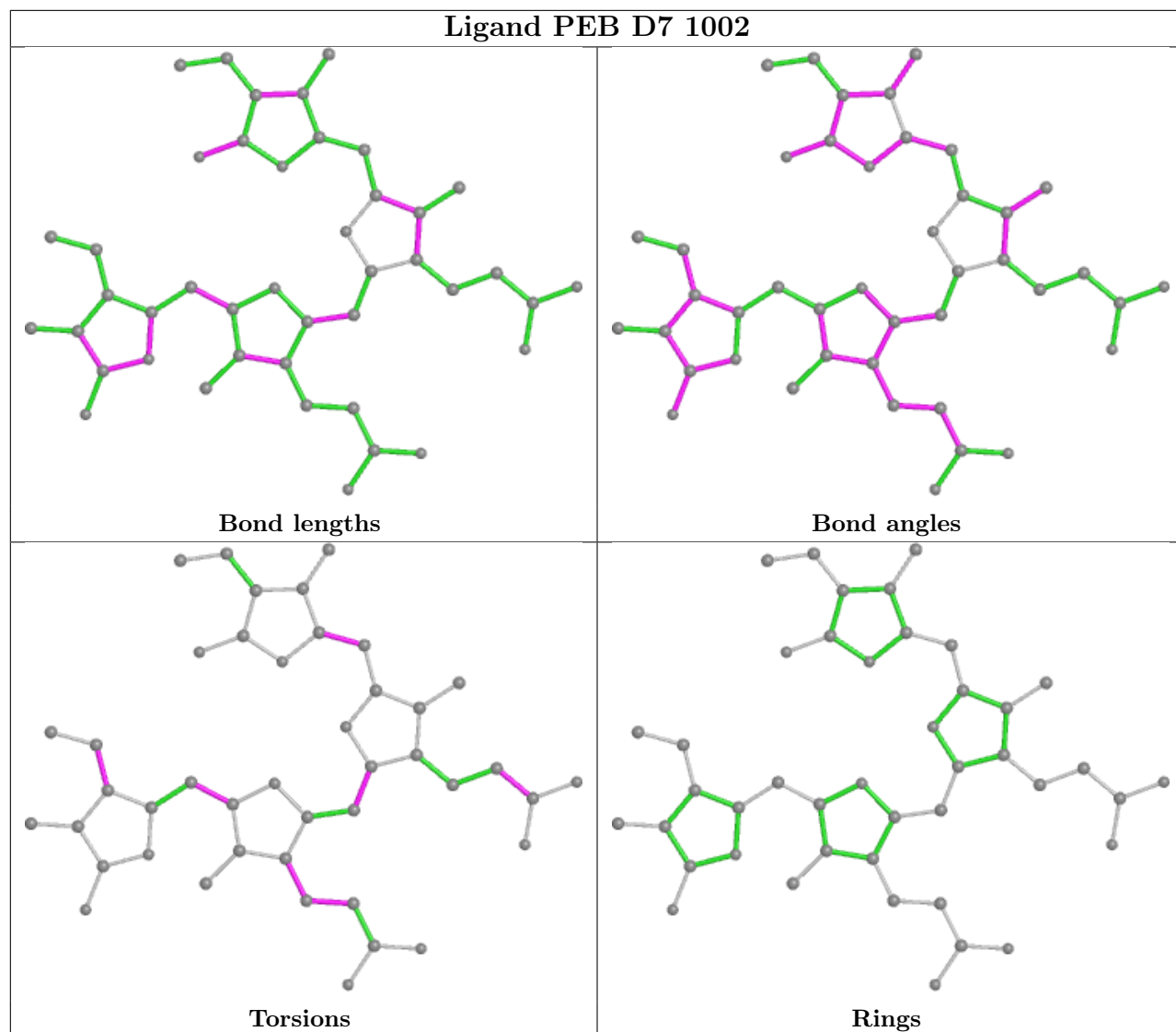


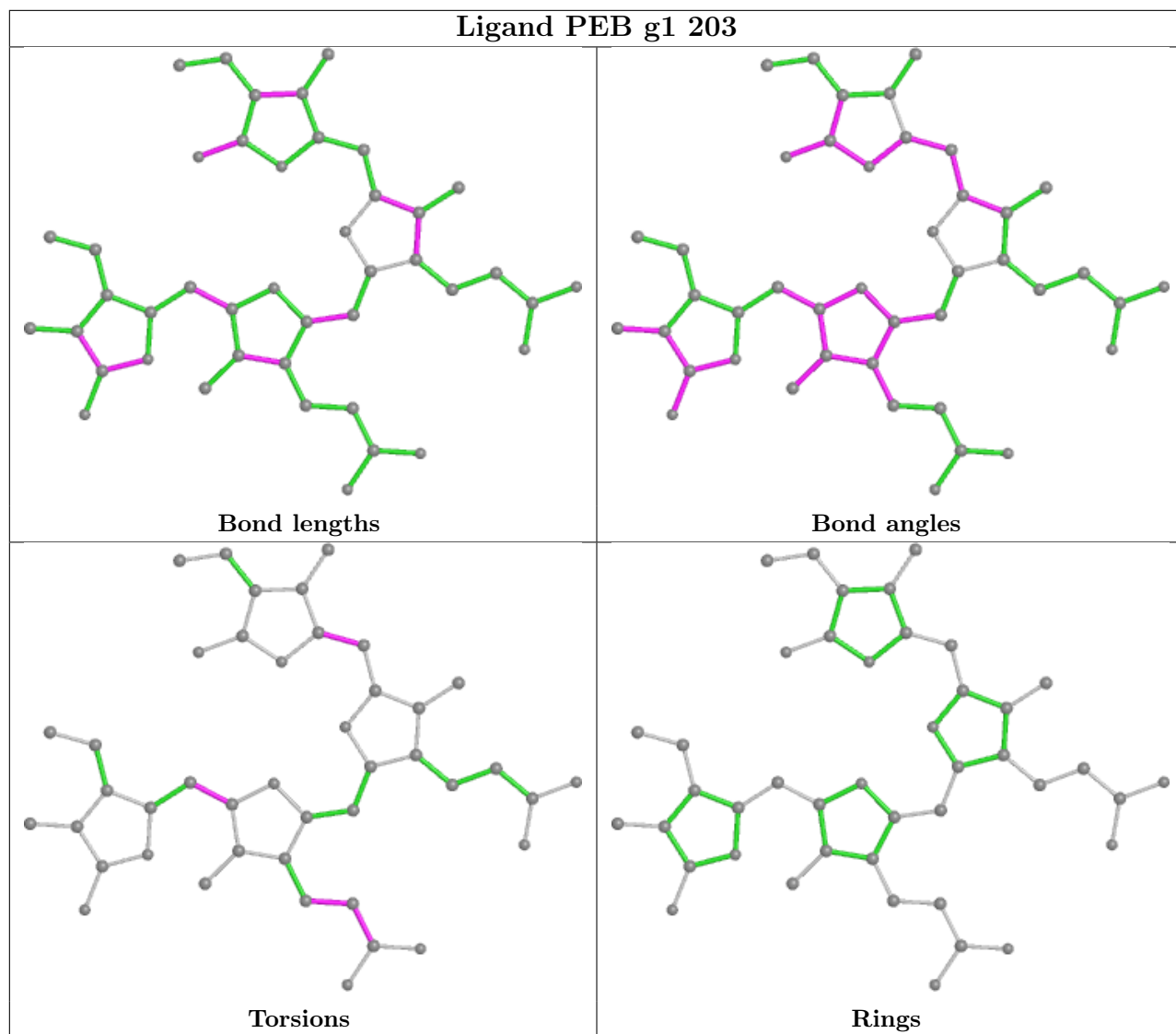


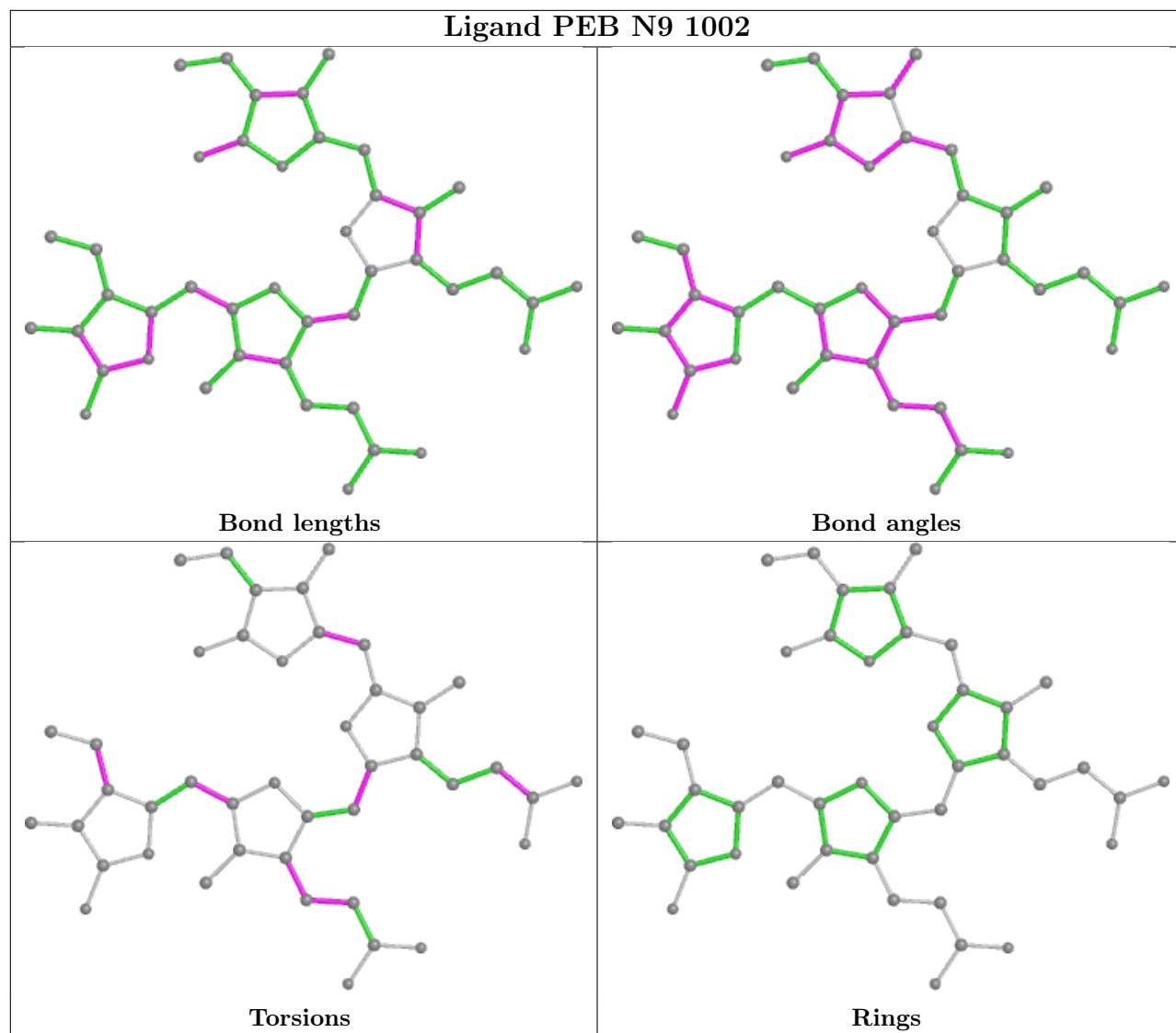


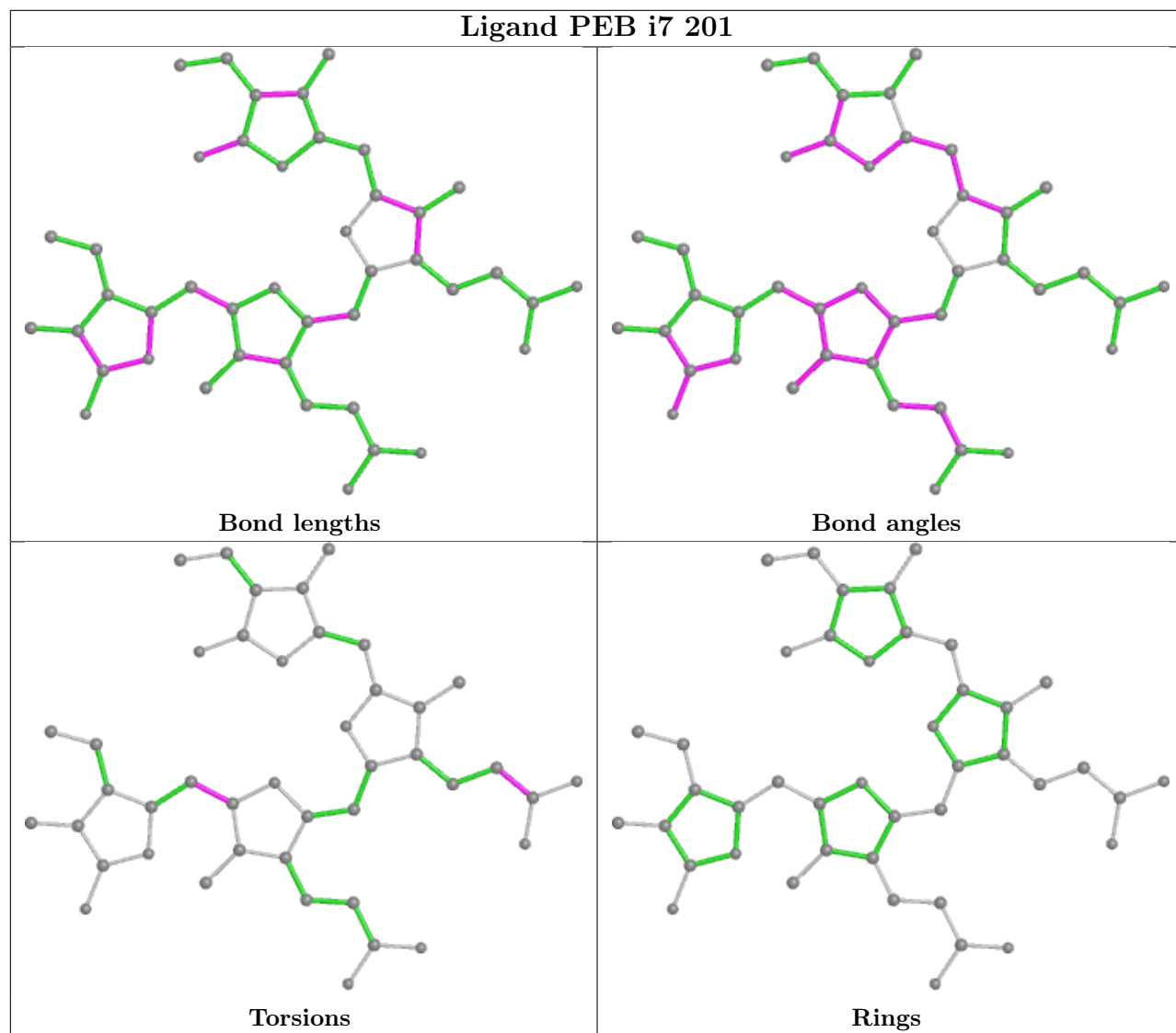


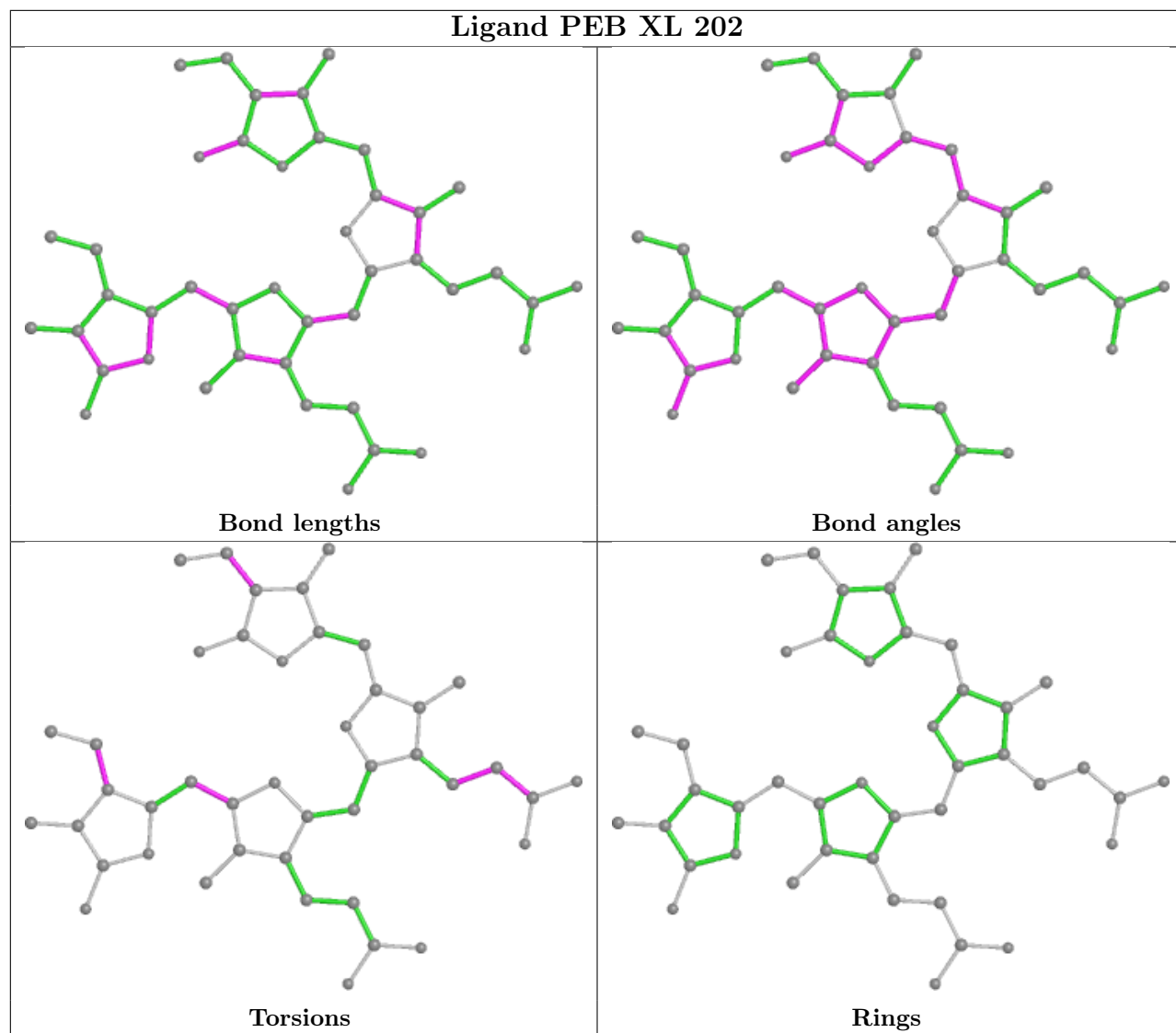


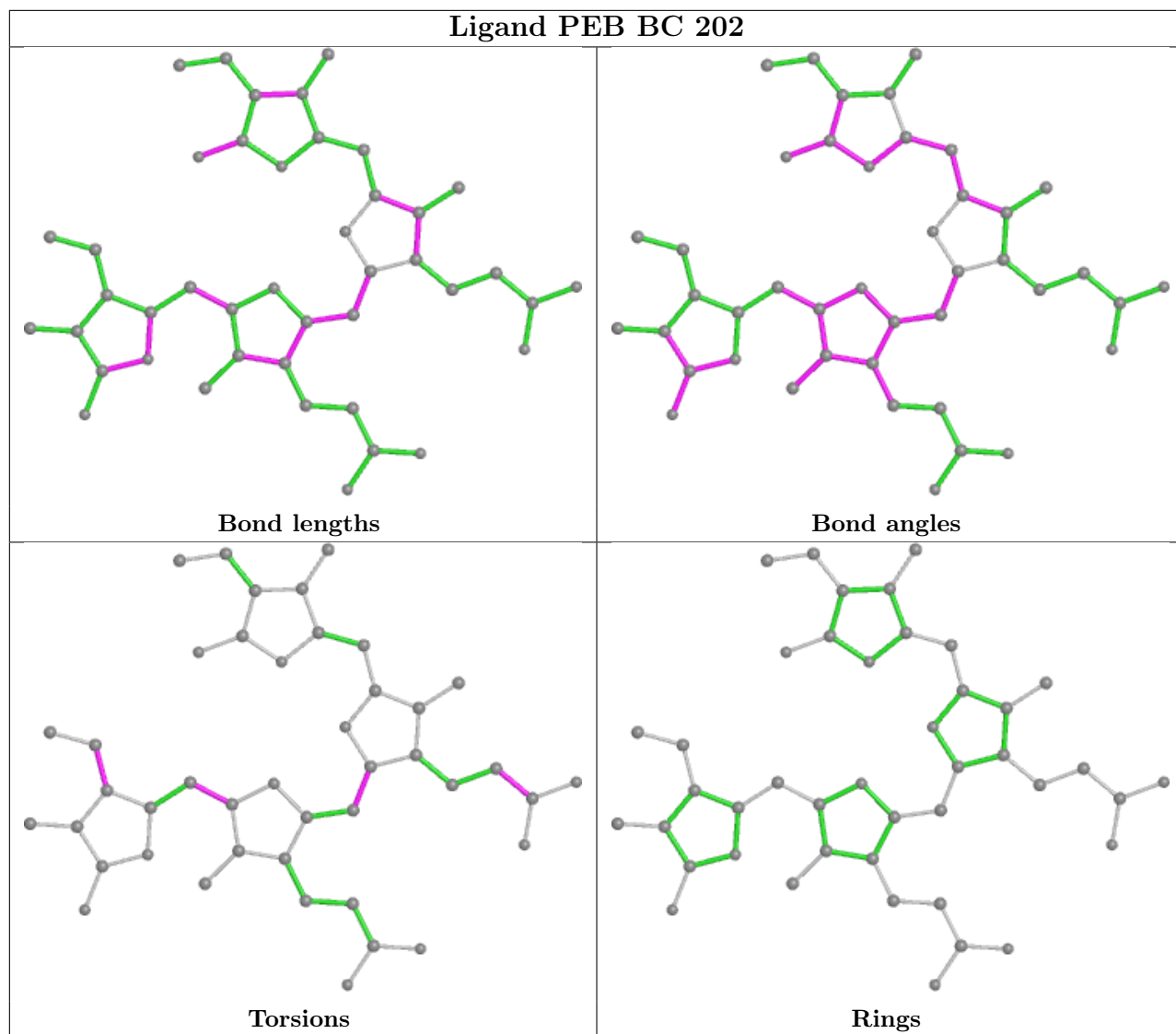


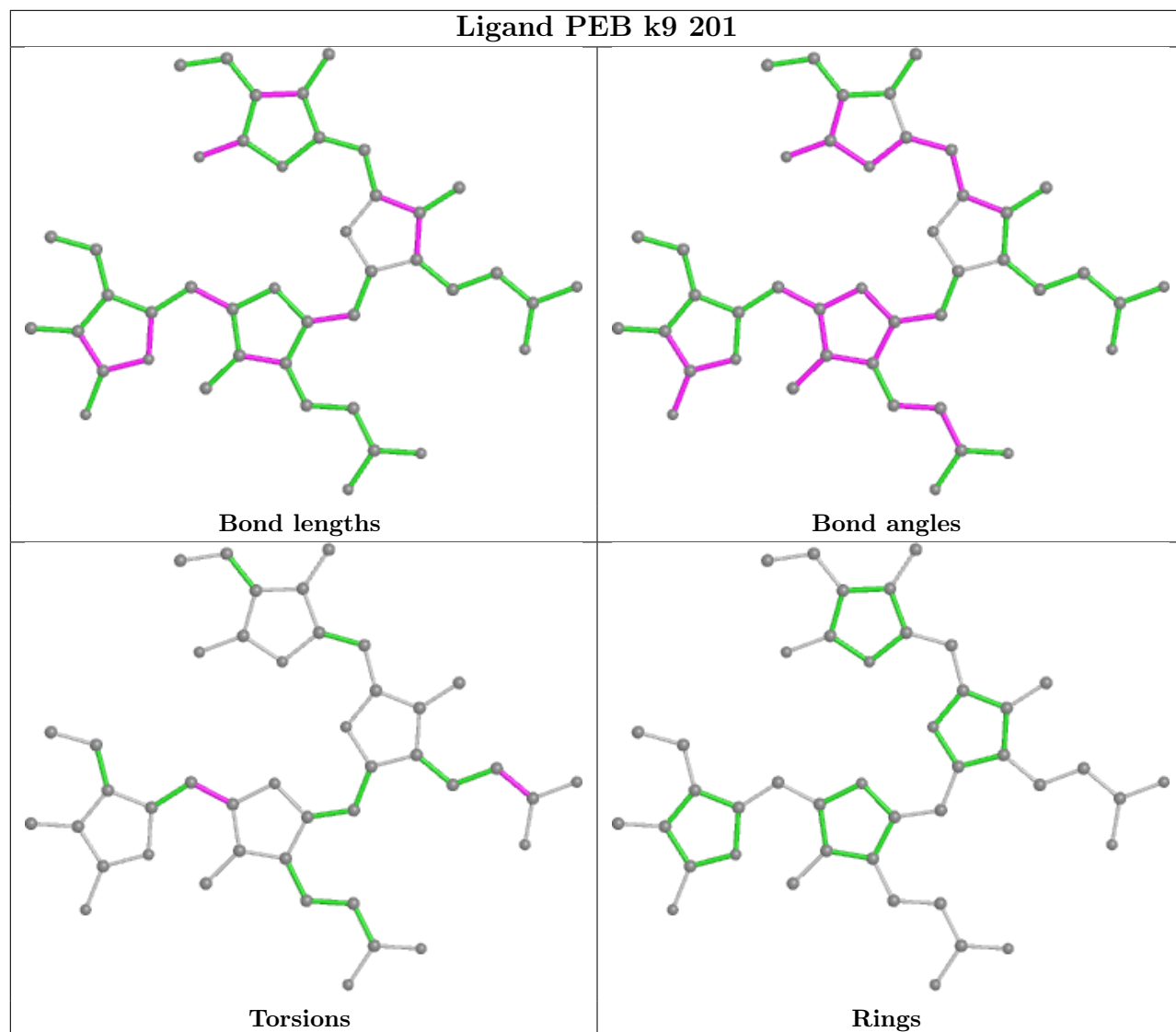


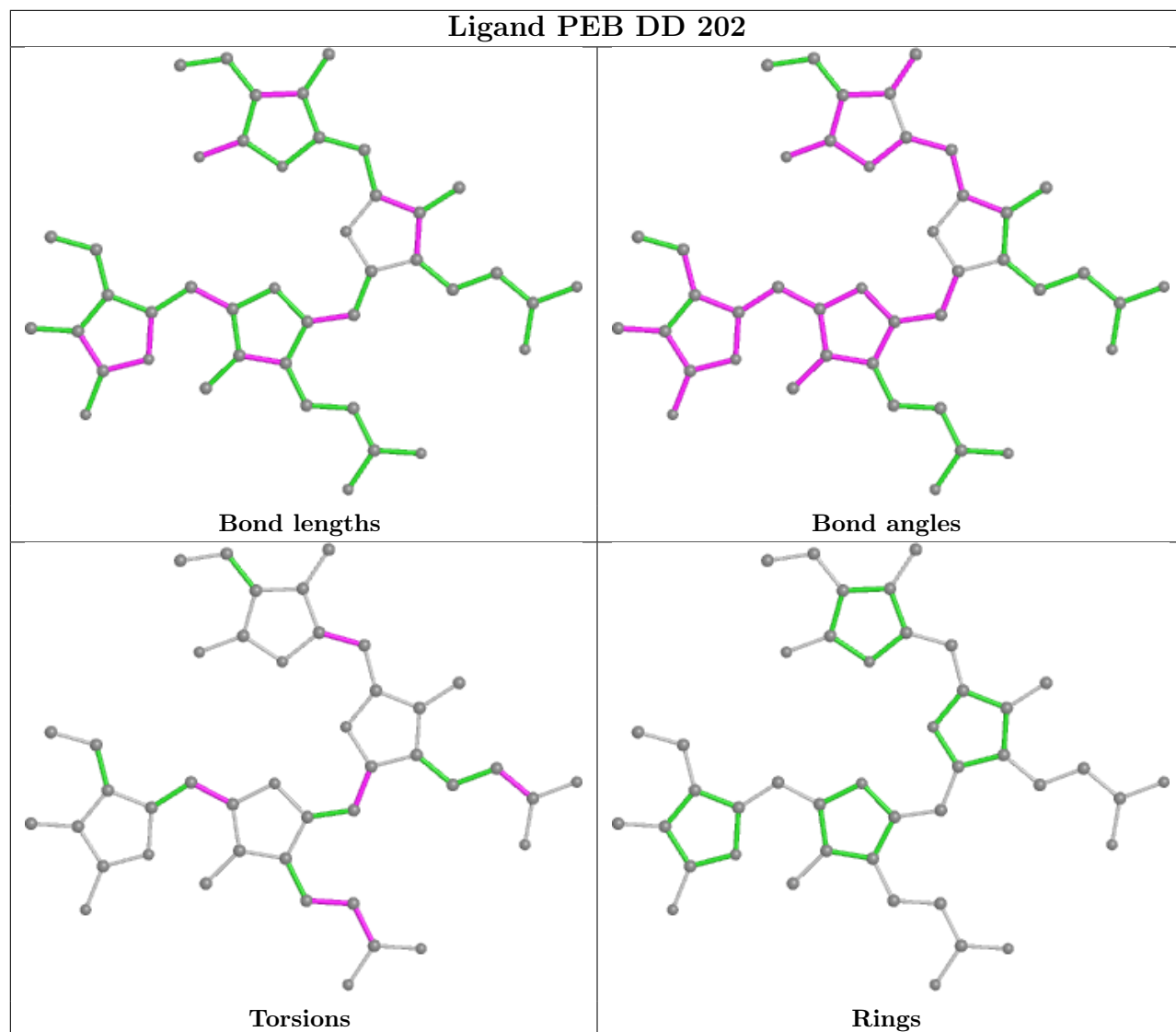


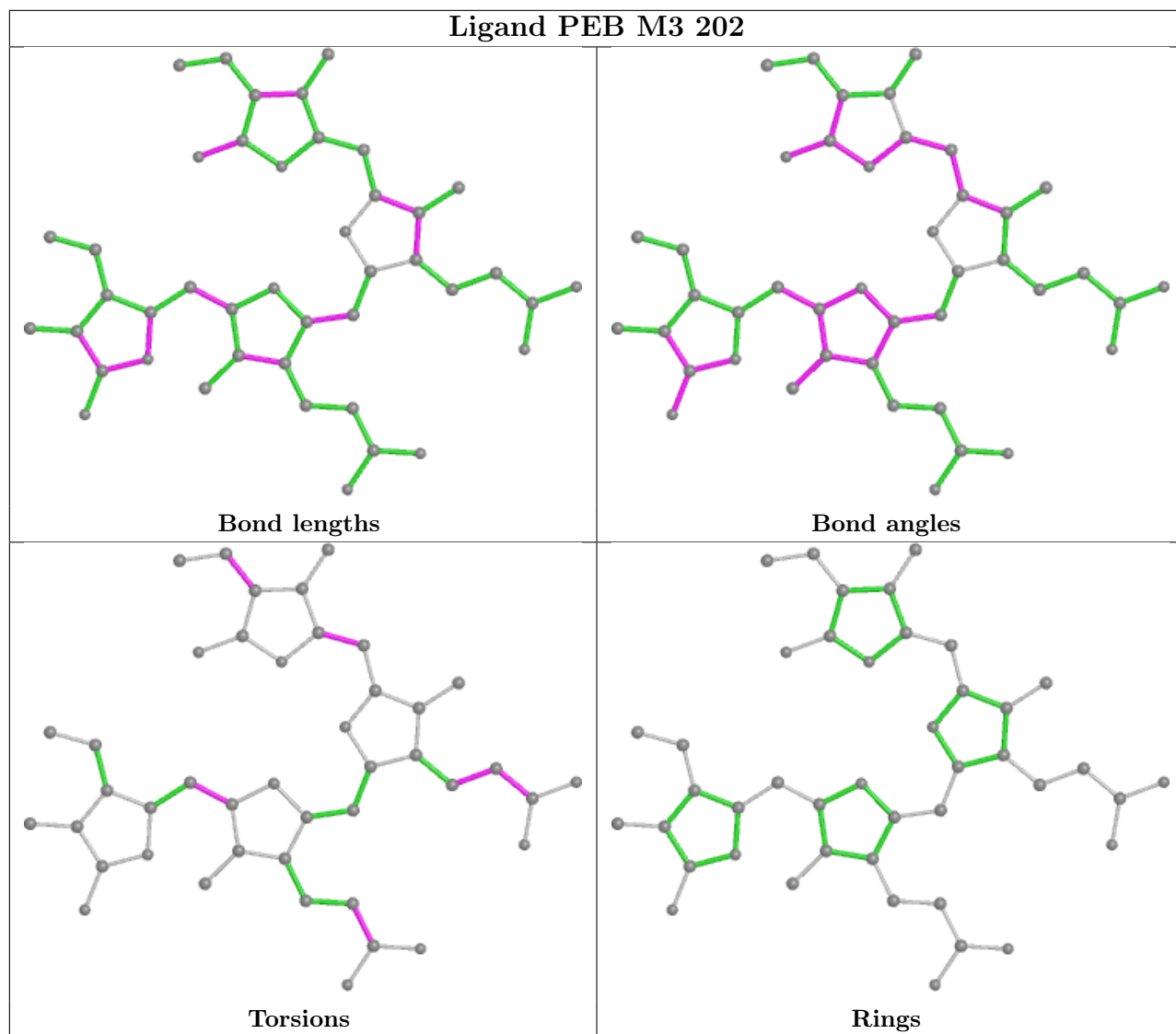


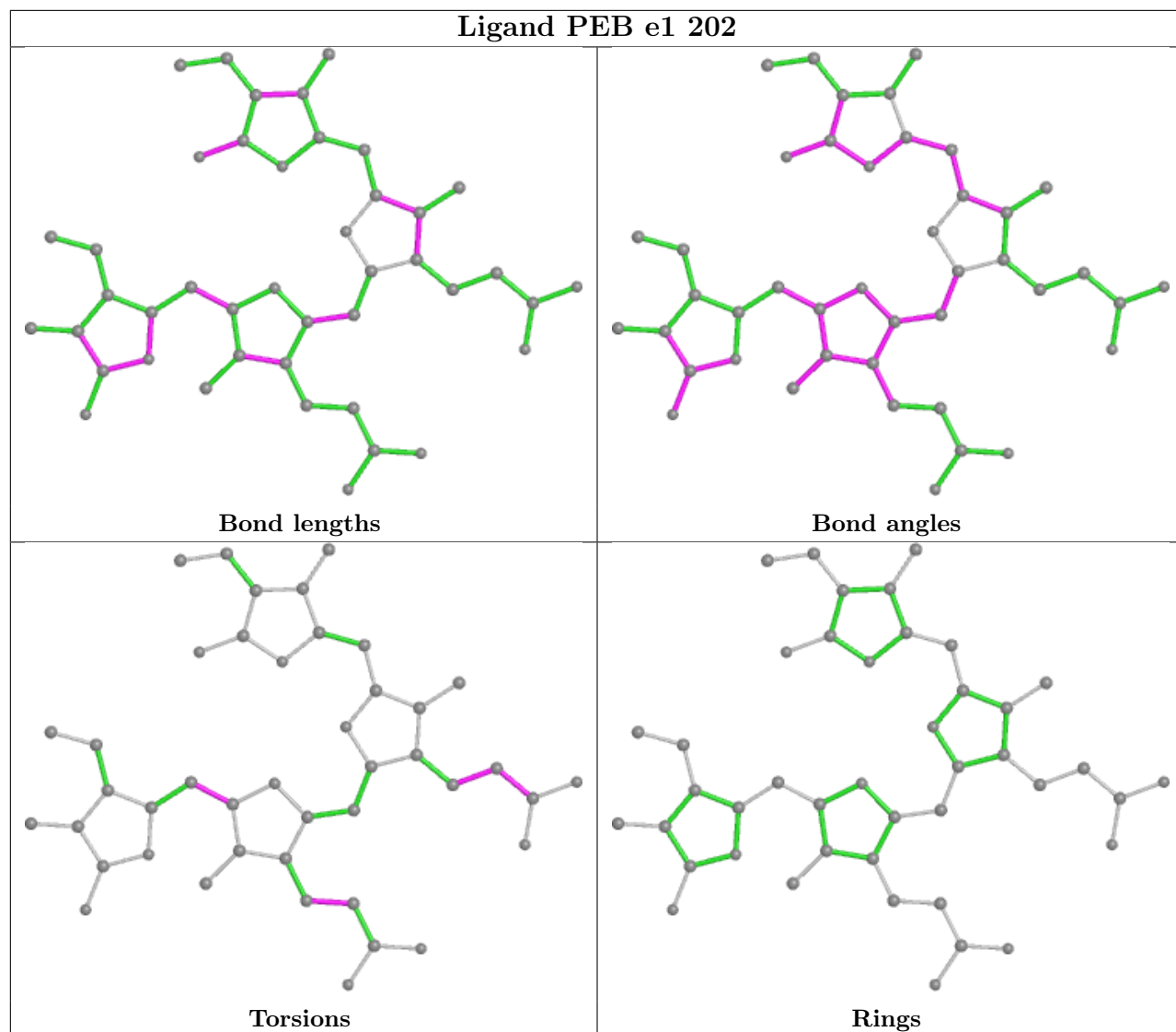


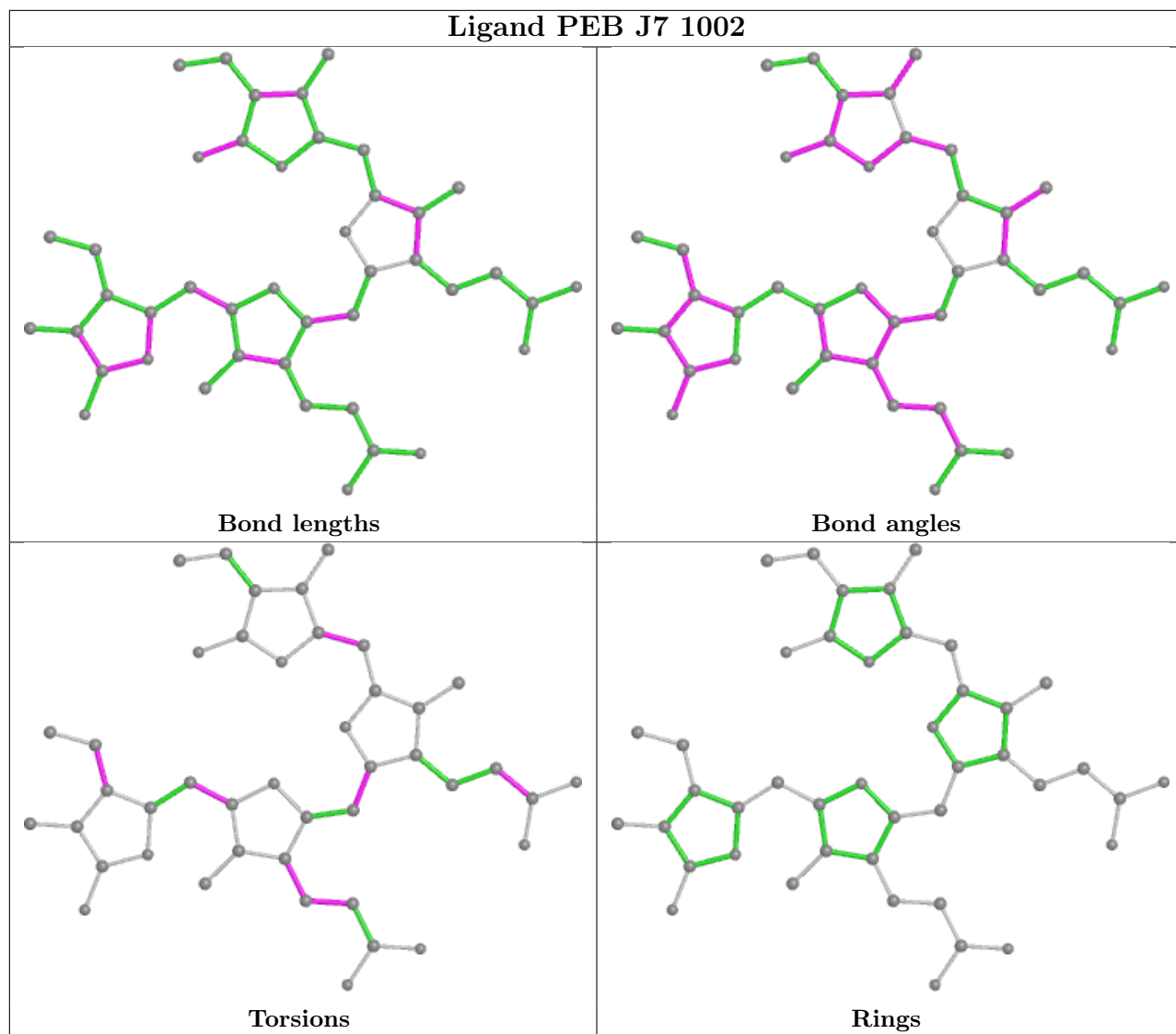


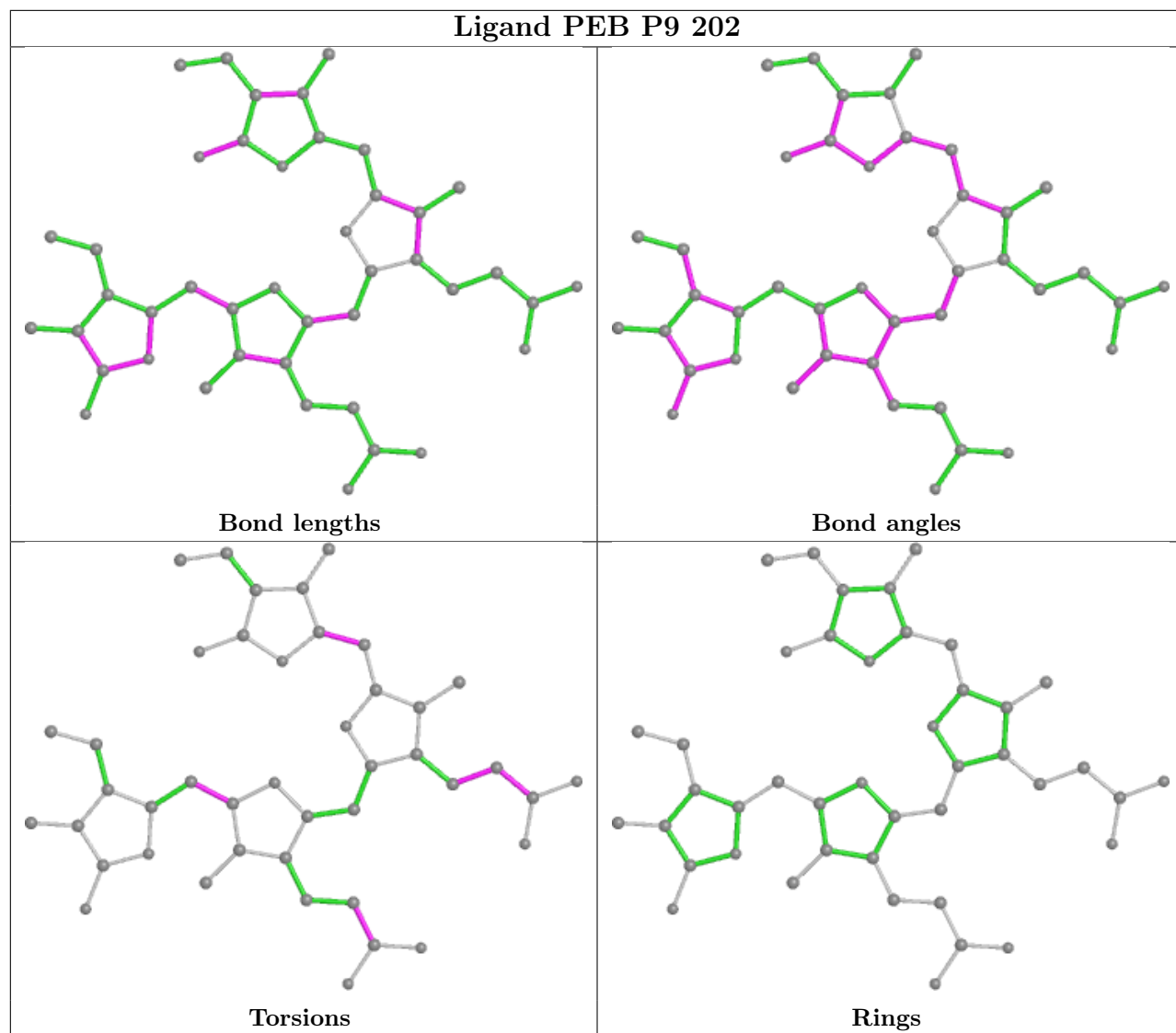


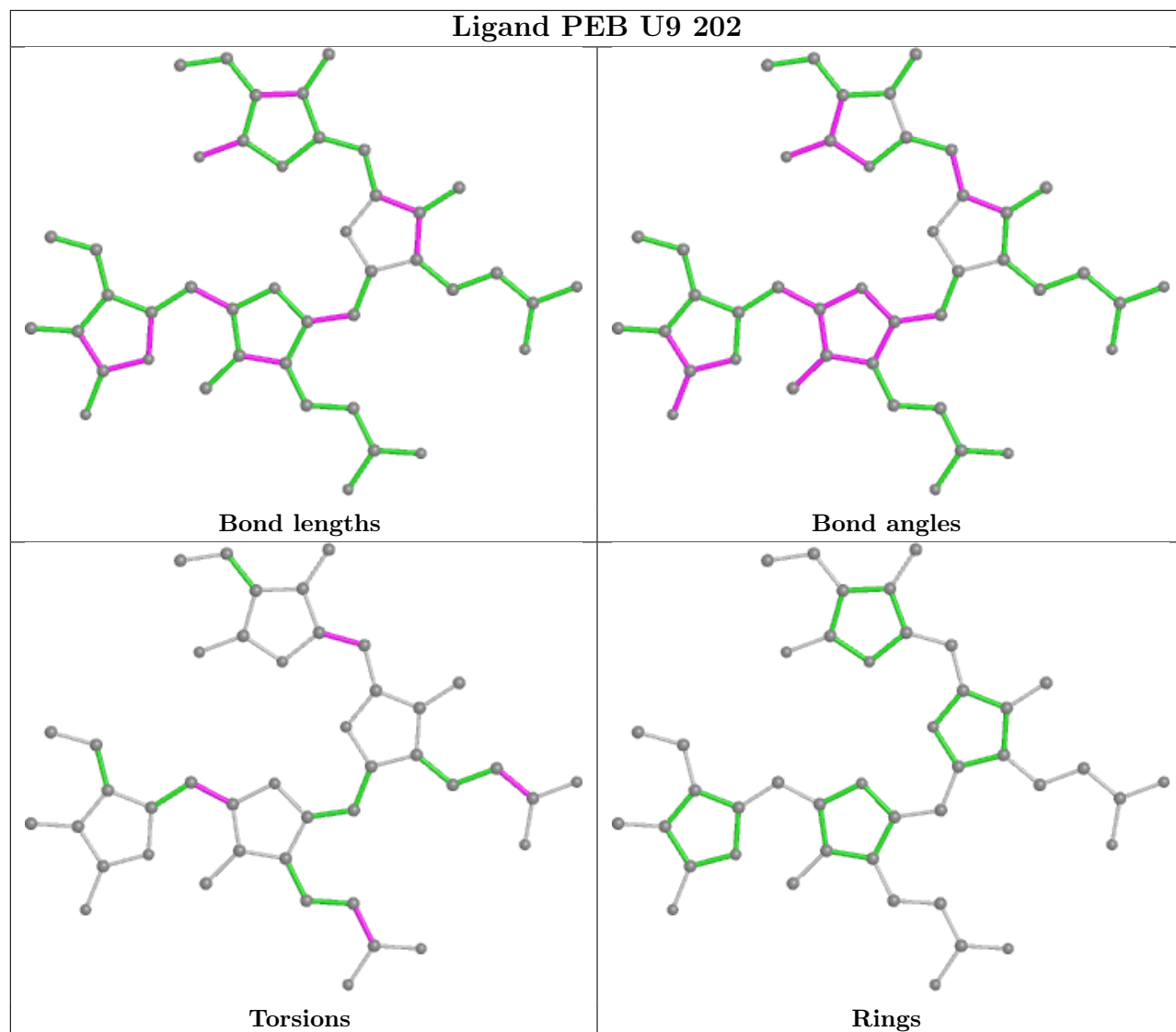


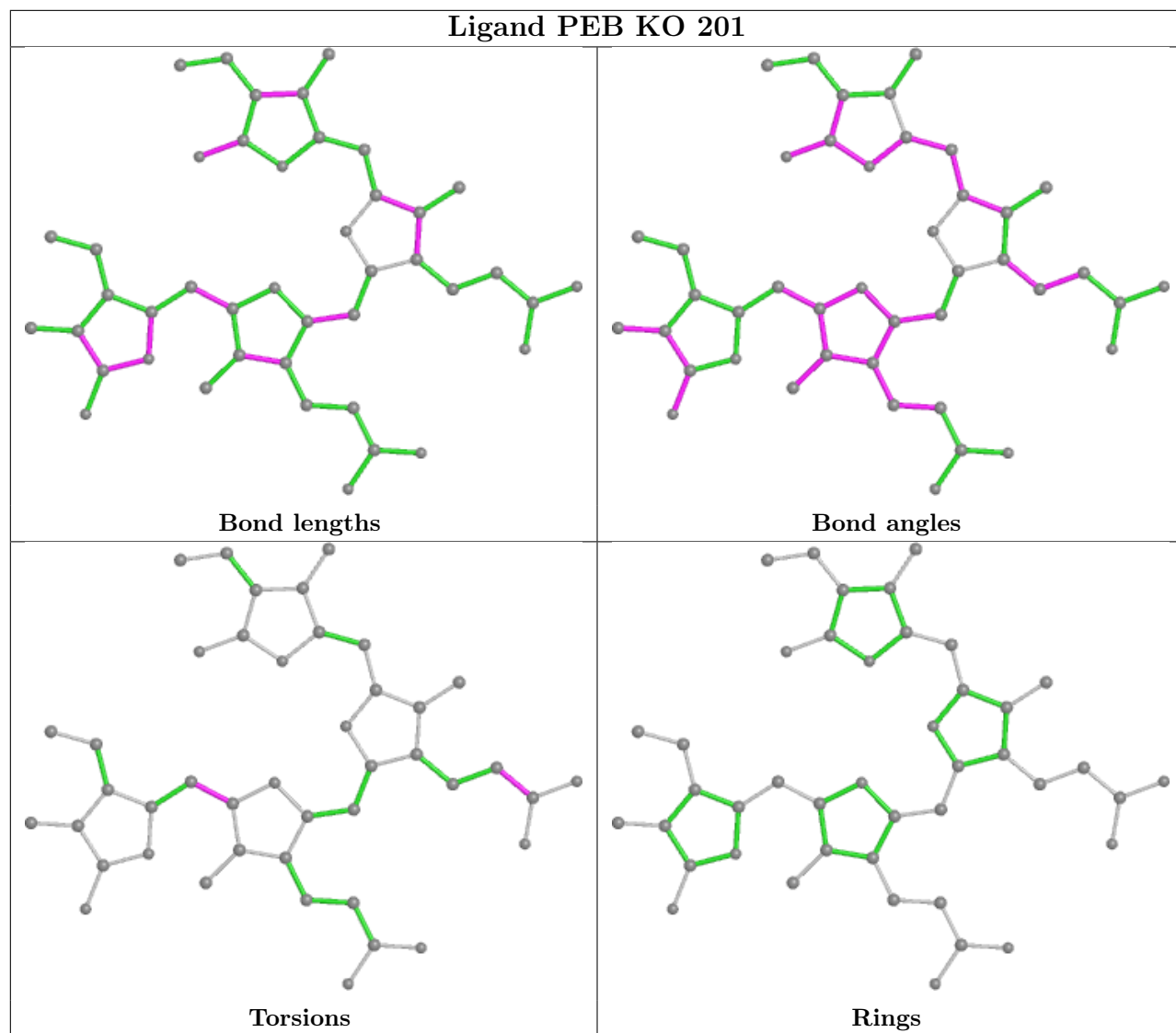


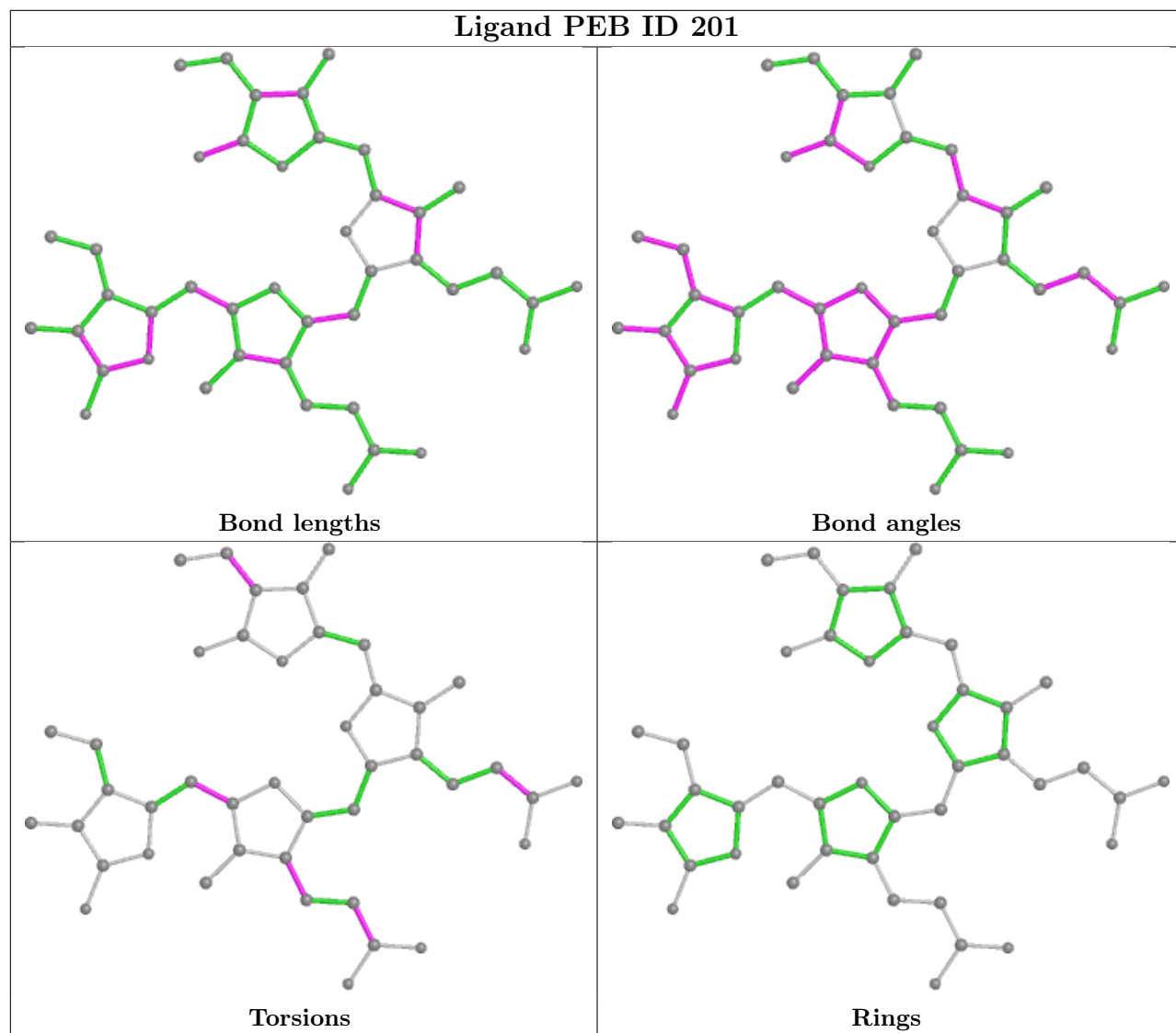


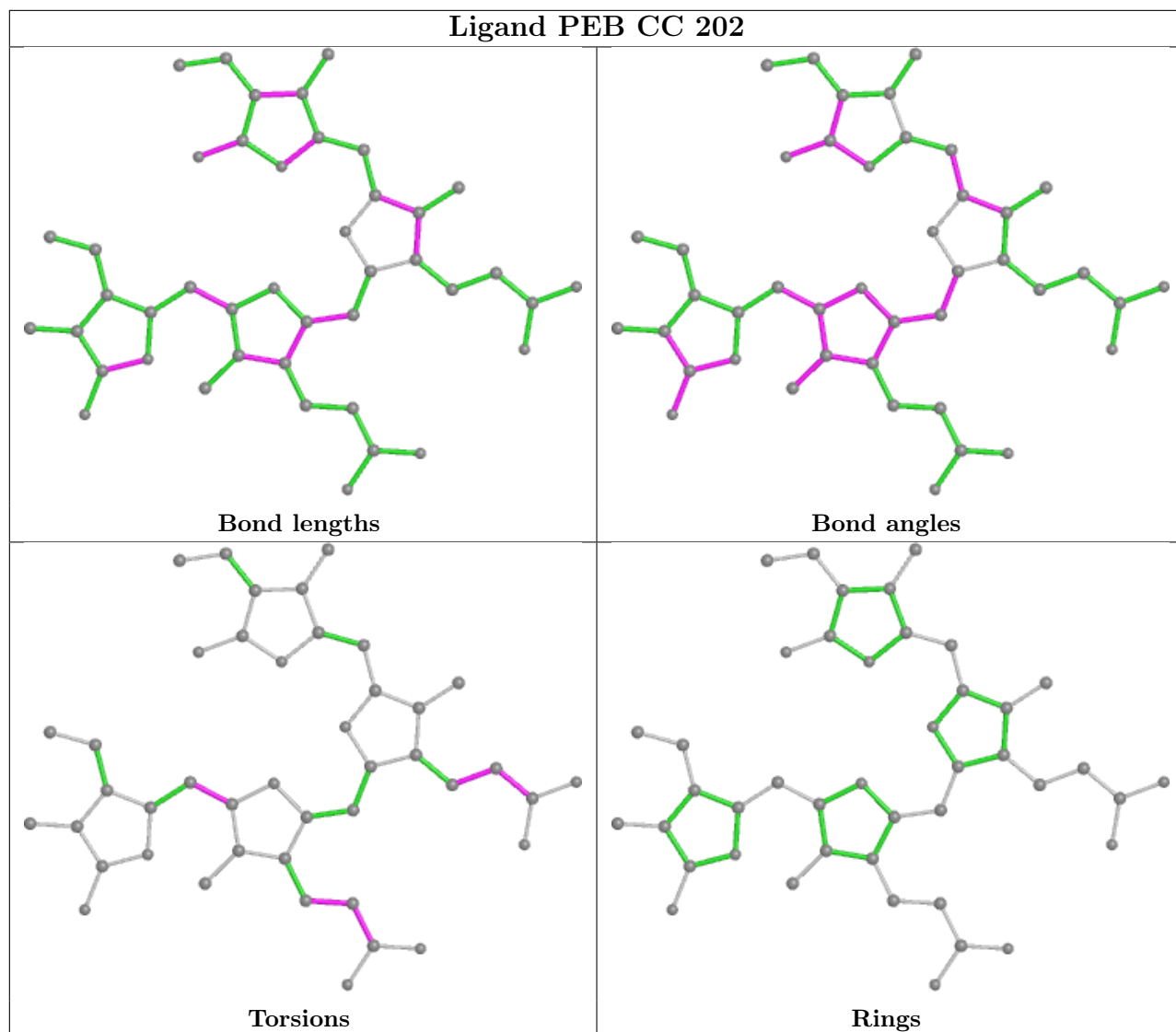


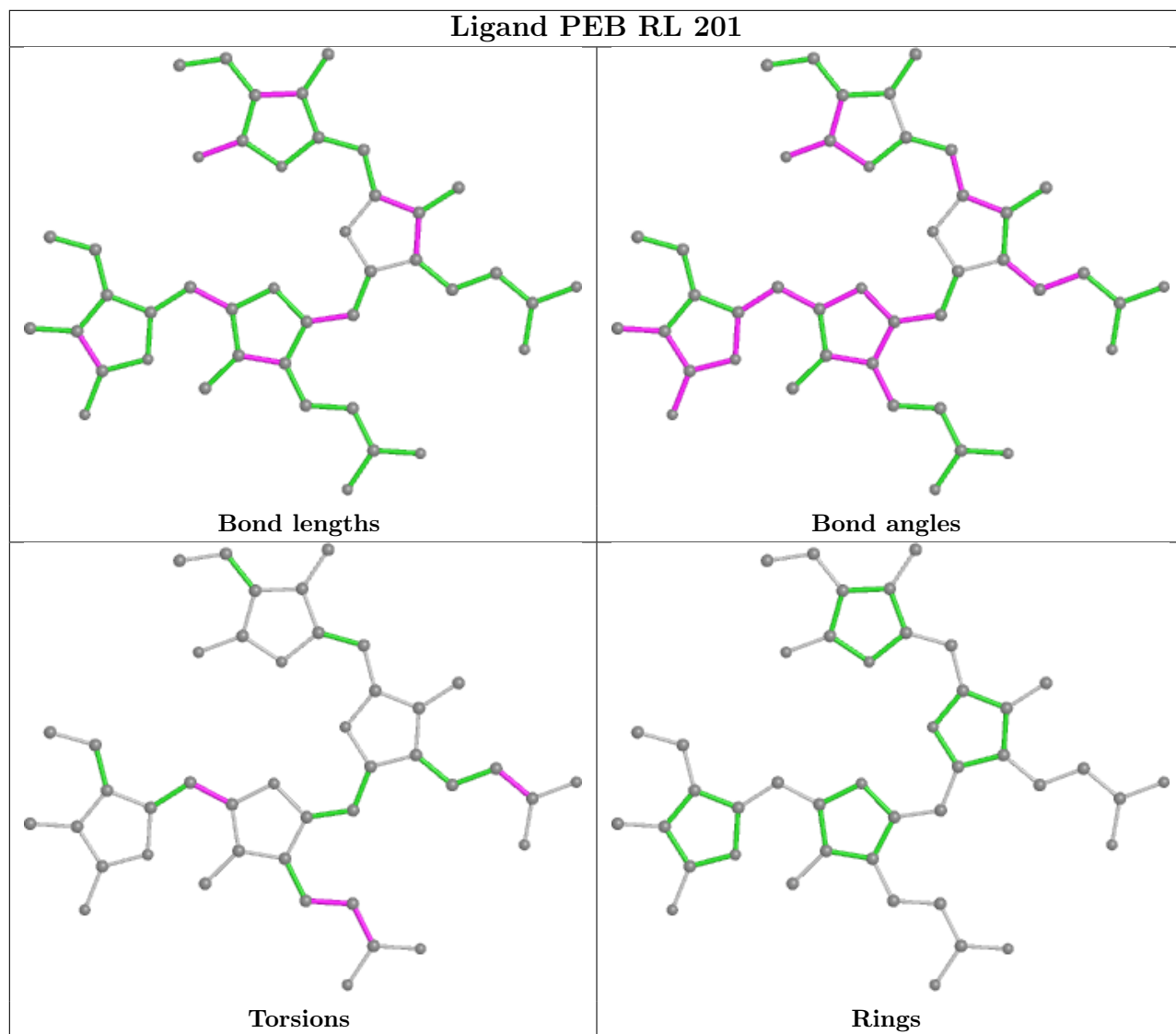


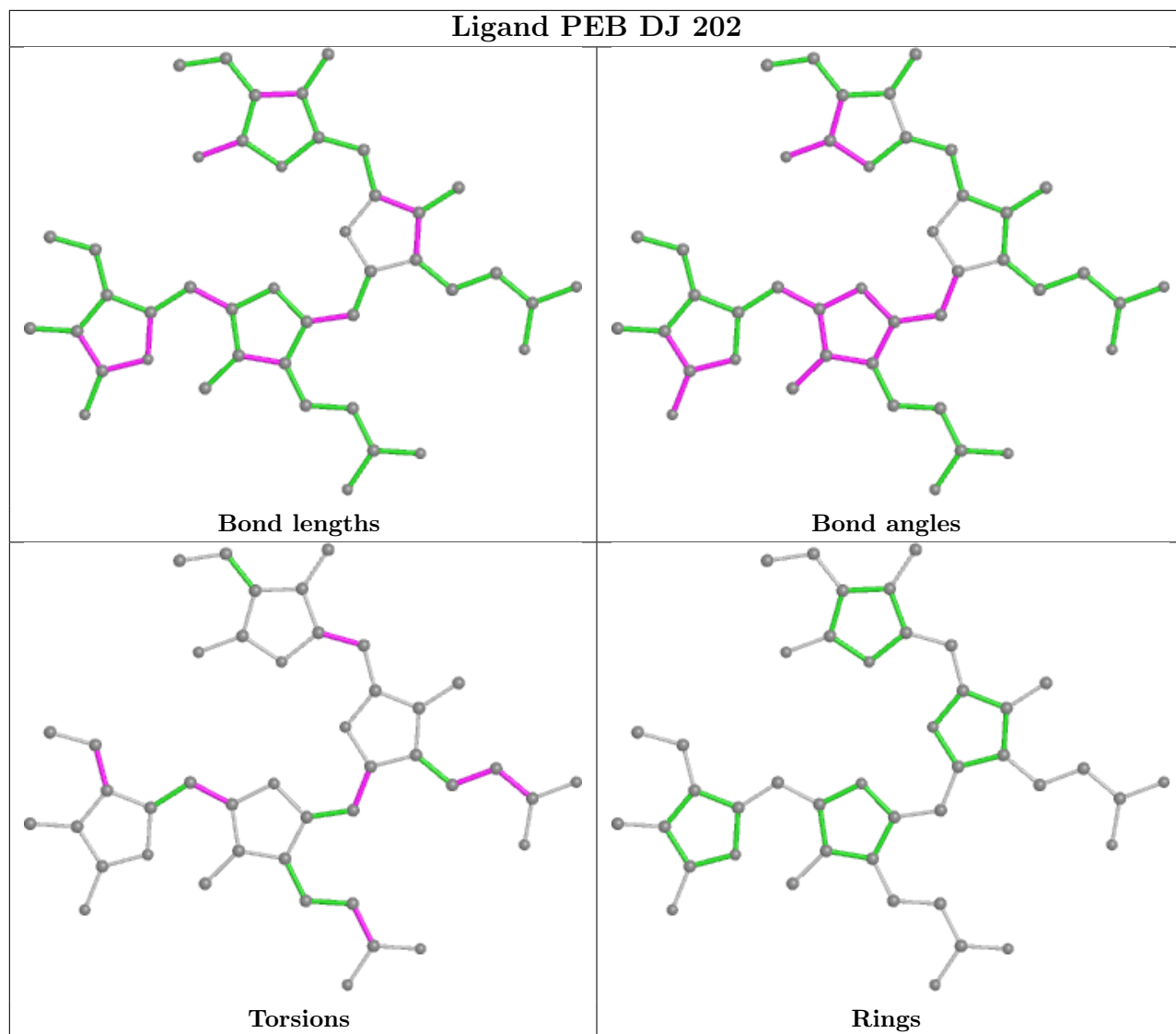


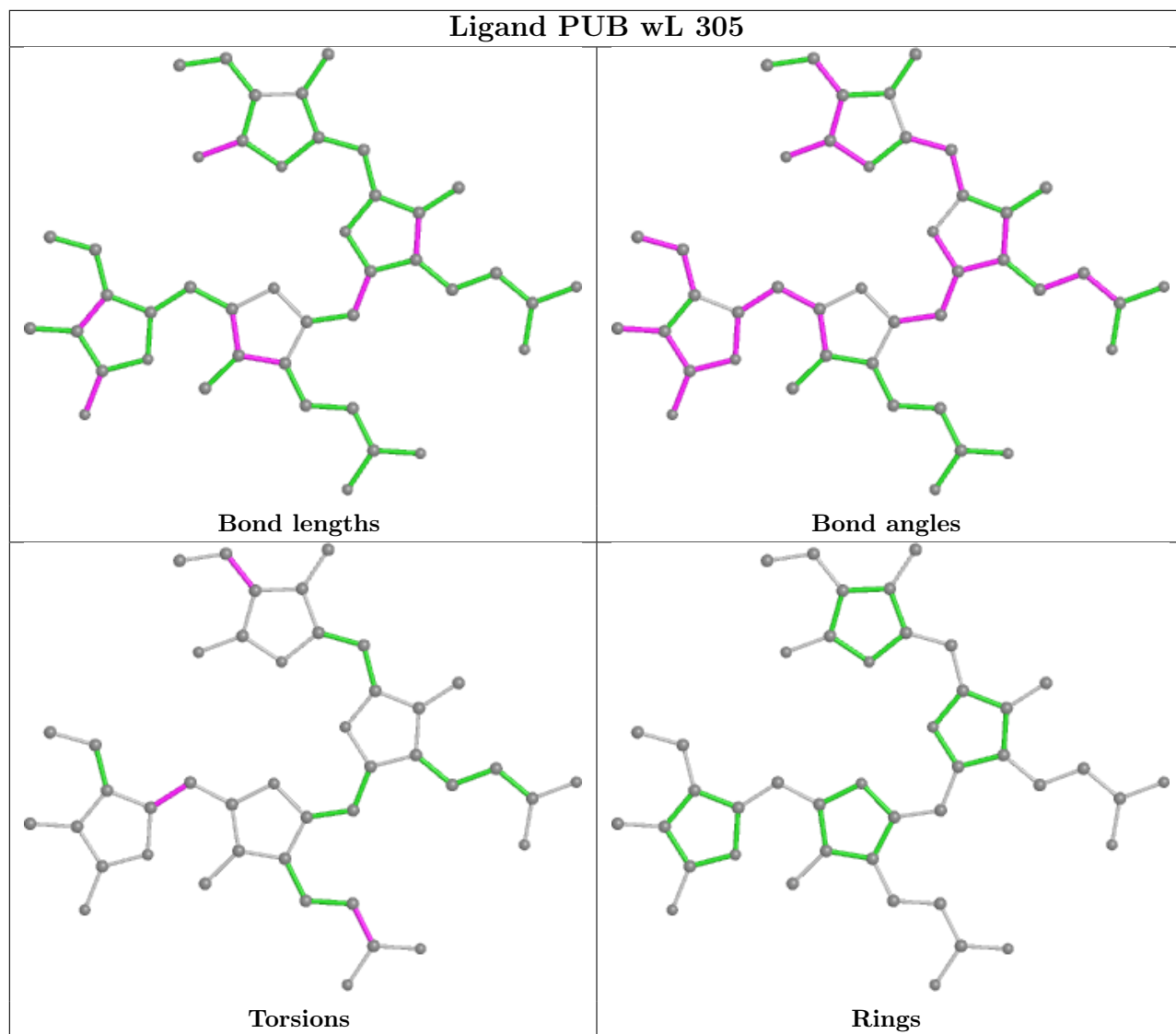


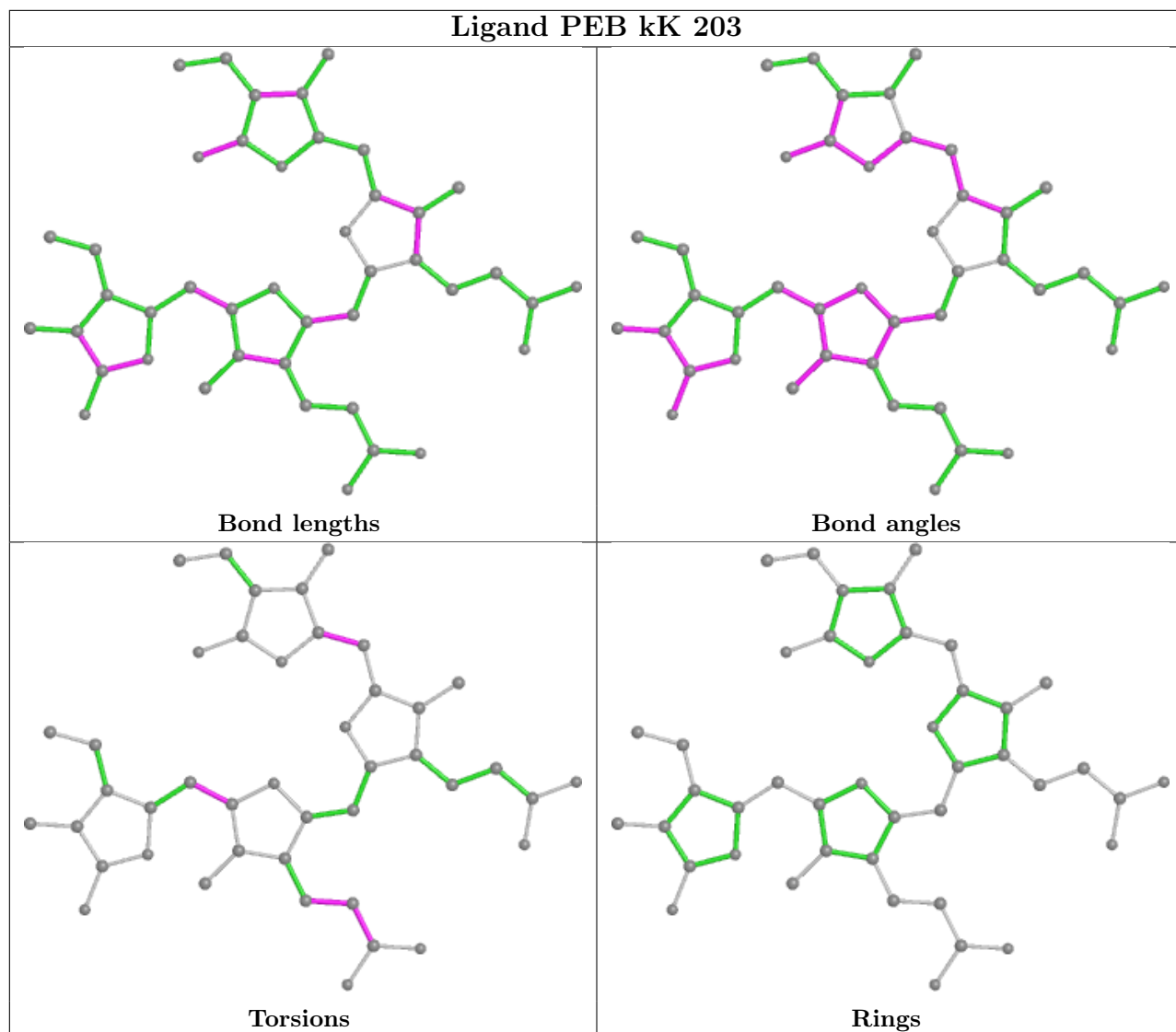


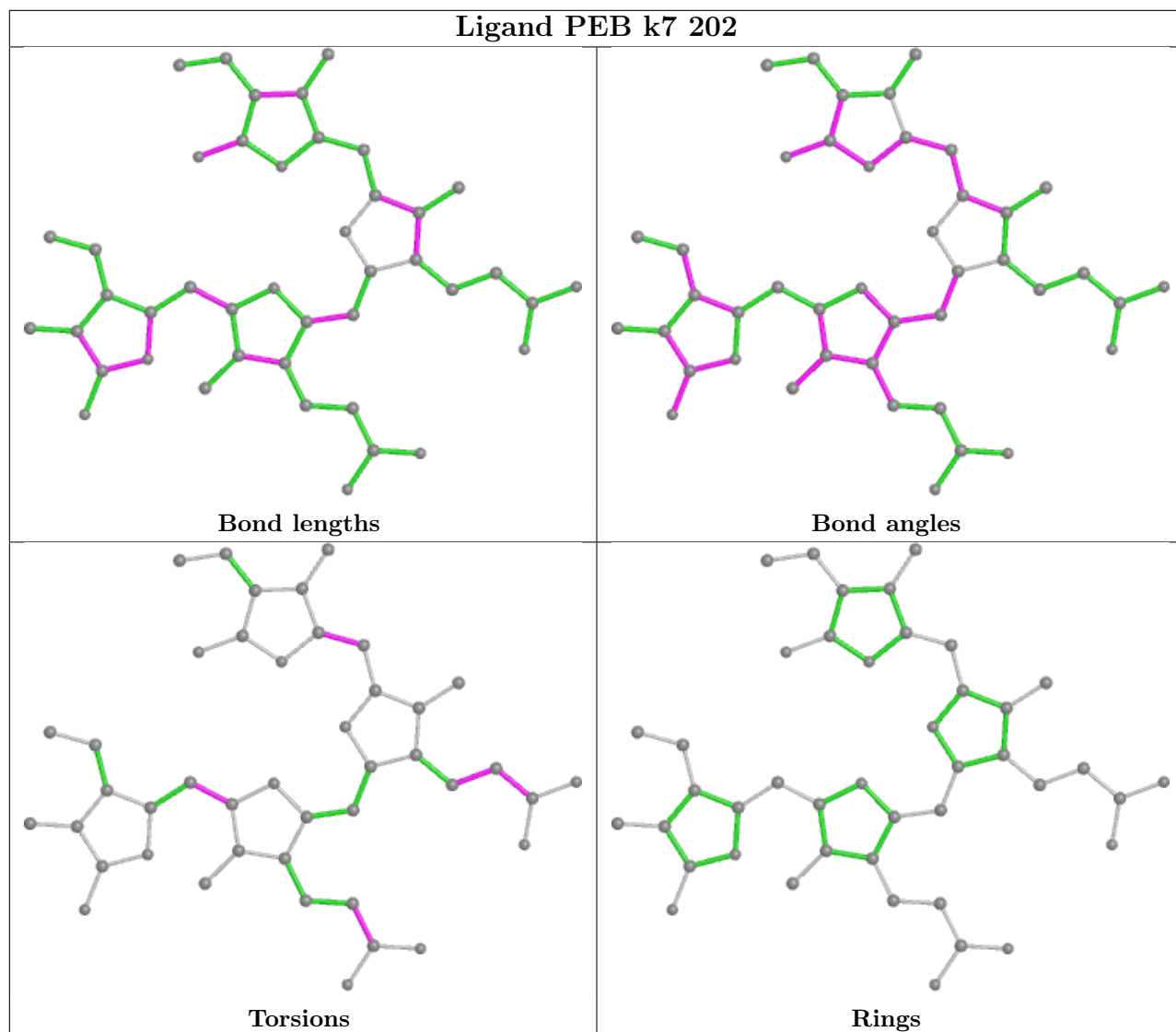


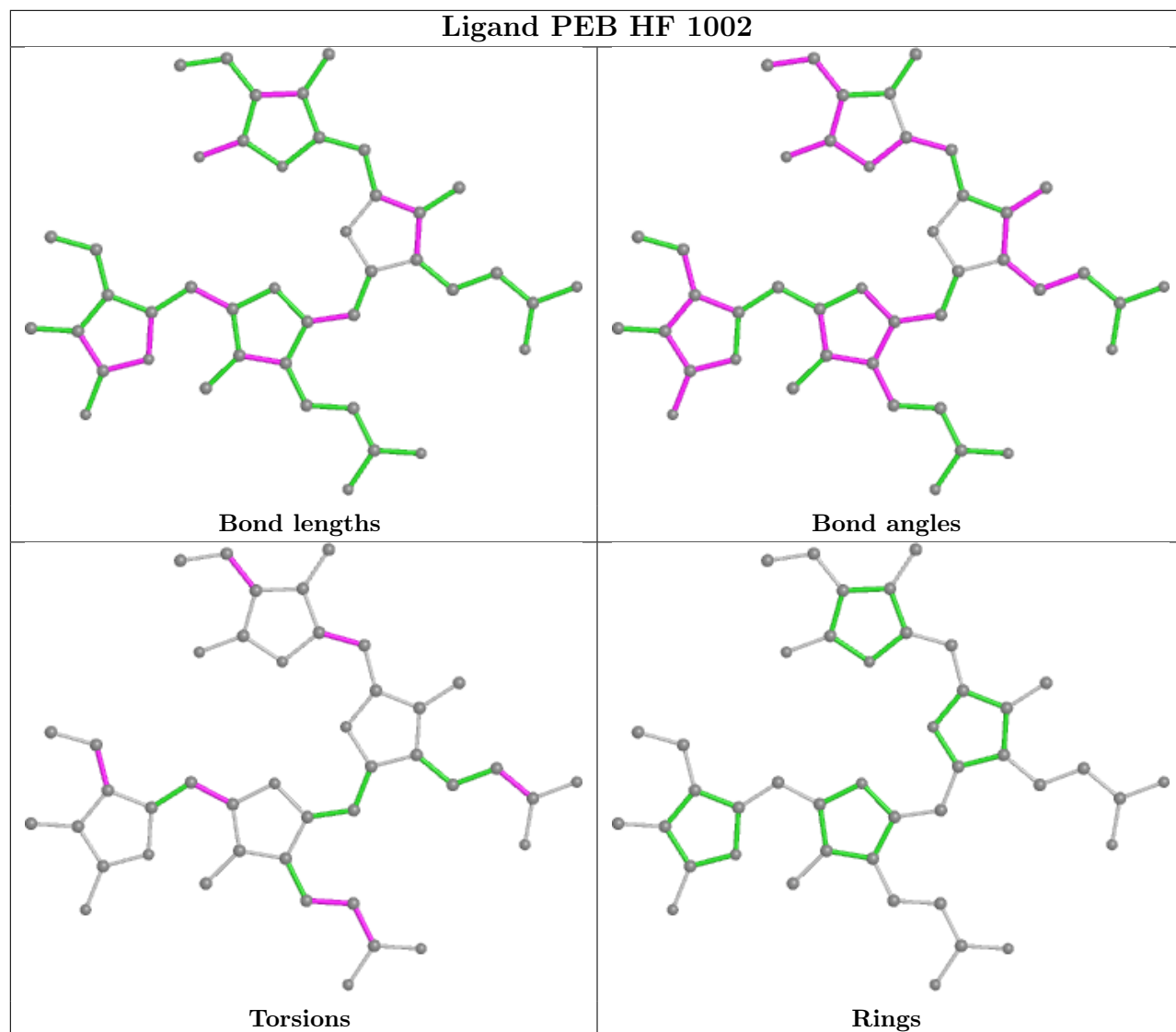


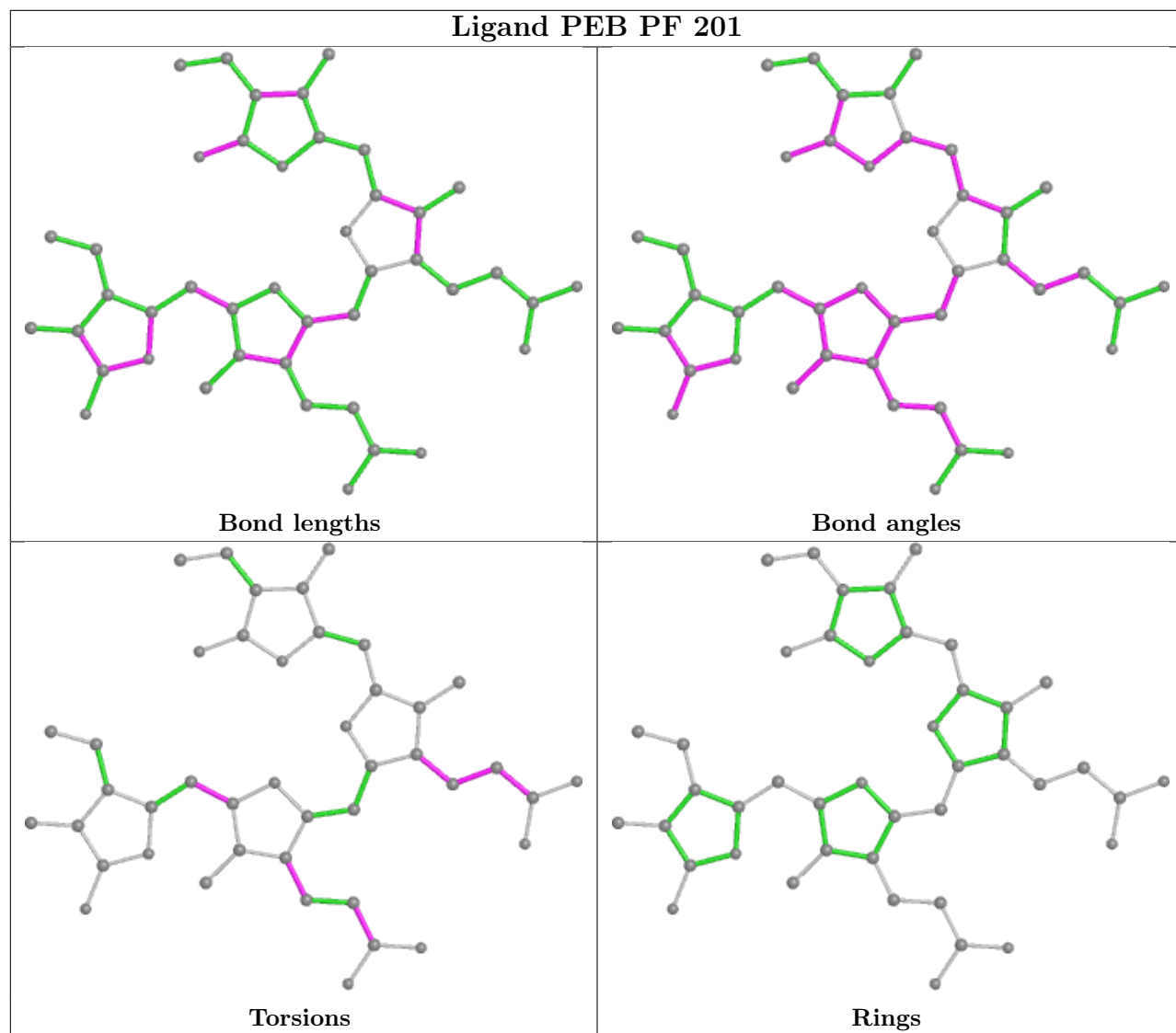


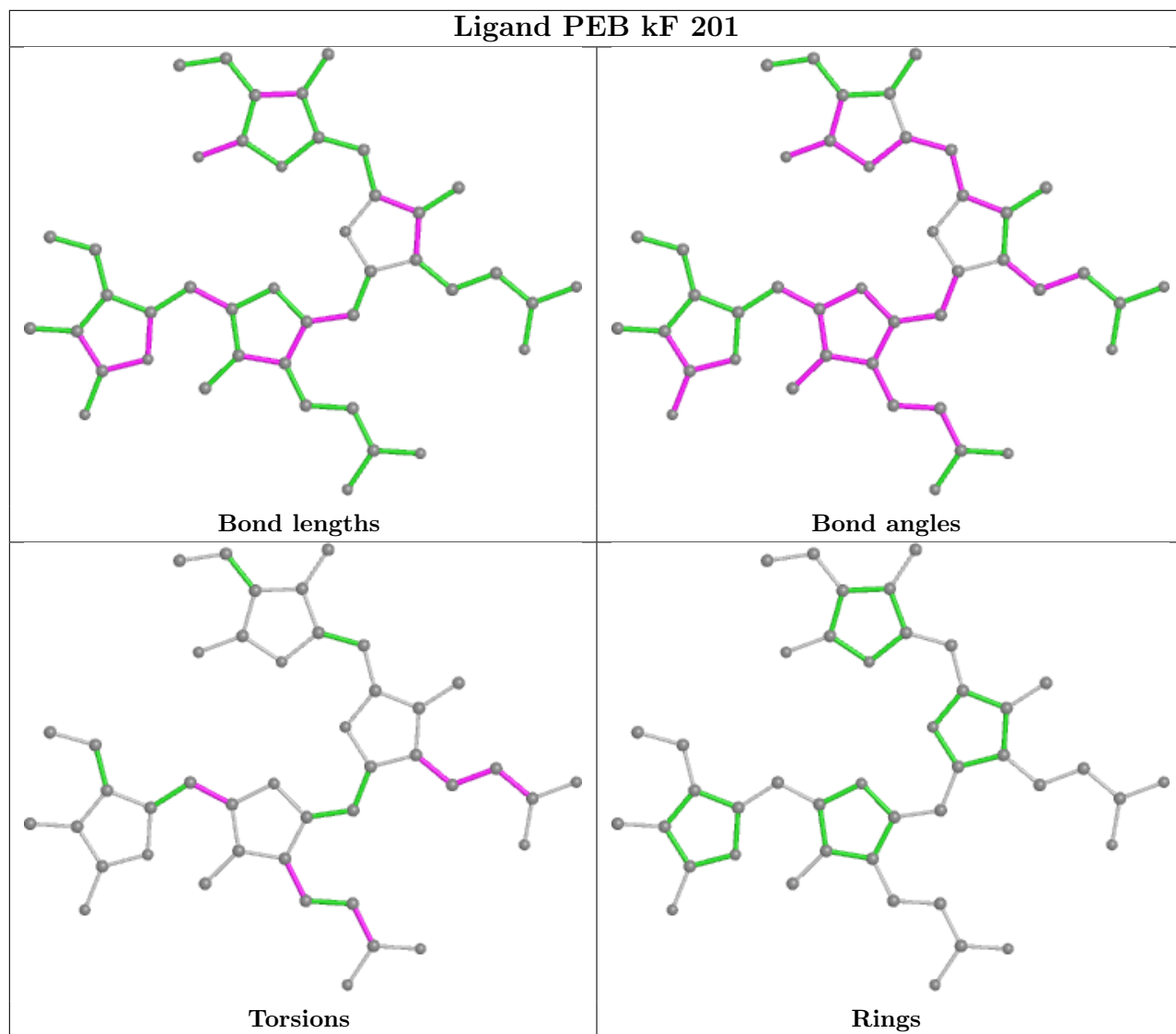


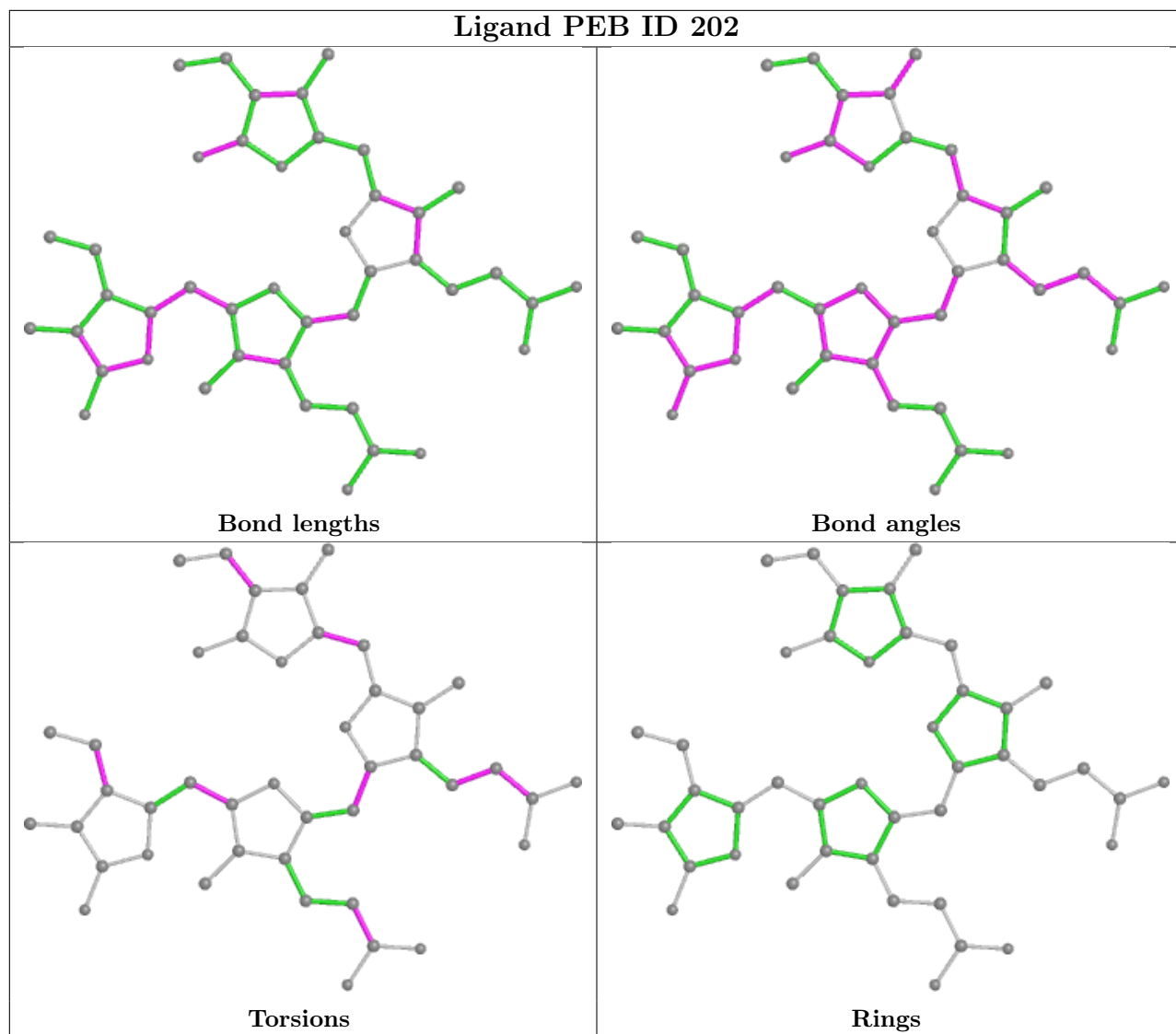


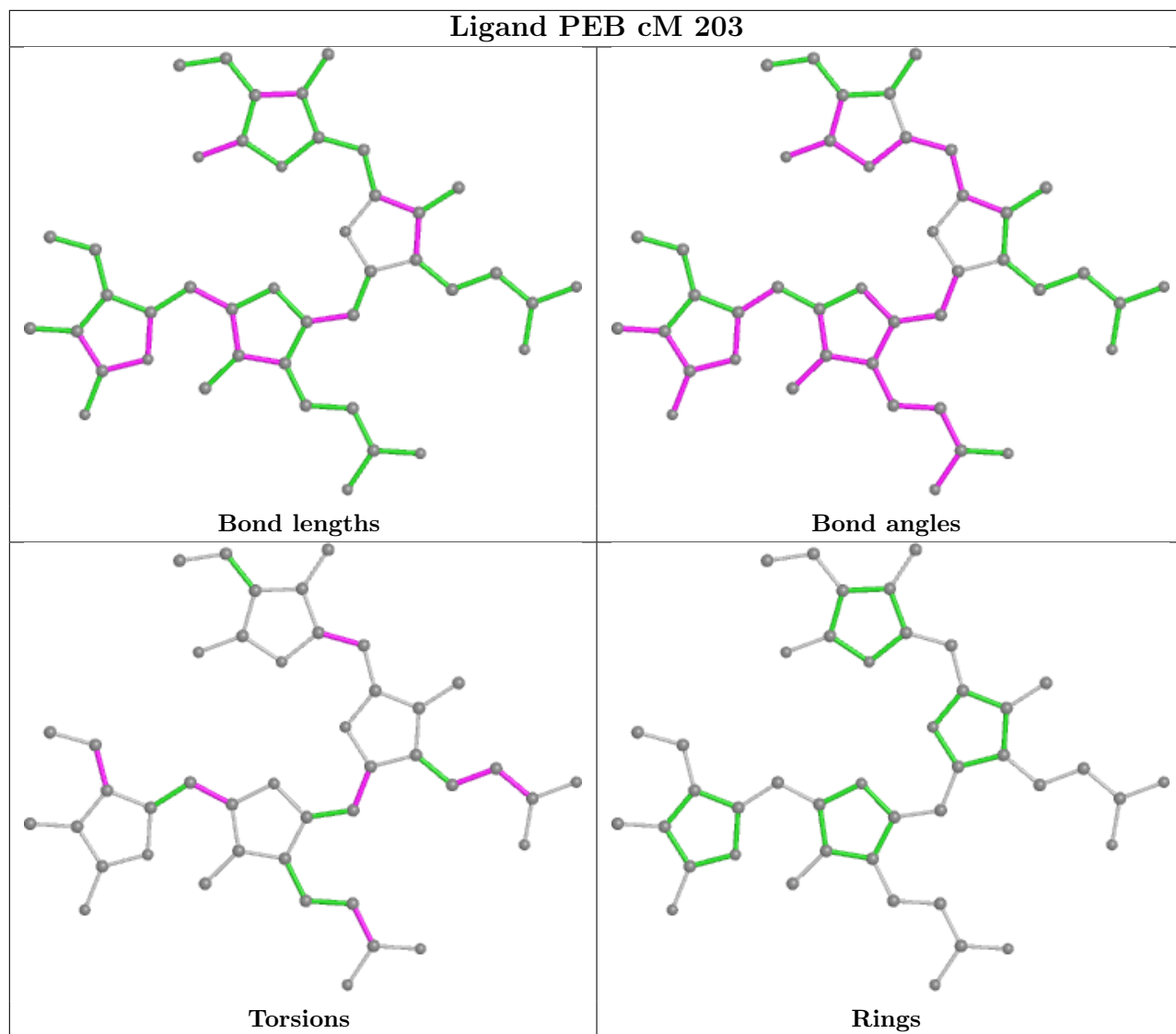


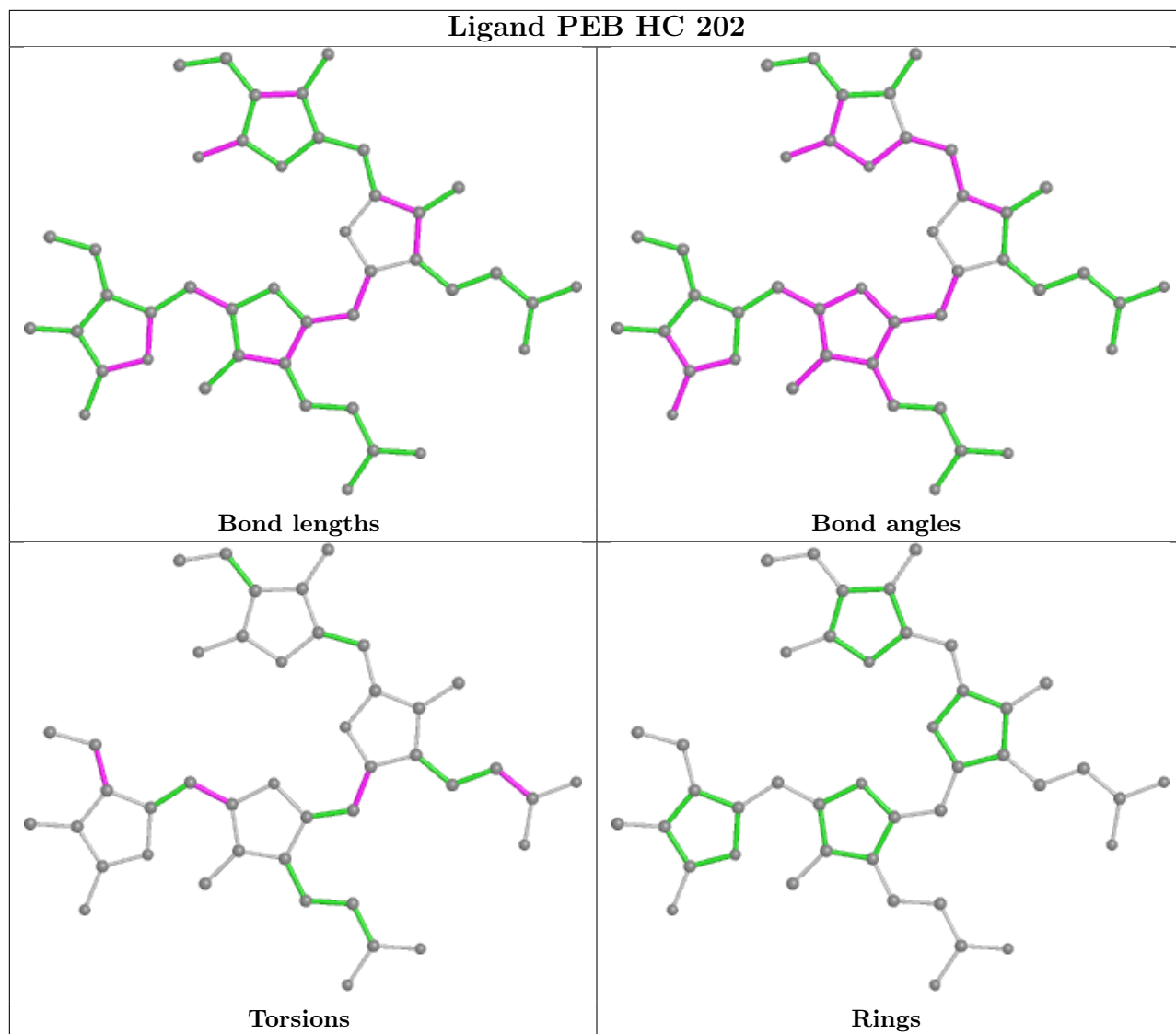


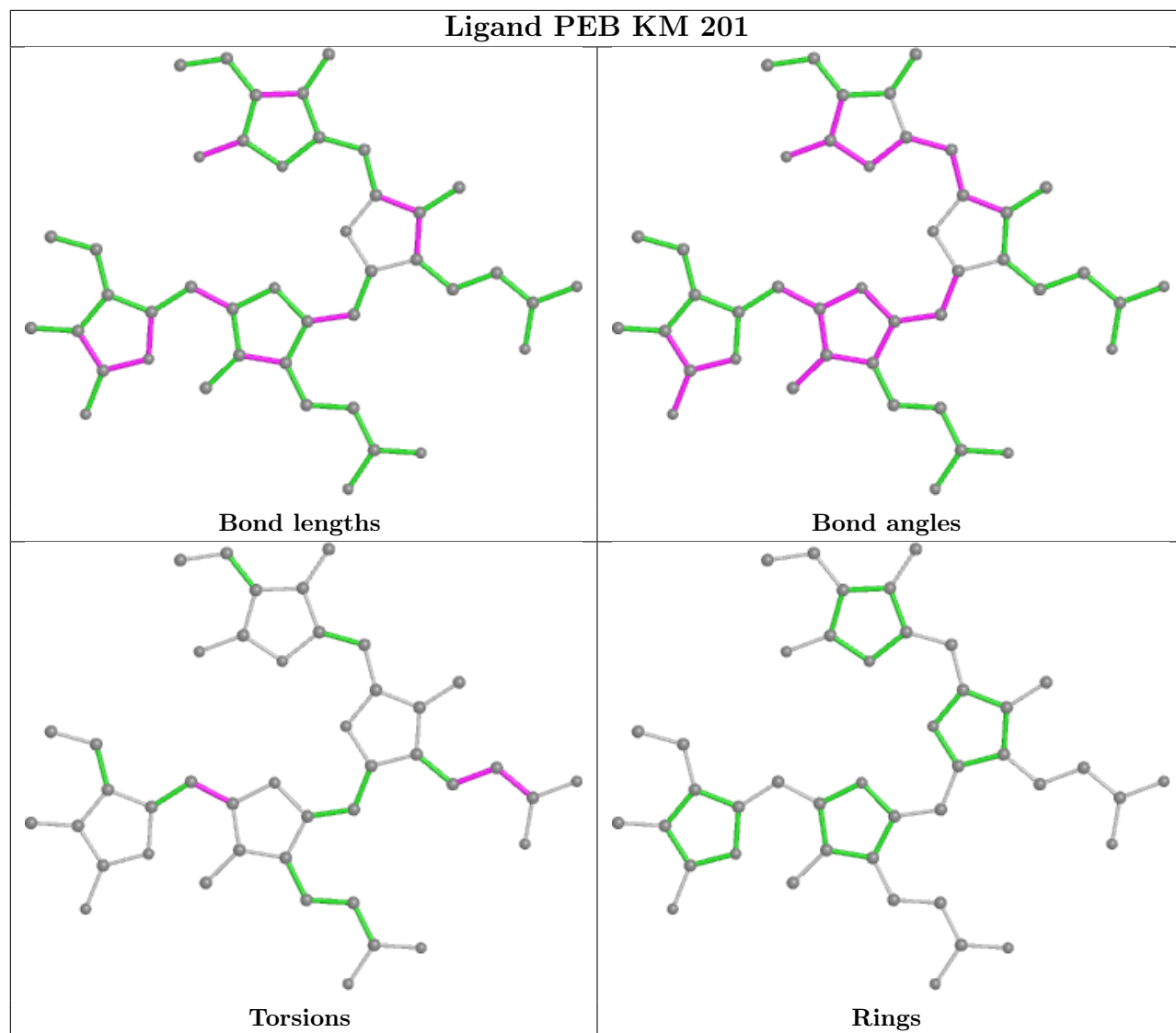


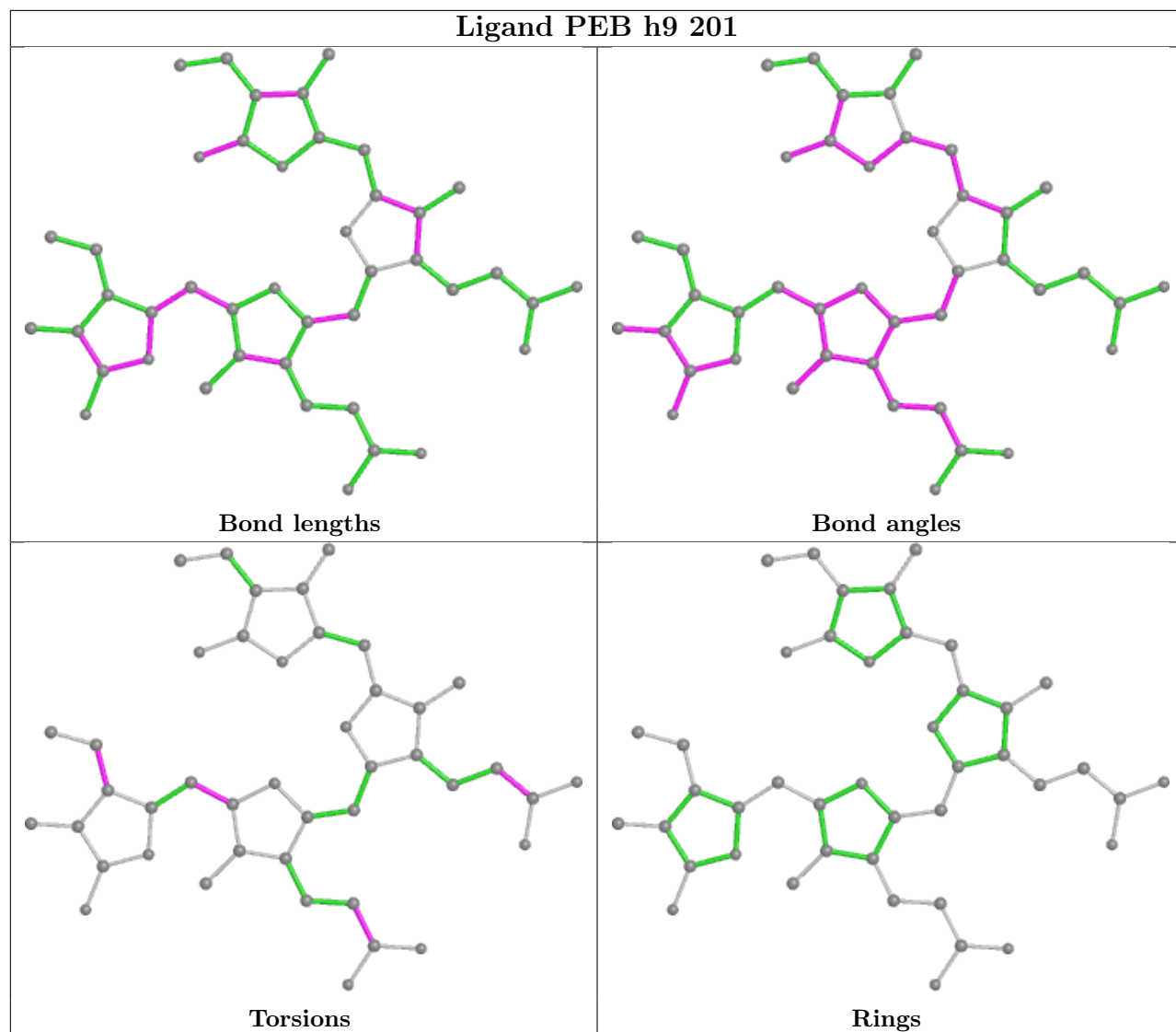


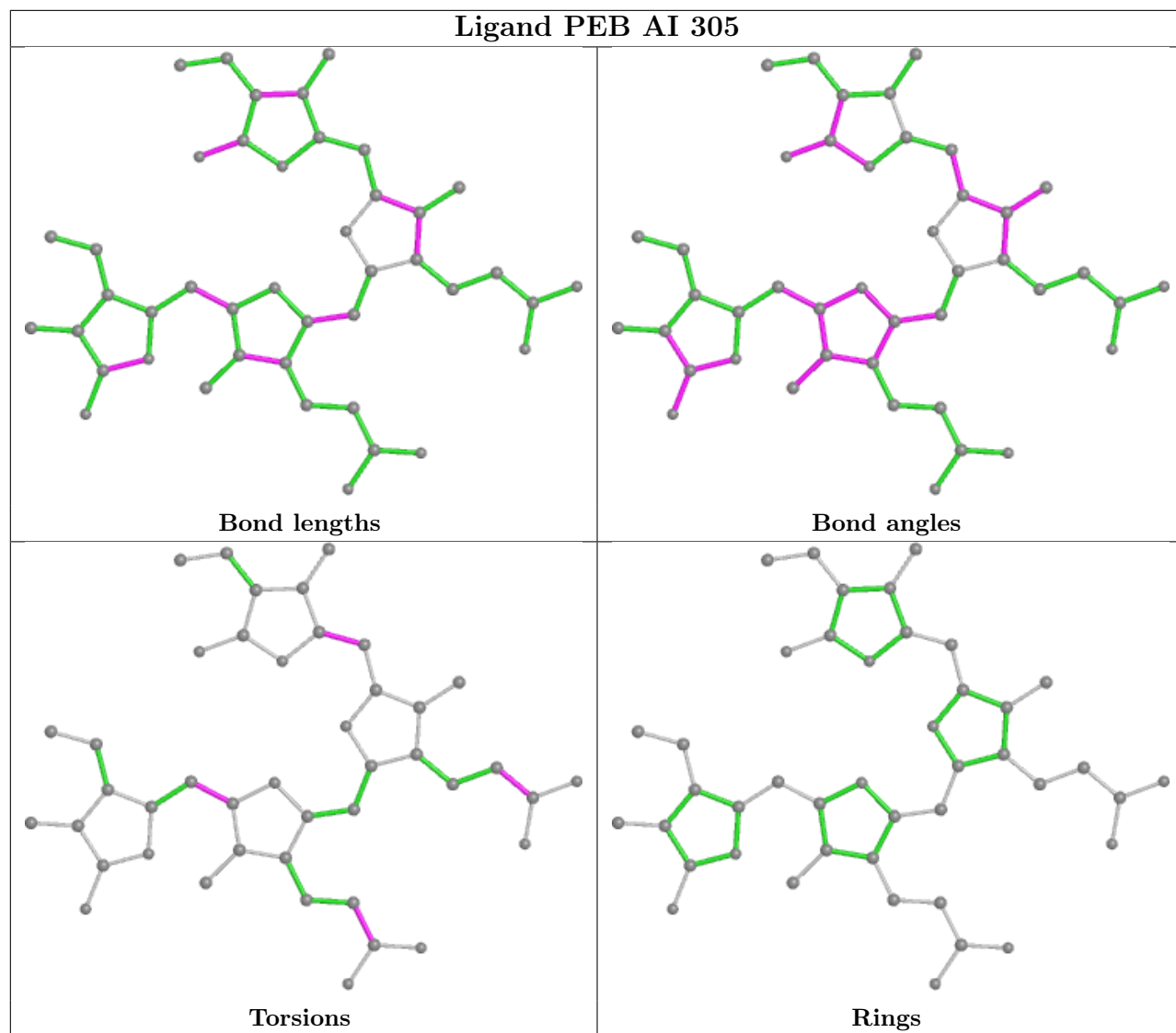


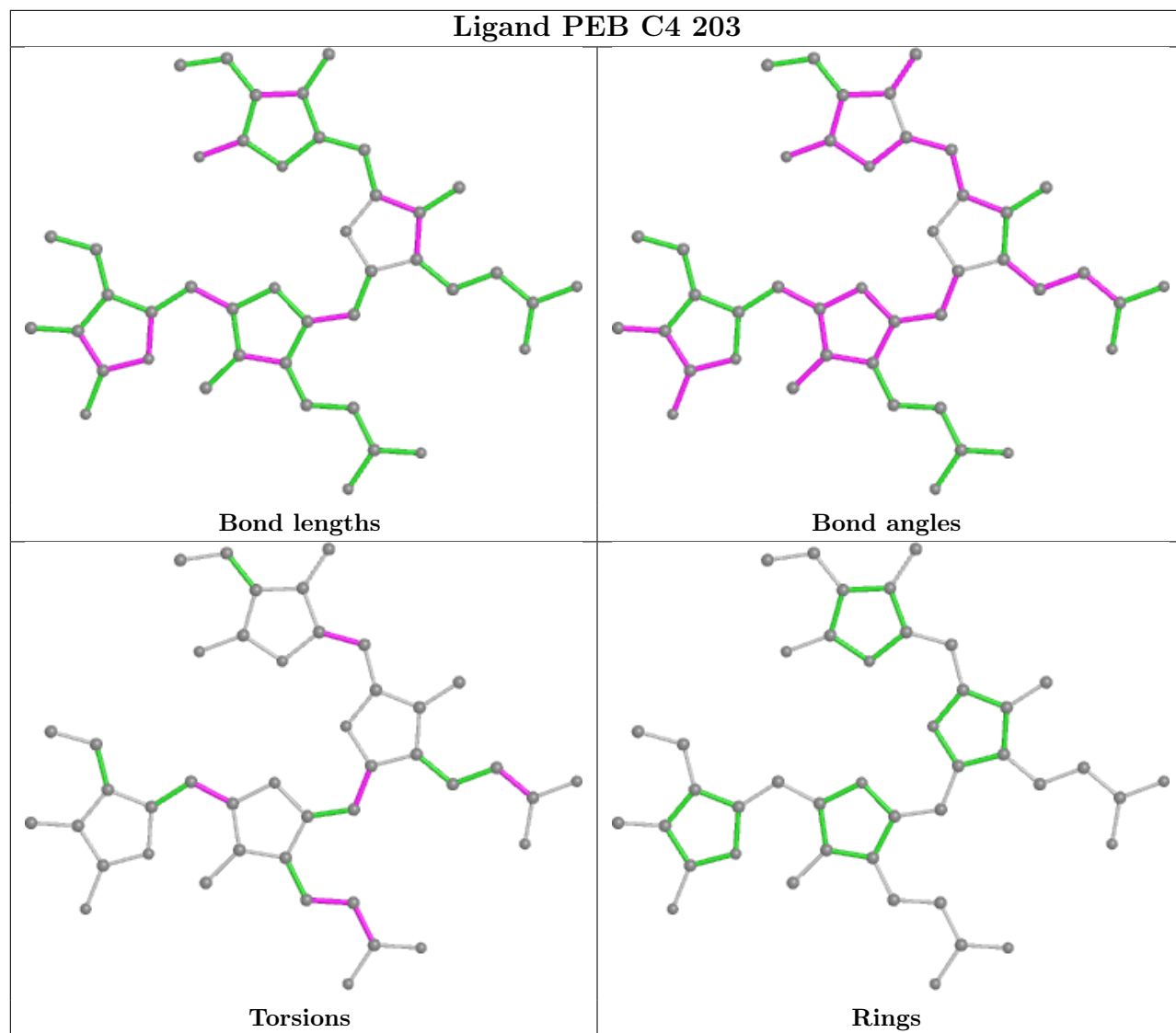


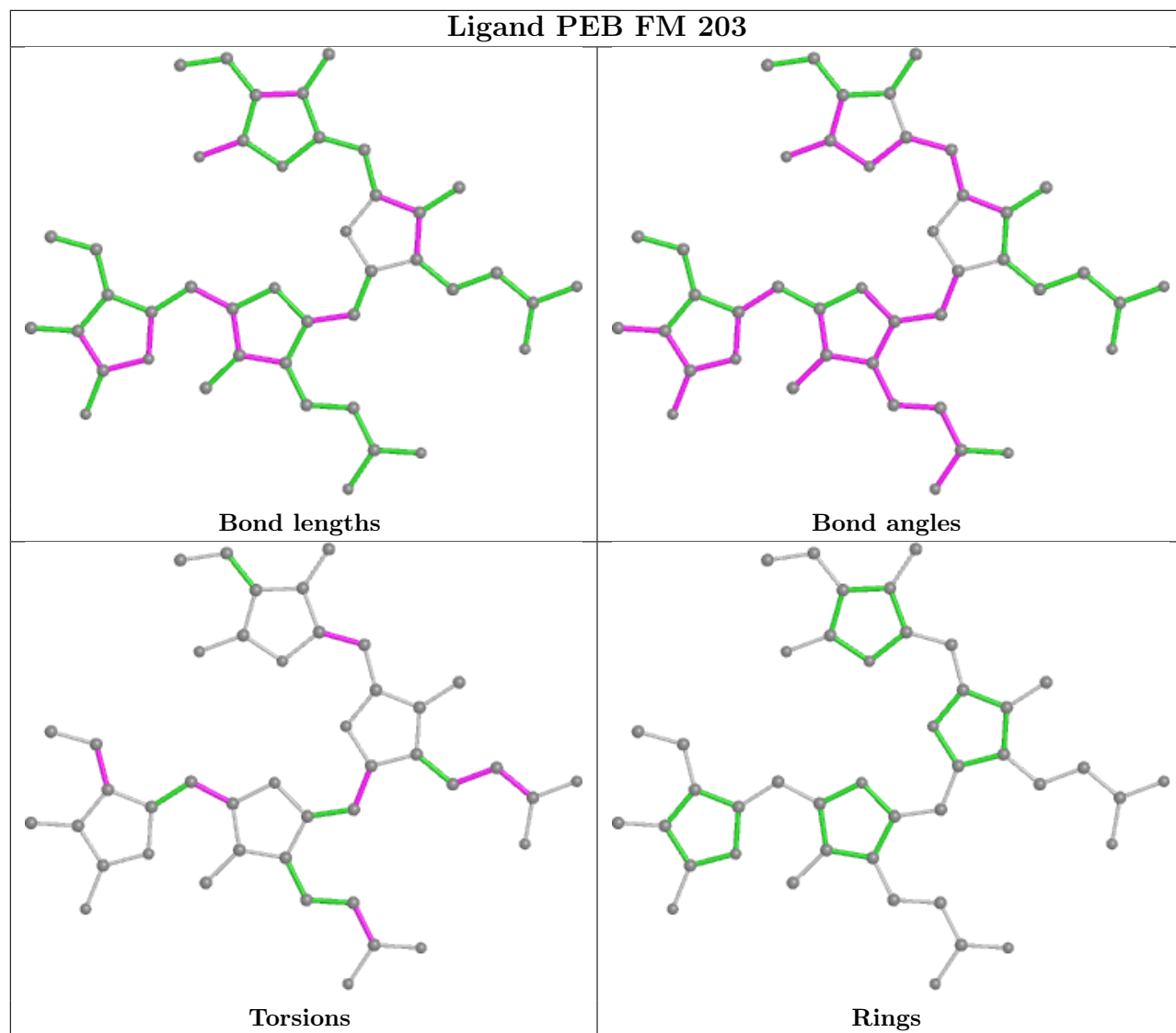


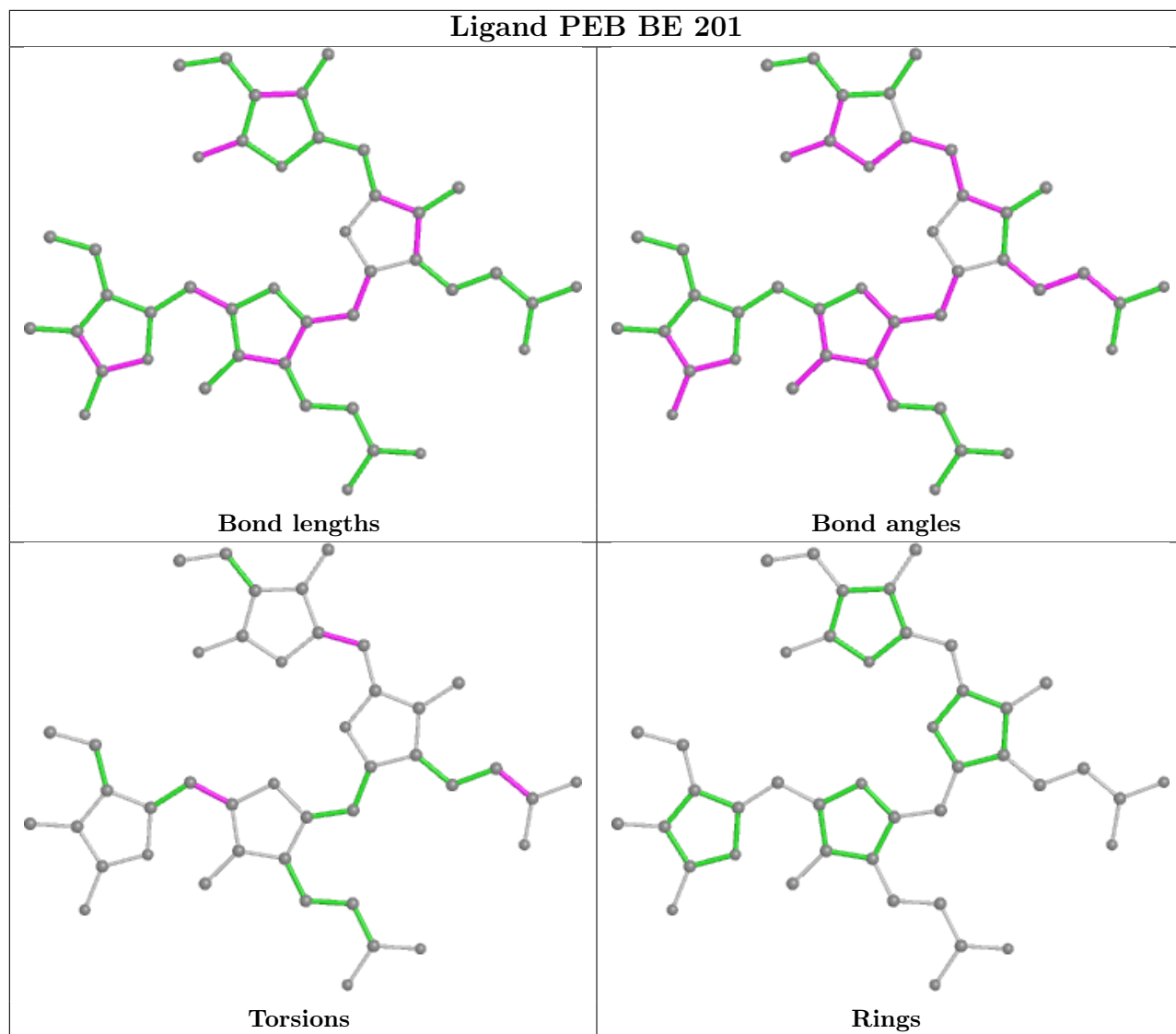


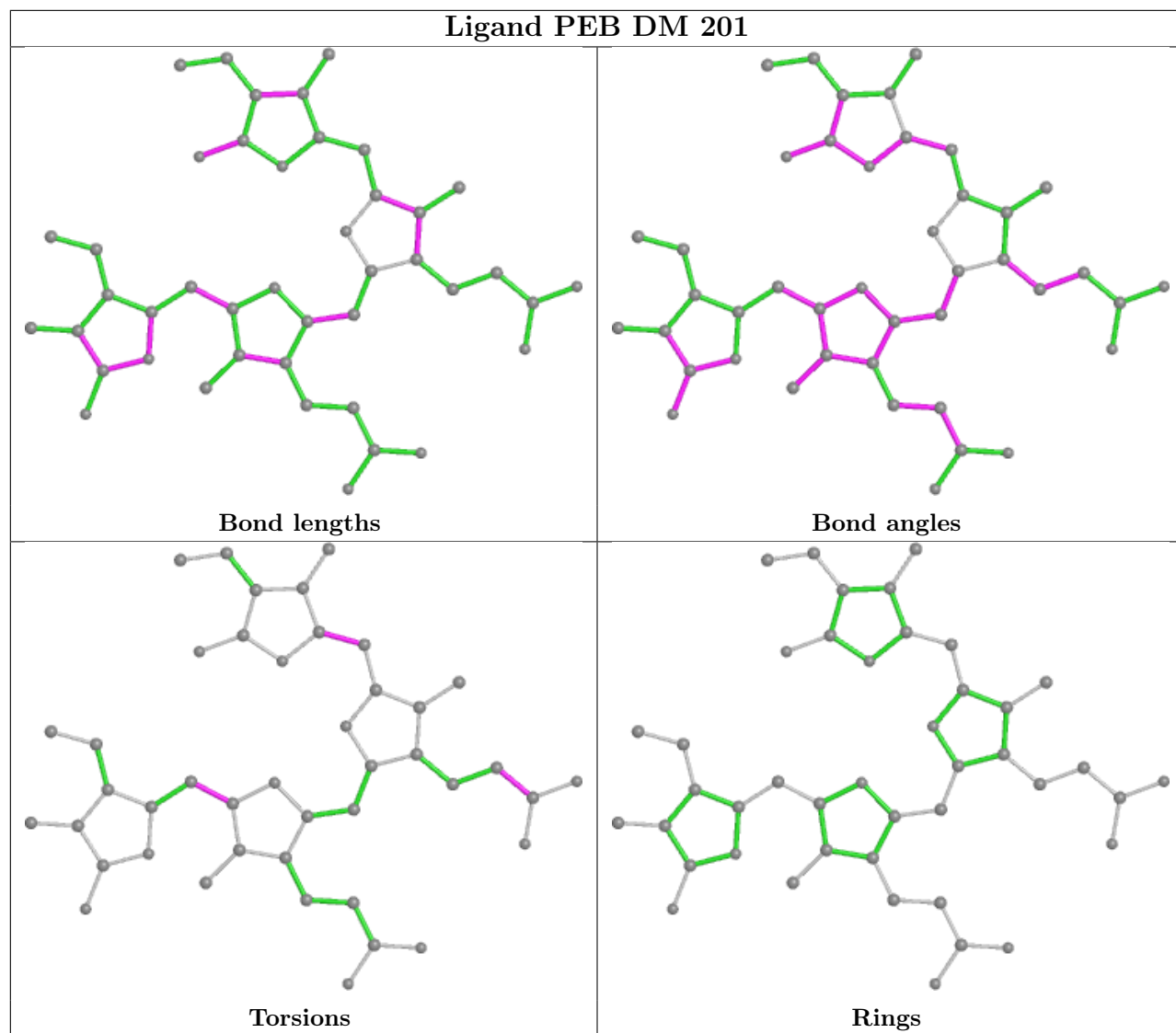


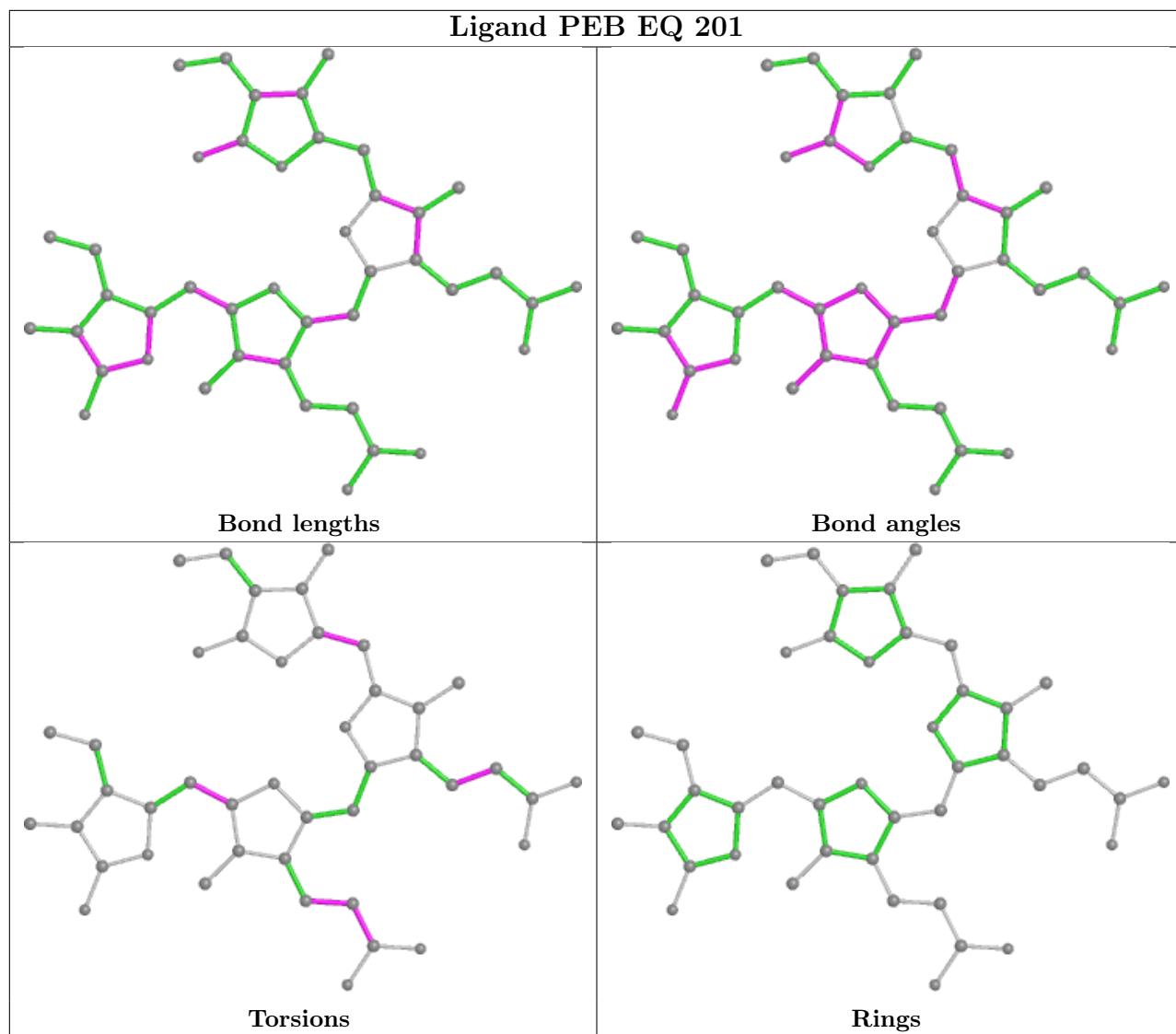


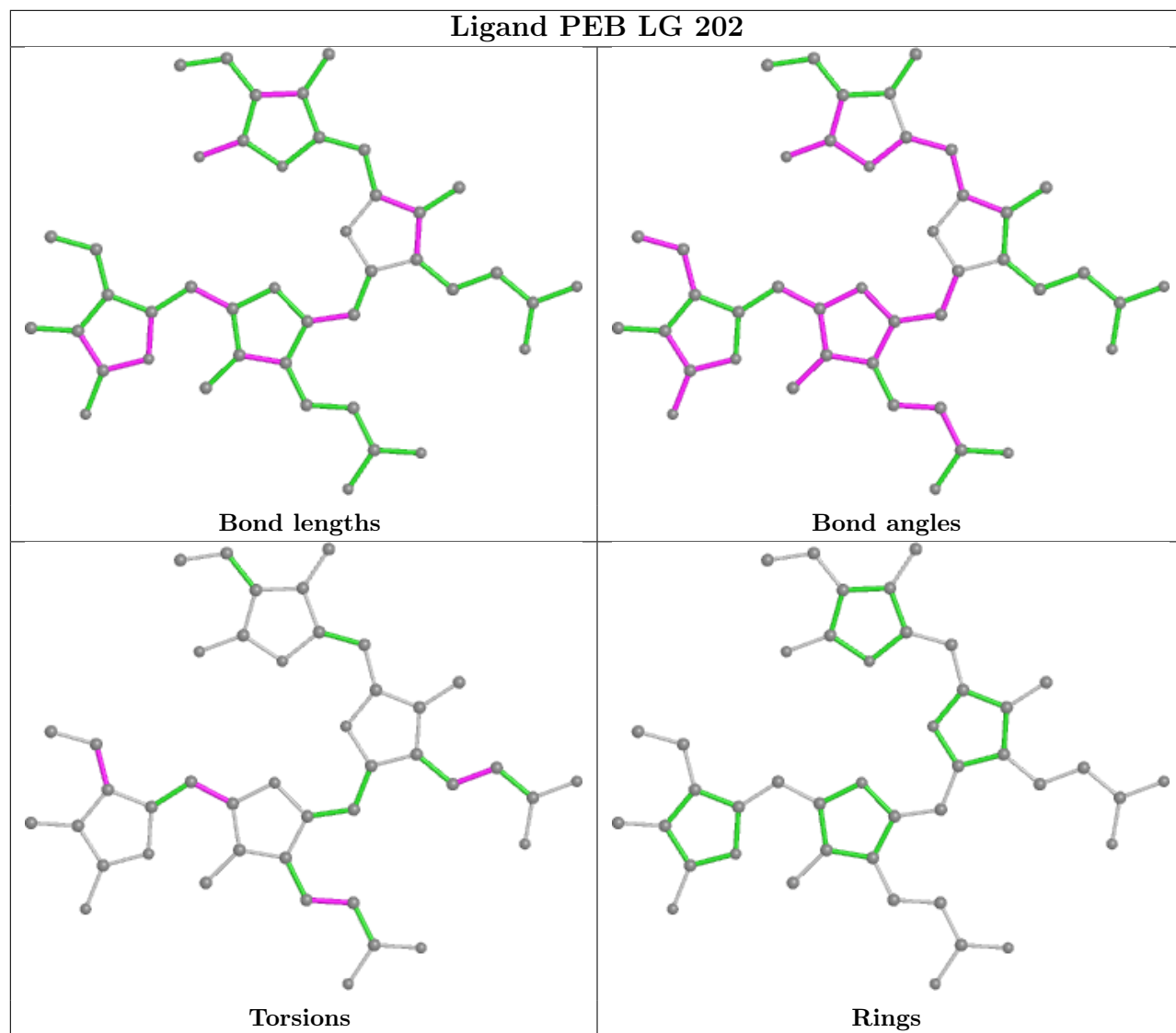


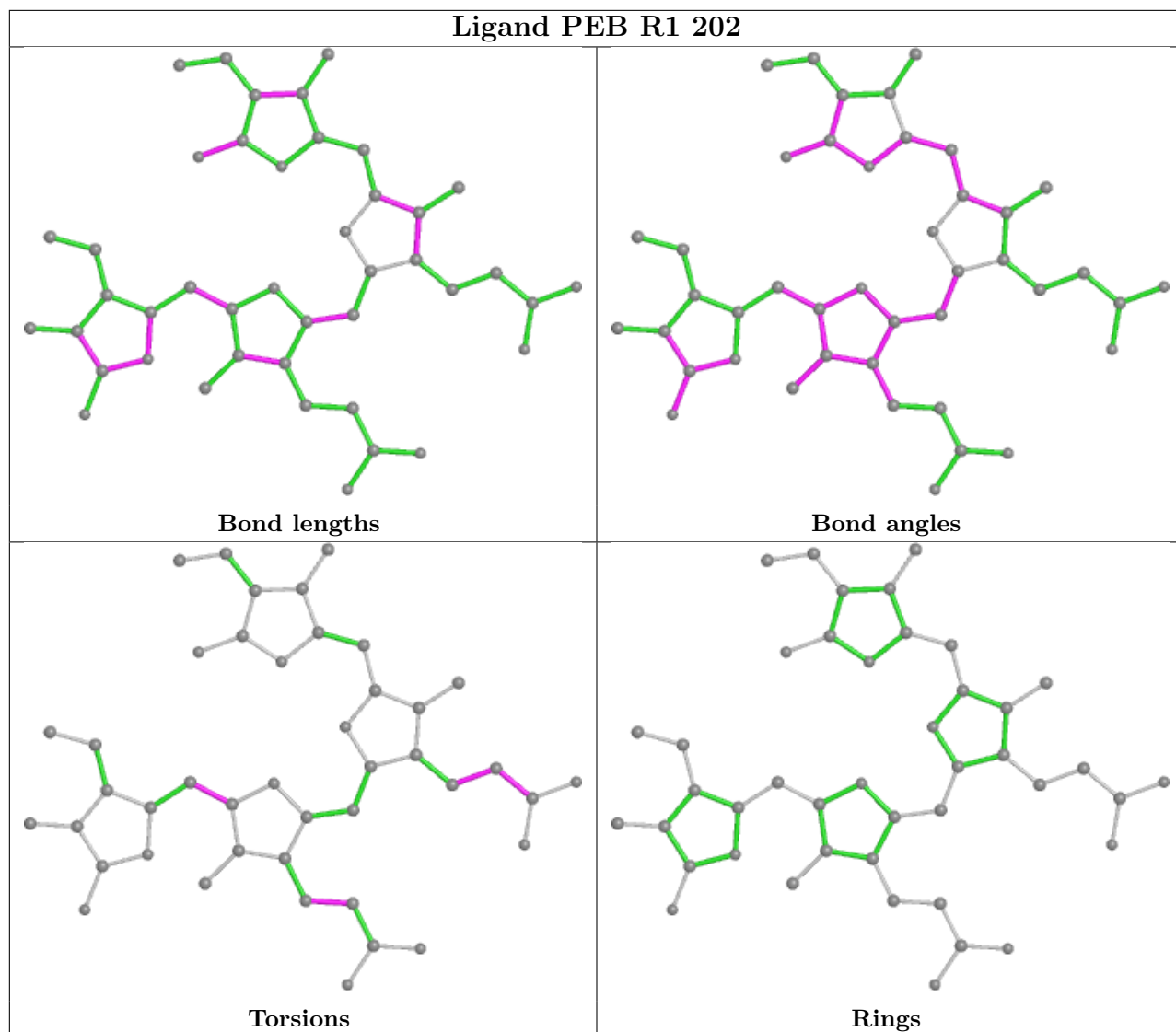


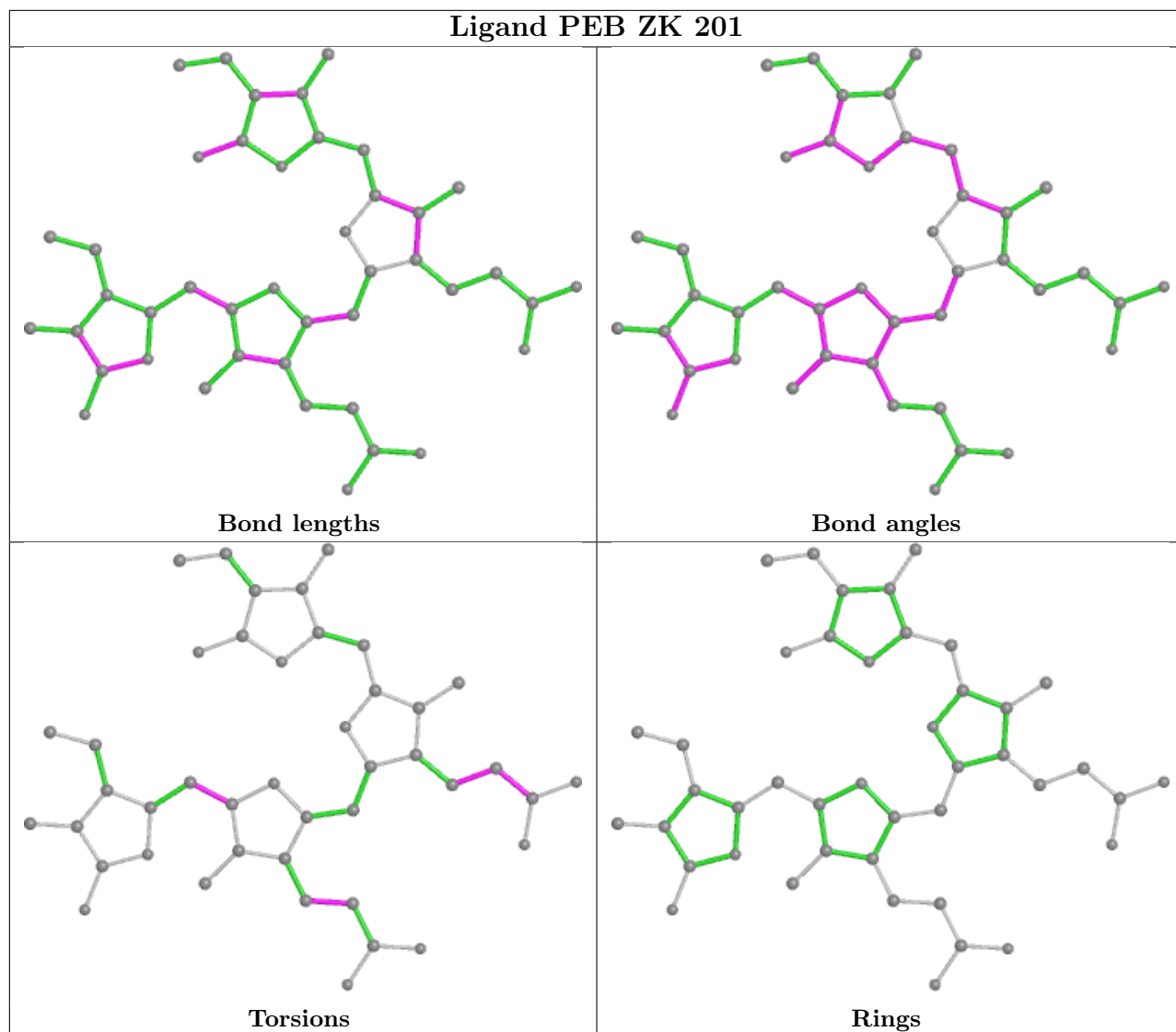


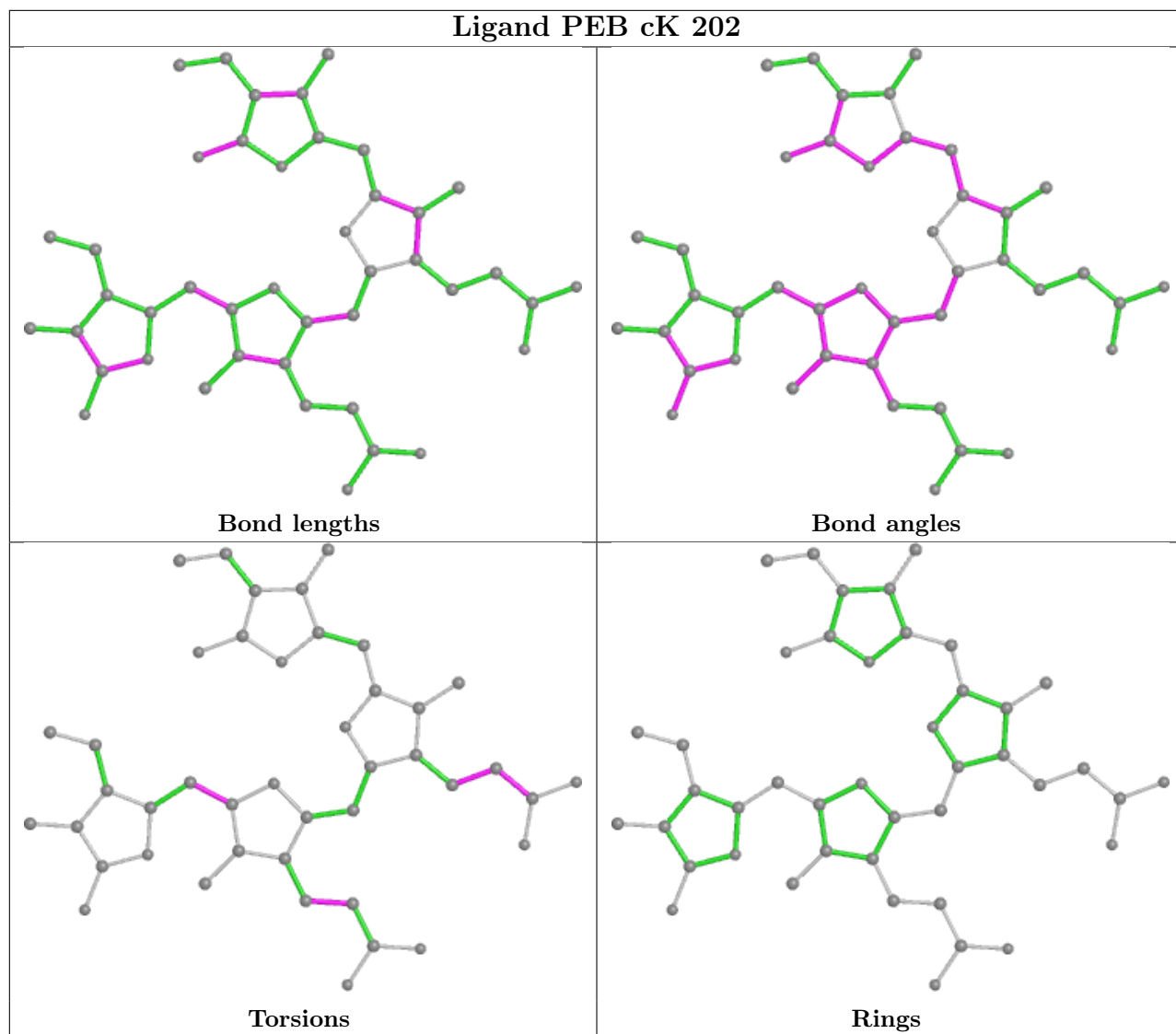


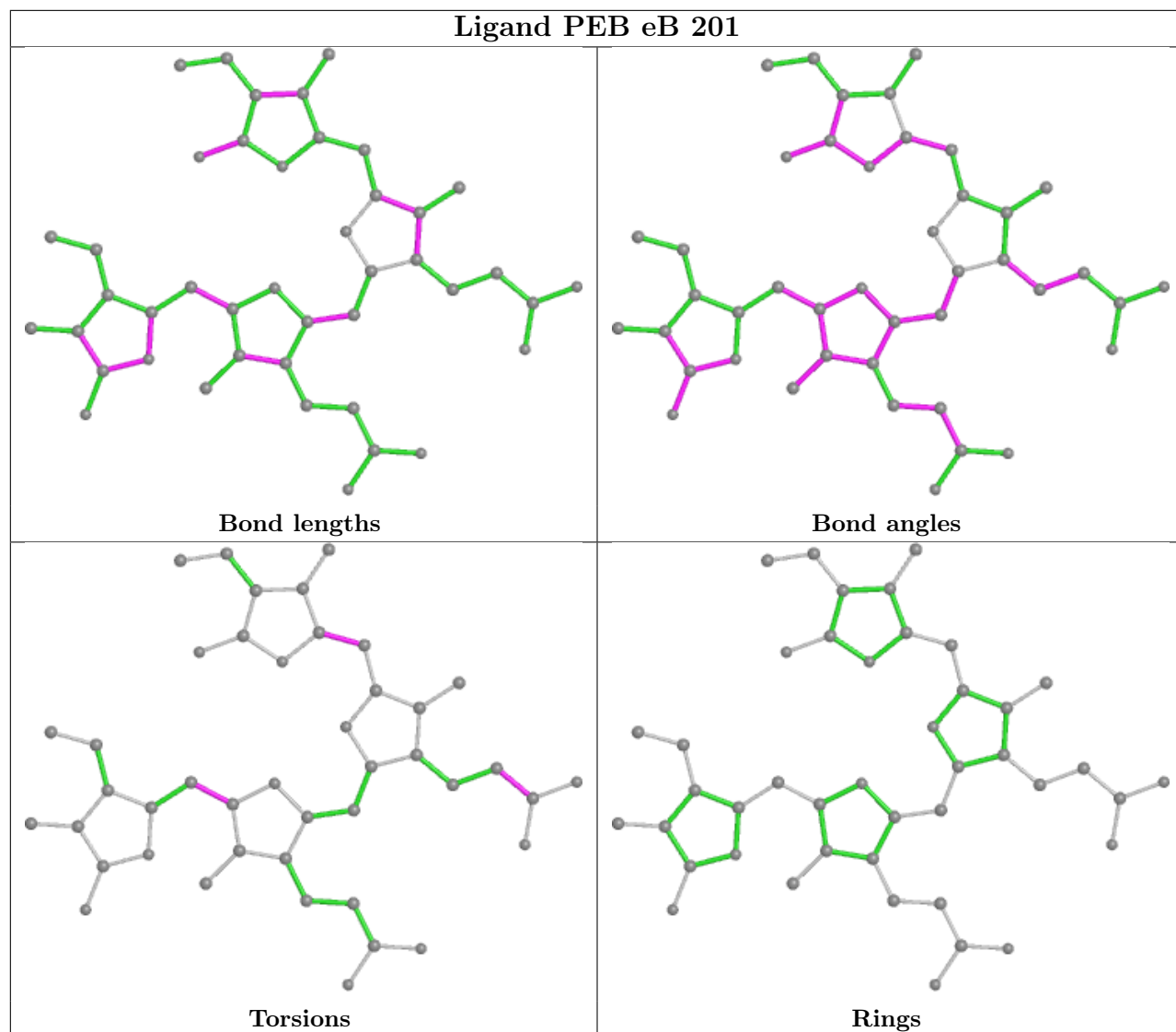


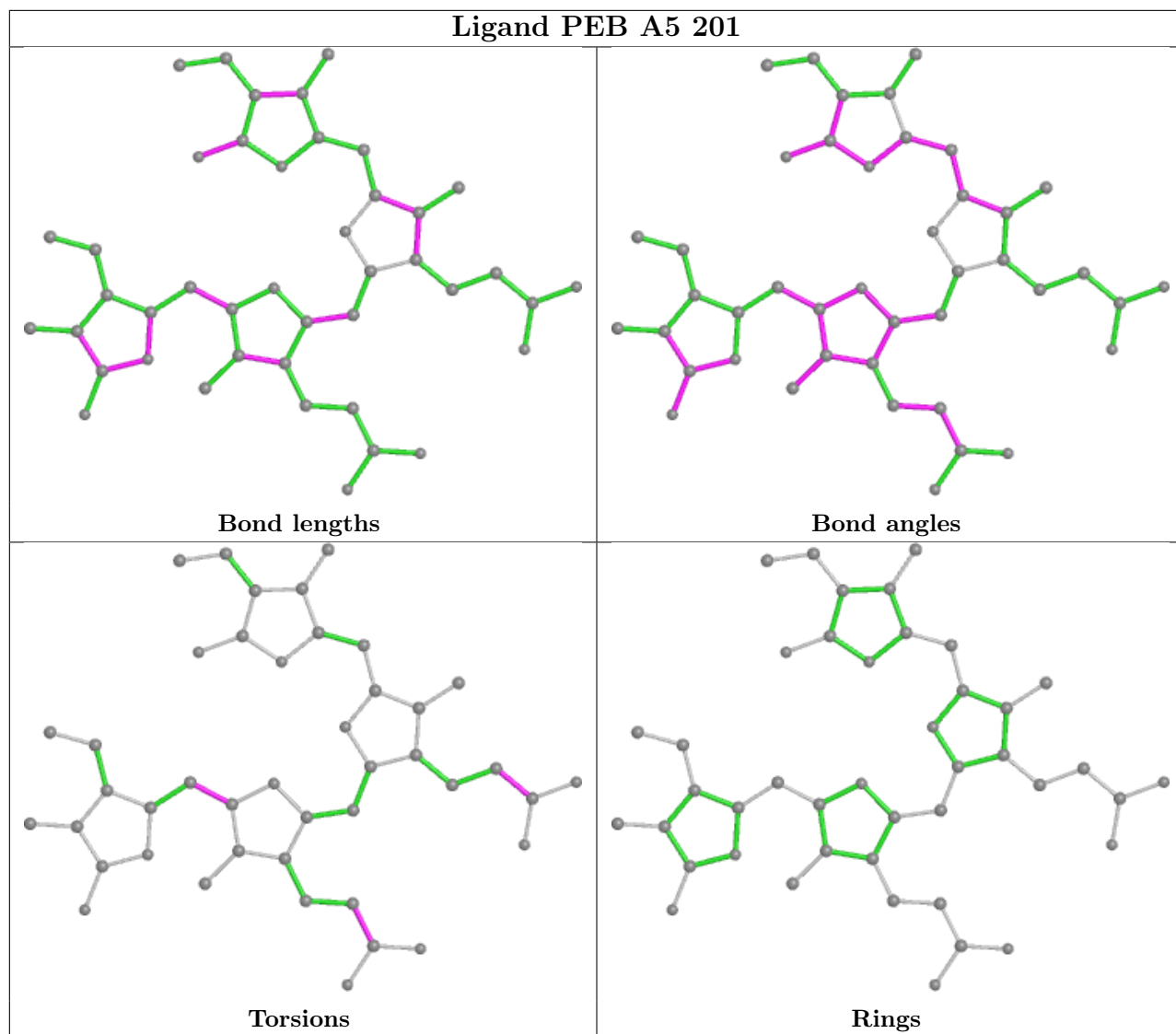


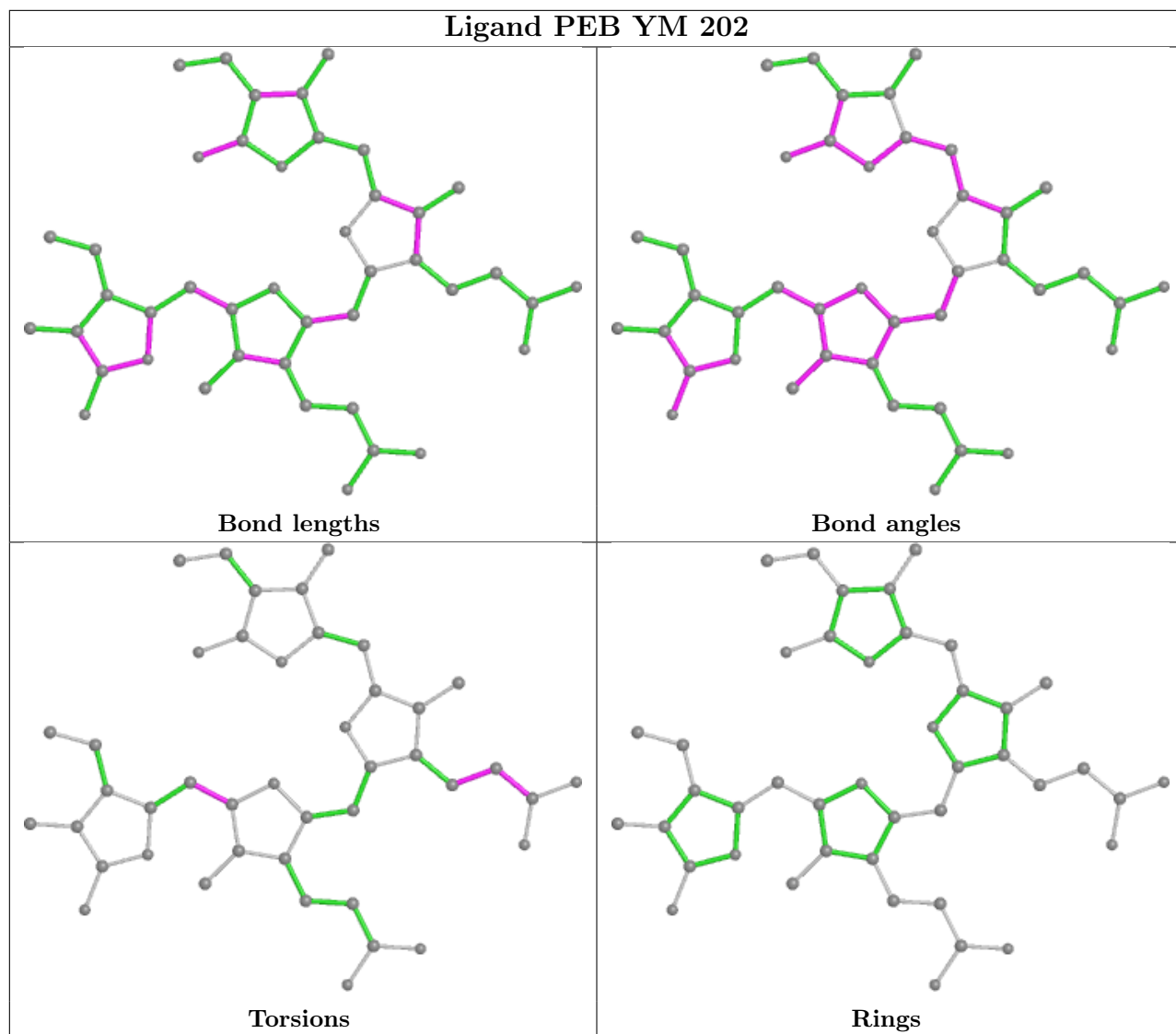


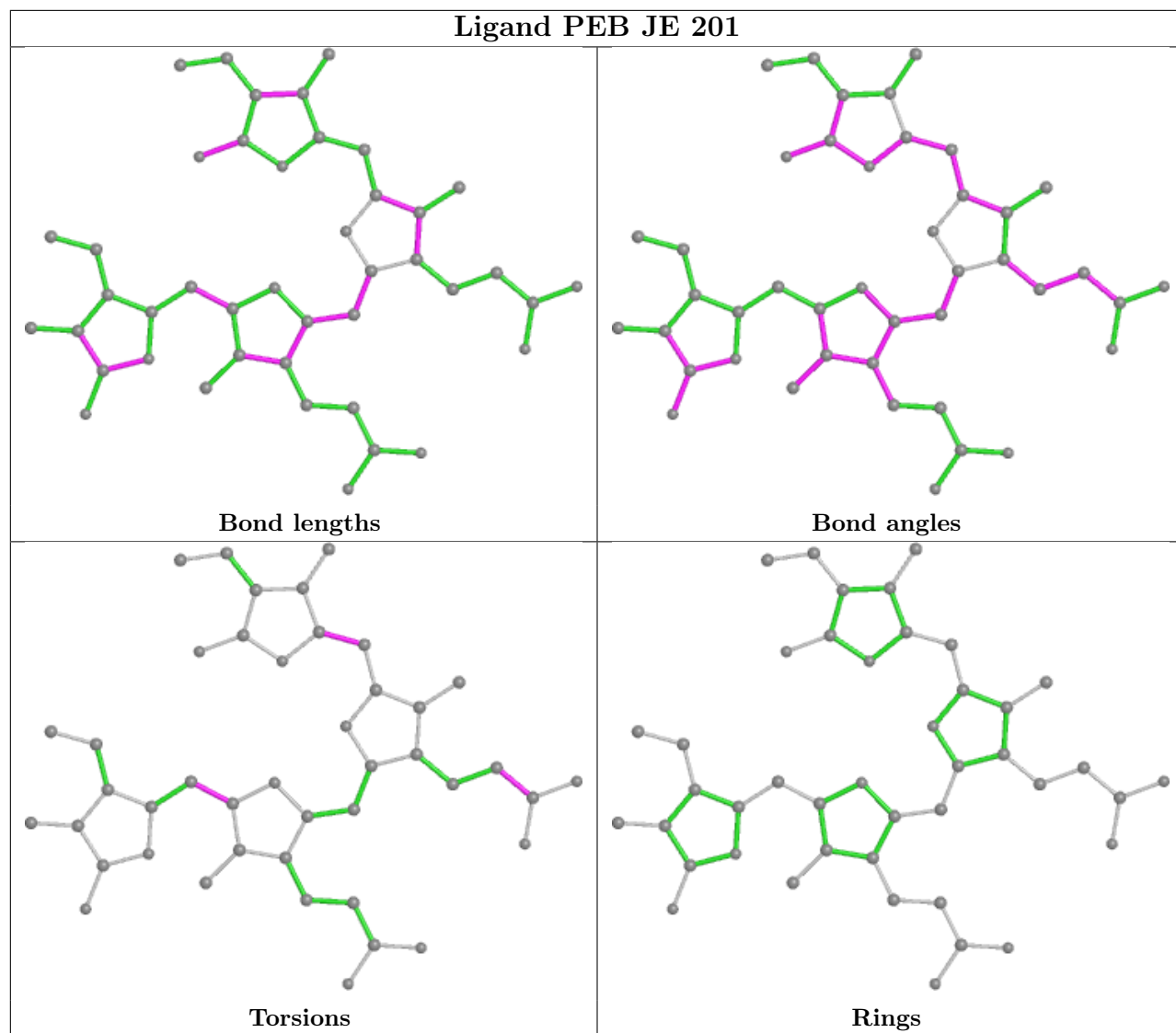


