Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 01:12 pm GMT

PDB ID	:	7PQD
EMDB ID	:	EMD-13590
Title	:	Cryo-EM structure of the dimeric Rhodobacter sphaeroides RC-LH1 core complex at 2.9 A: the structural basis for dimerisation
Authors	:	Qian, P.; Hunter, C.N.
Deposited on	:	2021-09-17
Resolution	:	2.90 Å(reported)

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

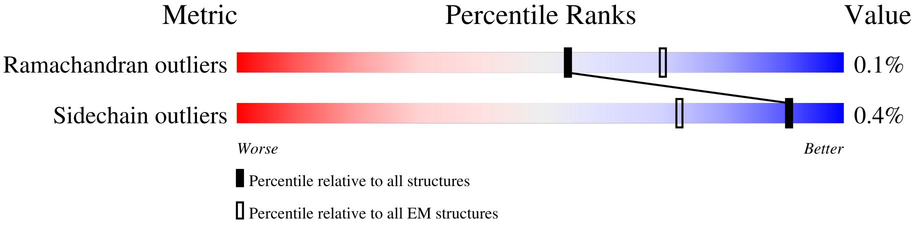
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

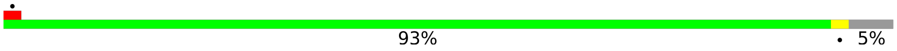
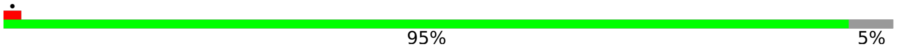
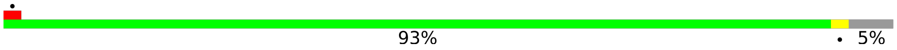
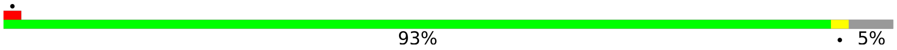
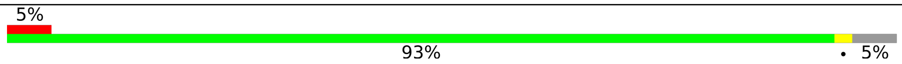
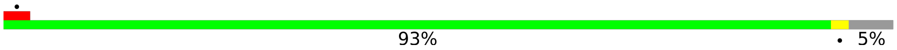
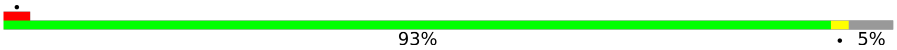
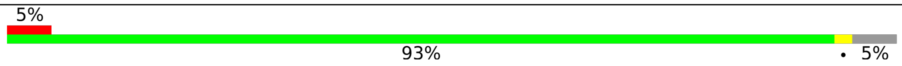
The reported resolution of this entry is 2.90 Å.

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 <=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	AA	58	
1	AB	58	
1	AC	58	
1	AD	58	
1	AE	58	
1	AF	58	
1	AG	58	
1	AH	58	
1	AI	58	

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Mol	Chain	Length	Quality of chain
1	AJ	58	• 95% 5%
1	AK	58	7% 93% • 5%
1	AL	58	17% 93% • 5%
1	AM	58	29% 93% • 5%
1	AN	58	47% 88% 12%
1	aa	58	78% • 21%
1	ab	58	• 93% • 5%
1	ac	58	• 95% 5%
1	ad	58	• 93% • 5%
1	ae	58	• 93% • 5%
1	af	58	5% 93% • 5%
1	ag	58	• 93% • 5%
1	ah	58	• 93% • 5%
1	ai	58	5% 93% • 5%
1	aj	58	• 95% 5%
1	ak	58	7% 93% • 5%
1	al	58	17% 93% • 5%
1	am	58	29% 93% • 5%
1	an	58	45% 88% 12%
2	BA	49	88% 12%
2	BB	49	88% 12%
2	BC	49	86% 14%
2	BD	49	• 88% 12%
2	BE	49	• 88% 12%
2	BF	49	8% 88% 12%

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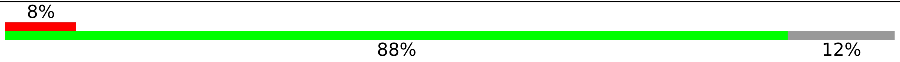
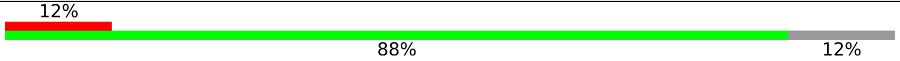
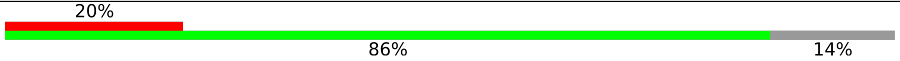
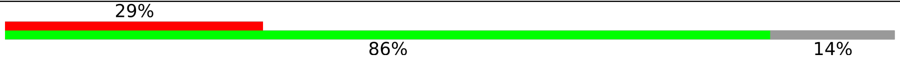
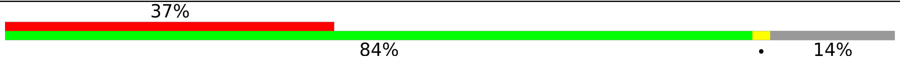
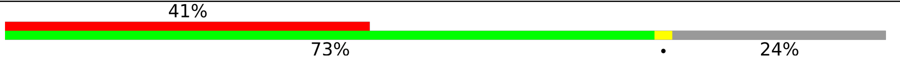
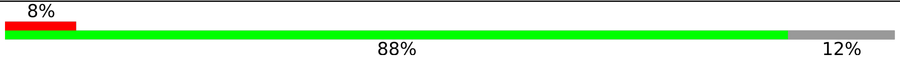
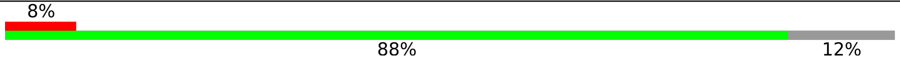
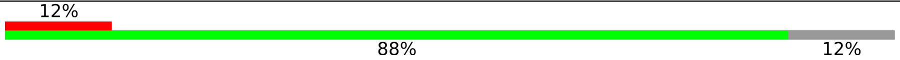
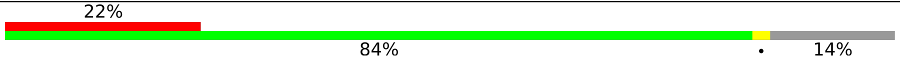
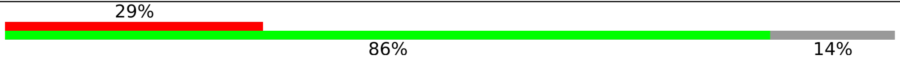
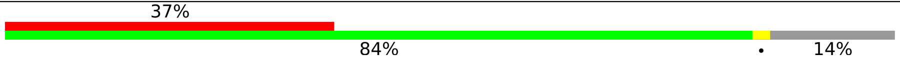
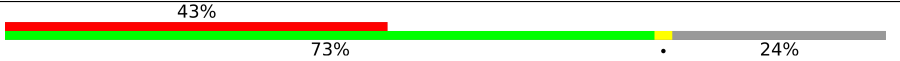
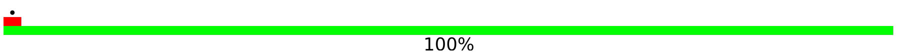
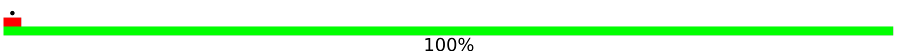
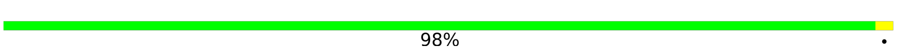
Mol	Chain	Length	Quality of chain
2	BG	49	
2	BH	49	
2	BI	49	
2	BJ	49	
2	BK	49	
2	BL	49	
2	BM	49	
2	BN	49	
2	ba	49	
2	bb	49	
2	bc	49	
2	bd	49	
2	be	49	
2	bf	49	
2	bg	49	
2	bh	49	
2	bi	49	
2	bj	49	
2	bk	49	
2	bl	49	
2	bm	49	
2	bn	49	
3	H	246	
3	h	246	
4	L	281	

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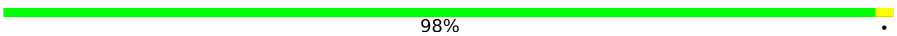
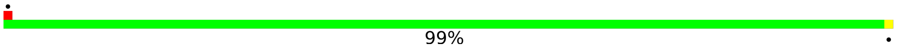
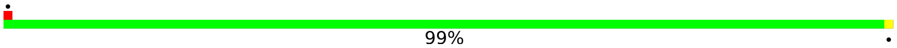
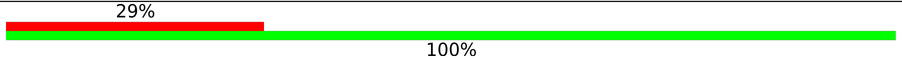
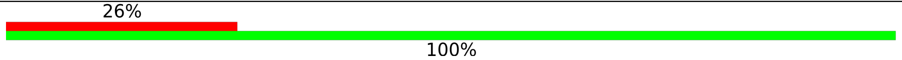
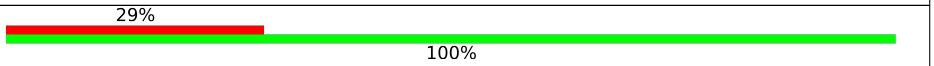
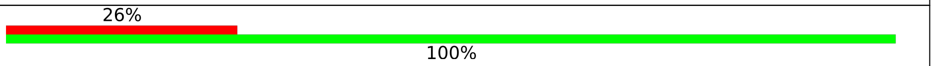
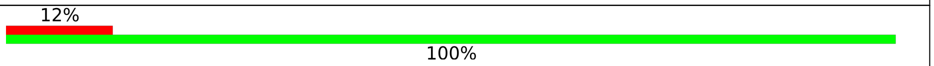
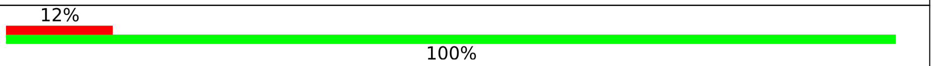
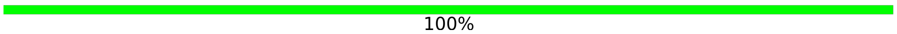
Mol	Chain	Length	Quality of chain
4	l	281	
5	M	307	
5	m	307	
6	UA	31	
6	UB	31	
6	ua	31	
6	ub	31	
7	UU	49	
7	uu	49	
8	X	55	
8	x	55	

2 Entry composition ⓘ

There are 19 unique types of molecules in this entry. The entry contains 45952 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 LH1-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	46	394	272	60	59	3	0	0
1	AB	55	462	314	74	71	3	0	0
1	AC	55	462	314	74	71	3	0	0
1	AD	55	462	314	74	71	3	0	0
1	AE	55	462	314	74	71	3	0	0
1	AF	55	462	314	74	71	3	0	0
1	AG	55	462	314	74	71	3	0	0
1	AH	55	462	314	74	71	3	0	0
1	AI	55	462	314	74	71	3	0	0
1	AJ	55	462	314	74	71	3	0	0
1	AK	55	462	314	74	71	3	0	0
1	AL	55	462	314	74	71	3	0	0
1	AM	55	462	314	74	71	3	0	0
1	AN	51	432	296	69	65	2	0	0
1	aa	46	394	272	60	59	3	0	0
1	ab	55	462	314	74	71	3	0	0
1	ac	55	462	314	74	71	3	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	ad	55	Total C N O S 462 314 74 71 3	0	0
1	ae	55	Total C N O S 462 314 74 71 3	0	0
1	af	55	Total C N O S 462 314 74 71 3	0	0
1	ag	55	Total C N O S 462 314 74 71 3	0	0
1	ah	55	Total C N O S 462 314 74 71 3	0	0
1	ai	55	Total C N O S 462 314 74 71 3	0	0
1	aj	55	Total C N O S 462 314 74 71 3	0	0
1	ak	55	Total C N O S 462 314 74 71 3	0	0
1	al	55	Total C N O S 462 314 74 71 3	0	0
1	am	55	Total C N O S 462 314 74 71 3	0	0
1	an	51	Total C N O S 432 296 69 65 2	0	0

- Molecule 2 is a protein called LH1-beta.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	BA	43	Total C N O S 351 236 55 59 1	0	0
2	BB	43	Total C N O S 351 236 55 59 1	0	0
2	BC	42	Total C N O S 343 230 54 58 1	0	0
2	BD	43	Total C N O S 351 236 55 59 1	0	0
2	BE	43	Total C N O S 351 236 55 59 1	0	0
2	BF	43	Total C N O S 351 236 55 59 1	0	0
2	BG	43	Total C N O S 351 236 55 59 1	0	0
2	BH	43	Total C N O S 351 236 55 59 1	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
2	BI	43	Total C N O S 351 236 55 59 1	0	0
2	BJ	43	Total C N O S 351 236 55 59 1	0	0
2	BK	42	Total C N O S 343 230 54 58 1	0	0
2	BL	42	Total C N O S 343 230 54 58 1	0	0
2	BM	42	Total C N O S 343 230 54 58 1	0	0
2	BN	37	Total C N O S 308 207 49 51 1	0	0
2	ba	43	Total C N O S 351 236 55 59 1	0	0
2	bb	43	Total C N O S 351 236 55 59 1	0	0
2	bc	42	Total C N O S 343 230 54 58 1	0	0
2	bd	43	Total C N O S 351 236 55 59 1	0	0
2	be	43	Total C N O S 351 236 55 59 1	0	0
2	bf	43	Total C N O S 351 236 55 59 1	0	0
2	bg	43	Total C N O S 351 236 55 59 1	0	0
2	bh	43	Total C N O S 351 236 55 59 1	0	0
2	bi	43	Total C N O S 351 236 55 59 1	0	0
2	bj	43	Total C N O S 351 236 55 59 1	0	0
2	bk	42	Total C N O S 343 230 54 58 1	0	0
2	bl	42	Total C N O S 343 230 54 58 1	0	0
2	bm	42	Total C N O S 343 230 54 58 1	0	0
2	bn	37	Total C N O S 308 207 49 51 1	0	0

- Molecule 3 is a protein called RC-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total 1866	C 1196	N 316	O 344	S 10	0	0
3	h	246	Total 1866	C 1196	N 316	O 344	S 10	0	0

- Molecule 4 is a protein called RC-L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total 2231	C 1507	N 355	O 361	S 8	0	0
4	l	281	Total 2231	C 1507	N 355	O 361	S 8	0	0

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	307	Total 2444	C 1630	N 400	O 403	S 11	0	0
5	m	307	Total 2444	C 1630	N 400	O 403	S 11	0	0

- Molecule 6 is a protein called PufZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UA	31	Total 244	C 165	N 39	O 35	S 5	0	0
6	UB	31	Total 244	C 165	N 39	O 35	S 5	0	0
6	ua	31	Total 244	C 165	N 39	O 35	S 5	0	0
6	ub	31	Total 244	C 165	N 39	O 35	S 5	0	0

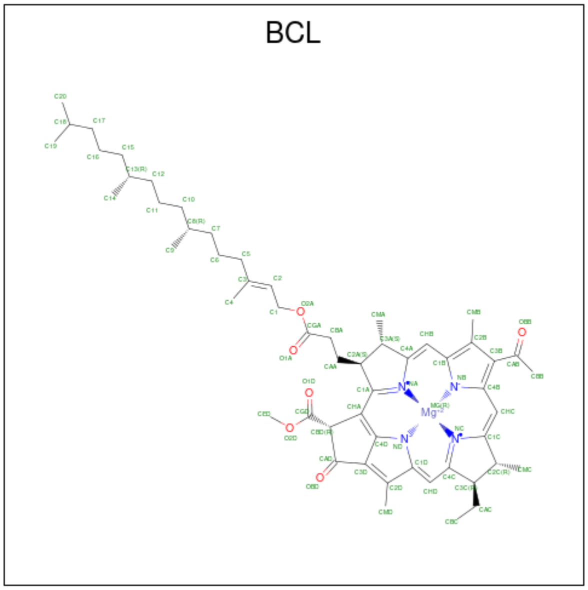
- Molecule 7 is a protein called PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UU	49	Total 362	C 247	N 56	O 56	S 3	0	0
7	uu	49	Total 362	C 247	N 56	O 56	S 3	0	0

- Molecule 8 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	X	55	424	281	74	66	3	0	0
8	x	55	424	281	74	66	3	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	AA	1	66	55	1	4	6	0
9	AB	1	66	55	1	4	6	0
9	AC	1	66	55	1	4	6	0
9	AD	1	66	55	1	4	6	0
9	AE	1	66	55	1	4	6	0
9	AF	1	66	55	1	4	6	0
9	AG	1	66	55	1	4	6	0
9	AH	1	66	55	1	4	6	0
9	AI	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
9	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	L	1	Total 132	C 110	Mg 2	N 8	O 12	0
9	L	1	Total 132	C 110	Mg 2	N 8	O 12	0

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Mol	Chain	Residues	Atoms	AltConf
9	M	1	Total C Mg N O 132 110 2 8 12	0
9	M	1	Total C Mg N O 132 110 2 8 12	0
9	aa	1	Total C Mg N O 66 55 1 4 6	0
9	ab	1	Total C Mg N O 66 55 1 4 6	0
9	ac	1	Total C Mg N O 66 55 1 4 6	0
9	ad	1	Total C Mg N O 66 55 1 4 6	0
9	ae	1	Total C Mg N O 66 55 1 4 6	0
9	af	1	Total C Mg N O 66 55 1 4 6	0
9	ag	1	Total C Mg N O 66 55 1 4 6	0
9	ah	1	Total C Mg N O 66 55 1 4 6	0
9	ai	1	Total C Mg N O 66 55 1 4 6	0
9	aj	1	Total C Mg N O 66 55 1 4 6	0
9	ak	1	Total C Mg N O 66 55 1 4 6	0
9	al	1	Total C Mg N O 66 55 1 4 6	0
9	am	1	Total C Mg N O 66 55 1 4 6	0
9	an	1	Total C Mg N O 66 55 1 4 6	0
9	ba	1	Total C Mg N O 66 55 1 4 6	0
9	bb	1	Total C Mg N O 66 55 1 4 6	0
9	bc	1	Total C Mg N O 66 55 1 4 6	0
9	bd	1	Total C Mg N O 66 55 1 4 6	0
9	be	1	Total C Mg N O 66 55 1 4 6	0

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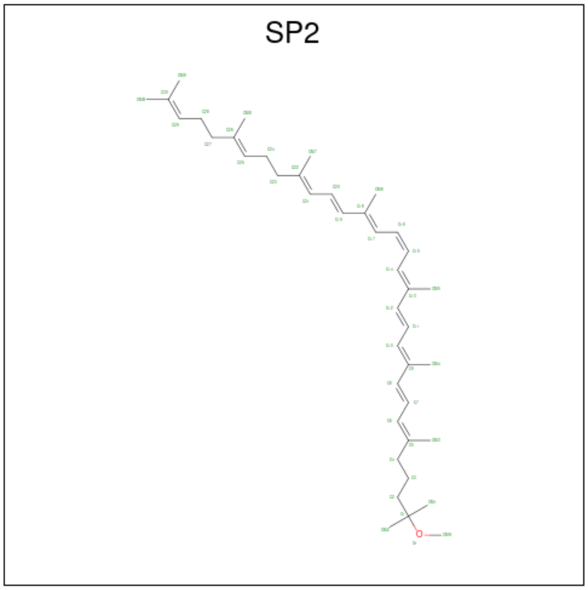
Mol	Chain	Residues	Atoms	AltConf
9	bf	1	Total C Mg N O 66 55 1 4 6	0
9	bg	1	Total C Mg N O 66 55 1 4 6	0
9	bh	1	Total C Mg N O 66 55 1 4 6	0
9	bi	1	Total C Mg N O 66 55 1 4 6	0
9	bj	1	Total C Mg N O 66 55 1 4 6	0
9	bk	1	Total C Mg N O 66 55 1 4 6	0
9	bl	1	Total C Mg N O 66 55 1 4 6	0
9	bm	1	Total C Mg N O 66 55 1 4 6	0
9	bn	1	Total C Mg N O 66 55 1 4 6	0
9	l	1	Total C Mg N O 132 110 2 8 12	0
9	l	1	Total C Mg N O 132 110 2 8 12	0
9	m	1	Total C Mg N O 132 110 2 8 12	0
9	m	1	Total C Mg N O 132 110 2 8 12	0

- Molecule 10 is 3,4-DIHYDROSPHEROIDENE (three-letter code: SP2) (formula: $C_{41}H_{62}O$).


SP2

Mol	Chain	Residues	Atoms	AltConf
10	AA	1	Total C O 42 41 1	0
10	AB	1	Total C O 126 123 3	0
10	AB	1	Total C O 126 123 3	0
10	AB	1	Total C O 126 123 3	0
10	AC	1	Total C O 84 82 2	0
10	AC	1	Total C O 84 82 2	0
10	AE	1	Total C O 42 41 1	0
10	AF	1	Total C O 84 82 2	0
10	AF	1	Total C O 84 82 2	0
10	AG	1	Total C O 42 41 1	0
10	AH	1	Total C O 42 41 1	0
10	AI	1	Total C O 84 82 2	0
10	AI	1	Total C O 84 82 2	0
10	AJ	1	Total C O 84 82 2	0

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Mol	Chain	Residues	Atoms	AltConf
10	AJ	1	Total C O 84 82 2	0
10	AK	1	Total C O 42 41 1	0
10	AM	1	Total C O 42 41 1	0
10	BA	1	Total C O 42 41 1	0
10	BC	1	Total C O 42 41 1	0
10	BE	1	Total C O 42 41 1	0
10	BF	1	Total C O 42 41 1	0
10	BH	1	Total C O 42 41 1	0
10	BJ	1	Total C O 42 41 1	0
10	BK	1	Total C O 42 41 1	0
10	BL	1	Total C O 84 82 2	0
10	BL	1	Total C O 84 82 2	0
10	M	1	Total C O 42 41 1	0
10	ab	1	Total C O 126 123 3	0
10	ab	1	Total C O 126 123 3	0
10	ab	1	Total C O 126 123 3	0
10	ac	1	Total C O 84 82 2	0
10	ac	1	Total C O 84 82 2	0
10	ad	1	Total C O 42 41 1	0
10	ae	1	Total C O 84 82 2	0
10	ae	1	Total C O 84 82 2	0

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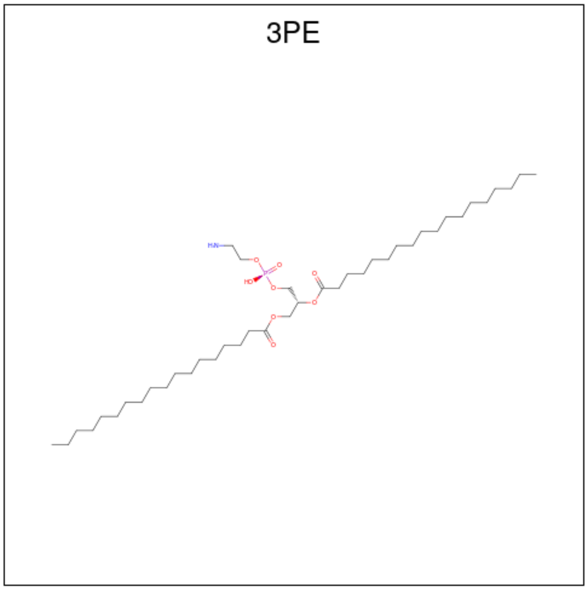
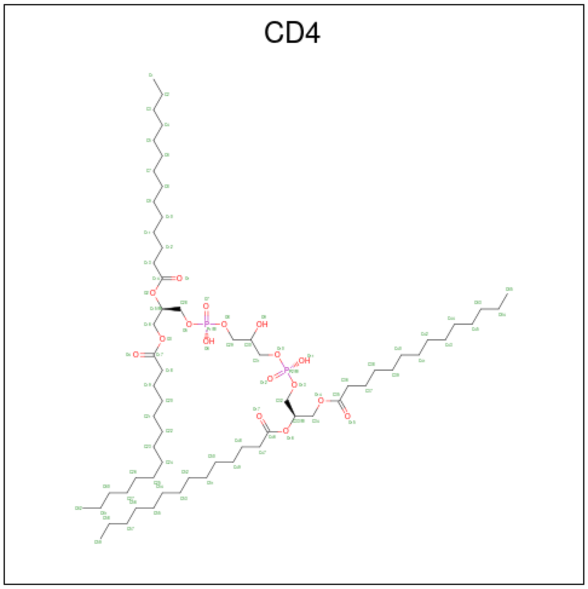
Mol	Chain	Residues	Atoms	AltConf
10	af	1	Total C O 126 123 3	0
10	af	1	Total C O 126 123 3	0
10	af	1	Total C O 126 123 3	0
10	ah	1	Total C O 42 41 1	0
10	ai	1	Total C O 84 82 2	0
10	ai	1	Total C O 84 82 2	0
10	aj	1	Total C O 84 82 2	0
10	aj	1	Total C O 84 82 2	0
10	ak	1	Total C O 42 41 1	0
10	al	1	Total C O 42 41 1	0
10	am	1	Total C O 42 41 1	0
10	ba	1	Total C O 42 41 1	0
10	bb	1	Total C O 42 41 1	0
10	bf	1	Total C O 42 41 1	0
10	bh	1	Total C O 42 41 1	0
10	bj	1	Total C O 42 41 1	0
10	bk	1	Total C O 42 41 1	0
10	bl	1	Total C O 42 41 1	0
10	m	1	Total C O 42 41 1	0

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



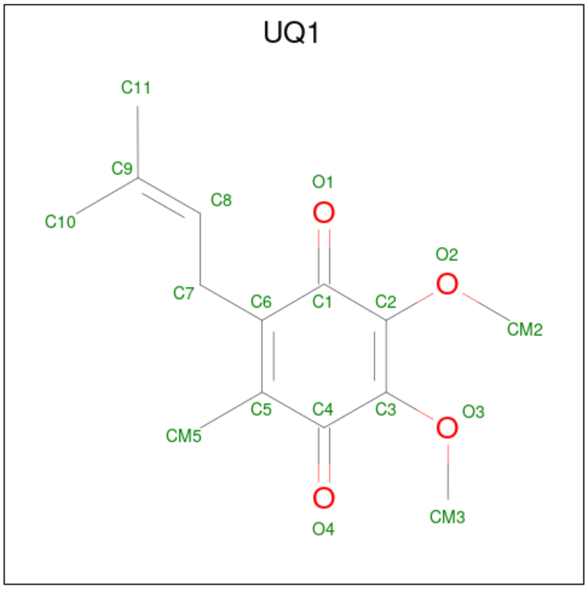
Mol	Chain	Residues	Atoms	AltConf
11	AC	1	Total C N O P 51 41 1 8 1	0
11	H	1	Total C N O P 51 41 1 8 1	0
11	ac	1	Total C N O P 51 41 1 8 1	0
11	h	1	Total C N O P 51 41 1 8 1	0

- Molecule 12 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula: $C_{65}H_{126}O_{17}P_2$).



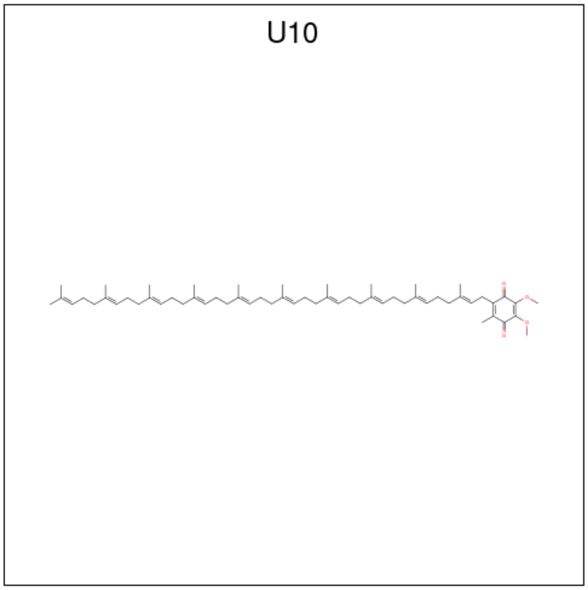
Mol	Chain	Residues	Atoms	AltConf
12	H	1	Total C O P 84 65 17 2	0
12	M	1	Total C O P 84 65 17 2	0
12	h	1	Total C O P 84 65 17 2	0
12	m	1	Total C O P 84 65 17 2	0

- Molecule 13 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



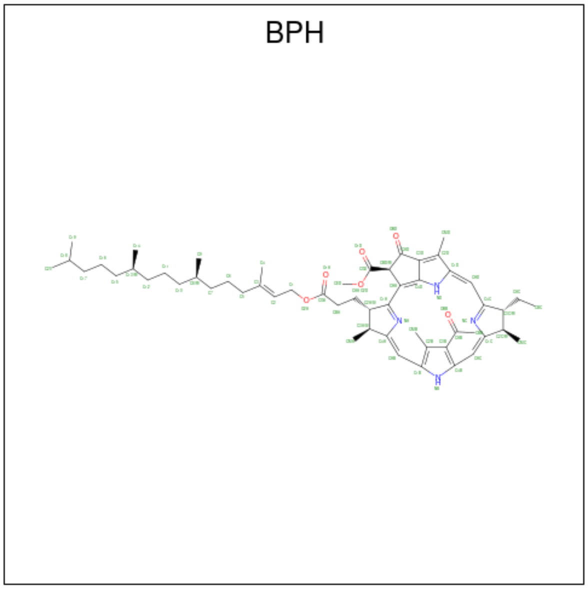
Mol	Chain	Residues	Atoms	AltConf
13	L	1	Total C O 18 14 4	0
13	l	1	Total C O 18 14 4	0

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



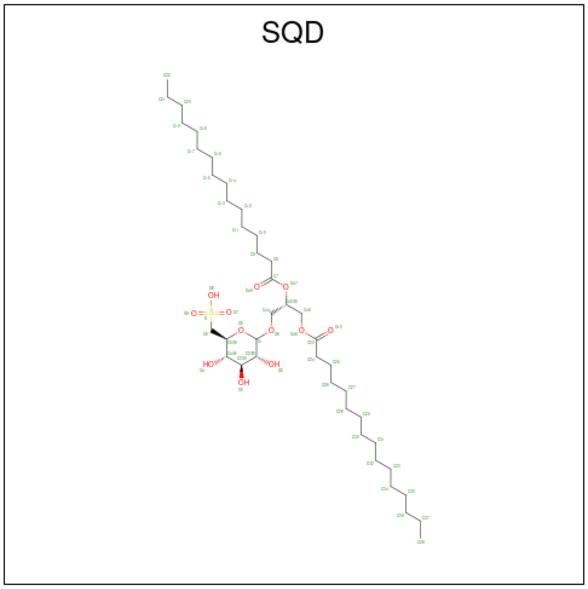
Mol	Chain	Residues	Atoms	AltConf
14	L	1	Total C O 63 59 4	0
14	M	1	Total C O 63 59 4	0
14	l	1	Total C O 63 59 4	0
14	m	1	Total C O 63 59 4	0

- Molecule 15 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



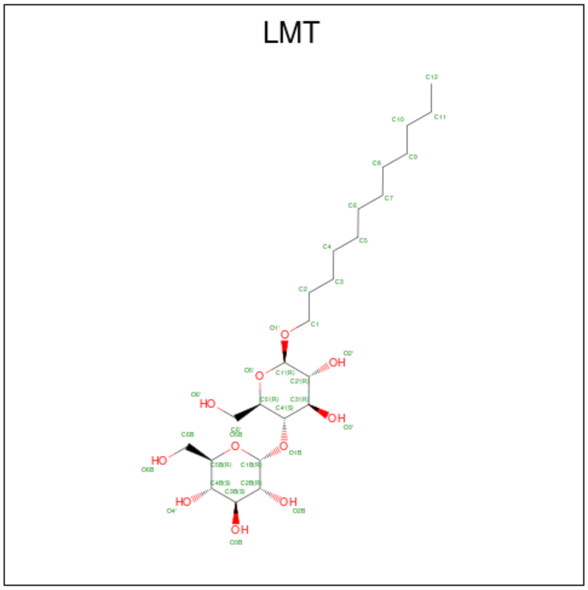
Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total 65	C 55	N 4	O 6	0
15	M	1	Total 65	C 55	N 4	O 6	0
15	l	1	Total 65	C 55	N 4	O 6	0
15	m	1	Total 65	C 55	N 4	O 6	0

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total 54	C 41	O 12	S 1	0
16	x	1	Total 54	C 41	O 12	S 1	0

- Molecule 17 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
17	M	1	Total C O 35 24 11	0
17	m	1	Total C O 35 24 11	0

- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
18	M	1	Total Fe 1 1	0
18	m	1	Total Fe 1 1	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	AltConf
19	AB	2	Total O 2 2	0
19	BB	1	Total O 1 1	0
19	H	18	Total O 18 18	0
19	L	27	Total O 27 27	0
19	M	19	Total O 19 19	0

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Mol	Chain	Residues	Atoms	AltConf
19	X	5	Total O 5 5	0
19	ab	3	Total O 3 3	0
19	h	18	Total O 18 18	0
19	l	27	Total O 27 27	0
19	m	19	Total O 19 19	0
19	x	5	Total O 5 5	0

3 Residue-property plots ⓘ

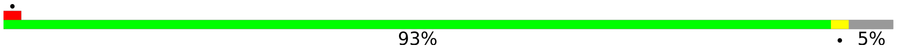
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

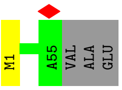
- Molecule 1: LH1-alpha

Chain AA:

- Molecule 1: LH1-alpha

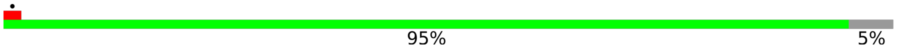
Chain AB:

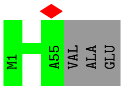




- Molecule 1: LH1-alpha

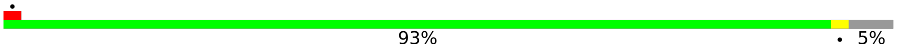
Chain AC:

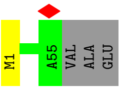




- Molecule 1: LH1-alpha

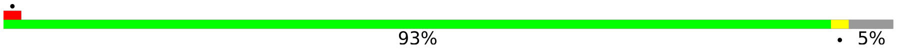
Chain AD:

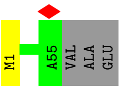




- Molecule 1: LH1-alpha

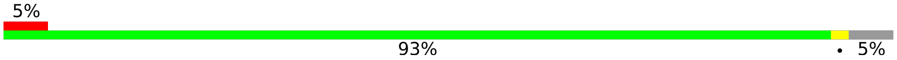
Chain AE:

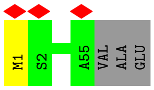




- Molecule 1: LH1-alpha

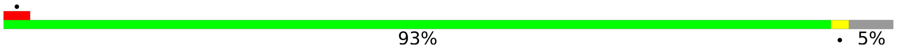
Chain AF:

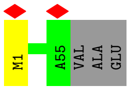




- Molecule 1: LH1-alpha

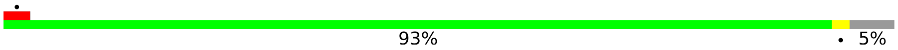
Chain AG:

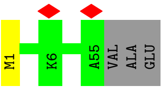




- Molecule 1: LH1-alpha

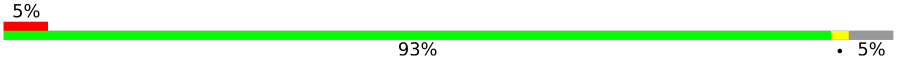
Chain AH:

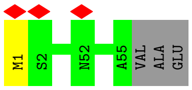




- Molecule 1: LH1-alpha

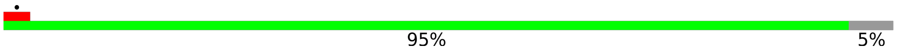
Chain AI:

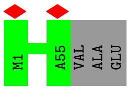




- Molecule 1: LH1-alpha

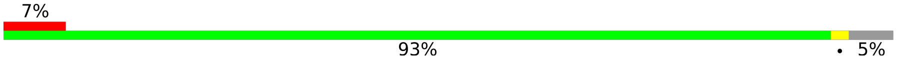
Chain AJ:

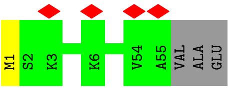




- Molecule 1: LH1-alpha

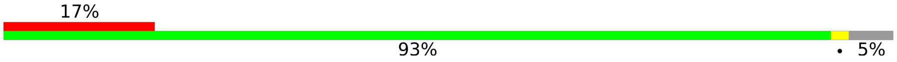
Chain AK:

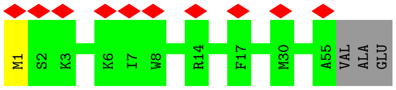




- Molecule 1: LH1-alpha

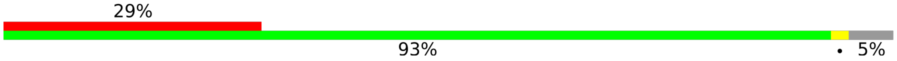
Chain AL:

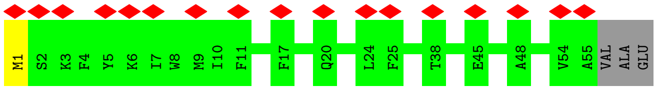




• Molecule 1: LH1-alpha

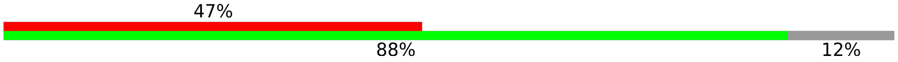
Chain AM:

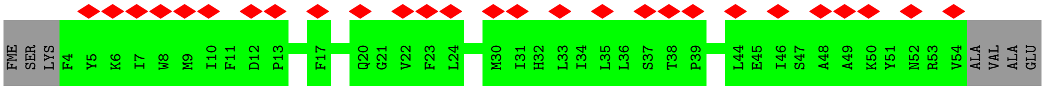




• Molecule 1: LH1-alpha

Chain AN:



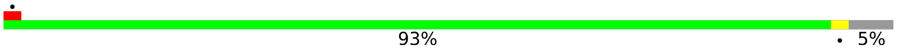


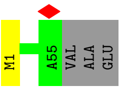
• Molecule 1: LH1-alpha

Chain aa:

• Molecule 1: LH1-alpha

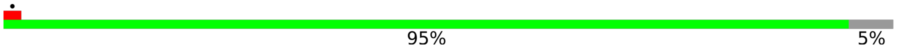
Chain ab:

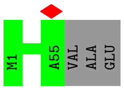




• Molecule 1: LH1-alpha

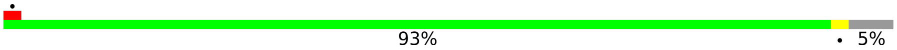
Chain ac:

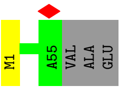




• Molecule 1: LH1-alpha

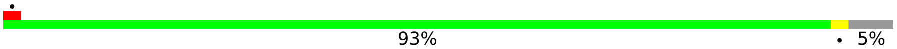
Chain ad:

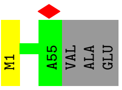




• Molecule 1: LH1-alpha

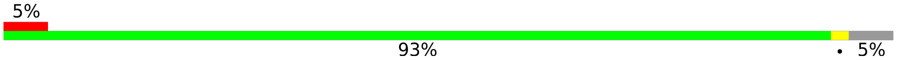
Chain ae:

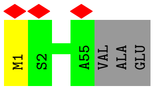




- Molecule 1: LH1-alpha

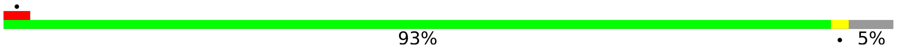
Chain af:

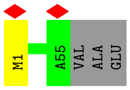




- Molecule 1: LH1-alpha

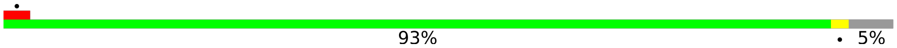
Chain ag:

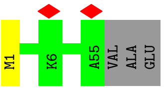




- Molecule 1: LH1-alpha

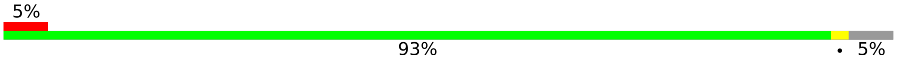
Chain ah:

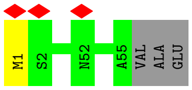




- Molecule 1: LH1-alpha

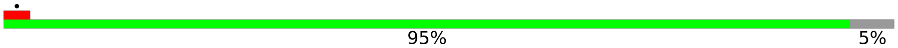
Chain ai:

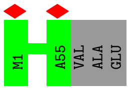




- Molecule 1: LH1-alpha

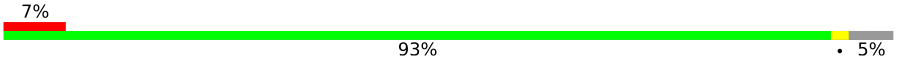
Chain aj:

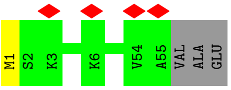




- Molecule 1: LH1-alpha

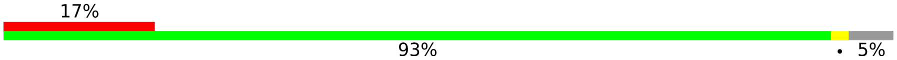
Chain ak:

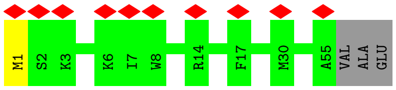




- Molecule 1: LH1-alpha

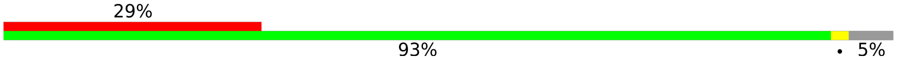
Chain al:

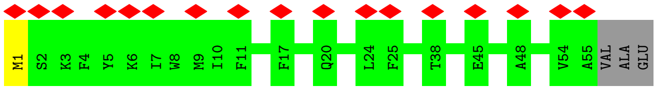




- Molecule 1: LH1-alpha

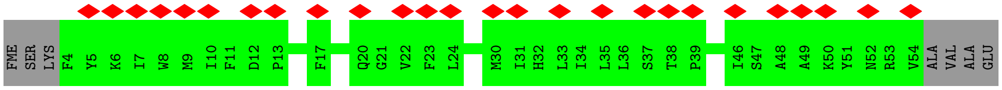
Chain am:





- Molecule 1: LH1-alpha

Chain an:



- Molecule 2: LH1-beta

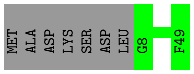
Chain BA:

- Molecule 2: LH1-beta

Chain BB:

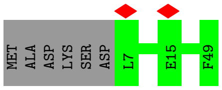
- Molecule 2: LH1-beta

Chain BC:



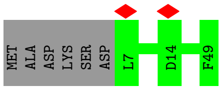
- Molecule 2: LH1-beta

Chain BD:



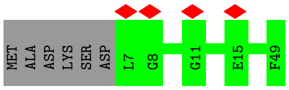
- Molecule 2: LH1-beta

Chain BE:



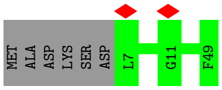
- Molecule 2: LH1-beta

Chain BF:



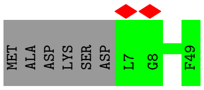
- Molecule 2: LH1-beta

Chain BG:



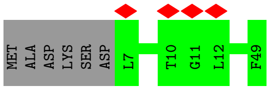
- Molecule 2: LH1-beta

Chain BH:



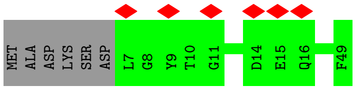
- Molecule 2: LH1-beta

Chain BI:



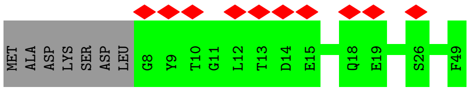
- Molecule 2: LH1-beta

Chain BJ:



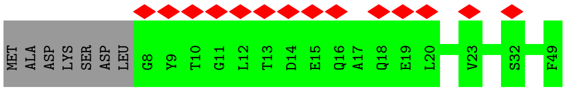
- Molecule 2: LH1-beta

Chain BK:



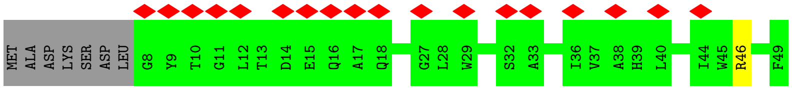
- Molecule 2: LH1-beta

Chain BL:



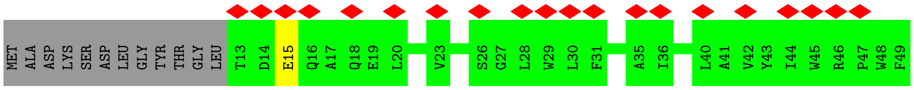
- Molecule 2: LH1-beta

Chain BM:



- Molecule 2: LH1-beta

Chain BN:



- Molecule 2: LH1-beta

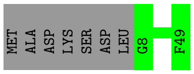
Chain ba:

- Molecule 2: LH1-beta

Chain bb:

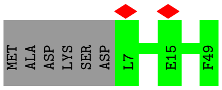
- Molecule 2: LH1-beta

Chain bc:



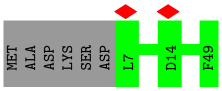
- Molecule 2: LH1-beta

Chain bd:



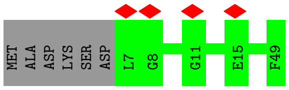
- Molecule 2: LH1-beta

Chain be:



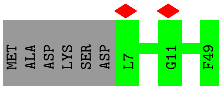
- Molecule 2: LH1-beta

Chain bf:



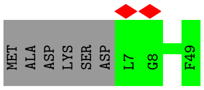
- Molecule 2: LH1-beta

Chain bg:



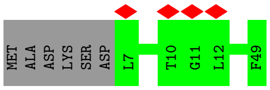
- Molecule 2: LH1-beta

Chain bh:



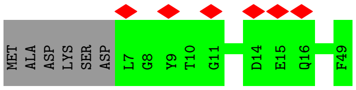
- Molecule 2: LH1-beta

Chain bi:



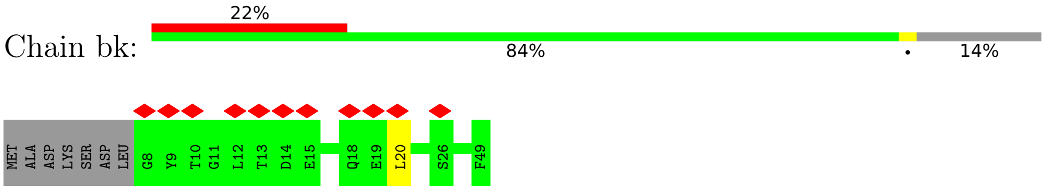
- Molecule 2: LH1-beta

Chain bj:



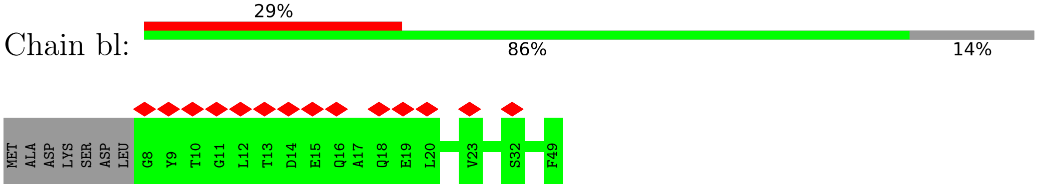
- Molecule 2: LH1-beta

Chain bk:



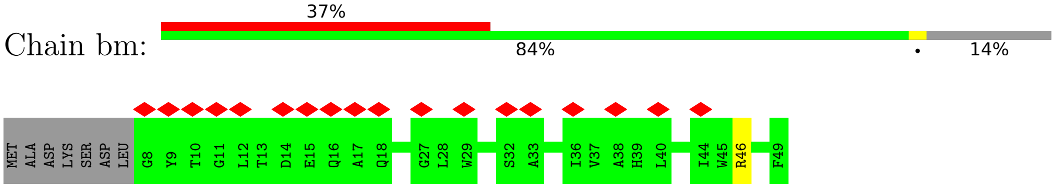
- Molecule 2: LH1-beta

Chain bl:



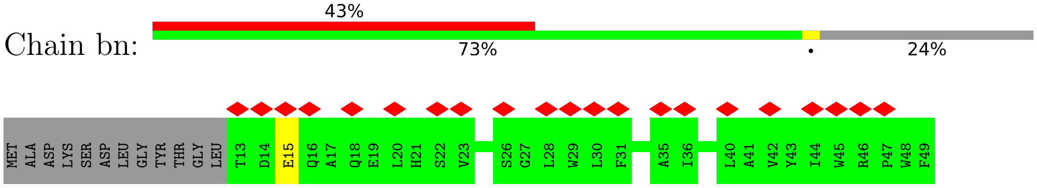
- Molecule 2: LH1-beta

Chain bm:



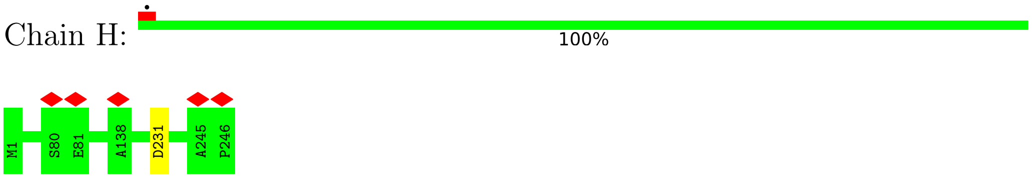
- Molecule 2: LH1-beta

Chain bn:



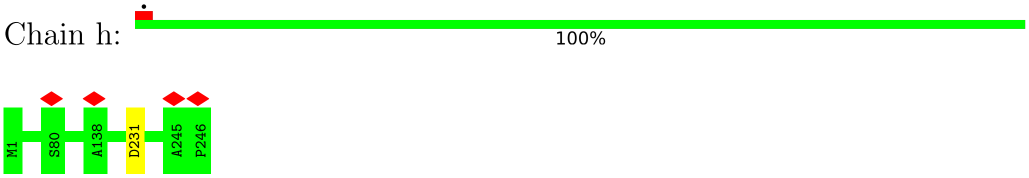
- Molecule 3: RC-H

Chain H:



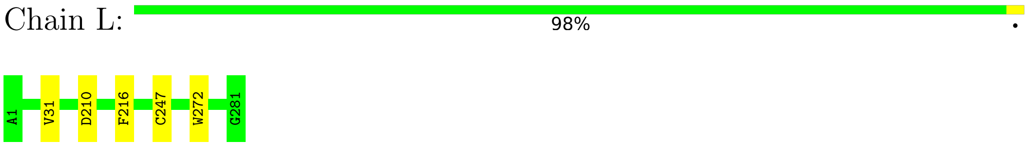
- Molecule 3: RC-H

Chain h:



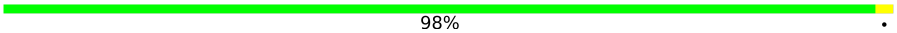
- Molecule 4: RC-L

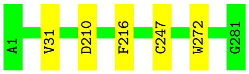
Chain L:



- Molecule 4: RC-L

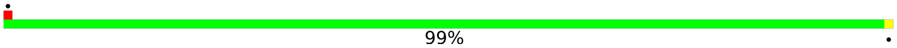
Chain l:





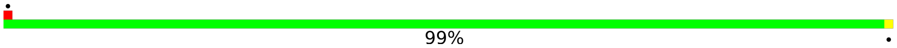
- Molecule 5: Reaction center protein M chain

Chain M:



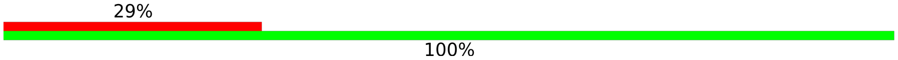
- Molecule 5: Reaction center protein M chain

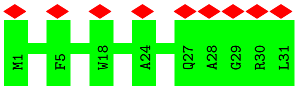
Chain m:



- Molecule 6: PufZ

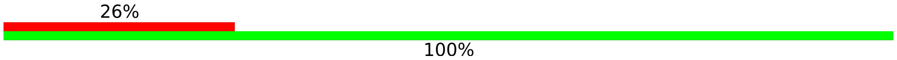
Chain UA:

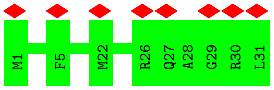




- Molecule 6: PufZ

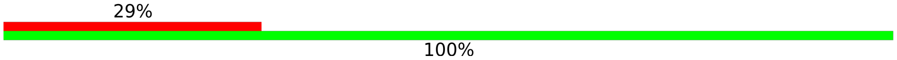
Chain UB:

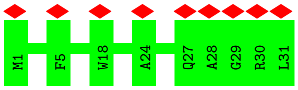




- Molecule 6: PufZ

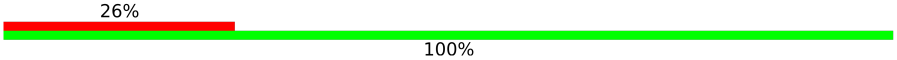
Chain ua:

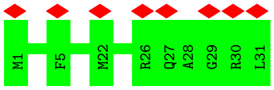




- Molecule 6: PufZ

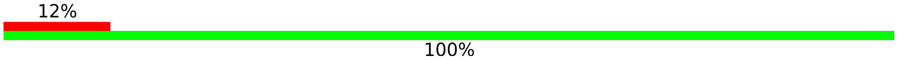
Chain ub:

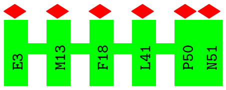




- Molecule 7: PufY

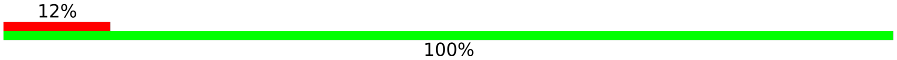
Chain UU:

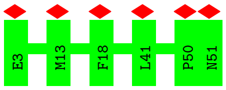




- Molecule 7: PufY

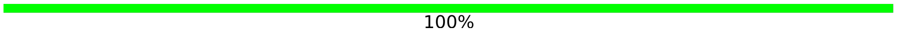
Chain uu:





- Molecule 8: PufX

Chain X:



There are no outlier residues recorded for this chain.

- Molecule 8: PufX

Chain x:

There are no outlier residues recorded for this chain.

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	58945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	45.36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0222	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CD4, BPH, U10, BCL, SP2, UQ1, FE, SQD, FME, LMT, 3PE

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	AA	0.26	0/397	0.46	0/539
1	AB	0.26	0/466	0.48	0/632
1	AC	0.26	0/466	0.51	0/632
1	AD	0.25	0/466	0.47	0/632
1	AE	0.26	0/466	0.51	0/632
1	AF	0.26	0/466	0.47	0/632
1	AG	0.26	0/466	0.50	0/632
1	AH	0.26	0/466	0.52	0/632
1	AI	0.25	0/466	0.47	0/632
1	AJ	0.26	0/466	0.49	0/632
1	AK	0.26	0/466	0.50	0/632
1	AL	0.26	0/466	0.51	0/632
1	AM	0.26	0/466	0.46	0/632
1	AN	0.26	0/446	0.51	0/606
1	aa	0.26	0/397	0.46	0/539
1	ab	0.25	0/466	0.48	0/632
1	ac	0.26	0/466	0.51	0/632
1	ad	0.25	0/466	0.47	0/632
1	ae	0.26	0/466	0.51	0/632
1	af	0.26	0/466	0.47	0/632
1	ag	0.26	0/466	0.50	0/632
1	ah	0.26	0/466	0.52	0/632
1	ai	0.26	0/466	0.47	0/632
1	aj	0.25	0/466	0.49	0/632
1	ak	0.26	0/466	0.50	0/632
1	al	0.27	0/466	0.50	0/632
1	am	0.26	0/466	0.47	0/632
1	an	0.26	0/446	0.51	0/606
2	BA	0.23	0/364	0.45	0/499
2	BB	0.23	0/364	0.44	0/499
2	BC	0.23	0/356	0.43	0/488
2	BD	0.24	0/364	0.43	0/499

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
2	BE	0.23	0/364	0.43	0/499
2	BF	0.23	0/364	0.44	0/499
2	BG	0.23	0/364	0.43	0/499
2	BH	0.23	0/364	0.44	0/499
2	BI	0.23	0/364	0.45	0/499
2	BJ	0.23	0/364	0.45	0/499
2	BK	0.23	0/356	0.48	0/488
2	BL	0.24	0/356	0.42	0/488
2	BM	0.23	0/356	0.41	0/488
2	BN	0.23	0/320	0.42	0/439
2	ba	0.23	0/364	0.46	0/499
2	bb	0.23	0/364	0.44	0/499
2	bc	0.23	0/356	0.43	0/488
2	bd	0.23	0/364	0.43	0/499
2	be	0.23	0/364	0.43	0/499
2	bf	0.23	0/364	0.44	0/499
2	bg	0.23	0/364	0.43	0/499
2	bh	0.23	0/364	0.44	0/499
2	bi	0.24	0/364	0.46	0/499
2	bj	0.23	0/364	0.44	0/499
2	bk	0.24	0/356	0.43	0/488
2	bl	0.23	0/356	0.43	0/488
2	bm	0.23	0/356	0.42	0/488
2	bn	0.24	0/320	0.41	0/439
3	H	0.24	0/1916	0.50	0/2609
3	h	0.24	0/1916	0.50	0/2609
4	L	0.26	0/2319	0.46	0/3175
4	l	0.26	0/2319	0.46	0/3175
5	M	0.24	0/2537	0.46	0/3464
5	m	0.24	0/2537	0.46	0/3464
6	UA	0.26	0/250	0.49	0/334
6	UB	0.27	0/250	0.49	0/334
6	ua	0.26	0/250	0.50	0/334
6	ub	0.27	0/250	0.49	0/334
7	UU	0.27	0/373	0.42	0/505
7	uu	0.27	0/373	0.42	0/505
8	X	0.24	0/436	0.54	0/589
8	x	0.24	0/436	0.53	0/589
All	All	0.25	0/39072	0.47	0/53242

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
2	BM	0	1
2	bm	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BM	46	ARG	Sidechain
2	bm	46	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AA	44/58 (76%)	43 (98%)	0	1 (2%)	6	23
1	AB	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AC	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AD	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AE	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AF	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AG	53/58 (91%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AH	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AI	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AJ	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AK	53/58 (91%)	53 (100%)	0	0	100	100
1	AL	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AM	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AN	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	aa	44/58 (76%)	43 (98%)	0	1 (2%)	6	23
1	ab	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ac	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ad	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ae	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	af	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ag	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ah	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ai	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	aj	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ak	53/58 (91%)	53 (100%)	0	0	100	100
1	al	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	am	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	an	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
2	BA	41/49 (84%)	41 (100%)	0	0	100	100
2	BB	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	BC	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	BD	41/49 (84%)	41 (100%)	0	0	100	100
2	BE	41/49 (84%)	41 (100%)	0	0	100	100
2	BF	41/49 (84%)	41 (100%)	0	0	100	100
2	BG	41/49 (84%)	41 (100%)	0	0	100	100
2	BH	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	BI	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	BJ	41/49 (84%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BK	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	BL	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	BM	40/49 (82%)	40 (100%)	0	0	100	100
2	BN	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
2	ba	41/49 (84%)	41 (100%)	0	0	100	100
2	bb	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	bc	40/49 (82%)	40 (100%)	0	0	100	100
2	bd	41/49 (84%)	41 (100%)	0	0	100	100
2	be	41/49 (84%)	41 (100%)	0	0	100	100
2	bf	41/49 (84%)	41 (100%)	0	0	100	100
2	bg	41/49 (84%)	41 (100%)	0	0	100	100
2	bh	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	bi	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	bj	41/49 (84%)	41 (100%)	0	0	100	100
2	bk	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	bl	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	bm	40/49 (82%)	40 (100%)	0	0	100	100
2	bn	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
3	H	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
3	h	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
4	L	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	34	66
4	l	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	34	66
5	M	305/307 (99%)	294 (96%)	10 (3%)	1 (0%)	41	71
5	m	305/307 (99%)	294 (96%)	10 (3%)	1 (0%)	41	71
6	UA	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
6	UB	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
6	ua	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
6	ub	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
7	UU	47/49 (96%)	47 (100%)	0	0	100	100
7	uu	47/49 (96%)	47 (100%)	0	0	100	100
8	X	53/55 (96%)	50 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	x	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
All	All	4558/4996 (91%)	4453 (98%)	99 (2%)	6 (0%)	54	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	SER
1	aa	2	SER
5	M	195	ASN
5	m	195	ASN
4	L	31	VAL
4	l	31	VAL

5.3.2 Protein sidechains ⓘ

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	AA	42/50 (84%)	42 (100%)	0	100	100
1	AB	48/50 (96%)	48 (100%)	0	100	100
1	AC	48/50 (96%)	48 (100%)	0	100	100
1	AD	48/50 (96%)	48 (100%)	0	100	100
1	AE	48/50 (96%)	48 (100%)	0	100	100
1	AF	48/50 (96%)	48 (100%)	0	100	100
1	AG	48/50 (96%)	48 (100%)	0	100	100
1	AH	48/50 (96%)	48 (100%)	0	100	100
1	AI	48/50 (96%)	48 (100%)	0	100	100
1	AJ	48/50 (96%)	48 (100%)	0	100	100
1	AK	48/50 (96%)	48 (100%)	0	100	100
1	AL	48/50 (96%)	48 (100%)	0	100	100
1	AM	48/50 (96%)	48 (100%)	0	100	100
1	AN	46/50 (92%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aa	42/50 (84%)	42 (100%)	0	100	100
1	ab	48/50 (96%)	48 (100%)	0	100	100
1	ac	48/50 (96%)	48 (100%)	0	100	100
1	ad	48/50 (96%)	48 (100%)	0	100	100
1	ae	48/50 (96%)	48 (100%)	0	100	100
1	af	48/50 (96%)	48 (100%)	0	100	100
1	ag	48/50 (96%)	48 (100%)	0	100	100
1	ah	48/50 (96%)	48 (100%)	0	100	100
1	ai	48/50 (96%)	48 (100%)	0	100	100
1	aj	48/50 (96%)	48 (100%)	0	100	100
1	ak	48/50 (96%)	48 (100%)	0	100	100
1	al	48/50 (96%)	48 (100%)	0	100	100
1	am	48/50 (96%)	48 (100%)	0	100	100
1	an	46/50 (92%)	46 (100%)	0	100	100
2	BA	35/40 (88%)	35 (100%)	0	100	100
2	BB	35/40 (88%)	35 (100%)	0	100	100
2	BC	34/40 (85%)	34 (100%)	0	100	100
2	BD	35/40 (88%)	35 (100%)	0	100	100
2	BE	35/40 (88%)	35 (100%)	0	100	100
2	BF	35/40 (88%)	35 (100%)	0	100	100
2	BG	35/40 (88%)	35 (100%)	0	100	100
2	BH	35/40 (88%)	35 (100%)	0	100	100
2	BI	35/40 (88%)	35 (100%)	0	100	100
2	BJ	35/40 (88%)	35 (100%)	0	100	100
2	BK	34/40 (85%)	34 (100%)	0	100	100
2	BL	34/40 (85%)	34 (100%)	0	100	100
2	BM	34/40 (85%)	34 (100%)	0	100	100
2	BN	31/40 (78%)	30 (97%)	1 (3%)	39	73
2	ba	35/40 (88%)	35 (100%)	0	100	100
2	bb	35/40 (88%)	35 (100%)	0	100	100
2	bc	34/40 (85%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	bd	35/40 (88%)	35 (100%)	0	100	100
2	be	35/40 (88%)	35 (100%)	0	100	100
2	bf	35/40 (88%)	35 (100%)	0	100	100
2	bg	35/40 (88%)	35 (100%)	0	100	100
2	bh	35/40 (88%)	35 (100%)	0	100	100
2	bi	35/40 (88%)	35 (100%)	0	100	100
2	bj	35/40 (88%)	35 (100%)	0	100	100
2	bk	34/40 (85%)	33 (97%)	1 (3%)	42	76
2	bl	34/40 (85%)	34 (100%)	0	100	100
2	bm	34/40 (85%)	34 (100%)	0	100	100
2	bn	31/40 (78%)	30 (97%)	1 (3%)	39	73
3	H	198/198 (100%)	197 (100%)	1 (0%)	88	96
3	h	198/198 (100%)	197 (100%)	1 (0%)	88	96
4	L	220/220 (100%)	216 (98%)	4 (2%)	59	85
4	l	220/220 (100%)	216 (98%)	4 (2%)	59	85
5	M	240/240 (100%)	238 (99%)	2 (1%)	81	94
5	m	240/240 (100%)	238 (99%)	2 (1%)	81	94
6	UA	22/22 (100%)	22 (100%)	0	100	100
6	UB	22/22 (100%)	22 (100%)	0	100	100
6	ua	22/22 (100%)	22 (100%)	0	100	100
6	ub	22/22 (100%)	22 (100%)	0	100	100
7	UU	33/33 (100%)	33 (100%)	0	100	100
7	uu	33/33 (100%)	33 (100%)	0	100	100
8	X	42/42 (100%)	42 (100%)	0	100	100
8	x	42/42 (100%)	42 (100%)	0	100	100
All	All	3846/4074 (94%)	3829 (100%)	17 (0%)	91	97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BN	15	GLU
3	H	231	ASP
4	L	210	ASP

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Mol	Chain	Res	Type
4	L	216	PHE
4	L	247	CYS
4	L	272	TRP
5	M	216	PHE
5	M	263	GLU
2	bk	20	LEU
2	bn	15	GLU
3	h	231	ASP
4	l	210	ASP
4	l	216	PHE
4	l	247	CYS
4	l	272	TRP
5	m	216	PHE
5	m	263	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	20	GLN
1	AB	20	GLN
1	AE	20	GLN
1	AF	52	ASN
2	BC	18	GLN
2	BJ	18	GLN
1	aa	20	GLN
1	ad	20	GLN
1	ae	20	GLN
1	af	52	ASN
2	bc	18	GLN
2	bj	18	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

26 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	$\#\|Z\| > 2$
1	FME	AA	1	1	8,9,10	0.92	0	7,9,11	0.93	0
1	FME	AC	1	1	8,9,10	0.96	0	7,9,11	0.91	0
1	FME	ab	1	1	8,9,10	0.91	0	7,9,11	1.29	1 (14%)
1	FME	al	1	1	8,9,10	0.90	0	7,9,11	1.22	1 (14%)
1	FME	ae	1	1	8,9,10	0.91	0	7,9,11	1.13	1 (14%)
1	FME	AB	1	1	8,9,10	0.91	0	7,9,11	1.29	1 (14%)
1	FME	AI	1	1	8,9,10	0.92	0	7,9,11	1.10	1 (14%)
1	FME	AJ	1	1	8,9,10	0.96	0	7,9,11	1.03	0
1	FME	ac	1	1	8,9,10	0.95	0	7,9,11	0.89	0
1	FME	ad	1	1	8,9,10	0.88	0	7,9,11	1.22	1 (14%)
1	FME	AL	1	1	8,9,10	0.90	0	7,9,11	1.22	1 (14%)
1	FME	ai	1	1	8,9,10	0.92	0	7,9,11	1.10	1 (14%)
1	FME	ah	1	1	8,9,10	0.91	0	7,9,11	1.05	1 (14%)
1	FME	ag	1	1	8,9,10	0.90	0	7,9,11	1.42	1 (14%)
1	FME	AE	1	1	8,9,10	0.91	0	7,9,11	1.13	1 (14%)
1	FME	af	1	1	8,9,10	0.91	0	7,9,11	1.27	1 (14%)
1	FME	ak	1	1	8,9,10	0.94	0	7,9,11	1.36	2 (28%)
1	FME	AF	1	1	8,9,10	0.91	0	7,9,11	1.28	1 (14%)
1	FME	AG	1	1	8,9,10	0.90	0	7,9,11	1.42	1 (14%)
1	FME	AH	1	1	8,9,10	0.91	0	7,9,11	1.06	1 (14%)
1	FME	aa	1	1	8,9,10	0.93	0	7,9,11	0.84	0
1	FME	AD	1	1	8,9,10	0.88	0	7,9,11	1.22	1 (14%)
1	FME	AM	1	1	8,9,10	0.91	0	7,9,11	1.11	1 (14%)
1	FME	aj	1	1	8,9,10	0.96	0	7,9,11	1.03	0
1	FME	am	1	1	8,9,10	0.91	0	7,9,11	1.11	1 (14%)
1	FME	AK	1	1	8,9,10	0.94	0	7,9,11	1.37	2 (28%)

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
1	FME	AA	1	1	-	1/7/9/11	-
1	FME	AC	1	1	-	1/7/9/11	-
1	FME	ab	1	1	-	0/7/9/11	-
1	FME	al	1	1	-	3/7/9/11	-
1	FME	ae	1	1	-	0/7/9/11	-
1	FME	AB	1	1	-	0/7/9/11	-
1	FME	AI	1	1	-	0/7/9/11	-
1	FME	AJ	1	1	-	4/7/9/11	-
1	FME	ac	1	1	-	1/7/9/11	-
1	FME	ad	1	1	-	0/7/9/11	-
1	FME	AL	1	1	-	3/7/9/11	-
1	FME	ai	1	1	-	0/7/9/11	-
1	FME	ah	1	1	-	0/7/9/11	-
1	FME	ag	1	1	-	1/7/9/11	-
1	FME	AE	1	1	-	0/7/9/11	-
1	FME	af	1	1	-	0/7/9/11	-
1	FME	ak	1	1	-	2/7/9/11	-
1	FME	AF	1	1	-	0/7/9/11	-
1	FME	AG	1	1	-	1/7/9/11	-
1	FME	AH	1	1	-	0/7/9/11	-
1	FME	aa	1	1	-	1/7/9/11	-
1	FME	AD	1	1	-	0/7/9/11	-
1	FME	AM	1	1	-	1/7/9/11	-
1	FME	aj	1	1	-	4/7/9/11	-
1	FME	am	1	1	-	1/7/9/11	-
1	FME	AK	1	1	-	2/7/9/11	-

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AG	1	FME	C-CA-N	3.16	115.44	109.73
1	ag	1	FME	C-CA-N	3.15	115.42	109.73
1	AB	1	FME	C-CA-N	2.71	114.63	109.73
1	ab	1	FME	C-CA-N	2.71	114.62	109.73
1	AF	1	FME	C-CA-N	2.61	114.44	109.73
1	af	1	FME	C-CA-N	2.60	114.42	109.73
1	ad	1	FME	C-CA-N	2.44	114.14	109.73
1	AD	1	FME	C-CA-N	2.44	114.13	109.73
1	al	1	FME	C-CA-N	2.38	114.03	109.73
1	AL	1	FME	C-CA-N	2.37	114.02	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AI	1	FME	C-CA-N	2.30	113.89	109.73
1	ai	1	FME	C-CA-N	2.30	113.88	109.73
1	AM	1	FME	C-CA-N	2.25	113.80	109.73
1	am	1	FME	C-CA-N	2.25	113.79	109.73
1	AE	1	FME	C-CA-N	2.25	113.79	109.73
1	ae	1	FME	C-CA-N	2.25	113.79	109.73
1	AK	1	FME	CA-N-CN	2.16	126.14	122.82
1	AH	1	FME	C-CA-N	2.15	113.62	109.73
1	ak	1	FME	CA-N-CN	2.13	126.09	122.82
1	AK	1	FME	C-CA-N	2.13	113.57	109.73
1	ah	1	FME	C-CA-N	2.11	113.55	109.73
1	ak	1	FME	C-CA-N	2.11	113.53	109.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1	FME	N-CA-CB-CG
1	AG	1	FME	O-C-CA-CB
1	AK	1	FME	O-C-CA-CB
1	ag	1	FME	O-C-CA-CB
1	ak	1	FME	O-C-CA-CB
1	AC	1	FME	N-CA-CB-CG
1	AJ	1	FME	N-CA-CB-CG
1	AL	1	FME	N-CA-CB-CG
1	aa	1	FME	N-CA-CB-CG
1	ac	1	FME	N-CA-CB-CG
1	aj	1	FME	N-CA-CB-CG
1	al	1	FME	N-CA-CB-CG
1	AJ	1	FME	C-CA-CB-CG
1	aj	1	FME	C-CA-CB-CG
1	AL	1	FME	CB-CG-SD-CE
1	al	1	FME	CB-CG-SD-CE
1	AJ	1	FME	CB-CG-SD-CE
1	aj	1	FME	CB-CG-SD-CE
1	AJ	1	FME	CA-CB-CG-SD
1	aj	1	FME	CA-CB-CG-SD
1	AK	1	FME	CA-CB-CG-SD
1	ak	1	FME	CA-CB-CG-SD
1	AM	1	FME	N-CA-CB-CG
1	am	1	FME	N-CA-CB-CG
1	AL	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	al	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 142 ligands modelled in this entry, 2 are monoatomic - leaving 140 for Mogul analysis.

