



Full wwPDB EM Validation Report ⓘ

Dec 21, 2022 – 12:41 PM EST

PDB ID : 8EQM
EMDB ID : EMD-28539
Title : Structure of a dimeric photosystem II complex acclimated to far-red light
Authors : Gisriel, C.J.; Shen, G.; Flesher, D.A.; Kurashov, V.; Golbeck, J.H.; Brudvig, G.W.; Amin, M.; Bryant, D.A.
Deposited on : 2022-10-08
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

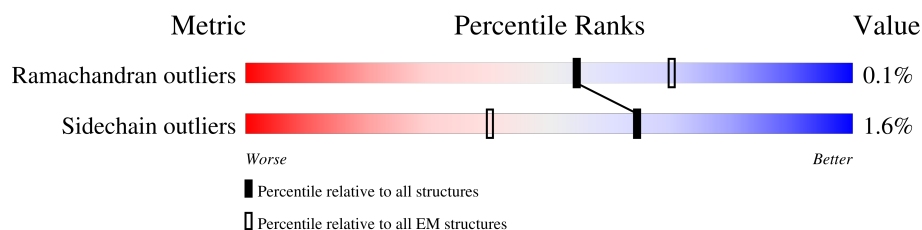
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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





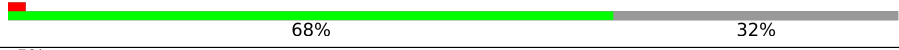
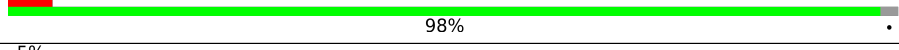
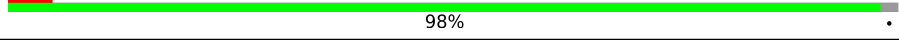

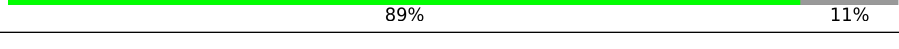
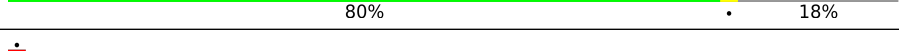
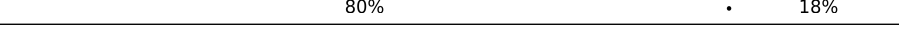
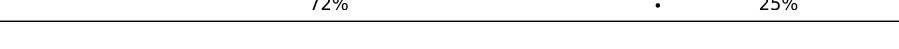
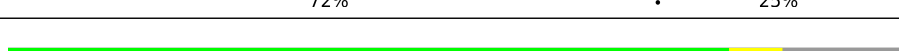



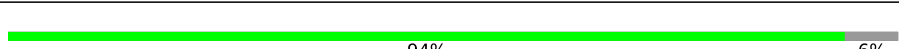
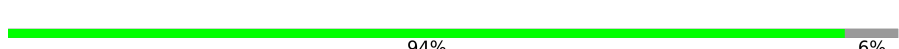




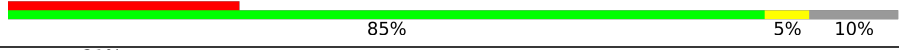


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	359	
1	a	359	
2	B	509	
2	b	509	
3	C	482	
3	c	482	
4	D	352	
4	d	352	
5	E	80	

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Mol	Chain	Length	Quality of chain
5	e	80	
6	F	44	
6	f	44	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	K	45	
9	k	45	
10	L	40	
10	l	40	
11	M	36	
11	m	36	
12	O	274	
12	o	274	
13	T	32	
13	t	32	
14	U	160	
14	u	160	
15	V	172	
15	v	172	
16	X	39	
16	x	39	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	404	X	-	-	-
20	CLA	A	405	X	-	-	-
20	CLA	A	407	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	609	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	C	504	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	511	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	C	513	X	-	-	-
20	CLA	C	514	X	-	-	-
20	CLA	D	403	X	-	-	-
20	CLA	D	404	X	-	-	-
20	CLA	H	101	X	-	-	-
20	CLA	a	404	X	-	-	-
20	CLA	a	405	X	-	-	-
20	CLA	a	407	X	-	-	-
20	CLA	b	601	X	-	-	-
20	CLA	b	602	X	-	-	-
20	CLA	b	603	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	610	X	-	-	-
20	CLA	b	611	X	-	-	-
20	CLA	b	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	c	502	X	-	-	-
20	CLA	c	503	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	c	513	X	-	-	-
20	CLA	c	514	X	-	-	-
20	CLA	d	403	X	-	-	-
20	CLA	d	404	X	-	-	-
20	CLA	h	101	X	-	-	-
29	CL7	D	401	X	-	-	-
29	CL7	d	401	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 42502 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2630	1723	431	461	15		
1	a	333	Total	C	N	O	S	0	0
			2630	1723	431	461	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	483	Total	C	N	O	S	0	0
			3784	2491	627	653	13		
2	b	483	Total	C	N	O	S	0	0
			3784	2491	627	653	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	453	Total	C	N	O	S	0	0
			3498	2290	591	604	13		
3	c	453	Total	C	N	O	S	0	0
			3498	2290	591	604	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	338	Total	C	N	O	S	1	0
			2709	1797	439	459	14		
4	d	338	Total	C	N	O	S	1	0
			2709	1797	439	459	14		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	48	Total	C	N	O	0	0
			371	246	59	66		
5	e	48	Total	C	N	O	0	0
			371	246	59	66		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			237	159	41	36	1		
6	f	30	Total	C	N	O	S	0	0
			237	159	41	36	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			479	318	76	83	2		
7	h	65	Total	C	N	O	S	0	0
			479	318	76	83	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			261	178	39	43	1		
8	i	34	Total	C	N	O	S	0	0
			261	178	39	43	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			291	203	45	43		
9	k	37	Total	C	N	O	0	0
			291	203	45	43		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	30	Total	C	N	O	0	0
			245	166	36	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	30	Total	C	N	O	0	0
			245	166	36	43		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			244	168	34	41	1		
11	m	31	Total	C	N	O	S	0	0
			244	168	34	41	1		

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	182	Total	C	N	O	S	0	0
			1238	788	221	228	1		
12	o	182	Total	C	N	O	S	0	0
			1238	788	221	228	1		

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	30	Total	C	N	O	S	0	0
			236	163	34	37	2		
13	t	30	Total	C	N	O	S	0	0
			236	163	34	37	2		

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	79	Total	C	N	O	0	0
			525	329	96	100		
14	u	79	Total	C	N	O	0	0
			525	329	96	100		

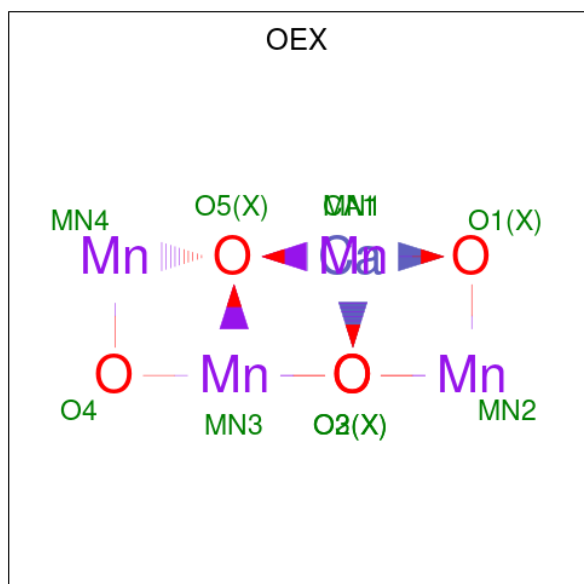
- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	131	Total	C	N	O	S	0	0
			826	518	153	151	4		
15	v	131	Total	C	N	O	S	0	0
			826	518	153	151	4		

- Molecule 16 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	35	Total	C	N	O	S	0	0
			261	174	41	44	2		
16	x	35	Total	C	N	O	S	0	0
			261	174	41	44	2		

- Molecule 17 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Ca	Mn	0
			5	1	4	
17	a	1	Total	Ca	Mn	0
			5	1	4	

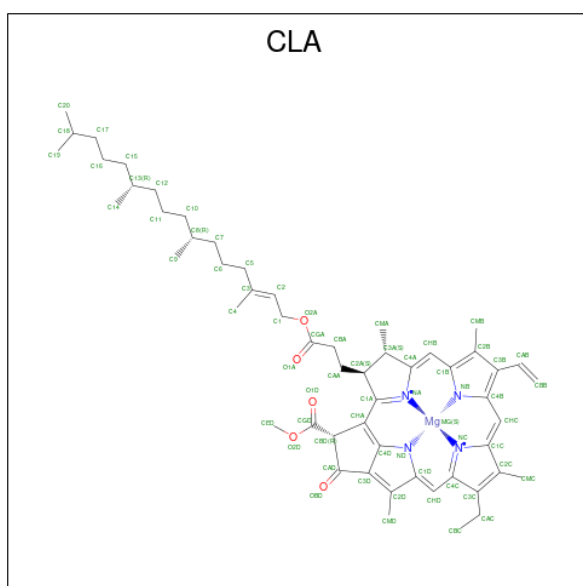
- Molecule 18 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	
18	a	1	Total	Fe	0
			1	1	

- Molecule 19 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total Cl 1 1	0
19	C	1	Total Cl 1 1	0
19	a	1	Total Cl 1 1	0
19	c	1	Total Cl 1 1	0

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 165	C 135	Mg 3	N 12	O 15	0
20	A	1	Total 165	C 135	Mg 3	N 12	O 15	0
20	A	1	Total 165	C 135	Mg 3	N 12	O 15	0
20	B	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	B	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	B	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	B	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	B	1	Total 695	C 575	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			695	575	12	48	60	
20	B	1	Total	C	Mg	N	O	0
			695	575	12	48	60	
20	B	1	Total	C	Mg	N	O	0
			695	575	12	48	60	
20	B	1	Total	C	Mg	N	O	0
			695	575	12	48	60	
20	B	1	Total	C	Mg	N	O	0
			695	575	12	48	60	
20	B	1	Total	C	Mg	N	O	0
			695	575	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	C	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	D	1	Total	C	Mg	N	O	0
			105	85	2	8	10	
20	D	1	Total	C	Mg	N	O	0
			105	85	2	8	10	

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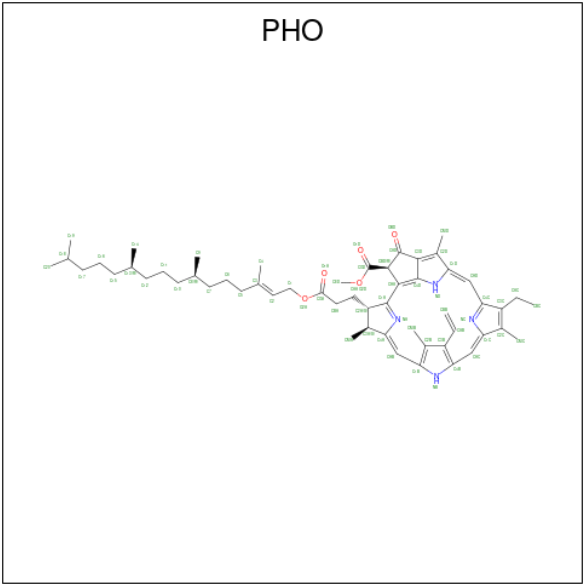
Mol	Chain	Residues	Atoms					AltConf
20	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	a	1	Total 165	C 135	Mg 3	N 12	O 15	0
20	a	1	Total 165	C 135	Mg 3	N 12	O 15	0
20	a	1	Total 165	C 135	Mg 3	N 12	O 15	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	b	1	Total 695	C 575	Mg 12	N 48	O 60	0
20	c	1	Total 685	C 565	Mg 12	N 48	O 60	0
20	c	1	Total 685	C 565	Mg 12	N 48	O 60	0
20	c	1	Total 685	C 565	Mg 12	N 48	O 60	0
20	c	1	Total 685	C 565	Mg 12	N 48	O 60	0
20	c	1	Total 685	C 565	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
20	c	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	c	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	c	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	c	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	c	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	c	1	Total	C	Mg	N	O	0
			685	565	12	48	60	
20	d	1	Total	C	Mg	N	O	0
			105	85	2	8	10	
20	d	1	Total	C	Mg	N	O	0
			105	85	2	8	10	
20	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



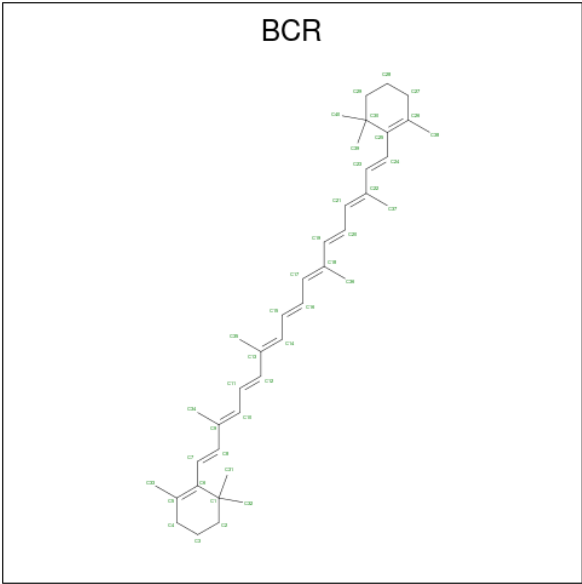
Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	N	O	0
			64	55	4	5	

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Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	N	O	0
			64	55	4	5	
21	a	1	Total	C	N	O	0
			64	55	4	5	
21	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



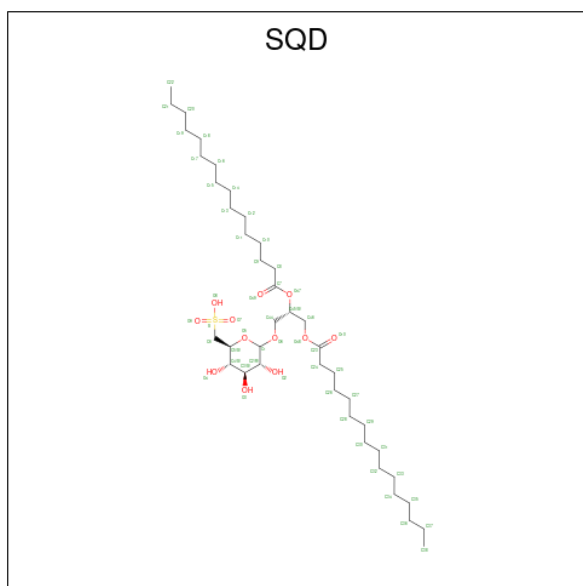
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			120	120	
22	B	1	Total	C	0
			120	120	
22	B	1	Total	C	0
			120	120	
22	C	1	Total	C	0
			60	60	
22	C	1	Total	C	0
			60	60	
22	D	1	Total	C	0
			26	26	
22	a	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
22	b	1	Total	C	0
			120	120	
22	b	1	Total	C	0
			120	120	
22	b	1	Total	C	0
			120	120	
22	c	1	Total	C	0
			60	60	
22	c	1	Total	C	0
			60	60	
22	d	1	Total	C	0
			26	26	

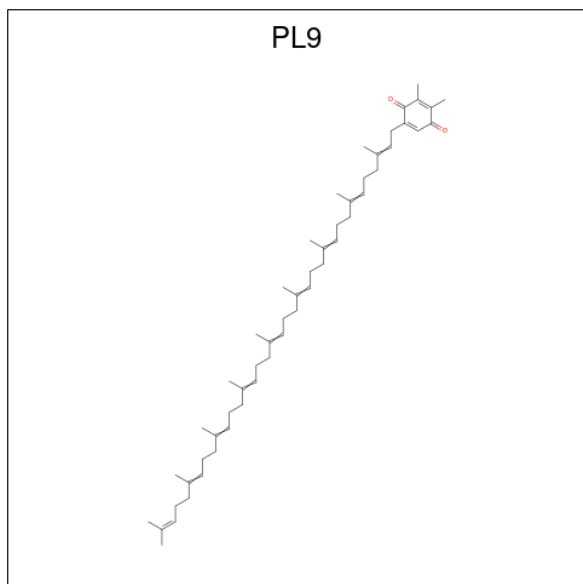
- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	S	0
			52	39	12	1	
23	L	1	Total	C	O	S	0
			54	41	12	1	
23	a	1	Total	C	O	S	0
			52	39	12	1	
23	l	1	Total	C	O	S	0
			54	41	12	1	

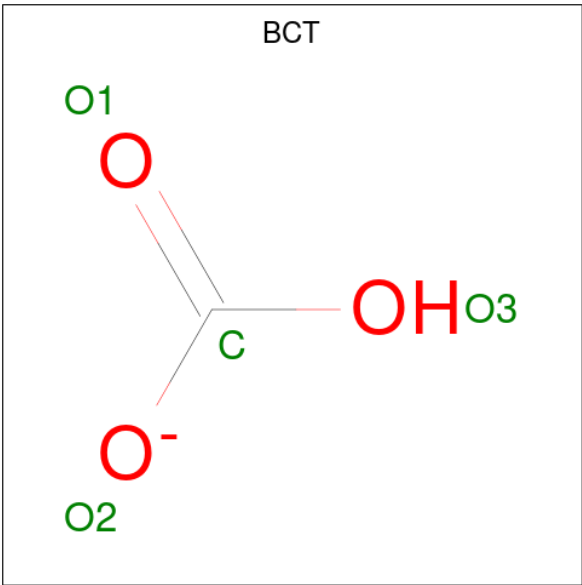
- Molecule 24 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18

,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



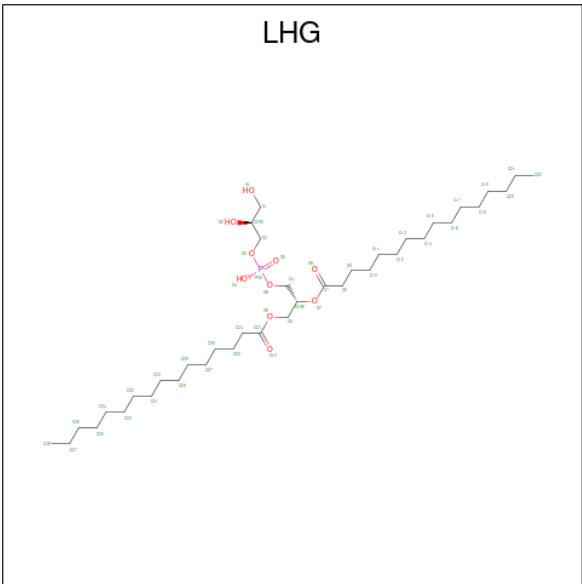
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			20	18	2	
24	D	1	Total	C	O	0
			45	43	2	
24	a	1	Total	C	O	0
			20	18	2	
24	d	1	Total	C	O	0
			45	43	2	

- Molecule 25 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			4	1	3	
25	a	1	Total	C	O	0
			4	1	3	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



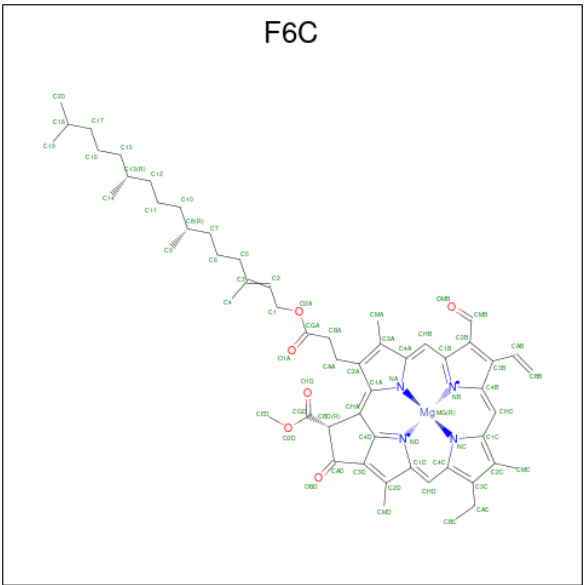
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	D	1	Total	C	O	P	0
			96	74	20	2	
26	D	1	Total	C	O	P	0
			96	74	20	2	
26	L	1	Total	C	O	P	0
			49	38	10	1	
26	a	1	Total	C	O	P	0
			37	26	10	1	
26	d	1	Total	C	O	P	0
			96	74	20	2	
26	d	1	Total	C	O	P	0
			96	74	20	2	
26	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is Chlorophyll F (three-letter code: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



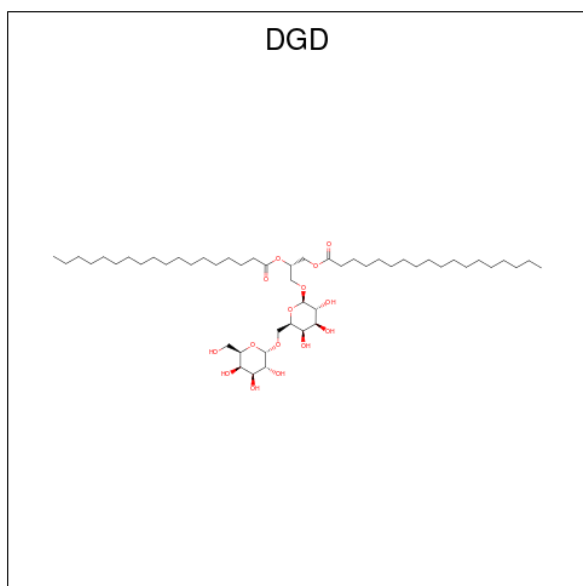
Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			193	160	3	12	18	
27	B	1	Total	C	Mg	N	O	0
			193	160	3	12	18	
27	B	1	Total	C	Mg	N	O	0
			193	160	3	12	18	
27	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total	C	Mg	N	O	0
			193	160	3	12	18	
27	b	1	Total	C	Mg	N	O	0
			193	160	3	12	18	
27	b	1	Total	C	Mg	N	O	0
			193	160	3	12	18	
27	c	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

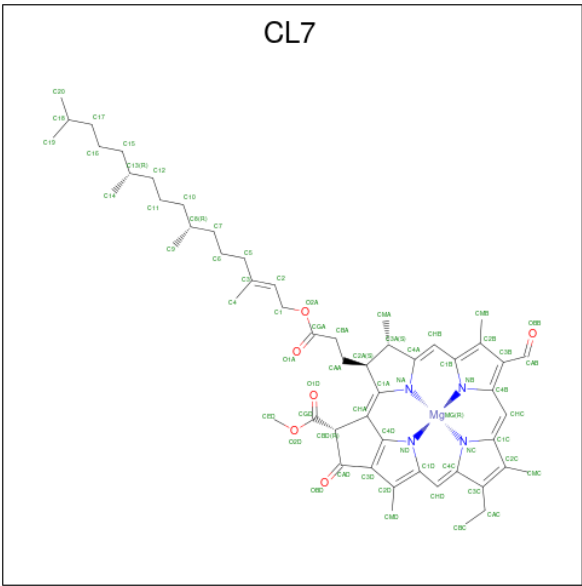
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	C	1	Total	C	O	0
			83	59	24	
28	C	1	Total	C	O	0
			83	59	24	
28	D	1	Total	C	O	0
			45	36	9	
28	c	1	Total	C	O	0
			83	59	24	
28	c	1	Total	C	O	0
			83	59	24	
28	d	1	Total	C	O	0
			45	36	9	

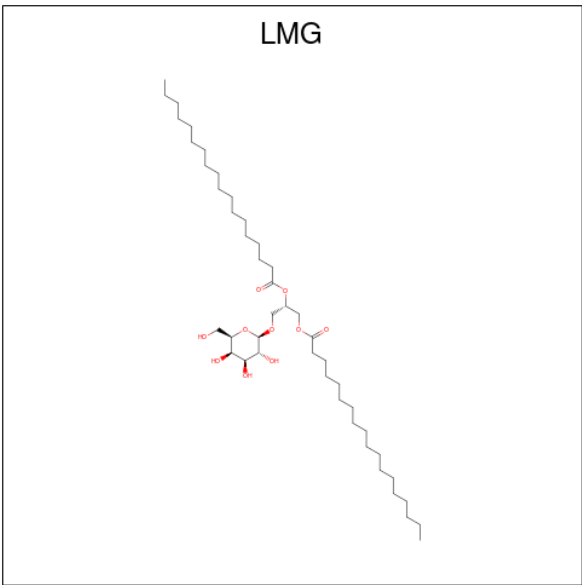
- Molecule 29 is CHLOROPHYLL D (three-letter code: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (la-

beled as "Ligand of Interest" by depositor).



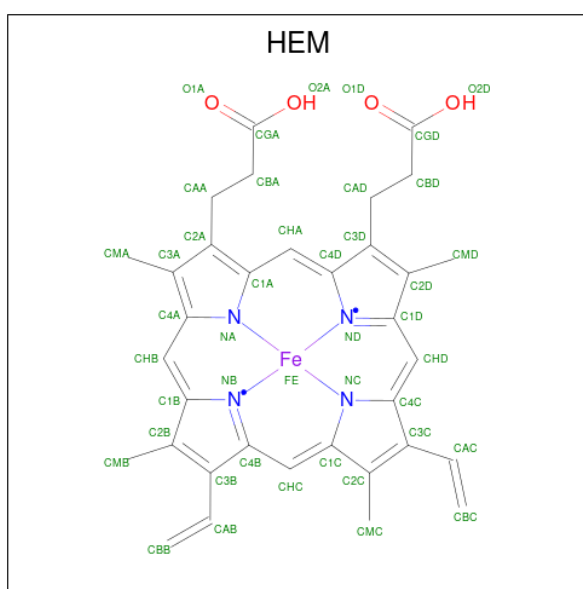
Mol	Chain	Residues	Atoms					AltConf
29	D	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
29	d	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



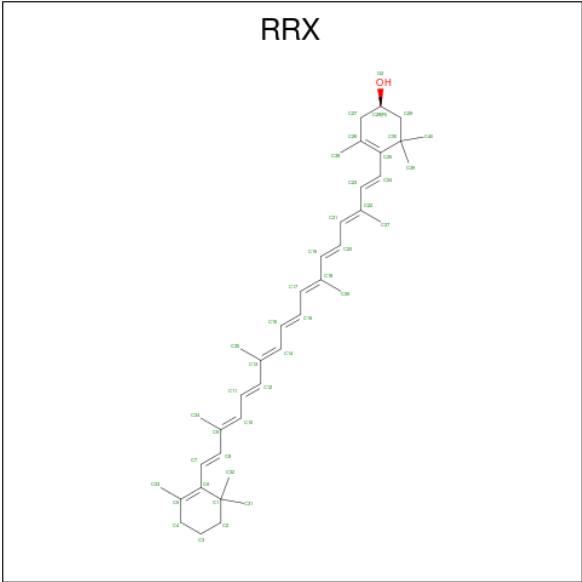
Mol	Chain	Residues	Atoms			AltConf
30	D	1	Total 33	C 23	O 10	0
30	M	1	Total 40	C 30	O 10	0
30	d	1	Total 33	C 23	O 10	0
30	m	1	Total 40	C 30	O 10	0

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



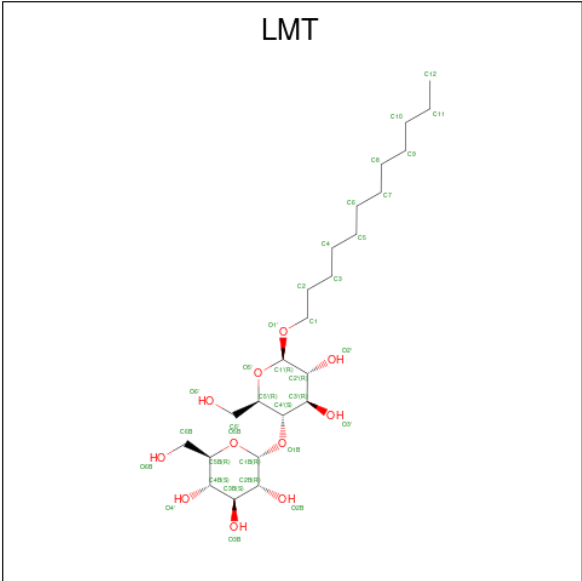
Mol	Chain	Residues	Atoms					AltConf
31	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
32	H	1	Total	C	O	0
			41	40	1	
32	h	1	Total	C	O	0
			41	40	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms			AltConf
34	A	75	Total	O		0
			75	75		
34	B	69	Total	O		0
			69	69		
34	C	63	Total	O		0
			63	63		
34	D	60	Total	O		0
			60	60		
34	E	1	Total	O		0
			1	1		
34	F	1	Total	O		0
			1	1		
34	H	7	Total	O		0
			7	7		
34	L	6	Total	O		0
			6	6		
34	M	4	Total	O		0
			4	4		
34	O	3	Total	O		0
			3	3		
34	T	5	Total	O		0
			5	5		
34	X	1	Total	O		0
			1	1		
34	a	75	Total	O		0
			75	75		
34	b	69	Total	O		0
			69	69		
34	c	63	Total	O		0
			63	63		
34	d	60	Total	O		0
			60	60		
34	e	1	Total	O		0
			1	1		
34	f	1	Total	O		0
			1	1		

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Mol	Chain	Residues	Atoms		AltConf
34	h	7	Total 7	O 7	0
34	l	6	Total 6	O 6	0
34	m	4	Total 4	O 4	0
34	o	3	Total 3	O 3	0
34	t	5	Total 5	O 5	0
34	x	1	Total 1	O 1	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: Photosystem II protein D1

Chain A:  91% • 7%



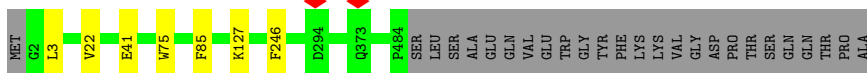
- Molecule 1: Photosystem II protein D1

Chain a:  91% • 7%



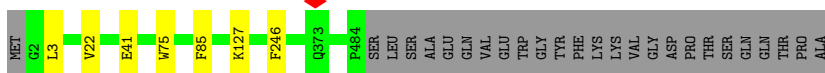
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  94% • 5%




- Molecule 2: Photosystem II CP47 reaction center protein

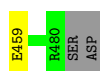
Chain b:  94% • 5%



- Molecule 3: Photosystem II CP43 reaction center protein

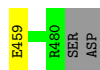
Chain C:  91% • 6%





- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 91% 6%



- Molecule 4: Photosystem II D2 protein

Chain D: 93%



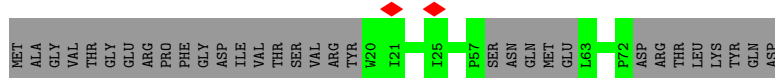
- Molecule 4: Photosystem II D2 protein

Chain d: 93%



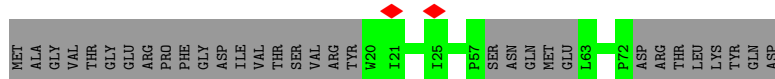
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 60% 40%



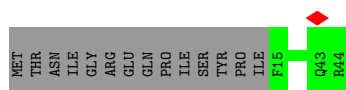
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 60% 40%

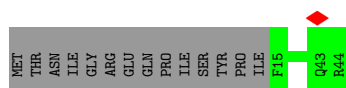


- Molecule 6: Cytochrome b559 subunit beta

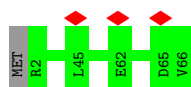
Chain F: 68% 32%



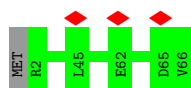
- Molecule 6: Cytochrome b559 subunit beta



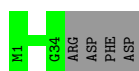
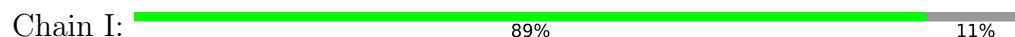
- Molecule 7: Photosystem II reaction center protein H



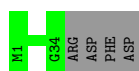
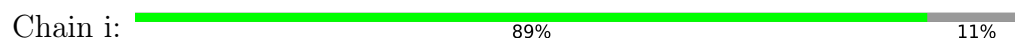
- Molecule 7: Photosystem II reaction center protein H



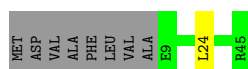
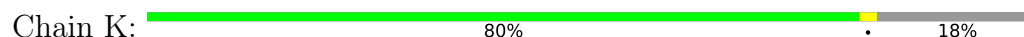
- Molecule 8: Photosystem II reaction center protein I



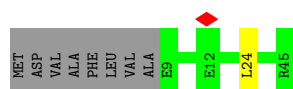
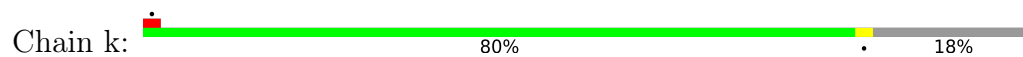
- Molecule 8: Photosystem II reaction center protein I



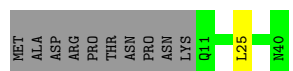
- Molecule 9: Photosystem II reaction center protein K



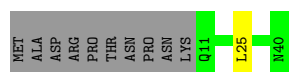
- Molecule 9: Photosystem II reaction center protein K



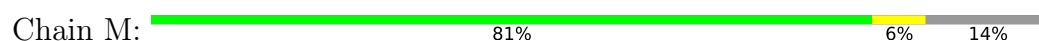
- Molecule 10: Photosystem II reaction center protein L



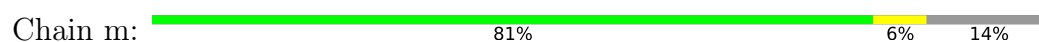
- Molecule 10: Photosystem II reaction center protein L



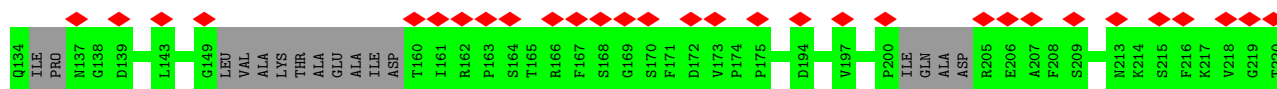
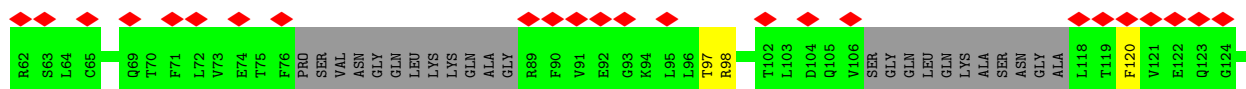
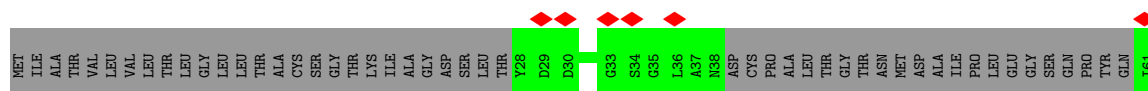
- Molecule 11: Photosystem II reaction center protein M

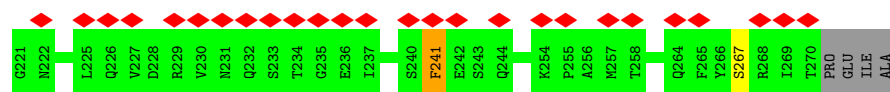


- Molecule 11: Photosystem II reaction center protein M



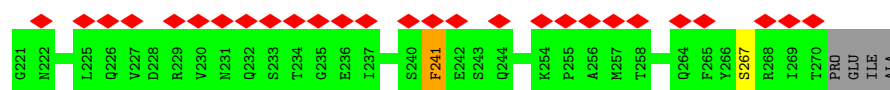
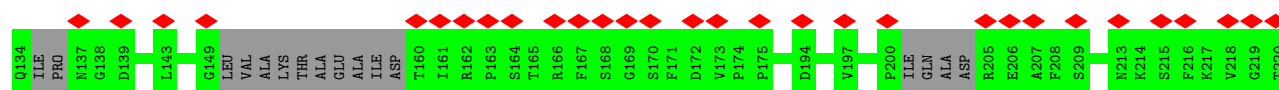
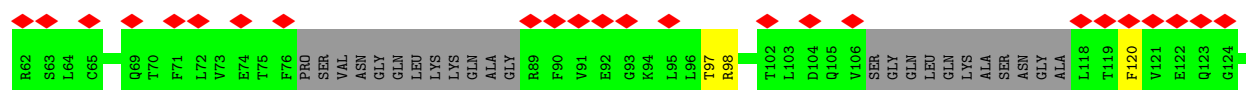
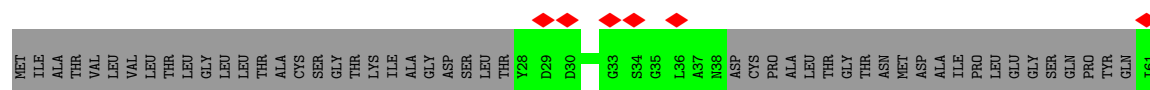
- Molecule 12: Photosystem II manganese-stabilizing polypeptide





- Molecule 12: Photosystem II manganese-stabilizing polypeptide

Chain o: 32% 65% 34%



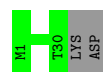
- Molecule 13: Photosystem II reaction center protein T

Chain T: 94% 6%



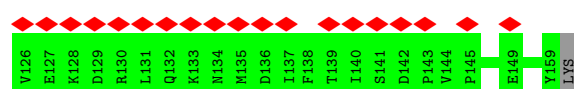
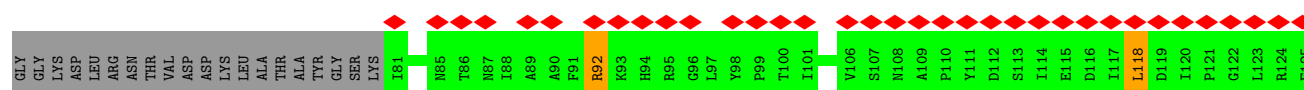
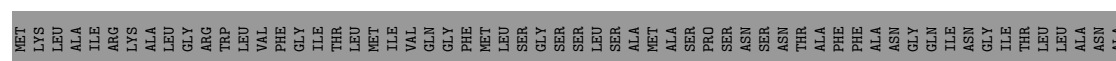
- Molecule 13: Photosystem II reaction center protein T

Chain t: 94% 6%

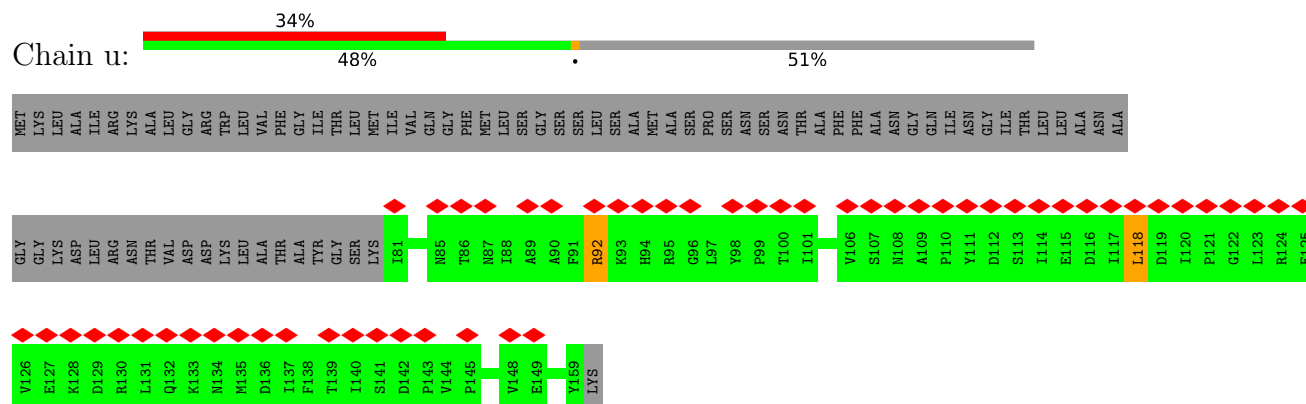


- Molecule 14: Photosystem II 12 kDa extrinsic protein

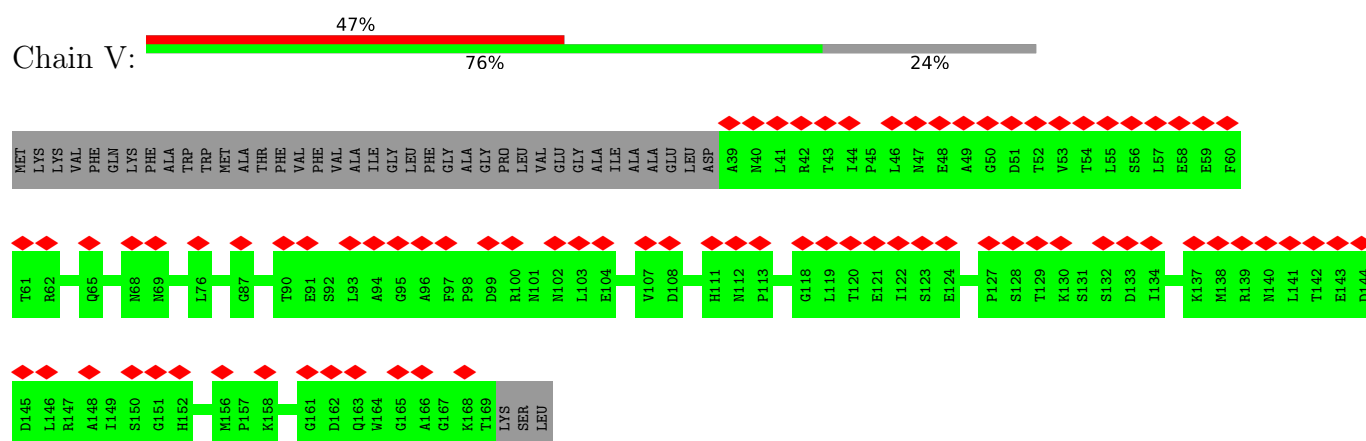
Chain U: 34% 48% 51%



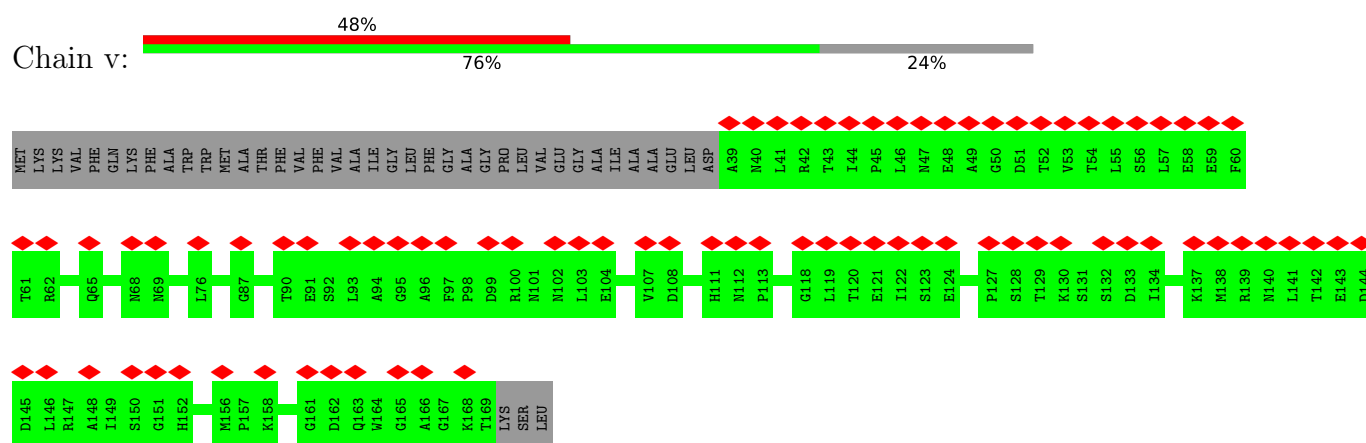
• Molecule 14: Photosystem II 12 kDa extrinsic protein



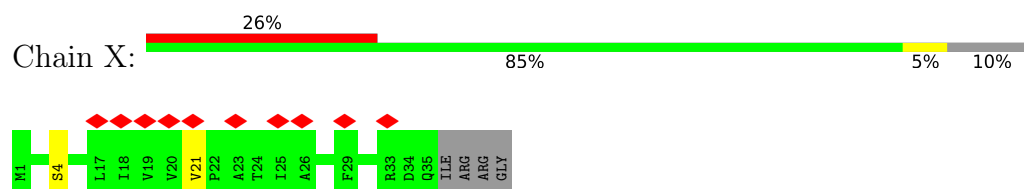
• Molecule 15: Cytochrome c-550




• Molecule 15: Cytochrome c-550

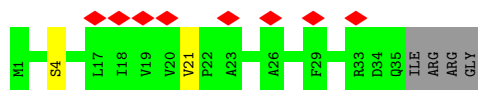


• Molecule 16: Photosystem II reaction center X protein



- Molecule 16: Photosystem II reaction center X protein

Chain x:  21% 85% 5% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90191	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 ($e^-/\text{\AA}^2$)	41.1	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0013	Depositor
Map size (\AA)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, BCT, CLA, BCR, F6C, LMT, SQD, PHO, CL7, CL, HEM, RRX, LHG, PL9, OEX, DGD, LMG

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	A	0.58	0/2716	0.69	1/3706 (0.0%)
1	a	0.58	0/2716	0.69	1/3706 (0.0%)
2	B	0.59	1/3922 (0.0%)	0.67	2/5346 (0.0%)
2	b	0.59	1/3922 (0.0%)	0.67	2/5346 (0.0%)
3	C	0.53	0/3616	0.69	4/4930 (0.1%)
3	c	0.53	0/3616	0.69	4/4930 (0.1%)
4	D	0.64	0/2804	0.73	10/3810 (0.3%)
4	d	0.64	0/2804	0.73	11/3810 (0.3%)
5	E	0.43	0/385	0.64	0/530
5	e	0.43	0/385	0.64	0/530
6	F	0.38	0/243	0.65	0/328
6	f	0.39	0/243	0.66	0/328
7	H	0.44	0/488	0.68	0/667
7	h	0.44	0/488	0.68	0/667
8	I	0.46	0/268	0.61	0/363
8	i	0.46	0/268	0.61	0/363
9	K	0.39	0/302	0.87	2/413 (0.5%)
9	k	0.39	0/302	0.87	2/413 (0.5%)
10	L	0.62	0/251	0.72	1/340 (0.3%)
10	l	0.62	0/251	0.71	1/340 (0.3%)
11	M	0.53	0/249	0.65	0/339
11	m	0.53	0/249	0.65	0/339
12	O	0.37	0/1256	0.71	2/1703 (0.1%)
12	o	0.37	0/1256	0.71	2/1703 (0.1%)
13	T	0.41	0/242	0.57	0/328
13	t	0.41	0/242	0.57	0/328
14	U	0.37	0/535	0.78	2/737 (0.3%)
14	u	0.37	0/535	0.78	2/737 (0.3%)
15	V	0.32	0/840	0.57	0/1157
15	v	0.32	0/840	0.57	0/1157
16	X	0.35	0/264	0.64	0/360

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	x	0.35	0/264	0.65	0/360
All	All	0.54	2/36762 (0.0%)	0.69	49/50114 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	c	0	2
12	O	0	1
12	o	0	1
16	X	0	1
16	x	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	22	VAL	CB-CG2	-7.47	1.37	1.52
2	B	22	VAL	CB-CG2	-7.45	1.37	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	279	LEU	CB-CG-CD1	-8.96	95.77	111.00
4	D	279	LEU	CB-CG-CD1	-8.95	95.78	111.00
9	K	24	LEU	CA-CB-CG	8.30	134.40	115.30
9	k	24	LEU	CA-CB-CG	8.30	134.40	115.30
3	c	234	GLU	CA-CB-CG	7.82	130.60	113.40
3	C	234	GLU	CA-CB-CG	7.80	130.55	113.40
14	U	118	LEU	CA-CB-CG	-7.28	98.55	115.30
14	u	118	LEU	CA-CB-CG	-7.28	98.57	115.30
2	B	3	LEU	CB-CG-CD2	-6.99	99.11	111.00
2	b	3	LEU	CB-CG-CD2	-6.97	99.14	111.00
12	O	98	ARG	NE-CZ-NH2	6.61	123.60	120.30
12	o	98	ARG	NE-CZ-NH2	6.61	123.60	120.30
4	D	213	ILE	CG1-CB-CG2	-6.24	97.67	111.40
4	d	213	ILE	CG1-CB-CG2	-6.23	97.69	111.40
4	d	294	ARG	CG-CD-NE	6.21	124.84	111.80
4	D	294	ARG	CG-CD-NE	6.21	124.84	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	317[A]	LYS	CB-CA-C	-5.89	98.61	110.40
4	d	317[B]	LYS	CB-CA-C	-5.89	98.61	110.40
4	D	317[A]	LYS	CB-CA-C	-5.89	98.62	110.40
4	D	317[B]	LYS	CB-CA-C	-5.89	98.62	110.40
14	U	92	ARG	CB-CG-CD	-5.79	96.54	111.60
14	u	92	ARG	CB-CG-CD	-5.79	96.56	111.60
12	o	241	PHE	CB-CG-CD2	5.77	124.84	120.80
12	O	241	PHE	CB-CG-CD2	5.72	124.80	120.80
1	a	258	ARG	NE-CZ-NH1	5.51	123.06	120.30
4	D	294	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	258	ARG	NE-CZ-NH1	5.43	123.01	120.30
4	d	294	ARG	NE-CZ-NH1	-5.41	117.60	120.30
4	D	18	LEU	CA-CB-CG	5.36	127.62	115.30
4	d	18	LEU	CA-CB-CG	5.34	127.59	115.30
4	d	235	PHE	CB-CG-CD1	5.33	124.53	120.80
4	d	272	LEU	CB-CG-CD1	-5.33	101.94	111.00
4	D	235	PHE	CB-CG-CD1	5.33	124.53	120.80
4	D	272	LEU	CB-CG-CD1	-5.33	101.95	111.00
3	C	394	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	c	394	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	c	201	LEU	CA-CB-CG	5.14	127.12	115.30
3	C	201	LEU	CA-CB-CG	5.13	127.10	115.30
3	c	381	ASP	CB-CG-OD1	5.08	122.87	118.30
9	K	24	LEU	CB-CG-CD1	5.07	119.62	111.00
4	d	152	VAL	CA-CB-CG2	-5.07	103.30	110.90
10	l	25	LEU	CB-CG-CD1	-5.07	102.39	111.00
4	D	152	VAL	CA-CB-CG2	-5.06	103.32	110.90
10	L	25	LEU	CB-CG-CD1	-5.05	102.42	111.00
9	k	24	LEU	CB-CG-CD1	5.04	119.56	111.00
2	b	246	PHE	N-CA-CB	5.02	119.64	110.60
3	C	381	ASP	CB-CG-OD1	5.02	122.81	118.30
4	d	235	PHE	CB-CG-CD2	-5.01	117.29	120.80
2	B	246	PHE	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	386	ASP	Peptide
3	C	388	GLN	Peptide
12	O	97	THR	Peptide
16	X	21	VAL	Peptide

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Mol	Chain	Res	Type	Group
3	c	386	ASP	Peptide
3	c	388	GLN	Peptide
12	o	97	THR	Peptide
16	x	21	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/359 (92%)	315 (95%)	16 (5%)	0	100	100
1	a	331/359 (92%)	315 (95%)	16 (5%)	0	100	100
2	B	481/509 (94%)	459 (95%)	22 (5%)	0	100	100
2	b	481/509 (94%)	459 (95%)	22 (5%)	0	100	100
3	C	451/482 (94%)	419 (93%)	30 (7%)	2 (0%)	34	57
3	c	451/482 (94%)	419 (93%)	30 (7%)	2 (0%)	34	57
4	D	337/352 (96%)	328 (97%)	9 (3%)	0	100	100
4	d	337/352 (96%)	328 (97%)	9 (3%)	0	100	100
5	E	44/80 (55%)	41 (93%)	3 (7%)	0	100	100
5	e	44/80 (55%)	41 (93%)	3 (7%)	0	100	100
6	F	28/44 (64%)	28 (100%)	0	0	100	100
6	f	28/44 (64%)	28 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
8	I	32/38 (84%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	32/38 (84%)	32 (100%)	0	0	100	100
9	K	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
9	k	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
10	L	28/40 (70%)	28 (100%)	0	0	100	100
10	l	28/40 (70%)	28 (100%)	0	0	100	100
11	M	29/36 (81%)	29 (100%)	0	0	100	100
11	m	29/36 (81%)	29 (100%)	0	0	100	100
12	O	168/274 (61%)	149 (89%)	19 (11%)	0	100	100
12	o	168/274 (61%)	149 (89%)	19 (11%)	0	100	100
13	T	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
13	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
14	U	77/160 (48%)	63 (82%)	14 (18%)	0	100	100
14	u	77/160 (48%)	63 (82%)	14 (18%)	0	100	100
15	V	129/172 (75%)	115 (89%)	14 (11%)	0	100	100
15	v	129/172 (75%)	115 (89%)	14 (11%)	0	100	100
16	X	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
16	x	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
All	All	4588/5456 (84%)	4312 (94%)	272 (6%)	4 (0%)	54	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	387	VAL
3	c	387	VAL
3	C	86	PRO
3	c	86	PRO

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	A	276/297 (93%)	271 (98%)	5 (2%)	59	80
1	a	276/297 (93%)	271 (98%)	5 (2%)	59	80
2	B	383/410 (93%)	379 (99%)	4 (1%)	76	90
2	b	383/410 (93%)	379 (99%)	4 (1%)	76	90
3	C	345/372 (93%)	336 (97%)	9 (3%)	46	72
3	c	345/372 (93%)	336 (97%)	9 (3%)	46	72
4	D	280/290 (97%)	277 (99%)	3 (1%)	73	88
4	d	280/290 (97%)	277 (99%)	3 (1%)	73	88
5	E	36/69 (52%)	36 (100%)	0	100	100
5	e	36/69 (52%)	36 (100%)	0	100	100
6	F	23/37 (62%)	23 (100%)	0	100	100
6	f	23/37 (62%)	23 (100%)	0	100	100
7	H	49/55 (89%)	49 (100%)	0	100	100
7	h	49/55 (89%)	49 (100%)	0	100	100
8	I	29/33 (88%)	29 (100%)	0	100	100
8	i	29/33 (88%)	29 (100%)	0	100	100
9	K	28/37 (76%)	28 (100%)	0	100	100
9	k	28/37 (76%)	28 (100%)	0	100	100
10	L	28/37 (76%)	28 (100%)	0	100	100
10	l	28/37 (76%)	28 (100%)	0	100	100
11	M	28/32 (88%)	26 (93%)	2 (7%)	14	29
11	m	28/32 (88%)	26 (93%)	2 (7%)	14	29
12	O	102/228 (45%)	99 (97%)	3 (3%)	42	68
12	o	102/228 (45%)	99 (97%)	3 (3%)	42	68
13	T	24/26 (92%)	24 (100%)	0	100	100
13	t	24/26 (92%)	24 (100%)	0	100	100
14	U	40/130 (31%)	38 (95%)	2 (5%)	24	47
14	u	40/130 (31%)	38 (95%)	2 (5%)	24	47
15	V	56/141 (40%)	56 (100%)	0	100	100
15	v	56/141 (40%)	56 (100%)	0	100	100
16	X	30/34 (88%)	29 (97%)	1 (3%)	38	64
16	x	30/34 (88%)	29 (97%)	1 (3%)	38	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3514/4456 (79%)	3456 (98%)	58 (2%)	64 81

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	42	LEU
1	A	293	THR
1	A	313	ARG
1	A	333	HIS
2	B	41	GLU
2	B	75	TRP
2	B	85	PHE
2	B	127	LYS
3	C	124	HIS
3	C	149	PHE
3	C	234	GLU
3	C	252	ILE
3	C	372	LEU
3	C	413	LEU
3	C	420	PHE
3	C	458	PHE
3	C	459	GLU
4	D	180	ARG
4	D	317[A]	LYS
4	D	317[B]	LYS
11	M	5	LYS
11	M	13	LEU
12	O	120	PHE
12	O	241	PHE
12	O	267	SER
14	U	92	ARG
14	U	118	LEU
16	X	4	SER
1	a	13	SER
1	a	42	LEU
1	a	293	THR
1	a	313	ARG
1	a	333	HIS
2	b	41	GLU
2	b	75	TRP
2	b	85	PHE

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Mol	Chain	Res	Type
2	b	127	LYS
3	c	124	HIS
3	c	149	PHE
3	c	234	GLU
3	c	252	ILE
3	c	372	LEU
3	c	413	LEU
3	c	420	PHE
3	c	458	PHE
3	c	459	GLU
4	d	180	ARG
4	d	317[A]	LYS
4	d	317[B]	LYS
11	m	5	LYS
11	m	13	LEU
12	o	120	PHE
12	o	241	PHE
12	o	267	SER
14	u	92	ARG
14	u	118	LEU
16	x	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	232	GLN
1	A	271	GLN
1	A	304	ASN
1	A	323	ASN
1	A	336	ASN
2	B	179	GLN
2	B	201	HIS
3	C	59	HIS
3	C	80	HIS
3	C	124	HIS
3	C	162	GLN
3	C	285	GLN
3	C	314	GLN
3	C	418	ASN
4	D	219	GLN
15	V	68	ASN

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Mol	Chain	Res	Type
16	X	32	GLN
16	X	35	GLN
1	a	166	GLN
1	a	232	GLN
1	a	304	ASN
1	a	323	ASN
1	a	336	ASN
2	b	179	GLN
2	b	201	HIS
3	c	59	HIS
3	c	80	HIS
3	c	124	HIS
3	c	162	GLN
3	c	285	GLN
3	c	314	GLN
3	c	418	ASN
4	d	219	GLN
15	v	68	ASN
16	x	32	GLN
16	x	35	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 132 ligands modelled in this entry, 6 are monoatomic - leaving 126 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
20	CLA	b	610	34	65,73,73	2.12	16 (24%)	76,113,113	2.82	28 (36%)
20	CLA	b	603	-	55,63,73	2.45	21 (38%)	64,101,113	2.79	23 (35%)
22	BCR	a	408	-	41,41,41	2.89	6 (14%)	56,56,56	6.38	21 (37%)
20	CLA	C	503	-	65,73,73	2.21	19 (29%)	76,113,113	2.65	28 (36%)
20	CLA	C	506	-	60,68,73	2.26	19 (31%)	70,107,113	2.74	24 (34%)
27	F6C	b	604	-	69,74,74	2.73	23 (33%)	70,114,114	3.26	29 (41%)
20	CLA	d	404	-	45,53,73	2.55	18 (40%)	52,89,113	3.04	20 (38%)
20	CLA	c	506	-	60,68,73	2.26	19 (31%)	70,107,113	2.74	24 (34%)
20	CLA	B	606	-	55,63,73	2.45	21 (38%)	64,101,113	2.77	23 (35%)
28	DGD	C	517	-	34,34,67	1.20	3 (8%)	42,42,81	1.31	3 (7%)
20	CLA	B	610	34	65,73,73	2.12	16 (24%)	76,113,113	2.82	28 (36%)
22	BCR	B	616	-	41,41,41	2.78	6 (14%)	56,56,56	6.51	27 (48%)
22	BCR	b	616	-	41,41,41	2.78	6 (14%)	56,56,56	6.51	27 (48%)
30	LMG	D	409	-	33,33,55	1.13	2 (6%)	41,41,63	1.23	4 (9%)
23	SQD	L	102	-	53,54,54	0.96	6 (11%)	62,65,65	1.96	15 (24%)
21	PHO	a	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.50	9 (19%)
32	RRX	h	102	-	42,42,42	1.71	8 (19%)	57,58,58	1.59	11 (19%)
20	CLA	d	403	-	60,68,73	2.29	21 (35%)	70,107,113	2.95	20 (28%)
20	CLA	A	407	-	50,58,73	2.57	20 (40%)	58,95,113	2.91	23 (39%)
20	CLA	c	510	-	65,73,73	2.17	17 (26%)	76,113,113	2.54	26 (34%)
20	CLA	C	502	-	60,68,73	2.30	18 (30%)	70,107,113	2.58	22 (31%)
24	PL9	A	410	-	20,20,55	3.17	7 (35%)	26,27,69	1.86	7 (26%)
31	HEM	V	201	15	41,50,50	1.49	5 (12%)	45,82,82	1.46	8 (17%)
20	CLA	b	615	-	60,68,73	2.16	18 (30%)	70,107,113	2.86	24 (34%)
20	CLA	b	608	-	55,63,73	2.44	19 (34%)	64,101,113	2.77	23 (35%)
20	CLA	B	609	-	45,53,73	2.57	17 (37%)	52,89,113	3.00	18 (34%)
31	HEM	v	201	15	41,50,50	1.49	5 (12%)	45,82,82	1.46	8 (17%)
20	CLA	c	504	-	65,73,73	2.22	19 (29%)	76,113,113	2.60	25 (32%)
22	BCR	c	518	-	20,20,41	2.53	3 (15%)	27,27,56	5.69	10 (37%)
20	CLA	B	611	-	65,73,73	2.16	20 (30%)	76,113,113	2.61	24 (31%)
20	CLA	B	615	-	60,68,73	2.16	18 (30%)	70,107,113	2.86	23 (32%)
20	CLA	a	405	34	50,58,73	2.47	18 (36%)	58,95,113	3.08	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	a	404	-	65,73,73	2.26	20 (30%)	76,113,113	2.58	23 (30%)
20	CLA	C	507	-	55,63,73	2.49	22 (40%)	64,101,113	2.94	28 (43%)
20	CLA	D	404	-	45,53,73	2.55	18 (40%)	52,89,113	3.04	19 (36%)
20	CLA	b	611	-	65,73,73	2.16	20 (30%)	76,113,113	2.60	23 (30%)
33	LMT	M	102	-	36,36,36	1.28	7 (19%)	47,47,47	0.98	0
20	CLA	h	101	-	50,58,73	2.43	18 (36%)	58,95,113	3.00	25 (43%)
30	LMG	M	101	-	40,40,55	1.12	4 (10%)	48,48,63	1.28	5 (10%)
22	BCR	C	515	-	41,41,41	2.85	6 (14%)	56,56,56	6.66	24 (42%)
27	F6C	B	607	34	64,69,74	2.87	26 (40%)	64,108,114	3.32	27 (42%)
20	CLA	B	601	-	45,53,73	2.54	17 (37%)	52,89,113	2.84	18 (34%)
23	SQD	A	409	-	51,52,54	0.38	1 (1%)	60,63,65	0.42	1 (1%)
24	PL9	D	406	-	45,45,55	2.02	11 (24%)	56,57,69	1.60	12 (21%)
20	CLA	b	601	-	45,53,73	2.53	17 (37%)	52,89,113	2.84	19 (36%)
22	BCR	B	618	-	41,41,41	2.94	7 (17%)	56,56,56	6.55	22 (39%)
26	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.31	6 (11%)
20	CLA	C	509	-	60,68,73	2.33	17 (28%)	70,107,113	2.63	26 (37%)
28	DGD	c	517	-	34,34,67	1.20	3 (8%)	42,42,81	1.31	3 (7%)
26	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.31	6 (11%)
23	SQD	l	102	-	53,54,54	0.96	6 (11%)	62,65,65	1.96	15 (24%)
30	LMG	m	101	-	40,40,55	1.12	4 (10%)	48,48,63	1.28	5 (10%)
20	CLA	c	507	-	55,63,73	2.49	22 (40%)	64,101,113	2.94	28 (43%)
22	BCR	A	408	-	41,41,41	2.89	6 (14%)	56,56,56	6.38	21 (37%)
20	CLA	c	511	-	65,73,73	2.21	19 (29%)	76,113,113	2.68	25 (32%)
25	BCT	a	411	18	2,3,3	1.09	0	2,3,3	4.44	2 (100%)
20	CLA	A	404	-	65,73,73	2.26	20 (30%)	76,113,113	2.57	23 (30%)
31	HEM	e	101	5	41,50,50	1.43	3 (7%)	45,82,82	1.40	6 (13%)
20	CLA	D	403	-	60,68,73	2.29	21 (35%)	70,107,113	2.95	20 (28%)
31	HEM	E	101	5	41,50,50	1.43	3 (7%)	45,82,82	1.41	7 (15%)
27	F6C	c	508	34	64,69,74	2.87	26 (40%)	64,108,114	3.32	27 (42%)
28	DGD	D	410	-	45,45,67	0.90	2 (4%)	53,53,81	1.21	2 (3%)
20	CLA	C	505	34	50,58,73	2.48	21 (42%)	58,95,113	2.94	23 (39%)
30	LMG	d	409	-	33,33,55	1.13	2 (6%)	41,41,63	1.23	4 (9%)
20	CLA	C	514	-	45,53,73	2.59	18 (40%)	52,89,113	2.89	22 (42%)
20	CLA	c	509	-	60,68,73	2.33	17 (28%)	70,107,113	2.63	26 (37%)
20	CLA	B	614	-	55,63,73	2.32	18 (32%)	64,101,113	2.74	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	F6C	B	613	-	69,74,74	2.69	23 (33%)	70,114,114	3.28	27 (38%)
32	RRX	H	102	-	42,42,42	1.70	8 (19%)	57,58,58	1.59	11 (19%)
21	PHO	A	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.50	9 (19%)
20	CLA	b	609	-	45,53,73	2.57	17 (37%)	52,89,113	3.00	18 (34%)
20	CLA	a	407	-	50,58,73	2.57	20 (40%)	58,95,113	2.91	23 (39%)
20	CLA	c	512	3	50,58,73	2.44	18 (36%)	58,95,113	3.15	25 (43%)
20	CLA	B	603	-	55,63,73	2.45	21 (38%)	64,101,113	2.79	23 (35%)
20	CLA	B	612	-	65,73,73	2.22	20 (30%)	76,113,113	2.72	26 (34%)
20	CLA	b	612	-	65,73,73	2.22	20 (30%)	76,113,113	2.72	25 (32%)
24	PL9	a	410	-	20,20,55	3.17	6 (30%)	26,27,69	1.86	7 (26%)
27	F6C	C	508	34	64,69,74	2.87	26 (40%)	64,108,114	3.32	27 (42%)
29	CL7	D	401	34	66,73,73	2.80	20 (30%)	65,113,113	2.40	15 (23%)
20	CLA	B	608	-	55,63,73	2.44	20 (36%)	64,101,113	2.77	23 (35%)
20	CLA	C	511	-	65,73,73	2.21	19 (29%)	76,113,113	2.68	25 (32%)
20	CLA	c	513	-	45,53,73	2.52	17 (37%)	52,89,113	2.84	20 (38%)
20	CLA	C	513	-	45,53,73	2.53	17 (37%)	52,89,113	2.84	20 (38%)
20	CLA	c	505	34	50,58,73	2.48	21 (42%)	58,95,113	2.94	23 (39%)
22	BCR	b	618	-	41,41,41	2.95	7 (17%)	56,56,56	6.55	22 (39%)
22	BCR	d	405	-	26,26,41	3.08	5 (19%)	34,34,56	7.90	12 (35%)
20	CLA	c	514	-	45,53,73	2.59	18 (40%)	52,89,113	2.89	22 (42%)
25	BCT	A	411	18	2,3,3	1.08	0	2,3,3	4.44	2 (100%)
26	LHG	D	408	-	46,46,48	0.94	2 (4%)	49,52,54	1.03	3 (6%)
23	SQD	a	409	-	51,52,54	0.38	1 (1%)	60,63,65	0.42	1 (1%)
33	LMT	m	102	-	36,36,36	1.28	7 (19%)	47,47,47	0.99	0
22	BCR	c	515	-	41,41,41	2.85	6 (14%)	56,56,56	6.66	24 (42%)
21	PHO	d	402	-	51,69,69	1.02	4 (7%)	47,99,99	1.26	4 (8%)
20	CLA	A	405	34	50,58,73	2.47	18 (36%)	58,95,113	3.07	26 (44%)
22	BCR	D	405	-	26,26,41	3.09	5 (19%)	34,34,56	7.90	12 (35%)
26	LHG	L	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.02	4 (7%)
21	PHO	D	402	-	51,69,69	1.01	4 (7%)	47,99,99	1.26	4 (8%)
26	LHG	l	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.02	4 (7%)
27	F6C	B	604	-	69,74,74	2.73	23 (33%)	70,114,114	3.26	29 (41%)
27	F6C	b	607	34	64,69,74	2.86	26 (40%)	64,108,114	3.32	27 (42%)
28	DGD	d	410	-	45,45,67	0.90	2 (4%)	53,53,81	1.21	2 (3%)
20	CLA	c	502	-	60,68,73	2.30	18 (30%)	70,107,113	2.58	22 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	B	617	-	41,41,41	2.89	6 (14%)	56,56,56	6.46	23 (41%)
22	BCR	b	617	-	41,41,41	2.89	6 (14%)	56,56,56	6.46	23 (41%)
26	LHG	a	412	-	36,36,48	1.05	4 (11%)	39,42,54	1.39	5 (12%)
22	BCR	C	518	-	20,20,41	2.53	3 (15%)	27,27,56	5.68	10 (37%)
20	CLA	B	602	-	65,73,73	2.26	21 (32%)	76,113,113	2.58	22 (28%)
20	CLA	b	602	-	65,73,73	2.26	21 (32%)	76,113,113	2.58	23 (30%)
20	CLA	b	606	-	55,63,73	2.45	21 (38%)	64,101,113	2.77	23 (35%)
28	DGD	C	516	-	50,50,67	1.29	8 (16%)	64,64,81	1.47	12 (18%)
20	CLA	C	510	-	65,73,73	2.17	17 (26%)	76,113,113	2.54	27 (35%)
28	DGD	c	516	-	50,50,67	1.29	8 (16%)	64,64,81	1.47	12 (18%)
20	CLA	b	605	-	65,73,73	2.24	19 (29%)	76,113,113	2.69	30 (39%)
26	LHG	A	412	1	36,36,48	1.05	4 (11%)	39,42,54	1.39	5 (12%)
29	CL7	d	401	34	66,73,73	2.81	20 (30%)	65,113,113	2.41	15 (23%)
20	CLA	C	504	-	65,73,73	2.22	19 (29%)	76,113,113	2.60	26 (34%)
20	CLA	H	101	-	50,58,73	2.43	18 (36%)	58,95,113	3.00	25 (43%)
20	CLA	b	614	-	55,63,73	2.32	18 (32%)	64,101,113	2.74	21 (32%)
27	F6C	b	613	-	69,74,74	2.69	23 (33%)	70,114,114	3.28	27 (38%)
26	LHG	d	408	-	46,46,48	0.94	2 (4%)	49,52,54	1.03	3 (6%)
20	CLA	C	512	3	50,58,73	2.44	18 (36%)	58,95,113	3.16	25 (43%)
20	CLA	c	503	-	65,73,73	2.21	19 (29%)	76,113,113	2.65	28 (36%)
20	CLA	B	605	-	65,73,73	2.24	19 (29%)	76,113,113	2.70	30 (39%)
24	PL9	d	406	-	45,45,55	2.02	11 (24%)	56,57,69	1.61	12 (21%)

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
20	CLA	b	610	34	1/1/15/20	16/37/115/115	-
20	CLA	b	603	-	1/1/13/20	10/25/103/115	-
22	BCR	a	408	-	-	6/29/63/63	0/2/2/2
20	CLA	C	503	-	1/1/15/20	14/37/115/115	-
20	CLA	C	506	-	1/1/14/20	16/31/109/115	-
27	F6C	b	604	-	-	18/41/97/97	-
20	CLA	d	404	-	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	506	-	1/1/14/20	16/31/109/115	-
20	CLA	B	606	-	1/1/13/20	9/25/103/115	-
28	DGD	C	517	-	-	13/28/48/95	0/1/1/2
20	CLA	B	610	34	1/1/15/20	16/37/115/115	-
22	BCR	B	616	-	-	12/29/63/63	0/2/2/2
22	BCR	b	616	-	-	12/29/63/63	0/2/2/2
30	LMG	D	409	-	-	7/28/48/70	0/1/1/1
23	SQD	L	102	-	-	19/49/69/69	0/1/1/1
21	PHO	a	406	-	-	18/37/103/103	0/5/6/6
32	RRX	h	102	-	-	20/29/65/65	0/2/2/2
20	CLA	d	403	-	1/1/14/20	7/31/109/115	-
20	CLA	A	407	-	1/1/12/20	6/19/97/115	-
20	CLA	c	510	-	1/1/15/20	10/37/115/115	-
20	CLA	C	502	-	1/1/14/20	10/31/109/115	-
24	PL9	A	410	-	-	5/11/31/73	0/1/1/1
31	HEM	V	201	15	-	4/12/54/54	-
20	CLA	b	615	-	1/1/14/20	11/31/109/115	-
20	CLA	b	608	-	1/1/13/20	9/25/103/115	-
20	CLA	B	609	-	1/1/11/20	7/13/91/115	-
31	HEM	v	201	15	-	4/12/54/54	-
20	CLA	c	504	-	1/1/15/20	18/37/115/115	-
22	BCR	c	518	-	-	6/13/30/63	0/1/1/2
20	CLA	B	611	-	1/1/15/20	16/37/115/115	-
20	CLA	B	615	-	1/1/14/20	11/31/109/115	-
20	CLA	a	405	34	1/1/12/20	7/19/97/115	-
20	CLA	a	404	-	1/1/15/20	8/37/115/115	-
20	CLA	C	507	-	1/1/13/20	12/25/103/115	-
20	CLA	D	404	-	1/1/11/20	9/13/91/115	-
20	CLA	b	611	-	1/1/15/20	16/37/115/115	-
33	LMT	M	102	-	-	7/21/61/61	0/2/2/2
20	CLA	h	101	-	1/1/12/20	5/19/97/115	-
30	LMG	M	101	-	-	10/35/55/70	0/1/1/1
22	BCR	C	515	-	-	6/29/63/63	0/2/2/2
27	F6C	B	607	34	-	22/35/91/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	601	-	1/1/11/20	11/13/91/115	-
23	SQD	A	409	-	-	26/47/67/69	0/1/1/1
24	PL9	D	406	-	-	15/41/61/73	0/1/1/1
20	CLA	b	601	-	1/1/11/20	11/13/91/115	-
22	BCR	B	618	-	-	11/29/63/63	0/2/2/2
26	LHG	d	407	-	-	28/53/53/53	-
20	CLA	C	509	-	1/1/14/20	11/31/109/115	-
28	DGD	c	517	-	-	13/28/48/95	0/1/1/2
26	LHG	D	407	-	-	28/53/53/53	-
23	SQD	l	102	-	-	19/49/69/69	0/1/1/1
30	LMG	m	101	-	-	10/35/55/70	0/1/1/1
20	CLA	c	507	-	1/1/13/20	12/25/103/115	-
22	BCR	A	408	-	-	6/29/63/63	0/2/2/2
20	CLA	c	511	-	1/1/15/20	19/37/115/115	-
20	CLA	A	404	-	1/1/15/20	8/37/115/115	-
31	HEM	e	101	5	-	6/12/54/54	-
20	CLA	D	403	-	1/1/14/20	7/31/109/115	-
31	HEM	E	101	5	-	6/12/54/54	-
27	F6C	c	508	34	-	21/35/91/97	-
28	DGD	D	410	-	-	12/39/59/95	0/1/1/2
20	CLA	C	505	34	1/1/12/20	7/19/97/115	-
30	LMG	d	409	-	-	7/28/48/70	0/1/1/1
20	CLA	C	514	-	1/1/11/20	5/13/91/115	-
20	CLA	c	509	-	1/1/14/20	11/31/109/115	-
20	CLA	B	614	-	1/1/13/20	9/25/103/115	-
27	F6C	B	613	-	-	20/41/97/97	-
32	RRX	H	102	-	-	20/29/65/65	0/2/2/2
21	PHO	A	406	-	-	18/37/103/103	0/5/6/6
20	CLA	b	609	-	1/1/11/20	7/13/91/115	-
20	CLA	a	407	-	1/1/12/20	6/19/97/115	-
20	CLA	c	512	3	1/1/12/20	9/19/97/115	-
20	CLA	B	603	-	1/1/13/20	10/25/103/115	-
20	CLA	B	612	-	1/1/15/20	16/37/115/115	-
20	CLA	b	612	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PL9	a	410	-	-	5/11/31/73	0/1/1/1
27	F6C	C	508	34	-	21/35/91/97	-
29	CL7	D	401	34	2/2/15/20	13/37/115/115	-
20	CLA	B	608	-	1/1/13/20	9/25/103/115	-
20	CLA	C	511	-	1/1/15/20	19/37/115/115	-
20	CLA	c	513	-	1/1/11/20	7/13/91/115	-
20	CLA	C	513	-	1/1/11/20	7/13/91/115	-
20	CLA	c	505	34	1/1/12/20	6/19/97/115	-
22	BCR	b	618	-	-	11/29/63/63	0/2/2/2
22	BCR	d	405	-	-	6/20/37/63	0/1/1/2
20	CLA	c	514	-	1/1/11/20	5/13/91/115	-
26	LHG	D	408	-	-	23/51/51/53	-
23	SQD	a	409	-	-	26/47/67/69	0/1/1/1
33	LMT	m	102	-	-	7/21/61/61	0/2/2/2
22	BCR	c	515	-	-	6/29/63/63	0/2/2/2
21	PHO	d	402	-	-	6/37/103/103	0/5/6/6
20	CLA	A	405	34	1/1/12/20	7/19/97/115	-
22	BCR	D	405	-	-	6/20/37/63	0/1/1/2
26	LHG	L	101	-	-	26/53/53/53	-
21	PHO	D	402	-	-	6/37/103/103	0/5/6/6
26	LHG	l	101	-	-	26/53/53/53	-
27	F6C	B	604	-	-	18/41/97/97	-
27	F6C	b	607	34	-	22/35/91/97	-
28	DGD	d	410	-	-	12/39/59/95	0/1/1/2
20	CLA	c	502	-	1/1/14/20	10/31/109/115	-
22	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	BCR	b	617	-	-	7/29/63/63	0/2/2/2
26	LHG	a	412	-	-	26/41/41/53	-
22	BCR	C	518	-	-	6/13/30/63	0/1/1/2
20	CLA	B	602	-	1/1/15/20	13/37/115/115	-
20	CLA	b	602	-	1/1/15/20	13/37/115/115	-
20	CLA	b	606	-	1/1/13/20	9/25/103/115	-
28	DGD	C	516	-	-	15/38/78/95	0/2/2/2
20	CLA	C	510	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	c	516	-	-	15/38/78/95	0/2/2/2
20	CLA	b	605	-	1/1/15/20	14/37/115/115	-
29	CL7	d	401	34	2/2/15/20	13/37/115/115	-
26	LHG	A	412	1	-	26/41/41/53	-
20	CLA	C	504	-	1/1/15/20	18/37/115/115	-
20	CLA	H	101	-	1/1/12/20	5/19/97/115	-
20	CLA	b	614	-	1/1/13/20	9/25/103/115	-
27	F6C	b	613	-	-	20/41/97/97	-
26	LHG	d	408	-	-	23/51/51/53	-
20	CLA	C	512	3	1/1/12/20	9/19/97/115	-
20	CLA	c	503	-	1/1/15/20	14/37/115/115	-
20	CLA	B	605	-	1/1/15/20	14/37/115/115	-
24	PL9	d	406	-	-	15/41/61/73	0/1/1/1