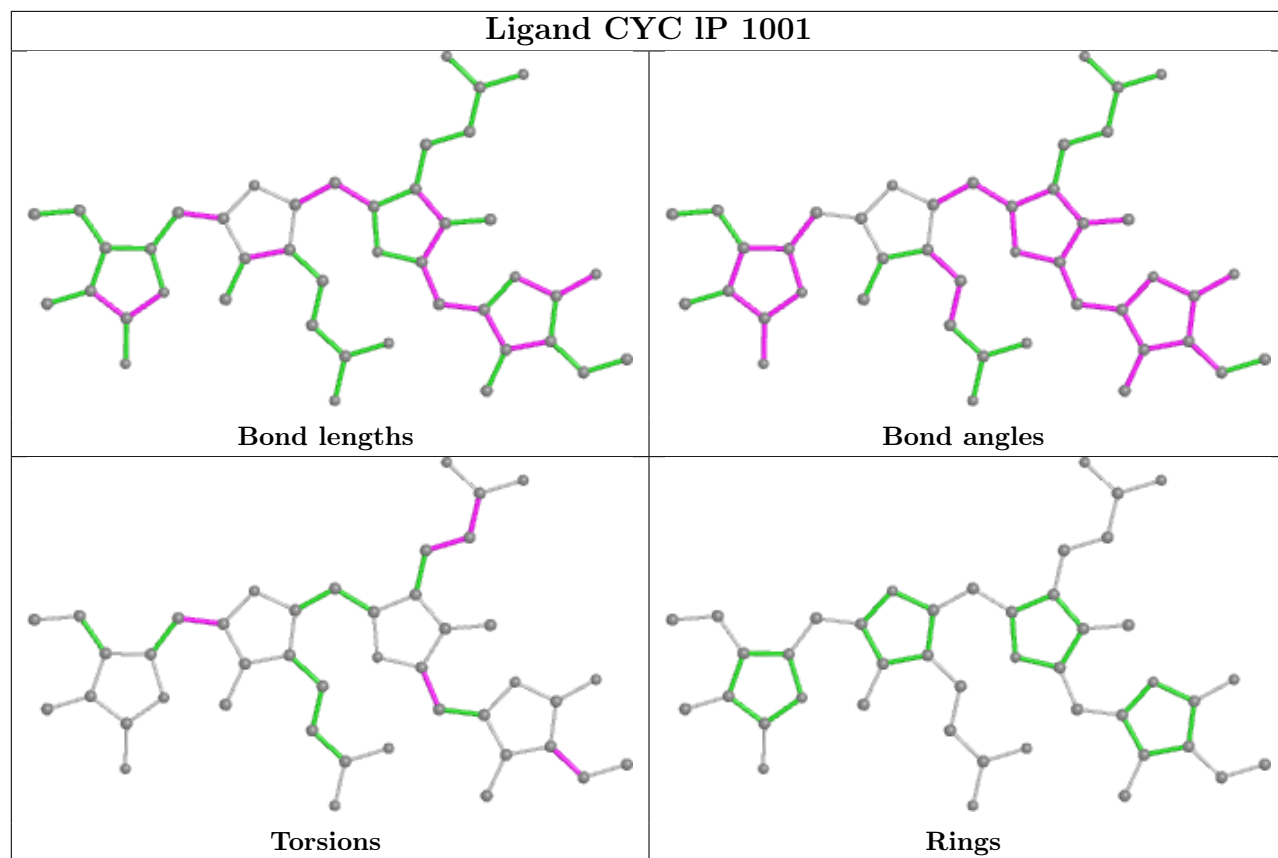


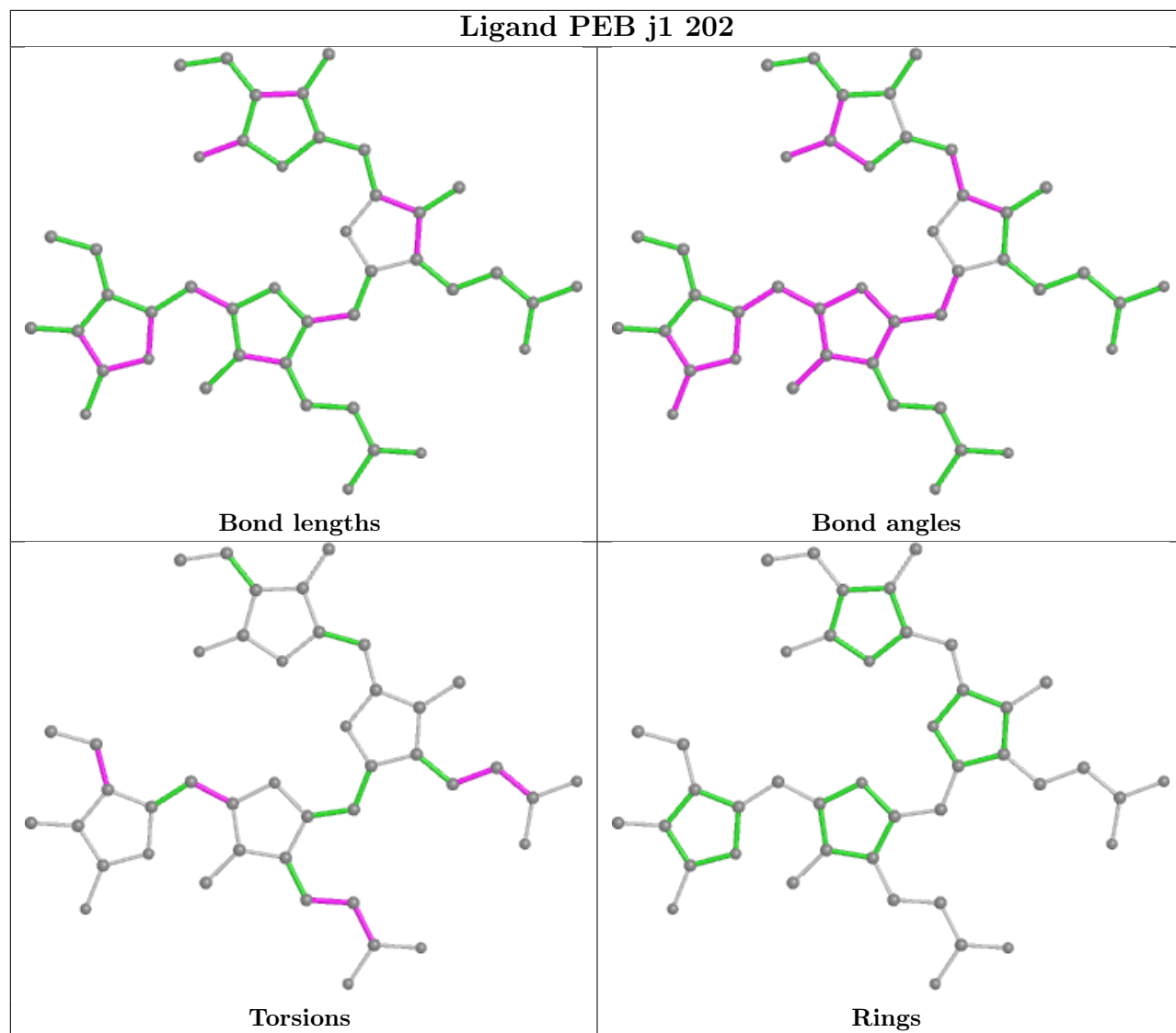


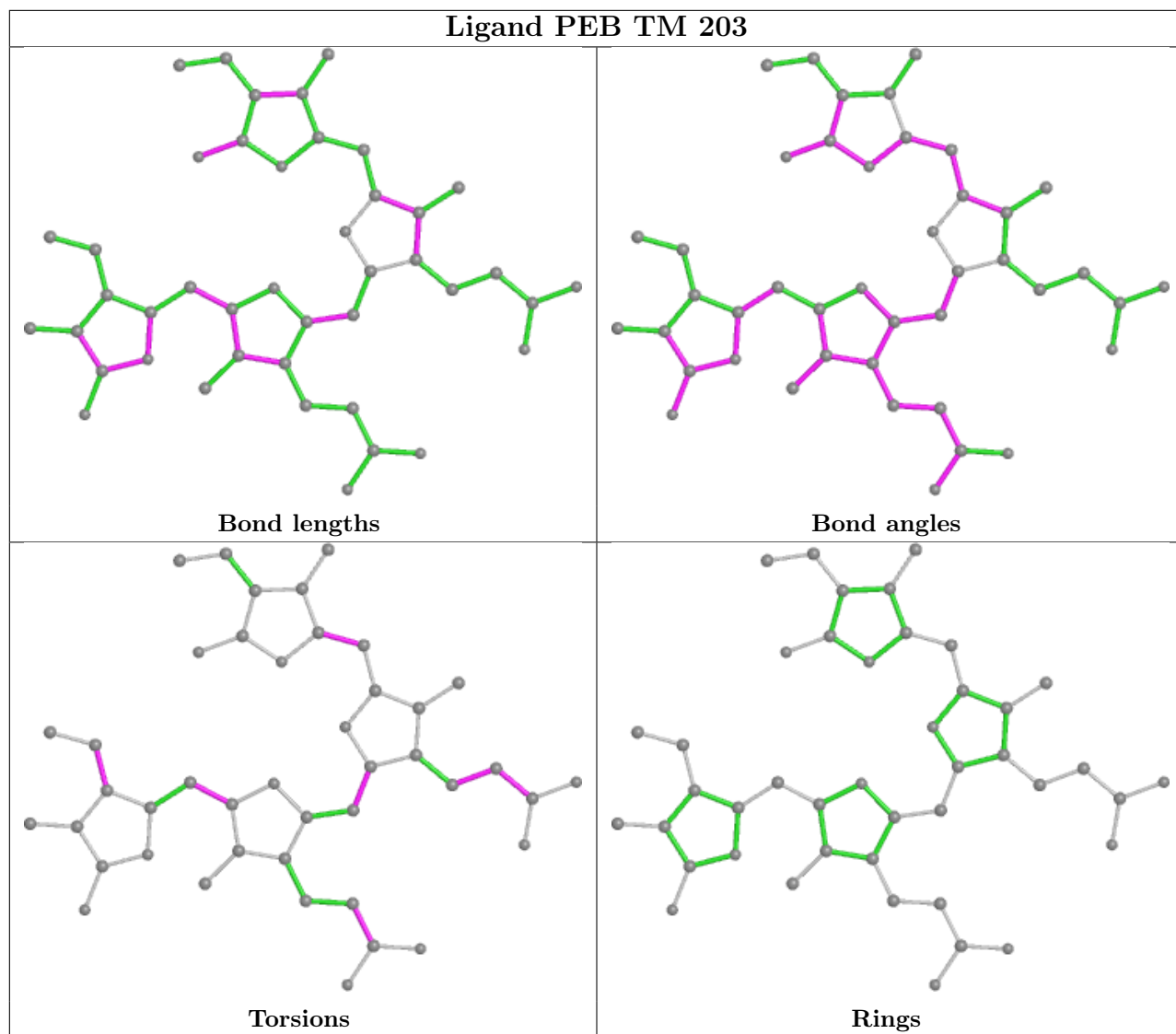


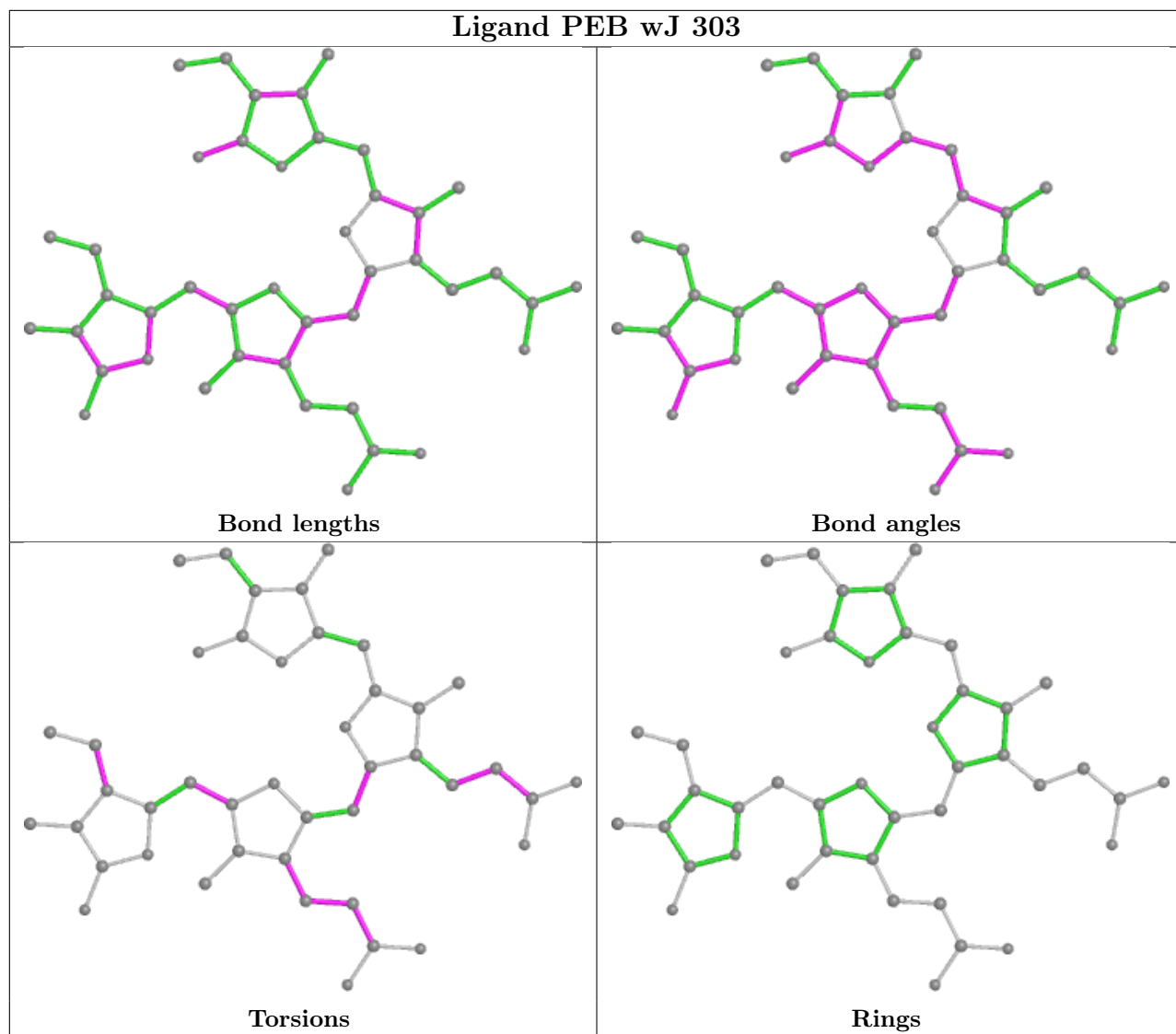


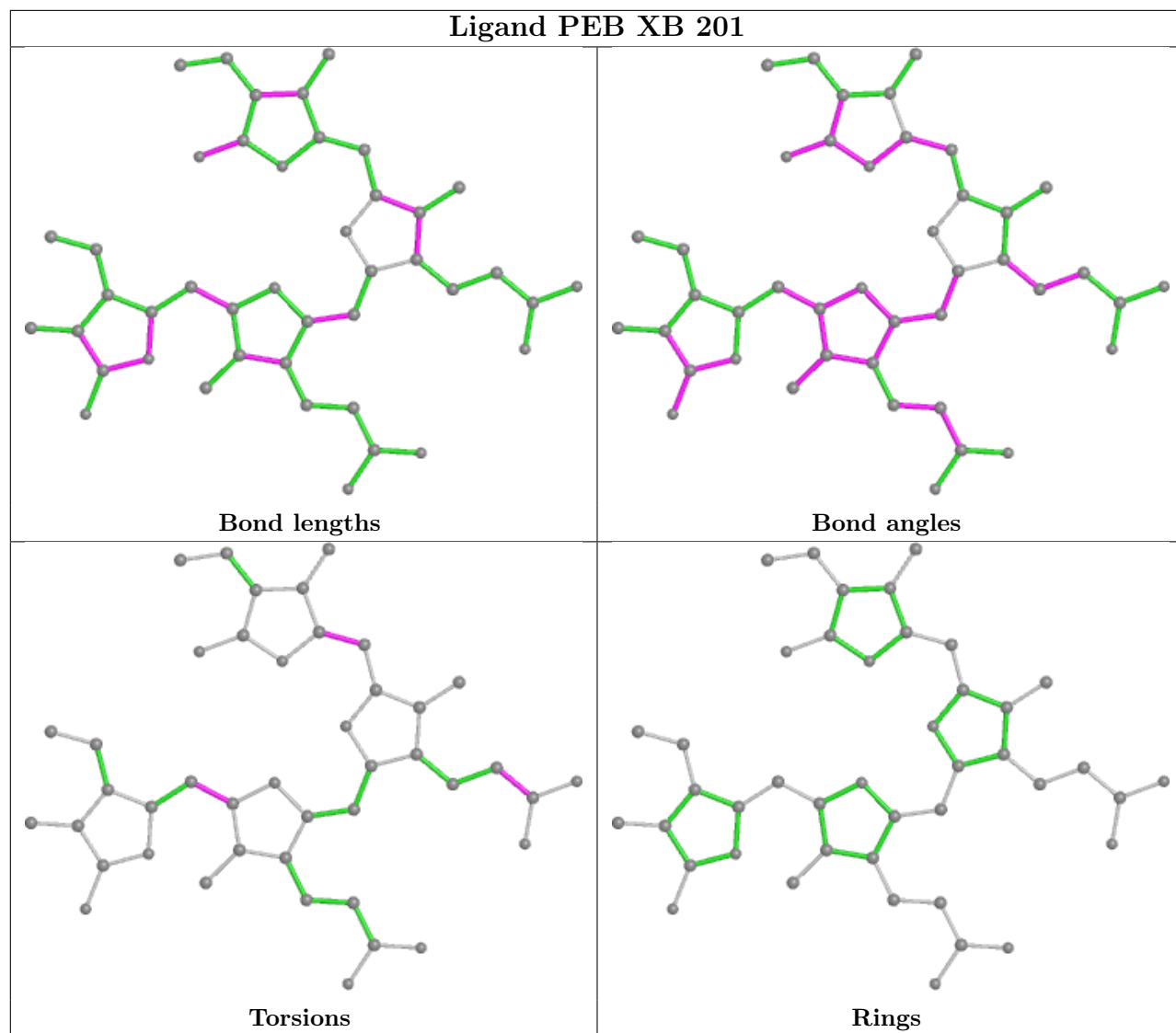


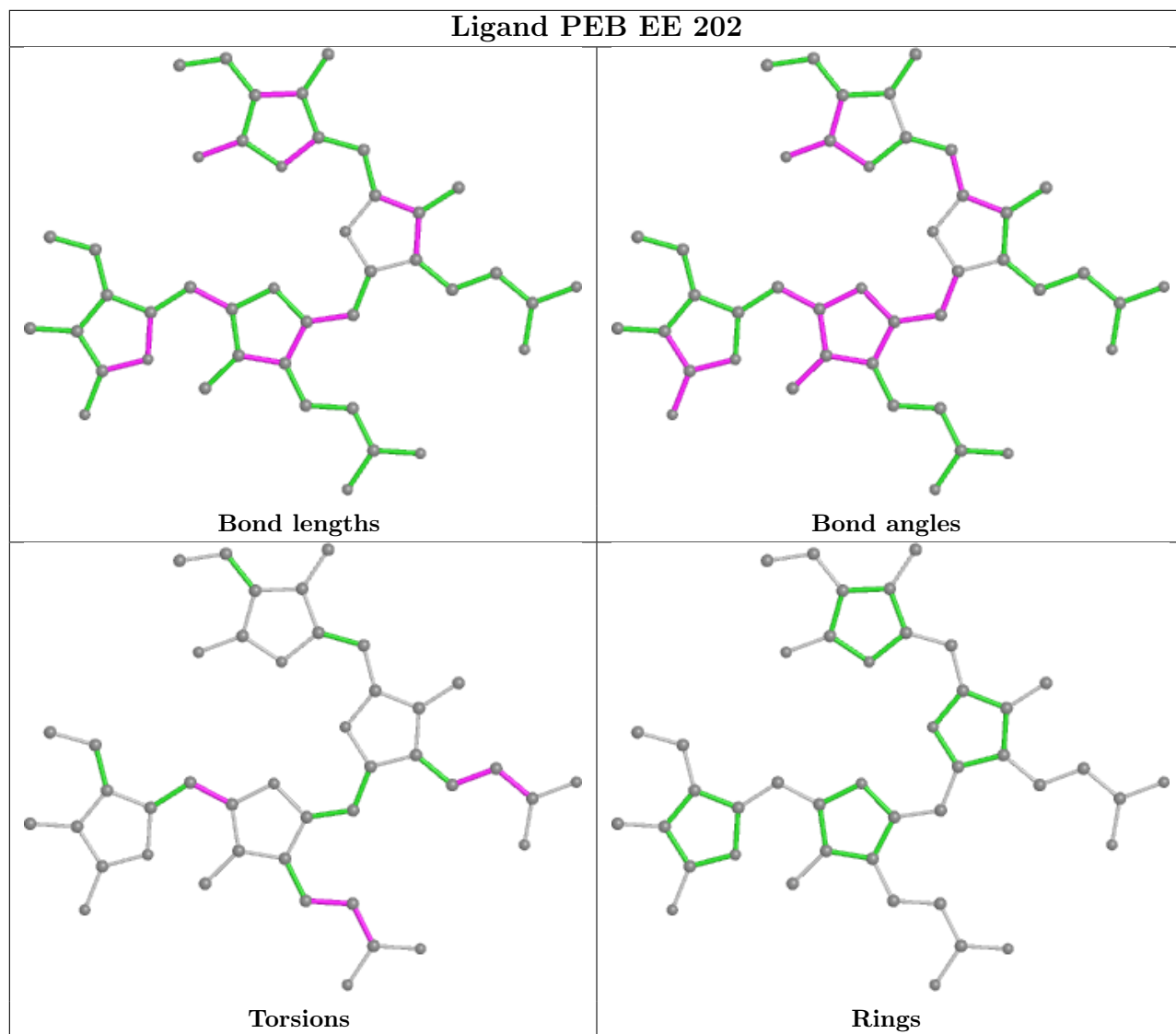


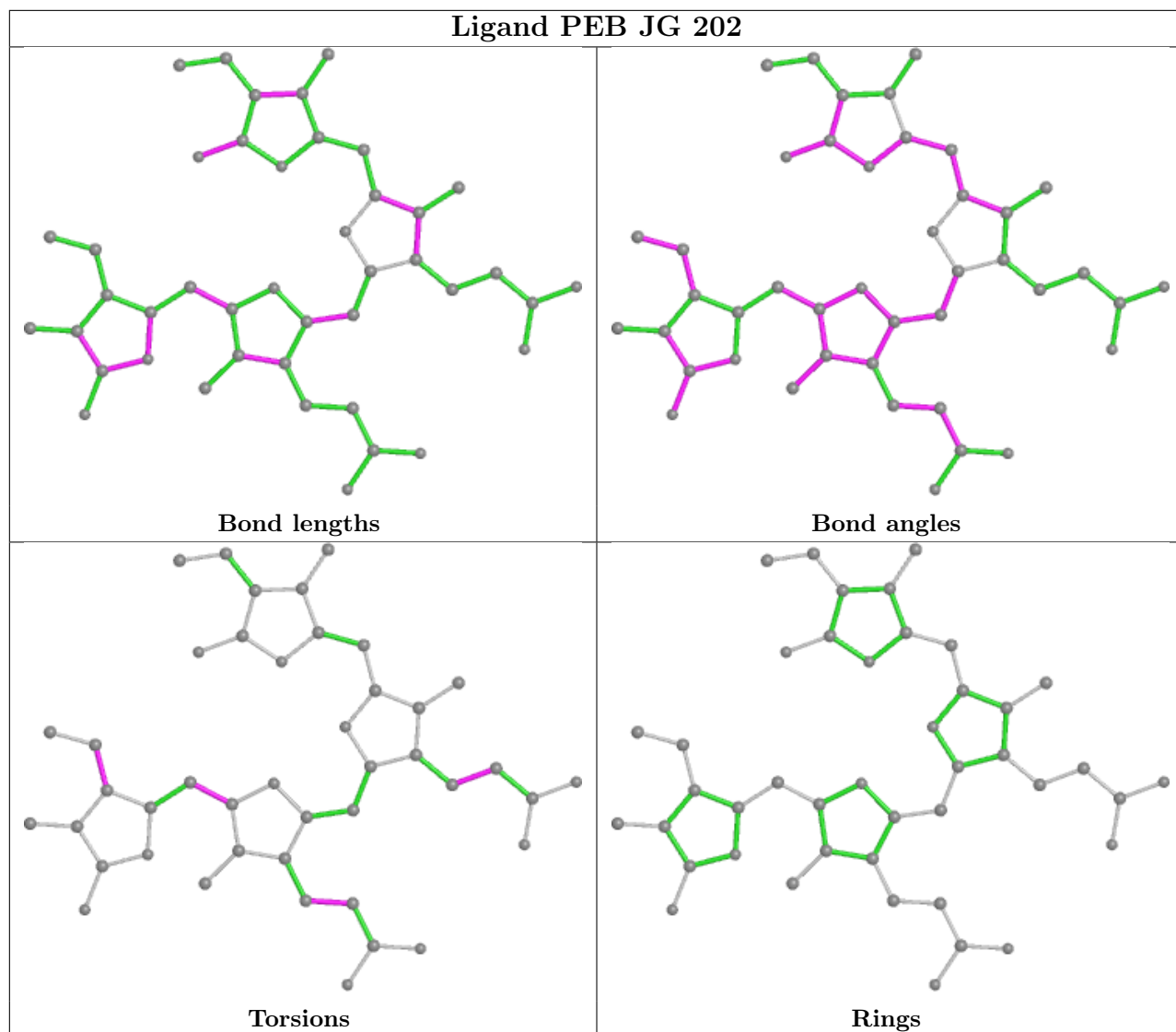


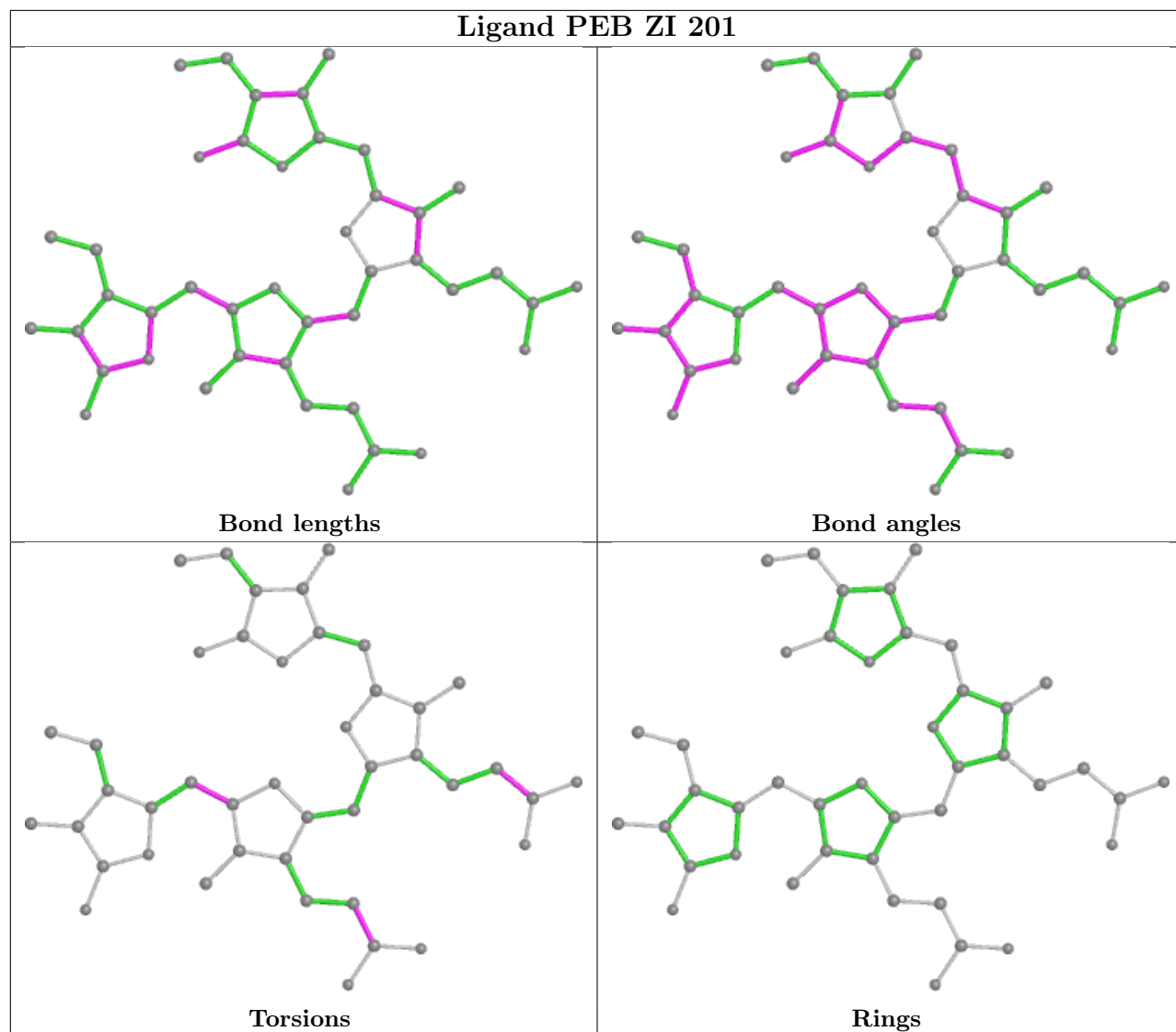


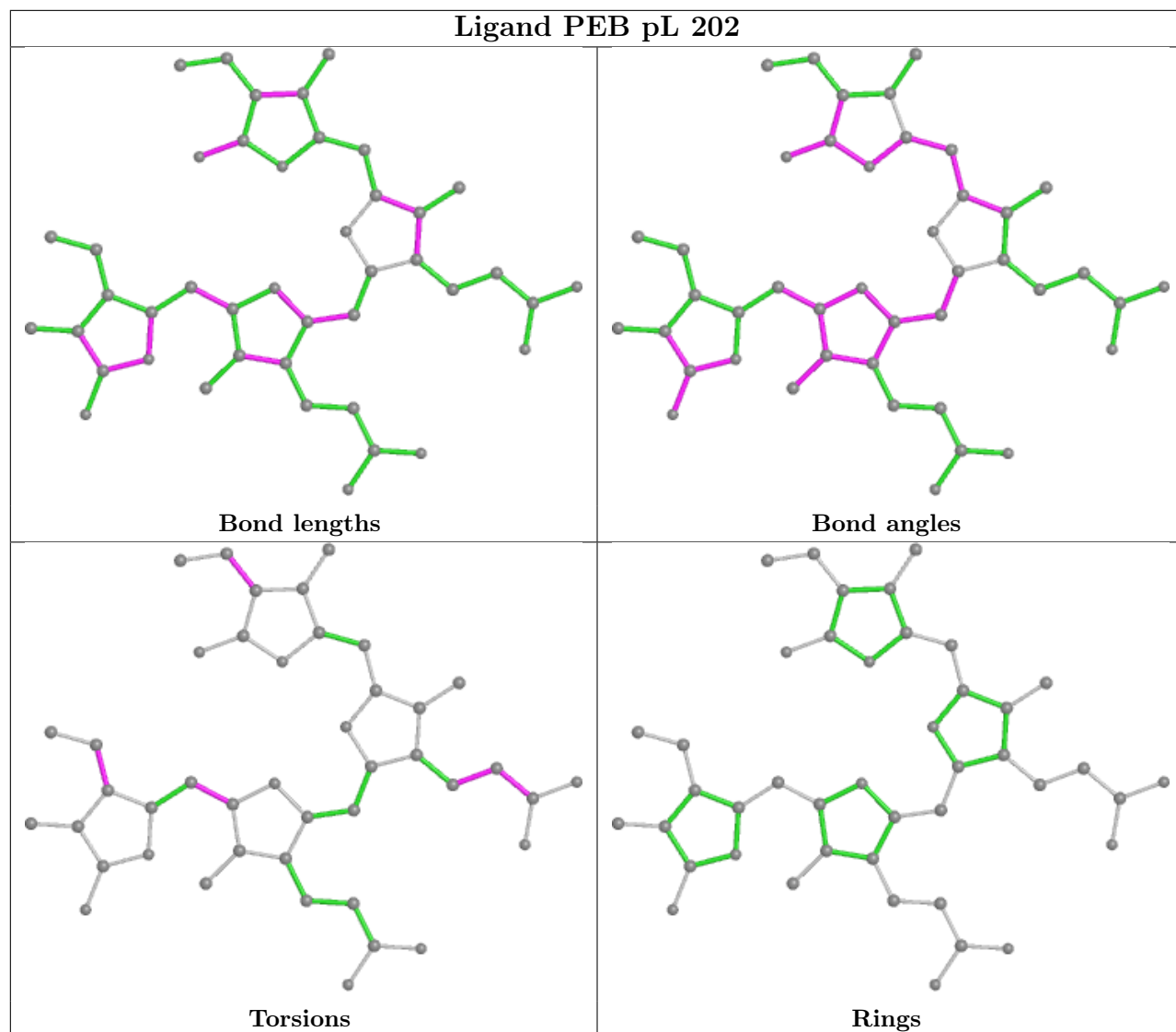


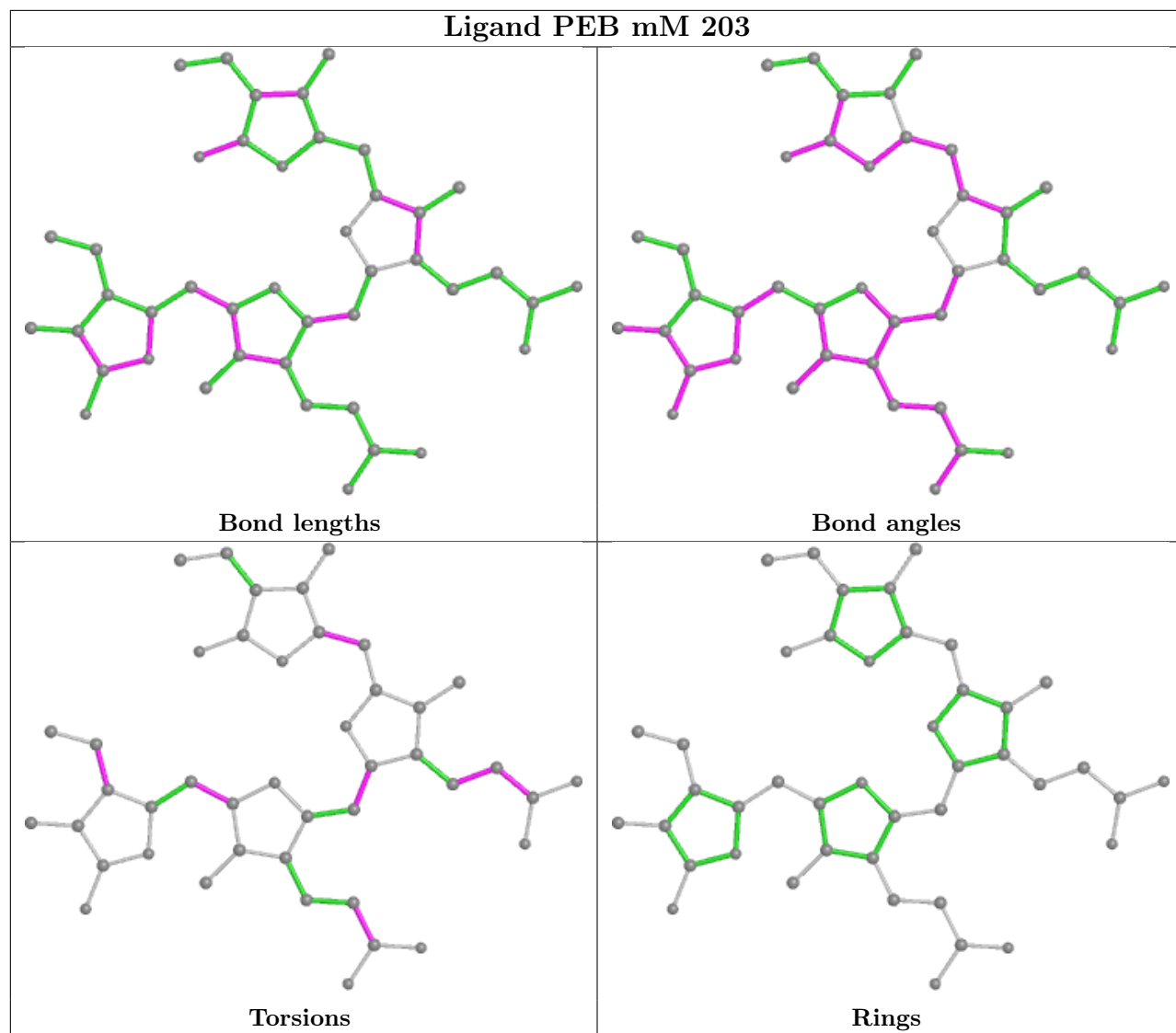


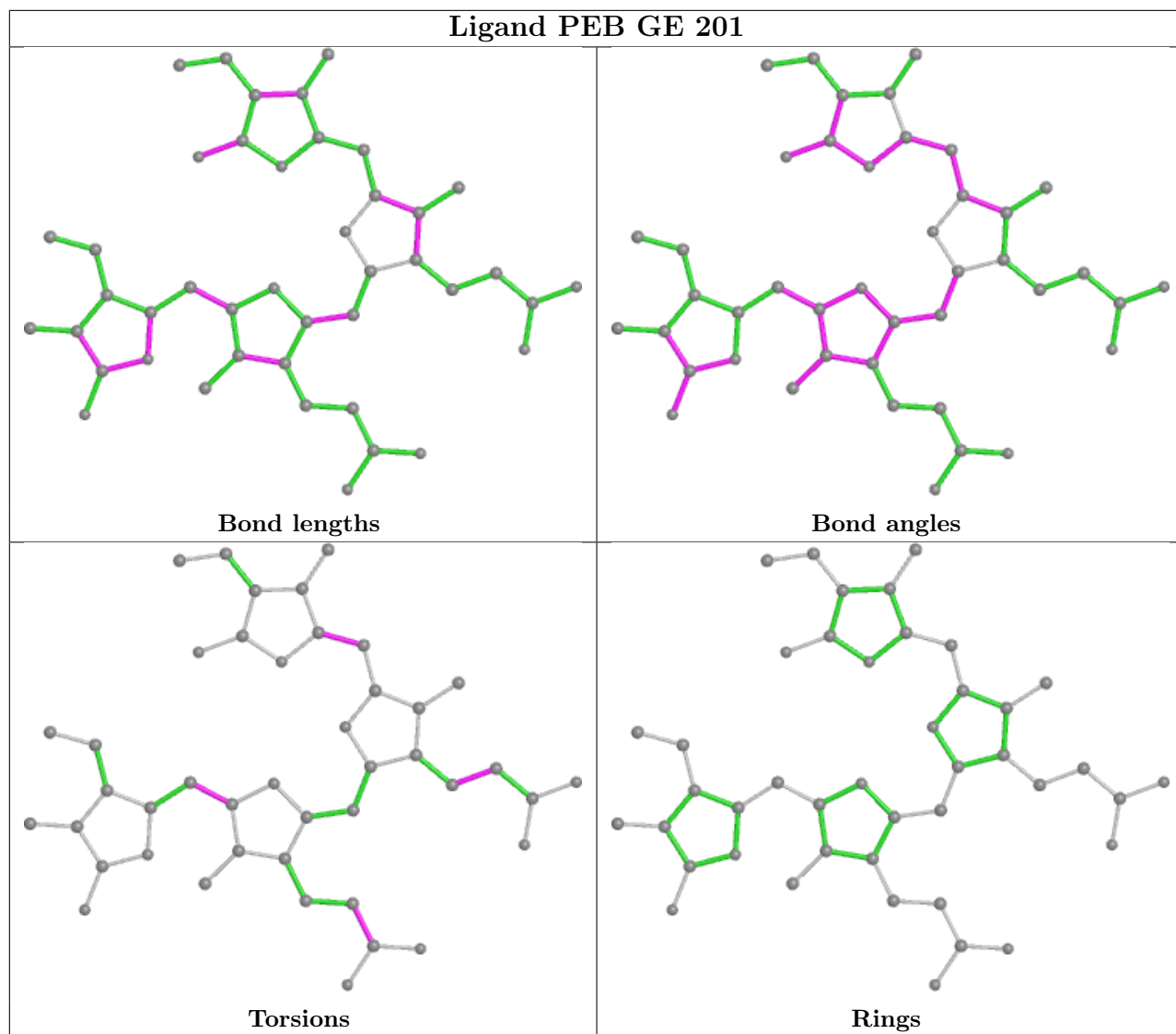


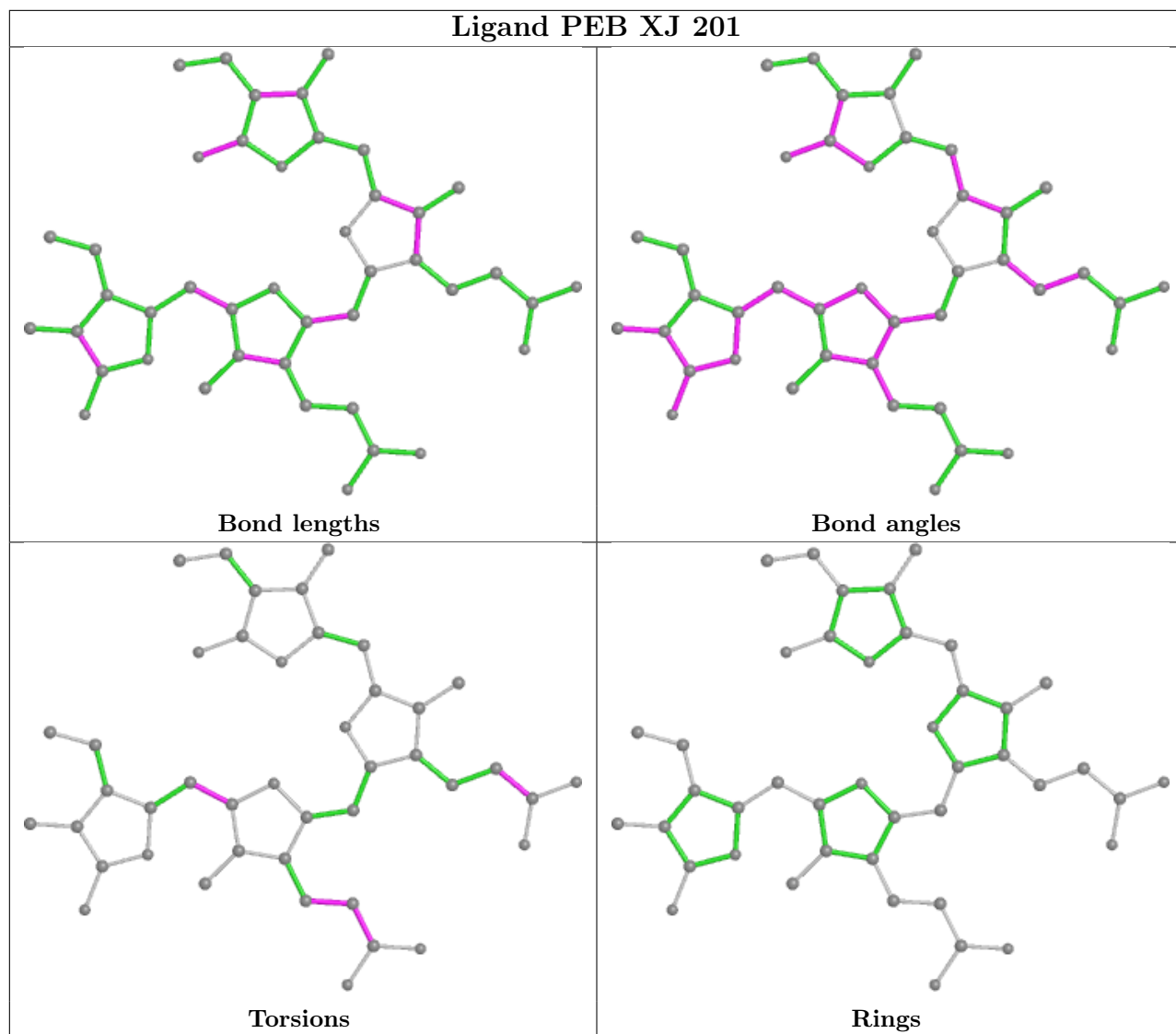


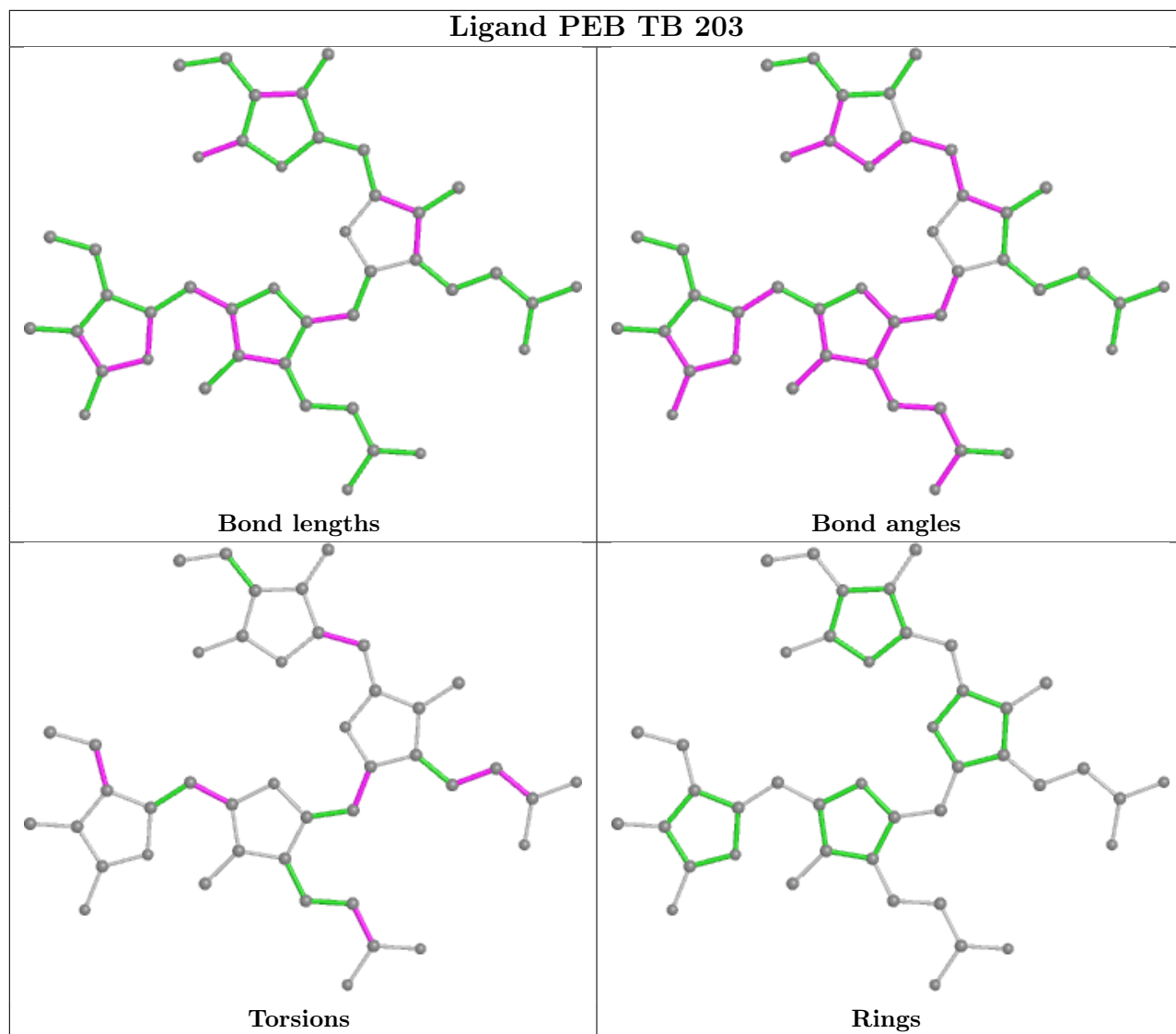


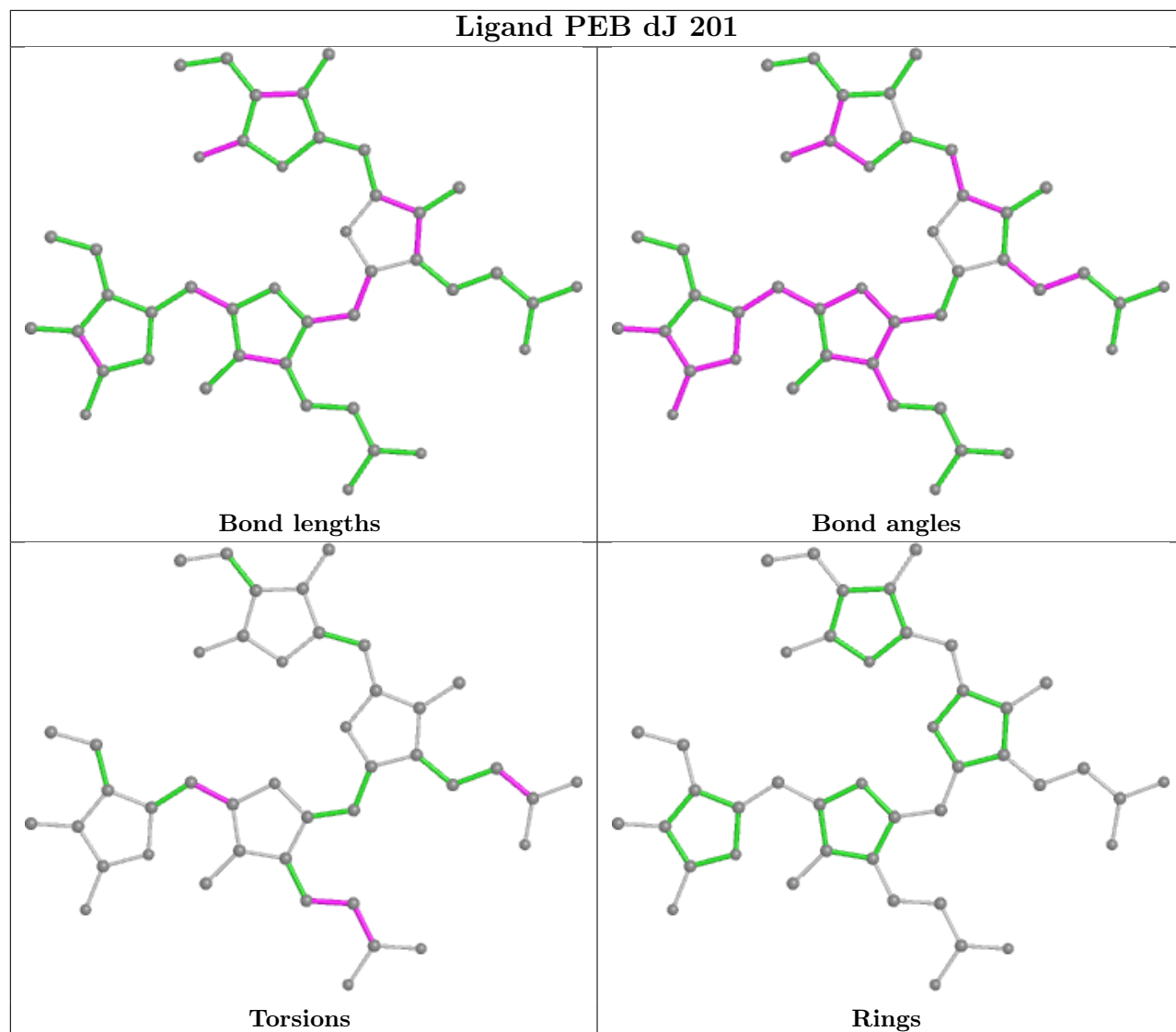


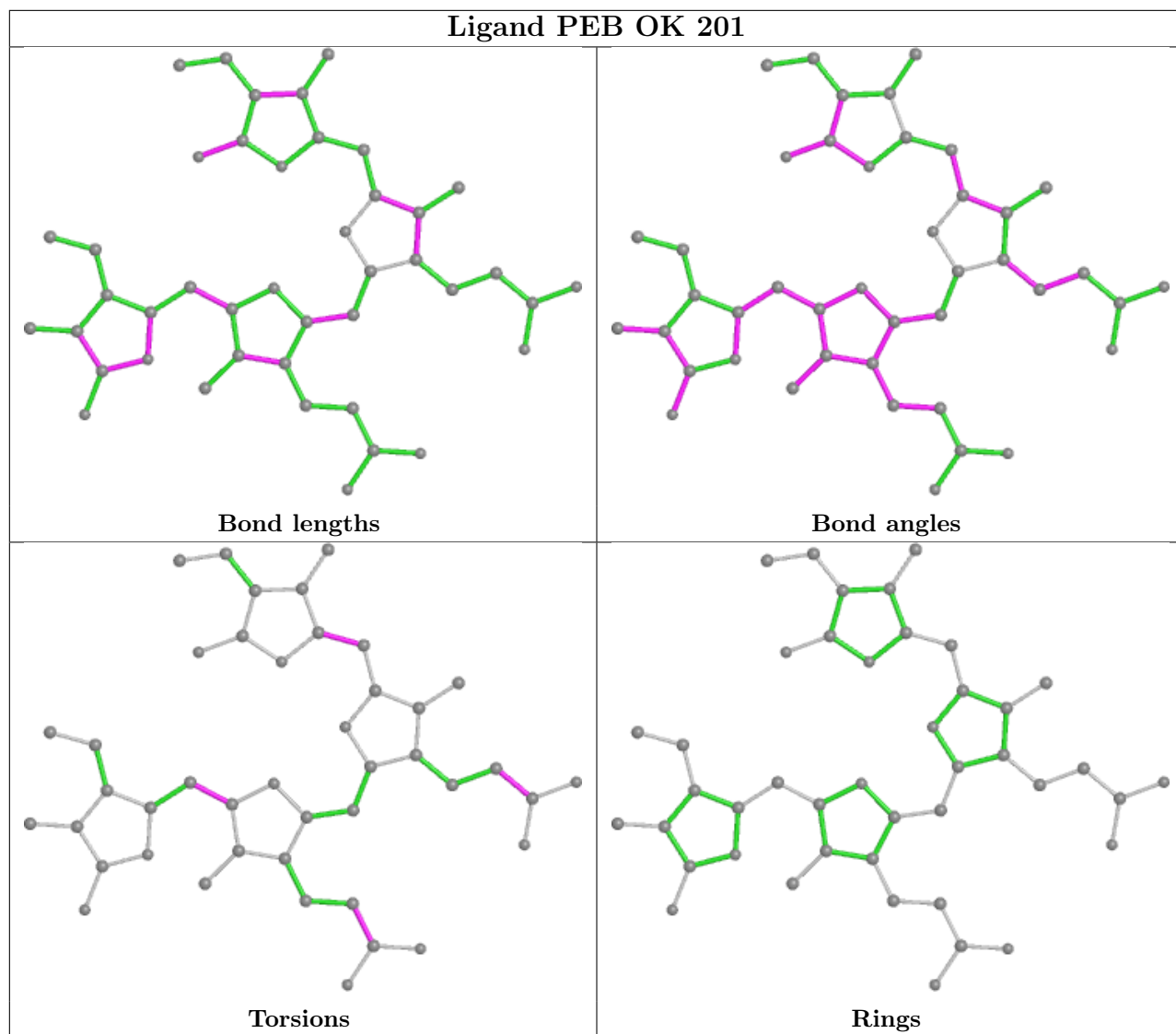


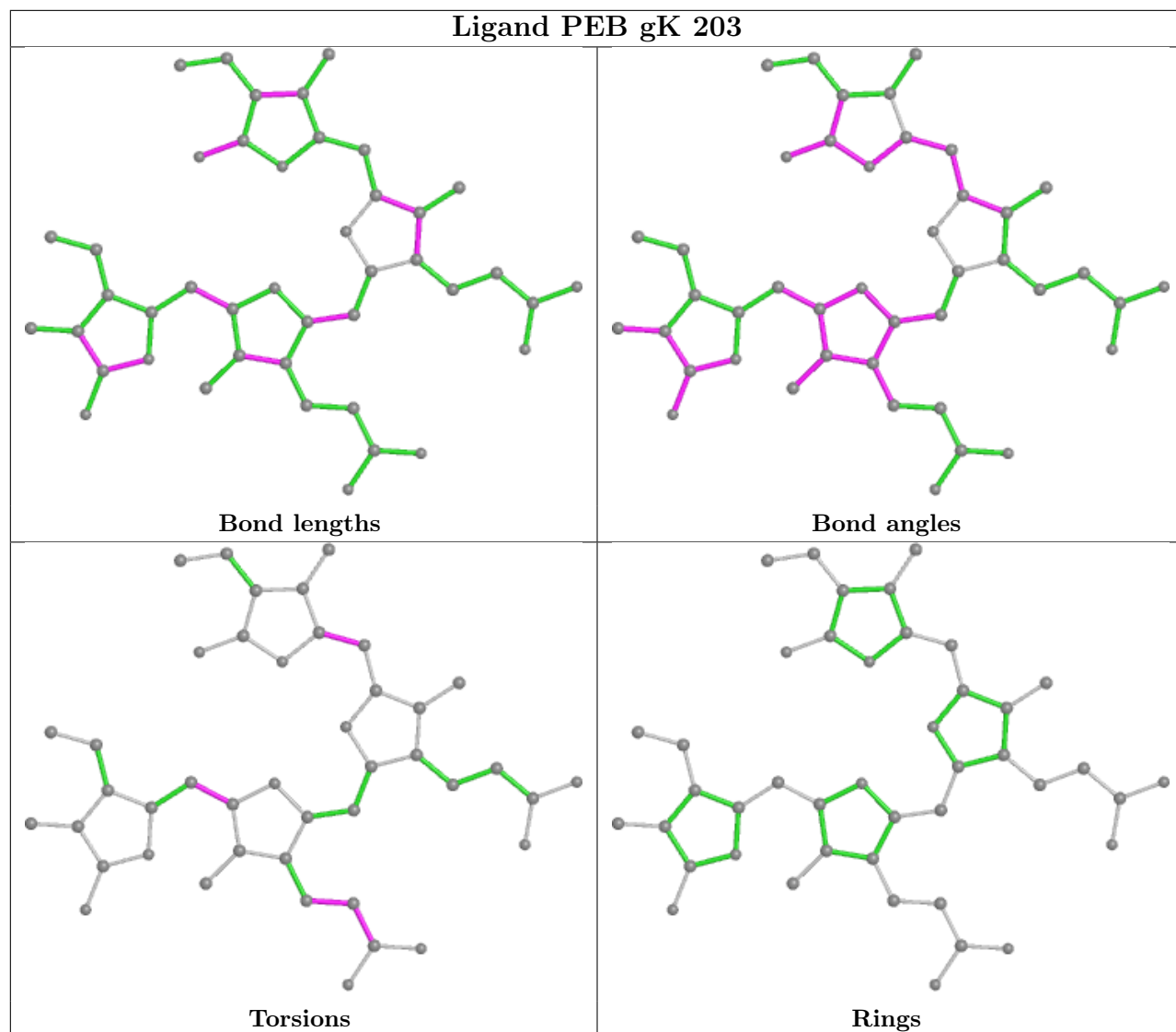


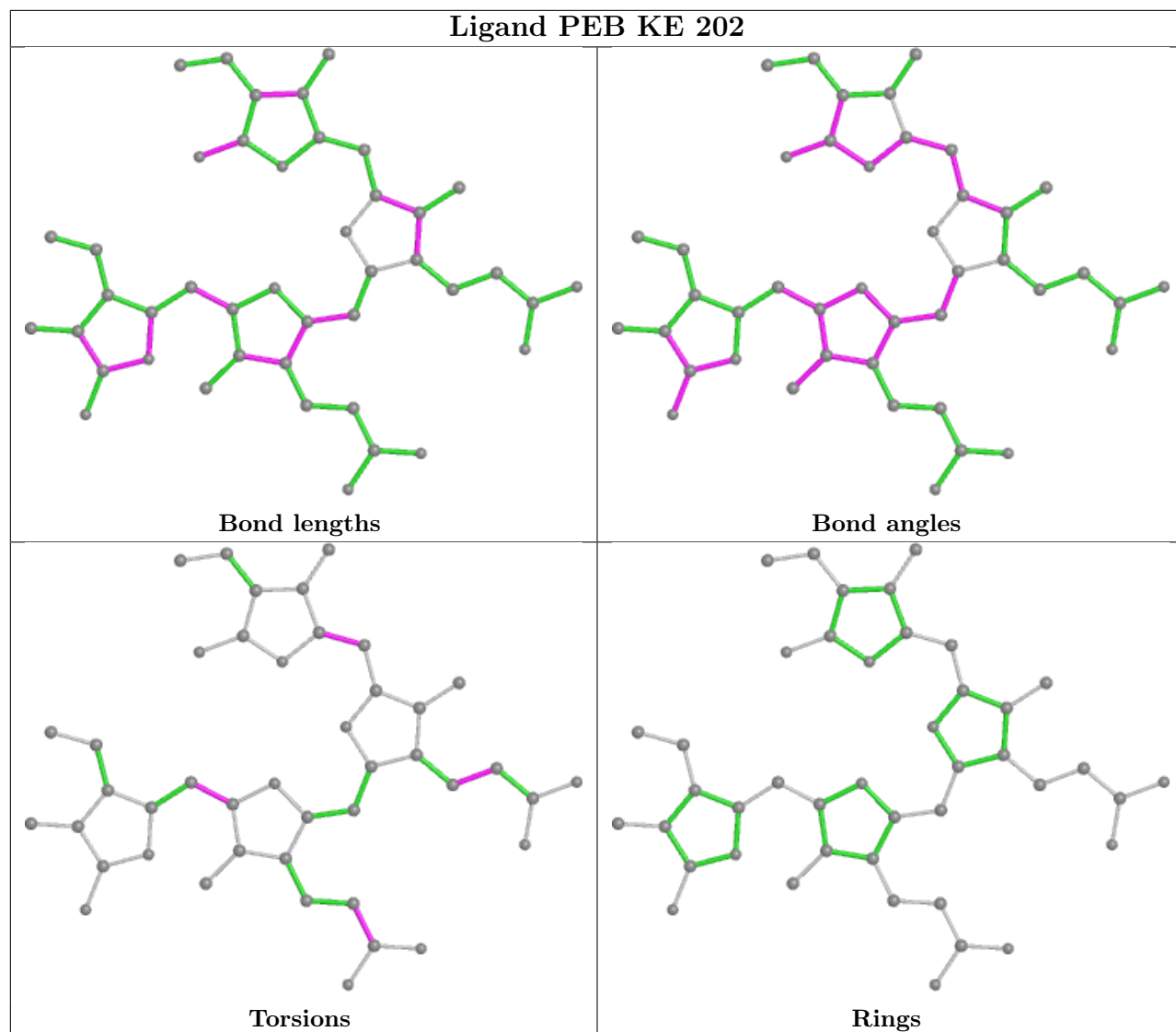


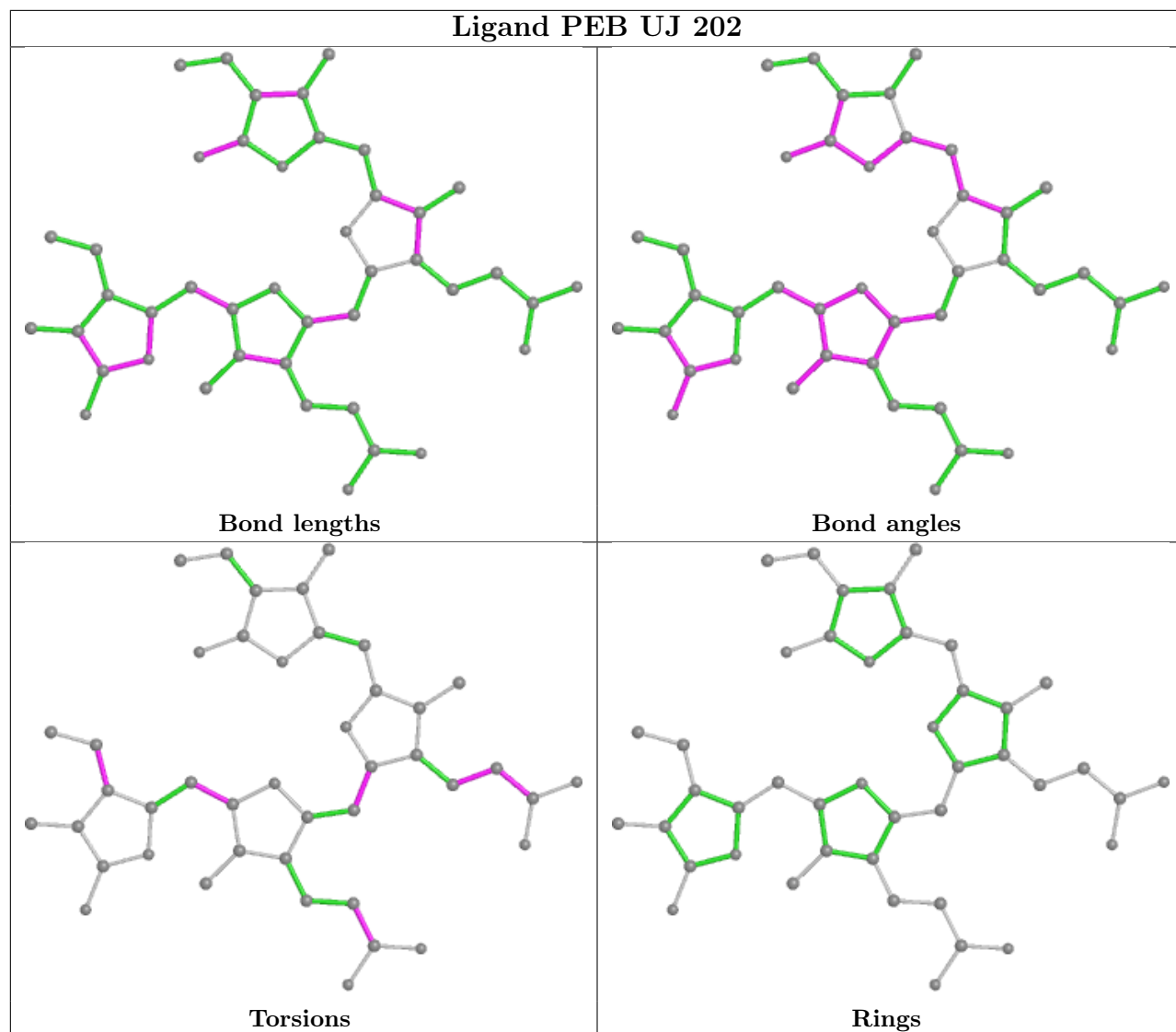


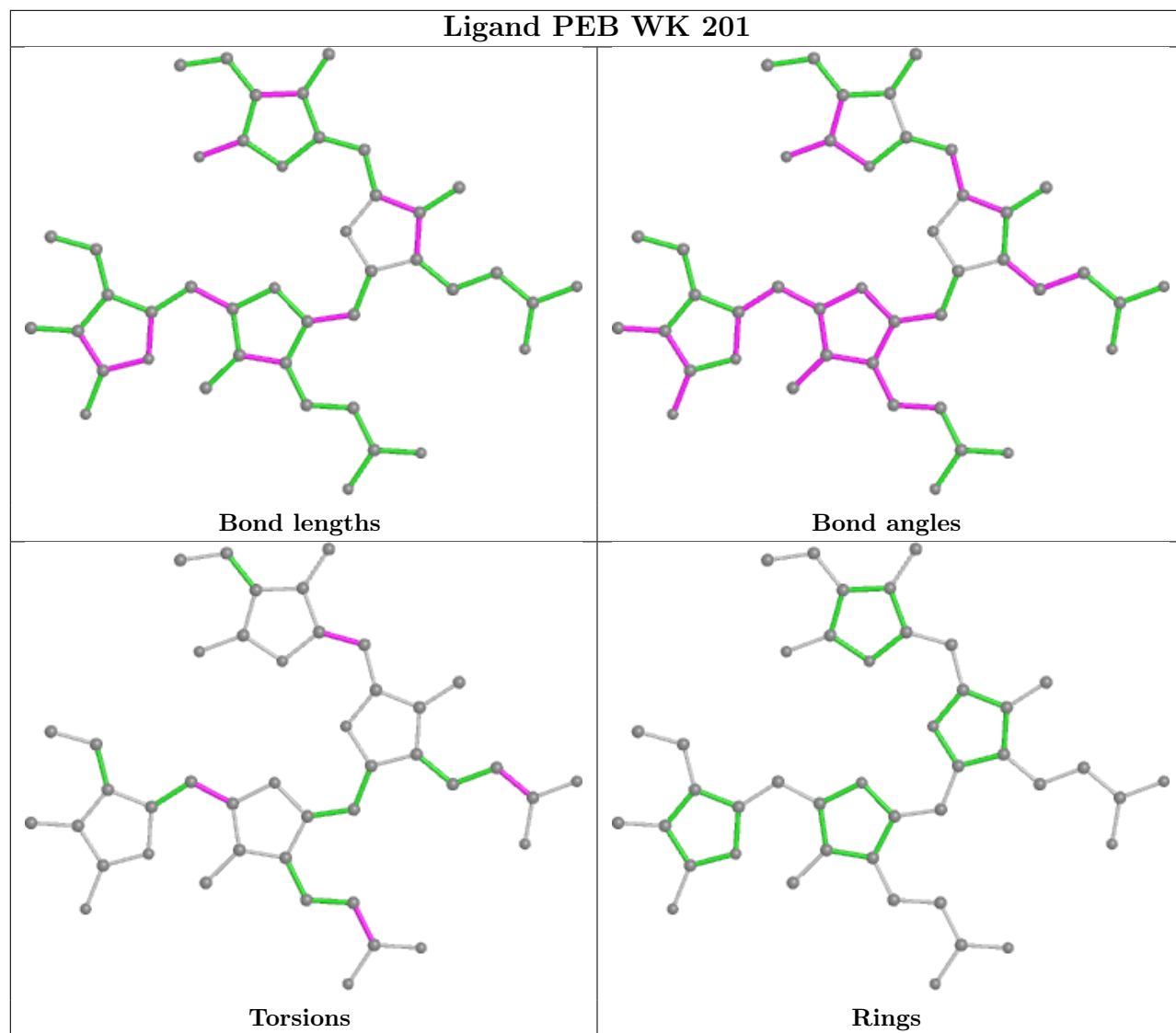


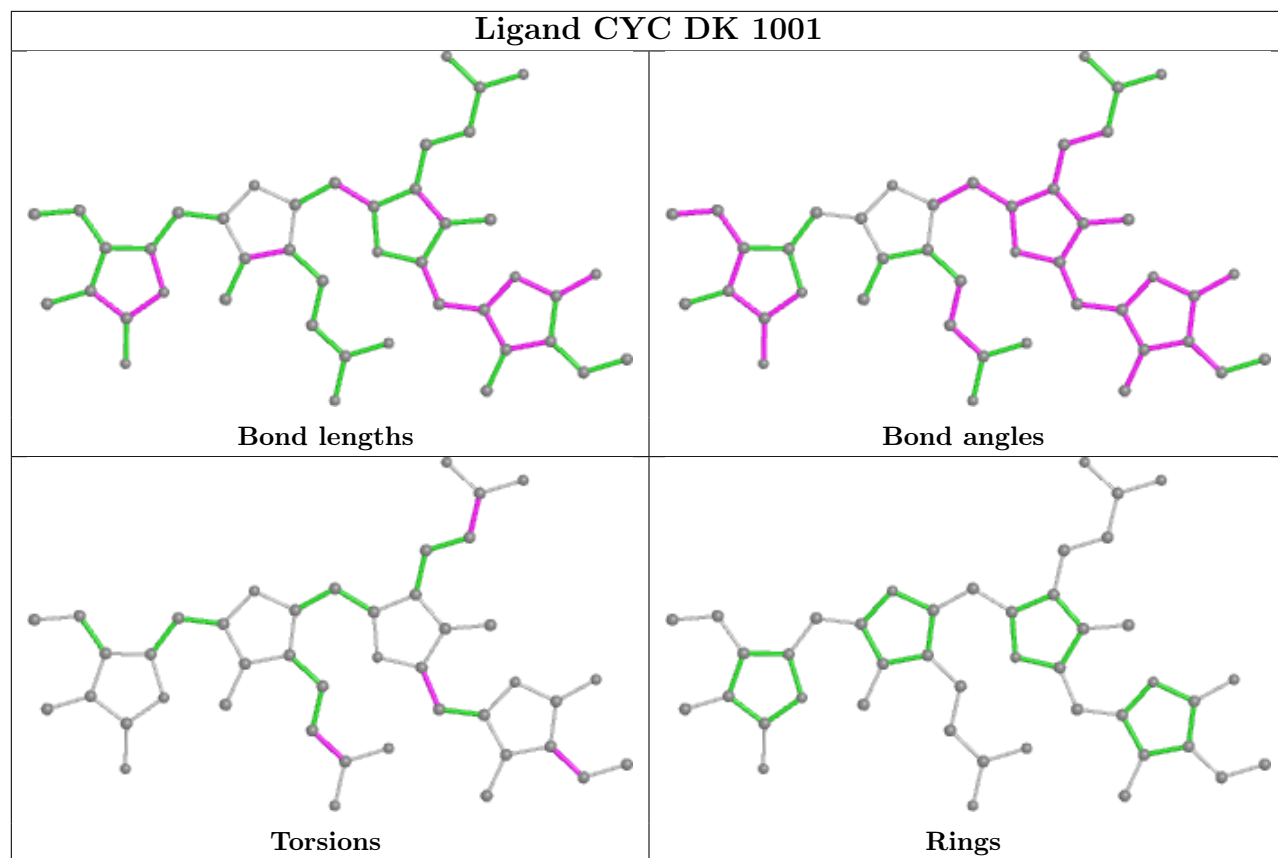


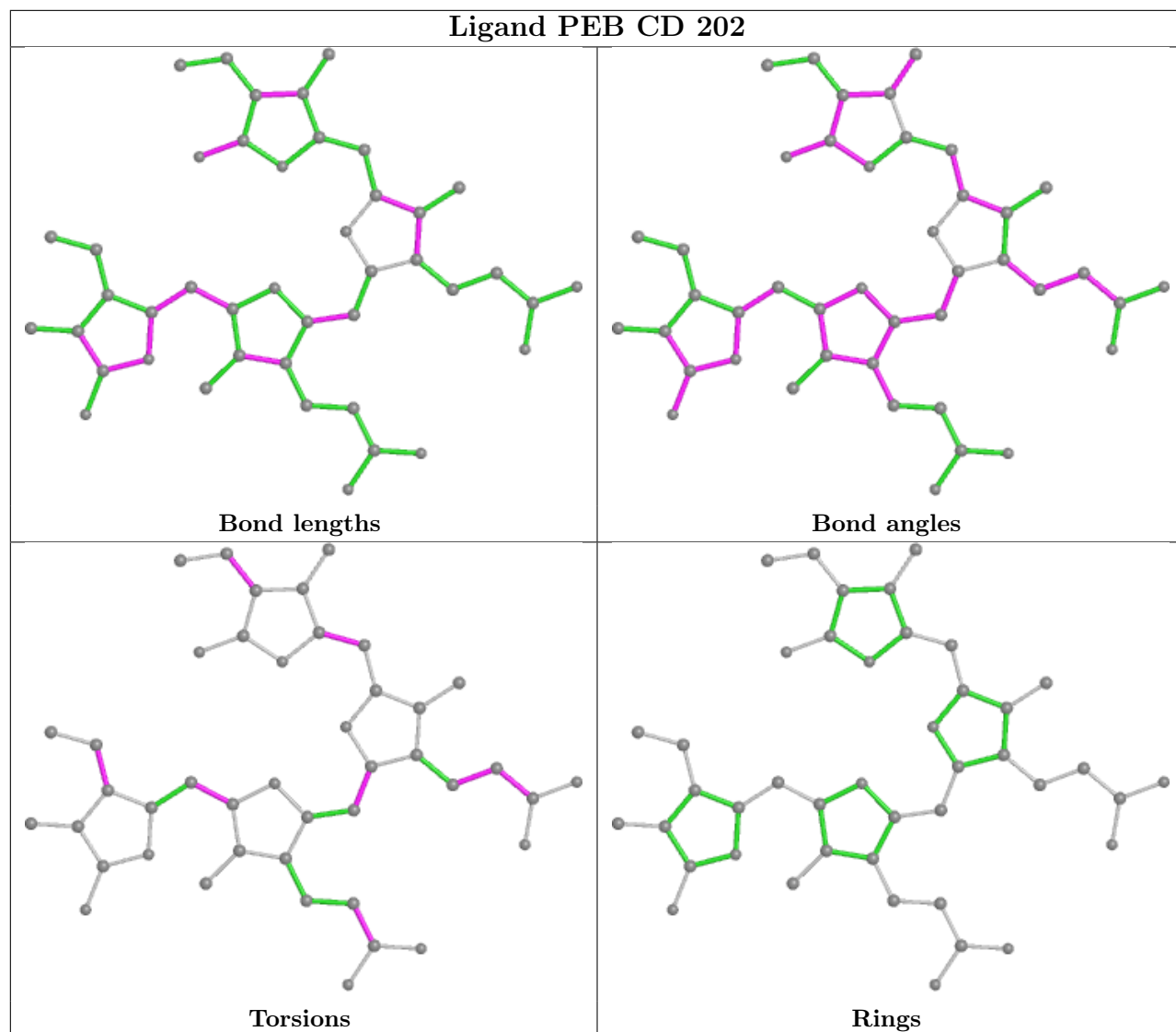


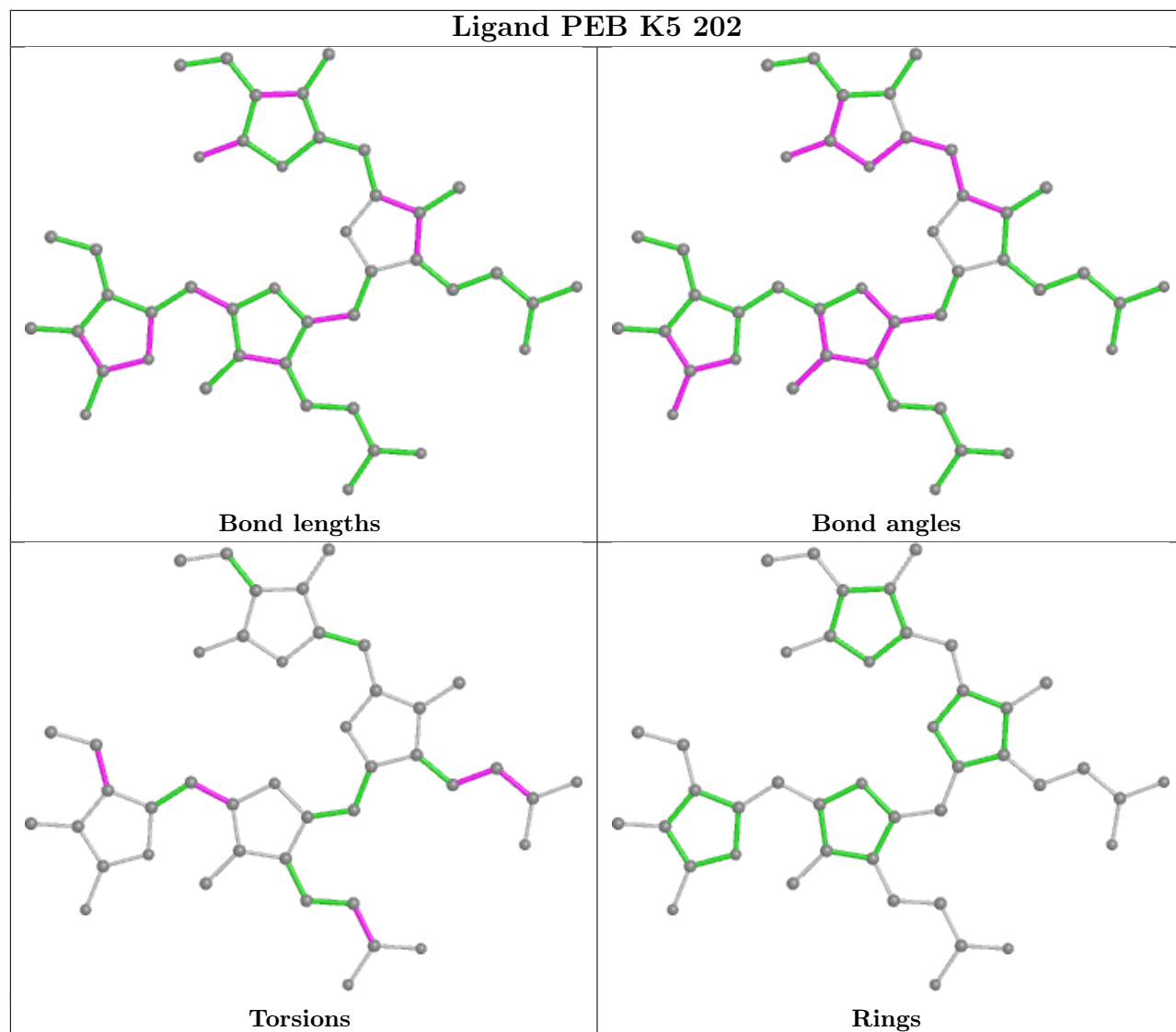


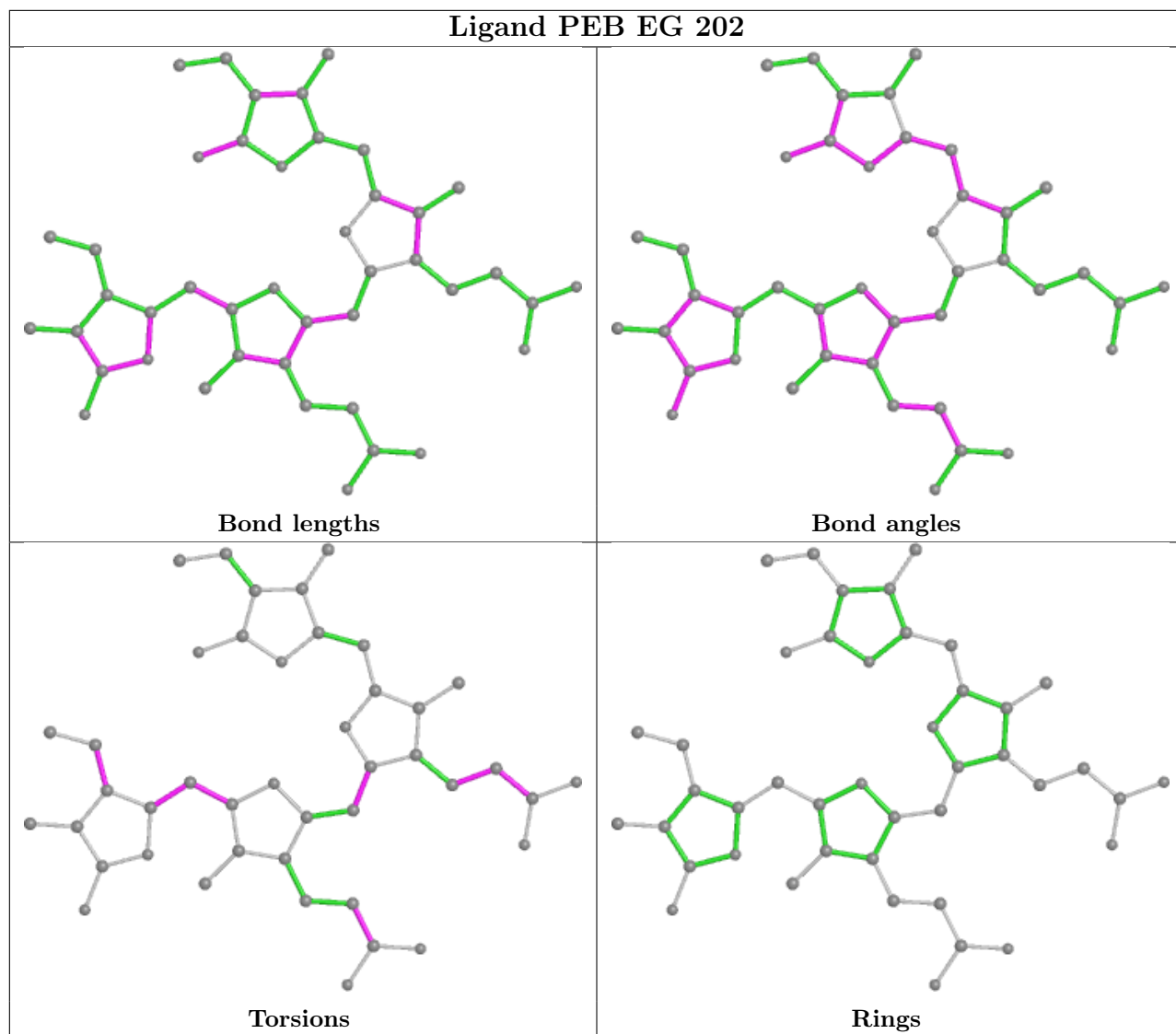


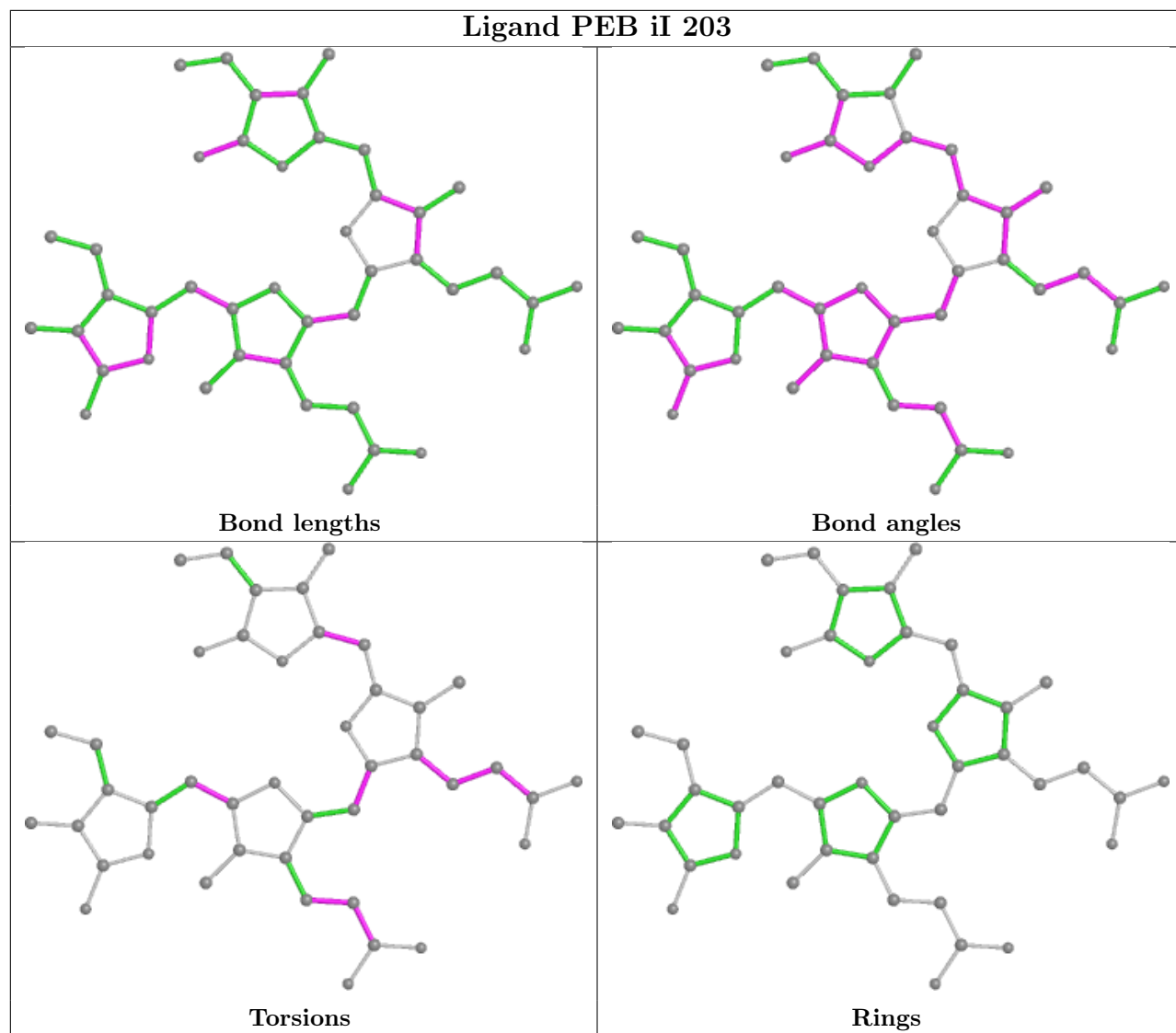


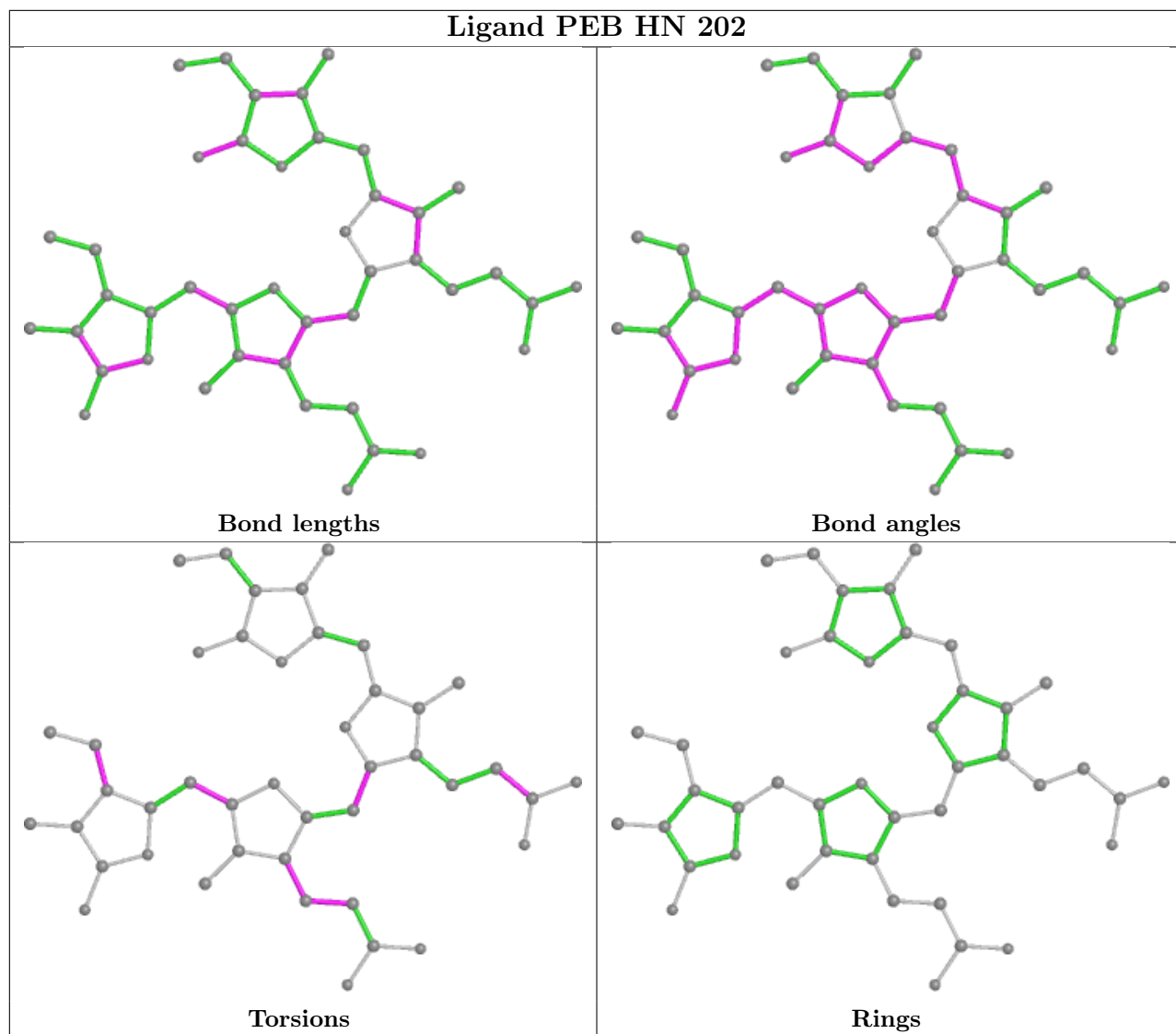


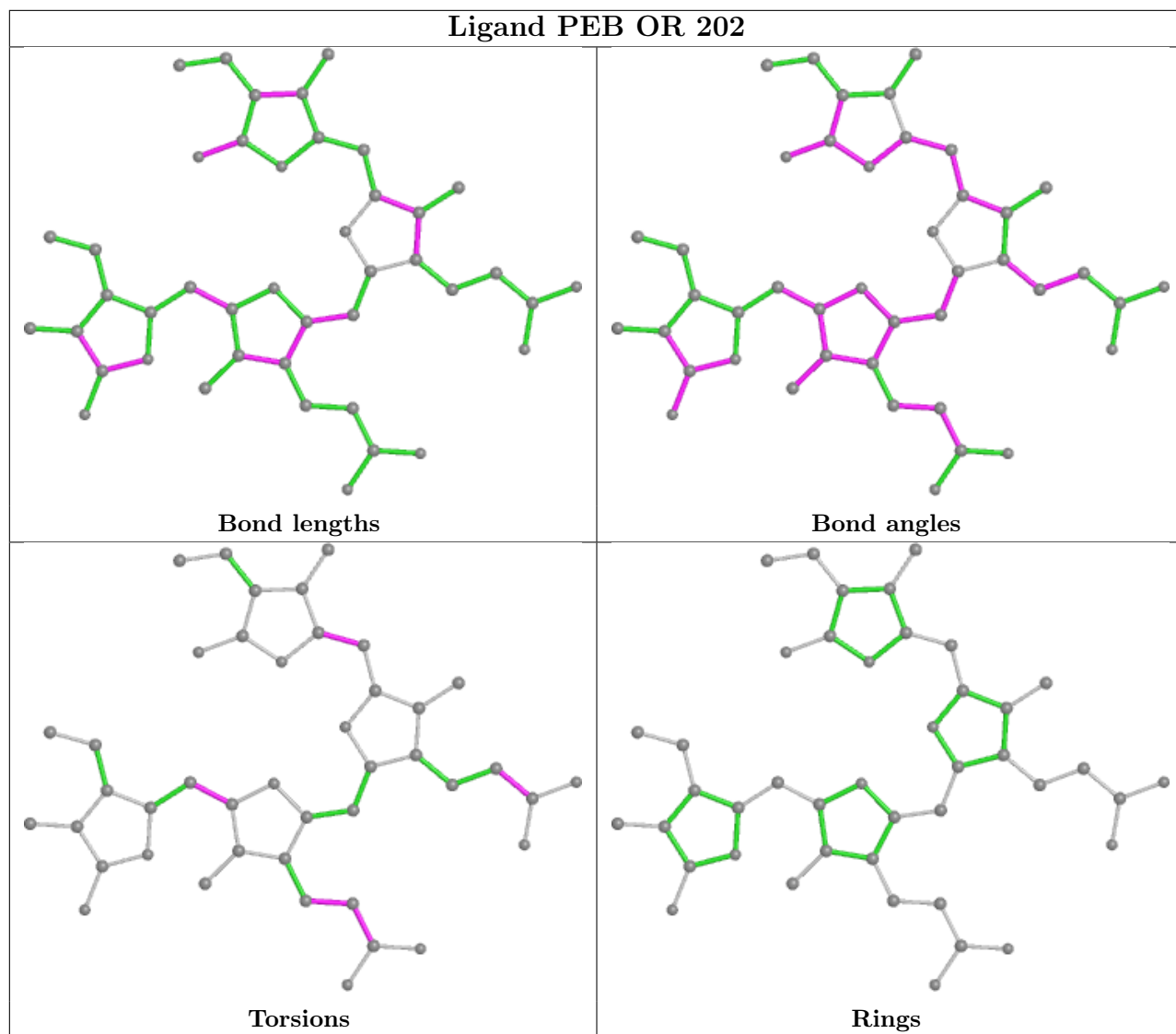


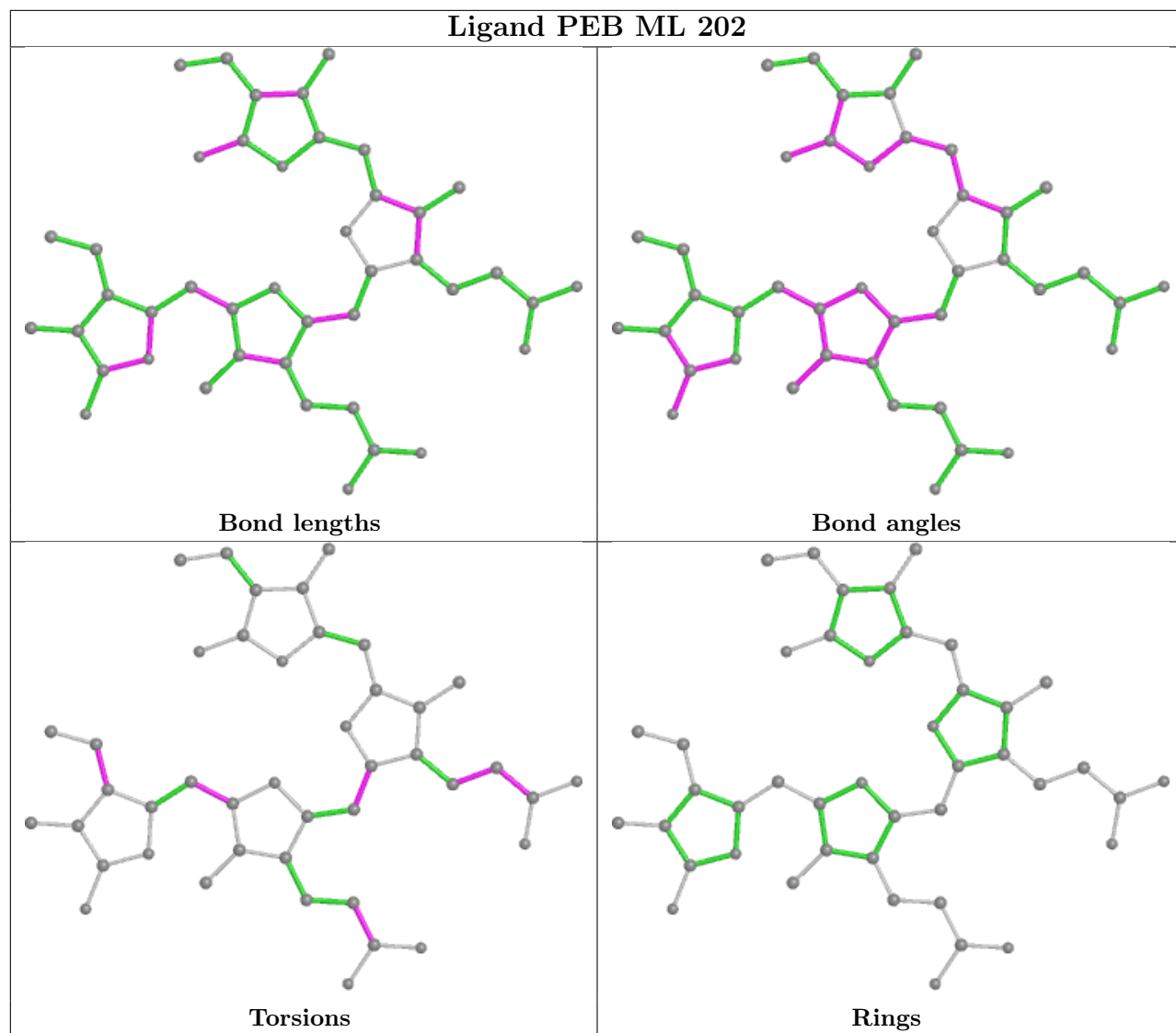


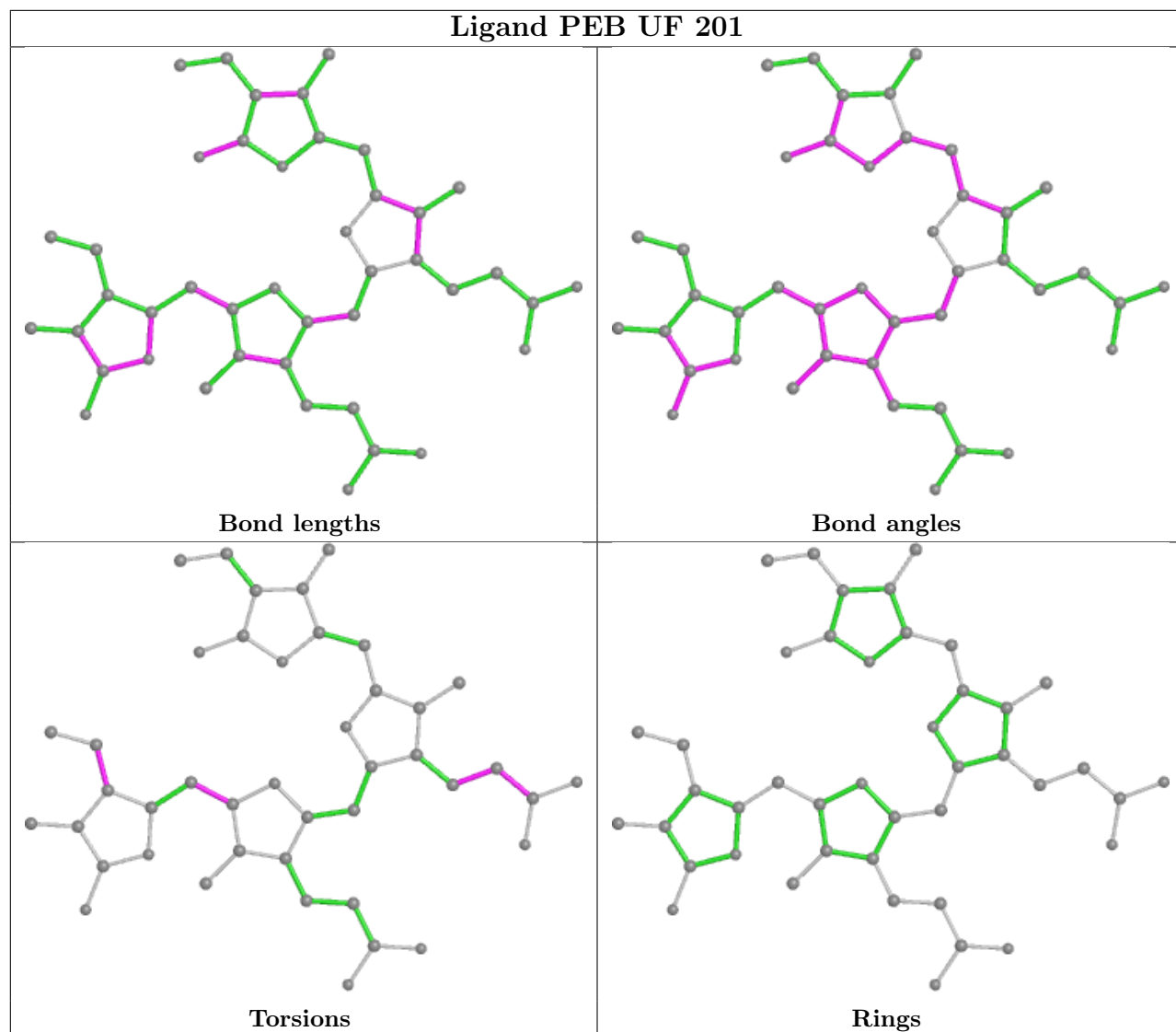


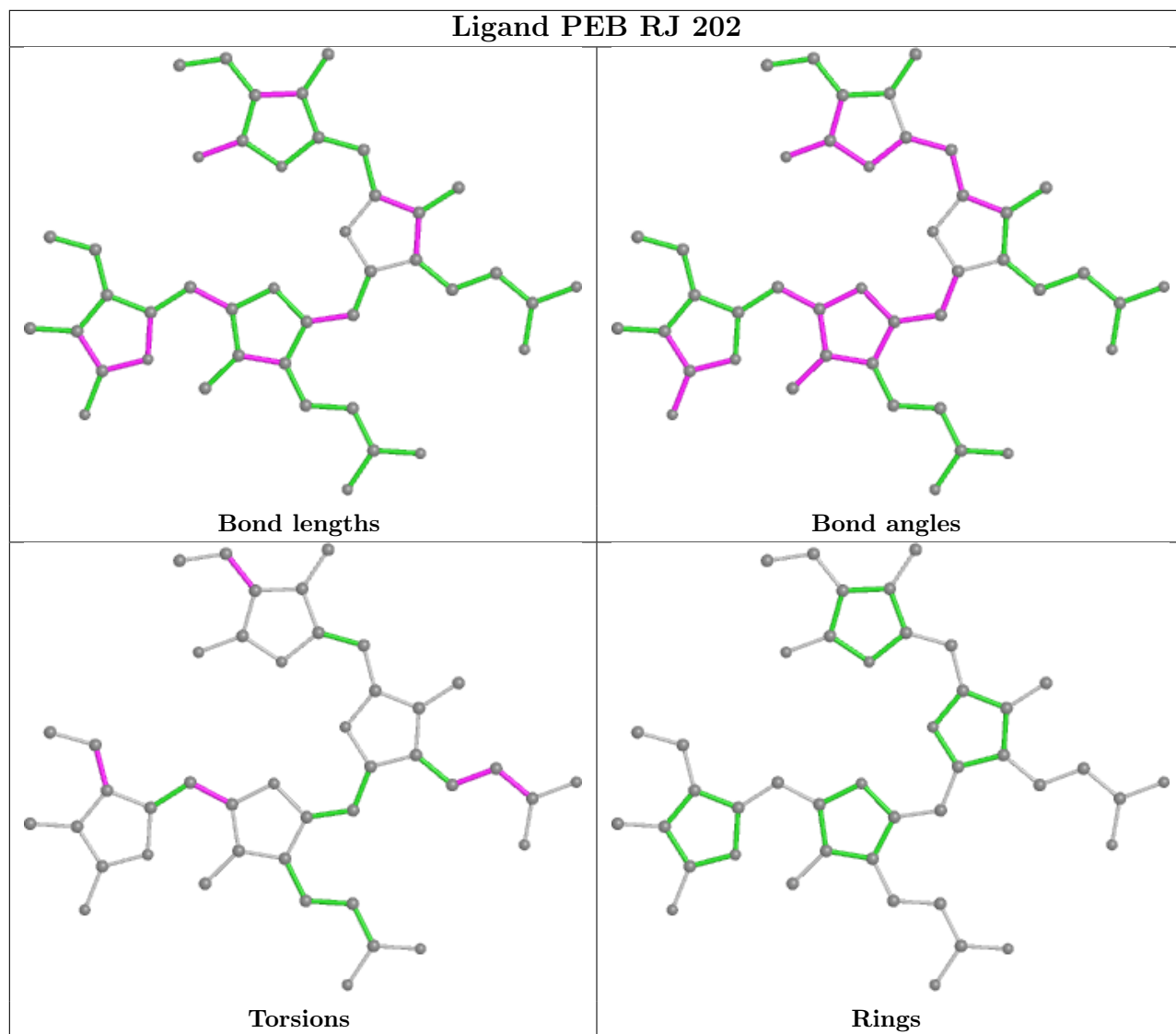


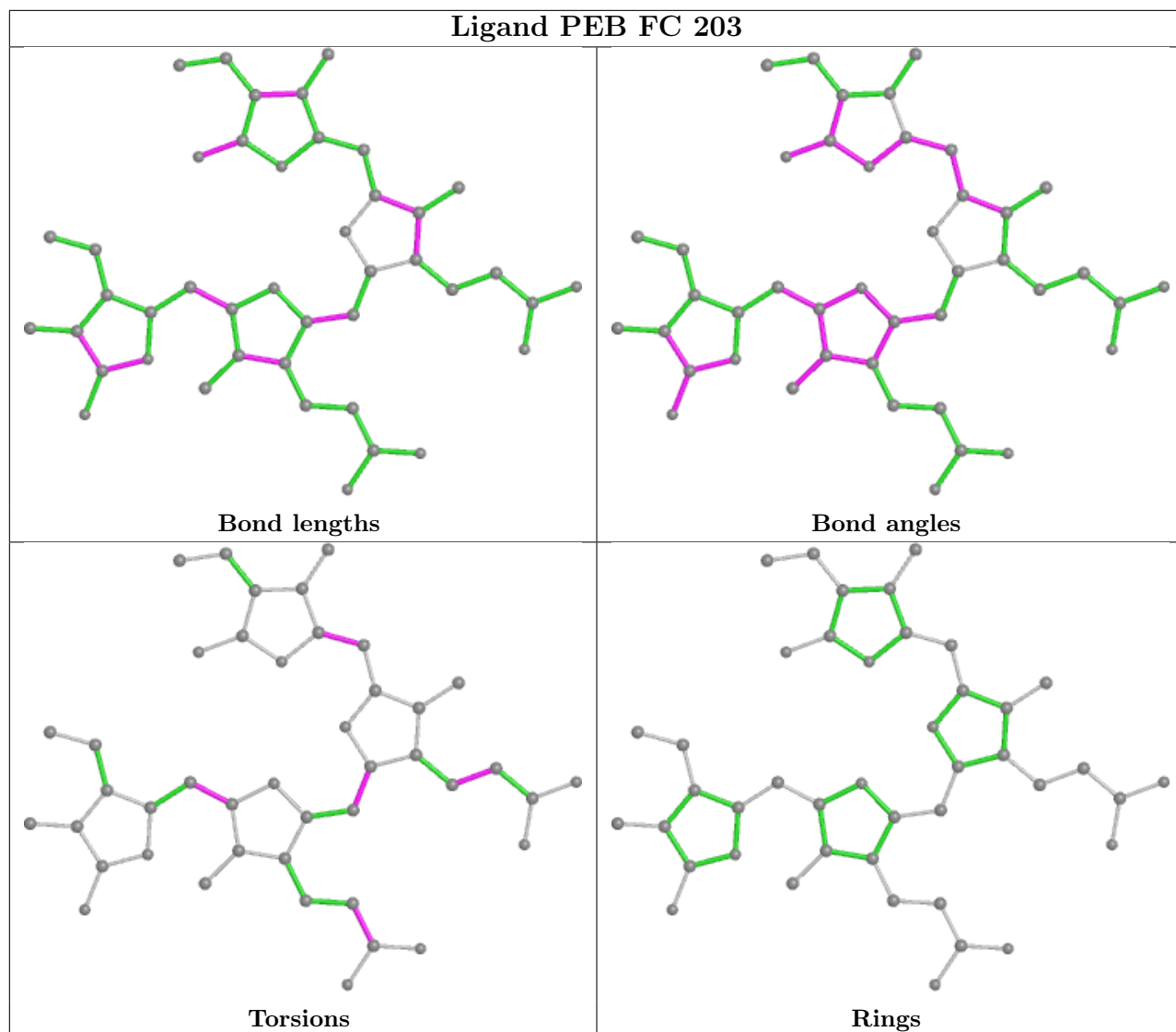


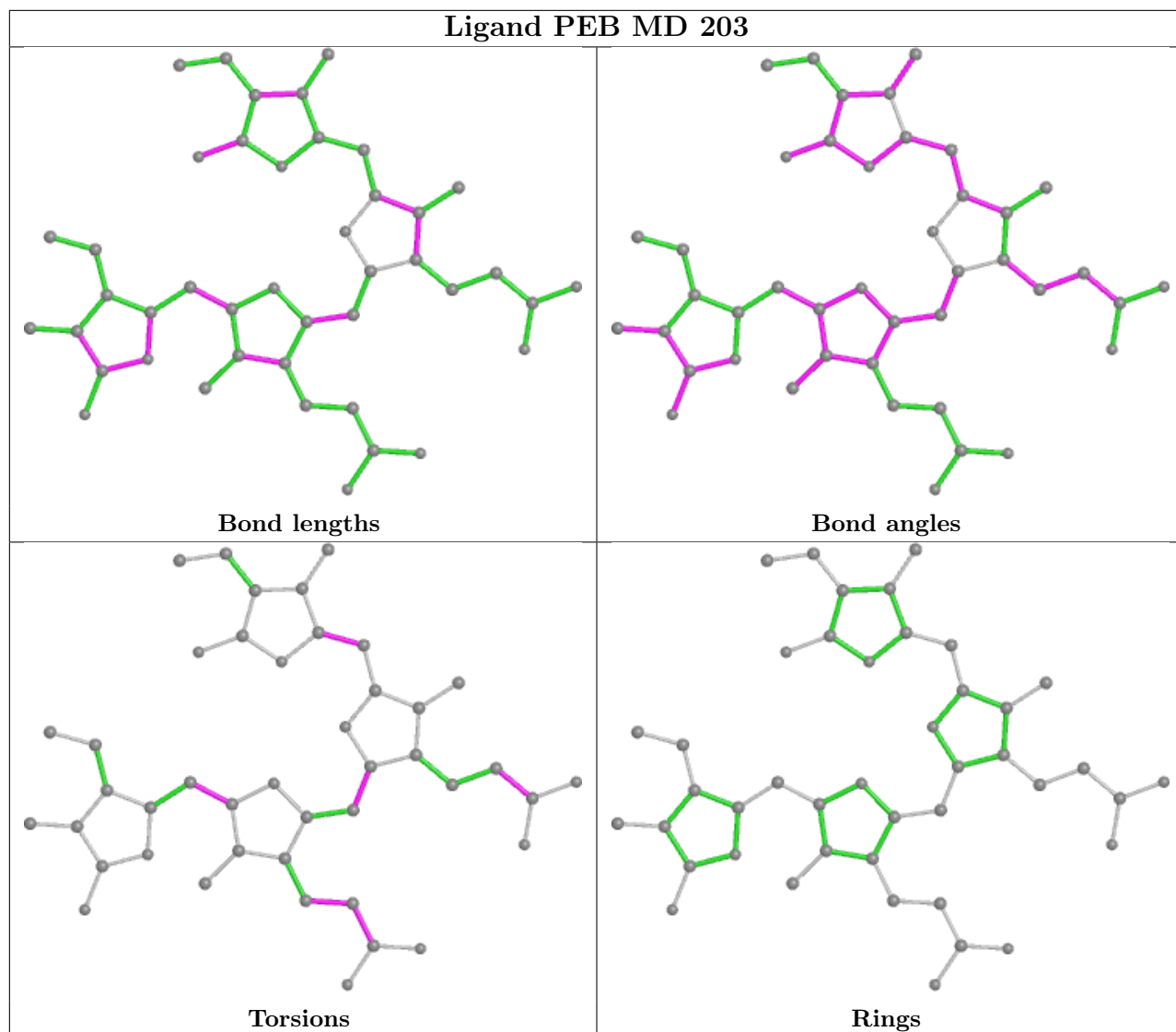


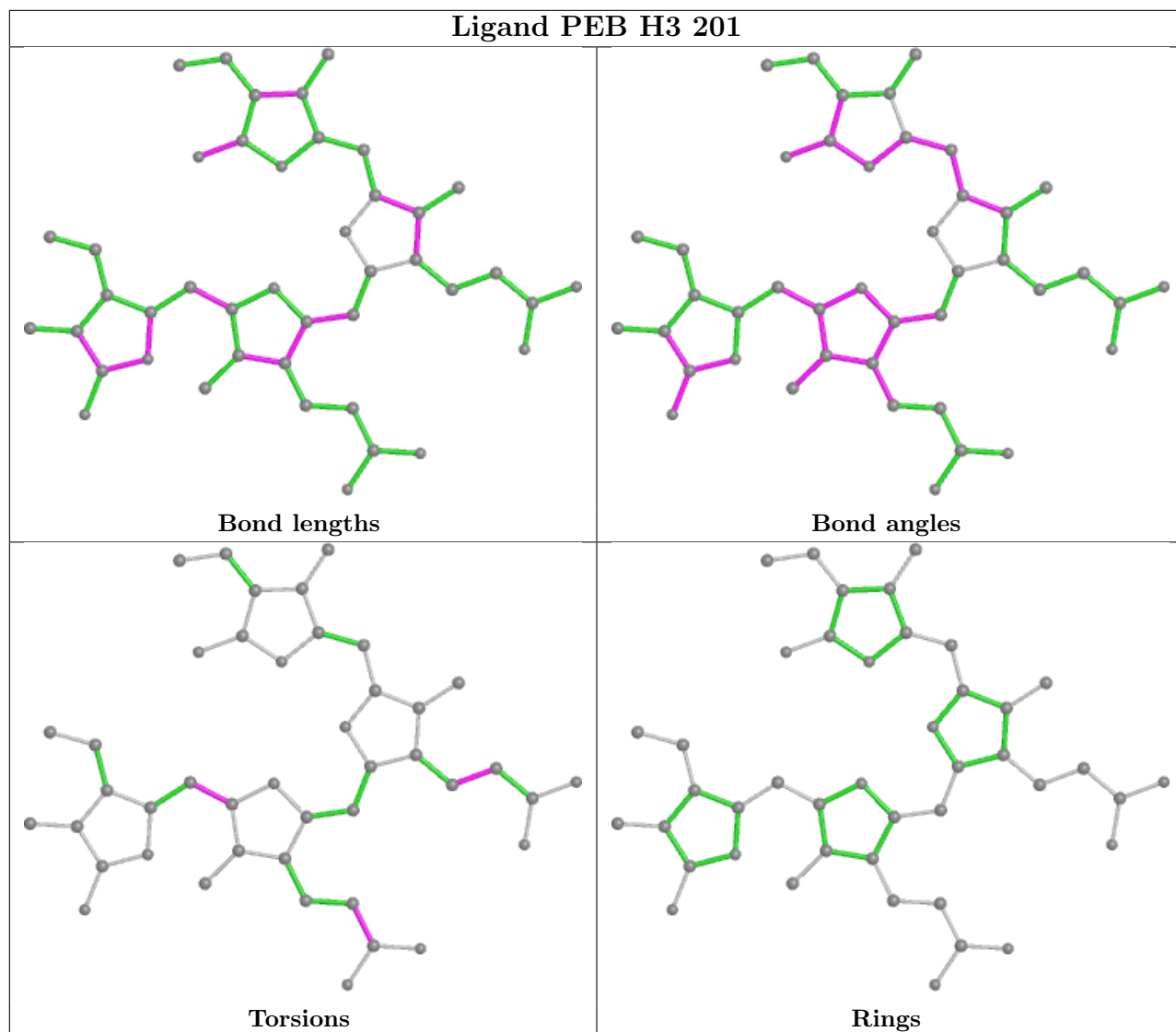


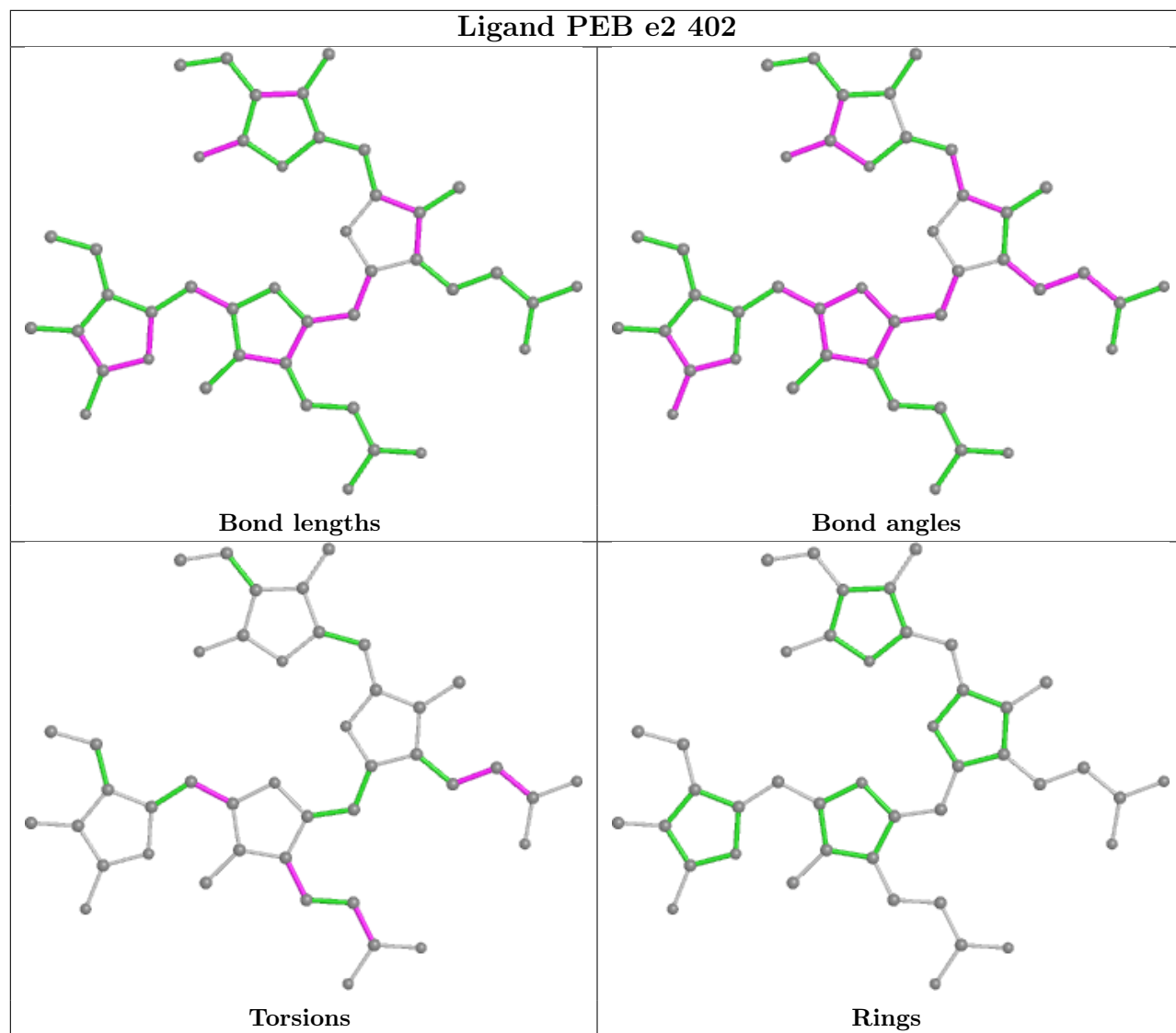


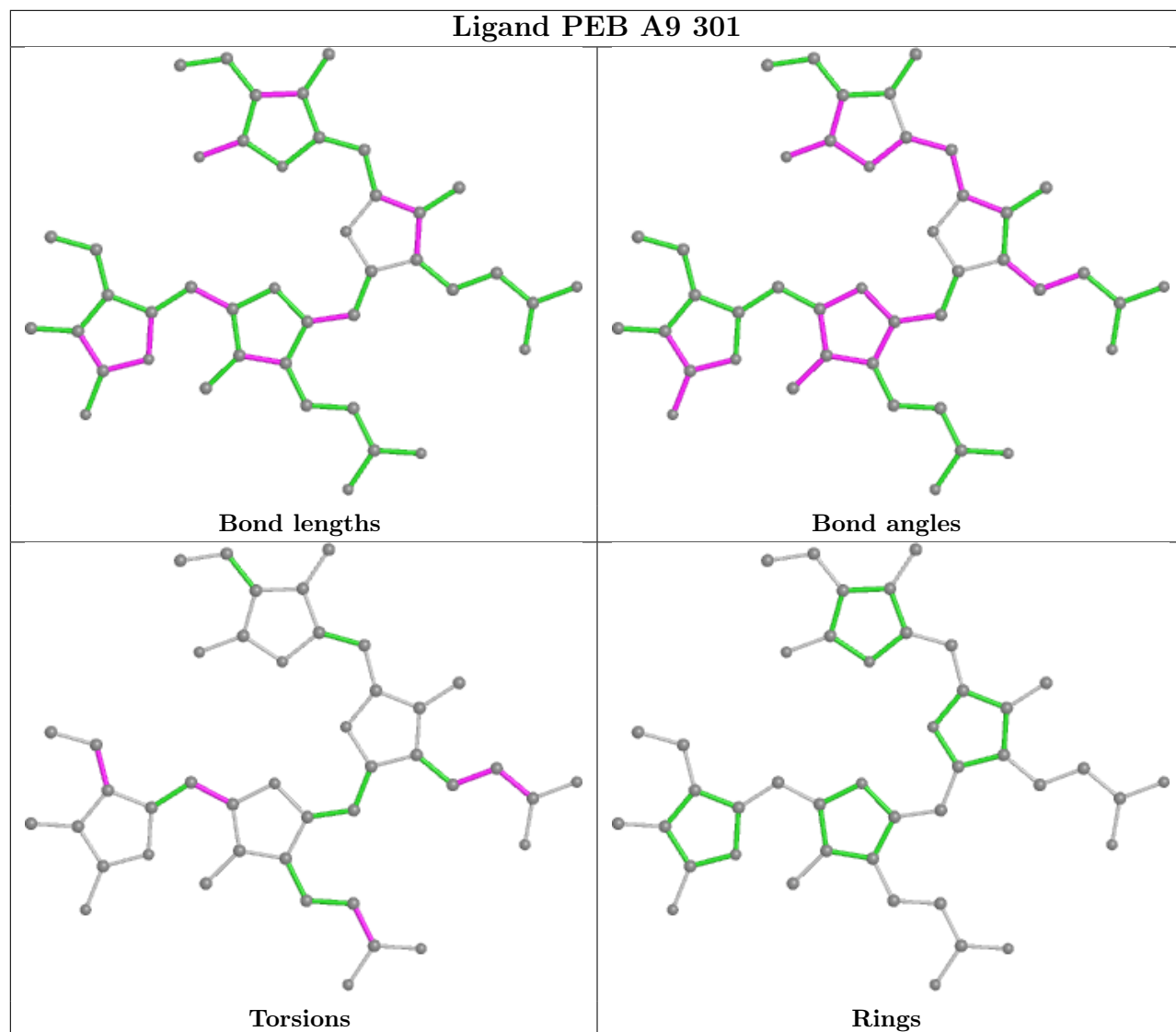


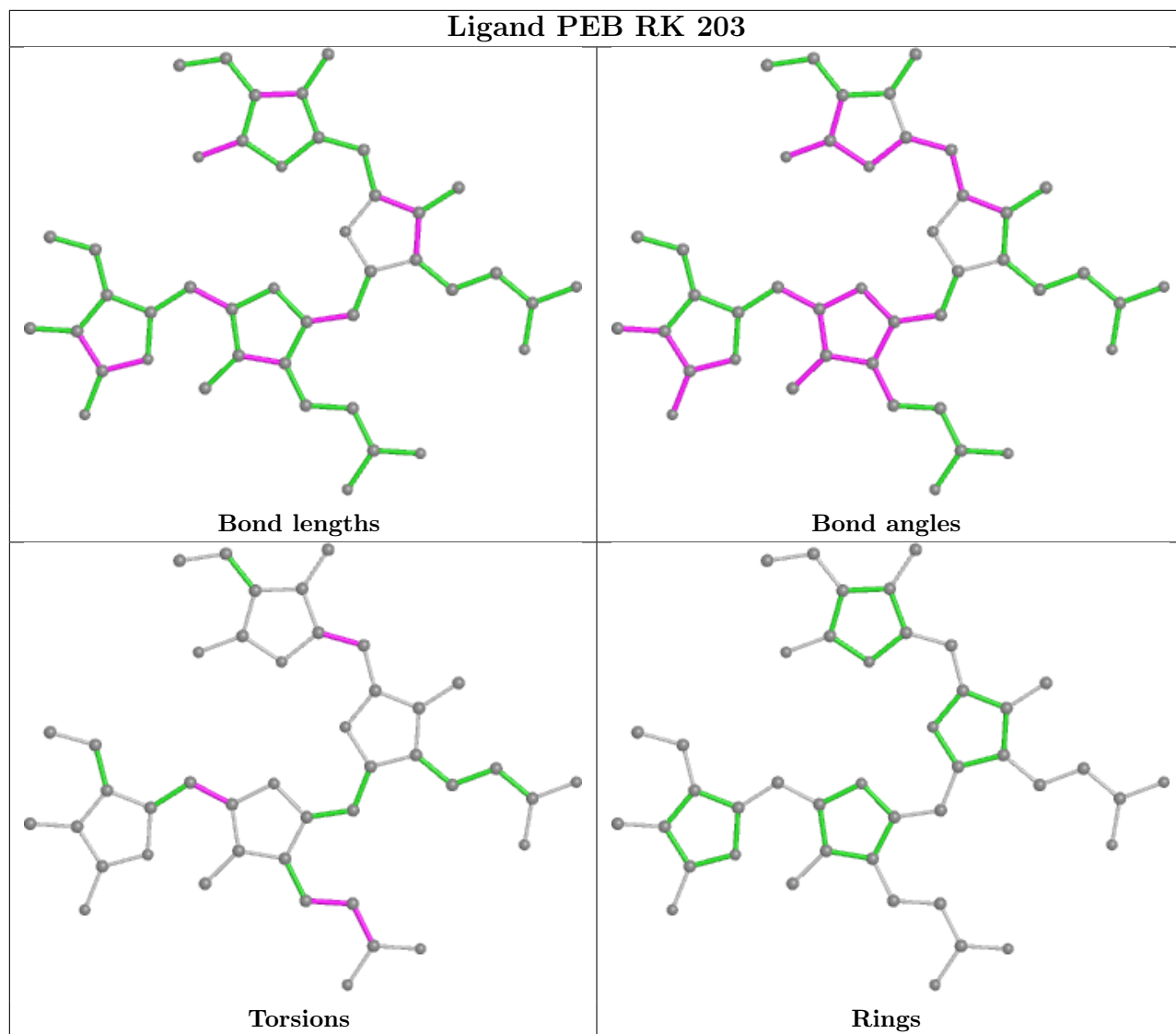


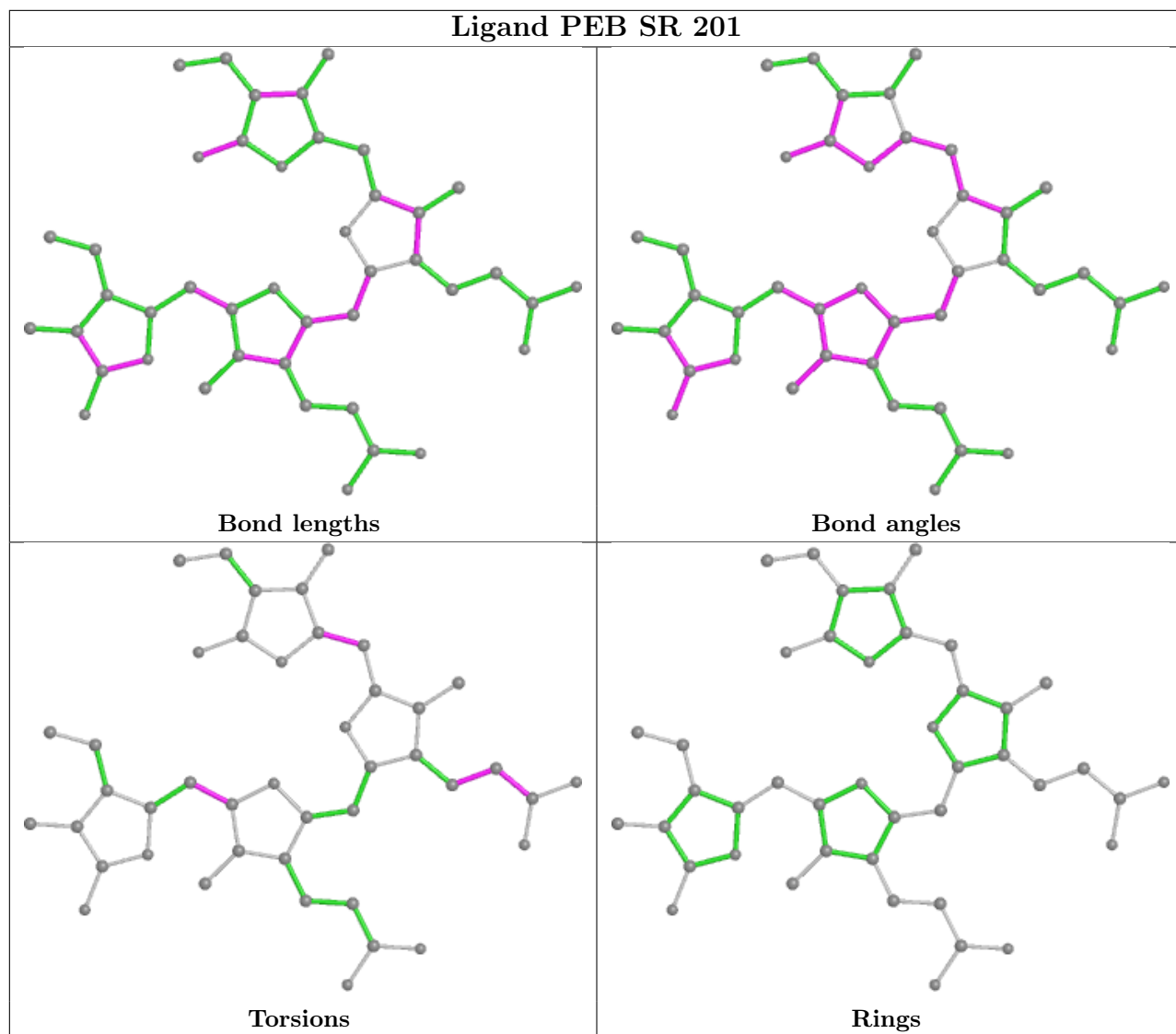


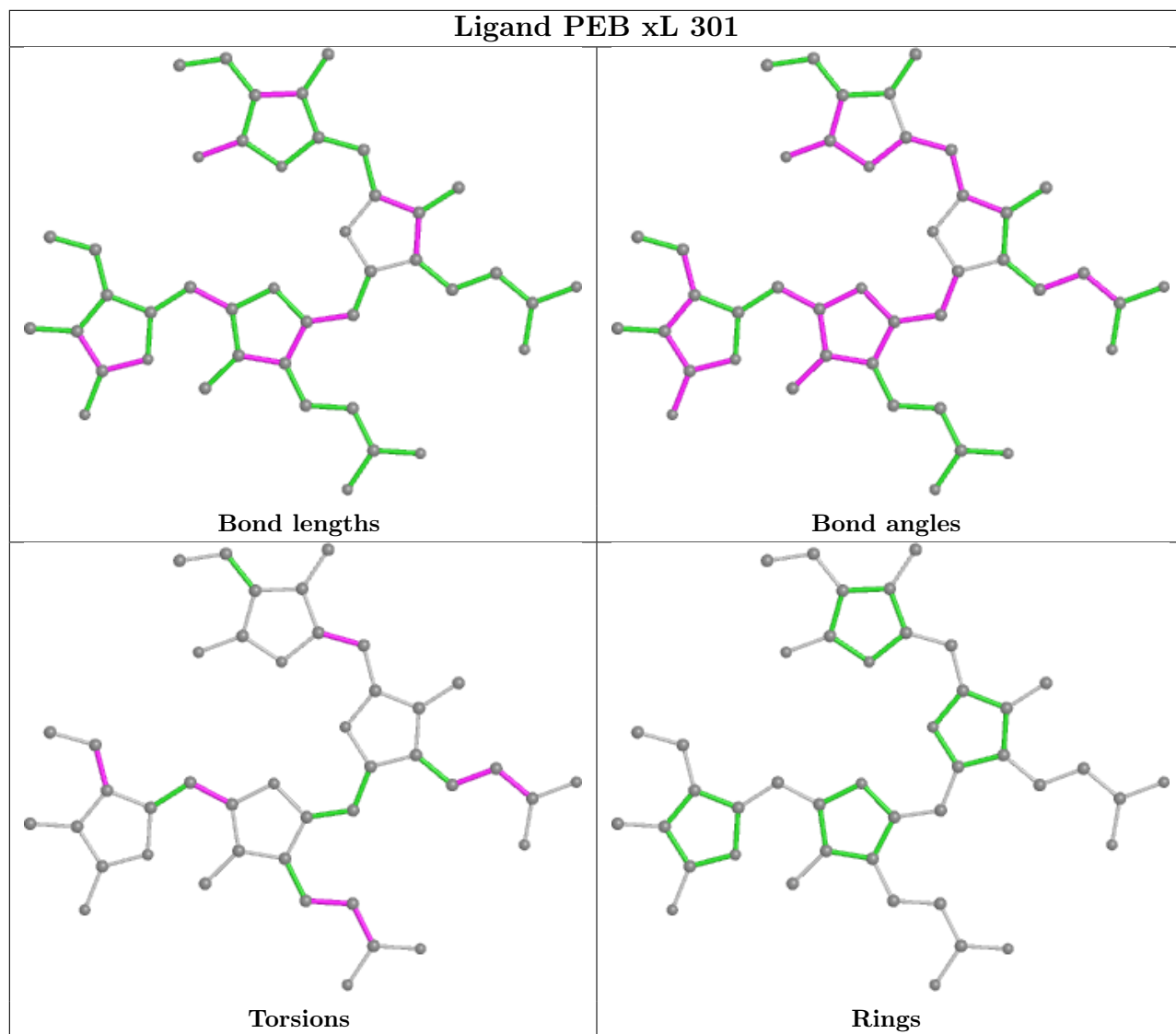


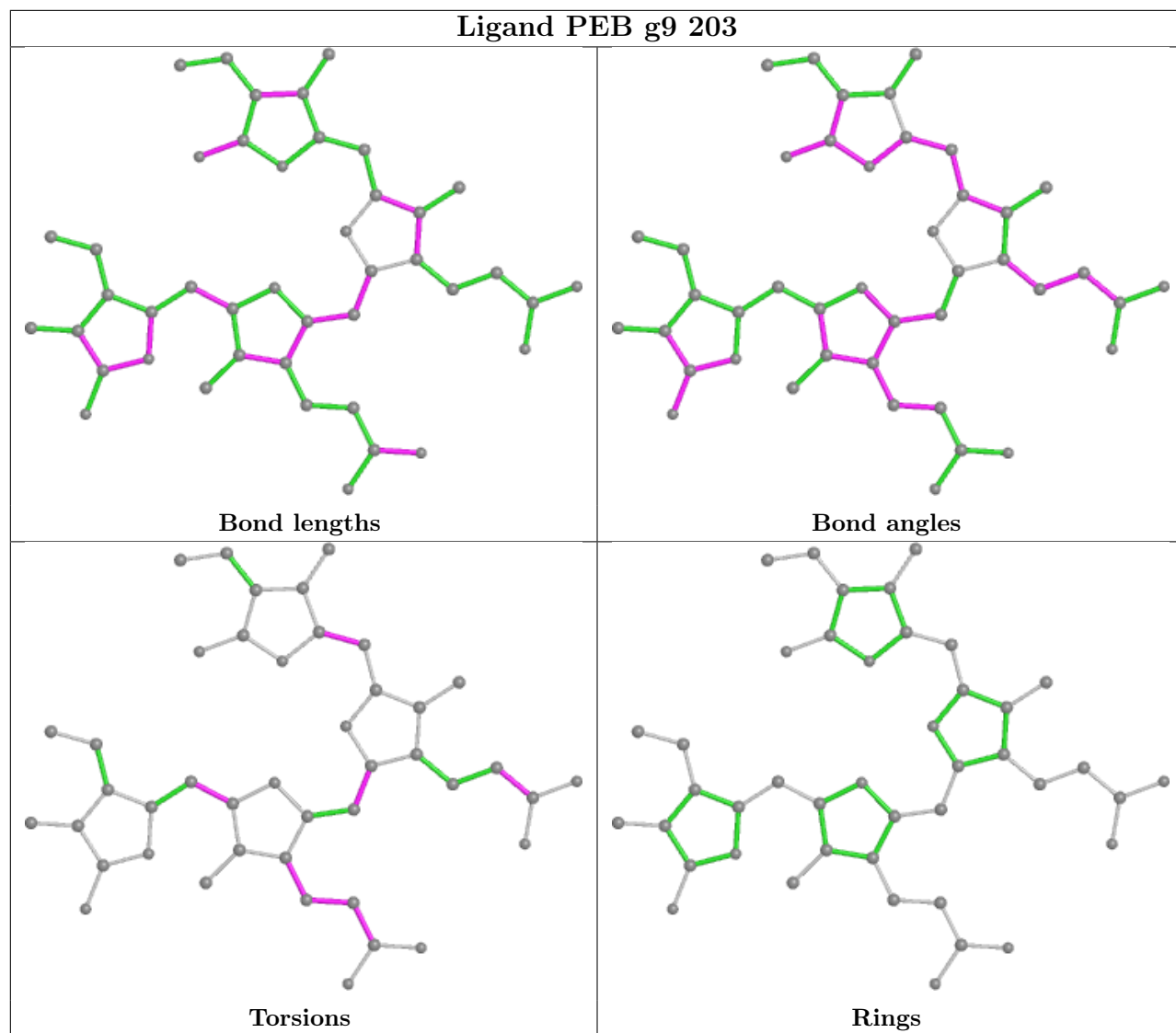


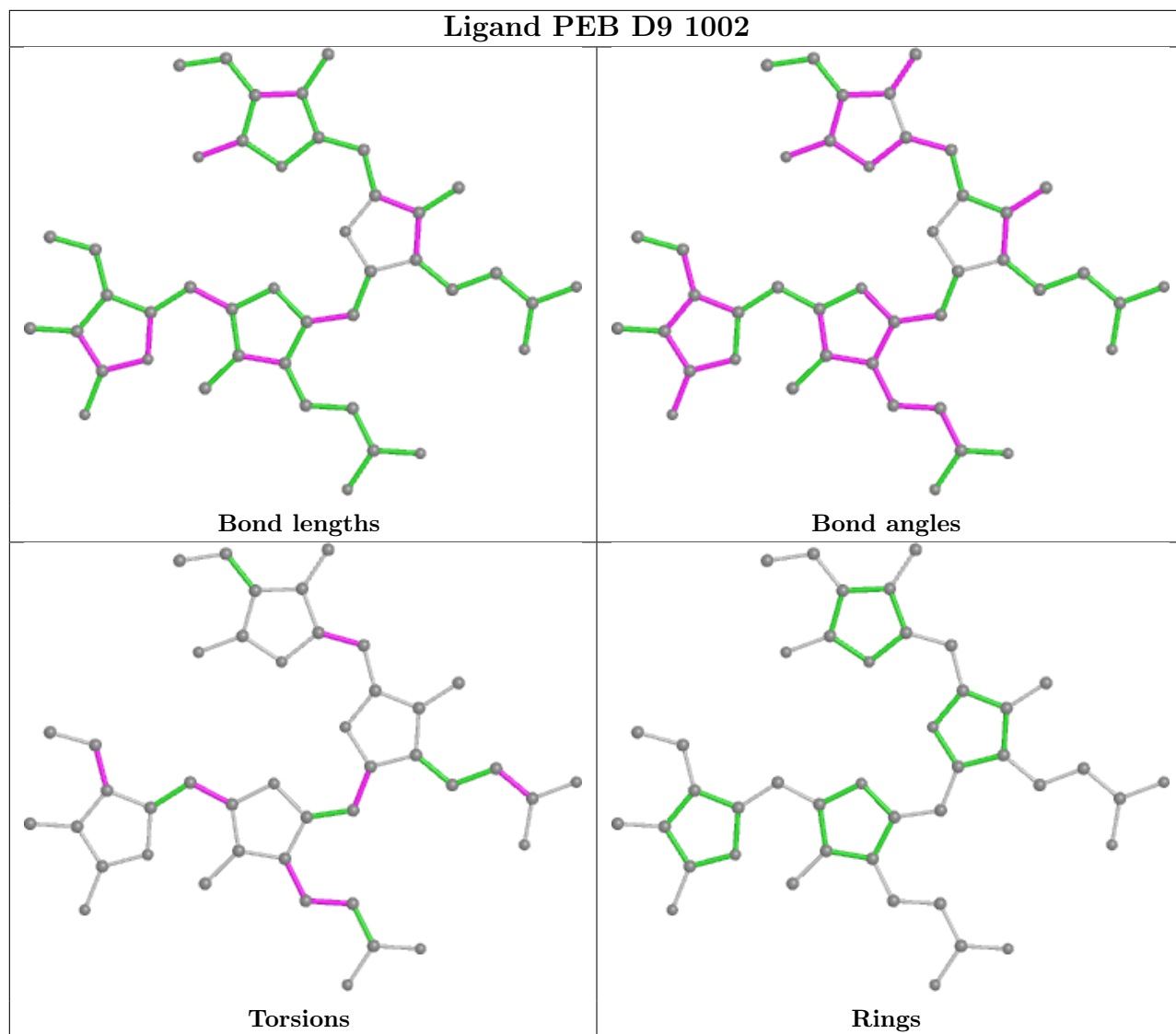


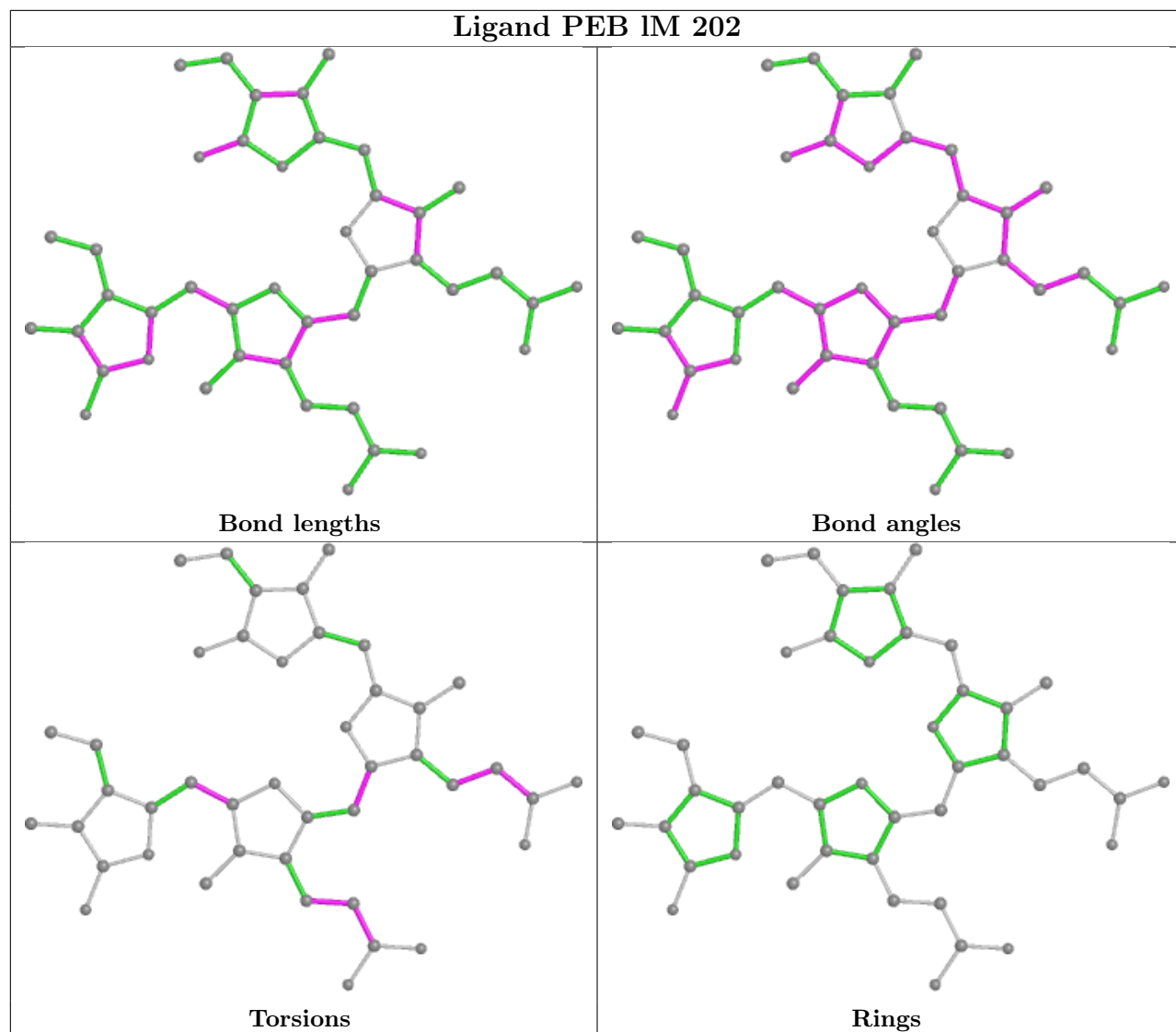


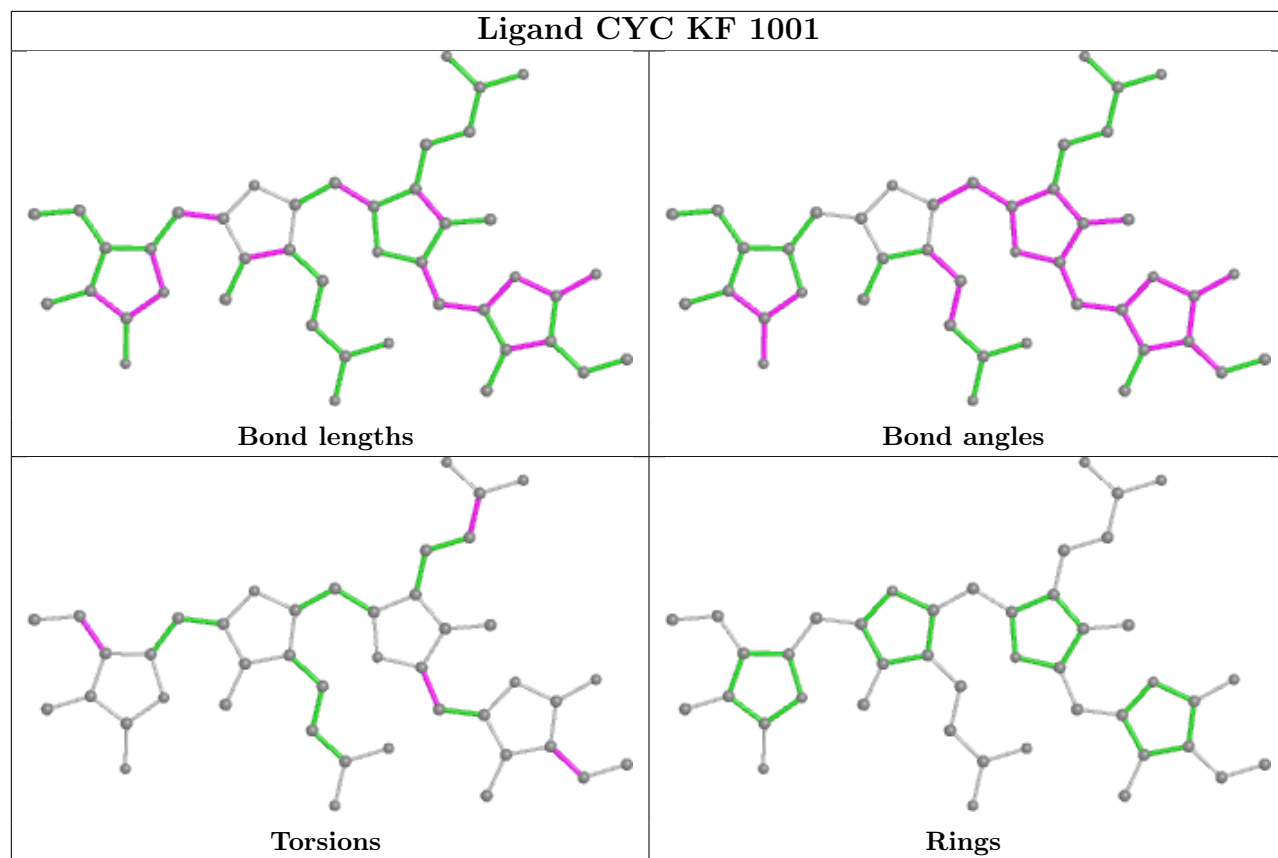


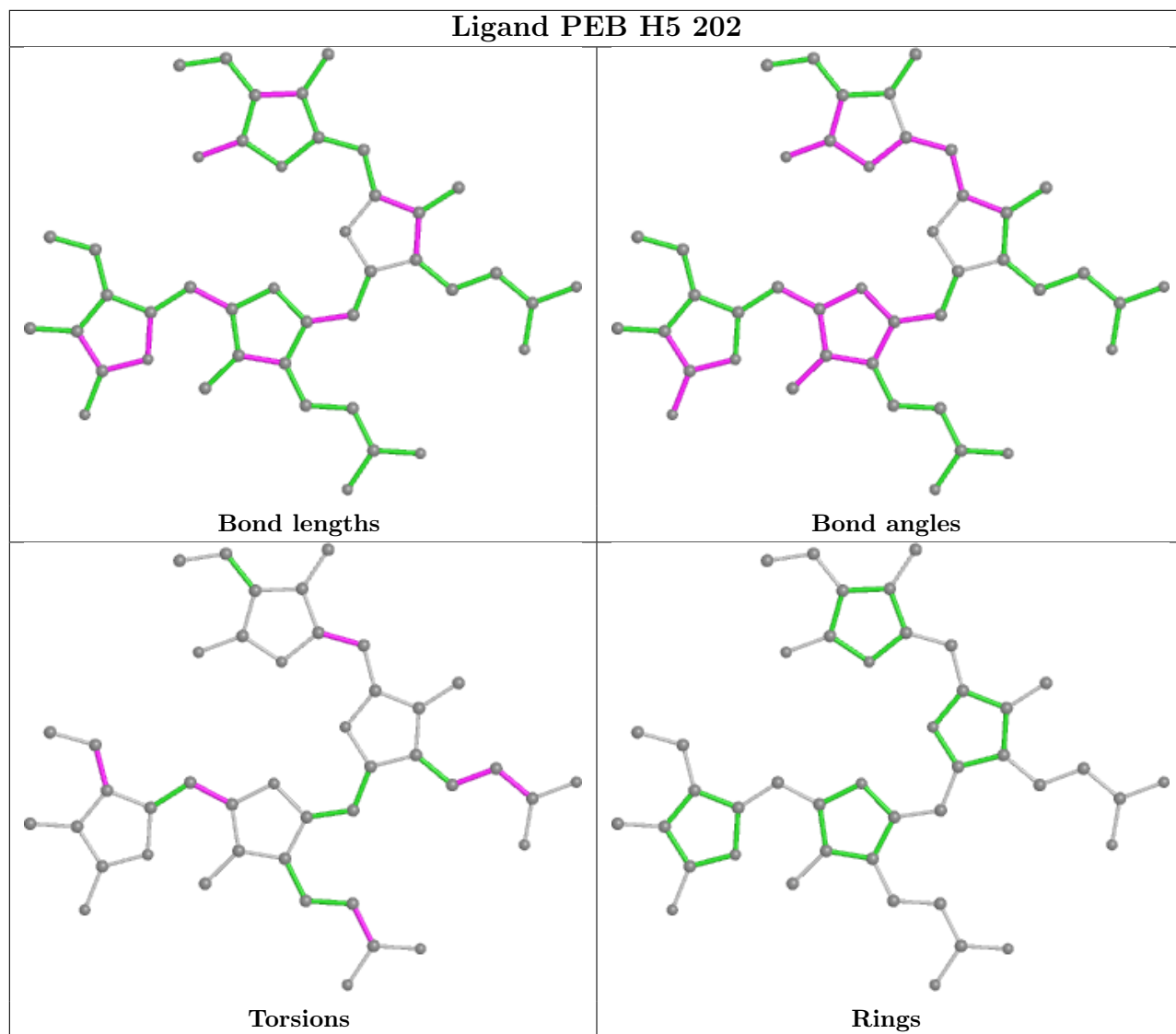


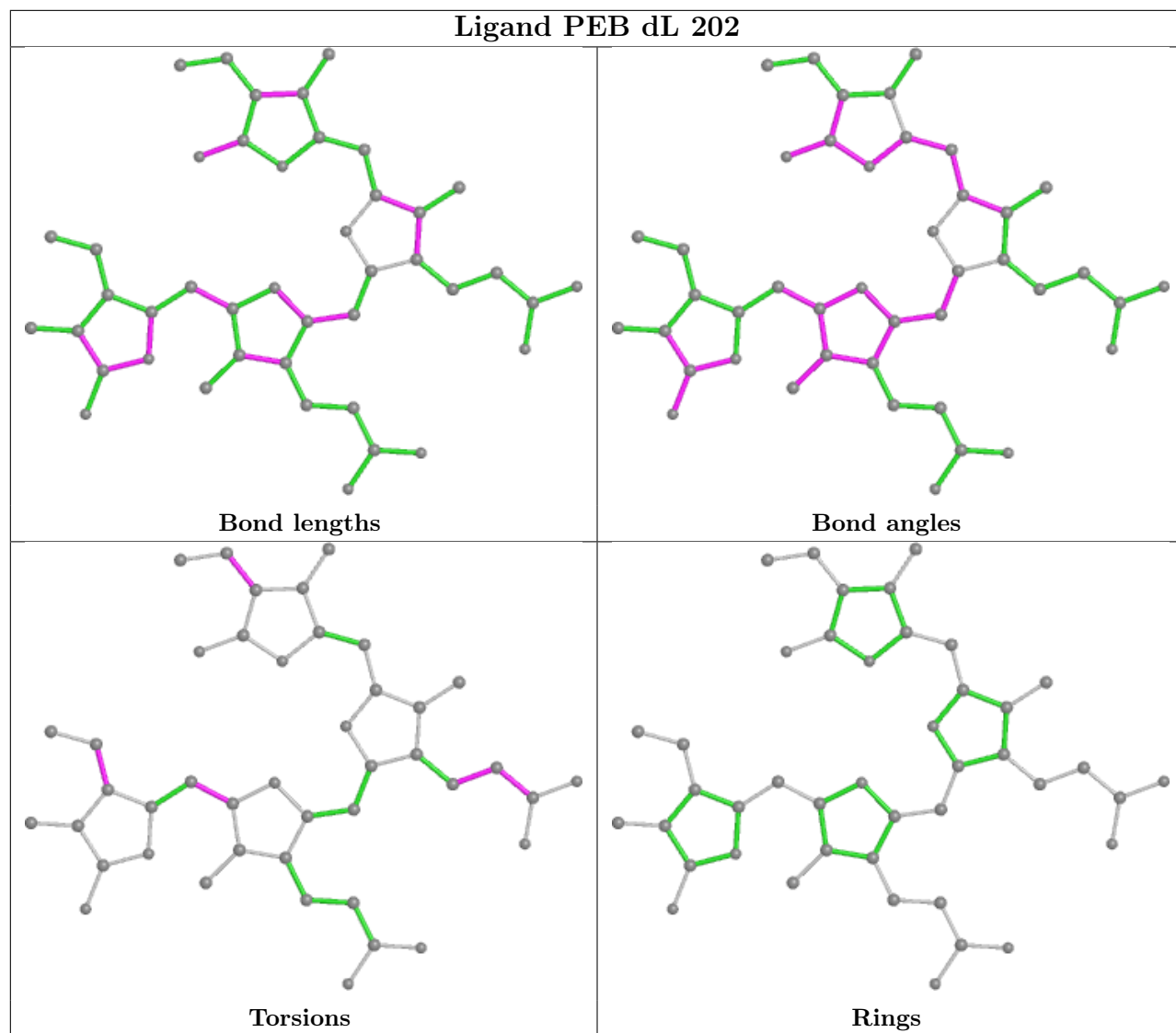


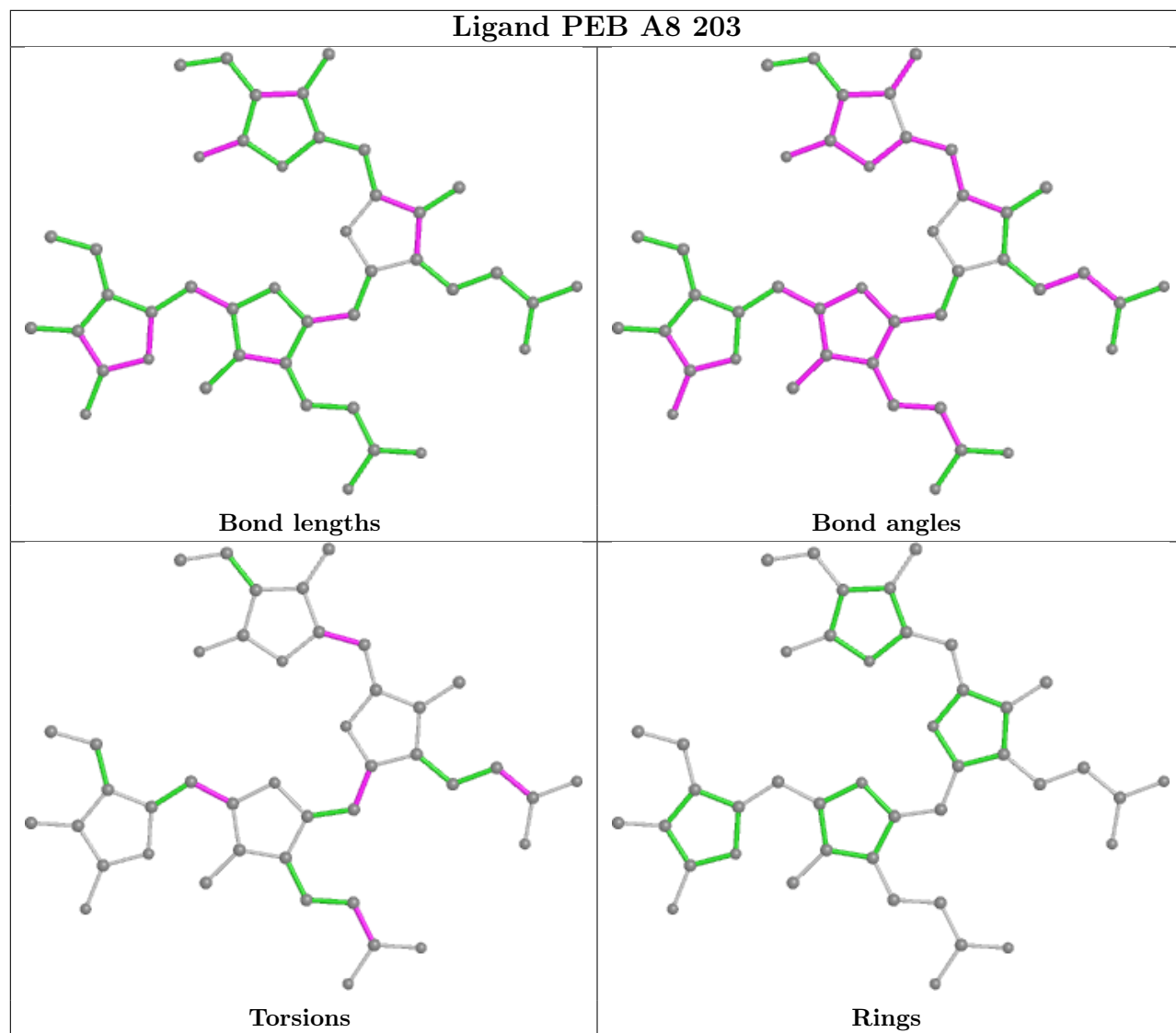