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	$\#\|Z\| > 2$
10	SP2	AB	102	-	41,41,41	0.24	0	47,50,50	0.31	0
10	SP2	ah	102	-	41,41,41	0.27	0	47,50,50	0.28	0
9	BCL	AA	1001	-	58,74,74	1.30	4 (6%)	69,115,115	1.38	9 (13%)
14	U10	l	303	-	63,63,63	2.70	17 (26%)	76,79,79	1.59	20 (26%)
10	SP2	af	102	-	41,41,41	0.29	0	47,50,50	0.27	0
10	SP2	AG	101	-	41,41,41	0.31	0	47,50,50	0.50	0
9	BCL	ae	101	-	58,74,74	1.29	4 (6%)	69,115,115	1.38	9 (13%)
9	BCL	AE	102	-	58,74,74	1.29	4 (6%)	69,115,115	1.38	9 (13%)
10	SP2	ba	101	-	41,41,41	0.25	0	47,50,50	0.40	0
15	BPH	L	305	-	51,70,70	0.87	1 (1%)	52,101,101	1.13	6 (11%)
9	BCL	BC	101	-	58,74,74	1.30	5 (8%)	69,115,115	1.53	13 (18%)
9	BCL	AL	1001	-	58,74,74	1.33	4 (6%)	69,115,115	1.35	10 (14%)
9	BCL	AD	1001	-	58,74,74	1.30	4 (6%)	69,115,115	1.38	9 (13%)
9	BCL	L	304	-	58,74,74	1.26	4 (6%)	69,115,115	1.30	10 (14%)
10	SP2	ak	102	-	41,41,41	0.25	0	47,50,50	0.44	0
10	SP2	BC	102	-	41,41,41	0.38	0	47,50,50	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	BCL	AH	101	-	58,74,74	1.33	5 (8%)	69,115,115	1.32	9 (13%)
9	BCL	AG	102	-	58,74,74	1.30	5 (8%)	69,115,115	1.34	9 (13%)
9	BCL	al	1001	-	58,74,74	1.33	4 (6%)	69,115,115	1.40	10 (14%)
13	UQ1	L	302	-	18,18,18	0.79	0	22,25,25	1.78	5 (22%)
17	LMT	M	1001	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	1 (2%)
15	BPH	M	1003	-	51,70,70	0.88	1 (1%)	52,101,101	1.18	7 (13%)
9	BCL	BH	102	-	58,74,74	1.31	4 (6%)	69,115,115	1.47	14 (20%)
12	CD4	m	1005	-	83,83,83	0.48	0	89,95,95	1.05	5 (5%)
9	BCL	AI	102	-	58,74,74	1.33	4 (6%)	69,115,115	1.40	10 (14%)
9	BCL	AC	101	-	58,74,74	1.30	5 (8%)	69,115,115	1.32	9 (13%)
10	SP2	BK	102	-	41,41,41	0.31	0	47,50,50	0.40	0
9	BCL	BE	1001	-	58,74,74	1.28	4 (6%)	69,115,115	1.42	11 (15%)
9	BCL	m	1004	-	58,74,74	1.25	3 (5%)	69,115,115	1.38	9 (13%)
9	BCL	bl	101	-	58,74,74	1.30	4 (6%)	69,115,115	1.33	11 (15%)
10	SP2	BE	1002	-	41,41,41	0.28	0	47,50,50	0.31	0
10	SP2	ab	103	-	41,41,41	0.22	0	47,50,50	0.35	0
9	BCL	ah	101	-	58,74,74	1.33	5 (8%)	69,115,115	1.32	9 (13%)
10	SP2	ae	102	-	41,41,41	0.34	0	47,50,50	0.31	0
10	SP2	ab	101	-	41,41,41	0.24	0	47,50,50	0.59	1 (2%)
9	BCL	ai	102	-	58,74,74	1.33	4 (6%)	69,115,115	1.41	10 (14%)
9	BCL	AM	1001	-	58,74,74	1.34	5 (8%)	69,115,115	1.35	9 (13%)
9	BCL	ac	102	-	58,74,74	1.30	5 (8%)	69,115,115	1.30	9 (13%)
10	SP2	AM	1000	-	41,41,41	0.27	0	47,50,50	0.42	0
16	SQD	L	306	-	53,54,54	1.50	4 (7%)	62,65,65	1.71	8 (12%)
9	BCL	BJ	102	-	58,74,74	1.27	5 (8%)	69,115,115	1.36	11 (15%)
10	SP2	ac	104	-	41,41,41	0.36	0	47,50,50	0.42	0
17	LMT	m	1001	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	1 (2%)
9	BCL	BK	101	-	58,74,74	1.29	5 (8%)	69,115,115	1.32	10 (14%)
10	SP2	af	104	-	41,41,41	0.31	0	47,50,50	0.32	0
10	SP2	aj	103	-	41,41,41	0.32	0	47,50,50	0.54	0
14	U10	m	1003	-	63,63,63	2.66	17 (26%)	76,79,79	1.75	18 (23%)
14	U10	M	1007	-	63,63,63	2.66	17 (26%)	76,79,79	1.74	18 (23%)
9	BCL	an	101	-	58,74,74	1.35	5 (8%)	69,115,115	1.32	10 (14%)
10	SP2	AF	101	-	41,41,41	0.27	0	47,50,50	0.27	0
9	BCL	bg	101	-	58,74,74	1.31	4 (6%)	69,115,115	1.34	11 (15%)
14	U10	L	303	-	63,63,63	2.70	17 (26%)	76,79,79	1.59	20 (26%)
10	SP2	AB	104	-	41,41,41	0.32	0	47,50,50	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	SP2	AE	101	-	41,41,41	0.34	0	47,50,50	0.40	0
10	SP2	ae	103	-	41,41,41	0.28	0	47,50,50	0.31	0
9	BCL	BD	101	-	58,74,74	1.29	4 (6%)	69,115,115	1.37	10 (14%)
9	BCL	BG	101	-	58,74,74	1.31	4 (6%)	69,115,115	1.36	11 (15%)
9	BCL	bk	101	-	58,74,74	1.29	5 (8%)	69,115,115	1.32	10 (14%)
9	BCL	M	1002	-	58,74,74	1.26	3 (5%)	69,115,115	1.42	11 (15%)
10	SP2	AB	103	-	41,41,41	0.30	0	47,50,50	0.55	1 (2%)
10	SP2	ai	103	-	41,41,41	0.44	0	47,50,50	0.82	2 (4%)
9	BCL	BI	101	-	58,74,74	1.30	4 (6%)	69,115,115	1.34	9 (13%)
10	SP2	BL	103	-	41,41,41	0.48	0	47,50,50	0.49	0
10	SP2	AJ	102	-	41,41,41	0.25	0	47,50,50	0.42	0
9	BCL	BF	101	-	58,74,74	1.31	4 (6%)	69,115,115	1.31	10 (14%)
10	SP2	bk	102	-	41,41,41	0.32	0	47,50,50	0.44	0
9	BCL	AB	101	-	58,74,74	1.34	5 (8%)	69,115,115	1.47	12 (17%)
10	SP2	bh	101	-	41,41,41	0.34	0	47,50,50	0.46	0
10	SP2	AC	103	-	41,41,41	0.31	0	47,50,50	0.37	0
9	BCL	bf	101	-	58,74,74	1.31	4 (6%)	69,115,115	1.31	10 (14%)
10	SP2	AF	103	-	41,41,41	0.30	0	47,50,50	0.31	0
10	SP2	AK	102	-	41,41,41	0.25	0	47,50,50	0.45	0
12	CD4	H	302	-	83,83,83	0.48	0	89,95,95	0.93	6 (6%)
10	SP2	BA	101	-	41,41,41	0.28	0	47,50,50	0.30	0
9	BCL	ad	1001	-	58,74,74	1.30	4 (6%)	69,115,115	1.39	9 (13%)
9	BCL	am	1001	-	58,74,74	1.34	5 (8%)	69,115,115	1.35	9 (13%)
11	3PE	AC	102	-	50,50,50	0.51	0	53,55,55	0.66	2 (3%)
16	SQD	x	100	-	53,54,54	1.49	4 (7%)	62,65,65	1.69	9 (14%)
9	BCL	aa	1001	-	58,74,74	1.30	4 (6%)	69,115,115	1.38	10 (14%)
11	3PE	h	301	-	50,50,50	0.52	0	53,55,55	0.49	1 (1%)
9	BCL	af	101	-	58,74,74	1.32	4 (6%)	69,115,115	1.33	9 (13%)
9	BCL	AN	101	-	58,74,74	1.35	5 (8%)	69,115,115	1.32	10 (14%)
9	BCL	bm	1001	-	58,74,74	1.30	5 (8%)	69,115,115	1.34	10 (14%)
10	SP2	AI	101	-	41,41,41	0.38	0	47,50,50	0.93	2 (4%)
10	SP2	BJ	101	-	41,41,41	0.24	0	47,50,50	0.30	0
10	SP2	bf	102	-	41,41,41	0.28	0	47,50,50	0.37	0
10	SP2	M	1005	-	41,41,41	0.29	0	47,50,50	0.50	0
9	BCL	AK	101	-	58,74,74	1.33	5 (8%)	69,115,115	1.41	10 (14%)
12	CD4	M	1004	-	83,83,83	0.48	0	89,95,95	1.05	5 (5%)
10	SP2	AH	102	-	41,41,41	0.27	0	47,50,50	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	BCL	bd	101	-	58,74,74	1.29	4 (6%)	69,115,115	1.37	10 (14%)
9	BCL	M	1008	-	58,74,74	1.25	3 (5%)	69,115,115	1.38	9 (13%)
9	BCL	ak	101	-	58,74,74	1.33	5 (8%)	69,115,115	1.40	10 (14%)
10	SP2	AC	104	-	41,41,41	0.34	0	47,50,50	0.42	0
10	SP2	AI	103	-	41,41,41	0.44	0	47,50,50	0.80	2 (4%)
9	BCL	l	301	-	58,74,74	1.26	4 (6%)	69,115,115	1.30	10 (14%)
9	BCL	ba	102	-	58,74,74	1.29	3 (5%)	69,115,115	1.44	12 (17%)
9	BCL	bi	101	-	58,74,74	1.29	4 (6%)	69,115,115	1.34	10 (14%)
9	BCL	BN	101	-	58,74,74	1.33	5 (8%)	69,115,115	1.37	10 (14%)
12	CD4	h	302	-	83,83,83	0.48	0	89,95,95	0.93	6 (6%)
9	BCL	bb	1001	-	58,74,74	1.29	4 (6%)	69,115,115	1.42	12 (17%)
9	BCL	bn	101	-	58,74,74	1.33	5 (8%)	69,115,115	1.37	10 (14%)
9	BCL	BB	1001	-	58,74,74	1.29	4 (6%)	69,115,115	1.41	12 (17%)
9	BCL	AF	102	-	58,74,74	1.31	4 (6%)	69,115,115	1.33	9 (13%)
15	BPH	l	302	-	51,70,70	0.87	1 (1%)	52,101,101	1.13	6 (11%)
10	SP2	BL	101	-	41,41,41	0.31	0	47,50,50	0.31	0
9	BCL	BL	102	-	58,74,74	1.30	4 (6%)	69,115,115	1.33	11 (15%)
10	SP2	bj	101	-	41,41,41	0.26	0	47,50,50	0.29	0
9	BCL	bj	102	-	58,74,74	1.27	5 (8%)	69,115,115	1.36	11 (15%)
9	BCL	ag	101	-	58,74,74	1.29	5 (8%)	69,115,115	1.34	9 (13%)
10	SP2	bb	1002	-	41,41,41	0.39	0	47,50,50	0.42	0
9	BCL	bc	101	-	58,74,74	1.30	5 (8%)	69,115,115	1.53	13 (18%)
10	SP2	al	1002	-	41,41,41	0.36	0	47,50,50	0.39	0
9	BCL	m	1006	-	58,74,74	1.26	3 (5%)	69,115,115	1.42	11 (15%)
9	BCL	aj	101	-	58,74,74	1.34	5 (8%)	69,115,115	1.40	12 (17%)
13	UQ1	l	304	-	18,18,18	0.79	0	22,25,25	1.78	5 (22%)
10	SP2	am	1000	-	41,41,41	0.23	0	47,50,50	0.39	0
10	SP2	bl	102	-	41,41,41	0.48	0	47,50,50	0.50	0
10	SP2	BH	101	-	41,41,41	0.31	0	47,50,50	0.51	0
9	BCL	bh	102	-	58,74,74	1.31	4 (6%)	69,115,115	1.47	14 (20%)
9	BCL	be	1001	-	58,74,74	1.28	4 (6%)	69,115,115	1.42	11 (15%)
9	BCL	BM	1001	-	58,74,74	1.30	5 (8%)	69,115,115	1.34	10 (14%)
10	SP2	ai	101	-	41,41,41	0.39	0	47,50,50	0.94	2 (4%)
9	BCL	BA	102	-	58,74,74	1.29	4 (6%)	69,115,115	1.44	12 (17%)
11	3PE	ac	101	-	50,50,50	0.51	0	53,55,55	0.66	2 (3%)
10	SP2	ad	1002	-	41,41,41	0.34	0	47,50,50	0.47	0
10	SP2	ac	103	-	41,41,41	0.23	0	47,50,50	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\vert Z\vert > 2$	Counts	RMSZ	$\#\vert Z\vert > 2$
10	SP2	m	1007	-	41,41,41	0.21	0	47,50,50	0.52	0
10	SP2	ab	104	-	41,41,41	0.25	0	47,50,50	0.30	0
9	BCL	AJ	101	-	58,74,74	1.34	5 (8%)	69,115,115	1.41	12 (17%)
9	BCL	l	305	-	58,74,74	1.26	4 (6%)	69,115,115	1.35	11 (15%)
10	SP2	AA	1002	-	41,41,41	0.21	0	47,50,50	0.58	1 (2%)
15	BPH	m	1002	-	51,70,70	0.88	1 (1%)	52,101,101	1.18	7 (13%)
10	SP2	BF	102	-	41,41,41	0.29	0	47,50,50	0.37	0
9	BCL	ab	102	-	58,74,74	1.34	4 (6%)	69,115,115	1.45	11 (15%)
10	SP2	af	103	-	41,41,41	0.34	0	47,50,50	0.40	0
10	SP2	aj	102	-	41,41,41	0.26	0	47,50,50	0.30	0
9	BCL	L	301	-	58,74,74	1.26	4 (6%)	69,115,115	1.35	11 (15%)
11	3PE	H	301	-	50,50,50	0.52	0	53,55,55	0.49	1 (1%)
10	SP2	AJ	103	-	41,41,41	0.36	0	47,50,50	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SP2	AB	102	-	-	3/47/47/47	-
10	SP2	ah	102	-	-	4/47/47/47	-
9	BCL	AA	1001	-	-	3/37/137/137	-
14	U10	l	303	-	-	16/63/87/87	0/1/1/1
10	SP2	af	102	-	-	5/47/47/47	-
10	SP2	AG	101	-	-	4/47/47/47	-
9	BCL	ae	101	-	-	6/37/137/137	-
9	BCL	AE	102	-	-	6/37/137/137	-
10	SP2	ba	101	-	-	7/47/47/47	-
15	BPH	L	305	-	-	6/37/105/105	0/5/6/6
9	BCL	BC	101	-	-	8/37/137/137	-
9	BCL	AL	1001	-	-	4/37/137/137	-
9	BCL	AD	1001	-	-	3/37/137/137	-
9	BCL	L	304	-	-	1/37/137/137	-
10	SP2	ak	102	-	-	8/47/47/47	-
10	SP2	BC	102	-	-	3/47/47/47	-
9	BCL	AH	101	-	-	4/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AG	102	-	-	0/37/137/137	-
9	BCL	al	1001	-	-	4/37/137/137	-
13	UQ1	L	302	-	-	4/9/33/33	0/1/1/1
17	LMT	M	1001	-	-	4/21/61/61	0/2/2/2
15	BPH	M	1003	-	-	4/37/105/105	0/5/6/6
9	BCL	BH	102	-	-	5/37/137/137	-
12	CD4	m	1005	-	-	12/94/94/94	-
9	BCL	AI	102	-	-	10/37/137/137	-
9	BCL	AC	101	-	-	6/37/137/137	-
10	SP2	BK	102	-	-	8/47/47/47	-
9	BCL	BE	1001	-	-	5/37/137/137	-
9	BCL	m	1004	-	-	1/37/137/137	-
9	BCL	bl	101	-	-	9/37/137/137	-
10	SP2	BE	1002	-	-	7/47/47/47	-
10	SP2	ab	103	-	-	5/47/47/47	-
9	BCL	ah	101	-	-	2/37/137/137	-
10	SP2	ae	102	-	-	1/47/47/47	-
10	SP2	ab	101	-	-	5/47/47/47	-
9	BCL	ai	102	-	-	10/37/137/137	-
9	BCL	AM	1001	-	-	0/37/137/137	-
9	BCL	ac	102	-	-	8/37/137/137	-
10	SP2	AM	1000	-	-	8/47/47/47	-
16	SQD	L	306	-	-	15/49/69/69	0/1/1/1
9	BCL	BJ	102	-	-	6/37/137/137	-
10	SP2	ac	104	-	-	7/47/47/47	-
17	LMT	m	1001	-	-	4/21/61/61	0/2/2/2
9	BCL	BK	101	-	-	6/37/137/137	-
10	SP2	af	104	-	-	3/47/47/47	-
10	SP2	aj	103	-	-	9/47/47/47	-
14	U10	m	1003	-	-	10/63/87/87	0/1/1/1
14	U10	M	1007	-	-	10/63/87/87	0/1/1/1
9	BCL	an	101	-	-	7/37/137/137	-
10	SP2	AF	101	-	-	6/47/47/47	-
9	BCL	bg	101	-	-	6/37/137/137	-
14	U10	L	303	-	-	16/63/87/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SP2	AB	104	-	-	6/47/47/47	-
10	SP2	AE	101	-	-	2/47/47/47	-
10	SP2	ae	103	-	-	7/47/47/47	-
9	BCL	BD	101	-	-	1/37/137/137	-
9	BCL	BG	101	-	-	4/37/137/137	-
9	BCL	bk	101	-	-	6/37/137/137	-
9	BCL	M	1002	-	-	2/37/137/137	-
10	SP2	AB	103	-	-	7/47/47/47	-
10	SP2	ai	103	-	-	3/47/47/47	-
9	BCL	BI	101	-	-	7/37/137/137	-
10	SP2	BL	103	-	-	2/47/47/47	-
10	SP2	AJ	102	-	-	5/47/47/47	-
9	BCL	BF	101	-	-	6/37/137/137	-
10	SP2	bk	102	-	-	6/47/47/47	-
9	BCL	AB	101	-	-	4/37/137/137	-
10	SP2	bh	101	-	-	2/47/47/47	-
10	SP2	AC	103	-	-	3/47/47/47	-
9	BCL	bf	101	-	-	7/37/137/137	-
10	SP2	AF	103	-	-	4/47/47/47	-
10	SP2	AK	102	-	-	8/47/47/47	-
12	CD4	H	302	-	-	21/94/94/94	-
10	SP2	BA	101	-	-	6/47/47/47	-
9	BCL	ad	1001	-	-	3/37/137/137	-
9	BCL	am	1001	-	-	0/37/137/137	-
11	3PE	AC	102	-	-	22/54/54/54	-
16	SQD	x	100	-	-	5/49/69/69	0/1/1/1
9	BCL	aa	1001	-	-	3/37/137/137	-
11	3PE	h	301	-	-	11/54/54/54	-
9	BCL	af	101	-	-	7/37/137/137	-
9	BCL	AN	101	-	-	6/37/137/137	-
9	BCL	bm	1001	-	-	9/37/137/137	-
10	SP2	AI	101	-	-	2/47/47/47	-
10	SP2	BJ	101	-	-	7/47/47/47	-
10	SP2	bf	102	-	-	2/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SP2	M	1005	-	-	3/47/47/47	-
9	BCL	AK	101	-	-	7/37/137/137	-
12	CD4	M	1004	-	-	12/94/94/94	-
10	SP2	AH	102	-	-	4/47/47/47	-
9	BCL	bd	101	-	-	1/37/137/137	-
9	BCL	M	1008	-	-	1/37/137/137	-
9	BCL	ak	101	-	-	8/37/137/137	-
10	SP2	AC	104	-	-	7/47/47/47	-
10	SP2	AI	103	-	-	4/47/47/47	-
9	BCL	l	301	-	-	1/37/137/137	-
9	BCL	ba	102	-	-	5/37/137/137	-
9	BCL	bi	101	-	-	7/37/137/137	-
9	BCL	BN	101	-	-	7/37/137/137	-
12	CD4	h	302	-	-	21/94/94/94	-
9	BCL	bb	1001	-	-	4/37/137/137	-
9	BCL	bn	101	-	-	7/37/137/137	-
9	BCL	BB	1001	-	-	4/37/137/137	-
9	BCL	AF	102	-	-	6/37/137/137	-
15	BPH	l	302	-	-	7/37/105/105	0/5/6/6
10	SP2	BL	101	-	-	5/47/47/47	-
9	BCL	BL	102	-	-	9/37/137/137	-
10	SP2	bj	101	-	-	7/47/47/47	-
9	BCL	bj	102	-	-	6/37/137/137	-
9	BCL	ag	101	-	-	0/37/137/137	-
10	SP2	bb	1002	-	-	9/47/47/47	-
9	BCL	bc	101	-	-	8/37/137/137	-
10	SP2	al	1002	-	-	4/47/47/47	-
9	BCL	m	1006	-	-	2/37/137/137	-
9	BCL	aj	101	-	-	5/37/137/137	-
13	UQ1	l	304	-	-	4/9/33/33	0/1/1/1
10	SP2	am	1000	-	-	2/47/47/47	-
10	SP2	bl	102	-	-	2/47/47/47	-
10	SP2	BH	101	-	-	5/47/47/47	-
9	BCL	bh	102	-	-	5/37/137/137	-
9	BCL	be	1001	-	-	5/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	BM	1001	-	-	9/37/137/137	-
10	SP2	ai	101	-	-	8/47/47/47	-
9	BCL	BA	102	-	-	5/37/137/137	-
11	3PE	ac	101	-	-	22/54/54/54	-
10	SP2	ad	1002	-	-	6/47/47/47	-
10	SP2	ac	103	-	-	2/47/47/47	-
10	SP2	m	1007	-	-	5/47/47/47	-
10	SP2	ab	104	-	-	4/47/47/47	-
9	BCL	AJ	101	-	-	5/37/137/137	-
9	BCL	l	305	-	-	1/37/137/137	-
10	SP2	AA	1002	-	-	5/47/47/47	-
15	BPH	m	1002	-	-	4/37/105/105	0/5/6/6
10	SP2	BF	102	-	-	2/47/47/47	-
9	BCL	ab	102	-	-	4/37/137/137	-
10	SP2	af	103	-	-	8/47/47/47	-
10	SP2	aj	102	-	-	4/47/47/47	-
9	BCL	L	301	-	-	1/37/137/137	-
11	3PE	H	301	-	-	11/54/54/54	-
10	SP2	AJ	103	-	-	8/47/47/47	-

All (366) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	x	100	SQD	O8-S	6.37	1.70	1.47
16	L	306	SQD	O8-S	6.36	1.70	1.47
14	l	303	U10	C43-C44	6.18	1.47	1.33
14	L	303	U10	C43-C44	6.18	1.47	1.33
14	M	1007	U10	C38-C39	6.17	1.47	1.33
14	m	1003	U10	C38-C39	6.17	1.47	1.33
14	l	303	U10	C48-C49	6.15	1.47	1.33
14	L	303	U10	C48-C49	6.15	1.47	1.33
14	L	303	U10	C23-C24	6.11	1.47	1.33
14	l	303	U10	C23-C24	6.11	1.47	1.33
14	m	1003	U10	C28-C29	6.09	1.47	1.33
14	M	1007	U10	C43-C44	6.09	1.47	1.33
14	M	1007	U10	C28-C29	6.09	1.47	1.33
14	m	1003	U10	C43-C44	6.08	1.47	1.33
14	L	303	U10	C33-C34	6.07	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	303	U10	C33-C34	6.06	1.47	1.33
14	m	1003	U10	C33-C34	6.06	1.47	1.33
14	L	303	U10	C18-C19	6.06	1.47	1.33
14	M	1007	U10	C33-C34	6.06	1.47	1.33
14	l	303	U10	C18-C19	6.06	1.47	1.33
14	L	303	U10	C38-C39	6.05	1.47	1.33
14	l	303	U10	C38-C39	6.04	1.47	1.33
14	M	1007	U10	C48-C49	6.04	1.47	1.33
14	m	1003	U10	C48-C49	6.04	1.47	1.33
14	L	303	U10	C28-C29	6.04	1.47	1.33
14	l	303	U10	C28-C29	6.04	1.47	1.33
14	m	1003	U10	C13-C14	6.01	1.47	1.33
14	M	1007	U10	C13-C14	6.01	1.47	1.33
14	m	1003	U10	C18-C19	6.01	1.47	1.33
14	M	1007	U10	C8-C9	6.01	1.47	1.33
14	M	1007	U10	C18-C19	6.01	1.47	1.33
14	m	1003	U10	C8-C9	6.01	1.47	1.33
14	l	303	U10	C8-C9	5.95	1.47	1.33
14	L	303	U10	C8-C9	5.95	1.47	1.33
14	M	1007	U10	C23-C24	5.95	1.47	1.33
14	m	1003	U10	C23-C24	5.95	1.47	1.33
14	L	303	U10	C13-C14	5.91	1.47	1.33
14	l	303	U10	C13-C14	5.90	1.47	1.33
9	al	1001	BCL	MG-NA	5.59	2.19	2.06
9	an	101	BCL	MG-NA	5.56	2.19	2.06
9	AJ	101	BCL	MG-NA	5.55	2.19	2.06
9	AN	101	BCL	MG-NA	5.54	2.19	2.06
9	AL	1001	BCL	MG-NA	5.54	2.19	2.06
9	AM	1001	BCL	MG-NA	5.52	2.19	2.06
9	aj	101	BCL	MG-NA	5.50	2.19	2.06
9	ah	101	BCL	MG-NA	5.50	2.19	2.06
9	AH	101	BCL	MG-NA	5.49	2.19	2.06
9	am	1001	BCL	MG-NA	5.48	2.19	2.06
14	l	303	U10	O4-C4	-5.48	1.23	1.36
14	L	303	U10	O4-C4	-5.47	1.23	1.36
9	af	101	BCL	MG-NA	5.46	2.19	2.06
9	AK	101	BCL	MG-NA	5.43	2.19	2.06
9	AA	1001	BCL	MG-NA	5.42	2.19	2.06
9	aa	1001	BCL	MG-NA	5.42	2.19	2.06
9	ak	101	BCL	MG-NA	5.42	2.19	2.06
9	AF	102	BCL	MG-NA	5.41	2.19	2.06
9	ab	102	BCL	MG-NA	5.41	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AB	101	BCL	MG-NA	5.40	2.19	2.06
9	AD	1001	BCL	MG-NA	5.36	2.19	2.06
9	ad	1001	BCL	MG-NA	5.36	2.19	2.06
9	bn	101	BCL	MG-NA	5.35	2.19	2.06
9	BN	101	BCL	MG-NA	5.34	2.19	2.06
9	ai	102	BCL	MG-NA	5.33	2.18	2.06
9	AI	102	BCL	MG-NA	5.32	2.18	2.06
9	ae	101	BCL	MG-NA	5.28	2.18	2.06
9	AE	102	BCL	MG-NA	5.27	2.18	2.06
14	l	303	U10	C53-C54	5.26	1.47	1.32
14	L	303	U10	C53-C54	5.26	1.47	1.32
9	bh	102	BCL	MG-NA	5.26	2.18	2.06
9	BH	102	BCL	MG-NA	5.25	2.18	2.06
9	ag	101	BCL	MG-NA	5.21	2.18	2.06
9	AG	102	BCL	MG-NA	5.21	2.18	2.06
9	M	1008	BCL	MG-NA	5.19	2.18	2.06
9	ac	102	BCL	MG-NA	5.19	2.18	2.06
9	m	1004	BCL	MG-NA	5.19	2.18	2.06
9	AC	101	BCL	MG-NA	5.19	2.18	2.06
9	BM	1001	BCL	MG-NA	5.17	2.18	2.06
9	bm	1001	BCL	MG-NA	5.17	2.18	2.06
9	bg	101	BCL	MG-NA	5.16	2.18	2.06
14	M	1007	U10	C53-C54	5.16	1.47	1.32
9	BG	101	BCL	MG-NA	5.16	2.18	2.06
9	ba	102	BCL	MG-NA	5.16	2.18	2.06
14	m	1003	U10	C53-C54	5.15	1.47	1.32
9	BA	102	BCL	MG-NA	5.15	2.18	2.06
9	be	1001	BCL	MG-NA	5.14	2.18	2.06
9	BE	1001	BCL	MG-NA	5.14	2.18	2.06
9	bl	101	BCL	MG-NA	5.13	2.18	2.06
9	BL	102	BCL	MG-NA	5.13	2.18	2.06
9	bd	101	BCL	MG-NA	5.12	2.18	2.06
9	BF	101	BCL	MG-NA	5.11	2.18	2.06
9	bf	101	BCL	MG-NA	5.11	2.18	2.06
9	BB	1001	BCL	MG-NA	5.11	2.18	2.06
9	BI	101	BCL	MG-NA	5.11	2.18	2.06
9	BD	101	BCL	MG-NA	5.10	2.18	2.06
14	l	303	U10	O3-C3	-5.10	1.24	1.36
9	bb	1001	BCL	MG-NA	5.10	2.18	2.06
9	bi	101	BCL	MG-NA	5.10	2.18	2.06
14	L	303	U10	O3-C3	-5.10	1.24	1.36
9	bc	101	BCL	MG-NA	5.06	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BK	101	BCL	MG-NA	5.05	2.18	2.06
9	bk	101	BCL	MG-NA	5.04	2.18	2.06
9	M	1002	BCL	MG-NA	5.04	2.18	2.06
9	BC	101	BCL	MG-NA	5.04	2.18	2.06
9	AN	101	BCL	C1B-NB	5.03	1.39	1.35
9	BJ	102	BCL	MG-NA	5.02	2.18	2.06
9	BF	101	BCL	C1B-NB	5.02	1.39	1.35
9	bj	102	BCL	MG-NA	5.02	2.18	2.06
9	BN	101	BCL	C1B-NB	5.02	1.39	1.35
9	m	1006	BCL	MG-NA	5.01	2.18	2.06
9	bf	101	BCL	C1B-NB	5.01	1.39	1.35
9	bn	101	BCL	C1B-NB	5.00	1.39	1.35
16	L	306	SQD	O7-S	-4.99	1.30	1.45
9	an	101	BCL	C1B-NB	4.99	1.39	1.35
16	x	100	SQD	O7-S	-4.99	1.30	1.45
9	bk	101	BCL	C1B-NB	4.98	1.39	1.35
9	AI	102	BCL	C1B-NB	4.98	1.39	1.35
9	BK	101	BCL	C1B-NB	4.97	1.39	1.35
9	ai	102	BCL	C1B-NB	4.97	1.39	1.35
9	al	1001	BCL	C1B-NB	4.97	1.39	1.35
9	AL	1001	BCL	C1B-NB	4.96	1.39	1.35
9	bm	1001	BCL	C1B-NB	4.96	1.39	1.35
9	aj	101	BCL	C1B-NB	4.95	1.39	1.35
9	BM	1001	BCL	C1B-NB	4.94	1.39	1.35
9	l	305	BCL	C1B-NB	4.93	1.39	1.35
9	L	301	BCL	C1B-NB	4.92	1.39	1.35
9	AJ	101	BCL	C1B-NB	4.92	1.39	1.35
9	BI	101	BCL	C1B-NB	4.91	1.39	1.35
9	bi	101	BCL	C1B-NB	4.91	1.39	1.35
9	AM	1001	BCL	C1B-NB	4.91	1.39	1.35
9	AG	102	BCL	C1B-NB	4.91	1.39	1.35
9	ac	102	BCL	C1B-NB	4.90	1.39	1.35
9	BG	101	BCL	C1B-NB	4.90	1.39	1.35
9	l	305	BCL	MG-NA	4.90	2.17	2.06
9	L	301	BCL	MG-NA	4.90	2.17	2.06
9	AC	101	BCL	C1B-NB	4.90	1.39	1.35
9	am	1001	BCL	C1B-NB	4.90	1.39	1.35
9	BL	102	BCL	C1B-NB	4.89	1.39	1.35
9	AH	101	BCL	C1B-NB	4.89	1.39	1.35
9	BC	101	BCL	C1B-NB	4.89	1.39	1.35
14	M	1007	U10	O4-C4	-4.89	1.24	1.36
14	m	1003	U10	O4-C4	-4.89	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	ag	101	BCL	C1B-NB	4.89	1.39	1.35
9	ah	101	BCL	C1B-NB	4.89	1.39	1.35
9	bg	101	BCL	C1B-NB	4.88	1.39	1.35
9	bl	101	BCL	C1B-NB	4.88	1.39	1.35
9	bc	101	BCL	C1B-NB	4.88	1.39	1.35
9	BB	1001	BCL	C1B-NB	4.88	1.39	1.35
9	bb	1001	BCL	C1B-NB	4.88	1.39	1.35
9	bd	101	BCL	C1B-NB	4.88	1.39	1.35
9	BD	101	BCL	C1B-NB	4.87	1.39	1.35
9	aa	1001	BCL	C1B-NB	4.87	1.39	1.35
9	ak	101	BCL	C1B-NB	4.87	1.39	1.35
9	AK	101	BCL	C1B-NB	4.86	1.39	1.35
9	bj	102	BCL	C1B-NB	4.86	1.39	1.35
9	AA	1001	BCL	C1B-NB	4.86	1.39	1.35
9	BJ	102	BCL	C1B-NB	4.85	1.39	1.35
9	be	1001	BCL	C1B-NB	4.85	1.39	1.35
9	BE	1001	BCL	C1B-NB	4.84	1.39	1.35
14	m	1003	U10	O3-C3	-4.83	1.25	1.36
14	M	1007	U10	O3-C3	-4.83	1.25	1.36
16	L	306	SQD	O9-S	-4.81	1.30	1.45
16	x	100	SQD	O9-S	-4.81	1.30	1.45
9	m	1006	BCL	C1B-NB	4.80	1.39	1.35
9	ae	101	BCL	C1B-NB	4.80	1.39	1.35
9	l	301	BCL	MG-NA	4.80	2.17	2.06
9	AE	102	BCL	C1B-NB	4.80	1.39	1.35
9	M	1002	BCL	C1B-NB	4.80	1.39	1.35
9	L	304	BCL	MG-NA	4.79	2.17	2.06
9	ba	102	BCL	C1B-NB	4.79	1.39	1.35
9	l	301	BCL	C1B-NB	4.79	1.39	1.35
9	L	304	BCL	C1B-NB	4.78	1.39	1.35
9	BA	102	BCL	C1B-NB	4.78	1.39	1.35
9	bh	102	BCL	C1B-NB	4.78	1.39	1.35
9	BH	102	BCL	C1B-NB	4.77	1.39	1.35
9	AF	102	BCL	C1B-NB	4.76	1.39	1.35
9	af	101	BCL	C1B-NB	4.76	1.39	1.35
9	AD	1001	BCL	C1B-NB	4.75	1.39	1.35
9	ad	1001	BCL	C1B-NB	4.73	1.39	1.35
9	AB	101	BCL	C1B-NB	4.71	1.39	1.35
9	ab	102	BCL	C1B-NB	4.71	1.39	1.35
9	M	1008	BCL	C1B-NB	4.67	1.39	1.35
9	m	1004	BCL	C1B-NB	4.66	1.39	1.35
16	L	306	SQD	C6-S	-4.24	1.61	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	x	100	SQD	C6-S	-4.22	1.61	1.77
9	bn	101	BCL	MG-NC	4.18	2.16	2.06
9	BN	101	BCL	MG-NC	4.14	2.16	2.06
9	BG	101	BCL	MG-NC	4.05	2.15	2.06
9	bg	101	BCL	MG-NC	4.04	2.15	2.06
9	AM	1001	BCL	MG-NC	4.02	2.15	2.06
9	ah	101	BCL	MG-NC	4.01	2.15	2.06
9	an	101	BCL	MG-NC	4.00	2.15	2.06
9	am	1001	BCL	MG-NC	4.00	2.15	2.06
9	AN	101	BCL	MG-NC	4.00	2.15	2.06
9	AH	101	BCL	MG-NC	3.99	2.15	2.06
9	AJ	101	BCL	MG-NC	3.99	2.15	2.06
9	aj	101	BCL	MG-NC	3.96	2.15	2.06
9	al	1001	BCL	MG-NC	3.96	2.15	2.06
9	af	101	BCL	MG-NC	3.95	2.15	2.06
9	AB	101	BCL	MG-NC	3.94	2.15	2.06
9	ab	102	BCL	MG-NC	3.93	2.15	2.06
9	ad	1001	BCL	MG-NC	3.93	2.15	2.06
9	AL	1001	BCL	MG-NC	3.92	2.15	2.06
9	AK	101	BCL	MG-NC	3.91	2.15	2.06
9	ak	101	BCL	MG-NC	3.91	2.15	2.06
9	AF	102	BCL	MG-NC	3.90	2.15	2.06
9	AD	1001	BCL	MG-NC	3.90	2.15	2.06
9	BF	101	BCL	MG-NC	3.88	2.15	2.06
9	bf	101	BCL	MG-NC	3.88	2.15	2.06
9	ai	102	BCL	MG-NC	3.88	2.15	2.06
9	AI	102	BCL	MG-NC	3.87	2.15	2.06
9	AA	1001	BCL	MG-NC	3.87	2.15	2.06
9	aa	1001	BCL	MG-NC	3.87	2.15	2.06
9	bh	102	BCL	MG-NC	3.84	2.15	2.06
9	BH	102	BCL	MG-NC	3.83	2.15	2.06
9	AC	101	BCL	MG-NC	3.82	2.15	2.06
9	BK	101	BCL	MG-NC	3.82	2.15	2.06
9	ae	101	BCL	MG-NC	3.81	2.15	2.06
9	ba	102	BCL	MG-NC	3.81	2.15	2.06
9	ac	102	BCL	MG-NC	3.81	2.15	2.06
9	BA	102	BCL	MG-NC	3.81	2.15	2.06
9	AE	102	BCL	MG-NC	3.80	2.15	2.06
9	bd	101	BCL	MG-NC	3.79	2.15	2.06
9	bk	101	BCL	MG-NC	3.79	2.15	2.06
9	BL	102	BCL	MG-NC	3.79	2.15	2.06
9	bl	101	BCL	MG-NC	3.79	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BE	1001	BCL	MG-NC	3.78	2.15	2.06
9	be	1001	BCL	MG-NC	3.78	2.15	2.06
9	BD	101	BCL	MG-NC	3.78	2.15	2.06
9	BM	1001	BCL	MG-NC	3.76	2.15	2.06
9	bi	101	BCL	MG-NC	3.76	2.15	2.06
9	BI	101	BCL	MG-NC	3.76	2.15	2.06
9	bm	1001	BCL	MG-NC	3.76	2.15	2.06
9	BB	1001	BCL	MG-NC	3.75	2.15	2.06
9	bb	1001	BCL	MG-NC	3.75	2.15	2.06
9	AG	102	BCL	MG-NC	3.72	2.15	2.06
9	ag	101	BCL	MG-NC	3.71	2.15	2.06
9	bj	102	BCL	MG-NC	3.70	2.15	2.06
9	BJ	102	BCL	MG-NC	3.70	2.15	2.06
9	M	1002	BCL	MG-NC	3.69	2.15	2.06
9	bc	101	BCL	MG-NC	3.68	2.15	2.06
9	BC	101	BCL	MG-NC	3.67	2.15	2.06
9	m	1006	BCL	MG-NC	3.67	2.15	2.06
9	l	301	BCL	MG-NC	3.66	2.15	2.06
9	L	304	BCL	MG-NC	3.66	2.15	2.06
15	M	1003	BPH	CBD-CGD	-3.63	1.47	1.52
15	m	1002	BPH	CBD-CGD	-3.63	1.47	1.52
15	L	305	BPH	CBD-CGD	-3.55	1.47	1.52
15	l	302	BPH	CBD-CGD	-3.54	1.47	1.52
9	L	301	BCL	MG-NC	3.41	2.14	2.06
9	l	305	BCL	MG-NC	3.40	2.14	2.06
9	M	1008	BCL	MG-NC	3.39	2.14	2.06
9	m	1004	BCL	MG-NC	3.38	2.14	2.06
14	l	303	U10	C4-C5	-3.30	1.39	1.48
14	L	303	U10	C4-C5	-3.30	1.39	1.48
14	m	1003	U10	C4-C5	-3.26	1.39	1.48
14	M	1007	U10	C4-C5	-3.26	1.39	1.48
14	m	1003	U10	C6-C5	-2.87	1.38	1.46
14	M	1007	U10	C6-C5	-2.87	1.38	1.46
14	L	303	U10	C3-C2	-2.79	1.40	1.48
14	l	303	U10	C3-C2	-2.79	1.40	1.48
14	L	303	U10	C6-C5	-2.76	1.38	1.46
14	l	303	U10	C6-C5	-2.75	1.38	1.46
17	m	1001	LMT	O3’-C3’	-2.71	1.36	1.43
17	M	1001	LMT	O3’-C3’	-2.70	1.36	1.43
14	M	1007	U10	C3-C2	-2.54	1.41	1.48
14	m	1003	U10	C3-C2	-2.54	1.41	1.48
9	bn	101	BCL	C4B-NB	2.53	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BN	101	BCL	C4B-NB	2.50	1.37	1.35
9	AH	101	BCL	C4B-NB	2.41	1.37	1.35
9	bg	101	BCL	C4B-NB	2.40	1.37	1.35
9	BG	101	BCL	C4B-NB	2.39	1.37	1.35
9	ah	101	BCL	C4B-NB	2.39	1.37	1.35
14	l	303	U10	C6-C1	2.37	1.39	1.35
14	L	303	U10	C6-C1	2.37	1.39	1.35
9	BM	1001	BCL	C4B-NB	2.35	1.37	1.35
9	AN	101	BCL	C4B-NB	2.35	1.37	1.35
9	bm	1001	BCL	C4B-NB	2.34	1.37	1.35
9	am	1001	BCL	C4B-NB	2.33	1.37	1.35
17	m	1001	LMT	O2'-C2'	-2.32	1.37	1.43
9	an	101	BCL	C4B-NB	2.31	1.37	1.35
17	M	1001	LMT	O2'-C2'	-2.31	1.37	1.43
17	m	1001	LMT	O3B-C3B	-2.31	1.37	1.43
17	M	1001	LMT	O3B-C3B	-2.31	1.37	1.43
9	AM	1001	BCL	C4B-NB	2.31	1.37	1.35
14	m	1003	U10	C6-C1	2.26	1.39	1.35
14	M	1007	U10	C6-C1	2.26	1.39	1.35
9	AF	102	BCL	C4B-NB	2.26	1.37	1.35
9	ag	101	BCL	C4B-NB	2.26	1.37	1.35
9	AG	102	BCL	C4B-NB	2.25	1.37	1.35
9	af	101	BCL	C4B-NB	2.25	1.37	1.35
9	ak	101	BCL	C4B-NB	2.25	1.37	1.35
9	BL	102	BCL	C4B-NB	2.24	1.37	1.35
9	bh	102	BCL	C4B-NB	2.24	1.37	1.35
9	AK	101	BCL	C4B-NB	2.23	1.37	1.35
9	bl	101	BCL	C4B-NB	2.23	1.37	1.35
9	BH	102	BCL	C4B-NB	2.23	1.37	1.35
17	M	1001	LMT	O2B-C2B	-2.19	1.37	1.43
17	m	1001	LMT	O2B-C2B	-2.19	1.37	1.43
9	AM	1001	BCL	OBD-CAD	2.18	1.25	1.22
14	m	1003	U10	C1-C2	-2.18	1.39	1.47
9	am	1001	BCL	OBD-CAD	2.18	1.25	1.22
9	bn	101	BCL	OBD-CAD	2.18	1.25	1.22
14	M	1007	U10	C1-C2	-2.17	1.39	1.47
14	L	303	U10	C1-C2	-2.17	1.39	1.47
14	l	303	U10	C1-C2	-2.17	1.39	1.47
9	BN	101	BCL	OBD-CAD	2.17	1.25	1.22
9	AI	102	BCL	C4B-NB	2.17	1.37	1.35
9	ai	102	BCL	C4B-NB	2.16	1.37	1.35
9	aj	101	BCL	C4B-NB	2.16	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BK	101	BCL	C4B-NB	2.14	1.37	1.35
9	bk	101	BCL	C4B-NB	2.13	1.37	1.35
9	AL	1001	BCL	C4B-NB	2.12	1.37	1.35
9	BJ	102	BCL	C4B-NB	2.12	1.37	1.35
9	ac	102	BCL	C4B-NB	2.12	1.37	1.35
9	bj	102	BCL	C4B-NB	2.12	1.37	1.35
9	AH	101	BCL	OBD-CAD	2.12	1.25	1.22
9	BI	101	BCL	C4B-NB	2.12	1.37	1.35
9	bi	101	BCL	C4B-NB	2.11	1.37	1.35
9	ah	101	BCL	OBD-CAD	2.11	1.25	1.22
9	AJ	101	BCL	C4B-NB	2.11	1.37	1.35
9	ag	101	BCL	OBD-CAD	2.10	1.25	1.22
9	AC	101	BCL	C4B-NB	2.10	1.37	1.35
9	AG	102	BCL	OBD-CAD	2.10	1.25	1.22
9	BD	101	BCL	C4B-NB	2.10	1.37	1.35
9	bd	101	BCL	C4B-NB	2.10	1.37	1.35
17	m	1001	LMT	O4’-C4B	-2.09	1.38	1.43
9	al	1001	BCL	C4B-NB	2.09	1.37	1.35
17	M	1001	LMT	O4’-C4B	-2.09	1.38	1.43
9	BE	1001	BCL	C4B-NB	2.09	1.37	1.35
9	AE	102	BCL	C4B-NB	2.09	1.37	1.35
9	ae	101	BCL	C4B-NB	2.09	1.37	1.35
9	be	1001	BCL	C4B-NB	2.09	1.37	1.35
9	bf	101	BCL	C4B-NB	2.09	1.37	1.35
9	BF	101	BCL	C4B-NB	2.08	1.37	1.35
9	AJ	101	BCL	OBD-CAD	2.08	1.25	1.22
9	aj	101	BCL	OBD-CAD	2.08	1.25	1.22
9	an	101	BCL	OBD-CAD	2.08	1.25	1.22
9	AN	101	BCL	OBD-CAD	2.07	1.25	1.22
9	bb	1001	BCL	OBD-CAD	2.07	1.25	1.22
9	BB	1001	BCL	OBD-CAD	2.06	1.25	1.22
9	L	304	BCL	OBD-CAD	2.06	1.25	1.22
9	bc	101	BCL	C4B-NB	2.06	1.37	1.35
9	l	301	BCL	OBD-CAD	2.06	1.25	1.22
9	ac	102	BCL	OBD-CAD	2.06	1.25	1.22
9	AC	101	BCL	OBD-CAD	2.05	1.25	1.22
9	BK	101	BCL	OBD-CAD	2.05	1.25	1.22
9	BC	101	BCL	C4B-NB	2.05	1.37	1.35
9	bk	101	BCL	OBD-CAD	2.05	1.25	1.22
9	AD	1001	BCL	C4B-NB	2.05	1.37	1.35
9	bj	102	BCL	OBD-CAD	2.04	1.25	1.22
9	AB	101	BCL	C4B-NB	2.03	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AA	1001	BCL	C4B-NB	2.03	1.37	1.35
9	AB	101	BCL	C5-C3	2.03	1.55	1.51
9	BJ	102	BCL	OBD-CAD	2.03	1.25	1.22
9	L	301	BCL	OBD-CAD	2.02	1.25	1.22
9	l	305	BCL	OBD-CAD	2.02	1.25	1.22
9	BM	1001	BCL	OBD-CAD	2.02	1.25	1.22
9	aa	1001	BCL	C4B-NB	2.02	1.37	1.35
9	bm	1001	BCL	OBD-CAD	2.02	1.25	1.22
9	AK	101	BCL	OBD-CAD	2.01	1.25	1.22
9	BC	101	BCL	OBD-CAD	2.01	1.25	1.22
9	ab	102	BCL	C4B-NB	2.01	1.37	1.35
9	ad	1001	BCL	C4B-NB	2.01	1.37	1.35
9	ak	101	BCL	OBD-CAD	2.01	1.25	1.22
9	BA	102	BCL	C4B-NB	2.01	1.37	1.35
9	bc	101	BCL	OBD-CAD	2.00	1.25	1.22