All (1620) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	410	PL9	C7-C3	-10.06	1.41	1.51
24	a	410	PL9	C7-C3	-10.06	1.41	1.51
27	B	604	F6C	MG-NA	9.21	2.24	2.05
27	b	604	F6C	MG-NA	9.21	2.24	2.05
27	c	508	F6C	MG-NA	9.19	2.24	2.05
27	B	607	F6C	MG-NA	9.18	2.24	2.05
27	C	508	F6C	MG-NA	9.17	2.24	2.05
27	b	607	F6C	MG-NA	9.17	2.24	2.05
27	b	613	F6C	MG-NA	8.91	2.23	2.05
27	B	613	F6C	MG-NA	8.89	2.23	2.05
29	d	401	CL7	CHD-C4C	8.88	1.47	1.35
29	D	401	CL7	CHD-C4C	8.83	1.47	1.35
22	b	618	BCR	C8-C9	-8.56	1.27	1.45
22	B	618	BCR	C8-C9	-8.56	1.27	1.45
22	b	618	BCR	C10-C9	-8.41	1.24	1.35
27	B	613	F6C	C1A-CHA	8.41	1.51	1.35
27	b	613	F6C	C1A-CHA	8.41	1.51	1.35
22	B	618	BCR	C10-C9	-8.39	1.24	1.35
22	B	618	BCR	C11-C10	-8.30	1.17	1.43
22	b	618	BCR	C11-C10	-8.30	1.17	1.43
22	b	617	BCR	C8-C9	-8.28	1.28	1.45
22	B	617	BCR	C8-C9	-8.26	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	401	CL7	MG-NA	8.23	2.22	2.05
29	d	401	CL7	MG-NA	8.23	2.22	2.05
22	C	515	BCR	C11-C10	-8.18	1.18	1.43
22	c	515	BCR	C11-C10	-8.18	1.18	1.43
22	A	408	BCR	C8-C9	-8.17	1.28	1.45
22	a	408	BCR	C8-C9	-8.17	1.28	1.45
22	A	408	BCR	C11-C10	-8.13	1.18	1.43
22	a	408	BCR	C11-C10	-8.13	1.18	1.43
22	B	617	BCR	C11-C10	-8.11	1.18	1.43
22	b	617	BCR	C11-C10	-8.11	1.18	1.43
22	d	405	BCR	C11-C10	-8.10	1.18	1.43
22	D	405	BCR	C11-C10	-8.09	1.18	1.43
22	c	515	BCR	C8-C9	-8.05	1.28	1.45
22	C	515	BCR	C8-C9	-8.03	1.28	1.45
22	b	616	BCR	C8-C9	-7.93	1.28	1.45
22	B	616	BCR	C8-C9	-7.93	1.28	1.45
22	b	616	BCR	C11-C10	-7.92	1.18	1.43
22	B	616	BCR	C11-C10	-7.91	1.18	1.43
22	A	408	BCR	C10-C9	-7.90	1.25	1.35
22	a	408	BCR	C10-C9	-7.90	1.25	1.35
27	B	604	F6C	C1A-CHA	7.86	1.50	1.35
27	b	604	F6C	C1A-CHA	7.84	1.50	1.35
29	d	401	CL7	C3D-C4D	-7.84	1.32	1.40
29	D	401	CL7	C3D-C4D	-7.80	1.32	1.40
22	D	405	BCR	C8-C9	-7.77	1.29	1.45
22	d	405	BCR	C8-C9	-7.75	1.29	1.45
22	B	617	BCR	C10-C9	-7.74	1.25	1.35
27	C	508	F6C	C2A-C3A	7.73	1.53	1.36
27	c	508	F6C	C2A-C3A	7.71	1.53	1.36
22	b	617	BCR	C10-C9	-7.71	1.25	1.35
27	B	607	F6C	C2A-C3A	7.70	1.53	1.36
27	b	607	F6C	C2A-C3A	7.70	1.53	1.36
22	C	518	BCR	C15-C14	-7.69	1.20	1.49
27	c	508	F6C	C1A-CHA	7.68	1.49	1.35
22	c	518	BCR	C15-C14	-7.68	1.20	1.49
22	B	617	BCR	C16-C17	-7.67	1.19	1.43
22	b	617	BCR	C16-C17	-7.67	1.19	1.43
27	C	508	F6C	C1A-CHA	7.64	1.49	1.35
22	c	515	BCR	C10-C9	-7.63	1.25	1.35
27	b	607	F6C	C1A-CHA	7.63	1.49	1.35
27	B	607	F6C	C1A-CHA	7.63	1.49	1.35
20	b	608	CLA	MG-NA	7.61	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	BCR	C20-C21	-7.60	1.19	1.43
22	b	617	BCR	C20-C21	-7.60	1.19	1.43
22	C	515	BCR	C10-C9	-7.59	1.25	1.35
29	d	401	CL7	CHC-C1C	7.59	1.45	1.35
20	B	608	CLA	MG-NA	7.59	2.24	2.06
22	A	408	BCR	C20-C21	-7.59	1.19	1.43
29	D	401	CL7	CHC-C1C	7.58	1.45	1.35
22	a	408	BCR	C20-C21	-7.57	1.20	1.43
20	B	601	CLA	MG-NA	7.53	2.24	2.06
20	b	601	CLA	MG-NA	7.53	2.24	2.06
22	c	518	BCR	C11-C10	-7.51	1.20	1.43
22	c	515	BCR	C20-C21	-7.50	1.20	1.43
20	B	603	CLA	MG-NA	7.50	2.24	2.06
22	C	515	BCR	C20-C21	-7.49	1.20	1.43
20	b	603	CLA	MG-NA	7.49	2.24	2.06
22	C	518	BCR	C11-C10	-7.49	1.20	1.43
22	B	618	BCR	C20-C21	-7.49	1.20	1.43
22	b	618	BCR	C20-C21	-7.48	1.20	1.43
20	b	602	CLA	MG-NA	7.47	2.24	2.06
22	C	515	BCR	C16-C17	-7.47	1.20	1.43
22	c	515	BCR	C16-C17	-7.46	1.20	1.43
20	C	504	CLA	MG-NA	7.46	2.24	2.06
20	B	602	CLA	MG-NA	7.46	2.24	2.06
20	A	404	CLA	MG-NA	7.46	2.24	2.06
22	A	408	BCR	C16-C17	-7.46	1.20	1.43
22	a	408	BCR	C16-C17	-7.46	1.20	1.43
20	c	504	CLA	MG-NA	7.45	2.24	2.06
20	A	407	CLA	MG-NA	7.45	2.24	2.06
20	B	606	CLA	MG-NA	7.45	2.24	2.06
20	a	407	CLA	MG-NA	7.45	2.24	2.06
20	a	404	CLA	MG-NA	7.45	2.24	2.06
27	b	604	F6C	C1A-NA	-7.45	1.27	1.37
20	b	606	CLA	MG-NA	7.44	2.24	2.06
27	B	604	F6C	C1A-NA	-7.42	1.27	1.37
22	b	616	BCR	C20-C21	-7.42	1.20	1.43
22	B	616	BCR	C20-C21	-7.40	1.20	1.43
22	b	618	BCR	C16-C17	-7.38	1.20	1.43
27	B	613	F6C	C1A-NA	-7.38	1.27	1.37
27	B	604	F6C	C2A-C3A	7.38	1.52	1.36
27	b	604	F6C	C2A-C3A	7.37	1.52	1.36
22	B	618	BCR	C16-C17	-7.37	1.20	1.43
27	b	613	F6C	C1A-NA	-7.35	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	BCR	C16-C17	-7.34	1.20	1.43
22	D	405	BCR	C16-C17	-7.33	1.20	1.43
22	b	616	BCR	C16-C17	-7.30	1.20	1.43
22	B	616	BCR	C16-C17	-7.30	1.20	1.43
20	C	510	CLA	MG-NA	7.29	2.23	2.06
20	c	510	CLA	MG-NA	7.28	2.23	2.06
20	C	513	CLA	MG-NA	7.23	2.23	2.06
20	c	513	CLA	MG-NA	7.23	2.23	2.06
20	d	404	CLA	MG-NA	7.23	2.23	2.06
20	B	609	CLA	MG-NA	7.23	2.23	2.06
22	B	616	BCR	C10-C9	-7.22	1.26	1.35
20	b	609	CLA	MG-NA	7.21	2.23	2.06
20	C	514	CLA	MG-NA	7.21	2.23	2.06
20	D	404	CLA	MG-NA	7.21	2.23	2.06
20	b	605	CLA	MG-NA	7.20	2.23	2.06
27	b	607	F6C	C1A-NA	-7.20	1.27	1.37
20	B	605	CLA	MG-NA	7.19	2.23	2.06
20	c	505	CLA	MG-NA	7.18	2.23	2.06
20	c	514	CLA	MG-NA	7.18	2.23	2.06
22	b	616	BCR	C10-C9	-7.17	1.26	1.35
20	C	505	CLA	MG-NA	7.17	2.23	2.06
27	B	607	F6C	C1A-NA	-7.16	1.27	1.37
20	C	503	CLA	MG-NA	7.15	2.23	2.06
20	A	405	CLA	MG-NA	7.13	2.23	2.06
20	c	503	CLA	MG-NA	7.12	2.23	2.06
20	a	405	CLA	MG-NA	7.11	2.23	2.06
27	c	508	F6C	C1A-NA	-7.09	1.28	1.37
27	C	508	F6C	C1A-NA	-7.05	1.28	1.37
20	C	511	CLA	MG-NA	7.03	2.23	2.06
20	c	511	CLA	MG-NA	7.01	2.22	2.06
20	h	101	CLA	MG-NA	6.97	2.22	2.06
20	b	614	CLA	MG-NA	6.96	2.22	2.06
20	B	614	CLA	MG-NA	6.96	2.22	2.06
20	H	101	CLA	MG-NA	6.95	2.22	2.06
24	d	406	PL9	C7-C3	-6.94	1.44	1.51
20	b	612	CLA	MG-NA	6.91	2.22	2.06
20	B	612	CLA	MG-NA	6.90	2.22	2.06
24	D	406	PL9	C7-C3	-6.89	1.44	1.51
22	d	405	BCR	C10-C9	-6.84	1.26	1.35
22	D	405	BCR	C10-C9	-6.83	1.26	1.35
20	B	615	CLA	MG-NA	6.82	2.22	2.06
20	b	615	CLA	MG-NA	6.81	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	512	CLA	MG-NA	6.81	2.22	2.06
20	C	512	CLA	MG-NA	6.80	2.22	2.06
20	C	507	CLA	MG-NA	6.78	2.22	2.06
20	c	507	CLA	MG-NA	6.78	2.22	2.06
20	B	610	CLA	MG-NA	6.77	2.22	2.06
20	b	610	CLA	MG-NA	6.77	2.22	2.06
20	c	502	CLA	MG-NA	6.76	2.22	2.06
20	C	502	CLA	MG-NA	6.74	2.22	2.06
20	C	506	CLA	MG-NA	6.66	2.22	2.06
20	c	506	CLA	MG-NA	6.64	2.22	2.06
20	B	611	CLA	MG-NA	6.64	2.22	2.06
20	b	611	CLA	MG-NA	6.63	2.22	2.06
20	c	509	CLA	MG-NA	6.56	2.21	2.06
20	C	509	CLA	MG-NA	6.54	2.21	2.06
20	d	403	CLA	MG-NA	6.40	2.21	2.06
20	D	403	CLA	MG-NA	6.39	2.21	2.06
27	B	613	F6C	C2A-C3A	6.25	1.50	1.36
27	b	613	F6C	C2A-C3A	6.25	1.50	1.36
27	B	613	F6C	C4A-NA	-5.89	1.30	1.37
27	b	613	F6C	C4A-NA	-5.89	1.30	1.37
24	D	406	PL9	C6-C1	-5.73	1.38	1.48
24	d	406	PL9	C6-C1	-5.72	1.38	1.48
27	B	604	F6C	C4A-NA	-5.72	1.30	1.37
27	b	604	F6C	C4A-NA	-5.72	1.30	1.37
20	C	507	CLA	C3C-C2C	5.48	1.48	1.36
20	c	507	CLA	C3C-C2C	5.47	1.48	1.36
20	d	403	CLA	C3B-C2B	5.28	1.47	1.40
20	c	514	CLA	C3B-C2B	5.27	1.47	1.40
20	a	404	CLA	CHC-C1C	5.26	1.48	1.35
20	C	514	CLA	C3B-C2B	5.25	1.47	1.40
20	a	404	CLA	O2D-CGD	5.25	1.46	1.33
20	B	603	CLA	CHC-C1C	5.25	1.48	1.35
20	D	403	CLA	C3B-C2B	5.24	1.47	1.40
29	d	401	CL7	O2A-C1	5.24	1.60	1.46
24	a	410	PL9	C7-C8	-5.24	1.43	1.50
20	b	603	CLA	CHC-C1C	5.24	1.48	1.35
20	A	404	CLA	CHC-C1C	5.23	1.48	1.35
24	A	410	PL9	C7-C8	-5.23	1.43	1.50
20	A	404	CLA	O2D-CGD	5.22	1.45	1.33
29	D	401	CL7	O2A-C1	5.21	1.60	1.46
20	A	407	CLA	CHC-C1C	5.21	1.48	1.35
20	a	407	CLA	CHC-C1C	5.21	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	509	CLA	C1D-ND	-5.20	1.31	1.37
20	B	606	CLA	CHC-C1C	5.20	1.48	1.35
20	B	602	CLA	O2D-CGD	5.19	1.45	1.33
20	a	407	CLA	O2D-CGD	5.19	1.45	1.33
27	c	508	F6C	CHC-C4B	5.18	1.48	1.35
27	c	508	F6C	O2D-CGD	5.18	1.45	1.33
20	b	602	CLA	O2D-CGD	5.18	1.45	1.33
20	b	606	CLA	CHC-C1C	5.18	1.48	1.35
27	C	508	F6C	CHC-C4B	5.18	1.48	1.35
20	B	602	CLA	CHC-C1C	5.17	1.48	1.35
20	C	509	CLA	C1D-ND	-5.17	1.31	1.37
20	c	507	CLA	O2A-C1	5.17	1.60	1.46
27	C	508	F6C	O2D-CGD	5.17	1.45	1.33
20	b	602	CLA	CHC-C1C	5.16	1.48	1.35
20	b	606	CLA	O2D-CGD	5.16	1.45	1.33
20	A	407	CLA	O2D-CGD	5.16	1.45	1.33
20	C	507	CLA	C3D-C4D	-5.15	1.32	1.44
20	c	502	CLA	C3B-C2B	5.15	1.47	1.40
27	B	607	F6C	CHC-C4B	5.15	1.48	1.35
20	C	507	CLA	O2A-C1	5.15	1.60	1.46
20	C	514	CLA	CHC-C1C	5.15	1.48	1.35
20	c	514	CLA	CHC-C1C	5.15	1.48	1.35
20	B	606	CLA	O2D-CGD	5.14	1.45	1.33
27	B	607	F6C	O2D-CGD	5.14	1.45	1.33
20	c	507	CLA	C3D-C4D	-5.14	1.32	1.44
20	C	503	CLA	O2D-CGD	5.14	1.45	1.33
27	b	607	F6C	O2D-CGD	5.14	1.45	1.33
27	b	607	F6C	CHC-C4B	5.14	1.48	1.35
20	c	503	CLA	O2D-CGD	5.13	1.45	1.33
20	C	512	CLA	O2A-C1	5.12	1.60	1.46
20	c	512	CLA	O2A-C1	5.12	1.60	1.46
20	d	403	CLA	C3D-C4D	-5.12	1.32	1.44
20	C	502	CLA	C3B-C2B	5.12	1.47	1.40
20	D	403	CLA	C3D-C4D	-5.12	1.32	1.44
20	b	603	CLA	O2D-CGD	5.10	1.45	1.33
20	B	603	CLA	O2D-CGD	5.10	1.45	1.33
20	a	407	CLA	O2A-C1	5.10	1.60	1.46
20	C	506	CLA	C1D-ND	-5.10	1.31	1.37
20	A	407	CLA	O2A-C1	5.10	1.60	1.46
27	C	508	F6C	O2A-C1	5.09	1.60	1.46
27	c	508	F6C	O2A-C1	5.09	1.60	1.46
20	B	615	CLA	O2A-C1	5.09	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	606	CLA	O2A-C1	5.08	1.60	1.46
20	b	615	CLA	O2A-C1	5.08	1.60	1.46
20	b	606	CLA	O2A-C1	5.07	1.60	1.46
27	B	607	F6C	O2A-C1	5.07	1.60	1.46
20	c	506	CLA	C1D-ND	-5.07	1.31	1.37
27	b	607	F6C	O2A-C1	5.07	1.60	1.46
20	c	510	CLA	O2A-C1	5.07	1.60	1.46
20	C	510	CLA	O2A-C1	5.06	1.60	1.46
20	B	612	CLA	CHC-C1C	5.05	1.47	1.35
20	h	101	CLA	O2A-C1	5.05	1.60	1.46
20	H	101	CLA	O2A-C1	5.05	1.60	1.46
20	B	603	CLA	O2A-C1	5.05	1.60	1.46
20	b	603	CLA	O2A-C1	5.05	1.60	1.46
20	c	502	CLA	O2A-C1	5.05	1.60	1.46
20	b	612	CLA	C1D-ND	-5.05	1.31	1.37
20	C	504	CLA	CHC-C1C	5.05	1.47	1.35
20	c	504	CLA	CHC-C1C	5.04	1.47	1.35
20	A	404	CLA	O2A-C1	5.04	1.60	1.46
20	b	602	CLA	O2A-C1	5.04	1.60	1.46
20	B	614	CLA	O2A-C1	5.03	1.60	1.46
20	a	405	CLA	C3D-C4D	-5.03	1.32	1.44
20	D	403	CLA	CHC-C1C	5.03	1.47	1.35
20	D	403	CLA	O2A-C1	5.03	1.60	1.46
20	B	602	CLA	O2A-C1	5.03	1.60	1.46
20	b	614	CLA	O2A-C1	5.03	1.60	1.46
20	C	502	CLA	O2A-C1	5.02	1.60	1.46
20	A	405	CLA	C3D-C4D	-5.02	1.32	1.44
20	b	612	CLA	CHC-C1C	5.02	1.47	1.35
20	a	404	CLA	O2A-C1	5.02	1.60	1.46
20	d	403	CLA	CHC-C1C	5.02	1.47	1.35
20	b	611	CLA	C1D-ND	-5.02	1.31	1.37
20	D	403	CLA	C1D-ND	-5.00	1.31	1.37
20	B	612	CLA	C1D-ND	-5.00	1.31	1.37
20	d	403	CLA	C1D-ND	-5.00	1.31	1.37
20	d	403	CLA	O2A-C1	5.00	1.60	1.46
20	C	510	CLA	C3D-C4D	-4.98	1.32	1.44
20	c	510	CLA	C3D-C4D	-4.98	1.32	1.44
20	B	611	CLA	C1D-ND	-4.98	1.31	1.37
20	B	601	CLA	O2D-CGD	4.98	1.45	1.33
20	a	405	CLA	O2A-C1	4.97	1.60	1.46
20	A	405	CLA	O2A-C1	4.96	1.60	1.46
20	C	503	CLA	O2A-C1	4.96	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	605	CLA	O2A-C1	4.96	1.60	1.46
20	c	503	CLA	C3D-C4D	-4.95	1.33	1.44
20	b	605	CLA	O2A-C1	4.95	1.60	1.46
20	b	601	CLA	O2D-CGD	4.95	1.45	1.33
20	c	503	CLA	O2A-C1	4.95	1.60	1.46
20	H	101	CLA	C3D-C4D	-4.94	1.33	1.44
20	C	511	CLA	C3D-C4D	-4.93	1.33	1.44
20	c	511	CLA	C3D-C4D	-4.93	1.33	1.44
20	b	608	CLA	O2A-C1	4.92	1.60	1.46
20	C	503	CLA	C3D-C4D	-4.92	1.33	1.44
20	B	608	CLA	O2A-C1	4.92	1.60	1.46
20	c	511	CLA	CHC-C1C	4.91	1.47	1.35
20	C	511	CLA	CHC-C1C	4.91	1.47	1.35
20	C	510	CLA	CHC-C1C	4.91	1.47	1.35
20	c	510	CLA	CHC-C1C	4.91	1.47	1.35
20	h	101	CLA	C3D-C4D	-4.90	1.33	1.44
20	b	611	CLA	C3D-C4D	-4.90	1.33	1.44
20	H	101	CLA	O2D-CGD	4.90	1.45	1.33
20	c	511	CLA	O2A-C1	4.90	1.59	1.46
20	c	514	CLA	O2D-CGD	4.90	1.45	1.33
20	b	605	CLA	C3D-C4D	-4.89	1.33	1.44
20	B	605	CLA	C3D-C4D	-4.89	1.33	1.44
20	B	601	CLA	CHC-C1C	4.89	1.47	1.35
20	h	101	CLA	O2D-CGD	4.89	1.45	1.33
31	v	201	HEM	C3C-C2C	-4.89	1.33	1.40
20	B	611	CLA	C3D-C4D	-4.89	1.33	1.44
20	b	614	CLA	CHC-C1C	4.89	1.47	1.35
20	C	511	CLA	O2A-C1	4.89	1.59	1.46
20	b	614	CLA	C3D-C4D	-4.89	1.33	1.44
20	c	509	CLA	C3D-C4D	-4.88	1.33	1.44
20	C	509	CLA	C3D-C4D	-4.88	1.33	1.44
20	b	601	CLA	CHC-C1C	4.88	1.47	1.35
20	C	507	CLA	O2D-CGD	4.88	1.45	1.33
20	B	614	CLA	CHC-C1C	4.87	1.47	1.35
20	c	507	CLA	O2D-CGD	4.87	1.45	1.33
20	C	514	CLA	O2D-CGD	4.87	1.45	1.33
20	B	614	CLA	C3D-C4D	-4.87	1.33	1.44
31	V	201	HEM	C3C-C2C	-4.86	1.33	1.40
20	C	502	CLA	O2D-CGD	4.86	1.45	1.33
20	D	404	CLA	CHC-C1C	4.84	1.47	1.35
20	C	505	CLA	CHC-C1C	4.84	1.47	1.35
20	c	505	CLA	CHC-C1C	4.84	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	502	CLA	O2D-CGD	4.83	1.45	1.33
20	B	609	CLA	O2D-CGD	4.83	1.45	1.33
20	B	608	CLA	O2D-CGD	4.83	1.45	1.33
20	b	609	CLA	O2D-CGD	4.83	1.45	1.33
27	B	607	F6C	CHD-C1D	4.83	1.47	1.35
20	b	608	CLA	O2D-CGD	4.82	1.45	1.33
20	C	505	CLA	O2D-CGD	4.82	1.45	1.33
20	c	505	CLA	O2D-CGD	4.82	1.45	1.33
27	b	607	F6C	CHD-C1D	4.82	1.47	1.35
20	B	609	CLA	C3D-C4D	-4.82	1.33	1.44
20	b	609	CLA	C3D-C4D	-4.82	1.33	1.44
27	C	508	F6C	CHD-C1D	4.82	1.47	1.35
20	d	404	CLA	CHC-C1C	4.82	1.47	1.35
20	b	611	CLA	O2A-C1	4.82	1.59	1.46
20	B	615	CLA	C3D-C4D	-4.81	1.33	1.44
27	c	508	F6C	CHD-C1D	4.81	1.47	1.35
20	B	611	CLA	O2A-C1	4.81	1.59	1.46
20	C	504	CLA	O2A-C1	4.81	1.59	1.46
20	C	513	CLA	CHC-C1C	4.80	1.47	1.35
20	B	605	CLA	O2D-CGD	4.80	1.44	1.33
20	b	605	CLA	O2D-CGD	4.80	1.44	1.33
20	a	407	CLA	C3B-C2B	4.80	1.47	1.40
20	c	513	CLA	CHC-C1C	4.80	1.47	1.35
20	B	605	CLA	C3B-C2B	4.80	1.47	1.40
20	C	506	CLA	O2A-C1	4.79	1.59	1.46
20	c	506	CLA	O2A-C1	4.79	1.59	1.46
20	b	615	CLA	C3D-C4D	-4.79	1.33	1.44
20	c	504	CLA	O2A-C1	4.79	1.59	1.46
20	C	509	CLA	O2A-C1	4.79	1.59	1.46
20	C	509	CLA	O2D-CGD	4.79	1.44	1.33
20	C	505	CLA	O2A-C1	4.78	1.59	1.46
20	c	509	CLA	O2D-CGD	4.78	1.44	1.33
20	D	404	CLA	C3D-C4D	-4.78	1.33	1.44
20	c	505	CLA	O2A-C1	4.78	1.59	1.46
20	A	407	CLA	C3B-C2B	4.78	1.47	1.40
20	d	404	CLA	C3D-C4D	-4.77	1.33	1.44
20	b	612	CLA	O2D-CGD	4.77	1.44	1.33
20	c	512	CLA	C3D-C4D	-4.77	1.33	1.44
20	c	509	CLA	O2A-C1	4.76	1.59	1.46
20	c	511	CLA	O2D-CGD	4.76	1.44	1.33
20	b	605	CLA	C3B-C2B	4.75	1.47	1.40
20	C	511	CLA	O2D-CGD	4.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	401	CL7	C1C-NC	-4.75	1.31	1.37
20	B	610	CLA	O2A-C1	4.75	1.59	1.46
24	A	410	PL9	C3-C4	-4.75	1.41	1.49
20	h	101	CLA	CHC-C1C	4.75	1.47	1.35
20	B	612	CLA	O2D-CGD	4.75	1.44	1.33
20	b	610	CLA	O2A-C1	4.75	1.59	1.46
20	C	512	CLA	C3D-C4D	-4.73	1.33	1.44
24	a	410	PL9	C3-C4	-4.73	1.41	1.49
20	H	101	CLA	CHC-C1C	4.72	1.47	1.35
27	b	604	F6C	CHC-C4B	4.72	1.47	1.35
20	B	606	CLA	C3B-C2B	4.72	1.46	1.40
20	a	405	CLA	O2D-CGD	4.71	1.44	1.33
20	A	405	CLA	O2D-CGD	4.70	1.44	1.33
20	c	507	CLA	CHC-C1C	4.70	1.47	1.35
20	A	404	CLA	C3B-C2B	4.70	1.46	1.40
20	b	612	CLA	C3B-C2B	4.70	1.46	1.40
20	C	504	CLA	C3B-C2B	4.70	1.46	1.40
20	b	602	CLA	C3B-C2B	4.70	1.46	1.40
27	B	604	F6C	CHC-C4B	4.69	1.47	1.35
20	C	507	CLA	CHC-C1C	4.69	1.47	1.35
20	C	506	CLA	C3D-C4D	-4.69	1.33	1.44
29	d	401	CL7	C1C-NC	-4.69	1.32	1.37
20	c	504	CLA	C3B-C2B	4.68	1.46	1.40
20	B	612	CLA	O2A-C1	4.68	1.59	1.46
20	B	602	CLA	C3B-C2B	4.68	1.46	1.40
20	b	612	CLA	O2A-C1	4.68	1.59	1.46
20	B	612	CLA	C3B-C2B	4.68	1.46	1.40
20	B	608	CLA	CHC-C1C	4.67	1.46	1.35
20	b	608	CLA	CHC-C1C	4.67	1.46	1.35
20	b	602	CLA	C3C-C2C	4.67	1.46	1.36
20	c	506	CLA	C3D-C4D	-4.67	1.33	1.44
20	C	506	CLA	O2D-CGD	4.66	1.44	1.33
20	c	506	CLA	O2D-CGD	4.66	1.44	1.33
20	B	602	CLA	C3C-C2C	4.66	1.46	1.36
20	b	615	CLA	O2D-CGD	4.66	1.44	1.33
20	b	606	CLA	C3B-C2B	4.66	1.46	1.40
20	D	404	CLA	C3B-C2B	4.65	1.46	1.40
20	d	404	CLA	C3B-C2B	4.65	1.46	1.40
20	a	404	CLA	C3B-C2B	4.65	1.46	1.40
20	a	404	CLA	C3C-C2C	4.65	1.46	1.36
20	B	603	CLA	C3C-C2C	4.64	1.46	1.36
20	B	615	CLA	O2D-CGD	4.64	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	610	CLA	C3D-C4D	-4.64	1.33	1.44
20	c	504	CLA	O2D-CGD	4.64	1.44	1.33
20	a	405	CLA	CHC-C1C	4.63	1.46	1.35
20	B	610	CLA	C3D-C4D	-4.63	1.33	1.44
20	b	610	CLA	O2D-CGD	4.63	1.44	1.33
20	A	404	CLA	C3C-C2C	4.63	1.46	1.36
20	c	513	CLA	C3D-C4D	-4.63	1.33	1.44
20	C	510	CLA	O2D-CGD	4.62	1.44	1.33
20	b	603	CLA	C3C-C2C	4.62	1.46	1.36
20	B	610	CLA	O2D-CGD	4.62	1.44	1.33
20	A	407	CLA	CHD-C1D	4.62	1.47	1.38
20	b	603	CLA	C3B-C2B	4.62	1.46	1.40
20	C	504	CLA	O2D-CGD	4.62	1.44	1.33
20	c	510	CLA	O2D-CGD	4.62	1.44	1.33
20	C	502	CLA	CHC-C1C	4.62	1.46	1.35
20	c	502	CLA	CHC-C1C	4.62	1.46	1.35
20	c	512	CLA	O2D-CGD	4.61	1.44	1.33
20	B	603	CLA	C3B-C2B	4.61	1.46	1.40
20	A	405	CLA	CHC-C1C	4.61	1.46	1.35
20	B	608	CLA	C1D-ND	-4.61	1.32	1.37
20	C	513	CLA	C3D-C4D	-4.61	1.33	1.44
20	C	512	CLA	O2D-CGD	4.61	1.44	1.33
27	B	604	F6C	O2A-C1	4.60	1.59	1.46
20	B	606	CLA	CHD-C1D	4.60	1.47	1.38
20	b	606	CLA	CHD-C1D	4.60	1.47	1.38
20	C	504	CLA	C3C-C2C	4.59	1.46	1.36
20	c	504	CLA	C3C-C2C	4.59	1.46	1.36
20	a	407	CLA	CHD-C1D	4.59	1.47	1.38
27	b	604	F6C	O2A-C1	4.59	1.59	1.46
20	b	608	CLA	C1D-ND	-4.59	1.32	1.37
20	a	407	CLA	C3C-C2C	4.59	1.46	1.36
20	A	404	CLA	CHD-C1D	4.58	1.47	1.38
20	b	602	CLA	CHD-C1D	4.58	1.47	1.38
20	A	407	CLA	C3C-C2C	4.58	1.46	1.36
20	B	615	CLA	CHC-C1C	4.57	1.46	1.35
20	b	606	CLA	C3C-C2C	4.57	1.46	1.36
20	C	511	CLA	C3B-C2B	4.57	1.46	1.40
20	B	602	CLA	CHD-C1D	4.57	1.47	1.38
20	a	404	CLA	CHD-C1D	4.57	1.47	1.38
20	c	511	CLA	C3B-C2B	4.56	1.46	1.40
20	B	606	CLA	C3C-C2C	4.56	1.46	1.36
20	b	615	CLA	CHC-C1C	4.55	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	609	CLA	CHC-C1C	4.55	1.46	1.35
20	b	609	CLA	CHC-C1C	4.55	1.46	1.35
20	B	603	CLA	CHD-C1D	4.55	1.47	1.38
27	B	613	F6C	O2A-C1	4.54	1.59	1.46
27	b	613	F6C	O2A-C1	4.53	1.58	1.46
20	C	514	CLA	C3D-C4D	-4.53	1.34	1.44
20	c	514	CLA	C3D-C4D	-4.53	1.34	1.44
20	b	603	CLA	CHD-C1D	4.53	1.47	1.38
20	B	611	CLA	O2D-CGD	4.53	1.44	1.33
20	b	614	CLA	O2D-CGD	4.52	1.44	1.33
20	C	506	CLA	CHC-C1C	4.52	1.46	1.35
27	b	613	F6C	CHC-C4B	4.52	1.46	1.35
20	c	506	CLA	CHC-C1C	4.51	1.46	1.35
20	C	512	CLA	C3B-C2B	4.51	1.46	1.40
20	b	609	CLA	MG-ND	-4.51	1.96	2.05
20	B	614	CLA	O2D-CGD	4.51	1.44	1.33
27	B	613	F6C	CHC-C4B	4.50	1.46	1.35
20	b	611	CLA	O2D-CGD	4.50	1.44	1.33
20	B	612	CLA	C3D-C4D	-4.50	1.34	1.44
20	b	612	CLA	C3D-C4D	-4.50	1.34	1.44
20	A	405	CLA	C3B-C2B	4.49	1.46	1.40
20	a	405	CLA	C3B-C2B	4.49	1.46	1.40
29	d	401	CL7	C3C-C2C	4.48	1.46	1.36
20	c	512	CLA	C3B-C2B	4.47	1.46	1.40
27	B	604	F6C	C3D-C4D	-4.47	1.32	1.43
20	B	609	CLA	MG-ND	-4.47	1.96	2.05
29	D	401	CL7	C3C-C2C	4.47	1.46	1.36
20	B	601	CLA	C3C-C2C	4.46	1.46	1.36
20	C	507	CLA	CHD-C1D	4.46	1.47	1.38
27	b	604	F6C	C3D-C4D	-4.46	1.32	1.43
20	c	511	CLA	C3C-C2C	4.46	1.46	1.36
20	b	601	CLA	C3C-C2C	4.46	1.46	1.36
20	C	511	CLA	C3C-C2C	4.46	1.46	1.36
24	D	406	PL9	C3-C4	-4.45	1.42	1.49
20	B	605	CLA	CHC-C1C	4.45	1.46	1.35
20	b	605	CLA	CHC-C1C	4.44	1.46	1.35
20	c	507	CLA	CHD-C1D	4.43	1.47	1.38
20	C	509	CLA	C1C-NC	-4.43	1.31	1.37
20	C	513	CLA	C3C-C2C	4.43	1.46	1.36
20	c	514	CLA	CHD-C1D	4.42	1.47	1.38
20	C	504	CLA	C3D-C4D	-4.42	1.34	1.44
20	c	504	CLA	C3D-C4D	-4.42	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	406	PL9	C3-C4	-4.42	1.42	1.49
20	C	513	CLA	C3B-C2B	4.41	1.46	1.40
27	B	604	F6C	CHD-C1D	4.41	1.46	1.35
20	c	509	CLA	C1C-NC	-4.41	1.31	1.37
20	C	514	CLA	CHD-C1D	4.41	1.47	1.38
27	b	604	F6C	CHD-C1D	4.41	1.46	1.35
20	c	502	CLA	C3C-C2C	4.41	1.46	1.36
20	b	610	CLA	CHC-C1C	4.40	1.46	1.35
20	d	404	CLA	O2D-CGD	4.40	1.43	1.33
20	c	513	CLA	C3C-C2C	4.40	1.46	1.36
20	c	505	CLA	C3D-C4D	-4.40	1.34	1.44
20	c	513	CLA	C3B-C2B	4.40	1.46	1.40
20	D	403	CLA	C3C-C2C	4.40	1.46	1.36
20	C	502	CLA	C3C-C2C	4.40	1.46	1.36
20	C	509	CLA	CHC-C1C	4.39	1.46	1.35
20	C	505	CLA	C3D-C4D	-4.39	1.34	1.44
27	b	604	F6C	O2D-CGD	4.39	1.43	1.33
27	B	613	F6C	C3D-C4D	-4.39	1.33	1.43
27	b	613	F6C	C3D-C4D	-4.39	1.33	1.43
20	c	512	CLA	C1D-ND	-4.39	1.32	1.37
20	c	509	CLA	CHC-C1C	4.39	1.46	1.35
20	C	512	CLA	C1D-ND	-4.38	1.32	1.37
20	D	404	CLA	O2D-CGD	4.38	1.43	1.33
20	D	404	CLA	C3C-C2C	4.38	1.46	1.36
20	c	513	CLA	CHD-C1D	4.38	1.46	1.38
27	B	604	F6C	O2D-CGD	4.38	1.43	1.33
20	d	403	CLA	C3C-C2C	4.38	1.46	1.36
20	c	510	CLA	C3C-C2C	4.37	1.46	1.36
20	d	404	CLA	C3C-C2C	4.37	1.46	1.36
20	C	505	CLA	C3B-C2B	4.37	1.46	1.40
20	B	605	CLA	C1C-NC	-4.37	1.31	1.37
20	C	510	CLA	C3C-C2C	4.36	1.46	1.36
20	B	610	CLA	CHC-C1C	4.36	1.46	1.35
20	C	513	CLA	CHD-C1D	4.36	1.46	1.38
20	c	511	CLA	CHD-C1D	4.35	1.46	1.38
20	C	512	CLA	CHC-C1C	4.35	1.46	1.35
29	d	401	CL7	O2D-CGD	4.34	1.43	1.33
20	C	513	CLA	O2D-CGD	4.34	1.43	1.33
20	b	605	CLA	C1C-NC	-4.34	1.31	1.37
20	a	404	CLA	C3D-C4D	-4.33	1.34	1.44
20	c	512	CLA	CHC-C1C	4.33	1.46	1.35
20	C	511	CLA	CHD-C1D	4.33	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	504	CLA	CHD-C1D	4.33	1.46	1.38
20	b	610	CLA	C3C-C2C	4.33	1.45	1.36
20	c	513	CLA	O2D-CGD	4.32	1.43	1.33
20	B	610	CLA	C3C-C2C	4.32	1.45	1.36
20	C	504	CLA	CHD-C1D	4.32	1.46	1.38
20	b	608	CLA	C3D-C4D	-4.31	1.34	1.44
20	c	505	CLA	C3B-C2B	4.31	1.46	1.40
20	B	608	CLA	C3D-C4D	-4.31	1.34	1.44
20	C	509	CLA	MG-ND	-4.31	1.97	2.05
29	D	401	CL7	O2D-CGD	4.31	1.43	1.33
20	B	603	CLA	C3D-C4D	-4.31	1.34	1.44
20	A	404	CLA	C3D-C4D	-4.31	1.34	1.44
20	c	509	CLA	MG-ND	-4.30	1.97	2.05
20	C	502	CLA	C3D-C4D	-4.30	1.34	1.44
20	C	509	CLA	C3B-C2B	4.29	1.46	1.40
20	c	502	CLA	C3D-C4D	-4.29	1.34	1.44
20	a	407	CLA	C3D-C4D	-4.29	1.34	1.44
20	b	606	CLA	C3D-C4D	-4.28	1.34	1.44
20	B	608	CLA	C3B-C2B	4.28	1.46	1.40
20	C	503	CLA	C3B-C2B	4.28	1.46	1.40
20	c	509	CLA	C3B-C2B	4.28	1.46	1.40
20	b	603	CLA	C3D-C4D	-4.28	1.34	1.44
20	c	502	CLA	CHD-C1D	4.28	1.46	1.38
20	A	407	CLA	C3D-C4D	-4.27	1.34	1.44
20	c	503	CLA	C3B-C2B	4.27	1.46	1.40
20	B	606	CLA	C3D-C4D	-4.27	1.34	1.44
20	C	503	CLA	CHC-C1C	4.27	1.45	1.35
20	c	503	CLA	CHC-C1C	4.27	1.45	1.35
20	C	502	CLA	CHD-C1D	4.26	1.46	1.38
20	b	601	CLA	C3D-C4D	-4.26	1.34	1.44
26	L	101	LHG	O8-C23	4.26	1.45	1.33
26	l	101	LHG	O8-C23	4.26	1.45	1.33
20	B	601	CLA	C3D-C4D	-4.25	1.34	1.44
20	c	503	CLA	CHD-C1D	4.25	1.46	1.38
20	b	608	CLA	C3B-C2B	4.25	1.46	1.40
27	b	613	F6C	O2D-CGD	4.25	1.43	1.33
20	C	503	CLA	CHD-C1D	4.24	1.46	1.38
20	b	602	CLA	C3D-C4D	-4.23	1.34	1.44
20	c	505	CLA	CHD-C1D	4.23	1.46	1.38
20	B	602	CLA	C3D-C4D	-4.23	1.34	1.44
20	C	505	CLA	C3C-C2C	4.23	1.45	1.36
20	b	614	CLA	C1D-ND	-4.22	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	401	CL7	C1A-NA	-4.22	1.27	1.38
27	B	613	F6C	O2D-CGD	4.22	1.43	1.33
29	D	401	CL7	C1A-NA	-4.22	1.27	1.38
20	C	505	CLA	CHD-C1D	4.22	1.46	1.38
20	c	505	CLA	C3C-C2C	4.22	1.45	1.36
20	b	610	CLA	C3B-C2B	4.21	1.46	1.40
20	b	609	CLA	C3C-C2C	4.20	1.45	1.36
20	C	514	CLA	C3C-C2C	4.20	1.45	1.36
20	c	514	CLA	C3C-C2C	4.20	1.45	1.36
20	B	614	CLA	C1D-ND	-4.20	1.32	1.37
20	C	512	CLA	C3C-C2C	4.20	1.45	1.36
20	B	609	CLA	C3C-C2C	4.19	1.45	1.36
20	B	610	CLA	C3B-C2B	4.19	1.46	1.40
32	h	102	RRX	C14-C13	4.19	1.41	1.35
20	D	403	CLA	O2D-CGD	4.19	1.43	1.33
20	d	403	CLA	O2D-CGD	4.19	1.43	1.33
32	h	102	RRX	C10-C9	4.18	1.41	1.35
32	H	102	RRX	C14-C13	4.18	1.41	1.35
20	c	503	CLA	C3C-C2C	4.18	1.45	1.36
24	a	410	PL9	C53-C6	-4.17	1.42	1.50
20	B	601	CLA	CHD-C1D	4.17	1.46	1.38
20	c	512	CLA	C3C-C2C	4.17	1.45	1.36
20	b	601	CLA	CHD-C1D	4.16	1.46	1.38
20	b	608	CLA	C3C-C2C	4.16	1.45	1.36
27	b	613	F6C	CHD-C1D	4.16	1.45	1.35
20	B	608	CLA	C3C-C2C	4.16	1.45	1.36
20	C	503	CLA	C3C-C2C	4.16	1.45	1.36
20	b	601	CLA	C3B-C2B	4.15	1.46	1.40
32	h	102	RRX	C17-C18	4.15	1.41	1.35
24	A	410	PL9	C53-C6	-4.15	1.42	1.50
20	A	405	CLA	CHD-C1D	4.15	1.46	1.38
32	H	102	RRX	C17-C18	4.14	1.41	1.35
20	B	601	CLA	C3B-C2B	4.14	1.46	1.40
32	h	102	RRX	C21-C22	4.14	1.41	1.35
20	a	405	CLA	CHD-C1D	4.14	1.46	1.38
27	B	613	F6C	CHD-C1D	4.14	1.45	1.35
20	b	609	CLA	C3B-C2B	4.13	1.46	1.40
30	D	409	LMG	O8-C28	4.13	1.45	1.33
29	d	401	CL7	C4C-NC	-4.13	1.32	1.37
32	H	102	RRX	C10-C9	4.13	1.41	1.35
32	H	102	RRX	C21-C22	4.13	1.41	1.35
30	d	409	LMG	O8-C28	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	609	CLA	C3B-C2B	4.12	1.46	1.40
30	m	101	LMG	O8-C28	4.12	1.45	1.33
30	d	409	LMG	O7-C10	4.12	1.45	1.34
30	M	101	LMG	O8-C28	4.12	1.45	1.33
20	B	609	CLA	C1D-ND	-4.11	1.32	1.37
30	D	409	LMG	O7-C10	4.10	1.45	1.34
20	b	605	CLA	C3C-C2C	4.10	1.45	1.36
20	b	609	CLA	C1D-ND	-4.10	1.32	1.37
20	C	503	CLA	C1C-NC	-4.09	1.31	1.37
20	c	503	CLA	C1C-NC	-4.09	1.31	1.37
29	D	401	CL7	C4C-NC	-4.09	1.32	1.37
27	C	508	F6C	C4A-NA	-4.08	1.32	1.37
20	B	605	CLA	C3C-C2C	4.08	1.45	1.36
20	C	509	CLA	C3C-C2C	4.08	1.45	1.36
20	b	611	CLA	C3B-C2B	4.07	1.46	1.40
20	c	509	CLA	C3C-C2C	4.07	1.45	1.36
20	B	609	CLA	CHD-C1D	4.07	1.46	1.38
20	b	609	CLA	CHD-C1D	4.06	1.46	1.38
20	D	404	CLA	CHD-C1D	4.06	1.46	1.38
27	B	607	F6C	C4A-NA	-4.06	1.32	1.37
20	H	101	CLA	CHD-C1D	4.05	1.46	1.38
20	h	101	CLA	CHD-C1D	4.04	1.46	1.38
27	c	508	F6C	C4A-NA	-4.03	1.32	1.37
20	b	611	CLA	CHC-C1C	4.03	1.45	1.35
29	D	401	CL7	OBD-CAD	4.02	1.27	1.22
20	b	615	CLA	C3B-C2B	4.02	1.45	1.40
20	d	404	CLA	CHD-C1D	4.02	1.46	1.38
20	b	605	CLA	C1D-ND	-4.02	1.32	1.37
20	B	611	CLA	C3B-C2B	4.01	1.45	1.40
20	c	507	CLA	C3B-C2B	4.01	1.45	1.40
26	A	412	LHG	O8-C23	4.01	1.45	1.33
26	D	408	LHG	O7-C7	4.00	1.45	1.34
20	B	610	CLA	CHD-C1D	4.00	1.46	1.38
20	b	614	CLA	C3C-C2C	4.00	1.45	1.36
20	B	614	CLA	C3C-C2C	4.00	1.45	1.36
20	B	611	CLA	CHC-C1C	4.00	1.45	1.35
29	d	401	CL7	OBD-CAD	4.00	1.27	1.22
26	a	412	LHG	O8-C23	3.99	1.45	1.33
20	b	610	CLA	CHD-C1D	3.98	1.46	1.38
27	b	607	F6C	C4A-NA	-3.98	1.32	1.37
26	d	408	LHG	O7-C7	3.97	1.45	1.34
20	B	605	CLA	C1D-ND	-3.97	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	507	CLA	C3B-C2B	3.97	1.45	1.40
20	B	615	CLA	C3B-C2B	3.97	1.45	1.40
20	C	510	CLA	CHD-C1D	3.95	1.46	1.38
20	C	506	CLA	C3C-C2C	3.95	1.45	1.36
20	b	612	CLA	C3C-C2C	3.94	1.45	1.36
20	H	101	CLA	C3C-C2C	3.94	1.45	1.36
20	C	502	CLA	CHD-C4C	3.94	1.48	1.39
20	c	510	CLA	CHD-C1D	3.93	1.46	1.38
20	B	612	CLA	C3C-C2C	3.93	1.45	1.36
20	c	506	CLA	C3C-C2C	3.93	1.45	1.36
27	c	508	F6C	CHB-C1B	3.93	1.48	1.39
20	c	502	CLA	CHD-C4C	3.93	1.48	1.39
20	B	606	CLA	CHD-C4C	3.92	1.48	1.39
20	b	606	CLA	CHD-C4C	3.92	1.48	1.39
20	D	404	CLA	C1D-ND	-3.92	1.33	1.37
20	d	404	CLA	C1D-ND	-3.92	1.33	1.37
20	h	101	CLA	C3C-C2C	3.92	1.45	1.36
27	B	607	F6C	CHB-C1B	3.92	1.48	1.39
20	c	507	CLA	CHD-C4C	3.91	1.48	1.39
20	B	614	CLA	CHD-C1D	3.91	1.46	1.38
27	C	508	F6C	CHB-C1B	3.91	1.48	1.39
27	b	607	F6C	CHB-C1B	3.91	1.48	1.39
20	B	603	CLA	CHD-C4C	3.90	1.48	1.39
20	b	611	CLA	CHD-C1D	3.90	1.46	1.38
20	b	611	CLA	C1C-NC	-3.89	1.32	1.37
20	b	614	CLA	CHD-C1D	3.89	1.45	1.38
20	B	611	CLA	CHD-C1D	3.88	1.45	1.38
20	B	602	CLA	CHD-C4C	3.88	1.48	1.39
20	C	514	CLA	CHD-C4C	3.88	1.48	1.39
20	c	514	CLA	CHD-C4C	3.88	1.48	1.39
20	a	404	CLA	CHD-C4C	3.88	1.48	1.39
20	C	507	CLA	CHD-C4C	3.88	1.48	1.39
20	b	602	CLA	CHD-C4C	3.88	1.48	1.39
20	b	603	CLA	CHD-C4C	3.88	1.48	1.39
20	c	506	CLA	C3B-C2B	3.87	1.45	1.40
20	b	602	CLA	OBD-CAD	3.87	1.29	1.22
20	A	404	CLA	CHD-C4C	3.87	1.48	1.39
20	B	611	CLA	C1C-NC	-3.87	1.32	1.37
20	a	407	CLA	CHD-C4C	3.87	1.48	1.39
26	d	407	LHG	O8-C23	3.87	1.44	1.33
20	a	405	CLA	C1C-NC	-3.87	1.32	1.37
20	A	407	CLA	CHD-C4C	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	610	CLA	C1D-ND	-3.86	1.33	1.37
26	D	407	LHG	O8-C23	3.86	1.44	1.33
20	B	602	CLA	OBD-CAD	3.85	1.29	1.22
20	a	405	CLA	C3C-C2C	3.85	1.44	1.36
20	b	615	CLA	C3C-C2C	3.85	1.44	1.36
20	d	404	CLA	CHD-C4C	3.85	1.48	1.39
20	A	405	CLA	C1C-NC	-3.84	1.32	1.37
20	C	510	CLA	C1D-ND	-3.83	1.33	1.37
20	A	405	CLA	C3C-C2C	3.83	1.44	1.36
20	B	615	CLA	C3C-C2C	3.82	1.44	1.36
30	M	101	LMG	O7-C10	3.82	1.45	1.34
30	m	101	LMG	O7-C10	3.82	1.45	1.34
20	c	504	CLA	CHD-C4C	3.82	1.47	1.39
27	b	607	F6C	C3D-C4D	-3.81	1.34	1.43
27	C	508	F6C	C3D-C4D	-3.81	1.34	1.43
27	c	508	F6C	C3D-C4D	-3.81	1.34	1.43
20	D	404	CLA	CHD-C4C	3.81	1.47	1.39
27	B	607	F6C	C3D-C4D	-3.80	1.34	1.43
20	C	506	CLA	C3B-C2B	3.80	1.45	1.40
20	b	610	CLA	C1D-ND	-3.80	1.33	1.37
20	C	504	CLA	CHD-C4C	3.80	1.47	1.39
20	c	510	CLA	C1D-ND	-3.78	1.33	1.37
20	h	101	CLA	C1D-ND	-3.78	1.33	1.37
20	C	510	CLA	MG-ND	-3.77	1.98	2.05
20	C	504	CLA	C1D-ND	-3.77	1.33	1.37
20	c	510	CLA	MG-ND	-3.77	1.98	2.05
20	B	603	CLA	OBD-CAD	3.77	1.29	1.22
20	b	603	CLA	OBD-CAD	3.77	1.29	1.22
27	C	508	F6C	OBD-CAD	3.75	1.28	1.22
20	H	101	CLA	C1D-ND	-3.75	1.33	1.37
20	b	608	CLA	CHD-C1D	3.75	1.45	1.38
27	c	508	F6C	OBD-CAD	3.74	1.28	1.22
20	c	506	CLA	MG-ND	-3.74	1.98	2.05
20	B	601	CLA	OBD-CAD	3.74	1.28	1.22
20	B	608	CLA	CHD-C1D	3.74	1.45	1.38
20	c	504	CLA	C1D-ND	-3.74	1.33	1.37
20	H	101	CLA	C3B-C2B	3.73	1.45	1.40
20	h	101	CLA	C3B-C2B	3.73	1.45	1.40
20	B	606	CLA	OBD-CAD	3.73	1.28	1.22
20	a	404	CLA	OBD-CAD	3.73	1.28	1.22
29	D	401	CL7	C3D-C2D	3.73	1.46	1.39
31	e	101	HEM	C3C-C2C	-3.72	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	401	CL7	C3D-C2D	3.72	1.46	1.39
27	B	613	F6C	CHB-C1B	3.72	1.47	1.39
20	C	502	CLA	C1D-ND	-3.71	1.33	1.37
20	c	502	CLA	C1D-ND	-3.71	1.33	1.37
20	A	404	CLA	OBD-CAD	3.71	1.28	1.22
27	B	607	F6C	OBD-CAD	3.70	1.28	1.22
27	b	607	F6C	OBD-CAD	3.70	1.28	1.22
20	b	601	CLA	OBD-CAD	3.70	1.28	1.22
27	b	613	F6C	CHB-C1B	3.70	1.47	1.39
20	b	606	CLA	OBD-CAD	3.70	1.28	1.22
20	C	506	CLA	MG-ND	-3.69	1.98	2.05
20	a	407	CLA	OBD-CAD	3.69	1.28	1.22
20	A	407	CLA	OBD-CAD	3.68	1.28	1.22
31	E	101	HEM	C3C-C2C	-3.68	1.35	1.40
20	C	505	CLA	CHD-C4C	3.67	1.47	1.39
20	C	513	CLA	OBD-CAD	3.67	1.28	1.22
20	c	505	CLA	CHD-C4C	3.66	1.47	1.39
20	a	405	CLA	CHD-C4C	3.65	1.47	1.39
20	A	405	CLA	CHD-C4C	3.64	1.47	1.39
20	c	513	CLA	OBD-CAD	3.64	1.28	1.22
26	D	407	LHG	O7-C7	3.63	1.44	1.34
20	c	505	CLA	C1D-ND	-3.63	1.33	1.37
20	c	507	CLA	C1D-ND	-3.62	1.33	1.37
20	C	511	CLA	CHD-C4C	3.62	1.47	1.39
20	c	511	CLA	CHD-C4C	3.62	1.47	1.39
20	C	506	CLA	CHD-C1D	3.62	1.45	1.38
20	b	610	CLA	C1C-NC	-3.62	1.32	1.37
20	c	506	CLA	CHD-C1D	3.62	1.45	1.38
20	B	605	CLA	CHD-C1D	3.62	1.45	1.38
20	b	605	CLA	CHD-C1D	3.62	1.45	1.38
26	d	407	LHG	O7-C7	3.61	1.44	1.34
20	C	514	CLA	OBD-CAD	3.60	1.28	1.22
26	D	408	LHG	O8-C23	3.59	1.43	1.33
20	C	507	CLA	C1D-ND	-3.59	1.33	1.37
26	d	408	LHG	O8-C23	3.58	1.43	1.33
20	b	601	CLA	CHD-C4C	3.58	1.47	1.39
20	b	615	CLA	CHD-C1D	3.58	1.45	1.38
24	D	406	PL9	C53-C6	-3.58	1.43	1.50
20	c	514	CLA	OBD-CAD	3.57	1.28	1.22
24	d	406	PL9	C53-C6	-3.57	1.43	1.50
20	B	610	CLA	C1C-NC	-3.57	1.32	1.37
20	C	505	CLA	C1D-ND	-3.57	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	601	CLA	CHD-C4C	3.57	1.47	1.39
20	C	513	CLA	CHD-C4C	3.57	1.47	1.39
20	c	513	CLA	CHD-C4C	3.56	1.47	1.39
26	l	101	LHG	O7-C7	3.56	1.44	1.34
20	D	403	CLA	CHD-C4C	3.56	1.47	1.39
20	C	509	CLA	CHD-C1D	3.56	1.45	1.38
20	B	615	CLA	CHD-C1D	3.56	1.45	1.38
20	d	403	CLA	CHD-C4C	3.55	1.47	1.39
20	B	608	CLA	C1B-NB	-3.55	1.32	1.35
20	c	509	CLA	CHD-C1D	3.55	1.45	1.38
20	A	405	CLA	C1D-ND	-3.55	1.33	1.37
20	a	405	CLA	C1D-ND	-3.55	1.33	1.37
31	E	101	HEM	C3C-CAC	3.55	1.55	1.47
31	e	101	HEM	C3C-CAC	3.55	1.55	1.47
20	b	614	CLA	C3B-C2B	3.55	1.45	1.40
20	b	608	CLA	C1B-NB	-3.54	1.32	1.35
26	L	101	LHG	O7-C7	3.54	1.44	1.34
20	b	615	CLA	C1C-NC	-3.54	1.32	1.37
20	B	615	CLA	C1C-NC	-3.53	1.32	1.37
20	B	609	CLA	C1C-NC	-3.53	1.32	1.37
20	c	513	CLA	C1D-ND	-3.53	1.33	1.37
29	d	401	CL7	C4D-ND	3.52	1.38	1.35
29	D	401	CL7	C4D-ND	3.52	1.38	1.35
20	b	615	CLA	C1D-ND	-3.52	1.33	1.37
20	C	513	CLA	C1D-ND	-3.51	1.33	1.37
20	C	511	CLA	C1D-ND	-3.50	1.33	1.37
20	b	609	CLA	C1C-NC	-3.50	1.32	1.37
20	c	506	CLA	C1C-NC	-3.50	1.32	1.37
20	B	614	CLA	C3B-C2B	3.50	1.45	1.40
20	B	615	CLA	C1D-ND	-3.49	1.33	1.37
20	C	502	CLA	OBD-CAD	3.49	1.28	1.22
20	C	506	CLA	C1C-NC	-3.49	1.32	1.37
20	b	608	CLA	MG-ND	-3.48	1.98	2.05
20	c	511	CLA	C1D-ND	-3.48	1.33	1.37
20	C	512	CLA	CHD-C1D	3.47	1.45	1.38
20	c	502	CLA	OBD-CAD	3.47	1.28	1.22
20	C	509	CLA	C1B-NB	-3.46	1.32	1.35
20	C	503	CLA	CHD-C4C	3.46	1.47	1.39
20	c	503	CLA	CHD-C4C	3.46	1.47	1.39
20	C	502	CLA	C1C-NC	-3.46	1.32	1.37
20	C	505	CLA	OBD-CAD	3.46	1.28	1.22
22	C	515	BCR	C11-C12	-3.46	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	615	CLA	CHD-C4C	3.46	1.47	1.39
20	B	608	CLA	CHD-C4C	3.45	1.47	1.39
20	C	510	CLA	CHD-C4C	3.45	1.47	1.39
20	B	615	CLA	CHD-C4C	3.45	1.47	1.39
20	B	611	CLA	C3C-C2C	3.45	1.44	1.36
20	c	505	CLA	OBD-CAD	3.45	1.28	1.22
22	c	515	BCR	C11-C12	-3.45	1.25	1.34
22	A	408	BCR	C11-C12	-3.45	1.25	1.34
20	h	101	CLA	C1C-NC	-3.44	1.32	1.37
20	B	608	CLA	MG-ND	-3.44	1.99	2.05
20	C	503	CLA	C1D-ND	-3.44	1.33	1.37
20	b	608	CLA	CHD-C4C	3.44	1.47	1.39
20	b	611	CLA	C3C-C2C	3.44	1.44	1.36
22	b	617	BCR	C11-C12	-3.44	1.25	1.34
22	B	617	BCR	C11-C12	-3.43	1.25	1.34
22	a	408	BCR	C11-C12	-3.43	1.25	1.34
20	C	509	CLA	CHD-C4C	3.43	1.47	1.39
20	b	614	CLA	CHD-C4C	3.43	1.47	1.39
20	c	510	CLA	CHD-C4C	3.43	1.47	1.39
20	c	509	CLA	C1B-NB	-3.43	1.32	1.35
20	c	502	CLA	C1C-NC	-3.43	1.32	1.37
20	c	512	CLA	CHD-C1D	3.43	1.45	1.38
20	B	614	CLA	CHD-C4C	3.43	1.47	1.39
20	c	509	CLA	CHD-C4C	3.43	1.47	1.39
20	H	101	CLA	C1C-NC	-3.42	1.32	1.37
20	B	609	CLA	CHD-C4C	3.42	1.47	1.39
20	b	609	CLA	CHD-C4C	3.42	1.47	1.39
20	b	612	CLA	CHD-C1D	3.42	1.45	1.38
20	B	610	CLA	CHD-C4C	3.41	1.47	1.39
20	C	514	CLA	C1D-ND	-3.40	1.33	1.37
20	B	612	CLA	CHD-C1D	3.40	1.45	1.38
20	c	503	CLA	C1D-ND	-3.39	1.33	1.37
20	B	608	CLA	OBD-CAD	3.39	1.28	1.22
20	h	101	CLA	CHD-C4C	3.39	1.47	1.39
20	H	101	CLA	CHD-C4C	3.37	1.46	1.39
20	b	610	CLA	CHD-C4C	3.37	1.46	1.39
20	C	511	CLA	OBD-CAD	3.37	1.28	1.22
24	A	410	PL9	C10-C9	-3.37	1.42	1.50
24	a	410	PL9	C10-C9	-3.36	1.42	1.50
20	c	514	CLA	C1D-ND	-3.35	1.33	1.37
20	b	608	CLA	OBD-CAD	3.35	1.28	1.22
20	C	511	CLA	C1C-NC	-3.35	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	511	CLA	C1C-NC	-3.35	1.32	1.37
26	A	412	LHG	O7-C7	3.34	1.43	1.34
31	v	201	HEM	C3C-CAC	3.34	1.54	1.47
22	d	405	BCR	C11-C12	-3.33	1.26	1.34
20	c	511	CLA	OBD-CAD	3.33	1.28	1.22
26	a	412	LHG	O7-C7	3.33	1.43	1.34
22	D	405	BCR	C11-C12	-3.33	1.26	1.34
20	b	614	CLA	MG-ND	-3.31	1.99	2.05
31	V	201	HEM	C3C-CAC	3.30	1.54	1.47
20	B	614	CLA	C1C-NC	-3.30	1.32	1.37
20	B	608	CLA	C1C-NC	-3.29	1.32	1.37
20	b	614	CLA	C1C-NC	-3.29	1.32	1.37
20	b	612	CLA	C1C-NC	-3.29	1.32	1.37
20	B	614	CLA	MG-ND	-3.29	1.99	2.05
20	b	608	CLA	C1C-NC	-3.28	1.32	1.37
20	B	612	CLA	C1C-NC	-3.28	1.32	1.37
28	c	516	DGD	O4D-C4D	-3.28	1.35	1.43
29	D	401	CL7	C3B-C2B	3.28	1.44	1.40
27	b	607	F6C	C3B-C2B	3.27	1.46	1.39
29	d	401	CL7	C3B-C2B	3.27	1.44	1.40
28	C	516	DGD	O4D-C4D	-3.27	1.35	1.43
27	B	607	F6C	C3B-C2B	3.27	1.46	1.39
20	C	512	CLA	CHD-C4C	3.27	1.46	1.39
27	c	508	F6C	C3B-C2B	3.26	1.46	1.39
29	d	401	CL7	C1B-NB	-3.26	1.32	1.35
20	c	514	CLA	C1C-NC	-3.26	1.32	1.37
20	C	507	CLA	OBD-CAD	3.26	1.28	1.22
23	l	102	SQD	O47-C7	3.26	1.43	1.34
20	c	512	CLA	CHD-C4C	3.26	1.46	1.39
20	B	601	CLA	C1D-ND	-3.25	1.33	1.37
20	C	506	CLA	OBD-CAD	3.25	1.28	1.22
20	B	611	CLA	CHD-C4C	3.25	1.46	1.39
23	L	102	SQD	O47-C7	3.25	1.43	1.34
22	b	616	BCR	C11-C12	-3.25	1.26	1.34
27	C	508	F6C	C3B-C2B	3.24	1.46	1.39
20	b	611	CLA	CHD-C4C	3.24	1.46	1.39
20	c	507	CLA	OBD-CAD	3.24	1.28	1.22
20	c	504	CLA	MG-ND	-3.24	1.99	2.05
20	b	601	CLA	C1D-ND	-3.23	1.33	1.37
22	B	616	BCR	C11-C12	-3.23	1.26	1.34
29	D	401	CL7	C1B-NB	-3.22	1.32	1.35
20	c	506	CLA	OBD-CAD	3.22	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	609	CLA	OBD-CAD	3.22	1.28	1.22
20	B	605	CLA	OBD-CAD	3.22	1.28	1.22
20	b	605	CLA	OBD-CAD	3.22	1.28	1.22
20	C	504	CLA	MG-ND	-3.22	1.99	2.05
20	c	503	CLA	MG-ND	-3.22	1.99	2.05
24	D	406	PL9	C52-C5	-3.22	1.44	1.50
22	B	618	BCR	C11-C12	-3.21	1.26	1.34
20	c	512	CLA	OBD-CAD	3.21	1.28	1.22
24	d	406	PL9	C52-C5	-3.21	1.44	1.50
20	C	512	CLA	OBD-CAD	3.21	1.28	1.22
20	b	611	CLA	OBD-CAD	3.21	1.28	1.22
22	b	618	BCR	C11-C12	-3.20	1.26	1.34
27	B	613	F6C	C1D-ND	-3.20	1.33	1.37
27	b	613	F6C	C1D-ND	-3.20	1.33	1.37
20	C	514	CLA	C1C-NC	-3.20	1.33	1.37
20	C	502	CLA	C3D-C2D	3.20	1.47	1.39
20	b	601	CLA	C3D-C2D	3.19	1.47	1.39
20	c	502	CLA	C3D-C2D	3.19	1.47	1.39
20	B	601	CLA	C3D-C2D	3.19	1.47	1.39
24	D	406	PL9	C31-C29	-3.19	1.44	1.51
20	C	503	CLA	MG-ND	-3.18	1.99	2.05
27	b	613	F6C	MG-ND	-3.18	1.98	2.06
24	d	406	PL9	C31-C29	-3.17	1.44	1.51
20	B	609	CLA	OBD-CAD	3.17	1.27	1.22
27	B	613	F6C	MG-ND	-3.17	1.98	2.06
27	B	604	F6C	C3B-C2B	3.16	1.46	1.39
20	B	611	CLA	OBD-CAD	3.16	1.27	1.22
20	a	405	CLA	MG-ND	-3.16	1.99	2.05
20	C	507	CLA	MG-ND	-3.15	1.99	2.05
20	C	503	CLA	OBD-CAD	3.15	1.27	1.22
20	c	507	CLA	MG-ND	-3.14	1.99	2.05
31	E	101	HEM	CAB-C3B	3.14	1.56	1.47
31	e	101	HEM	CAB-C3B	3.14	1.56	1.47
20	A	405	CLA	MG-ND	-3.14	1.99	2.05
20	B	612	CLA	CHD-C4C	3.13	1.46	1.39
20	b	612	CLA	CHD-C4C	3.13	1.46	1.39
27	B	604	F6C	C1D-ND	-3.13	1.33	1.37
27	b	604	F6C	C1D-ND	-3.13	1.33	1.37
27	b	604	F6C	C3B-C2B	3.13	1.46	1.39
20	a	404	CLA	MG-NC	3.12	2.13	2.06
28	C	516	DGD	O5D-C6D	-3.12	1.38	1.43
20	C	509	CLA	OBD-CAD	3.12	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	606	CLA	MG-NC	3.12	2.13	2.06
20	C	506	CLA	CHD-C4C	3.11	1.46	1.39
20	D	403	CLA	C1C-NC	-3.11	1.33	1.37
20	c	506	CLA	CHD-C4C	3.11	1.46	1.39
28	c	516	DGD	O5D-C6D	-3.11	1.38	1.43
20	C	507	CLA	C1C-NC	-3.11	1.33	1.37
20	B	606	CLA	MG-NC	3.10	2.13	2.06
20	B	602	CLA	MG-NC	3.10	2.13	2.06
20	d	403	CLA	C1C-NC	-3.10	1.33	1.37
20	B	610	CLA	OBD-CAD	3.10	1.27	1.22
20	c	503	CLA	OBD-CAD	3.10	1.27	1.22
20	c	509	CLA	OBD-CAD	3.09	1.27	1.22
20	b	603	CLA	MG-NC	3.09	2.13	2.06
20	A	404	CLA	MG-NC	3.09	2.13	2.06
20	D	404	CLA	C1C-NC	-3.09	1.33	1.37
20	B	605	CLA	CHD-C4C	3.08	1.46	1.39
20	B	603	CLA	MG-NC	3.08	2.13	2.06
20	c	507	CLA	C1C-NC	-3.08	1.33	1.37
20	d	404	CLA	C1C-NC	-3.07	1.33	1.37
28	C	516	DGD	O2G-C2G	-3.07	1.38	1.46
31	V	201	HEM	CAB-C3B	3.07	1.55	1.47
20	b	605	CLA	CHD-C4C	3.07	1.46	1.39
20	b	602	CLA	MG-NC	3.07	2.13	2.06
20	B	609	CLA	C3D-C2D	3.06	1.47	1.39
20	A	407	CLA	MG-NC	3.06	2.13	2.06
20	a	407	CLA	MG-NC	3.06	2.13	2.06
20	b	610	CLA	OBD-CAD	3.06	1.27	1.22
28	c	516	DGD	O2G-C2G	-3.06	1.38	1.46
20	C	513	CLA	MG-ND	-3.05	1.99	2.05
20	B	605	CLA	MG-ND	-3.05	1.99	2.05
31	v	201	HEM	CAB-C3B	3.04	1.55	1.47
20	b	605	CLA	C4B-NB	-3.03	1.32	1.35
20	B	612	CLA	MG-ND	-3.03	1.99	2.05
20	b	612	CLA	MG-ND	-3.03	1.99	2.05
20	C	504	CLA	OBD-CAD	3.03	1.27	1.22
20	d	403	CLA	CHD-C1D	3.02	1.44	1.38
20	b	609	CLA	C3D-C2D	3.02	1.47	1.39
20	b	605	CLA	MG-ND	-3.02	1.99	2.05
20	c	504	CLA	OBD-CAD	3.02	1.27	1.22
27	B	607	F6C	C1D-C2D	3.02	1.50	1.44
27	c	508	F6C	C3D-C2D	3.02	1.47	1.39
20	a	407	CLA	C3D-C2D	3.01	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	513	CLA	C1C-NC	-3.01	1.33	1.37
20	D	403	CLA	CHD-C1D	3.01	1.44	1.38
20	c	513	CLA	C1C-NC	-3.01	1.33	1.37
20	c	513	CLA	MG-ND	-3.01	1.99	2.05
27	C	508	F6C	C3D-C2D	3.00	1.47	1.39
20	C	512	CLA	C1C-NC	-3.00	1.33	1.37
20	c	512	CLA	C1C-NC	-3.00	1.33	1.37
20	b	601	CLA	MG-NC	3.00	2.13	2.06
20	C	512	CLA	MG-ND	-3.00	1.99	2.05
20	B	601	CLA	MG-NC	2.99	2.13	2.06
20	b	612	CLA	OBD-CAD	2.99	1.27	1.22
20	c	512	CLA	MG-ND	-2.99	1.99	2.05
27	B	604	F6C	CHB-C1B	2.99	1.46	1.39
27	b	604	F6C	CHB-C1B	2.99	1.46	1.39
27	B	604	F6C	MG-ND	-2.99	1.99	2.06
20	B	612	CLA	OBD-CAD	2.99	1.27	1.22
27	b	604	F6C	OBD-CAD	2.99	1.27	1.22
20	B	606	CLA	C3D-C2D	2.98	1.47	1.39
27	b	604	F6C	MG-ND	-2.98	1.99	2.06
27	c	508	F6C	C3C-C2C	2.98	1.46	1.37
20	A	407	CLA	C3D-C2D	2.98	1.47	1.39
27	b	607	F6C	C1D-C2D	2.98	1.50	1.44
27	C	508	F6C	C1D-C2D	2.98	1.50	1.44
27	c	508	F6C	C1D-C2D	2.98	1.50	1.44
27	B	604	F6C	OBD-CAD	2.98	1.27	1.22
27	B	607	F6C	C3C-C2C	2.98	1.46	1.37
27	b	607	F6C	C3C-C2C	2.98	1.46	1.37
20	b	603	CLA	C3D-C2D	2.98	1.47	1.39
20	B	603	CLA	C3D-C2D	2.98	1.47	1.39
20	B	605	CLA	C4B-NB	-2.98	1.32	1.35
20	d	403	CLA	MG-ND	-2.98	1.99	2.05
20	d	404	CLA	MG-ND	-2.98	1.99	2.05
20	b	606	CLA	C3D-C2D	2.97	1.47	1.39
20	a	404	CLA	C3D-C2D	2.97	1.47	1.39
27	b	604	F6C	C1A-C2A	2.97	1.52	1.45
20	A	404	CLA	C3D-C2D	2.97	1.47	1.39
20	c	504	CLA	MG-NC	2.96	2.13	2.06
27	C	508	F6C	C3C-C2C	2.96	1.46	1.37
20	D	404	CLA	MG-ND	-2.96	1.99	2.05
27	B	607	F6C	C3D-C2D	2.96	1.47	1.39
20	B	602	CLA	C3D-C2D	2.96	1.47	1.39
20	D	403	CLA	MG-ND	-2.96	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	602	CLA	C3D-C2D	2.95	1.47	1.39
29	D	401	CL7	C1A-CHA	2.95	1.51	1.38
29	d	401	CL7	C1A-CHA	2.95	1.51	1.38
27	b	607	F6C	C3D-C2D	2.95	1.47	1.39
27	B	604	F6C	C1A-C2A	2.94	1.51	1.45
20	C	504	CLA	MG-NC	2.93	2.13	2.06
27	b	613	F6C	C3B-C2B	2.93	1.46	1.39
20	B	601	CLA	MG-ND	-2.93	2.00	2.05
20	H	101	CLA	MG-ND	-2.92	2.00	2.05
20	A	405	CLA	OBD-CAD	2.92	1.27	1.22
20	C	507	CLA	C1B-NB	-2.92	1.32	1.35
20	b	601	CLA	MG-ND	-2.91	2.00	2.05
27	B	613	F6C	C3B-C2B	2.91	1.46	1.39
20	c	513	CLA	MG-NC	2.90	2.13	2.06
21	a	406	PHO	CAC-C3C	-2.90	1.47	1.52
20	C	513	CLA	MG-NC	2.90	2.13	2.06
29	d	401	CL7	C4A-NA	-2.90	1.30	1.38
20	h	101	CLA	MG-ND	-2.89	2.00	2.05
20	b	608	CLA	C3D-C2D	2.89	1.47	1.39
20	C	505	CLA	MG-ND	-2.88	2.00	2.05
20	a	405	CLA	OBD-CAD	2.88	1.27	1.22
20	C	505	CLA	C1C-NC	-2.88	1.33	1.37
29	D	401	CL7	C4A-NA	-2.88	1.30	1.38
20	c	505	CLA	C1C-NC	-2.88	1.33	1.37
20	B	608	CLA	C3D-C2D	2.88	1.47	1.39
27	B	613	F6C	OBD-CAD	2.87	1.27	1.22
20	c	507	CLA	C1B-NB	-2.87	1.32	1.35
21	A	406	PHO	CAC-C3C	-2.86	1.47	1.52
20	c	509	CLA	C3D-C2D	2.85	1.46	1.39
20	c	505	CLA	MG-ND	-2.84	2.00	2.05
20	B	610	CLA	C1B-NB	-2.84	1.32	1.35
27	b	613	F6C	C3D-C2D	2.84	1.46	1.39
20	c	514	CLA	C3D-C2D	2.84	1.46	1.39
29	d	401	CL7	C1D-ND	-2.83	1.32	1.35
20	C	509	CLA	C3D-C2D	2.83	1.46	1.39
20	C	514	CLA	C3D-C2D	2.83	1.46	1.39
20	C	502	CLA	MG-ND	-2.83	2.00	2.05
27	b	613	F6C	OBD-CAD	2.83	1.27	1.22
20	C	506	CLA	C3D-C2D	2.83	1.46	1.39
20	D	404	CLA	C3D-C2D	2.83	1.46	1.39
20	c	505	CLA	C3D-C2D	2.83	1.46	1.39
20	d	404	CLA	C3D-C2D	2.83	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	608	CLA	MG-NC	2.82	2.13	2.06
20	D	404	CLA	MG-NC	2.82	2.13	2.06
20	d	404	CLA	MG-NC	2.82	2.13	2.06
27	B	613	F6C	C3D-C2D	2.82	1.46	1.39
20	C	505	CLA	C3D-C2D	2.82	1.46	1.39
20	c	511	CLA	MG-ND	-2.82	2.00	2.05
20	c	502	CLA	MG-ND	-2.81	2.00	2.05
20	c	507	CLA	C3D-C2D	2.81	1.46	1.39
20	b	608	CLA	MG-NC	2.81	2.12	2.06
20	c	506	CLA	C3D-C2D	2.81	1.46	1.39
20	b	601	CLA	C4D-CHA	2.81	1.48	1.38
27	c	508	F6C	CMB-C2B	2.80	1.51	1.45
20	B	601	CLA	C4D-CHA	2.80	1.48	1.38
20	C	507	CLA	C3D-C2D	2.80	1.46	1.39
24	d	406	PL9	C7-C8	-2.79	1.46	1.50
20	D	403	CLA	OBD-CAD	2.78	1.27	1.22
29	d	401	CL7	MG-NC	2.78	2.11	2.05
20	B	610	CLA	C3D-C2D	2.78	1.46	1.39
20	b	610	CLA	C3D-C2D	2.78	1.46	1.39
29	D	401	CL7	MG-NC	2.78	2.11	2.05
27	C	508	F6C	CMB-C2B	2.78	1.51	1.45
20	b	611	CLA	C1B-NB	-2.78	1.32	1.35
20	d	403	CLA	OBD-CAD	2.77	1.27	1.22
20	b	610	CLA	MG-ND	-2.77	2.00	2.05
24	D	406	PL9	C7-C8	-2.77	1.46	1.50
20	h	101	CLA	OBD-CAD	2.77	1.27	1.22
20	C	511	CLA	MG-ND	-2.77	2.00	2.05
20	B	615	CLA	C3D-C2D	2.77	1.46	1.39
20	b	615	CLA	C3D-C2D	2.77	1.46	1.39
20	c	504	CLA	C3D-C2D	2.77	1.46	1.39
29	D	401	CL7	C1D-ND	-2.76	1.32	1.35
20	H	101	CLA	OBD-CAD	2.76	1.27	1.22
27	B	607	F6C	CMB-C2B	2.76	1.51	1.45
33	M	102	LMT	O2B-C2B	-2.76	1.36	1.43
33	m	102	LMT	O2B-C2B	-2.75	1.36	1.43
20	c	512	CLA	C3D-C2D	2.75	1.46	1.39
20	C	513	CLA	C3D-C2D	2.75	1.46	1.39
20	C	504	CLA	C3D-C2D	2.74	1.46	1.39
20	C	503	CLA	C3D-C2D	2.74	1.46	1.39
20	C	513	CLA	C4D-CHA	2.74	1.48	1.38
20	c	510	CLA	C4B-CHC	2.74	1.48	1.41
20	c	503	CLA	C3D-C2D	2.74	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	513	CLA	C3D-C2D	2.74	1.46	1.39
20	c	513	CLA	C4D-CHA	2.74	1.48	1.38
20	B	610	CLA	MG-ND	-2.74	2.00	2.05
27	b	607	F6C	CMB-C2B	2.74	1.51	1.45
32	h	102	RRX	C23-C22	-2.74	1.40	1.45
20	C	510	CLA	C4B-CHC	2.74	1.48	1.41
20	C	506	CLA	MG-NC	2.74	2.12	2.06
20	C	512	CLA	C3D-C2D	2.74	1.46	1.39
20	c	510	CLA	C1C-NC	-2.73	1.33	1.37
20	c	506	CLA	MG-NC	2.73	2.12	2.06
20	C	510	CLA	C1C-NC	-2.73	1.33	1.37
32	H	102	RRX	C23-C22	-2.73	1.40	1.45
20	b	610	CLA	C1B-NB	-2.73	1.32	1.35
20	B	611	CLA	C1B-NB	-2.73	1.32	1.35
21	D	402	PHO	CMD-C2D	-2.73	1.45	1.51
21	d	402	PHO	CMD-C2D	-2.72	1.45	1.51
20	C	514	CLA	MG-ND	-2.72	2.00	2.05
20	c	514	CLA	MG-ND	-2.72	2.00	2.05
32	h	102	RRX	C8-C9	-2.72	1.40	1.45
20	D	404	CLA	C1B-CHB	2.71	1.48	1.41
20	B	605	CLA	MG-NC	2.70	2.12	2.06
20	b	605	CLA	MG-NC	2.70	2.12	2.06
32	H	102	RRX	C8-C9	-2.70	1.40	1.45
20	A	407	CLA	C1D-ND	-2.70	1.34	1.37
20	B	612	CLA	MG-NC	2.70	2.12	2.06
20	d	404	CLA	C1B-CHB	2.69	1.48	1.41
20	B	614	CLA	OBD-CAD	2.69	1.27	1.22
20	c	505	CLA	C4D-CHA	2.69	1.48	1.38
20	B	603	CLA	C1D-ND	-2.69	1.34	1.37
27	b	604	F6C	CHB-C4A	-2.69	1.33	1.38
27	B	604	F6C	CHB-C4A	-2.69	1.33	1.38
20	c	502	CLA	C4D-CHA	2.69	1.47	1.38
20	B	615	CLA	MG-ND	-2.69	2.00	2.05
20	b	614	CLA	OBD-CAD	2.68	1.27	1.22
20	a	407	CLA	C1D-ND	-2.68	1.34	1.37
20	C	505	CLA	C4D-CHA	2.68	1.47	1.38
20	C	510	CLA	OBD-CAD	2.68	1.27	1.22
20	c	510	CLA	OBD-CAD	2.68	1.27	1.22
20	a	404	CLA	C4D-CHA	2.68	1.47	1.38
20	b	612	CLA	MG-NC	2.68	2.12	2.06
20	a	407	CLA	C4D-CHA	2.68	1.47	1.38
20	b	609	CLA	MG-NC	2.67	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	609	CLA	MG-NC	2.67	2.12	2.06
20	B	608	CLA	C4D-CHA	2.67	1.47	1.38
20	C	502	CLA	C4D-CHA	2.67	1.47	1.38
20	A	404	CLA	C4D-CHA	2.67	1.47	1.38
20	b	614	CLA	C4D-CHA	2.67	1.47	1.38
20	b	608	CLA	C4D-CHA	2.66	1.47	1.38
20	A	407	CLA	C4D-CHA	2.66	1.47	1.38
20	B	614	CLA	MG-NC	2.66	2.12	2.06
20	b	614	CLA	MG-NC	2.65	2.12	2.06
20	C	504	CLA	C4D-CHA	2.65	1.47	1.38
20	b	615	CLA	MG-ND	-2.65	2.00	2.05
20	b	602	CLA	C4D-CHA	2.65	1.47	1.38
20	B	614	CLA	C4D-CHA	2.65	1.47	1.38
20	B	606	CLA	C1D-ND	-2.65	1.34	1.37
20	B	606	CLA	C4D-CHA	2.65	1.47	1.38
20	B	603	CLA	C4D-CHA	2.64	1.47	1.38
20	b	603	CLA	C4D-CHA	2.64	1.47	1.38
27	c	508	F6C	C1C-CHC	2.64	1.48	1.41
27	C	508	F6C	C1C-CHC	2.64	1.48	1.41
28	C	517	DGD	C4D-C3D	2.64	1.59	1.52
20	B	606	CLA	C1B-CHB	2.64	1.48	1.41
20	b	606	CLA	C1B-CHB	2.64	1.48	1.41
20	c	504	CLA	C4D-CHA	2.64	1.47	1.38
28	c	517	DGD	C4D-C3D	2.64	1.59	1.52
20	A	404	CLA	C1B-CHB	2.64	1.48	1.41
20	B	602	CLA	C4D-CHA	2.64	1.47	1.38
24	D	406	PL9	C26-C24	-2.63	1.45	1.51
27	B	607	F6C	C1C-CHC	2.63	1.48	1.41
33	M	102	LMT	O2'-C2'	-2.63	1.36	1.43
20	a	404	CLA	C1D-ND	-2.63	1.34	1.37
20	b	603	CLA	C1D-ND	-2.63	1.34	1.37
27	b	607	F6C	C1C-CHC	2.63	1.48	1.41
20	C	510	CLA	MG-NC	2.63	2.12	2.06
20	a	404	CLA	C1B-CHB	2.63	1.48	1.41
20	C	510	CLA	C3D-C2D	2.63	1.46	1.39
20	b	610	CLA	C4D-CHA	2.62	1.47	1.38
33	m	102	LMT	O2'-C2'	-2.62	1.36	1.43
30	m	101	LMG	C37-C36	-2.62	1.33	1.51
20	b	606	CLA	C4D-CHA	2.62	1.47	1.38
20	B	610	CLA	C4D-CHA	2.62	1.47	1.38
20	b	606	CLA	C1D-ND	-2.62	1.34	1.37
20	C	503	CLA	C1B-NB	-2.62	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	606	CLA	C4B-CHC	2.62	1.48	1.41
24	d	406	PL9	C26-C24	-2.62	1.45	1.51
20	A	404	CLA	C1D-ND	-2.62	1.34	1.37
20	B	602	CLA	C1D-C2D	2.62	1.50	1.45
20	B	601	CLA	C1C-NC	-2.62	1.33	1.37
20	b	601	CLA	C1C-NC	-2.62	1.33	1.37
20	c	510	CLA	C3D-C2D	2.62	1.46	1.39
20	c	504	CLA	C1C-NC	-2.61	1.33	1.37
20	B	603	CLA	C4B-CHC	2.61	1.48	1.41
30	M	101	LMG	C37-C36	-2.61	1.33	1.51
20	b	602	CLA	C1D-C2D	2.61	1.50	1.45
20	C	506	CLA	C1B-NB	-2.61	1.32	1.35
20	c	510	CLA	MG-NC	2.61	2.12	2.06
20	b	605	CLA	C3D-C2D	2.61	1.46	1.39
20	B	606	CLA	C4B-CHC	2.61	1.48	1.41
29	d	401	CL7	C3A-C4A	-2.61	1.47	1.52
20	B	602	CLA	C1B-CHB	2.61	1.48	1.41
20	B	605	CLA	C3D-C2D	2.61	1.46	1.39
20	B	615	CLA	C4D-CHA	2.61	1.47	1.38
20	b	615	CLA	C4D-CHA	2.61	1.47	1.38
33	M	102	LMT	O3'-C3'	-2.60	1.36	1.43
20	a	407	CLA	C1D-C2D	2.60	1.50	1.45
20	A	407	CLA	C1B-CHB	2.60	1.48	1.41
20	a	407	CLA	C1B-CHB	2.60	1.48	1.41
20	A	407	CLA	C1D-C2D	2.60	1.50	1.45
33	m	102	LMT	O3'-C3'	-2.60	1.36	1.43
20	b	603	CLA	C4B-CHC	2.59	1.48	1.41
27	C	508	F6C	C4A-C3A	2.59	1.50	1.45
20	b	612	CLA	C4D-CHA	2.59	1.47	1.38
29	D	401	CL7	C3A-C4A	-2.59	1.47	1.52
20	A	405	CLA	MG-NC	2.59	2.12	2.06
20	b	602	CLA	C1B-CHB	2.59	1.48	1.41
21	A	406	PHO	CMD-C2D	-2.59	1.45	1.51
27	b	607	F6C	C4C-CHD	2.59	1.48	1.41
20	B	603	CLA	C1D-C2D	2.59	1.50	1.45
20	B	606	CLA	C1D-C2D	2.59	1.50	1.45
20	b	606	CLA	C1D-C2D	2.59	1.50	1.45
20	a	404	CLA	C4B-CHC	2.59	1.48	1.41
20	B	612	CLA	C4D-CHA	2.59	1.47	1.38
20	B	603	CLA	C1B-CHB	2.58	1.48	1.41
20	b	611	CLA	C3D-C2D	2.58	1.46	1.39
20	A	404	CLA	C4B-CHC	2.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	101	CLA	MG-NC	2.57	2.12	2.06
20	h	101	CLA	MG-NC	2.57	2.12	2.06
27	c	508	F6C	C4A-C3A	2.57	1.50	1.45
20	a	405	CLA	MG-NC	2.57	2.12	2.06
20	c	503	CLA	C1B-NB	-2.57	1.32	1.35
21	a	406	PHO	CMD-C2D	-2.57	1.45	1.51
20	A	407	CLA	C4B-CHC	2.57	1.48	1.41
20	a	407	CLA	C4B-CHC	2.57	1.48	1.41
20	C	504	CLA	C1C-NC	-2.57	1.34	1.37
27	c	508	F6C	C4C-CHD	2.57	1.48	1.41
27	C	508	F6C	C4C-CHD	2.57	1.48	1.41
20	c	506	CLA	C1B-NB	-2.57	1.32	1.35
20	b	603	CLA	C1B-CHB	2.57	1.48	1.41
28	d	410	DGD	O2G-C2G	-2.57	1.40	1.46
20	c	507	CLA	MG-NC	2.56	2.12	2.06
27	B	607	F6C	C4A-C3A	2.56	1.50	1.45
27	B	607	F6C	C4C-CHD	2.56	1.48	1.41
20	a	404	CLA	C1D-C2D	2.56	1.50	1.45
20	B	611	CLA	C3D-C2D	2.56	1.46	1.39
20	b	603	CLA	C1D-C2D	2.56	1.50	1.45
20	A	404	CLA	C1D-C2D	2.56	1.50	1.45
27	b	607	F6C	C4A-C3A	2.55	1.50	1.45
20	C	514	CLA	C4D-CHA	2.55	1.47	1.38
20	c	514	CLA	C4D-CHA	2.55	1.47	1.38
20	c	511	CLA	C4D-CHA	2.55	1.47	1.38
20	C	511	CLA	C4D-CHA	2.55	1.47	1.38
20	B	602	CLA	C4B-CHC	2.54	1.48	1.41
20	b	602	CLA	C4B-CHC	2.54	1.48	1.41
28	D	410	DGD	O2G-C2G	-2.54	1.40	1.46
20	C	507	CLA	MG-NC	2.54	2.12	2.06
28	C	516	DGD	O3E-C3E	-2.53	1.37	1.43
20	c	505	CLA	MG-NC	2.53	2.12	2.06
27	b	613	F6C	C4B-NB	-2.53	1.34	1.37
20	C	514	CLA	C4B-CHC	2.53	1.48	1.41
20	C	507	CLA	C4B-NB	-2.53	1.33	1.35
20	C	512	CLA	C1B-CHB	2.52	1.48	1.41
28	c	516	DGD	O3E-C3E	-2.52	1.37	1.43
20	C	505	CLA	MG-NC	2.52	2.12	2.06
20	c	507	CLA	C4B-NB	-2.52	1.33	1.35
20	c	512	CLA	C1B-CHB	2.52	1.48	1.41
20	C	503	CLA	C4D-CHA	2.51	1.47	1.38
20	c	503	CLA	C4D-CHA	2.51	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	514	CLA	C4B-CHC	2.51	1.48	1.41
20	B	602	CLA	C1D-ND	-2.51	1.34	1.37
27	B	613	F6C	C4B-NB	-2.50	1.34	1.37
20	A	405	CLA	C3D-C2D	2.50	1.46	1.39
20	a	405	CLA	C3D-C2D	2.50	1.46	1.39
20	b	609	CLA	C4D-CHA	2.50	1.47	1.38
20	d	404	CLA	OBD-CAD	2.50	1.26	1.22
20	c	506	CLA	C4D-CHA	2.50	1.47	1.38
20	c	507	CLA	C4D-CHA	2.50	1.47	1.38
20	B	609	CLA	C4D-CHA	2.50	1.47	1.38
20	C	507	CLA	C4D-CHA	2.50	1.47	1.38
20	H	101	CLA	C4D-CHA	2.50	1.47	1.38
20	B	614	CLA	C3D-C2D	2.49	1.45	1.39
20	C	506	CLA	C4D-CHA	2.49	1.47	1.38
27	B	607	F6C	C2B-C1B	2.49	1.49	1.44
27	b	607	F6C	C2B-C1B	2.49	1.49	1.44
20	D	404	CLA	OBD-CAD	2.49	1.26	1.22
20	c	514	CLA	MG-NC	2.49	2.12	2.06
20	b	614	CLA	C3D-C2D	2.49	1.45	1.39
20	h	101	CLA	C4D-CHA	2.48	1.47	1.38
20	b	612	CLA	C3D-C2D	2.47	1.45	1.39
20	c	510	CLA	C4D-CHA	2.47	1.47	1.38
27	b	604	F6C	C1C-NC	-2.47	1.33	1.35
20	b	605	CLA	C1B-CHB	2.47	1.47	1.41
20	C	510	CLA	C4D-CHA	2.47	1.47	1.38
20	b	602	CLA	C1D-ND	-2.47	1.34	1.37
20	d	404	CLA	C4D-CHA	2.47	1.47	1.38
27	C	508	F6C	C2B-C1B	2.46	1.49	1.44
27	c	508	F6C	C2B-C1B	2.46	1.49	1.44
20	B	612	CLA	C3D-C2D	2.46	1.45	1.39
20	C	514	CLA	MG-NC	2.46	2.12	2.06
20	c	504	CLA	C4B-CHC	2.45	1.47	1.41
20	C	510	CLA	C3B-C2B	2.45	1.43	1.40
20	B	605	CLA	C1B-CHB	2.45	1.47	1.41
20	D	404	CLA	C4D-CHA	2.45	1.47	1.38
20	c	512	CLA	C1B-NB	-2.44	1.33	1.35
20	c	510	CLA	C3B-C2B	2.44	1.43	1.40
20	C	504	CLA	C4B-CHC	2.43	1.47	1.41
27	B	613	F6C	CHB-C4A	-2.43	1.33	1.38
20	C	512	CLA	C1B-NB	-2.43	1.33	1.35
27	B	604	F6C	C1C-NC	-2.43	1.33	1.35
27	b	613	F6C	CHB-C4A	-2.43	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	611	CLA	MG-ND	-2.42	2.01	2.05
20	c	511	CLA	MG-NC	2.42	2.12	2.06
20	c	503	CLA	MG-NC	2.42	2.12	2.06
20	C	509	CLA	C4D-CHA	2.42	1.47	1.38
20	A	405	CLA	C4D-CHA	2.41	1.47	1.38
20	a	405	CLA	C4D-CHA	2.41	1.47	1.38
20	D	403	CLA	C3D-C2D	2.41	1.45	1.39
20	b	611	CLA	MG-ND	-2.40	2.01	2.05
20	b	611	CLA	MG-NC	2.40	2.12	2.06
20	C	511	CLA	MG-NC	2.40	2.12	2.06
20	d	403	CLA	C3D-C2D	2.40	1.45	1.39
20	C	503	CLA	MG-NC	2.39	2.12	2.06
20	c	509	CLA	C4D-CHA	2.39	1.46	1.38
20	B	612	CLA	C4B-CHC	2.38	1.47	1.41
20	b	612	CLA	C4B-CHC	2.38	1.47	1.41
20	b	601	CLA	C4B-CHC	2.38	1.47	1.41
24	D	406	PL9	C35-C34	-2.38	1.44	1.50
24	d	406	PL9	C35-C34	-2.37	1.44	1.50
20	B	611	CLA	MG-NC	2.37	2.11	2.06
20	d	403	CLA	C1B-CHB	2.37	1.47	1.41
20	H	101	CLA	C3D-C2D	2.37	1.45	1.39
20	h	101	CLA	C3D-C2D	2.37	1.45	1.39
28	C	516	DGD	O1G-C1G	-2.36	1.39	1.45
20	D	403	CLA	C1B-CHB	2.36	1.47	1.41
20	B	601	CLA	C4B-CHC	2.36	1.47	1.41
27	B	607	F6C	C1A-C2A	2.36	1.50	1.45
20	b	605	CLA	C1B-NB	-2.36	1.33	1.35
24	a	410	PL9	C6-C1	-2.36	1.44	1.48
24	A	410	PL9	C6-C1	-2.35	1.44	1.48
20	D	404	CLA	C4C-C3C	2.35	1.49	1.45
27	b	607	F6C	C1A-C2A	2.35	1.50	1.45
33	m	102	LMT	O1'-C1'	-2.34	1.36	1.40
20	B	615	CLA	C1B-NB	-2.34	1.33	1.35
20	b	615	CLA	C1B-NB	-2.34	1.33	1.35
33	M	102	LMT	O1'-C1'	-2.34	1.36	1.40
20	B	605	CLA	C4D-CHA	2.34	1.46	1.38
20	B	605	CLA	C1B-NB	-2.34	1.33	1.35
20	a	404	CLA	C1C-NC	-2.34	1.34	1.37
20	d	404	CLA	C4C-C3C	2.33	1.49	1.45
20	C	511	CLA	C3D-C2D	2.33	1.45	1.39
20	c	511	CLA	C3D-C2D	2.33	1.45	1.39
28	c	517	DGD	O4D-C4D	-2.32	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	101	LHG	O7-C5	-2.32	1.40	1.46
28	c	516	DGD	O1G-C1G	-2.32	1.39	1.45
27	B	604	F6C	C3C-C2C	2.32	1.44	1.37
27	b	604	F6C	C3C-C2C	2.32	1.44	1.37
20	c	514	CLA	C1B-CHB	2.32	1.47	1.41
20	b	605	CLA	C4D-CHA	2.32	1.46	1.38
20	C	514	CLA	C1B-CHB	2.31	1.47	1.41
20	b	606	CLA	MG-ND	-2.31	2.01	2.05
20	B	602	CLA	C1C-NC	-2.31	1.34	1.37
27	B	613	F6C	C3C-C2C	2.30	1.44	1.37
26	l	101	LHG	O7-C5	-2.30	1.40	1.46
23	L	102	SQD	O2-C2	-2.30	1.37	1.43
20	C	502	CLA	MG-NC	2.30	2.11	2.06
20	B	601	CLA	C1B-CHB	2.30	1.47	1.41
28	C	517	DGD	O4D-C4D	-2.30	1.37	1.43
20	b	612	CLA	CMA-C3A	-2.30	1.48	1.53
20	c	514	CLA	C1D-C2D	2.30	1.49	1.45
23	l	102	SQD	O2-C2	-2.30	1.37	1.43
23	L	102	SQD	O48-C23	2.30	1.40	1.33
20	C	511	CLA	C1B-CHB	2.30	1.47	1.41
20	b	601	CLA	C1B-CHB	2.30	1.47	1.41
27	b	613	F6C	C3C-C2C	2.30	1.44	1.37
20	B	603	CLA	MG-ND	-2.29	2.01	2.05
20	b	603	CLA	MG-ND	-2.29	2.01	2.05
20	D	404	CLA	C4B-CHC	2.29	1.47	1.41
20	d	404	CLA	C4B-CHC	2.29	1.47	1.41
20	B	612	CLA	CMA-C3A	-2.29	1.48	1.53
20	b	611	CLA	C4D-CHA	2.29	1.46	1.38
22	C	518	BCR	C1-C6	-2.29	1.50	1.53
20	c	502	CLA	MG-NC	2.29	2.11	2.06
20	B	615	CLA	OBD-CAD	2.29	1.26	1.22
20	b	615	CLA	OBD-CAD	2.29	1.26	1.22
20	c	513	CLA	C1B-CHB	2.28	1.47	1.41
33	M	102	LMT	O3B-C3B	-2.28	1.37	1.43
33	m	102	LMT	O3B-C3B	-2.28	1.37	1.43
20	b	612	CLA	C1B-CHB	2.28	1.47	1.41
20	c	512	CLA	C4D-CHA	2.28	1.46	1.38
23	l	102	SQD	O48-C23	2.28	1.40	1.33
20	B	611	CLA	C4D-CHA	2.28	1.46	1.38
20	b	609	CLA	C1B-CHB	2.28	1.47	1.41
20	c	511	CLA	C1B-CHB	2.28	1.47	1.41
20	A	404	CLA	C1C-NC	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	606	CLA	C4C-C3C	2.27	1.49	1.45
20	b	606	CLA	C1C-NC	-2.27	1.34	1.37
20	C	513	CLA	C1B-CHB	2.27	1.47	1.41
20	D	403	CLA	C4B-CHC	2.27	1.47	1.41
20	C	514	CLA	C1D-C2D	2.27	1.49	1.45
28	c	516	DGD	O2E-C2E	-2.27	1.37	1.43
28	C	516	DGD	O2E-C2E	-2.27	1.37	1.43
20	C	512	CLA	C4D-CHA	2.27	1.46	1.38
20	d	403	CLA	C4B-CHC	2.27	1.47	1.41
20	B	609	CLA	C1B-CHB	2.26	1.47	1.41
20	B	606	CLA	MG-ND	-2.26	2.01	2.05
20	a	404	CLA	MG-ND	-2.26	2.01	2.05
20	b	603	CLA	C4C-C3C	2.26	1.48	1.45
20	B	606	CLA	C1C-NC	-2.26	1.34	1.37
20	B	612	CLA	C1B-CHB	2.26	1.47	1.41
20	C	503	CLA	C1B-CHB	2.26	1.47	1.41
20	c	503	CLA	C1B-CHB	2.26	1.47	1.41
20	A	407	CLA	MG-ND	-2.25	2.01	2.05
20	A	404	CLA	MG-ND	-2.25	2.01	2.05
24	D	406	PL9	C36-C34	-2.25	1.46	1.51
24	d	406	PL9	C36-C34	-2.25	1.46	1.51
20	b	602	CLA	C1C-NC	-2.25	1.34	1.37
27	C	508	F6C	C1D-ND	-2.25	1.34	1.37
27	c	508	F6C	C1D-ND	-2.25	1.34	1.37
20	a	407	CLA	MG-ND	-2.25	2.01	2.05
20	C	511	CLA	C1B-NB	-2.25	1.33	1.35
20	c	511	CLA	C1B-NB	-2.25	1.33	1.35
20	a	407	CLA	C1C-NC	-2.25	1.34	1.37
21	d	402	PHO	CAC-C3C	-2.25	1.48	1.52
33	m	102	LMT	O4'-C4B	-2.25	1.37	1.43
20	B	603	CLA	C1C-NC	-2.24	1.34	1.37
20	b	603	CLA	C1C-NC	-2.24	1.34	1.37
20	b	602	CLA	C4C-C3C	2.24	1.48	1.45
20	A	407	CLA	C4C-C3C	2.24	1.48	1.45
27	c	508	F6C	C1A-C2A	2.24	1.50	1.45
20	A	407	CLA	C1C-NC	-2.24	1.34	1.37
20	c	505	CLA	C1B-CHB	2.23	1.47	1.41
20	b	606	CLA	C4C-C3C	2.23	1.48	1.45
20	b	602	CLA	MG-ND	-2.23	2.01	2.05
27	B	604	F6C	C1C-CHC	2.23	1.47	1.41
27	B	607	F6C	C1D-ND	-2.23	1.34	1.37
20	B	603	CLA	C4C-C3C	2.23	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	602	CLA	C4C-C3C	2.23	1.48	1.45
21	a	406	PHO	CMC-C2C	-2.23	1.46	1.51
21	D	402	PHO	CAC-C3C	-2.22	1.48	1.52
20	C	511	CLA	C4B-CHC	2.22	1.47	1.41
22	c	518	BCR	C1-C6	-2.22	1.50	1.53
27	b	604	F6C	C1C-CHC	2.22	1.47	1.41
20	C	507	CLA	C4C-C3C	2.22	1.48	1.45
20	C	502	CLA	C4B-CHC	2.22	1.47	1.41
20	c	502	CLA	C4B-CHC	2.22	1.47	1.41
20	A	404	CLA	C4C-C3C	2.22	1.48	1.45
20	C	505	CLA	C1B-CHB	2.22	1.47	1.41
20	H	101	CLA	C4B-CHC	2.22	1.47	1.41
20	h	101	CLA	C4B-CHC	2.22	1.47	1.41
20	A	405	CLA	C1B-CHB	2.22	1.47	1.41
27	C	508	F6C	C1A-C2A	2.22	1.50	1.45
33	M	102	LMT	O4'-C4B	-2.21	1.37	1.43
20	b	615	CLA	C4B-CHC	2.21	1.47	1.41
27	B	604	F6C	C4C-CHD	2.21	1.47	1.41
21	A	406	PHO	CMC-C2C	-2.21	1.46	1.51
20	C	513	CLA	C4B-CHC	2.21	1.47	1.41
27	b	604	F6C	C4C-CHD	2.21	1.47	1.41
20	B	612	CLA	C1B-NB	-2.21	1.33	1.35
32	H	102	RRX	C19-C18	-2.21	1.41	1.45
20	a	407	CLA	C4C-C3C	2.21	1.48	1.45
20	a	405	CLA	C1B-CHB	2.21	1.47	1.41
20	c	511	CLA	C4B-CHC	2.21	1.47	1.41
20	B	602	CLA	MG-ND	-2.21	2.01	2.05
20	C	506	CLA	C4B-CHC	2.20	1.47	1.41
20	C	505	CLA	C1B-NB	-2.20	1.33	1.35
20	B	615	CLA	C4B-CHC	2.20	1.47	1.41
26	A	412	LHG	O7-C5	-2.20	1.41	1.46
20	a	404	CLA	C4C-C3C	2.20	1.48	1.45
32	h	102	RRX	C19-C18	-2.20	1.41	1.45
20	c	513	CLA	C4B-CHC	2.20	1.47	1.41
26	a	412	LHG	O7-C5	-2.20	1.41	1.46
32	h	102	RRX	C12-C13	-2.20	1.41	1.45
20	C	512	CLA	MG-NC	2.19	2.11	2.06
20	c	507	CLA	C4C-C3C	2.19	1.48	1.45
22	B	618	BCR	C21-C22	-2.19	1.32	1.35
27	B	613	F6C	C4D-CHA	2.19	1.48	1.42
27	b	607	F6C	C1D-ND	-2.19	1.34	1.37
20	c	512	CLA	MG-NC	2.19	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	613	F6C	C4C-CHD	2.18	1.47	1.41
20	c	506	CLA	C4B-CHC	2.18	1.47	1.41
20	b	612	CLA	C1B-NB	-2.18	1.33	1.35
27	b	613	F6C	C4D-CHA	2.18	1.48	1.42
23	a	409	SQD	O8-S	2.18	1.55	1.47
27	B	613	F6C	C2B-C1B	2.18	1.49	1.44
20	D	403	CLA	C3A-C2A	-2.17	1.48	1.54
20	c	505	CLA	C1B-NB	-2.17	1.33	1.35
20	c	505	CLA	C1D-C2D	2.17	1.49	1.45
20	d	403	CLA	C3A-C2A	-2.17	1.48	1.54
27	b	613	F6C	C4C-CHD	2.17	1.47	1.41
21	d	402	PHO	C1C-NC	-2.17	1.31	1.38
32	H	102	RRX	C12-C13	-2.17	1.41	1.45
22	b	618	BCR	C21-C22	-2.16	1.32	1.35
27	b	613	F6C	C2B-C1B	2.16	1.49	1.44
28	D	410	DGD	O2D-C2D	-2.16	1.37	1.43
28	d	410	DGD	O2D-C2D	-2.16	1.37	1.43
23	A	409	SQD	O8-S	2.16	1.55	1.47
20	C	505	CLA	C4B-CHC	2.16	1.47	1.41
20	B	611	CLA	CMB-C2B	-2.16	1.47	1.51
21	D	402	PHO	C1C-NC	-2.15	1.31	1.38
20	C	505	CLA	C1D-C2D	2.15	1.49	1.45
20	D	403	CLA	MG-NC	2.15	2.11	2.06
20	c	505	CLA	C4B-CHC	2.15	1.47	1.41
20	d	403	CLA	C2A-C1A	-2.15	1.47	1.52
20	c	507	CLA	C4B-CHC	2.14	1.47	1.41
23	l	102	SQD	O4-C4	-2.14	1.37	1.43
20	b	611	CLA	CMB-C2B	-2.14	1.47	1.51
23	L	102	SQD	O4-C4	-2.14	1.37	1.43
20	C	507	CLA	C4B-CHC	2.14	1.46	1.41
21	a	406	PHO	CBD-CGD	-2.14	1.49	1.52
20	D	403	CLA	C2A-C1A	-2.13	1.47	1.52
20	b	609	CLA	C4B-NB	-2.13	1.33	1.35
20	b	608	CLA	C4B-CHC	2.13	1.46	1.41
27	C	508	F6C	MG-ND	-2.13	2.01	2.06
21	A	406	PHO	CBD-CGD	-2.13	1.49	1.52
31	V	201	HEM	CMD-C2D	2.12	1.55	1.50
20	d	403	CLA	MG-NC	2.12	2.11	2.06
20	H	101	CLA	C1B-CHB	2.12	1.46	1.41
31	v	201	HEM	CMD-C2D	2.12	1.55	1.50
27	c	508	F6C	MG-ND	-2.11	2.01	2.06
20	b	614	CLA	C4B-CHC	2.11	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	101	CLA	C1B-CHB	2.11	1.46	1.41
28	C	516	DGD	O4E-C4E	-2.11	1.38	1.43
20	B	608	CLA	C4B-CHC	2.11	1.46	1.41
20	C	504	CLA	C1D-C2D	2.11	1.49	1.45
28	c	517	DGD	O2G-C2G	-2.11	1.41	1.46
27	b	607	F6C	MG-ND	-2.11	2.01	2.06
20	B	614	CLA	C4B-CHC	2.10	1.46	1.41
28	c	516	DGD	O4E-C4E	-2.10	1.38	1.43
28	C	517	DGD	O2G-C2G	-2.10	1.41	1.46
20	A	405	CLA	C4B-CHC	2.10	1.46	1.41
20	a	405	CLA	C4B-CHC	2.10	1.46	1.41
20	d	403	CLA	C4D-CHA	2.10	1.45	1.38
20	c	504	CLA	C1D-C2D	2.09	1.49	1.45
20	B	609	CLA	C4B-NB	-2.09	1.33	1.35
20	D	403	CLA	C1B-NB	-2.09	1.33	1.35
26	a	412	LHG	O8-C6	-2.09	1.40	1.45
20	B	614	CLA	C1B-CHB	2.09	1.46	1.41
20	b	611	CLA	C1B-CHB	2.09	1.46	1.41
20	B	611	CLA	C1A-CHA	2.09	1.51	1.43
20	b	602	CLA	C1C-C2C	2.09	1.48	1.44
20	b	608	CLA	C1A-CHA	2.09	1.51	1.43
28	c	516	DGD	O6D-C5D	-2.09	1.39	1.44
23	l	102	SQD	O3-C3	-2.09	1.38	1.43
27	C	508	F6C	C4B-NB	-2.08	1.34	1.37
27	b	607	F6C	C4B-NB	-2.08	1.34	1.37
23	L	102	SQD	O48-C46	-2.08	1.40	1.45
20	b	611	CLA	C1A-CHA	2.08	1.51	1.43
27	B	607	F6C	MG-ND	-2.08	2.01	2.06
27	b	604	F6C	C4B-NB	-2.08	1.34	1.37
20	D	403	CLA	C4D-CHA	2.08	1.45	1.38
20	c	507	CLA	C1D-C2D	2.08	1.49	1.45
24	d	406	PL9	C5-C4	-2.08	1.39	1.47
20	c	503	CLA	C4B-NB	-2.08	1.33	1.35
20	b	614	CLA	C1B-CHB	2.08	1.46	1.41
27	B	604	F6C	C4B-NB	-2.08	1.34	1.37
20	B	611	CLA	C1B-CHB	2.08	1.46	1.41
27	b	607	F6C	C4D-CHA	2.08	1.47	1.42
28	C	516	DGD	O6D-C5D	-2.07	1.39	1.44
20	B	608	CLA	C1A-CHA	2.07	1.51	1.43
20	C	503	CLA	C4B-NB	-2.07	1.33	1.35
27	b	604	F6C	CMB-C2B	2.07	1.49	1.45
27	B	607	F6C	C4B-NB	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	406	PL9	C5-C4	-2.07	1.39	1.47
27	B	607	F6C	C4D-CHA	2.07	1.47	1.42
23	l	102	SQD	O48-C46	-2.07	1.40	1.45
27	c	508	F6C	C4B-NB	-2.06	1.34	1.37
20	C	502	CLA	C1D-C2D	2.06	1.49	1.45
20	d	403	CLA	C1B-NB	-2.06	1.33	1.35
23	L	102	SQD	O3-C3	-2.06	1.38	1.43
26	A	412	LHG	O8-C6	-2.06	1.40	1.45
20	c	505	CLA	C1A-CHA	2.06	1.51	1.43
20	B	602	CLA	C1C-C2C	2.06	1.48	1.44
20	C	509	CLA	MG-NC	2.06	2.11	2.06
31	V	201	HEM	CMB-C2B	2.06	1.55	1.50
21	D	402	PHO	CMC-C2C	-2.06	1.46	1.51
21	d	402	PHO	CMC-C2C	-2.06	1.46	1.51
31	v	201	HEM	CMB-C2B	2.06	1.55	1.50
20	C	505	CLA	C1A-CHA	2.05	1.51	1.43
20	B	603	CLA	C1C-C2C	2.05	1.48	1.44
27	B	613	F6C	C1A-C2A	2.05	1.50	1.45
27	b	613	F6C	C1A-C2A	2.05	1.50	1.45
27	B	604	F6C	CMB-C2B	2.05	1.49	1.45
20	c	502	CLA	C1D-C2D	2.05	1.49	1.45
20	C	507	CLA	C1D-C2D	2.04	1.49	1.45
27	C	508	F6C	C4D-CHA	2.04	1.47	1.42
33	m	102	LMT	O5'-C5'	-2.04	1.39	1.44
33	M	102	LMT	O5'-C5'	-2.04	1.39	1.44
20	B	615	CLA	MG-NC	2.03	2.11	2.06
20	c	509	CLA	MG-NC	2.03	2.11	2.06
20	c	507	CLA	C1B-CHB	2.03	1.46	1.41
20	C	504	CLA	C1B-CHB	2.03	1.46	1.41
20	b	603	CLA	C1C-C2C	2.03	1.48	1.44
20	b	606	CLA	C1C-C2C	2.03	1.48	1.44
20	b	615	CLA	MG-NC	2.02	2.11	2.06
30	m	101	LMG	C19-C18	-2.02	1.33	1.49
20	C	506	CLA	C1B-CHB	2.02	1.46	1.41
26	D	407	LHG	O7-C5	-2.02	1.41	1.46
30	M	101	LMG	C19-C18	-2.02	1.33	1.49
20	C	507	CLA	C1B-CHB	2.01	1.46	1.41
20	c	506	CLA	C1B-CHB	2.01	1.46	1.41
27	c	508	F6C	C4D-CHA	2.01	1.47	1.42
24	A	410	PL9	C11-C9	-2.01	1.47	1.51
20	B	608	CLA	C1B-CHB	2.00	1.46	1.41
20	c	504	CLA	C1B-CHB	2.00	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	606	CLA	C1C-C2C	2.00	1.48	1.44
26	d	407	LHG	O7-C5	-2.00	1.41	1.46