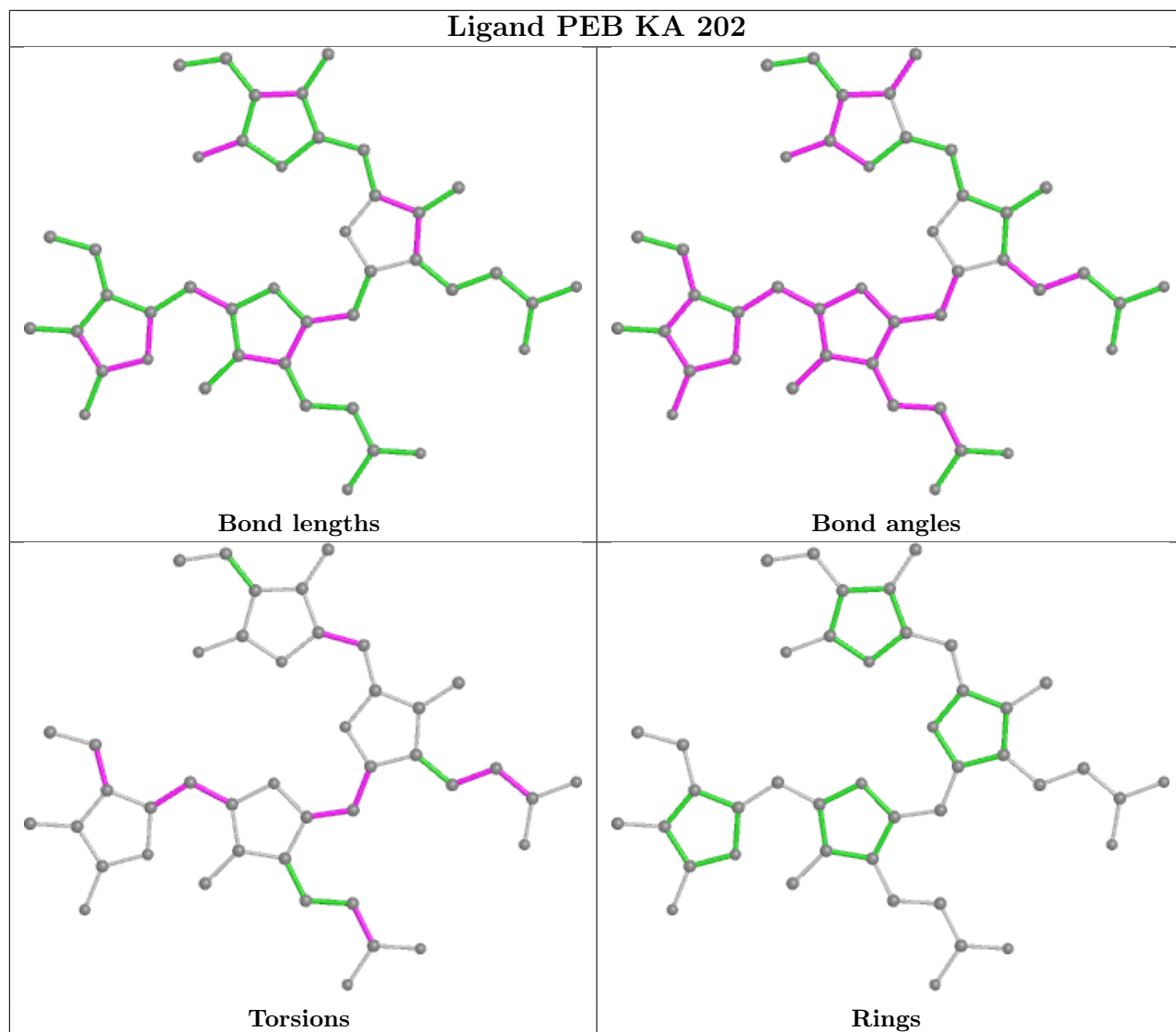


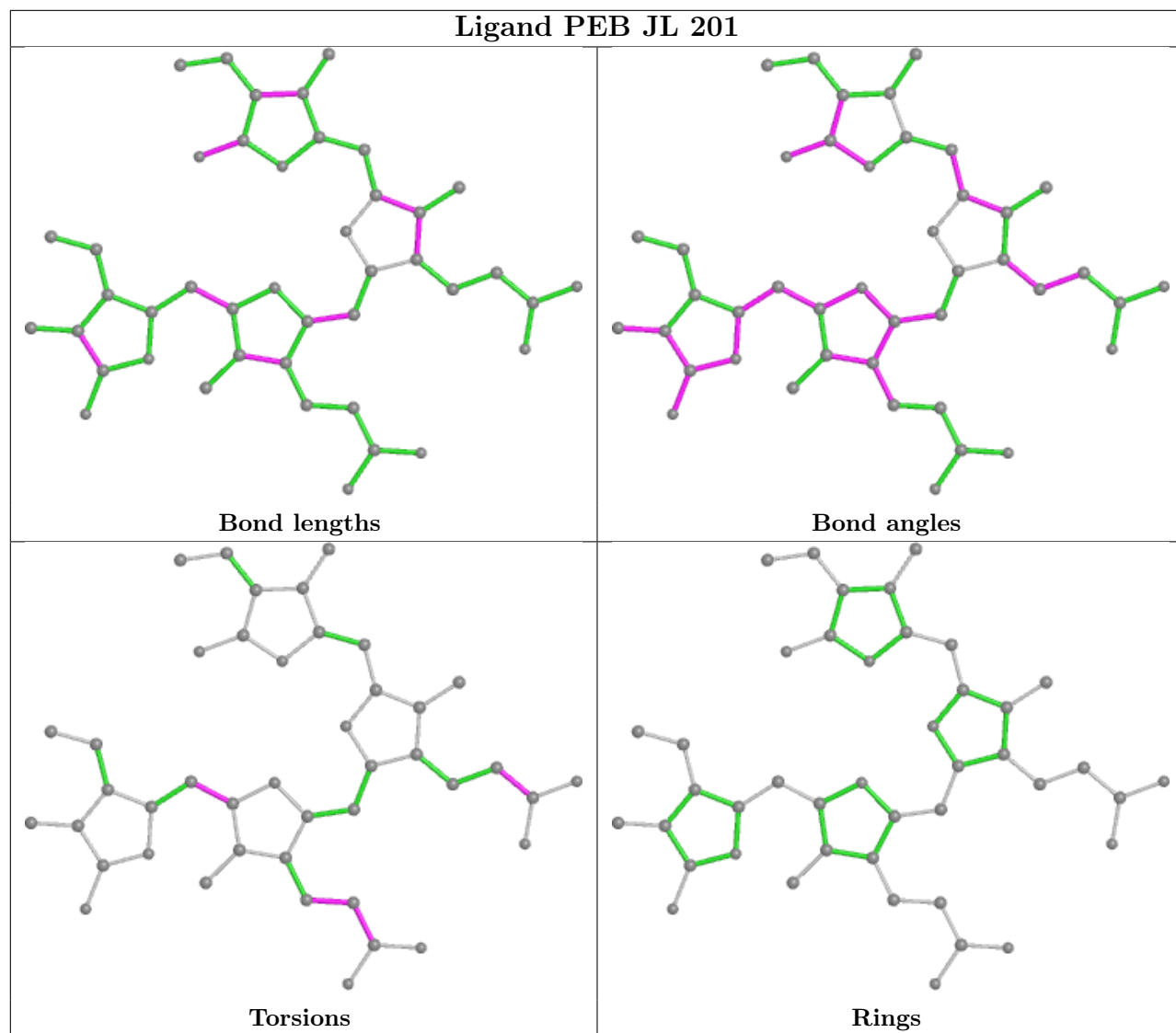


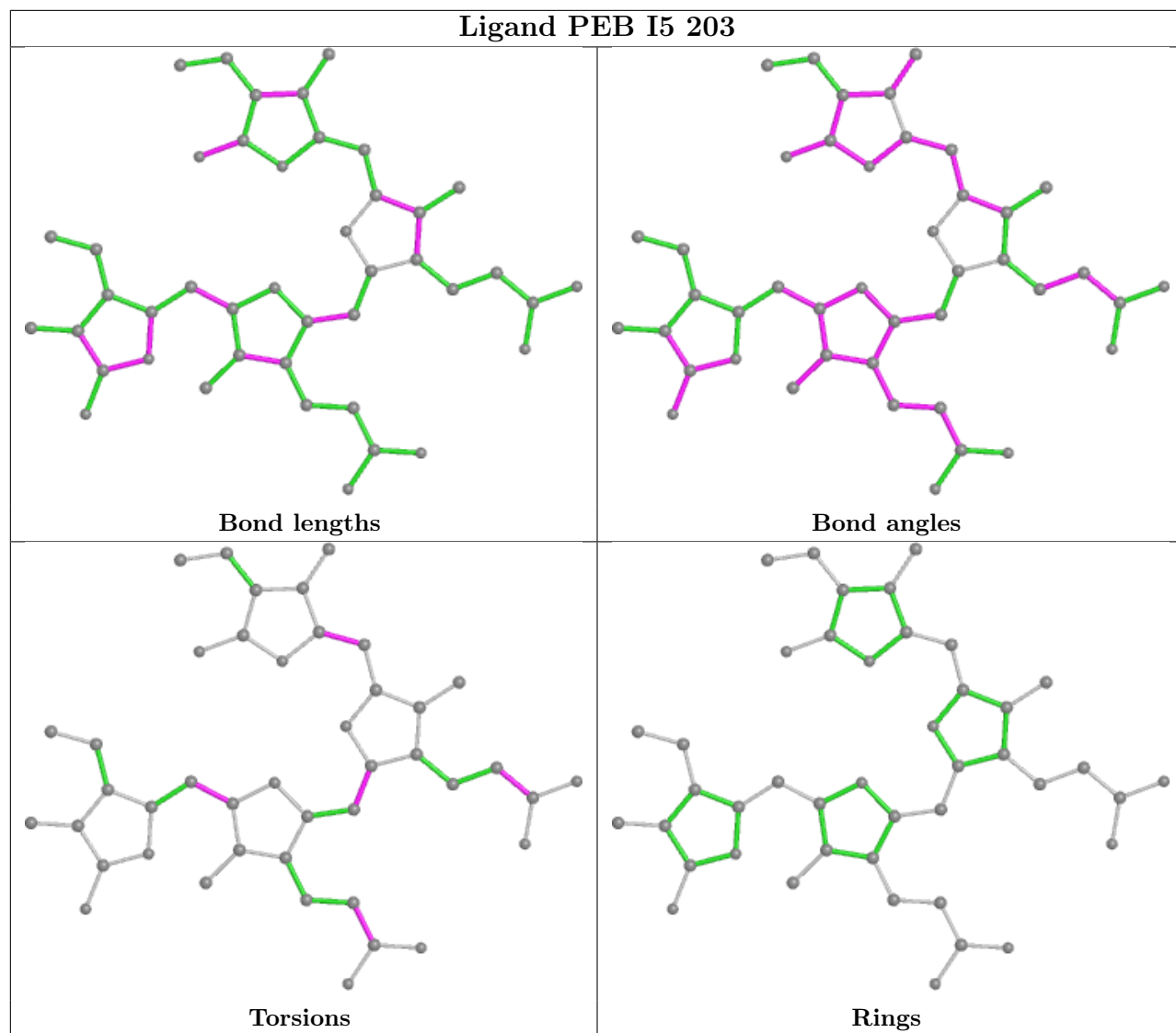


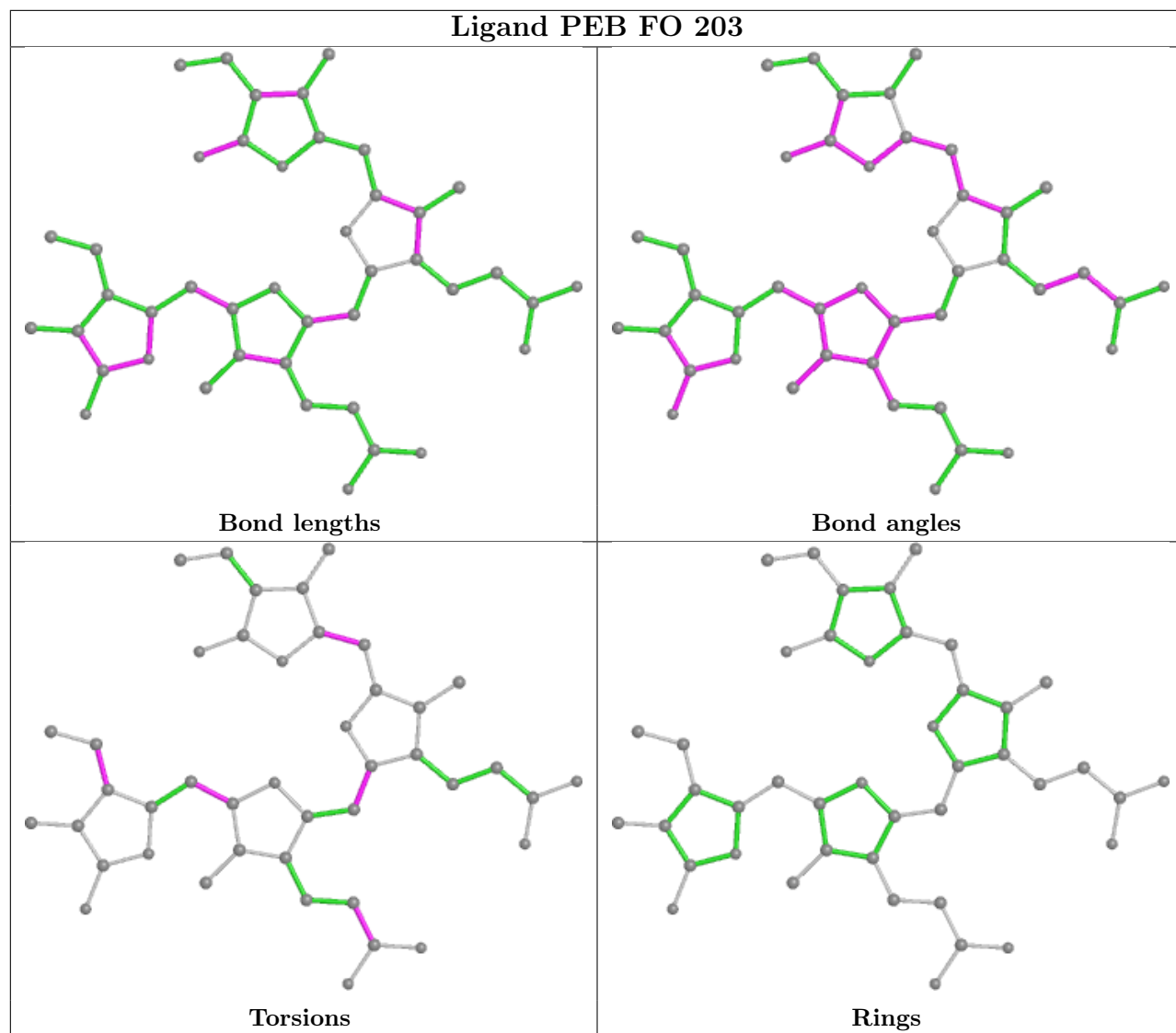


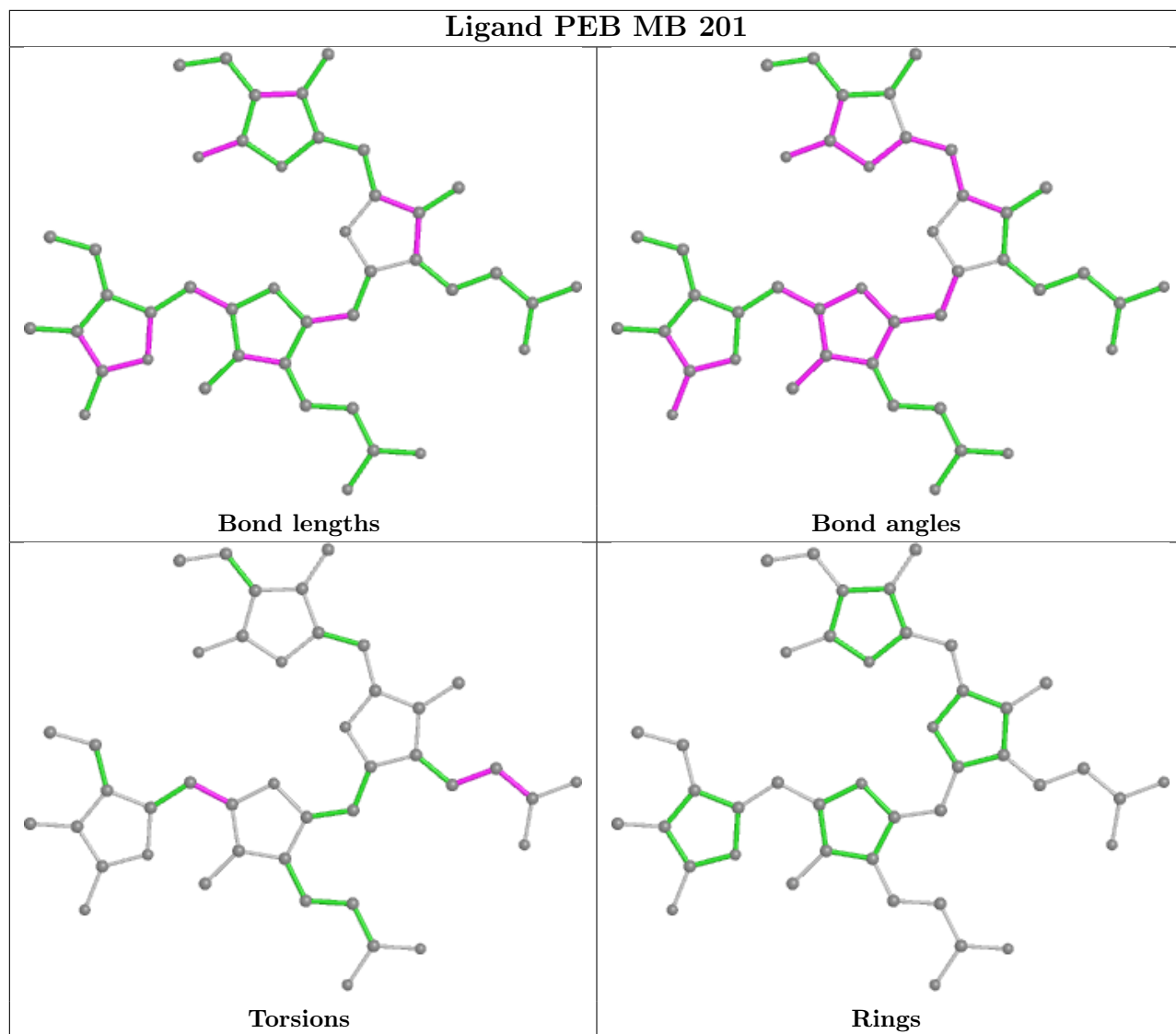


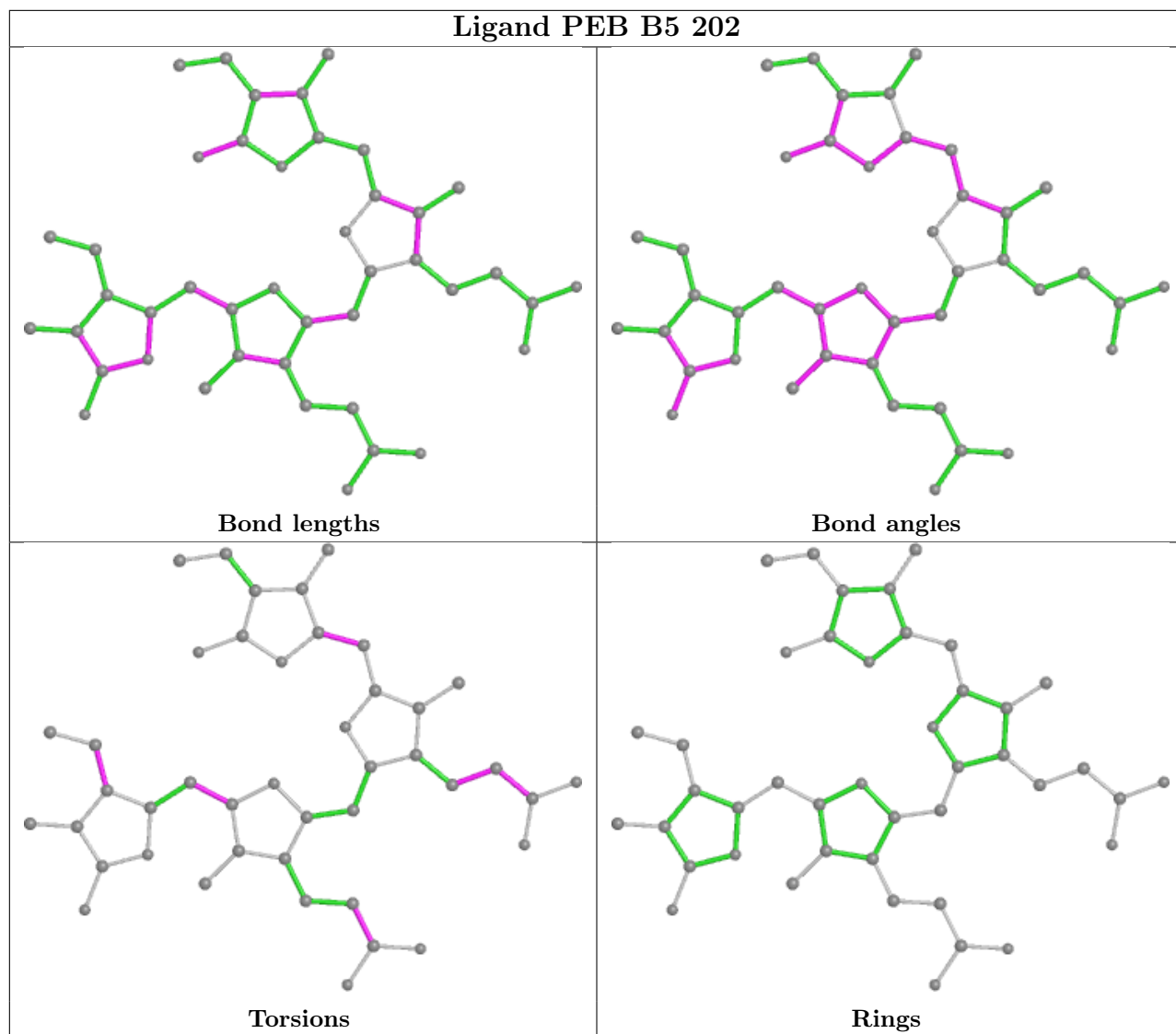


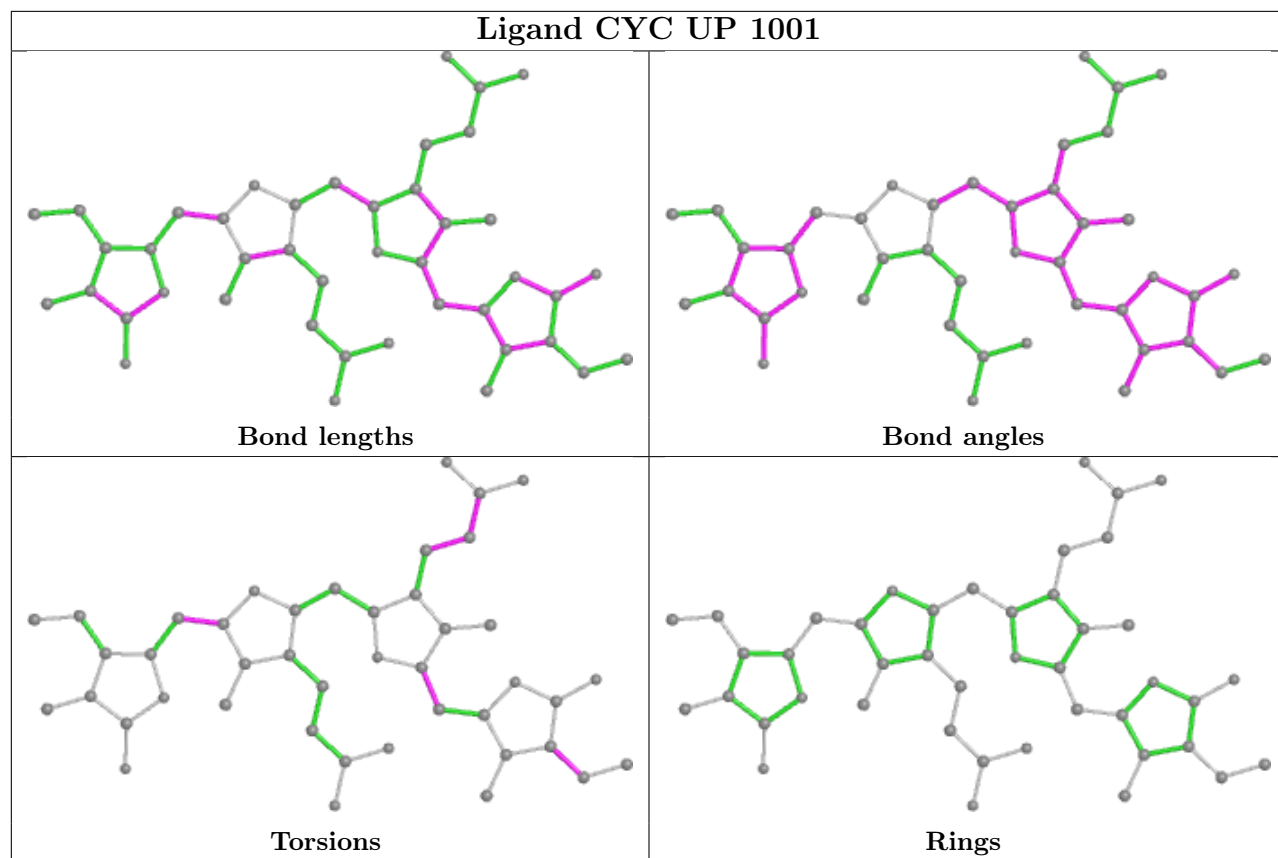


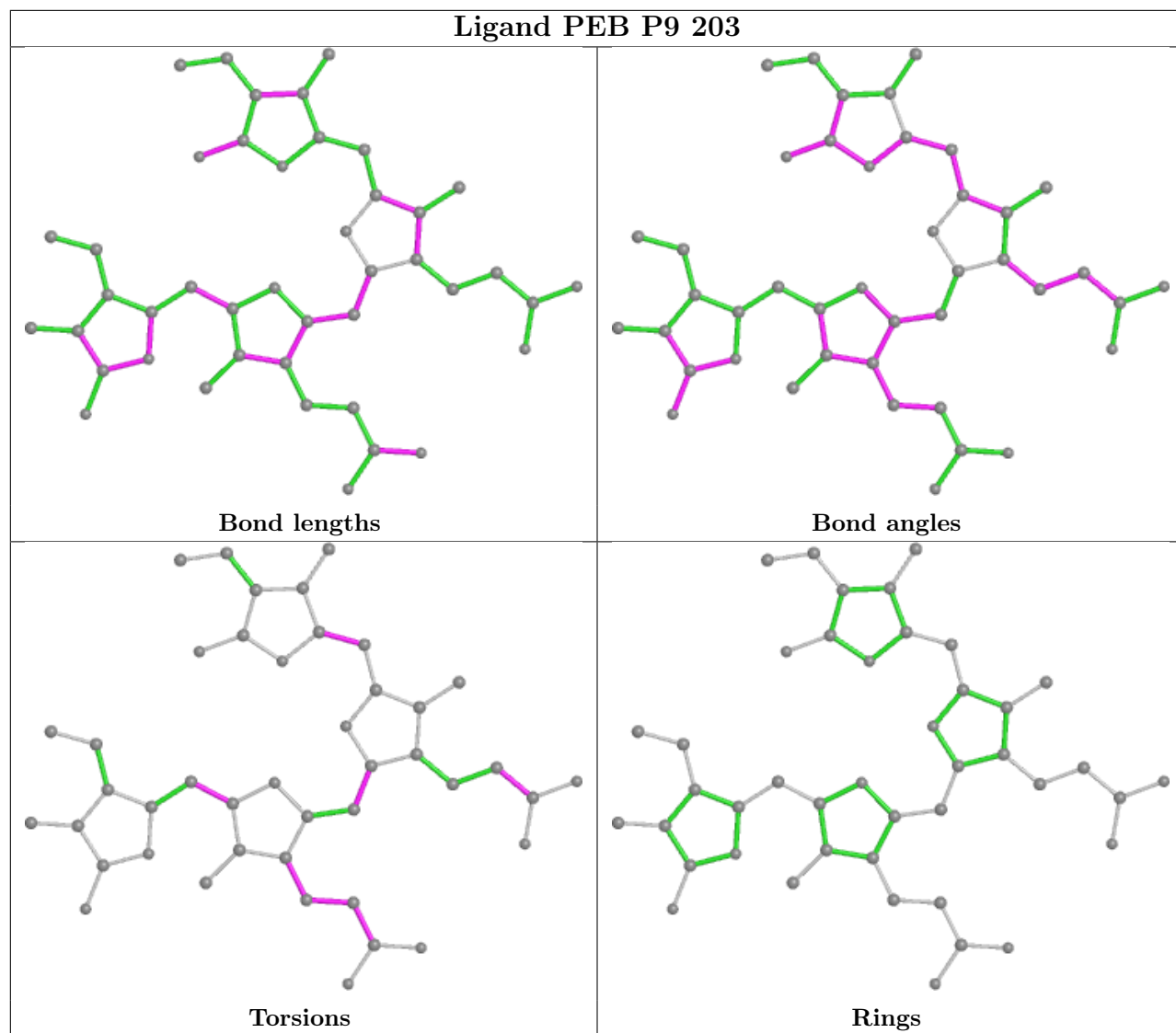


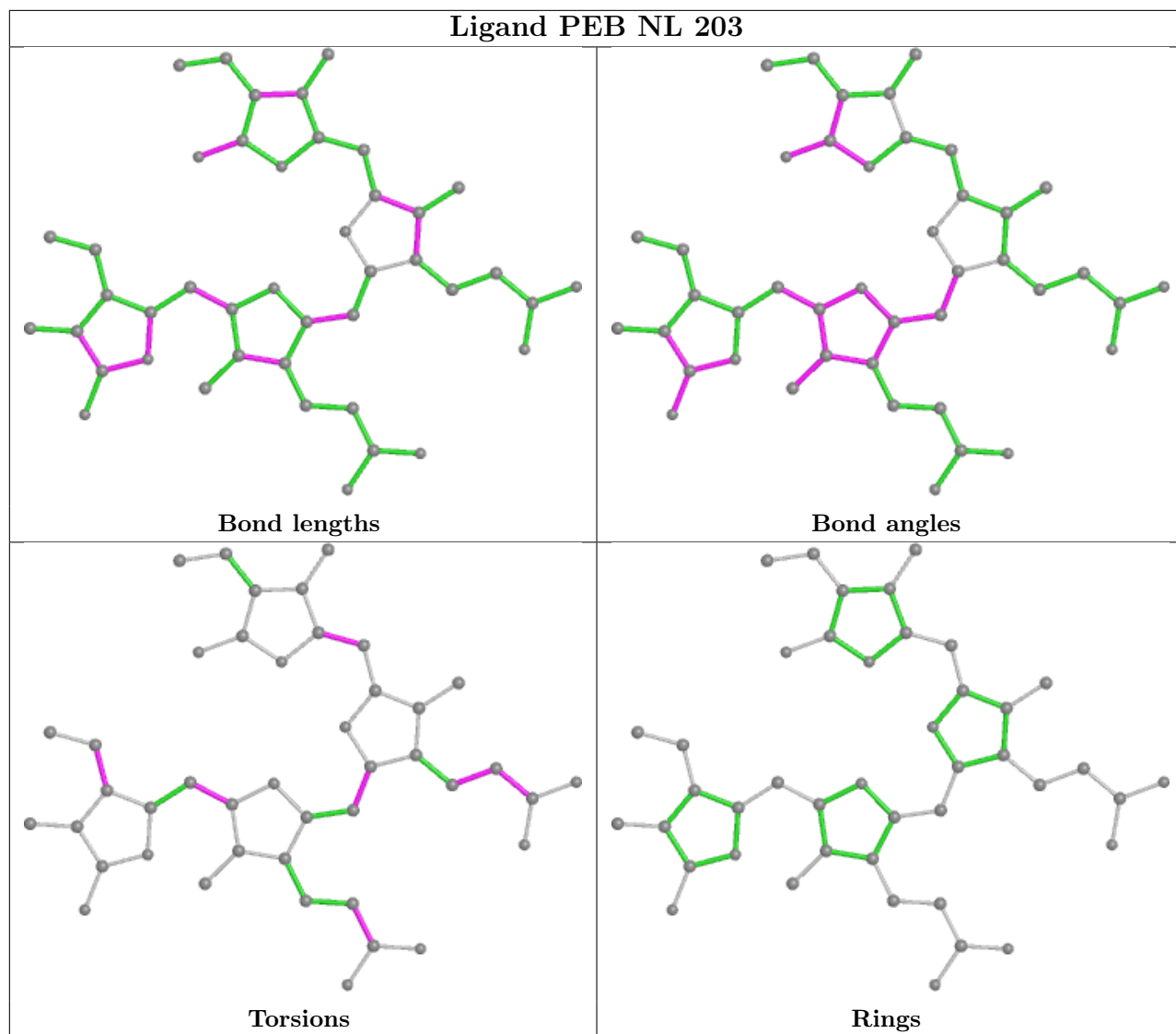


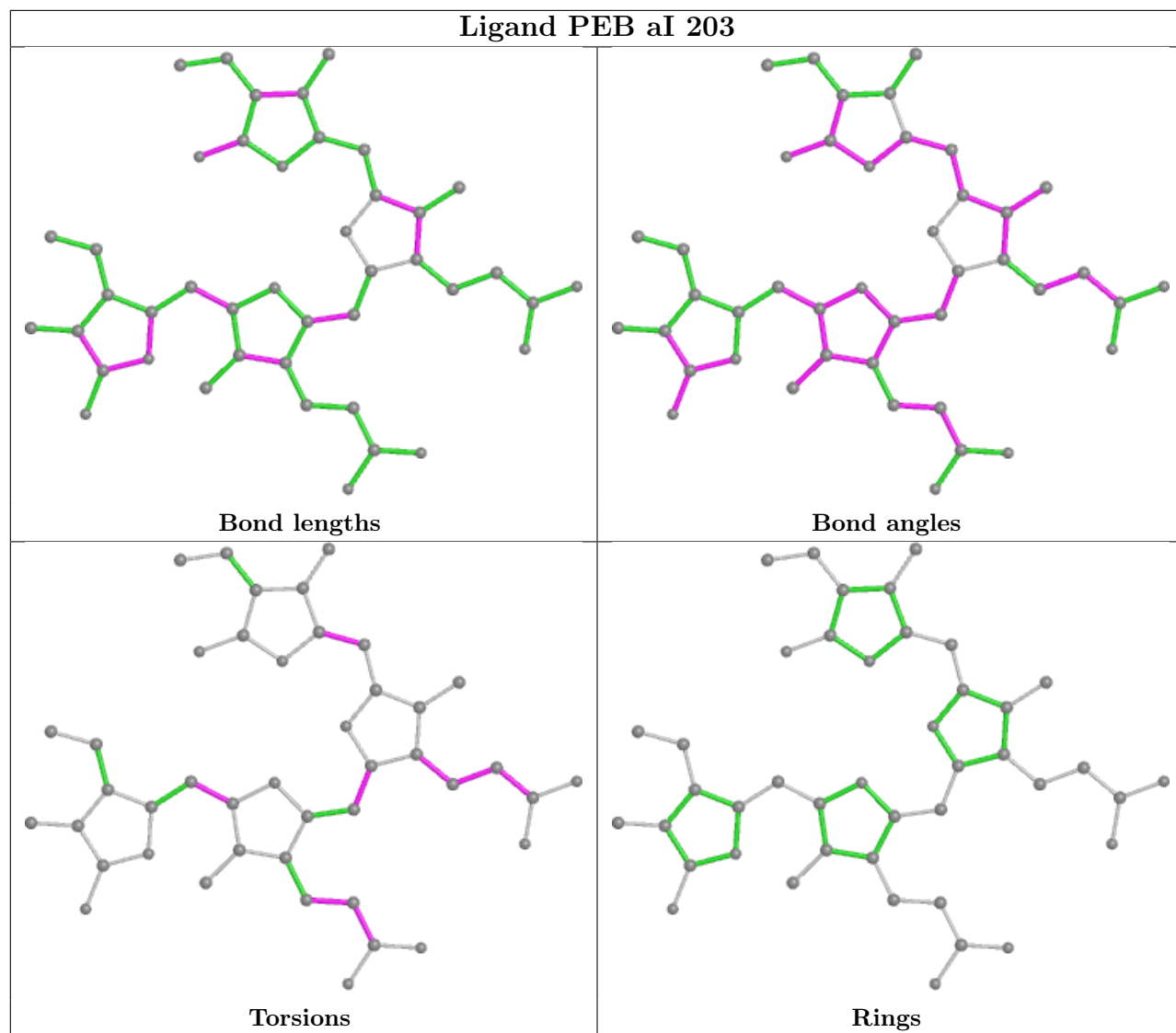


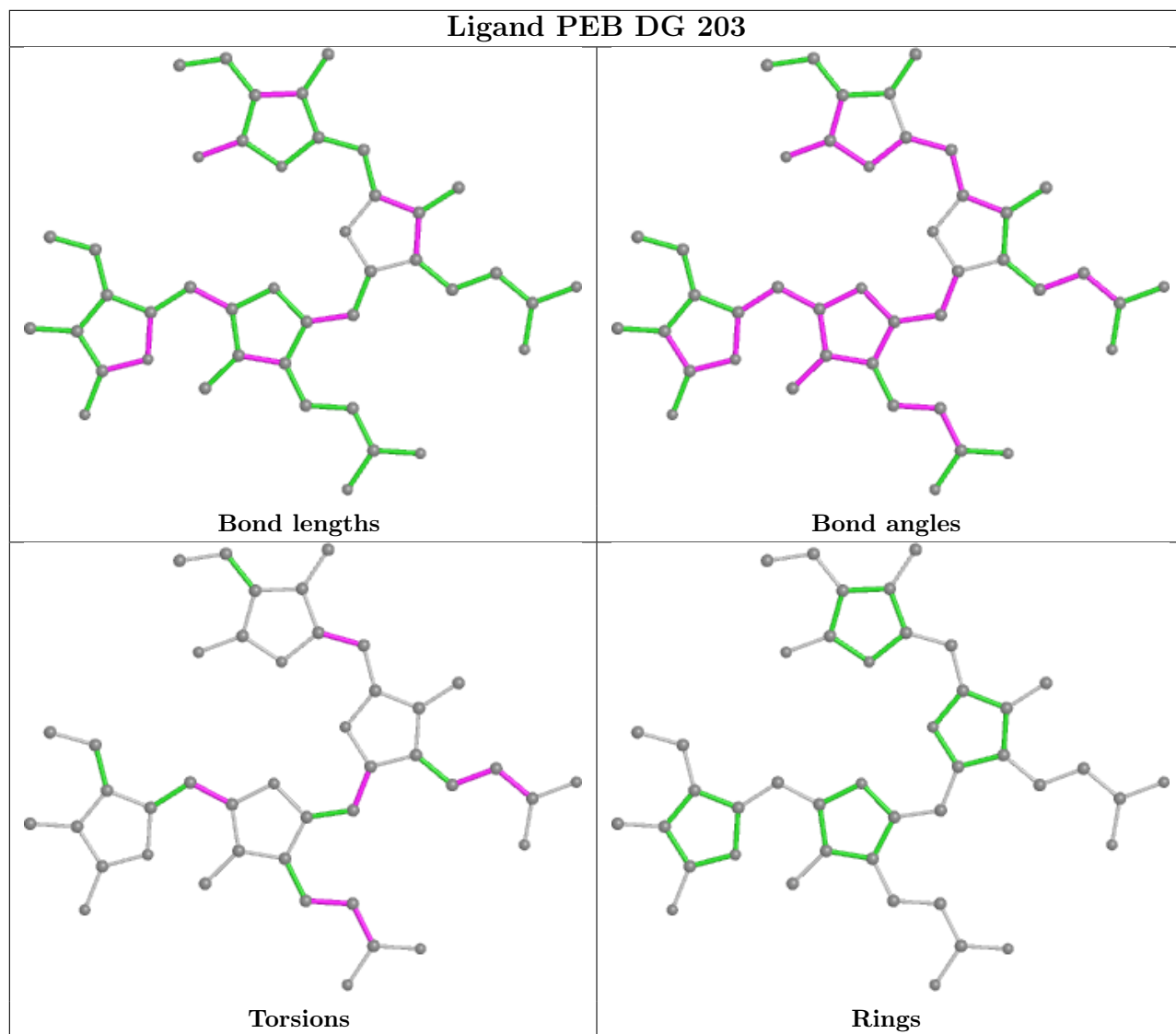


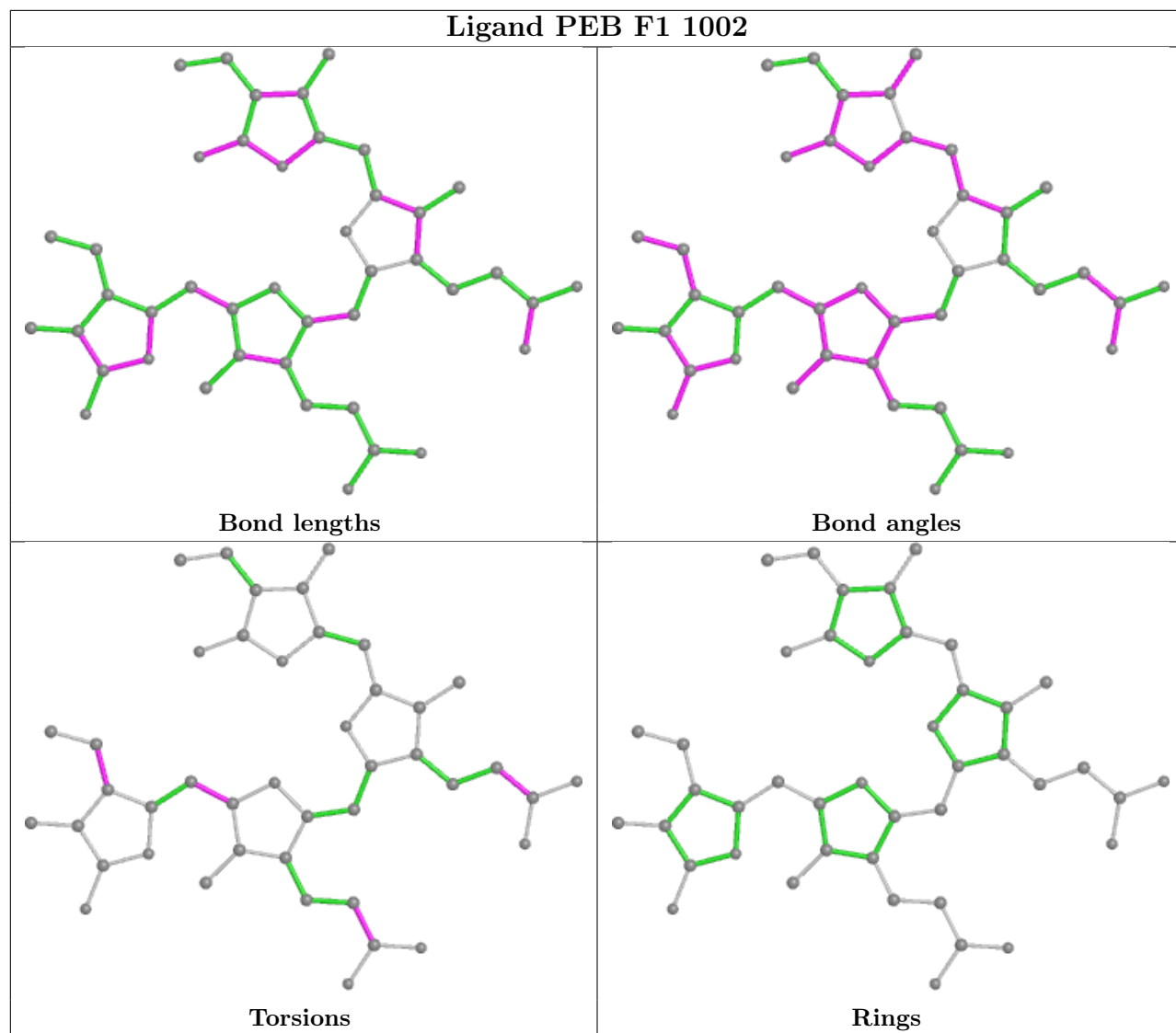


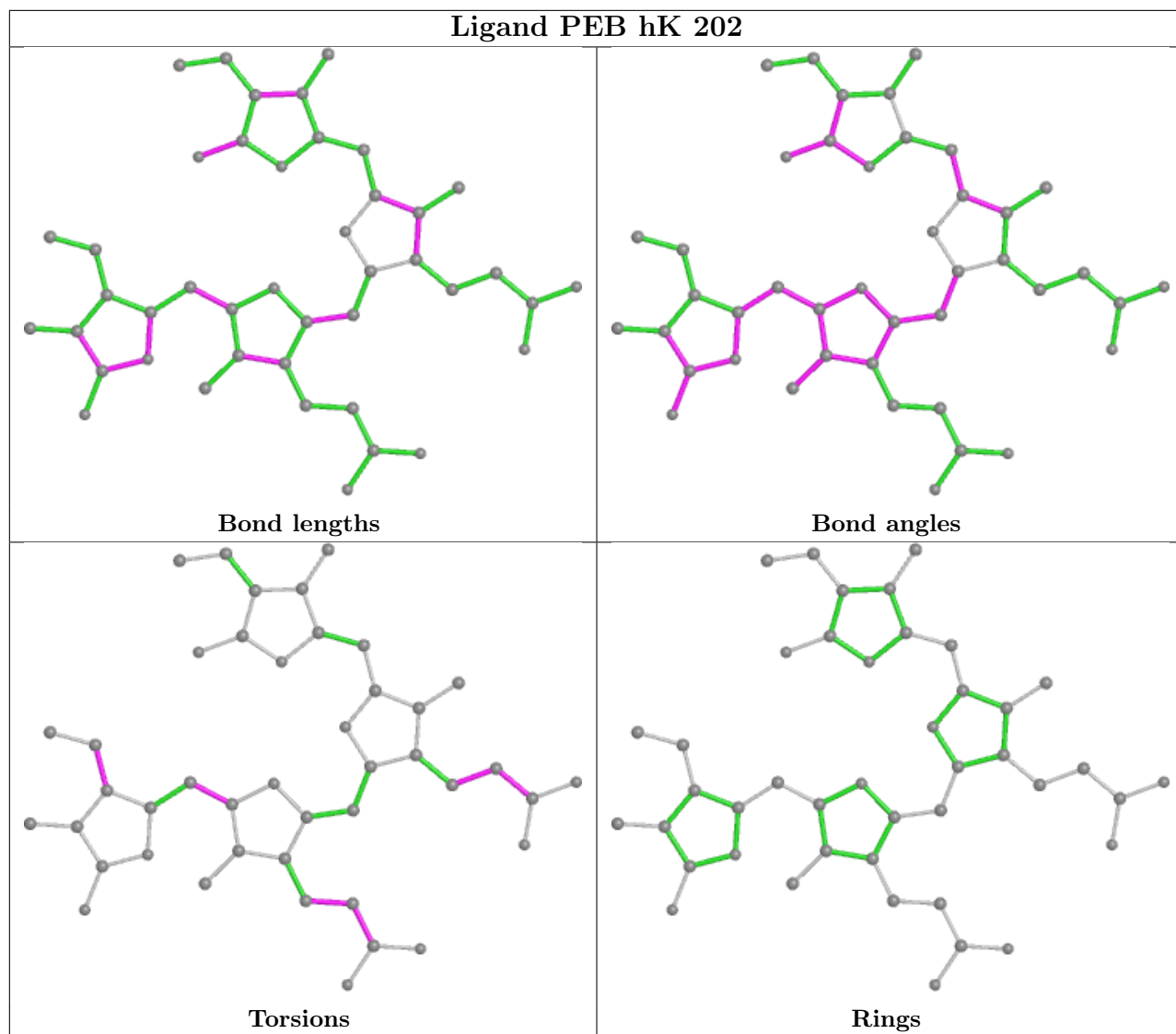


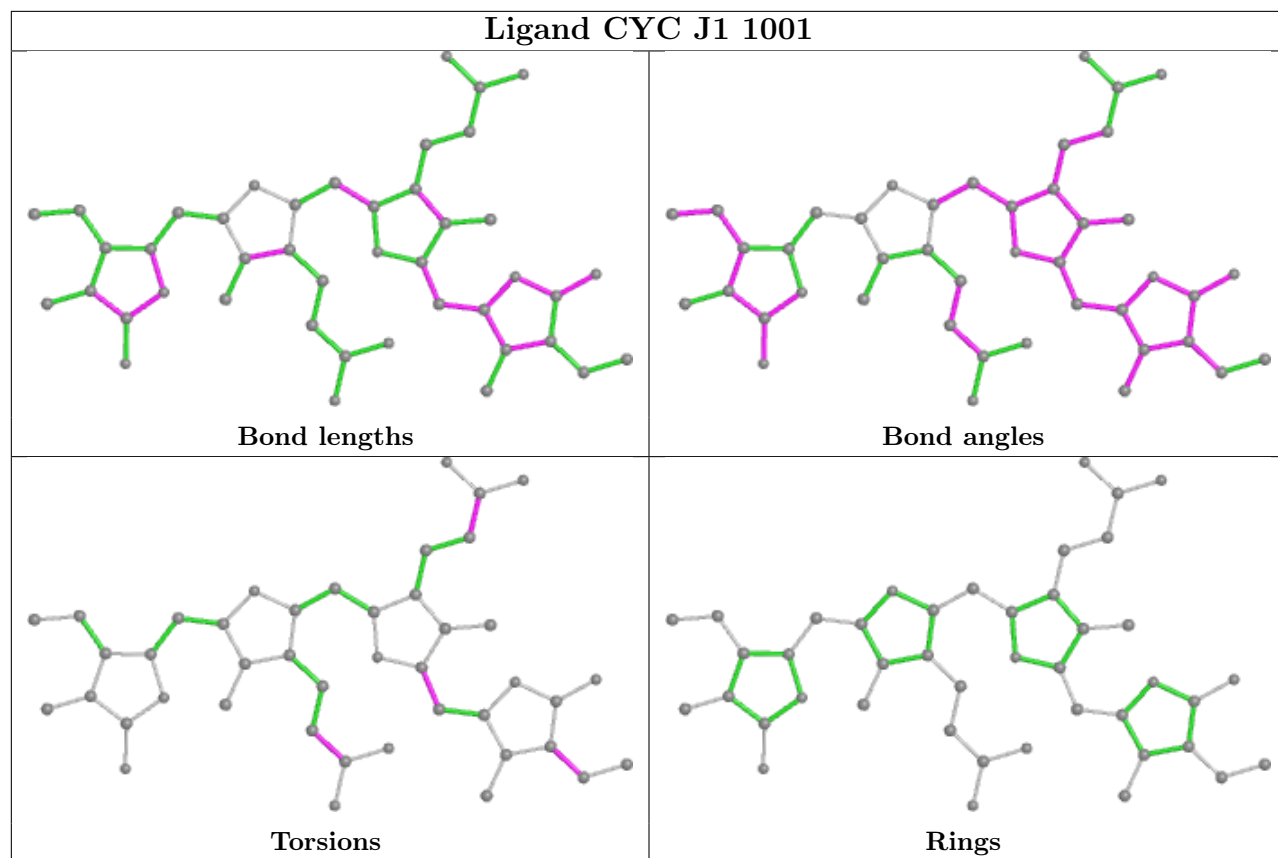


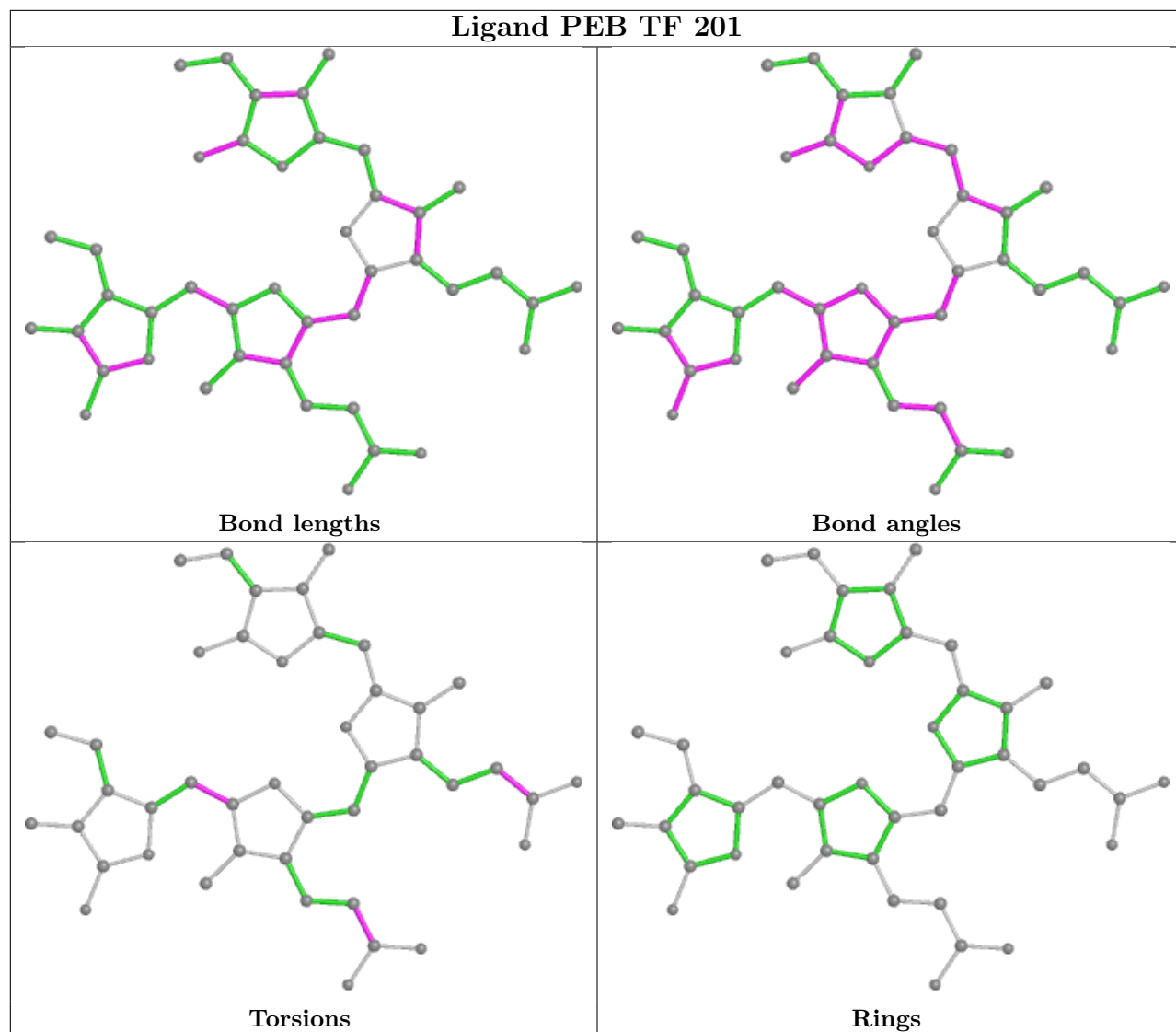


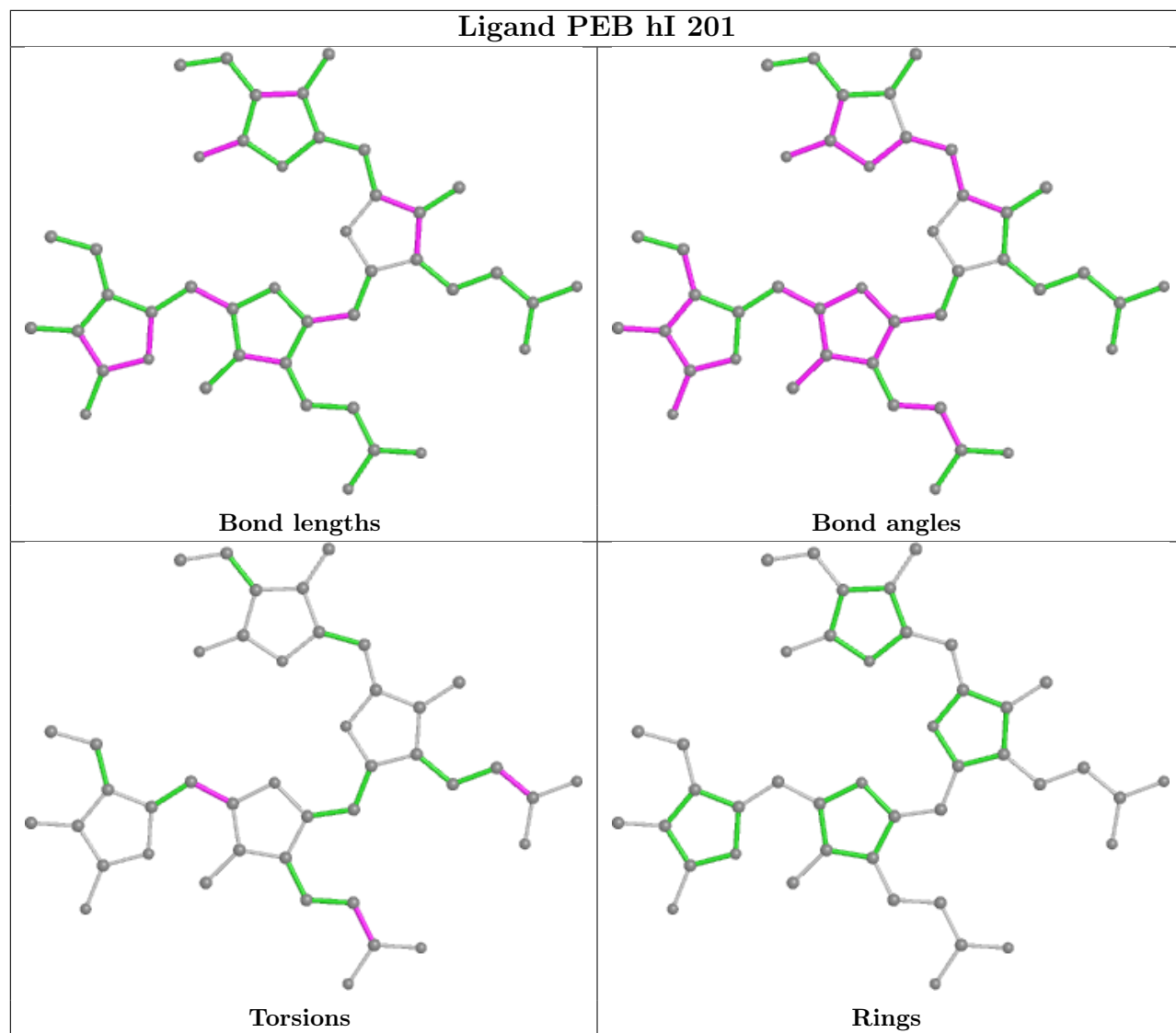


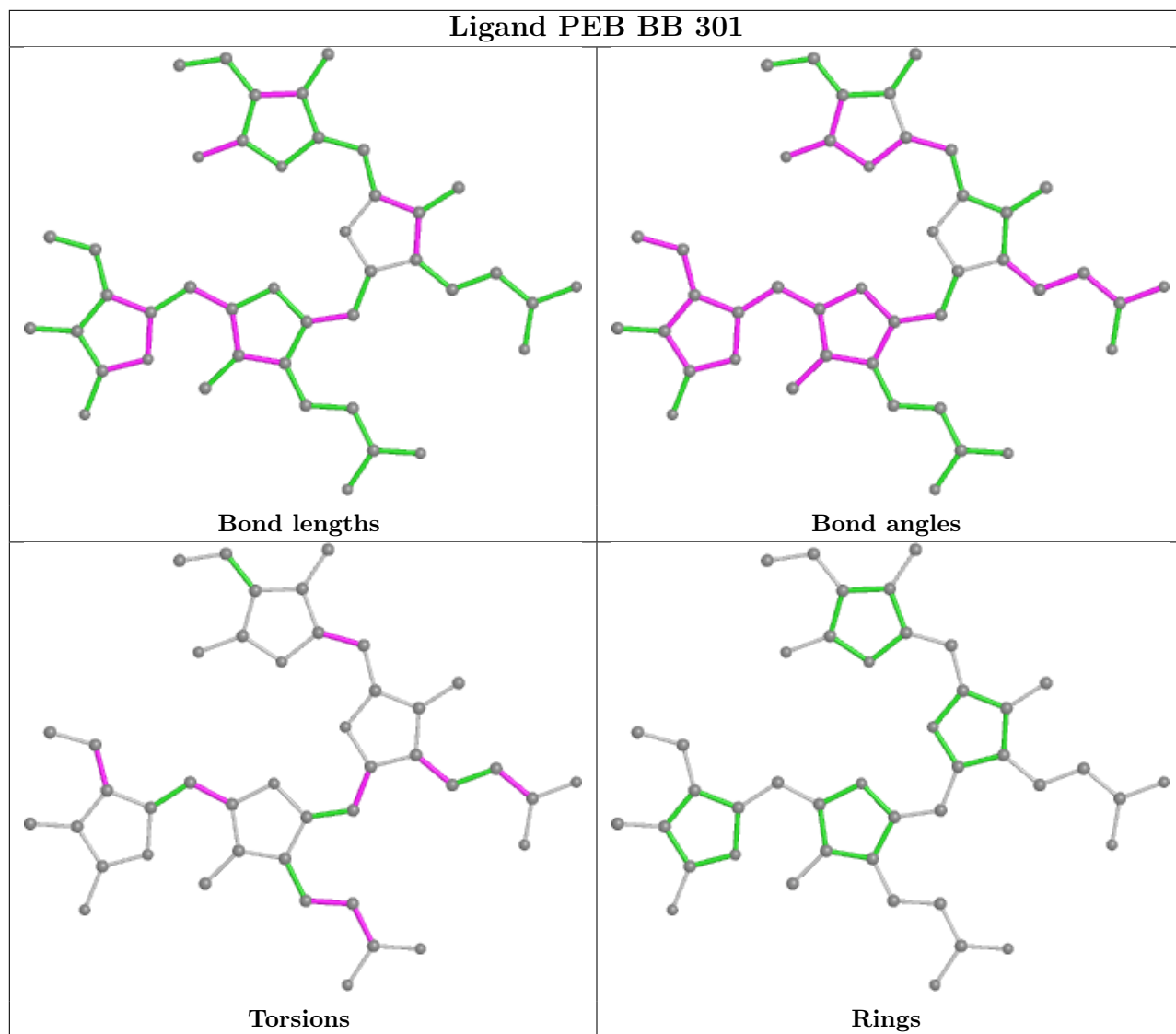


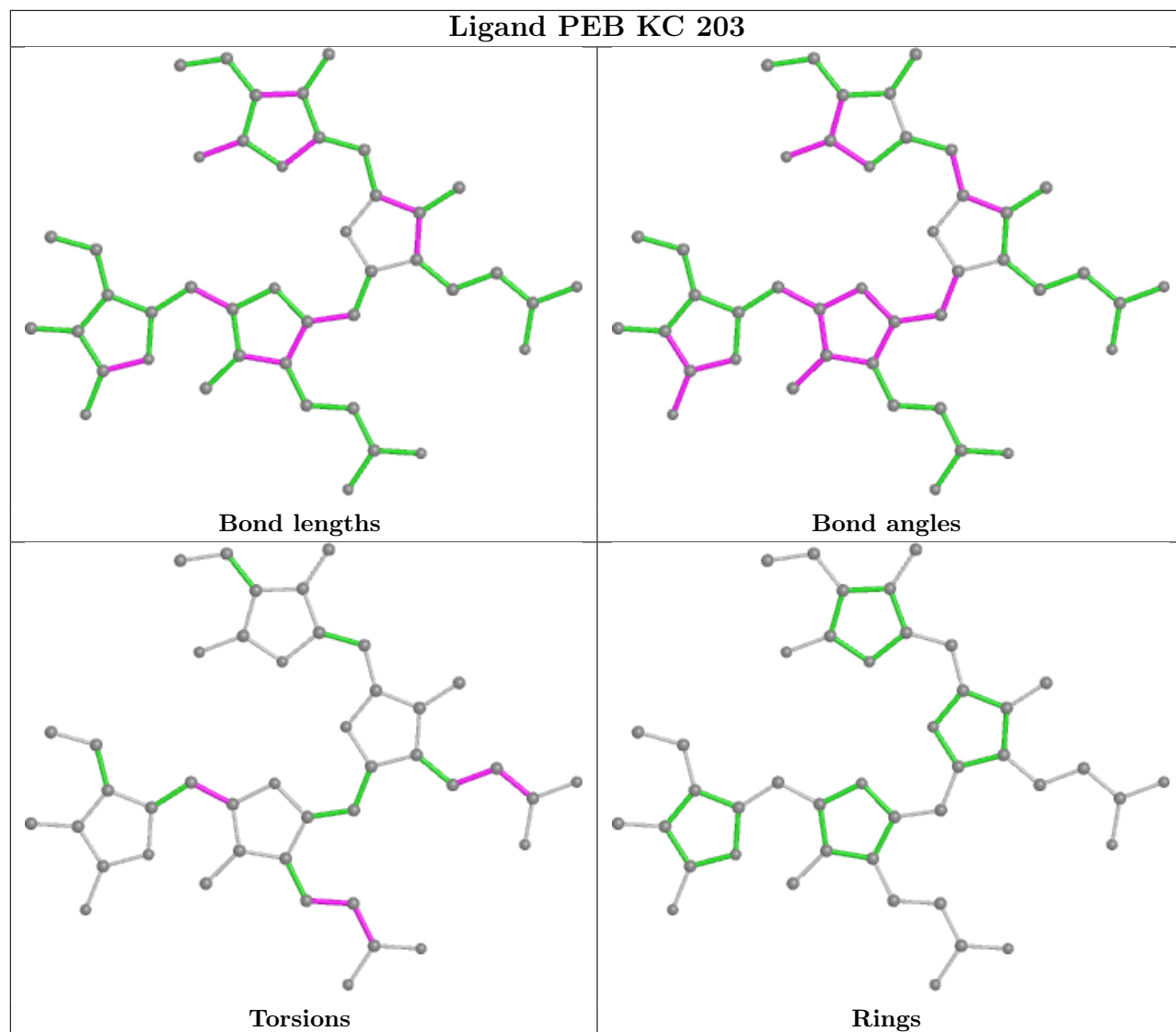


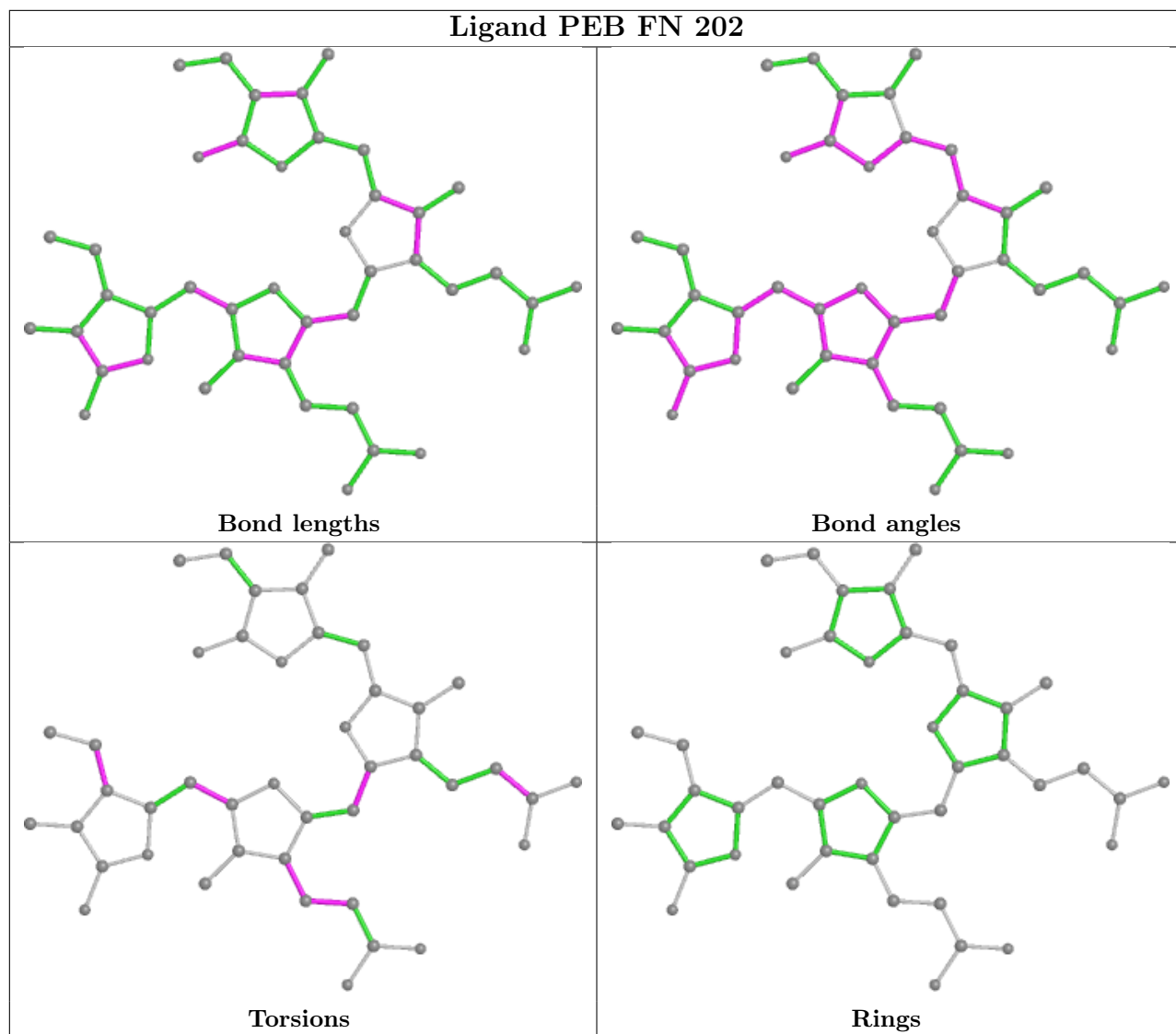


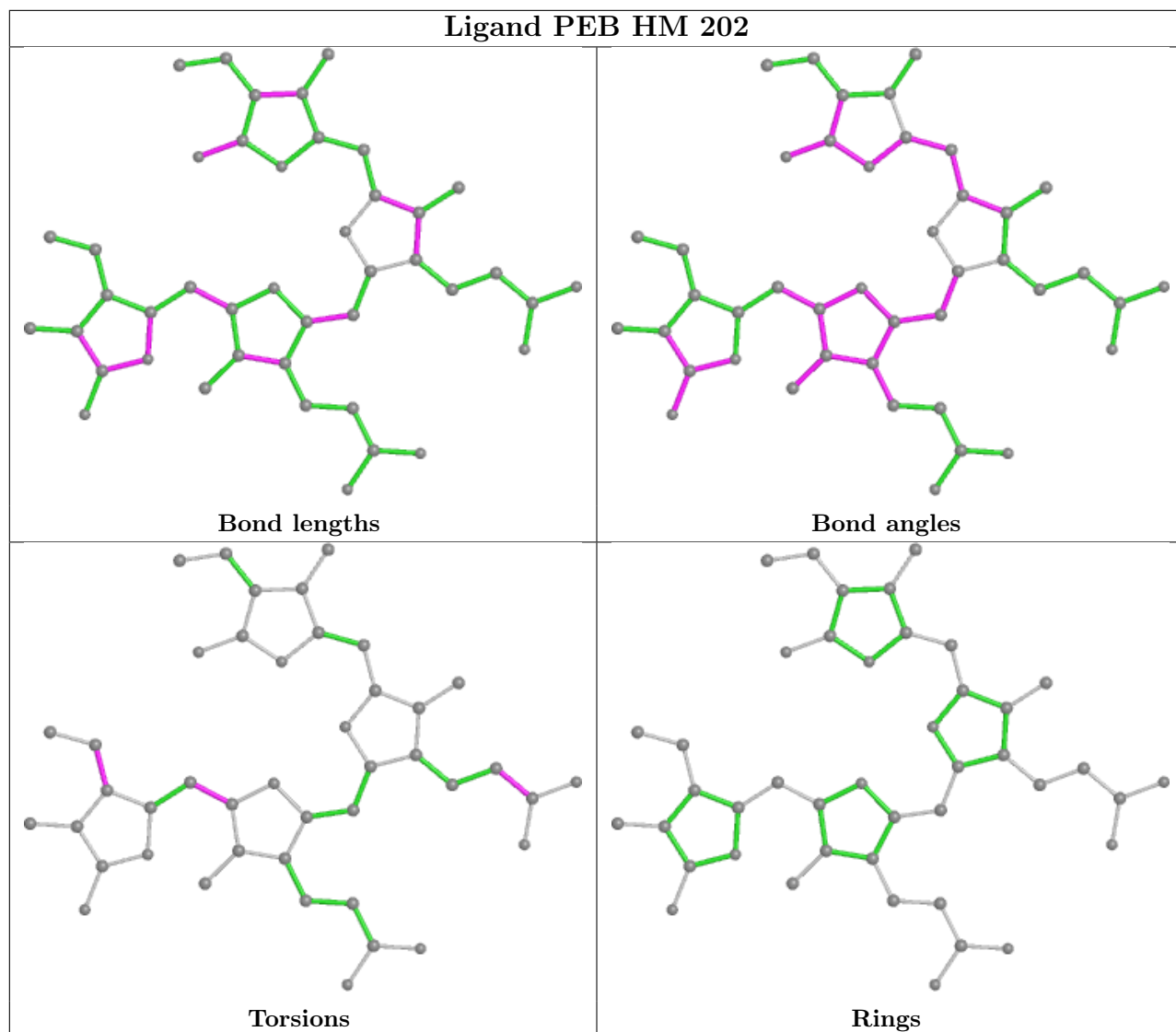


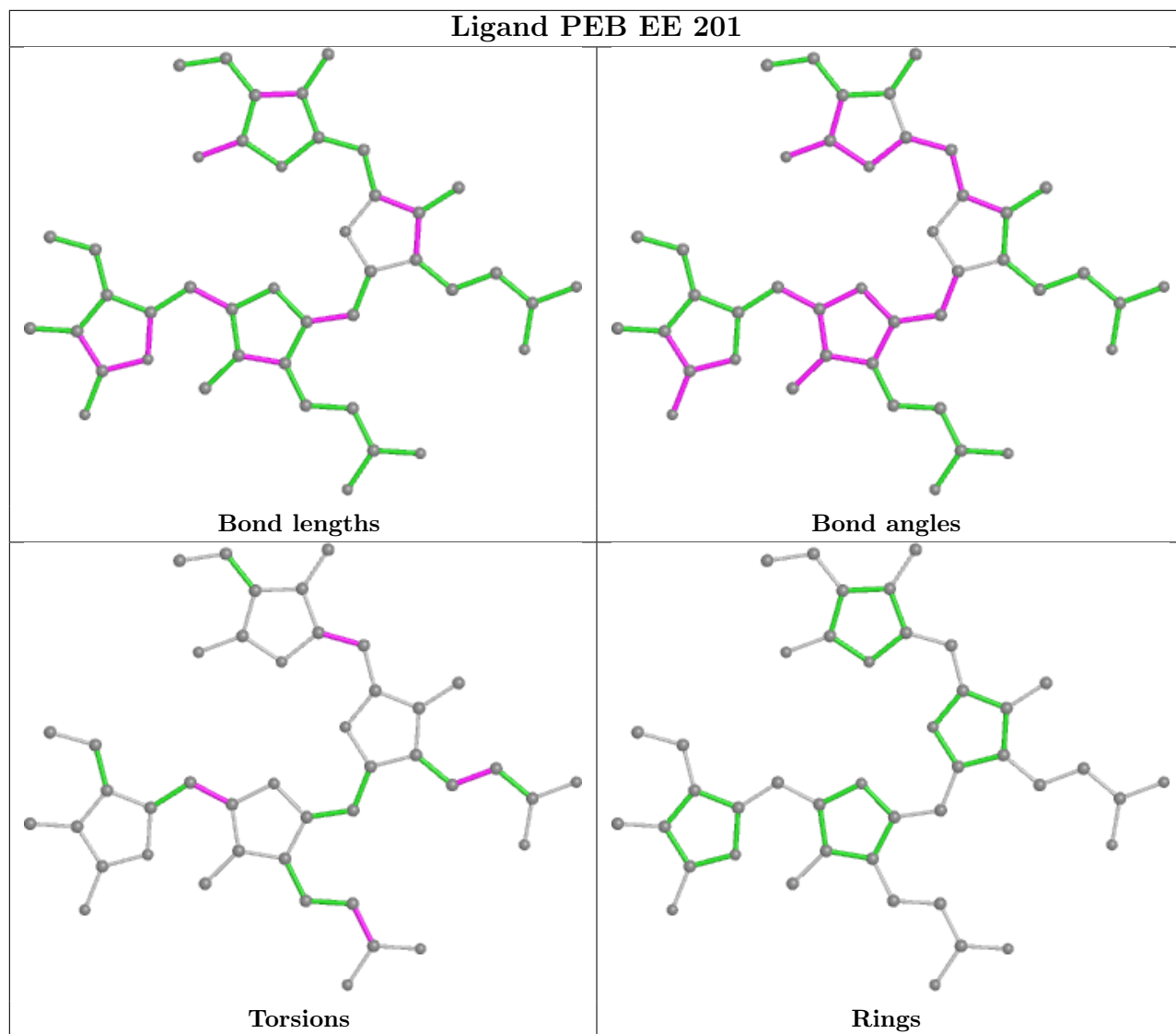


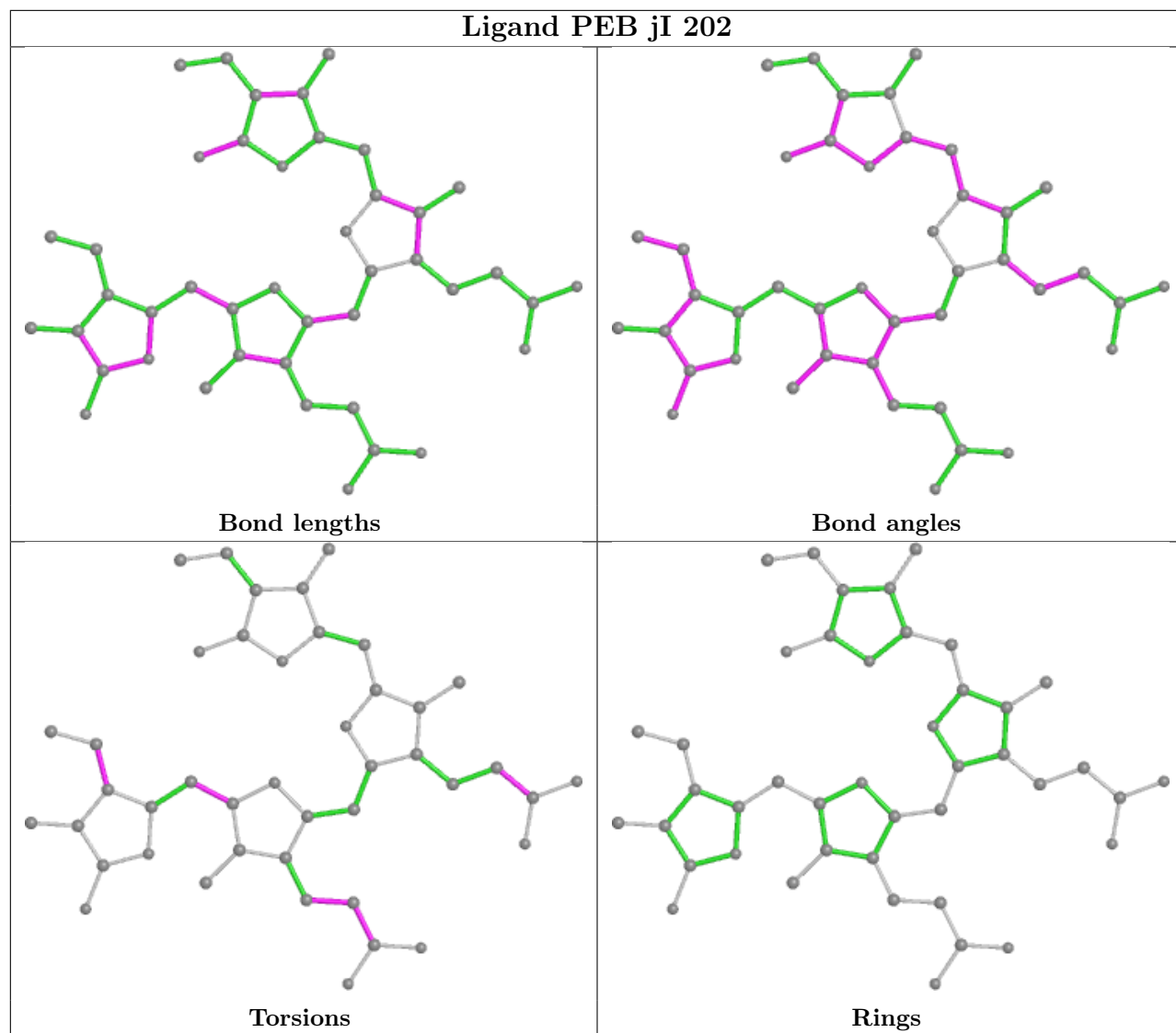


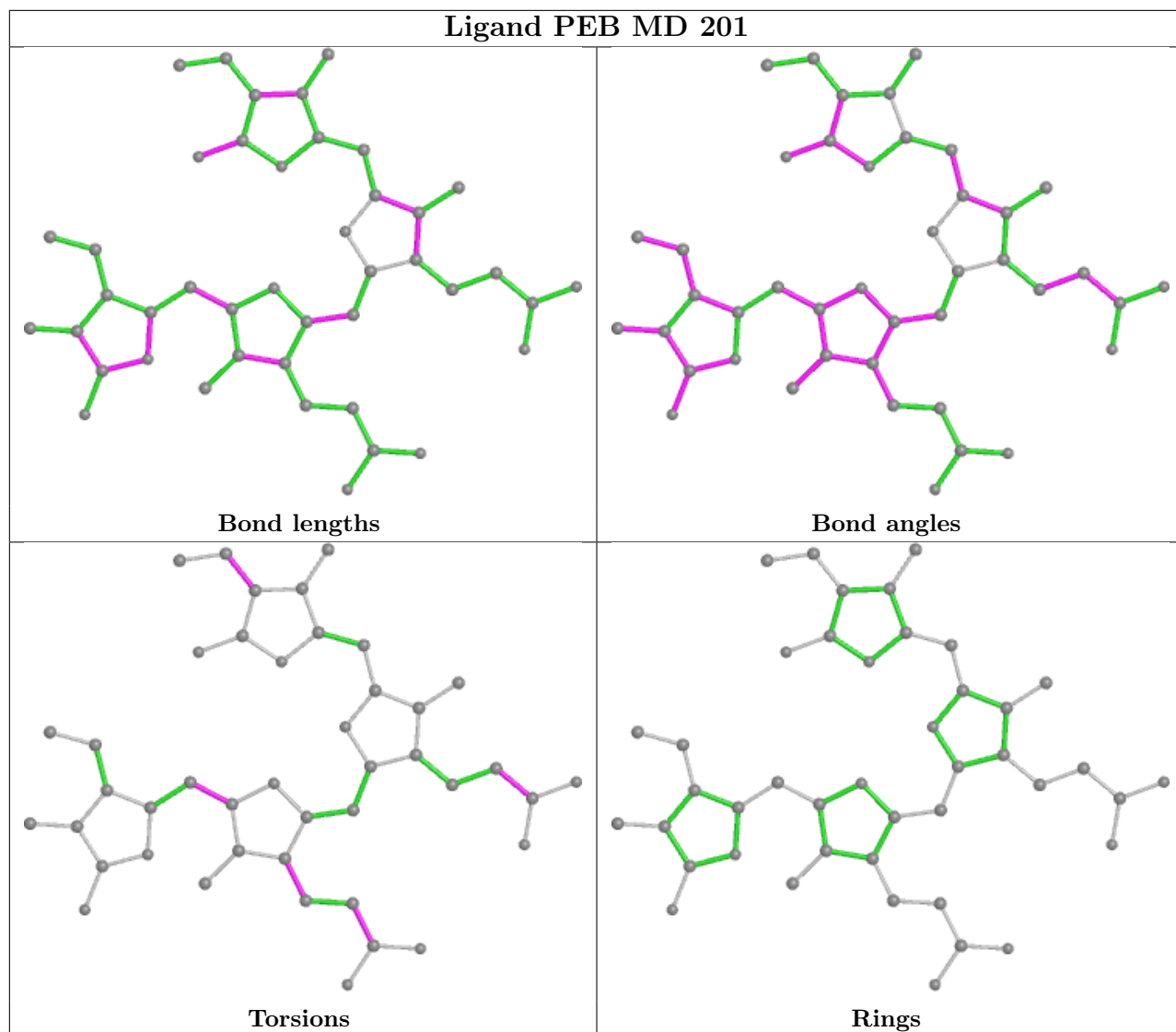


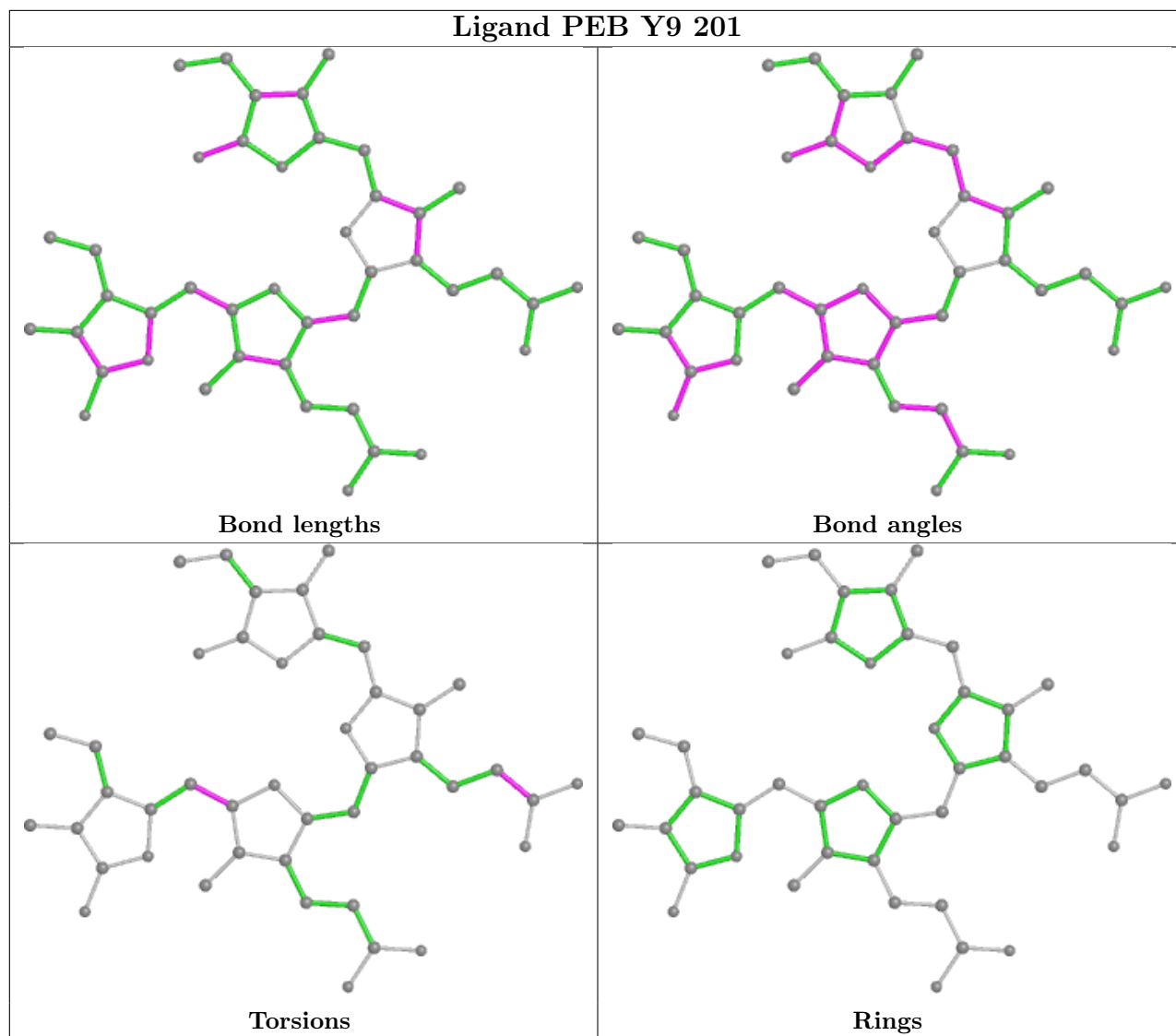


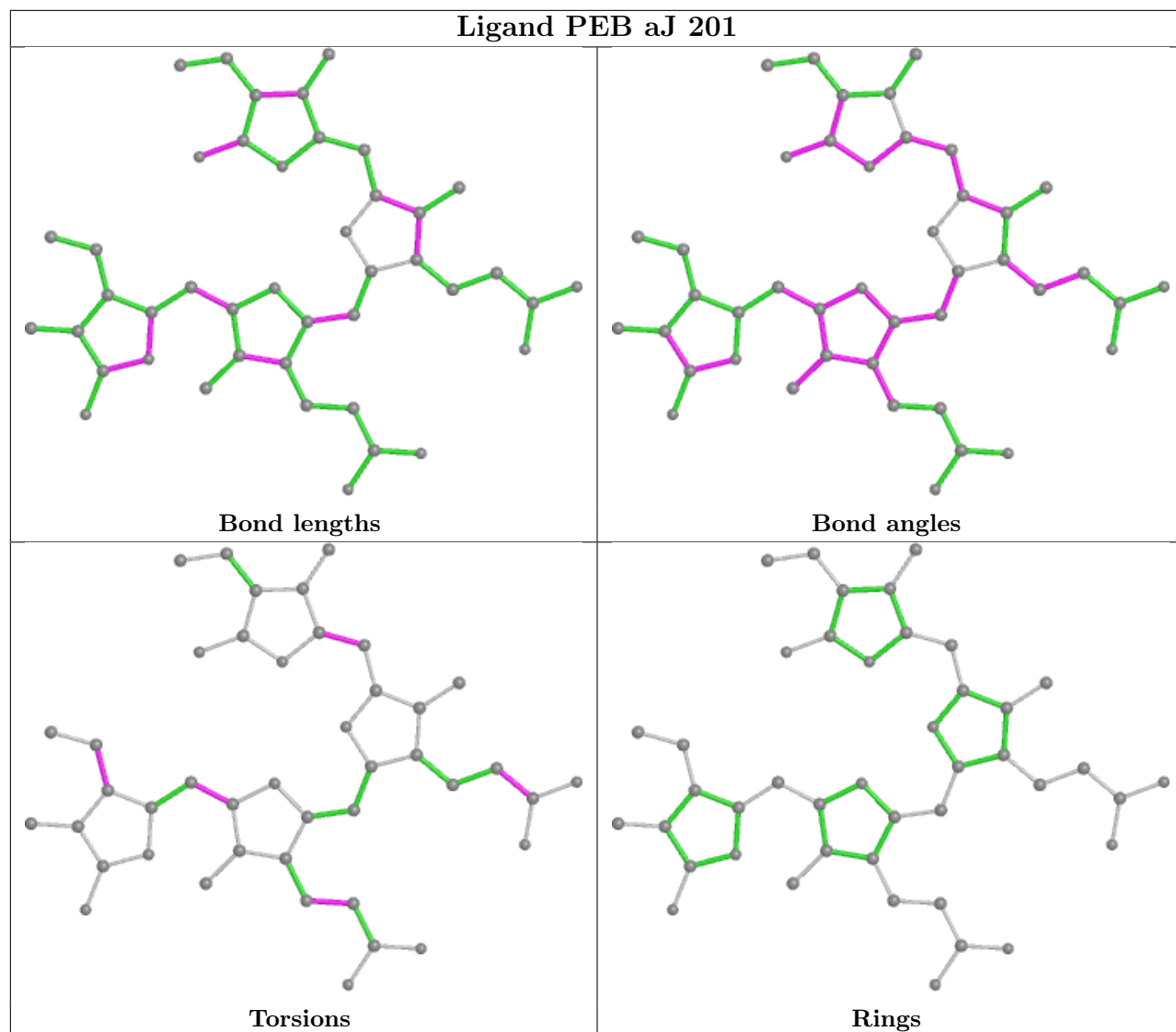


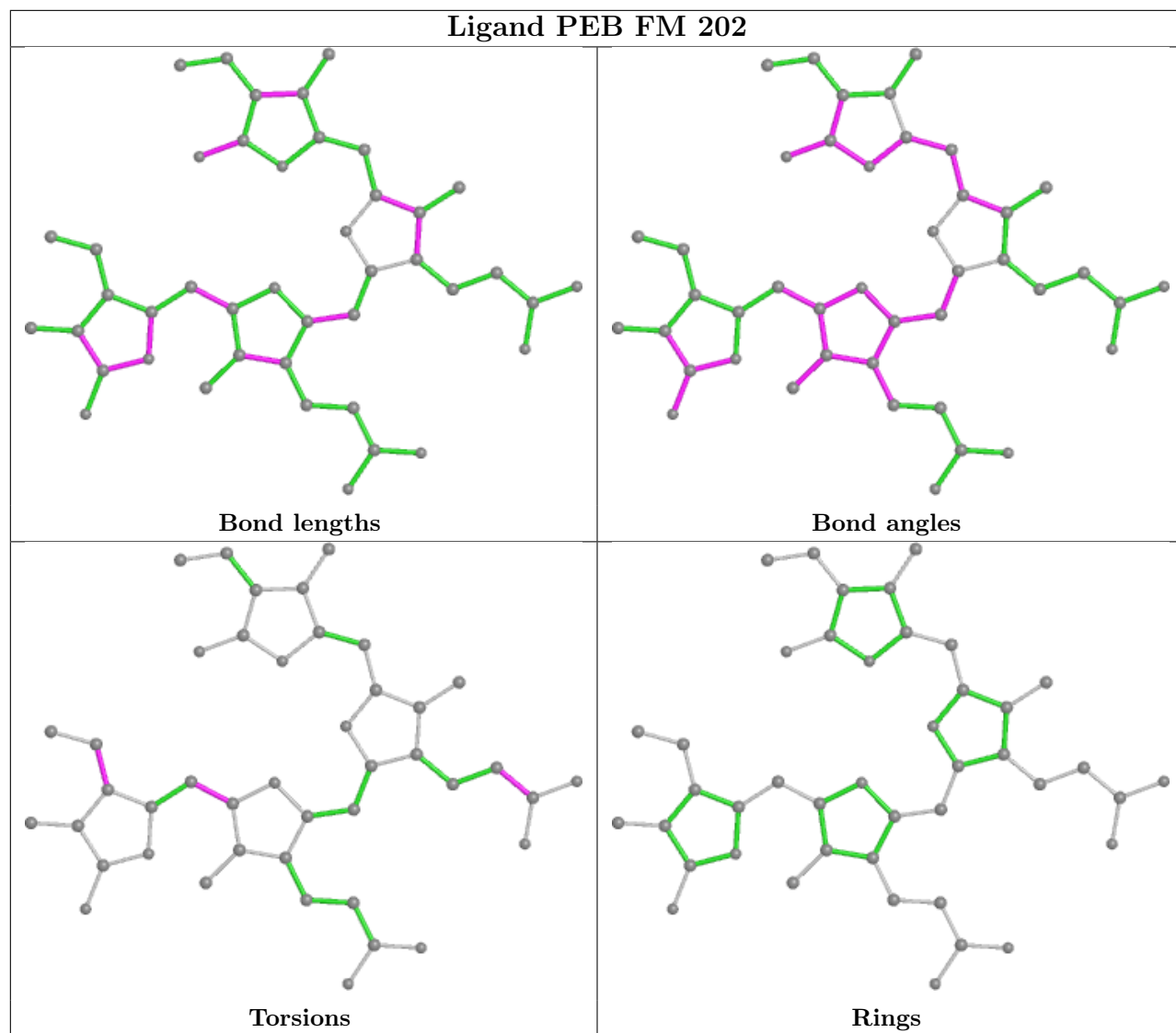


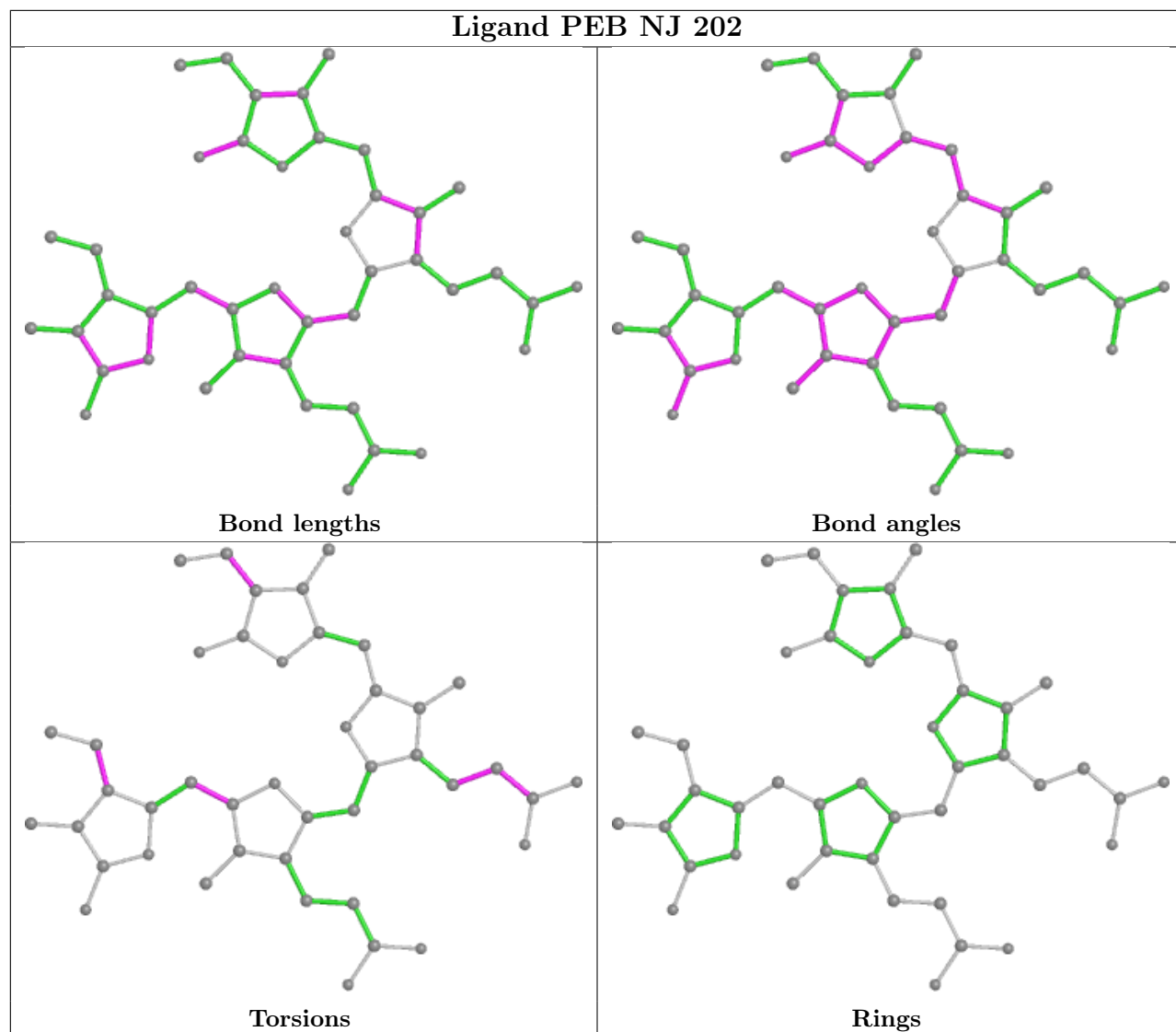


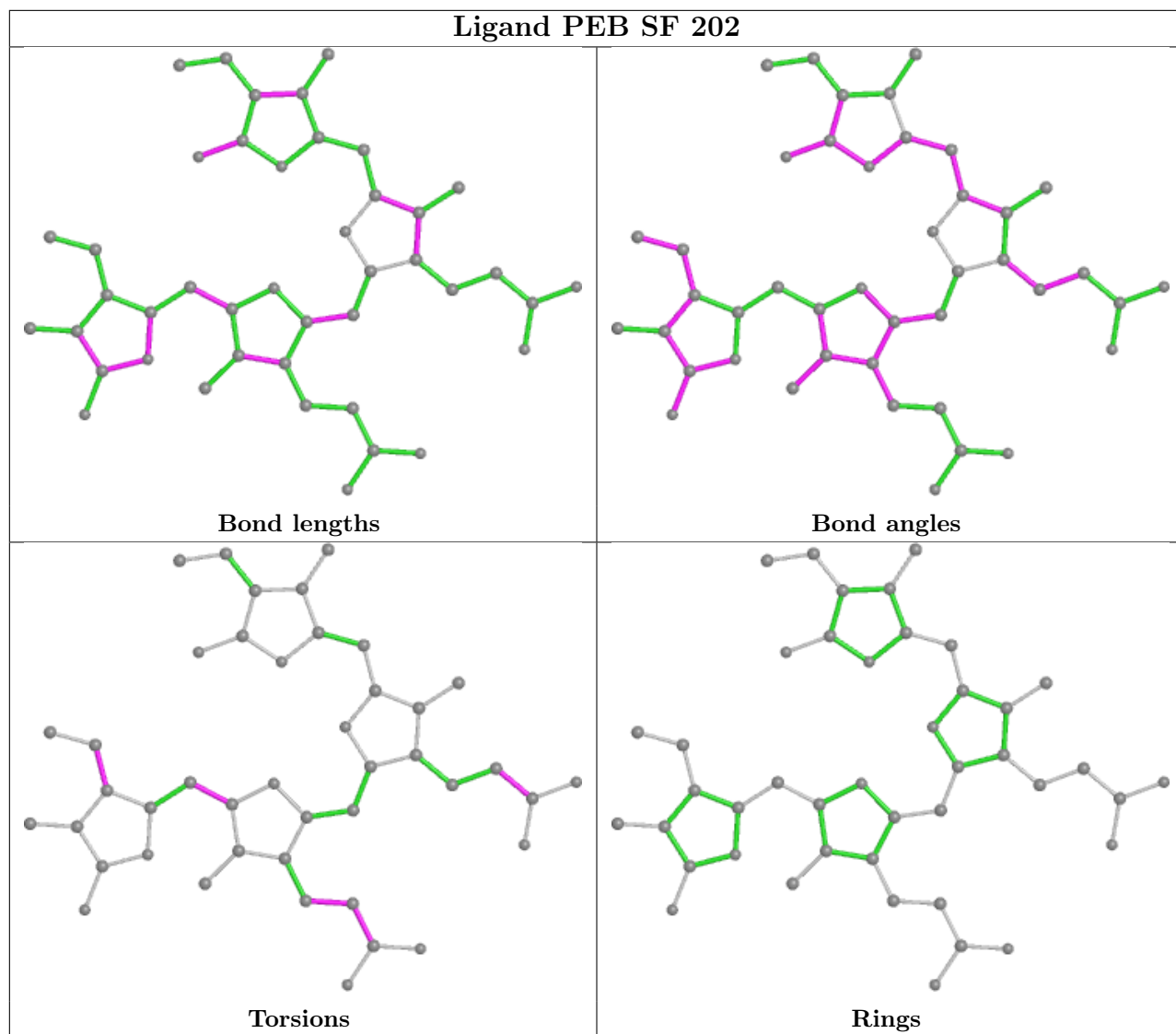


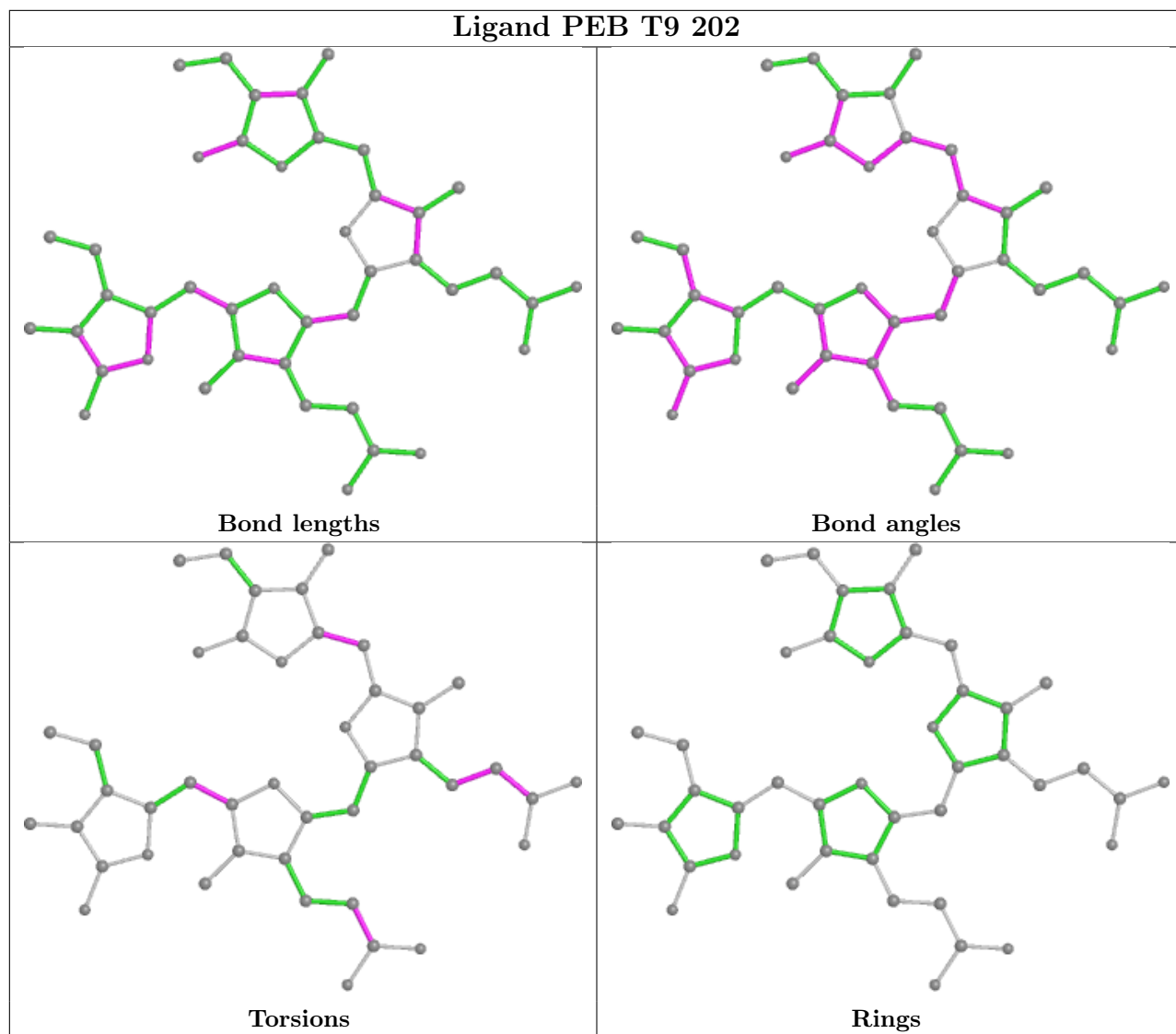


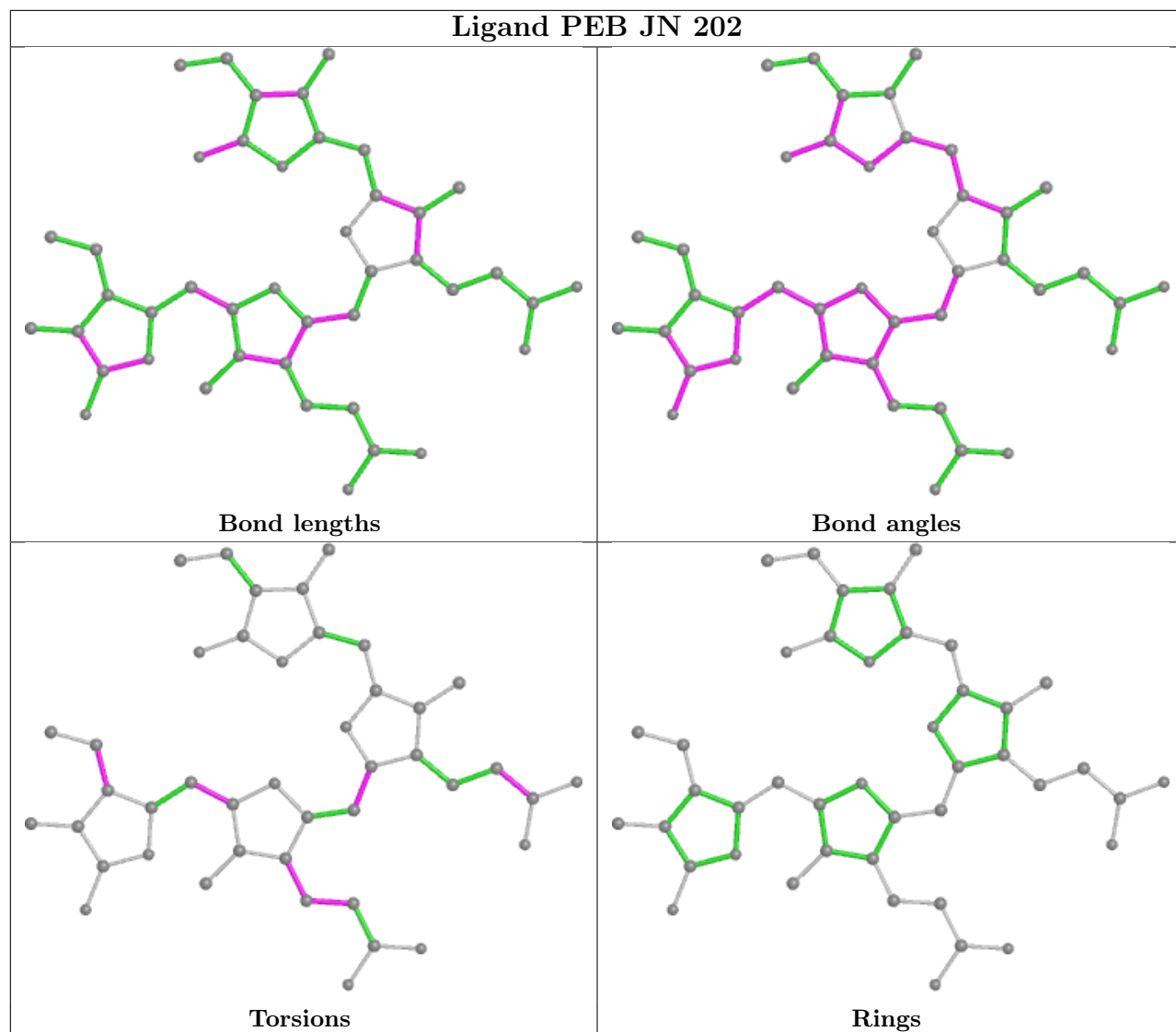


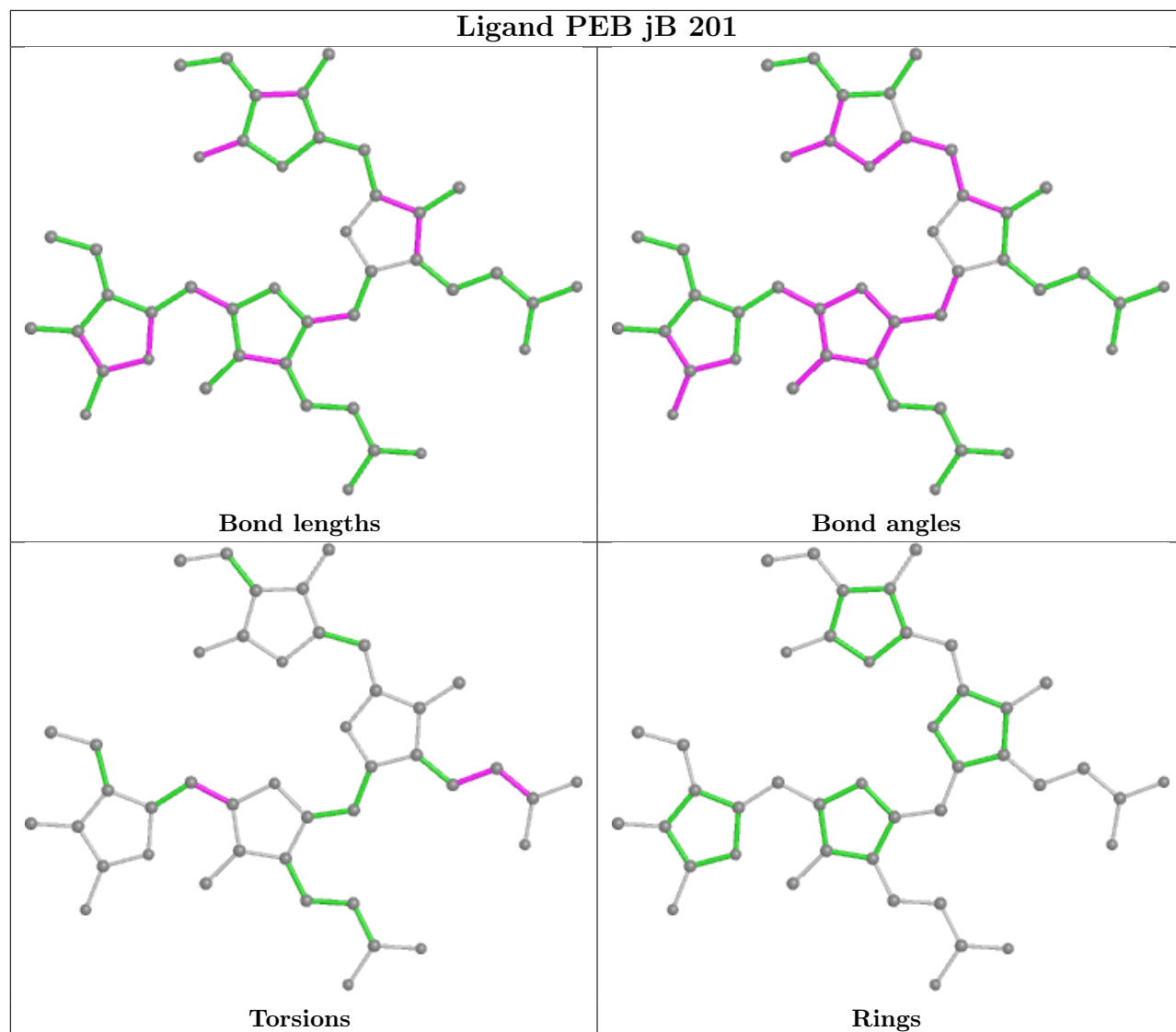


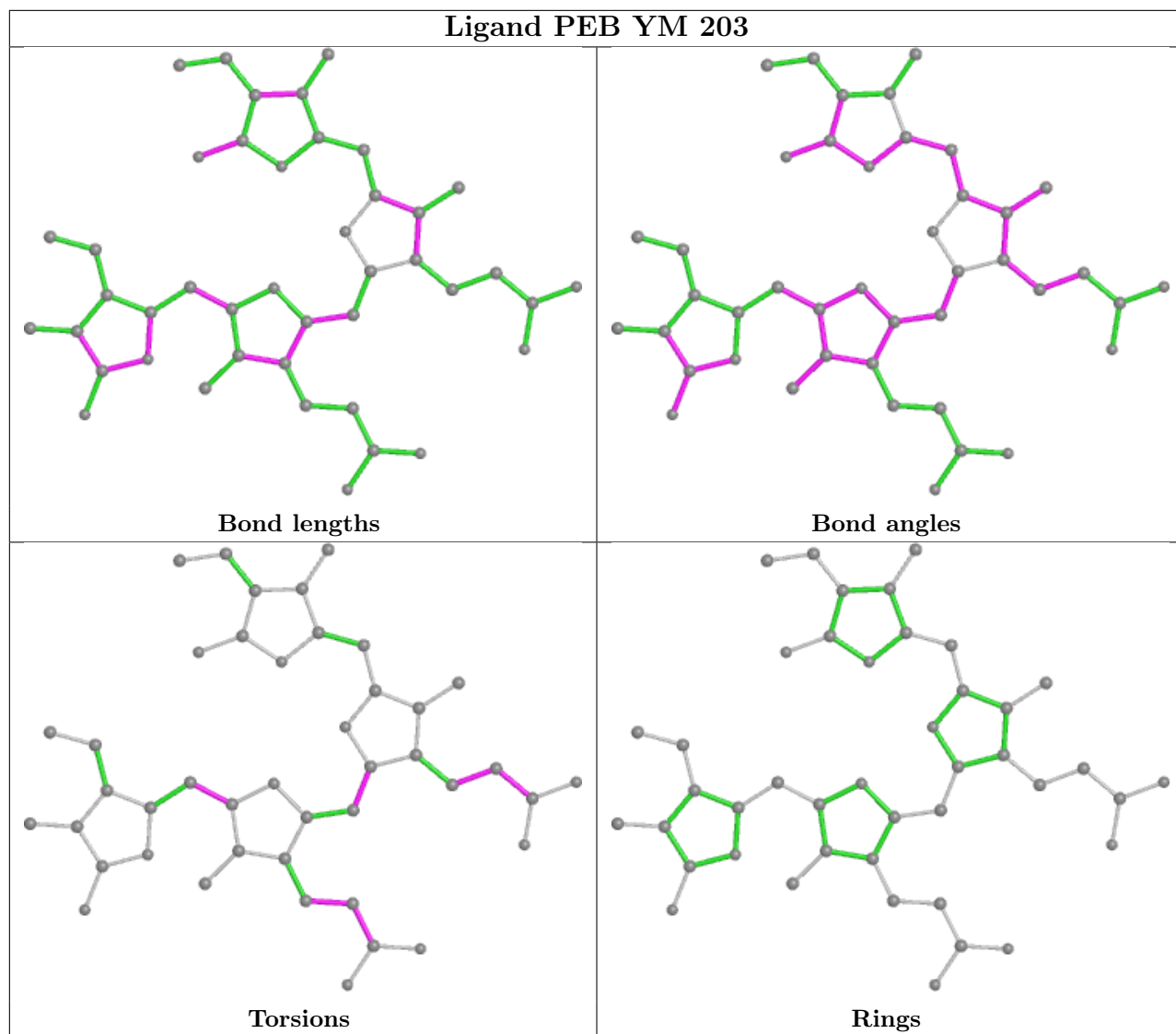


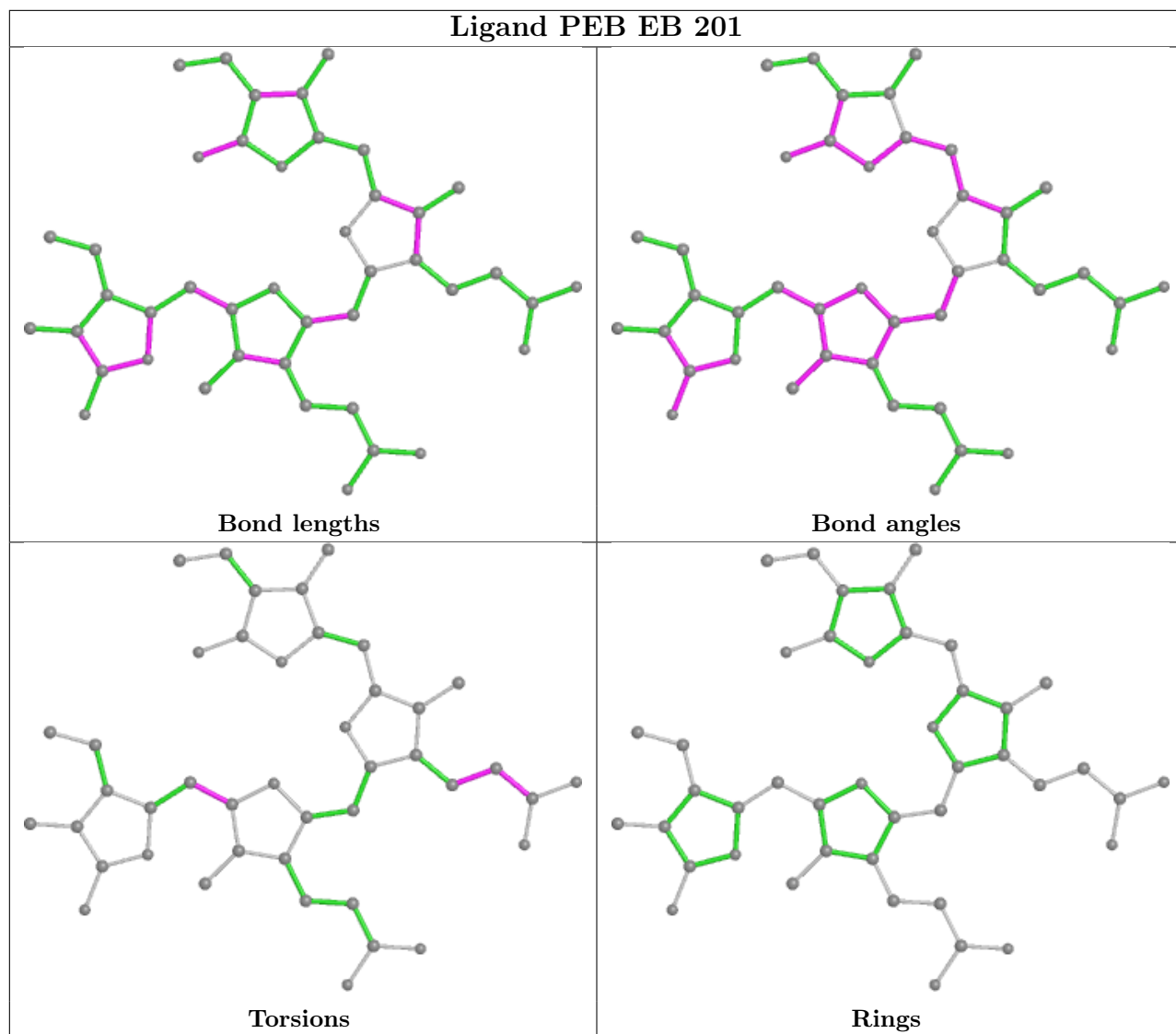


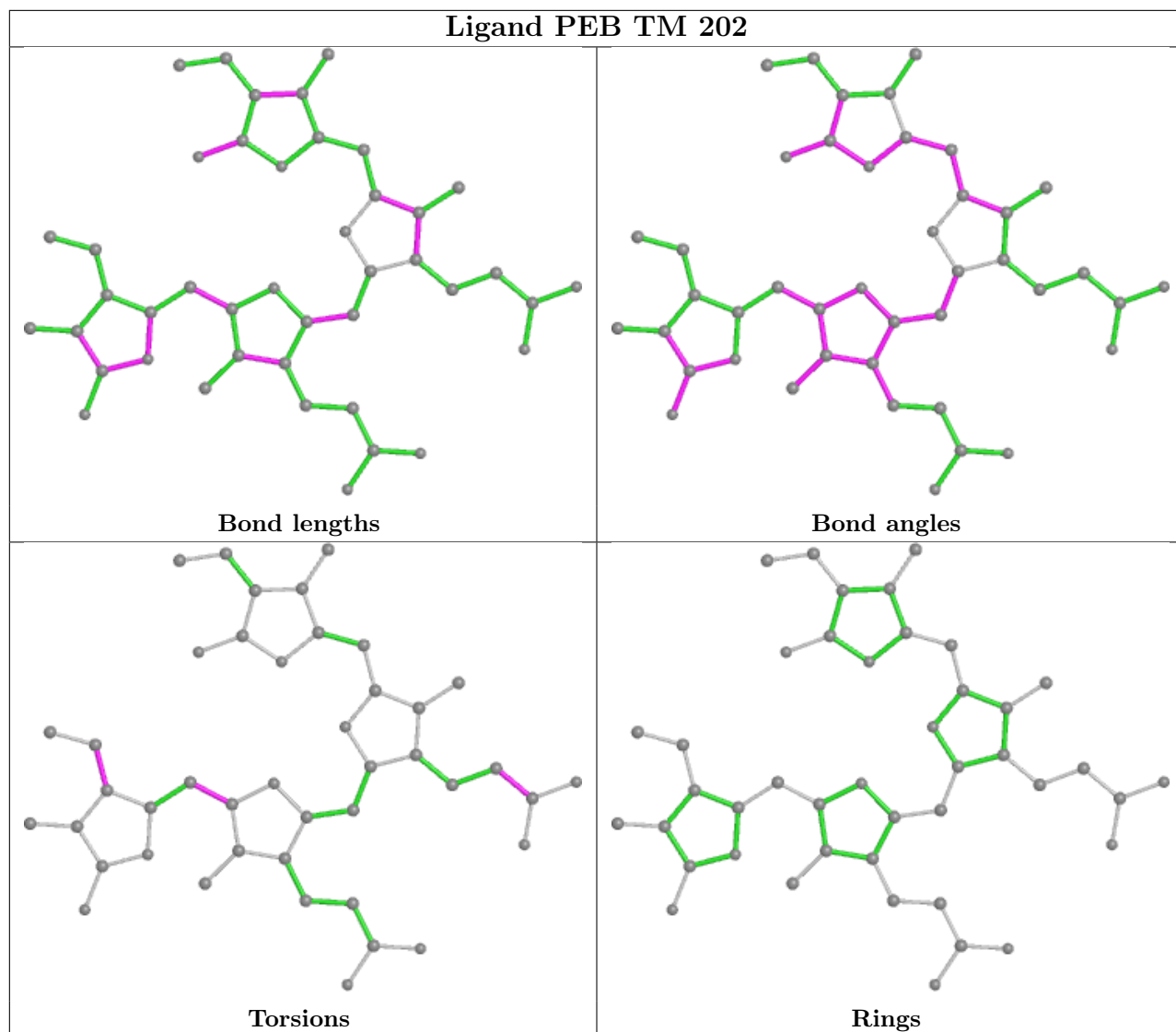


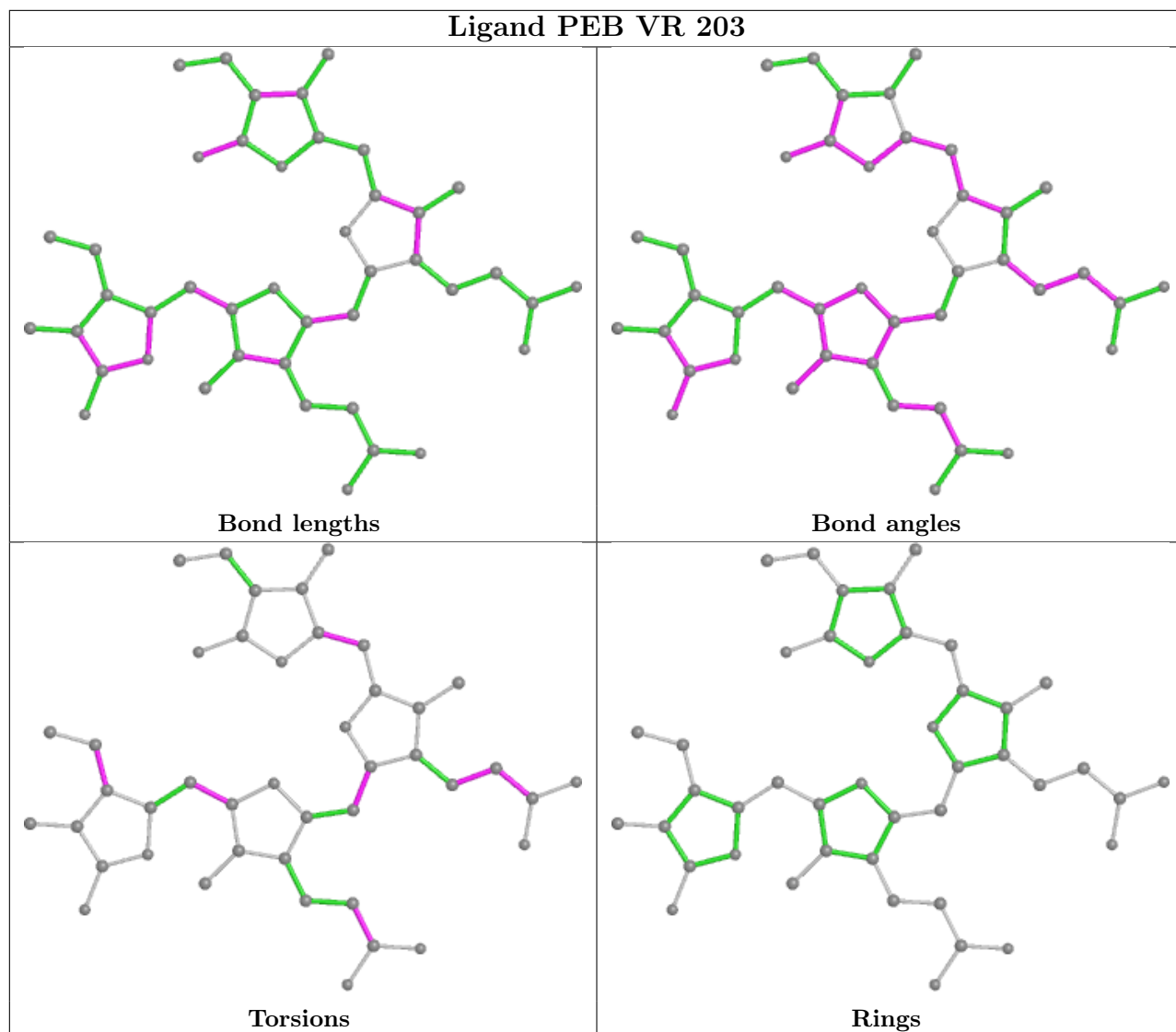


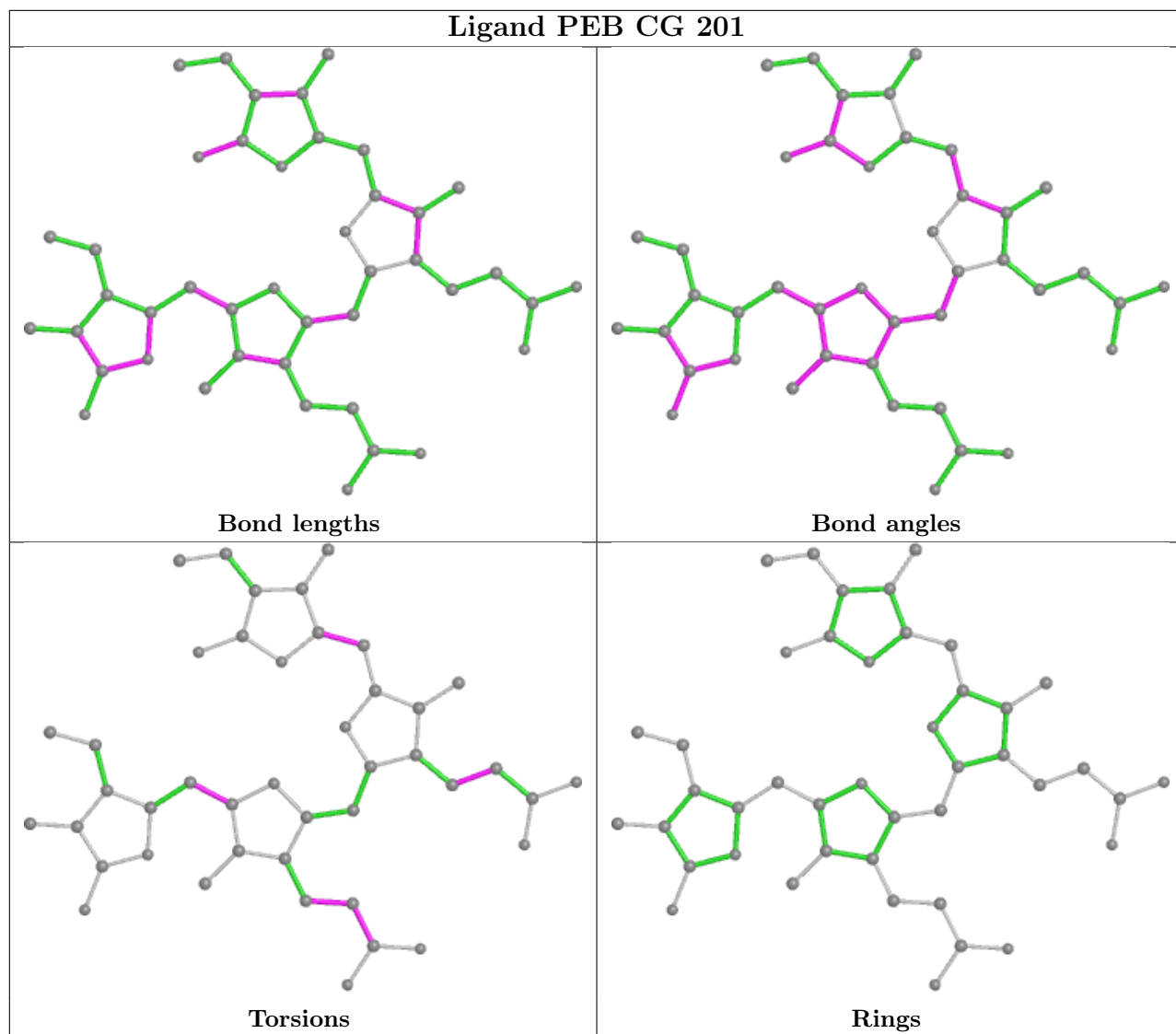


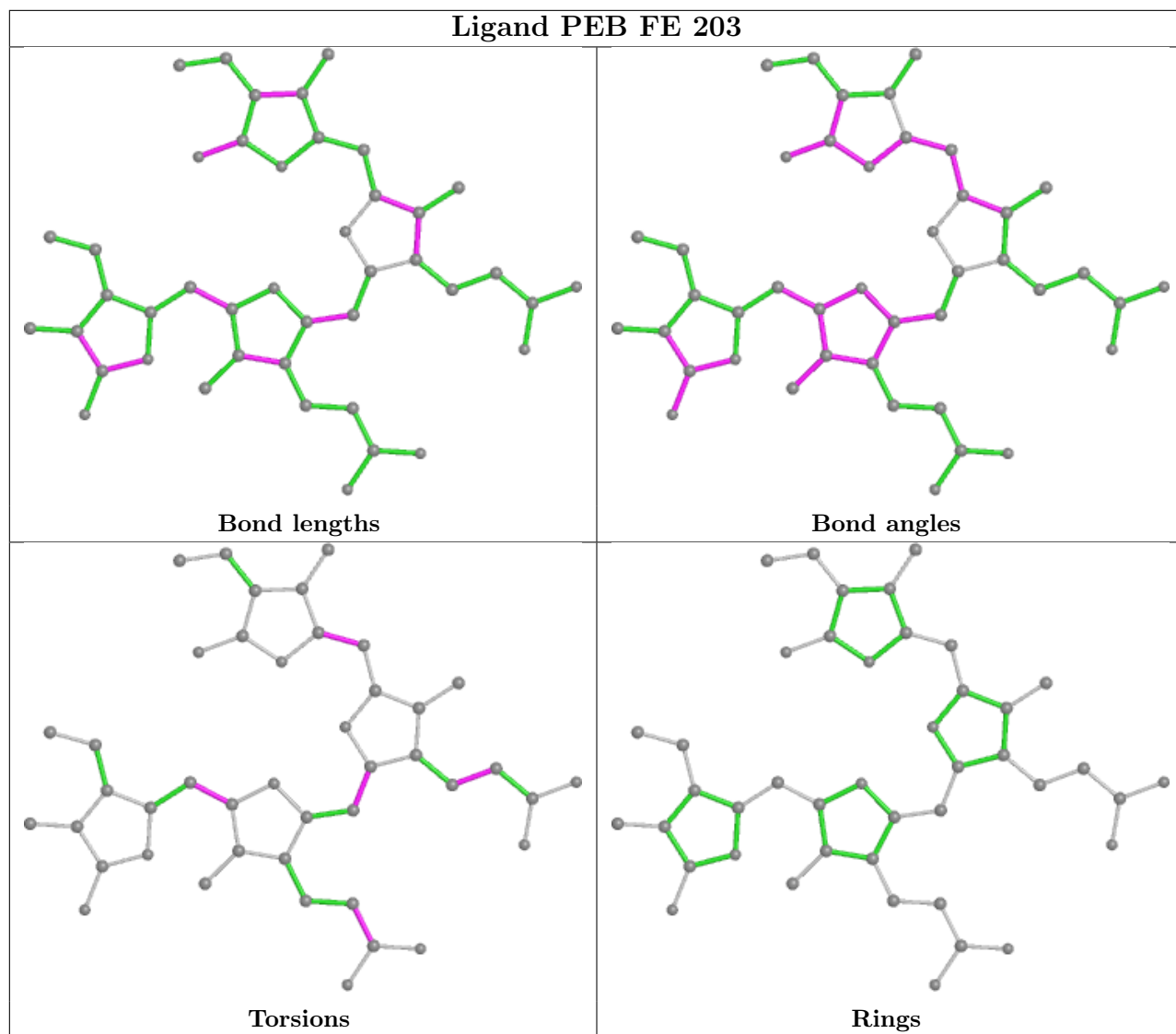


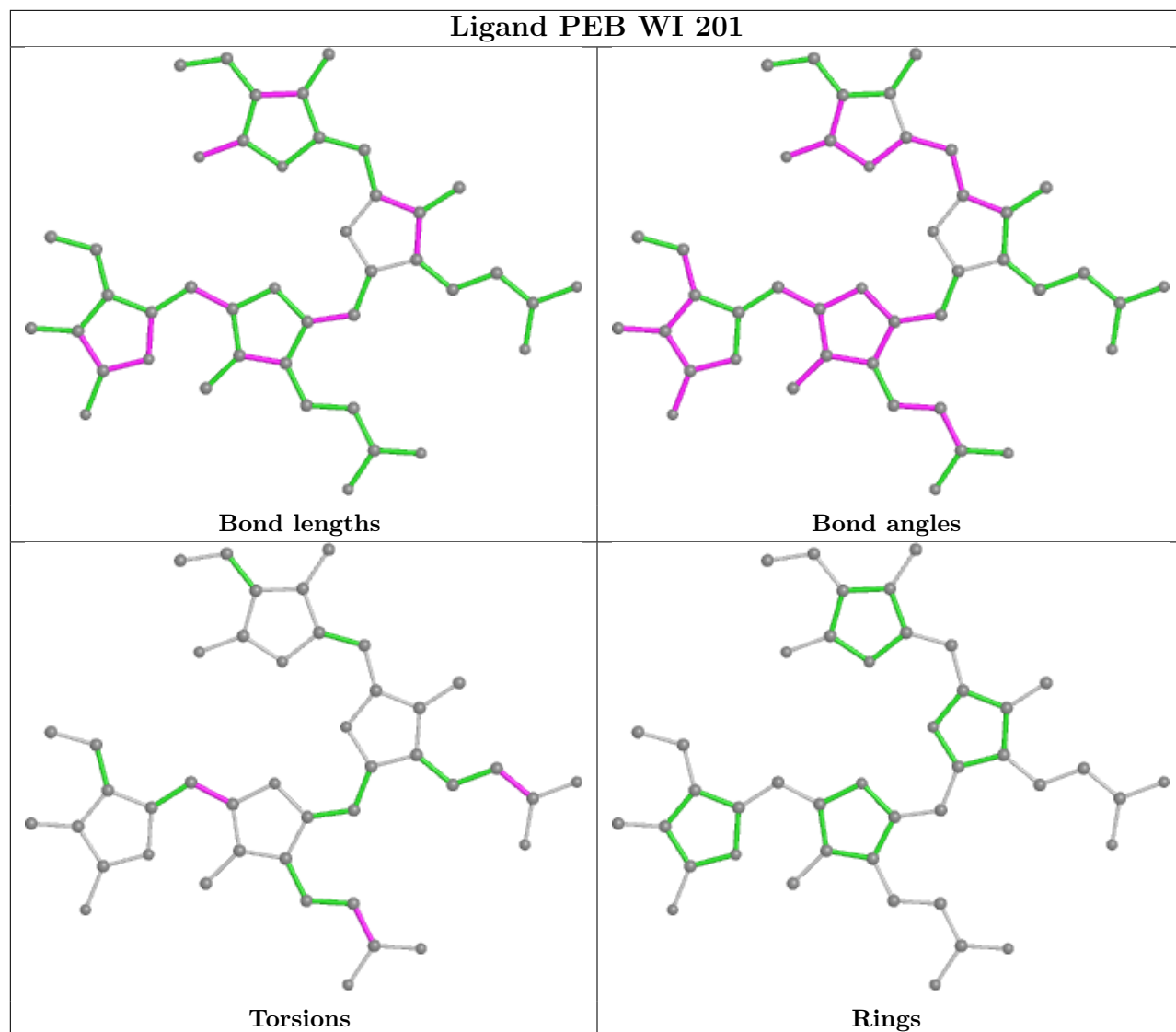


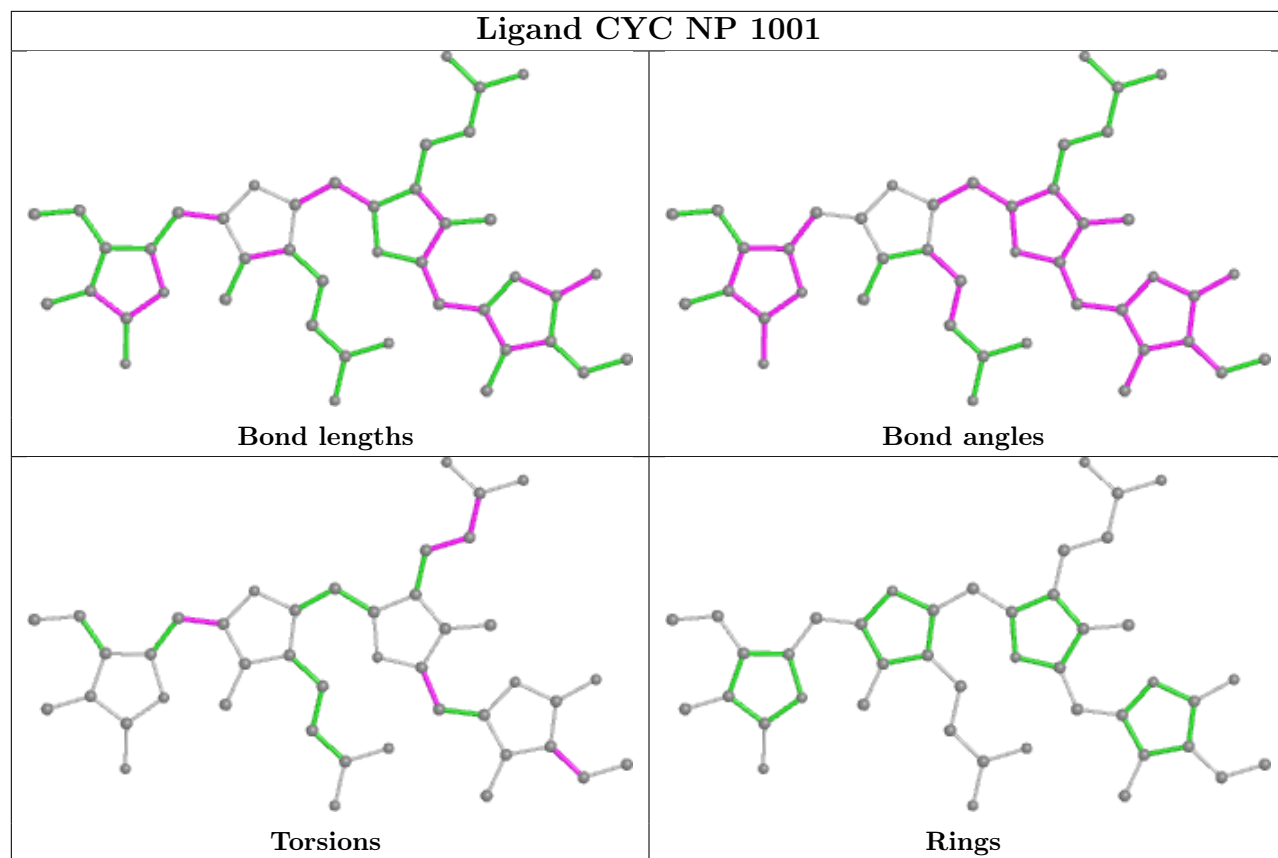


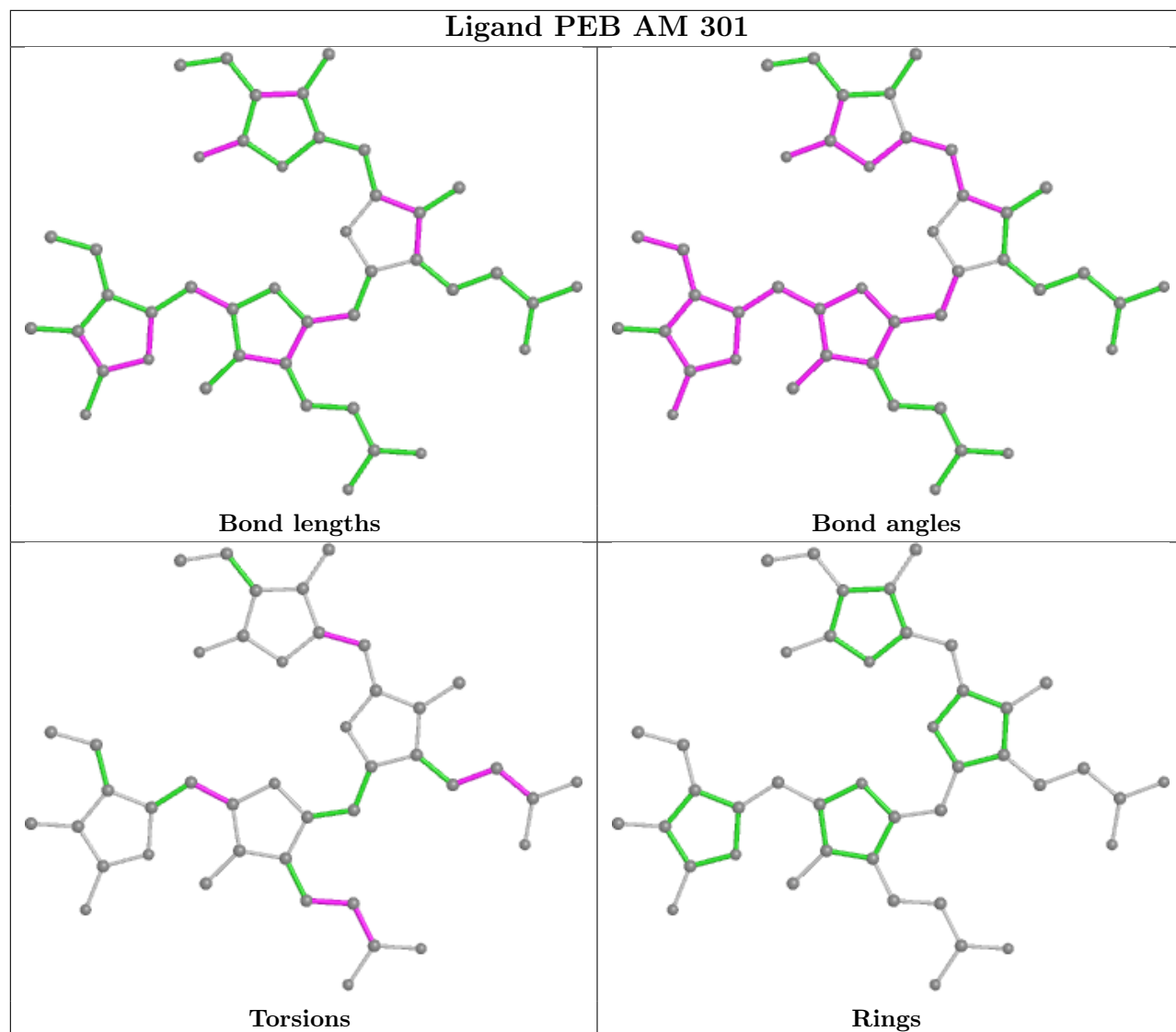


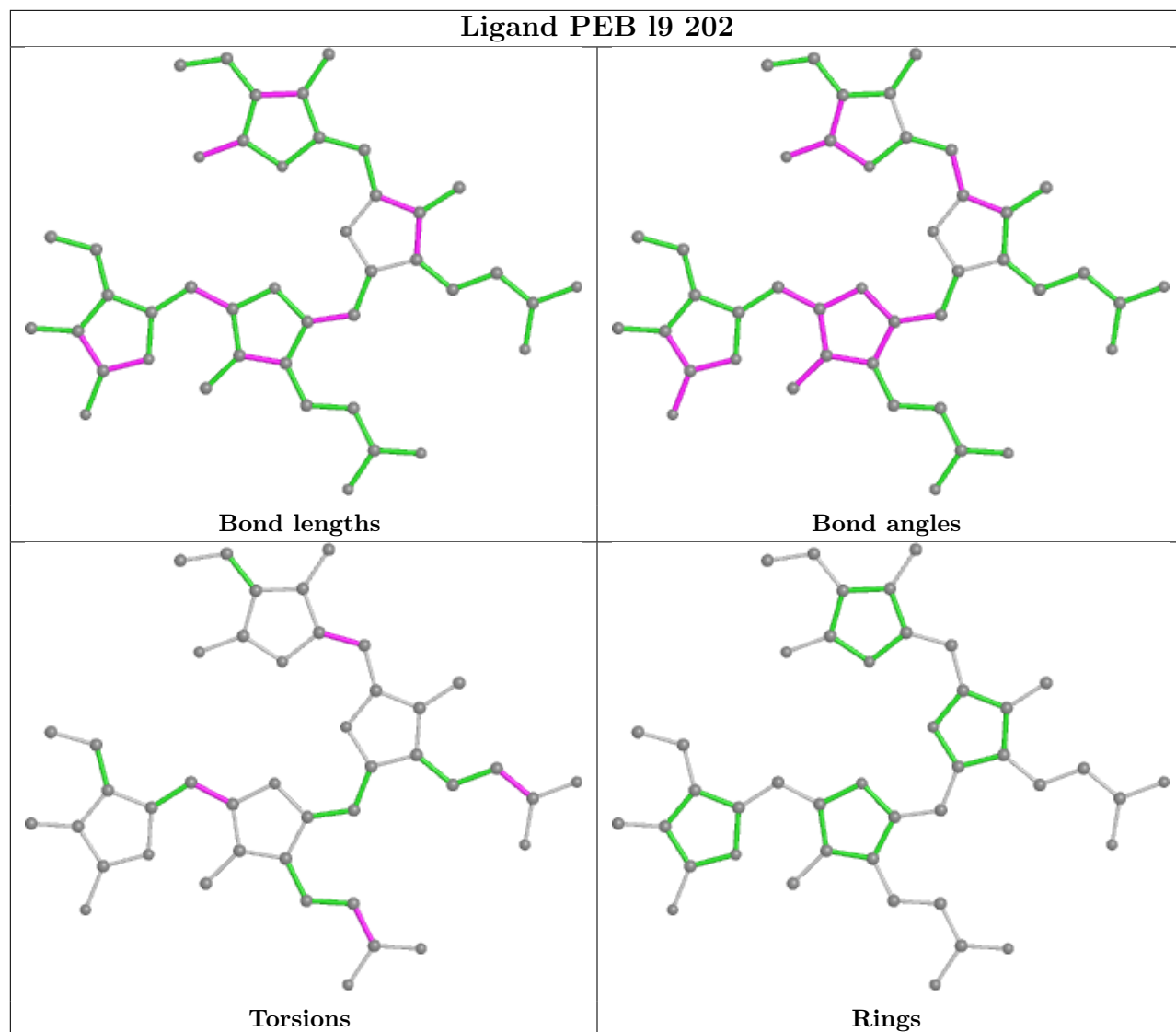


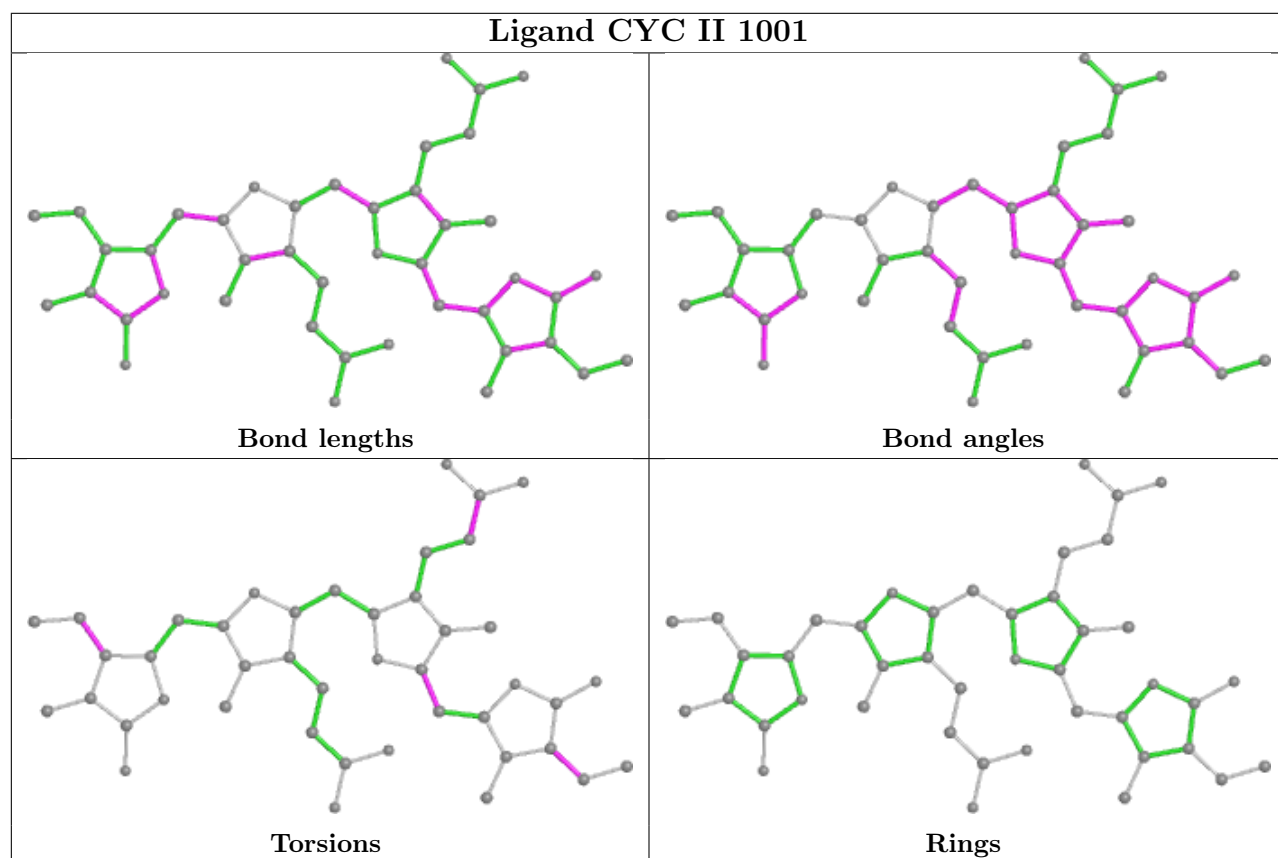
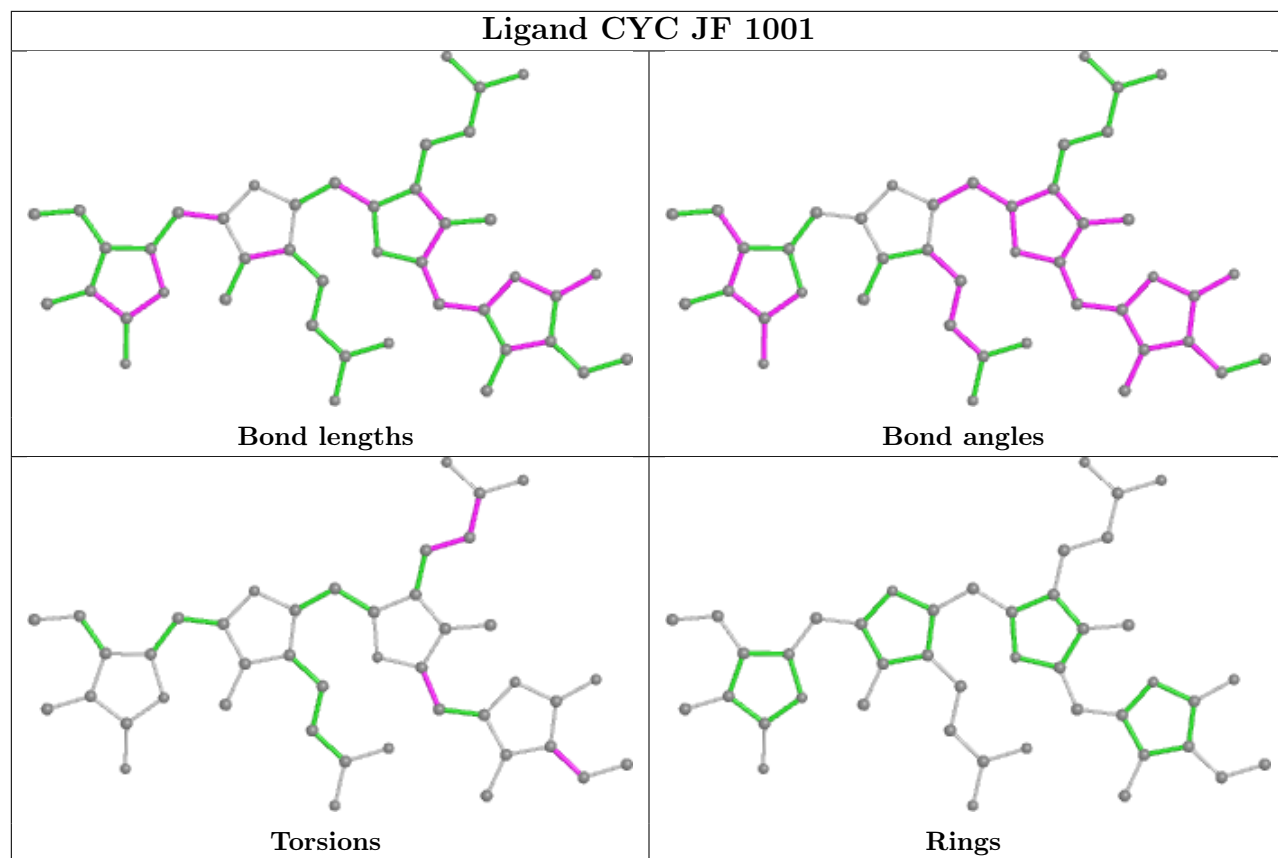