All (833) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	x	100	SQD	O8-S-C6	-6.75	94.98	105.74
16	L	306	SQD	O8-S-C6	-6.73	95.01	105.74
16	x	100	SQD	O7-S-C6	5.54	113.52	106.94
16	L	306	SQD	O7-S-C6	5.47	113.44	106.94
16	x	100	SQD	O9-S-C6	5.35	113.30	106.94
16	L	306	SQD	O9-S-C6	5.27	113.20	106.94
13	l	304	UQ1	C6-C5-C4	4.81	122.98	119.18
13	L	302	UQ1	C6-C5-C4	4.80	122.98	119.18
9	am	1001	BCL	CMB-C2B-C1B	-4.48	121.58	128.46
9	AM	1001	BCL	CMB-C2B-C1B	-4.45	121.62	128.46
9	m	1004	BCL	CMB-C2B-C1B	-4.42	121.67	128.46
9	M	1008	BCL	CMB-C2B-C1B	-4.42	121.67	128.46
9	AH	101	BCL	CMB-C2B-C1B	-4.41	121.69	128.46
9	al	1001	BCL	CMB-C2B-C1B	-4.40	121.70	128.46
9	AK	101	BCL	CMB-C2B-C1B	-4.40	121.70	128.46
9	AL	1001	BCL	CMB-C2B-C1B	-4.40	121.70	128.46
9	m	1006	BCL	CMB-C2B-C1B	-4.39	121.72	128.46
9	ak	101	BCL	CMB-C2B-C1B	-4.38	121.73	128.46
9	AE	102	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
9	AA	1001	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
9	AF	102	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
9	aa	1001	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
9	ae	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AD	1001	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
9	af	101	BCL	CMB-C2B-C1B	-4.35	121.77	128.46
9	ad	1001	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
9	M	1002	BCL	CMB-C2B-C1B	-4.34	121.80	128.46
10	AI	101	SP2	C20-C19-C18	4.32	138.56	126.42
9	AI	102	BCL	CMB-C2B-C1B	-4.32	121.83	128.46
9	ai	102	BCL	CMB-C2B-C1B	-4.32	121.83	128.46
9	ah	101	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
9	bl	101	BCL	CMB-C2B-C1B	-4.30	121.85	128.46
9	BL	102	BCL	CMB-C2B-C1B	-4.29	121.87	128.46
9	AJ	101	BCL	CMB-C2B-C1B	-4.29	121.87	128.46
9	aj	101	BCL	CMB-C2B-C1B	-4.28	121.88	128.46
9	BC	101	BCL	C1-C2-C3	-4.28	118.64	126.04
9	bc	101	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
9	BC	101	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
9	bc	101	BCL	C1-C2-C3	-4.28	118.64	126.04
9	bg	101	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
9	BG	101	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
9	bi	101	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
9	BI	101	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
9	ac	102	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
9	BN	101	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
9	bh	102	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
9	be	1001	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
9	BD	101	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
9	BJ	102	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
9	bd	101	BCL	CMB-C2B-C1B	-4.26	121.92	128.46
9	ab	102	BCL	CMB-C2B-C1B	-4.25	121.92	128.46
9	BH	102	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
9	BE	1001	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
9	AB	101	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
9	bj	102	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
9	BM	1001	BCL	CMB-C2B-C1B	-4.25	121.94	128.46
9	bn	101	BCL	CMB-C2B-C1B	-4.25	121.94	128.46
9	bm	1001	BCL	CMB-C2B-C1B	-4.24	121.94	128.46
9	AC	101	BCL	CMB-C2B-C1B	-4.24	121.95	128.46
9	bb	1001	BCL	CMB-C2B-C1B	-4.24	121.95	128.46
9	ag	101	BCL	CMB-C2B-C1B	-4.24	121.95	128.46
9	ba	102	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
9	AG	102	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
9	BA	102	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
9	L	304	BCL	CMB-C2B-C1B	-4.21	121.99	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BB	1001	BCL	CMB-C2B-C1B	-4.21	121.99	128.46
9	l	301	BCL	CMB-C2B-C1B	-4.21	121.99	128.46
9	an	101	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
9	BK	101	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
9	bk	101	BCL	CMB-C2B-C1B	-4.14	122.09	128.46
9	bf	101	BCL	CMB-C2B-C1B	-4.12	122.14	128.46
9	AN	101	BCL	CMB-C2B-C1B	-4.12	122.14	128.46
9	BF	101	BCL	CMB-C2B-C1B	-4.12	122.14	128.46
9	l	305	BCL	CMB-C2B-C1B	-3.98	122.34	128.46
9	L	301	BCL	CMB-C2B-C1B	-3.98	122.34	128.46
13	l	304	UQ1	CM3-O3-C3	3.90	130.30	116.47
13	L	302	UQ1	CM3-O3-C3	3.90	130.29	116.47
9	AB	101	BCL	C4A-NA-C1A	3.77	108.40	106.71
9	M	1008	BCL	C4A-NA-C1A	3.77	108.40	106.71
9	m	1004	BCL	C4A-NA-C1A	3.76	108.40	106.71
12	m	1005	CD4	O2-C14-C13	3.76	119.60	111.50
12	M	1004	CD4	O2-C14-C13	3.75	119.58	111.50
9	ab	102	BCL	C4A-NA-C1A	3.74	108.39	106.71
9	L	301	BCL	CAD-C3D-C4D	-3.74	106.39	108.47
9	bb	1001	BCL	C1-C2-C3	-3.73	119.58	126.04
9	l	305	BCL	CAD-C3D-C4D	-3.73	106.39	108.47
14	m	1003	U10	C3M-O3-C3	3.69	129.53	116.47
14	M	1007	U10	C3M-O3-C3	3.68	129.52	116.47
10	ai	101	SP2	C20-C19-C18	3.65	136.68	126.42
9	AI	102	BCL	CAD-C3D-C4D	-3.62	106.45	108.47
9	ai	102	BCL	CAD-C3D-C4D	-3.61	106.46	108.47
9	BB	1001	BCL	C1-C2-C3	-3.61	119.80	126.04
9	M	1002	BCL	CAD-C3D-C4D	-3.54	106.50	108.47
9	m	1006	BCL	CAD-C3D-C4D	-3.54	106.50	108.47
9	AE	102	BCL	C4A-NA-C1A	3.52	108.29	106.71
9	al	1001	BCL	CAD-C3D-C4D	-3.52	106.51	108.47
9	BA	102	BCL	C4A-NA-C1A	3.51	108.28	106.71
9	ba	102	BCL	C4A-NA-C1A	3.49	108.27	106.71
14	m	1003	U10	C47-C48-C49	-3.49	119.27	127.66
14	M	1007	U10	C47-C48-C49	-3.48	119.29	127.66
16	x	100	SQD	O8-S-O9	-3.47	102.79	111.27
9	ae	101	BCL	C4A-NA-C1A	3.47	108.27	106.71
9	ag	101	BCL	C4A-NA-C1A	3.45	108.26	106.71
9	m	1004	BCL	CAD-C3D-C4D	-3.45	106.55	108.47
9	AL	1001	BCL	CAD-C3D-C4D	-3.45	106.55	108.47
14	l	303	U10	C12-C13-C14	-3.45	119.36	127.66
14	L	303	U10	C12-C13-C14	-3.45	119.36	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1008	BCL	CAD-C3D-C4D	-3.44	106.55	108.47
9	AK	101	BCL	C4A-NA-C1A	3.44	108.25	106.71
14	M	1007	U10	C4M-O4-C4	3.44	128.65	116.47
14	m	1003	U10	C4M-O4-C4	3.44	128.65	116.47
9	ak	101	BCL	C4A-NA-C1A	3.43	108.25	106.71
9	AG	102	BCL	C4A-NA-C1A	3.42	108.25	106.71
16	L	306	SQD	O8-S-O9	-3.40	102.95	111.27
9	be	1001	BCL	C4A-NA-C1A	3.39	108.23	106.71
9	bh	102	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
9	BH	102	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
9	BI	101	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
9	AI	102	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
9	AE	102	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
9	ai	102	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
9	bi	101	BCL	OBD-CAD-CBD	-3.37	121.07	125.89
9	ag	101	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
9	ae	101	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
9	AD	1001	BCL	C4A-NA-C1A	3.37	108.22	106.71
9	AG	102	BCL	OBD-CAD-CBD	-3.37	121.09	125.89
9	aj	101	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
9	AJ	101	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
9	bd	101	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
9	AN	101	BCL	CAD-C3D-C4D	-3.36	106.60	108.47
9	BF	101	BCL	OBD-CAD-CBD	-3.35	121.10	125.89
9	bf	101	BCL	OBD-CAD-CBD	-3.35	121.10	125.89
9	BD	101	BCL	OBD-CAD-CBD	-3.35	121.10	125.89
9	am	1001	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
9	an	101	BCL	CAD-C3D-C4D	-3.35	106.60	108.47
9	AM	1001	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
9	ae	101	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
9	be	1001	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
9	an	101	BCL	CHA-C1A-NA	-3.34	118.75	126.40
9	BE	1001	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
9	AE	102	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
9	bn	101	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
9	BE	1001	BCL	C4A-NA-C1A	3.33	108.20	106.71
9	BN	101	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
9	L	301	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
9	l	305	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
9	aa	1001	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
9	AA	1001	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	BB	1001	BCL	OBD-CAD-CBD	-3.32	121.15	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BK	101	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	m	1004	BCL	CHA-C1A-NA	-3.32	118.79	126.40
14	m	1003	U10	C35-C34-C36	3.32	120.86	115.27
9	bl	101	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	bm	1001	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	BL	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	BM	1001	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	bk	101	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	L	304	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
9	ac	102	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
9	l	301	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
14	M	1007	U10	C35-C34-C36	3.32	120.85	115.27
9	bb	1001	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
9	M	1008	BCL	CHA-C1A-NA	-3.32	118.80	126.40
9	AD	1001	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
9	AN	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
9	ad	1001	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
9	af	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
9	ah	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
9	an	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
9	AH	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
9	AM	1001	BCL	C4A-NA-C1A	3.31	108.19	106.71
9	AA	1001	BCL	C4A-NA-C1A	3.31	108.19	106.71
9	AC	101	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
9	AF	102	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
9	BG	101	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
9	BJ	102	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
9	AB	101	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
9	bj	102	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
15	M	1003	BPH	OBD-CAD-CBD	-3.31	120.97	125.82
15	m	1002	BPH	OBD-CAD-CBD	-3.31	120.97	125.82
9	ab	102	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
9	AN	101	BCL	CHA-C1A-NA	-3.30	118.83	126.40
9	BA	102	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
17	M	1001	LMT	C3'-C4'-C5'	-3.30	103.35	110.93
9	ba	102	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
17	m	1001	LMT	C3'-C4'-C5'	-3.30	103.36	110.93
9	bg	101	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
9	BC	101	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
9	ad	1001	BCL	C4A-NA-C1A	3.29	108.19	106.71
9	am	1001	BCL	C4A-NA-C1A	3.29	108.19	106.71
14	m	1003	U10	C30-C29-C31	3.29	120.81	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bc	101	BCL	OBD-CAD-CBD	-3.29	121.20	125.89
9	AF	102	BCL	C4A-NA-C1A	3.28	108.18	106.71
14	M	1007	U10	C30-C29-C31	3.28	120.78	115.27
9	bc	101	BCL	C4A-NA-C1A	3.28	108.18	106.71
9	AK	101	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
9	ak	101	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
9	al	1001	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
9	aa	1001	BCL	C4A-NA-C1A	3.27	108.17	106.71
14	m	1003	U10	C42-C43-C44	-3.27	119.80	127.66
9	AL	1001	BCL	OBD-CAD-CBD	-3.26	121.23	125.89
14	M	1007	U10	C42-C43-C44	-3.26	119.81	127.66
9	m	1004	BCL	OBD-CAD-CBD	-3.25	121.25	125.89
9	M	1008	BCL	OBD-CAD-CBD	-3.25	121.25	125.89
9	ak	101	BCL	CAD-C3D-C4D	-3.24	106.66	108.47
9	AK	101	BCL	CAD-C3D-C4D	-3.24	106.67	108.47
9	bh	102	BCL	C4A-NA-C1A	3.22	108.16	106.71
9	BC	101	BCL	C4A-NA-C1A	3.22	108.15	106.71
9	am	1001	BCL	CMB-C2B-C3B	3.22	130.70	124.68
9	bi	101	BCL	CAD-C3D-C4D	-3.21	106.68	108.47
9	BH	102	BCL	C4A-NA-C1A	3.21	108.15	106.71
9	BI	101	BCL	CAD-C3D-C4D	-3.21	106.68	108.47
9	M	1002	BCL	OBD-CAD-CBD	-3.20	121.32	125.89
9	m	1006	BCL	OBD-CAD-CBD	-3.20	121.32	125.89
9	m	1006	BCL	CMB-C2B-C3B	3.20	130.67	124.68
9	AM	1001	BCL	CMB-C2B-C3B	3.20	130.67	124.68
9	al	1001	BCL	C1-C2-C3	-3.20	120.52	126.04
15	l	302	BPH	OBD-CAD-CBD	-3.18	121.16	125.82
9	AG	102	BCL	CAD-C3D-C4D	-3.18	106.70	108.47
15	L	305	BPH	OBD-CAD-CBD	-3.18	121.16	125.82
9	M	1002	BCL	CMB-C2B-C3B	3.17	130.60	124.68
9	AD	1001	BCL	CMB-C2B-C3B	3.17	130.60	124.68
9	ad	1001	BCL	CMB-C2B-C3B	3.17	130.60	124.68
9	AK	101	BCL	CMB-C2B-C3B	3.17	130.60	124.68
9	AE	102	BCL	CMB-C2B-C3B	3.16	130.60	124.68
9	AF	102	BCL	CMB-C2B-C3B	3.16	130.60	124.68
9	al	1001	BCL	CMB-C2B-C3B	3.16	130.60	124.68
9	AL	1001	BCL	CMB-C2B-C3B	3.16	130.60	124.68
9	af	101	BCL	C4A-NA-C1A	3.16	108.13	106.71
9	ae	101	BCL	CMB-C2B-C3B	3.16	130.59	124.68
9	ag	101	BCL	CAD-C3D-C4D	-3.16	106.71	108.47
9	AH	101	BCL	CMB-C2B-C3B	3.16	130.59	124.68
9	m	1004	BCL	CMB-C2B-C3B	3.16	130.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	al	1001	BCL	CHA-C1A-NA	-3.16	119.17	126.40
9	M	1008	BCL	CMB-C2B-C3B	3.16	130.58	124.68
9	ak	101	BCL	CMB-C2B-C3B	3.15	130.58	124.68
9	af	101	BCL	CMB-C2B-C3B	3.15	130.57	124.68
9	ab	102	BCL	CAD-C3D-C4D	-3.15	106.71	108.47
9	AB	101	BCL	CAD-C3D-C4D	-3.14	106.72	108.47
9	AL	1001	BCL	CHA-C1A-NA	-3.14	119.21	126.40
9	AA	1001	BCL	CMB-C2B-C3B	3.14	130.55	124.68
9	aa	1001	BCL	CMB-C2B-C3B	3.14	130.55	124.68
9	ab	102	BCL	CHA-C1A-NA	-3.13	119.22	126.40
9	bn	101	BCL	CAD-C3D-C4D	-3.13	106.72	108.47
9	ai	102	BCL	CHA-C1A-NA	-3.13	119.23	126.40
9	AI	102	BCL	CHA-C1A-NA	-3.13	119.23	126.40
14	m	1003	U10	C25-C24-C26	3.13	120.53	115.27
9	AB	101	BCL	CHA-C1A-NA	-3.12	119.24	126.40
16	L	306	SQD	O5-C1-O6	-3.12	102.58	109.97
14	M	1007	U10	C25-C24-C26	3.12	120.52	115.27
9	AJ	101	BCL	CMB-C2B-C3B	3.10	130.48	124.68
9	AC	101	BCL	CHA-C1A-NA	-3.10	119.29	126.40
9	ai	102	BCL	CMB-C2B-C3B	3.10	130.48	124.68
9	AI	102	BCL	CMB-C2B-C3B	3.10	130.48	124.68
9	ah	101	BCL	CMB-C2B-C3B	3.10	130.48	124.68
9	AM	1001	BCL	CHA-C1A-NA	-3.10	119.30	126.40
9	af	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
9	am	1001	BCL	CHA-C1A-NA	-3.10	119.31	126.40
9	ac	102	BCL	CHA-C1A-NA	-3.09	119.32	126.40
9	AH	101	BCL	CAD-C3D-C4D	-3.09	106.75	108.47
9	AH	101	BCL	CHA-C1A-NA	-3.09	119.33	126.40
9	aj	101	BCL	CMB-C2B-C3B	3.09	130.45	124.68
9	aa	1001	BCL	CHA-C1A-NA	-3.08	119.33	126.40
9	AF	102	BCL	CHA-C1A-NA	-3.08	119.33	126.40
9	AD	1001	BCL	CHA-C1A-NA	-3.08	119.34	126.40
9	ab	102	BCL	CMB-C2B-C3B	3.08	130.45	124.68
9	AA	1001	BCL	CHA-C1A-NA	-3.08	119.34	126.40
9	BN	101	BCL	CAD-C3D-C4D	-3.08	106.75	108.47
14	m	1003	U10	C17-C18-C19	-3.08	120.24	127.66
9	bj	102	BCL	C4A-NA-C1A	3.08	108.09	106.71
14	M	1007	U10	C17-C18-C19	-3.08	120.25	127.66
9	ad	1001	BCL	CHA-C1A-NA	-3.07	119.36	126.40
9	bb	1001	BCL	CMB-C2B-C3B	3.07	130.43	124.68
9	BF	101	BCL	CAD-C3D-C4D	-3.07	106.76	108.47
9	bf	101	BCL	CAD-C3D-C4D	-3.07	106.76	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	304	BCL	CMB-C2B-C3B	3.07	130.42	124.68
9	bc	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
9	l	301	BCL	CMB-C2B-C3B	3.07	130.42	124.68
9	BC	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
9	AB	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
9	ac	102	BCL	CMB-C2B-C3B	3.07	130.41	124.68
14	l	303	U10	C25-C24-C26	3.07	120.43	115.27
9	bg	101	BCL	CMB-C2B-C3B	3.06	130.41	124.68
9	BG	101	BCL	CMB-C2B-C3B	3.06	130.41	124.68
9	BJ	102	BCL	C4A-NA-C1A	3.06	108.08	106.71
9	aj	101	BCL	C4A-NA-C1A	3.06	108.08	106.71
9	BF	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
9	ba	102	BCL	CMB-C2B-C3B	3.06	130.40	124.68
9	bf	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
14	L	303	U10	C25-C24-C26	3.06	120.42	115.27
9	BA	102	BCL	CMB-C2B-C3B	3.06	130.40	124.68
9	bl	101	BCL	CMB-C2B-C3B	3.06	130.40	124.68
9	BB	1001	BCL	CMB-C2B-C3B	3.05	130.39	124.68
14	M	1007	U10	C10-C9-C11	3.05	120.41	115.27
9	BJ	102	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
9	bj	102	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
14	m	1003	U10	C10-C9-C11	3.05	120.41	115.27
9	BJ	102	BCL	CMB-C2B-C3B	3.05	130.39	124.68
9	ah	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
9	BL	102	BCL	CMB-C2B-C3B	3.05	130.39	124.68
9	bi	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
9	BD	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
9	bd	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
14	l	303	U10	C30-C29-C31	3.05	120.40	115.27
9	BI	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
9	BH	102	BCL	CHA-C1A-NA	-3.05	119.42	126.40
9	AC	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
14	M	1007	U10	C22-C23-C24	-3.05	120.32	127.66
9	ba	102	BCL	CHA-C1A-NA	-3.05	119.42	126.40
9	bn	101	BCL	CHA-C1A-NA	-3.05	119.42	126.40
16	x	100	SQD	O8-S-O7	-3.04	103.83	111.27
14	m	1003	U10	C22-C23-C24	-3.04	120.33	127.66
9	bj	102	BCL	CMB-C2B-C3B	3.04	130.37	124.68
14	L	303	U10	C30-C29-C31	3.04	120.39	115.27
9	ag	101	BCL	CMB-C2B-C3B	3.04	130.37	124.68
9	BN	101	BCL	CMB-C2B-C3B	3.04	130.37	124.68
9	bb	1001	BCL	CHA-C1A-NA	-3.04	119.44	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bh	102	BCL	CHA-C1A-NA	-3.04	119.44	126.40
9	AK	101	BCL	CHA-C1A-NA	-3.04	119.44	126.40
9	BB	1001	BCL	CHA-C1A-NA	-3.04	119.44	126.40
9	BA	102	BCL	CHA-C1A-NA	-3.04	119.44	126.40
9	AJ	101	BCL	CHA-C1A-NA	-3.04	119.44	126.40
9	BN	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
9	bn	101	BCL	CMB-C2B-C3B	3.03	130.35	124.68
15	L	305	BPH	CMB-C2B-C3B	3.03	130.35	124.68
9	BK	101	BCL	CAD-C3D-C4D	-3.03	106.78	108.47
9	BD	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
9	bd	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
9	AG	102	BCL	CMB-C2B-C3B	3.03	130.35	124.68
9	bh	102	BCL	CMB-C2B-C3B	3.03	130.34	124.68
9	BE	1001	BCL	CMB-C2B-C3B	3.03	130.34	124.68
15	l	302	BPH	CMB-C2B-C3B	3.03	130.34	124.68
9	BG	101	BCL	C4A-NA-C1A	3.03	108.07	106.71
9	ah	101	BCL	C4A-NA-C1A	3.03	108.07	106.71
9	be	1001	BCL	CMB-C2B-C3B	3.03	130.34	124.68
9	ak	101	BCL	CHA-C1A-NA	-3.03	119.47	126.40
9	BE	1001	BCL	CHA-C1A-NA	-3.02	119.47	126.40
9	BH	102	BCL	CMB-C2B-C3B	3.02	130.34	124.68
9	bg	101	BCL	C4A-NA-C1A	3.02	108.06	106.71
14	L	303	U10	C40-C39-C41	3.02	120.35	115.27
9	ae	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
9	be	1001	BCL	CHA-C1A-NA	-3.02	119.49	126.40
9	BM	1001	BCL	CMB-C2B-C3B	3.02	130.32	124.68
9	bi	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
9	bm	1001	BCL	CMB-C2B-C3B	3.02	130.32	124.68
14	l	303	U10	C40-C39-C41	3.02	120.34	115.27
9	bg	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
9	an	101	BCL	CMB-C2B-C3B	3.01	130.32	124.68
9	BI	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
9	ah	101	BCL	CAD-C3D-C4D	-3.01	106.79	108.47
9	BM	1001	BCL	C4A-NA-C1A	3.01	108.06	106.71
9	AE	102	BCL	CHA-C1A-NA	-3.01	119.51	126.40
9	BG	101	BCL	CHA-C1A-NA	-3.01	119.51	126.40
9	bm	1001	BCL	C4A-NA-C1A	3.01	108.06	106.71
9	bc	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40
9	aj	101	BCL	CHA-C1A-NA	-3.00	119.54	126.40
10	ai	103	SP2	C15-C16-C17	3.00	129.61	123.47
9	BK	101	BCL	CMB-C2B-C3B	2.99	130.28	124.68
9	BC	101	BCL	CHA-C1A-NA	-2.99	119.54	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	306	SQD	O8-S-O7	-2.99	103.97	111.27
9	BM	1001	BCL	CHA-C1A-NA	-2.99	119.56	126.40
9	bk	101	BCL	CAD-C3D-C4D	-2.99	106.80	108.47
9	bm	1001	BCL	CHA-C1A-NA	-2.99	119.56	126.40
9	bk	101	BCL	CMB-C2B-C3B	2.99	130.26	124.68
9	M	1002	BCL	CHA-C1A-NA	-2.98	119.57	126.40
9	AN	101	BCL	CMB-C2B-C3B	2.98	130.25	124.68
9	bf	101	BCL	CMB-C2B-C3B	2.97	130.24	124.68
9	BF	101	BCL	CMB-C2B-C3B	2.97	130.24	124.68
9	L	301	BCL	CHA-C1A-NA	-2.97	119.60	126.40
9	AJ	101	BCL	C4A-NA-C1A	2.97	108.04	106.71
9	m	1006	BCL	CHA-C1A-NA	-2.97	119.60	126.40
9	l	305	BCL	CHA-C1A-NA	-2.97	119.60	126.40
9	BA	102	BCL	CBA-CAA-C2A	2.96	122.60	113.86
9	ba	102	BCL	CBA-CAA-C2A	2.96	122.59	113.86
9	AD	1001	BCL	CAD-C3D-C4D	-2.95	106.82	108.47
9	AJ	101	BCL	CAD-C3D-C4D	-2.95	106.83	108.47
9	bl	101	BCL	CAD-C3D-C4D	-2.94	106.83	108.47
9	BK	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
15	M	1003	BPH	CMB-C2B-C3B	2.93	130.17	124.68
15	m	1002	BPH	CMB-C2B-C3B	2.93	130.17	124.68
9	L	301	BCL	C2A-C1A-CHA	2.93	128.98	123.86
9	ad	1001	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
9	BJ	102	BCL	CHA-C1A-NA	-2.93	119.69	126.40
9	l	305	BCL	C2A-C1A-CHA	2.93	128.98	123.86
9	bl	101	BCL	CHA-C1A-NA	-2.93	119.70	126.40
9	bk	101	BCL	CHA-C1A-NA	-2.92	119.70	126.40
9	l	305	BCL	CMB-C2B-C3B	2.92	130.15	124.68
9	L	301	BCL	CMB-C2B-C3B	2.92	130.15	124.68
9	AG	102	BCL	CHA-C1A-NA	-2.92	119.71	126.40
9	bj	102	BCL	CHA-C1A-NA	-2.92	119.71	126.40
9	ag	101	BCL	CHA-C1A-NA	-2.92	119.71	126.40
9	BL	102	BCL	CHA-C1A-NA	-2.92	119.72	126.40
9	BD	101	BCL	CAD-C3D-C4D	-2.91	106.84	108.47
9	bd	101	BCL	CAD-C3D-C4D	-2.91	106.85	108.47
14	M	1007	U10	C20-C19-C21	2.90	120.16	115.27
14	m	1003	U10	C20-C19-C21	2.90	120.16	115.27
9	BL	102	BCL	CAD-C3D-C4D	-2.90	106.85	108.47
9	BM	1001	BCL	CAD-C3D-C4D	-2.90	106.86	108.47
10	AI	103	SP2	C15-C16-C17	2.90	129.41	123.47
9	aj	101	BCL	CAD-C3D-C4D	-2.88	106.86	108.47
14	l	303	U10	C10-C9-C11	2.88	120.11	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bm	1001	BCL	CAD-C3D-C4D	-2.87	106.87	108.47
14	L	303	U10	C10-C9-C11	2.87	120.10	115.27
9	BB	1001	BCL	CAD-C3D-C4D	-2.87	106.87	108.47
9	BG	101	BCL	CAD-C3D-C4D	-2.86	106.88	108.47
9	bb	1001	BCL	CAD-C3D-C4D	-2.86	106.88	108.47
9	BD	101	BCL	C2A-C1A-CHA	2.86	128.86	123.86
9	bd	101	BCL	C2A-C1A-CHA	2.86	128.86	123.86
9	bg	101	BCL	CAD-C3D-C4D	-2.85	106.88	108.47
9	bn	101	BCL	C4A-NA-C1A	2.85	107.99	106.71
9	bd	101	BCL	C4A-NA-C1A	2.85	107.99	106.71
9	BD	101	BCL	C4A-NA-C1A	2.84	107.98	106.71
12	M	1004	CD4	O16-C46-C47	2.84	117.62	111.50
12	m	1005	CD4	O16-C46-C47	2.84	117.62	111.50
9	BN	101	BCL	C4A-NA-C1A	2.84	107.98	106.71
14	L	303	U10	C7-C8-C9	-2.83	122.09	126.79
9	AH	101	BCL	C4A-NA-C1A	2.82	107.97	106.71
14	l	303	U10	C7-C8-C9	-2.81	122.11	126.79
9	bh	102	BCL	C1-O2A-CGA	2.81	123.82	116.44
9	bk	101	BCL	C4A-NA-C1A	2.81	107.97	106.71
9	BH	102	BCL	C1-O2A-CGA	2.81	123.82	116.44
12	H	302	CD4	O16-C46-C47	2.81	117.55	111.50
9	AC	101	BCL	CAD-C3D-C4D	-2.81	106.91	108.47
9	ac	102	BCL	CAD-C3D-C4D	-2.81	106.91	108.47
12	h	302	CD4	O16-C46-C47	2.80	117.55	111.50
14	M	1007	U10	C12-C13-C14	-2.80	120.93	127.66
14	m	1003	U10	C12-C13-C14	-2.79	120.94	127.66
12	M	1004	CD4	O3-C17-C18	2.79	120.67	111.91
12	m	1005	CD4	O3-C17-C18	2.79	120.67	111.91
9	L	304	BCL	CAD-C3D-C4D	-2.78	106.92	108.47
9	BL	102	BCL	C4A-NA-C1A	2.78	107.96	106.71
9	AJ	101	BCL	C1-C2-C3	2.78	130.85	126.04
9	l	301	BCL	CAD-C3D-C4D	-2.77	106.92	108.47
9	m	1006	BCL	C2A-C1A-CHA	2.77	128.70	123.86
9	M	1002	BCL	C2A-C1A-CHA	2.76	128.69	123.86
9	BE	1001	BCL	CBA-CAA-C2A	2.76	122.00	113.86
9	BK	101	BCL	C4A-NA-C1A	2.76	107.94	106.71
9	aa	1001	BCL	CAD-C3D-C4D	-2.75	106.94	108.47
9	bl	101	BCL	C4A-NA-C1A	2.75	107.94	106.71
9	AA	1001	BCL	CAD-C3D-C4D	-2.75	106.94	108.47
9	L	304	BCL	C2A-C1A-CHA	2.75	128.66	123.86
9	l	301	BCL	C2A-C1A-CHA	2.75	128.66	123.86
9	be	1001	BCL	CBA-CAA-C2A	2.74	121.96	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	304	BCL	CHA-C1A-NA	-2.74	120.12	126.40
9	l	301	BCL	CHA-C1A-NA	-2.74	120.13	126.40
9	ba	102	BCL	CAD-C3D-C4D	-2.72	106.95	108.47
9	BA	102	BCL	CAD-C3D-C4D	-2.72	106.95	108.47
14	l	303	U10	C45-C44-C46	2.71	119.84	115.27
9	AF	102	BCL	CAD-C3D-C4D	-2.71	106.96	108.47
9	af	101	BCL	CAD-C3D-C4D	-2.71	106.96	108.47
14	L	303	U10	C45-C44-C46	2.71	119.82	115.27
9	am	1001	BCL	CAD-C3D-C4D	-2.70	106.96	108.47
9	AM	1001	BCL	CAD-C3D-C4D	-2.69	106.97	108.47
9	AN	101	BCL	C4A-NA-C1A	2.69	107.92	106.71
9	l	305	BCL	C4A-NA-C1A	2.69	107.91	106.71
9	AB	101	BCL	C1-C2-C3	2.69	130.69	126.04
9	L	301	BCL	C4A-NA-C1A	2.68	107.91	106.71
14	l	303	U10	C47-C48-C49	-2.67	121.22	127.66
9	BB	1001	BCL	C4A-NA-C1A	2.67	107.91	106.71
14	L	303	U10	C47-C48-C49	-2.67	121.24	127.66
9	BC	101	BCL	CAD-C3D-C4D	-2.66	106.99	108.47
12	H	302	CD4	O2-C14-C13	2.66	117.23	111.50
10	ai	101	SP2	C15-C16-C17	2.66	128.91	123.47
12	h	302	CD4	O2-C14-C13	2.65	117.22	111.50
9	bb	1001	BCL	C4A-NA-C1A	2.65	107.90	106.71
9	al	1001	BCL	C4A-NA-C1A	2.65	107.90	106.71
9	bc	101	BCL	CAD-C3D-C4D	-2.65	107.00	108.47
9	m	1004	BCL	C2A-C1A-CHA	2.64	128.48	123.86
9	M	1008	BCL	C2A-C1A-CHA	2.63	128.46	123.86
9	AK	101	BCL	C2A-C1A-CHA	2.62	128.45	123.86
9	BH	102	BCL	CAD-C3D-C4D	-2.62	107.01	108.47
9	bh	102	BCL	CAD-C3D-C4D	-2.62	107.01	108.47
14	M	1007	U10	C15-C14-C16	2.62	119.68	115.27
9	be	1001	BCL	CAD-C3D-C4D	-2.62	107.01	108.47
9	af	101	BCL	C2A-C1A-CHA	2.62	128.43	123.86
9	ak	101	BCL	C2A-C1A-CHA	2.62	128.43	123.86
14	m	1003	U10	C15-C14-C16	2.62	119.67	115.27
9	BI	101	BCL	C4A-NA-C1A	2.61	107.88	106.71
9	bf	101	BCL	C4A-NA-C1A	2.61	107.88	106.71
9	ba	102	BCL	C2A-C1A-CHA	2.61	128.42	123.86
9	BE	1001	BCL	CAD-C3D-C4D	-2.61	107.02	108.47
9	BA	102	BCL	C2A-C1A-CHA	2.60	128.41	123.86
9	AL	1001	BCL	C4A-NA-C1A	2.60	107.87	106.71
9	ab	102	BCL	C2A-C1A-CHA	2.59	128.39	123.86
9	AA	1001	BCL	C2A-C1A-CHA	2.59	128.39	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	aa	1001	BCL	C2A-C1A-CHA	2.59	128.39	123.86
9	bi	101	BCL	C4A-NA-C1A	2.59	107.87	106.71
9	BF	101	BCL	C4A-NA-C1A	2.59	107.87	106.71
9	BH	102	BCL	C2A-C1A-CHA	2.58	128.38	123.86
16	x	100	SQD	O9-S-O7	2.58	122.89	113.95
9	bh	102	BCL	C2A-C1A-CHA	2.58	128.37	123.86
9	AC	101	BCL	C4A-NA-C1A	2.58	107.86	106.71
16	L	306	SQD	O9-S-O7	2.57	122.85	113.95
9	AB	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
9	AF	102	BCL	C2A-C1A-CHA	2.56	128.33	123.86
9	BG	101	BCL	C1-O2A-CGA	2.56	123.15	116.44
9	m	1006	BCL	C4A-NA-C1A	2.55	107.85	106.71
9	bc	101	BCL	C1-O2A-CGA	2.54	123.12	116.44
9	ac	102	BCL	C4A-NA-C1A	2.54	107.85	106.71
9	an	101	BCL	C4A-NA-C1A	2.54	107.85	106.71
9	ab	102	BCL	C1-C2-C3	2.54	130.43	126.04
9	AB	101	BCL	OBB-CAB-CBB	-2.54	114.46	120.17
9	M	1008	BCL	OBB-CAB-CBB	-2.54	114.46	120.17
9	M	1002	BCL	C4A-NA-C1A	2.54	107.85	106.71
9	BA	102	BCL	C1-O2A-CGA	2.53	123.09	116.44
9	m	1004	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
9	AC	101	BCL	OBB-CAB-CBB	-2.53	114.48	120.17
9	BK	101	BCL	OBB-CAB-CBB	-2.53	114.48	120.17
13	l	304	UQ1	O4-C4-C3	2.53	126.29	120.93
14	L	303	U10	C20-C19-C21	2.53	119.52	115.27
14	l	303	U10	C20-C19-C21	2.52	119.51	115.27
9	BC	101	BCL	C1-O2A-CGA	2.52	123.06	116.44
9	AH	101	BCL	OBB-CAB-CBB	-2.52	114.50	120.17
13	L	302	UQ1	O4-C4-C3	2.52	126.28	120.93
9	bk	101	BCL	OBB-CAB-CBB	-2.52	114.50	120.17
9	AM	1001	BCL	C2A-C1A-CHA	2.52	128.26	123.86
9	ah	101	BCL	OBB-CAB-CBB	-2.52	114.50	120.17
9	bh	102	BCL	OBB-CAB-CBB	-2.52	114.51	120.17
9	BH	102	BCL	OBB-CAB-CBB	-2.51	114.51	120.17
9	ac	102	BCL	OBB-CAB-CBB	-2.51	114.52	120.17
9	ba	102	BCL	C1-O2A-CGA	2.51	123.04	116.44
9	bj	102	BCL	CMD-C2D-C3D	2.51	129.38	124.68
9	AG	102	BCL	C2A-C1A-CHA	2.51	128.25	123.86
9	ab	102	BCL	OBB-CAB-CBB	-2.51	114.52	120.17
9	BM	1001	BCL	CMD-C2D-C3D	2.51	129.37	124.68
9	ag	101	BCL	C2A-C1A-CHA	2.50	128.24	123.86
9	ai	102	BCL	OBB-CAB-CBB	-2.50	114.53	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	m	1006	BCL	OBB-CAB-CBB	-2.50	114.53	120.17
9	AD	1001	BCL	C2A-C1A-CHA	2.50	128.24	123.86
9	bm	1001	BCL	CMD-C2D-C3D	2.50	129.36	124.68
9	AI	102	BCL	OBB-CAB-CBB	-2.50	114.54	120.17
9	BJ	102	BCL	CMD-C2D-C3D	2.50	129.36	124.68
9	AM	1001	BCL	OBB-CAB-CBB	-2.50	114.55	120.17
9	AJ	101	BCL	OBB-CAB-CBB	-2.49	114.56	120.17
9	am	1001	BCL	C2A-C1A-CHA	2.49	128.22	123.86
14	m	1003	U10	C56-C54-C55	2.49	120.10	114.60
9	am	1001	BCL	OBB-CAB-CBB	-2.49	114.57	120.17
9	aj	101	BCL	OBB-CAB-CBB	-2.49	114.57	120.17
9	aj	101	BCL	C1-C2-C3	2.49	130.35	126.04
9	bh	102	BCL	C1-C2-C3	2.48	130.34	126.04
9	AK	101	BCL	C1-C2-C3	2.48	130.33	126.04
14	M	1007	U10	C56-C54-C55	2.48	120.08	114.60
14	l	303	U10	C17-C18-C19	-2.48	121.69	127.66
14	L	303	U10	C17-C18-C19	-2.48	121.70	127.66
9	ba	102	BCL	OBB-CAB-CBB	-2.47	114.60	120.17
9	BA	102	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
9	bn	101	BCL	CMD-C2D-C3D	2.47	129.30	124.68
9	ad	1001	BCL	C2A-C1A-CHA	2.47	128.18	123.86
9	af	101	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
9	l	305	BCL	C1-O2A-CGA	2.47	122.92	116.44
9	be	1001	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
9	AF	102	BCL	OBB-CAB-CBB	-2.47	114.62	120.17
9	bg	101	BCL	C1-O2A-CGA	2.47	122.92	116.44
9	bg	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
9	AJ	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
9	AA	1001	BCL	OBB-CAB-CBB	-2.47	114.62	120.17
9	BE	1001	BCL	OBB-CAB-CBB	-2.47	114.62	120.17
9	al	1001	BCL	C2A-C1A-CHA	2.46	128.17	123.86
9	al	1001	BCL	OBB-CAB-CBB	-2.46	114.62	120.17
9	M	1002	BCL	OBB-CAB-CBB	-2.46	114.62	120.17
9	ak	101	BCL	OBB-CAB-CBB	-2.46	114.63	120.17
9	aa	1001	BCL	OBB-CAB-CBB	-2.46	114.63	120.17
9	AL	1001	BCL	OBB-CAB-CBB	-2.46	114.64	120.17
9	bf	101	BCL	CMD-C2D-C3D	2.46	129.28	124.68
9	BH	102	BCL	C1-C2-C3	2.46	130.29	126.04
9	BG	101	BCL	OBB-CAB-CBB	-2.46	114.64	120.17
9	be	1001	BCL	CMD-C2D-C3D	2.46	129.28	124.68
9	AK	101	BCL	OBB-CAB-CBB	-2.46	114.64	120.17
9	BF	101	BCL	CMD-C2D-C3D	2.46	129.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bl	101	BCL	CMD-C2D-C3D	2.46	129.28	124.68
9	bg	101	BCL	OBB-CAB-CBB	-2.46	114.64	120.17
9	L	301	BCL	C1-O2A-CGA	2.46	122.89	116.44
13	L	302	UQ1	C7-C6-C1	-2.45	115.53	118.48
9	AL	1001	BCL	C1-C2-C3	-2.45	121.80	126.04
9	bf	101	BCL	OBB-CAB-CBB	-2.45	114.65	120.17
9	BF	101	BCL	OBB-CAB-CBB	-2.45	114.65	120.17
9	AL	1001	BCL	C2A-C1A-CHA	2.45	128.15	123.86
9	BG	101	BCL	C2A-C1A-CHA	2.45	128.15	123.86
9	BN	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
9	BD	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
9	bd	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
9	aj	101	BCL	C2A-C1A-CHA	2.45	128.14	123.86
9	AE	102	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
9	ae	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
9	bn	101	BCL	OBB-CAB-CBB	-2.44	114.67	120.17
9	BM	1001	BCL	C2A-C1A-CHA	2.44	128.13	123.86
9	BE	1001	BCL	CMD-C2D-C3D	2.44	129.25	124.68
10	AI	101	SP2	C15-C16-C17	2.44	128.48	123.47
9	bd	101	BCL	CMD-C2D-C3D	2.44	129.25	124.68
9	l	305	BCL	CMD-C2D-C3D	2.44	129.24	124.68
9	L	301	BCL	CMD-C2D-C3D	2.44	129.24	124.68
9	bc	101	BCL	C2A-C1A-CHA	2.44	128.12	123.86
9	BC	101	BCL	C2A-C1A-CHA	2.44	128.12	123.86
9	BJ	102	BCL	OBB-CAB-CBB	-2.43	114.69	120.17
9	bj	102	BCL	OBB-CAB-CBB	-2.43	114.69	120.17
9	M	1002	BCL	C1-O2A-CGA	2.43	122.82	116.44
12	h	302	CD4	C15-O2-C14	2.43	123.77	117.79
9	ag	101	BCL	OBB-CAB-CBB	-2.43	114.71	120.17
9	bm	1001	BCL	C2A-C1A-CHA	2.42	128.10	123.86
12	H	302	CD4	C15-O2-C14	2.42	123.75	117.79
9	BD	101	BCL	CMD-C2D-C3D	2.42	129.21	124.68
9	BL	102	BCL	CMD-C2D-C3D	2.42	129.20	124.68
9	BG	101	BCL	CMD-C2D-C3D	2.41	129.19	124.68
9	L	304	BCL	OBB-CAB-CBB	-2.41	114.74	120.17
9	l	301	BCL	OBB-CAB-CBB	-2.41	114.74	120.17
13	l	304	UQ1	C7-C6-C1	-2.41	115.57	118.48
15	l	302	BPH	OBB-CAB-CBB	-2.41	114.74	120.17
9	bg	101	BCL	CMD-C2D-C3D	2.41	129.19	124.68
9	bc	101	BCL	OBB-CAB-CBB	-2.41	114.74	120.17
14	L	303	U10	C50-C49-C51	2.41	119.33	115.27
9	BN	101	BCL	CMD-C2D-C3D	2.41	129.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BC	101	BCL	OBB-CAB-CBB	-2.41	114.75	120.17
15	L	305	BPH	OBB-CAB-CBB	-2.41	114.75	120.17
9	m	1006	BCL	C1-O2A-CGA	2.41	122.76	116.44
9	AG	102	BCL	OBB-CAB-CBB	-2.41	114.75	120.17
15	M	1003	BPH	CMD-C2D-C3D	2.41	129.18	124.68
14	l	303	U10	C50-C49-C51	2.40	119.32	115.27
15	m	1002	BPH	CMD-C2D-C3D	2.40	129.18	124.68
9	AD	1001	BCL	OBB-CAB-CBB	-2.40	114.76	120.17
9	bi	101	BCL	OBB-CAB-CBB	-2.40	114.76	120.17
9	BI	101	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
9	BE	1001	BCL	C2A-C1A-CHA	2.40	128.05	123.86
9	an	101	BCL	C2A-C1A-CHA	2.40	128.05	123.86
15	L	305	BPH	CMD-C2D-C3D	2.39	129.16	124.68
9	ad	1001	BCL	OBB-CAB-CBB	-2.39	114.78	120.17
9	BK	101	BCL	CMD-C2D-C3D	2.39	129.15	124.68
15	l	302	BPH	CMD-C2D-C3D	2.39	129.15	124.68
9	BM	1001	BCL	OBB-CAB-CBB	-2.39	114.79	120.17
9	M	1002	BCL	CMD-C2D-C3D	2.39	129.15	124.68
9	be	1001	BCL	C2A-C1A-CHA	2.39	128.04	123.86
9	bm	1001	BCL	OBB-CAB-CBB	-2.39	114.79	120.17
9	ba	102	BCL	CMD-C2D-C3D	2.39	129.15	124.68
9	BA	102	BCL	CMD-C2D-C3D	2.39	129.14	124.68
9	m	1006	BCL	CMD-C2D-C3D	2.39	129.14	124.68
9	AE	102	BCL	C2A-C1A-CHA	2.38	128.03	123.86
9	bk	101	BCL	CMD-C2D-C3D	2.38	129.13	124.68
9	BC	101	BCL	CMD-C2D-C3D	2.38	129.13	124.68
9	BF	101	BCL	C2A-C1A-CHA	2.37	128.01	123.86
9	bh	102	BCL	C6-C5-C3	2.37	119.67	113.45
9	ae	101	BCL	C2A-C1A-CHA	2.37	128.00	123.86
9	BH	102	BCL	CMD-C2D-C3D	2.37	129.11	124.68
14	l	303	U10	C1M-C1-C6	-2.37	120.54	124.40
9	bf	101	BCL	C2A-C1A-CHA	2.37	128.00	123.86
9	bl	101	BCL	OBB-CAB-CBB	-2.37	114.84	120.17
9	bc	101	BCL	CMD-C2D-C3D	2.37	129.11	124.68
14	L	303	U10	C35-C34-C36	2.37	119.25	115.27
14	l	303	U10	C35-C34-C36	2.37	119.25	115.27
14	L	303	U10	C1M-C1-C6	-2.37	120.54	124.40
9	BL	102	BCL	OBB-CAB-CBB	-2.36	114.85	120.17
9	bh	102	BCL	CMD-C2D-C3D	2.36	129.10	124.68
9	BH	102	BCL	C6-C5-C3	2.36	119.64	113.45
9	AN	101	BCL	C2A-C1A-CHA	2.35	127.98	123.86
12	H	302	CD4	O3-C17-C18	2.35	119.29	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	h	302	CD4	O3-C17-C18	2.35	119.29	111.91
9	l	301	BCL	C4A-NA-C1A	2.35	107.76	106.71
9	AN	101	BCL	OBB-CAB-CBB	-2.35	114.88	120.17
9	bb	1001	BCL	CMD-C2D-C3D	2.35	129.07	124.68
9	L	304	BCL	C4A-NA-C1A	2.34	107.76	106.71
9	L	304	BCL	CMD-C2D-C3D	2.34	129.05	124.68
9	l	301	BCL	CMD-C2D-C3D	2.33	129.04	124.68
9	ah	101	BCL	C2A-C1A-CHA	2.33	127.94	123.86
14	L	303	U10	C56-C54-C55	2.33	119.76	114.60
14	l	303	U10	C56-C54-C55	2.33	119.75	114.60
9	an	101	BCL	OBB-CAB-CBB	-2.33	114.92	120.17
9	bb	1001	BCL	OBB-CAB-CBB	-2.33	114.92	120.17
9	BB	1001	BCL	CMD-C2D-C3D	2.33	129.04	124.68
14	l	303	U10	C15-C14-C16	2.33	119.19	115.27
14	L	303	U10	C15-C14-C16	2.33	119.19	115.27
9	an	101	BCL	CMD-C2D-C3D	2.33	129.03	124.68
9	bi	101	BCL	CMD-C2D-C3D	2.33	129.03	124.68
9	AN	101	BCL	CMD-C2D-C3D	2.32	129.03	124.68
9	AH	101	BCL	C2A-C1A-CHA	2.32	127.92	123.86
9	BI	101	BCL	CMD-C2D-C3D	2.32	129.03	124.68
12	m	1005	CD4	O14-C35-C36	2.32	119.19	111.91
9	BB	1001	BCL	OBB-CAB-CBB	-2.32	114.95	120.17
12	M	1004	CD4	O14-C35-C36	2.32	119.18	111.91
9	bb	1001	BCL	C2A-C1A-CHA	2.31	127.90	123.86
9	BF	101	BCL	C4B-C3B-CAB	-2.31	122.66	127.13
9	bf	101	BCL	C4B-C3B-CAB	-2.31	122.66	127.13
9	AB	101	BCL	O2A-CGA-O1A	-2.31	117.76	123.59
9	BB	1001	BCL	C2A-C1A-CHA	2.31	127.90	123.86
11	AC	102	3PE	O12-P-O14	2.31	123.64	112.24
9	AI	102	BCL	C2A-C1A-CHA	2.30	127.89	123.86
11	ac	101	3PE	O12-P-O14	2.30	123.63	112.24
9	ai	102	BCL	C2A-C1A-CHA	2.30	127.89	123.86
9	AD	1001	BCL	CMD-C2D-C3D	2.30	128.99	124.68
16	x	100	SQD	O5-C1-O6	-2.30	104.52	109.97
14	l	303	U10	C32-C33-C34	-2.30	122.12	127.66
9	M	1008	BCL	CMD-C2D-C3D	2.30	128.98	124.68
9	ad	1001	BCL	CMD-C2D-C3D	2.30	128.98	124.68
9	m	1004	BCL	CMD-C2D-C3D	2.30	128.98	124.68
14	L	303	U10	C32-C33-C34	-2.30	122.13	127.66
9	AB	101	BCL	CMD-C2D-C3D	2.29	128.97	124.68
9	ab	102	BCL	CMD-C2D-C3D	2.29	128.97	124.68
11	H	301	3PE	O12-P-O14	2.29	123.55	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	m	1002	BPH	O2D-CGD-CBD	2.29	113.89	111.00
9	ah	101	BCL	CMD-C2D-C3D	2.28	128.95	124.68
15	M	1003	BPH	O2D-CGD-CBD	2.28	113.89	111.00
9	aj	101	BCL	CMD-C2D-C3D	2.28	128.95	124.68
9	ae	101	BCL	CMD-C2D-C3D	2.28	128.95	124.68
14	M	1007	U10	O3-C3-C4	-2.28	115.04	123.64
9	ai	102	BCL	CMD-C2D-C3D	2.28	128.94	124.68
9	AI	102	BCL	CMD-C2D-C3D	2.28	128.94	124.68
14	m	1003	U10	O3-C3-C4	-2.28	115.04	123.64
9	AJ	101	BCL	CMD-C2D-C3D	2.28	128.94	124.68
11	h	301	3PE	O12-P-O14	2.28	123.50	112.24
9	AE	102	BCL	CMD-C2D-C3D	2.28	128.94	124.68
9	AH	101	BCL	CMD-C2D-C3D	2.28	128.94	124.68
9	bj	102	BCL	C2A-C1A-CHA	2.27	127.83	123.86
9	ak	101	BCL	C1-C2-C3	2.27	129.97	126.04
13	l	304	UQ1	C8-C7-C6	2.27	118.17	112.05
13	L	302	UQ1	C8-C7-C6	2.27	118.17	112.05
9	bc	101	BCL	CAA-CBA-CGA	2.27	119.88	113.25
9	BC	101	BCL	CAA-CBA-CGA	2.27	119.88	113.25
9	bi	101	BCL	C2A-C1A-CHA	2.27	127.82	123.86
9	AK	101	BCL	CMD-C2D-C3D	2.27	128.92	124.68
15	L	305	BPH	C1-C2-C3	-2.26	122.13	126.04
9	BN	101	BCL	C1-O2A-CGA	2.26	122.38	116.44
9	ak	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
9	ai	102	BCL	C4A-NA-C1A	2.26	107.72	106.71
9	AF	102	BCL	CMD-C2D-C3D	2.26	128.91	124.68
15	l	302	BPH	C1-C2-C3	-2.26	122.13	126.04
9	AI	102	BCL	C4A-NA-C1A	2.26	107.72	106.71
9	BI	101	BCL	C2A-C1A-CHA	2.26	127.81	123.86
9	AC	101	BCL	CMD-C2D-C3D	2.26	128.90	124.68
9	af	101	BCL	CMD-C2D-C3D	2.26	128.90	124.68
9	l	305	BCL	OBB-CAB-CBB	-2.26	115.09	120.17
9	BJ	102	BCL	C2A-C1A-CHA	2.25	127.80	123.86
9	L	301	BCL	OBB-CAB-CBB	-2.25	115.09	120.17
9	ac	102	BCL	CMD-C2D-C3D	2.25	128.90	124.68
9	BB	1001	BCL	C1-O2A-CGA	2.25	122.35	116.44
14	L	303	U10	C42-C43-C44	-2.25	122.24	127.66
9	AM	1001	BCL	CMD-C2D-C3D	2.25	128.89	124.68
15	m	1002	BPH	CAC-C3C-C4C	2.25	118.76	113.73
9	am	1001	BCL	CMD-C2D-C3D	2.25	128.88	124.68
15	M	1003	BPH	CAC-C3C-C4C	2.25	118.76	113.73
14	l	303	U10	C42-C43-C44	-2.24	122.28	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AG	102	BCL	CMD-C2D-C3D	2.23	128.86	124.68
9	ag	101	BCL	CMD-C2D-C3D	2.23	128.85	124.68
9	bl	101	BCL	C2A-C1A-CHA	2.22	127.75	123.86
9	l	305	BCL	C4B-C3B-CAB	-2.22	122.83	127.13
9	L	301	BCL	C4B-C3B-CAB	-2.22	122.84	127.13
9	BL	102	BCL	C2A-C1A-CHA	2.22	127.74	123.86
9	AL	1001	BCL	CMD-C2D-C3D	2.22	128.83	124.68
10	ai	103	SP2	C19-C18-C17	2.22	122.34	118.94
10	AI	103	SP2	C19-C18-C17	2.22	122.34	118.94
9	al	1001	BCL	CMD-C2D-C3D	2.21	128.82	124.68
9	bb	1001	BCL	C1-O2A-CGA	2.21	122.25	116.44
9	bn	101	BCL	C1-O2A-CGA	2.21	122.24	116.44
11	ac	101	3PE	O21-C2-C1	2.21	116.40	108.40
11	AC	102	3PE	O21-C2-C1	2.20	116.37	108.40
9	AA	1001	BCL	CMD-C2D-C3D	2.19	128.78	124.68
9	BD	101	BCL	C1-C2-C3	-2.19	122.25	126.04
9	aa	1001	BCL	CMD-C2D-C3D	2.19	128.78	124.68
9	bl	101	BCL	C1-O2A-CGA	2.19	122.18	116.44
9	L	304	BCL	C4B-C3B-CAB	-2.18	122.91	127.13
9	l	301	BCL	C4B-C3B-CAB	-2.18	122.91	127.13
9	BL	102	BCL	C1-O2A-CGA	2.18	122.16	116.44
16	x	100	SQD	O5-C5-C4	2.18	113.65	109.69
10	ab	101	SP2	C28-C29-C30	2.17	135.18	127.75
14	m	1003	U10	C52-C53-C54	-2.16	120.35	127.75
16	x	100	SQD	O48-C23-O10	-2.16	118.13	123.59
14	M	1007	U10	C52-C53-C54	-2.16	120.35	127.75
14	l	303	U10	C3M-O3-C3	2.16	124.13	116.47
14	L	303	U10	O3-C3-C4	-2.16	115.49	123.64
14	L	303	U10	C3M-O3-C3	2.16	124.13	116.47
14	l	303	U10	O3-C3-C4	-2.16	115.49	123.64
9	BH	102	BCL	C4B-C3B-CAB	-2.15	122.98	127.13
9	bh	102	BCL	C4B-C3B-CAB	-2.15	122.98	127.13
9	ba	102	BCL	C4B-C3B-CAB	-2.14	122.99	127.13
15	M	1003	BPH	OBB-CAB-CBB	-2.14	115.35	120.17
9	bd	101	BCL	C1-C2-C3	-2.14	122.34	126.04
9	BK	101	BCL	C2A-C1A-CHA	2.14	127.60	123.86
15	L	305	BPH	O2D-CGD-CBD	2.14	113.70	111.00
14	M	1007	U10	O2-C2-C1	-2.14	114.43	120.73
14	m	1003	U10	O2-C2-C1	-2.14	114.43	120.73
15	l	302	BPH	O2D-CGD-CBD	2.14	113.70	111.00
10	AA	1002	SP2	C28-C29-C30	2.14	135.05	127.75
15	m	1002	BPH	OBB-CAB-CBB	-2.14	115.36	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BA	102	BCL	C4B-C3B-CAB	-2.13	123.01	127.13
12	h	302	CD4	O14-C35-C36	2.13	118.59	111.91
10	AB	103	SP2	C3-C2-C1	2.13	124.68	114.13
12	H	302	CD4	O14-C35-C36	2.13	118.59	111.91
9	M	1002	BCL	C4B-C3B-CAB	-2.12	123.03	127.13
9	m	1006	BCL	C4B-C3B-CAB	-2.11	123.04	127.13
9	AB	101	BCL	C4B-C3B-CAB	-2.11	123.05	127.13
9	BL	102	BCL	CAA-CBA-CGA	2.11	119.41	113.25
9	ab	102	BCL	C4B-C3B-CAB	-2.10	123.06	127.13
9	BE	1001	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
9	be	1001	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
9	bj	102	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
9	bk	101	BCL	C4B-C3B-CAB	-2.10	123.08	127.13
12	M	1004	CD4	C49-C48-C47	-2.10	105.66	113.19
12	m	1005	CD4	C49-C48-C47	-2.10	105.66	113.19
9	bk	101	BCL	C2A-C1A-CHA	2.09	127.52	123.86
9	BJ	102	BCL	C4B-C3B-CAB	-2.09	123.09	127.13
9	bm	1001	BCL	C4B-C3B-CAB	-2.09	123.09	127.13
9	aj	101	BCL	C6-C5-C3	2.08	118.92	113.45
9	BB	1001	BCL	C4B-C3B-CAB	-2.08	123.10	127.13
9	BK	101	BCL	C4B-C3B-CAB	-2.08	123.10	127.13
9	BM	1001	BCL	C4B-C3B-CAB	-2.08	123.10	127.13
9	bb	1001	BCL	C4B-C3B-CAB	-2.08	123.12	127.13
9	bn	101	BCL	C2A-C1A-CHA	2.08	127.49	123.86
9	bl	101	BCL	CAA-CBA-CGA	2.07	119.30	113.25
9	ac	102	BCL	C2A-C1A-CHA	2.06	127.47	123.86
12	h	302	CD4	C33-O16-C46	2.06	122.87	117.79
12	H	302	CD4	C33-O16-C46	2.06	122.86	117.79
9	AC	101	BCL	C2A-C1A-CHA	2.06	127.46	123.86
9	BN	101	BCL	C2A-C1A-CHA	2.05	127.44	123.86
14	m	1003	U10	C50-C49-C48	-2.05	118.42	123.68
14	M	1007	U10	C50-C49-C48	-2.05	118.43	123.68
9	BC	101	BCL	C4B-C3B-CAB	-2.04	123.18	127.13
9	bj	102	BCL	C1-O2A-CGA	2.04	121.79	116.44
16	L	306	SQD	O6-C44-C45	-2.04	105.98	110.90
9	AN	101	BCL	C4B-C3B-CAB	-2.03	123.20	127.13
9	AJ	101	BCL	C4B-C3B-CAB	-2.03	123.21	127.13
9	bc	101	BCL	C4B-C3B-CAB	-2.03	123.21	127.13
9	BJ	102	BCL	C1-O2A-CGA	2.03	121.76	116.44
9	aj	101	BCL	C4B-C3B-CAB	-2.03	123.22	127.13
9	BH	102	BCL	CAA-CBA-CGA	2.02	119.15	113.25
9	BG	101	BCL	C4B-C3B-CAB	-2.02	123.23	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	101	BCL	C6-C5-C3	2.02	118.74	113.45
9	an	101	BCL	C4B-C3B-CAB	-2.01	123.24	127.13
15	M	1003	BPH	C1-C2-C3	-2.01	122.56	126.04
15	m	1002	BPH	C1-C2-C3	-2.01	122.56	126.04
9	bg	101	BCL	C4B-C3B-CAB	-2.01	123.24	127.13
9	bh	102	BCL	CAA-CBA-CGA	2.01	119.13	113.25
14	l	303	U10	C6-C1-C2	2.01	120.77	119.18
9	ai	102	BCL	C4B-C3B-CAB	-2.01	123.25	127.13
14	L	303	U10	C6-C1-C2	2.01	120.77	119.18
9	bi	101	BCL	C1C-NC-C4C	2.00	107.61	106.71
9	aa	1001	BCL	C4B-C3B-CAB	-2.00	123.26	127.13
9	AI	102	BCL	C4B-C3B-CAB	-2.00	123.26	127.13

There are no chirality outliers.

All (818) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AJ	101	BCL	C4-C3-C5-C6
9	AK	101	BCL	CHA-CBD-CGD-O1D
9	AK	101	BCL	CHA-CBD-CGD-O2D
9	AK	101	BCL	C2-C3-C5-C6
9	AK	101	BCL	C4-C3-C5-C6
9	BA	102	BCL	C3A-C2A-CAA-CBA
9	BB	1001	BCL	C1A-C2A-CAA-CBA
9	BF	101	BCL	C1A-C2A-CAA-CBA
9	BH	102	BCL	O2A-C1-C2-C3
9	BJ	102	BCL	C1A-C2A-CAA-CBA
9	BL	102	BCL	C1A-C2A-CAA-CBA
9	aj	101	BCL	C4-C3-C5-C6
9	ak	101	BCL	CHA-CBD-CGD-O1D
9	ak	101	BCL	CHA-CBD-CGD-O2D
9	ak	101	BCL	C2-C3-C5-C6
9	ak	101	BCL	C4-C3-C5-C6
9	an	101	BCL	C11-C12-C13-C14
9	ba	102	BCL	C3A-C2A-CAA-CBA
9	bb	1001	BCL	C1A-C2A-CAA-CBA
9	bf	101	BCL	C1A-C2A-CAA-CBA
9	bh	102	BCL	O2A-C1-C2-C3
9	bj	102	BCL	C1A-C2A-CAA-CBA
9	bl	101	BCL	C1A-C2A-CAA-CBA
10	AA	1002	SP2	C27-C28-C29-C30
10	AC	104	SP2	C11-C12-C13-CM5

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Mol	Chain	Res	Type	Atoms
10	AF	101	SP2	O1-C1-C2-C3
10	AI	103	SP2	CM6-C18-C19-C20
10	AJ	103	SP2	O1-C1-C2-C3
10	AJ	103	SP2	CM1-C1-C2-C3
10	AJ	103	SP2	CM2-C1-C2-C3
10	AJ	103	SP2	C7-C8-C9-CM4
10	AK	102	SP2	C7-C8-C9-CM4
10	AK	102	SP2	C7-C8-C9-C10
10	AM	1000	SP2	O1-C1-C2-C3
10	AM	1000	SP2	CM2-C1-C2-C3
10	BE	1002	SP2	C1-C2-C3-C4
10	BF	102	SP2	C11-C12-C13-CM5
10	BF	102	SP2	C11-C12-C13-C14
10	BK	102	SP2	O1-C1-C2-C3
10	BK	102	SP2	C11-C12-C13-CM5
10	BL	101	SP2	O1-C1-C2-C3
10	BL	103	SP2	C11-C12-C13-CM5
10	BL	103	SP2	C11-C12-C13-C14
10	ab	101	SP2	CM1-C1-C2-C3
10	ab	101	SP2	C27-C28-C29-C30
10	ac	104	SP2	C11-C12-C13-CM5
10	ad	1002	SP2	CM1-C1-C2-C3
10	af	103	SP2	CM1-C1-C2-C3
10	af	103	SP2	CM2-C1-C2-C3
10	af	104	SP2	C11-C12-C13-CM5
10	ai	101	SP2	O1-C1-C2-C3
10	ai	101	SP2	CM1-C1-C2-C3
10	ai	101	SP2	CM2-C1-C2-C3
10	ai	103	SP2	CM6-C18-C19-C20
10	aj	102	SP2	C25-C26-C27-C28
10	aj	102	SP2	CM8-C26-C27-C28
10	aj	103	SP2	CM2-C1-C2-C3
10	ak	102	SP2	C7-C8-C9-CM4
10	ak	102	SP2	C7-C8-C9-C10
10	al	1002	SP2	CM1-C1-C2-C3
10	ba	101	SP2	O1-C1-C2-C3
10	ba	101	SP2	CM1-C1-C2-C3
10	ba	101	SP2	CM2-C1-C2-C3
10	bb	1002	SP2	C3-C4-C5-CM3
10	bb	1002	SP2	C3-C4-C5-C6
10	bf	102	SP2	C11-C12-C13-CM5
10	bf	102	SP2	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
10	bj	101	SP2	O1-C1-C2-C3
10	bj	101	SP2	CM2-C1-C2-C3
10	bl	102	SP2	C11-C12-C13-CM5
10	bl	102	SP2	C11-C12-C13-C14
11	AC	102	3PE	C11-O13-P-O12
11	AC	102	3PE	O13-C11-C12-N
11	ac	101	3PE	C11-O13-P-O12
11	ac	101	3PE	O13-C11-C12-N
12	H	302	CD4	O8-C29-C30-O9
12	H	302	CD4	C30-C31-O10-P2
12	M	1004	CD4	O16-C33-C34-O14
12	h	302	CD4	O8-C29-C30-O9
12	h	302	CD4	C30-C31-O10-P2
12	m	1005	CD4	O16-C33-C34-O14
14	L	303	U10	C24-C26-C27-C28
14	l	303	U10	C24-C26-C27-C28
16	L	306	SQD	C2-C1-O6-C44
16	L	306	SQD	O5-C1-O6-C44
9	AD	1001	BCL	C3-C5-C6-C7
10	AG	101	SP2	C2-C3-C4-C5
9	AJ	101	BCL	C2-C3-C5-C6
9	ad	1001	BCL	C3-C5-C6-C7
10	AG	101	SP2	CM8-C26-C27-C28
10	af	103	SP2	CM8-C26-C27-C28
10	m	1007	SP2	C3-C4-C5-CM3
9	aj	101	BCL	C2-C3-C5-C6
10	AG	101	SP2	C25-C26-C27-C28
10	af	103	SP2	C25-C26-C27-C28
10	m	1007	SP2	C3-C4-C5-C6
10	BA	101	SP2	C26-C27-C28-C29
10	ac	103	SP2	C22-C23-C24-C25
10	ba	101	SP2	C26-C27-C28-C29
10	ae	103	SP2	C1-C2-C3-C4
12	H	302	CD4	O8-C29-C30-C31
12	h	302	CD4	O8-C29-C30-C31
17	M	1001	LMT	C2B-C1B-O1B-C4'
17	m	1001	LMT	C2B-C1B-O1B-C4'
10	AJ	102	SP2	CM8-C26-C27-C28
10	AJ	102	SP2	C25-C26-C27-C28
9	AN	101	BCL	C11-C10-C8-C9
9	AN	101	BCL	C11-C12-C13-C14
9	BL	102	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	bl	101	BCL	C6-C7-C8-C9
10	AF	103	SP2	C11-C12-C13-CM5
10	BC	102	SP2	C11-C12-C13-CM5
10	ab	104	SP2	C11-C12-C13-CM5
10	bk	102	SP2	C11-C12-C13-CM5
10	AI	103	SP2	C17-C18-C19-C20
10	ai	103	SP2	C17-C18-C19-C20
17	M	1001	LMT	O5B-C1B-O1B-C4’
17	m	1001	LMT	O5B-C1B-O1B-C4’
11	ac	101	3PE	C31-C32-C33-C34
13	L	302	UQ1	C2-C3-O3-CM3
13	l	304	UQ1	C2-C3-O3-CM3
14	M	1007	U10	C4-C3-O3-C3M
14	m	1003	U10	C4-C3-O3-C3M
9	bi	101	BCL	C2A-CAA-CBA-CGA
10	BL	101	SP2	C26-C27-C28-C29
10	aj	103	SP2	C22-C23-C24-C25
10	al	1002	SP2	C26-C27-C28-C29
11	H	301	3PE	C21-C22-C23-C24
11	h	301	3PE	C21-C22-C23-C24
9	ae	101	BCL	C10-C11-C12-C13
10	AB	104	SP2	C1-C2-C3-C4
10	BA	101	SP2	C1-C2-C3-C4
9	AF	102	BCL	C5-C6-C7-C8
9	AL	1001	BCL	C15-C16-C17-C18
9	af	101	BCL	C5-C6-C7-C8
9	al	1001	BCL	C15-C16-C17-C18
12	M	1004	CD4	C32-O13-P2-O10
12	m	1005	CD4	C32-O13-P2-O10
9	AE	102	BCL	C10-C11-C12-C13
11	AC	102	3PE	C31-C32-C33-C34
9	AD	1001	BCL	C4-C3-C5-C6
10	M	1005	SP2	C3-C4-C5-CM3
10	bb	1002	SP2	CM8-C26-C27-C28
9	BC	101	BCL	C5-C6-C7-C8
9	BC	101	BCL	C2A-CAA-CBA-CGA
9	bc	101	BCL	C2A-CAA-CBA-CGA
9	bc	101	BCL	C5-C6-C7-C8
10	AB	104	SP2	CM8-C26-C27-C28
14	M	1007	U10	C50-C49-C51-C52
14	m	1003	U10	C50-C49-C51-C52
10	ac	104	SP2	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	bb	1002	SP2	C25-C26-C27-C28
9	AJ	101	BCL	C11-C10-C8-C9
9	an	101	BCL	C11-C10-C8-C9
15	M	1003	BPH	C6-C7-C8-C9
15	m	1002	BPH	C6-C7-C8-C9
11	AC	102	3PE	C21-C22-C23-C24
11	ac	101	3PE	C21-C22-C23-C24
11	ac	101	3PE	C34-C35-C36-C37
9	BI	101	BCL	C2A-CAA-CBA-CGA
10	ai	101	SP2	CM6-C18-C19-C20
10	BK	102	SP2	C11-C12-C13-C14
10	ai	101	SP2	C17-C18-C19-C20
11	H	301	3PE	C22-C23-C24-C25
11	H	301	3PE	C2A-C2B-C2C-C2D
11	h	301	3PE	C22-C23-C24-C25
11	AC	102	3PE	C34-C35-C36-C37
11	h	301	3PE	C2A-C2B-C2C-C2D
9	AC	101	BCL	C3A-C2A-CAA-CBA
9	AI	102	BCL	C3A-C2A-CAA-CBA
9	BB	1001	BCL	C3A-C2A-CAA-CBA
9	BF	101	BCL	C3A-C2A-CAA-CBA
9	BJ	102	BCL	C3A-C2A-CAA-CBA
9	BK	101	BCL	C3A-C2A-CAA-CBA
9	BL	102	BCL	C3A-C2A-CAA-CBA
9	ac	102	BCL	C3A-C2A-CAA-CBA
9	ai	102	BCL	C3A-C2A-CAA-CBA
9	bb	1001	BCL	C3A-C2A-CAA-CBA
9	bf	101	BCL	C3A-C2A-CAA-CBA
9	bj	102	BCL	C3A-C2A-CAA-CBA
9	bk	101	BCL	C3A-C2A-CAA-CBA
9	bl	101	BCL	C3A-C2A-CAA-CBA
10	AI	103	SP2	C1-C2-C3-C4
17	M	1001	LMT	O5'-C5'-C6'-O6'
17	m	1001	LMT	O5'-C5'-C6'-O6'
10	ac	104	SP2	CM8-C26-C27-C28
9	AD	1001	BCL	C2-C3-C5-C6
9	BA	102	BCL	C2-C3-C5-C6
9	ba	102	BCL	C2-C3-C5-C6
10	AB	104	SP2	C25-C26-C27-C28
10	AC	104	SP2	C25-C26-C27-C28
10	AA	1002	SP2	C2-C3-C4-C5
11	ac	101	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
16	L	306	SQD	C15-C16-C17-C18
9	bm	1001	BCL	C5-C6-C7-C8
11	AC	102	3PE	C24-C25-C26-C27
12	H	302	CD4	C47-C48-C49-C50
12	h	302	CD4	C47-C48-C49-C50
9	BM	1001	BCL	C5-C6-C7-C8
9	BA	102	BCL	C4-C3-C5-C6
9	ad	1001	BCL	C4-C3-C5-C6
9	ba	102	BCL	C4-C3-C5-C6
10	AC	104	SP2	CM8-C26-C27-C28
14	L	303	U10	C35-C34-C36-C37
14	l	303	U10	C35-C34-C36-C37
9	AJ	101	BCL	C11-C10-C8-C7
9	AN	101	BCL	C11-C10-C8-C7
9	BL	102	BCL	C6-C7-C8-C10
9	ad	1001	BCL	C2-C3-C5-C6
9	ae	101	BCL	C11-C10-C8-C7
9	al	1001	BCL	C6-C7-C8-C10
9	an	101	BCL	C11-C10-C8-C7
9	bl	101	BCL	C6-C7-C8-C10
10	ab	103	SP2	C3-C4-C5-C6
14	L	303	U10	C33-C34-C36-C37
14	M	1007	U10	C48-C49-C51-C52
14	l	303	U10	C33-C34-C36-C37
14	m	1003	U10	C48-C49-C51-C52
15	M	1003	BPH	C6-C7-C8-C10
15	m	1002	BPH	C6-C7-C8-C10
9	ak	101	BCL	C8-C10-C11-C12
14	L	303	U10	C4-C3-O3-C3M
14	l	303	U10	C4-C3-O3-C3M
12	H	302	CD4	C6-C7-C8-C9
12	h	302	CD4	C6-C7-C8-C9
11	AC	102	3PE	O11-C1-C2-O21
11	ac	101	3PE	O11-C1-C2-O21
10	ab	103	SP2	C3-C4-C5-CM3
10	M	1005	SP2	C3-C4-C5-C6
9	AA	1001	BCL	C11-C12-C13-C14
9	AE	102	BCL	C11-C10-C8-C9
9	AL	1001	BCL	C6-C7-C8-C9
9	BJ	102	BCL	C14-C13-C15-C16
9	aa	1001	BCL	C11-C12-C13-C14
9	ae	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
9	al	1001	BCL	C6-C7-C8-C9
10	AI	101	SP2	CM6-C18-C19-C20
10	M	1005	SP2	C11-C12-C13-CM5
10	ad	1002	SP2	C11-C12-C13-CM5
9	BH	102	BCL	C10-C11-C12-C13
9	BJ	102	BCL	C5-C6-C7-C8
9	bh	102	BCL	C10-C11-C12-C13
9	bj	102	BCL	C5-C6-C7-C8
10	AI	101	SP2	C17-C18-C19-C20
9	AC	101	BCL	C1A-C2A-CAA-CBA
9	AI	102	BCL	C1A-C2A-CAA-CBA
9	BK	101	BCL	C1A-C2A-CAA-CBA
9	ac	102	BCL	C1A-C2A-CAA-CBA
9	ai	102	BCL	C1A-C2A-CAA-CBA
9	bk	101	BCL	C1A-C2A-CAA-CBA
11	H	301	3PE	O11-C1-C2-C3
11	h	301	3PE	O11-C1-C2-C3
11	ac	101	3PE	C39-C3A-C3B-C3C
9	bl	101	BCL	C4-C3-C5-C6
9	BD	101	BCL	C2A-CAA-CBA-CGA
12	M	1004	CD4	C41-C42-C43-C44
12	m	1005	CD4	C41-C42-C43-C44
16	L	306	SQD	O6-C44-C45-C46
9	AC	101	BCL	C15-C16-C17-C18
9	AF	102	BCL	C15-C16-C17-C18
9	BL	102	BCL	C4-C3-C5-C6
9	BM	1001	BCL	C4-C3-C5-C6
9	be	1001	BCL	C4-C3-C5-C6
9	bm	1001	BCL	C4-C3-C5-C6
10	AB	102	SP2	C3-C4-C5-CM3
10	AB	104	SP2	CM7-C22-C23-C24
10	bb	1002	SP2	CM7-C22-C23-C24
14	L	303	U10	C15-C14-C16-C17
14	L	303	U10	C50-C49-C51-C52
14	M	1007	U10	C35-C34-C36-C37
14	l	303	U10	C15-C14-C16-C17
14	l	303	U10	C50-C49-C51-C52
14	m	1003	U10	C35-C34-C36-C37
9	bl	101	BCL	C2-C3-C5-C6
10	AB	102	SP2	C3-C4-C5-C6
10	bb	1002	SP2	C21-C22-C23-C24
12	h	302	CD4	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
9	AK	101	BCL	C8-C10-C11-C12
9	af	101	BCL	C15-C16-C17-C18
10	bh	101	SP2	C1-C2-C3-C4
9	bd	101	BCL	C2A-CAA-CBA-CGA
9	BG	101	BCL	C2-C1-O2A-CGA
9	BI	101	BCL	C2-C1-O2A-CGA
9	bg	101	BCL	C2-C1-O2A-CGA
9	bi	101	BCL	C2-C1-O2A-CGA
11	h	301	3PE	O11-C1-C2-O21
12	H	302	CD4	O2-C15-C28-O5
12	h	302	CD4	O2-C15-C28-O5
12	H	302	CD4	C17-C18-C19-C20
12	M	1004	CD4	C42-C43-C44-C45
12	m	1005	CD4	C42-C43-C44-C45
11	AC	102	3PE	O21-C2-C3-O31
11	ac	101	3PE	O21-C2-C3-O31
9	bg	101	BCL	C4-C3-C5-C6
10	AJ	103	SP2	CM7-C22-C23-C24
10	AM	1000	SP2	C3-C4-C5-CM3
10	ai	101	SP2	C3-C4-C5-CM3
9	AA	1001	BCL	C11-C12-C13-C15
9	AE	102	BCL	C11-C10-C8-C7
9	AL	1001	BCL	C6-C7-C8-C10
9	BF	101	BCL	C12-C13-C15-C16
9	BJ	102	BCL	C12-C13-C15-C16
9	BL	102	BCL	C2-C3-C5-C6
9	aa	1001	BCL	C11-C12-C13-C15
9	ac	102	BCL	C11-C12-C13-C15
9	bf	101	BCL	C12-C13-C15-C16
9	bj	102	BCL	C12-C13-C15-C16
10	AB	104	SP2	C21-C22-C23-C24
14	M	1007	U10	C33-C34-C36-C37
14	m	1003	U10	C33-C34-C36-C37
9	BF	101	BCL	C14-C13-C15-C16
9	ac	102	BCL	C11-C12-C13-C14
9	bf	101	BCL	C14-C13-C15-C16
9	bj	102	BCL	C14-C13-C15-C16
11	AC	102	3PE	C39-C3A-C3B-C3C
10	AJ	103	SP2	C7-C8-C9-C10
10	ac	104	SP2	C11-C12-C13-C14
9	bc	101	BCL	C3-C5-C6-C7
11	AC	102	3PE	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
11	AC	102	3PE	O11-C1-C2-C3
11	ac	101	3PE	O11-C1-C2-C3
9	BC	101	BCL	C3-C5-C6-C7
9	BH	102	BCL	C5-C6-C7-C8
10	BA	101	SP2	C3-C4-C5-CM3
10	af	103	SP2	C3-C4-C5-CM3
9	bg	101	BCL	C2-C3-C5-C6
10	AJ	103	SP2	C21-C22-C23-C24
10	AM	1000	SP2	C3-C4-C5-C6
14	L	303	U10	C48-C49-C51-C52
14	l	303	U10	C48-C49-C51-C52
11	ac	101	3PE	C3D-C3E-C3F-C3G
9	bh	102	BCL	C5-C6-C7-C8
12	M	1004	CD4	O3-C17-C18-C19
12	m	1005	CD4	O3-C17-C18-C19
11	H	301	3PE	C2-C1-O11-P
11	h	301	3PE	C2-C1-O11-P
9	BE	1001	BCL	C3A-C2A-CAA-CBA
9	be	1001	BCL	C3A-C2A-CAA-CBA
12	H	302	CD4	C1-C2-C3-C4
12	h	302	CD4	C1-C2-C3-C4
10	AF	101	SP2	CM2-C1-C2-C3
10	AM	1000	SP2	CM1-C1-C2-C3
10	BK	102	SP2	CM2-C1-C2-C3
10	BL	101	SP2	CM2-C1-C2-C3
10	ab	101	SP2	CM2-C1-C2-C3
10	ad	1002	SP2	CM2-C1-C2-C3
10	af	102	SP2	CM2-C1-C2-C3
10	aj	103	SP2	CM1-C1-C2-C3
10	al	1002	SP2	CM2-C1-C2-C3
10	bj	101	SP2	CM1-C1-C2-C3
11	H	301	3PE	C28-C29-C2A-C2B
11	h	301	3PE	C28-C29-C2A-C2B
16	L	306	SQD	C13-C14-C15-C16
9	BN	101	BCL	O2A-C1-C2-C3
9	bn	101	BCL	O2A-C1-C2-C3
9	BE	1001	BCL	C4-C3-C5-C6
9	BM	1001	BCL	C2-C3-C5-C6
16	x	100	SQD	C27-C28-C29-C30
9	ac	102	BCL	C15-C16-C17-C18
16	L	306	SQD	C27-C28-C29-C30
11	H	301	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
10	BA	101	SP2	C3-C4-C5-C6
10	af	103	SP2	C3-C4-C5-C6
9	BM	1001	BCL	C11-C10-C8-C9
9	aj	101	BCL	C11-C10-C8-C9
9	bm	1001	BCL	C11-C10-C8-C9
11	AC	102	3PE	C35-C36-C37-C38
9	ai	102	BCL	C8-C10-C11-C12
9	AB	101	BCL	C4C-C3C-CAC-CBC
9	BC	101	BCL	C4C-C3C-CAC-CBC
9	bc	101	BCL	C4C-C3C-CAC-CBC
10	AC	104	SP2	C11-C12-C13-C14
11	ac	101	3PE	C35-C36-C37-C38
10	ab	103	SP2	CM8-C26-C27-C28
9	bm	1001	BCL	C2-C3-C5-C6
14	L	303	U10	C13-C14-C16-C17
14	l	303	U10	C13-C14-C16-C17
9	L	304	BCL	CAD-CBD-CGD-O2D
9	l	301	BCL	CAD-CBD-CGD-O2D
15	L	305	BPH	CAD-CBD-CGD-O2D
15	l	302	BPH	CAD-CBD-CGD-O2D
10	AJ	102	SP2	CM7-C22-C23-C24
10	BE	1002	SP2	CM8-C26-C27-C28
10	ae	103	SP2	CM8-C26-C27-C28
10	ab	103	SP2	C25-C26-C27-C28
13	L	302	UQ1	C4-C3-O3-CM3
13	l	304	UQ1	C4-C3-O3-CM3
12	M	1004	CD4	C32-C33-C34-O14
12	m	1005	CD4	C32-C33-C34-O14
12	h	302	CD4	C9-C10-C11-C12
12	H	302	CD4	O16-C33-C34-O14
12	h	302	CD4	O16-C33-C34-O14
12	H	302	CD4	C9-C10-C11-C12
9	bc	101	BCL	C4-C3-C5-C6
10	AC	103	SP2	CM7-C22-C23-C24
10	AM	1000	SP2	CM7-C22-C23-C24
10	aj	102	SP2	CM7-C22-C23-C24
10	am	1000	SP2	CM7-C22-C23-C24
10	BE	1002	SP2	C11-C12-C13-CM5
10	BK	102	SP2	C7-C8-C9-CM4
10	ae	103	SP2	C7-C8-C9-CM4
10	ae	103	SP2	C11-C12-C13-CM5
10	m	1007	SP2	C11-C12-C13-CM5

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Mol	Chain	Res	Type	Atoms
9	BA	102	BCL	C1A-C2A-CAA-CBA
9	ba	102	BCL	C1A-C2A-CAA-CBA
9	bi	101	BCL	C1A-C2A-CAA-CBA
9	BJ	102	BCL	C2-C1-O2A-CGA
9	BL	102	BCL	C2-C1-O2A-CGA
9	bj	102	BCL	C2-C1-O2A-CGA
9	bl	101	BCL	C2-C1-O2A-CGA
11	AC	102	3PE	C3A-C3B-C3C-C3D
12	H	302	CD4	C30-C29-O8-P1
12	h	302	CD4	C30-C29-O8-P1
10	ai	101	SP2	C3-C4-C5-C6
12	M	1004	CD4	C32-O13-P2-O11
12	m	1005	CD4	C32-O13-P2-O11
12	H	302	CD4	C16-C15-C28-O5
12	h	302	CD4	C16-C15-C28-O5
10	aj	103	SP2	C27-C28-C29-C30
11	AC	102	3PE	C12-C11-O13-P
9	AI	102	BCL	C8-C10-C11-C12
9	BC	101	BCL	C4-C3-C5-C6
10	BK	102	SP2	CM8-C26-C27-C28
10	bk	102	SP2	CM8-C26-C27-C28
9	BH	102	BCL	C12-C13-C15-C16
9	BK	101	BCL	C6-C7-C8-C10
9	bc	101	BCL	C2-C3-C5-C6
9	bh	102	BCL	C12-C13-C15-C16
9	bk	101	BCL	C6-C7-C8-C10
11	ac	101	3PE	C3A-C3B-C3C-C3D
9	BL	102	BCL	C2A-CAA-CBA-CGA
9	bl	101	BCL	C2A-CAA-CBA-CGA
10	ad	1002	SP2	O1-C1-C2-C3
10	af	102	SP2	O1-C1-C2-C3
10	af	103	SP2	O1-C1-C2-C3
10	aj	103	SP2	O1-C1-C2-C3
12	H	302	CD4	C32-C33-C34-O14
12	h	302	CD4	C32-C33-C34-O14
12	m	1005	CD4	C6-C7-C8-C9
16	L	306	SQD	O6-C44-C45-O47
12	M	1004	CD4	C6-C7-C8-C9
9	BC	101	BCL	C2-C3-C5-C6
10	AM	1000	SP2	C21-C22-C23-C24
9	ak	101	BCL	C11-C10-C8-C9
9	AI	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	bn	101	BCL	C3-C5-C6-C7
14	L	303	U10	C49-C51-C52-C53
9	BA	102	BCL	C2A-CAA-CBA-CGA
9	ba	102	BCL	C2A-CAA-CBA-CGA
10	ah	102	SP2	C7-C8-C9-CM4
9	BN	101	BCL	C3-C5-C6-C7
10	BJ	101	SP2	C2-C3-C4-C5
14	L	303	U10	C5-C4-O4-C4M
14	l	303	U10	C5-C4-O4-C4M
10	BJ	101	SP2	CM7-C22-C23-C24
16	L	306	SQD	C12-C13-C14-C15
10	ae	103	SP2	C25-C26-C27-C28
10	aj	102	SP2	C21-C22-C23-C24
12	H	302	CD4	C16-C15-O2-C14
12	h	302	CD4	C16-C15-O2-C14
9	bb	1001	BCL	C2A-CAA-CBA-CGA
9	AH	101	BCL	C2-C1-O2A-CGA
9	BB	1001	BCL	C2-C1-O2A-CGA
9	BN	101	BCL	C2-C1-O2A-CGA
9	af	101	BCL	C2-C1-O2A-CGA
9	bb	1001	BCL	C2-C1-O2A-CGA
9	bn	101	BCL	C2-C1-O2A-CGA
9	M	1008	BCL	CAA-CBA-CGA-O2A
10	bj	101	SP2	CM8-C26-C27-C28
10	BE	1002	SP2	C25-C26-C27-C28
10	am	1000	SP2	C21-C22-C23-C24
10	AB	103	SP2	CM1-C1-O1-CMA
14	L	303	U10	C29-C31-C32-C33
14	l	303	U10	C29-C31-C32-C33
14	l	303	U10	C49-C51-C52-C53
10	bj	101	SP2	CM7-C22-C23-C24
9	BM	1001	BCL	C11-C10-C8-C7
9	aj	101	BCL	C11-C10-C8-C7
9	bm	1001	BCL	C11-C10-C8-C7
10	BK	102	SP2	C25-C26-C27-C28
10	bk	102	SP2	C25-C26-C27-C28
9	m	1004	BCL	CAA-CBA-CGA-O2A
9	BK	101	BCL	C6-C7-C8-C9
9	bk	101	BCL	C6-C7-C8-C9
10	AJ	103	SP2	C27-C28-C29-C30
9	BB	1001	BCL	C2A-CAA-CBA-CGA
9	ai	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	ai	101	SP2	C1-C2-C3-C4
10	m	1007	SP2	C1-C2-C3-C4
10	BH	101	SP2	C11-C12-C13-CM5
16	x	100	SQD	C13-C14-C15-C16
10	ae	103	SP2	C7-C8-C9-C10
10	AA	1002	SP2	C3-C4-C5-CM3
10	ba	101	SP2	CM8-C26-C27-C28
9	be	1001	BCL	C2-C3-C5-C6
11	H	301	3PE	C3D-C3E-C3F-C3G
11	h	301	3PE	C3D-C3E-C3F-C3G
12	m	1005	CD4	C18-C19-C20-C21
16	x	100	SQD	C17-C18-C19-C20
12	H	302	CD4	C40-C41-C42-C43
12	M	1004	CD4	C18-C19-C20-C21
12	h	302	CD4	C40-C41-C42-C43
15	L	305	BPH	C8-C10-C11-C12
15	l	302	BPH	C8-C10-C11-C12
10	bk	102	SP2	C9-C10-C11-C12
14	M	1007	U10	C39-C41-C42-C43
14	m	1003	U10	C39-C41-C42-C43
10	BJ	101	SP2	CM8-C26-C27-C28
9	BE	1001	BCL	C2-C3-C5-C6
9	AC	101	BCL	C2A-CAA-CBA-CGA
9	AI	102	BCL	C2A-CAA-CBA-CGA
9	BG	101	BCL	C2A-CAA-CBA-CGA
9	ac	102	BCL	C2A-CAA-CBA-CGA
9	bg	101	BCL	C2A-CAA-CBA-CGA
12	M	1004	CD4	C33-C32-O13-P2
12	m	1005	CD4	C33-C32-O13-P2
10	bb	1002	SP2	C1-C2-C3-C4
10	bk	102	SP2	C1-C2-C3-C4
10	ab	104	SP2	CM7-C22-C23-C24
10	AJ	102	SP2	C21-C22-C23-C24
9	bl	101	BCL	C11-C10-C8-C9
12	M	1004	CD4	C28-C15-C16-O3
12	m	1005	CD4	C28-C15-C16-O3
11	ac	101	3PE	C33-C34-C35-C36
9	AI	102	BCL	C16-C17-C18-C19
15	L	305	BPH	O2A-C1-C2-C3
15	l	302	BPH	O2A-C1-C2-C3
11	ac	101	3PE	C26-C27-C28-C29
10	AH	102	SP2	C7-C8-C9-CM4