All (2189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	BCR	C16-C17-C18	23.20	160.41	127.31
22	B	618	BCR	C16-C17-C18	23.19	160.40	127.31
22	c	518	BCR	C11-C10-C9	22.88	159.97	127.31
22	C	518	BCR	C11-C10-C9	22.84	159.91	127.31
22	C	515	BCR	C16-C17-C18	22.16	158.94	127.31
22	c	515	BCR	C16-C17-C18	22.16	158.94	127.31
22	D	405	BCR	C16-C17-C18	21.92	158.59	127.31
22	d	405	BCR	C16-C17-C18	21.91	158.58	127.31
22	B	617	BCR	C20-C21-C22	21.73	158.32	127.31
22	b	617	BCR	C20-C21-C22	21.70	158.28	127.31
22	D	405	BCR	C20-C19-C18	21.66	149.49	126.59
22	d	405	BCR	C20-C19-C18	21.63	149.46	126.59
22	c	515	BCR	C20-C21-C22	21.45	157.93	127.31
22	C	515	BCR	C20-C21-C22	21.43	157.89	127.31
22	b	618	BCR	C20-C21-C22	21.21	157.59	127.31
22	B	618	BCR	C20-C21-C22	21.20	157.57	127.31
22	a	408	BCR	C15-C16-C17	20.69	165.87	123.47
22	A	408	BCR	C15-C16-C17	20.67	165.82	123.47
22	c	515	BCR	C15-C16-C17	20.53	165.52	123.47
22	C	515	BCR	C15-C16-C17	20.52	165.51	123.47
22	B	616	BCR	C15-C16-C17	20.51	165.50	123.47
22	b	616	BCR	C15-C16-C17	20.49	165.46	123.47
22	b	617	BCR	C15-C16-C17	20.34	165.14	123.47
22	B	617	BCR	C15-C16-C17	20.33	165.12	123.47
22	A	408	BCR	C20-C21-C22	20.29	156.27	127.31
22	a	408	BCR	C20-C21-C22	20.29	156.27	127.31
22	B	616	BCR	C20-C21-C22	20.26	156.23	127.31
22	b	616	BCR	C20-C21-C22	20.25	156.22	127.31
22	B	616	BCR	C16-C17-C18	18.93	154.32	127.31
22	b	616	BCR	C16-C17-C18	18.90	154.28	127.31
22	a	408	BCR	C16-C17-C18	18.89	154.26	127.31
22	A	408	BCR	C16-C17-C18	18.85	154.22	127.31
22	d	405	BCR	C15-C16-C17	18.84	162.06	123.47
22	D	405	BCR	C15-C16-C17	18.84	162.06	123.47
22	b	617	BCR	C16-C17-C18	18.32	153.45	127.31
22	B	617	BCR	C16-C17-C18	18.29	153.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	BCR	C15-C16-C17	17.49	159.30	123.47
22	B	618	BCR	C15-C16-C17	17.46	159.25	123.47
22	a	408	BCR	C10-C11-C12	17.13	176.68	123.22
22	d	405	BCR	C10-C11-C12	17.12	176.64	123.22
22	D	405	BCR	C10-C11-C12	17.12	176.64	123.22
22	A	408	BCR	C10-C11-C12	17.12	176.63	123.22
22	B	616	BCR	C10-C11-C12	17.01	176.31	123.22
22	b	616	BCR	C10-C11-C12	17.01	176.28	123.22
22	B	617	BCR	C10-C11-C12	16.97	176.19	123.22
22	b	617	BCR	C10-C11-C12	16.97	176.17	123.22
22	c	515	BCR	C10-C11-C12	16.96	176.15	123.22
22	C	515	BCR	C10-C11-C12	16.94	176.10	123.22
22	b	618	BCR	C10-C11-C12	16.87	175.86	123.22
22	B	618	BCR	C10-C11-C12	16.87	175.85	123.22
22	b	616	BCR	C11-C10-C9	14.40	147.86	127.31
22	B	616	BCR	C11-C10-C9	14.36	147.81	127.31
22	B	618	BCR	C16-C15-C14	14.35	152.87	123.47
22	b	618	BCR	C16-C15-C14	14.33	152.82	123.47
22	B	618	BCR	C21-C20-C19	13.60	165.66	123.22
22	b	618	BCR	C21-C20-C19	13.60	165.66	123.22
22	D	405	BCR	C11-C10-C9	13.50	146.57	127.31
22	B	617	BCR	C11-C10-C9	13.48	146.55	127.31
22	d	405	BCR	C11-C10-C9	13.46	146.52	127.31
22	b	617	BCR	C11-C10-C9	13.44	146.49	127.31
22	a	408	BCR	C21-C20-C19	13.35	164.88	123.22
22	A	408	BCR	C21-C20-C19	13.35	164.87	123.22
22	B	617	BCR	C21-C20-C19	12.90	163.48	123.22
22	b	617	BCR	C21-C20-C19	12.88	163.42	123.22
22	b	616	BCR	C21-C20-C19	12.85	163.31	123.22
22	B	616	BCR	C21-C20-C19	12.84	163.29	123.22
22	B	616	BCR	C16-C15-C14	12.83	149.76	123.47
22	b	616	BCR	C16-C15-C14	12.83	149.75	123.47
22	d	405	BCR	C16-C15-C14	12.70	149.49	123.47
22	D	405	BCR	C16-C15-C14	12.69	149.47	123.47
22	b	617	BCR	C16-C15-C14	12.66	149.41	123.47
22	B	617	BCR	C16-C15-C14	12.66	149.41	123.47
22	c	518	BCR	C10-C11-C12	12.32	161.67	123.22
22	C	518	BCR	C10-C11-C12	12.32	161.66	123.22
22	c	515	BCR	C11-C10-C9	12.14	144.63	127.31
22	C	515	BCR	C11-C10-C9	12.09	144.57	127.31
22	C	515	BCR	C21-C20-C19	11.97	160.56	123.22
22	c	515	BCR	C21-C20-C19	11.96	160.54	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	515	BCR	C16-C15-C14	11.80	147.65	123.47
22	C	515	BCR	C16-C15-C14	11.80	147.64	123.47
22	a	408	BCR	C16-C15-C14	11.73	147.50	123.47
22	A	408	BCR	C16-C15-C14	11.72	147.49	123.47
22	C	515	BCR	C11-C12-C13	11.69	159.25	126.42
22	c	515	BCR	C11-C12-C13	11.69	159.25	126.42
22	B	618	BCR	C11-C10-C9	11.61	143.88	127.31
22	b	618	BCR	C11-C10-C9	11.61	143.87	127.31
22	A	408	BCR	C11-C12-C13	11.55	158.87	126.42
22	a	408	BCR	C11-C12-C13	11.55	158.86	126.42
22	a	408	BCR	C11-C10-C9	11.45	143.65	127.31
22	A	408	BCR	C11-C10-C9	11.43	143.62	127.31
22	d	405	BCR	C11-C12-C13	11.40	158.44	126.42
22	D	405	BCR	C11-C12-C13	11.38	158.40	126.42
22	B	618	BCR	C11-C12-C13	10.85	156.89	126.42
22	b	618	BCR	C11-C12-C13	10.85	156.89	126.42
27	B	604	F6C	CAA-C2A-C3A	-10.76	107.83	127.88
27	b	604	F6C	CAA-C2A-C3A	-10.76	107.83	127.88
22	B	616	BCR	C11-C12-C13	10.59	156.16	126.42
22	b	616	BCR	C11-C12-C13	10.58	156.14	126.42
27	B	613	F6C	CAA-C2A-C3A	-10.54	108.25	127.88
27	b	613	F6C	CAA-C2A-C3A	-10.52	108.28	127.88
22	b	617	BCR	C11-C12-C13	10.31	155.37	126.42
22	B	617	BCR	C11-C12-C13	10.30	155.35	126.42
27	B	604	F6C	CMD-C2D-C1D	10.29	140.71	125.04
27	b	604	F6C	CMD-C2D-C1D	10.25	140.65	125.04
29	D	401	CL7	C2C-C1C-NC	9.63	117.20	110.10
29	d	401	CL7	C2C-C1C-NC	9.61	117.18	110.10
27	b	613	F6C	C1C-C2C-C3C	-9.52	100.38	107.00
27	C	508	F6C	C1D-ND-C4D	-9.50	102.43	106.71
27	B	613	F6C	C1C-C2C-C3C	-9.50	100.39	107.00
27	c	508	F6C	C1D-ND-C4D	-9.47	102.45	106.71
27	b	607	F6C	C1D-ND-C4D	-9.45	102.46	106.71
27	B	607	F6C	C1D-ND-C4D	-9.38	102.49	106.71
20	c	511	CLA	CMD-C2D-C1D	9.34	141.18	124.71
27	b	607	F6C	CAA-C2A-C3A	-9.34	110.49	127.88
27	B	607	F6C	CAA-C2A-C3A	-9.33	110.50	127.88
20	C	511	CLA	CMD-C2D-C1D	9.32	141.13	124.71
27	c	508	F6C	CMD-C2D-C1D	9.24	139.12	125.04
27	C	508	F6C	CMD-C2D-C1D	9.21	139.06	125.04
27	b	607	F6C	CMD-C2D-C1D	9.16	138.99	125.04
27	B	607	F6C	CMD-C2D-C1D	9.15	138.98	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	613	F6C	CMD-C2D-C1D	9.07	138.85	125.04
27	B	613	F6C	CMD-C2D-C1D	9.03	138.80	125.04
27	c	508	F6C	CAA-C2A-C3A	-8.86	111.37	127.88
27	C	508	F6C	CAA-C2A-C3A	-8.86	111.39	127.88
20	a	405	CLA	CMD-C2D-C1D	8.64	139.94	124.71
20	A	405	CLA	CMD-C2D-C1D	8.63	139.92	124.71
20	D	403	CLA	C2D-C1D-ND	8.56	116.41	110.10
20	d	403	CLA	C2D-C1D-ND	8.53	116.39	110.10
20	c	507	CLA	CMD-C2D-C1D	8.30	139.35	124.71
20	B	612	CLA	C2D-C1D-ND	8.30	116.22	110.10
20	C	507	CLA	CMD-C2D-C1D	8.30	139.34	124.71
20	b	612	CLA	C2D-C1D-ND	8.29	116.21	110.10
20	B	610	CLA	CMD-C2D-C1D	8.28	139.31	124.71
20	b	610	CLA	CMD-C2D-C1D	8.28	139.31	124.71
20	b	602	CLA	CMD-C2D-C1D	8.19	139.16	124.71
20	B	602	CLA	CMD-C2D-C1D	8.19	139.15	124.71
20	B	603	CLA	CMD-C2D-C1D	8.18	139.12	124.71
20	b	603	CLA	CMD-C2D-C1D	8.18	139.12	124.71
20	C	514	CLA	CMD-C2D-C1D	8.17	139.10	124.71
20	c	514	CLA	CMD-C2D-C1D	8.16	139.10	124.71
20	b	612	CLA	C4A-NA-C1A	8.16	110.37	106.71
20	B	612	CLA	C4A-NA-C1A	8.14	110.36	106.71
20	H	101	CLA	CMD-C2D-C1D	8.13	139.03	124.71
20	a	407	CLA	CMD-C2D-C1D	8.12	139.03	124.71
20	A	407	CLA	CMD-C2D-C1D	8.12	139.02	124.71
22	b	616	BCR	C20-C19-C18	8.11	149.21	126.42
20	B	606	CLA	CMD-C2D-C1D	8.11	139.01	124.71
20	C	510	CLA	CMD-C2D-C1D	8.11	139.00	124.71
20	c	510	CLA	CMD-C2D-C1D	8.11	139.00	124.71
20	h	101	CLA	CMD-C2D-C1D	8.11	139.00	124.71
22	B	616	BCR	C20-C19-C18	8.10	149.16	126.42
20	b	606	CLA	CMD-C2D-C1D	8.10	138.98	124.71
23	l	102	SQD	O6-C1-C2	8.09	120.94	108.30
20	b	615	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	L	102	SQD	O6-C1-C2	8.07	120.90	108.30
20	B	615	CLA	C2D-C1D-ND	8.06	116.05	110.10
20	A	404	CLA	CMD-C2D-C1D	8.05	138.90	124.71
20	B	615	CLA	CMD-C2D-C1D	8.05	138.89	124.71
20	C	503	CLA	CMD-C2D-C1D	8.04	138.89	124.71
20	b	615	CLA	CMD-C2D-C1D	8.04	138.88	124.71
22	C	515	BCR	C20-C19-C18	8.04	148.99	126.42
20	a	404	CLA	CMD-C2D-C1D	8.03	138.87	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	503	CLA	CMD-C2D-C1D	8.03	138.86	124.71
22	c	515	BCR	C20-C19-C18	8.03	148.97	126.42
27	B	607	F6C	C1C-C2C-C3C	-8.02	101.41	107.00
20	c	512	CLA	C2D-C1D-ND	8.01	116.00	110.10
20	C	512	CLA	C2D-C1D-ND	8.00	116.00	110.10
27	b	607	F6C	C1C-C2C-C3C	-7.98	101.44	107.00
27	c	508	F6C	C1C-C2C-C3C	-7.96	101.46	107.00
20	b	611	CLA	CMD-C2D-C1D	7.94	138.71	124.71
20	B	611	CLA	CMD-C2D-C1D	7.94	138.71	124.71
20	c	505	CLA	CMD-C2D-C1D	7.94	138.70	124.71
27	C	508	F6C	C1C-C2C-C3C	-7.93	101.48	107.00
20	C	505	CLA	CMD-C2D-C1D	7.92	138.66	124.71
20	b	608	CLA	C2D-C1D-ND	7.83	115.88	110.10
20	C	504	CLA	CMD-C2D-C1D	7.83	138.52	124.71
20	c	504	CLA	CMD-C2D-C1D	7.83	138.52	124.71
20	C	503	CLA	C2C-C1C-NC	7.82	117.30	109.97
20	c	503	CLA	C2C-C1C-NC	7.79	117.27	109.97
22	C	518	BCR	C11-C12-C13	7.77	148.24	126.42
20	B	608	CLA	C2D-C1D-ND	7.77	115.83	110.10
22	c	518	BCR	C11-C12-C13	7.77	148.23	126.42
20	B	610	CLA	C2D-C1D-ND	7.73	115.80	110.10
20	B	609	CLA	C2D-C1D-ND	7.71	115.78	110.10
20	b	610	CLA	C2D-C1D-ND	7.70	115.78	110.10
20	b	609	CLA	C2D-C1D-ND	7.69	115.77	110.10
20	D	403	CLA	CMD-C2D-C1D	7.67	138.24	124.71
27	B	604	F6C	O2D-CGD-CBD	7.66	124.88	111.27
27	b	604	F6C	O2D-CGD-CBD	7.66	124.88	111.27
20	d	404	CLA	CMD-C2D-C1D	7.66	138.21	124.71
20	d	403	CLA	CMD-C2D-C1D	7.66	138.21	124.71
20	D	404	CLA	CMD-C2D-C1D	7.65	138.20	124.71
20	c	507	CLA	O2A-C1-C2	7.64	128.70	108.64
20	C	507	CLA	O2A-C1-C2	7.63	128.68	108.64
20	c	509	CLA	C2D-C1D-ND	7.59	115.70	110.10
20	C	512	CLA	C4A-NA-C1A	7.58	110.11	106.71
20	B	611	CLA	C4A-NA-C1A	7.58	110.11	106.71
20	c	512	CLA	C4A-NA-C1A	7.58	110.11	106.71
20	C	509	CLA	C2D-C1D-ND	7.57	115.69	110.10
20	b	611	CLA	C4A-NA-C1A	7.56	110.11	106.71
20	B	605	CLA	C2D-C1D-ND	7.56	115.67	110.10
20	B	614	CLA	CMD-C2D-C1D	7.55	138.01	124.71
27	B	613	F6C	CAA-C2A-C1A	-7.53	107.36	128.11
20	b	605	CLA	C2D-C1D-ND	7.53	115.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	614	CLA	CMD-C2D-C1D	7.53	137.98	124.71
27	b	613	F6C	CAA-C2A-C1A	-7.53	107.38	128.11
20	C	506	CLA	C4A-NA-C1A	7.49	110.07	106.71
20	c	506	CLA	C4A-NA-C1A	7.48	110.07	106.71
20	b	610	CLA	C2C-C1C-NC	7.40	116.90	109.97
20	b	601	CLA	CMD-C2D-C1D	7.40	137.75	124.71
20	B	601	CLA	CMD-C2D-C1D	7.39	137.73	124.71
20	a	405	CLA	C2C-C1C-NC	7.38	116.88	109.97
20	B	610	CLA	C2C-C1C-NC	7.35	116.86	109.97
20	A	405	CLA	C2C-C1C-NC	7.33	116.84	109.97
20	B	605	CLA	CMD-C2D-C1D	7.31	137.60	124.71
20	b	605	CLA	CMD-C2D-C1D	7.31	137.59	124.71
20	c	512	CLA	CMD-C2D-C1D	7.30	137.59	124.71
20	C	512	CLA	CMD-C2D-C1D	7.29	137.56	124.71
20	C	506	CLA	O2D-CGD-CBD	7.28	124.20	111.27
20	c	506	CLA	O2D-CGD-CBD	7.28	124.20	111.27
20	C	513	CLA	C2C-C1C-NC	7.22	116.74	109.97
20	c	513	CLA	C2C-C1C-NC	7.19	116.71	109.97
20	C	502	CLA	CMD-C2D-C1D	7.16	137.33	124.71
20	c	502	CLA	CMD-C2D-C1D	7.15	137.32	124.71
20	D	404	CLA	C2D-C1D-ND	7.09	115.33	110.10
20	d	404	CLA	C2D-C1D-ND	7.09	115.33	110.10
20	b	602	CLA	C2D-C1D-ND	7.08	115.32	110.10
20	B	602	CLA	C2D-C1D-ND	7.05	115.30	110.10
20	C	506	CLA	C2C-C1C-NC	7.03	116.56	109.97
20	c	506	CLA	C2C-C1C-NC	7.01	116.54	109.97
20	B	614	CLA	C2D-C1D-ND	7.01	115.27	110.10
20	H	101	CLA	C2D-C1D-ND	7.01	115.27	110.10
20	C	507	CLA	C2C-C1C-NC	6.99	116.52	109.97
20	b	614	CLA	C2D-C1D-ND	6.99	115.26	110.10
20	h	101	CLA	C2D-C1D-ND	6.98	115.25	110.10
22	B	618	BCR	C20-C19-C18	6.98	146.02	126.42
22	b	618	BCR	C20-C19-C18	6.97	146.01	126.42
20	c	507	CLA	C2C-C1C-NC	6.97	116.50	109.97
20	b	614	CLA	C4A-NA-C1A	6.94	109.83	106.71
20	d	403	CLA	O2A-C1-C2	6.93	126.86	108.64
20	B	609	CLA	C2C-C1C-NC	6.92	116.46	109.97
20	c	505	CLA	C2D-C1D-ND	6.92	115.20	110.10
20	D	403	CLA	O2A-C1-C2	6.92	126.82	108.64
20	b	609	CLA	C2C-C1C-NC	6.92	116.45	109.97
20	B	614	CLA	C4A-NA-C1A	6.91	109.81	106.71
20	C	505	CLA	C2D-C1D-ND	6.91	115.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	605	CLA	C2C-C1C-NC	6.90	116.44	109.97
20	b	605	CLA	C2C-C1C-NC	6.89	116.43	109.97
20	b	615	CLA	C4A-NA-C1A	6.87	109.80	106.71
20	b	605	CLA	C4A-NA-C1A	6.86	109.79	106.71
20	C	506	CLA	C2D-C1D-ND	6.85	115.16	110.10
20	B	615	CLA	C4A-NA-C1A	6.85	109.79	106.71
20	a	404	CLA	C2D-C1D-ND	6.84	115.15	110.10
20	A	407	CLA	C2D-C1D-ND	6.84	115.15	110.10
20	c	506	CLA	C2D-C1D-ND	6.84	115.14	110.10
20	A	404	CLA	C2D-C1D-ND	6.84	115.14	110.10
20	B	605	CLA	C4A-NA-C1A	6.83	109.78	106.71
20	B	601	CLA	C2D-C1D-ND	6.82	115.13	110.10
20	B	603	CLA	C2D-C1D-ND	6.82	115.13	110.10
20	b	601	CLA	C2D-C1D-ND	6.81	115.12	110.10
20	b	606	CLA	C2D-C1D-ND	6.79	115.11	110.10
20	B	606	CLA	C2D-C1D-ND	6.78	115.10	110.10
20	D	404	CLA	O2D-CGD-CBD	6.78	123.32	111.27
20	a	407	CLA	C2D-C1D-ND	6.78	115.10	110.10
20	b	603	CLA	C2D-C1D-ND	6.77	115.09	110.10
20	B	601	CLA	C2C-C1C-NC	6.76	116.31	109.97
20	b	601	CLA	C2C-C1C-NC	6.76	116.31	109.97
20	d	404	CLA	O2D-CGD-CBD	6.74	123.25	111.27
20	C	504	CLA	C2D-C1D-ND	6.71	115.05	110.10
20	c	504	CLA	C2D-C1D-ND	6.70	115.04	110.10
20	h	101	CLA	C4A-NA-C1A	6.69	109.71	106.71
20	C	513	CLA	CMD-C2D-C1D	6.68	136.48	124.71
20	c	513	CLA	CMD-C2D-C1D	6.68	136.48	124.71
29	d	401	CL7	CMD-C2D-C1D	6.66	138.70	128.46
20	b	608	CLA	C2C-C1C-NC	6.65	116.20	109.97
29	D	401	CL7	CMD-C2D-C1D	6.64	138.67	128.46
20	C	511	CLA	C2C-C1C-NC	6.64	116.19	109.97
20	B	608	CLA	C2C-C1C-NC	6.63	116.19	109.97
22	A	408	BCR	C20-C19-C18	6.62	145.01	126.42
20	C	514	CLA	C2D-C1D-ND	6.62	114.98	110.10
22	a	408	BCR	C20-C19-C18	6.62	145.00	126.42
27	C	508	F6C	CAA-C2A-C1A	-6.61	109.92	128.11
20	H	101	CLA	C4A-NA-C1A	6.61	109.68	106.71
27	c	508	F6C	CAA-C2A-C1A	-6.60	109.93	128.11
20	c	511	CLA	C2C-C1C-NC	6.60	116.16	109.97
20	C	502	CLA	C2D-C1D-ND	6.60	114.97	110.10
20	c	514	CLA	C2D-C1D-ND	6.60	114.97	110.10
27	b	613	F6C	CMA-C3A-C4A	-6.59	113.09	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	613	F6C	CMA-C3A-C4A	-6.58	113.11	124.71
20	c	502	CLA	C2D-C1D-ND	6.56	114.94	110.10
20	B	611	CLA	O2A-C1-C2	6.55	125.85	108.64
20	b	611	CLA	O2A-C1-C2	6.54	125.83	108.64
20	C	503	CLA	C4A-NA-C1A	6.54	109.65	106.71
20	B	608	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	C	518	BCR	C7-C8-C9	-6.52	116.38	126.23
20	b	608	CLA	C4A-NA-C1A	6.51	109.63	106.71
20	b	608	CLA	CMD-C2D-C1D	6.50	136.18	124.71
22	c	518	BCR	C7-C8-C9	-6.50	116.41	126.23
20	a	407	CLA	C2C-C1C-NC	6.50	116.06	109.97
20	B	606	CLA	C2C-C1C-NC	6.50	116.06	109.97
20	c	503	CLA	C4A-NA-C1A	6.49	109.63	106.71
20	a	404	CLA	C2C-C1C-NC	6.49	116.05	109.97
20	A	407	CLA	C2C-C1C-NC	6.49	116.05	109.97
20	b	606	CLA	C2C-C1C-NC	6.48	116.04	109.97
20	c	509	CLA	CMD-C2D-C1D	6.47	136.12	124.71
20	B	608	CLA	CMD-C2D-C1D	6.47	136.11	124.71
27	B	604	F6C	C3A-C4A-NA	6.47	114.87	110.10
20	C	509	CLA	CMD-C2D-C1D	6.47	136.11	124.71
27	b	604	F6C	C3A-C4A-NA	6.46	114.86	110.10
20	A	404	CLA	C2C-C1C-NC	6.44	116.00	109.97
20	c	504	CLA	C2C-C1C-NC	6.42	115.99	109.97
20	B	612	CLA	O2D-CGD-CBD	6.42	122.67	111.27
20	B	603	CLA	C2C-C1C-NC	6.41	115.97	109.97
20	C	504	CLA	C2C-C1C-NC	6.41	115.97	109.97
20	b	603	CLA	C2C-C1C-NC	6.40	115.97	109.97
20	b	612	CLA	O2D-CGD-CBD	6.40	122.65	111.27
20	B	611	CLA	C2D-C1D-ND	6.38	114.81	110.10
20	b	615	CLA	C2C-C1C-NC	6.38	115.95	109.97
20	C	512	CLA	C2C-C1C-NC	6.37	115.94	109.97
20	a	405	CLA	C1C-C2C-C3C	-6.36	100.27	106.96
20	b	611	CLA	C2D-C1D-ND	6.36	114.79	110.10
20	B	615	CLA	C2C-C1C-NC	6.36	115.93	109.97
20	b	610	CLA	CHD-C1D-ND	-6.36	118.61	124.45
20	c	511	CLA	O2D-CGD-CBD	6.35	122.56	111.27
20	A	405	CLA	C1C-C2C-C3C	-6.34	100.29	106.96
20	C	511	CLA	O2D-CGD-CBD	6.34	122.53	111.27
20	B	610	CLA	O2D-CGD-CBD	6.34	122.53	111.27
20	C	513	CLA	C2D-C1D-ND	6.34	114.77	110.10
20	b	610	CLA	O2D-CGD-CBD	6.33	122.52	111.27
20	B	610	CLA	CHD-C1D-ND	-6.33	118.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	512	CLA	C2C-C1C-NC	6.32	115.89	109.97
20	d	403	CLA	C1D-ND-C4D	-6.32	101.85	106.33
20	D	403	CLA	C1D-ND-C4D	-6.31	101.85	106.33
20	c	513	CLA	C2D-C1D-ND	6.31	114.75	110.10
20	b	601	CLA	O2D-CGD-CBD	6.31	122.47	111.27
22	B	617	BCR	C20-C19-C18	6.30	144.11	126.42
20	D	403	CLA	C4A-NA-C1A	6.30	109.54	106.71
20	d	403	CLA	C4A-NA-C1A	6.29	109.53	106.71
20	B	601	CLA	O2D-CGD-CBD	6.29	122.44	111.27
20	D	403	CLA	CHD-C1D-ND	-6.29	118.67	124.45
22	b	617	BCR	C20-C19-C18	6.28	144.07	126.42
27	B	604	F6C	C1D-ND-C4D	-6.28	103.88	106.71
20	h	101	CLA	O2D-CGD-CBD	6.26	122.39	111.27
20	d	403	CLA	CHD-C1D-ND	-6.26	118.70	124.45
27	b	604	F6C	C1D-ND-C4D	-6.25	103.89	106.71
20	a	405	CLA	C2D-C1D-ND	6.25	114.71	110.10
20	H	101	CLA	O2D-CGD-CBD	6.25	122.37	111.27
20	C	510	CLA	O2D-CGD-CBD	6.23	122.34	111.27
20	c	510	CLA	O2D-CGD-CBD	6.23	122.34	111.27
20	A	405	CLA	C2D-C1D-ND	6.22	114.69	110.10
20	B	602	CLA	C2C-C1C-NC	6.20	115.78	109.97
27	b	604	F6C	C1C-C2C-C3C	-6.20	102.69	107.00
27	B	604	F6C	C1C-C2C-C3C	-6.19	102.69	107.00
20	B	609	CLA	CMD-C2D-C1D	6.18	135.61	124.71
20	b	602	CLA	C2C-C1C-NC	6.17	115.75	109.97
20	b	609	CLA	CMD-C2D-C1D	6.16	135.56	124.71
20	C	510	CLA	O2A-CGA-O1A	-6.16	108.06	123.59
20	c	510	CLA	O2A-CGA-O1A	-6.15	108.08	123.59
20	C	505	CLA	C4A-NA-C1A	6.14	109.47	106.71
20	D	404	CLA	C2C-C1C-NC	6.14	115.72	109.97
20	C	510	CLA	C2D-C1D-ND	6.13	114.62	110.10
20	C	512	CLA	C1C-C2C-C3C	-6.13	100.52	106.96
20	c	510	CLA	C2D-C1D-ND	6.12	114.61	110.10
20	c	512	CLA	C1C-C2C-C3C	-6.12	100.52	106.96
27	b	604	F6C	C1A-C2A-C3A	-6.12	100.53	106.97
20	C	502	CLA	C2C-C1C-NC	6.12	115.70	109.97
20	c	505	CLA	C4A-NA-C1A	6.11	109.45	106.71
20	b	615	CLA	C3D-C2D-C1D	-6.10	97.50	105.83
20	C	505	CLA	C2C-C1C-NC	6.10	115.68	109.97
20	c	502	CLA	C2C-C1C-NC	6.09	115.68	109.97
20	B	615	CLA	C3D-C2D-C1D	-6.09	97.52	105.83
27	B	604	F6C	C1A-C2A-C3A	-6.09	100.56	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	404	CLA	C2C-C1C-NC	6.08	115.67	109.97
20	B	610	CLA	C1C-C2C-C3C	-6.08	100.56	106.96
20	b	610	CLA	C1C-C2C-C3C	-6.08	100.57	106.96
20	b	611	CLA	C2C-C1C-NC	6.07	115.66	109.97
20	C	507	CLA	CHD-C1D-ND	-6.07	118.88	124.45
20	B	611	CLA	C2C-C1C-NC	6.07	115.66	109.97
23	l	102	SQD	O7-S-C6	6.06	114.14	106.94
23	L	102	SQD	O7-S-C6	6.05	114.14	106.94
20	C	503	CLA	O2D-CGD-CBD	6.05	122.02	111.27
20	c	503	CLA	O2D-CGD-CBD	6.05	122.01	111.27
20	h	101	CLA	C2C-C1C-NC	6.04	115.63	109.97
20	c	505	CLA	C2C-C1C-NC	6.04	115.63	109.97
20	H	101	CLA	C2C-C1C-NC	6.02	115.61	109.97
20	c	507	CLA	CHD-C1D-ND	-6.02	118.92	124.45
27	B	607	F6C	CAA-C2A-C1A	-6.01	111.55	128.11
20	c	510	CLA	C2C-C1C-NC	6.01	115.60	109.97
27	b	607	F6C	CAA-C2A-C1A	-6.00	111.60	128.11
20	C	510	CLA	C2C-C1C-NC	5.99	115.58	109.97
20	C	511	CLA	C1C-C2C-C3C	-5.98	100.67	106.96
20	A	405	CLA	C4A-NA-C1A	5.98	109.39	106.71
20	c	511	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
20	D	403	CLA	C2C-C1C-NC	5.94	115.54	109.97
20	c	502	CLA	C4A-NA-C1A	5.94	109.38	106.71
20	B	610	CLA	C3D-C2D-C1D	-5.92	97.75	105.83
20	b	610	CLA	C3D-C2D-C1D	-5.92	97.75	105.83
20	d	403	CLA	C2C-C1C-NC	5.92	115.52	109.97
20	C	511	CLA	C4A-NA-C1A	5.91	109.36	106.71
20	C	502	CLA	CHD-C1D-ND	-5.89	119.04	124.45
20	b	609	CLA	C1C-C2C-C3C	-5.89	100.76	106.96
20	c	511	CLA	C2D-C1D-ND	5.89	114.44	110.10
20	b	615	CLA	O2D-CGD-CBD	5.87	121.70	111.27
20	c	502	CLA	CHD-C1D-ND	-5.87	119.06	124.45
20	a	405	CLA	C4A-NA-C1A	5.86	109.34	106.71
20	B	615	CLA	O2D-CGD-CBD	5.85	121.67	111.27
20	B	609	CLA	C1C-C2C-C3C	-5.85	100.80	106.96
20	C	502	CLA	C4A-NA-C1A	5.83	109.33	106.71
20	B	612	CLA	CMD-C2D-C1D	5.81	134.96	124.71
20	b	612	CLA	CMD-C2D-C1D	5.81	134.95	124.71
20	C	503	CLA	C2D-C1D-ND	5.81	114.39	110.10
20	c	503	CLA	C2D-C1D-ND	5.80	114.38	110.10
20	c	511	CLA	C4A-NA-C1A	5.80	109.31	106.71
20	C	511	CLA	C2D-C1D-ND	5.80	114.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	614	CLA	O2D-CGD-CBD	5.79	121.56	111.27
20	A	405	CLA	O2A-CGA-O1A	-5.79	108.97	123.59
22	C	515	BCR	C24-C23-C22	-5.79	117.49	126.23
20	d	403	CLA	O2A-CGA-O1A	-5.78	109.01	123.59
20	b	614	CLA	O2D-CGD-CBD	5.77	121.53	111.27
22	c	515	BCR	C24-C23-C22	-5.77	117.51	126.23
20	D	403	CLA	O2A-CGA-O1A	-5.77	109.03	123.59
20	a	405	CLA	O2A-CGA-O1A	-5.77	109.03	123.59
20	b	602	CLA	C1D-ND-C4D	-5.76	102.24	106.33
27	B	604	F6C	O2A-C1-C2	5.75	123.74	108.64
20	c	514	CLA	CHD-C1D-ND	-5.74	119.18	124.45
20	C	514	CLA	CHD-C1D-ND	-5.74	119.18	124.45
27	b	604	F6C	O2A-C1-C2	5.73	123.70	108.64
20	b	614	CLA	C2C-C1C-NC	5.73	115.34	109.97
20	B	612	CLA	C2C-C1C-NC	5.73	115.34	109.97
20	C	504	CLA	O2D-CGD-CBD	5.72	121.44	111.27
20	C	505	CLA	O2D-CGD-CBD	5.72	121.43	111.27
20	b	612	CLA	C2C-C1C-NC	5.71	115.32	109.97
20	B	608	CLA	O2D-CGD-CBD	5.71	121.41	111.27
20	c	504	CLA	O2D-CGD-CBD	5.70	121.40	111.27
20	c	505	CLA	O2D-CGD-CBD	5.70	121.39	111.27
20	b	609	CLA	O2D-CGD-CBD	5.70	121.39	111.27
20	B	609	CLA	O2D-CGD-CBD	5.70	121.39	111.27
20	B	614	CLA	C2C-C1C-NC	5.69	115.31	109.97
20	b	609	CLA	C1D-ND-C4D	-5.69	102.29	106.33
20	b	608	CLA	O2D-CGD-CBD	5.69	121.38	111.27
20	B	602	CLA	C1D-ND-C4D	-5.68	102.30	106.33
20	C	509	CLA	CMB-C2B-C3B	5.68	135.31	124.68
20	B	609	CLA	C4A-NA-C1A	5.68	109.26	106.71
20	c	509	CLA	CMB-C2B-C3B	5.66	135.27	124.68
20	B	609	CLA	C1D-ND-C4D	-5.65	102.32	106.33
20	b	615	CLA	C1C-C2C-C3C	-5.62	101.04	106.96
20	c	513	CLA	C4A-NA-C1A	5.62	109.23	106.71
20	B	615	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
20	C	513	CLA	C4A-NA-C1A	5.61	109.23	106.71
20	C	513	CLA	C1C-C2C-C3C	-5.59	101.08	106.96
20	b	614	CLA	C3D-C2D-C1D	-5.58	98.22	105.83
20	c	513	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
27	b	607	F6C	C1A-C2A-C3A	-5.57	101.11	106.97
27	B	607	F6C	C1A-C2A-C3A	-5.57	101.11	106.97
27	C	508	F6C	C2D-C1D-ND	5.56	115.18	109.97
27	c	508	F6C	C2D-C1D-ND	5.56	115.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	614	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
20	d	403	CLA	C3D-C2D-C1D	-5.55	98.25	105.83
20	C	512	CLA	O2D-CGD-CBD	5.55	121.14	111.27
20	D	403	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
20	c	512	CLA	O2D-CGD-CBD	5.53	121.10	111.27
20	c	509	CLA	C3D-C2D-C1D	-5.52	98.30	105.83
20	C	509	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
20	B	611	CLA	C3D-C2D-C1D	-5.50	98.32	105.83
20	a	404	CLA	C1D-ND-C4D	-5.50	102.42	106.33
20	B	603	CLA	C1D-ND-C4D	-5.50	102.43	106.33
20	B	610	CLA	C4A-NA-C1A	5.50	109.18	106.71
20	b	609	CLA	C4A-NA-C1A	5.50	109.18	106.71
20	b	611	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
20	b	610	CLA	C4A-NA-C1A	5.50	109.18	106.71
20	D	404	CLA	CHD-C1D-ND	-5.49	119.41	124.45
27	c	508	F6C	C1A-C2A-C3A	-5.49	101.19	106.97
20	b	603	CLA	C1D-ND-C4D	-5.49	102.44	106.33
20	c	512	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
20	C	512	CLA	C3D-C2D-C1D	-5.48	98.36	105.83
20	A	404	CLA	C1D-ND-C4D	-5.47	102.45	106.33
20	d	404	CLA	CHD-C1D-ND	-5.47	119.43	124.45
20	c	504	CLA	C1C-C2C-C3C	-5.47	101.21	106.96
20	C	504	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
27	C	508	F6C	C1A-C2A-C3A	-5.46	101.22	106.97
27	B	607	F6C	C2D-C1D-ND	5.45	115.08	109.97
27	b	607	F6C	C2D-C1D-ND	5.45	115.08	109.97
20	b	606	CLA	C1D-ND-C4D	-5.43	102.48	106.33
20	c	505	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
27	b	613	F6C	C3D-C2D-C1D	-5.42	97.98	105.83
20	A	405	CLA	O2A-C1-C2	5.41	122.86	108.64
20	c	509	CLA	O2A-CGA-O1A	-5.41	109.94	123.59
20	b	608	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
20	B	610	CLA	O2A-C1-C2	5.40	122.83	108.64
20	b	610	CLA	O2A-C1-C2	5.40	122.83	108.64
27	B	613	F6C	C3D-C2D-C1D	-5.40	98.01	105.83
20	C	509	CLA	O2A-CGA-O1A	-5.40	109.97	123.59
20	C	514	CLA	C2C-C1C-NC	5.40	115.03	109.97
20	B	605	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
20	C	505	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
20	a	405	CLA	O2A-C1-C2	5.39	122.81	108.64
20	H	101	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
20	B	608	CLA	C3D-C2D-C1D	-5.38	98.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	101	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
20	b	605	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
20	c	514	CLA	C2C-C1C-NC	5.38	115.01	109.97
20	b	609	CLA	CHD-C1D-ND	-5.37	119.52	124.45
20	B	606	CLA	C1D-ND-C4D	-5.36	102.53	106.33
20	B	609	CLA	CHD-C1D-ND	-5.36	119.53	124.45
20	c	506	CLA	O2A-CGA-O1A	-5.36	110.08	123.59
20	A	407	CLA	C1D-ND-C4D	-5.35	102.53	106.33
20	C	510	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
20	B	610	CLA	O2A-CGA-O1A	-5.35	110.10	123.59
20	b	605	CLA	O2A-C1-C2	5.34	122.68	108.64
20	B	605	CLA	O2A-C1-C2	5.34	122.68	108.64
20	C	506	CLA	O2A-CGA-O1A	-5.34	110.11	123.59
20	b	610	CLA	O2A-CGA-O1A	-5.33	110.13	123.59
20	C	507	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
20	c	506	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
20	c	507	CLA	O2D-CGD-CBD	5.33	120.74	111.27
20	C	506	CLA	C1C-C2C-C3C	-5.33	101.36	106.96
20	c	512	CLA	CHD-C1D-ND	-5.33	119.56	124.45
29	d	401	CL7	C1A-NA-C4A	5.33	109.53	106.30
20	C	507	CLA	O2D-CGD-CBD	5.32	120.72	111.27
20	a	407	CLA	C1D-ND-C4D	-5.32	102.56	106.33
20	c	510	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
20	C	504	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
20	c	507	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
20	a	407	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
20	D	403	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
20	C	512	CLA	CHD-C1D-ND	-5.31	119.58	124.45
20	c	504	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
20	a	405	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
20	a	404	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
20	d	403	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
20	A	405	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
29	D	401	CL7	C1A-NA-C4A	5.28	109.50	106.30
20	A	407	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
22	C	518	BCR	C15-C14-C13	5.27	158.10	127.65
20	b	606	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
20	B	601	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
20	D	404	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
20	d	404	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
20	C	509	CLA	C2C-C1C-NC	5.26	114.90	109.97
20	c	509	CLA	C2C-C1C-NC	5.26	114.90	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	601	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
20	B	603	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
20	c	503	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
22	c	518	BCR	C15-C14-C13	5.26	158.03	127.65
20	b	601	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
20	C	506	CLA	O2A-C1-C2	5.26	122.45	108.64
20	c	506	CLA	O2A-C1-C2	5.25	122.44	108.64
20	B	606	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
20	B	601	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
20	C	505	CLA	CHD-C1D-ND	-5.24	119.64	124.45
20	A	404	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
20	c	512	CLA	C1D-ND-C4D	-5.24	102.61	106.33
20	b	603	CLA	O2D-CGD-CBD	5.24	120.57	111.27
20	C	503	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
20	C	512	CLA	C1D-ND-C4D	-5.23	102.62	106.33
20	b	603	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
20	A	407	CLA	O2D-CGD-CBD	5.23	120.56	111.27
20	B	612	CLA	C1D-ND-C4D	-5.23	102.62	106.33
20	a	407	CLA	O2D-CGD-CBD	5.22	120.55	111.27
20	b	612	CLA	O2A-C1-C2	5.22	122.36	108.64
20	B	612	CLA	O2A-C1-C2	5.22	122.35	108.64
20	c	512	CLA	O2A-C1-C2	5.22	122.35	108.64
20	B	603	CLA	O2D-CGD-CBD	5.21	120.53	111.27
20	C	512	CLA	O2A-C1-C2	5.21	122.33	108.64
20	b	612	CLA	C1D-ND-C4D	-5.21	102.64	106.33
20	c	505	CLA	CHD-C1D-ND	-5.20	119.67	124.45
20	B	612	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
20	B	602	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
20	b	612	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
20	c	514	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
23	L	102	SQD	O47-C7-C8	5.18	122.66	111.50
20	b	615	CLA	CHD-C1D-ND	-5.18	119.69	124.45
20	C	503	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
20	b	602	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
20	c	503	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
20	B	602	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
20	B	615	CLA	CHD-C1D-ND	-5.17	119.71	124.45
23	l	102	SQD	O47-C7-C8	5.16	122.62	111.50
20	b	602	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
20	C	514	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
20	C	513	CLA	O2A-CGA-O1A	-5.15	110.45	123.30
20	c	513	CLA	O2A-CGA-O1A	-5.15	110.47	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	404	CLA	C1D-ND-C4D	-5.15	102.68	106.33
20	d	404	CLA	C1D-ND-C4D	-5.15	102.68	106.33
20	C	502	CLA	C1C-C2C-C3C	-5.15	101.55	106.96
20	c	503	CLA	O2A-C1-C2	5.14	122.13	108.64
27	B	607	F6C	O2D-CGD-CBD	5.13	120.39	111.27
20	c	502	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
27	b	607	F6C	O2D-CGD-CBD	5.13	120.39	111.27
20	A	407	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
20	c	504	CLA	O2A-CGA-O1A	-5.12	110.66	123.59
20	C	503	CLA	O2A-C1-C2	5.12	122.10	108.64
20	C	504	CLA	O2A-CGA-O1A	-5.12	110.67	123.59
27	B	613	F6C	O2A-CGA-O1A	-5.11	110.69	123.59
20	C	502	CLA	C3D-C2D-C1D	-5.10	98.86	105.83
20	a	407	CLA	C3D-C2D-C1D	-5.10	98.86	105.83
20	a	404	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
20	c	507	CLA	C4A-NA-C1A	5.10	109.00	106.71
20	A	404	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
20	c	502	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
27	b	613	F6C	O2A-CGA-O1A	-5.09	110.76	123.59
27	b	613	F6C	C2D-C1D-ND	5.07	114.72	109.97
20	B	606	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
20	c	502	CLA	O2D-CGD-CBD	5.07	120.28	111.27
27	B	613	F6C	C1A-C2A-C3A	-5.07	101.63	106.97
27	b	613	F6C	C1A-C2A-C3A	-5.07	101.63	106.97
20	A	405	CLA	CHD-C1D-ND	-5.07	119.80	124.45
20	B	603	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
20	a	405	CLA	CHD-C1D-ND	-5.06	119.81	124.45
20	B	606	CLA	O2D-CGD-CBD	5.06	120.25	111.27
20	C	504	CLA	CHD-C1D-ND	-5.06	119.81	124.45
20	c	504	CLA	CHD-C1D-ND	-5.06	119.81	124.45
20	b	606	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
20	b	609	CLA	O2A-CGA-O1A	-5.05	110.70	123.30
20	C	502	CLA	O2D-CGD-CBD	5.05	120.25	111.27
20	C	507	CLA	C4A-NA-C1A	5.05	108.98	106.71
20	B	609	CLA	O2A-CGA-O1A	-5.05	110.71	123.30
20	b	606	CLA	O2D-CGD-CBD	5.05	120.24	111.27
27	B	613	F6C	C2D-C1D-ND	5.04	114.69	109.97
20	B	615	CLA	C1D-ND-C4D	-5.03	102.76	106.33
27	b	613	F6C	C1D-ND-C4D	-5.03	104.44	106.71
20	C	505	CLA	C1C-C2C-C3C	-5.03	101.67	106.96
27	c	508	F6C	O2D-CGD-CBD	5.03	120.20	111.27
27	B	613	F6C	C1D-ND-C4D	-5.02	104.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	603	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
20	A	407	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	C	508	F6C	O2D-CGD-CBD	5.02	120.18	111.27
20	B	605	CLA	C1D-ND-C4D	-5.01	102.78	106.33
20	b	602	CLA	CHD-C1D-ND	-5.01	119.85	124.45
20	b	603	CLA	CHD-C1D-ND	-5.01	119.85	124.45
24	A	410	PL9	C7-C3-C4	5.01	120.95	116.88
20	b	615	CLA	C1D-ND-C4D	-5.00	102.78	106.33
20	c	505	CLA	O2A-CGA-O1A	-5.00	110.97	123.59
20	H	101	CLA	C1D-ND-C4D	-5.00	102.78	106.33
20	c	509	CLA	C4A-NA-C1A	5.00	108.95	106.71
20	B	602	CLA	CHD-C1D-ND	-5.00	119.86	124.45
20	B	603	CLA	CHD-C1D-ND	-5.00	119.86	124.45
20	C	505	CLA	O2A-CGA-O1A	-5.00	110.98	123.59
20	B	608	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
20	c	505	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
20	b	608	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
27	B	607	F6C	O2A-CGA-O1A	-4.99	111.00	123.59
20	a	404	CLA	CHD-C1D-ND	-4.99	119.87	124.45
20	b	606	CLA	CHD-C1D-ND	-4.98	119.87	124.45
24	a	410	PL9	C7-C3-C4	4.98	120.93	116.88
20	a	407	CLA	CHD-C1D-ND	-4.98	119.88	124.45
27	b	607	F6C	O2A-CGA-O1A	-4.98	111.03	123.59
20	A	404	CLA	CHD-C1D-ND	-4.97	119.89	124.45
20	b	605	CLA	C1D-ND-C4D	-4.96	102.81	106.33
20	h	101	CLA	C1D-ND-C4D	-4.95	102.82	106.33
27	c	508	F6C	O2A-CGA-O1A	-4.94	111.12	123.59
20	C	511	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
20	B	606	CLA	CHD-C1D-ND	-4.94	119.92	124.45
20	a	404	CLA	O2A-CGA-O1A	-4.94	111.13	123.59
27	C	508	F6C	O2A-CGA-O1A	-4.94	111.14	123.59
20	C	506	CLA	CMD-C2D-C1D	4.94	133.41	124.71
20	c	511	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
20	A	404	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
20	C	513	CLA	O2D-CGD-CBD	4.93	120.03	111.27
20	b	606	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
20	C	509	CLA	O2D-CGD-CBD	4.93	120.02	111.27
20	c	506	CLA	CMD-C2D-C1D	4.93	133.39	124.71
24	d	406	PL9	C7-C3-C4	4.92	120.88	116.88
20	C	512	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
20	c	513	CLA	O2D-CGD-CBD	4.92	120.01	111.27
20	c	509	CLA	O2D-CGD-CBD	4.92	120.01	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	603	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
20	c	512	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
20	B	603	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
20	B	606	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
20	h	101	CLA	O2A-C1-C2	4.91	121.54	108.64
20	H	101	CLA	O2A-C1-C2	4.91	121.54	108.64
20	C	509	CLA	C4A-NA-C1A	4.90	108.91	106.71
20	B	602	CLA	C4A-NA-C1A	4.90	108.91	106.71
20	b	601	CLA	O2A-CGA-O1A	-4.89	111.10	123.30
20	B	601	CLA	O2A-CGA-O1A	-4.89	111.11	123.30
20	C	511	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
20	c	502	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
20	C	502	CLA	O2A-CGA-O1A	-4.88	111.27	123.59
27	B	607	F6C	C3A-C4A-NA	4.88	113.70	110.10
27	C	508	F6C	C3A-C4A-NA	4.87	113.70	110.10
20	b	614	CLA	C1C-C2C-C3C	-4.87	101.83	106.96
20	c	511	CLA	O2A-CGA-O1A	-4.87	111.31	123.59
20	b	602	CLA	C4A-NA-C1A	4.86	108.89	106.71
20	B	614	CLA	C1C-C2C-C3C	-4.86	101.85	106.96
27	b	607	F6C	C3A-C4A-NA	4.86	113.68	110.10
24	D	406	PL9	C7-C3-C4	4.85	120.82	116.88
20	c	510	CLA	C1C-C2C-C3C	-4.84	101.86	106.96
20	a	404	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	B	602	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	A	404	CLA	O2D-CGD-CBD	4.84	119.86	111.27
20	C	510	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
20	b	602	CLA	O2D-CGD-CBD	4.83	119.86	111.27
27	c	508	F6C	C3A-C4A-NA	4.83	113.67	110.10
20	B	602	CLA	O2A-CGA-O1A	-4.83	111.40	123.59
20	b	602	CLA	O2A-CGA-O1A	-4.83	111.40	123.59
20	c	511	CLA	CHD-C1D-ND	-4.83	120.02	124.45
29	d	401	CL7	O2A-CGA-O1A	-4.83	111.41	123.59
27	b	604	F6C	O2A-CGA-O1A	-4.83	111.41	123.59
29	D	401	CL7	O2A-CGA-O1A	-4.82	111.43	123.59
27	B	604	F6C	O2A-CGA-O1A	-4.81	111.46	123.59
20	B	614	CLA	O2A-CGA-O1A	-4.81	111.46	123.59
20	d	403	CLA	CAA-C2A-C3A	-4.81	99.62	112.78
20	b	614	CLA	O2A-CGA-O1A	-4.80	111.47	123.59
27	B	613	F6C	C3A-C4A-NA	4.80	113.64	110.10
20	D	403	CLA	CAA-C2A-C3A	-4.80	99.63	112.78
27	c	508	F6C	C3D-C2D-C1D	-4.80	98.89	105.83
27	C	508	F6C	C3D-C2D-C1D	-4.79	98.89	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	612	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
20	b	612	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
20	B	602	CLA	O2A-C1-C2	4.79	121.23	108.64
27	c	508	F6C	O2A-C1-C2	4.79	121.22	108.64
20	C	511	CLA	CHD-C1D-ND	-4.78	120.06	124.45
20	b	602	CLA	O2A-C1-C2	4.78	121.19	108.64
27	C	508	F6C	O2A-C1-C2	4.77	121.18	108.64
27	b	607	F6C	O2A-C1-C2	4.77	121.18	108.64
27	B	607	F6C	O2A-C1-C2	4.77	121.17	108.64
20	B	609	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
27	b	613	F6C	C3A-C4A-NA	4.76	113.61	110.10
27	B	607	F6C	C3D-C2D-C1D	-4.76	98.94	105.83
20	h	101	CLA	O2A-CGA-O1A	-4.76	111.59	123.59
20	A	405	CLA	O2A-CGA-CBA	4.76	126.83	111.91
20	C	507	CLA	C2D-C1D-ND	4.75	113.61	110.10
20	C	514	CLA	O2D-CGD-CBD	4.75	119.71	111.27
20	a	405	CLA	O2A-CGA-CBA	4.75	126.82	111.91
20	b	610	CLA	C1D-ND-C4D	-4.75	102.96	106.33
20	H	101	CLA	O2A-CGA-O1A	-4.74	111.62	123.59
27	b	607	F6C	C3D-C2D-C1D	-4.74	98.97	105.83
20	B	610	CLA	C1D-ND-C4D	-4.74	102.97	106.33
20	c	514	CLA	O2D-CGD-CBD	4.73	119.68	111.27
20	c	507	CLA	C2D-C1D-ND	4.73	113.59	110.10
20	a	405	CLA	O2D-CGD-CBD	4.73	119.68	111.27
27	B	604	F6C	C1-C2-C3	-4.73	117.86	126.04
20	b	609	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
26	d	407	LHG	O7-C7-C8	4.72	121.68	111.50
26	D	407	LHG	O7-C7-C8	4.72	121.67	111.50
27	b	604	F6C	C1-C2-C3	-4.71	117.89	126.04
27	B	613	F6C	CMA-C3A-C2A	-4.71	113.32	126.12
20	a	407	CLA	O2A-C1-C2	4.71	121.01	108.64
20	A	407	CLA	O2A-C1-C2	4.71	121.00	108.64
20	D	404	CLA	O2A-CGA-O1A	-4.71	111.57	123.30
20	a	407	CLA	O2A-CGA-O1A	-4.71	111.72	123.59
25	a	411	BCT	O2-C-O1	4.70	131.75	119.55
20	d	404	CLA	O2A-CGA-O1A	-4.70	111.57	123.30
25	A	411	BCT	O2-C-O1	4.70	131.75	119.55
20	A	405	CLA	O2D-CGD-CBD	4.70	119.62	111.27
20	A	407	CLA	O2A-CGA-O1A	-4.70	111.73	123.59
27	b	613	F6C	CMA-C3A-C2A	-4.69	113.37	126.12
20	A	404	CLA	O2A-C1-C2	4.69	120.97	108.64
20	c	513	CLA	C3D-C2D-C1D	-4.69	99.43	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	404	CLA	O2A-C1-C2	4.69	120.97	108.64
20	c	514	CLA	C1D-ND-C4D	-4.69	103.00	106.33
20	C	514	CLA	C1D-ND-C4D	-4.69	103.00	106.33
20	C	507	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
20	C	513	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
20	c	507	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
20	D	403	CLA	O2A-CGA-CBA	4.67	126.56	111.91
20	d	403	CLA	O2A-CGA-CBA	4.67	126.56	111.91
20	C	511	CLA	O2A-C1-C2	4.67	120.90	108.64
20	c	511	CLA	O2A-C1-C2	4.67	120.90	108.64
20	c	514	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
20	C	514	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
20	D	404	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
20	C	509	CLA	CHD-C1D-ND	-4.65	120.18	124.45
20	c	509	CLA	CHD-C1D-ND	-4.64	120.19	124.45
20	B	612	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
20	B	606	CLA	O2A-C1-C2	4.63	120.80	108.64
20	c	510	CLA	CHD-C1D-ND	-4.63	120.20	124.45
20	b	606	CLA	O2A-C1-C2	4.63	120.79	108.64
20	d	404	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
20	b	612	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
22	A	408	BCR	C24-C23-C22	-4.60	119.28	126.23
20	b	611	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
22	a	408	BCR	C24-C23-C22	-4.59	119.30	126.23
20	C	514	CLA	C4A-NA-C1A	4.59	108.77	106.71
20	c	514	CLA	C4A-NA-C1A	4.59	108.77	106.71
20	C	510	CLA	CHD-C1D-ND	-4.59	120.24	124.45
20	C	514	CLA	O2A-CGA-O1A	-4.57	111.91	123.30
20	B	611	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
20	d	404	CLA	C4A-NA-C1A	4.57	108.76	106.71
20	B	603	CLA	O2A-C1-C2	4.56	120.62	108.64
20	c	507	CLA	O2A-CGA-O1A	-4.56	112.09	123.59
20	C	507	CLA	O2A-CGA-O1A	-4.56	112.09	123.59
20	b	603	CLA	O2A-C1-C2	4.55	120.59	108.64
20	c	514	CLA	O2A-CGA-O1A	-4.55	111.97	123.30
20	B	605	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	b	605	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	D	404	CLA	C4A-NA-C1A	4.53	108.74	106.71
24	A	410	PL9	C7-C3-C2	-4.53	117.34	123.30
24	a	410	PL9	C7-C3-C2	-4.53	117.34	123.30
20	D	404	CLA	O2D-CGD-O1D	-4.52	115.00	123.84
20	d	404	CLA	O2D-CGD-O1D	-4.52	115.01	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	608	CLA	CMB-C2B-C3B	4.52	133.13	124.68
20	B	608	CLA	CMB-C2B-C3B	4.51	133.11	124.68
20	H	101	CLA	CHD-C1D-ND	-4.50	120.31	124.45
20	C	507	CLA	CMB-C2B-C3B	4.49	133.09	124.68
20	c	507	CLA	CMB-C2B-C3B	4.49	133.09	124.68
22	C	515	BCR	C3-C4-C5	-4.49	106.05	114.08
20	B	614	CLA	CHD-C1D-ND	-4.49	120.33	124.45
22	c	515	BCR	C3-C4-C5	-4.49	106.06	114.08
20	C	505	CLA	C1-C2-C3	-4.49	119.49	126.75
29	D	401	CL7	C1C-C2C-C3C	-4.49	100.39	106.94
29	d	401	CL7	C1C-C2C-C3C	-4.48	100.39	106.94
20	c	505	CLA	C1-C2-C3	-4.48	119.51	126.75
20	h	101	CLA	CHD-C1D-ND	-4.47	120.35	124.45
20	C	504	CLA	O2A-C1-C2	4.46	120.37	108.64
20	b	614	CLA	CHD-C1D-ND	-4.46	120.36	124.45
29	D	401	CL7	O2D-CGD-CBD	4.46	119.19	111.27
20	B	603	CLA	C4A-NA-C1A	4.46	108.71	106.71
20	c	504	CLA	O2A-C1-C2	4.45	120.33	108.64
29	d	401	CL7	O2D-CGD-CBD	4.45	119.18	111.27
20	c	504	CLA	O2A-CGA-CBA	4.45	125.87	111.91
20	b	603	CLA	C4A-NA-C1A	4.44	108.70	106.71
20	C	504	CLA	O2A-CGA-CBA	4.44	125.84	111.91
20	C	506	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
28	c	517	DGD	O3G-C3G-C2G	-4.43	100.22	110.90
20	c	506	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
28	C	517	DGD	O3G-C3G-C2G	-4.42	100.23	110.90
27	B	613	F6C	O2D-CGD-CBD	4.42	119.12	111.27
20	D	403	CLA	CMB-C2B-C3B	4.40	132.92	124.68
27	b	613	F6C	O2D-CGD-CBD	4.40	119.09	111.27
21	A	406	PHO	CMB-C2B-C3B	4.40	132.91	124.68
21	a	406	PHO	CMB-C2B-C3B	4.39	132.90	124.68
20	c	509	CLA	O2A-C1-C2	4.39	120.17	108.64
22	b	618	BCR	C15-C14-C13	-4.39	121.04	127.31
20	d	403	CLA	CMB-C2B-C3B	4.39	132.89	124.68
26	a	412	LHG	O7-C7-C8	4.39	120.95	111.50
20	C	510	CLA	C4A-NA-C1A	4.38	108.68	106.71
22	B	618	BCR	C15-C14-C13	-4.38	121.06	127.31
20	a	404	CLA	C4A-NA-C1A	4.38	108.68	106.71
26	A	412	LHG	O7-C7-C8	4.38	120.94	111.50
20	C	509	CLA	O2A-C1-C2	4.38	120.15	108.64
20	C	506	CLA	O2D-CGD-O1D	-4.38	115.28	123.84
20	c	506	CLA	O2D-CGD-O1D	-4.38	115.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	613	F6C	C4A-NA-C1A	4.37	109.44	106.33
20	B	608	CLA	O2A-CGA-O1A	-4.37	112.57	123.59
20	b	608	CLA	O2A-CGA-O1A	-4.37	112.57	123.59
20	c	511	CLA	C1D-ND-C4D	-4.37	103.23	106.33
20	c	504	CLA	C4A-NA-C1A	4.35	108.66	106.71
20	C	513	CLA	C1D-ND-C4D	-4.35	103.25	106.33
21	d	402	PHO	CMB-C2B-C3B	4.35	132.81	124.68
20	c	510	CLA	C4A-NA-C1A	4.35	108.66	106.71
20	b	605	CLA	O2A-CGA-O1A	-4.35	112.62	123.59
20	C	505	CLA	C1D-ND-C4D	-4.34	103.25	106.33
21	D	402	PHO	CMB-C2B-C3B	4.34	132.80	124.68
20	B	605	CLA	O2A-CGA-O1A	-4.34	112.64	123.59
27	B	613	F6C	C4A-NA-C1A	4.33	109.41	106.33
20	A	404	CLA	C4A-NA-C1A	4.32	108.65	106.71
20	B	605	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
20	c	513	CLA	C1D-ND-C4D	-4.32	103.27	106.33
20	b	611	CLA	O2D-CGD-CBD	4.32	118.94	111.27
20	c	505	CLA	C1D-ND-C4D	-4.31	103.27	106.33
20	b	605	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
20	C	504	CLA	C4A-NA-C1A	4.31	108.64	106.71
20	B	611	CLA	O2D-CGD-CBD	4.30	118.92	111.27
20	B	610	CLA	CAA-C2A-C3A	-4.30	101.00	112.78
20	b	610	CLA	CAA-C2A-C3A	-4.30	101.00	112.78
20	C	512	CLA	O2A-CGA-CBA	4.26	125.28	111.91
20	c	512	CLA	O2A-CGA-CBA	4.26	125.28	111.91
20	C	511	CLA	C1D-ND-C4D	-4.26	103.31	106.33
20	B	615	CLA	O2A-CGA-O1A	-4.25	112.86	123.59
20	b	615	CLA	O2A-CGA-O1A	-4.25	112.87	123.59
30	M	101	LMG	O7-C10-C11	4.24	120.64	111.50
30	m	101	LMG	O7-C10-C11	4.24	120.64	111.50
20	B	606	CLA	C4A-NA-C1A	4.24	108.61	106.71
20	B	611	CLA	CMB-C2B-C3B	4.24	132.60	124.68
20	B	601	CLA	CHD-C1D-ND	-4.23	120.56	124.45
20	b	611	CLA	CMB-C2B-C3B	4.22	132.58	124.68
20	a	405	CLA	C1D-ND-C4D	-4.22	103.34	106.33
20	c	503	CLA	CHD-C1D-ND	-4.22	120.58	124.45
20	C	504	CLA	C1D-ND-C4D	-4.22	103.34	106.33
20	c	504	CLA	C1D-ND-C4D	-4.21	103.34	106.33
20	C	503	CLA	CHD-C1D-ND	-4.21	120.58	124.45
30	D	409	LMG	O7-C10-C11	4.21	120.57	111.50
20	c	506	CLA	O2A-CGA-CBA	4.20	125.09	111.91
20	b	601	CLA	CHD-C1D-ND	-4.20	120.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	506	CLA	O2A-CGA-CBA	4.20	125.08	111.91
28	C	516	DGD	O3G-C3G-C2G	-4.19	100.78	110.90
30	d	409	LMG	O7-C10-C11	4.19	120.53	111.50
28	c	516	DGD	O3G-C3G-C2G	-4.19	100.79	110.90
20	c	503	CLA	O2A-CGA-O1A	-4.19	113.02	123.59
20	A	405	CLA	C1D-ND-C4D	-4.18	103.36	106.33
20	C	503	CLA	O2A-CGA-O1A	-4.18	113.03	123.59
26	d	408	LHG	O7-C7-C8	4.18	120.51	111.50
22	A	408	BCR	C38-C26-C25	-4.18	119.84	124.53
20	b	606	CLA	C4A-NA-C1A	4.17	108.58	106.71
26	D	408	LHG	O7-C7-C8	4.17	120.48	111.50
25	a	411	BCT	O3-C-O1	-4.17	108.74	119.55
20	C	514	CLA	CMB-C2B-C3B	4.17	132.47	124.68
32	h	102	RRX	C37-C22-C21	-4.16	117.09	122.92
25	A	411	BCT	O3-C-O1	-4.16	108.75	119.55
20	B	611	CLA	CHD-C1D-ND	-4.16	120.63	124.45
29	D	401	CL7	O2A-CGA-CBA	4.16	124.95	111.91
29	d	401	CL7	O2A-CGA-CBA	4.16	124.95	111.91
32	H	102	RRX	C37-C22-C21	-4.15	117.11	122.92
20	B	614	CLA	C4-C3-C5	4.15	122.24	115.27
22	a	408	BCR	C38-C26-C25	-4.14	119.88	124.53
20	b	614	CLA	C4-C3-C5	4.13	122.22	115.27
20	b	611	CLA	CHD-C1D-ND	-4.13	120.66	124.45
20	c	514	CLA	CMB-C2B-C3B	4.13	132.40	124.68
22	c	518	BCR	C33-C5-C6	-4.12	119.91	124.53
32	h	102	RRX	C34-C9-C10	-4.11	117.17	122.92
20	c	506	CLA	C1D-ND-C4D	-4.10	103.42	106.33
20	C	506	CLA	C1D-ND-C4D	-4.09	103.43	106.33
20	B	605	CLA	O2A-CGA-CBA	4.09	124.76	111.91
32	H	102	RRX	C34-C9-C10	-4.09	117.19	122.92
20	b	605	CLA	O2A-CGA-CBA	4.09	124.74	111.91
20	C	502	CLA	CMB-C2B-C3B	4.09	132.33	124.68
20	H	101	CLA	OBD-CAD-C3D	-4.09	118.68	128.52
20	c	502	CLA	CMB-C2B-C3B	4.08	132.32	124.68
20	b	608	CLA	CHD-C1D-ND	-4.08	120.70	124.45
20	h	101	CLA	OBD-CAD-C3D	-4.08	118.70	128.52
27	B	604	F6C	C3D-C2D-C1D	-4.07	99.93	105.83
20	c	511	CLA	O2A-CGA-CBA	4.07	124.68	111.91
20	C	511	CLA	O2A-CGA-CBA	4.07	124.68	111.91
20	B	608	CLA	CHD-C1D-ND	-4.07	120.72	124.45
22	C	518	BCR	C33-C5-C6	-4.07	119.96	124.53
27	b	604	F6C	C3D-C2D-C1D	-4.06	99.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	615	CLA	O2A-CGA-CBA	4.04	124.58	111.91
20	b	615	CLA	O2A-CGA-CBA	4.04	124.58	111.91
20	b	612	CLA	CMB-C2B-C3B	4.03	132.21	124.68
20	B	614	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
20	D	403	CLA	O2D-CGD-CBD	4.02	118.41	111.27
22	B	616	BCR	C36-C18-C17	-4.01	117.30	122.92
20	A	407	CLA	C4A-NA-C1A	4.01	108.51	106.71
20	c	509	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
20	d	403	CLA	O2D-CGD-CBD	4.01	118.39	111.27
22	b	616	BCR	C36-C18-C17	-4.01	117.31	122.92
20	b	614	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
20	C	509	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
20	B	612	CLA	CMB-C2B-C3B	4.01	132.17	124.68
20	C	502	CLA	C1D-ND-C4D	-4.01	103.49	106.33
27	B	604	F6C	CMA-C3A-C4A	-3.99	117.69	124.71
27	b	604	F6C	CMA-C3A-C4A	-3.98	117.71	124.71
20	c	502	CLA	C1D-ND-C4D	-3.98	103.51	106.33
20	b	614	CLA	C1D-ND-C4D	-3.97	103.51	106.33
20	B	614	CLA	C1D-ND-C4D	-3.97	103.52	106.33
20	B	603	CLA	O2A-CGA-CBA	3.97	124.36	111.91
20	b	603	CLA	O2A-CGA-CBA	3.97	124.36	111.91
20	a	407	CLA	C4A-NA-C1A	3.97	108.49	106.71
20	B	612	CLA	O2A-CGA-CBA	3.97	124.35	111.91
27	B	607	F6C	O2A-CGA-CBA	3.96	124.33	111.91
20	B	611	CLA	O2A-CGA-O1A	-3.95	113.61	123.59
20	b	612	CLA	O2A-CGA-CBA	3.95	124.32	111.91
27	b	607	F6C	O2A-CGA-CBA	3.95	124.30	111.91
20	b	611	CLA	O2A-CGA-O1A	-3.94	113.65	123.59
20	c	513	CLA	O2D-CGD-O1D	-3.93	116.14	123.84
20	C	513	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
20	B	611	CLA	O2A-CGA-CBA	3.93	124.25	111.91
20	b	611	CLA	O2A-CGA-CBA	3.93	124.25	111.91
27	C	508	F6C	O2A-CGA-CBA	3.93	124.24	111.91
20	B	601	CLA	C4A-NA-C1A	3.93	108.47	106.71
27	c	508	F6C	O2A-CGA-CBA	3.93	124.23	111.91
29	D	401	CL7	O2A-C1-C2	3.93	118.95	108.64
29	d	401	CL7	O2A-C1-C2	3.92	118.93	108.64
20	b	608	CLA	C1D-ND-C4D	-3.92	103.55	106.33
22	B	617	BCR	C1-C6-C5	-3.91	117.10	122.61
27	B	604	F6C	C2D-C1D-ND	3.91	113.64	109.97
20	a	404	CLA	O2A-CGA-CBA	3.91	124.18	111.91
20	d	404	CLA	CAC-C3C-C4C	3.91	129.88	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	508	F6C	C4A-C3A-C2A	-3.91	101.23	106.94
20	A	404	CLA	O2A-CGA-CBA	3.91	124.17	111.91
29	d	401	CL7	C3A-C4A-CHB	-3.91	117.90	123.70
22	B	617	BCR	C24-C23-C22	-3.91	120.33	126.23
20	b	612	CLA	C3C-C4C-NC	3.90	114.95	110.57
20	b	601	CLA	C4A-NA-C1A	3.89	108.46	106.71
20	B	606	CLA	O2A-CGA-CBA	3.89	124.13	111.91
29	D	401	CL7	C3A-C4A-CHB	-3.89	117.92	123.70
20	b	606	CLA	O2A-CGA-CBA	3.89	124.12	111.91
27	b	604	F6C	C2D-C1D-ND	3.89	113.61	109.97
20	B	612	CLA	C3C-C4C-NC	3.89	114.93	110.57
20	c	507	CLA	CAC-C3C-C2C	3.88	134.17	127.53
20	D	404	CLA	CAC-C3C-C4C	3.88	129.85	124.81
27	c	508	F6C	C4A-C3A-C2A	-3.88	101.28	106.94
22	b	617	BCR	C1-C6-C5	-3.88	117.16	122.61
22	b	617	BCR	C24-C23-C22	-3.87	120.38	126.23
20	C	507	CLA	CAC-C3C-C2C	3.87	134.15	127.53
20	h	101	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
20	H	101	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
20	a	407	CLA	C1-C2-C3	-3.86	120.51	126.75
27	B	607	F6C	C4A-C3A-C2A	-3.85	101.32	106.94
27	b	607	F6C	C4A-C3A-C2A	-3.85	101.32	106.94
27	b	613	F6C	O2A-C1-C2	3.84	118.74	108.64
20	A	407	CLA	C1-C2-C3	-3.84	120.53	126.75
27	B	613	F6C	O2A-C1-C2	3.84	118.73	108.64
20	b	615	CLA	O2A-C1-C2	3.84	118.72	108.64
20	b	615	CLA	C4-C3-C5	3.84	121.73	115.27
20	B	615	CLA	C4-C3-C5	3.84	121.73	115.27
20	B	601	CLA	C1D-ND-C4D	-3.84	103.61	106.33
20	b	601	CLA	C1D-ND-C4D	-3.83	103.61	106.33
20	B	615	CLA	O2A-C1-C2	3.83	118.71	108.64
22	a	408	BCR	C7-C8-C9	-3.83	120.44	126.23
20	B	608	CLA	C1D-ND-C4D	-3.83	103.61	106.33
20	C	509	CLA	C1D-ND-C4D	-3.83	103.61	106.33
26	D	407	LHG	C5-O7-C7	-3.83	108.37	117.79
22	b	617	BCR	C15-C14-C13	-3.83	121.85	127.31
22	A	408	BCR	C7-C8-C9	-3.83	120.45	126.23
32	h	102	RRX	C15-C16-C17	3.82	131.29	123.47
26	d	407	LHG	C5-O7-C7	-3.82	108.39	117.79
20	c	509	CLA	C1D-ND-C4D	-3.82	103.62	106.33
20	c	506	CLA	C1-C2-C3	-3.81	119.45	126.04
32	H	102	RRX	C15-C16-C17	3.81	131.28	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	BCR	C15-C14-C13	-3.81	121.87	127.31
20	C	506	CLA	C1-C2-C3	-3.81	119.46	126.04
20	a	407	CLA	O2A-CGA-CBA	3.79	123.80	111.91
20	A	407	CLA	O2A-CGA-CBA	3.78	123.78	111.91
20	C	503	CLA	O2A-CGA-CBA	3.78	123.78	111.91
20	c	509	CLA	O2A-CGA-CBA	3.78	123.77	111.91
20	c	503	CLA	O2A-CGA-CBA	3.78	123.76	111.91
22	A	408	BCR	C33-C5-C6	-3.77	120.29	124.53
20	C	509	CLA	O2A-CGA-CBA	3.77	123.75	111.91
20	B	605	CLA	C1-C2-C3	-3.77	119.52	126.04
20	b	605	CLA	C1-C2-C3	-3.77	119.53	126.04
20	c	506	CLA	C3C-C4C-NC	3.77	114.80	110.57
22	c	515	BCR	C4-C5-C6	-3.76	117.27	122.73
22	a	408	BCR	C33-C5-C6	-3.76	120.31	124.53
20	C	506	CLA	C3C-C4C-NC	3.76	114.78	110.57
22	C	515	BCR	C4-C5-C6	-3.75	117.28	122.73
27	B	613	F6C	O2A-CGA-CBA	3.75	123.69	111.91
27	B	604	F6C	C4A-C3A-C2A	-3.75	101.47	106.94
27	b	613	F6C	O2A-CGA-CBA	3.74	123.66	111.91
32	h	102	RRX	C16-C15-C14	3.74	131.13	123.47
27	b	604	F6C	C4A-C3A-C2A	-3.73	101.50	106.94
32	H	102	RRX	C16-C15-C14	3.72	131.10	123.47
22	b	616	BCR	C7-C8-C9	-3.72	120.61	126.23
20	C	505	CLA	O2A-C1-C2	3.71	118.39	108.64
20	c	505	CLA	O2A-C1-C2	3.71	118.38	108.64
20	B	611	CLA	C1-C2-C3	-3.70	119.64	126.04
20	b	602	CLA	O2A-CGA-CBA	3.70	123.51	111.91
20	b	611	CLA	C1-C2-C3	-3.70	119.65	126.04
20	B	602	CLA	O2A-CGA-CBA	3.69	123.49	111.91
20	B	612	CLA	CHD-C1D-ND	-3.68	121.07	124.45
22	B	616	BCR	C7-C8-C9	-3.68	120.68	126.23
20	c	510	CLA	C1D-ND-C4D	-3.67	103.73	106.33
22	C	515	BCR	C38-C26-C25	-3.67	120.41	124.53
22	c	515	BCR	C38-C26-C25	-3.67	120.41	124.53
20	c	503	CLA	C1D-ND-C4D	-3.65	103.74	106.33
20	b	612	CLA	CHD-C1D-ND	-3.64	121.11	124.45
20	C	510	CLA	C1D-ND-C4D	-3.64	103.75	106.33
20	C	502	CLA	C1-C2-C3	-3.63	119.76	126.04
22	B	616	BCR	C37-C22-C21	-3.63	117.84	122.92
20	C	509	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
20	B	612	CLA	CMC-C2C-C1C	3.62	130.55	125.04
20	c	502	CLA	C1-C2-C3	-3.62	119.79	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	612	CLA	CMC-C2C-C1C	3.61	130.53	125.04
22	b	616	BCR	C37-C22-C21	-3.61	117.87	122.92
27	B	604	F6C	CMD-C2D-C3D	-3.60	119.33	127.61
22	a	408	BCR	C37-C22-C21	-3.59	117.89	122.92
20	C	503	CLA	C1D-ND-C4D	-3.59	103.78	106.33
27	B	613	F6C	C4A-C3A-C2A	-3.59	101.70	106.94
20	B	609	CLA	O2A-CGA-CBA	3.59	125.55	114.03
27	b	604	F6C	CMD-C2D-C3D	-3.58	119.37	127.61
20	d	404	CLA	CMA-C3A-C4A	3.58	121.39	111.77
20	b	609	CLA	O2A-CGA-CBA	3.58	125.52	114.03
22	A	408	BCR	C37-C22-C21	-3.57	117.92	122.92
20	D	404	CLA	CMA-C3A-C4A	3.57	121.36	111.77
27	b	613	F6C	C4A-C3A-C2A	-3.57	101.73	106.94
20	B	605	CLA	CHD-C1D-ND	-3.56	121.18	124.45
20	c	509	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
20	B	612	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
22	B	616	BCR	C1-C6-C5	-3.55	117.61	122.61
20	b	612	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
20	b	605	CLA	CHD-C1D-ND	-3.54	121.20	124.45
22	b	618	BCR	C7-C8-C9	-3.54	120.89	126.23
27	B	604	F6C	OMB-CMB-C2B	-3.53	117.71	125.69
22	b	616	BCR	C1-C6-C5	-3.52	117.65	122.61
20	D	404	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
27	b	604	F6C	OMB-CMB-C2B	-3.52	117.73	125.69
20	b	614	CLA	O2A-CGA-CBA	3.52	122.94	111.91
22	B	618	BCR	C7-C8-C9	-3.52	120.92	126.23
20	B	614	CLA	O2A-CGA-CBA	3.51	122.92	111.91
20	d	404	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
20	B	609	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
23	l	102	SQD	O9-S-O7	-3.50	101.85	113.95
20	b	609	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
23	L	102	SQD	O9-S-O7	-3.50	101.85	113.95
28	C	516	DGD	O6D-C1D-O3G	-3.49	101.71	109.97
28	c	516	DGD	O6D-C1D-O3G	-3.48	101.73	109.97
20	h	101	CLA	O2A-CGA-CBA	3.48	122.83	111.91
20	H	101	CLA	O2A-CGA-CBA	3.46	122.78	111.91
20	C	507	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
20	C	512	CLA	C1-C2-C3	-3.46	121.16	126.75
20	c	507	CLA	CAA-C2A-C3A	-3.46	103.31	112.78
20	B	601	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
20	C	505	CLA	O2A-CGA-CBA	3.45	122.75	111.91
20	c	505	CLA	O2A-CGA-CBA	3.45	122.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	512	CLA	C1-C2-C3	-3.45	121.17	126.75
20	b	601	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
31	e	101	HEM	CMC-C2C-C3C	3.43	131.10	124.68
20	c	511	CLA	CMD-C2D-C3D	-3.43	119.72	127.61
31	E	101	HEM	CMC-C2C-C3C	3.43	131.09	124.68
27	C	508	F6C	C3D-C4D-ND	3.41	115.16	110.17
27	B	604	F6C	CHB-C4A-C3A	-3.41	118.32	125.48
27	b	607	F6C	C3D-C4D-ND	3.41	115.16	110.17
20	c	505	CLA	CMB-C2B-C3B	3.41	131.06	124.68
27	b	604	F6C	CHB-C4A-C3A	-3.41	118.33	125.48
20	C	511	CLA	CMD-C2D-C3D	-3.41	119.78	127.61
27	c	508	F6C	C3D-C4D-ND	3.41	115.15	110.17
31	V	201	HEM	CBA-CAA-C2A	-3.40	106.81	112.62
32	H	102	RRX	C36-C18-C17	-3.40	118.16	122.92
27	B	607	F6C	C3D-C4D-ND	3.40	115.14	110.17
22	b	617	BCR	C33-C5-C4	3.39	120.13	113.62
27	b	604	F6C	O2A-CGA-CBA	3.39	122.55	111.91
24	d	406	PL9	C36-C34-C33	-3.39	114.26	121.12
32	H	102	RRX	C35-C13-C14	-3.39	118.18	122.92
31	v	201	HEM	CBA-CAA-C2A	-3.39	106.84	112.62
20	C	505	CLA	CMB-C2B-C3B	3.39	131.02	124.68
20	C	513	CLA	O2A-CGA-CBA	3.39	124.91	114.03
32	h	102	RRX	C35-C13-C14	-3.39	118.18	122.92
22	B	617	BCR	C33-C5-C4	3.38	120.12	113.62
23	L	102	SQD	O9-S-C6	3.38	110.96	106.94
23	l	102	SQD	O9-S-C6	3.38	110.96	106.94
20	c	510	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
20	C	505	CLA	CMA-C3A-C4A	3.37	120.84	111.77
27	B	604	F6C	O2A-CGA-CBA	3.37	122.49	111.91
20	h	101	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
20	H	101	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
20	c	513	CLA	O2A-CGA-CBA	3.37	124.86	114.03
24	D	406	PL9	C36-C34-C33	-3.37	114.30	121.12
20	B	608	CLA	O2A-CGA-CBA	3.37	122.48	111.91
26	a	412	LHG	C5-O7-C7	-3.37	109.50	117.79
20	C	507	CLA	O2A-CGA-CBA	3.37	122.47	111.91
26	A	412	LHG	C5-O7-C7	-3.37	109.50	117.79
20	C	510	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
20	c	505	CLA	CMA-C3A-C4A	3.36	120.81	111.77
22	B	616	BCR	C24-C23-C22	-3.36	121.15	126.23
20	c	507	CLA	O2A-CGA-CBA	3.36	122.45	111.91
20	b	608	CLA	O2A-CGA-CBA	3.36	122.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	h	102	RRX	C36-C18-C17	-3.35	118.22	122.92
22	b	616	BCR	C24-C23-C22	-3.35	121.17	126.23
27	b	604	F6C	C4A-NA-C1A	3.35	108.71	106.33
20	b	608	CLA	O2A-C1-C2	3.35	117.43	108.64
20	B	608	CLA	C3C-C4C-NC	3.34	114.32	110.57
20	B	608	CLA	O2A-C1-C2	3.34	117.42	108.64
29	d	401	CL7	C3C-C4C-NC	3.34	112.60	110.18
20	C	505	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
20	c	505	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
20	b	608	CLA	C3C-C4C-NC	3.33	114.30	110.57
20	b	614	CLA	CMC-C2C-C1C	3.32	130.10	125.04
27	B	604	F6C	O1D-CGD-CBD	-3.32	117.69	124.48
20	b	615	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
20	B	614	CLA	CMC-C2C-C1C	3.31	130.08	125.04
27	B	604	F6C	C4A-NA-C1A	3.31	108.69	106.33
27	b	604	F6C	O1D-CGD-CBD	-3.30	117.72	124.48
22	c	515	BCR	C34-C9-C10	-3.30	118.31	122.92
22	B	616	BCR	C23-C22-C21	3.30	124.00	118.94
27	b	604	F6C	O2D-CGD-O1D	-3.30	117.39	123.84
31	v	201	HEM	C4C-CHD-C1D	3.29	126.90	122.56
22	b	616	BCR	C23-C22-C21	3.29	123.99	118.94
28	C	517	DGD	O6D-C1D-O3G	-3.29	102.18	109.97
20	C	511	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	c	511	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
22	C	515	BCR	C34-C9-C10	-3.29	118.32	122.92
20	c	509	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
27	b	613	F6C	O2D-CGD-O1D	-3.28	117.42	123.84
28	c	517	DGD	O6D-C1D-O3G	-3.28	102.20	109.97
20	B	615	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
26	L	101	LHG	O7-C7-C8	3.28	118.57	111.50
31	V	201	HEM	C4C-CHD-C1D	3.28	126.89	122.56
27	B	613	F6C	O2D-CGD-O1D	-3.28	117.42	123.84
26	l	101	LHG	O7-C7-C8	3.28	118.57	111.50
27	B	604	F6C	O2D-CGD-O1D	-3.28	117.43	123.84
20	B	611	CLA	CAC-C3C-C4C	3.28	129.06	124.81
20	C	509	CLA	CAA-C2A-C3A	-3.27	103.81	112.78
24	D	406	PL9	C7-C8-C9	-3.27	121.34	126.79
20	B	614	CLA	O2A-C1-C2	3.27	117.23	108.64
20	b	614	CLA	O2A-C1-C2	3.27	117.23	108.64
22	b	617	BCR	C4-C5-C6	-3.27	117.98	122.73
24	d	406	PL9	C7-C8-C9	-3.27	121.35	126.79
20	C	514	CLA	CMC-C2C-C1C	3.27	130.01	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	507	CLA	C1D-ND-C4D	-3.26	104.02	106.33
22	B	617	BCR	C4-C5-C6	-3.26	117.99	122.73
26	a	412	LHG	O8-C23-C24	3.26	122.13	111.91
20	c	504	CLA	CMB-C2B-C3B	3.26	130.77	124.68
29	D	401	CL7	C3C-C4C-NC	3.26	112.54	110.18
20	c	514	CLA	CMC-C2C-C1C	3.26	130.00	125.04
26	A	412	LHG	O8-C23-C24	3.26	122.13	111.91
27	B	607	F6C	C4A-NA-C1A	3.25	108.65	106.33
20	b	611	CLA	CAC-C3C-C4C	3.25	129.03	124.81
26	D	407	LHG	O8-C23-C24	3.25	122.11	111.91
20	c	510	CLA	O2A-CGA-CBA	3.24	122.08	111.91
20	C	512	CLA	CMB-C2B-C3B	3.24	130.74	124.68
20	c	507	CLA	C1D-ND-C4D	-3.24	104.04	106.33
20	c	512	CLA	CMB-C2B-C3B	3.24	130.73	124.68
20	C	513	CLA	CMA-C3A-C4A	3.24	120.47	111.77
27	C	508	F6C	C4A-NA-C1A	3.23	108.63	106.33
27	c	508	F6C	C4A-NA-C1A	3.23	108.63	106.33
20	C	504	CLA	CMB-C2B-C3B	3.23	130.73	124.68
20	A	405	CLA	CMB-C2B-C3B	3.23	130.73	124.68
20	a	405	CLA	CMB-C2B-C3B	3.23	130.73	124.68
26	d	407	LHG	O8-C23-C24	3.23	122.05	111.91
20	C	510	CLA	O2A-CGA-CBA	3.23	122.05	111.91
20	c	513	CLA	CMA-C3A-C4A	3.23	120.46	111.77
20	b	610	CLA	O2A-CGA-CBA	3.22	122.01	111.91
20	B	610	CLA	O2A-CGA-CBA	3.22	122.00	111.91
20	c	510	CLA	CAA-CBA-CGA	3.21	122.64	113.25
27	b	607	F6C	C4A-NA-C1A	3.21	108.62	106.33
20	C	510	CLA	CAA-CBA-CGA	3.21	122.63	113.25
21	A	406	PHO	C1-C2-C3	3.20	131.58	126.04
21	a	406	PHO	C1-C2-C3	3.20	131.58	126.04
20	B	605	CLA	C3C-C4C-NC	3.20	114.16	110.57
20	B	610	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
20	b	605	CLA	C3C-C4C-NC	3.19	114.15	110.57
29	D	401	CL7	C1-O2A-CGA	3.19	124.82	116.44
20	b	615	CLA	OBD-CAD-C3D	-3.19	120.84	128.52
29	d	401	CL7	C1-O2A-CGA	3.19	124.80	116.44
20	b	610	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
20	A	404	CLA	C1-C2-C3	-3.18	120.54	126.04
20	C	507	CLA	CMC-C2C-C3C	3.18	134.74	126.12
20	c	502	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
22	A	408	BCR	C19-C18-C17	3.18	123.82	118.94
20	a	404	CLA	C1-C2-C3	-3.17	120.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	408	BCR	C19-C18-C17	3.17	123.81	118.94
20	B	615	CLA	OBD-CAD-C3D	-3.17	120.90	128.52
20	C	502	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
20	c	507	CLA	CMC-C2C-C3C	3.17	134.71	126.12
20	C	513	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	C	511	CLA	C4D-C3D-CAD	3.16	111.82	108.10
20	a	407	CLA	CMA-C3A-C4A	3.16	120.27	111.77
20	c	511	CLA	C4D-C3D-CAD	3.15	111.81	108.10
20	C	510	CLA	O2A-C1-C2	3.15	116.92	108.64
20	H	101	CLA	C1-C2-C3	-3.15	121.65	126.75
20	h	101	CLA	C4D-C3D-CAD	3.15	111.81	108.10
22	b	616	BCR	C19-C18-C17	3.15	123.78	118.94
20	h	101	CLA	C1-C2-C3	-3.15	121.65	126.75
20	A	407	CLA	CMA-C3A-C4A	3.15	120.24	111.77
22	B	616	BCR	C19-C18-C17	3.15	123.77	118.94
20	B	606	CLA	CMA-C3A-C4A	3.14	120.22	111.77
20	B	608	CLA	C4-C3-C5	3.14	120.56	115.27
20	b	606	CLA	CMA-C3A-C4A	3.14	120.22	111.77
20	c	513	CLA	CHD-C1D-ND	-3.14	121.57	124.45
20	c	510	CLA	O2A-C1-C2	3.14	116.88	108.64
20	b	608	CLA	C4-C3-C5	3.13	120.54	115.27
20	H	101	CLA	C4D-C3D-CAD	3.13	111.79	108.10
27	C	508	F6C	C1-C2-C3	-3.13	120.62	126.04
27	c	508	F6C	C1-C2-C3	-3.13	120.63	126.04
20	a	405	CLA	C1-C2-C3	-3.13	121.69	126.75
22	b	617	BCR	C19-C18-C17	3.12	123.74	118.94
27	b	613	F6C	C1-C2-C3	-3.12	120.64	126.04
22	a	408	BCR	C36-C18-C17	-3.12	118.55	122.92
22	b	617	BCR	C36-C18-C17	-3.12	118.56	122.92
22	A	408	BCR	C36-C18-C17	-3.12	118.56	122.92
32	h	102	RRX	C12-C13-C14	3.11	123.72	118.94
22	B	617	BCR	C19-C18-C17	3.11	123.72	118.94
24	D	406	PL9	C7-C3-C2	-3.10	119.22	123.30
32	H	102	RRX	C12-C13-C14	3.10	123.70	118.94
27	B	613	F6C	C1-C2-C3	-3.10	120.68	126.04
24	d	406	PL9	C7-C3-C2	-3.10	119.23	123.30
32	H	102	RRX	C19-C18-C17	3.09	123.69	118.94
20	c	510	CLA	C3C-C4C-NC	3.09	114.04	110.57
20	C	510	CLA	C3C-C4C-NC	3.09	114.04	110.57
20	b	603	CLA	C3D-C4D-ND	3.09	115.24	110.24
20	B	601	CLA	O2A-CGA-CBA	3.09	123.96	114.03
20	d	403	CLA	C3D-C4D-ND	3.09	115.24	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	405	CLA	C1-C2-C3	-3.09	121.75	126.75
22	B	617	BCR	C36-C18-C17	-3.09	118.59	122.92
27	b	613	F6C	OMB-CMB-C2B	-3.09	118.71	125.69
20	B	603	CLA	C3D-C4D-ND	3.08	115.23	110.24
27	B	613	F6C	OMB-CMB-C2B	-3.08	118.72	125.69
26	l	101	LHG	O8-C23-C24	3.08	121.57	111.91
20	b	601	CLA	O2A-CGA-CBA	3.08	123.91	114.03
32	h	102	RRX	C19-C18-C17	3.08	123.66	118.94
27	B	604	F6C	CAA-C2A-C1A	-3.07	119.64	128.11
20	B	609	CLA	C3C-C4C-NC	3.07	114.02	110.57
27	b	604	F6C	CAA-C2A-C1A	-3.07	119.65	128.11
20	D	403	CLA	C3D-C4D-ND	3.07	115.21	110.24
26	L	101	LHG	O8-C23-C24	3.07	121.55	111.91
20	b	603	CLA	CMA-C3A-C4A	3.07	120.03	111.77
20	B	603	CLA	CMA-C3A-C4A	3.06	120.01	111.77
20	b	609	CLA	C3C-C4C-NC	3.06	114.01	110.57
22	c	515	BCR	C33-C5-C4	3.06	119.50	113.62
20	b	602	CLA	C3D-C4D-ND	3.06	115.19	110.24
20	C	504	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
28	d	410	DGD	O6D-C1D-O3G	-3.06	102.73	109.97
22	C	515	BCR	C33-C5-C4	3.06	119.49	113.62
20	c	504	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
20	b	605	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
29	D	401	CL7	CMC-C2C-C3C	3.05	134.40	126.12
20	c	512	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
20	b	601	CLA	CMA-C3A-C4A	3.05	119.97	111.77
29	d	401	CL7	CMC-C2C-C3C	3.05	134.40	126.12
28	D	410	DGD	O6D-C1D-O3G	-3.05	102.76	109.97
20	C	512	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
20	C	503	CLA	C1-C2-C3	-3.04	120.78	126.04
20	b	612	CLA	C4-C3-C5	3.04	120.39	115.27
20	B	612	CLA	C4-C3-C5	3.04	120.38	115.27
20	a	404	CLA	C3D-C4D-ND	3.04	115.15	110.24
20	B	605	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
20	B	601	CLA	CMA-C3A-C4A	3.04	119.94	111.77
20	c	506	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	b	606	CLA	C1-C2-C3	-3.03	120.80	126.04
20	c	503	CLA	C1-C2-C3	-3.03	120.80	126.04
22	A	408	BCR	C34-C9-C10	-3.03	118.68	122.92
20	B	601	CLA	C3C-C4C-NC	3.03	113.97	110.57
20	C	506	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	a	408	BCR	C34-C9-C10	-3.03	118.68	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	606	CLA	C1-C2-C3	-3.03	120.81	126.04
20	B	602	CLA	C3D-C4D-ND	3.03	115.13	110.24
20	b	601	CLA	C3C-C4C-NC	3.03	113.96	110.57
31	V	201	HEM	C4D-ND-C1D	3.02	108.19	105.07
27	b	607	F6C	C1-C2-C3	-3.02	120.82	126.04
20	A	404	CLA	C3D-C4D-ND	3.02	115.12	110.24
27	B	607	F6C	C1-C2-C3	-3.01	120.83	126.04
20	A	404	CLA	CMA-C3A-C4A	3.01	119.87	111.77
20	b	603	CLA	C1-C2-C3	-3.01	120.83	126.04
20	c	511	CLA	CMB-C2B-C3B	3.01	130.30	124.68
20	a	404	CLA	CMA-C3A-C4A	3.01	119.85	111.77
20	B	603	CLA	C1-C2-C3	-3.00	120.85	126.04
20	a	407	CLA	C3D-C4D-ND	3.00	115.10	110.24
20	B	609	CLA	C3D-C4D-ND	3.00	115.08	110.24
20	C	511	CLA	CMB-C2B-C3B	3.00	130.28	124.68
20	C	510	CLA	CMC-C2C-C1C	2.99	129.60	125.04
20	B	610	CLA	CMB-C2B-C3B	2.99	130.28	124.68
20	b	609	CLA	C3D-C4D-ND	2.99	115.08	110.24
31	v	201	HEM	C4D-ND-C1D	2.99	108.16	105.07
20	b	606	CLA	C3D-C4D-ND	2.99	115.08	110.24
20	b	602	CLA	CMA-C3A-C4A	2.99	119.80	111.77
20	d	404	CLA	C3D-C4D-ND	2.99	115.07	110.24
20	D	404	CLA	C3D-C4D-ND	2.98	115.06	110.24
20	C	502	CLA	O2A-CGA-CBA	2.98	121.26	111.91
20	c	502	CLA	O2A-CGA-CBA	2.98	121.26	111.91
20	B	606	CLA	C3D-C4D-ND	2.98	115.06	110.24
20	C	506	CLA	CMC-C2C-C1C	2.98	129.58	125.04
20	b	610	CLA	CMB-C2B-C3B	2.98	130.25	124.68
20	B	602	CLA	CMA-C3A-C4A	2.98	119.77	111.77
20	c	503	CLA	CMC-C2C-C3C	2.97	134.19	126.12
20	c	510	CLA	CMC-C2C-C1C	2.97	129.57	125.04
20	A	407	CLA	C3D-C4D-ND	2.97	115.05	110.24
31	E	101	HEM	C4D-ND-C1D	2.97	108.14	105.07
27	b	607	F6C	CHA-C1A-C2A	-2.96	121.81	129.84
20	C	503	CLA	CMC-C2C-C3C	2.96	134.16	126.12
20	c	506	CLA	CMC-C2C-C1C	2.95	129.53	125.04
27	B	607	F6C	CHA-C1A-C2A	-2.95	121.84	129.84
26	d	407	LHG	O8-C23-O10	-2.94	116.16	123.59
22	b	617	BCR	C7-C8-C9	-2.94	121.79	126.23
26	D	407	LHG	O8-C23-O10	-2.94	116.17	123.59
20	B	605	CLA	CAC-C3C-C4C	2.94	128.63	124.81
20	b	605	CLA	CAC-C3C-C4C	2.94	128.63	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	611	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
22	B	617	BCR	C7-C8-C9	-2.94	121.80	126.23
20	b	605	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	B	605	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
21	A	406	PHO	O1D-CGD-CBD	2.93	129.62	124.74
22	B	616	BCR	C34-C9-C10	-2.93	118.81	122.92
22	b	616	BCR	C34-C9-C10	-2.93	118.81	122.92
20	b	608	CLA	CMC-C2C-C1C	2.93	129.50	125.04
21	a	406	PHO	O1D-CGD-CBD	2.93	129.62	124.74
21	d	402	PHO	O2D-CGD-O1D	-2.93	118.11	123.84
31	e	101	HEM	C4D-ND-C1D	2.93	108.10	105.07
22	D	405	BCR	C34-C9-C10	-2.93	118.82	122.92
20	B	608	CLA	CMC-C2C-C1C	2.93	129.50	125.04
20	C	504	CLA	CAA-CBA-CGA	-2.92	104.71	113.25
20	B	608	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	c	504	CLA	CAA-CBA-CGA	-2.92	104.72	113.25
20	b	611	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
30	M	101	LMG	O1-C1-C2	2.92	112.86	108.30
21	d	402	PHO	O1D-CGD-CBD	2.92	129.60	124.74
22	C	515	BCR	C35-C13-C12	2.92	122.67	118.08
20	C	513	CLA	C3C-C4C-NC	2.91	113.84	110.57
21	D	402	PHO	O2D-CGD-O1D	-2.91	118.14	123.84
22	d	405	BCR	C34-C9-C10	-2.91	118.84	122.92
20	D	404	CLA	O2A-CGA-CBA	2.91	123.39	114.03
20	d	404	CLA	O2A-CGA-CBA	2.91	123.38	114.03
22	c	515	BCR	C35-C13-C12	2.91	122.66	118.08
30	M	101	LMG	O8-C28-C29	2.90	121.02	111.91
20	c	513	CLA	C3C-C4C-NC	2.90	113.83	110.57
27	c	508	F6C	CHA-C1A-C2A	-2.90	121.97	129.84
21	D	402	PHO	O1D-CGD-CBD	2.90	129.57	124.74
30	m	101	LMG	O1-C1-C2	2.90	112.83	108.30
20	b	608	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
27	C	508	F6C	CHA-C1A-C2A	-2.90	121.98	129.84
20	b	614	CLA	C3C-C4C-NC	2.90	113.82	110.57
30	m	101	LMG	O8-C28-C29	2.90	121.00	111.91
20	C	514	CLA	CAA-CBA-CGA	-2.90	104.82	112.51
20	H	101	CLA	C3C-C4C-NC	2.90	113.82	110.57
20	h	101	CLA	C3C-C4C-NC	2.90	113.82	110.57
24	d	406	PL9	C22-C23-C24	-2.89	120.69	127.66
20	C	512	CLA	CMC-C2C-C1C	2.89	129.44	125.04
20	c	514	CLA	CAA-CBA-CGA	-2.89	104.83	112.51
20	B	614	CLA	C3C-C4C-NC	2.89	113.81	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	406	PL9	C22-C23-C24	-2.89	120.71	127.66
21	a	406	PHO	O2D-CGD-O1D	-2.88	118.20	123.84
20	c	512	CLA	CMC-C2C-C1C	2.88	129.43	125.04
31	v	201	HEM	CBD-CAD-C3D	-2.88	104.63	112.63
31	V	201	HEM	CBD-CAD-C3D	-2.87	104.65	112.63
20	b	611	CLA	C4D-C3D-CAD	2.87	111.48	108.10
21	A	406	PHO	O2D-CGD-O1D	-2.87	118.23	123.84
20	B	611	CLA	C4D-C3D-CAD	2.87	111.47	108.10
27	B	607	F6C	CHD-C1D-ND	-2.86	119.86	124.20
20	C	509	CLA	OBD-CAD-C3D	-2.86	121.63	128.52
27	b	607	F6C	CHD-C1D-ND	-2.86	119.87	124.20
20	B	609	CLA	CMC-C2C-C1C	2.85	129.38	125.04
20	b	609	CLA	CMC-C2C-C1C	2.85	129.38	125.04
20	c	509	CLA	OBD-CAD-C3D	-2.84	121.69	128.52
22	c	518	BCR	C34-C9-C10	-2.84	118.95	122.92
20	a	404	CLA	C4-C3-C5	2.83	120.04	115.27
20	b	611	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
20	B	605	CLA	C4D-C3D-CAD	2.83	111.43	108.10
27	C	508	F6C	CHD-C1D-ND	-2.82	119.92	124.20
20	A	404	CLA	C4-C3-C5	2.82	120.02	115.27
20	B	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
20	b	605	CLA	C4D-C3D-CAD	2.82	111.42	108.10
20	B	606	CLA	C4-C3-C5	2.81	120.00	115.27
20	a	404	CLA	CMC-C2C-C1C	2.81	129.32	125.04
22	C	518	BCR	C34-C9-C10	-2.81	118.99	122.92
20	b	612	CLA	C1-C2-C3	-2.81	121.19	126.04
20	B	603	CLA	CMC-C2C-C1C	2.81	129.31	125.04
20	b	606	CLA	C4-C3-C5	2.81	119.99	115.27
27	c	508	F6C	CHD-C1D-ND	-2.81	119.94	124.20
24	d	406	PL9	C20-C19-C21	2.81	119.99	115.27
20	B	612	CLA	C1-C2-C3	-2.80	121.19	126.04
24	D	406	PL9	C20-C19-C21	2.80	119.98	115.27
20	b	603	CLA	C4-C3-C5	2.80	119.98	115.27
20	a	405	CLA	C1-O2A-CGA	2.80	123.79	116.44
20	b	603	CLA	CMC-C2C-C1C	2.80	129.30	125.04
27	c	508	F6C	C4-C3-C5	2.80	119.98	115.27
20	b	606	CLA	CMC-C2C-C1C	2.80	129.30	125.04
20	B	606	CLA	CMC-C2C-C1C	2.80	129.30	125.04
20	c	503	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
20	C	503	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
20	b	602	CLA	C1-C2-C3	-2.79	121.22	126.04
20	c	507	CLA	CMD-C2D-C3D	-2.79	121.20	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	603	CLA	C4-C3-C5	2.79	119.96	115.27
20	c	509	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
20	A	405	CLA	C1-O2A-CGA	2.79	123.76	116.44
20	C	510	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
20	C	512	CLA	C1-O2A-CGA	2.78	123.75	116.44
20	c	510	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
20	C	507	CLA	CMD-C2D-C3D	-2.78	121.22	127.61
27	C	508	F6C	C4-C3-C5	2.78	119.94	115.27
20	B	602	CLA	C4-C3-C5	2.78	119.94	115.27
20	B	602	CLA	C1-C2-C3	-2.78	121.24	126.04
24	A	410	PL9	O2-C1-C6	2.77	125.39	120.59
20	A	404	CLA	CMC-C2C-C1C	2.77	129.26	125.04
20	c	512	CLA	C1-O2A-CGA	2.77	123.72	116.44
24	a	410	PL9	O2-C1-C6	2.77	125.38	120.59
20	b	602	CLA	C4-C3-C5	2.77	119.92	115.27
20	C	512	CLA	CBC-CAC-C3C	-2.77	104.81	112.43
20	c	504	CLA	CMC-C2C-C1C	2.76	129.25	125.04
20	c	512	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
22	b	616	BCR	C30-C25-C24	2.76	123.59	115.78
22	B	616	BCR	C30-C25-C24	2.76	123.59	115.78
20	B	610	CLA	CMA-C3A-C4A	2.76	119.19	111.77
22	C	515	BCR	C29-C30-C25	-2.76	106.24	110.48
20	C	509	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
20	a	407	CLA	CMC-C2C-C1C	2.75	129.23	125.04
20	b	610	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	A	406	PHO	CMC-C2C-C3C	2.75	130.13	124.94
20	C	504	CLA	CMC-C2C-C1C	2.75	129.23	125.04
20	C	503	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
21	a	406	PHO	CMC-C2C-C3C	2.75	130.12	124.94
27	b	607	F6C	C4-C3-C5	2.74	119.89	115.27
22	c	515	BCR	C29-C30-C25	-2.74	106.26	110.48
27	B	607	F6C	C4-C3-C5	2.73	119.86	115.27
20	A	407	CLA	CMC-C2C-C1C	2.73	129.20	125.04
20	C	504	CLA	CMA-C3A-C4A	2.73	119.11	111.77
20	c	503	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
30	M	101	LMG	C7-O1-C1	-2.72	108.42	113.74
20	c	502	CLA	C3D-C4D-ND	2.72	114.64	110.24
20	c	504	CLA	CMA-C3A-C4A	2.72	119.08	111.77
20	B	611	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	C	515	BCR	C7-C8-C9	-2.72	122.13	126.23
20	D	403	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
20	C	502	CLA	C3D-C4D-ND	2.72	114.63	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	516	DGD	C1E-O6E-C5E	2.71	119.02	113.69
20	B	605	CLA	CED-O2D-CGD	2.71	122.07	115.94
20	b	605	CLA	CED-O2D-CGD	2.71	122.07	115.94
30	m	101	LMG	C7-O1-C1	-2.71	108.44	113.74
28	C	516	DGD	C1E-O6E-C5E	2.71	119.01	113.69
20	C	504	CLA	C3C-C4C-NC	2.71	113.61	110.57
20	c	509	CLA	C4-C3-C5	2.71	119.83	115.27
20	d	403	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
20	C	514	CLA	O2A-CGA-CBA	2.71	122.72	114.03
22	c	515	BCR	C7-C8-C9	-2.70	122.15	126.23
20	c	514	CLA	O2A-CGA-CBA	2.70	122.71	114.03
20	H	101	CLA	CAC-C3C-C4C	2.70	128.32	124.81
20	h	101	CLA	CAC-C3C-C4C	2.70	128.32	124.81
20	c	504	CLA	C3C-C4C-NC	2.70	113.60	110.57
20	C	503	CLA	C3B-C4B-NB	2.70	112.70	109.21
20	C	502	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
20	c	514	CLA	C3D-C4D-ND	2.70	114.60	110.24
27	B	613	F6C	CHD-C1D-ND	-2.69	120.12	124.20
20	c	507	CLA	C3C-C4C-NC	2.69	113.59	110.57
22	b	617	BCR	C38-C26-C25	-2.69	121.50	124.53
20	c	510	CLA	C6-C5-C3	-2.69	106.40	113.45
20	c	502	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
27	b	613	F6C	CHD-C1D-ND	-2.69	120.12	124.20
20	C	507	CLA	C3C-C4C-NC	2.69	113.58	110.57
20	C	509	CLA	C4-C3-C5	2.69	119.79	115.27
20	C	514	CLA	C3D-C4D-ND	2.69	114.58	110.24
20	c	503	CLA	C3B-C4B-NB	2.68	112.68	109.21
20	c	514	CLA	C4D-C3D-CAD	2.68	111.25	108.10
20	A	405	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
20	c	513	CLA	CMB-C2B-C3B	2.68	129.69	124.68
20	C	510	CLA	C6-C5-C3	-2.68	106.43	113.45
22	B	617	BCR	C38-C26-C25	-2.68	121.52	124.53
20	b	611	CLA	C1D-ND-C4D	-2.68	104.43	106.33
20	D	403	CLA	CAA-C2A-C1A	-2.68	103.21	111.97
20	a	405	CLA	CMD-C2D-C3D	-2.67	121.46	127.61
20	C	513	CLA	CMB-C2B-C3B	2.67	129.67	124.68
20	d	403	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
20	C	514	CLA	C4D-C3D-CAD	2.67	111.24	108.10
27	b	607	F6C	CMA-C3A-C4A	-2.66	120.03	124.71
20	b	610	CLA	C4-C3-C5	2.66	119.74	115.27
20	B	610	CLA	C4-C3-C5	2.66	119.74	115.27
20	B	601	CLA	CMC-C2C-C1C	2.66	129.08	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	BCR	C24-C23-C22	-2.66	122.22	126.23
20	C	512	CLA	CMA-C3A-C4A	2.65	118.90	111.77
20	c	512	CLA	CMA-C3A-C4A	2.65	118.90	111.77
20	b	601	CLA	CMC-C2C-C1C	2.65	129.07	125.04
20	d	403	CLA	C4-C3-C5	2.65	119.72	115.27
22	B	618	BCR	C24-C23-C22	-2.64	122.24	126.23
27	B	607	F6C	CMA-C3A-C4A	-2.64	120.06	124.71
22	B	616	BCR	C3-C4-C5	-2.64	109.36	114.08
22	b	616	BCR	C3-C4-C5	-2.64	109.36	114.08
20	C	503	CLA	C3C-C4C-NC	2.64	113.53	110.57
27	B	613	F6C	CHB-C4A-C3A	-2.64	119.94	125.48
20	c	510	CLA	C1-C2-C3	-2.64	121.48	126.04
20	D	404	CLA	CMC-C2C-C1C	2.64	129.05	125.04
20	c	509	CLA	CAC-C3C-C4C	2.63	128.23	124.81
20	D	403	CLA	C4-C3-C5	2.63	119.69	115.27
20	C	509	CLA	CAC-C3C-C4C	2.63	128.22	124.81
22	b	617	BCR	C28-C27-C26	-2.62	109.39	114.08
20	c	503	CLA	C3C-C4C-NC	2.62	113.51	110.57
20	b	610	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
20	A	404	CLA	C3C-C4C-NC	2.62	113.51	110.57
20	c	506	CLA	CMB-C2B-C3B	2.62	129.58	124.68
20	C	510	CLA	C1-C2-C3	-2.62	121.51	126.04
20	c	512	CLA	C3D-C4D-ND	2.62	114.47	110.24
20	C	512	CLA	C3D-C4D-ND	2.62	114.47	110.24
20	B	610	CLA	CHC-C1C-C2C	-2.62	119.49	126.72
27	b	613	F6C	CHB-C4A-C3A	-2.61	120.00	125.48
20	b	611	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
20	c	507	CLA	C3D-C4D-ND	2.61	114.46	110.24
22	B	617	BCR	C28-C27-C26	-2.61	109.42	114.08
20	B	611	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
22	A	408	BCR	C33-C5-C4	2.61	118.62	113.62
20	C	506	CLA	CMB-C2B-C3B	2.61	129.56	124.68
20	C	507	CLA	C3D-C4D-ND	2.60	114.45	110.24
20	C	504	CLA	C1-C2-C3	-2.60	121.54	126.04
20	a	404	CLA	CMB-C2B-C3B	2.60	129.55	124.68
20	b	612	CLA	CHD-C4C-C3C	-2.60	121.02	124.84
22	a	408	BCR	C33-C5-C4	2.60	118.61	113.62
20	a	404	CLA	C3C-C4C-NC	2.60	113.49	110.57
20	d	404	CLA	CMC-C2C-C1C	2.60	129.00	125.04
27	b	604	F6C	CMC-C2C-C3C	2.60	129.84	124.94
20	c	504	CLA	C1-C2-C3	-2.60	121.55	126.04
20	H	101	CLA	C4C-C3C-C2C	-2.59	103.12	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	101	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
20	A	404	CLA	CMB-C2B-C3B	2.59	129.53	124.68
20	b	606	CLA	C3C-C4C-NC	2.59	113.47	110.57
27	b	604	F6C	CHD-C1D-ND	-2.59	120.28	124.20
20	A	405	CLA	CMA-C3A-C4A	2.59	118.72	111.77
20	B	612	CLA	CHD-C4C-C3C	-2.59	121.04	124.84
20	C	511	CLA	C1-O2A-CGA	2.58	123.23	116.44
22	b	616	BCR	C15-C14-C13	-2.58	123.62	127.31
22	d	405	BCR	C1-C6-C5	-2.58	118.97	122.61
27	B	604	F6C	CHD-C1D-ND	-2.58	120.29	124.20
20	a	407	CLA	C3C-C4C-NC	2.58	113.46	110.57
20	c	503	CLA	C4D-C3D-CAD	2.58	111.13	108.10
20	b	603	CLA	CMB-C2B-C3B	2.58	129.50	124.68
27	B	604	F6C	CMC-C2C-C3C	2.58	129.80	124.94
20	a	405	CLA	CMA-C3A-C4A	2.58	118.70	111.77
22	a	408	BCR	C35-C13-C12	2.57	122.13	118.08
22	B	616	BCR	C15-C14-C13	-2.57	123.64	127.31
20	c	511	CLA	C1-O2A-CGA	2.57	123.19	116.44
20	c	507	CLA	CHB-C4A-NA	2.57	128.07	124.51
20	b	606	CLA	CMB-C2B-C3B	2.57	129.48	124.68
20	B	606	CLA	C3C-C4C-NC	2.57	113.45	110.57
20	a	407	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
20	b	615	CLA	CHB-C4A-NA	2.57	128.06	124.51
31	V	201	HEM	CMA-C3A-C4A	-2.56	124.52	128.46
31	v	201	HEM	CMA-C3A-C4A	-2.56	124.52	128.46
22	A	408	BCR	C35-C13-C12	2.56	122.11	118.08
20	A	407	CLA	C3C-C4C-NC	2.56	113.44	110.57
27	B	613	F6C	CMC-C2C-C3C	2.56	129.77	124.94
22	D	405	BCR	C7-C8-C9	-2.56	122.37	126.23
22	D	405	BCR	C1-C6-C5	-2.56	119.01	122.61
20	A	407	CLA	CMB-C2B-C3B	2.56	129.47	124.68
20	C	507	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	d	405	BCR	C7-C8-C9	-2.56	122.37	126.23
20	B	615	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	b	605	CLA	CMB-C2B-C3B	2.55	129.46	124.68
20	b	612	CLA	C3D-C4D-ND	2.55	114.37	110.24
20	B	603	CLA	CMB-C2B-C3B	2.55	129.46	124.68
22	b	616	BCR	C38-C26-C25	-2.55	121.66	124.53
20	B	605	CLA	CMB-C2B-C3B	2.55	129.45	124.68
20	c	513	CLA	C4D-C3D-CAD	2.55	111.10	108.10
22	B	618	BCR	C30-C25-C26	-2.55	119.02	122.61
22	B	618	BCR	C1-C6-C5	-2.55	119.03	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	604	F6C	CHB-C4A-NA	2.55	126.79	124.45
22	C	515	BCR	C34-C9-C8	2.55	122.09	118.08
22	c	518	BCR	C31-C1-C6	-2.55	106.17	110.30
27	B	604	F6C	CHB-C4A-NA	2.54	126.79	124.45
20	C	503	CLA	C4D-C3D-CAD	2.54	111.09	108.10
27	b	613	F6C	CMC-C2C-C3C	2.54	129.74	124.94
22	C	518	BCR	C31-C1-C6	-2.54	106.17	110.30
20	A	407	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
20	C	513	CLA	C4D-C3D-CAD	2.54	111.09	108.10
22	b	618	BCR	C1-C6-C5	-2.54	119.04	122.61
22	B	616	BCR	C38-C26-C25	-2.54	121.68	124.53
20	B	606	CLA	CMB-C2B-C3B	2.54	129.43	124.68
20	a	407	CLA	CMB-C2B-C3B	2.54	129.43	124.68
20	b	602	CLA	CMB-C2B-C3B	2.54	129.43	124.68
20	C	512	CLA	CAA-CBA-CGA	-2.54	105.84	113.25
22	B	616	BCR	C40-C30-C25	2.54	114.42	110.30
20	C	511	CLA	C3C-C4C-NC	2.54	113.42	110.57
27	b	604	F6C	C1-O2A-CGA	2.54	123.10	116.44
20	B	603	CLA	C3C-C4C-NC	2.53	113.41	110.57
22	b	616	BCR	C40-C30-C25	2.53	114.41	110.30
22	c	515	BCR	C34-C9-C8	2.53	122.06	118.08
20	B	612	CLA	C3D-C4D-ND	2.53	114.33	110.24
20	c	512	CLA	CAA-CBA-CGA	-2.53	105.87	113.25
28	C	516	DGD	O3G-C1D-C2D	-2.52	104.36	108.30
20	B	602	CLA	CMB-C2B-C3B	2.52	129.40	124.68
22	b	618	BCR	C30-C25-C26	-2.52	119.06	122.61
27	c	508	F6C	CMA-C3A-C4A	-2.52	120.27	124.71
22	c	515	BCR	C12-C13-C14	-2.52	115.08	118.94
20	a	404	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
20	A	404	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
20	C	511	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
20	C	503	CLA	C1-O2A-CGA	2.51	123.03	116.44
20	c	511	CLA	C3C-C4C-NC	2.51	113.39	110.57
24	A	410	PL9	O1-C4-C3	-2.51	117.95	120.72
27	B	604	F6C	C1-O2A-CGA	2.51	123.03	116.44
22	C	515	BCR	C1-C6-C7	2.51	122.87	115.78
28	c	516	DGD	O3G-C1D-C2D	-2.51	104.39	108.30
27	C	508	F6C	CHB-C4A-C3A	-2.51	120.22	125.48
20	c	503	CLA	C1-O2A-CGA	2.50	123.02	116.44
20	c	511	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
20	B	602	CLA	CMC-C2C-C1C	2.50	128.85	125.04
20	c	510	CLA	C11-C12-C13	-2.50	107.83	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	613	F6C	C4-C3-C5	2.50	119.48	115.27
27	B	607	F6C	CHB-C4A-C3A	-2.50	120.24	125.48
24	d	406	PL9	C31-C32-C33	-2.50	103.67	111.88
29	d	401	CL7	O2D-CGD-O1D	-2.50	118.95	123.84
29	D	401	CL7	O2D-CGD-O1D	-2.50	118.96	123.84
22	c	515	BCR	C1-C6-C7	2.50	122.84	115.78
20	C	506	CLA	C3D-C4D-ND	2.50	114.28	110.24
20	B	601	CLA	CMB-C2B-C3B	2.50	129.35	124.68
27	C	508	F6C	CMA-C3A-C4A	-2.49	120.32	124.71
24	a	410	PL9	O1-C4-C3	-2.49	117.97	120.72
20	C	510	CLA	C11-C12-C13	-2.49	107.86	115.92
24	D	406	PL9	C31-C32-C33	-2.49	103.69	111.88
20	C	514	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
22	C	515	BCR	C12-C13-C14	-2.49	115.12	118.94
20	C	513	CLA	C3D-C4D-ND	2.49	114.27	110.24
20	c	513	CLA	C3D-C4D-ND	2.49	114.27	110.24
27	B	607	F6C	OMB-CMB-C2B	-2.49	120.06	125.69
27	b	607	F6C	OMB-CMB-C2B	-2.49	120.06	125.69
20	C	504	CLA	C3D-C4D-ND	2.49	114.26	110.24
20	c	506	CLA	C3D-C4D-ND	2.49	114.26	110.24
20	b	610	CLA	C3D-C4D-ND	2.49	114.26	110.24
20	B	605	CLA	C3D-C4D-ND	2.49	114.26	110.24
20	b	603	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
20	b	603	CLA	CMD-C2D-C3D	-2.49	121.90	127.61
20	b	602	CLA	CMC-C2C-C1C	2.48	128.82	125.04
20	b	603	CLA	C3C-C4C-NC	2.48	113.36	110.57
20	c	514	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
22	b	618	BCR	C23-C22-C21	2.48	122.75	118.94
20	c	504	CLA	C3D-C4D-ND	2.48	114.25	110.24
21	A	406	PHO	C4-C3-C2	-2.48	117.31	123.68
20	C	502	CLA	O2A-C1-C2	2.48	115.16	108.64
20	c	502	CLA	O2A-C1-C2	2.48	115.16	108.64
20	a	407	CLA	C5-C3-C4	2.48	120.08	114.60
27	b	613	F6C	C4-C3-C5	2.48	119.44	115.27
27	c	508	F6C	CHB-C4A-C3A	-2.48	120.28	125.48
26	A	412	LHG	O8-C23-O10	-2.48	117.34	123.59
20	b	601	CLA	CMB-C2B-C3B	2.48	129.31	124.68
22	c	518	BCR	C33-C5-C4	2.48	118.37	113.62
20	B	603	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
20	A	407	CLA	C5-C3-C4	2.47	120.06	114.60
21	a	406	PHO	C4-C3-C2	-2.47	117.34	123.68
27	b	607	F6C	CHB-C4A-C3A	-2.47	120.30	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	610	CLA	C3D-C4D-ND	2.47	114.23	110.24
20	b	605	CLA	C3D-C4D-ND	2.47	114.23	110.24
20	c	504	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
22	B	618	BCR	C23-C22-C21	2.46	122.72	118.94
20	c	509	CLA	C3C-C4C-NC	2.46	113.33	110.57
20	B	603	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
22	C	518	BCR	C33-C5-C4	2.46	118.34	113.62
20	B	608	CLA	C1-O2A-CGA	2.46	122.90	116.44
20	d	404	CLA	CMB-C2B-C3B	2.46	129.28	124.68
20	D	404	CLA	CMB-C2B-C3B	2.45	129.27	124.68
22	D	405	BCR	C3-C4-C5	-2.45	109.70	114.08
22	d	405	BCR	C3-C4-C5	-2.45	109.70	114.08
27	c	508	F6C	OMB-CMB-C2B	-2.45	120.14	125.69
26	a	412	LHG	O8-C23-O10	-2.45	117.41	123.59
27	C	508	F6C	OMB-CMB-C2B	-2.45	120.15	125.69
20	c	503	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
20	b	606	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
20	C	506	CLA	C1-O2A-CGA	2.45	122.86	116.44
20	C	504	CLA	CAA-C2A-C3A	-2.45	106.08	112.78
27	c	508	F6C	O2D-CGD-O1D	-2.45	119.05	123.84
20	B	606	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
20	c	506	CLA	C1-O2A-CGA	2.44	122.86	116.44
20	b	608	CLA	C1-O2A-CGA	2.44	122.85	116.44
20	a	405	CLA	C3D-C4D-ND	2.44	114.19	110.24
27	b	604	F6C	C4-C3-C5	2.44	119.38	115.27
27	c	508	F6C	CMD-C2D-C3D	-2.44	122.00	127.61
20	C	503	CLA	C4-C3-C5	2.44	119.38	115.27
20	c	503	CLA	C4-C3-C5	2.44	119.38	115.27
32	H	102	RRX	C8-C9-C10	2.44	122.69	118.94
20	C	509	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	d	401	CL7	CMB-C2B-C3B	2.44	129.24	124.68
20	c	514	CLA	CAC-C3C-C4C	2.44	127.97	124.81
27	B	604	F6C	C4-C3-C5	2.44	119.37	115.27
20	B	605	CLA	OBD-CAD-C3D	-2.44	122.65	128.52
20	A	405	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
20	c	503	CLA	CMA-C3A-C4A	2.44	118.32	111.77
32	h	102	RRX	C23-C22-C21	2.44	122.68	118.94
32	H	102	RRX	C23-C22-C21	2.43	122.68	118.94
20	b	605	CLA	OBD-CAD-C3D	-2.43	122.66	128.52
27	B	607	F6C	O2D-CGD-O1D	-2.43	119.08	123.84
20	C	509	CLA	C3C-C4C-NC	2.43	113.30	110.57
26	D	407	LHG	O7-C7-O9	-2.43	117.83	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	615	CLA	CBA-CAA-C2A	-2.43	106.69	113.86
20	C	503	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
20	C	503	CLA	CMA-C3A-C4A	2.43	118.30	111.77
20	b	605	CLA	C3B-C4B-NB	2.43	112.35	109.21
20	A	405	CLA	C3D-C4D-ND	2.43	114.17	110.24
20	B	605	CLA	C3B-C4B-NB	2.43	112.35	109.21
20	c	505	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
20	c	509	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
20	b	615	CLA	CBA-CAA-C2A	-2.43	106.70	113.86
27	b	607	F6C	O2D-CGD-O1D	-2.43	119.09	123.84
29	D	401	CL7	CMB-C2B-C3B	2.43	129.22	124.68
26	d	407	LHG	O7-C7-O9	-2.43	117.84	123.70
32	h	102	RRX	C8-C9-C10	2.42	122.66	118.94
20	b	602	CLA	C3C-C4C-NC	2.42	113.29	110.57
22	B	618	BCR	C33-C5-C4	2.42	118.27	113.62
27	b	607	F6C	CMD-C2D-C3D	-2.42	122.04	127.61
26	A	412	LHG	O7-C7-O9	-2.42	117.85	123.70
26	a	412	LHG	O7-C7-O9	-2.42	117.85	123.70
20	b	610	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
22	a	408	BCR	C34-C9-C8	2.42	121.89	118.08
20	a	405	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
27	C	508	F6C	CMD-C2D-C3D	-2.42	122.05	127.61
27	C	508	F6C	O2D-CGD-O1D	-2.42	119.11	123.84
20	h	101	CLA	C3D-C4D-ND	2.42	114.15	110.24
20	b	602	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
22	A	408	BCR	C34-C9-C8	2.42	121.89	118.08
22	b	618	BCR	C33-C5-C4	2.42	118.26	113.62
22	b	617	BCR	C3-C4-C5	-2.41	109.77	114.08
20	C	505	CLA	C5-C3-C4	2.41	119.94	114.60
20	H	101	CLA	C3D-C4D-ND	2.41	114.14	110.24
20	B	610	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
22	B	617	BCR	C3-C4-C5	-2.41	109.77	114.08
20	C	514	CLA	CAC-C3C-C4C	2.41	127.94	124.81
20	B	602	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
20	c	505	CLA	C5-C3-C4	2.41	119.92	114.60
20	C	502	CLA	C1-O2A-CGA	2.41	122.76	116.44
20	C	505	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
20	c	502	CLA	C1-O2A-CGA	2.41	122.76	116.44
20	b	612	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
20	B	606	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
27	B	607	F6C	CMD-C2D-C3D	-2.41	122.08	127.61
20	B	602	CLA	C3C-C4C-NC	2.40	113.27	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	405	CLA	CMC-C2C-C1C	2.40	128.70	125.04
20	b	606	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
20	c	511	CLA	C3D-C4D-ND	2.40	114.12	110.24
20	c	512	CLA	C4D-C3D-CAD	2.40	110.92	108.10
20	c	510	CLA	C4-C3-C5	2.40	119.30	115.27
21	A	406	PHO	C5-C3-C2	2.40	125.97	121.12
20	C	514	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
20	C	512	CLA	C4D-C3D-CAD	2.40	110.92	108.10
20	a	407	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
20	B	615	CLA	C4-C3-C2	-2.39	117.54	123.68
20	c	505	CLA	C3D-C4D-ND	2.39	114.11	110.24
22	b	617	BCR	C39-C30-C25	-2.39	106.42	110.30
20	B	608	CLA	C1-C2-C3	-2.39	121.91	126.04
20	B	602	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
20	B	605	CLA	CMC-C2C-C3C	2.39	132.60	126.12
20	b	605	CLA	CMC-C2C-C3C	2.39	132.60	126.12
20	b	615	CLA	C4-C3-C2	-2.39	117.56	123.68
20	a	405	CLA	C4D-C3D-CAD	2.38	110.91	108.10
21	a	406	PHO	C5-C3-C2	2.38	125.94	121.12
27	B	604	F6C	C3D-C4D-ND	2.38	113.65	110.17
20	C	511	CLA	C3D-C4D-ND	2.38	114.09	110.24
20	C	505	CLA	C3D-C4D-ND	2.38	114.09	110.24
20	B	612	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
28	C	516	DGD	C3D-C4D-C5D	-2.38	105.99	110.24
20	c	514	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
20	A	407	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
22	b	617	BCR	C33-C5-C6	-2.38	121.86	124.53
20	d	403	CLA	C4D-C3D-CAD	2.38	110.90	108.10
22	B	617	BCR	C39-C30-C25	-2.38	106.45	110.30
28	c	516	DGD	C3D-C4D-C5D	-2.37	106.00	110.24
20	A	405	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	L	102	SQD	O47-C45-C44	2.37	116.99	108.40
20	b	602	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
28	c	517	DGD	C1D-C2D-C3D	-2.37	105.06	110.00
20	b	615	CLA	CMC-C2C-C1C	2.37	128.65	125.04
22	B	617	BCR	C33-C5-C6	-2.37	121.86	124.53
20	B	602	CLA	C4D-C3D-CAD	2.37	110.89	108.10
20	C	506	CLA	C4D-C3D-CAD	2.37	110.89	108.10
28	C	517	DGD	C1D-C2D-C3D	-2.37	105.06	110.00
20	b	608	CLA	C6-C5-C3	-2.37	107.24	113.45
20	b	608	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
20	c	514	CLA	C3C-C4C-NC	2.37	113.23	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	405	CLA	C4D-C3D-CAD	2.37	110.89	108.10
20	B	608	CLA	C6-C5-C3	-2.37	107.25	113.45
20	b	608	CLA	C1-C2-C3	-2.37	121.95	126.04
22	a	408	BCR	C3-C4-C5	-2.37	109.85	114.08
20	b	602	CLA	C4D-C3D-CAD	2.36	110.88	108.10
22	B	618	BCR	C33-C5-C6	-2.36	121.87	124.53
20	b	609	CLA	OBD-CAD-C3D	-2.36	122.83	128.52
23	l	102	SQD	O47-C45-C44	2.36	116.96	108.40
20	B	608	CLA	CMB-C2B-C1B	-2.36	124.83	128.46
20	C	510	CLA	C4-C3-C5	2.36	119.24	115.27
21	D	402	PHO	CMC-C2C-C3C	2.36	129.39	124.94
22	A	408	BCR	C3-C4-C5	-2.36	109.86	114.08
30	d	409	LMG	O8-C28-C29	2.36	119.31	111.91
20	D	403	CLA	C4D-C3D-CAD	2.36	110.87	108.10
20	B	609	CLA	OBD-CAD-C3D	-2.36	122.85	128.52
20	c	506	CLA	C4D-C3D-CAD	2.36	110.87	108.10
26	D	407	LHG	C6-C5-C4	-2.35	106.22	111.79
26	d	408	LHG	O8-C23-O10	-2.35	117.65	123.59
22	b	616	BCR	C33-C5-C4	2.35	118.14	113.62
30	D	409	LMG	O8-C28-C29	2.35	119.29	111.91
27	b	604	F6C	C3D-C4D-ND	2.35	113.61	110.17
20	B	615	CLA	CMC-C2C-C1C	2.35	128.62	125.04
26	D	408	LHG	O8-C23-O10	-2.35	117.66	123.59
20	C	514	CLA	C3C-C4C-NC	2.35	113.21	110.57
21	d	402	PHO	CMC-C2C-C3C	2.35	129.37	124.94
22	b	618	BCR	C33-C5-C6	-2.35	121.89	124.53
20	A	404	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
20	B	612	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	c	507	CLA	C4C-C3C-C2C	-2.34	103.48	106.90
22	B	616	BCR	C33-C5-C4	2.34	118.11	113.62
26	d	407	LHG	C6-C5-C4	-2.34	106.25	111.79
20	C	512	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
22	B	618	BCR	C34-C9-C10	-2.34	119.64	122.92
20	c	512	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
20	C	507	CLA	C4C-C3C-C2C	-2.34	103.49	106.90
20	c	507	CLA	C4-C3-C5	2.34	119.20	115.27
22	c	518	BCR	C35-C13-C14	-2.34	116.80	123.71
20	b	612	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	C	518	BCR	C35-C13-C14	-2.34	116.80	123.71
20	b	615	CLA	C3C-C4C-NC	2.34	113.19	110.57
22	b	618	BCR	C34-C9-C10	-2.33	119.65	122.92
20	D	403	CLA	OBD-CAD-C3D	-2.33	122.90	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	101	CLA	CMB-C2B-C1B	2.33	132.05	128.46
20	c	503	CLA	CMB-C2B-C3B	2.33	129.04	124.68
20	C	505	CLA	CMC-C2C-C1C	2.33	128.59	125.04
27	B	607	F6C	CMC-C2C-C3C	2.33	129.33	124.94
20	a	404	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
20	d	403	CLA	OBD-CAD-C3D	-2.33	122.92	128.52
20	c	514	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
20	b	608	CLA	CAC-C3C-C4C	2.32	127.83	124.81
20	H	101	CLA	CMB-C2B-C1B	2.32	132.03	128.46
26	L	101	LHG	C9-C8-C7	-2.32	105.17	113.62
26	l	101	LHG	C9-C8-C7	-2.32	105.17	113.62
23	L	102	SQD	O47-C7-O49	-2.32	118.09	123.70
31	E	101	HEM	CBA-CAA-C2A	-2.32	108.66	112.62
20	C	514	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	e	101	HEM	CBA-CAA-C2A	-2.32	108.66	112.62
23	l	102	SQD	C45-O47-C7	2.32	123.50	117.79
20	c	506	CLA	CHB-C4A-NA	2.32	127.72	124.51
20	B	608	CLA	CAC-C3C-C4C	2.32	127.82	124.81
20	C	507	CLA	C4-C3-C5	2.32	119.17	115.27
20	B	615	CLA	C3C-C4C-NC	2.31	113.17	110.57
23	L	102	SQD	C45-O47-C7	2.31	123.48	117.79
23	L	102	SQD	C1-C2-C3	-2.31	105.18	110.00
23	l	102	SQD	C1-C2-C3	-2.31	105.18	110.00
20	C	505	CLA	C3C-C4C-NC	2.31	113.16	110.57
20	c	505	CLA	CMC-C2C-C1C	2.31	128.56	125.04
27	b	607	F6C	CMC-C2C-C3C	2.31	129.30	124.94
20	C	503	CLA	CMB-C2B-C3B	2.31	129.00	124.68
20	C	506	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	l	102	SQD	O47-C7-O49	-2.30	118.14	123.70
20	b	610	CLA	C4-C3-C2	-2.30	117.77	123.68
20	a	404	CLA	C4D-C3D-CAD	2.30	110.81	108.10
22	b	618	BCR	C36-C18-C17	-2.30	119.70	122.92
21	a	406	PHO	CBA-CAA-C2A	-2.30	107.08	113.81
27	C	508	F6C	CMC-C2C-C3C	2.30	129.28	124.94
20	B	610	CLA	C4-C3-C2	-2.30	117.77	123.68
27	c	508	F6C	CMC-C2C-C3C	2.30	129.28	124.94
20	c	507	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
20	B	609	CLA	CMB-C2B-C3B	2.30	128.98	124.68
20	b	609	CLA	CMB-C2B-C3B	2.30	128.98	124.68
20	C	507	CLA	C4D-C3D-CAD	2.30	110.80	108.10
20	b	610	CLA	C7-C6-C5	-2.30	107.12	113.36
20	B	610	CLA	C7-C6-C5	-2.29	107.13	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	503	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
21	A	406	PHO	CBA-CAA-C2A	-2.29	107.11	113.81
20	c	503	CLA	C3D-C4D-ND	2.29	113.95	110.24
21	a	406	PHO	C1B-NB-C4B	2.29	111.79	107.09
20	B	610	CLA	CMC-C2C-C3C	2.29	132.33	126.12
20	c	507	CLA	C4D-C3D-CAD	2.29	110.79	108.10
22	B	618	BCR	C3-C4-C5	-2.29	110.00	114.08
20	c	503	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
21	A	406	PHO	C1B-NB-C4B	2.28	111.78	107.09
20	c	505	CLA	C3C-C4C-NC	2.28	113.13	110.57
28	C	516	DGD	O5D-C6D-C5D	-2.28	104.82	109.05
20	c	502	CLA	C4-C3-C5	2.28	119.11	115.27
20	C	507	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
22	b	618	BCR	C3-C4-C5	-2.28	110.00	114.08
20	b	610	CLA	CMC-C2C-C3C	2.28	132.31	126.12
22	B	618	BCR	C36-C18-C17	-2.28	119.73	122.92
20	A	404	CLA	C4D-C3D-CAD	2.28	110.78	108.10
20	b	610	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
20	C	502	CLA	C4-C3-C5	2.28	119.10	115.27
20	a	405	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
20	c	511	CLA	C1-C2-C3	-2.27	122.11	126.04
20	B	615	CLA	C1-C2-C3	-2.27	122.11	126.04
28	c	516	DGD	O5D-C6D-C5D	-2.27	104.84	109.05
30	d	409	LMG	C8-O7-C10	-2.27	112.20	117.79
20	C	511	CLA	C1-C2-C3	-2.27	122.12	126.04
24	a	410	PL9	O2-C1-C2	-2.27	116.58	121.78
20	C	503	CLA	C3D-C4D-ND	2.27	113.91	110.24
30	D	409	LMG	C8-O7-C10	-2.27	112.21	117.79
20	b	615	CLA	C1-C2-C3	-2.26	122.13	126.04
20	A	405	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
20	C	512	CLA	C3C-C4C-NC	2.26	113.11	110.57
20	B	610	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
27	c	508	F6C	CMA-C3A-C2A	-2.26	119.98	126.12
23	L	102	SQD	O48-C46-C45	-2.26	101.85	108.43
27	C	508	F6C	CMA-C3A-C2A	-2.26	119.98	126.12
20	b	603	CLA	C4D-C3D-CAD	2.26	110.76	108.10
24	A	410	PL9	O2-C1-C2	-2.26	116.61	121.78
23	l	102	SQD	O48-C46-C45	-2.26	101.86	108.43
20	b	606	CLA	CAC-C3C-C4C	2.26	127.74	124.81
20	c	510	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
20	b	606	CLA	C4D-C3D-CAD	2.25	110.75	108.10
27	B	607	F6C	CMA-C3A-C2A	-2.25	120.00	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	101	CLA	C5-C3-C4	2.25	119.57	114.60
20	h	101	CLA	C5-C3-C4	2.25	119.57	114.60
20	B	603	CLA	C4D-C3D-CAD	2.25	110.75	108.10
28	c	516	DGD	O6E-C5E-C6E	-2.25	100.84	106.44
20	c	505	CLA	C4D-C3D-CAD	2.25	110.75	108.10
20	C	507	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
20	B	605	CLA	C1-O2A-CGA	2.25	122.34	116.44
20	B	606	CLA	C4D-C3D-CAD	2.25	110.75	108.10
20	a	404	CLA	CAC-C3C-C4C	2.25	127.72	124.81
27	b	607	F6C	CMA-C3A-C2A	-2.25	120.02	126.12
20	b	614	CLA	CHD-C4C-C3C	-2.25	121.54	124.84
20	B	610	CLA	C3C-C4C-NC	2.24	113.09	110.57
20	c	507	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
20	a	407	CLA	C4D-C3D-CAD	2.24	110.74	108.10
20	B	606	CLA	CAC-C3C-C4C	2.24	127.72	124.81
28	D	410	DGD	C1D-C2D-C3D	-2.24	105.33	110.00
20	C	503	CLA	C4C-C3C-C2C	-2.24	103.63	106.90
20	b	605	CLA	C1-O2A-CGA	2.24	122.32	116.44
28	d	410	DGD	C1D-C2D-C3D	-2.24	105.33	110.00
23	L	102	SQD	O48-C23-O10	-2.24	117.94	123.59
20	C	507	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
24	d	406	PL9	C27-C28-C29	-2.24	122.27	127.66
28	c	516	DGD	O2E-C2E-C1E	-2.24	104.61	110.05
20	A	404	CLA	CAC-C3C-C4C	2.24	127.71	124.81
28	C	516	DGD	O6E-C5E-C6E	-2.24	100.87	106.44
20	C	510	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
27	b	613	F6C	C4A-CHB-C1B	2.24	130.88	126.06
20	c	512	CLA	C3C-C4C-NC	2.23	113.08	110.57
20	B	614	CLA	CHD-C4C-C3C	-2.23	121.56	124.84
20	B	608	CLA	C4C-C3C-C2C	-2.23	103.65	106.90
20	H	101	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
20	c	507	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
20	c	503	CLA	C4C-C3C-C2C	-2.23	103.65	106.90
20	B	611	CLA	C3B-C4B-NB	2.23	112.09	109.21
28	C	516	DGD	O2E-C2E-C1E	-2.23	104.64	110.05
27	B	613	F6C	C4A-CHB-C1B	2.23	130.86	126.06
20	b	608	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
20	H	101	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
20	C	505	CLA	C4D-C3D-CAD	2.22	110.71	108.10
23	l	102	SQD	C4-C3-C2	2.22	114.70	110.82
20	b	611	CLA	C3B-C4B-NB	2.22	112.08	109.21
24	D	406	PL9	C27-C28-C29	-2.22	122.31	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	l	102	SQD	O48-C23-O10	-2.22	117.99	123.59
20	h	101	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
20	C	510	CLA	C3D-C4D-ND	2.22	113.82	110.24
20	c	507	CLA	C3B-C4B-NB	2.22	112.07	109.21
20	B	605	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
20	h	101	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
20	d	404	CLA	C3C-C4C-NC	2.21	113.05	110.57
20	B	611	CLA	C7-C6-C5	-2.21	107.36	113.36
24	D	406	PL9	C8-C7-C3	2.21	118.21	111.98
20	c	510	CLA	C3D-C4D-ND	2.21	113.81	110.24
20	C	509	CLA	CED-O2D-CGD	2.21	120.92	115.94
20	c	509	CLA	CED-O2D-CGD	2.20	120.92	115.94
20	b	605	CLA	CHC-C1C-C2C	-2.20	120.62	126.72
24	d	406	PL9	C8-C7-C3	2.20	118.21	111.98
20	c	507	CLA	C1-O2A-CGA	2.20	122.22	116.44
31	v	201	HEM	CMB-C2B-C1B	-2.20	121.69	125.04
20	A	407	CLA	C4D-C3D-CAD	2.20	110.69	108.10
23	L	102	SQD	C4-C3-C2	2.20	114.67	110.82
20	b	611	CLA	C7-C6-C5	-2.20	107.38	113.36
20	b	610	CLA	C3C-C4C-NC	2.20	113.04	110.57
20	C	507	CLA	C1-O2A-CGA	2.20	122.22	116.44
20	B	615	CLA	C3D-C4D-ND	2.20	113.79	110.24
20	C	507	CLA	C3B-C4B-NB	2.20	112.05	109.21
22	c	515	BCR	C23-C22-C21	2.19	122.31	118.94
20	C	511	CLA	CAC-C3C-C2C	2.19	131.28	127.53
20	c	514	CLA	CMA-C3A-C4A	2.19	117.66	111.77
20	C	513	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
22	C	515	BCR	C1-C6-C5	-2.19	119.53	122.61
20	C	511	CLA	C3B-C4B-NB	2.19	112.04	109.21
22	D	405	BCR	C35-C13-C12	2.18	121.52	118.08
20	b	615	CLA	C3D-C4D-ND	2.18	113.77	110.24
20	c	513	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
20	D	404	CLA	C3C-C4C-NC	2.18	113.02	110.57
22	C	515	BCR	C23-C22-C21	2.18	122.29	118.94
31	V	201	HEM	CMB-C2B-C1B	-2.18	121.72	125.04
20	c	511	CLA	CAC-C3C-C2C	2.18	131.26	127.53
20	c	504	CLA	C4-C3-C5	2.18	118.94	115.27
20	C	504	CLA	C11-C12-C13	-2.18	108.88	115.92
20	C	514	CLA	CMA-C3A-C4A	2.18	117.63	111.77
20	c	512	CLA	C5-C3-C4	2.18	119.42	114.60
20	c	511	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
22	d	405	BCR	C35-C13-C12	2.18	121.50	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	614	CLA	CMB-C2B-C3B	2.17	128.75	124.68
20	C	506	CLA	C4C-C3C-C2C	-2.17	103.73	106.90
20	A	405	CLA	C3C-C4C-NC	2.17	113.01	110.57
20	b	605	CLA	C4-C3-C5	2.17	118.93	115.27
20	a	405	CLA	C3C-C4C-NC	2.17	113.01	110.57
20	b	614	CLA	CMB-C2B-C3B	2.17	128.74	124.68
20	B	612	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
20	b	612	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
20	C	504	CLA	C4-C3-C5	2.17	118.92	115.27
20	c	504	CLA	C11-C12-C13	-2.17	108.91	115.92
20	C	512	CLA	C5-C3-C4	2.17	119.39	114.60
20	B	605	CLA	CAA-C2A-C1A	2.17	119.08	111.97
20	c	506	CLA	C4C-C3C-C2C	-2.17	103.74	106.90
20	b	605	CLA	CAA-C2A-C1A	2.16	119.07	111.97
30	M	101	LMG	C8-O7-C10	-2.16	112.46	117.79
20	C	511	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
22	B	616	BCR	C1-C6-C7	2.16	121.89	115.78
22	c	515	BCR	C1-C6-C5	-2.16	119.57	122.61
30	m	101	LMG	C8-O7-C10	-2.16	112.47	117.79
20	c	511	CLA	C3B-C4B-NB	2.16	112.00	109.21
22	b	616	BCR	C1-C6-C7	2.16	121.89	115.78
20	B	605	CLA	C4-C3-C5	2.16	118.90	115.27
20	b	614	CLA	CAC-C3C-C4C	2.16	127.61	124.81
20	B	614	CLA	CAC-C3C-C4C	2.15	127.60	124.81
20	C	510	CLA	CHB-C4A-NA	2.15	127.48	124.51
20	c	506	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
20	C	506	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
23	l	102	SQD	C44-O6-C1	2.13	117.90	113.74
20	c	510	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	C	510	CLA	C4D-C3D-CAD	2.13	110.61	108.10
20	b	605	CLA	C12-C11-C10	2.13	123.01	113.24
26	D	408	LHG	O8-C23-C24	2.13	118.58	111.91
20	B	605	CLA	C12-C11-C10	2.13	123.00	113.24
20	b	601	CLA	C3D-C4D-ND	2.12	113.67	110.24
20	C	513	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
20	C	503	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
24	a	410	PL9	C2-C3-C4	2.12	121.72	118.80
20	c	503	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
26	d	408	LHG	O8-C23-C24	2.12	118.56	111.91
28	C	516	DGD	C7B-C6B-C5B	-2.12	103.67	114.42
28	c	516	DGD	C7B-C6B-C5B	-2.12	103.67	114.42
22	b	616	BCR	C4-C5-C6	-2.12	119.66	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	102	SQD	O8-S-C6	2.12	109.11	105.74
22	B	616	BCR	C4-C5-C6	-2.12	119.66	122.73
20	B	601	CLA	C3D-C4D-ND	2.12	113.66	110.24
31	e	101	HEM	C3D-C4D-ND	-2.12	107.81	110.17
20	c	513	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
23	L	102	SQD	C44-O6-C1	2.11	117.87	113.74
31	E	101	HEM	C3D-C4D-ND	-2.11	107.81	110.17
20	b	615	CLA	C6-C5-C3	-2.11	107.92	113.45
20	B	605	CLA	CBA-CAA-C2A	2.11	120.09	113.86
23	l	102	SQD	O8-S-C6	2.11	109.10	105.74
20	C	502	CLA	C3C-C4C-NC	2.11	112.94	110.57
28	c	516	DGD	O2D-C2D-C1D	-2.11	104.92	110.05
20	b	605	CLA	CBA-CAA-C2A	2.11	120.08	113.86
24	A	410	PL9	C2-C3-C4	2.11	121.70	118.80
20	C	509	CLA	C3D-C4D-ND	2.11	113.64	110.24
20	c	513	CLA	CMC-C2C-C1C	2.10	128.24	125.04
20	c	502	CLA	C3C-C4C-NC	2.10	112.93	110.57
20	C	513	CLA	CMC-C2C-C1C	2.10	128.24	125.04
24	A	410	PL9	C7-C8-C9	-2.10	123.30	126.79
24	D	406	PL9	C41-C39-C40	2.10	119.24	114.60
22	b	618	BCR	C37-C22-C21	-2.10	119.98	122.92
24	d	406	PL9	C41-C39-C40	2.10	119.24	114.60
20	b	612	CLA	CAC-C3C-C4C	2.10	127.53	124.81
20	B	612	CLA	CAC-C3C-C4C	2.10	127.53	124.81
20	a	405	CLA	C5-C3-C4	2.10	119.23	114.60
28	C	516	DGD	O2D-C2D-C1D	-2.10	104.95	110.05
20	c	509	CLA	C3D-C4D-ND	2.10	113.63	110.24
20	A	407	CLA	CAC-C3C-C4C	2.09	127.53	124.81
20	B	603	CLA	CAC-C3C-C4C	2.09	127.53	124.81
20	B	615	CLA	C6-C5-C3	-2.09	107.97	113.45
20	B	612	CLA	C16-C15-C13	-2.09	109.15	115.92
20	b	612	CLA	C16-C15-C13	-2.09	109.15	115.92
20	A	405	CLA	C5-C3-C4	2.09	119.22	114.60
20	B	609	CLA	CAA-C2A-C1A	2.09	118.83	111.97
22	c	515	BCR	C37-C22-C21	-2.09	119.99	122.92
29	d	401	CL7	C6-C5-C3	-2.09	107.97	113.45
24	a	410	PL9	C7-C8-C9	-2.09	123.32	126.79
20	b	609	CLA	CAA-C2A-C1A	2.09	118.81	111.97
20	a	407	CLA	CAC-C3C-C4C	2.09	127.52	124.81
20	c	510	CLA	C4D-C3D-CAD	2.09	110.55	108.10
24	D	406	PL9	C32-C33-C34	-2.08	122.64	127.66
20	c	502	CLA	C7-C6-C5	-2.08	107.70	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	509	CLA	C1-C2-C3	-2.08	122.44	126.04
22	B	618	BCR	C37-C22-C21	-2.08	120.01	122.92
22	C	515	BCR	C37-C22-C21	-2.08	120.01	122.92
20	c	509	CLA	C1-C2-C3	-2.08	122.45	126.04
24	d	406	PL9	C32-C33-C34	-2.08	122.66	127.66
20	C	502	CLA	C7-C6-C5	-2.08	107.72	113.36
20	a	405	CLA	CED-O2D-CGD	2.07	120.63	115.94
29	D	401	CL7	C6-C5-C3	-2.07	108.02	113.45
20	a	405	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
22	b	616	BCR	C33-C5-C6	-2.07	122.21	124.53
31	E	101	HEM	CMB-C2B-C1B	-2.07	121.89	125.04
20	C	505	CLA	CMD-C2D-C3D	-2.06	122.86	127.61
20	b	610	CLA	C1-C2-C3	-2.06	122.47	126.04
32	h	102	RRX	C1-C6-C5	-2.06	119.71	122.61
20	c	505	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
31	e	101	HEM	CMB-C2B-C1B	-2.06	121.90	125.04
20	A	405	CLA	CED-O2D-CGD	2.06	120.60	115.94
20	c	504	CLA	C6-C5-C3	-2.06	108.06	113.45
20	b	603	CLA	CAC-C3C-C4C	2.06	127.48	124.81
20	B	610	CLA	C1-C2-C3	-2.06	122.49	126.04
20	c	504	CLA	CMD-C2D-C3D	-2.06	122.89	127.61
20	C	510	CLA	C4C-C3C-C2C	-2.05	103.90	106.90
24	d	406	PL9	C36-C37-C38	-2.05	105.13	111.88
20	b	610	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	H	102	RRX	C1-C6-C5	-2.05	119.72	122.61
31	E	101	HEM	C3B-C2B-C1B	2.05	108.01	106.49
22	b	618	BCR	C28-C27-C26	-2.05	110.42	114.08
24	D	406	PL9	C36-C37-C38	-2.05	105.14	111.88
22	B	616	BCR	C33-C5-C6	-2.05	122.23	124.53
20	C	504	CLA	C6-C5-C3	-2.05	108.08	113.45
20	c	509	CLA	C4D-C3D-CAD	2.05	110.51	108.10
20	C	504	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
23	A	409	SQD	O8-S-C6	-2.05	102.48	105.74
27	B	613	F6C	CHA-C1A-C2A	-2.05	124.29	129.84
27	b	613	F6C	CHA-C1A-C2A	-2.05	124.29	129.84
31	V	201	HEM	C3C-C4C-NC	-2.04	107.08	110.94
20	c	510	CLA	C4C-C3C-C2C	-2.04	103.92	106.90
23	a	409	SQD	O8-S-C6	-2.04	102.48	105.74
31	v	201	HEM	C3C-C4C-NC	-2.04	107.09	110.94
28	C	516	DGD	C1D-C2D-C3D	-2.04	105.74	110.00
22	B	618	BCR	C28-C27-C26	-2.04	110.43	114.08
20	A	405	CLA	O2D-CGD-O1D	-2.04	119.84	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	516	DGD	C1D-C2D-C3D	-2.04	105.75	110.00
26	L	101	LHG	C5-O7-C7	-2.04	112.77	117.79
20	B	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
20	B	601	CLA	C4D-C3D-CAD	2.04	110.50	108.10
23	l	102	SQD	O5-C5-C4	2.04	113.39	109.69
26	l	101	LHG	C5-O7-C7	-2.04	112.78	117.79
20	c	502	CLA	C3B-C4B-NB	2.04	111.84	109.21
20	b	614	CLA	C3D-C4D-ND	2.03	113.53	110.24
28	C	516	DGD	CBB-CAB-C9B	-2.03	104.10	114.42
28	c	516	DGD	CBB-CAB-C9B	-2.03	104.10	114.42
20	B	610	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
27	B	604	F6C	CHA-C1A-NA	-2.03	120.70	124.60
20	b	610	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
23	L	102	SQD	O5-C5-C4	2.03	113.38	109.69
20	b	601	CLA	C4D-C3D-CAD	2.03	110.49	108.10
27	B	613	F6C	CHB-C4A-NA	2.03	126.32	124.45
20	C	509	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
31	e	101	HEM	C3B-C2B-C1B	2.03	107.99	106.49
20	c	506	CLA	CAC-C3C-C4C	2.03	127.44	124.81
20	C	509	CLA	C4D-C3D-CAD	2.03	110.48	108.10
20	C	506	CLA	CAC-C3C-C4C	2.02	127.44	124.81
20	b	601	CLA	CAC-C3C-C4C	2.02	127.44	124.81
20	C	502	CLA	C3B-C4B-NB	2.02	111.83	109.21
20	b	611	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
20	B	614	CLA	C3D-C4D-ND	2.02	113.51	110.24
20	b	611	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
20	c	509	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
20	b	614	CLA	C1-O2A-CGA	2.02	121.74	116.44
20	B	611	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
20	h	101	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
30	D	409	LMG	O7-C10-O9	-2.01	118.84	123.70
22	b	617	BCR	C35-C13-C12	2.01	121.25	118.08
20	C	511	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
20	c	511	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
20	C	504	CLA	CHA-C1A-NA	-2.01	121.79	126.40
20	B	614	CLA	C1-O2A-CGA	2.01	121.72	116.44
22	B	616	BCR	C24-C25-C26	-2.01	116.59	121.46
22	B	617	BCR	C35-C13-C12	2.01	121.24	118.08
20	B	611	CLA	C1-O2A-CGA	2.01	121.71	116.44
27	b	604	F6C	CHA-C1A-NA	-2.01	120.75	124.60
31	E	101	HEM	CAD-CBD-CGD	-2.01	109.28	113.60
20	H	101	CLA	O1D-CGD-CBD	-2.01	120.38	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	613	F6C	CHB-C4A-NA	2.01	126.30	124.45
20	b	602	CLA	CAC-C3C-C4C	2.00	127.41	124.81
20	B	611	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
20	d	404	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
31	V	201	HEM	C3D-C4D-ND	-2.00	107.94	110.17
31	v	201	HEM	C3D-C4D-ND	-2.00	107.94	110.17
20	b	615	CLA	C4D-C3D-CAD	2.00	110.46	108.10
30	d	409	LMG	O7-C10-O9	-2.00	118.86	123.70
22	b	616	BCR	C24-C25-C26	-2.00	116.61	121.46
20	B	612	CLA	CHC-C1C-NC	-2.00	121.17	124.20
20	C	510	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