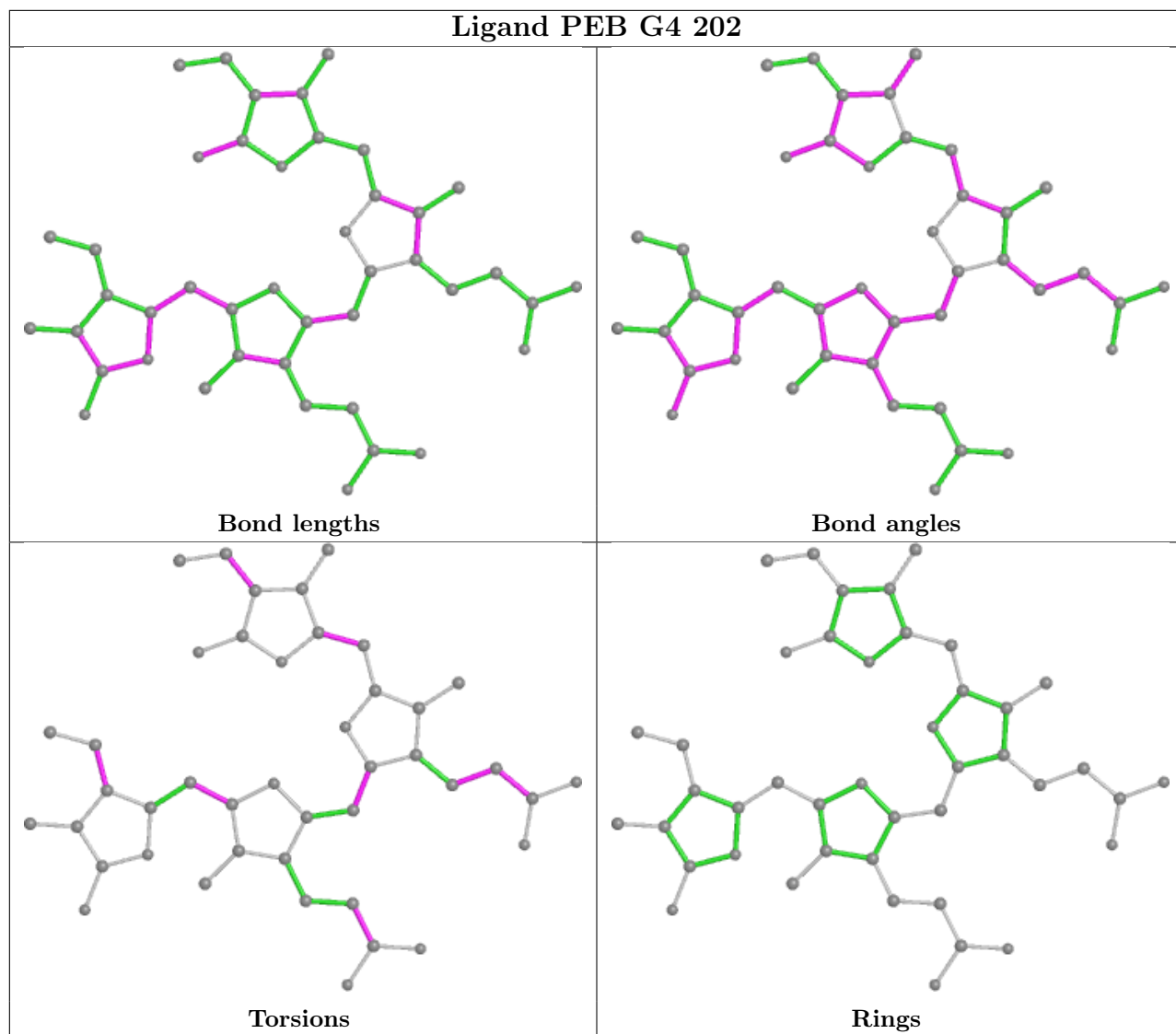


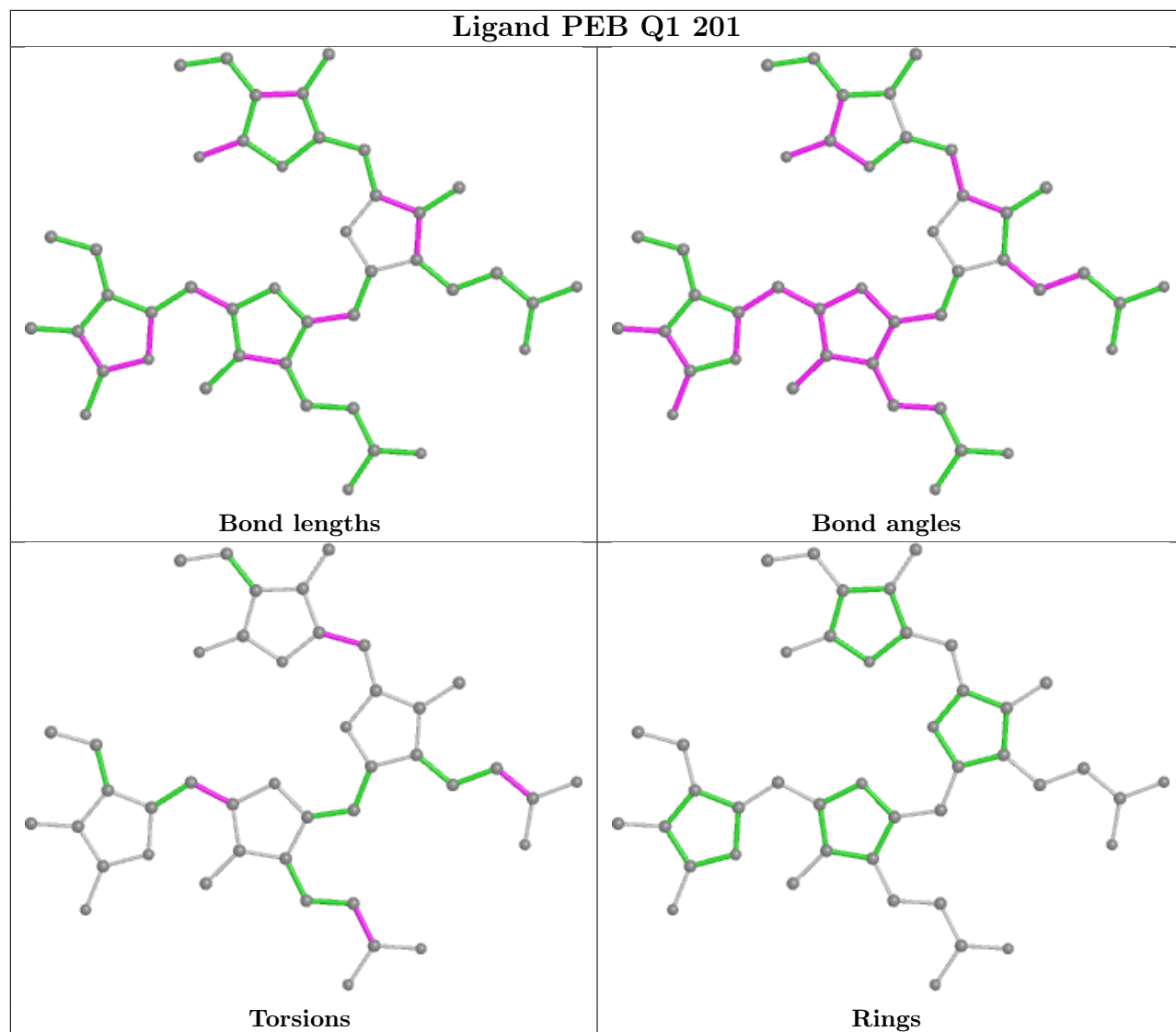


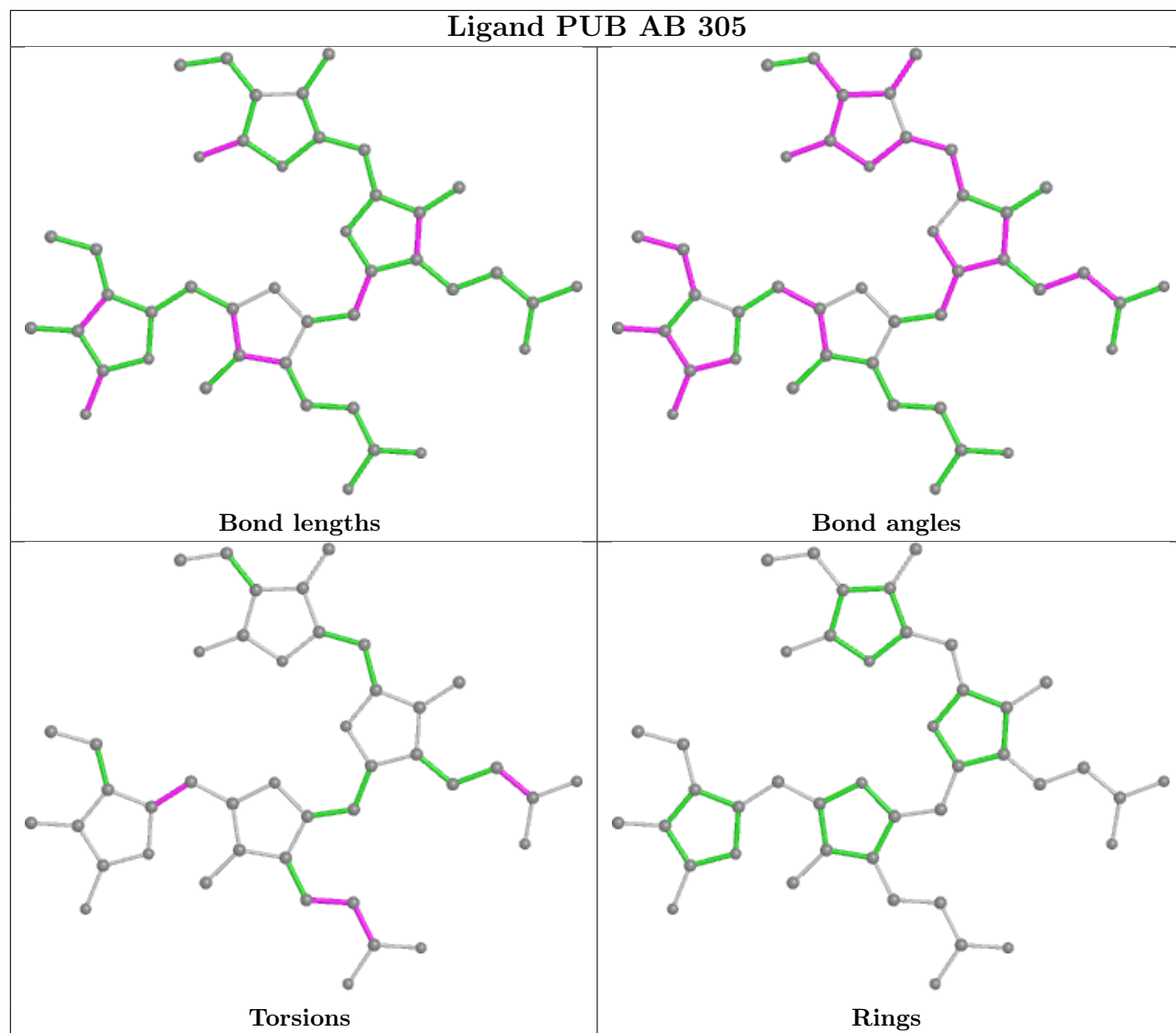


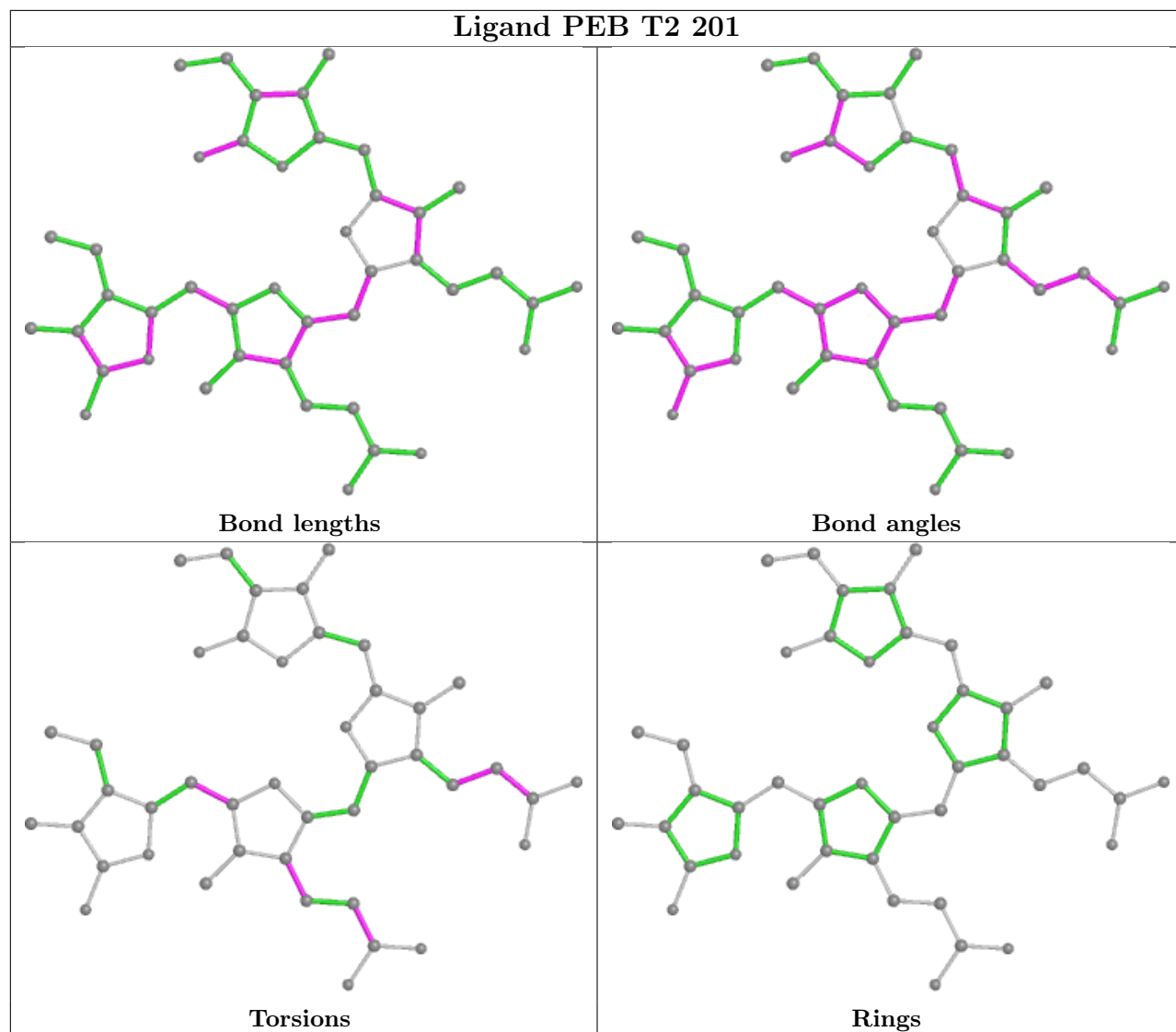


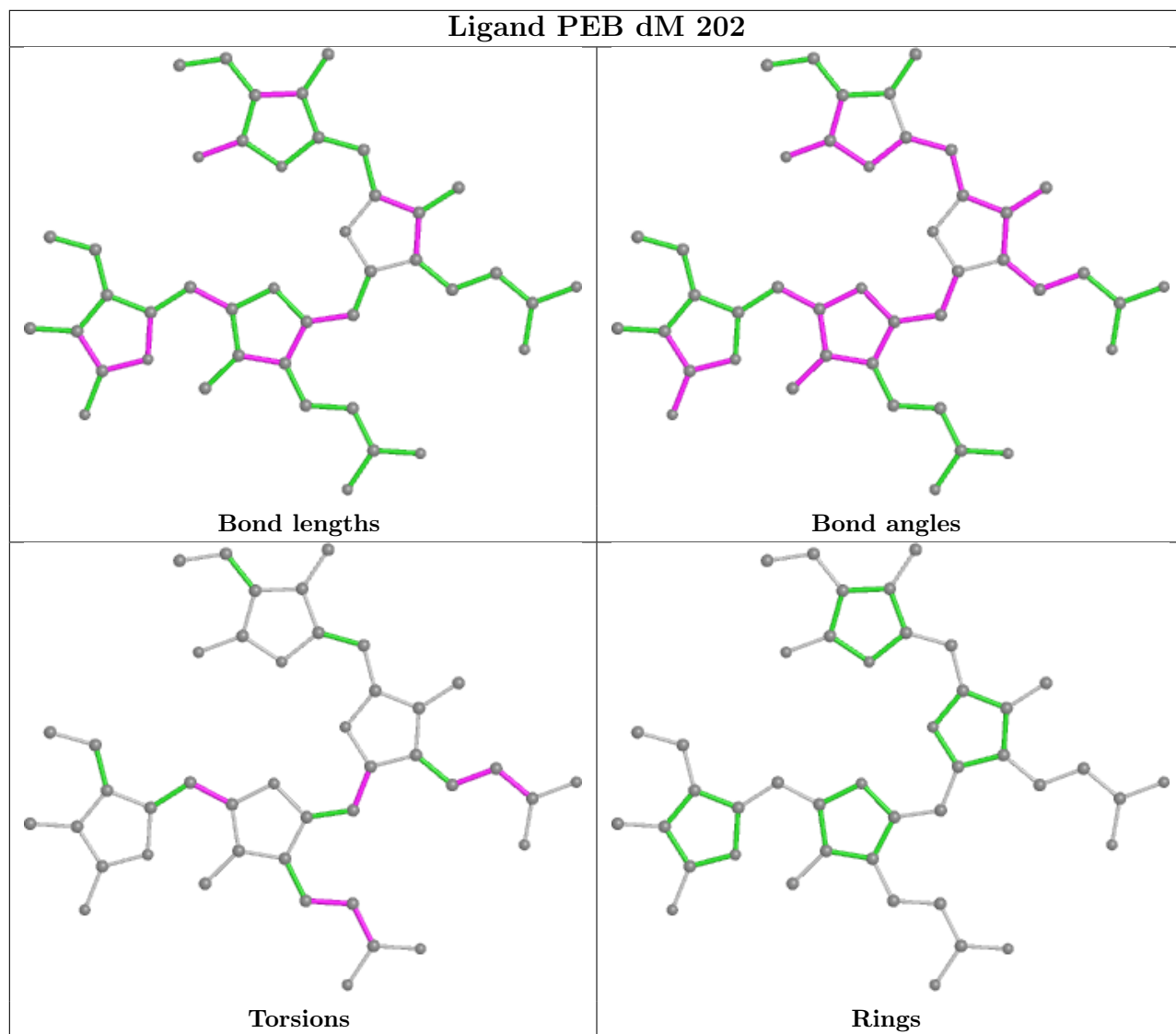


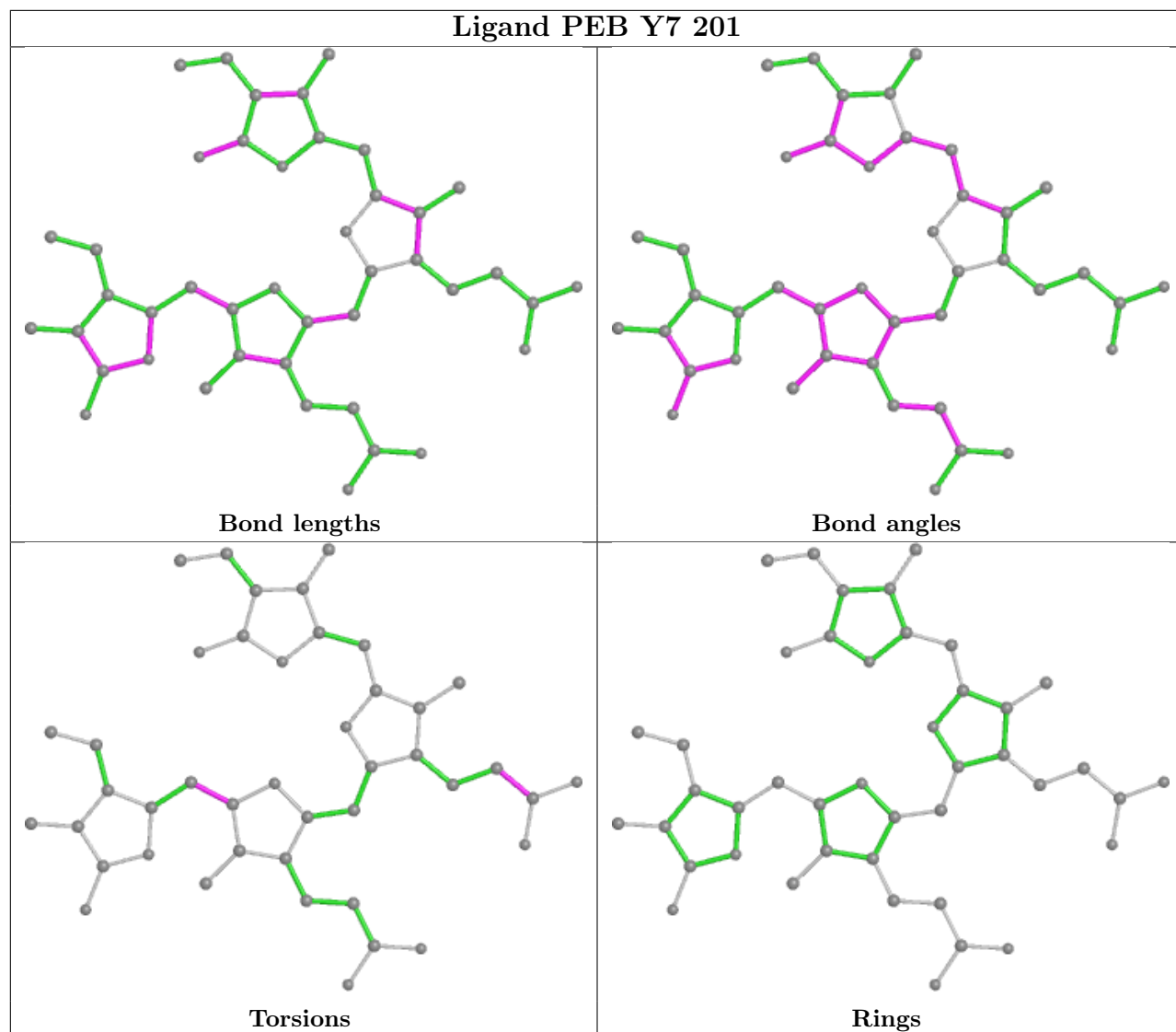


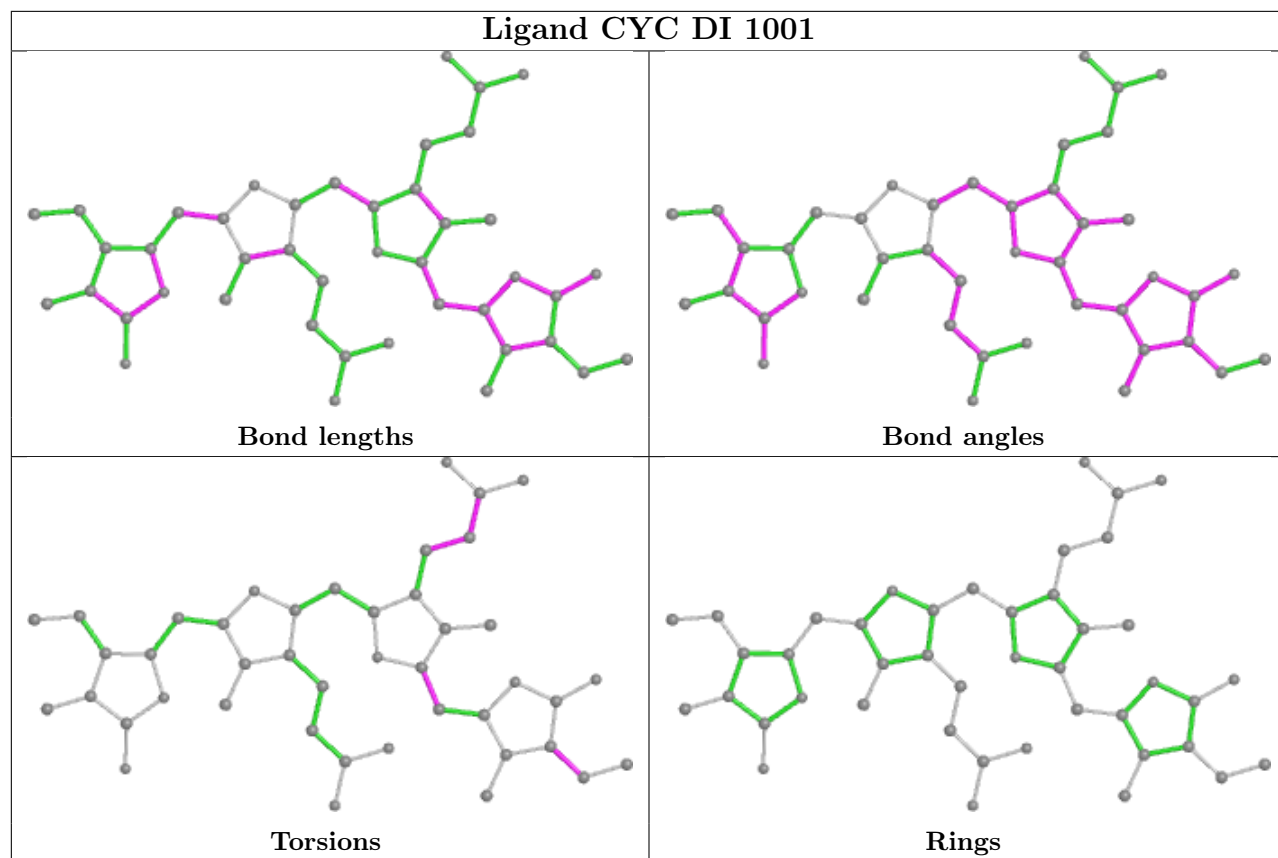


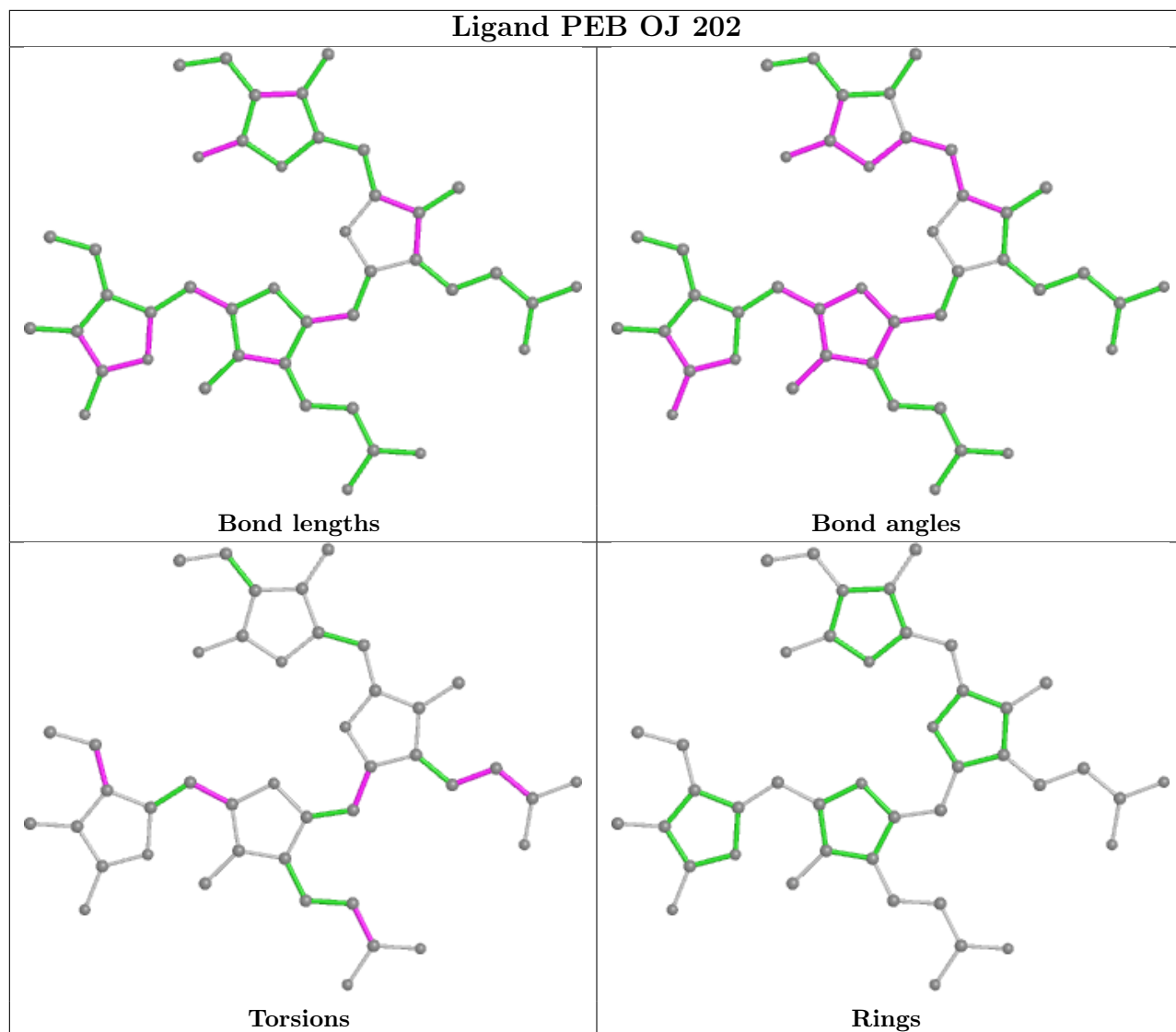


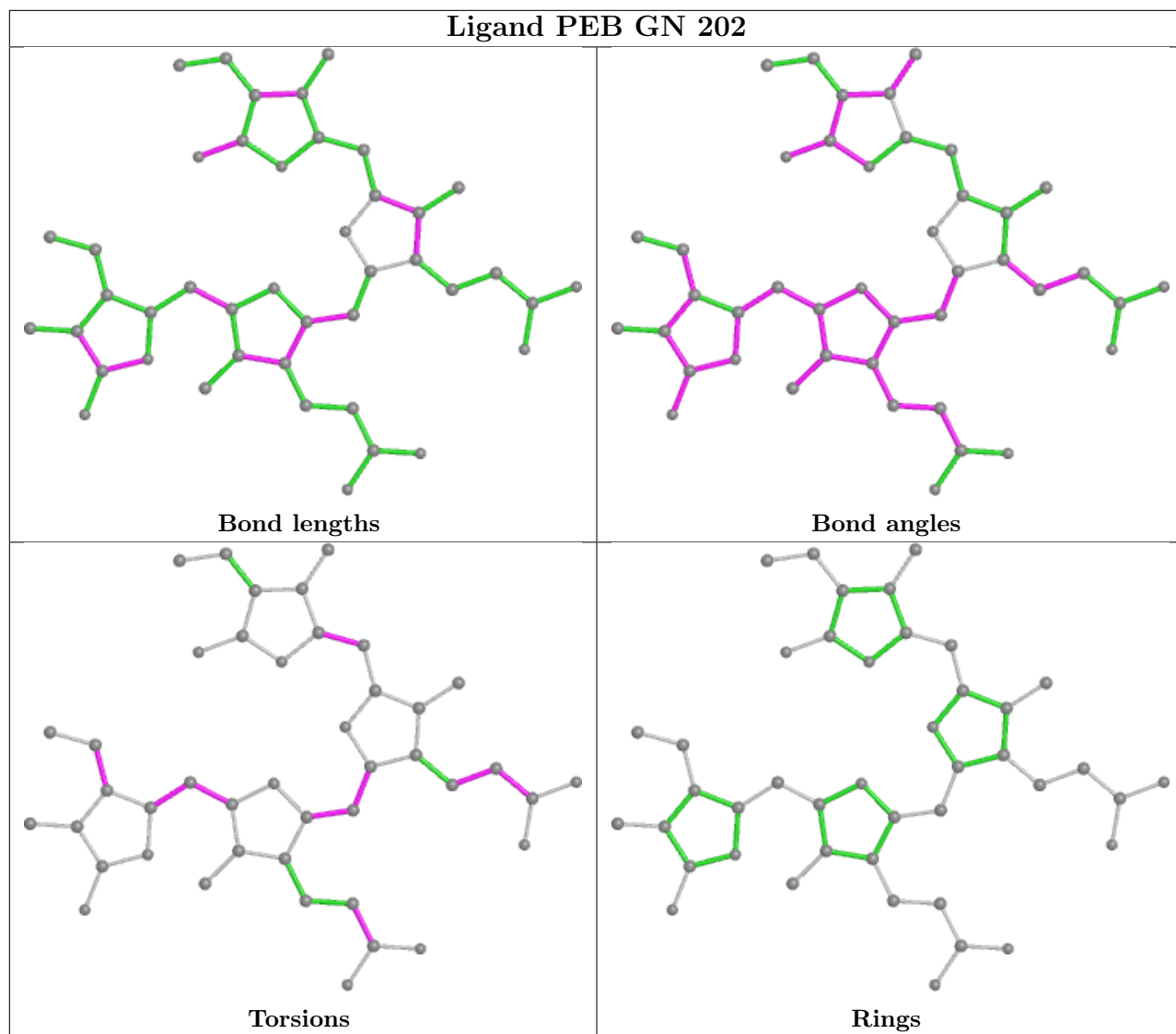


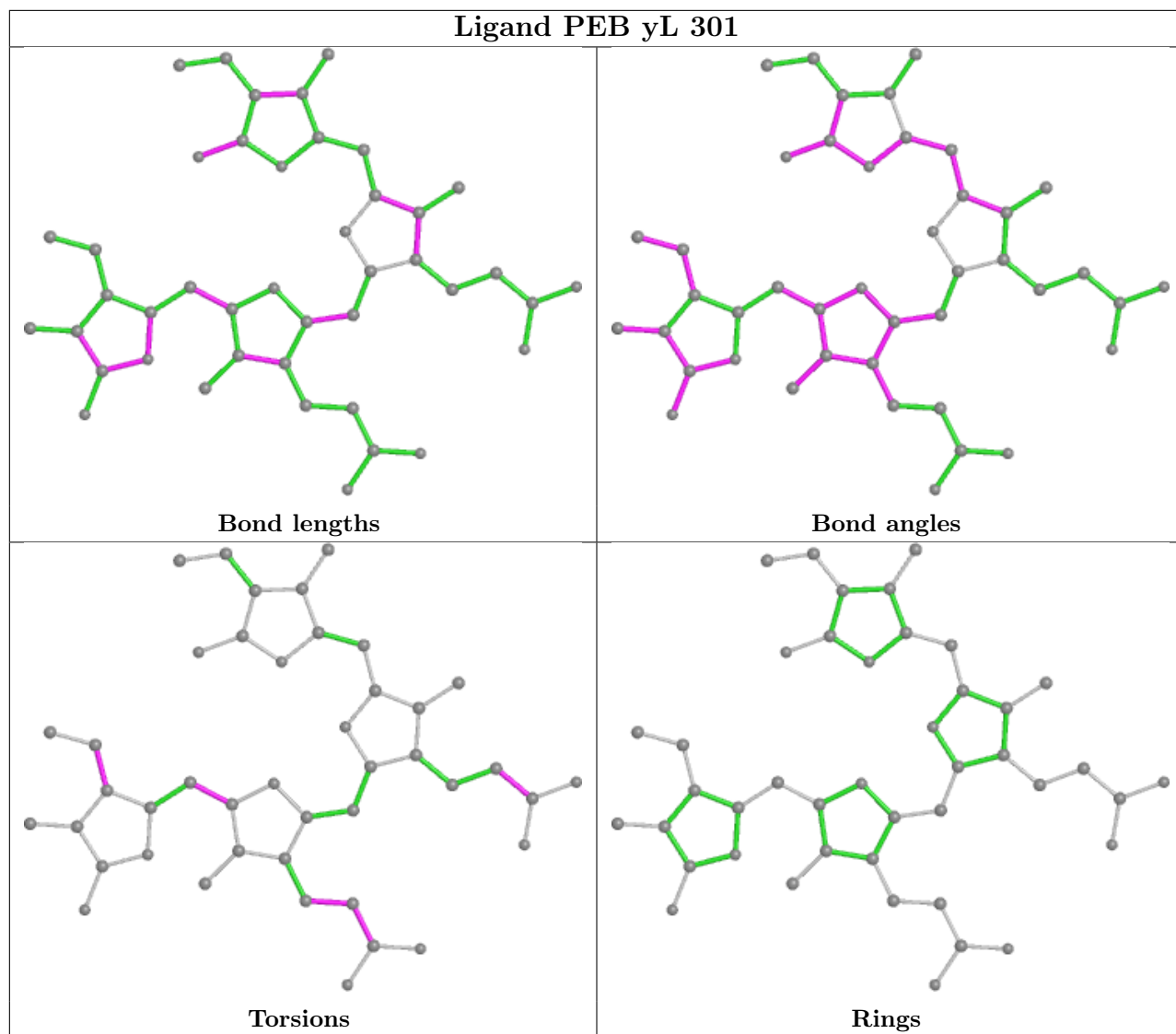


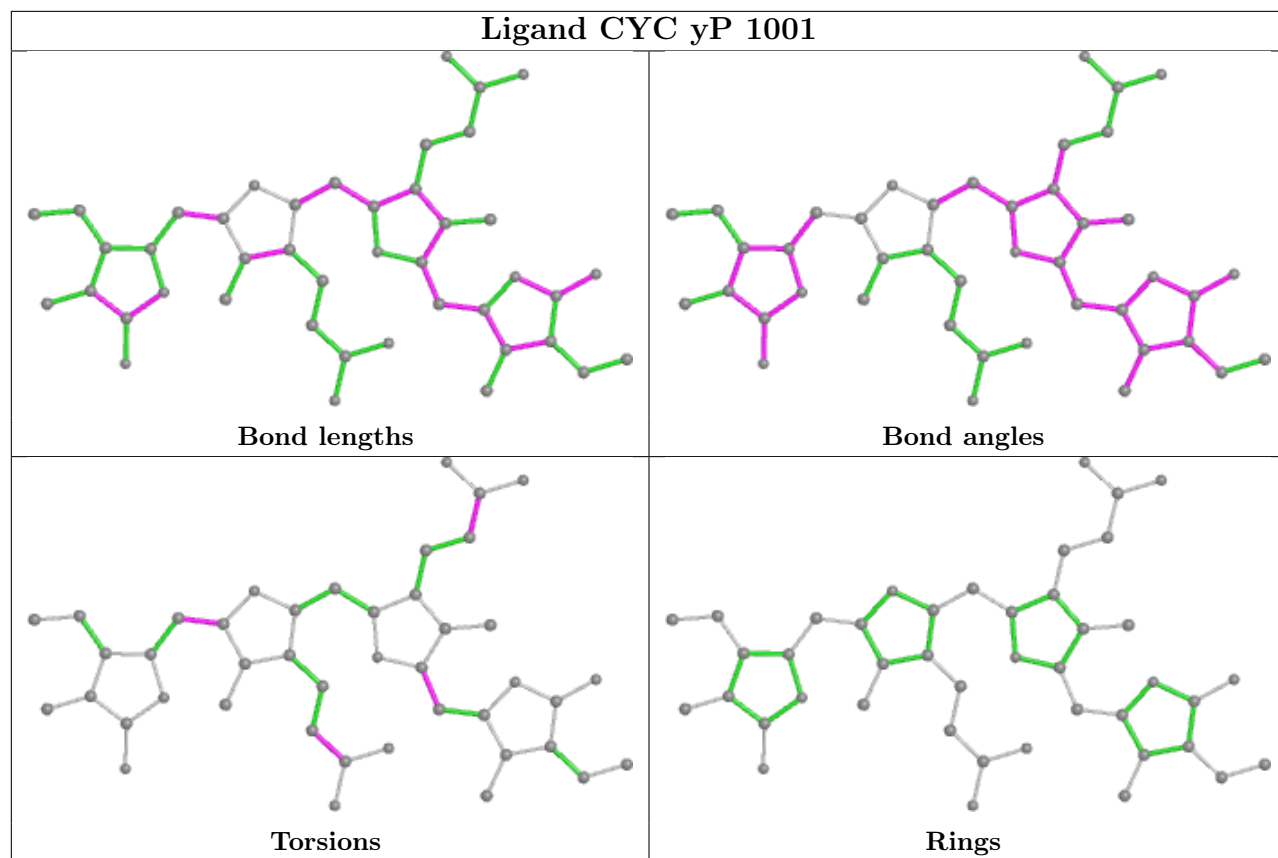


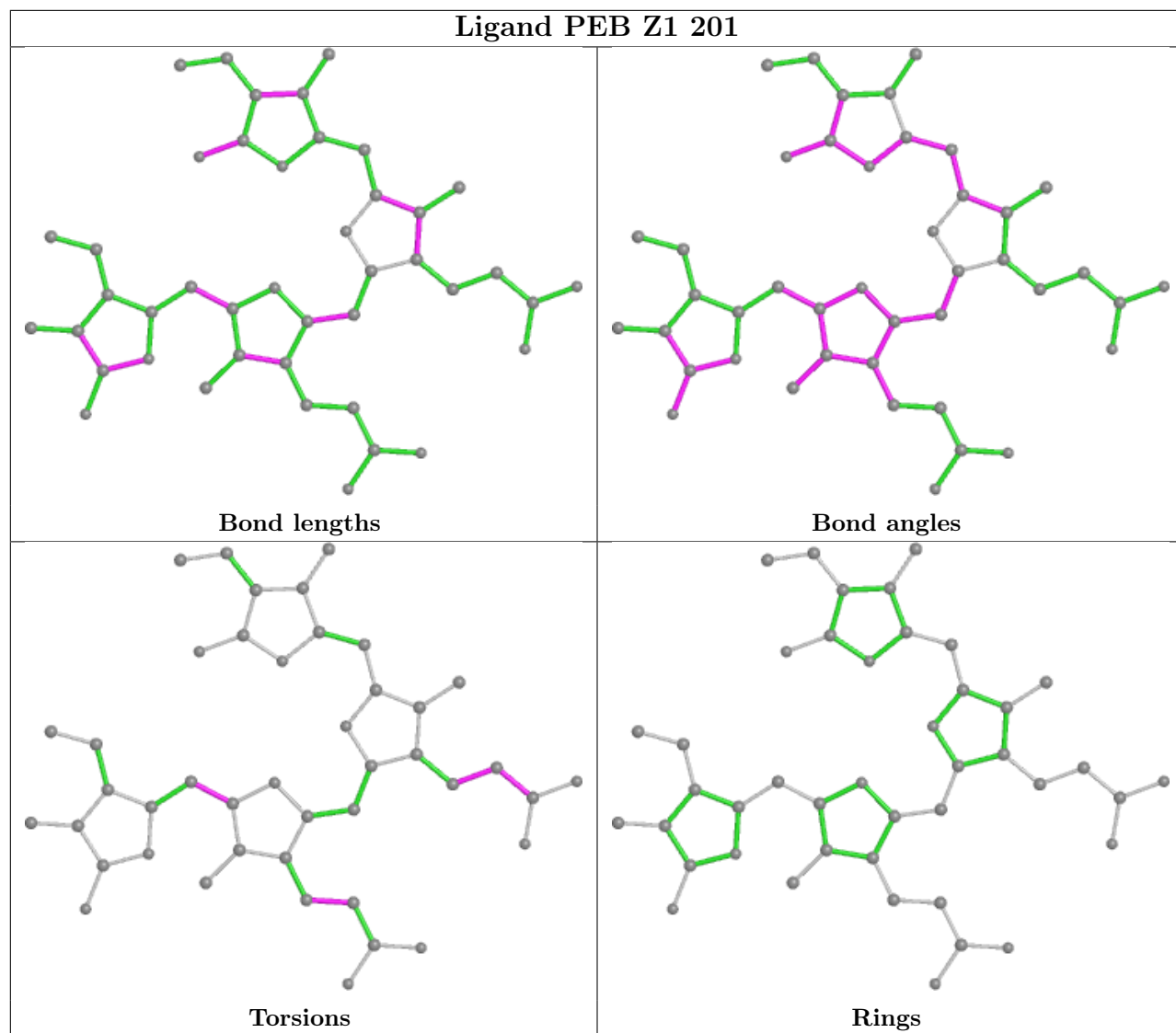


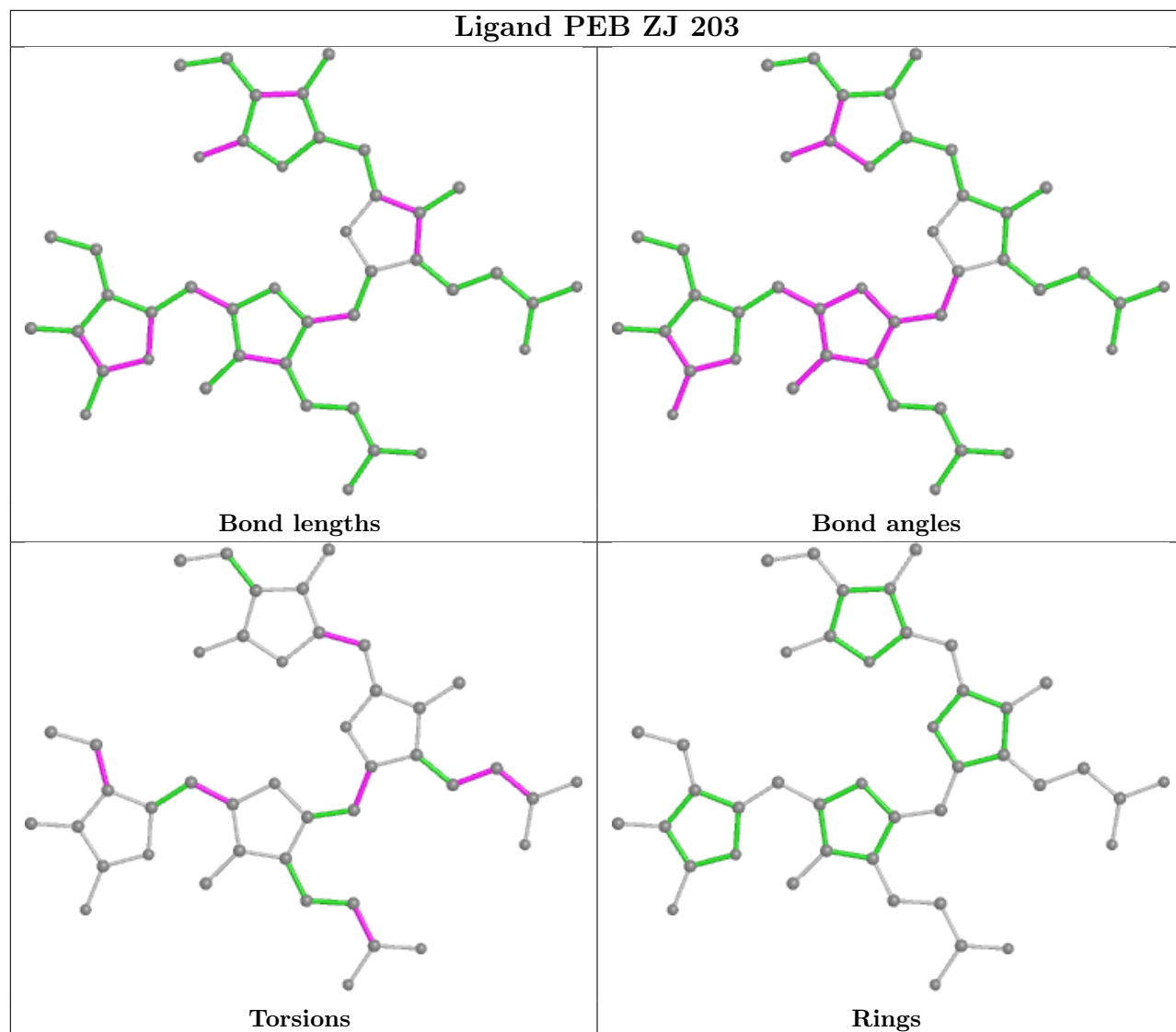


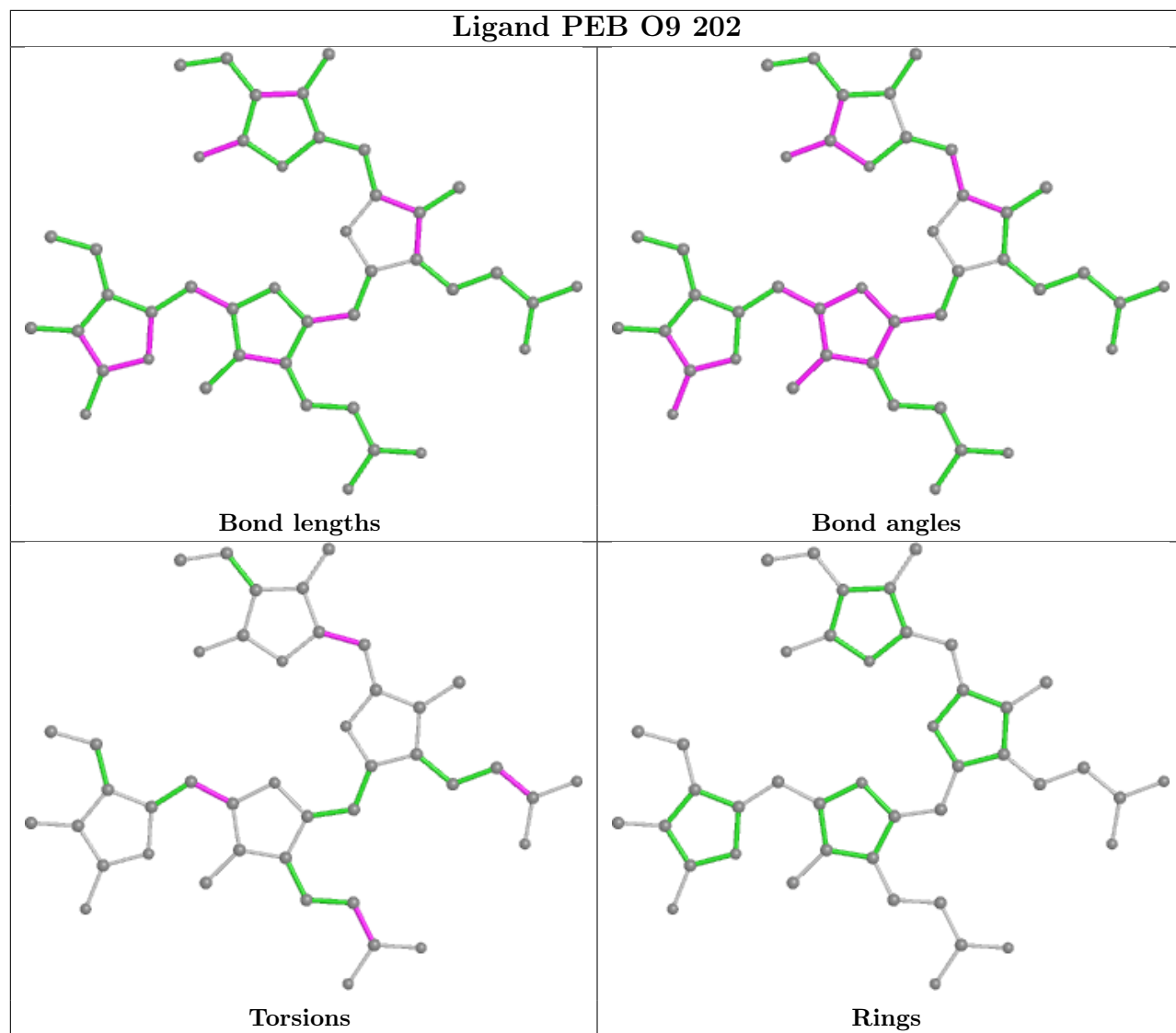


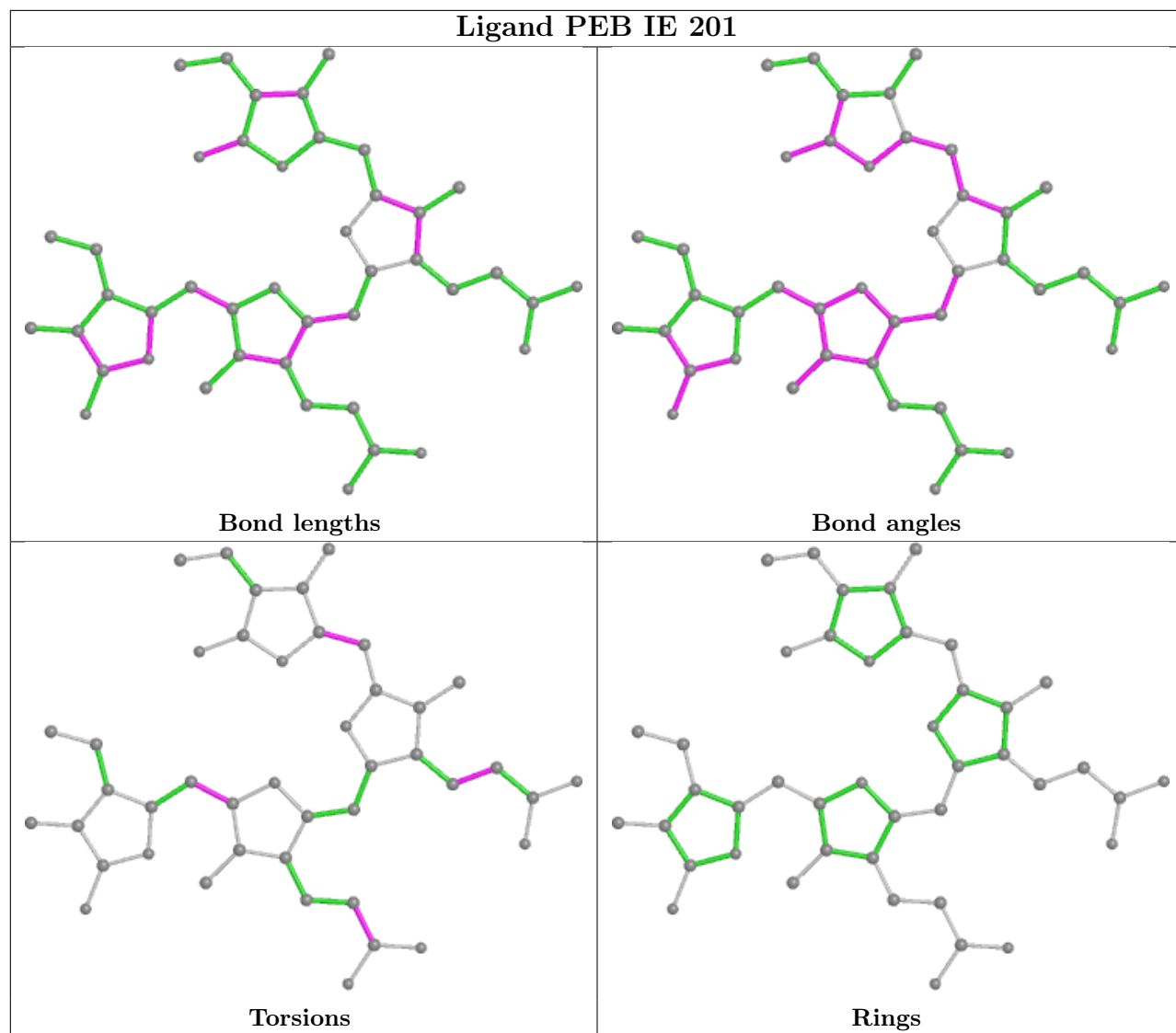


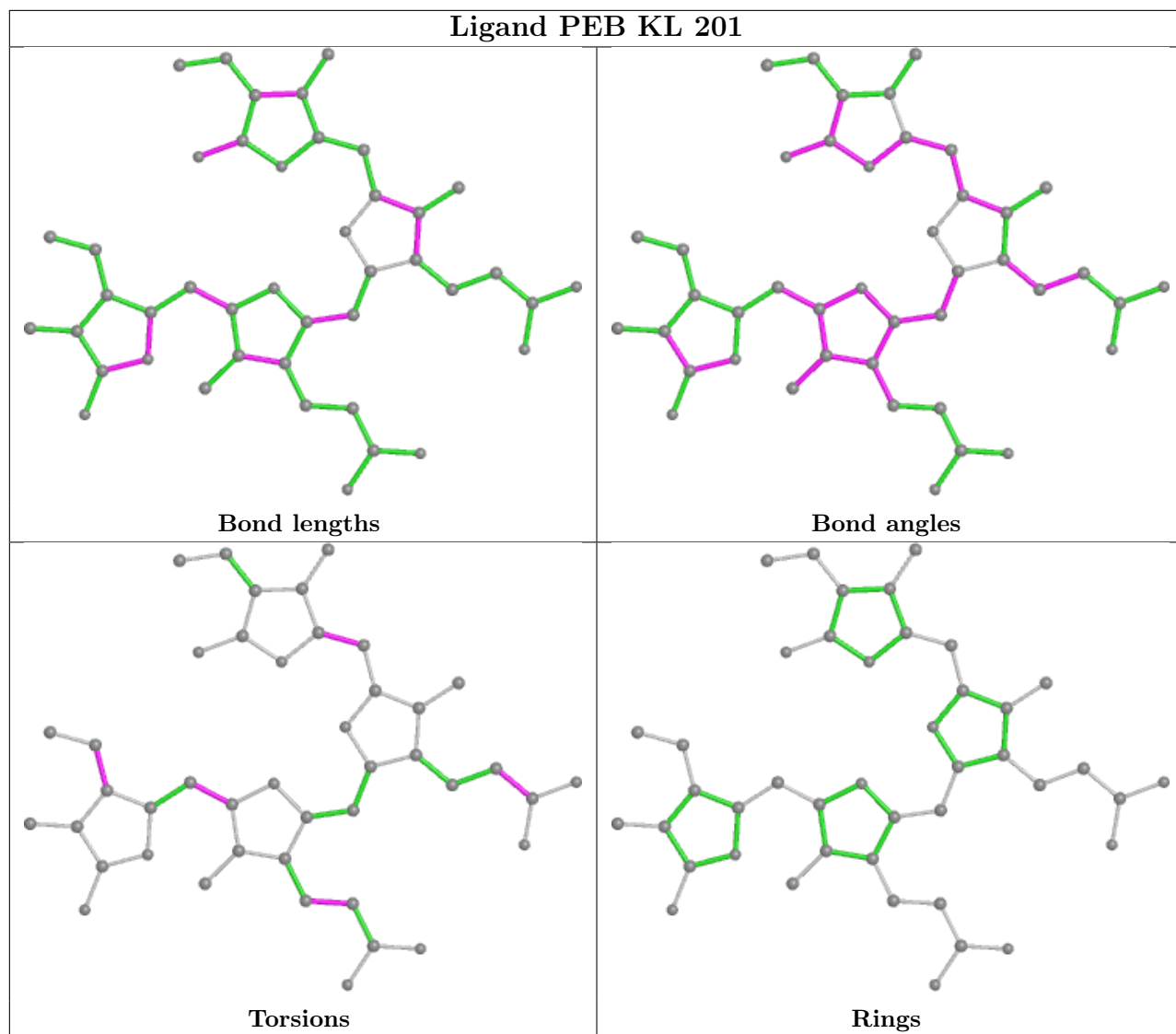


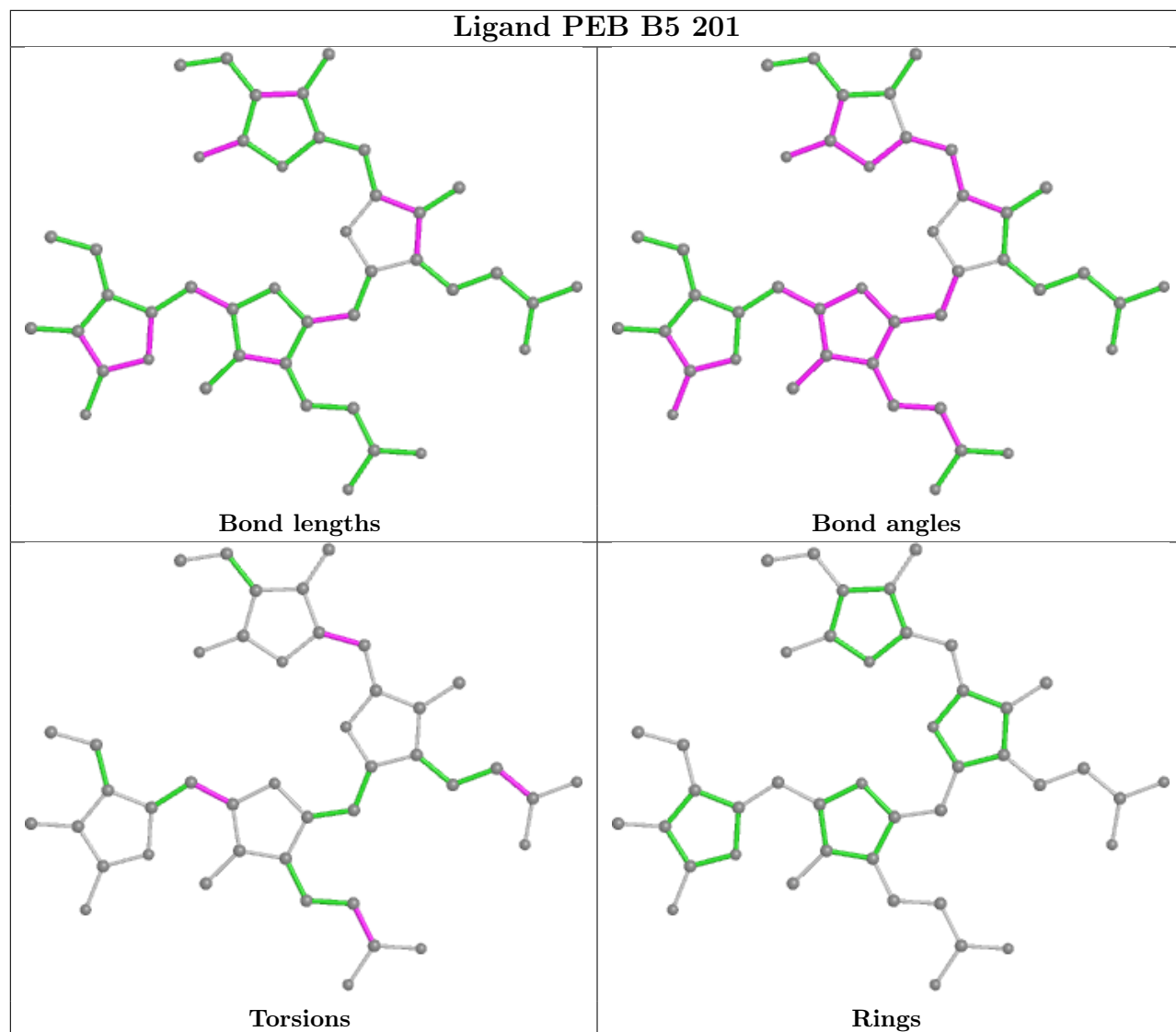


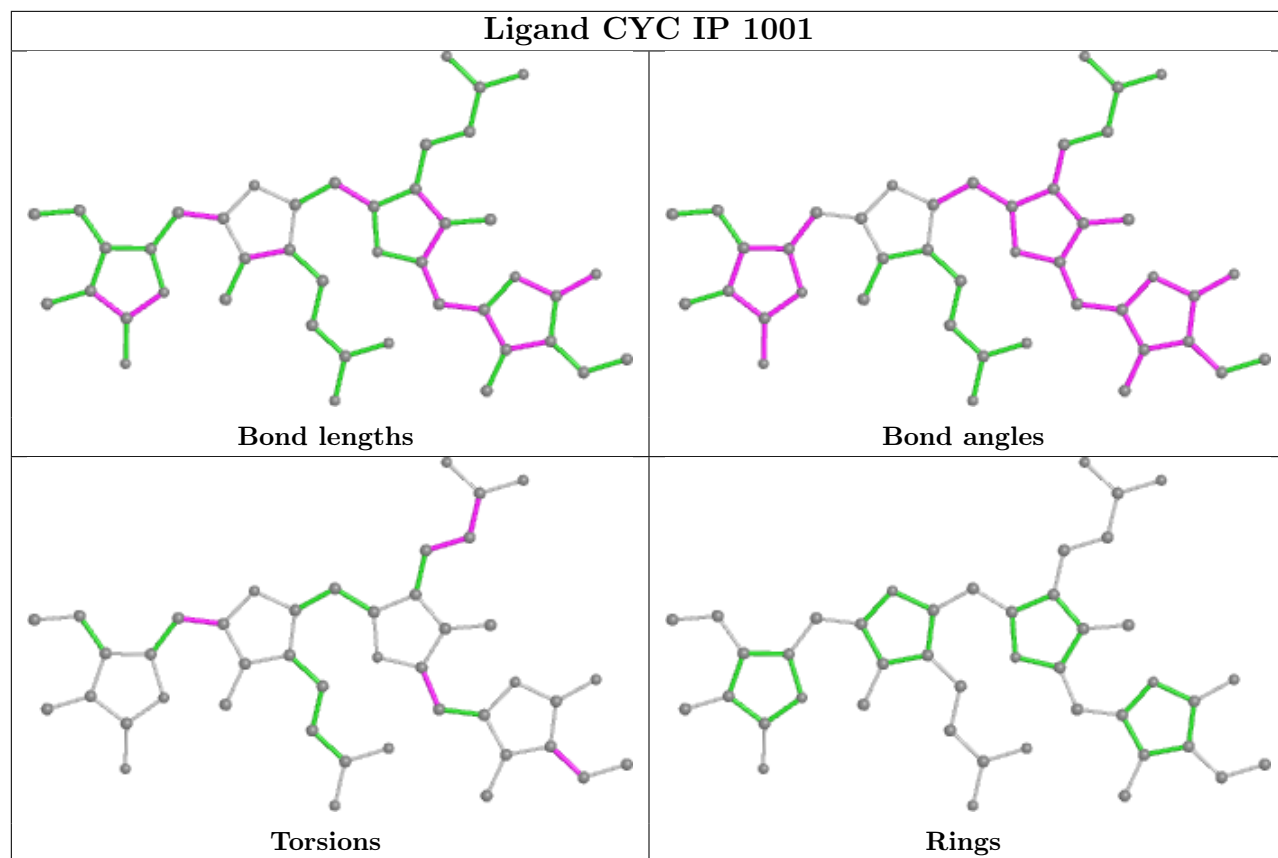


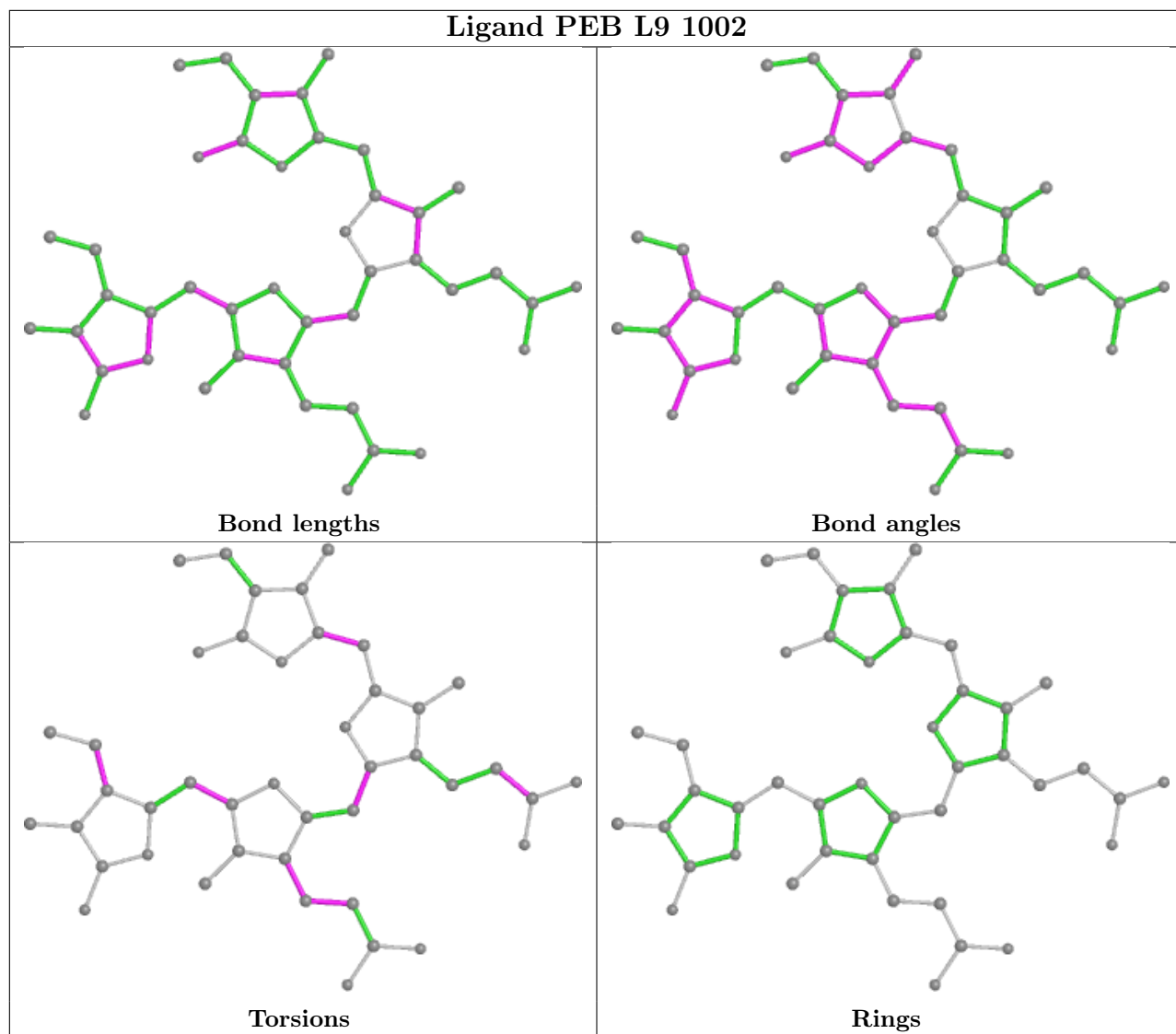


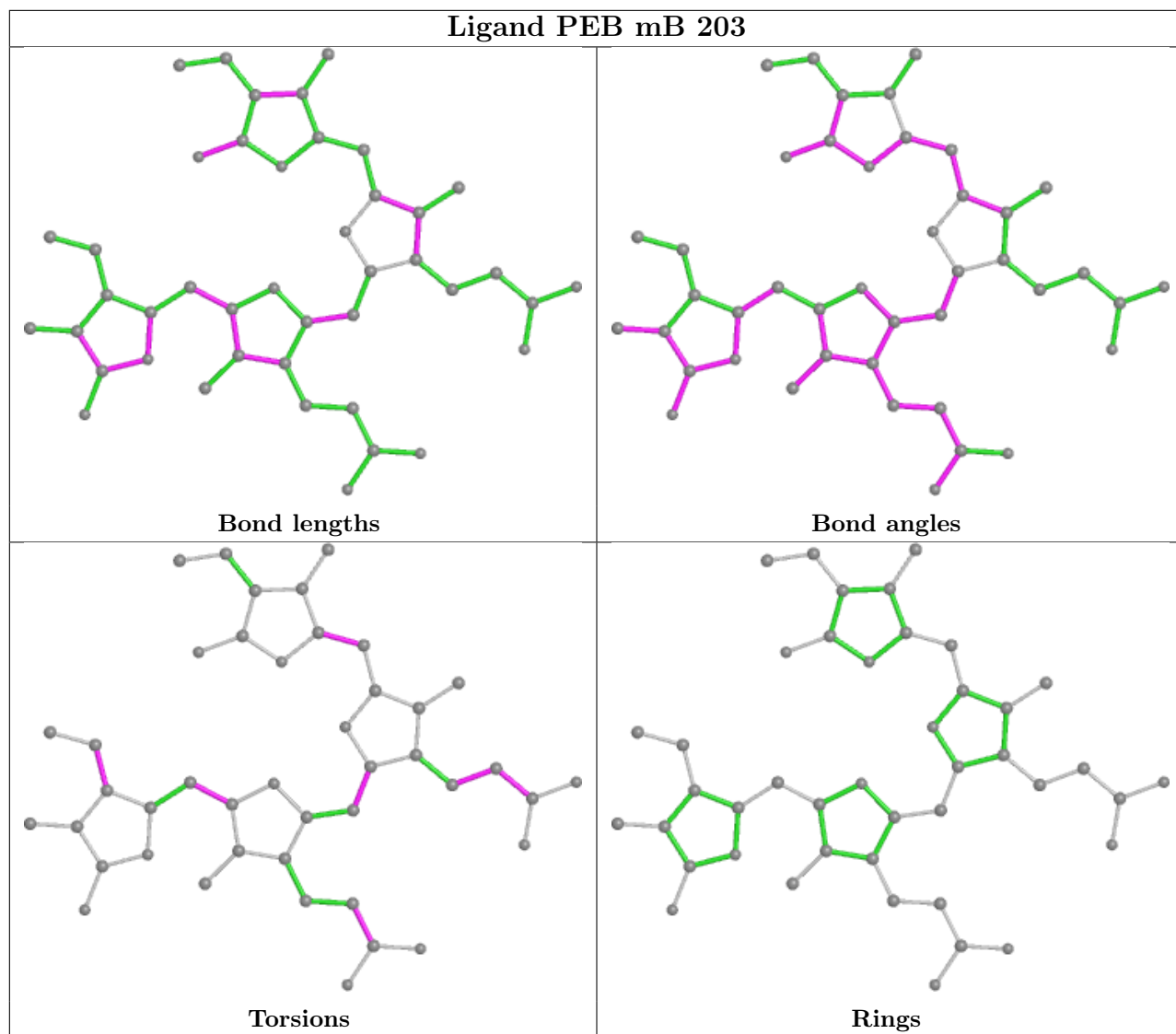


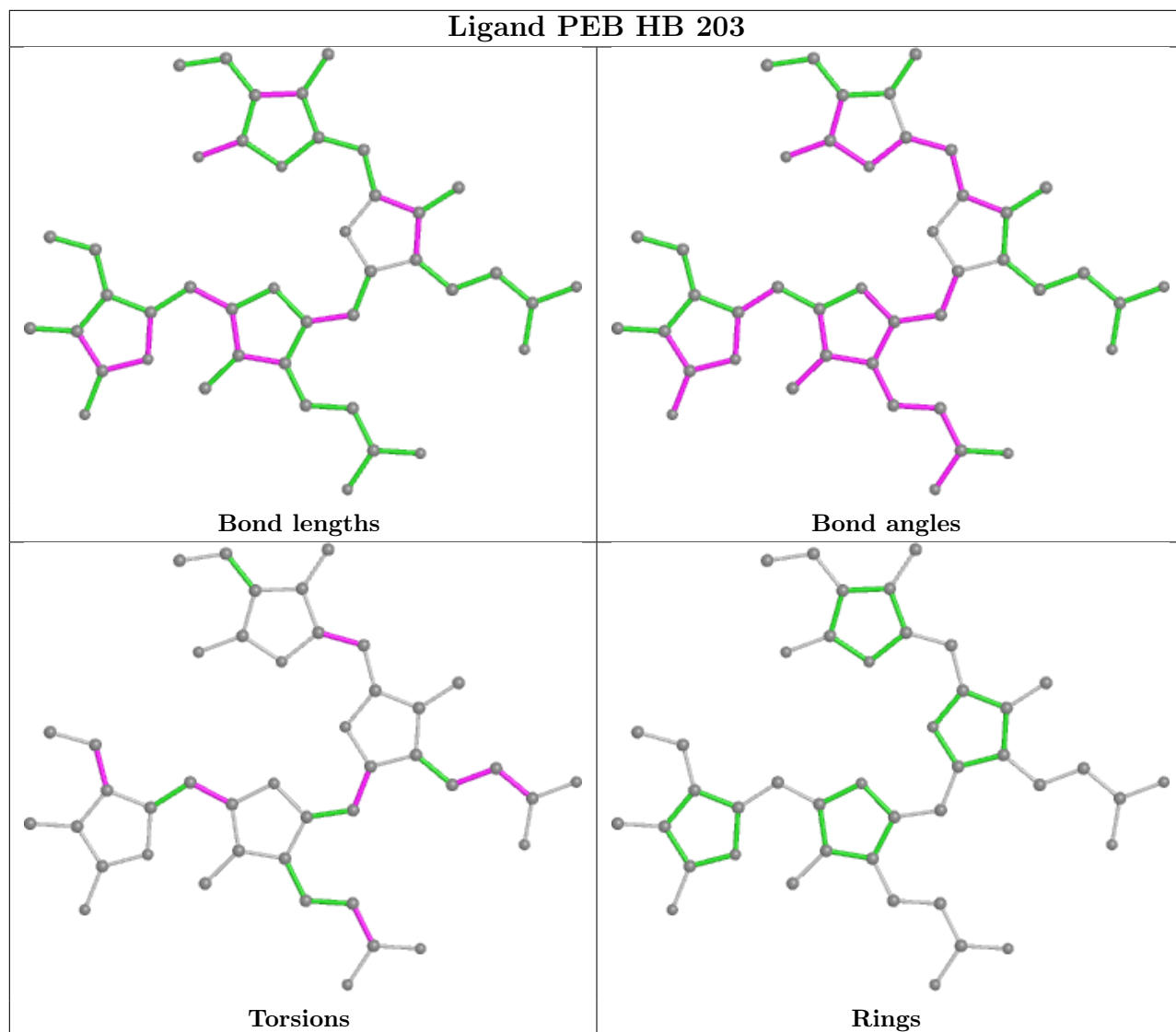


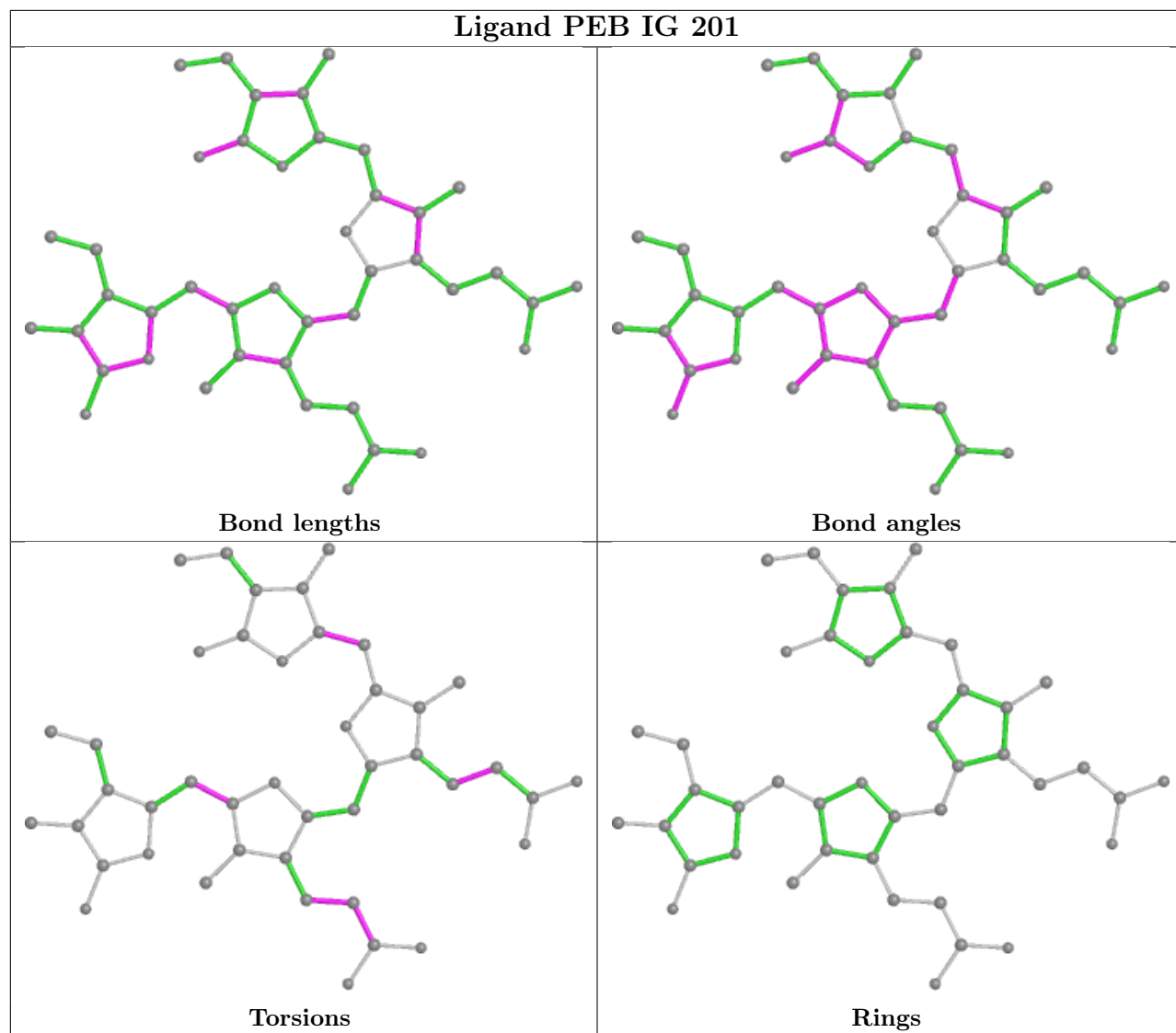


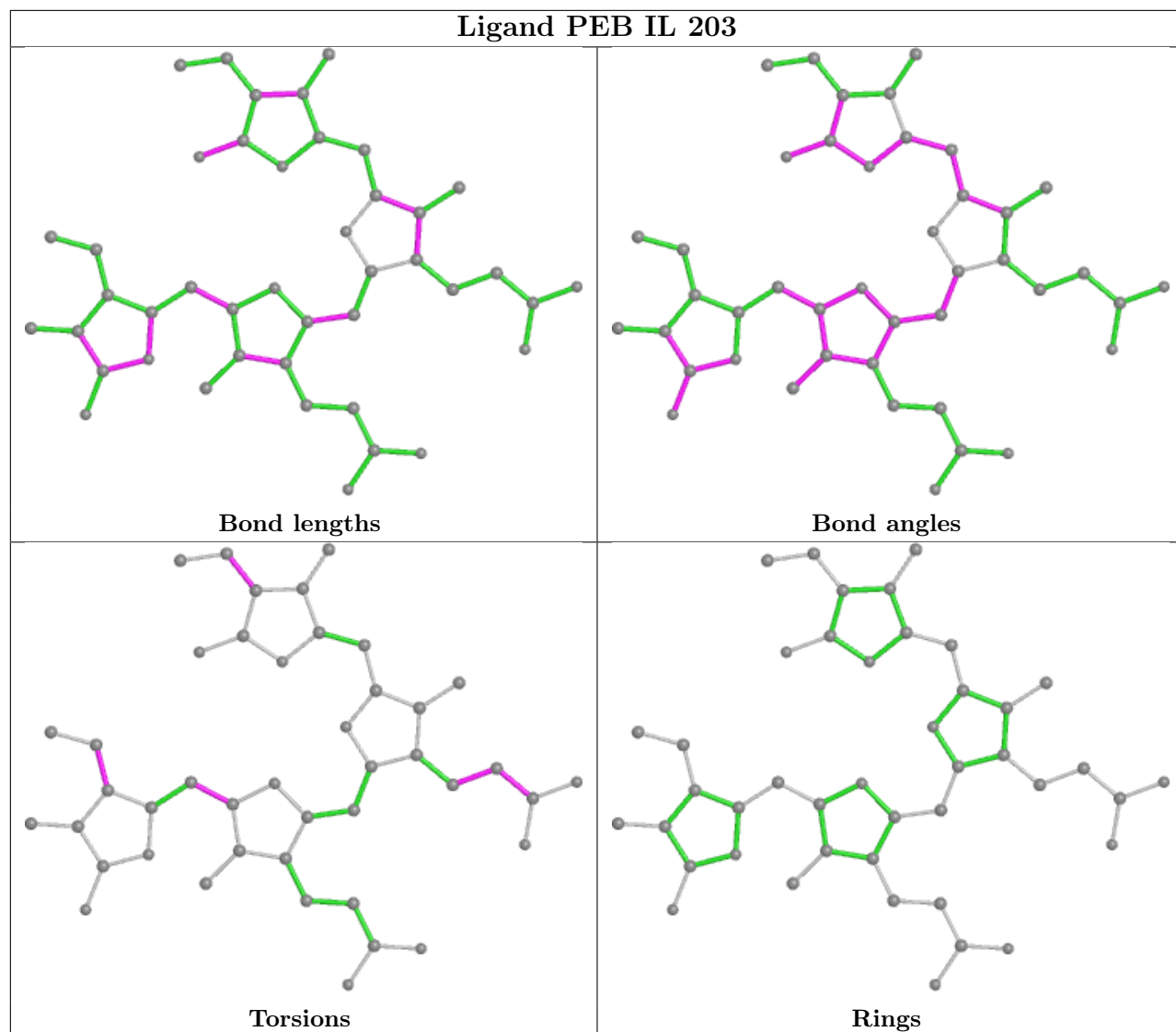


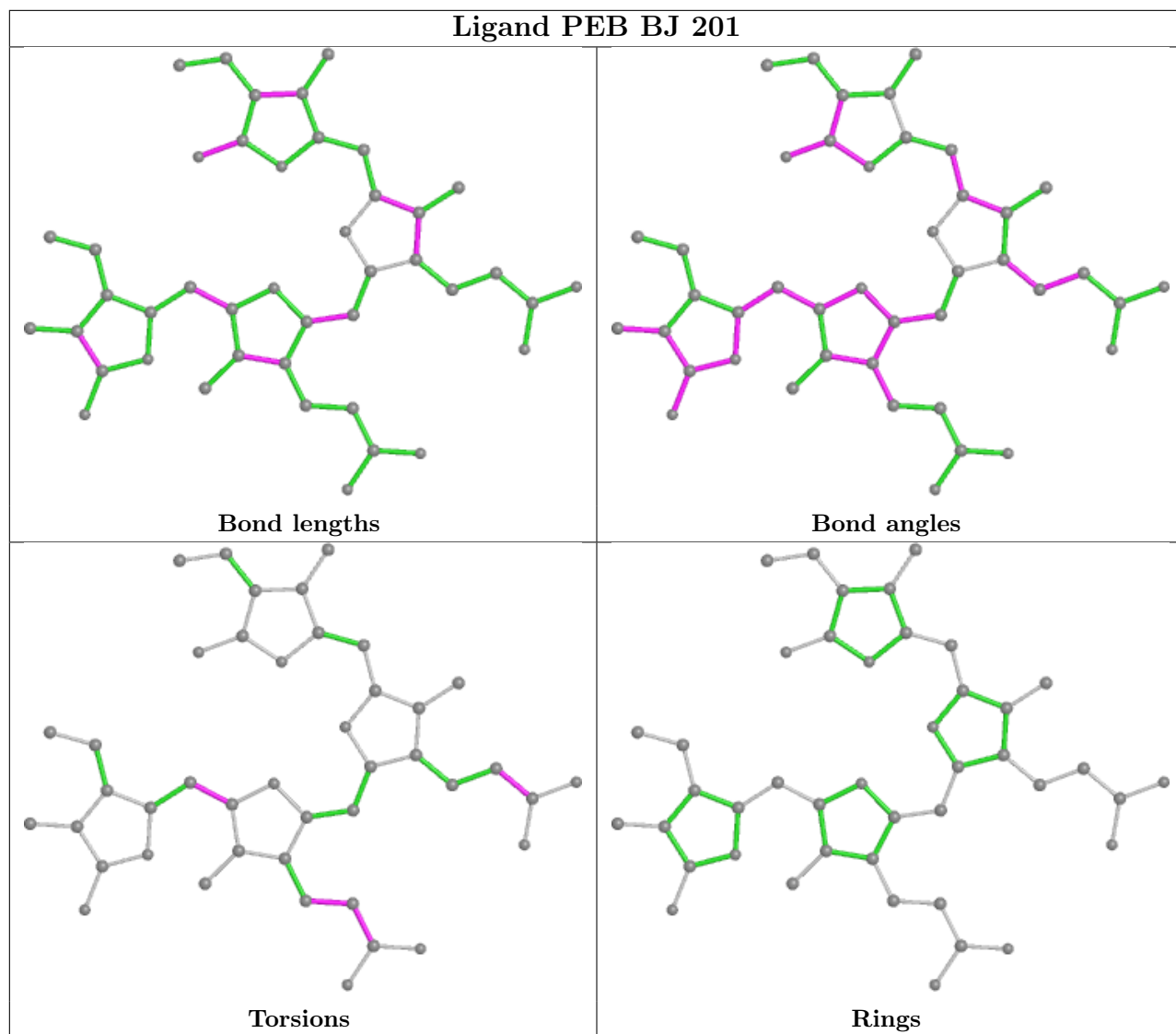


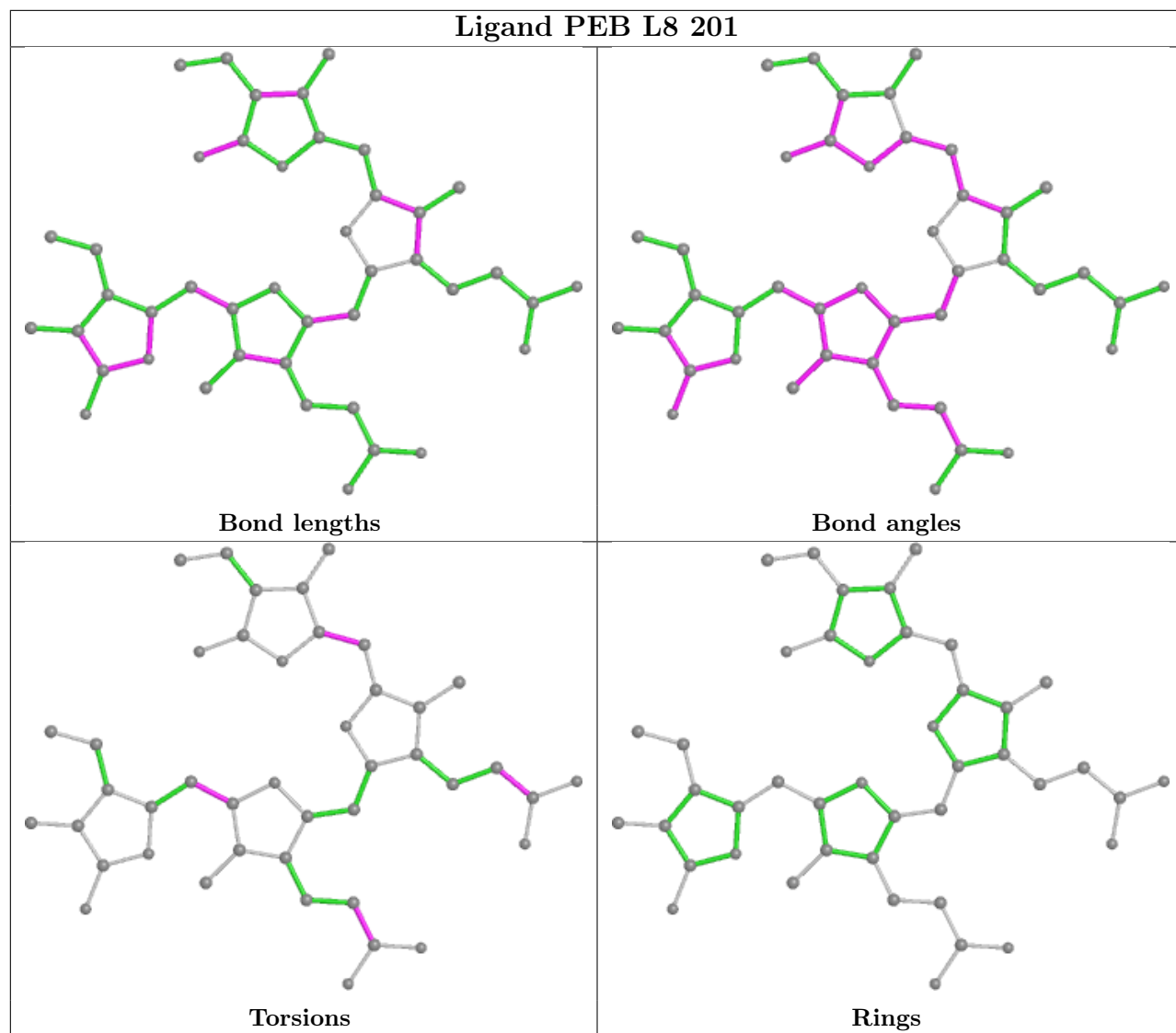


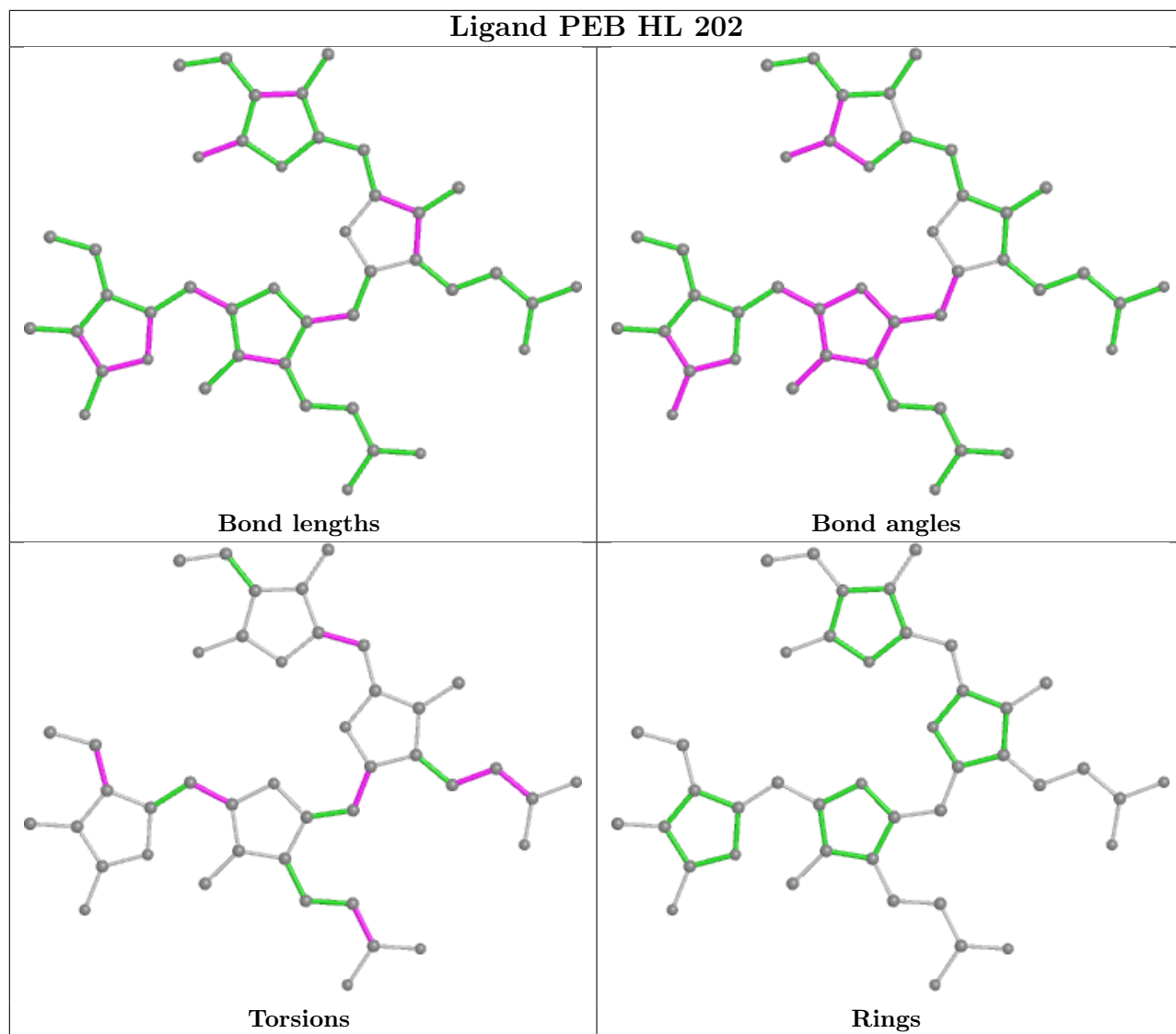


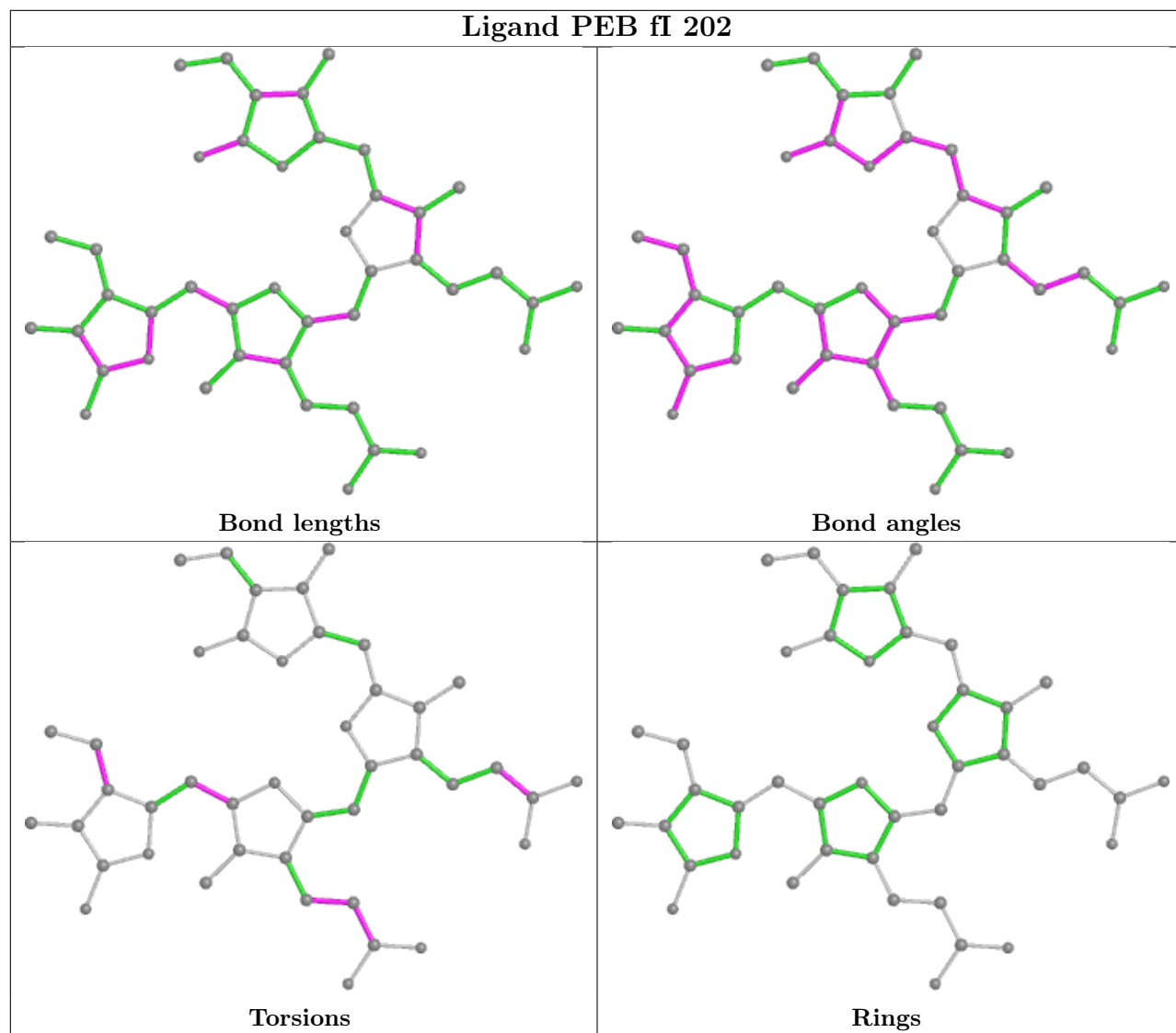


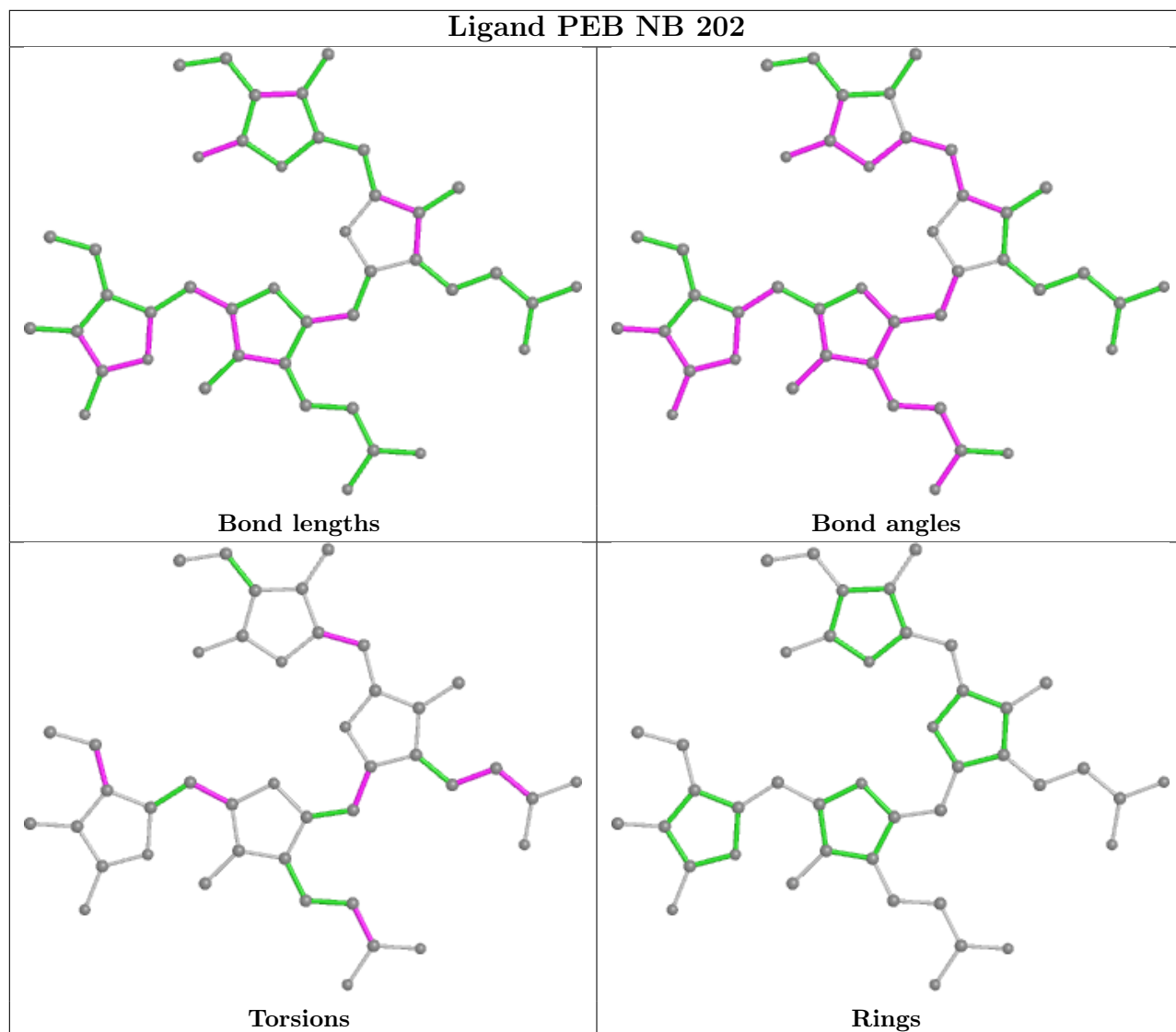


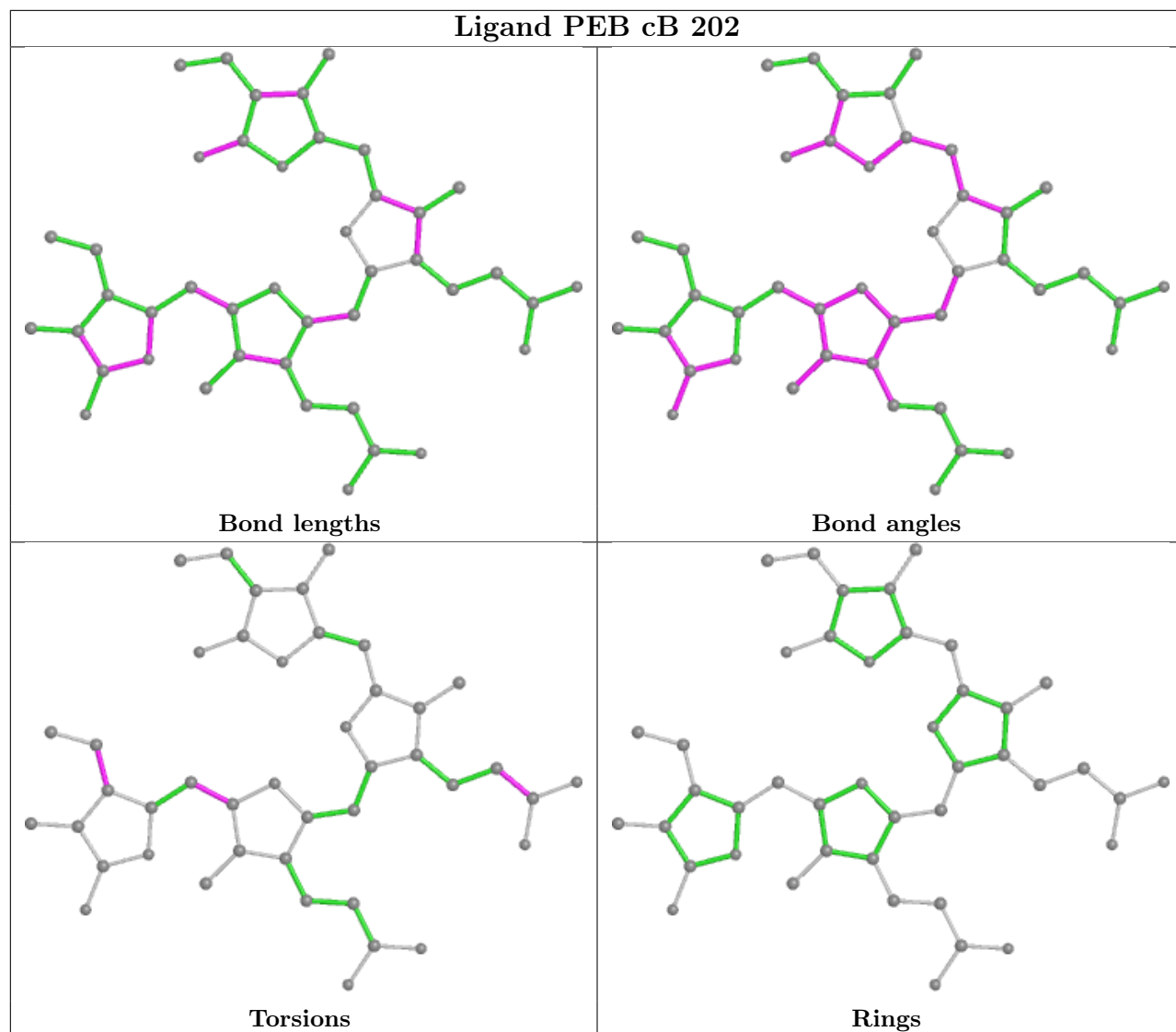


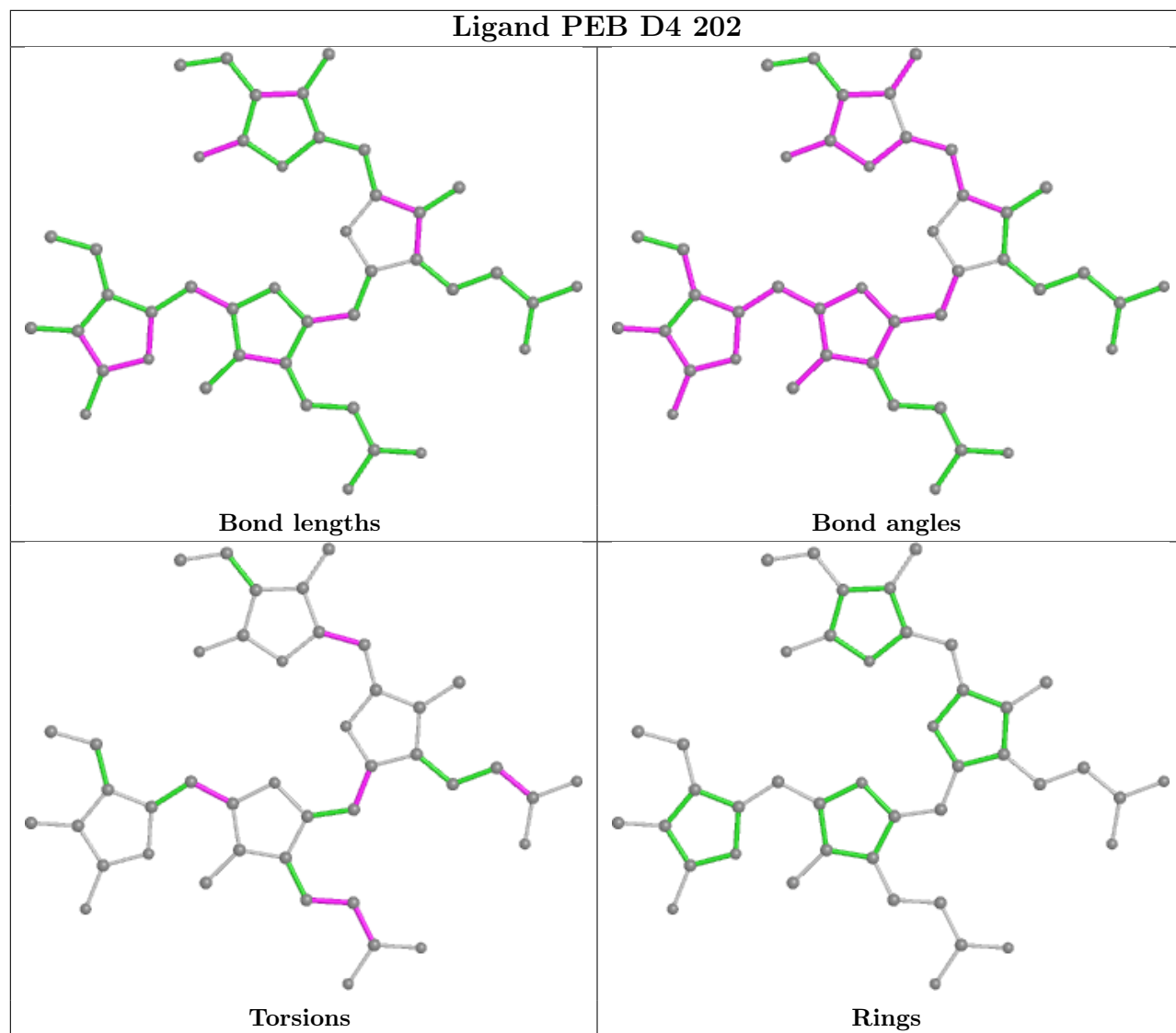


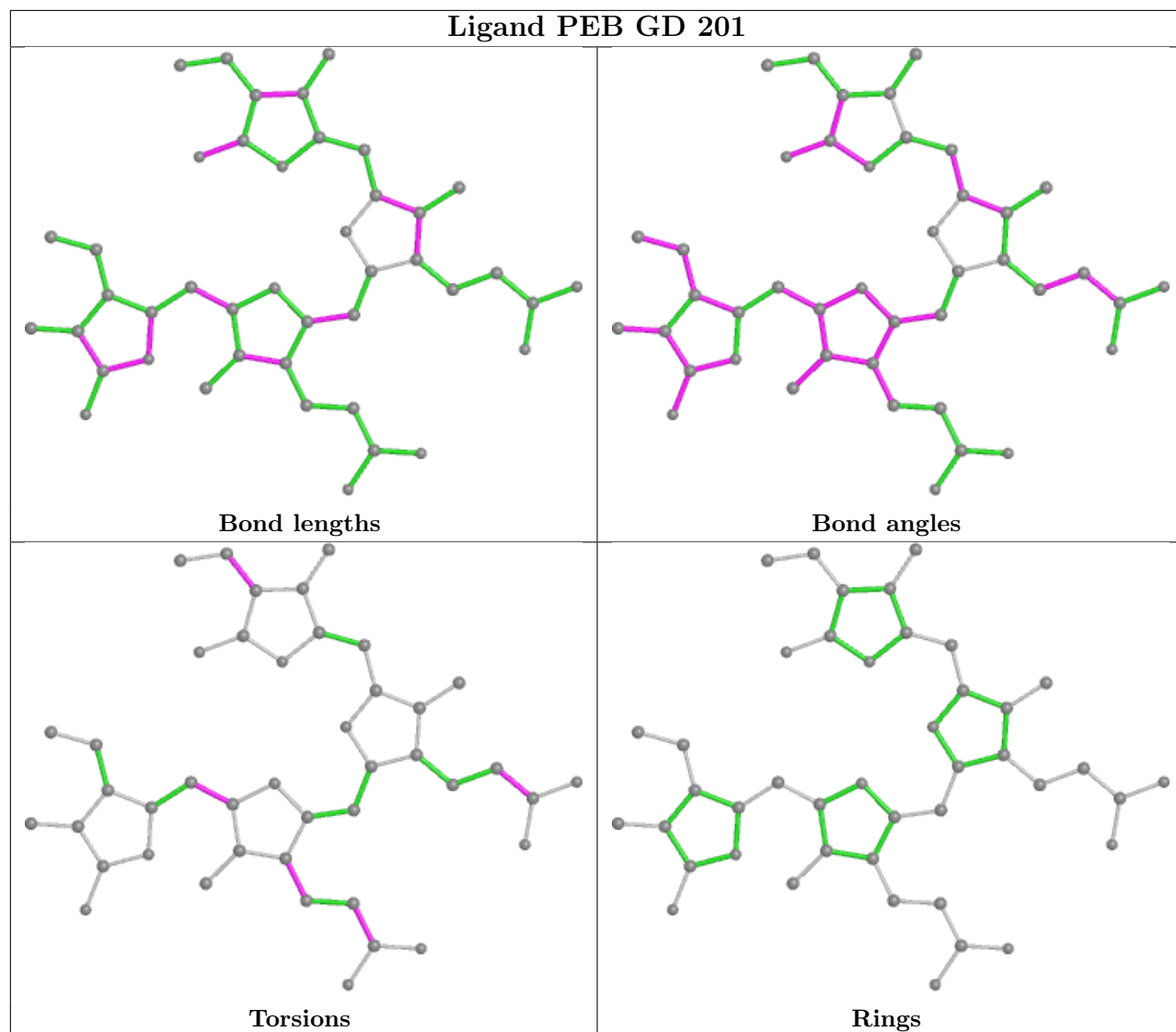


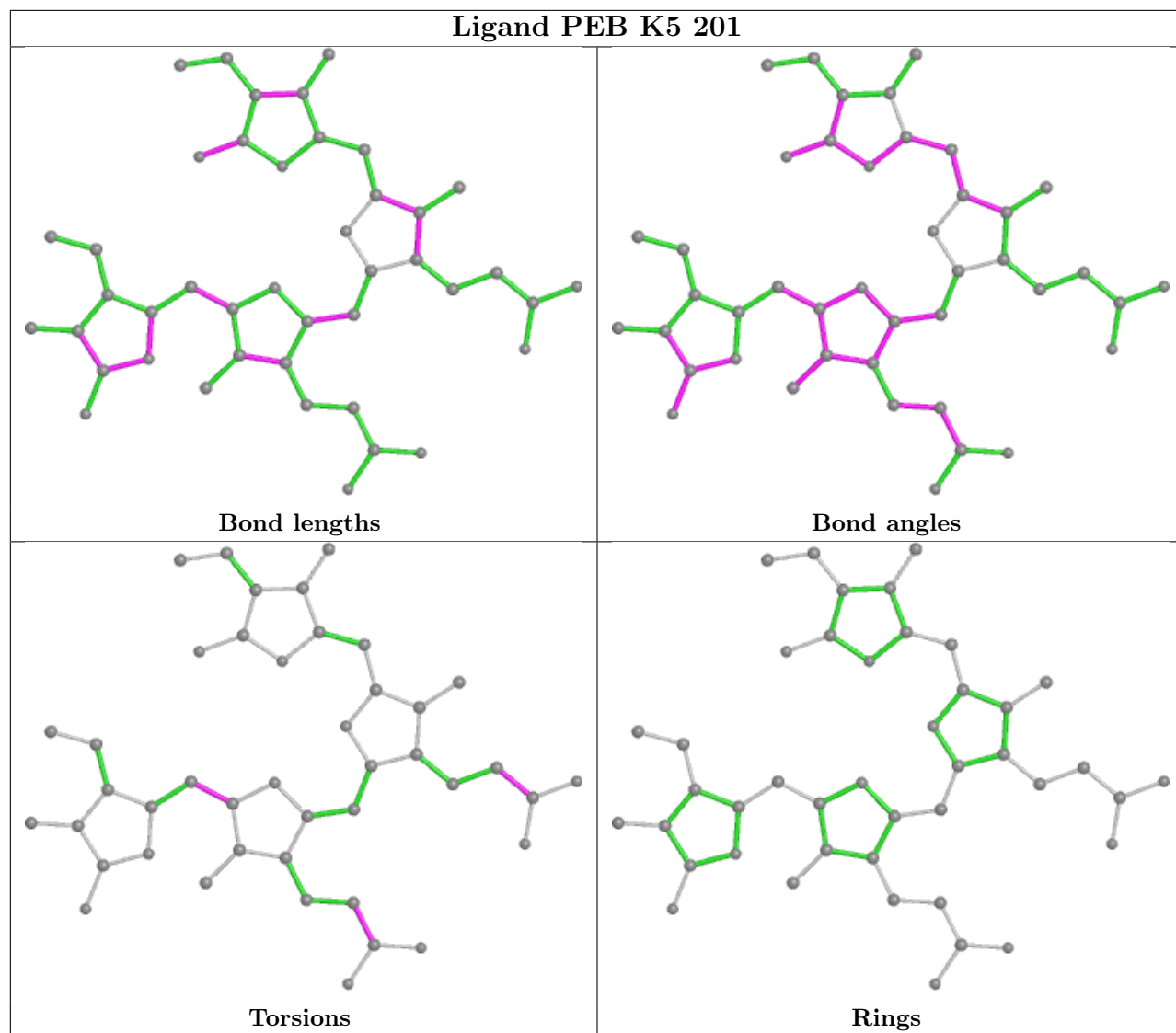


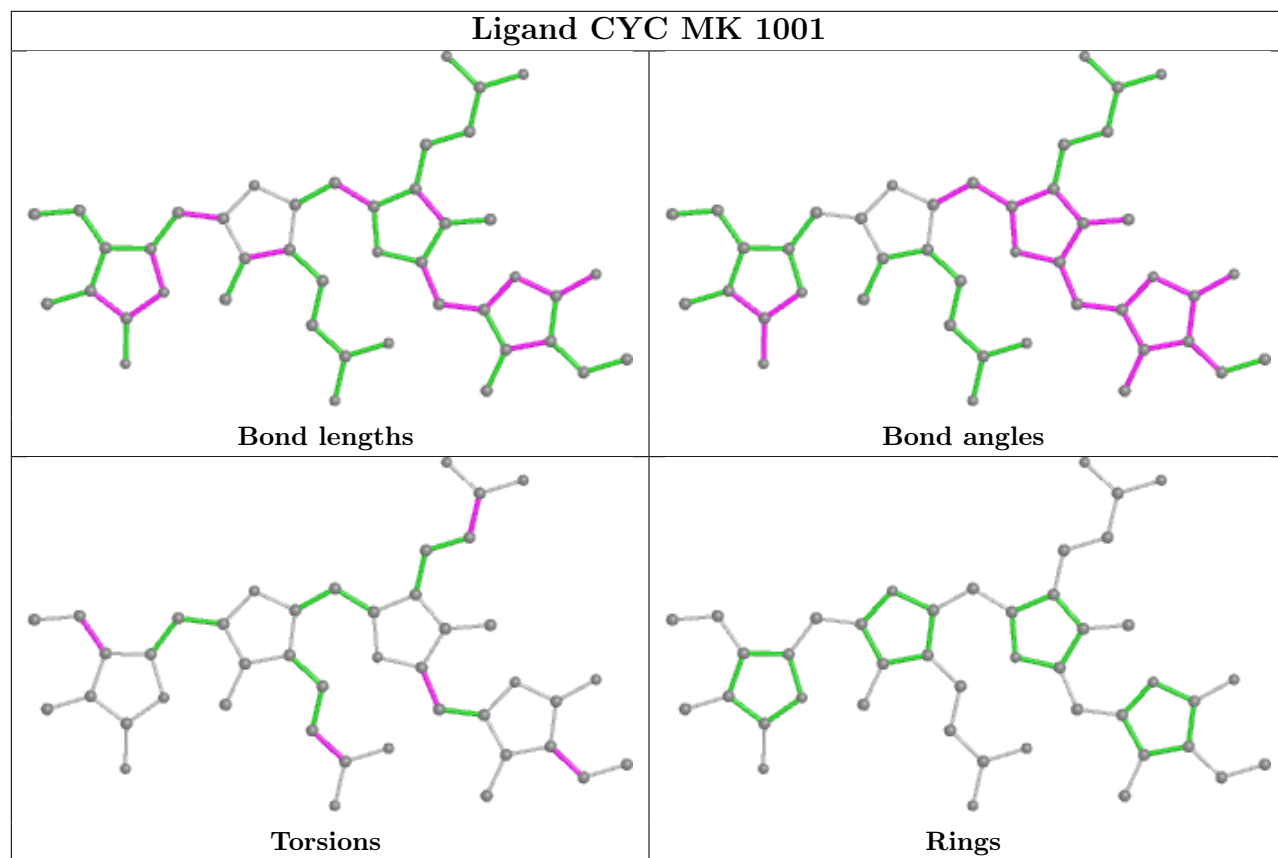


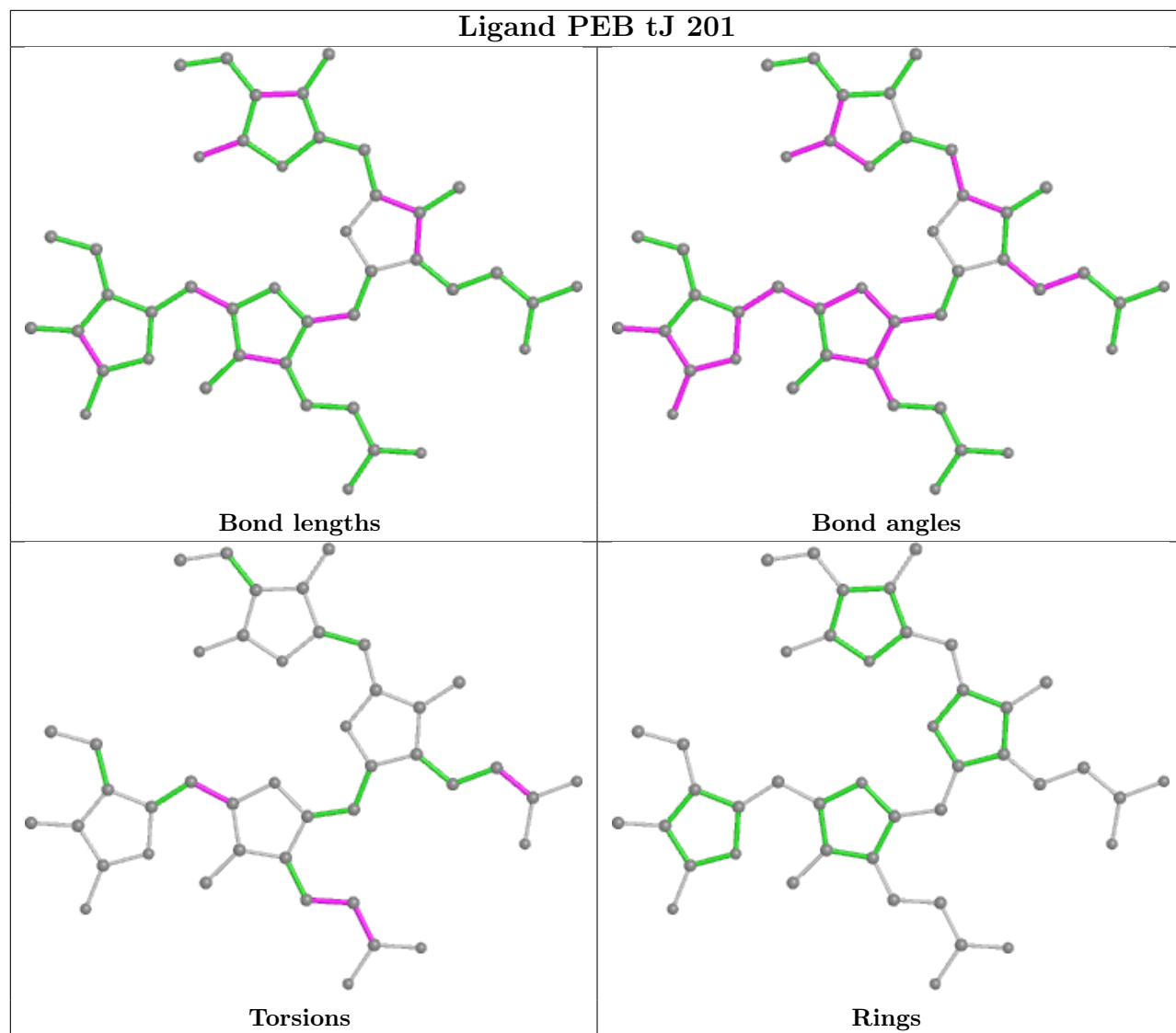


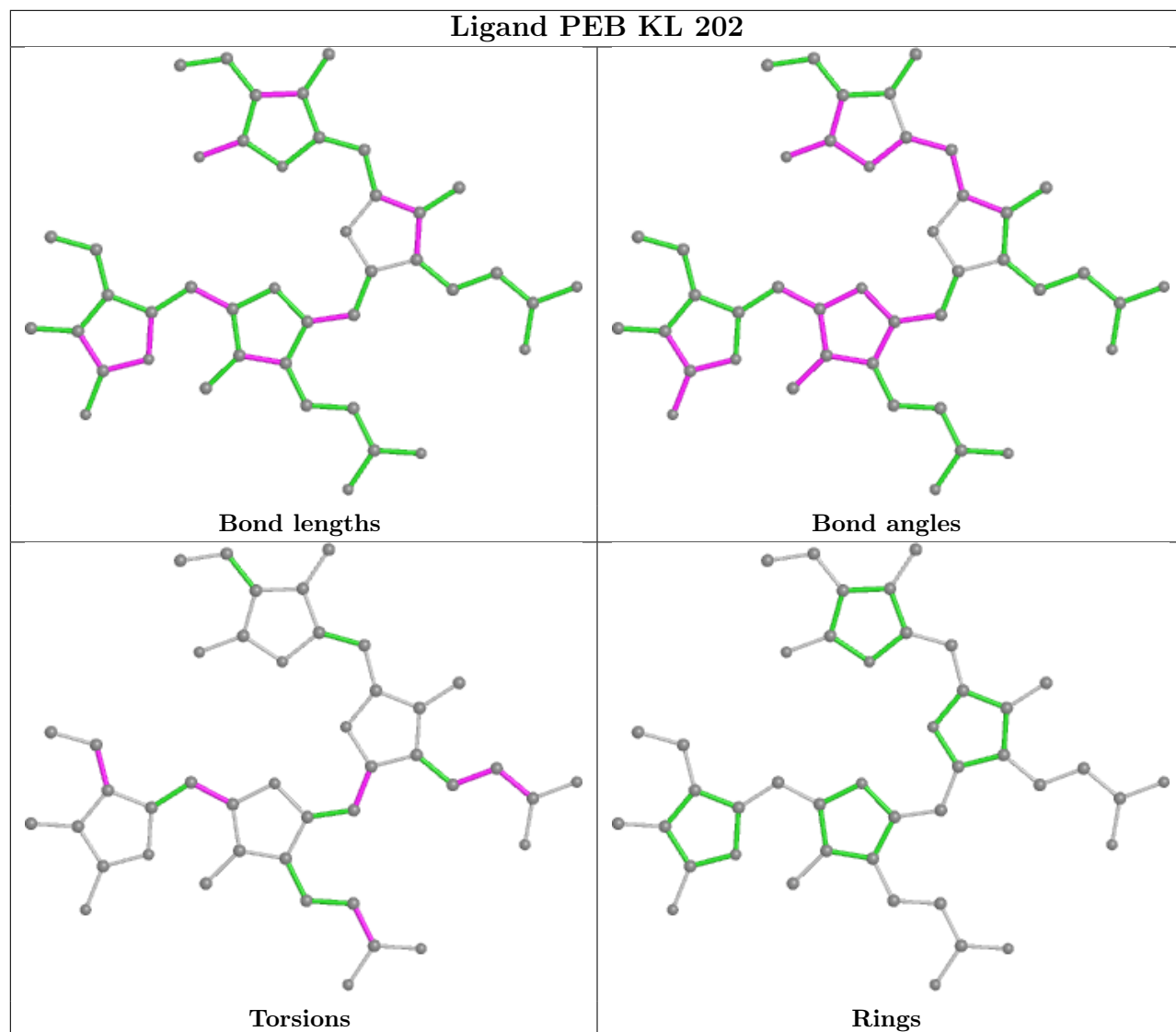


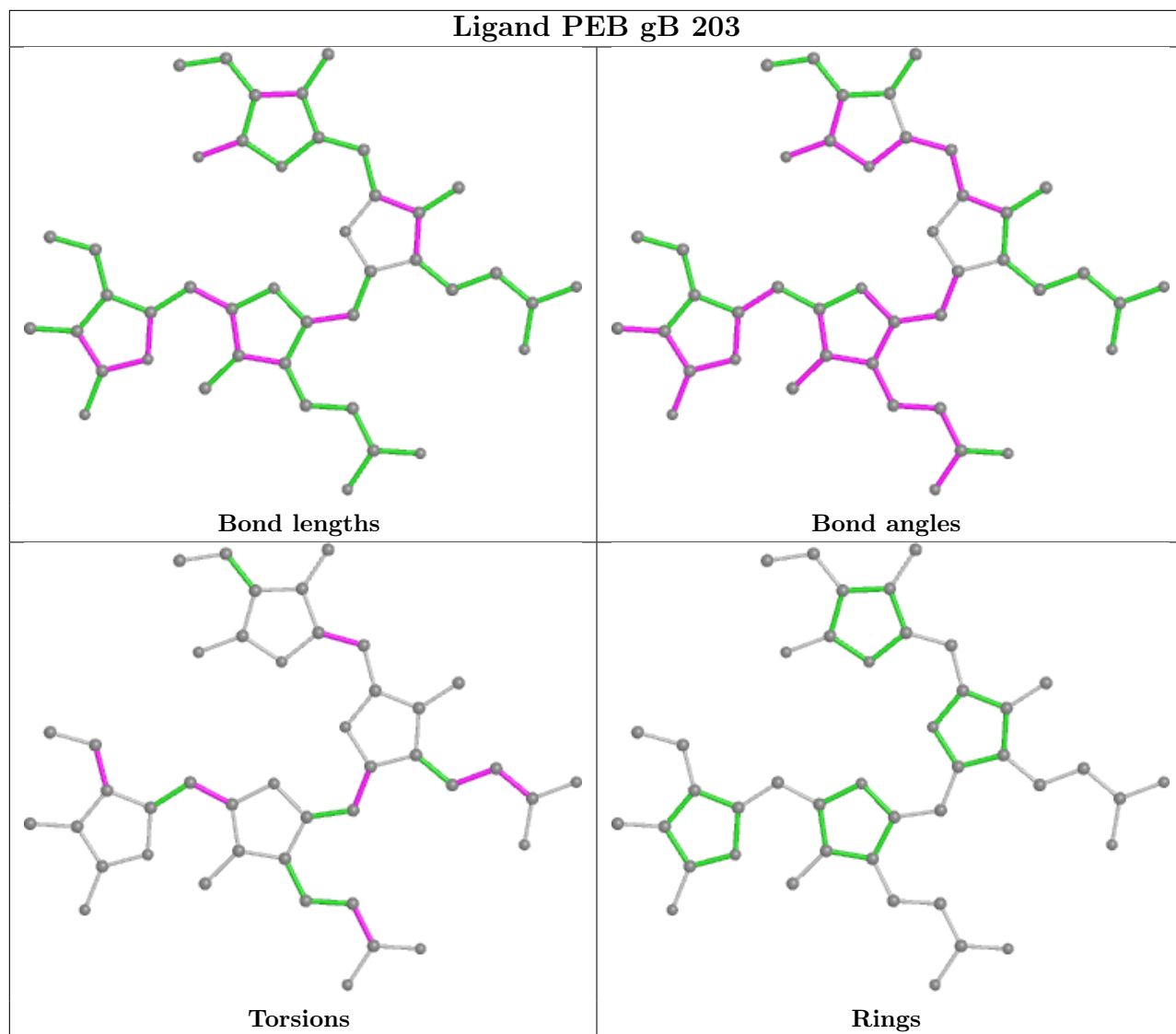


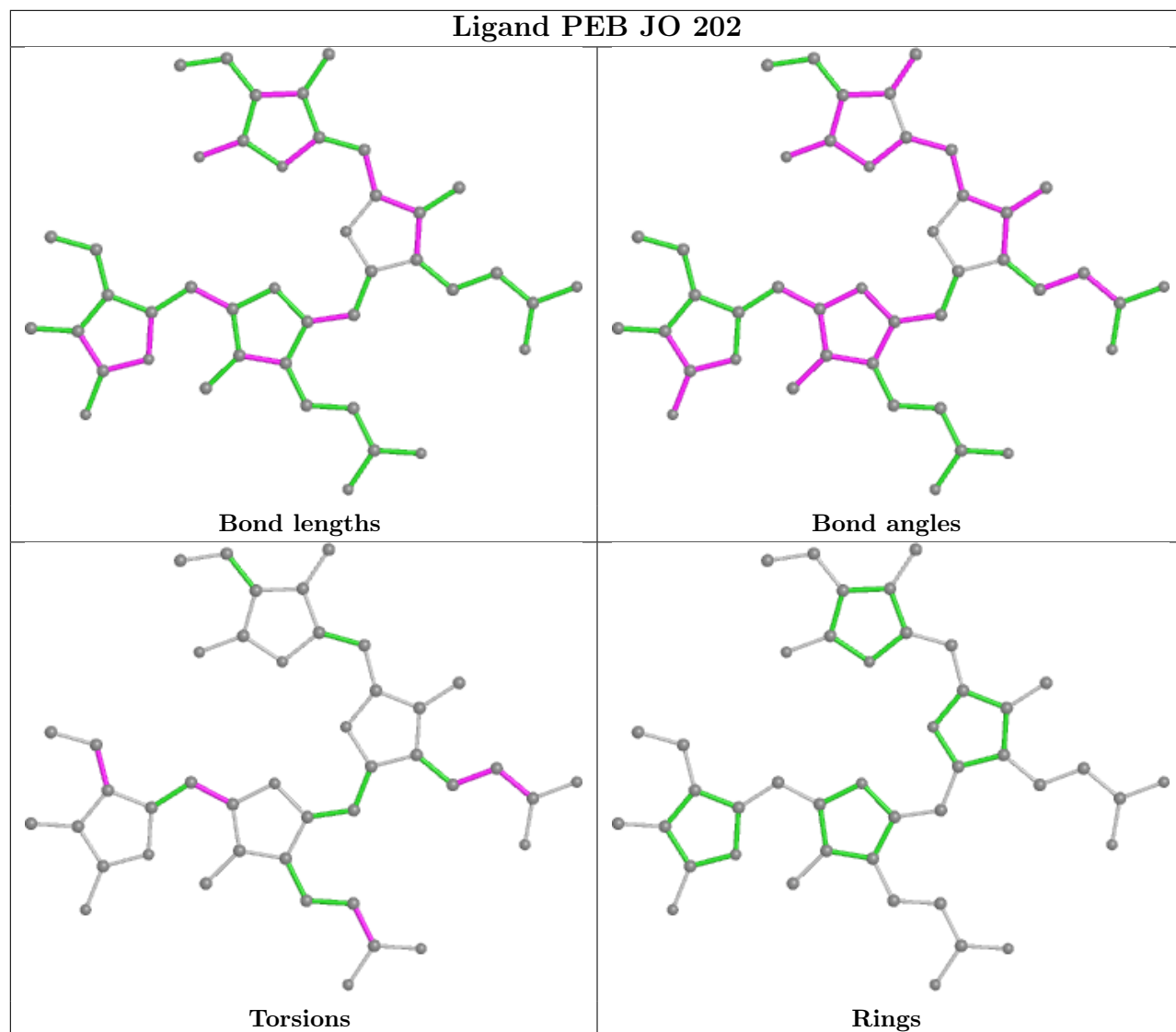


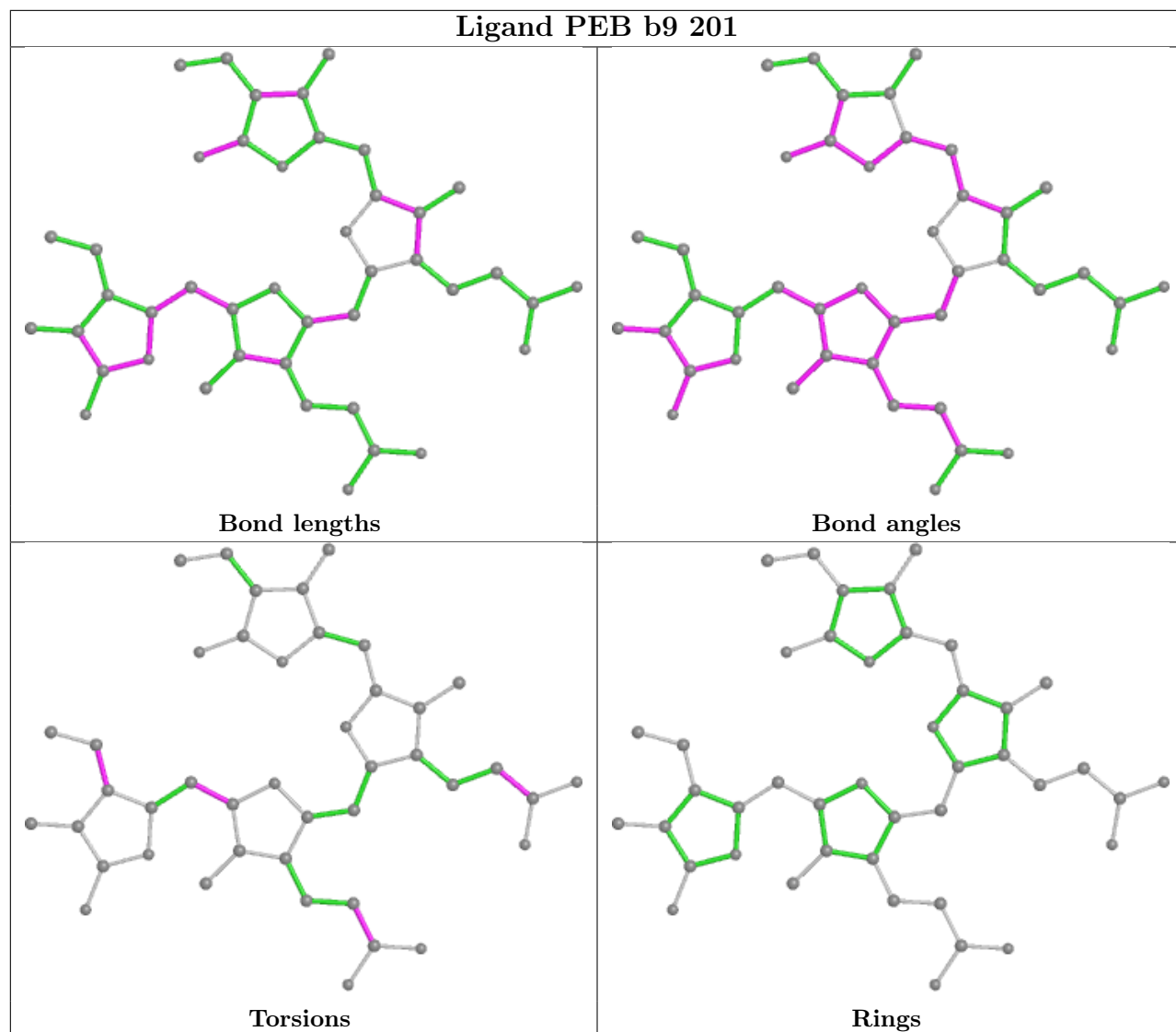


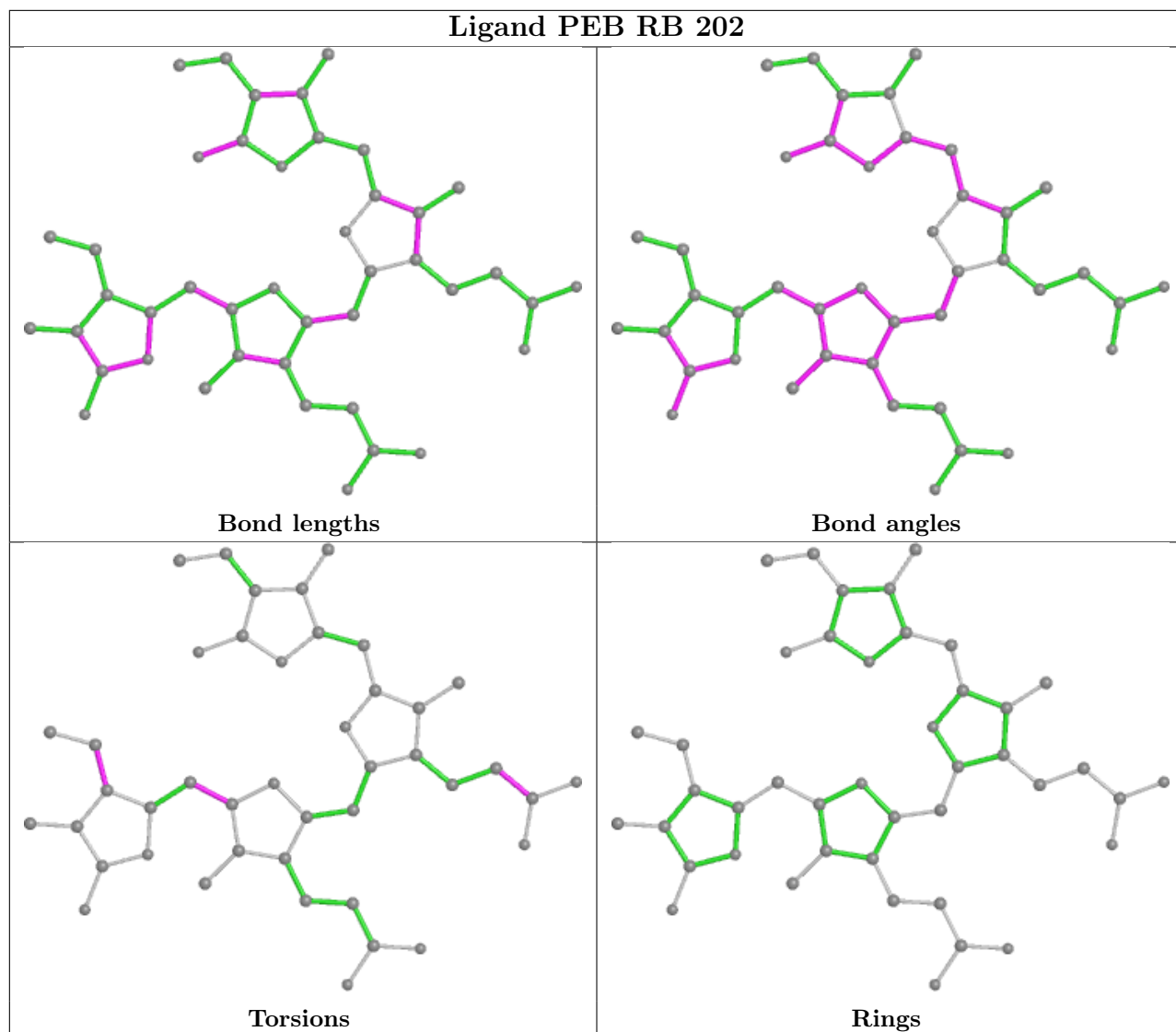


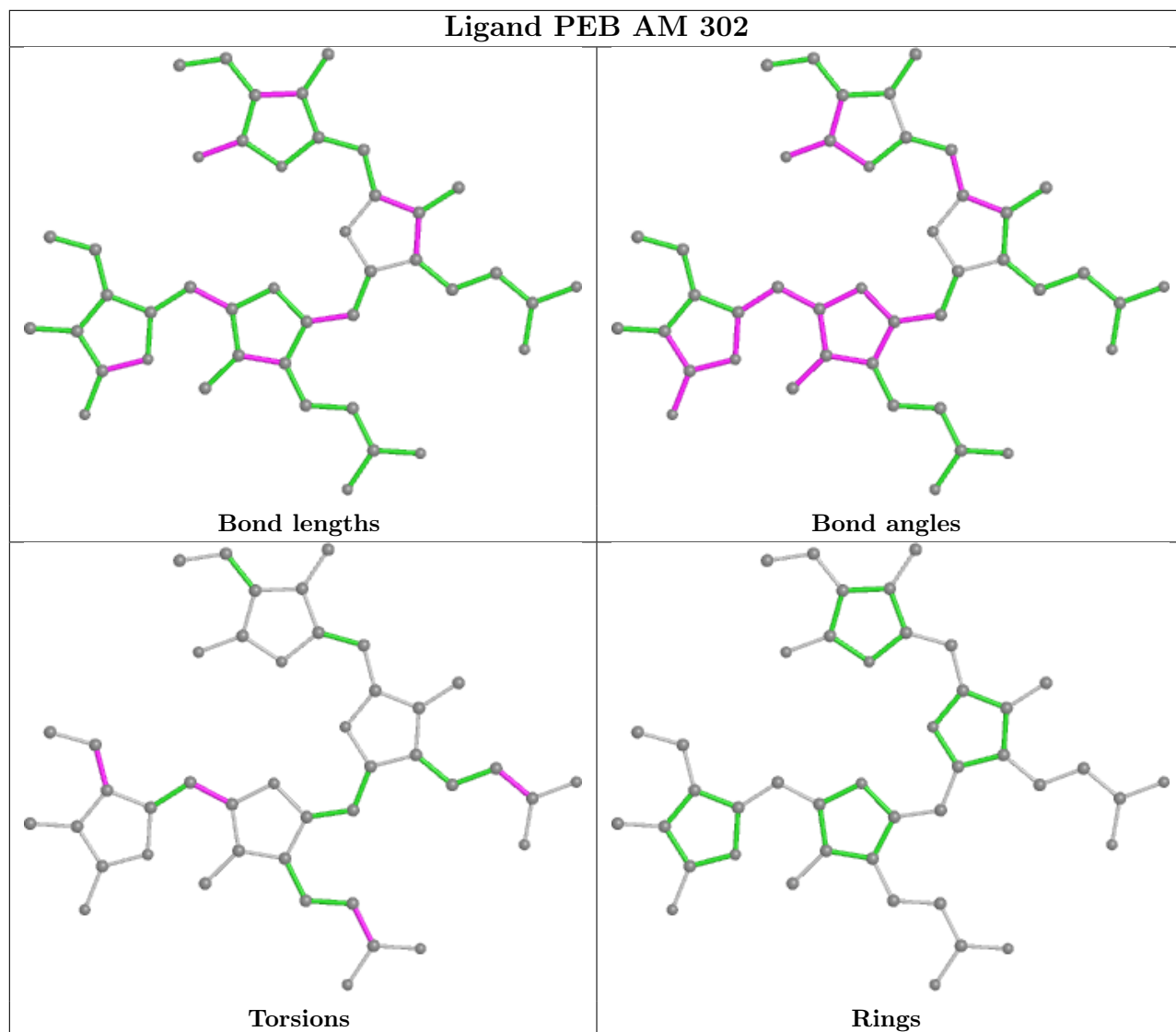


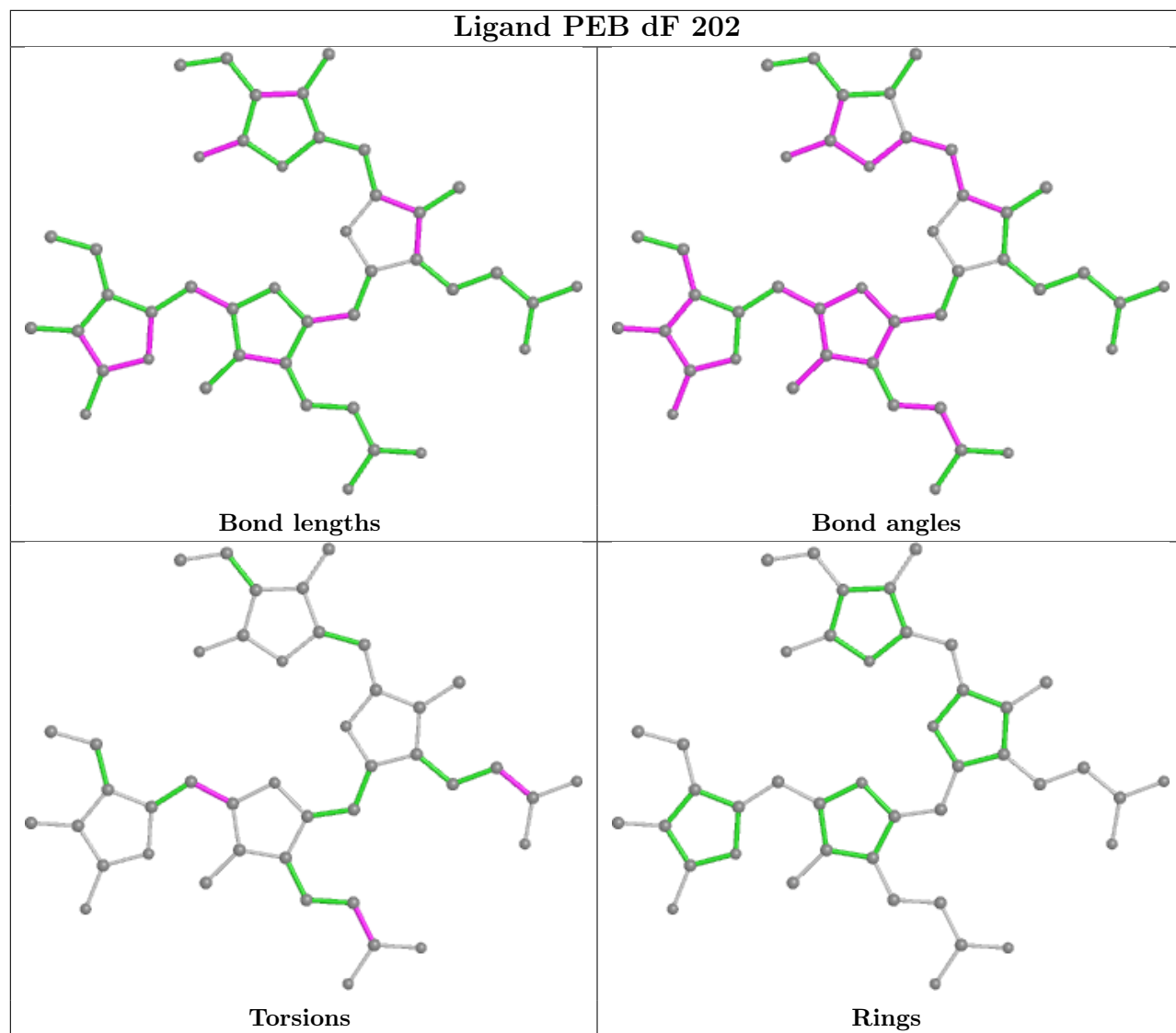


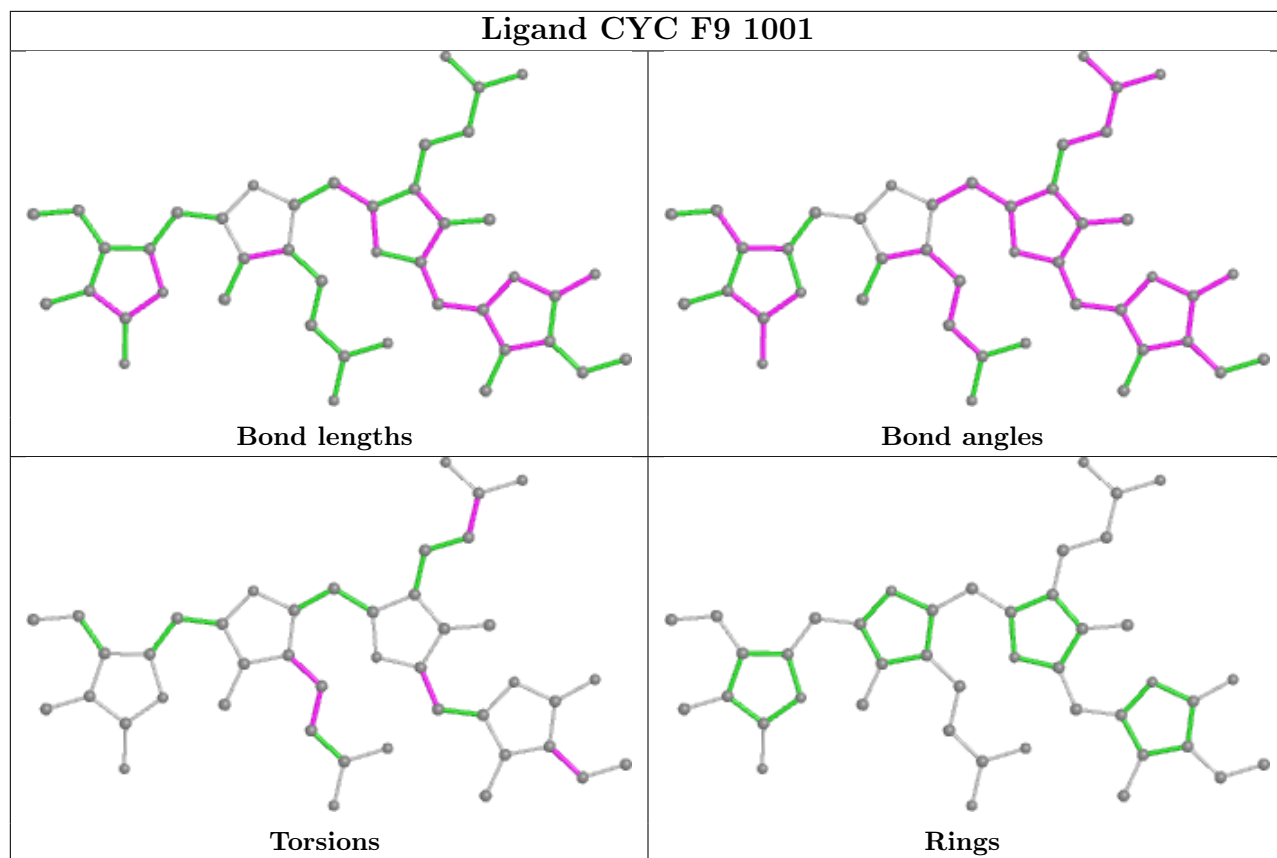


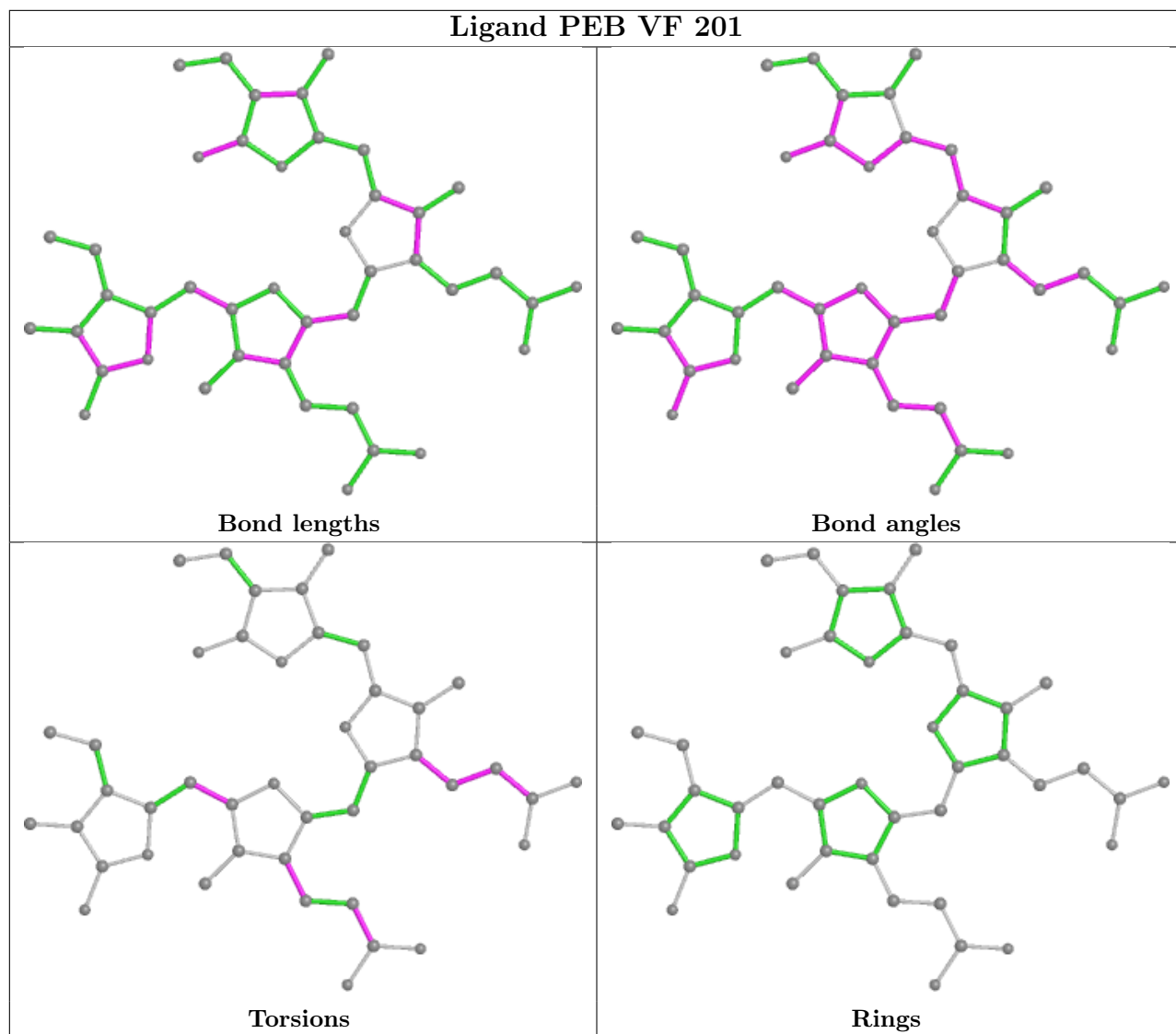


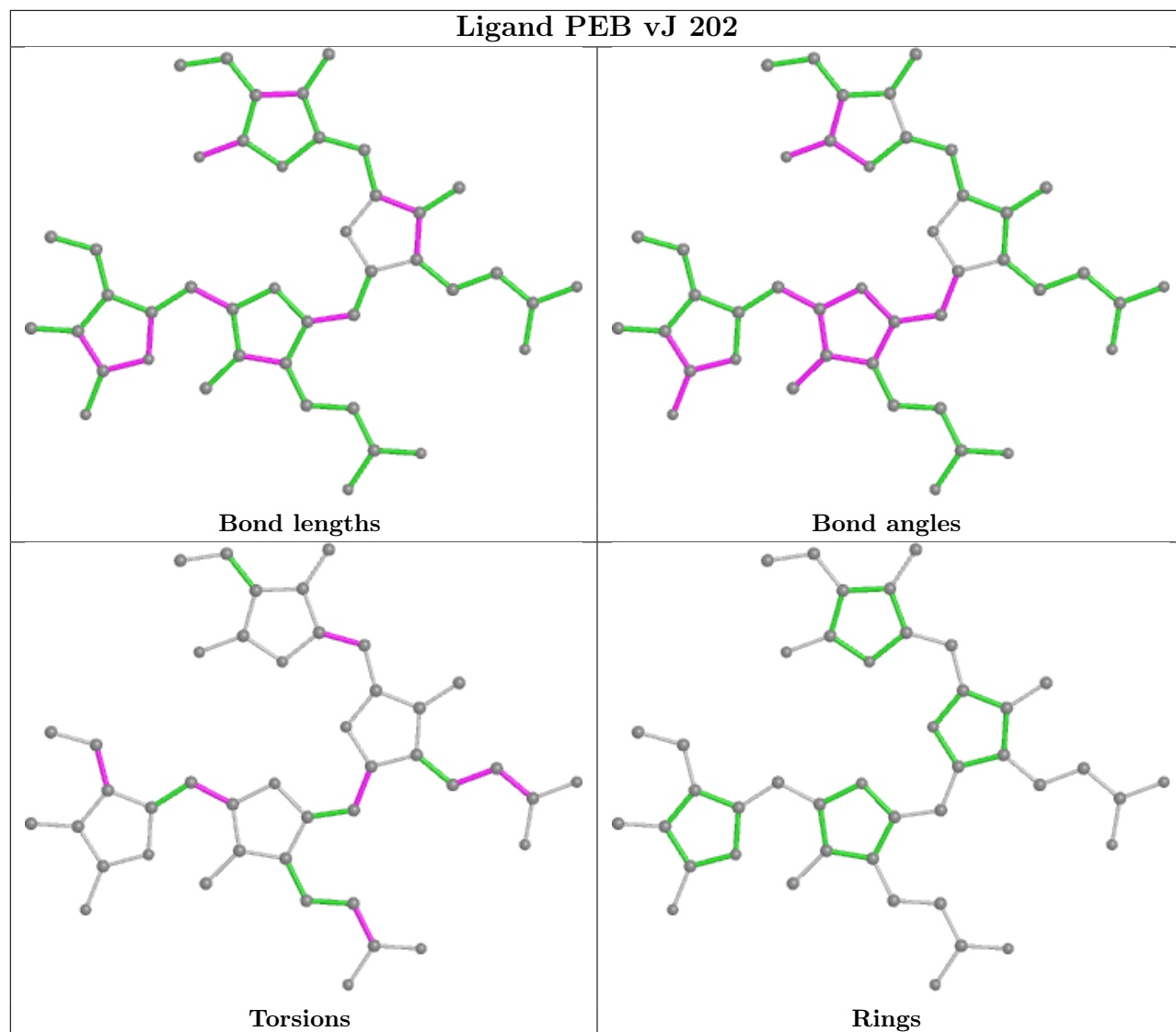


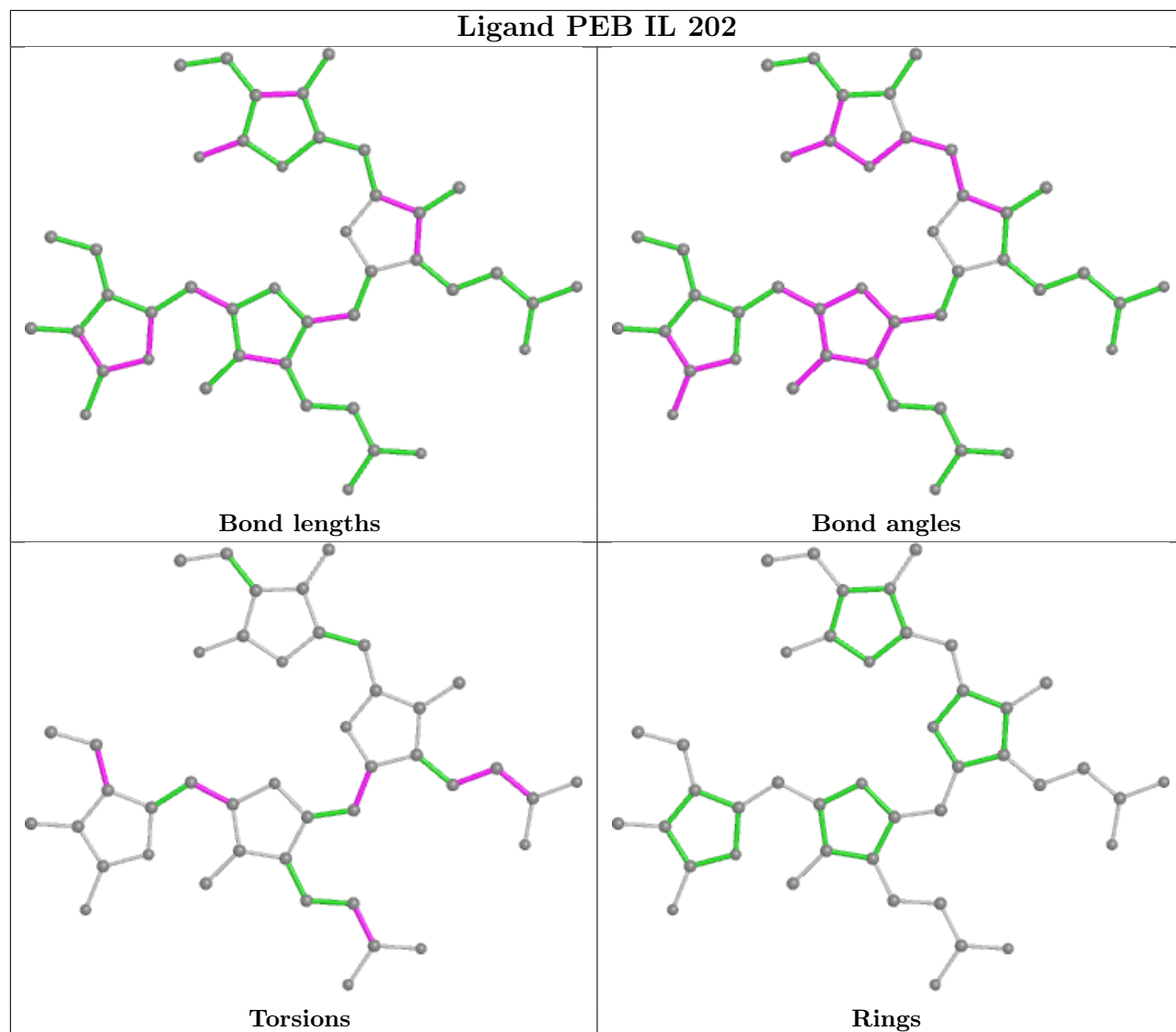


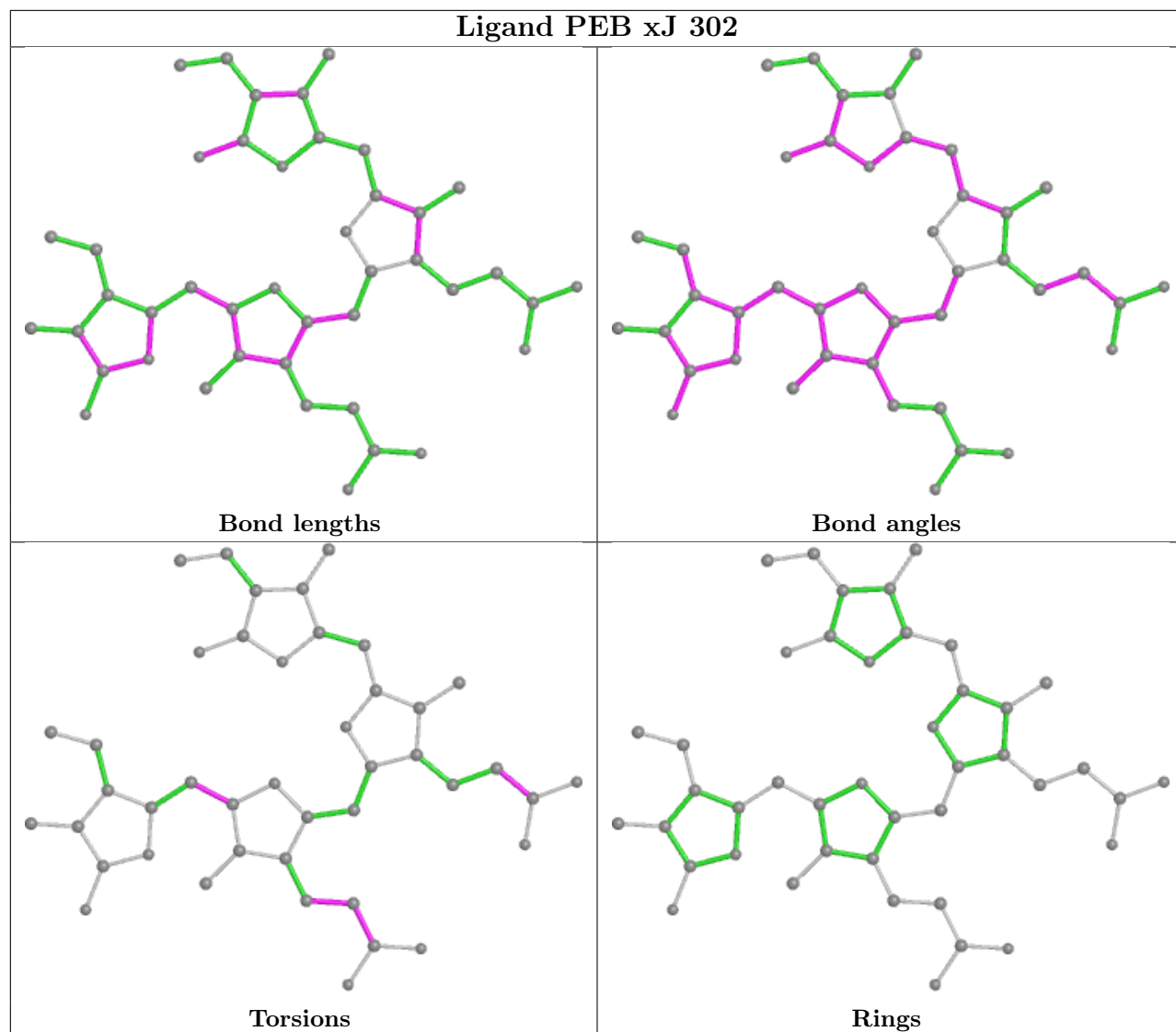


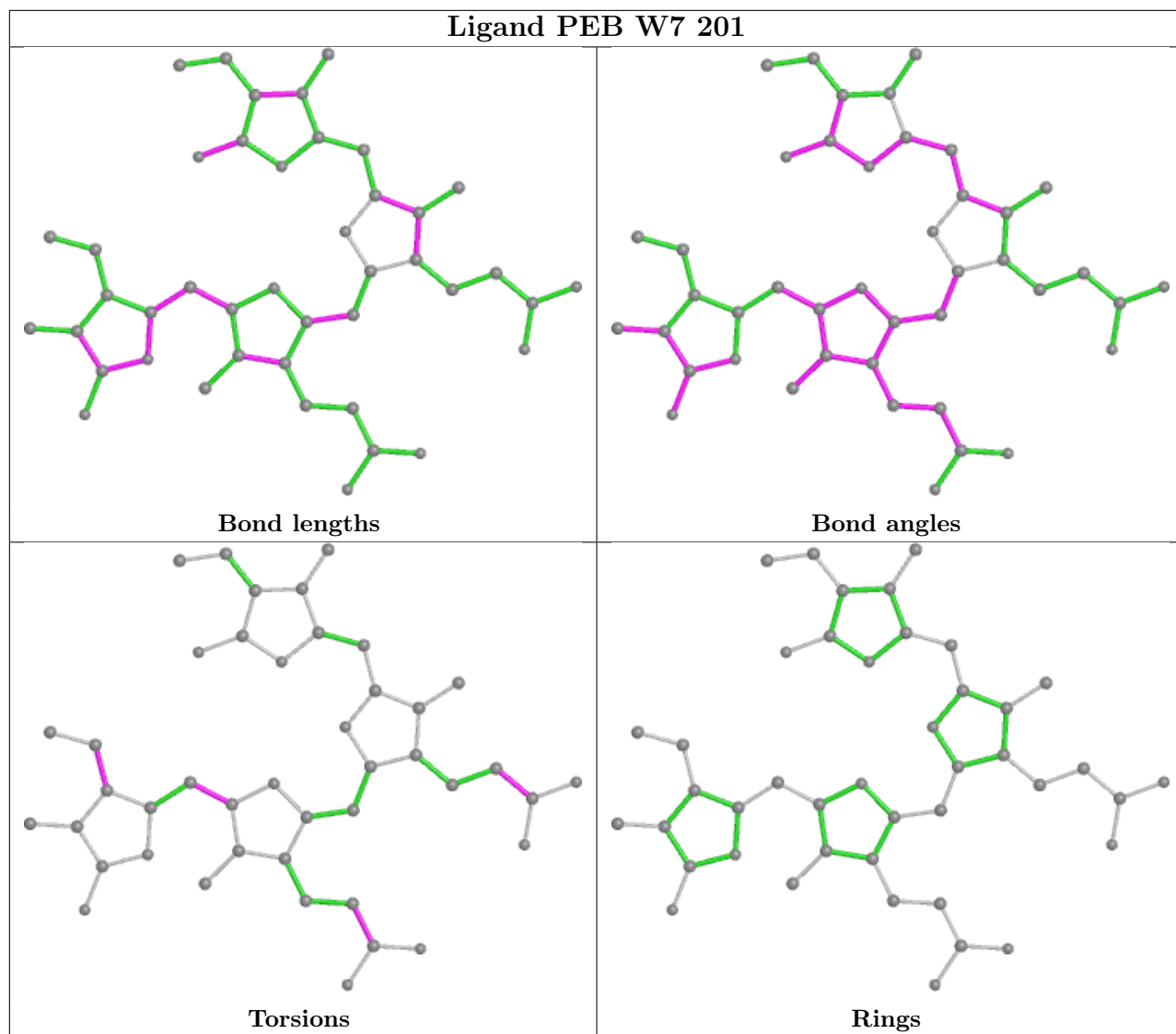


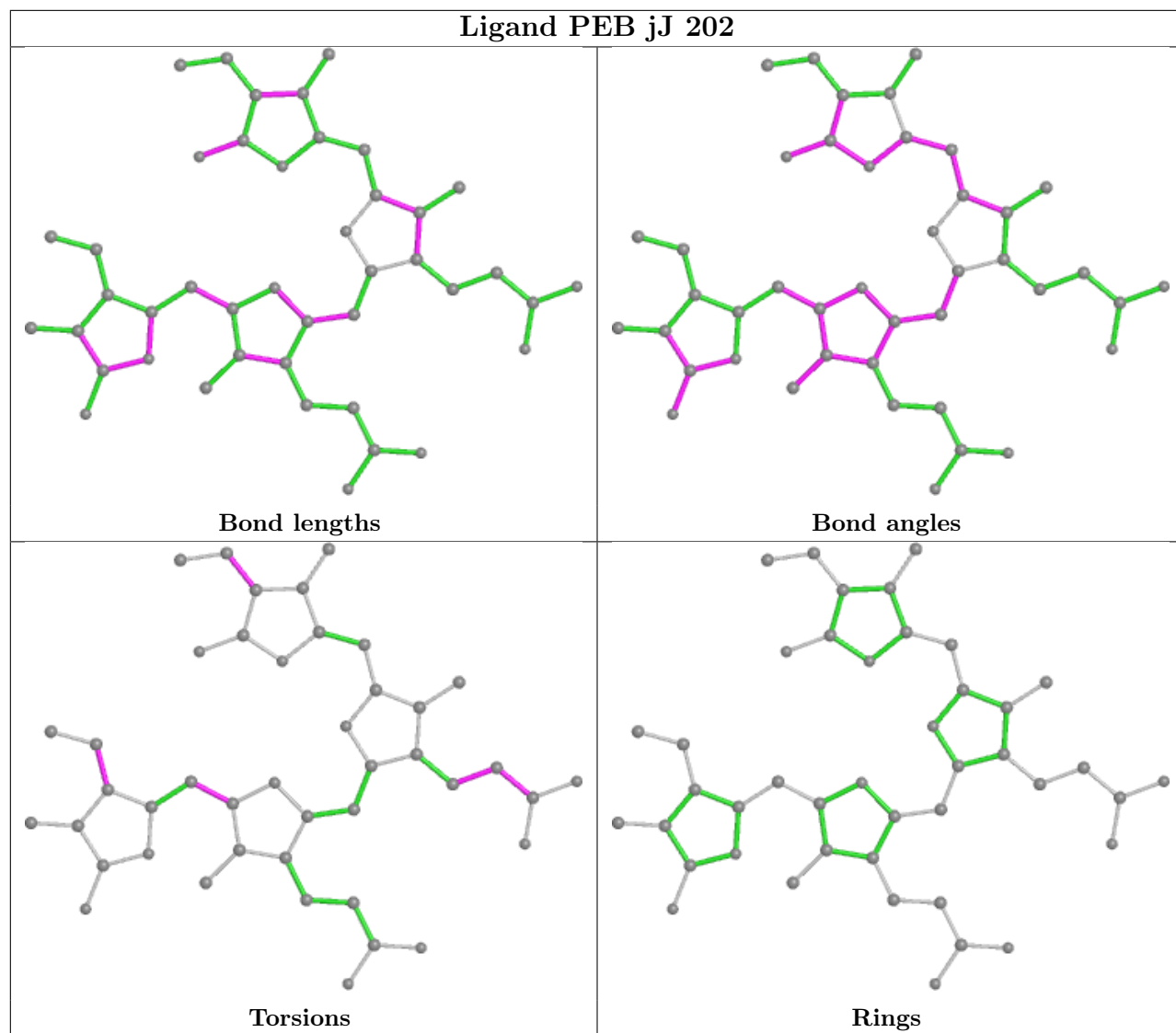


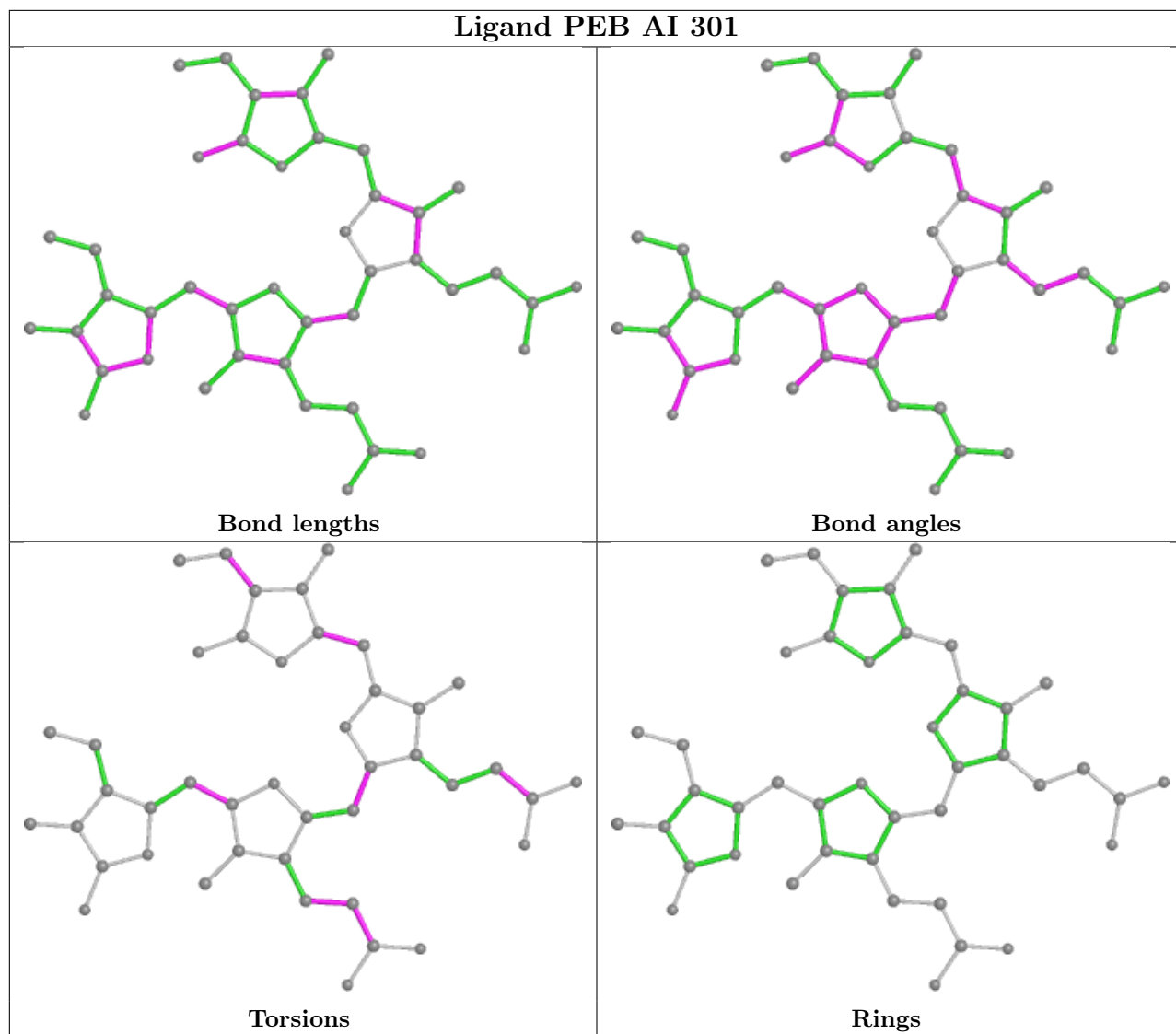


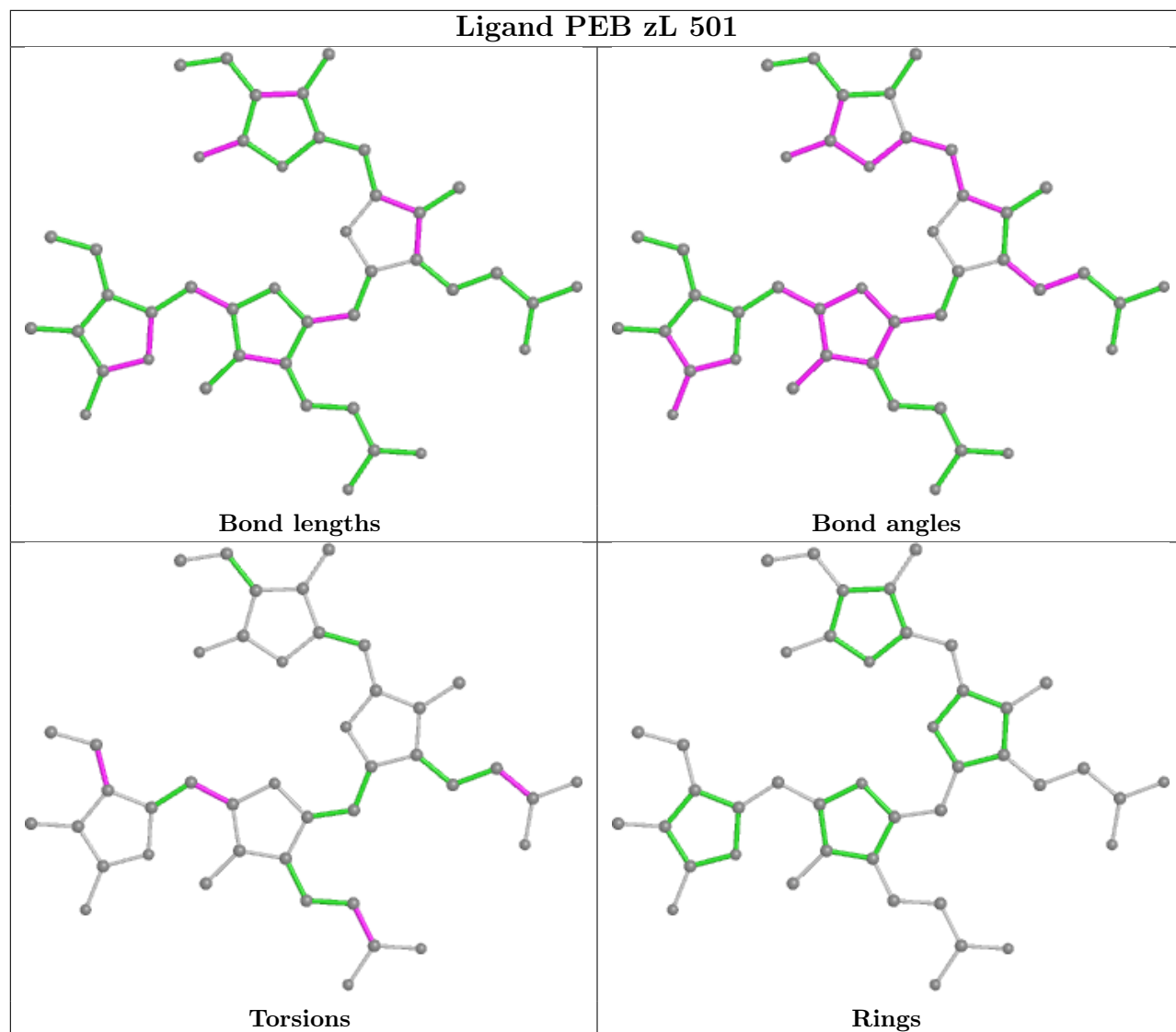


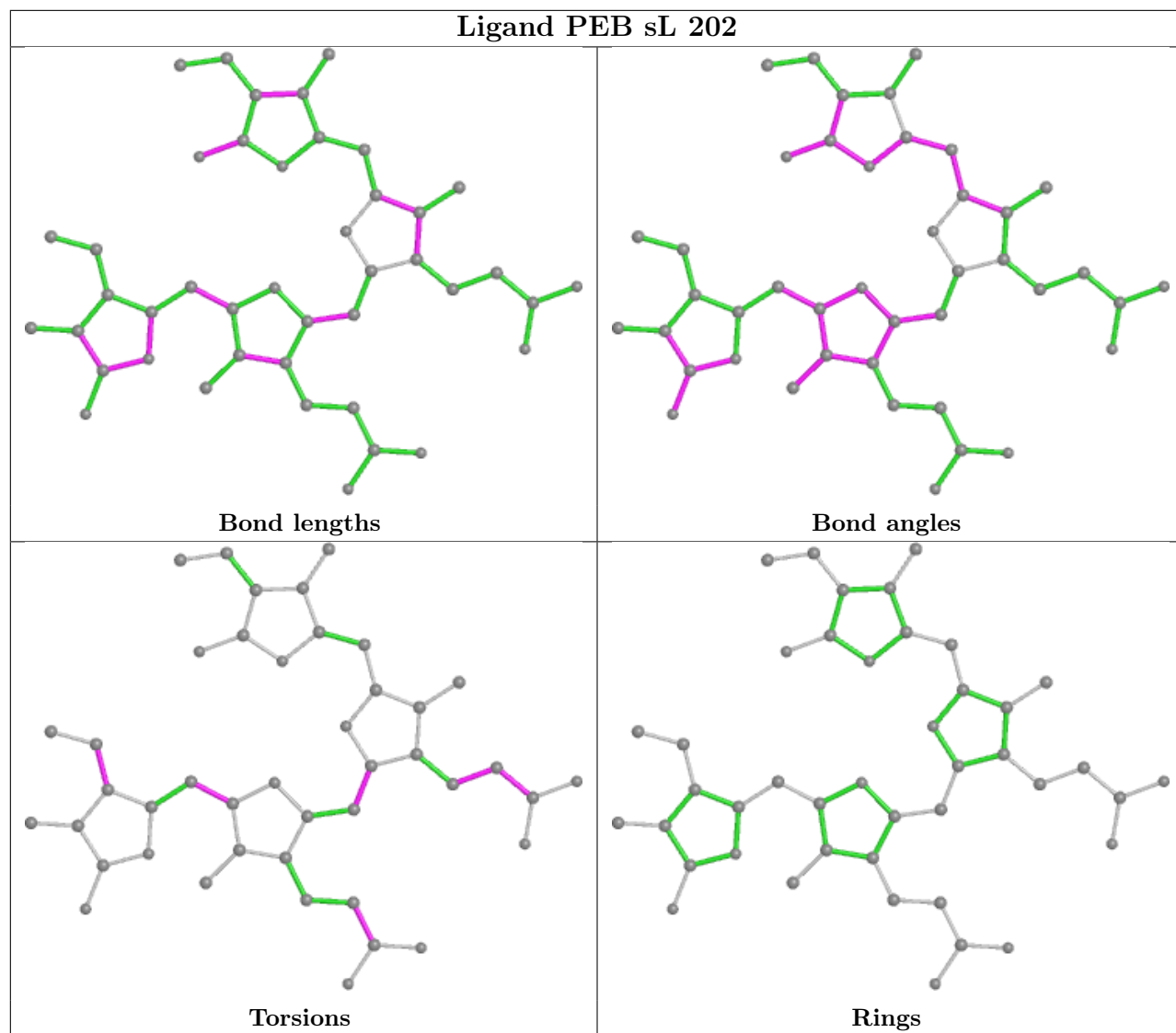


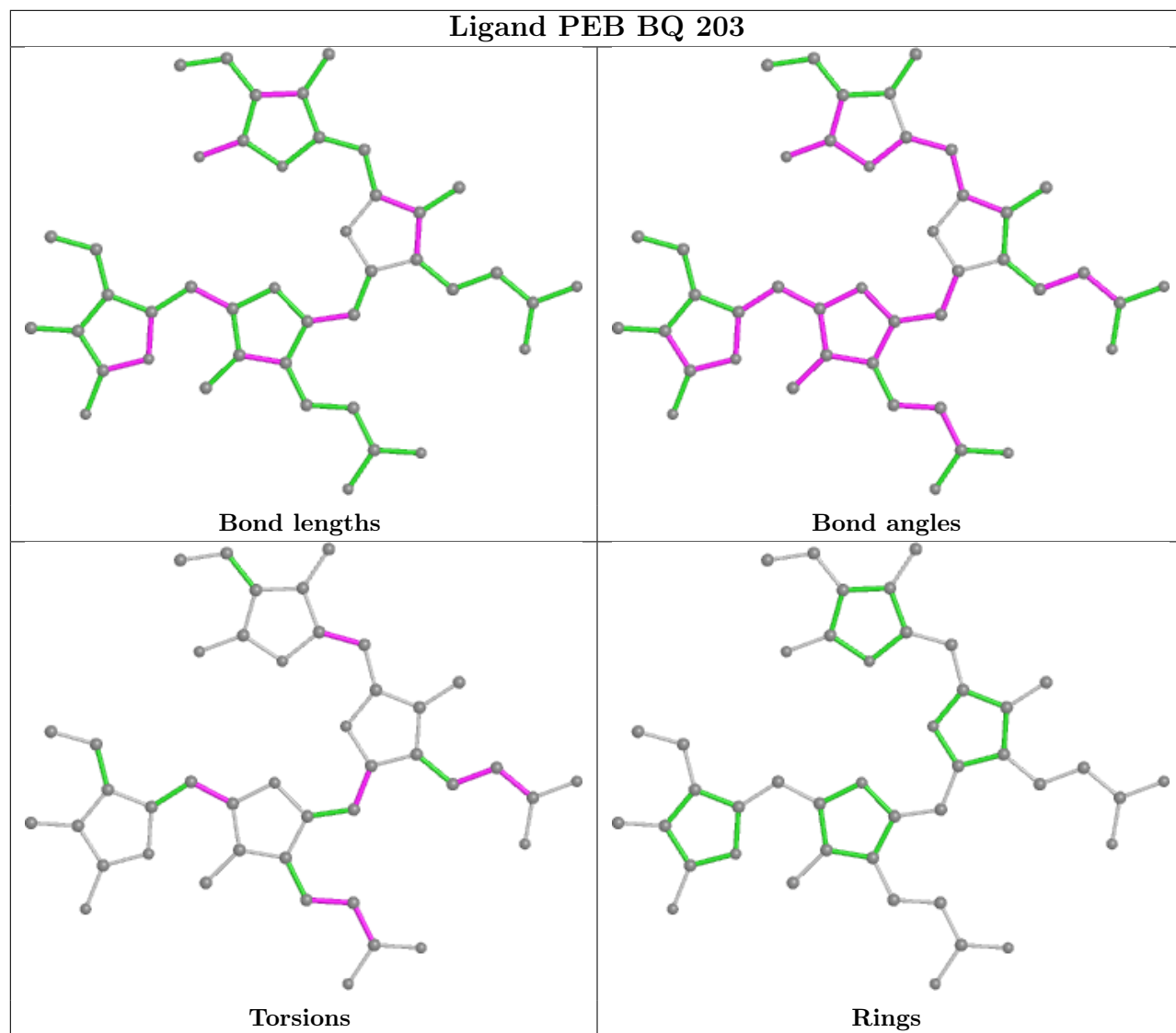


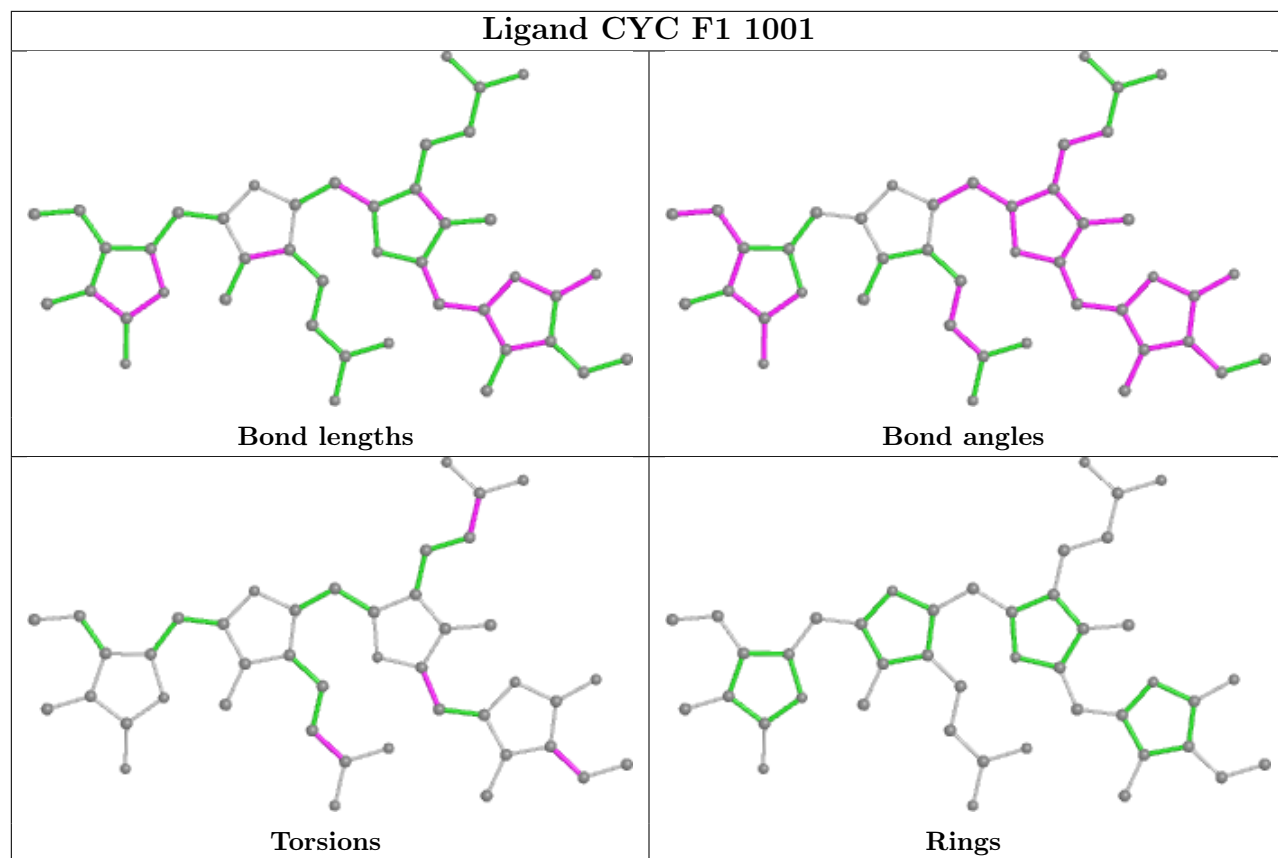


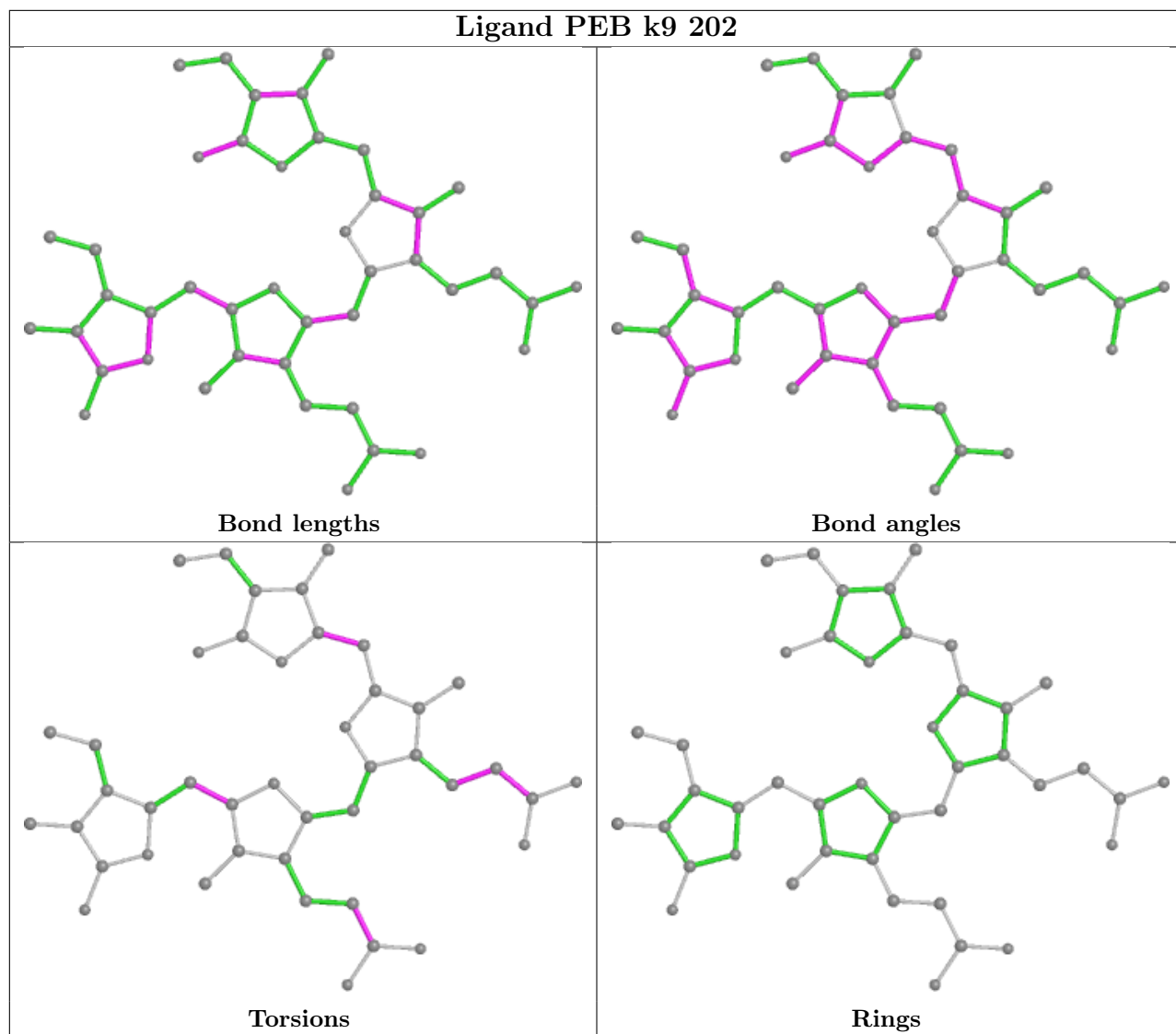


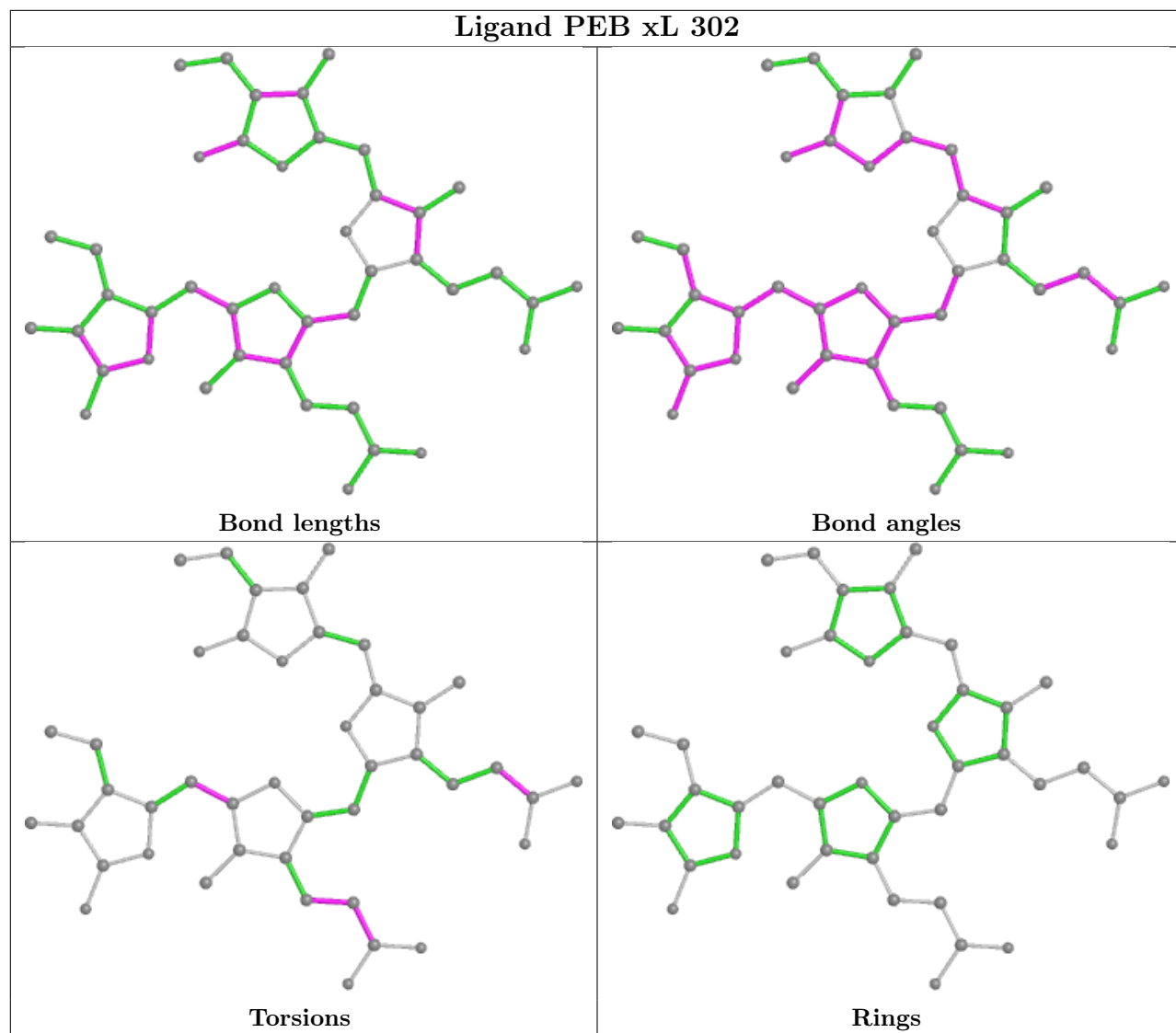


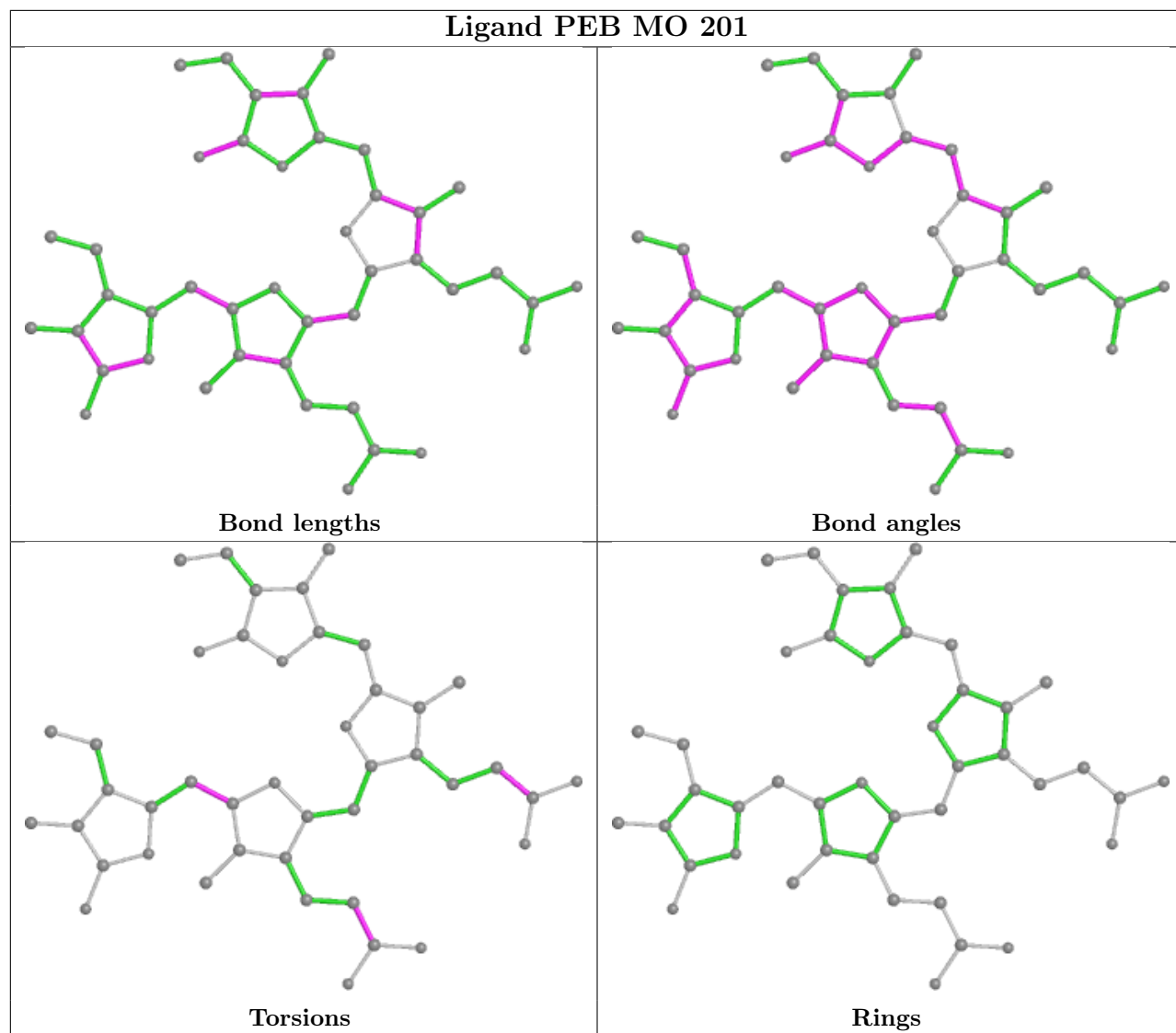


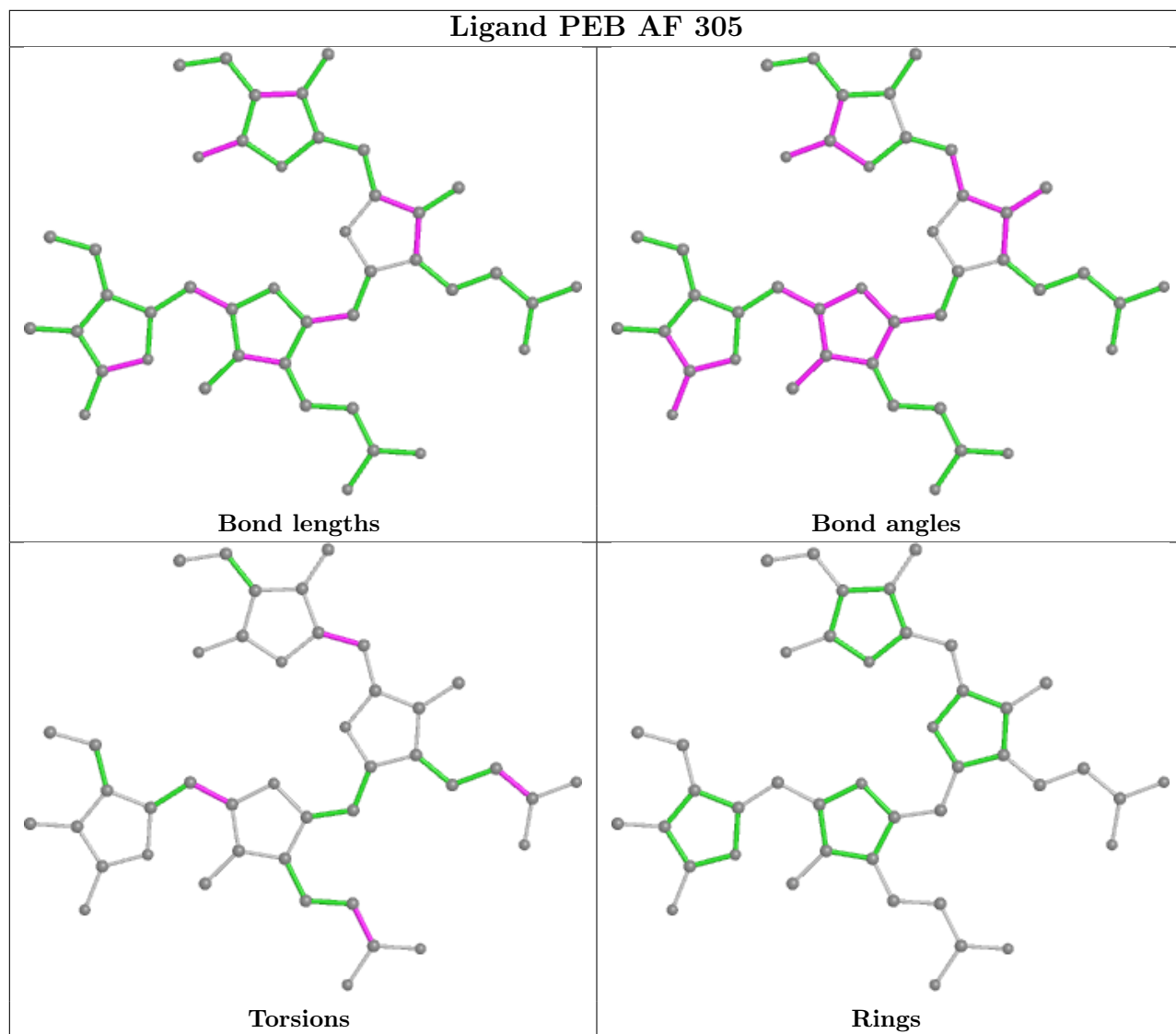


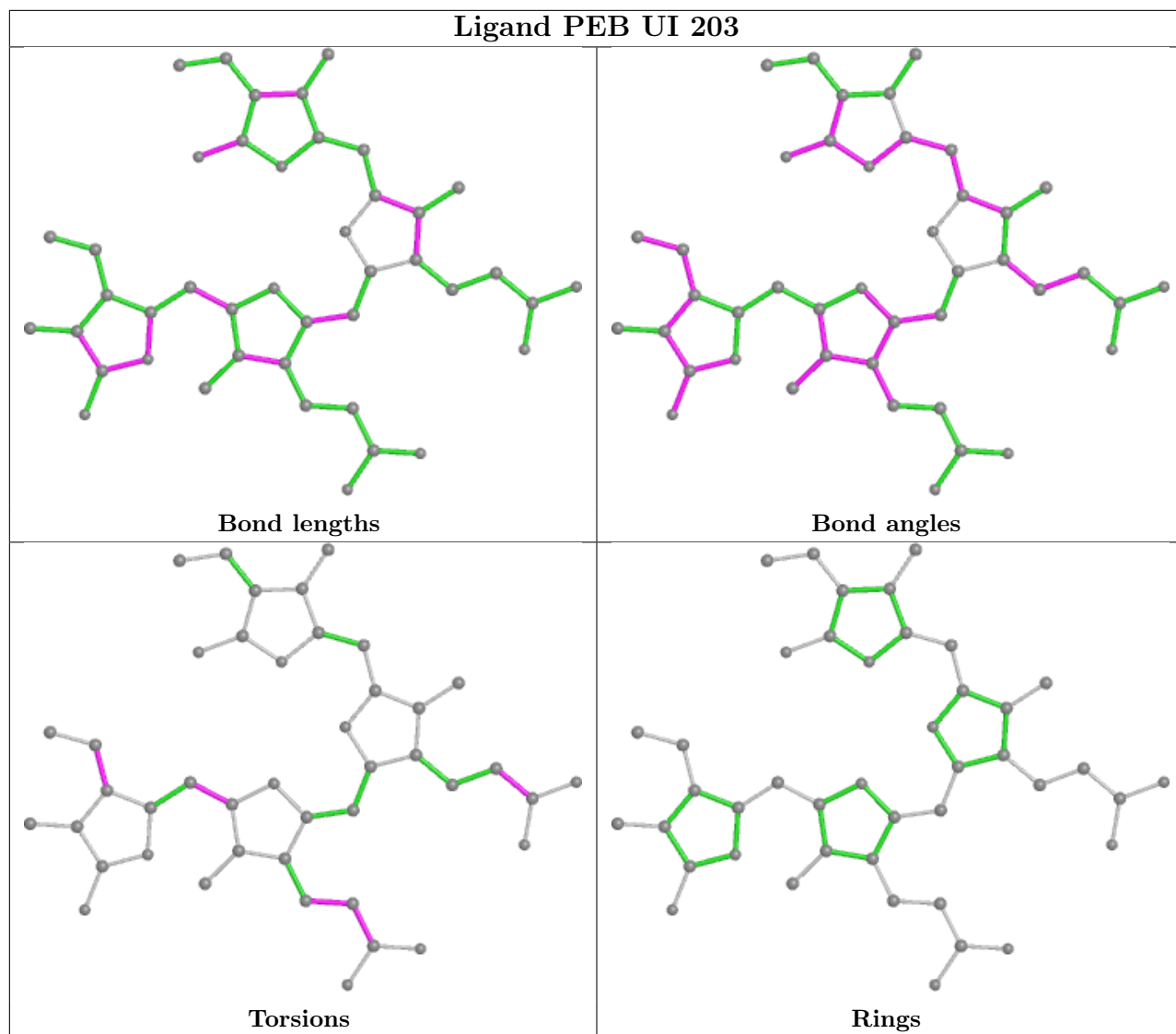


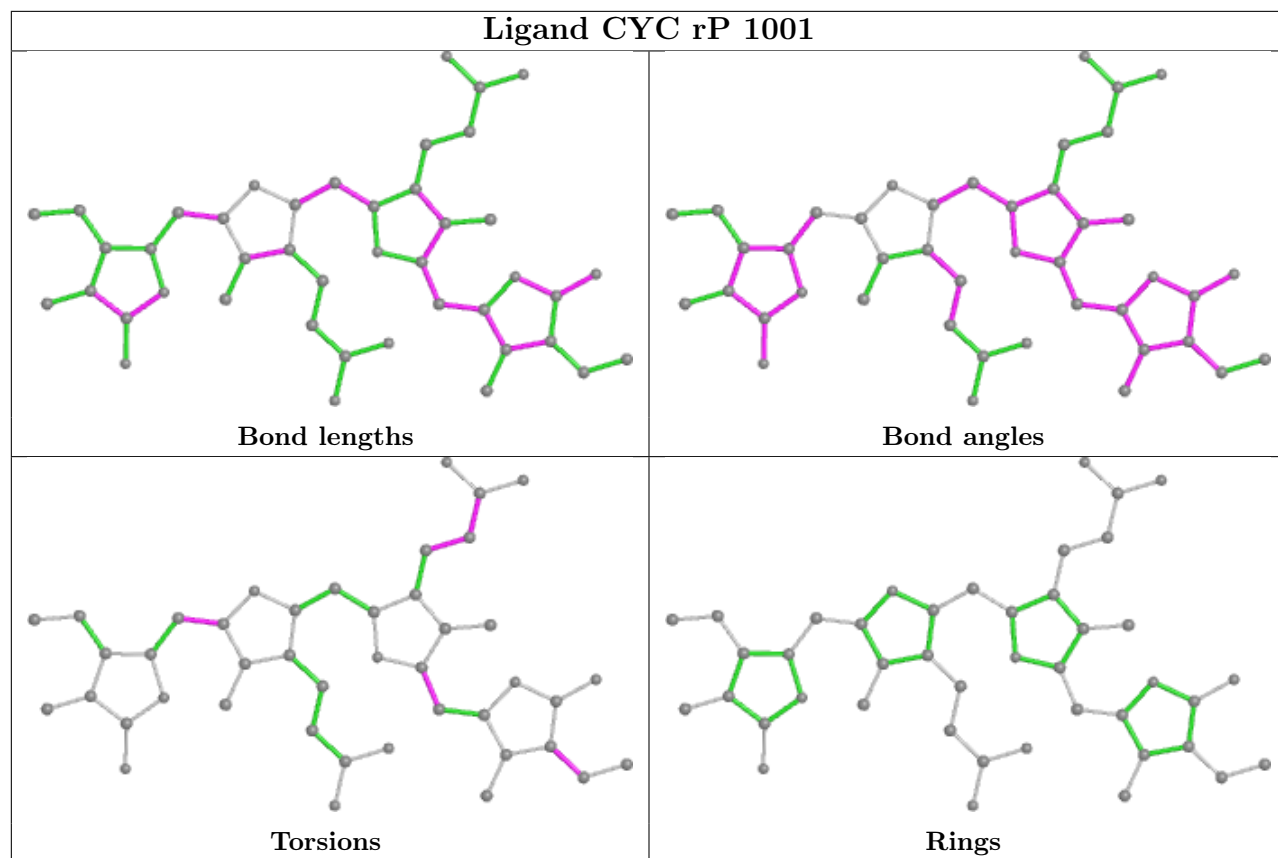


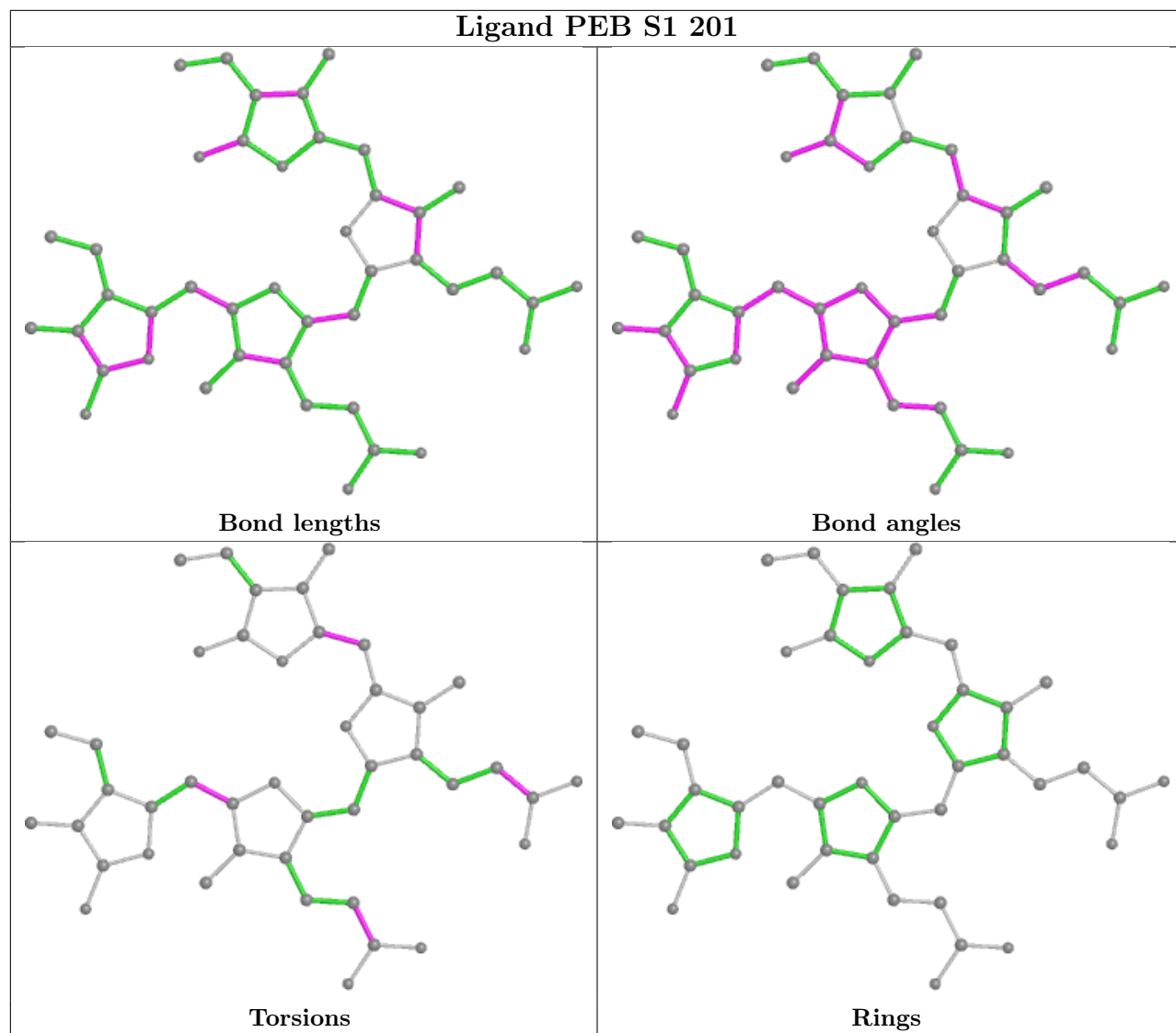


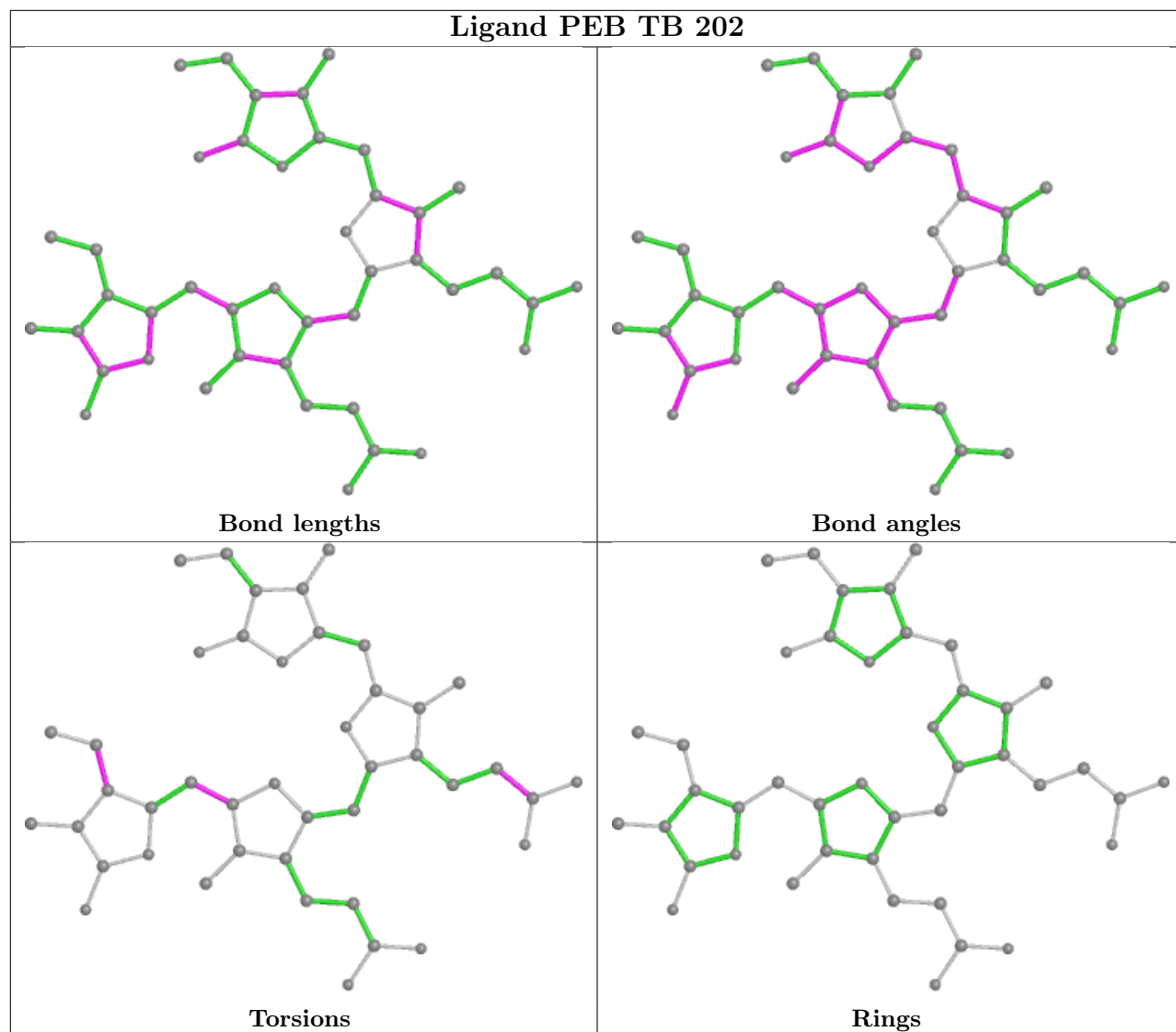


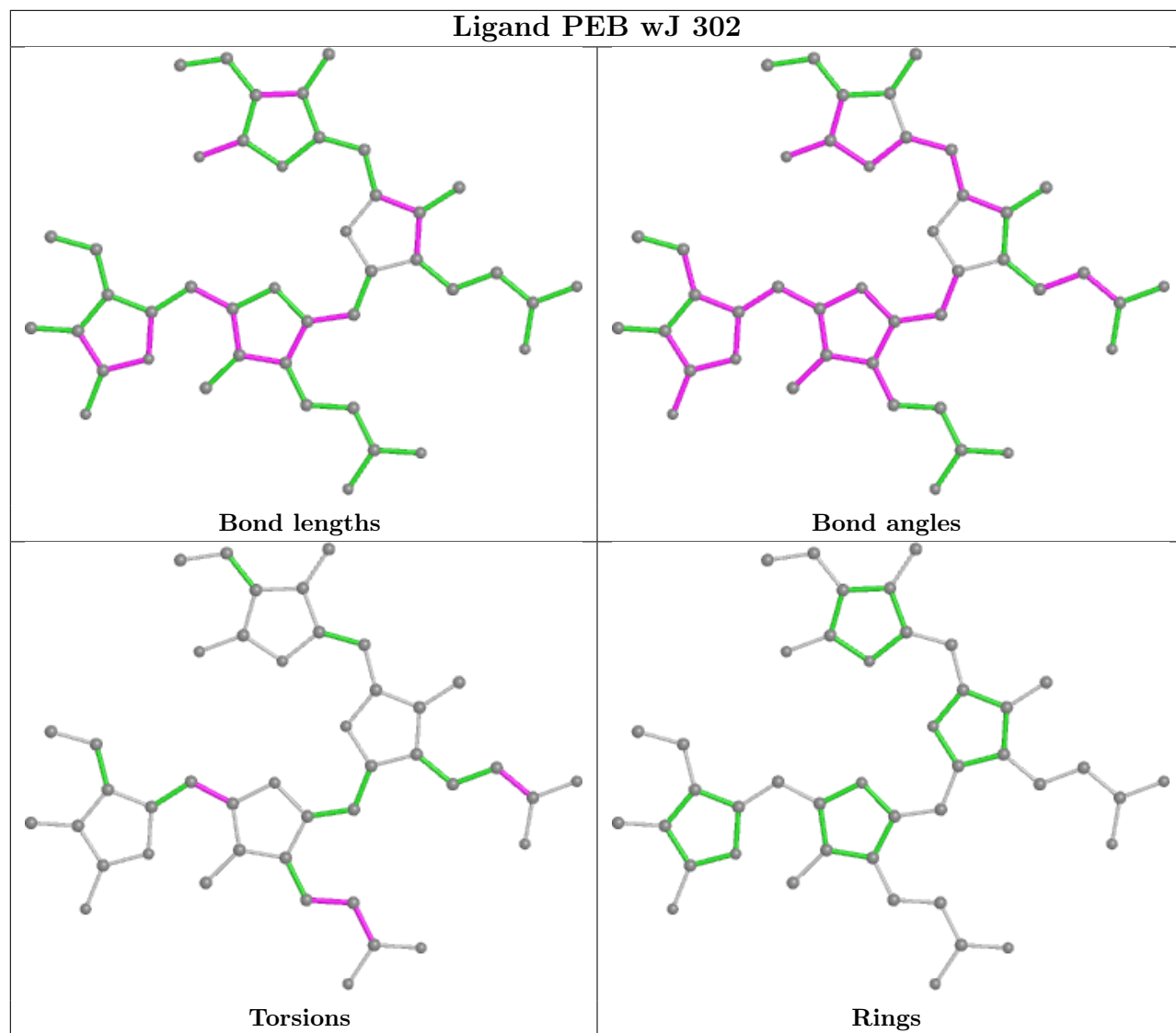


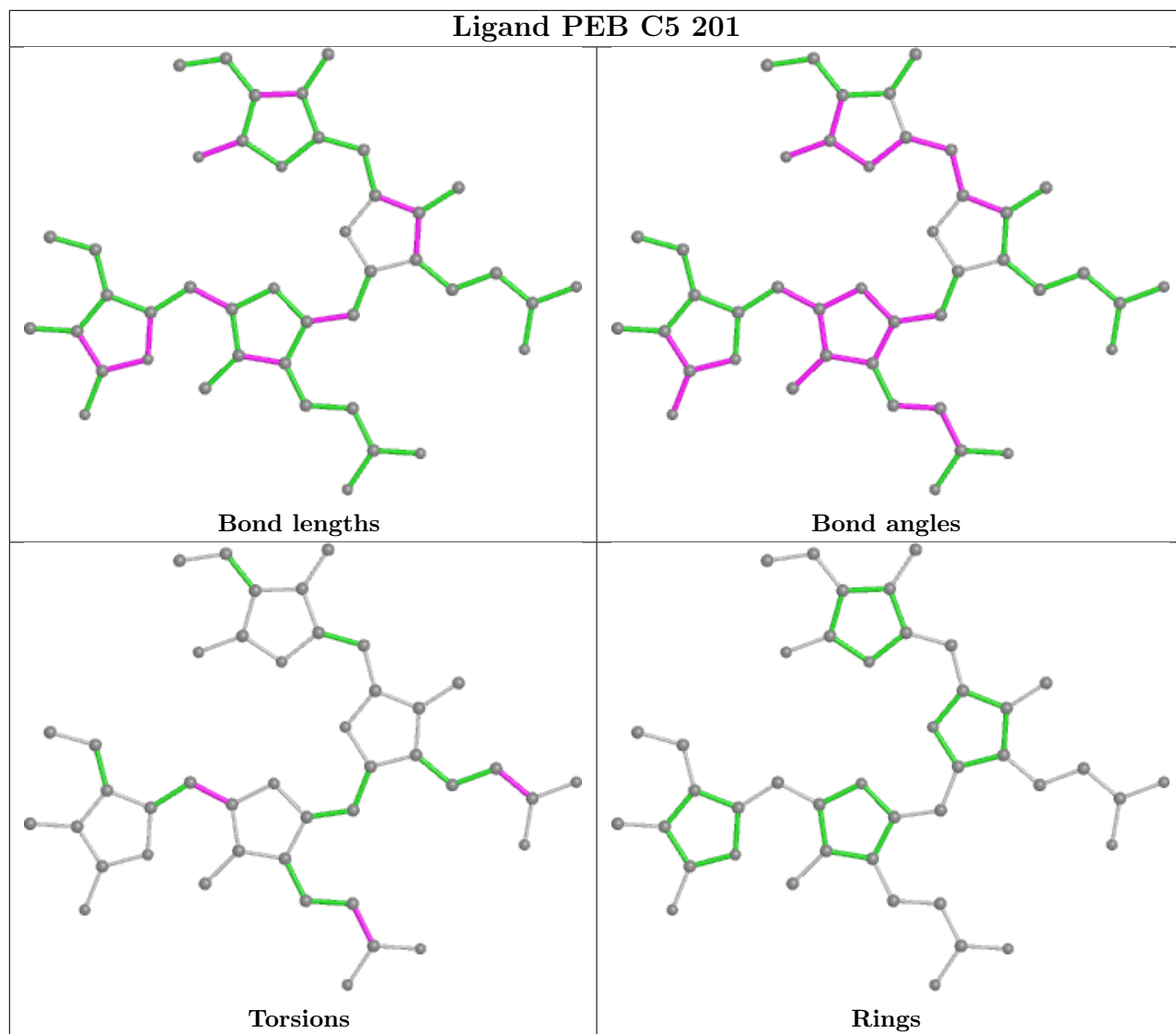


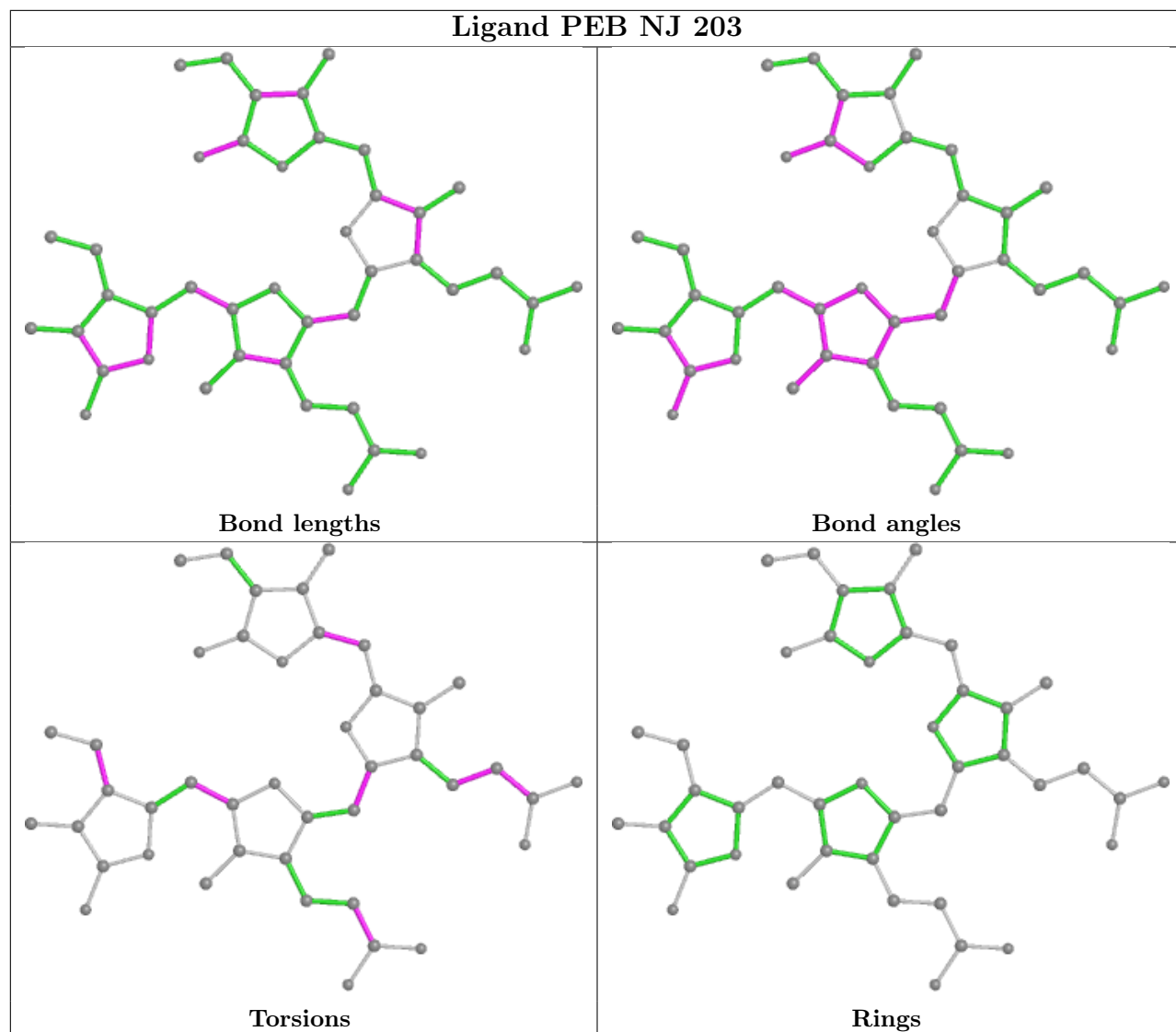


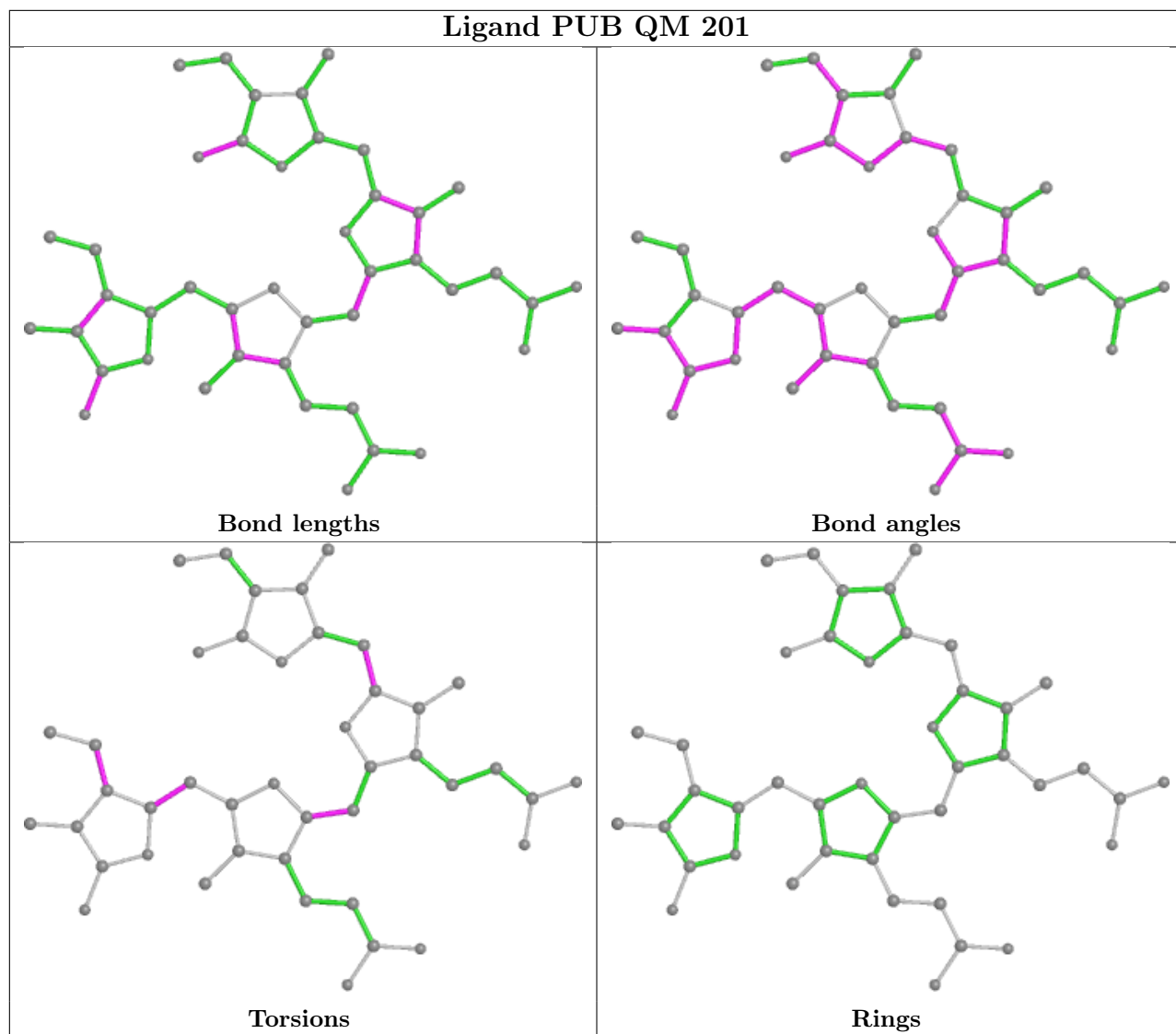


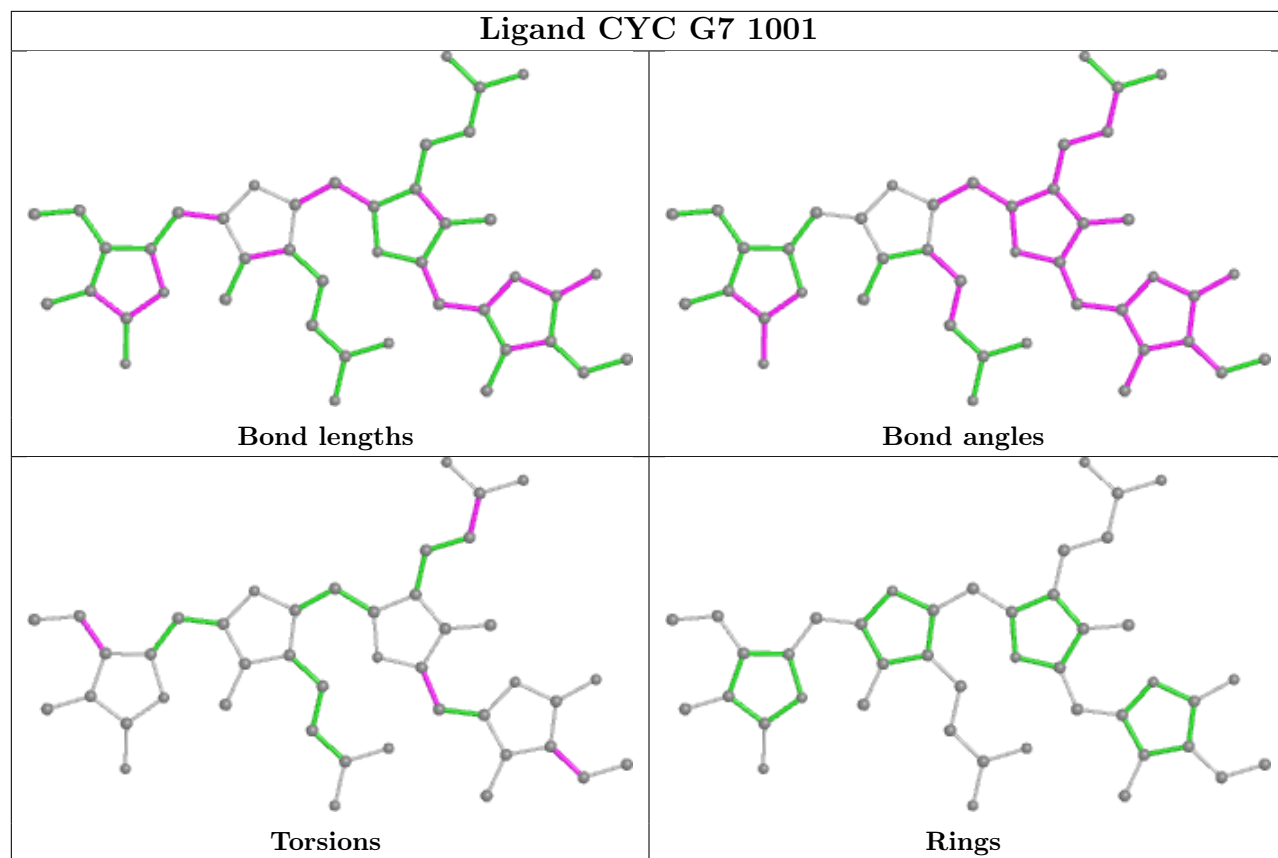


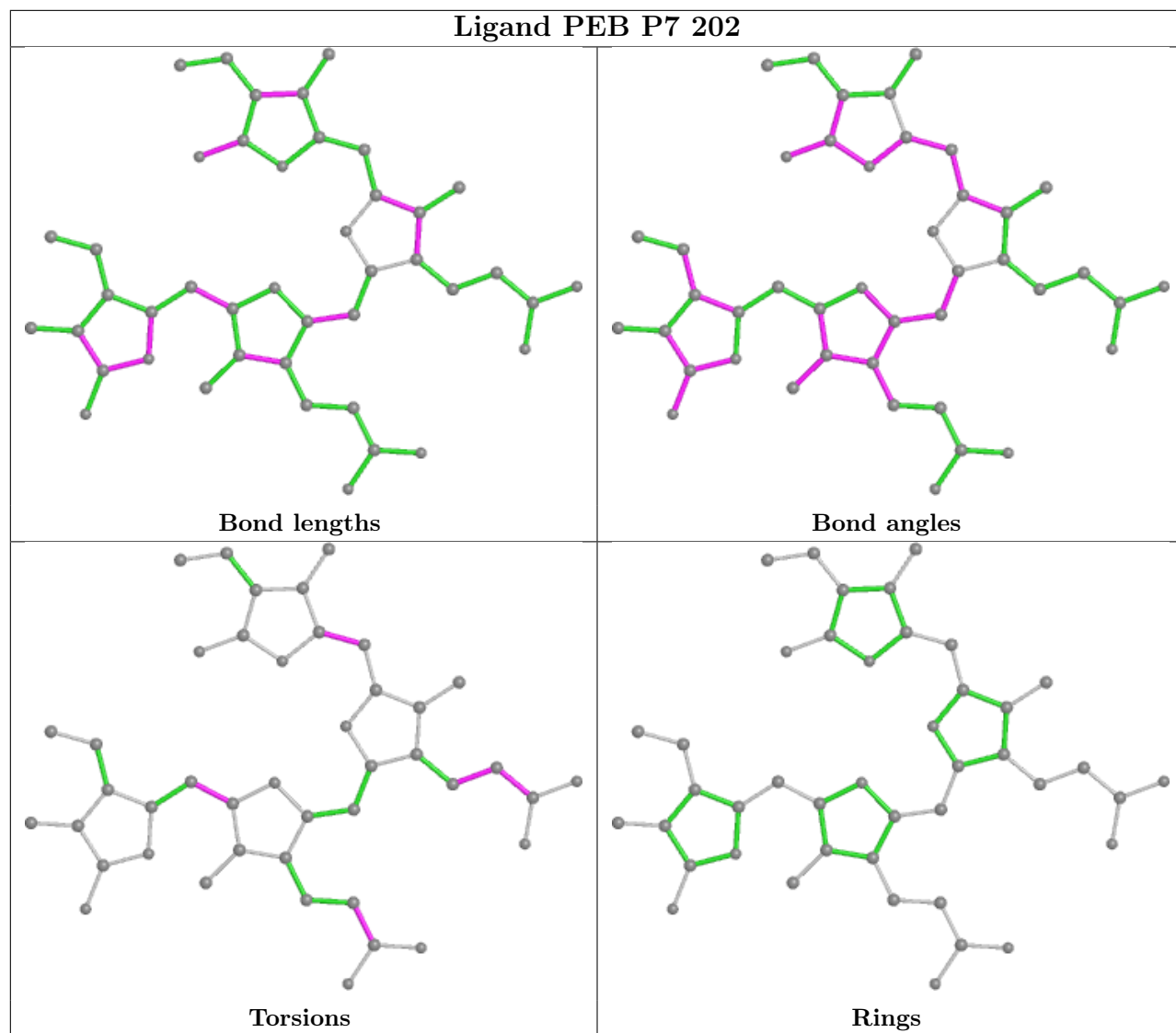


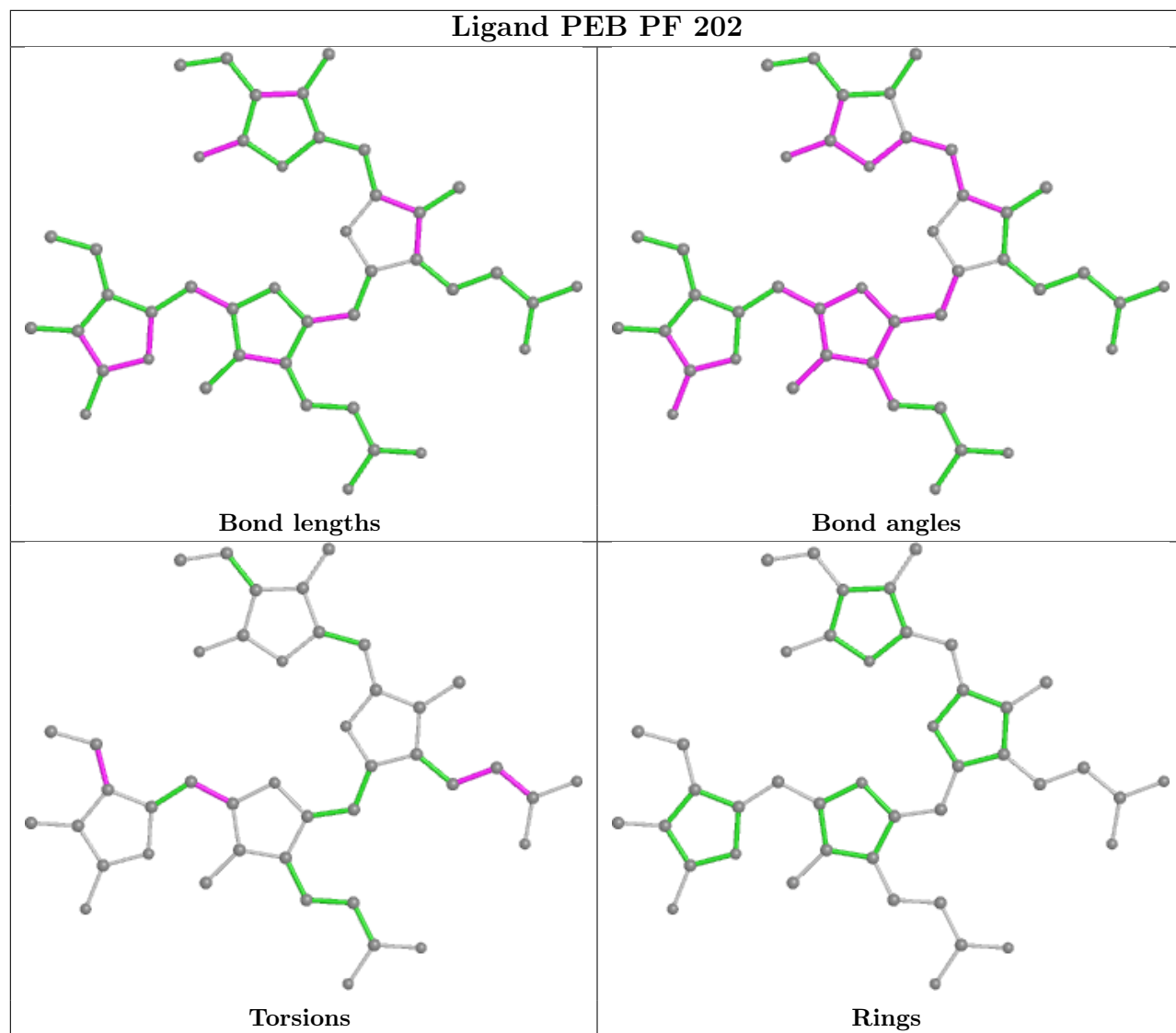


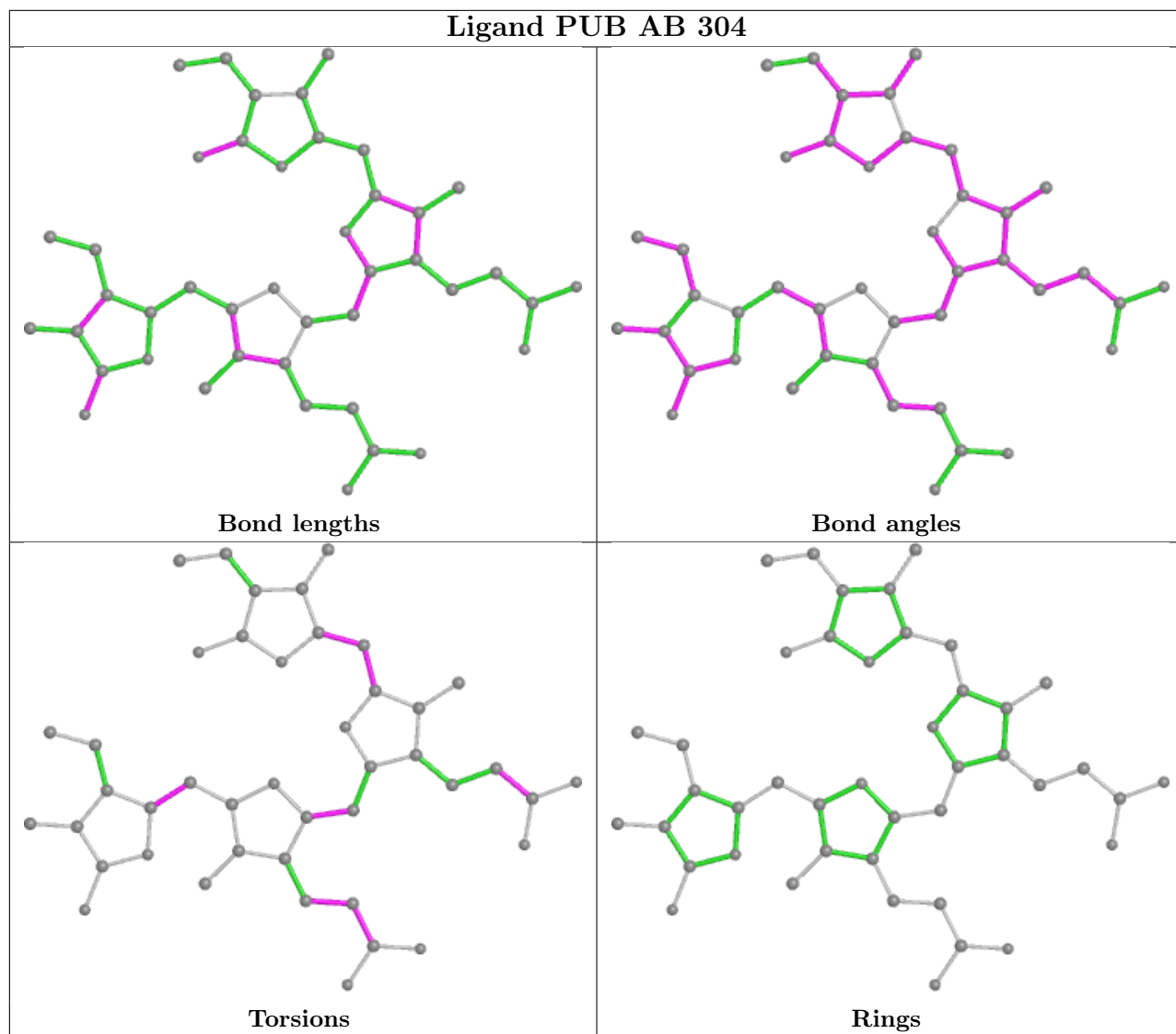


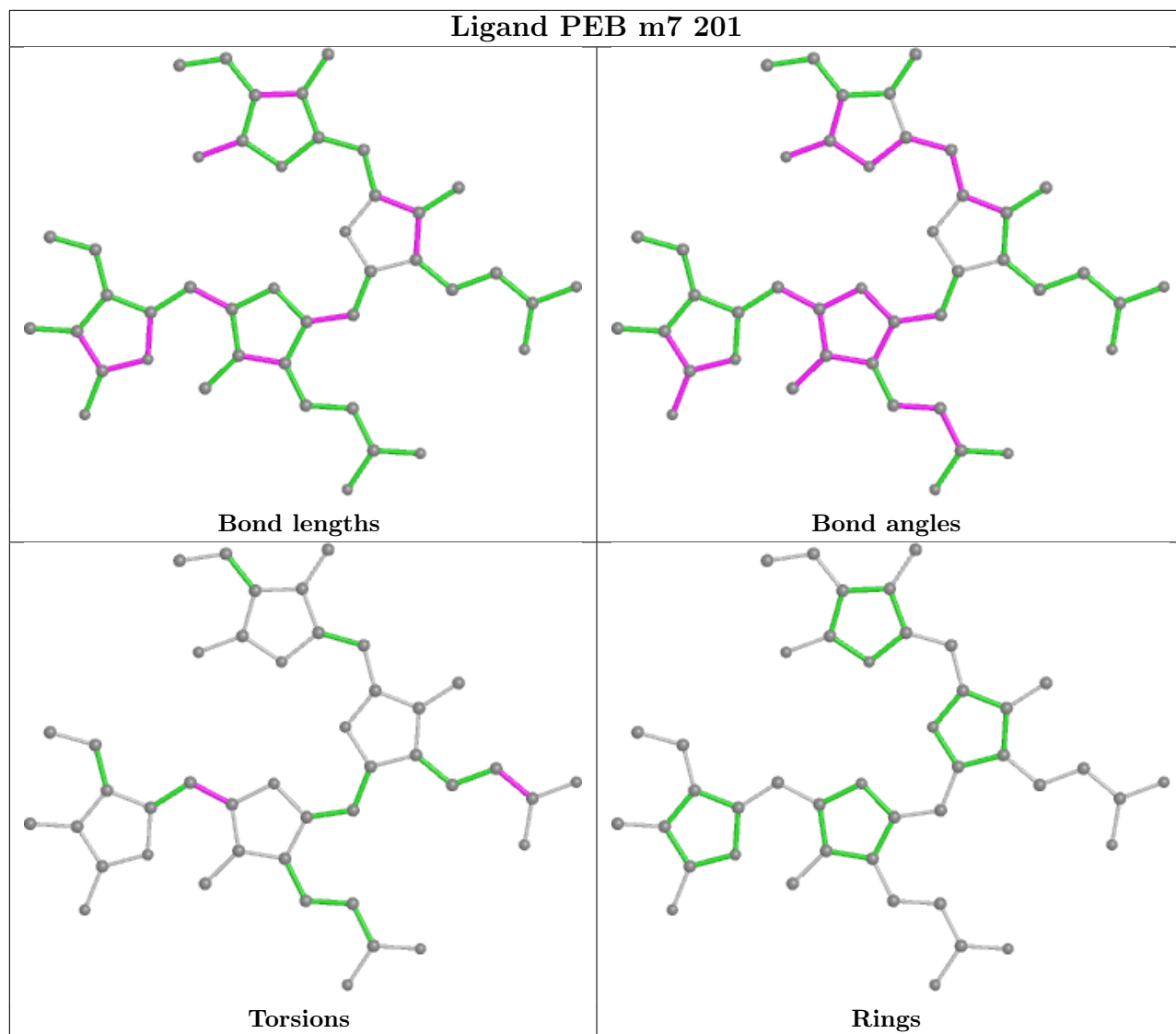


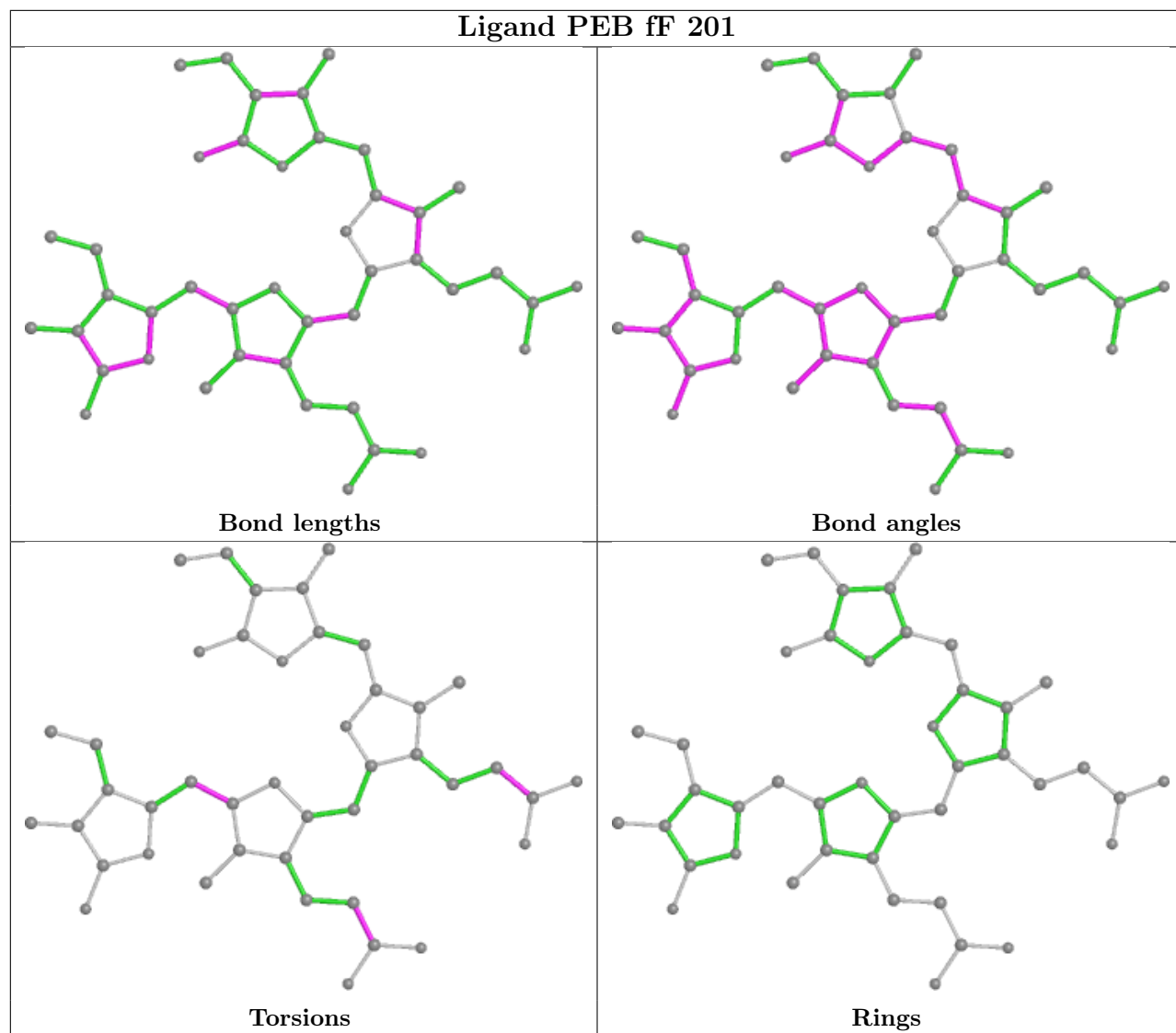


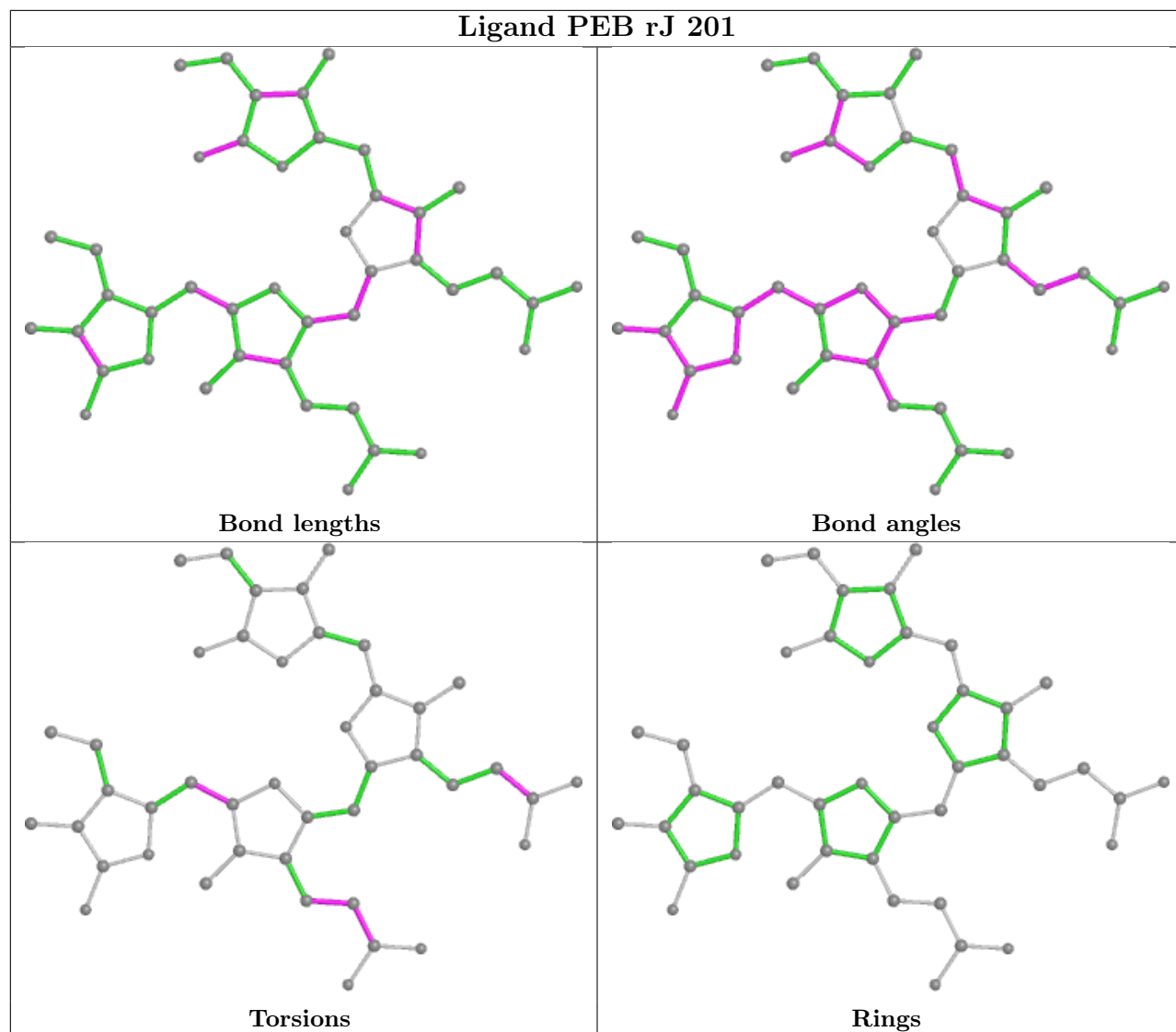


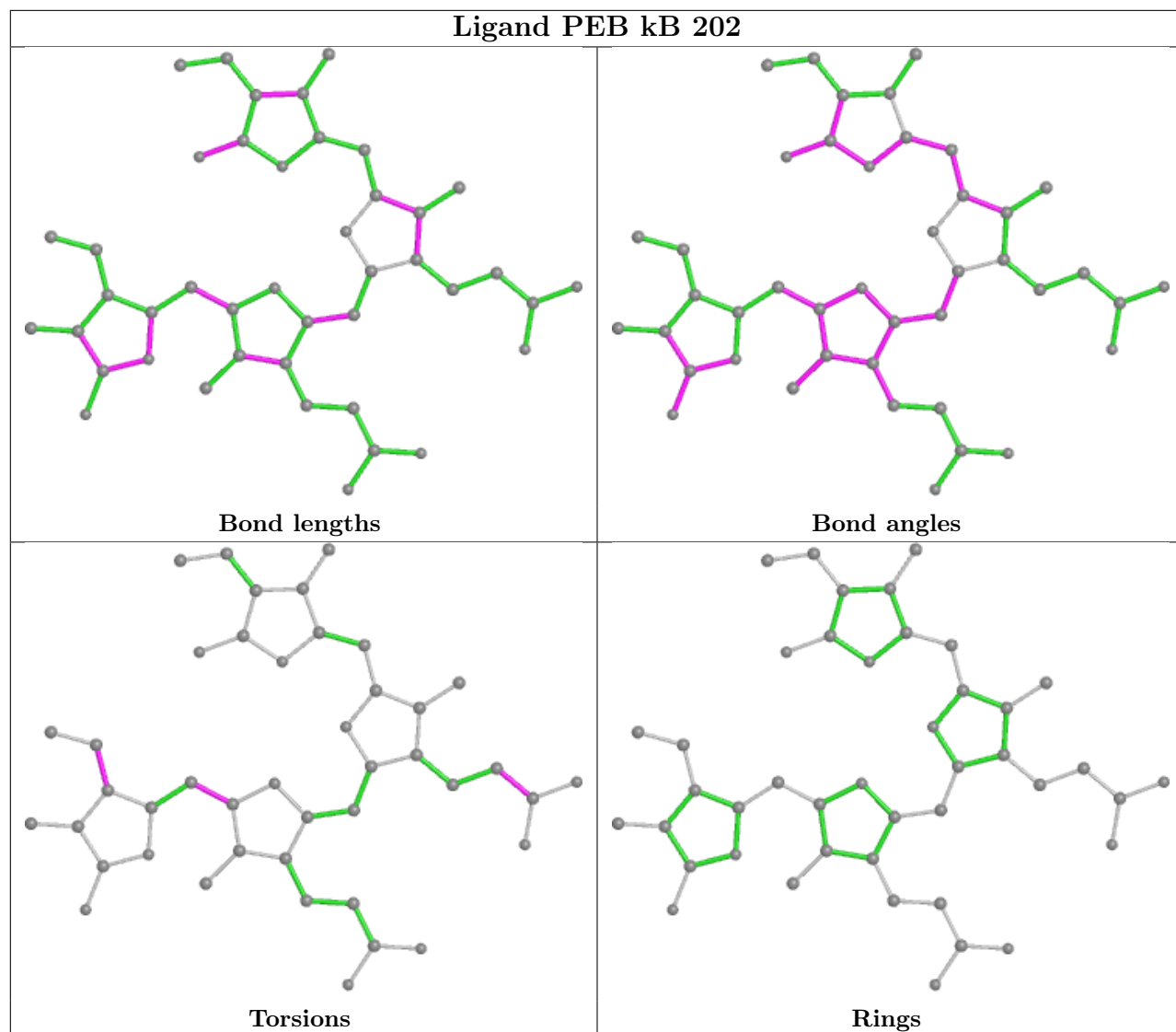


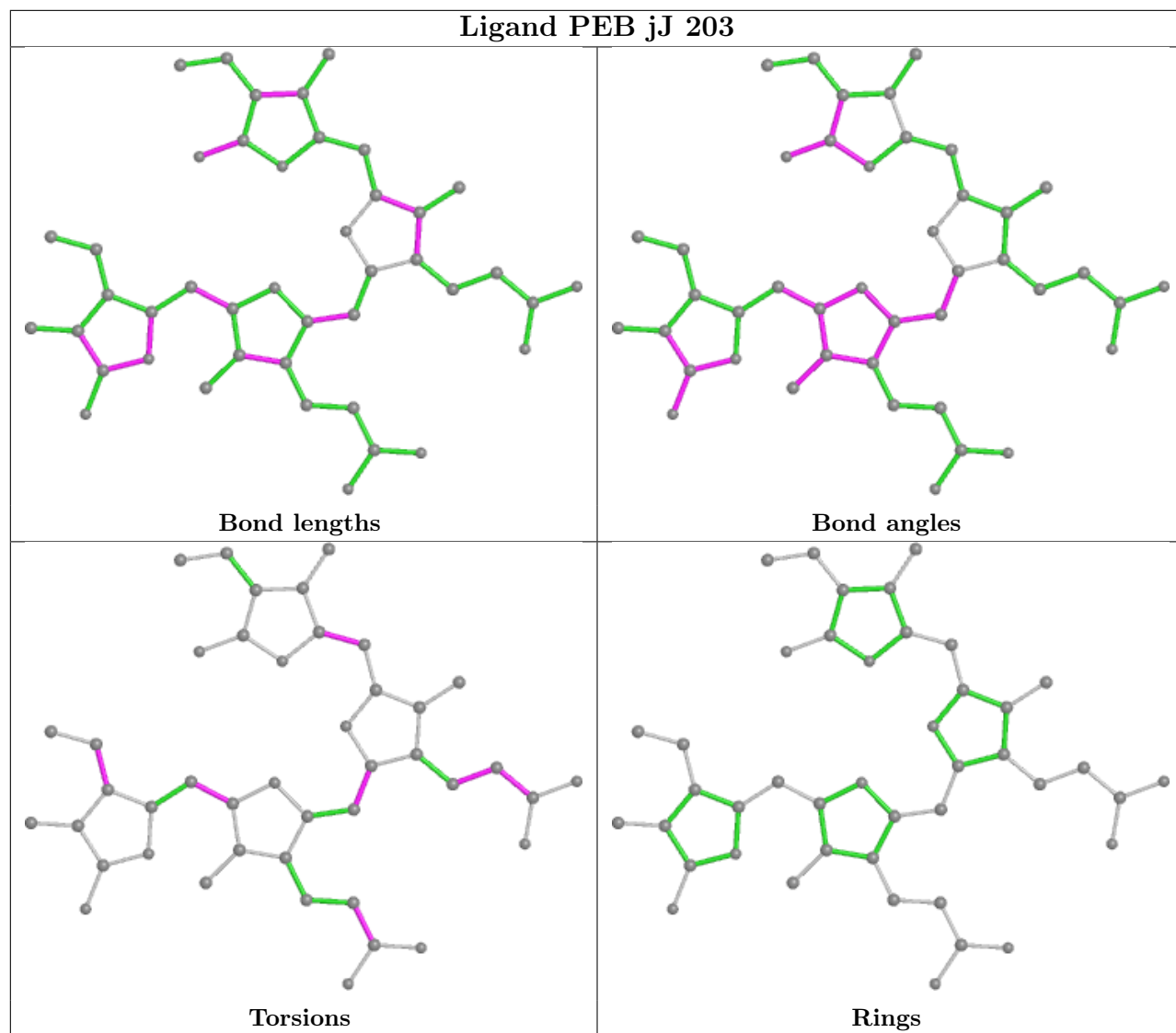


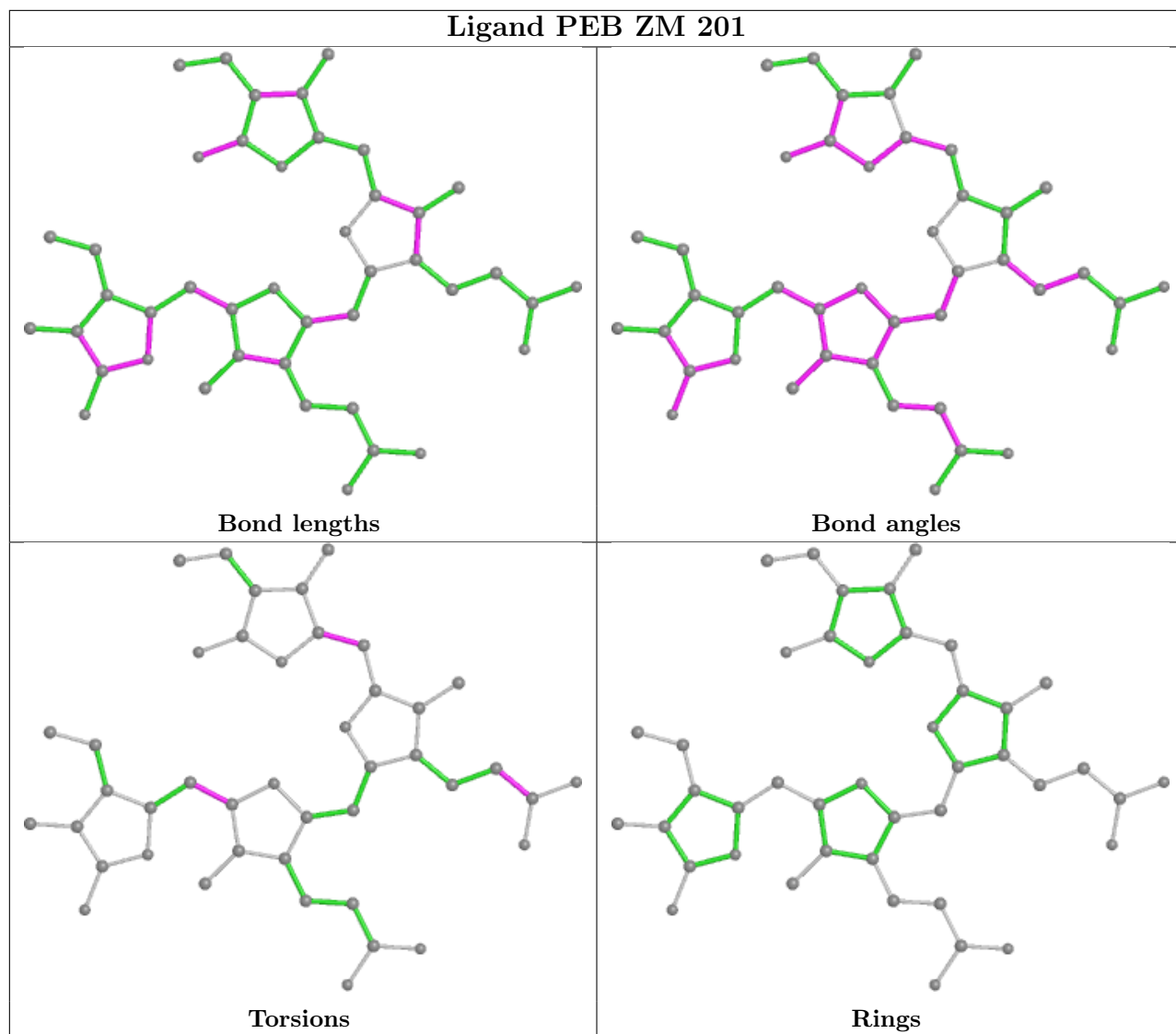


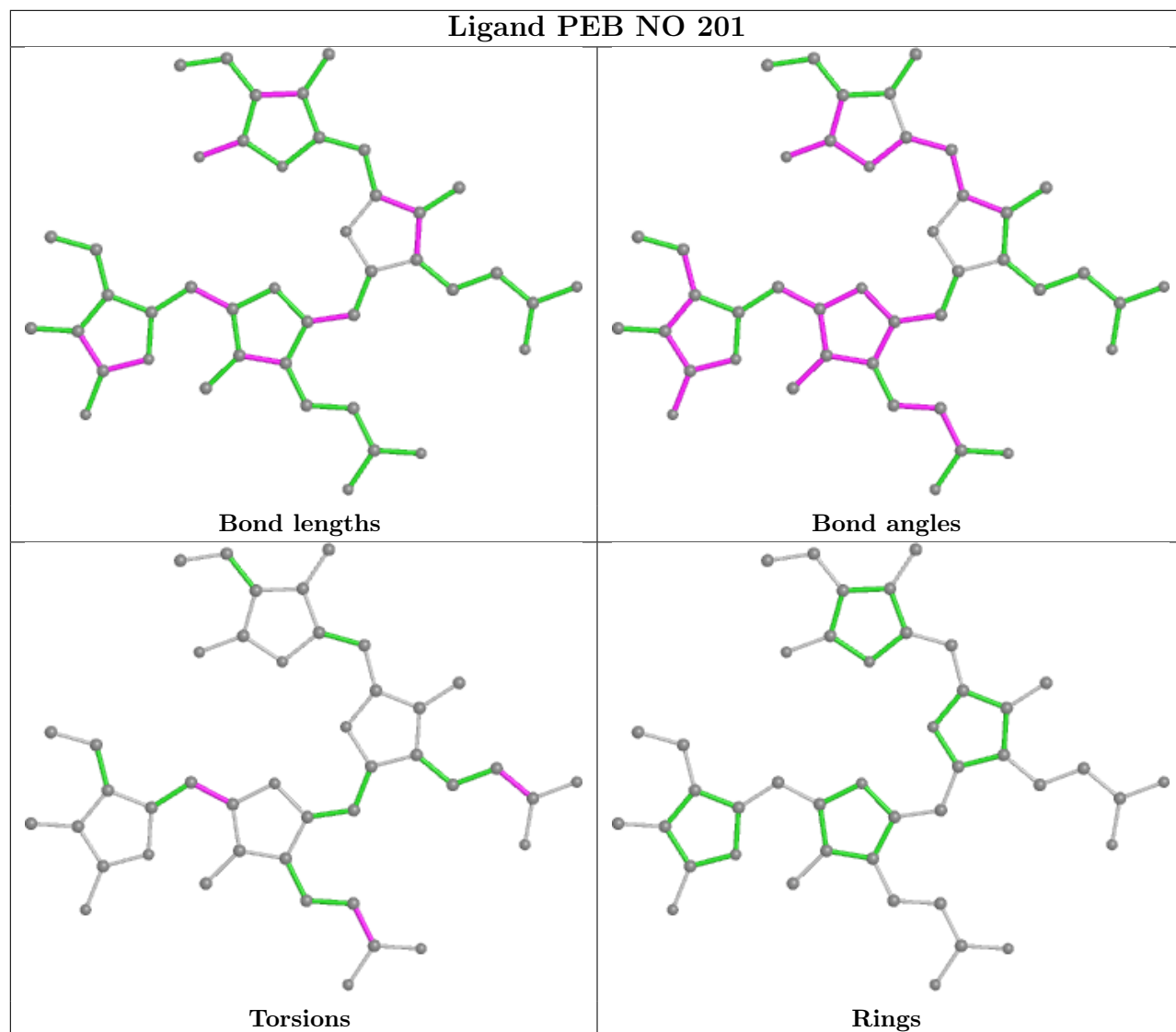


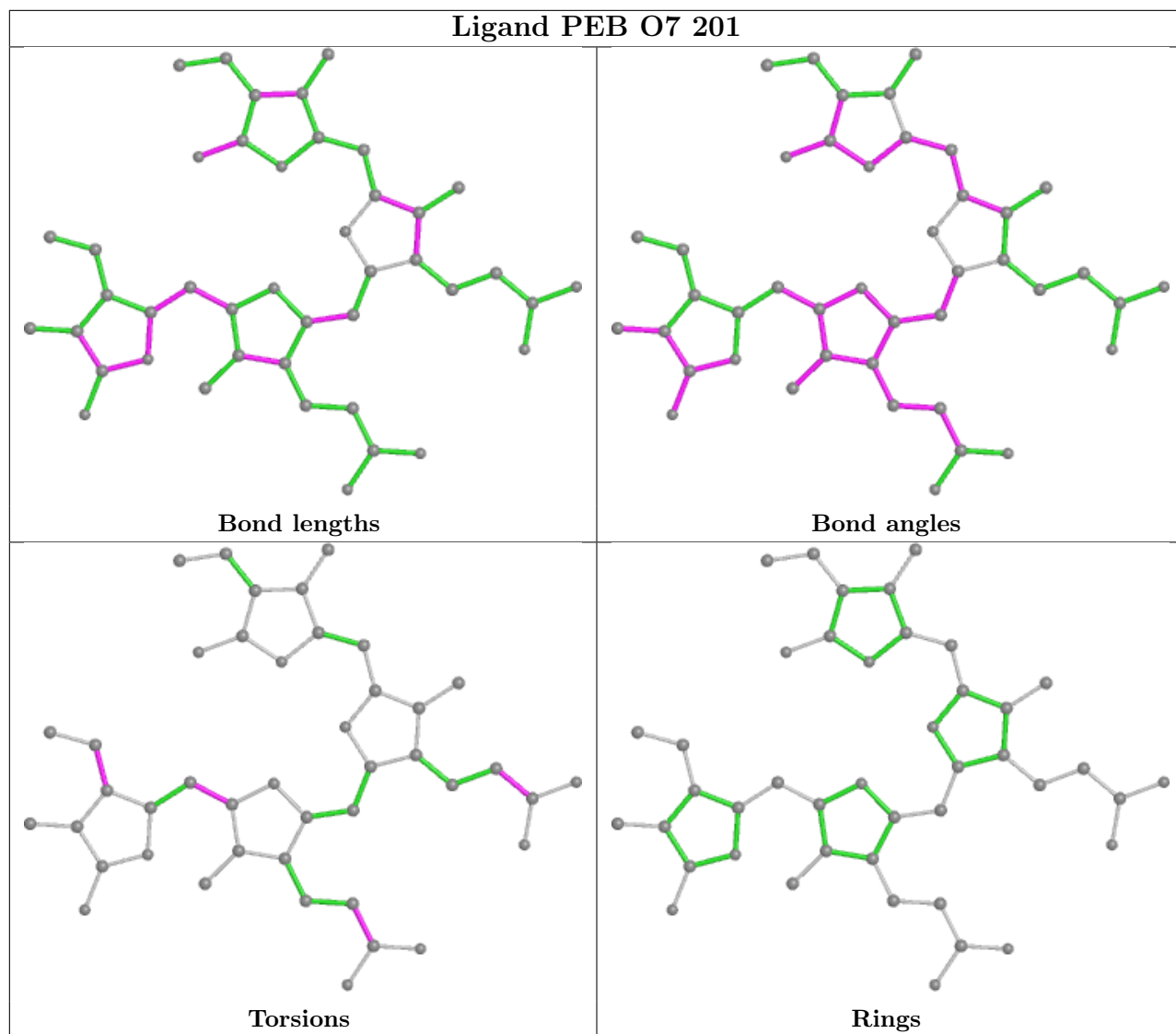


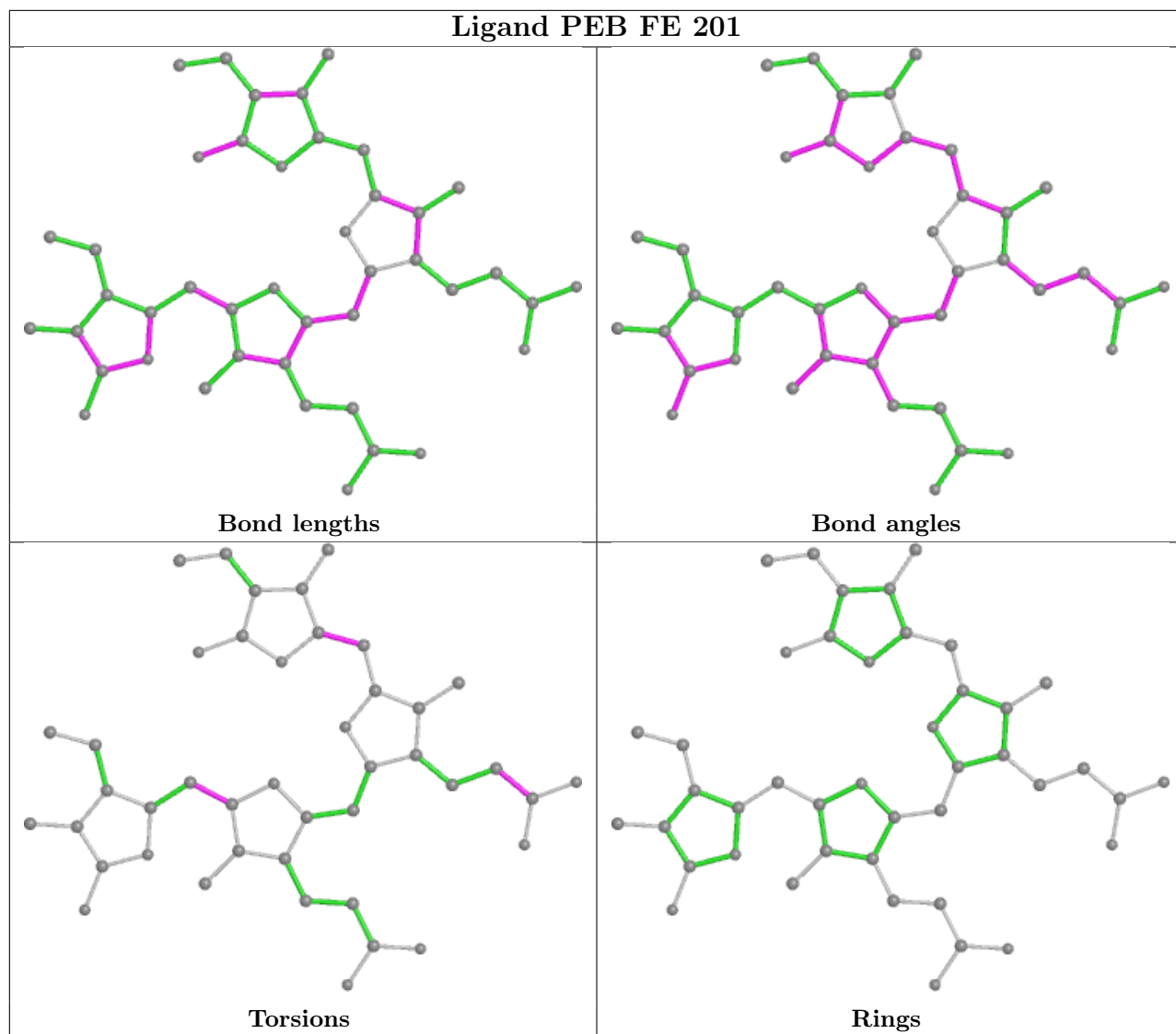


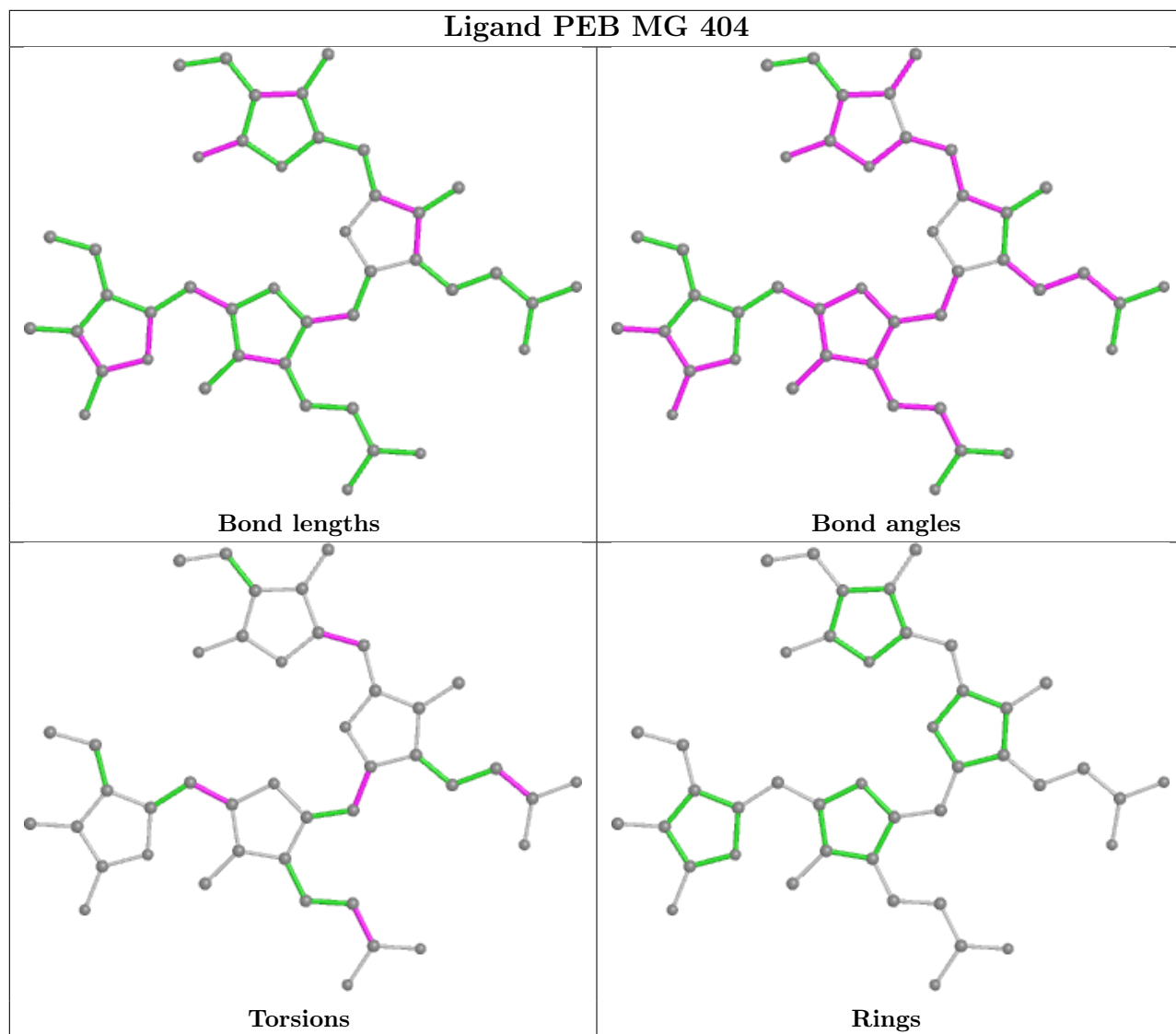


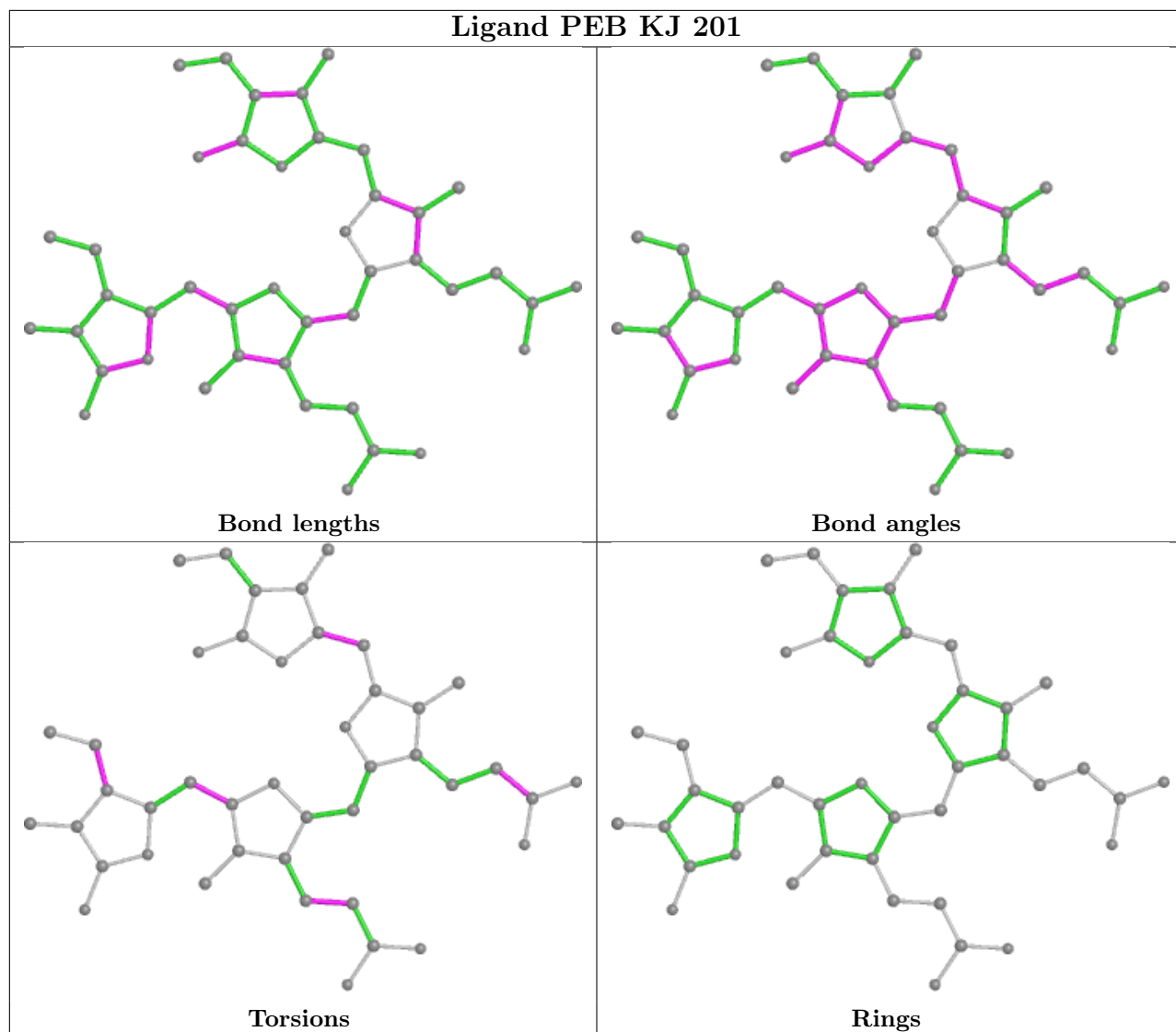


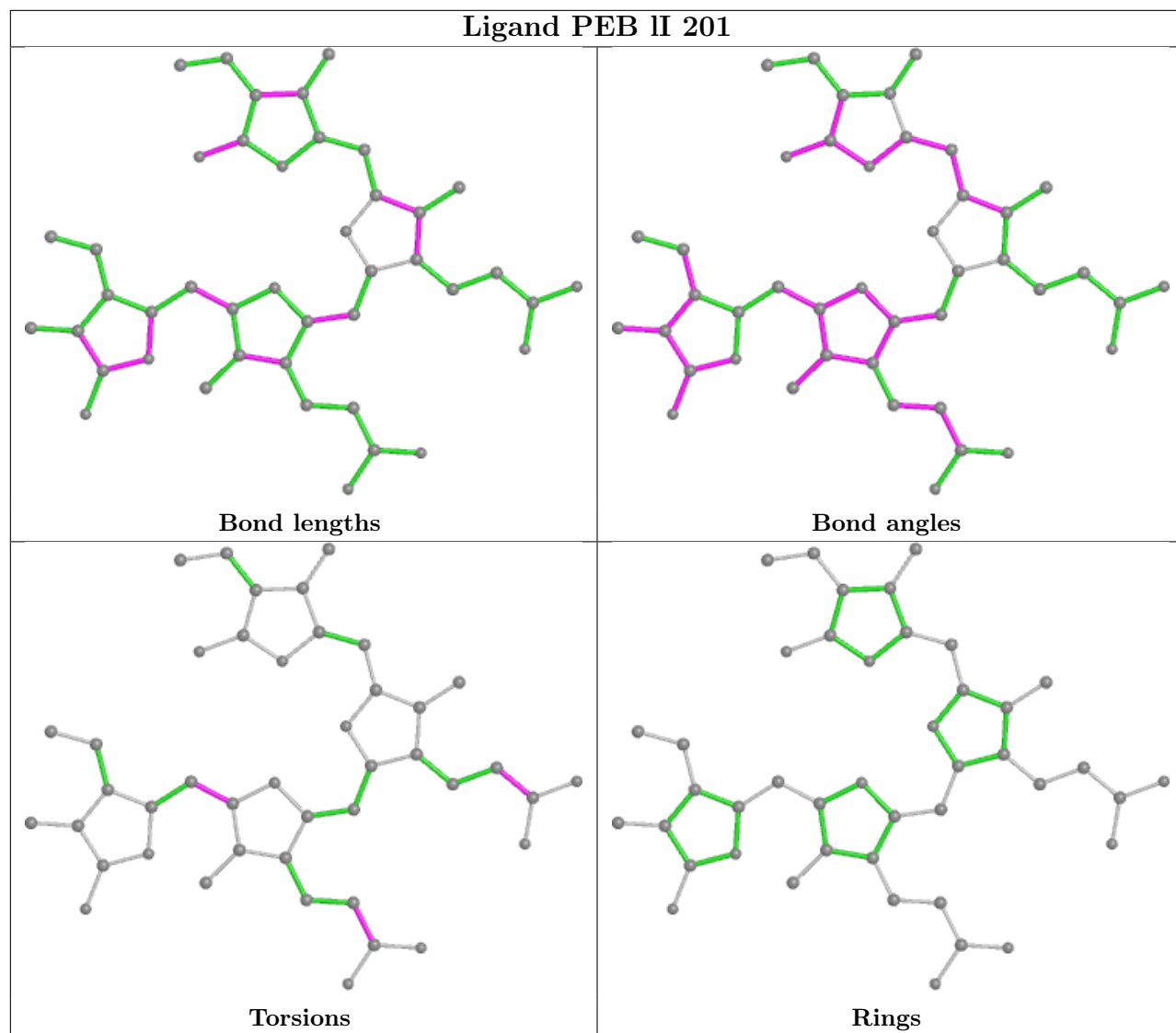


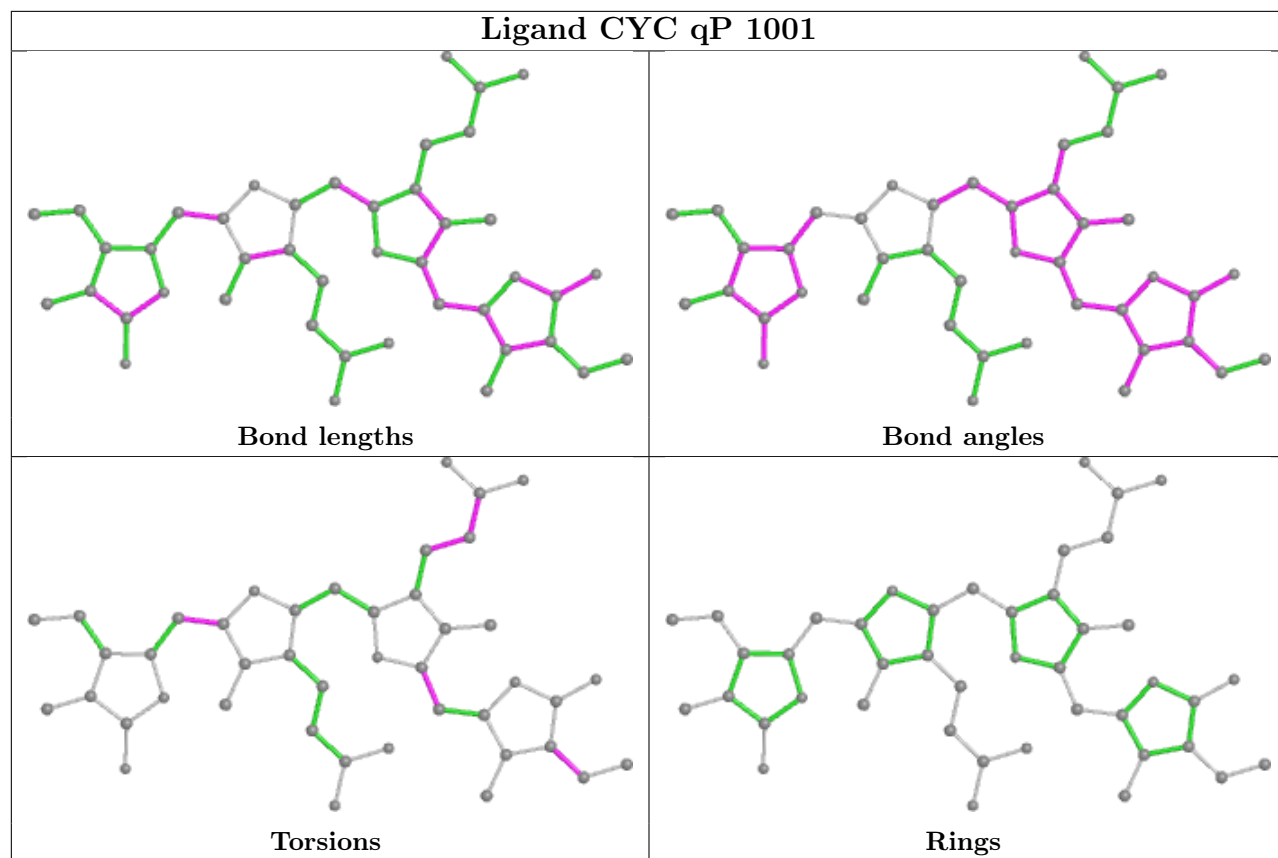


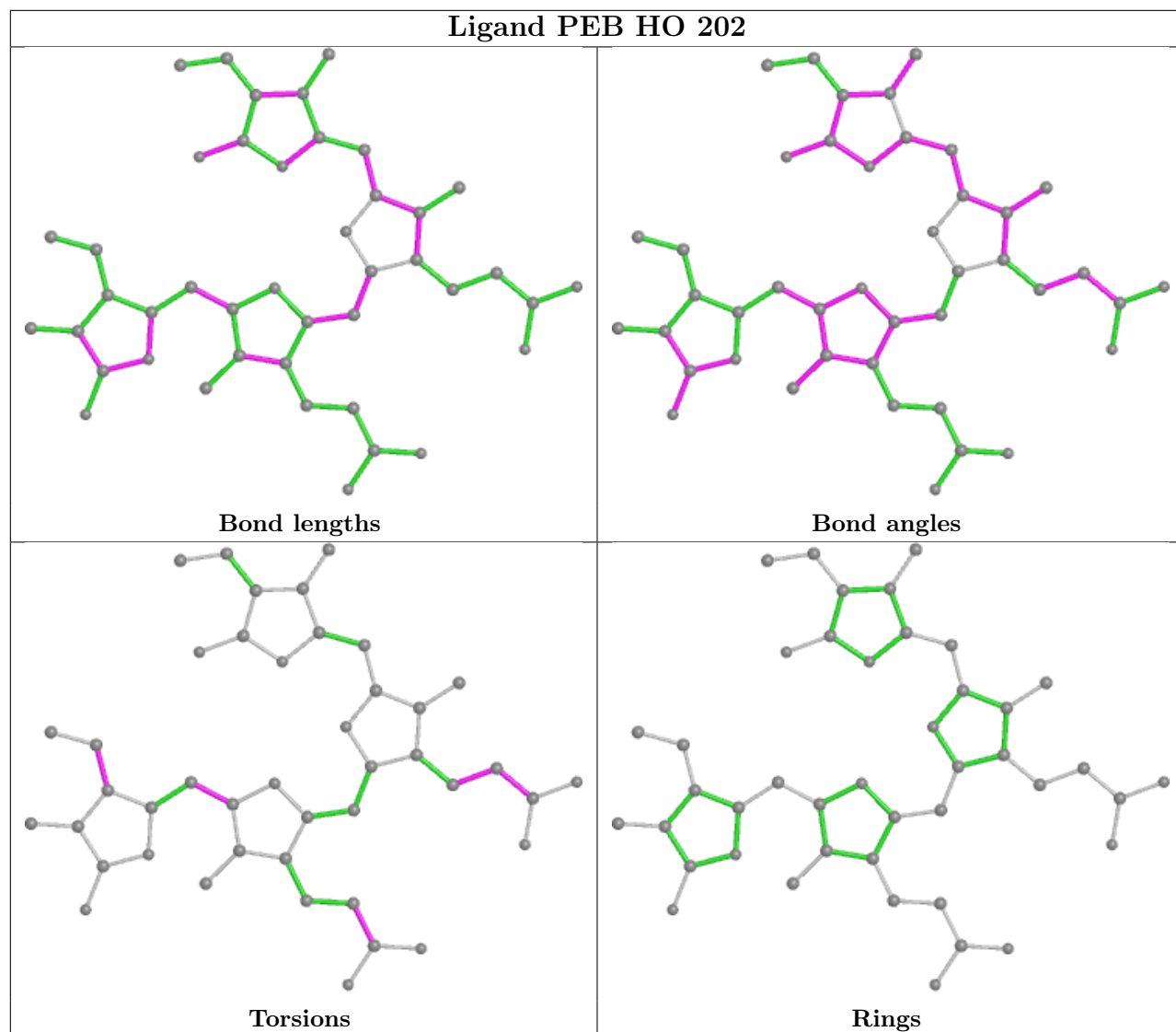


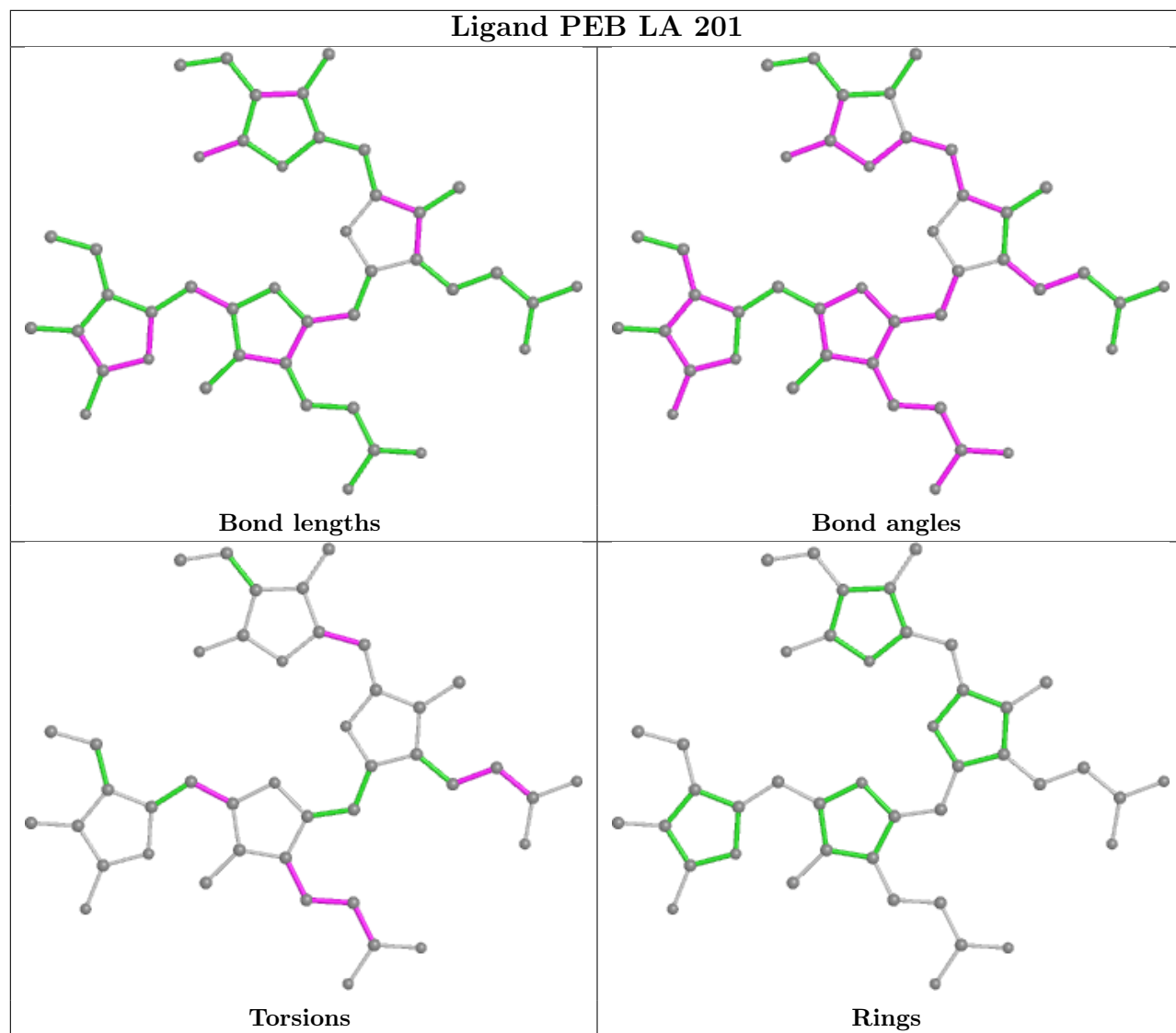


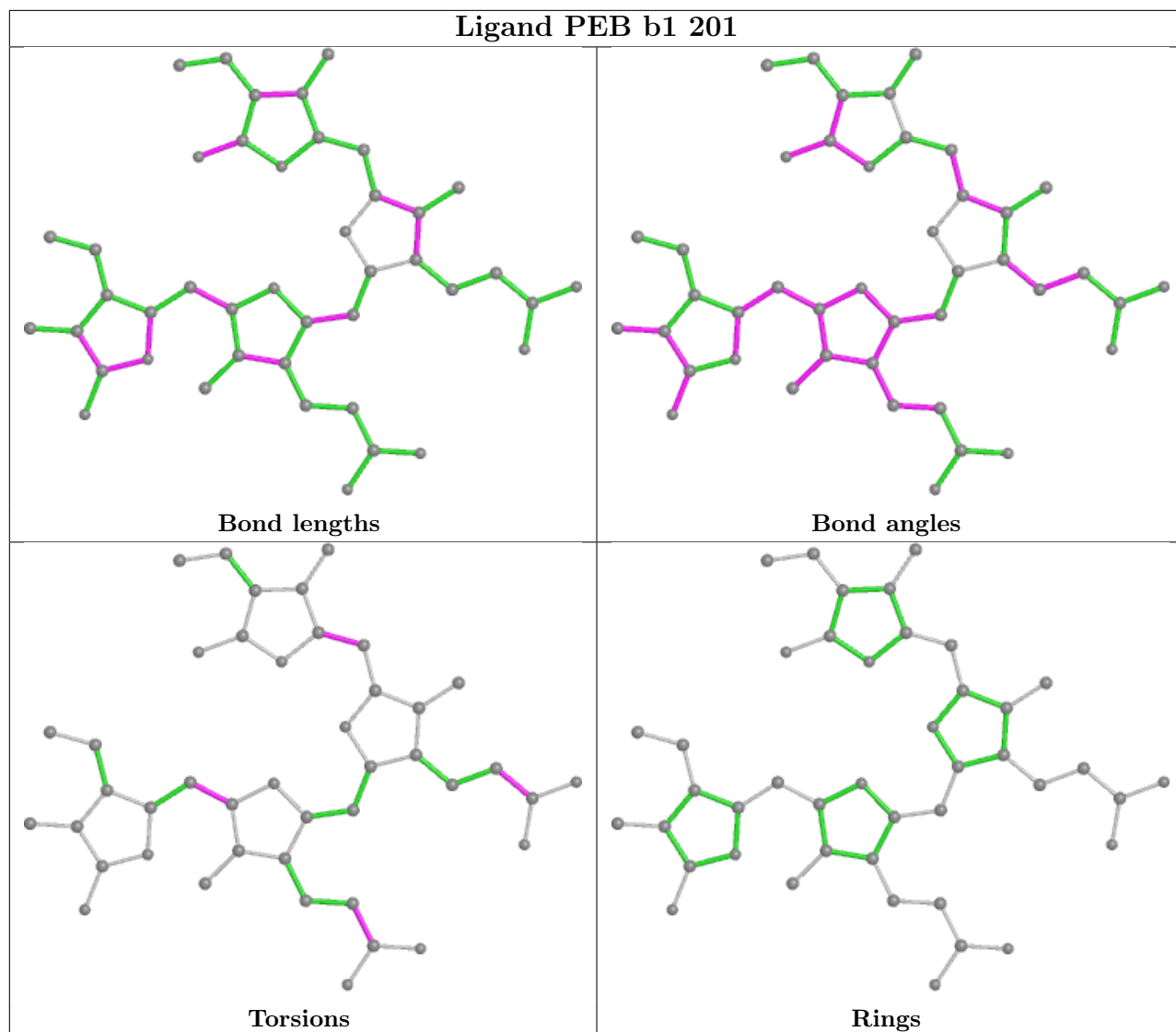


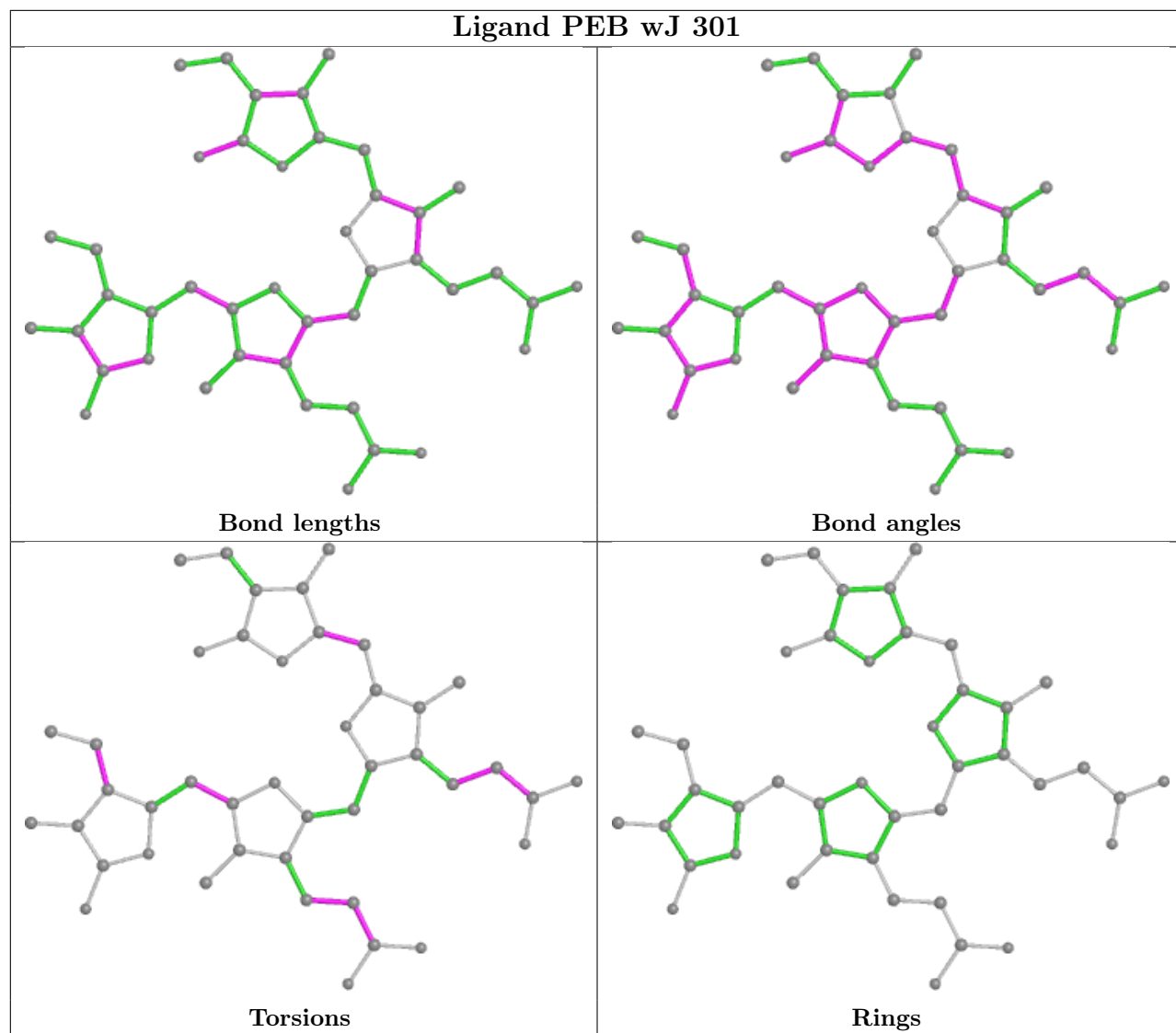


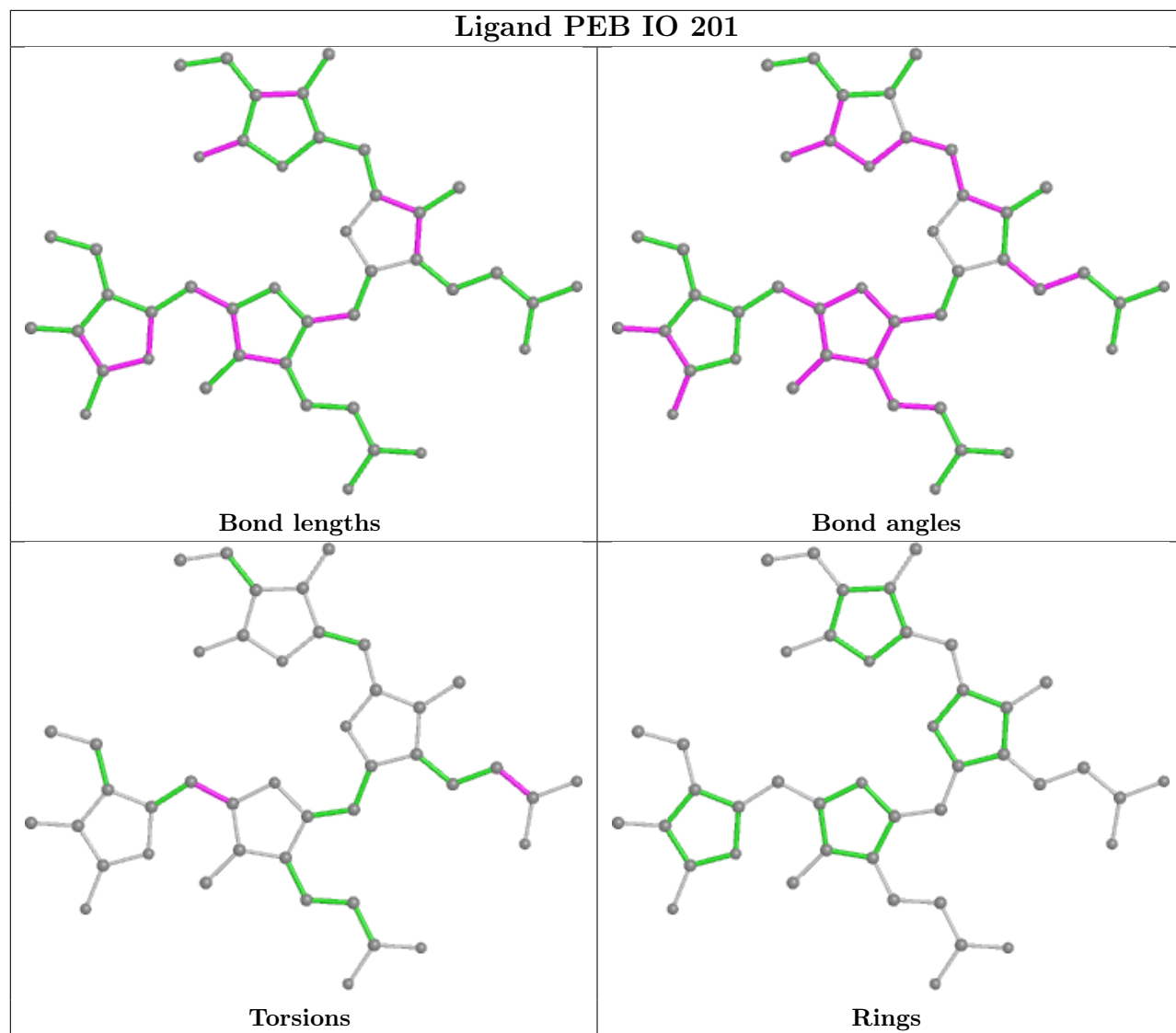


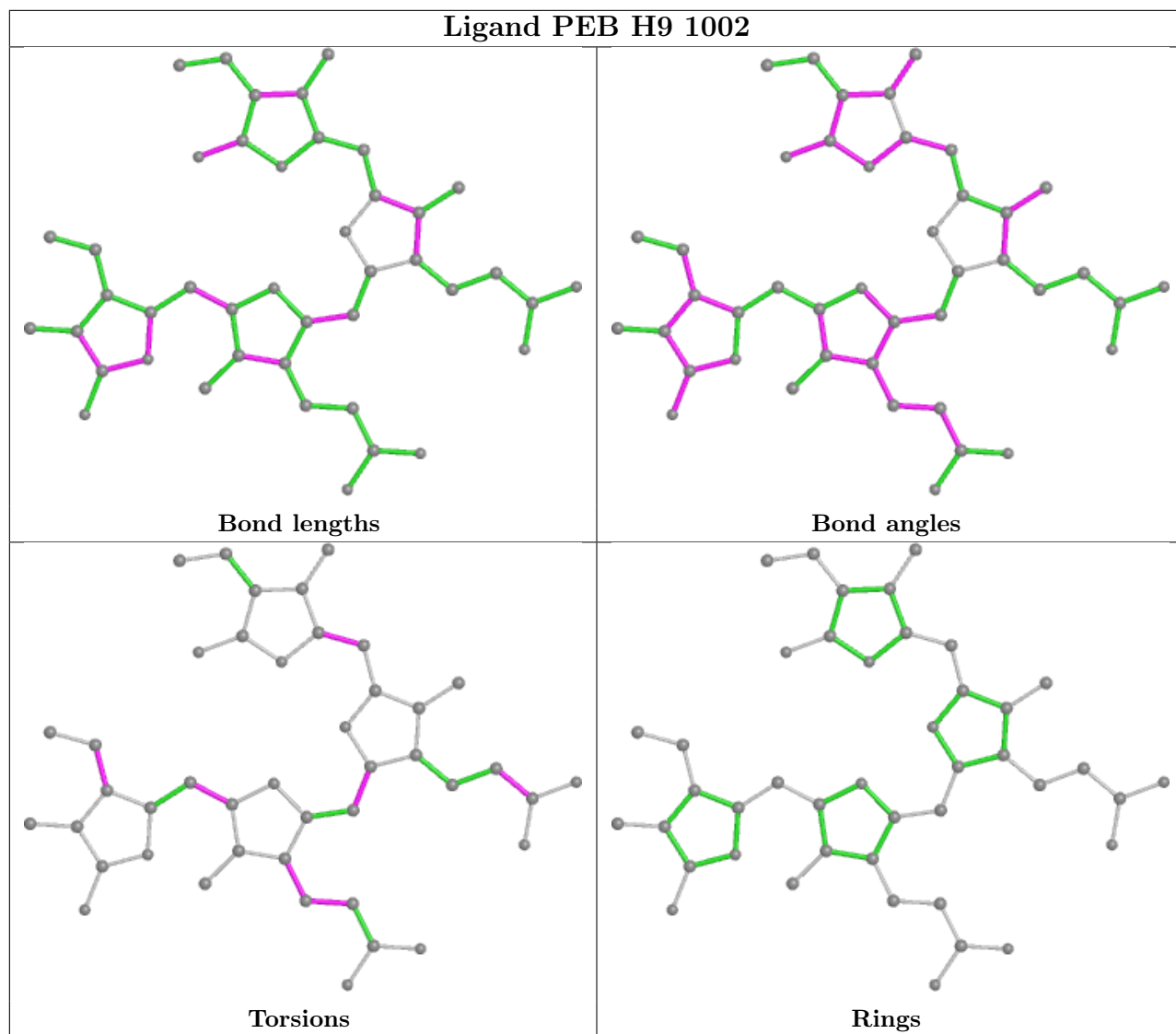


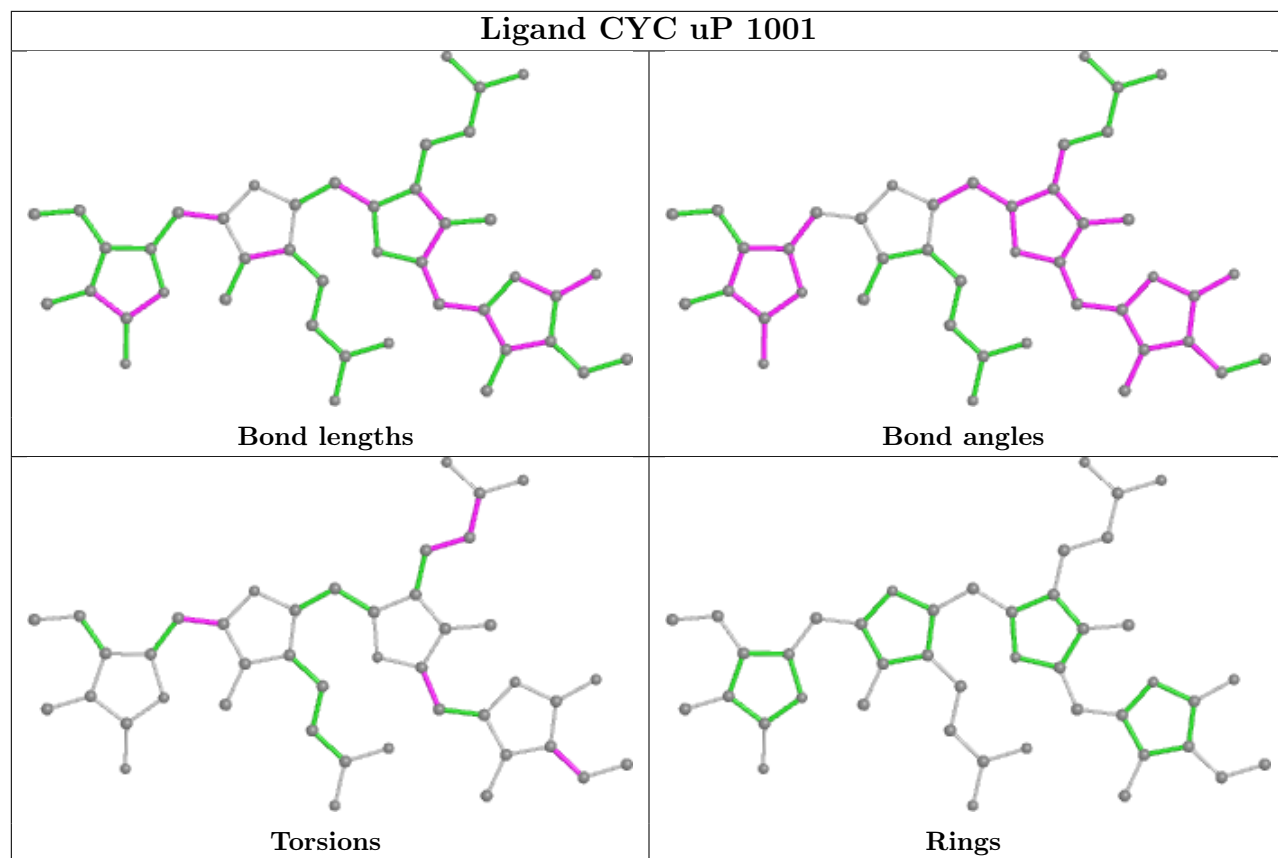


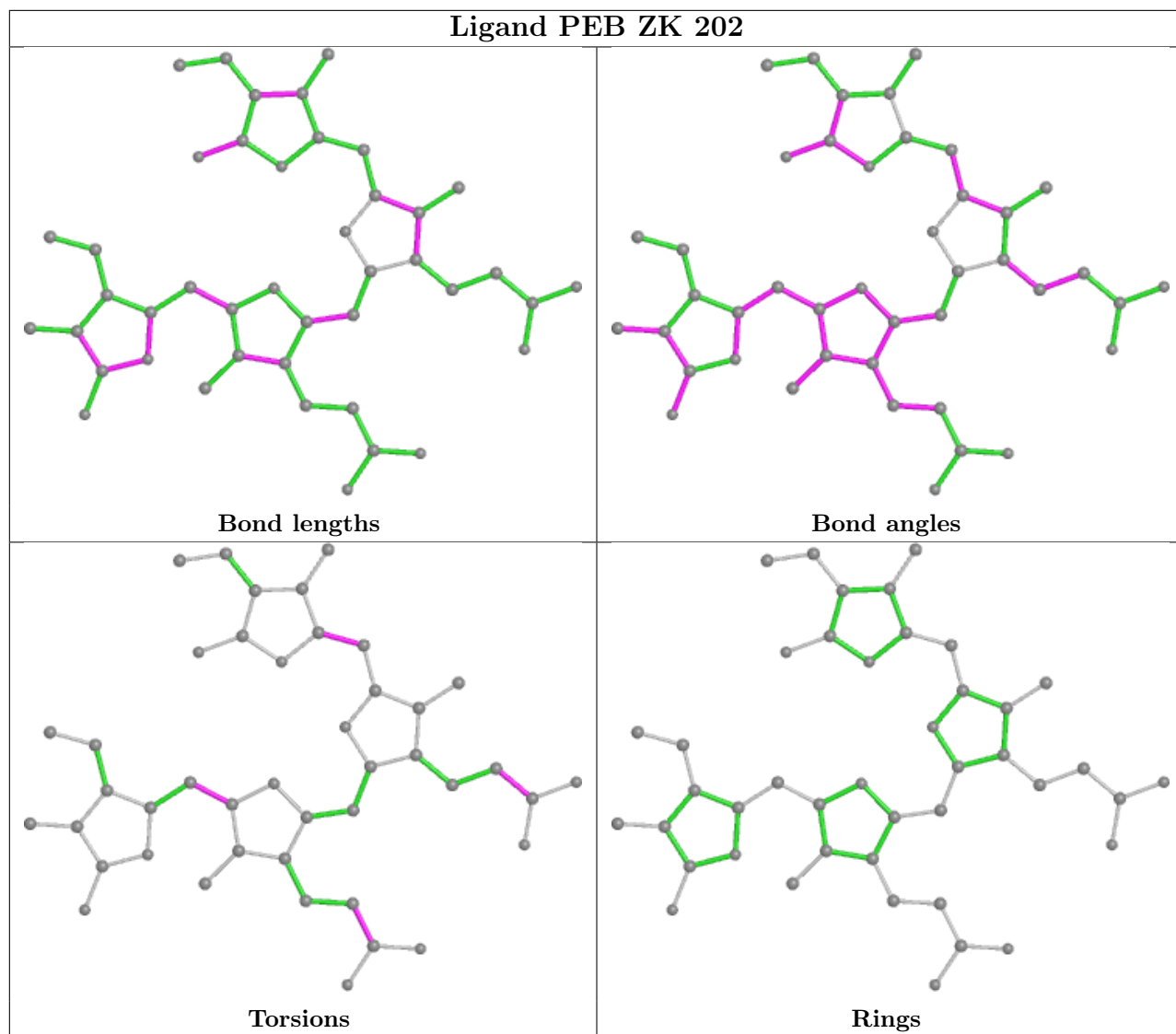


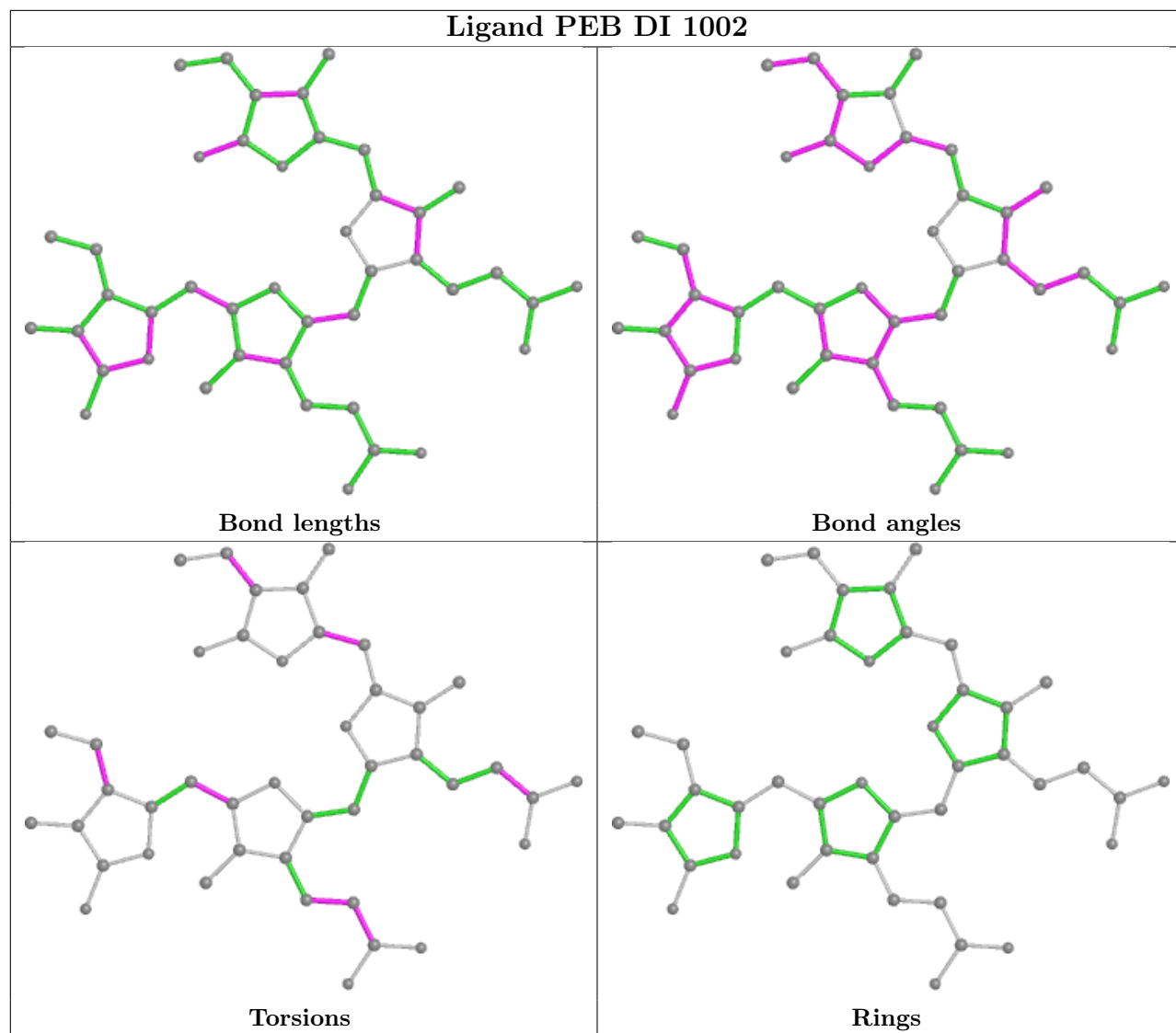


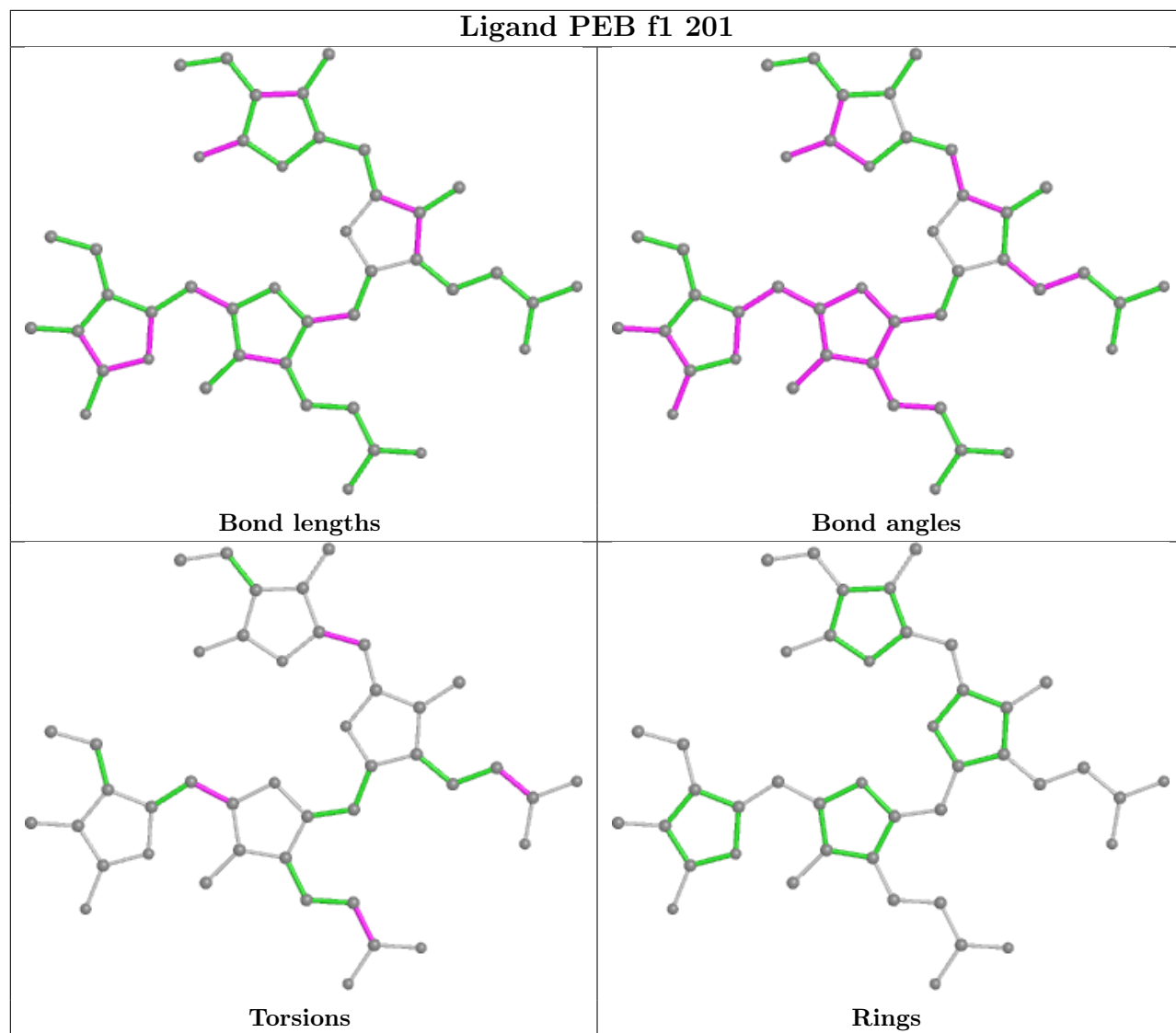


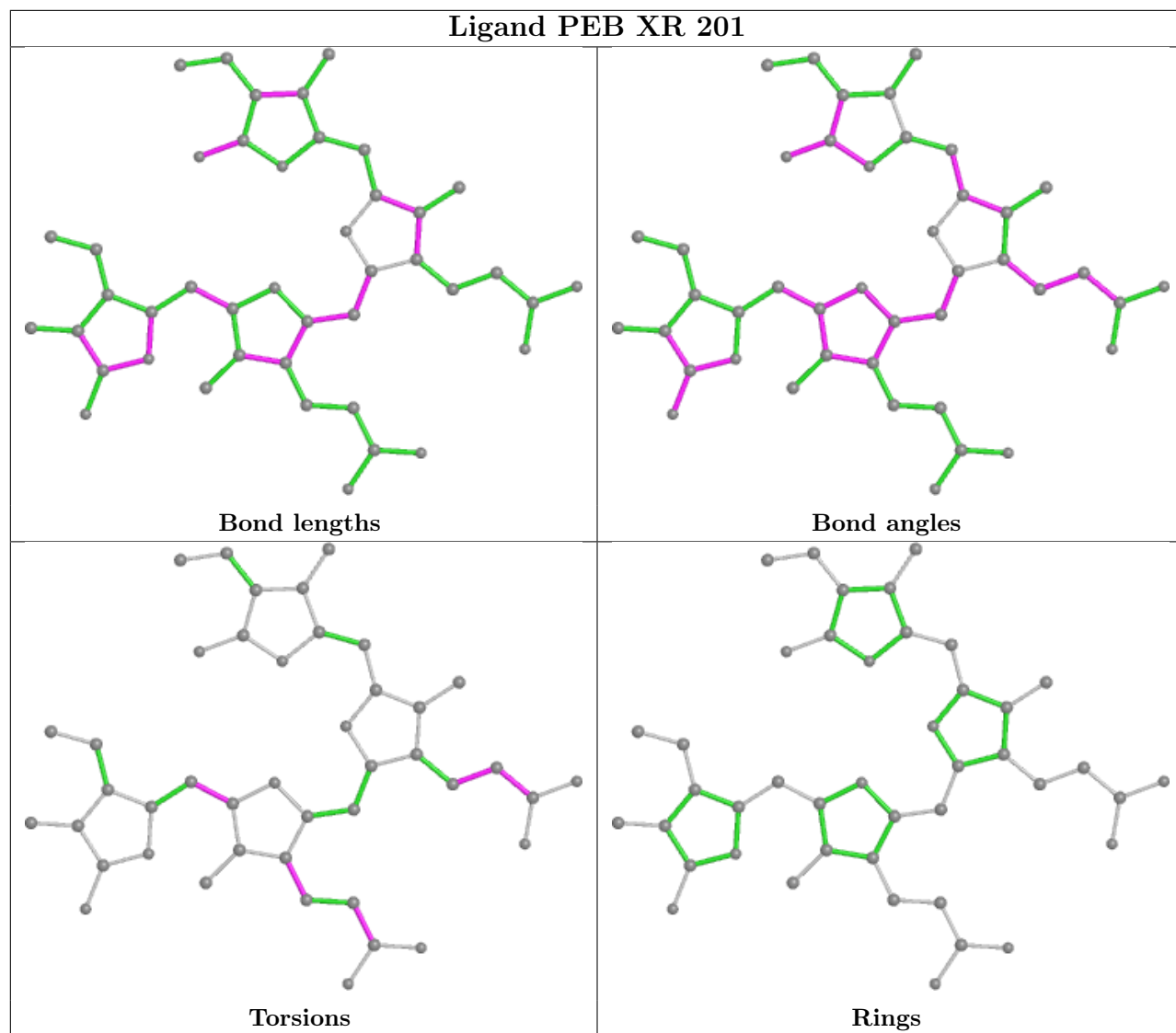


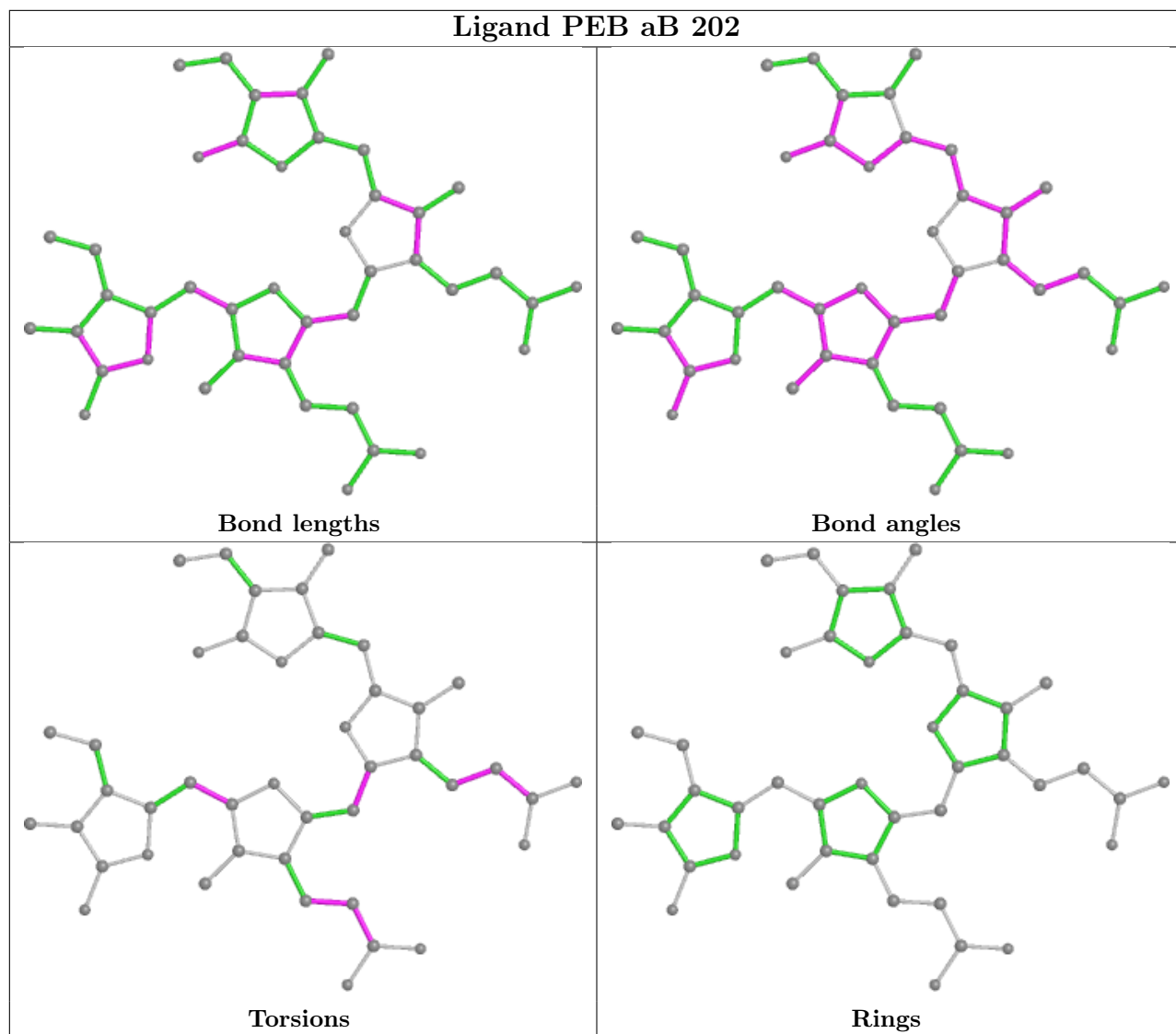


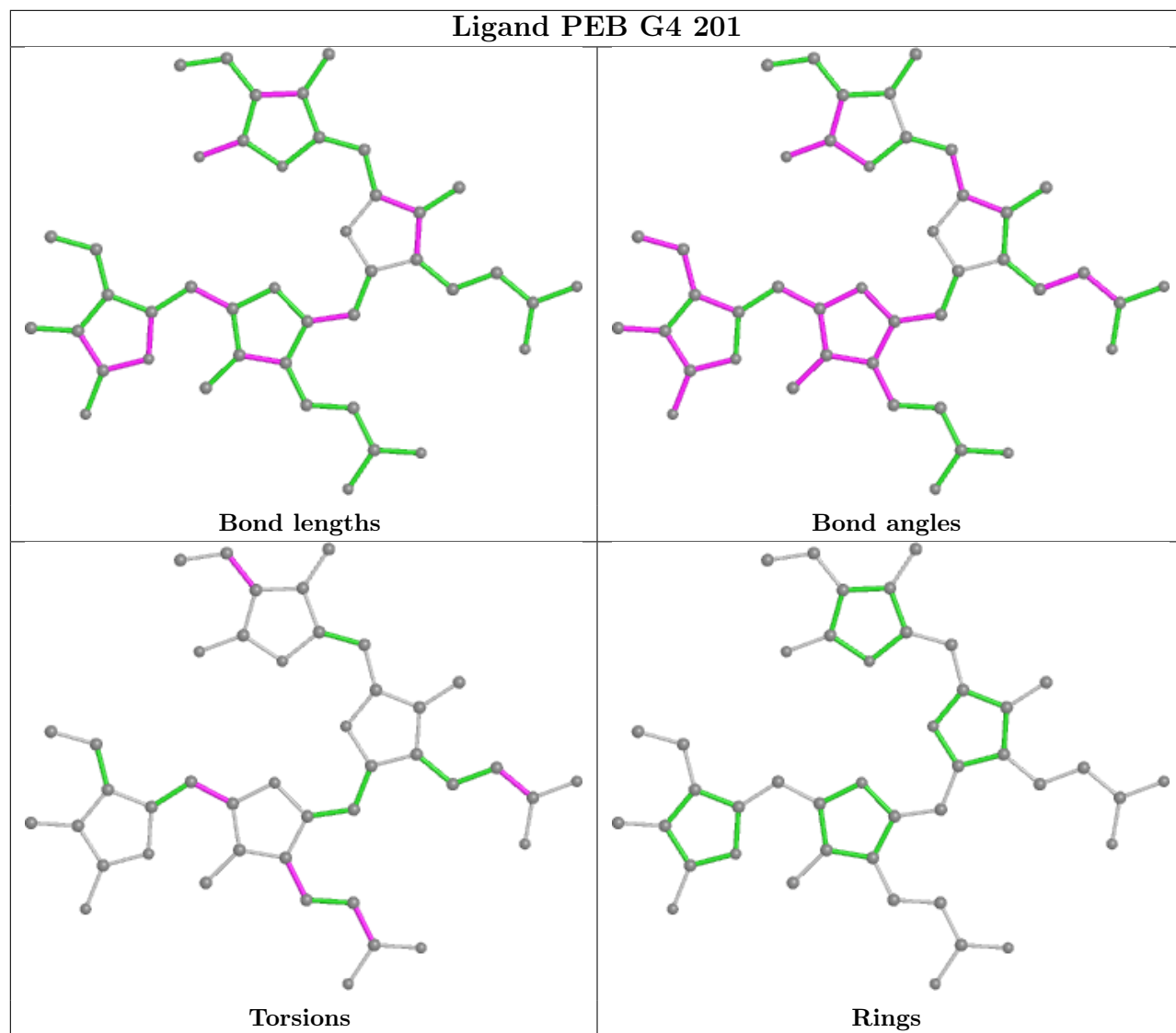


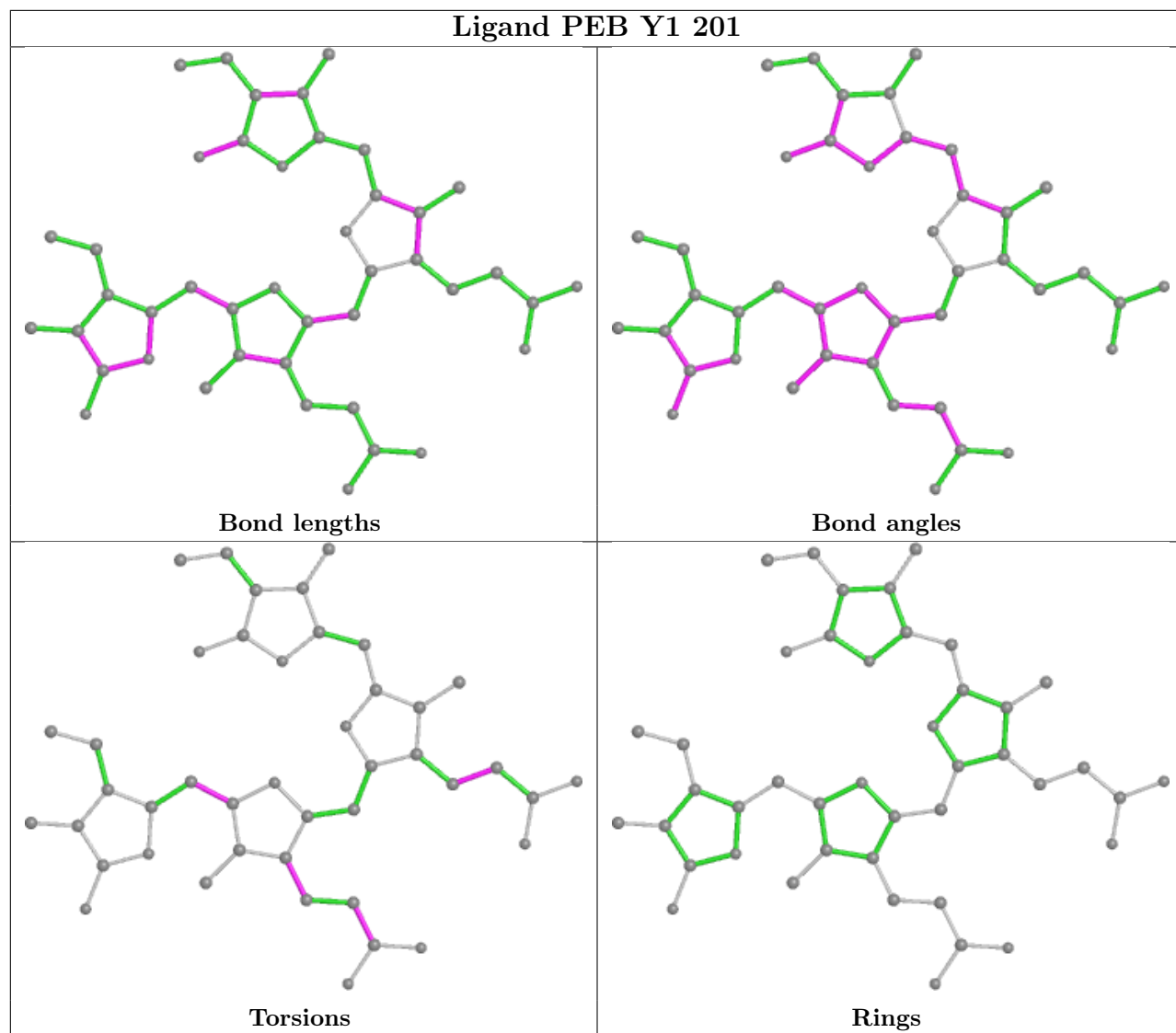


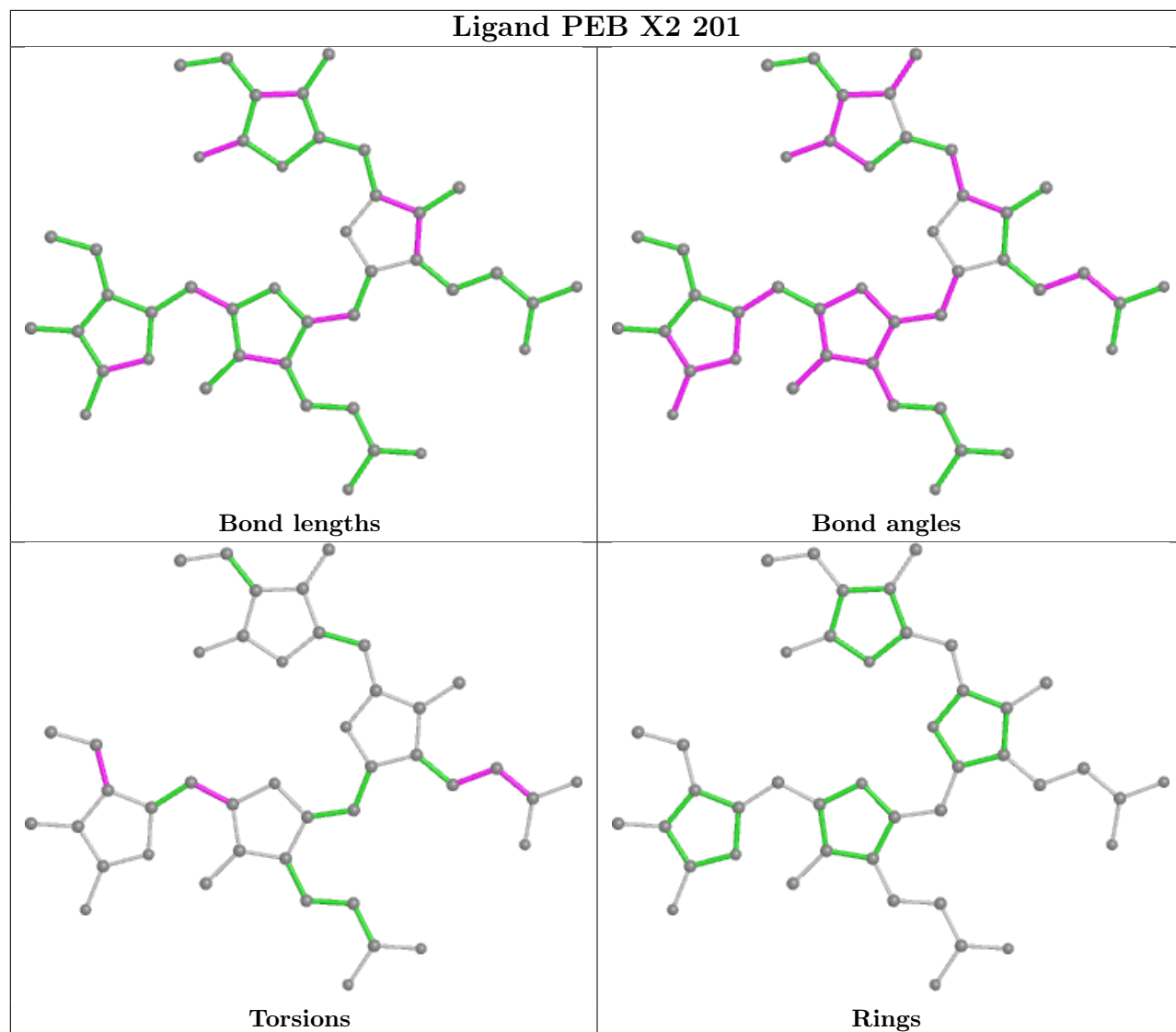


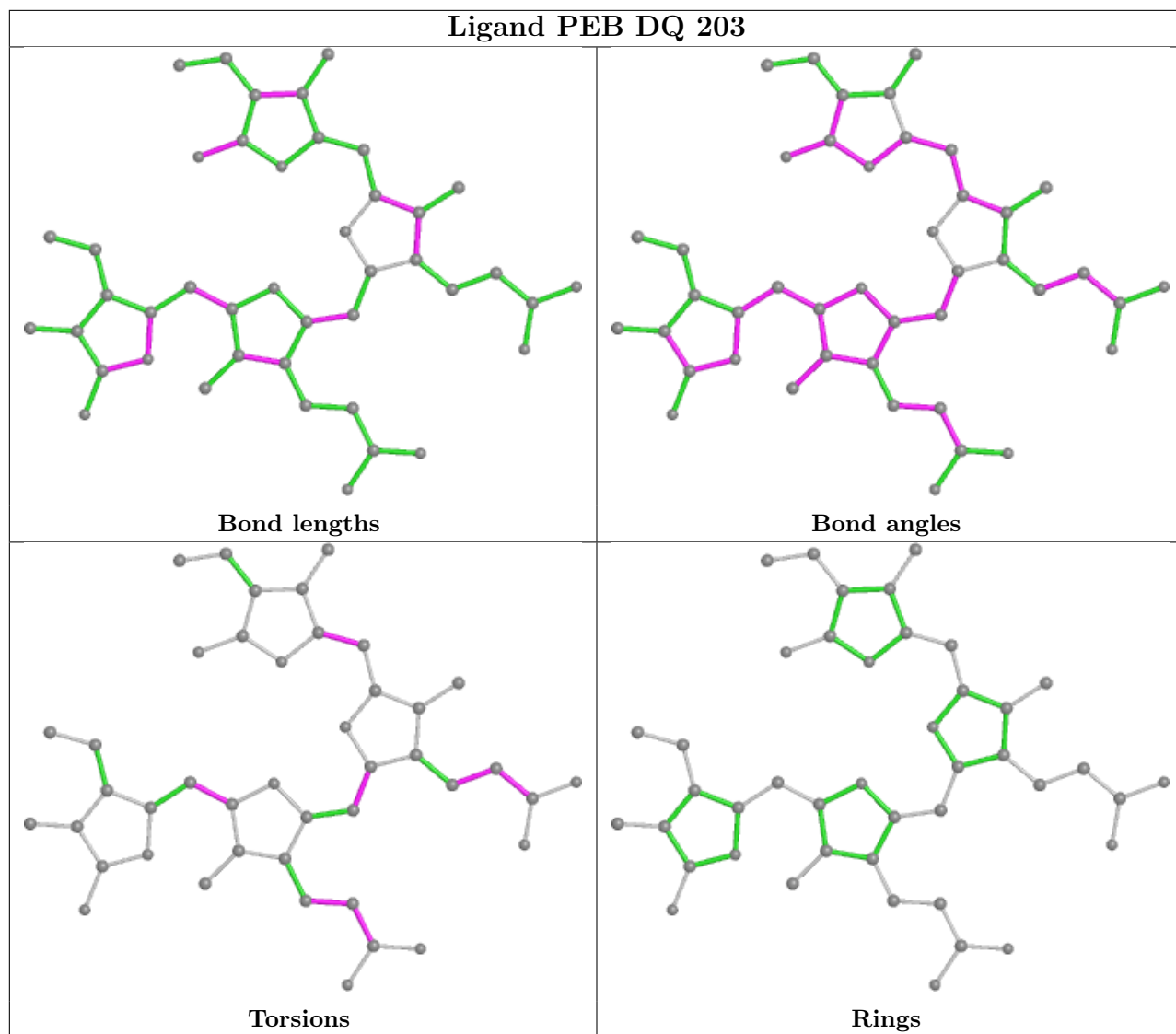


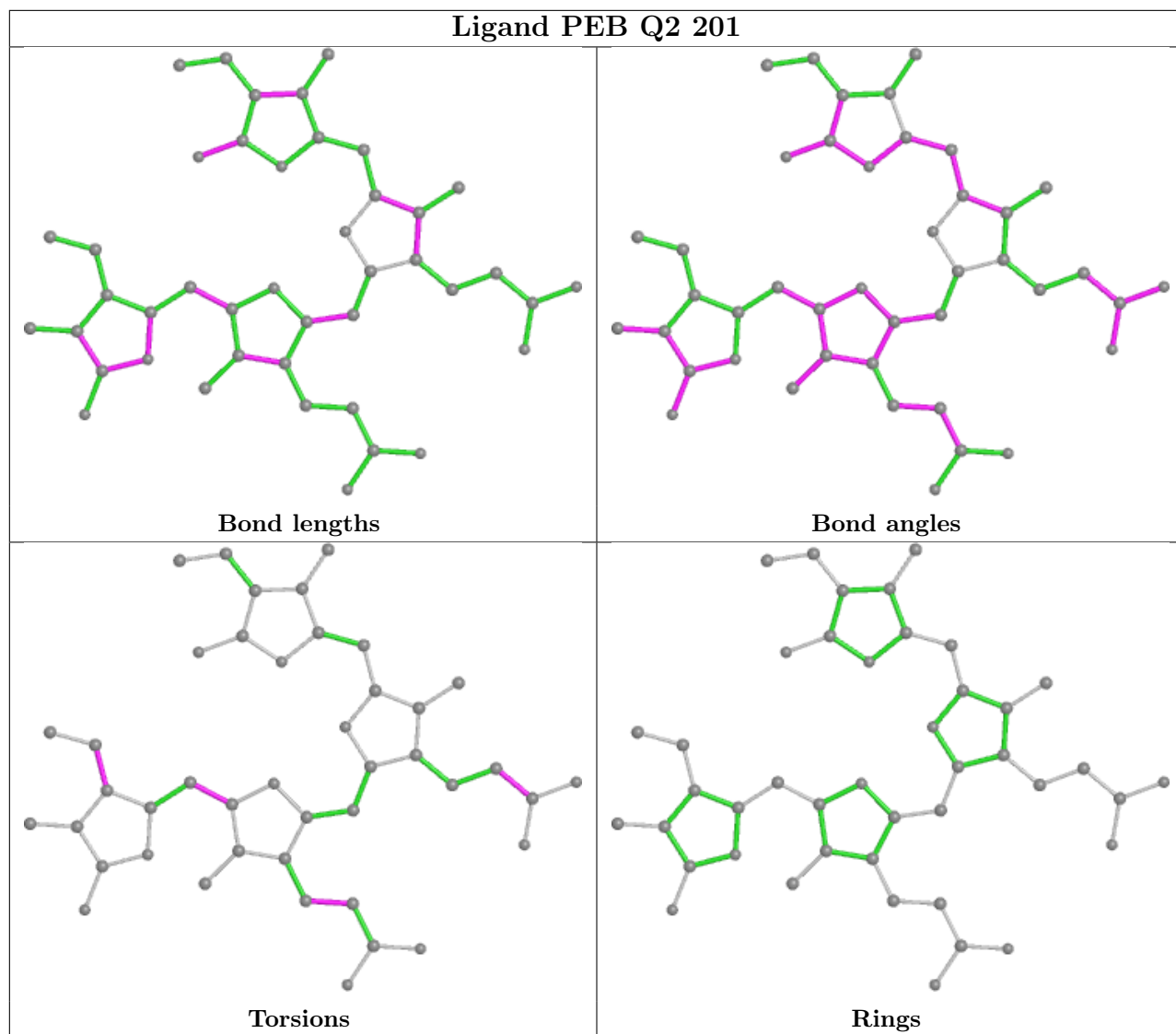


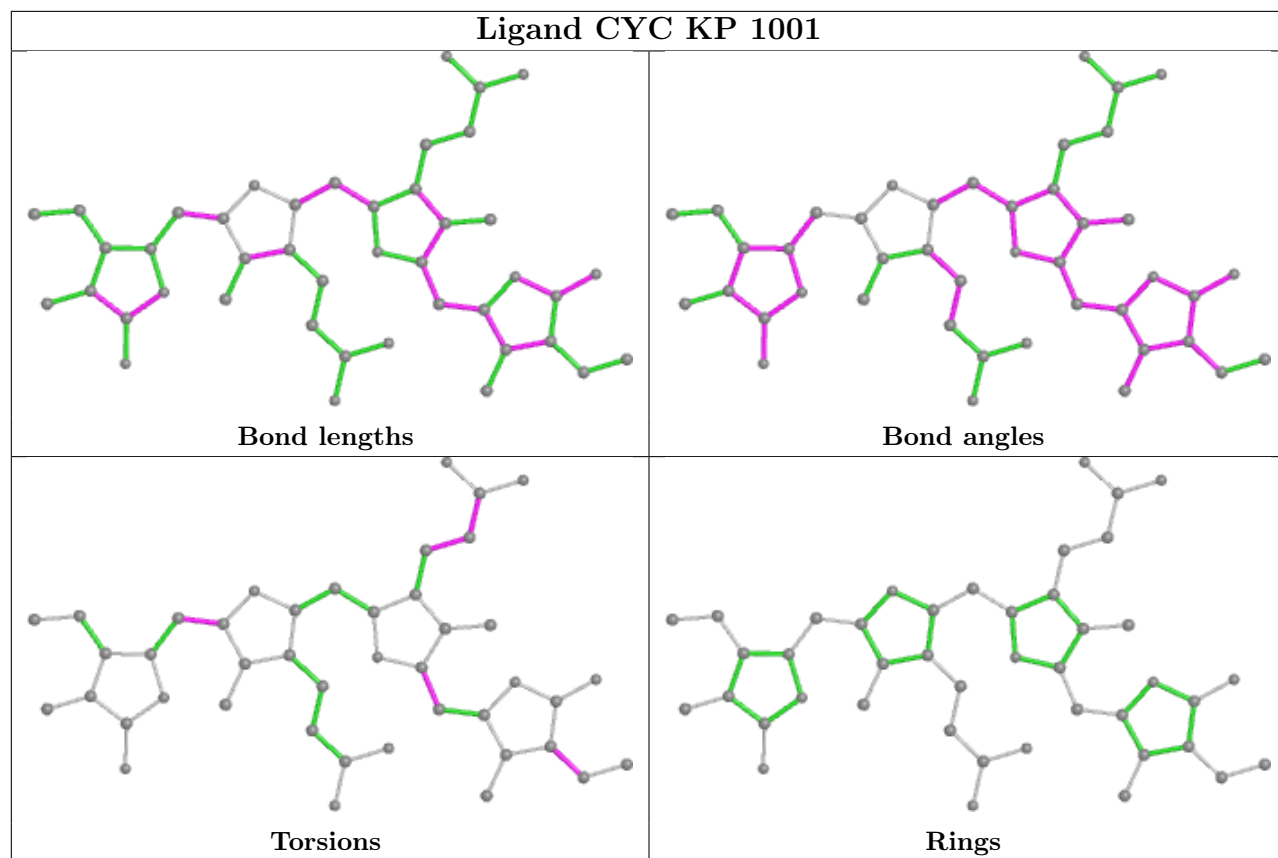


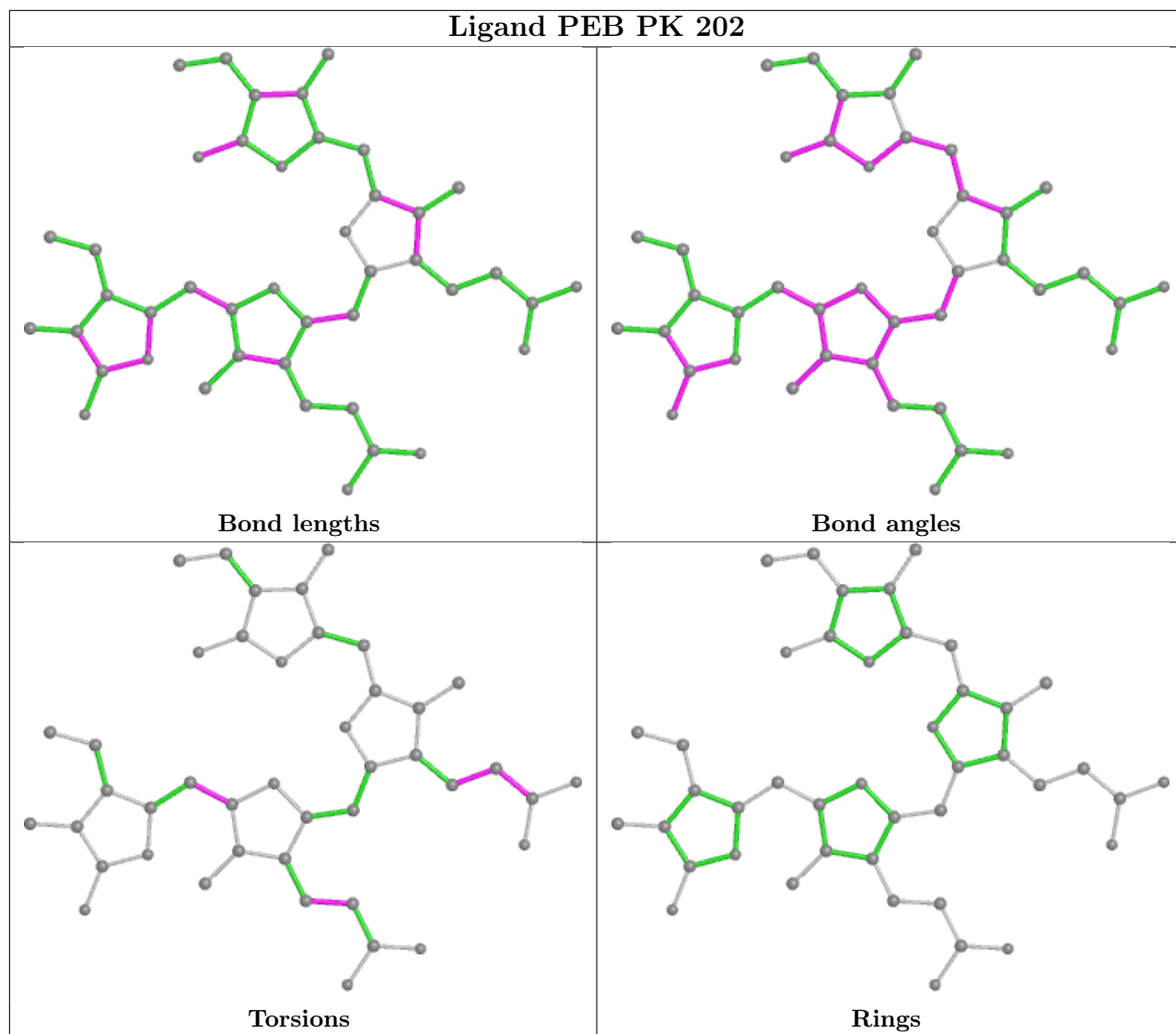


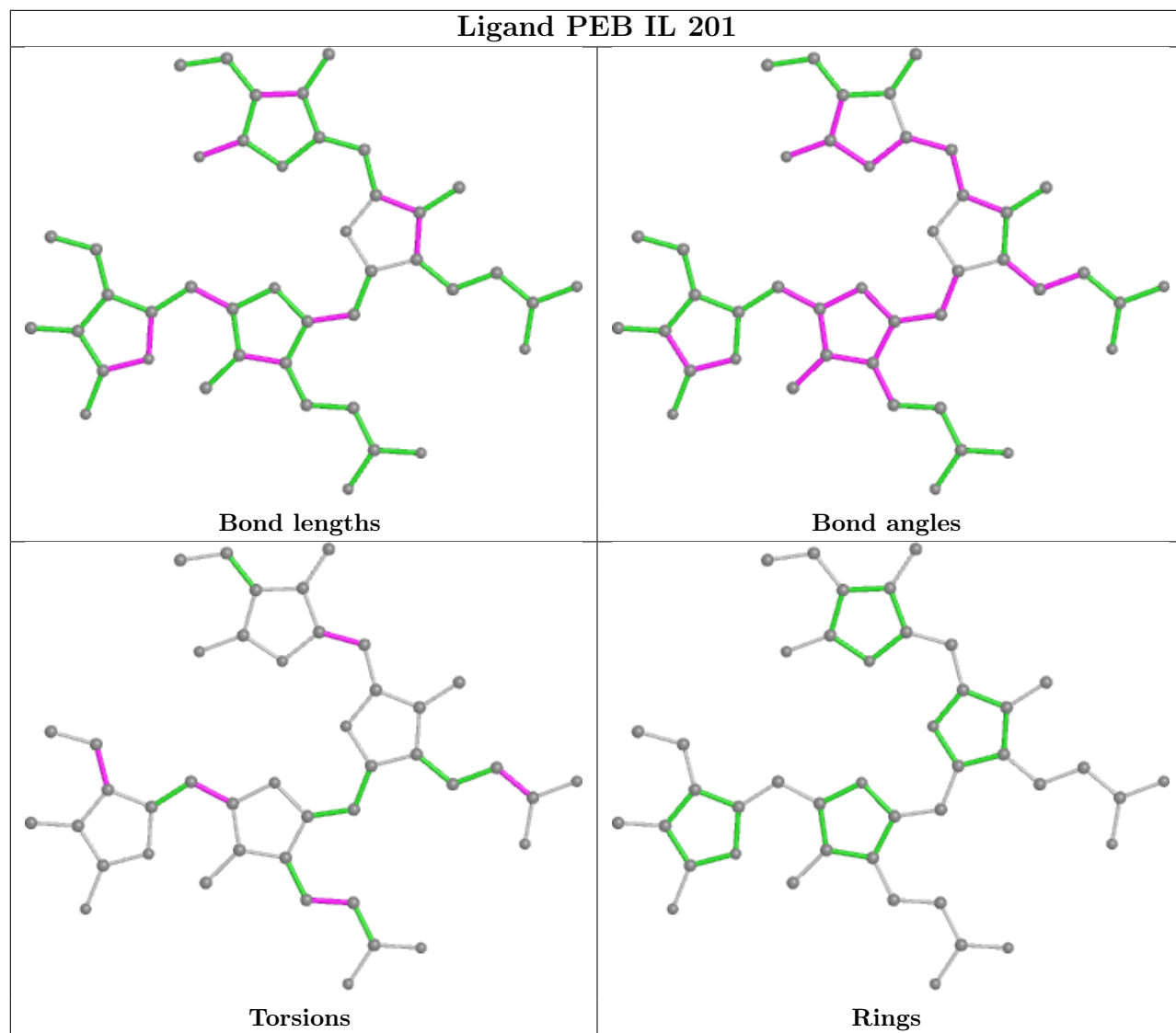


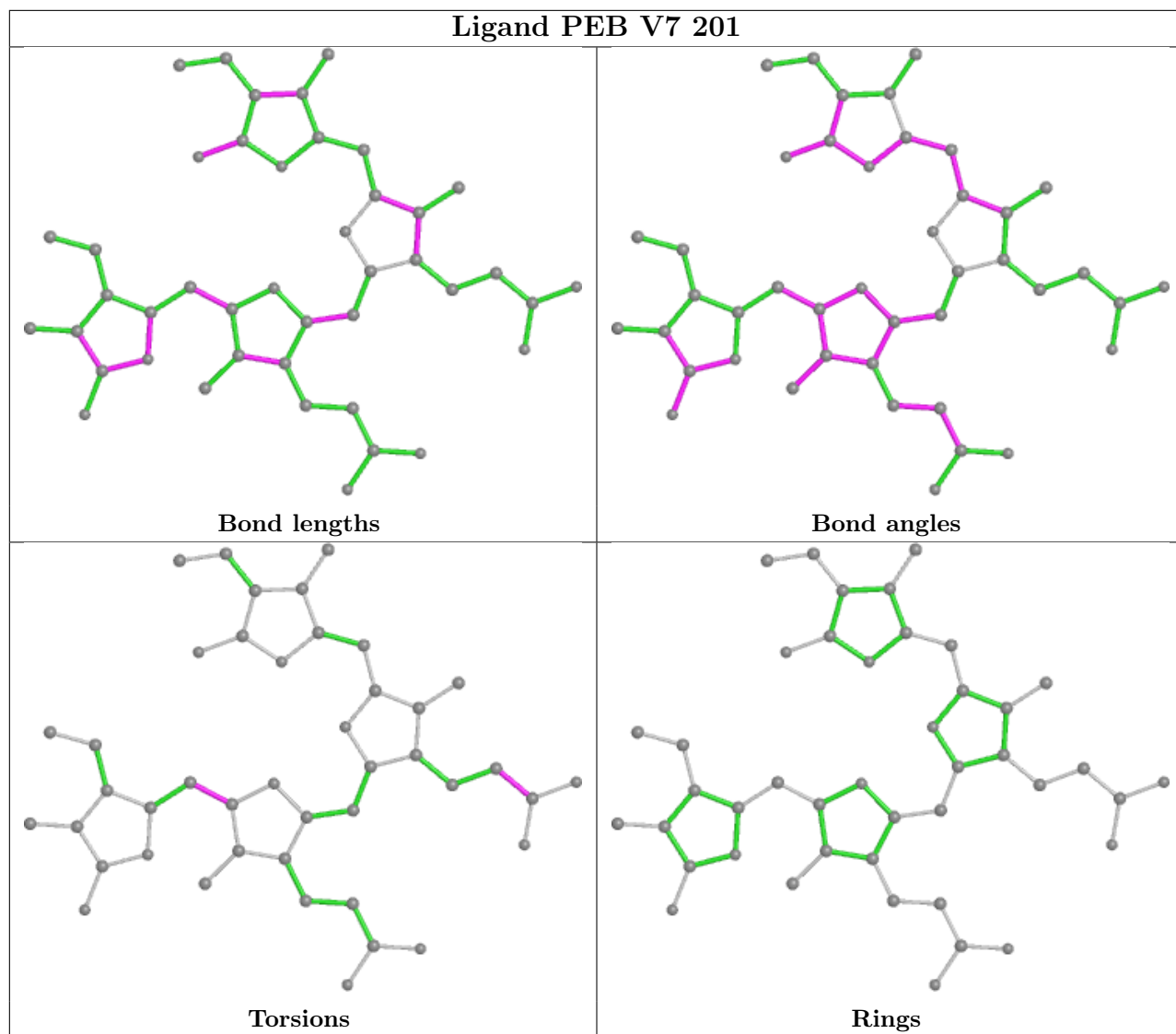


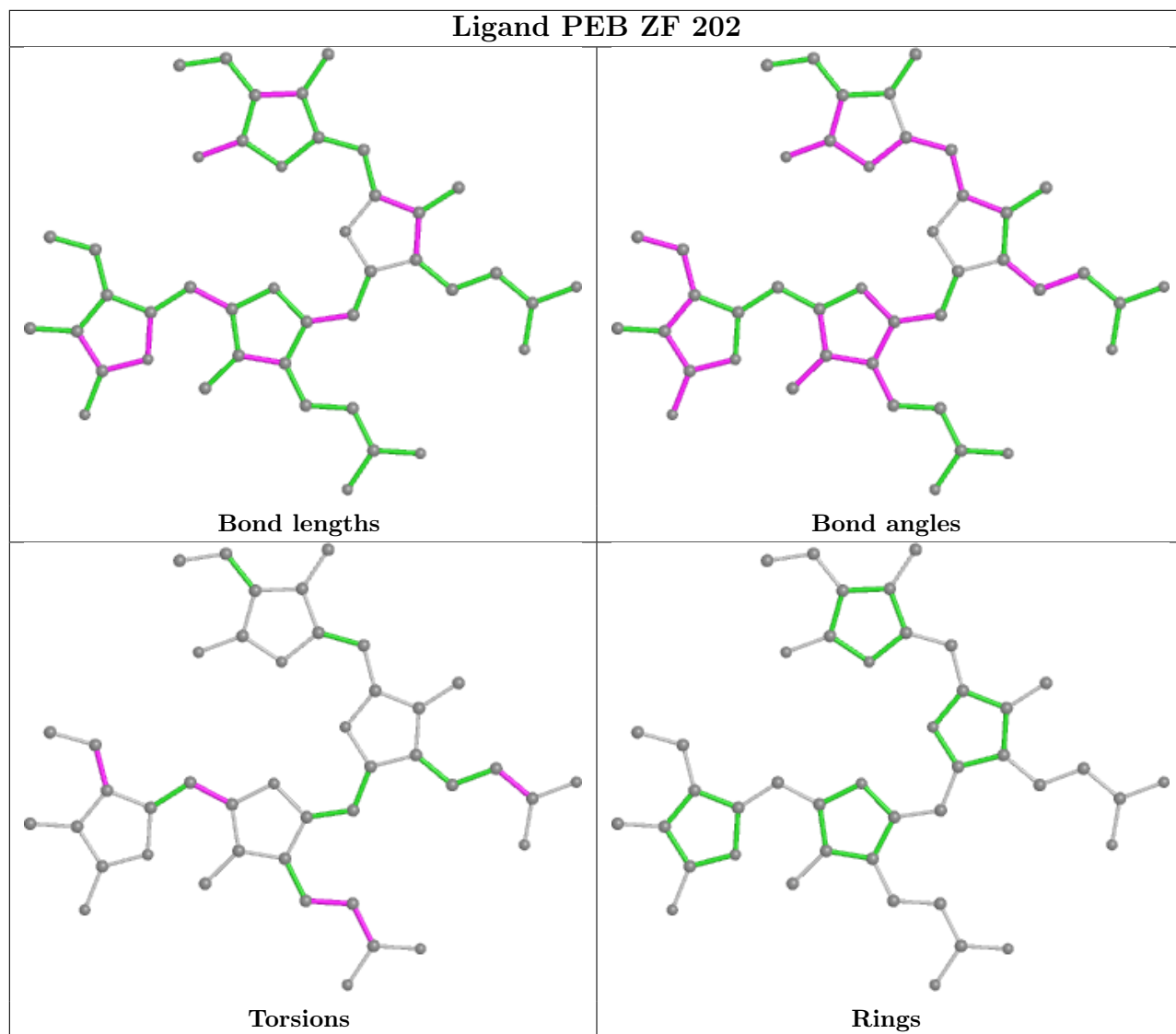


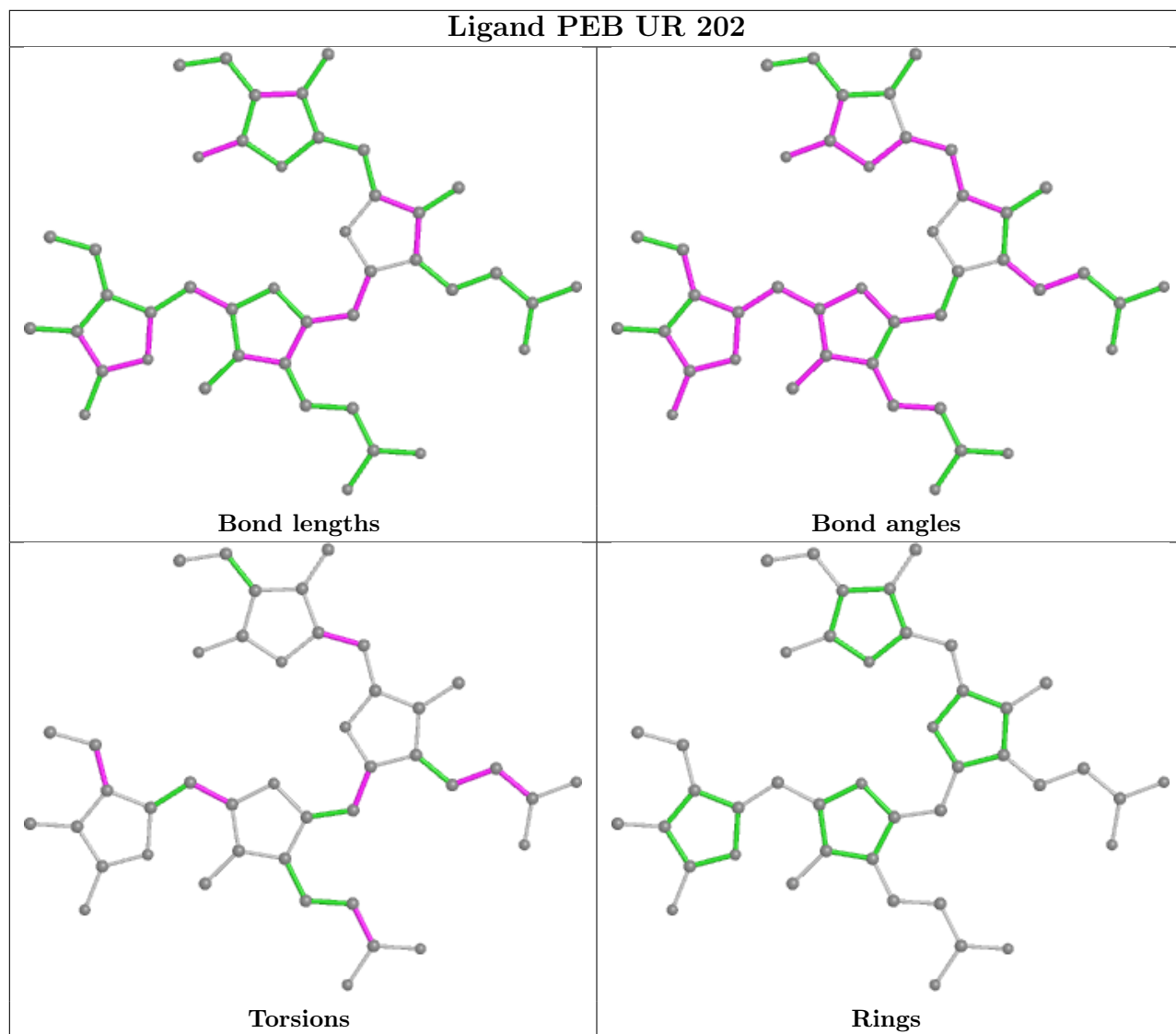


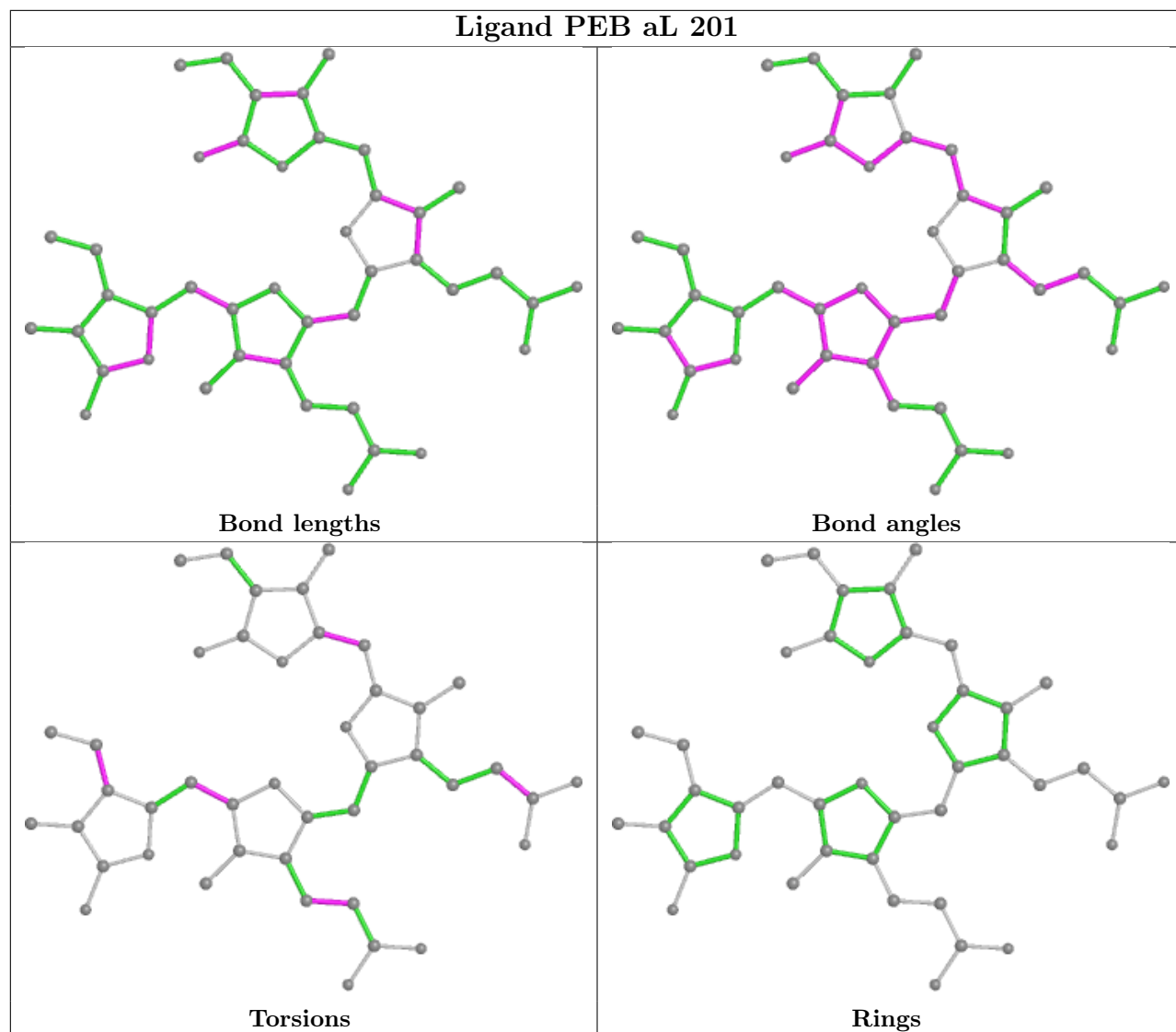


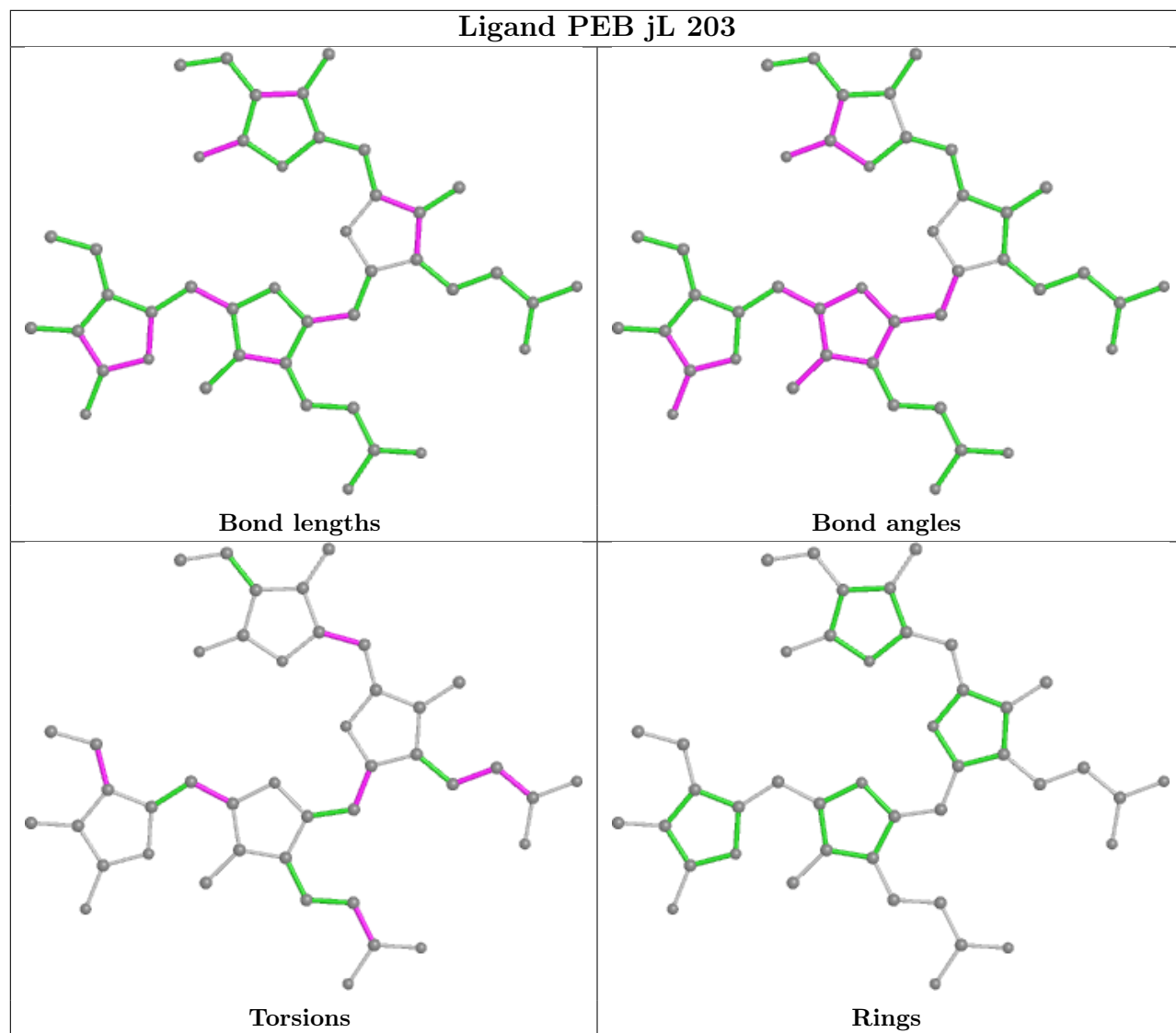


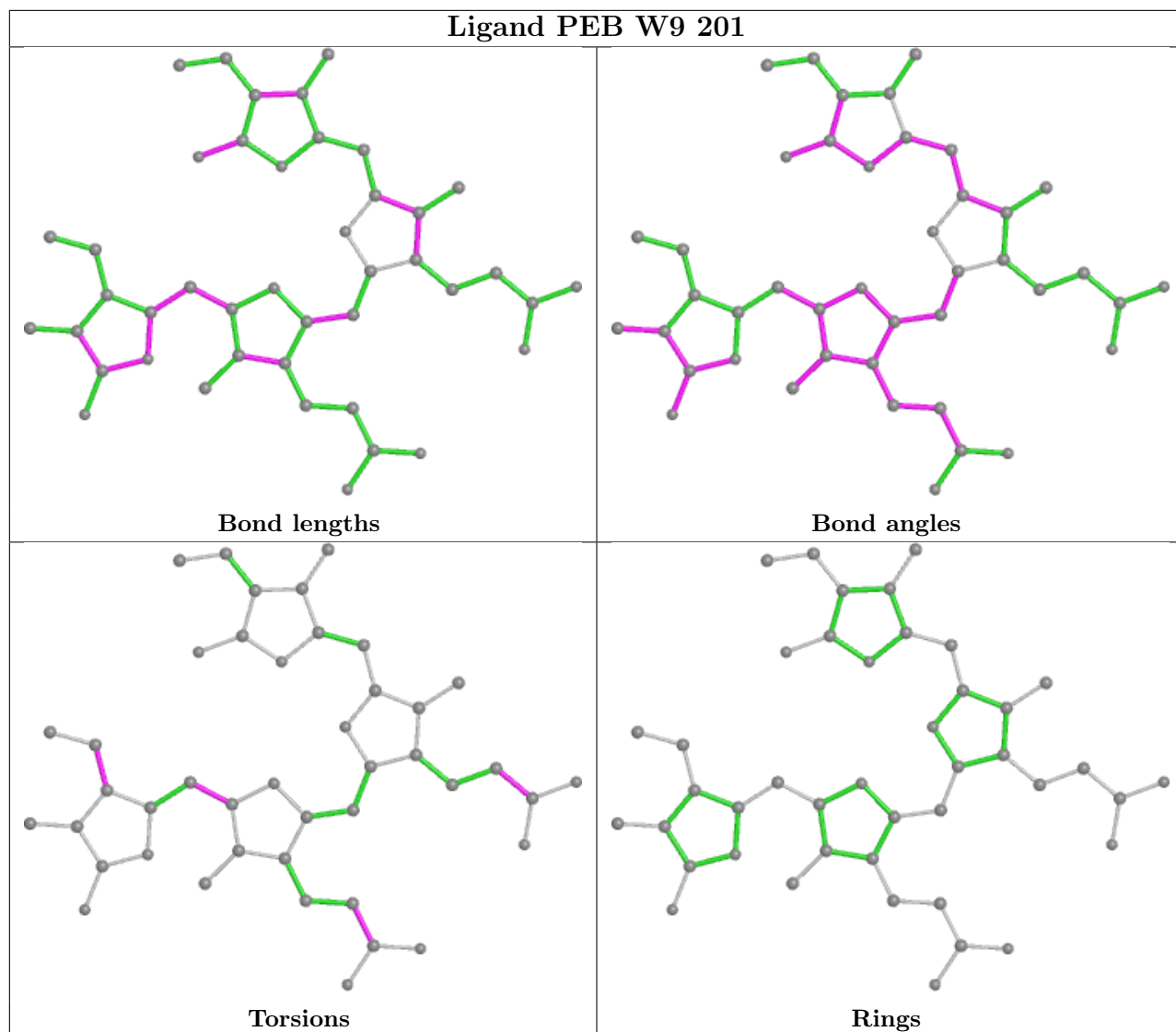


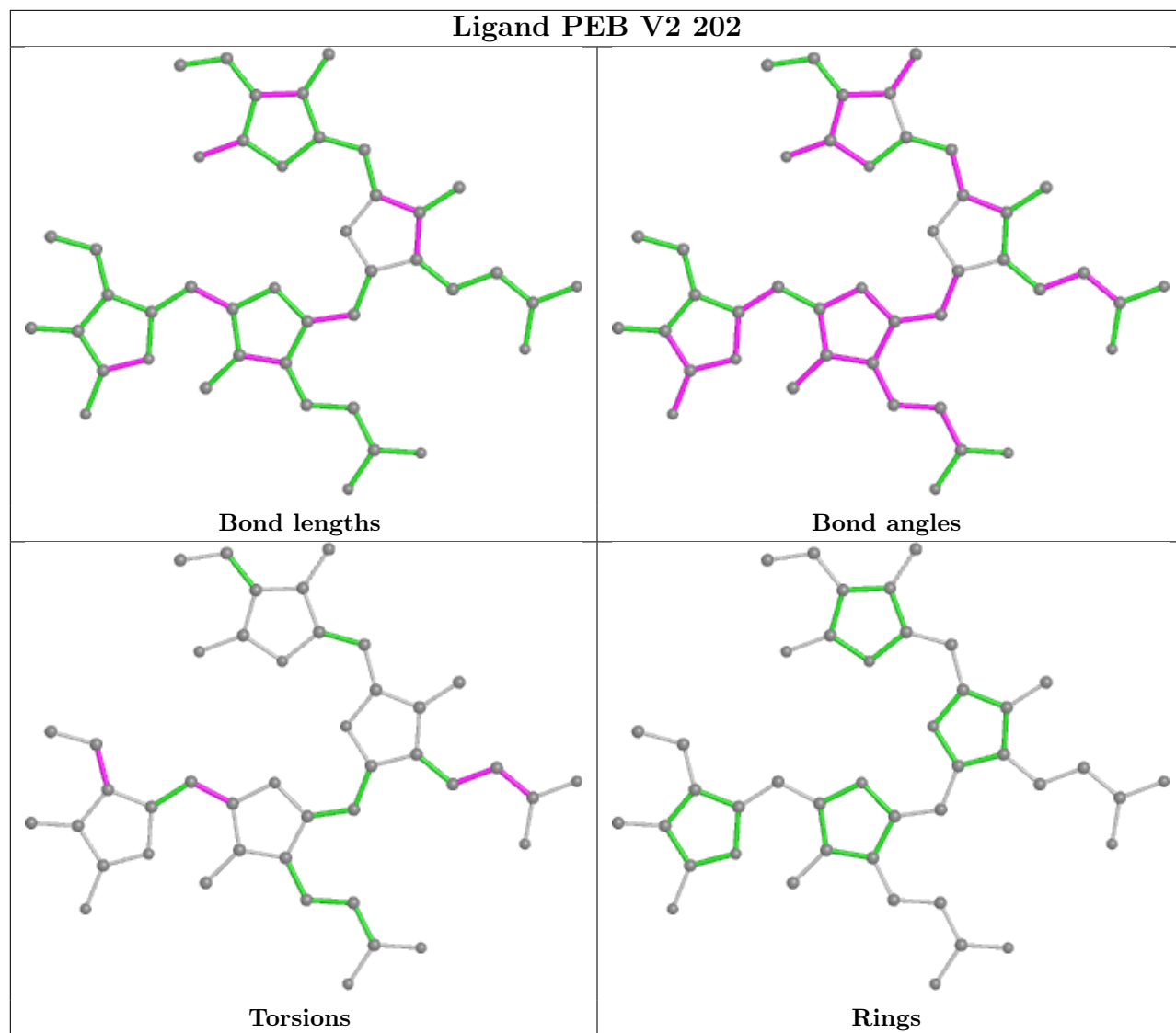


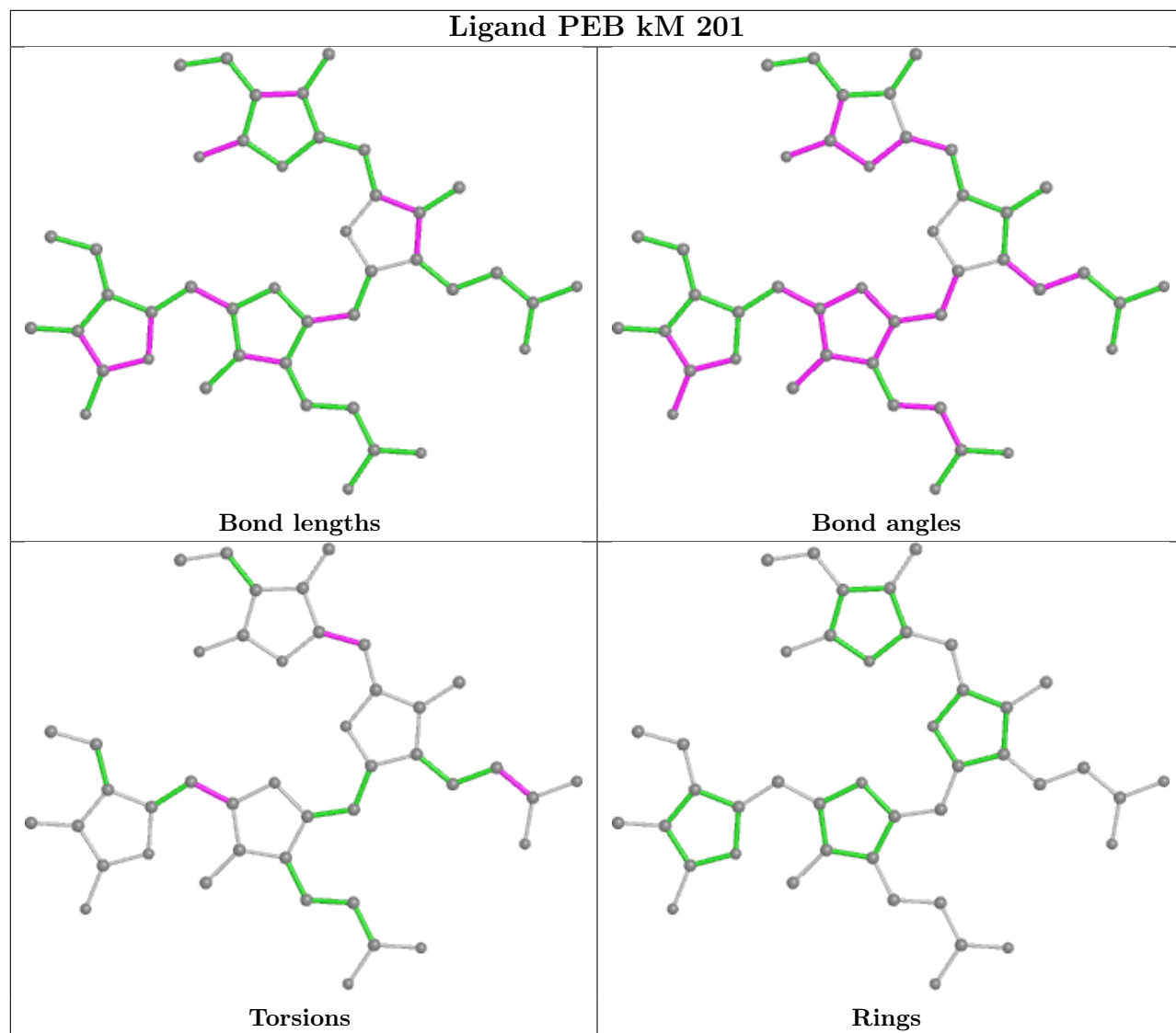


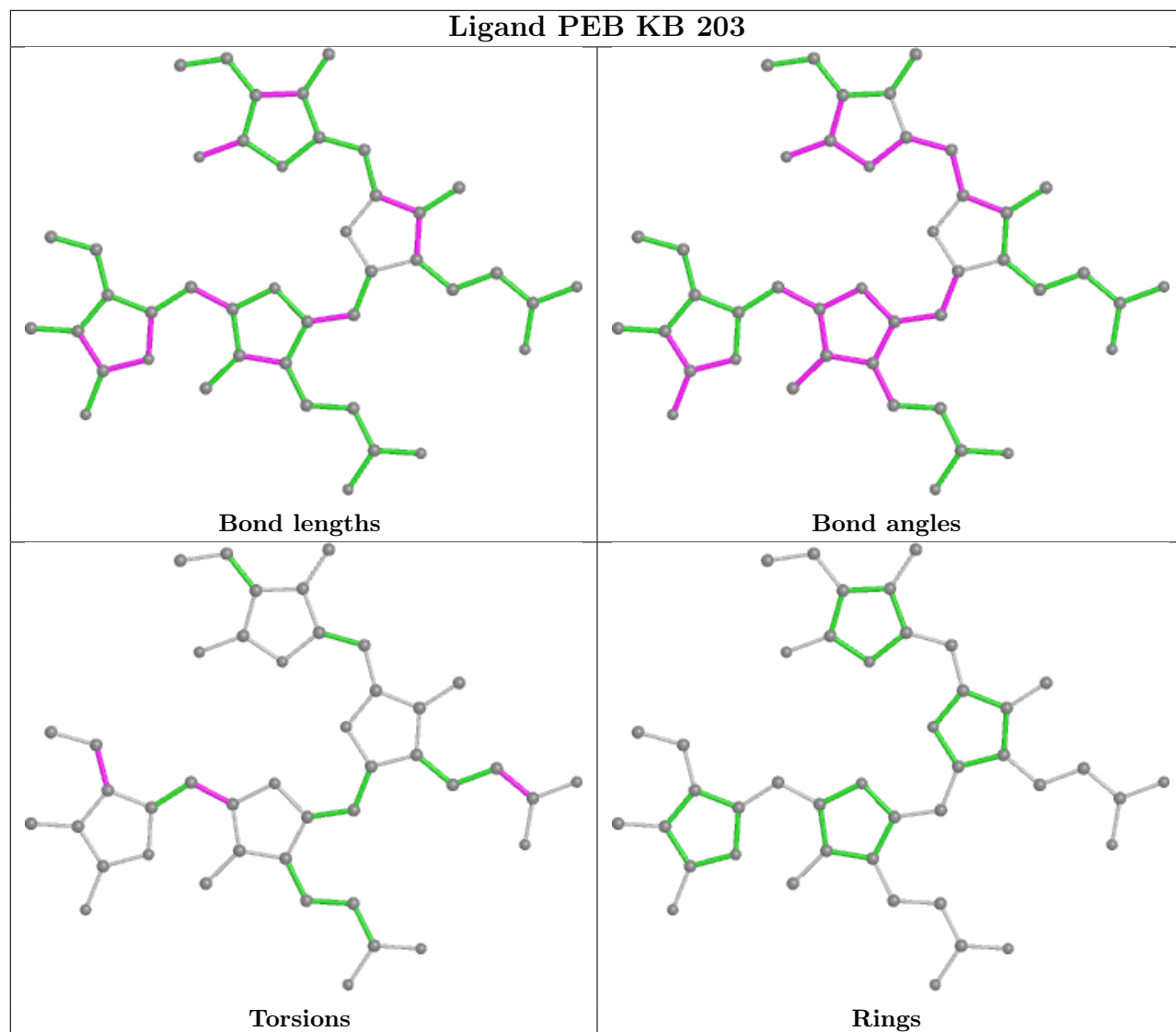


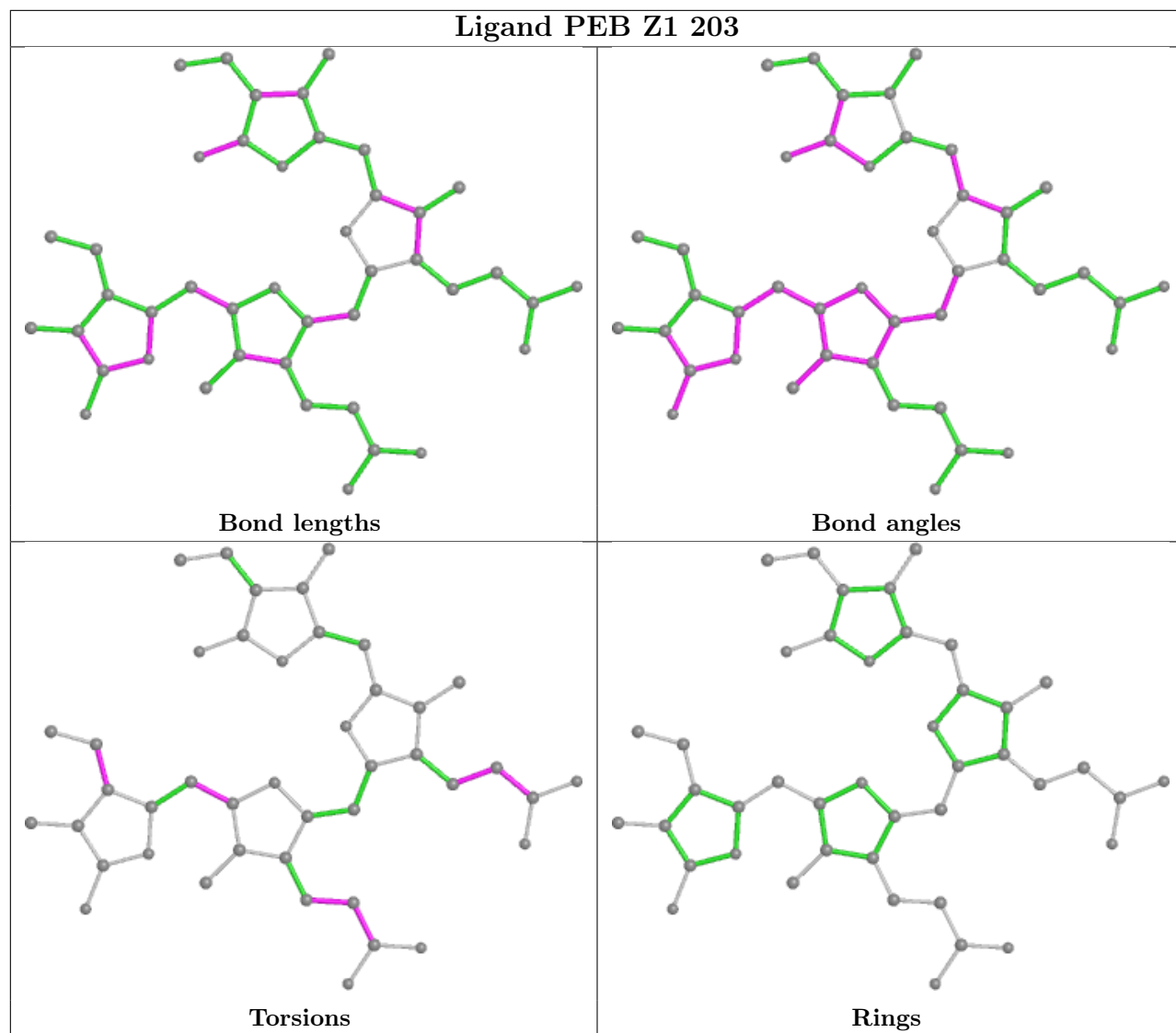


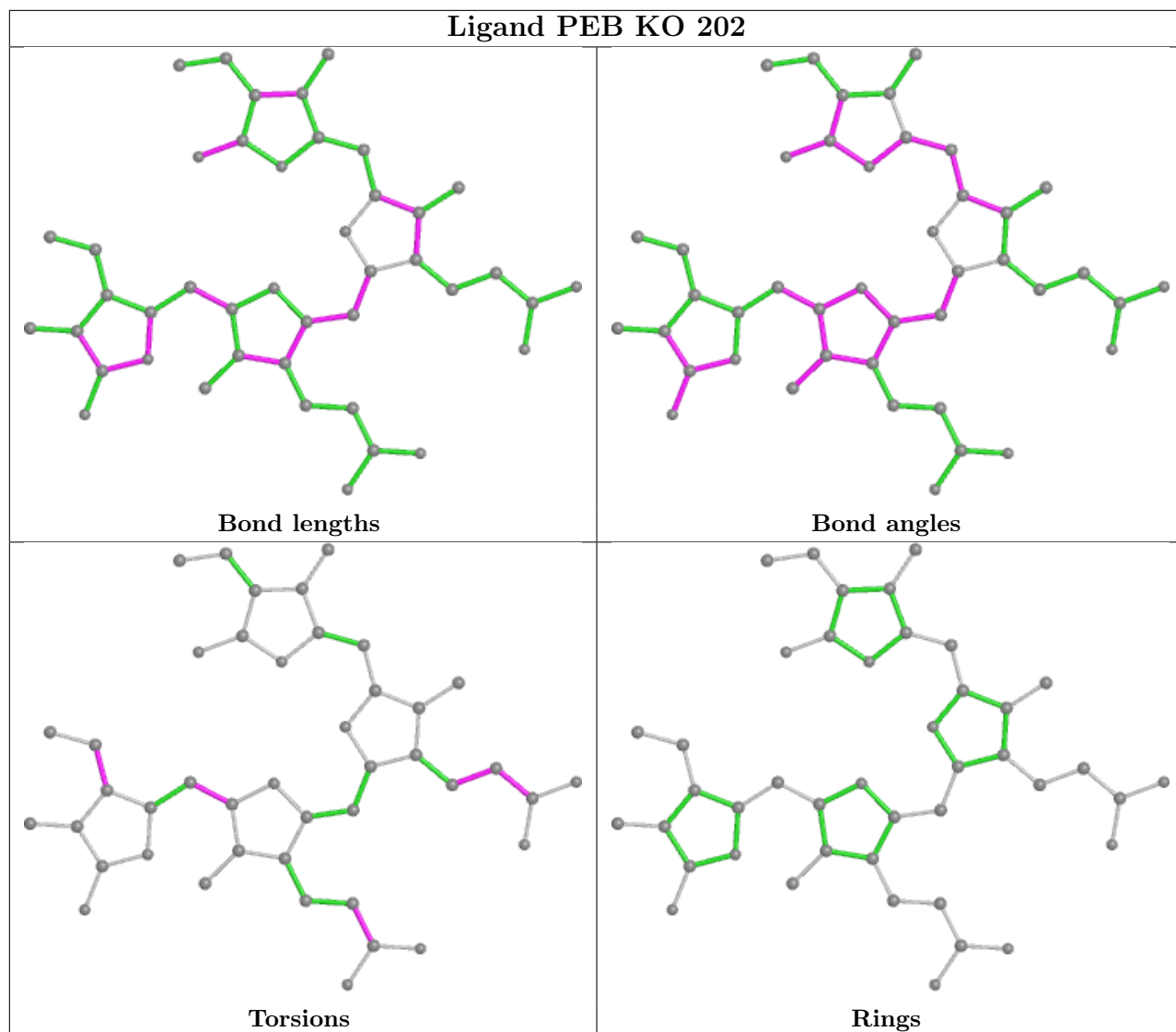