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Mol	Chain	Res	Type	Atoms
10	AK	102	SP2	C11-C12-C13-CM5
10	ak	102	SP2	C11-C12-C13-CM5
9	AA	1001	BCL	C15-C16-C17-C18
10	AB	103	SP2	CM7-C22-C23-C24
10	BA	101	SP2	CM8-C26-C27-C28
10	aj	103	SP2	C3-C4-C5-CM3
9	BE	1001	BCL	C1A-C2A-CAA-CBA
9	BG	101	BCL	C1A-C2A-CAA-CBA
9	BI	101	BCL	C1A-C2A-CAA-CBA
9	be	1001	BCL	C1A-C2A-CAA-CBA
9	bg	101	BCL	C1A-C2A-CAA-CBA
9	AN	101	BCL	C11-C12-C13-C15
9	an	101	BCL	C11-C12-C13-C15
11	AC	102	3PE	C26-C27-C28-C29
9	aa	1001	BCL	C15-C16-C17-C18
14	L	303	U10	C3-C4-O4-C4M
14	l	303	U10	C3-C4-O4-C4M
13	L	302	UQ1	C6-C7-C8-C9
13	l	304	UQ1	C6-C7-C8-C9
9	AN	101	BCL	C15-C16-C17-C18
9	ai	102	BCL	C16-C17-C18-C19
9	an	101	BCL	C15-C16-C17-C18
12	H	302	CD4	C18-C19-C20-C21
10	AC	104	SP2	CM7-C22-C23-C24
10	AF	101	SP2	C3-C4-C5-CM3
14	L	303	U10	C25-C24-C26-C27
14	l	303	U10	C25-C24-C26-C27
10	AJ	102	SP2	C1-C2-C3-C4
12	h	302	CD4	C18-C19-C20-C21
16	L	306	SQD	C11-C12-C13-C14
9	ai	102	BCL	C3-C5-C6-C7
10	BH	101	SP2	C3-C4-C5-CM3
10	ac	104	SP2	CM7-C22-C23-C24
14	L	303	U10	C12-C11-C9-C10
14	l	303	U10	C12-C11-C9-C10
10	BA	101	SP2	C25-C26-C27-C28
10	ab	104	SP2	C21-C22-C23-C24
9	BL	102	BCL	C11-C10-C8-C9
11	H	301	3PE	C37-C38-C39-C3A
9	AN	101	BCL	C5-C6-C7-C8
11	h	301	3PE	C37-C38-C39-C3A
10	BH	101	SP2	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	BH	101	SP2	C9-C10-C11-C12
10	BK	102	SP2	C9-C10-C11-C12
16	L	306	SQD	C26-C27-C28-C29
9	af	101	BCL	C4-C3-C5-C6
10	AF	103	SP2	CM8-C26-C27-C28
10	AK	102	SP2	CM7-C22-C23-C24
10	BJ	101	SP2	C3-C4-C5-CM3
10	ad	1002	SP2	CM7-C22-C23-C24
10	ak	102	SP2	CM7-C22-C23-C24
10	ak	102	SP2	CM8-C26-C27-C28
9	ab	102	BCL	C4C-C3C-CAC-CBC
10	ab	104	SP2	C11-C12-C13-C14
9	AI	102	BCL	C16-C17-C18-C20
10	AC	103	SP2	C21-C22-C23-C24
10	BJ	101	SP2	C21-C22-C23-C24
10	aj	103	SP2	C3-C4-C5-C6
10	ba	101	SP2	C25-C26-C27-C28
10	bj	101	SP2	C21-C22-C23-C24
11	AC	102	3PE	C33-C34-C35-C36
9	an	101	BCL	C3-C5-C6-C7
9	AF	102	BCL	C4-C3-C5-C6
10	AK	102	SP2	CM8-C26-C27-C28
10	af	104	SP2	CM8-C26-C27-C28
10	AB	103	SP2	C2-C1-O1-CMA
9	ak	101	BCL	C11-C10-C8-C7
10	AK	102	SP2	C25-C26-C27-C28
10	ac	104	SP2	C21-C22-C23-C24
10	ak	102	SP2	C25-C26-C27-C28
9	ae	101	BCL	C8-C10-C11-C12
16	L	306	SQD	C9-C10-C11-C12
10	bh	101	SP2	C5-C6-C7-C8
9	af	101	BCL	CAA-CBA-CGA-O2A
11	AC	102	3PE	O31-C31-C32-C33
10	AA	1002	SP2	C23-C24-C25-C26
11	ac	101	3PE	O31-C31-C32-C33
9	M	1002	BCL	C4-C3-C5-C6
9	m	1006	BCL	C4-C3-C5-C6
10	BL	101	SP2	C3-C4-C5-CM3
10	ab	101	SP2	C3-C4-C5-CM3
10	ah	102	SP2	CM7-C22-C23-C24
10	al	1002	SP2	C3-C4-C5-CM3
10	AB	103	SP2	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
10	AF	101	SP2	C3-C4-C5-C6
10	AF	103	SP2	C25-C26-C27-C28
10	bj	101	SP2	C25-C26-C27-C28
14	L	303	U10	C23-C24-C26-C27
14	l	303	U10	C23-C24-C26-C27
9	ai	102	BCL	C16-C17-C18-C20
12	m	1005	CD4	C3-C4-C5-C6
12	M	1004	CD4	C3-C4-C5-C6
9	BG	101	BCL	C3A-C2A-CAA-CBA
9	BI	101	BCL	C3A-C2A-CAA-CBA
9	bg	101	BCL	C3A-C2A-CAA-CBA
9	bi	101	BCL	C3A-C2A-CAA-CBA
10	AB	103	SP2	C1-C2-C3-C4
10	AE	101	SP2	C1-C2-C3-C4
10	AG	101	SP2	C1-C2-C3-C4
10	af	103	SP2	C1-C2-C3-C4
10	ba	101	SP2	C1-C2-C3-C4
9	L	301	BCL	CAD-CBD-CGD-O2D
9	l	305	BCL	CAD-CBD-CGD-O2D
11	AC	102	3PE	C1-C2-O21-C21
11	ac	101	3PE	C1-C2-O21-C21
15	M	1003	BPH	CAD-CBD-CGD-O2D
15	m	1002	BPH	CAD-CBD-CGD-O2D
9	AB	101	BCL	C2A-CAA-CBA-CGA
10	AB	103	SP2	C2-C3-C4-C5
10	AE	101	SP2	CM7-C22-C23-C24
10	AH	102	SP2	CM7-C22-C23-C24
10	BC	102	SP2	CM7-C22-C23-C24
10	ae	102	SP2	CM7-C22-C23-C24
10	af	102	SP2	C3-C4-C5-CM3
10	ah	102	SP2	C3-C4-C5-CM3
10	aj	103	SP2	CM7-C22-C23-C24
12	H	302	CD4	C53-C54-C55-C56
10	AA	1002	SP2	C3-C4-C5-C6
10	AC	104	SP2	C21-C22-C23-C24
10	BH	101	SP2	C3-C4-C5-C6
10	ak	102	SP2	C21-C22-C23-C24
14	L	303	U10	C12-C11-C9-C8
14	l	303	U10	C12-C11-C9-C8
9	AC	101	BCL	CAA-CBA-CGA-O2A
9	ac	102	BCL	CAA-CBA-CGA-O2A
11	AC	102	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
10	AB	102	SP2	C7-C8-C9-C10
10	BE	1002	SP2	C7-C8-C9-C10
10	ab	103	SP2	C7-C8-C9-C10
10	af	104	SP2	C11-C12-C13-C14
10	bk	102	SP2	C11-C12-C13-C14
14	M	1007	U10	C5-C4-O4-C4M
14	m	1003	U10	C5-C4-O4-C4M
10	AB	104	SP2	C26-C27-C28-C29
10	AC	104	SP2	C22-C23-C24-C25
10	bb	1002	SP2	C26-C27-C28-C29
11	H	301	3PE	C3F-C3G-C3H-C3I
12	h	302	CD4	C53-C54-C55-C56
11	AC	102	3PE	C1-C2-C3-O31
11	ac	101	3PE	C1-C2-C3-O31
10	ab	101	SP2	C23-C24-C25-C26
9	an	101	BCL	C5-C6-C7-C8
9	AF	102	BCL	CAA-CBA-CGA-O2A
11	ac	101	3PE	O21-C21-C22-C23
9	BF	101	BCL	O2A-C1-C2-C3
9	BI	101	BCL	O2A-C1-C2-C3
9	bf	101	BCL	O2A-C1-C2-C3
9	bi	101	BCL	O2A-C1-C2-C3
15	M	1003	BPH	O2A-C1-C2-C3
15	m	1002	BPH	O2A-C1-C2-C3
11	h	301	3PE	C3F-C3G-C3H-C3I
12	H	302	CD4	C48-C49-C50-C51
9	AB	101	BCL	CHA-CBD-CGD-O1D
9	AE	102	BCL	CHA-CBD-CGD-O1D
9	AE	102	BCL	CHA-CBD-CGD-O2D
9	AH	101	BCL	CHA-CBD-CGD-O1D
9	AH	101	BCL	CHA-CBD-CGD-O2D
9	AI	102	BCL	CHA-CBD-CGD-O1D
9	AI	102	BCL	CHA-CBD-CGD-O2D
9	AJ	101	BCL	CHA-CBD-CGD-O2D
9	ab	102	BCL	CHA-CBD-CGD-O1D
9	ae	101	BCL	CHA-CBD-CGD-O1D
9	ae	101	BCL	CHA-CBD-CGD-O2D
9	ah	101	BCL	CHA-CBD-CGD-O1D
9	ah	101	BCL	CHA-CBD-CGD-O2D
9	ai	102	BCL	CHA-CBD-CGD-O1D
9	ai	102	BCL	CHA-CBD-CGD-O2D
9	aj	101	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	bf	101	BCL	CHA-CBD-CGD-O2D
10	bb	1002	SP2	C5-C6-C7-C8
10	AH	102	SP2	C3-C4-C5-CM3
10	AK	102	SP2	C21-C22-C23-C24
12	h	302	CD4	C48-C49-C50-C51
14	m	1003	U10	C36-C37-C38-C39
10	AB	103	SP2	CM2-C1-O1-CMA
16	L	306	SQD	C29-C30-C31-C32
9	AE	102	BCL	C8-C10-C11-C12
15	l	302	BPH	CHA-CBD-CGD-O2D
10	AI	103	SP2	C23-C24-C25-C26
14	M	1007	U10	C36-C37-C38-C39
16	x	100	SQD	C26-C27-C28-C29
9	AF	102	BCL	C2-C3-C5-C6
9	af	101	BCL	C2-C3-C5-C6
9	bn	101	BCL	C11-C12-C13-C15
10	AH	102	SP2	C21-C22-C23-C24
10	BJ	101	SP2	C25-C26-C27-C28
10	BL	101	SP2	C3-C4-C5-C6
10	af	102	SP2	C3-C4-C5-C6
10	ah	102	SP2	C21-C22-C23-C24
10	aj	103	SP2	C21-C22-C23-C24
9	BH	102	BCL	C14-C13-C15-C16
9	BK	101	BCL	C11-C10-C8-C9
9	BN	101	BCL	C11-C12-C13-C14
9	bh	102	BCL	C14-C13-C15-C16
9	bk	101	BCL	C11-C10-C8-C9
9	bn	101	BCL	C11-C12-C13-C14
14	M	1007	U10	C3-C4-O4-C4M
14	m	1003	U10	C3-C4-O4-C4M
13	L	302	UQ1	C1-C2-O2-CM2
13	l	304	UQ1	C1-C2-O2-CM2
10	ai	103	SP2	C23-C24-C25-C26
14	M	1007	U10	C16-C17-C18-C19
14	m	1003	U10	C16-C17-C18-C19
10	BE	1002	SP2	C7-C8-C9-CM4
9	BN	101	BCL	C5-C6-C7-C8
10	AF	103	SP2	C11-C12-C13-C14
10	m	1007	SP2	C11-C12-C13-C14
9	BC	101	BCL	C1A-C2A-CAA-CBA
9	BM	1001	BCL	C1A-C2A-CAA-CBA
9	bc	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	bm	1001	BCL	C1A-C2A-CAA-CBA
9	AC	101	BCL	CAA-CBA-CGA-O1A
12	H	302	CD4	C54-C55-C56-C57
12	h	302	CD4	C54-C55-C56-C57
10	AF	101	SP2	C27-C28-C29-C30
10	af	102	SP2	C27-C28-C29-C30
11	ac	101	3PE	O32-C31-C32-C33
9	bn	101	BCL	C5-C6-C7-C8
9	be	1001	BCL	C2A-CAA-CBA-CGA
9	bm	1001	BCL	C2A-CAA-CBA-CGA
10	AM	1000	SP2	C1-C2-C3-C4
9	BF	101	BCL	CAA-CBA-CGA-O2A
9	bf	101	BCL	CAA-CBA-CGA-O2A
9	bm	1001	BCL	CAA-CBA-CGA-O2A
9	bm	1001	BCL	CAA-CBA-CGA-O1A
15	l	302	BPH	C2-C3-C5-C6
9	m	1006	BCL	C10-C11-C12-C13
9	AF	102	BCL	CAA-CBA-CGA-O1A
11	AC	102	3PE	O22-C21-C22-C23
10	ac	104	SP2	C22-C23-C24-C25
16	x	100	SQD	C29-C30-C31-C32
9	M	1002	BCL	C10-C11-C12-C13
11	AC	102	3PE	O32-C31-C32-C33
16	L	306	SQD	O49-C7-C8-C9
9	BE	1001	BCL	C2A-CAA-CBA-CGA
9	ac	102	BCL	CAA-CBA-CGA-O1A
9	AK	101	BCL	C15-C16-C17-C18
9	bn	101	BCL	CAA-CBA-CGA-O2A
9	BM	1001	BCL	CAA-CBA-CGA-O1A
11	ac	101	3PE	O22-C21-C22-C23
10	ac	103	SP2	C3-C4-C5-CM3
9	AB	101	BCL	CAD-CBD-CGD-O1D
9	AI	102	BCL	CAD-CBD-CGD-O1D
9	ab	102	BCL	CAD-CBD-CGD-O1D
9	ai	102	BCL	CAD-CBD-CGD-O1D
11	ac	101	3PE	C12-C11-O13-P
12	H	302	CD4	C32-C33-O16-C46
12	H	302	CD4	C34-C33-O16-C46
12	h	302	CD4	C32-C33-O16-C46
12	h	302	CD4	C34-C33-O16-C46
9	af	101	BCL	CAA-CBA-CGA-O1A
9	BM	1001	BCL	CAA-CBA-CGA-O2A

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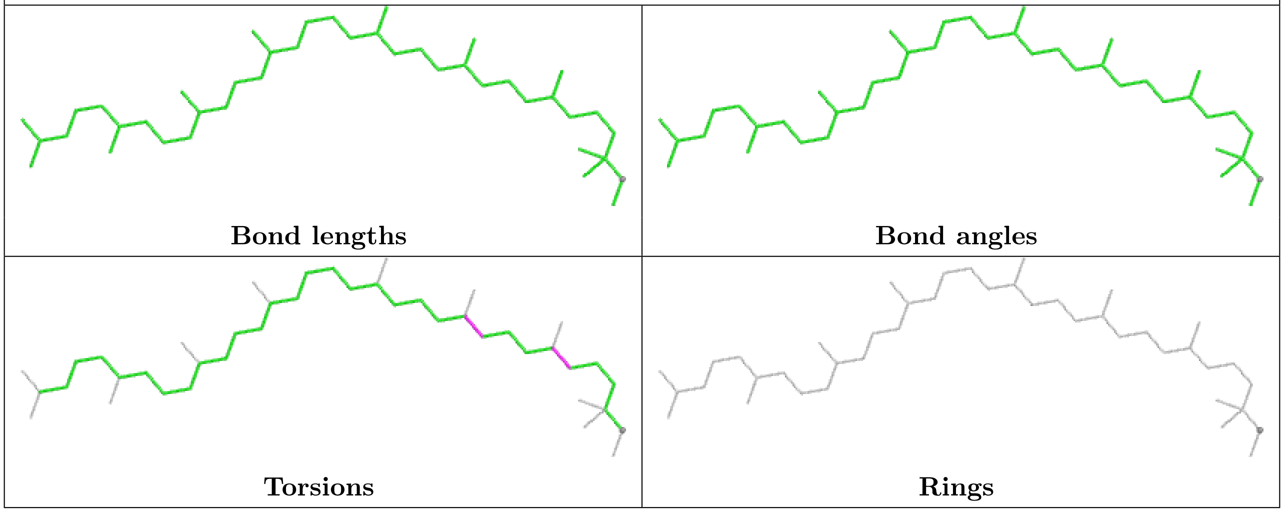
Mol	Chain	Res	Type	Atoms
9	BN	101	BCL	CAA-CBA-CGA-O2A
9	bi	101	BCL	CAA-CBA-CGA-O2A
9	AK	101	BCL	C11-C10-C8-C9
15	L	305	BPH	C11-C10-C8-C9
15	l	302	BPH	C11-C10-C8-C9
9	ab	102	BCL	C8-C10-C11-C12
9	bi	101	BCL	CAA-CBA-CGA-O1A
16	L	306	SQD	C10-C11-C12-C13
11	h	301	3PE	C39-C3A-C3B-C3C
10	AF	101	SP2	CM7-C22-C23-C24
9	BC	101	BCL	C8-C10-C11-C12
10	AC	103	SP2	C7-C8-C9-CM4
11	H	301	3PE	C39-C3A-C3B-C3C
9	BK	101	BCL	C11-C10-C8-C7
9	BN	101	BCL	C11-C12-C13-C15
9	bk	101	BCL	C11-C10-C8-C7
10	BJ	101	SP2	C3-C4-C5-C6
15	L	305	BPH	C2-C3-C5-C6
9	BI	101	BCL	CAA-CBA-CGA-O1A
9	AH	101	BCL	CAA-CBA-CGA-O2A
9	BI	101	BCL	CAA-CBA-CGA-O2A
16	L	306	SQD	O47-C7-C8-C9
9	bc	101	BCL	C8-C10-C11-C12
10	AK	102	SP2	C11-C12-C13-C14
10	BC	102	SP2	C11-C12-C13-C14
10	BE	1002	SP2	C11-C12-C13-C14
10	ad	1002	SP2	C11-C12-C13-C14
10	ae	103	SP2	C11-C12-C13-C14
10	ak	102	SP2	C11-C12-C13-C14
17	M	1001	LMT	C2-C1-O1'-C1'
17	m	1001	LMT	C2-C1-O1'-C1'
9	ak	101	BCL	C15-C16-C17-C18
9	BM	1001	BCL	C2A-CAA-CBA-CGA
9	AL	1001	BCL	C10-C11-C12-C13
15	L	305	BPH	C4-C3-C5-C6
15	l	302	BPH	C4-C3-C5-C6
9	al	1001	BCL	C10-C11-C12-C13

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 then 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.

Ligand SP2 AB 102



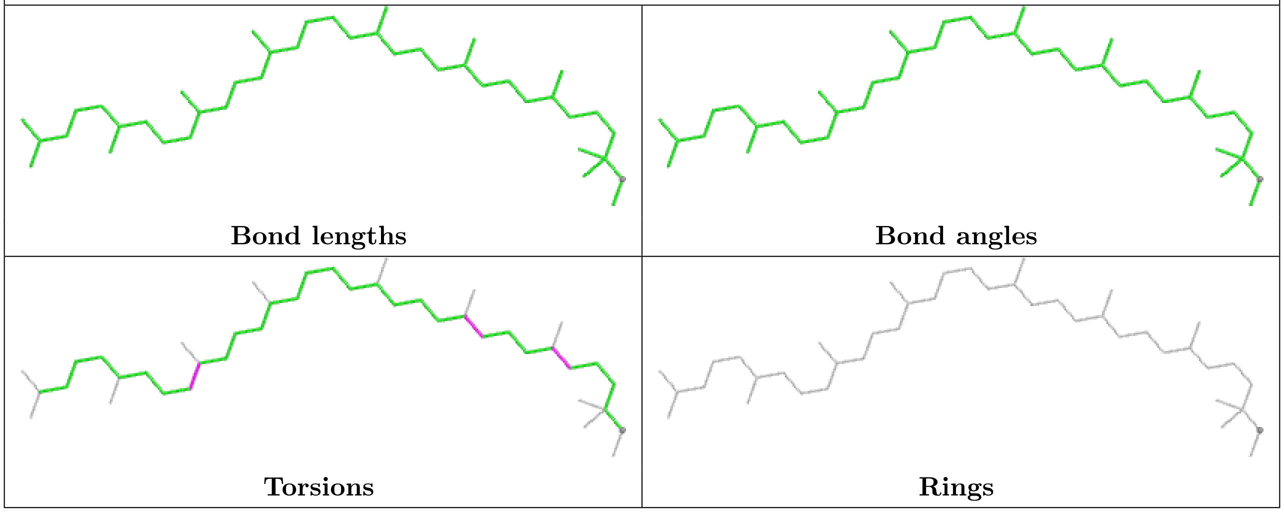
Bond lengths

Bond angles

Torsions

Rings

Ligand SP2 ah 102



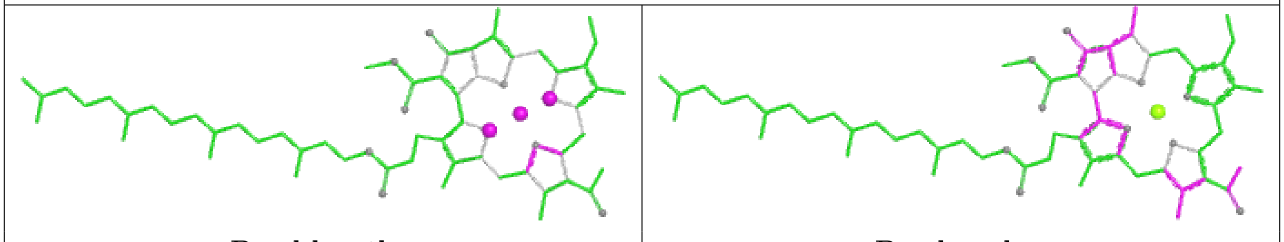
Bond lengths

Bond angles

Torsions

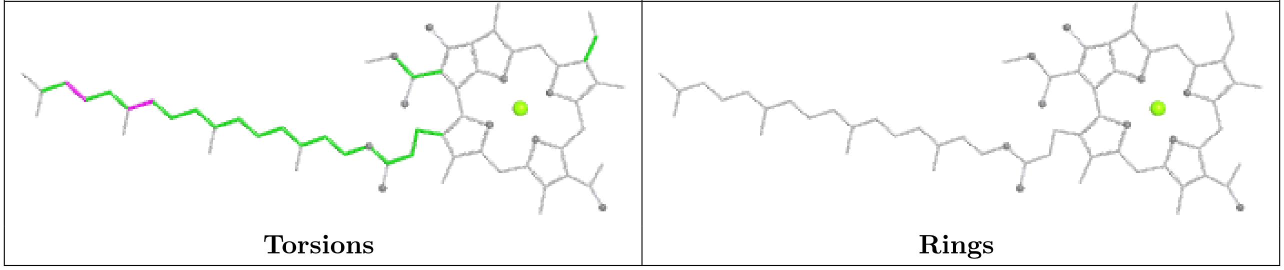
Rings

Ligand BCL AA 1001



Bond lengths

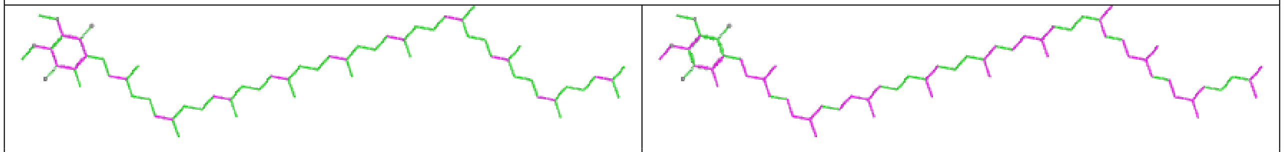
Bond angles



Torsions

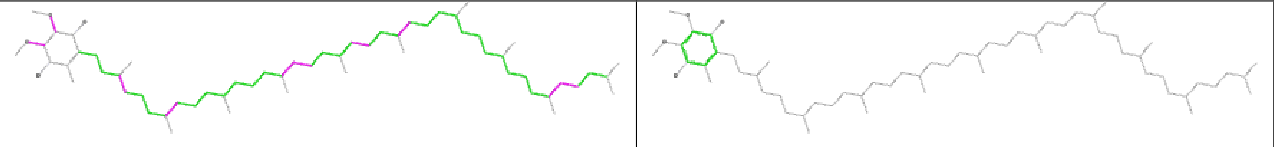
Rings

Ligand U10 l 303



Bond lengths

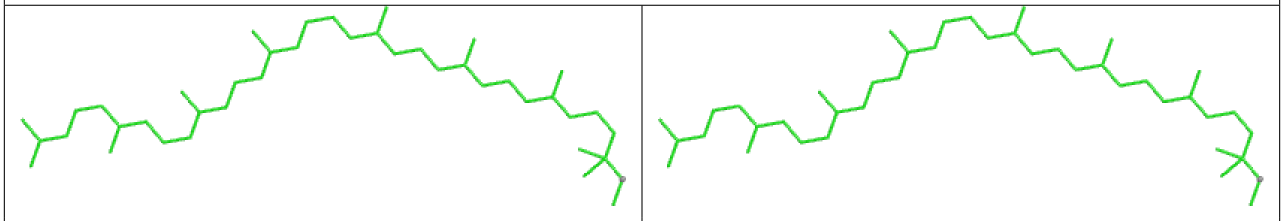
Bond angles



Torsions

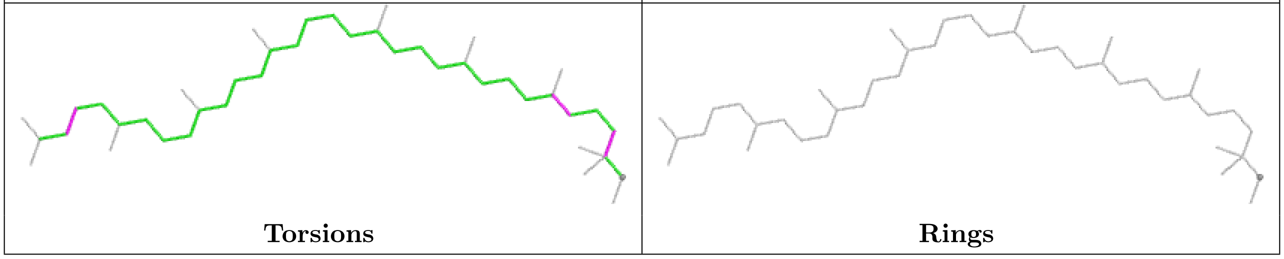
Rings

Ligand SP2 af 102



Bond lengths

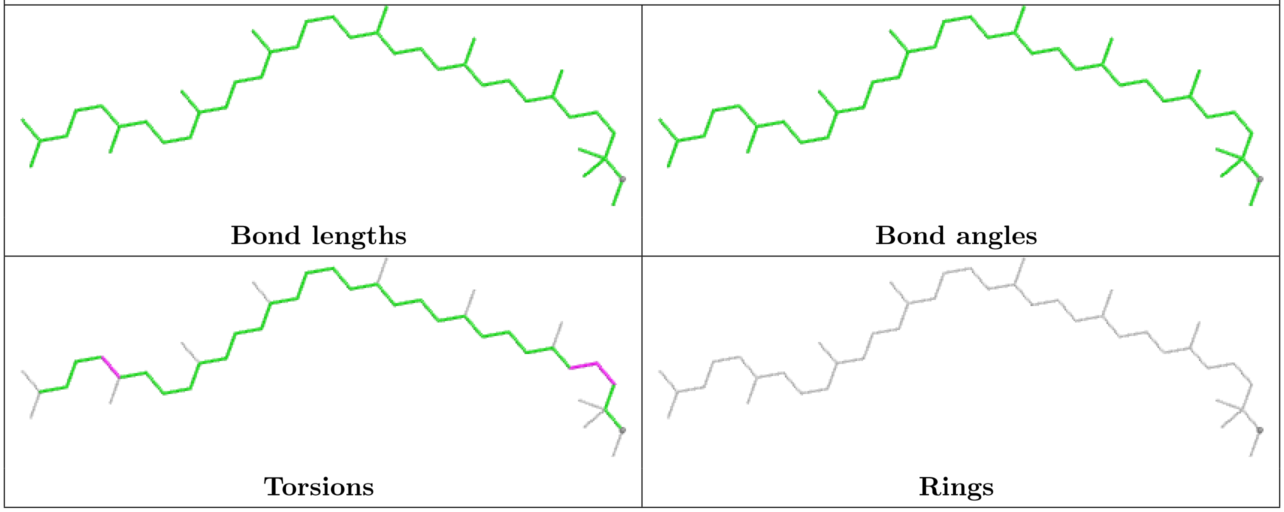
Bond angles



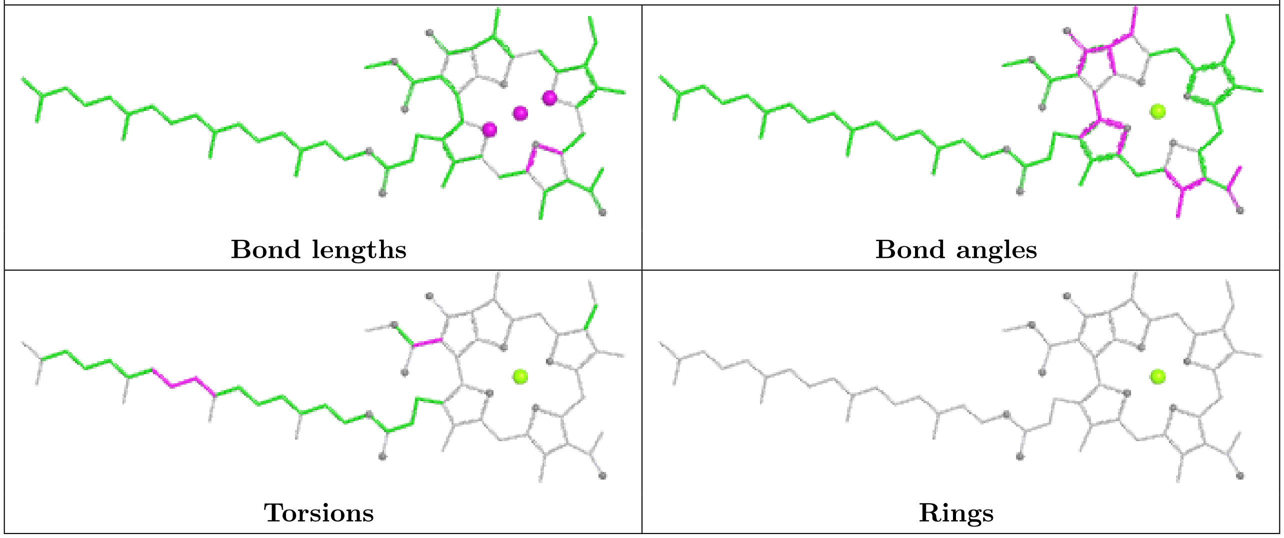
Torsions

Rings

Ligand SP2 AG 101



Ligand BCL ae 101



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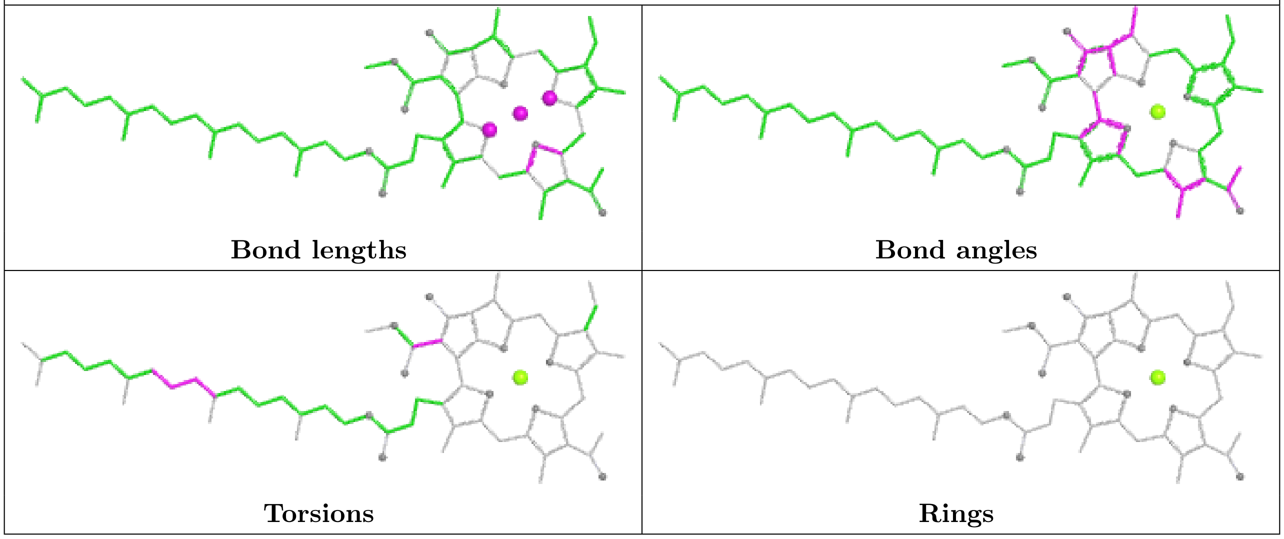
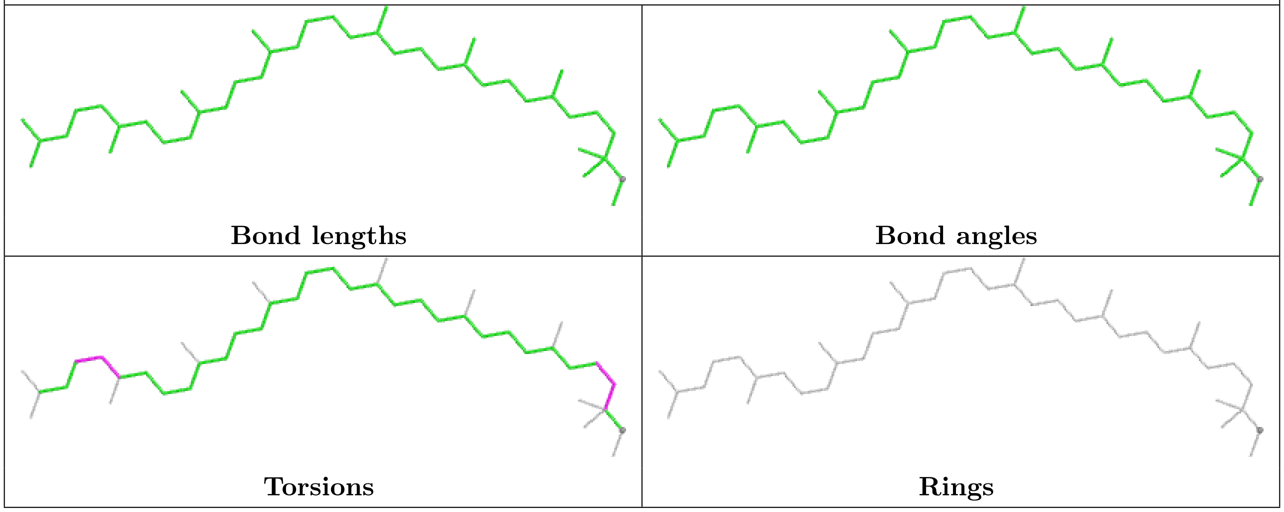


Ligand SP2 ba 101



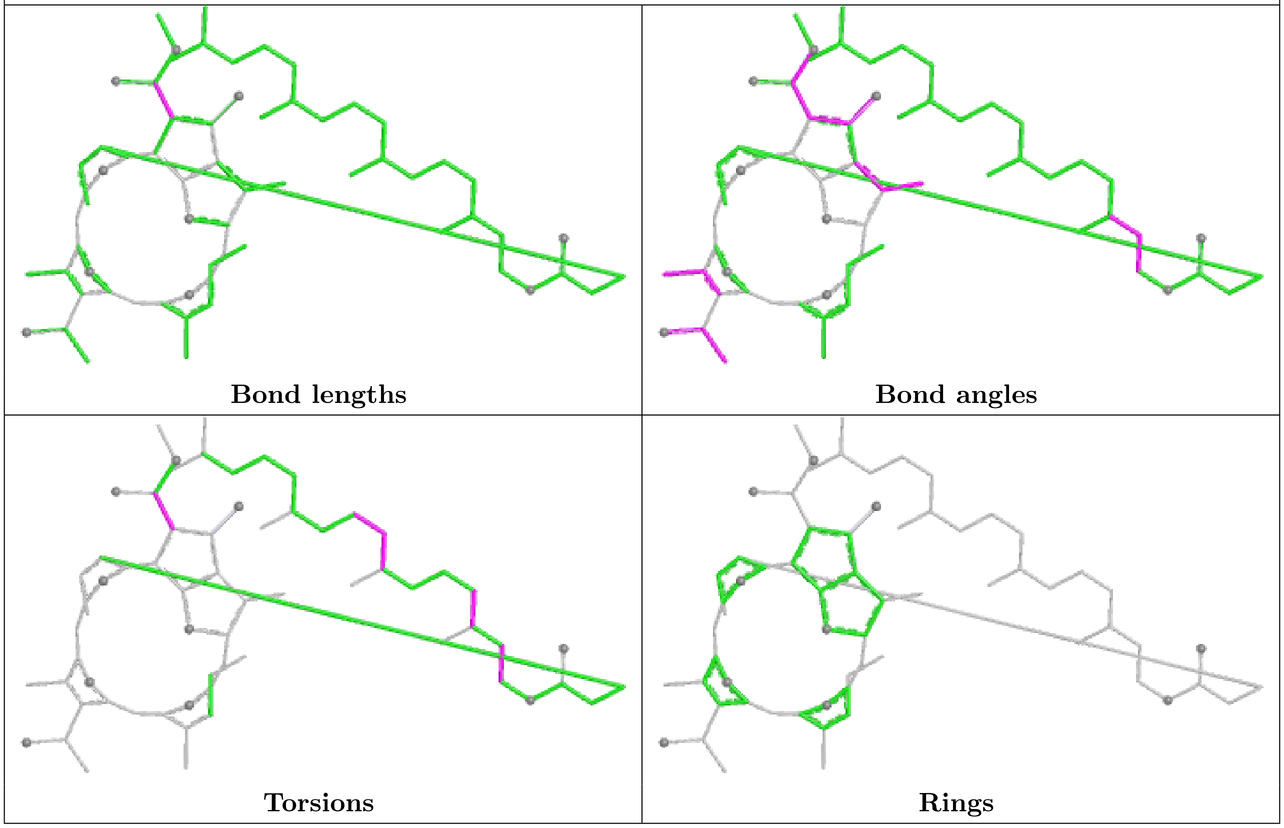
Bond lengths

Bond angles

Torsions

Rings

Ligand BPH L 305



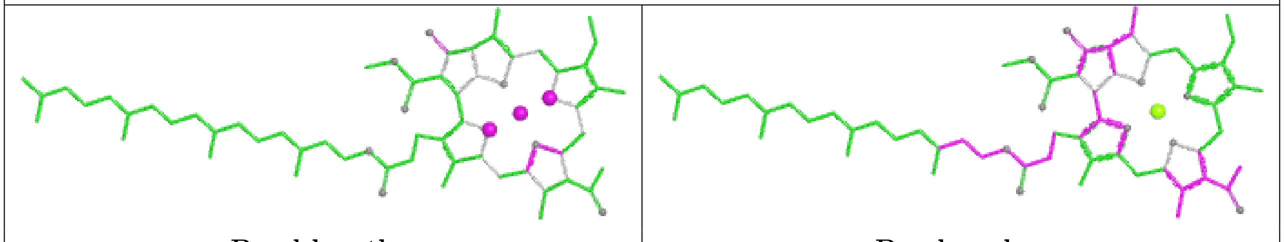
Bond lengths

Bond angles

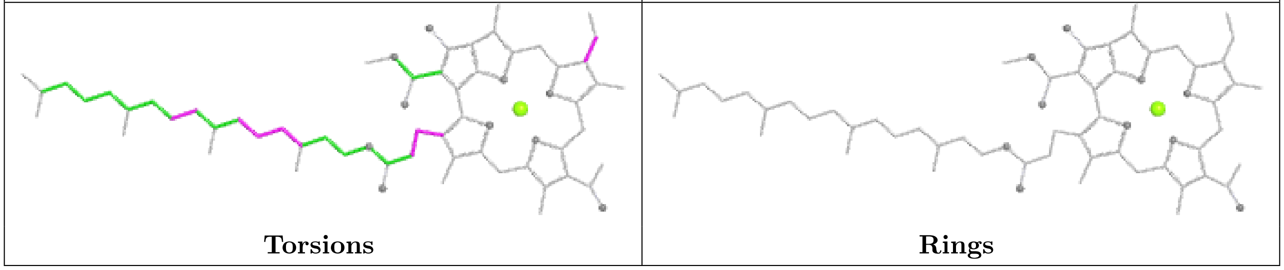
Torsions

Rings

Ligand BCL BC 101

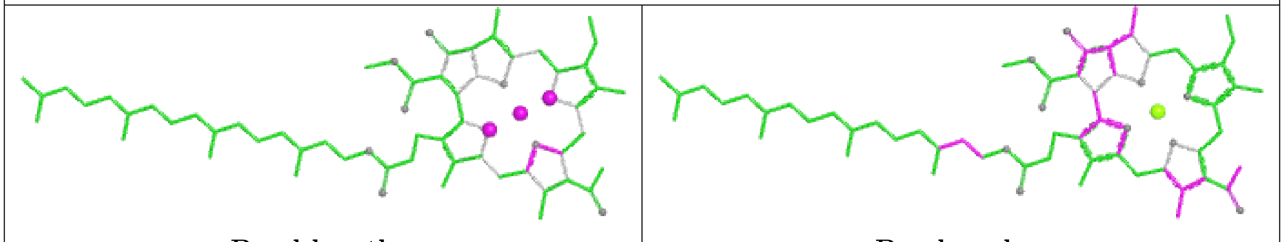


Bond lengths Bond angles

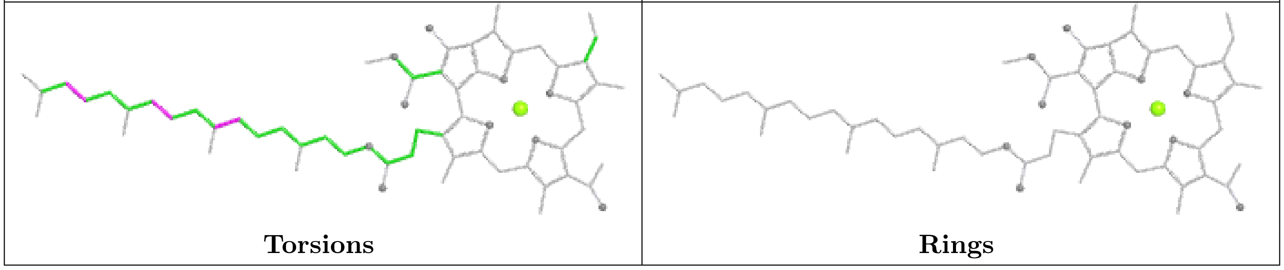


Torsions Rings

Ligand BCL AL 1001

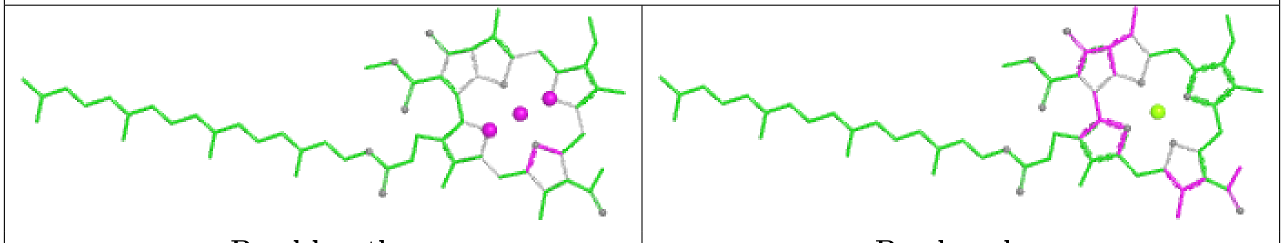


Bond lengths Bond angles

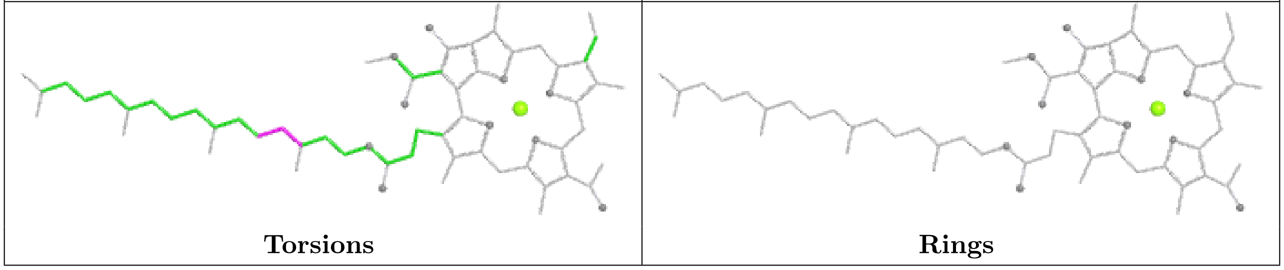


Torsions Rings

Ligand BCL AD 1001

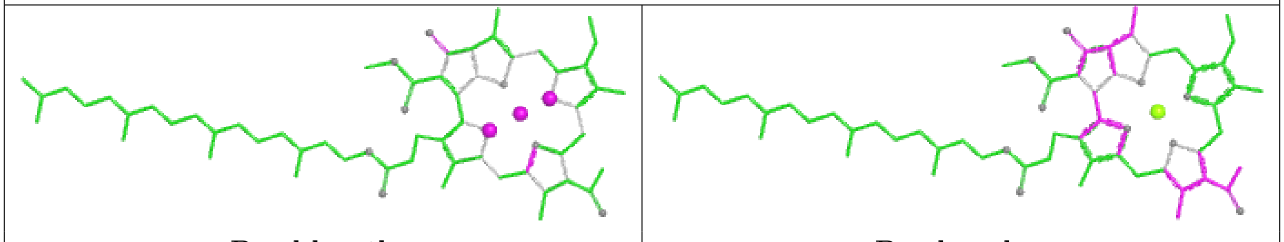


Bond lengths Bond angles

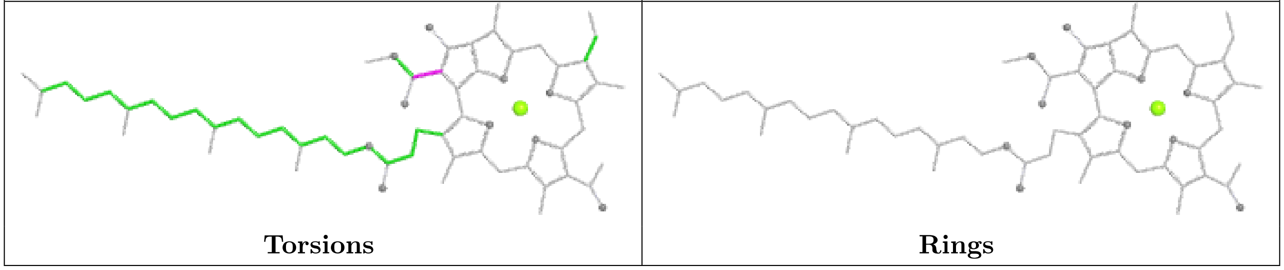


Torsions Rings

Ligand BCL L 304

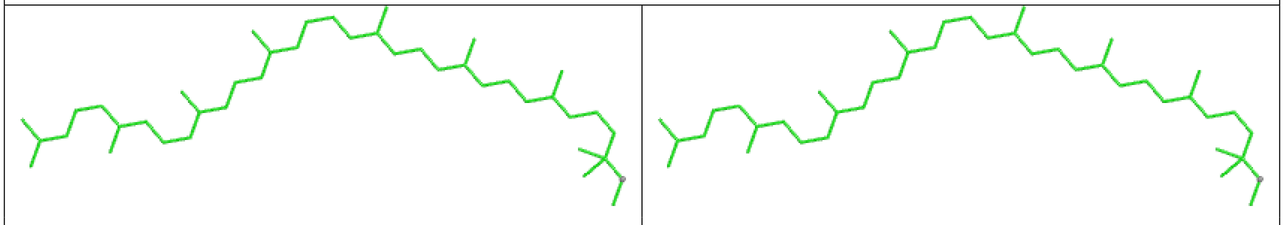


Bond lengths Bond angles

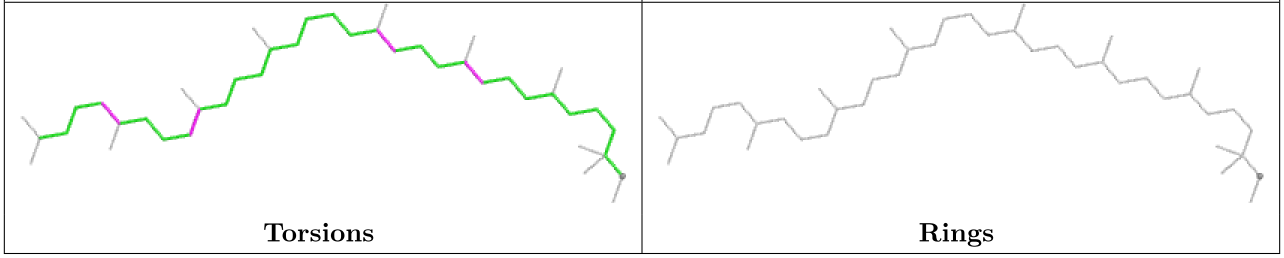


Torsions Rings

Ligand SP2 ak 102

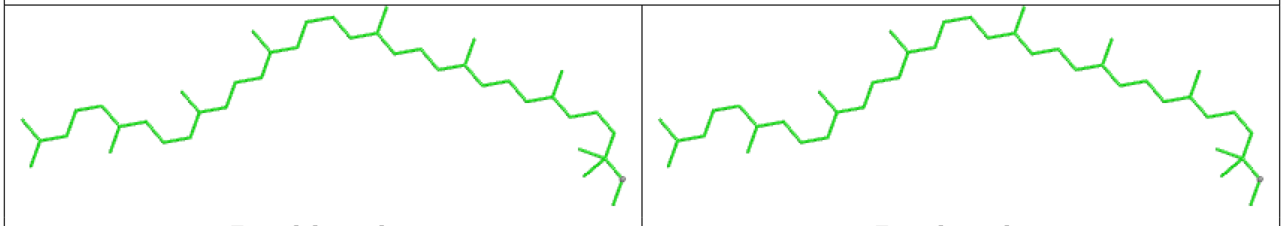


Bond lengths Bond angles

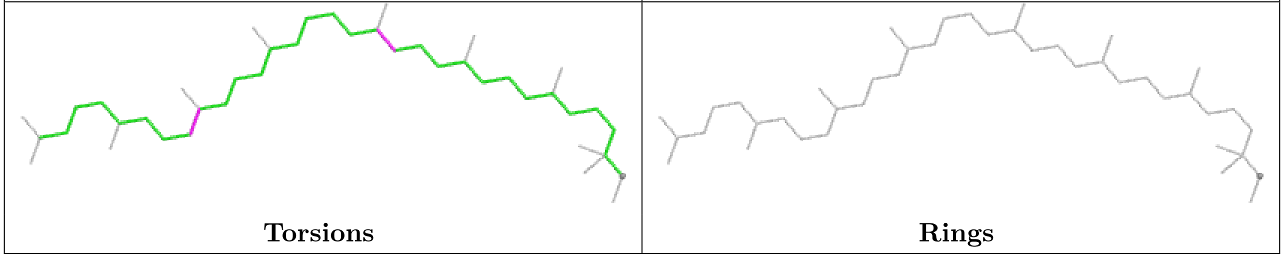


Torsions Rings

Ligand SP2 BC 102

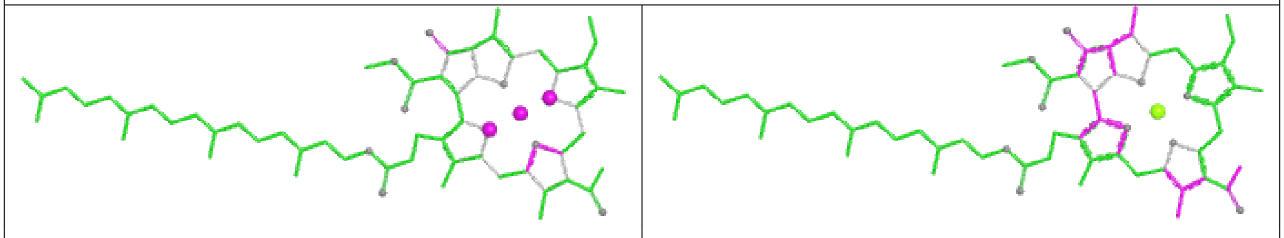


Bond lengths Bond angles

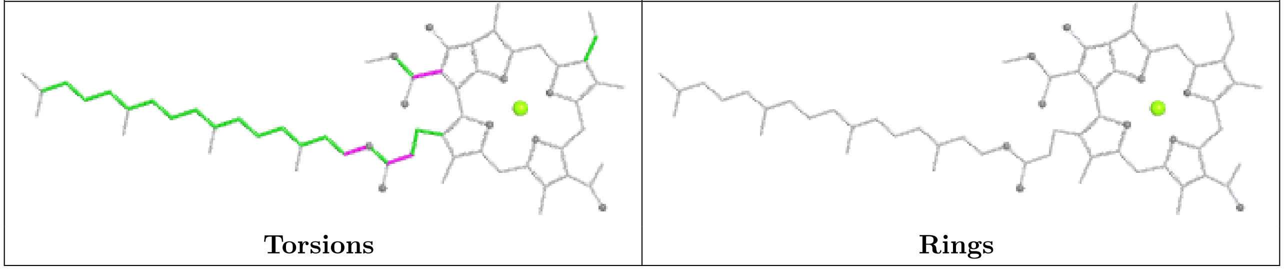


Torsions Rings

Ligand BCL AH 101

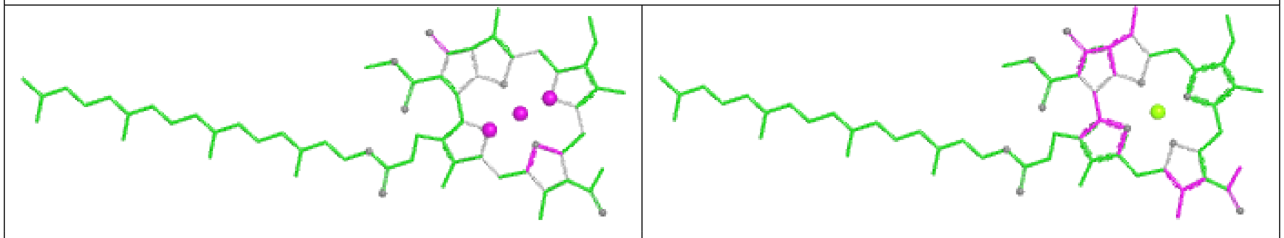


Bond lengths Bond angles

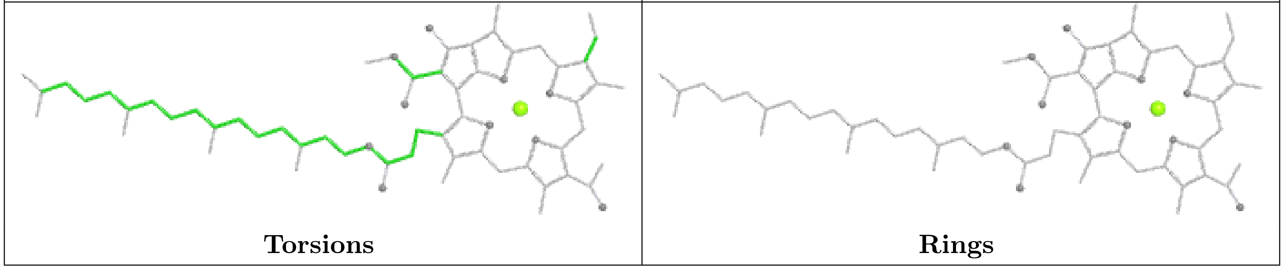


Torsions Rings

Ligand BCL AG 102

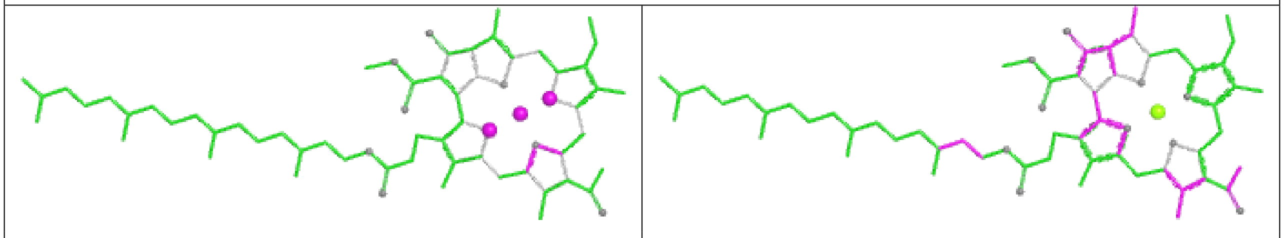


Bond lengths Bond angles

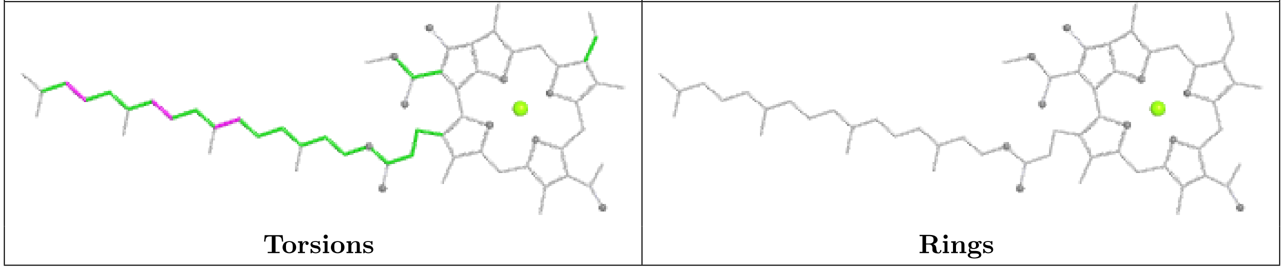


Torsions Rings

Ligand BCL al 1001

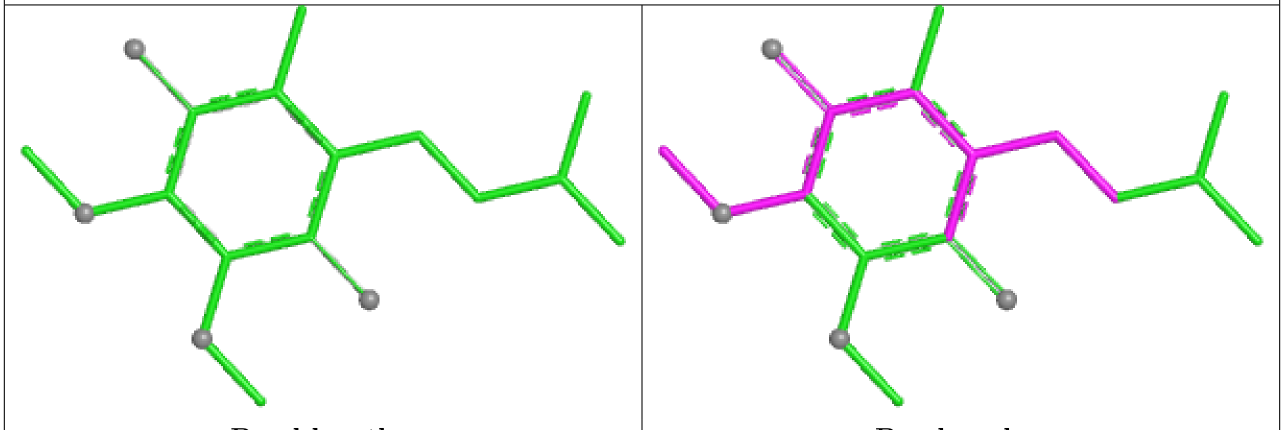


Bond lengths Bond angles



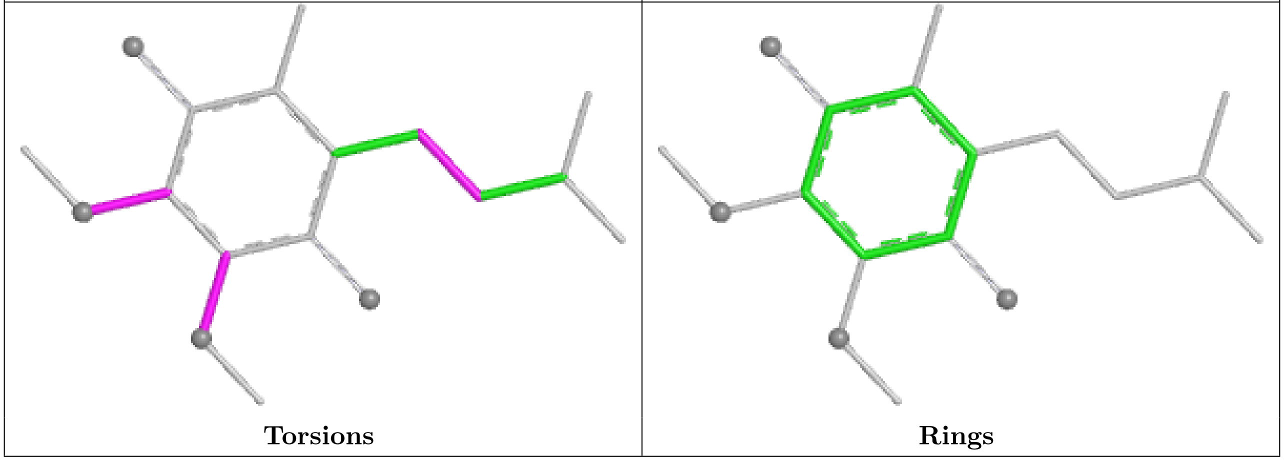
Torsions Rings

Ligand UQ1 L 302



Bond lengths

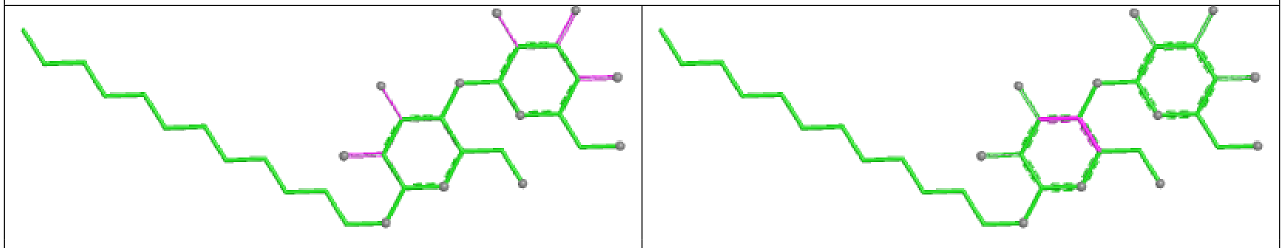
Bond angles



Torsions

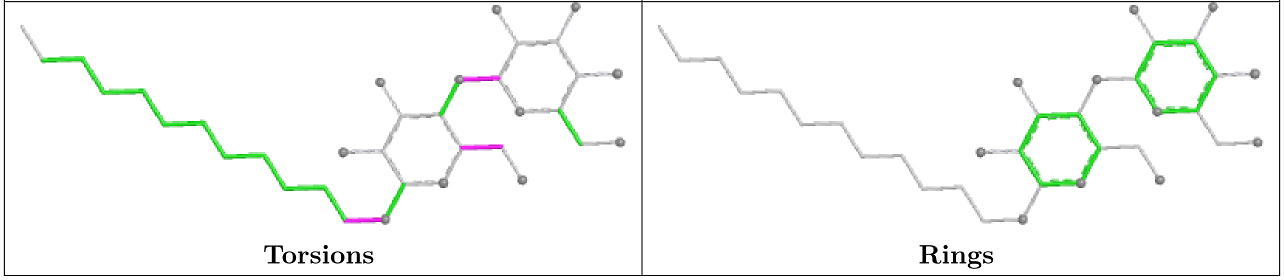
Rings

Ligand LMT M 1001



Bond lengths

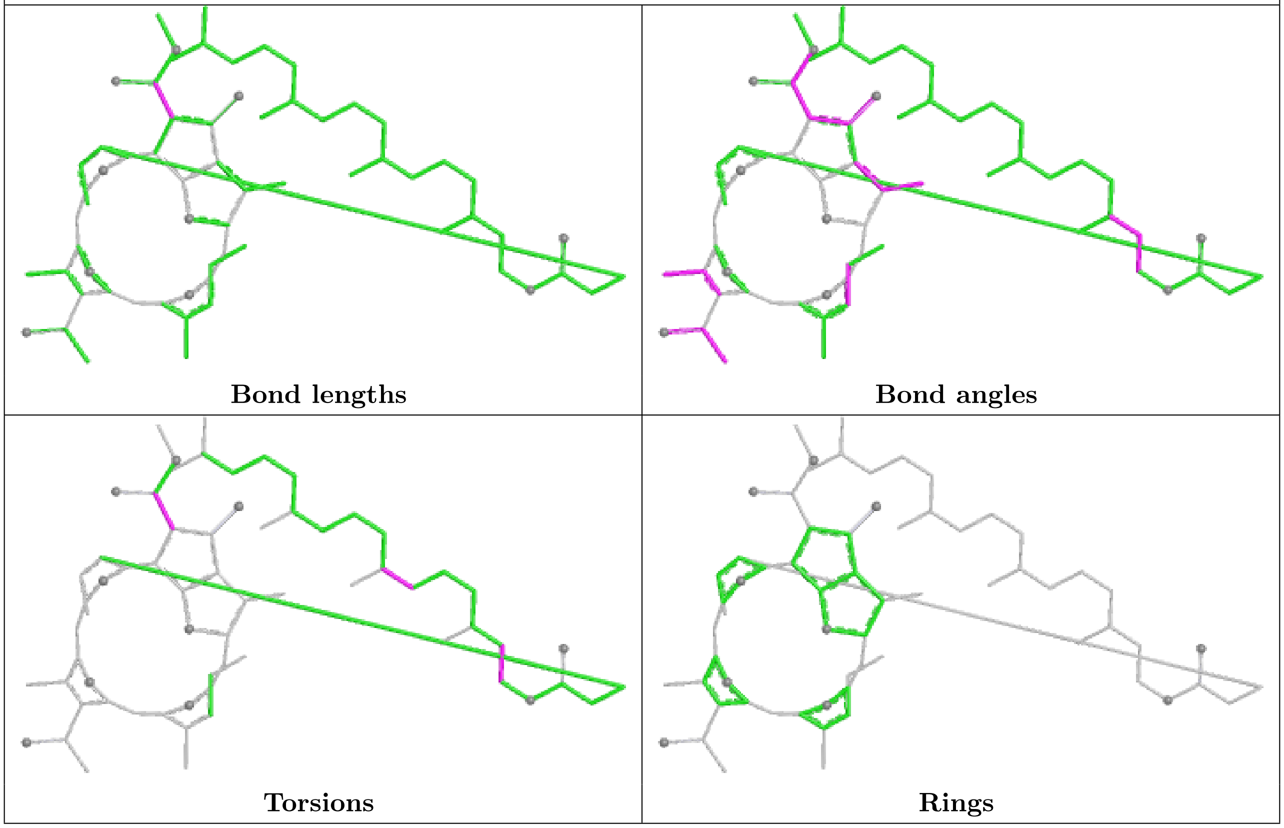
Bond angles



Torsions

Rings

Ligand BPH M 1003



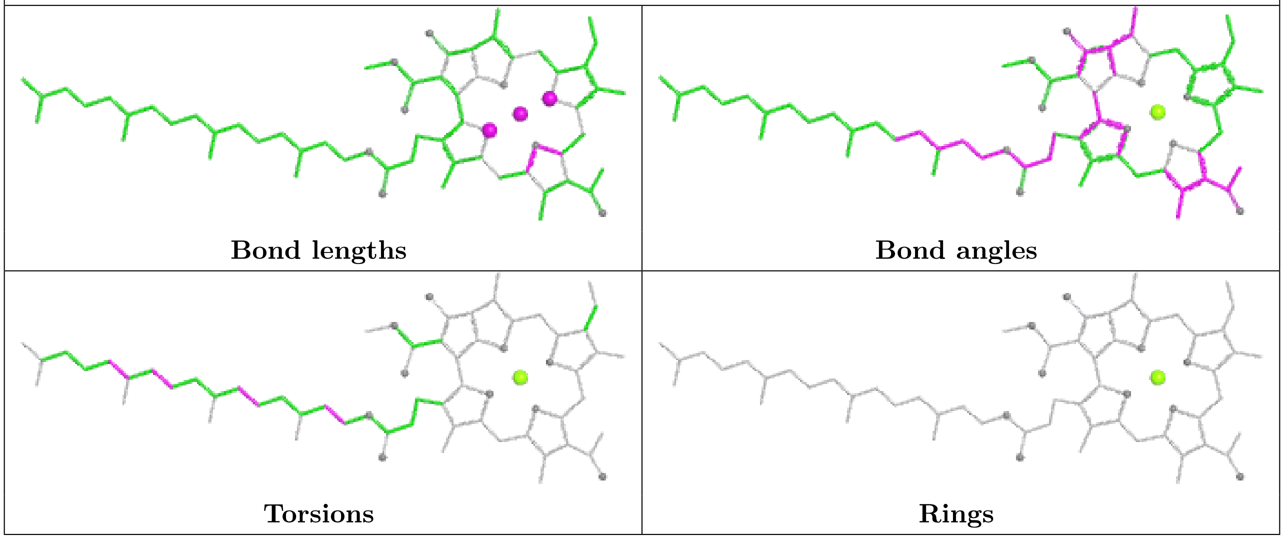
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL BH 102