All (64) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	404	CLA	ND
20	A	405	CLA	ND
20	A	407	CLA	ND
20	B	601	CLA	ND
20	B	602	CLA	ND
20	B	603	CLA	ND
20	B	605	CLA	ND
20	B	606	CLA	ND
20	B	608	CLA	ND
20	B	609	CLA	ND
20	B	610	CLA	ND
20	B	611	CLA	ND
20	B	612	CLA	ND
20	B	614	CLA	ND
20	B	615	CLA	ND
20	C	502	CLA	ND
20	C	503	CLA	ND
20	C	504	CLA	ND
20	C	505	CLA	ND
20	C	506	CLA	ND
20	C	507	CLA	ND
20	C	509	CLA	ND
20	C	510	CLA	ND
20	C	511	CLA	ND
20	C	512	CLA	ND
20	C	513	CLA	ND
20	C	514	CLA	ND

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Mol	Chain	Res	Type	Atom
20	D	403	CLA	ND
20	D	404	CLA	ND
20	H	101	CLA	ND
20	a	404	CLA	ND
20	a	405	CLA	ND
20	a	407	CLA	ND
20	b	601	CLA	ND
20	b	602	CLA	ND
20	b	603	CLA	ND
20	b	605	CLA	ND
20	b	606	CLA	ND
20	b	608	CLA	ND
20	b	609	CLA	ND
20	b	610	CLA	ND
20	b	611	CLA	ND
20	b	612	CLA	ND
20	b	614	CLA	ND
20	b	615	CLA	ND
20	c	502	CLA	ND
20	c	503	CLA	ND
20	c	504	CLA	ND
20	c	505	CLA	ND
20	c	506	CLA	ND
20	c	507	CLA	ND
20	c	509	CLA	ND
20	c	510	CLA	ND
20	c	511	CLA	ND
20	c	512	CLA	ND
20	c	513	CLA	ND
20	c	514	CLA	ND
20	d	403	CLA	ND
20	d	404	CLA	ND
20	h	101	CLA	ND
29	D	401	CL7	NC
29	D	401	CL7	NA
29	d	401	CL7	NC
29	d	401	CL7	NA

All (1509) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	404	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	404	CLA	O1D-CGD-O2D-CED
20	A	405	CLA	CBA-CGA-O2A-C1
20	A	405	CLA	O1A-CGA-O2A-C1
20	A	405	CLA	CHA-CBD-CGD-O1D
20	A	405	CLA	CHA-CBD-CGD-O2D
20	B	601	CLA	CHA-CBD-CGD-O1D
20	B	601	CLA	CHA-CBD-CGD-O2D
20	B	601	CLA	CAD-CBD-CGD-O1D
20	B	602	CLA	O2A-C1-C2-C3
20	B	605	CLA	C1A-C2A-CAA-CBA
20	B	606	CLA	CHA-CBD-CGD-O1D
20	B	606	CLA	CHA-CBD-CGD-O2D
20	B	606	CLA	CBD-CGD-O2D-CED
20	B	608	CLA	C3A-C2A-CAA-CBA
20	B	610	CLA	C1A-C2A-CAA-CBA
20	B	611	CLA	CHA-CBD-CGD-O1D
20	B	611	CLA	CHA-CBD-CGD-O2D
20	B	611	CLA	CBD-CGD-O2D-CED
20	B	612	CLA	CHA-CBD-CGD-O1D
20	B	612	CLA	CHA-CBD-CGD-O2D
20	B	612	CLA	CAD-CBD-CGD-O1D
20	B	612	CLA	CAD-CBD-CGD-O2D
20	B	614	CLA	C4-C3-C5-C6
20	C	504	CLA	CBD-CGD-O2D-CED
20	C	505	CLA	CHA-CBD-CGD-O1D
20	C	505	CLA	CHA-CBD-CGD-O2D
20	C	505	CLA	CAD-CBD-CGD-O1D
20	C	507	CLA	CBD-CGD-O2D-CED
20	C	507	CLA	O2A-C1-C2-C3
20	C	509	CLA	CHA-CBD-CGD-O1D
20	C	509	CLA	CHA-CBD-CGD-O2D
20	C	510	CLA	C2-C1-O2A-CGA
20	C	510	CLA	C6-C7-C8-C9
20	C	513	CLA	CAD-CBD-CGD-O1D
20	C	513	CLA	CAD-CBD-CGD-O2D
20	C	514	CLA	CHA-CBD-CGD-O1D
20	a	404	CLA	CBD-CGD-O2D-CED
20	a	404	CLA	O1D-CGD-O2D-CED
20	a	405	CLA	CBA-CGA-O2A-C1
20	a	405	CLA	O1A-CGA-O2A-C1
20	a	405	CLA	CHA-CBD-CGD-O1D
20	a	405	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	b	601	CLA	CHA-CBD-CGD-O1D
20	b	601	CLA	CHA-CBD-CGD-O2D
20	b	601	CLA	CAD-CBD-CGD-O1D
20	b	602	CLA	O2A-C1-C2-C3
20	b	605	CLA	C1A-C2A-CAA-CBA
20	b	606	CLA	CHA-CBD-CGD-O1D
20	b	606	CLA	CHA-CBD-CGD-O2D
20	b	606	CLA	CBD-CGD-O2D-CED
20	b	608	CLA	C3A-C2A-CAA-CBA
20	b	610	CLA	C1A-C2A-CAA-CBA
20	b	611	CLA	CHA-CBD-CGD-O1D
20	b	611	CLA	CHA-CBD-CGD-O2D
20	b	611	CLA	CBD-CGD-O2D-CED
20	b	612	CLA	CHA-CBD-CGD-O1D
20	b	612	CLA	CHA-CBD-CGD-O2D
20	b	612	CLA	CAD-CBD-CGD-O1D
20	b	612	CLA	CAD-CBD-CGD-O2D
20	b	614	CLA	C4-C3-C5-C6
20	c	504	CLA	CBD-CGD-O2D-CED
20	c	505	CLA	CHA-CBD-CGD-O1D
20	c	505	CLA	CHA-CBD-CGD-O2D
20	c	505	CLA	CAD-CBD-CGD-O1D
20	c	507	CLA	CBD-CGD-O2D-CED
20	c	507	CLA	O2A-C1-C2-C3
20	c	509	CLA	CHA-CBD-CGD-O1D
20	c	509	CLA	CHA-CBD-CGD-O2D
20	c	510	CLA	C2-C1-O2A-CGA
20	c	510	CLA	C6-C7-C8-C9
20	c	513	CLA	CAD-CBD-CGD-O1D
20	c	513	CLA	CAD-CBD-CGD-O2D
20	c	514	CLA	CHA-CBD-CGD-O1D
21	A	406	PHO	O2A-C1-C2-C3
21	A	406	PHO	C2-C3-C5-C6
21	A	406	PHO	C4-C3-C5-C6
21	a	406	PHO	O2A-C1-C2-C3
21	a	406	PHO	C2-C3-C5-C6
21	a	406	PHO	C4-C3-C5-C6
22	B	616	BCR	C7-C8-C9-C10
22	B	616	BCR	C7-C8-C9-C34
22	B	616	BCR	C11-C10-C9-C8
22	B	616	BCR	C11-C10-C9-C34
22	B	616	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	616	BCR	C17-C18-C19-C20
22	B	616	BCR	C36-C18-C19-C20
22	B	617	BCR	C7-C8-C9-C10
22	B	617	BCR	C7-C8-C9-C34
22	B	618	BCR	C7-C8-C9-C10
22	B	618	BCR	C7-C8-C9-C34
22	B	618	BCR	C11-C10-C9-C8
22	B	618	BCR	C11-C10-C9-C34
22	B	618	BCR	C21-C22-C23-C24
22	B	618	BCR	C37-C22-C23-C24
22	B	618	BCR	C23-C24-C25-C30
22	C	515	BCR	C5-C6-C7-C8
22	C	518	BCR	C1-C6-C7-C8
22	C	518	BCR	C11-C12-C13-C14
22	C	518	BCR	C11-C12-C13-C35
22	D	405	BCR	C1-C6-C7-C8
22	D	405	BCR	C11-C10-C9-C8
22	D	405	BCR	C11-C10-C9-C34
22	D	405	BCR	C36-C18-C19-C20
22	b	616	BCR	C7-C8-C9-C10
22	b	616	BCR	C7-C8-C9-C34
22	b	616	BCR	C11-C10-C9-C8
22	b	616	BCR	C11-C10-C9-C34
22	b	616	BCR	C10-C11-C12-C13
22	b	616	BCR	C17-C18-C19-C20
22	b	616	BCR	C36-C18-C19-C20
22	b	617	BCR	C7-C8-C9-C10
22	b	617	BCR	C7-C8-C9-C34
22	b	618	BCR	C7-C8-C9-C10
22	b	618	BCR	C7-C8-C9-C34
22	b	618	BCR	C11-C10-C9-C8
22	b	618	BCR	C11-C10-C9-C34
22	b	618	BCR	C21-C22-C23-C24
22	b	618	BCR	C37-C22-C23-C24
22	b	618	BCR	C23-C24-C25-C30
22	c	515	BCR	C5-C6-C7-C8
22	c	518	BCR	C1-C6-C7-C8
22	c	518	BCR	C11-C12-C13-C14
22	c	518	BCR	C11-C12-C13-C35
22	d	405	BCR	C1-C6-C7-C8
22	d	405	BCR	C11-C10-C9-C8
22	d	405	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
22	d	405	BCR	C36-C18-C19-C20
23	A	409	SQD	C8-C7-O47-C45
23	A	409	SQD	O5-C5-C6-S
23	L	102	SQD	C8-C7-O47-C45
23	L	102	SQD	C5-C6-S-O7
23	a	409	SQD	C8-C7-O47-C45
23	a	409	SQD	O5-C5-C6-S
23	l	102	SQD	C8-C7-O47-C45
23	l	102	SQD	C5-C6-S-O7
24	A	410	PL9	C7-C8-C9-C10
24	A	410	PL9	C7-C8-C9-C11
24	A	410	PL9	C12-C13-C14-C15
24	D	406	PL9	C7-C8-C9-C11
24	D	406	PL9	C12-C11-C9-C8
24	D	406	PL9	C20-C19-C21-C22
24	D	406	PL9	C27-C28-C29-C30
24	D	406	PL9	C27-C28-C29-C31
24	D	406	PL9	C32-C33-C34-C35
24	D	406	PL9	C32-C33-C34-C36
24	D	406	PL9	C37-C38-C39-C40
24	a	410	PL9	C7-C8-C9-C10
24	a	410	PL9	C7-C8-C9-C11
24	a	410	PL9	C12-C13-C14-C15
24	d	406	PL9	C7-C8-C9-C11
24	d	406	PL9	C12-C11-C9-C8
24	d	406	PL9	C20-C19-C21-C22
24	d	406	PL9	C27-C28-C29-C30
24	d	406	PL9	C27-C28-C29-C31
24	d	406	PL9	C32-C33-C34-C35
24	d	406	PL9	C32-C33-C34-C36
24	d	406	PL9	C37-C38-C39-C40
26	A	412	LHG	C4-O6-P-O4
26	A	412	LHG	C24-C23-O8-C6
26	D	407	LHG	C4-O6-P-O3
26	D	407	LHG	C4-O6-P-O4
26	D	407	LHG	C4-O6-P-O5
26	D	408	LHG	C3-O3-P-O5
26	D	408	LHG	C8-C7-O7-C5
26	L	101	LHG	O1-C1-C2-C3
26	a	412	LHG	C4-O6-P-O4
26	a	412	LHG	C24-C23-O8-C6
26	d	407	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
26	d	407	LHG	C4-O6-P-O4
26	d	407	LHG	C4-O6-P-O5
26	d	408	LHG	C3-O3-P-O5
26	d	408	LHG	C8-C7-O7-C5
26	l	101	LHG	O1-C1-C2-C3
27	B	604	F6C	C1A-C2A-CAA-CBA
27	B	604	F6C	C1B-C2B-CMB-OMB
27	B	604	F6C	C3B-C2B-CMB-OMB
27	B	604	F6C	C4-C3-C5-C6
27	B	607	F6C	C1A-C2A-CAA-CBA
27	B	607	F6C	CAD-CBD-CGD-O1D
27	B	607	F6C	CHA-CBD-CGD-O1D
27	B	607	F6C	CHA-CBD-CGD-O2D
27	B	607	F6C	C3B-C2B-CMB-OMB
27	B	607	F6C	C2-C1-O2A-CGA
27	B	613	F6C	C1A-C2A-CAA-CBA
27	B	613	F6C	C1B-C2B-CMB-OMB
27	B	613	F6C	C3B-C2B-CMB-OMB
27	B	613	F6C	C11-C12-C13-C14
27	C	508	F6C	C2B-C3B-CAB-CBB
27	C	508	F6C	CBD-CGD-O2D-CED
27	b	604	F6C	C1A-C2A-CAA-CBA
27	b	604	F6C	C1B-C2B-CMB-OMB
27	b	604	F6C	C3B-C2B-CMB-OMB
27	b	604	F6C	C4-C3-C5-C6
27	b	607	F6C	C1A-C2A-CAA-CBA
27	b	607	F6C	CAD-CBD-CGD-O1D
27	b	607	F6C	CHA-CBD-CGD-O1D
27	b	607	F6C	CHA-CBD-CGD-O2D
27	b	607	F6C	C3B-C2B-CMB-OMB
27	b	607	F6C	C2-C1-O2A-CGA
27	b	613	F6C	C1A-C2A-CAA-CBA
27	b	613	F6C	C1B-C2B-CMB-OMB
27	b	613	F6C	C3B-C2B-CMB-OMB
27	b	613	F6C	C11-C12-C13-C14
27	c	508	F6C	C2B-C3B-CAB-CBB
27	c	508	F6C	CBD-CGD-O2D-CED
28	C	517	DGD	O6D-C1D-O3G-C3G
29	D	401	CL7	C2-C1-O2A-CGA
29	D	401	CL7	C1A-C2A-CAA-CBA
29	D	401	CL7	C3A-C2A-CAA-CBA
29	d	401	CL7	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	d	401	CL7	C1A-C2A-CAA-CBA
29	d	401	CL7	C3A-C2A-CAA-CBA
31	E	101	HEM	C2A-CAA-CBA-CGA
31	e	101	HEM	C2A-CAA-CBA-CGA
32	H	102	RRX	C22-C23-C24-C25
32	H	102	RRX	C37-C22-C23-C24
32	H	102	RRX	C21-C22-C23-C24
32	H	102	RRX	C20-C21-C22-C23
32	H	102	RRX	C20-C21-C22-C37
32	H	102	RRX	C16-C17-C18-C19
32	H	102	RRX	C16-C17-C18-C36
32	H	102	RRX	C35-C13-C14-C15
32	H	102	RRX	C12-C13-C14-C15
32	H	102	RRX	C11-C10-C9-C34
32	H	102	RRX	C11-C10-C9-C8
32	H	102	RRX	C6-C7-C8-C9
32	h	102	RRX	C22-C23-C24-C25
32	h	102	RRX	C37-C22-C23-C24
32	h	102	RRX	C21-C22-C23-C24
32	h	102	RRX	C20-C21-C22-C23
32	h	102	RRX	C20-C21-C22-C37
32	h	102	RRX	C16-C17-C18-C19
32	h	102	RRX	C16-C17-C18-C36
32	h	102	RRX	C35-C13-C14-C15
32	h	102	RRX	C12-C13-C14-C15
32	h	102	RRX	C11-C10-C9-C34
32	h	102	RRX	C11-C10-C9-C8
32	h	102	RRX	C6-C7-C8-C9
20	C	507	CLA	C2C-C3C-CAC-CBC
20	C	507	CLA	C4C-C3C-CAC-CBC
20	c	507	CLA	C2C-C3C-CAC-CBC
20	c	507	CLA	C4C-C3C-CAC-CBC
20	C	514	CLA	O1D-CGD-O2D-CED
20	c	514	CLA	O1D-CGD-O2D-CED
20	B	610	CLA	CBD-CGD-O2D-CED
20	B	612	CLA	CBD-CGD-O2D-CED
20	C	511	CLA	CBD-CGD-O2D-CED
20	C	514	CLA	CBD-CGD-O2D-CED
20	H	101	CLA	CBD-CGD-O2D-CED
20	b	610	CLA	CBD-CGD-O2D-CED
20	b	612	CLA	CBD-CGD-O2D-CED
20	c	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	c	514	CLA	CBD-CGD-O2D-CED
20	h	101	CLA	CBD-CGD-O2D-CED
26	A	412	LHG	O10-C23-O8-C6
26	a	412	LHG	O10-C23-O8-C6
20	B	606	CLA	O1D-CGD-O2D-CED
20	B	611	CLA	O1D-CGD-O2D-CED
20	C	507	CLA	O1D-CGD-O2D-CED
20	b	606	CLA	O1D-CGD-O2D-CED
20	b	611	CLA	O1D-CGD-O2D-CED
20	c	507	CLA	O1D-CGD-O2D-CED
27	C	508	F6C	O1D-CGD-O2D-CED
27	c	508	F6C	O1D-CGD-O2D-CED
24	A	410	PL9	C12-C13-C14-C16
24	D	406	PL9	C37-C38-C39-C41
24	a	410	PL9	C12-C13-C14-C16
24	d	406	PL9	C37-C38-C39-C41
20	B	603	CLA	CBD-CGD-O2D-CED
20	B	608	CLA	CBD-CGD-O2D-CED
20	B	609	CLA	CBD-CGD-O2D-CED
20	C	503	CLA	CBD-CGD-O2D-CED
20	C	512	CLA	CBD-CGD-O2D-CED
20	C	513	CLA	CBD-CGD-O2D-CED
20	b	603	CLA	CBD-CGD-O2D-CED
20	b	608	CLA	CBD-CGD-O2D-CED
20	b	609	CLA	CBD-CGD-O2D-CED
20	c	503	CLA	CBD-CGD-O2D-CED
20	c	512	CLA	CBD-CGD-O2D-CED
20	c	513	CLA	CBD-CGD-O2D-CED
27	B	613	F6C	CBD-CGD-O2D-CED
27	b	613	F6C	CBD-CGD-O2D-CED
20	B	603	CLA	O1A-CGA-O2A-C1
20	b	603	CLA	O1A-CGA-O2A-C1
28	C	517	DGD	O1A-C1A-O1G-C1G
28	c	517	DGD	O1A-C1A-O1G-C1G
20	B	612	CLA	O1D-CGD-O2D-CED
20	C	504	CLA	O1D-CGD-O2D-CED
20	c	504	CLA	O1D-CGD-O2D-CED
20	b	612	CLA	O1D-CGD-O2D-CED
23	A	409	SQD	O49-C7-O47-C45
23	L	102	SQD	O49-C7-O47-C45
23	a	409	SQD	O49-C7-O47-C45
23	l	102	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
26	D	408	LHG	O9-C7-O7-C5
26	d	408	LHG	O9-C7-O7-C5
20	C	506	CLA	O1A-CGA-O2A-C1
20	c	506	CLA	O1A-CGA-O2A-C1
20	B	610	CLA	C3-C5-C6-C7
20	b	610	CLA	C3-C5-C6-C7
21	A	406	PHO	C3-C5-C6-C7
21	a	406	PHO	C3-C5-C6-C7
27	B	604	F6C	C3-C5-C6-C7
27	b	604	F6C	C3-C5-C6-C7
29	D	401	CL7	C3-C5-C6-C7
29	d	401	CL7	C3-C5-C6-C7
27	C	508	F6C	CBA-CGA-O2A-C1
27	c	508	F6C	CBA-CGA-O2A-C1
28	C	517	DGD	C2A-C1A-O1G-C1G
28	c	517	DGD	C2A-C1A-O1G-C1G
29	D	401	CL7	CBA-CGA-O2A-C1
29	d	401	CL7	CBA-CGA-O2A-C1
20	C	510	CLA	C8-C10-C11-C12
20	c	510	CLA	C8-C10-C11-C12
30	M	101	LMG	C4-C5-C6-O5
30	m	101	LMG	C4-C5-C6-O5
20	B	614	CLA	C2-C3-C5-C6
20	b	614	CLA	C2-C3-C5-C6
24	D	406	PL9	C18-C19-C21-C22
24	d	406	PL9	C18-C19-C21-C22
20	A	407	CLA	C2A-CAA-CBA-CGA
20	B	611	CLA	C2A-CAA-CBA-CGA
20	C	510	CLA	C2A-CAA-CBA-CGA
20	a	407	CLA	C2A-CAA-CBA-CGA
20	b	611	CLA	C2A-CAA-CBA-CGA
20	c	510	CLA	C2A-CAA-CBA-CGA
20	C	510	CLA	O1A-CGA-O2A-C1
20	c	510	CLA	O1A-CGA-O2A-C1
23	A	409	SQD	O10-C23-O48-C46
23	a	409	SQD	O10-C23-O48-C46
20	B	606	CLA	C3-C5-C6-C7
20	B	615	CLA	C3-C5-C6-C7
20	b	606	CLA	C3-C5-C6-C7
20	b	615	CLA	C3-C5-C6-C7
27	B	613	F6C	C3-C5-C6-C7
27	b	613	F6C	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	B	603	CLA	CBA-CGA-O2A-C1
20	B	608	CLA	CBA-CGA-O2A-C1
20	B	610	CLA	CBA-CGA-O2A-C1
20	C	509	CLA	CBA-CGA-O2A-C1
20	C	510	CLA	CBA-CGA-O2A-C1
20	C	511	CLA	CBA-CGA-O2A-C1
20	C	512	CLA	CBA-CGA-O2A-C1
20	H	101	CLA	CBA-CGA-O2A-C1
20	b	603	CLA	CBA-CGA-O2A-C1
20	b	608	CLA	CBA-CGA-O2A-C1
20	b	610	CLA	CBA-CGA-O2A-C1
20	c	509	CLA	CBA-CGA-O2A-C1
20	c	510	CLA	CBA-CGA-O2A-C1
20	c	511	CLA	CBA-CGA-O2A-C1
20	c	512	CLA	CBA-CGA-O2A-C1
20	h	101	CLA	CBA-CGA-O2A-C1
21	D	402	PHO	CBD-CGD-O2D-CED
21	d	402	PHO	CBD-CGD-O2D-CED
27	C	508	F6C	O1A-CGA-O2A-C1
27	c	508	F6C	O1A-CGA-O2A-C1
29	D	401	CL7	O1A-CGA-O2A-C1
29	d	401	CL7	O1A-CGA-O2A-C1
22	B	618	BCR	C15-C16-C17-C18
22	b	618	BCR	C15-C16-C17-C18
20	D	403	CLA	CBD-CGD-O2D-CED
20	d	403	CLA	CBD-CGD-O2D-CED
21	A	406	PHO	CBD-CGD-O2D-CED
21	a	406	PHO	CBD-CGD-O2D-CED
20	C	503	CLA	C3-C5-C6-C7
20	c	503	CLA	C3-C5-C6-C7
20	B	605	CLA	CBA-CGA-O2A-C1
20	b	605	CLA	CBA-CGA-O2A-C1
20	B	608	CLA	O1A-CGA-O2A-C1
20	C	511	CLA	O1A-CGA-O2A-C1
20	H	101	CLA	O1A-CGA-O2A-C1
20	b	608	CLA	O1A-CGA-O2A-C1
20	c	511	CLA	O1A-CGA-O2A-C1
20	h	101	CLA	O1A-CGA-O2A-C1
21	A	406	PHO	O1A-CGA-O2A-C1
21	a	406	PHO	O1A-CGA-O2A-C1
20	C	511	CLA	O1D-CGD-O2D-CED
20	c	511	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	M	101	LMG	C11-C10-O7-C8
30	m	101	LMG	C11-C10-O7-C8
20	B	605	CLA	CBD-CGD-O2D-CED
20	b	605	CLA	CBD-CGD-O2D-CED
20	B	610	CLA	O1D-CGD-O2D-CED
20	b	610	CLA	O1D-CGD-O2D-CED
30	D	409	LMG	O6-C5-C6-O5
30	d	409	LMG	O6-C5-C6-O5
20	C	507	CLA	C3-C5-C6-C7
20	C	511	CLA	C3-C5-C6-C7
20	c	507	CLA	C3-C5-C6-C7
20	c	511	CLA	C3-C5-C6-C7
20	C	506	CLA	CBA-CGA-O2A-C1
20	c	506	CLA	CBA-CGA-O2A-C1
21	A	406	PHO	CBA-CGA-O2A-C1
21	a	406	PHO	CBA-CGA-O2A-C1
23	A	409	SQD	C24-C23-O48-C46
23	a	409	SQD	C24-C23-O48-C46
20	B	605	CLA	O1A-CGA-O2A-C1
20	C	512	CLA	O1A-CGA-O2A-C1
20	b	605	CLA	O1A-CGA-O2A-C1
20	c	512	CLA	O1A-CGA-O2A-C1
27	B	604	F6C	C2A-CAA-CBA-CGA
27	b	604	F6C	C2A-CAA-CBA-CGA
30	M	101	LMG	O6-C5-C6-O5
30	m	101	LMG	O6-C5-C6-O5
20	B	603	CLA	C4-C3-C5-C6
20	b	603	CLA	C4-C3-C5-C6
27	C	508	F6C	C4-C3-C5-C6
27	c	508	F6C	C4-C3-C5-C6
20	B	603	CLA	C2-C3-C5-C6
20	b	603	CLA	C2-C3-C5-C6
27	B	604	F6C	C2-C3-C5-C6
27	C	508	F6C	C2-C3-C5-C6
27	b	604	F6C	C2-C3-C5-C6
27	c	508	F6C	C2-C3-C5-C6
20	B	601	CLA	C2A-CAA-CBA-CGA
20	b	601	CLA	C2A-CAA-CBA-CGA
29	D	401	CL7	C2A-CAA-CBA-CGA
29	d	401	CL7	C2A-CAA-CBA-CGA
20	C	509	CLA	O1A-CGA-O2A-C1
20	c	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	L	102	SQD	O5-C1-O6-C44
23	l	102	SQD	O5-C1-O6-C44
28	c	517	DGD	O6D-C1D-O3G-C3G
24	D	406	PL9	C9-C11-C12-C13
24	d	406	PL9	C9-C11-C12-C13
20	B	602	CLA	CBA-CGA-O2A-C1
20	b	602	CLA	CBA-CGA-O2A-C1
26	D	408	LHG	C11-C10-C9-C8
26	d	408	LHG	C11-C10-C9-C8
20	H	101	CLA	O1D-CGD-O2D-CED
20	h	101	CLA	O1D-CGD-O2D-CED
20	B	608	CLA	O1D-CGD-O2D-CED
20	b	608	CLA	O1D-CGD-O2D-CED
23	A	409	SQD	C28-C29-C30-C31
23	a	409	SQD	C28-C29-C30-C31
26	L	101	LHG	C1-C2-C3-O3
26	l	101	LHG	C1-C2-C3-O3
30	M	101	LMG	O9-C10-O7-C8
30	m	101	LMG	O9-C10-O7-C8
20	B	610	CLA	O1A-CGA-O2A-C1
20	b	610	CLA	O1A-CGA-O2A-C1
20	B	605	CLA	C3-C5-C6-C7
20	b	605	CLA	C3-C5-C6-C7
20	B	612	CLA	CBA-CGA-O2A-C1
20	B	615	CLA	CBA-CGA-O2A-C1
20	C	507	CLA	CBA-CGA-O2A-C1
20	b	612	CLA	CBA-CGA-O2A-C1
20	b	615	CLA	CBA-CGA-O2A-C1
20	c	507	CLA	CBA-CGA-O2A-C1
22	b	616	BCR	C9-C10-C11-C12
32	H	102	RRX	C15-C16-C17-C18
32	h	102	RRX	C15-C16-C17-C18
26	A	412	LHG	O6-C4-C5-O7
26	a	412	LHG	O6-C4-C5-O7
20	C	504	CLA	C15-C16-C17-C18
20	c	504	CLA	C15-C16-C17-C18
21	A	406	PHO	C10-C11-C12-C13
21	a	406	PHO	C10-C11-C12-C13
26	D	408	LHG	O2-C2-C3-O3
26	d	408	LHG	O2-C2-C3-O3
20	B	605	CLA	C11-C12-C13-C14
20	B	610	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	b	605	CLA	C11-C12-C13-C14
20	b	610	CLA	C14-C13-C15-C16
27	B	607	F6C	C6-C7-C8-C9
27	B	613	F6C	C11-C10-C8-C9
27	C	508	F6C	C11-C10-C8-C9
27	b	607	F6C	C6-C7-C8-C9
27	b	613	F6C	C11-C10-C8-C9
27	c	508	F6C	C11-C10-C8-C9
20	C	503	CLA	O1D-CGD-O2D-CED
20	c	503	CLA	O1D-CGD-O2D-CED
20	B	614	CLA	CBD-CGD-O2D-CED
20	b	614	CLA	CBD-CGD-O2D-CED
22	B	617	BCR	C11-C12-C13-C35
22	C	518	BCR	C7-C8-C9-C34
22	b	617	BCR	C11-C12-C13-C35
22	c	518	BCR	C7-C8-C9-C34
28	C	517	DGD	O1B-C1B-O2G-C2G
28	c	517	DGD	O1B-C1B-O2G-C2G
20	C	507	CLA	O1A-CGA-O2A-C1
20	c	507	CLA	O1A-CGA-O2A-C1
20	B	612	CLA	C10-C11-C12-C13
20	C	503	CLA	C5-C6-C7-C8
20	C	511	CLA	C10-C11-C12-C13
20	b	612	CLA	C10-C11-C12-C13
20	c	503	CLA	C5-C6-C7-C8
20	c	511	CLA	C10-C11-C12-C13
27	C	508	F6C	C8-C10-C11-C12
27	c	508	F6C	C8-C10-C11-C12
20	C	513	CLA	O1D-CGD-O2D-CED
20	c	513	CLA	O1D-CGD-O2D-CED
20	b	603	CLA	O1D-CGD-O2D-CED
21	D	402	PHO	C3-C5-C6-C7
21	d	402	PHO	C3-C5-C6-C7
20	B	602	CLA	C13-C15-C16-C17
20	B	606	CLA	C5-C6-C7-C8
20	B	610	CLA	C8-C10-C11-C12
20	C	503	CLA	C15-C16-C17-C18
20	C	511	CLA	C15-C16-C17-C18
20	b	602	CLA	C13-C15-C16-C17
20	b	606	CLA	C5-C6-C7-C8
20	b	610	CLA	C8-C10-C11-C12
20	c	503	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	c	511	CLA	C15-C16-C17-C18
28	D	410	DGD	C1B-C2B-C3B-C4B
28	d	410	DGD	C1B-C2B-C3B-C4B
20	B	603	CLA	O1D-CGD-O2D-CED
20	B	602	CLA	C10-C11-C12-C13
20	B	611	CLA	C13-C15-C16-C17
20	b	602	CLA	C10-C11-C12-C13
20	b	611	CLA	C13-C15-C16-C17
29	D	401	CL7	C15-C16-C17-C18
29	d	401	CL7	C15-C16-C17-C18
27	B	613	F6C	O1D-CGD-O2D-CED
27	b	613	F6C	O1D-CGD-O2D-CED
23	A	409	SQD	C23-C24-C25-C26
23	a	409	SQD	C23-C24-C25-C26
26	A	412	LHG	C23-C24-C25-C26
26	a	412	LHG	C23-C24-C25-C26
27	B	607	F6C	C5-C6-C7-C8
27	b	607	F6C	C5-C6-C7-C8
20	B	609	CLA	O1D-CGD-O2D-CED
20	b	609	CLA	O1D-CGD-O2D-CED
20	B	612	CLA	C2-C1-O2A-CGA
20	C	504	CLA	C2-C1-O2A-CGA
20	b	612	CLA	C2-C1-O2A-CGA
20	c	504	CLA	C2-C1-O2A-CGA
20	C	506	CLA	C10-C11-C12-C13
20	c	506	CLA	C10-C11-C12-C13
23	L	102	SQD	C7-C8-C9-C10
23	l	102	SQD	C7-C8-C9-C10
27	B	607	F6C	C2A-CAA-CBA-CGA
27	b	607	F6C	C2A-CAA-CBA-CGA
27	B	613	F6C	C11-C10-C8-C7
27	b	613	F6C	C11-C10-C8-C7
20	B	615	CLA	O1A-CGA-O2A-C1
20	b	615	CLA	O1A-CGA-O2A-C1
22	B	616	BCR	C9-C10-C11-C12
20	C	512	CLA	O1D-CGD-O2D-CED
20	c	512	CLA	O1D-CGD-O2D-CED
20	C	504	CLA	C5-C6-C7-C8
20	c	504	CLA	C5-C6-C7-C8
20	B	603	CLA	C2C-C3C-CAC-CBC
20	b	603	CLA	C2C-C3C-CAC-CBC
27	B	604	F6C	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	b	604	F6C	C13-C15-C16-C17
26	A	412	LHG	C7-C8-C9-C10
26	a	412	LHG	C7-C8-C9-C10
22	B	617	BCR	C10-C11-C12-C13
22	b	617	BCR	C10-C11-C12-C13
32	H	102	RRX	C18-C19-C20-C21
32	h	102	RRX	C18-C19-C20-C21
20	B	608	CLA	C5-C6-C7-C8
20	C	503	CLA	C8-C10-C11-C12
20	C	511	CLA	C13-C15-C16-C17
20	b	608	CLA	C5-C6-C7-C8
20	c	503	CLA	C8-C10-C11-C12
20	c	511	CLA	C13-C15-C16-C17
20	B	602	CLA	O1A-CGA-O2A-C1
20	B	612	CLA	O1A-CGA-O2A-C1
20	b	602	CLA	O1A-CGA-O2A-C1
20	b	612	CLA	O1A-CGA-O2A-C1
20	B	612	CLA	C8-C10-C11-C12
20	B	612	CLA	C13-C15-C16-C17
20	C	502	CLA	C8-C10-C11-C12
20	b	612	CLA	C8-C10-C11-C12
20	b	612	CLA	C13-C15-C16-C17
20	c	502	CLA	C8-C10-C11-C12
29	D	401	CL7	C13-C15-C16-C17
29	d	401	CL7	C13-C15-C16-C17
26	A	412	LHG	C3-O3-P-O6
26	A	412	LHG	C4-O6-P-O3
26	D	407	LHG	C3-O3-P-O6
26	D	408	LHG	C3-O3-P-O6
26	L	101	LHG	C4-O6-P-O3
26	a	412	LHG	C3-O3-P-O6
26	a	412	LHG	C4-O6-P-O3
26	d	407	LHG	C3-O3-P-O6
26	d	408	LHG	C3-O3-P-O6
26	l	101	LHG	C4-O6-P-O3
26	L	101	LHG	C23-C24-C25-C26
26	l	101	LHG	C23-C24-C25-C26
27	B	607	F6C	CBA-CGA-O2A-C1
27	b	607	F6C	CBA-CGA-O2A-C1
20	d	404	CLA	CBD-CGD-O2D-CED
20	B	611	CLA	C8-C10-C11-C12
20	b	611	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	D	404	CLA	CBD-CGD-O2D-CED
20	B	602	CLA	C2A-CAA-CBA-CGA
20	B	606	CLA	C2A-CAA-CBA-CGA
20	b	602	CLA	C2A-CAA-CBA-CGA
20	b	606	CLA	C2A-CAA-CBA-CGA
20	C	509	CLA	C11-C12-C13-C14
20	c	509	CLA	C11-C12-C13-C14
20	C	504	CLA	CBA-CGA-O2A-C1
20	c	504	CLA	CBA-CGA-O2A-C1
23	A	409	SQD	C34-C35-C36-C37
23	a	409	SQD	C34-C35-C36-C37
26	l	101	LHG	C34-C35-C36-C37
22	A	408	BCR	C11-C10-C9-C34
22	a	408	BCR	C11-C10-C9-C34
23	A	409	SQD	C25-C26-C27-C28
23	a	409	SQD	C25-C26-C27-C28
26	L	101	LHG	C34-C35-C36-C37
20	C	506	CLA	C11-C12-C13-C15
20	c	506	CLA	C11-C12-C13-C15
27	C	508	F6C	C11-C12-C13-C14
27	c	508	F6C	C11-C12-C13-C14
23	A	409	SQD	C15-C16-C17-C18
23	a	409	SQD	C15-C16-C17-C18
26	L	101	LHG	C18-C19-C20-C21
26	l	101	LHG	C18-C19-C20-C21
23	L	102	SQD	C46-C45-O47-C7
23	l	102	SQD	C46-C45-O47-C7
27	C	508	F6C	C10-C11-C12-C13
21	D	402	PHO	O1D-CGD-O2D-CED
21	d	402	PHO	O1D-CGD-O2D-CED
28	D	410	DGD	CBA-CCA-CDA-CEA
28	d	410	DGD	CBA-CCA-CDA-CEA
27	c	508	F6C	C10-C11-C12-C13
26	L	101	LHG	O2-C2-C3-O3
26	l	101	LHG	O2-C2-C3-O3
26	L	101	LHG	C29-C30-C31-C32
26	l	101	LHG	C29-C30-C31-C32
33	M	102	LMT	O1'-C1-C2-C3
33	m	102	LMT	O1'-C1-C2-C3
22	A	408	BCR	C11-C10-C9-C8
22	a	408	BCR	C11-C10-C9-C8
28	C	517	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	C2D-C1D-O3G-C3G
26	D	408	LHG	C27-C28-C29-C30
26	d	408	LHG	C27-C28-C29-C30
20	C	504	CLA	O1A-CGA-O2A-C1
20	c	504	CLA	O1A-CGA-O2A-C1
27	B	607	F6C	O1A-CGA-O2A-C1
27	b	607	F6C	O1A-CGA-O2A-C1
21	A	406	PHO	O1D-CGD-O2D-CED
21	a	406	PHO	O1D-CGD-O2D-CED
26	D	407	LHG	C34-C35-C36-C37
26	d	407	LHG	C34-C35-C36-C37
32	H	102	RRX	C36-C18-C19-C20
32	h	102	RRX	C36-C18-C19-C20
26	D	407	LHG	O1-C1-C2-C3
26	d	407	LHG	O1-C1-C2-C3
32	H	102	RRX	C17-C18-C19-C20
32	h	102	RRX	C17-C18-C19-C20
23	L	102	SQD	C32-C33-C34-C35
23	l	102	SQD	C32-C33-C34-C35
26	A	412	LHG	C26-C27-C28-C29
26	D	407	LHG	C18-C19-C20-C21
26	a	412	LHG	C26-C27-C28-C29
26	d	407	LHG	C18-C19-C20-C21
20	B	601	CLA	CBD-CGD-O2D-CED
20	b	601	CLA	CBD-CGD-O2D-CED
26	D	407	LHG	C7-C8-C9-C10
26	D	407	LHG	C23-C24-C25-C26
26	d	407	LHG	C7-C8-C9-C10
26	d	407	LHG	C23-C24-C25-C26
23	A	409	SQD	C11-C10-C9-C8
23	a	409	SQD	C11-C10-C9-C8
23	l	102	SQD	C9-C10-C11-C12
26	D	407	LHG	C28-C29-C30-C31
26	L	101	LHG	C26-C27-C28-C29
26	d	407	LHG	C28-C29-C30-C31
26	l	101	LHG	C26-C27-C28-C29
28	D	410	DGD	C6B-C7B-C8B-C9B
28	d	410	DGD	C6B-C7B-C8B-C9B
20	B	614	CLA	C6-C7-C8-C10
20	b	614	CLA	C6-C7-C8-C10
27	B	607	F6C	C11-C12-C13-C15
27	C	508	F6C	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	b	607	F6C	C11-C12-C13-C15
27	c	508	F6C	C11-C12-C13-C15
26	D	408	LHG	O6-C4-C5-C6
26	d	408	LHG	O6-C4-C5-C6
23	L	102	SQD	C9-C10-C11-C12
26	L	101	LHG	C15-C16-C17-C18
26	l	101	LHG	C15-C16-C17-C18
28	C	516	DGD	C8B-C9B-CAB-CBB
29	D	401	CL7	C2C-C3C-CAC-CBC
29	d	401	CL7	C2C-C3C-CAC-CBC
26	L	101	LHG	C13-C14-C15-C16
26	l	101	LHG	C13-C14-C15-C16
28	c	516	DGD	C8B-C9B-CAB-CBB
23	A	409	SQD	C9-C10-C11-C12
23	A	409	SQD	C13-C14-C15-C16
23	a	409	SQD	C9-C10-C11-C12
23	a	409	SQD	C13-C14-C15-C16
20	B	605	CLA	C3A-C2A-CAA-CBA
20	B	615	CLA	C3A-C2A-CAA-CBA
20	C	513	CLA	C3A-C2A-CAA-CBA
20	b	605	CLA	C3A-C2A-CAA-CBA
20	b	615	CLA	C3A-C2A-CAA-CBA
20	c	513	CLA	C3A-C2A-CAA-CBA
33	M	102	LMT	C2-C1-O1'-C1'
33	m	102	LMT	C2-C1-O1'-C1'
20	C	509	CLA	C11-C12-C13-C15
20	c	509	CLA	C11-C12-C13-C15
27	B	607	F6C	C11-C12-C13-C14
27	b	607	F6C	C11-C12-C13-C14
20	A	407	CLA	C2C-C3C-CAC-CBC
20	a	407	CLA	C2C-C3C-CAC-CBC
23	a	409	SQD	C30-C31-C32-C33
20	D	403	CLA	O1D-CGD-O2D-CED
20	d	403	CLA	O1D-CGD-O2D-CED
23	A	409	SQD	C30-C31-C32-C33
26	D	407	LHG	C32-C33-C34-C35
26	d	407	LHG	C32-C33-C34-C35
27	C	508	F6C	C1A-C2A-CAA-CBA
27	c	508	F6C	C1A-C2A-CAA-CBA
20	C	506	CLA	C4-C3-C5-C6
20	c	506	CLA	C4-C3-C5-C6
20	C	506	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	c	506	CLA	C2-C3-C5-C6
26	A	412	LHG	C25-C26-C27-C28
26	D	407	LHG	C29-C30-C31-C32
26	L	101	LHG	C17-C18-C19-C20
26	a	412	LHG	C25-C26-C27-C28
26	d	407	LHG	C29-C30-C31-C32
26	l	101	LHG	C17-C18-C19-C20
20	C	506	CLA	C2A-CAA-CBA-CGA
20	c	506	CLA	C2A-CAA-CBA-CGA
26	D	407	LHG	O1-C1-C2-O2
26	d	407	LHG	O1-C1-C2-O2
26	L	101	LHG	C25-C26-C27-C28
26	l	101	LHG	C25-C26-C27-C28
28	D	410	DGD	C7B-C8B-C9B-CAB
28	d	410	DGD	C7B-C8B-C9B-CAB
28	C	517	DGD	C1A-C2A-C3A-C4A
28	c	517	DGD	C1A-C2A-C3A-C4A
20	B	614	CLA	C3-C5-C6-C7
20	b	614	CLA	C3-C5-C6-C7
28	C	516	DGD	C4D-C5D-C6D-O5D
28	c	516	DGD	C4D-C5D-C6D-O5D
20	C	505	CLA	CBA-CGA-O2A-C1
20	c	505	CLA	CBA-CGA-O2A-C1
26	D	408	LHG	C13-C14-C15-C16
26	d	408	LHG	C13-C14-C15-C16
20	C	512	CLA	C2-C1-O2A-CGA
20	c	512	CLA	C2-C1-O2A-CGA
27	B	604	F6C	C2-C1-O2A-CGA
27	b	604	F6C	C2-C1-O2A-CGA
28	C	516	DGD	O6D-C5D-C6D-O5D
28	c	516	DGD	O6D-C5D-C6D-O5D
20	C	504	CLA	C8-C10-C11-C12
20	c	504	CLA	C8-C10-C11-C12
20	C	506	CLA	C11-C12-C13-C14
20	c	506	CLA	C11-C12-C13-C14
22	A	408	BCR	C23-C24-C25-C26
22	B	616	BCR	C1-C6-C7-C8
22	B	616	BCR	C5-C6-C7-C8
22	B	616	BCR	C23-C24-C25-C26
22	B	616	BCR	C23-C24-C25-C30
22	B	618	BCR	C1-C6-C7-C8
22	B	618	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	618	BCR	C23-C24-C25-C26
22	C	515	BCR	C1-C6-C7-C8
22	C	515	BCR	C23-C24-C25-C26
22	C	515	BCR	C23-C24-C25-C30
22	C	518	BCR	C5-C6-C7-C8
22	D	405	BCR	C5-C6-C7-C8
22	a	408	BCR	C23-C24-C25-C26
22	b	616	BCR	C1-C6-C7-C8
22	b	616	BCR	C5-C6-C7-C8
22	b	616	BCR	C23-C24-C25-C26
22	b	616	BCR	C23-C24-C25-C30
22	b	618	BCR	C1-C6-C7-C8
22	b	618	BCR	C5-C6-C7-C8
22	b	618	BCR	C23-C24-C25-C26
22	c	515	BCR	C1-C6-C7-C8
22	c	515	BCR	C23-C24-C25-C26
22	c	515	BCR	C23-C24-C25-C30
22	c	518	BCR	C5-C6-C7-C8
22	d	405	BCR	C5-C6-C7-C8
23	a	409	SQD	C14-C15-C16-C17
20	B	606	CLA	CBA-CGA-O2A-C1
20	b	606	CLA	CBA-CGA-O2A-C1
23	A	409	SQD	C14-C15-C16-C17
26	A	412	LHG	C28-C29-C30-C31
26	a	412	LHG	C28-C29-C30-C31
27	B	604	F6C	C15-C16-C17-C18
27	b	604	F6C	C15-C16-C17-C18
26	D	407	LHG	C9-C10-C11-C12
26	d	407	LHG	C9-C10-C11-C12
20	C	506	CLA	C6-C7-C8-C10
20	c	506	CLA	C6-C7-C8-C10
21	A	406	PHO	C11-C10-C8-C7
21	a	406	PHO	C11-C10-C8-C7
20	C	505	CLA	O1A-CGA-O2A-C1
20	c	505	CLA	O1A-CGA-O2A-C1
20	B	610	CLA	C10-C11-C12-C13
20	b	610	CLA	C10-C11-C12-C13
20	A	404	CLA	CBA-CGA-O2A-C1
20	D	403	CLA	CBA-CGA-O2A-C1
20	a	404	CLA	CBA-CGA-O2A-C1
20	d	403	CLA	CBA-CGA-O2A-C1
27	B	613	F6C	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	b	613	F6C	CBA-CGA-O2A-C1
26	D	408	LHG	C11-C12-C13-C14
26	d	408	LHG	C11-C12-C13-C14
20	A	404	CLA	C2A-CAA-CBA-CGA
20	A	405	CLA	C2A-CAA-CBA-CGA
20	B	608	CLA	C2A-CAA-CBA-CGA
20	C	513	CLA	C2A-CAA-CBA-CGA
20	a	404	CLA	C2A-CAA-CBA-CGA
20	a	405	CLA	C2A-CAA-CBA-CGA
20	b	608	CLA	C2A-CAA-CBA-CGA
20	c	513	CLA	C2A-CAA-CBA-CGA
20	C	511	CLA	C5-C6-C7-C8
20	c	511	CLA	C5-C6-C7-C8
28	C	516	DGD	C9B-CAB-CBB-CCB
28	c	516	DGD	C9B-CAB-CBB-CCB
26	D	408	LHG	C23-C24-C25-C26
26	d	408	LHG	C23-C24-C25-C26
20	C	509	CLA	C8-C10-C11-C12
20	c	509	CLA	C8-C10-C11-C12
26	D	407	LHG	C27-C28-C29-C30
26	d	407	LHG	C27-C28-C29-C30
20	B	605	CLA	O1D-CGD-O2D-CED
26	L	101	LHG	C11-C12-C13-C14
26	l	101	LHG	C11-C12-C13-C14
20	b	605	CLA	O1D-CGD-O2D-CED
26	A	412	LHG	C8-C7-O7-C5
26	D	407	LHG	C8-C7-O7-C5
26	a	412	LHG	C8-C7-O7-C5
26	d	407	LHG	C8-C7-O7-C5
28	C	517	DGD	C2B-C1B-O2G-C2G
28	c	517	DGD	C2B-C1B-O2G-C2G
22	d	405	BCR	C10-C11-C12-C13
23	L	102	SQD	C16-C17-C18-C19
23	l	102	SQD	C16-C17-C18-C19
27	C	508	F6C	C4B-C3B-CAB-CBB
27	c	508	F6C	C4B-C3B-CAB-CBB
30	M	101	LMG	C31-C32-C33-C34
30	m	101	LMG	C31-C32-C33-C34
26	A	412	LHG	O9-C7-O7-C5
26	D	407	LHG	O9-C7-O7-C5
26	a	412	LHG	O9-C7-O7-C5
26	d	407	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	B	607	F6C	C3-C5-C6-C7
27	b	607	F6C	C3-C5-C6-C7
28	C	516	DGD	O6E-C5E-C6E-O5E
28	c	516	DGD	O6E-C5E-C6E-O5E
20	B	606	CLA	O1A-CGA-O2A-C1
20	b	606	CLA	O1A-CGA-O2A-C1
28	C	517	DGD	C2B-C3B-C4B-C5B
28	c	517	DGD	C2B-C3B-C4B-C5B
24	A	410	PL9	C4-C3-C7-C8
24	D	406	PL9	C4-C3-C7-C8
24	a	410	PL9	C4-C3-C7-C8
24	d	406	PL9	C4-C3-C7-C8
20	B	605	CLA	C14-C13-C15-C16
20	C	506	CLA	C6-C7-C8-C9
20	b	605	CLA	C14-C13-C15-C16
20	c	506	CLA	C6-C7-C8-C9
21	A	406	PHO	C11-C10-C8-C9
21	a	406	PHO	C11-C10-C8-C9
21	a	406	PHO	C8-C10-C11-C12
22	A	408	BCR	C36-C18-C19-C20
22	a	408	BCR	C36-C18-C19-C20
21	A	406	PHO	C8-C10-C11-C12
20	A	407	CLA	C1A-C2A-CAA-CBA
20	B	608	CLA	C1A-C2A-CAA-CBA
20	B	615	CLA	C1A-C2A-CAA-CBA
20	C	502	CLA	C1A-C2A-CAA-CBA
20	C	503	CLA	C1A-C2A-CAA-CBA
20	C	504	CLA	C1A-C2A-CAA-CBA
20	C	507	CLA	C1A-C2A-CAA-CBA
20	C	509	CLA	C1A-C2A-CAA-CBA
20	C	512	CLA	C1A-C2A-CAA-CBA
20	D	404	CLA	C1A-C2A-CAA-CBA
20	a	407	CLA	C1A-C2A-CAA-CBA
20	b	608	CLA	C1A-C2A-CAA-CBA
20	b	615	CLA	C1A-C2A-CAA-CBA
20	c	502	CLA	C1A-C2A-CAA-CBA
20	c	503	CLA	C1A-C2A-CAA-CBA
20	c	504	CLA	C1A-C2A-CAA-CBA
20	c	507	CLA	C1A-C2A-CAA-CBA
20	c	509	CLA	C1A-C2A-CAA-CBA
20	c	512	CLA	C1A-C2A-CAA-CBA
20	d	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	H	102	RRX	C9-C10-C11-C12
32	h	102	RRX	C9-C10-C11-C12
20	C	506	CLA	C5-C6-C7-C8
20	c	506	CLA	C5-C6-C7-C8
26	D	408	LHG	C28-C29-C30-C31
20	C	506	CLA	C3-C5-C6-C7
20	c	506	CLA	C3-C5-C6-C7
26	d	408	LHG	C28-C29-C30-C31
27	B	613	F6C	O1A-CGA-O2A-C1
27	b	613	F6C	O1A-CGA-O2A-C1
28	C	516	DGD	C6B-C7B-C8B-C9B
28	c	516	DGD	C6B-C7B-C8B-C9B
28	C	517	DGD	C4A-C5A-C6A-C7A
28	c	517	DGD	C4A-C5A-C6A-C7A
20	B	603	CLA	C4C-C3C-CAC-CBC
20	b	603	CLA	C4C-C3C-CAC-CBC
20	A	404	CLA	O1A-CGA-O2A-C1
20	a	404	CLA	O1A-CGA-O2A-C1
20	B	603	CLA	C3-C5-C6-C7
20	b	603	CLA	C3-C5-C6-C7
26	D	407	LHG	C4-C5-C6-O8
26	d	407	LHG	C4-C5-C6-O8
30	M	101	LMG	O1-C7-C8-C9
26	D	408	LHG	C10-C11-C12-C13
26	d	408	LHG	C10-C11-C12-C13
20	b	602	CLA	C2C-C3C-CAC-CBC
20	C	504	CLA	C3-C5-C6-C7
20	c	504	CLA	C3-C5-C6-C7
20	B	602	CLA	C2C-C3C-CAC-CBC
30	M	101	LMG	C28-C29-C30-C31
30	m	101	LMG	C28-C29-C30-C31
23	L	102	SQD	C24-C25-C26-C27
23	l	102	SQD	C24-C25-C26-C27
23	A	409	SQD	C46-C45-O47-C7
23	a	409	SQD	C46-C45-O47-C7
20	C	502	CLA	C2A-CAA-CBA-CGA
20	c	502	CLA	C2A-CAA-CBA-CGA
21	A	406	PHO	C5-C6-C7-C8
21	a	406	PHO	C5-C6-C7-C8
20	B	614	CLA	O1D-CGD-O2D-CED
20	b	614	CLA	O1D-CGD-O2D-CED
26	L	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	l	101	LHG	C7-C8-C9-C10
20	D	404	CLA	O1D-CGD-O2D-CED
20	d	404	CLA	O1D-CGD-O2D-CED
23	A	409	SQD	C17-C18-C19-C20
23	a	409	SQD	C17-C18-C19-C20
20	B	615	CLA	C10-C11-C12-C13
20	b	615	CLA	C10-C11-C12-C13
28	C	517	DGD	C5B-C6B-C7B-C8B
33	M	102	LMT	C1-C2-C3-C4
33	m	102	LMT	C1-C2-C3-C4
28	c	517	DGD	C5B-C6B-C7B-C8B
20	D	403	CLA	O1A-CGA-O2A-C1
20	d	403	CLA	O1A-CGA-O2A-C1
28	D	410	DGD	O1A-C1A-O1G-C1G
28	d	410	DGD	O1A-C1A-O1G-C1G
20	B	611	CLA	C16-C17-C18-C20
20	b	611	CLA	C16-C17-C18-C20
26	D	407	LHG	C11-C10-C9-C8
26	d	407	LHG	C11-C10-C9-C8
20	B	605	CLA	C11-C12-C13-C15
20	B	610	CLA	C12-C13-C15-C16
20	B	612	CLA	C6-C7-C8-C10
20	C	511	CLA	C11-C10-C8-C7
20	b	605	CLA	C11-C12-C13-C15
20	b	610	CLA	C12-C13-C15-C16
20	b	612	CLA	C6-C7-C8-C10
20	c	511	CLA	C11-C10-C8-C7
20	C	511	CLA	C11-C10-C8-C9
20	c	511	CLA	C11-C10-C8-C9
27	B	604	F6C	C11-C12-C13-C14
27	b	604	F6C	C11-C12-C13-C14
22	B	617	BCR	C11-C12-C13-C14
20	A	407	CLA	CBA-CGA-O2A-C1
20	a	407	CLA	CBA-CGA-O2A-C1
30	D	409	LMG	C4-C5-C6-O5
30	d	409	LMG	C4-C5-C6-O5
20	B	614	CLA	C6-C7-C8-C9
20	b	614	CLA	C6-C7-C8-C9
33	M	102	LMT	O5'-C1'-O1'-C1
33	m	102	LMT	O5'-C1'-O1'-C1
26	A	412	LHG	O6-C4-C5-C6
26	L	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	a	412	LHG	O6-C4-C5-C6
26	l	101	LHG	O6-C4-C5-C6
20	C	509	CLA	C3-C5-C6-C7
20	c	509	CLA	C3-C5-C6-C7
22	D	405	BCR	C10-C11-C12-C13
27	C	508	F6C	C5-C6-C7-C8
27	c	508	F6C	C5-C6-C7-C8
20	b	601	CLA	O1D-CGD-O2D-CED
20	C	502	CLA	C4-C3-C5-C6
20	C	503	CLA	C4-C3-C5-C6
20	c	502	CLA	C4-C3-C5-C6
20	c	503	CLA	C4-C3-C5-C6
20	C	502	CLA	C2-C3-C5-C6
20	c	502	CLA	C2-C3-C5-C6
26	A	412	LHG	C27-C28-C29-C30
26	a	412	LHG	C27-C28-C29-C30
20	B	601	CLA	O1D-CGD-O2D-CED
20	A	405	CLA	C3A-C2A-CAA-CBA
20	B	601	CLA	C3A-C2A-CAA-CBA
20	B	610	CLA	C3A-C2A-CAA-CBA
20	B	611	CLA	C3A-C2A-CAA-CBA
20	D	403	CLA	C3A-C2A-CAA-CBA
20	a	405	CLA	C3A-C2A-CAA-CBA
20	b	601	CLA	C3A-C2A-CAA-CBA
20	b	610	CLA	C3A-C2A-CAA-CBA
20	b	611	CLA	C3A-C2A-CAA-CBA
20	d	403	CLA	C3A-C2A-CAA-CBA
26	A	412	LHG	C9-C10-C11-C12
26	a	412	LHG	C9-C10-C11-C12
20	B	611	CLA	C16-C17-C18-C19
20	b	611	CLA	C16-C17-C18-C19
31	E	101	HEM	C3D-CAD-CBD-CGD
31	e	101	HEM	C3D-CAD-CBD-CGD
26	A	412	LHG	C31-C32-C33-C34
26	a	412	LHG	C31-C32-C33-C34
23	L	102	SQD	C44-C45-C46-O48
23	l	102	SQD	C44-C45-C46-O48
30	m	101	LMG	O1-C7-C8-C9
26	L	101	LHG	C19-C20-C21-C22
26	l	101	LHG	C19-C20-C21-C22
20	A	404	CLA	C3-C5-C6-C7
20	a	404	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	A	412	LHG	C30-C31-C32-C33
26	D	408	LHG	C31-C32-C33-C34
26	a	412	LHG	C30-C31-C32-C33
26	d	408	LHG	C31-C32-C33-C34
20	C	511	CLA	C16-C17-C18-C19
26	L	101	LHG	C3-O3-P-O6
26	l	101	LHG	C3-O3-P-O6
23	A	409	SQD	C35-C36-C37-C38
23	L	102	SQD	C34-C35-C36-C37
23	a	409	SQD	C35-C36-C37-C38
21	D	402	PHO	C8-C10-C11-C12
21	d	402	PHO	C8-C10-C11-C12
23	l	102	SQD	C34-C35-C36-C37
26	L	101	LHG	O6-C4-C5-O7
26	l	101	LHG	O6-C4-C5-O7
20	c	511	CLA	C16-C17-C18-C19
27	B	613	F6C	C16-C17-C18-C20
27	b	613	F6C	C16-C17-C18-C20
26	D	408	LHG	C29-C30-C31-C32
26	d	408	LHG	C29-C30-C31-C32
28	C	516	DGD	CAB-CBB-CCB-CDB
28	c	516	DGD	CAB-CBB-CCB-CDB
29	d	401	CL7	C4C-C3C-CAC-CBC
29	D	401	CL7	C4C-C3C-CAC-CBC
20	A	407	CLA	C4C-C3C-CAC-CBC
30	M	101	LMG	O1-C7-C8-O7
30	m	101	LMG	O1-C7-C8-O7
20	a	407	CLA	C4C-C3C-CAC-CBC
26	D	408	LHG	C1-C2-C3-O3
26	d	408	LHG	C1-C2-C3-O3
20	B	611	CLA	C14-C13-C15-C16
20	B	612	CLA	C11-C12-C13-C14
20	C	509	CLA	C11-C10-C8-C9
20	b	611	CLA	C14-C13-C15-C16
20	b	612	CLA	C11-C12-C13-C14
20	c	509	CLA	C11-C10-C8-C9
21	A	406	PHO	C14-C13-C15-C16
21	a	406	PHO	C14-C13-C15-C16
23	L	102	SQD	C11-C10-C9-C8
23	l	102	SQD	C11-C10-C9-C8
22	A	408	BCR	C23-C24-C25-C30
22	a	408	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
32	H	102	RRX	C23-C24-C25-C26
32	h	102	RRX	C23-C24-C25-C26
26	A	412	LHG	C32-C33-C34-C35
26	a	412	LHG	C32-C33-C34-C35
22	b	617	BCR	C11-C12-C13-C14
20	C	504	CLA	C16-C17-C18-C19
20	c	504	CLA	C16-C17-C18-C19
20	A	407	CLA	O1A-CGA-O2A-C1
20	B	610	CLA	C11-C10-C8-C7
20	B	611	CLA	C12-C13-C15-C16
20	B	612	CLA	C11-C12-C13-C15
20	C	510	CLA	C6-C7-C8-C10
20	D	403	CLA	C11-C10-C8-C7
20	b	610	CLA	C11-C10-C8-C7
20	b	611	CLA	C12-C13-C15-C16
20	b	612	CLA	C11-C12-C13-C15
20	c	510	CLA	C6-C7-C8-C10
20	d	403	CLA	C11-C10-C8-C7
21	A	406	PHO	C12-C13-C15-C16
21	a	406	PHO	C12-C13-C15-C16
27	B	604	F6C	C11-C12-C13-C15
27	B	613	F6C	C6-C7-C8-C10
27	B	613	F6C	C11-C12-C13-C15
27	b	604	F6C	C11-C12-C13-C15
27	b	613	F6C	C6-C7-C8-C10
27	b	613	F6C	C11-C12-C13-C15
20	a	407	CLA	O1A-CGA-O2A-C1
20	B	615	CLA	C8-C10-C11-C12
20	b	615	CLA	C8-C10-C11-C12
20	C	511	CLA	C16-C17-C18-C20
20	c	511	CLA	C16-C17-C18-C20
27	B	613	F6C	C16-C17-C18-C19
27	b	613	F6C	C16-C17-C18-C19
23	A	409	SQD	C16-C17-C18-C19
23	a	409	SQD	C16-C17-C18-C19
20	B	605	CLA	CAD-CBD-CGD-O2D
20	B	610	CLA	CAD-CBD-CGD-O2D
20	B	614	CLA	CAD-CBD-CGD-O2D
20	C	502	CLA	CAD-CBD-CGD-O2D
20	C	510	CLA	CAD-CBD-CGD-O2D
20	b	605	CLA	CAD-CBD-CGD-O2D
20	b	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	b	614	CLA	CAD-CBD-CGD-O2D
20	c	502	CLA	CAD-CBD-CGD-O2D
20	c	510	CLA	CAD-CBD-CGD-O2D
28	C	516	DGD	O6E-C1E-O5D-C6D
28	c	516	DGD	O6E-C1E-O5D-C6D
30	M	101	LMG	O6-C1-O1-C7
30	m	101	LMG	O6-C1-O1-C7
21	D	402	PHO	C2C-C3C-CAC-CBC
21	d	402	PHO	C2C-C3C-CAC-CBC
26	D	408	LHG	O6-C4-C5-O7
26	d	408	LHG	O6-C4-C5-O7
23	l	102	SQD	C17-C18-C19-C20
23	L	102	SQD	C17-C18-C19-C20
20	B	609	CLA	CHA-CBD-CGD-O1D
20	B	609	CLA	CHA-CBD-CGD-O2D
20	C	503	CLA	CHA-CBD-CGD-O1D
20	C	504	CLA	CHA-CBD-CGD-O1D
20	C	504	CLA	CHA-CBD-CGD-O2D
20	C	506	CLA	CHA-CBD-CGD-O1D
20	C	506	CLA	CHA-CBD-CGD-O2D
20	C	507	CLA	CHA-CBD-CGD-O1D
20	C	507	CLA	CHA-CBD-CGD-O2D
20	C	511	CLA	CHA-CBD-CGD-O1D
20	C	511	CLA	CHA-CBD-CGD-O2D
20	C	514	CLA	CHA-CBD-CGD-O2D
20	b	609	CLA	CHA-CBD-CGD-O1D
20	b	609	CLA	CHA-CBD-CGD-O2D
20	c	503	CLA	CHA-CBD-CGD-O1D
20	c	504	CLA	CHA-CBD-CGD-O1D
20	c	504	CLA	CHA-CBD-CGD-O2D
20	c	506	CLA	CHA-CBD-CGD-O1D
20	c	506	CLA	CHA-CBD-CGD-O2D
20	c	507	CLA	CHA-CBD-CGD-O1D
20	c	507	CLA	CHA-CBD-CGD-O2D
20	c	511	CLA	CHA-CBD-CGD-O1D
20	c	511	CLA	CHA-CBD-CGD-O2D
20	c	514	CLA	CHA-CBD-CGD-O2D
20	c	503	CLA	C2C-C3C-CAC-CBC
20	C	503	CLA	C2C-C3C-CAC-CBC
23	L	102	SQD	O47-C45-C46-O48
23	l	102	SQD	O47-C45-C46-O48
26	A	412	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
26	a	412	LHG	O7-C5-C6-O8
28	D	410	DGD	O1G-C1G-C2G-O2G
28	d	410	DGD	O1G-C1G-C2G-O2G
26	L	101	LHG	O1-C1-C2-O2
26	l	101	LHG	O1-C1-C2-O2
21	A	406	PHO	C6-C7-C8-C9
21	a	406	PHO	C6-C7-C8-C9
27	B	613	F6C	C6-C7-C8-C9
27	b	613	F6C	C6-C7-C8-C9
23	A	409	SQD	C32-C33-C34-C35
20	D	404	CLA	C2C-C3C-CAC-CBC
20	d	404	CLA	C2C-C3C-CAC-CBC
23	a	409	SQD	C32-C33-C34-C35
20	B	605	CLA	C5-C6-C7-C8
23	A	409	SQD	C4-C5-C6-S
23	L	102	SQD	C5-C6-S-O8
23	a	409	SQD	C4-C5-C6-S
23	l	102	SQD	C5-C6-S-O8
20	C	502	CLA	CBD-CGD-O2D-CED
20	c	502	CLA	CBD-CGD-O2D-CED
20	b	605	CLA	C5-C6-C7-C8
22	A	408	BCR	C17-C18-C19-C20
22	C	518	BCR	C7-C8-C9-C10
22	a	408	BCR	C17-C18-C19-C20
22	c	518	BCR	C7-C8-C9-C10
20	C	513	CLA	C1A-C2A-CAA-CBA
20	c	513	CLA	C1A-C2A-CAA-CBA
26	D	408	LHG	C2-C3-O3-P
26	d	408	LHG	C2-C3-O3-P
26	D	407	LHG	C13-C14-C15-C16
26	d	407	LHG	C13-C14-C15-C16
26	A	412	LHG	C3-O3-P-O4
26	A	412	LHG	C3-O3-P-O5
26	D	407	LHG	C3-O3-P-O4
26	D	407	LHG	C3-O3-P-O5
26	D	408	LHG	C3-O3-P-O4
26	L	101	LHG	C4-O6-P-O5
26	a	412	LHG	C3-O3-P-O4
26	a	412	LHG	C3-O3-P-O5
26	d	407	LHG	C3-O3-P-O4
26	d	407	LHG	C3-O3-P-O5
26	d	408	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
26	l	101	LHG	C4-O6-P-O5
23	A	409	SQD	C27-C28-C29-C30
23	a	409	SQD	C27-C28-C29-C30
26	D	407	LHG	C10-C11-C12-C13
26	d	407	LHG	C10-C11-C12-C13
26	d	407	LHG	C12-C13-C14-C15
20	B	609	CLA	CAD-CBD-CGD-O1D
20	C	503	CLA	CAD-CBD-CGD-O1D
20	C	504	CLA	CAD-CBD-CGD-O1D
20	C	506	CLA	CAD-CBD-CGD-O1D
20	C	507	CLA	CAD-CBD-CGD-O1D
20	C	511	CLA	CAD-CBD-CGD-O1D
20	b	609	CLA	CAD-CBD-CGD-O1D
20	c	503	CLA	CAD-CBD-CGD-O1D
20	c	504	CLA	CAD-CBD-CGD-O1D
20	c	506	CLA	CAD-CBD-CGD-O1D
20	c	507	CLA	CAD-CBD-CGD-O1D
20	c	511	CLA	CAD-CBD-CGD-O1D
23	L	102	SQD	O5-C5-C6-S
23	l	102	SQD	O5-C5-C6-S
26	D	407	LHG	C12-C13-C14-C15
28	D	410	DGD	CCA-CDA-CEA-CFA
28	d	410	DGD	CCA-CDA-CEA-CFA
20	C	510	CLA	C11-C10-C8-C7
20	c	510	CLA	C11-C10-C8-C7
21	A	406	PHO	C6-C7-C8-C10
21	a	406	PHO	C6-C7-C8-C10
27	B	604	F6C	C12-C13-C15-C16
27	B	607	F6C	C11-C10-C8-C7
27	b	604	F6C	C12-C13-C15-C16
27	b	607	F6C	C11-C10-C8-C7
28	C	516	DGD	C1B-C2B-C3B-C4B
28	D	410	DGD	C1A-C2A-C3A-C4A
28	c	516	DGD	C1B-C2B-C3B-C4B
31	V	201	HEM	C2A-CAA-CBA-CGA
31	v	201	HEM	C2A-CAA-CBA-CGA
27	B	613	F6C	C13-C15-C16-C17
27	b	613	F6C	C13-C15-C16-C17
28	d	410	DGD	C1A-C2A-C3A-C4A
26	A	412	LHG	C4-C5-C6-O8
26	a	412	LHG	C4-C5-C6-O8
27	B	607	F6C	C1B-C2B-CMB-OMB