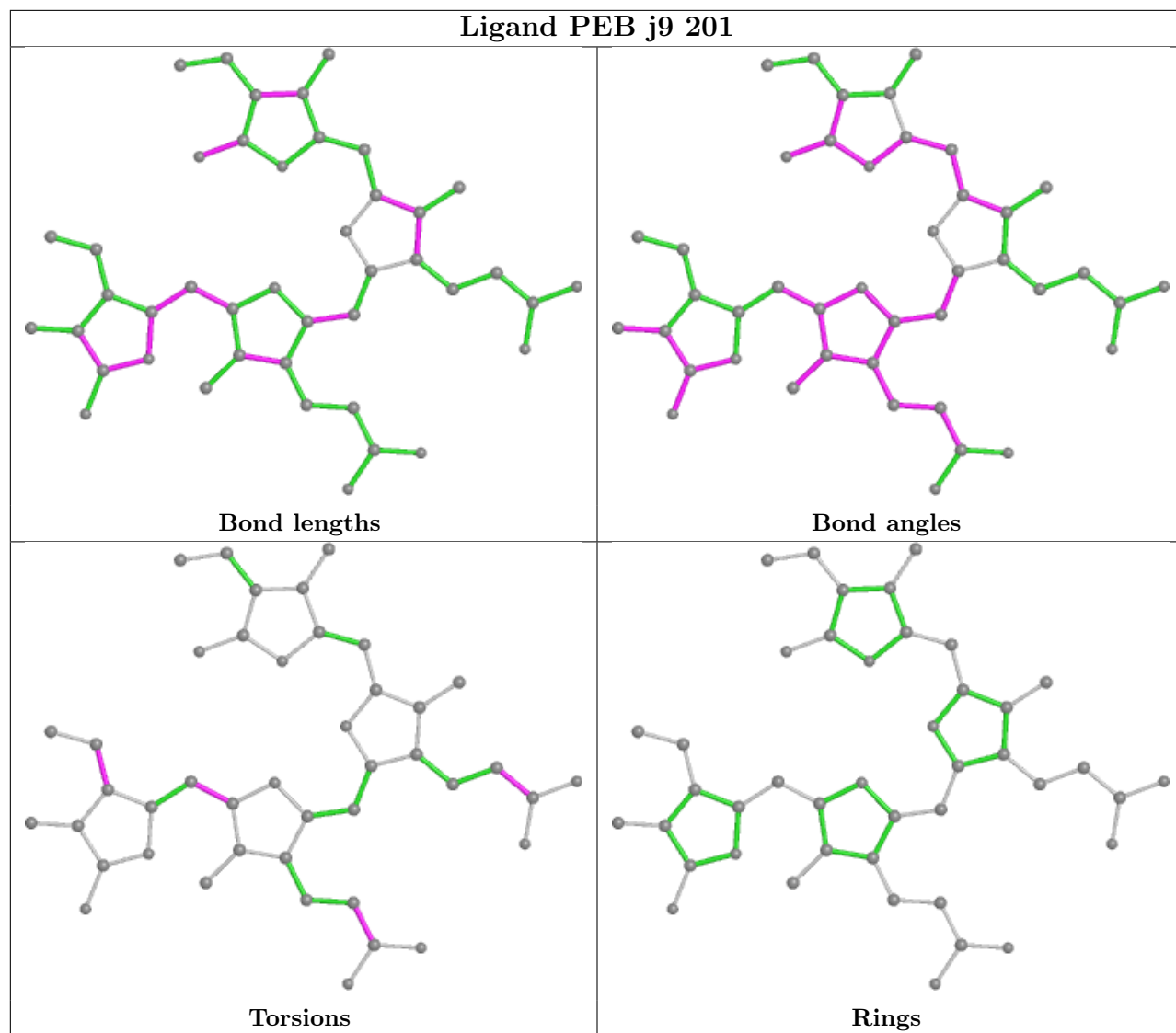


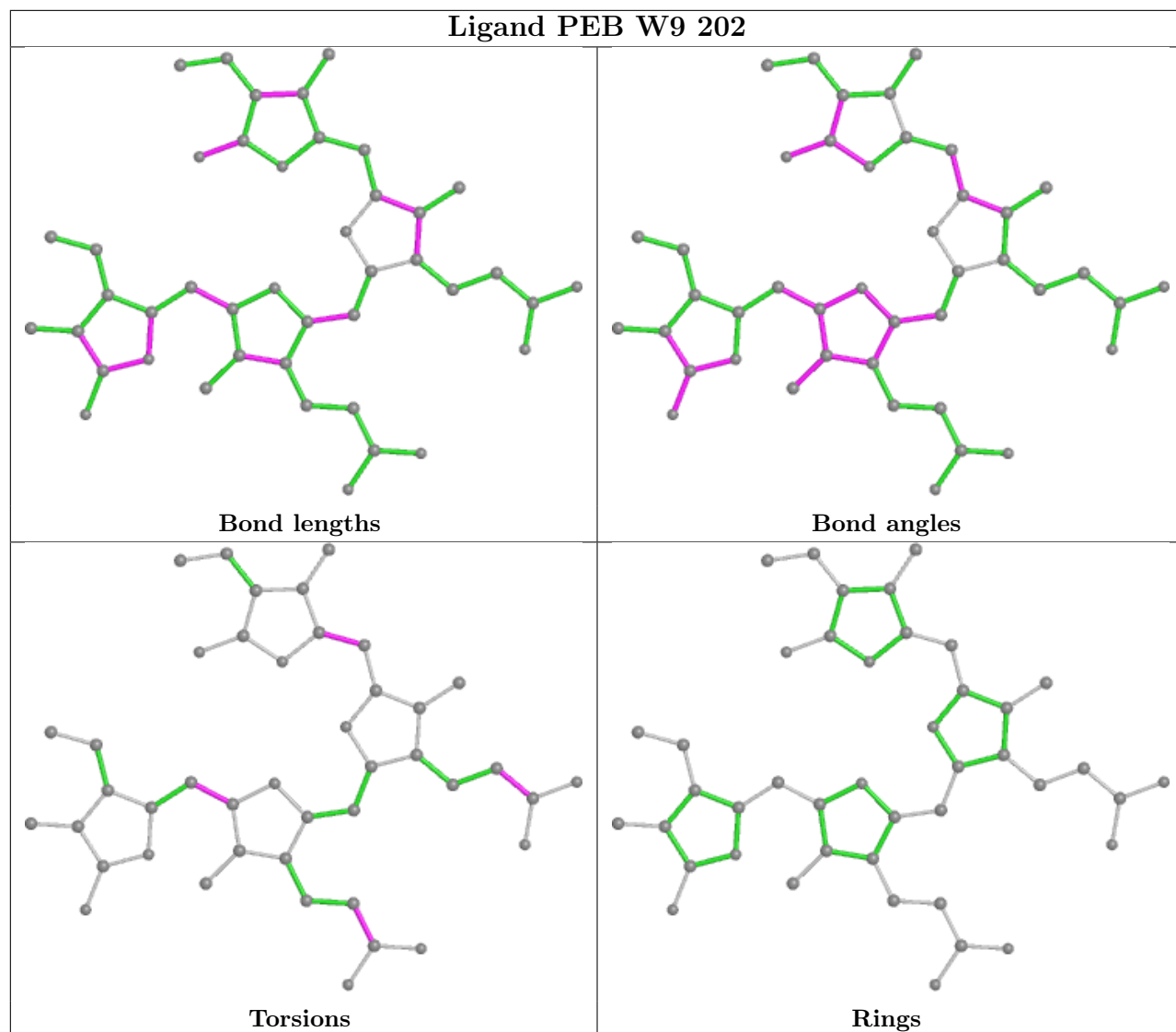


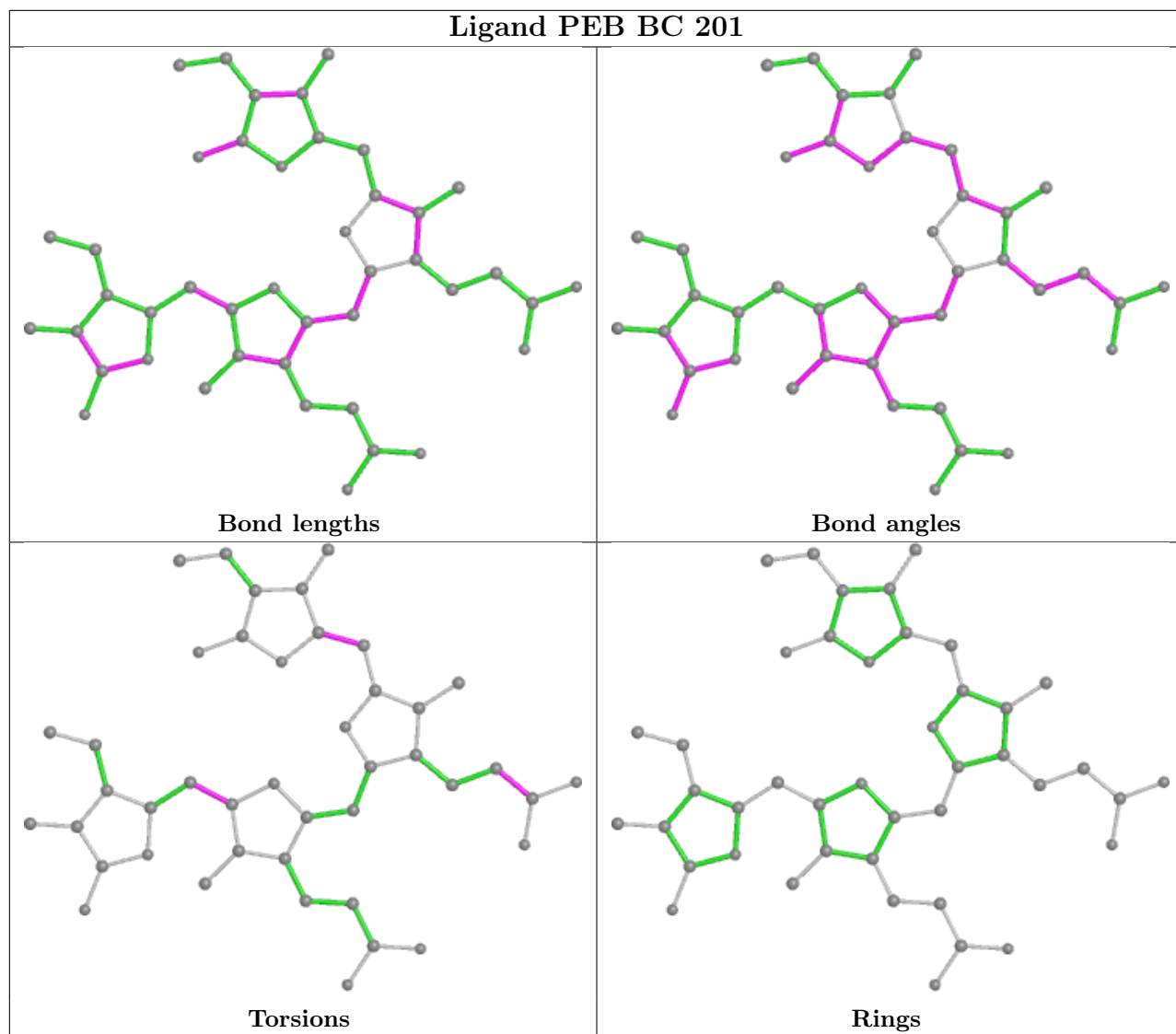


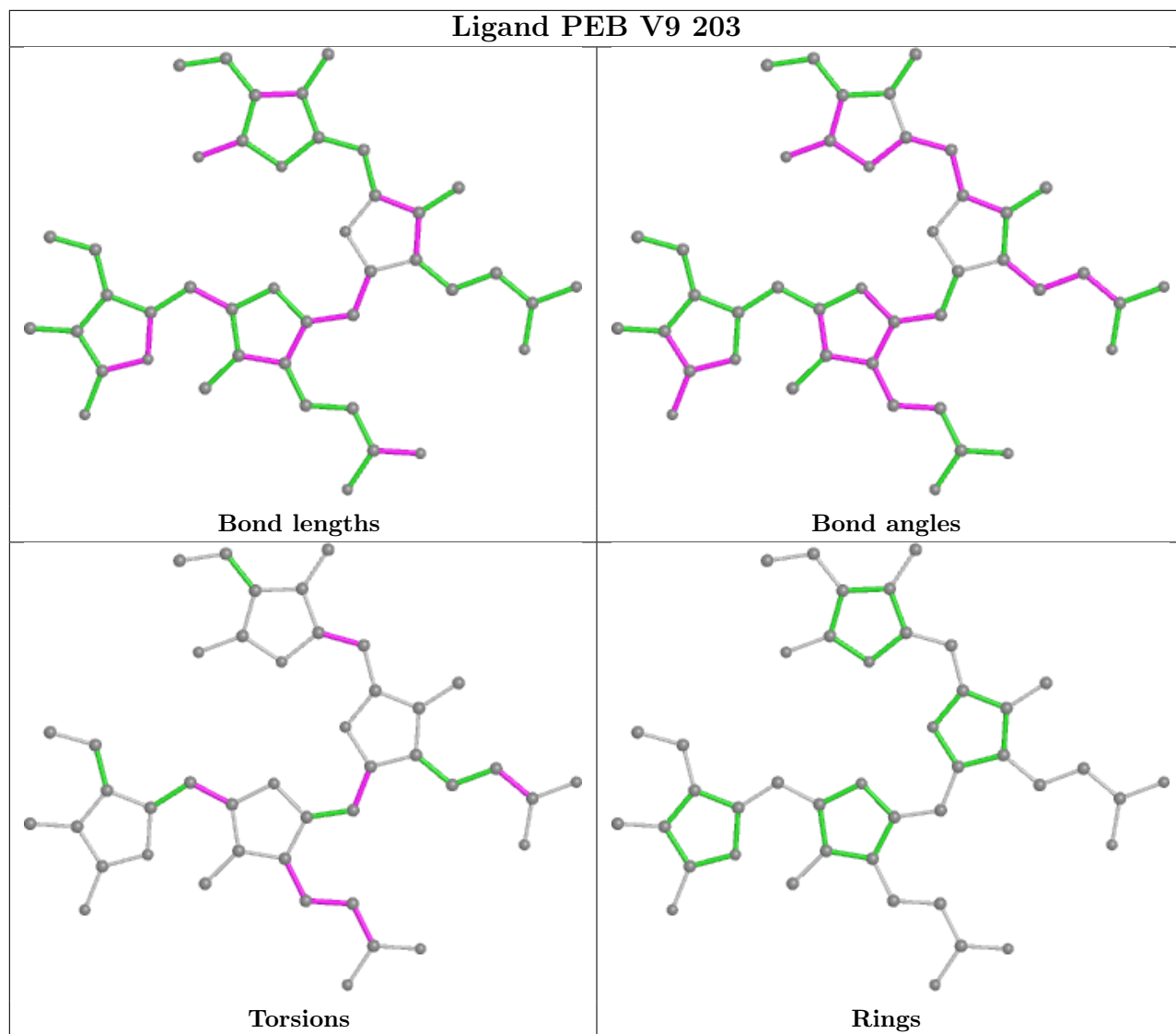


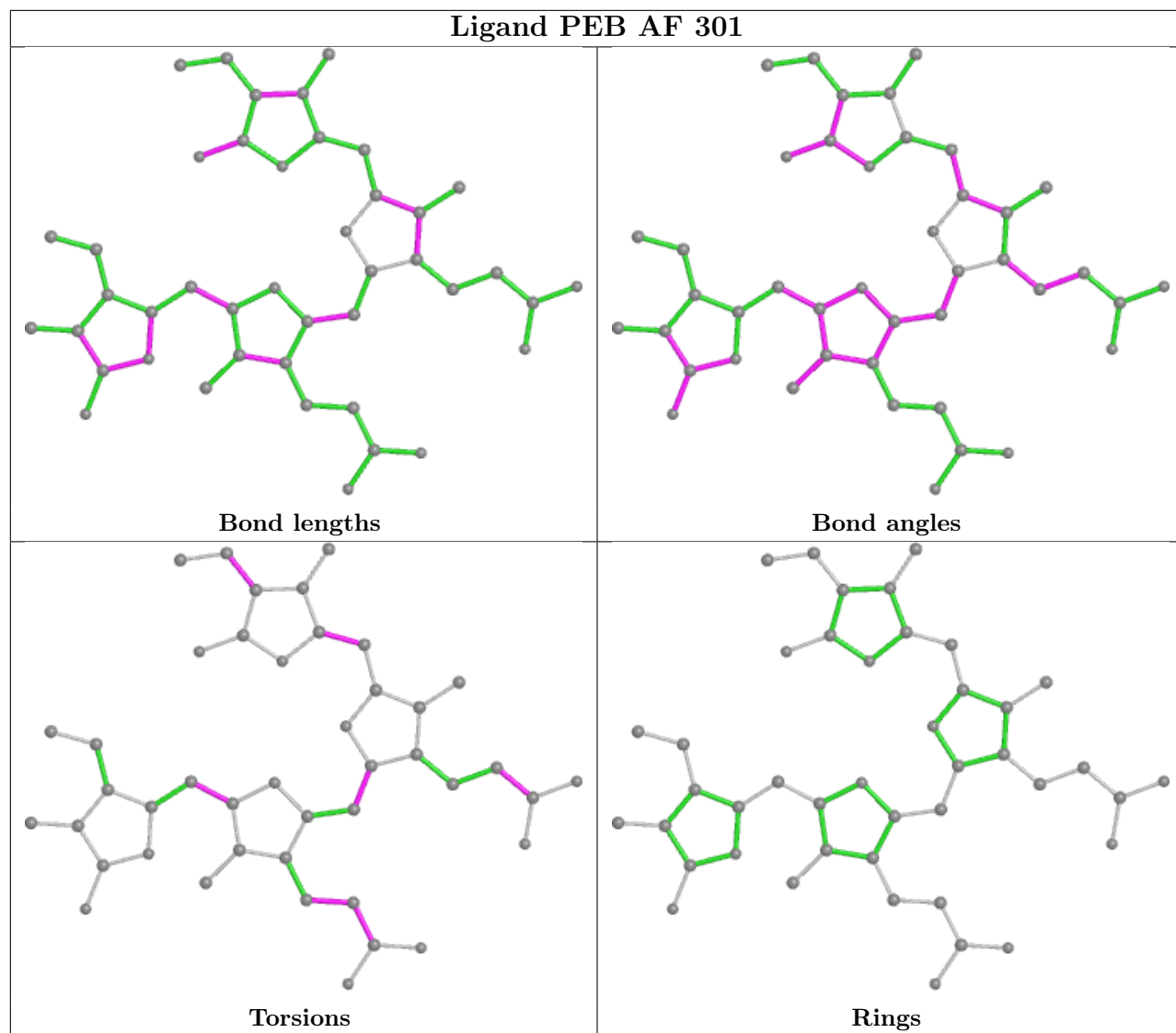


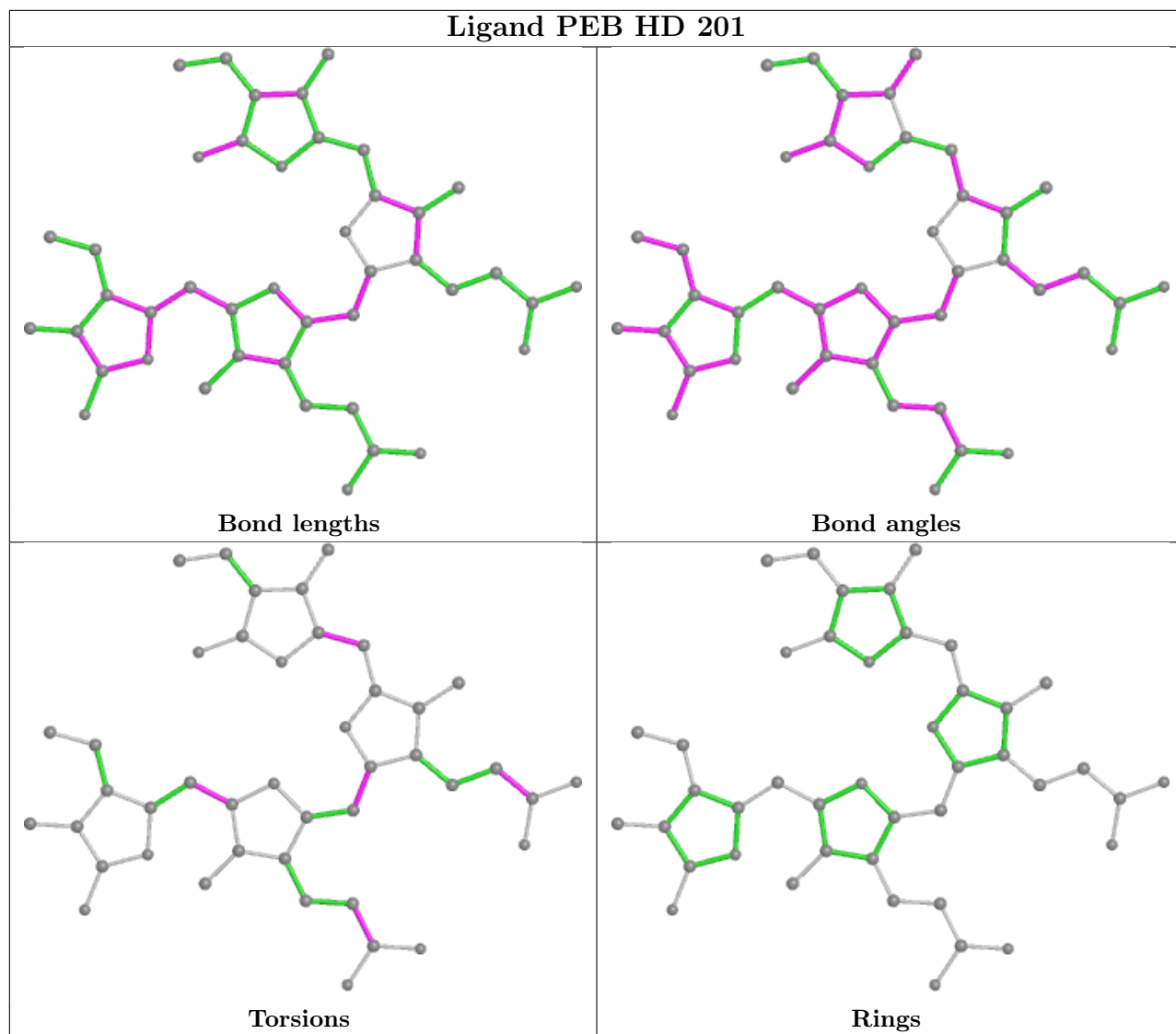


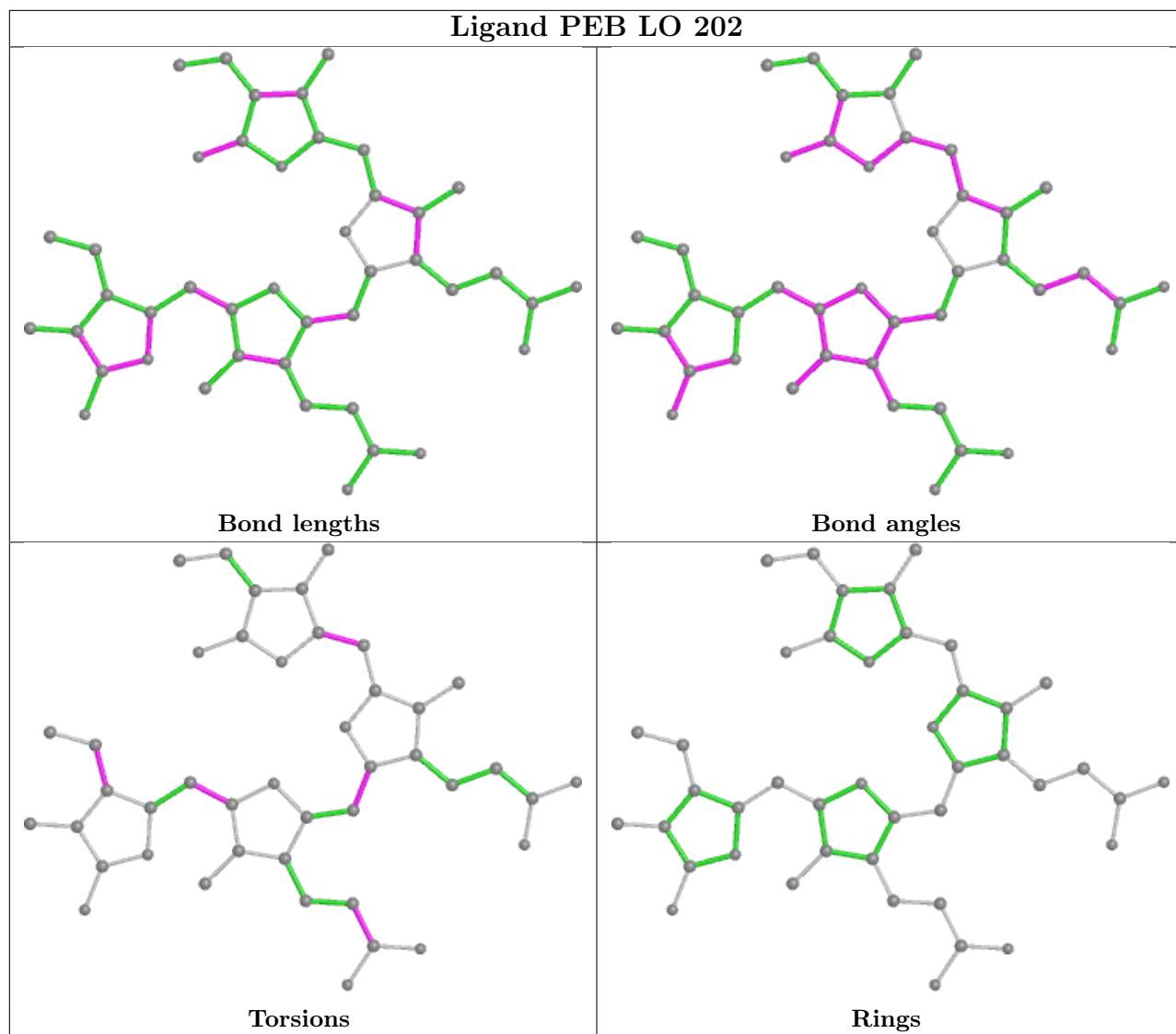


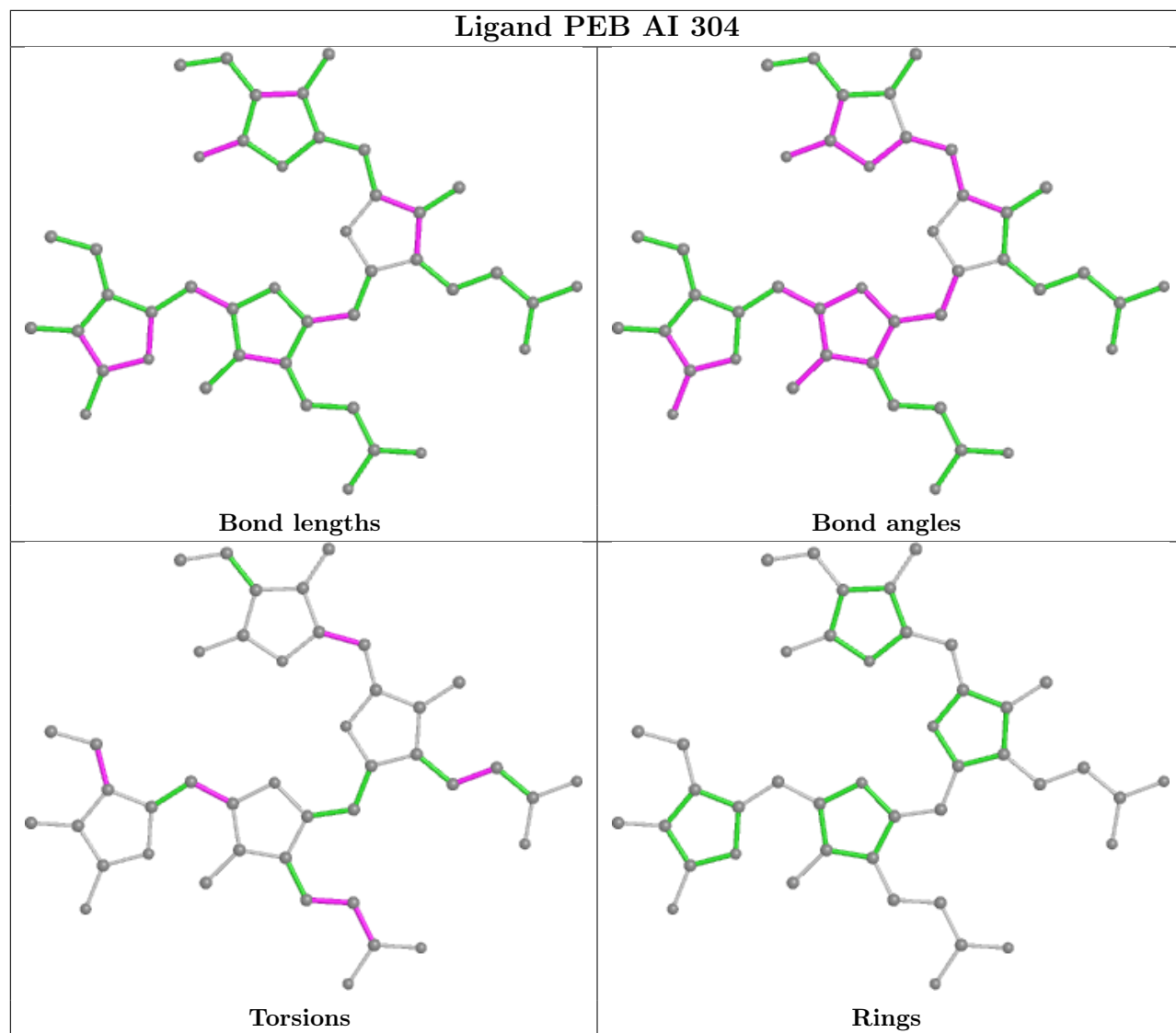


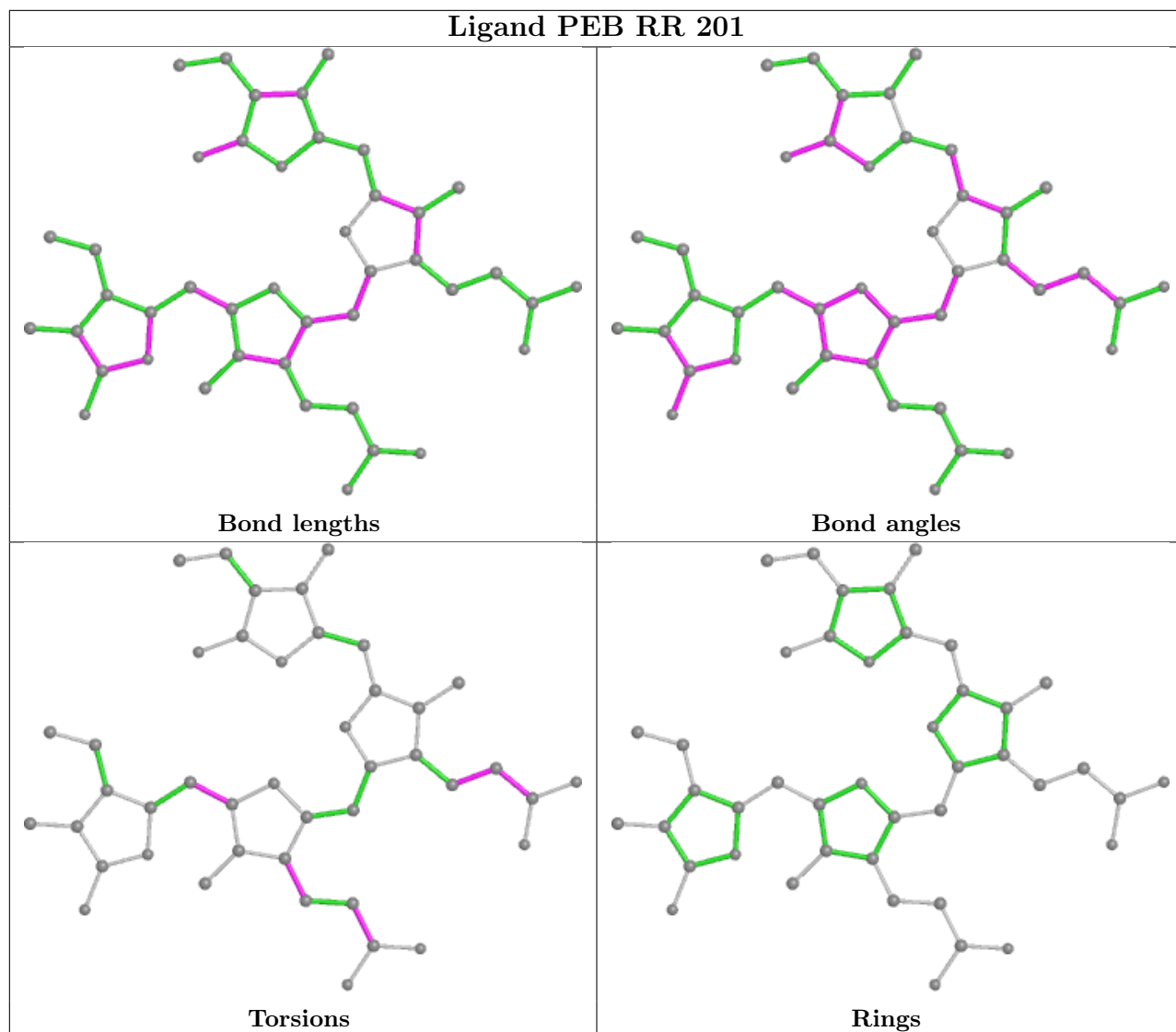


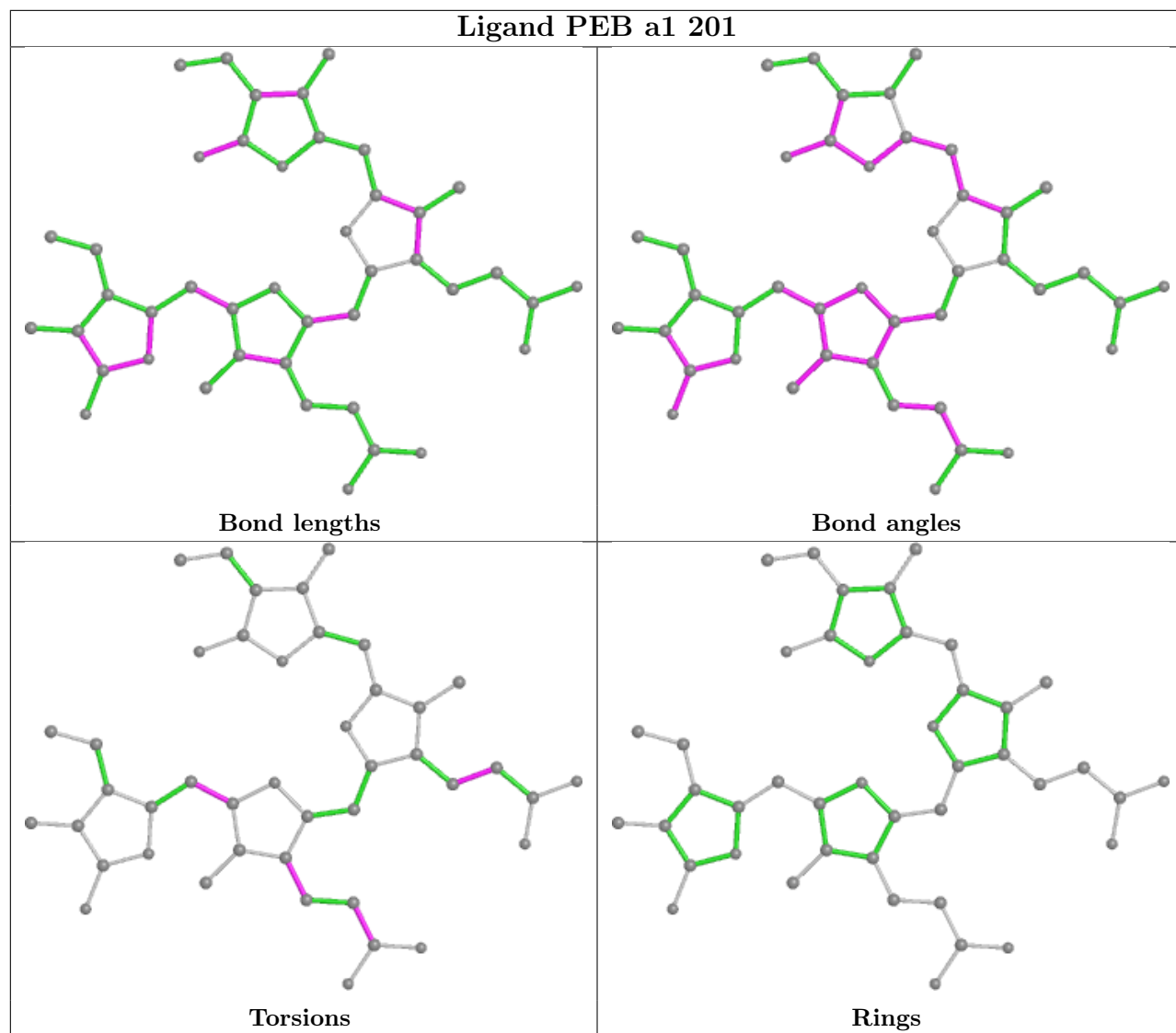


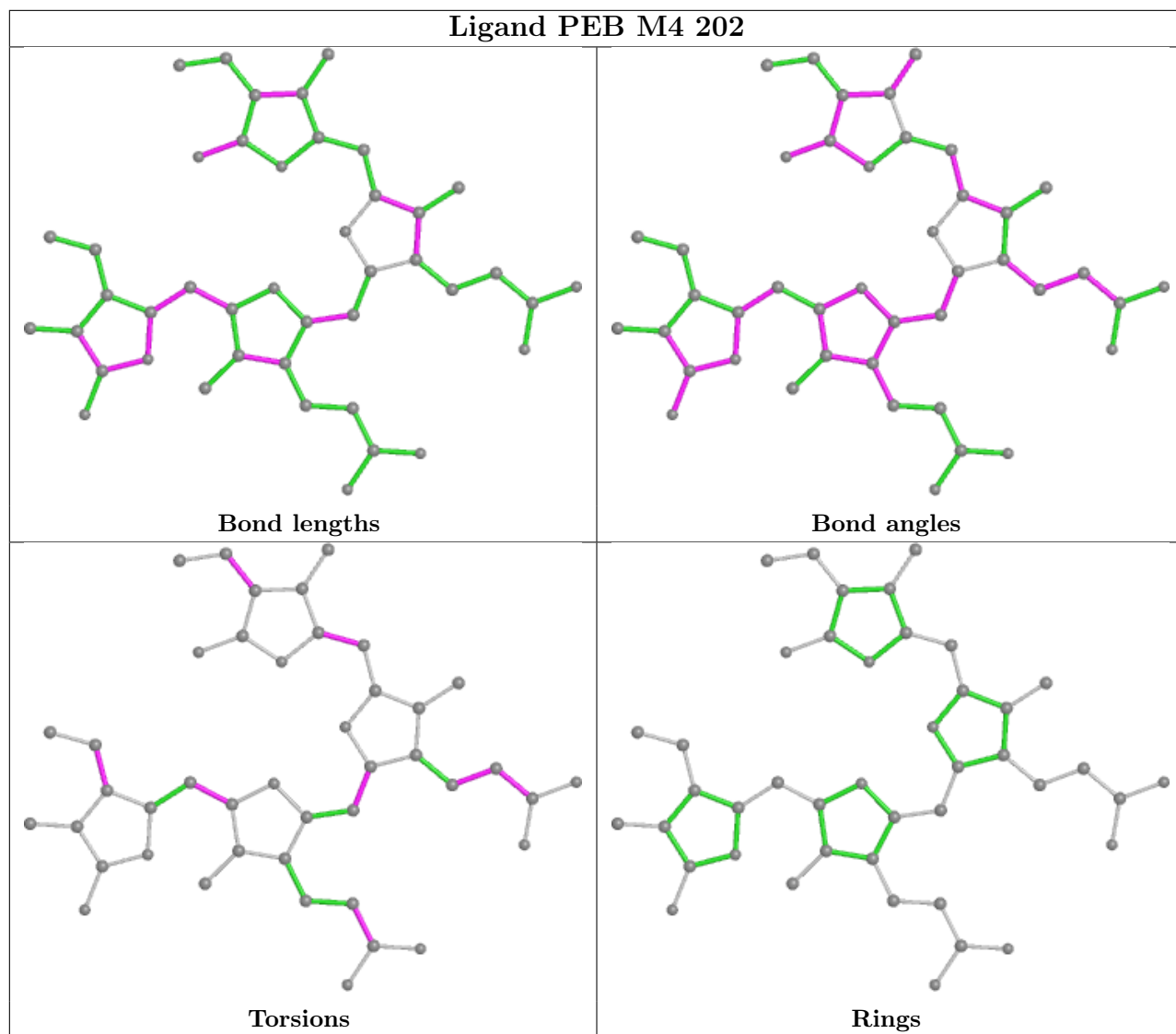


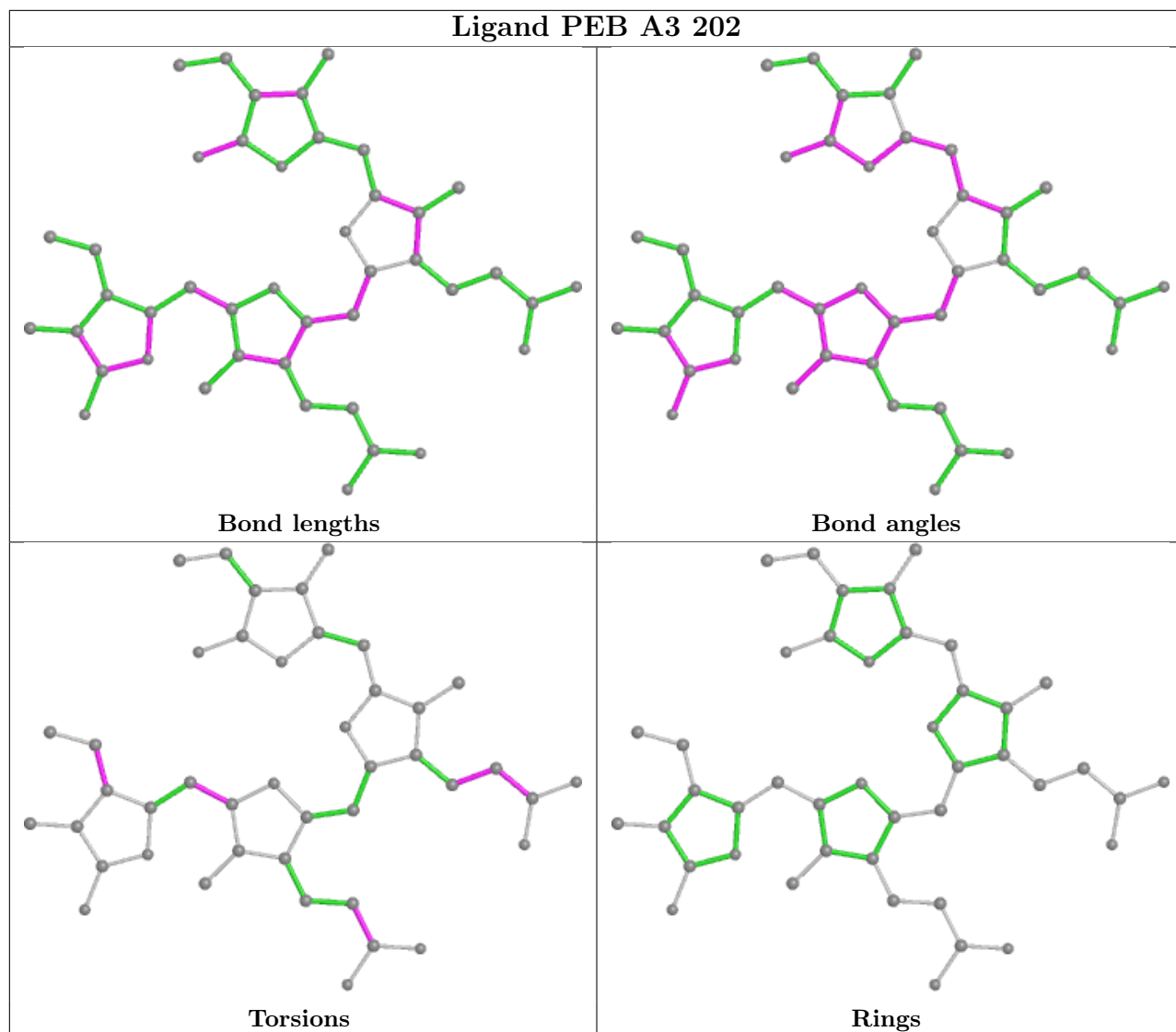


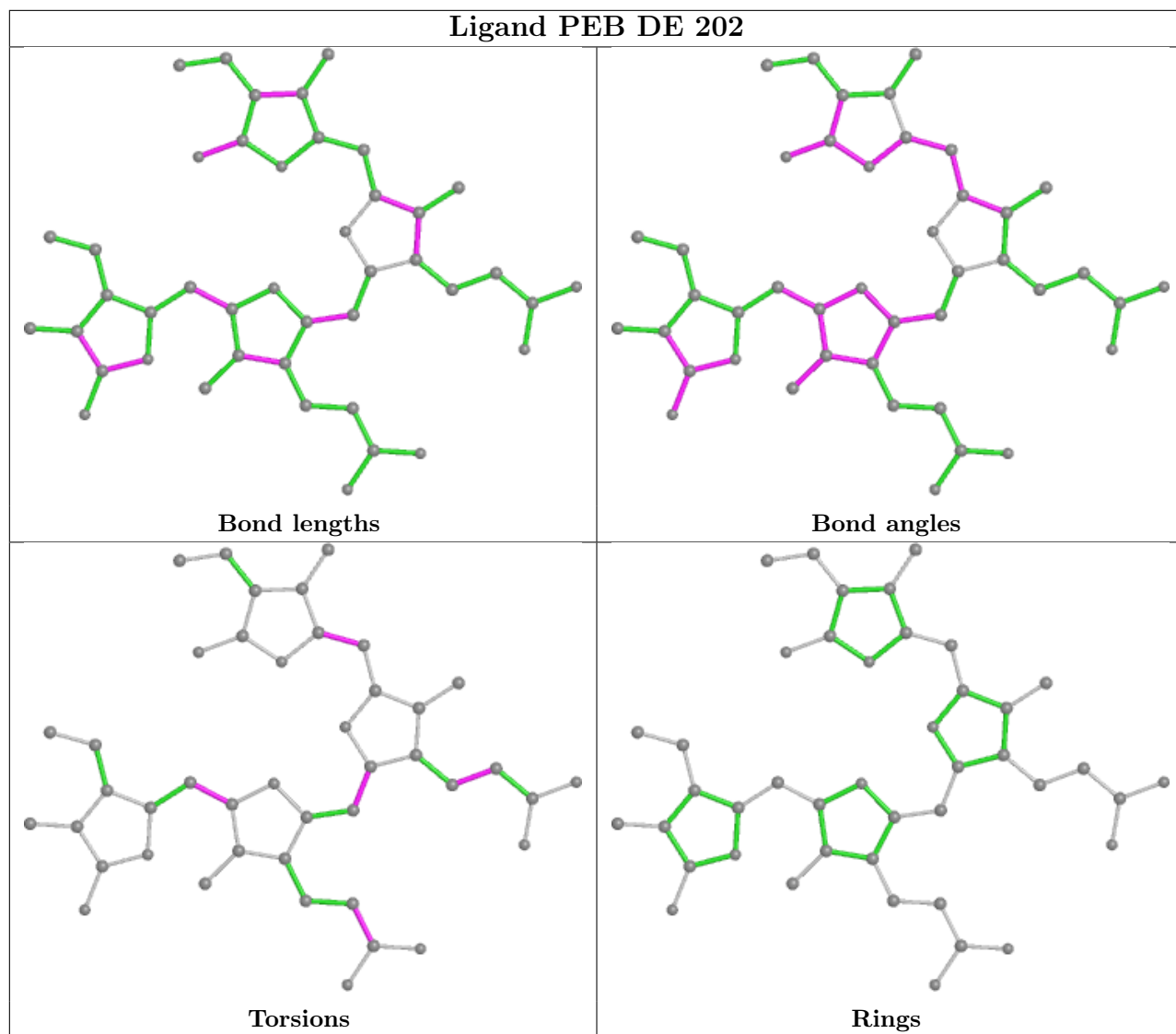


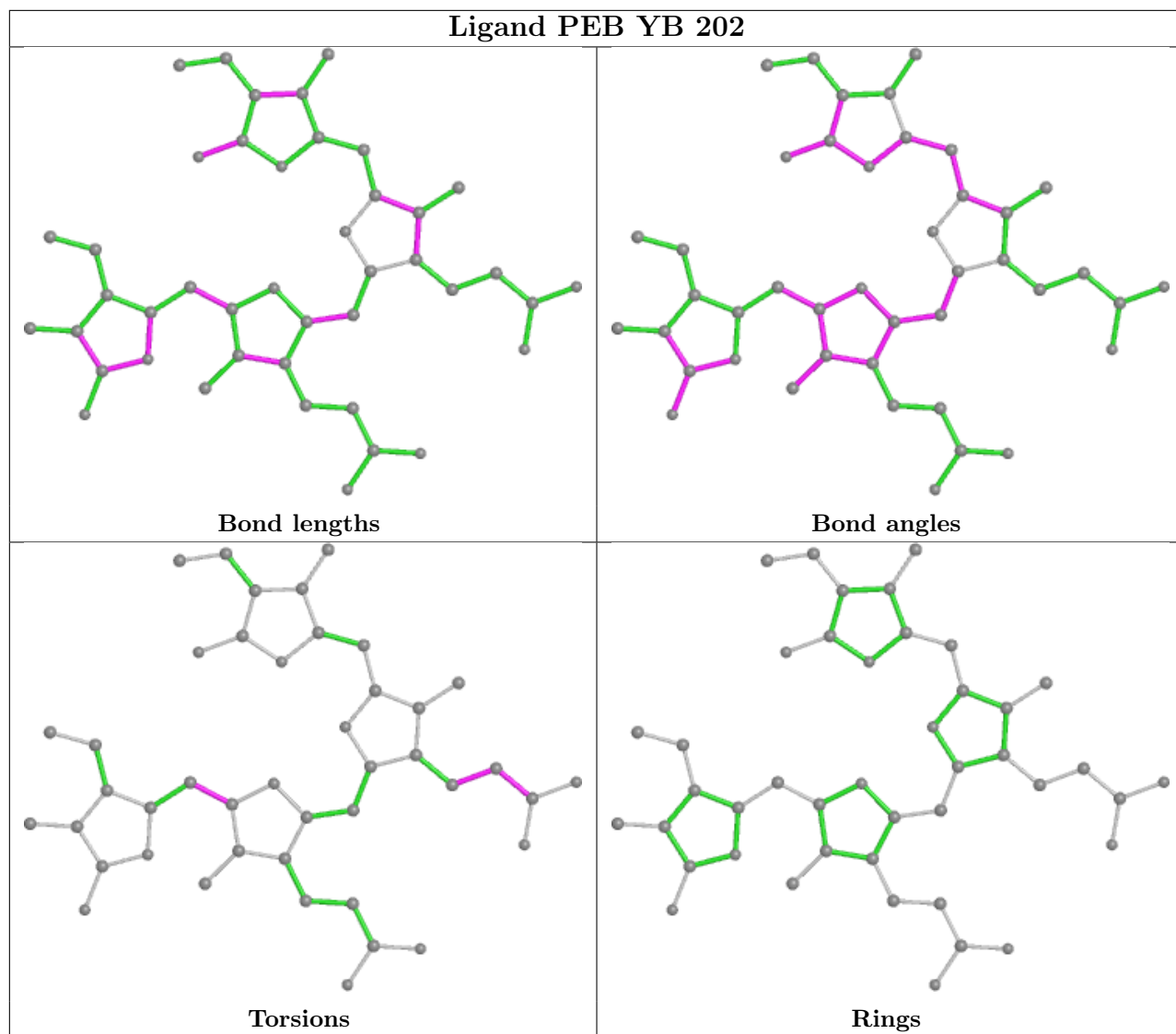


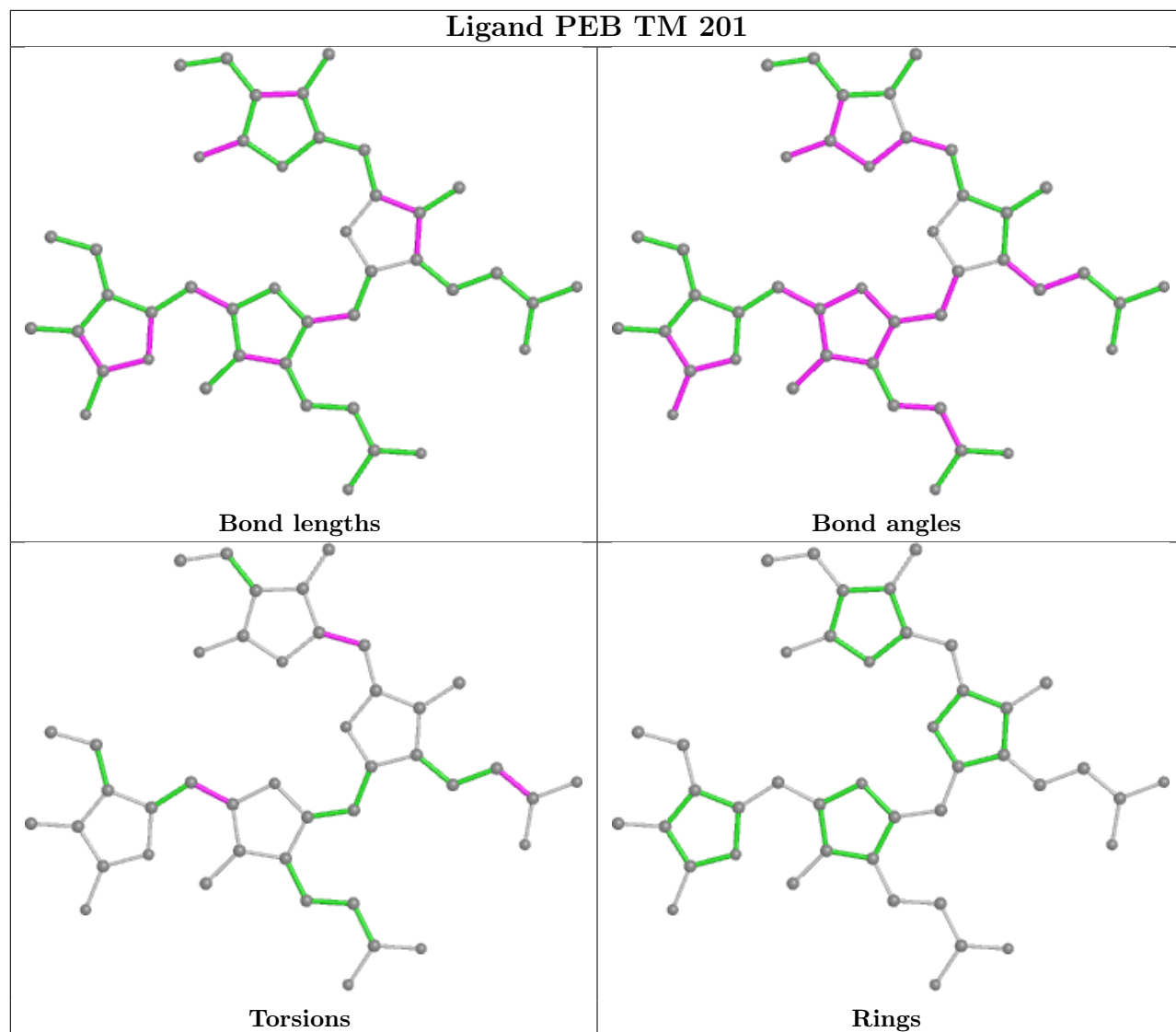


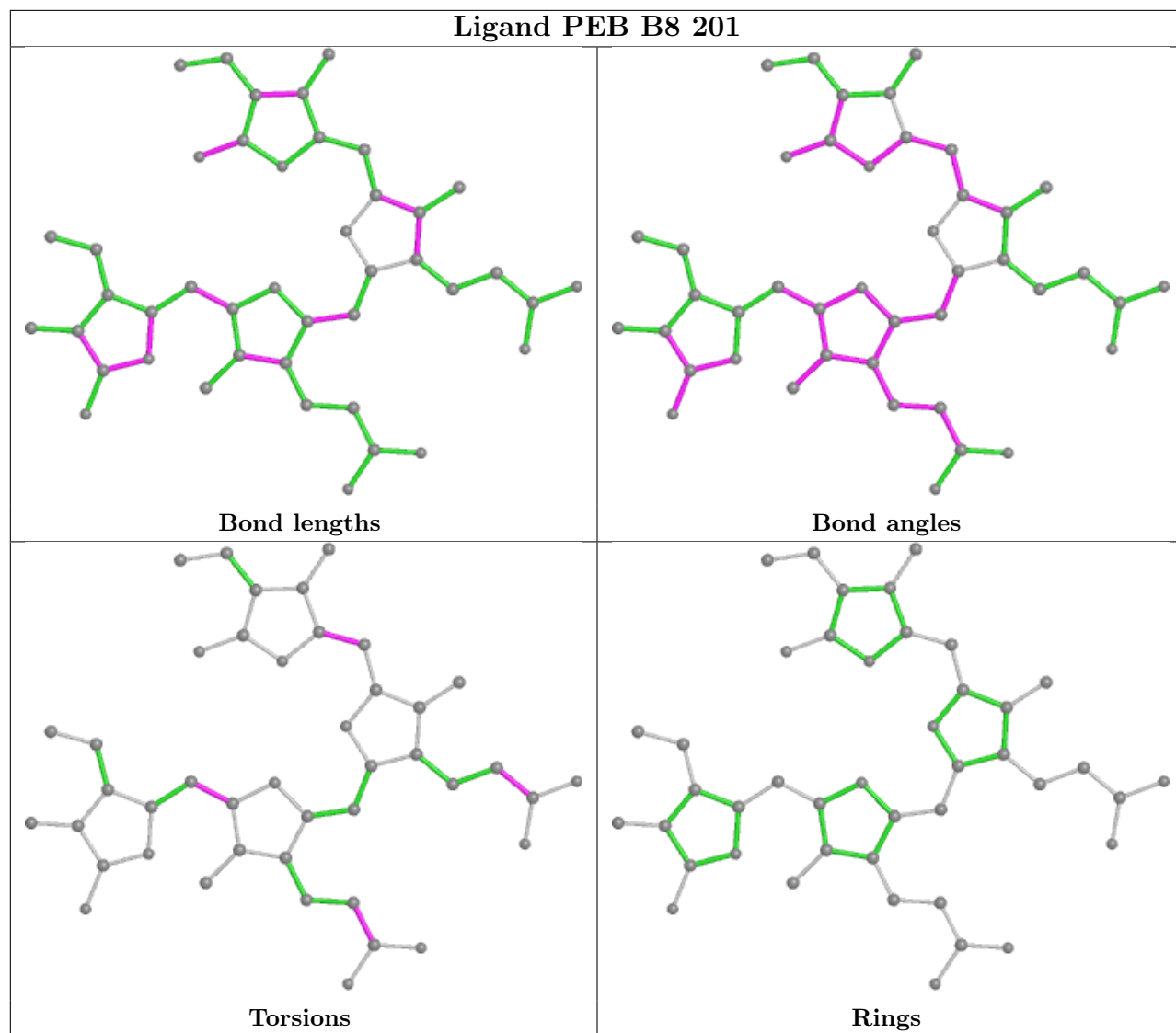


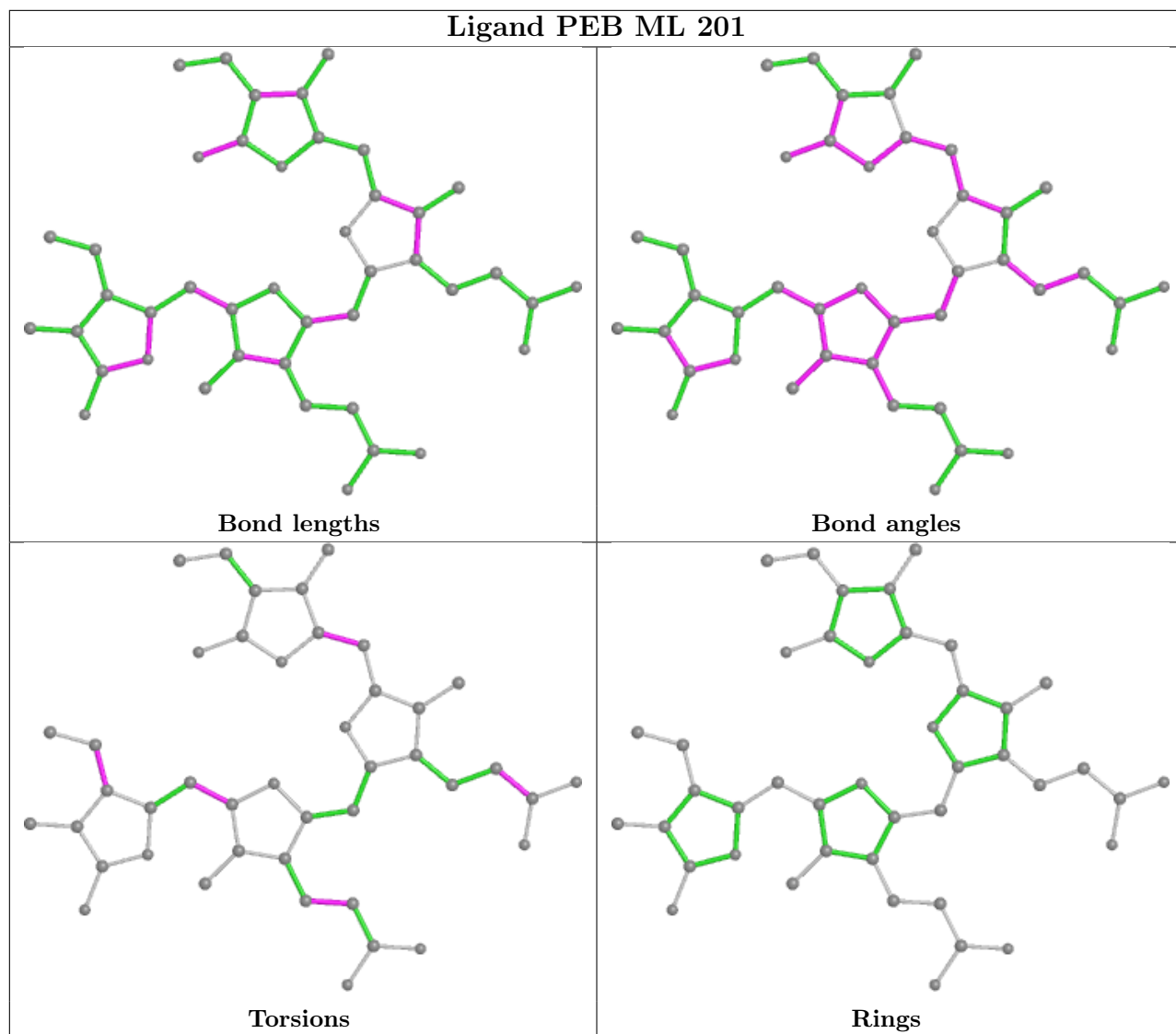


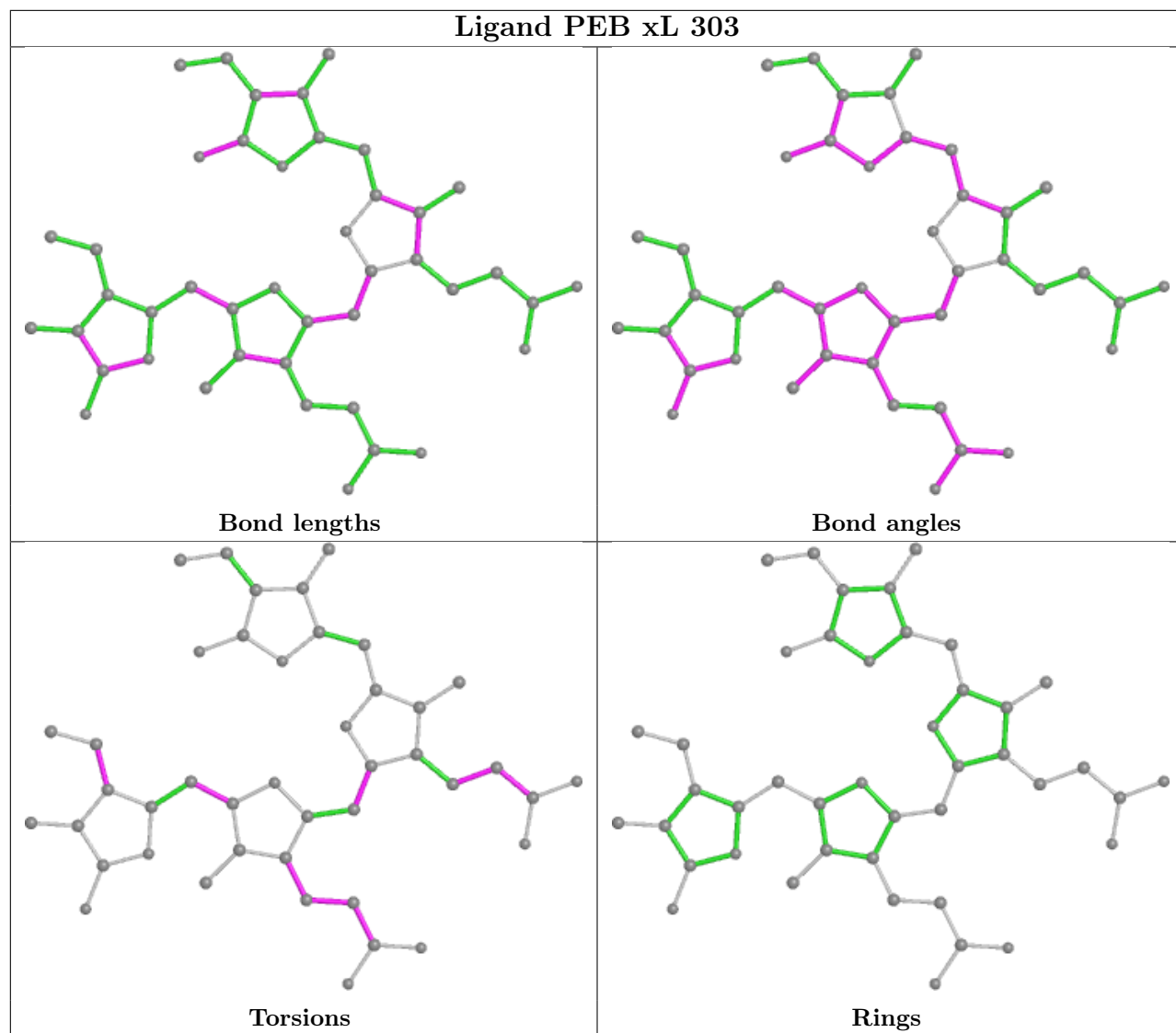


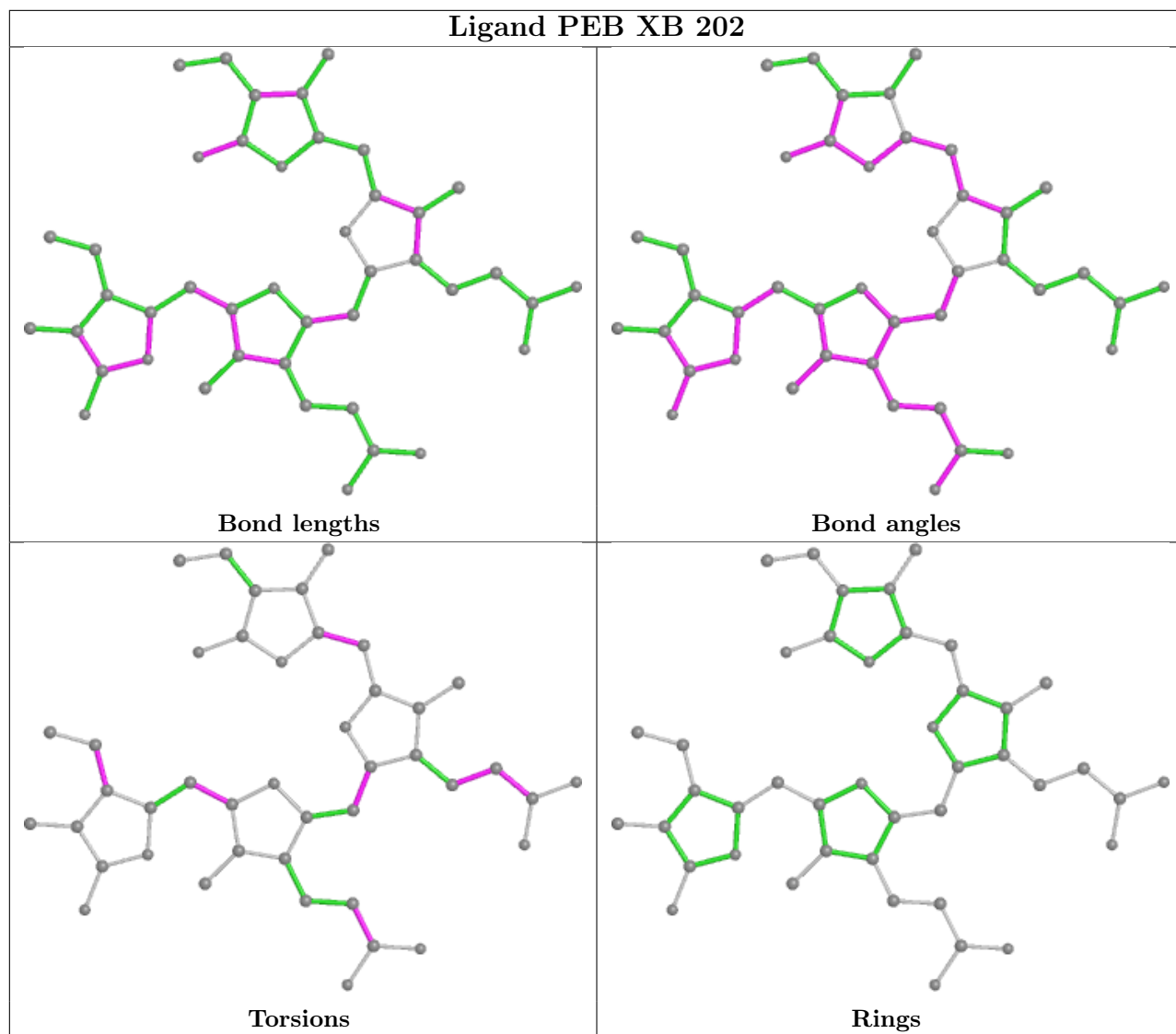


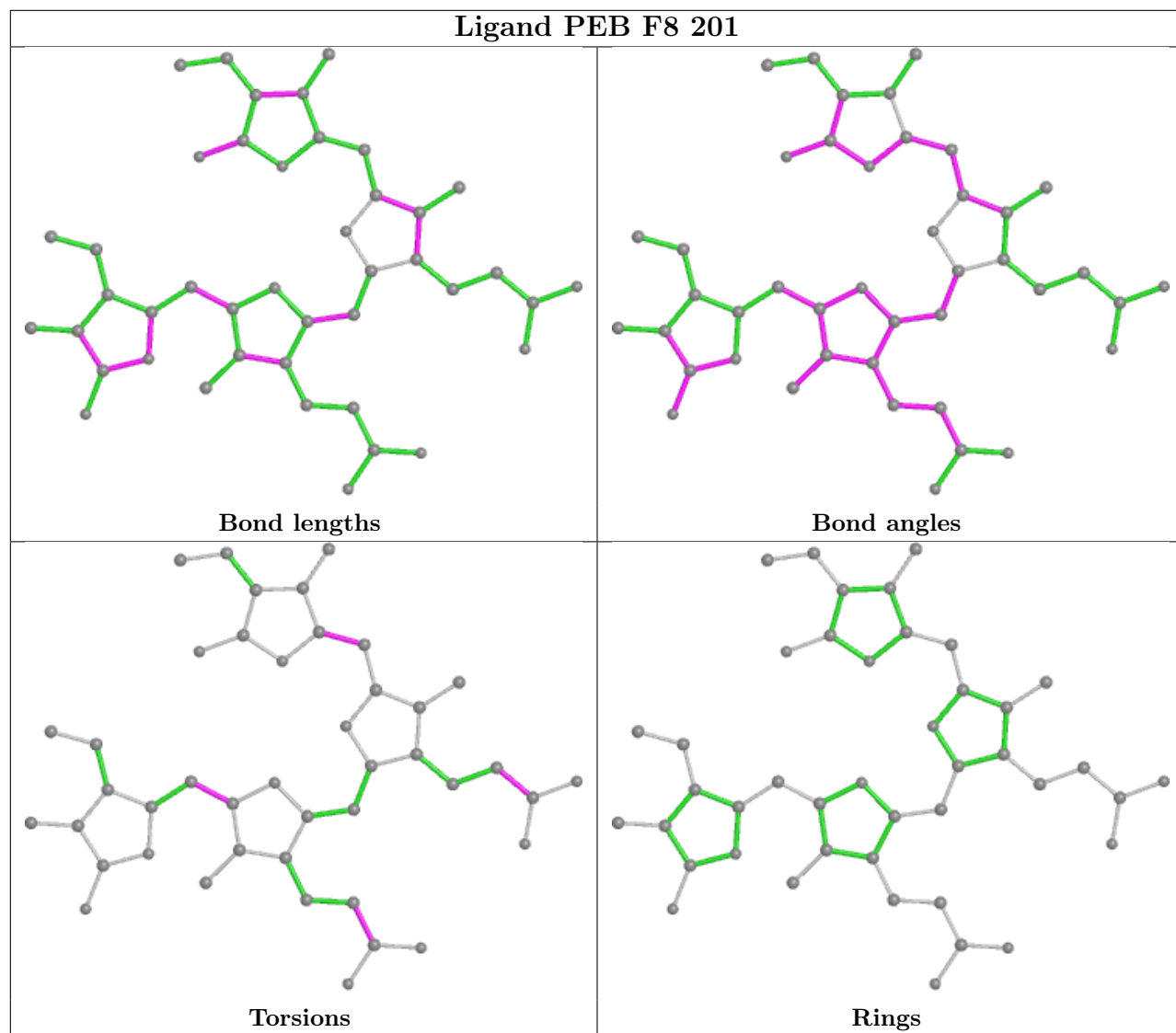


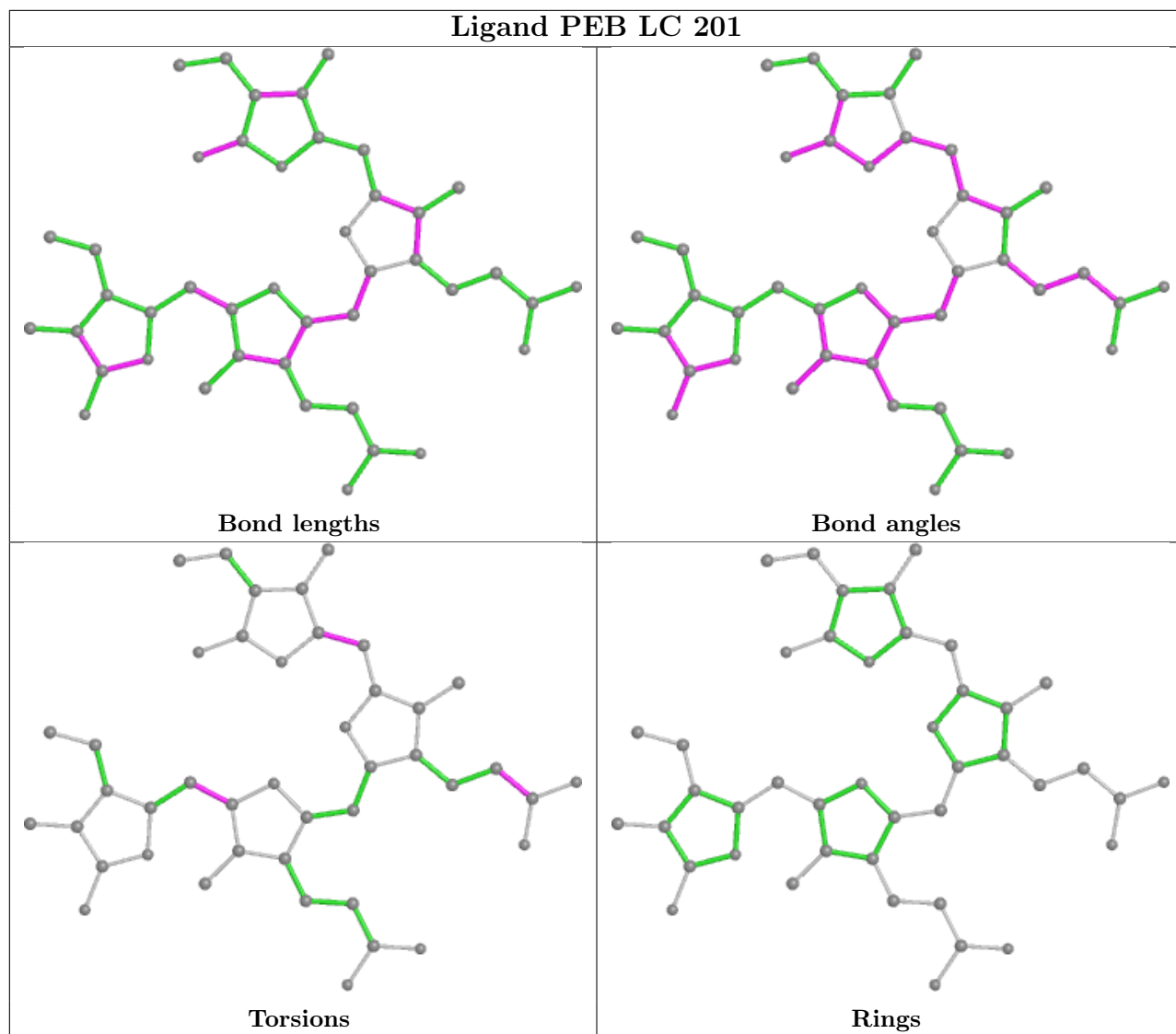


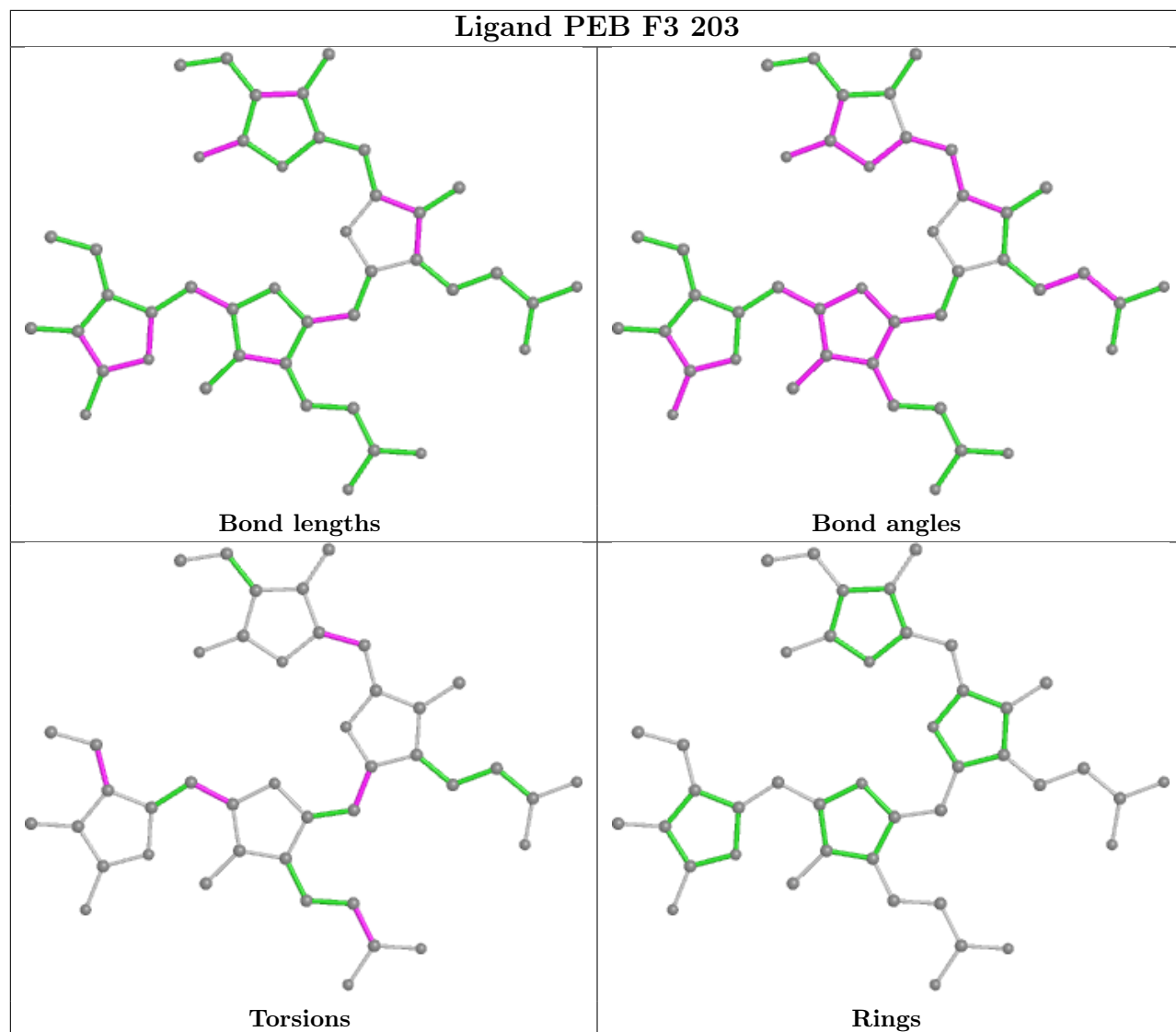


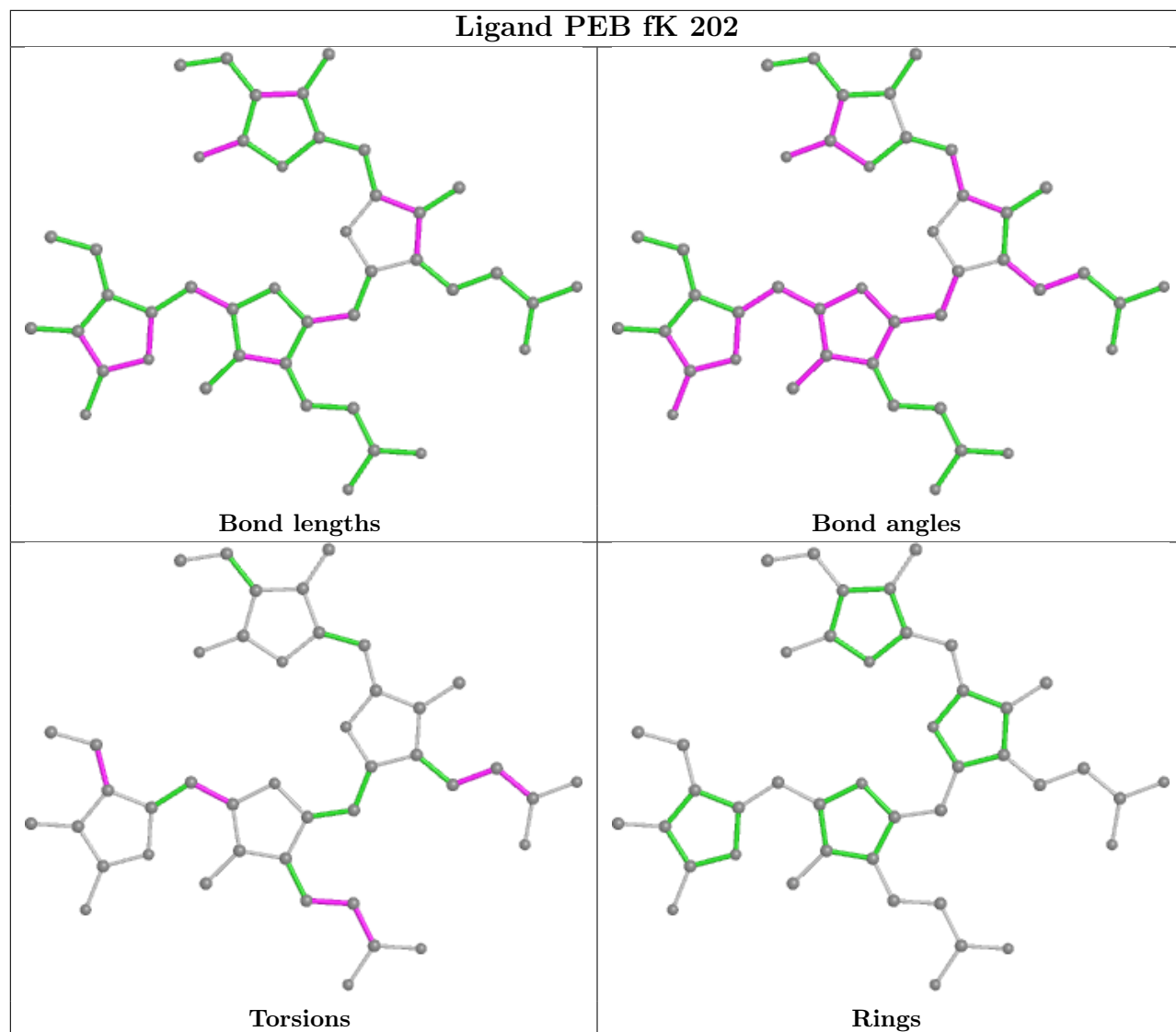


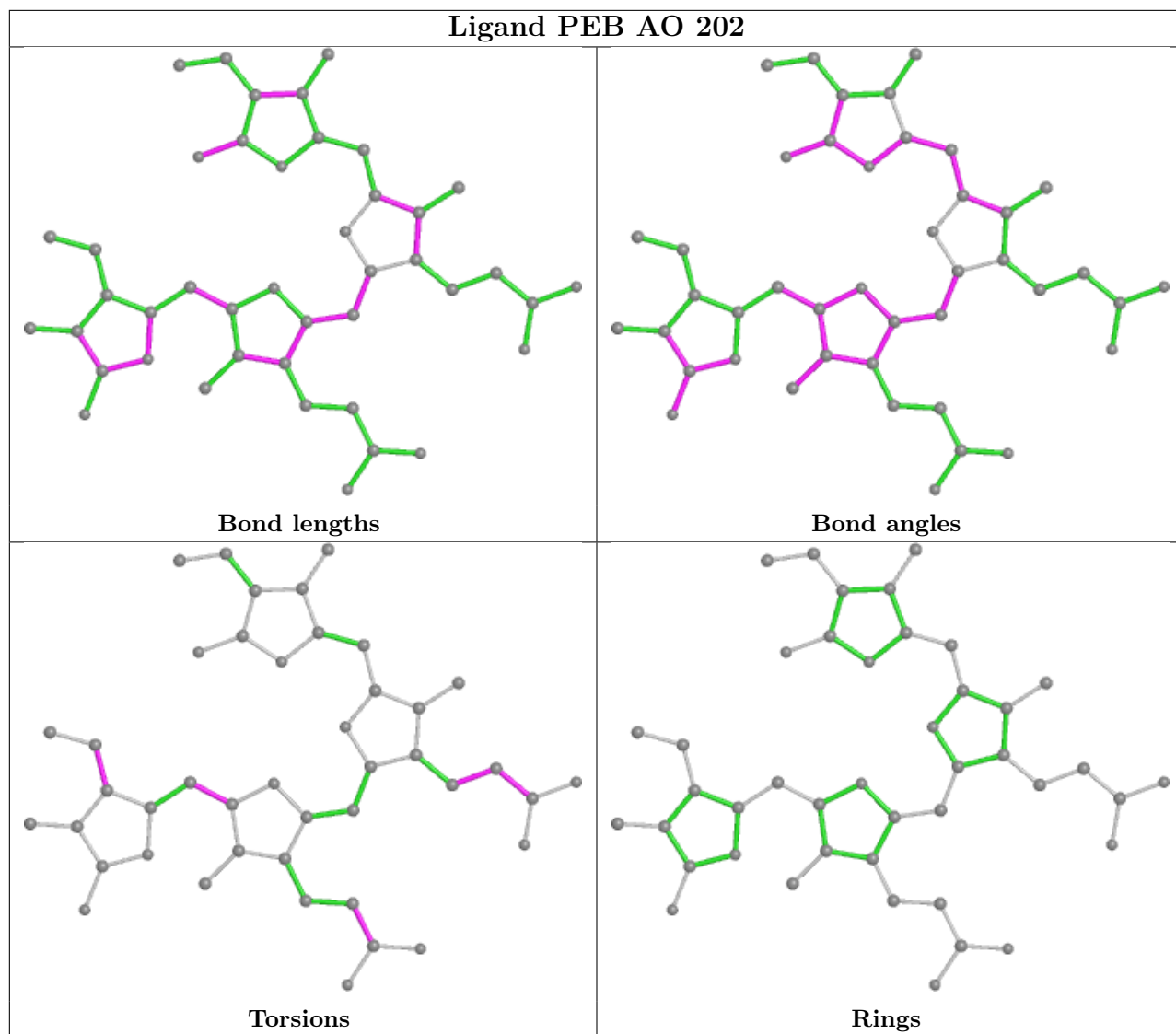


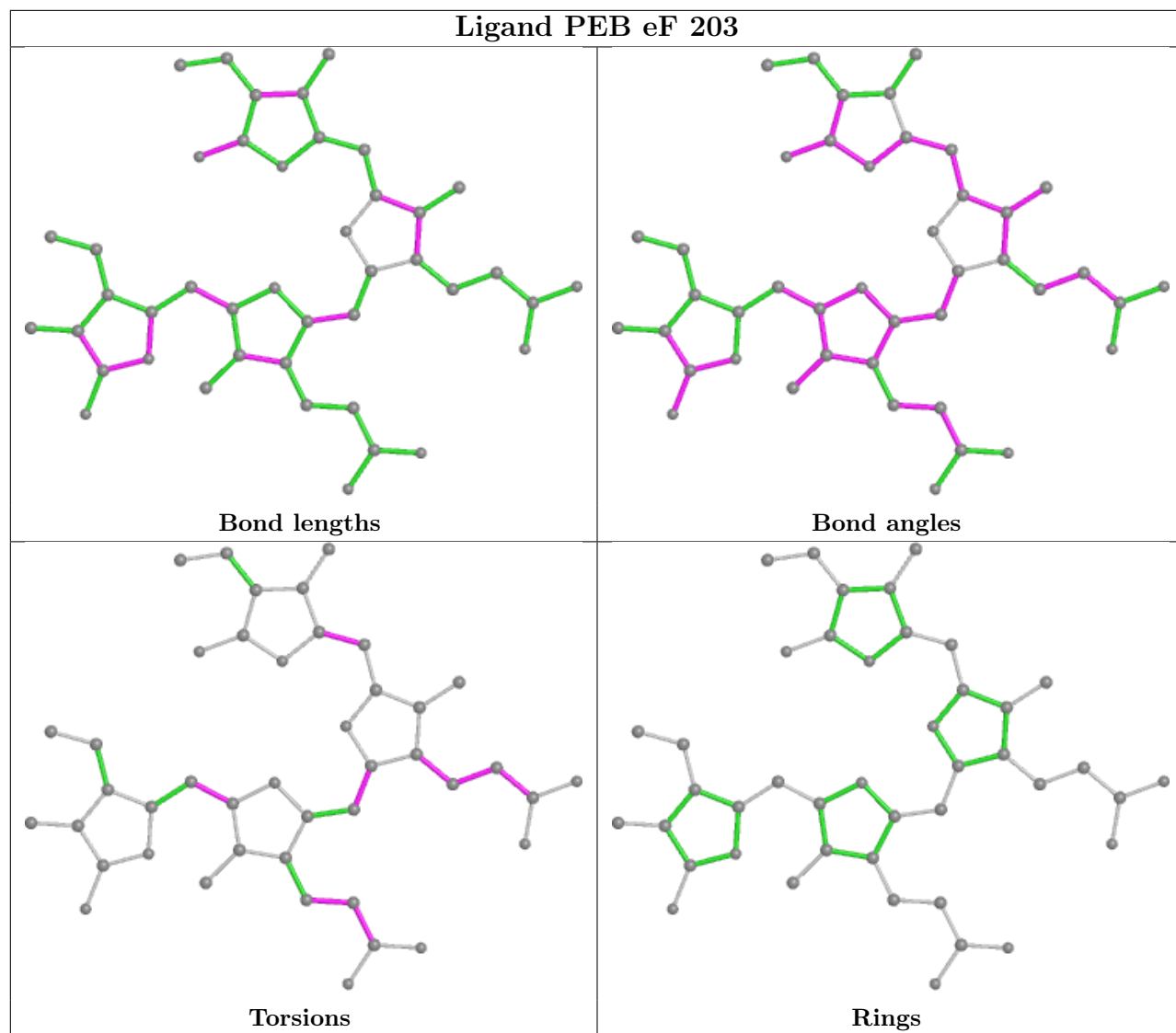


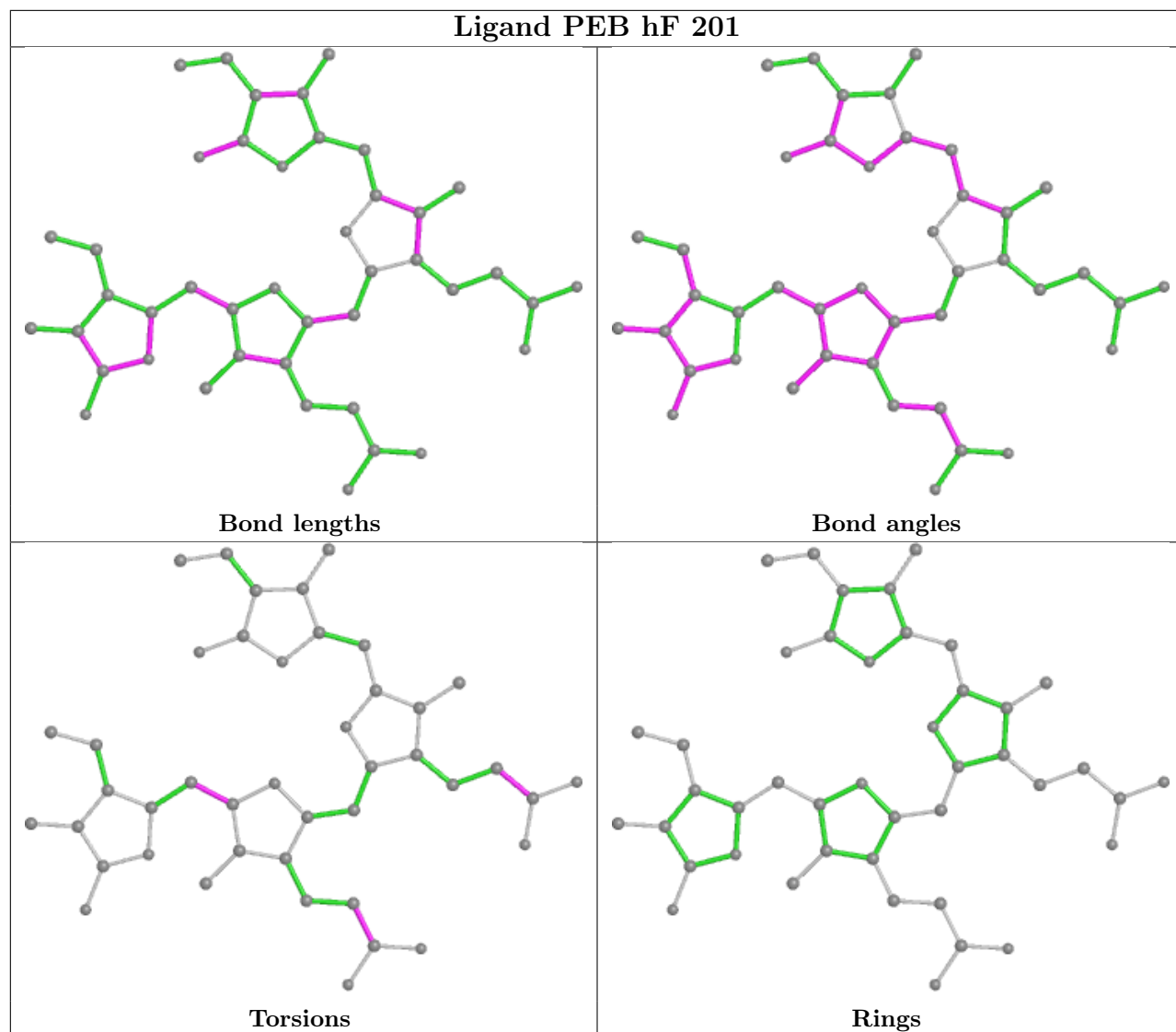


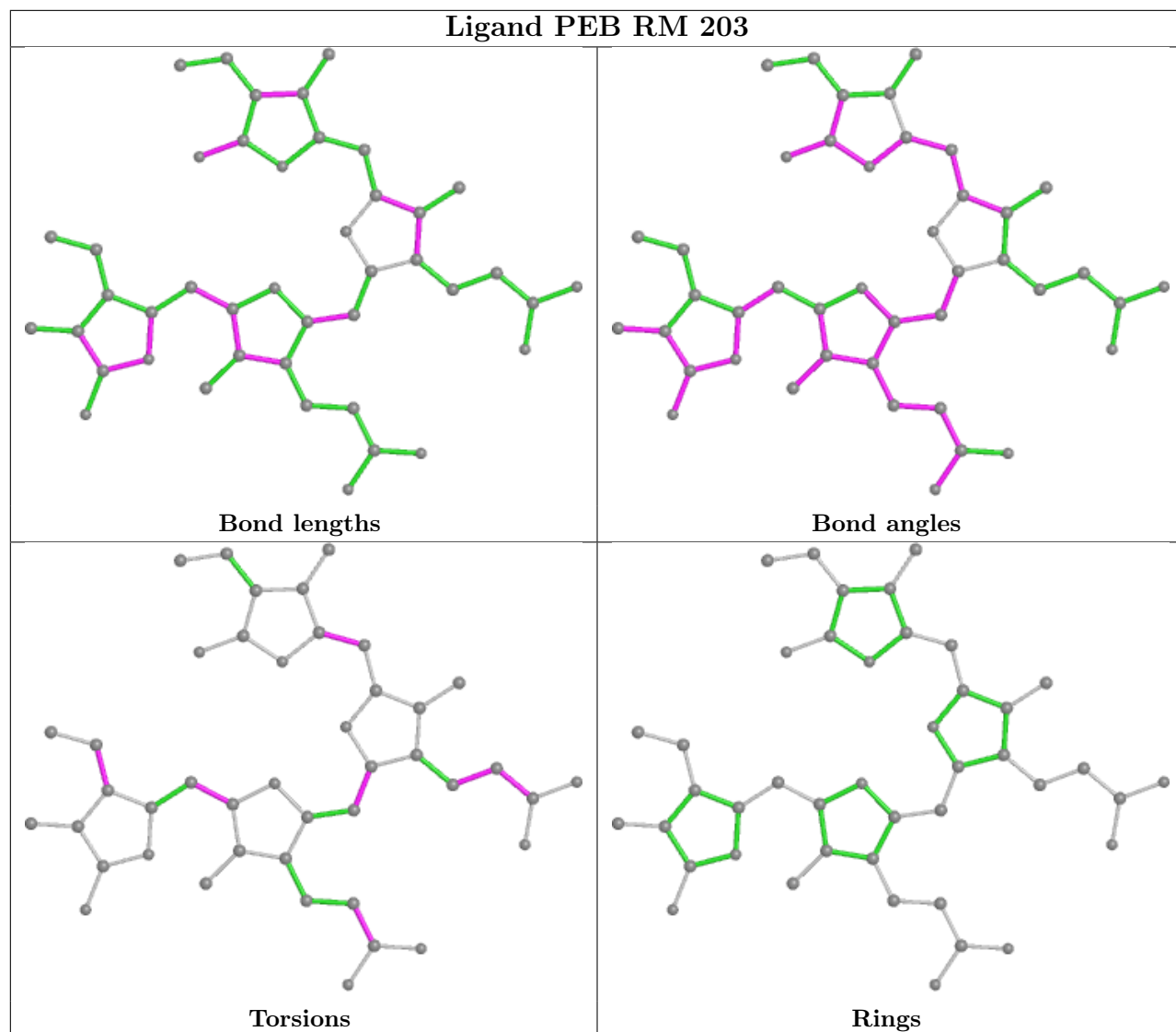


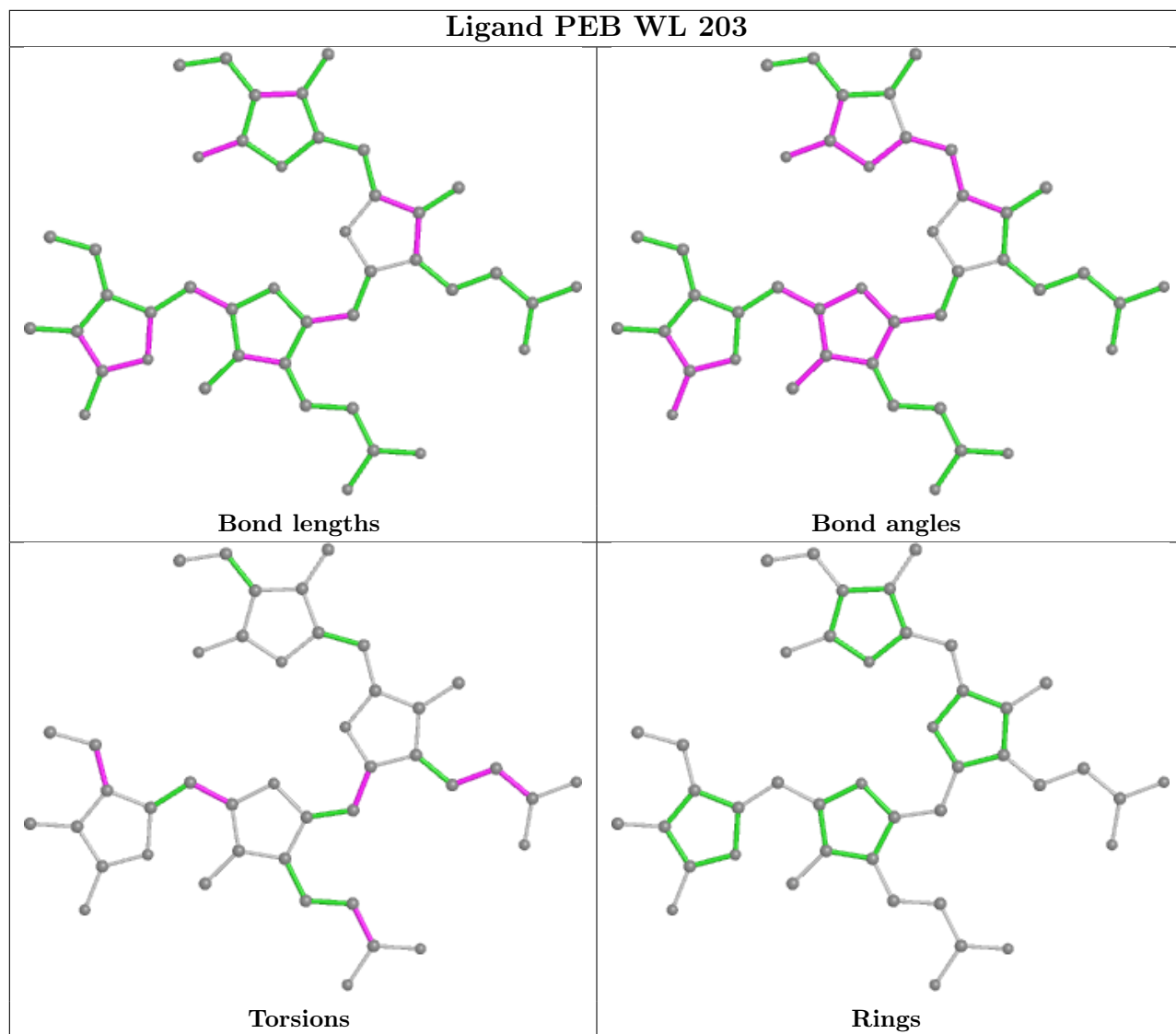


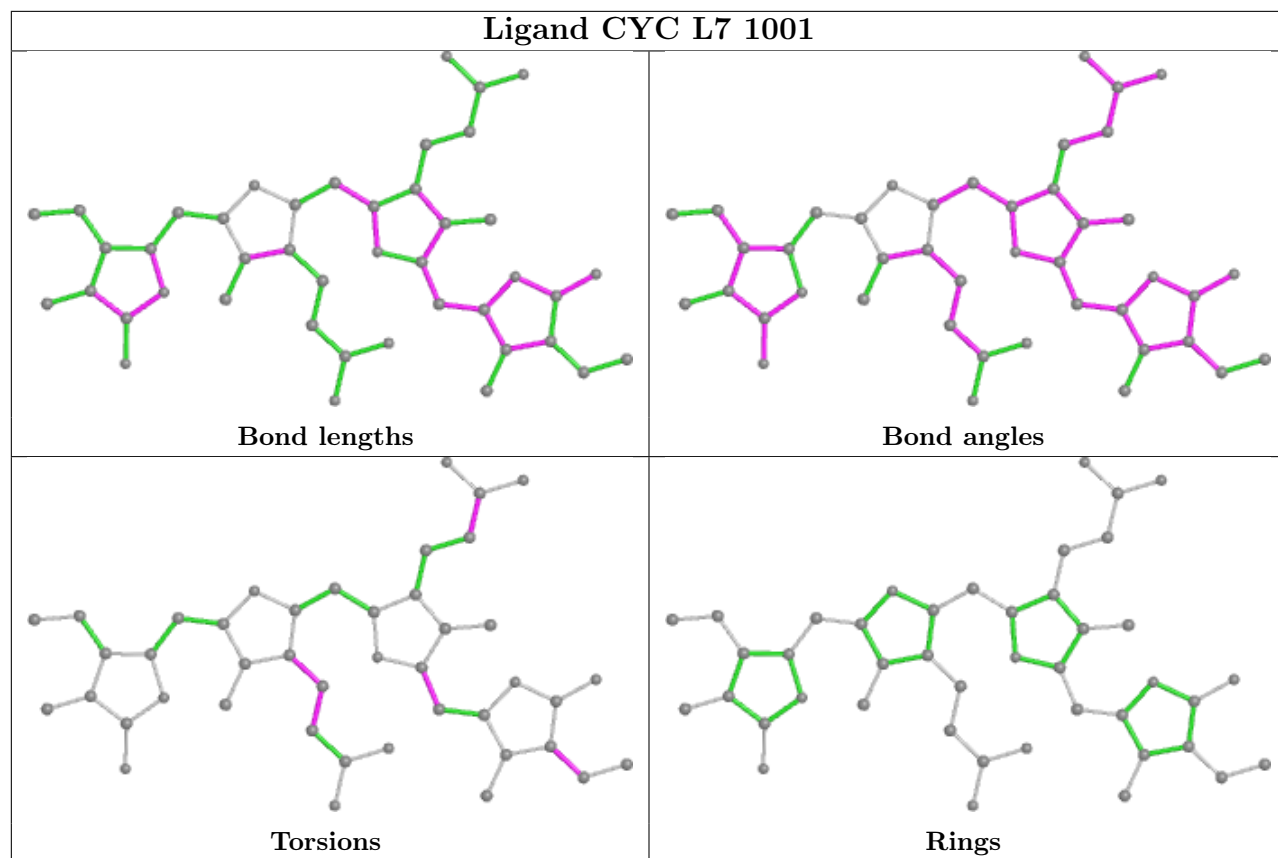


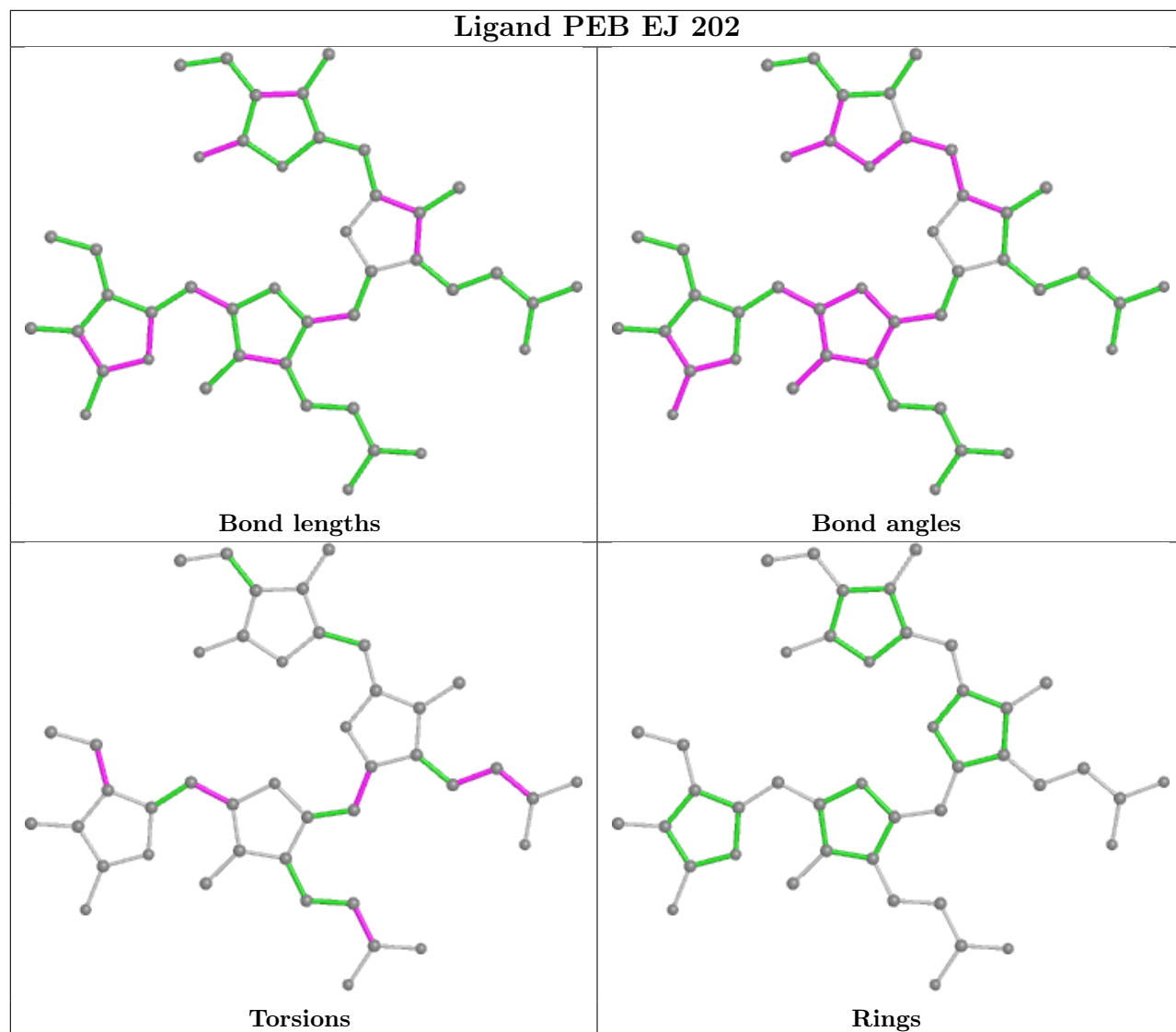


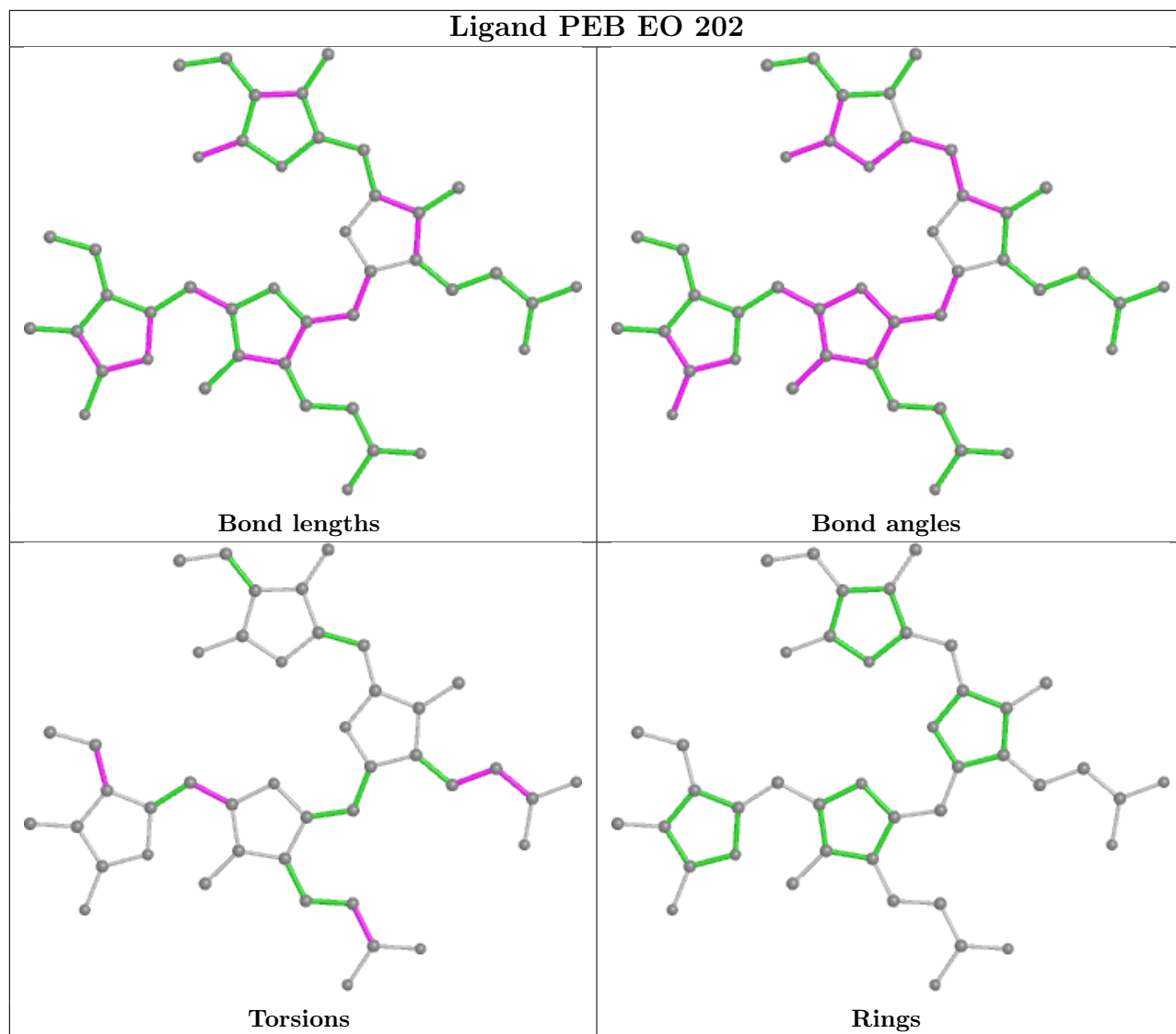


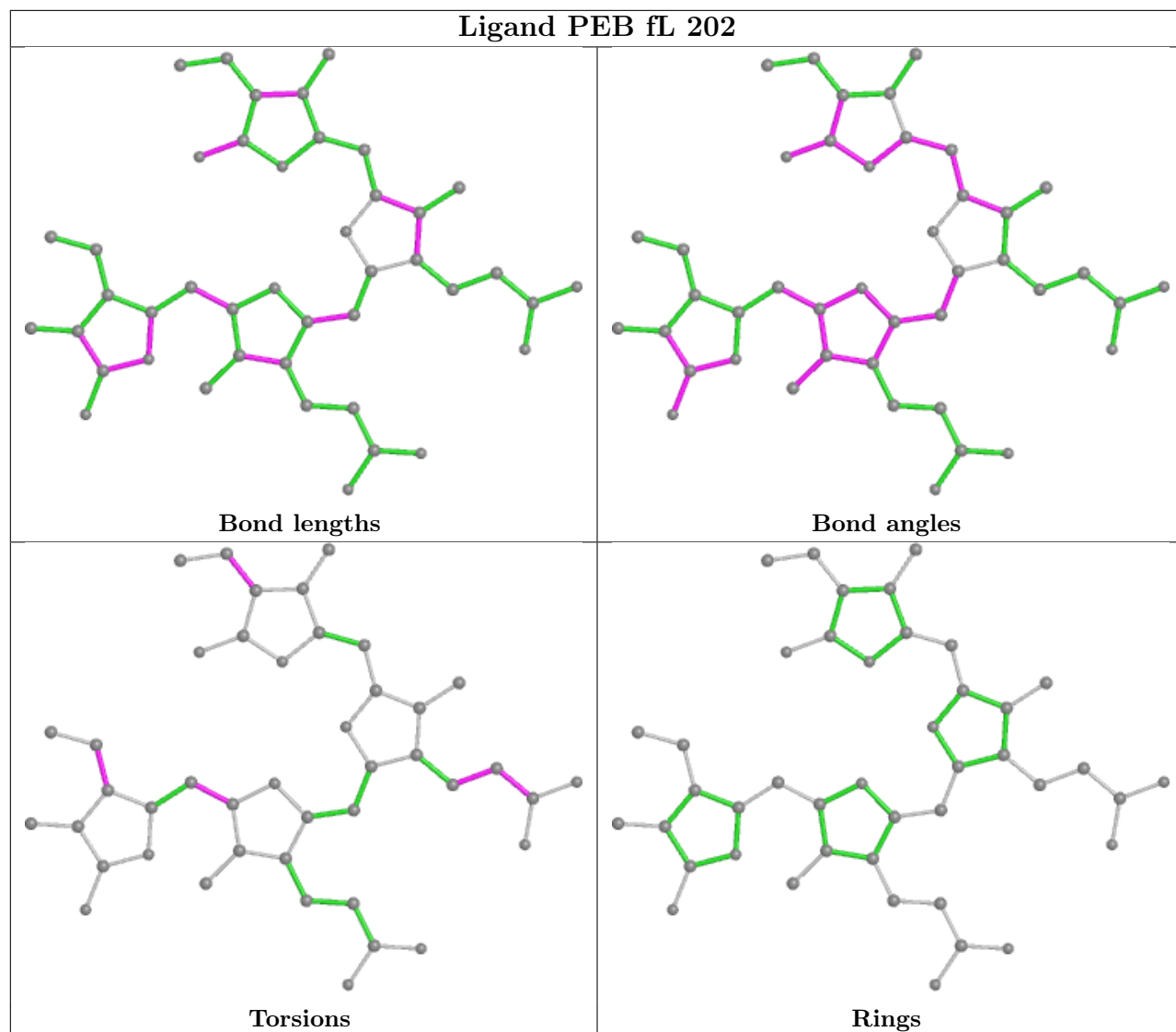


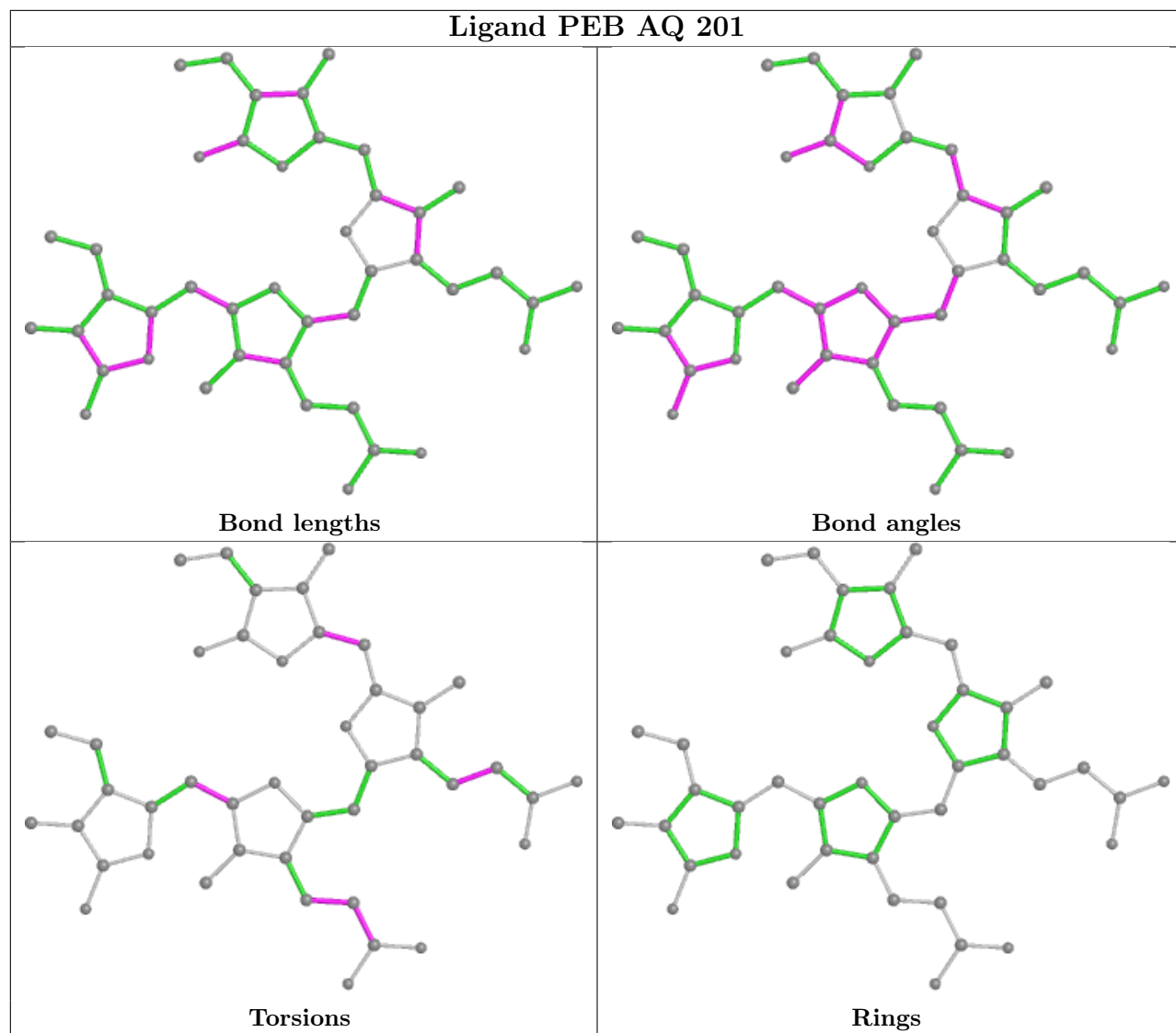


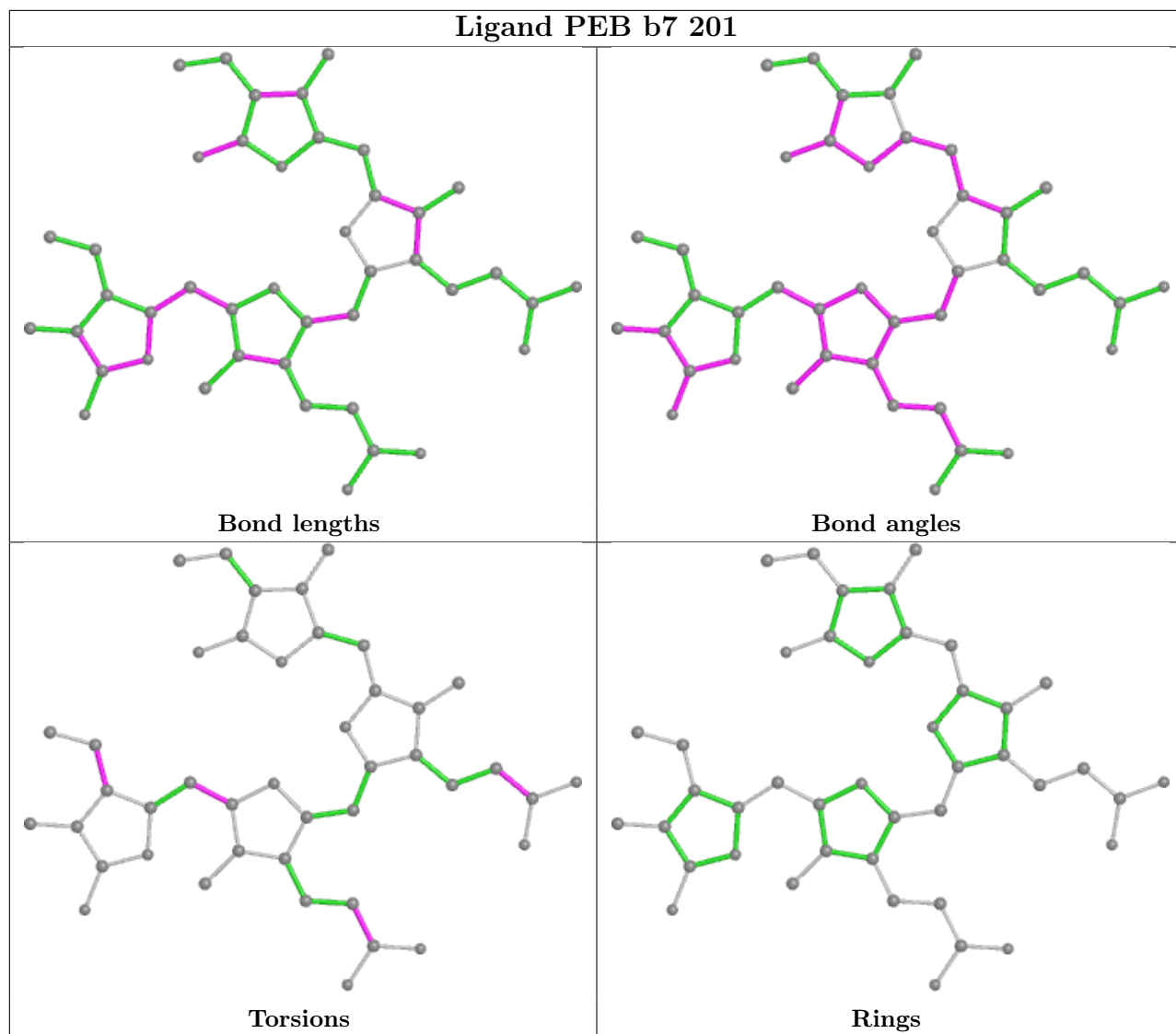


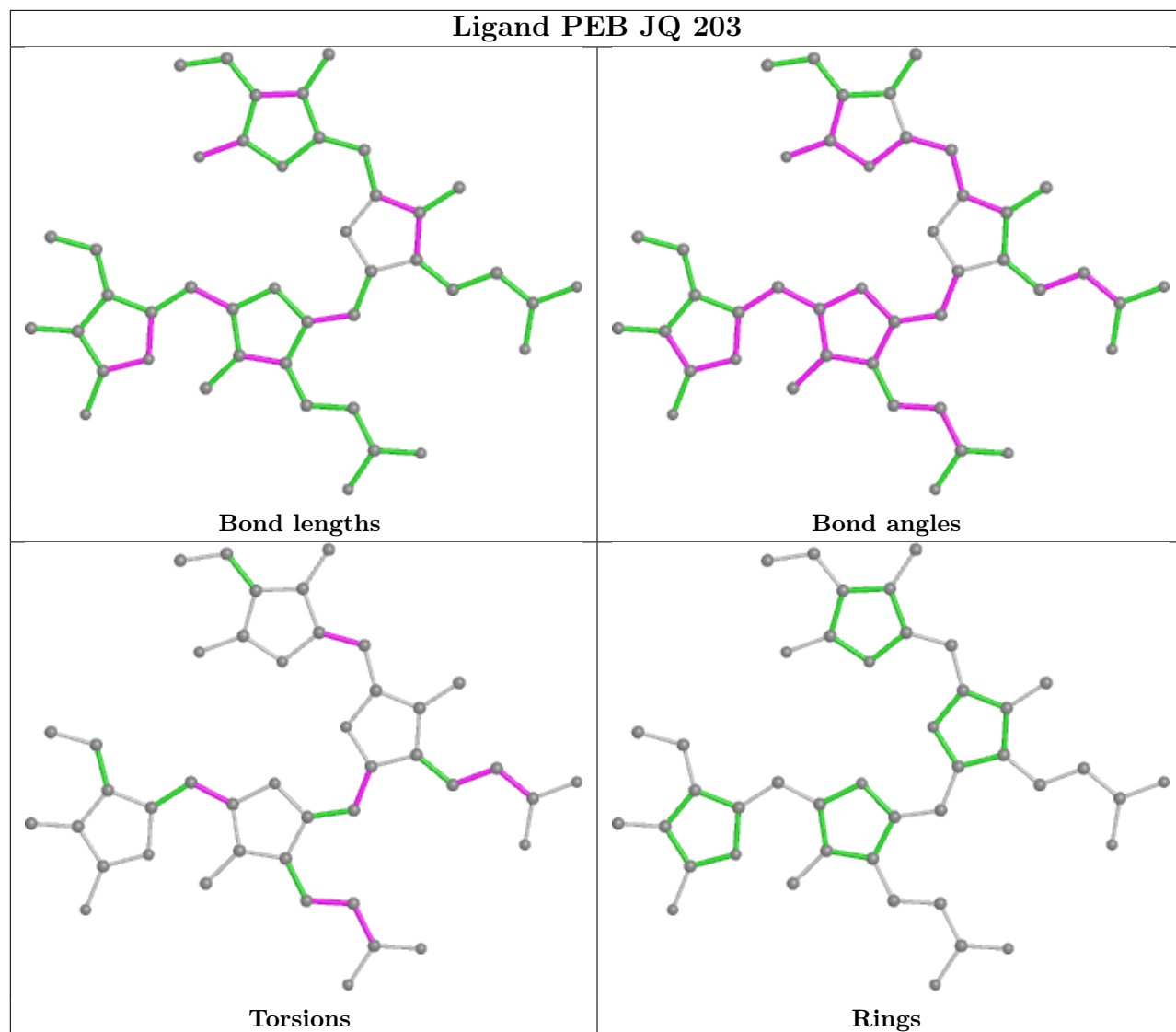


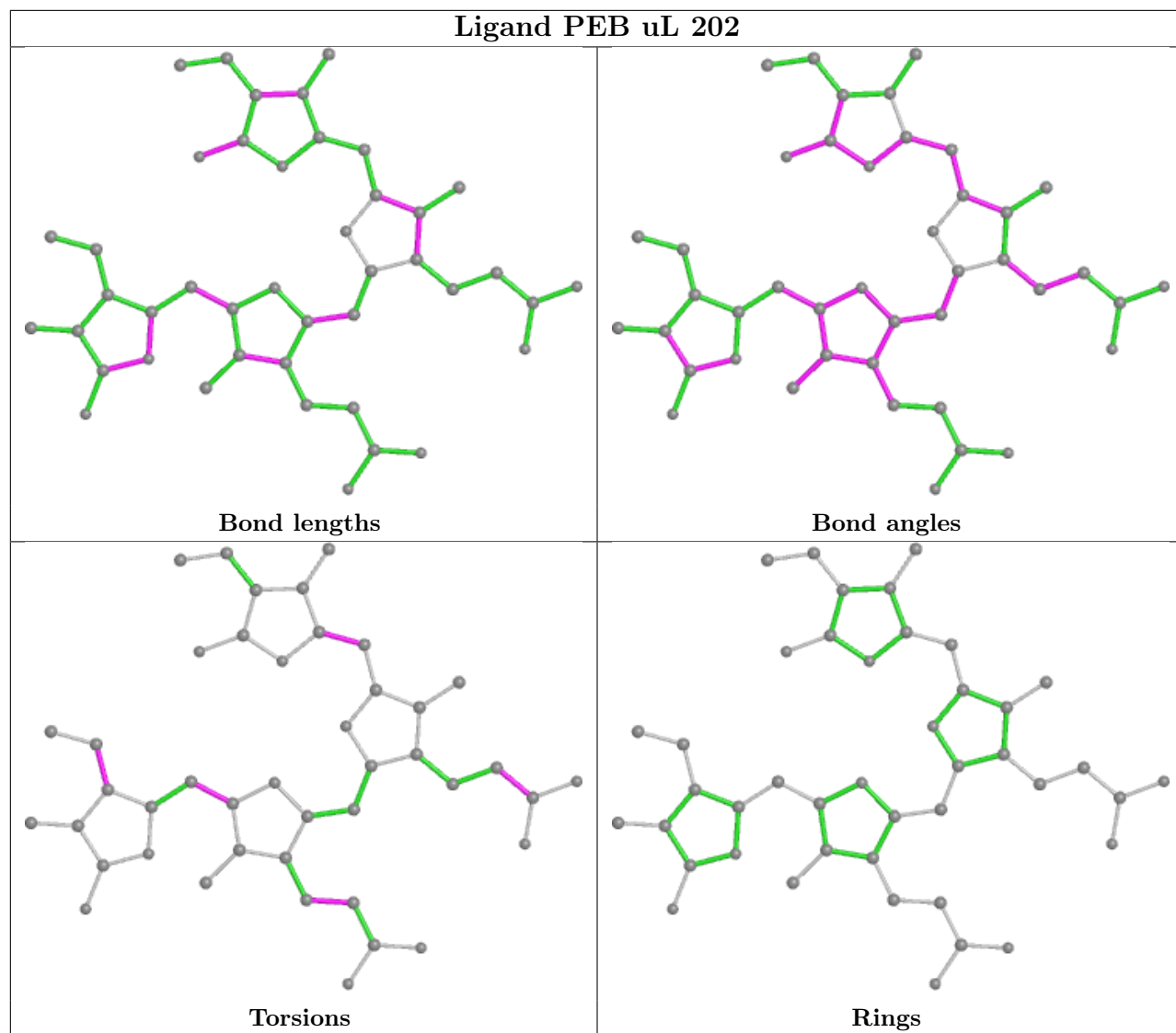


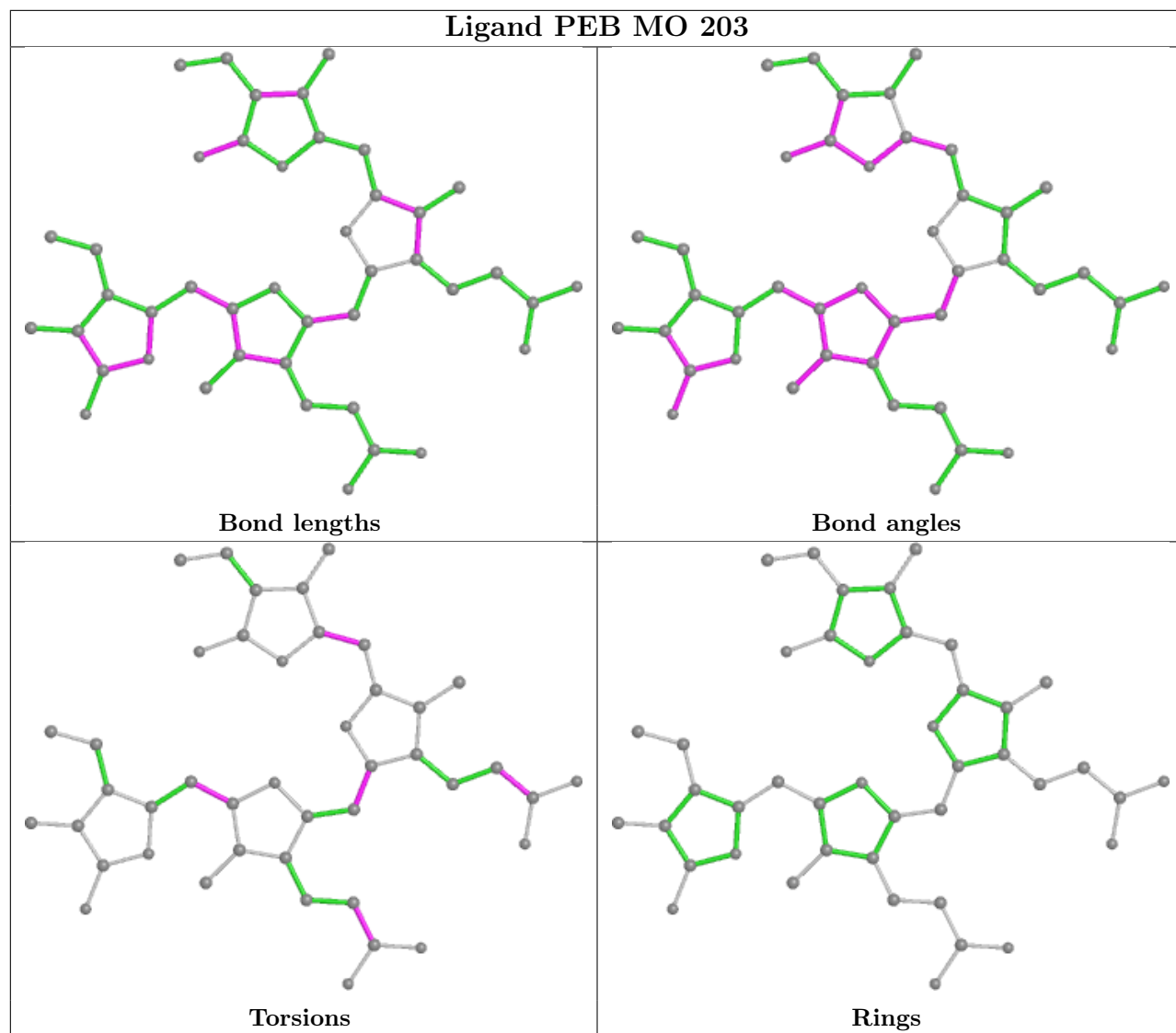


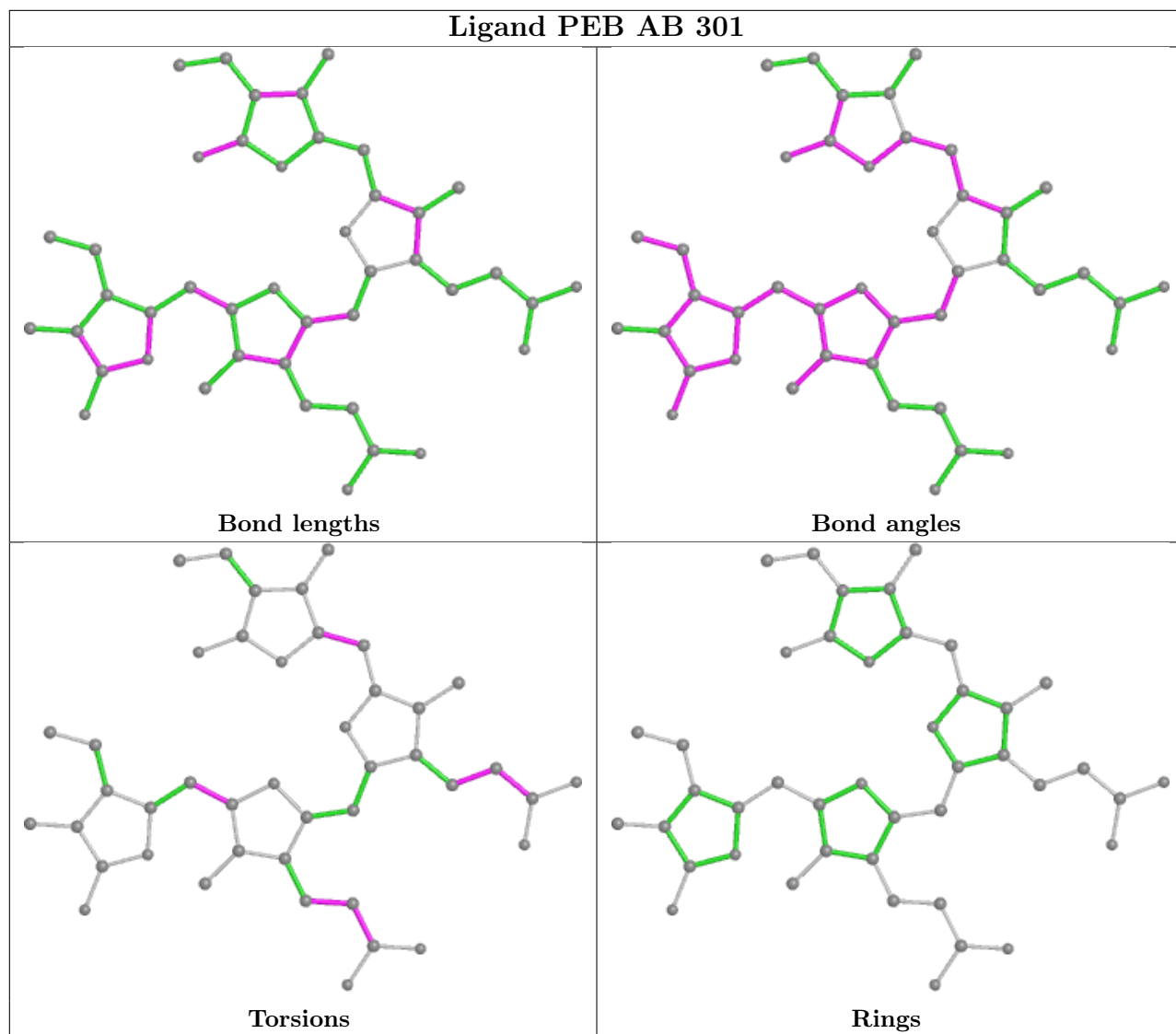


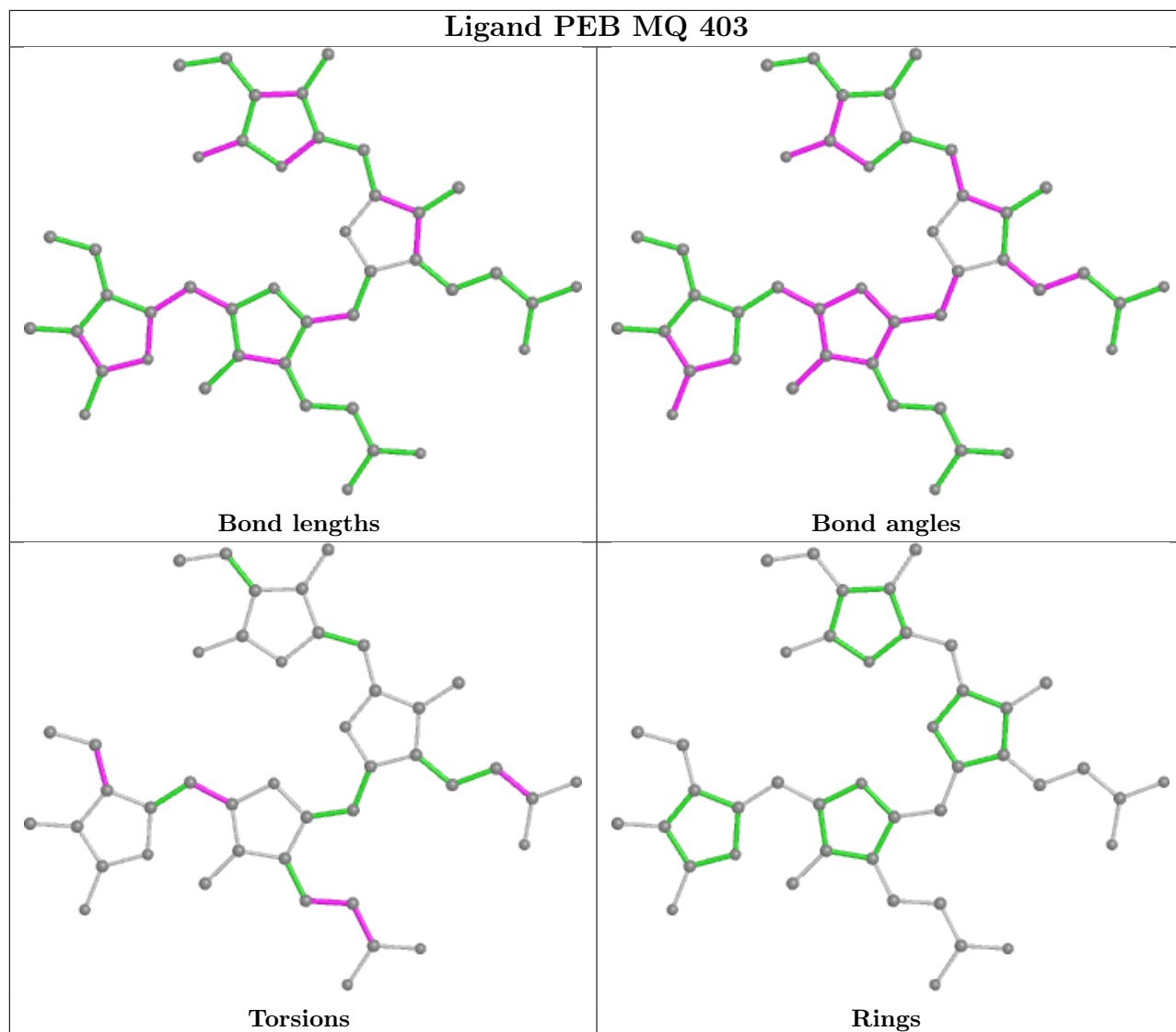


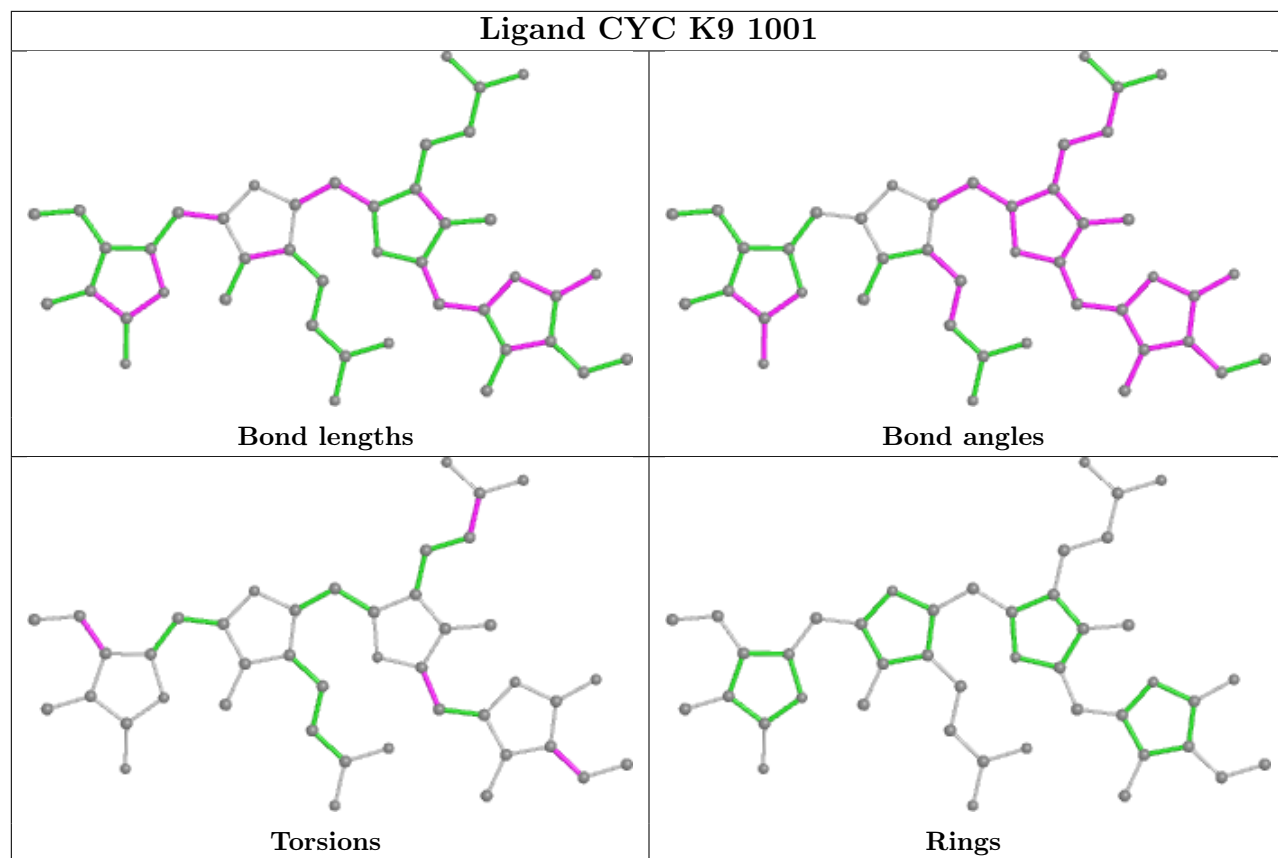


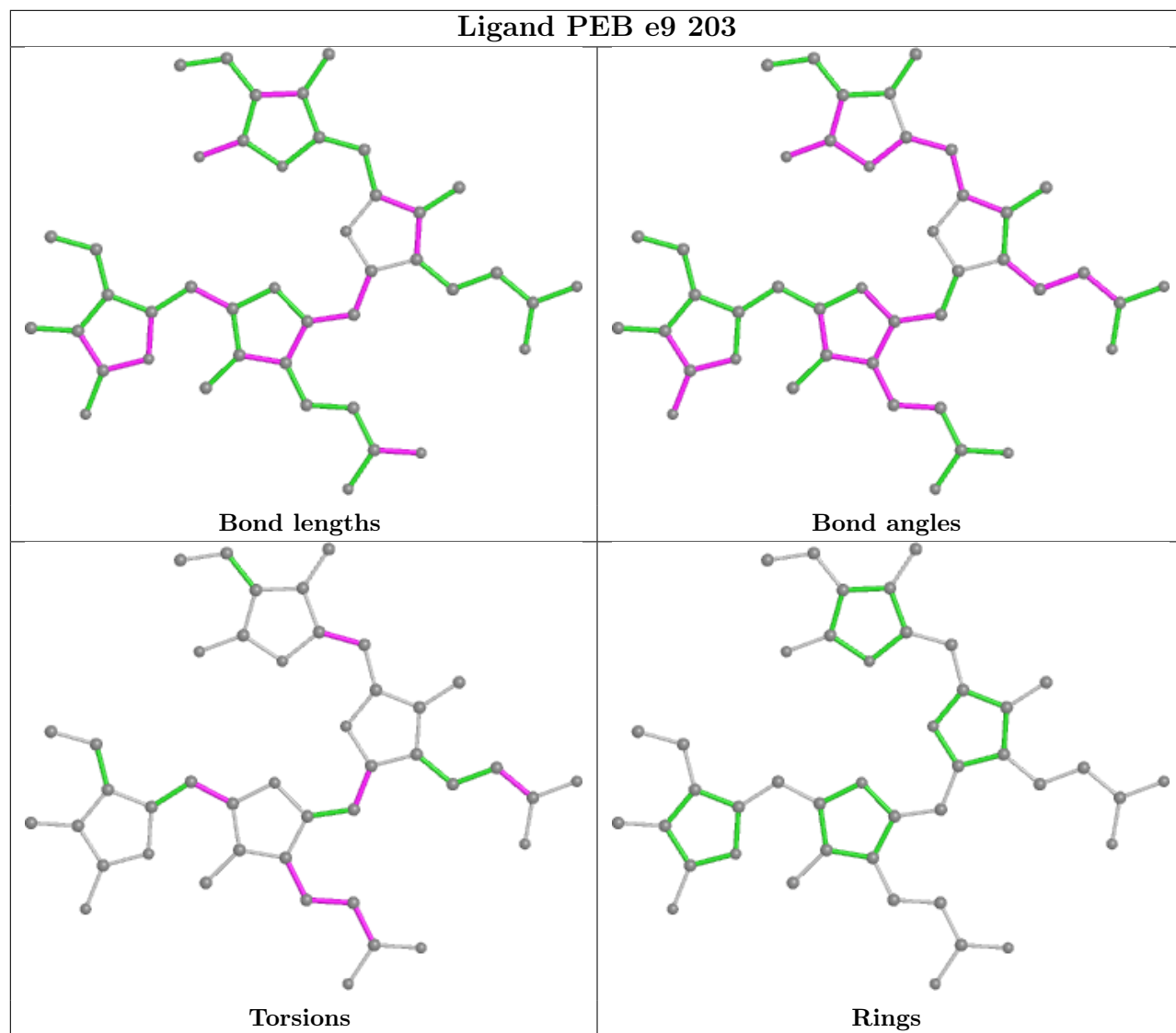


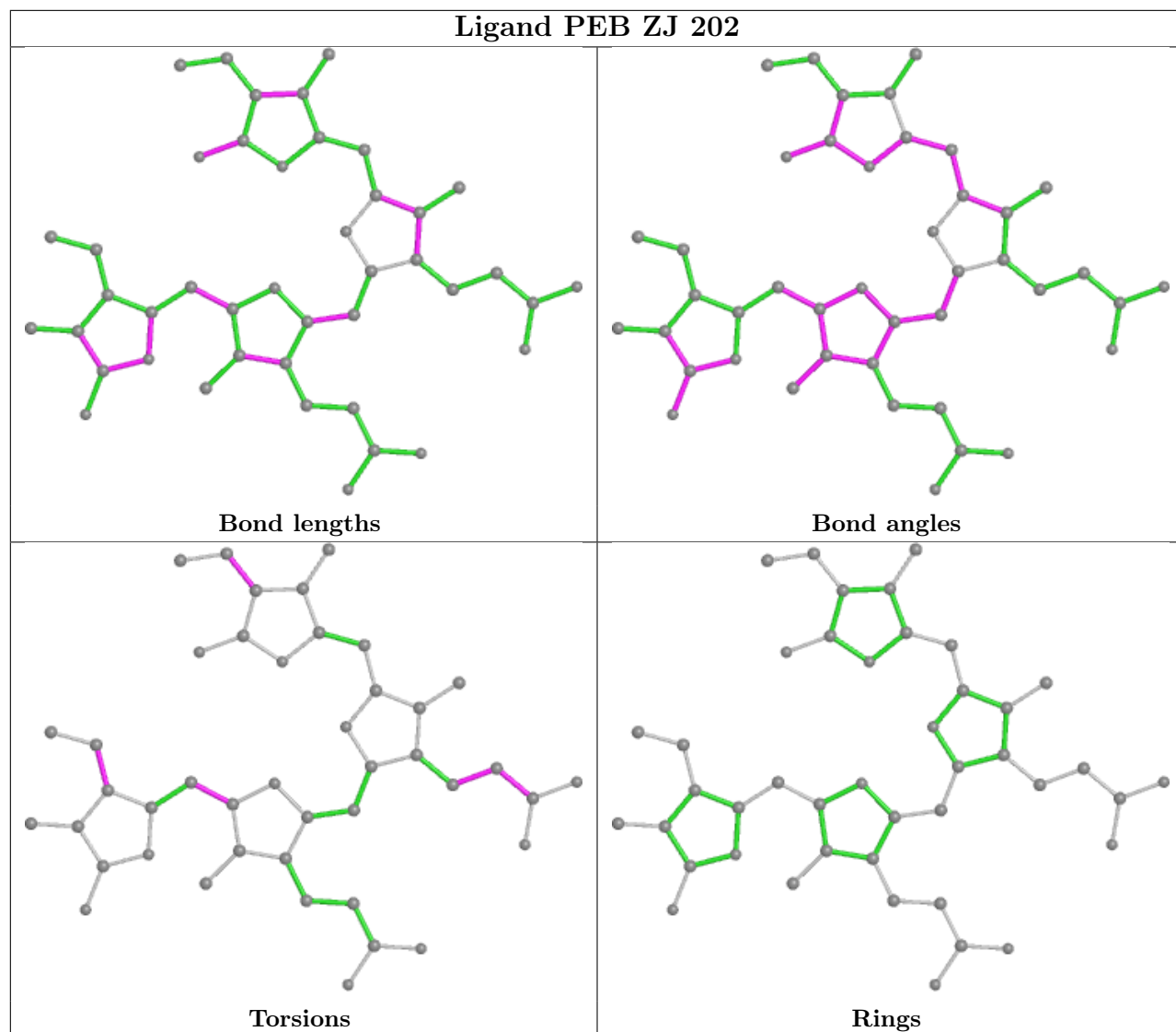


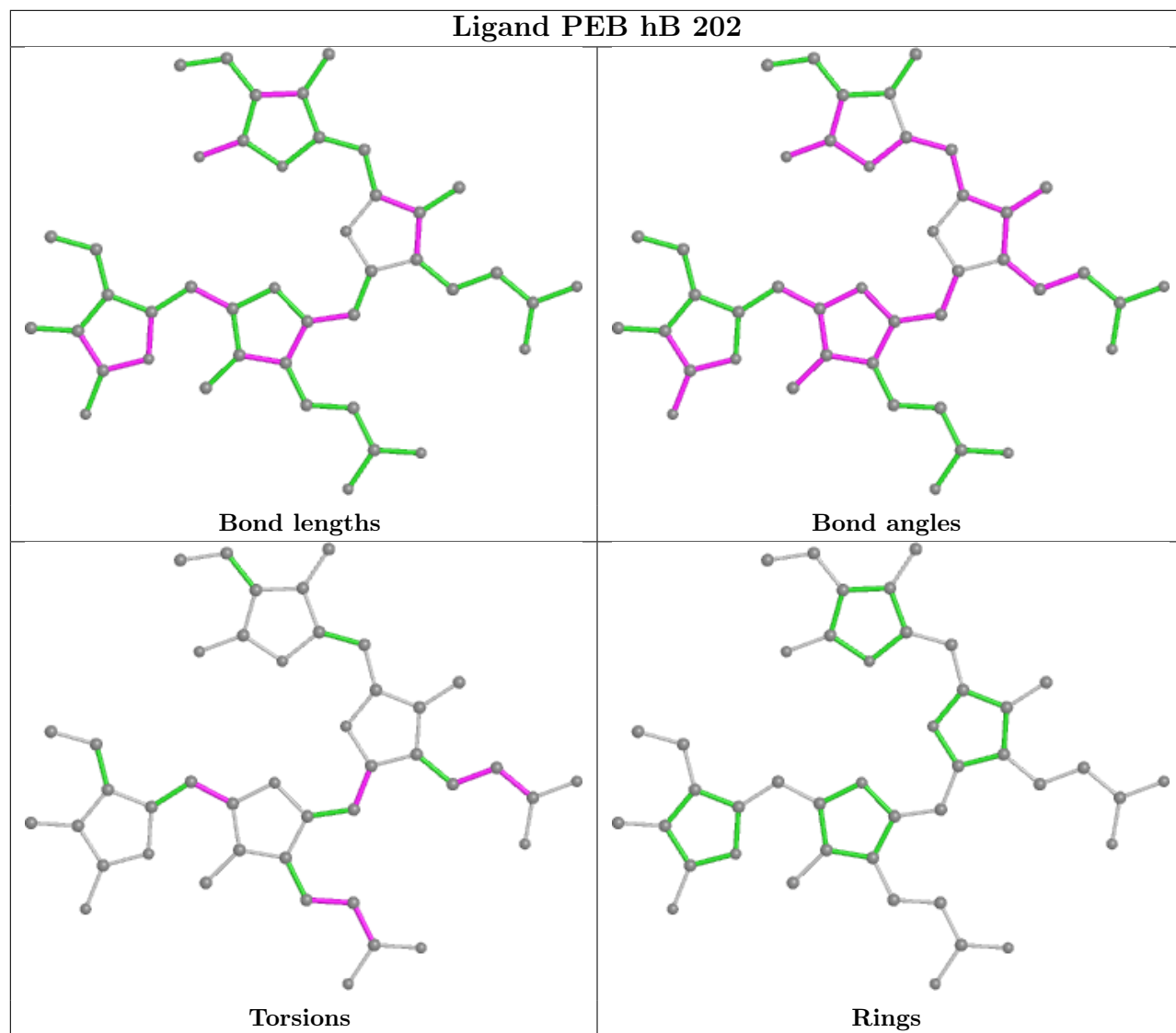


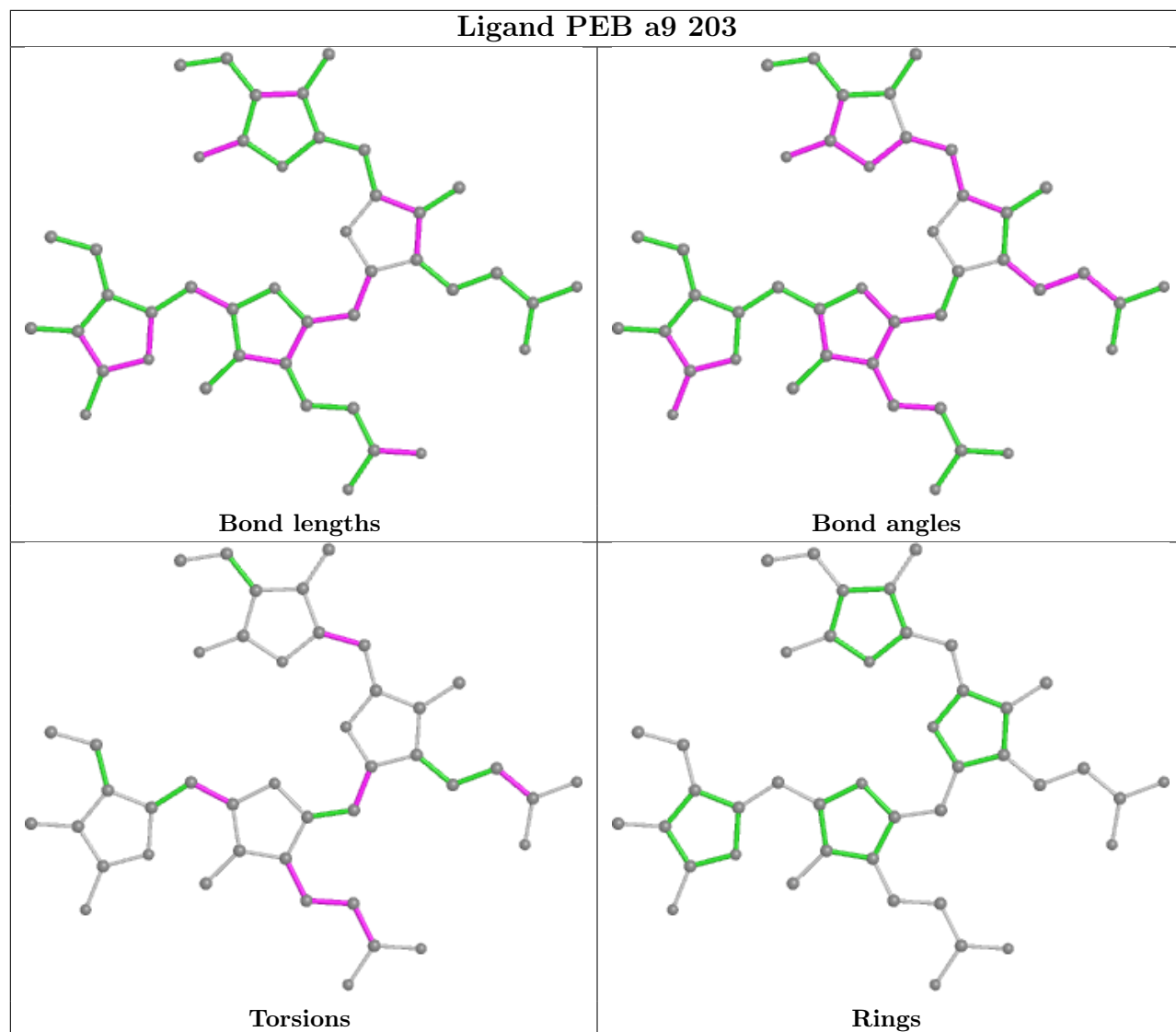


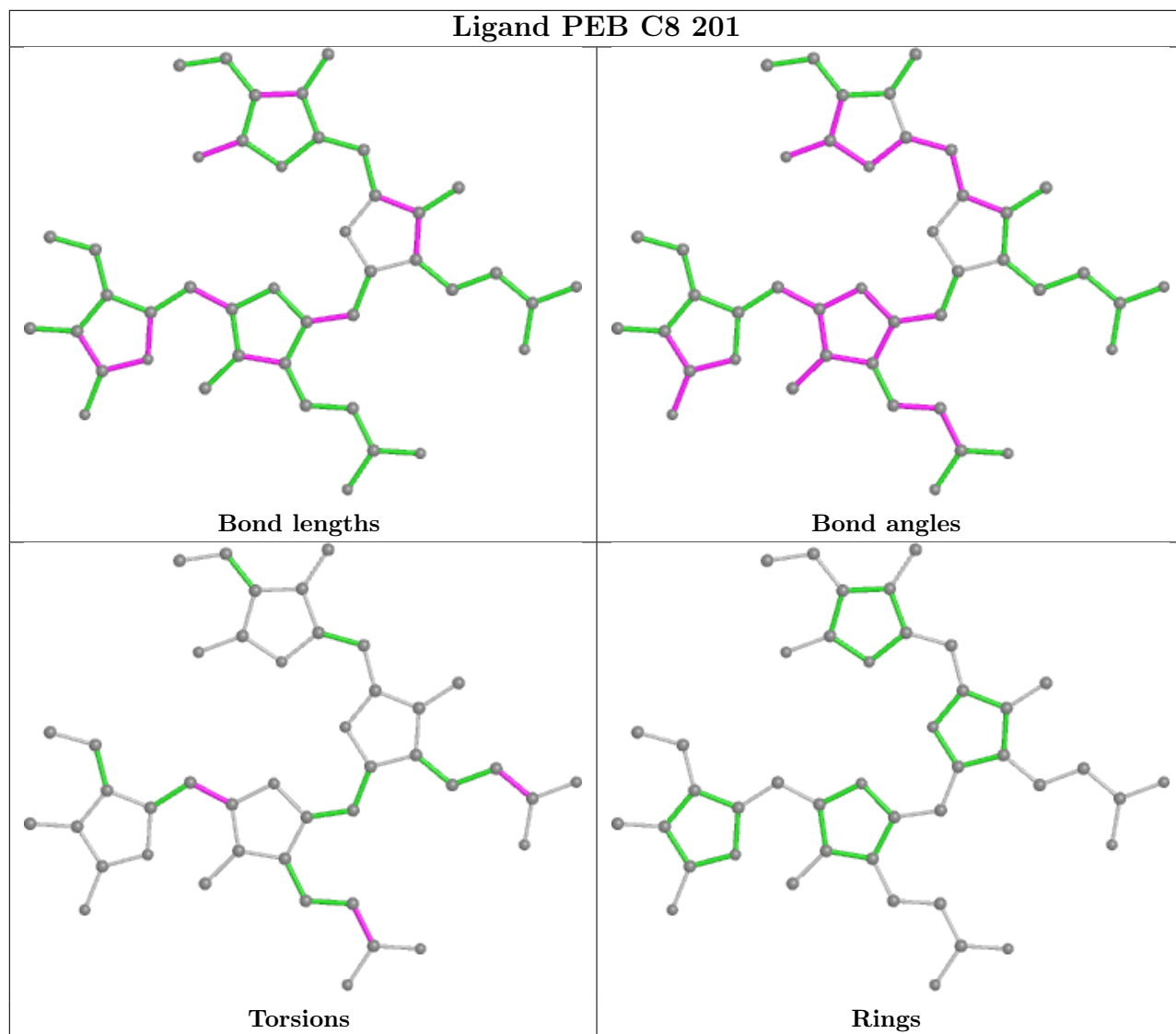


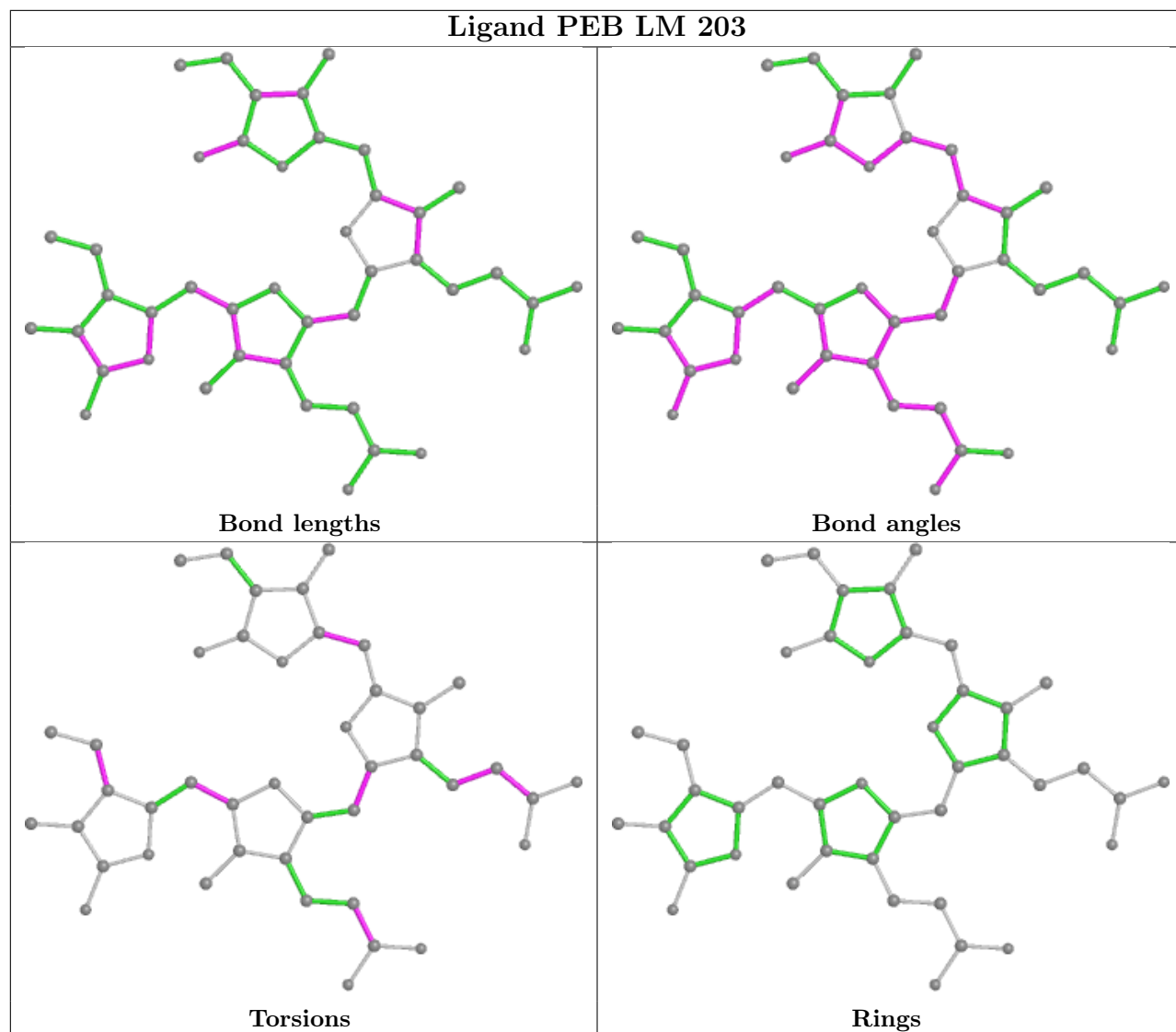


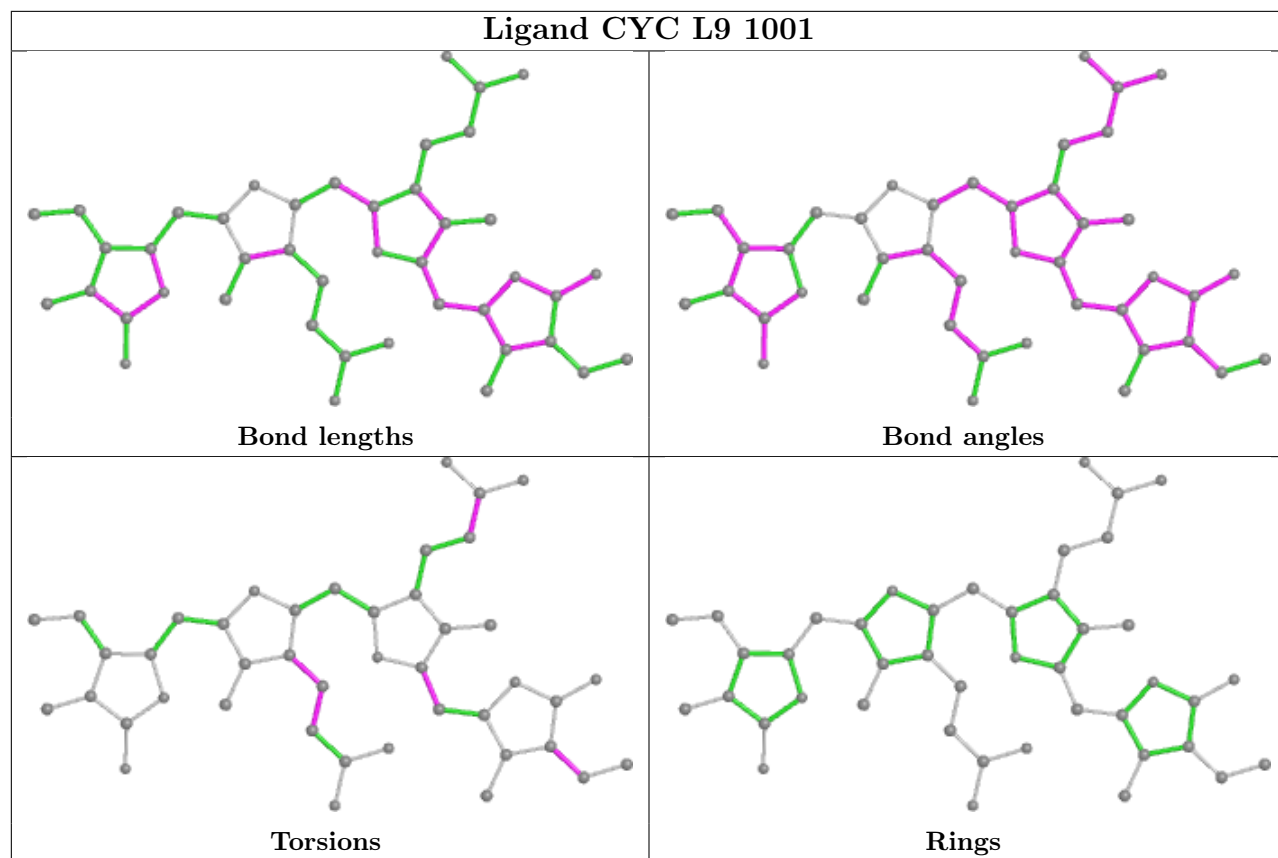


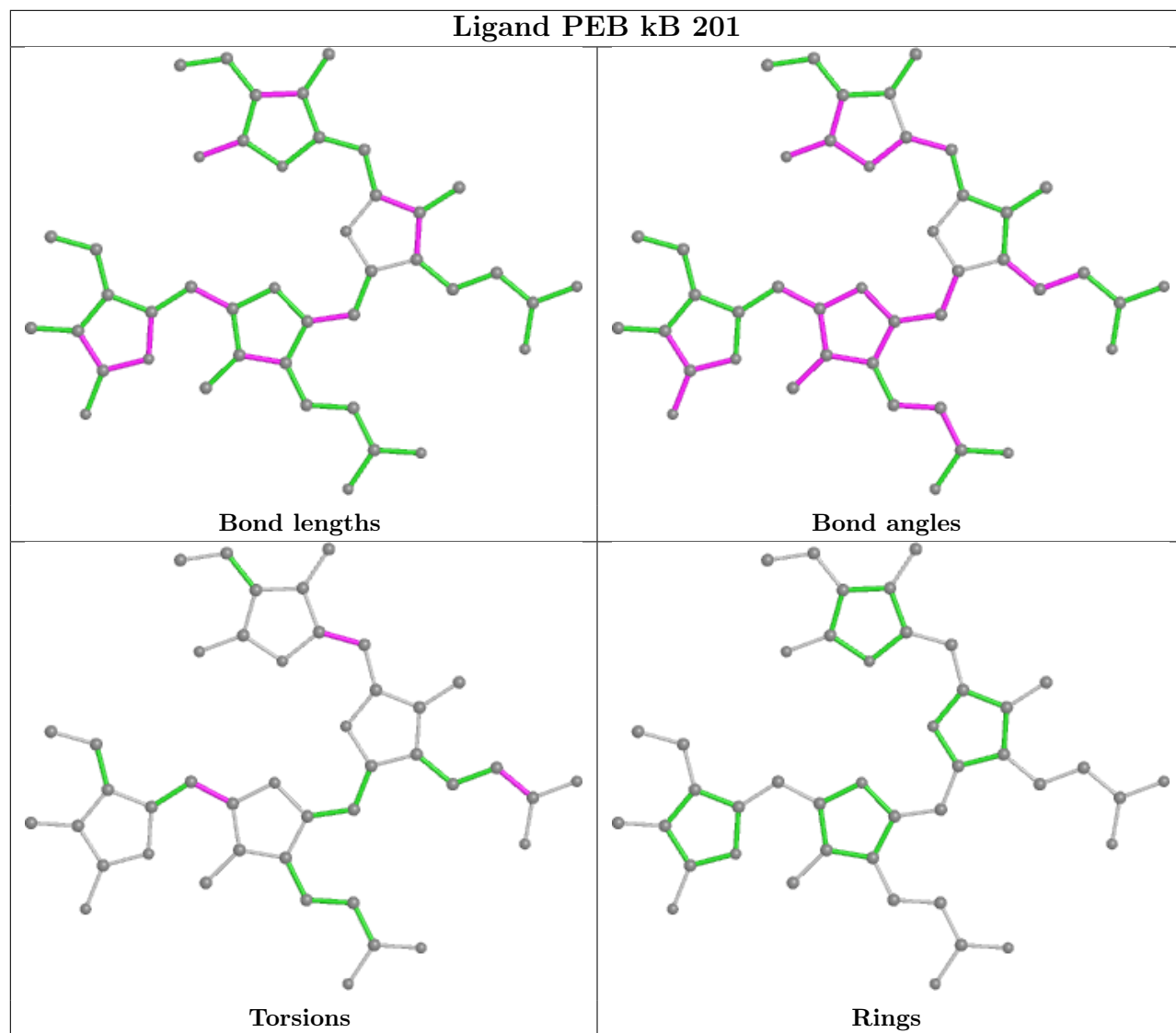


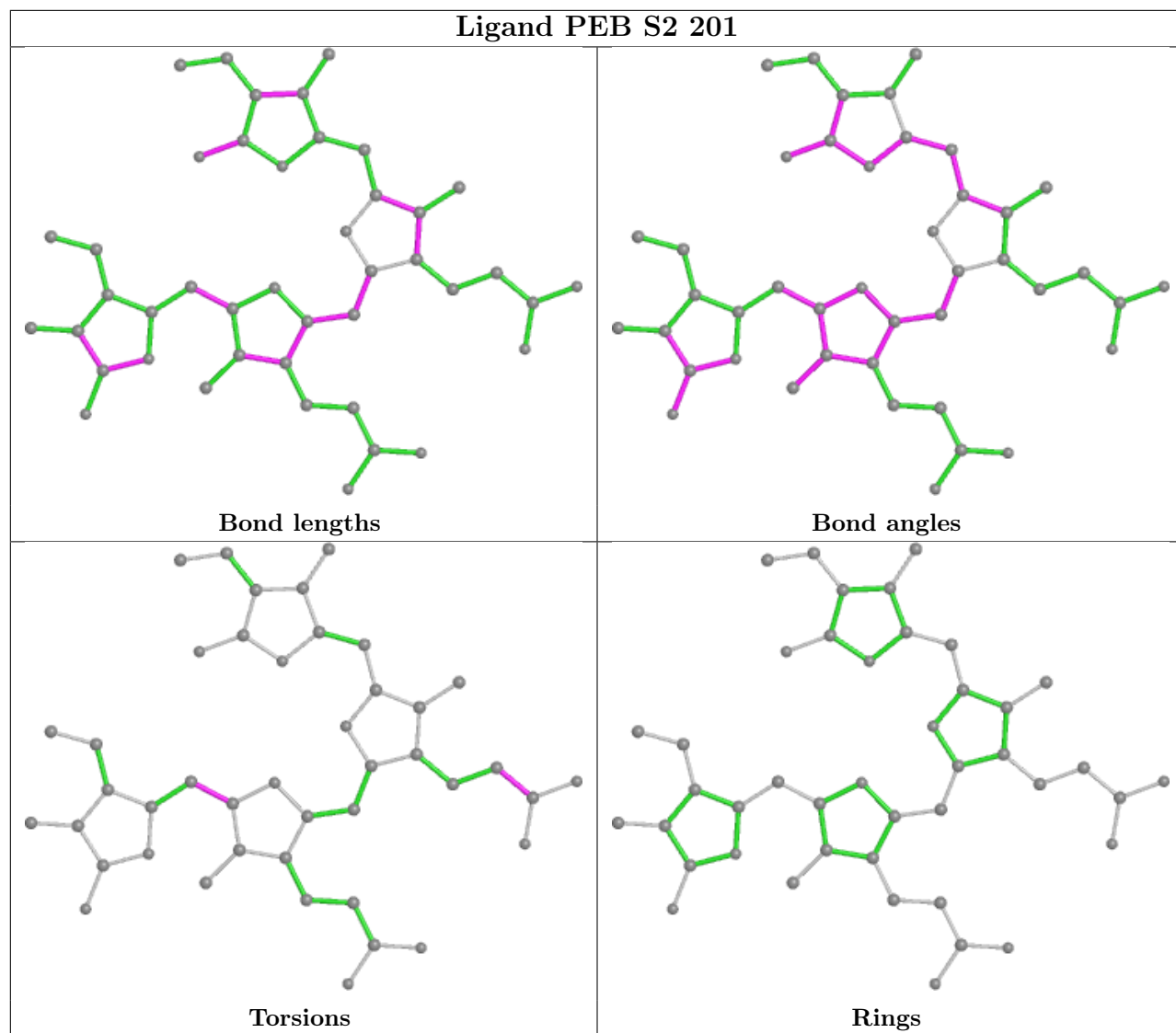


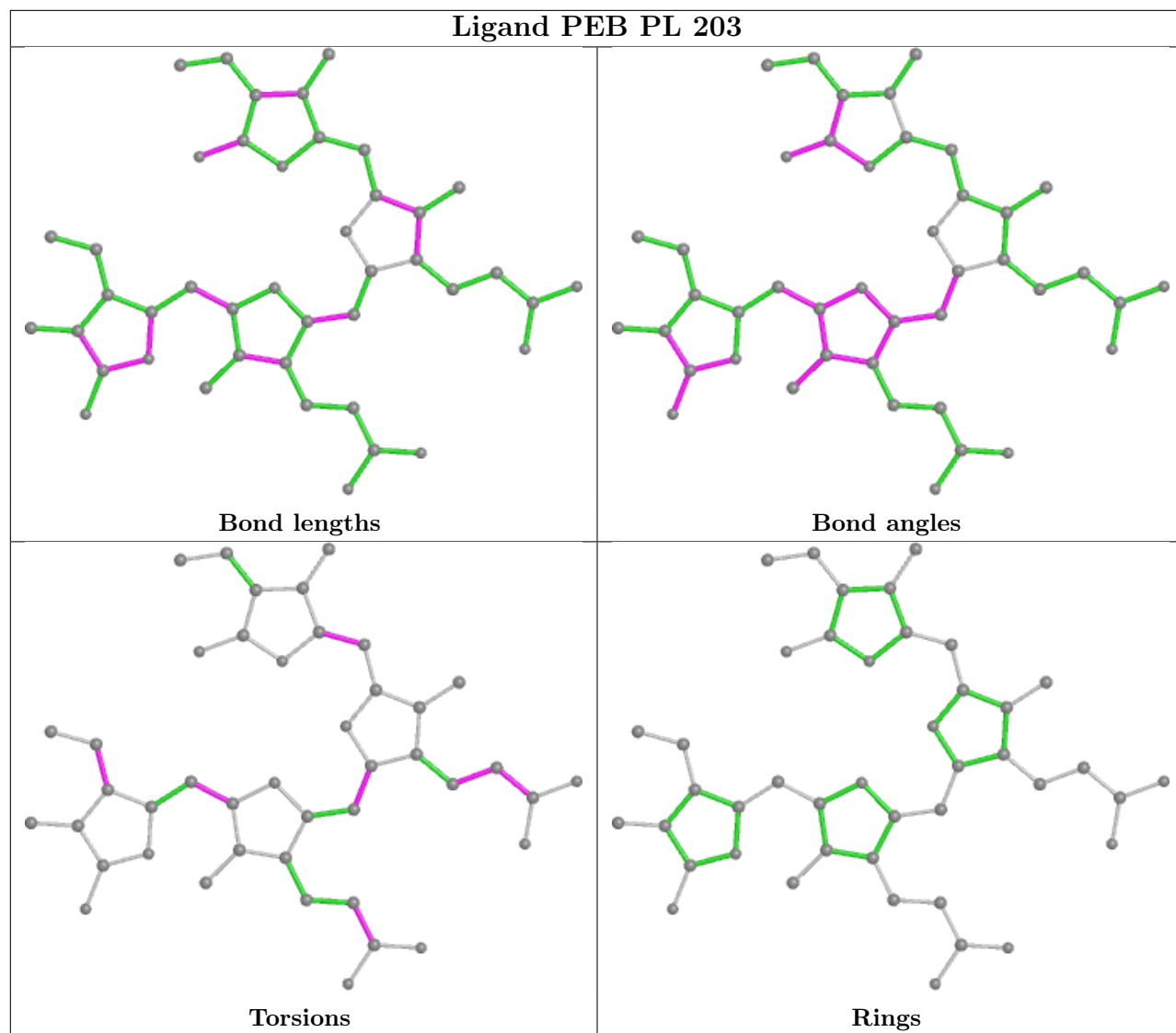


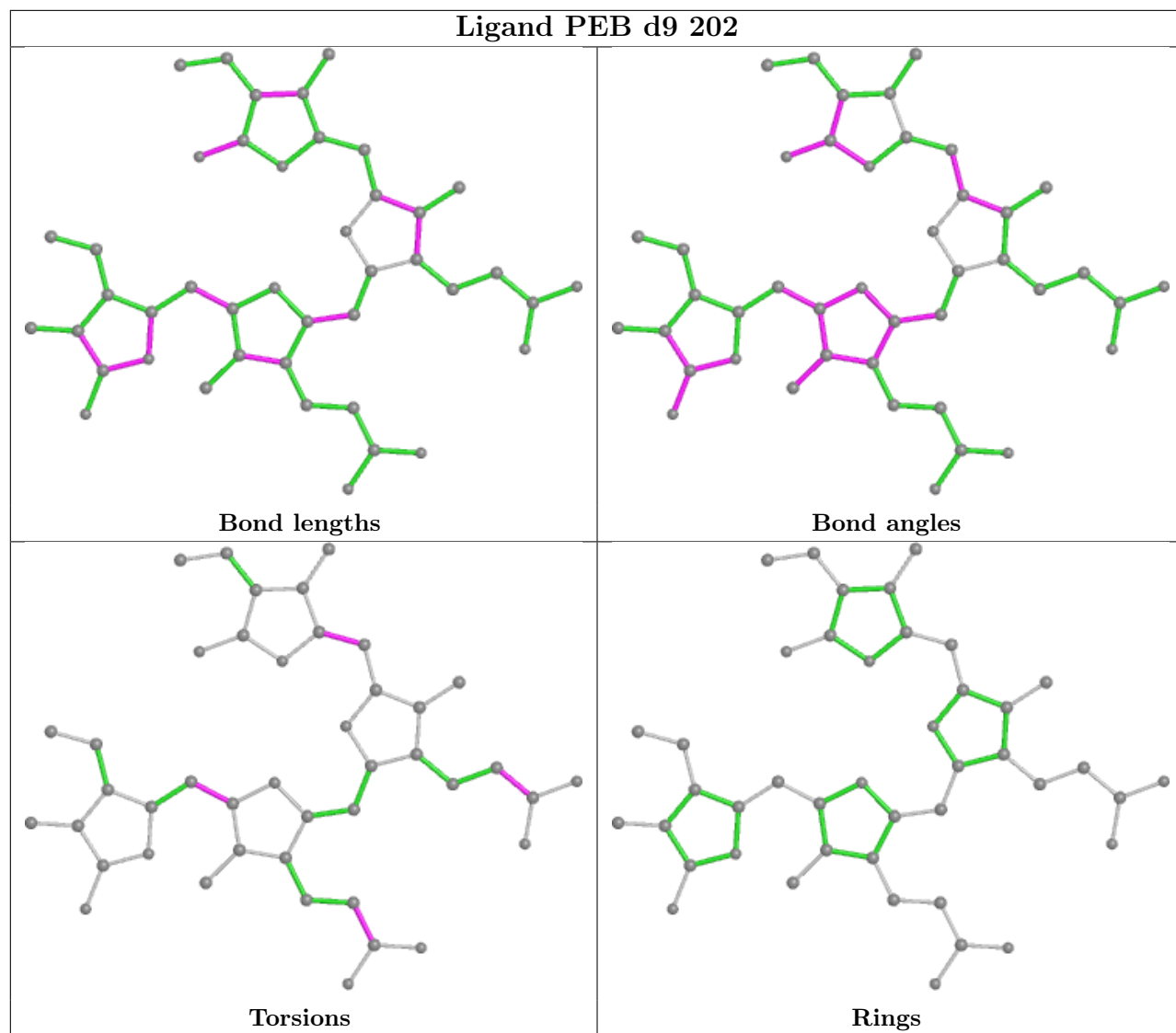


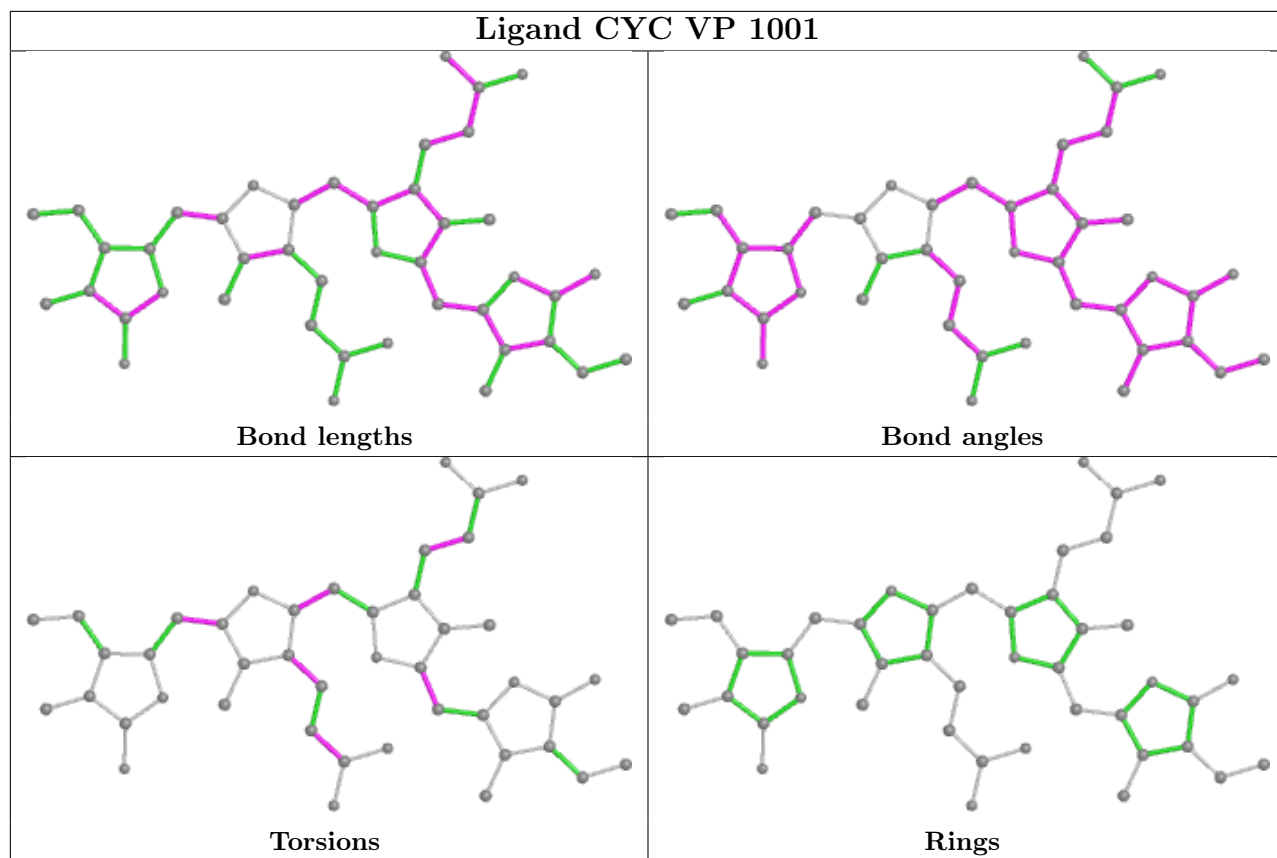


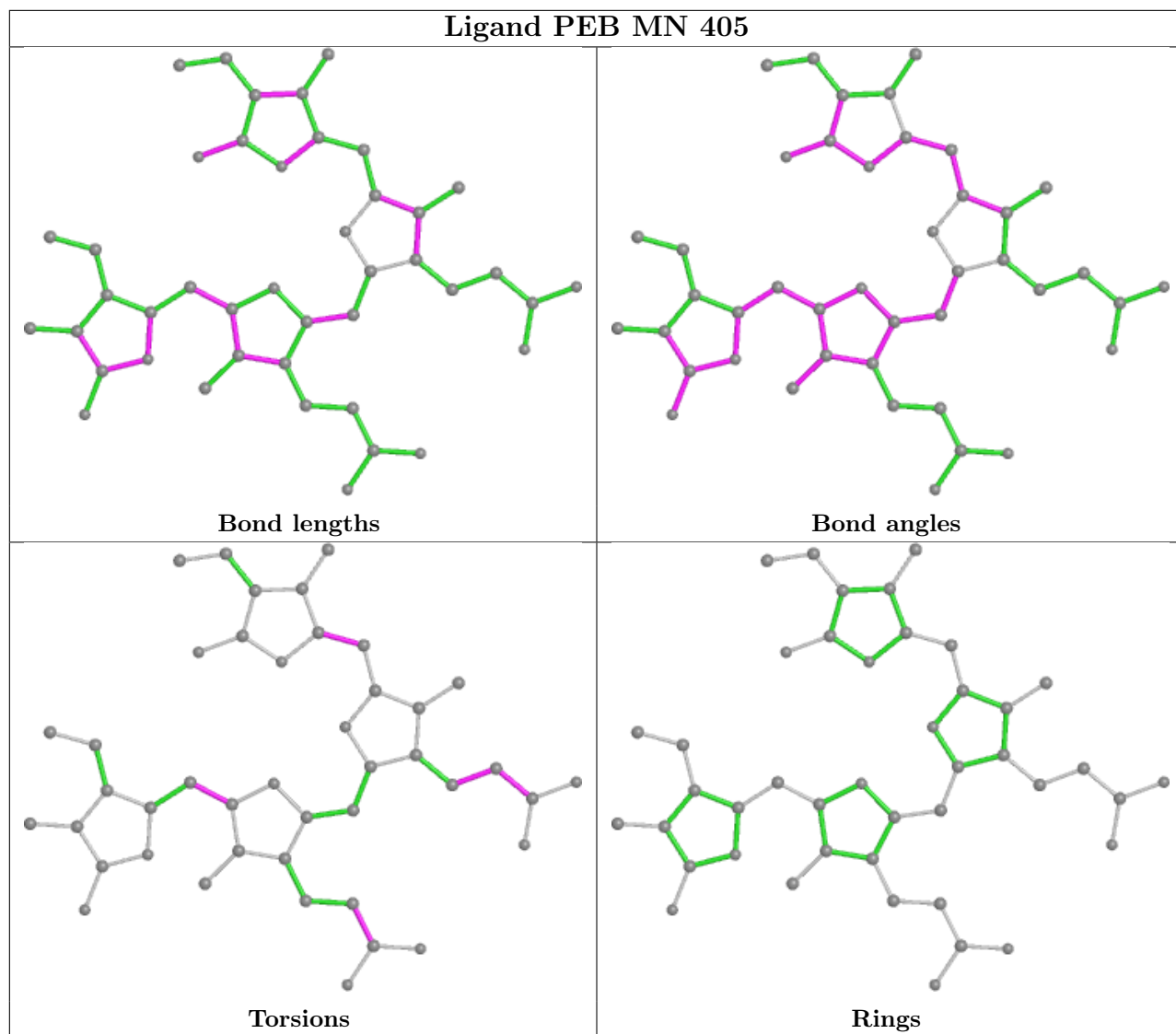


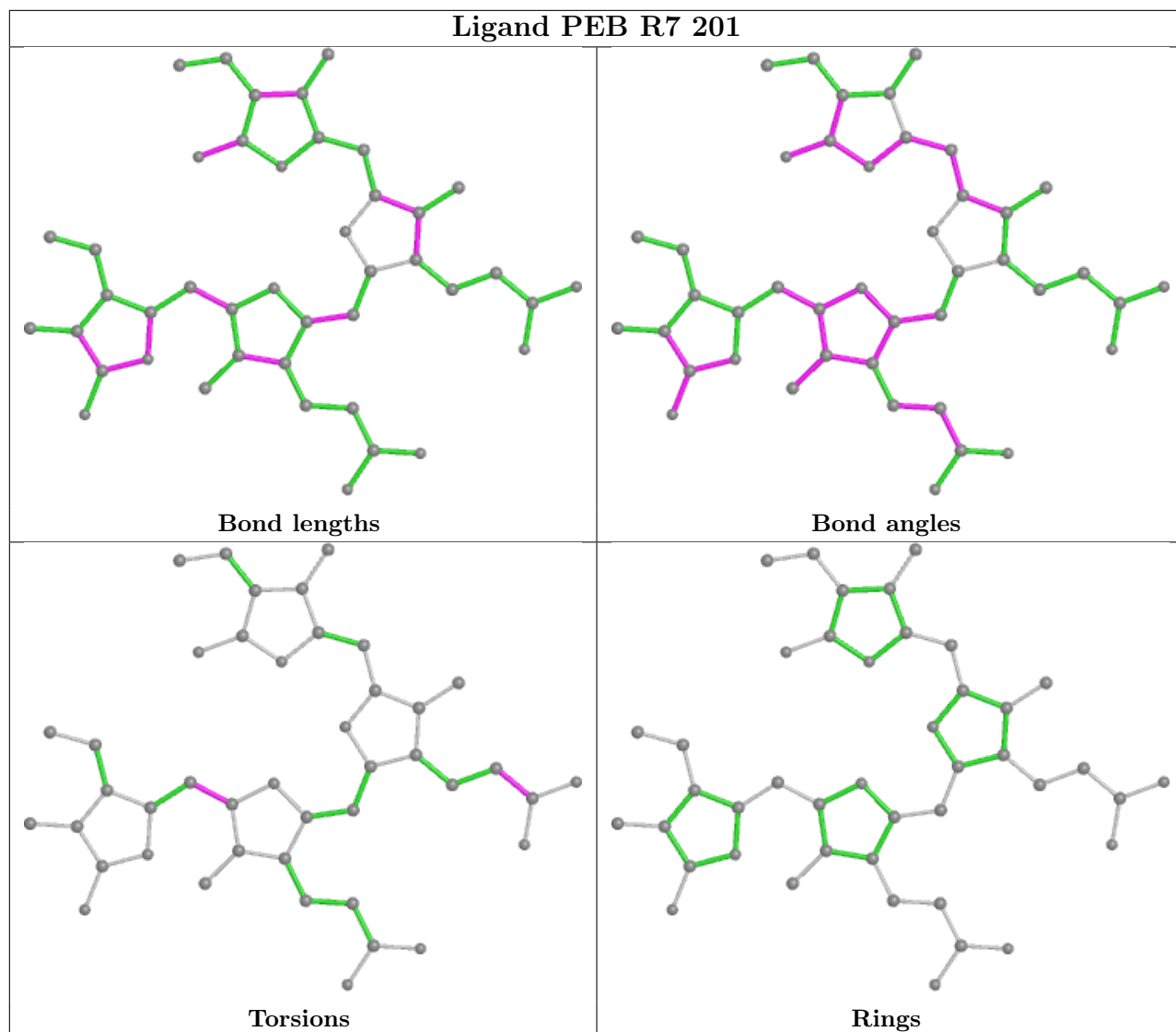


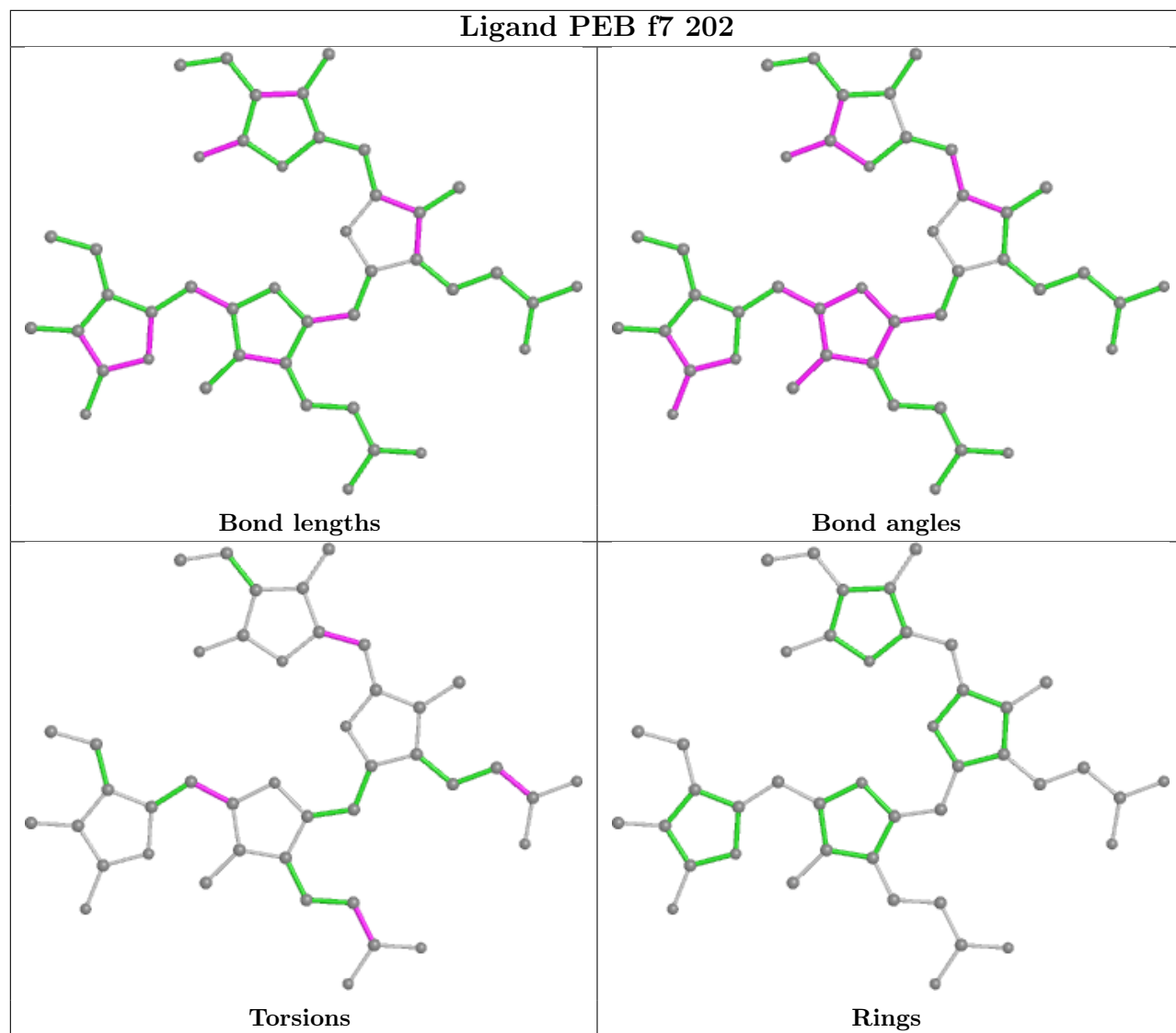


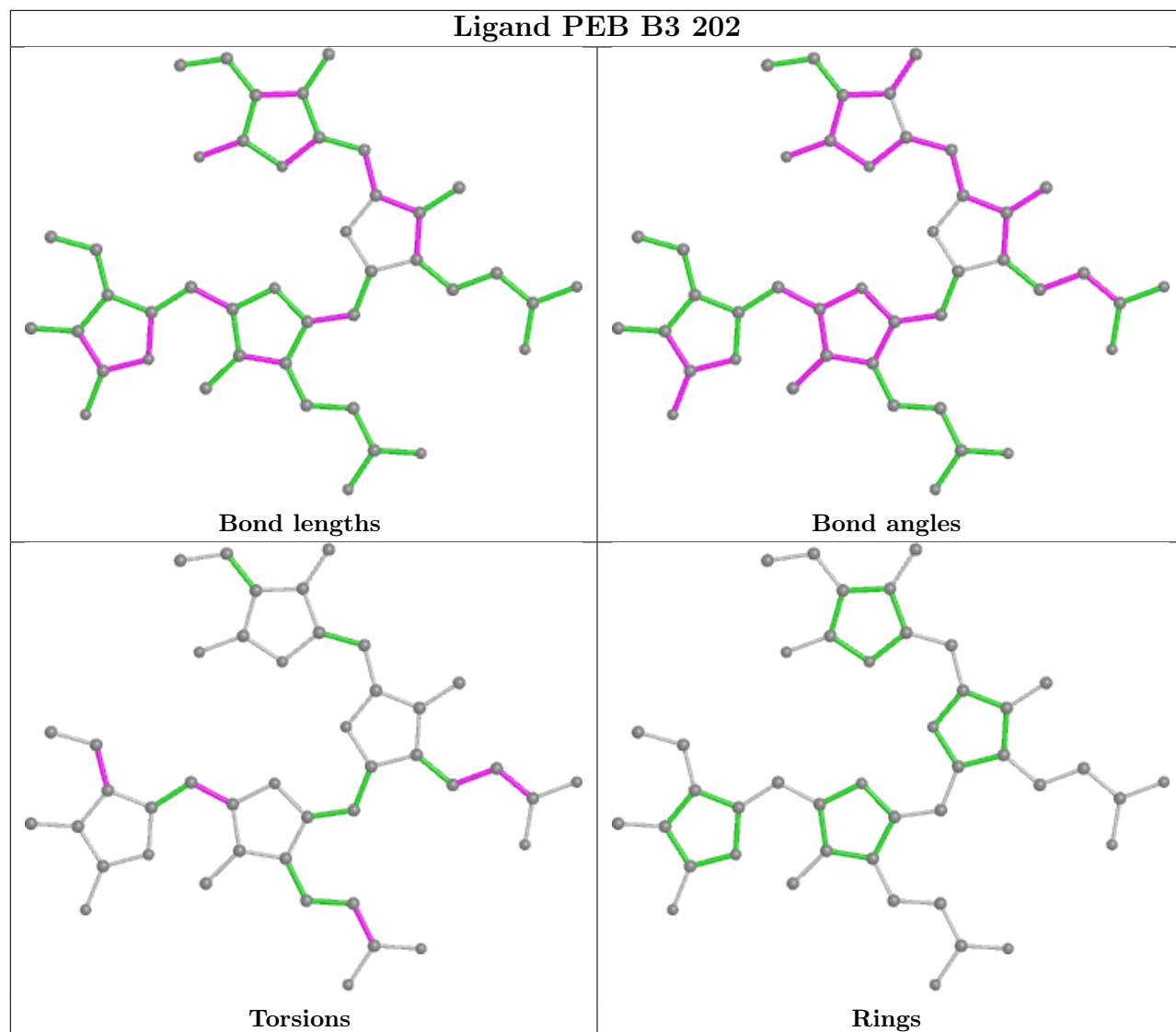


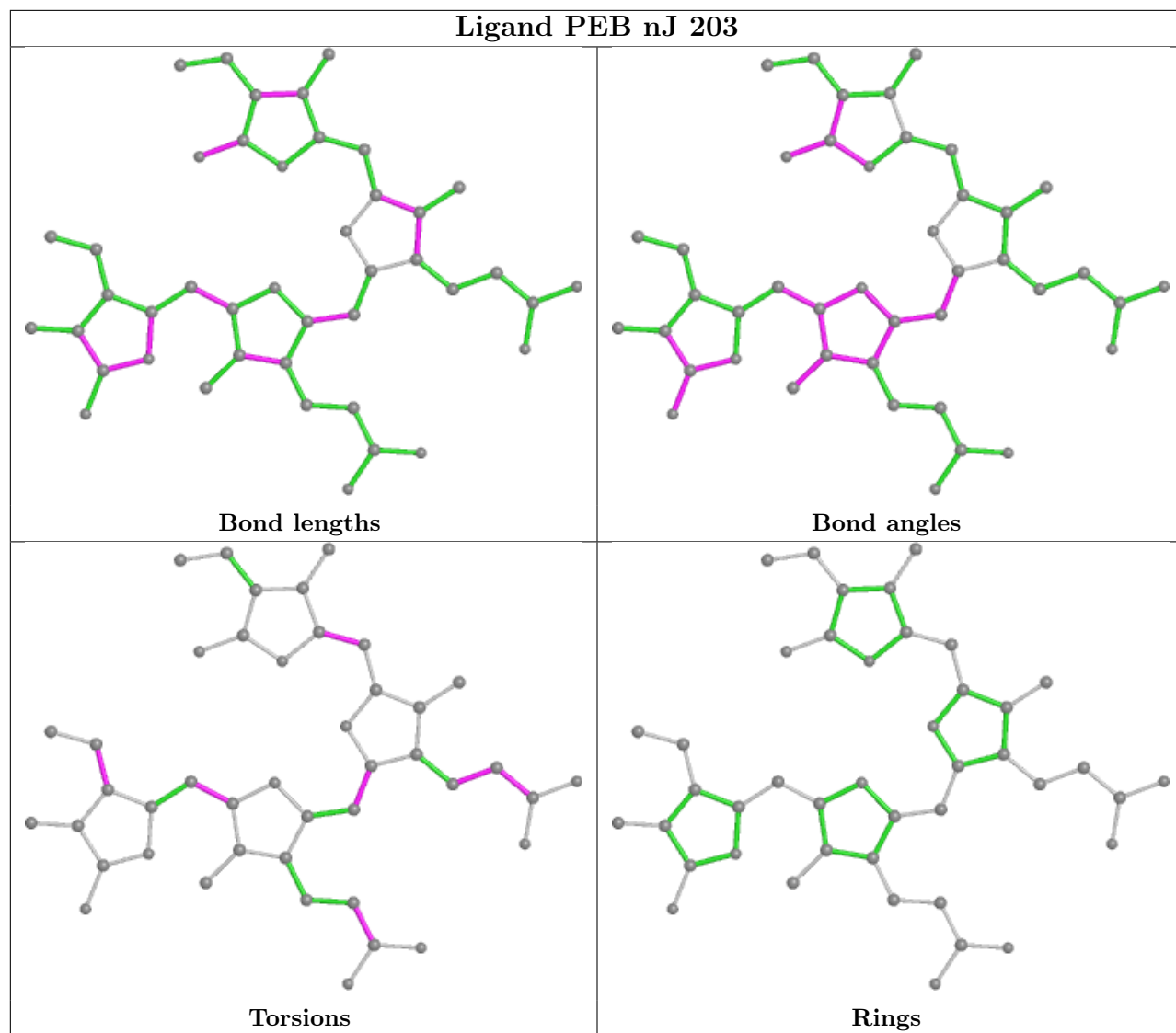


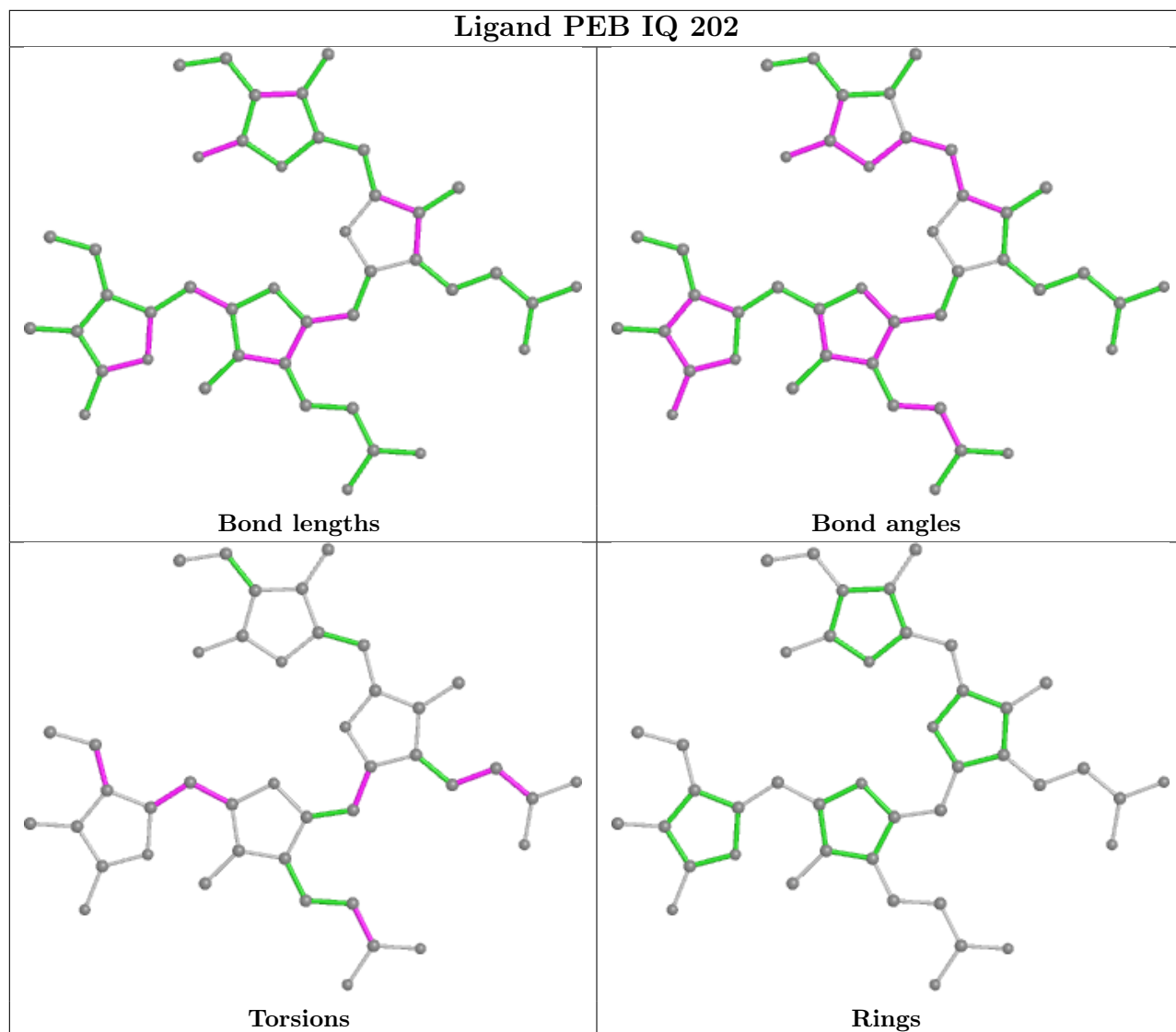


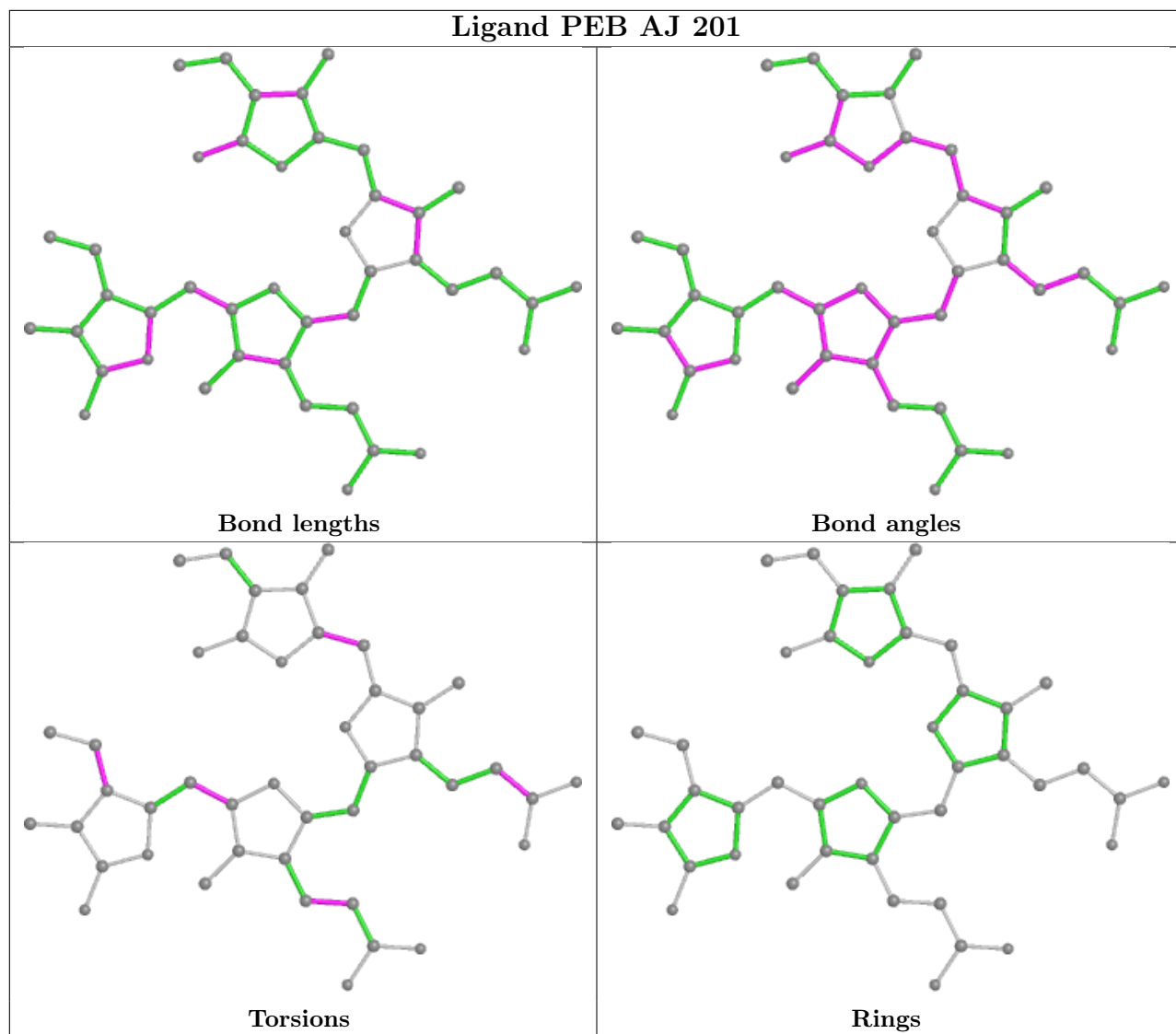


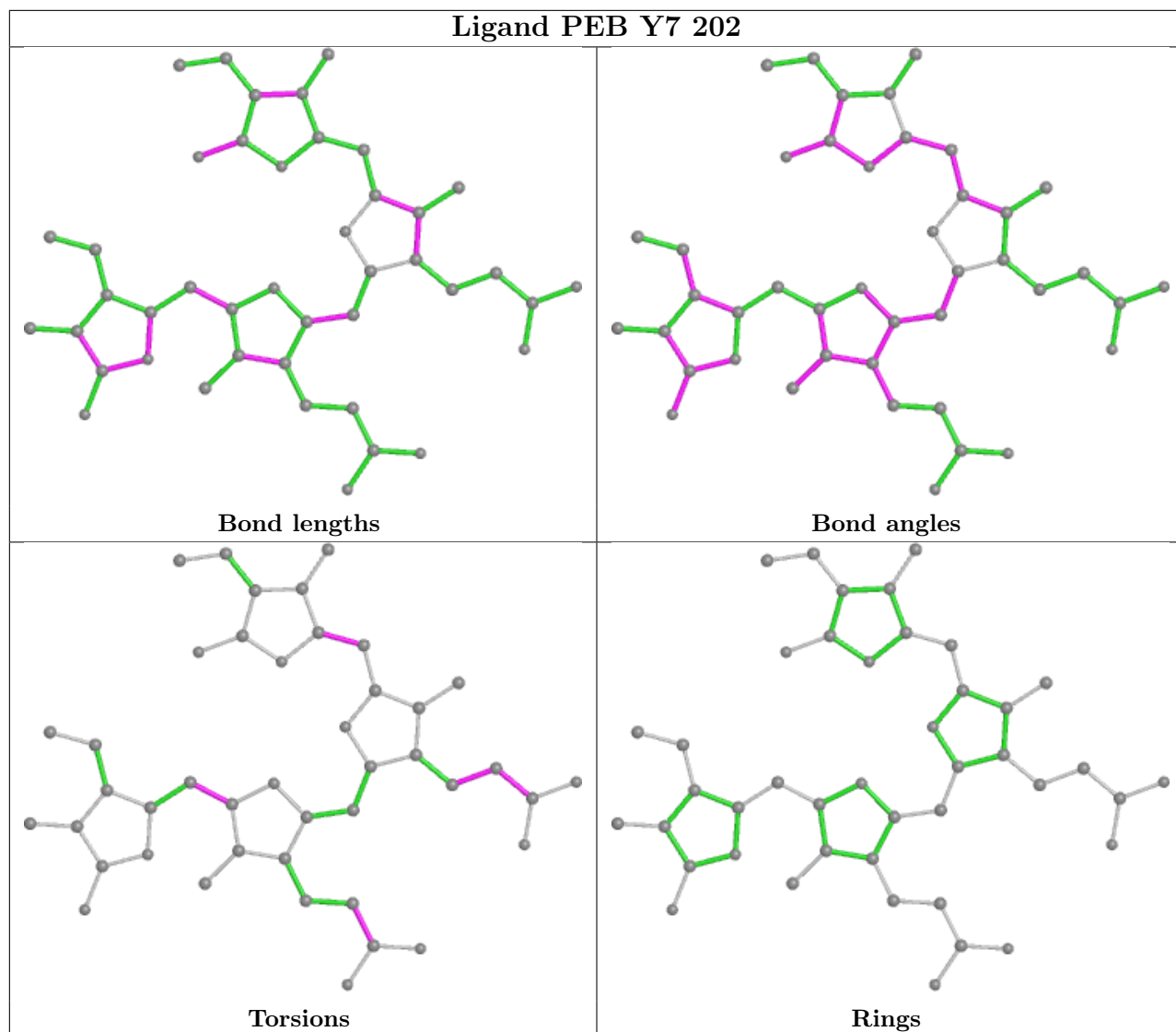


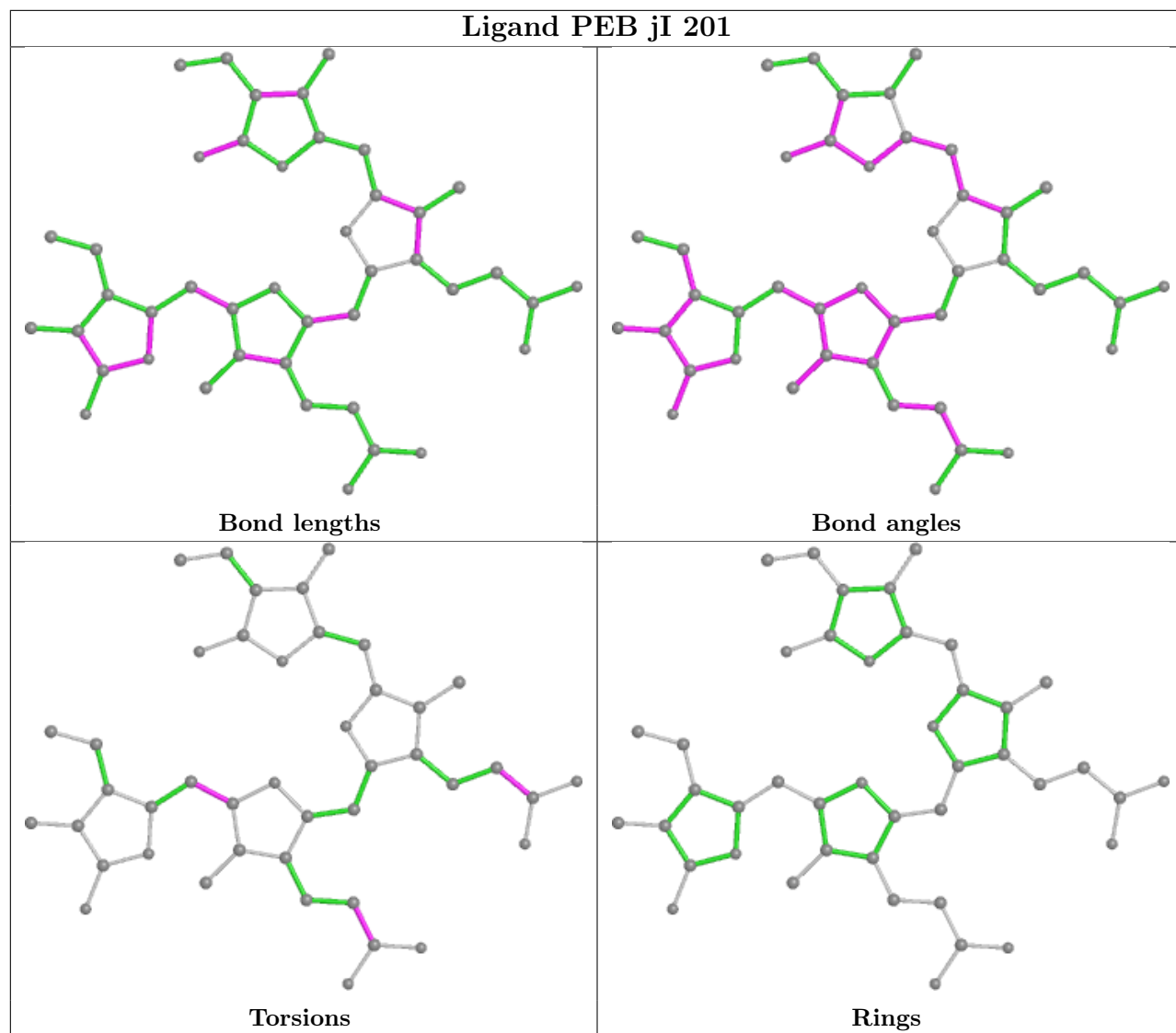


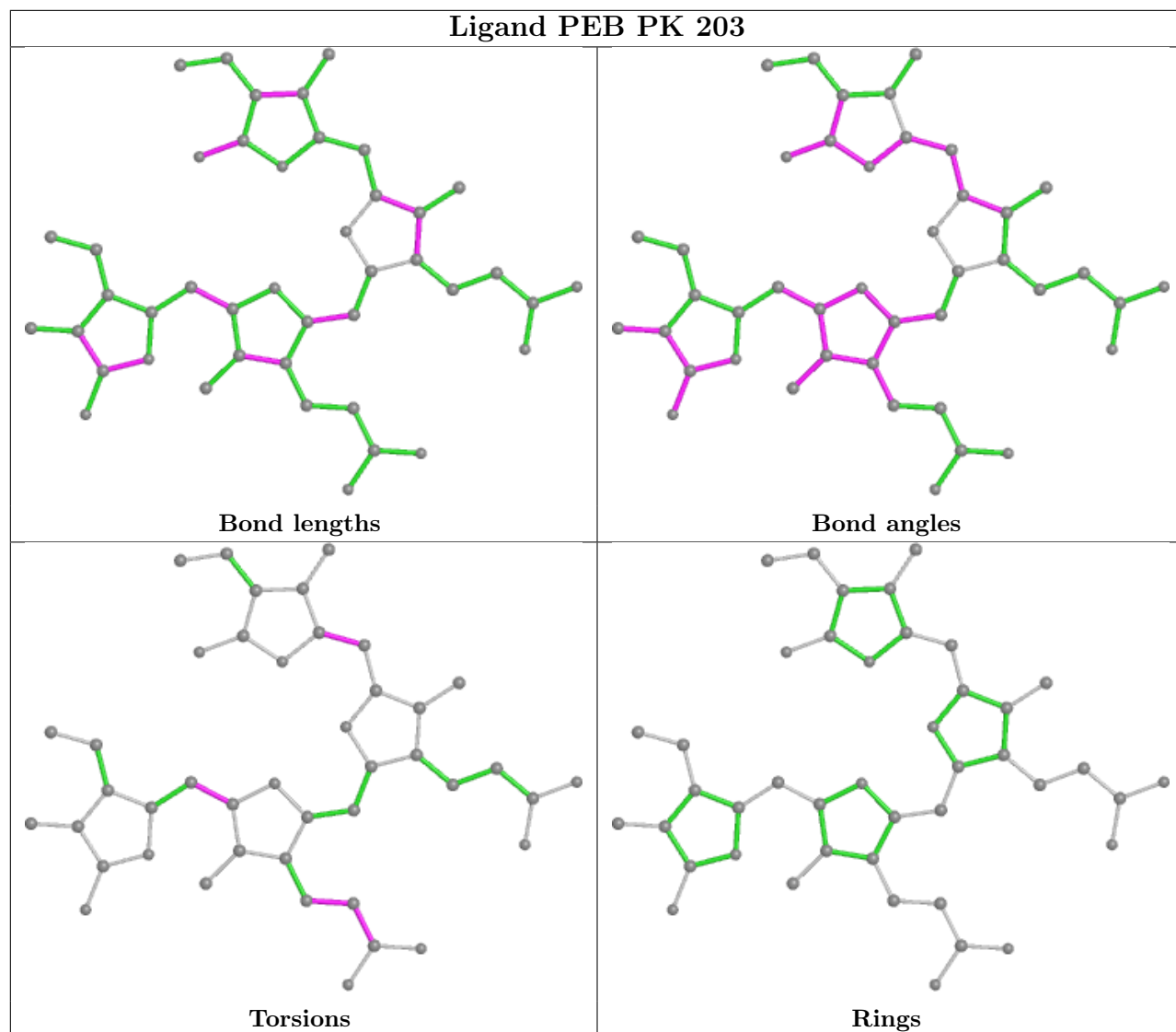


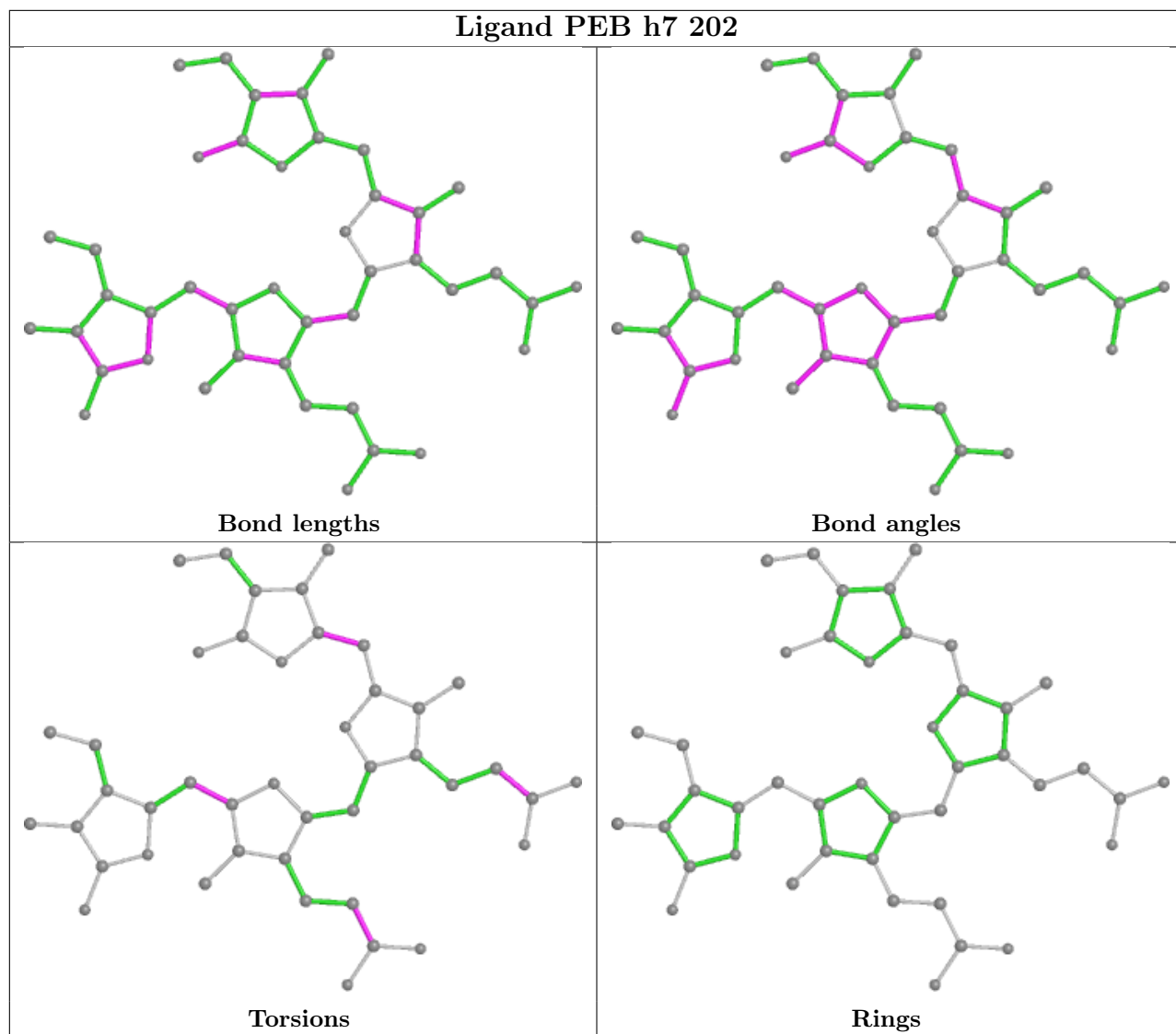


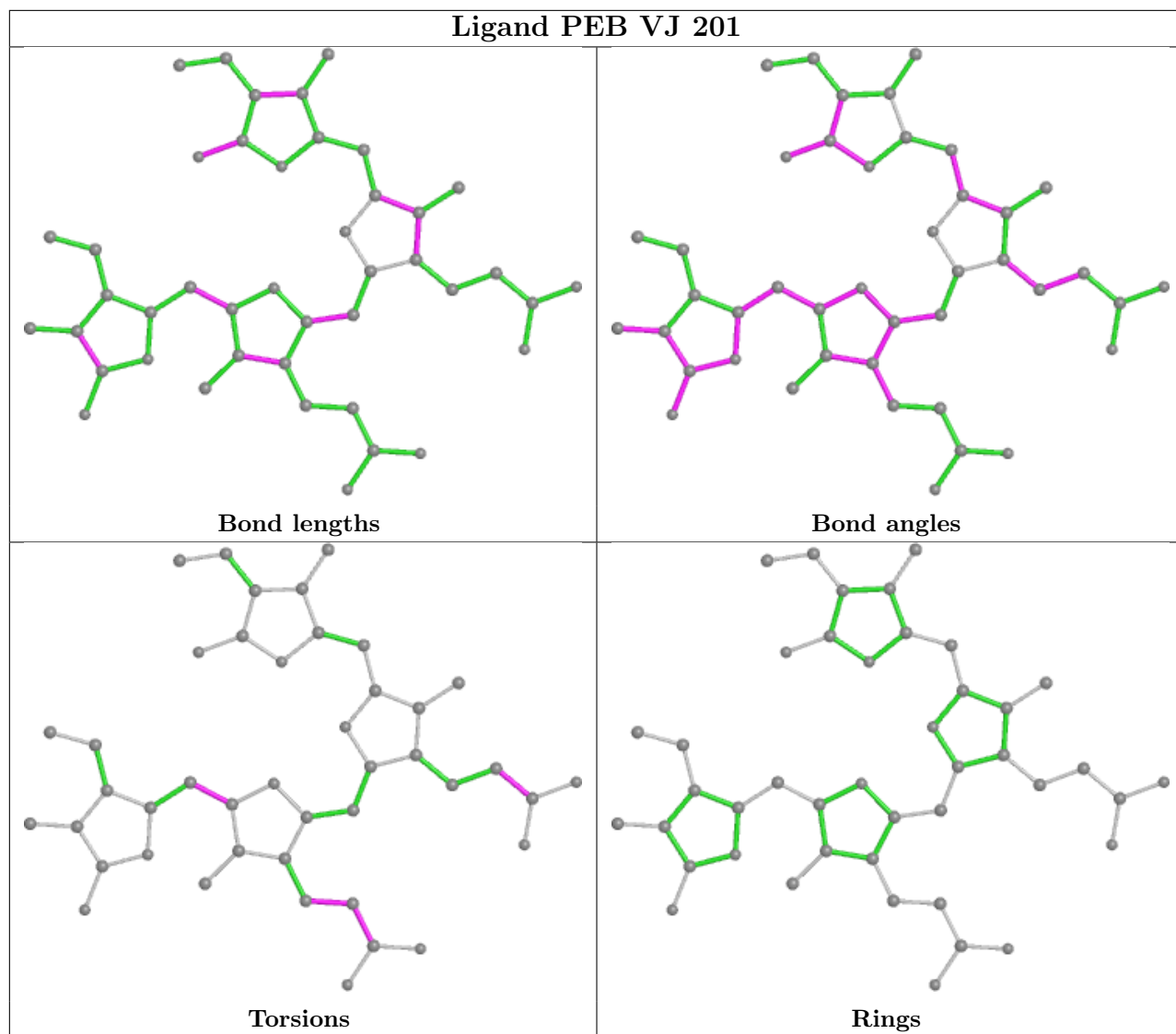


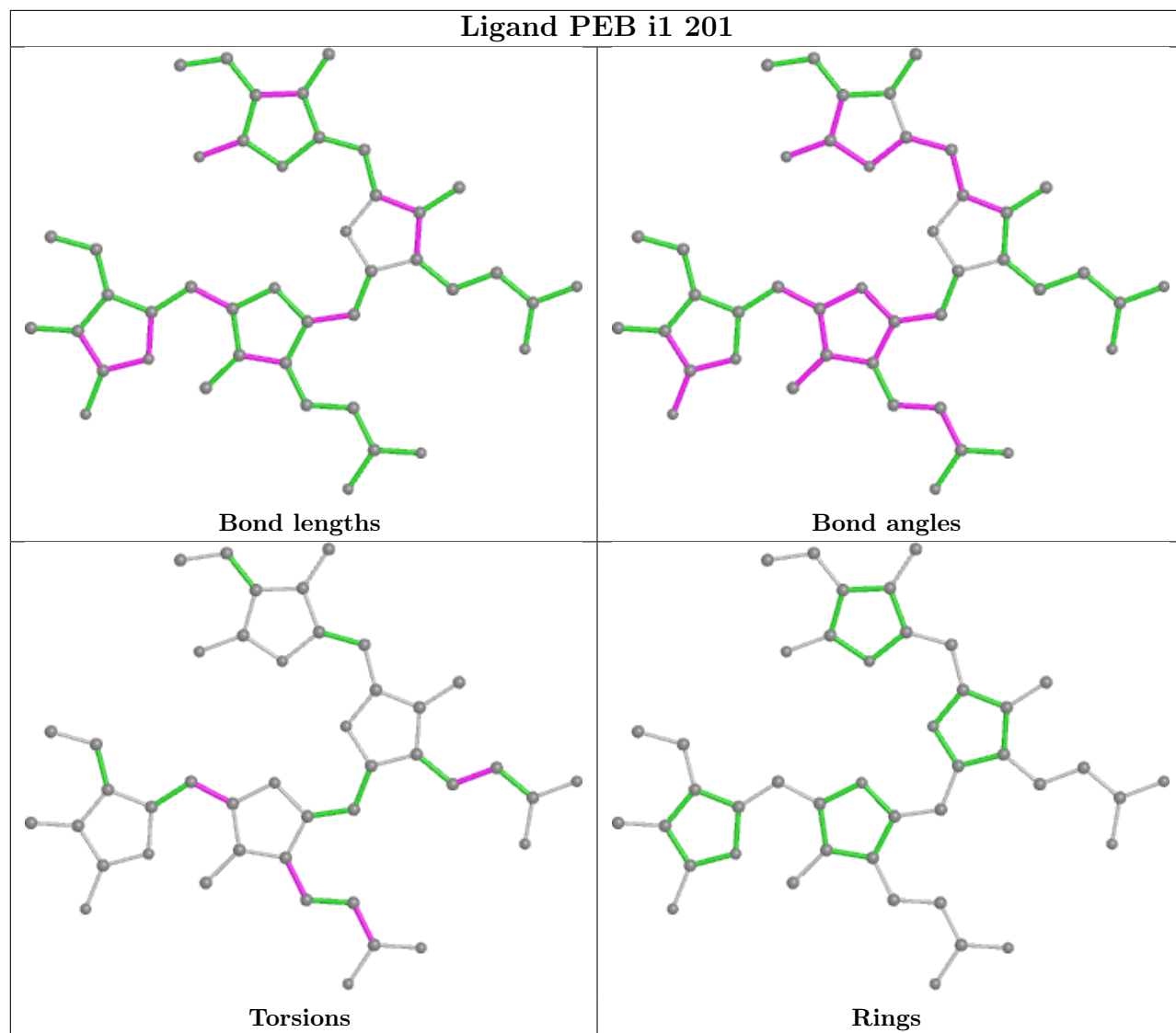


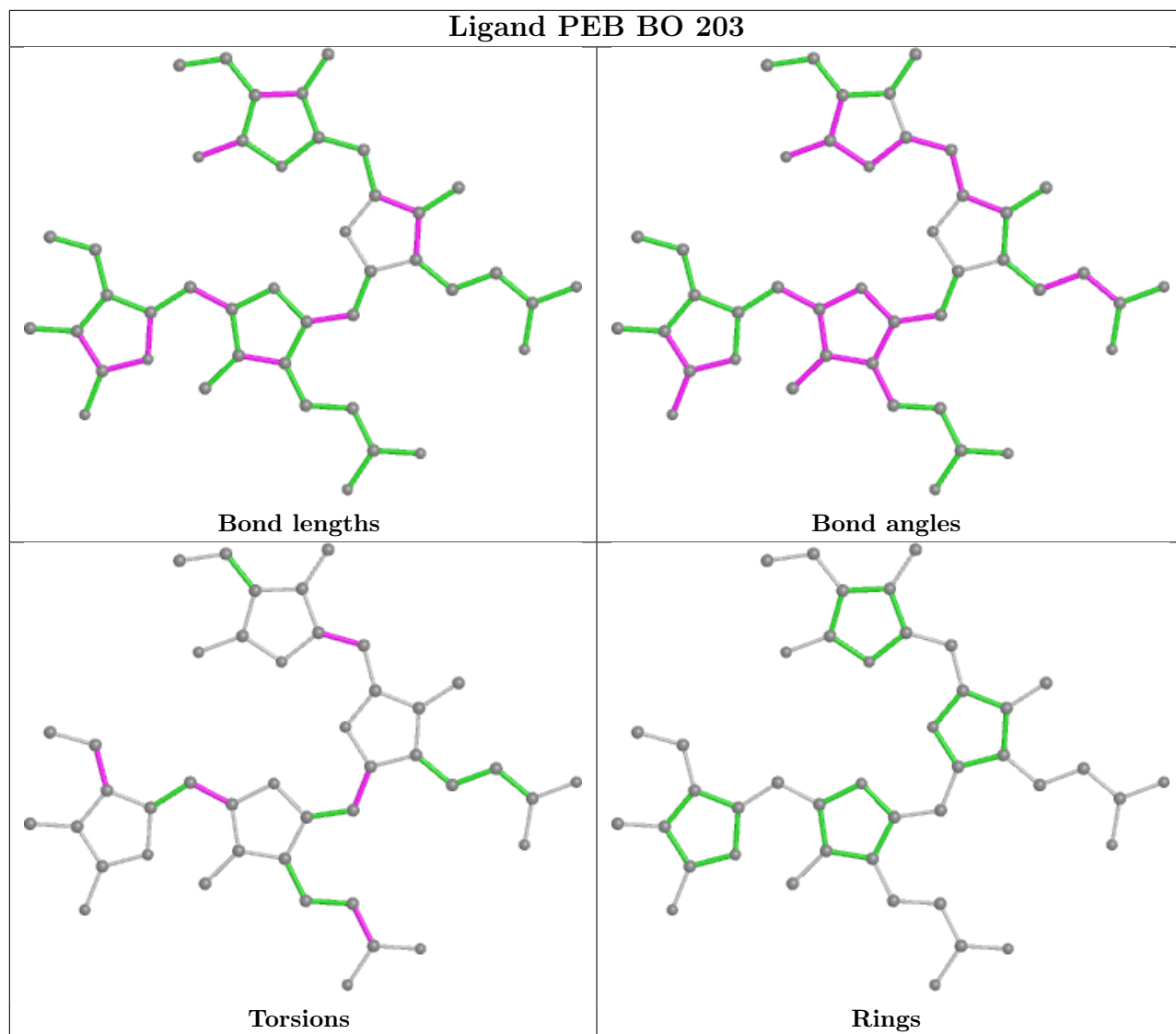


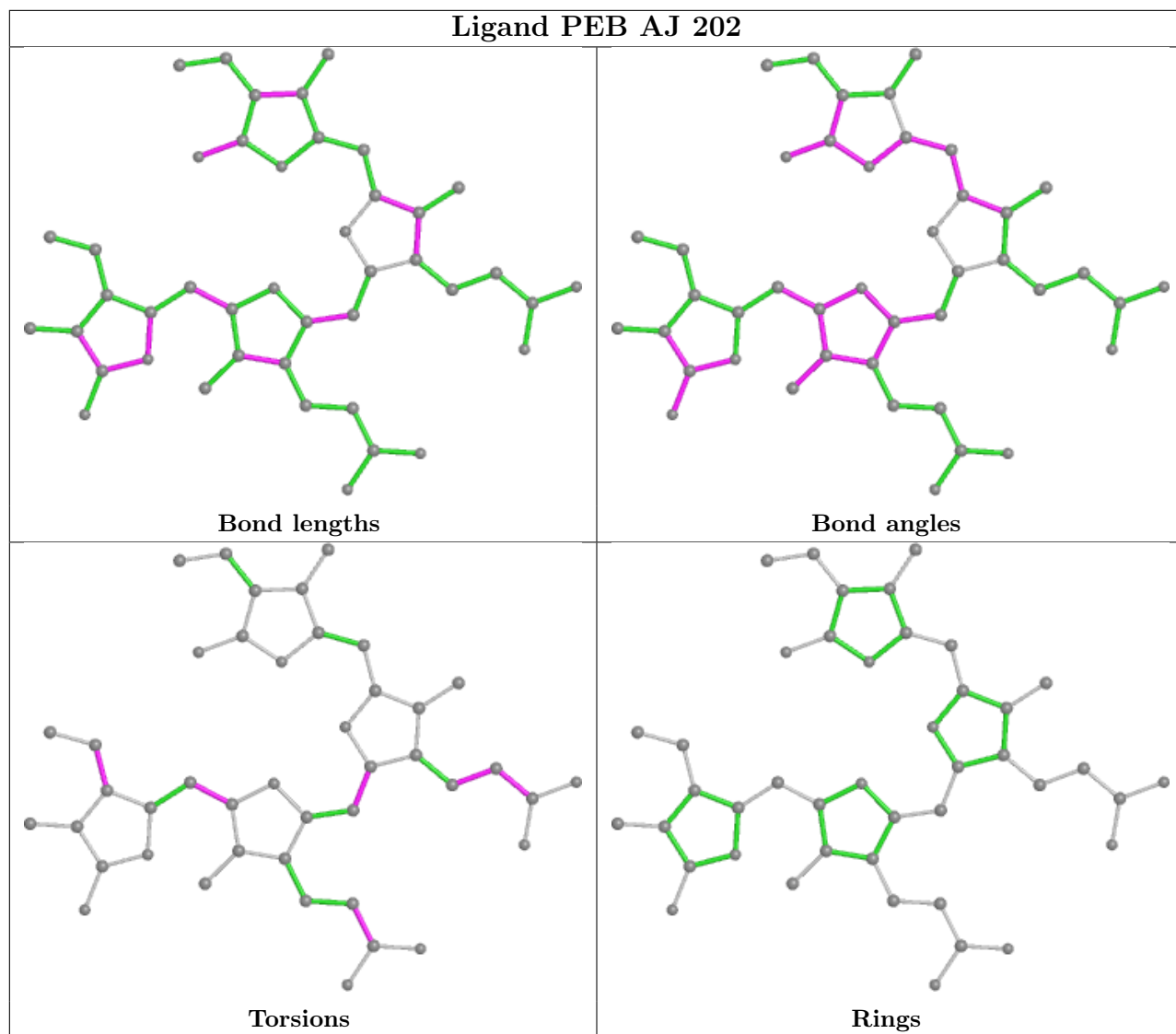


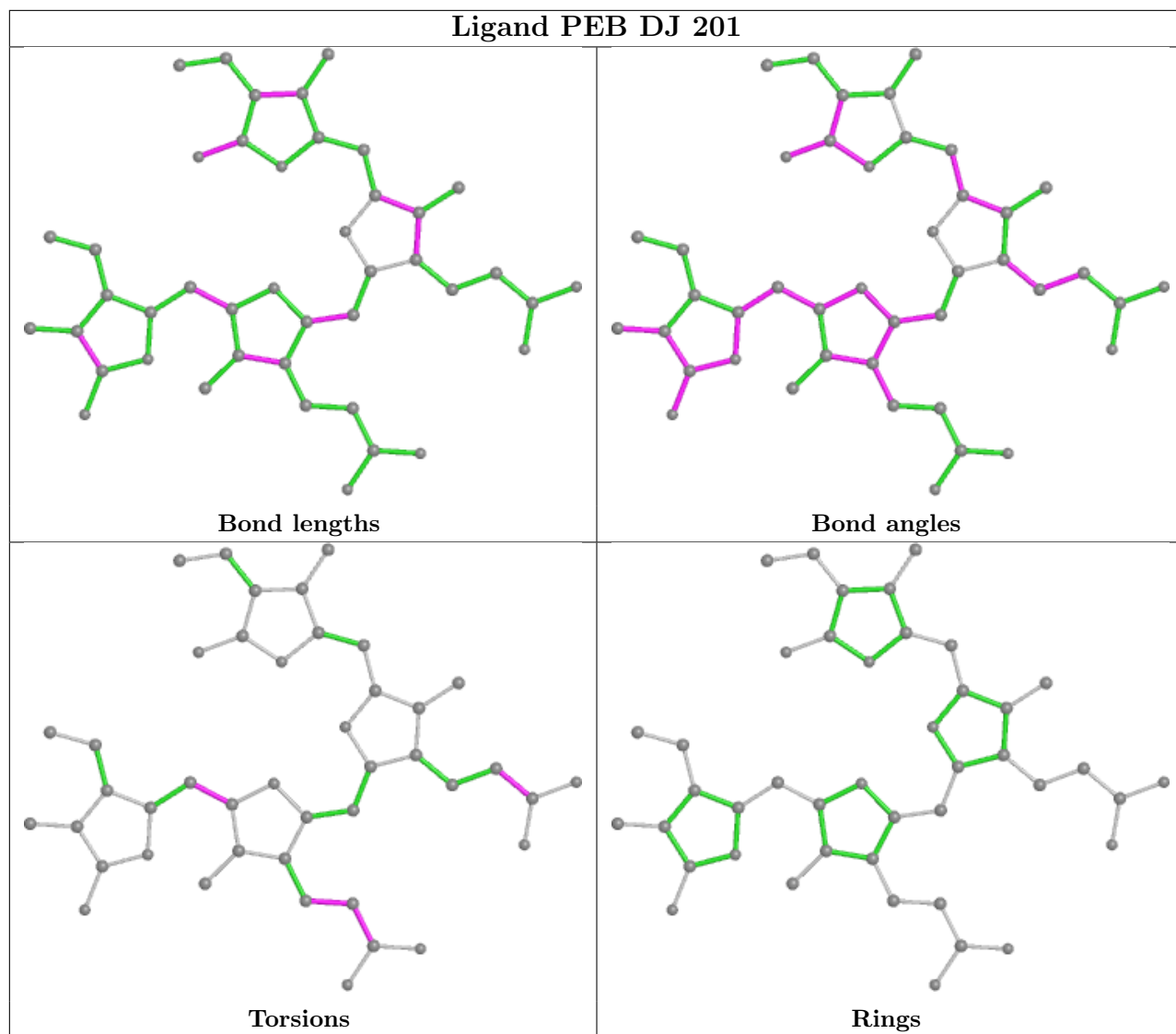


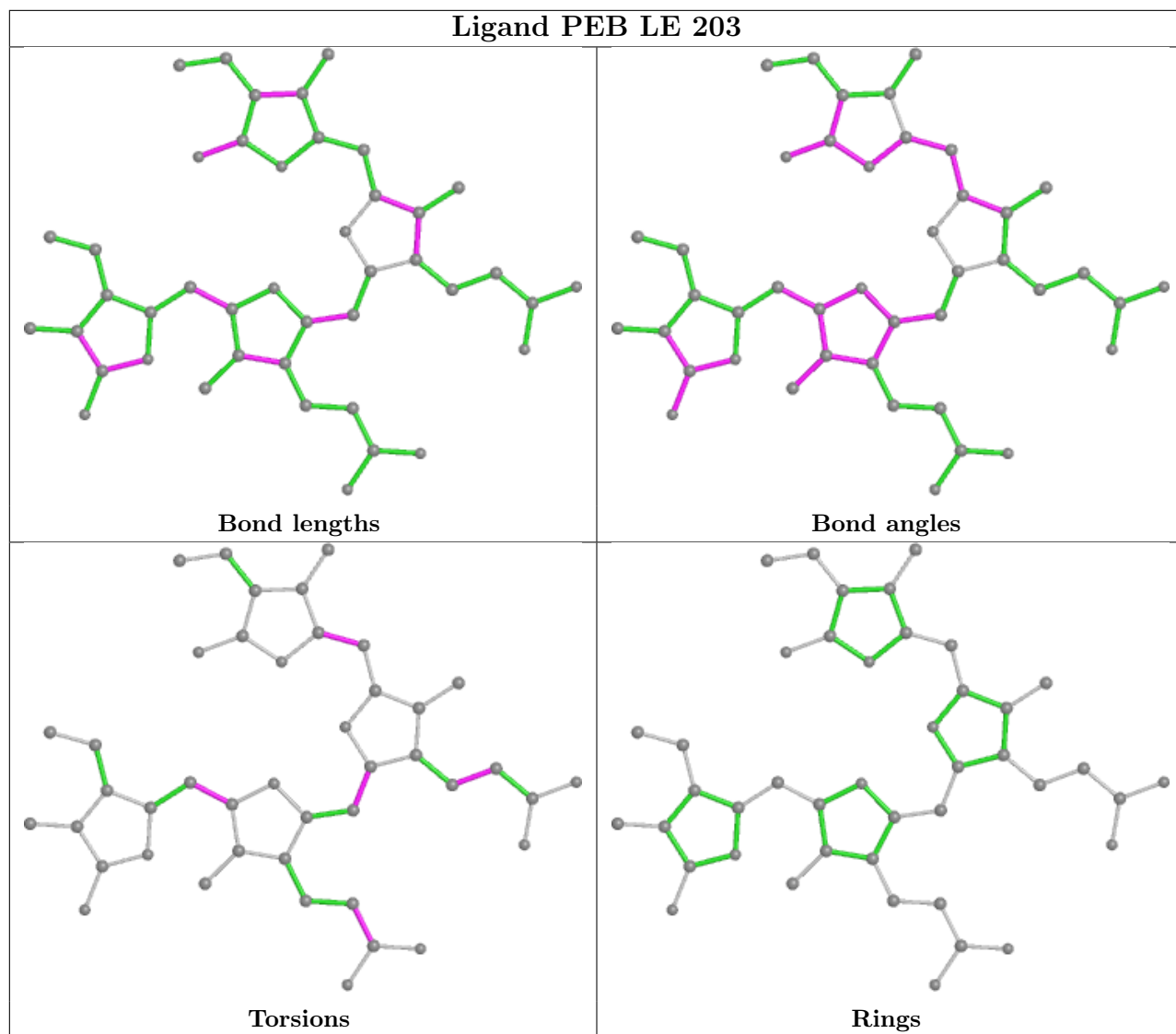


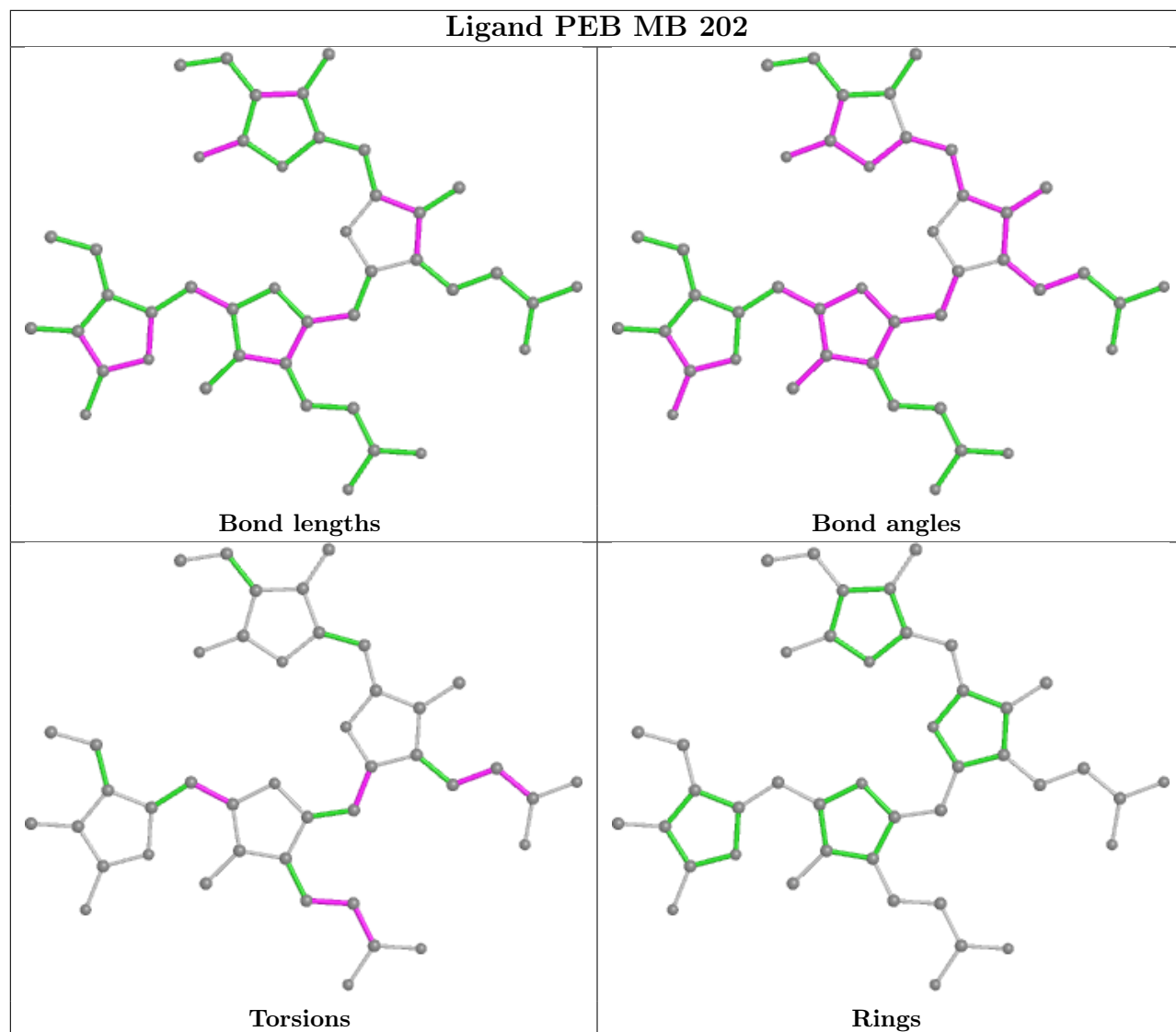


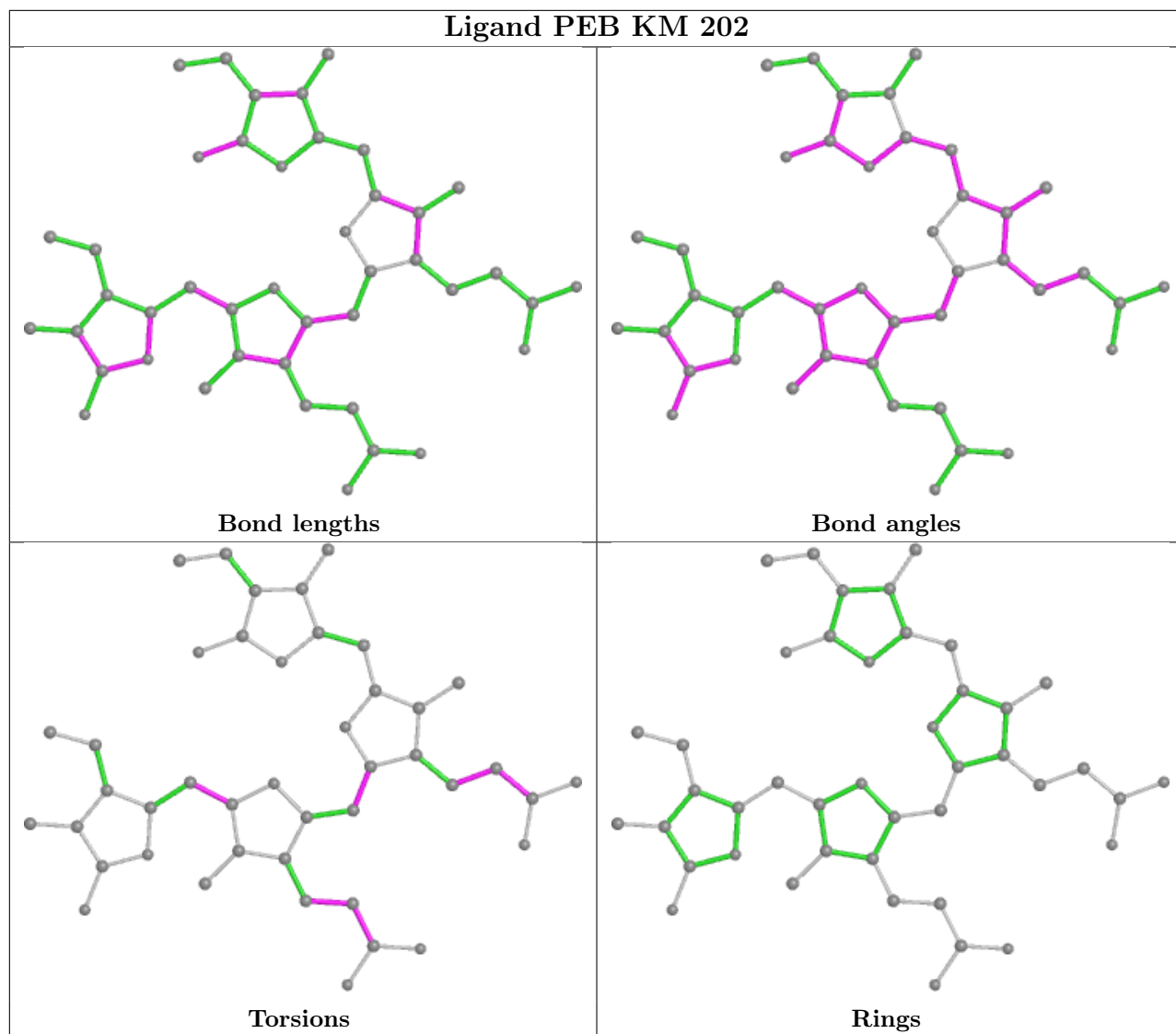


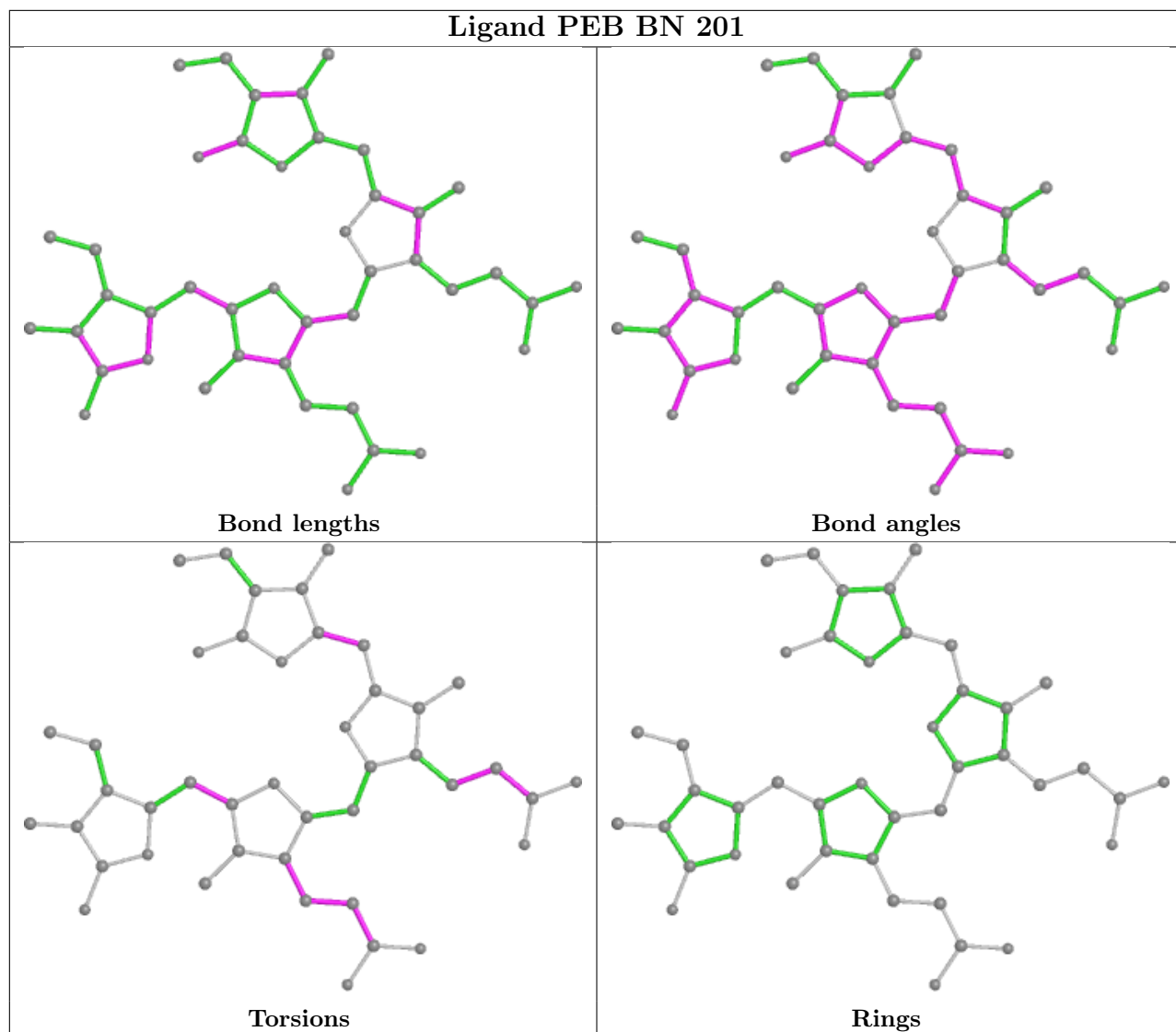


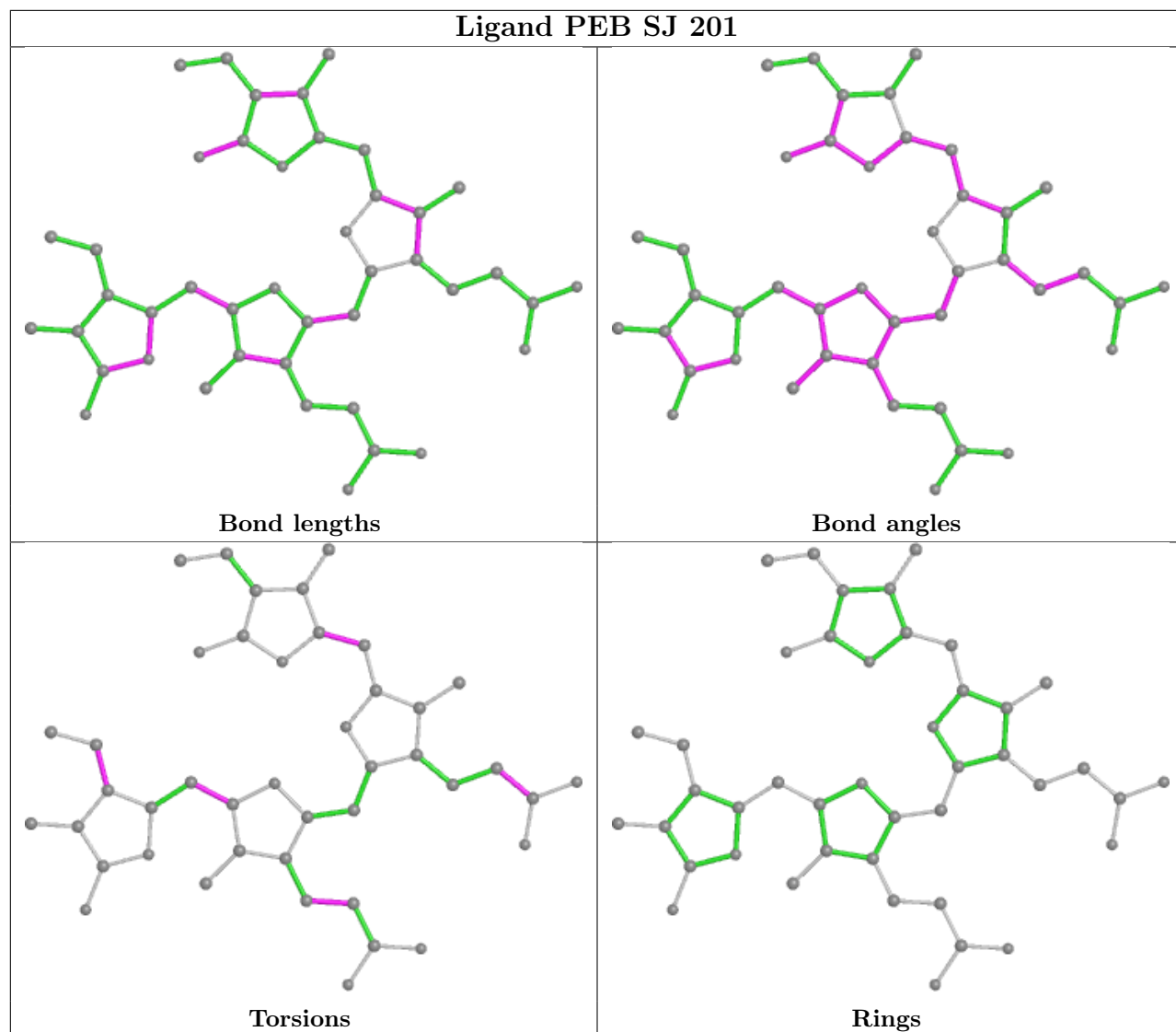


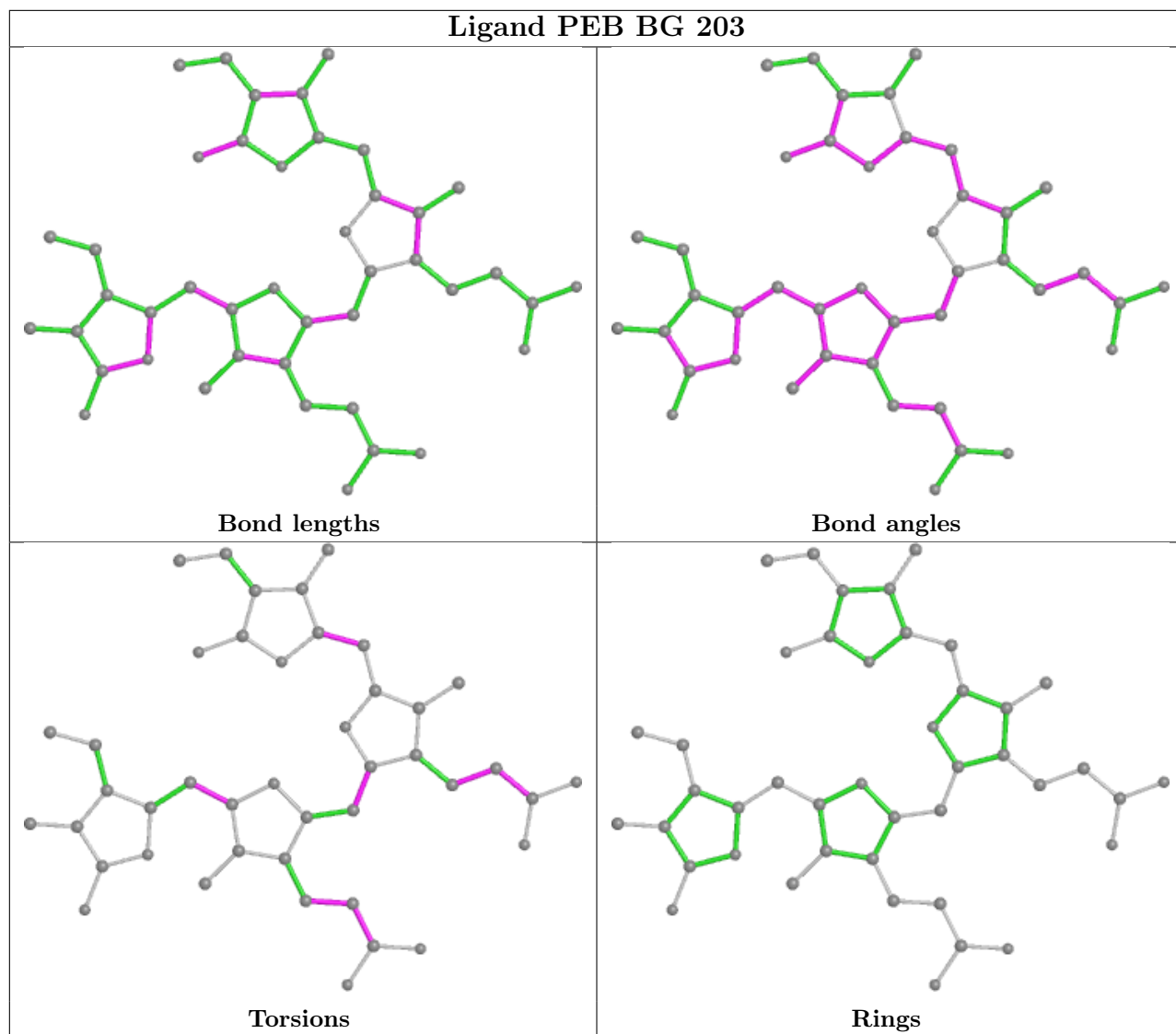


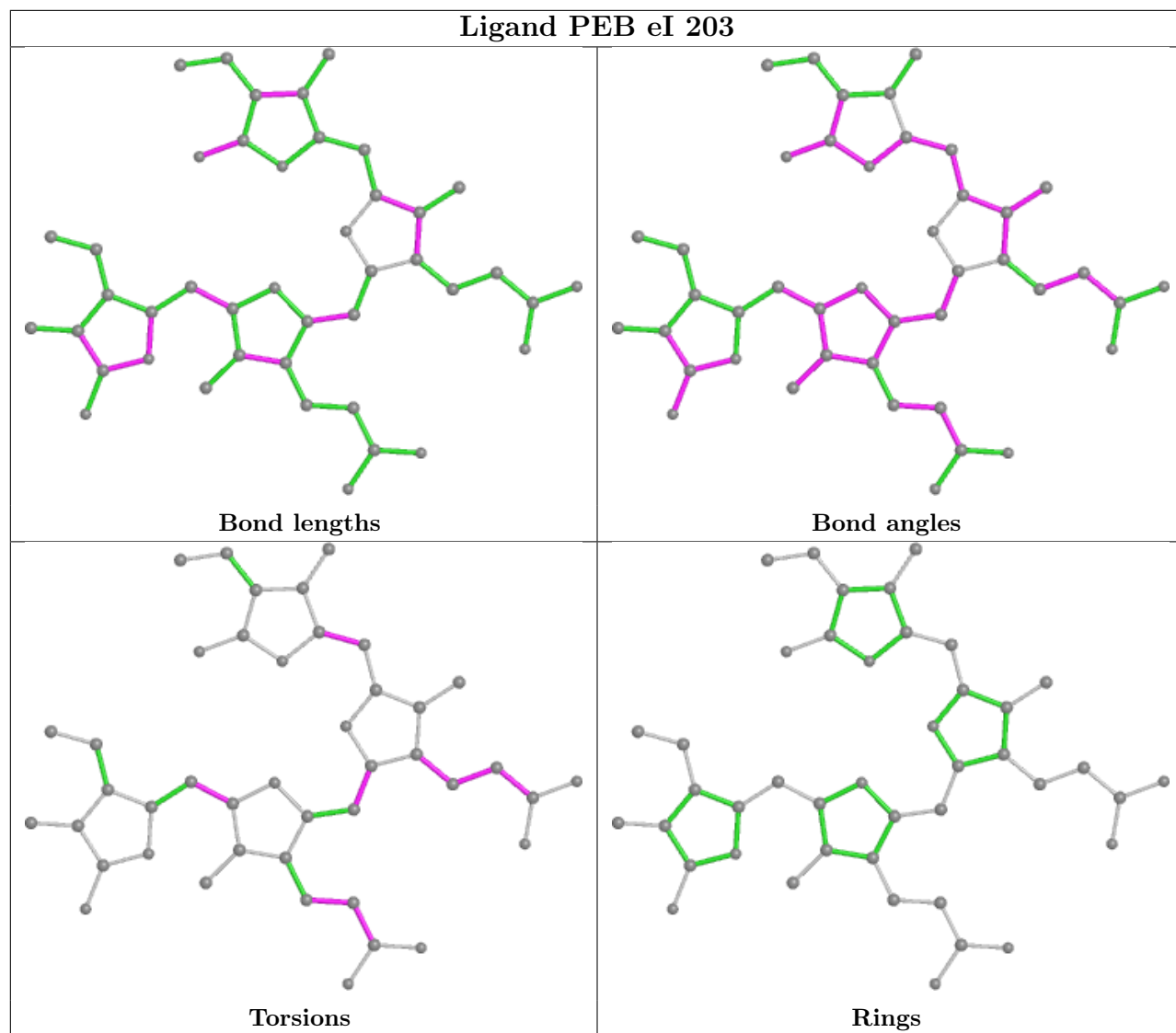


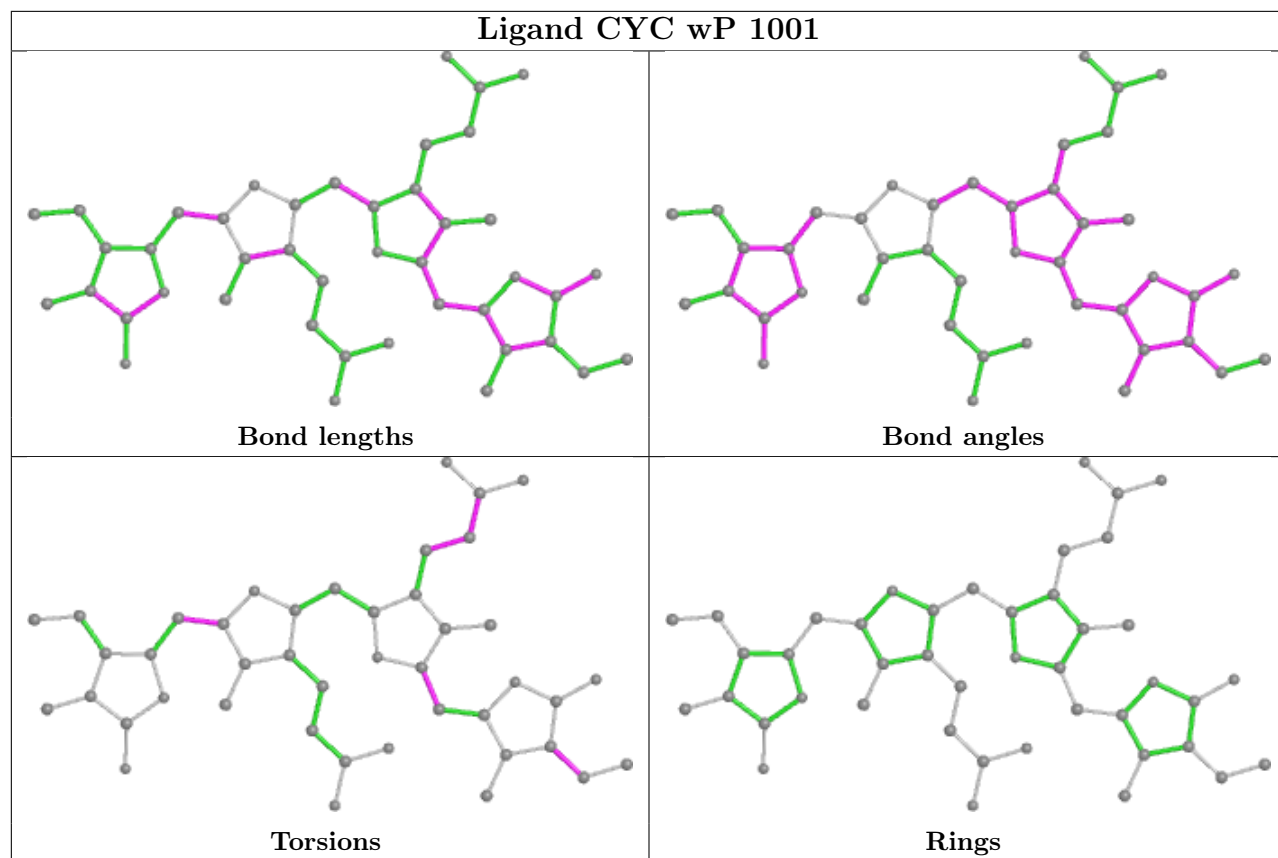


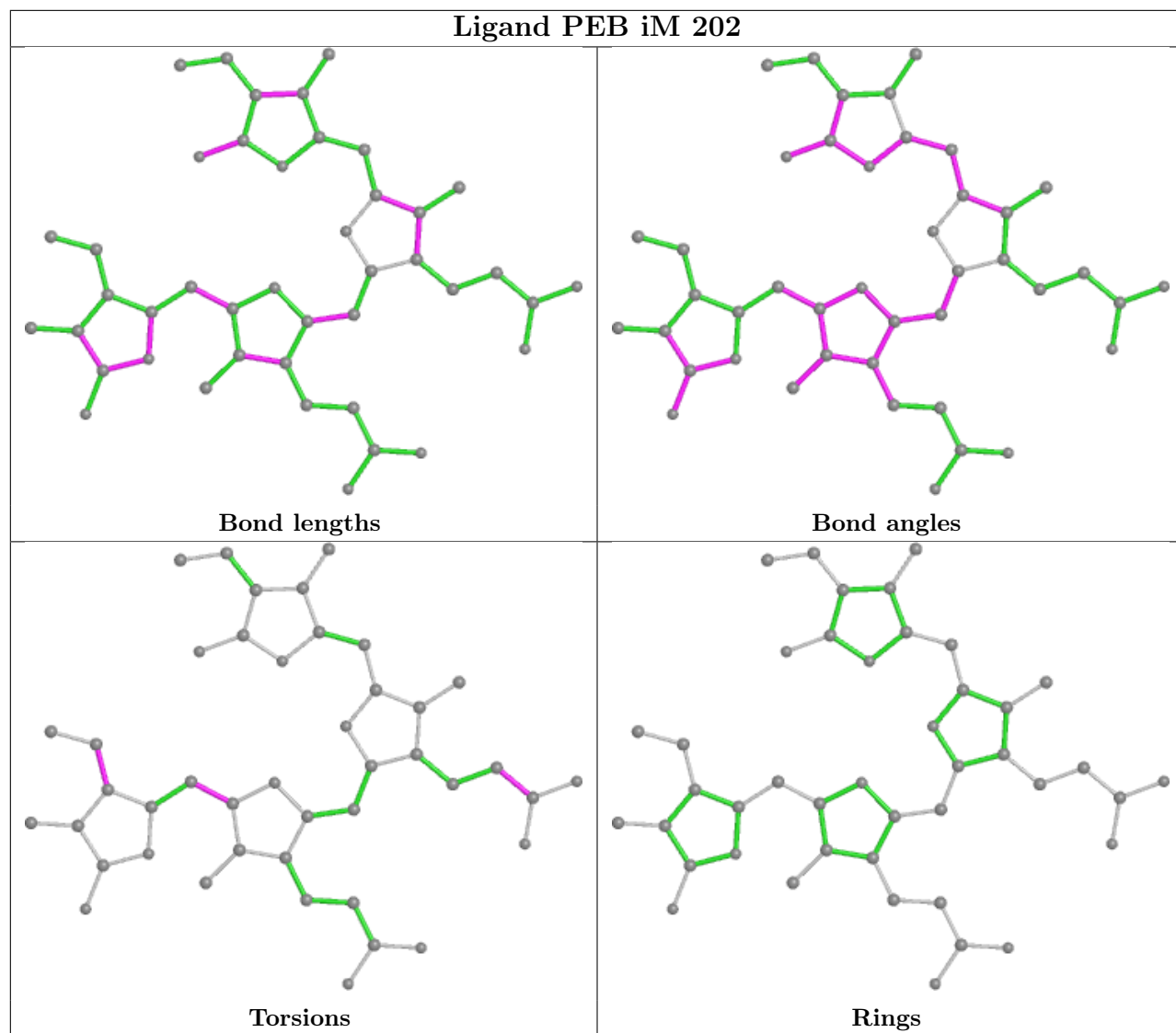


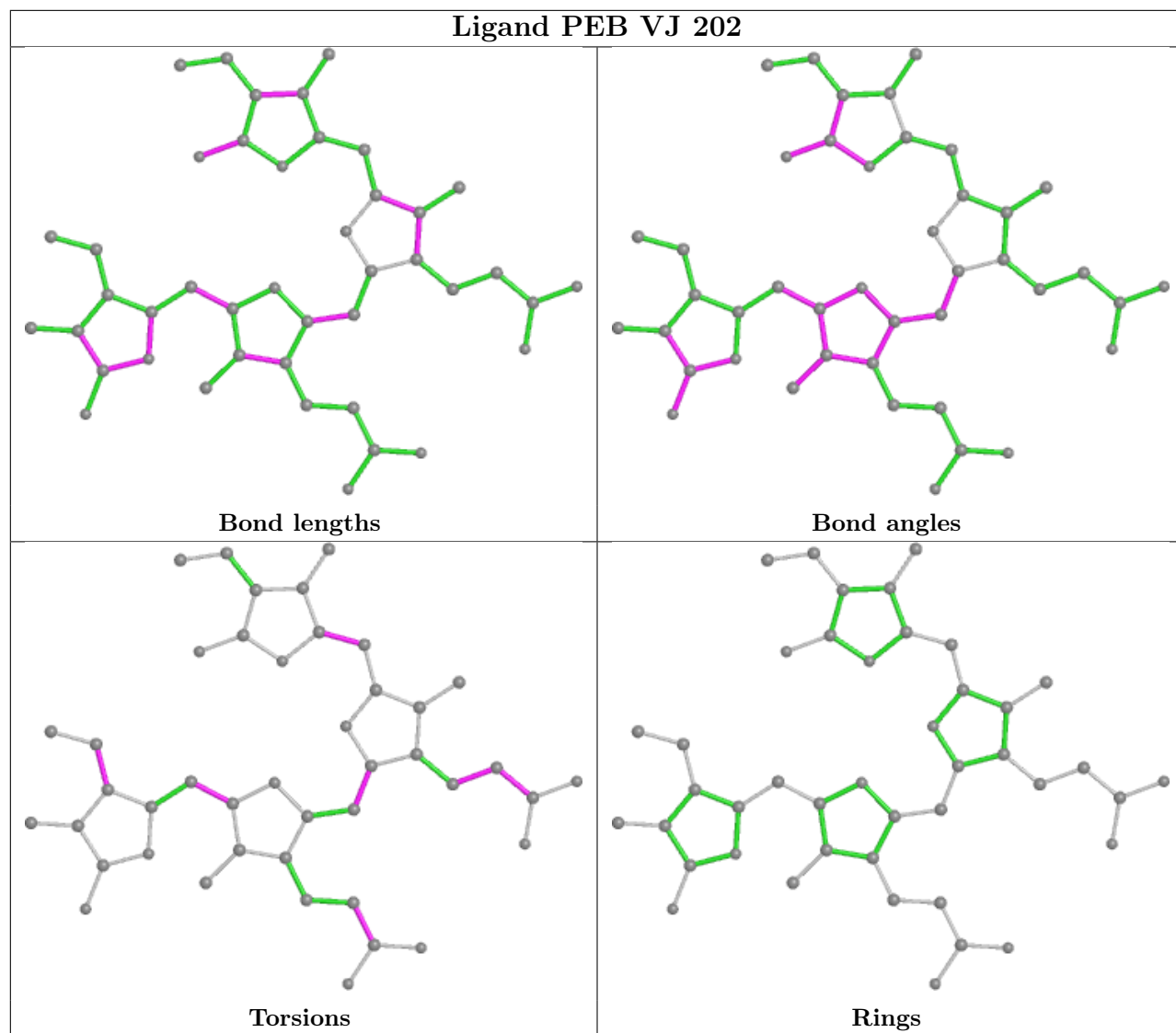


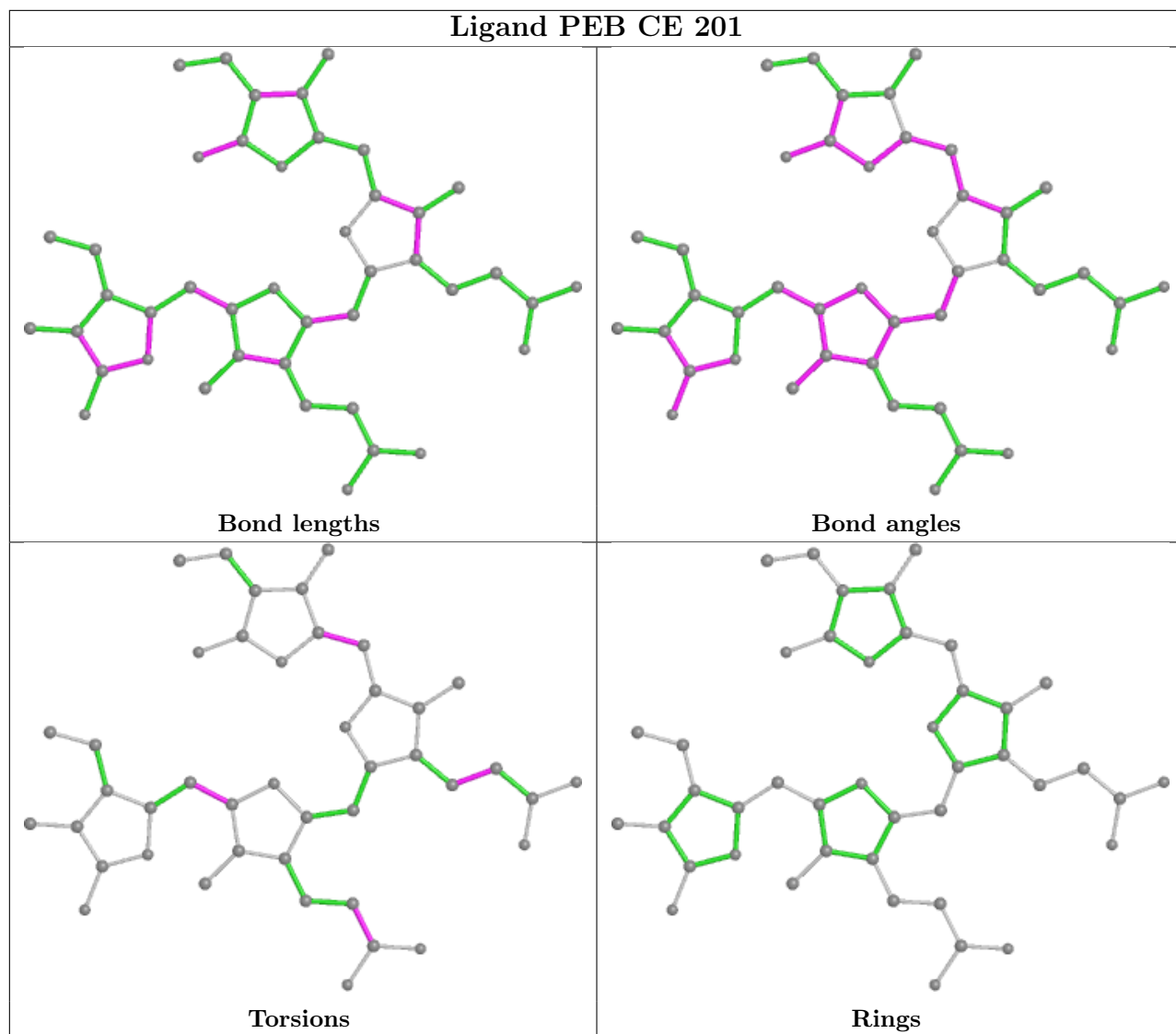


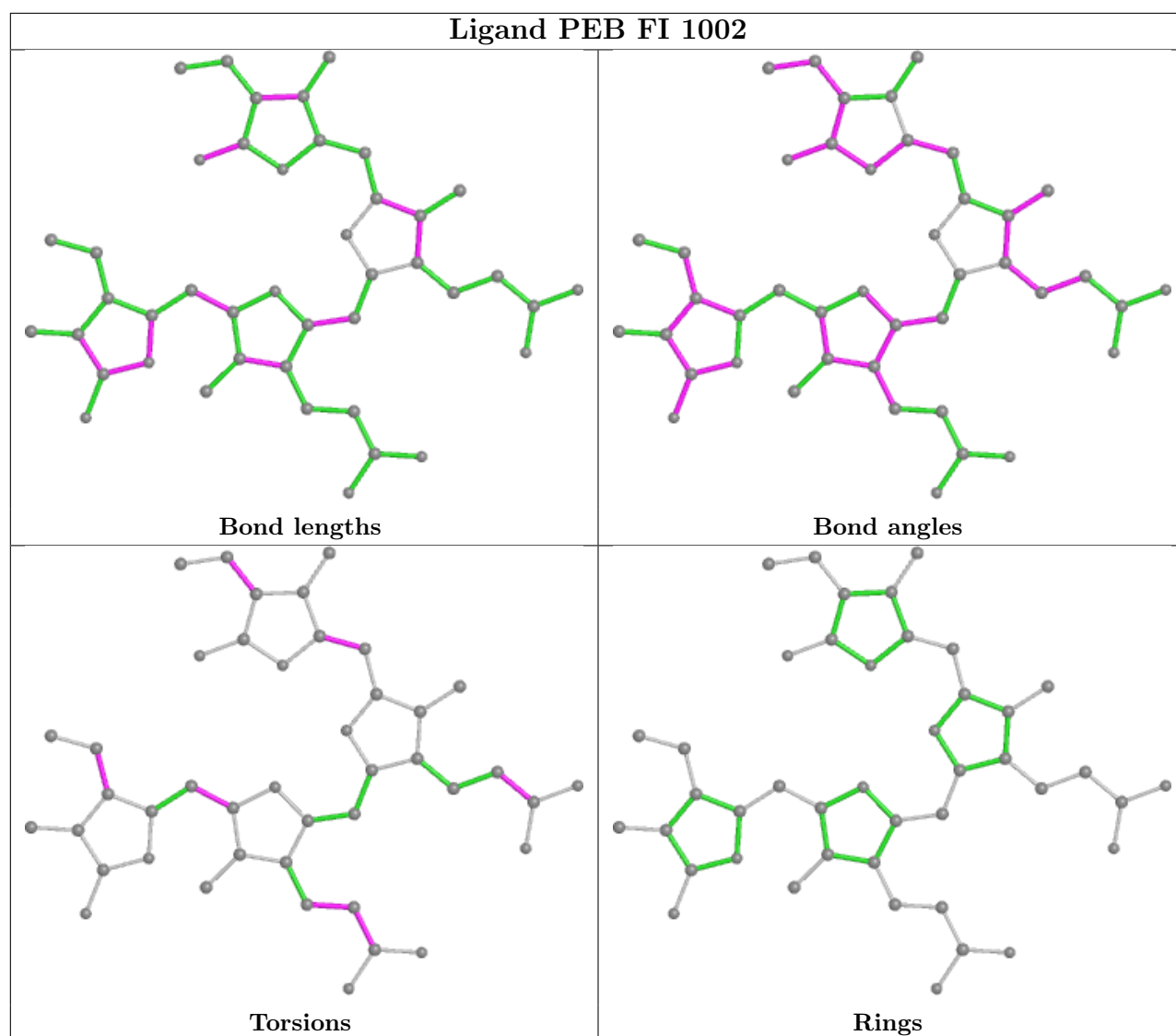












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

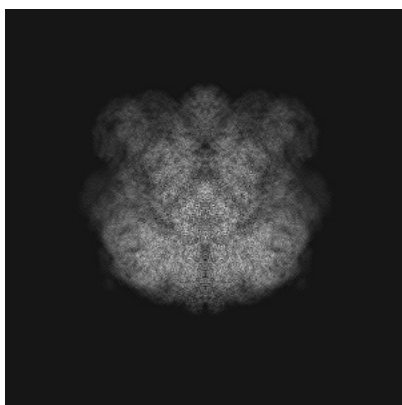
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31393. These allow visual inspection of the internal detail of the map and identification of artifacts.

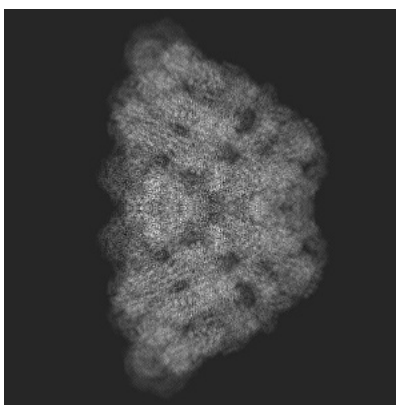
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

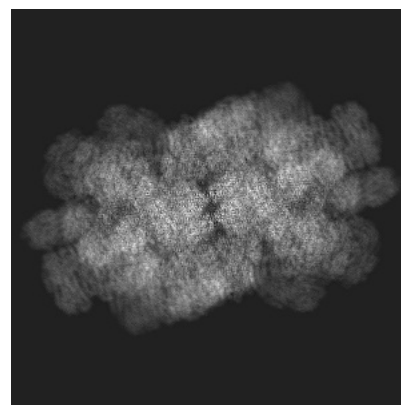
6.1.1 Primary map



X



Y



Z

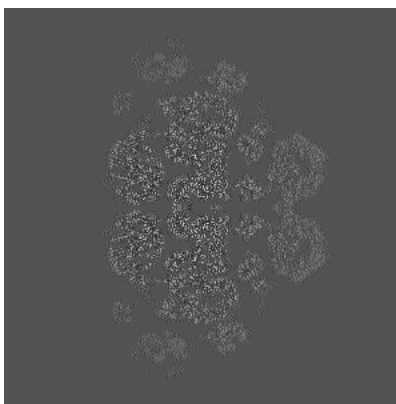
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

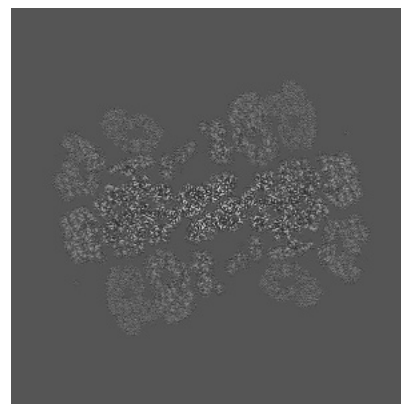
6.2.1 Primary map



X Index: 290



Y Index: 290



Z Index: 290

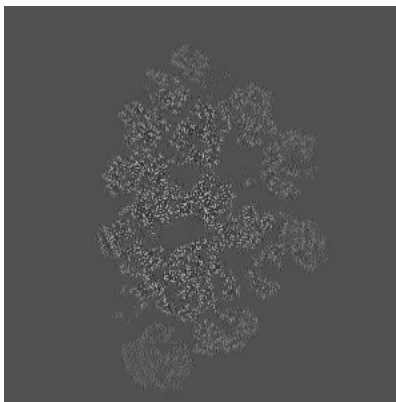
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

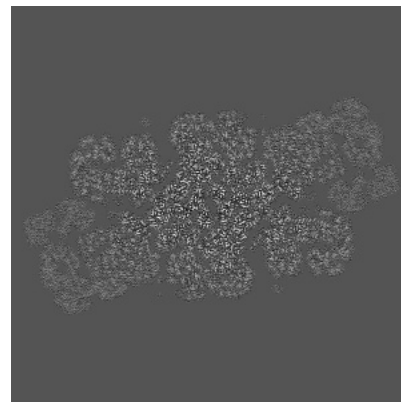
6.3.1 Primary map



X Index: 322



Y Index: 271

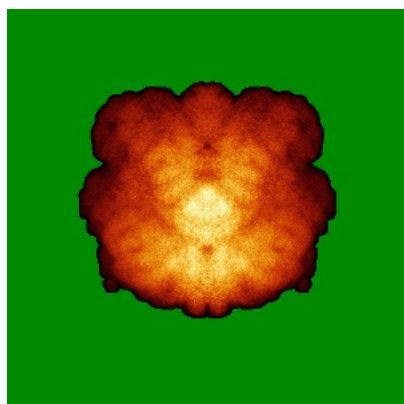


Z Index: 217

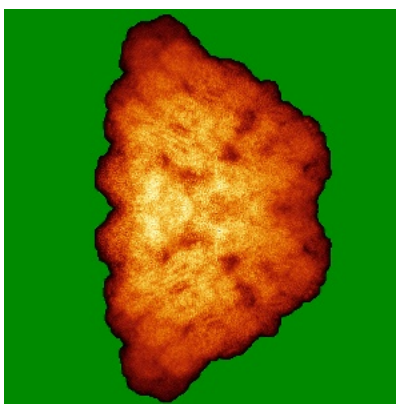
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

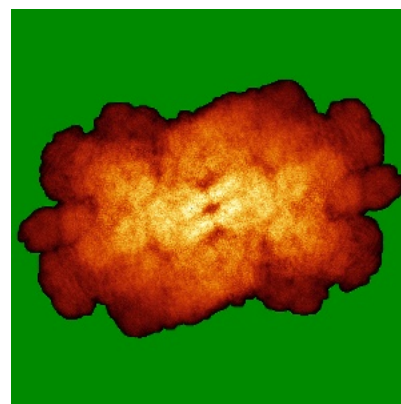
6.4.1 Primary map



X



Y

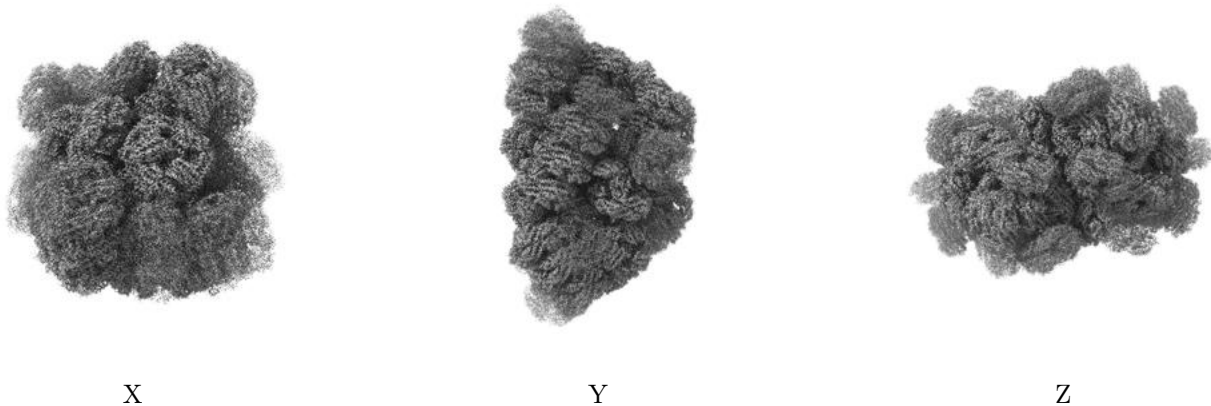


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

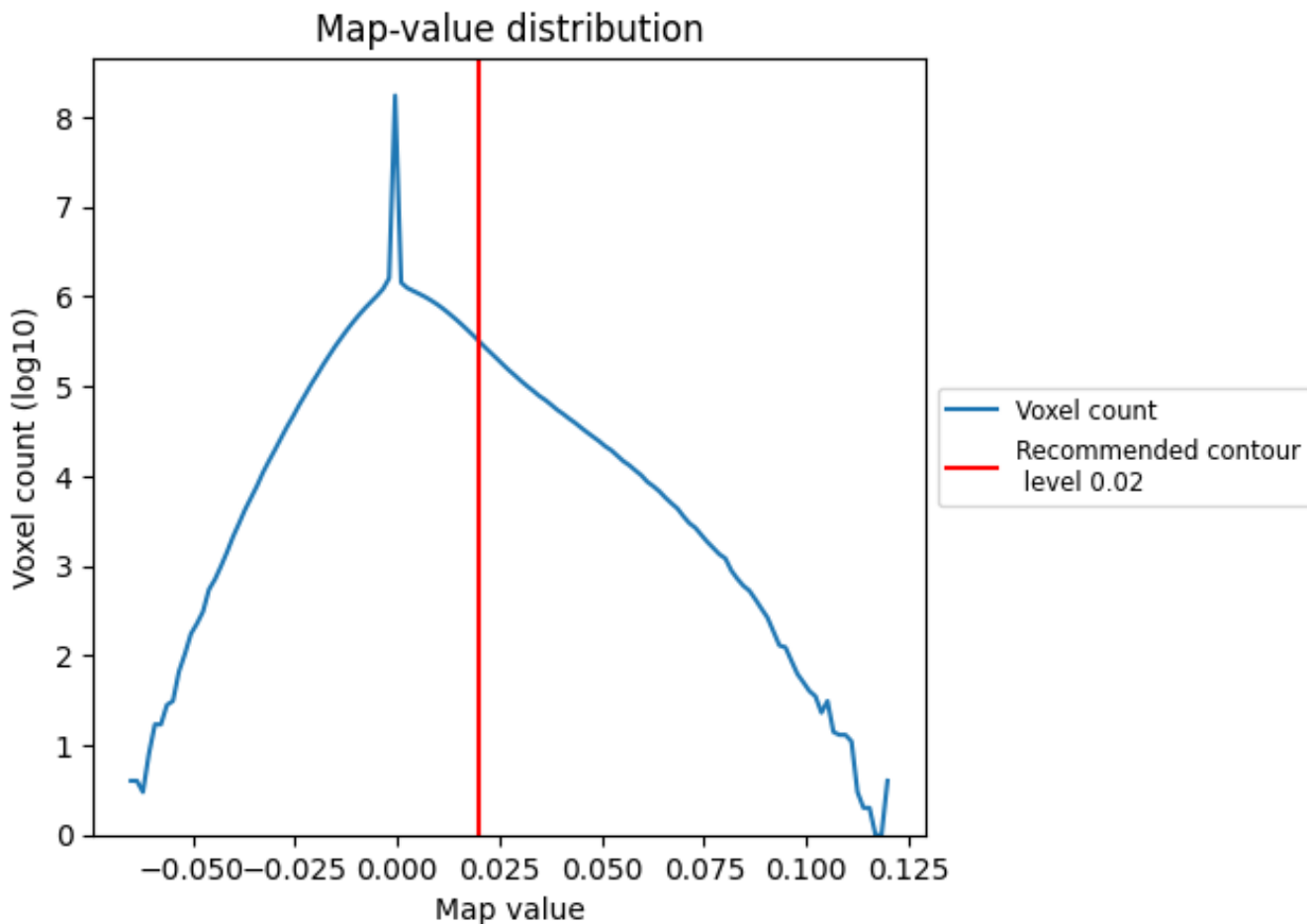
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

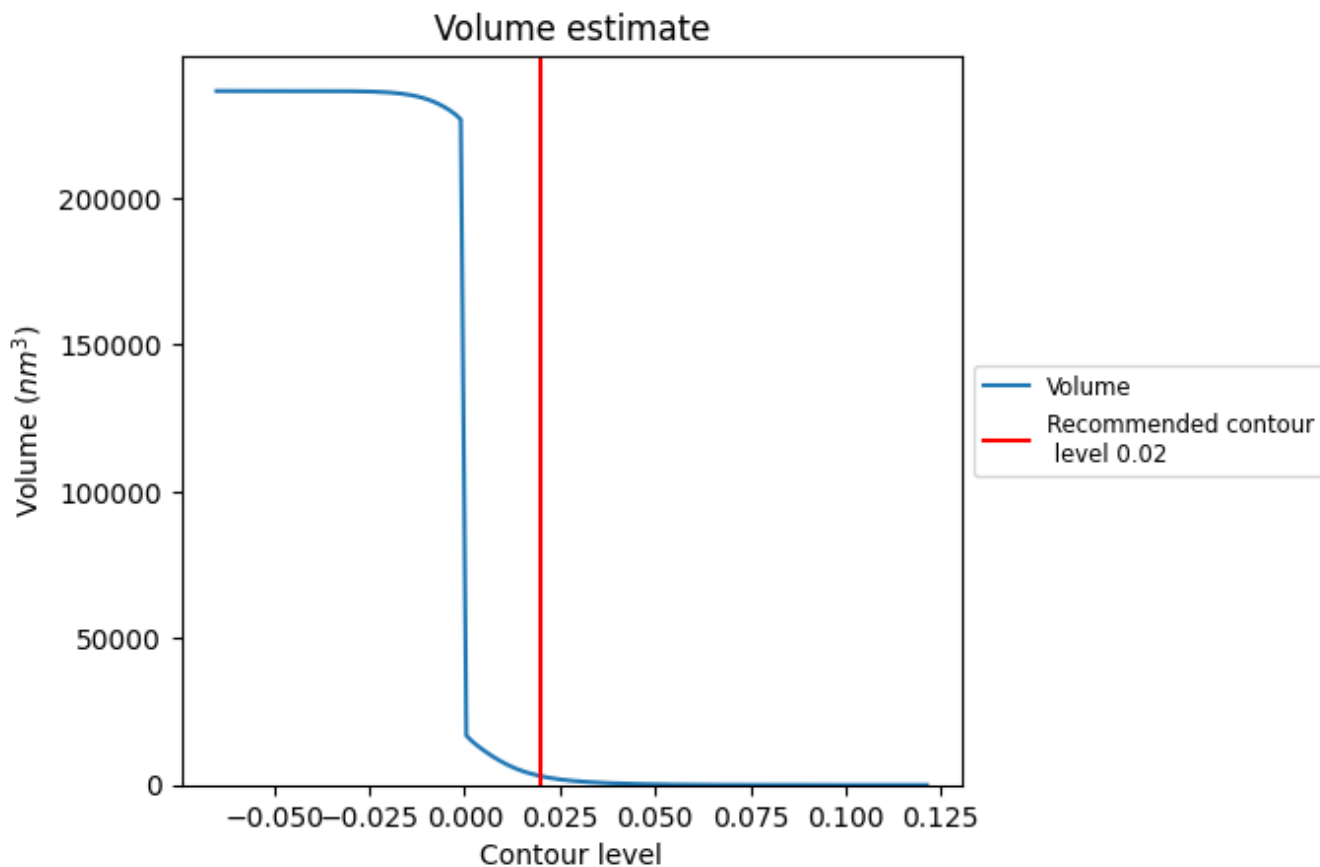
This section contains the results of statistical analysis of the map.

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.

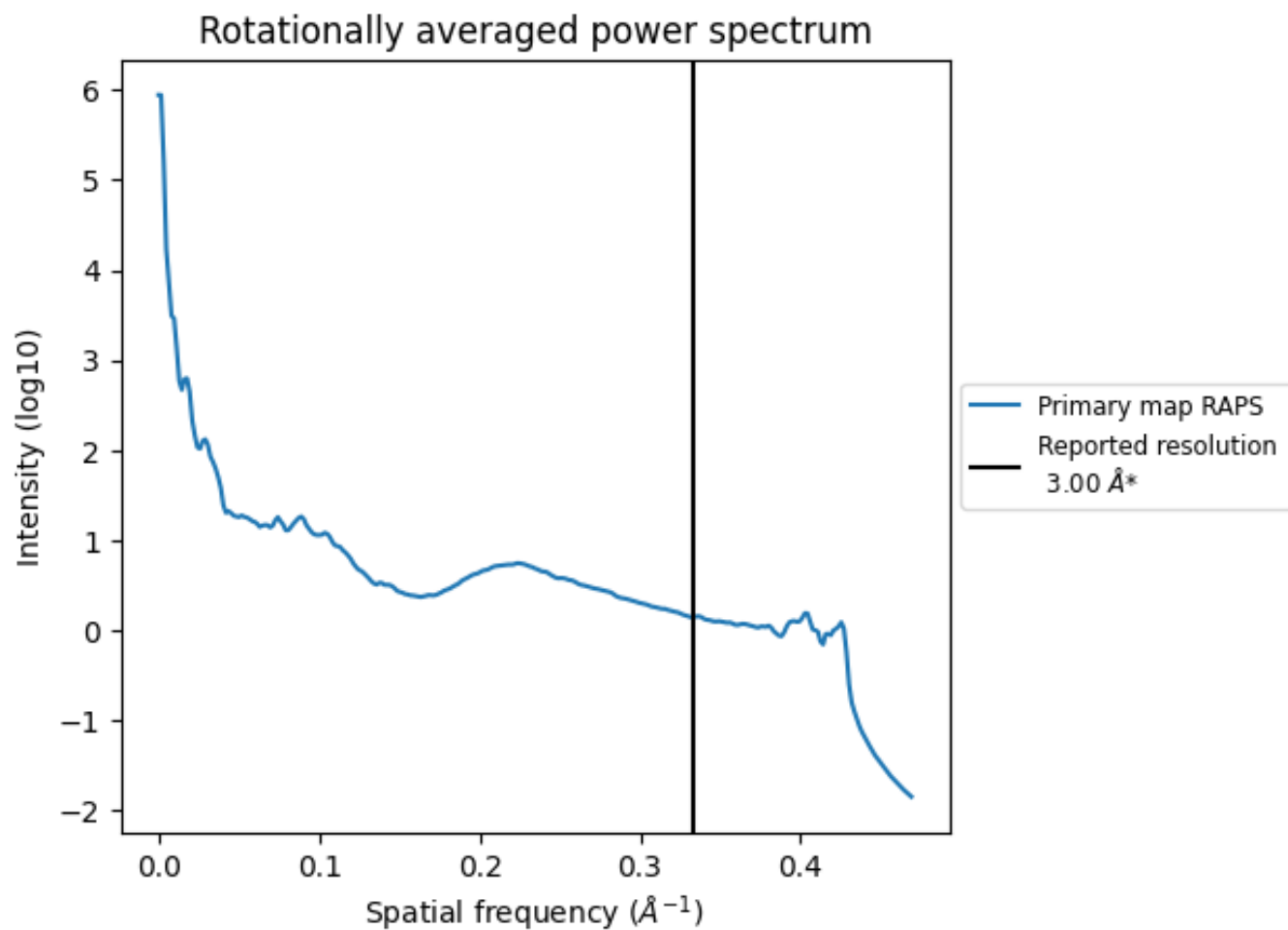