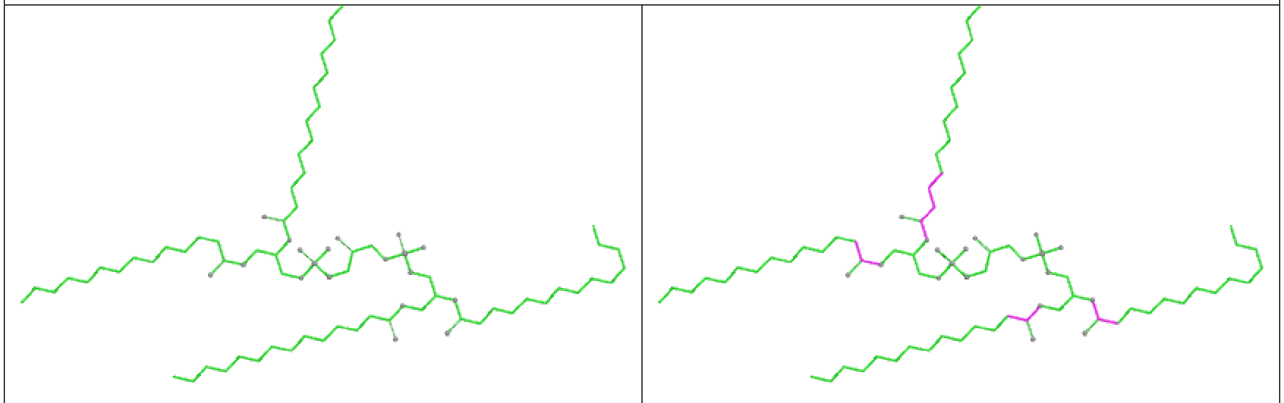
Bond lengths

Bond angles

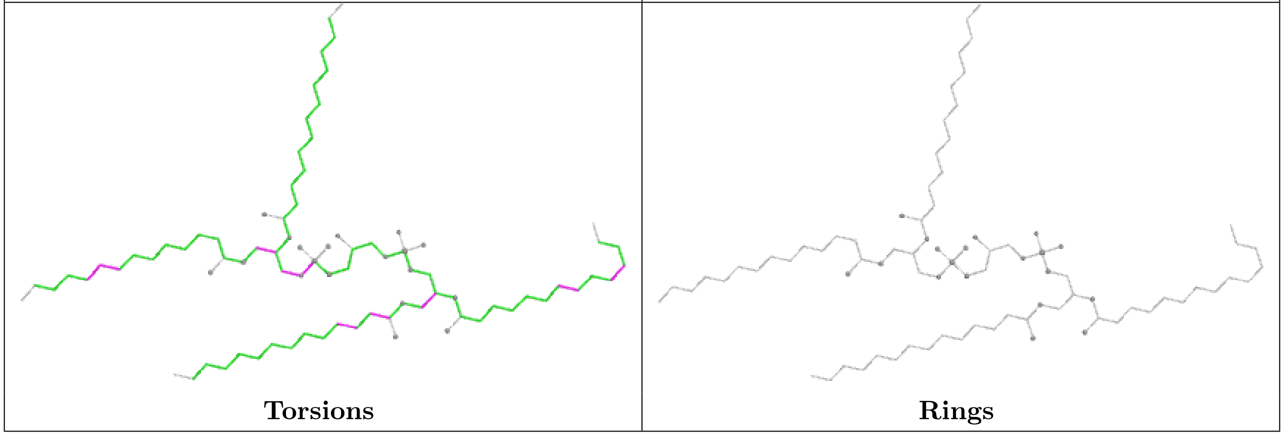
Torsions

Rings

Ligand CD4 m 1005

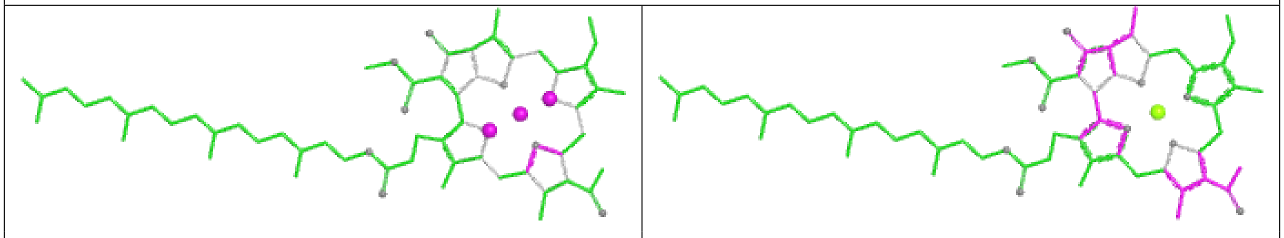


Bond lengths Bond angles

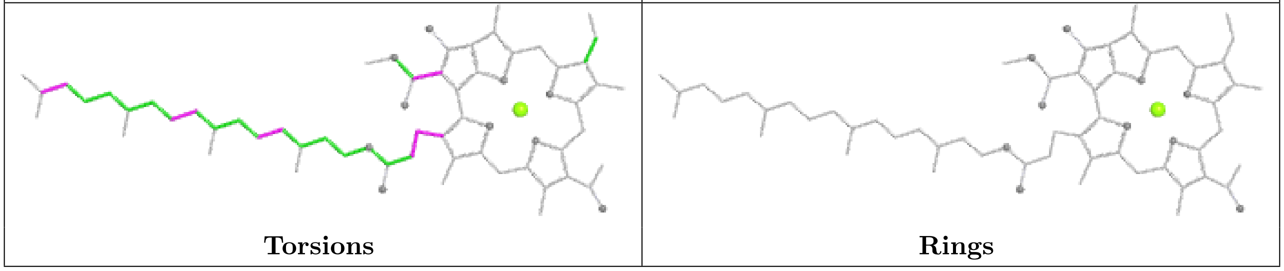


Torsions Rings

Ligand BCL AI 102

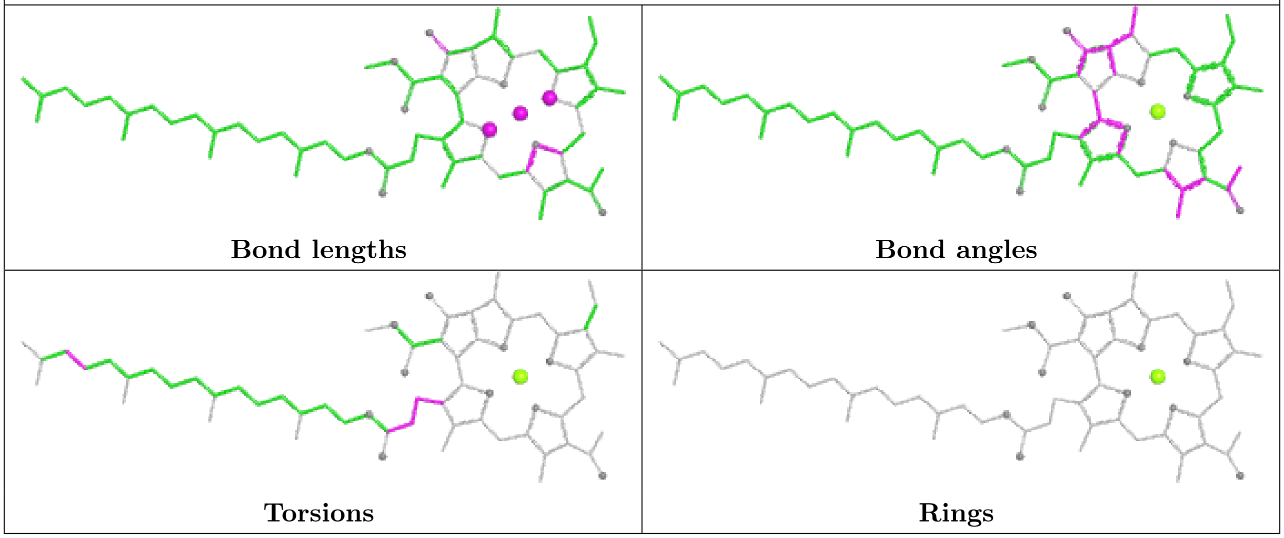


Bond lengths Bond angles

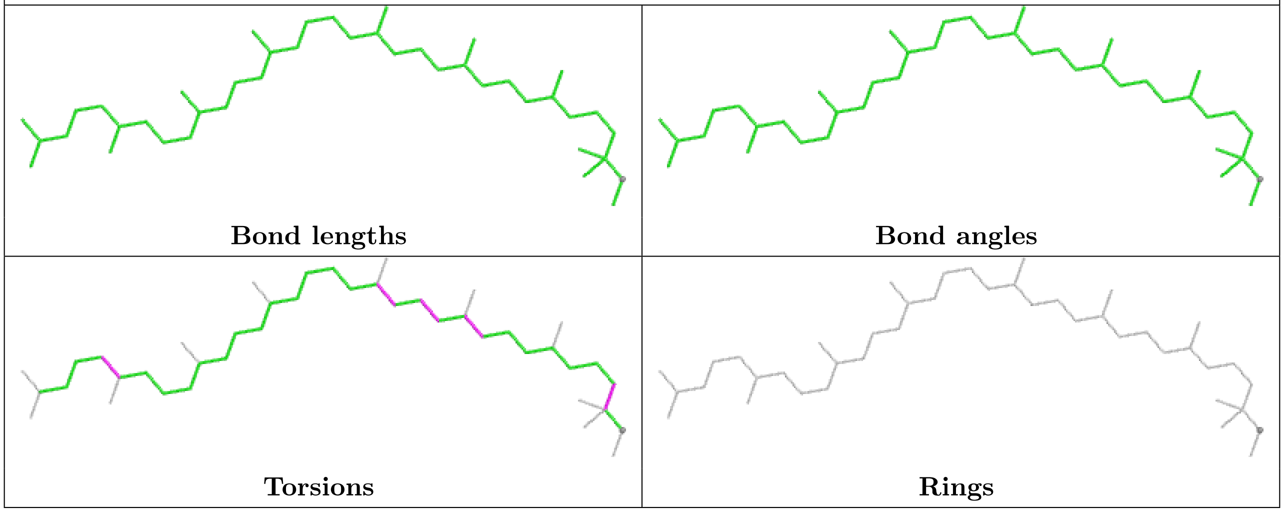


Torsions Rings

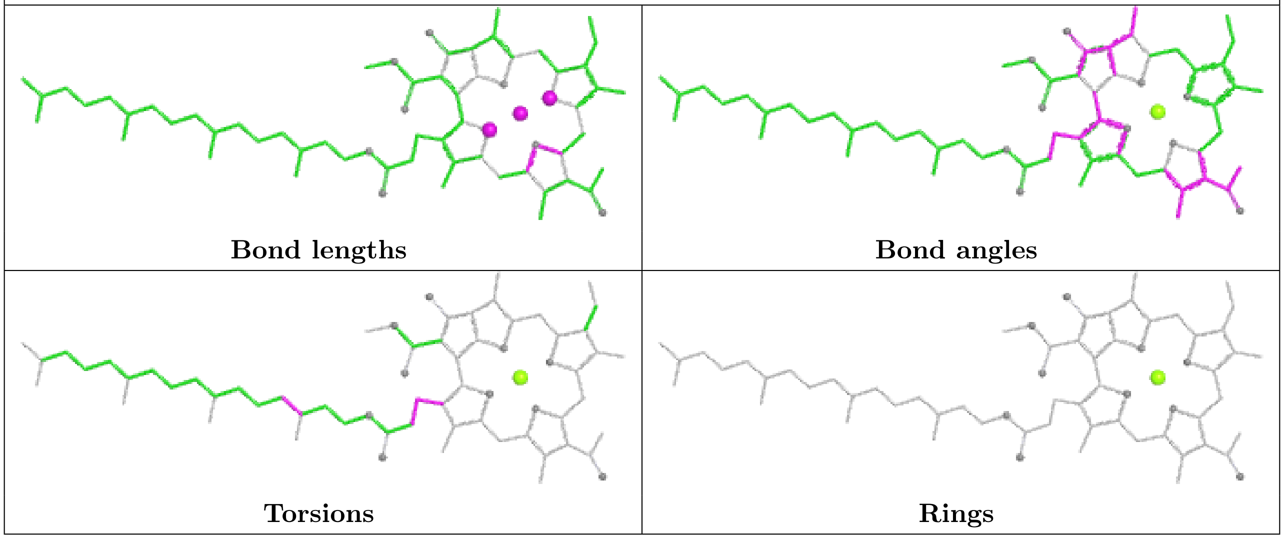
Ligand BCL AC 101


Bond lengths
Bond angles
Torsions
Rings

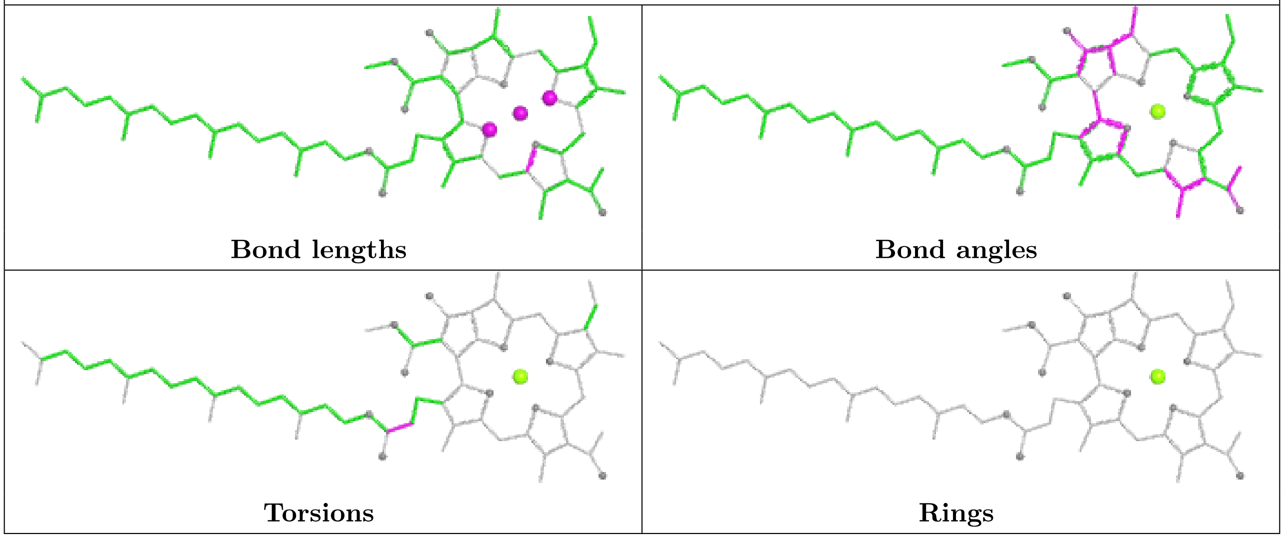
Ligand SP2 BK 102


Bond lengths
Bond angles
Torsions
Rings

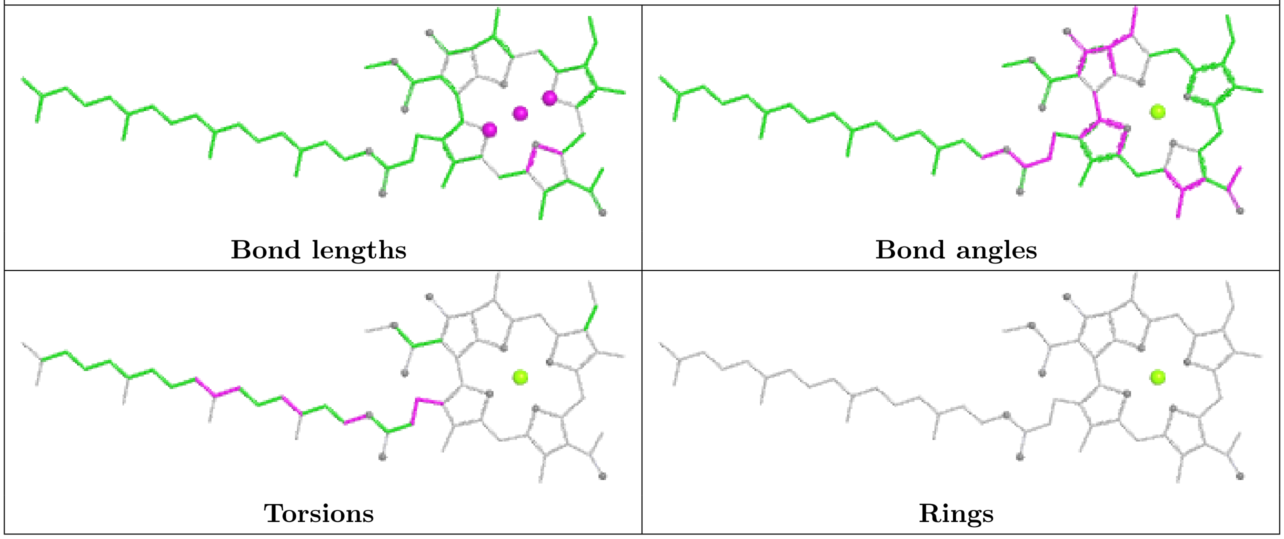
Ligand BCL BE 1001


Bond lengths
Bond angles
Torsions
Rings

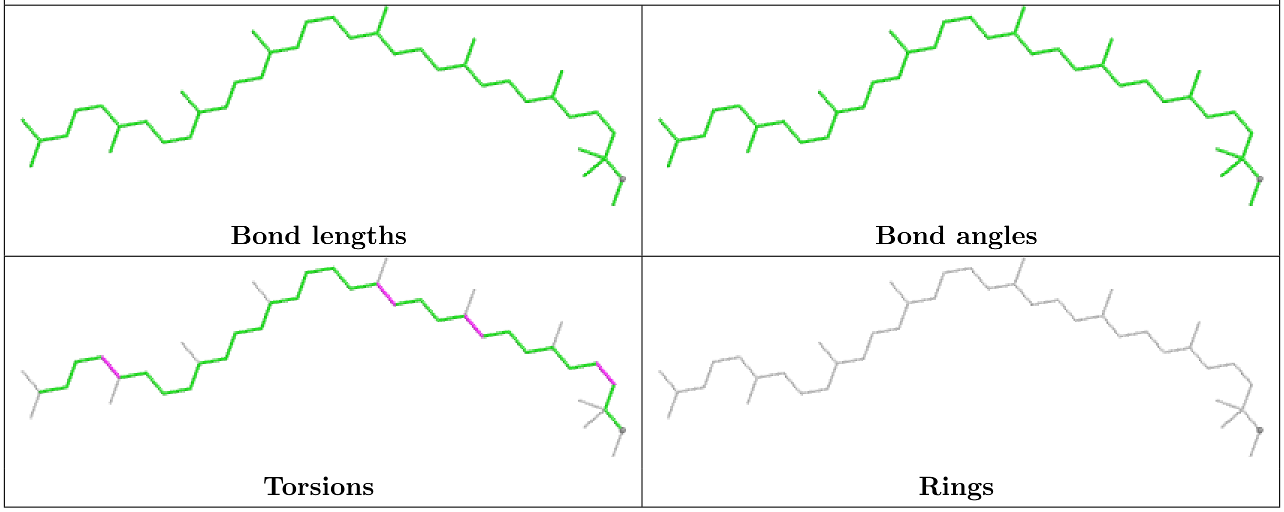
Ligand BCL m 1004



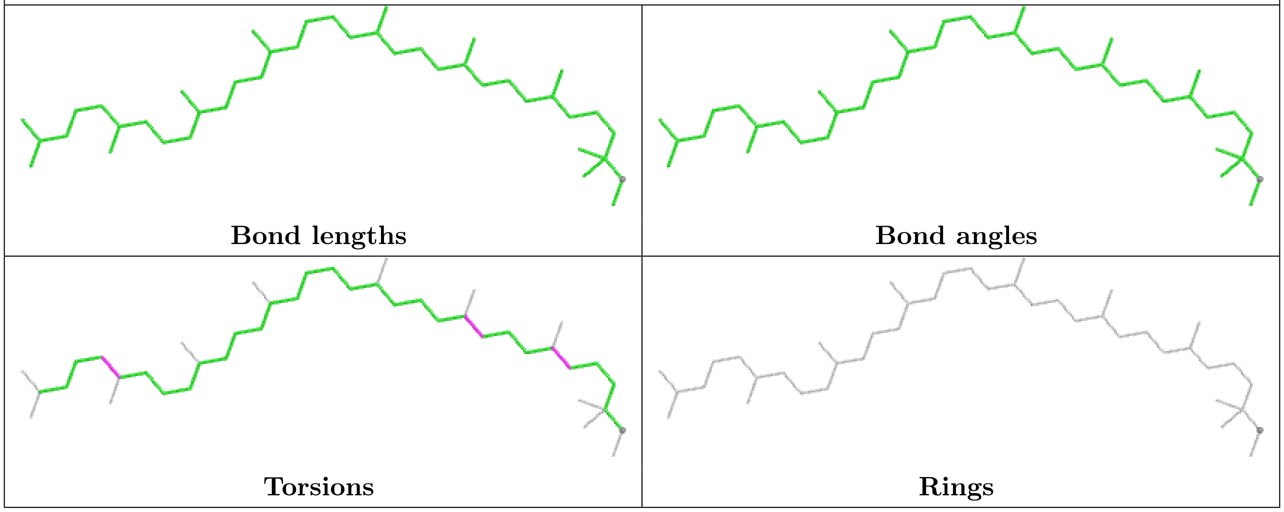
Ligand BCL bl 101



Ligand SP2 BE 1002



Ligand SP2 ab 103



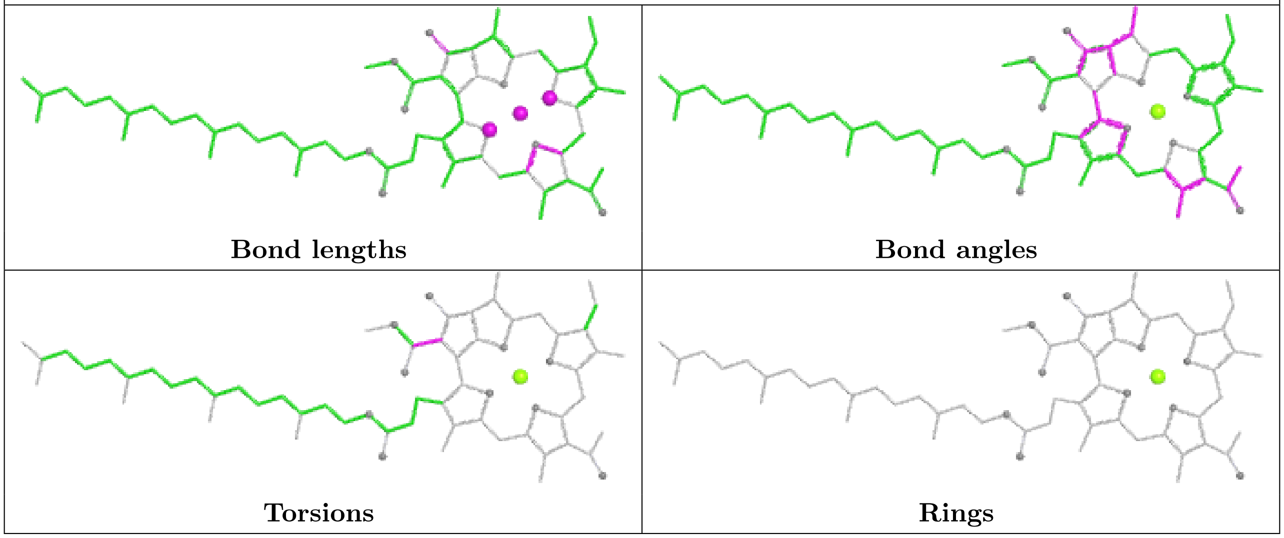
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL ah 101



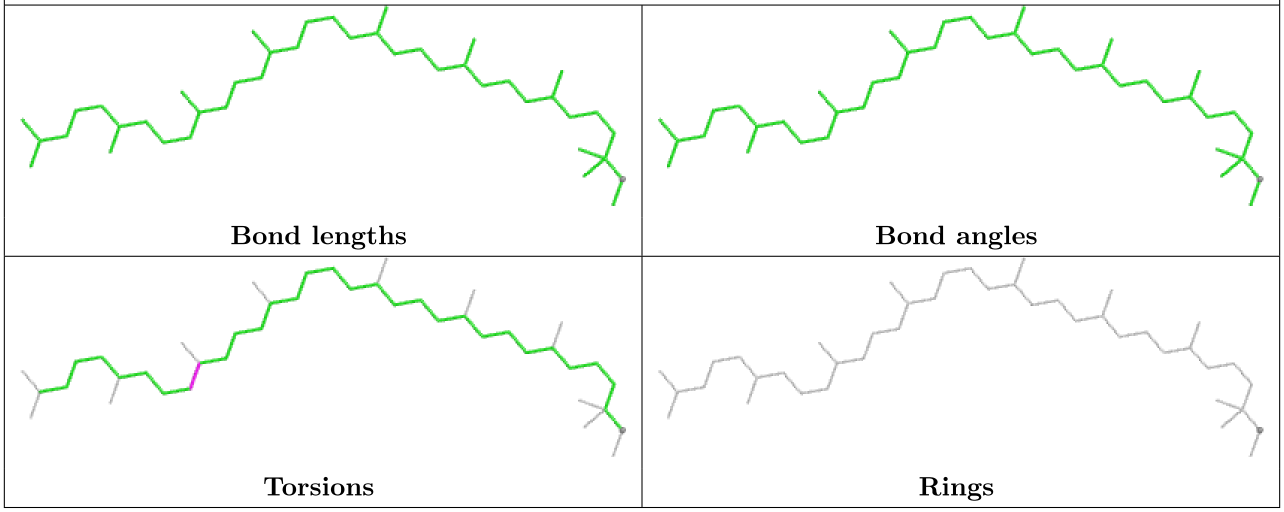
Bond lengths

Bond angles

Torsions

Rings

Ligand SP2 ae 102



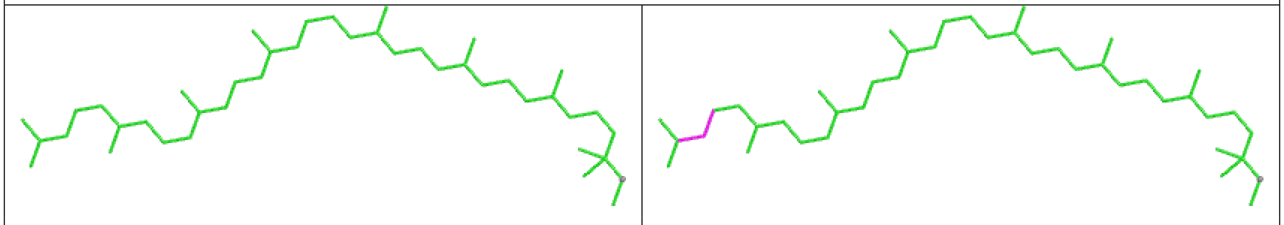
Bond lengths

Bond angles

Torsions

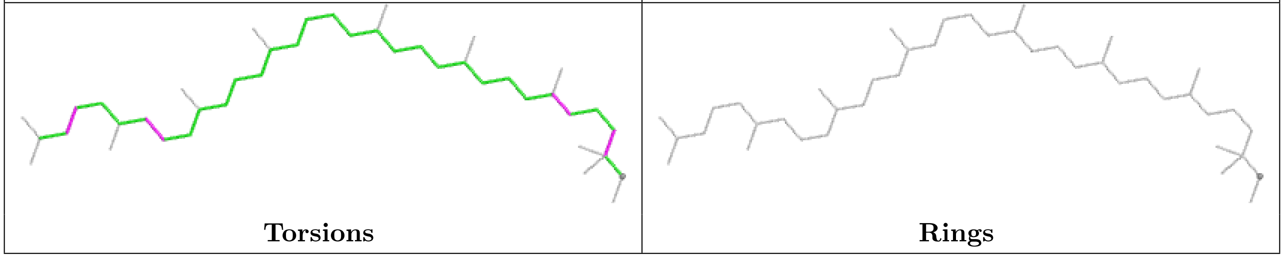
Rings

Ligand SP2 ab 101



Bond lengths

Bond angles



Torsions

Rings

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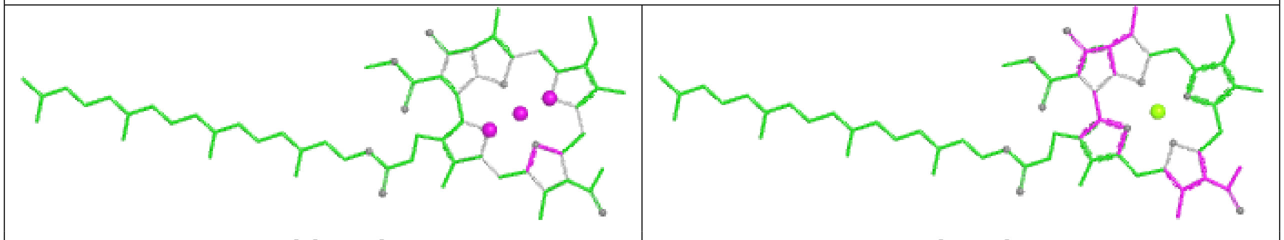
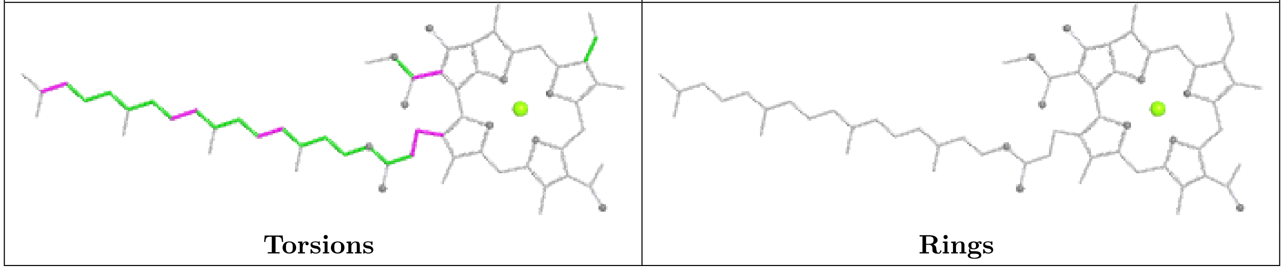


Bond lengths

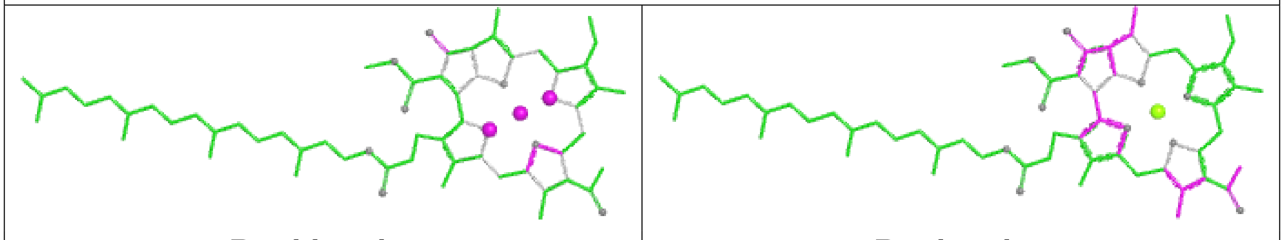
Bond angles



Torsions

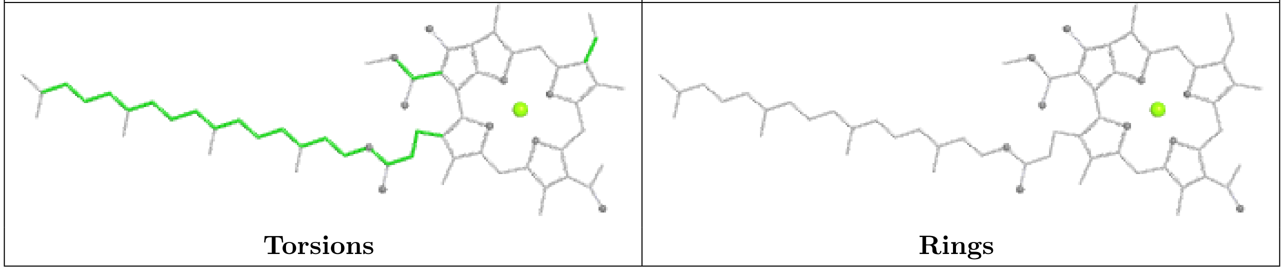
Rings

Ligand BCL AM 1001



Bond lengths

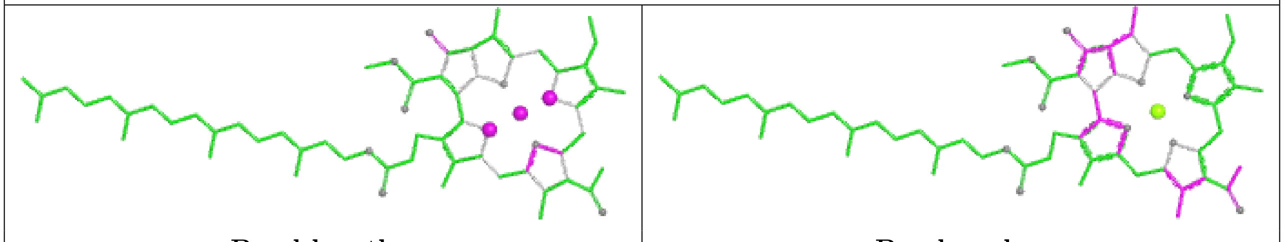
Bond angles



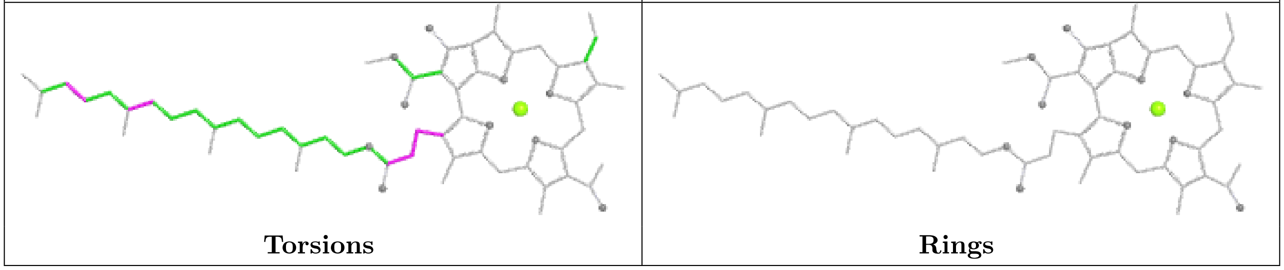
Torsions

Rings

Ligand BCL ac 102

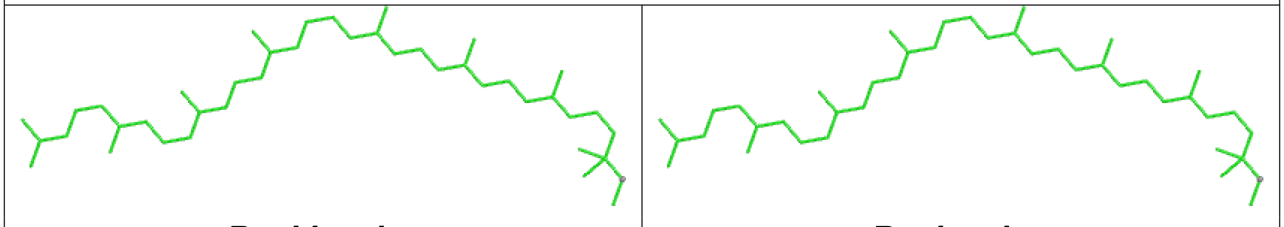


Bond lengths **Bond angles**

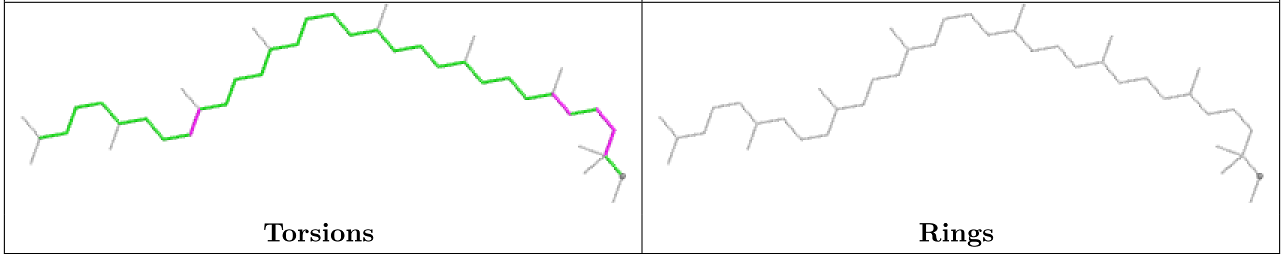


Torsions **Rings**

Ligand SP2 AM 1000

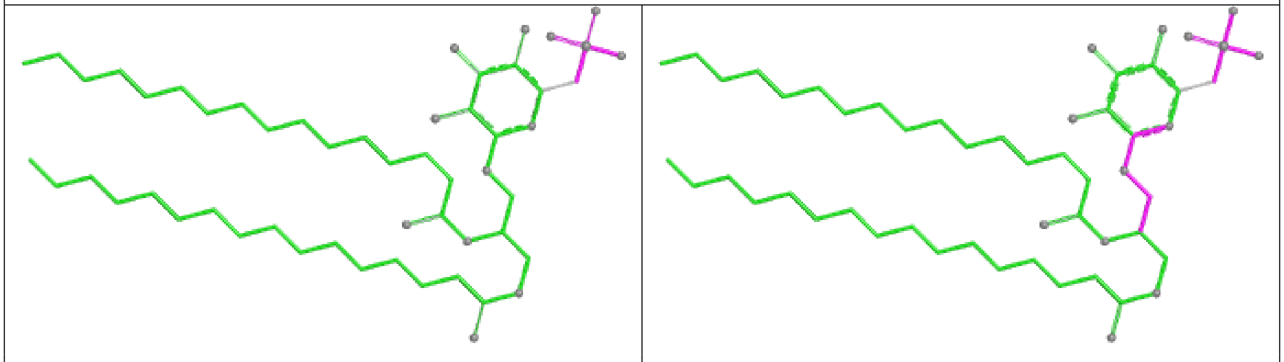


Bond lengths **Bond angles**



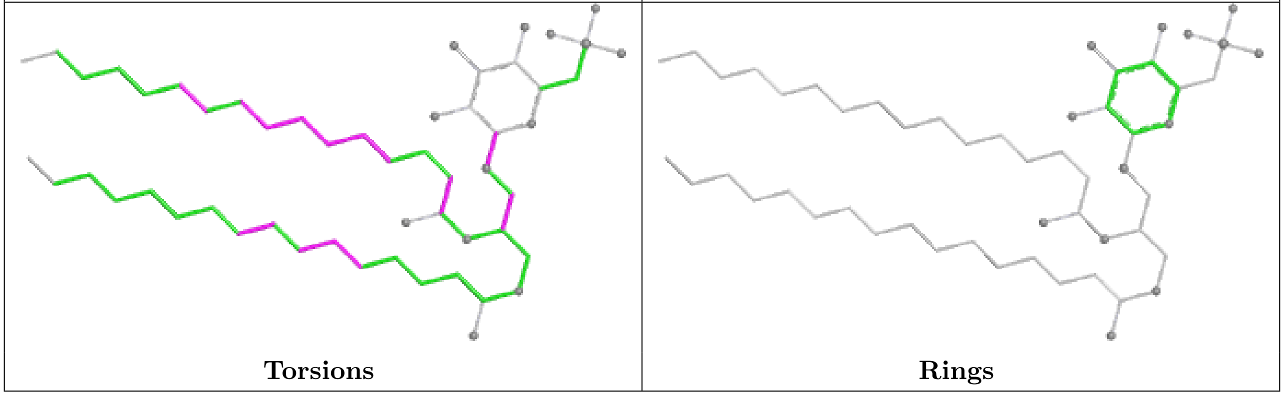
Torsions **Rings**

Ligand SQD L 306



Bond lengths

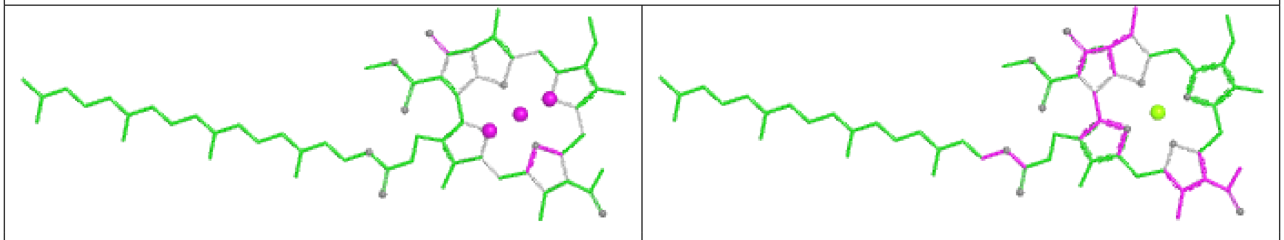
Bond angles



Torsions

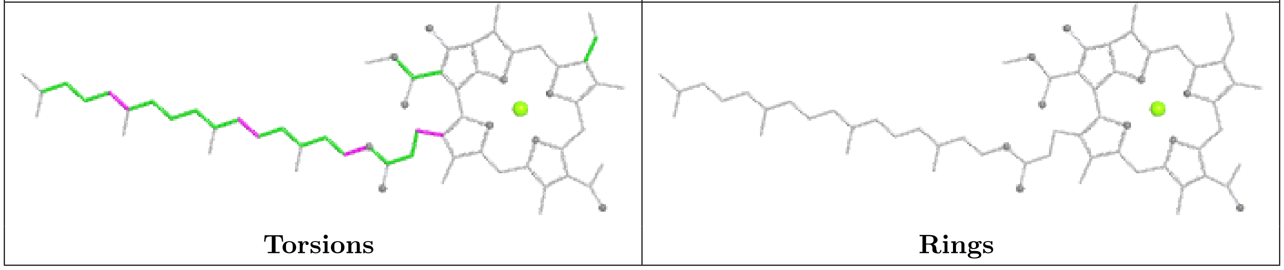
Rings

Ligand BCL BJ 102



Bond lengths

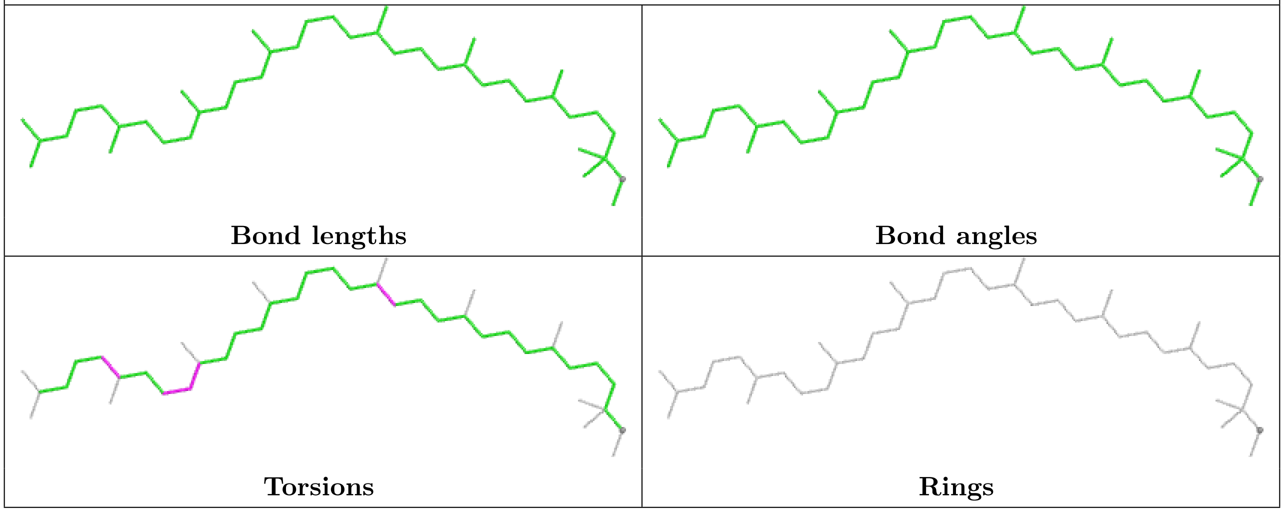
Bond angles



Torsions

Rings

Ligand SP2 ac 104



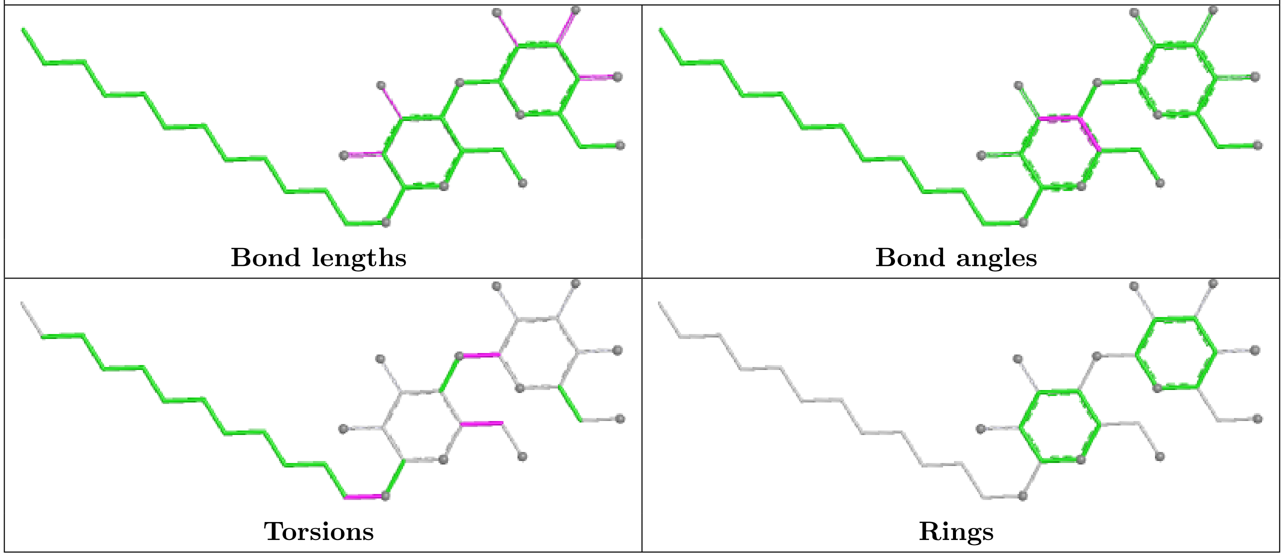
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT m 1001



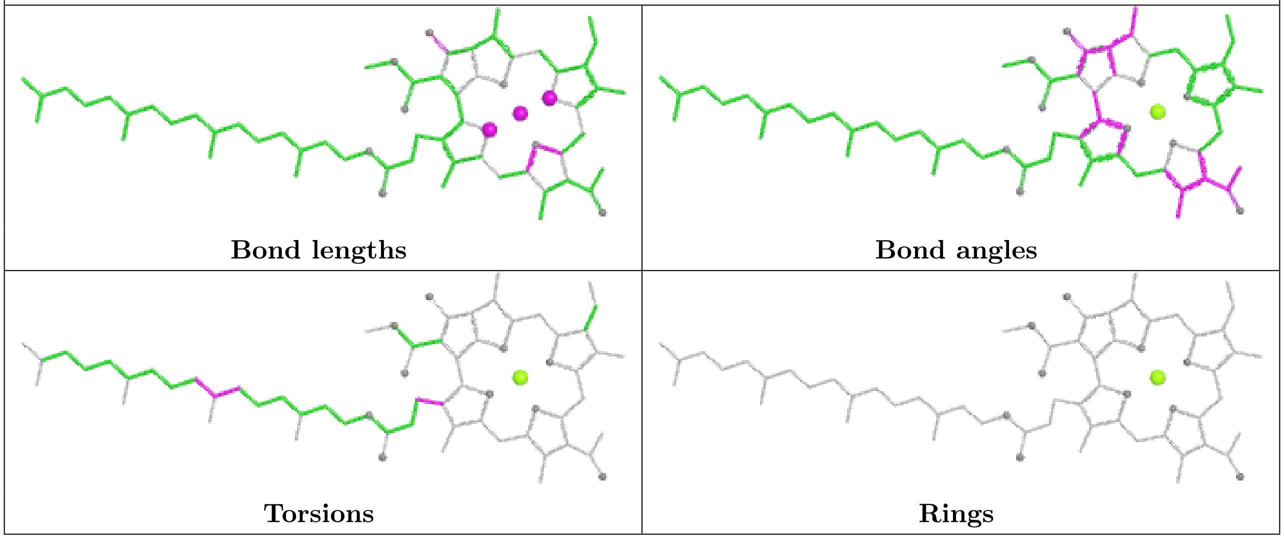
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL BK 101



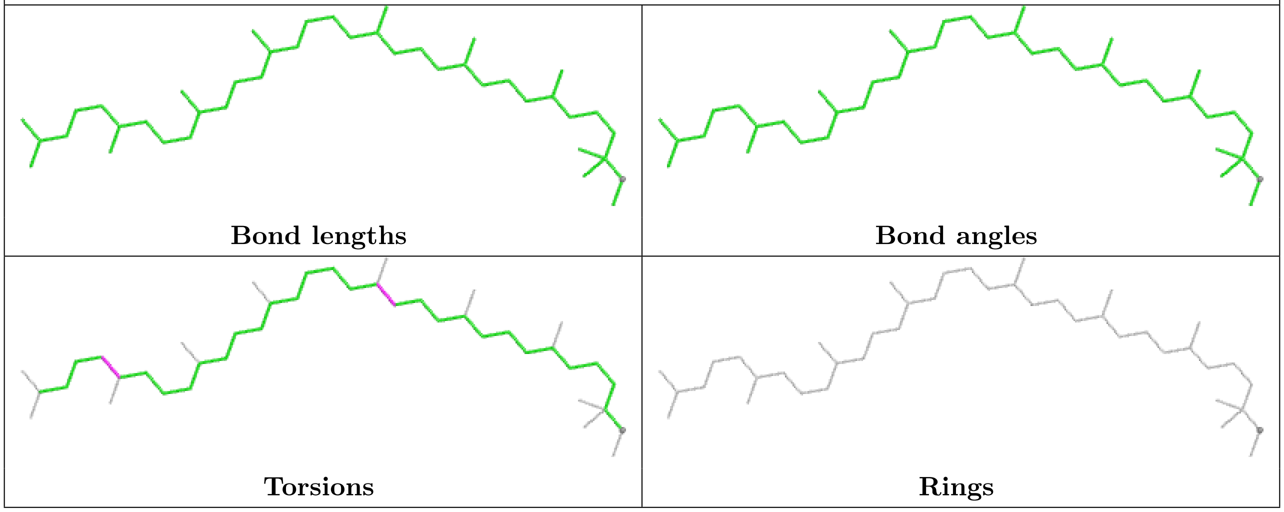
Bond lengths

Bond angles

Torsions

Rings

Ligand SP2 af 104



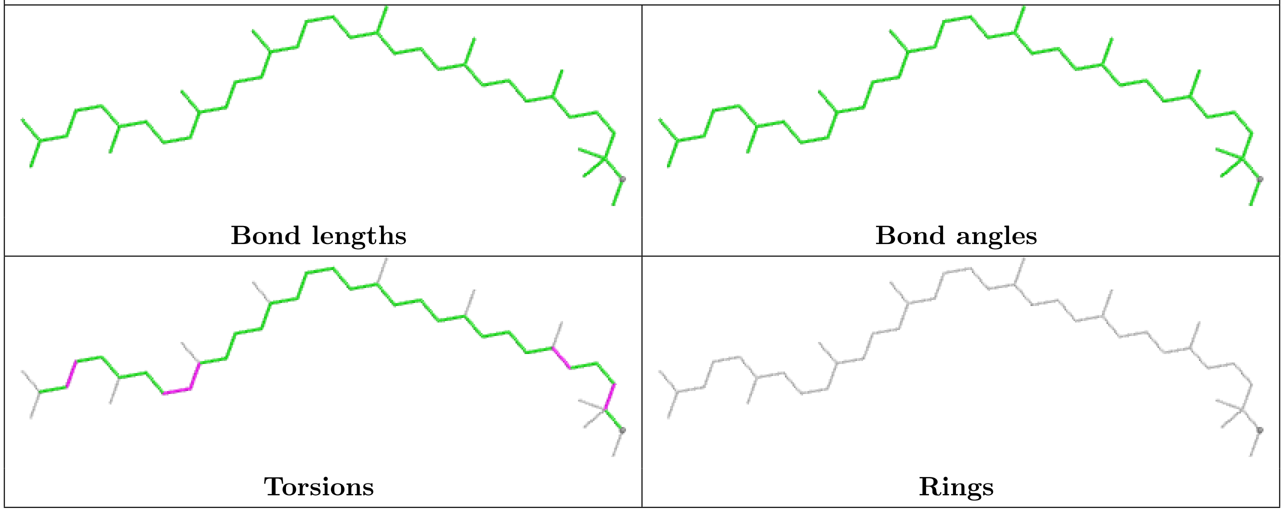
Bond lengths

Bond angles

Torsions

Rings

Ligand SP2 aj 103



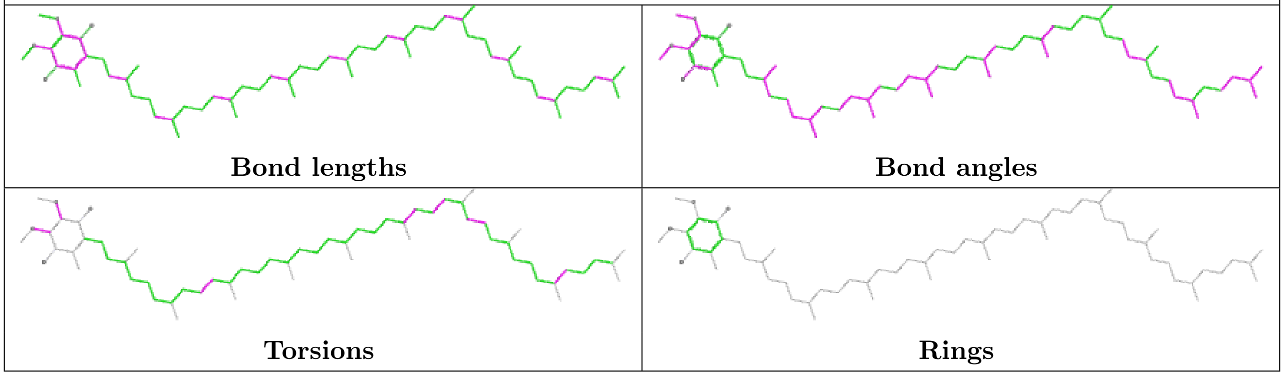
Bond lengths

Bond angles

Torsions

Rings

Ligand U10 m 1003



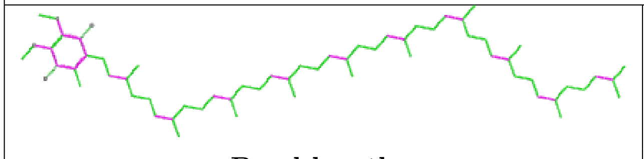
Bond lengths

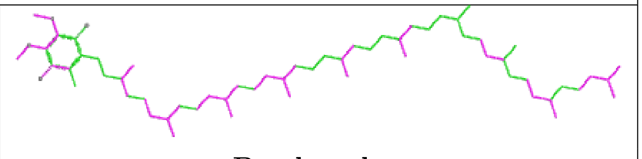
Bond angles

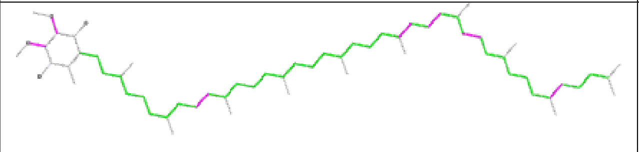
Torsions

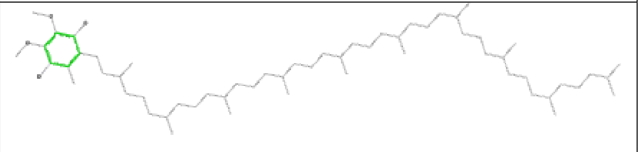
Rings

Ligand U10 M 1007

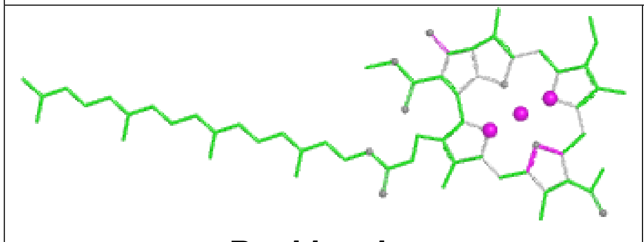

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL an 101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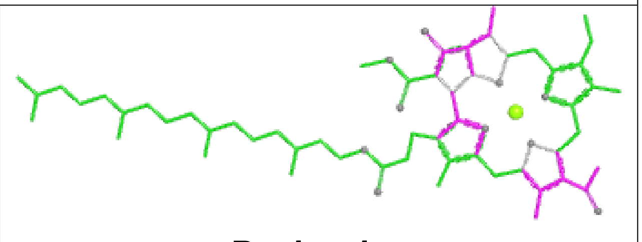
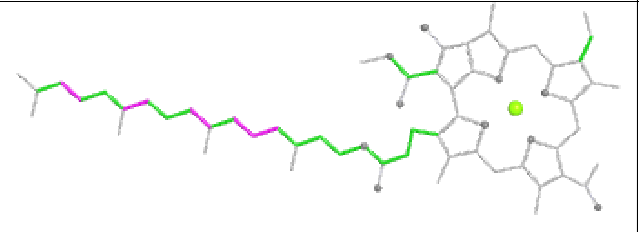

Bond angles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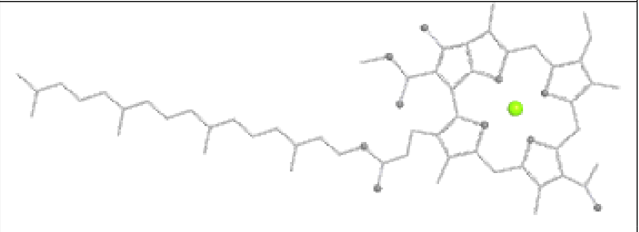
Rings

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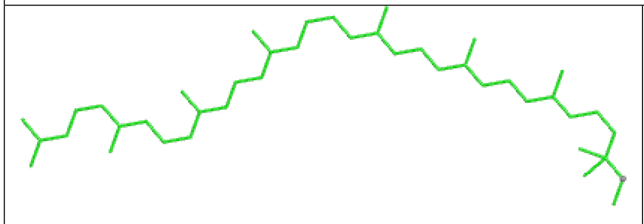
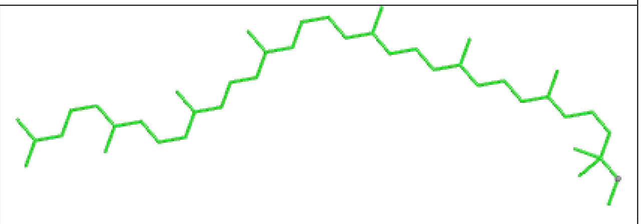
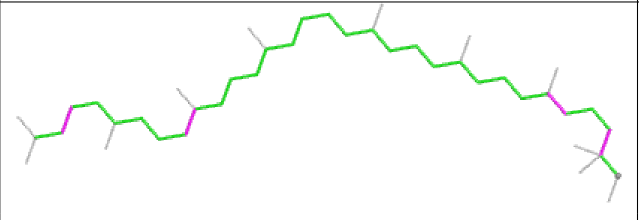
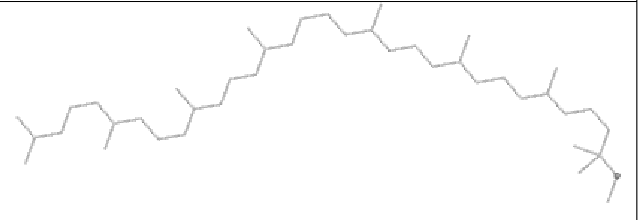
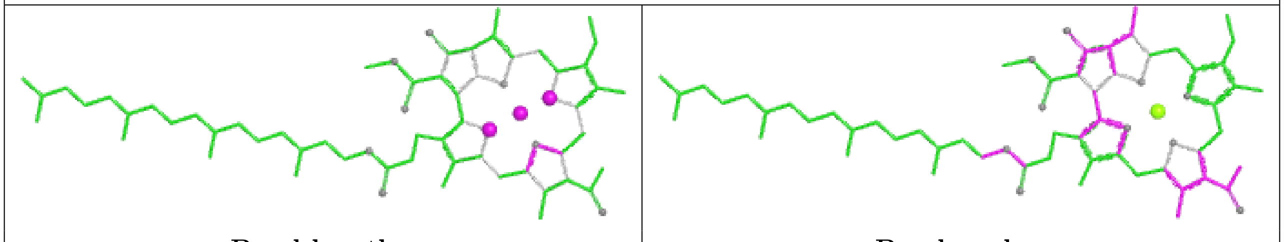

Bond lengths


Bond angles


Torsions

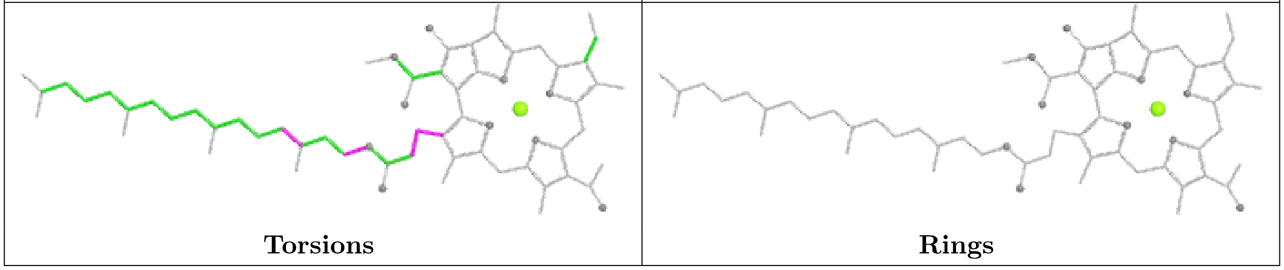

Rings

Ligand BCL bg 101



Bond lengths

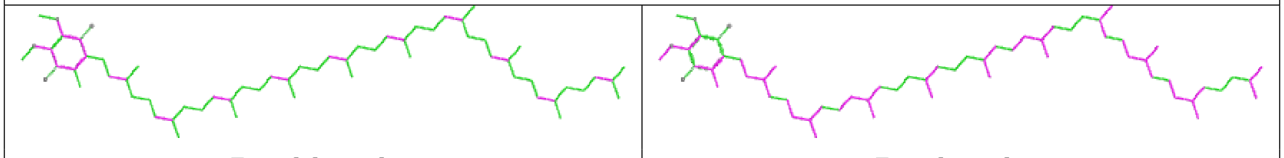
Bond angles



Torsions

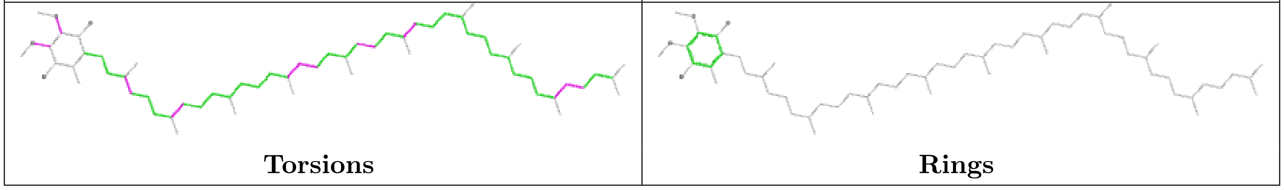
Rings

Ligand U10 L 303



Bond lengths

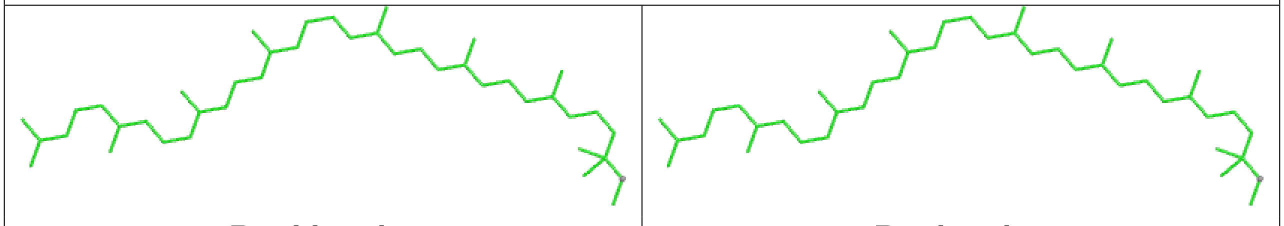
Bond angles



Torsions

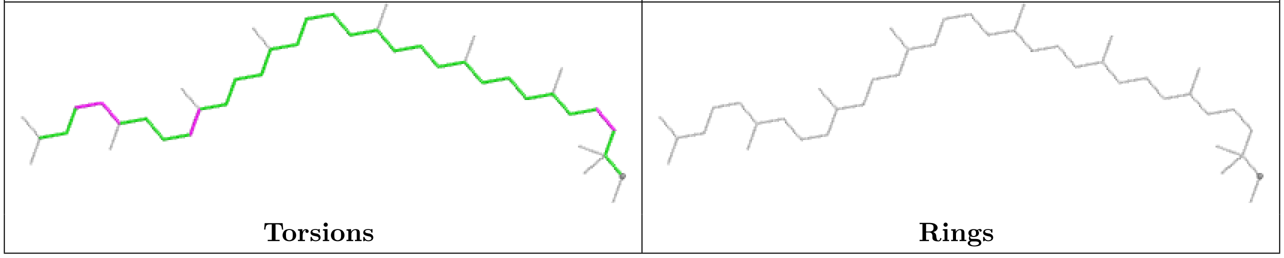
Rings

Ligand SP2 AB 104



Bond lengths

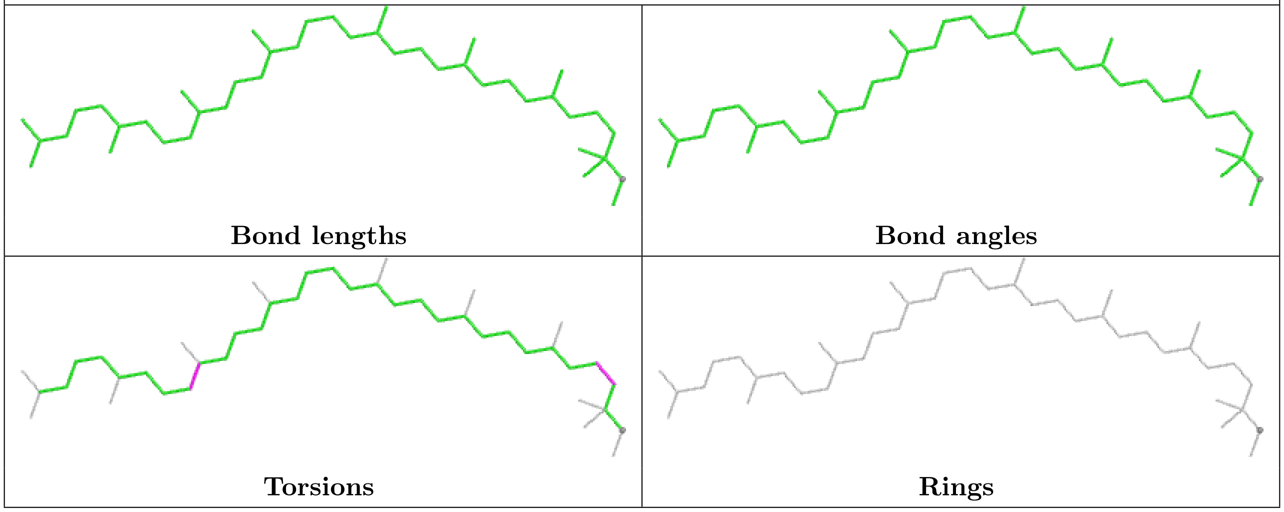
Bond angles



Torsions

Rings

Ligand SP2 AE 101



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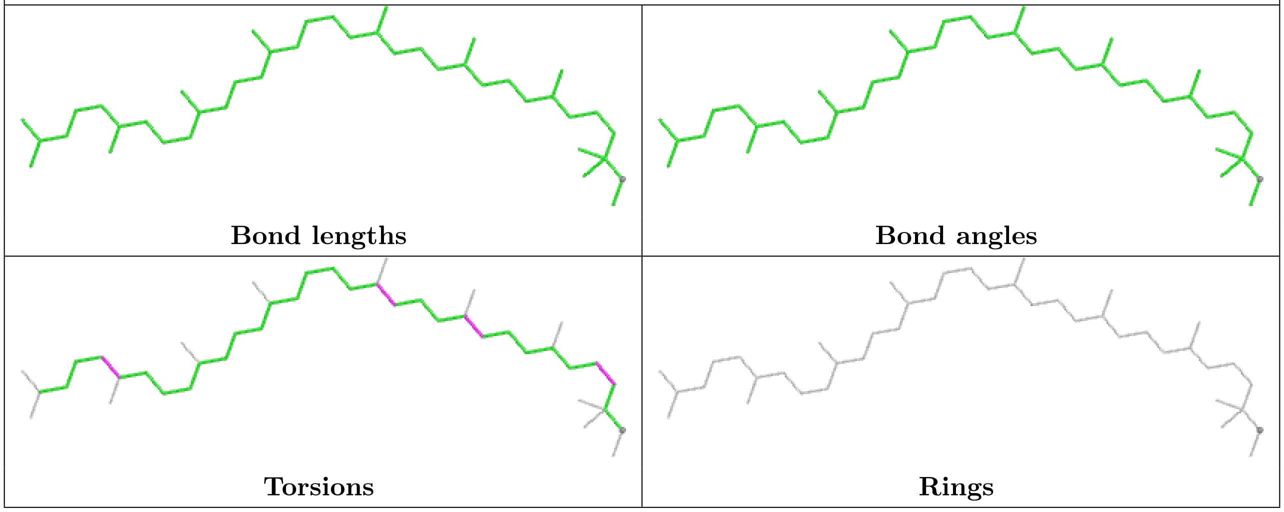
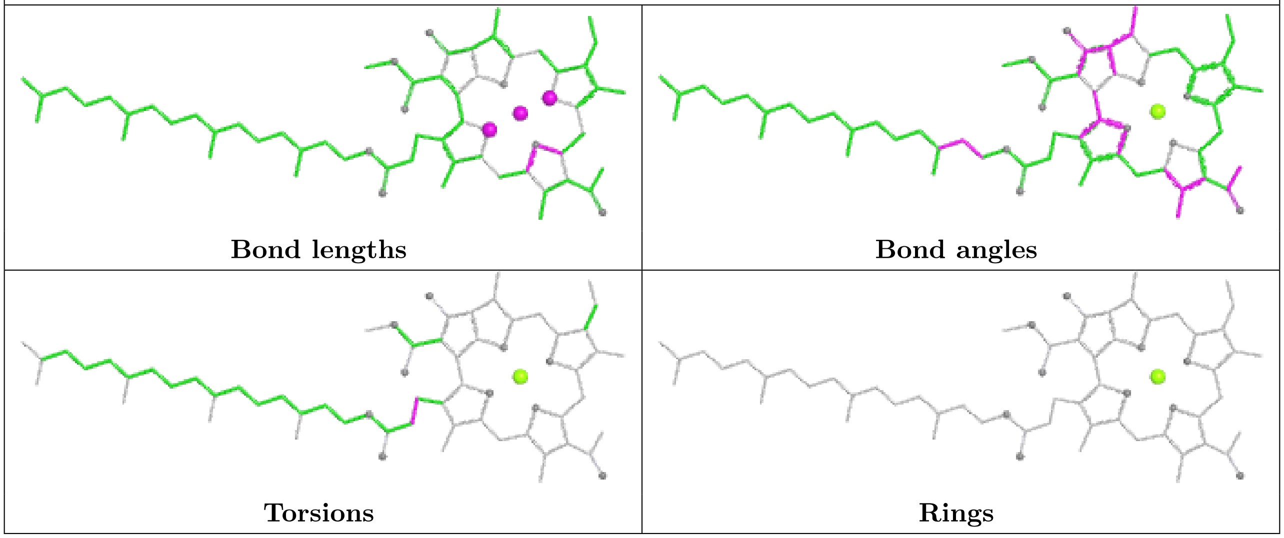


Ligand BCL BD 101



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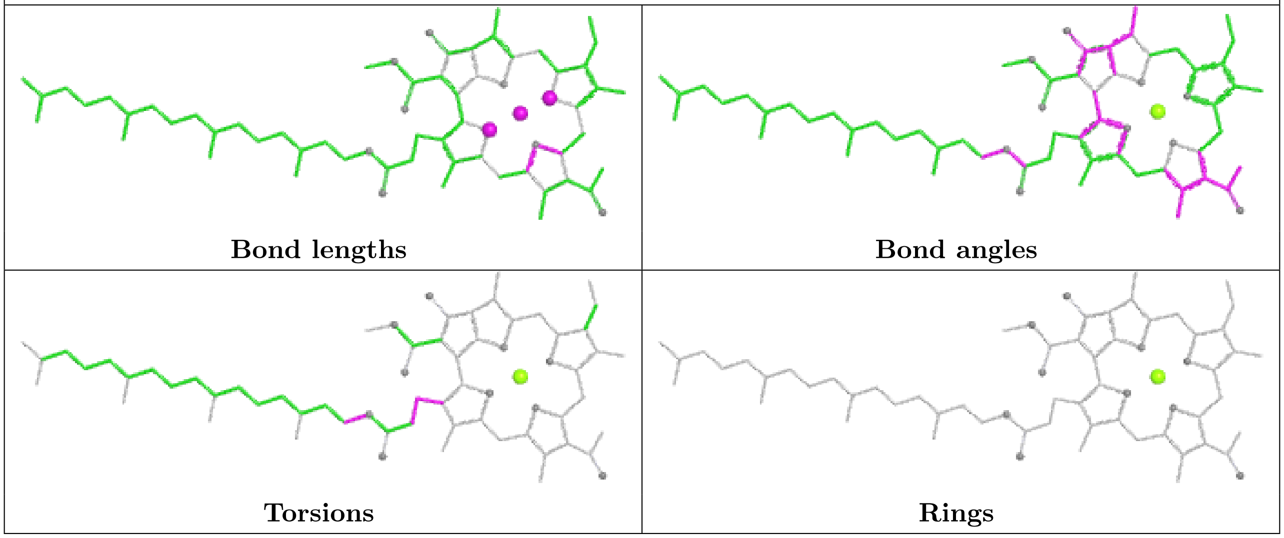