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Mol	Chain	Res	Type	Atoms
27	b	607	F6C	C1B-C2B-CMB-OMB
26	D	407	LHG	O7-C5-C6-O8
26	d	407	LHG	O7-C5-C6-O8
30	M	101	LMG	C8-C7-O1-C1
30	m	101	LMG	C8-C7-O1-C1
20	C	503	CLA	C2-C3-C5-C6
20	c	503	CLA	C2-C3-C5-C6
20	D	403	CLA	C11-C10-C8-C9
20	d	403	CLA	C11-C10-C8-C9
31	V	201	HEM	C3D-CAD-CBD-CGD
31	v	201	HEM	C3D-CAD-CBD-CGD
32	H	102	RRX	C10-C11-C12-C13
32	h	102	RRX	C10-C11-C12-C13
28	D	410	DGD	C7A-C8A-C9A-CAA
28	d	410	DGD	C7A-C8A-C9A-CAA
26	a	412	LHG	C29-C30-C31-C32
26	A	412	LHG	C29-C30-C31-C32
20	B	610	CLA	C2-C1-O2A-CGA
20	b	610	CLA	C2-C1-O2A-CGA
20	C	503	CLA	C4C-C3C-CAC-CBC
20	c	503	CLA	C4C-C3C-CAC-CBC
26	A	412	LHG	C11-C10-C9-C8
26	a	412	LHG	C11-C10-C9-C8
26	D	407	LHG	C11-C12-C13-C14
26	d	407	LHG	C11-C12-C13-C14
26	d	408	LHG	C15-C16-C17-C18
22	B	617	BCR	C23-C24-C25-C26
22	b	617	BCR	C23-C24-C25-C26
26	D	408	LHG	C15-C16-C17-C18
20	C	505	CLA	C2A-CAA-CBA-CGA
20	c	505	CLA	C2A-CAA-CBA-CGA
28	C	516	DGD	C2E-C1E-O5D-C6D
28	c	516	DGD	C2E-C1E-O5D-C6D
20	C	509	CLA	C11-C10-C8-C7
20	c	509	CLA	C11-C10-C8-C7
27	B	604	F6C	C14-C13-C15-C16
27	B	607	F6C	C11-C10-C8-C9
27	b	604	F6C	C14-C13-C15-C16
27	b	607	F6C	C11-C10-C8-C9
27	B	604	F6C	C16-C17-C18-C19
27	b	604	F6C	C16-C17-C18-C19
26	a	412	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	A	412	LHG	C24-C25-C26-C27
31	E	101	HEM	CAA-CBA-CGA-O2A
31	V	201	HEM	CAA-CBA-CGA-O1A
31	e	101	HEM	CAA-CBA-CGA-O2A
31	v	201	HEM	CAA-CBA-CGA-O1A
22	C	515	BCR	C19-C20-C21-C22
22	c	515	BCR	C19-C20-C21-C22
20	B	612	CLA	C3-C5-C6-C7
20	b	612	CLA	C3-C5-C6-C7
29	D	401	CL7	C5-C6-C7-C8
29	d	401	CL7	C5-C6-C7-C8
28	C	517	DGD	C4B-C5B-C6B-C7B
28	c	517	DGD	C4B-C5B-C6B-C7B
22	C	515	BCR	C10-C11-C12-C13
23	a	409	SQD	C31-C32-C33-C34
23	A	409	SQD	C31-C32-C33-C34
20	B	615	CLA	C2-C1-O2A-CGA
20	B	610	CLA	C15-C16-C17-C18
20	b	610	CLA	C15-C16-C17-C18
30	D	409	LMG	O9-C10-O7-C8
20	B	610	CLA	C6-C7-C8-C9
20	B	615	CLA	C11-C10-C8-C9
20	b	610	CLA	C6-C7-C8-C9
20	b	615	CLA	C11-C10-C8-C9
33	M	102	LMT	C9-C10-C11-C12
30	d	409	LMG	O9-C10-O7-C8
33	m	102	LMT	C9-C10-C11-C12
20	D	404	CLA	C2A-CAA-CBA-CGA
20	d	404	CLA	C2A-CAA-CBA-CGA
20	B	602	CLA	C16-C17-C18-C20
20	b	602	CLA	C16-C17-C18-C20
27	C	508	F6C	O2A-C1-C2-C3
27	c	508	F6C	O2A-C1-C2-C3
31	E	101	HEM	CAD-CBD-CGD-O2D
31	V	201	HEM	CAA-CBA-CGA-O2A
31	e	101	HEM	CAD-CBD-CGD-O2D
31	v	201	HEM	CAA-CBA-CGA-O2A
20	A	405	CLA	C1A-C2A-CAA-CBA
20	B	601	CLA	C1A-C2A-CAA-CBA
20	B	611	CLA	C1A-C2A-CAA-CBA
20	a	405	CLA	C1A-C2A-CAA-CBA
20	b	601	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	b	611	CLA	C1A-C2A-CAA-CBA
20	a	404	CLA	C16-C17-C18-C20
31	e	101	HEM	CAD-CBD-CGD-O1D
28	C	516	DGD	C2A-C3A-C4A-C5A
28	c	516	DGD	C2A-C3A-C4A-C5A
31	E	101	HEM	CAD-CBD-CGD-O1D
20	A	404	CLA	C16-C17-C18-C20
26	D	408	LHG	C7-C8-C9-C10
20	b	602	CLA	C4C-C3C-CAC-CBC
33	M	102	LMT	C11-C10-C9-C8
33	m	102	LMT	C11-C10-C9-C8
20	B	602	CLA	C4C-C3C-CAC-CBC
26	d	408	LHG	C7-C8-C9-C10
20	c	502	CLA	O1D-CGD-O2D-CED
20	C	502	CLA	O1D-CGD-O2D-CED
23	A	409	SQD	C33-C34-C35-C36
20	b	615	CLA	C2-C1-O2A-CGA
23	a	409	SQD	C33-C34-C35-C36
31	E	101	HEM	CAA-CBA-CGA-O1A
31	e	101	HEM	CAA-CBA-CGA-O1A
20	B	611	CLA	C11-C10-C8-C9
20	b	611	CLA	C11-C10-C8-C9
20	B	602	CLA	C5-C6-C7-C8
20	b	602	CLA	C5-C6-C7-C8
20	C	506	CLA	C8-C10-C11-C12
20	c	506	CLA	C8-C10-C11-C12
20	B	615	CLA	C2A-CAA-CBA-CGA
20	b	615	CLA	C2A-CAA-CBA-CGA
22	B	617	BCR	C23-C24-C25-C30
22	b	617	BCR	C23-C24-C25-C30
32	H	102	RRX	C23-C24-C25-C30
32	h	102	RRX	C23-C24-C25-C30
28	c	516	DGD	C4B-C5B-C6B-C7B
28	C	516	DGD	C4B-C5B-C6B-C7B
20	B	602	CLA	C4-C3-C5-C6
20	b	602	CLA	C4-C3-C5-C6
26	D	408	LHG	C9-C10-C11-C12
26	d	408	LHG	C9-C10-C11-C12
30	D	409	LMG	C11-C10-O7-C8
30	d	409	LMG	C11-C10-O7-C8
26	L	101	LHG	C10-C11-C12-C13
20	C	514	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	c	514	CLA	C2A-CAA-CBA-CGA
26	l	101	LHG	C10-C11-C12-C13
28	D	410	DGD	C3A-C4A-C5A-C6A
28	d	410	DGD	C3A-C4A-C5A-C6A
33	M	102	LMT	C5-C6-C7-C8
33	m	102	LMT	C5-C6-C7-C8
23	l	102	SQD	C19-C20-C21-C22
20	B	602	CLA	C2-C3-C5-C6
20	B	605	CLA	C12-C13-C15-C16
20	B	615	CLA	C6-C7-C8-C10
20	b	602	CLA	C2-C3-C5-C6
20	b	605	CLA	C12-C13-C15-C16
20	b	615	CLA	C6-C7-C8-C10
27	b	604	F6C	C10-C11-C12-C13
23	L	102	SQD	C19-C20-C21-C22
30	D	409	LMG	O7-C10-C11-C12
27	B	604	F6C	C10-C11-C12-C13
28	d	410	DGD	O2G-C1B-C2B-C3B
30	d	409	LMG	O7-C10-C11-C12
20	C	512	CLA	C2A-CAA-CBA-CGA
20	c	512	CLA	C2A-CAA-CBA-CGA
27	B	607	F6C	C4C-C3C-CAC-CBC
27	b	607	F6C	C4C-C3C-CAC-CBC
28	D	410	DGD	O2G-C1B-C2B-C3B
20	C	504	CLA	C4-C3-C5-C6
20	c	504	CLA	C4-C3-C5-C6
24	D	406	PL9	C12-C11-C9-C10
24	d	406	PL9	C12-C11-C9-C10
27	B	613	F6C	C4-C3-C5-C6
27	b	613	F6C	C4-C3-C5-C6
20	d	404	CLA	CAA-CBA-CGA-O2A
20	B	611	CLA	C11-C12-C13-C14
20	b	611	CLA	C11-C12-C13-C14
20	B	608	CLA	C3-C5-C6-C7
20	b	608	CLA	C3-C5-C6-C7
20	D	404	CLA	CAA-CBA-CGA-O2A
21	D	402	PHO	C3A-C2A-CAA-CBA
21	d	402	PHO	C3A-C2A-CAA-CBA
27	c	508	F6C	CAA-CBA-CGA-O2A
20	B	601	CLA	CAD-CBD-CGD-O2D
20	C	505	CLA	CAD-CBD-CGD-O2D
20	H	101	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	b	601	CLA	CAD-CBD-CGD-O2D
20	h	101	CLA	CAD-CBD-CGD-O2D
21	A	406	PHO	CAD-CBD-CGD-O2D
21	a	406	PHO	CAD-CBD-CGD-O2D
27	B	604	F6C	CAD-CBD-CGD-O2D
27	B	607	F6C	CAD-CBD-CGD-O2D
27	b	604	F6C	CAD-CBD-CGD-O2D
27	b	607	F6C	CAD-CBD-CGD-O2D
20	C	512	CLA	CAA-CBA-CGA-O2A
20	c	512	CLA	CAA-CBA-CGA-O2A
27	C	508	F6C	CAA-CBA-CGA-O2A
28	C	516	DGD	O2G-C1B-C2B-C3B
28	c	516	DGD	O2G-C1B-C2B-C3B
28	D	410	DGD	C4B-C5B-C6B-C7B
28	d	410	DGD	C4B-C5B-C6B-C7B
27	B	613	F6C	C15-C16-C17-C18
27	b	613	F6C	C15-C16-C17-C18
27	B	607	F6C	C2C-C3C-CAC-CBC
27	b	607	F6C	C2C-C3C-CAC-CBC
20	B	609	CLA	CAA-CBA-CGA-O2A
20	b	609	CLA	CAA-CBA-CGA-O2A
20	D	404	CLA	CAA-CBA-CGA-O1A
20	d	404	CLA	CAA-CBA-CGA-O1A
20	C	503	CLA	CHA-CBD-CGD-O2D
20	D	404	CLA	CHA-CBD-CGD-O1D
20	D	404	CLA	CHA-CBD-CGD-O2D
20	c	503	CLA	CHA-CBD-CGD-O2D
20	d	404	CLA	CHA-CBD-CGD-O1D
20	d	404	CLA	CHA-CBD-CGD-O2D
27	C	508	F6C	CHA-CBD-CGD-O2D
27	c	508	F6C	CHA-CBD-CGD-O2D
29	D	401	CL7	CHA-CBD-CGD-O2D
29	d	401	CL7	CHA-CBD-CGD-O2D
20	A	404	CLA	C4-C3-C5-C6
20	a	404	CLA	C4-C3-C5-C6
30	D	409	LMG	C11-C12-C13-C14
30	d	409	LMG	C11-C12-C13-C14
20	C	502	CLA	CAA-CBA-CGA-O2A
20	c	502	CLA	CAA-CBA-CGA-O2A
23	A	409	SQD	O48-C23-C24-C25
23	a	409	SQD	O48-C23-C24-C25
28	C	517	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	O1G-C1G-C2G-O2G
20	B	609	CLA	CAA-CBA-CGA-O1A
20	b	609	CLA	CAA-CBA-CGA-O1A
27	B	607	F6C	CAA-CBA-CGA-O2A
27	b	607	F6C	CAA-CBA-CGA-O2A
20	B	611	CLA	C11-C10-C8-C7
20	b	611	CLA	C11-C10-C8-C7
27	C	508	F6C	C11-C10-C8-C7
27	c	508	F6C	C11-C10-C8-C7
20	B	605	CLA	C11-C10-C8-C9
20	C	504	CLA	C6-C7-C8-C9
20	b	605	CLA	C11-C10-C8-C9
20	c	504	CLA	C6-C7-C8-C9
20	B	602	CLA	C16-C17-C18-C19
20	C	504	CLA	C16-C17-C18-C20
20	c	504	CLA	C16-C17-C18-C20
20	b	602	CLA	C16-C17-C18-C19
27	c	508	F6C	C3A-C2A-CAA-CBA
20	C	511	CLA	C2-C3-C5-C6
20	c	511	CLA	C2-C3-C5-C6
27	c	508	F6C	CAA-CBA-CGA-O1A
30	D	409	LMG	O9-C10-C11-C12
30	d	409	LMG	O9-C10-C11-C12
27	C	508	F6C	CAA-CBA-CGA-O1A
26	D	407	LHG	C33-C34-C35-C36
26	d	407	LHG	C33-C34-C35-C36
28	C	516	DGD	C1G-C2G-C3G-O3G
28	c	516	DGD	C1G-C2G-C3G-O3G
23	L	102	SQD	C11-C12-C13-C14
23	l	102	SQD	C11-C12-C13-C14
26	L	101	LHG	C3-O3-P-O5
26	l	101	LHG	C3-O3-P-O5
23	A	409	SQD	O10-C23-C24-C25
23	a	409	SQD	O10-C23-C24-C25
26	L	101	LHG	O7-C7-C8-C9
26	l	101	LHG	O7-C7-C8-C9
22	c	515	BCR	C10-C11-C12-C13
20	C	512	CLA	CAA-CBA-CGA-O1A
28	c	516	DGD	O1B-C1B-C2B-C3B
20	B	601	CLA	CAA-CBA-CGA-O2A
20	b	601	CLA	CAA-CBA-CGA-O2A
27	C	508	F6C	C3A-C2A-CAA-CBA

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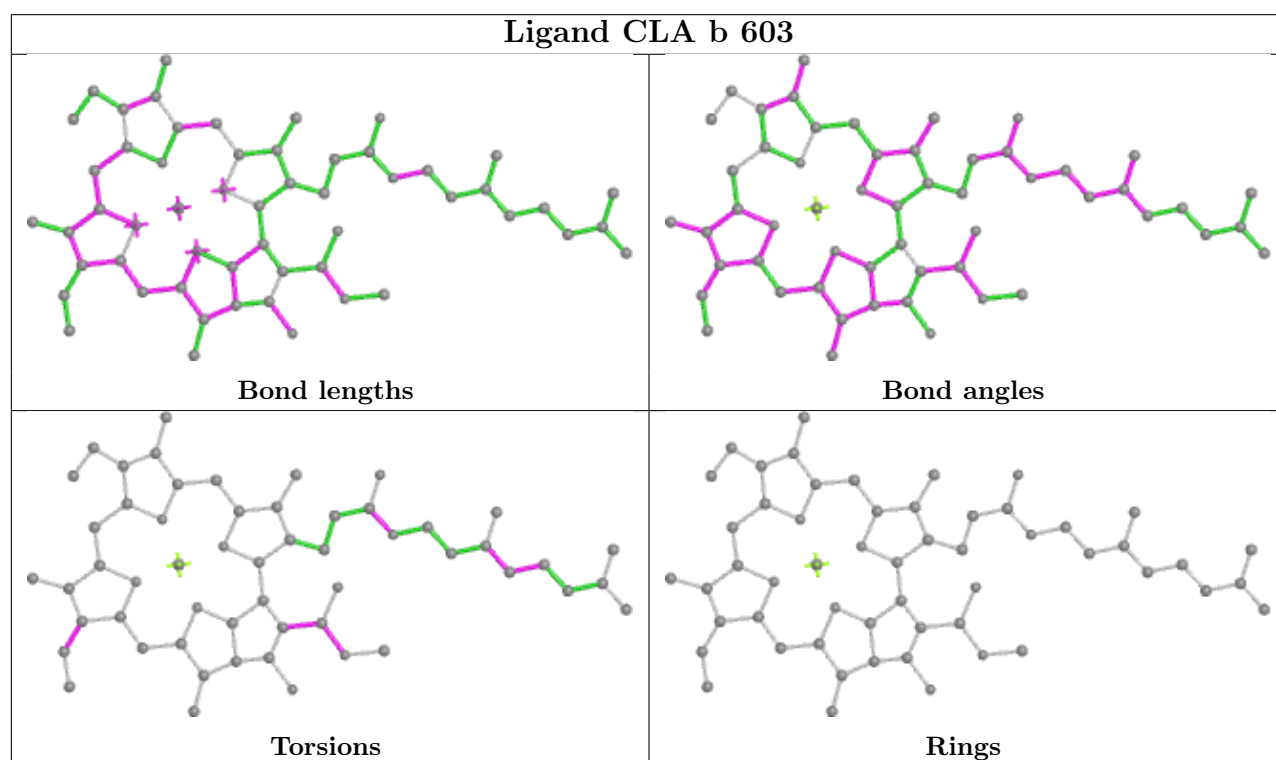
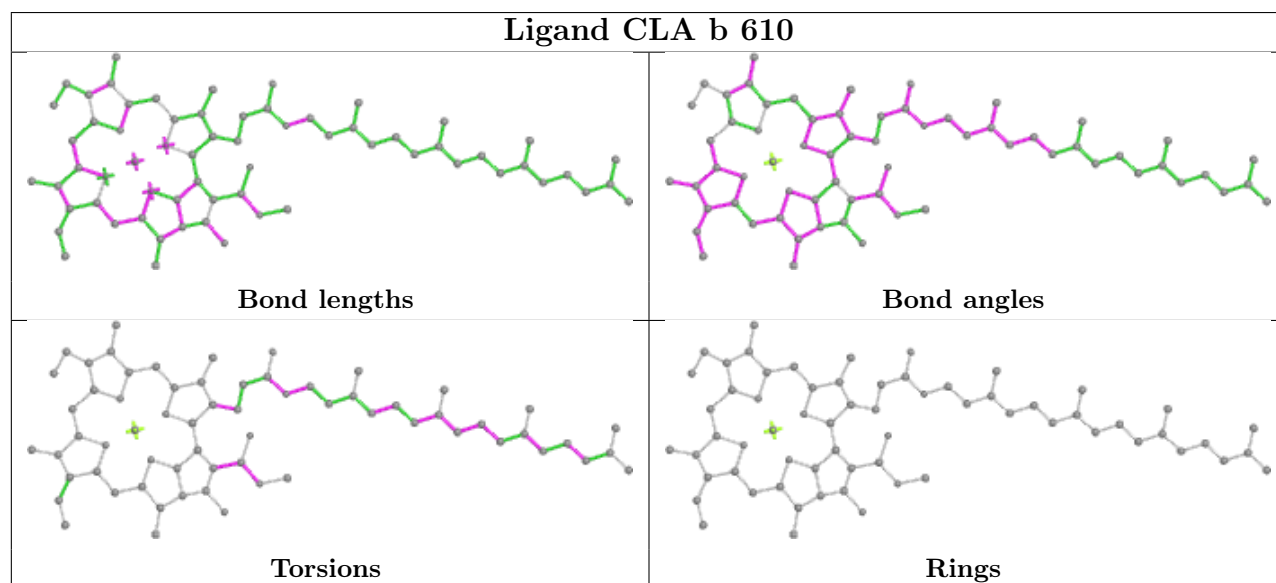
Mol	Chain	Res	Type	Atoms
27	B	613	F6C	CAA-CBA-CGA-O2A
27	b	613	F6C	CAA-CBA-CGA-O2A
26	L	101	LHG	C12-C13-C14-C15
26	d	407	LHG	C17-C18-C19-C20
20	c	512	CLA	CAA-CBA-CGA-O1A
28	C	516	DGD	O1B-C1B-C2B-C3B
26	D	407	LHG	C17-C18-C19-C20
26	l	101	LHG	C12-C13-C14-C15
20	B	603	CLA	CAD-CBD-CGD-O1D
20	b	603	CLA	CAD-CBD-CGD-O1D
27	B	604	F6C	O1A-CGA-O2A-C1
27	b	604	F6C	O1A-CGA-O2A-C1
20	B	614	CLA	CAA-CBA-CGA-O2A
20	C	510	CLA	C11-C10-C8-C9
20	c	510	CLA	C11-C10-C8-C9
20	b	614	CLA	CAA-CBA-CGA-O2A
20	c	511	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	O1G-C1A-C2A-C3A
28	c	517	DGD	O1G-C1A-C2A-C3A
20	C	504	CLA	CAA-CBA-CGA-O2A
20	c	504	CLA	CAA-CBA-CGA-O2A
20	C	502	CLA	CAA-CBA-CGA-O1A
20	c	502	CLA	CAA-CBA-CGA-O1A
20	C	511	CLA	CAA-CBA-CGA-O2A
26	D	408	LHG	O7-C7-C8-C9
26	d	408	LHG	O7-C7-C8-C9
20	B	601	CLA	CAA-CBA-CGA-O1A
20	b	601	CLA	CAA-CBA-CGA-O1A
26	l	101	LHG	O9-C7-C8-C9
27	b	607	F6C	CAA-CBA-CGA-O1A
24	D	406	PL9	C19-C21-C22-C23
24	D	406	PL9	C29-C31-C32-C33
24	d	406	PL9	C19-C21-C22-C23
24	d	406	PL9	C29-C31-C32-C33
26	L	101	LHG	O9-C7-C8-C9
27	B	607	F6C	CAA-CBA-CGA-O1A
20	C	511	CLA	C4-C3-C5-C6
20	c	511	CLA	C4-C3-C5-C6

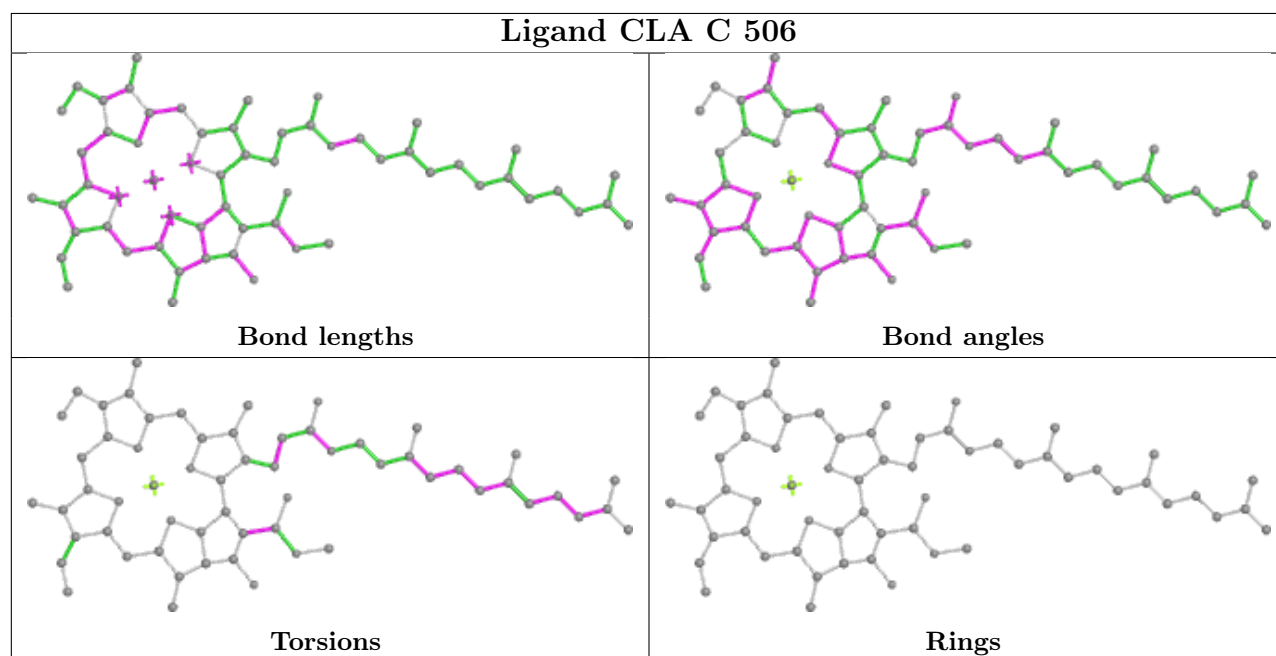
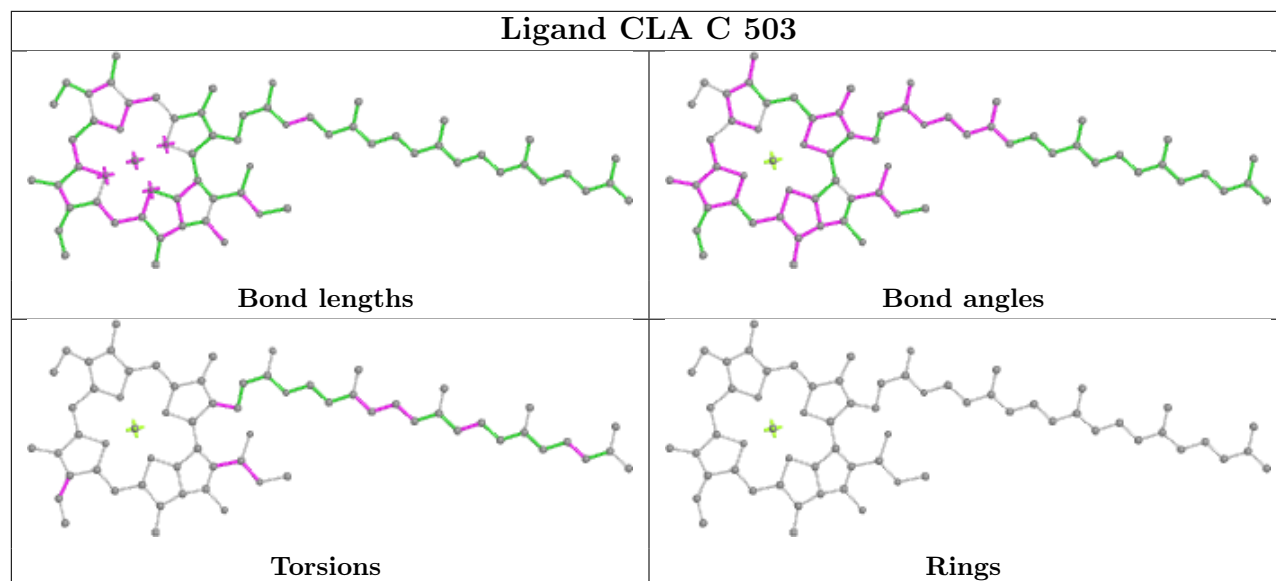
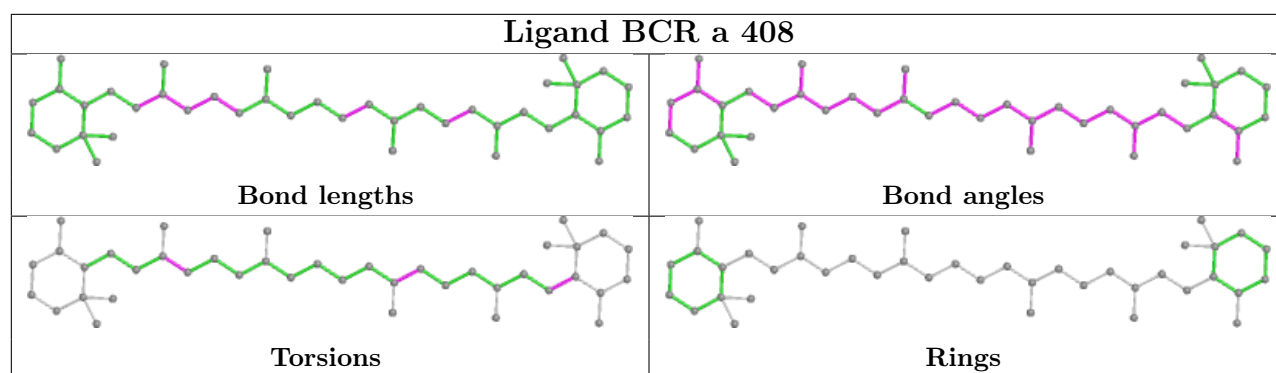
There are no ring outliers.

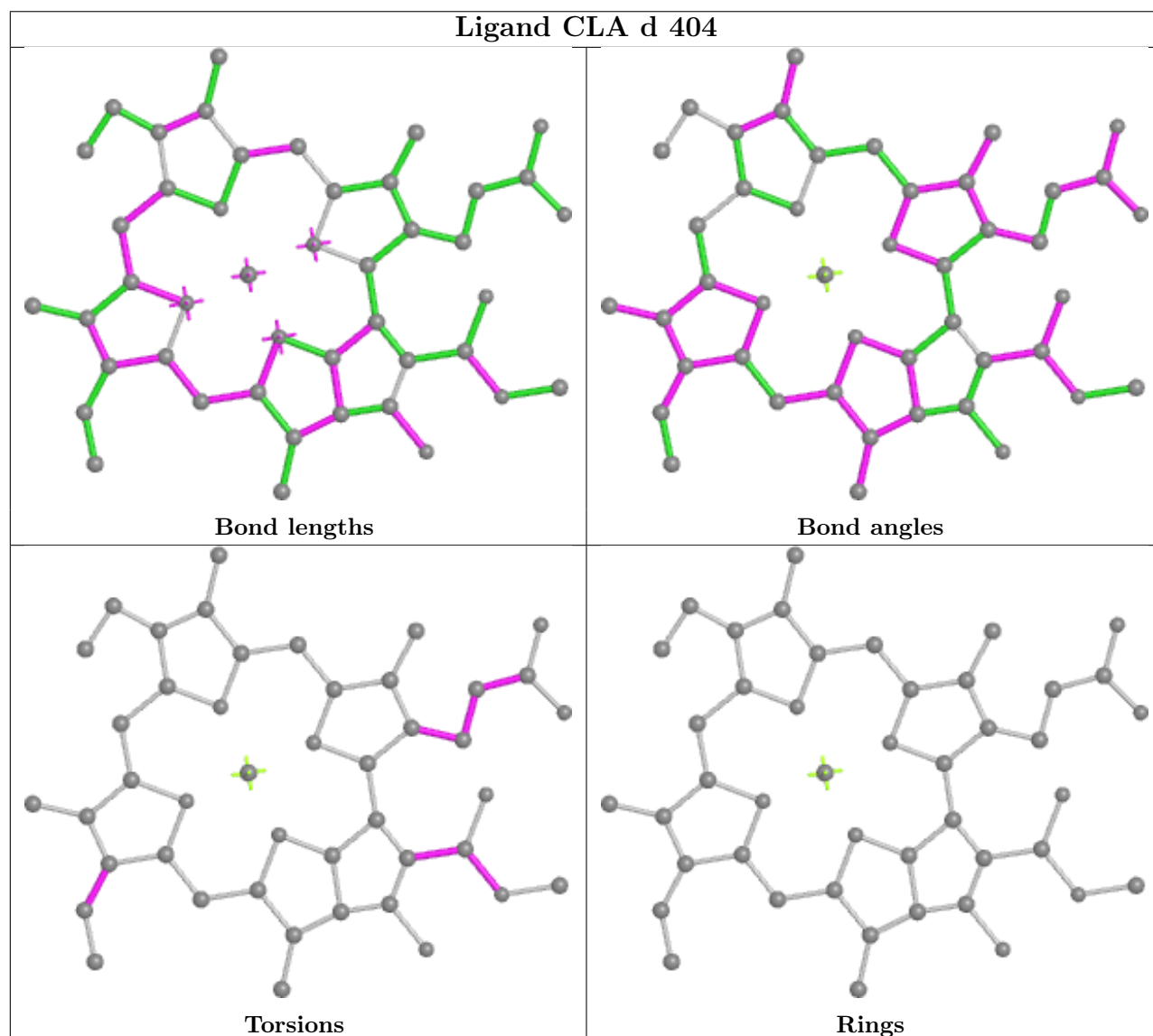
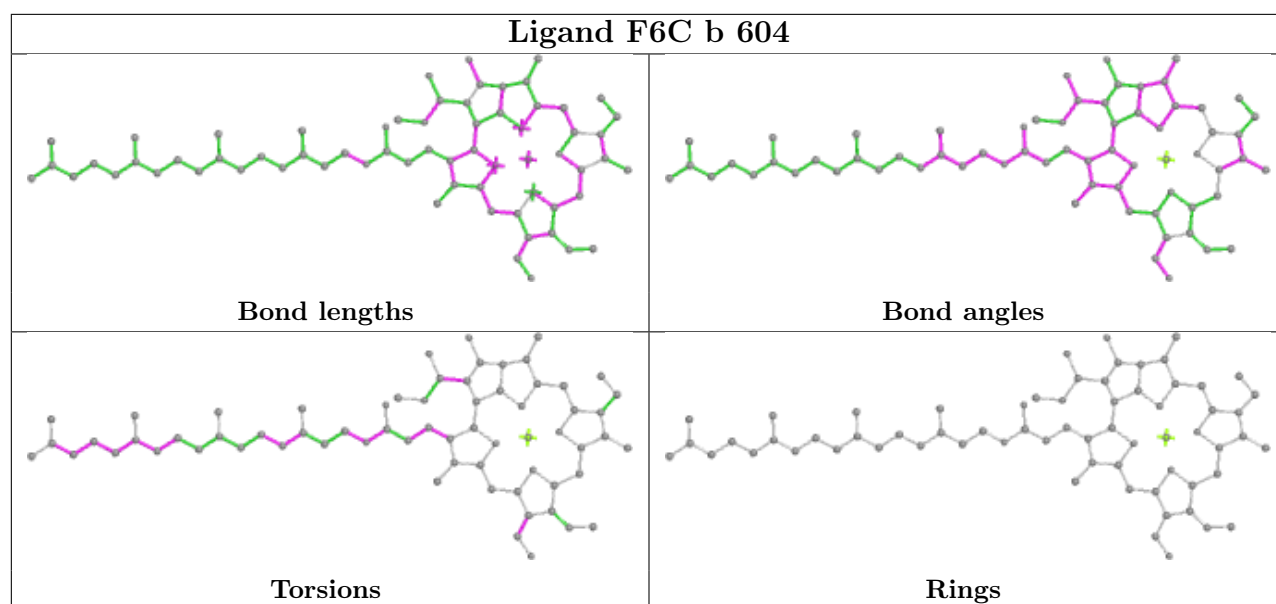
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

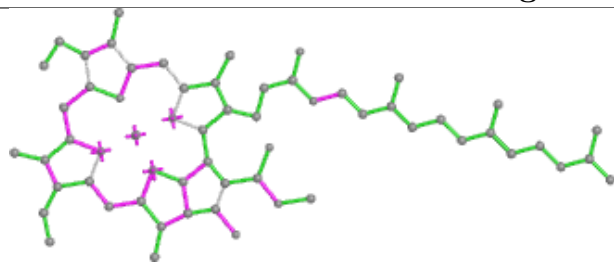
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



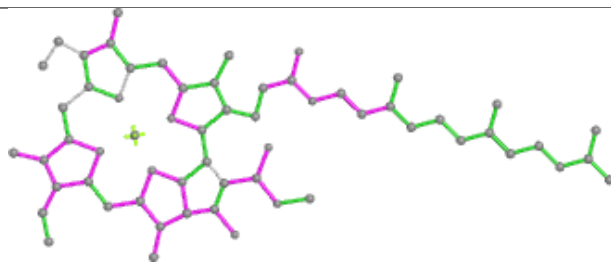




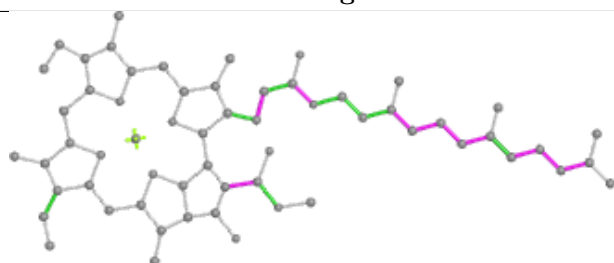
Ligand CLA c 506



Bond lengths



Bond angles

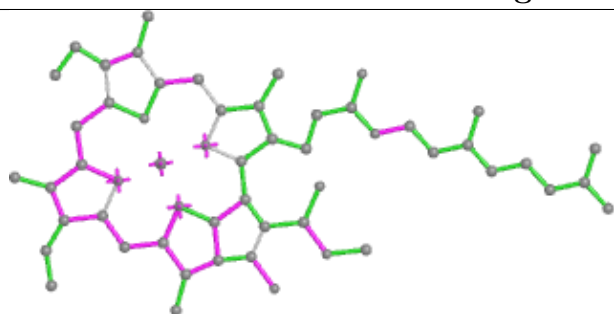


Torsions

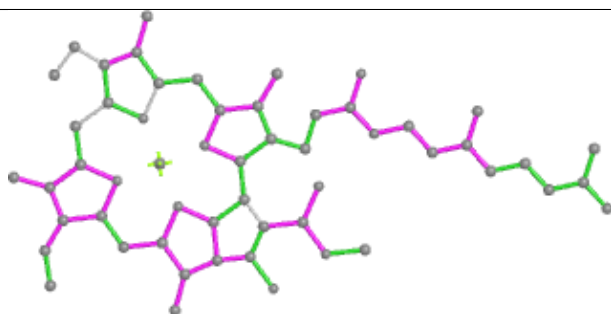


Rings

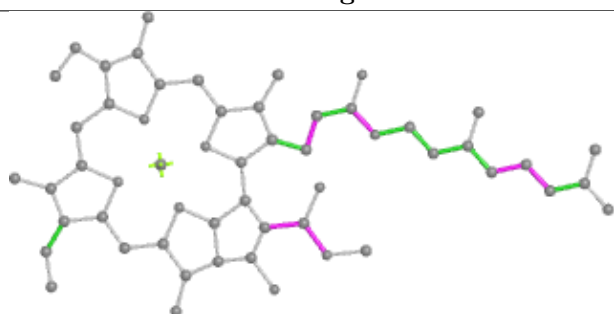
Ligand CLA B 606



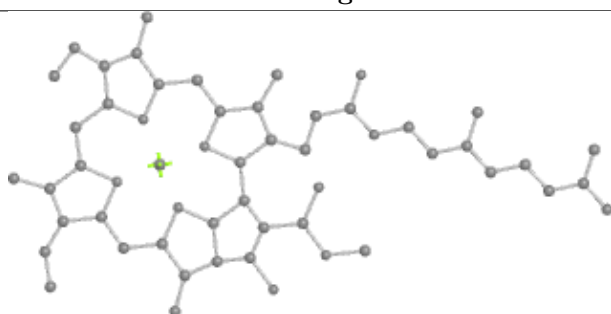
Bond lengths



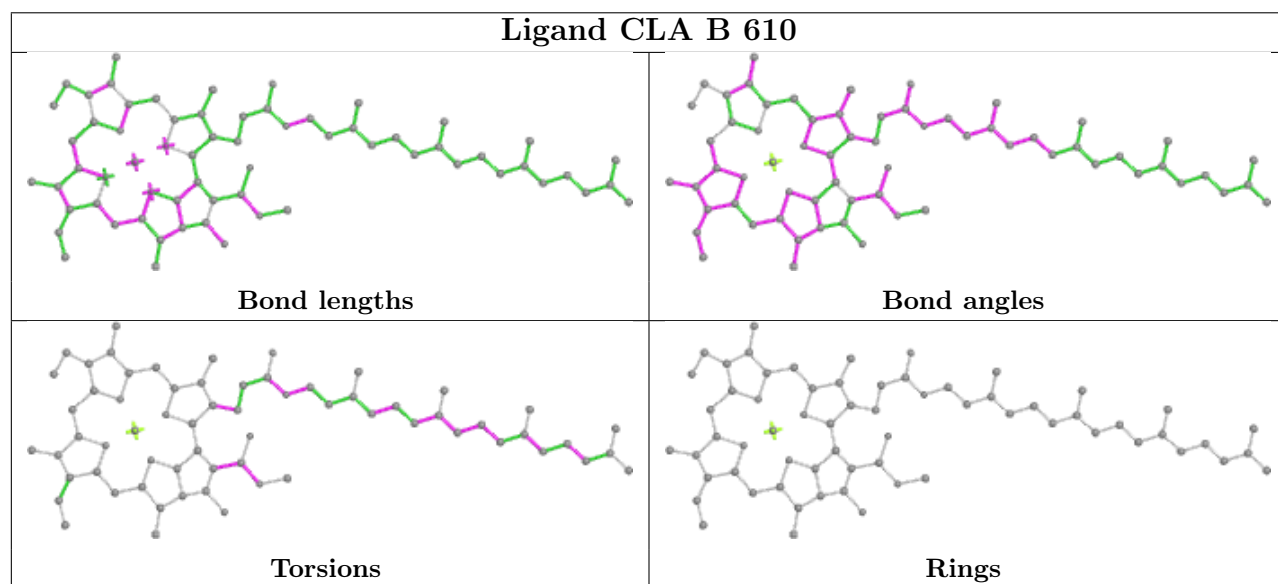
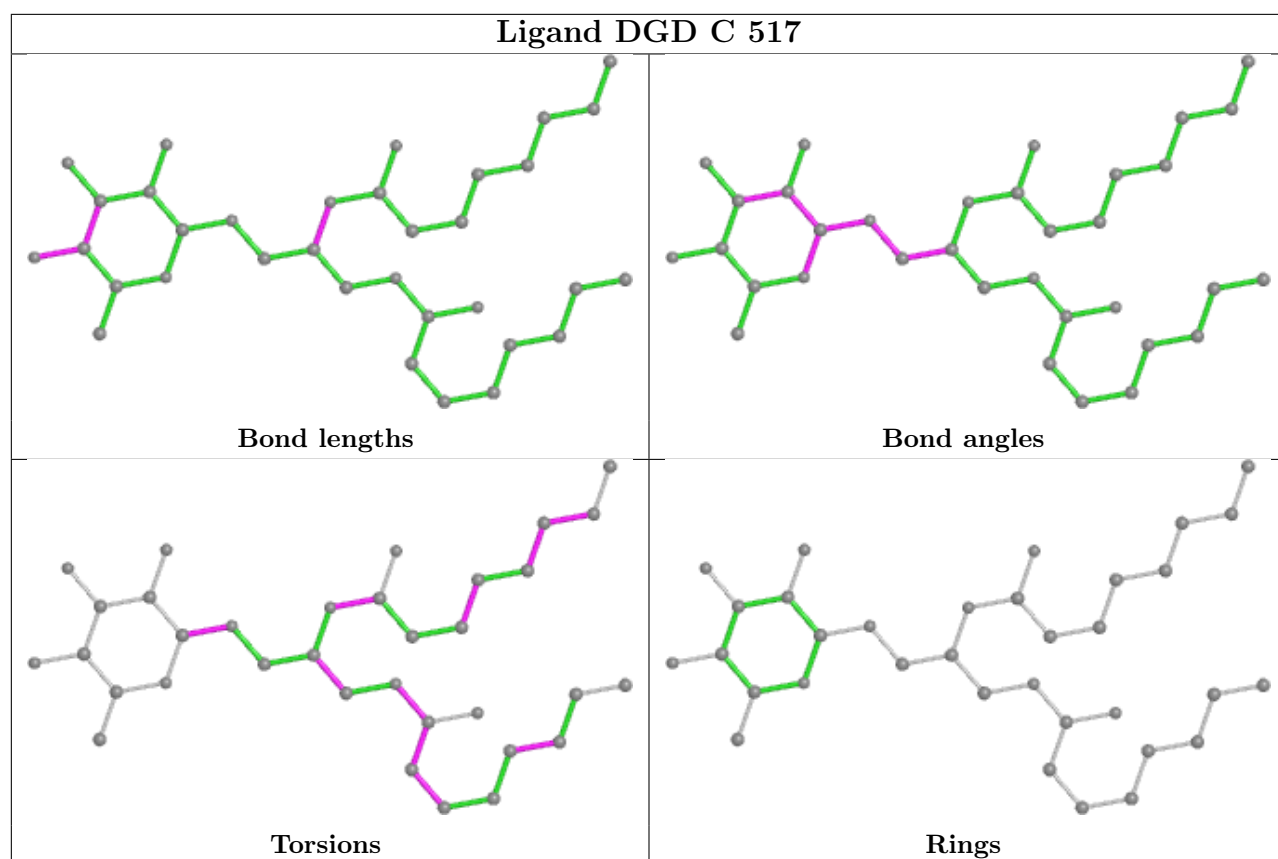
Bond angles

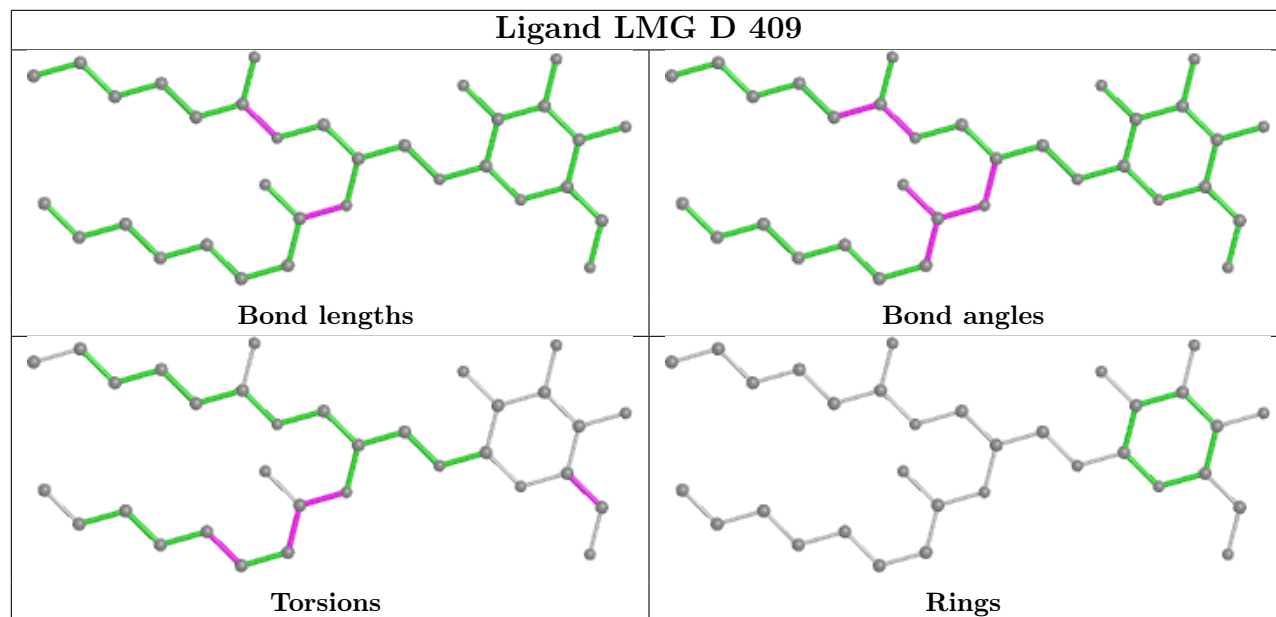
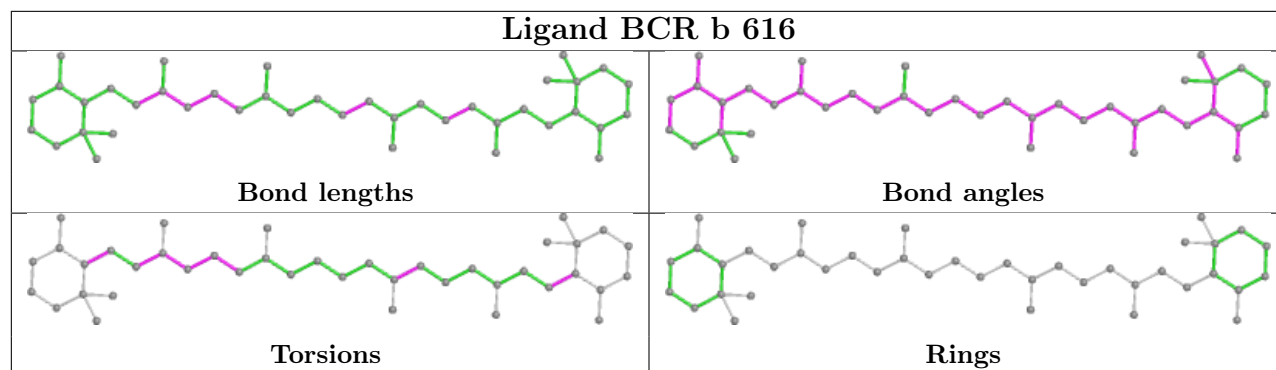
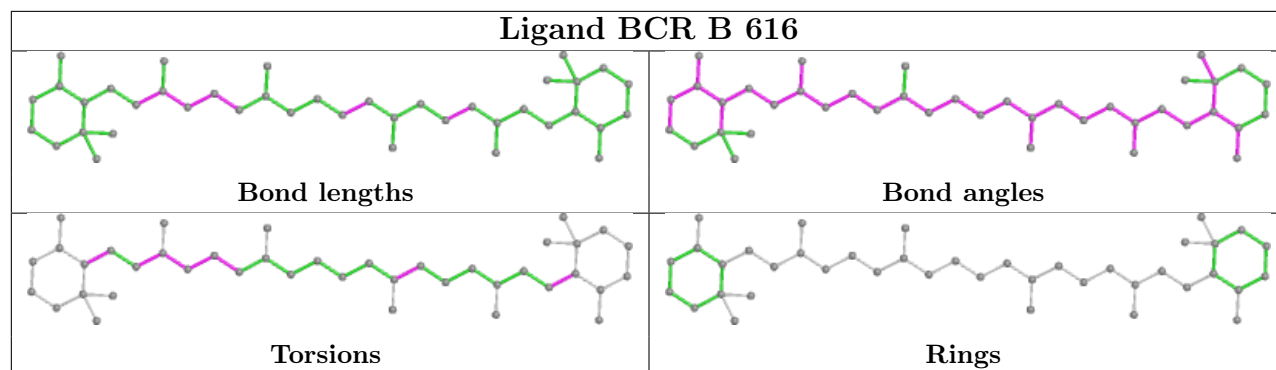


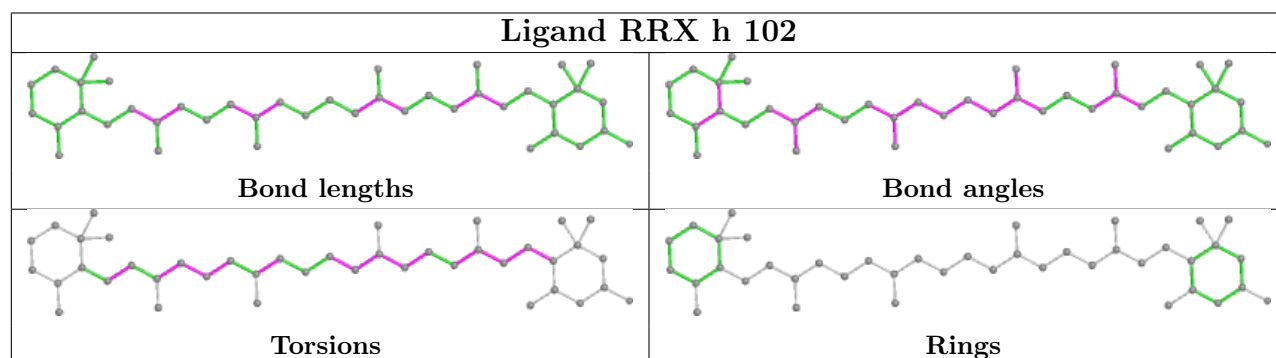
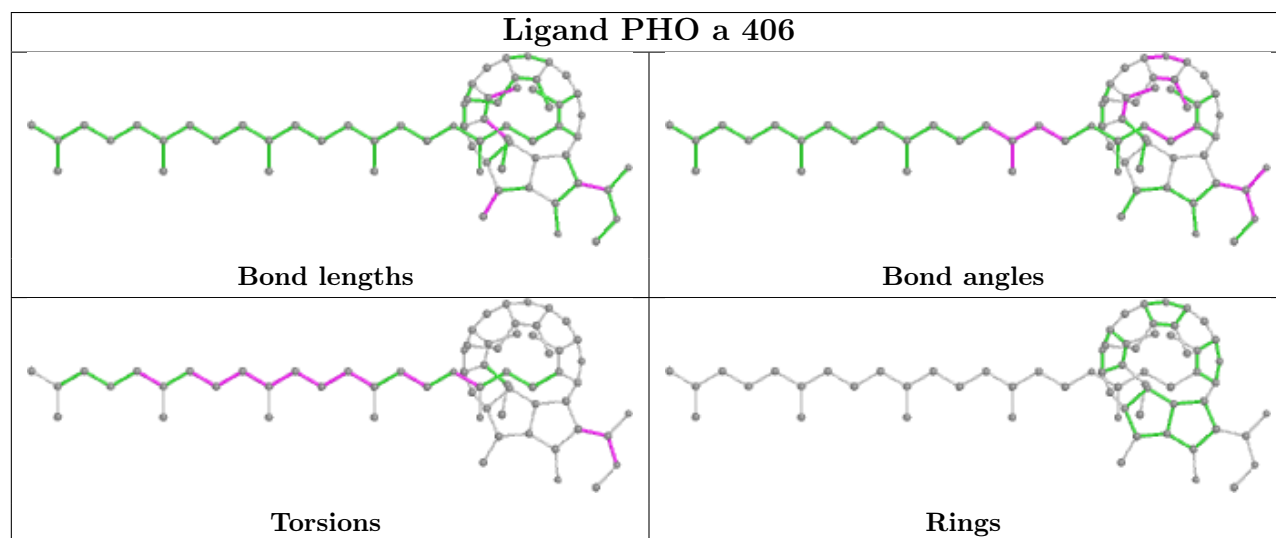
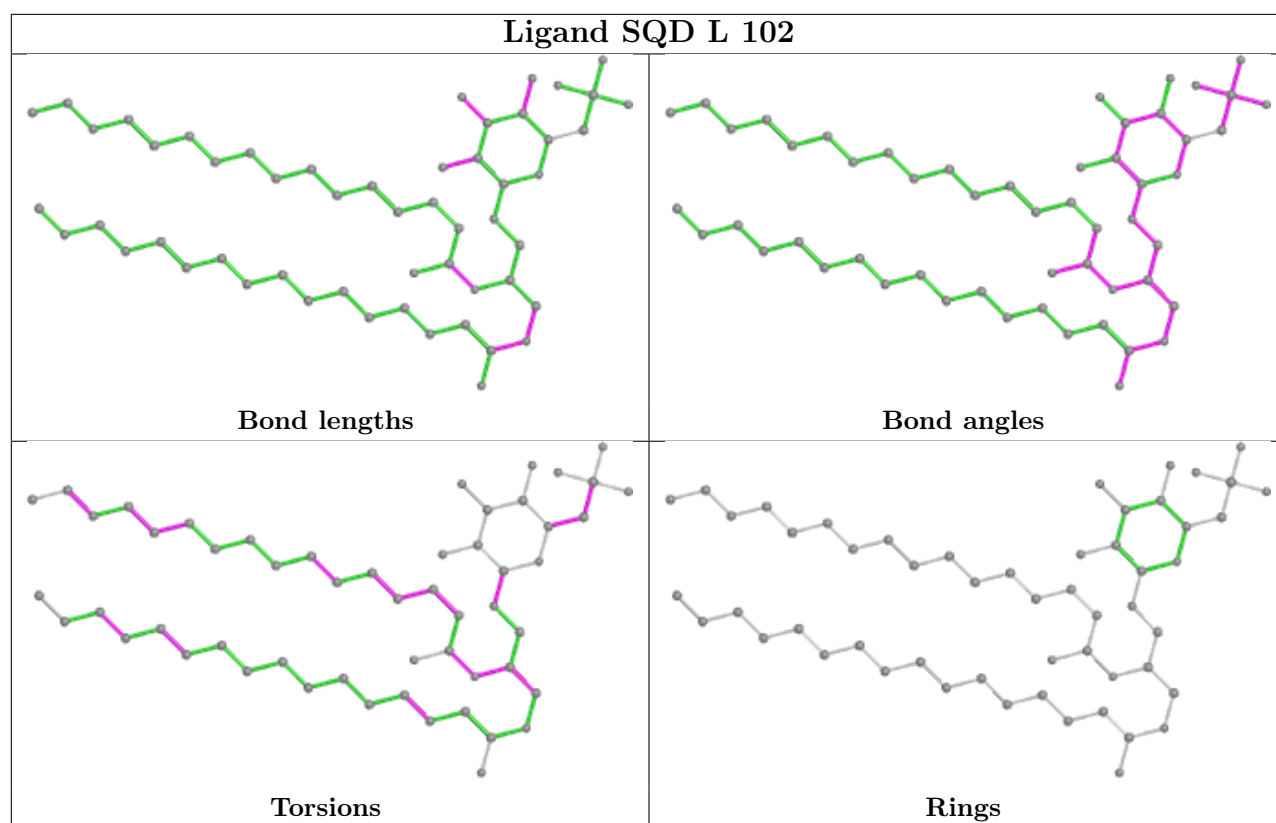
Torsions



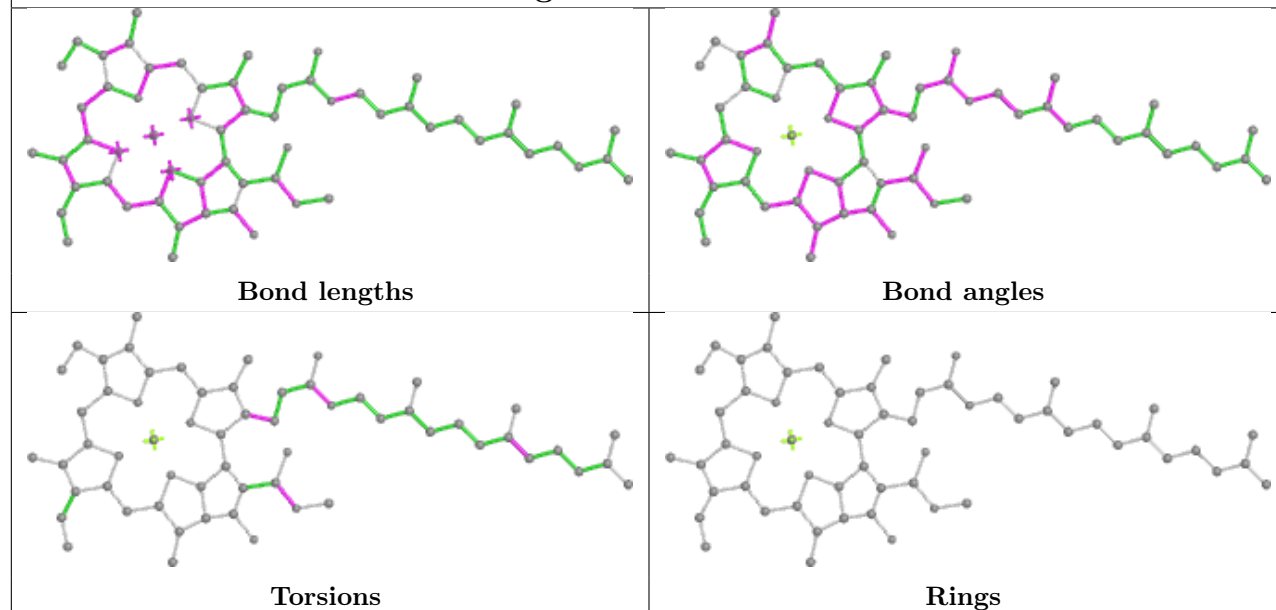
Rings



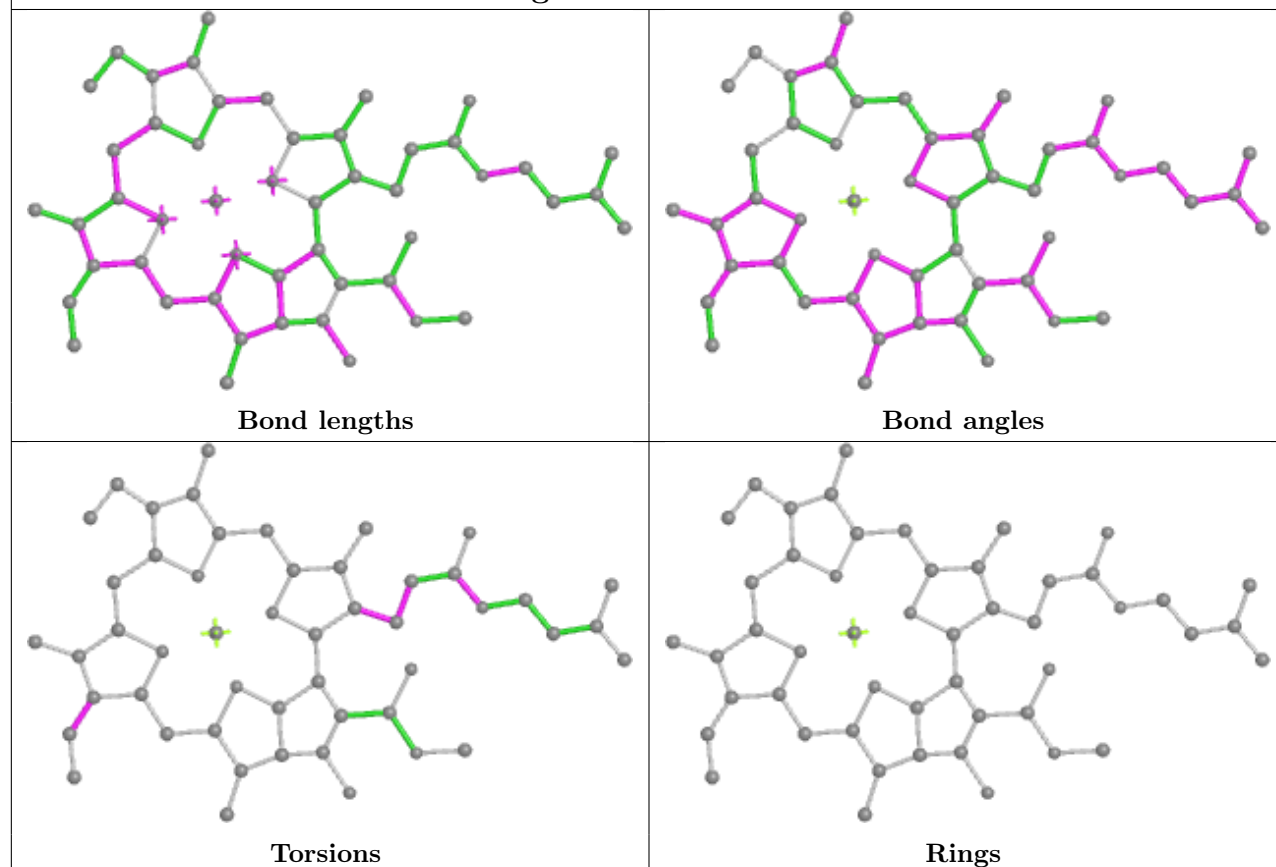




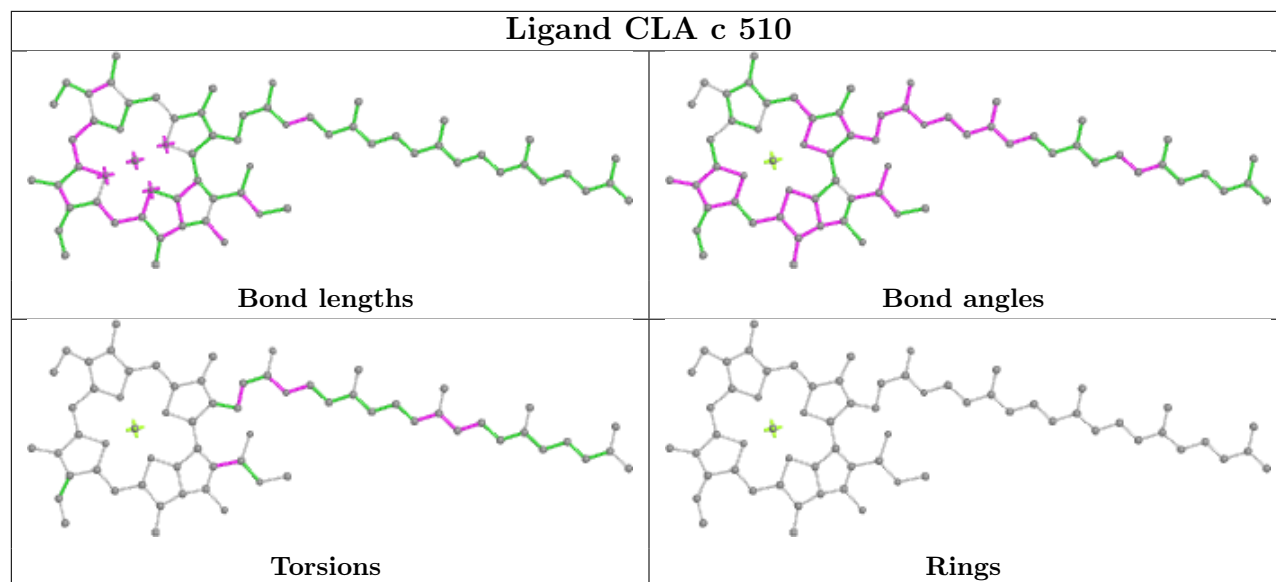
Ligand CLA d 403



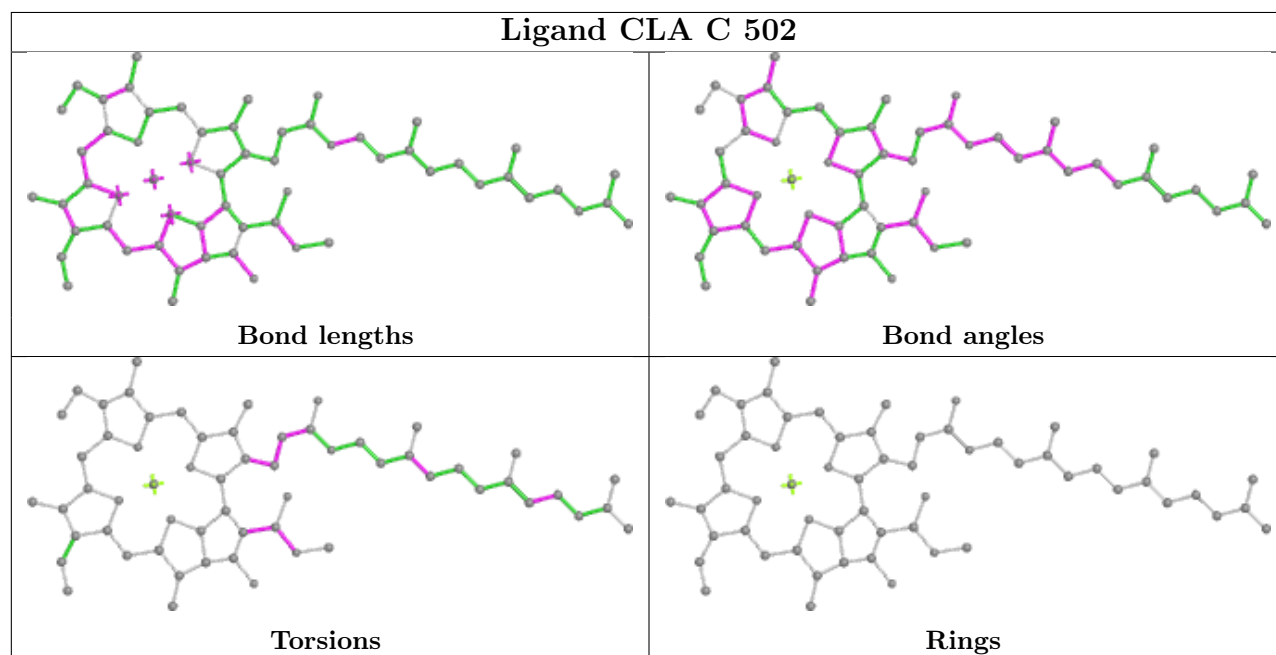
Ligand CLA A 407

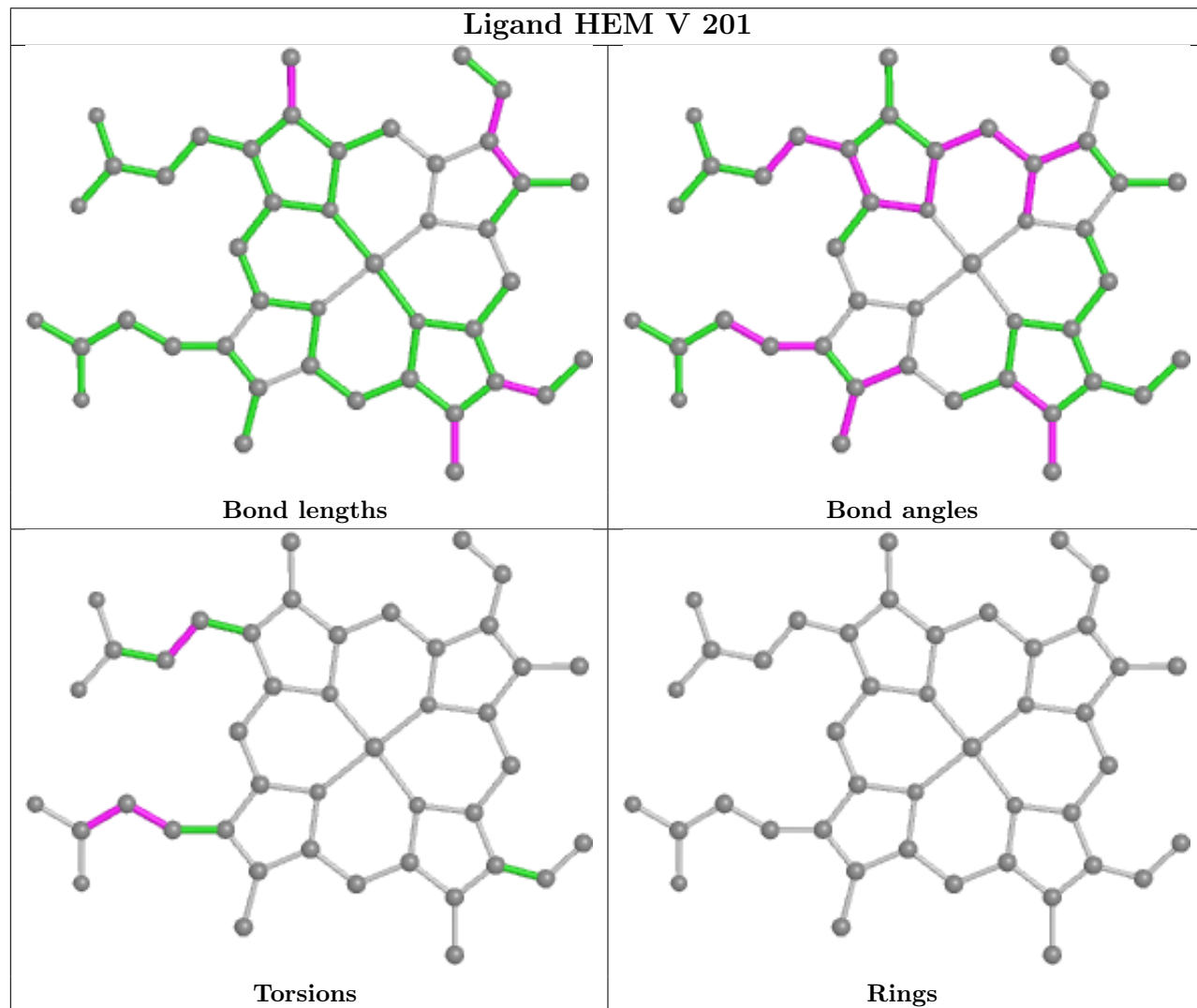
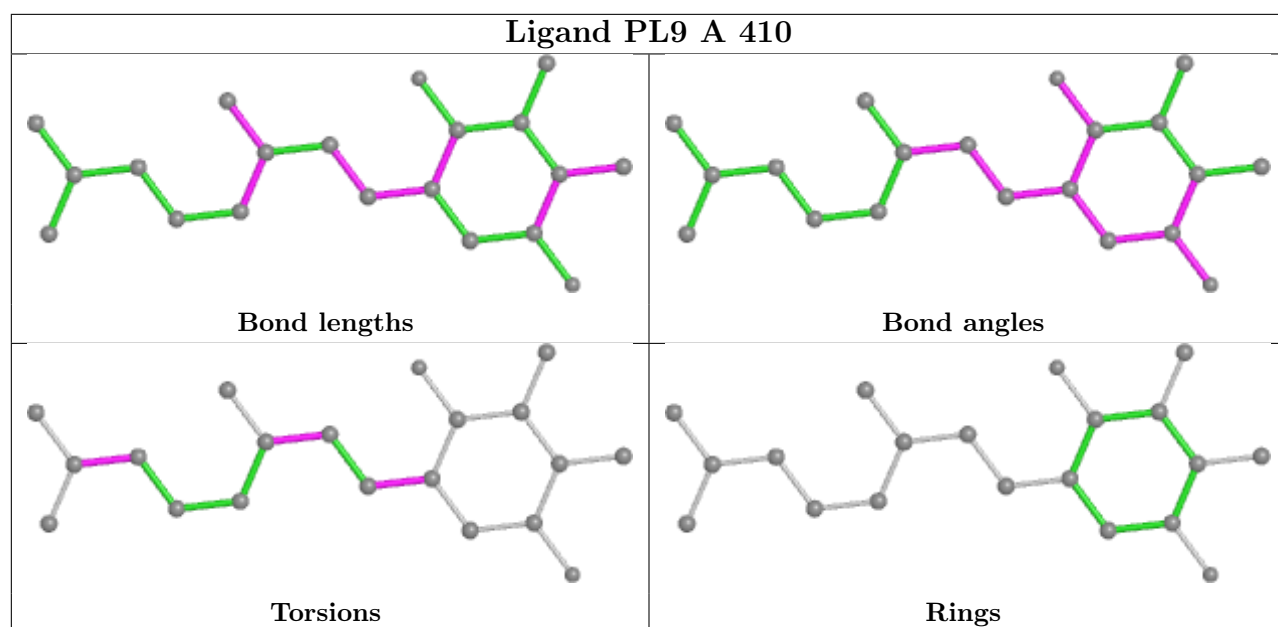