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3006 nm^3 ; this corresponds to an approximate mass of 2716 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 0.333 Å⁻¹

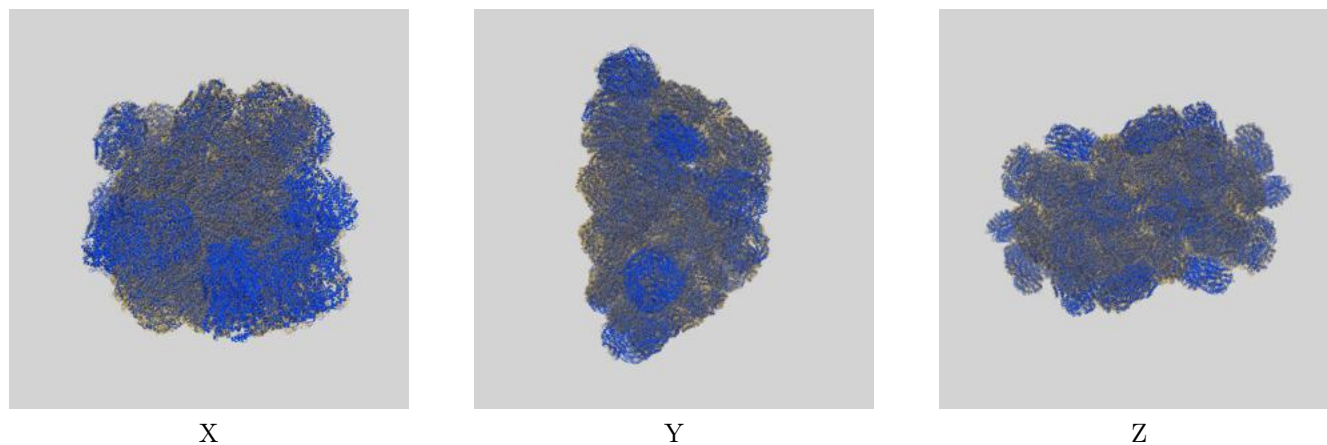
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

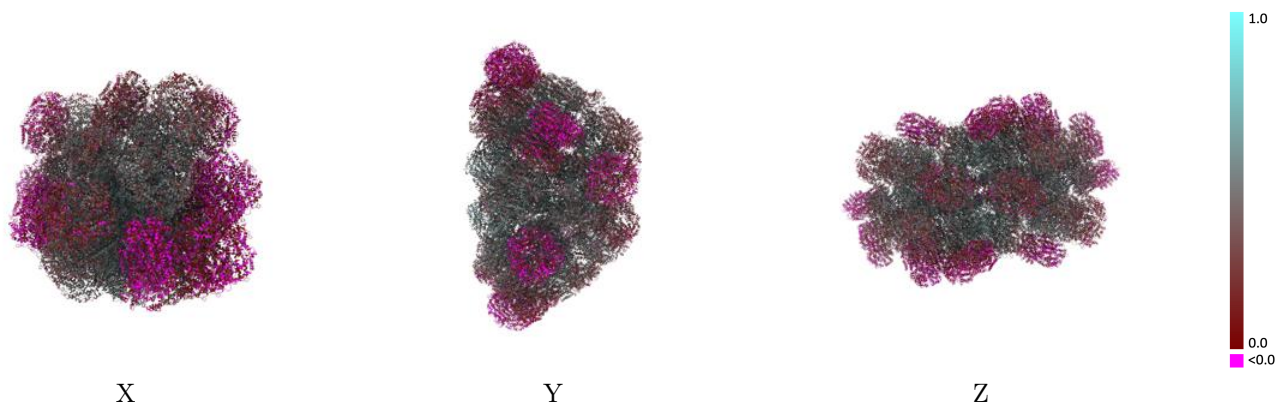
This section contains information regarding the fit between EMDB map EMD-31393 and PDB model 7EZX. Per-residue inclusion information can be found in section 3 on page 136.

9.1 Map-model overlay [i](#)



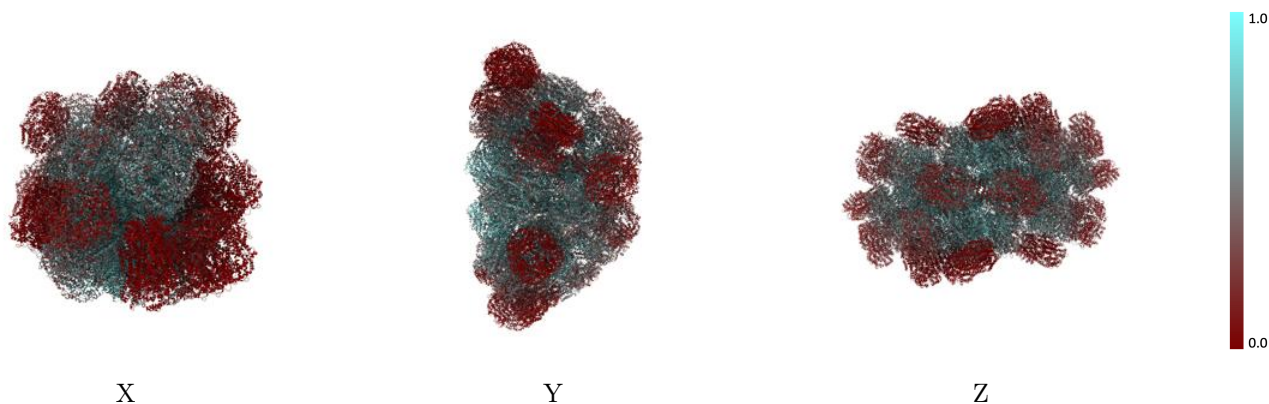
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



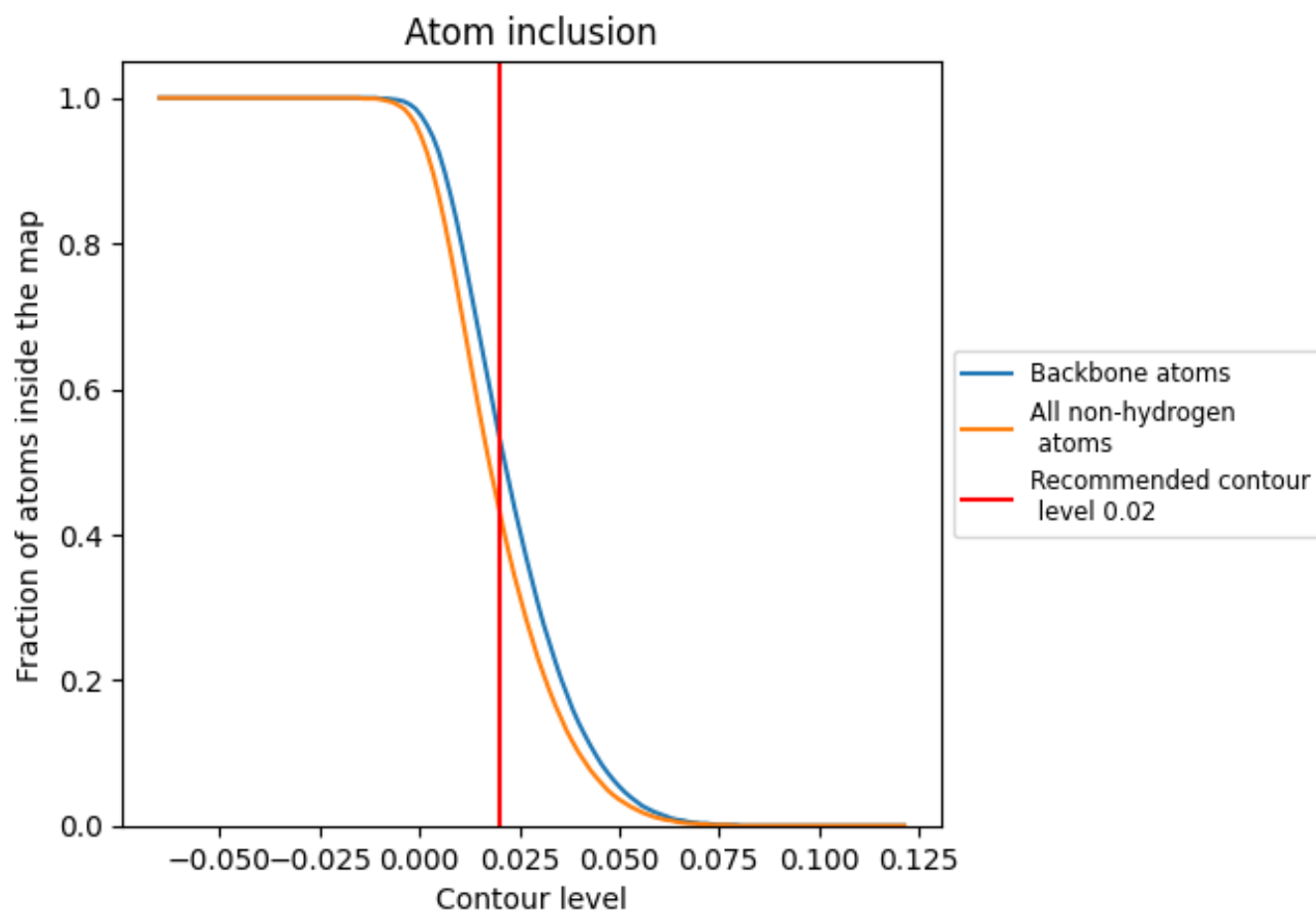
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 53% of all backbone atoms, 43% 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	 0.4330	 0.3580
1P	 0.8010	 0.5930
2P	 0.7070	 0.5460
3P	 0.7460	 0.5620
4P	 0.7640	 0.5730
A1	 0.0690	 0.1470
A3	 0.6740	 0.4950
A5	 0.0320	 0.1800
A7	 0.5670	 0.4590
A8	 0.0310	 0.1830
A9	 0.5670	 0.4600
AA	 0.0120	 0.0270
AB	 0.1980	 0.2990
AC	 0.0370	 0.0570
AE	 0.0380	 0.0560
AF	 0.3850	 0.3680
AG	 0.0110	 0.0240
AI	 0.3830	 0.3670
AJ	 0.5360	 0.4260
AK	 0.0650	 0.1500
AL	 0.5290	 0.4200
AM	 0.1990	 0.3000
AN	 0.0140	 0.0330
AO	 0.6770	 0.5020
AP	 0.6920	 0.4990
AQ	 0.0110	 0.0200
B1	 0.5950	 0.4650
B3	 0.5890	 0.4590
B4	 0.2360	 0.2570
B5	 0.1220	 0.2730
B7	 0.8120	 0.5680
B8	 0.1150	 0.2790
B9	 0.8150	 0.5740
BA	 0.0090	 0.0390
BB	 0.5720	 0.4690























































































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Chain	Atom inclusion	Q-score
BC	0.0370	0.0800
BD	0.2360	0.2570
BE	0.0360	0.0820
BF	0.7370	0.5270
BG	0.0170	0.0910
BI	0.7400	0.5250
BJ	0.4870	0.3810
BK	0.5950	0.4580
BL	0.5000	0.3980
BM	0.5710	0.4710
BN	0.0110	0.0380
BO	0.5960	0.4640
BP	0.7410	0.5240
BQ	0.0180	0.0940
C1	0.3030	0.3140
C3	0.4610	0.3940
C4	0.2490	0.2710
C5	0.0140	0.1360
C7	0.8450	0.5720
C8	0.0130	0.1380
C9	0.8360	0.5750
CA	0.0110	0.0180
CB	0.6470	0.4950
CC	0.0740	0.1300
CD	0.2490	0.2710
CE	0.0710	0.1320
CF	0.7330	0.5380
CG	0.0090	0.0270
CI	0.7320	0.5450
CJ	0.5250	0.4110
CK	0.2960	0.3100
CL	0.5260	0.4170
CM	0.6520	0.4970
CN	0.0120	0.0210
CO	0.4640	0.3980
CP	0.6520	0.4590
CQ	0.0080	0.0260
D1	0.2580	0.2830
D3	0.6430	0.4900
D4	0.3670	0.3420
D5	0.0510	0.2170
D7	0.8090	0.5680

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Chain	Atom inclusion	Q-score
D8	 0.0510	 0.2130
D9	 0.8080	 0.5700
DA	 0.0080	 0.0270
DB	 0.5260	 0.4300
DC	 0.0900	 0.1420
DD	 0.3690	 0.3420
DE	 0.0900	 0.1420
DF	 0.6830	 0.4980
DG	 0.0080	 0.0470
DI	 0.6840	 0.4990
DJ	 0.5610	 0.4460
DK	 0.2680	 0.2850
DL	 0.5560	 0.4380
DM	 0.5230	 0.4300
DN	 0.0090	 0.0270
DO	 0.6380	 0.4830
DP	 0.7400	 0.4920
DQ	 0.0090	 0.0520
E1	 0.7280	 0.5280
E3	 0.4340	 0.3640
E4	 0.3390	 0.3150
E5	 0.4760	 0.4280
E7	 0.8070	 0.5670
E8	 0.4740	 0.4280
E9	 0.8080	 0.5750
EA	 0.0140	 0.0450
EB	 0.4860	 0.4170
EC	 0.0350	 0.0760
ED	 0.3400	 0.3130
EE	 0.0350	 0.0770
EF	 0.7620	 0.5600
EG	 0.0100	 0.0330
EI	 0.7600	 0.5550
EJ	 0.6040	 0.4530
EK	 0.7280	 0.5300
EL	 0.6060	 0.4490
EM	 0.4910	 0.4190
EN	 0.0150	 0.0470
EO	 0.4400	 0.3700
EP	 0.7350	 0.4910
EQ	 0.0100	 0.0390
F1	 0.4890	 0.4170

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Chain	Atom inclusion	Q-score
F3	0.5210	0.4120
F4	0.3200	0.3160
F5	0.4860	0.4310
F7	0.7390	0.5280
F8	0.4880	0.4300
F9	0.7530	0.5440
FA	0.0350	0.1250
FB	0.6430	0.4680
FC	0.0480	0.0870
FD	0.3280	0.3150
FE	0.0470	0.0870
FF	0.6780	0.5180
FG	0.0170	0.0700
FI	0.6830	0.5170
FJ	0.6890	0.4780
FK	0.4920	0.4190
FL	0.6980	0.4920
FM	0.6420	0.4670
FN	0.0360	0.1320
FO	0.5190	0.4110
FP	0.8010	0.5580
FQ	0.0180	0.0730
G1	0.4050	0.3670
G3	0.4570	0.3870
G4	0.1900	0.2260
G5	0.3210	0.3360
G7	0.8450	0.6000
G8	0.3240	0.3340
G9	0.8540	0.5990
GA	0.0410	0.0870
GB	0.4570	0.3940
GC	0.1010	0.1560
GD	0.1950	0.2310
GE	0.0960	0.1540
GF	0.8180	0.5740
GG	0.0140	0.0220
GI	0.8220	0.5790
GJ	0.7510	0.5180
GK	0.3940	0.3590
GL	0.7590	0.5230
GM	0.4610	0.3990
GN	0.0380	0.0860





















































































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Chain	Atom inclusion	Q-score
GO	0.4520	0.3890
GP	0.7790	0.5360
GQ	0.0140	0.0230
H1	0.5400	0.4200
H3	0.4370	0.3720
H4	0.2490	0.2680
H5	0.5370	0.4570
H7	0.7700	0.5520
H8	0.5400	0.4540
H9	0.7710	0.5570
HA	0.0210	0.0580
HB	0.5500	0.4460
HC	0.0910	0.1360
HD	0.2550	0.2790
HE	0.0910	0.1330
HF	0.7580	0.5570
HG	0.0110	0.0380
HI	0.7600	0.5610
HJ	0.6820	0.4860
HK	0.5520	0.4370
HL	0.6880	0.4940
HM	0.5450	0.4500
HN	0.0180	0.0590
HO	0.4350	0.3800
HP	0.7350	0.5180
HQ	0.0110	0.0440
I1	0.7370	0.5350
I3	0.6030	0.4670
I4	0.4630	0.3880
I5	0.6430	0.4640
I7	0.8320	0.5850
I8	0.6400	0.4570
I9	0.8330	0.5890
IA	0.0110	0.0340
IB	0.6130	0.4680
IC	0.0700	0.1410
ID	0.4680	0.3850
IE	0.0660	0.1420
IF	0.8100	0.5670
IG	0.0110	0.0750
II	0.8090	0.5690