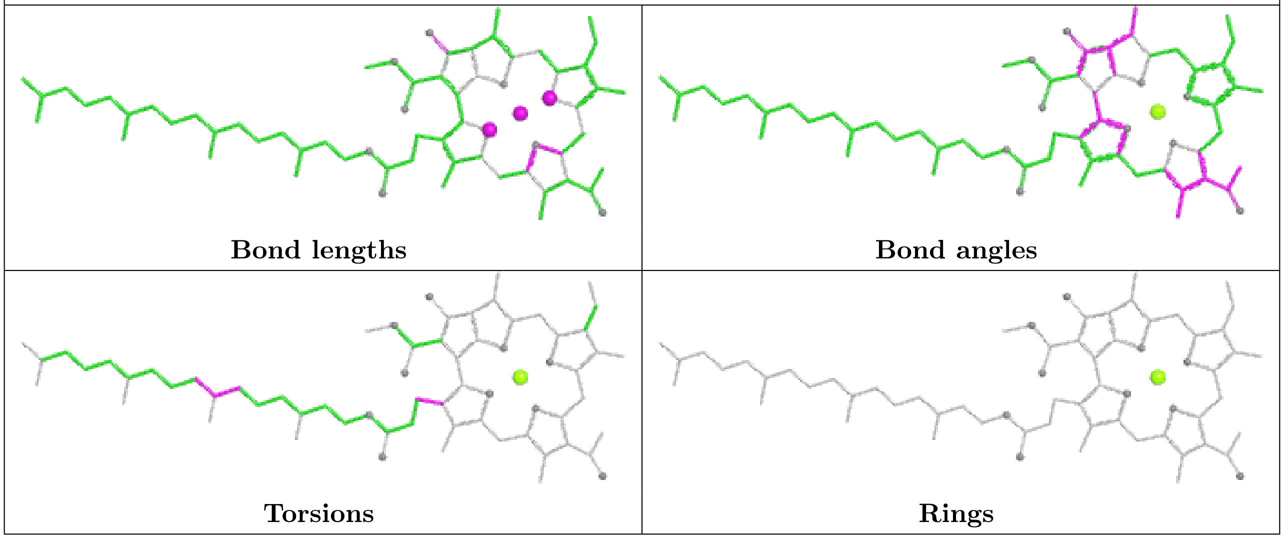
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL bk 101



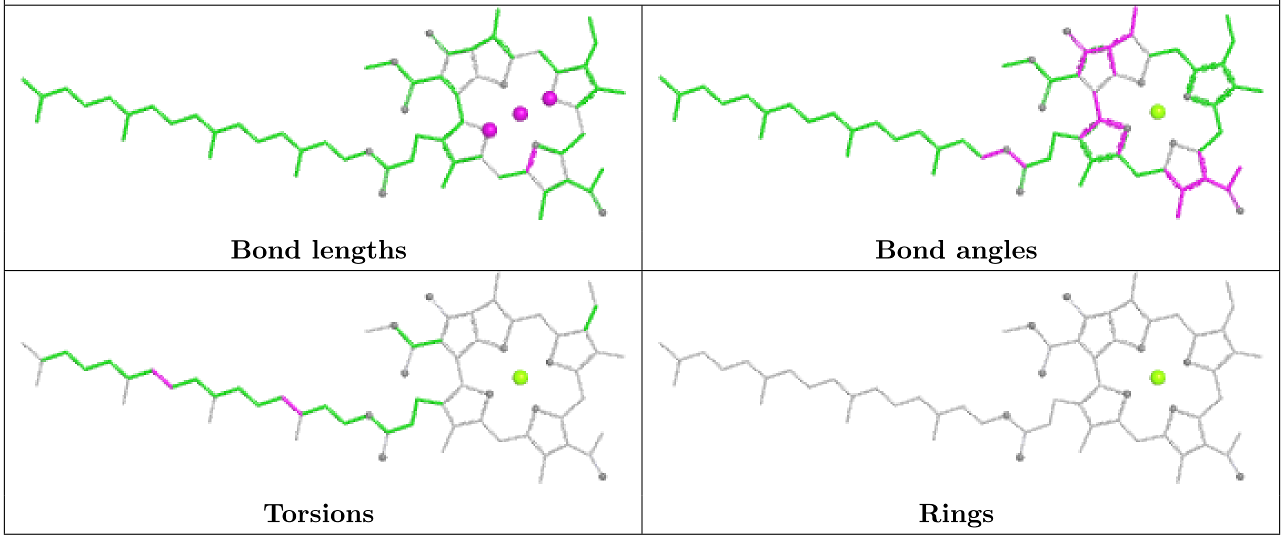
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 1002



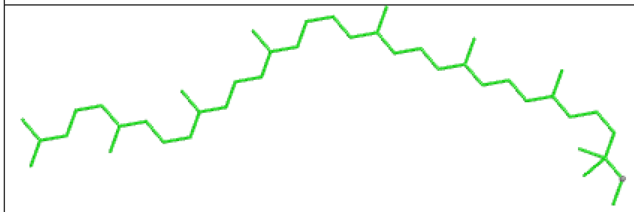
Bond lengths

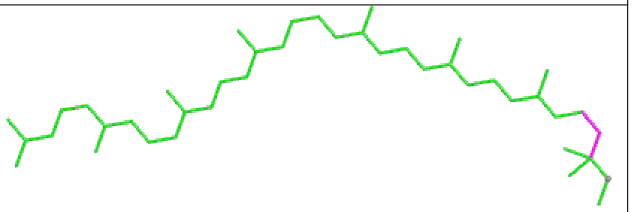
Bond angles

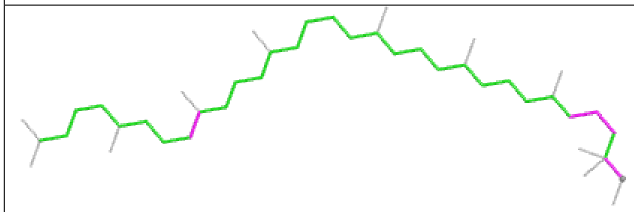
Torsions

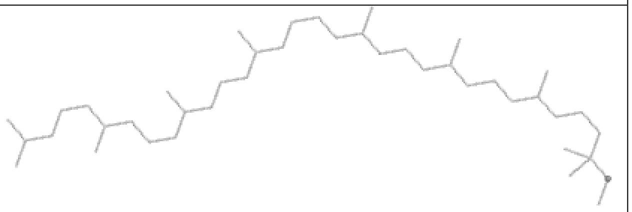
Rings

Ligand SP2 AB 103


Bond lengths


Bond angles


Torsions


Rings

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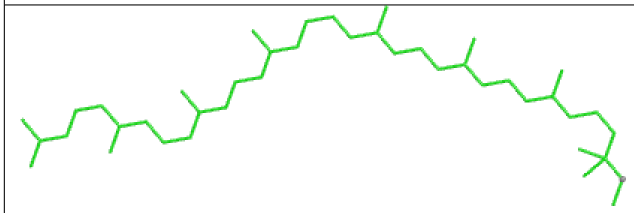
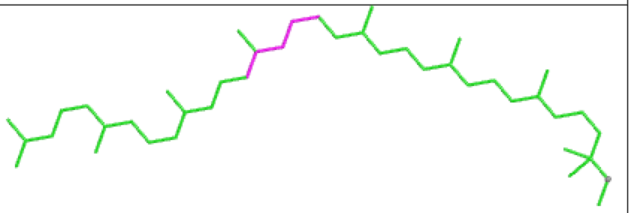
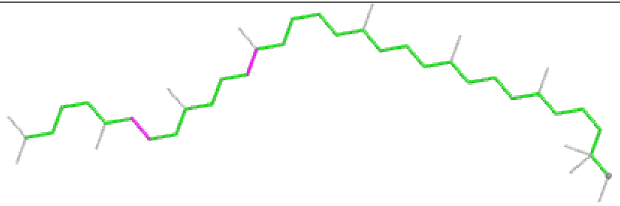
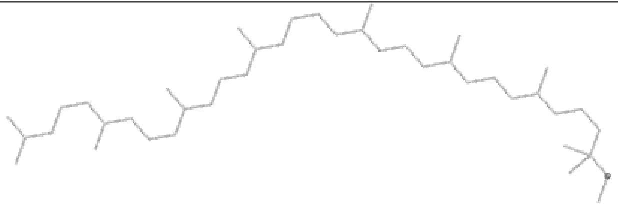
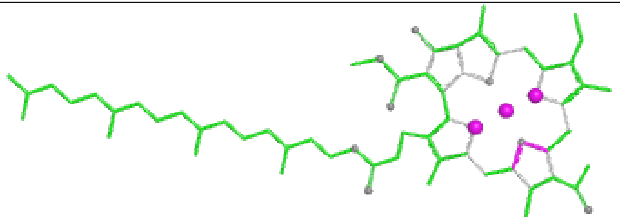

Bond lengths

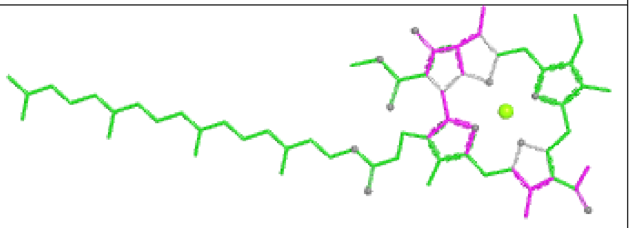

Bond angles

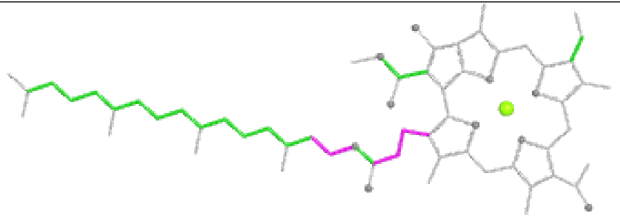

Torsions

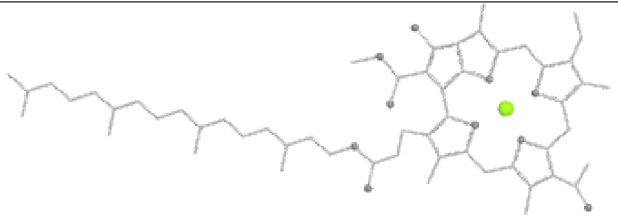

Rings

Ligand BCL BI 101

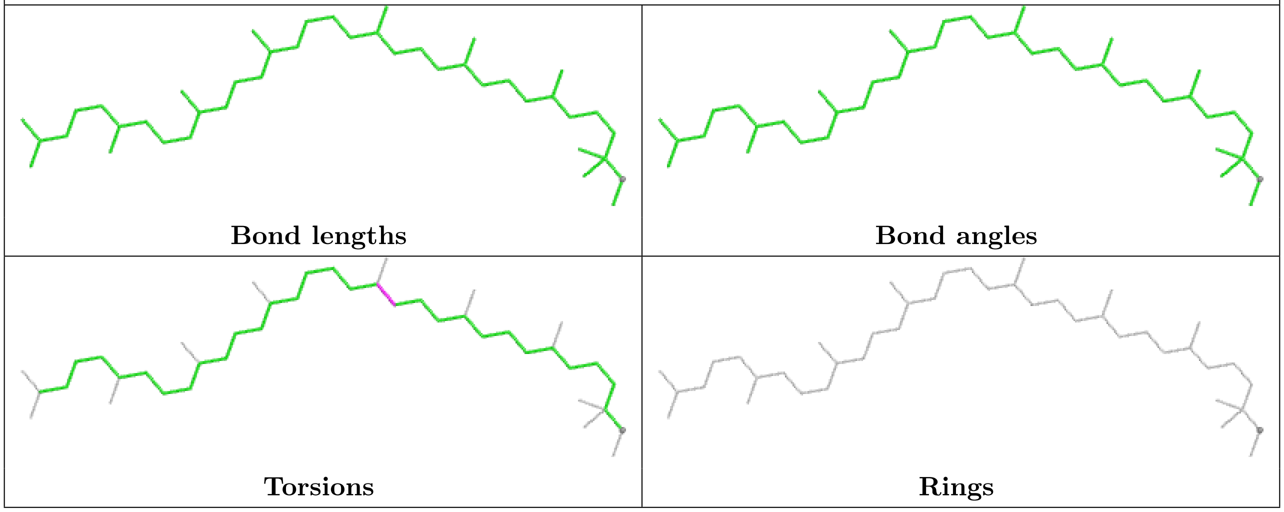

Bond lengths


Bond angles


Torsions


Rings

Ligand SP2 BL 103



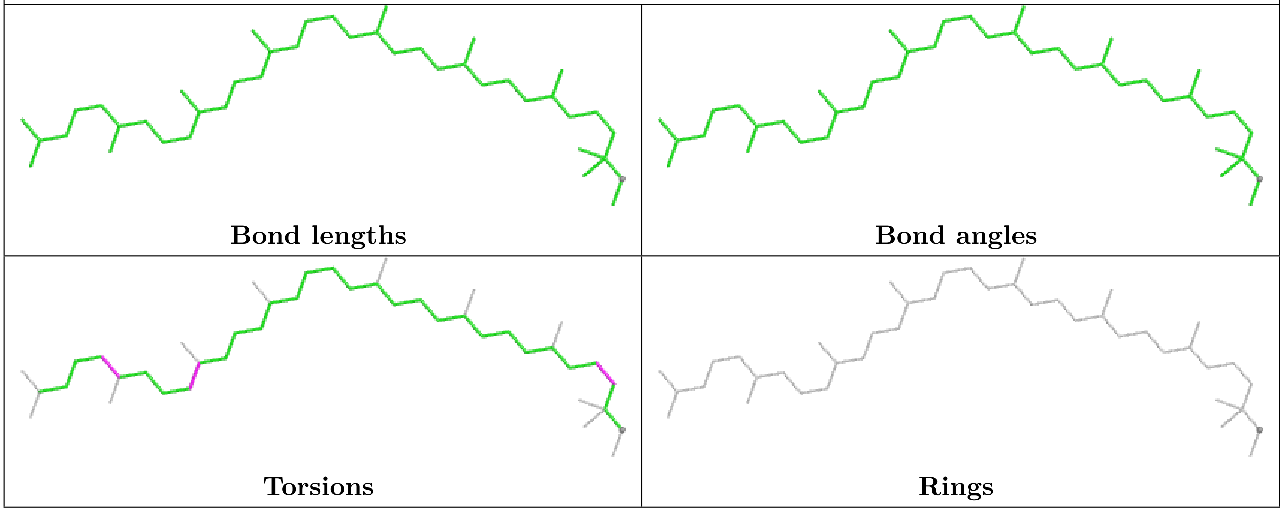
Bond lengths

Bond angles

Torsions

Rings

Ligand SP2 AJ 102



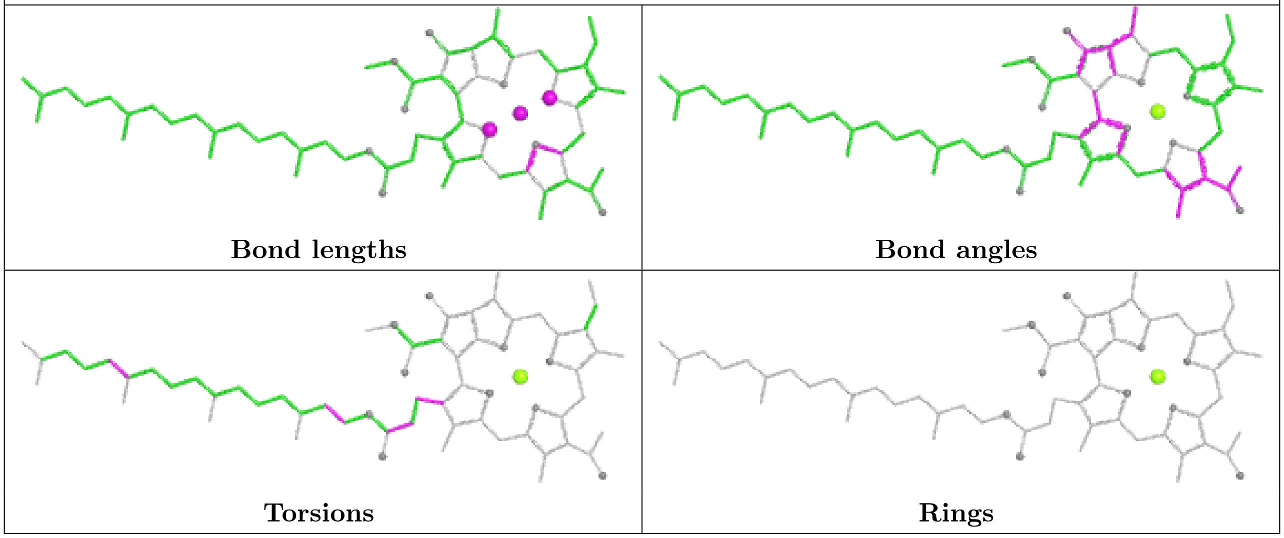
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL BF 101



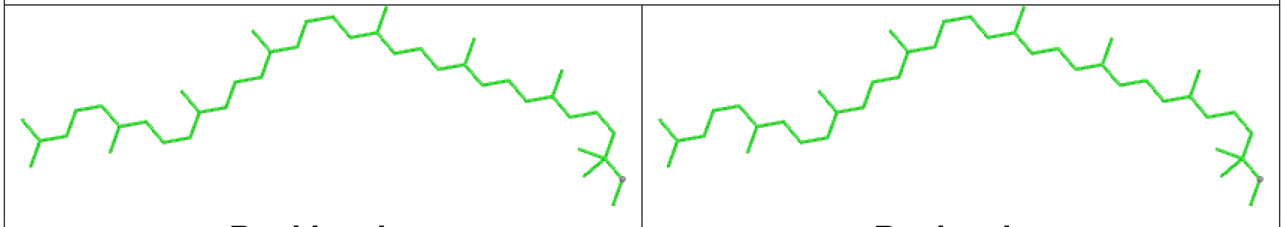
Bond lengths

Bond angles

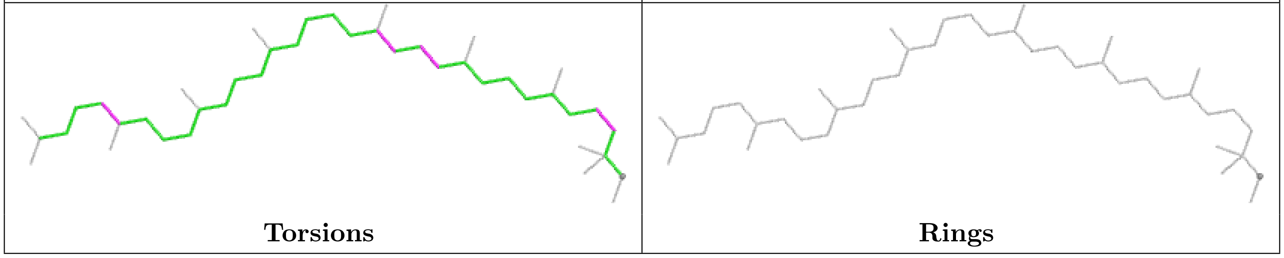
Torsions

Rings

Ligand SP2 bk 102

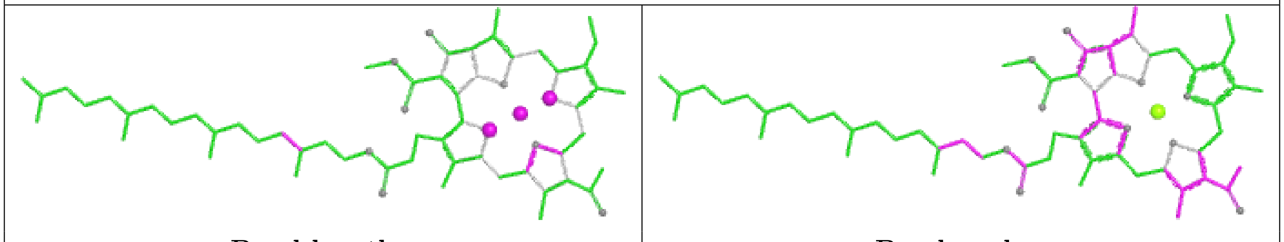


Bond lengths Bond angles

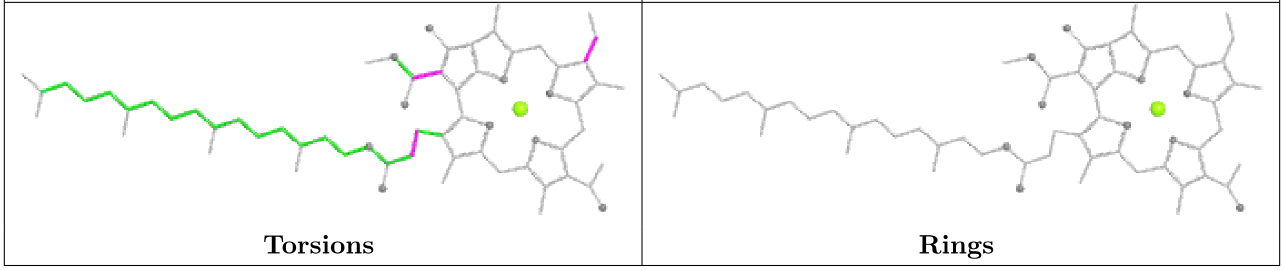


Torsions Rings

Ligand BCL AB 101

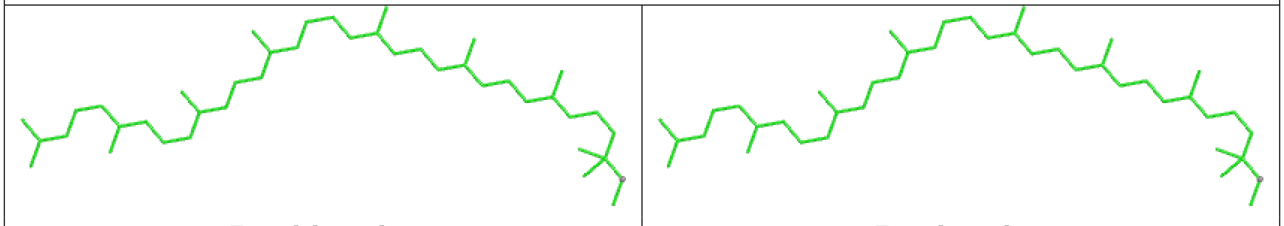


Bond lengths Bond angles

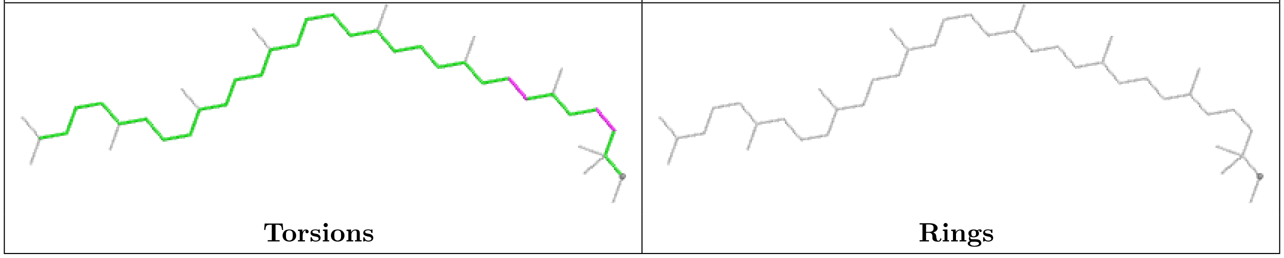


Torsions Rings

Ligand SP2 bh 101

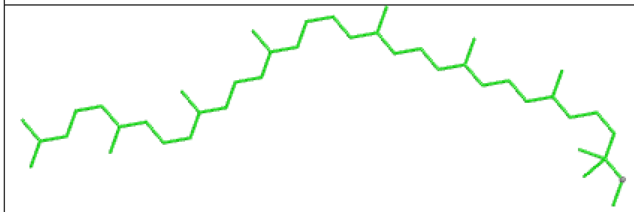


Bond lengths Bond angles

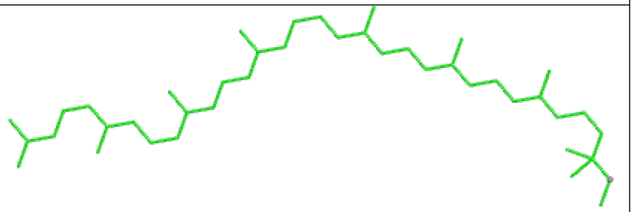


Torsions Rings

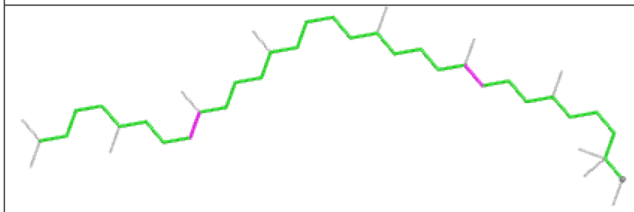
Ligand SP2 AC 103



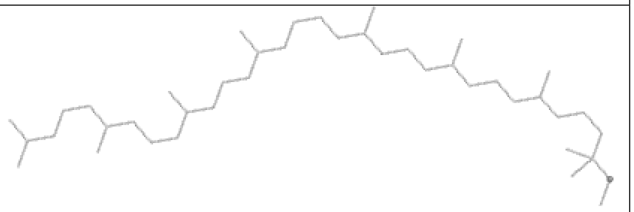
Bond lengths



Bond angles

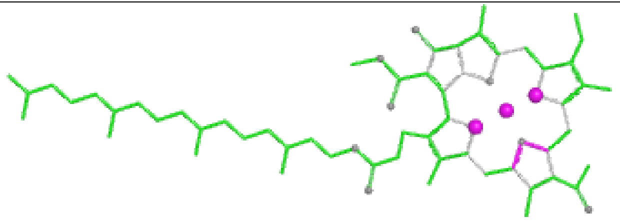


Torsions

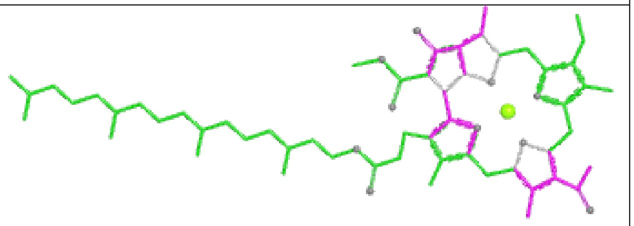


Rings

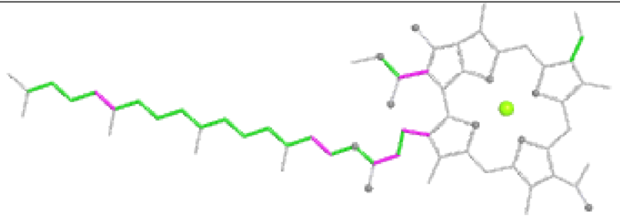
Ligand BCL bf 101



Bond lengths



Bond angles



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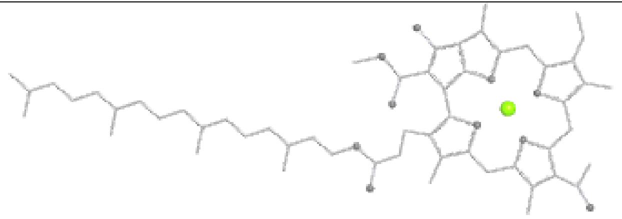
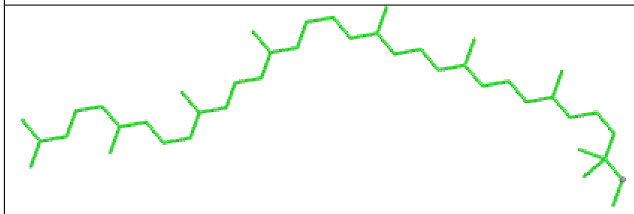
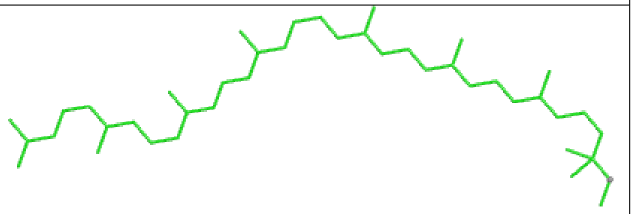


Rings

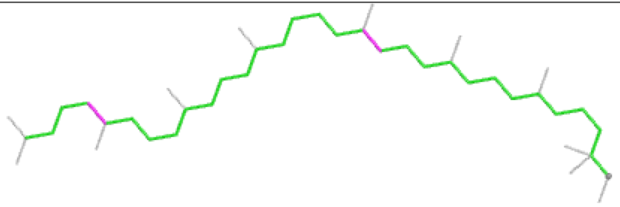
Ligand SP2 AF 103



Bond lengths



Bond angles



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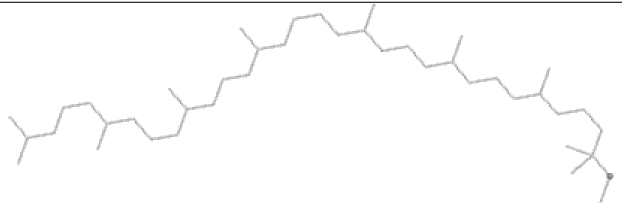
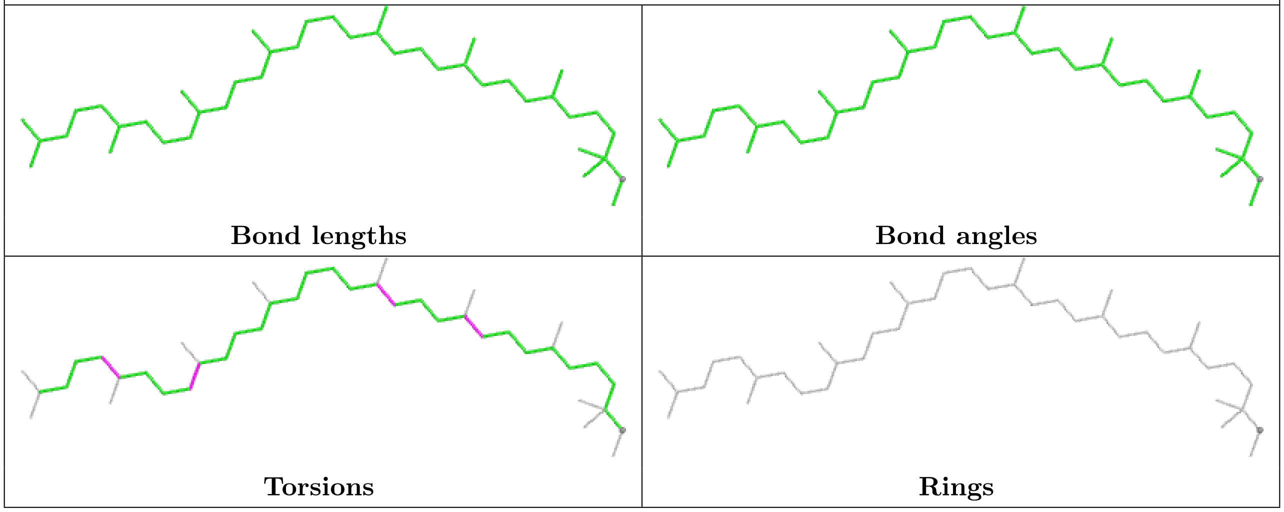


Rings

Ligand SP2 AK 102



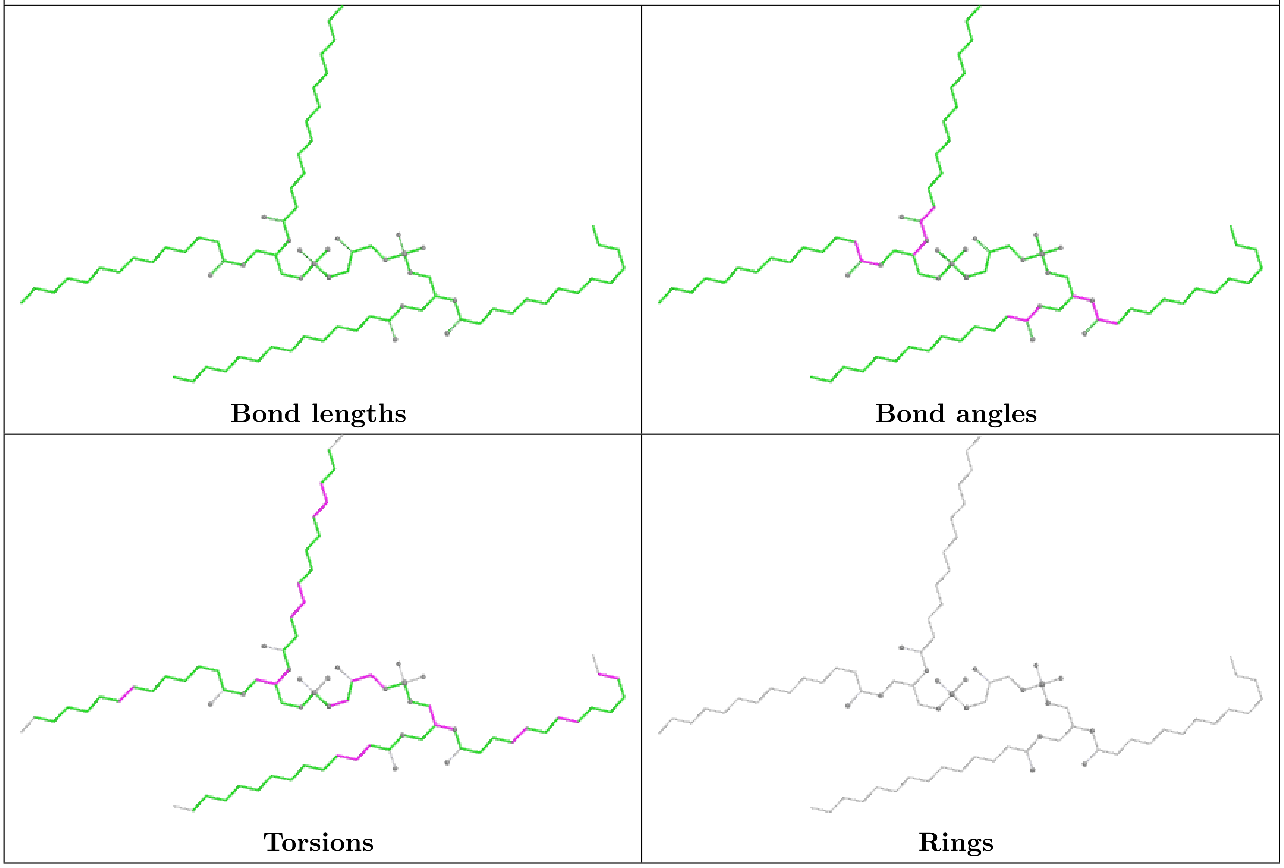
Bond lengths

Bond angles

Torsions

Rings

Ligand CD4 H 302



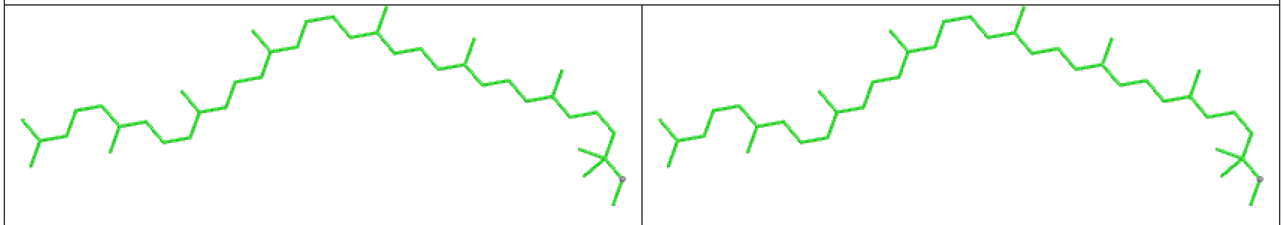
Bond lengths

Bond angles

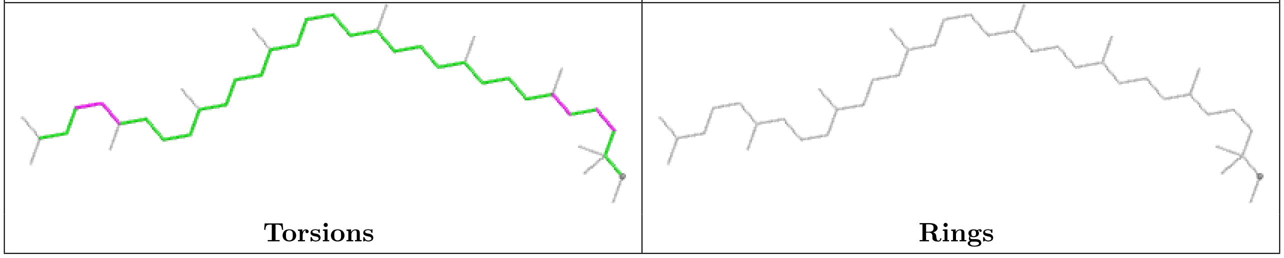
Torsions

Rings

Ligand SP2 BA 101

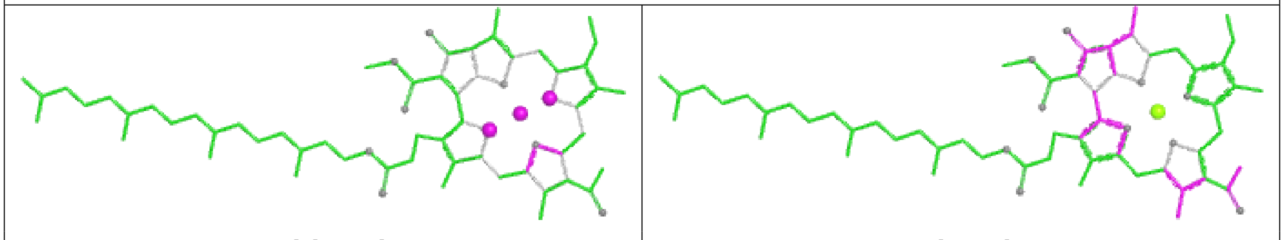


Bond lengths Bond angles

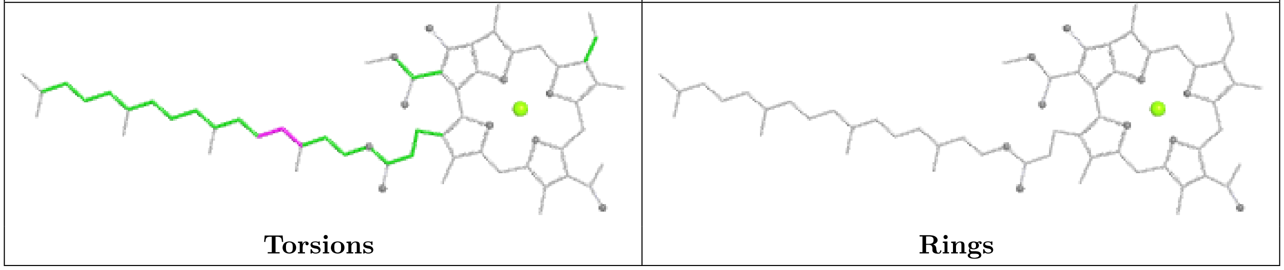


Torsions Rings

Ligand BCL ad 1001



Bond lengths Bond angles



Torsions Rings

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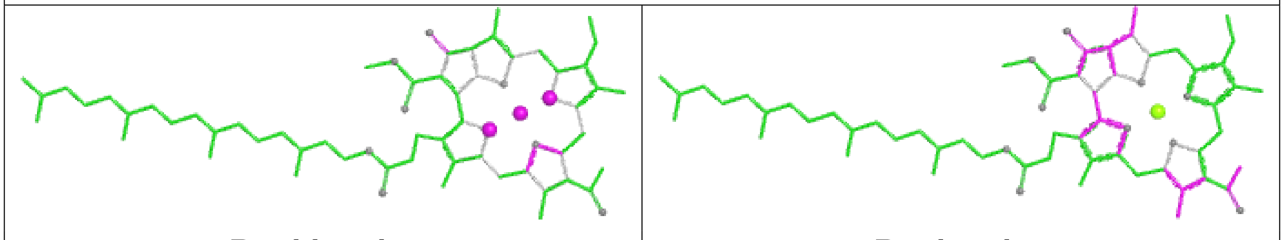
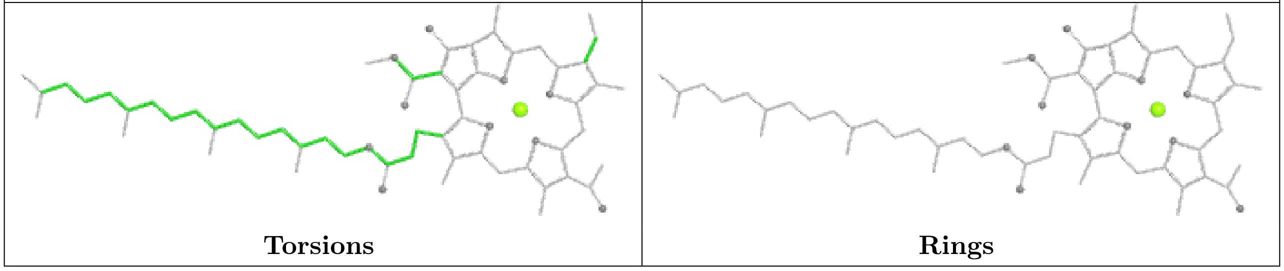
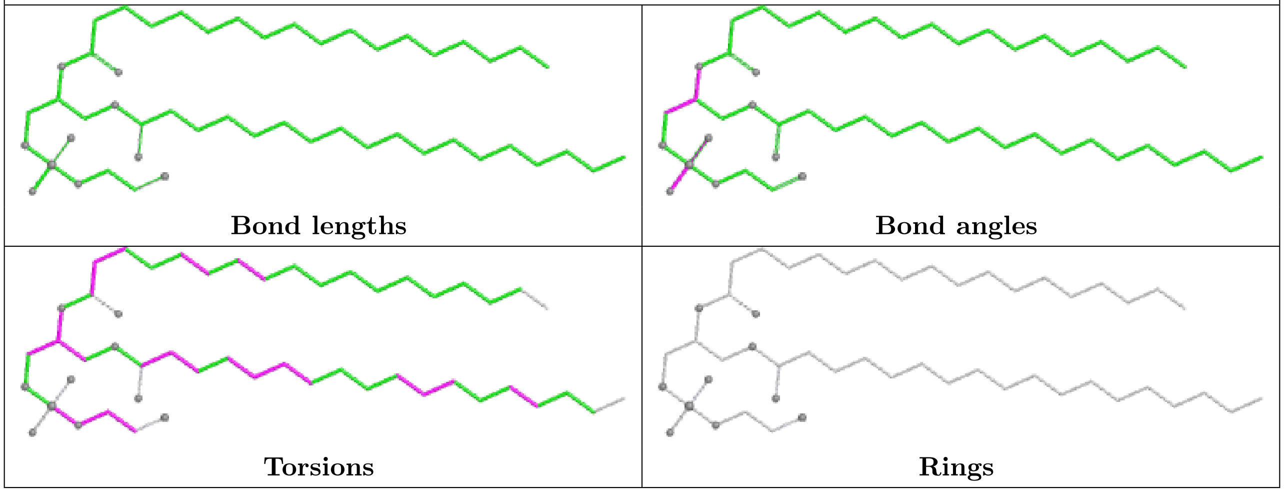


Bond lengths Bond angles



Torsions Rings

Ligand 3PE AC 102



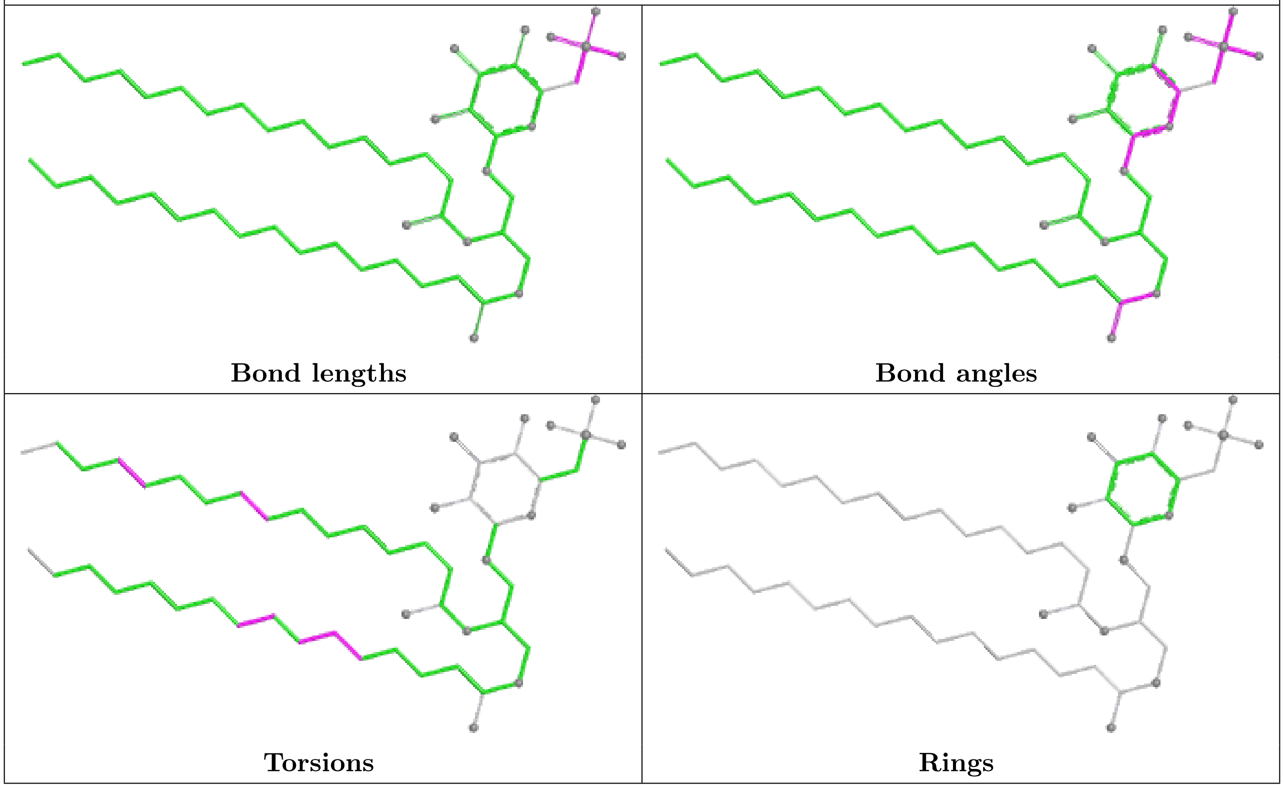
Bond lengths

Bond angles

Torsions

Rings

Ligand SQD x 100



Bond lengths

Bond angles

Torsions

Rings

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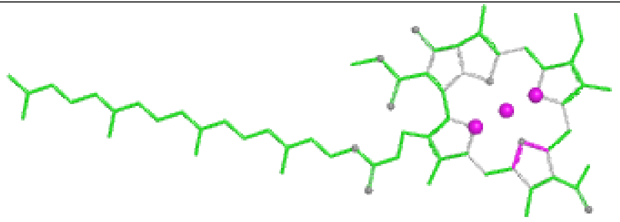
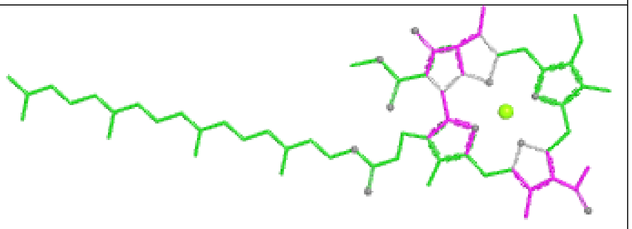
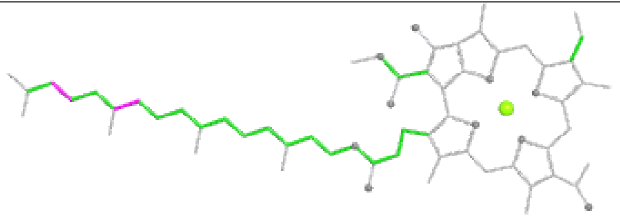


Bond lengths



Bond angles



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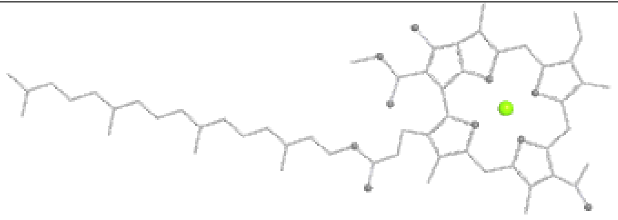
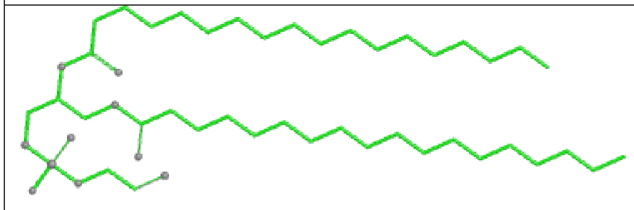


Rings

Ligand 3PE h 301



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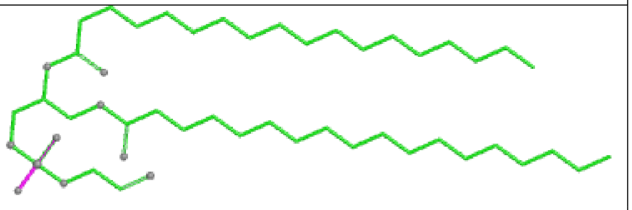
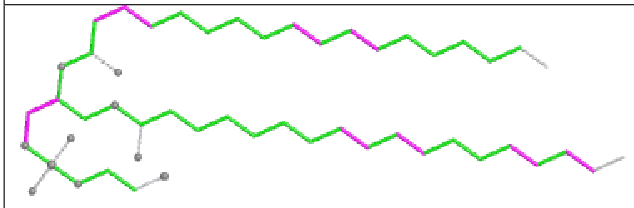


Bond angles



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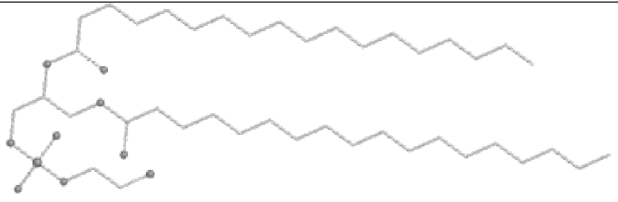
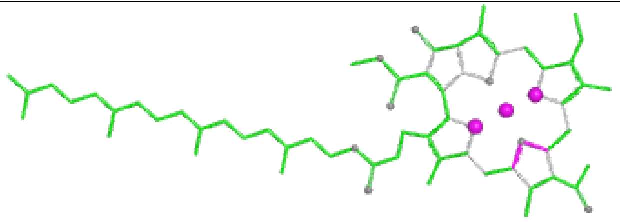


Rings

Ligand BCL af 101



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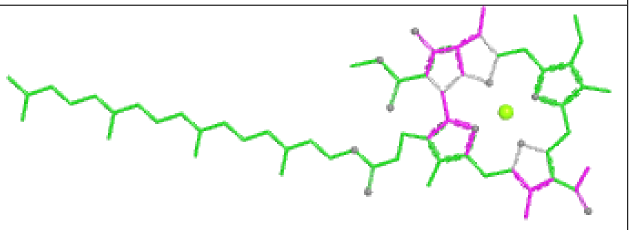
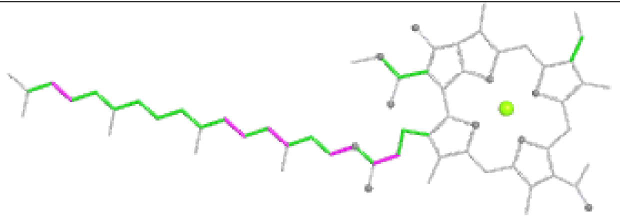


Bond angles



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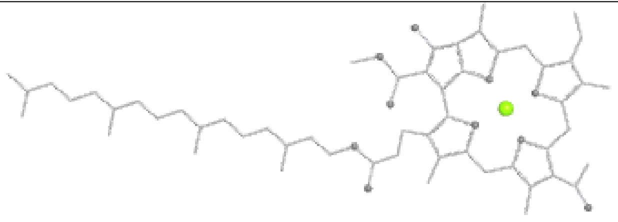
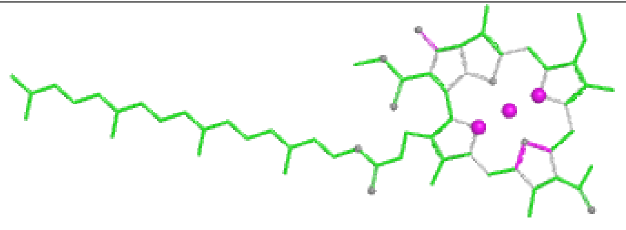


Rings

Ligand BCL AN 101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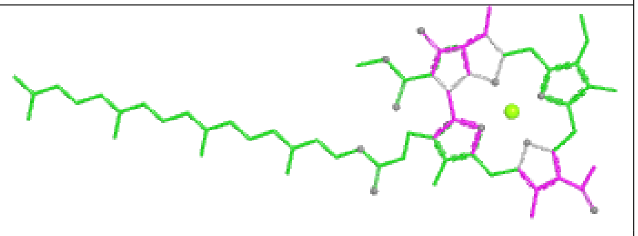
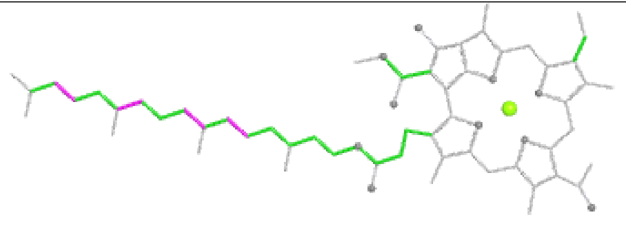

Bond angles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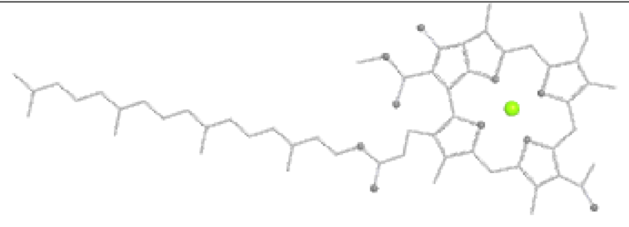
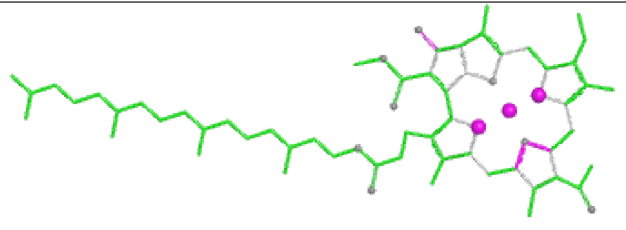

Rings

Ligand BCL bm 1001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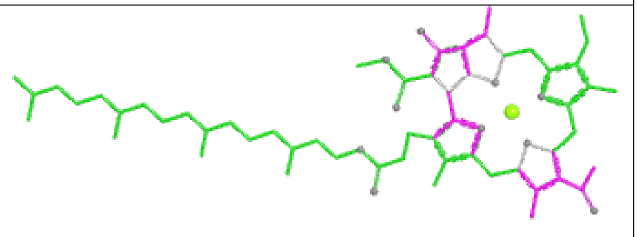
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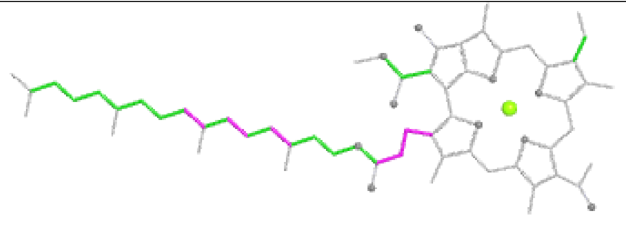
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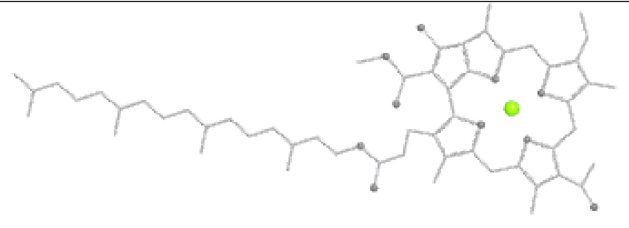
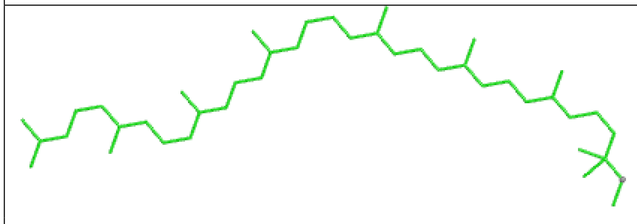

Rings

Ligand SP2 AI 101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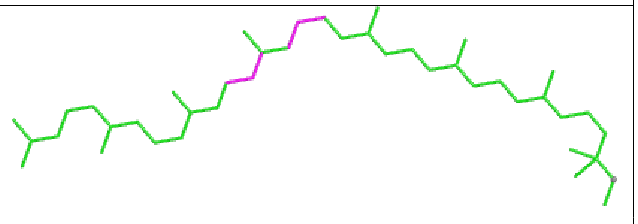
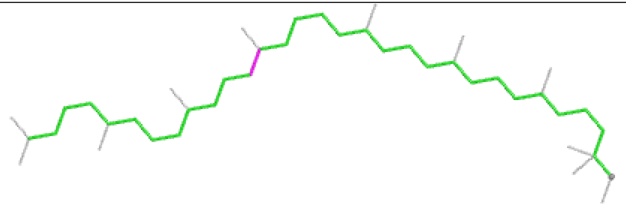

Bond angles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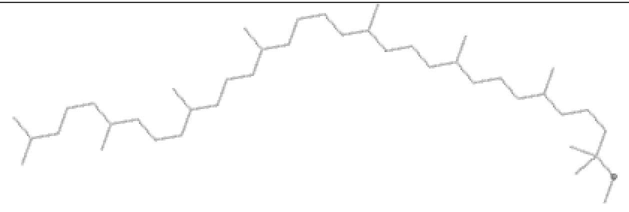
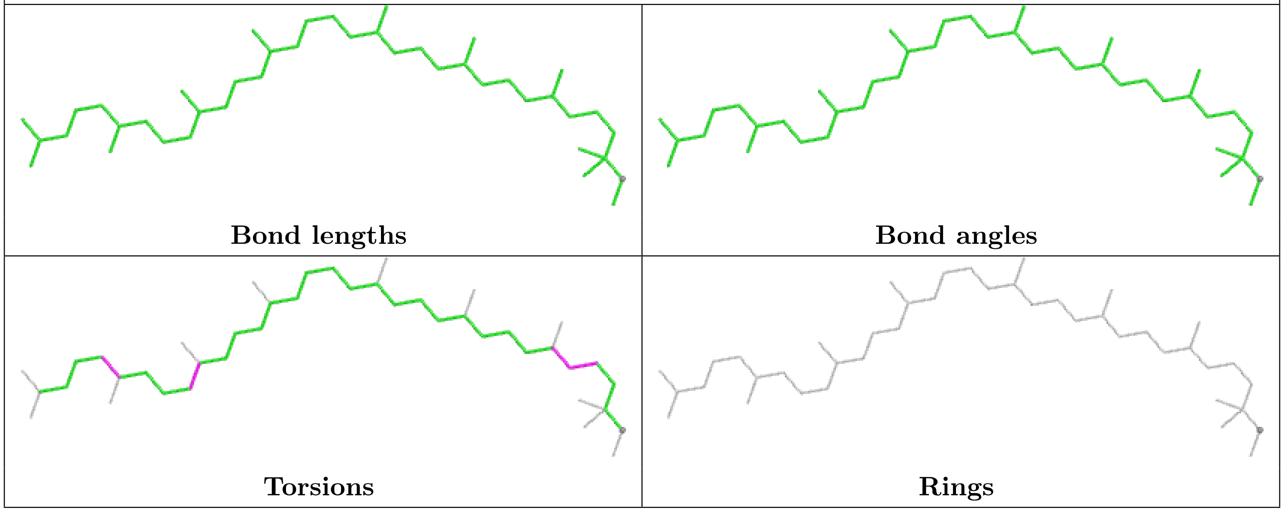
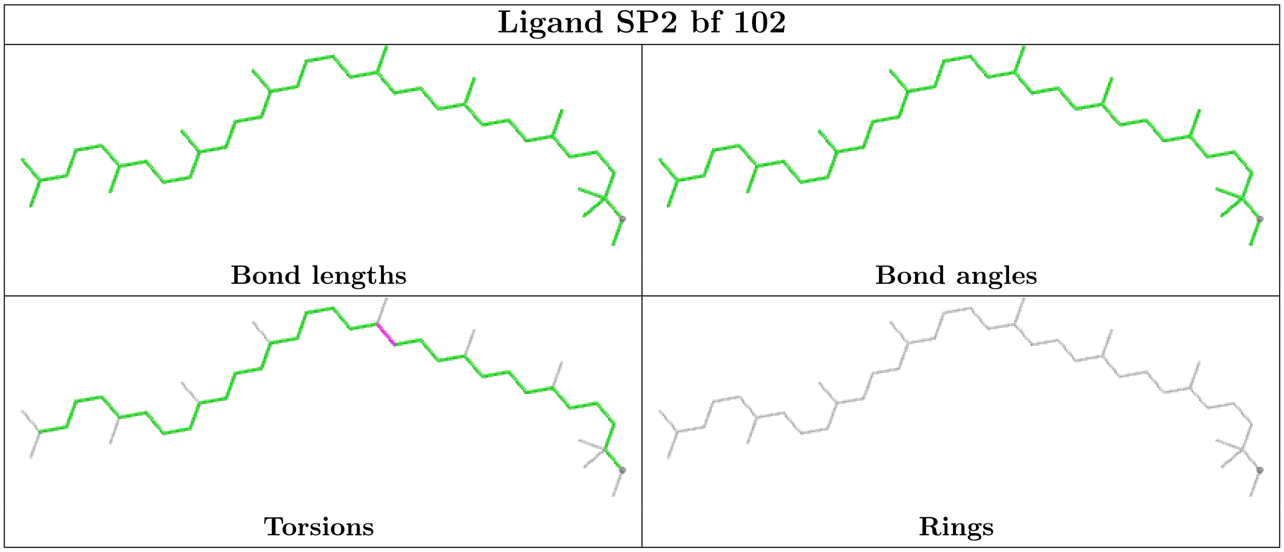

Rings

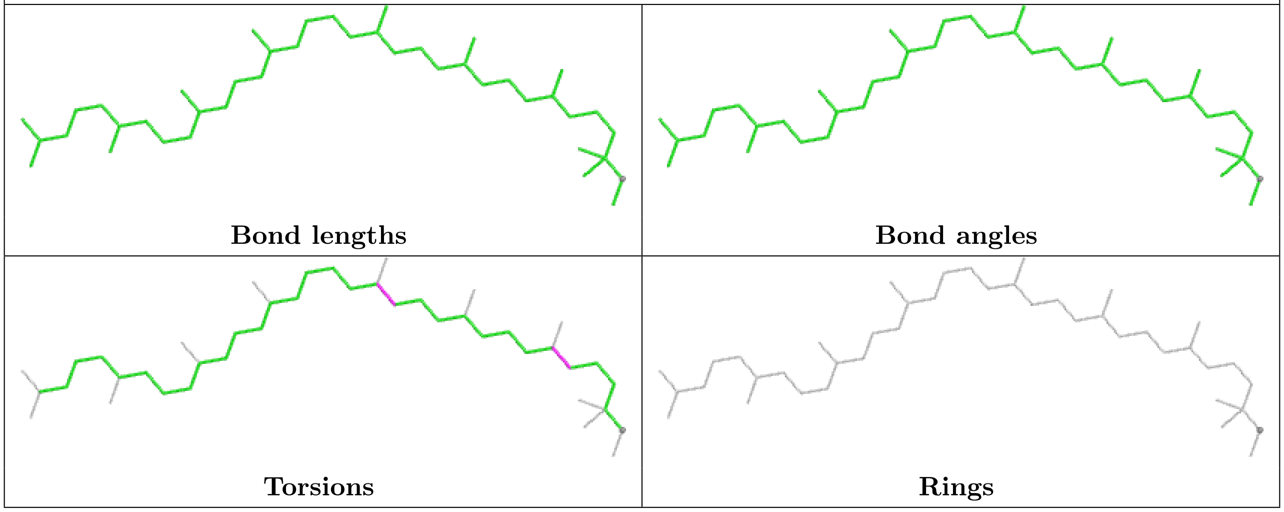
Ligand SP2 BJ 101



Ligand SP2 bf 102



Ligand SP2 M 1005



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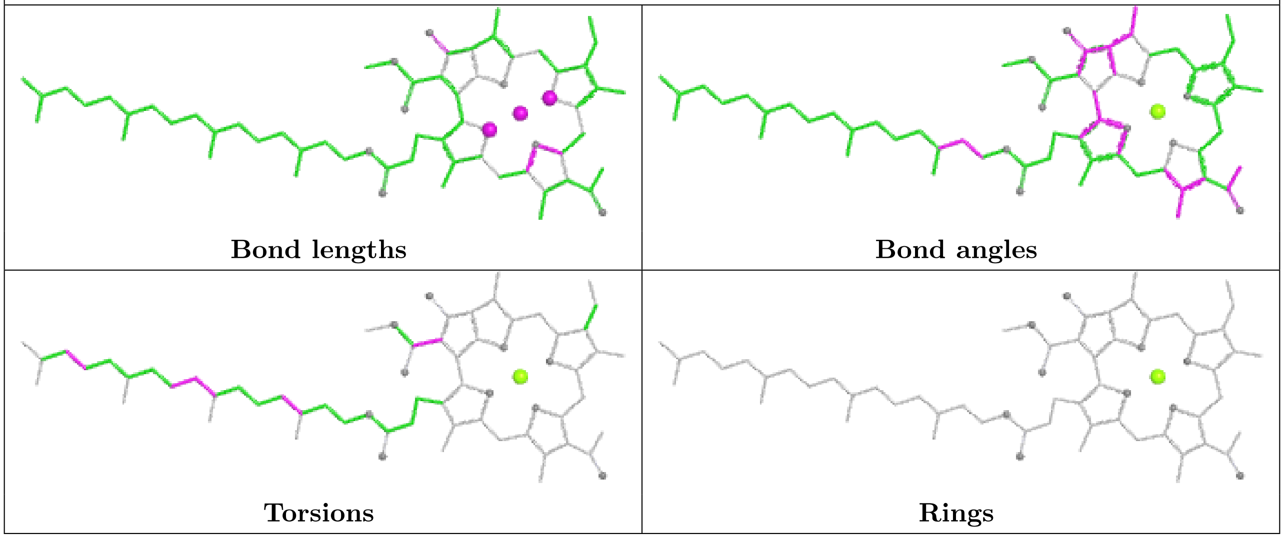

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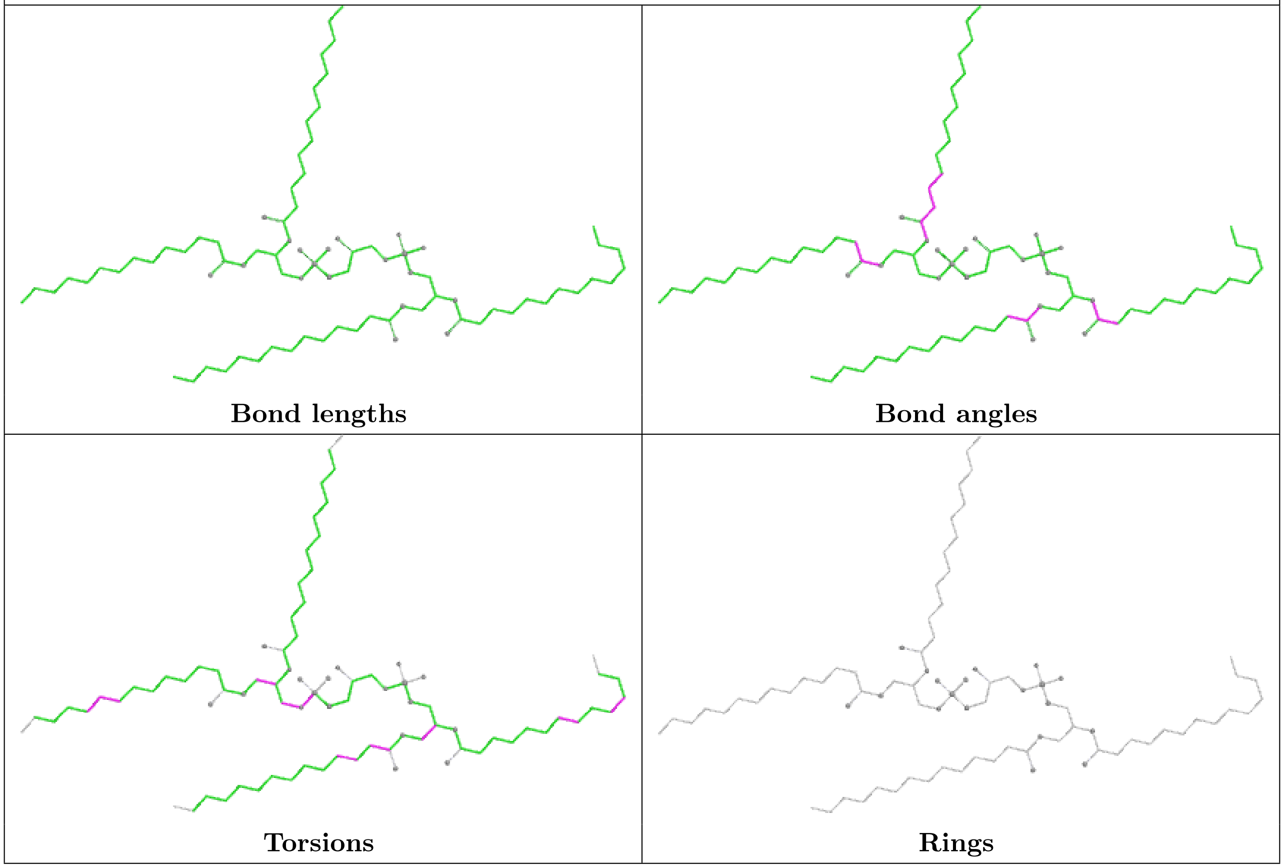