Ligand CLA c 510

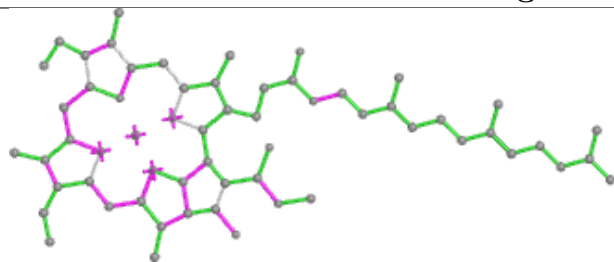


Ligand CLA C 502

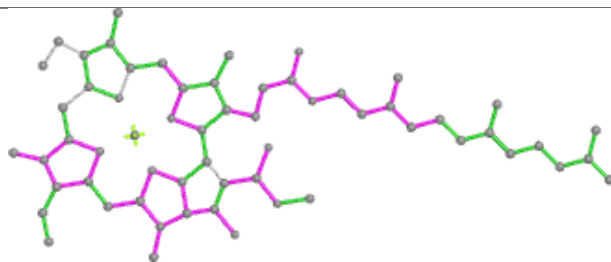




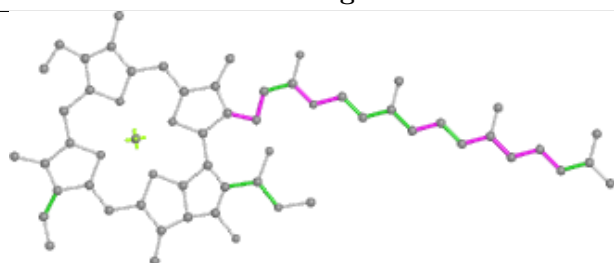
Ligand CLA b 615



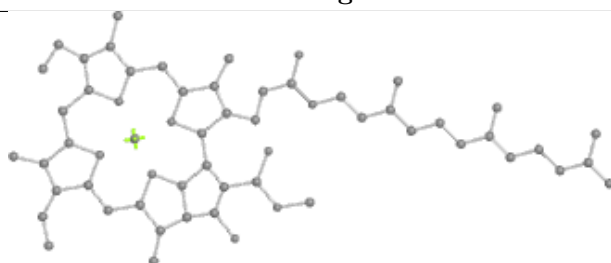
Bond lengths



Bond angles

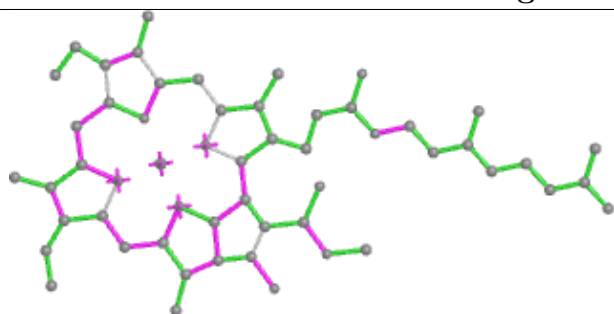


Torsions

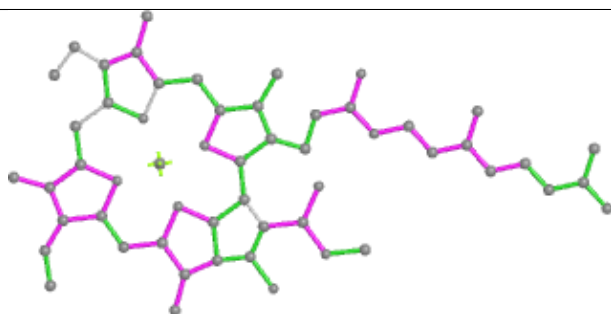


Rings

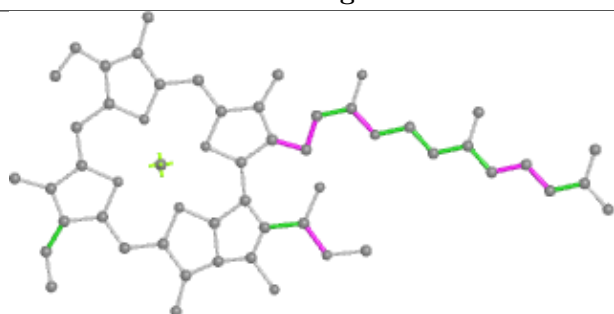
Ligand CLA b 608



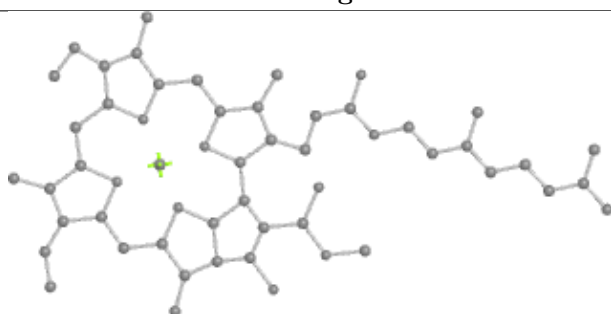
Bond lengths



Bond angles

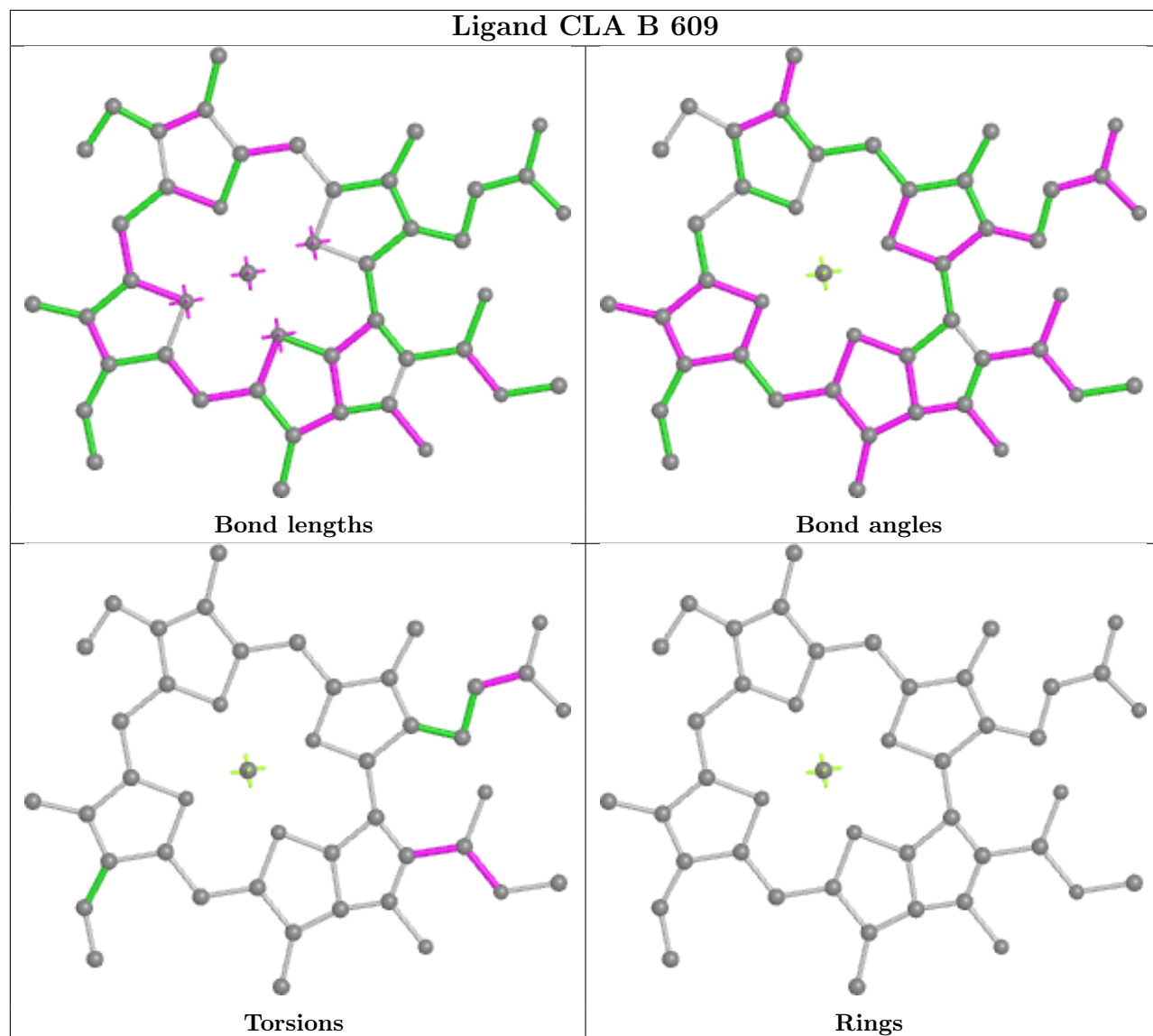


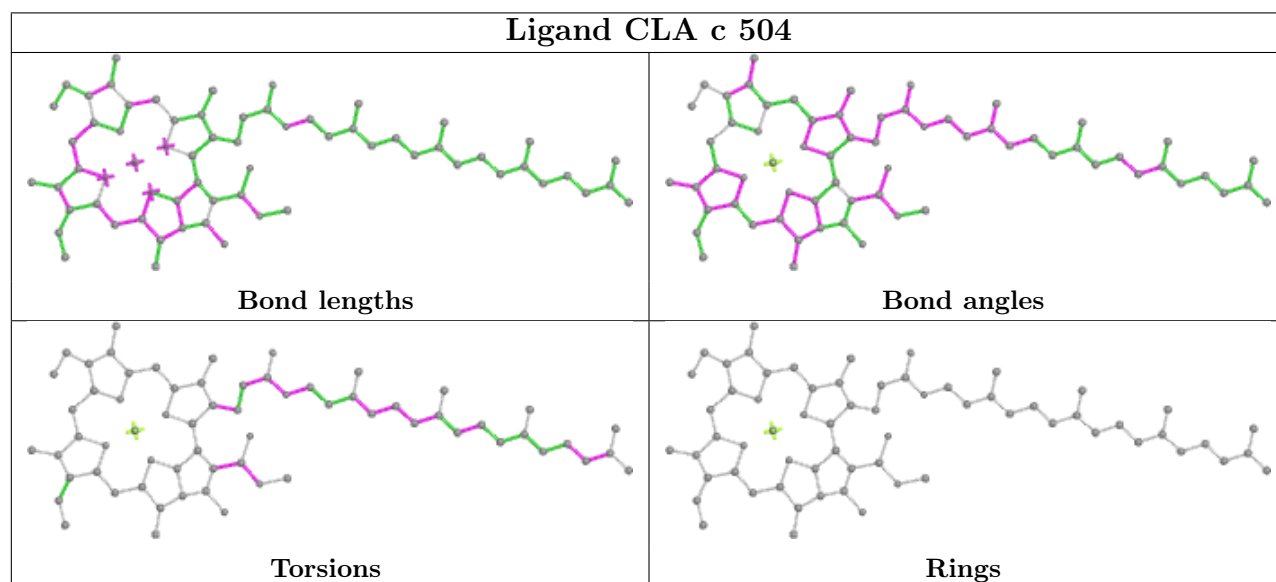
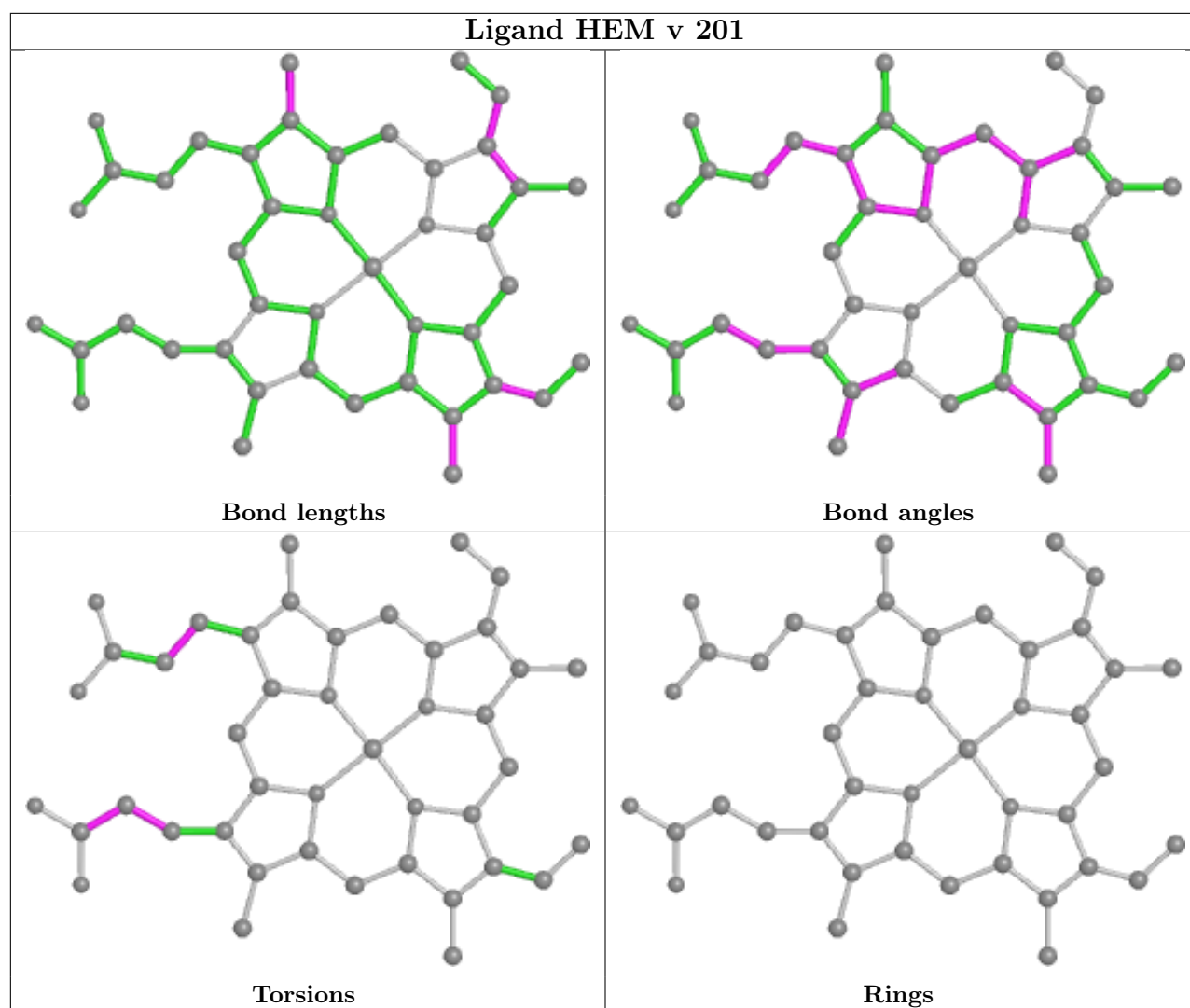
Torsions

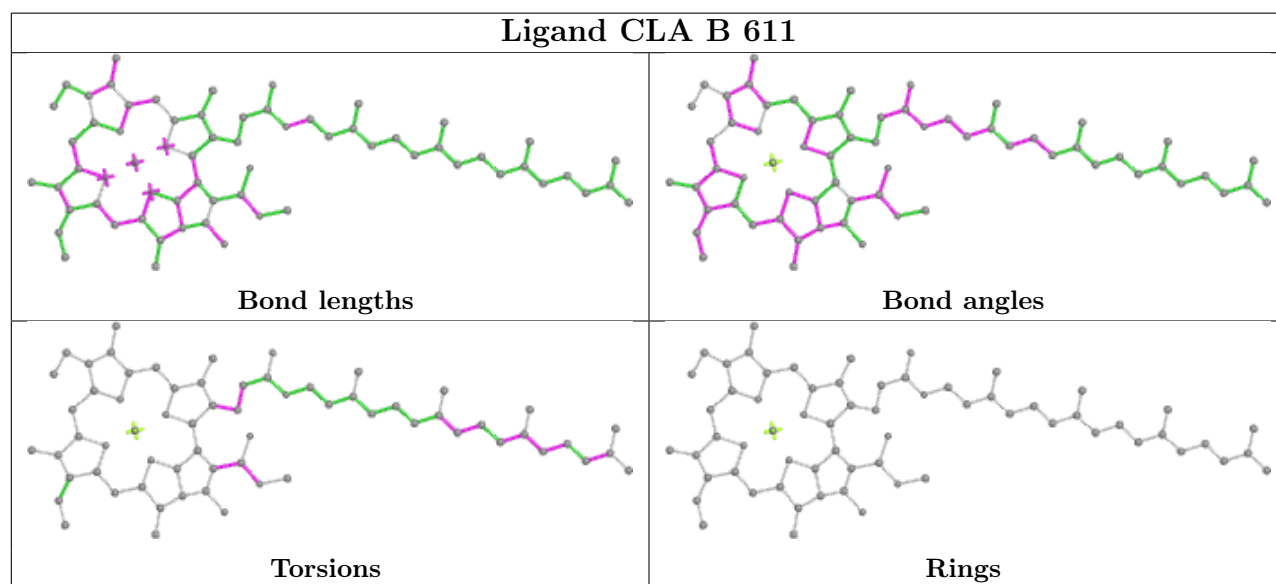
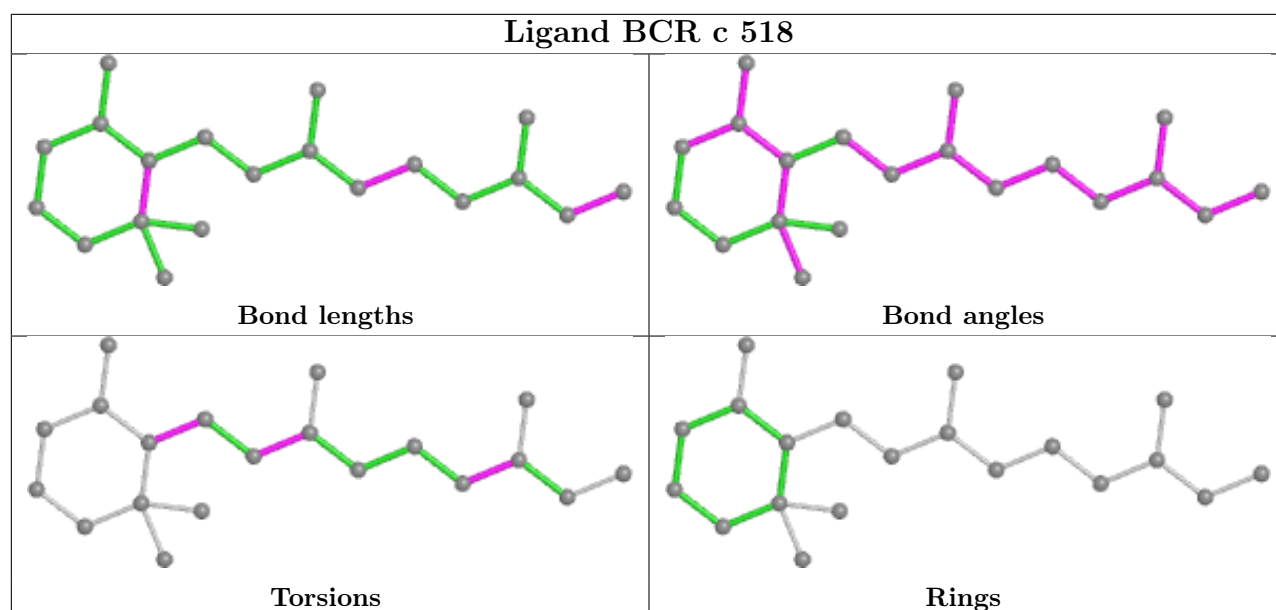


Rings

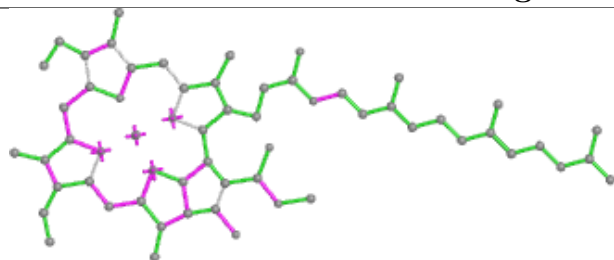
Ligand CLA B 609



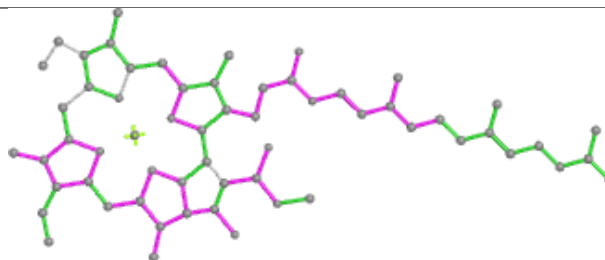




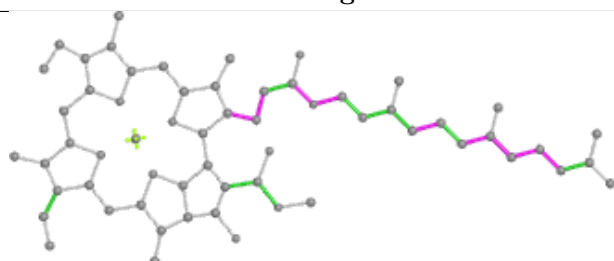
Ligand CLA B 615



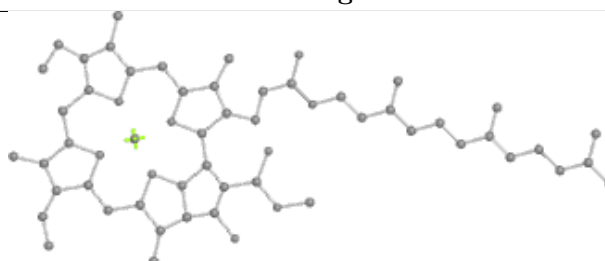
Bond lengths



Bond angles

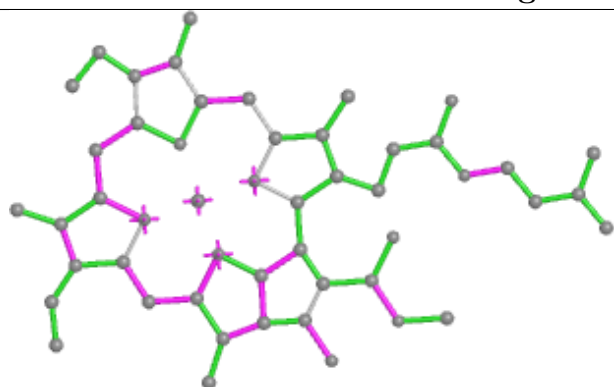


Torsions

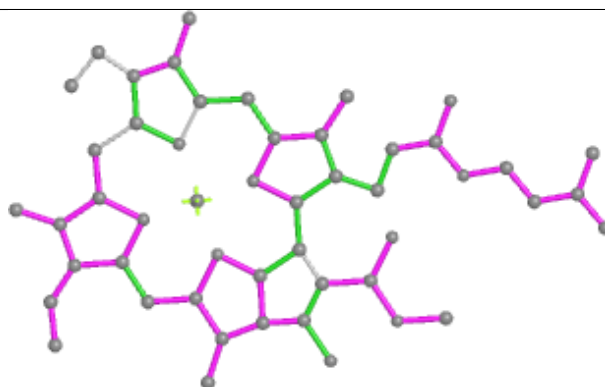


Rings

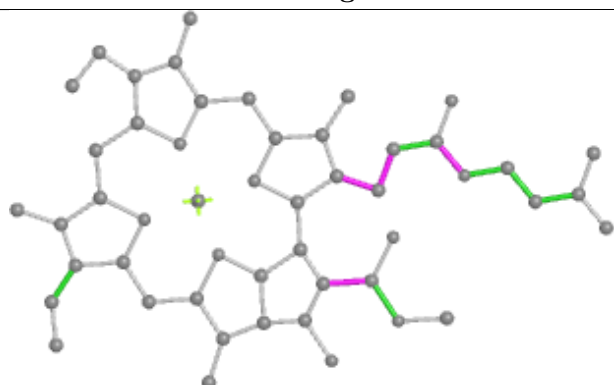
Ligand CLA a 405



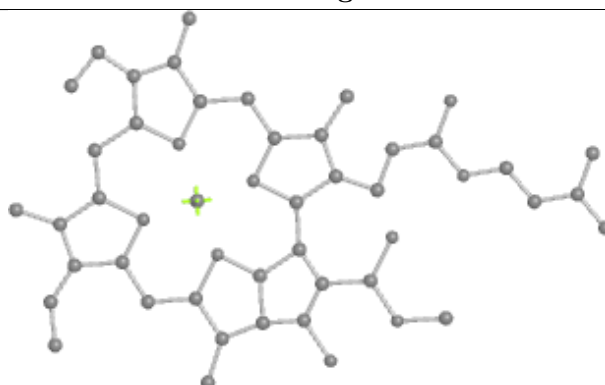
Bond lengths



Bond angles

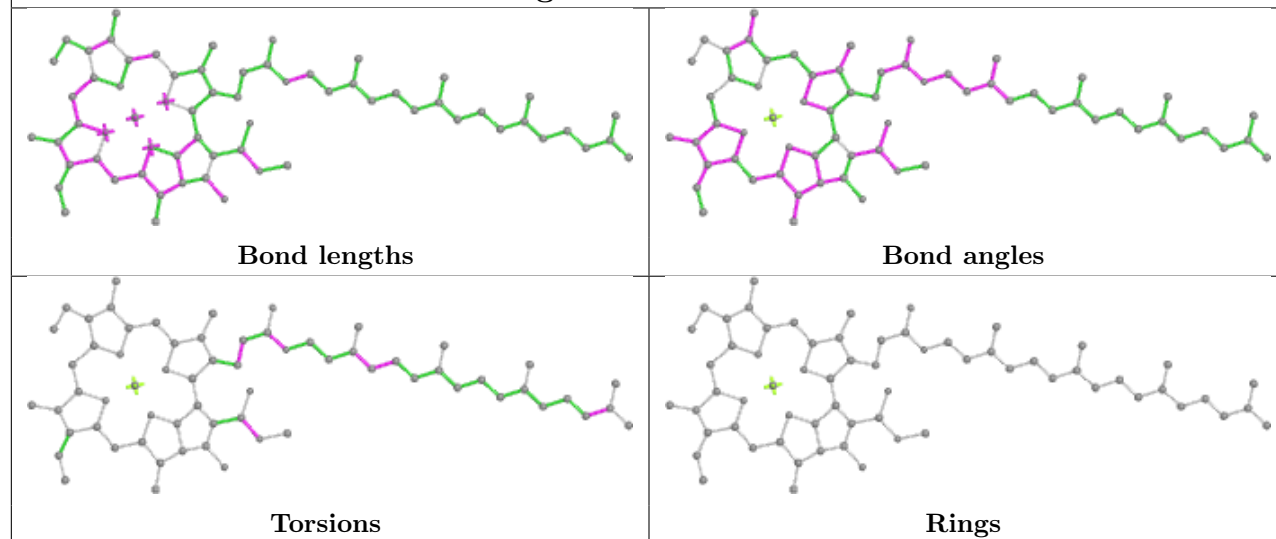


Torsions

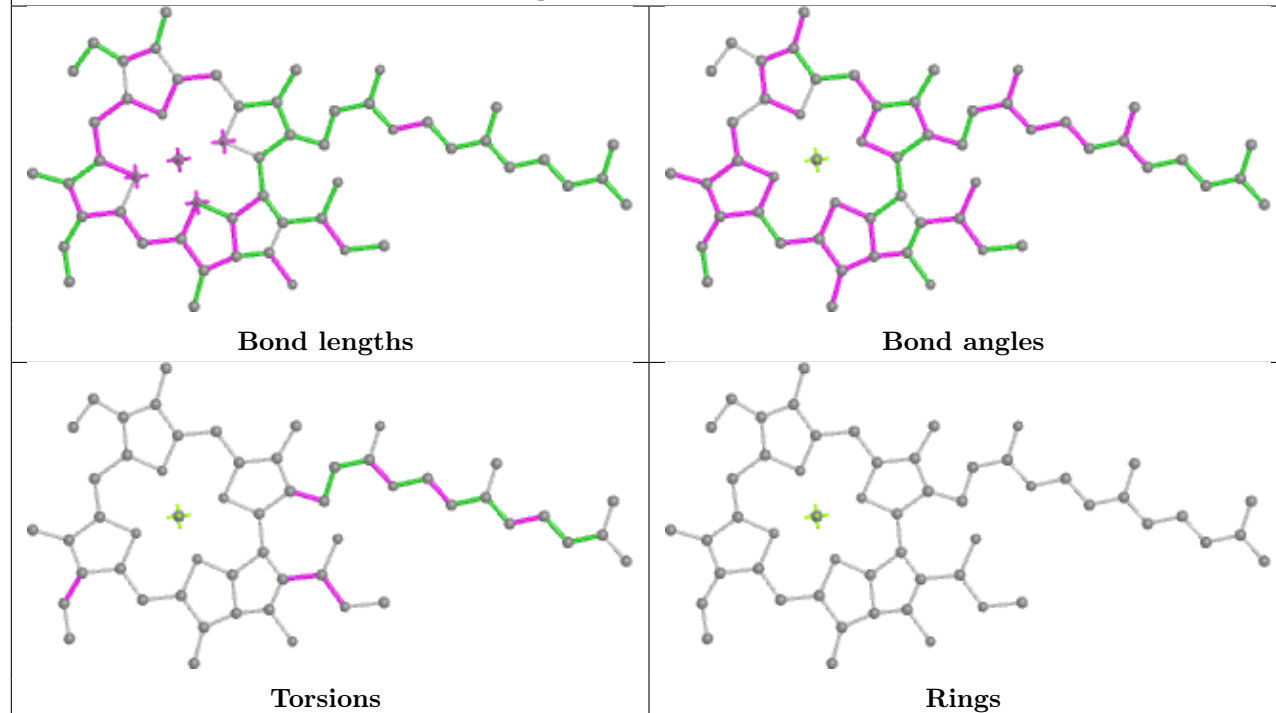


Rings

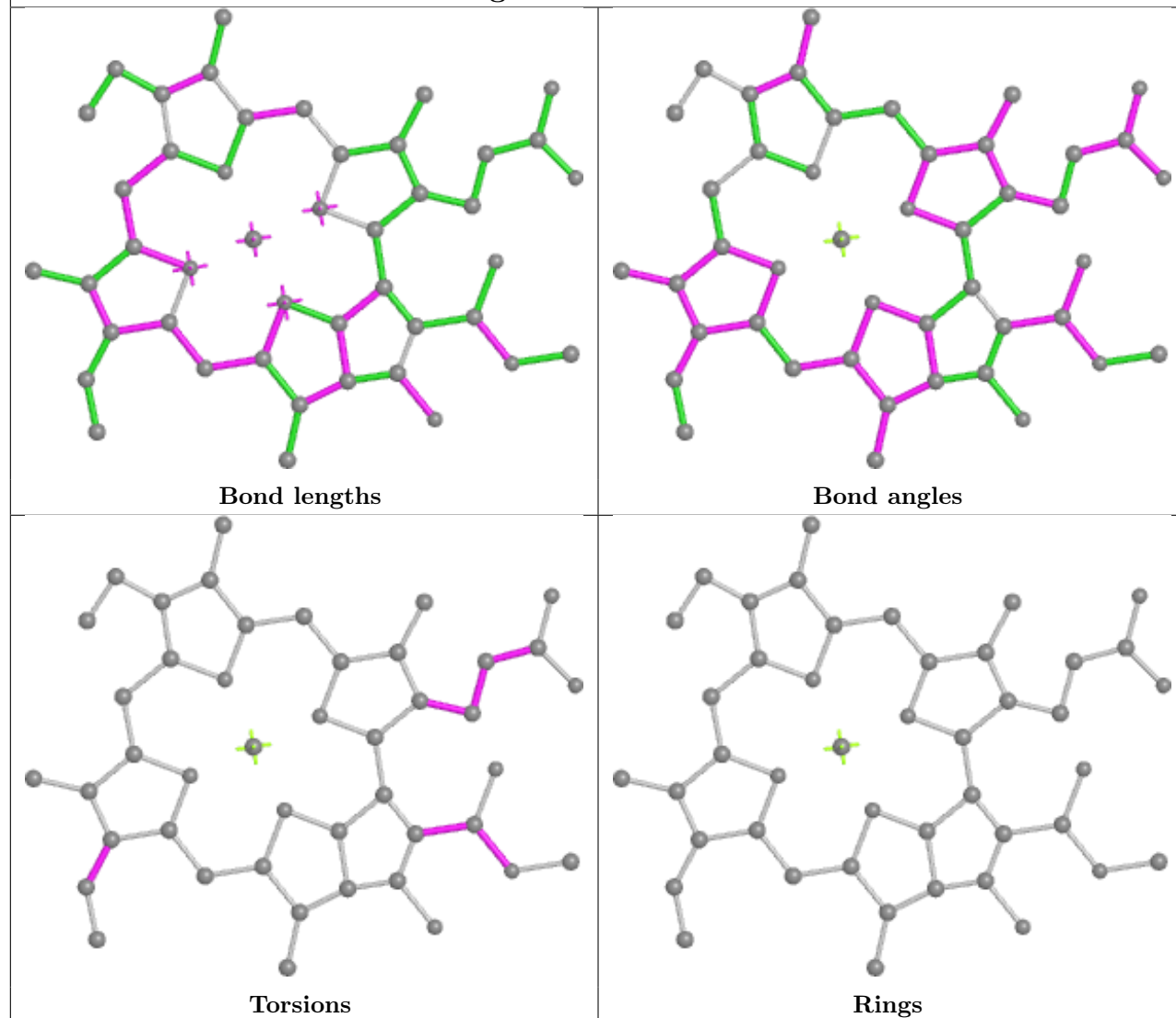
Ligand CLA a 404



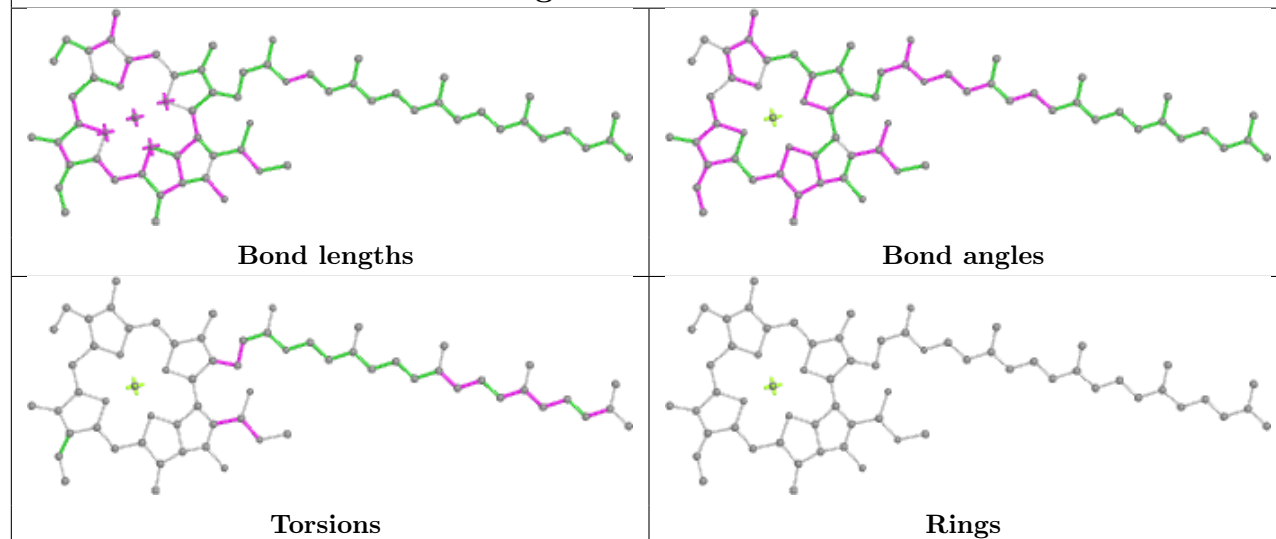
Ligand CLA C 507

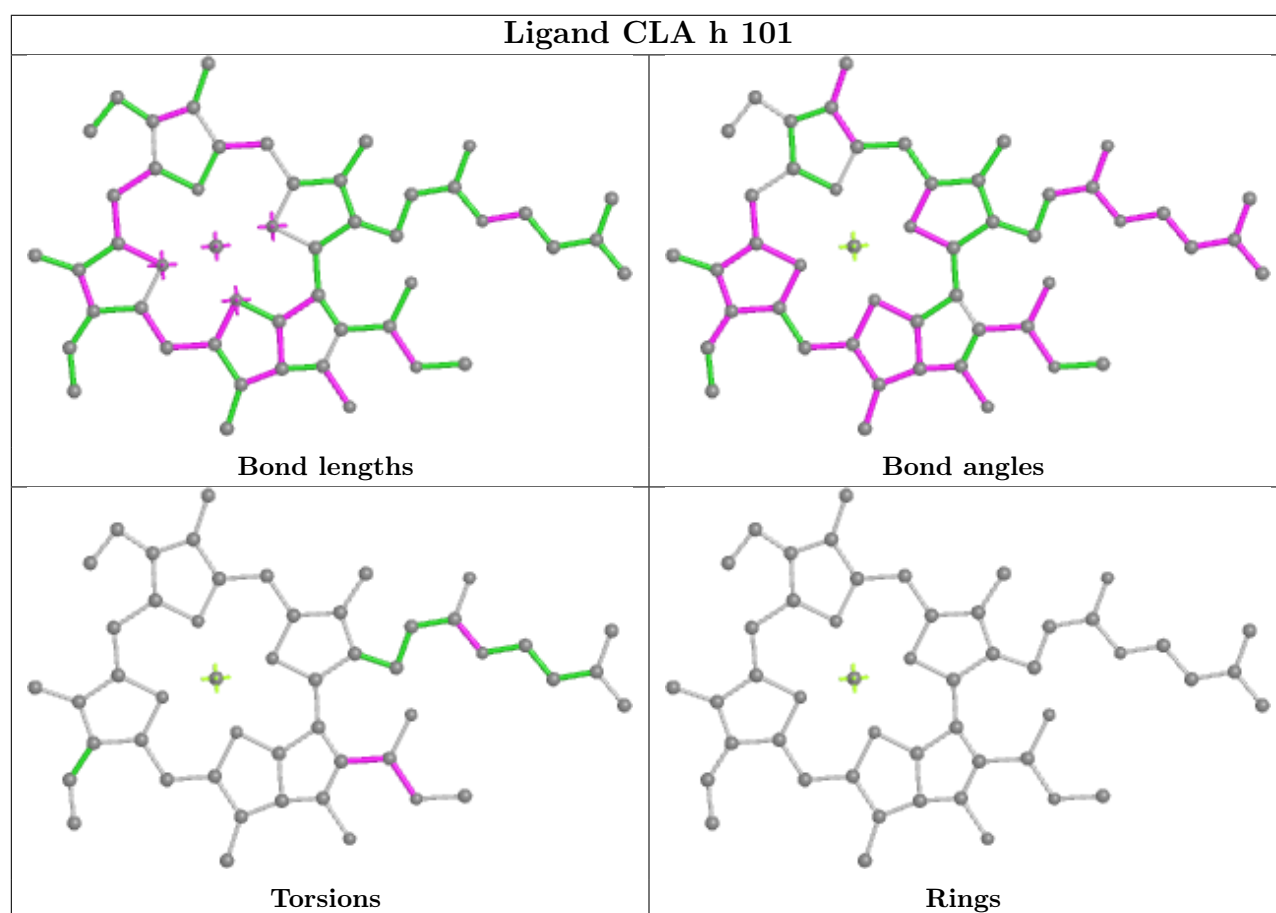
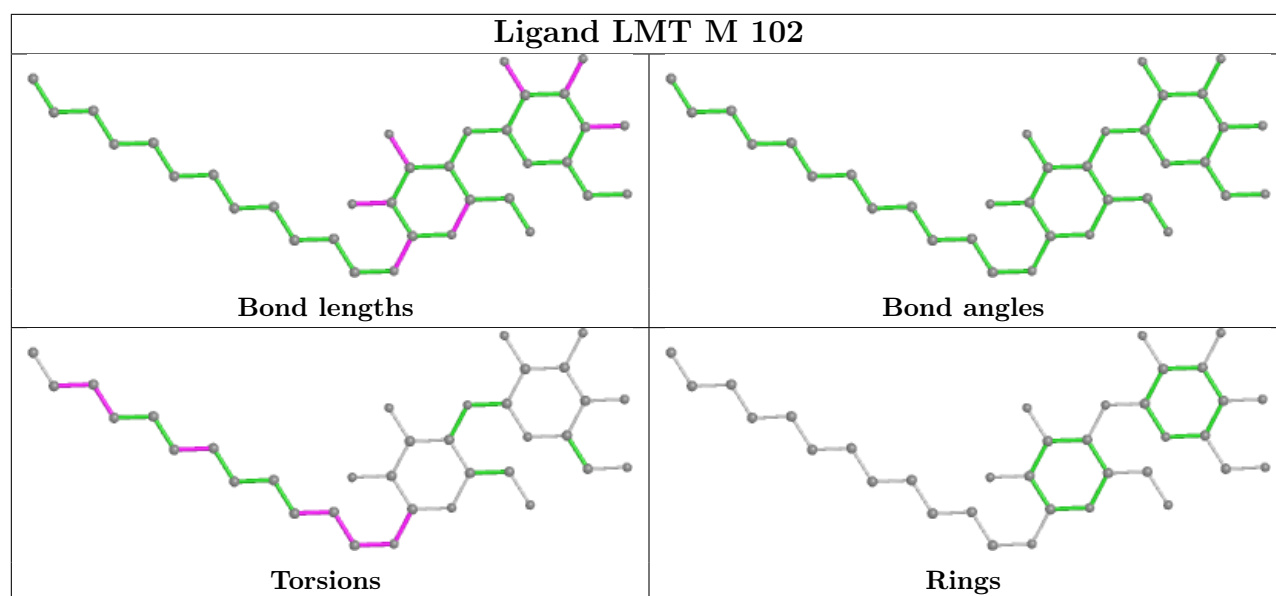


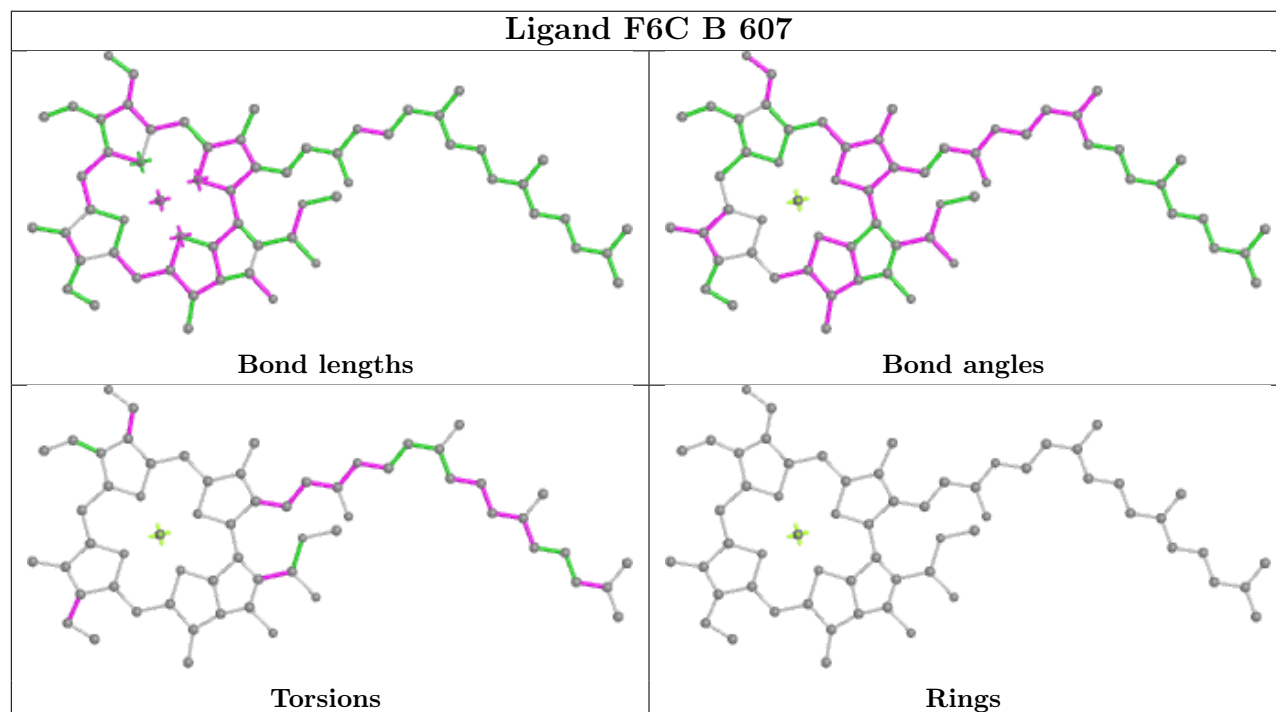
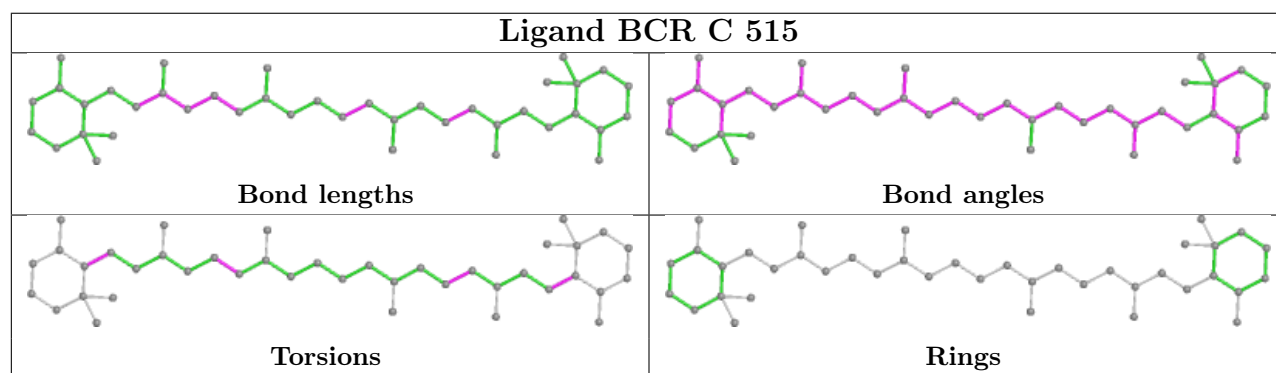
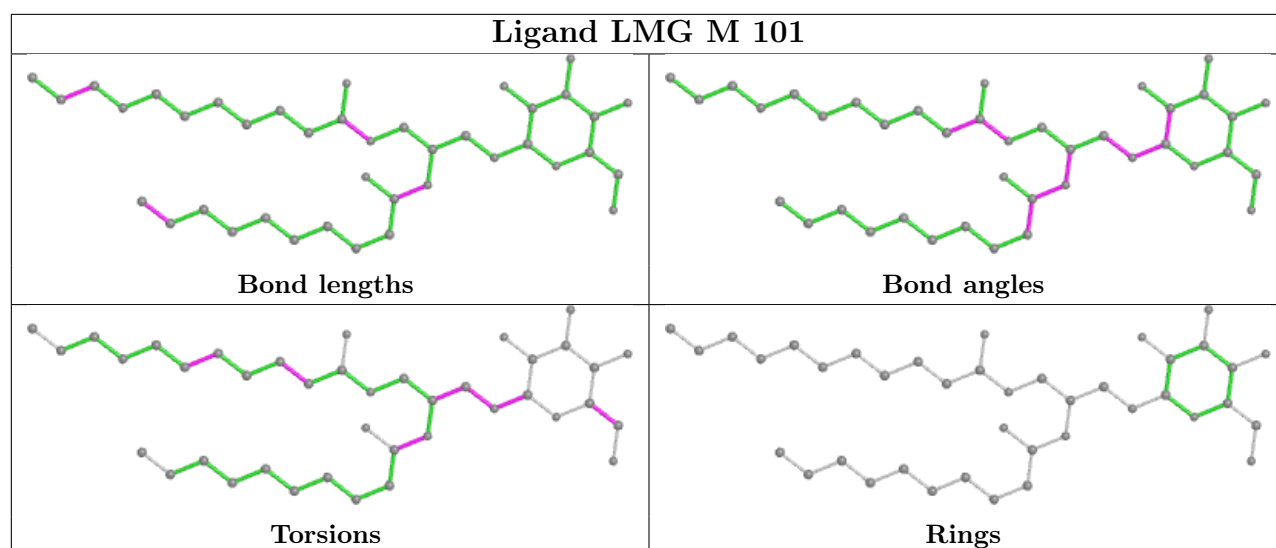
Ligand CLA D 404

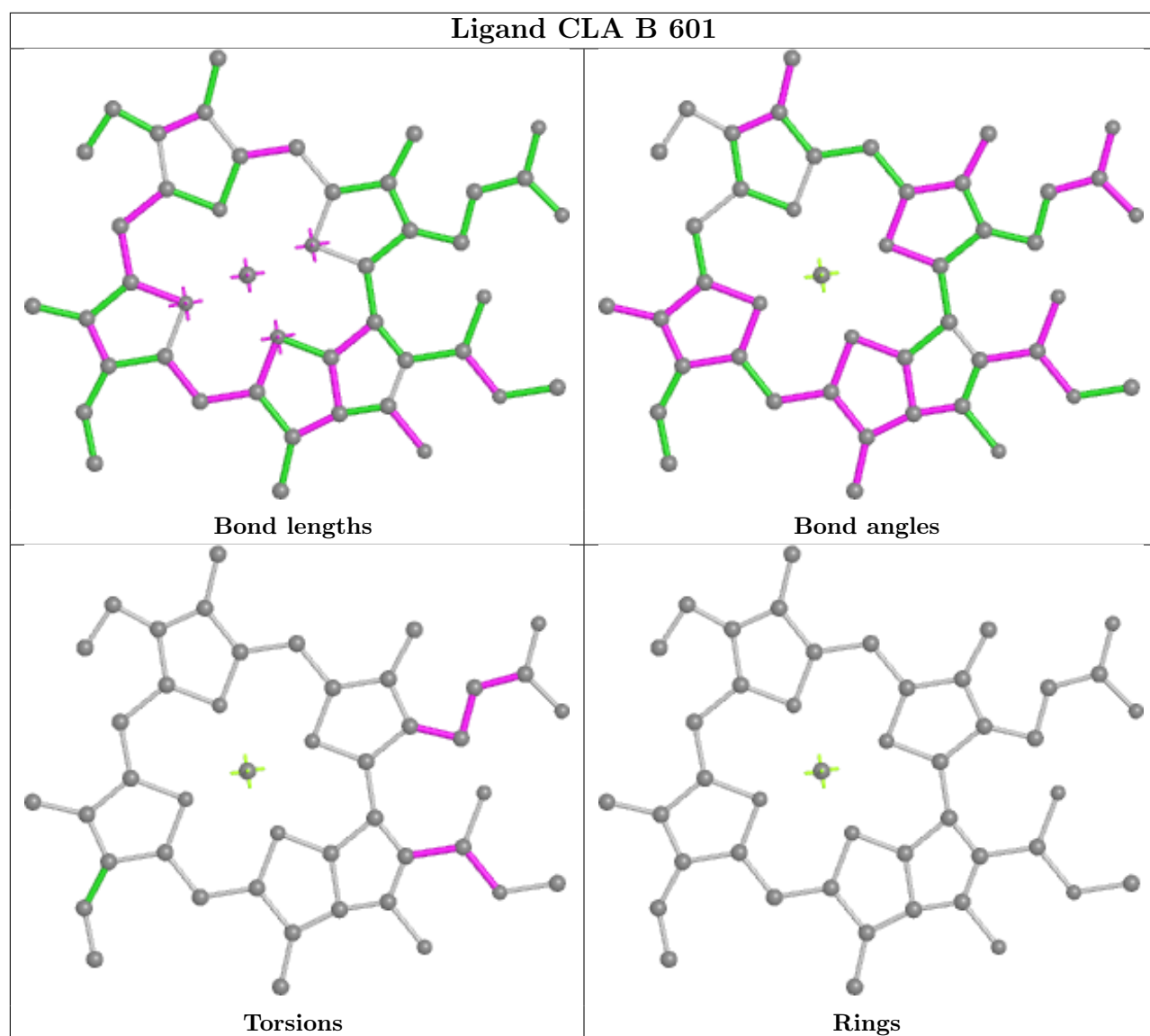


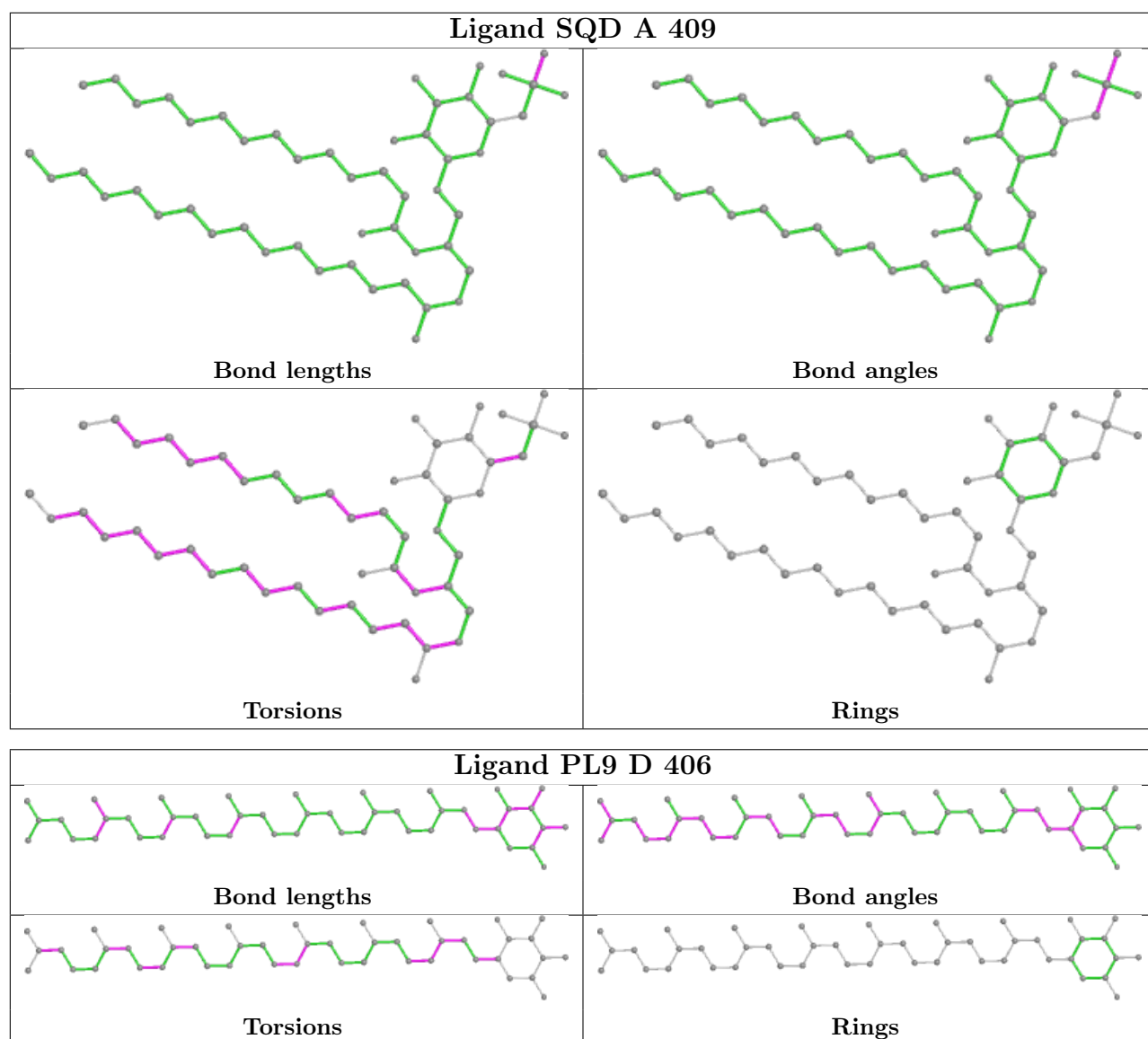
Ligand CLA b 611



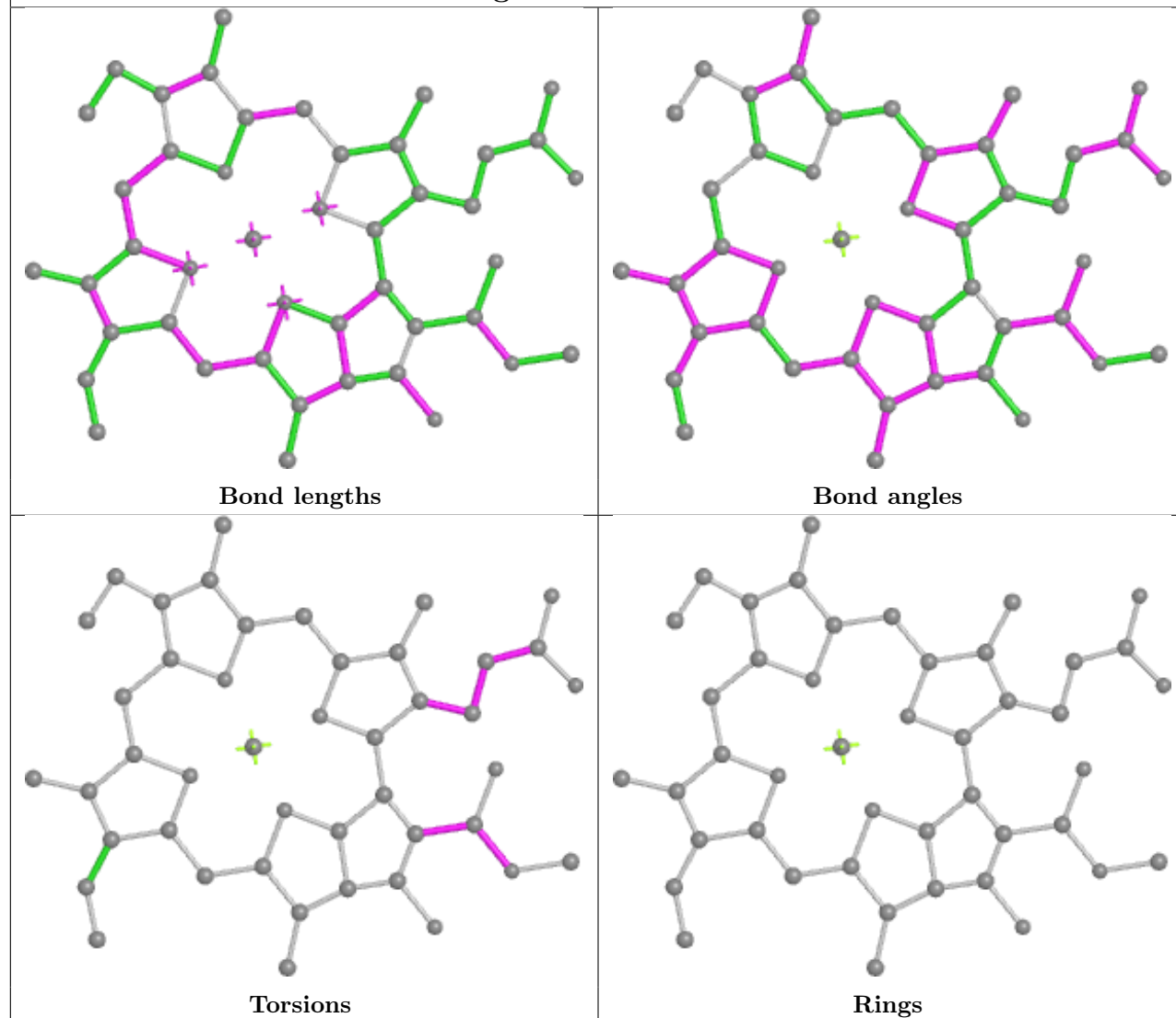




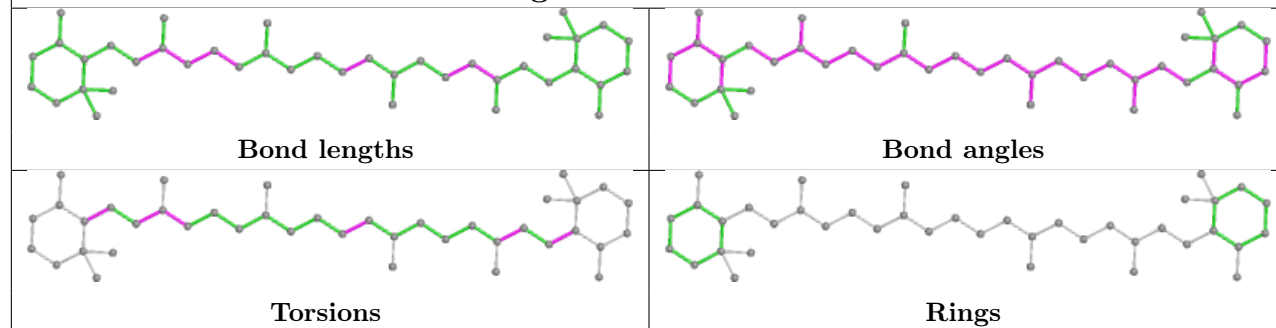


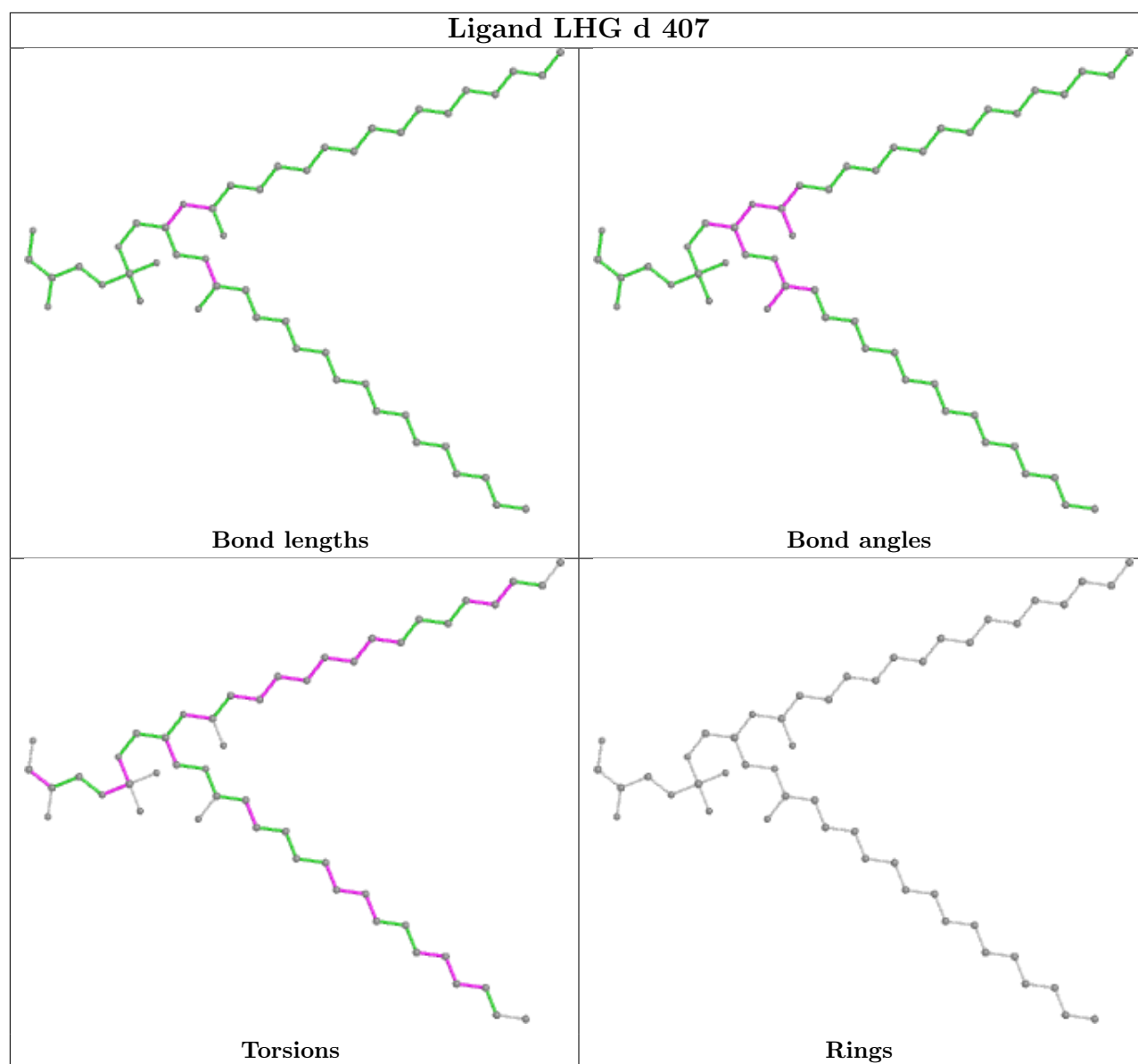


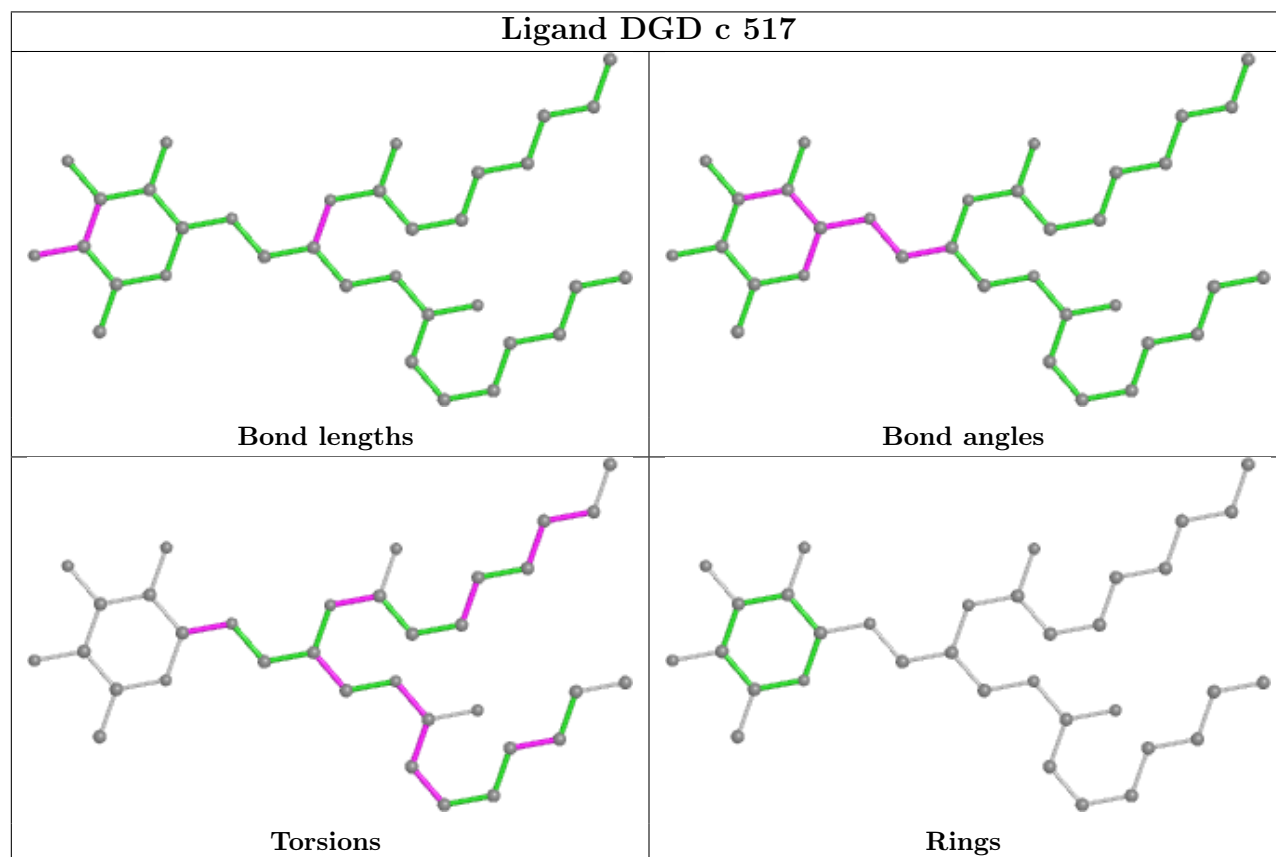
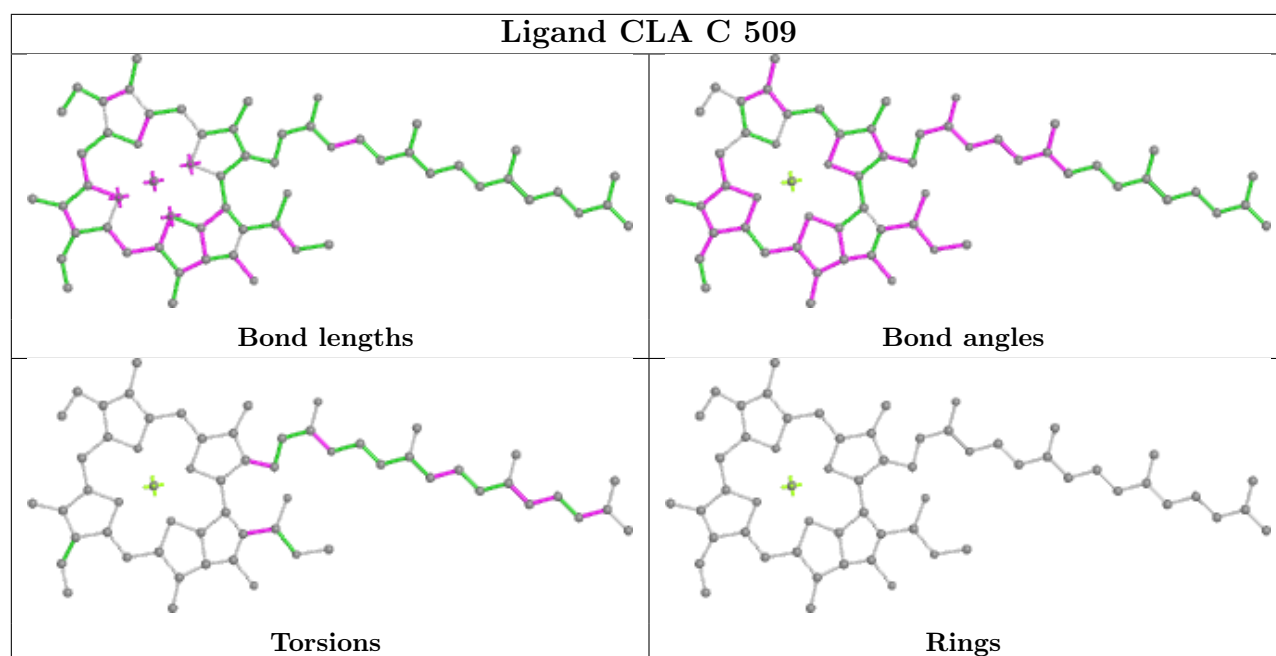
Ligand CLA b 601

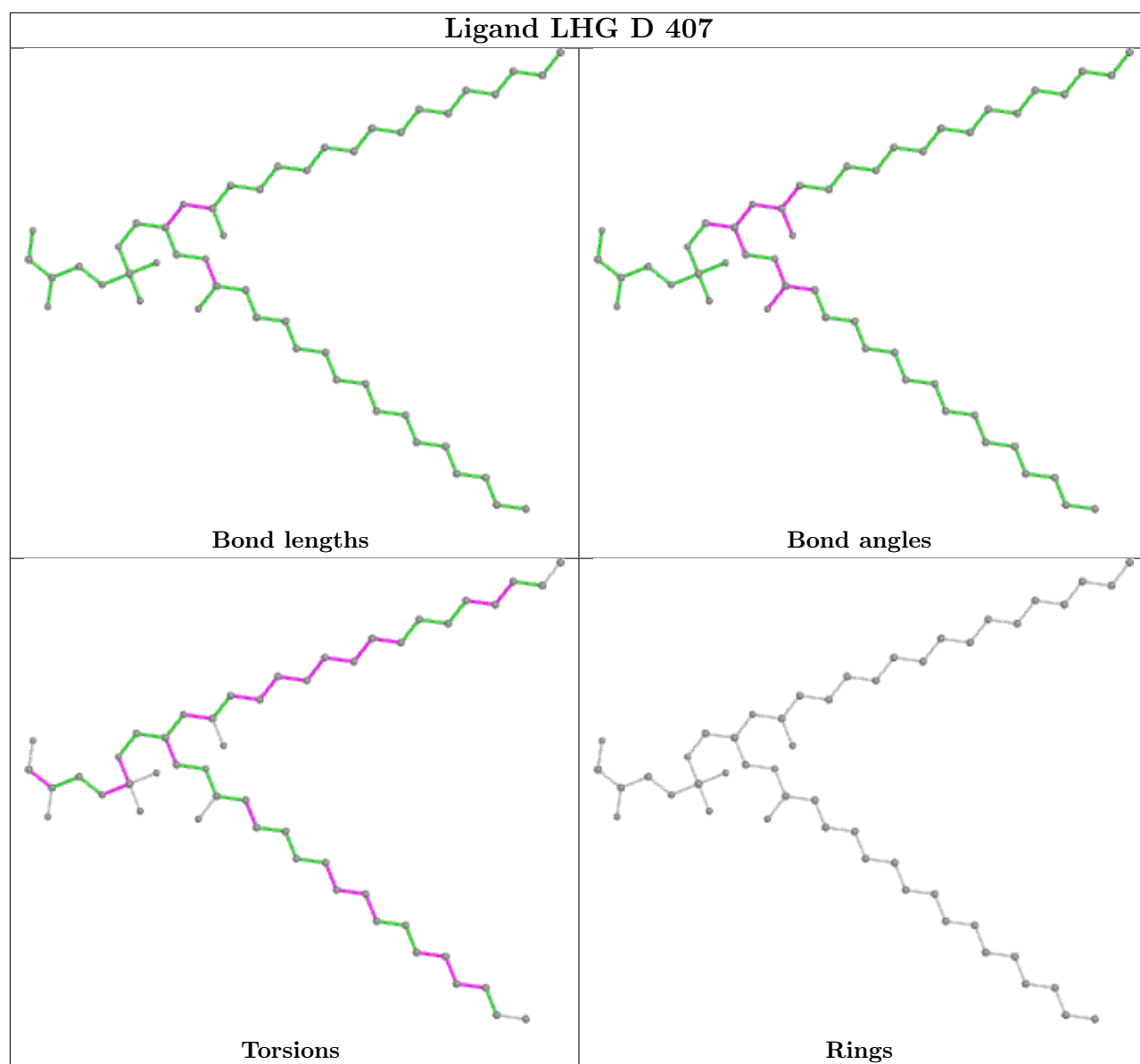


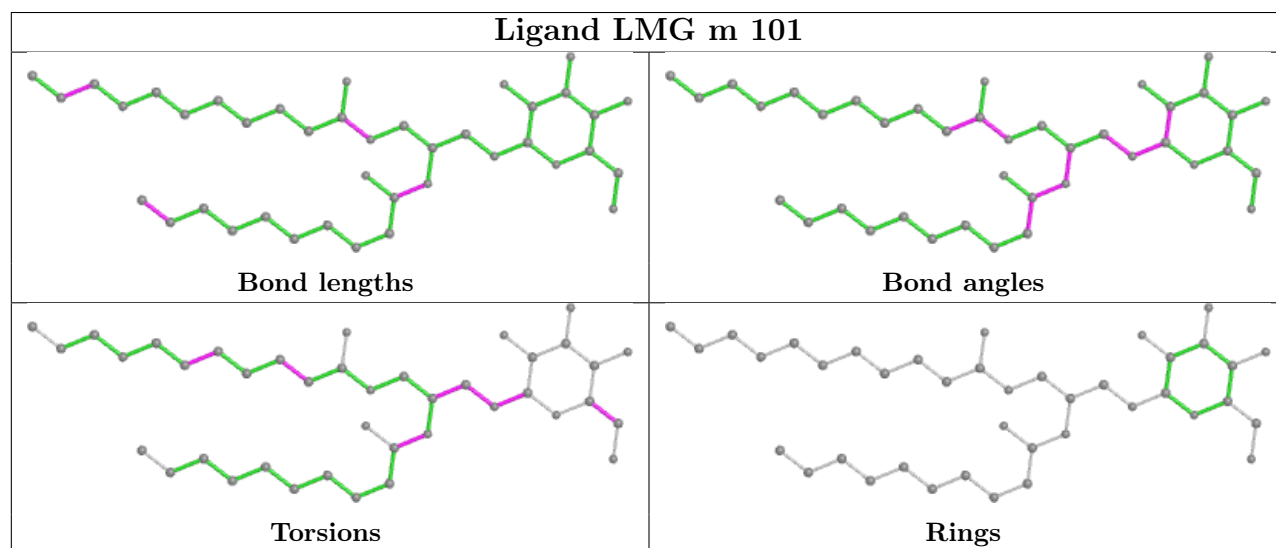
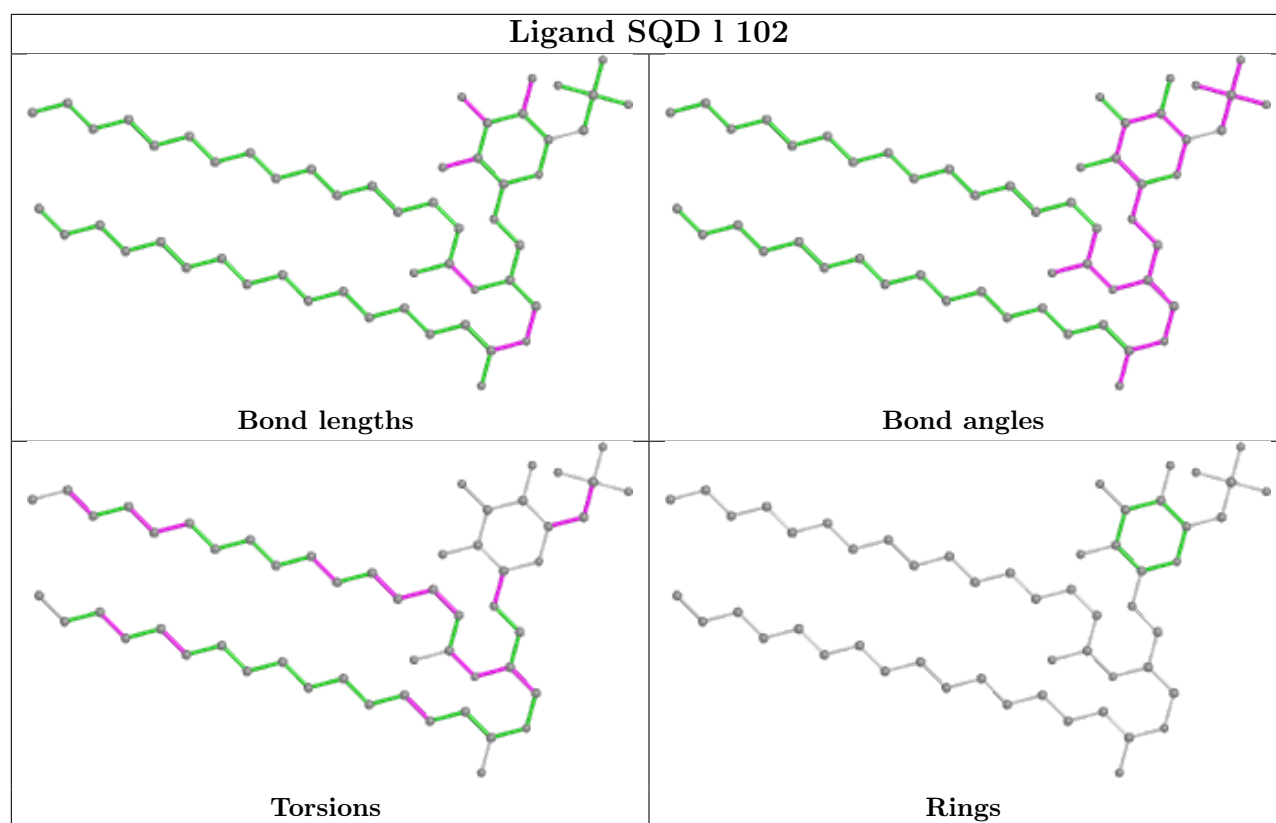
Ligand BCR B 618

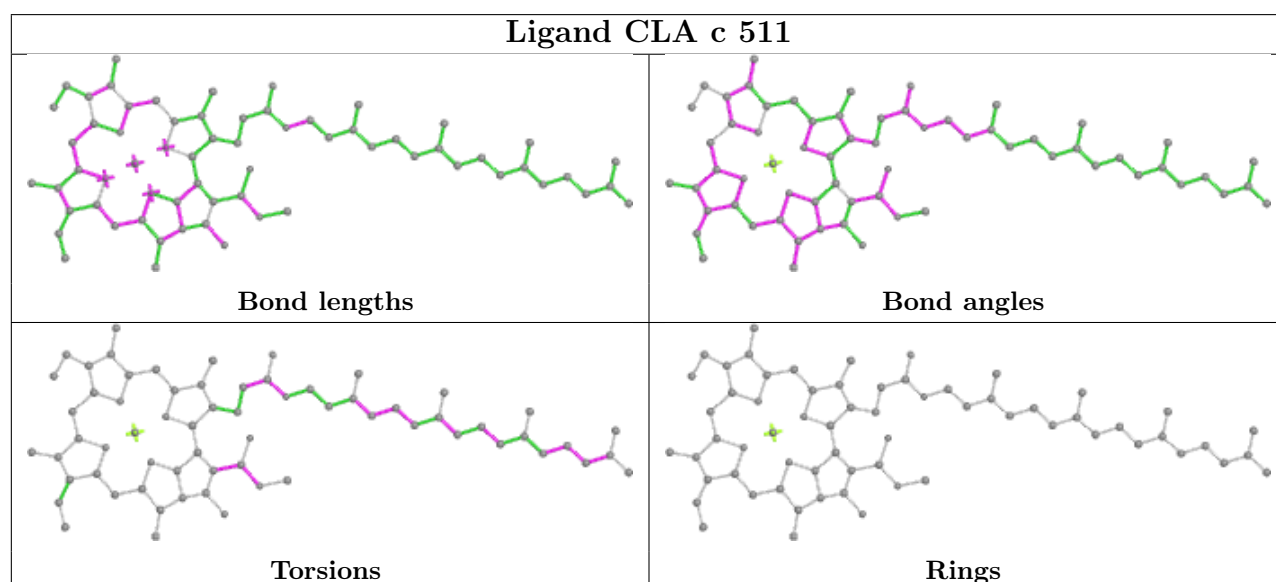
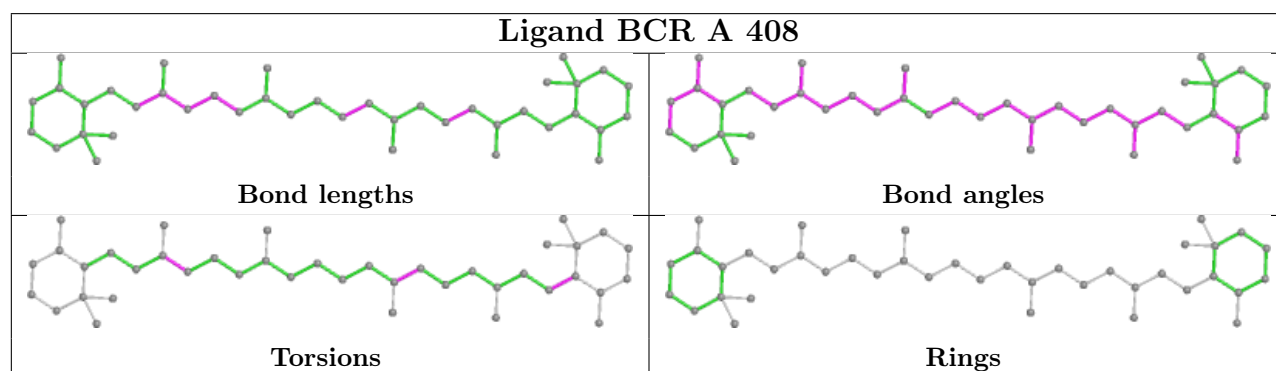
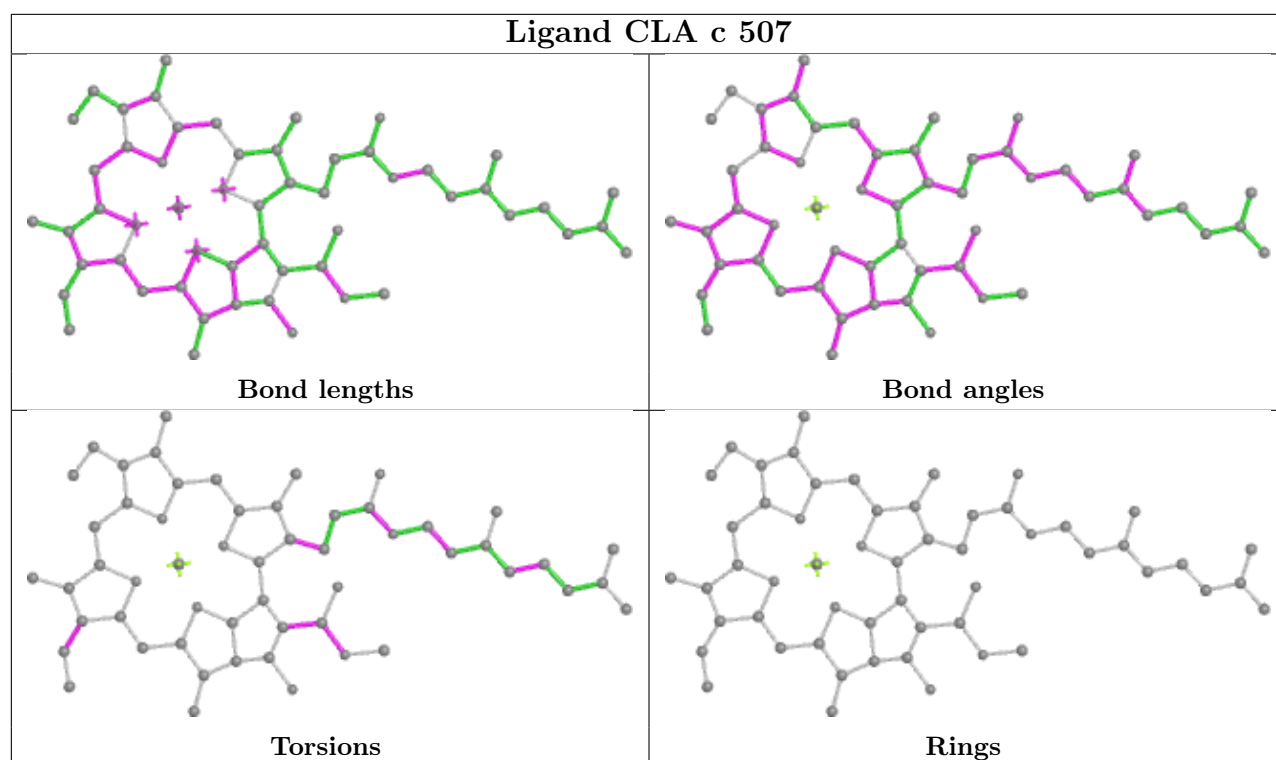


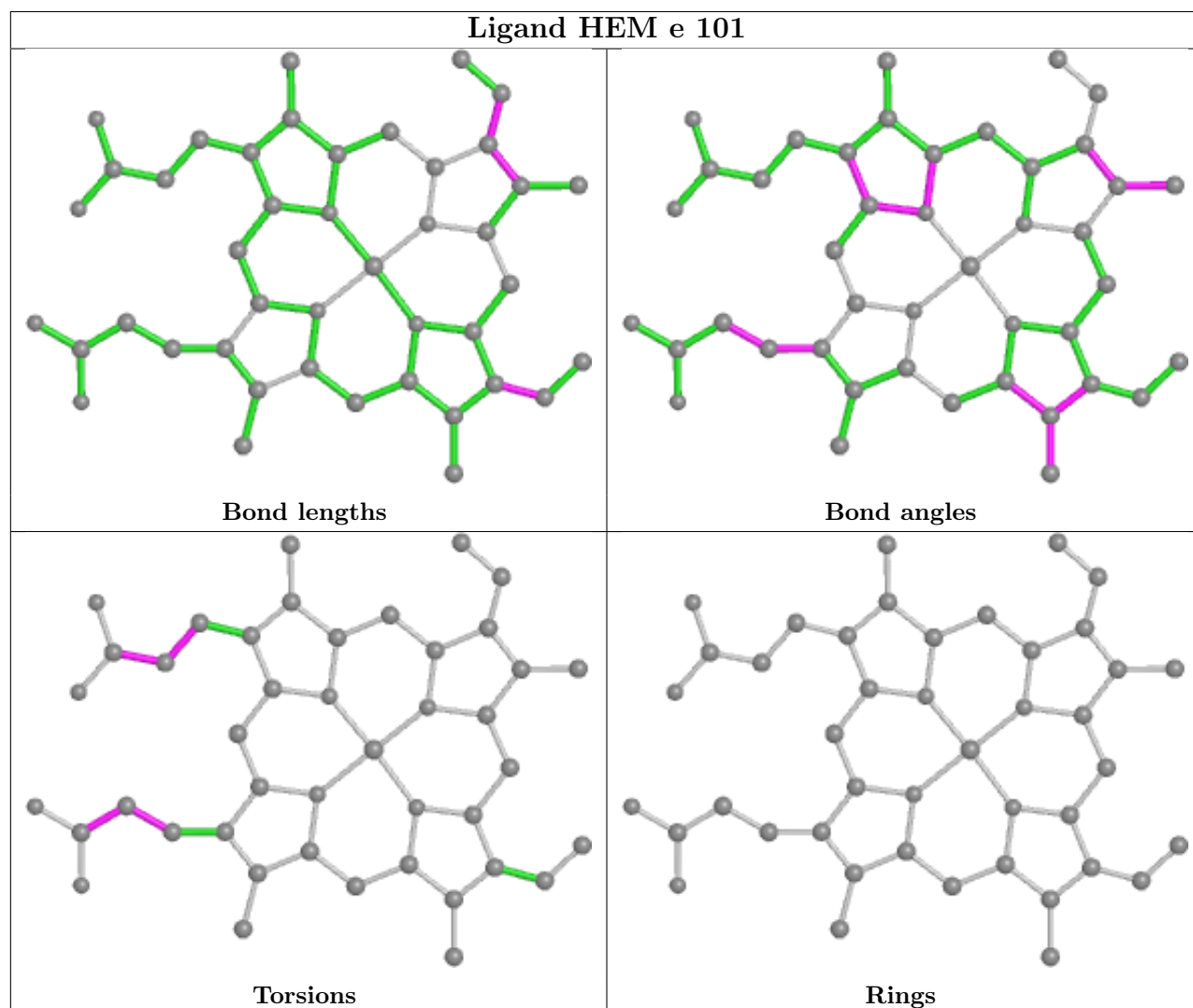
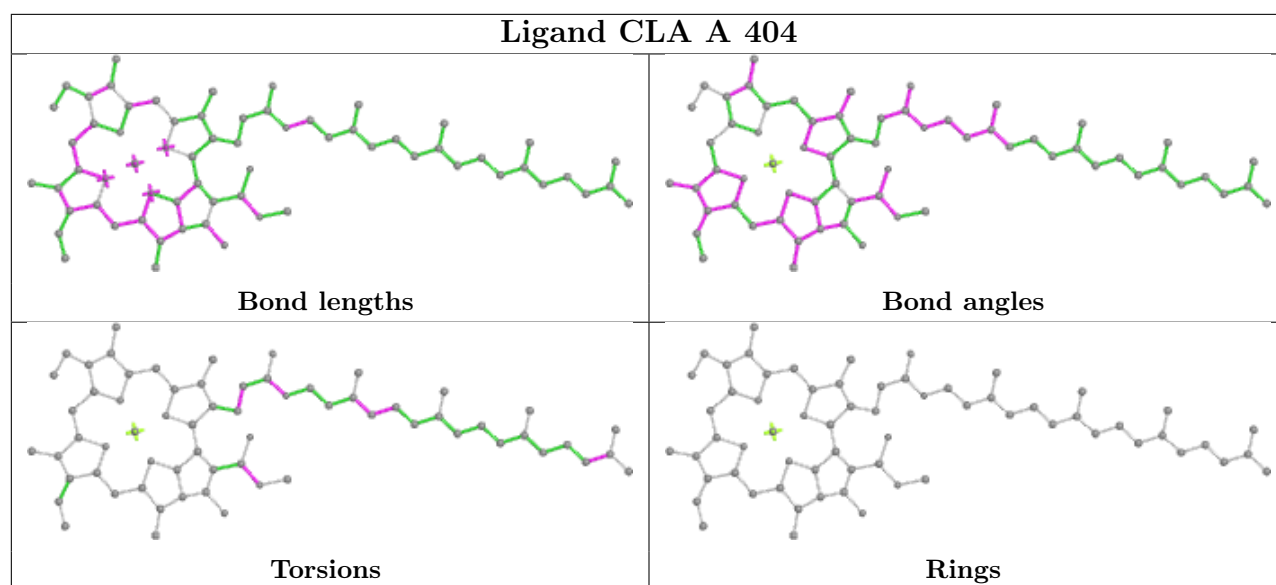