IJ	0.7300	0.5200





















































































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Chain	Atom inclusion	Q-score
IK	 0.7400	 0.5360
IL	 0.7270	 0.5170
IM	 0.6050	 0.4660
IN	 0.0090	 0.0280
IO	 0.5970	 0.4660
IP	 0.8340	 0.5860
IQ	 0.0100	 0.0740
J1	 0.5130	 0.4220
J3	 0.7390	 0.5350
J4	 0.1720	 0.2200
J5	 0.7120	 0.5230
J7	 0.8120	 0.5570
J8	 0.7120	 0.5190
J9	 0.8130	 0.5550
JA	 0.0100	 0.0350
JB	 0.5410	 0.4470
JC	 0.0300	 0.0890
JD	 0.1680	 0.2200
JE	 0.0330	 0.0860
JF	 0.8120	 0.5690
JG	 0.0220	 0.1200
JI	 0.8160	 0.5760
JJ	 0.6600	 0.4940
JK	 0.5150	 0.4250
JL	 0.6670	 0.5010
JM	 0.5460	 0.4480
JN	 0.0070	 0.0340
JO	 0.7400	 0.5340
JP	 0.7870	 0.5560
JQ	 0.0190	 0.1200
K1	 0.4830	 0.4140
K3	 0.7540	 0.5360
K4	 0.1600	 0.1990
K5	 0.4850	 0.4120
K7	 0.8280	 0.5730
K8	 0.4840	 0.4120
K9	 0.8430	 0.5880
KA	 0.0090	 0.0150
KB	 0.6980	 0.5190
KC	 0.0460	 0.0820
KD	 0.1590	 0.1980
KE	 0.0460	 0.0860





















































































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Chain	Atom inclusion	Q-score
KF	 0.7660	 0.5560
KG	 0.0120	 0.0830
KI	 0.7710	 0.5610
KJ	 0.6170	 0.4410
KK	 0.4860	 0.4180
KL	 0.6310	 0.4570
KM	 0.6910	 0.5180
KN	 0.0080	 0.0170
KO	 0.7510	 0.5370
KP	 0.7150	 0.5100
KQ	 0.0120	 0.0770
L1	 0.6910	 0.5110
L3	 0.6210	 0.4850
L4	 0.2050	 0.2400
L5	 0.5460	 0.4460
L7	 0.7820	 0.5510
L8	 0.5410	 0.4390
L9	 0.7910	 0.5560
LA	 0.0140	 0.0190
LB	 0.6820	 0.5030
LC	 0.1230	 0.1900
LD	 0.2010	 0.2410
LE	 0.1200	 0.1880
LF	 0.7400	 0.5340
LG	 0.0170	 0.0710
LI	 0.7390	 0.5330
LJ	 0.7400	 0.5150
LK	 0.6900	 0.5120
LL	 0.7450	 0.5140
LM	 0.6970	 0.5080
LN	 0.0140	 0.0190
LO	 0.6190	 0.4910
LP	 0.7510	 0.5010
LQ	 0.0180	 0.0860
M1	 0.3130	 0.2940
M2	 0.3810	 0.3270
M3	 0.5320	 0.4050
M4	 0.2360	 0.2480
M7	 0.8390	 0.5740
M9	 0.8500	 0.5950
MA	 0.0260	 0.0750
MB	 0.7400	 0.5360

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Chain	Atom inclusion	Q-score
MC	 0.1530	 0.1960
MD	 0.2260	 0.2390
ME	 0.1500	 0.1870
MF	 0.8160	 0.5810
MG	 0.0180	 0.0900
MI	 0.8190	 0.5850
MJ	 0.4290	 0.3720
MK	 0.3170	 0.2930
ML	 0.4370	 0.3740
MM	 0.7440	 0.5370
MN	 0.0210	 0.0740
MO	 0.5390	 0.4110
MP	 0.7520	 0.5250
MQ	 0.0260	 0.1110
MR	 0.3870	 0.3380
N1	 0.3610	 0.3230
N2	 0.4860	 0.4000
N3	 0.3620	 0.3330
N7	 0.8170	 0.5670
N9	 0.8130	 0.5640
NB	 0.7480	 0.5330
NF	 0.7290	 0.5290
NI	 0.7370	 0.5300
NJ	 0.4510	 0.3900
NK	 0.3670	 0.3260
NL	 0.4500	 0.3960
NM	 0.7480	 0.5320
NO	 0.3670	 0.3240
NP	 0.8090	 0.5670
NR	 0.4820	 0.3990
O1	 0.2300	 0.2790
O2	 0.6140	 0.4530
O3	 0.5460	 0.4280
O7	 0.6760	 0.4980
O9	 0.6760	 0.5020
OB	 0.5080	 0.4260
OF	 0.6330	 0.4950
OI	 0.6360	 0.5010
OJ	 0.5190	 0.4260
OK	 0.2300	 0.2800
OL	 0.5210	 0.4310
OM	 0.5070	 0.4310





















































































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Chain	Atom inclusion	Q-score
OO	0.5500	0.4330
OP	0.7090	0.5010
OR	0.6190	0.4560
P1	0.4100	0.3910
P2	0.5380	0.4350
P7	0.7000	0.5120
P9	0.7020	0.5180
PB	0.4120	0.3740
PF	0.6300	0.4840
PI	0.6340	0.4900
PJ	0.5330	0.4390
PK	0.4060	0.3920
PL	0.5390	0.4460
PM	0.4120	0.3750
PP	0.7930	0.5300
PR	0.5360	0.4310
Q1	0.2790	0.3130
Q2	0.5570	0.4310
Q7	0.7450	0.5290
Q9	0.7440	0.5330
QB	0.4150	0.3640
QF	0.5370	0.4400
QI	0.5390	0.4430
QJ	0.4970	0.4280
QK	0.2800	0.3070
QL	0.5020	0.4300
QM	0.4150	0.3610
QP	0.8290	0.5660
QR	0.5610	0.4340
R1	0.1950	0.2420
R2	0.5240	0.4300
R7	0.7790	0.5470
R9	0.7760	0.5520
RB	0.5560	0.4460
RF	0.6080	0.4830
RI	0.6140	0.4870
RJ	0.5490	0.4430
RK	0.1920	0.2430
RL	0.5580	0.4480
RM	0.5550	0.4440
RP	0.7910	0.5260
RR	0.5190	0.4330





















































































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Chain	Atom inclusion	Q-score
S1	 0.2420	 0.2700
S2	 0.5960	 0.4650
S7	 0.7330	 0.5410
S9	 0.7350	 0.5450
SB	 0.3820	 0.3610
SF	 0.5650	 0.4500
SI	 0.5650	 0.4520
SJ	 0.6200	 0.4480
SK	 0.2460	 0.2760
SL	 0.6240	 0.4620
SM	 0.3860	 0.3610
SP	 0.8210	 0.5620
SR	 0.5920	 0.4630
T1	 0.2390	 0.2820
T2	 0.6910	 0.5140
T7	 0.6950	 0.5250
T9	 0.7020	 0.5340
TB	 0.5170	 0.4350
TF	 0.6630	 0.4980
TI	 0.6550	 0.4980
TJ	 0.6380	 0.4900
TK	 0.2380	 0.2820
TL	 0.6470	 0.4950
TM	 0.5150	 0.4390
TP	 0.7840	 0.5270
TR	 0.6840	 0.5140
U1	 0.1460	 0.2190
U2	 0.4560	 0.3930
U7	 0.7240	 0.5170
U9	 0.7250	 0.5230
UB	 0.5720	 0.4560
UF	 0.5510	 0.4490
UI	 0.5530	 0.4430
UJ	 0.6140	 0.4740
UK	 0.1500	 0.2220
UL	 0.6160	 0.4750
UM	 0.5770	 0.4680
UP	 0.8590	 0.5930
UR	 0.4600	 0.3970
V1	 0.1840	 0.2560
V2	 0.3530	 0.3210
V7	 0.7910	 0.5610

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Chain	Atom inclusion	Q-score
V9	 0.7950	 0.5610
VB	 0.4570	 0.4060
VF	 0.5290	 0.4350
VI	 0.5270	 0.4410
VJ	 0.4980	 0.4090
VK	 0.1900	 0.2590