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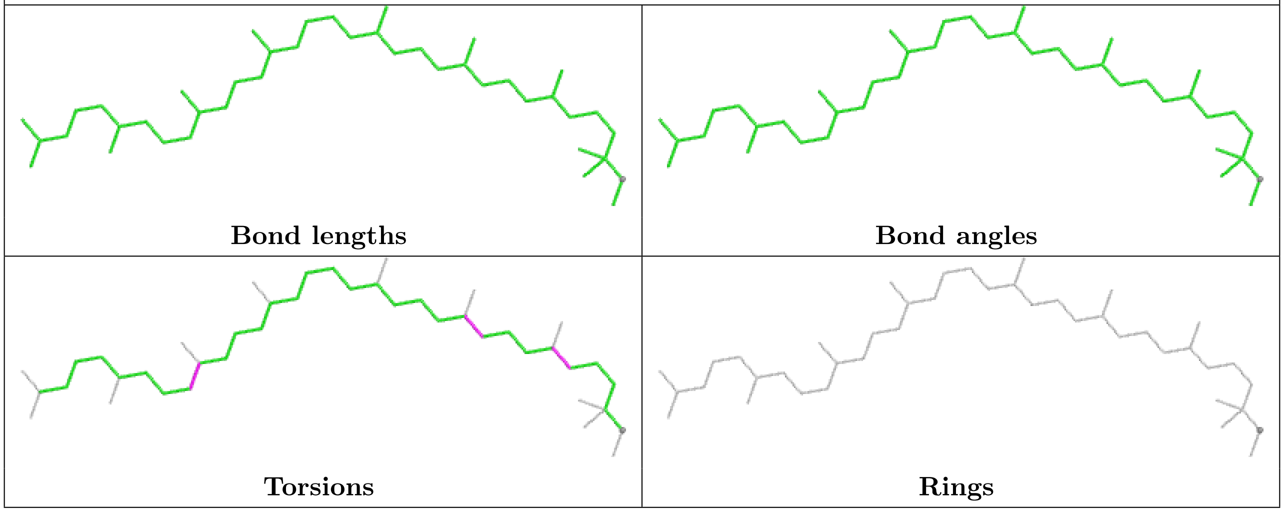


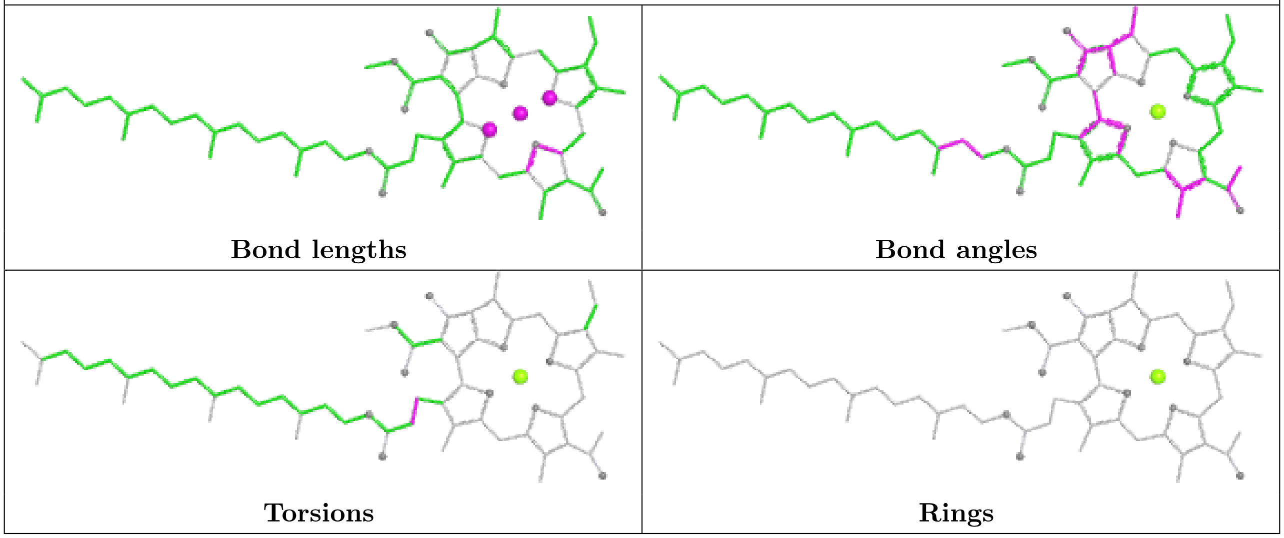
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL bd 101



Bond lengths

Bond angles

Torsions

Rings

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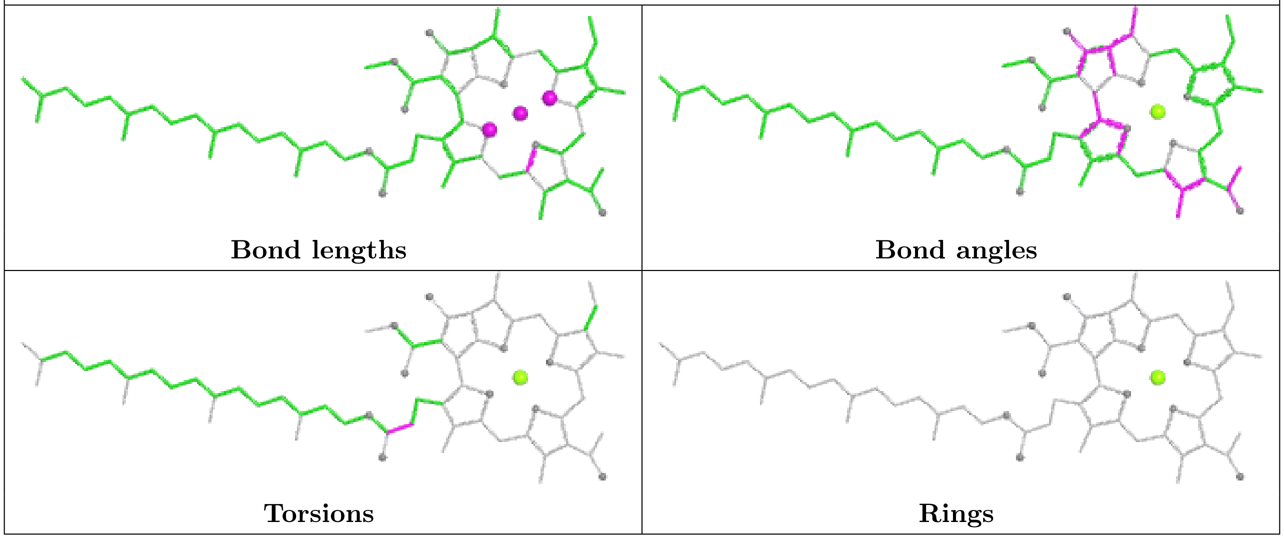


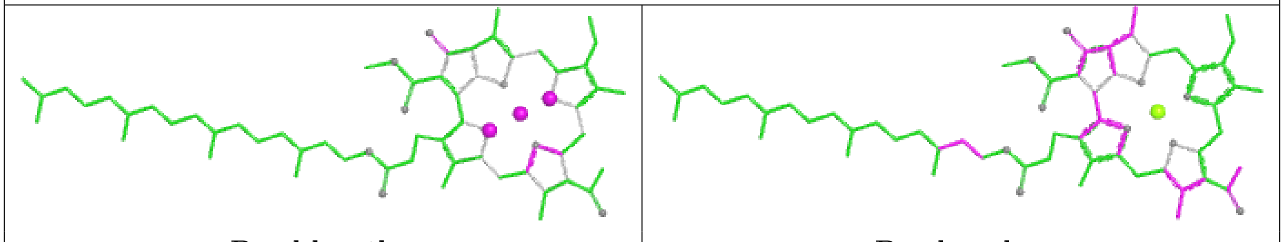
Bond lengths

Bond angles

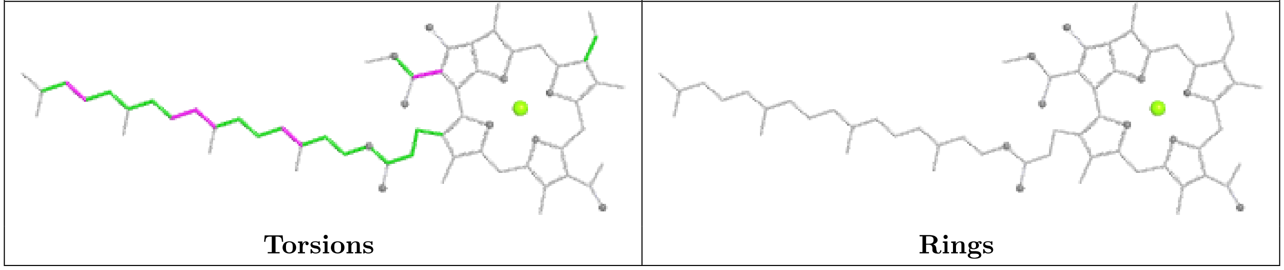
Torsions

Rings

Ligand BCL ak 101

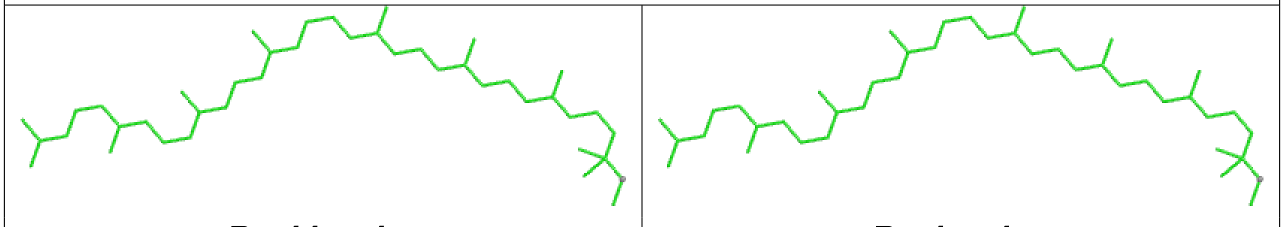


Bond lengths Bond angles

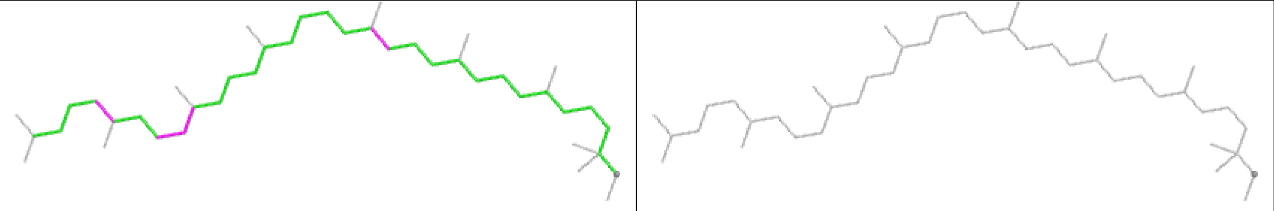


Torsions Rings

Ligand SP2 AC 104

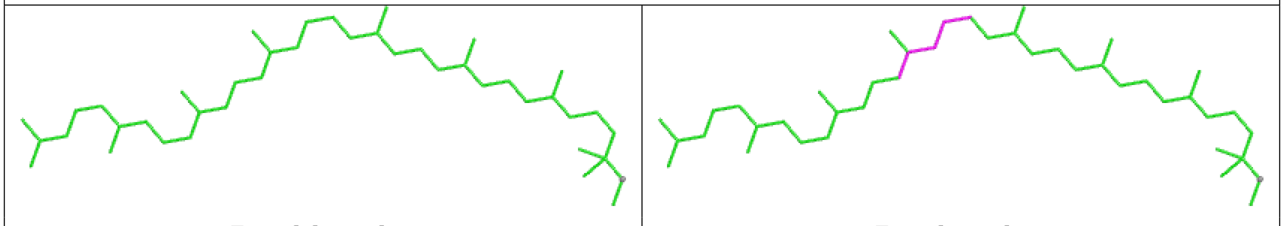


Bond lengths Bond angles

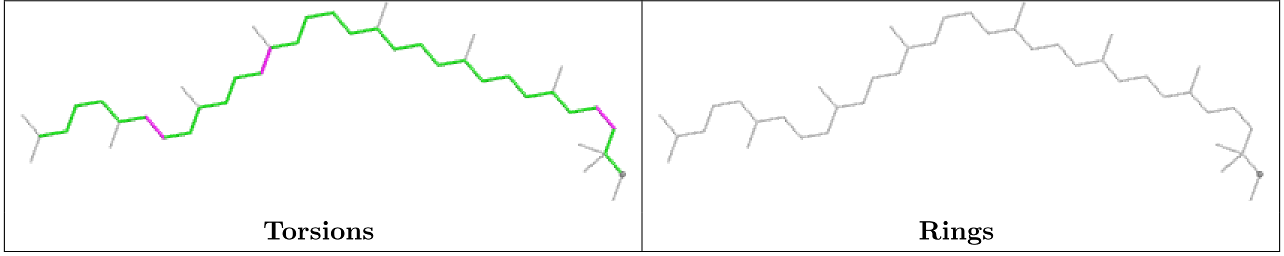


Torsions Rings

Ligand SP2 AI 103

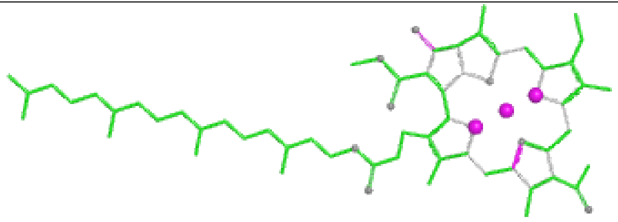


Bond lengths Bond angles

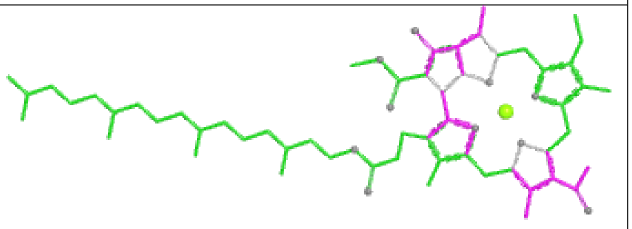


Torsions Rings

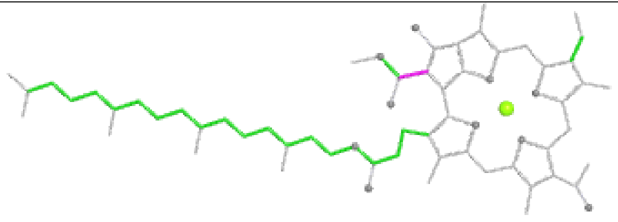
Ligand BCL l 301



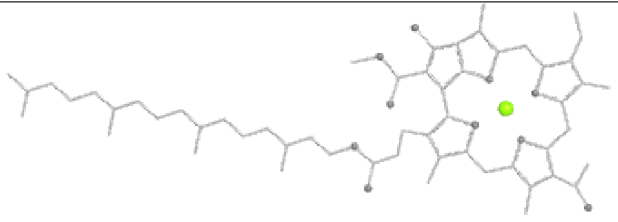
Bond lengths



Bond angles

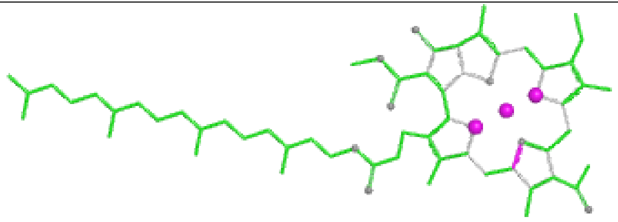


Torsions

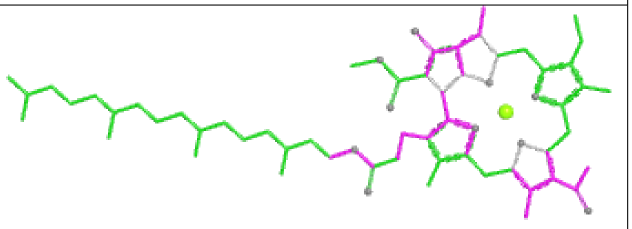


Rings

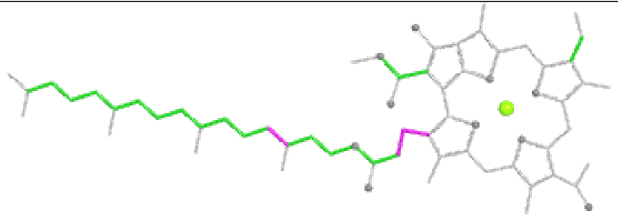
Ligand BCL ba 102



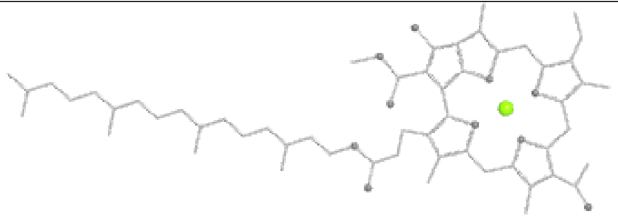
Bond lengths



Bond angles

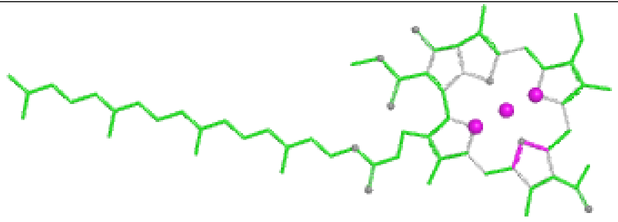


Torsions



Rings

Ligand BCL bi 101



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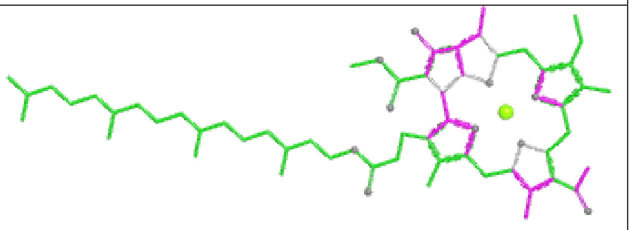

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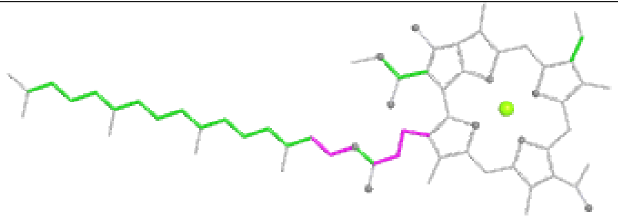

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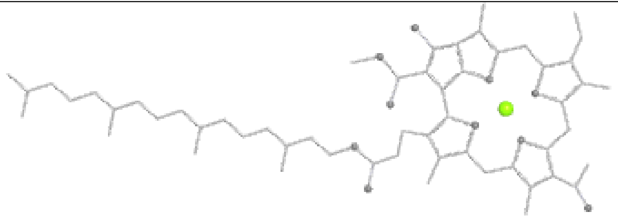

Rings

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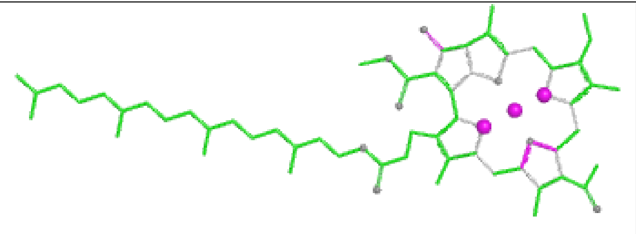
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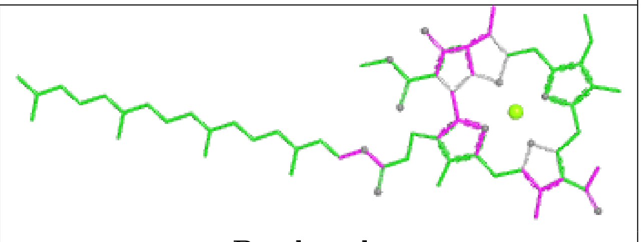
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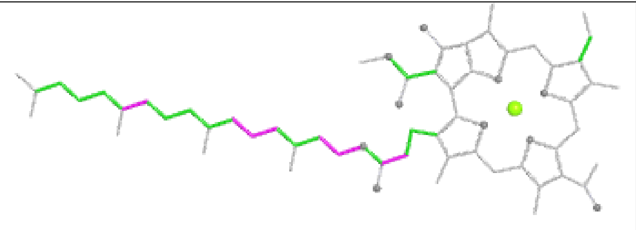
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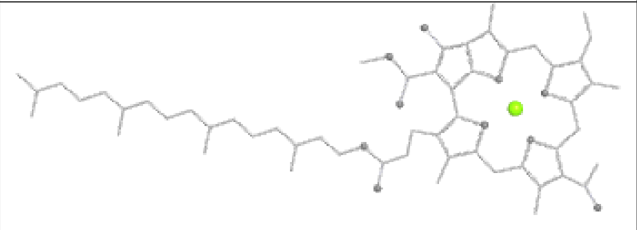
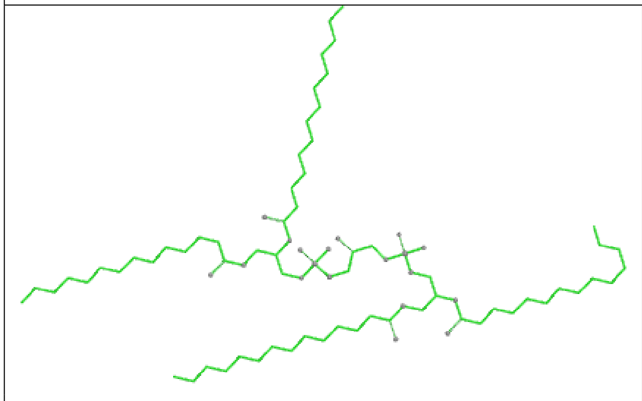

Rings

Ligand CD4 h 302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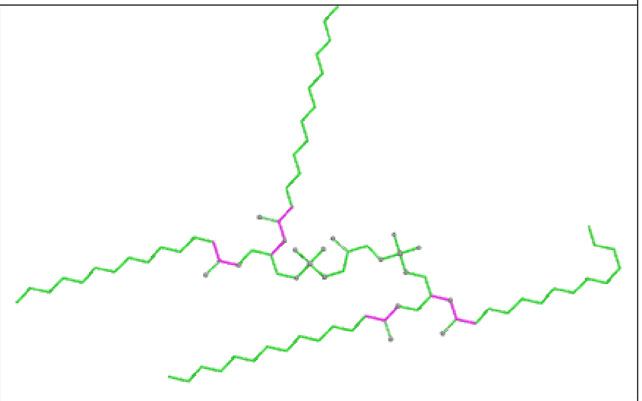
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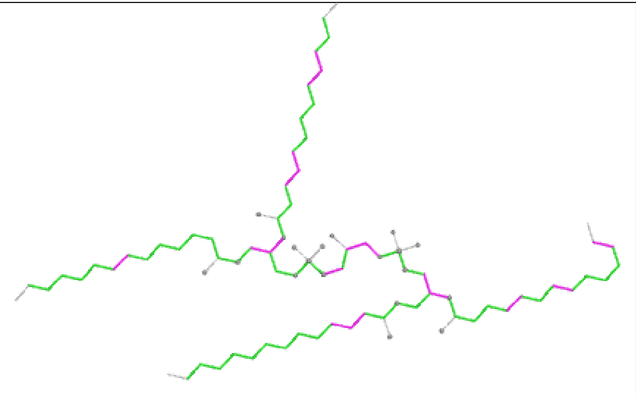
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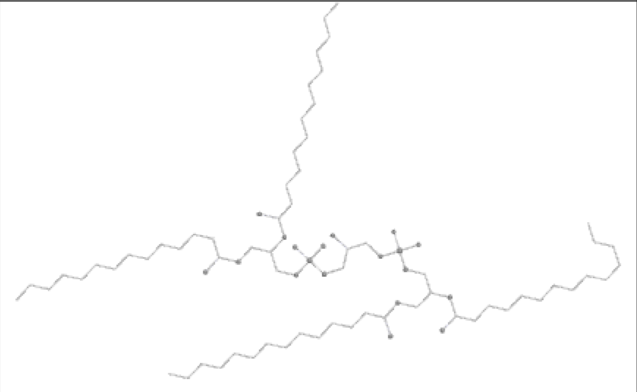
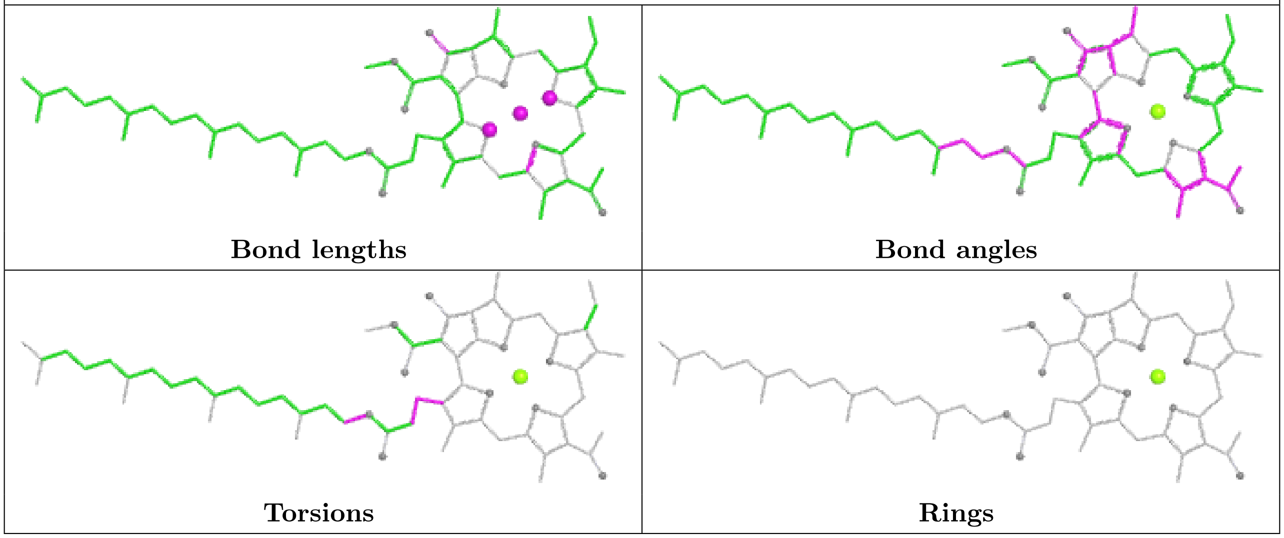

Rings

Ligand BCL bb 1001



Bond lengths

Bond angles

Torsions

Rings

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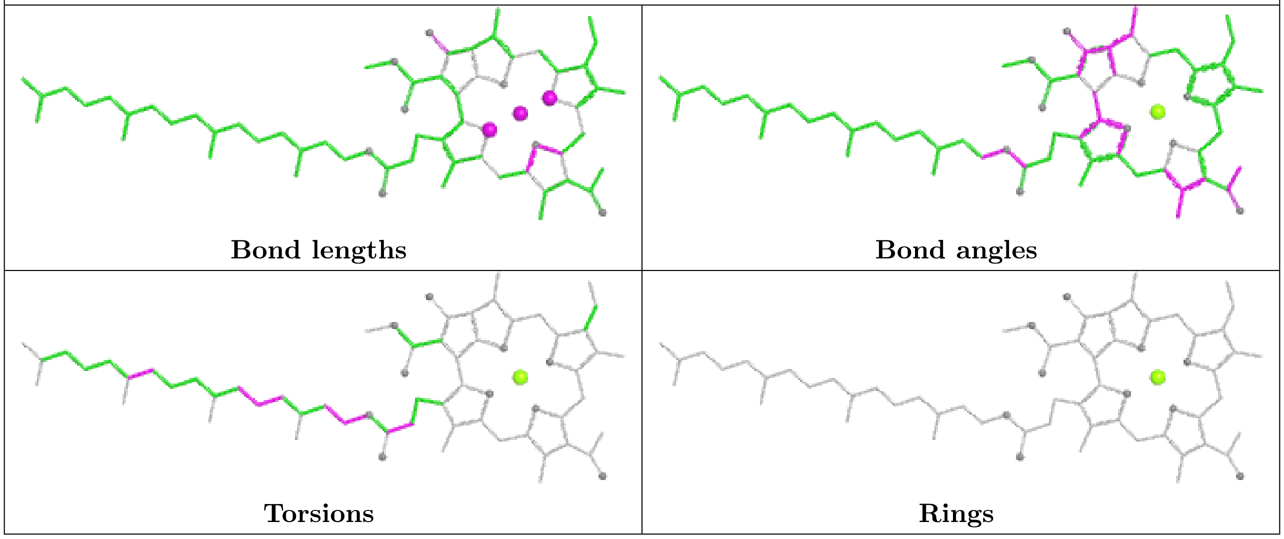

Bond lengths

Bond angles

Torsions

Rings

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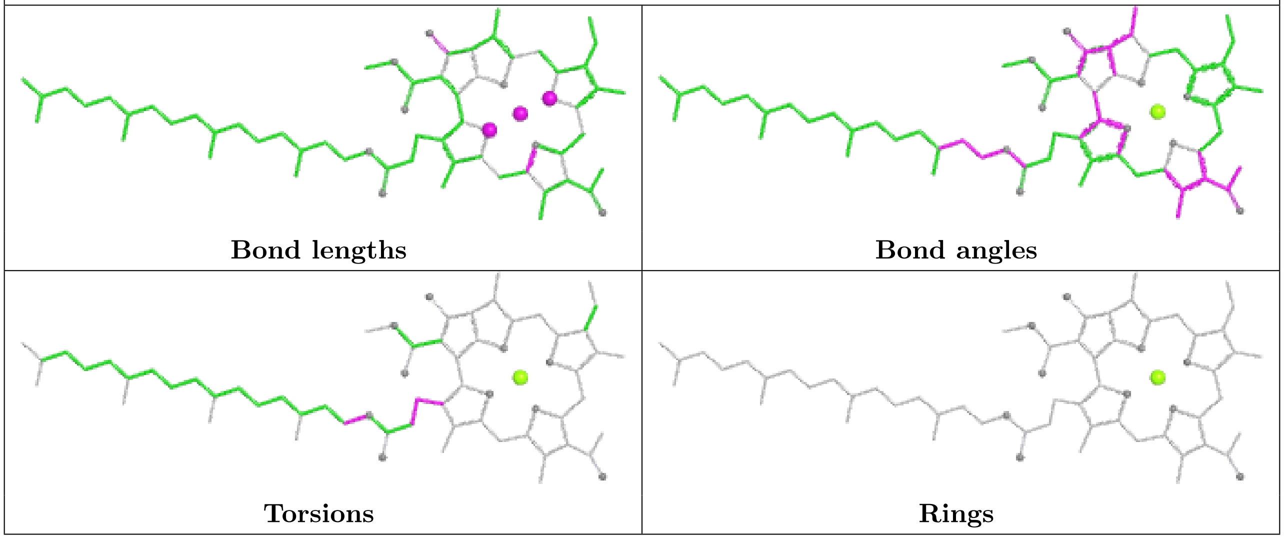

Bond lengths

Bond angles

Torsions

Rings

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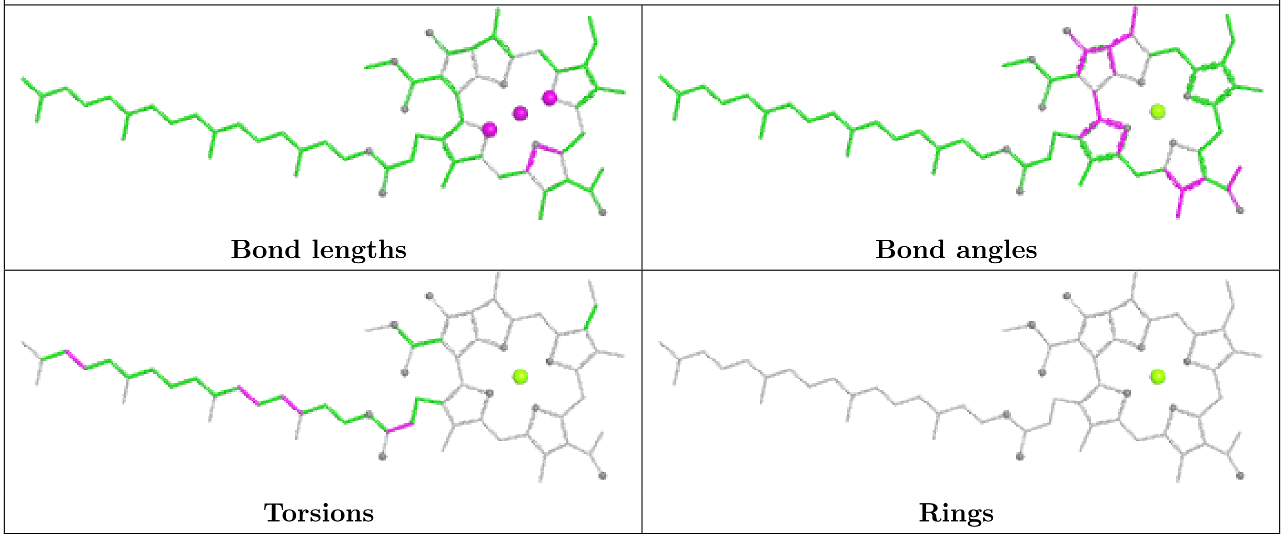


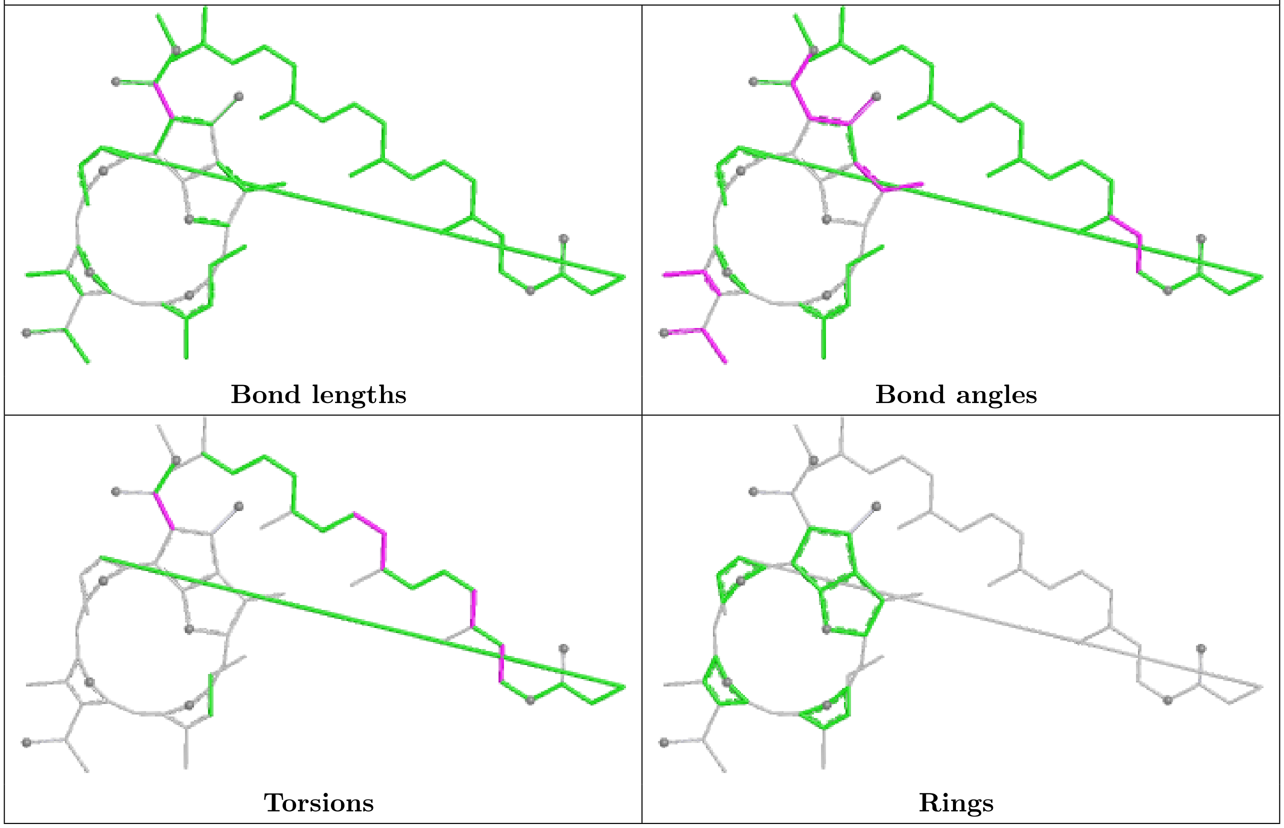
Bond lengths

Bond angles

Torsions

Rings

Ligand BPH l 302



Bond lengths

Bond angles

Torsions

Rings

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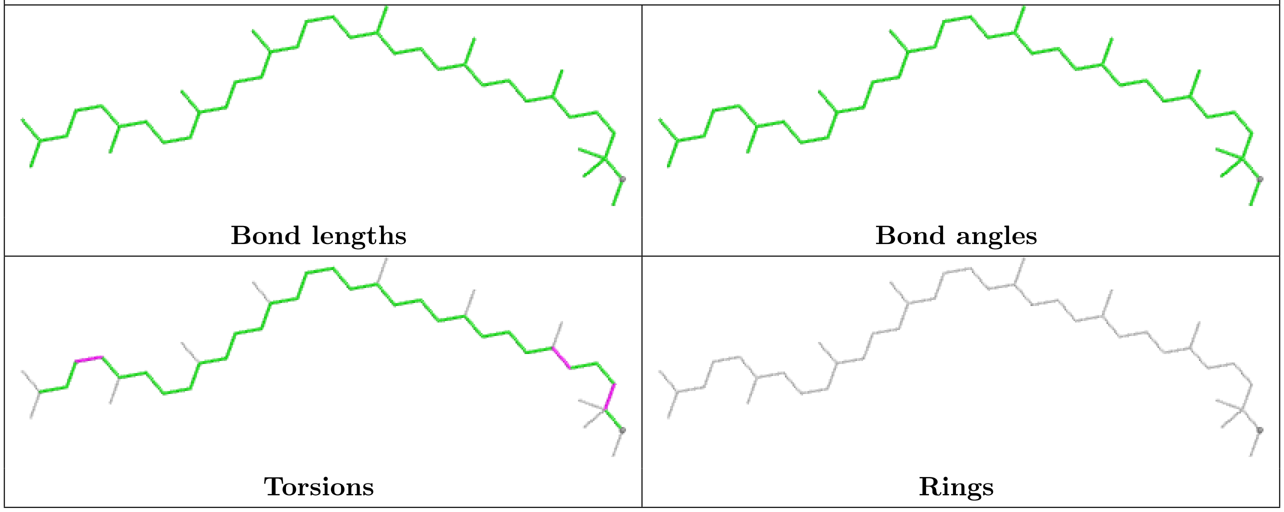

Bond lengths

Bond angles

Torsions

Rings

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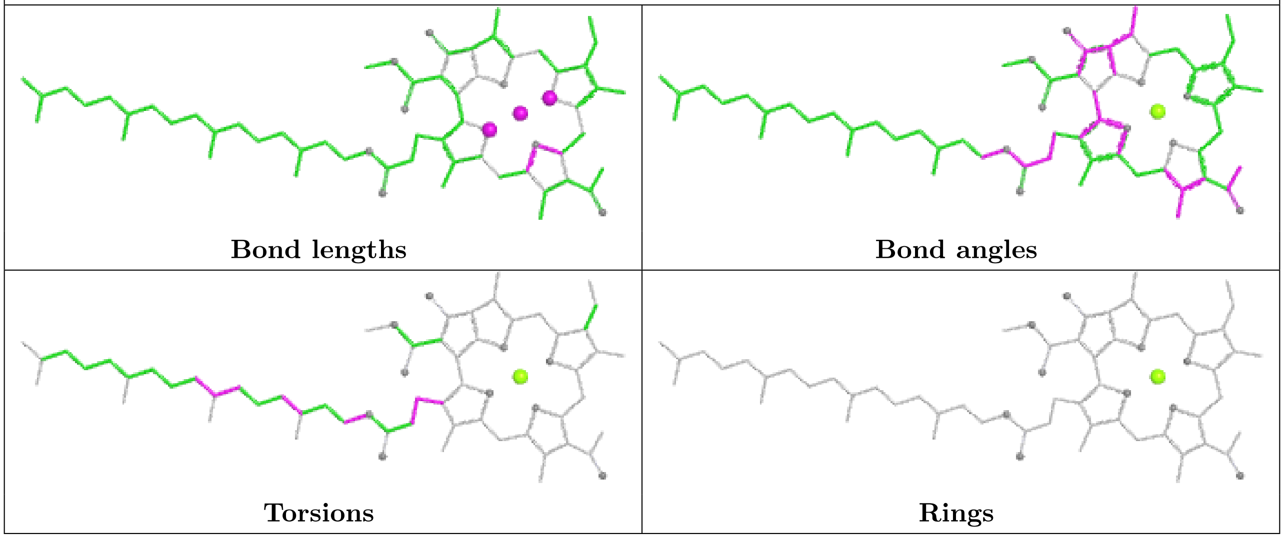

Bond lengths

Bond angles

Torsions

Rings

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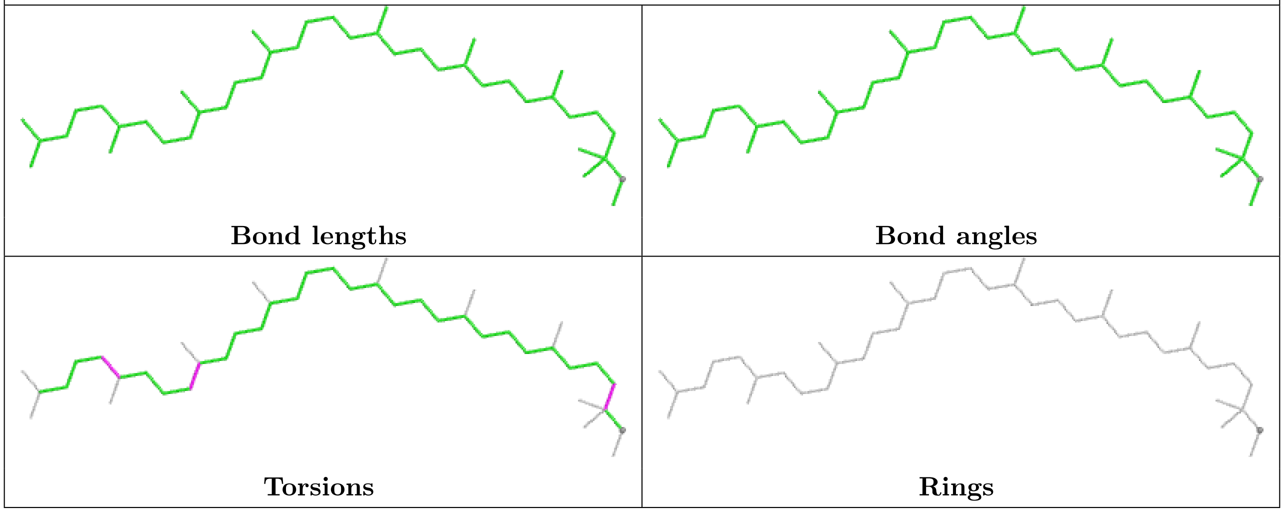

Bond lengths

Bond angles

Torsions

Rings

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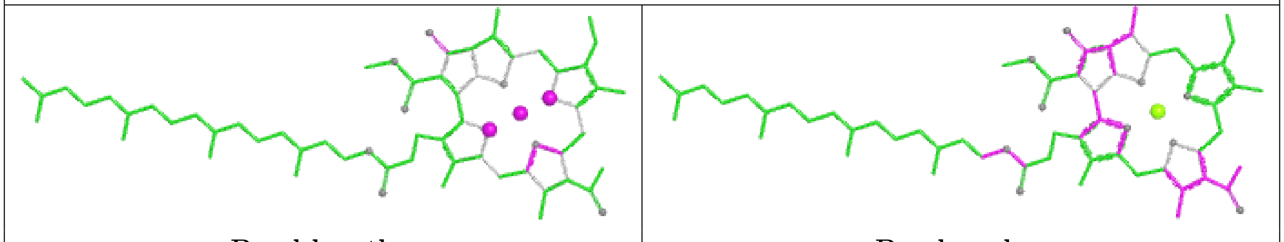
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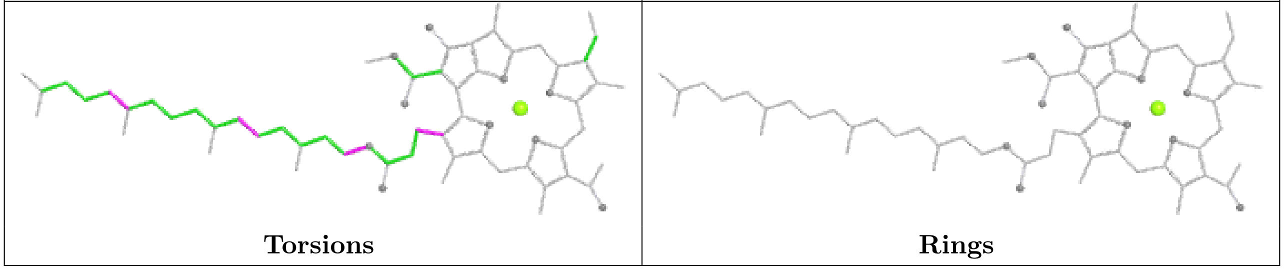
Torsions Rings

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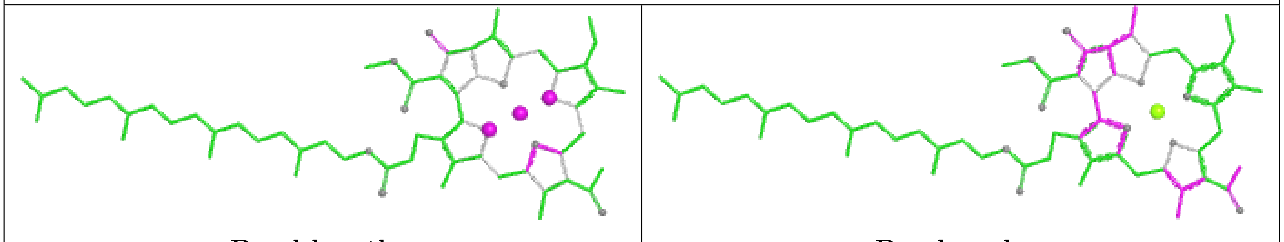
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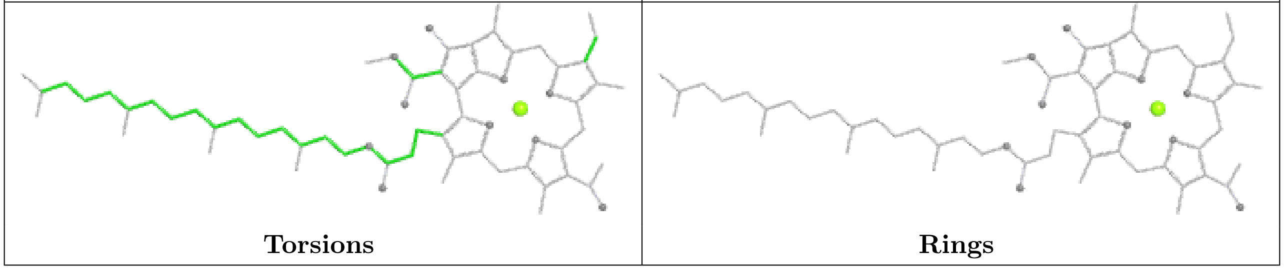
Torsions Rings

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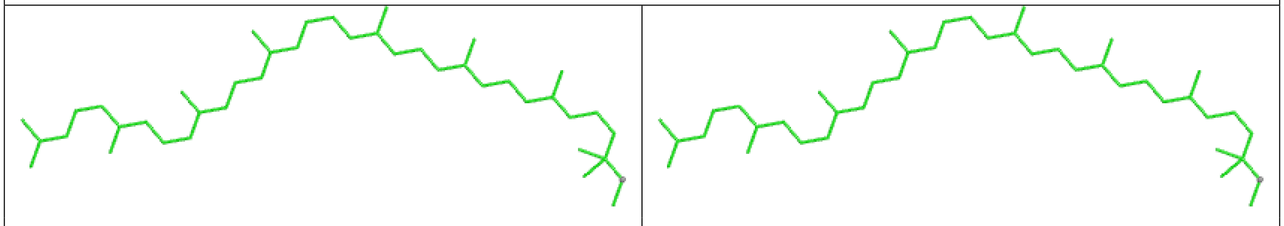
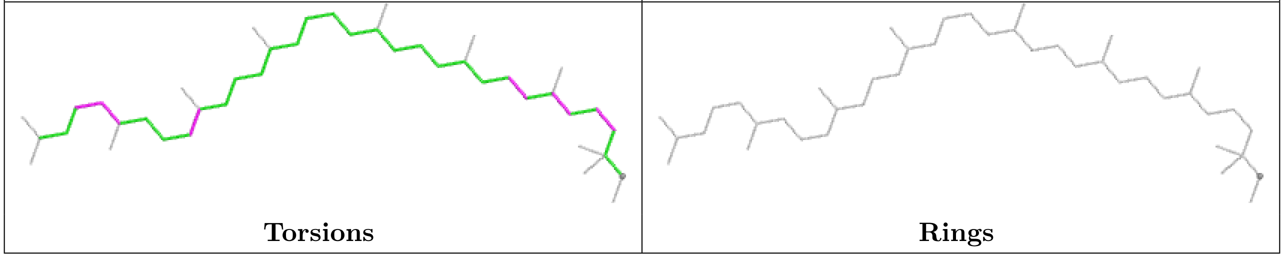

Bond lengths Bond angles


Torsions Rings

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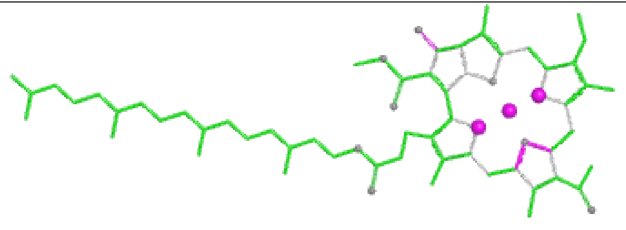
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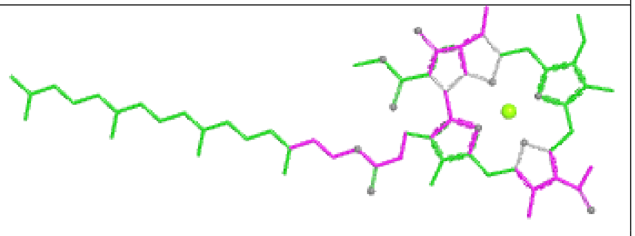
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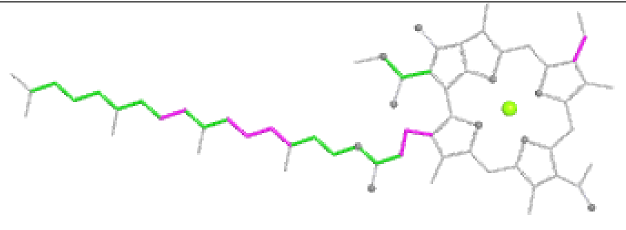
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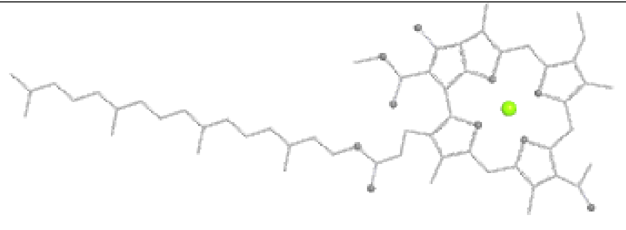
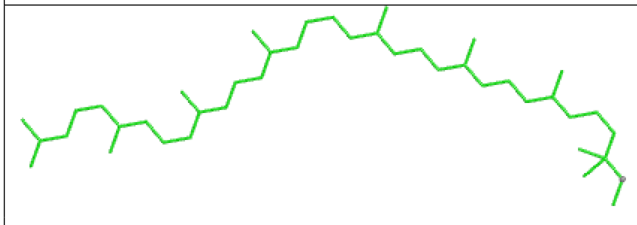

Rings

Ligand SP2 al 1002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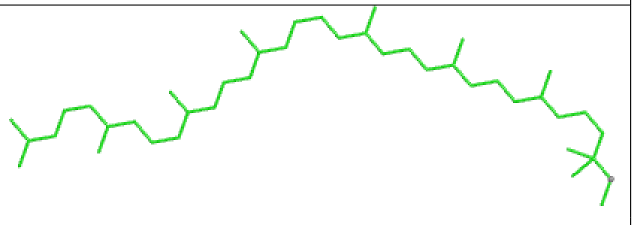
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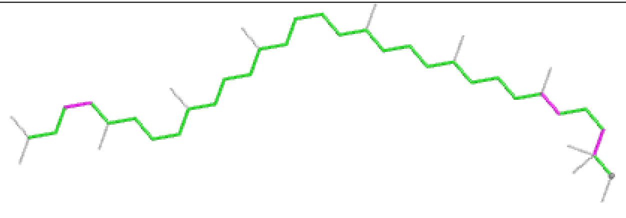
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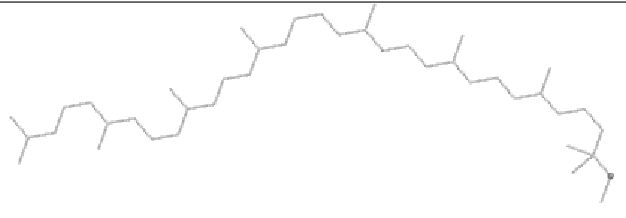
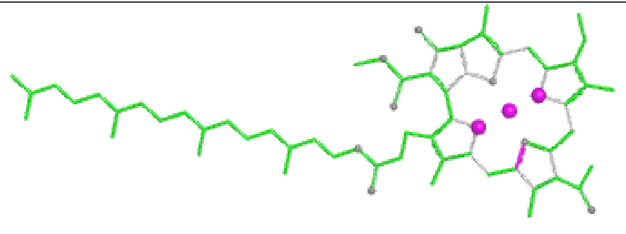

Rings

Ligand BCL m 1006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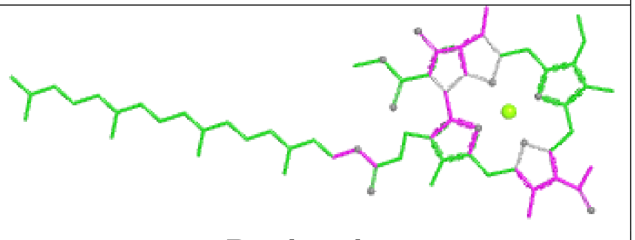
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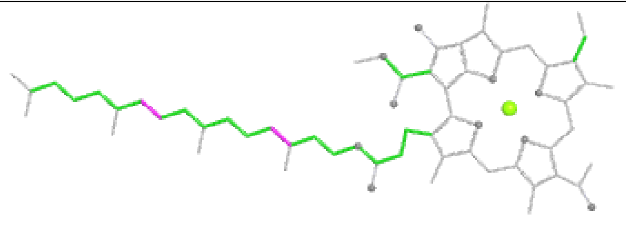
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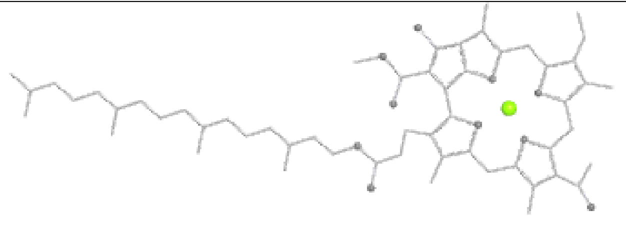
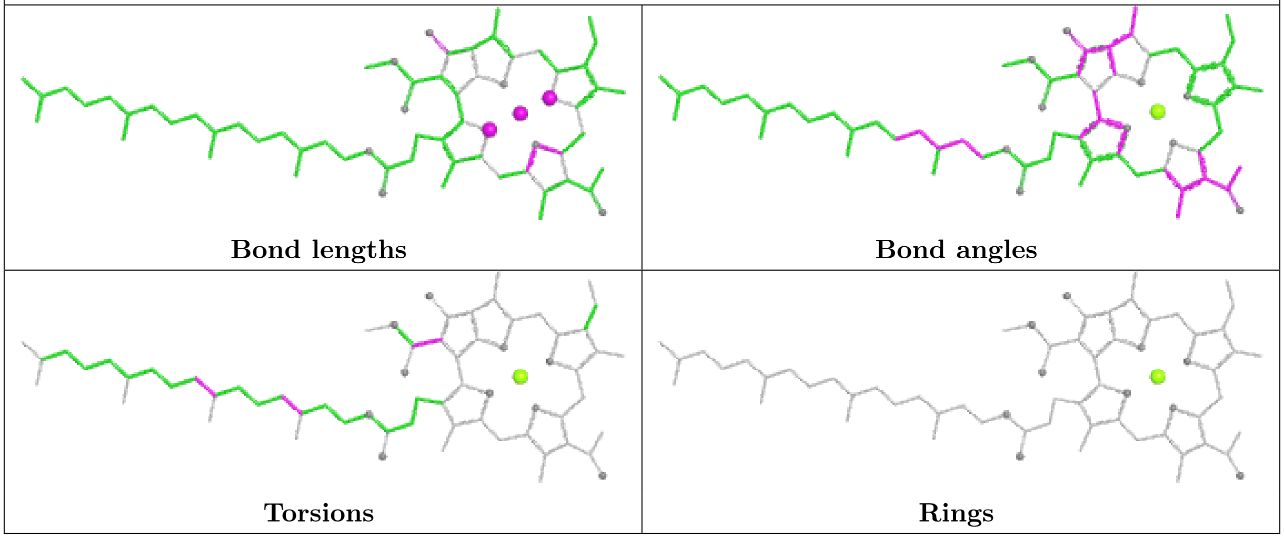

Rings

Ligand BCL aj 101



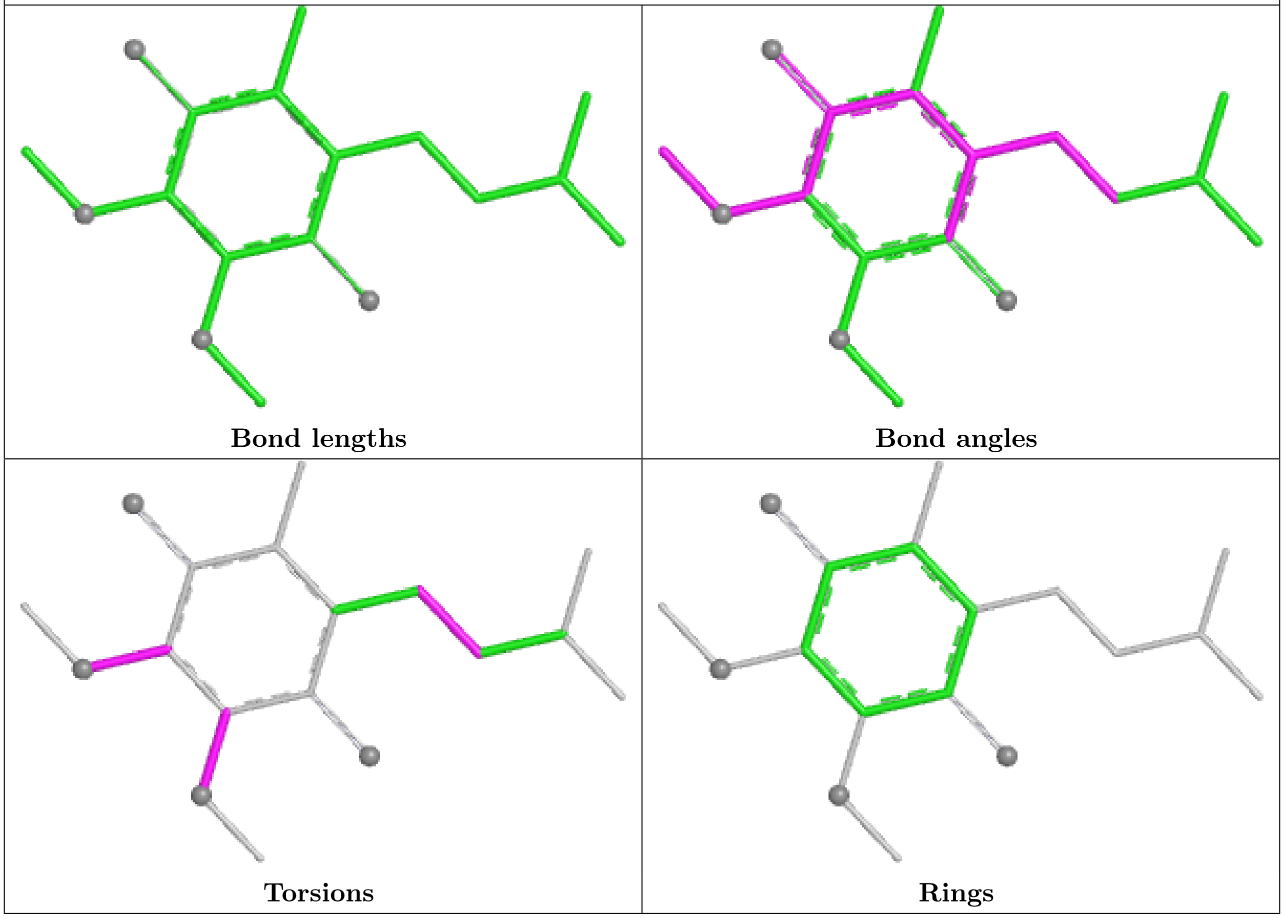
Bond lengths

Bond angles

Torsions

Rings

Ligand UQ1 l 304



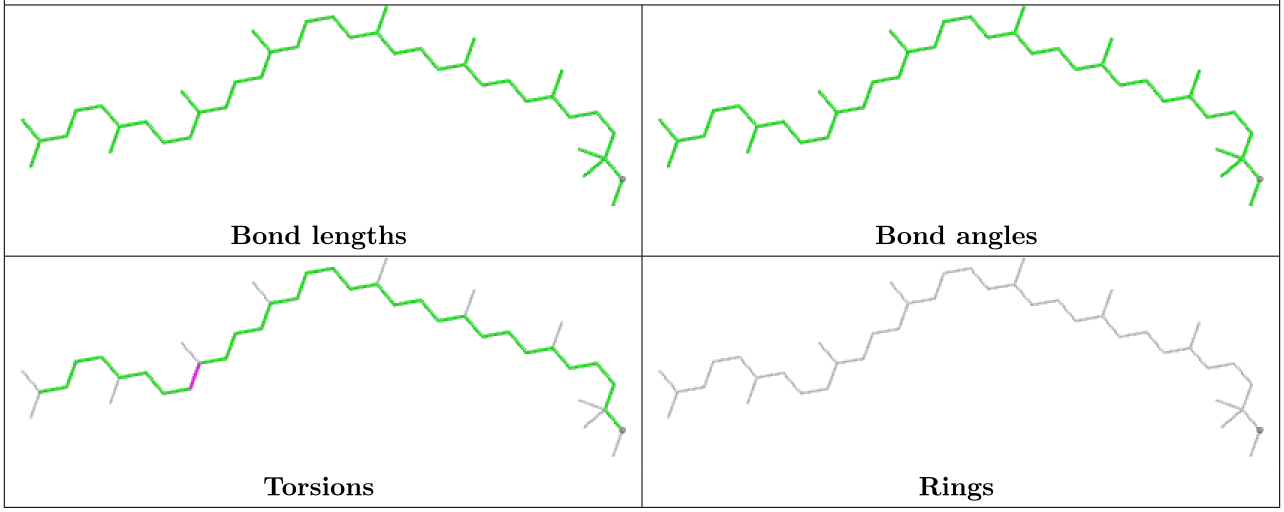
Bond lengths

Bond angles

Torsions

Rings

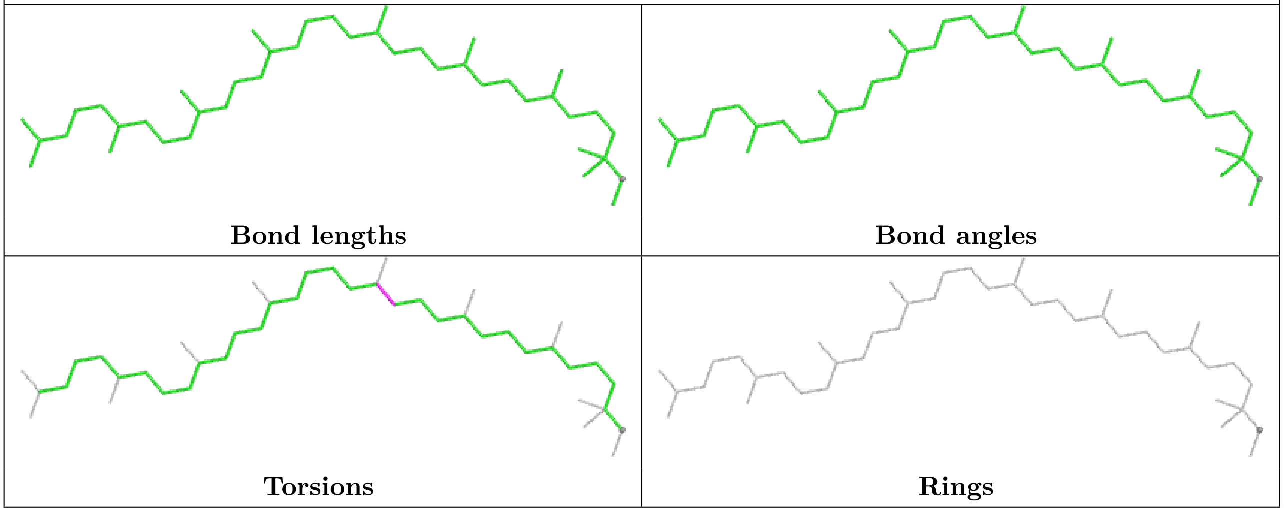
Ligand SP2 am 1000



Bond lengths Bond angles

Torsions Rings

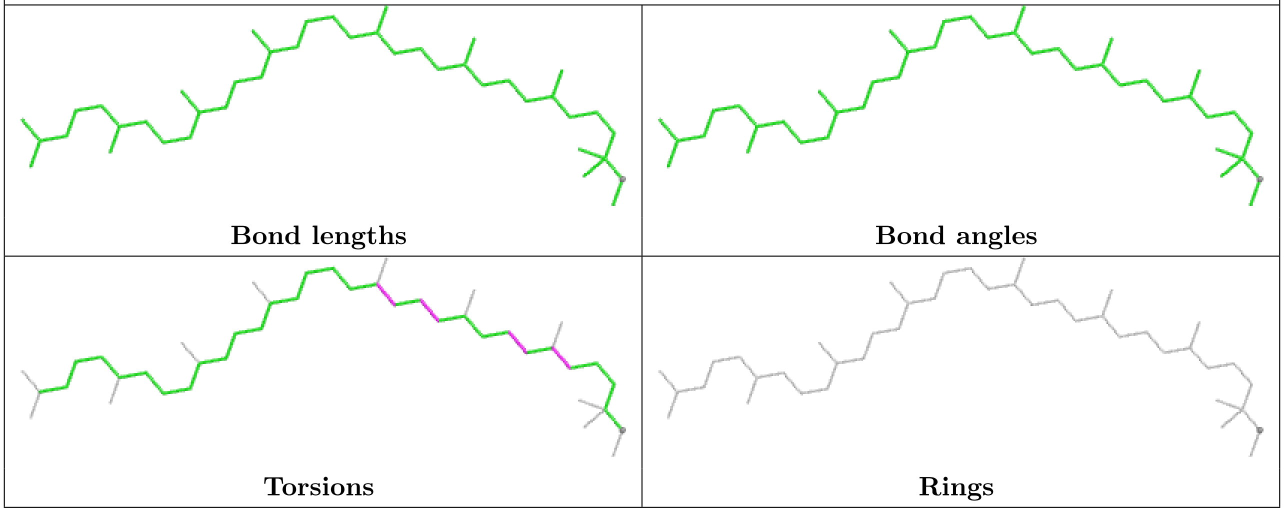
Ligand SP2 bl 102



Bond lengths Bond angles

Torsions Rings

Ligand SP2 BH 101



Bond lengths Bond angles

Torsions Rings

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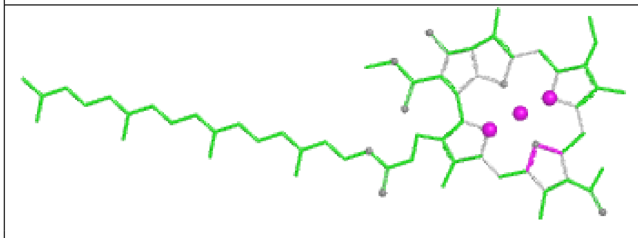
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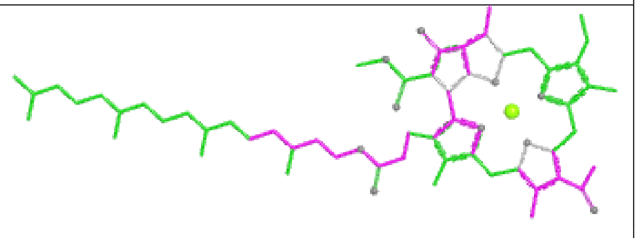
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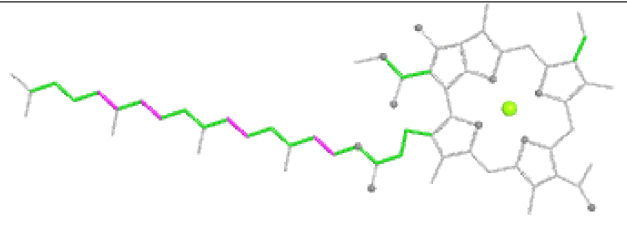
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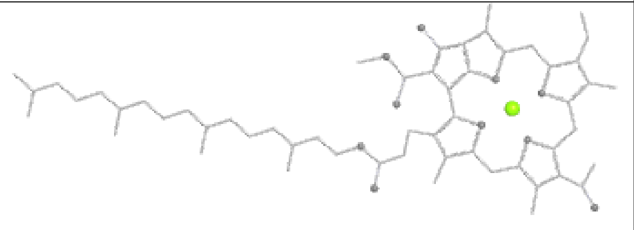
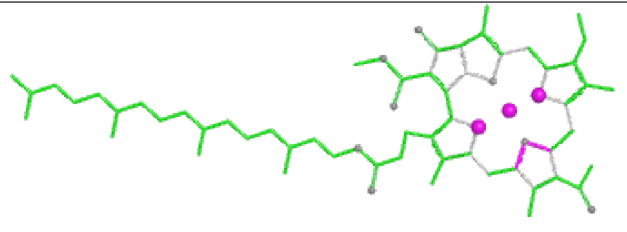