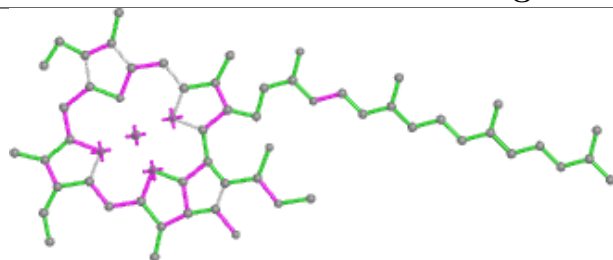




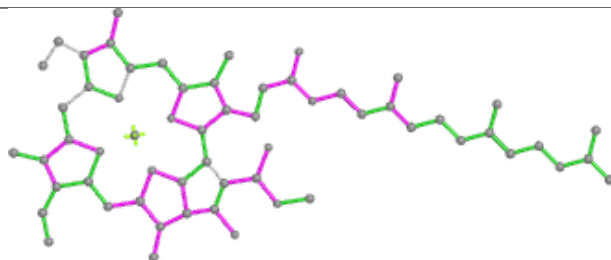




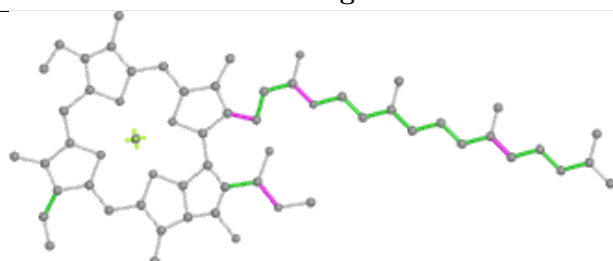
Ligand CLA D 403



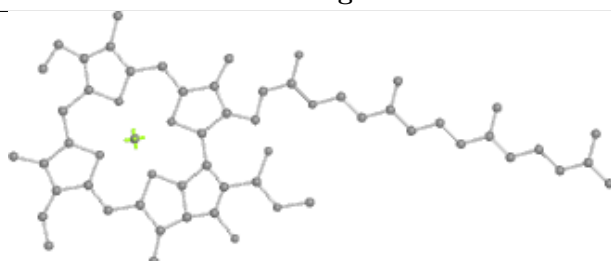
Bond lengths



Bond angles

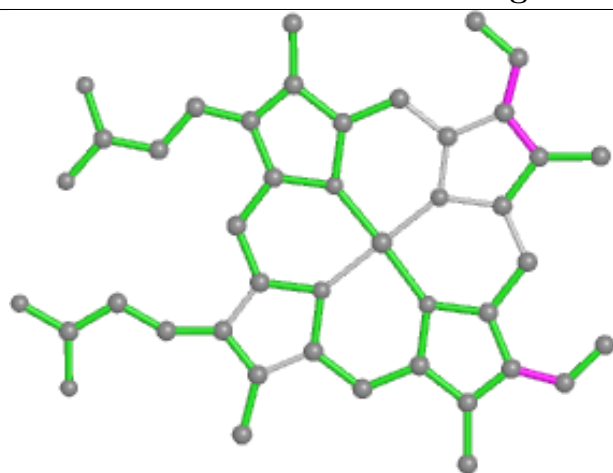


Torsions

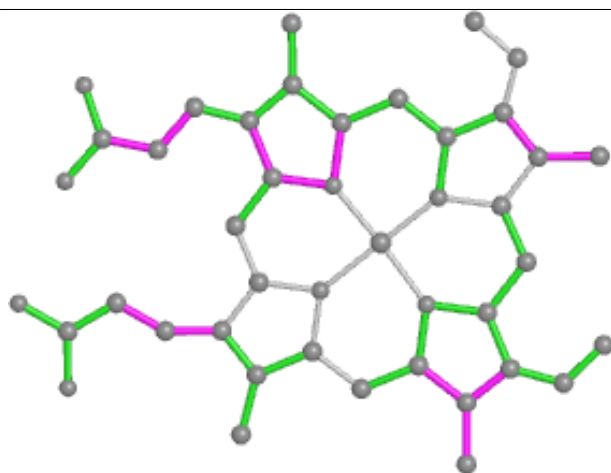


Rings

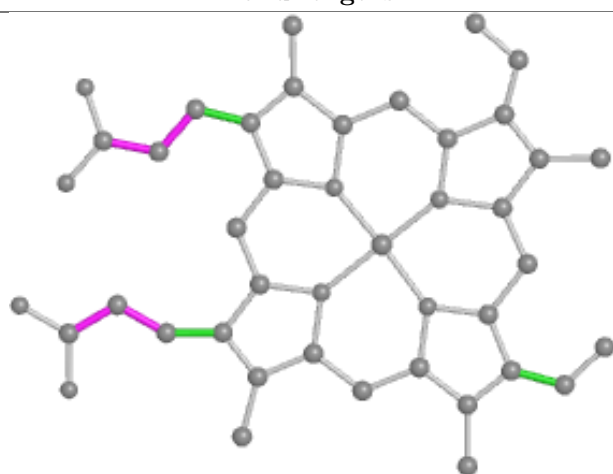
Ligand HEM E 101



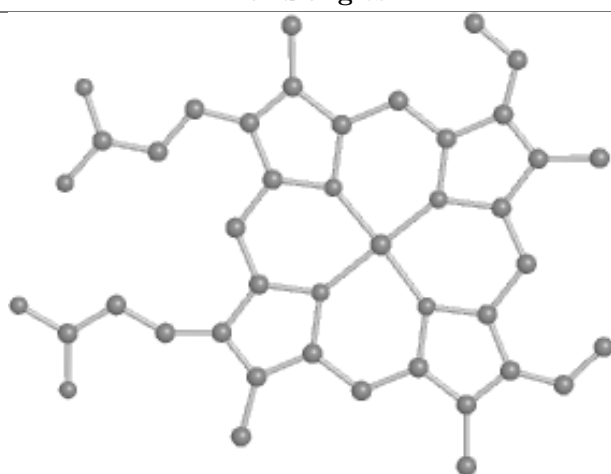
Bond lengths



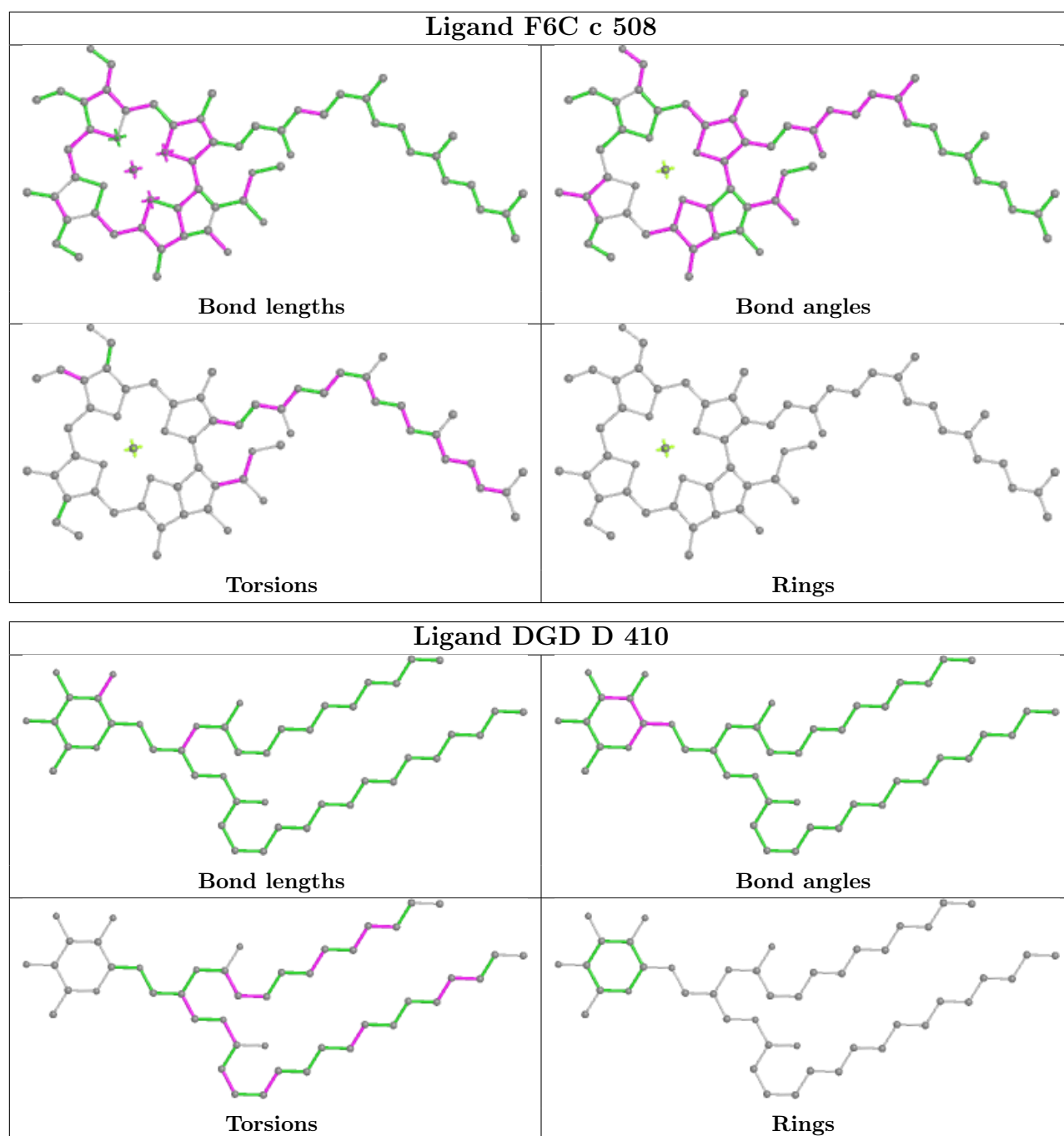
Bond angles

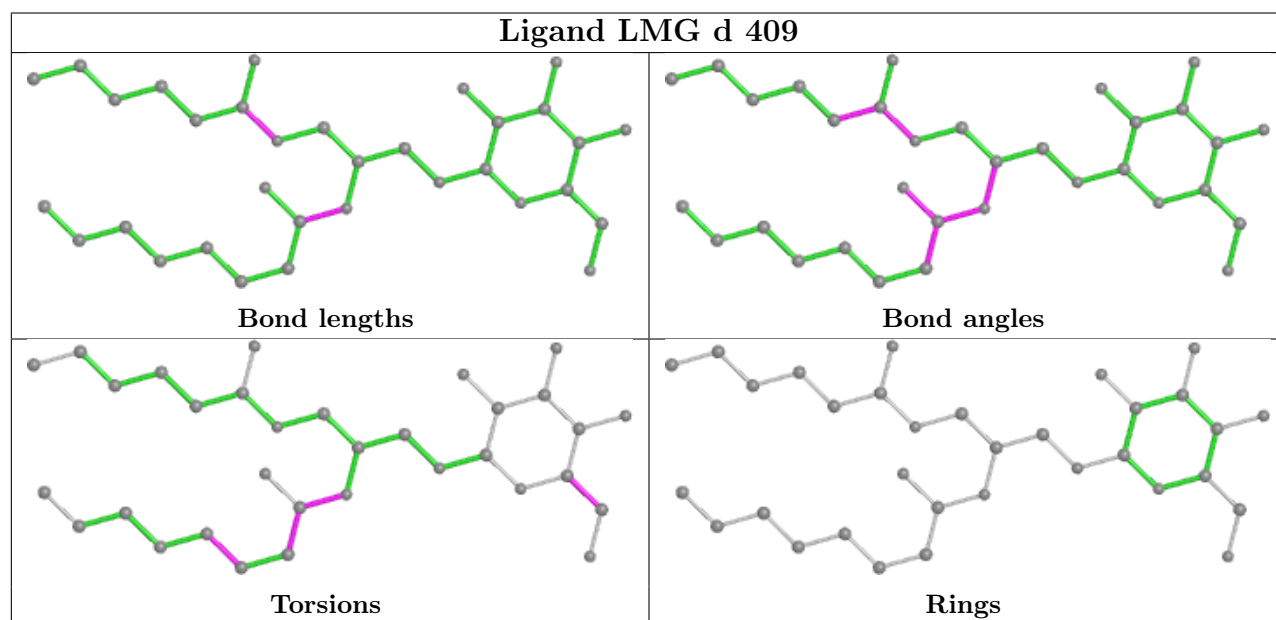
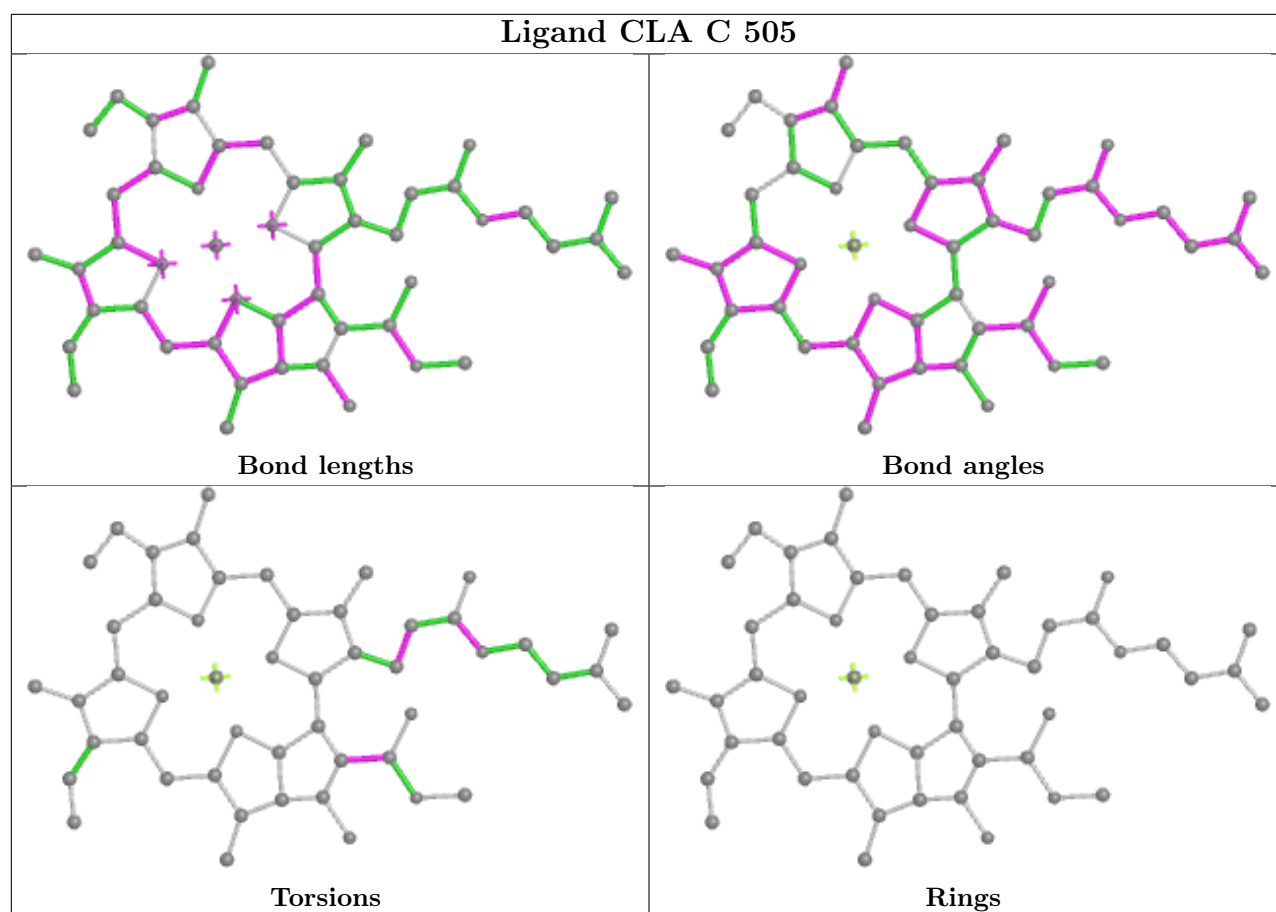


Torsions

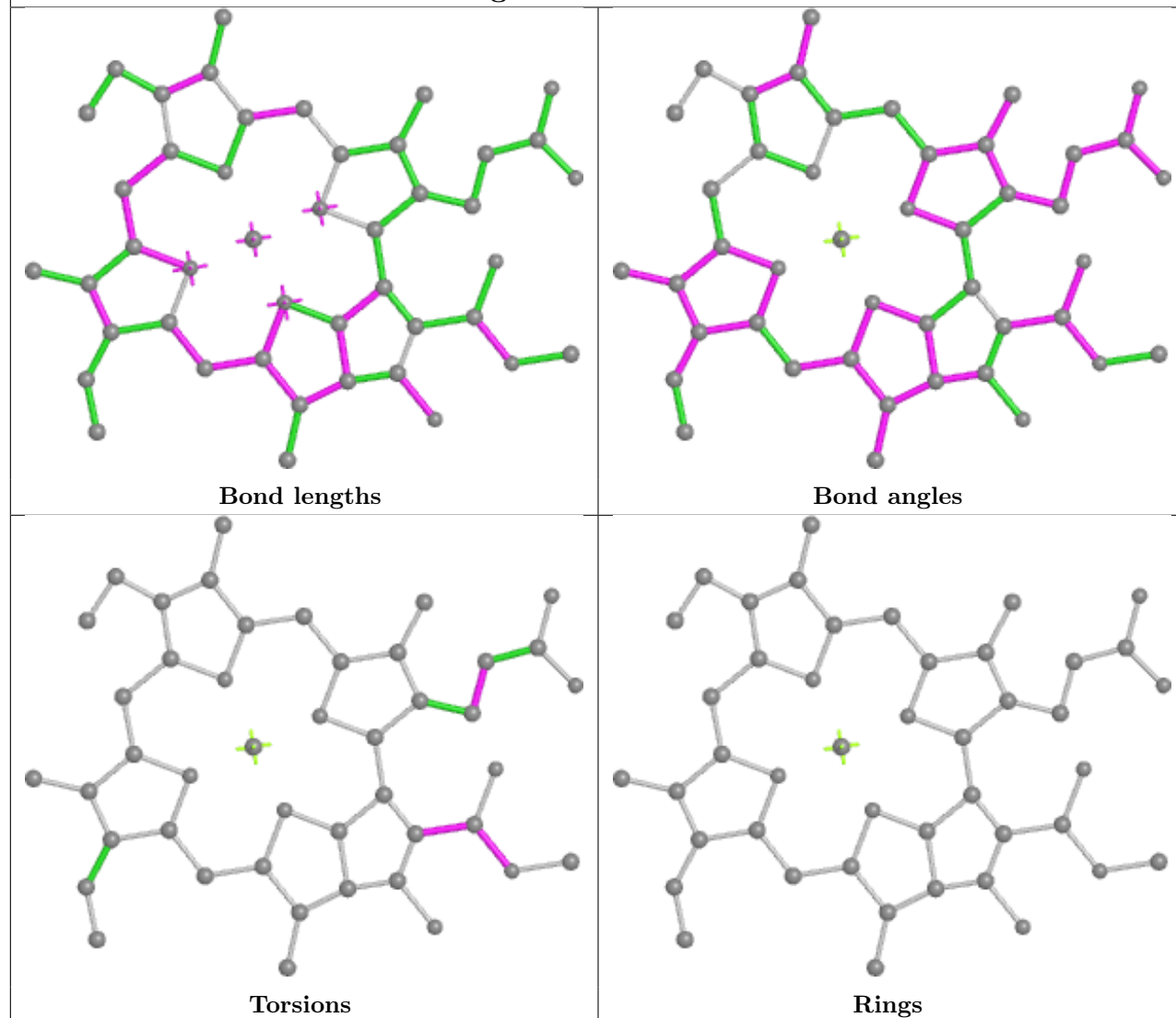


Rings

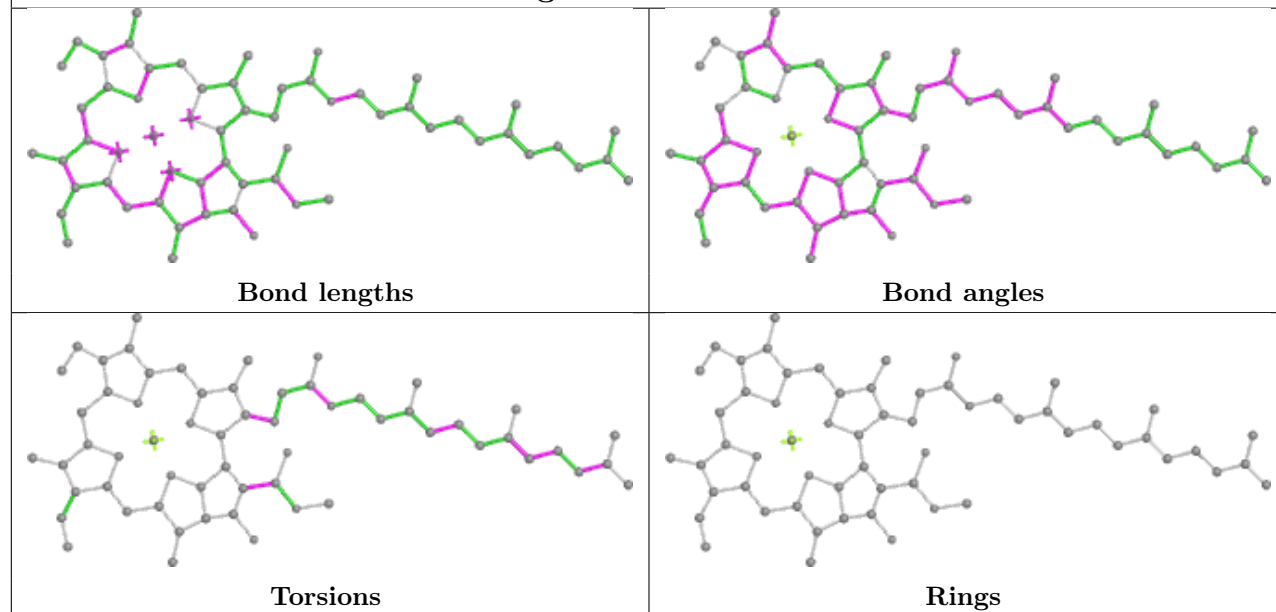


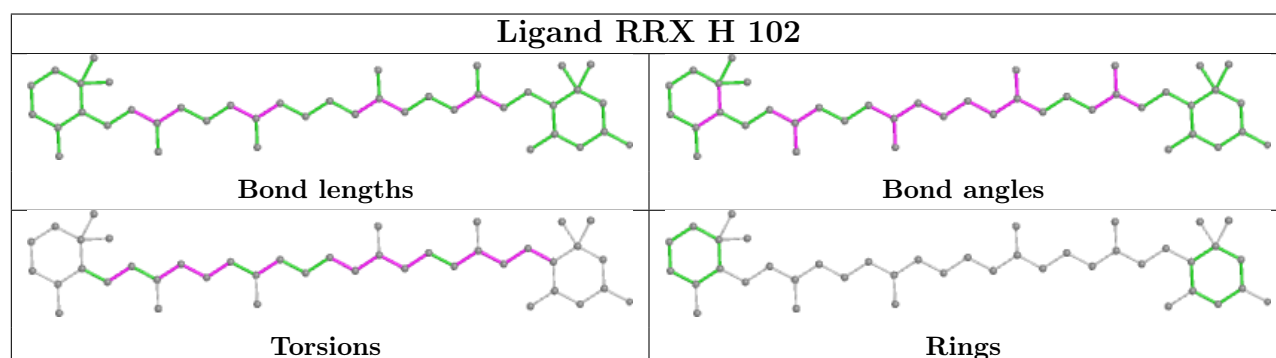
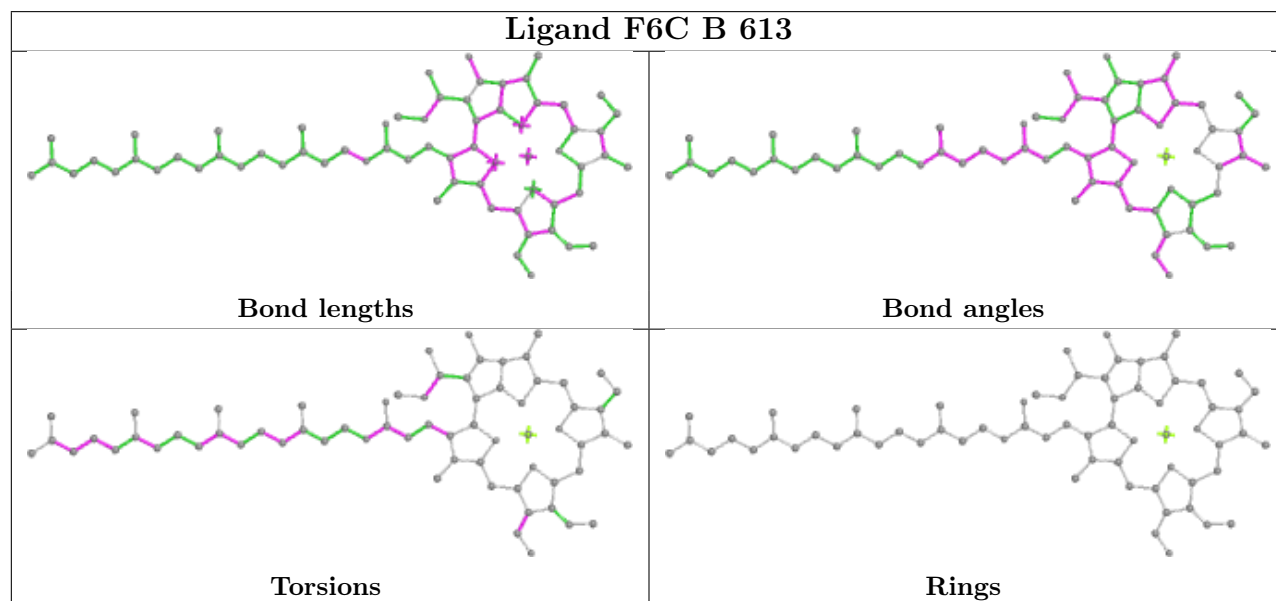
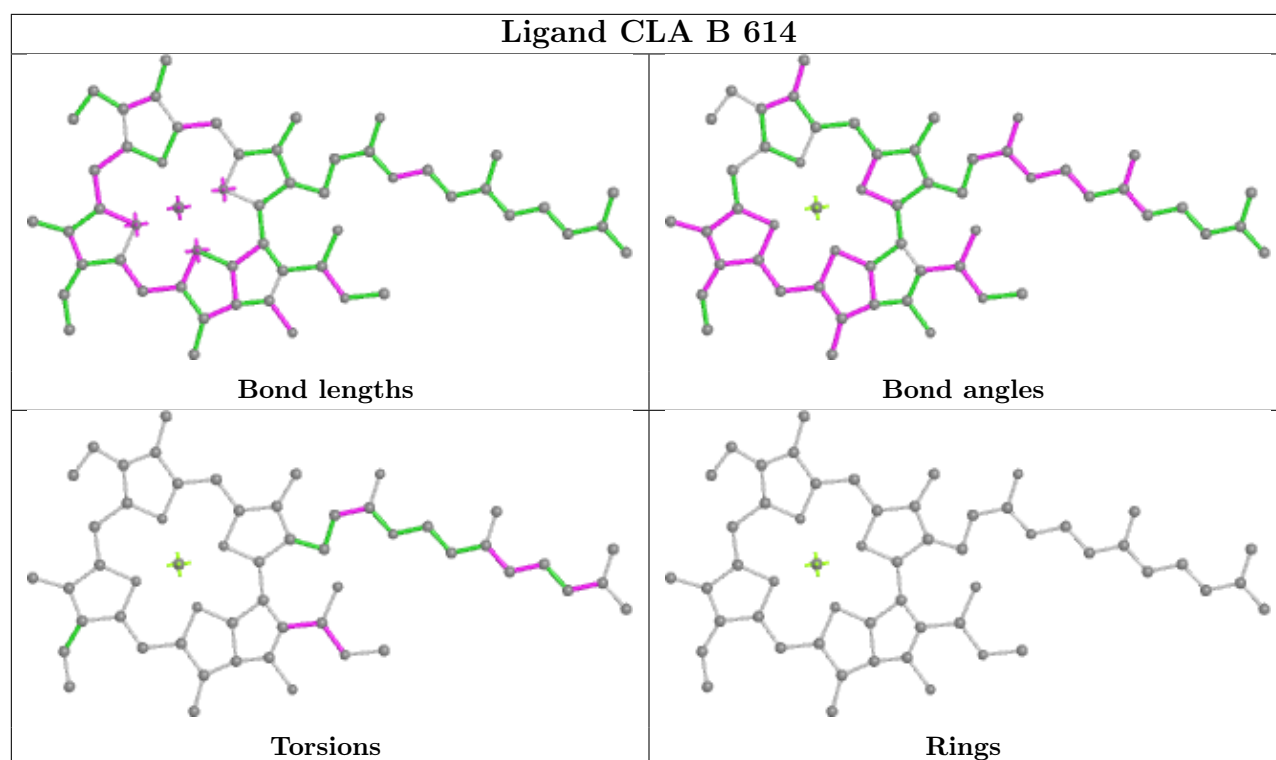


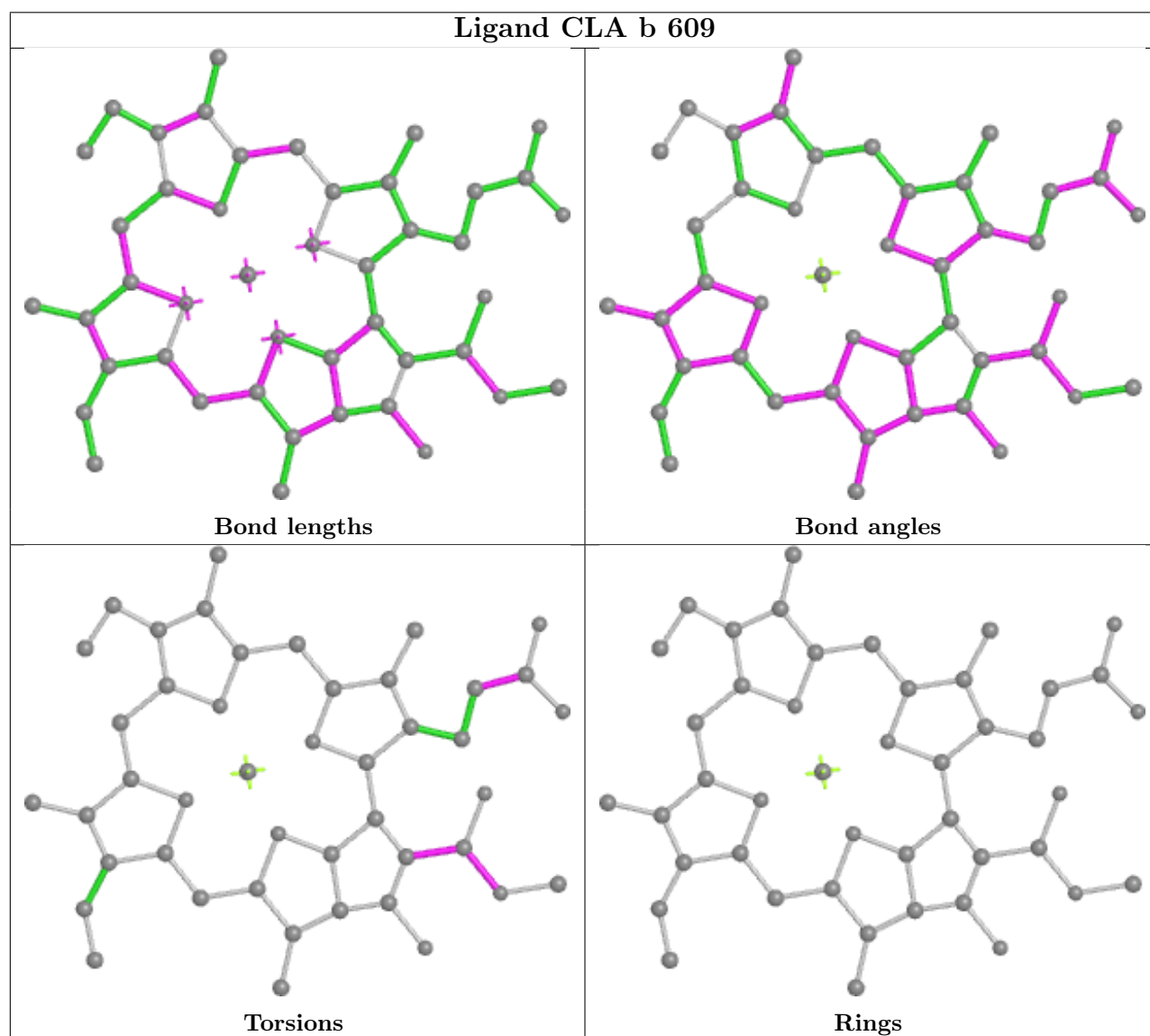
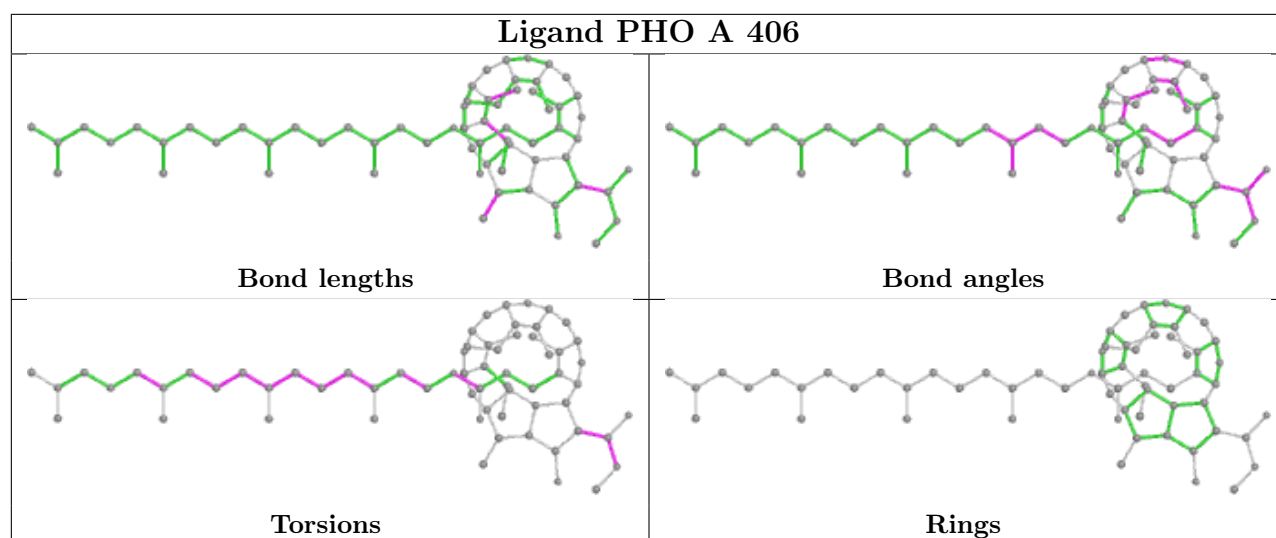
Ligand CLA C 514

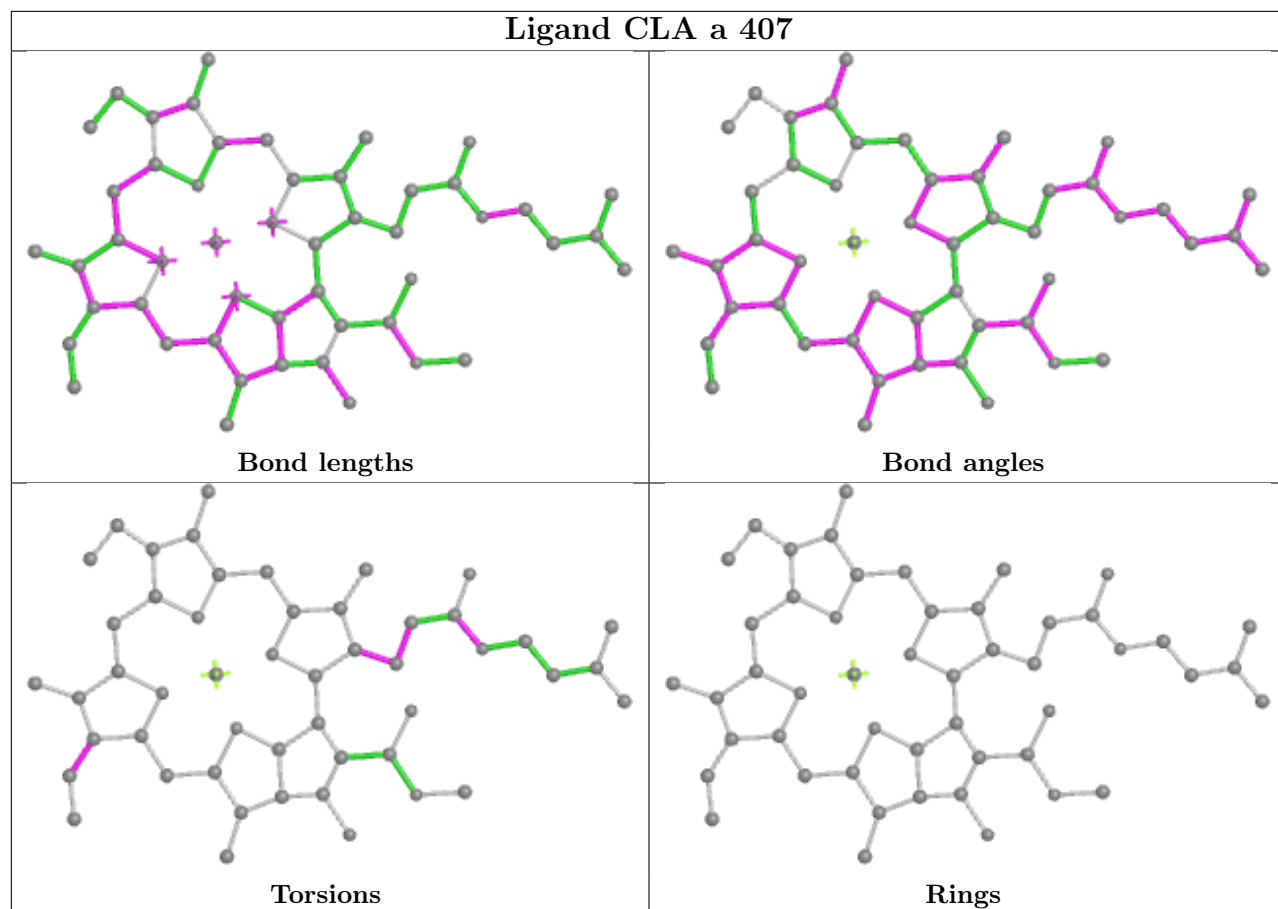


Ligand CLA c 509

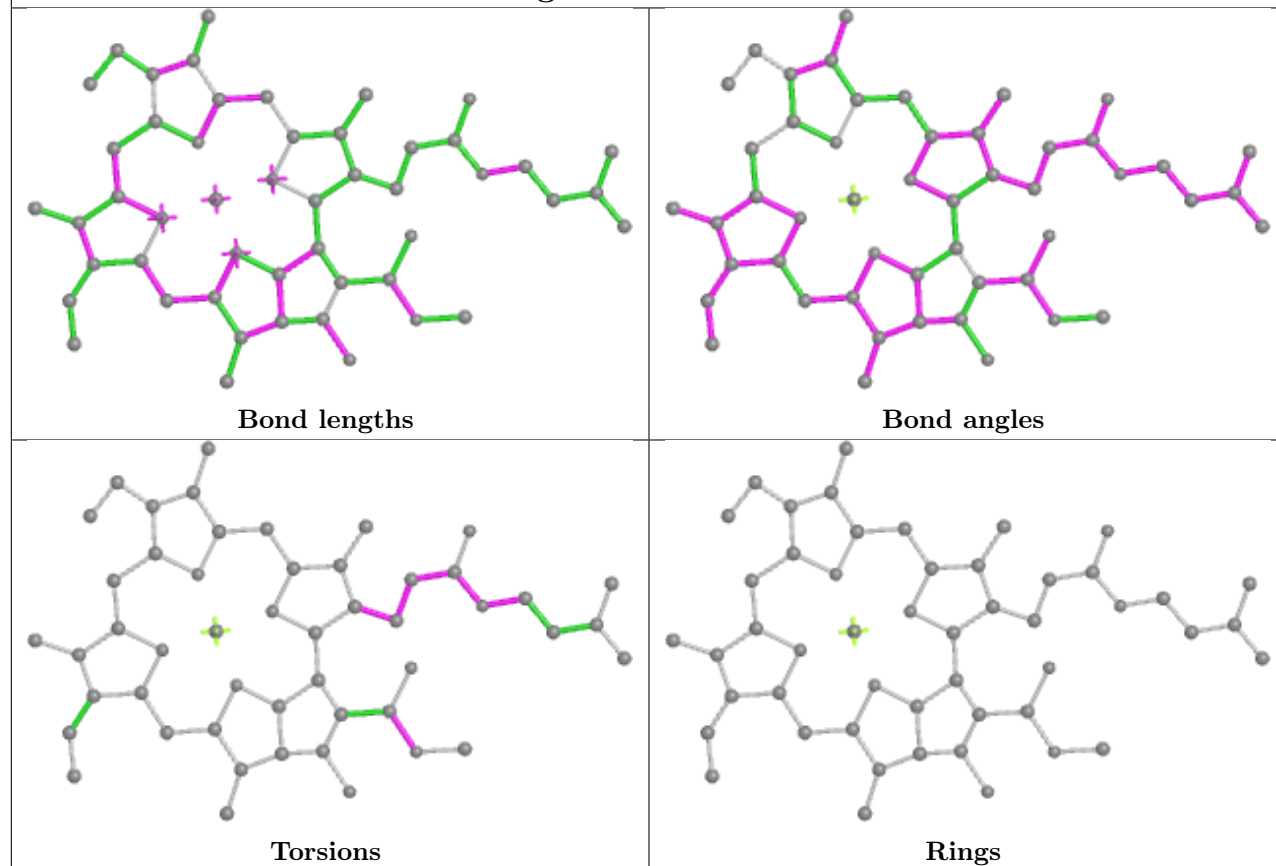




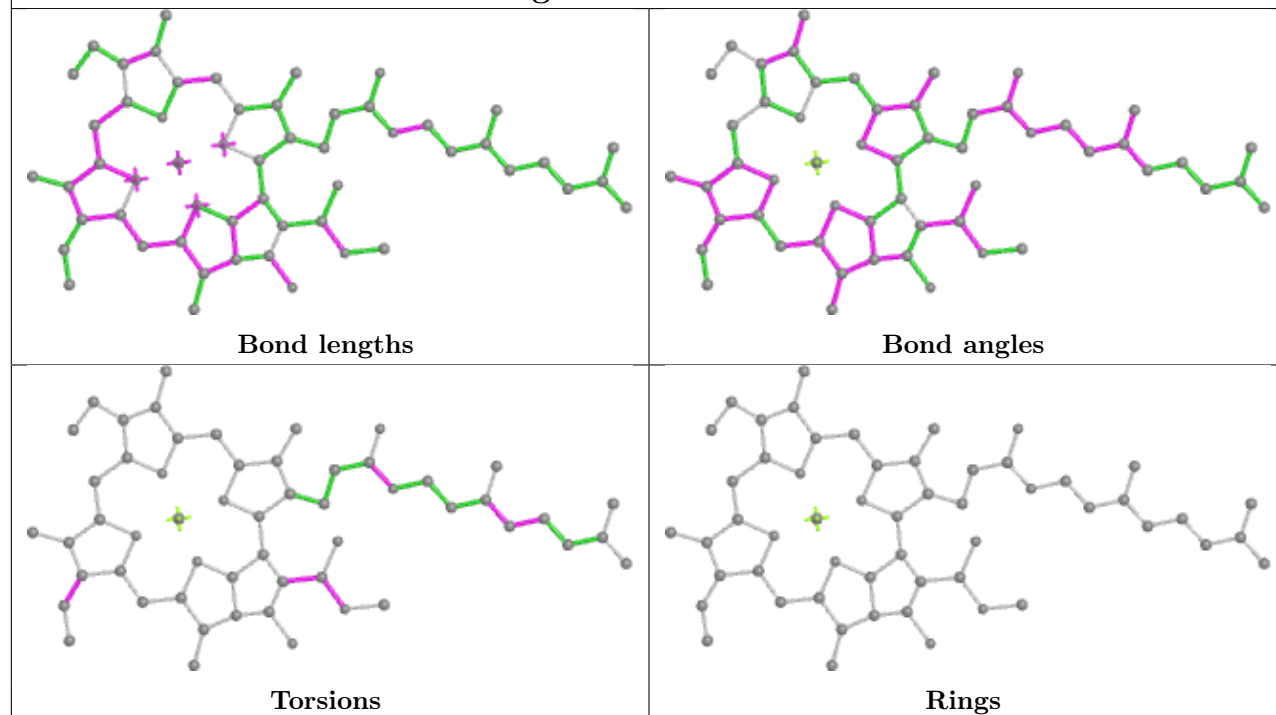


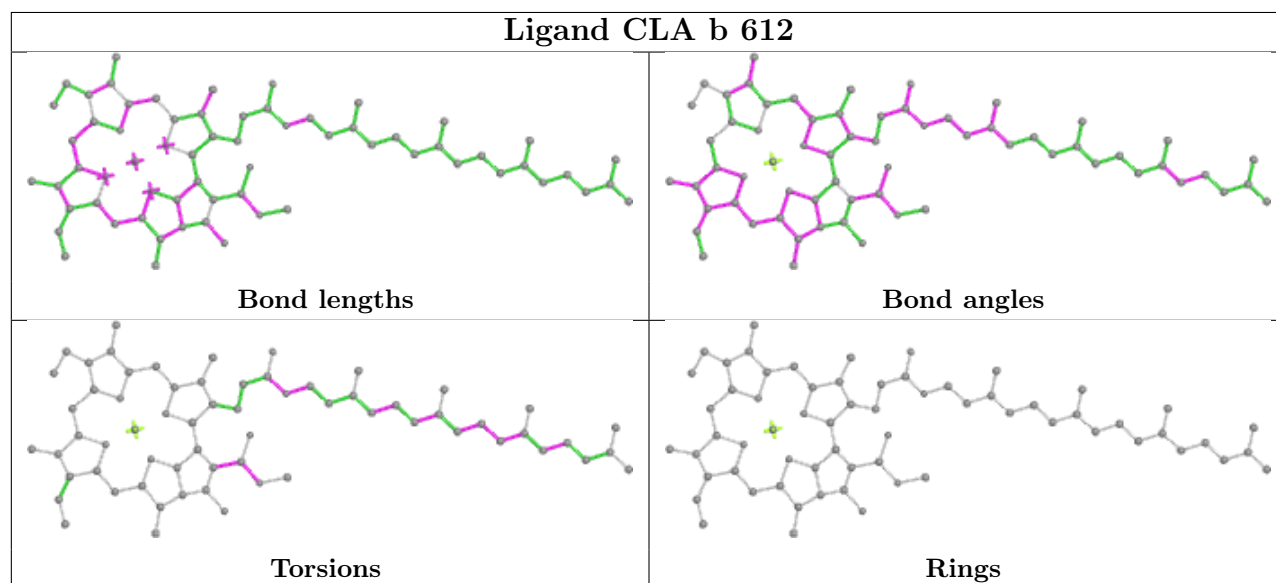
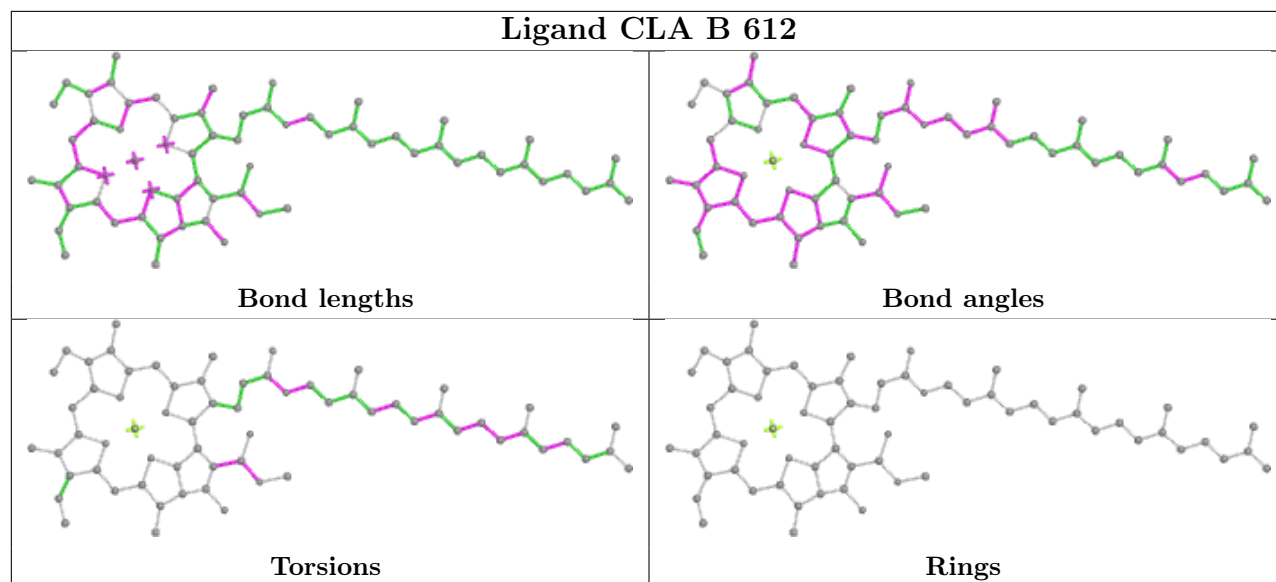


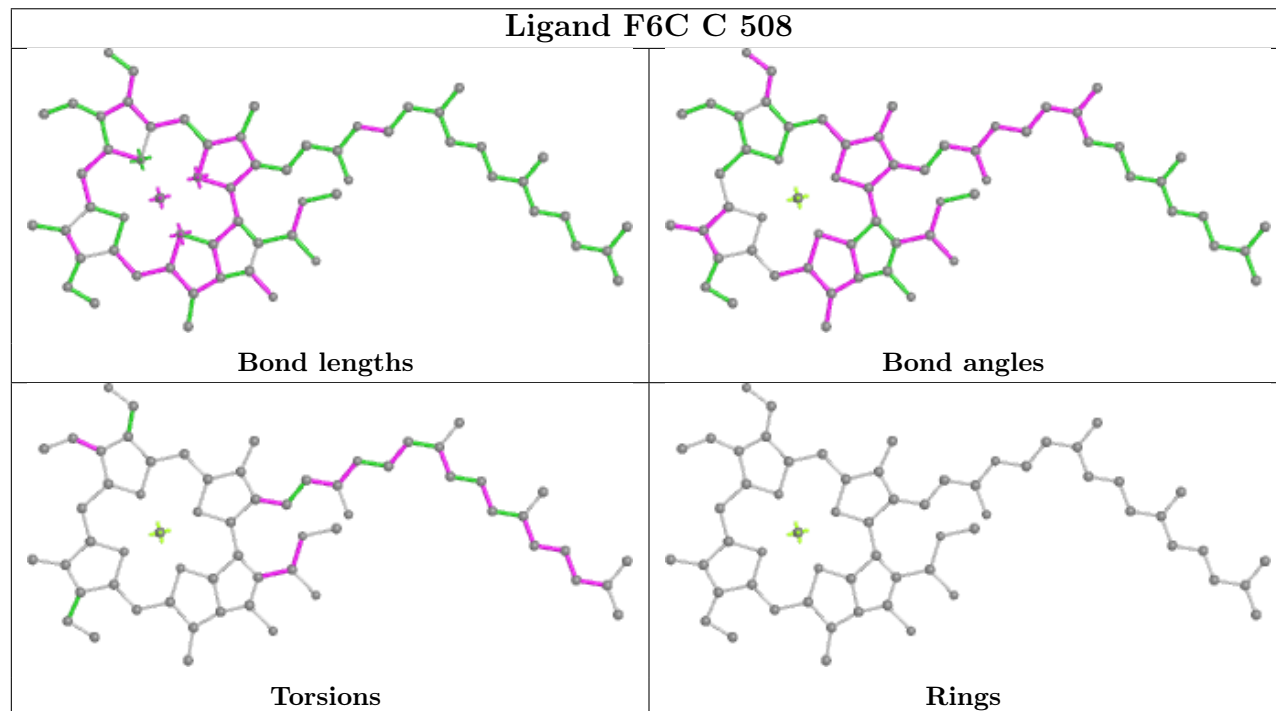
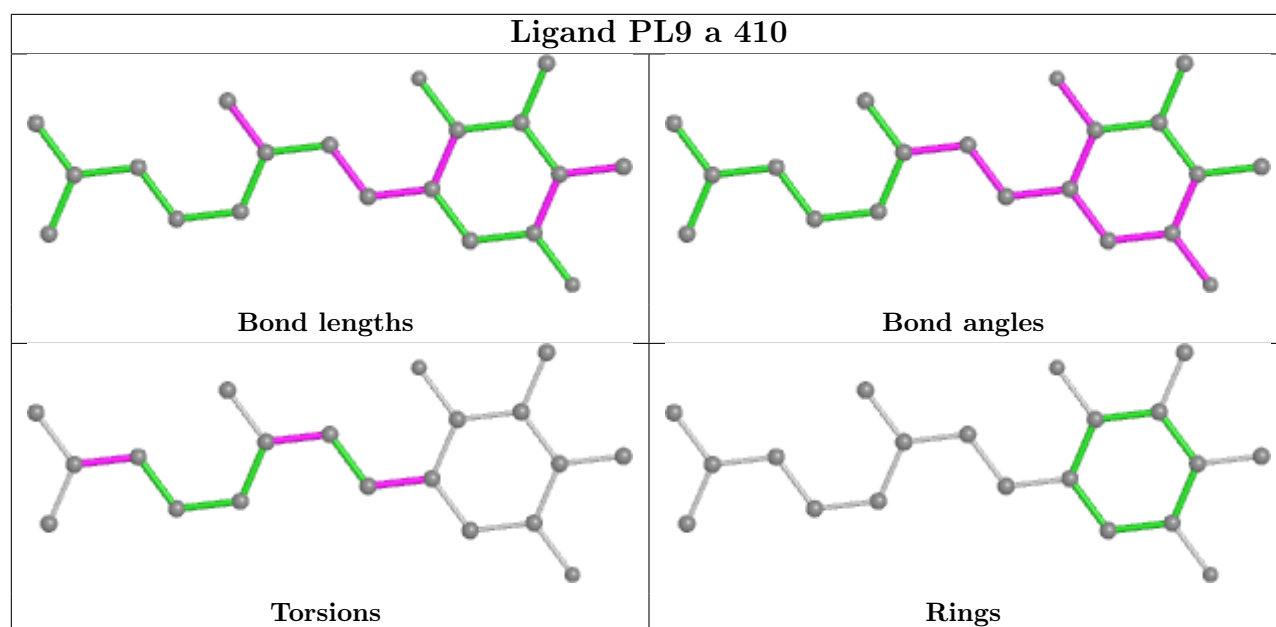
Ligand CLA c 512

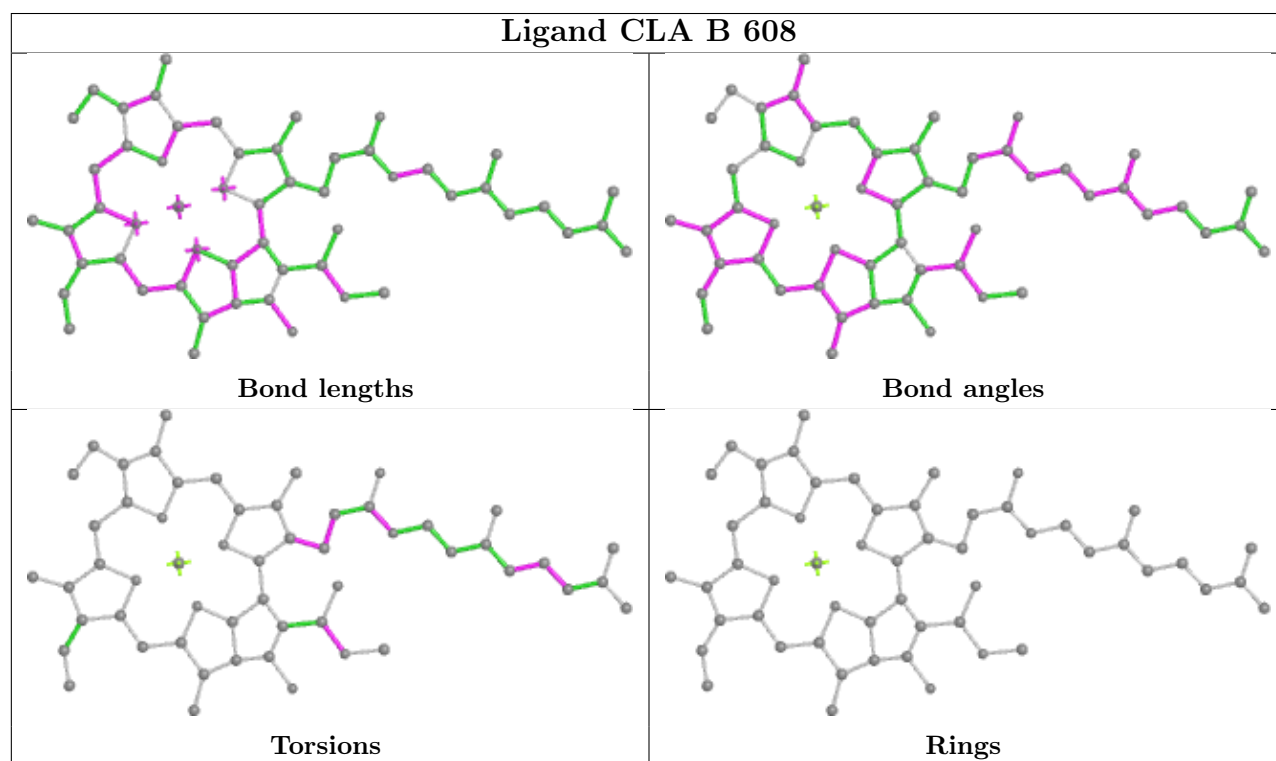
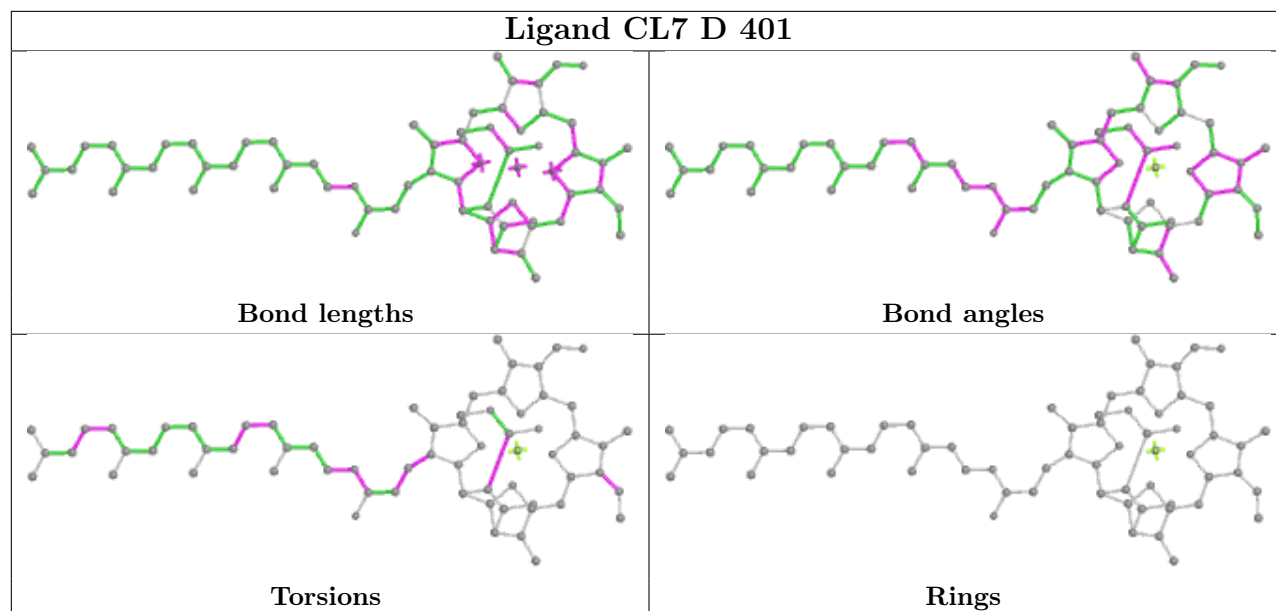


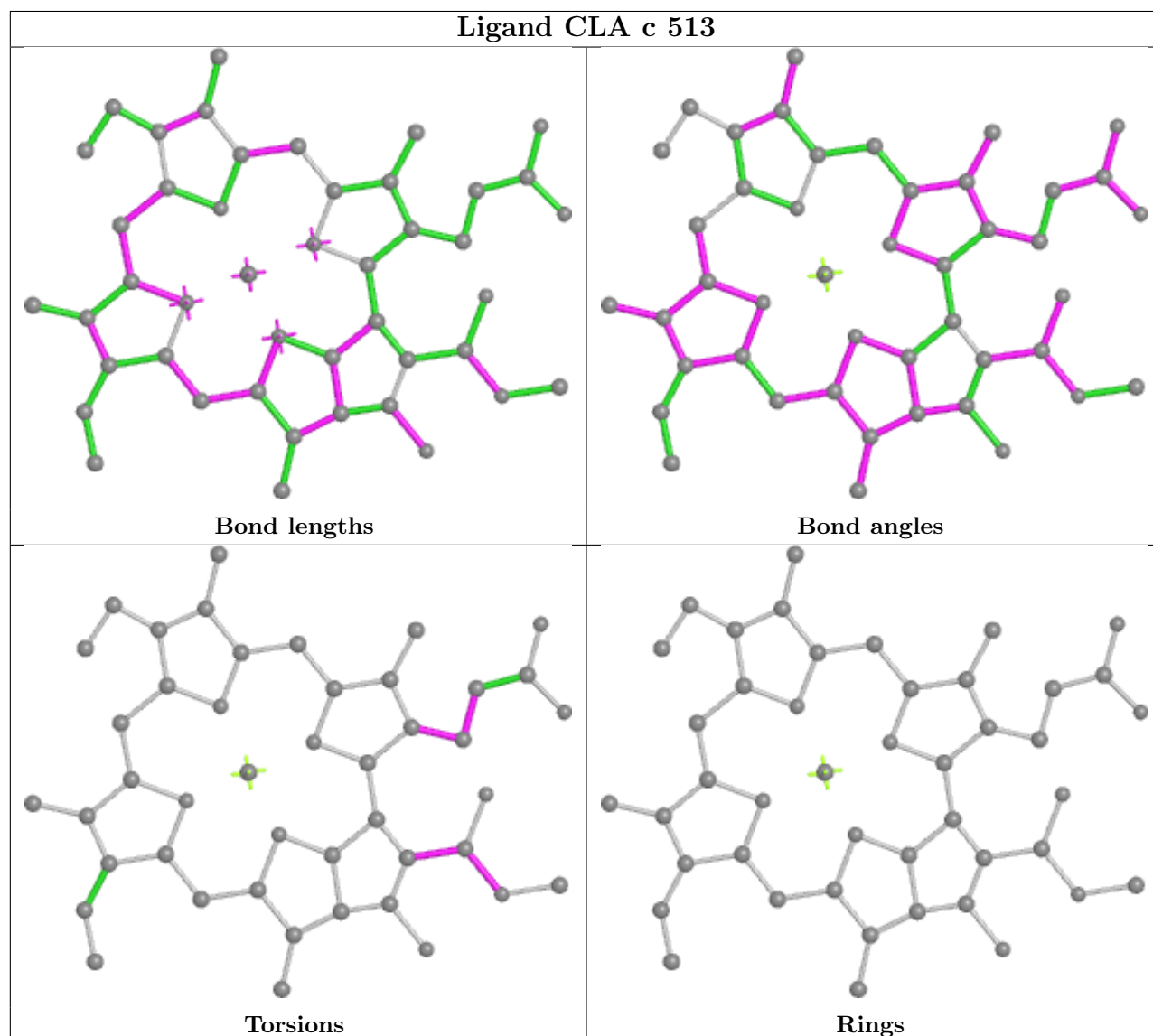
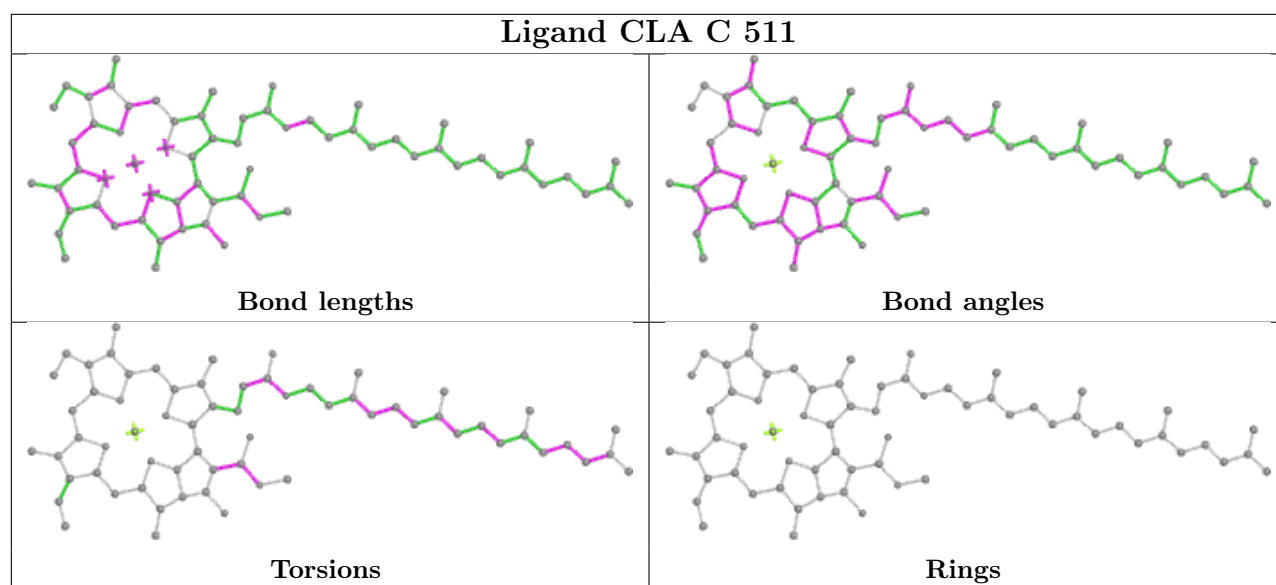
Ligand CLA B 603

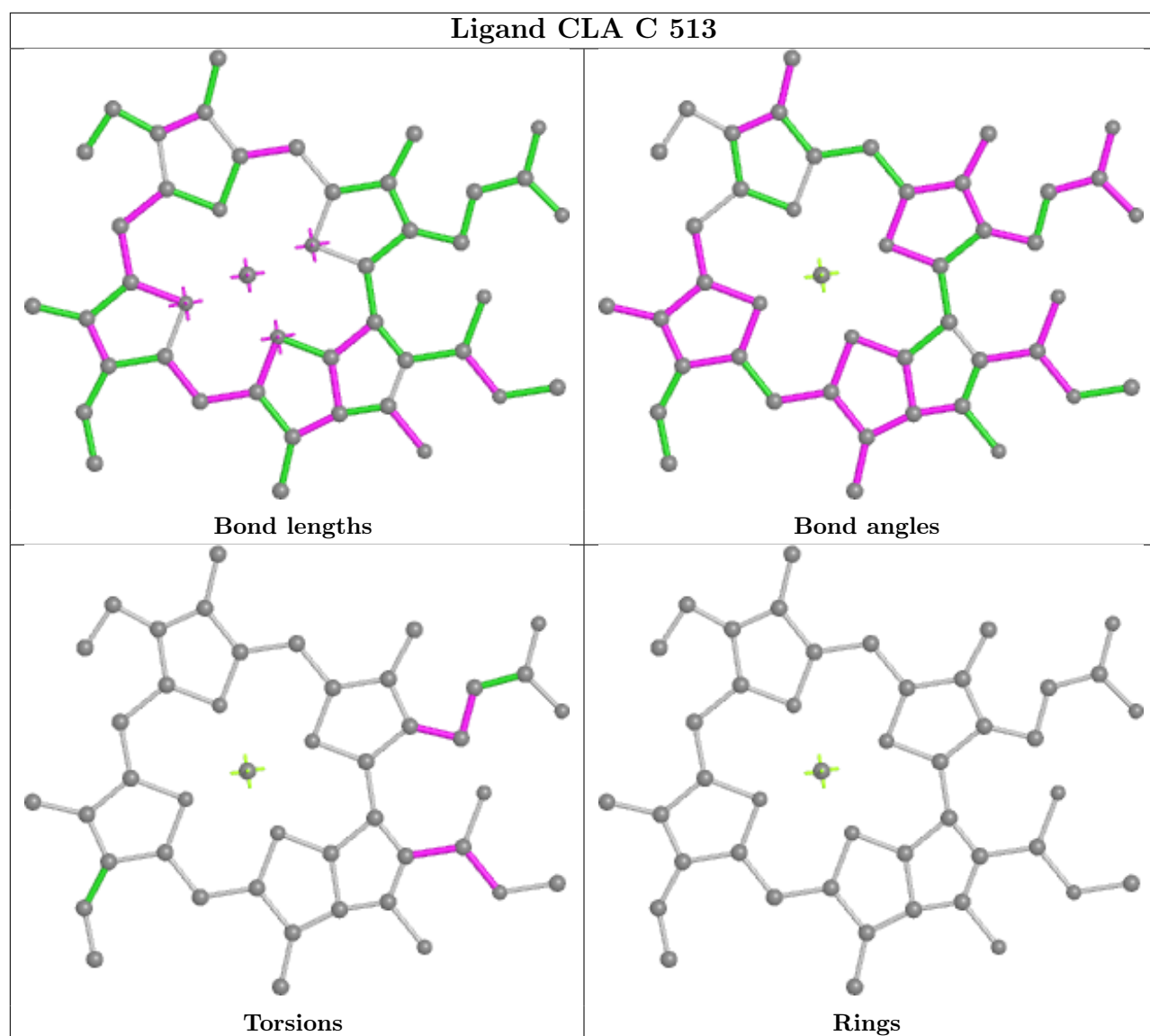


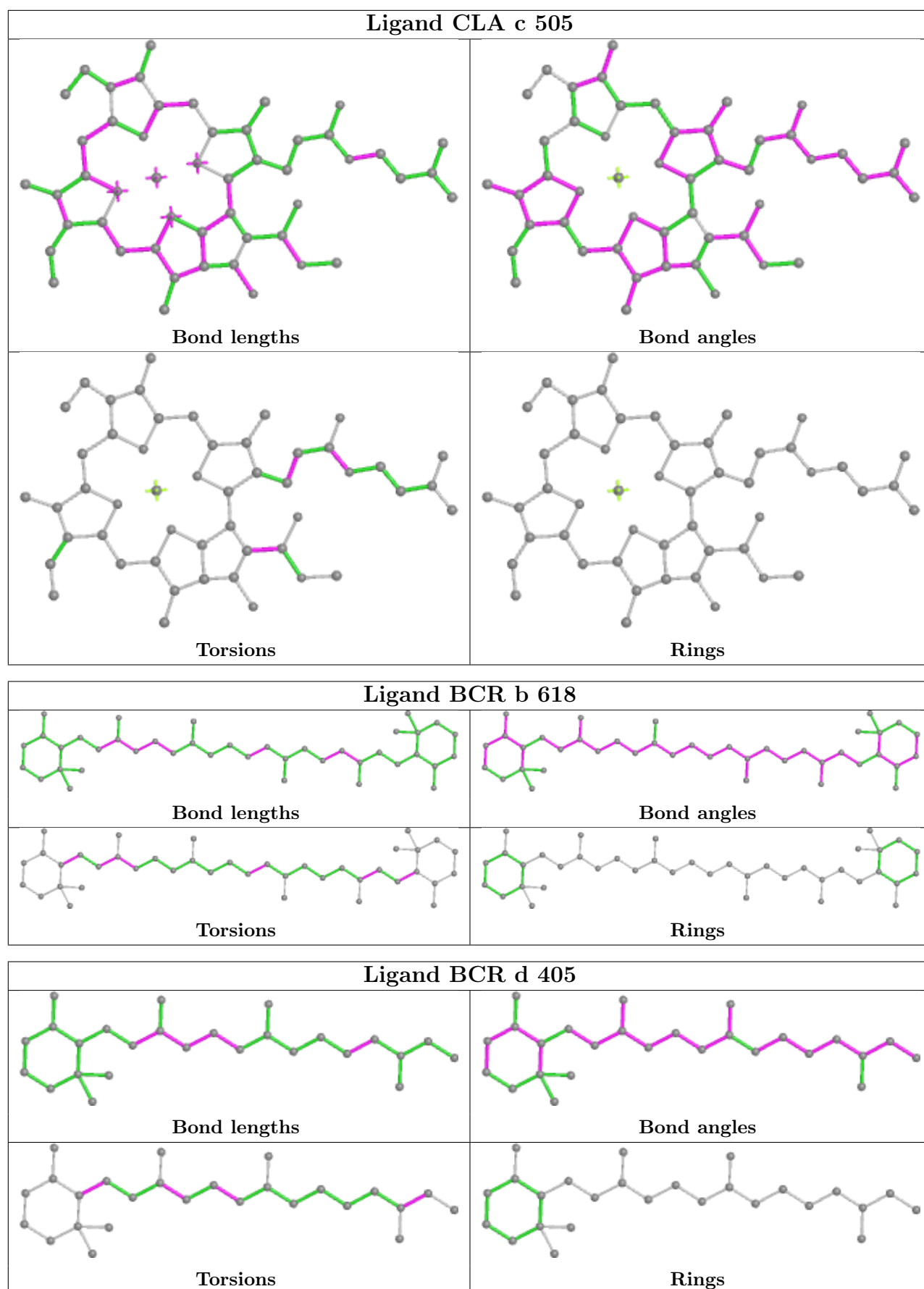




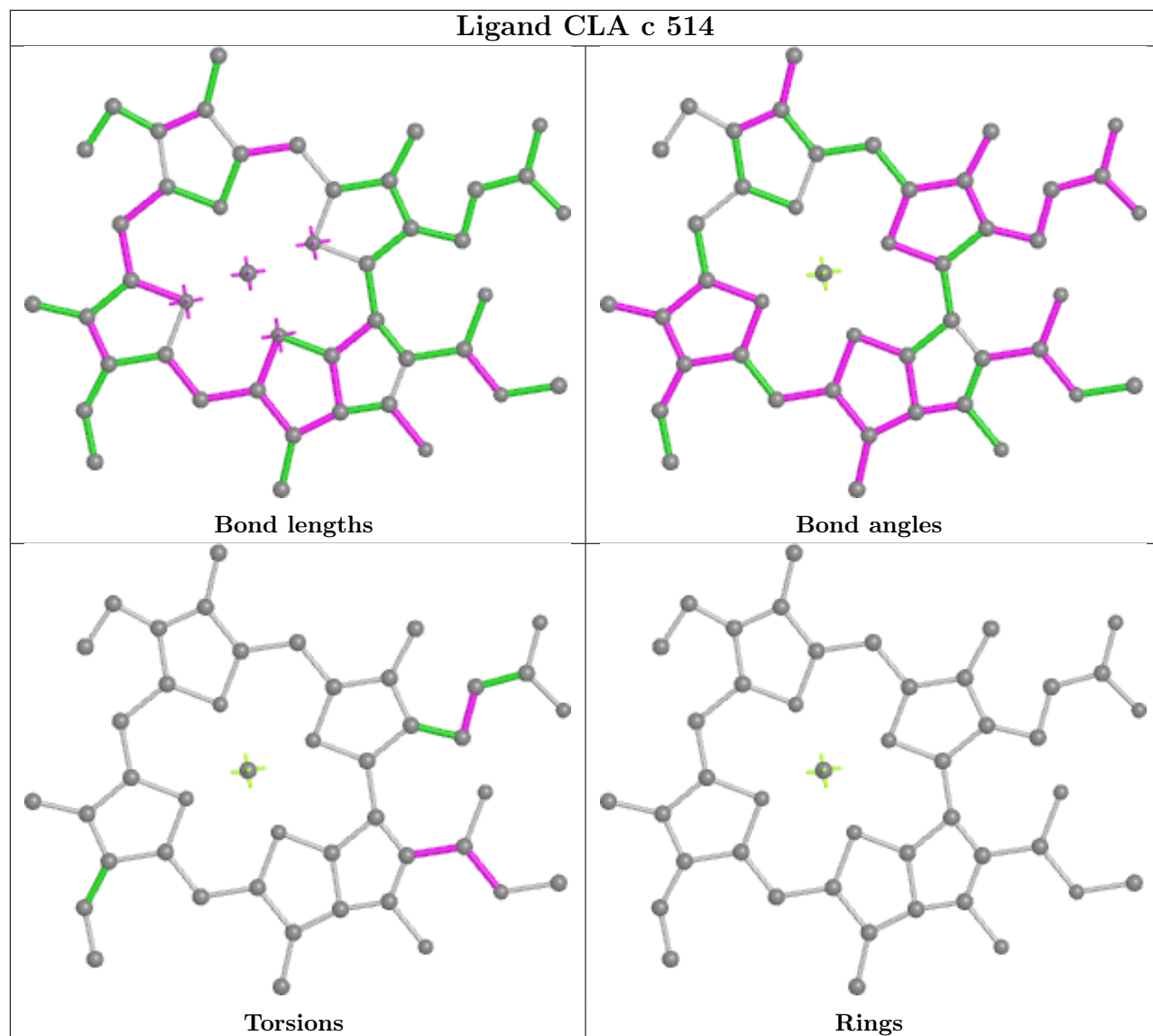


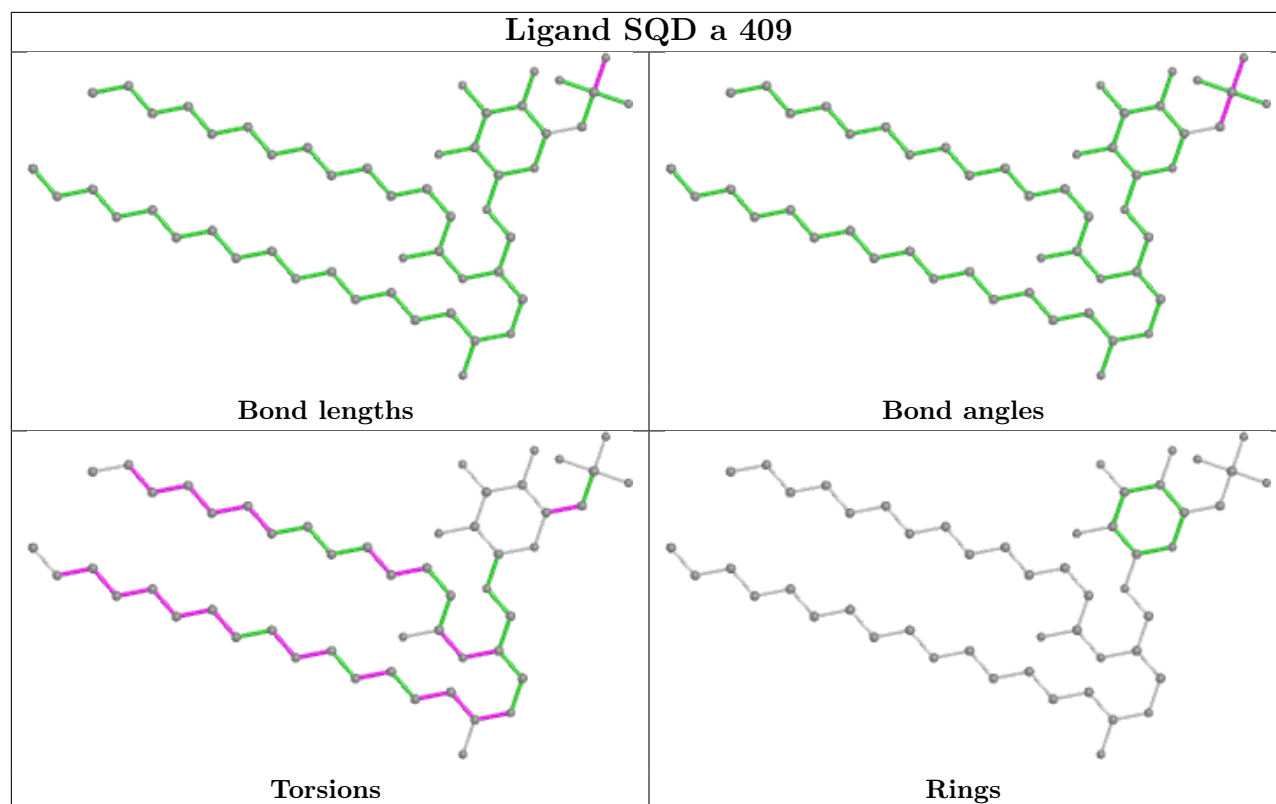
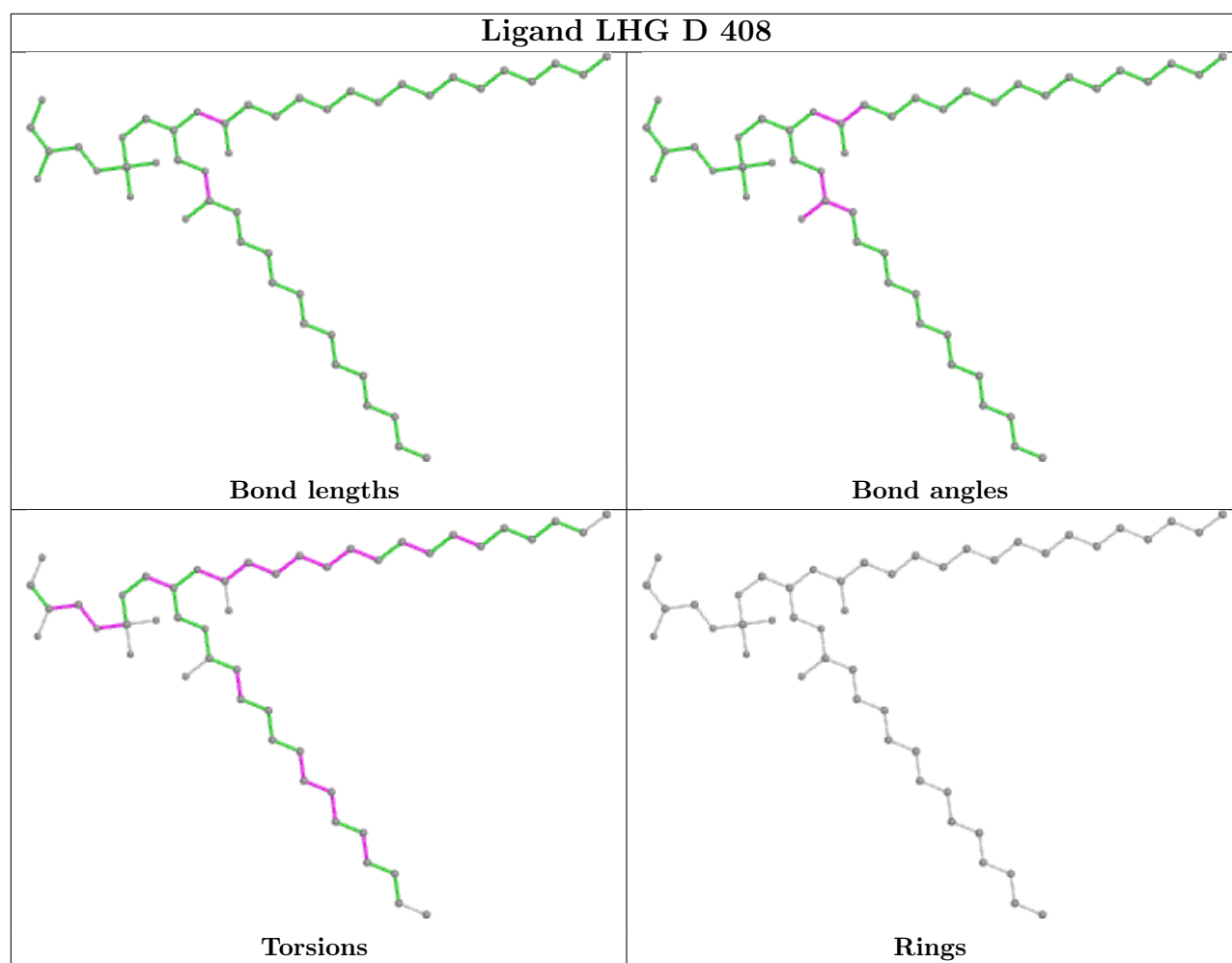


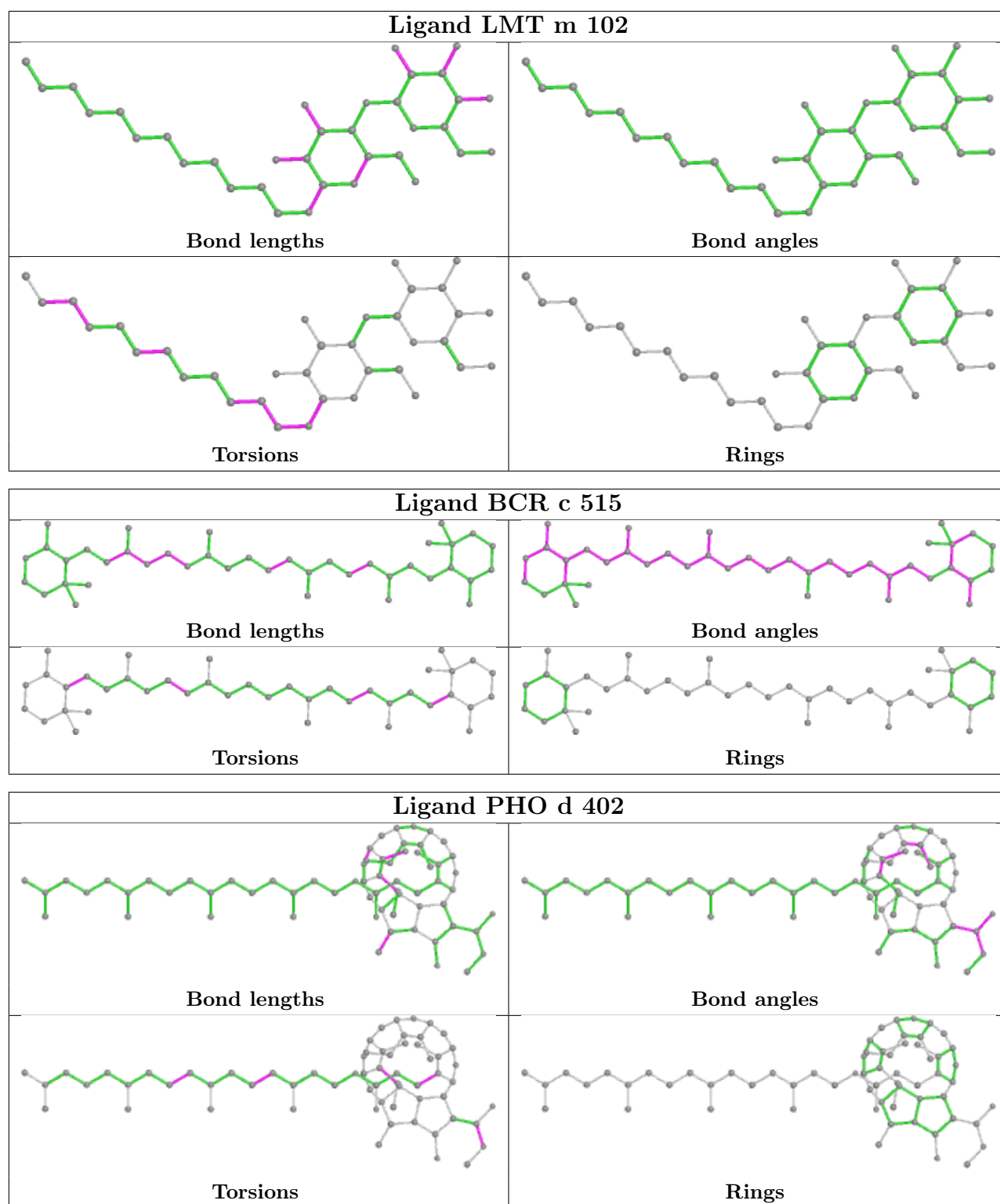


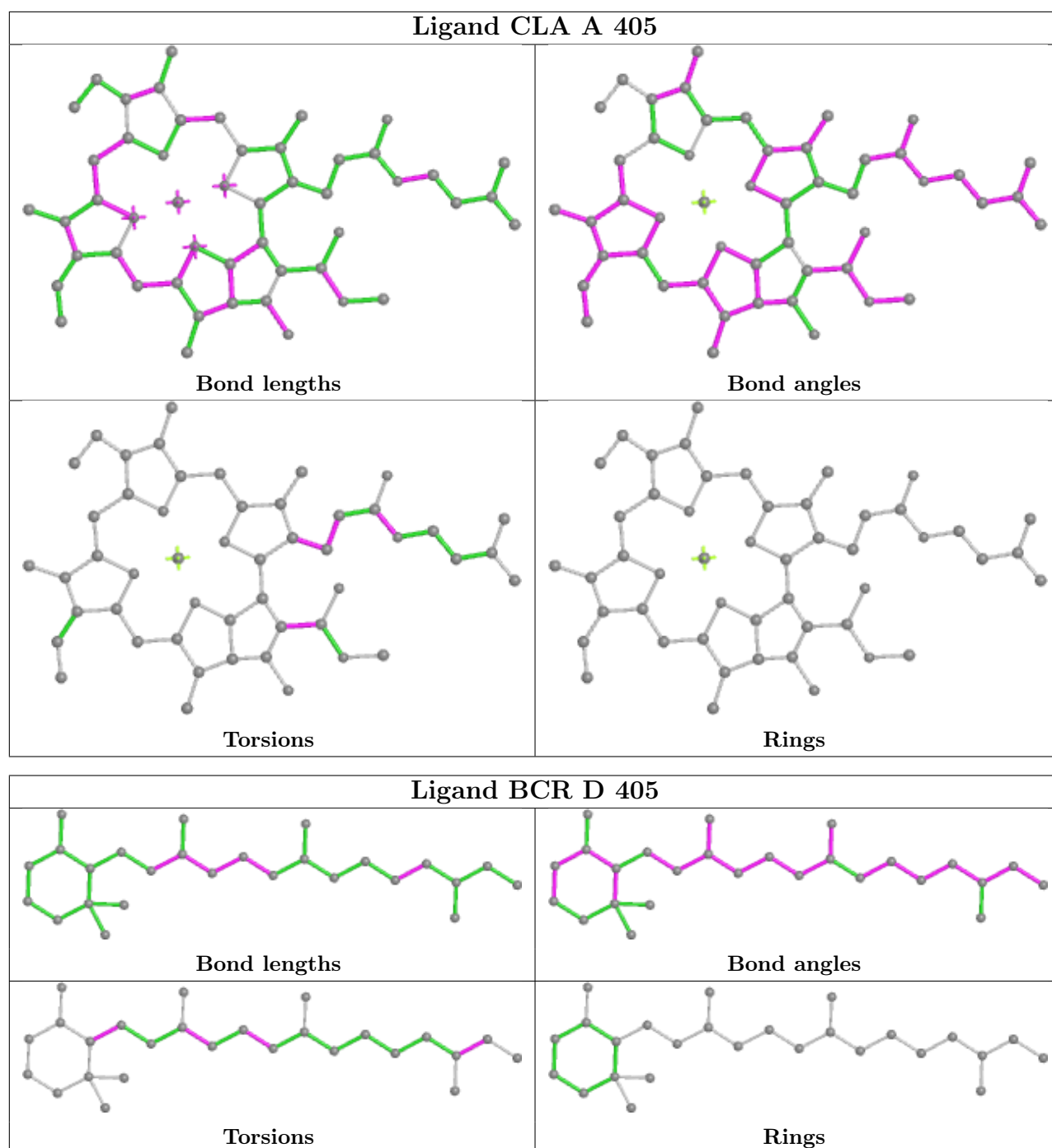


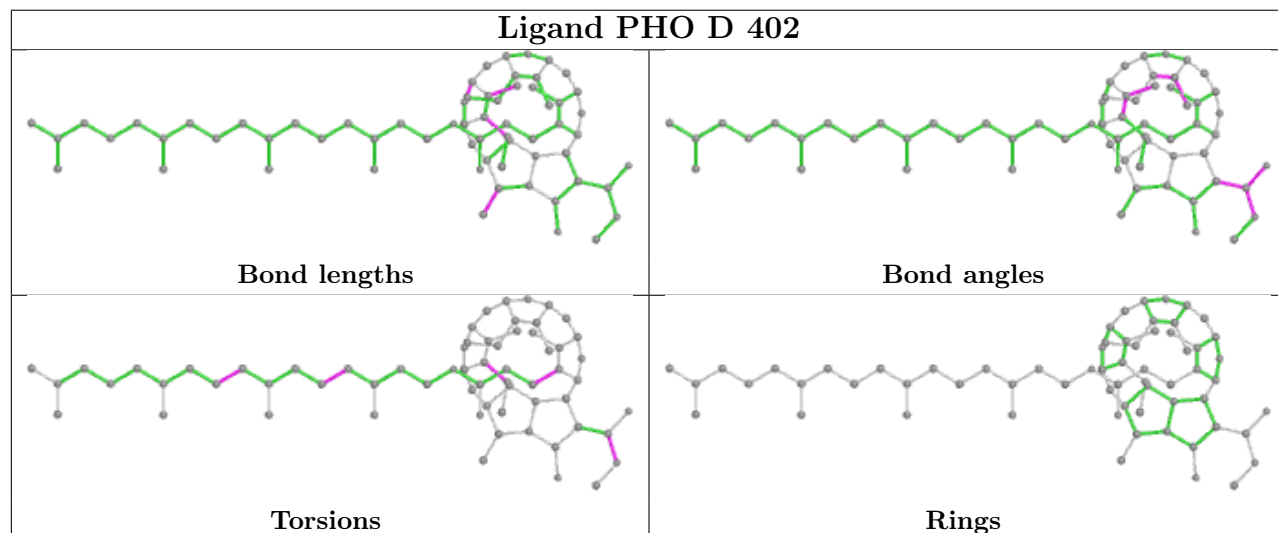
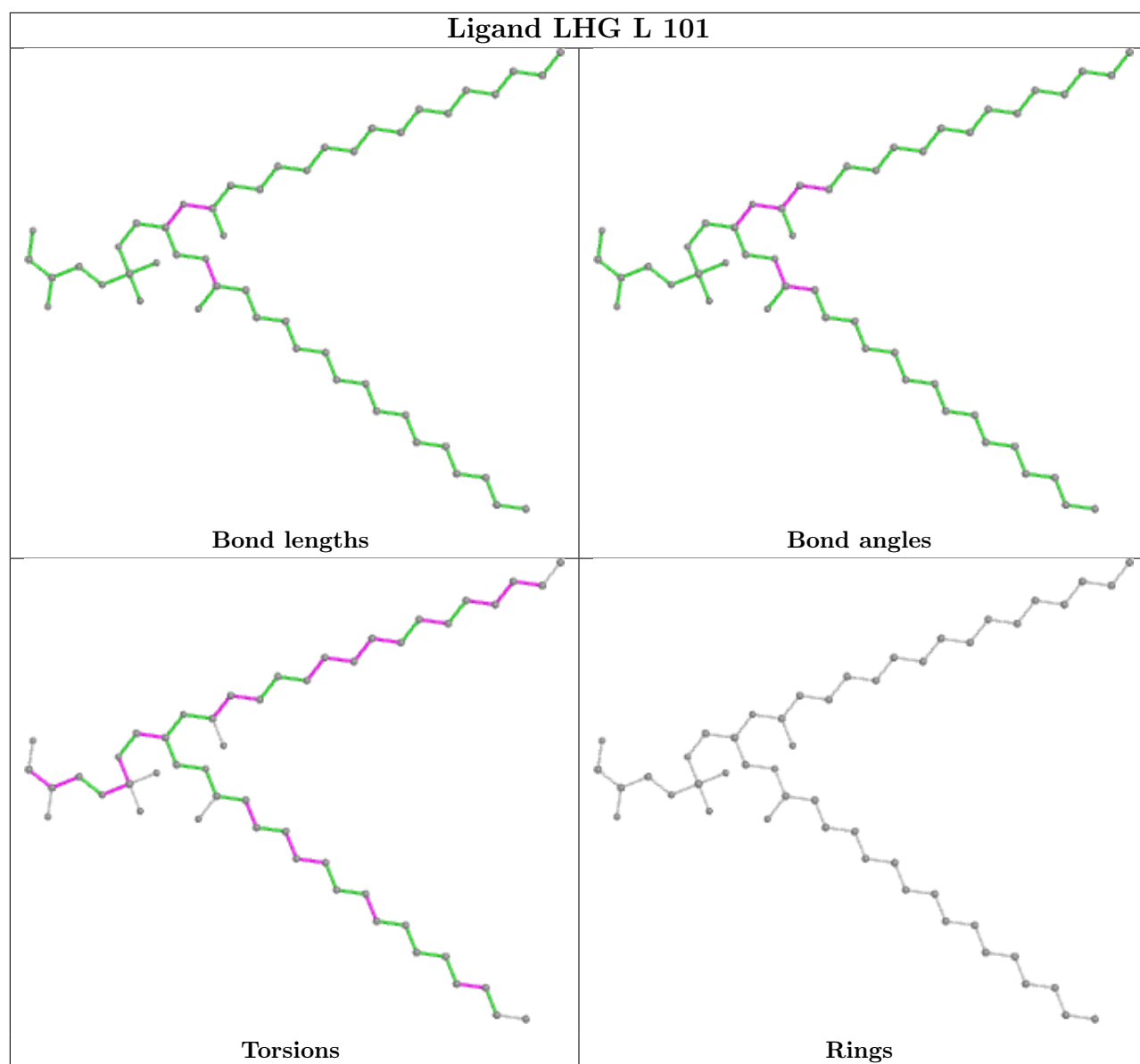
Ligand CLA c 514

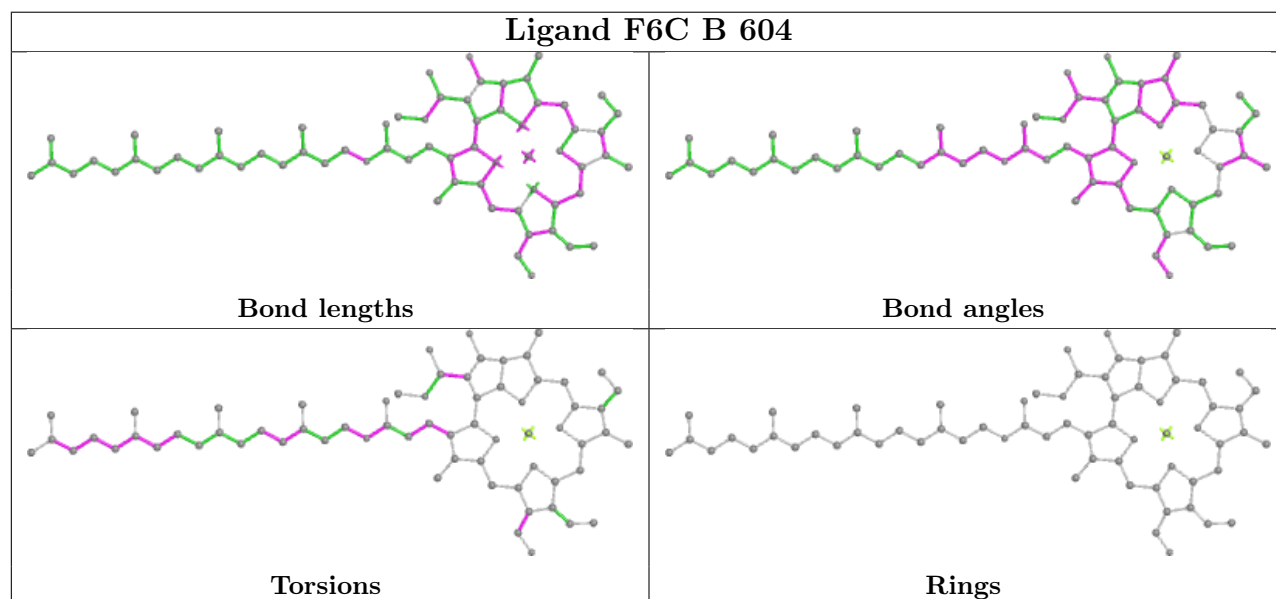
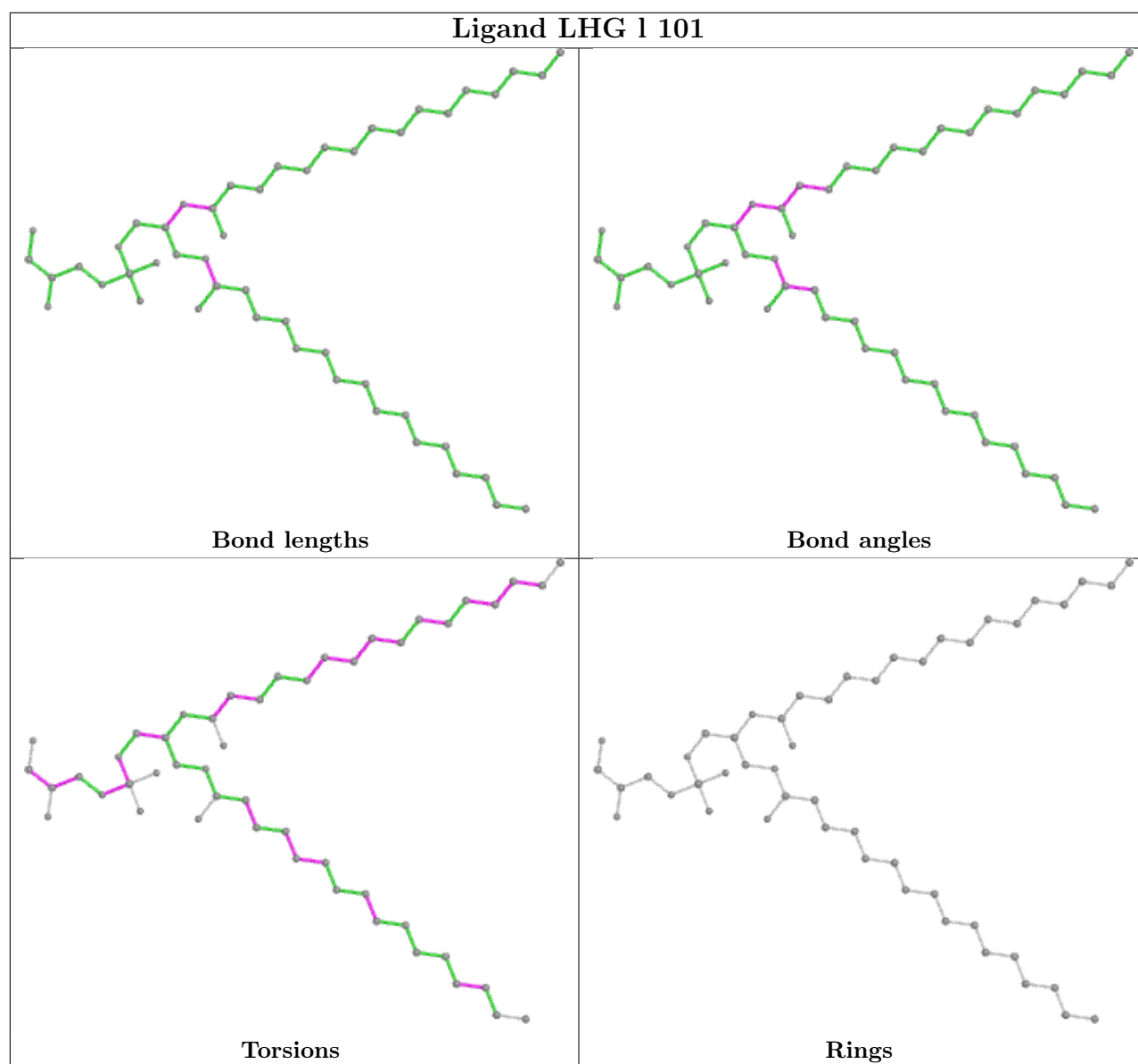