VL	 0.5140	 0.4130
VM	 0.4550	 0.4060
VP	 0.7470	 0.5580
VR	 0.3520	 0.3250
W1	 0.1290	 0.1740
W2	 0.4220	 0.3610
W7	 0.7080	 0.5190
W9	 0.7140	 0.5270
WB	 0.6780	 0.5150
WF	 0.6380	 0.4890
WI	 0.6370	 0.4900
WJ	 0.5380	 0.4220
WK	 0.1300	 0.1760
WL	 0.5470	 0.4280
WM	 0.6810	 0.5150
WP	 0.7840	 0.5900
WR	 0.4190	 0.3600
X1	 0.3370	 0.3640
X2	 0.5510	 0.4570
X7	 0.7790	 0.5530
X9	 0.7830	 0.5600
XB	 0.6110	 0.4790
XF	 0.6800	 0.5230
XI	 0.6840	 0.5270
XJ	 0.6500	 0.4860
XK	 0.3400	 0.3620
XL	 0.6480	 0.4880
XM	 0.6190	 0.4840
XP	 0.8550	 0.6050
XR	 0.5550	 0.4600
Y1	 0.1950	 0.2540
Y7	 0.6750	 0.5020
Y9	 0.6850	 0.5120
YB	 0.6400	 0.4960
YF	 0.7040	 0.5280
YI	 0.7140	 0.5330

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Chain	Atom inclusion	Q-score
YJ	0.0960	0.1130
YK	0.1880	0.2550
YL	0.0950	0.1180
YM	0.6420	0.5030
YP	0.8020	0.5920
Z1	0.1210	0.1860
Z7	0.6970	0.5010
Z9	0.7040	0.5110
ZB	0.6920	0.5120
ZF	0.6520	0.4990
ZI	0.6510	0.4970
ZJ	0.1110	0.1350
ZK	0.1200	0.1850
ZL	0.1170	0.1330
ZM	0.6960	0.5210
ZP	0.7060	0.5470
a1	0.1050	0.1590
a7	0.7220	0.5080
a9	0.7300	0.5160
aB	0.1990	0.3080
aF	0.5610	0.4540
aI	0.5630	0.4590
aJ	0.1930	0.2190
aK	0.1040	0.1610
aL	0.1930	0.2200
aM	0.1980	0.3130
aP	0.7500	0.5660
b1	0.0540	0.0950
b7	0.4930	0.3940
b9	0.5000	0.3990
bB	0.6780	0.4980
bF	0.4800	0.4160
bI	0.4770	0.4160
bJ	0.2130	0.2240
bK	0.0580	0.0960
bL	0.2180	0.2330
bM	0.6720	0.4940
bP	0.7620	0.5710
c1	0.0800	0.1740
c7	0.4460	0.3870
c9	0.4560	0.3890
cB	0.1140	0.2190

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Chain	Atom inclusion	Q-score
cF	█ 0.4320	█ 0.4060
cI	█ 0.4340	█ 0.4080
cJ	█ 0.1850	█ 0.2160
cK	█ 0.0820	█ 0.1770
cL	█ 0.1810	█ 0.2220
cM	█ 0.1120	█ 0.2220
cP	█ 0.6940	█ 0.4970
d1	█ 0.0600	█ 0.1020
d4	█ 0.3220	█ 0.2860
d7	█ 0.5490	█ 0.4500
d9	█ 0.5460	█ 0.4520
dB	█ 0.1750	█ 0.2800
dD	█ 0.3520	█ 0.3250
dF	█ 0.3350	█ 0.3150
dI	█ 0.3390	█ 0.3170
dJ	█ 0.1360	█ 0.1860
dK	█ 0.0580	█ 0.1030
dL	█ 0.1350	█ 0.1850
dM	█ 0.1740	█ 0.2810
dP	█ 0.7500	█ 0.4920
e1	█ 0.0460	█ 0.0860
e2	█ 0.4980	█ 0.3770
e7	█ 0.6080	█ 0.4870
e9	█ 0.6100	█ 0.4870
eB	█ 0.3450	█ 0.3970
eF	█ 0.3620	█ 0.3580
eI	█ 0.3650	█ 0.3600
eJ	█ 0.1620	█ 0.1830
eK	█ 0.0460	█ 0.0880
eL	█ 0.1630	█ 0.1840
eM	█ 0.3470	█ 0.4040
eP	█ 0.6500	█ 0.4610
eR	█ 0.4730	█ 0.3480
f1	█ 0.0670	█ 0.1320
f7	█ 0.4800	█ 0.3960
f9	█ 0.4730	█ 0.3930
fB	█ 0.0900	█ 0.1660
fF	█ 0.2990	█ 0.3030
fI	█ 0.3020	█ 0.3040
fJ	█ 0.2530	█ 0.2880
fK	█ 0.0710	█ 0.1370
fL	█ 0.2580	█ 0.2890

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Chain	Atom inclusion	Q-score
fM	0.0870	0.1680
fP	0.7990	0.5580
g1	0.0660	0.1250
g7	0.4290	0.3880
g9	0.4310	0.3890
gB	0.0810	0.1520
gF	0.3770	0.3550
gI	0.3800	0.3540
gJ	0.1560	0.2020
gK	0.0630	0.1300
gL	0.1590	0.2010
gM	0.0750	0.1520
gP	0.7480	0.4980
h1	0.0380	0.0730
h7	0.5170	0.4340
h9	0.5190	0.4340
hB	0.1290	0.2340
hF	0.2280	0.2660
hI	0.2240	0.2640
hJ	0.1170	0.1620
hK	0.0350	0.0760
hL	0.1200	0.1580
hM	0.1310	0.2330
hP	0.7330	0.5150
i1	0.0470	0.1020
i7	0.6070	0.4830
i9	0.6000	0.4860
iB	0.2080	0.3100
iF	0.2440	0.2850
iI	0.2380	0.2850
iJ	0.2110	0.2480
iK	0.0480	0.1050
iL	0.2050	0.2490
iM	0.2070	0.3130
iP	0.7810	0.5350
j1	0.0410	0.0830
j7	0.4570	0.3850
j9	0.4500	0.3880
jB	0.1050	0.2080
jF	0.3400	0.3340
jI	0.3360	0.3320
jJ	0.2770	0.3000









































































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Chain	Atom inclusion	Q-score
jK	0.0450	0.0830
jL	0.2730	0.2990
jM	0.1050	0.2100
jP	0.7270	0.5150
k1	0.0310	0.1040
k6	0.7730	0.6030
k7	0.4560	0.3930
k9	0.4650	0.3960
kB	0.1410	0.2320
kF	0.4940	0.4310
kH	0.7760	0.6060
kI	0.4900	0.4330
kJ	0.0080	0.0370
kK	0.0330	0.1060
kL	0.0100	0.0400
kM	0.1390	0.2300
kP	0.8360	0.5830
l1	0.0250	0.0520
l7	0.5400	0.4290
l9	0.5560	0.4330
lB	0.2980	0.3490
lF	0.3900	0.3730
lI	0.3940	0.3760
lJ	0.0100	0.0320
lK	0.0250	0.0460
lL	0.0110	0.0310
lM	0.2950	0.3600
lP	0.7950	0.5530
m1	0.0320	0.0470
m7	0.5780	0.4660
m9	0.5710	0.4700
mB	0.2240	0.3160
mF	0.2740	0.2810
mI	0.2700	0.2860
mJ	0.0100	0.0360
mK	0.0320	0.0460
mL	0.0120	0.0350
mM	0.2240	0.3170
mP	0.7190	0.5090
nJ	0.0110	0.0220
nL	0.0110	0.0230
nP	0.7520	0.5010

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Chain	Atom inclusion	Q-score
oJ	 0.0150	 0.0220
oL	 0.0150	 0.0220
oP	 0.7500	 0.5240
pJ	 0.0160	 0.0280
pL	 0.0140	 0.0250
pP	 0.8230	 0.5750
qJ	 0.0140	 0.0500
qL	 0.0120	 0.0470
qP	 0.7130	 0.5040
rJ	 0.0160	 0.0620
rL	 0.0150	 0.0630
rP	 0.7860	 0.5290
sJ	 0.0150	 0.0450
sL	 0.0130	 0.0460
sP	 0.8290	 0.5650
tJ	 0.0130	 0.0390
tL	 0.0130	 0.0360
tP	 0.7830	 0.5350
uJ	 0.0120	 0.0080
uL	 0.0080	 0.0100
uP	 0.8200	 0.5630
vJ	 0.0180	 0.0660
vL	 0.0160	 0.0630
vP	 0.7870	 0.5260
wJ	 0.2660	 0.2830
wL	 0.2670	 0.2880
wP	 0.8620	 0.5950
xJ	 0.0110	 0.0530
xL	 0.0120	 0.0400
xP	 0.7400	 0.5590
yJ	 0.6260	 0.5070
yL	 0.6230	 0.5050
yP	 0.7810	 0.5880
zJ	 0.7150	 0.5140
zL	 0.7130	 0.5130
zP	 0.8450	 0.6020