Rings

Ligand BCL be 1001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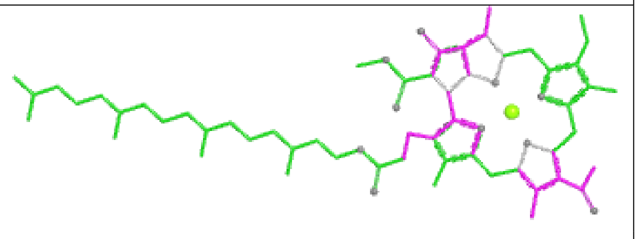
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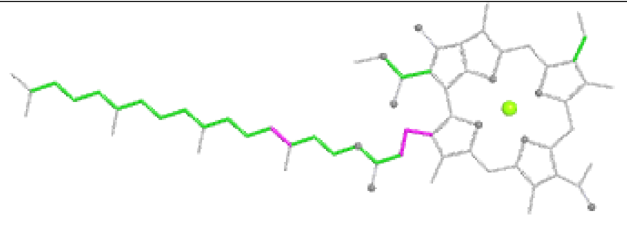
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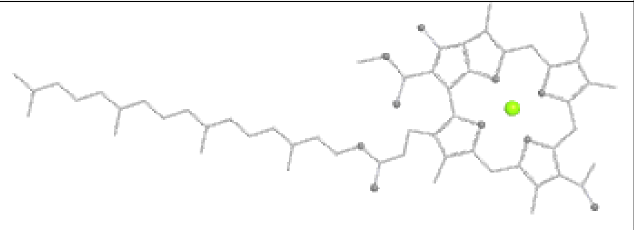
Rings

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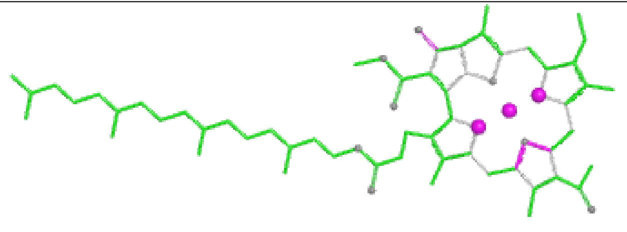
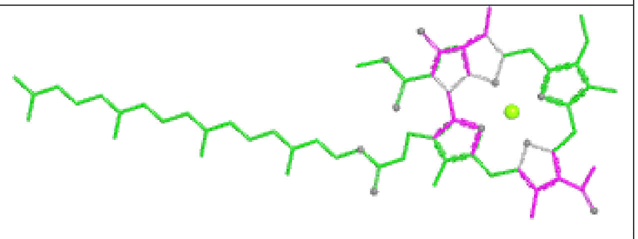
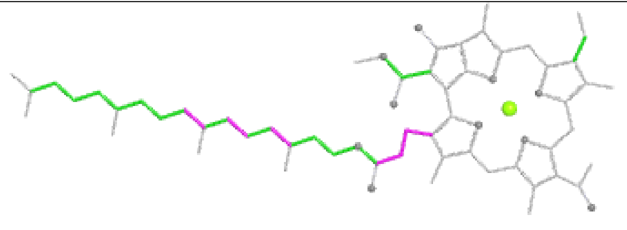

Bond lengths


Bond angles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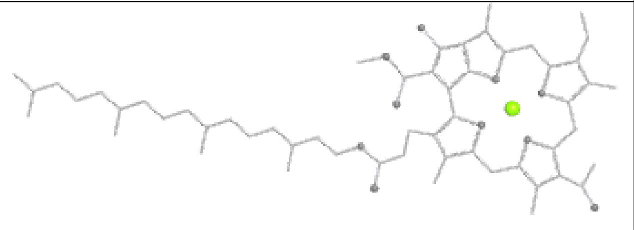
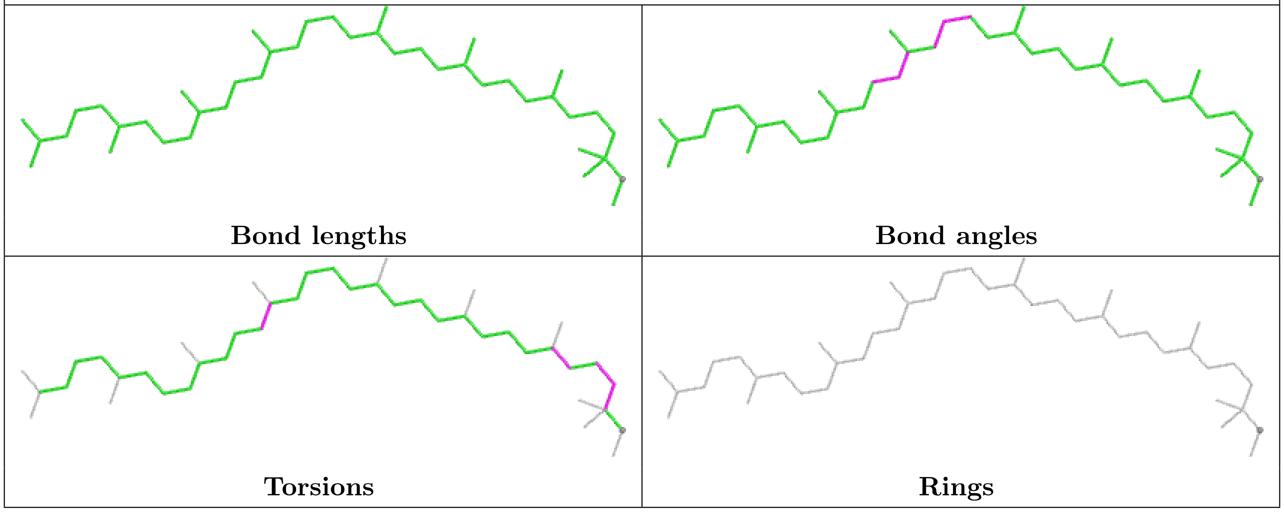
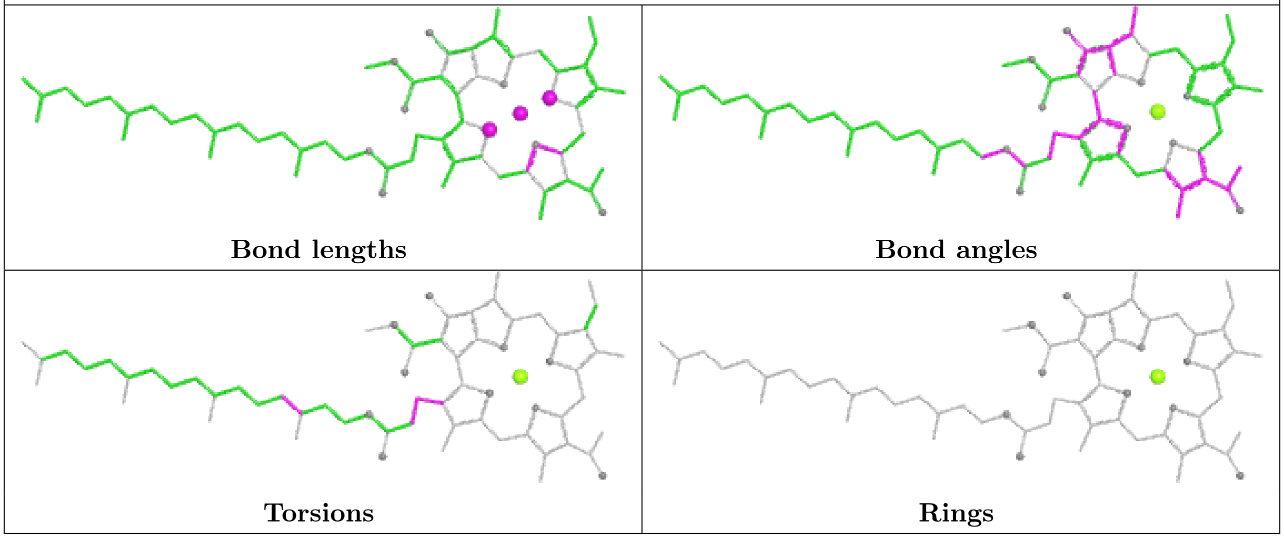

Rings

Ligand SP2 ai 101


Bond lengths
Bond angles
Torsions
Rings

Ligand BCL BA 102


Bond lengths
Bond angles
Torsions
Rings

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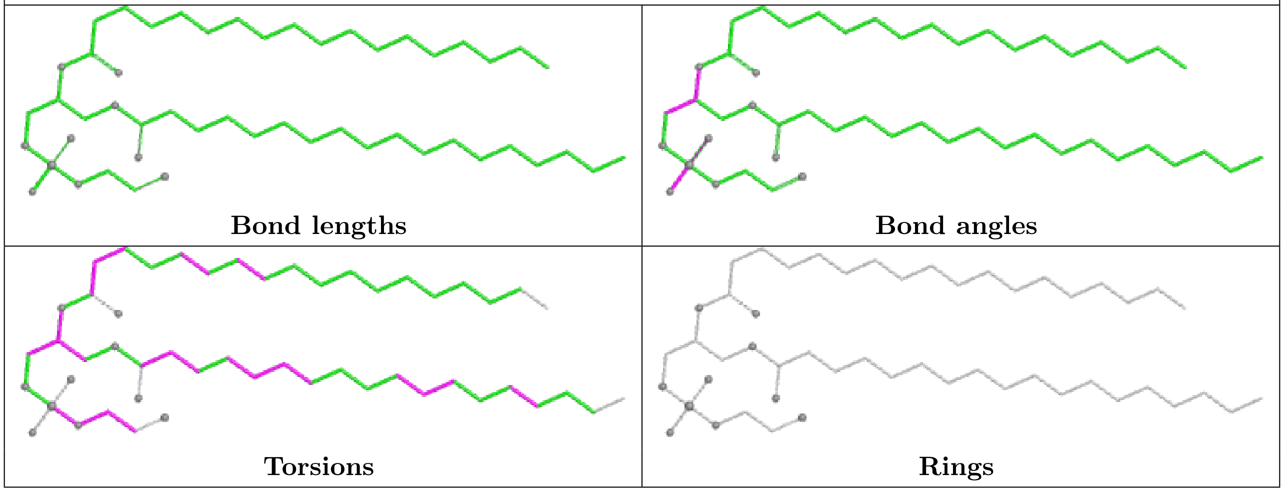
Bond lengths
Bond angles
Torsions
Rings

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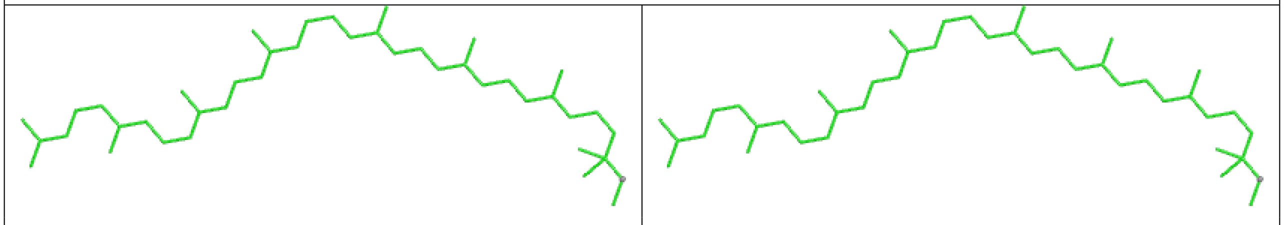
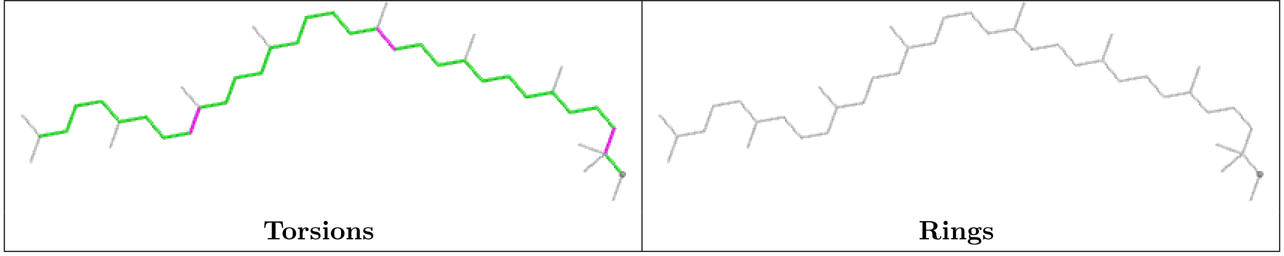


Bond lengths

Bond angles



Torsions

Rings

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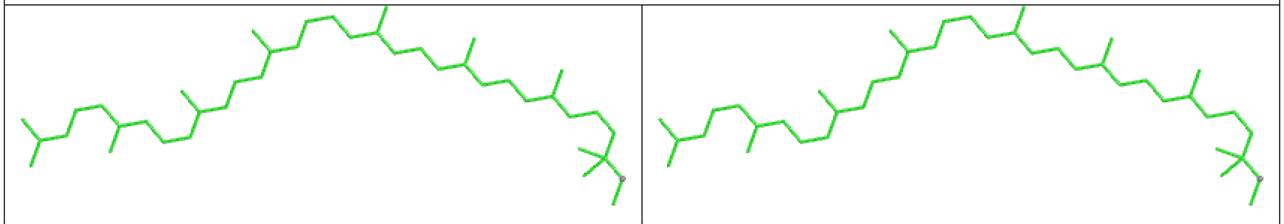

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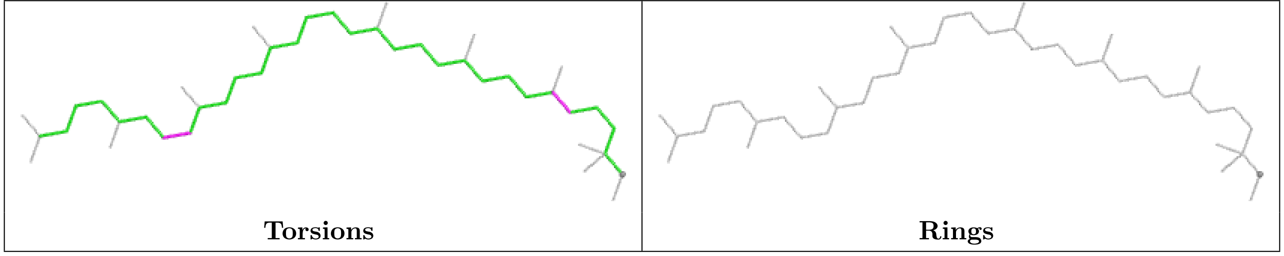
Bond angles



Torsions

Rings

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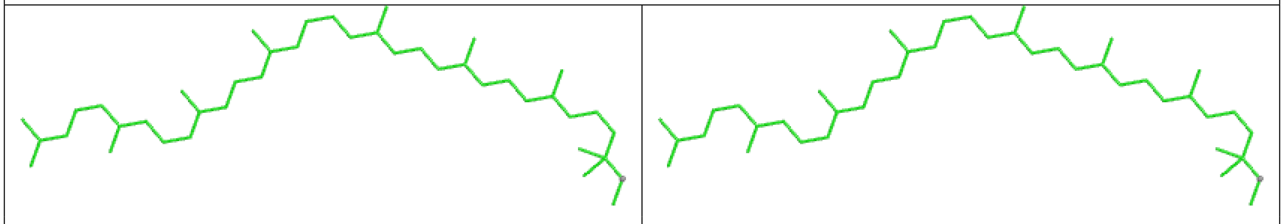
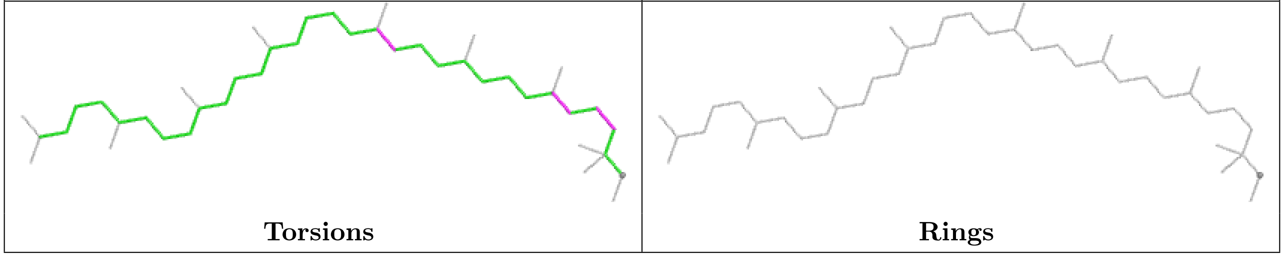


Bond lengths

Bond angles



Torsions

Rings

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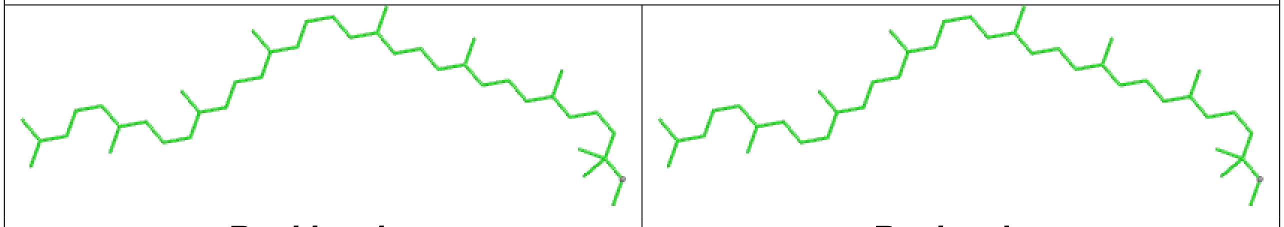
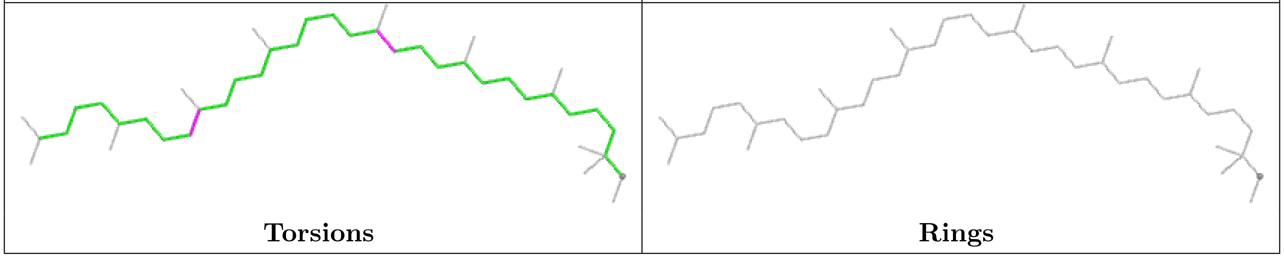


Bond lengths

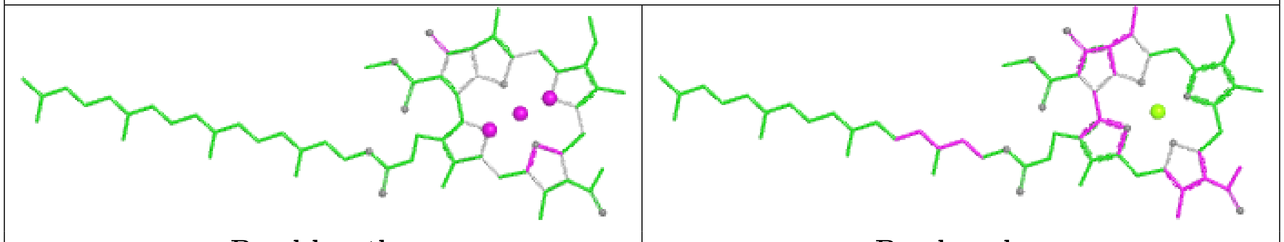
Bond angles



Torsions

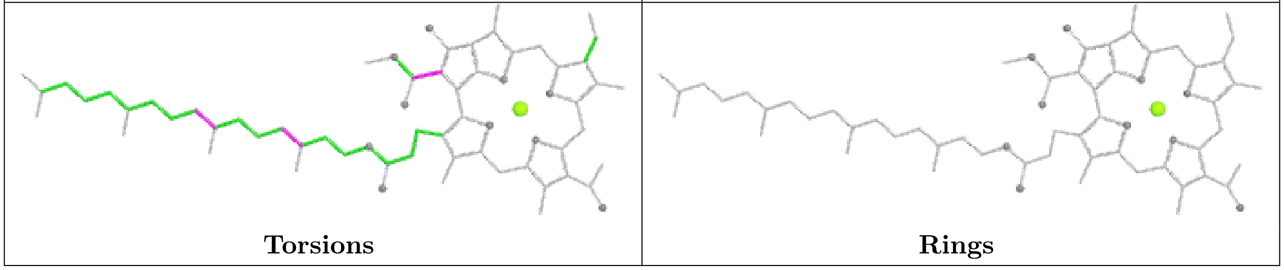
Rings

Ligand BCL AJ 101



Bond lengths

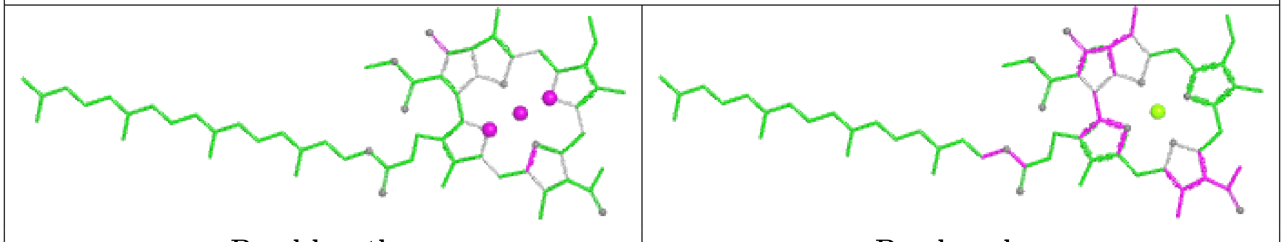
Bond angles



Torsions

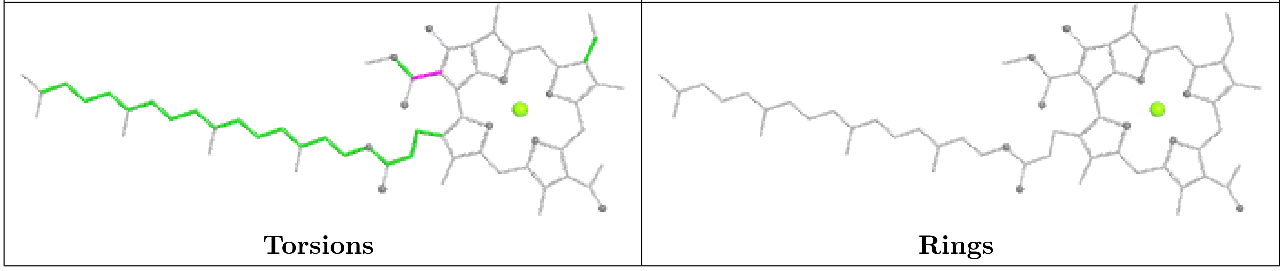
Rings

Ligand BCL l 305



Bond lengths

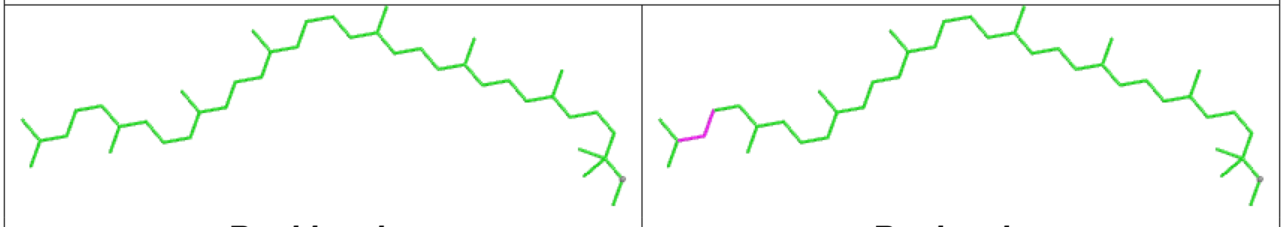
Bond angles



Torsions

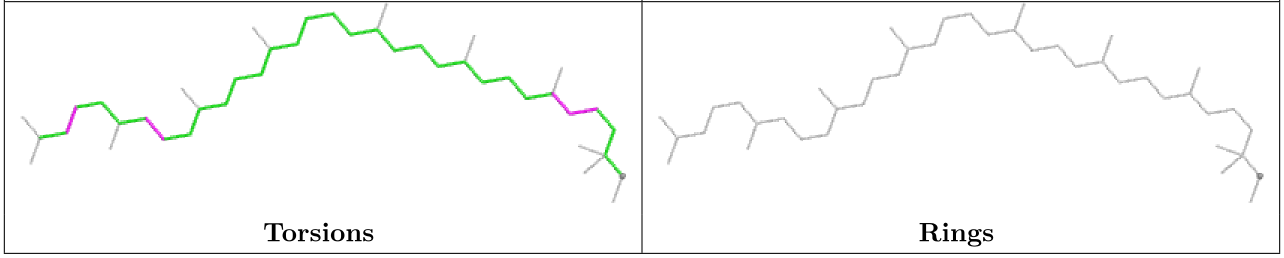
Rings

Ligand SP2 AA 1002



Bond lengths

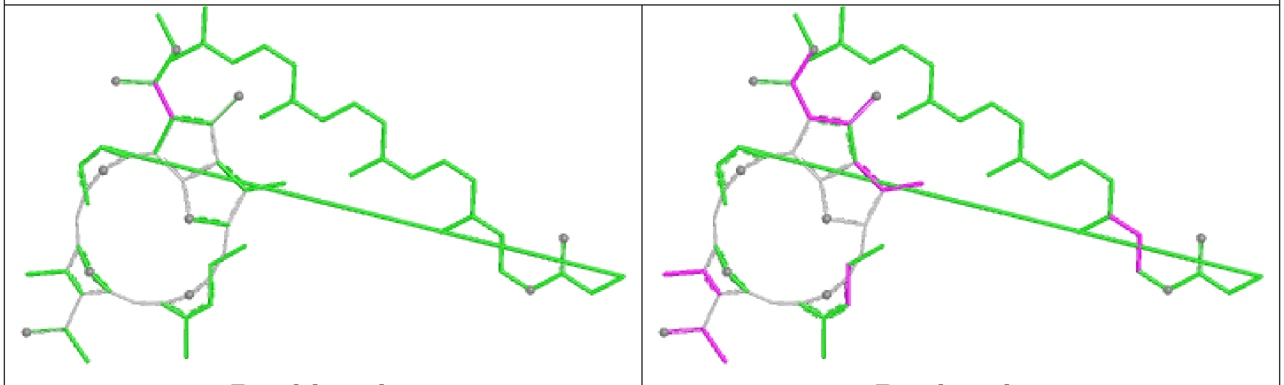
Bond angles



Torsions

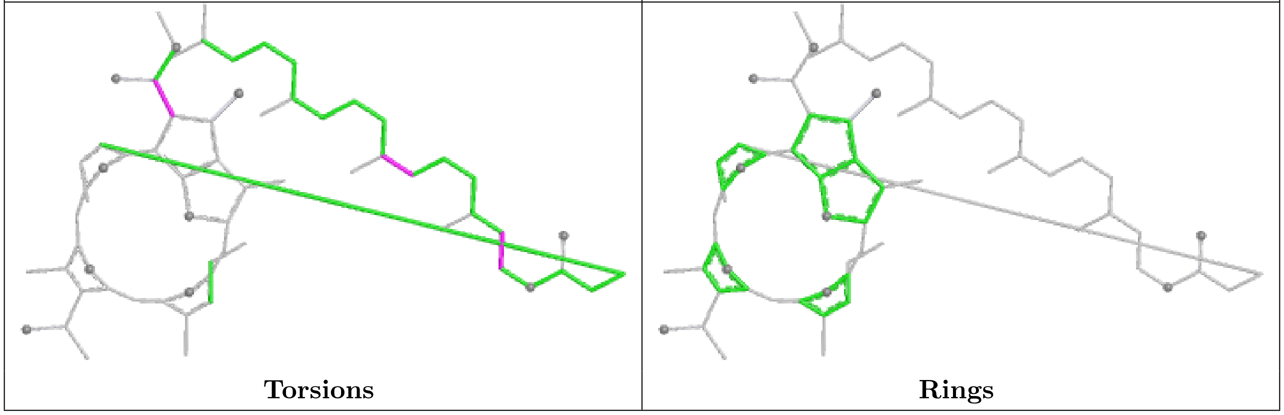
Rings

Ligand BPH m 1002



Bond lengths

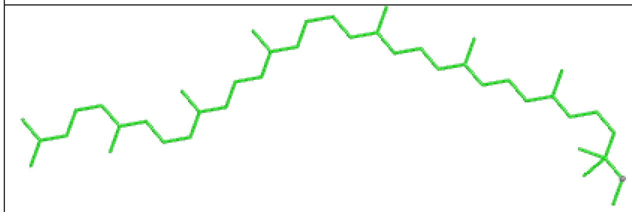
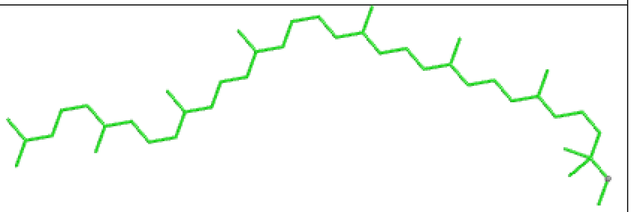
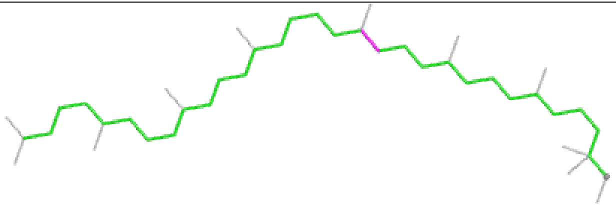
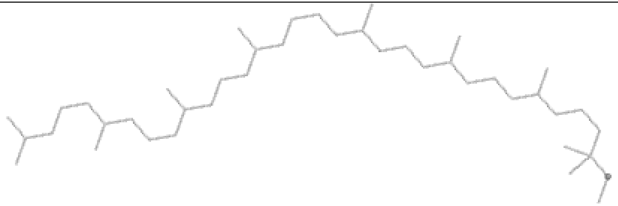
Bond angles



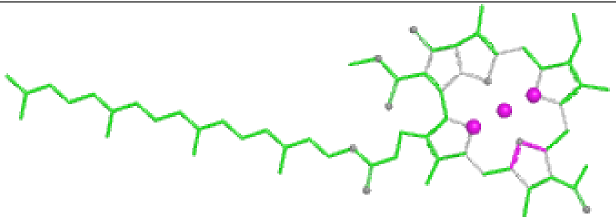
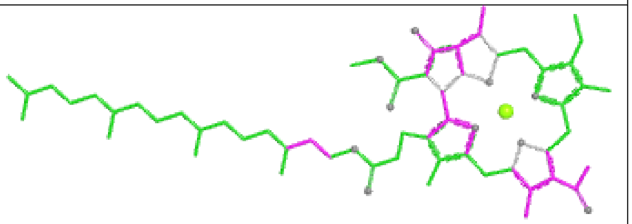
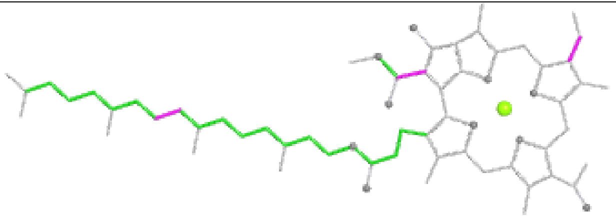
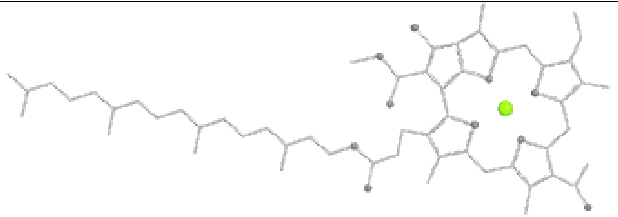
Torsions

Rings

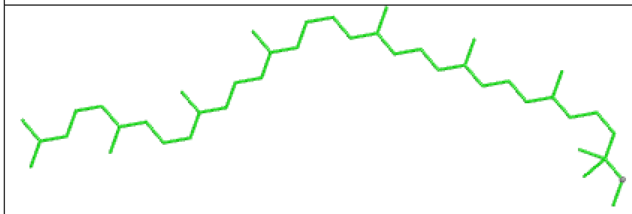
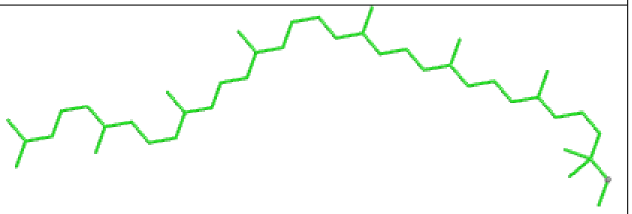
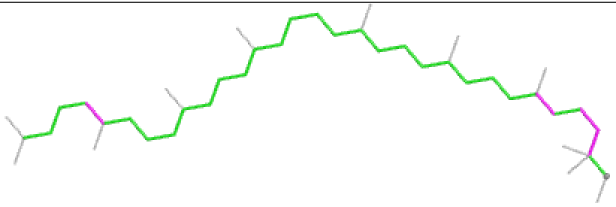
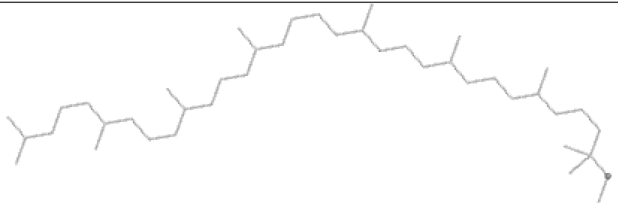
Ligand SP2 BF 102

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

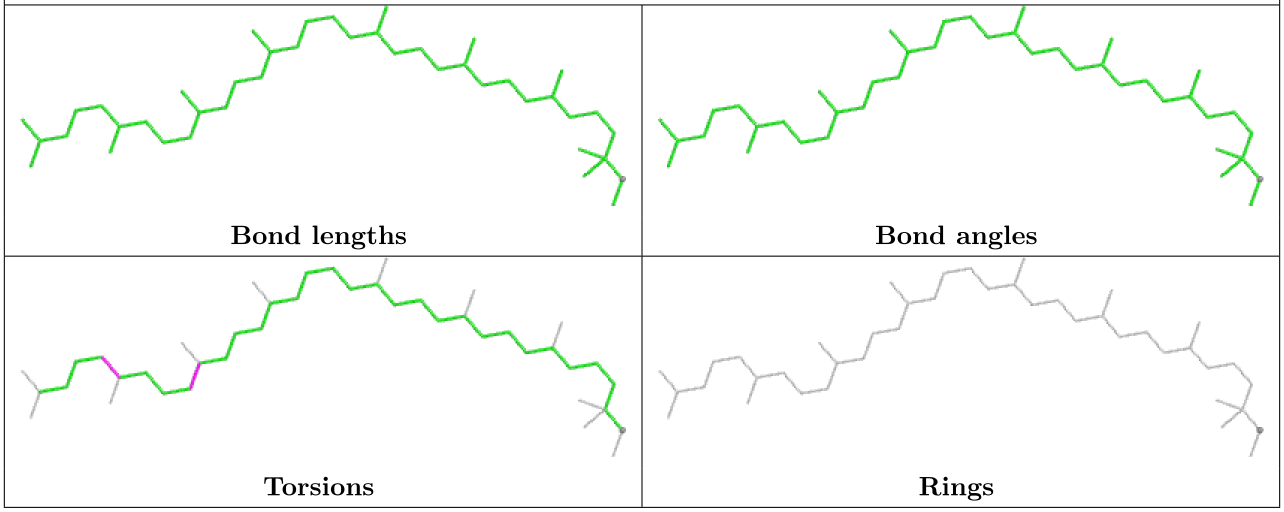
Ligand BCL ab 102

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand SP2 af 103

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand SP2 aj 102



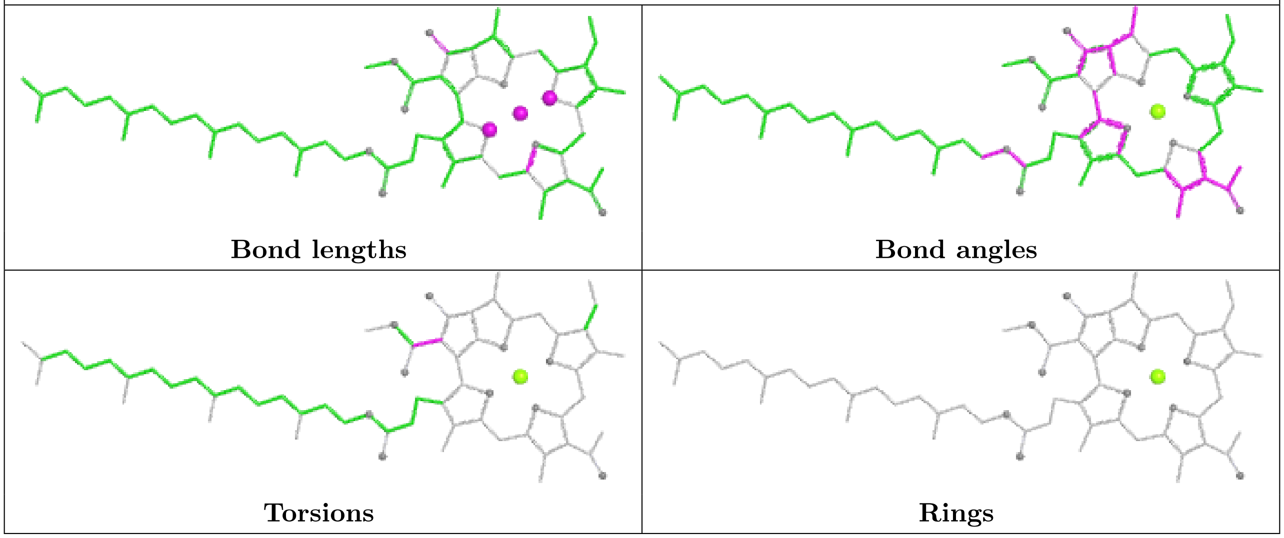
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 301



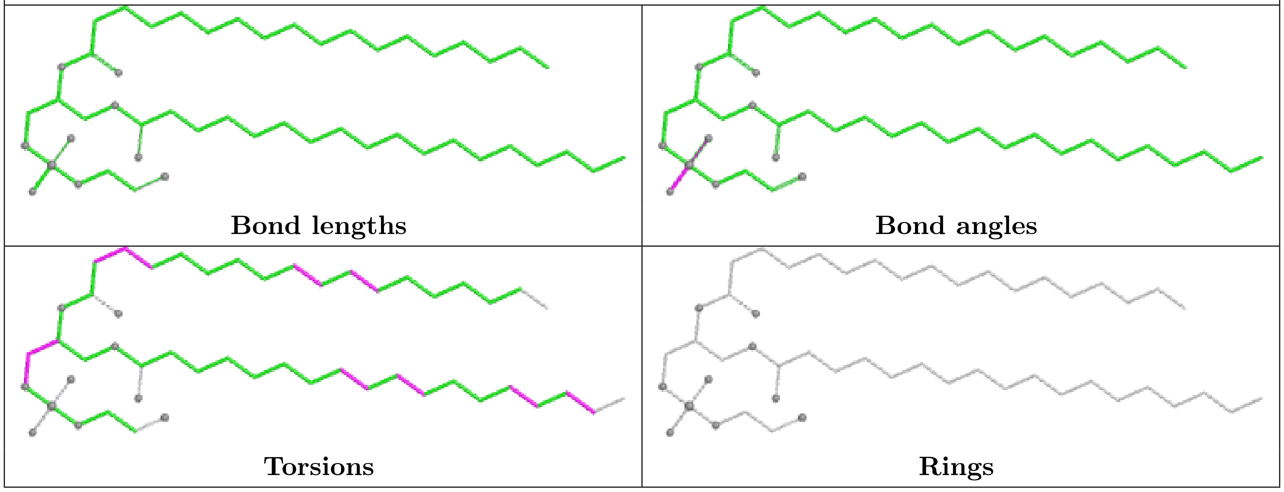
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE H 301



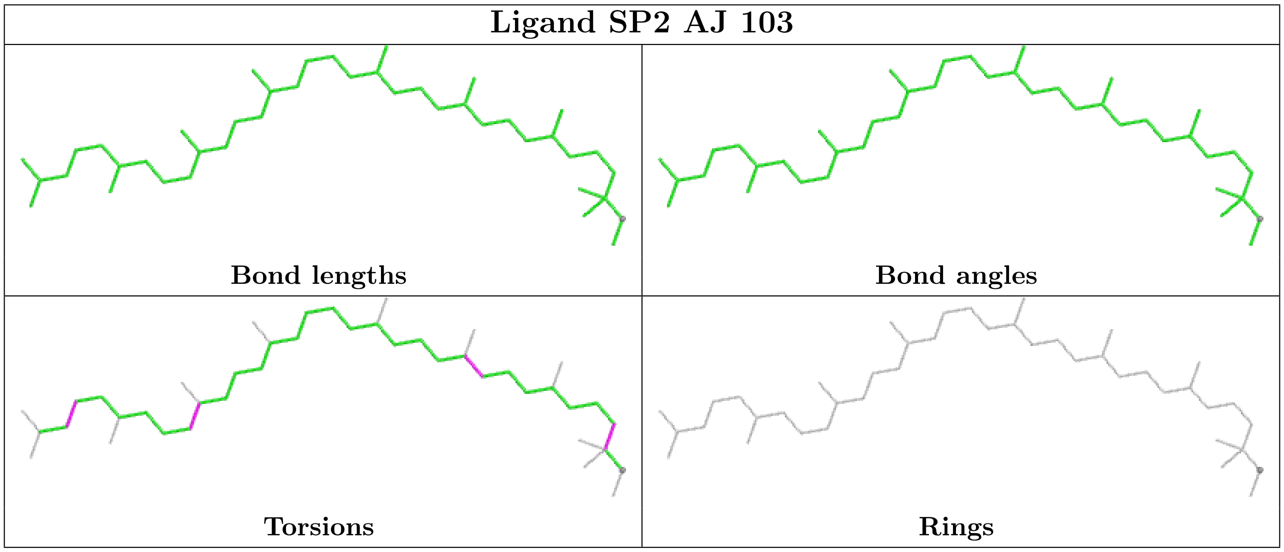
Bond lengths

Bond angles

Torsions

Rings

Ligand SP2 AJ 103



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

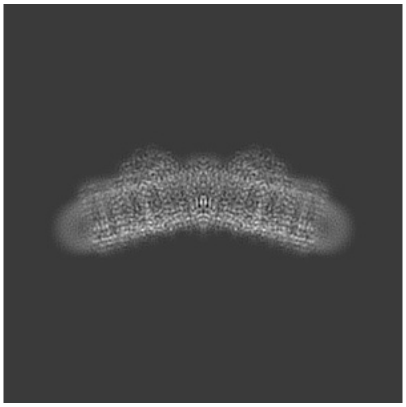
6 Map visualisation ⓘ

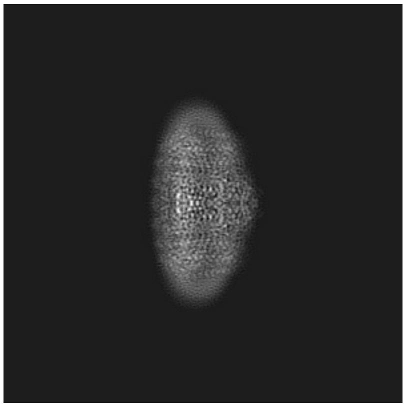
This section contains visualisations of the EMDB entry EMD-13590. These allow visual inspection of the internal detail of the map and identification of artifacts.

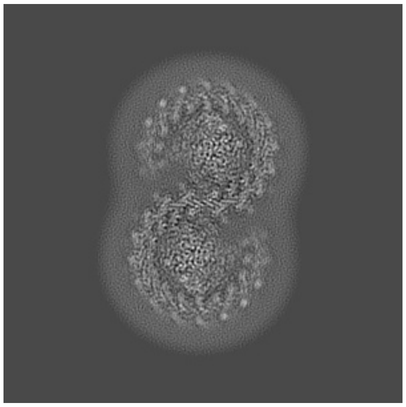
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map


X

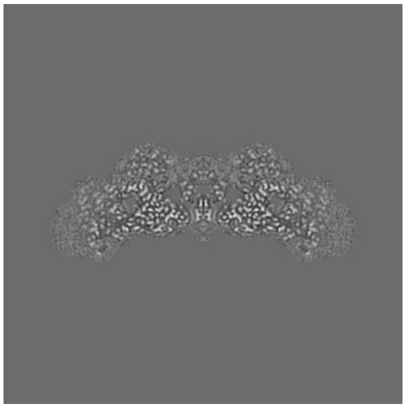

Y


Z

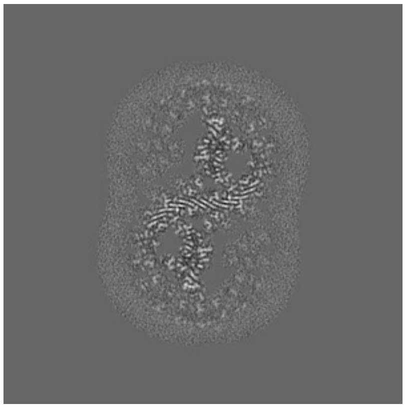
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map


X Index: 256


Y Index: 256


Z Index: 256

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map

X Index: 239 Y Index: 187 Z Index: 236

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

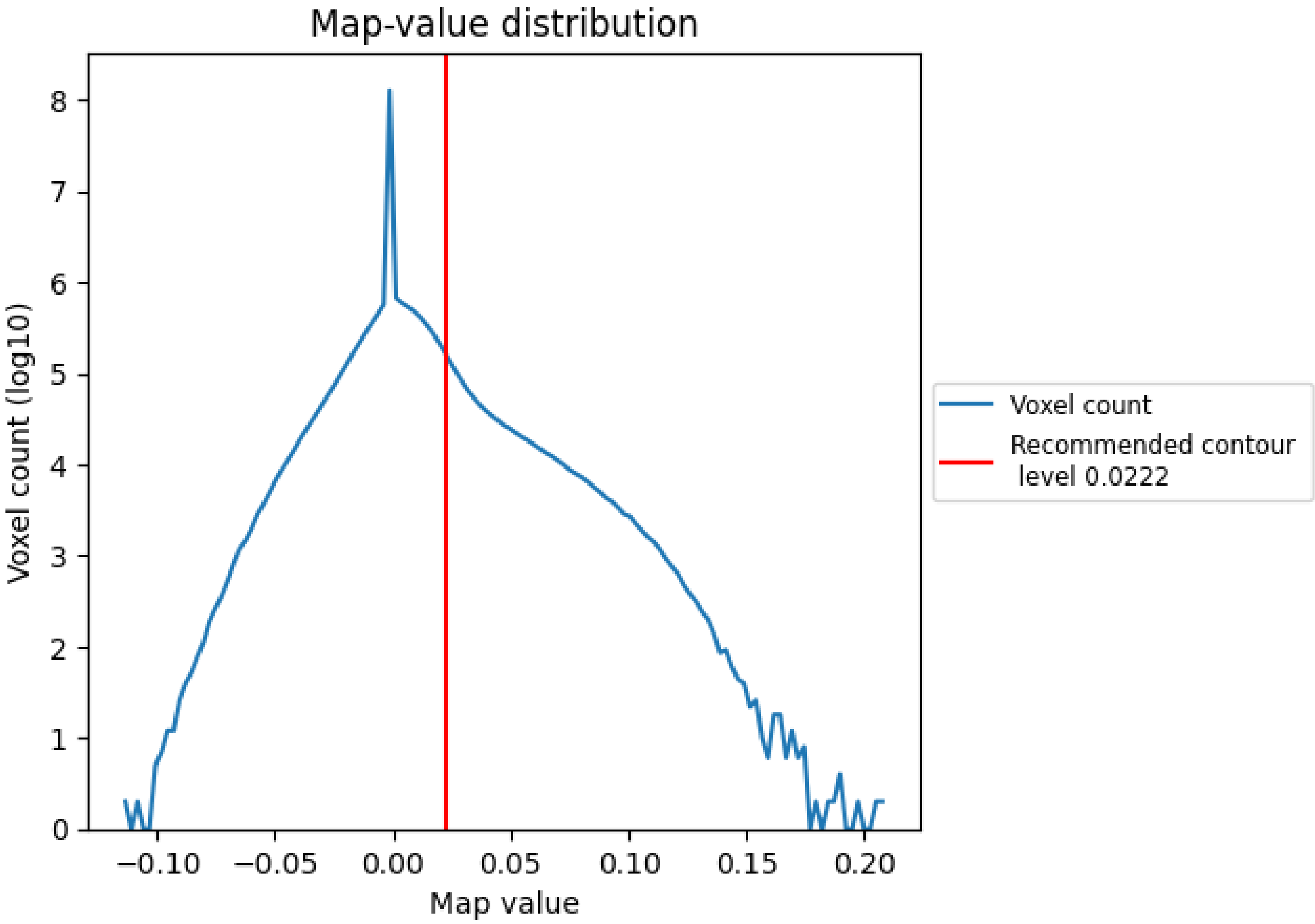
6.5 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

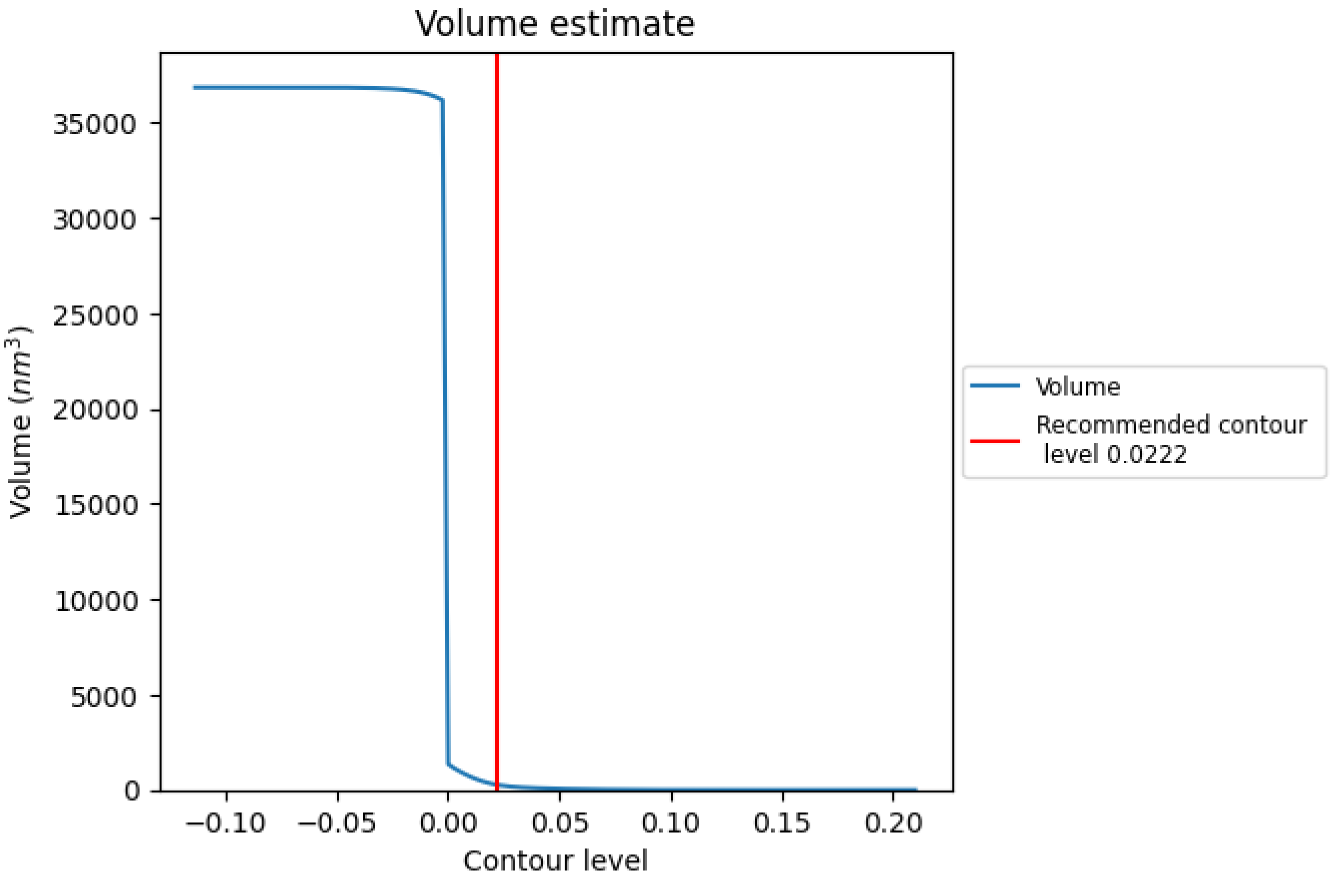
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

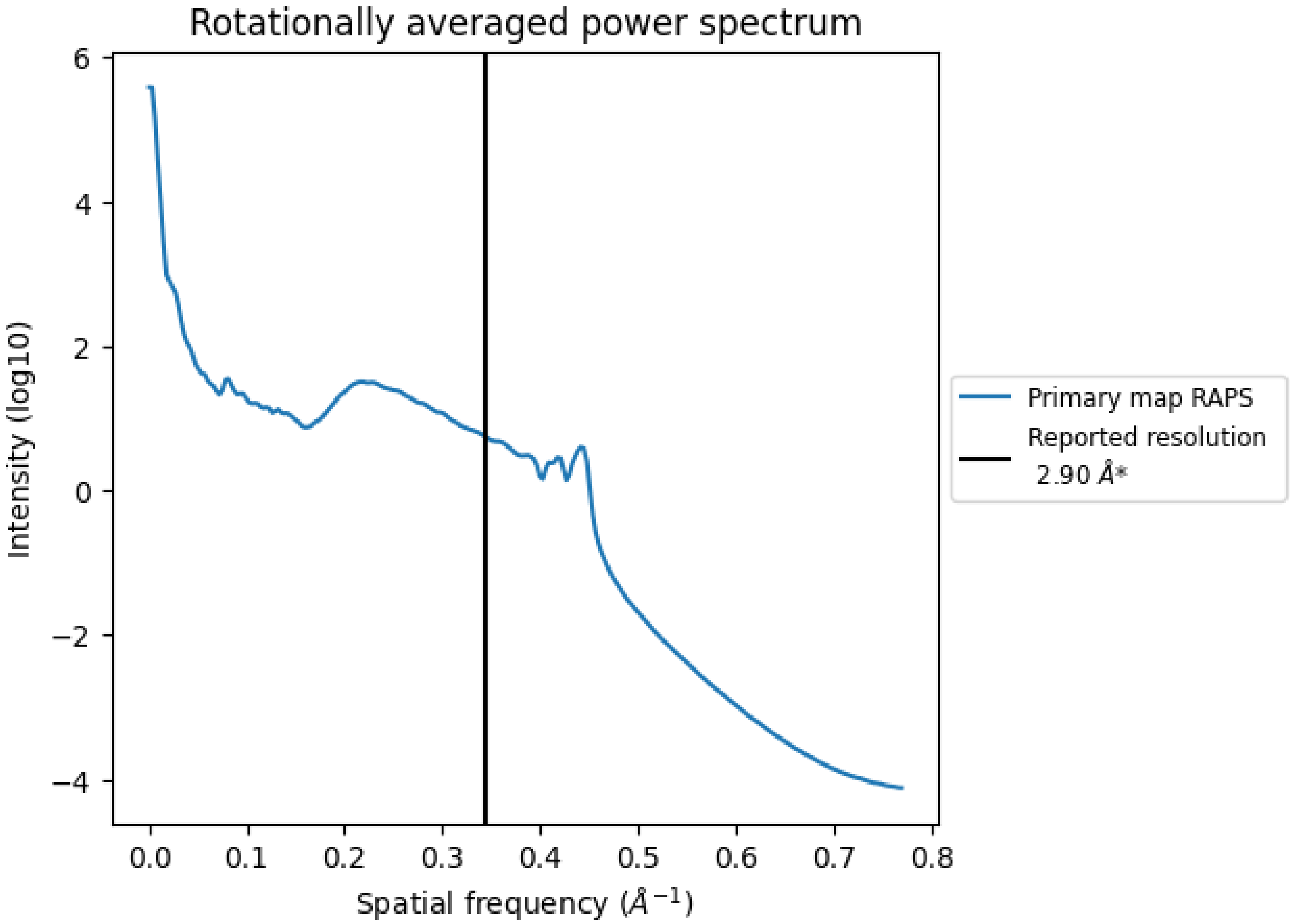
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 271 nm^3; this corresponds to an approximate mass of 245 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)

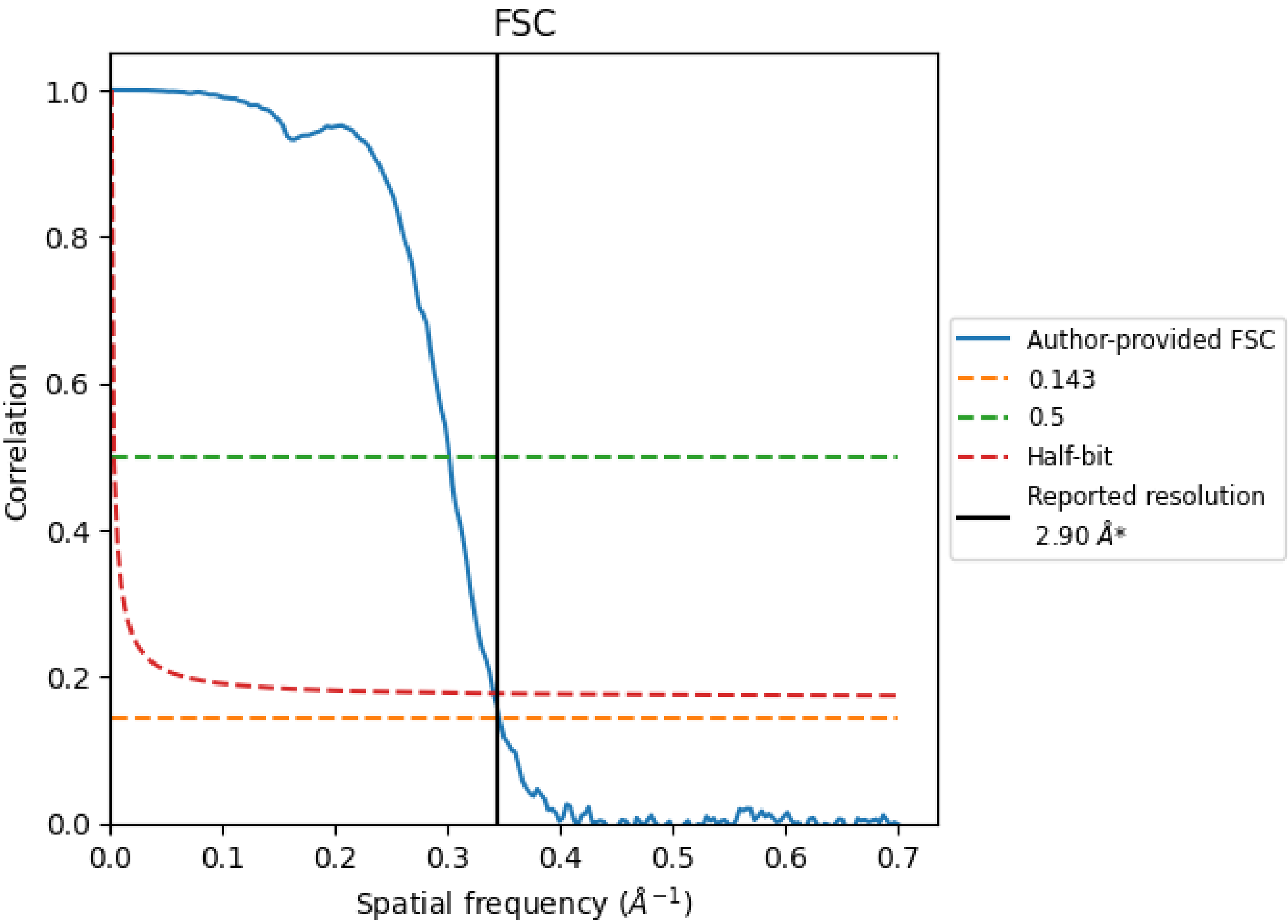


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8.2 Resolution estimates ⓘ

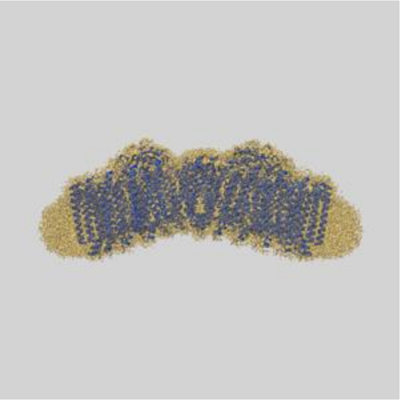
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.31	2.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

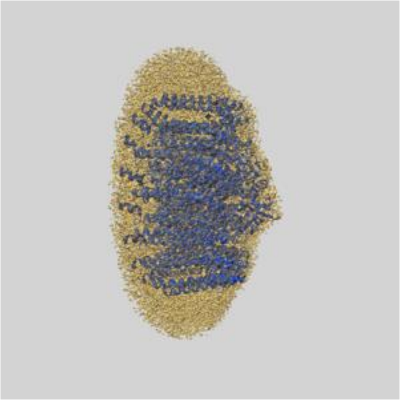
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-13590 and PDB model 7PQD. Per-residue inclusion information can be found in section 3 on page 23.

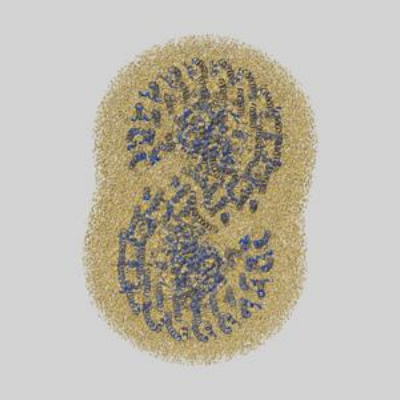
9.1 Map-model overlay ⓘ



X



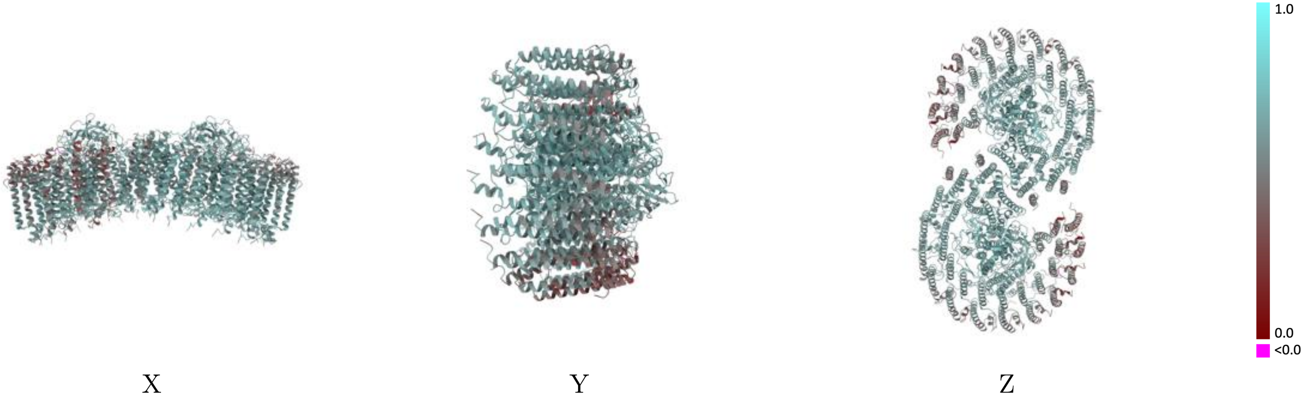
Y



Z

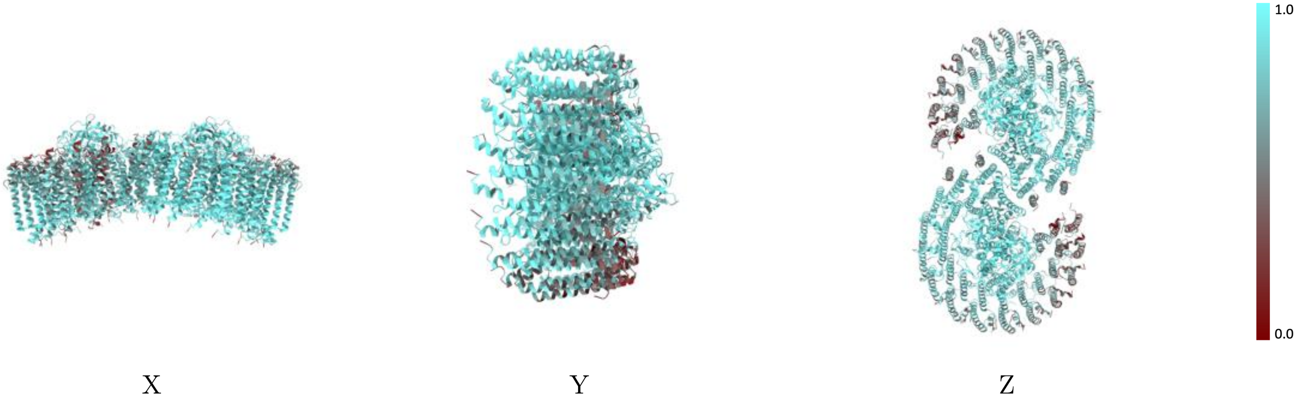
The images above show the 3D surface view of the map at the recommended contour level 0.0222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



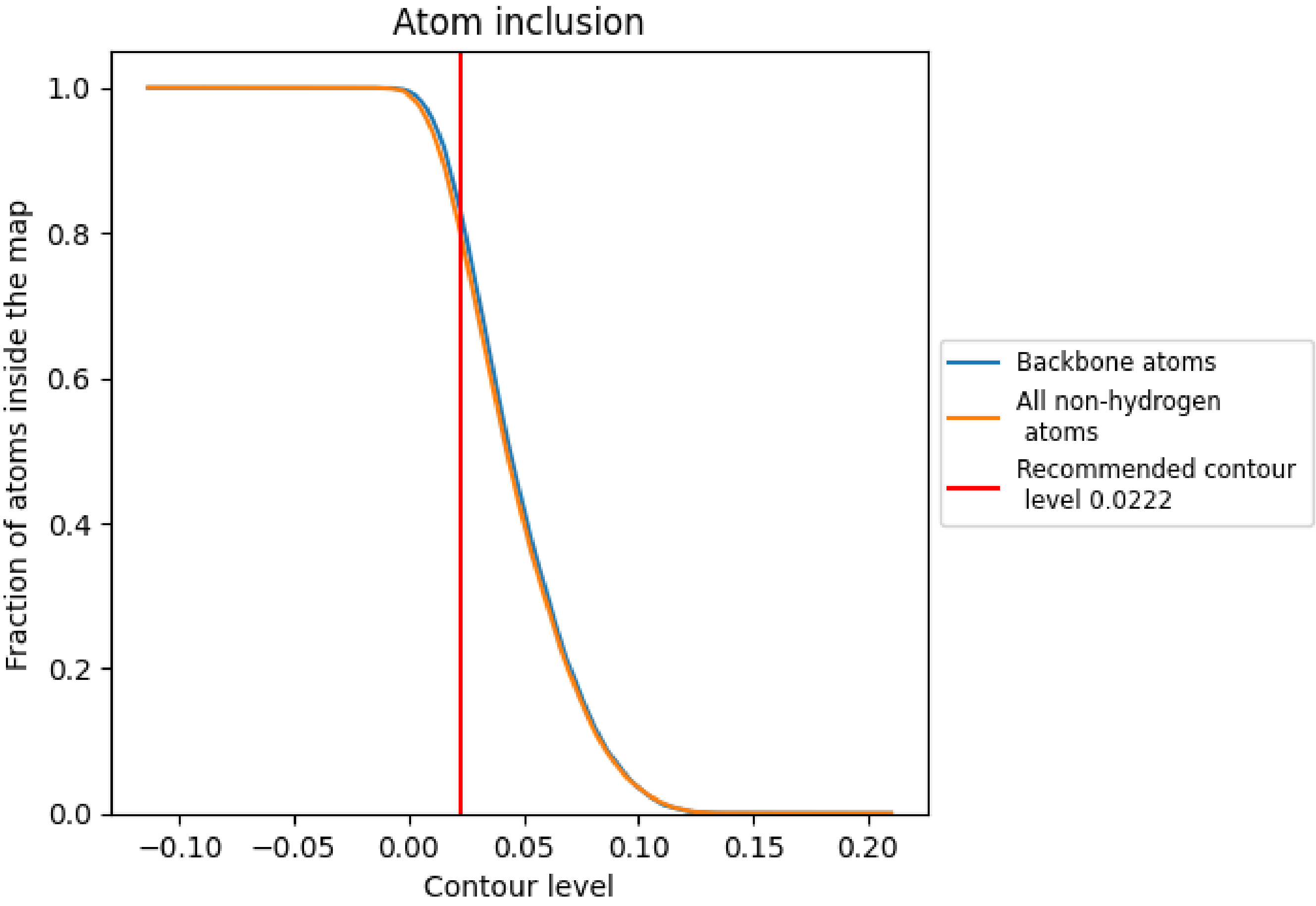
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0222).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 80% 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 (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8033	0.5820
AA	0.9286	0.6410
AB	0.9061	0.6380
AC	0.8591	0.6070
AD	0.8967	0.6180
AE	0.8649	0.6020
AF	0.7839	0.5740
AG	0.7946	0.5730
AH	0.8036	0.5820
AI	0.7772	0.5600
AJ	0.7538	0.5510
AK	0.7171	0.5250
AL	0.6530	0.4990
AM	0.5297	0.4500
AN	0.4244	0.4020
BA	0.9172	0.6430
BB	0.9062	0.6310
BC	0.8497	0.6010
BD	0.8321	0.5970
BE	0.7852	0.5670
BF	0.7360	0.5340
BG	0.7728	0.5640
BH	0.7315	0.5280
BI	0.7383	0.5350
BJ	0.7114	0.5300
BK	0.6219	0.4780
BL	0.5447	0.4430
BM	0.4761	0.3910
BN	0.4132	0.3840
H	0.8817	0.6140
L	0.9617	0.6740
M	0.9422	0.6590
UA	0.5294	0.4460
UB	0.5756	0.5110
UU	0.6657	0.5290

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Chain	Atom inclusion	Q-score
X	0.9279	0.6460
aa	0.9263	0.6390
ab	0.9124	0.6400
ac	0.8514	0.6090
ad	0.8721	0.6040
ae	0.8375	0.5880
af	0.7778	0.5690
ag	0.8070	0.5770
ah	0.7982	0.5810
ai	0.7739	0.5580
aj	0.7571	0.5500
ak	0.7117	0.5230
al	0.6378	0.4960
am	0.5261	0.4480
an	0.4306	0.4000
ba	0.9105	0.6440
bb	0.8904	0.6310
bc	0.8866	0.6120
bd	0.8321	0.5960
be	0.8173	0.5830
bf	0.7338	0.5340
bg	0.7753	0.5620
bh	0.7293	0.5270
bi	0.7309	0.5360
bj	0.7069	0.5280
bk	0.6219	0.4850
bl	0.5444	0.4400
bm	0.4761	0.3890
bn	0.4077	0.3840
h	0.8807	0.6140
l	0.9637	0.6740
m	0.9429	0.6600
ua	0.5252	0.4480
ub	0.5756	0.5080
uu	0.6657	0.5310
x	0.9170	0.6390