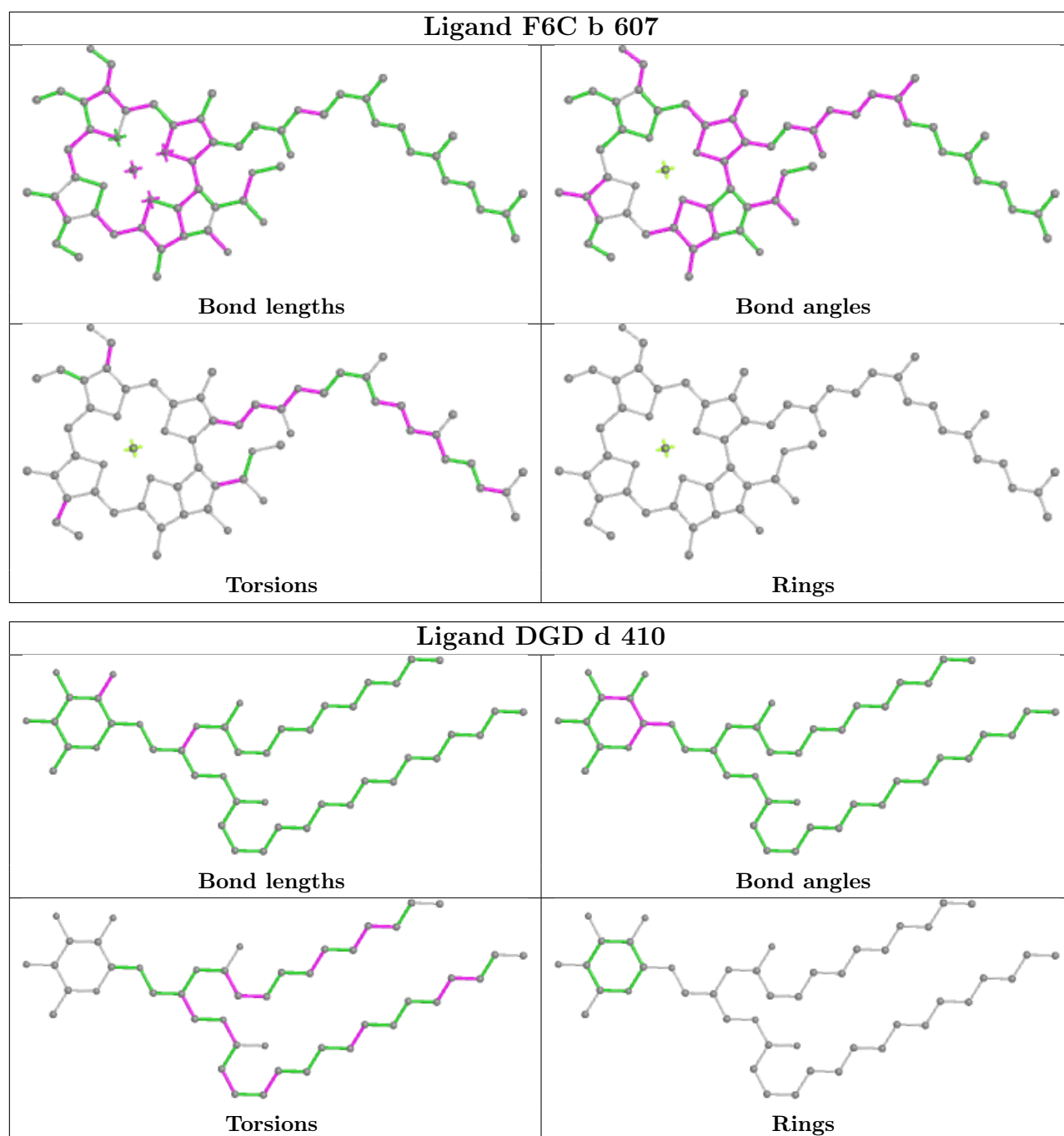


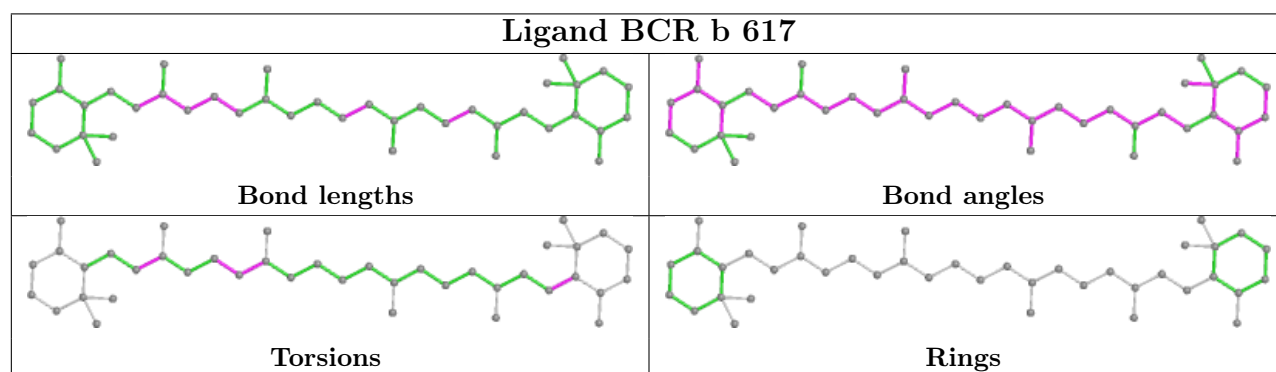
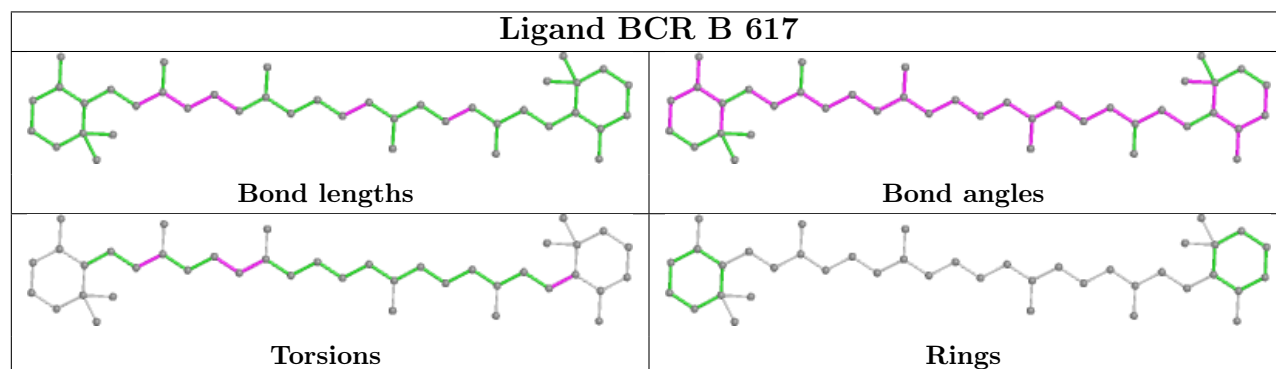
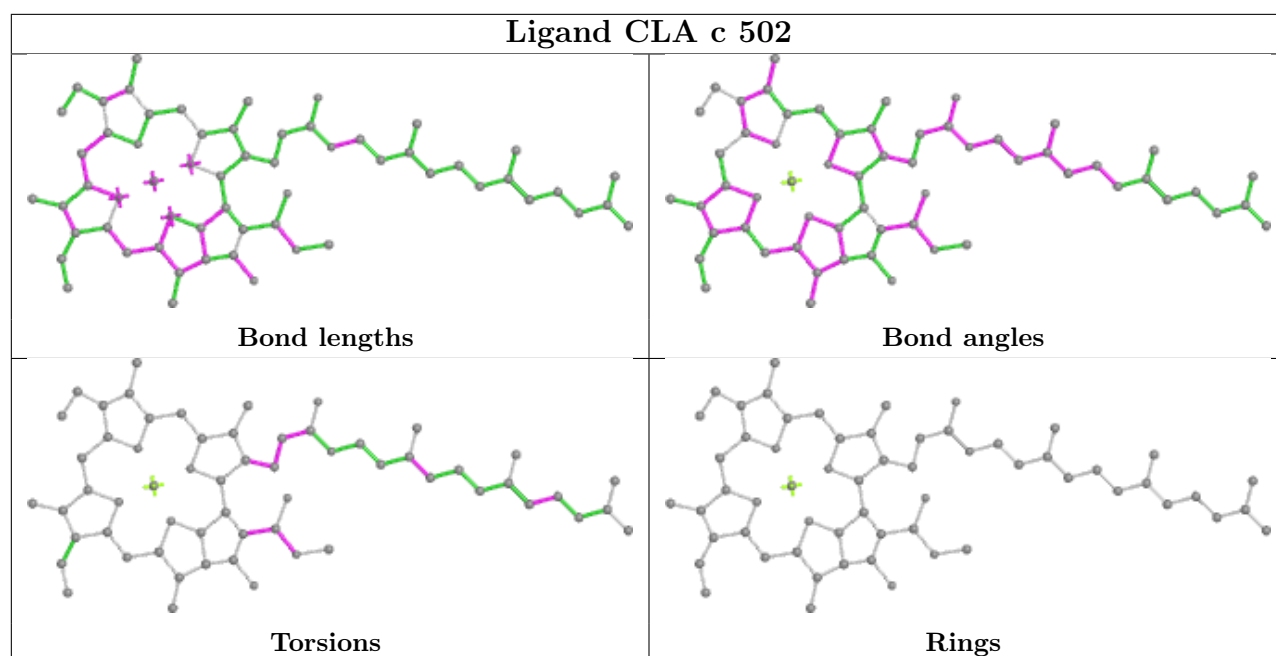




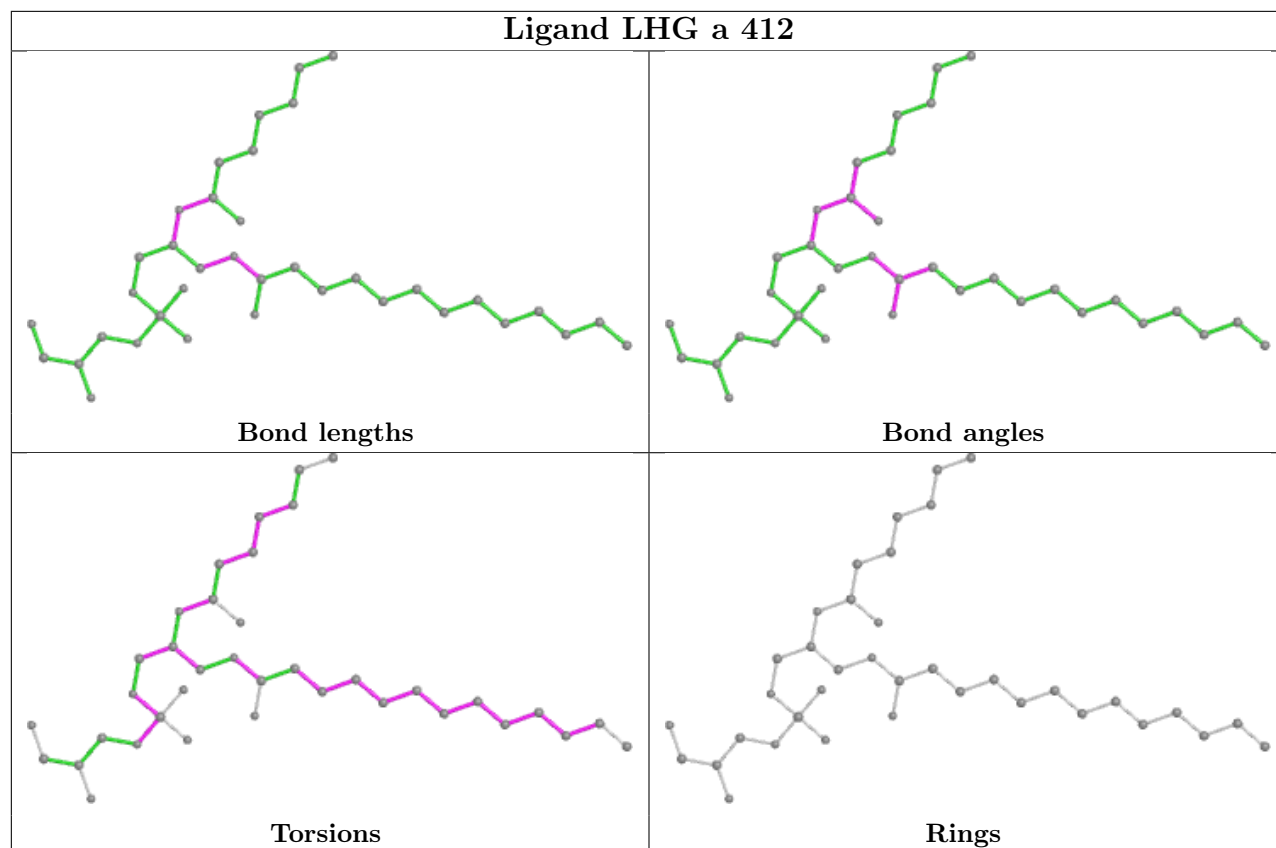




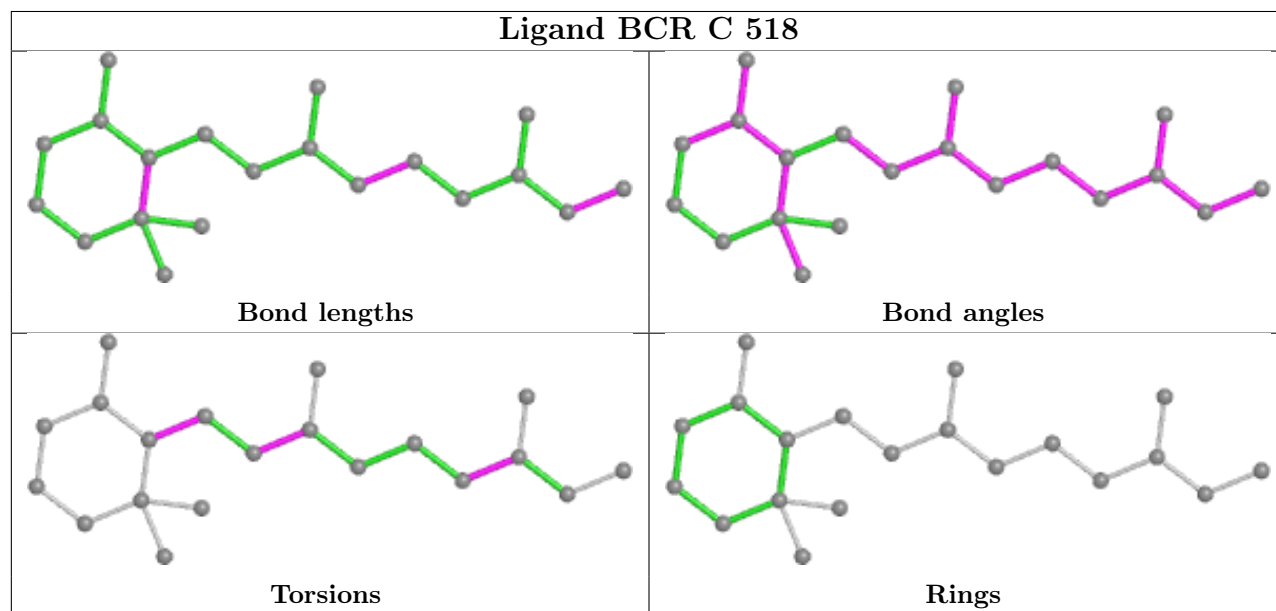


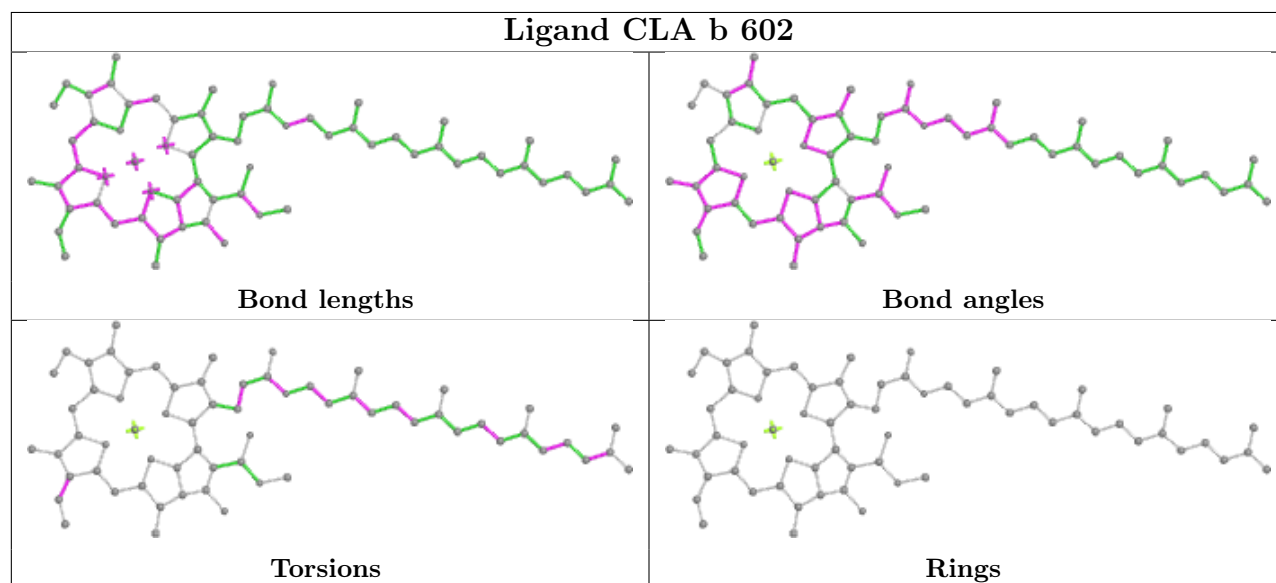
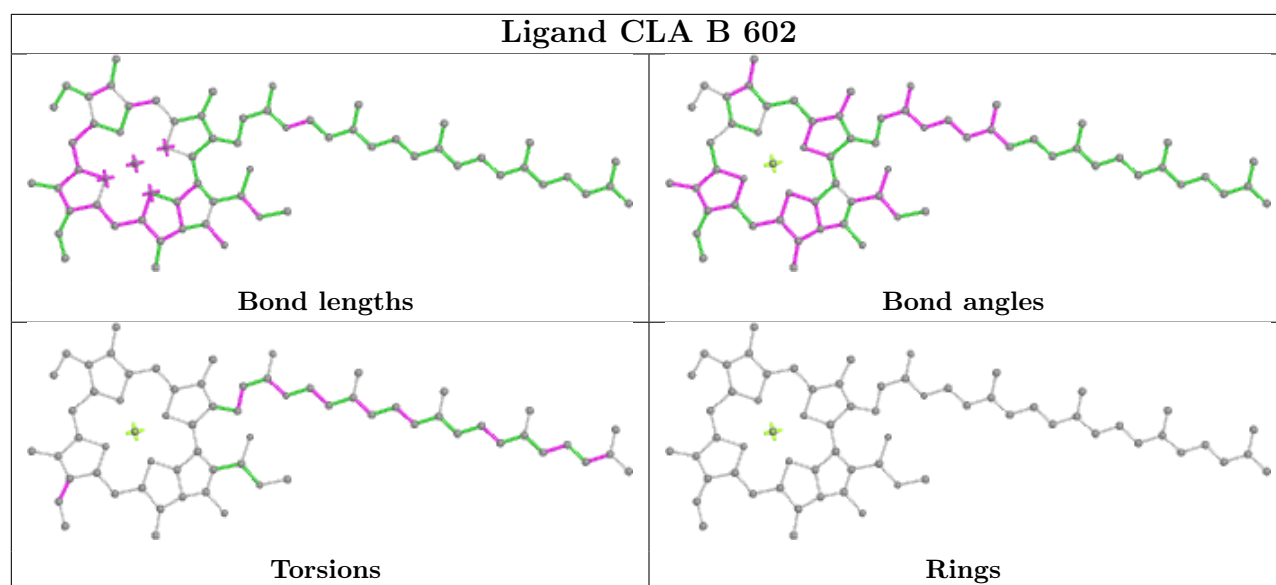


Ligand LHG a 412

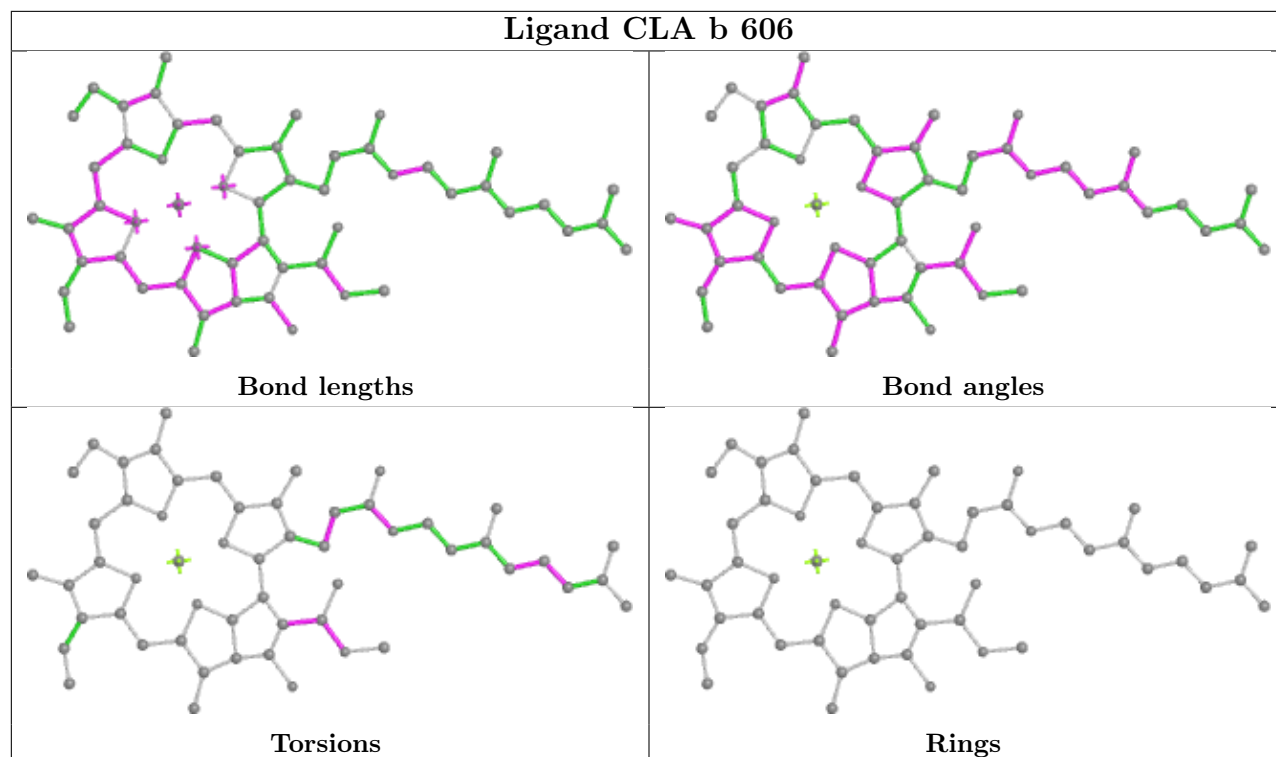


Ligand BCR C 518

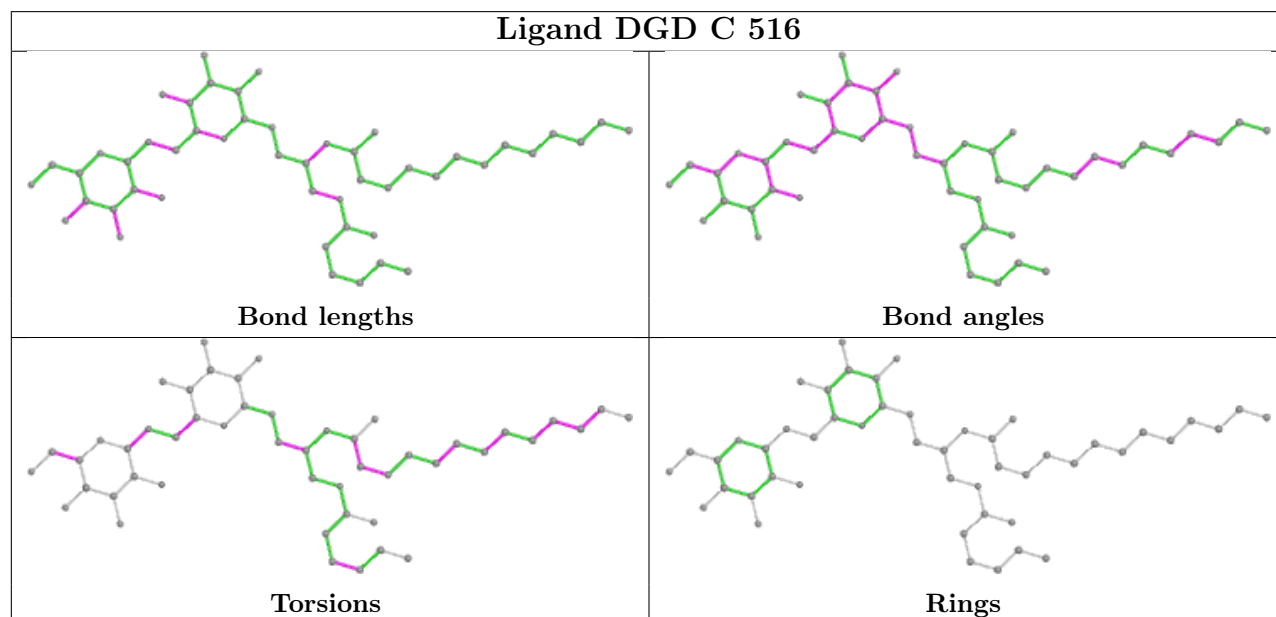


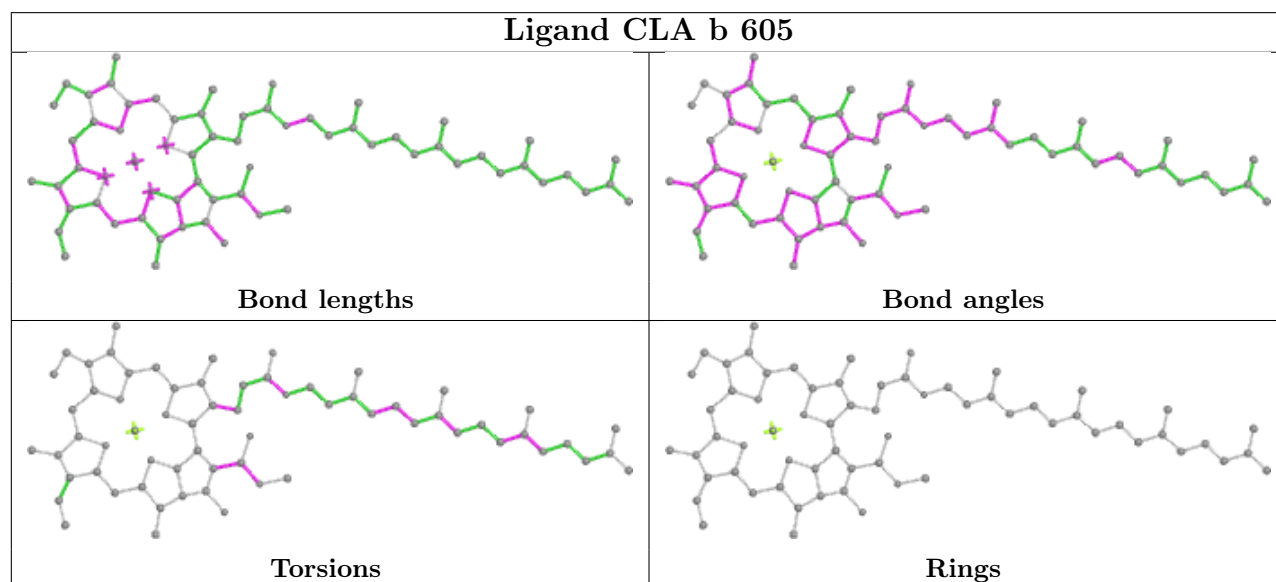
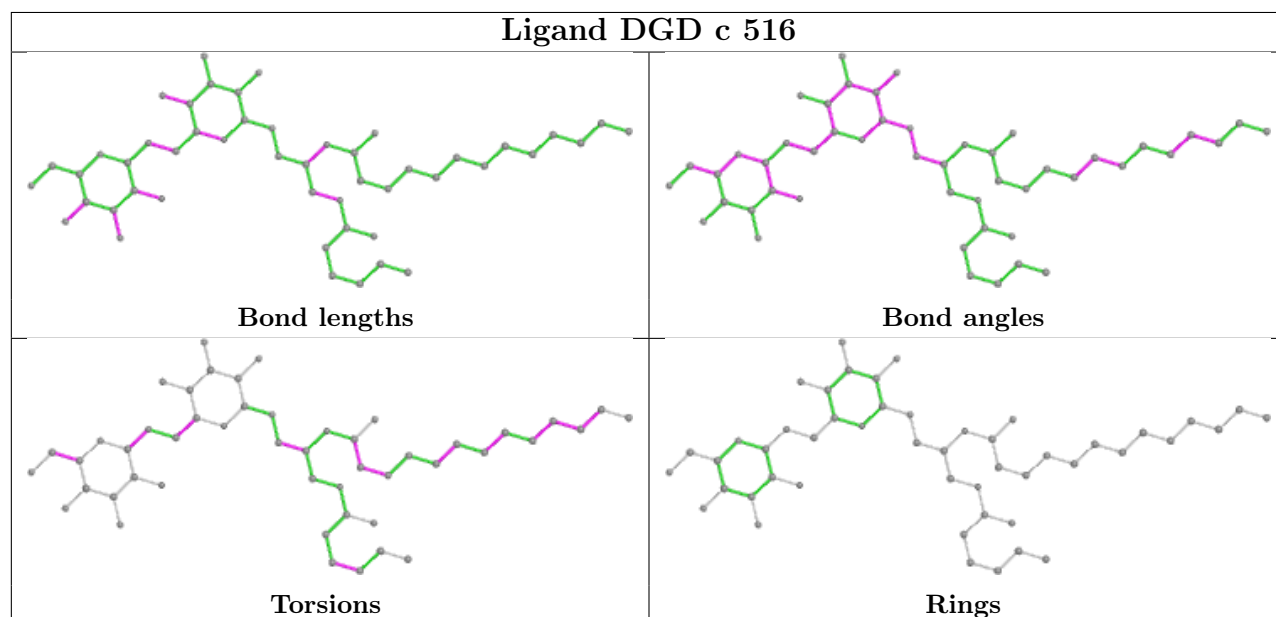
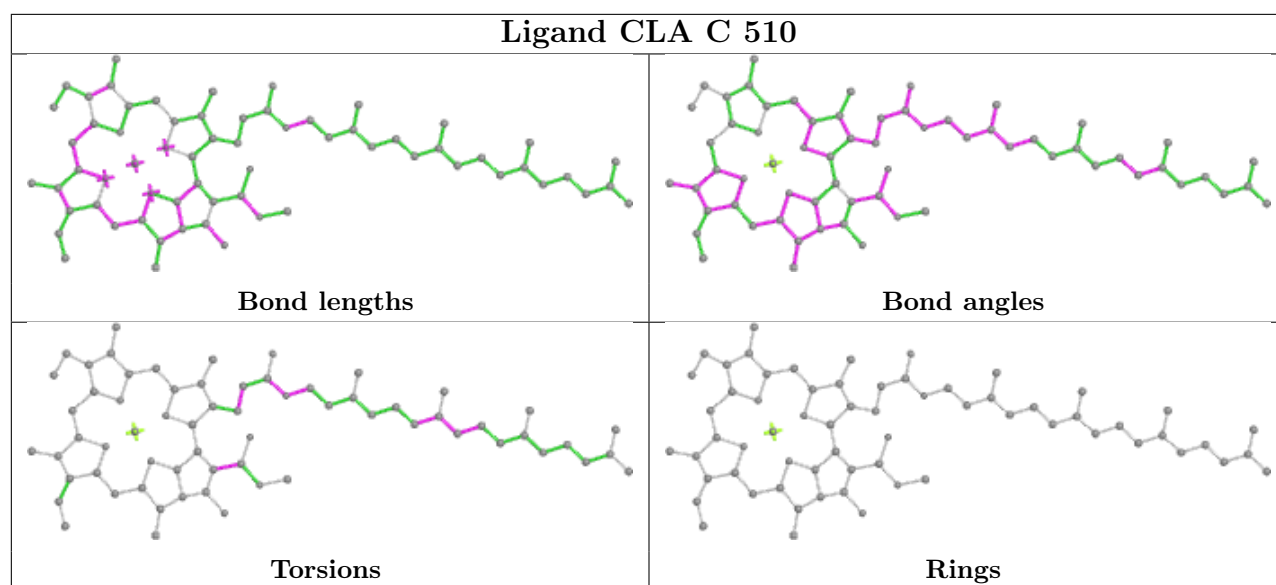


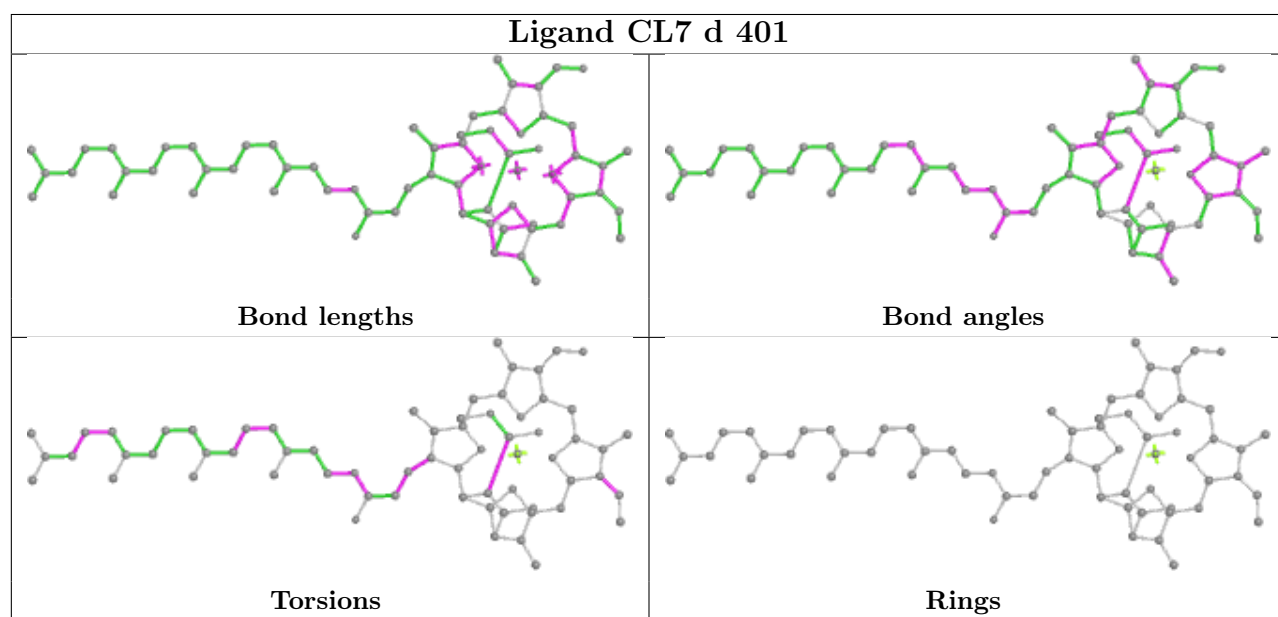
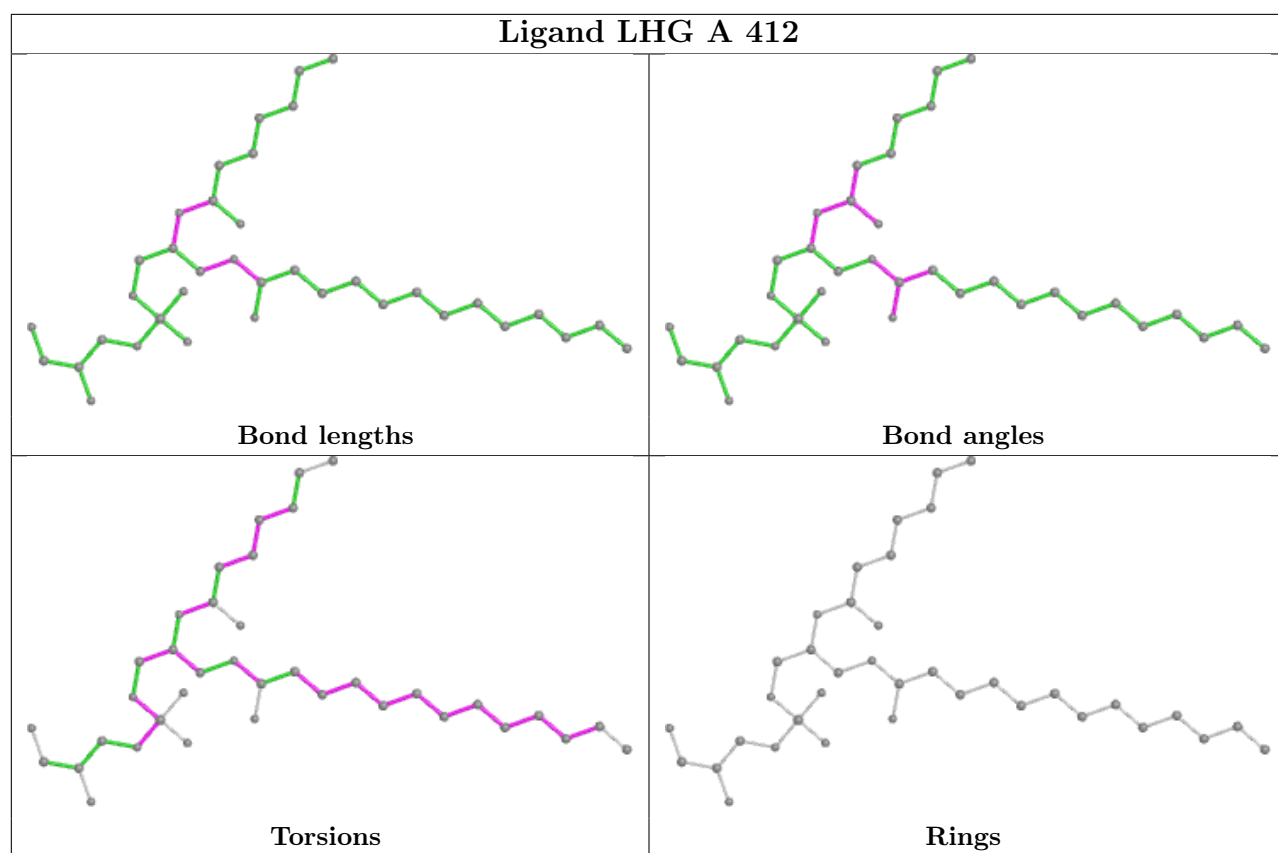
Ligand CLA b 606



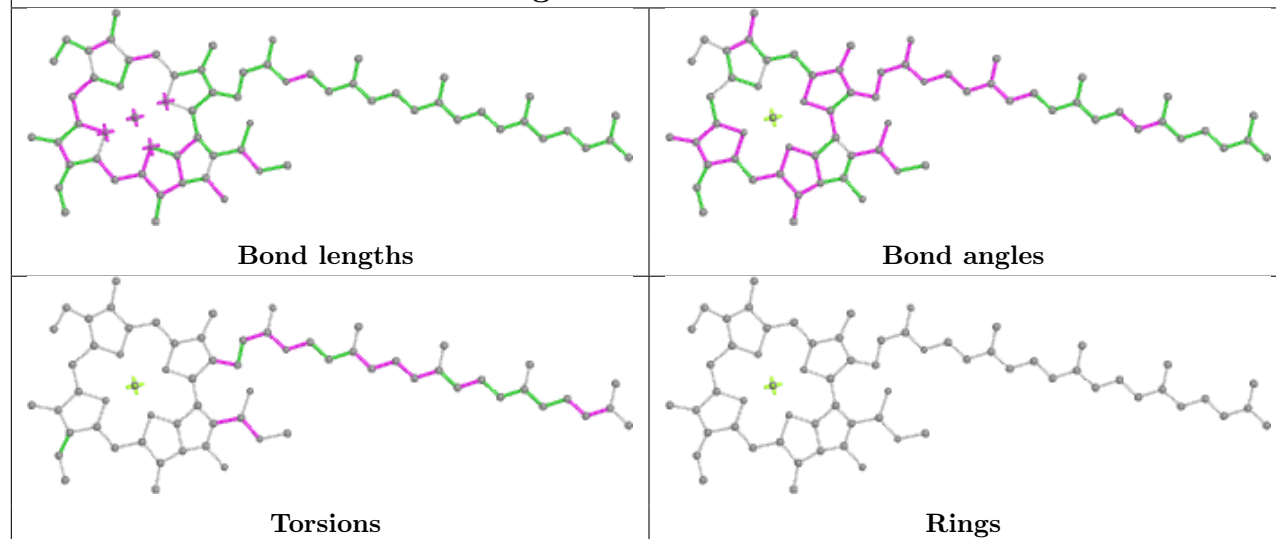
Ligand DGD C 516



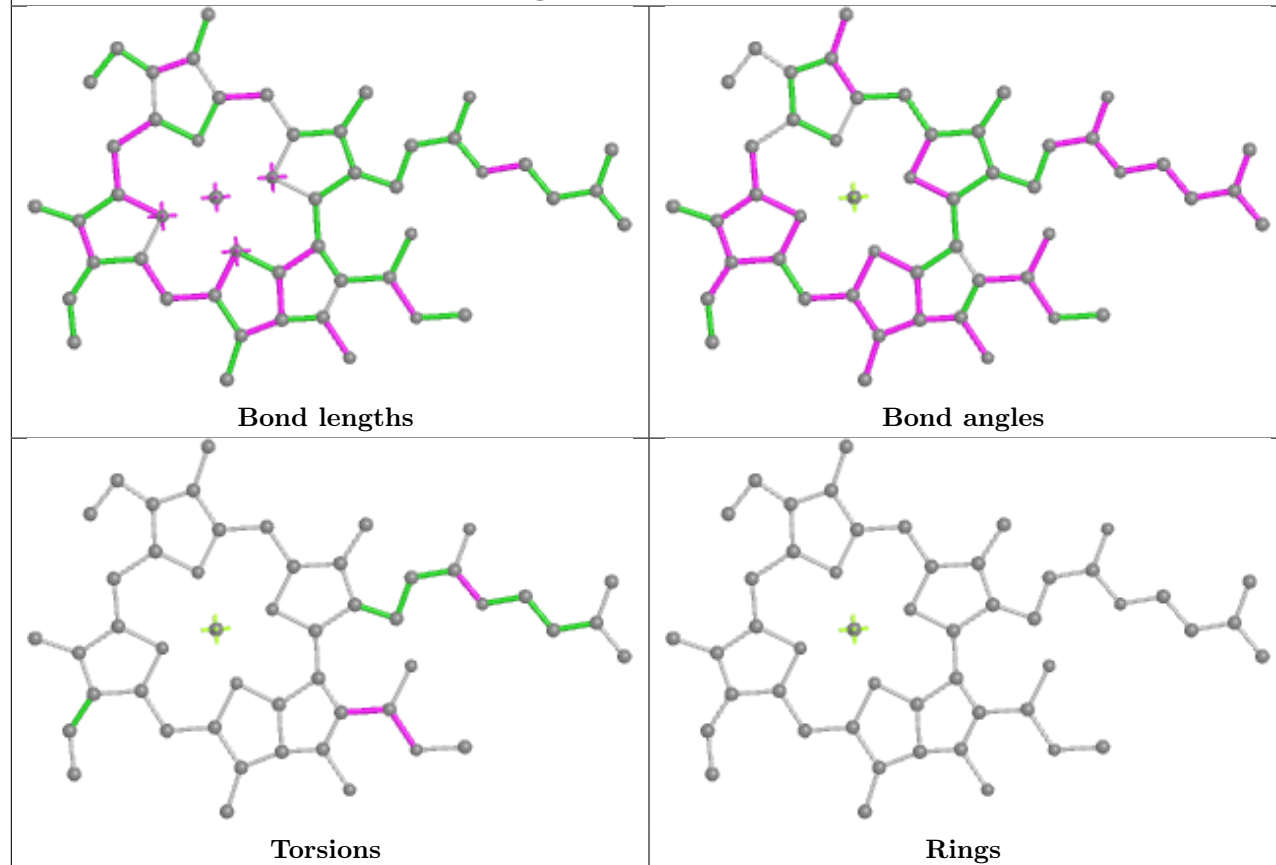


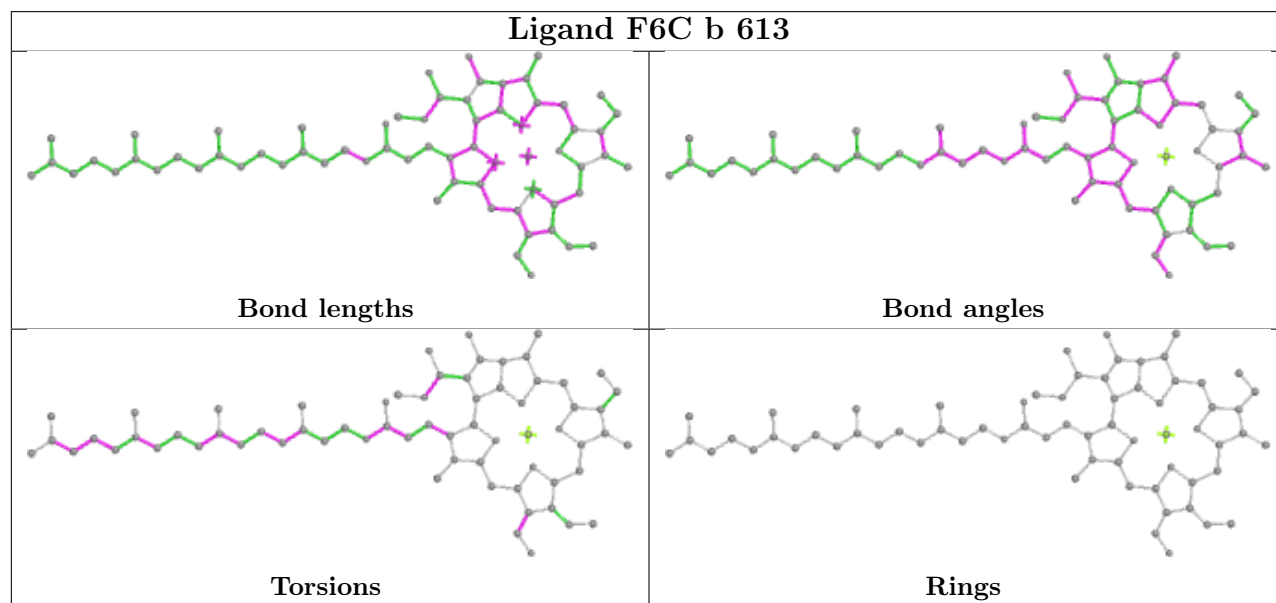
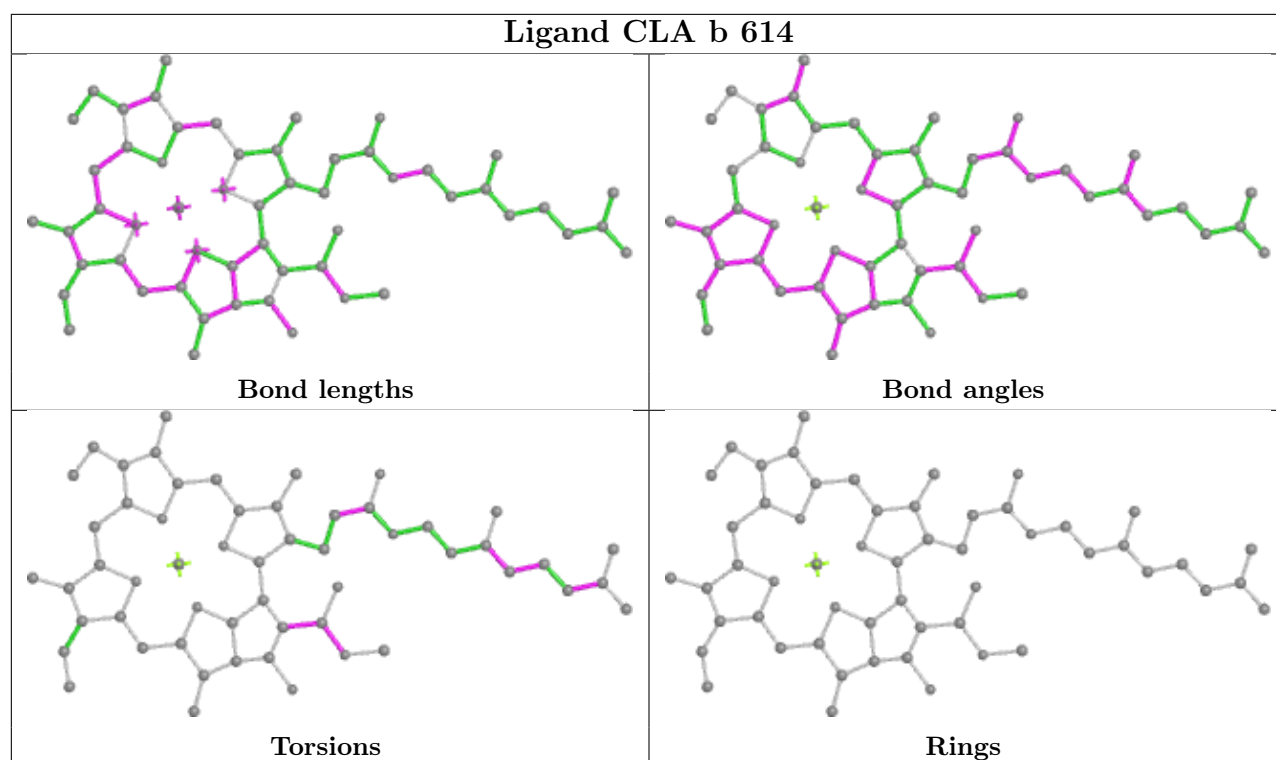


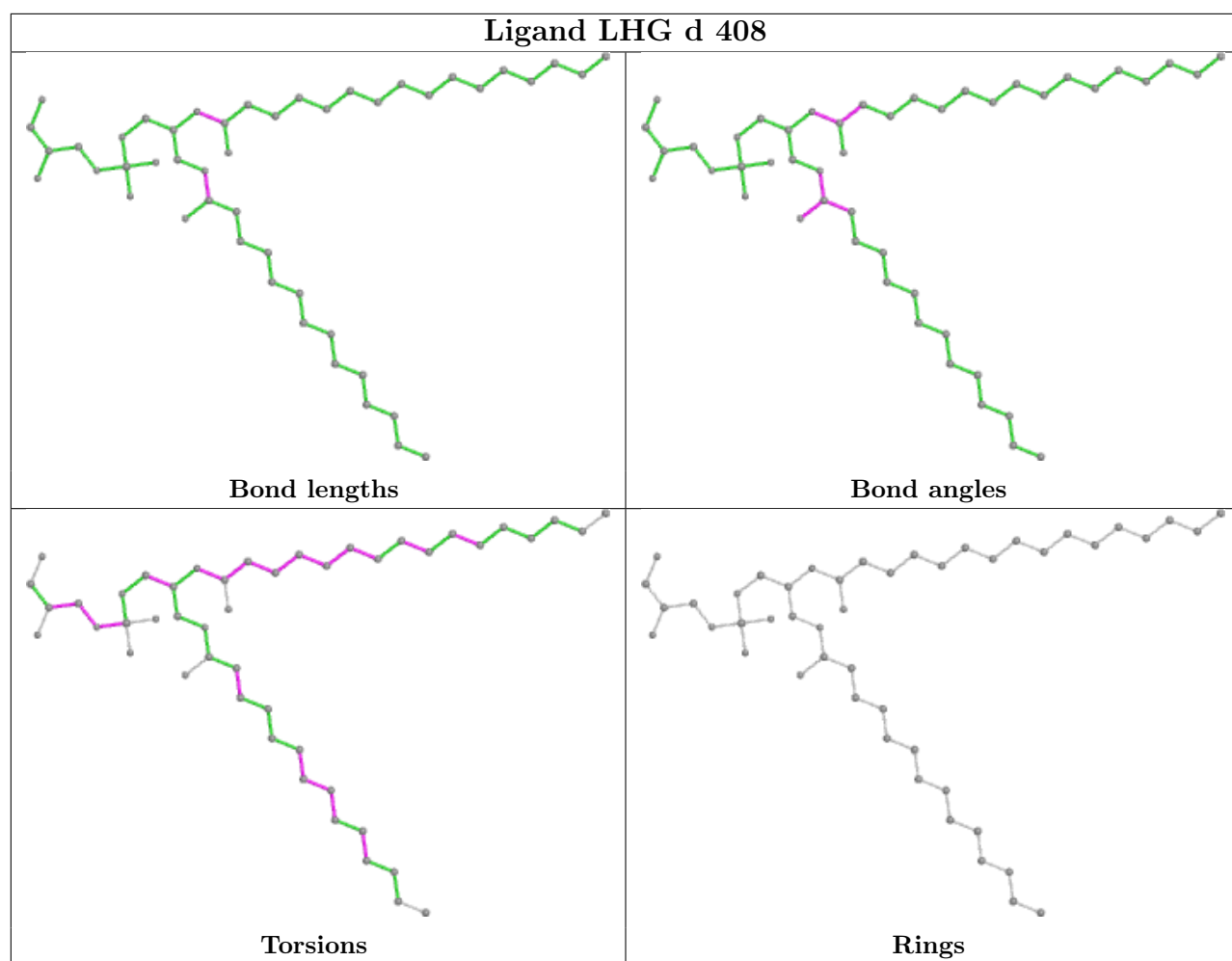
Ligand CLA C 504

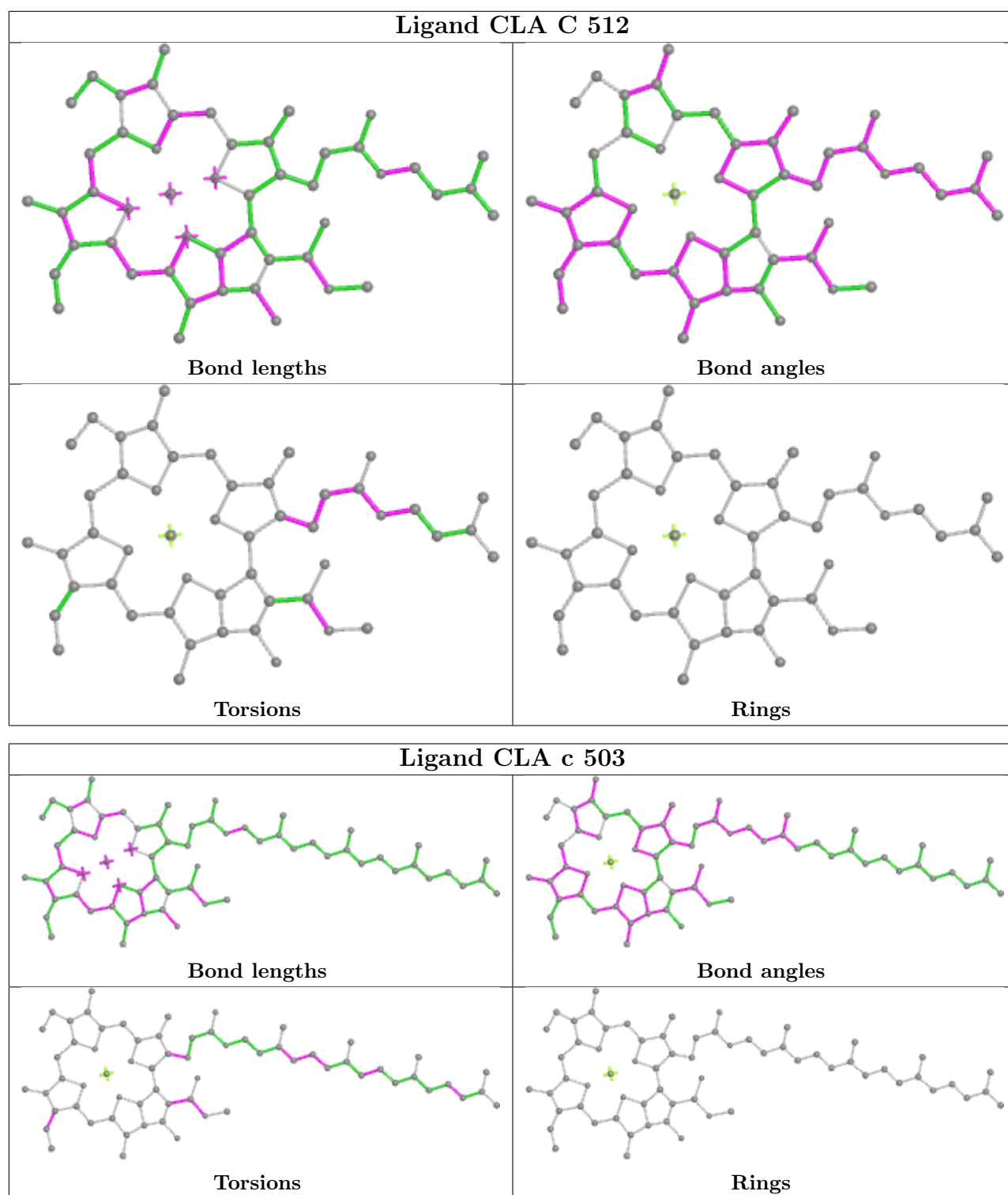


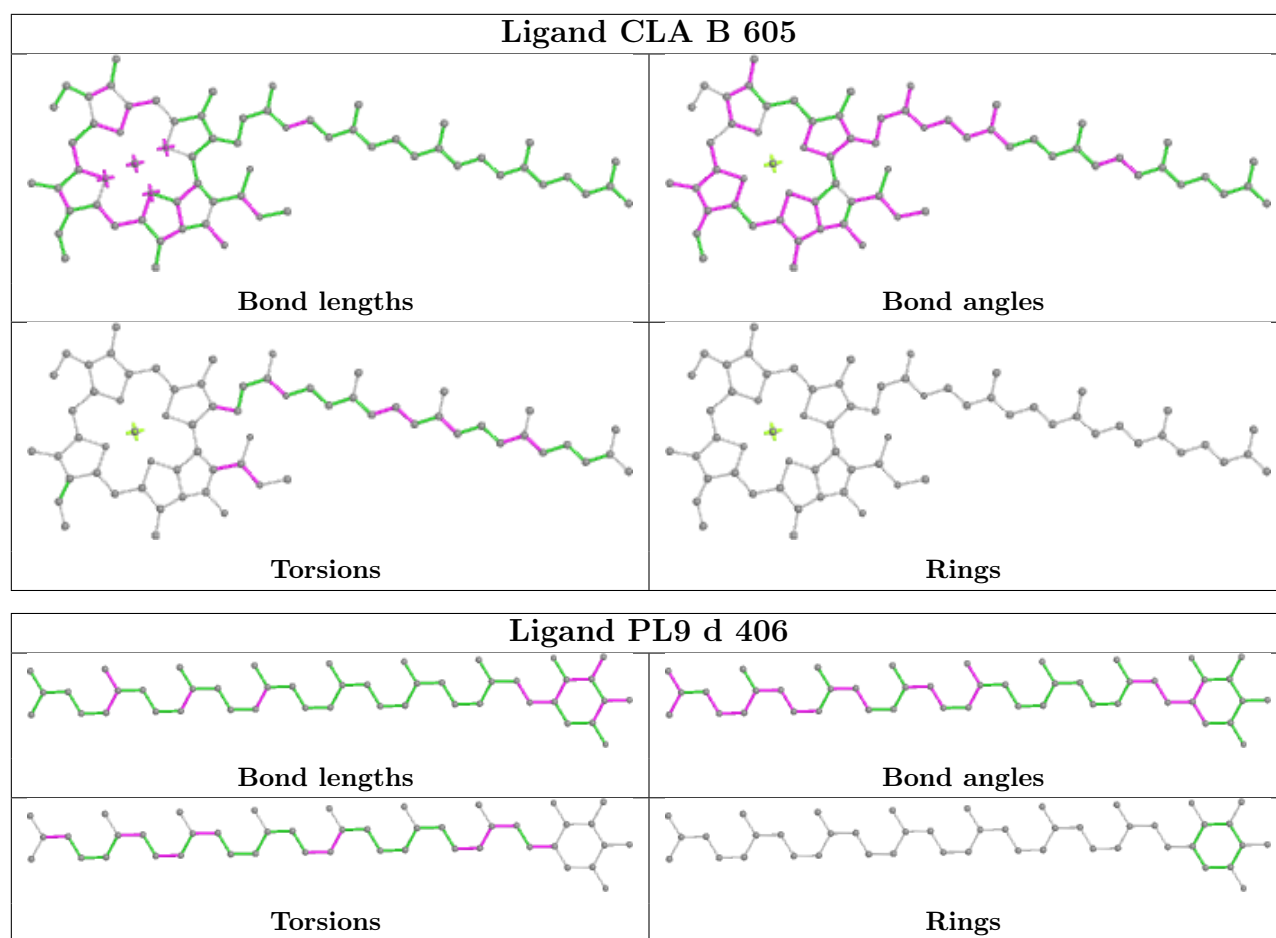
Ligand CLA H 101











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

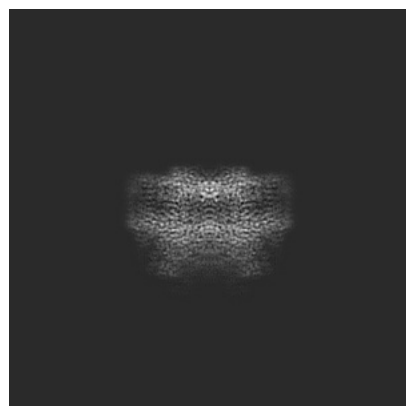
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28539. These allow visual inspection of the internal detail of the map and identification of artifacts.

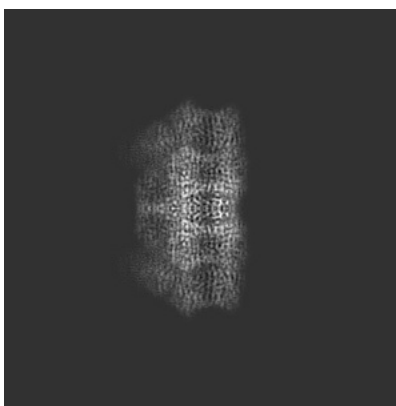
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

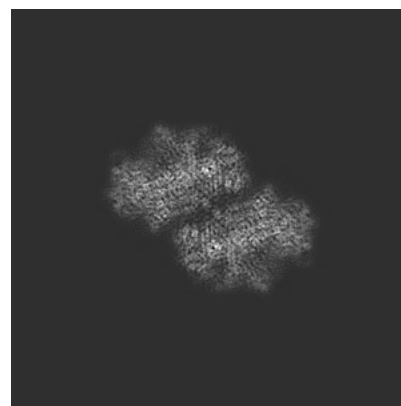
6.1.1 Primary map



X

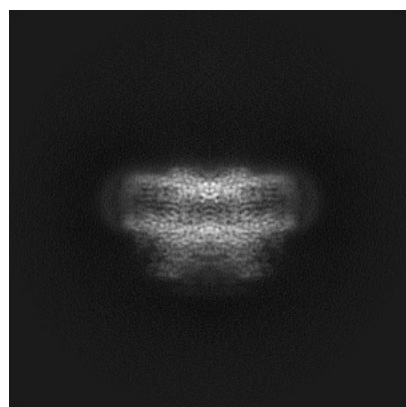


Y

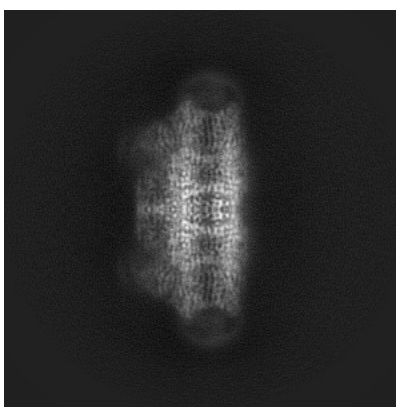


Z

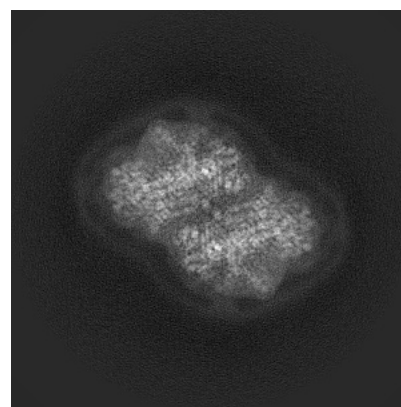
6.1.2 Raw map



X



Y

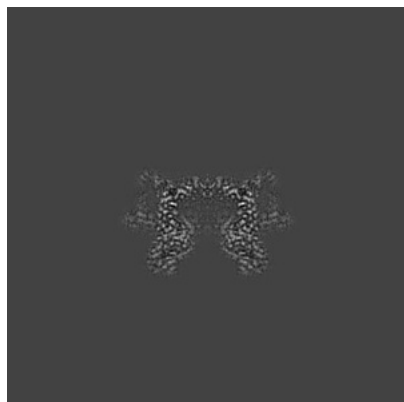


Z

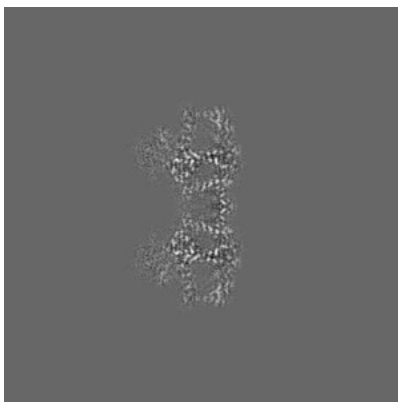
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

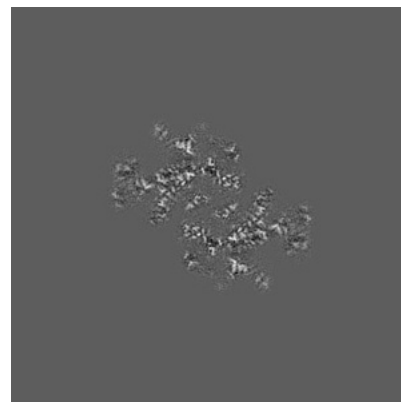
6.2.1 Primary map



X Index: 192

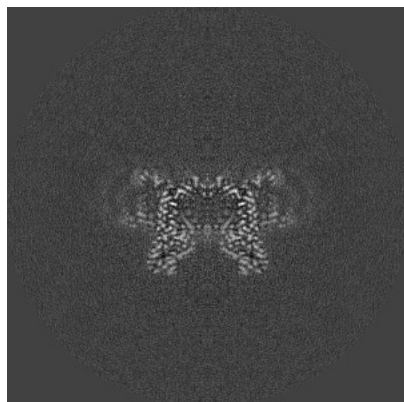


Y Index: 192

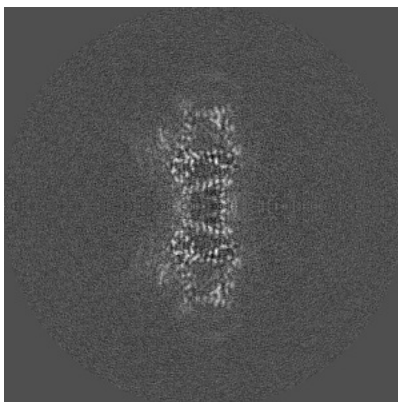


Z Index: 192

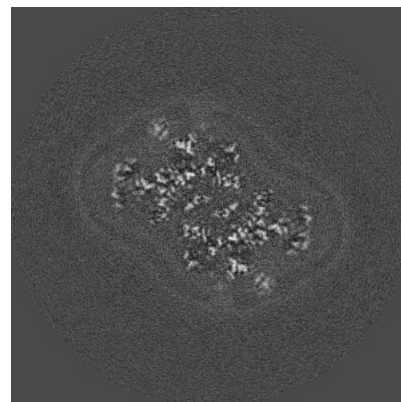
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

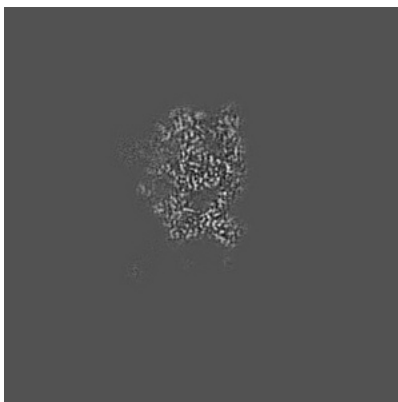
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

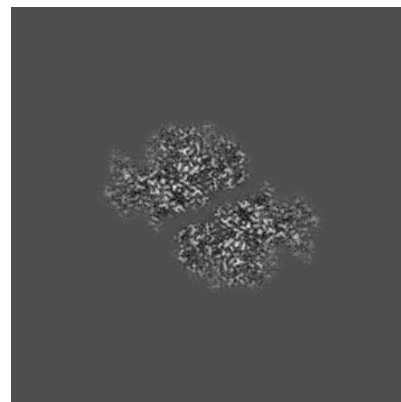
6.3.1 Primary map



X Index: 168

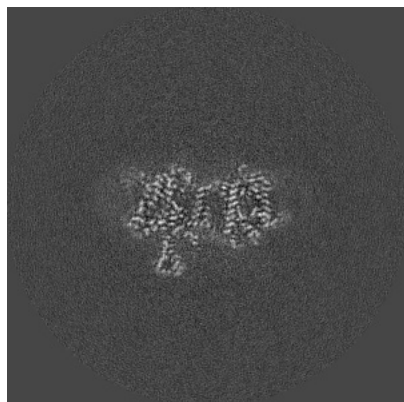


Y Index: 166

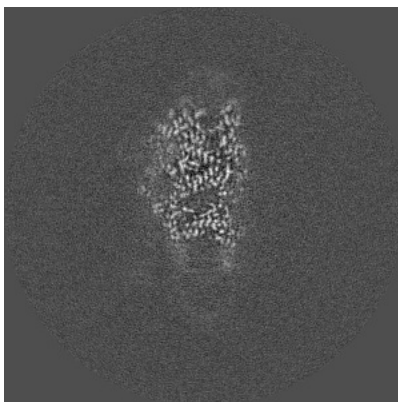


Z Index: 175

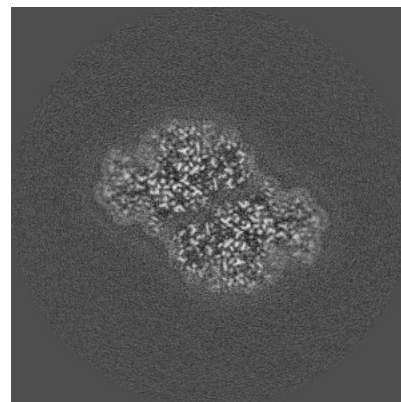
6.3.2 Raw map



X Index: 209



Y Index: 167

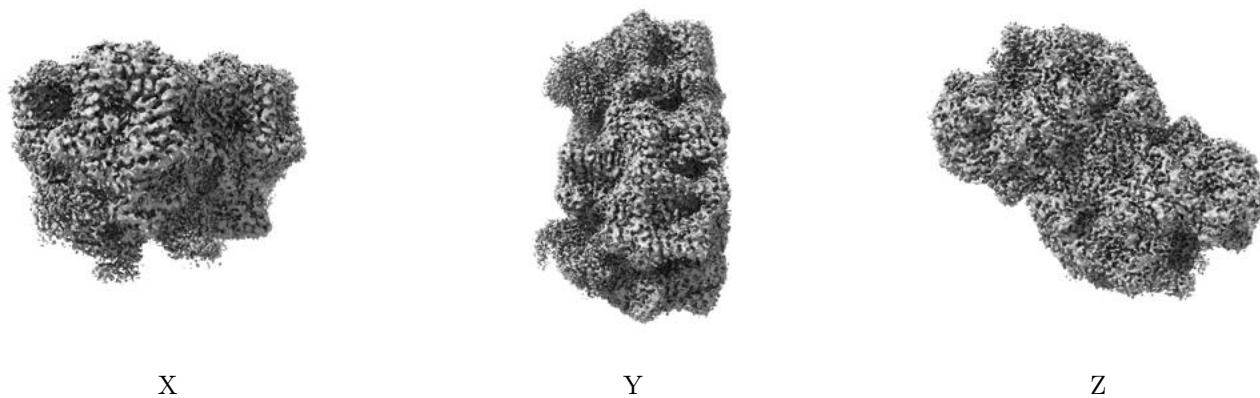


Z Index: 175

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

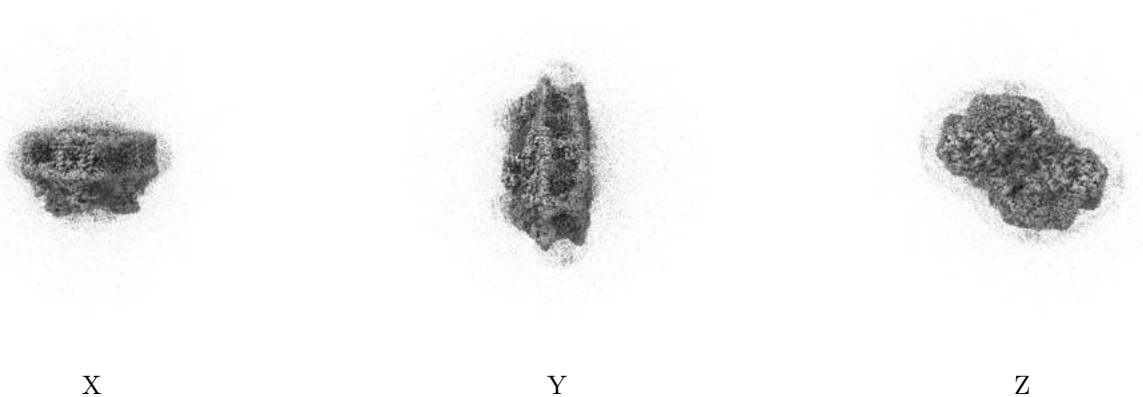
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

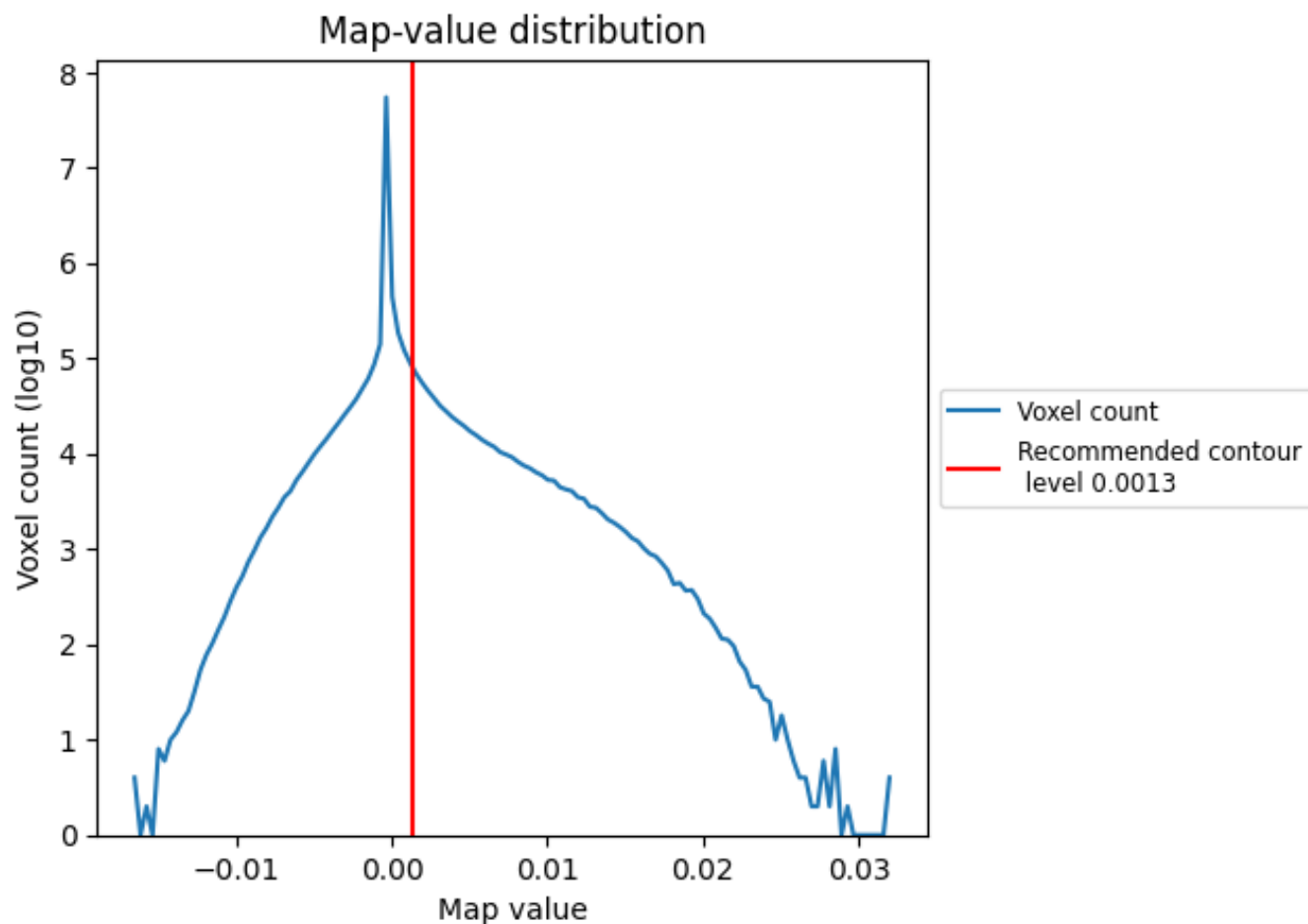
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

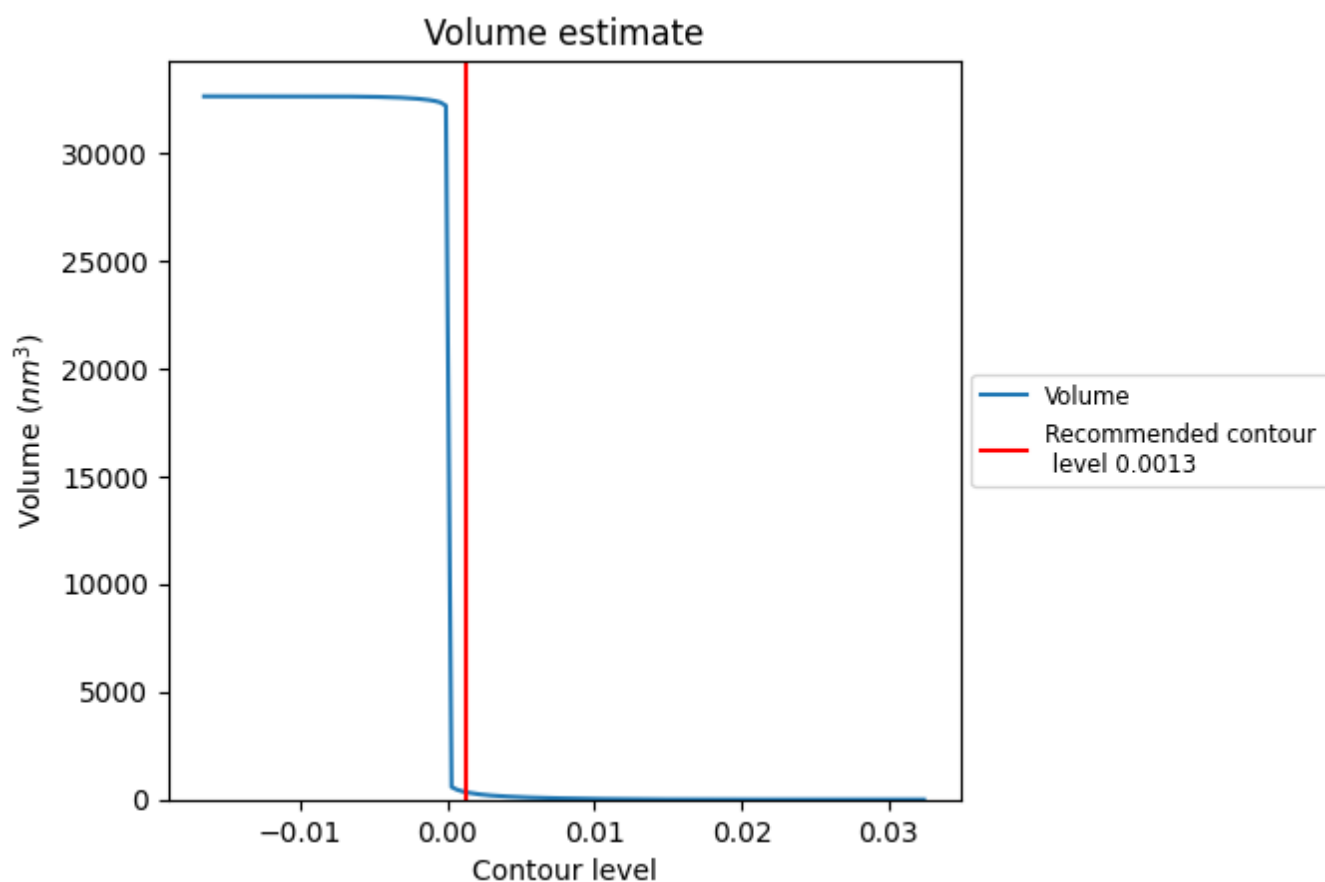
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

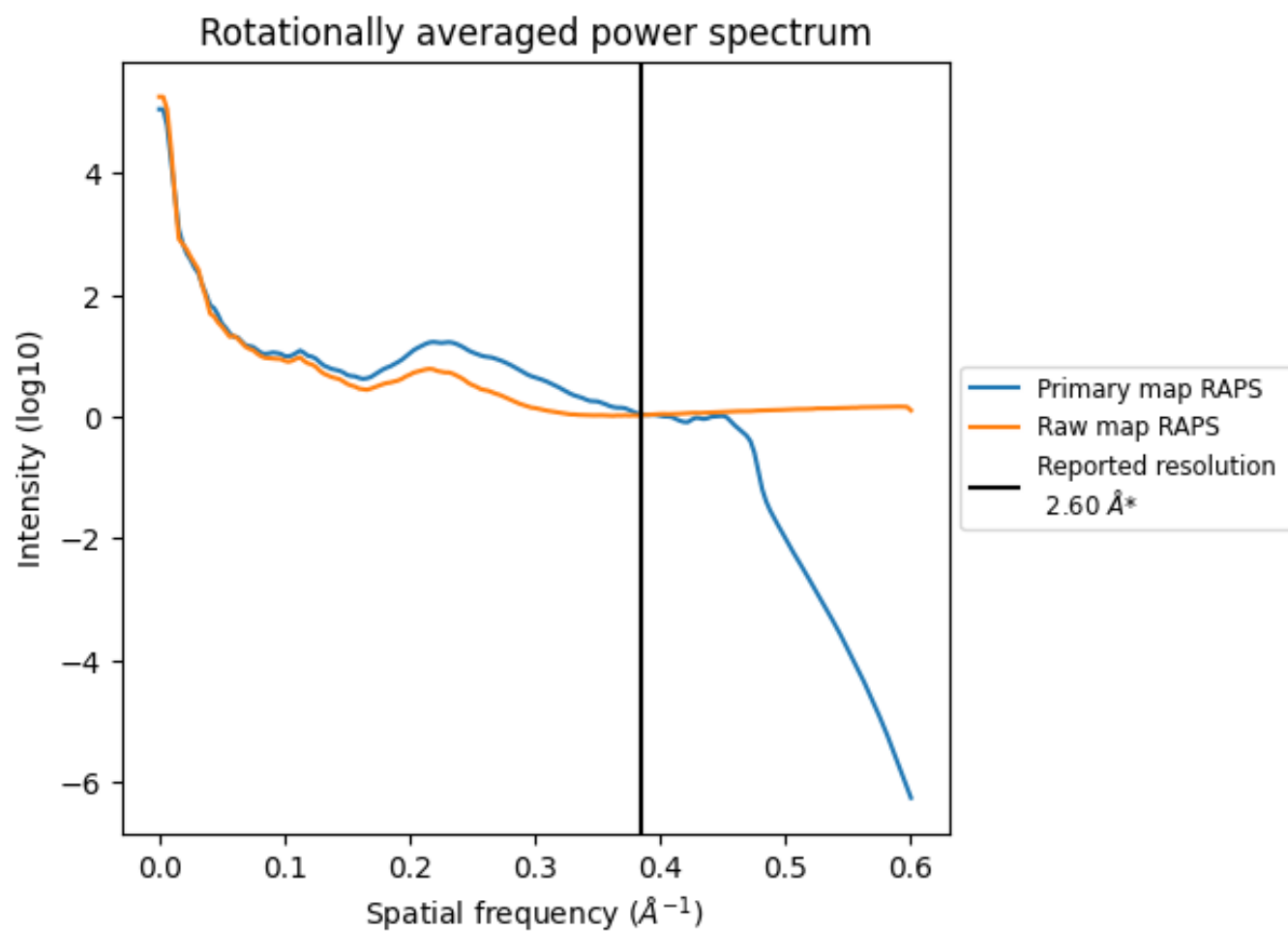
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 340 nm^3 ; this corresponds to an approximate mass of 308 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 ⓘ

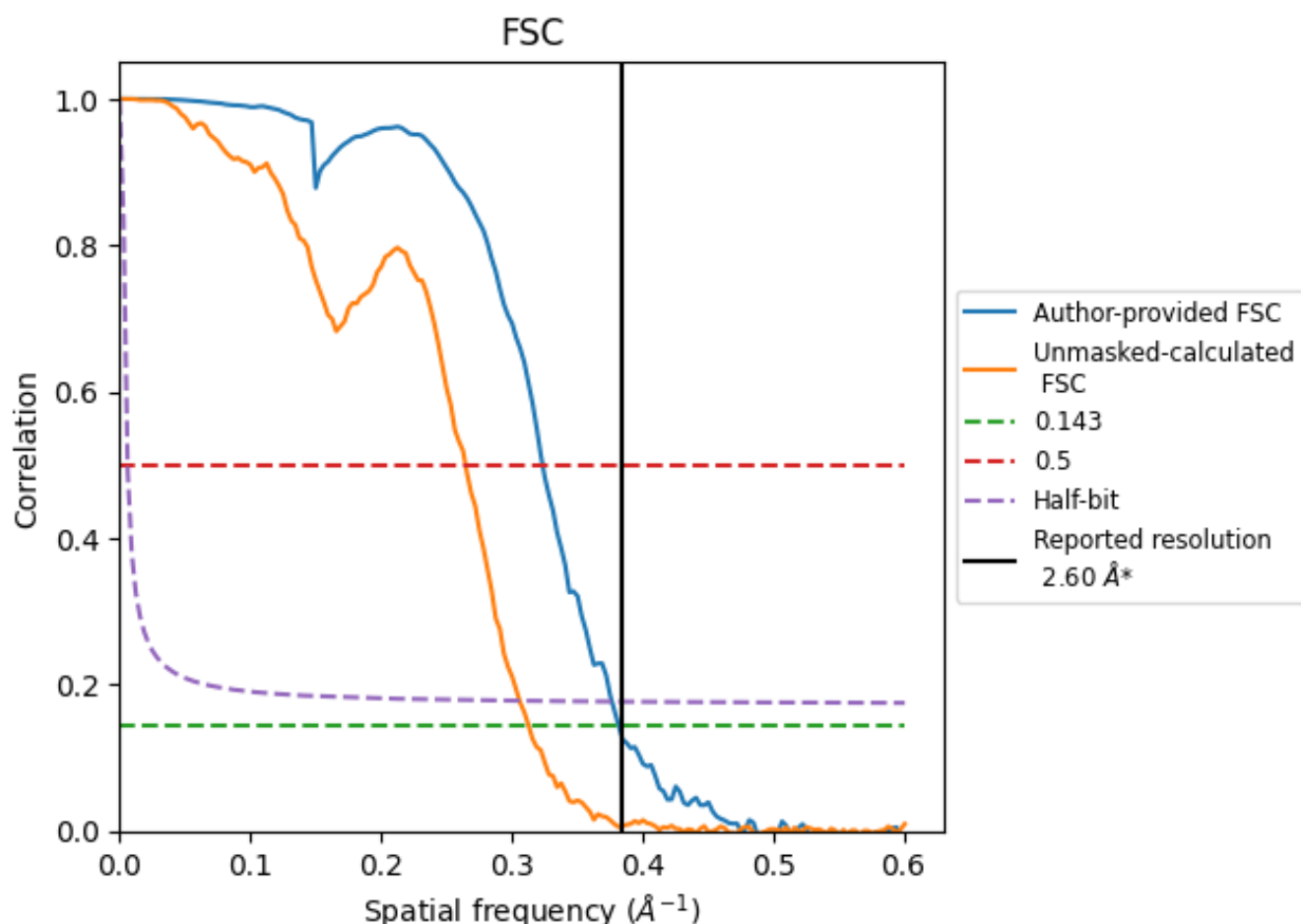


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

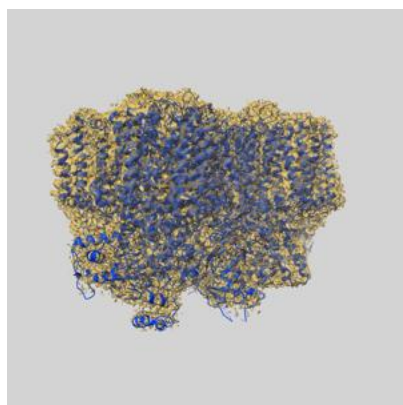
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.09	2.65
Unmasked-calculated*	3.19	3.78	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.6 by more than 10 %

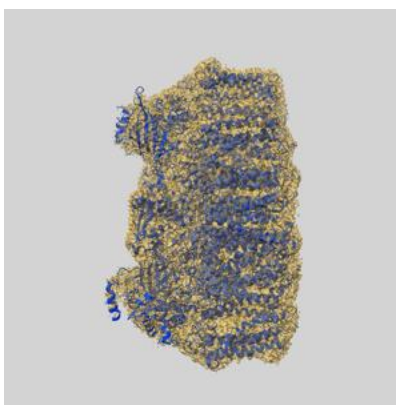
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28539 and PDB model 8EQM. Per-residue inclusion information can be found in section [3](#) on page [25](#).

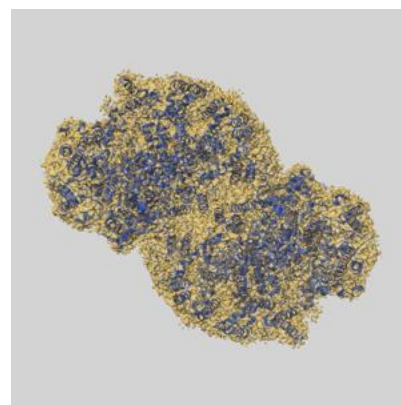
9.1 Map-model overlay [i](#)



X



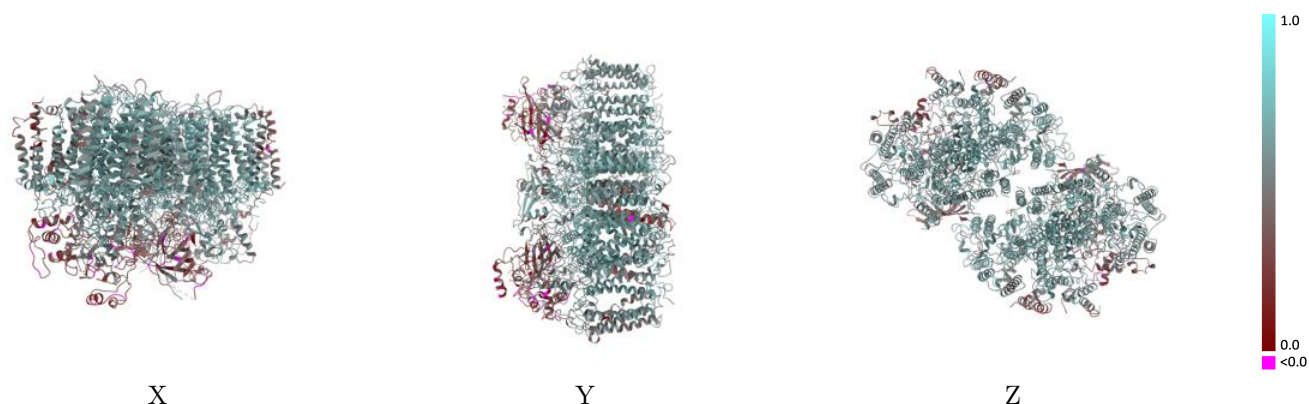
Y



Z

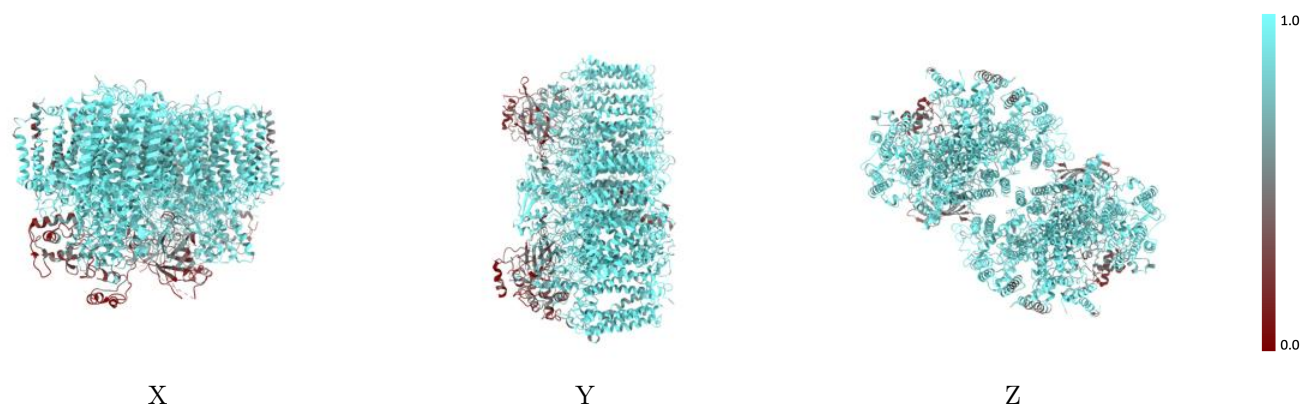
The images above show the 3D surface view of the map at the recommended contour level 0.0013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



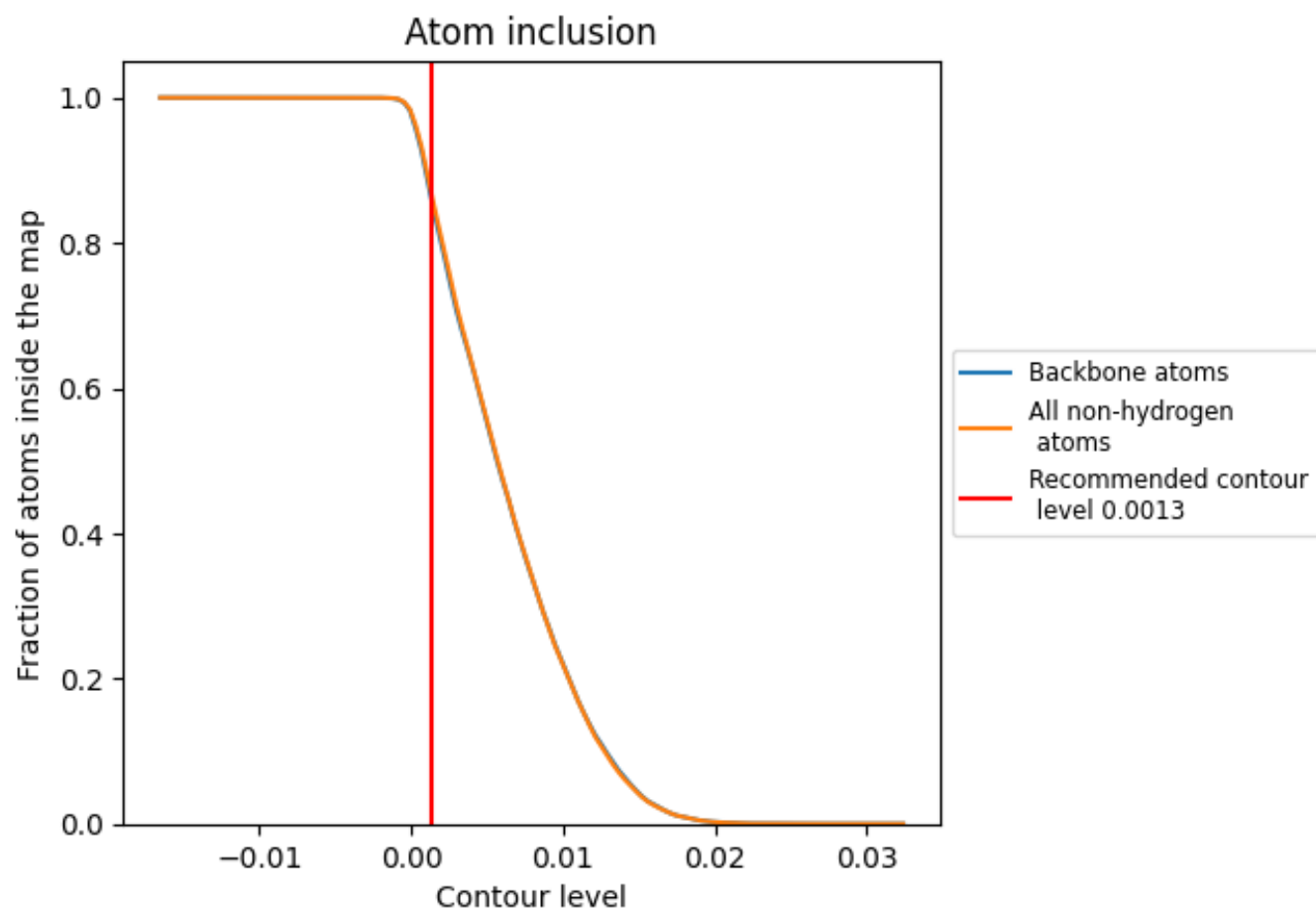
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0013).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (0.0013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8721	 0.5530
A	 0.9648	 0.6260
B	 0.9451	 0.6120
C	 0.9313	 0.5520
D	 0.9647	 0.6280
E	 0.9002	 0.4990
F	 0.8836	 0.4900
H	 0.8875	 0.5460
I	 0.9419	 0.5700
K	 0.8246	 0.4550
L	 0.9477	 0.6220
M	 0.9340	 0.5750
O	 0.4787	 0.3290
T	 0.9227	 0.5840
U	 0.3333	 0.2590
V	 0.4182	 0.2930
X	 0.6371	 0.3290
a	 0.9651	 0.6260
b	 0.9453	 0.6110
c	 0.9301	 0.5520
d	 0.9647	 0.6290
e	 0.9002	 0.4980
f	 0.8879	 0.4910
h	 0.8911	 0.5510
i	 0.9419	 0.5750
k	 0.8246	 0.4510
l	 0.9477	 0.6210
m	 0.9277	 0.5740
o	 0.4762	 0.3280
t	 0.9185	 0.5830
u	 0.3275	 0.2570
v	 0.4217	 0.2930
x	 0.6486	 0.3270

